



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:29 AM JST

PDB ID : 7C9R / pdb_00007c9r
EMDB ID : EMD-30314
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF THIORHODOVIBRIO STRAIN 970
Authors : Tani, K.; Kanno, R.; Makino, Y.; Hall, M.; Takenouchi, M.; Imanishi, M.; Yu, L.-J.; Overmann, J.; Madigan, M.T.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2020-06-07
Resolution : 2.82 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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)

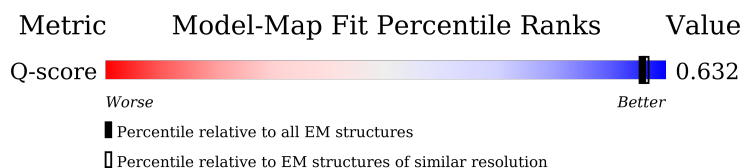
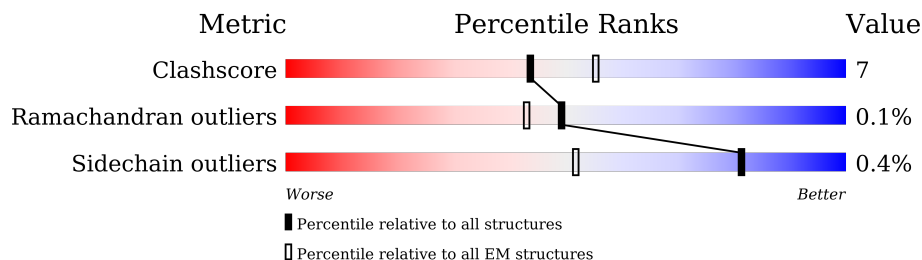
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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	11795 (2.32 - 3.32)

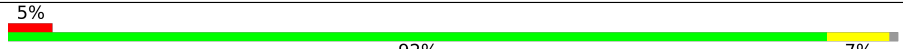
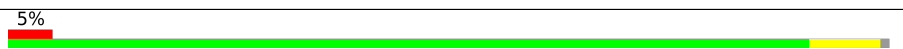
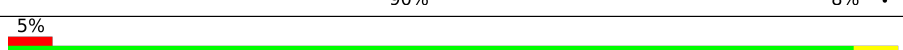
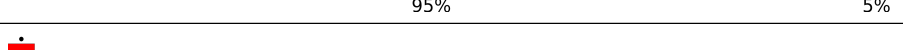
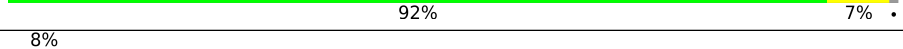
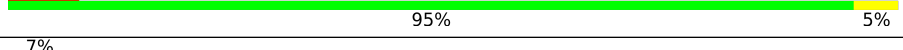
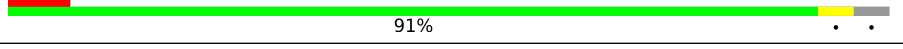
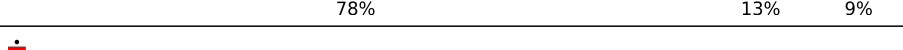
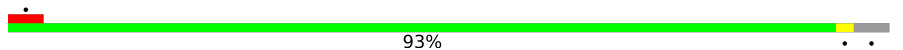
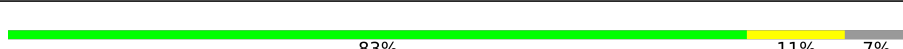
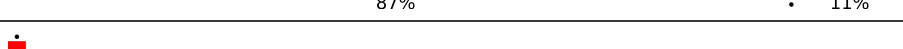
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	396	66% 12% 21%
2	L	273	85% 14%
3	M	324	90% 8%

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Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
4	H	258	
5	A	73	
5	D	73	
5	F	73	
5	I	73	
5	K	73	
5	O	73	
6	4	46	
6	B	46	
6	P	46	
7	0	46	
7	2	46	
7	6	46	
7	8	46	
7	E	46	
7	G	46	
7	J	46	
7	N	46	
7	R	46	
7	T	46	
7	V	46	
7	X	46	
7	Z	46	
8	Q	81	
9	1	77	

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Mol	Chain	Length	Quality of chain
9	3	77	6% 87% 5% • 5%
9	5	77	8% 91% 5% •
9	7	77	5% 87% 8% 5%
9	S	77	10% 81% 13% 6%
9	U	77	6% 90% • 6%
9	W	77	• 88% 5% • 5%
9	Y	77	5% 88% 6% 5%
10	9	86	5% 88% 9% •

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 29228 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
			2433	1536	423	458	16		

- Molecule 2 is a protein called L subunit of the reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	272	Total	C	N	O	S	0	0
			2161	1459	350	344	8		

- 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
			2535	1700	408	416	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	257	Total	C	N	O	S	0	0
			2017	1298	348	366	5		

- Molecule 5 is a protein called Alpha subunit 1 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	70	Total	C	N	O	S	0	0
			563	373	89	96	5		
5	D	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	F	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	I	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	O	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	43	Total	C	N	O	S	0	0
			352	236	55	58	3		
6	P	42	Total	C	N	O	S	0	0
			343	230	53	57	3		
6	4	44	Total	C	N	O	S	0	0
			361	241	56	61	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	G	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	J	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	N	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	R	44	Total	C	N	O	S	0	0
			361	241	56	62	2		
7	T	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	V	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	X	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	Z	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	2	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	6	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	8	42	Total	C	N	O	S	0	0
			343	230	53	58	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	41	Total	C	N	O	S	0	0
			337	227	52	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	78	Total	C	N	O	S	0	0
			628	416	101	107	4		

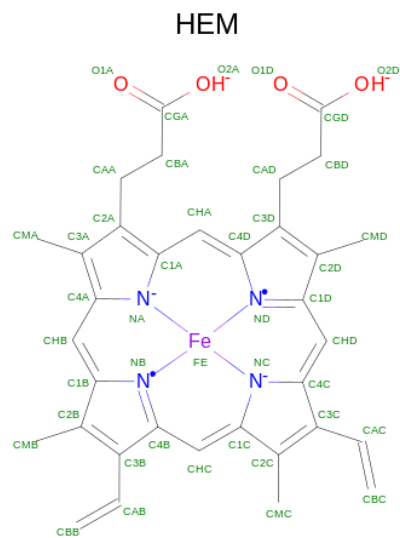
- Molecule 9 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	72	Total	C	N	O	S	0	0
			579	382	92	99	6		
9	U	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	W	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	Y	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	1	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	3	73	Total	C	N	O	S	0	0
			584	386	93	100	5		
9	5	74	Total	C	N	O	S	0	0
			589	389	94	101	5		
9	7	73	Total	C	N	O	S	0	0
			584	386	93	100	5		

- Molecule 10 is a protein called Alpha subunit 2 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	84	Total	C	N	O	S	0	0
			668	440	113	111	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

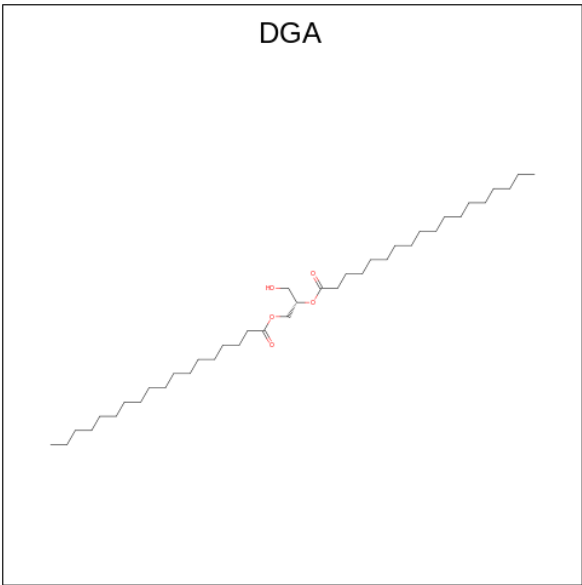
Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total 1	Ca 1	0
13	A	1	Total 1	Ca 1	0
13	D	1	Total 1	Ca 1	0
13	F	1	Total 1	Ca 1	0

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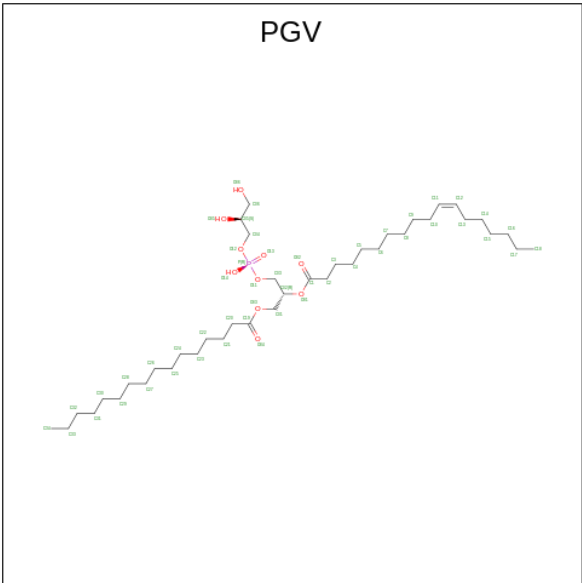
Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total 1	Ca 1	0
13	K	1	Total 1	Ca 1	0
13	O	1	Total 1	Ca 1	0
13	Q	1	Total 1	Ca 1	0
13	S	1	Total 1	Ca 1	0
13	U	1	Total 1	Ca 1	0
13	W	1	Total 1	Ca 1	0
13	Y	1	Total 1	Ca 1	0
13	1	1	Total 1	Ca 1	0
13	3	1	Total 1	Ca 1	0
13	5	1	Total 1	Ca 1	0
13	7	1	Total 1	Ca 1	0
13	9	1	Total 1	Ca 1	0

- Molecule 14 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			AltConf
14	C	1	Total	C	O	0
			32	28	4	

- 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).



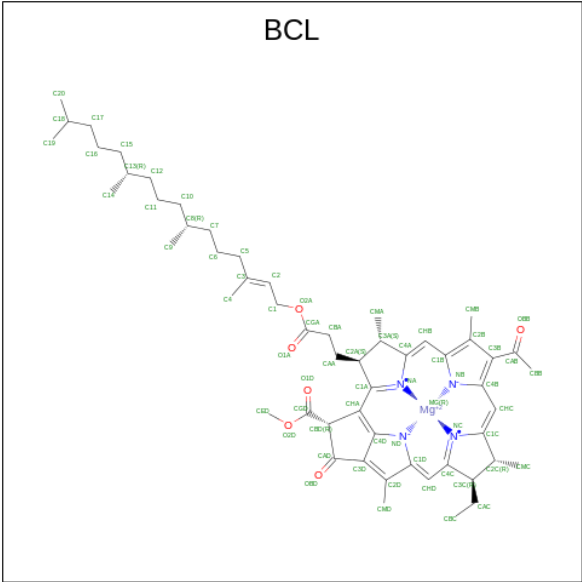
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			16	9	6	1	
15	L	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			39	28	10	1	
15	H	1	Total	C	O	P	0
			36	25	10	1	
15	A	1	Total	C	O	P	0
			23	12	10	1	
15	D	1	Total	C	O	P	0
			43	32	10	1	
15	F	1	Total	C	O	P	0
			34	25	8	1	
15	F	1	Total	C	O	P	0
			37	26	10	1	
15	I	1	Total	C	O	P	0
			41	32	8	1	
15	K	1	Total	C	O	P	0
			36	25	10	1	
15	K	1	Total	C	O	P	0
			19	10	8	1	
15	K	1	Total	C	O	P	0
			43	34	8	1	
15	O	1	Total	C	O	P	0
			44	33	10	1	
15	Q	1	Total	C	O	P	0
			38	27	10	1	
15	Y	1	Total	C	O	P	0
			27	18	8	1	
15	1	1	Total	C	O	P	0
			26	17	8	1	
15	3	1	Total	C	O	P	0
			47	36	10	1	
15	5	1	Total	C	O	P	0
			47	36	10	1	
15	9	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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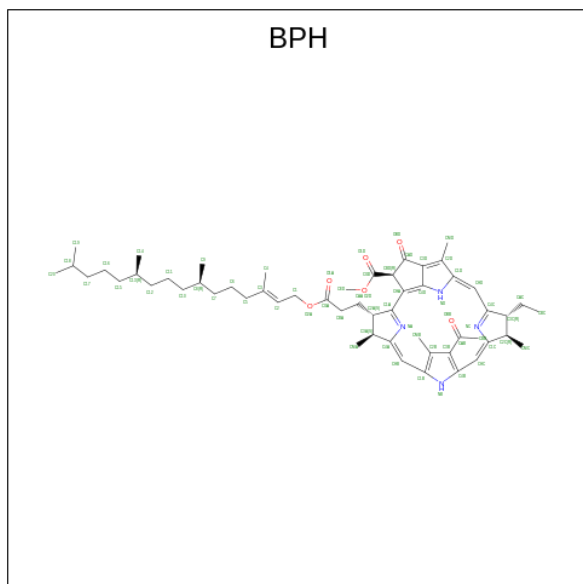
Mol	Chain	Residues	Atoms					AltConf
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total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

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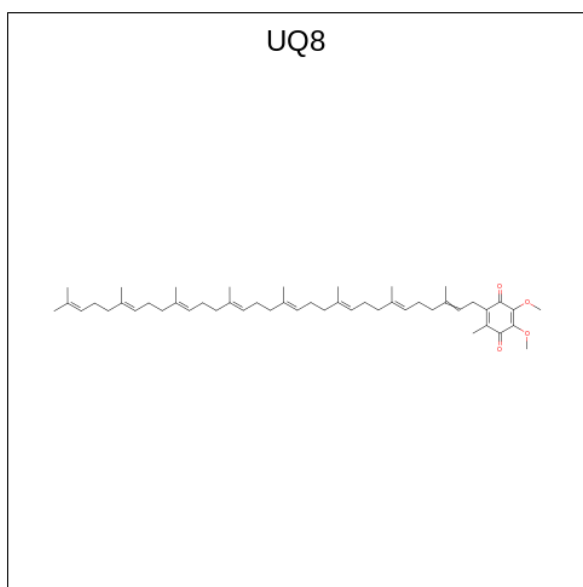
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	9	1	66	55	1	4	6	0

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



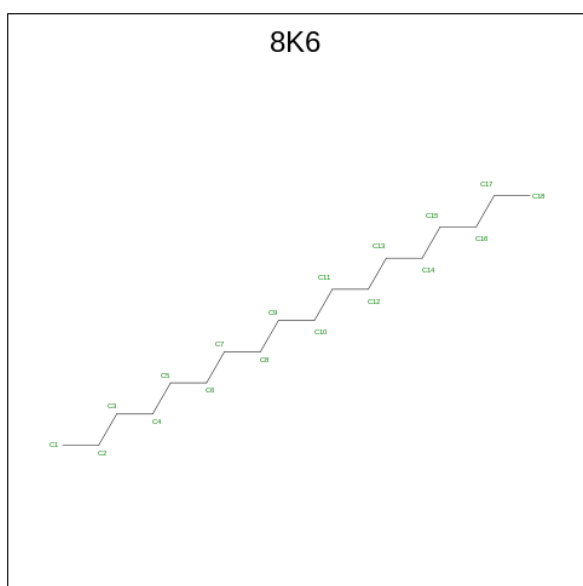
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	L	1	65	55	4	6	0
17	M	1	65	55	4	6	0

- 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
			33	29	4	

- Molecule 19 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).

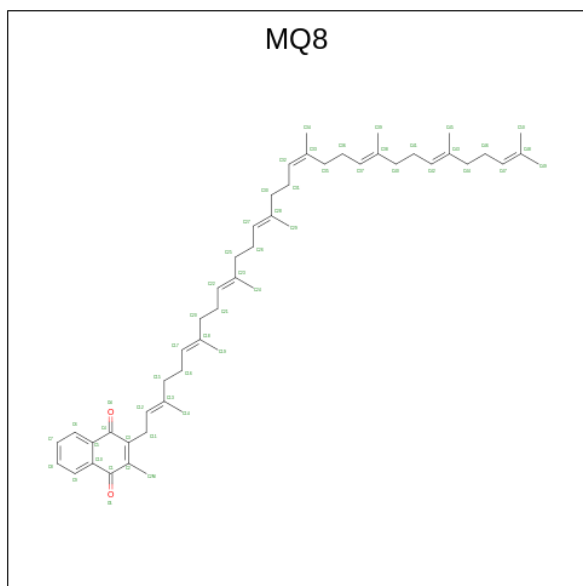


Mol	Chain	Residues	Atoms		AltConf
19	L	1	Total	C	0
			18	18	
19	5	1	Total	C	0
			15	15	

- Molecule 20 is FE (III) ION (CCD ID: FE) (formula: Fe).

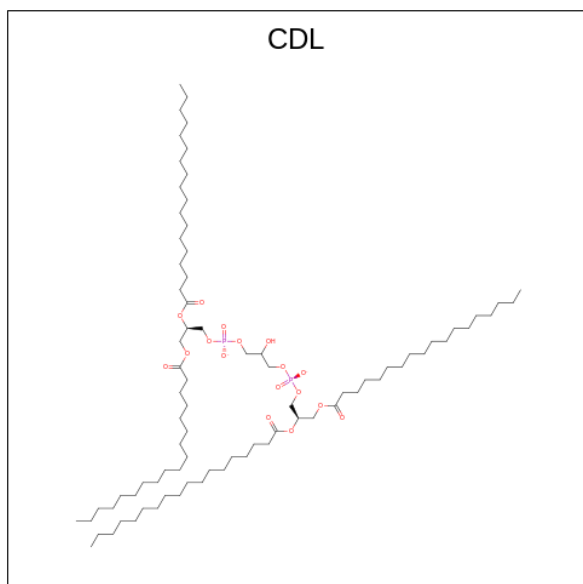
Mol	Chain	Residues	Atoms		AltConf
20	M	1	Total	Fe	0
			1	1	

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



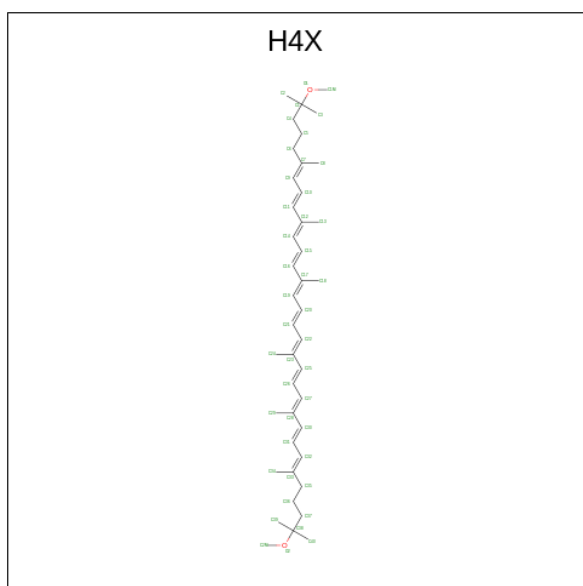
Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			53	51	2	

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



Mol	Chain	Residues	Atoms				AltConf
22	H	1	Total	C	O	P	0
			73	54	17	2	
22	S	1	Total	C	O	P	0
			74	55	17	2	
22	Y	1	Total	C	O	P	0
			30	14	14	2	

- Molecule 23 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26-undecaene (CCD ID: H4X) (formula: C₄₂H₆₄O₂).



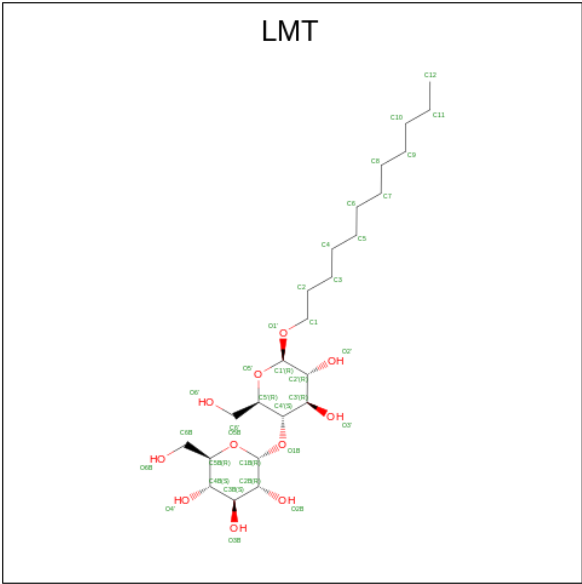
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			44	42	2	
23	E	1	Total	C	O	0
			44	42	2	
23	G	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	P	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
23	Q	1	Total	C	O	0
			44	42	2	
23	U	1	Total	C	O	0
			44	42	2	
23	V	1	Total	C	O	0
			44	42	2	
23	Z	1	Total	C	O	0
			44	42	2	
23	2	1	Total	C	O	0
			44	42	2	
23	4	1	Total	C	O	0
			44	42	2	
23	5	1	Total	C	O	0
			44	42	2	
23	6	1	Total	C	O	0
			44	42	2	
23	7	1	Total	C	O	0
			44	42	2	

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



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

Continued on next page...

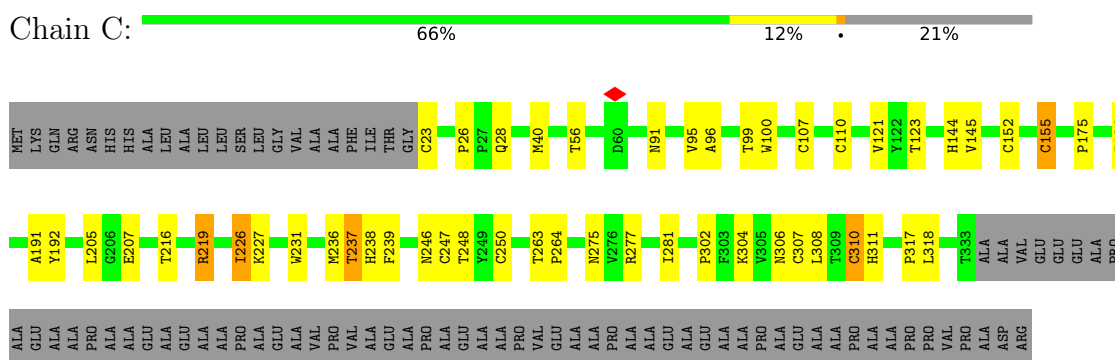
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
24	E	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	N	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	T	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	4	1	Total	C	O	0
			35	24	11	
24	6	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	0	1	Total	C	O	0
			35	24	11	

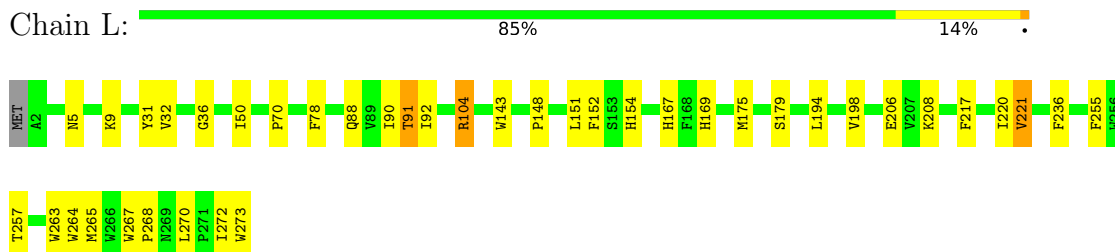
3 Residue-property plots

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.

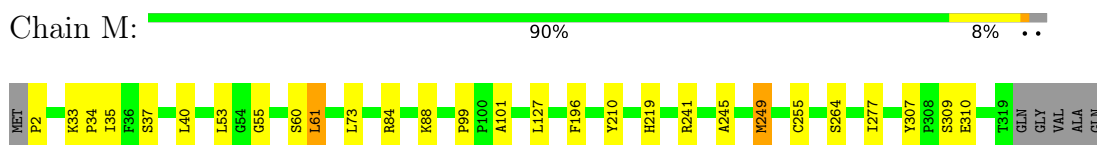
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



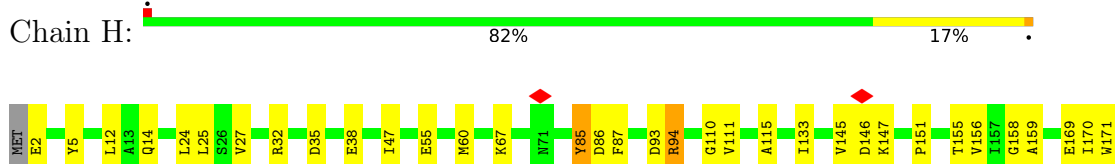
- Molecule 2: L subunit of the reaction center



- Molecule 3: Reaction center protein M chain

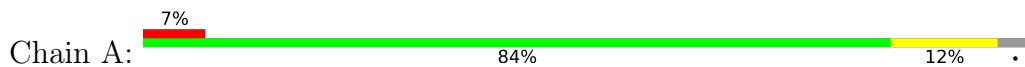


- Molecule 4: Photosynthetic reaction center, subunit H, bacterial





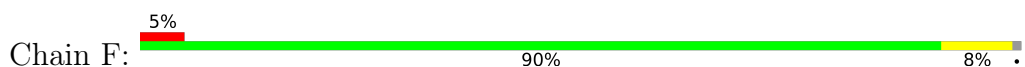
- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



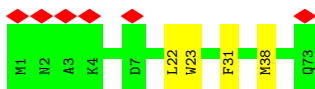
- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



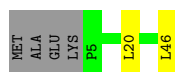
- Molecule 6: Antenna complex alpha/beta subunit

Chain B:  80% 13% 7%

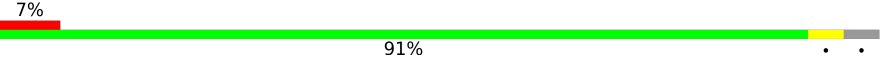


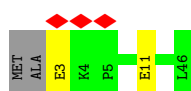
- Molecule 6: Antenna complex alpha/beta subunit

Chain P:  87% 9%



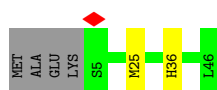
- Molecule 6: Antenna complex alpha/beta subunit

Chain 4:  7% 91%



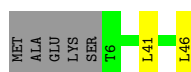
- Molecule 7: Antenna complex alpha/beta subunit

Chain E:  87% 9%



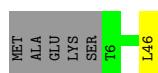
- Molecule 7: Antenna complex alpha/beta subunit

Chain G:  85% 11%



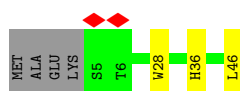
- Molecule 7: Antenna complex alpha/beta subunit

Chain J:  87% 11%

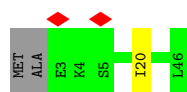


- Molecule 7: Antenna complex alpha/beta subunit

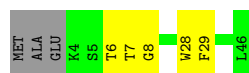
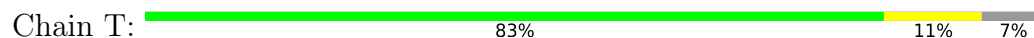
Chain N:  85% 7% 9%



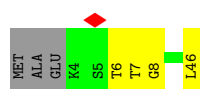
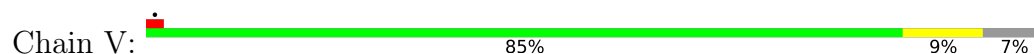
- Molecule 7: Antenna complex alpha/beta subunit



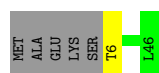
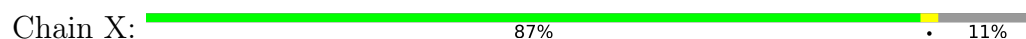
- Molecule 7: Antenna complex alpha/beta subunit



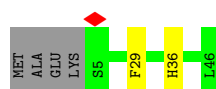
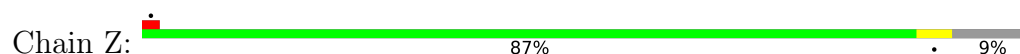
- Molecule 7: Antenna complex alpha/beta subunit



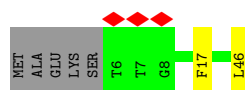
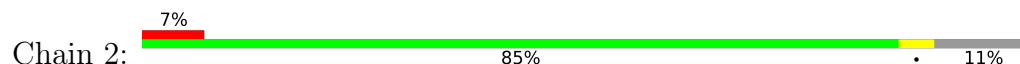
- Molecule 7: Antenna complex alpha/beta subunit



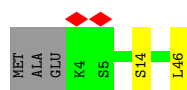
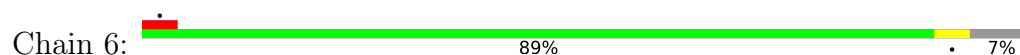
- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



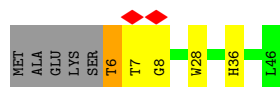
- Molecule 7: Antenna complex alpha/beta subunit

Chain 8:  78% 13% 9%



- Molecule 7: Antenna complex alpha/beta subunit

Chain 0:  78% 9% 11%



- Molecule 8: Antenna complex alpha/beta subunit

Chain Q:  6% 85% 11%

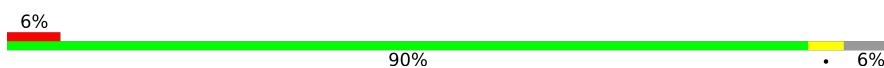


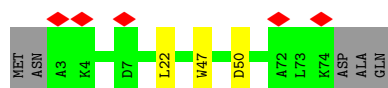
- Molecule 9: LHC domain-containing protein

Chain S:  10% 81% 13% 6%

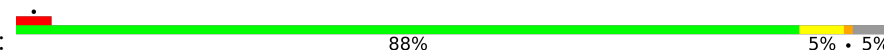


- Molecule 9: LHC domain-containing protein

Chain U:  6% 90% 6%

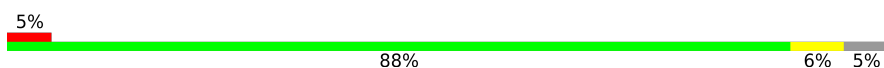


- Molecule 9: LHC domain-containing protein

Chain W:  88% 5% 5%

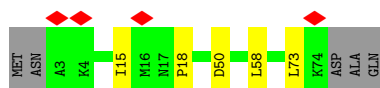
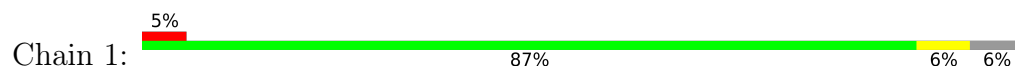


- Molecule 9: LHC domain-containing protein

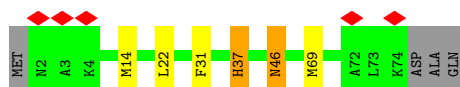
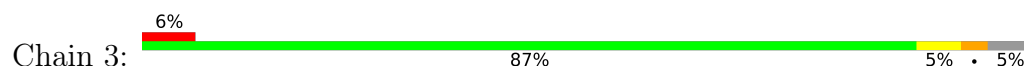
Chain Y:  5% 88% 6% 5%



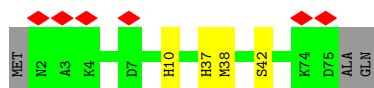
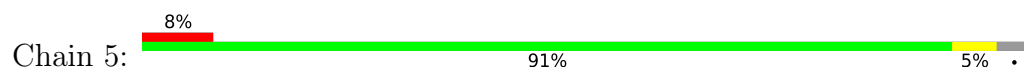
- Molecule 9: LHC domain-containing protein



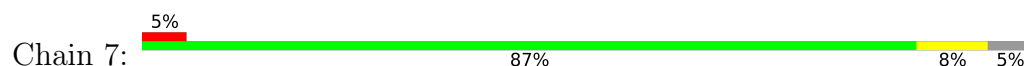
- Molecule 9: LHC domain-containing protein



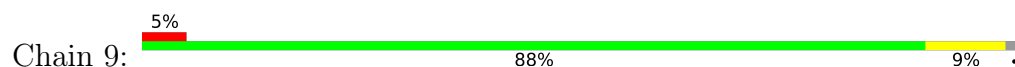
- Molecule 9: LHC domain-containing protein



- Molecule 9: LHC domain-containing protein



- Molecule 10: Alpha subunit 2 of light-harvesting 1 complex



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105234	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.263	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.037	Depositor
Map size ($\text{\AA}$)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, BPH, BCL, H4X, CDL, 8K6, MG, LMT, FE, UQ8, DGA, MQ8, CA, HEM

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	0.89	6/2503 (0.2%)	1.09	11/3423 (0.3%)
2	L	0.87	5/2244 (0.2%)	1.05	6/3068 (0.2%)
3	M	0.78	2/2633 (0.1%)	1.03	3/3599 (0.1%)
4	H	0.63	0/2069	1.01	2/2811 (0.1%)
5	A	0.91	1/579 (0.2%)	0.98	0/787
5	D	0.81	1/596 (0.2%)	0.97	0/810
5	F	0.80	0/596	0.92	0/810
5	I	0.75	1/604 (0.2%)	0.90	0/820
5	K	0.76	0/596	0.91	1/810 (0.1%)
5	O	0.80	0/604	0.93	0/820
6	4	0.69	0/374	0.73	0/506
6	B	1.02	3/365 (0.8%)	0.83	0/494
6	P	0.74	0/356	0.71	0/482
7	0	0.79	1/349 (0.3%)	0.91	0/474
7	2	0.64	0/349	0.69	0/474
7	6	0.76	0/364	0.78	0/493
7	8	0.78	0/355	0.79	0/482
7	E	0.81	1/355 (0.3%)	0.75	0/482
7	G	0.76	0/349	0.72	0/474
7	J	0.73	0/349	0.71	0/474
7	N	0.77	1/355 (0.3%)	0.72	0/482
7	R	0.72	0/373	0.81	0/505
7	T	0.69	0/364	0.72	0/493
7	V	0.72	0/364	0.76	0/493
7	X	0.67	0/349	0.75	1/474 (0.2%)
7	Z	0.69	1/355 (0.3%)	0.71	0/482
8	Q	0.67	0/649	0.93	0/881
9	1	0.78	0/592	0.88	0/805
9	3	0.78	1/600 (0.2%)	0.93	1/816 (0.1%)
9	5	0.79	0/605	0.85	0/823
9	7	0.88	1/600 (0.2%)	1.07	2/816 (0.2%)
9	S	0.82	0/595	1.00	1/808 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	U	0.82	0/592	0.89	0/805
9	W	0.73	0/600	0.86	0/816
9	Y	0.75	1/600 (0.2%)	0.86	0/816
10	9	0.70	0/690	1.14	0/941
All	All	0.78	26/24872 (0.1%)	0.95	28/33849 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
5	A	0	1
5	K	0	1
7	0	0	1
9	1	0	1
All	All	0	5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	ARG	CZ-NH1	18.83	1.59	1.32
1	C	219	ARG	NE-CZ	14.01	1.48	1.33
6	B	42	TYR	CZ-OH	11.38	1.61	1.38
2	L	167	HIS	CE1-NE2	8.83	1.41	1.32
2	L	154	HIS	CE1-NE2	8.28	1.40	1.32

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	C	219	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	C	155	CYS	CB-CA-C	-6.85	98.14	109.65
5	K	46	ASN	OD1-CG-ND2	-6.70	115.91	122.60
1	C	219	ARG	CB-CA-C	6.48	119.56	109.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	0	6	THR	Peptide
9	1	15	ILE	Mainchain
5	A	68	GLU	Mainchain
1	C	219	ARG	Sidechain
5	K	42	SER	Mainchain

5.2 Too-close contacts

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	2433	0	2339	57	0
2	L	2161	0	2138	33	0
3	M	2535	0	2502	24	0
4	H	2017	0	2015	39	0
5	A	563	0	565	8	0
5	D	580	0	579	2	0
5	F	580	0	579	4	0
5	I	588	0	591	4	0
5	K	580	0	579	8	0
5	O	588	0	591	6	0
6	4	361	0	354	3	0
6	B	352	0	348	3	0
6	P	343	0	336	1	0
7	0	337	0	332	9	0
7	2	337	0	332	2	0
7	6	352	0	350	2	0
7	8	343	0	337	5	0
7	E	343	0	337	1	0
7	G	337	0	332	2	0
7	J	337	0	332	1	0
7	N	343	0	337	2	0
7	R	361	0	356	2	0
7	T	352	0	350	4	0
7	V	352	0	350	3	0
7	X	337	0	332	0	0
7	Z	343	0	337	1	0
8	Q	628	0	617	8	0
9	1	576	0	578	5	0
9	3	584	0	584	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	5	589	0	586	4	0
9	7	584	0	584	2	0
9	S	579	0	583	10	0
9	U	576	0	578	3	0
9	W	584	0	582	5	0
9	Y	584	0	582	5	0
10	9	668	0	673	7	0
11	C	172	0	120	29	0
12	C	1	0	0	0	0
13	1	1	0	0	0	0
13	3	1	0	0	0	0
13	5	1	0	0	0	0
13	7	1	0	0	0	0
13	9	1	0	0	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	I	1	0	0	0	0
13	K	1	0	0	0	0
13	O	1	0	0	0	0
13	Q	1	0	0	0	0
13	S	1	0	0	0	0
13	U	1	0	0	0	0
13	W	1	0	0	0	0
13	Y	1	0	0	0	0
14	C	32	0	45	6	0
15	1	26	0	25	0	0
15	3	47	0	65	4	0
15	5	47	0	65	4	0
15	9	47	0	65	2	0
15	A	23	0	18	0	0
15	C	16	0	11	0	0
15	D	43	0	59	0	0
15	F	71	0	83	2	0
15	H	36	0	42	1	0
15	I	41	0	53	0	0
15	K	98	0	117	3	0
15	L	47	0	62	3	0
15	M	39	0	48	1	0
15	O	44	0	61	5	0
15	Q	38	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Y	27	0	27	6	0
16	1	66	0	74	4	0
16	2	66	0	74	2	0
16	3	132	0	148	11	0
16	5	132	0	148	8	0
16	7	127	0	135	7	0
16	9	132	0	148	7	0
16	A	66	0	74	7	0
16	B	66	0	74	2	0
16	D	132	0	148	5	0
16	F	132	0	148	5	0
16	I	66	0	74	4	0
16	J	66	0	73	4	0
16	K	132	0	147	10	0
16	L	132	0	148	9	0
16	M	132	0	148	8	0
16	O	132	0	147	5	0
16	Q	132	0	147	8	0
16	S	66	0	74	6	0
16	T	66	0	74	3	0
16	U	132	0	147	9	0
16	W	66	0	74	3	0
16	X	66	0	74	2	0
16	Y	132	0	148	3	0
17	L	65	0	76	7	0
17	M	65	0	76	7	0
18	L	66	0	78	7	0
19	5	15	0	29	0	0
19	L	18	0	38	1	0
20	M	1	0	0	0	0
21	M	53	0	72	2	0
22	H	73	0	90	3	0
22	S	74	0	95	1	0
22	Y	30	0	17	0	0
23	2	44	0	0	0	0
23	4	44	0	0	0	0
23	5	44	0	0	0	0
23	6	44	0	0	0	0
23	7	44	0	0	0	0
23	B	44	0	0	0	0
23	E	44	0	0	1	0
23	G	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	88	0	0	0	0
23	O	88	0	0	1	0
23	P	44	0	0	0	0
23	Q	44	0	0	0	0
23	U	44	0	0	0	0
23	V	44	0	0	0	0
23	Z	44	0	0	0	0
24	0	35	0	46	1	0
24	2	35	0	46	2	0
24	4	35	0	46	3	0
24	6	35	0	46	2	0
24	8	70	0	92	5	0
24	B	70	0	92	5	0
24	E	35	0	46	2	0
24	G	35	0	46	1	0
24	J	35	0	46	2	0
24	N	35	0	46	3	0
24	P	35	0	46	2	0
24	R	35	0	46	2	0
24	T	35	0	46	2	0
24	V	35	0	46	1	0
24	X	35	0	46	2	0
24	Z	35	0	46	1	0
All	All	29228	0	28934	379	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 7.

The worst 5 of 379 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:247:CYS:SG	11:C:403:HEM:HAB	1.52	1.47
1:C:247:CYS:SG	11:C:403:HEM:CAB	2.07	1.42
1:C:307:CYS:SG	11:C:404:HEM:HAB	1.66	1.36
1:C:155:CYS:SG	11:C:402:HEM:HAC	1.73	1.29
1:C:310:CYS:SG	11:C:404:HEM:CAC	2.28	1.21

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	309/396 (78%)	287 (93%)	22 (7%)	0	100	100
2	L	270/273 (99%)	251 (93%)	19 (7%)	0	100	100
3	M	316/324 (98%)	303 (96%)	13 (4%)	0	100	100
4	H	255/258 (99%)	231 (91%)	21 (8%)	3 (1%)	10	31
5	A	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
5	D	70/73 (96%)	70 (100%)	0	0	100	100
5	F	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
5	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
5	K	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
5	O	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
6	4	42/46 (91%)	40 (95%)	2 (5%)	0	100	100
6	B	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
7	0	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	6	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	8	40/46 (87%)	38 (95%)	1 (2%)	1 (2%)	4	15
7	E	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	G	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	J	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	N	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	R	42/46 (91%)	42 (100%)	0	0	100	100
7	T	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	V	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	X	39/46 (85%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Z	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
8	Q	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
9	1	70/77 (91%)	69 (99%)	1 (1%)	0	100	100
9	3	71/77 (92%)	70 (99%)	1 (1%)	0	100	100
9	5	72/77 (94%)	72 (100%)	0	0	100	100
9	7	71/77 (92%)	71 (100%)	0	0	100	100
9	S	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	U	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	W	71/77 (92%)	71 (100%)	0	0	100	100
9	Y	71/77 (92%)	71 (100%)	0	0	100	100
10	9	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
All	All	2937/3208 (92%)	2819 (96%)	114 (4%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	86	ASP
7	8	6	THR
4	H	257	VAL
4	H	256	SER

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	266/314 (85%)	265 (100%)	1 (0%)	84	94
2	L	217/218 (100%)	216 (100%)	1 (0%)	81	93
3	M	256/260 (98%)	255 (100%)	1 (0%)	84	94
4	H	211/212 (100%)	208 (99%)	3 (1%)	59	84
5	A	62/65 (95%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	64/65 (98%)	64 (100%)	0	100	100
5	F	64/65 (98%)	63 (98%)	1 (2%)	55	82
5	I	65/65 (100%)	65 (100%)	0	100	100
5	K	64/65 (98%)	64 (100%)	0	100	100
5	O	65/65 (100%)	65 (100%)	0	100	100
6	4	38/39 (97%)	38 (100%)	0	100	100
6	B	37/39 (95%)	36 (97%)	1 (3%)	39	72
6	P	36/39 (92%)	35 (97%)	1 (3%)	38	71
7	0	35/39 (90%)	35 (100%)	0	100	100
7	2	35/39 (90%)	35 (100%)	0	100	100
7	6	37/39 (95%)	37 (100%)	0	100	100
7	8	36/39 (92%)	36 (100%)	0	100	100
7	E	36/39 (92%)	36 (100%)	0	100	100
7	G	35/39 (90%)	35 (100%)	0	100	100
7	J	35/39 (90%)	35 (100%)	0	100	100
7	N	36/39 (92%)	36 (100%)	0	100	100
7	R	38/39 (97%)	38 (100%)	0	100	100
7	T	37/39 (95%)	37 (100%)	0	100	100
7	V	37/39 (95%)	37 (100%)	0	100	100
7	X	35/39 (90%)	35 (100%)	0	100	100
7	Z	36/39 (92%)	36 (100%)	0	100	100
8	Q	67/70 (96%)	67 (100%)	0	100	100
9	1	63/68 (93%)	63 (100%)	0	100	100
9	3	64/68 (94%)	64 (100%)	0	100	100
9	5	64/68 (94%)	64 (100%)	0	100	100
9	7	64/68 (94%)	63 (98%)	1 (2%)	55	82
9	S	64/68 (94%)	64 (100%)	0	100	100
9	U	63/68 (93%)	63 (100%)	0	100	100
9	W	64/68 (94%)	63 (98%)	1 (2%)	55	82
9	Y	64/68 (94%)	64 (100%)	0	100	100
10	9	72/74 (97%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2562/2706 (95%)	2551 (100%)	11 (0%)	81 94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	70	LYS
6	P	20	LEU
9	7	54	VAL
9	W	58	LEU
4	H	27	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
9	W	48	HIS
9	W	59	GLN
9	7	59	GLN
3	M	259	ASN
3	M	202	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 19 are monoatomic - leaving 105 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
19	8K6	5	106	-	14,14,17	0.29	0	13,13,16	0.11	0
15	PGV	Q	101	-	37,37,50	1.09	3 (8%)	40,43,56	1.47	6 (15%)
16	BCL	Y	104	7	69,74,74	1.85	14 (20%)	83,115,115	2.24	25 (30%)
23	H4X	Q	105	-	43,43,43	2.25	12 (27%)	50,54,54	2.30	22 (44%)
16	BCL	9	103	10	69,74,74	1.71	15 (21%)	83,115,115	2.26	22 (26%)
16	BCL	2	102	7	69,74,74	1.66	12 (17%)	83,115,115	2.37	25 (30%)
23	H4X	U	104	-	43,43,43	2.35	14 (32%)	50,54,54	2.05	14 (28%)
15	PGV	K	102	-	18,18,50	1.27	1 (5%)	20,22,56	1.10	1 (5%)
14	DGA	C	407	1	31,31,43	0.61	0	33,33,45	0.77	1 (3%)
15	PGV	A	101	-	22,22,50	1.50	4 (18%)	23,27,56	1.55	6 (26%)
16	BCL	F	105	7	69,74,74	1.92	16 (23%)	83,115,115	2.18	20 (24%)
16	BCL	U	102	9	69,74,74	1.79	17 (24%)	83,115,115	2.40	26 (31%)
11	HEM	C	401	1	50,50,50	1.73	13 (26%)	66,82,82	2.01	22 (33%)
24	LMT	G	102	-	36,36,36	0.85	2 (5%)	47,47,47	1.69	8 (17%)
23	H4X	O	106	-	43,43,43	2.44	17 (39%)	50,54,54	2.05	18 (36%)
23	H4X	5	105	-	43,43,43	2.24	12 (27%)	50,54,54	2.10	14 (28%)
24	LMT	J	102	-	36,36,36	0.90	2 (5%)	47,47,47	1.75	11 (23%)
15	PGV	D	101	-	42,42,50	0.95	2 (4%)	45,48,56	1.52	7 (15%)
15	PGV	3	101	-	46,46,50	1.05	2 (4%)	48,52,56	1.40	8 (16%)
24	LMT	N	101	-	36,36,36	0.83	1 (2%)	47,47,47	1.53	6 (12%)
24	LMT	R	101	-	36,36,36	0.85	2 (5%)	47,47,47	1.36	8 (17%)
11	HEM	C	403	1	50,50,50	1.44	6 (12%)	66,82,82	2.24	25 (37%)
16	BCL	3	103	9	69,74,74	1.75	15 (21%)	83,115,115	2.09	24 (28%)
23	H4X	K	103	-	43,43,43	2.18	11 (25%)	50,54,54	2.00	21 (42%)
16	BCL	W	102	9	69,74,74	1.76	15 (21%)	83,115,115	2.25	22 (26%)
15	PGV	F	101	-	33,33,50	1.34	2 (6%)	36,38,56	1.65	10 (27%)
16	BCL	K	108	7	69,74,74	1.87	16 (23%)	83,115,115	2.21	28 (33%)
24	LMT	0	101	-	36,36,36	0.83	2 (5%)	47,47,47	1.37	7 (14%)
16	BCL	K	105	5	69,74,74	1.84	14 (20%)	83,115,115	2.12	24 (28%)
16	BCL	S	103	9	69,74,74	1.75	15 (21%)	83,115,115	2.15	19 (22%)
24	LMT	B	104	-	36,36,36	1.13	3 (8%)	47,47,47	1.38	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BPH	M	404	-	59,70,70	1.04	5 (8%)	61,101,101	1.28	5 (8%)
16	BCL	1	102	9	69,74,74	1.82	15 (21%)	83,115,115	2.29	23 (27%)
21	MQ8	M	405	-	54,54,54	0.80	3 (5%)	66,69,69	0.85	1 (1%)
24	LMT	2	103	-	36,36,36	0.92	3 (8%)	47,47,47	1.91	13 (27%)
15	PGV	M	406	-	38,38,50	1.15	2 (5%)	41,44,56	1.19	3 (7%)
24	LMT	B	102	-	36,36,36	0.53	0	47,47,47	1.16	3 (6%)
23	H4X	Z	101	-	43,43,43	2.28	11 (25%)	50,54,54	1.87	11 (22%)
24	LMT	6	102	-	36,36,36	0.94	3 (8%)	47,47,47	1.68	8 (17%)
24	LMT	P	102	-	36,36,36	0.92	1 (2%)	47,47,47	1.36	6 (12%)
16	BCL	I	102	5	69,74,74	1.73	15 (21%)	83,115,115	2.27	22 (26%)
24	LMT	8	102	-	36,36,36	0.74	0	47,47,47	1.32	6 (12%)
11	HEM	C	404	1	50,50,50	1.54	8 (16%)	66,82,82	1.97	16 (24%)
15	PGV	Y	105	-	26,26,50	1.37	2 (7%)	30,31,56	1.28	5 (16%)
16	BCL	O	104	5	69,74,74	1.98	17 (24%)	83,115,115	2.27	23 (27%)
16	BCL	L	301	2	69,74,74	1.92	14 (20%)	83,115,115	2.40	32 (38%)
23	H4X	G	101	-	43,43,43	2.29	14 (32%)	50,54,54	2.16	18 (36%)
23	H4X	4	101	-	43,43,43	2.13	12 (27%)	50,54,54	1.90	16 (32%)
16	BCL	A	102	5	69,74,74	1.84	17 (24%)	83,115,115	2.41	19 (22%)
16	BCL	X	101	7	69,74,74	2.00	16 (23%)	83,115,115	2.26	25 (30%)
15	PGV	K	106	-	42,42,50	1.06	2 (4%)	46,47,56	1.03	3 (6%)
15	PGV	F	104	-	36,36,50	1.11	2 (5%)	39,42,56	1.49	6 (15%)
18	UQ8	L	303	-	33,33,53	1.70	4 (12%)	40,43,67	2.02	13 (32%)
11	HEM	C	402	1	50,50,50	1.77	11 (22%)	66,82,82	2.10	24 (36%)
17	BPH	L	302	-	59,70,70	0.89	3 (5%)	61,101,101	1.17	3 (4%)
16	BCL	T	101	7	69,74,74	1.82	16 (23%)	83,115,115	2.23	27 (32%)
23	H4X	P	101	-	43,43,43	2.34	14 (32%)	50,54,54	1.92	17 (34%)
23	H4X	E	101	-	43,43,43	2.49	13 (30%)	50,54,54	2.18	15 (30%)
23	H4X	O	101	-	43,43,43	2.25	15 (34%)	50,54,54	2.50	19 (38%)
16	BCL	5	103	9	69,74,74	1.89	19 (27%)	83,115,115	2.28	24 (28%)
24	LMT	X	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.36	5 (10%)
24	LMT	4	102	-	36,36,36	0.96	3 (8%)	47,47,47	1.76	9 (19%)
16	BCL	Q	104	7	69,74,74	2.05	20 (28%)	83,115,115	2.43	30 (36%)
16	BCL	D	103	-	69,74,74	1.73	15 (21%)	83,115,115	2.28	18 (21%)
22	CDL	S	101	-	73,73,99	0.48	0	79,85,111	0.81	3 (3%)
15	PGV	5	101	-	46,46,50	1.05	2 (4%)	49,52,56	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	H	302	-	72,72,99	0.45	0	78,84,111	1.01	5 (6%)
16	BCL	9	104	7	69,74,74	1.99	12 (17%)	83,115,115	2.12	26 (31%)
16	BCL	3	104	6	69,74,74	1.97	15 (21%)	83,115,115	2.28	29 (34%)
24	LMT	8	101	-	36,36,36	0.56	0	47,47,47	0.78	0
18	UQ8	L	306	-	33,33,53	1.67	2 (6%)	40,43,67	1.86	11 (27%)
16	BCL	J	101	7	69,74,74	1.87	15 (21%)	83,115,115	2.17	25 (30%)
23	H4X	V	101	-	43,43,43	2.32	13 (30%)	50,54,54	2.67	17 (34%)
23	H4X	B	101	-	43,43,43	2.22	13 (30%)	50,54,54	2.06	19 (38%)
15	PGV	1	103	-	25,25,50	1.37	2 (8%)	29,30,56	1.57	3 (10%)
16	BCL	D	104	7	69,74,74	2.01	18 (26%)	83,115,115	2.10	18 (21%)
15	PGV	C	408	-	15,15,50	1.45	3 (20%)	18,19,56	2.34	5 (27%)
24	LMT	Z	102	-	36,36,36	0.83	1 (2%)	47,47,47	1.62	10 (21%)
24	LMT	T	102	-	36,36,36	0.91	2 (5%)	47,47,47	1.49	9 (19%)
15	PGV	K	101	-	35,35,50	1.20	2 (5%)	38,41,56	1.14	5 (13%)
16	BCL	B	103	6	69,74,74	2.07	16 (23%)	83,115,115	2.31	29 (34%)
23	H4X	7	104	-	43,43,43	2.34	12 (27%)	50,54,54	2.18	14 (28%)
22	CDL	Y	103	-	29,29,99	0.59	0	33,38,111	0.84	1 (3%)
16	BCL	7	103	7	69,74,74	2.02	16 (23%)	83,115,115	2.07	21 (25%)
15	PGV	H	301	-	35,35,50	1.27	3 (8%)	38,41,56	1.92	5 (13%)
16	BCL	M	402	3	69,74,74	1.75	13 (18%)	83,115,115	2.43	21 (25%)
16	BCL	Q	103	8	69,74,74	1.84	16 (23%)	83,115,115	2.10	21 (25%)
24	LMT	E	102	-	36,36,36	0.92	2 (5%)	47,47,47	1.53	9 (19%)
16	BCL	5	104	7	69,74,74	1.88	15 (21%)	83,115,115	2.26	25 (30%)
16	BCL	O	105	6	69,74,74	1.96	15 (21%)	83,115,115	2.32	27 (32%)
15	PGV	L	305	-	46,46,50	1.05	2 (4%)	49,52,56	1.45	6 (12%)
16	BCL	U	103	7	69,74,74	2.13	15 (21%)	83,115,115	2.20	23 (27%)
15	PGV	9	101	-	46,46,50	0.95	2 (4%)	48,52,56	1.12	4 (8%)
16	BCL	Y	102	9	69,74,74	1.83	14 (20%)	83,115,115	2.32	25 (30%)
24	LMT	V	102	-	36,36,36	0.90	0	47,47,47	1.72	7 (14%)
15	PGV	I	103	-	40,40,50	1.01	2 (5%)	44,45,56	1.17	7 (15%)
16	BCL	F	103	5	69,74,74	1.71	13 (18%)	83,115,115	2.25	22 (26%)
19	8K6	L	307	-	17,17,17	0.45	0	16,16,16	0.17	0
23	H4X	2	101	-	43,43,43	2.25	10 (23%)	50,54,54	1.90	16 (32%)
16	BCL	7	102	9	64,69,74	1.76	15 (23%)	77,109,115	2.23	24 (31%)
23	H4X	K	107	-	43,43,43	2.20	11 (25%)	50,54,54	1.95	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCL	M	403	3	69,74,74	1.71	13 (18%)	83,115,115	2.43	27 (32%)
16	BCL	L	304	2	69,74,74	1.83	15 (21%)	83,115,115	3.17	27 (32%)
23	H4X	6	101	-	43,43,43	2.29	12 (27%)	50,54,54	2.19	19 (38%)
15	PGV	O	102	-	43,43,50	0.93	2 (4%)	46,49,56	1.23	3 (6%)

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
19	8K6	5	106	-	-	4/12/12/15	-
15	PGV	Q	101	-	-	21/42/42/55	-
16	BCL	Y	104	7	-	18/41/137/137	-
23	H4X	Q	105	-	-	11/51/51/51	-
16	BCL	9	103	10	-	21/41/137/137	-
16	BCL	2	102	7	-	15/41/137/137	-
23	H4X	U	104	-	-	5/51/51/51	-
15	PGV	K	102	-	-	5/20/20/55	-
14	DGA	C	407	1	-	20/32/32/45	-
15	PGV	A	101	-	-	10/26/26/55	-
16	BCL	F	105	7	-	14/41/137/137	-
16	BCL	U	102	9	-	14/41/137/137	-
11	HEM	C	401	1	-	9/14/54/54	-
24	LMT	G	102	-	-	12/21/61/61	0/2/2/2
23	H4X	O	106	-	-	8/51/51/51	-
23	H4X	5	105	-	-	10/51/51/51	-
24	LMT	J	102	-	-	10/21/61/61	0/2/2/2
15	PGV	D	101	-	-	14/47/47/55	-
15	PGV	3	101	-	-	24/51/51/55	-
24	LMT	N	101	-	-	11/21/61/61	0/2/2/2
24	LMT	R	101	-	-	9/21/61/61	0/2/2/2
11	HEM	C	403	1	-	4/14/54/54	-
16	BCL	3	103	9	-	17/41/137/137	-
23	H4X	K	103	-	-	10/51/51/51	-
16	BCL	W	102	9	-	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PGV	F	101	-	-	13/35/35/55	-
16	BCL	K	108	7	-	19/41/137/137	-
24	LMT	O	101	-	-	11/21/61/61	0/2/2/2
16	BCL	K	105	5	-	22/41/137/137	-
16	BCL	S	103	9	-	5/41/137/137	-
24	LMT	B	104	-	-	12/21/61/61	0/2/2/2
17	BPH	M	404	-	-	19/37/105/105	0/5/6/6
16	BCL	1	102	9	-	9/41/137/137	-
21	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
24	LMT	2	103	-	-	10/21/61/61	0/2/2/2
15	PGV	M	406	-	-	21/43/43/55	-
24	LMT	B	102	-	-	13/21/61/61	0/2/2/2
23	H4X	Z	101	-	-	8/51/51/51	-
24	LMT	6	102	-	-	10/21/61/61	0/2/2/2
24	LMT	P	102	-	-	12/21/61/61	0/2/2/2
16	BCL	I	102	5	-	13/41/137/137	-
24	LMT	8	102	-	-	11/21/61/61	0/2/2/2
11	HEM	C	404	1	-	7/14/54/54	-
15	PGV	Y	105	-	-	9/28/28/55	-
16	BCL	O	104	5	-	13/41/137/137	-
16	BCL	L	301	2	-	8/41/137/137	-
23	H4X	G	101	-	-	7/51/51/51	-
23	H4X	4	101	-	-	10/51/51/51	-
16	BCL	A	102	5	-	14/41/137/137	-
16	BCL	X	101	7	-	16/41/137/137	-
15	PGV	K	106	-	-	17/44/44/55	-
15	PGV	F	104	-	-	23/41/41/55	-
18	UQ8	L	303	-	-	6/27/51/75	0/1/1/1
11	HEM	C	402	1	-	7/14/54/54	-
17	BPH	L	302	-	-	17/37/105/105	0/5/6/6
16	BCL	T	101	7	-	16/41/137/137	-
23	H4X	P	101	-	-	6/51/51/51	-
23	H4X	E	101	-	-	5/51/51/51	-
23	H4X	O	101	-	-	14/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	5	103	9	-	14/41/137/137	-
24	LMT	X	102	-	-	11/21/61/61	0/2/2/2
24	LMT	4	102	-	-	11/21/61/61	0/2/2/2
16	BCL	Q	104	7	-	14/41/137/137	-
16	BCL	D	103	-	-	6/41/137/137	-
22	CDL	S	101	-	-	35/84/84/110	-
15	PGV	5	101	-	-	23/51/51/55	-
22	CDL	H	302	-	-	29/83/83/110	-
16	BCL	9	104	7	-	14/41/137/137	-
16	BCL	3	104	6	-	17/41/137/137	-
24	LMT	8	101	-	-	8/21/61/61	0/2/2/2
18	UQ8	L	306	-	-	7/27/51/75	0/1/1/1
16	BCL	J	101	7	-	15/41/137/137	-
23	H4X	V	101	-	-	11/51/51/51	-
23	H4X	B	101	-	-	3/51/51/51	-
15	PGV	1	103	-	-	11/27/27/55	-
16	BCL	D	104	7	-	16/41/137/137	-
15	PGV	C	408	-	-	10/15/15/55	-
24	LMT	Z	102	-	-	11/21/61/61	0/2/2/2
24	LMT	T	102	-	-	11/21/61/61	0/2/2/2
15	PGV	K	101	-	-	18/40/40/55	-
16	BCL	B	103	6	-	14/41/137/137	-
23	H4X	7	104	-	-	7/51/51/51	-
22	CDL	Y	103	-	-	13/35/35/110	-
16	BCL	7	103	7	-	14/41/137/137	-
15	PGV	H	301	-	-	17/40/40/55	-
16	BCL	M	402	3	-	15/41/137/137	-
16	BCL	Q	103	8	-	17/41/137/137	-
24	LMT	E	102	-	-	12/21/61/61	0/2/2/2
16	BCL	5	104	7	-	18/41/137/137	-
16	BCL	O	105	6	-	17/41/137/137	-
15	PGV	L	305	-	-	14/51/51/55	-
16	BCL	U	103	7	-	15/41/137/137	-
15	PGV	9	101	-	-	23/51/51/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	Y	102	9	-	10/41/137/137	-
24	LMT	V	102	-	-	10/21/61/61	0/2/2/2
15	PGV	I	103	-	-	19/42/42/55	-
16	BCL	F	103	5	-	13/41/137/137	-
19	8K6	L	307	-	-	11/15/15/15	-
23	H4X	2	101	-	-	10/51/51/51	-
16	BCL	7	102	9	-	8/35/131/137	-
23	H4X	K	107	-	-	9/51/51/51	-
16	BCL	M	403	3	-	13/41/137/137	-
16	BCL	L	304	2	-	7/41/137/137	-
23	H4X	6	101	-	-	5/51/51/51	-
15	PGV	O	102	-	-	23/48/48/55	-

The worst 5 of 890 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	306	UQ8	C6-C1	8.07	1.49	1.35
18	L	303	UQ8	C6-C1	7.22	1.48	1.35
16	U	103	BCL	C3D-C4D	-6.72	1.29	1.44
16	L	301	BCL	O2D-CGD	6.54	1.49	1.33
16	B	103	BCL	C3D-C4D	-6.29	1.30	1.44

The worst 5 of 1510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	304	BCL	O2D-CGD-CBD	15.70	139.16	111.27
16	L	304	BCL	O2D-CGD-O1D	-13.24	97.96	123.84
16	2	102	BCL	C2B-C1B-NB	10.28	117.13	110.23
16	Q	104	BCL	C2B-C1B-NB	10.01	116.94	110.23
16	B	103	BCL	C2B-C1B-NB	9.87	116.85	110.23

There are no chirality outliers.

5 of 1344 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	HEM	C2B-C3B-CAB-CBB
11	C	401	HEM	C4B-C3B-CAB-CBB
11	C	402	HEM	C2C-C3C-CAC-CBC
11	C	402	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	C	404	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

80 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	101	PGV	1	0
16	Y	104	BCL	2	0
16	9	103	BCL	6	0
16	2	102	BCL	2	0
14	C	407	DGA	6	0
16	F	105	BCL	2	0
16	U	102	BCL	7	0
11	C	401	HEM	6	0
24	G	102	LMT	1	0
23	O	106	H4X	1	0
24	J	102	LMT	2	0
15	3	101	PGV	4	0
24	N	101	LMT	3	0
24	R	101	LMT	2	0
11	C	403	HEM	9	0
16	3	103	BCL	6	0
16	W	102	BCL	3	0
16	K	108	BCL	3	0
24	0	101	LMT	1	0
16	K	105	BCL	7	0
16	S	103	BCL	6	0
24	B	104	LMT	2	0
17	M	404	BPH	7	0
16	1	102	BCL	4	0
21	M	405	MQ8	2	0
24	2	103	LMT	2	0
15	M	406	PGV	1	0
24	B	102	LMT	3	0
24	6	102	LMT	2	0
24	P	102	LMT	2	0
16	I	102	BCL	4	0
24	8	102	LMT	3	0
11	C	404	HEM	9	0
15	Y	105	PGV	6	0
16	O	104	BCL	2	0
16	L	301	BCL	5	0

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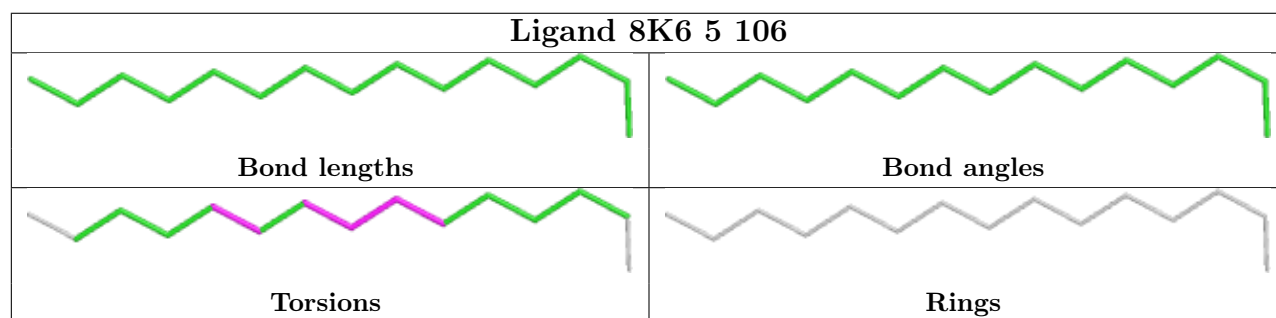
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	101	H4X	1	0
16	A	102	BCL	7	0
16	X	101	BCL	2	0
15	F	104	PGV	2	0
11	C	402	HEM	5	0
17	L	302	BPH	7	0
16	T	101	BCL	3	0
23	E	101	H4X	1	0
16	5	103	BCL	6	0
24	X	102	LMT	2	0
24	4	102	LMT	3	0
16	Q	104	BCL	3	0
16	D	103	BCL	4	0
22	S	101	CDL	1	0
15	5	101	PGV	4	0
22	H	302	CDL	3	0
16	9	104	BCL	1	0
16	3	104	BCL	5	0
24	8	101	LMT	2	0
18	L	306	UQ8	7	0
16	J	101	BCL	4	0
16	D	104	BCL	1	0
24	Z	102	LMT	1	0
24	T	102	LMT	2	0
15	K	101	PGV	3	0
16	B	103	BCL	2	0
16	7	103	BCL	3	0
15	H	301	PGV	1	0
16	M	402	BCL	2	0
16	Q	103	BCL	5	0
24	E	102	LMT	2	0
16	5	104	BCL	2	0
16	O	105	BCL	3	0
15	L	305	PGV	3	0
16	U	103	BCL	2	0
15	9	101	PGV	2	0
16	Y	102	BCL	1	0
24	V	102	LMT	1	0
16	F	103	BCL	3	0
19	L	307	8K6	1	0
16	7	102	BCL	4	0
16	M	403	BCL	6	0

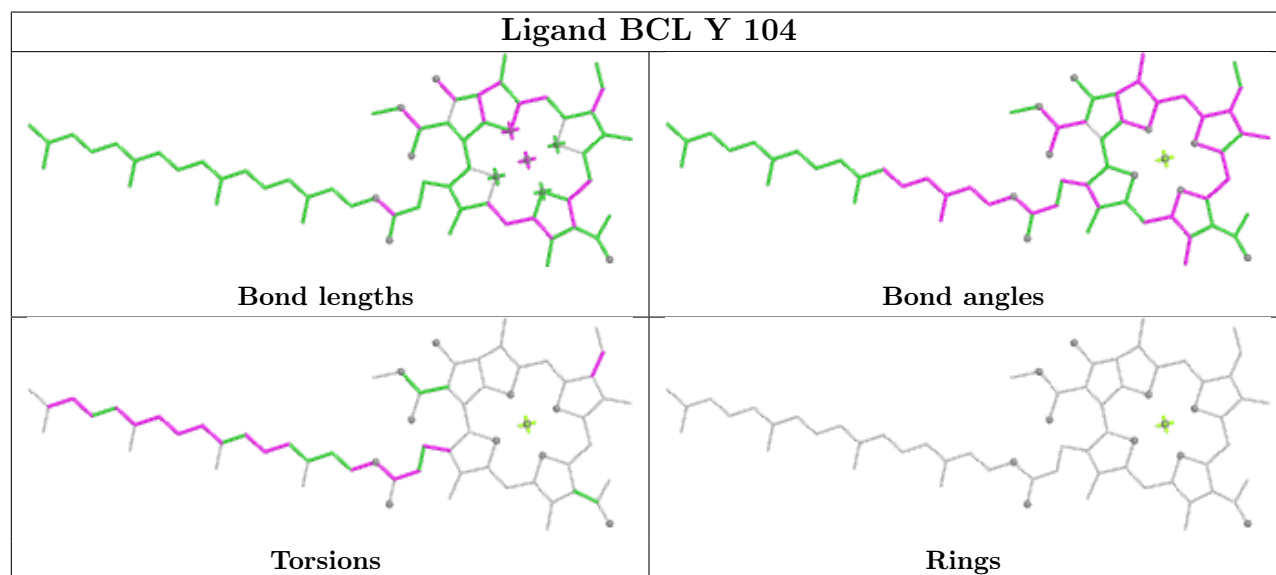
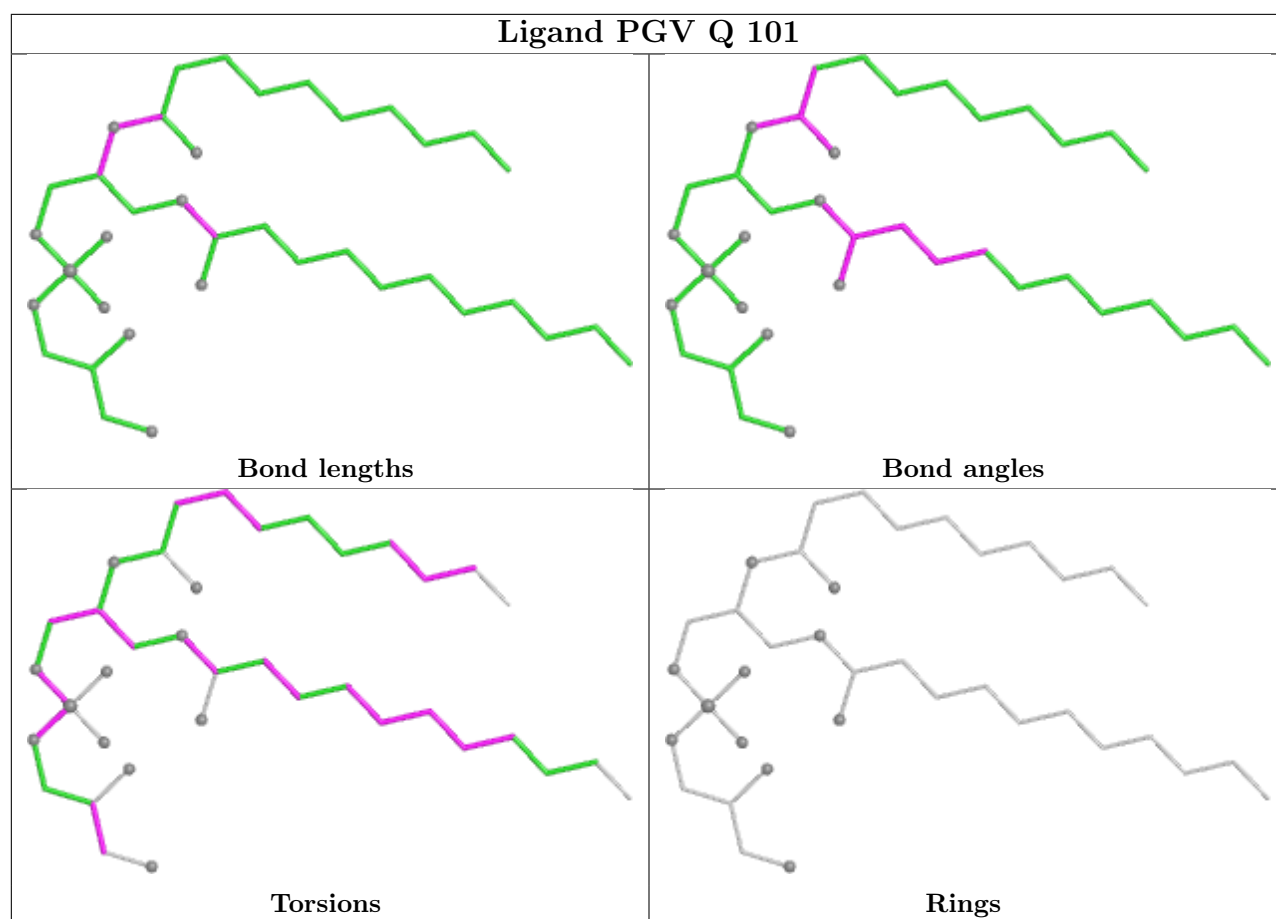
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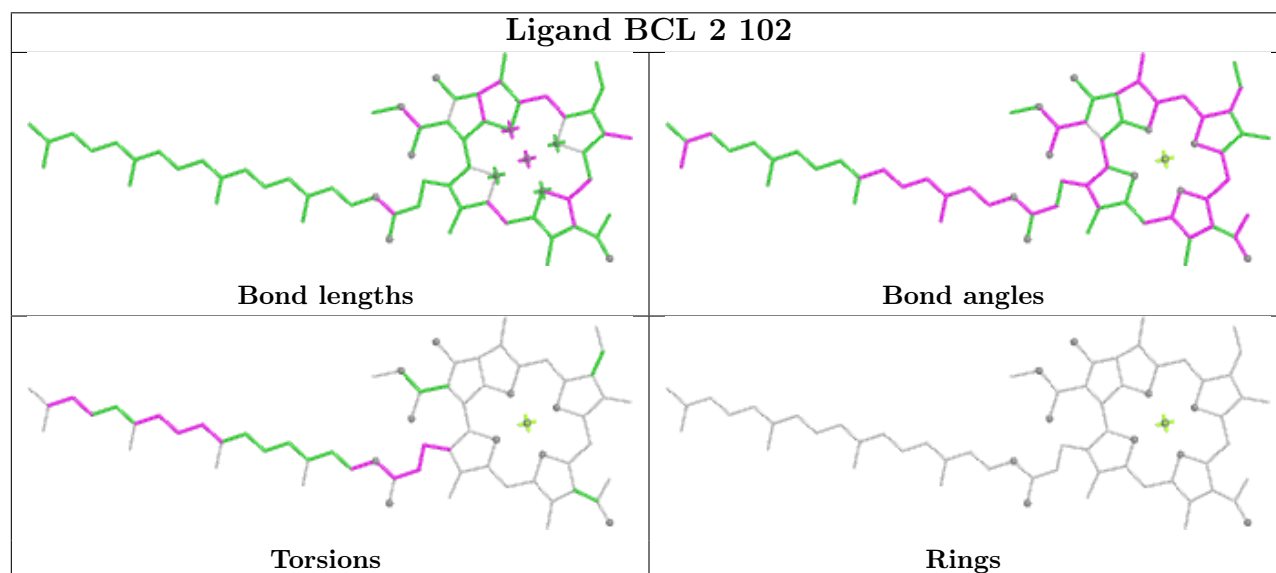
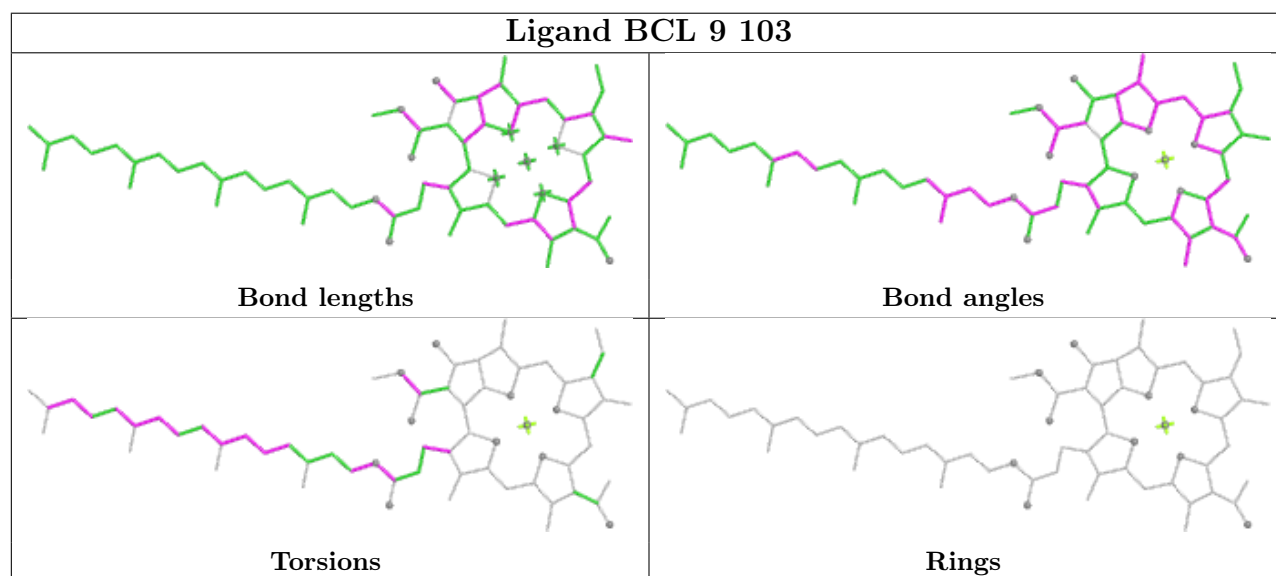
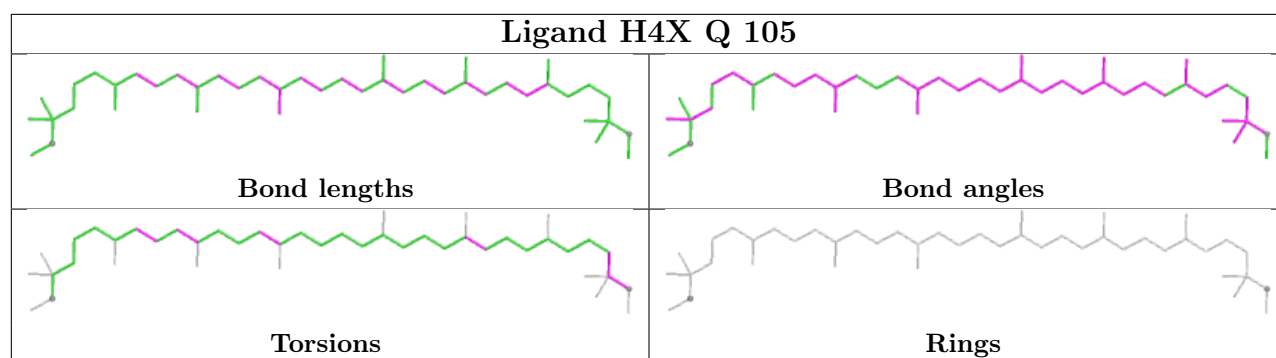
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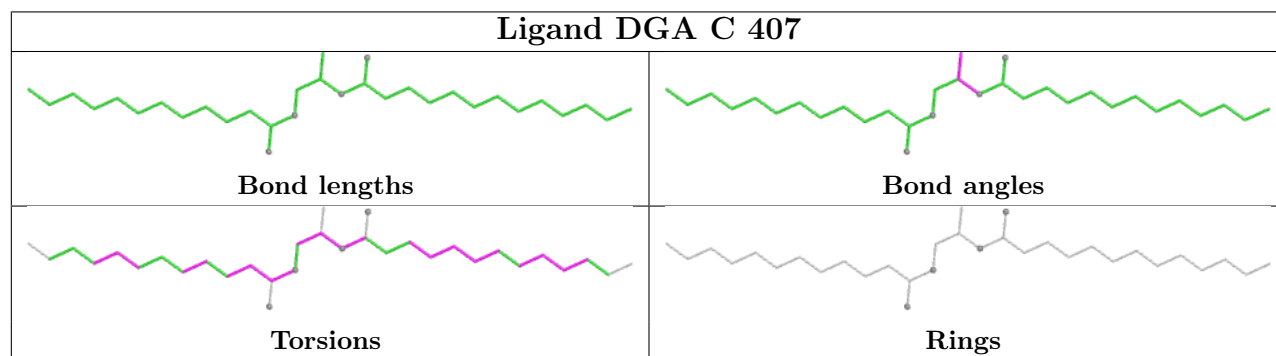
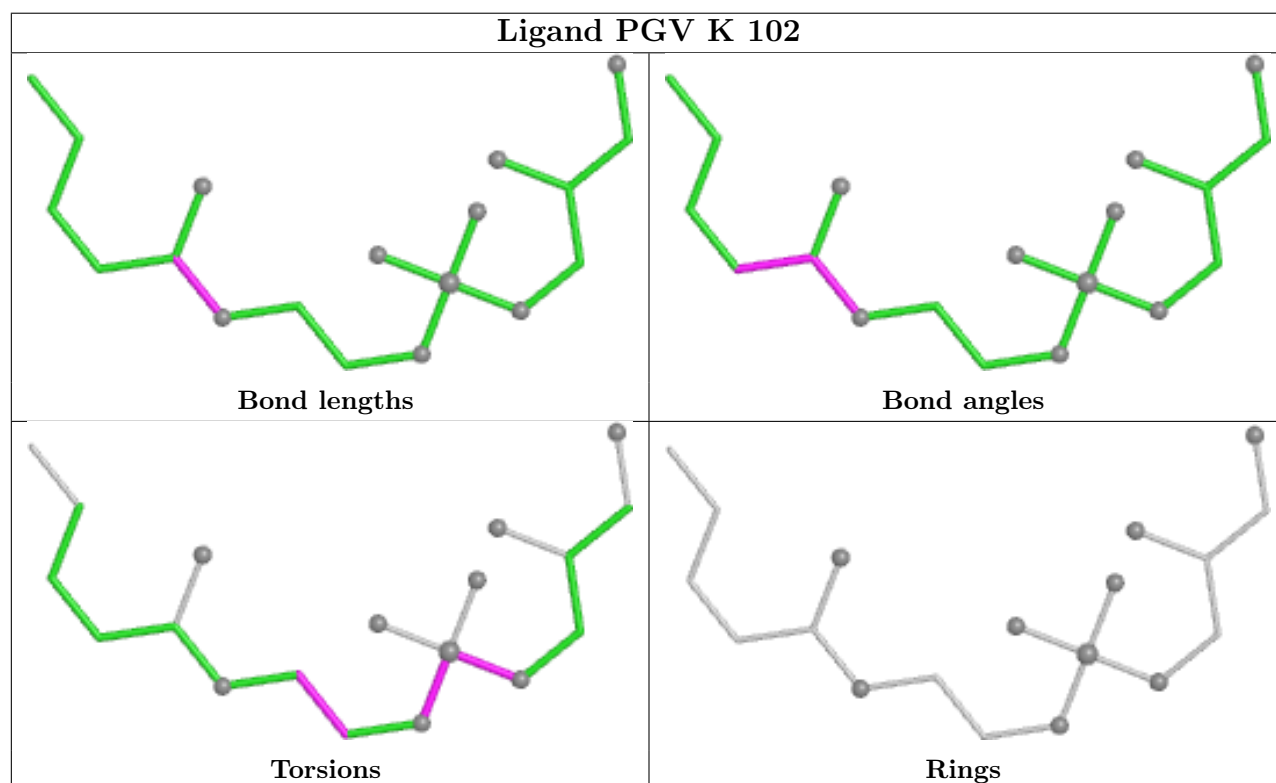
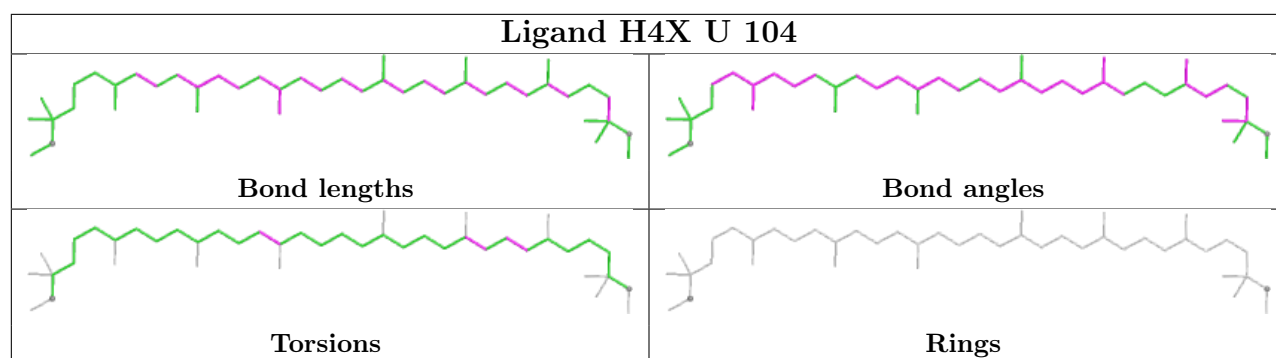
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	L	304	BCL	4	0
15	O	102	PGV	5	0

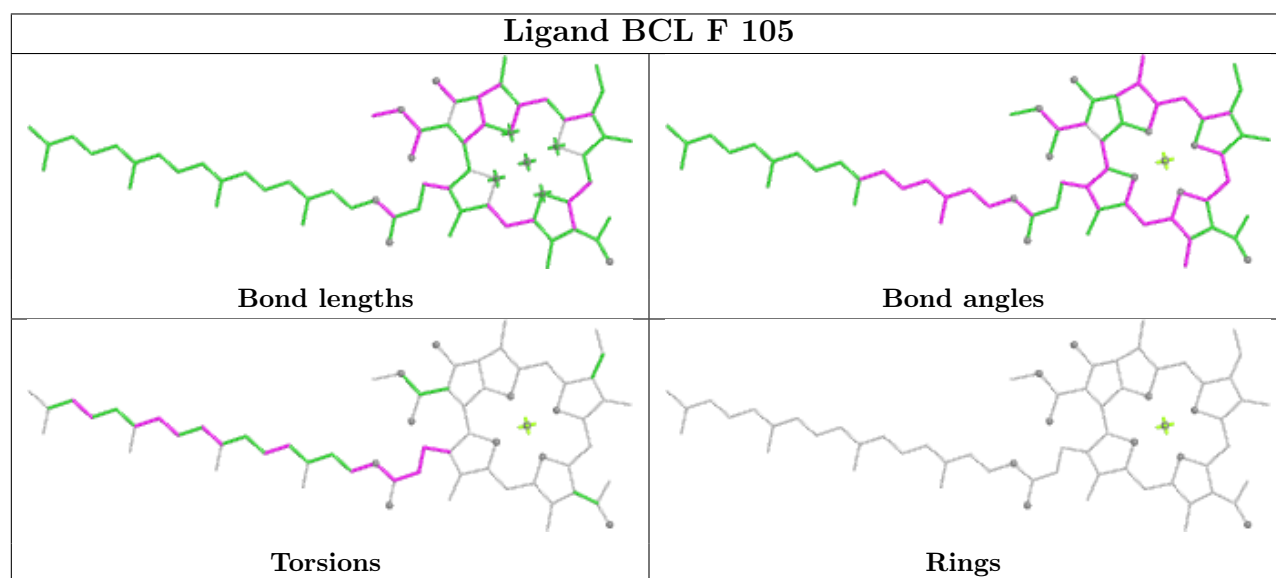
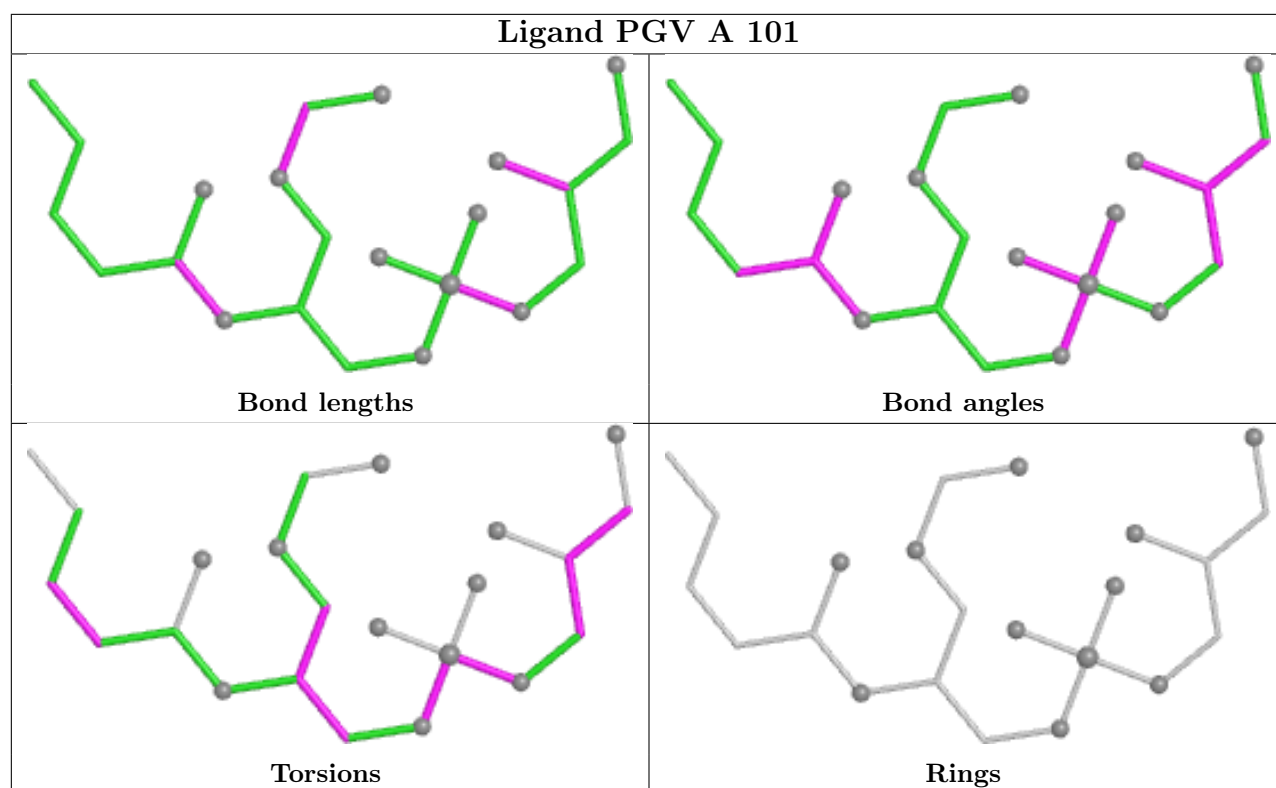
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

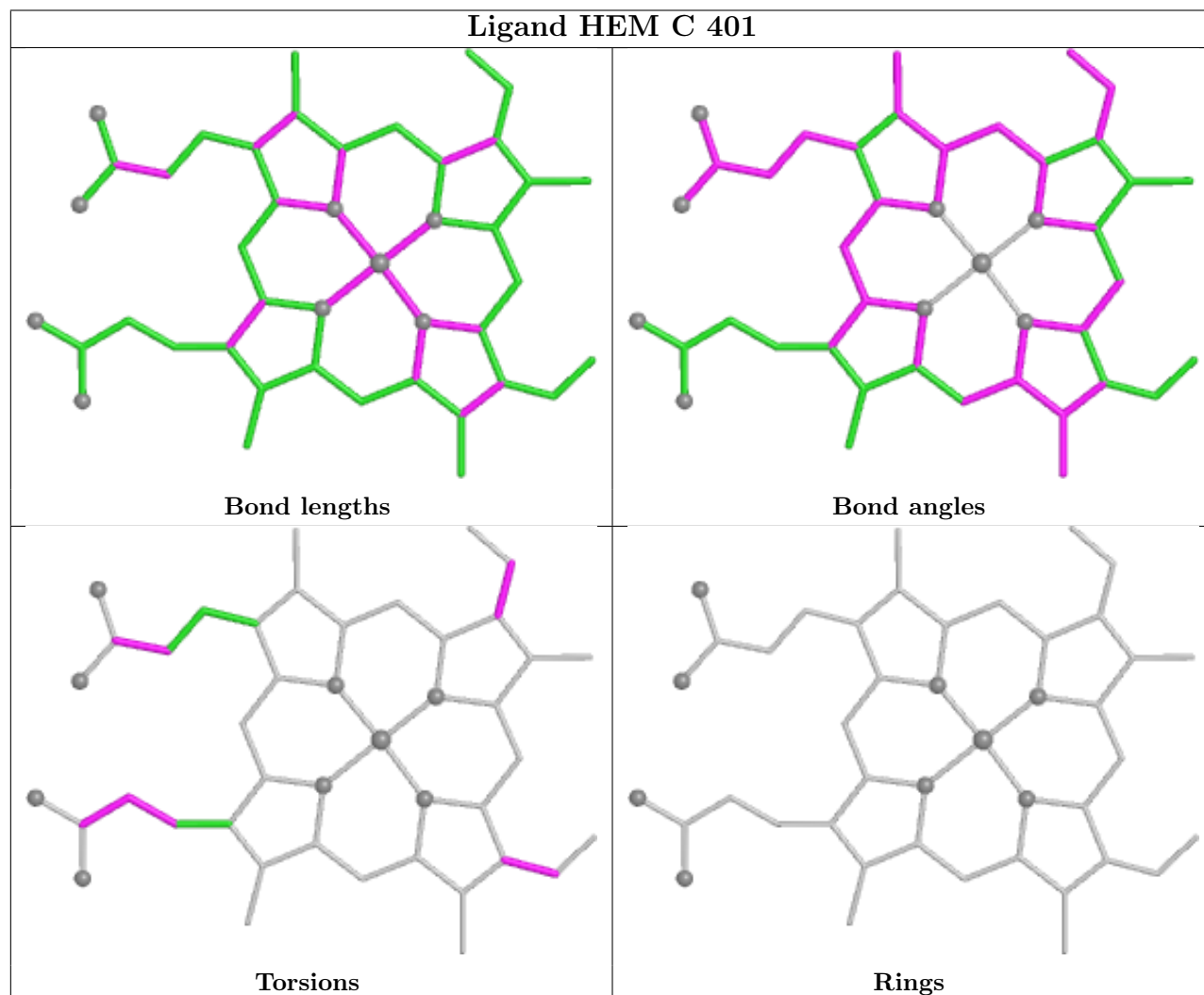
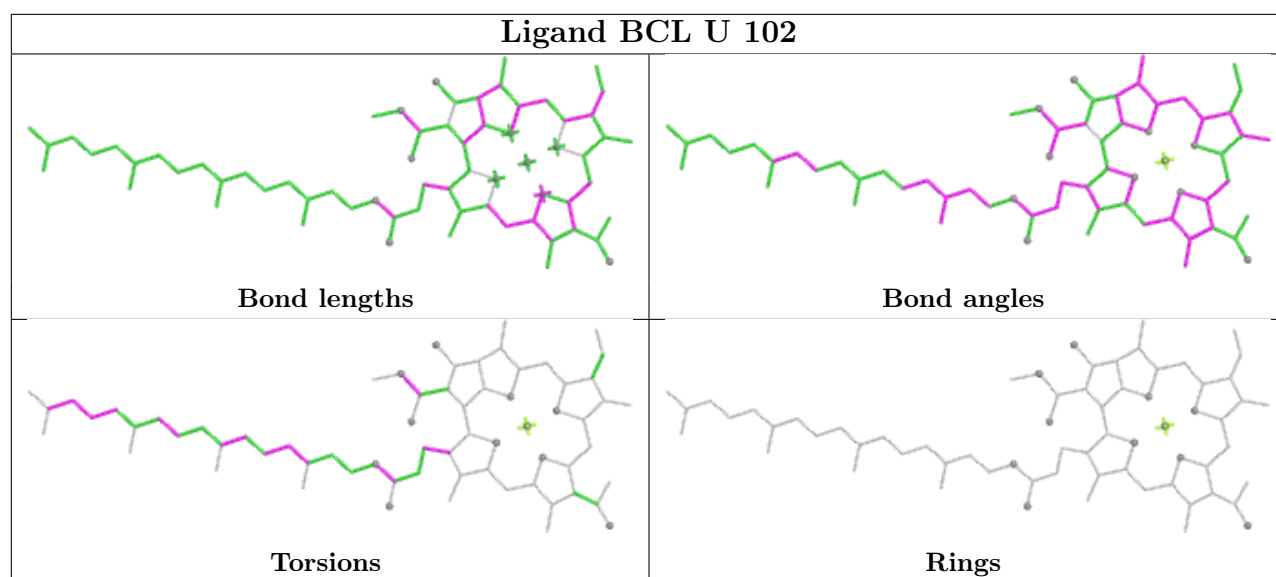


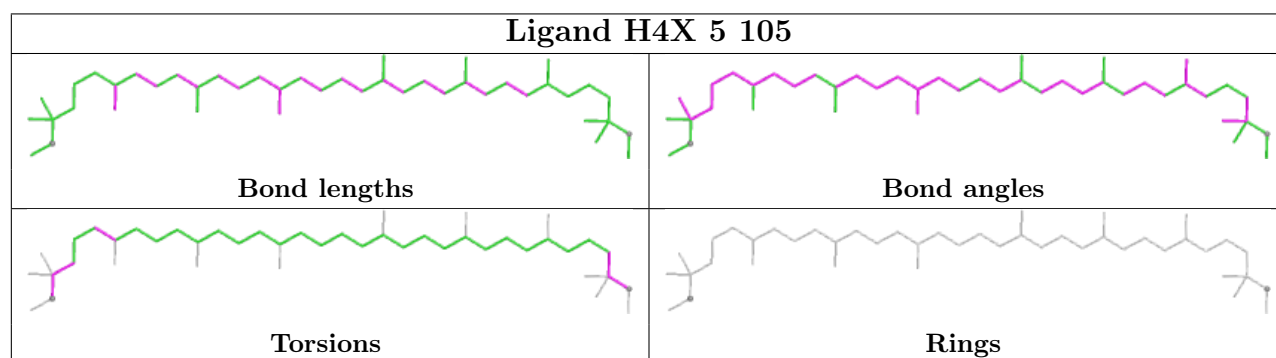
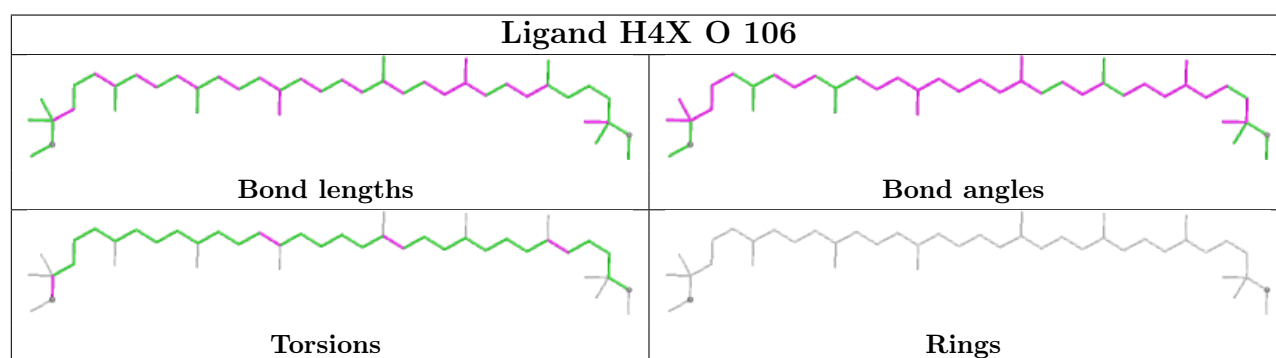
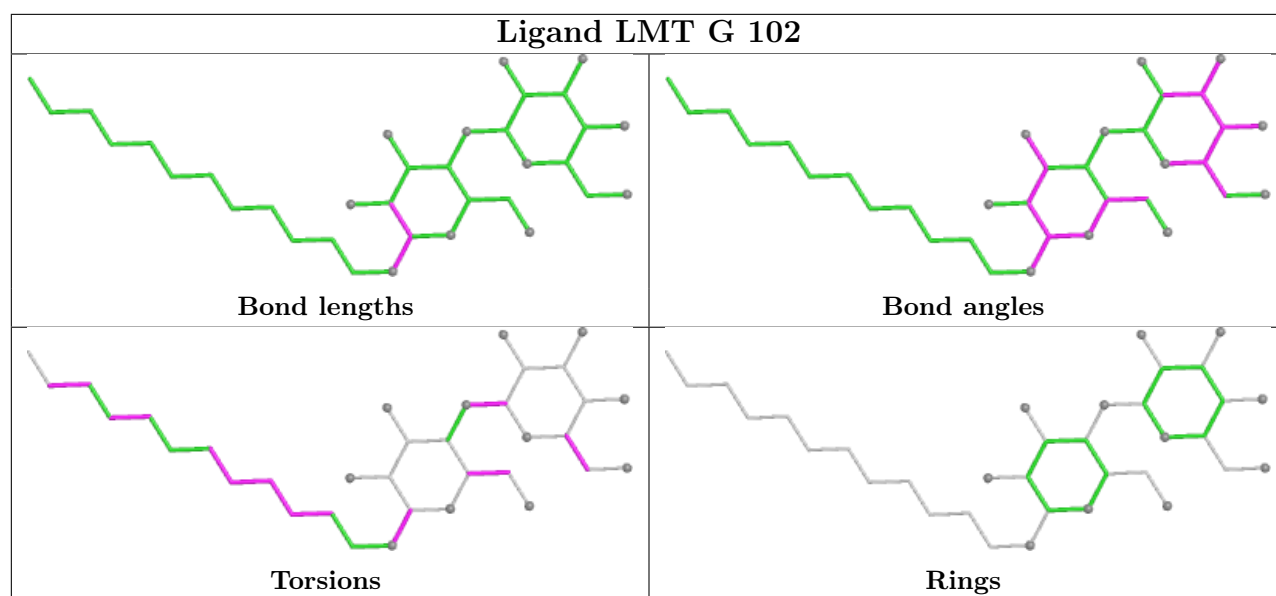


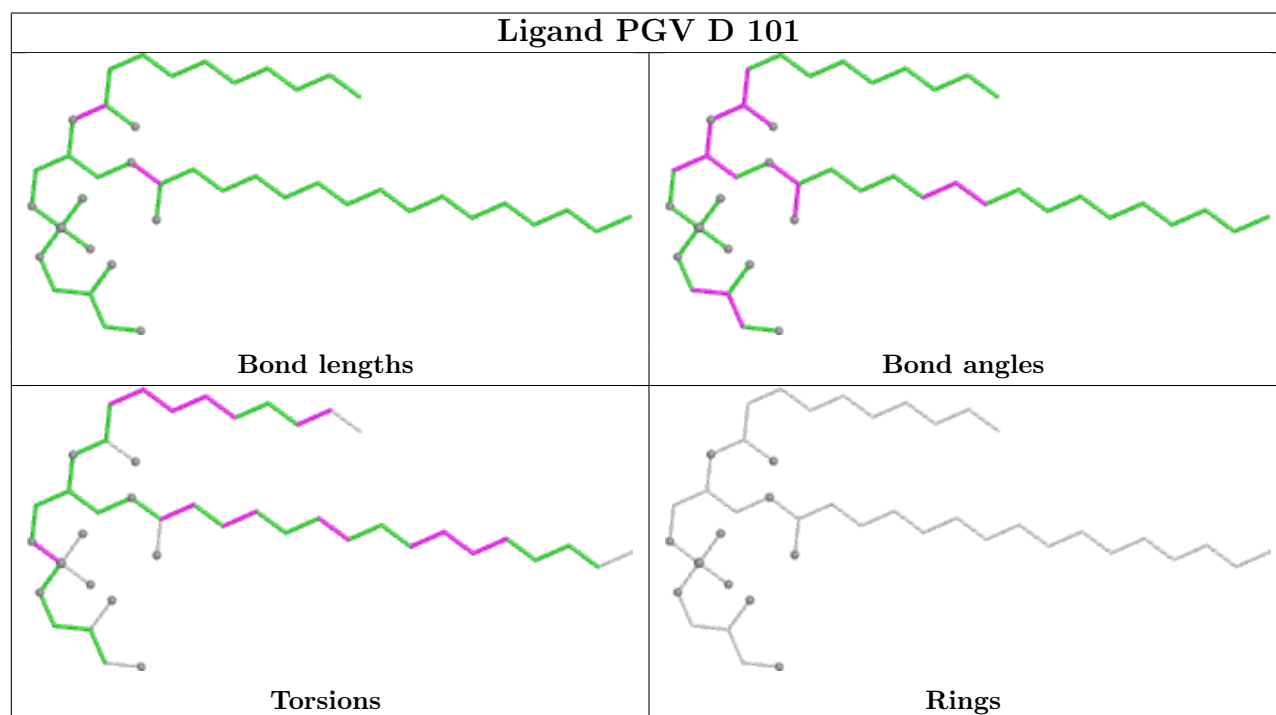
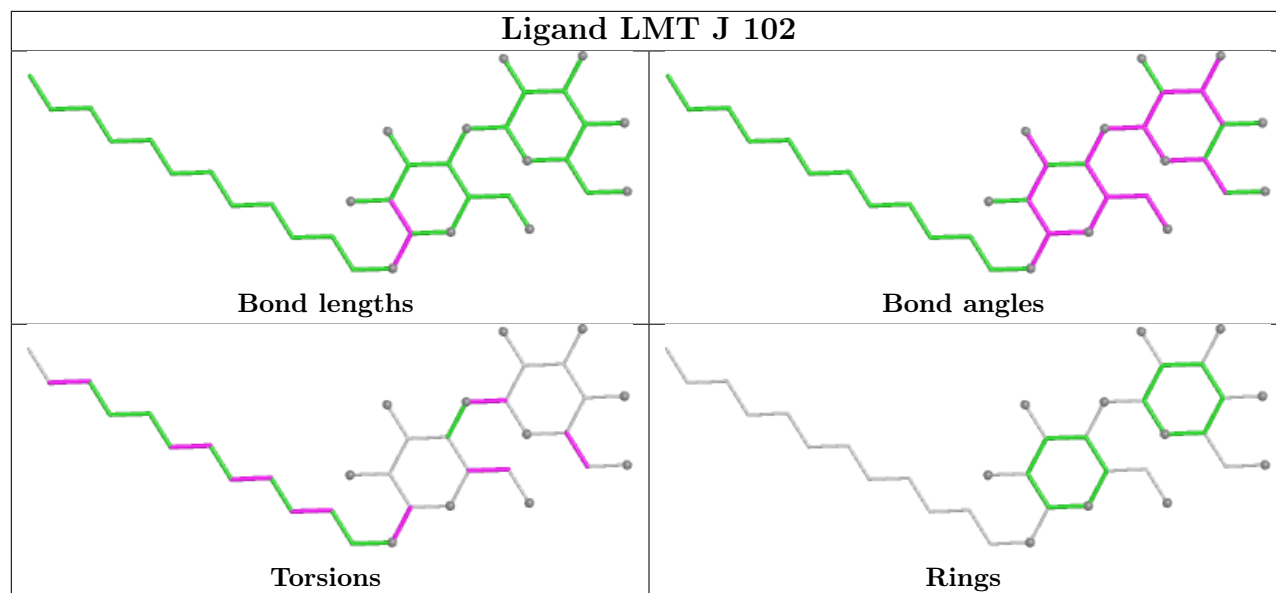


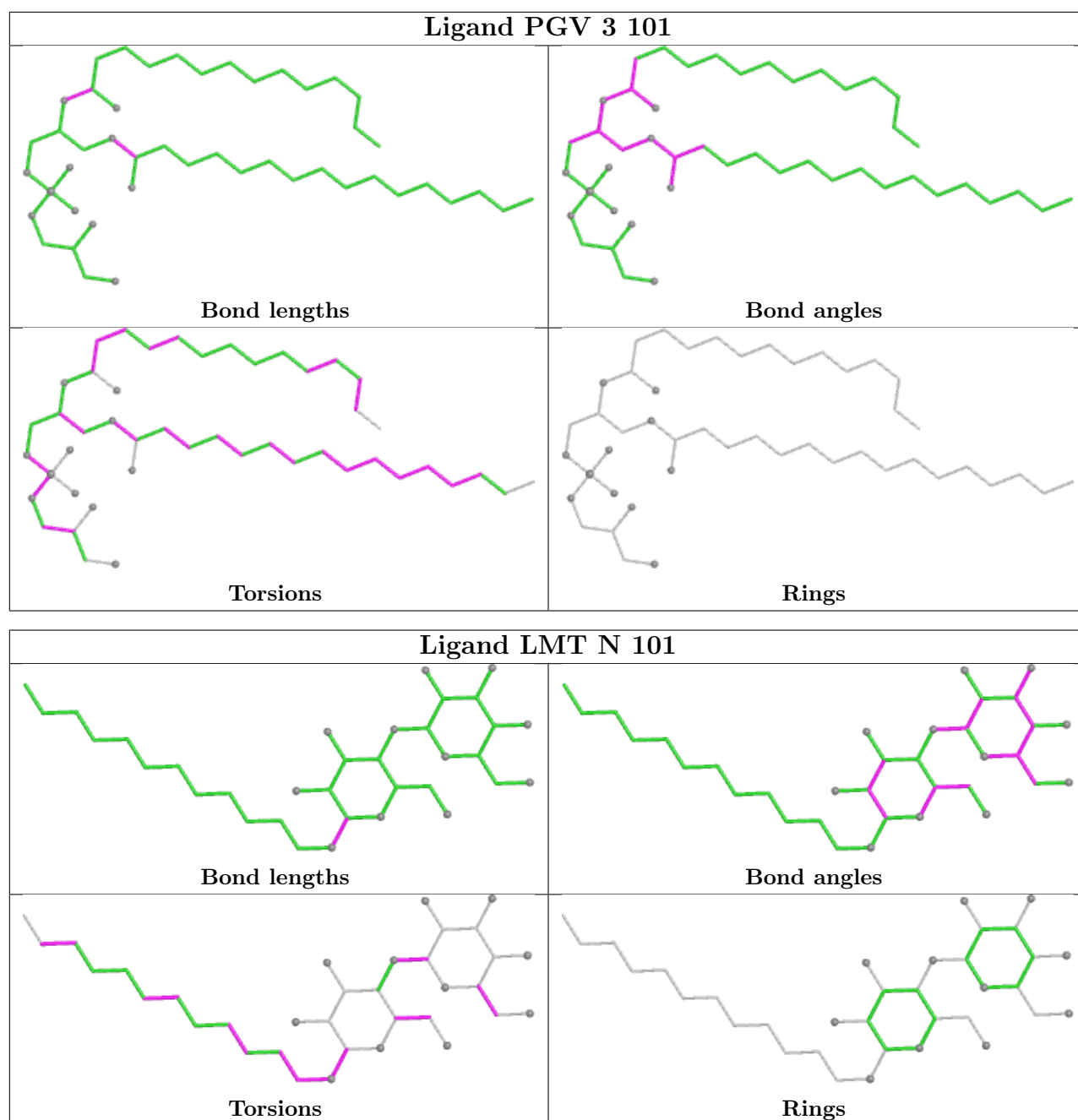


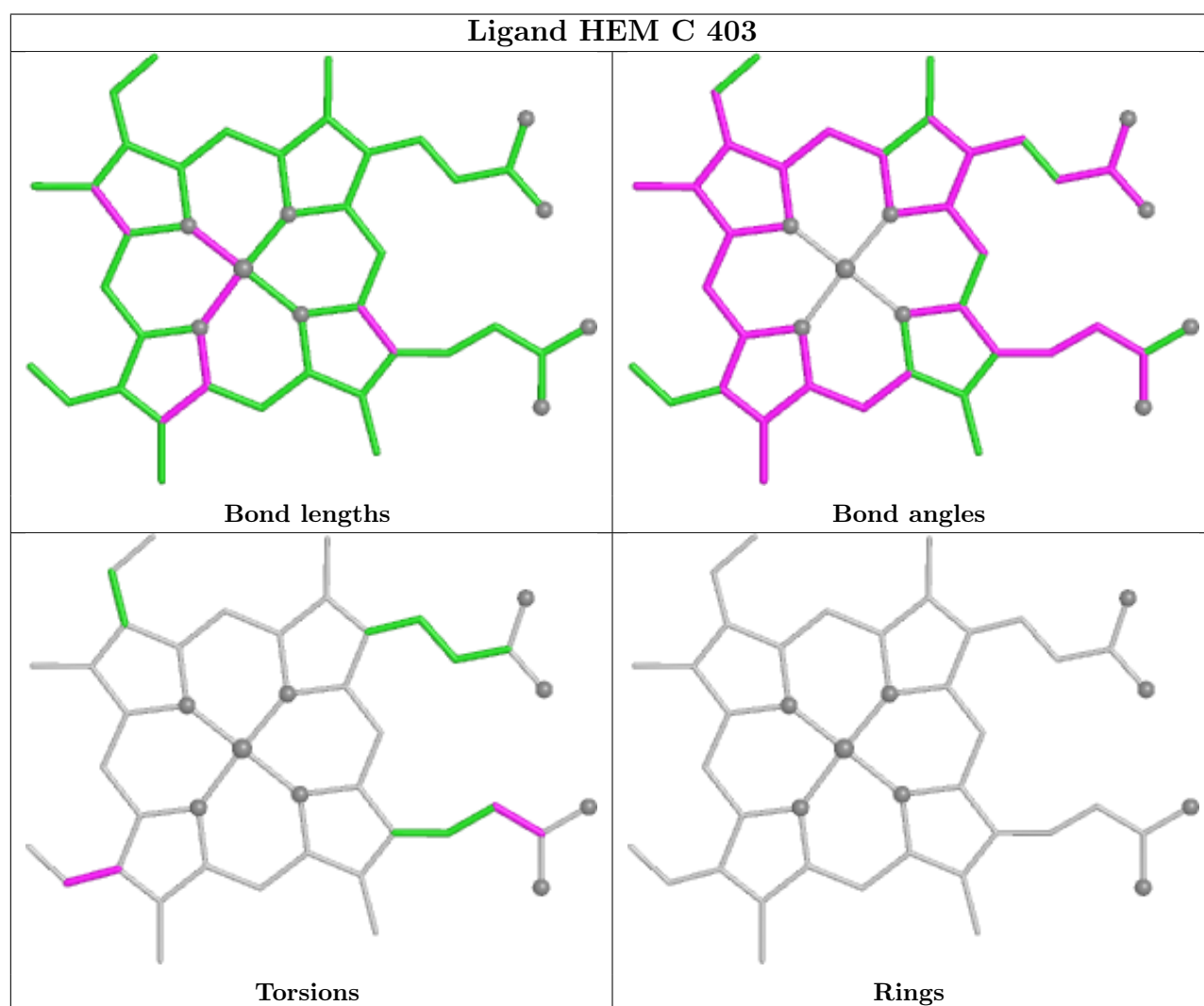
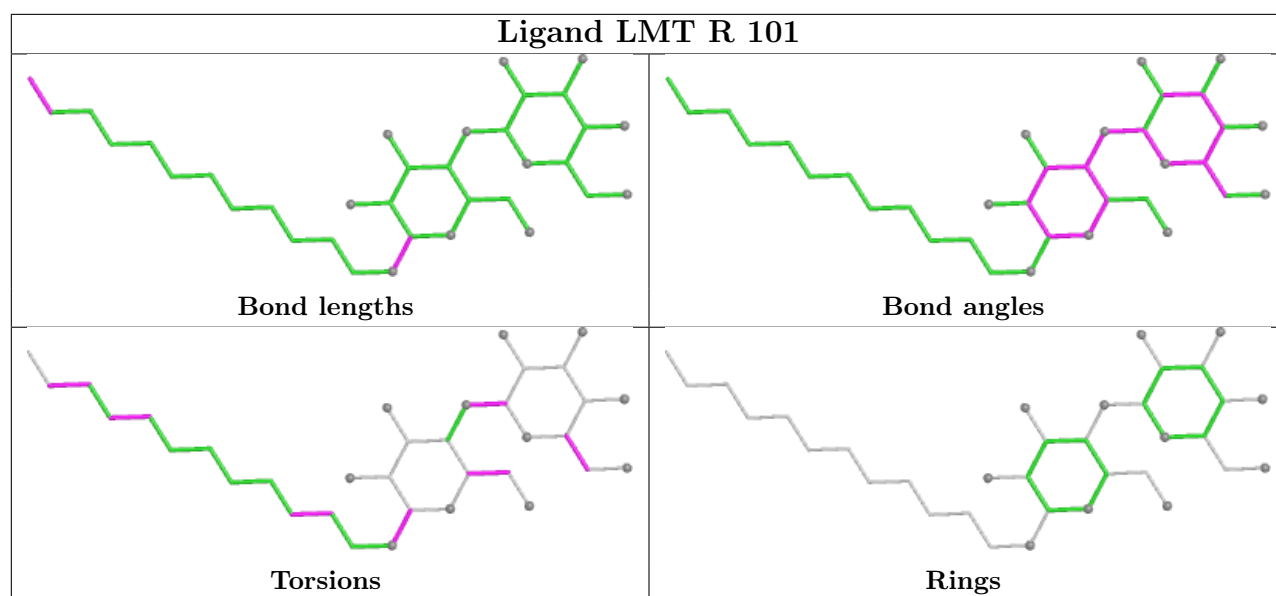


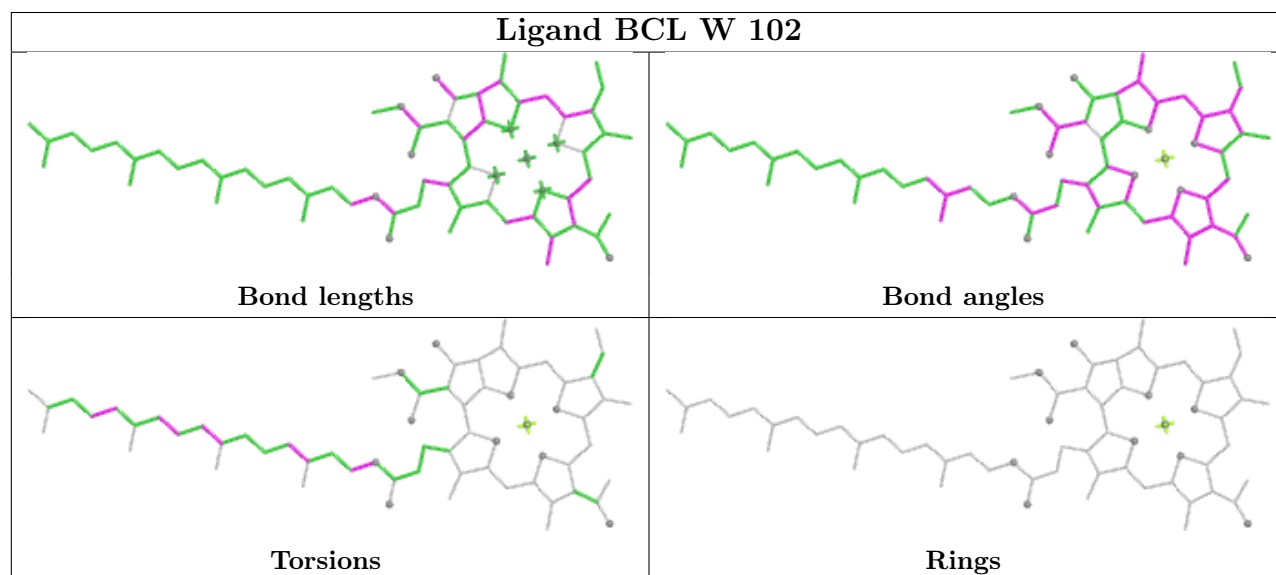
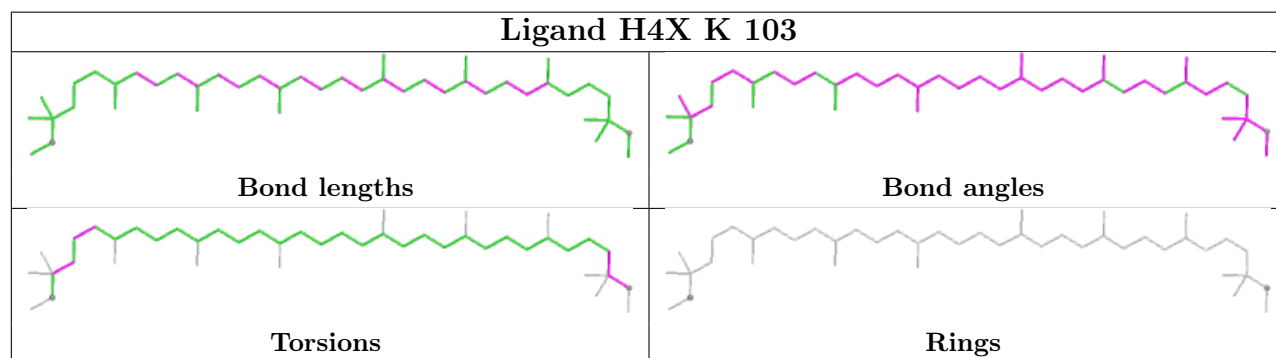
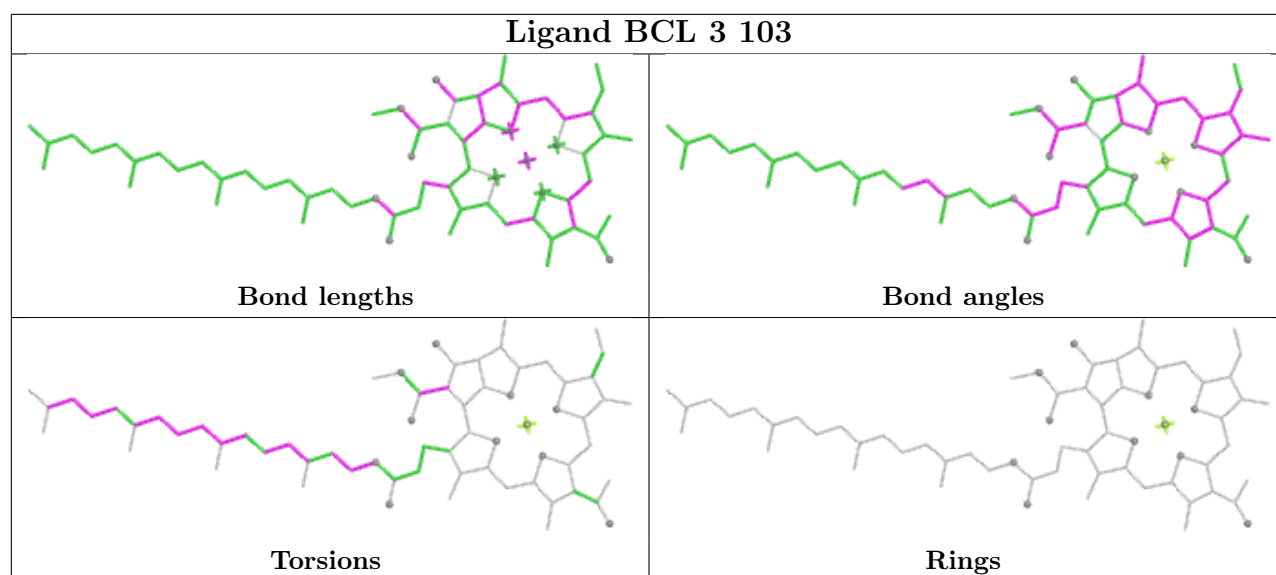


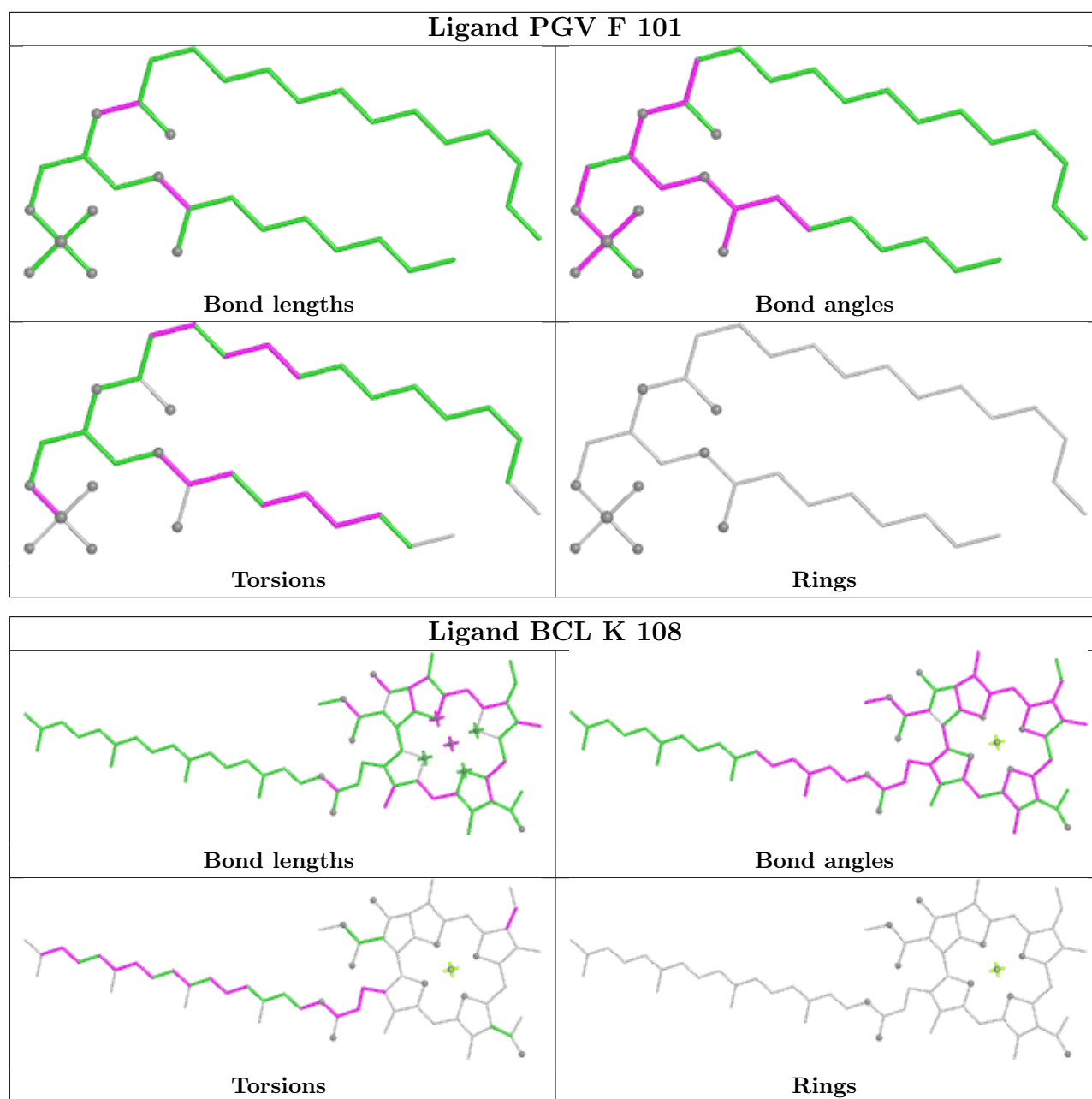


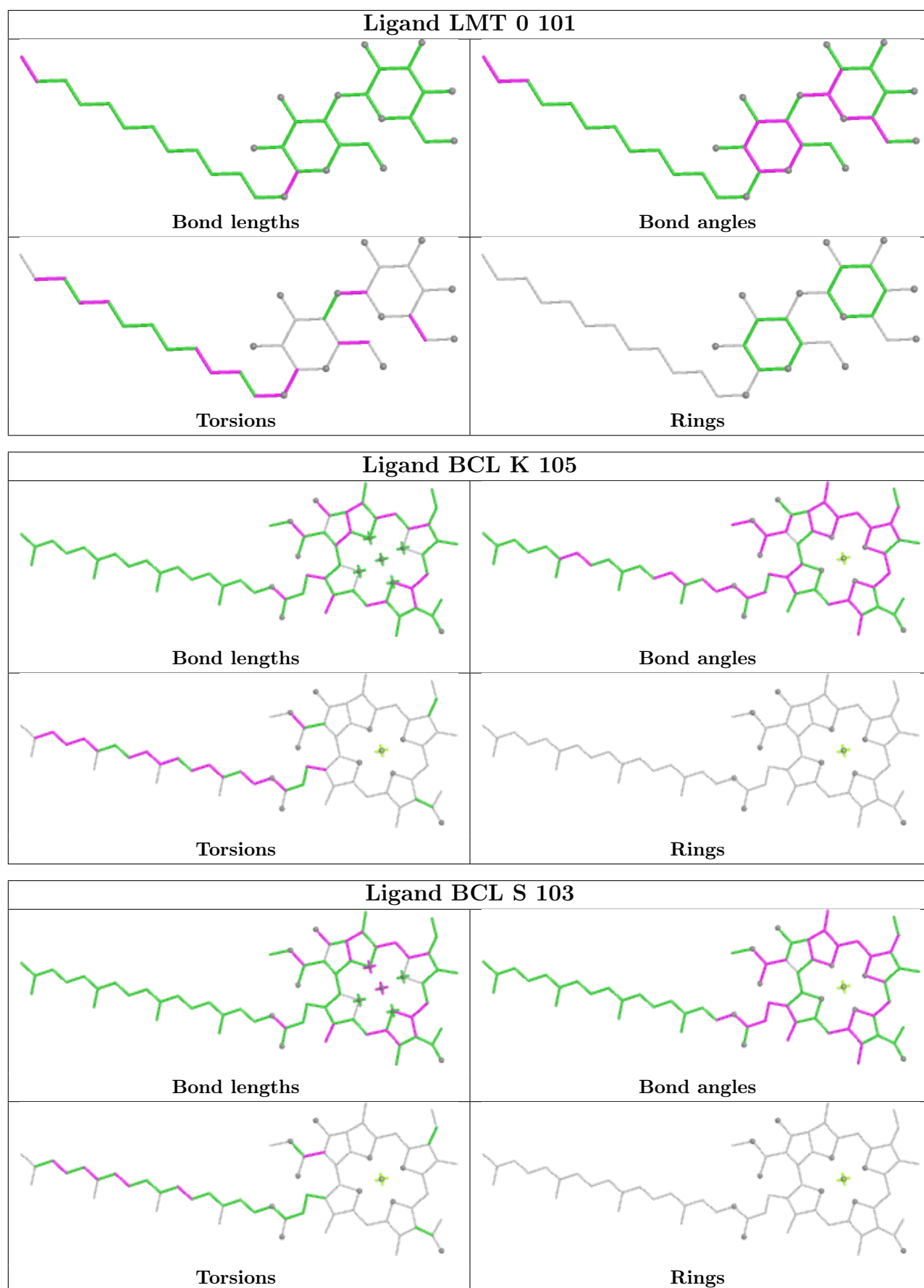


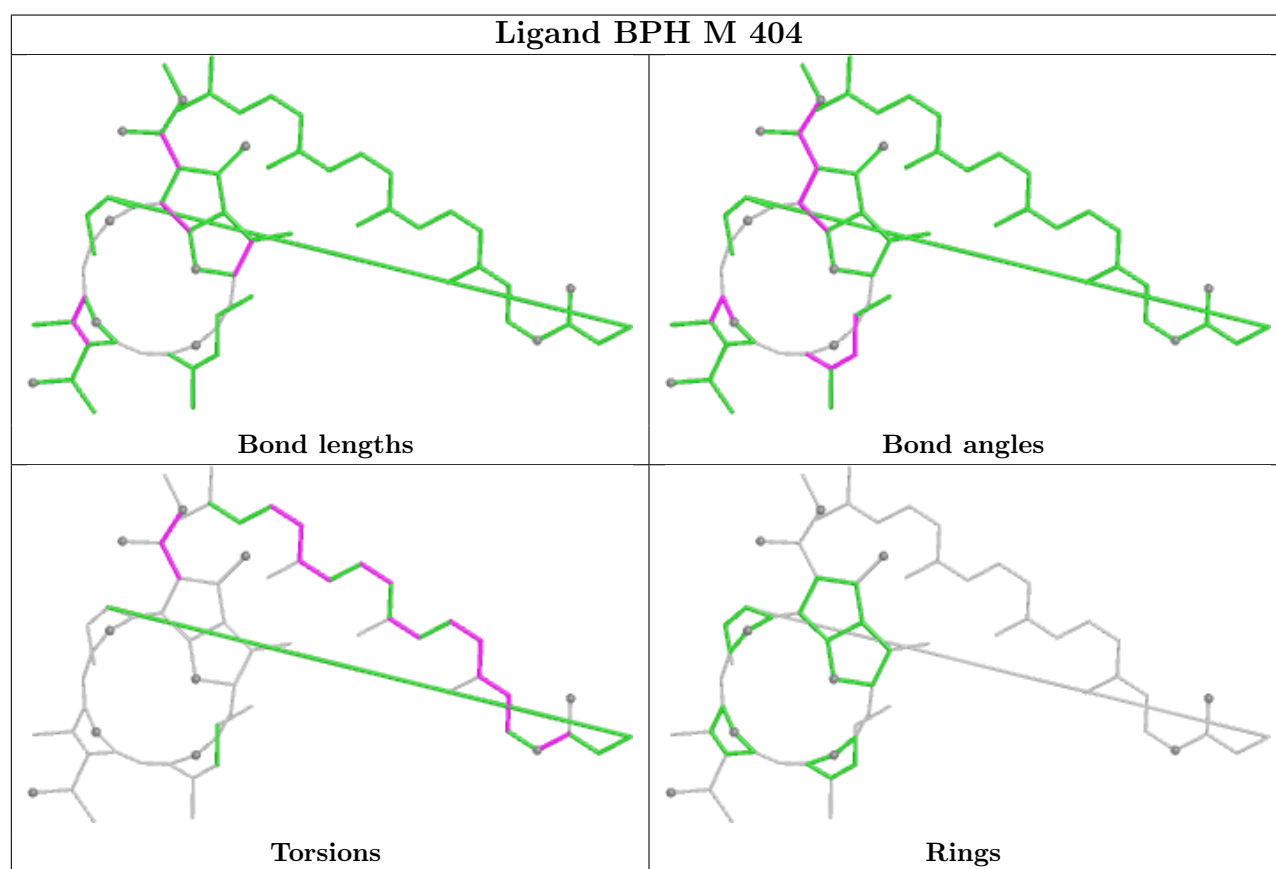
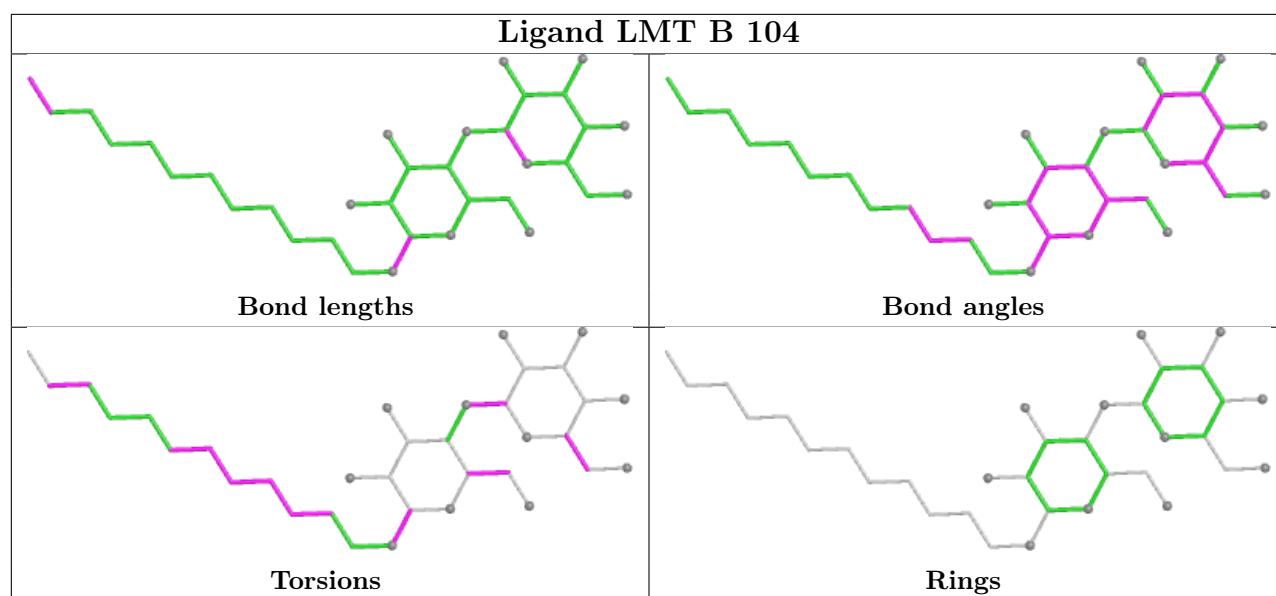


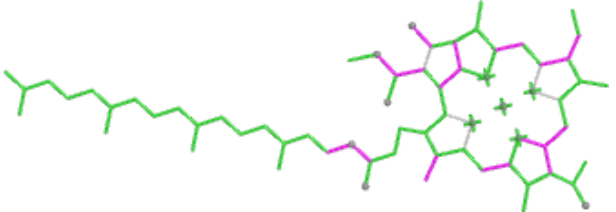
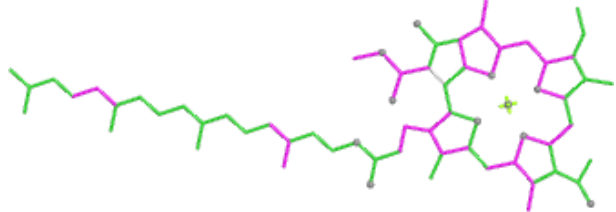
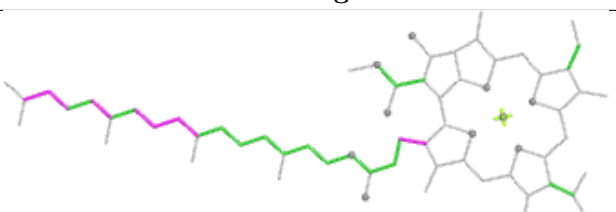
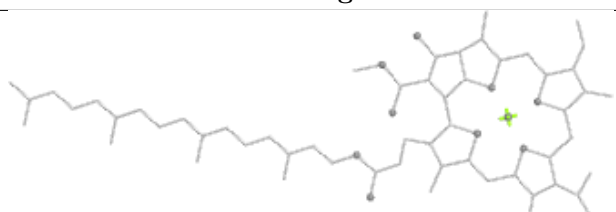
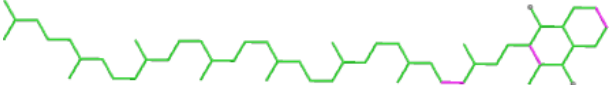
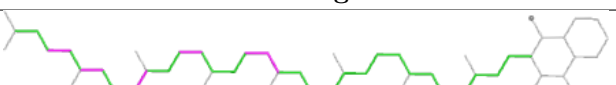
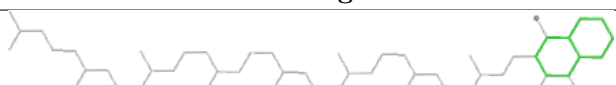
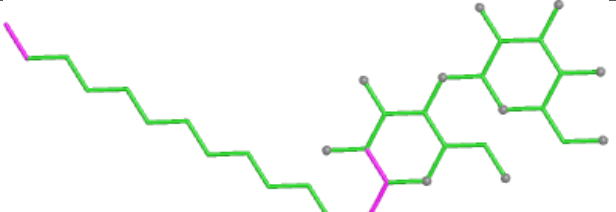
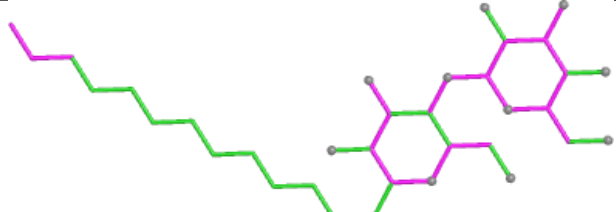
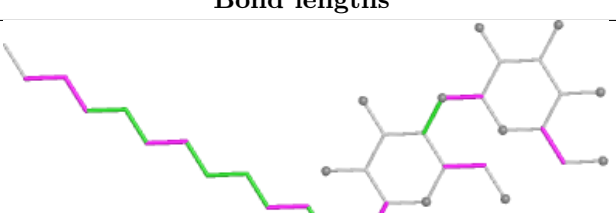
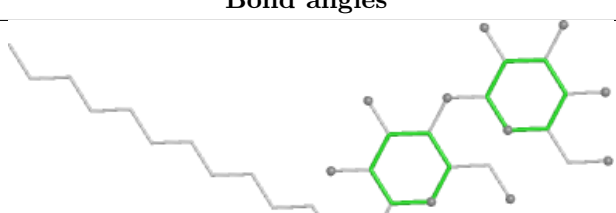


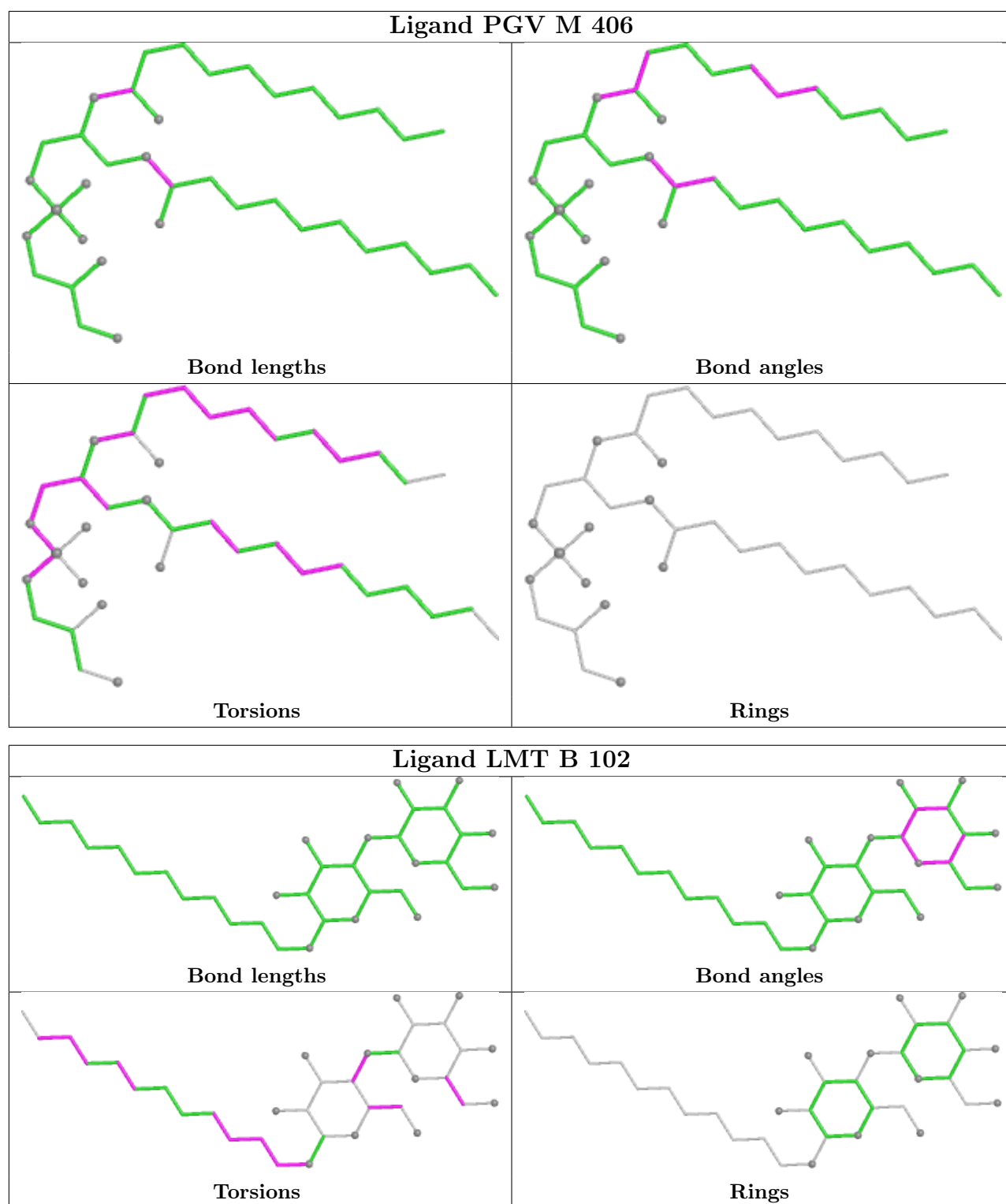


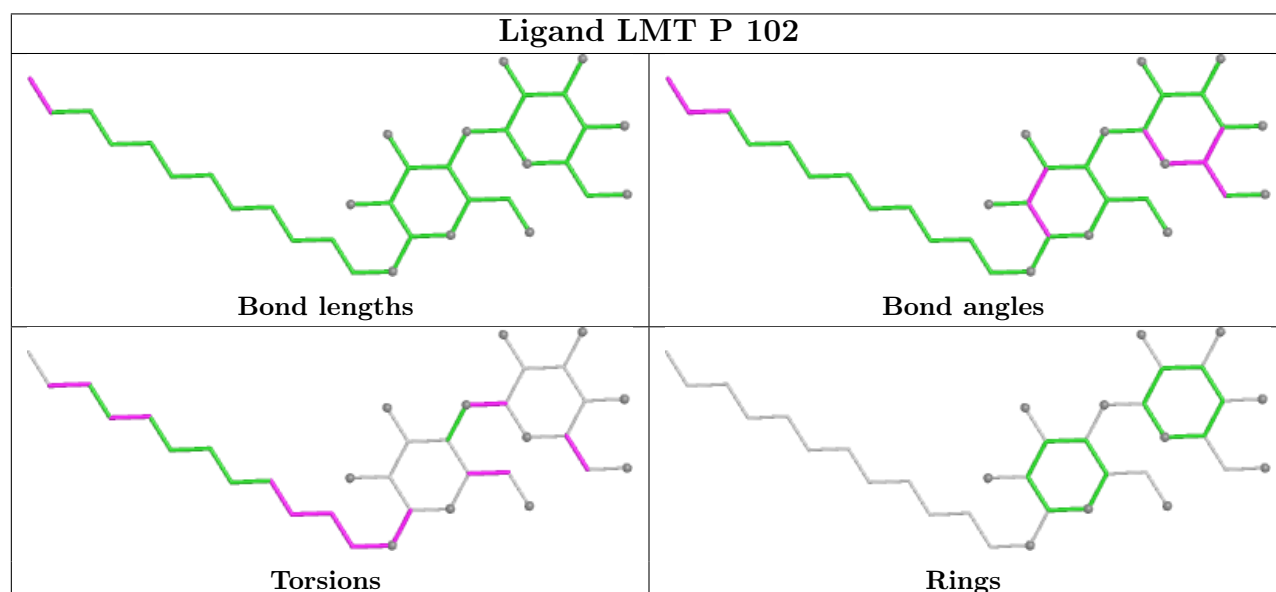
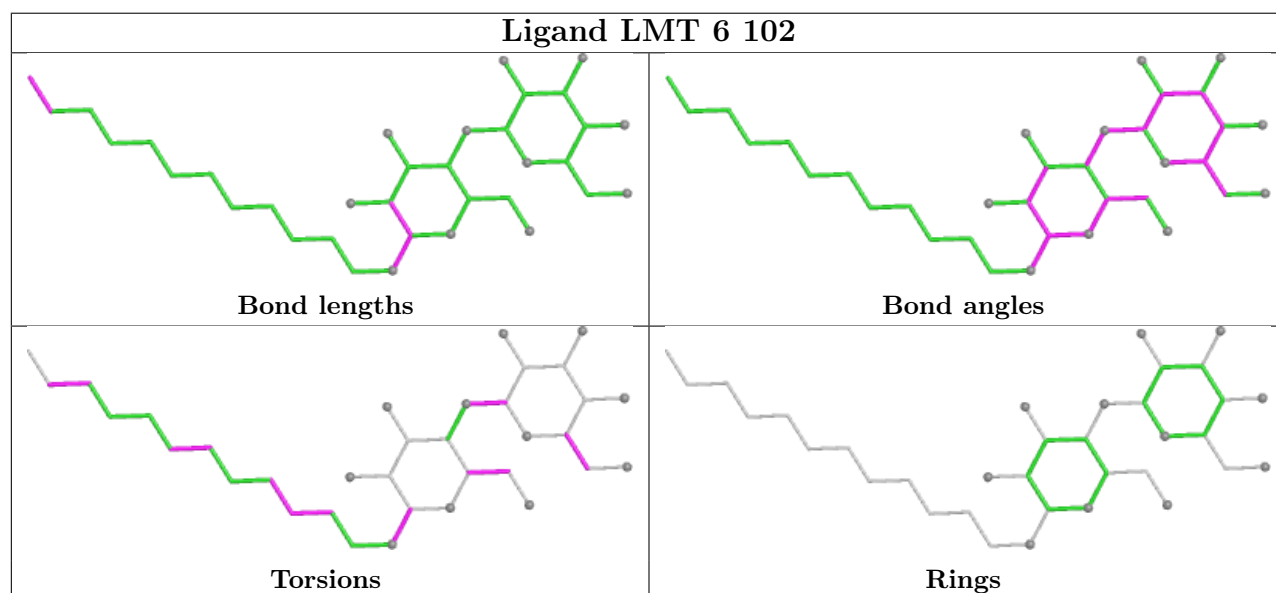
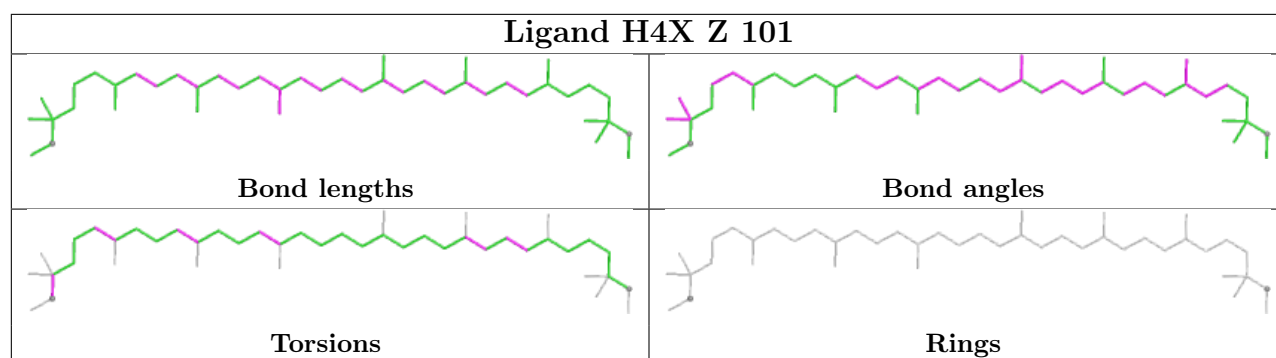


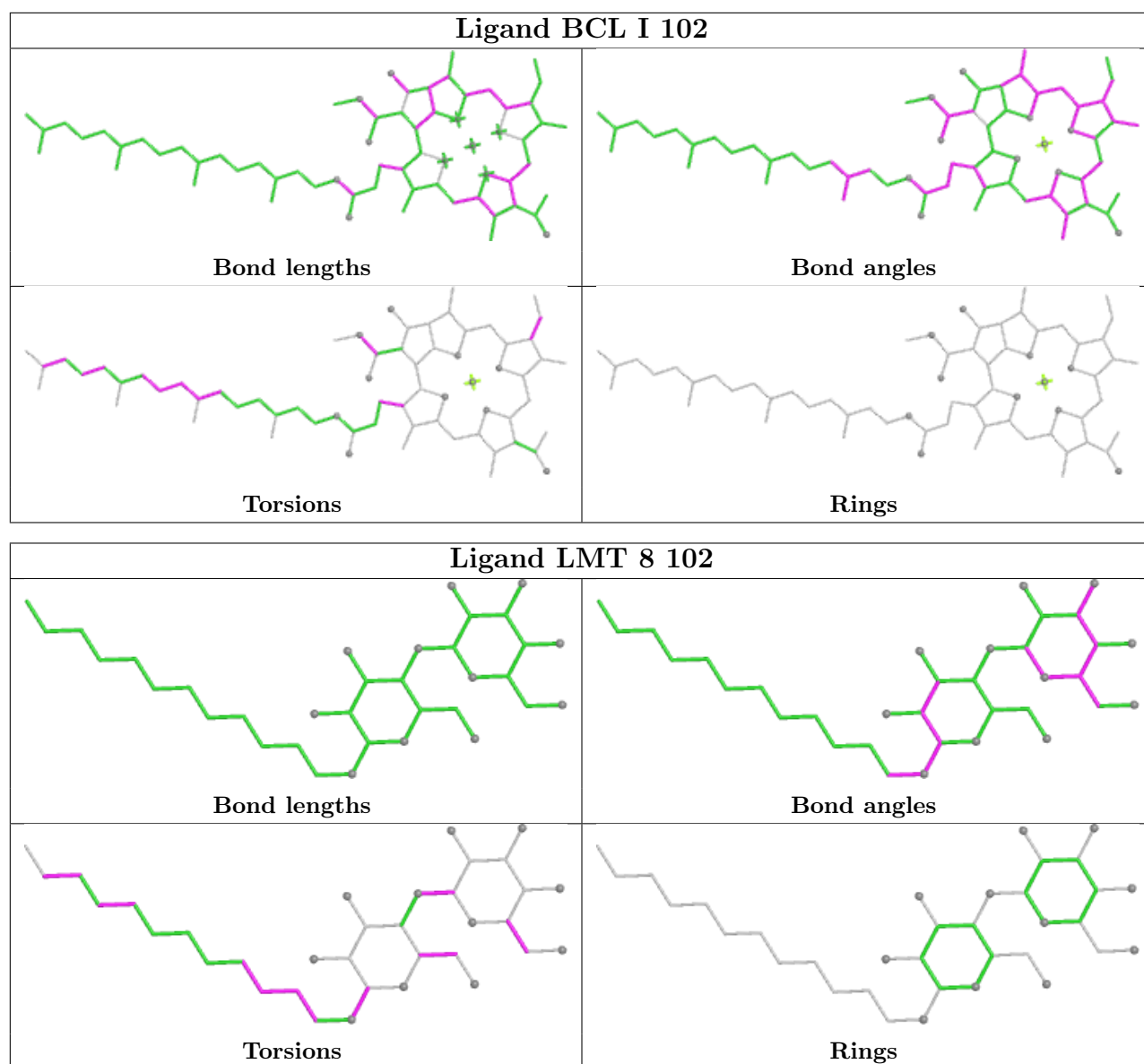


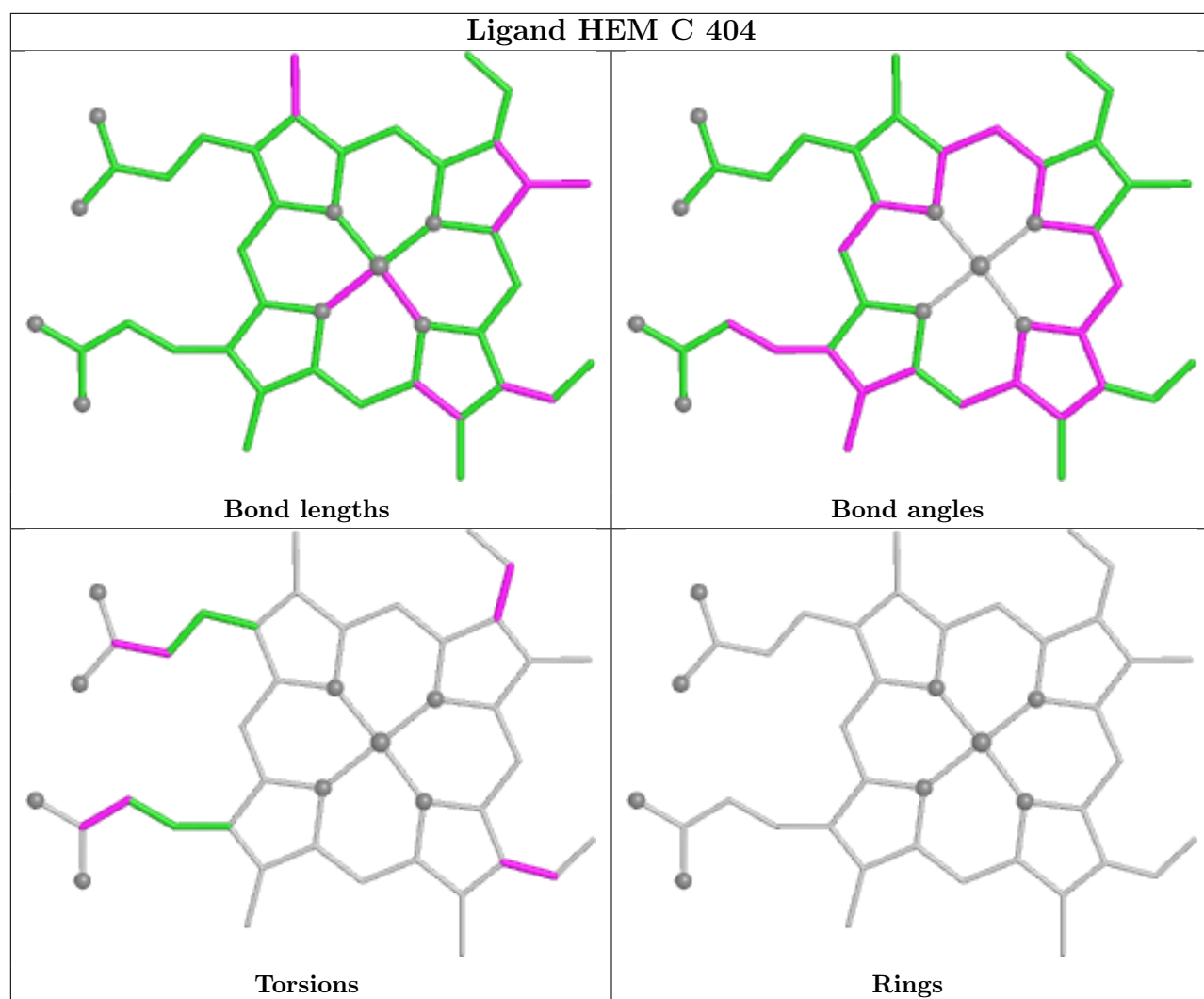


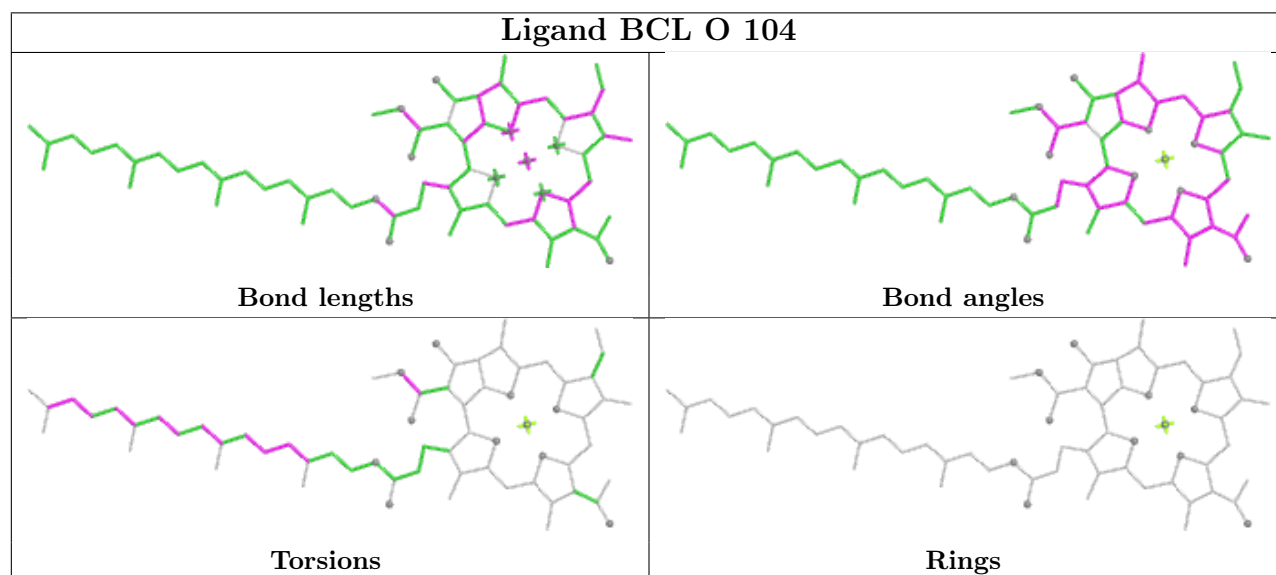
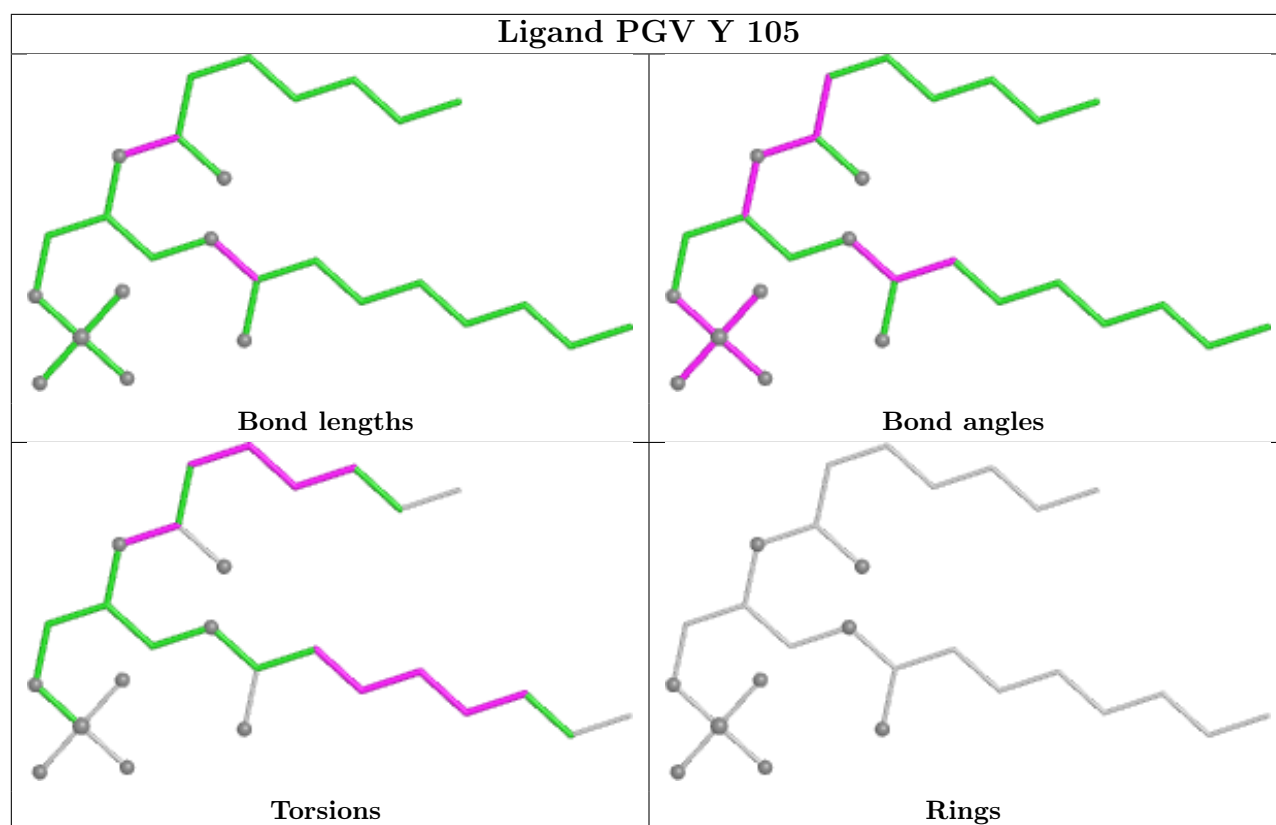
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MQ8 M 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT 2 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

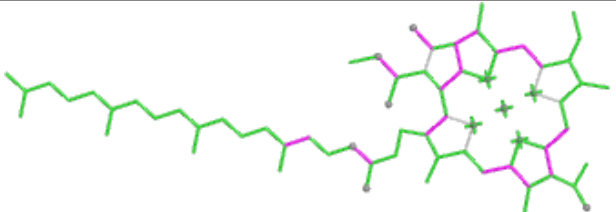
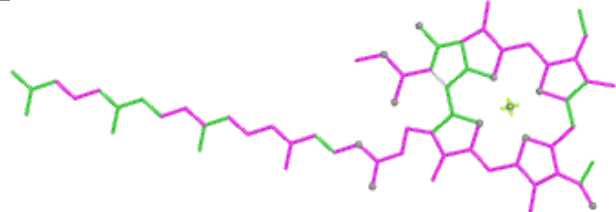
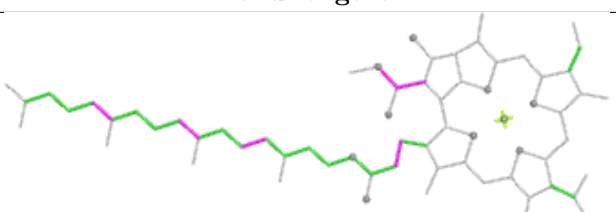
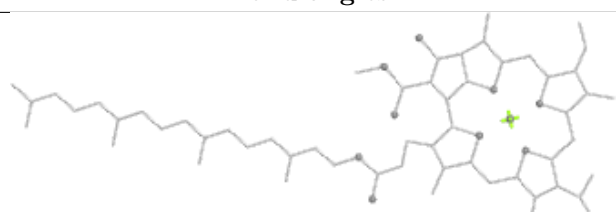
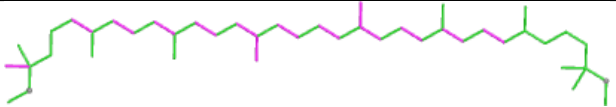
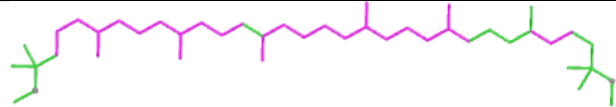
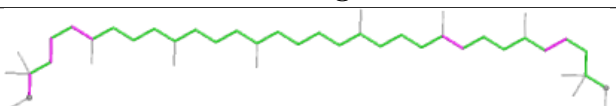
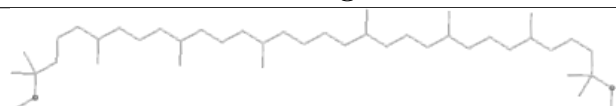
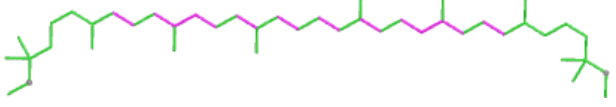
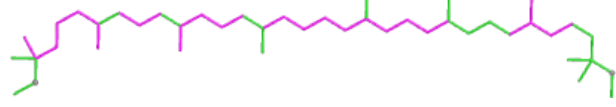
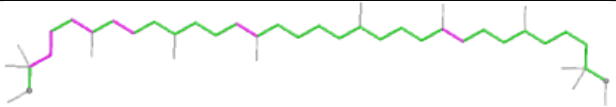
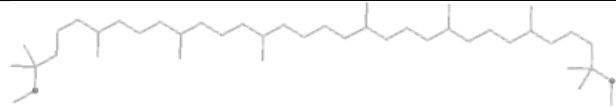


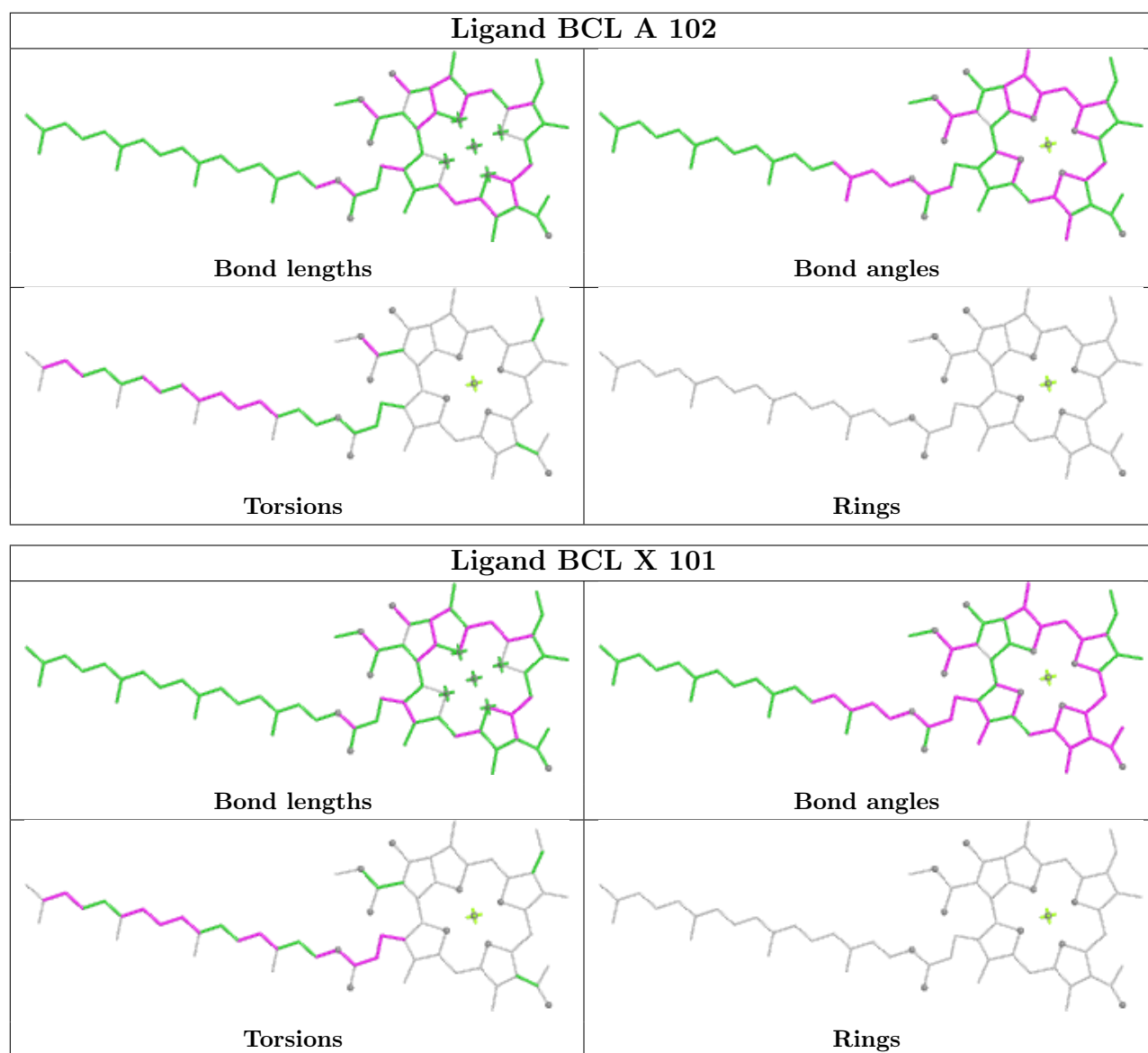


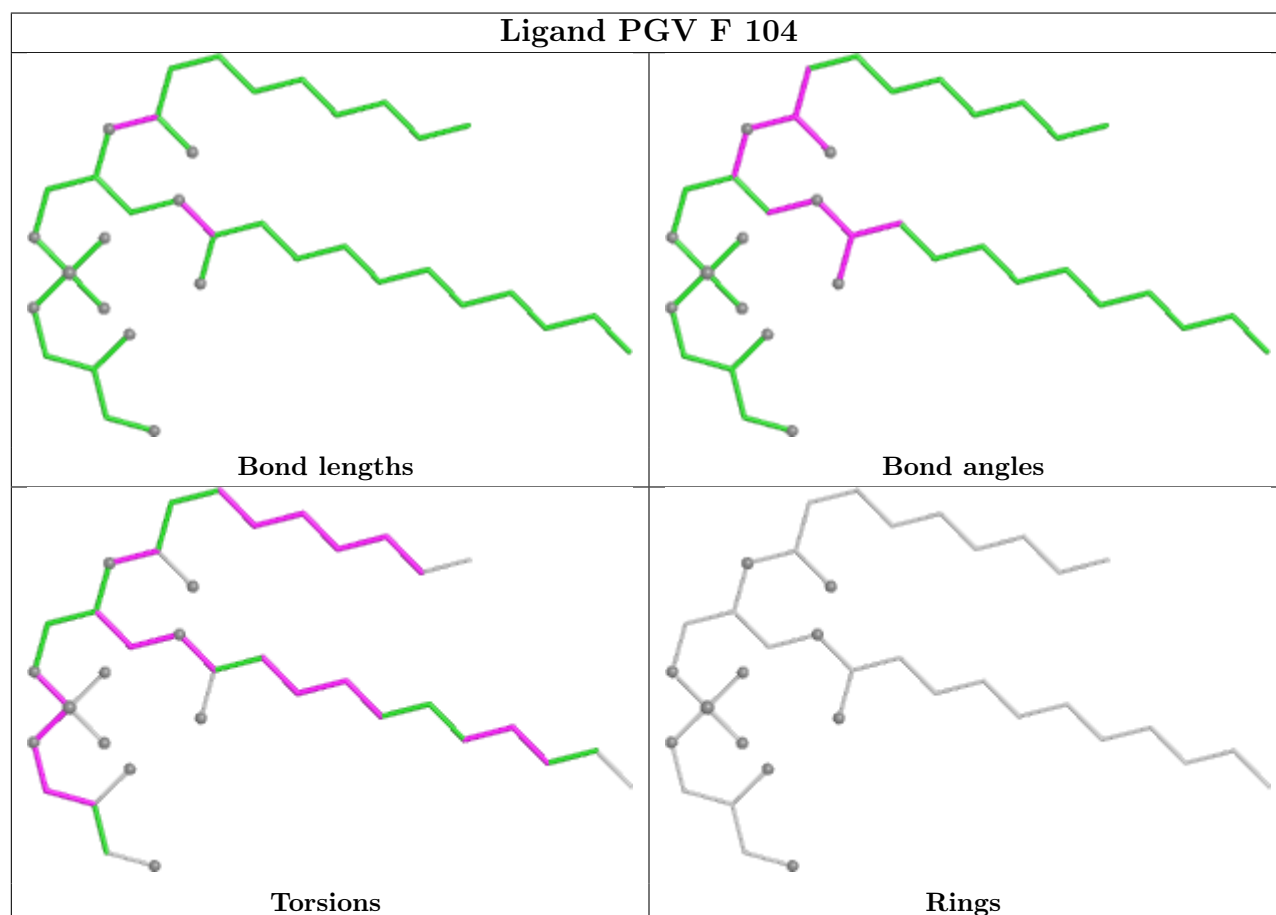
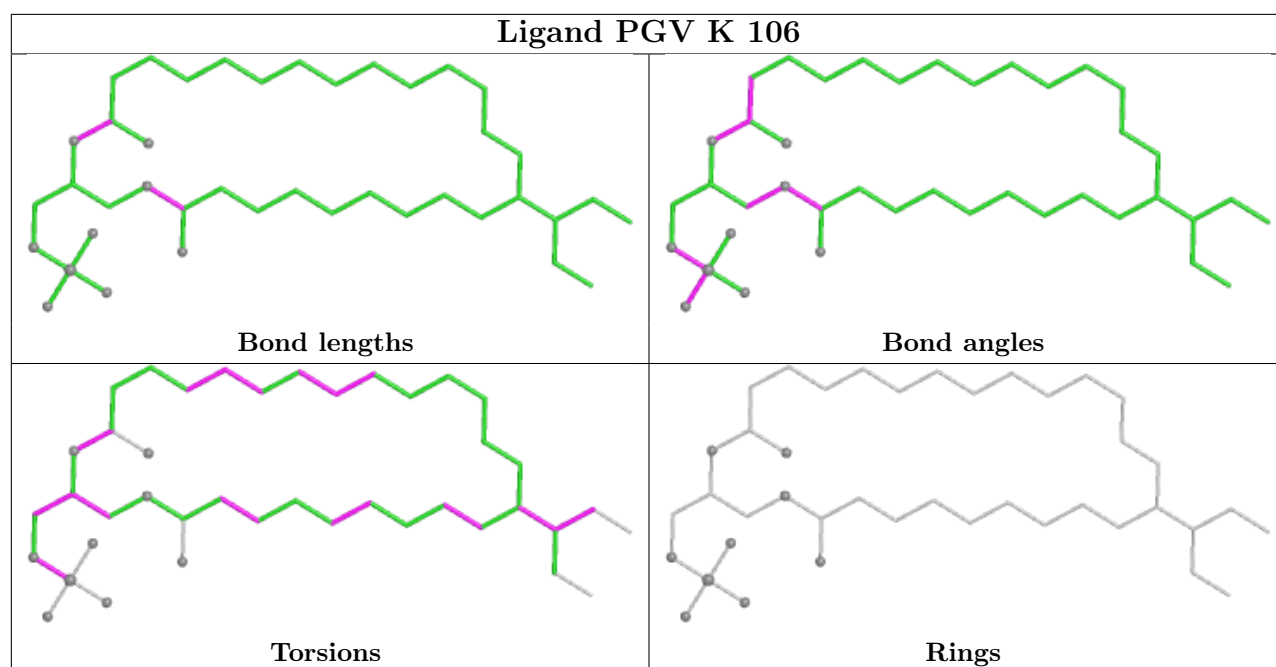


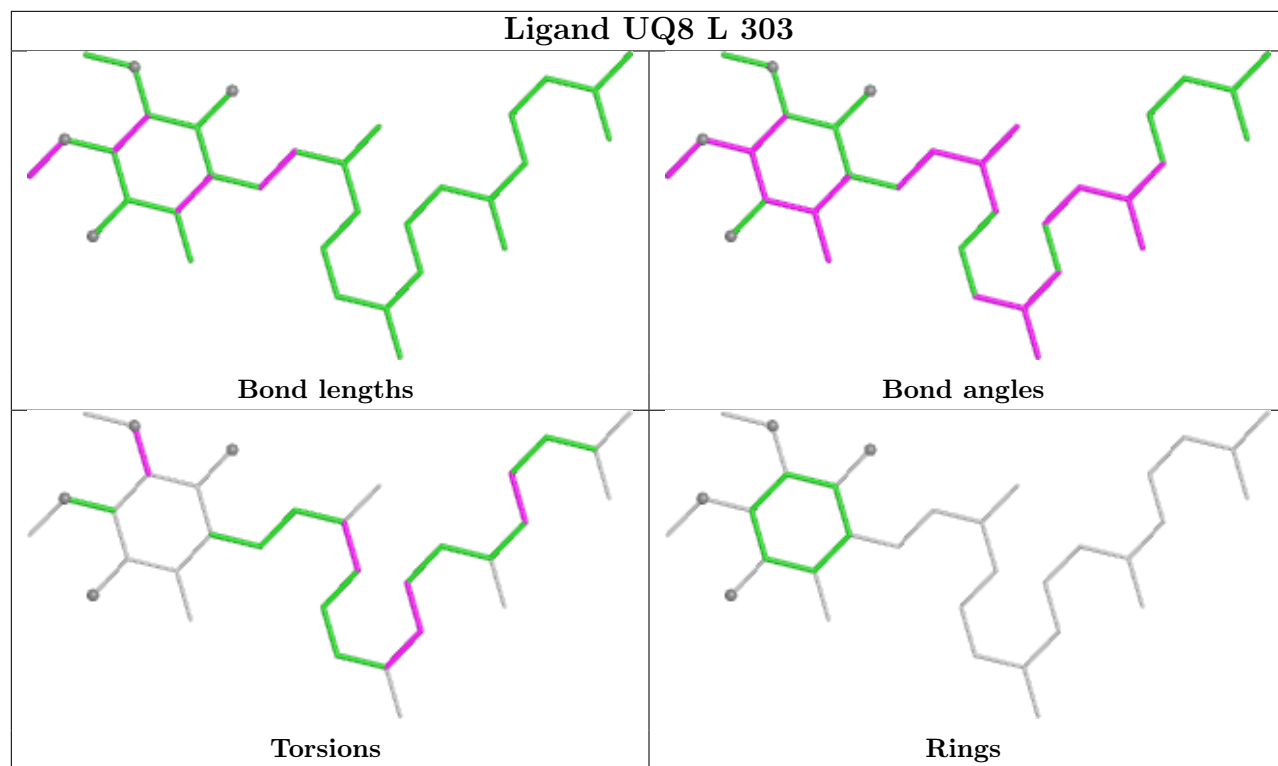


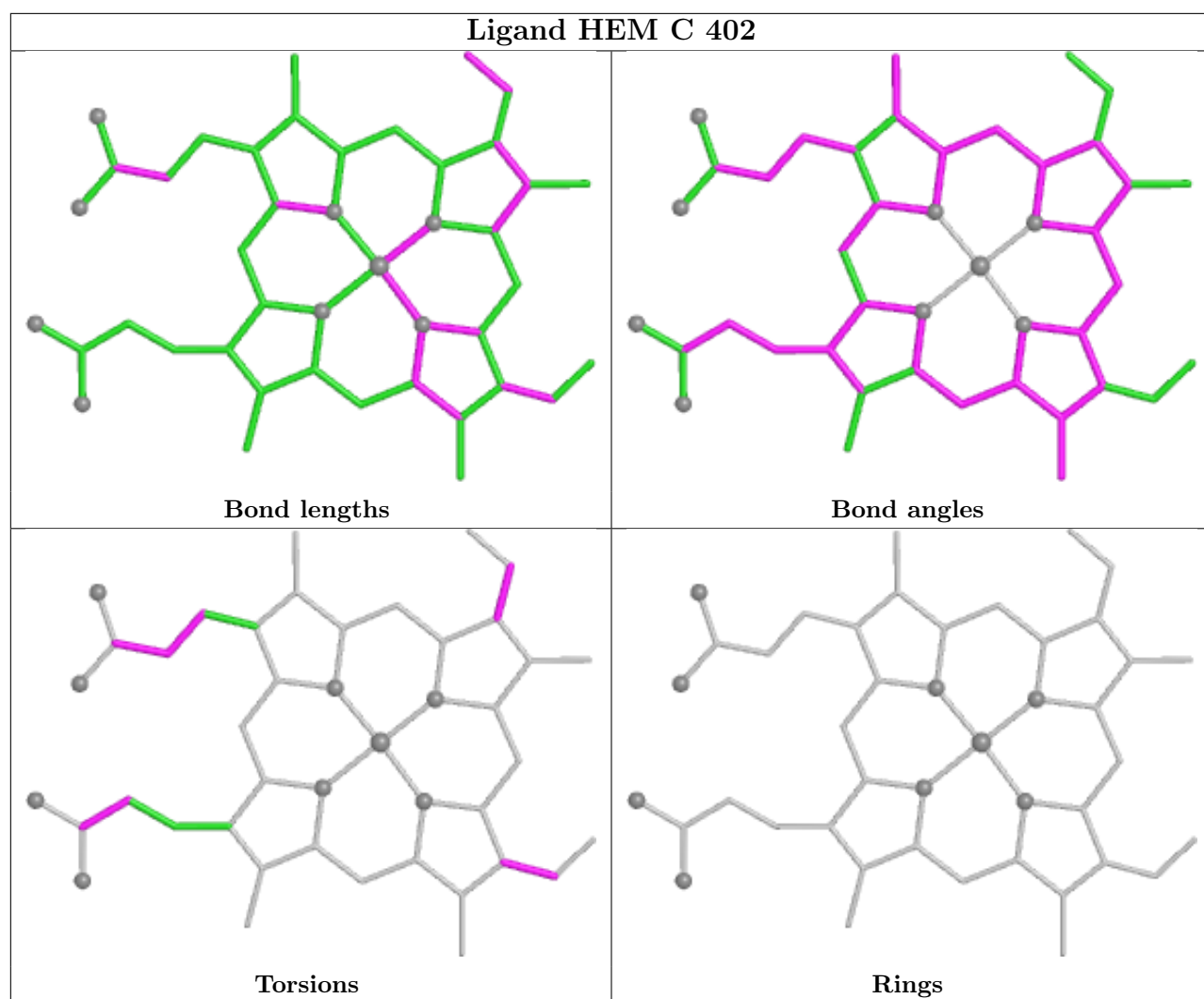


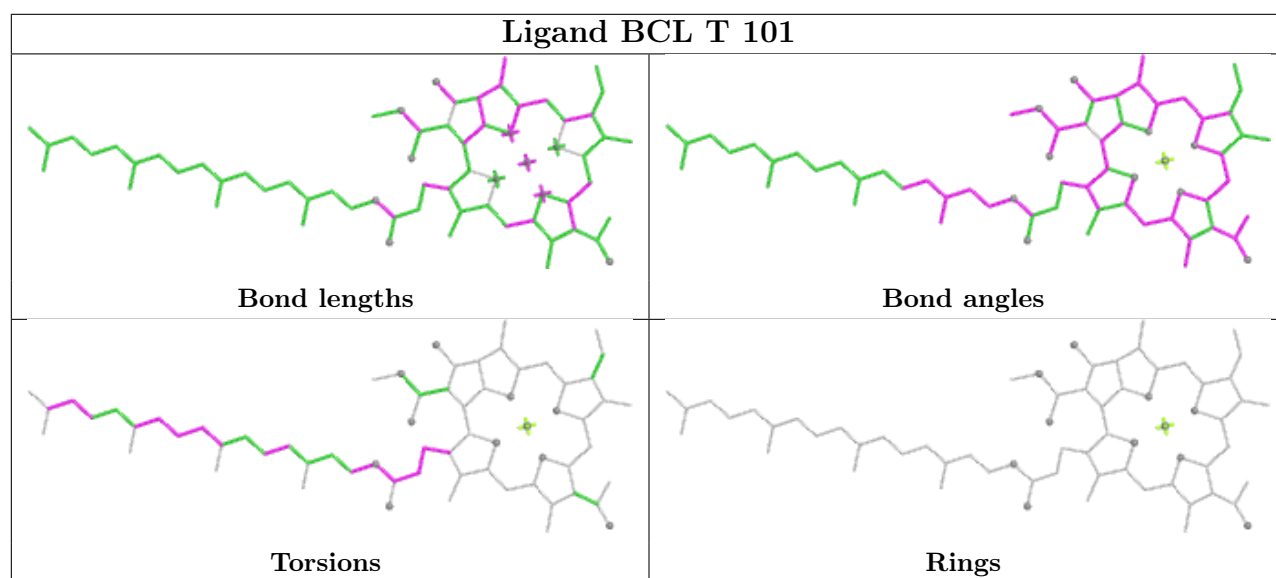
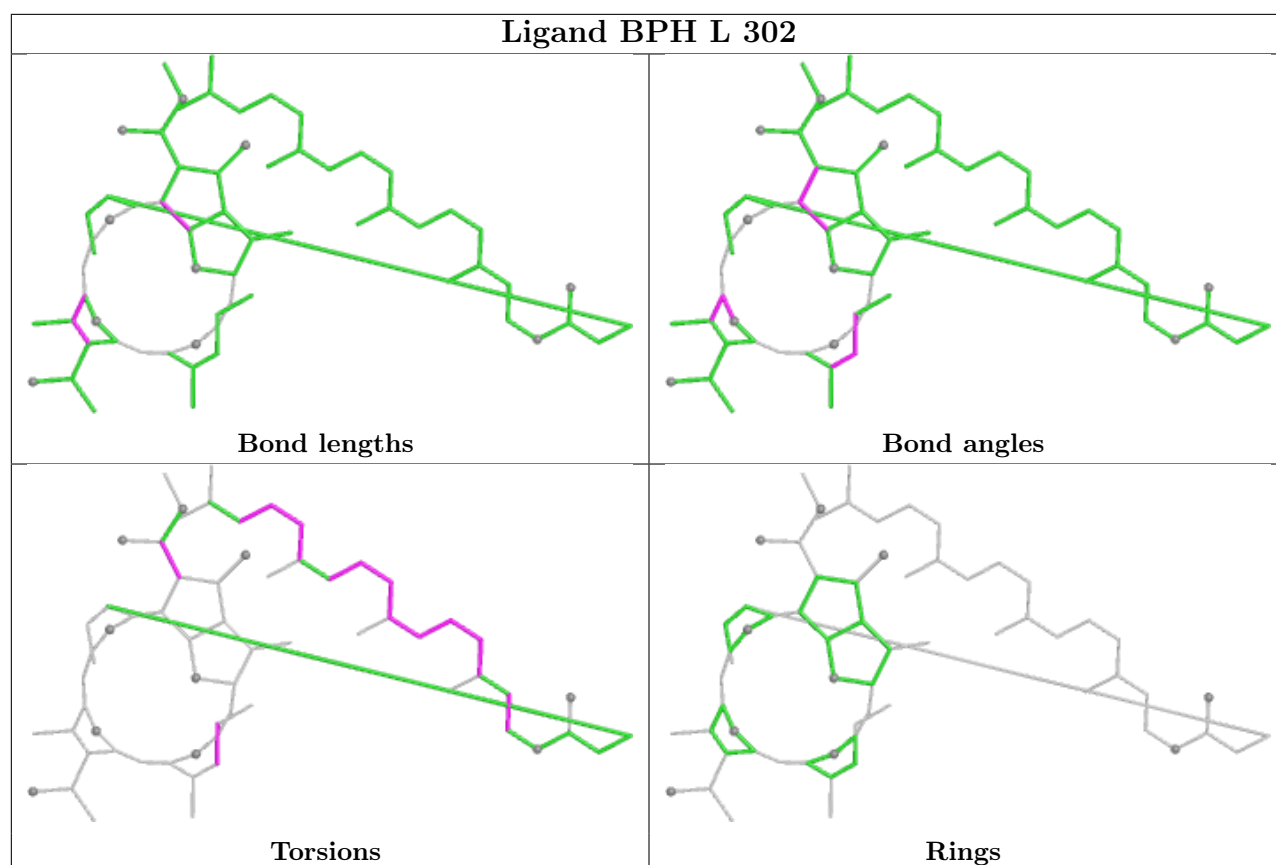
Ligand BCL L 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand H4X G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand H4X 4 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

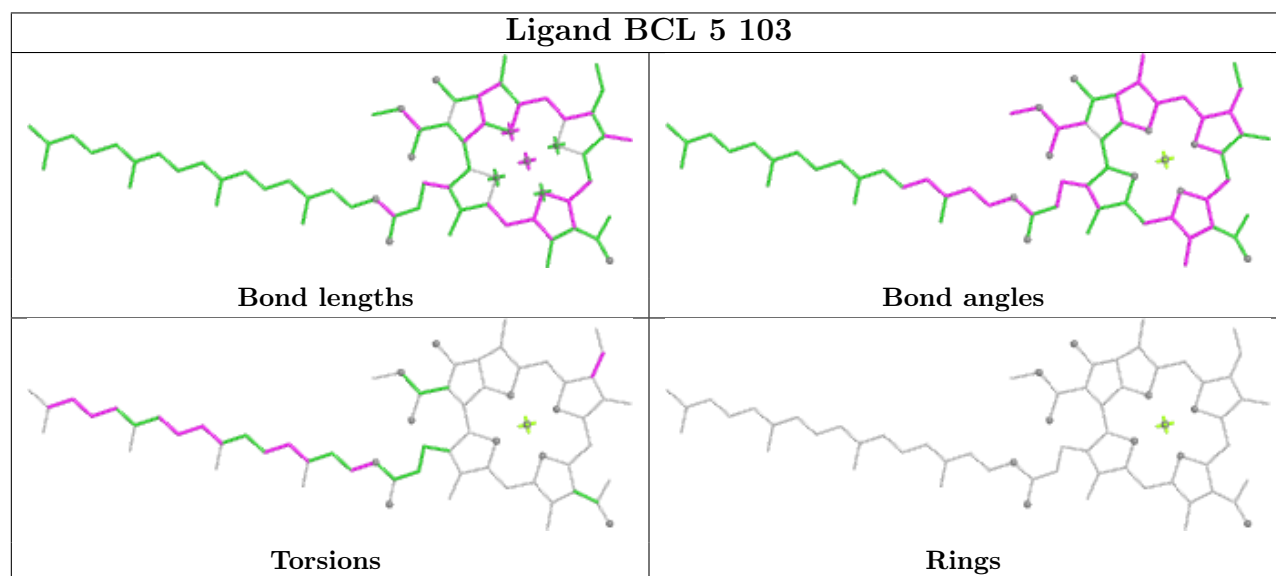
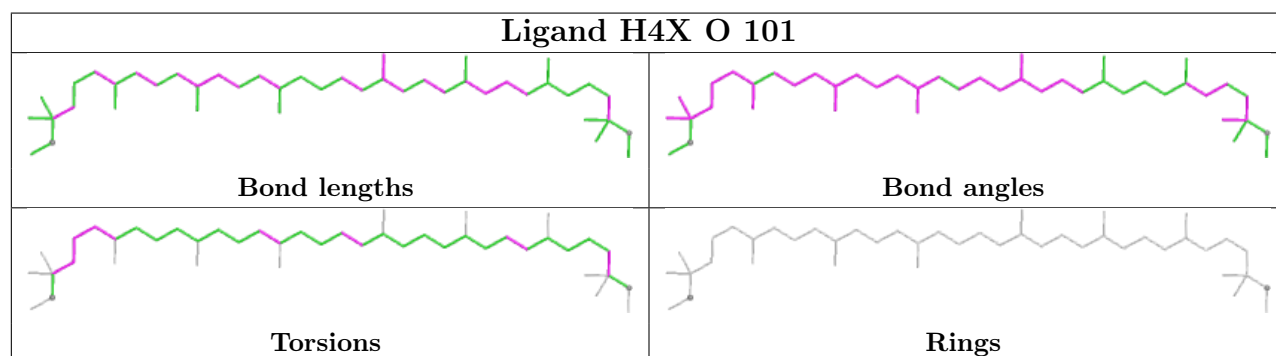
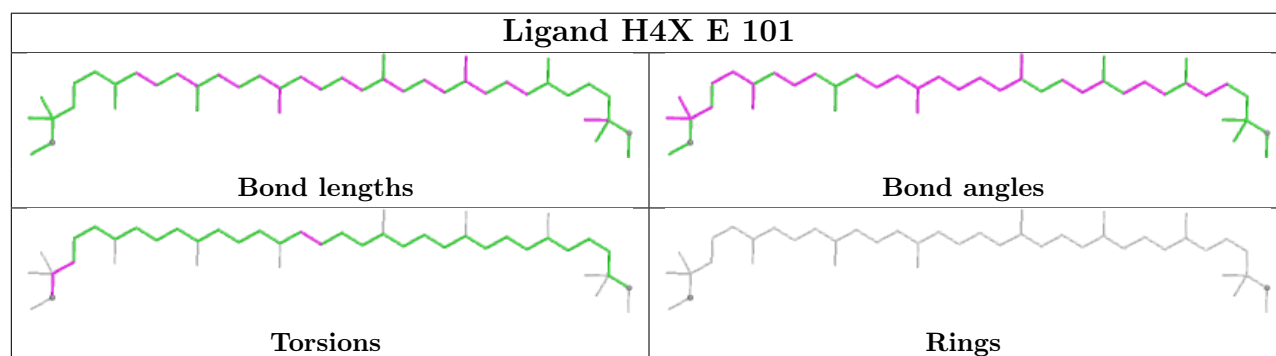
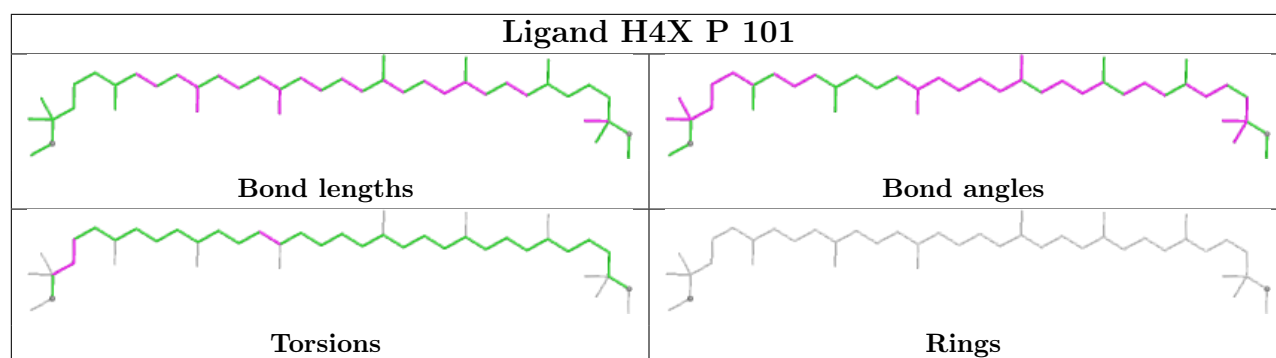


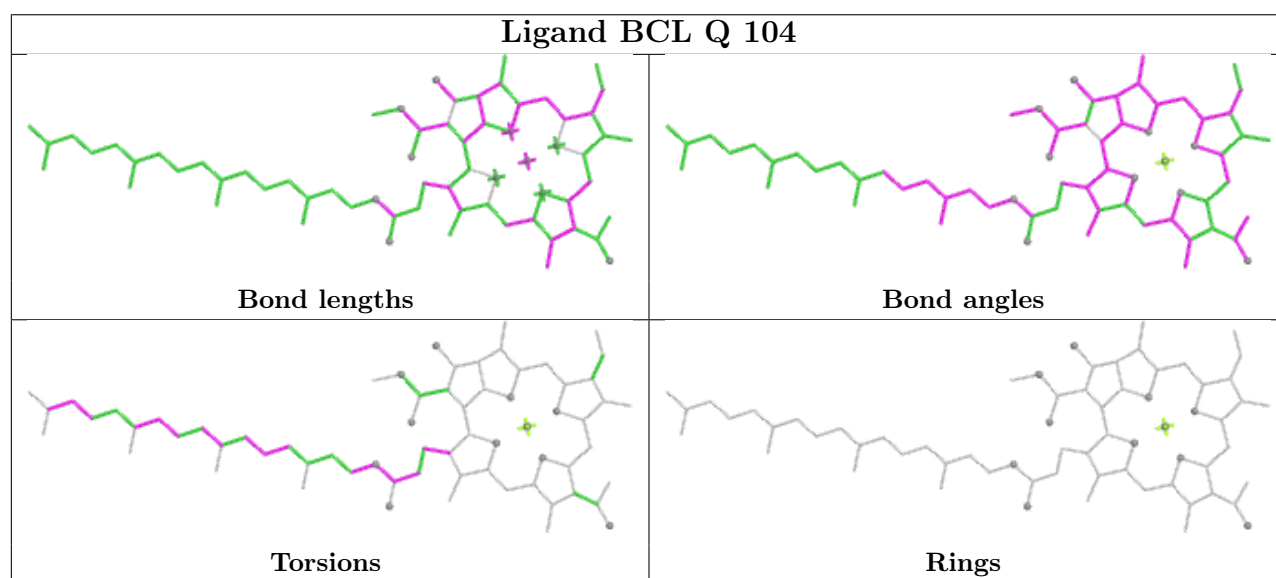
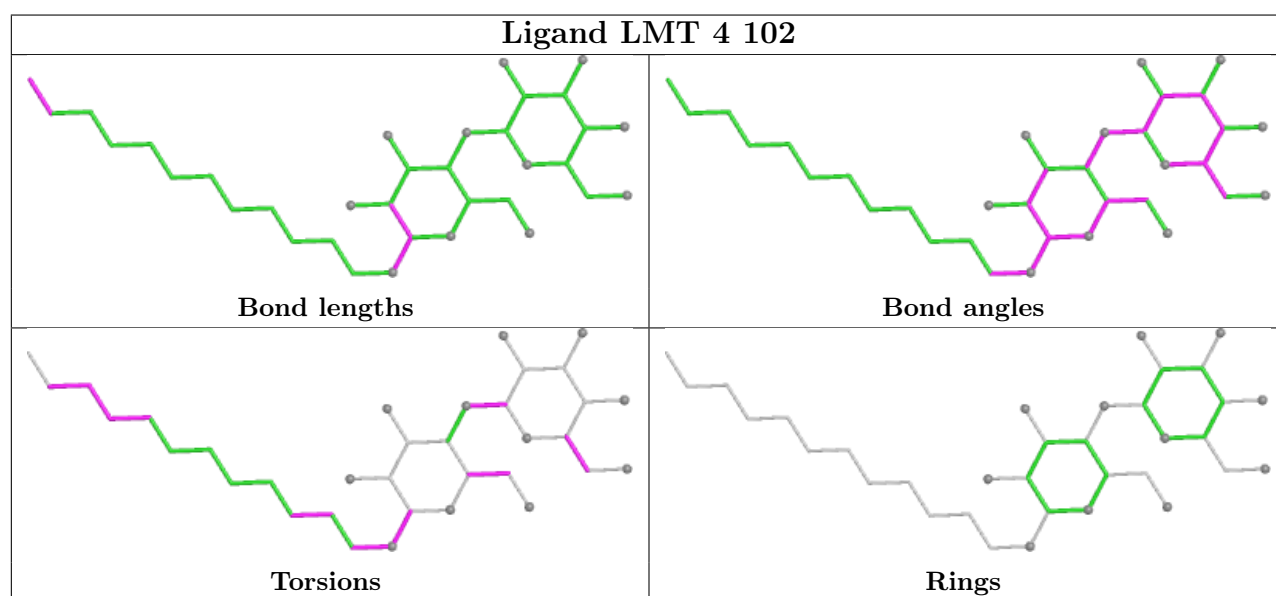
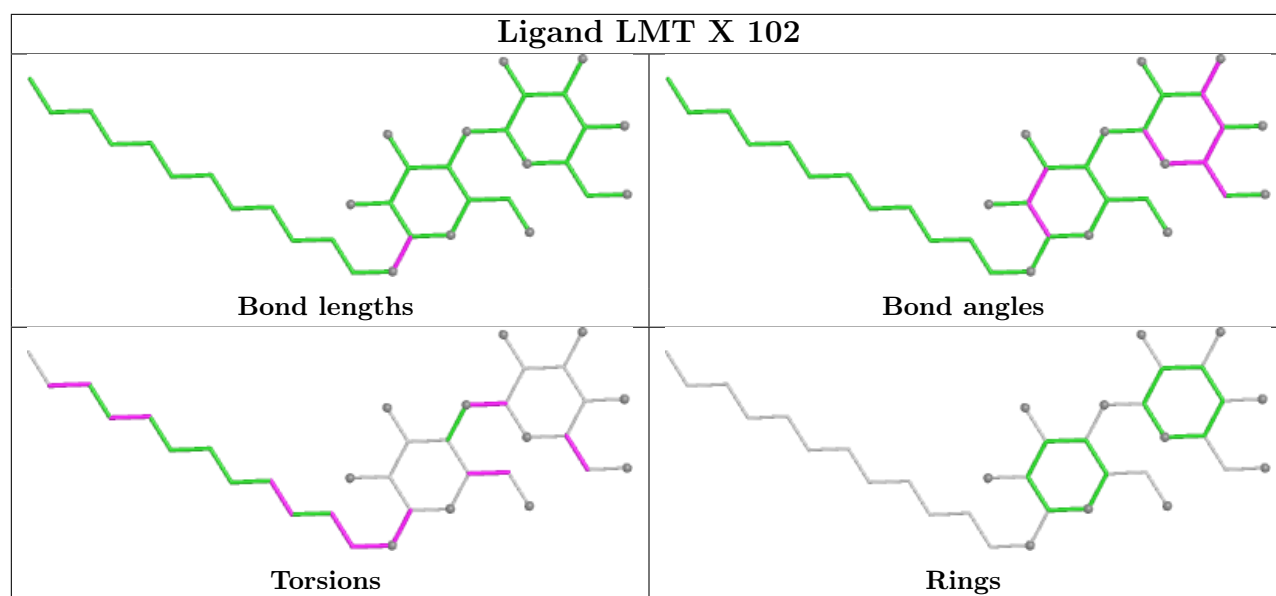


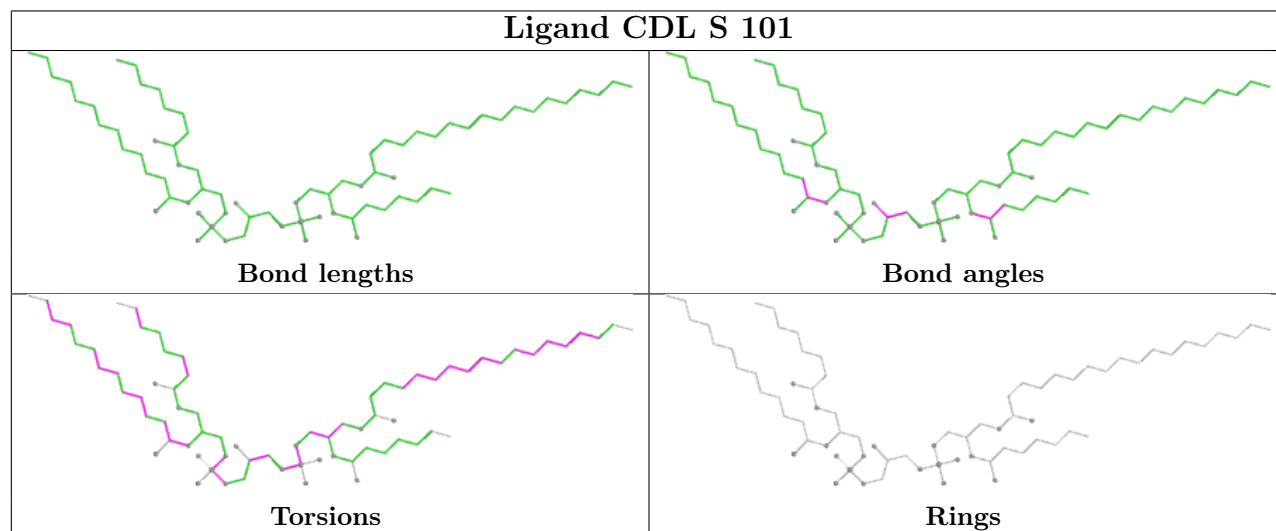
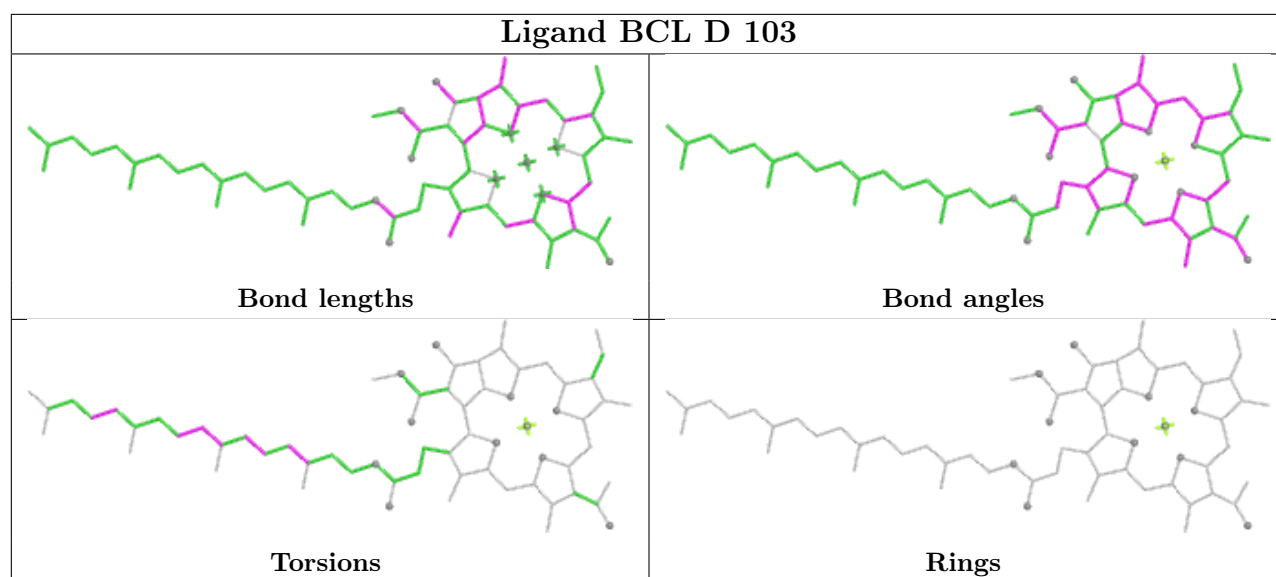


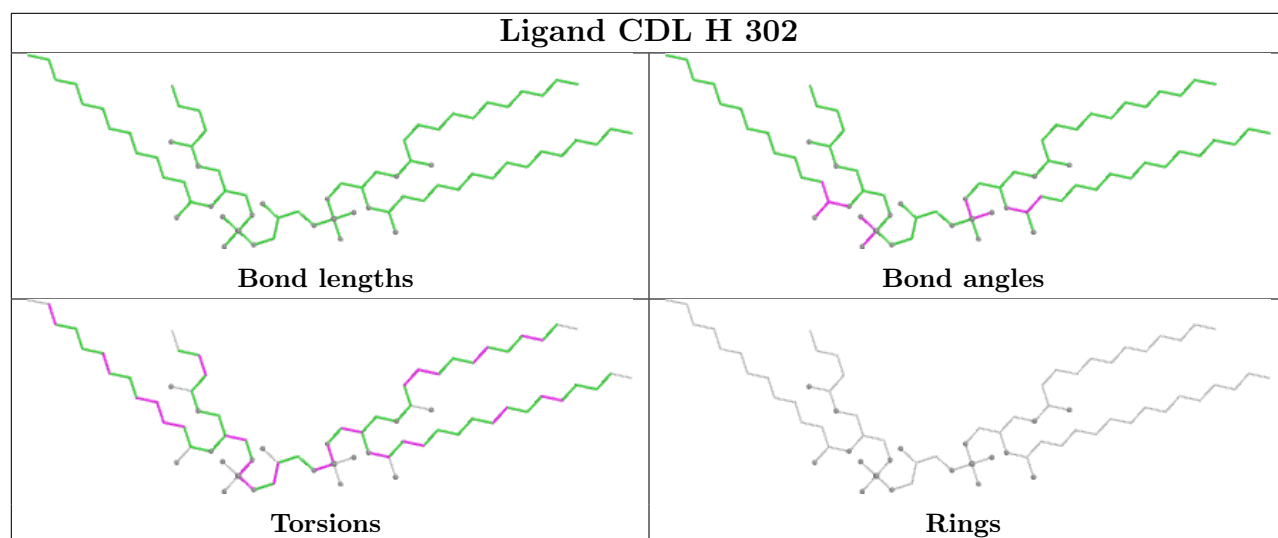
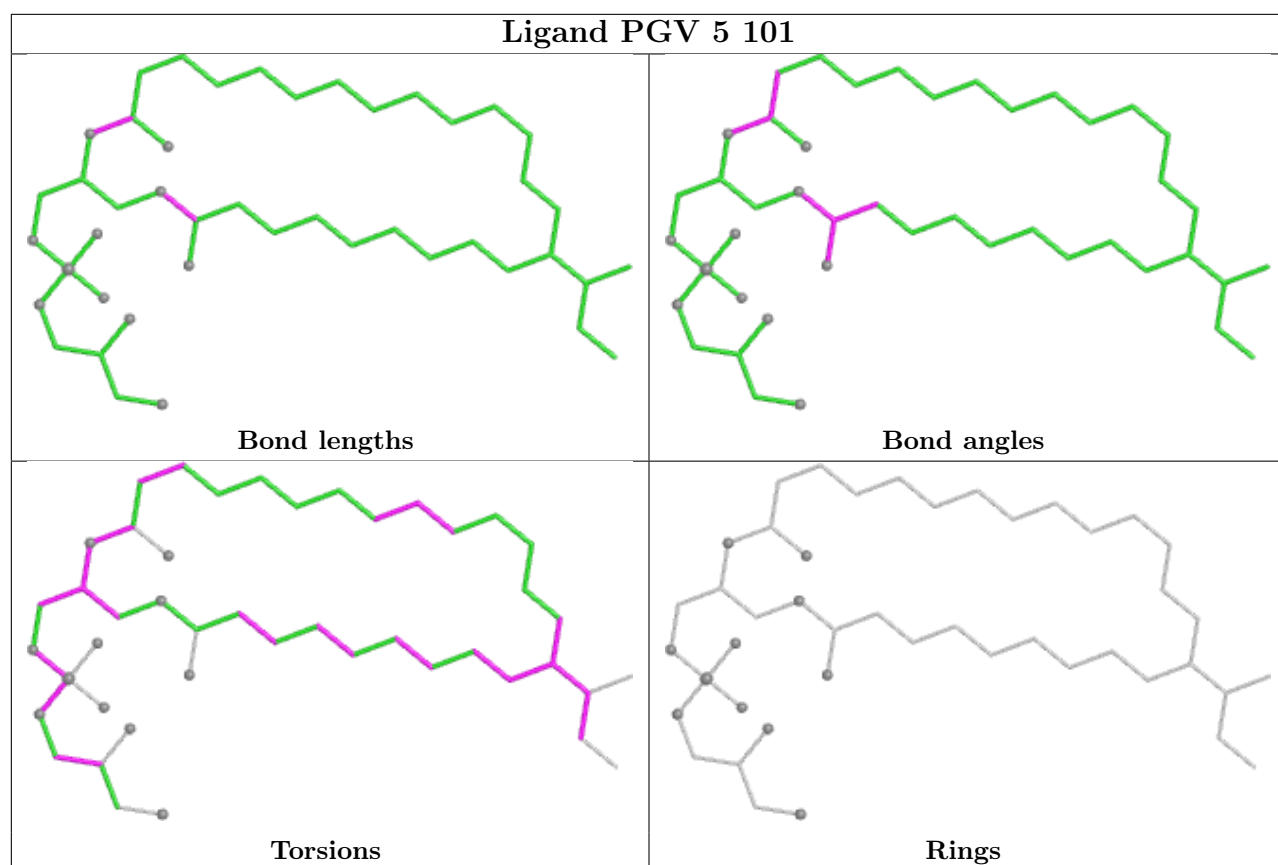


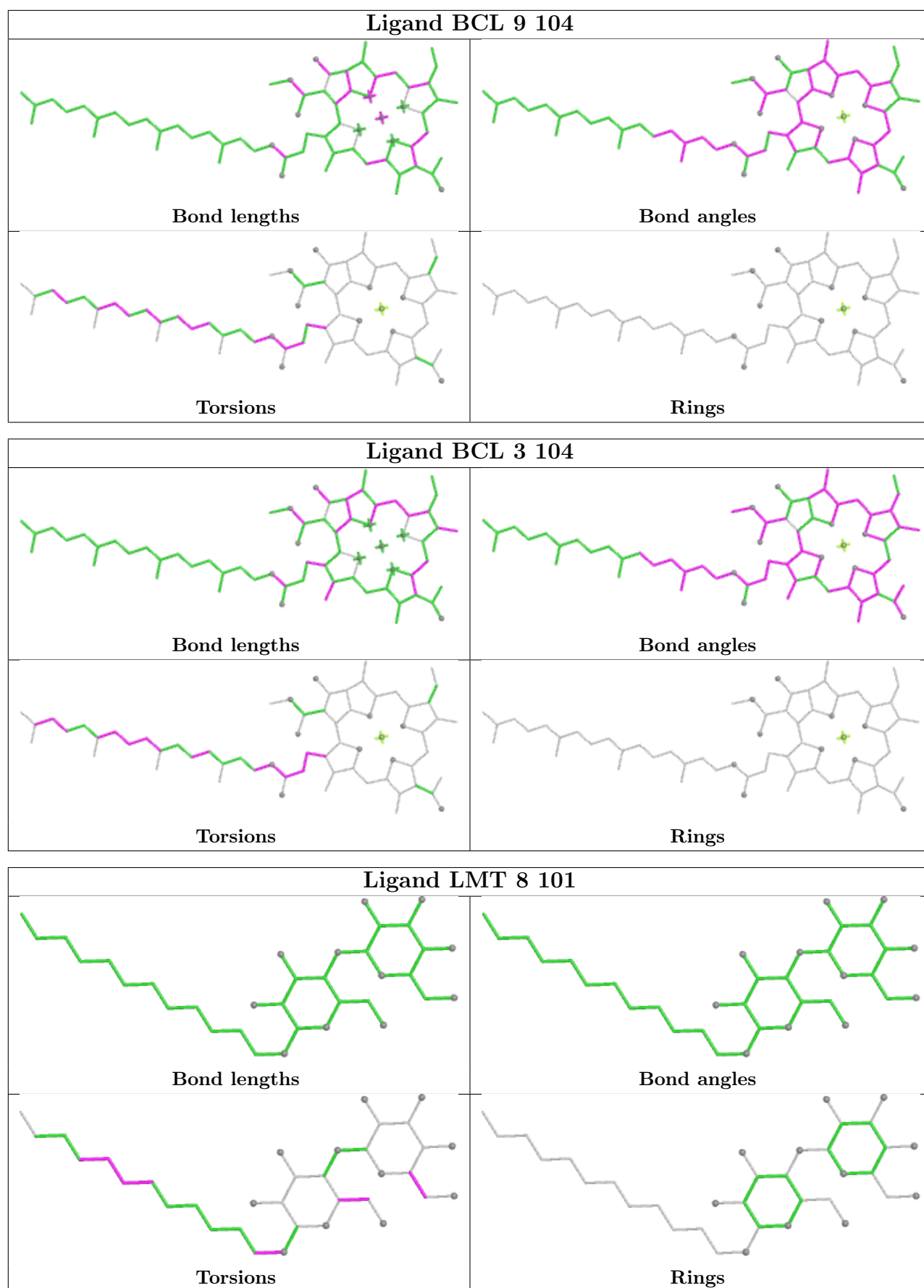


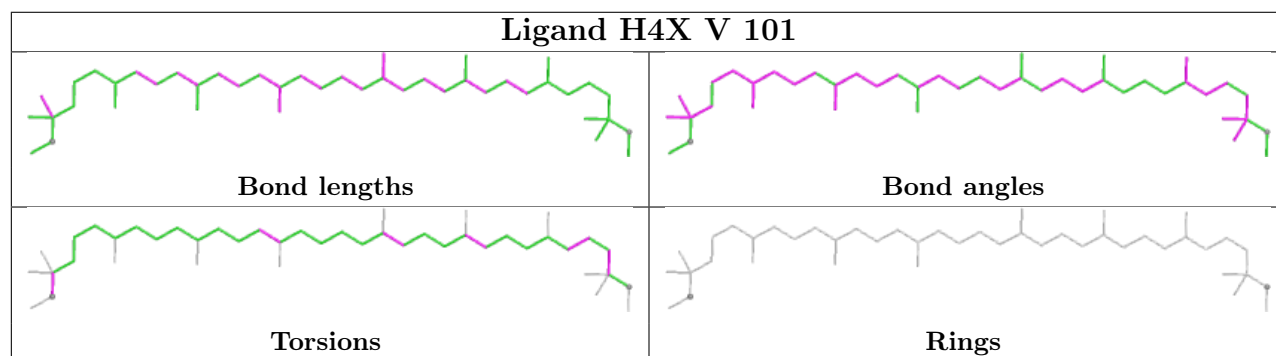
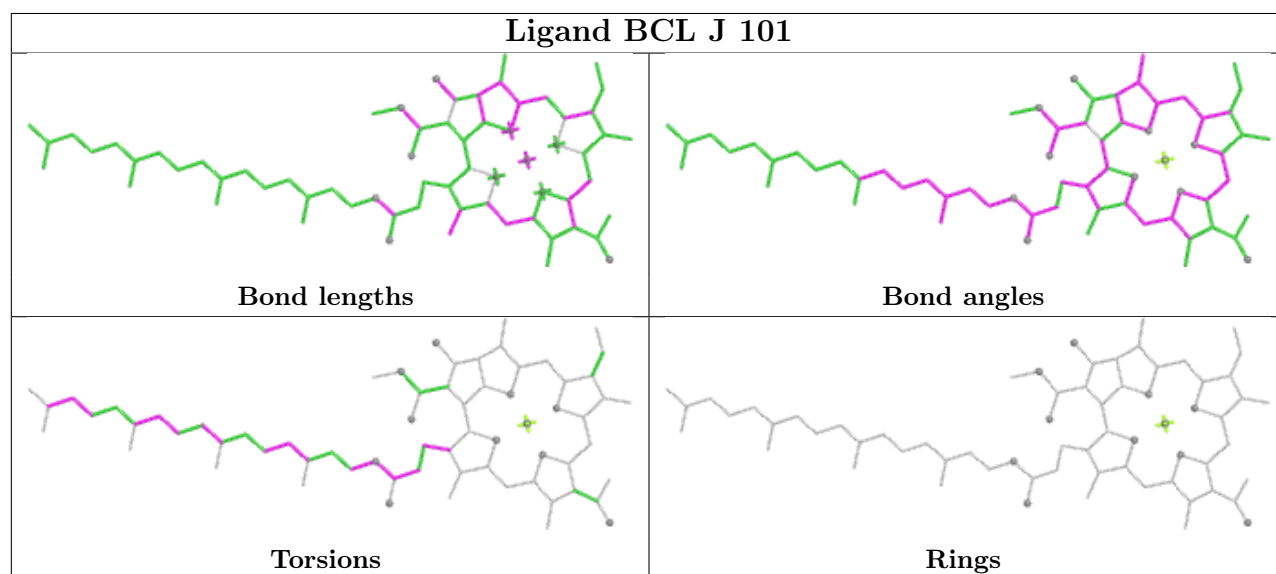
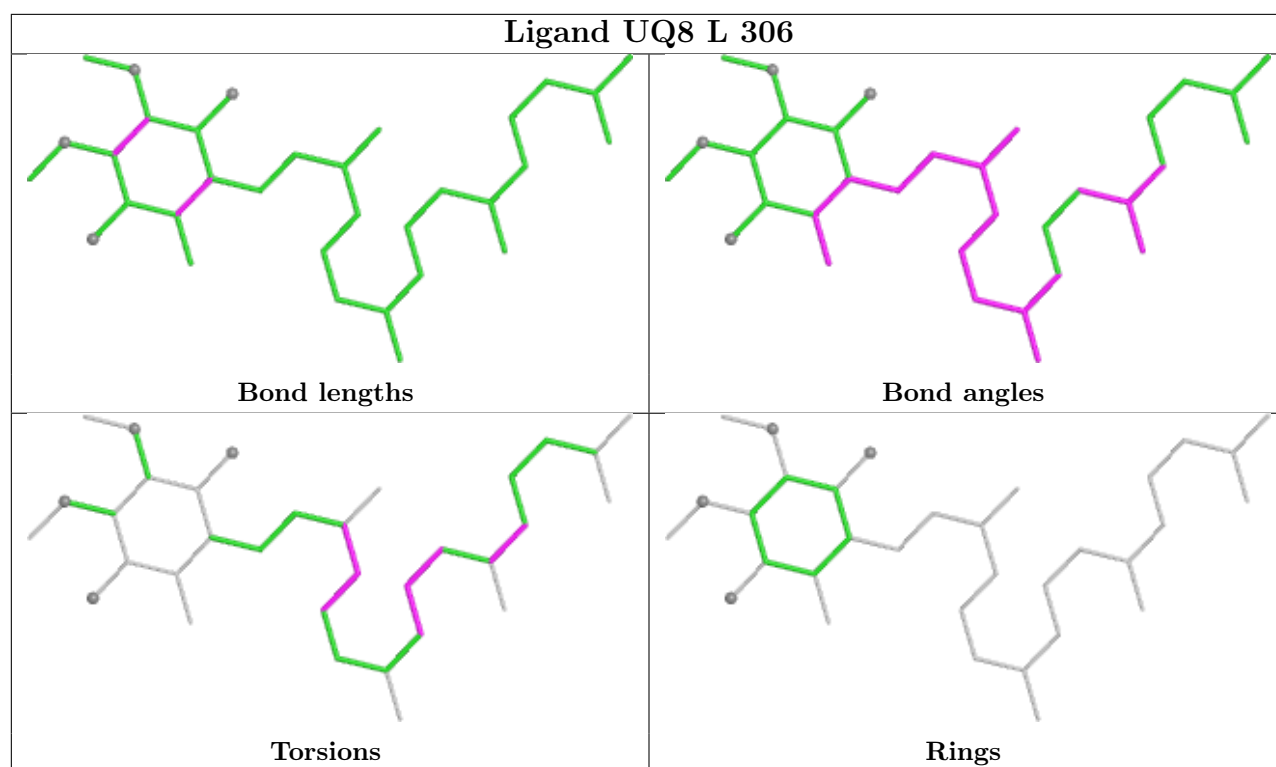


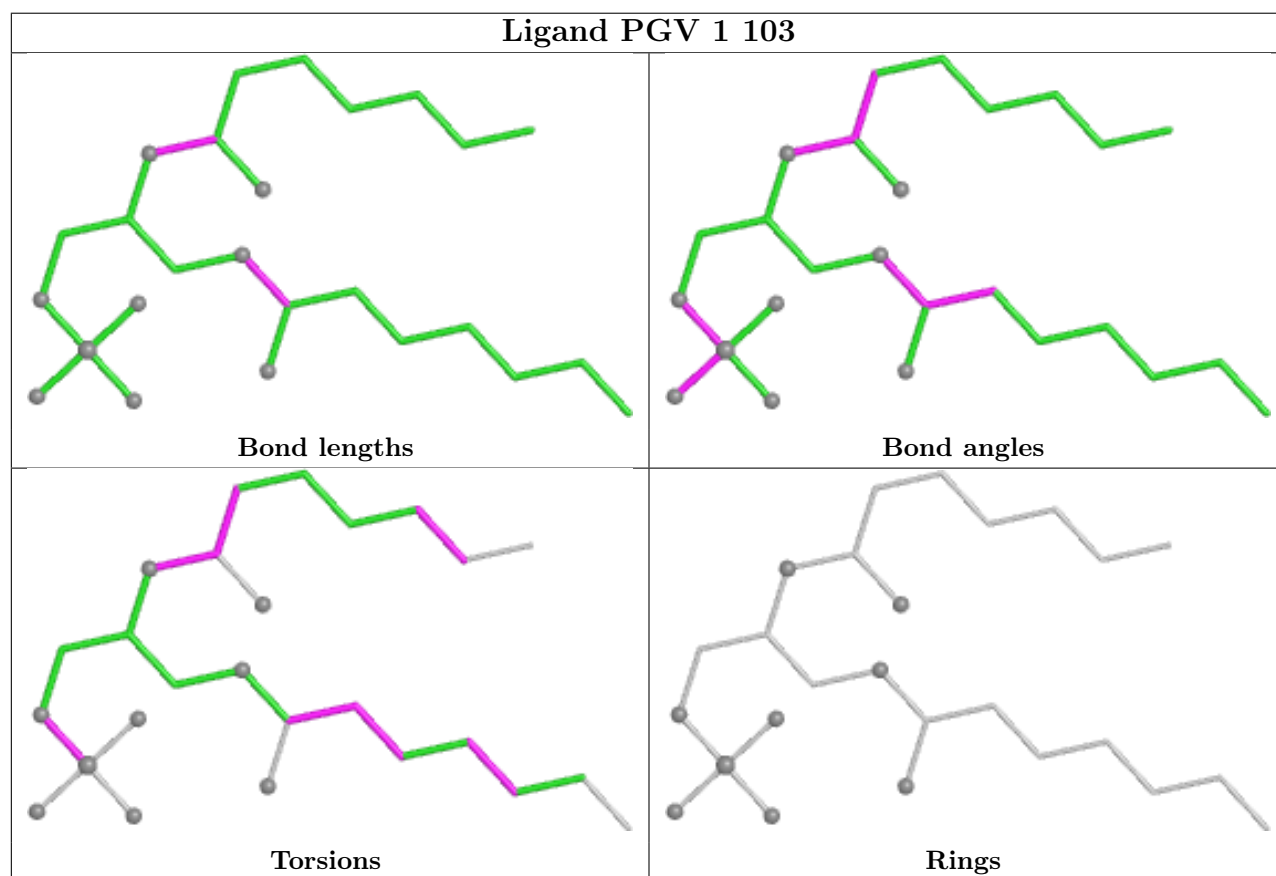
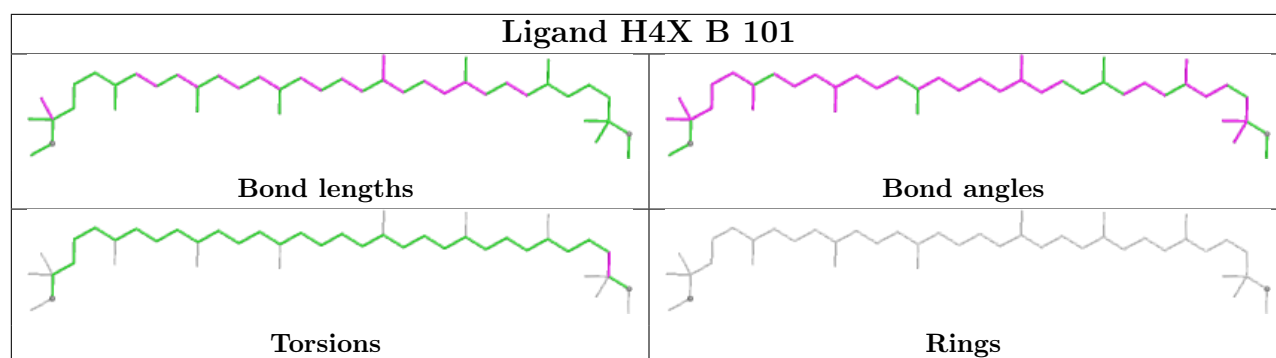


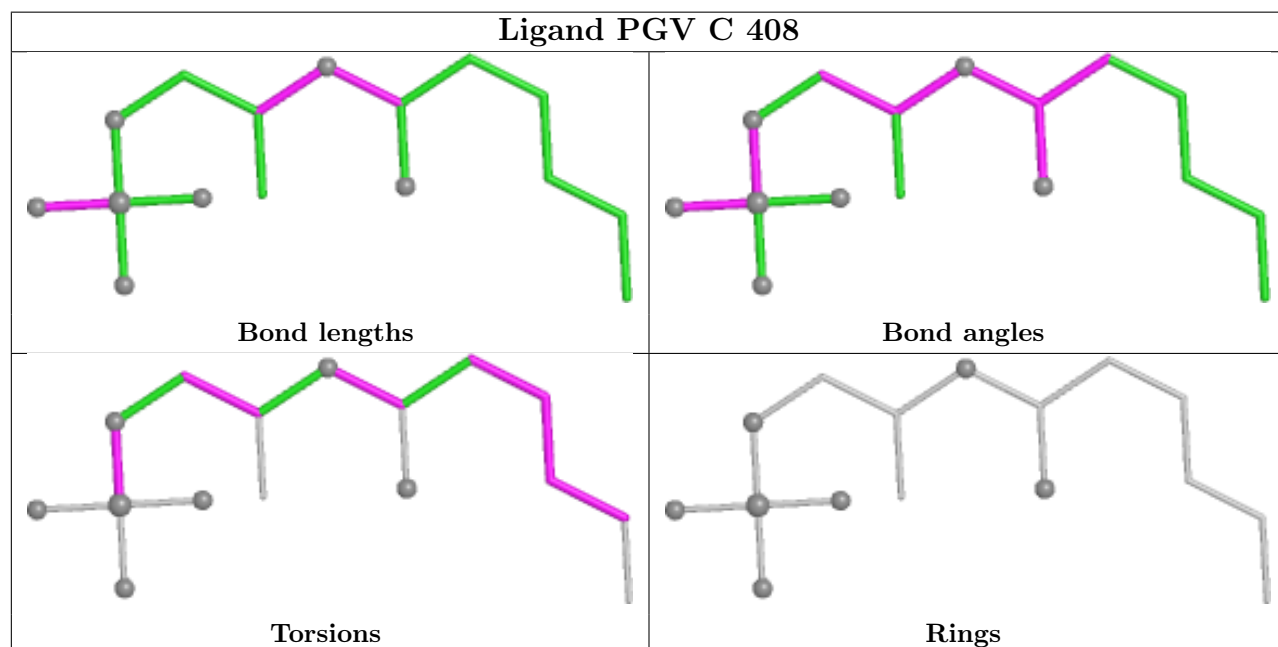
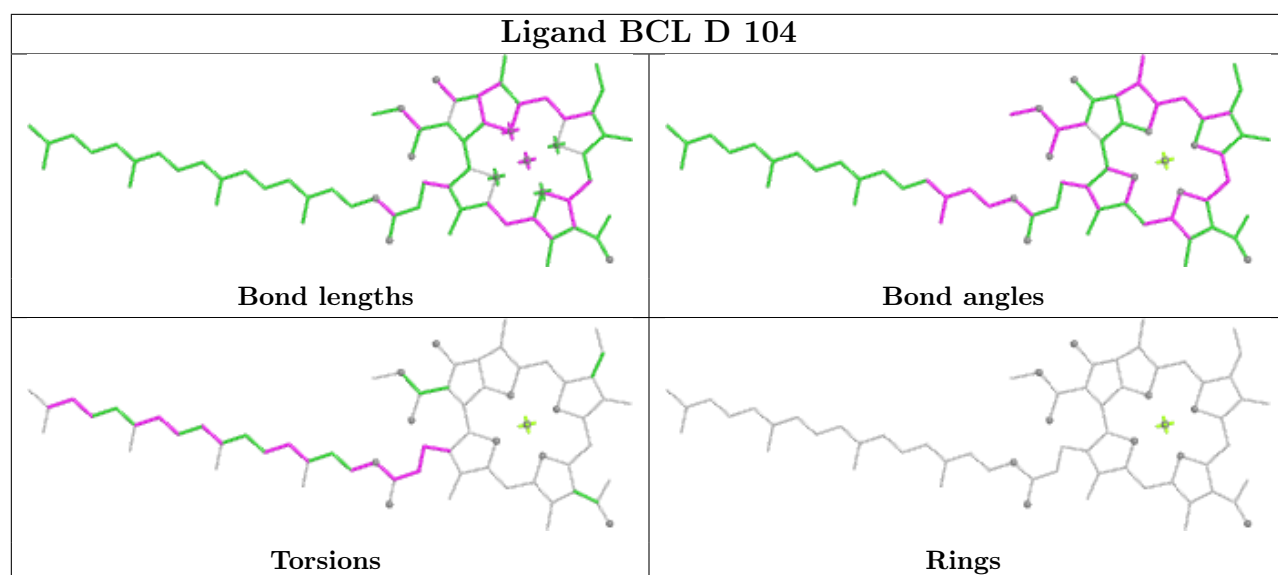


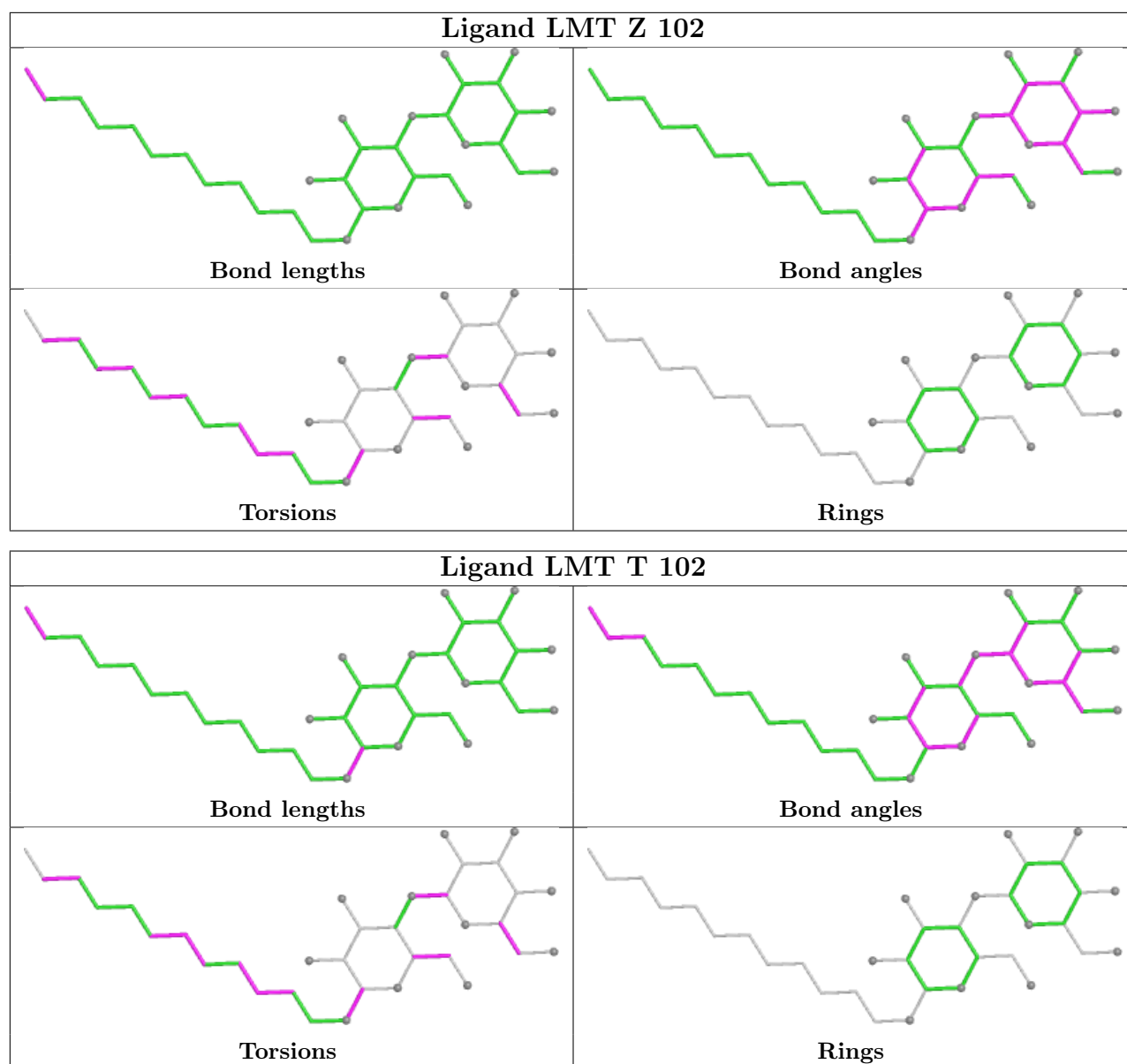


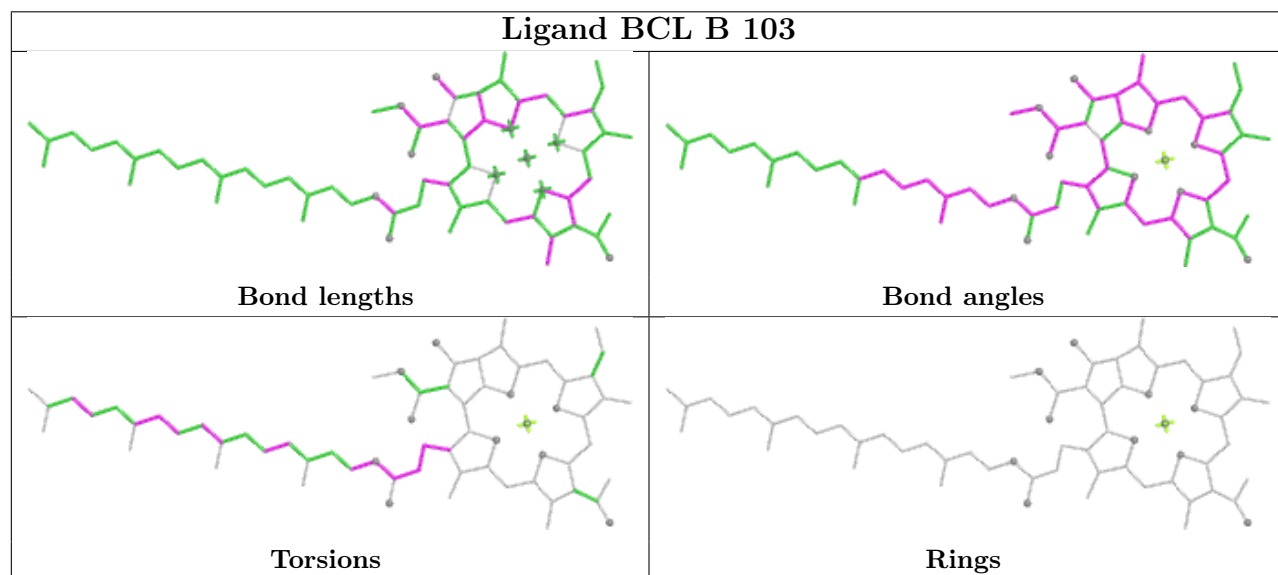
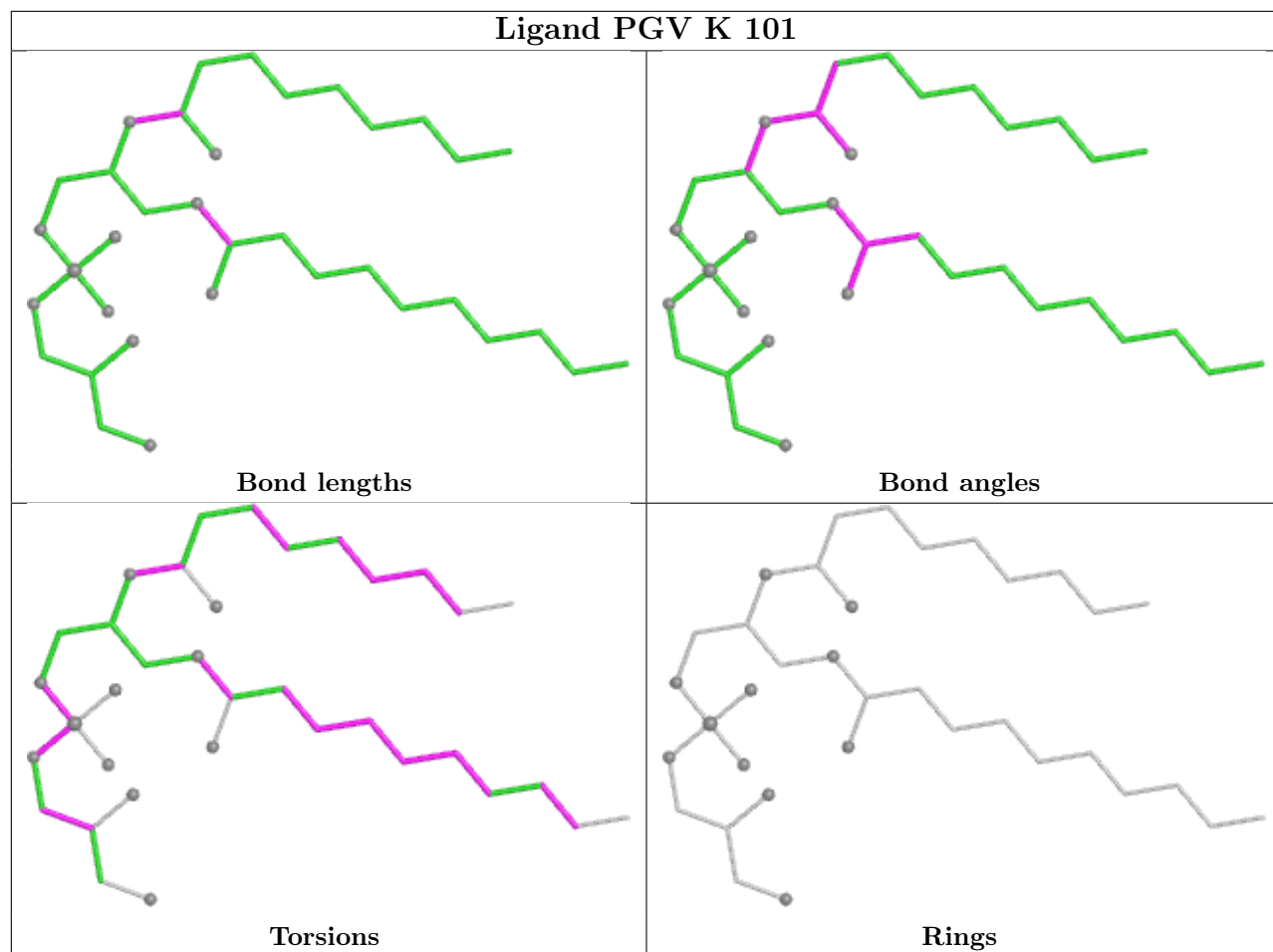


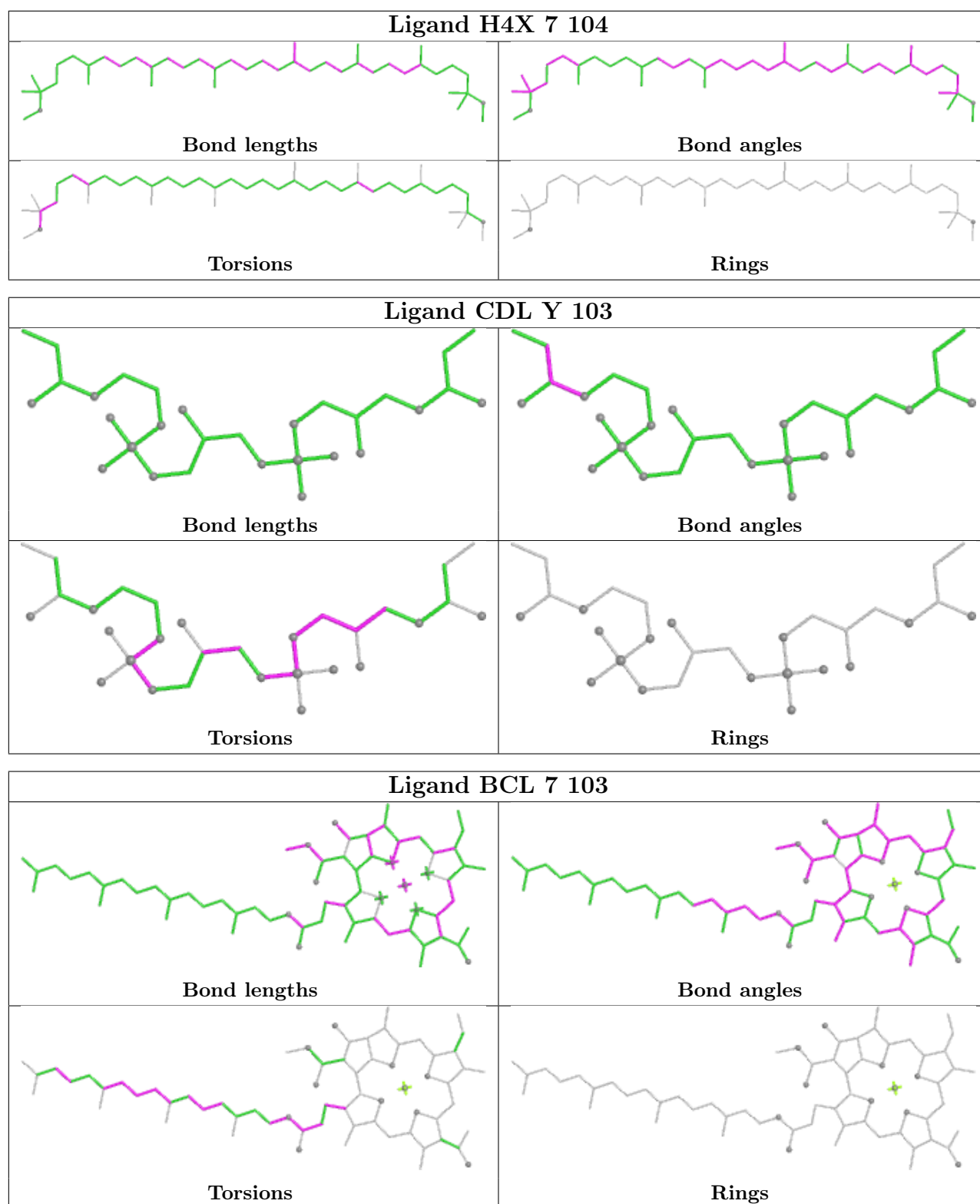


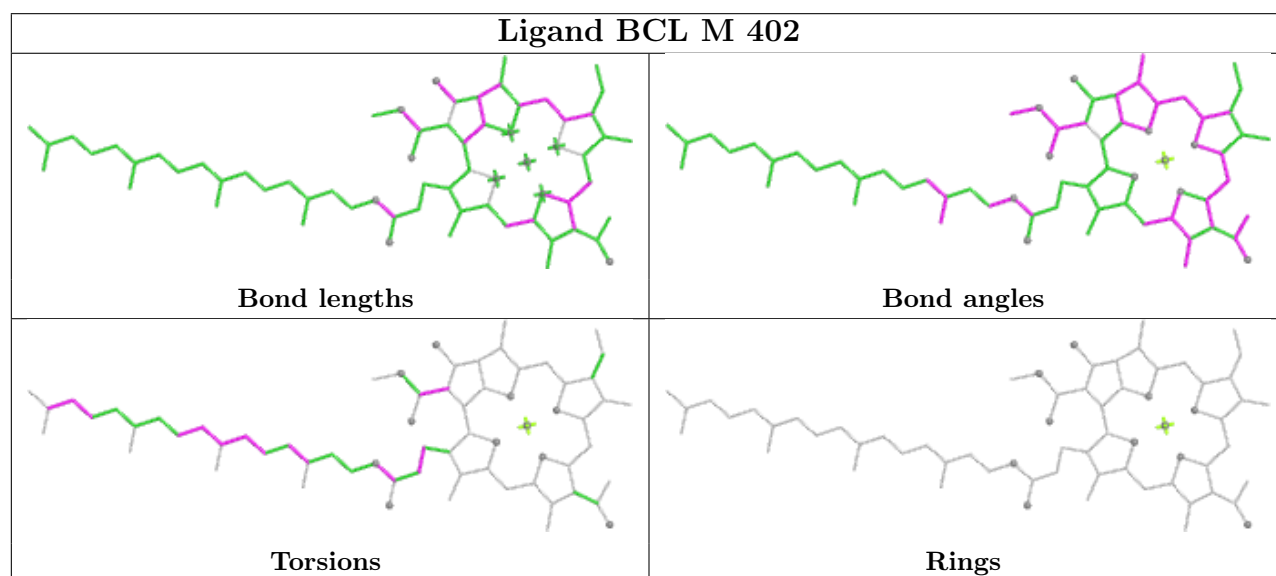
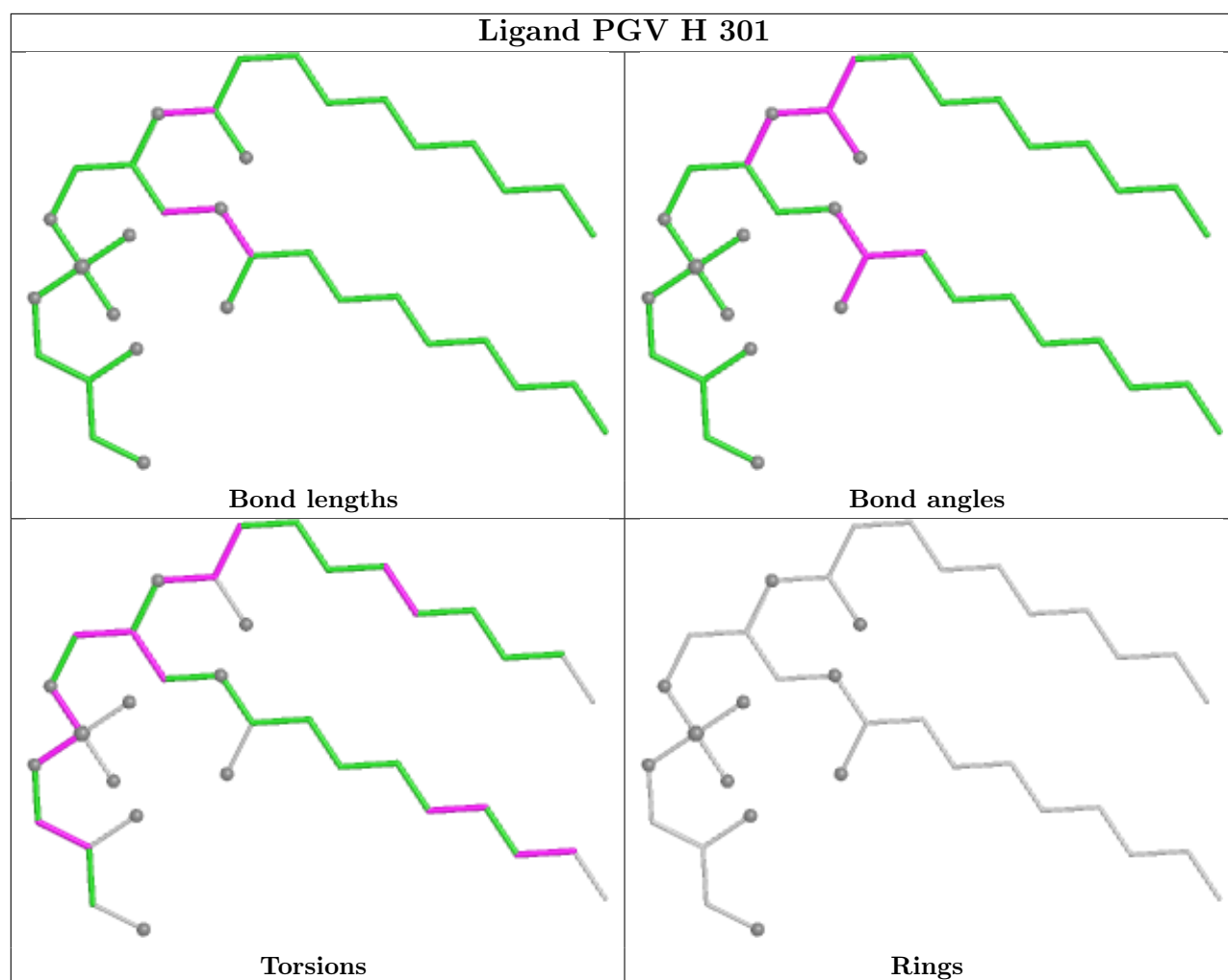


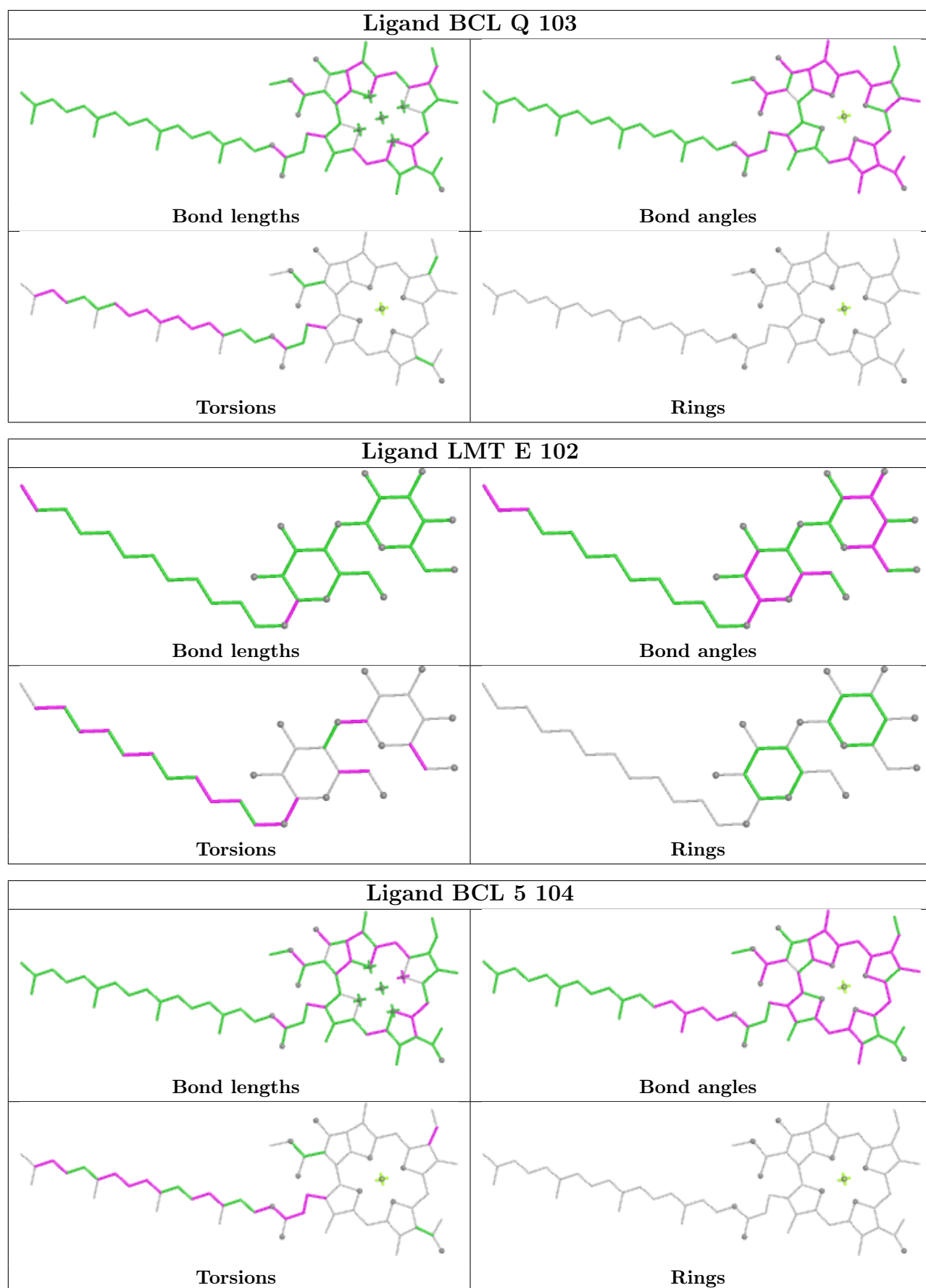


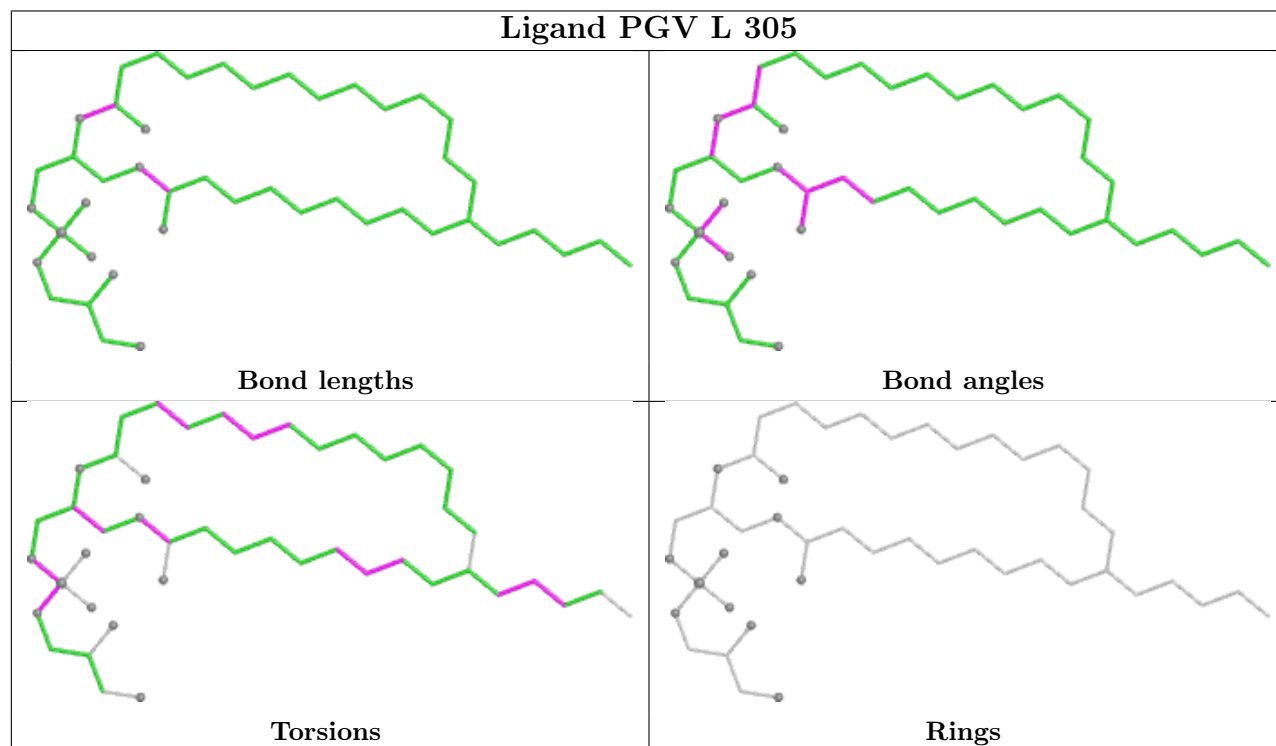
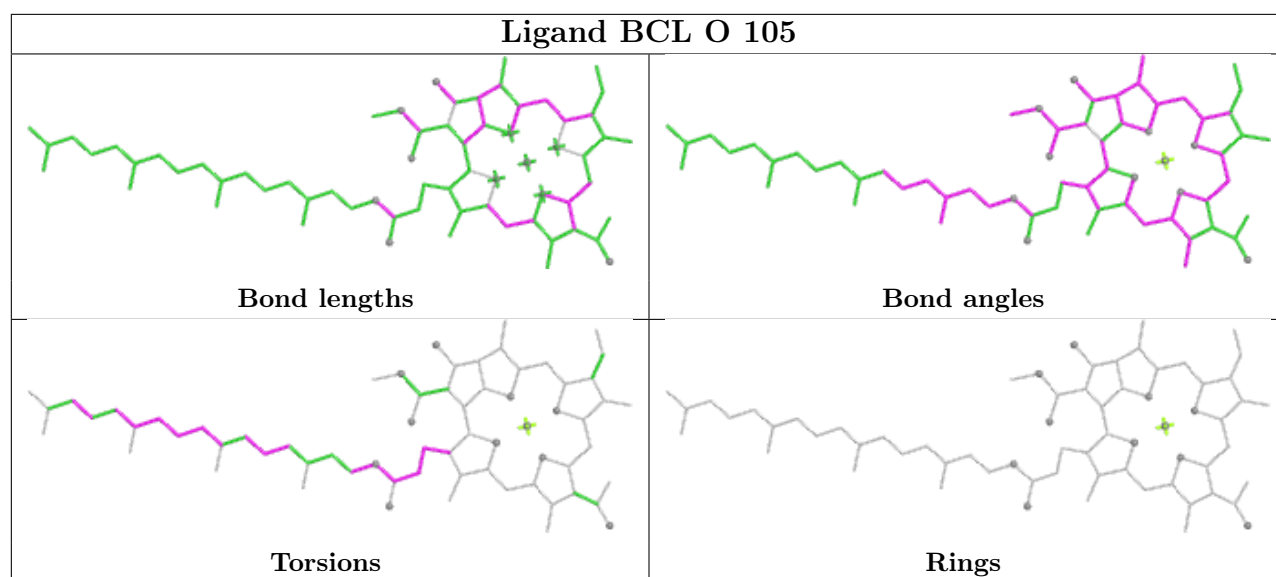


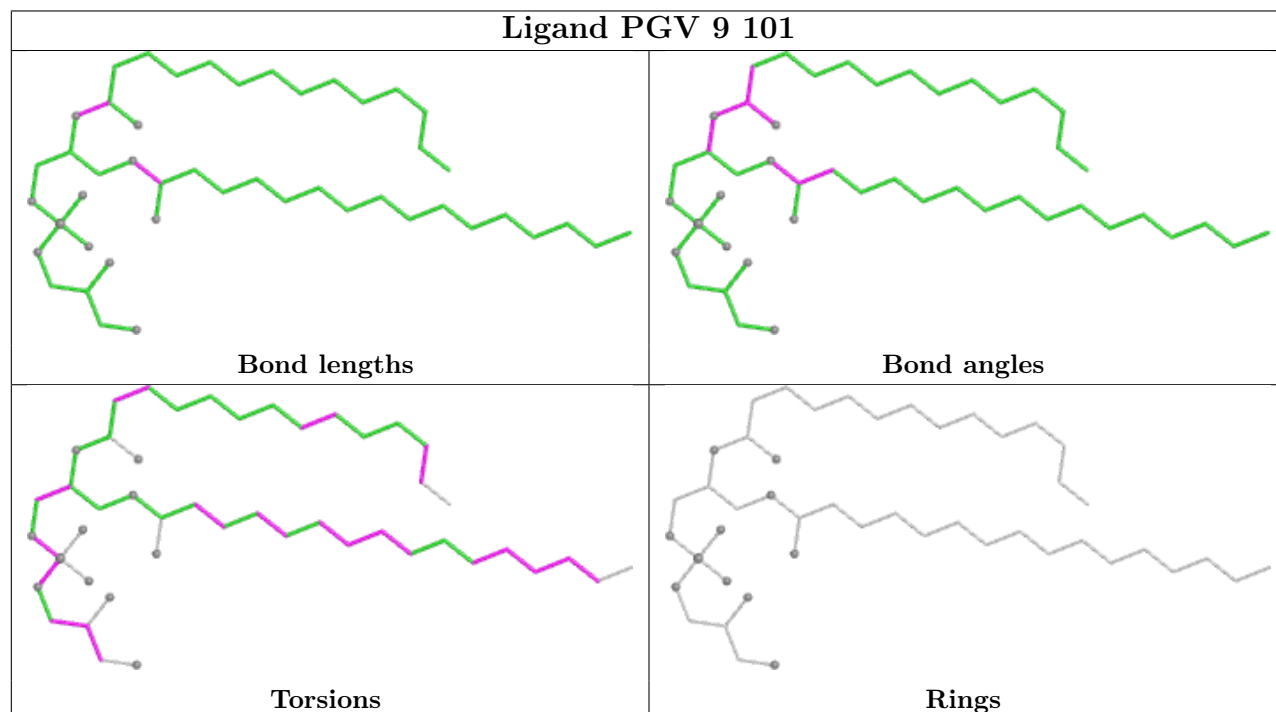
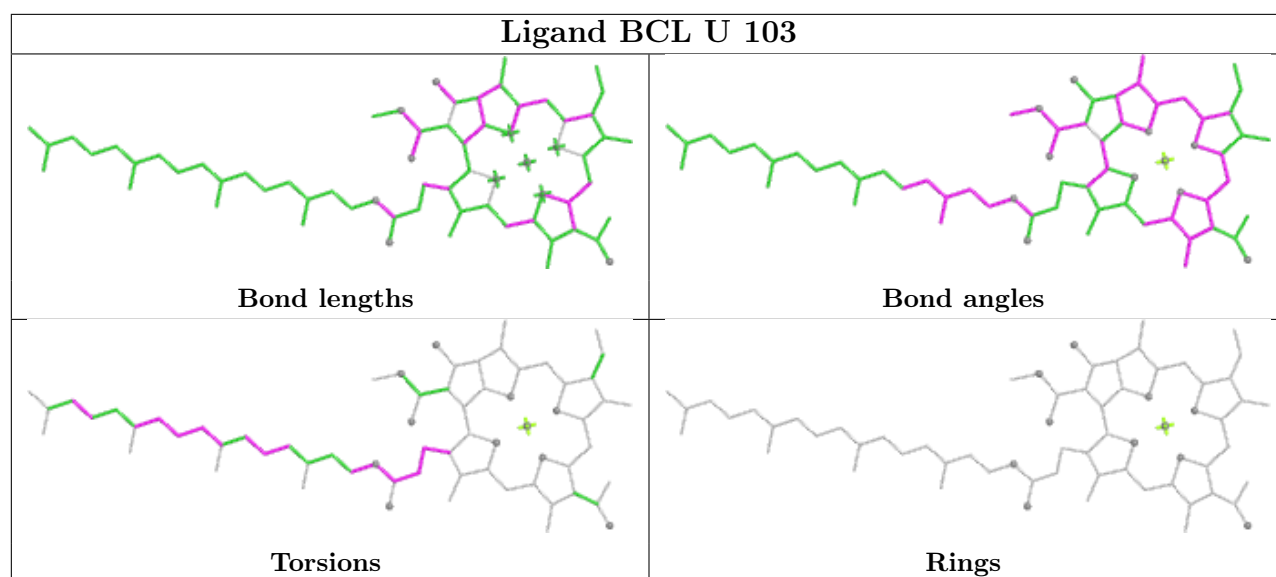


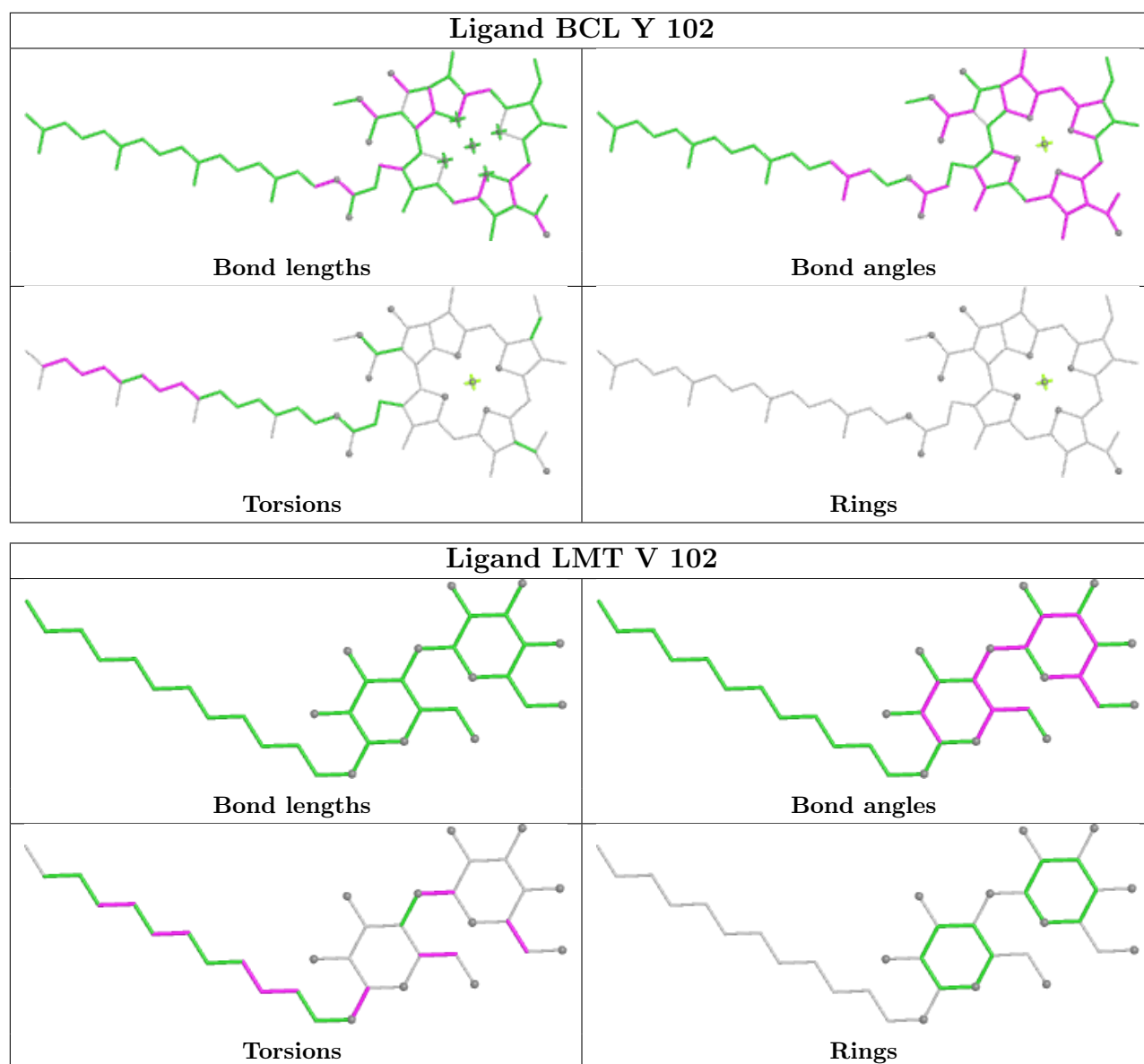


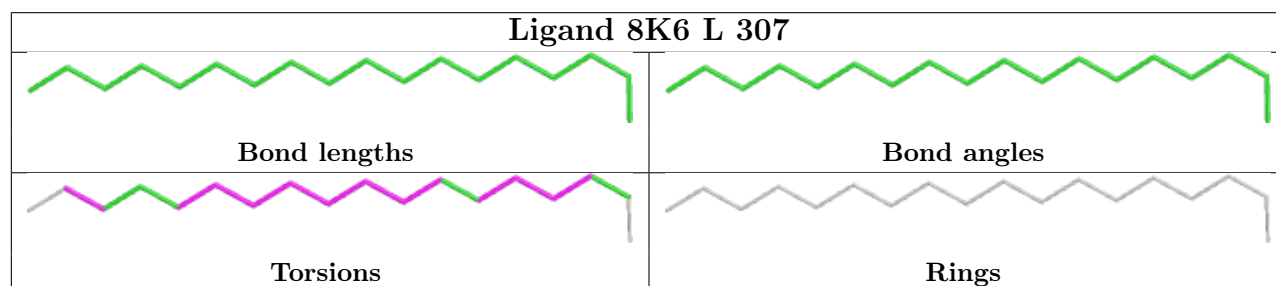
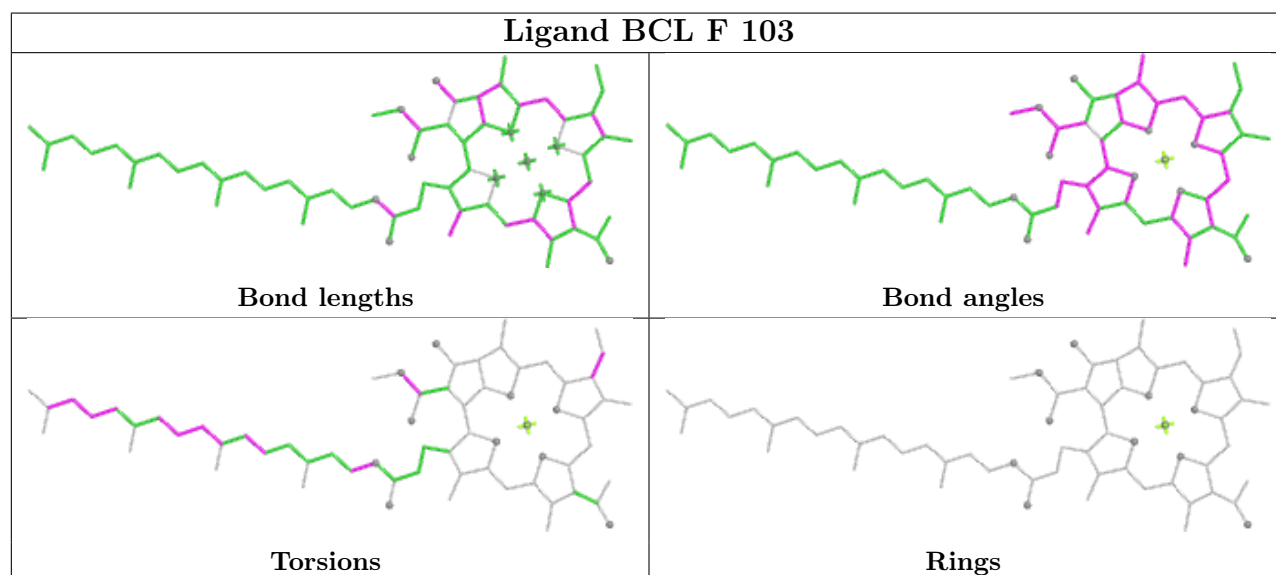
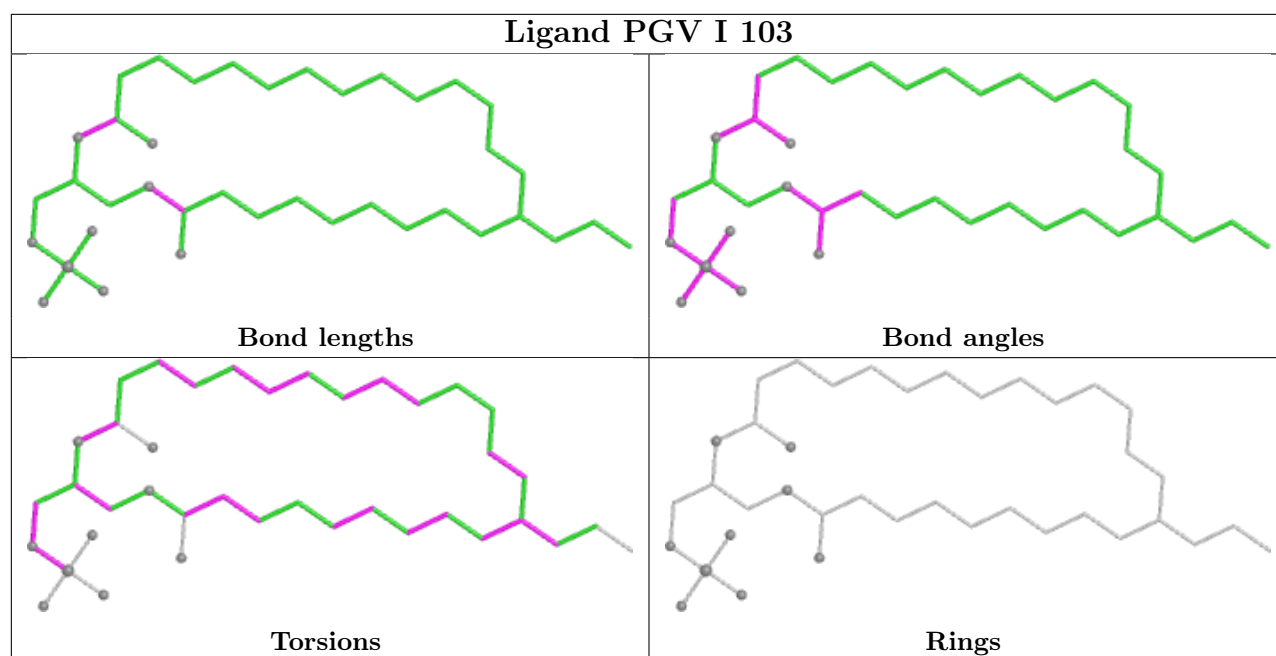


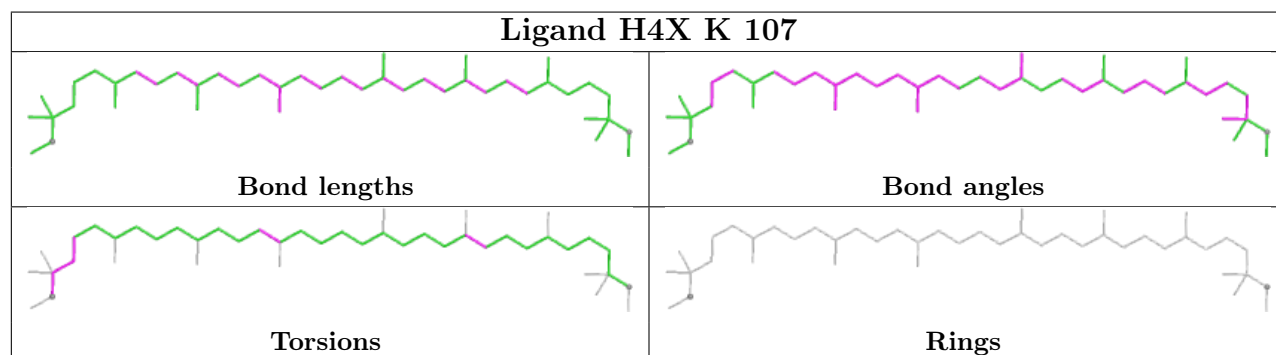
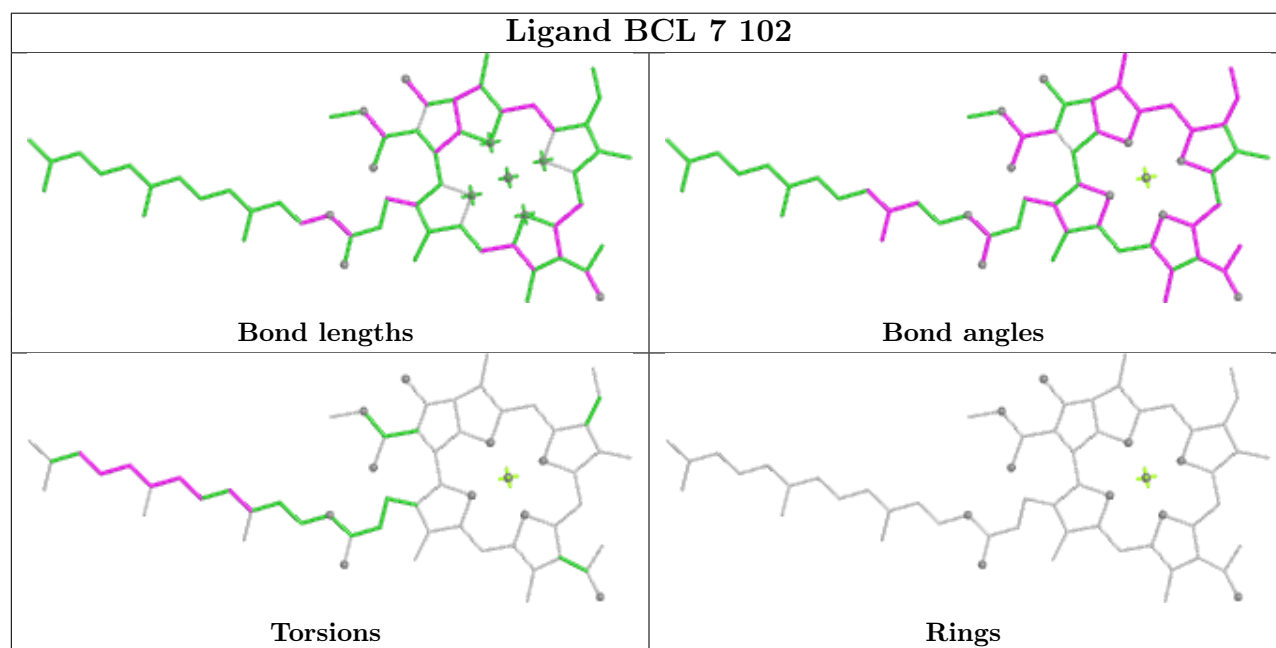
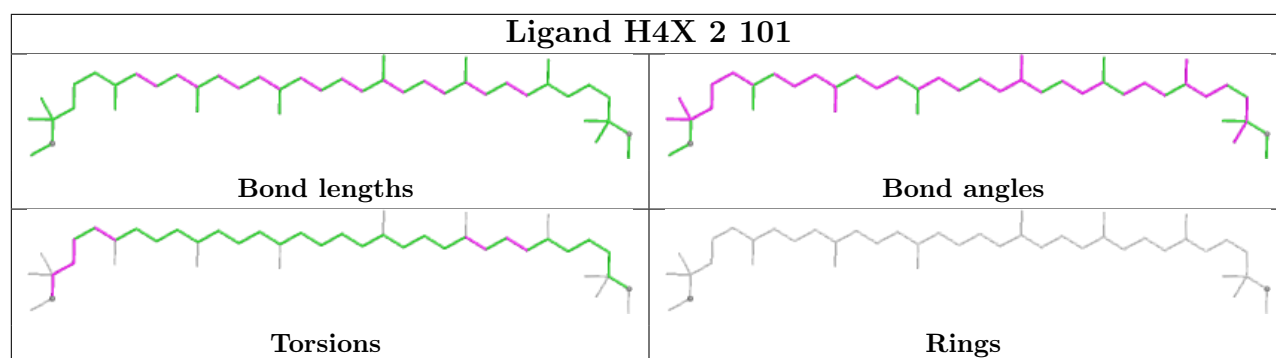


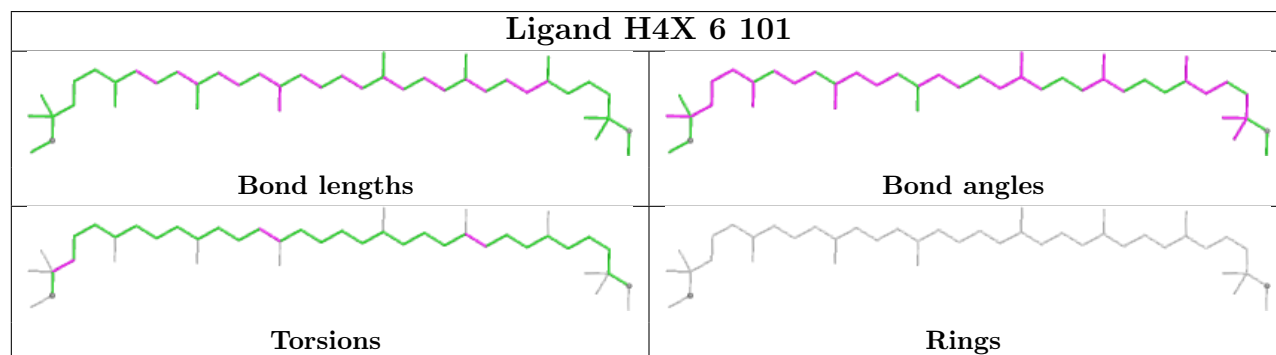
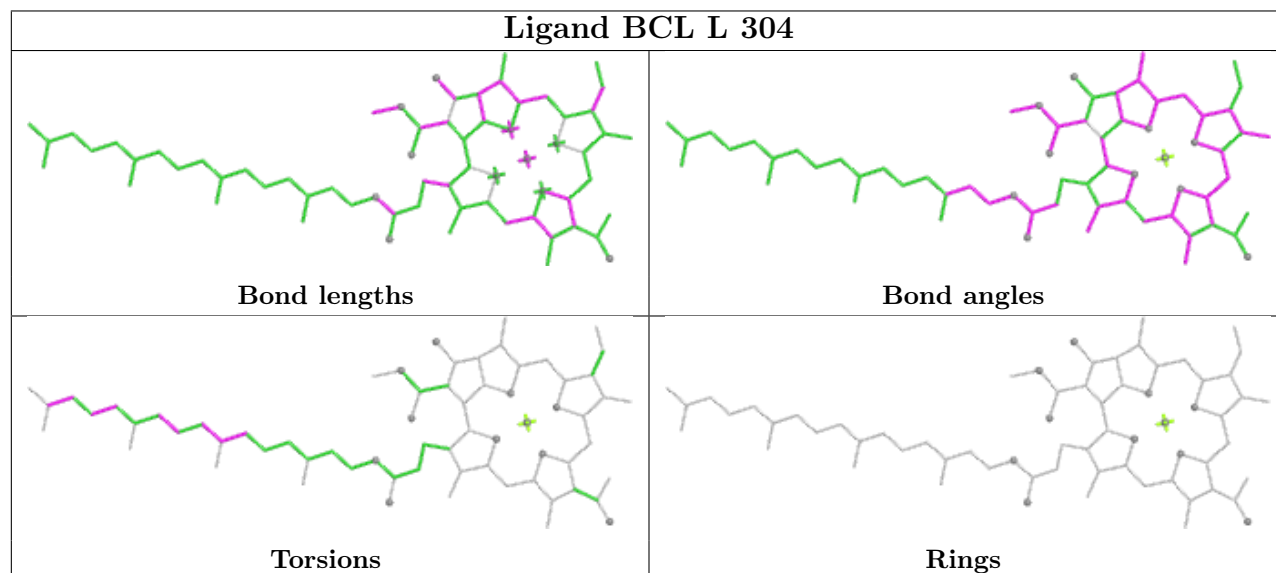
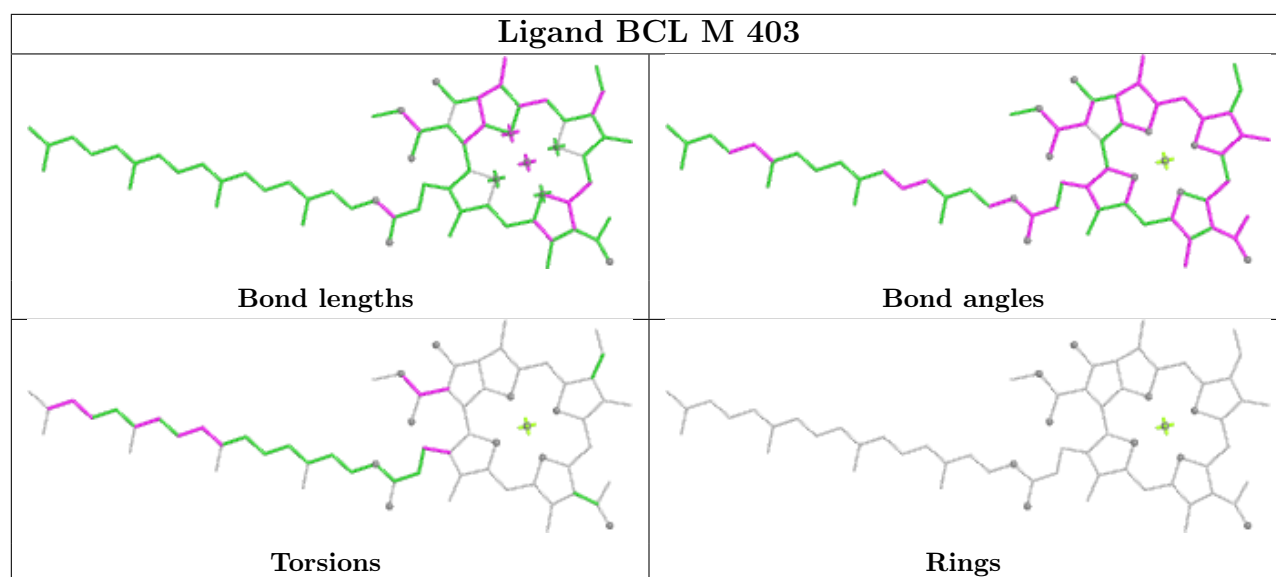


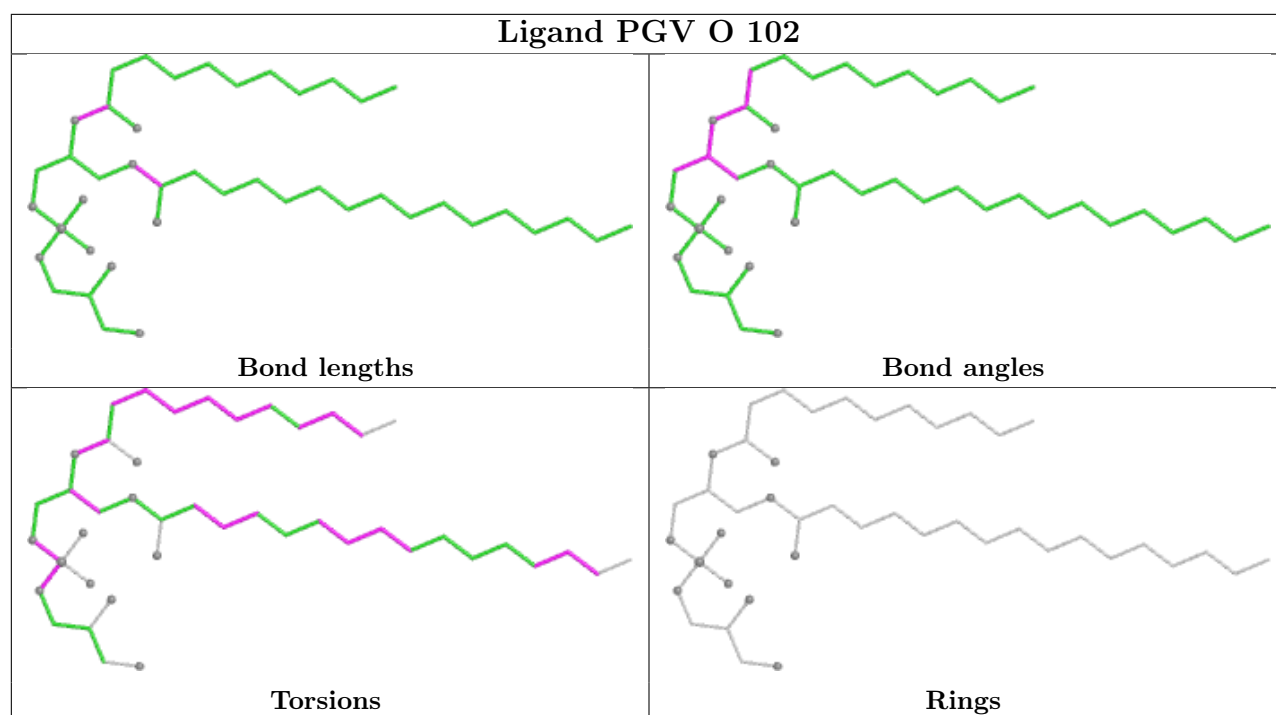












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

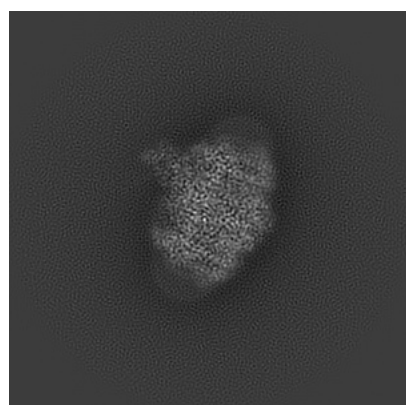
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30314. These allow visual inspection of the internal detail of the map and identification of artifacts.

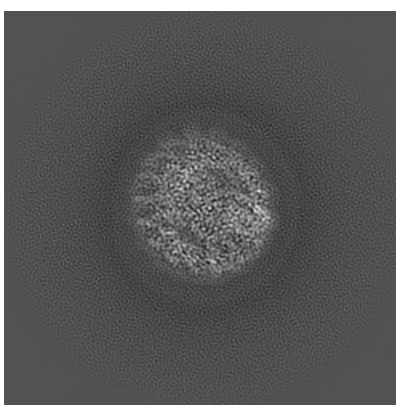
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

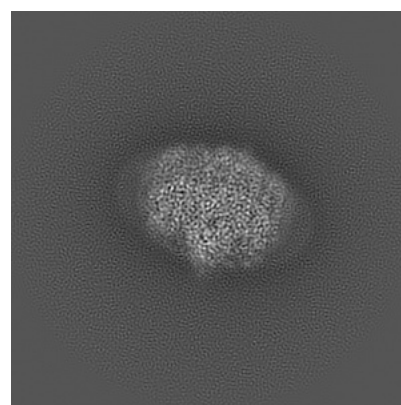
6.1.1 Primary map



X



Y

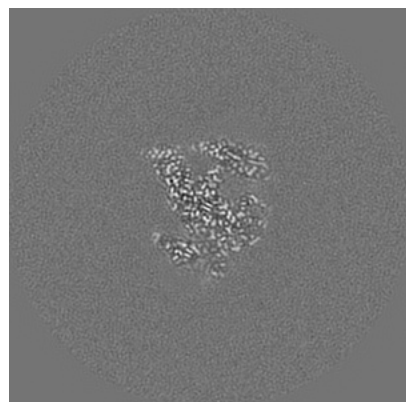


Z

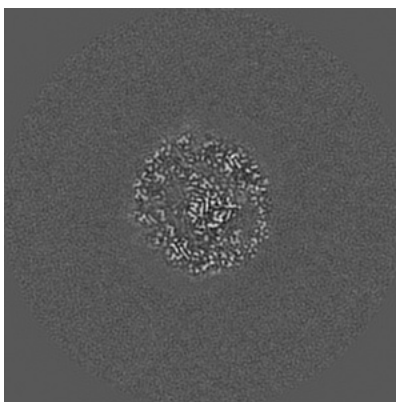
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

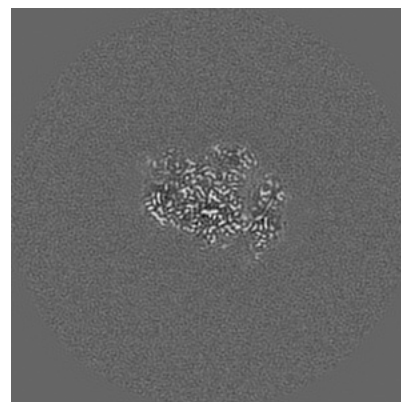
6.2.1 Primary map



X Index: 200



Y Index: 200

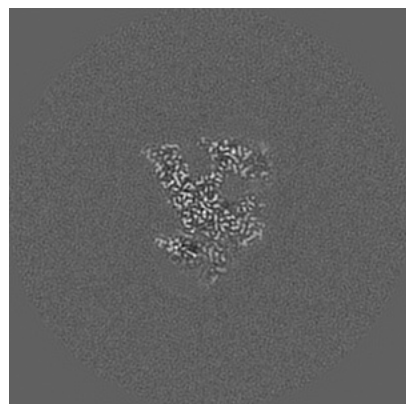


Z Index: 200

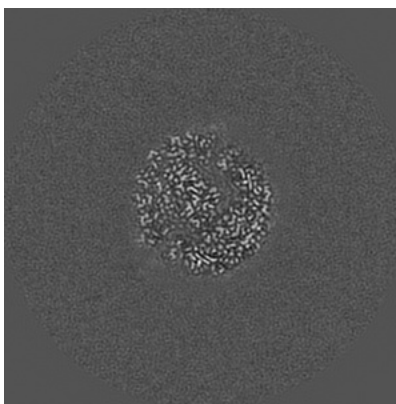
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

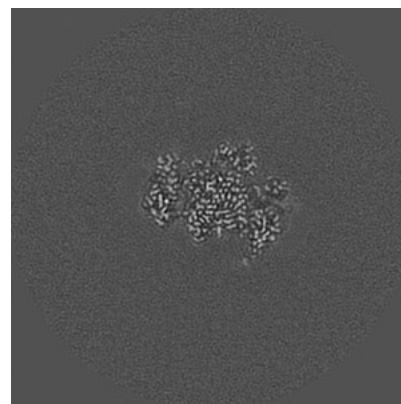
6.3.1 Primary map



X Index: 197



Y Index: 211

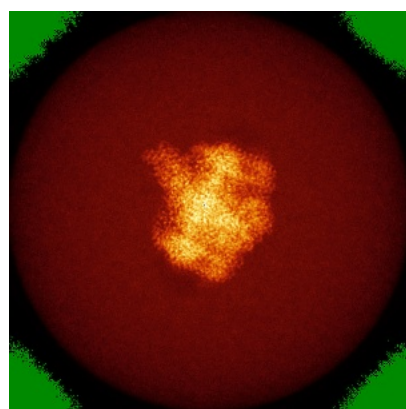


Z Index: 190

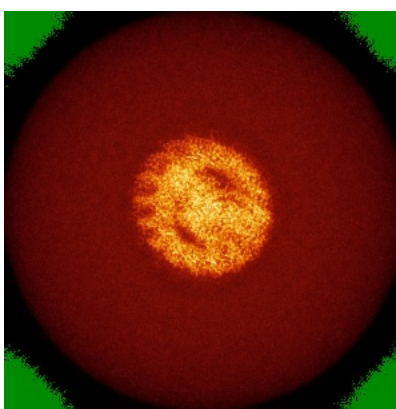
The images above show the largest variance slices of the map in three orthogonal directions.

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

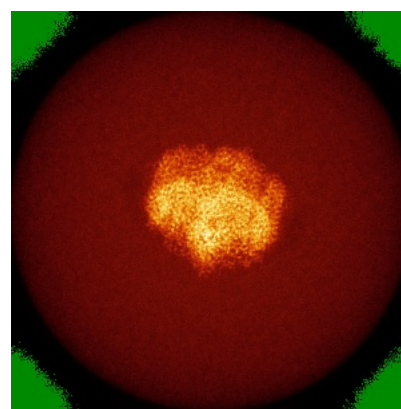
6.4.1 Primary map



X



Y

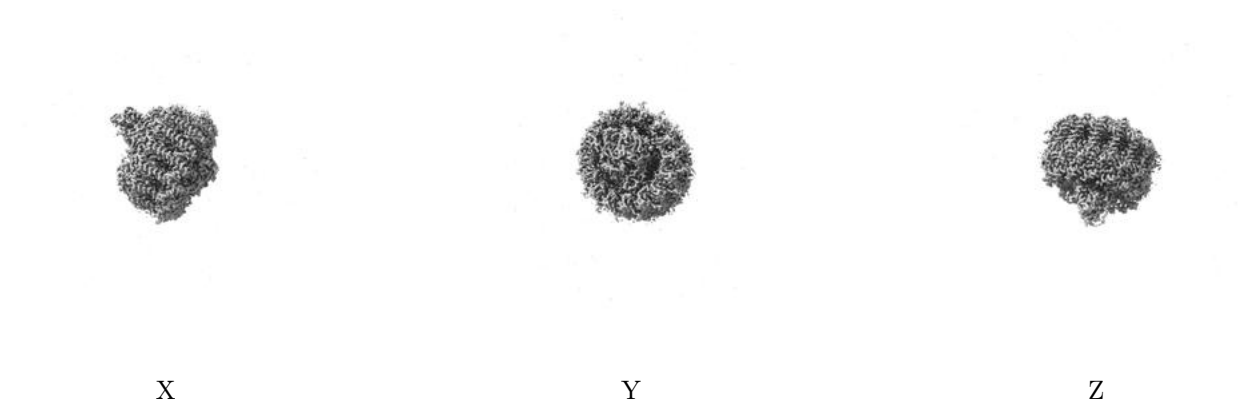


Z

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 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

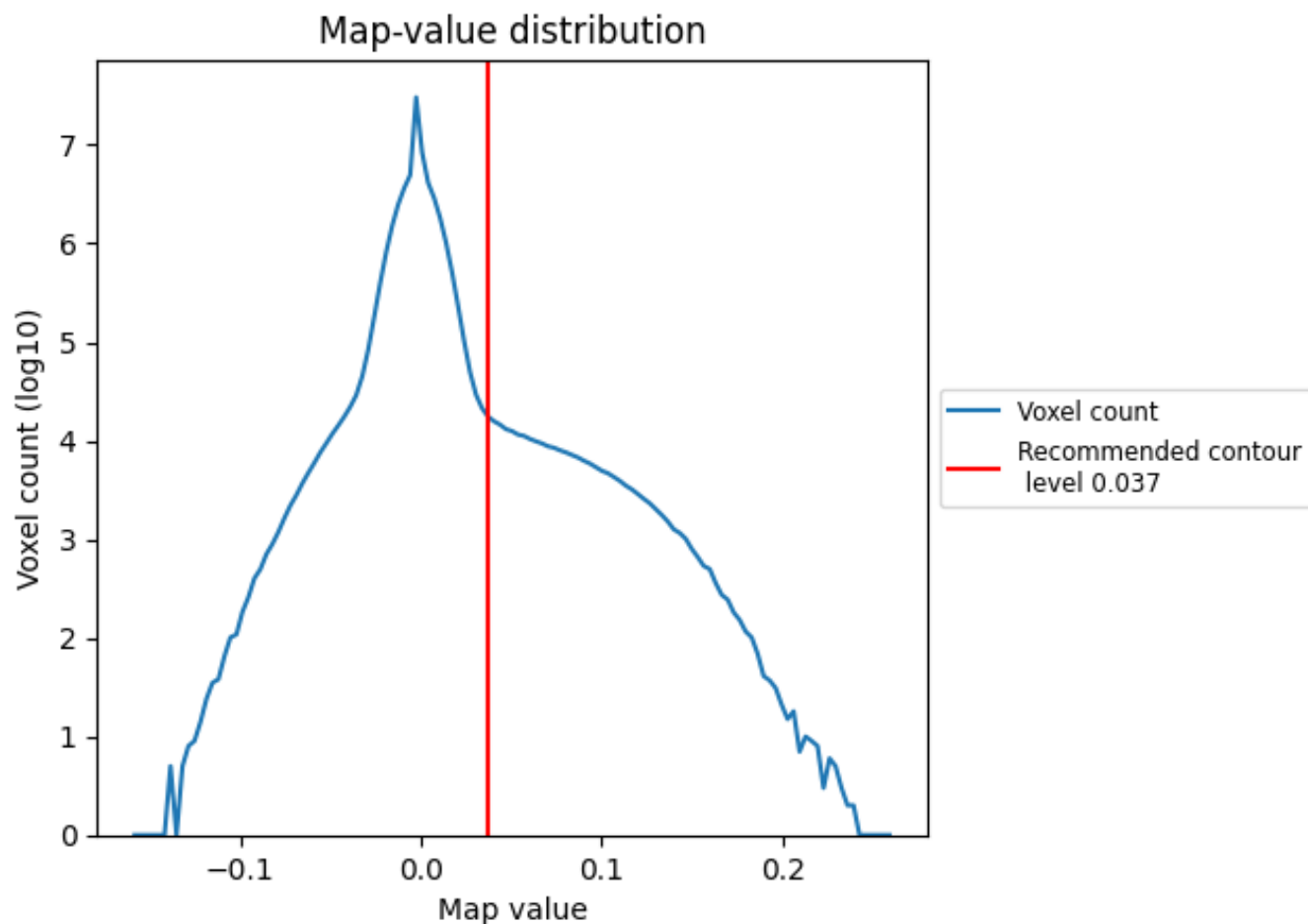
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

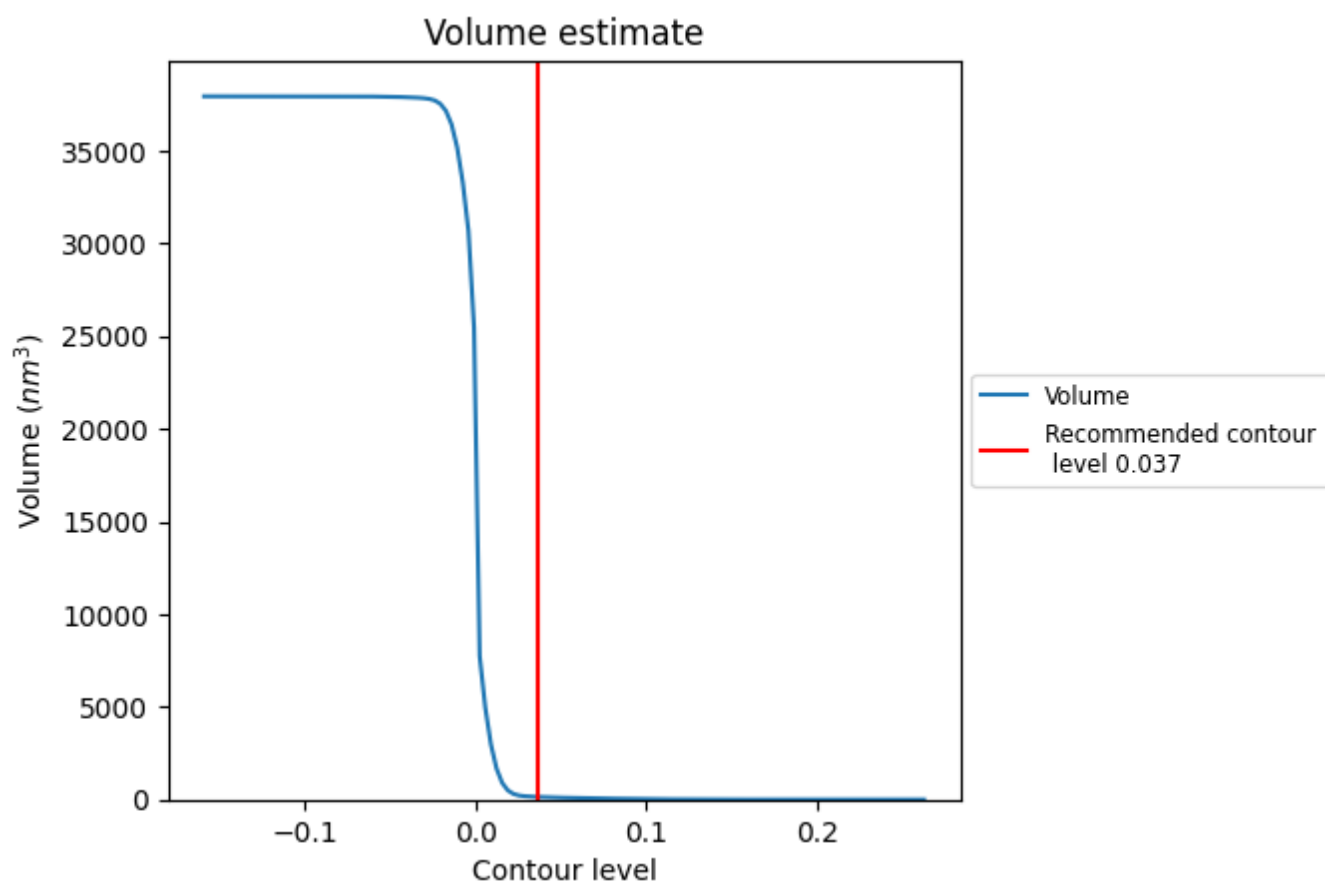
This section contains the results of statistical analysis of the map.

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.

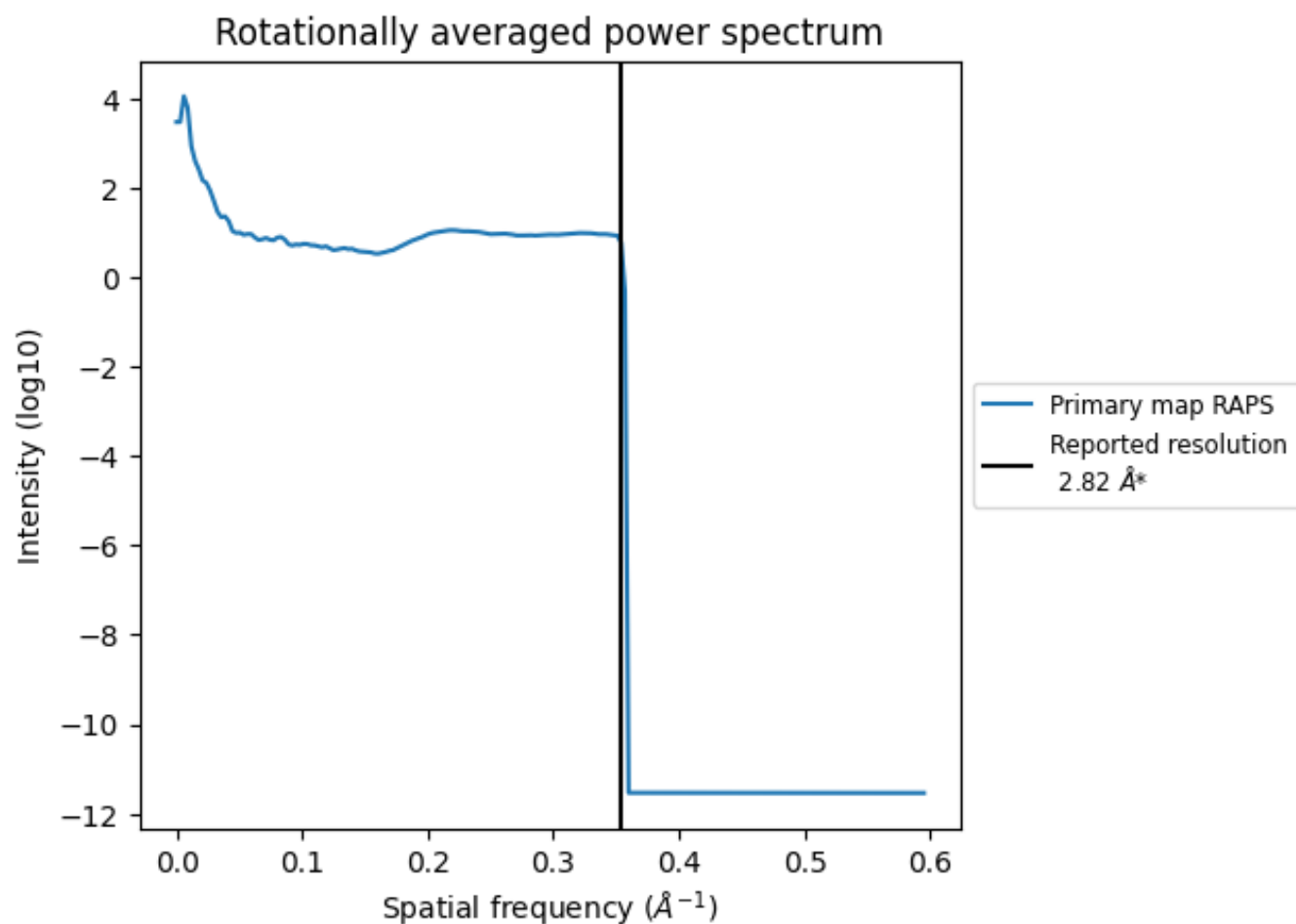
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 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 ⓘ

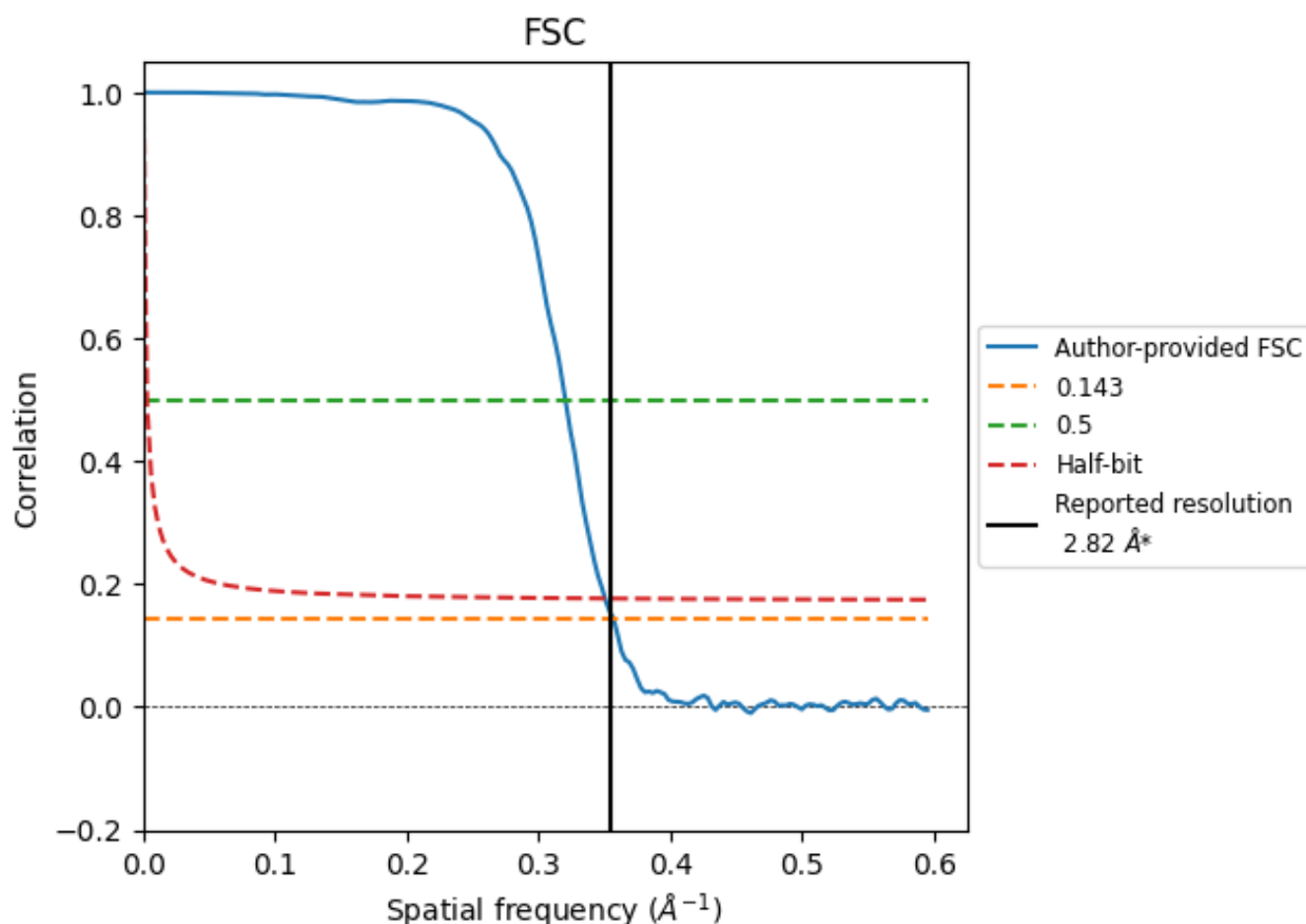


*Reported resolution corresponds to spatial frequency of 0.355 $\text{\AA}^{-1}$

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 0.355 Å⁻¹

8.2 Resolution estimates [i](#)

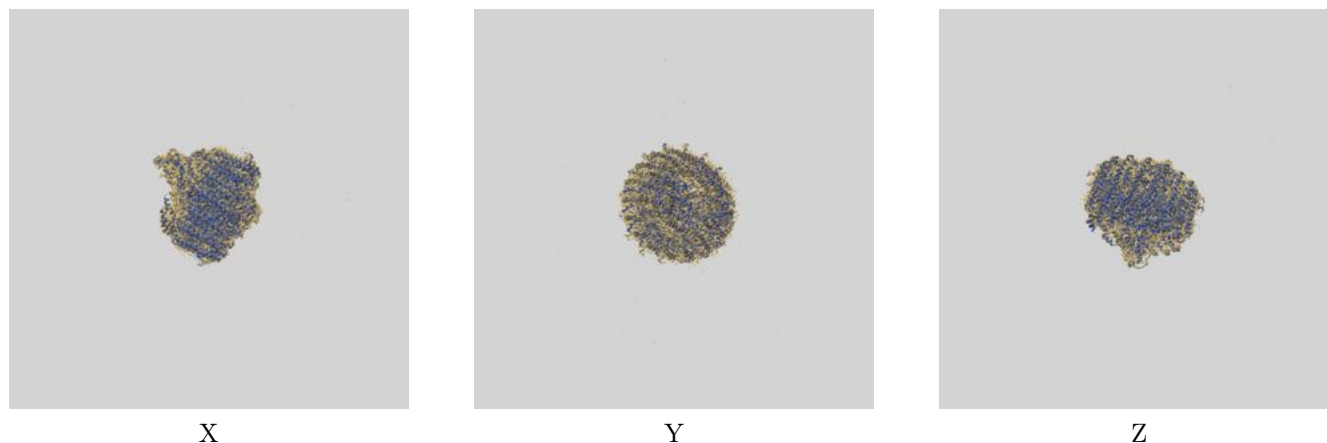
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.80	3.12	2.85
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

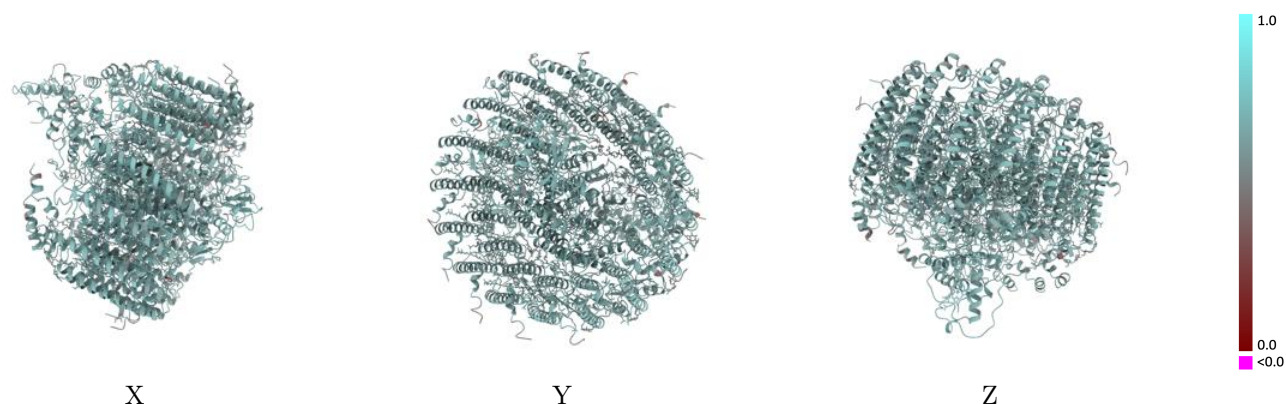
This section contains information regarding the fit between EMDB map EMD-30314 and PDB model 7C9R. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



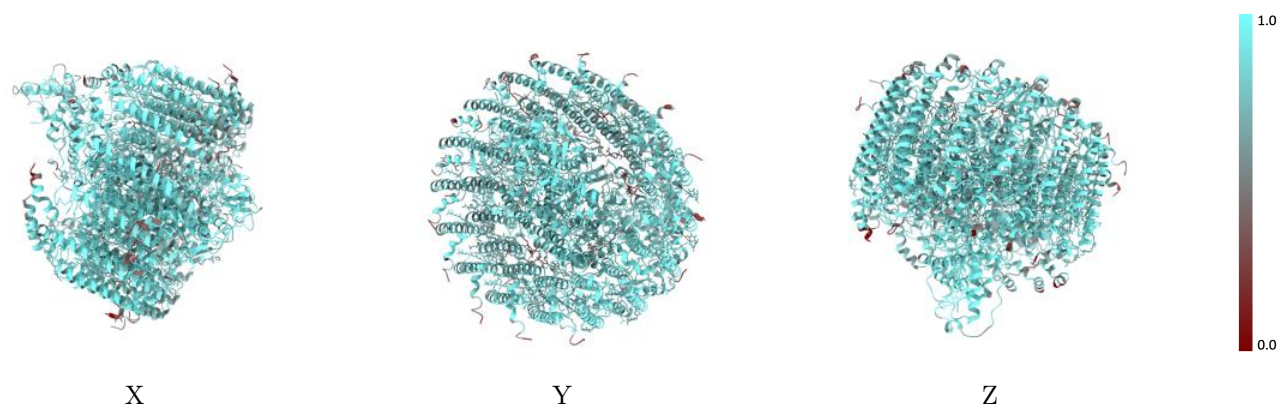
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



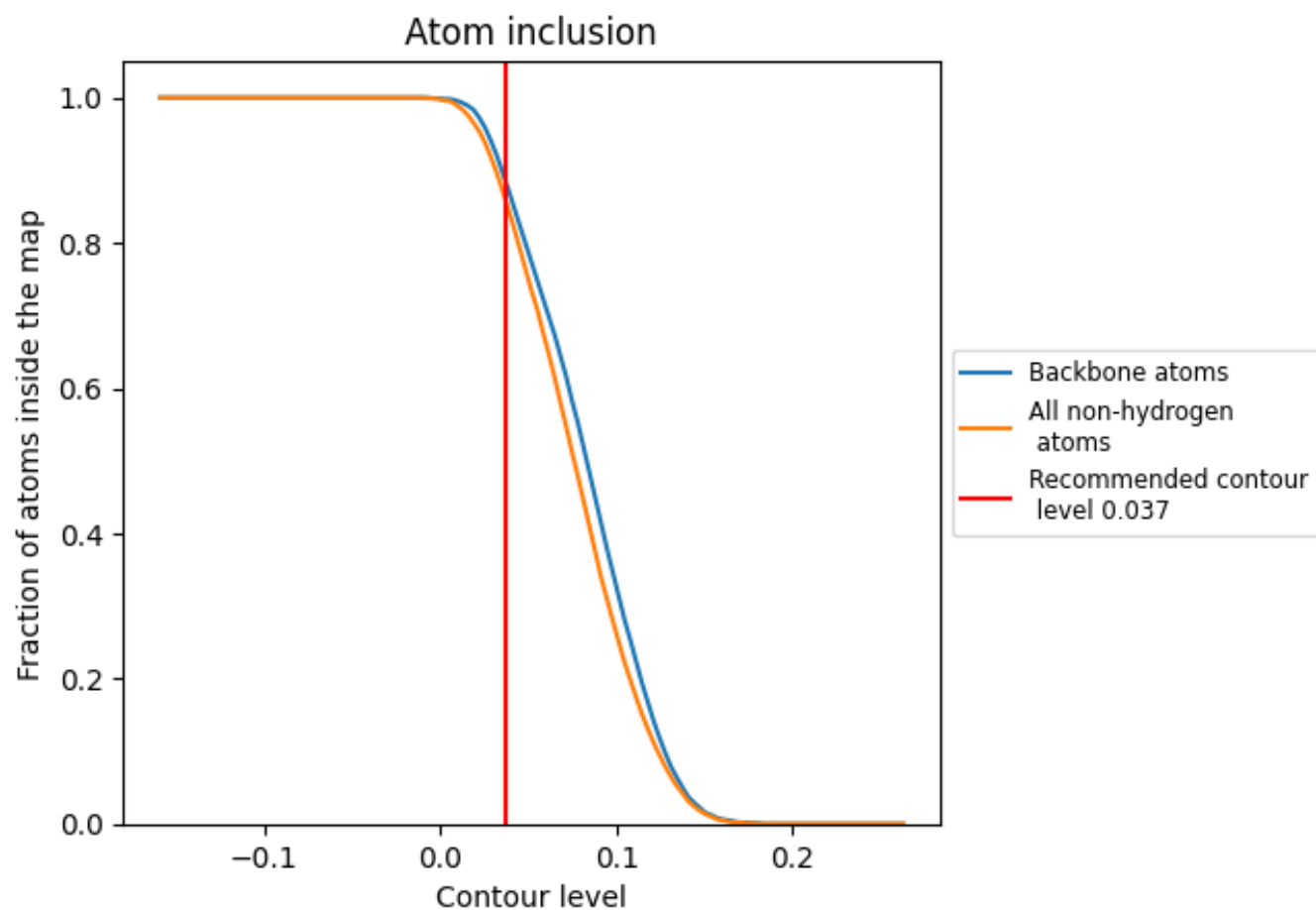
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.6320
0	 0.8250	 0.6030
1	 0.8120	 0.6140
2	 0.8200	 0.6170
3	 0.7930	 0.6150
4	 0.8500	 0.6250
5	 0.8260	 0.6250
6	 0.8680	 0.6300
7	 0.8500	 0.6270
8	 0.7890	 0.6050
9	 0.8730	 0.6380
A	 0.8540	 0.6280
B	 0.8560	 0.6260
C	 0.9080	 0.6420
D	 0.8430	 0.6300
E	 0.8580	 0.6330
F	 0.8320	 0.6270
G	 0.8610	 0.6300
H	 0.8520	 0.6330
I	 0.8340	 0.6240
J	 0.8780	 0.6320
K	 0.8210	 0.6290
L	 0.9390	 0.6520
M	 0.9220	 0.6520
N	 0.8500	 0.6250
O	 0.8420	 0.6280
P	 0.8610	 0.6310
Q	 0.8810	 0.6350
R	 0.8390	 0.6160
S	 0.7630	 0.6090
T	 0.8490	 0.6300
U	 0.8580	 0.6310
V	 0.8450	 0.6240
W	 0.8350	 0.6180
X	 0.8480	 0.6220



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Chain	Atom inclusion	Q-score
Y	 0.7860	 0.6140
Z	 0.8440	 0.6250