



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 11:59 AM UTC

PDB ID : 8WDV / pdb_00008wdv
EMDB ID : EMD-37466
Title : Photosynthetic LH1-RC complex from the purple sulfur bacterium *Allochro-
matium vinosum* purified by Ca²⁺-DEAE
Authors : Tani, K.; Kanno, R.; Harada, A.; Kobayashi, A.; Minamino, A.; Nakamura,
N.; Ji, X.-C.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.;
Iwasaki, K.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on : 2023-09-16
Resolution : 2.24 Å (reported)
Based on initial model : 7VRJ

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

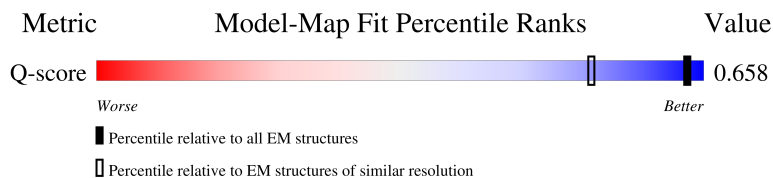
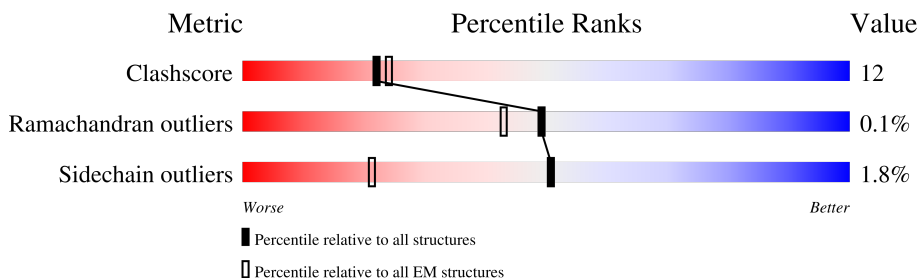
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3381 (1.75 - 2.74)

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	C	383	
2	L	278	
3	M	325	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	H	259	
5	1	44	
5	5	44	
5	7	44	
5	9	44	
5	A	44	
5	I	44	
5	K	44	
5	O	44	
5	Q	44	
6	0	46	
6	2	46	
6	4	46	
6	6	46	
6	8	46	
6	B	46	
6	J	46	
6	N	46	
6	P	46	
6	R	46	
7	D	64	
7	F	64	
7	S	64	
7	U	64	
7	W	64	

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Mol	Chain	Length	Quality of chain
7	Y	64	
8	E	47	
8	G	47	
8	T	47	
8	V	47	
8	X	47	
8	Z	47	
9	3	66	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 26261 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	311	Total	C	N	O	S	0	0
			2429	1535	418	460	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	277	Total	C	N	O	S	0	0
			2210	1489	354	357	10		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2533	1702	405	414	12		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	259	Total	C	N	O	S	1	0
			1993	1281	339	366	7		

- Molecule 5 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	I	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	K	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	O	44	Total	C	N	O	S	0	0
			366	251	59	55	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	1	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	5	43	Total	C	N	O	S	0	0
			355	245	57	52	1		
5	7	41	Total	C	N	O		0	0
			341	237	55	49			
5	9	43	Total	C	N	O	S	0	0
			359	248	58	52	1		

- Molecule 6 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	44	Total	C	N	O	S	0	0
			359	238	58	61	2		
6	J	40	Total	C	N	O	S	0	0
			331	223	53	54	1		
6	N	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	P	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	R	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	2	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	4	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	6	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	8	34	Total	C	N	O	S	0	0
			287	197	46	43	1		
6	0	42	Total	C	N	O	S	0	0
			345	231	55	57	2		

- Molecule 7 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	50	Total	C	N	O	S	0	0
			407	276	63	66	2		
7	F	49	Total	C	N	O	S	0	0
			397	270	62	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	51	Total	C	N	O	S	0	0
			412	279	64	67	2		
7	U	51	Total	C	N	O	S	0	0
			412	279	64	67	2		
7	W	54	Total	C	N	O	S	0	0
			431	291	67	71	2		
7	Y	64	Total	C	N	O	S	0	0
			511	341	83	85	2		

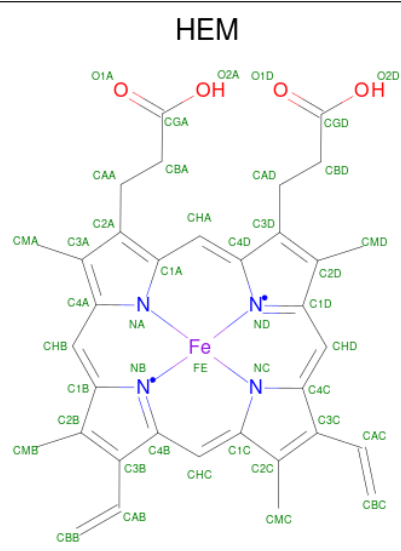
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	G	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	T	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	V	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	X	42	Total	C	N	O	S	0	0
			349	234	54	58	3		
8	Z	41	Total	C	N	O	S	0	0
			343	231	53	56	3		

- Molecule 9 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	62	Total	C	N	O	S	0	0
			489	332	76	78	3		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total 1	Mg 1	0

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

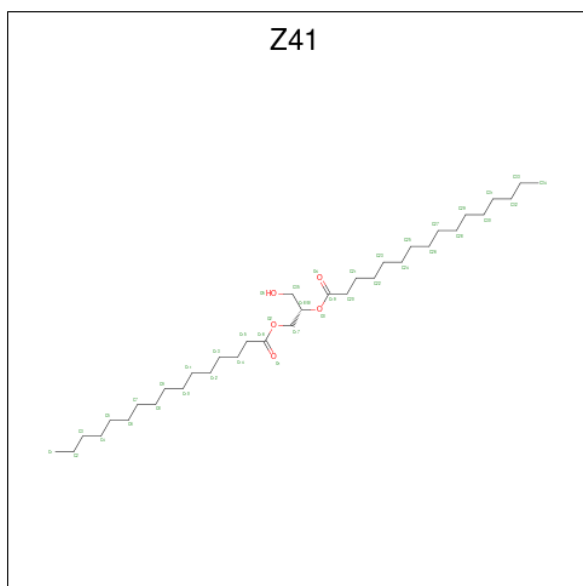
Mol	Chain	Residues	Atoms	AltConf
12	C	1	Total Ca 1 1	0
12	M	1	Total Ca 1 1	0
12	D	1	Total Ca 1 1	0
12	F	1	Total Ca 1 1	0

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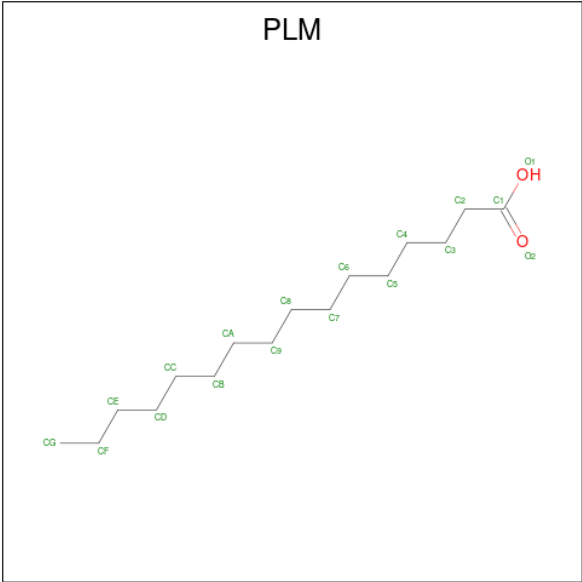
Mol	Chain	Residues	Atoms		AltConf
12	S	1	Total	Ca	0
			1	1	
12	U	1	Total	Ca	0
			1	1	
12	W	1	Total	Ca	0
			1	1	
12	Y	1	Total	Ca	0
			1	1	

- Molecule 13 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula: $C_{35}H_{68}O_5$).



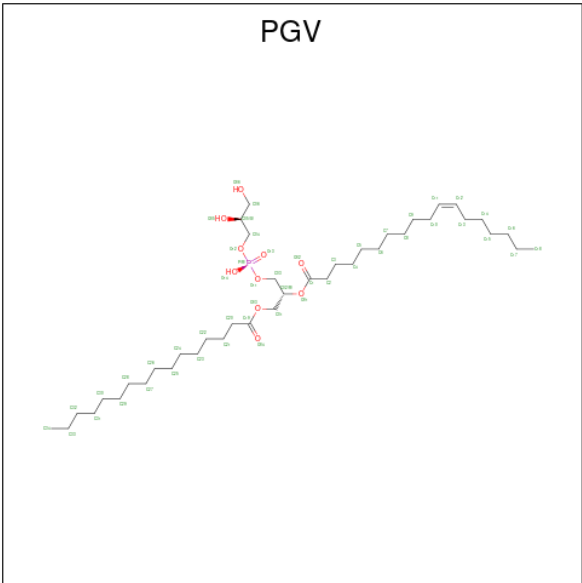
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			35	31	4	

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	C	1	Total	C	O	0
			12	11	1	

- Molecule 15 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



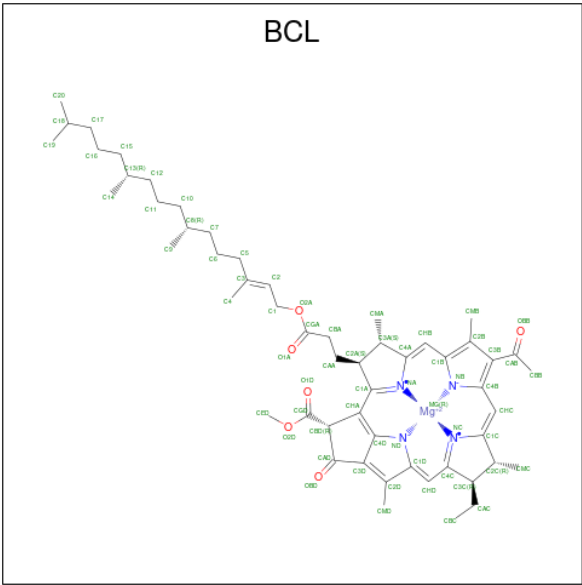
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			31	20	10	1	
15	L	1	Total	C	O	P	0
			29	18	10	1	

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Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			35	24	10	1	
15	L	1	Total	C	O	P	0
			33	22	10	1	
15	M	1	Total	C	O	P	0
			37	26	10	1	
15	M	1	Total	C	O	P	0
			27	18	8	1	
15	H	1	Total	C	O	P	0
			36	25	10	1	
15	D	1	Total	C	O	P	0
			39	28	10	1	
15	F	1	Total	C	O	P	0
			36	25	10	1	
15	1	1	Total	C	O	P	0
			27	18	8	1	

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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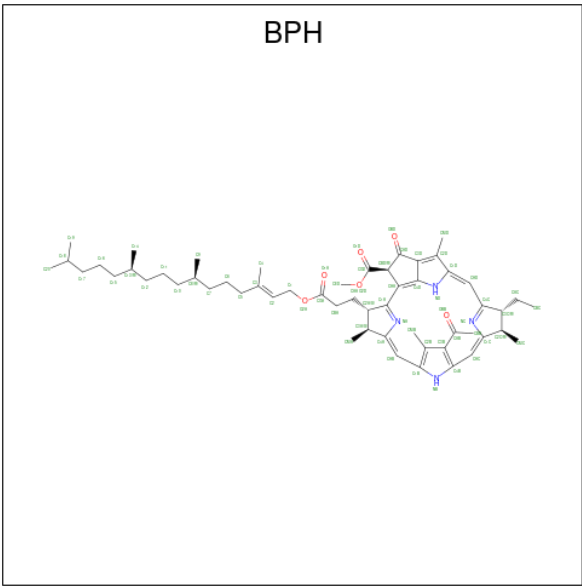
Mol	Chain	Residues	Atoms					AltConf
16	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	I	1	Total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

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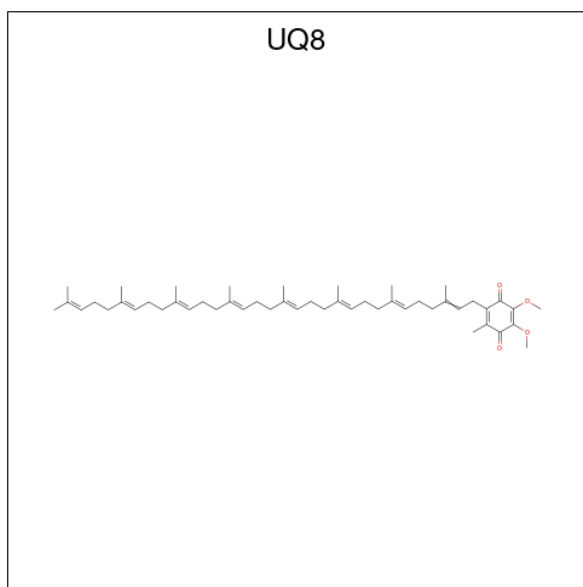
Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).

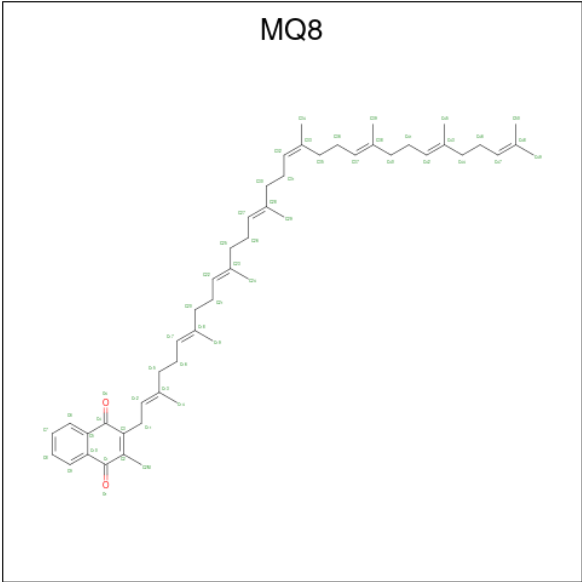


Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			33	29	4	
18	L	1	Total	C	O	0
			53	49	4	
18	L	1	Total	C	O	0
			53	49	4	

- Molecule 19 is FE (III) ION (CCD ID: FE) (formula: Fe).

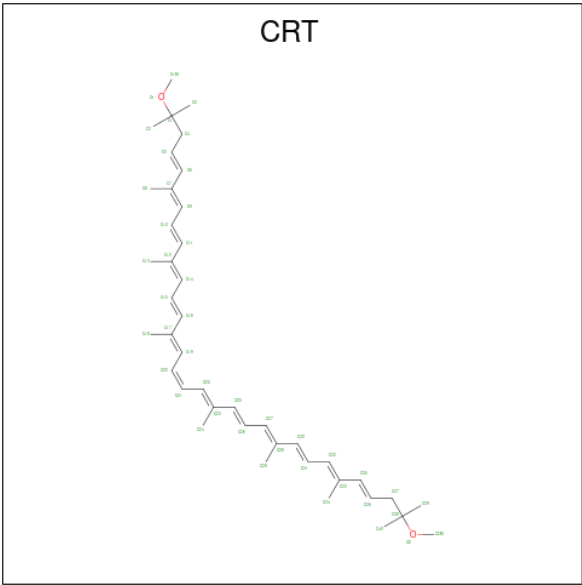
Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Fe	0
			1	1	

- Molecule 20 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			AltConf
20	M	1	Total	C	O	0
			53	51	2	

- Molecule 21 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



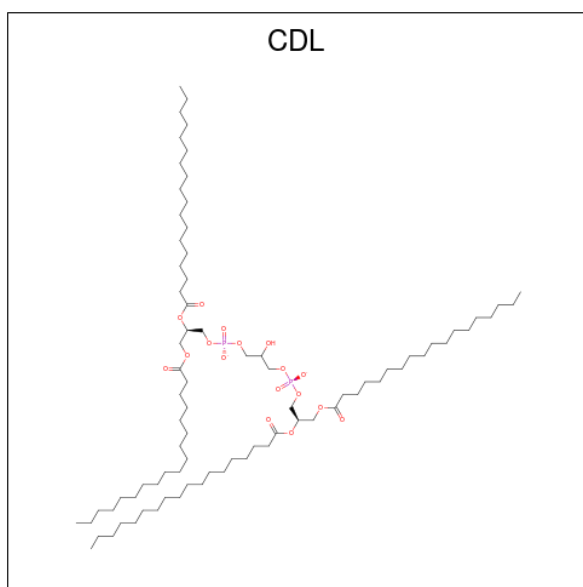
Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			44	42	2	
21	B	1	Total	C	O	0
			44	42	2	
21	E	1	Total	C	O	0
			44	42	2	

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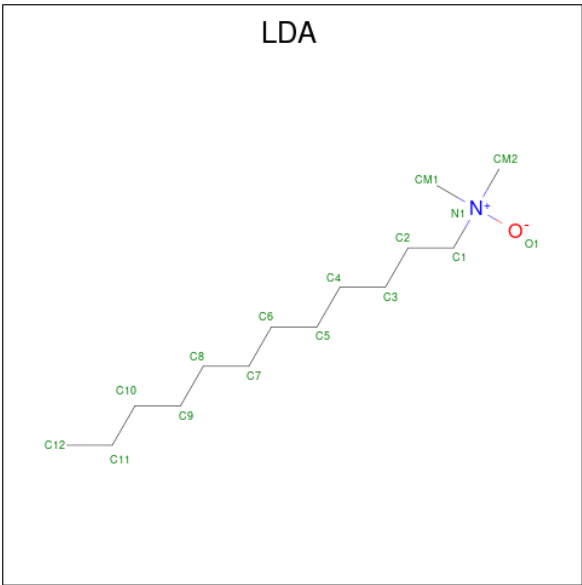
Mol	Chain	Residues	Atoms			AltConf
21	G	1	Total	C	O	0
			44	42	2	
21	K	1	Total	C	O	0
			44	42	2	
21	N	1	Total	C	O	0
			44	42	2	
21	Q	1	Total	C	O	0
			44	42	2	
21	R	1	Total	C	O	0
			44	42	2	
21	T	1	Total	C	O	0
			44	42	2	
21	V	1	Total	C	O	0
			44	42	2	
21	X	1	Total	C	O	0
			44	42	2	
21	Z	1	Total	C	O	0
			44	42	2	
21	2	1	Total	C	O	0
			44	42	2	
21	4	1	Total	C	O	0
			44	42	2	
21	7	1	Total	C	O	0
			44	42	2	
21	8	1	Total	C	O	0
			44	42	2	
21	0	1	Total	C	O	0
			44	42	2	

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



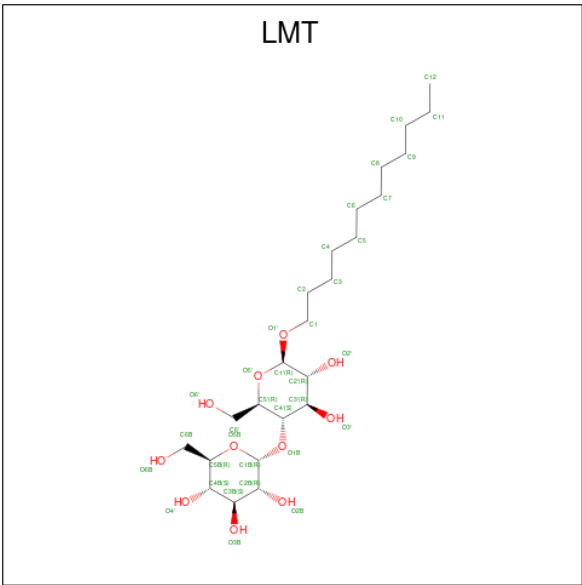
Mol	Chain	Residues	Atoms				AltConf
22	M	1	Total	C	O	P	0
			39	21	16	2	
22	M	1	Total	C	O	P	0
			95	76	17	2	
22	M	1	Total	C	O	P	0
			84	65	17	2	
22	H	1	Total	C	O	P	0
			79	60	17	2	
22	D	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 23 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				AltConf
23	M	1	Total	C	N	O	0
			16	14	1	1	
23	O	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			35	24	11	
24	E	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	J	1	Total	C	O	0
			35	24	11	
24	P	1	Total	C	O	0
			35	24	11	
24	P	1	Total	C	O	0
			35	24	11	
24	R	1	Total	C	O	0
			35	24	11	
24	V	1	Total	C	O	0
			35	24	11	
24	X	1	Total	C	O	0
			35	24	11	
24	Z	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	
24	5	1	Total	C	O	0
			31	20	11	
24	8	1	Total	C	O	0
			35	24	11	
24	0	1	Total	C	O	0
			35	24	11	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	C	134	Total	O	0
			134	134	
25	L	50	Total	O	0
			50	50	

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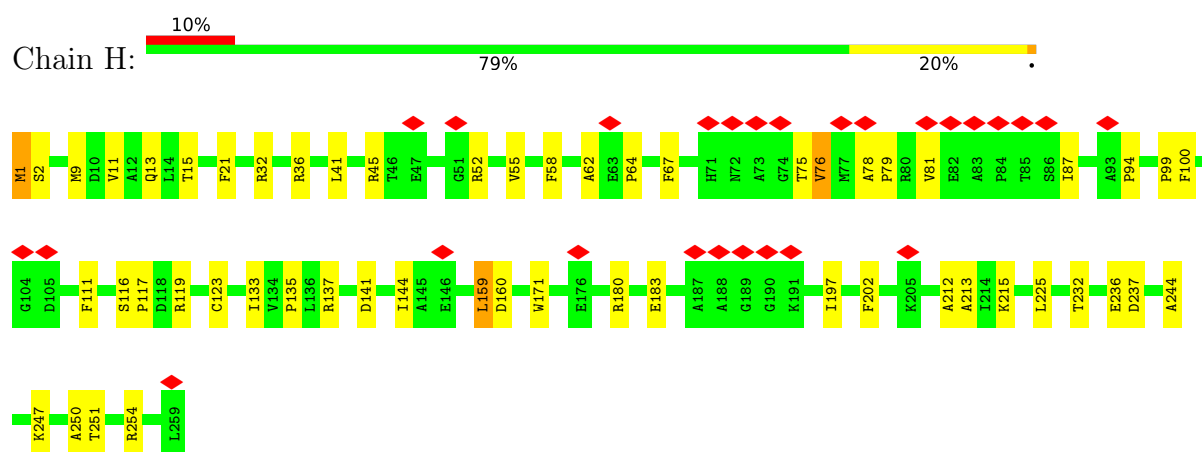
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Mol	Chain	Residues	Atoms		AltConf
25	M	73	Total 73	O 73	0
25	H	16	Total 16	O 16	0
25	A	2	Total 2	O 2	0
25	D	7	Total 7	O 7	0
25	E	2	Total 2	O 2	0
25	F	3	Total 3	O 3	0
25	I	2	Total 2	O 2	0
25	K	1	Total 1	O 1	0
25	Q	3	Total 3	O 3	0
25	R	1	Total 1	O 1	0
25	S	6	Total 6	O 6	0
25	T	4	Total 4	O 4	0
25	U	12	Total 12	O 12	0
25	V	3	Total 3	O 3	0
25	W	6	Total 6	O 6	0
25	X	2	Total 2	O 2	0
25	Y	8	Total 8	O 8	0
25	Z	2	Total 2	O 2	0
25	1	1	Total 1	O 1	0
25	2	1	Total 1	O 1	0
25	3	10	Total 10	O 10	0

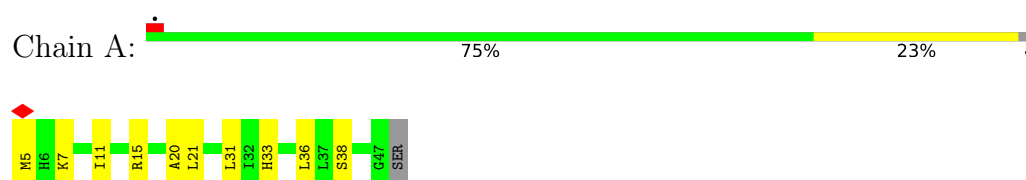
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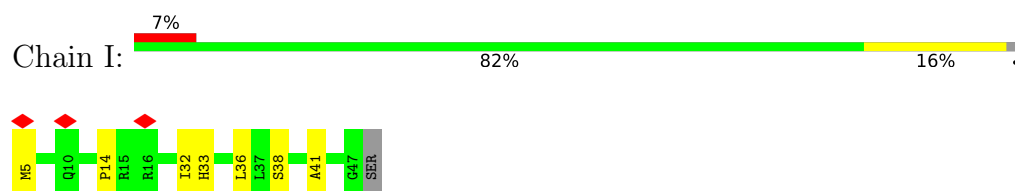
Mol	Chain	Residues	Atoms		AltConf
25	5	1	Total 1	O 1	0
25	7	1	Total 1	O 1	0
25	9	3	Total 3	O 3	0



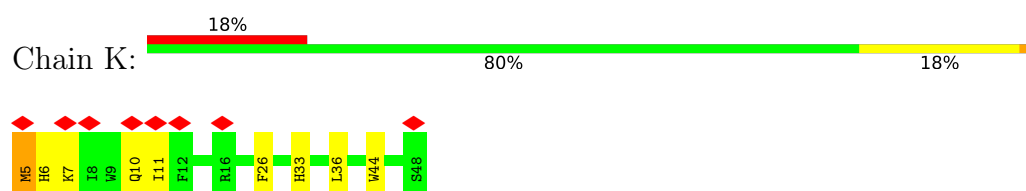
- Molecule 5: Antenna complex alpha/beta subunit



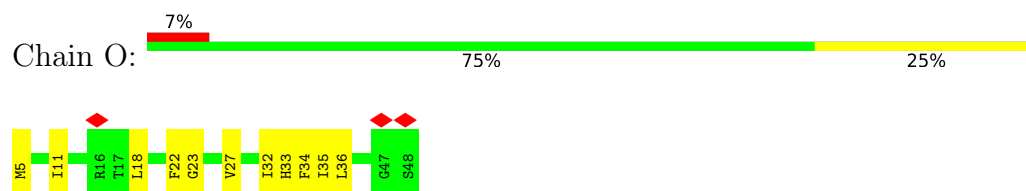
- Molecule 5: Antenna complex alpha/beta subunit



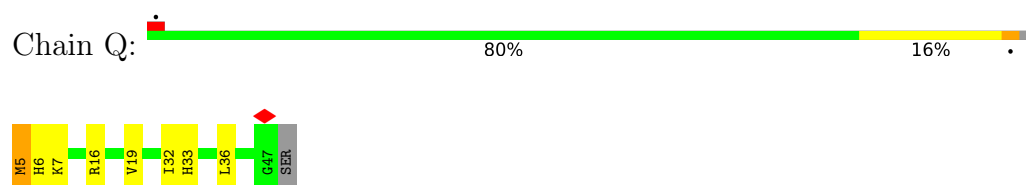
- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit

Chain 1:  70% 27%



- Molecule 5: Antenna complex alpha/beta subunit

Chain 5:  11% 80% 16%



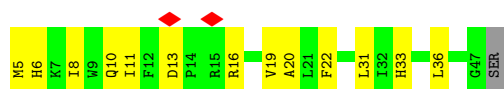
- Molecule 5: Antenna complex alpha/beta subunit

Chain 7:  11% 68% 23% 7%



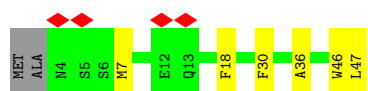
- Molecule 5: Antenna complex alpha/beta subunit

Chain 9:  5% 68% 30%



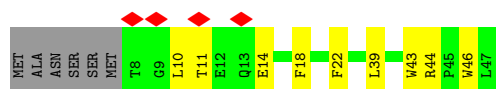
- Molecule 6: Antenna complex alpha/beta subunit

Chain B:  9% 83% 13%



- Molecule 6: Antenna complex alpha/beta subunit

Chain J:  9% 67% 20% 13%

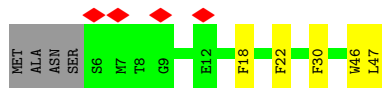
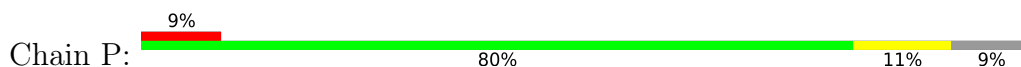


- Molecule 6: Antenna complex alpha/beta subunit

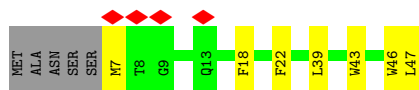
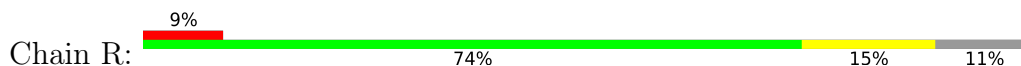
Chain N:  11% 67% 15% 17%



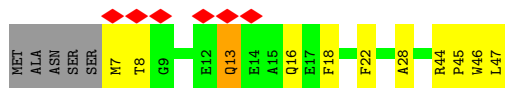
- Molecule 6: Antenna complex alpha/beta subunit



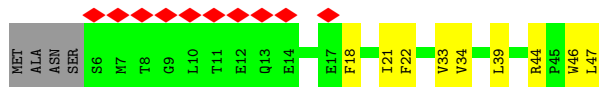
- Molecule 6: Antenna complex alpha/beta subunit



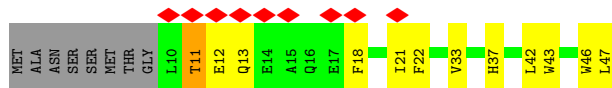
- Molecule 6: Antenna complex alpha/beta subunit



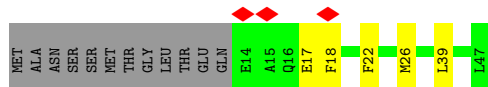
- Molecule 6: Antenna complex alpha/beta subunit



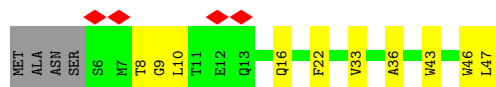
- Molecule 6: Antenna complex alpha/beta subunit



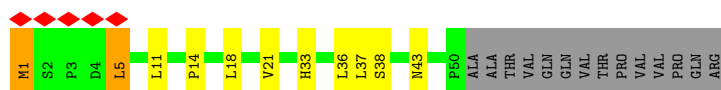
- Molecule 6: Antenna complex alpha/beta subunit



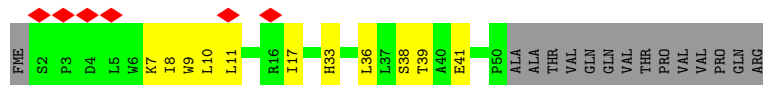
- Molecule 6: Antenna complex alpha/beta subunit



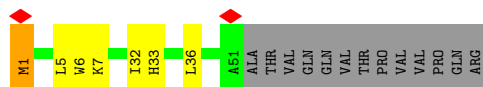
- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



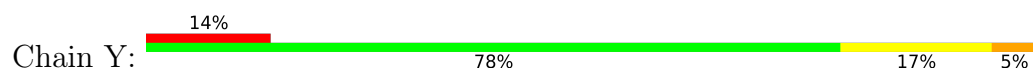
- Molecule 7: Antenna complex alpha/beta subunit

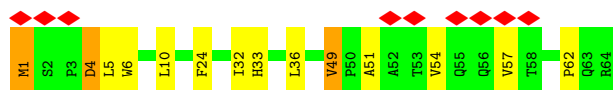


- Molecule 7: Antenna complex alpha/beta subunit

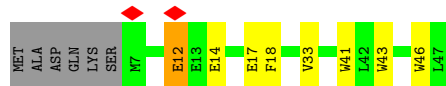


- Molecule 7: Antenna complex alpha/beta subunit

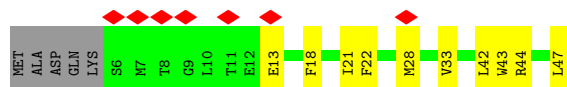




- Molecule 8: Antenna complex alpha/beta subunit



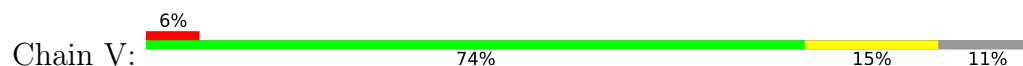
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



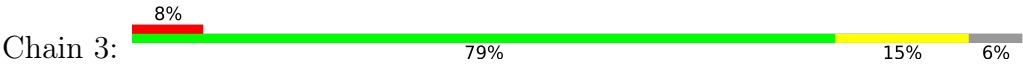
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 9: Antenna complex alpha/beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219233	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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: HEM, Z41, CDL, CRT, CA, UQ8, PLM, FE, LMT, LDA, BPH, PGV, MQ8, FME, BCL, MG

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	C	0.19	0/2502	0.31	0/3426
2	L	0.19	0/2295	0.29	0/3135
3	M	0.20	0/2632	0.27	0/3601
4	H	0.13	0/2039	0.24	0/2776
5	1	0.14	0/362	0.21	0/492
5	5	0.14	0/358	0.25	0/488
5	7	0.15	0/354	0.23	0/483
5	9	0.15	0/362	0.24	0/492
5	A	0.16	0/362	0.23	0/492
5	I	0.14	0/362	0.20	0/492
5	K	0.13	0/369	0.20	0/500
5	O	0.15	0/369	0.22	0/500
5	Q	0.17	0/362	0.22	0/492
6	0	0.13	0/357	0.26	0/485
6	2	0.12	0/351	0.16	0/477
6	4	0.11	0/357	0.18	0/485
6	6	0.09	0/332	0.16	0/452
6	8	0.11	0/299	0.19	0/407
6	B	0.12	0/371	0.17	0/504
6	J	0.11	0/343	0.19	0/467
6	N	0.11	0/332	0.16	0/452
6	P	0.12	0/357	0.17	0/485
6	R	0.13	0/351	0.15	0/477
7	D	0.14	0/409	0.25	0/561
7	F	0.13	0/409	0.23	0/561
7	S	0.15	0/414	0.21	0/568
7	U	0.15	0/414	0.21	0/568
7	W	0.15	0/433	0.25	0/595
7	Y	0.14	0/515	0.29	0/709
8	E	0.12	0/355	0.17	0/480
8	G	0.11	0/361	0.18	0/488
8	T	0.14	0/361	0.18	0/488

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	V	0.13	0/361	0.17	0/488
8	X	0.13	0/361	0.16	0/488
8	Z	0.12	0/355	0.18	0/480
9	3	0.15	0/506	0.22	0/688
All	All	0.16	0/21432	0.24	0/29222

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2429	0	2328	55	0
2	L	2210	0	2166	50	0
3	M	2533	0	2490	51	0
4	H	1993	0	1994	43	0
5	1	359	0	371	10	0
5	5	355	0	360	7	0
5	7	341	0	346	14	0
5	9	359	0	371	10	0
5	A	359	0	371	8	0
5	I	359	0	371	7	0
5	K	366	0	376	12	0
5	O	366	0	376	10	0
5	Q	359	0	371	10	0
6	0	345	0	334	10	0
6	2	339	0	329	12	0
6	4	345	0	334	10	0
6	6	320	0	310	8	0
6	8	287	0	278	6	0
6	B	359	0	345	7	0
6	J	331	0	320	10	0
6	N	320	0	310	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	345	0	334	5	0
6	R	339	0	329	8	0
7	D	407	0	424	10	0
7	F	397	0	413	9	0
7	S	412	0	429	7	0
7	U	412	0	429	12	0
7	W	431	0	450	12	0
7	Y	511	0	535	11	0
8	E	343	0	336	11	0
8	G	349	0	341	10	0
8	T	349	0	341	11	0
8	V	349	0	341	10	0
8	X	349	0	341	11	0
8	Z	343	0	336	12	0
9	3	489	0	497	10	0
10	C	172	0	120	22	0
11	C	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	F	1	0	0	0	0
12	M	1	0	0	0	0
12	S	1	0	0	0	0
12	U	1	0	0	0	0
12	W	1	0	0	0	0
12	Y	1	0	0	0	0
13	C	35	0	0	0	0
14	C	12	0	18	3	0
15	1	27	0	25	3	0
15	C	31	0	32	2	0
15	D	39	0	51	4	0
15	F	36	0	42	3	0
15	H	36	0	42	3	0
15	L	97	0	104	11	0
15	M	64	0	74	3	0
16	0	66	0	74	8	0
16	1	66	0	74	3	0
16	2	66	0	74	10	0
16	3	66	0	74	6	0
16	4	66	0	74	6	0
16	5	66	0	74	6	0
16	6	66	0	74	6	0
16	7	61	0	61	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	8	66	0	74	4	0
16	9	66	0	74	4	0
16	A	66	0	74	1	0
16	B	66	0	74	8	0
16	D	66	0	74	4	0
16	E	66	0	74	7	0
16	F	66	0	74	1	0
16	G	66	0	74	5	0
16	I	66	0	74	5	0
16	J	66	0	74	5	0
16	K	66	0	74	6	0
16	L	132	0	148	8	0
16	M	132	0	148	8	0
16	N	66	0	74	7	0
16	O	66	0	74	3	0
16	P	66	0	74	8	0
16	Q	66	0	74	4	0
16	R	66	0	74	7	0
16	S	66	0	74	6	0
16	T	66	0	74	10	0
16	U	66	0	74	5	0
16	V	66	0	74	8	0
16	W	66	0	74	2	0
16	X	66	0	74	7	0
16	Y	66	0	74	3	0
16	Z	66	0	74	8	0
17	L	65	0	76	5	0
17	M	65	0	76	7	0
18	L	139	0	187	25	0
19	M	1	0	0	0	0
20	M	53	0	72	4	0
21	0	44	0	60	4	0
21	2	44	0	60	7	0
21	4	44	0	60	11	0
21	7	44	0	60	10	0
21	8	44	0	60	7	0
21	B	44	0	60	5	0
21	E	44	0	60	4	0
21	G	44	0	60	7	0
21	K	44	0	60	9	0
21	M	44	0	60	5	0
21	N	44	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	44	0	60	8	0
21	R	44	0	60	5	0
21	T	44	0	60	7	0
21	V	44	0	60	3	0
21	X	44	0	60	9	0
21	Z	44	0	60	6	0
22	D	58	0	60	3	0
22	H	79	0	105	2	0
22	M	218	0	289	13	0
23	M	16	0	31	0	0
23	O	16	0	31	1	0
24	0	35	0	46	3	0
24	2	70	0	92	4	0
24	4	35	0	46	2	0
24	5	31	0	35	1	0
24	8	35	0	46	4	0
24	B	35	0	46	3	0
24	E	35	0	46	2	0
24	G	70	0	92	6	0
24	H	35	0	46	3	0
24	J	35	0	46	2	0
24	M	35	0	46	2	0
24	P	70	0	92	5	0
24	R	35	0	46	2	0
24	V	35	0	46	2	0
24	X	35	0	46	0	0
24	Z	35	0	46	2	0
25	1	1	0	0	0	0
25	2	1	0	0	0	0
25	3	10	0	0	0	0
25	5	1	0	0	0	0
25	7	1	0	0	0	0
25	9	3	0	0	0	0
25	A	2	0	0	0	0
25	C	134	0	0	1	0
25	D	7	0	0	0	0
25	E	2	0	0	0	0
25	F	3	0	0	0	0
25	H	16	0	0	0	0
25	I	2	0	0	0	0
25	K	1	0	0	0	0
25	L	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	M	73	0	0	3	0
25	Q	3	0	0	0	0
25	R	1	0	0	0	0
25	S	6	0	0	0	0
25	T	4	0	0	0	0
25	U	12	0	0	0	0
25	V	3	0	0	0	0
25	W	6	0	0	0	0
25	X	2	0	0	0	0
25	Y	8	0	0	0	0
25	Z	2	0	0	0	0
All	All	26261	0	26696	606	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 12.

The worst 5 of 606 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:CYS:SG	10:C:402:HEM:HAC	1.62	1.39
1:C:250:CYS:SG	10:C:403:HEM:HAC	1.60	1.39
1:C:310:CYS:SG	10:C:404:HEM:CAC	2.15	1.34
1:C:155:CYS:SG	10:C:402:HEM:CAC	2.15	1.33
1:C:250:CYS:SG	10:C:403:HEM:CAC	2.19	1.30

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	C	309/383 (81%)	301 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	275/278 (99%)	269 (98%)	6 (2%)	0	100	100
3	M	316/325 (97%)	311 (98%)	5 (2%)	0	100	100
4	H	258/259 (100%)	249 (96%)	9 (4%)	0	100	100
5	1	41/44 (93%)	41 (100%)	0	0	100	100
5	5	41/44 (93%)	38 (93%)	2 (5%)	1 (2%)	4	1
5	7	39/44 (89%)	39 (100%)	0	0	100	100
5	9	41/44 (93%)	40 (98%)	1 (2%)	0	100	100
5	A	41/44 (93%)	41 (100%)	0	0	100	100
5	I	41/44 (93%)	41 (100%)	0	0	100	100
5	K	42/44 (96%)	42 (100%)	0	0	100	100
5	O	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	Q	41/44 (93%)	40 (98%)	0	1 (2%)	4	1
6	0	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
6	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
6	4	40/46 (87%)	40 (100%)	0	0	100	100
6	6	36/46 (78%)	36 (100%)	0	0	100	100
6	8	32/46 (70%)	32 (100%)	0	0	100	100
6	B	42/46 (91%)	42 (100%)	0	0	100	100
6	J	38/46 (83%)	38 (100%)	0	0	100	100
6	N	36/46 (78%)	36 (100%)	0	0	100	100
6	P	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
6	R	39/46 (85%)	39 (100%)	0	0	100	100
7	D	48/64 (75%)	46 (96%)	2 (4%)	0	100	100
7	F	47/64 (73%)	45 (96%)	2 (4%)	0	100	100
7	S	49/64 (77%)	49 (100%)	0	0	100	100
7	U	49/64 (77%)	49 (100%)	0	0	100	100
7	W	52/64 (81%)	49 (94%)	3 (6%)	0	100	100
7	Y	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
8	E	39/47 (83%)	39 (100%)	0	0	100	100
8	G	40/47 (85%)	40 (100%)	0	0	100	100
8	T	40/47 (85%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	40/47 (85%)	40 (100%)	0	0	100	100
8	X	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
8	Z	39/47 (83%)	39 (100%)	0	0	100	100
9	3	60/66 (91%)	60 (100%)	0	0	100	100
All	All	2514/2833 (89%)	2465 (98%)	47 (2%)	2 (0%)	49	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Q	6	HIS
5	5	6	HIS

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	C	265/311 (85%)	264 (100%)	1 (0%)	84	88
2	L	223/224 (100%)	219 (98%)	4 (2%)	51	61
3	M	252/257 (98%)	249 (99%)	3 (1%)	63	72
4	H	206/206 (100%)	200 (97%)	6 (3%)	37	44
5	1	37/38 (97%)	37 (100%)	0	100	100
5	5	36/38 (95%)	34 (94%)	2 (6%)	19	18
5	7	36/38 (95%)	35 (97%)	1 (3%)	38	45
5	9	37/38 (97%)	36 (97%)	1 (3%)	39	47
5	A	37/38 (97%)	36 (97%)	1 (3%)	39	47
5	I	37/38 (97%)	37 (100%)	0	100	100
5	K	38/38 (100%)	38 (100%)	0	100	100
5	O	38/38 (100%)	38 (100%)	0	100	100
5	Q	37/38 (97%)	37 (100%)	0	100	100
6	0	35/38 (92%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2	34/38 (90%)	32 (94%)	2 (6%)	18	16
6	4	35/38 (92%)	35 (100%)	0	100	100
6	6	32/38 (84%)	28 (88%)	4 (12%)	4	2
6	8	28/38 (74%)	27 (96%)	1 (4%)	31	36
6	B	37/38 (97%)	37 (100%)	0	100	100
6	J	33/38 (87%)	33 (100%)	0	100	100
6	N	32/38 (84%)	32 (100%)	0	100	100
6	P	35/38 (92%)	35 (100%)	0	100	100
6	R	34/38 (90%)	34 (100%)	0	100	100
7	D	43/55 (78%)	42 (98%)	1 (2%)	44	53
7	F	43/55 (78%)	43 (100%)	0	100	100
7	S	43/55 (78%)	42 (98%)	1 (2%)	44	53
7	U	43/55 (78%)	41 (95%)	2 (5%)	23	24
7	W	45/55 (82%)	45 (100%)	0	100	100
7	Y	55/55 (100%)	50 (91%)	5 (9%)	9	5
8	E	35/40 (88%)	34 (97%)	1 (3%)	37	44
8	G	36/40 (90%)	35 (97%)	1 (3%)	38	45
8	T	36/40 (90%)	36 (100%)	0	100	100
8	V	36/40 (90%)	36 (100%)	0	100	100
8	X	36/40 (90%)	36 (100%)	0	100	100
8	Z	35/40 (88%)	34 (97%)	1 (3%)	37	44
9	3	48/52 (92%)	48 (100%)	0	100	100
All	All	2148/2342 (92%)	2110 (98%)	38 (2%)	51	61

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	2	16	GLN
5	7	11	ILE
5	5	6	HIS
6	6	13	GLN
5	9	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	O	10	GLN
5	Q	10	GLN
6	8	24	GLN
8	Z	24	GLN
6	2	13	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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	$\# Z > 2$
7	FME	U	1	7	8,9,10	0.57	0	8,9,11	0.85	1 (12%)
5	FME	Q	5	5	8,9,10	0.55	0	8,9,11	0.96	1 (12%)
7	FME	S	1	7	8,9,10	0.56	0	8,9,11	0.89	1 (12%)
7	FME	W	1	7	8,9,10	0.56	0	8,9,11	0.99	1 (12%)
5	FME	I	5	5	8,9,10	0.53	0	8,9,11	1.10	1 (12%)
5	FME	5	5	5	8,9,10	0.55	0	8,9,11	0.95	1 (12%)
5	FME	9	5	5	8,9,10	0.54	0	8,9,11	1.06	1 (12%)
7	FME	D	1	7	8,9,10	0.54	0	8,9,11	1.04	1 (12%)
4	FME	H	1	4	8,9,10	0.54	0	8,9,11	0.96	1 (12%)
5	FME	O	5	5	8,9,10	0.55	0	8,9,11	0.94	1 (12%)
5	FME	K	5	5	8,9,10	0.53	0	8,9,11	1.18	1 (12%)
5	FME	1	5	5	8,9,10	0.54	0	8,9,11	0.92	1 (12%)
7	FME	Y	1	7	8,9,10	0.55	0	8,9,11	0.93	1 (12%)
5	FME	A	5	5	8,9,10	0.53	0	8,9,11	1.07	1 (12%)

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

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1	FME	O-C-CA	-2.76	117.68	124.77
5	K	5	FME	O-C-CA	-2.75	117.69	124.77
5	I	5	FME	O-C-CA	-2.75	117.70	124.77
5	9	5	FME	O-C-CA	-2.71	117.79	124.77
5	A	5	FME	O-C-CA	-2.69	117.85	124.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
5	K	5	FME	CB-CA-N-CN
5	Q	5	FME	O1-CN-N-CA
5	Q	5	FME	CB-CA-N-CN
5	Q	5	FME	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	5	FME	3	0
7	S	1	FME	1	0
7	W	1	FME	1	0
7	D	1	FME	1	0
4	H	1	FME	1	0
5	K	5	FME	1	0
7	Y	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 10 are monoatomic - leaving 101 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	$\# Z > 2$
21	CRT	K	101	-	43,43,43	0.67	0	48,54,54	2.31	17 (35%)
16	BCL	P	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.18	24 (30%)
24	LMT	4	103	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
16	BCL	B	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.18	25 (31%)
16	BCL	7	102	-	64,69,74	1.85	17 (26%)	73,109,115	2.28	23 (31%)
14	PLM	C	408	1	10,11,17	0.33	0	9,10,17	0.33	0
21	CRT	2	103	-	43,43,43	0.67	0	48,54,54	2.21	18 (37%)
15	PGV	D	501	-	38,38,50	1.02	2 (5%)	41,44,56	1.19	3 (7%)
16	BCL	Z	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.19	22 (27%)
21	CRT	M	407	-	43,43,43	0.59	0	48,54,54	2.43	17 (35%)
16	BCL	4	101	-	69,74,74	1.79	19 (27%)	79,115,115	2.20	24 (30%)
10	HEM	C	403	1	50,50,50	1.62	9 (18%)	67,82,82	1.61	10 (14%)
21	CRT	G	103	-	43,43,43	0.63	0	48,54,54	2.05	16 (33%)
24	LMT	2	101	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	E	101	-	36,36,36	0.43	0	47,47,47	0.81	1 (2%)
21	CRT	Q	101	-	43,43,43	0.65	0	48,54,54	2.31	15 (31%)
21	CRT	V	103	-	43,43,43	0.64	0	48,54,54	2.31	19 (39%)
16	BCL	I	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.22	22 (27%)
13	Z4I	C	407	-	34,34,39	0.29	0	36,36,41	0.30	0
24	LMT	2	104	-	36,36,36	0.42	0	47,47,47	0.67	1 (2%)
16	BCL	L	307	-	69,74,74	1.78	17 (24%)	79,115,115	2.17	20 (25%)
16	BCL	J	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.20	23 (29%)
24	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	1.00	3 (6%)
15	PGV	L	309	-	32,32,50	1.14	2 (6%)	35,38,56	1.30	3 (8%)
16	BCL	Q	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.24	23 (29%)
24	LMT	5	101	-	32,32,36	0.43	0	43,43,47	1.14	3 (6%)
16	BCL	N	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.19	22 (27%)
10	HEM	C	402	1	50,50,50	1.60	9 (18%)	67,82,82	1.64	12 (17%)
16	BCL	L	301	-	69,74,74	1.77	17 (24%)	79,115,115	2.22	23 (29%)
16	BCL	T	101	-	69,74,74	1.76	15 (21%)	79,115,115	2.16	20 (25%)
22	CDL	D	502	-	57,57,99	1.11	4 (7%)	63,69,111	1.20	5 (7%)
16	BCL	8	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.20	24 (30%)
15	PGV	F	501	-	35,35,50	1.09	2 (5%)	38,41,56	1.16	3 (7%)
24	LMT	B	101	-	36,36,36	0.42	0	47,47,47	0.68	1 (2%)
16	BCL	X	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.15	22 (27%)
16	BCL	G	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.20	22 (27%)
16	BCL	W	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.24	22 (27%)
24	LMT	8	101	-	36,36,36	0.39	0	47,47,47	0.77	2 (4%)
24	LMT	G	101	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
16	BCL	2	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.20	23 (29%)
21	CRT	X	103	-	43,43,43	0.61	0	48,54,54	2.18	17 (35%)
16	BCL	M	403	-	69,74,74	1.77	19 (27%)	79,115,115	2.17	24 (30%)
17	BPH	L	302	-	59,70,70	0.80	3 (5%)	59,101,101	0.93	3 (5%)
24	LMT	P	101	-	36,36,36	0.41	0	47,47,47	0.61	0
22	CDL	M	412	-	83,83,99	1.04	4 (4%)	89,95,111	1.17	6 (6%)
21	CRT	7	101	-	43,43,43	0.65	0	48,54,54	1.90	10 (20%)
23	LDA	O	501	-	13,15,15	2.18	2 (15%)	14,17,17	0.50	0
15	PGV	L	306	-	34,34,50	1.09	2 (5%)	37,40,56	1.18	4 (10%)
15	PGV	L	305	-	28,28,50	1.21	2 (7%)	31,34,56	1.25	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CRT	B	103	-	43,43,43	0.62	0	48,54,54	2.09	16 (33%)
16	BCL	Y	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.22	22 (27%)
22	CDL	H	302	-	78,78,99	1.02	4 (5%)	84,90,111	1.09	6 (7%)
22	CDL	M	411	-	94,94,99	0.95	4 (4%)	100,106,111	1.10	7 (7%)
21	CRT	8	103	-	43,43,43	0.62	0	48,54,54	2.06	15 (31%)
15	PGV	M	410	-	26,26,50	1.29	2 (7%)	29,31,56	1.39	6 (20%)
22	CDL	M	409	-	38,38,99	1.31	3 (7%)	43,49,111	1.18	3 (6%)
23	LDA	M	413	-	13,15,15	2.20	2 (15%)	14,17,17	0.50	0
21	CRT	0	103	-	43,43,43	0.62	0	48,54,54	2.04	16 (33%)
16	BCL	0	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.15	23 (29%)
24	LMT	G	104	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
15	PGV	1	401	-	26,26,50	1.29	2 (7%)	29,31,56	1.20	2 (6%)
16	BCL	9	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.20	23 (29%)
21	CRT	4	102	-	43,43,43	0.65	0	48,54,54	2.21	16 (33%)
18	UQ8	L	304	-	53,53,53	1.23	2 (3%)	66,67,67	1.71	16 (24%)
16	BCL	M	404	-	69,74,74	1.80	17 (24%)	79,115,115	2.37	26 (32%)
17	BPH	M	405	-	59,70,70	0.79	4 (6%)	59,101,101	0.86	3 (5%)
16	BCL	U	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.21	20 (25%)
16	BCL	S	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.19	22 (27%)
16	BCL	V	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.15	22 (27%)
24	LMT	R	103	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
18	UQ8	L	308	-	53,53,53	1.26	2 (3%)	66,67,67	1.61	16 (24%)
16	BCL	3	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.27	24 (30%)
21	CRT	T	102	-	43,43,43	0.63	0	48,54,54	2.16	17 (35%)
16	BCL	6	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.18	25 (31%)
16	BCL	D	503	-	69,74,74	1.78	17 (24%)	79,115,115	2.25	21 (26%)
15	PGV	H	301	-	35,35,50	1.08	2 (5%)	38,41,56	1.23	4 (10%)
24	LMT	H	303	-	36,36,36	0.38	0	47,47,47	0.79	1 (2%)
24	LMT	V	101	-	36,36,36	0.39	0	47,47,47	0.75	0
15	PGV	C	409	-	30,30,50	1.17	2 (6%)	33,36,56	1.13	4 (12%)
20	MQ8	M	406	-	54,54,54	1.33	2 (3%)	67,69,69	1.51	14 (20%)
10	HEM	C	401	1	50,50,50	1.61	9 (18%)	67,82,82	1.67	14 (20%)
16	BCL	R	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.16	23 (29%)
21	CRT	R	102	-	43,43,43	0.62	0	48,54,54	2.06	16 (33%)
15	PGV	M	408	-	36,36,50	1.07	2 (5%)	39,42,56	1.17	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEM	C	404	1	50,50,50	1.63	10 (20%)	67,82,82	1.62	11 (16%)
21	CRT	N	102	-	43,43,43	0.61	0	48,54,54	2.13	17 (35%)
16	BCL	F	502	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	22 (27%)
24	LMT	M	414	-	36,36,36	0.39	0	47,47,47	0.77	0
24	LMT	X	101	-	36,36,36	0.42	0	47,47,47	0.83	1 (2%)
24	LMT	O	101	-	36,36,36	0.40	0	47,47,47	0.78	1 (2%)
16	BCL	O	502	-	69,74,74	1.78	18 (26%)	79,115,115	2.26	22 (27%)
24	LMT	J	102	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
24	LMT	P	103	-	36,36,36	0.38	0	47,47,47	0.72	1 (2%)
18	UQ8	L	303	-	33,33,53	1.51	2 (6%)	42,43,67	1.64	10 (23%)
16	BCL	E	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.21	23 (29%)
21	CRT	Z	103	-	43,43,43	0.62	0	48,54,54	2.12	17 (35%)
16	BCL	A	101	-	69,74,74	1.77	18 (26%)	79,115,115	2.28	22 (27%)
16	BCL	K	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.26	24 (30%)
21	CRT	E	103	-	43,43,43	0.61	0	48,54,54	2.17	17 (35%)
16	BCL	5	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.23	23 (29%)
16	BCL	1	402	-	69,74,74	1.78	17 (24%)	79,115,115	2.20	24 (30%)

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
21	CRT	K	101	-	-	11/51/51/51	-
16	BCL	P	102	-	-	21/41/137/137	-
24	LMT	4	103	-	-	2/21/61/61	0/2/2/2
16	BCL	B	102	-	-	17/41/137/137	-
16	BCL	7	102	-	-	12/35/131/137	-
14	PLM	C	408	1	-	2/9/9/15	-
21	CRT	2	103	-	-	2/51/51/51	-
15	PGV	D	501	-	-	14/43/43/55	-
16	BCL	Z	102	-	-	16/41/137/137	-
21	CRT	M	407	-	-	8/51/51/51	-
16	BCL	4	101	-	-	8/41/137/137	-
10	HEM	C	403	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CRT	G	103	-	-	5/51/51/51	-
24	LMT	2	101	-	-	2/21/61/61	0/2/2/2
24	LMT	E	101	-	-	2/21/61/61	0/2/2/2
21	CRT	Q	101	-	-	8/51/51/51	-
21	CRT	V	103	-	-	5/51/51/51	-
16	BCL	I	101	-	-	12/41/137/137	-
13	Z41	C	407	-	-	5/35/35/41	-
24	LMT	2	104	-	-	3/21/61/61	0/2/2/2
16	BCL	L	307	-	-	12/41/137/137	-
16	BCL	J	101	-	-	14/41/137/137	-
24	LMT	Z	101	-	-	5/21/61/61	0/2/2/2
15	PGV	L	309	-	-	6/37/37/55	-
16	BCL	Q	102	-	-	11/41/137/137	-
24	LMT	5	101	-	-	5/17/57/61	0/2/2/2
16	BCL	N	101	-	-	15/41/137/137	-
10	HEM	C	402	1	-	7/14/54/54	-
16	BCL	L	301	-	-	8/41/137/137	-
16	BCL	T	101	-	-	17/41/137/137	-
22	CDL	D	502	-	-	21/67/67/110	-
16	BCL	8	102	-	-	15/41/137/137	-
15	PGV	F	501	-	-	4/40/40/55	-
24	LMT	B	101	-	-	1/21/61/61	0/2/2/2
16	BCL	X	102	-	-	16/41/137/137	-
16	BCL	G	102	-	-	18/41/137/137	-
16	BCL	W	101	-	-	20/41/137/137	-
24	LMT	8	101	-	-	2/21/61/61	0/2/2/2
24	LMT	G	101	-	-	5/21/61/61	0/2/2/2
16	BCL	2	102	-	-	14/41/137/137	-
21	CRT	X	103	-	-	4/51/51/51	-
16	BCL	M	403	-	-	5/41/137/137	-
17	BPH	L	302	-	-	3/37/105/105	0/5/6/6
24	LMT	P	101	-	-	4/21/61/61	0/2/2/2
22	CDL	M	412	-	-	30/93/93/110	-
21	CRT	7	101	-	-	5/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LDA	O	501	-	-	0/13/13/13	-
15	PGV	L	306	-	-	6/39/39/55	-
15	PGV	L	305	-	-	14/33/33/55	-
21	CRT	B	103	-	-	1/51/51/51	-
16	BCL	Y	101	-	-	18/41/137/137	-
22	CDL	H	302	-	-	22/89/89/110	-
22	CDL	M	411	-	-	28/105/105/110	-
21	CRT	8	103	-	-	3/51/51/51	-
15	PGV	M	410	-	-	7/28/28/55	-
22	CDL	M	409	-	-	18/48/48/110	-
23	LDA	M	413	-	-	3/13/13/13	-
21	CRT	0	103	-	-	2/51/51/51	-
16	BCL	0	102	-	-	16/41/137/137	-
24	LMT	G	104	-	-	2/21/61/61	0/2/2/2
15	PGV	1	401	-	-	12/30/30/55	-
16	BCL	9	101	-	-	16/41/137/137	-
21	CRT	4	102	-	-	7/51/51/51	-
18	UQ8	L	304	-	-	14/51/75/75	0/1/1/1
16	BCL	M	404	-	-	10/41/137/137	-
17	BPH	M	405	-	-	4/37/105/105	0/5/6/6
16	BCL	U	101	-	-	18/41/137/137	-
16	BCL	S	101	-	-	11/41/137/137	-
16	BCL	V	102	-	-	21/41/137/137	-
24	LMT	R	103	-	-	7/21/61/61	0/2/2/2
18	UQ8	L	308	-	-	7/51/75/75	0/1/1/1
16	BCL	3	101	-	-	10/41/137/137	-
21	CRT	T	102	-	-	5/51/51/51	-
16	BCL	6	101	-	-	14/41/137/137	-
16	BCL	D	503	-	-	8/41/137/137	-
15	PGV	H	301	-	-	15/40/40/55	-
24	LMT	H	303	-	-	1/21/61/61	0/2/2/2
24	LMT	V	101	-	-	9/21/61/61	0/2/2/2
15	PGV	C	409	-	-	5/35/35/55	-
20	MQ8	M	406	-	-	5/47/67/67	0/2/2/2
10	HEM	C	401	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	R	101	-	-	13/41/137/137	-
21	CRT	R	102	-	-	2/51/51/51	-
15	PGV	M	408	-	-	5/41/41/55	-
10	HEM	C	404	1	-	6/14/54/54	-
21	CRT	N	102	-	-	5/51/51/51	-
16	BCL	F	502	-	-	12/41/137/137	-
24	LMT	M	414	-	-	7/21/61/61	0/2/2/2
24	LMT	X	101	-	-	4/21/61/61	0/2/2/2
24	LMT	O	101	-	-	5/21/61/61	0/2/2/2
16	BCL	O	502	-	-	16/41/137/137	-
24	LMT	J	102	-	-	3/21/61/61	0/2/2/2
24	LMT	P	103	-	-	1/21/61/61	0/2/2/2
18	UQ8	L	303	-	-	4/27/51/75	0/1/1/1
16	BCL	E	102	-	-	13/41/137/137	-
21	CRT	Z	103	-	-	8/51/51/51	-
16	BCL	A	101	-	-	13/41/137/137	-
16	BCL	K	102	-	-	10/41/137/137	-
21	CRT	E	103	-	-	0/51/51/51	-
16	BCL	5	102	-	-	9/41/137/137	-
16	BCL	1	402	-	-	17/41/137/137	-

The worst 5 of 722 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	406	MQ8	C3-C2	8.01	1.49	1.35
18	L	308	UQ8	C6-C1	7.75	1.49	1.35
18	L	304	UQ8	C6-C1	7.70	1.49	1.35
18	L	303	UQ8	C6-C1	7.54	1.48	1.35
23	M	413	LDA	O1-N1	-6.81	1.25	1.42

The worst 5 of 1287 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	404	BCL	CMD-C2D-C1D	8.44	139.59	124.73
16	7	102	BCL	CMD-C2D-C1D	8.13	139.05	124.73
16	A	101	BCL	CMD-C2D-C1D	8.08	138.96	124.73
16	F	502	BCL	CMD-C2D-C1D	8.06	138.92	124.73
16	I	101	BCL	CMD-C2D-C1D	8.02	138.85	124.73

There are no chirality outliers.

5 of 924 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	401	HEM	C2B-C3B-CAB-CBB
10	C	402	HEM	C2B-C3B-CAB-CBB
10	C	402	HEM	C2C-C3C-CAC-CBC
10	C	403	HEM	C2B-C3B-CAB-CBB
10	C	403	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

97 monomers are involved in 428 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	101	CRT	9	0
16	P	102	BCL	8	0
24	4	103	LMT	2	0
16	B	102	BCL	8	0
16	7	102	BCL	6	0
14	C	408	PLM	3	0
21	2	103	CRT	7	0
15	D	501	PGV	4	0
16	Z	102	BCL	8	0
21	M	407	CRT	5	0
16	4	101	BCL	6	0
10	C	403	HEM	4	0
21	G	103	CRT	7	0
24	2	101	LMT	1	0
24	E	101	LMT	2	0
21	Q	101	CRT	8	0
21	V	103	CRT	3	0
16	I	101	BCL	5	0
24	2	104	LMT	3	0
16	L	307	BCL	7	0
16	J	101	BCL	5	0
24	Z	101	LMT	2	0
15	L	309	PGV	4	0
16	Q	102	BCL	4	0
24	5	101	LMT	1	0
16	N	101	BCL	7	0
10	C	402	HEM	7	0
16	L	301	BCL	1	0
16	T	101	BCL	10	0
22	D	502	CDL	3	0

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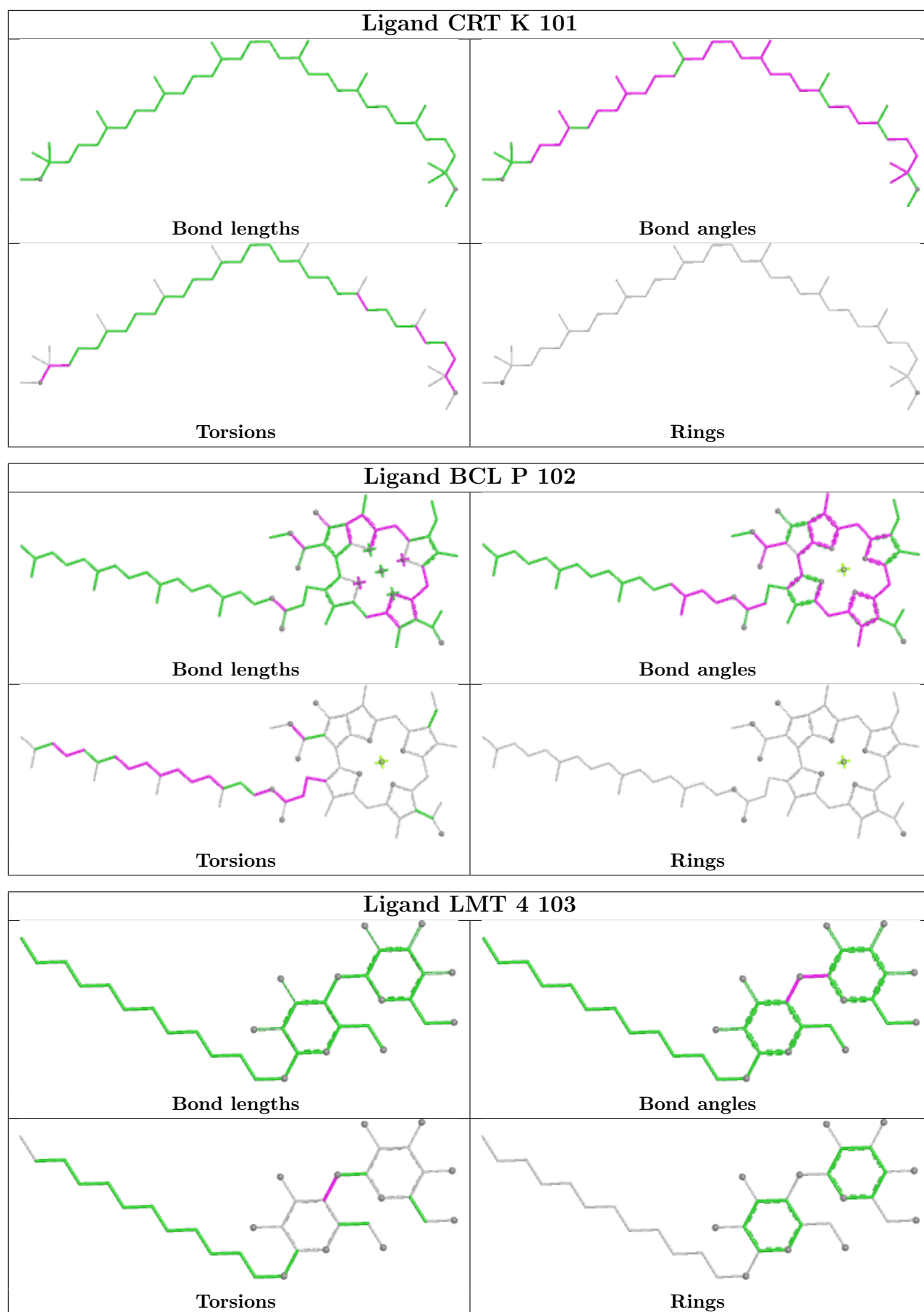
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	8	102	BCL	4	0
15	F	501	PGV	3	0
24	B	101	LMT	3	0
16	X	102	BCL	7	0
16	G	102	BCL	5	0
16	W	101	BCL	2	0
24	8	101	LMT	4	0
24	G	101	LMT	2	0
16	2	102	BCL	10	0
21	X	103	CRT	9	0
16	M	403	BCL	2	0
17	L	302	BPH	5	0
24	P	101	LMT	2	0
22	M	412	CDL	7	0
21	7	101	CRT	10	0
23	O	501	LDA	1	0
15	L	306	PGV	3	0
15	L	305	PGV	4	0
21	B	103	CRT	5	0
16	Y	101	BCL	3	0
22	H	302	CDL	2	0
22	M	411	CDL	5	0
21	8	103	CRT	7	0
15	M	410	PGV	3	0
22	M	409	CDL	1	0
21	0	103	CRT	4	0
16	0	102	BCL	8	0
24	G	104	LMT	4	0
15	1	401	PGV	3	0
16	9	101	BCL	4	0
21	4	102	CRT	11	0
18	L	304	UQ8	12	0
16	M	404	BCL	6	0
17	M	405	BPH	7	0
16	U	101	BCL	5	0
16	S	101	BCL	6	0
16	V	102	BCL	8	0
24	R	103	LMT	2	0
18	L	308	UQ8	9	0
16	3	101	BCL	6	0
21	T	102	CRT	7	0
16	6	101	BCL	6	0

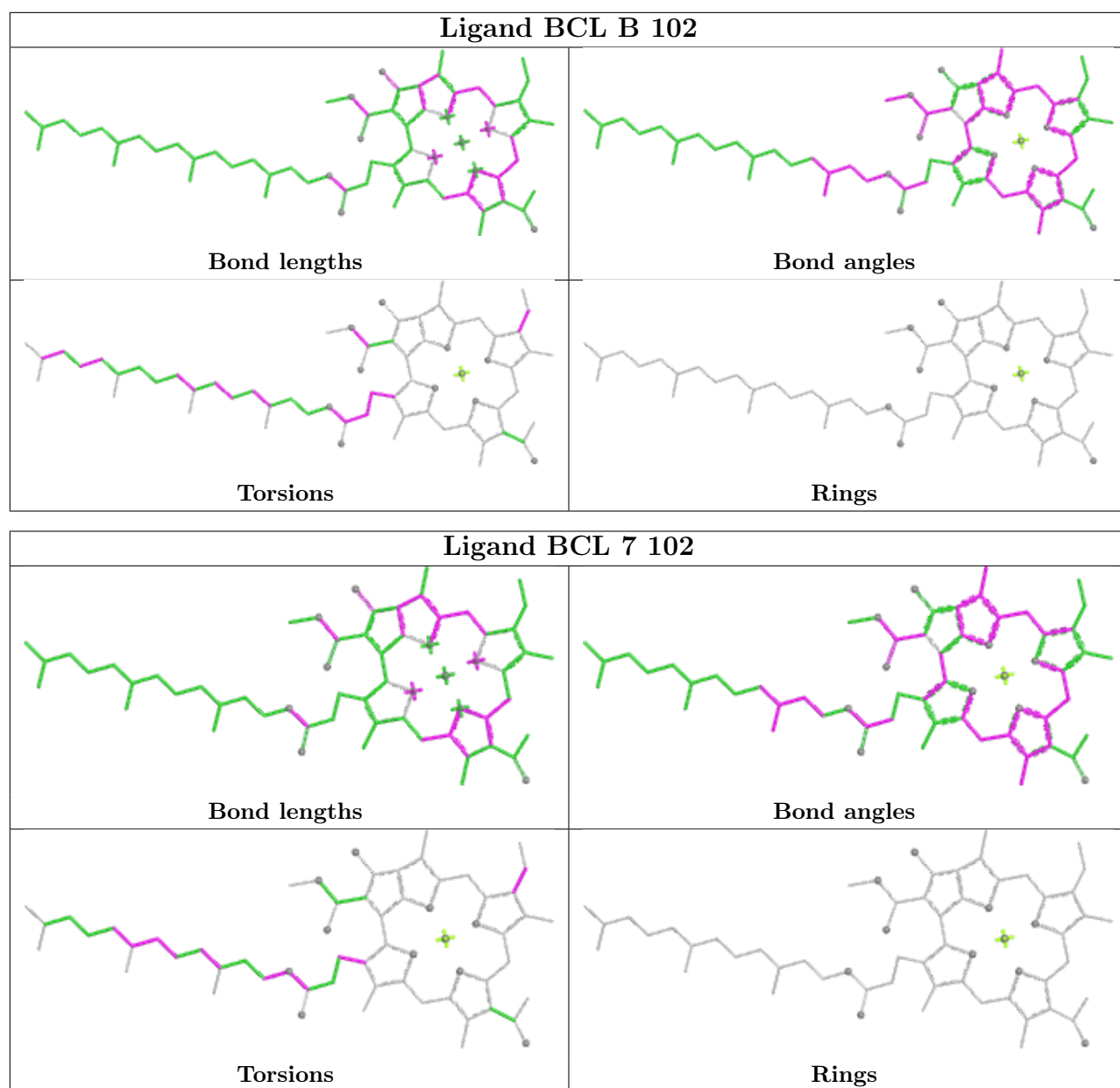
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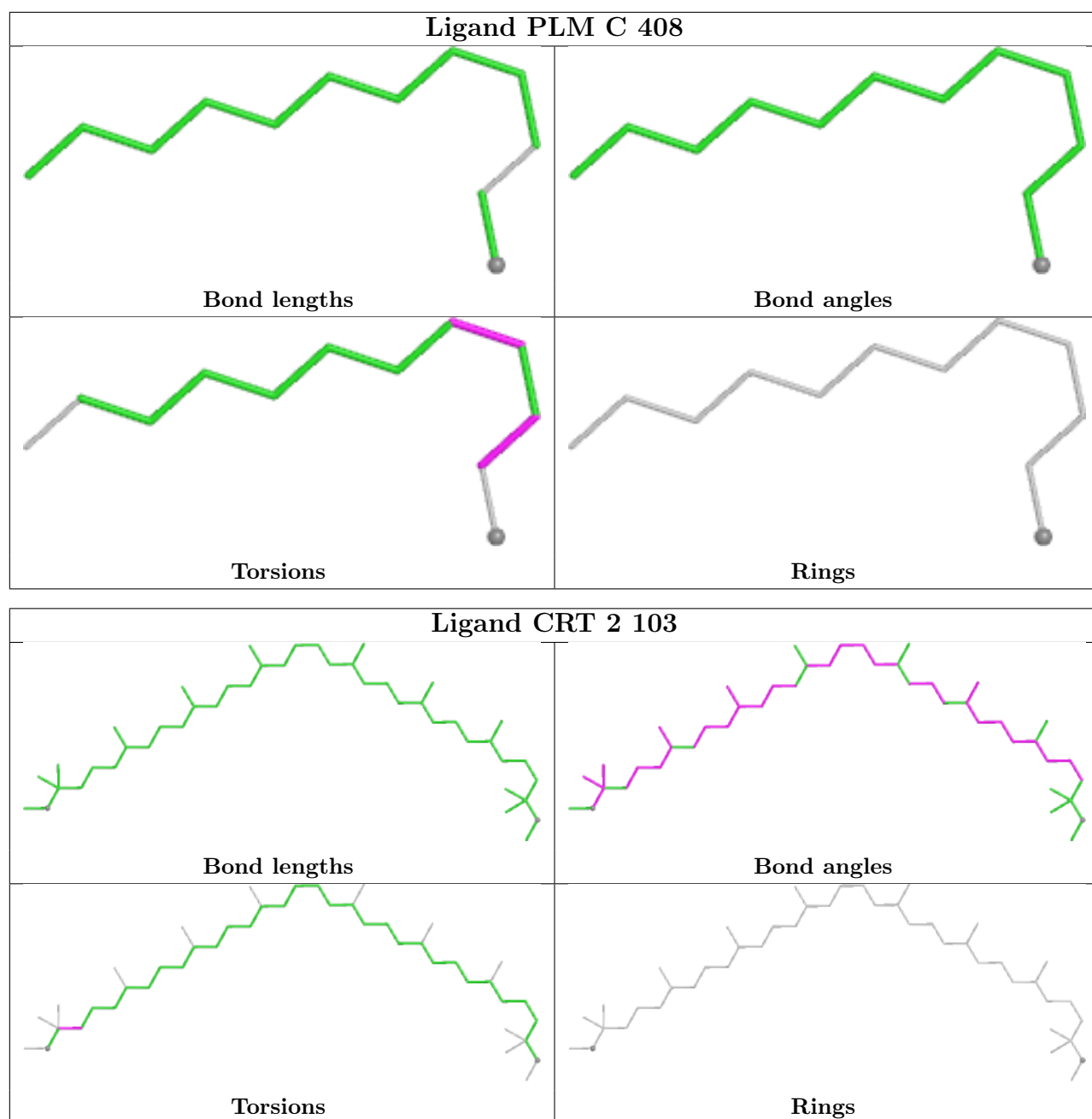
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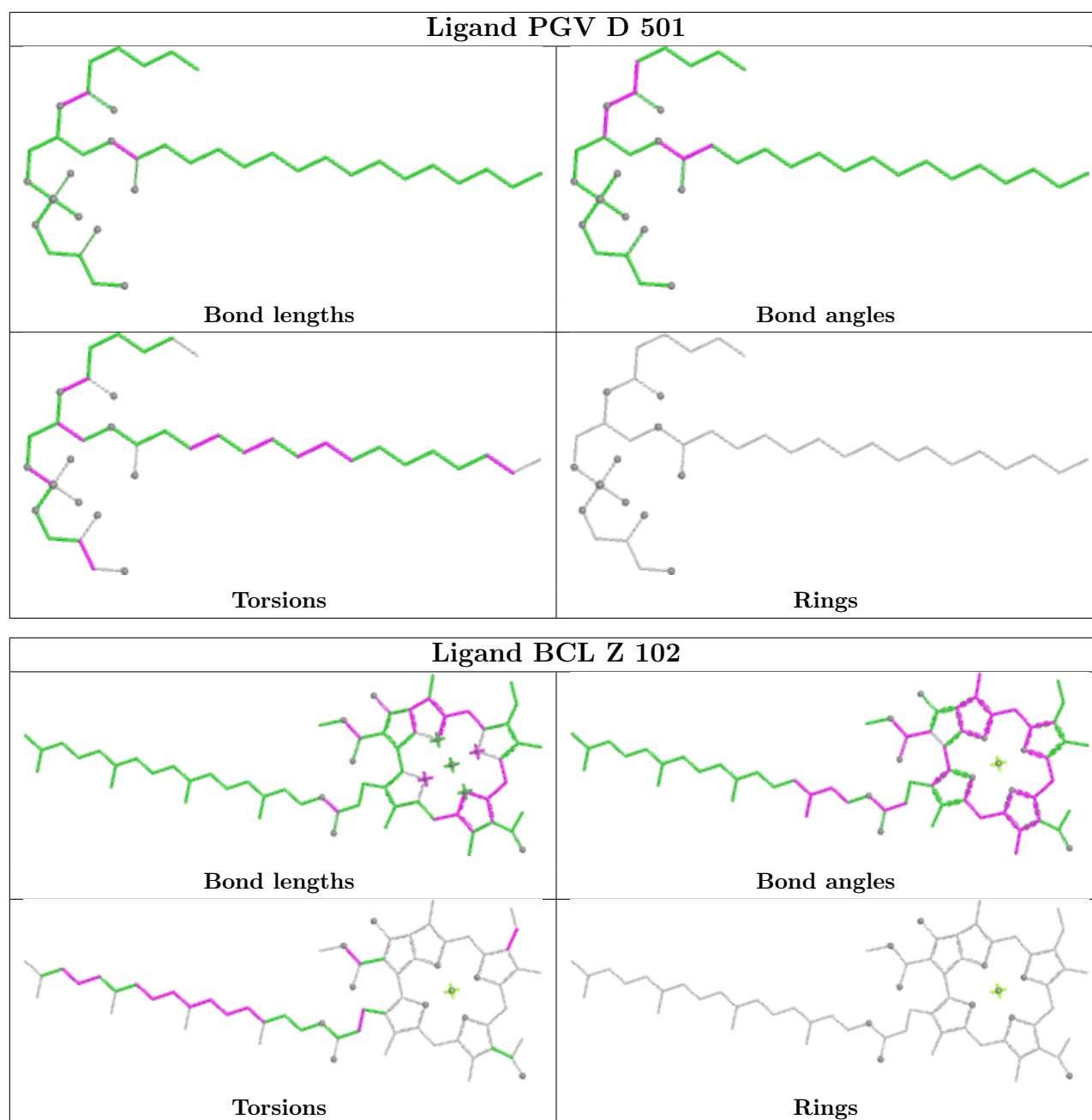
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	503	BCL	4	0
15	H	301	PGV	3	0
24	H	303	LMT	3	0
24	V	101	LMT	2	0
15	C	409	PGV	2	0
20	M	406	MQ8	4	0
10	C	401	HEM	7	0
16	R	101	BCL	7	0
21	R	102	CRT	5	0
10	C	404	HEM	4	0
21	N	102	CRT	1	0
16	F	502	BCL	1	0
24	M	414	LMT	2	0
24	O	101	LMT	3	0
16	O	502	BCL	3	0
24	J	102	LMT	2	0
24	P	103	LMT	3	0
18	L	303	UQ8	4	0
16	E	102	BCL	7	0
21	Z	103	CRT	6	0
16	A	101	BCL	1	0
16	K	102	BCL	6	0
21	E	103	CRT	4	0
16	5	102	BCL	6	0
16	1	402	BCL	3	0

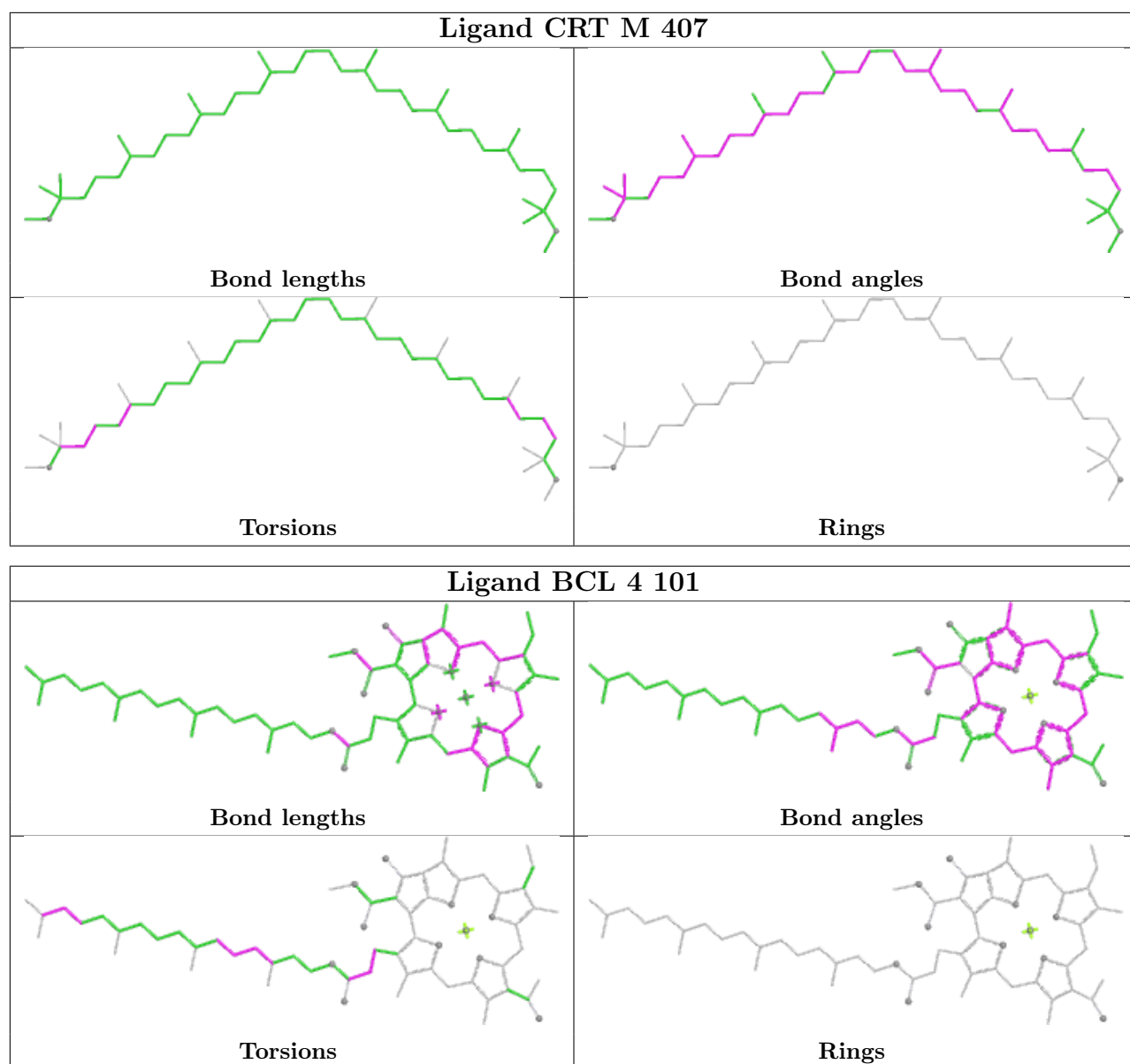
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

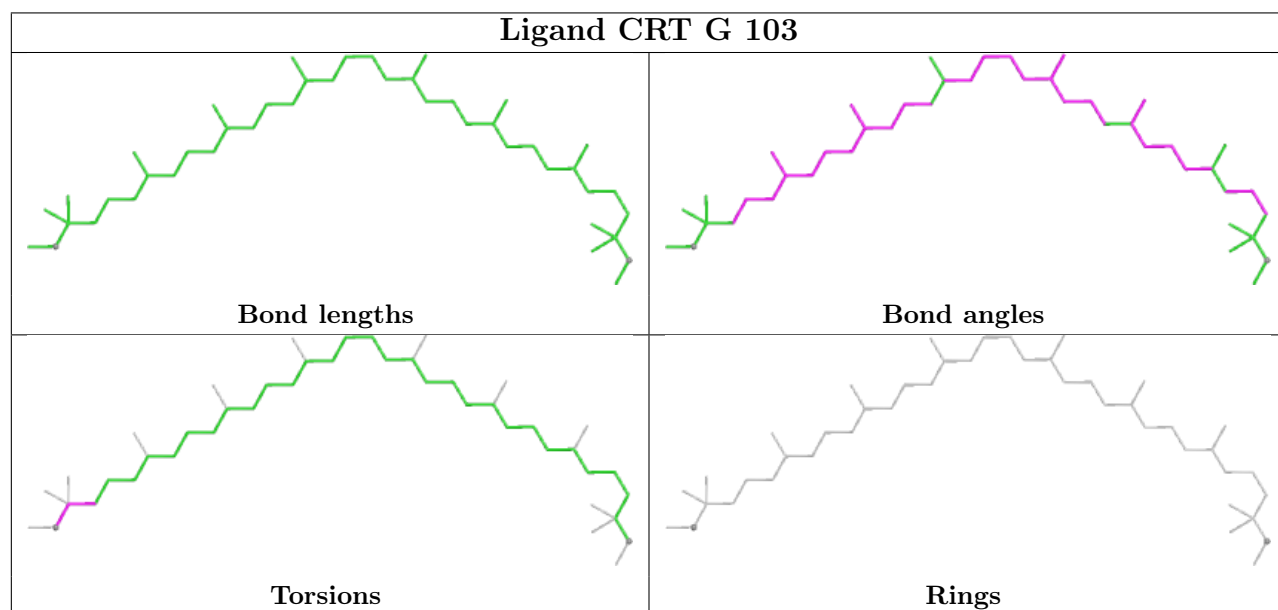
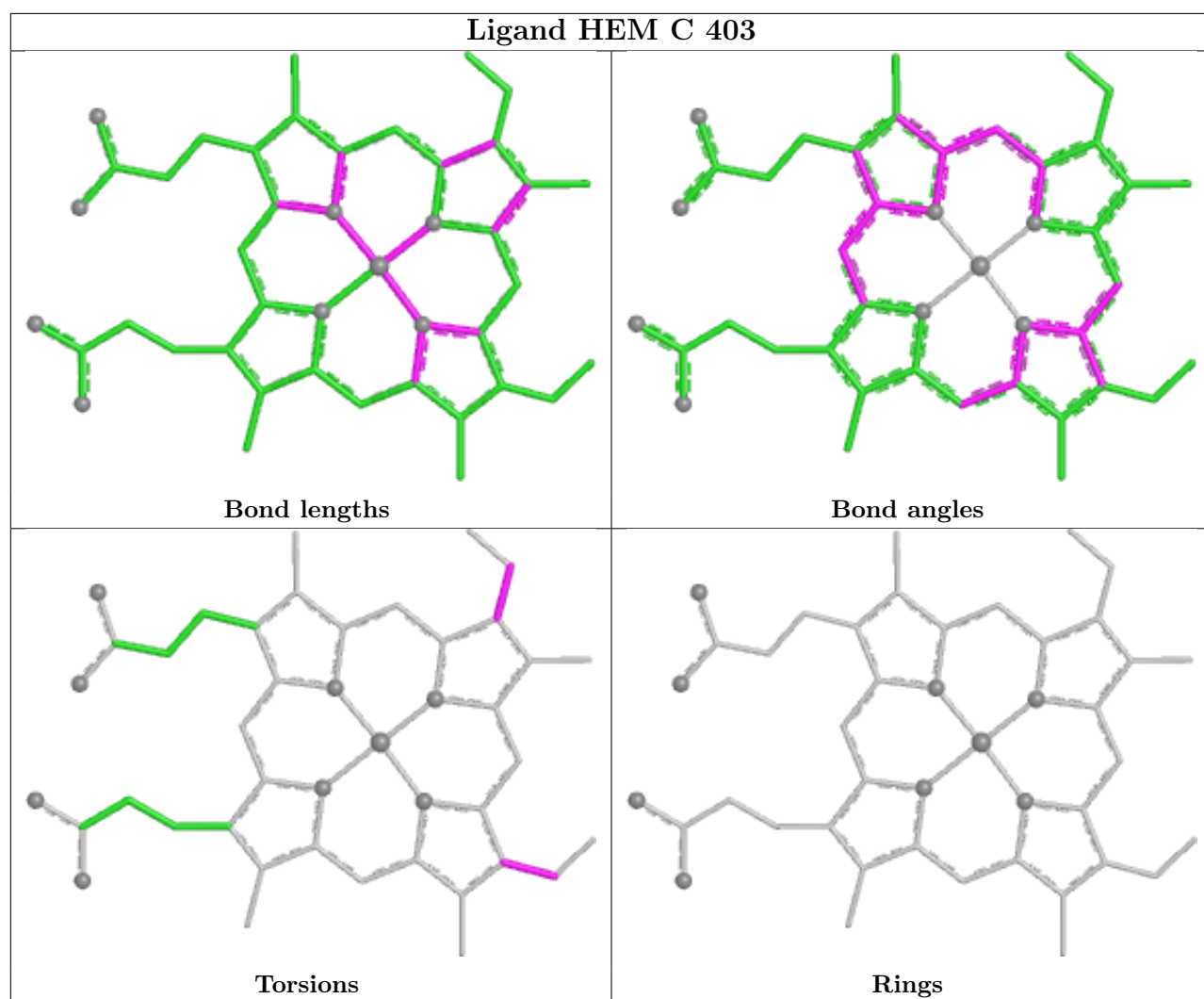


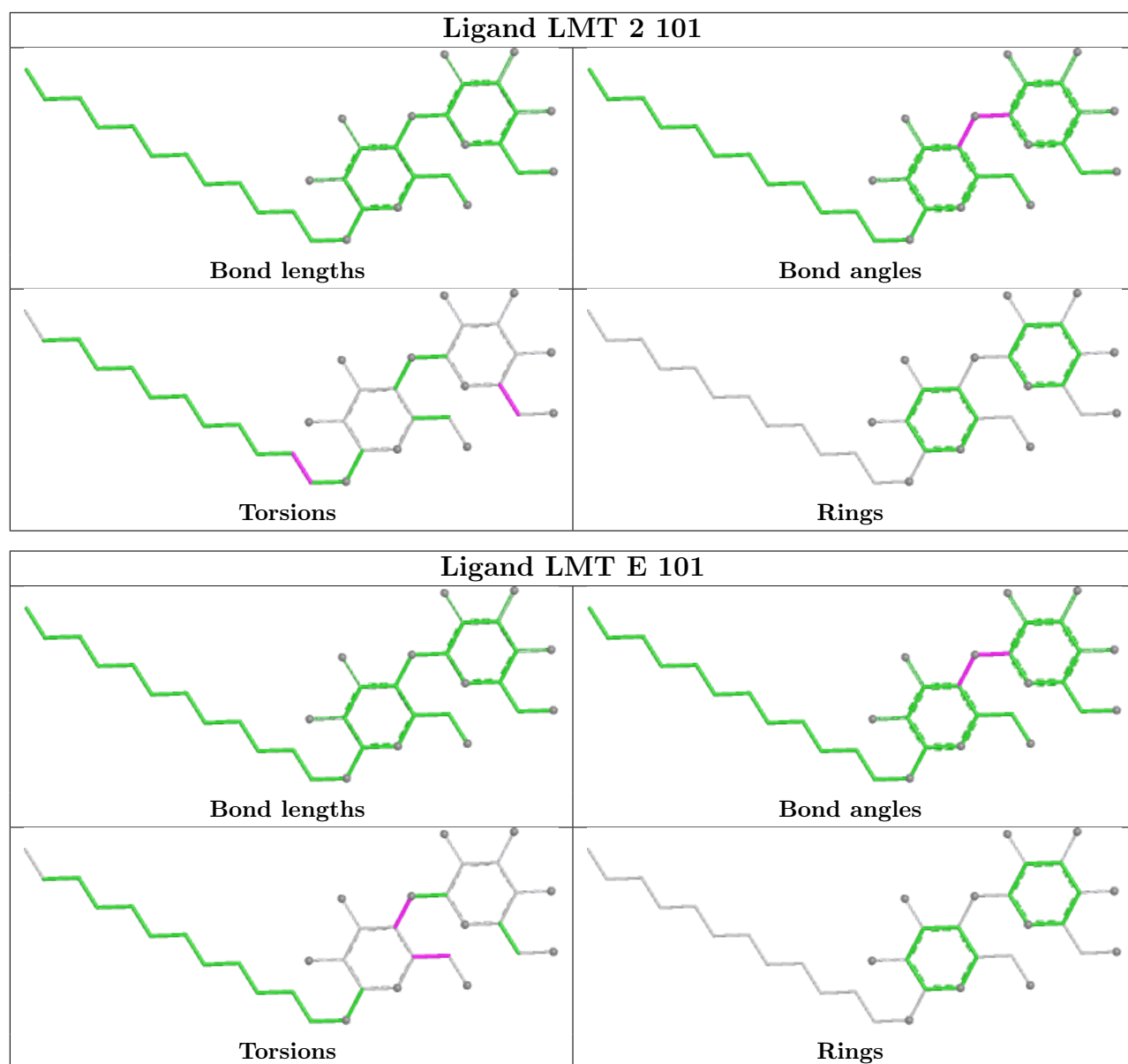


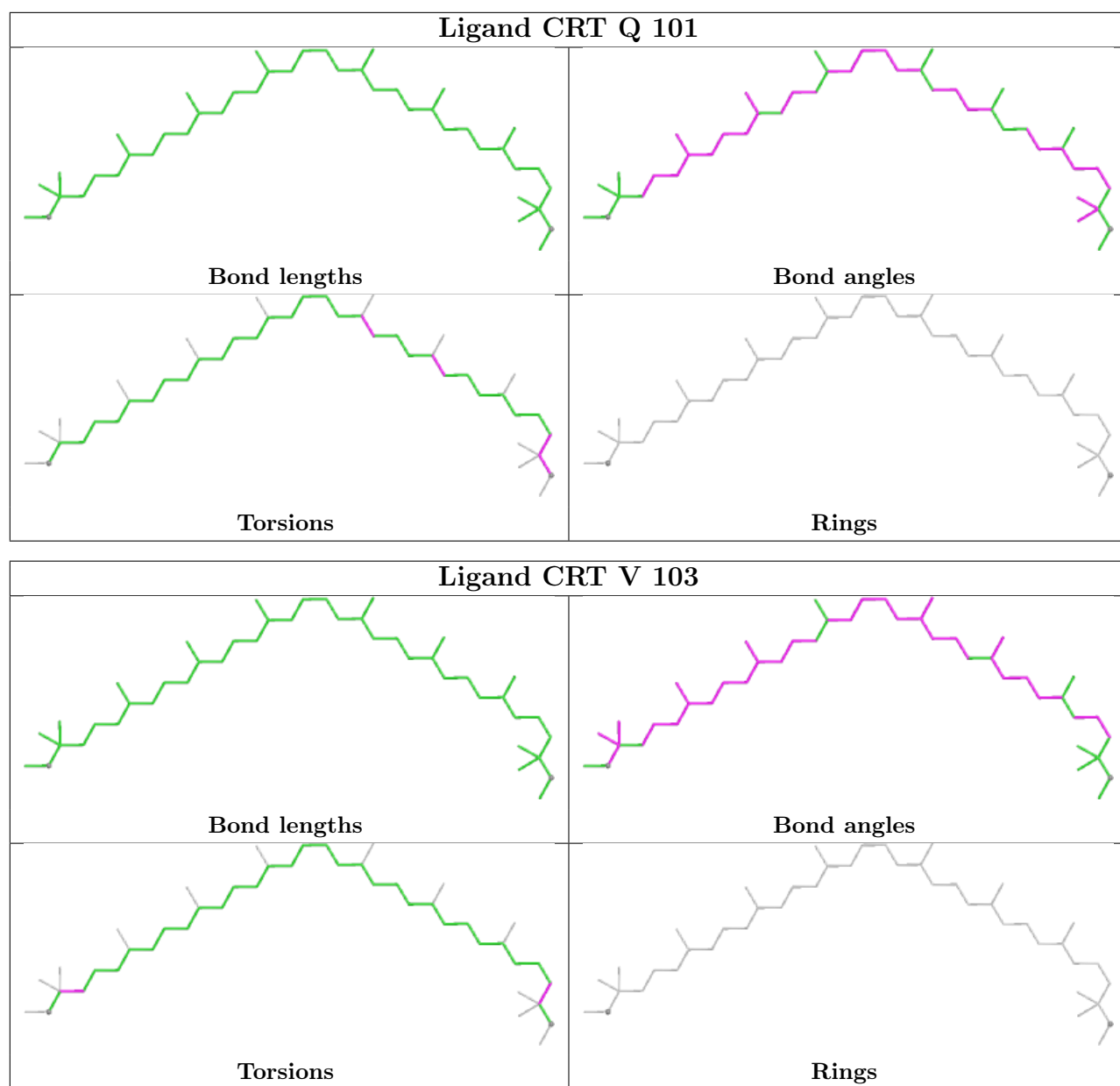


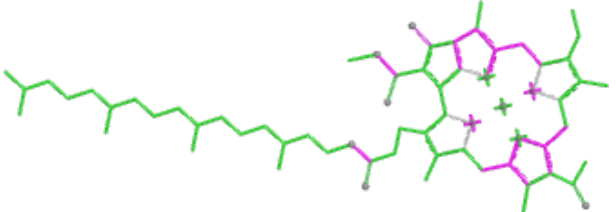
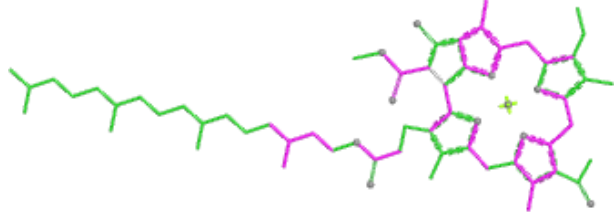
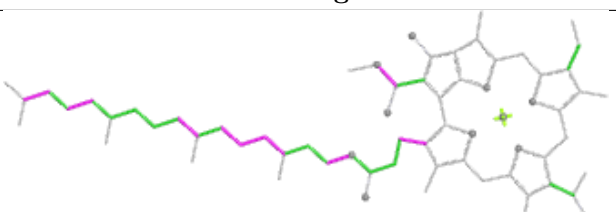
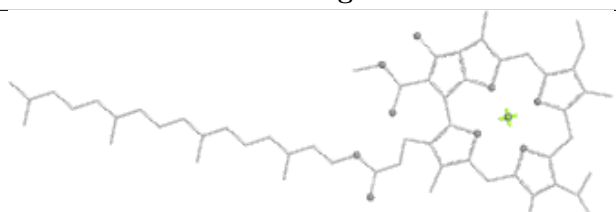
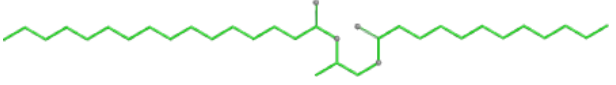
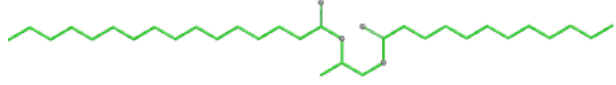
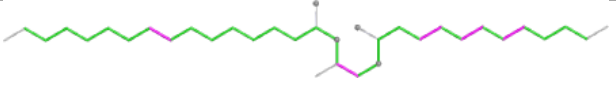
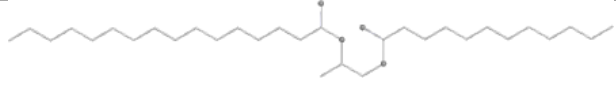
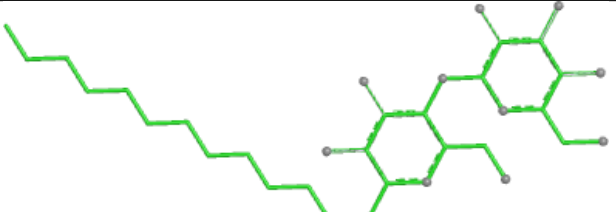
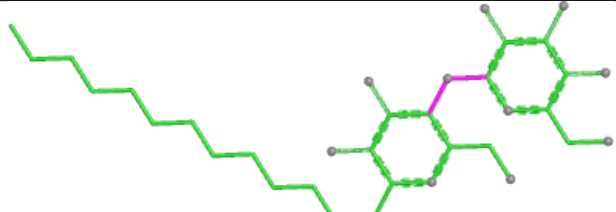
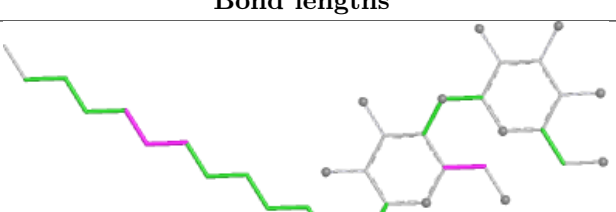
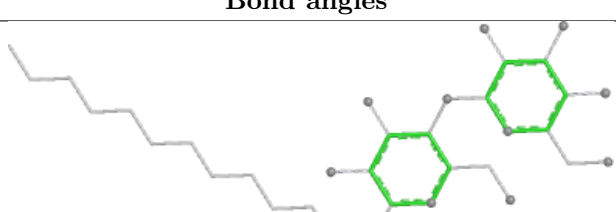


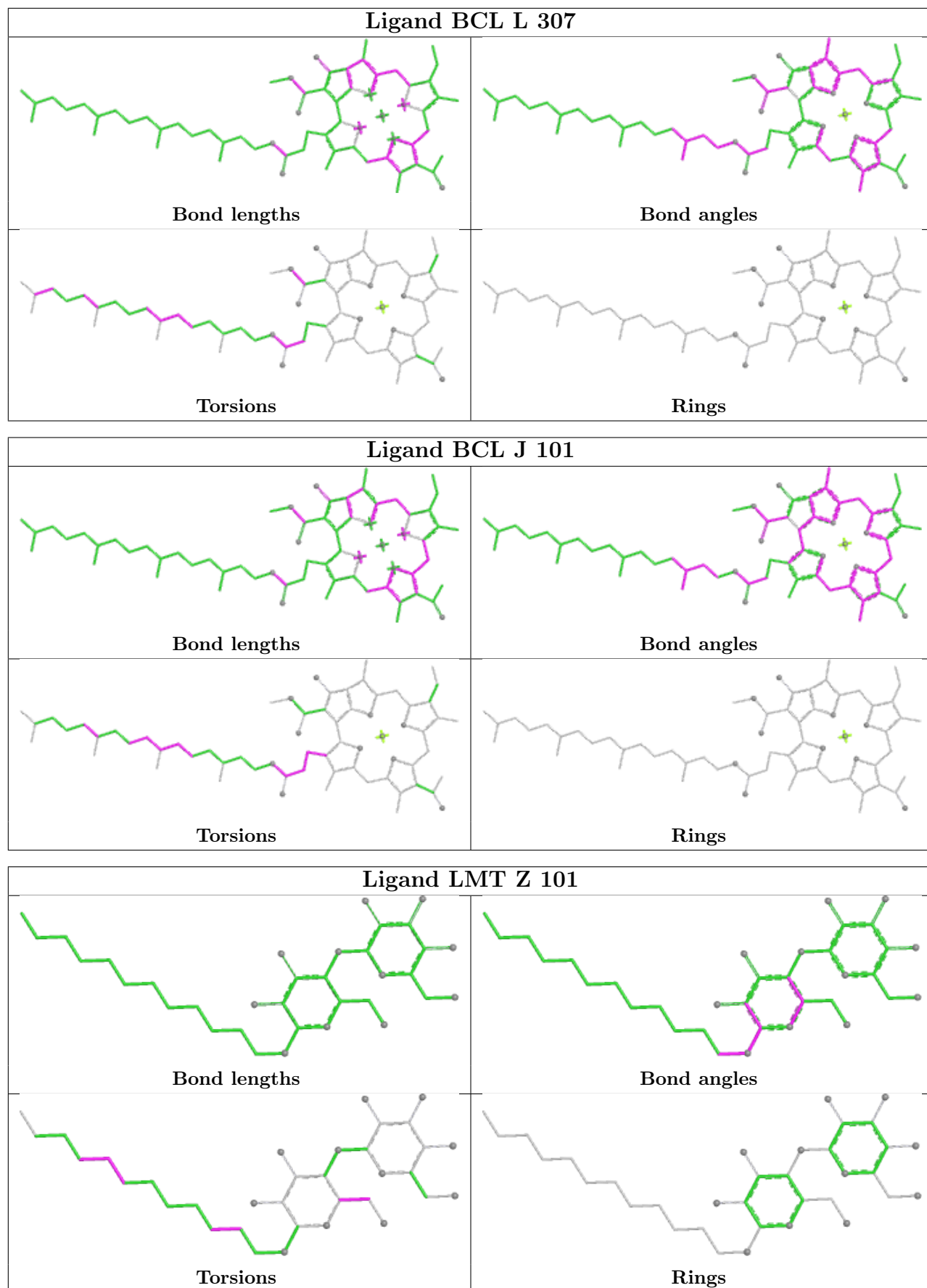


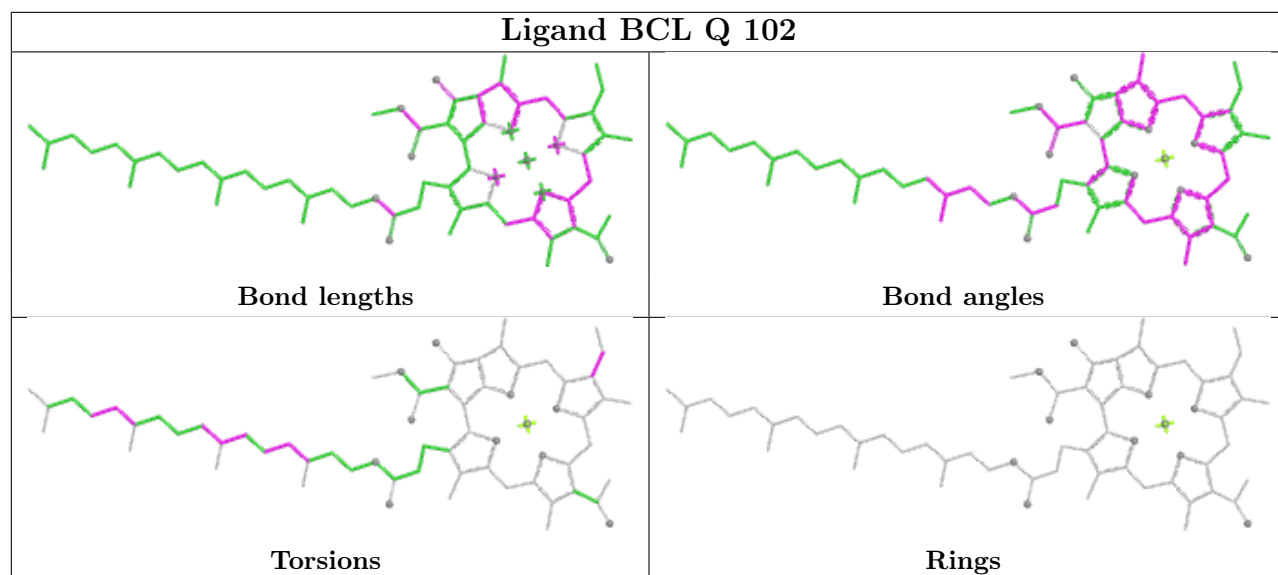
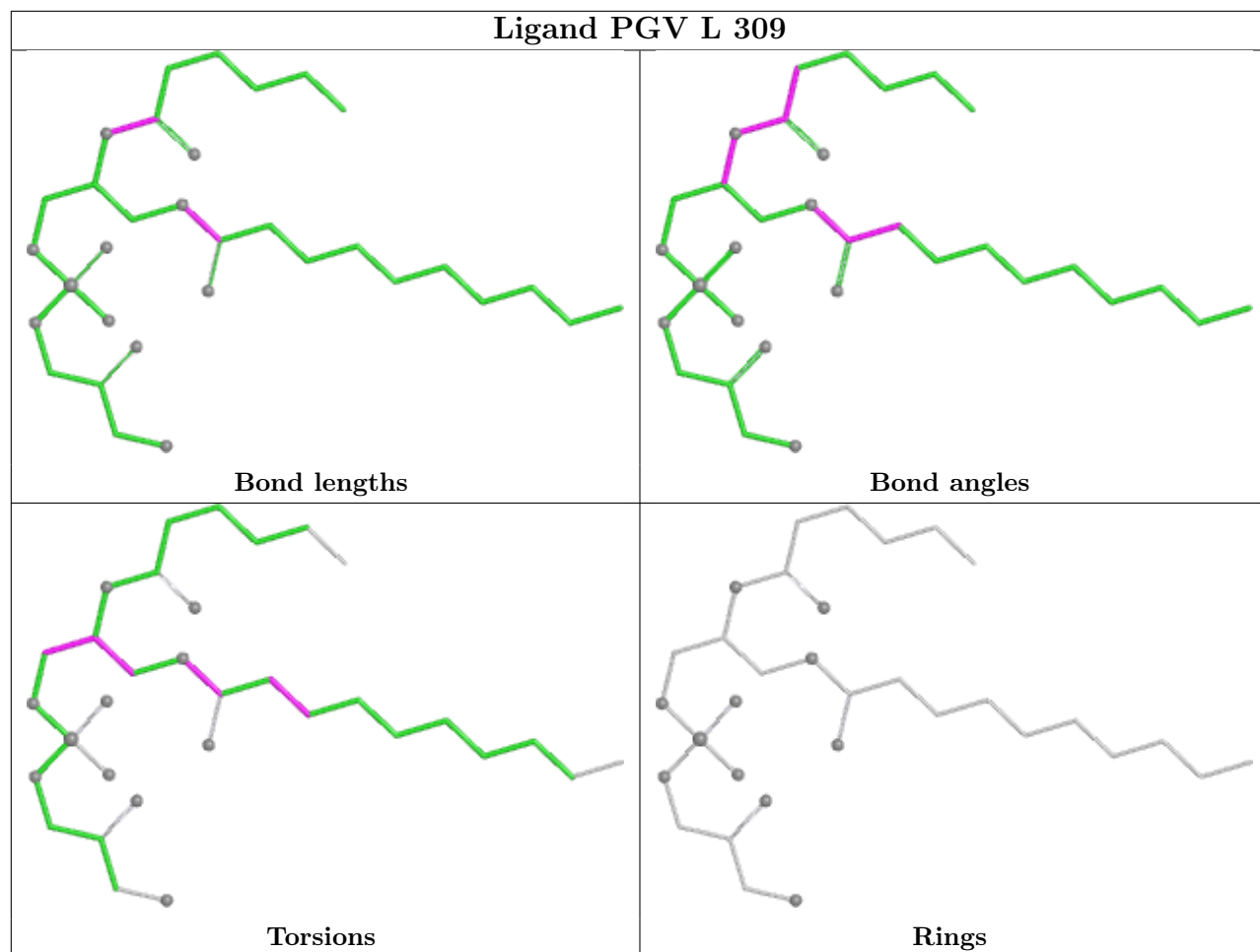


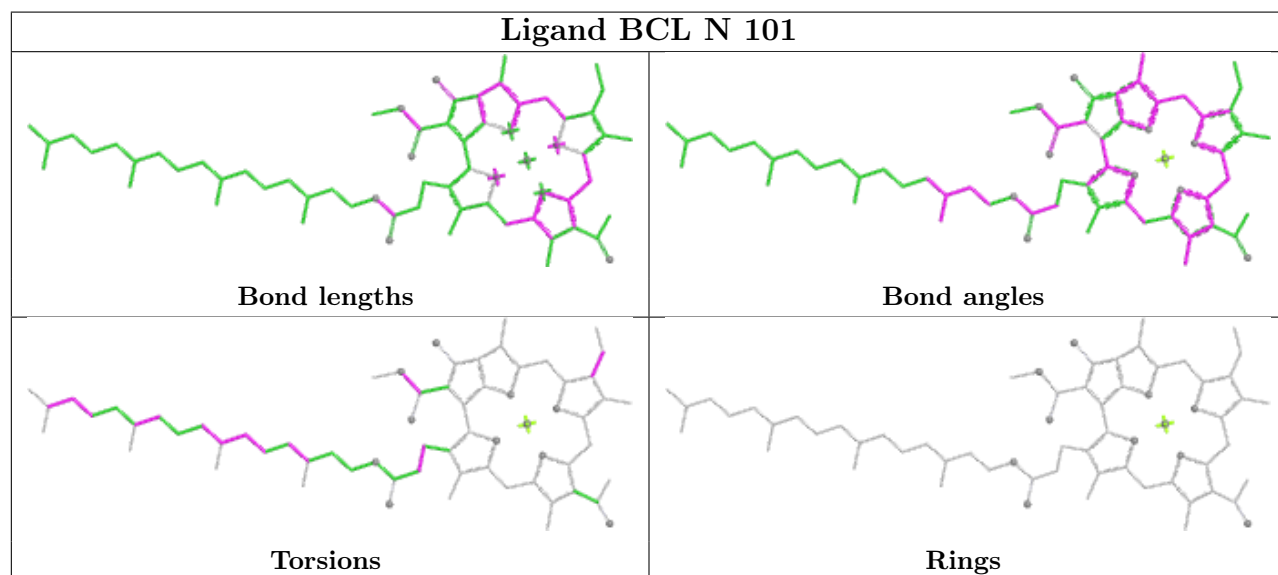
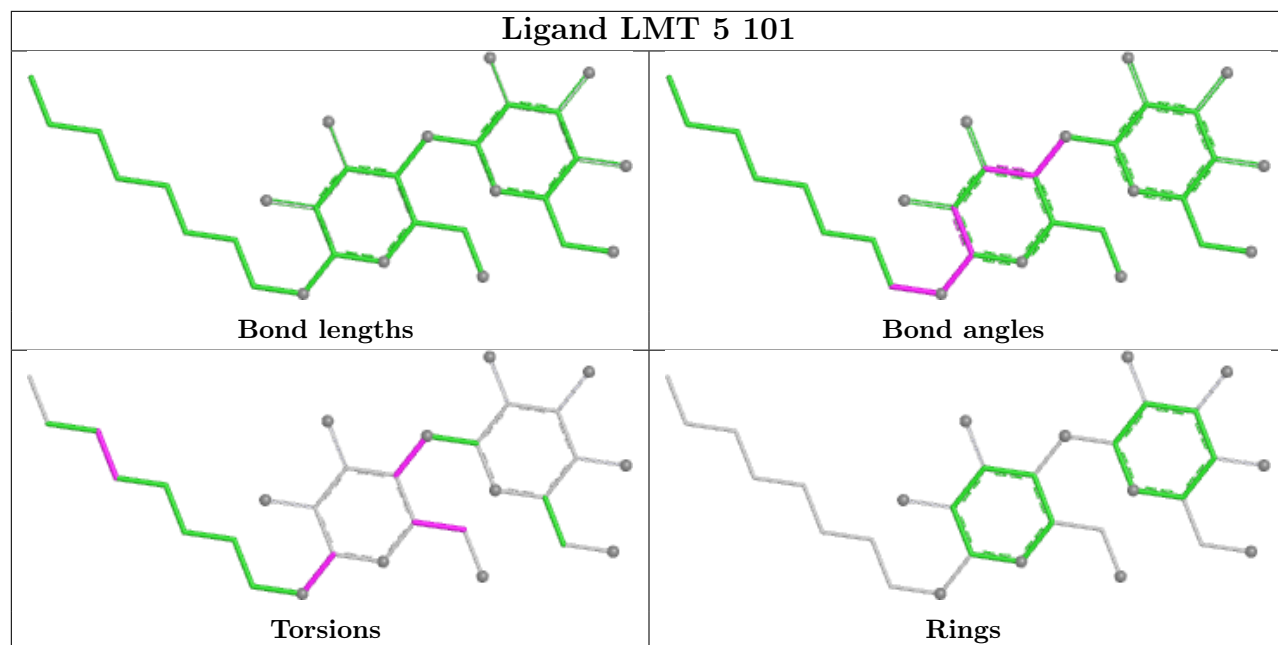


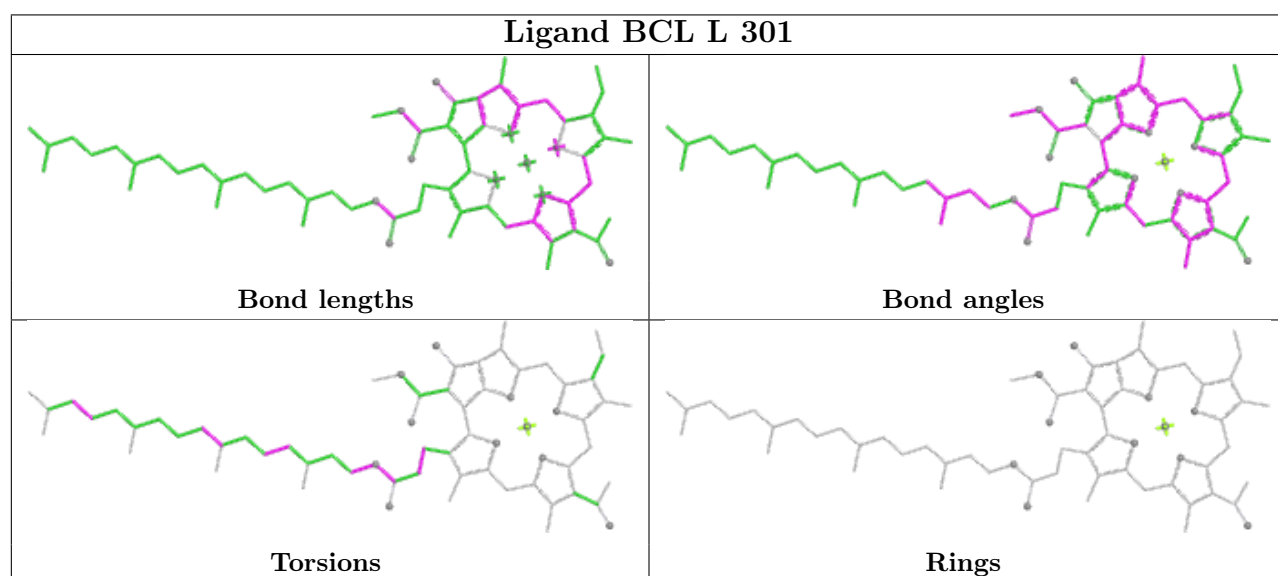
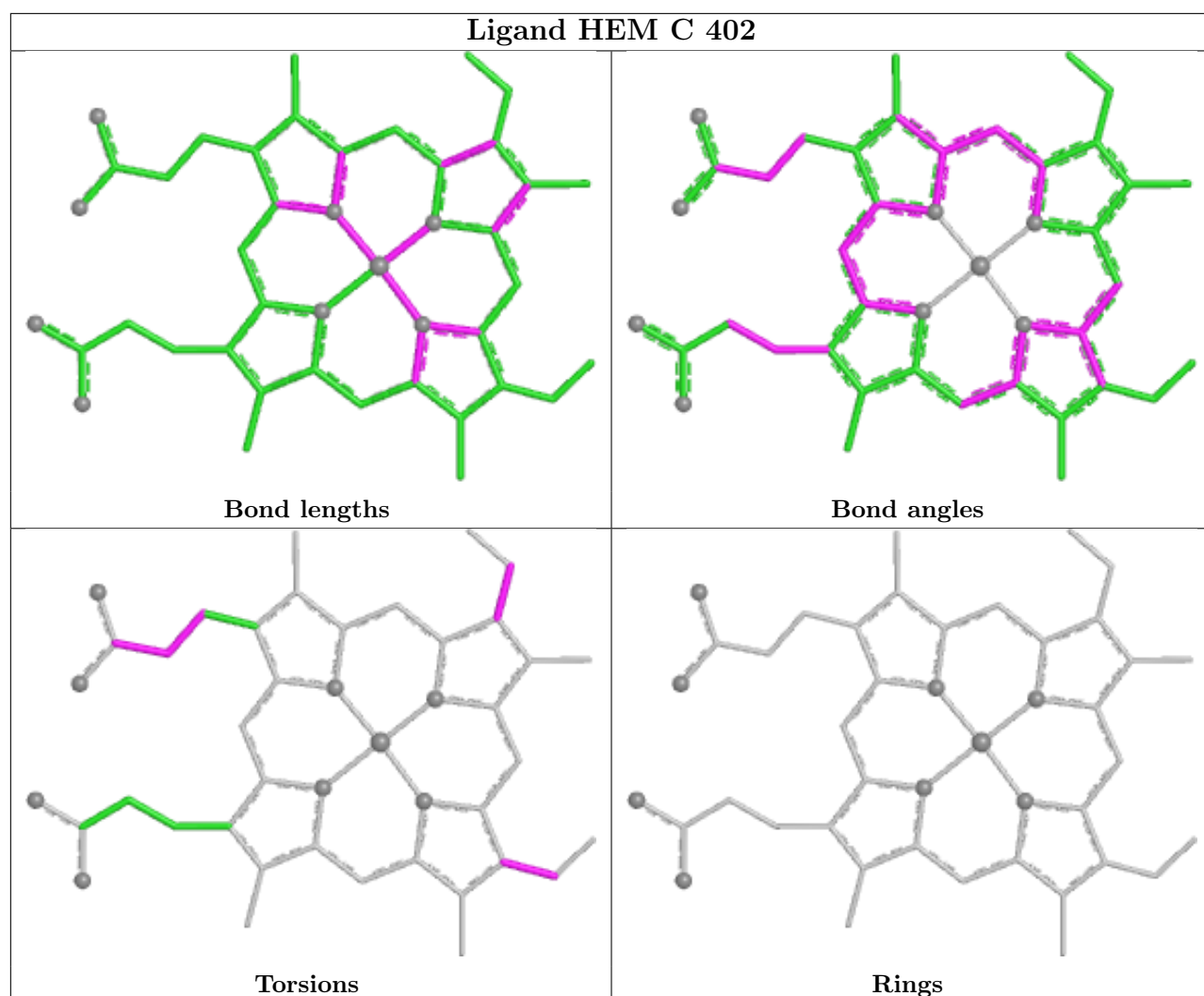


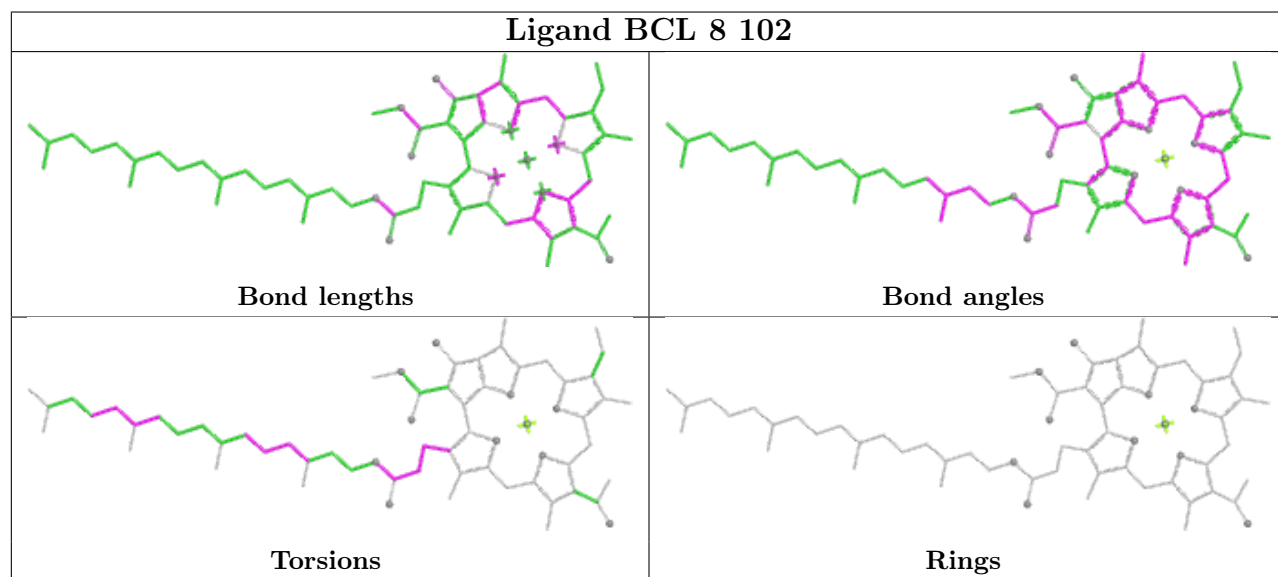
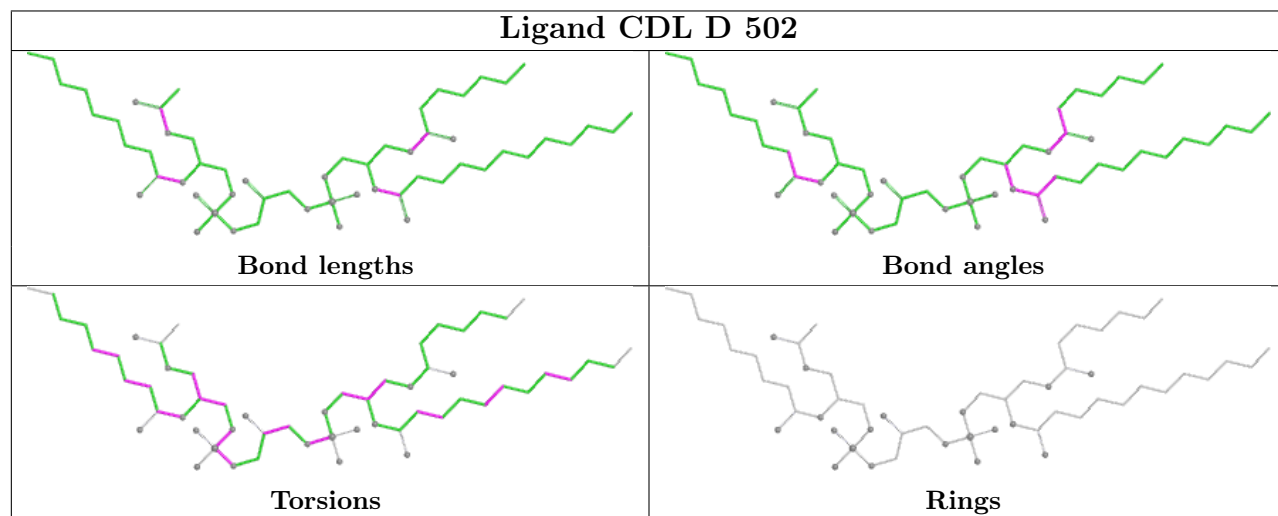
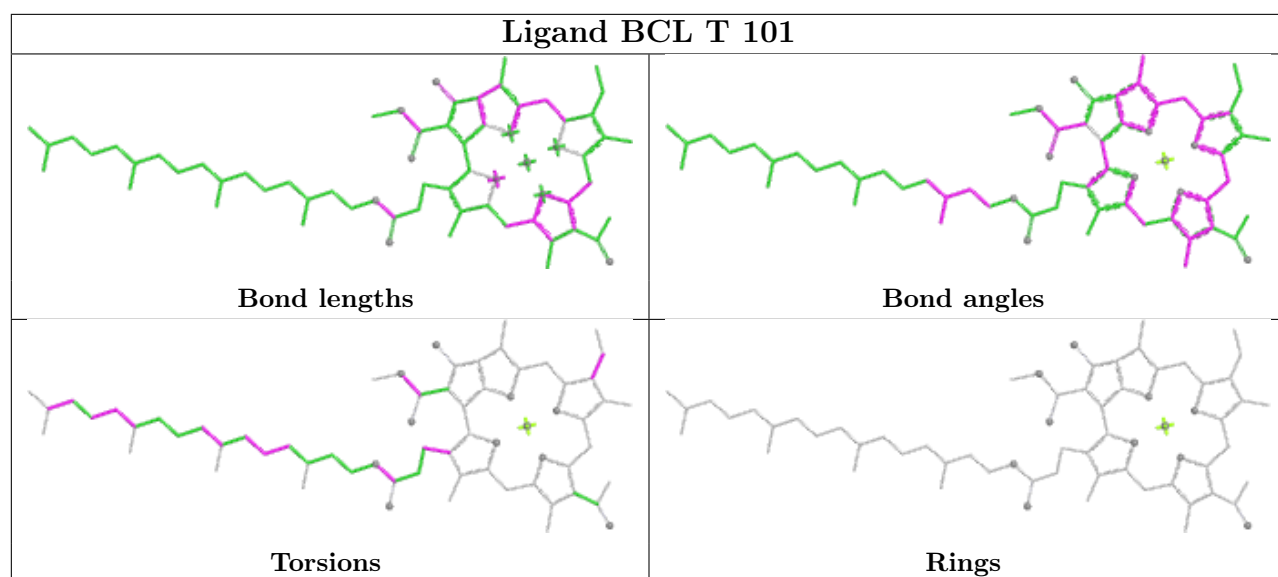
Ligand BCL I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand Z41 C 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT 2 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

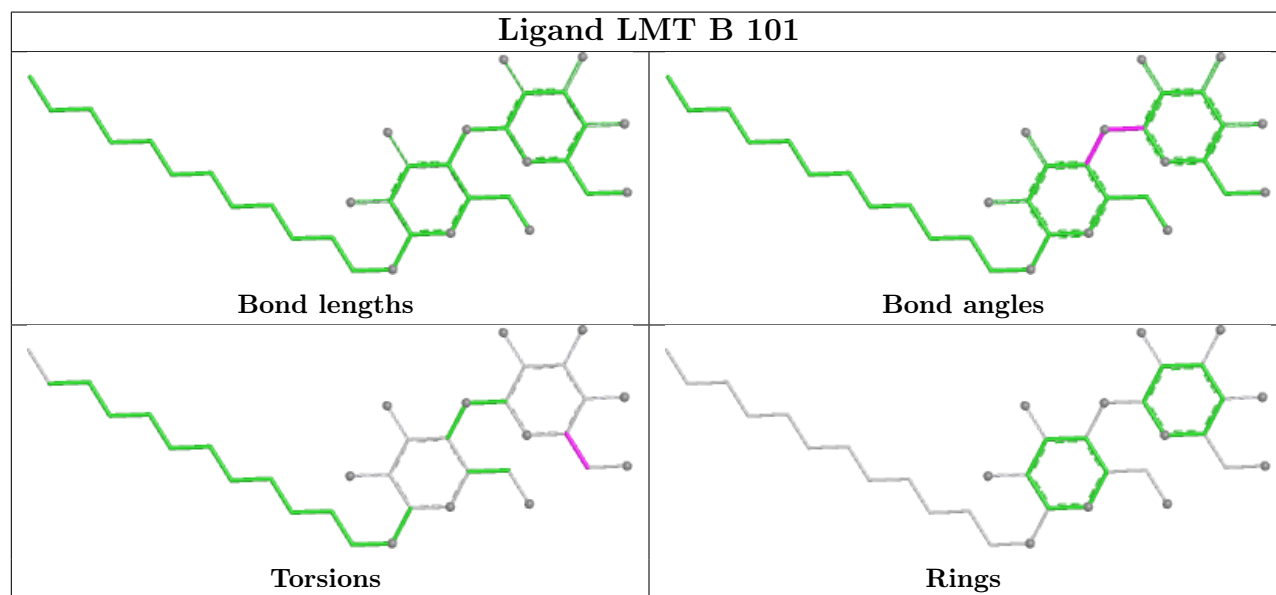
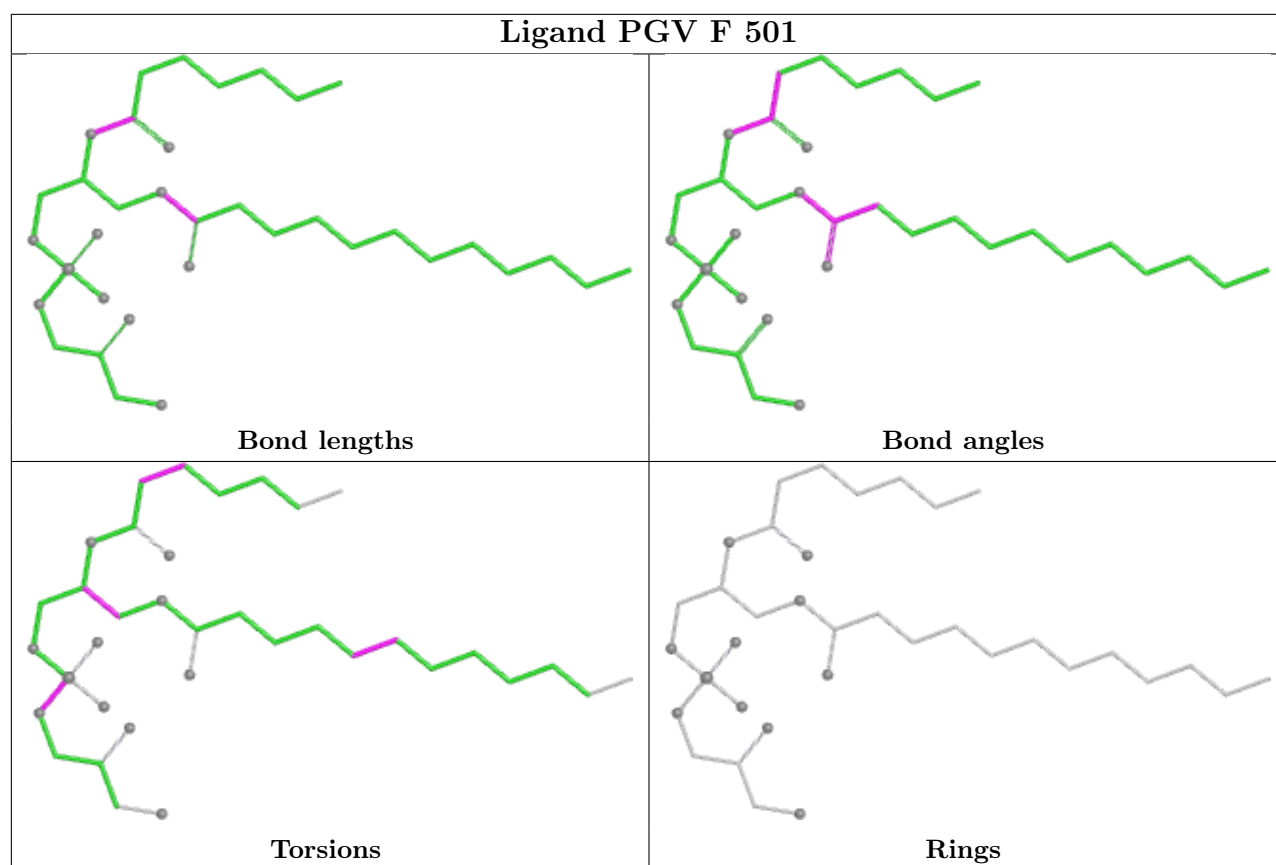


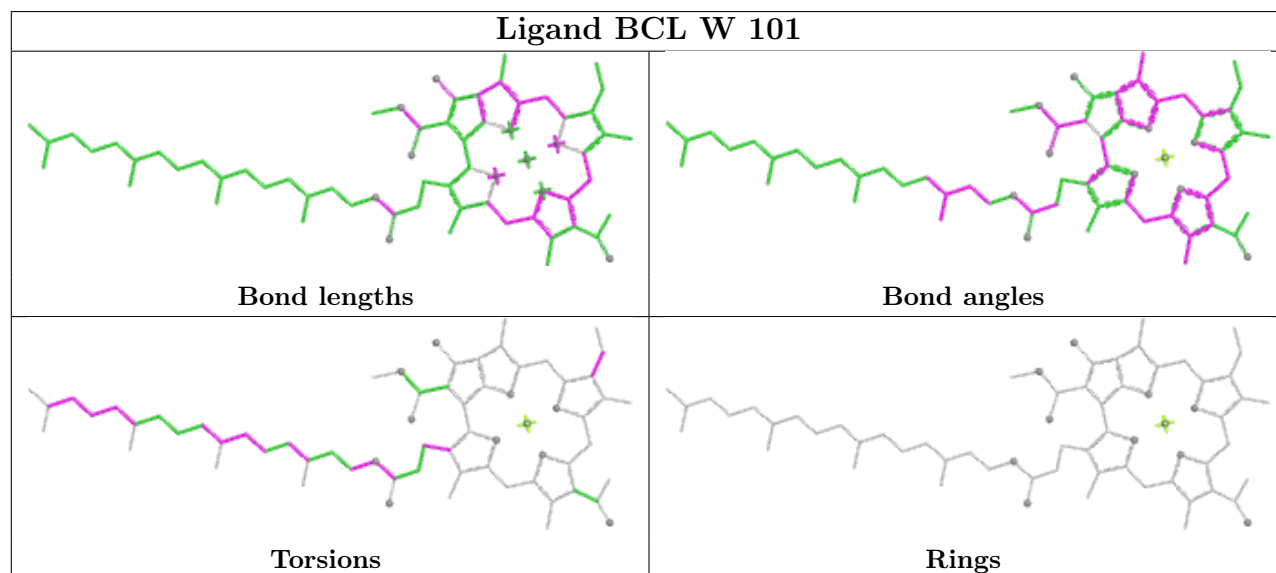
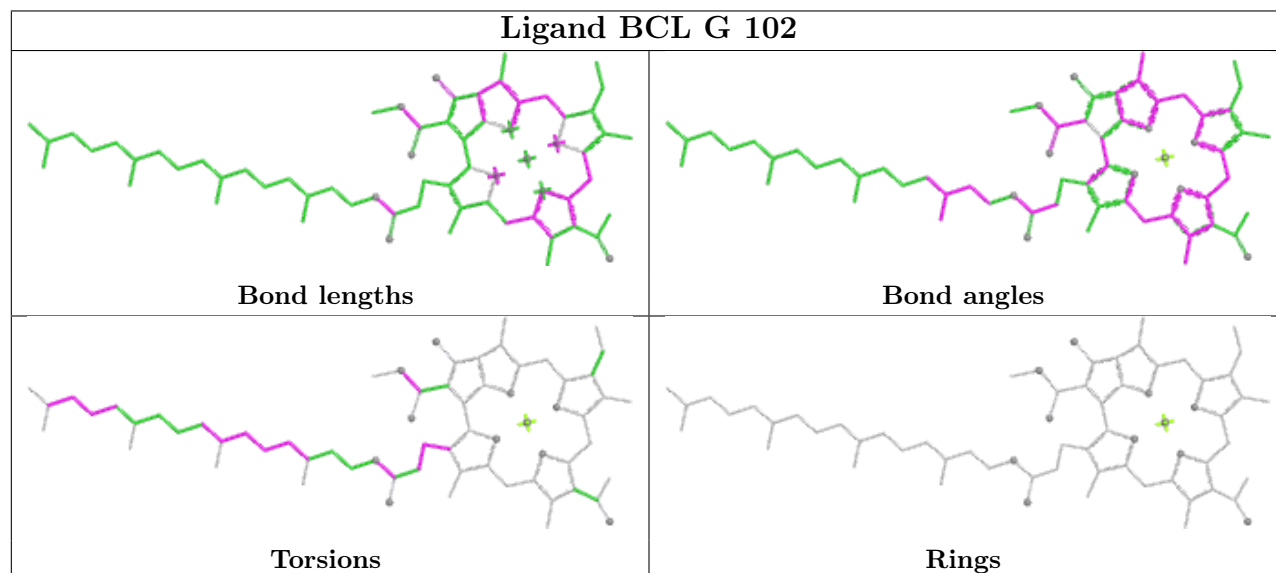
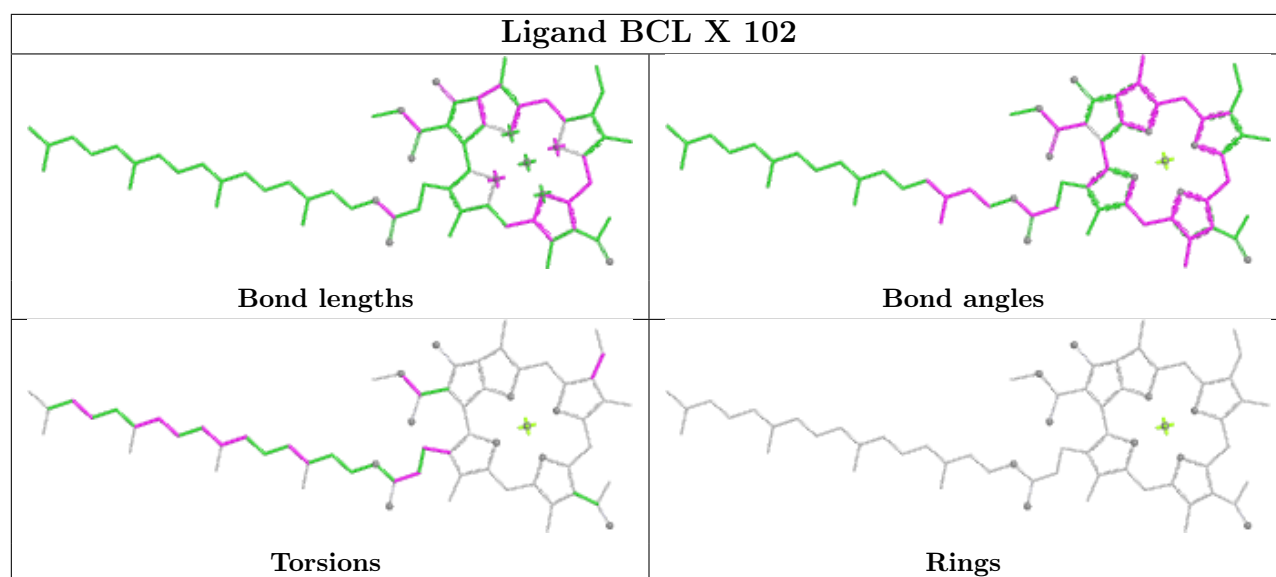


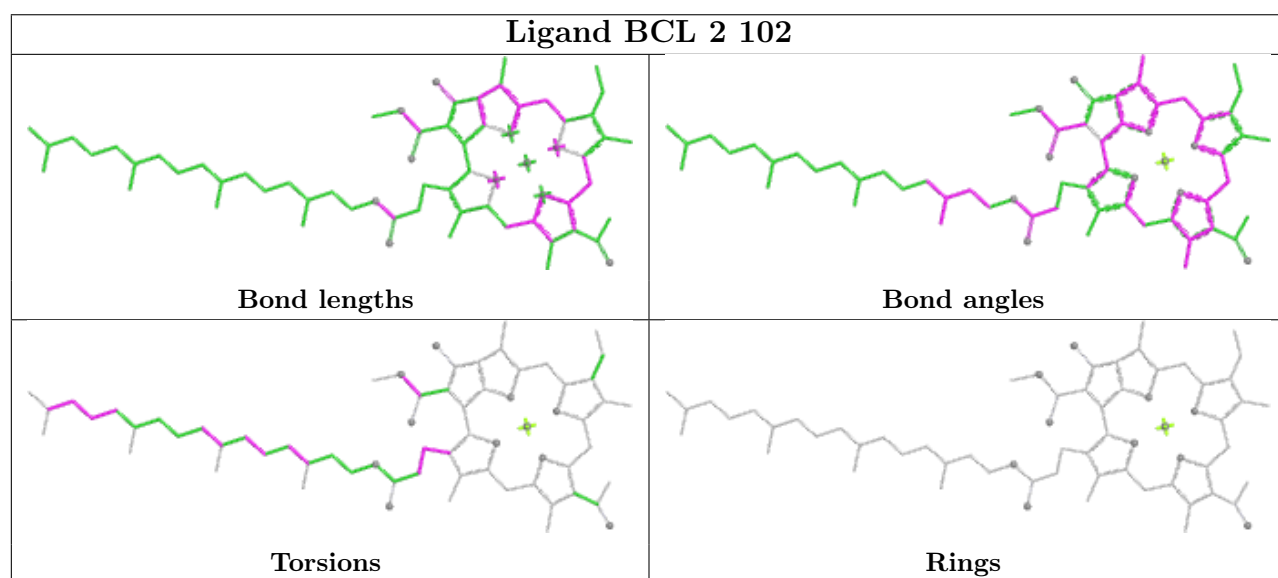
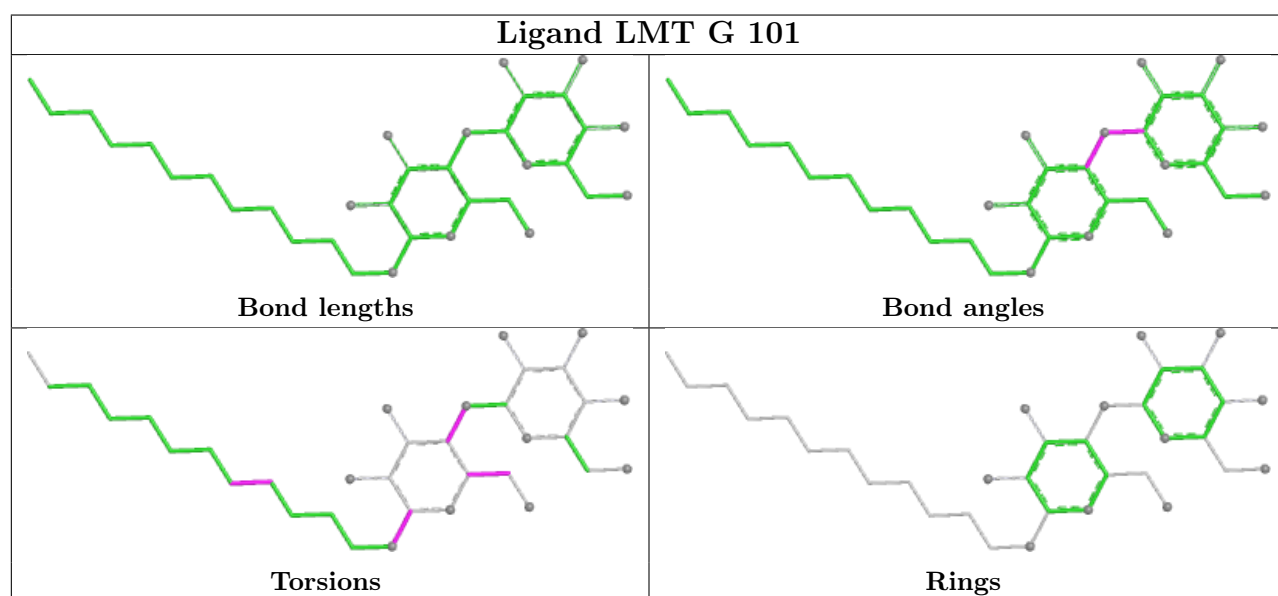
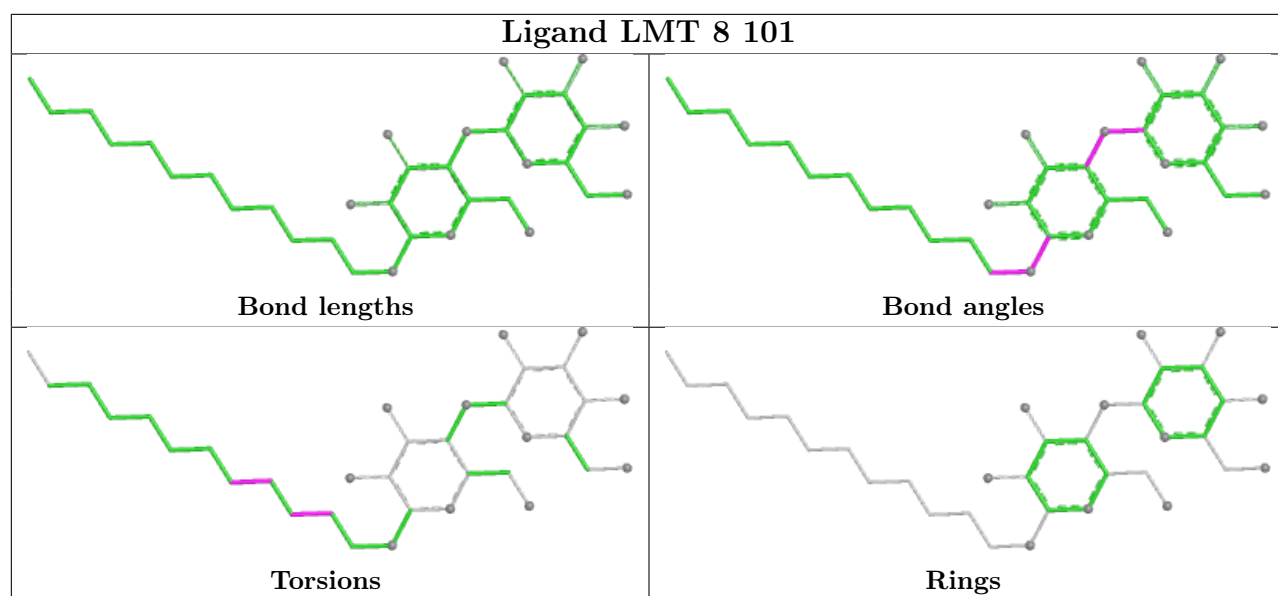


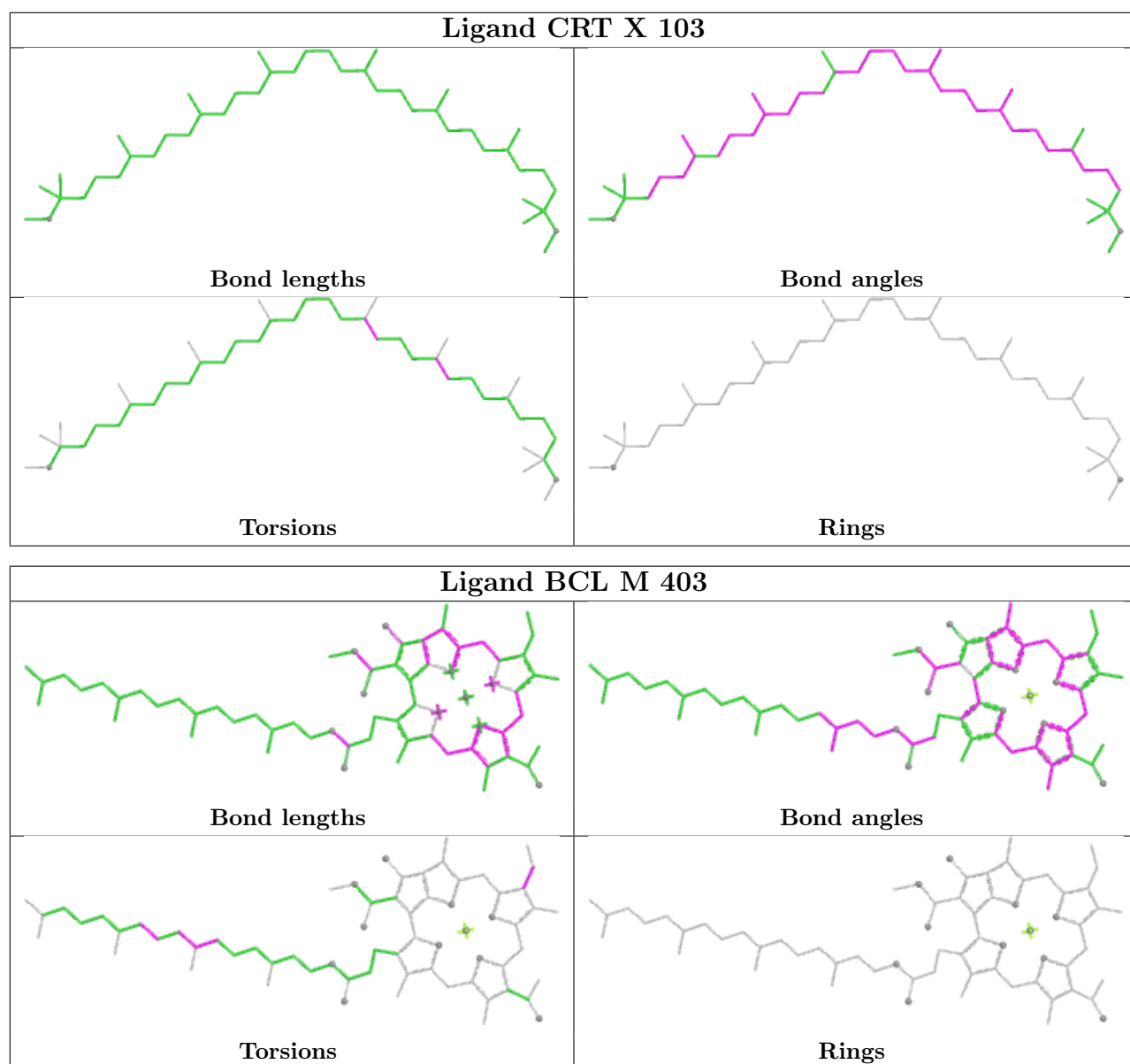


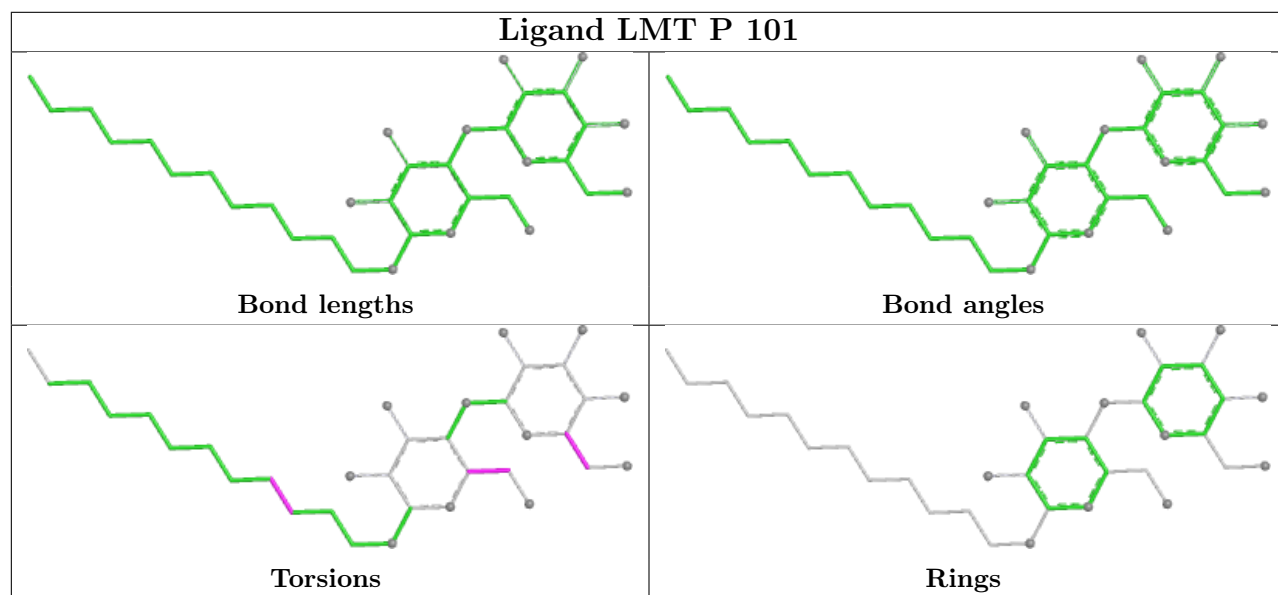
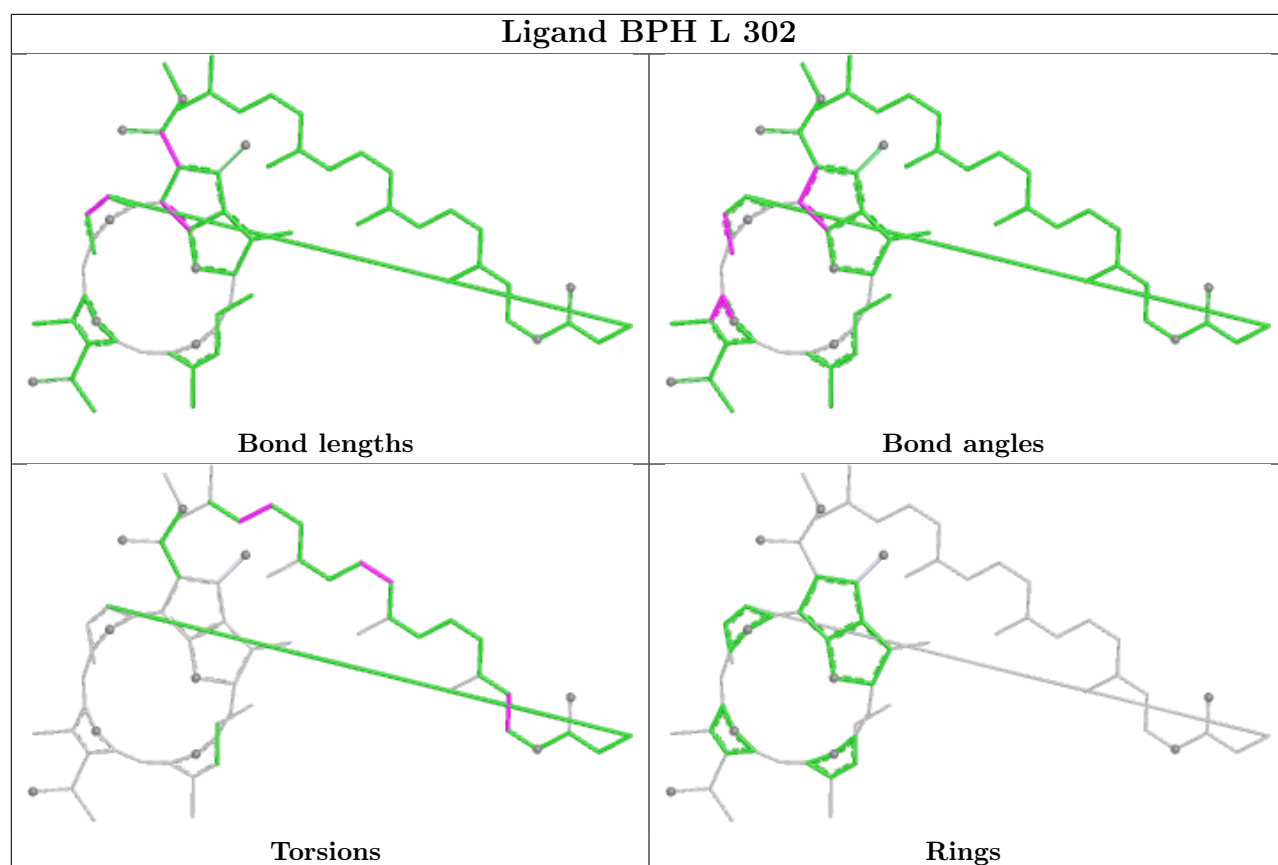


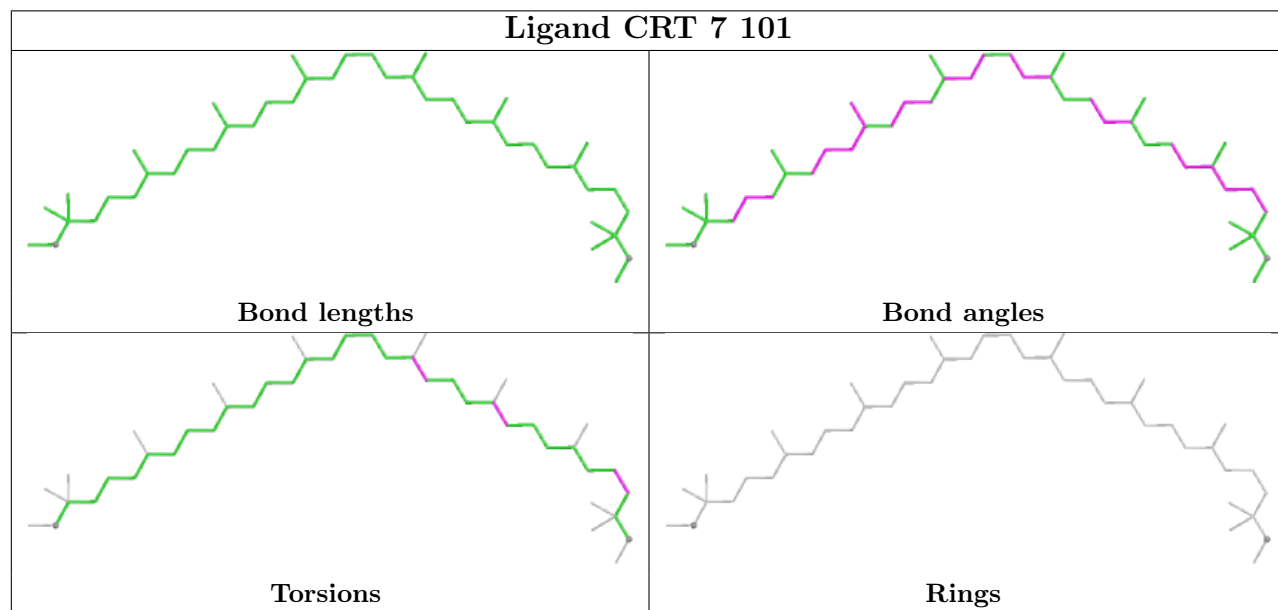
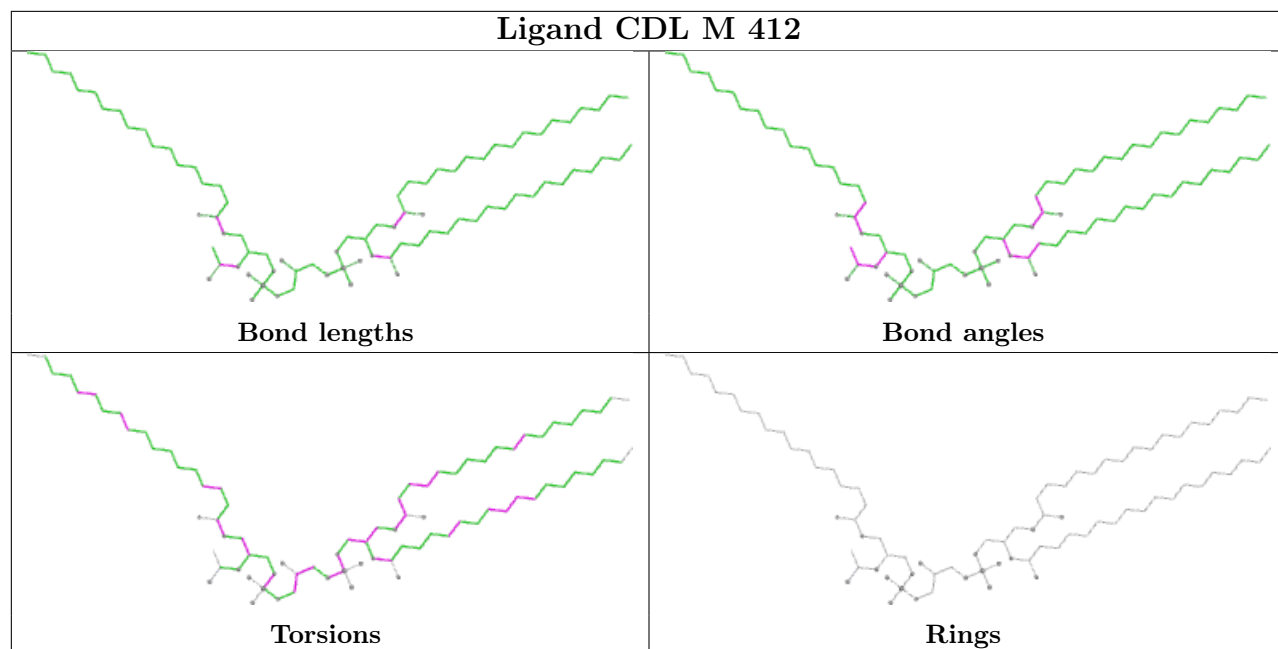


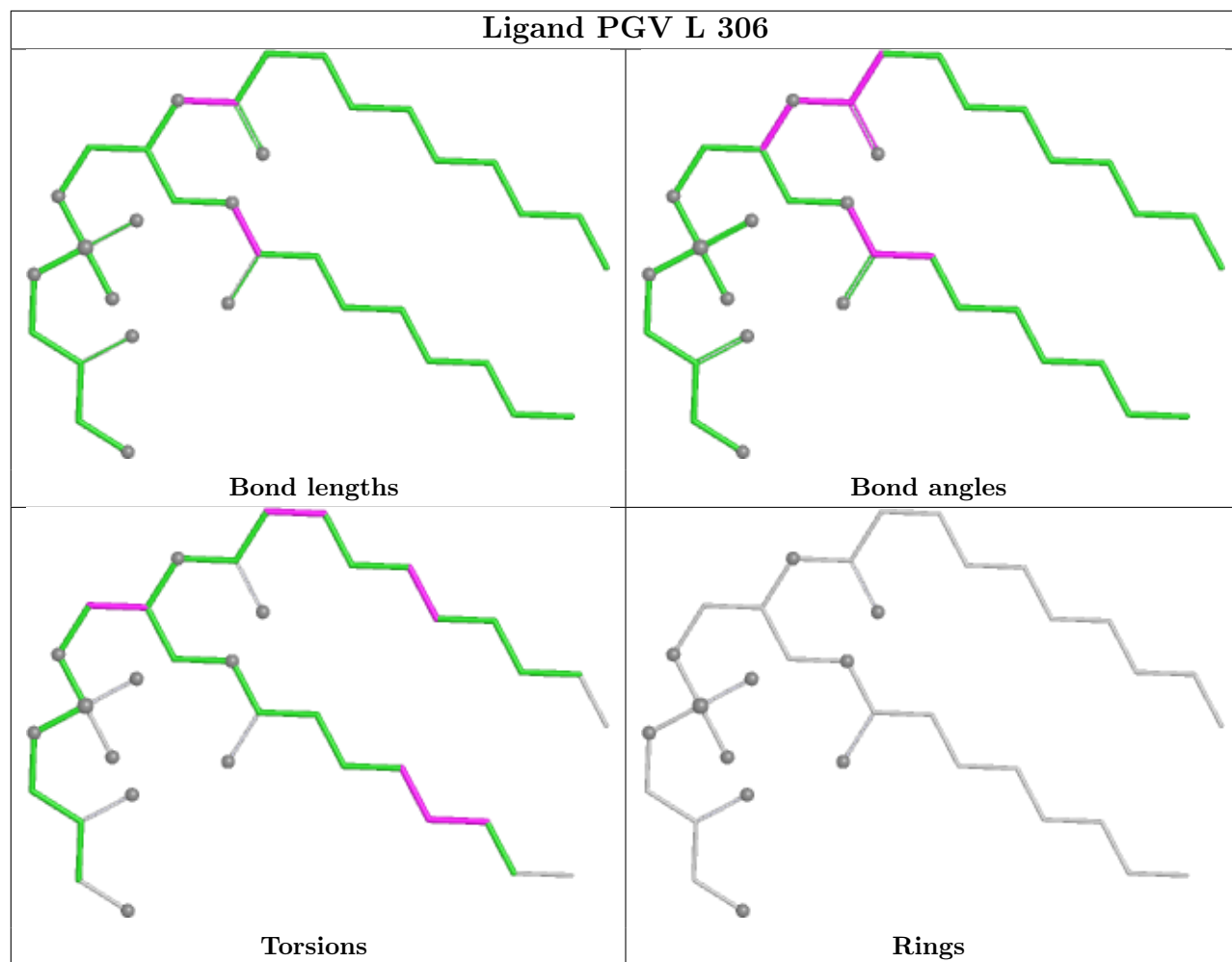


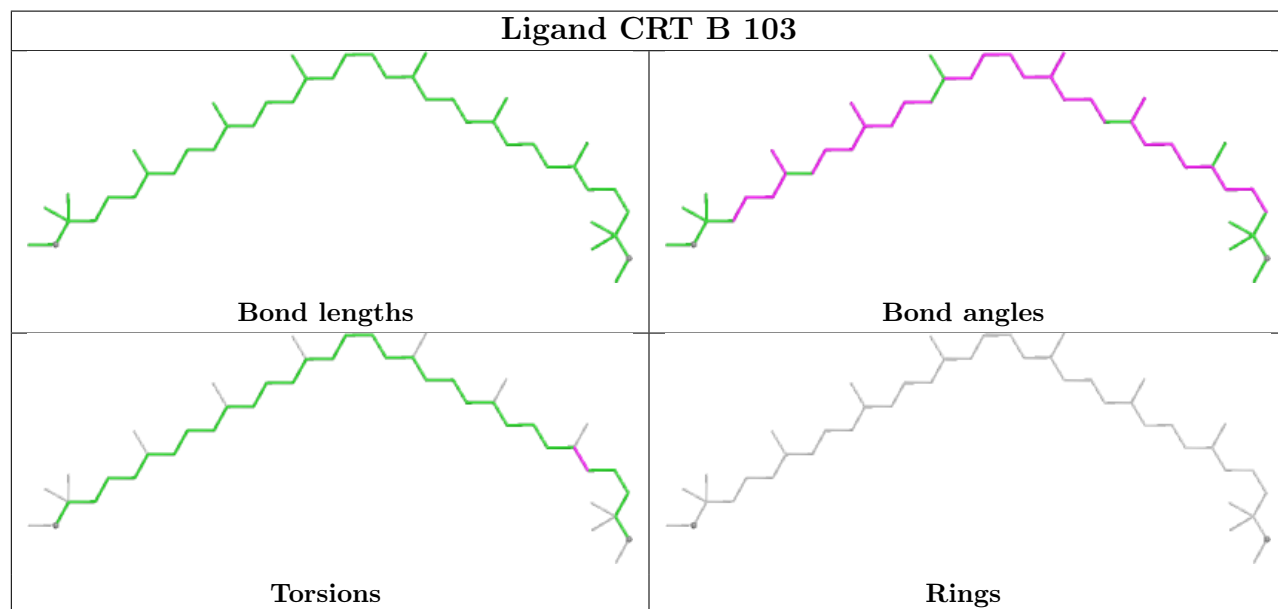
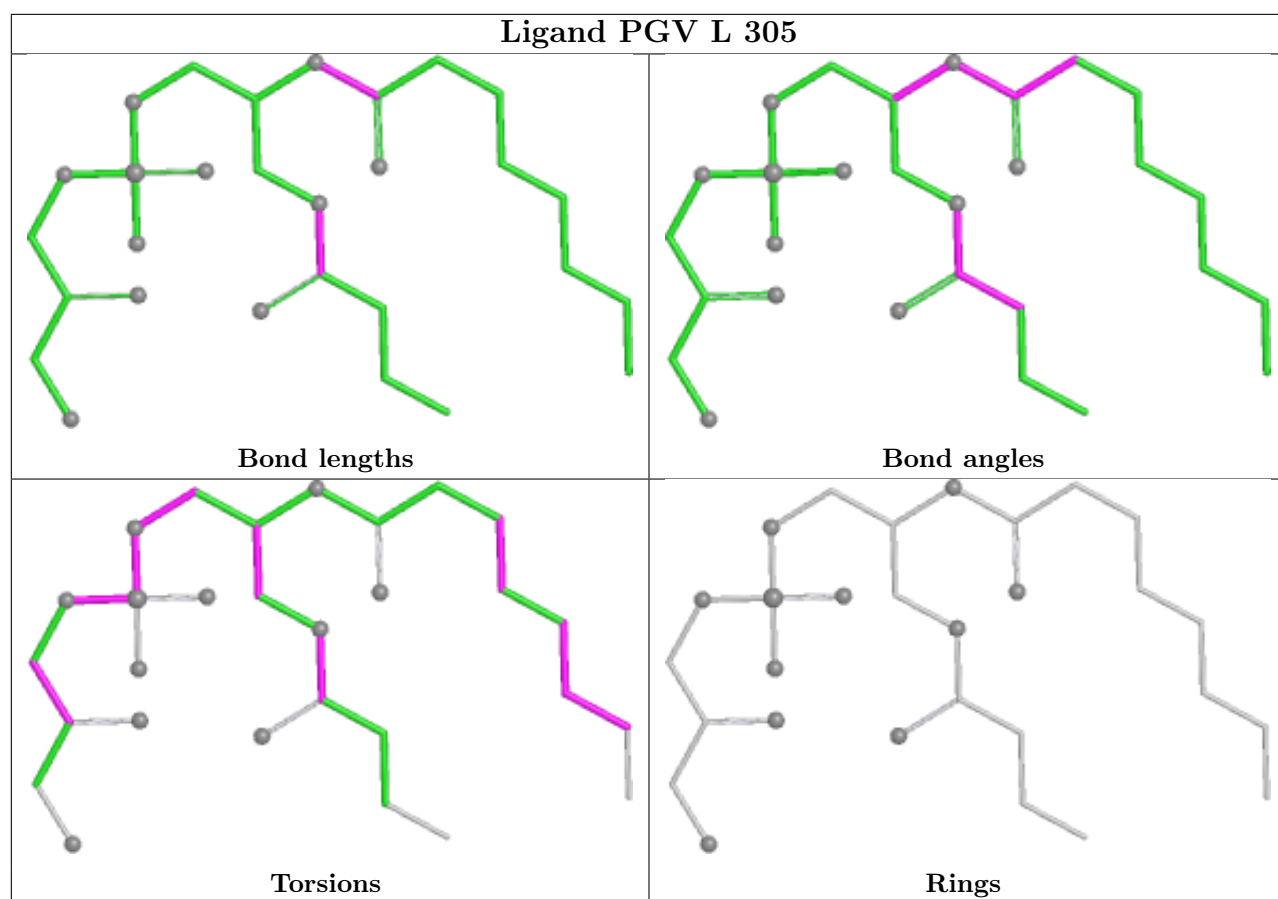


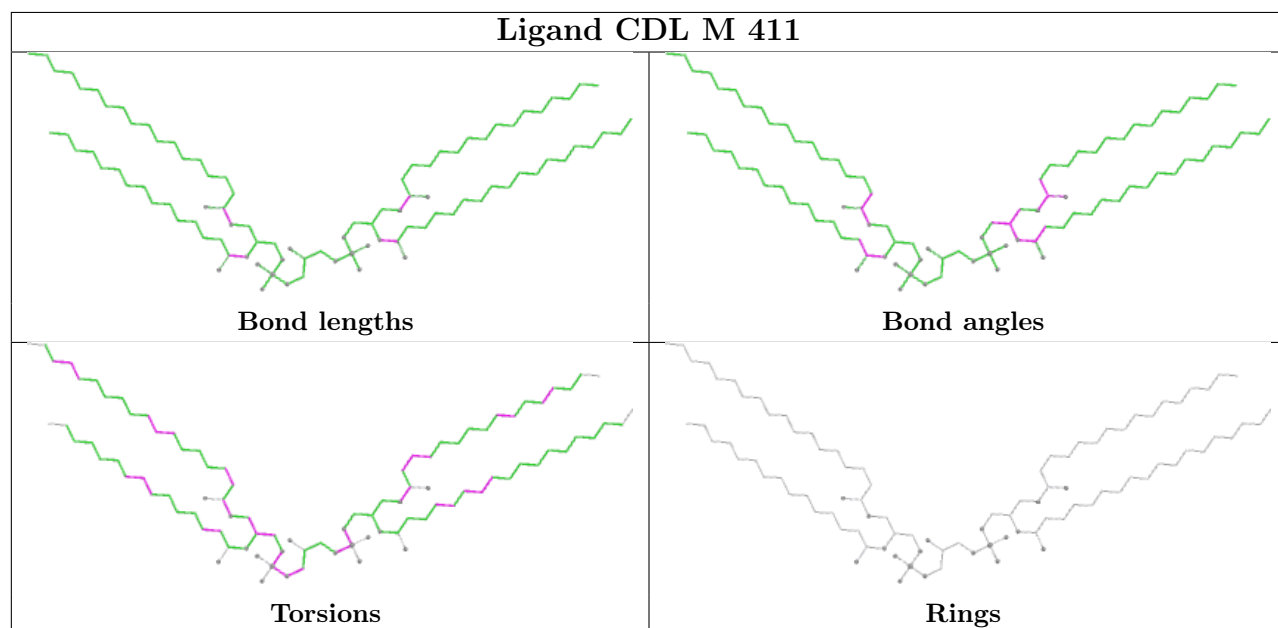
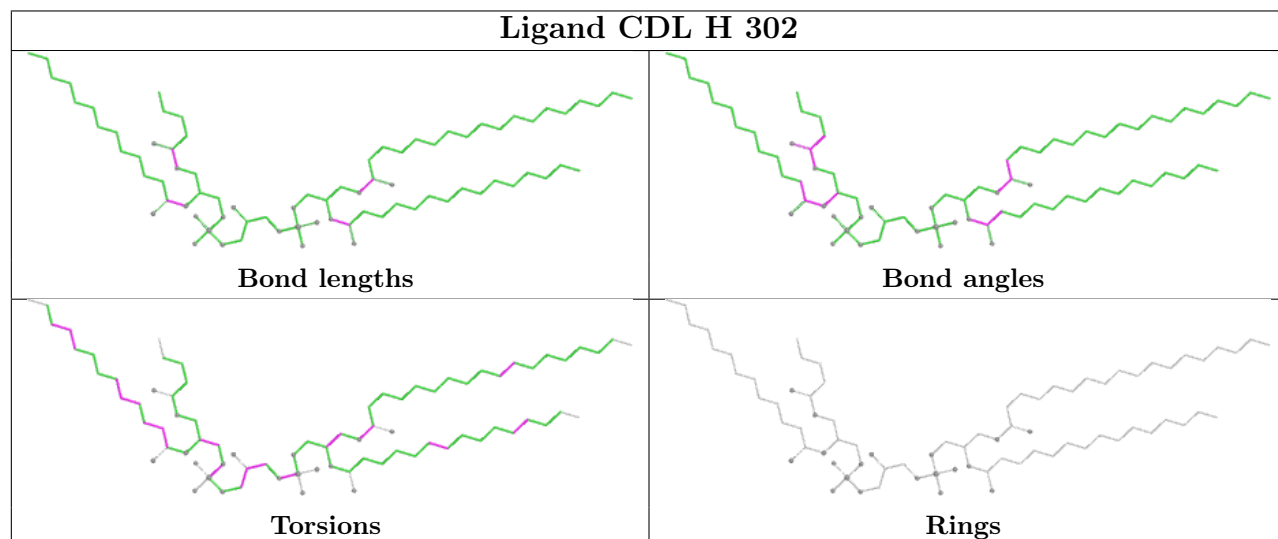
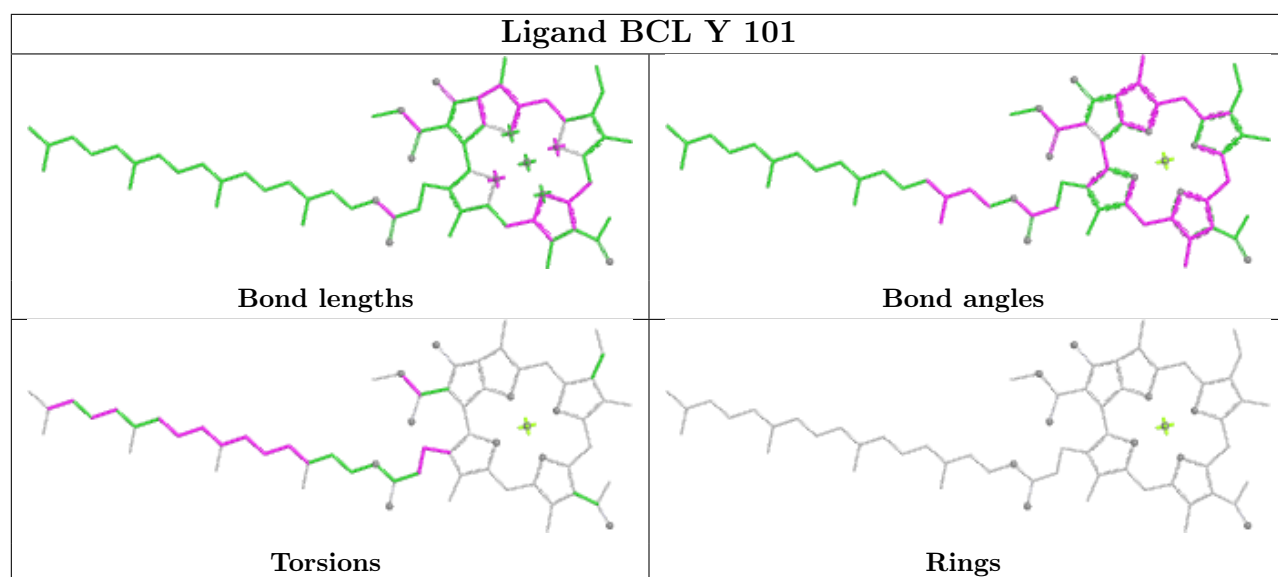


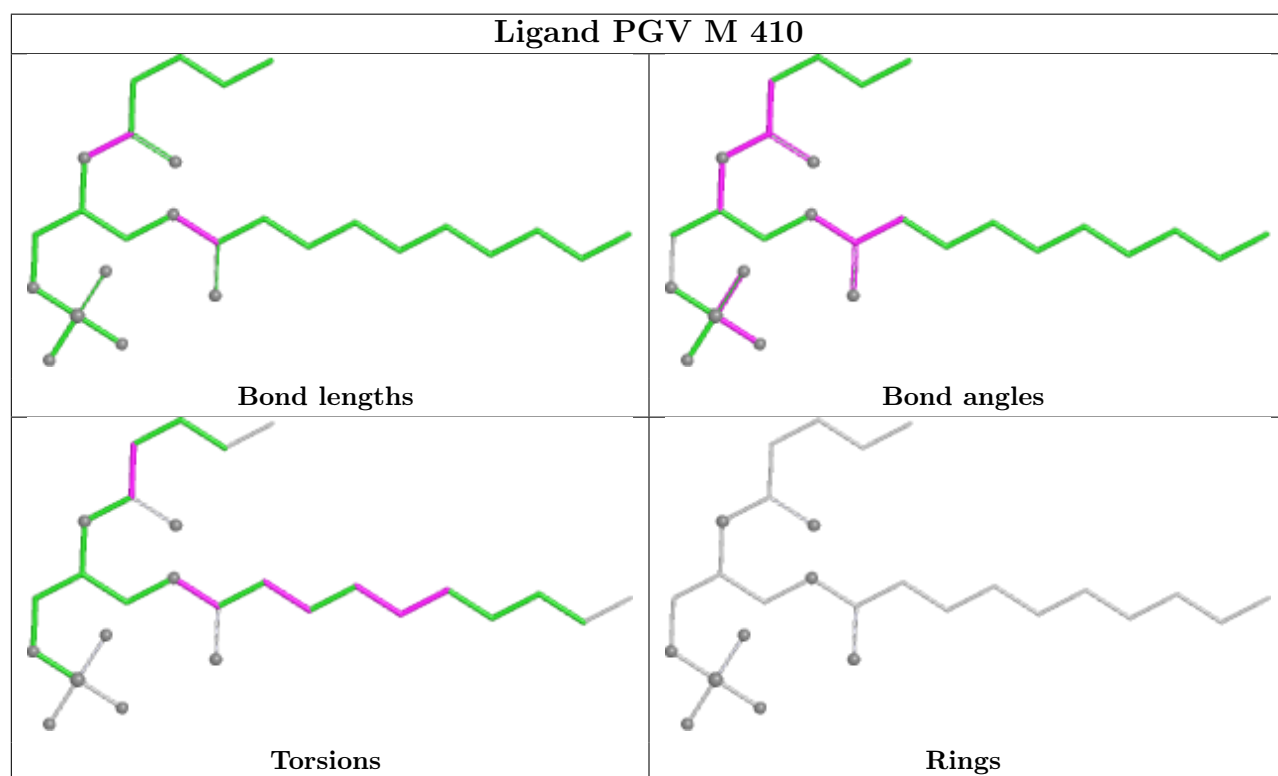
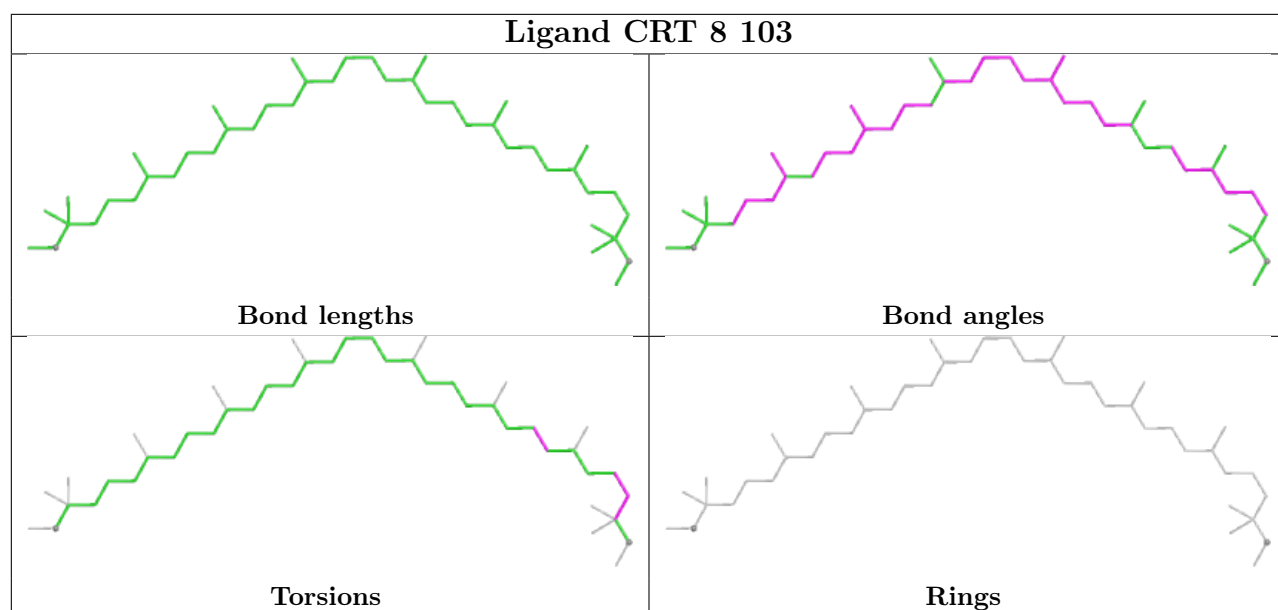


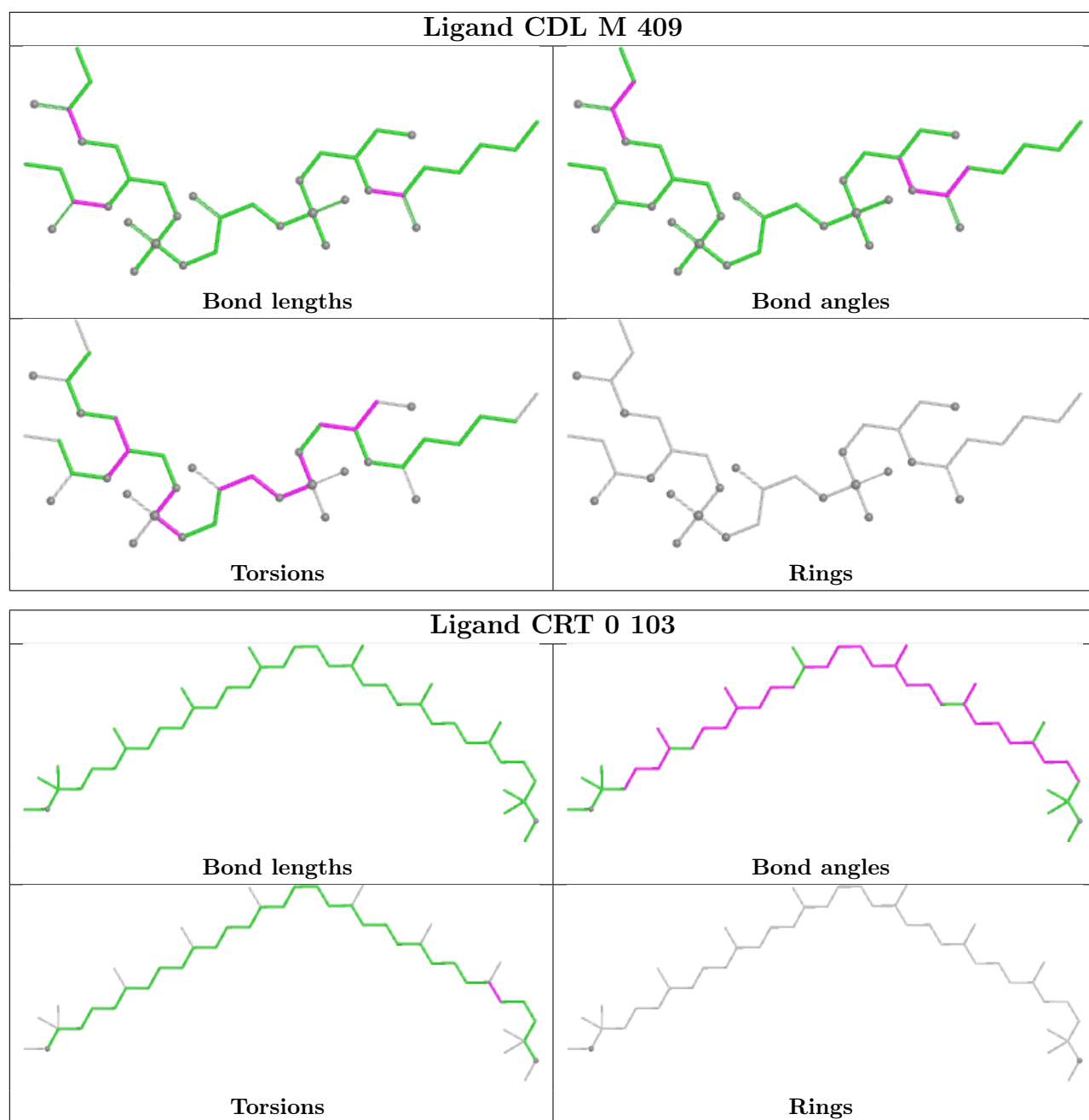


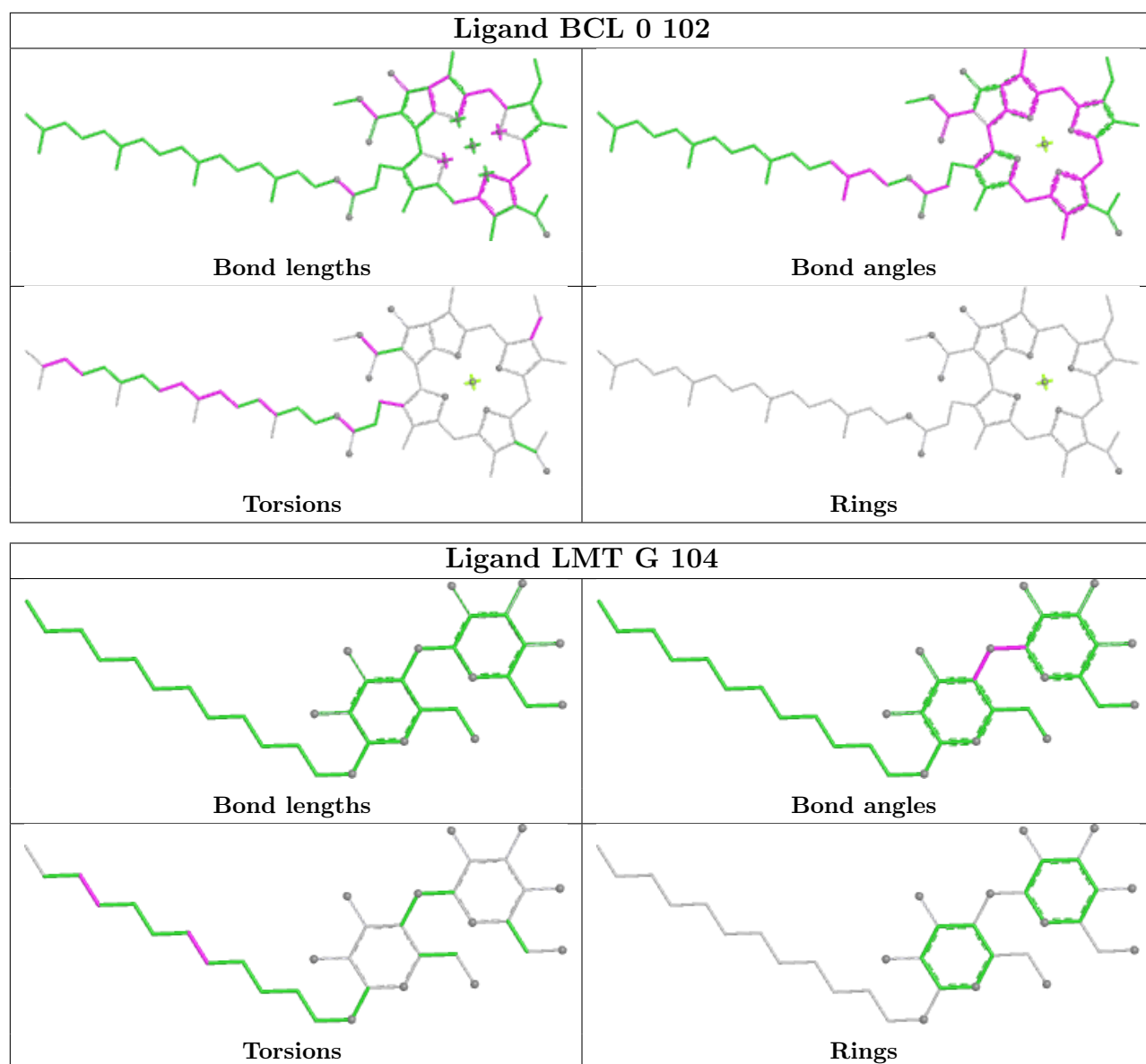


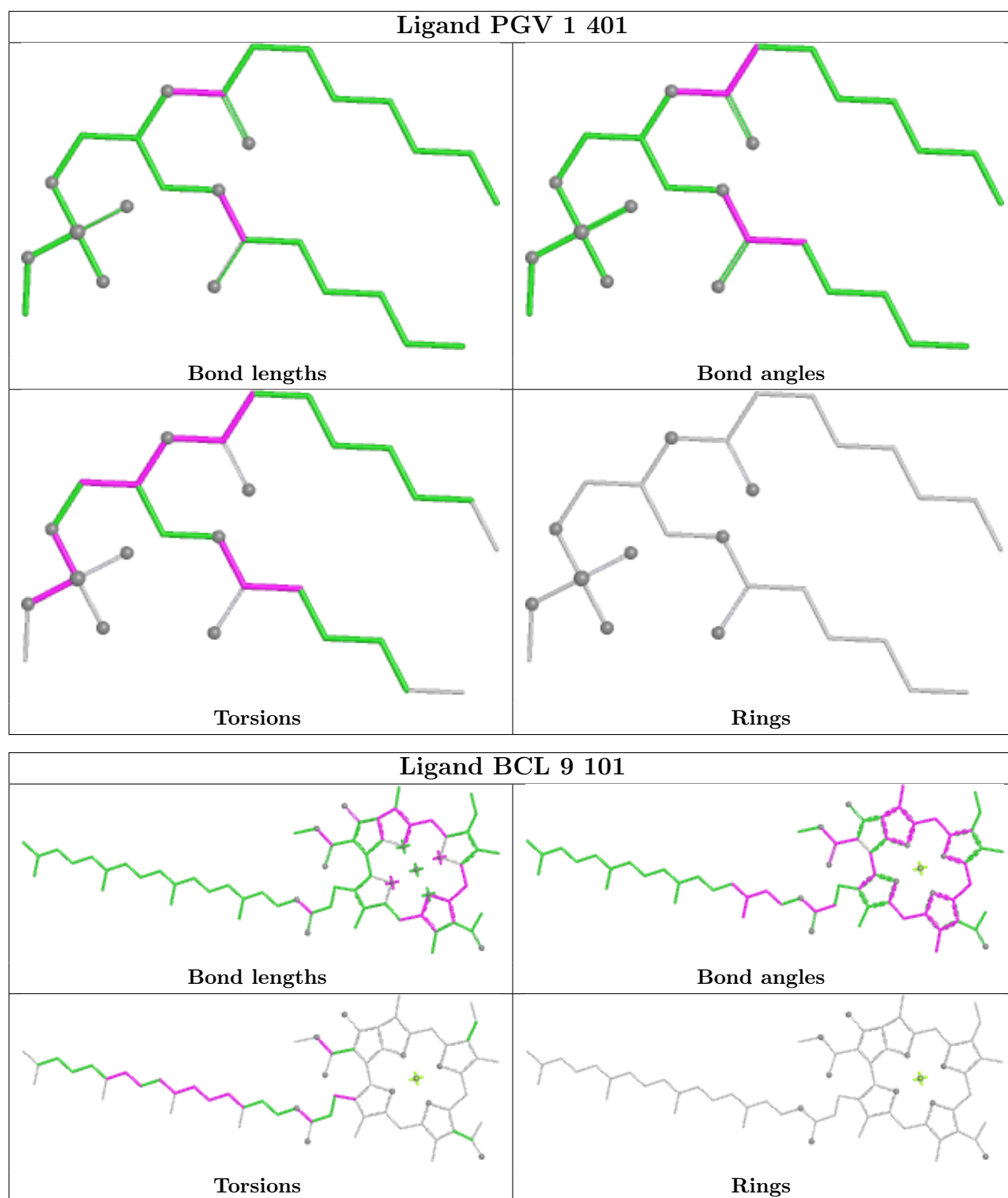


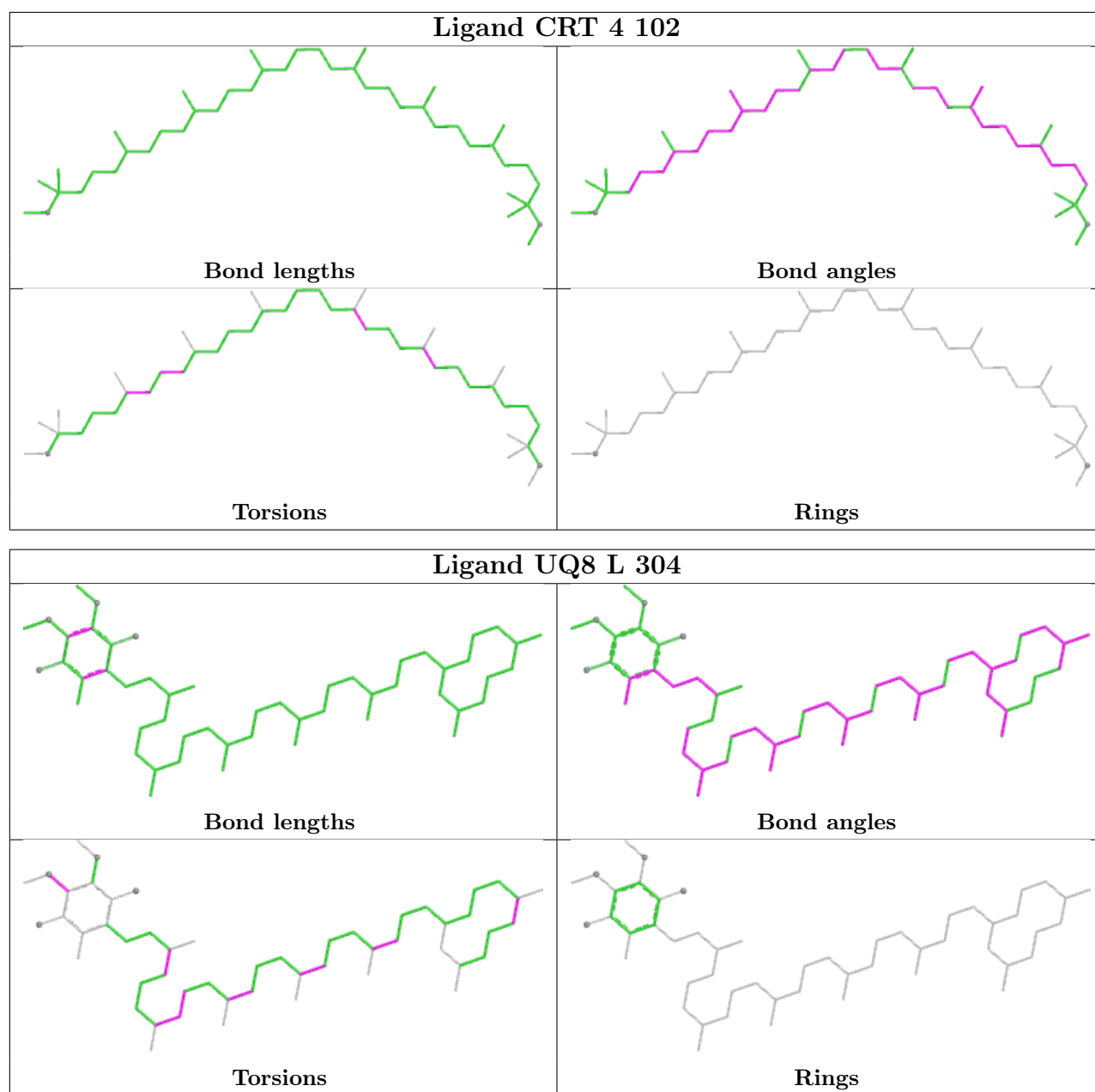


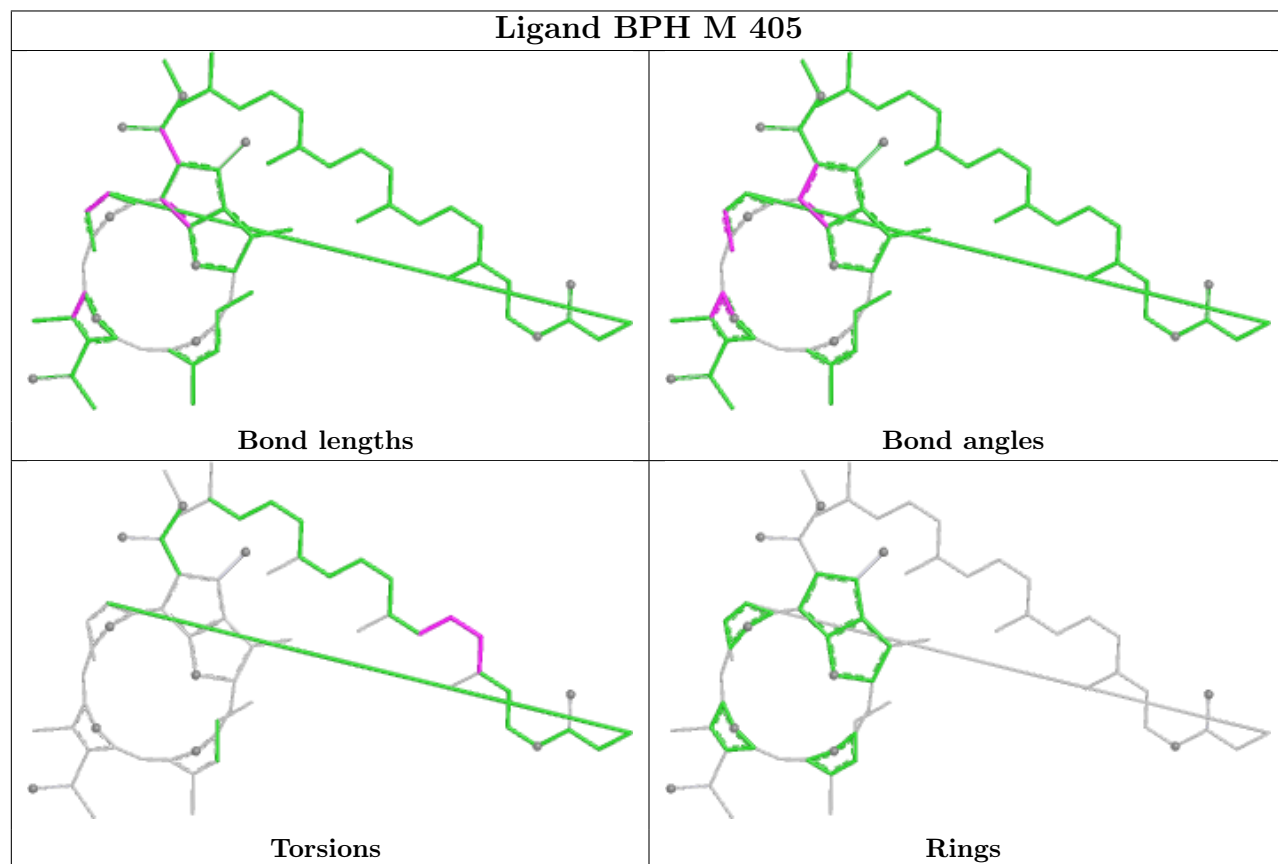
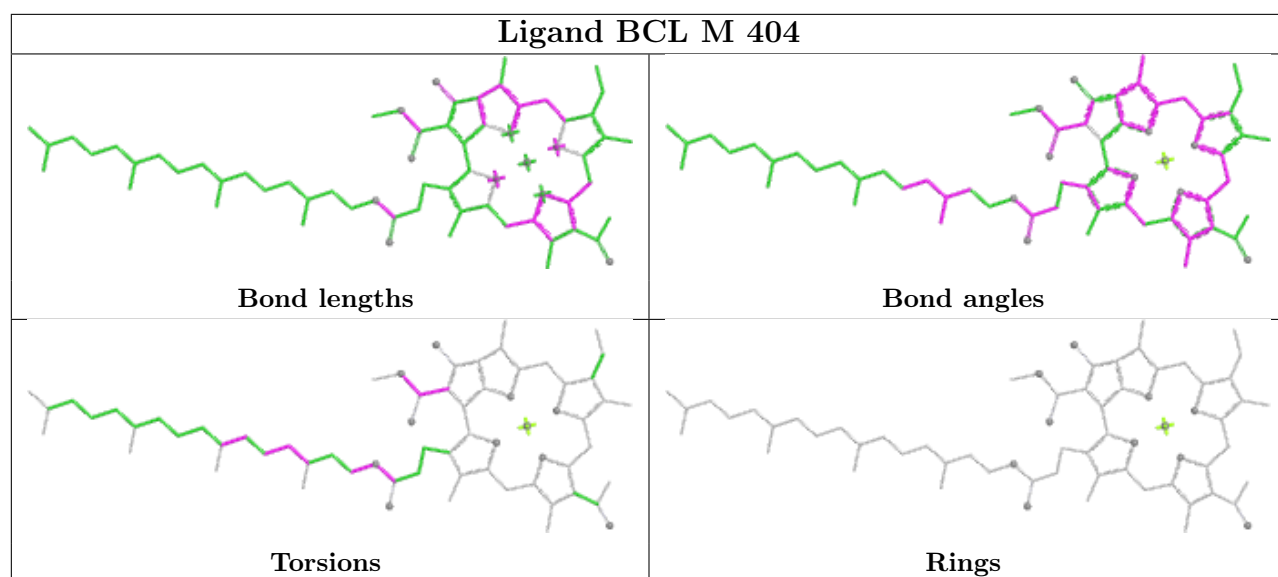


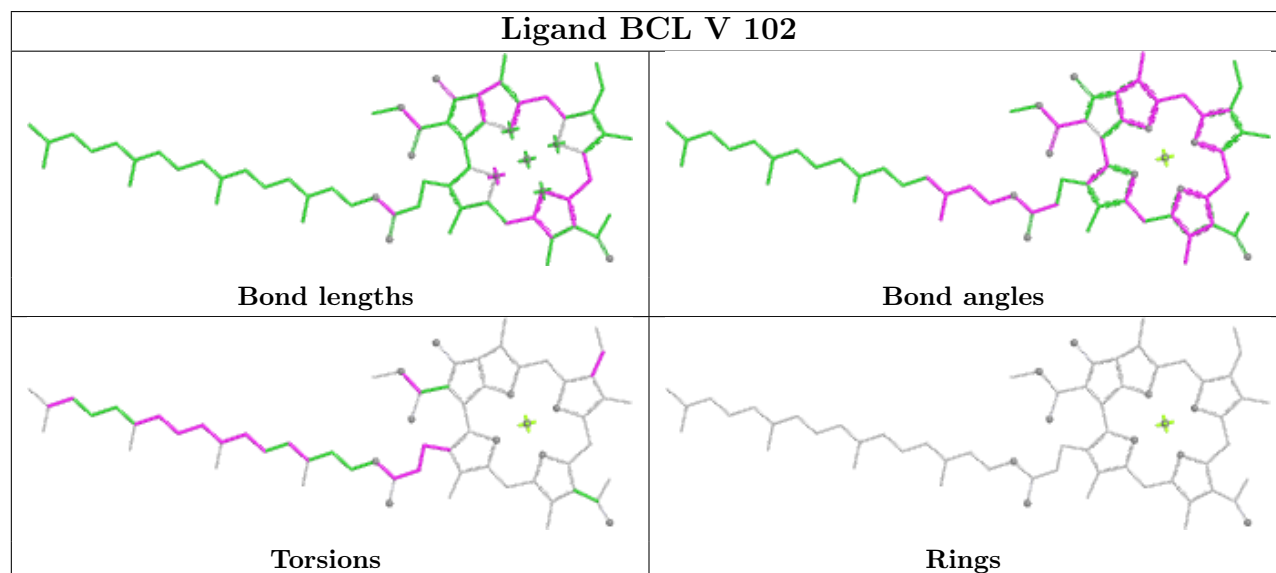
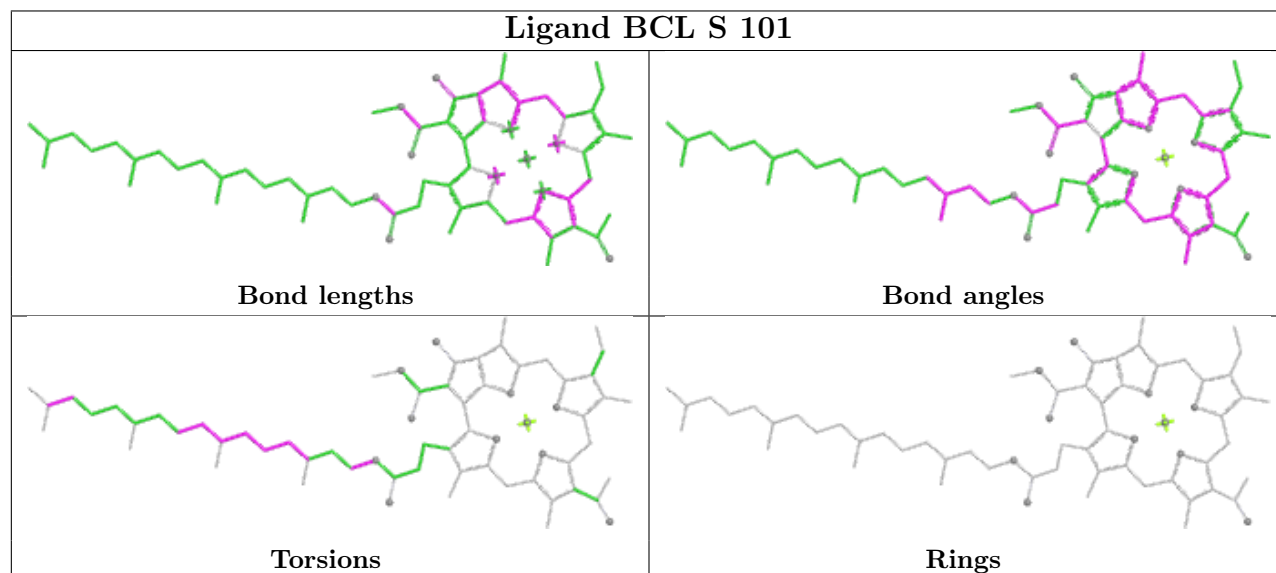
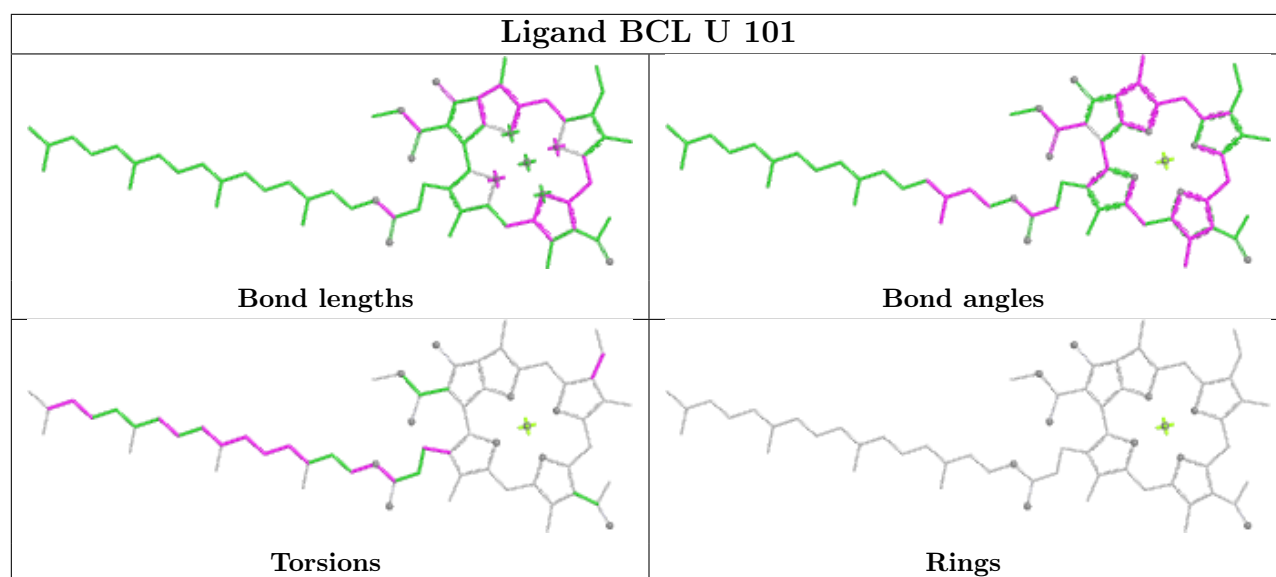


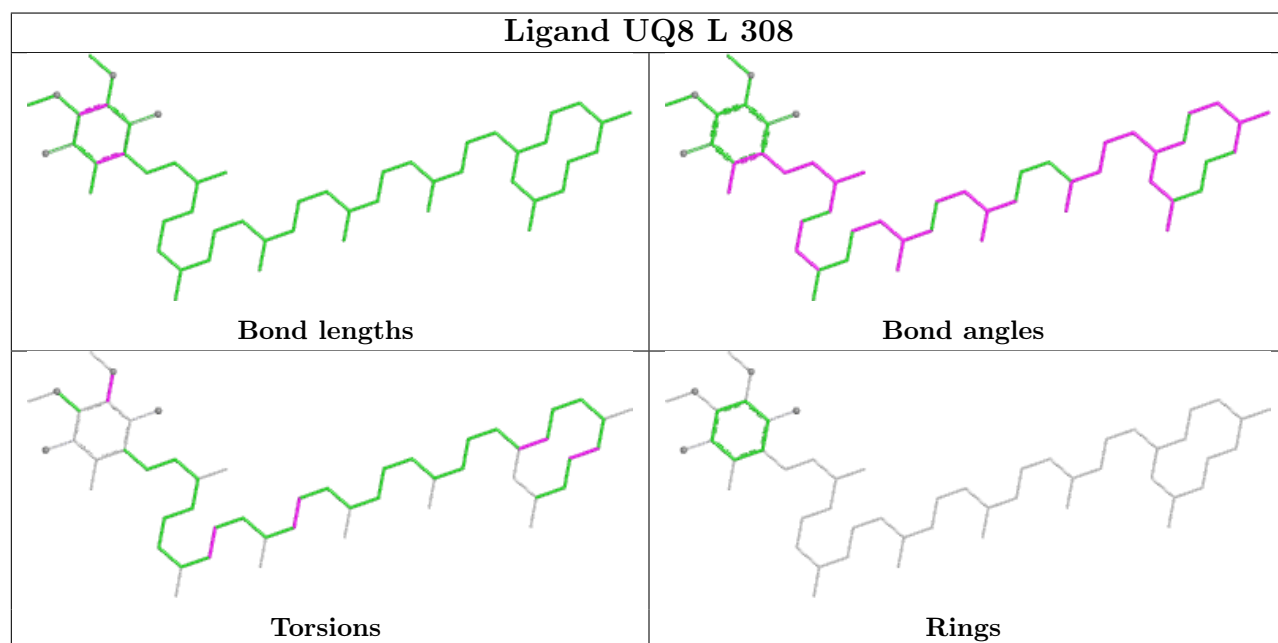
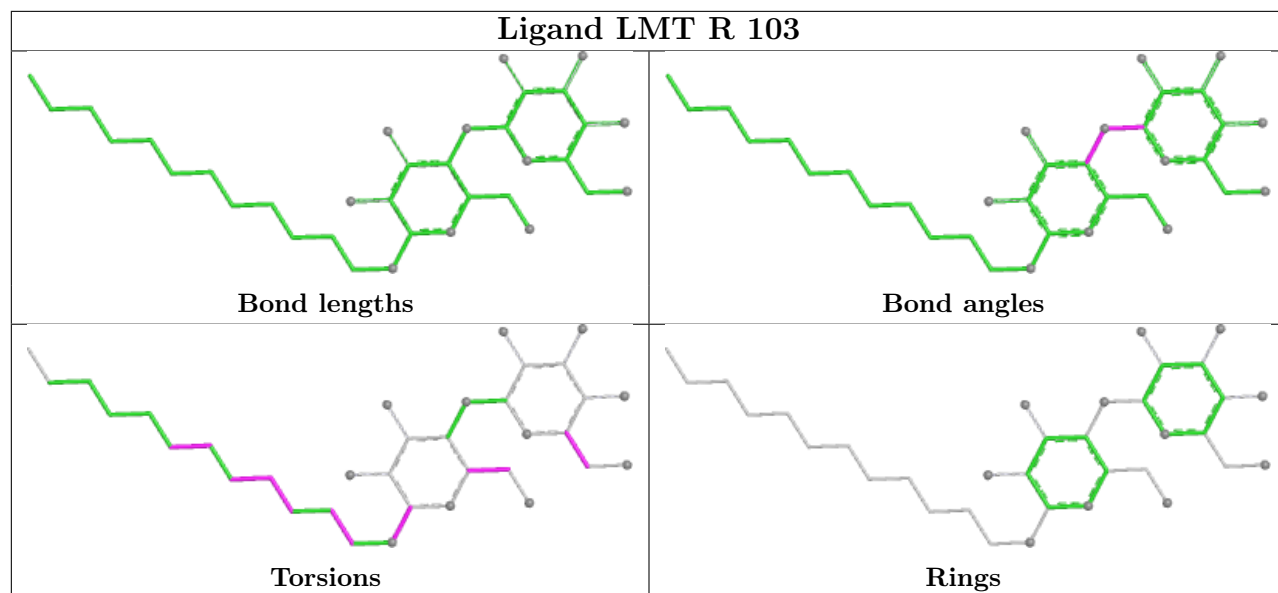


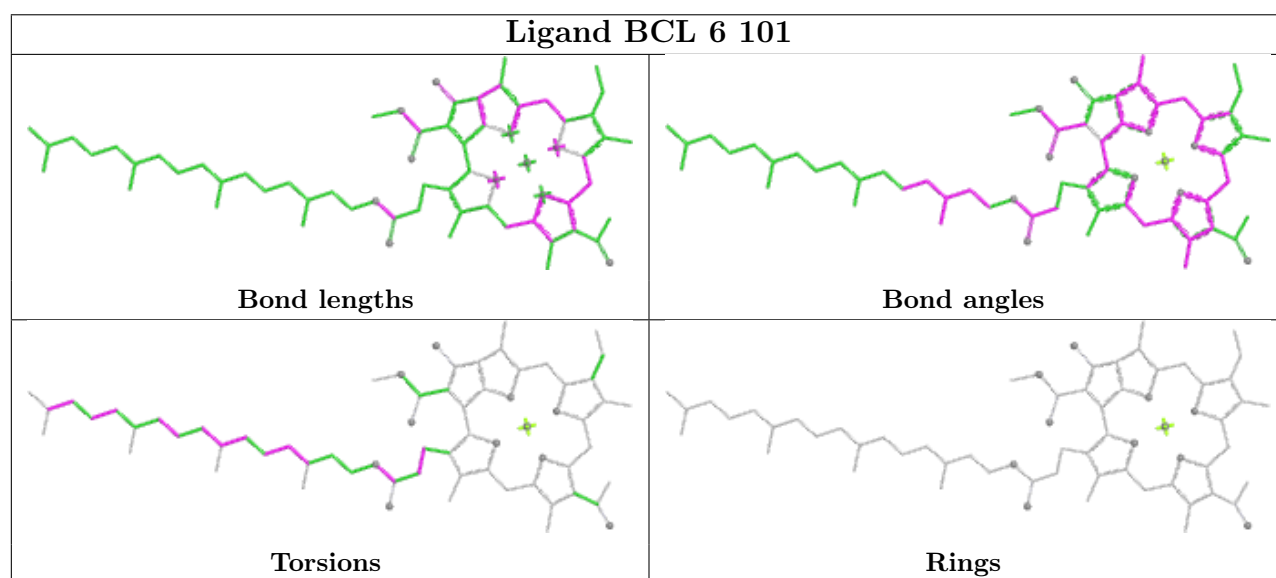
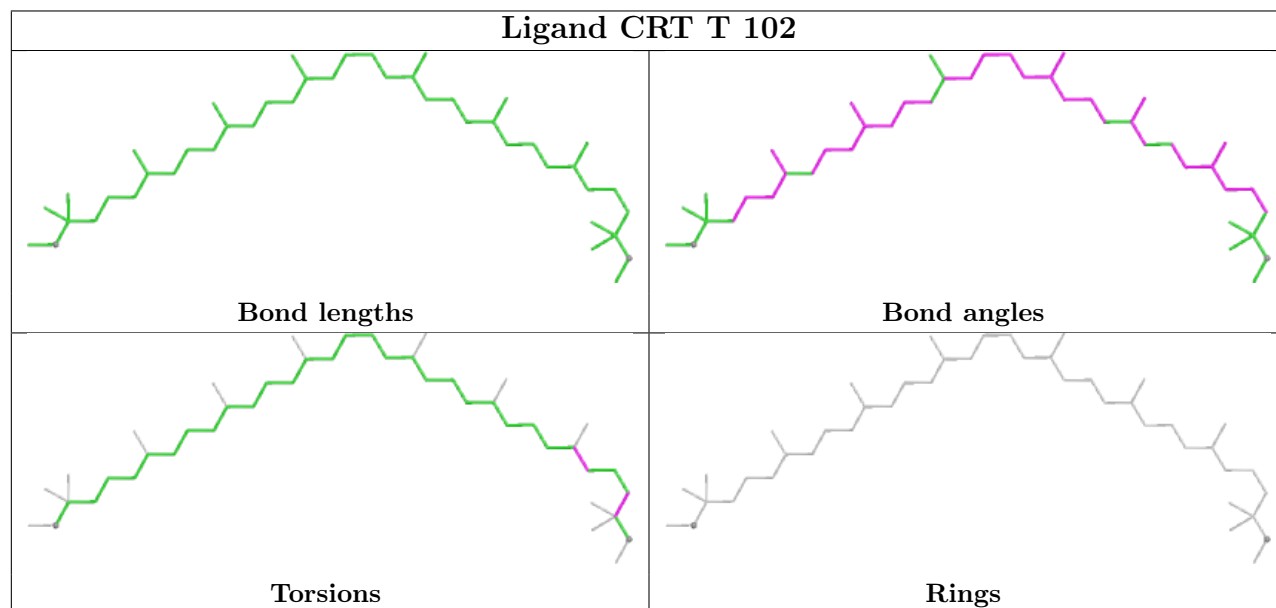
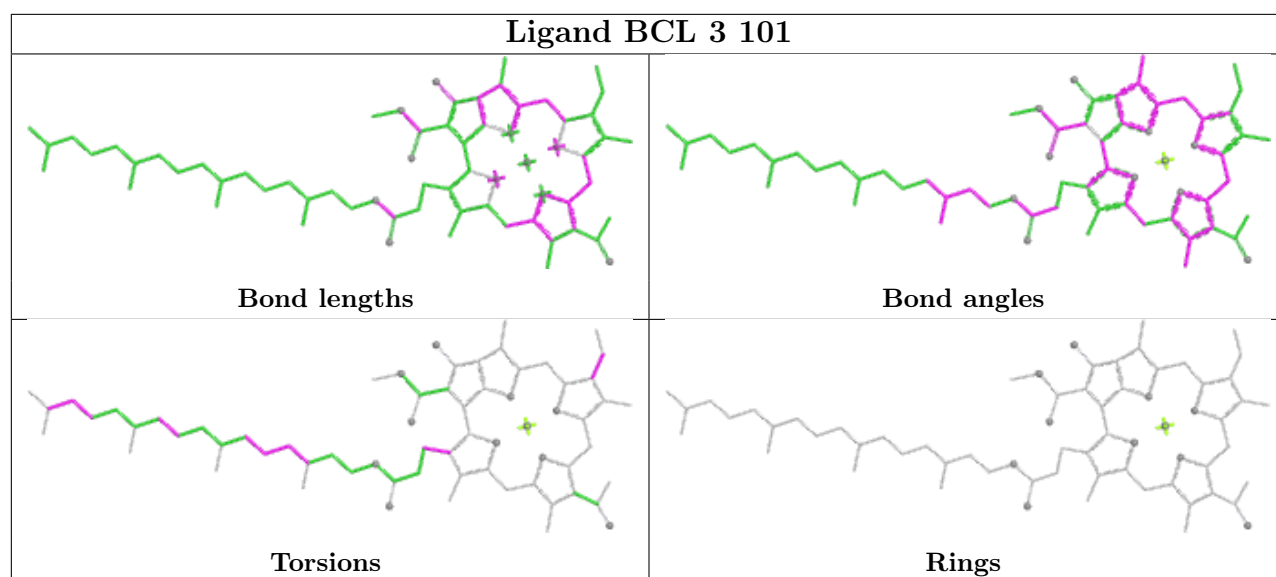


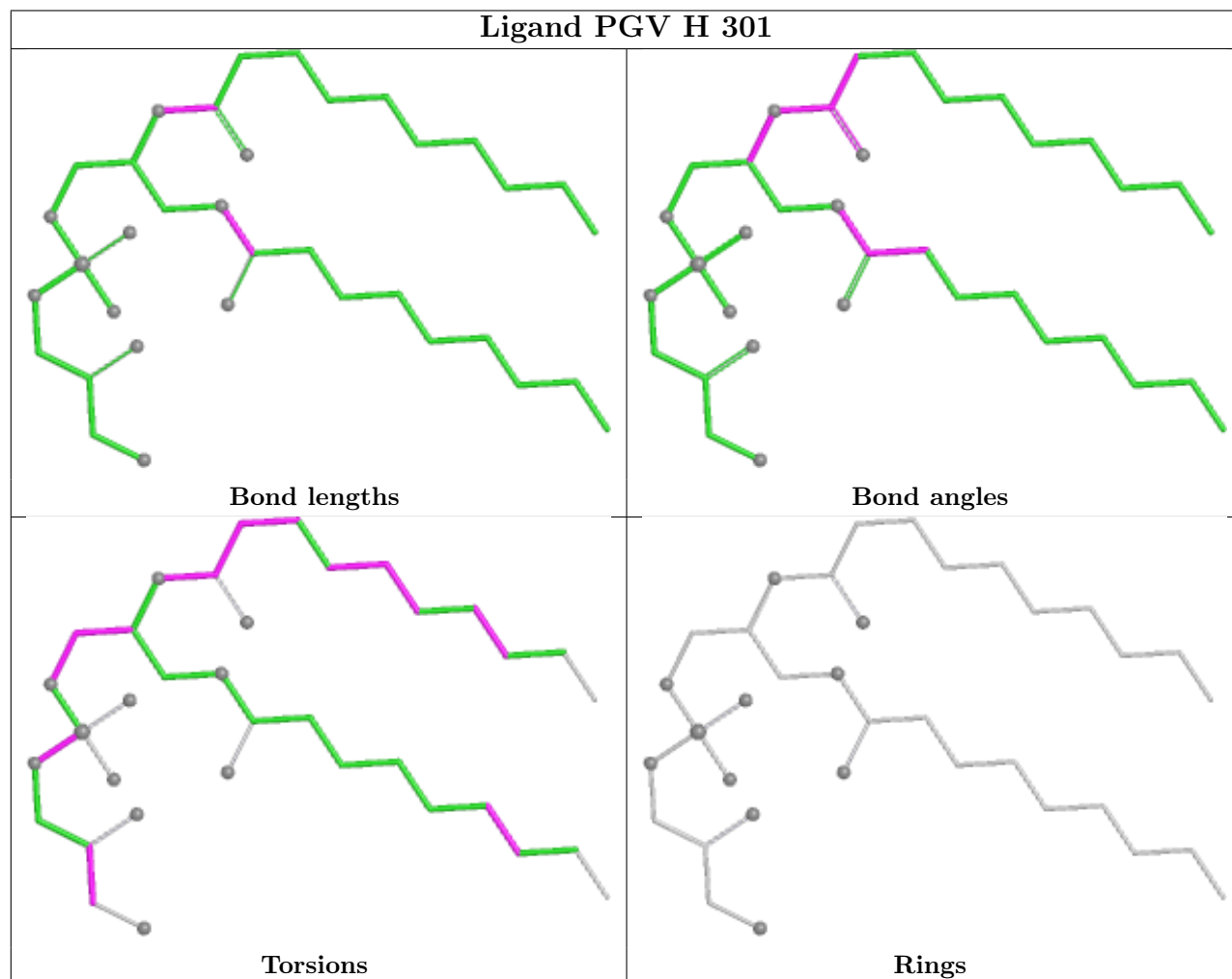
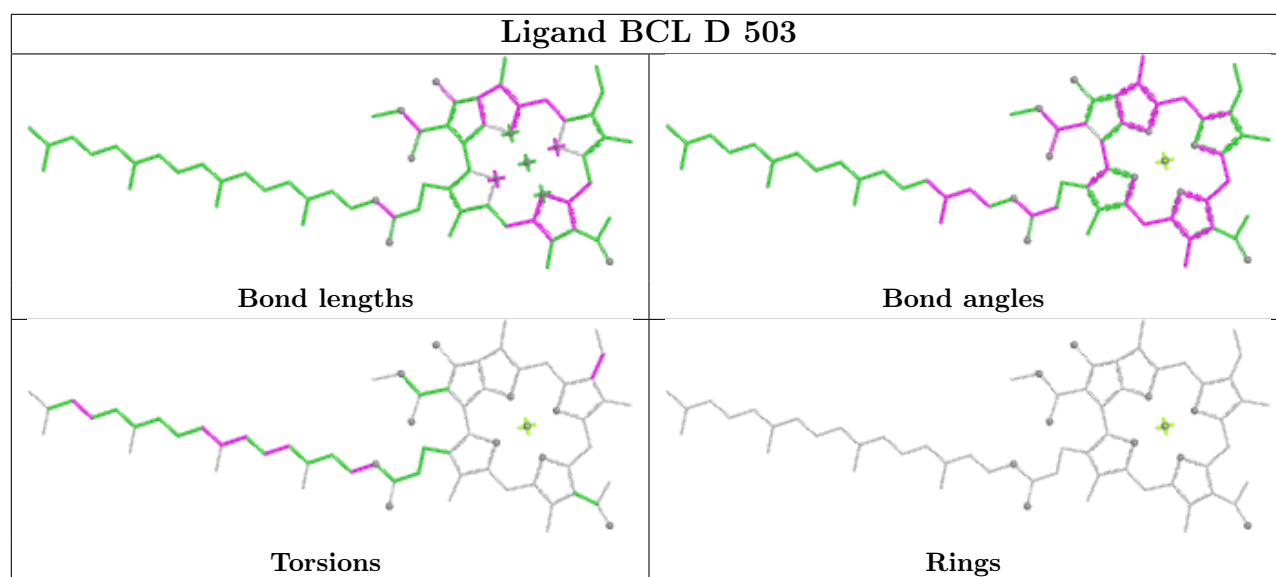


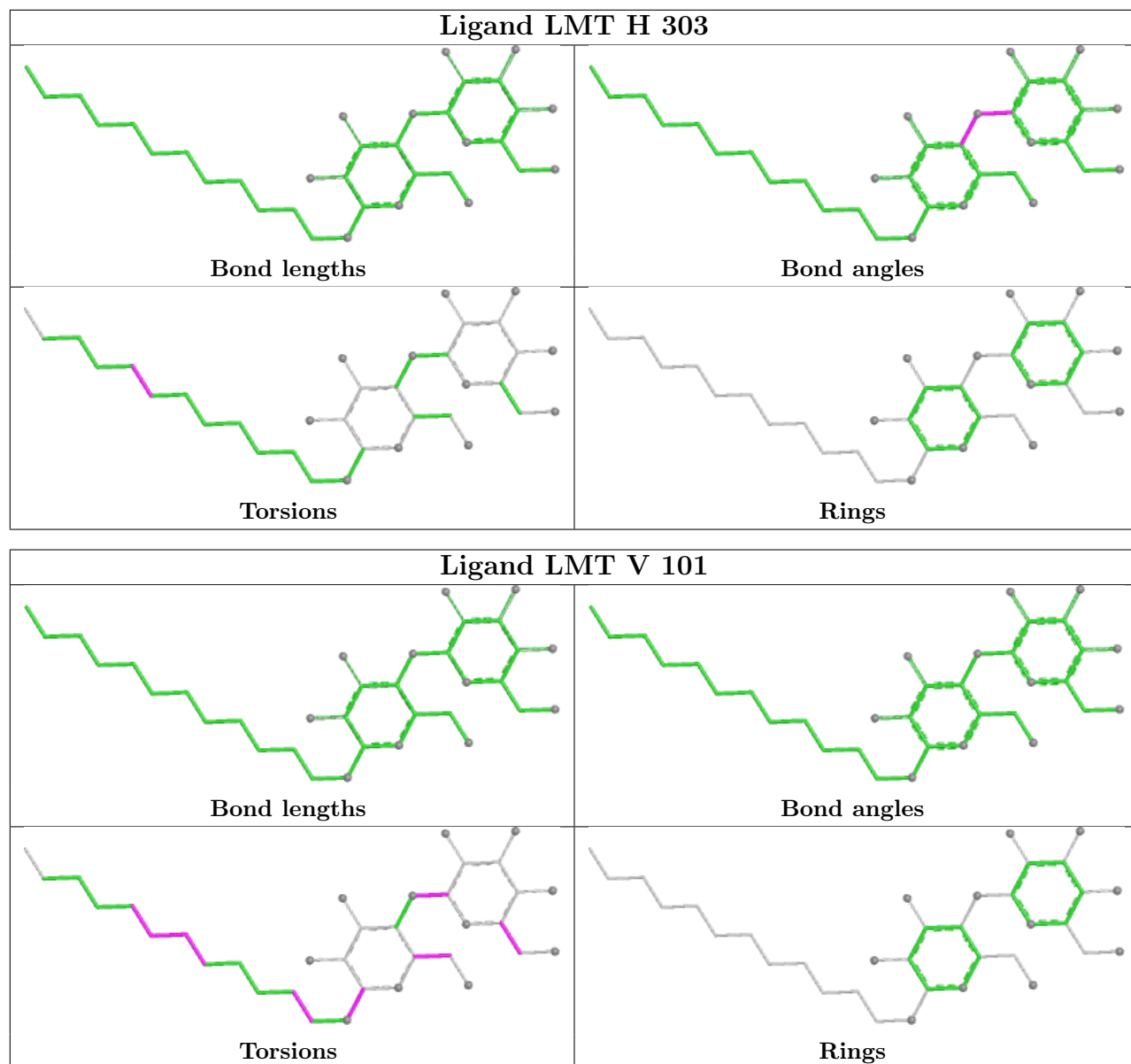


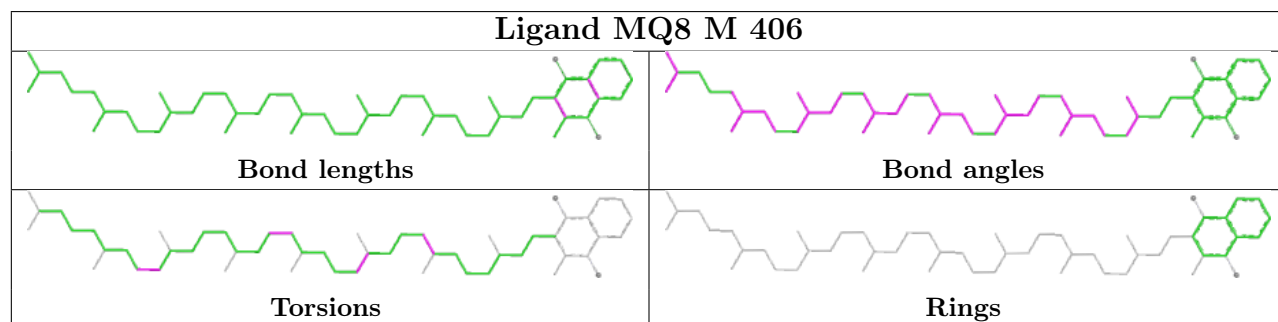
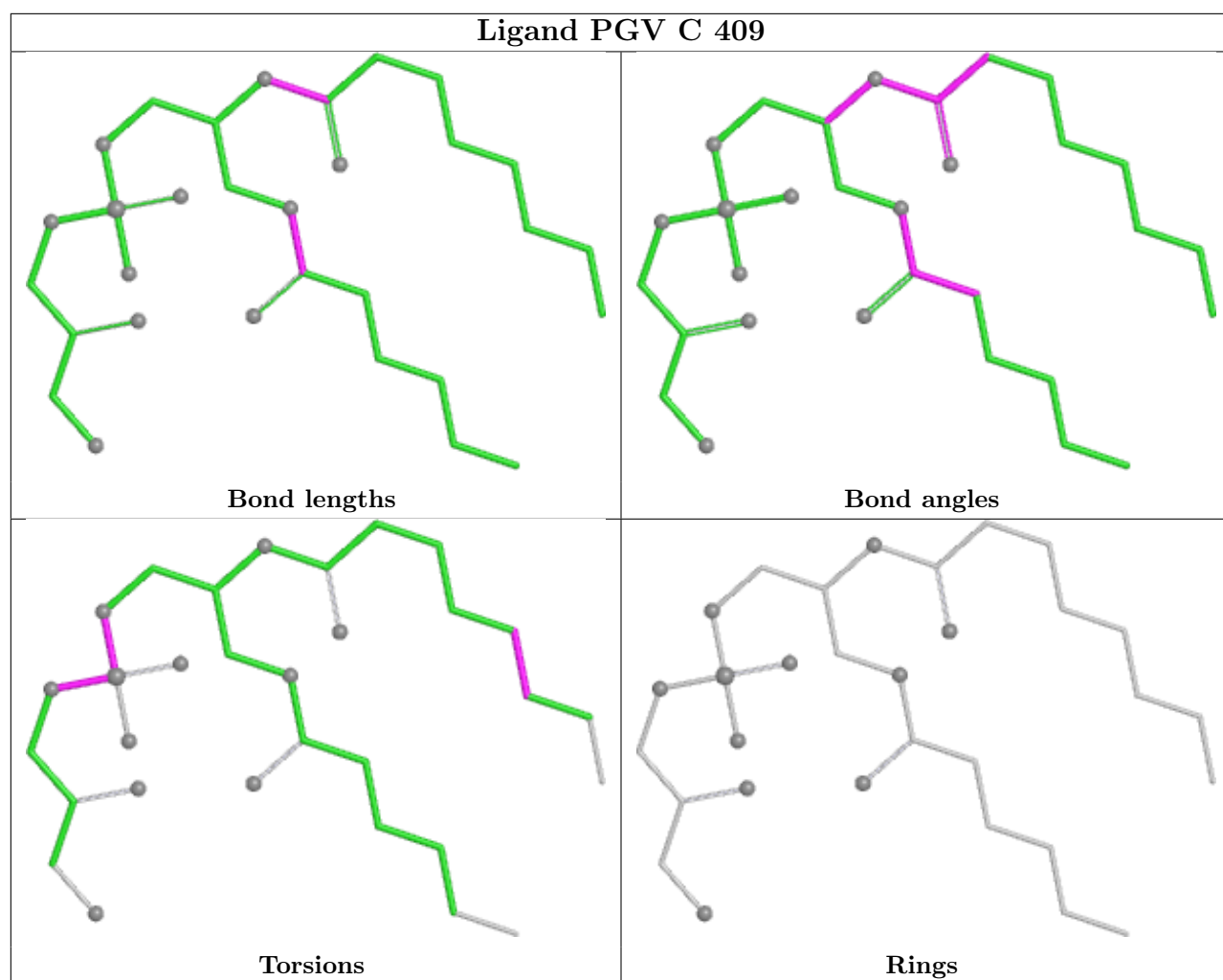


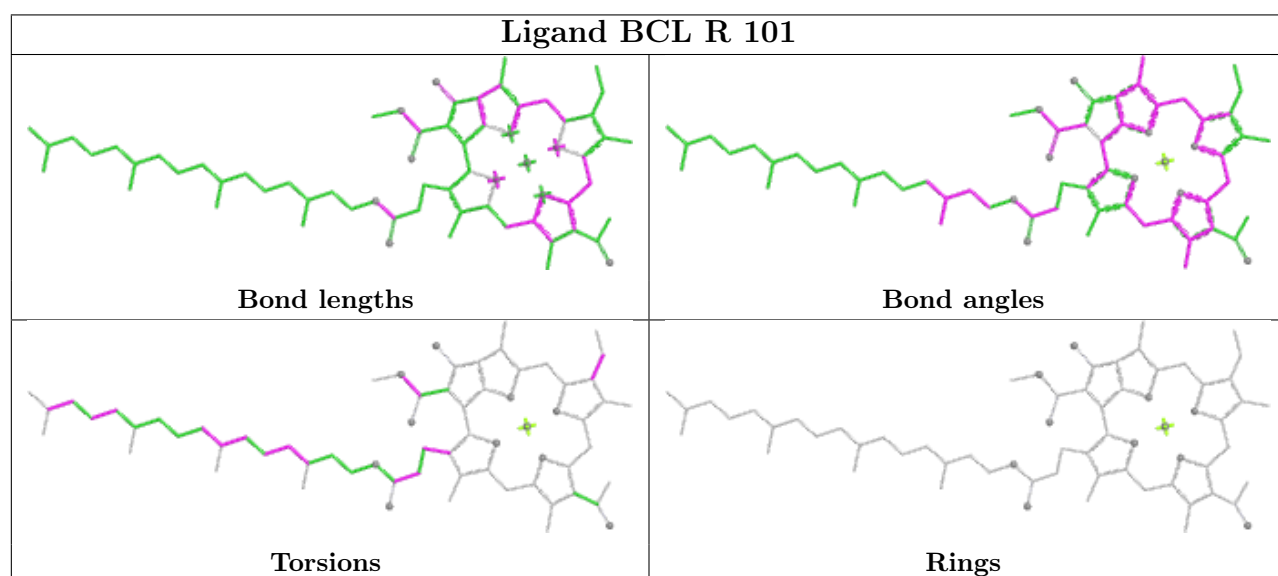
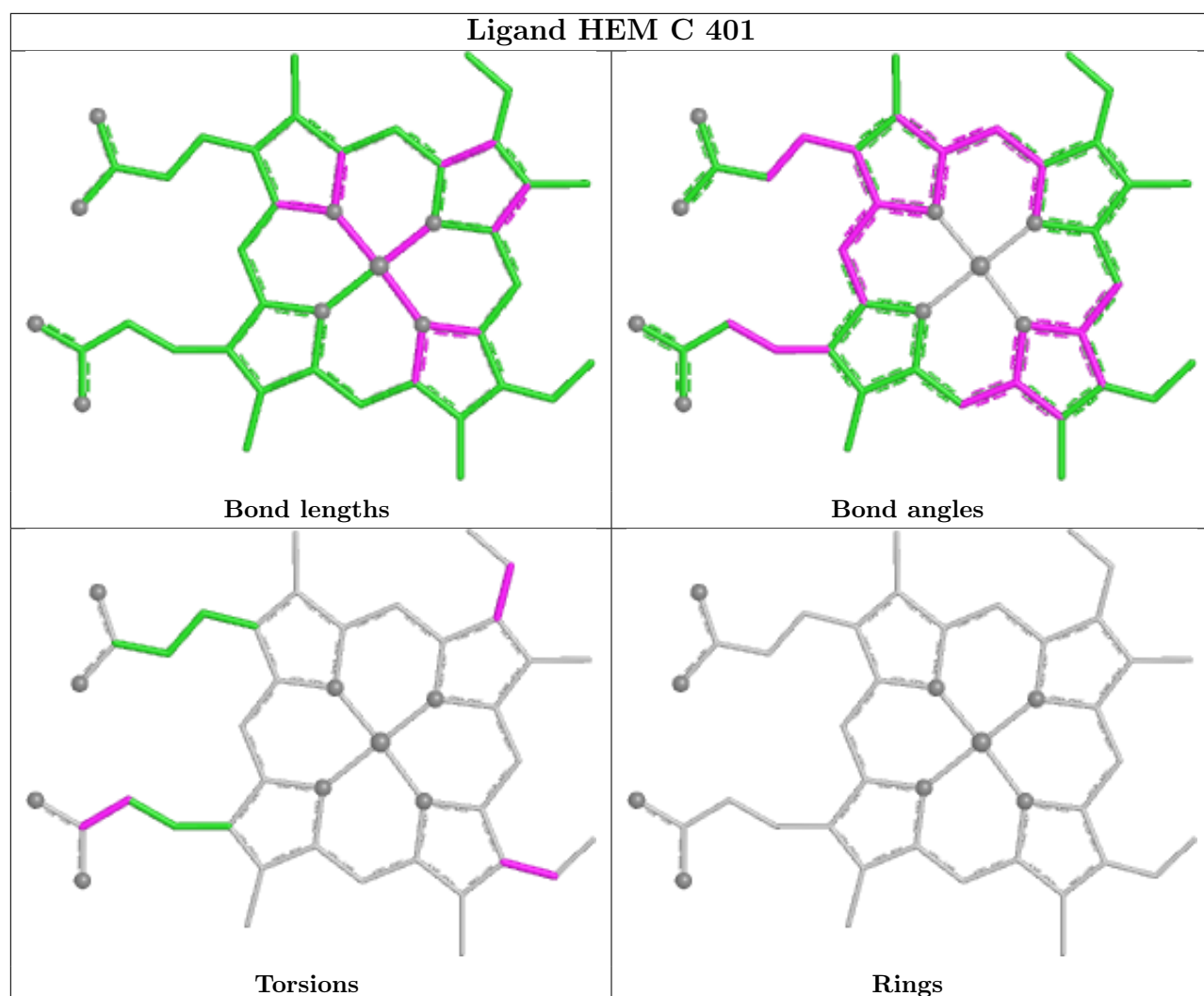


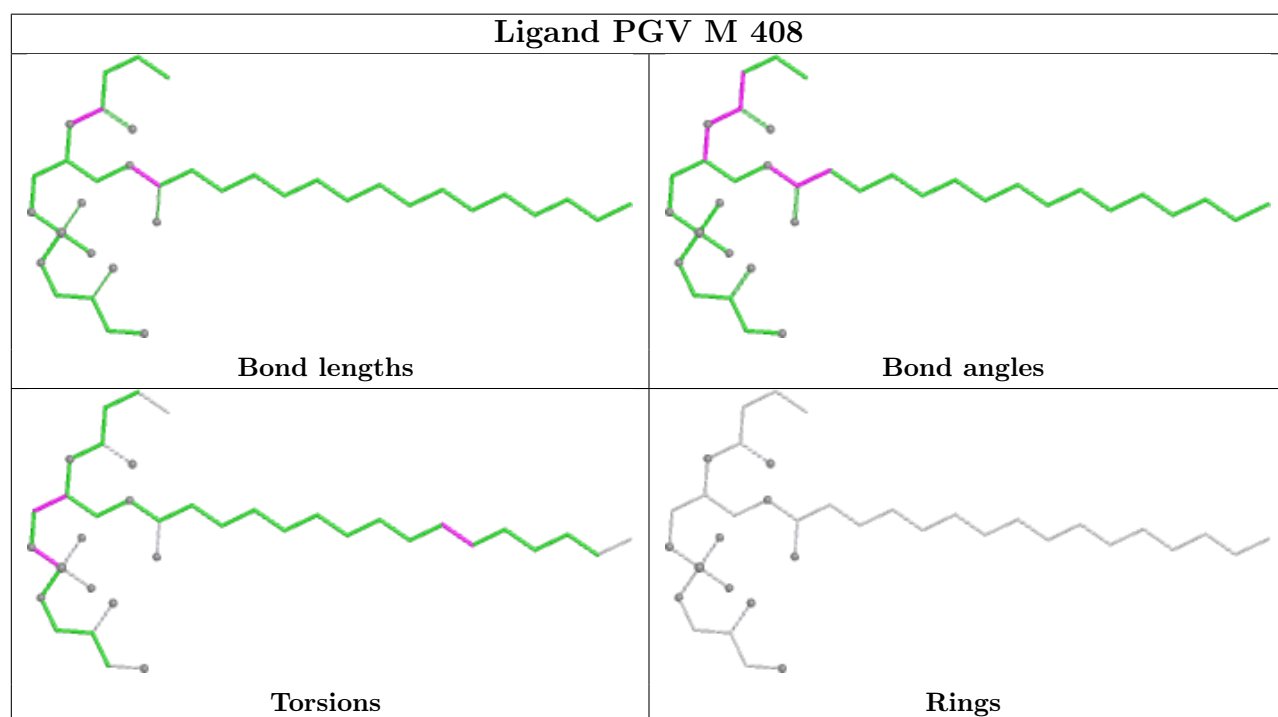
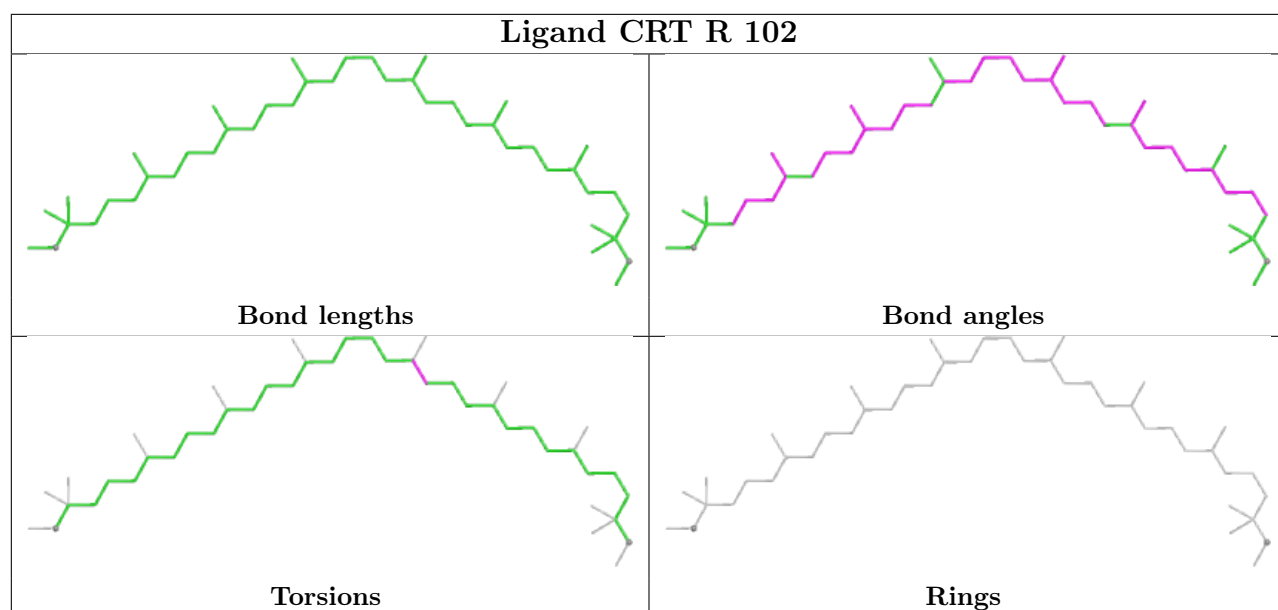


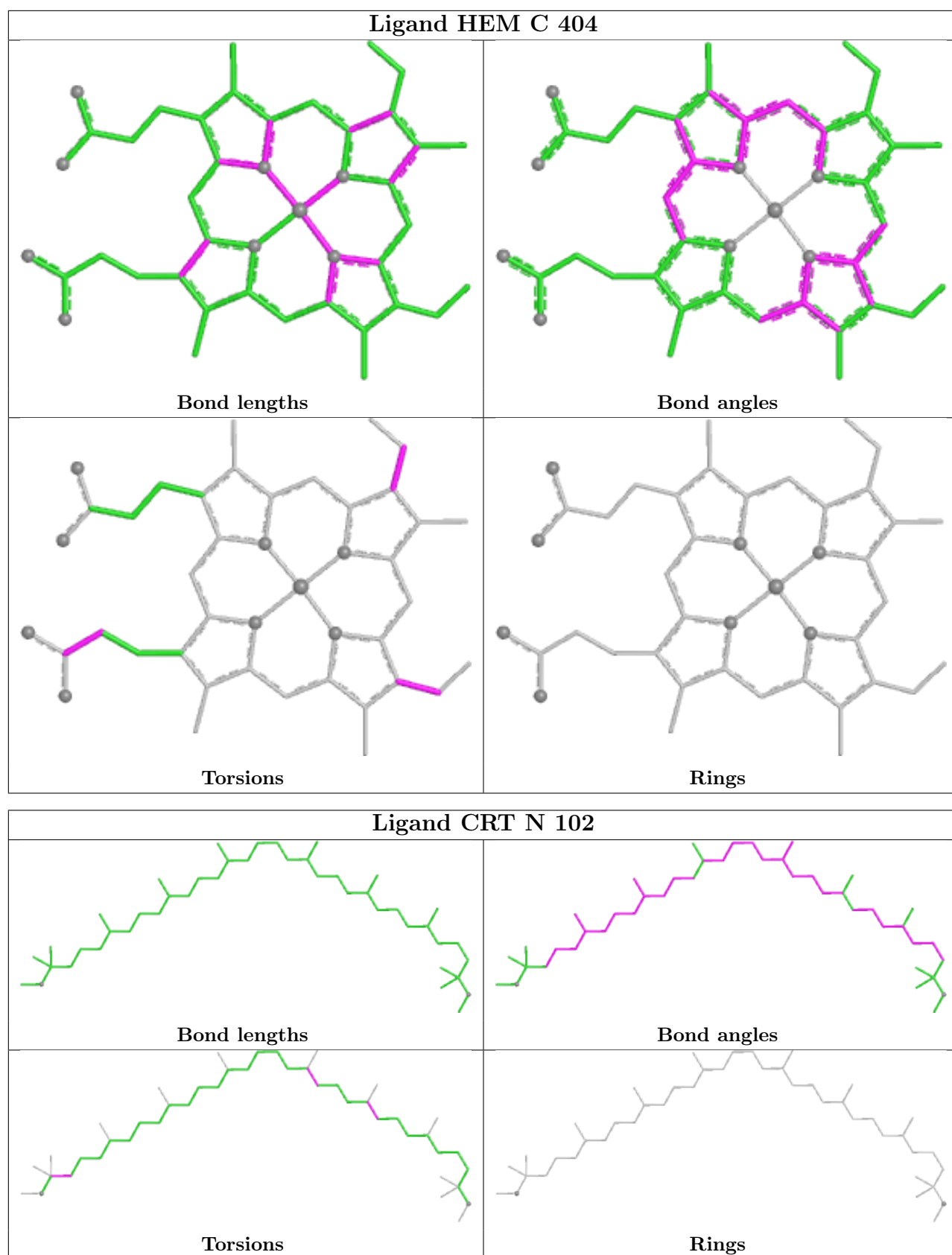


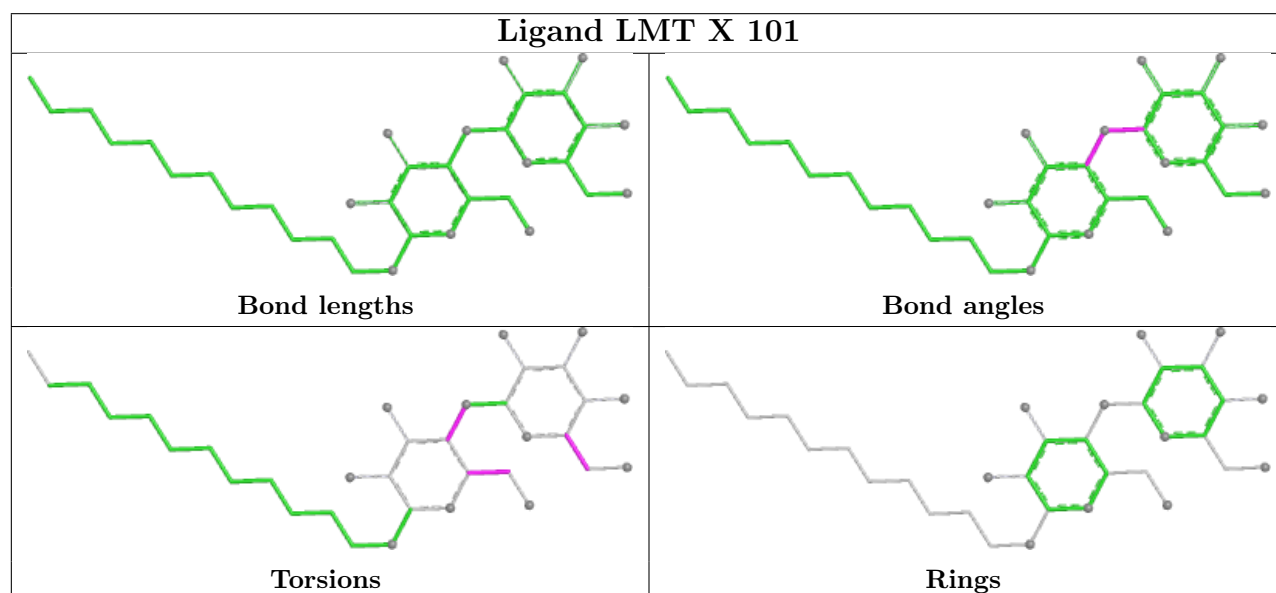
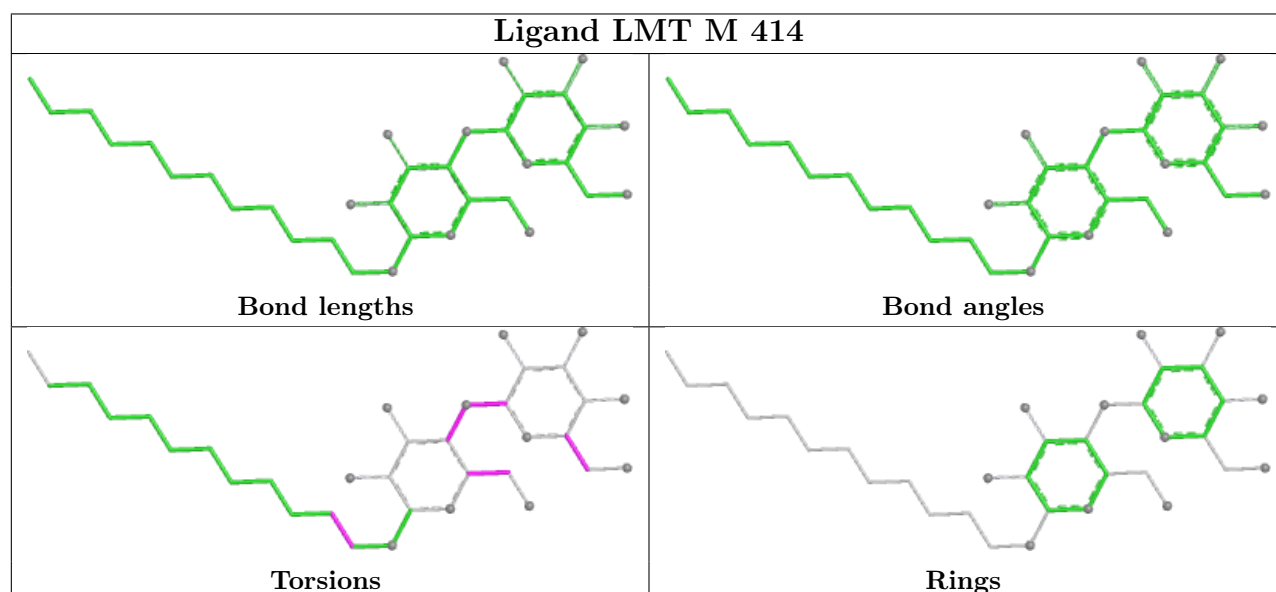
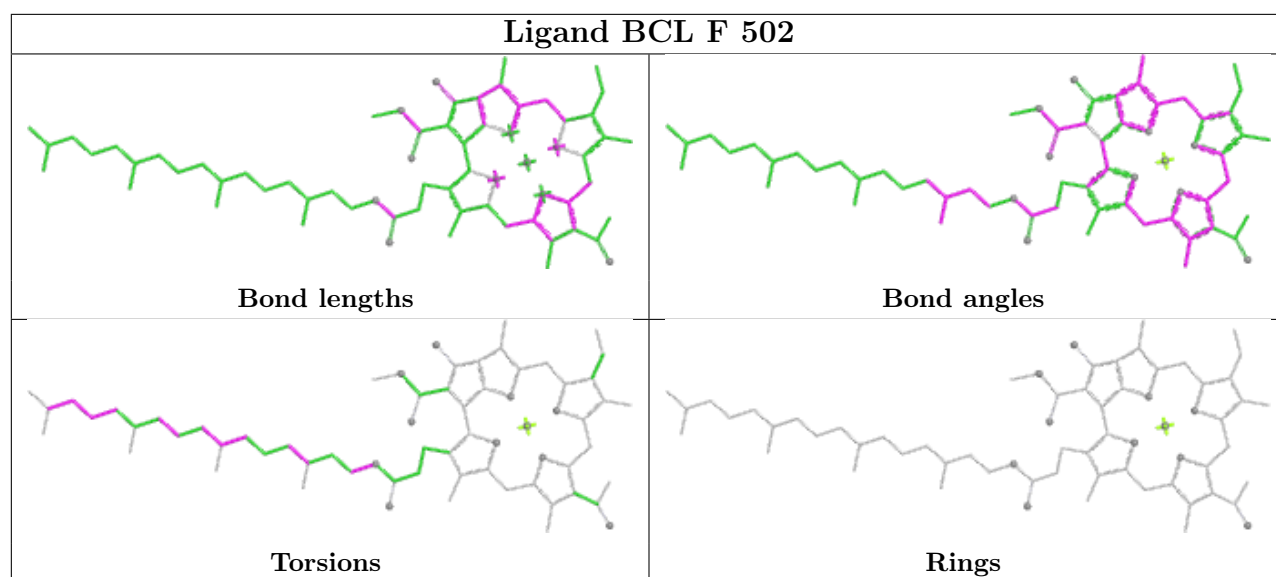


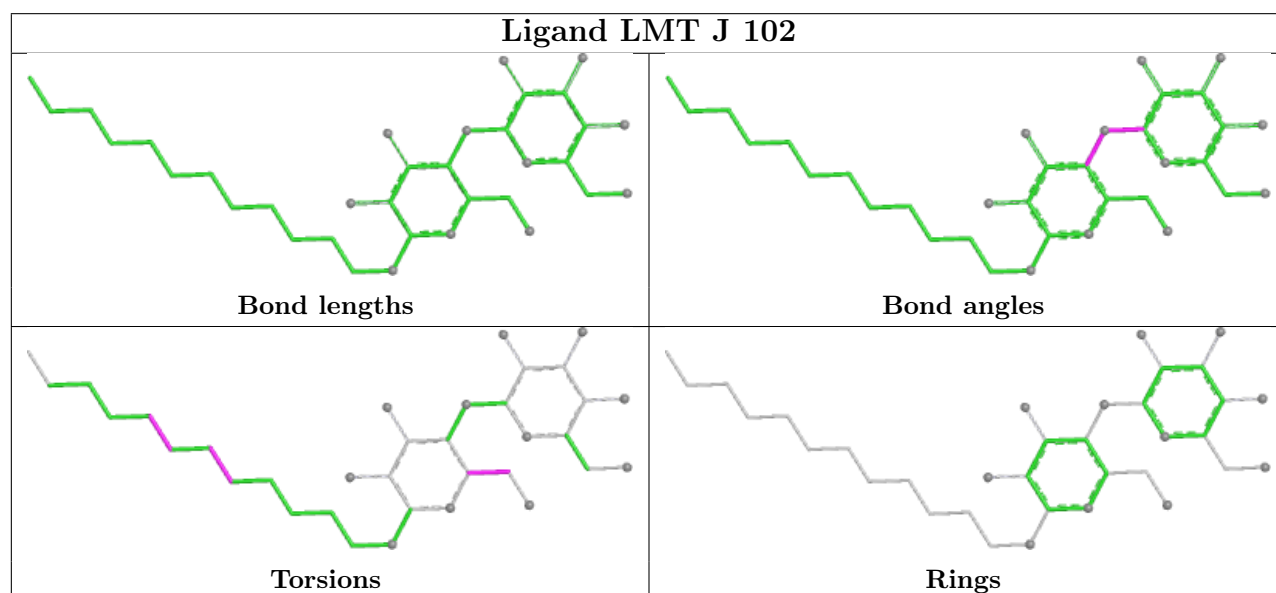
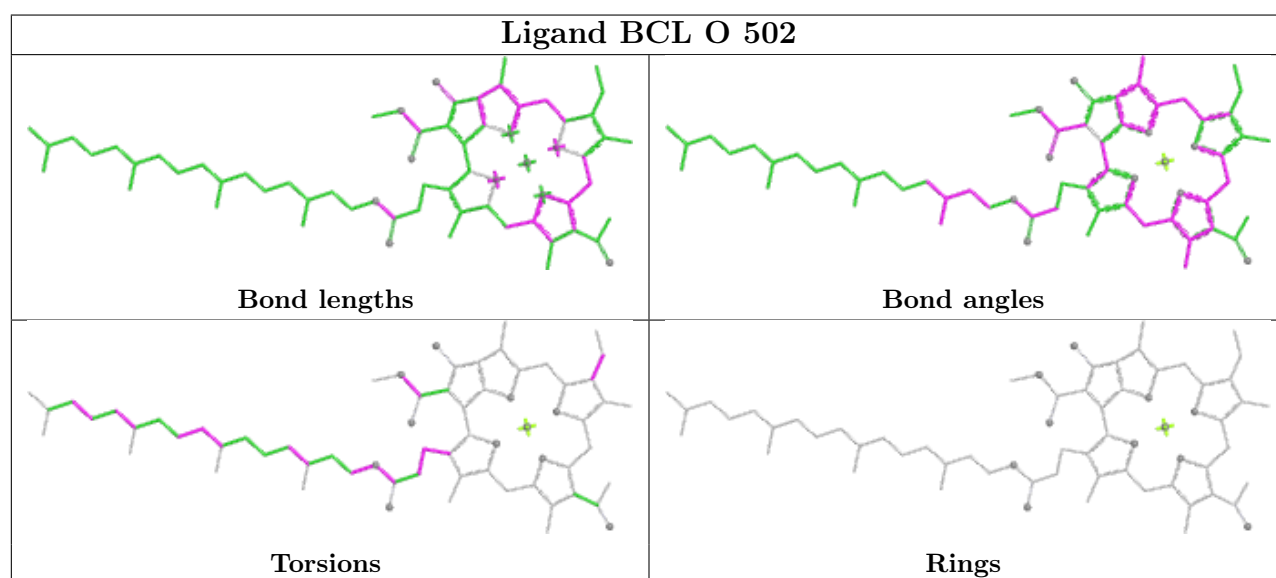
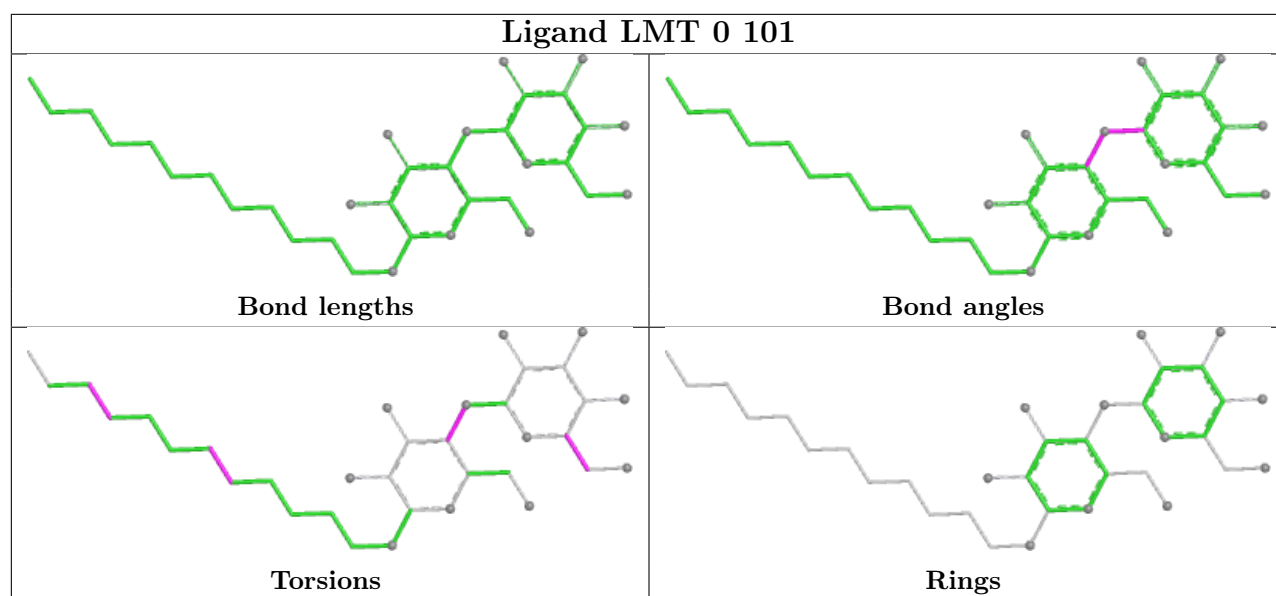


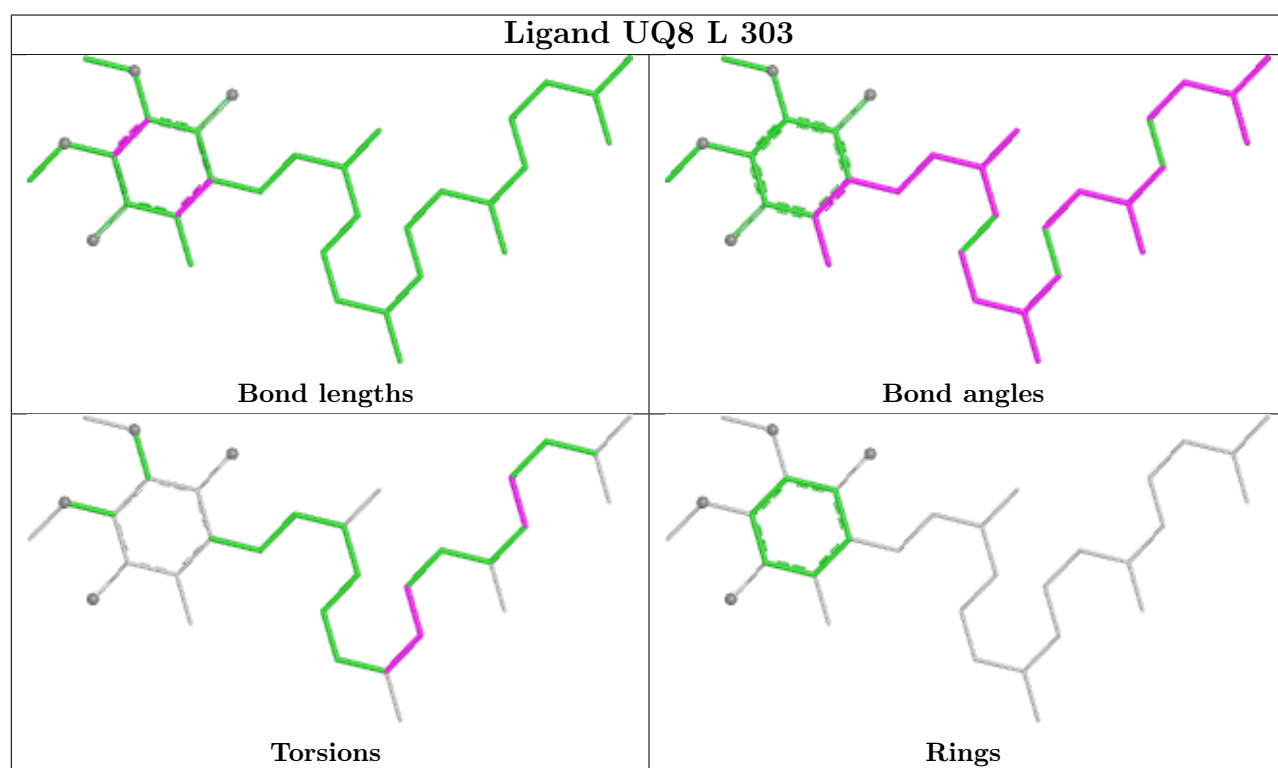
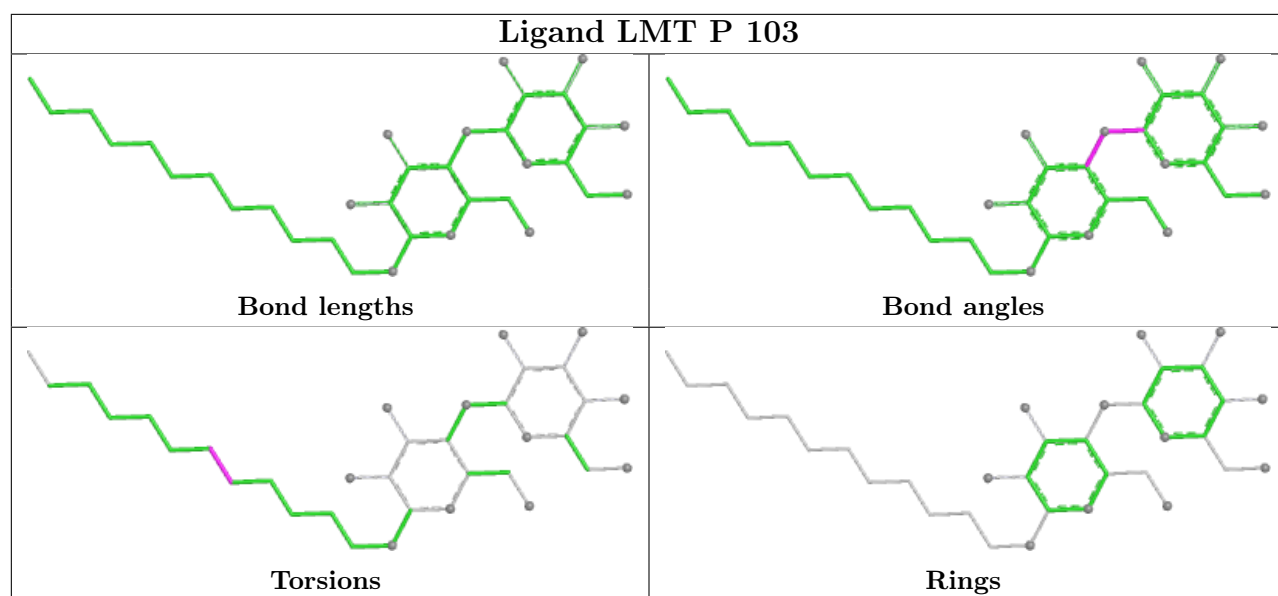


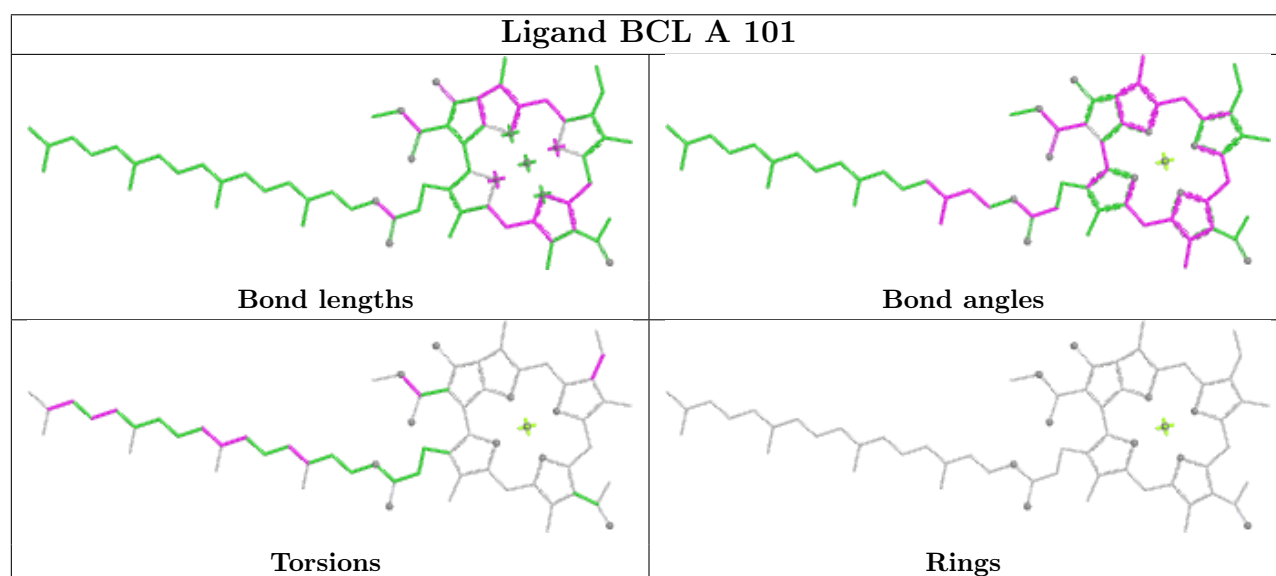
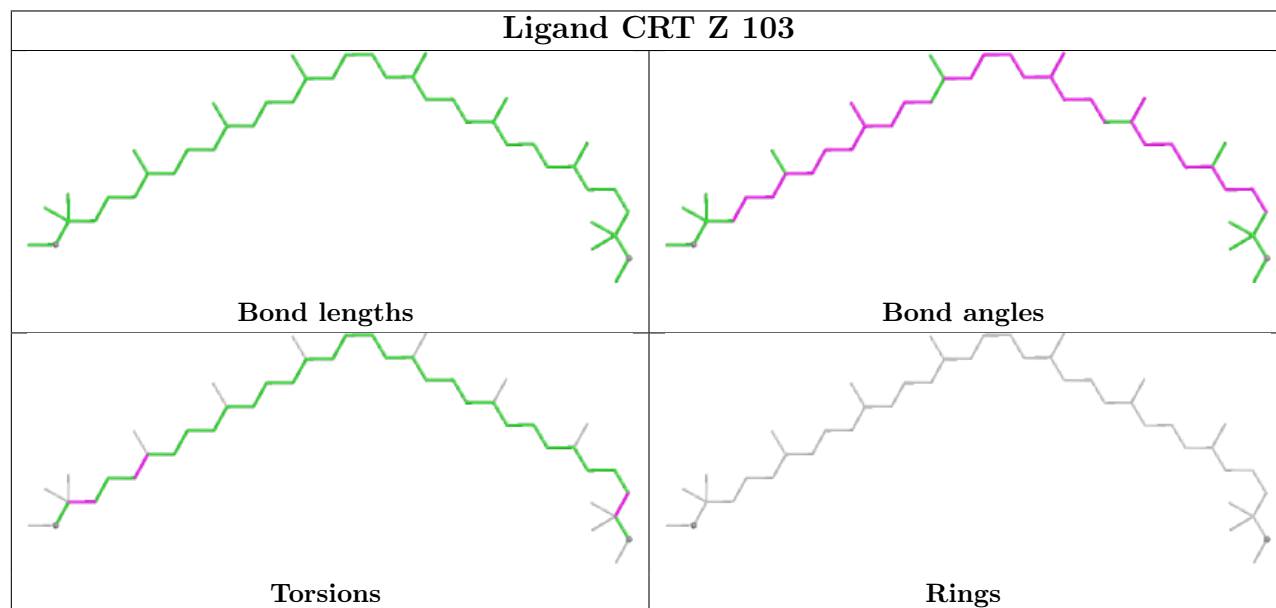
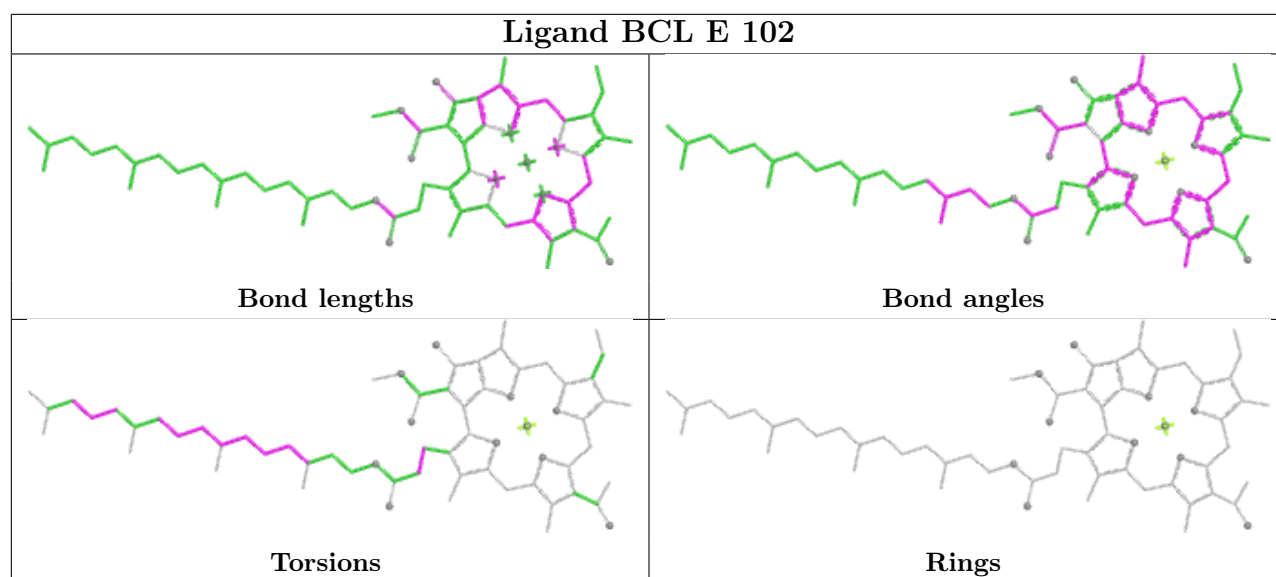


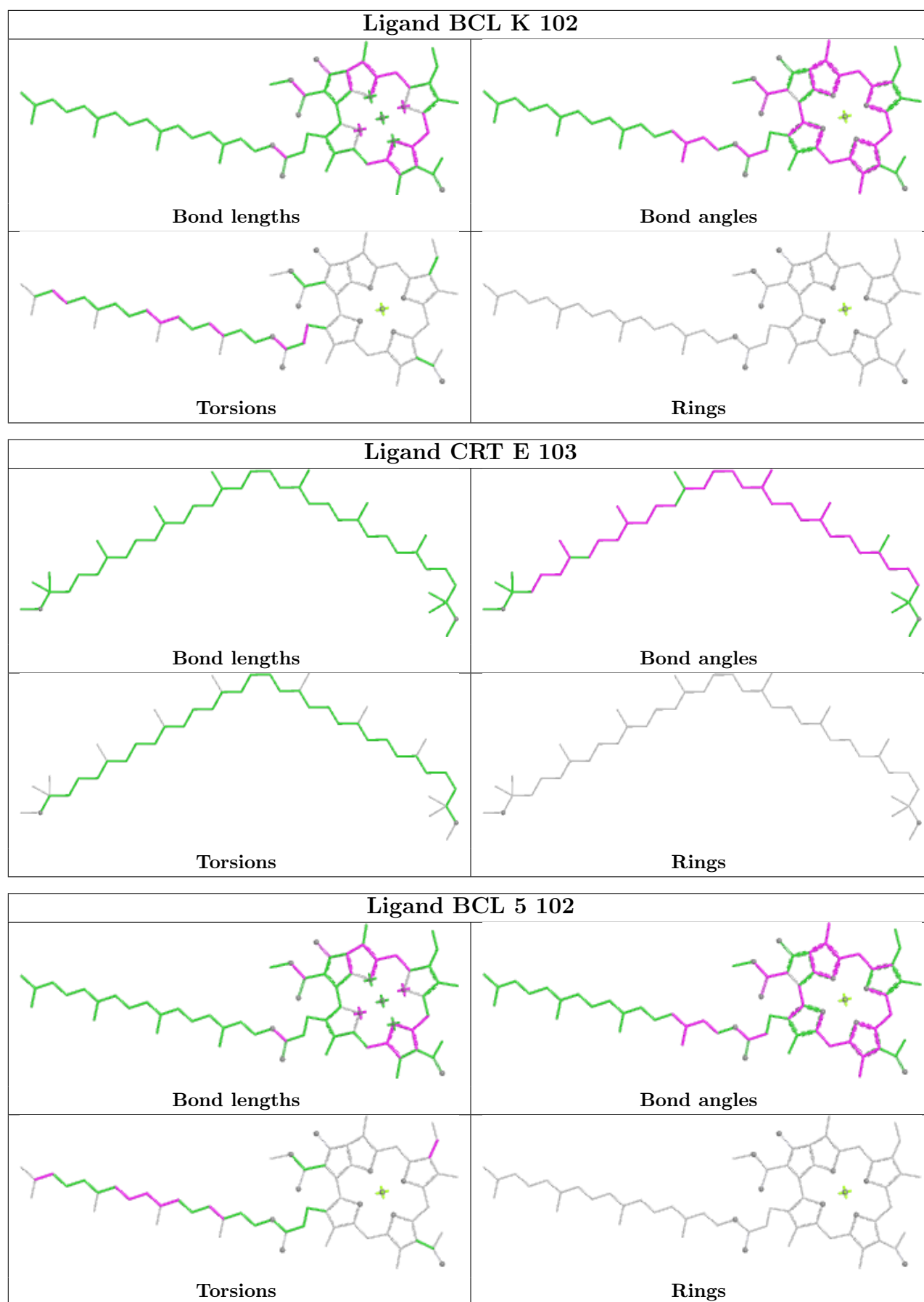


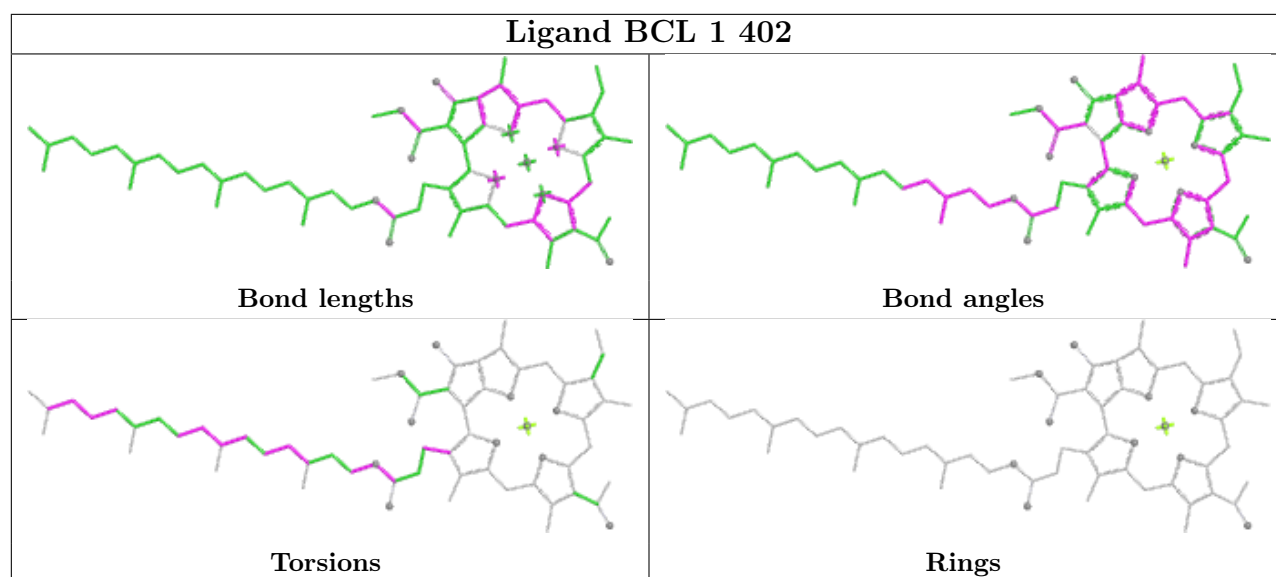












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

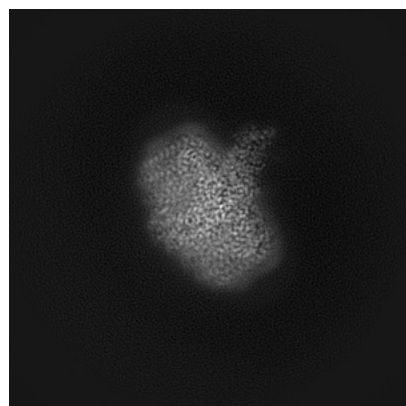
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37466. These allow visual inspection of the internal detail of the map and identification of artifacts.

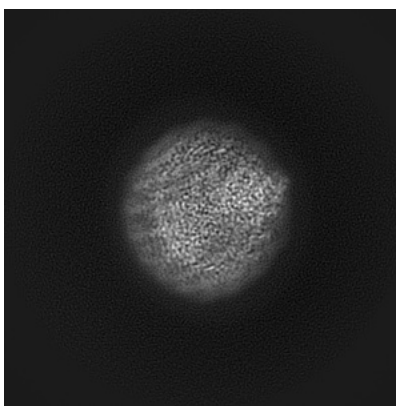
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

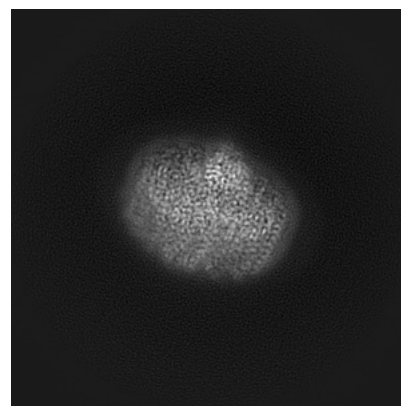
6.1.1 Primary map



X

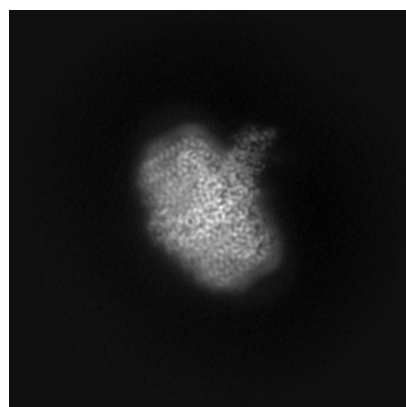


Y

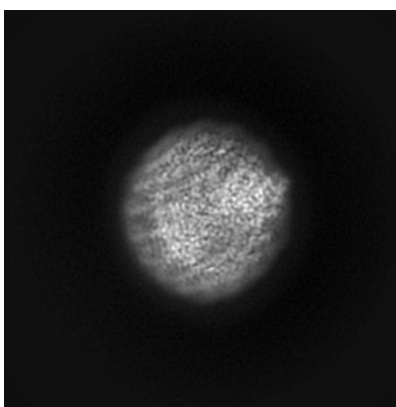


Z

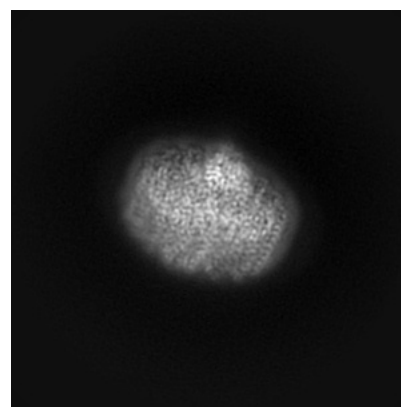
6.1.2 Raw map



X



Y

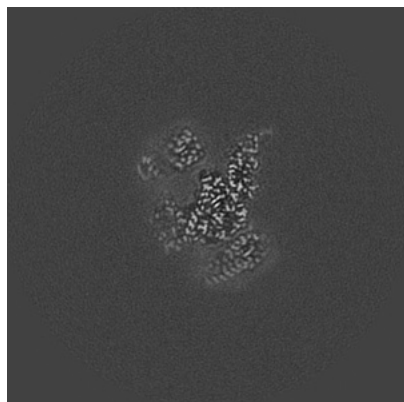


Z

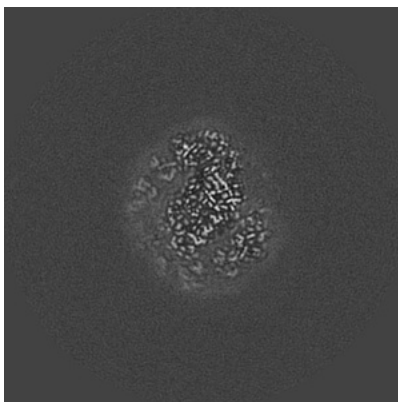
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

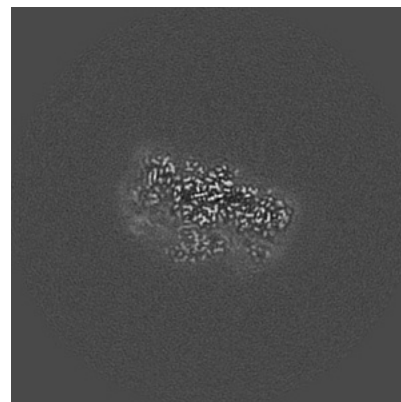
6.2.1 Primary map



X Index: 180

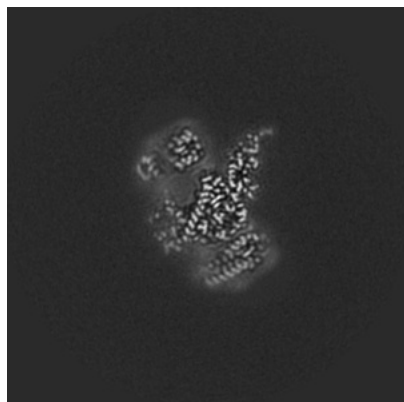


Y Index: 180

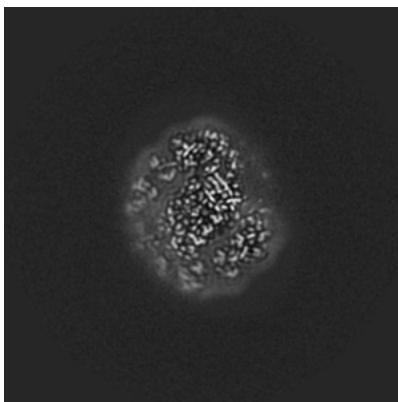


Z Index: 180

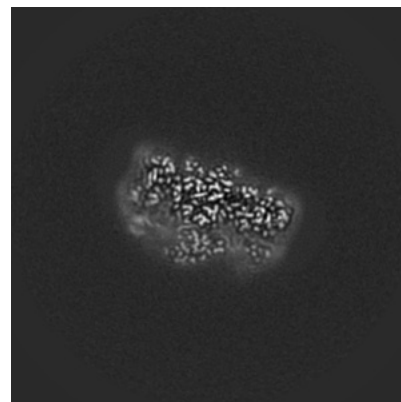
6.2.2 Raw map



X Index: 180



Y Index: 180

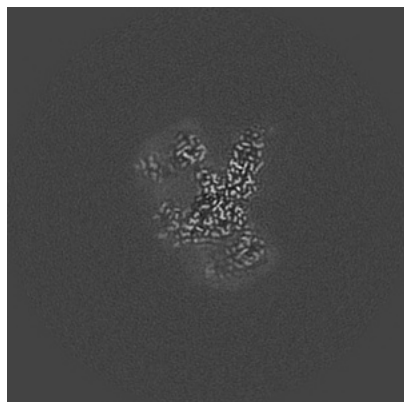


Z Index: 180

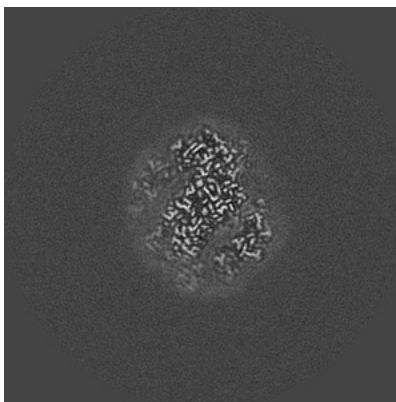
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

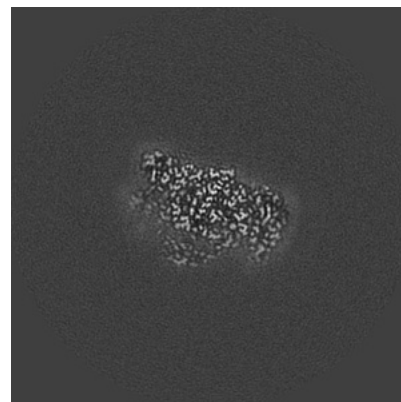
6.3.1 Primary map



X Index: 184

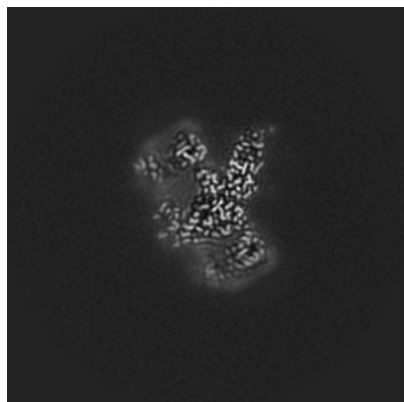


Y Index: 178

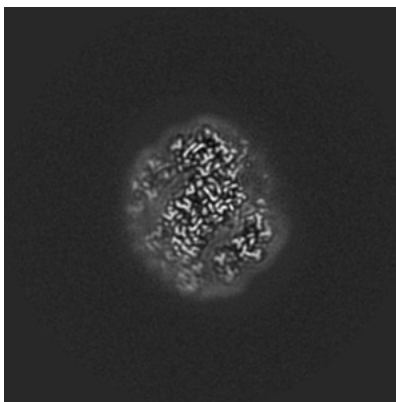


Z Index: 173

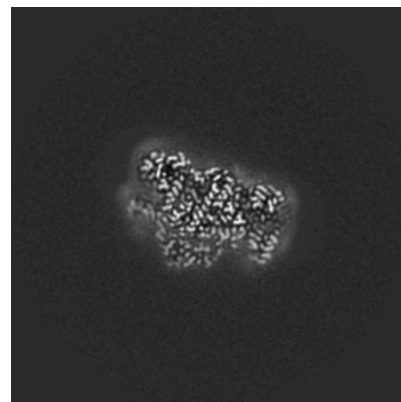
6.3.2 Raw map



X Index: 184



Y Index: 178

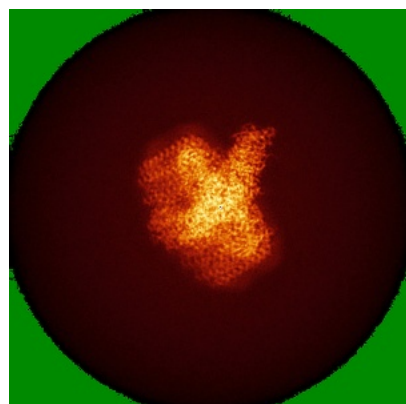


Z Index: 169

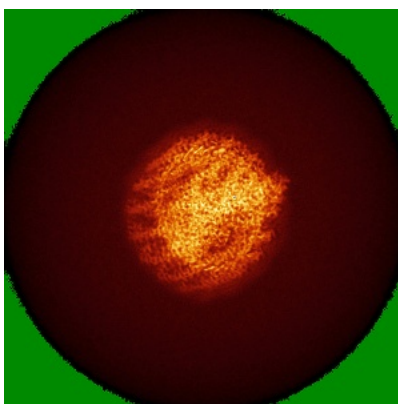
The images above show the largest variance slices of the map in three orthogonal directions.

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

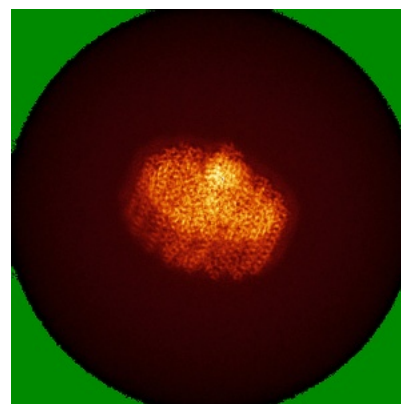
6.4.1 Primary map



X

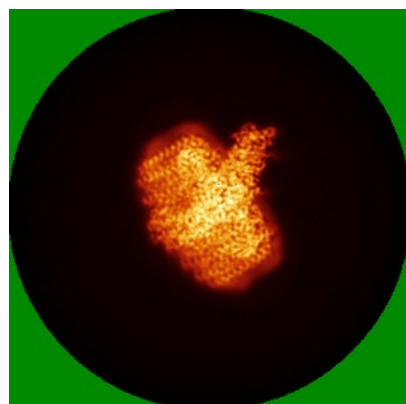


Y

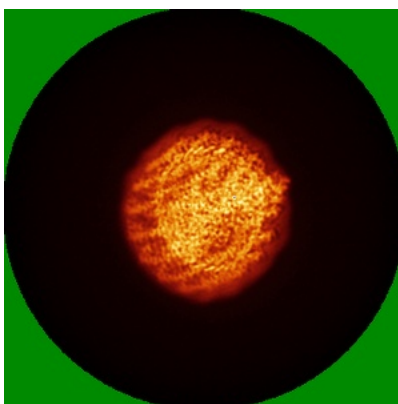


Z

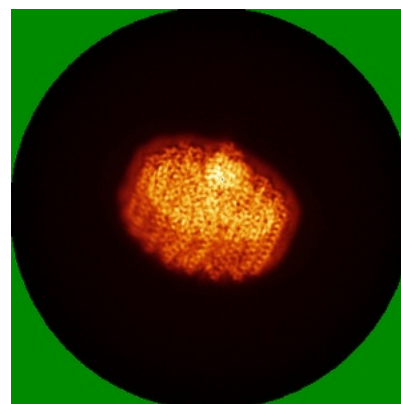
6.4.2 Raw map



X



Y

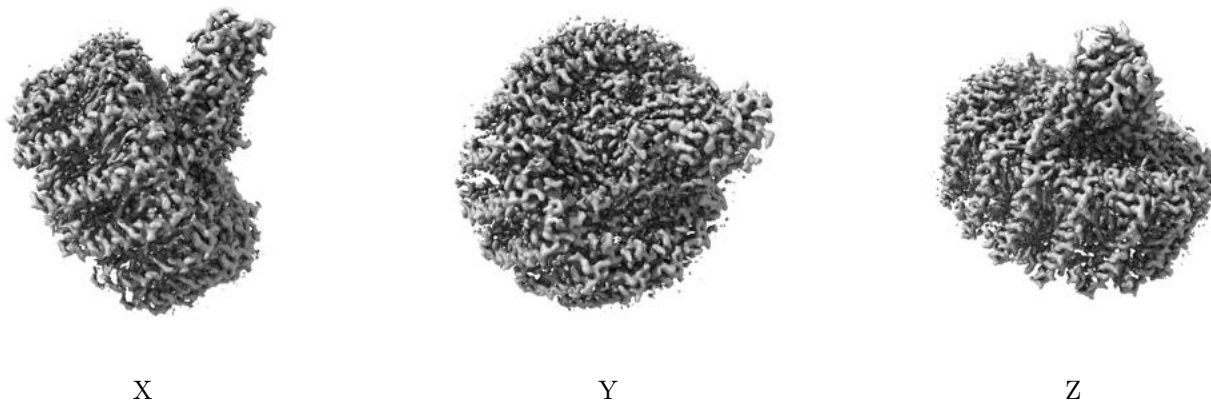


Z

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.

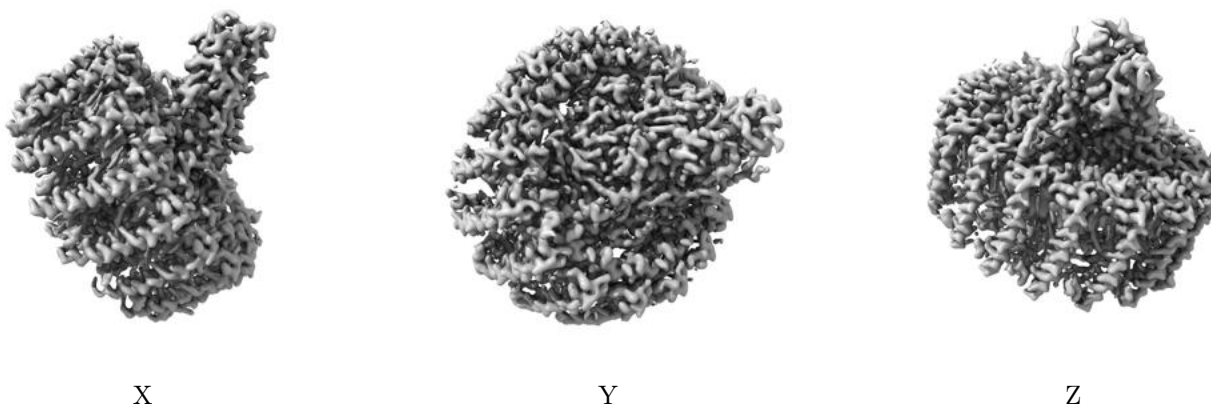
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

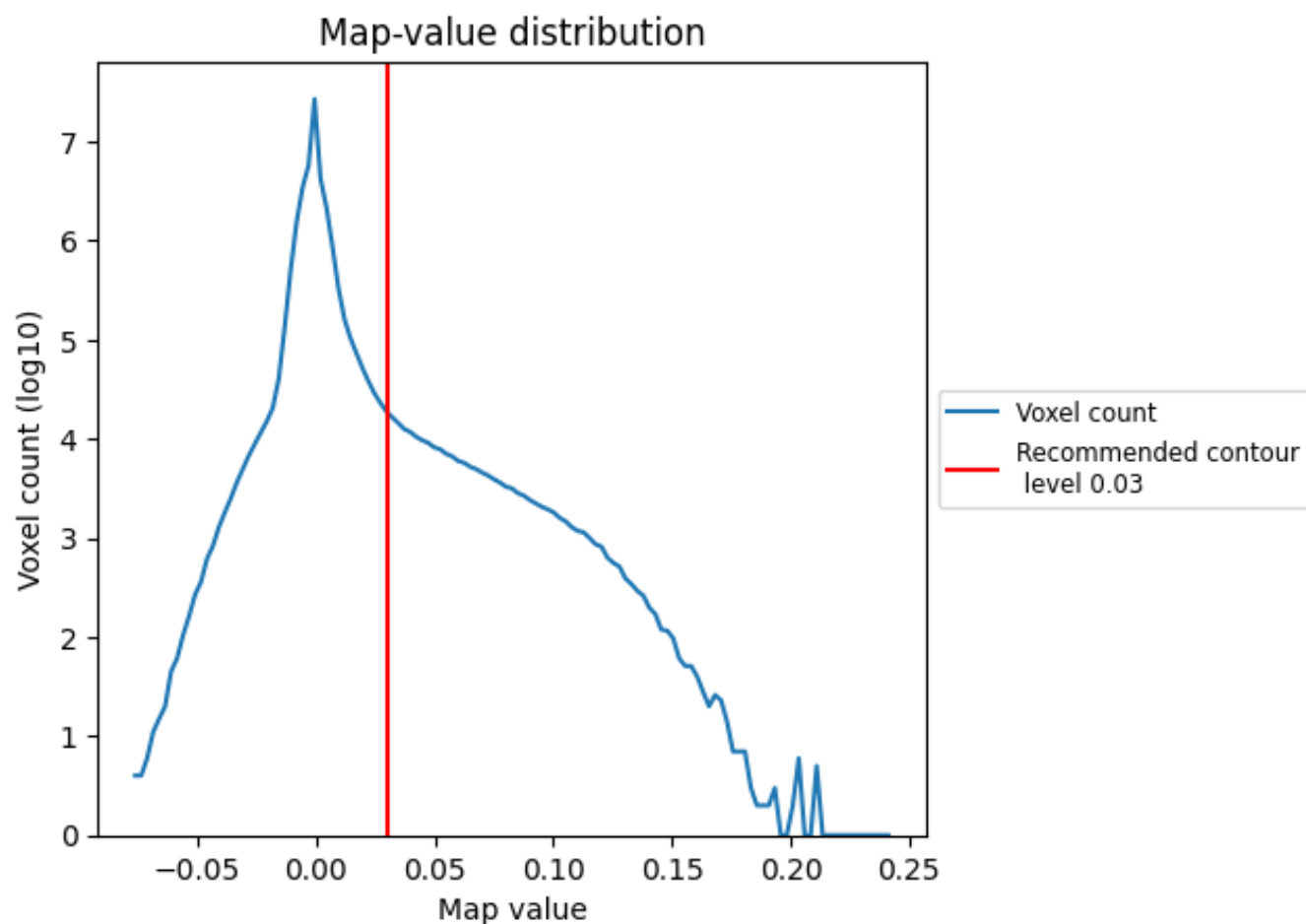
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

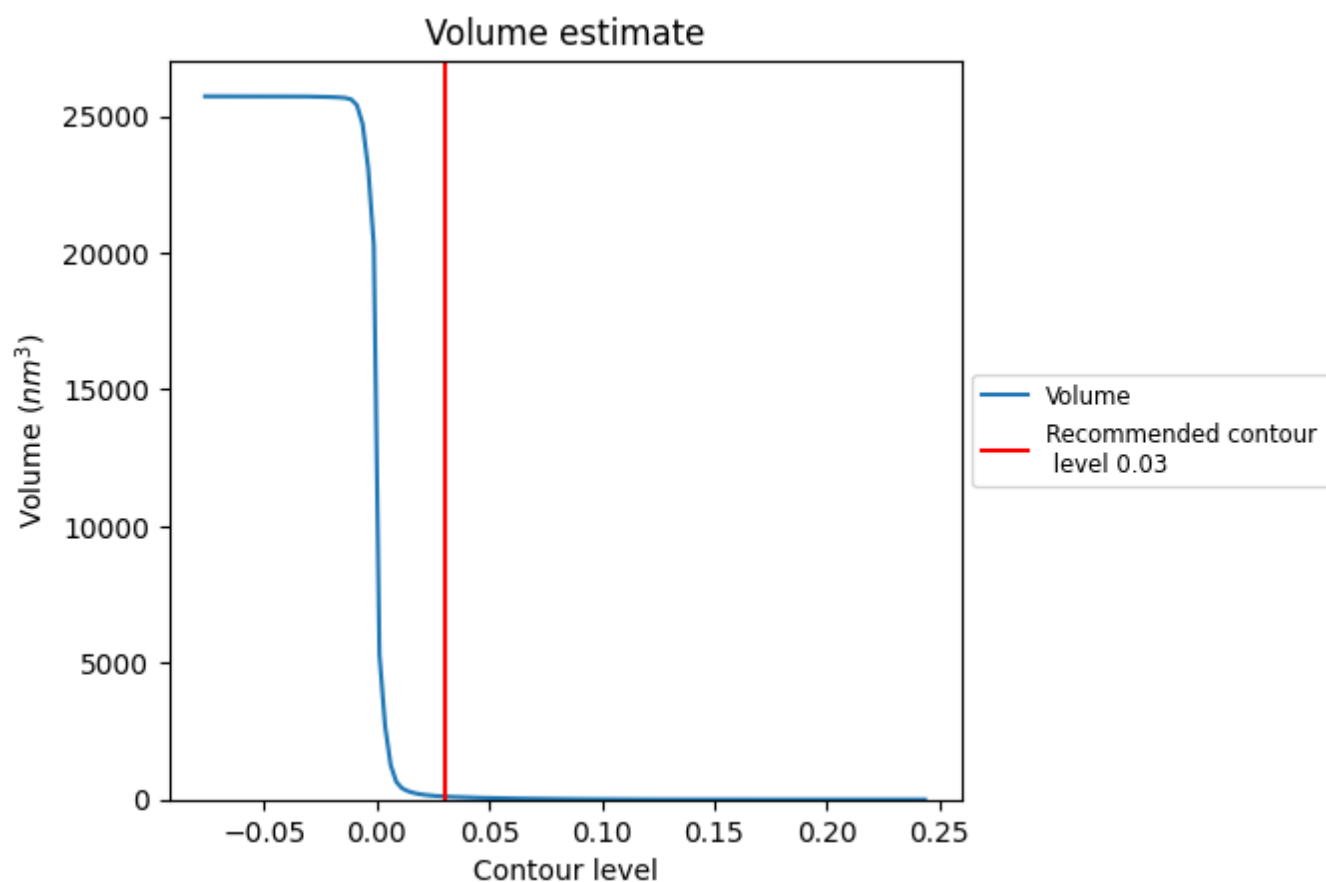
This section contains the results of statistical analysis of the map.

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.

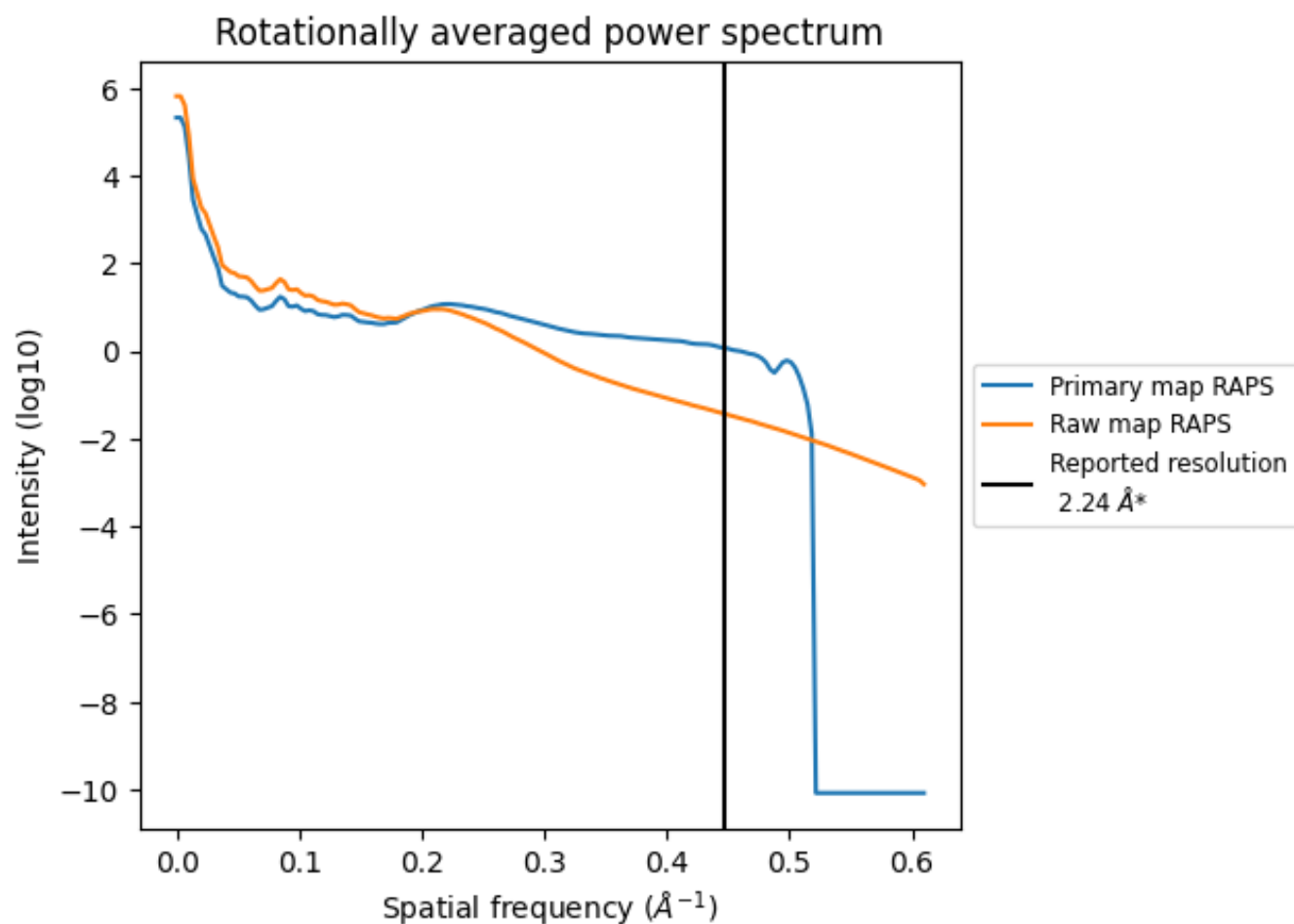
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm^3 ; this corresponds to an approximate mass of 102 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 ⓘ

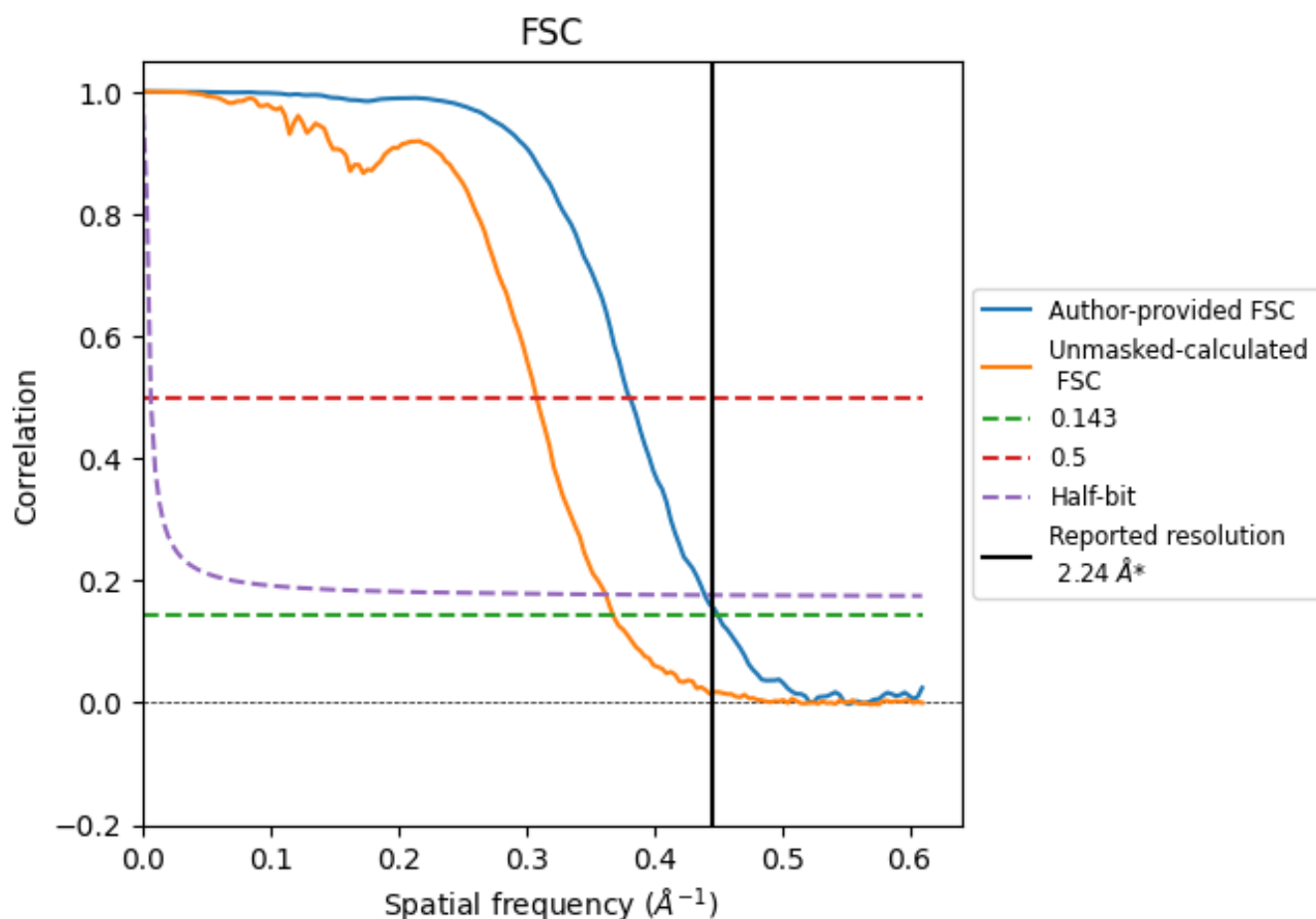


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

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 0.446 Å⁻¹

8.2 Resolution estimates [i](#)

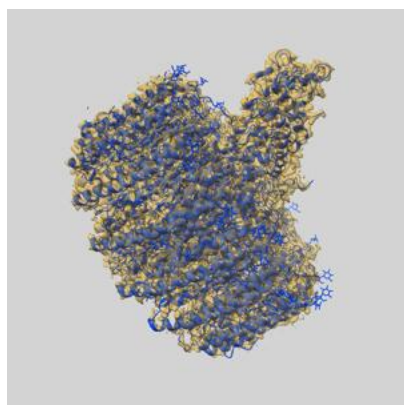
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.22	2.63	2.27
Unmasked-calculated*	2.72	3.24	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.24 by more than 10 %

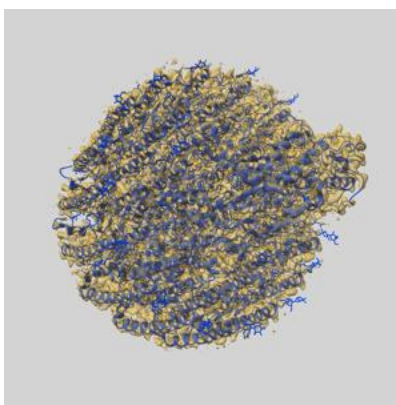
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37466 and PDB model 8WDV. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

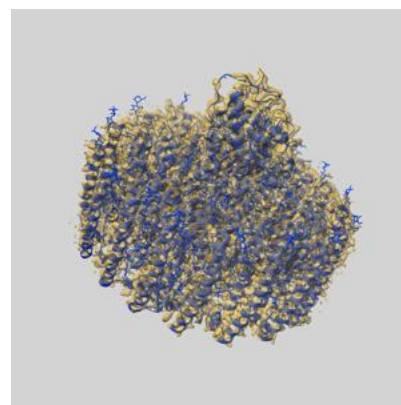
9.1 Map-model overlay [i](#)



X



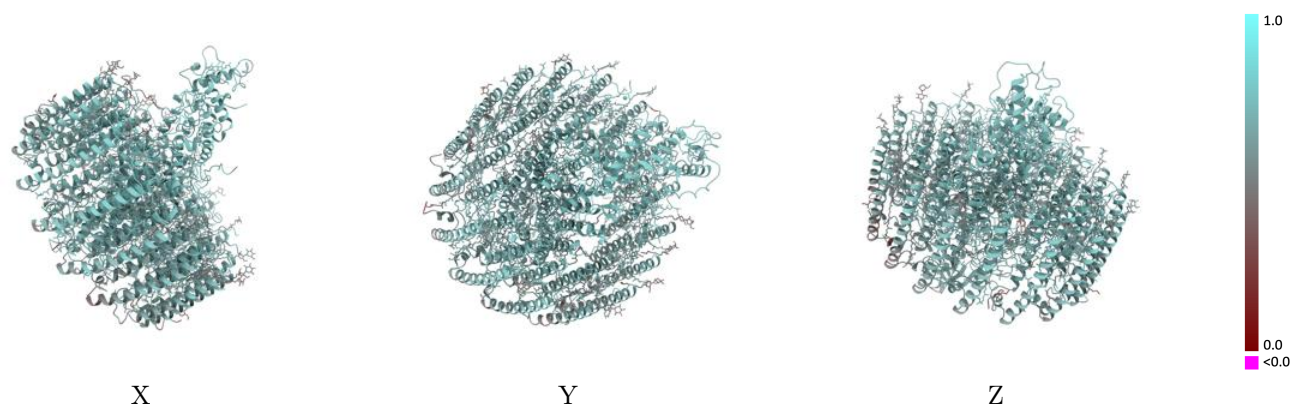
Y



Z

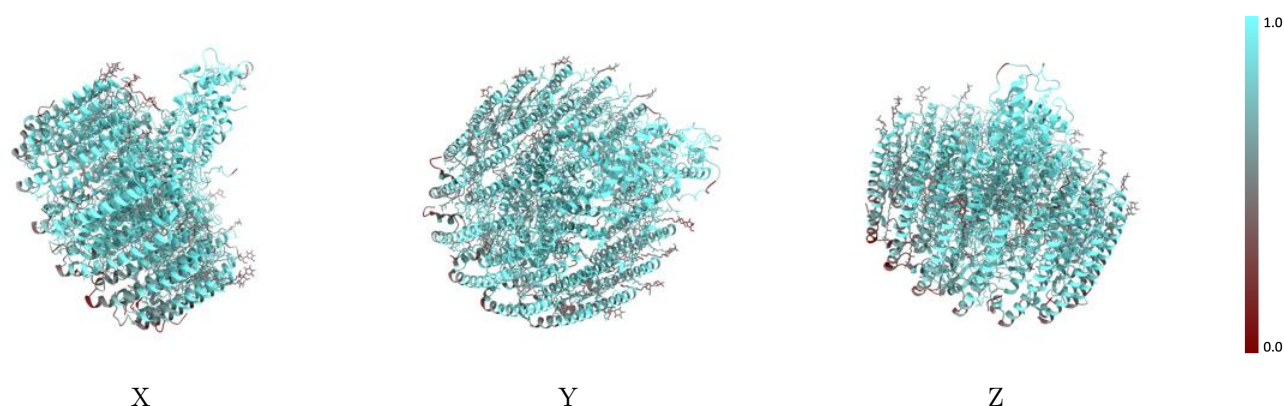
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



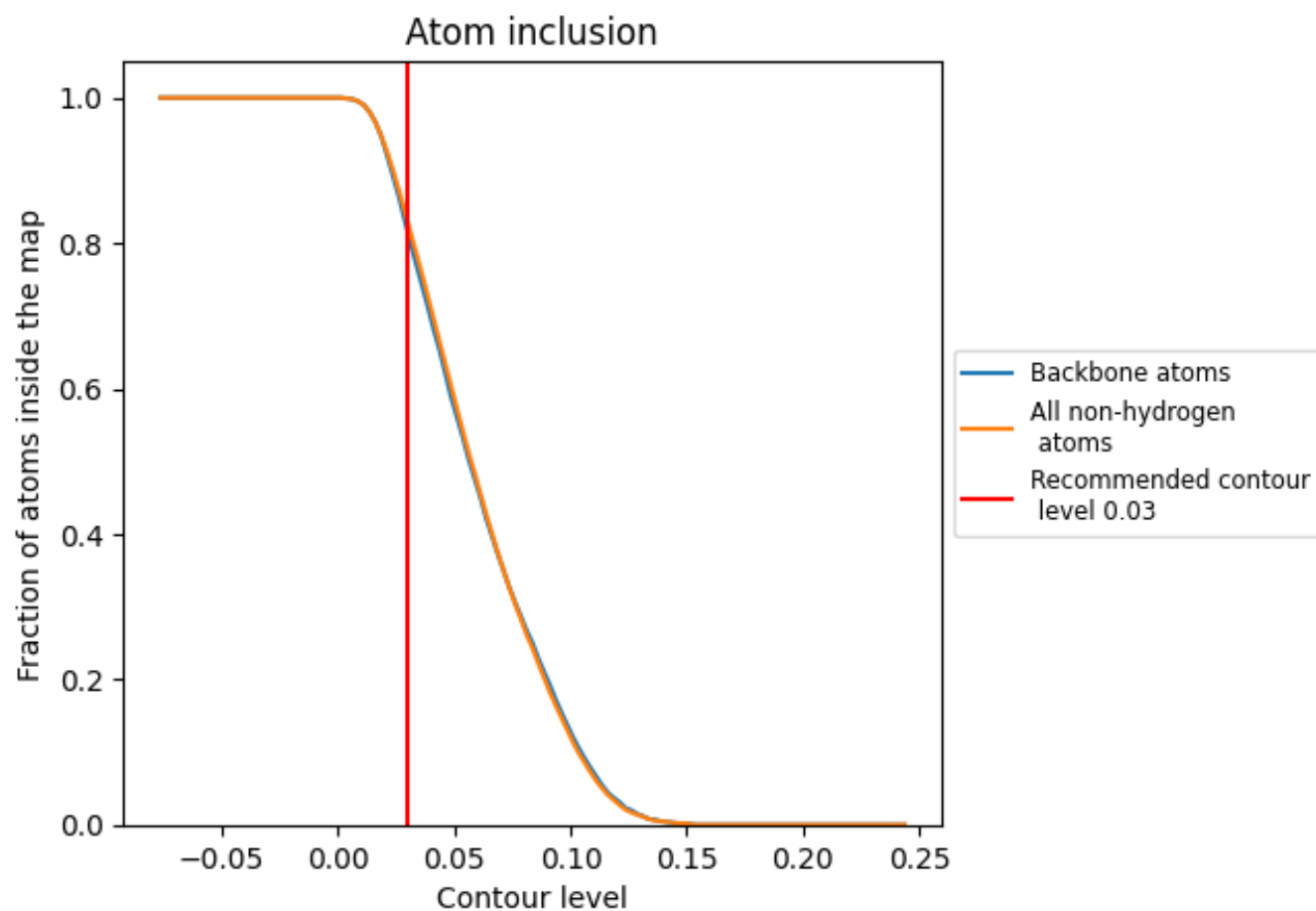
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.6580
0	 0.7650	 0.6280
1	 0.8150	 0.6430
2	 0.6960	 0.6040
3	 0.8110	 0.6480
4	 0.6440	 0.5770
5	 0.7650	 0.6040
6	 0.6760	 0.5750
7	 0.7660	 0.6160
8	 0.7020	 0.5930
9	 0.8460	 0.6580
A	 0.8940	 0.6750
B	 0.7940	 0.6350
C	 0.9510	 0.7090
D	 0.7750	 0.6370
E	 0.7850	 0.6330
F	 0.7180	 0.6200
G	 0.6630	 0.5930
H	 0.7680	 0.6550
I	 0.8100	 0.6400
J	 0.7160	 0.6030
K	 0.7400	 0.6140
L	 0.9290	 0.7070
M	 0.9120	 0.7000
N	 0.7460	 0.6180
O	 0.8540	 0.6600
P	 0.7610	 0.6250
Q	 0.9020	 0.6800
R	 0.8250	 0.6570
S	 0.8850	 0.6740
T	 0.8640	 0.6690
U	 0.8740	 0.6720
V	 0.8140	 0.6490
W	 0.8130	 0.6500
X	 0.7960	 0.6420



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Chain	Atom inclusion	Q-score
Y	 0.7380	 0.6250
Z	 0.7910	 0.6290