



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:00 AM UTC

PDB ID : 8IUN / pdb_00008iun
EMDB ID : EMD-35727
Title : Cryo-EM structure of the CRT-LESS RC-LH core complex from *roseiflexus castenholzii*
Authors : Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on : 2023-03-24
Resolution : 2.85 Å(reported)

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:

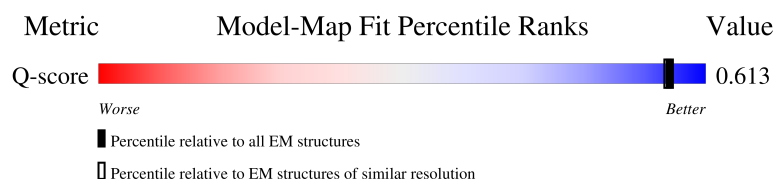
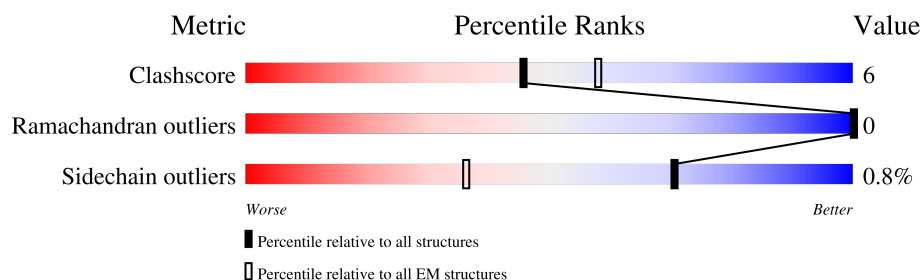
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.85 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.



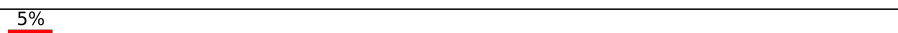
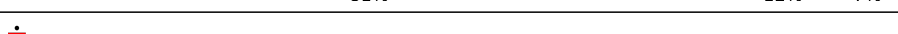
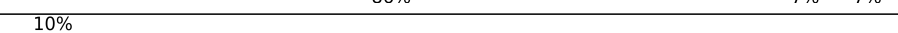
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	0	55	5% 80% 11% 9%
1	2	55	16% 80% 11% 9%
1	4	55	5% 87% • 9%
1	6	55	• 80% 11% 9%

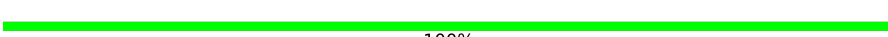
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Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	L	641	
2	M	641	
3	1	42	
3	3	42	
3	5	42	
3	7	42	
3	9	42	
3	A	42	
3	D	42	
3	F	42	
3	H	42	
3	J	42	
3	N	42	
3	P	42	

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Mol	Chain	Length	Quality of chain
3	R	42	
3	T	42	
3	V	42	
4	Y	39	
5	h	63	
6	C	320	
7	Z	10	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	UNL	9	103	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 24285 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 Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	U	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	S	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	Q	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	O	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	K	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	I	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	G	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	E	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	B	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	0	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	8	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	6	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	4	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	2	50	Total 416	C 280	N 69	O 66	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		
2	L	286	Total	C	N	O	S	0	0
			2278	1527	367	376	8		

- Molecule 3 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	J	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	N	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	P	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	R	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	3	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	5	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	7	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	D	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 4 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

- Molecule 5 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

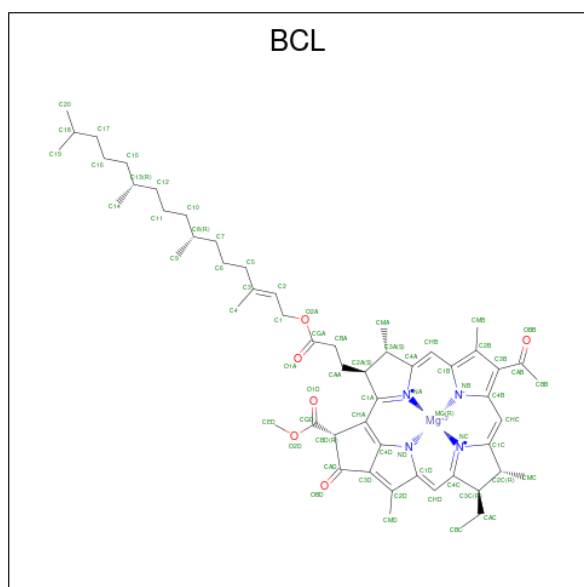
- Molecule 6 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	308	Total	C	N	O	S	0	0
			2347	1492	400	433	22		

- Molecule 7 is a protein called reaction center unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	10	Total	C	N	O	0	0
			51	31	10	10		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0

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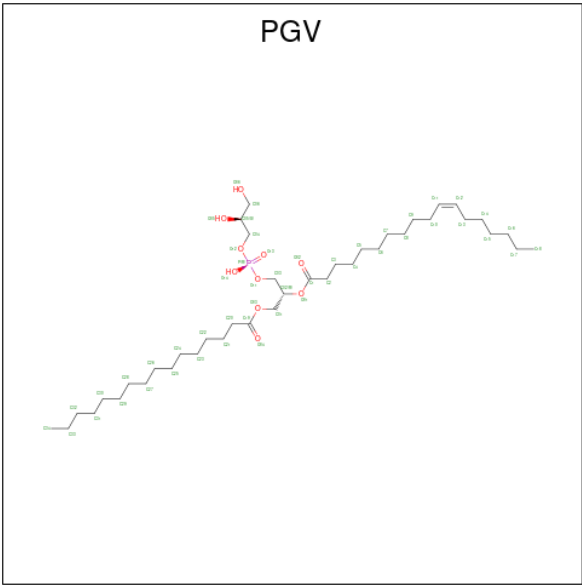
Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



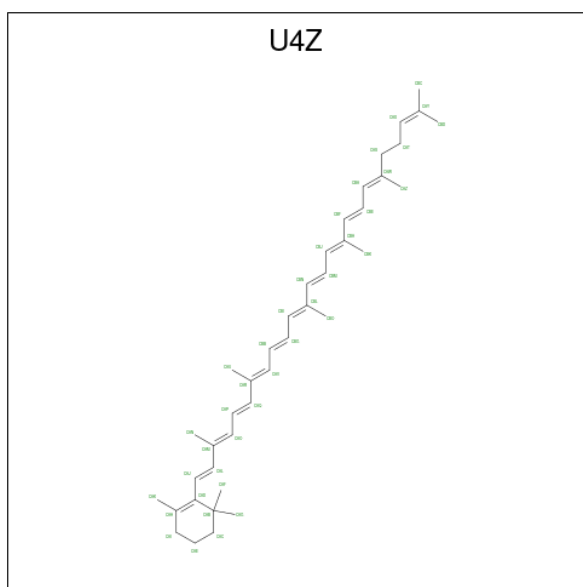
Mol	Chain	Residues	Atoms				AltConf
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	S	1	Total	C	O	P	0
			44	33	10	1	
9	O	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	I	1	Total	C	O	P	0
			44	33	10	1	

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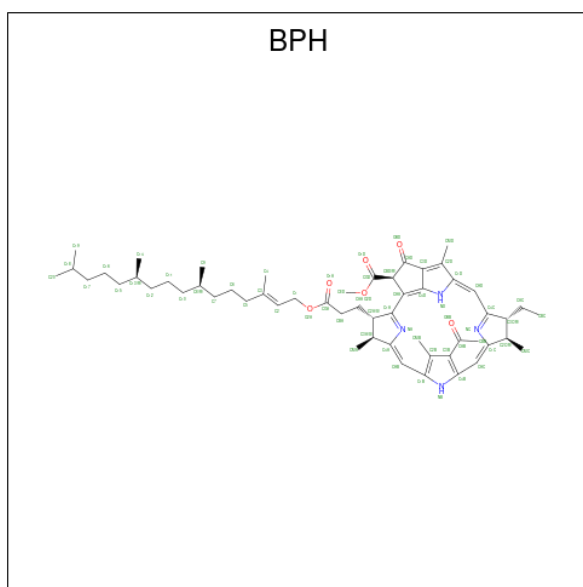
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	8	1	Total	C	O	P	0
			44	33	10	1	
9	6	1	Total	C	O	P	0
			44	33	10	1	
9	4	1	Total	C	O	P	0
			44	33	10	1	
9	M	1	Total	C	O	P	0
			35	24	10	1	
9	L	1	Total	C	O	P	0
			51	40	10	1	
9	L	1	Total	C	O	P	0
			33	23	9	1	
9	L	1	Total	C	O	P	0
			35	24	10	1	
9	N	1	Total	C	O	P	0
			24	13	10	1	
9	1	1	Total	C	O	P	0
			36	27	8	1	
9	h	1	Total	C	O	P	0
			46	37	8	1	
9	C	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 10 is gamma-Carotene (CCD ID: U4Z) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
10	0	1	Total C 40 40	0
10	J	1	Total C 40 40	0
10	R	1	Total C 40 40	0
10	3	1	Total C 40 40	0
10	D	1	Total C 40 40	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

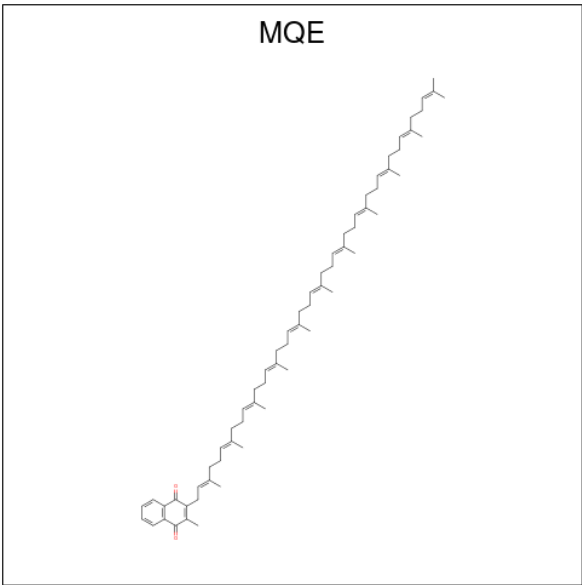


Mol	Chain	Residues	Atoms				AltConf
11	M	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

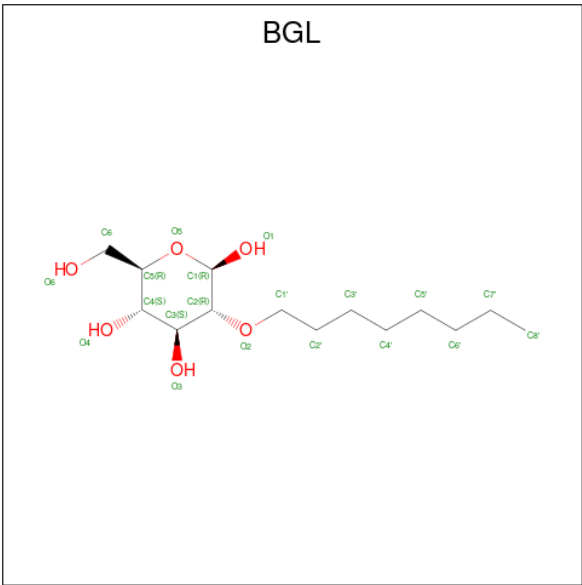
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Mn	0
			1	1	

- Molecule 13 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (CCD ID: MQE) (formula: C₆₆H₉₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			68	66	2	
13	L	1	Total	C	O	0
			53	51	2	

- Molecule 14 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



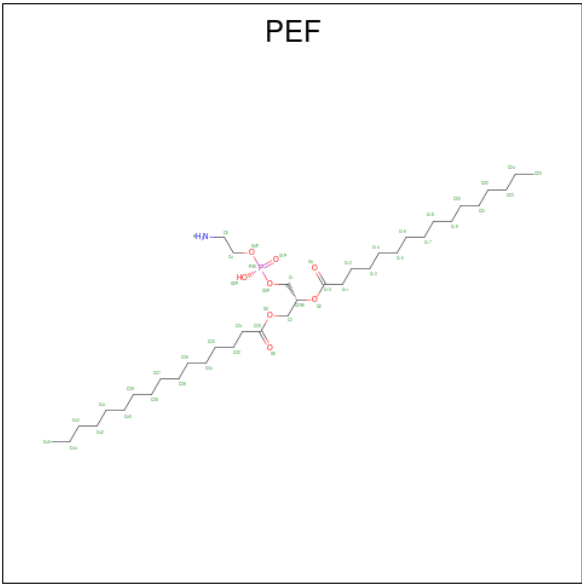
Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			20	14	6	
14	M	1	Total	C	O	0
			20	14	6	

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Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	H	1	Total	C	O	0
			20	14	6	
14	Y	1	Total	C	O	0
			20	14	6	
14	Y	1	Total	C	O	0
			20	14	6	
14	C	1	Total	C	O	0
			20	14	6	

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



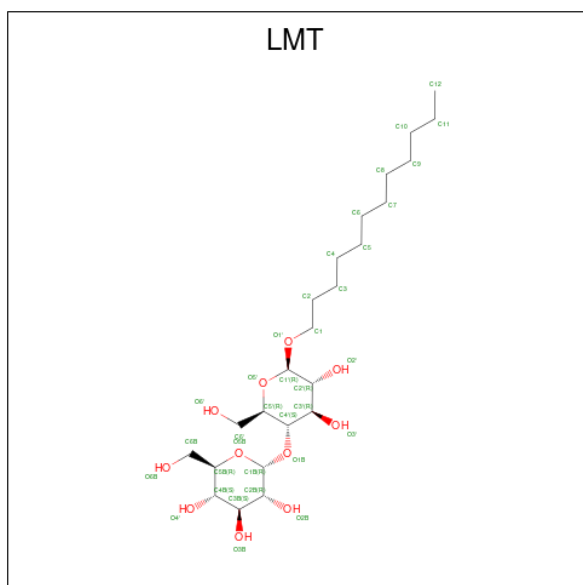
Mol	Chain	Residues	Atoms					AltConf
15	M	1	Total	C	N	O	P	0
			21	11	1	8	1	
15	L	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	h	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			35	24	11	
16	H	1	Total	C	O	0
			35	24	11	
16	T	1	Total	C	O	0
			35	24	11	
16	1	1	Total	C	O	0
			35	24	11	
16	D	1	Total	C	O	0
			35	24	11	

- Molecule 17 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

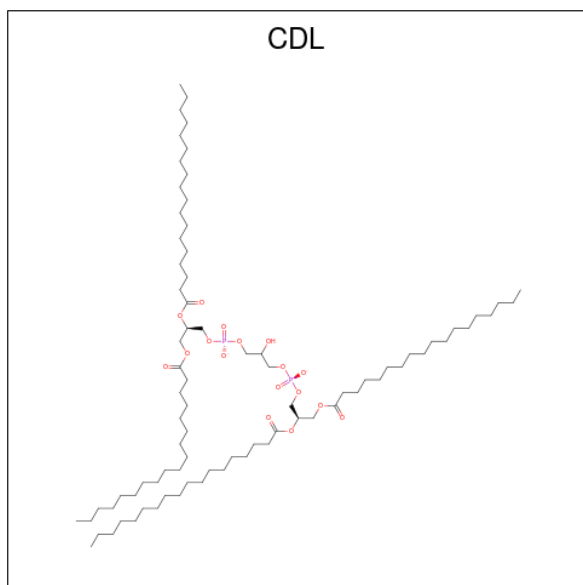
Mol	Chain	Residues	Atoms		AltConf
17	M	3	Total	C	0
			44	44	
17	L	3	Total	C	0
			30	30	

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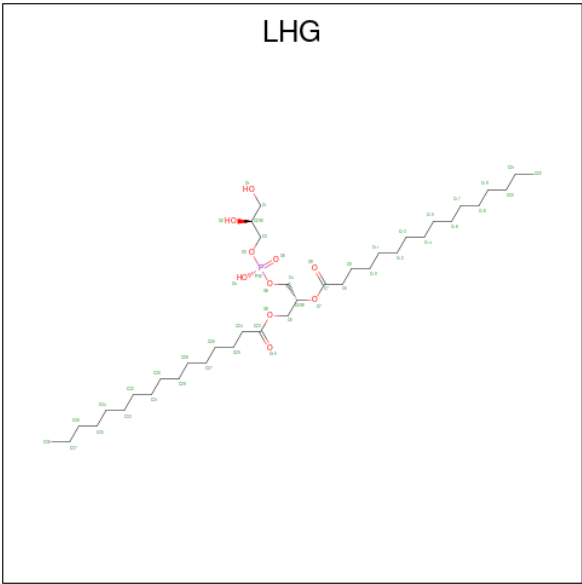
Mol	Chain	Residues	Atoms		AltConf
17	H	1	Total	C	0
			13	13	
17	V	2	Total	C	0
			26	26	
17	1	1	Total	C	0
			18	18	
17	9	2	Total	C	0
			36	36	
17	A	1	Total	C	0
			18	18	
17	D	1	Total	C	0
			12	12	
17	F	1	Total	C	0
			15	15	
17	Y	1	Total	C	0
			14	14	
17	h	2	Total	C	0
			24	24	
17	C	2	Total	C	0
			34	34	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



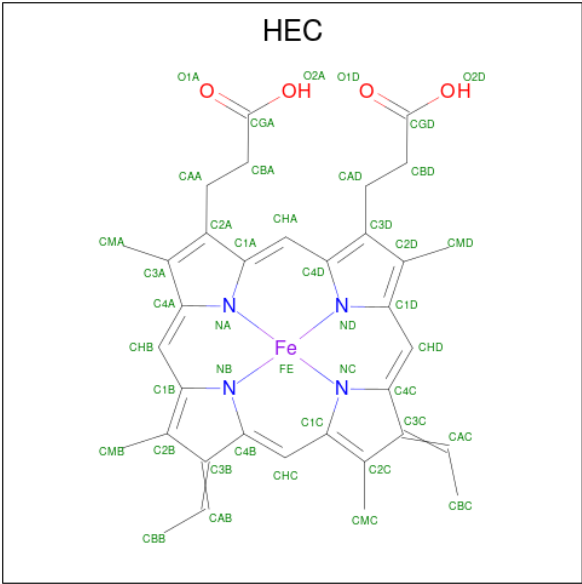
Mol	Chain	Residues	Atoms				AltConf
18	P	1	Total	C	O	P	0
			50	31	17	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	h	1	Total	C	O	0
			24	20	4	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
21	C	1	Total	Ca	0
			1	1	

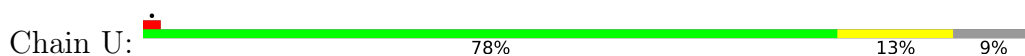
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

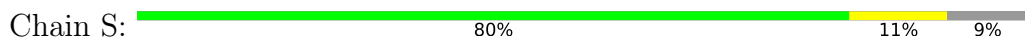
- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit



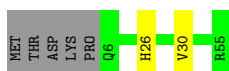
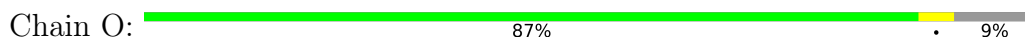
- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit

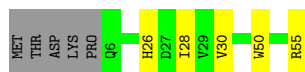


- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit

Chain K:  82% 9% 9%



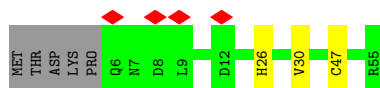
- Molecule 1: Antenna complex alpha/beta subunit

Chain I:  75% 16% 9%



- Molecule 1: Antenna complex alpha/beta subunit

Chain G:  7% 85% 5% 9%



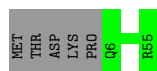
- Molecule 1: Antenna complex alpha/beta subunit

Chain E:  80% 11% 9%



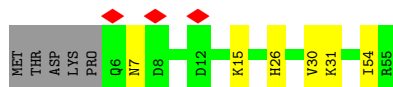
- Molecule 1: Antenna complex alpha/beta subunit

Chain B:  91% 9%



- Molecule 1: Antenna complex alpha/beta subunit

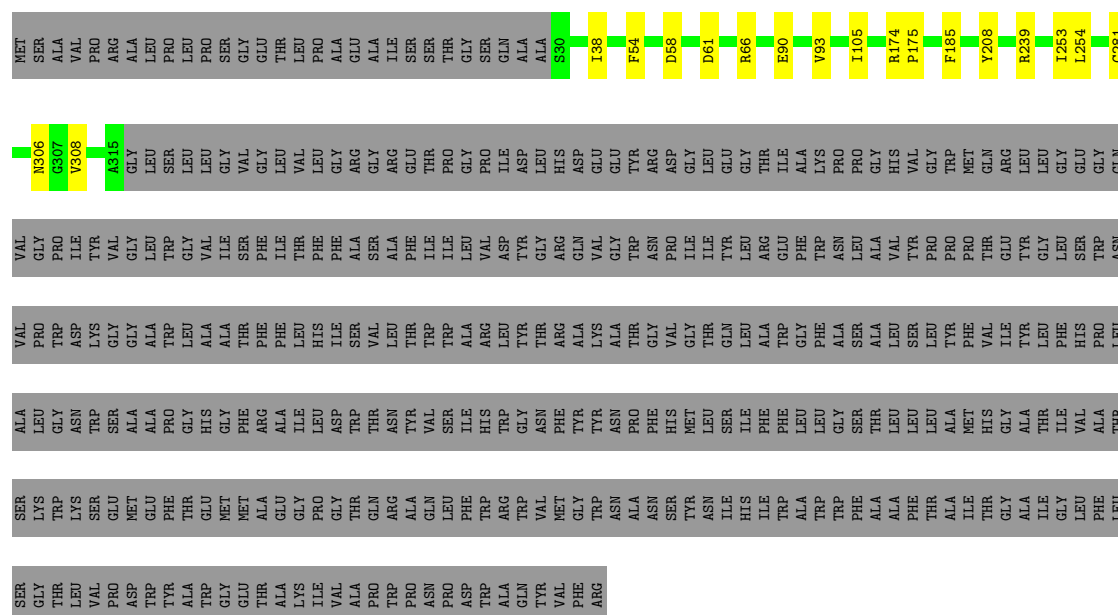
Chain 0:  5% 80% 11% 9%



- Molecule 1: Antenna complex alpha/beta subunit

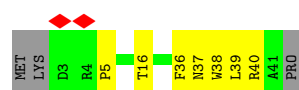
Chain 8:  69% 22% 9%

Chain L:  42% 55%



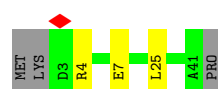
- Molecule 3: Alpha subunit of light-harvesting 1

Chain H:  5% 76% 17% 7%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain J:  86% 7% 7%



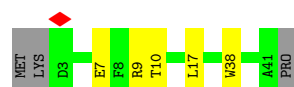
- Molecule 3: Alpha subunit of light-harvesting 1

Chain N:  83% 10% 7%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain P:  81% 12% 7%



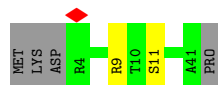
- Molecule 3: Alpha subunit of light-harvesting 1

Chain R:  90% 7%



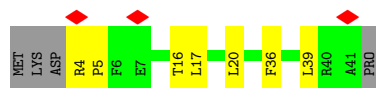
- Molecule 3: Alpha subunit of light-harvesting 1

Chain T:  86% 5% 10%



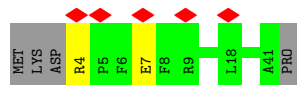
- Molecule 3: Alpha subunit of light-harvesting 1

Chain V:  74% 17% 10%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain 1:  86% 5% 10%



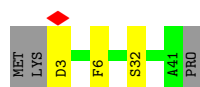
- Molecule 3: Alpha subunit of light-harvesting 1

Chain 3:  81% 12% 7%



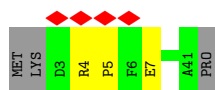
- Molecule 3: Alpha subunit of light-harvesting 1

Chain 5:  86% 7% 7%

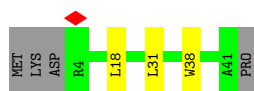
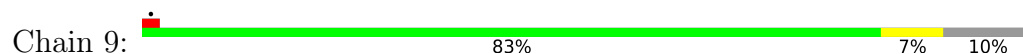


- Molecule 3: Alpha subunit of light-harvesting 1

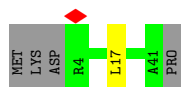
Chain 7:  86% 7% 7%



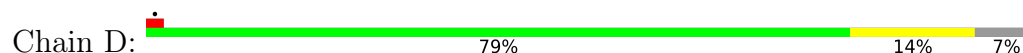
- Molecule 3: Alpha subunit of light-harvesting 1



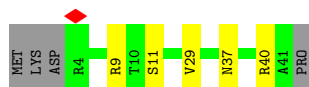
- Molecule 3: Alpha subunit of light-harvesting 1



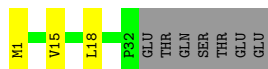
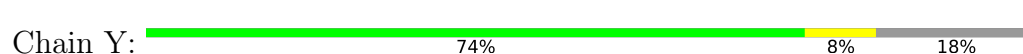
- Molecule 3: Alpha subunit of light-harvesting 1



- Molecule 3: Alpha subunit of light-harvesting 1



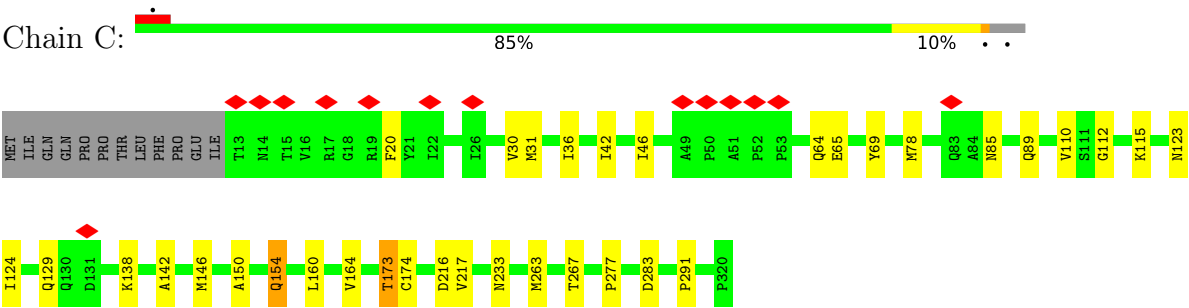
- Molecule 4: reaction center small polypeptide



- Molecule 5: reaction center small polypeptide



- Molecule 6: Cytochrome subunit of photosynthetic reaction center



- Molecule 7: reaction center unknown polypeptide



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	373675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.500	Depositor
Minimum map value	-1.414	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.307	Depositor
Map size ($\text{\AA}$)	320.4, 320.4, 320.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.89, 0.89, 0.89	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LHG, CDL, PEF, BPH, U4Z, MQE, BCL, PGV, UNL, HEC, MN, LMT, BGL

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	0	0.20	0/432	0.32	0/597
1	2	0.16	0/432	0.27	0/597
1	4	0.17	0/432	0.28	0/597
1	6	0.18	0/432	0.28	0/597
1	8	0.19	0/432	0.30	0/597
1	B	0.20	0/432	0.37	0/597
1	E	0.20	0/432	0.31	0/597
1	G	0.18	0/432	0.30	0/597
1	I	0.18	0/432	0.29	0/597
1	K	0.20	0/432	0.32	0/597
1	O	0.19	0/432	0.30	0/597
1	Q	0.24	0/432	0.35	0/597
1	S	0.20	0/432	0.31	0/597
1	U	0.21	0/432	0.33	0/597
1	W	0.16	0/432	0.27	0/597
2	L	0.41	0/2360	0.58	1/3220 (0.0%)
2	M	0.66	1/2597 (0.0%)	0.49	2/3566 (0.1%)
3	1	0.16	0/307	0.25	0/417
3	3	0.15	0/315	0.25	0/428
3	5	0.17	0/315	0.37	0/428
3	7	0.19	0/315	0.29	0/428
3	9	0.22	0/307	0.37	0/417
3	A	0.19	0/307	0.29	0/417
3	D	0.18	0/315	0.27	0/428
3	F	0.16	0/307	0.28	0/417
3	H	0.36	0/315	0.48	0/428
3	J	0.18	0/315	0.35	0/428
3	N	0.43	0/315	0.66	0/428
3	P	0.17	0/315	0.32	0/428
3	R	0.18	0/315	0.28	0/428
3	T	0.29	0/307	0.42	0/417
3	V	0.18	0/307	0.35	0/417

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Y	0.20	0/268	0.38	0/370
5	h	0.19	0/374	0.29	0/513
6	C	0.39	0/2409	0.57	0/3288
7	Z	1.30	0/51	1.58	0/70
All	All	0.36	1/19216 (0.0%)	0.43	3/26336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	355	PRO	N-CD	-29.75	1.06	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	185	PHE	CA-CB-CG	8.63	122.43	113.80
2	M	355	PRO	N-CD-CG	7.76	114.85	103.20
2	M	375	VAL	N-CA-C	-5.22	100.97	108.48

There are no chirality outliers.

There are no planarity outliers.

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	0	416	0	413	6	0
1	2	416	0	413	3	0
1	4	416	0	413	1	0
1	6	416	0	413	3	0
1	8	416	0	413	12	0
1	B	416	0	413	0	0
1	E	416	0	413	5	0
1	G	416	0	413	2	0
1	I	416	0	413	9	0
1	K	416	0	413	6	0
1	O	416	0	413	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	416	0	413	7	0
1	S	416	0	413	6	0
1	U	416	0	413	5	0
1	W	416	0	413	6	0
2	L	2278	0	2235	16	0
2	M	2488	0	2373	27	0
3	1	300	0	316	2	0
3	3	308	0	320	4	0
3	5	308	0	320	3	0
3	7	308	0	320	2	0
3	9	300	0	316	11	0
3	A	300	0	316	1	0
3	D	308	0	320	8	0
3	F	300	0	316	6	0
3	H	308	0	320	7	0
3	J	308	0	320	2	0
3	N	308	0	320	4	0
3	P	308	0	320	4	0
3	R	308	0	320	1	0
3	T	300	0	316	2	0
3	V	300	0	316	12	0
4	Y	259	0	272	2	0
5	h	362	0	365	2	0
6	C	2347	0	2301	29	0
7	Z	51	0	49	0	0
8	0	132	0	148	8	0
8	1	66	0	74	3	0
8	2	132	0	148	7	0
8	3	132	0	148	0	0
8	4	66	0	74	6	0
8	5	66	0	74	2	0
8	6	132	0	148	4	0
8	7	66	0	74	1	0
8	8	132	0	148	4	0
8	9	66	0	74	0	0
8	A	132	0	148	3	0
8	B	66	0	74	2	0
8	D	66	0	74	3	0
8	E	132	0	148	10	0
8	F	66	0	74	3	0
8	G	132	0	148	3	0
8	H	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	132	0	148	3	0
8	J	66	0	74	0	0
8	K	132	0	148	1	0
8	L	132	0	148	8	0
8	M	66	0	74	2	0
8	N	66	0	74	3	0
8	O	132	0	148	4	0
8	P	66	0	74	2	0
8	Q	132	0	148	4	0
8	R	66	0	74	3	0
8	S	132	0	148	4	0
8	T	66	0	74	0	0
8	U	132	0	148	7	0
8	V	66	0	74	8	0
8	W	132	0	148	6	0
9	0	88	0	122	2	0
9	1	36	0	43	1	0
9	4	44	0	61	1	0
9	6	44	0	61	1	0
9	8	44	0	61	1	0
9	C	51	0	76	1	0
9	E	88	0	122	2	0
9	I	44	0	61	3	0
9	K	88	0	122	3	0
9	L	119	0	154	3	0
9	M	35	0	38	5	0
9	N	24	0	18	0	0
9	O	44	0	61	1	0
9	S	44	0	61	1	0
9	U	88	0	122	2	0
9	h	46	0	69	2	0
10	0	40	0	0	0	0
10	3	40	0	0	2	0
10	D	40	0	0	0	0
10	J	40	0	0	0	0
10	R	40	0	0	1	0
11	L	130	0	152	3	0
11	M	65	0	76	2	0
12	M	1	0	0	0	0
13	L	53	0	0	0	0
13	M	68	0	0	1	0
14	C	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	20	0	28	0	0
14	L	80	0	112	1	0
14	M	60	0	84	2	0
14	Y	40	0	56	0	0
15	L	88	0	131	3	0
15	M	21	0	15	0	0
15	h	41	0	55	4	0
16	1	35	0	46	1	0
16	D	35	0	46	3	0
16	H	35	0	46	2	0
16	M	35	0	46	2	0
16	T	35	0	46	2	0
17	1	18	0	0	0	0
17	9	36	0	0	10	0
17	A	18	0	0	0	0
17	C	34	0	0	0	0
17	D	12	0	0	0	0
17	F	15	0	0	0	0
17	H	13	0	0	0	0
17	L	30	0	0	0	0
17	M	44	0	0	0	0
17	V	26	0	0	0	0
17	Y	14	0	0	0	0
17	h	24	0	0	0	0
18	P	50	0	44	2	0
19	h	24	0	34	5	0
20	C	172	0	120	5	0
21	C	1	0	0	0	0
All	All	24285	0	24535	302	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 6.

The worst 5 of 302 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:31:LEU:HD23	17:9:103:UNL:C11	1.59	1.32
3:9:31:LEU:HD21	17:9:103:UNL:C14	1.62	1.27
3:9:31:LEU:CD2	17:9:103:UNL:C11	2.23	1.16
8:2:102:BCL:HBB2	6:C:20:PHE:CE1	1.85	1.10
3:V:20:LEU:HD12	8:V:101:BCL:C4	1.86	1.05

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	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	2	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	4	48/55 (87%)	48 (100%)	0	0	100	100
1	6	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	8	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	B	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	E	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	G	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
1	I	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	K	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	O	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	Q	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	S	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	U	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	W	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
2	L	284/641 (44%)	272 (96%)	12 (4%)	0	100	100
2	M	304/641 (47%)	294 (97%)	10 (3%)	0	100	100
3	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	3	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	5	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	7	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	9	36/42 (86%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
3	D	37/42 (88%)	37 (100%)	0	0	100	100
3	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	H	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	J	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
3	N	37/42 (88%)	37 (100%)	0	0	100	100
3	P	37/42 (88%)	37 (100%)	0	0	100	100
3	R	37/42 (88%)	37 (100%)	0	0	100	100
3	T	36/42 (86%)	36 (100%)	0	0	100	100
3	V	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
4	Y	30/39 (77%)	29 (97%)	1 (3%)	0	100	100
5	h	45/63 (71%)	45 (100%)	0	0	100	100
6	C	306/320 (96%)	290 (95%)	16 (5%)	0	100	100
7	Z	8/10 (80%)	8 (100%)	0	0	100	100
All	All	2246/3169 (71%)	2166 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	0	44/49 (90%)	44 (100%)	0	100	100
1	2	44/49 (90%)	43 (98%)	1 (2%)	44	68
1	4	44/49 (90%)	44 (100%)	0	100	100
1	6	44/49 (90%)	43 (98%)	1 (2%)	44	68
1	8	44/49 (90%)	44 (100%)	0	100	100
1	B	44/49 (90%)	44 (100%)	0	100	100
1	E	44/49 (90%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	44/49 (90%)	44 (100%)	0	100	100
1	I	44/49 (90%)	44 (100%)	0	100	100
1	K	44/49 (90%)	44 (100%)	0	100	100
1	O	44/49 (90%)	44 (100%)	0	100	100
1	Q	44/49 (90%)	44 (100%)	0	100	100
1	S	44/49 (90%)	44 (100%)	0	100	100
1	U	44/49 (90%)	44 (100%)	0	100	100
1	W	44/49 (90%)	44 (100%)	0	100	100
2	L	232/511 (45%)	229 (99%)	3 (1%)	61	79
2	M	244/511 (48%)	240 (98%)	4 (2%)	55	76
3	1	33/37 (89%)	33 (100%)	0	100	100
3	3	34/37 (92%)	34 (100%)	0	100	100
3	5	34/37 (92%)	34 (100%)	0	100	100
3	7	34/37 (92%)	34 (100%)	0	100	100
3	9	33/37 (89%)	32 (97%)	1 (3%)	36	61
3	A	33/37 (89%)	33 (100%)	0	100	100
3	D	34/37 (92%)	34 (100%)	0	100	100
3	F	33/37 (89%)	33 (100%)	0	100	100
3	H	34/37 (92%)	34 (100%)	0	100	100
3	J	34/37 (92%)	34 (100%)	0	100	100
3	N	34/37 (92%)	34 (100%)	0	100	100
3	P	34/37 (92%)	34 (100%)	0	100	100
3	R	34/37 (92%)	34 (100%)	0	100	100
3	T	33/37 (89%)	33 (100%)	0	100	100
3	V	33/37 (89%)	33 (100%)	0	100	100
4	Y	29/36 (81%)	28 (97%)	1 (3%)	32	58
5	h	36/50 (72%)	35 (97%)	1 (3%)	38	62
6	C	250/262 (95%)	247 (99%)	3 (1%)	63	80
7	Z	1/1 (100%)	1 (100%)	0	100	100
All	All	1956/2661 (74%)	1941 (99%)	15 (1%)	70	86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	281	CYS
6	C	173	THR
2	L	308	VAL
6	C	217	VAL
5	h	18	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	89	GLN
6	C	226	GLN
6	C	225	ASN
3	J	37	ASN
6	C	83	GLN

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 128 ligands modelled in this entry, 2 are monoatomic and 20 are unknown - leaving 106 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	3	101	-	69,74,74	1.82	18 (26%)	79,115,115	2.28	26 (32%)
8	BCL	L	703	-	69,74,74	1.80	17 (24%)	79,115,115	2.35	24 (30%)
8	BCL	F	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.21	20 (25%)
9	PGV	6	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.16	4 (8%)
8	BCL	M	701	-	69,74,74	1.82	17 (24%)	79,115,115	2.41	23 (29%)
10	U4Z	D	101	-	40,40,40	1.46	6 (15%)	51,51,51	1.51	12 (23%)
8	BCL	H	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.33	22 (27%)
8	BCL	3	103	-	69,74,74	1.79	18 (26%)	79,115,115	2.25	20 (25%)
15	PEF	M	708	-	20,20,46	1.54	2 (10%)	23,25,51	1.64	3 (13%)
8	BCL	O	101	-	69,74,74	1.82	18 (26%)	79,115,115	2.15	21 (26%)
9	PGV	L	712	-	34,34,50	1.09	2 (5%)	37,40,56	1.22	4 (10%)
20	HEC	C	501	6	46,50,50	1.82	5 (10%)	58,82,82	1.86	4 (6%)
9	PGV	h	102	-	45,45,50	0.98	2 (4%)	48,50,56	1.21	5 (10%)
8	BCL	E	102	-	69,74,74	1.80	18 (26%)	79,115,115	2.32	23 (29%)
8	BCL	4	101	-	69,74,74	1.76	20 (28%)	79,115,115	2.27	25 (31%)
8	BCL	5	101	-	69,74,74	1.77	16 (23%)	79,115,115	2.22	24 (30%)
9	PGV	N	102	-	23,23,50	1.32	2 (8%)	26,29,56	1.36	3 (11%)
14	BGL	M	707	-	20,20,20	0.35	0	24,25,25	0.85	1 (4%)
14	BGL	C	507	-	20,20,20	0.37	0	24,25,25	0.64	0
8	BCL	6	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.09	23 (29%)
9	PGV	E	104	-	43,43,50	0.97	2 (4%)	46,49,56	1.10	4 (8%)
14	BGL	L	714	-	20,20,20	0.37	0	24,25,25	0.56	0
8	BCL	7	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.28	24 (30%)
14	BGL	L	708	-	20,20,20	0.41	0	24,25,25	0.76	0
8	BCL	W	101	-	69,74,74	1.82	19 (27%)	79,115,115	2.10	20 (25%)
14	BGL	Y	103	-	20,20,20	0.40	0	24,25,25	0.64	0
10	U4Z	R	101	-	40,40,40	1.45	7 (17%)	51,51,51	1.49	13 (25%)
14	BGL	H	103	-	20,20,20	0.36	0	24,25,25	0.60	0
9	PGV	4	102	-	43,43,50	0.98	2 (4%)	46,49,56	1.08	4 (8%)
10	U4Z	J	101	-	40,40,40	1.47	7 (17%)	51,51,51	1.59	15 (29%)
8	BCL	G	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.18	28 (35%)
11	BPH	L	701	-	59,70,70	0.78	2 (3%)	59,101,101	1.00	3 (5%)
8	BCL	0	101	-	69,74,74	1.80	16 (23%)	79,115,115	2.18	25 (31%)
8	BCL	V	101	-	69,74,74	1.75	18 (26%)	79,115,115	2.16	19 (24%)
16	LMT	H	102	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
8	BCL	8	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.05	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BGL	M	706	-	20,20,20	0.44	0	24,25,25	0.63	0
16	LMT	D	104	-	36,36,36	0.40	0	47,47,47	0.77	0
8	BCL	B	101	-	69,74,74	1.86	19 (27%)	79,115,115	2.24	22 (27%)
9	PGV	I	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.28	4 (8%)
9	PGV	U	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.11	4 (8%)
19	LHG	h	101	-	23,23,48	0.30	0	24,24,54	0.73	1 (4%)
8	BCL	L	702	-	69,74,74	1.80	16 (23%)	79,115,115	2.29	22 (27%)
8	BCL	Q	102	-	69,74,74	1.80	18 (26%)	79,115,115	2.20	21 (26%)
9	PGV	K	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.04	4 (8%)
8	BCL	8	102	-	69,74,74	1.72	18 (26%)	79,115,115	2.32	25 (31%)
8	BCL	W	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.37	26 (32%)
8	BCL	R	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.27	21 (26%)
20	HEC	C	502	6	46,50,50	1.83	3 (6%)	58,82,82	1.89	4 (6%)
8	BCL	U	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.82	30 (37%)
8	BCL	S	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.06	22 (27%)
8	BCL	2	102	-	69,74,74	1.77	19 (27%)	79,115,115	2.43	28 (35%)
8	BCL	0	102	-	69,74,74	1.76	21 (30%)	79,115,115	2.27	24 (30%)
9	PGV	L	711	-	32,32,50	0.85	1 (3%)	34,37,56	1.10	2 (5%)
13	MQE	M	704	-	69,69,69	0.39	0	85,87,87	0.44	1 (1%)
8	BCL	E	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.08	22 (27%)
8	BCL	D	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.29	24 (30%)
9	PGV	U	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.10	4 (8%)
14	BGL	L	715	-	20,20,20	0.35	0	24,25,25	0.94	1 (4%)
9	PGV	K	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.04	2 (4%)
8	BCL	2	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.06	23 (29%)
9	PGV	L	706	-	50,50,50	0.91	2 (4%)	53,56,56	1.00	2 (3%)
8	BCL	1	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.27	21 (26%)
9	PGV	O	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.16	3 (6%)
9	PGV	1	102	-	35,35,50	1.12	2 (5%)	38,40,56	1.21	4 (10%)
8	BCL	A	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.20	22 (27%)
8	BCL	K	102	-	69,74,74	1.80	20 (28%)	79,115,115	2.17	23 (29%)
9	PGV	E	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.14	3 (6%)
9	PGV	0	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.18	4 (8%)
8	BCL	N	101	-	69,74,74	1.75	17 (24%)	79,115,115	2.25	20 (25%)
8	BCL	P	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.25	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BPH	L	704	-	59,70,70	0.88	3 (5%)	59,101,101	0.95	2 (3%)
8	BCL	A	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.20	23 (29%)
20	HEC	C	503	6	46,50,50	1.83	4 (8%)	58,82,82	1.93	4 (6%)
15	PEF	h	103	-	40,40,46	1.02	2 (5%)	43,45,51	1.14	3 (6%)
8	BCL	G	102	-	69,74,74	1.80	19 (27%)	79,115,115	2.35	22 (27%)
8	BCL	Q	101	-	69,74,74	1.78	16 (23%)	79,115,115	2.14	21 (26%)
8	BCL	S	102	-	69,74,74	1.80	22 (31%)	79,115,115	2.32	24 (30%)
8	BCL	O	102	-	69,74,74	1.75	18 (26%)	79,115,115	2.33	25 (31%)
15	PEF	L	713	-	46,46,46	0.95	2 (4%)	49,51,51	1.10	4 (8%)
10	U4Z	0	103	-	40,40,40	1.47	6 (15%)	51,51,51	1.53	13 (25%)
8	BCL	U	101	-	69,74,74	1.80	18 (26%)	79,115,115	2.14	24 (30%)
14	BGL	Y	101	-	20,20,20	0.38	0	24,25,25	0.78	0
8	BCL	9	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.26	23 (29%)
8	BCL	I	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.14	23 (29%)
9	PGV	C	506	21	50,50,50	0.87	2 (4%)	53,56,56	1.12	4 (7%)
11	BPH	M	702	-	59,70,70	0.85	2 (3%)	59,101,101	0.99	3 (5%)
15	PEF	L	717	-	40,40,46	1.01	2 (5%)	43,45,51	1.08	2 (4%)
8	BCL	T	101	-	69,74,74	1.77	20 (28%)	79,115,115	2.27	20 (25%)
8	BCL	6	102	-	69,74,74	1.82	18 (26%)	79,115,115	2.31	22 (27%)
9	PGV	0	105	-	43,43,50	0.97	2 (4%)	46,49,56	1.18	4 (8%)
8	BCL	J	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	21 (26%)
16	LMT	M	709	-	36,36,36	0.37	0	47,47,47	0.97	3 (6%)
14	BGL	M	710	-	20,20,20	0.39	0	24,25,25	0.60	0
20	HEC	C	504	6	46,50,50	1.86	4 (8%)	58,82,82	1.84	5 (8%)
8	BCL	I	102	-	69,74,74	1.77	20 (28%)	79,115,115	2.23	20 (25%)
10	U4Z	3	102	-	40,40,40	1.47	9 (22%)	51,51,51	1.57	14 (27%)
8	BCL	K	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.10	23 (29%)
9	PGV	S	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.13	5 (10%)
9	PGV	8	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.17	4 (8%)
16	LMT	T	102	-	36,36,36	0.51	1 (2%)	47,47,47	1.05	3 (6%)
14	BGL	L	709	-	20,20,20	0.39	0	24,25,25	0.49	0
13	MQE	L	705	-	54,54,69	0.35	0	67,69,87	0.72	2 (2%)
16	LMT	1	104	-	36,36,36	0.39	0	47,47,47	0.80	1 (2%)
18	CDL	P	102	-	49,49,99	1.29	4 (8%)	55,61,111	1.31	6 (10%)
9	PGV	M	705	-	34,34,50	1.12	2 (5%)	37,40,56	1.11	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	3	101	-	-	11/41/137/137	-
8	BCL	L	703	-	-	17/41/137/137	-
8	BCL	F	101	-	-	20/41/137/137	-
9	PGV	6	103	-	-	15/48/48/55	-
8	BCL	M	701	-	-	18/41/137/137	-
10	U4Z	D	101	-	-	4/36/53/53	0/1/1/1
8	BCL	H	101	-	-	16/41/137/137	-
8	BCL	3	103	-	-	14/41/137/137	-
15	PEF	M	708	-	-	9/23/23/50	-
8	BCL	O	101	-	-	12/41/137/137	-
9	PGV	L	712	-	-	15/39/39/55	-
20	HEC	C	501	6	-	5/14/54/54	-
9	PGV	h	102	-	-	11/47/47/55	-
8	BCL	E	102	-	-	22/41/137/137	-
8	BCL	4	101	-	-	16/41/137/137	-
8	BCL	5	101	-	-	14/41/137/137	-
9	PGV	N	102	-	-	0/28/28/55	-
14	BGL	M	707	-	-	1/11/31/31	0/1/1/1
14	BGL	C	507	-	-	1/11/31/31	0/1/1/1
8	BCL	6	101	-	-	10/41/137/137	-
9	PGV	E	104	-	-	10/48/48/55	-
14	BGL	L	714	-	-	2/11/31/31	0/1/1/1
8	BCL	7	101	-	-	12/41/137/137	-
14	BGL	L	708	-	-	3/11/31/31	0/1/1/1
8	BCL	W	101	-	-	17/41/137/137	-
14	BGL	Y	103	-	-	3/11/31/31	0/1/1/1
10	U4Z	R	101	-	-	4/36/53/53	0/1/1/1
14	BGL	H	103	-	-	2/11/31/31	0/1/1/1
9	PGV	4	102	-	-	16/48/48/55	-
10	U4Z	J	101	-	-	4/36/53/53	0/1/1/1
8	BCL	G	101	-	-	15/41/137/137	-
11	BPH	L	701	-	-	14/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	0	101	-	-	11/41/137/137	-
8	BCL	V	101	-	-	19/41/137/137	-
16	LMT	H	102	-	-	6/21/61/61	0/2/2/2
8	BCL	8	101	-	-	14/41/137/137	-
14	BGL	M	706	-	-	3/11/31/31	0/1/1/1
16	LMT	D	104	-	-	10/21/61/61	0/2/2/2
8	BCL	B	101	-	-	15/41/137/137	-
9	PGV	I	103	-	-	10/48/48/55	-
9	PGV	U	104	-	-	12/48/48/55	-
19	LHG	h	101	-	-	19/23/23/53	-
8	BCL	L	702	-	-	14/41/137/137	-
8	BCL	Q	102	-	-	19/41/137/137	-
9	PGV	K	103	-	-	13/48/48/55	-
8	BCL	8	102	-	-	11/41/137/137	-
8	BCL	W	102	-	-	19/41/137/137	-
8	BCL	R	102	-	-	12/41/137/137	-
20	HEC	C	502	6	-	4/14/54/54	-
8	BCL	U	102	-	-	21/41/137/137	-
8	BCL	S	101	-	-	17/41/137/137	-
8	BCL	2	102	-	-	21/41/137/137	-
8	BCL	0	102	-	-	20/41/137/137	-
9	PGV	L	711	-	-	9/36/36/55	-
13	MQE	M	704	-	-	10/65/85/85	0/2/2/2
8	BCL	E	101	-	-	15/41/137/137	-
8	BCL	D	102	-	-	13/41/137/137	-
9	PGV	U	103	-	-	11/48/48/55	-
14	BGL	L	715	-	-	1/11/31/31	0/1/1/1
9	PGV	K	104	-	-	15/48/48/55	-
8	BCL	2	101	-	-	13/41/137/137	-
9	PGV	L	706	-	-	14/55/55/55	-
8	BCL	1	101	-	-	13/41/137/137	-
9	PGV	O	103	-	-	17/48/48/55	-
9	PGV	1	102	-	-	12/37/37/55	-
8	BCL	A	102	-	-	10/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	K	102	-	-	20/41/137/137	-
9	PGV	E	103	-	-	13/48/48/55	-
9	PGV	O	104	-	-	15/48/48/55	-
8	BCL	N	101	-	-	17/41/137/137	-
8	BCL	P	101	-	-	8/41/137/137	-
11	BPH	L	704	-	-	11/37/105/105	0/5/6/6
8	BCL	A	101	-	-	15/41/137/137	-
20	HEC	C	503	6	-	4/14/54/54	-
15	PEF	h	103	-	-	18/44/44/50	-
8	BCL	G	102	-	-	24/41/137/137	-
8	BCL	Q	101	-	-	14/41/137/137	-
8	BCL	S	102	-	-	19/41/137/137	-
8	BCL	O	102	-	-	18/41/137/137	-
15	PEF	L	713	-	-	14/50/50/50	-
10	U4Z	O	103	-	-	2/36/53/53	0/1/1/1
8	BCL	U	101	-	-	10/41/137/137	-
14	BGL	Y	101	-	-	2/11/31/31	0/1/1/1
8	BCL	9	101	-	-	13/41/137/137	-
8	BCL	I	101	-	-	10/41/137/137	-
9	PGV	C	506	21	-	20/55/55/55	-
11	BPH	M	702	-	-	22/37/105/105	0/5/6/6
15	PEF	L	717	-	-	11/44/44/50	-
8	BCL	T	101	-	-	15/41/137/137	-
8	BCL	6	102	-	-	20/41/137/137	-
9	PGV	O	105	-	-	10/48/48/55	-
8	BCL	J	102	-	-	14/41/137/137	-
16	LMT	M	709	-	-	13/21/61/61	0/2/2/2
14	BGL	M	710	-	-	1/11/31/31	0/1/1/1
20	HEC	C	504	6	-	6/14/54/54	-
8	BCL	I	102	-	-	23/41/137/137	-
10	U4Z	3	102	-	-	4/36/53/53	0/1/1/1
8	BCL	K	101	-	-	15/41/137/137	-
9	PGV	S	103	-	-	10/48/48/55	-
9	PGV	8	103	-	-	14/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	T	102	-	-	8/21/61/61	0/2/2/2
14	BGL	L	709	-	-	0/11/31/31	0/1/1/1
13	MQE	L	705	-	-	6/47/67/85	0/2/2/2
16	LMT	1	104	-	-	3/21/61/61	0/2/2/2
18	CDL	P	102	-	-	24/60/60/110	-
9	PGV	M	705	-	-	10/39/39/55	-

The worst 5 of 974 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	503	HEC	CAC-C3C	6.46	1.56	1.35
20	C	504	HEC	CAC-C3C	6.40	1.55	1.35
20	C	502	HEC	CAC-C3C	6.39	1.55	1.35
20	C	501	HEC	CAC-C3C	6.29	1.55	1.35
20	C	504	HEC	CAB-C3B	6.26	1.55	1.35

The worst 5 of 1302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	102	BCL	C2B-C1B-NB	11.07	121.80	110.33
20	C	503	HEC	CBB-CAB-C3B	-9.08	109.28	127.43
8	U	102	BCL	C4A-NA-C1A	8.83	110.71	106.68
8	E	102	BCL	CMD-C2D-C1D	8.21	139.19	124.73
20	C	501	HEC	CBB-CAB-C3B	-8.21	111.03	127.43

There are no chirality outliers.

5 of 1272 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C4C-C3C-CAC-CBC
8	W	102	BCL	C2-C1-O2A-CGA
8	W	102	BCL	C2C-C3C-CAC-CBC
8	U	102	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

72 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	703	BCL	2	0

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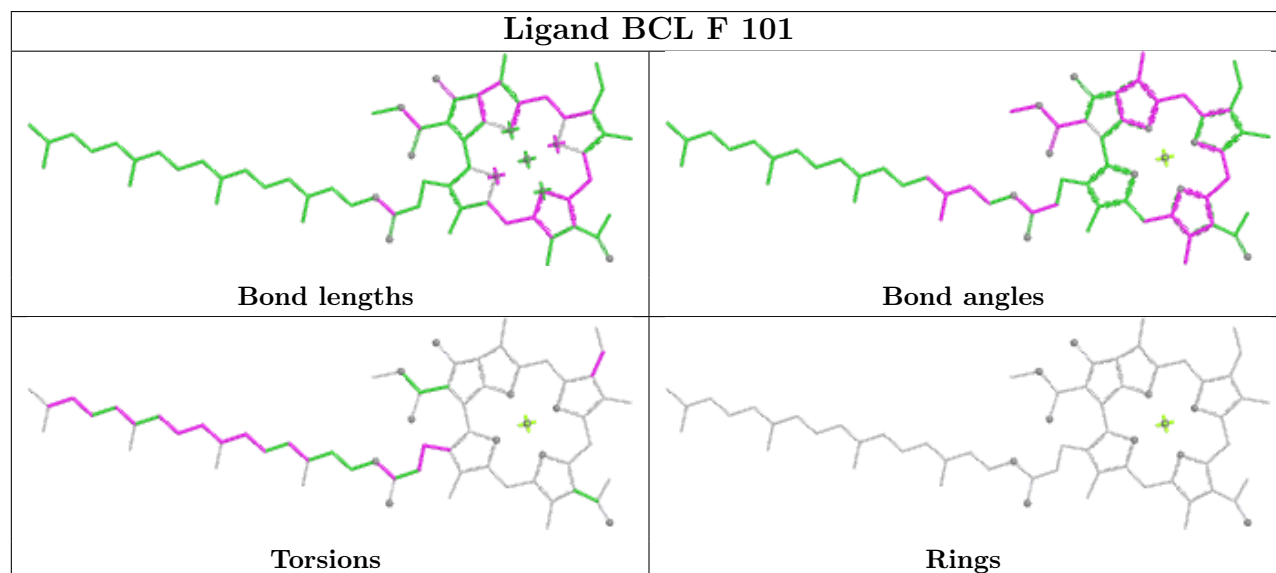
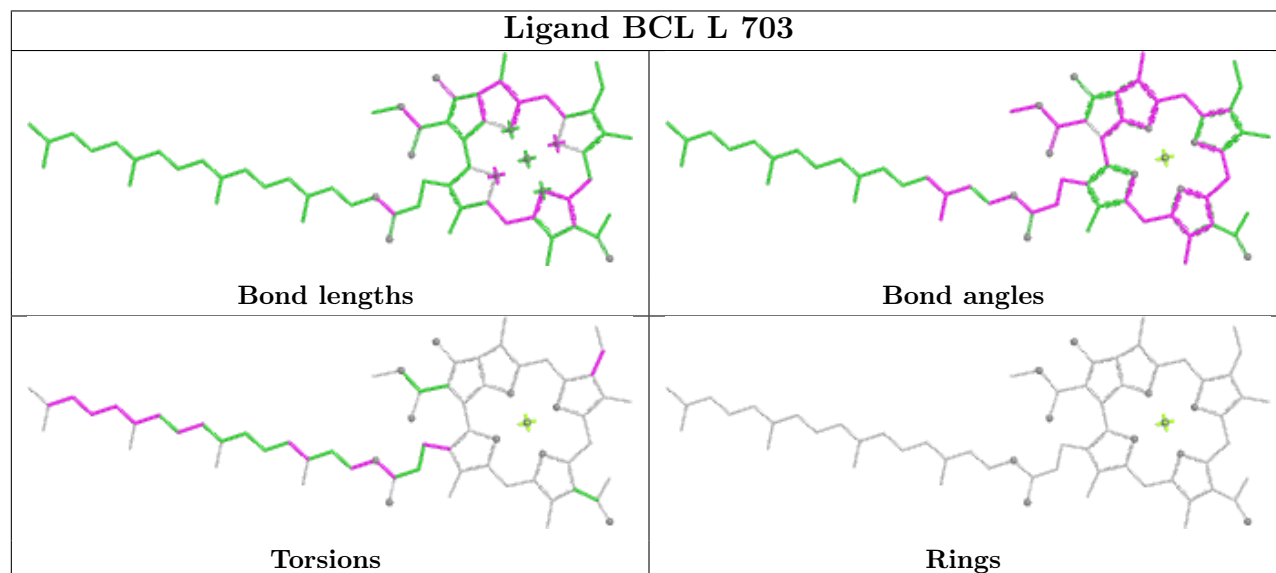
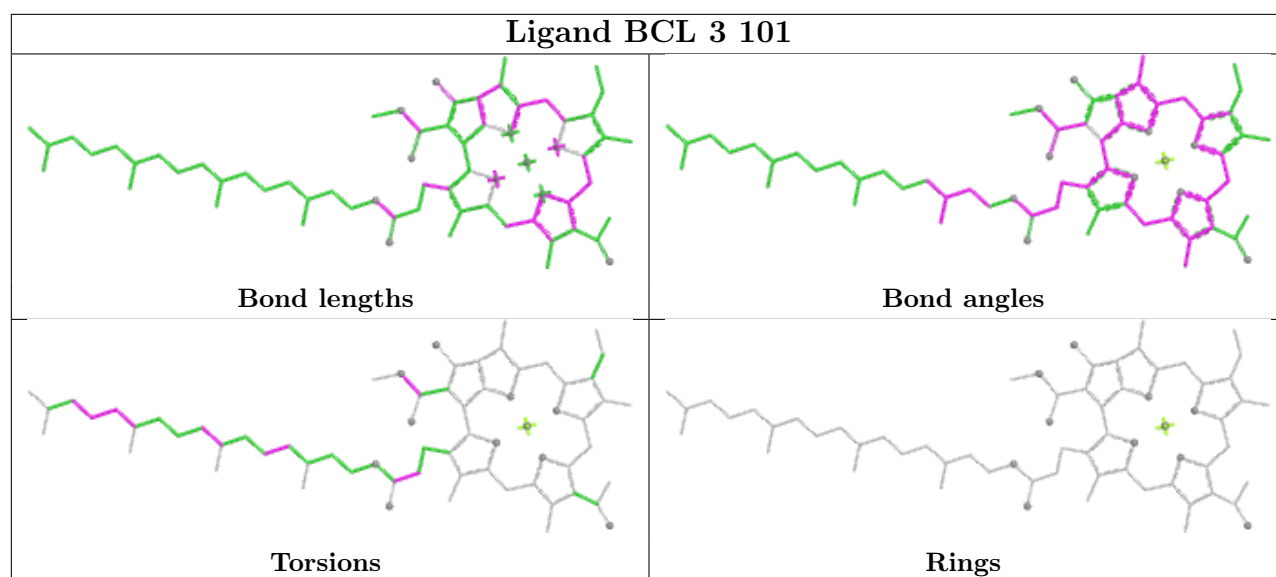
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	BCL	3	0
9	6	103	PGV	1	0
8	M	701	BCL	2	0
8	H	101	BCL	1	0
20	C	501	HEC	2	0
9	h	102	PGV	2	0
8	E	102	BCL	3	0
8	4	101	BCL	6	0
8	5	101	BCL	2	0
8	6	101	BCL	1	0
8	7	101	BCL	1	0
8	W	101	BCL	3	0
10	R	101	U4Z	1	0
9	4	102	PGV	1	0
8	G	101	BCL	1	0
8	V	101	BCL	8	0
16	H	102	LMT	2	0
8	8	101	BCL	1	0
16	D	104	LMT	3	0
8	B	101	BCL	2	0
9	I	103	PGV	3	0
19	h	101	LHG	5	0
8	L	702	BCL	6	0
8	Q	102	BCL	2	0
9	K	103	PGV	2	0
8	8	102	BCL	3	0
8	W	102	BCL	3	0
8	R	102	BCL	3	0
8	U	102	BCL	4	0
8	2	102	BCL	7	0
8	0	102	BCL	8	0
9	L	711	PGV	3	0
13	M	704	MQE	1	0
8	E	101	BCL	7	0
8	D	102	BCL	3	0
9	U	103	PGV	2	0
14	L	715	BGL	1	0
9	K	104	PGV	1	0
8	1	101	BCL	3	0
9	O	103	PGV	1	0
9	1	102	PGV	1	0
8	A	102	BCL	3	0

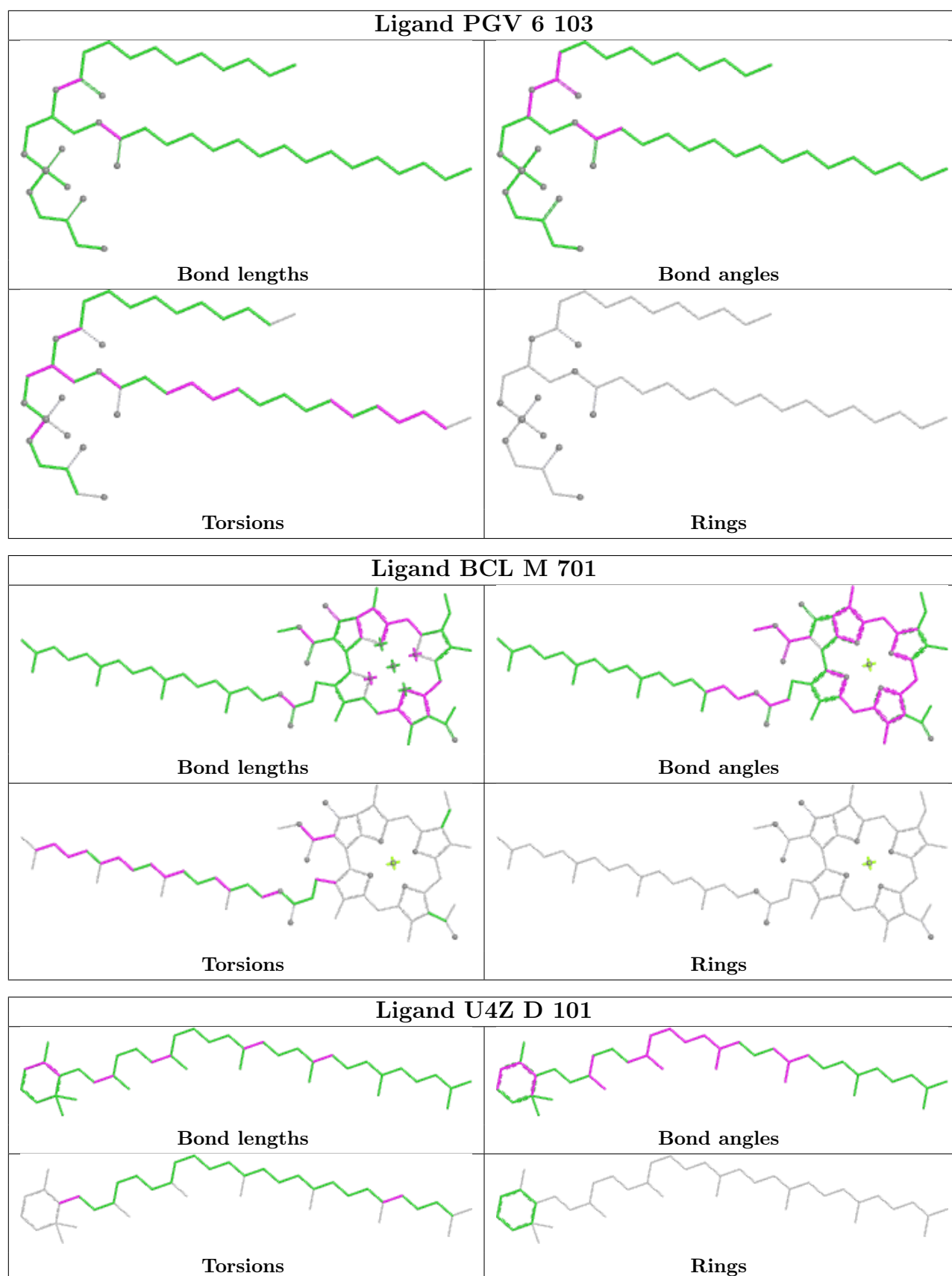
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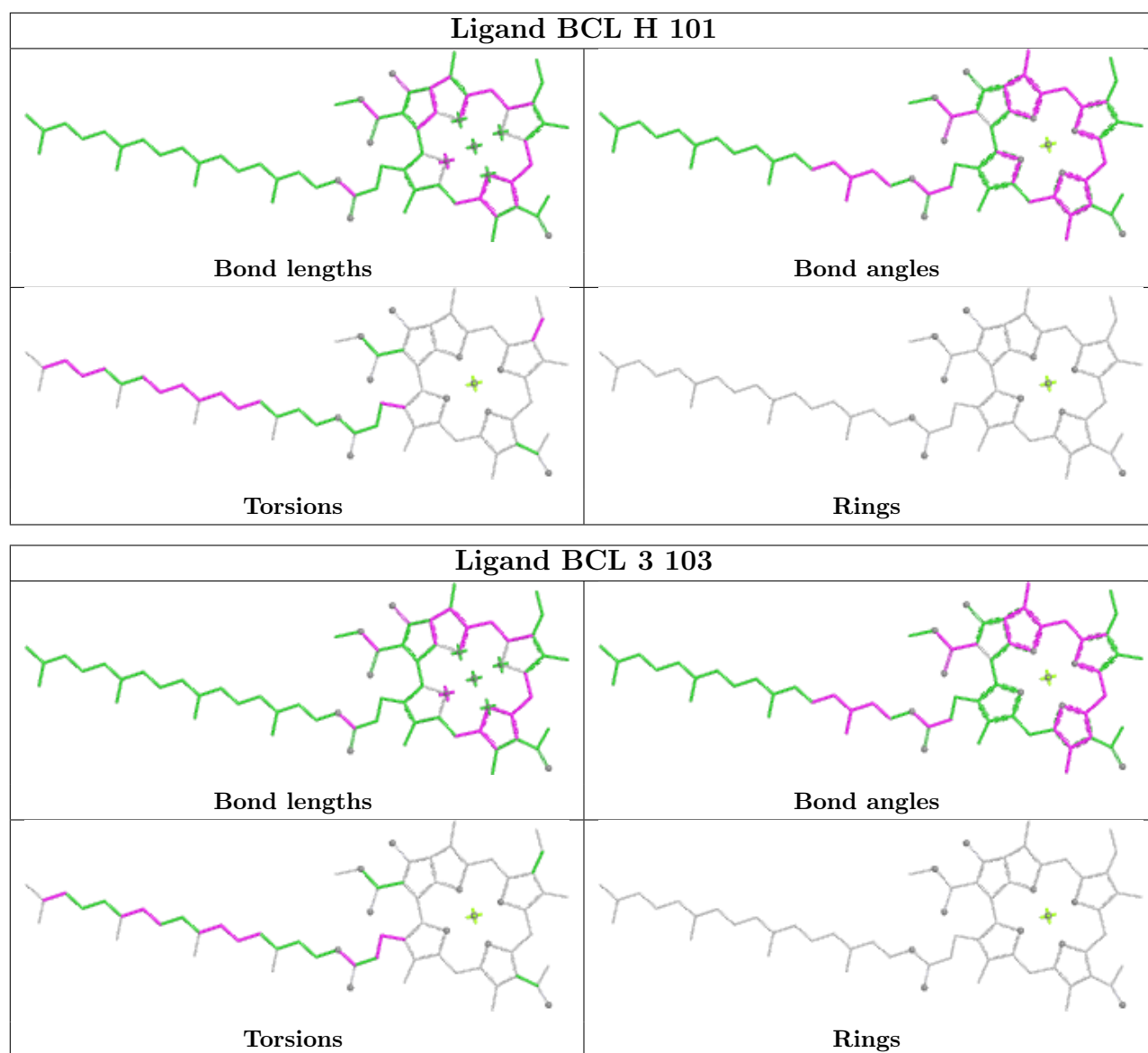
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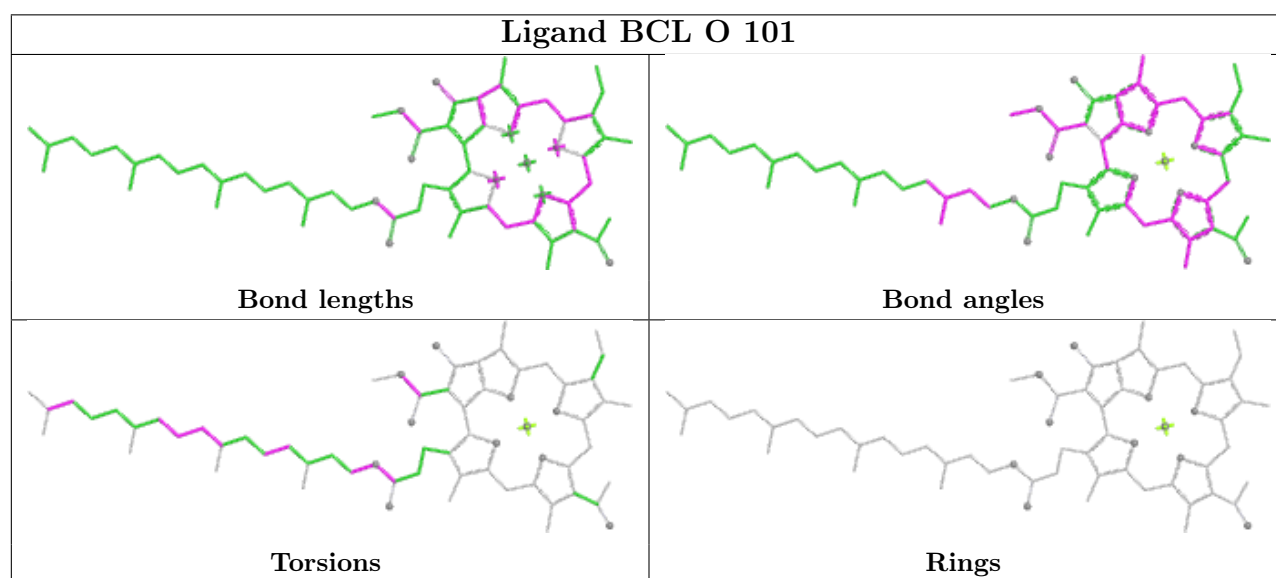
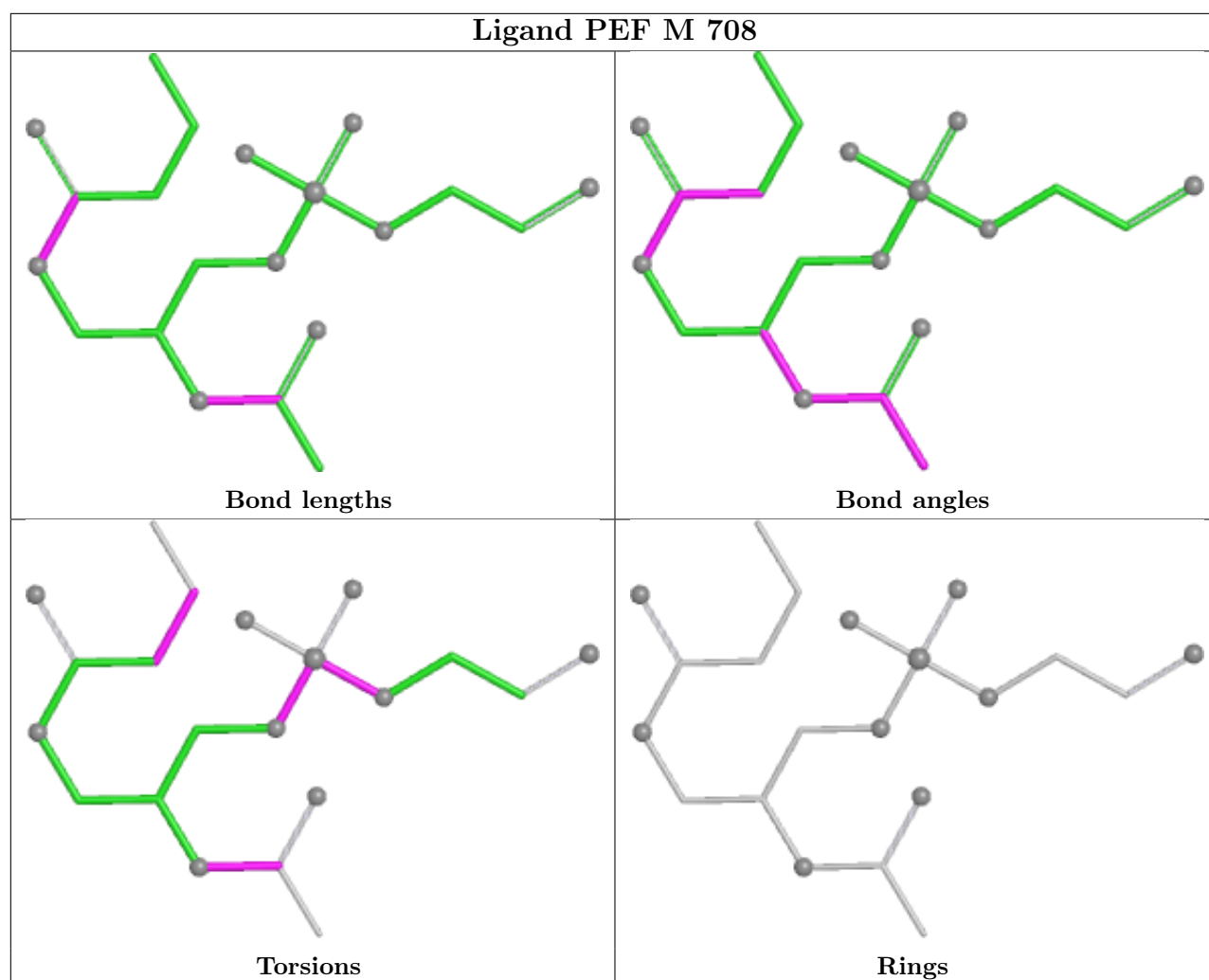
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	102	BCL	1	0
9	E	103	PGV	2	0
9	O	104	PGV	2	0
8	N	101	BCL	3	0
8	P	101	BCL	2	0
11	L	704	BPH	3	0
15	h	103	PEF	4	0
8	G	102	BCL	2	0
8	Q	101	BCL	2	0
8	S	102	BCL	4	0
8	O	102	BCL	4	0
15	L	713	PEF	2	0
8	U	101	BCL	3	0
8	I	101	BCL	1	0
9	C	506	PGV	1	0
11	M	702	BPH	2	0
15	L	717	PEF	2	0
8	6	102	BCL	3	0
16	M	709	LMT	2	0
14	M	710	BGL	2	0
20	C	504	HEC	3	0
8	I	102	BCL	2	0
10	3	102	U4Z	2	0
9	S	103	PGV	1	0
9	8	103	PGV	1	0
16	T	102	LMT	2	0
16	1	104	LMT	1	0
18	P	102	CDL	2	0
9	M	705	PGV	5	0

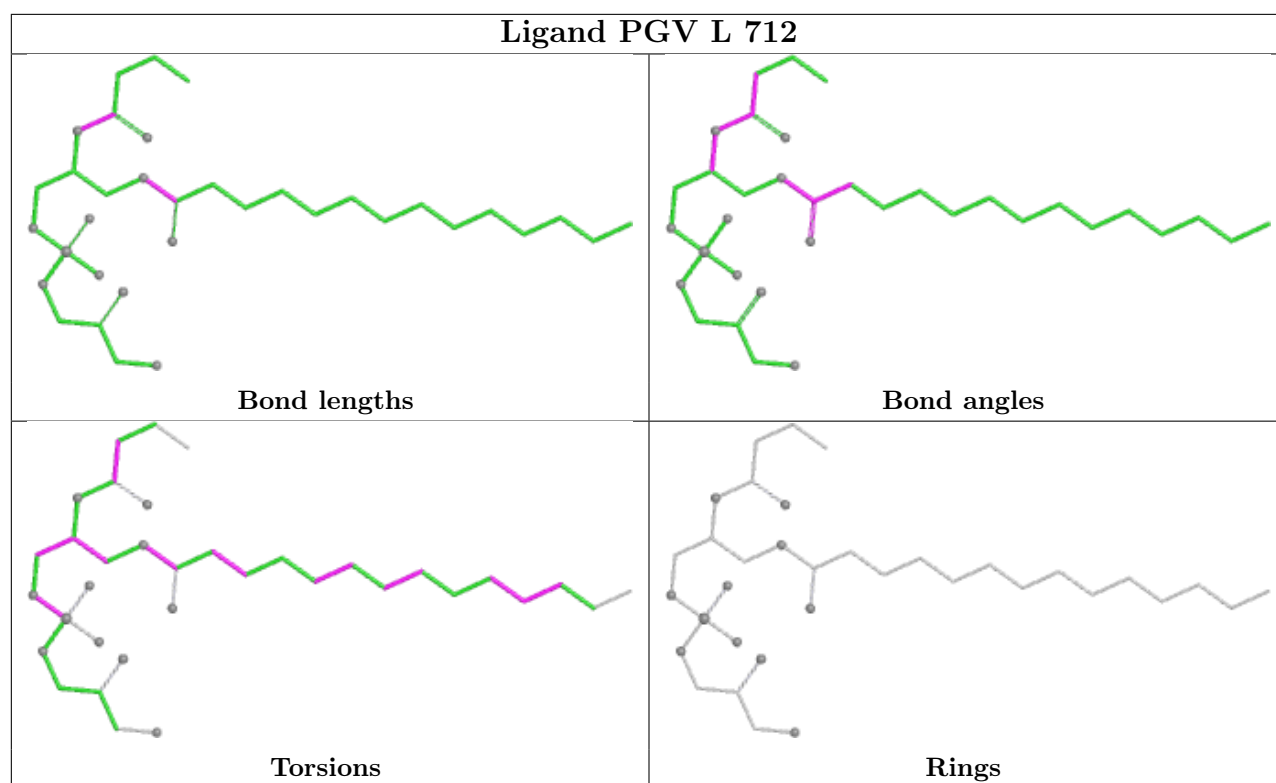
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



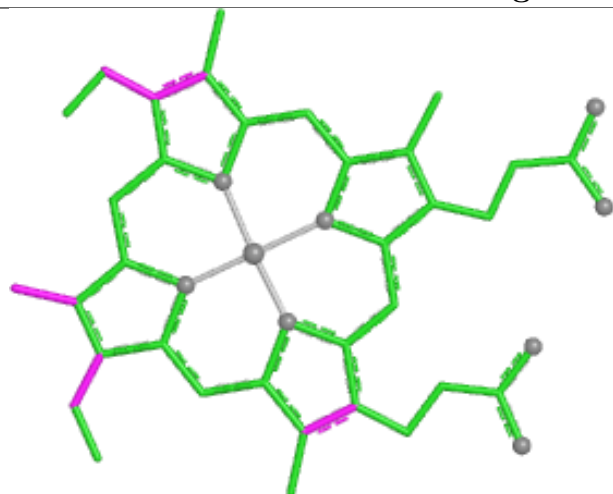




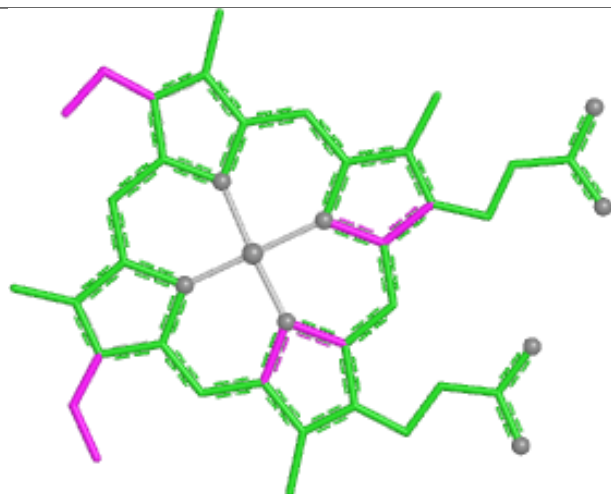




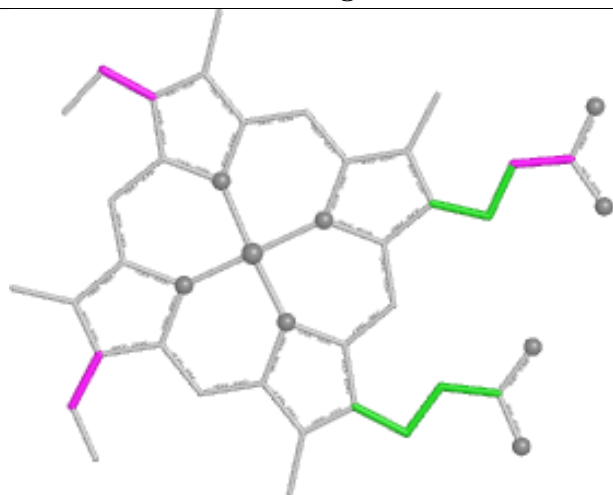
Ligand HEC C 501



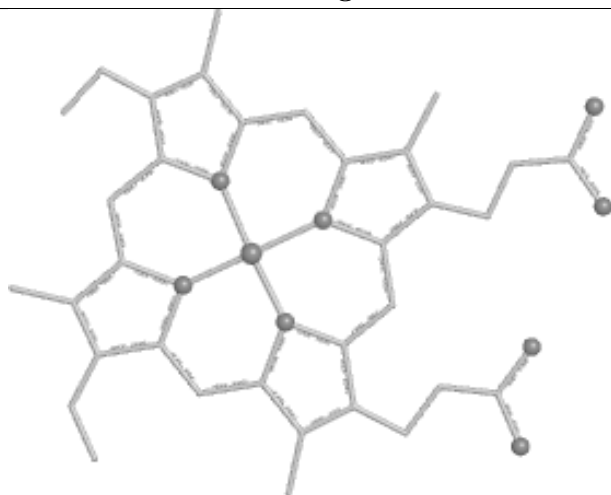
Bond lengths



Bond angles

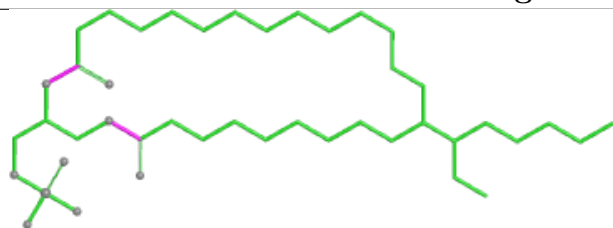


Torsions

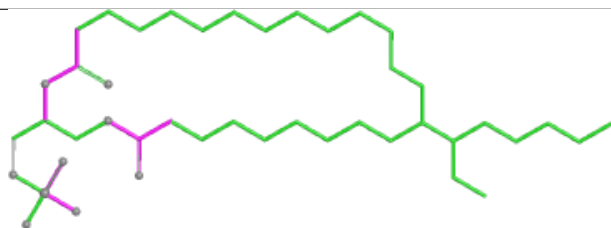


Rings

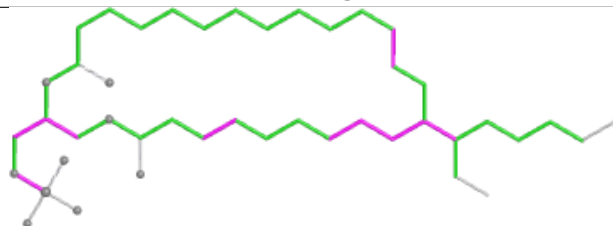
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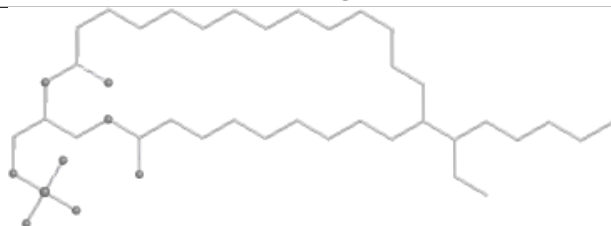
Bond lengths



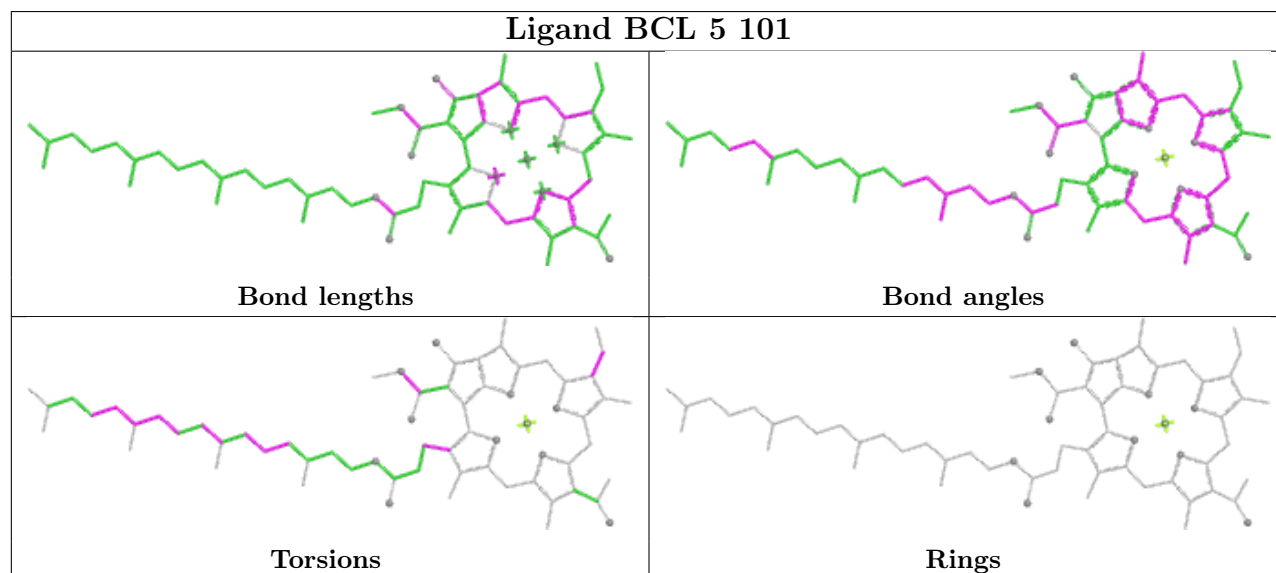
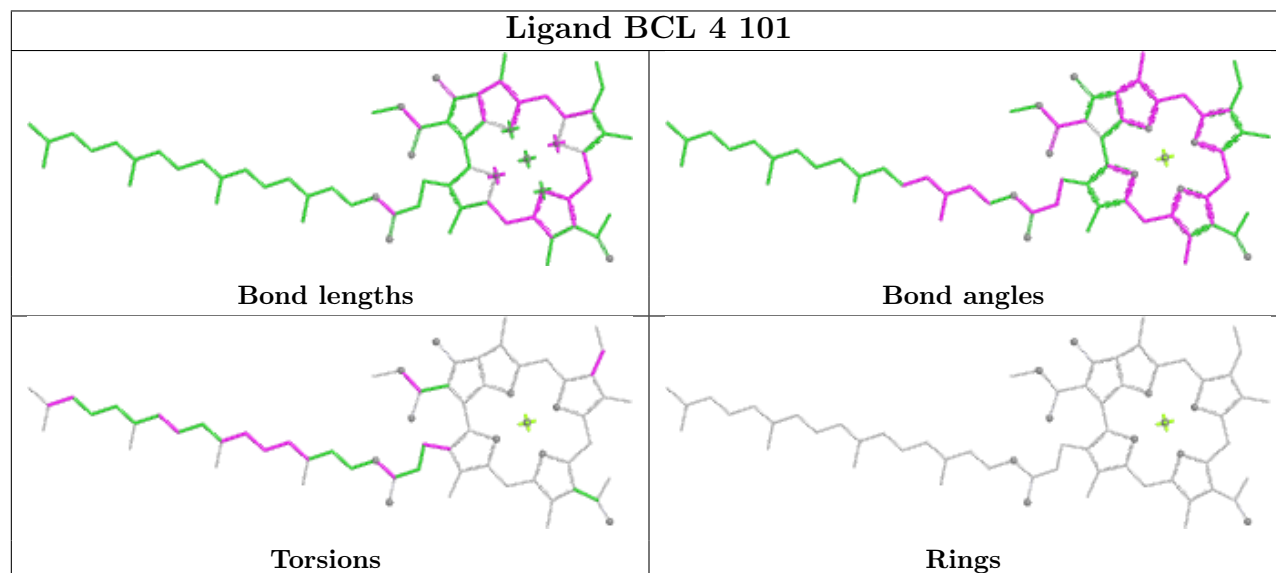
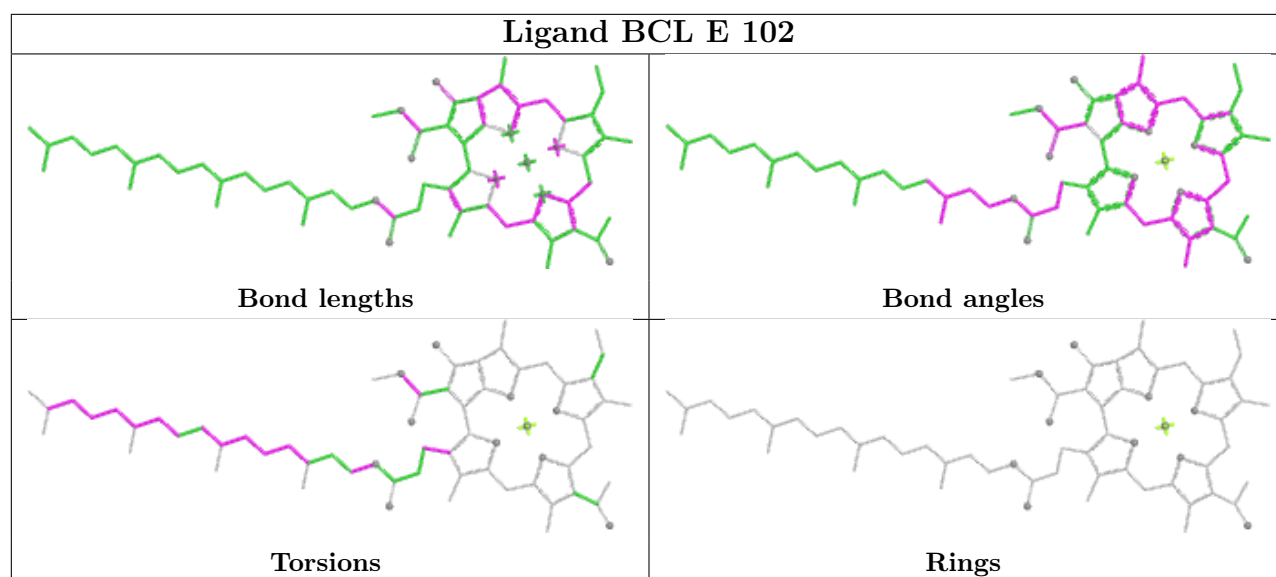
Bond angles

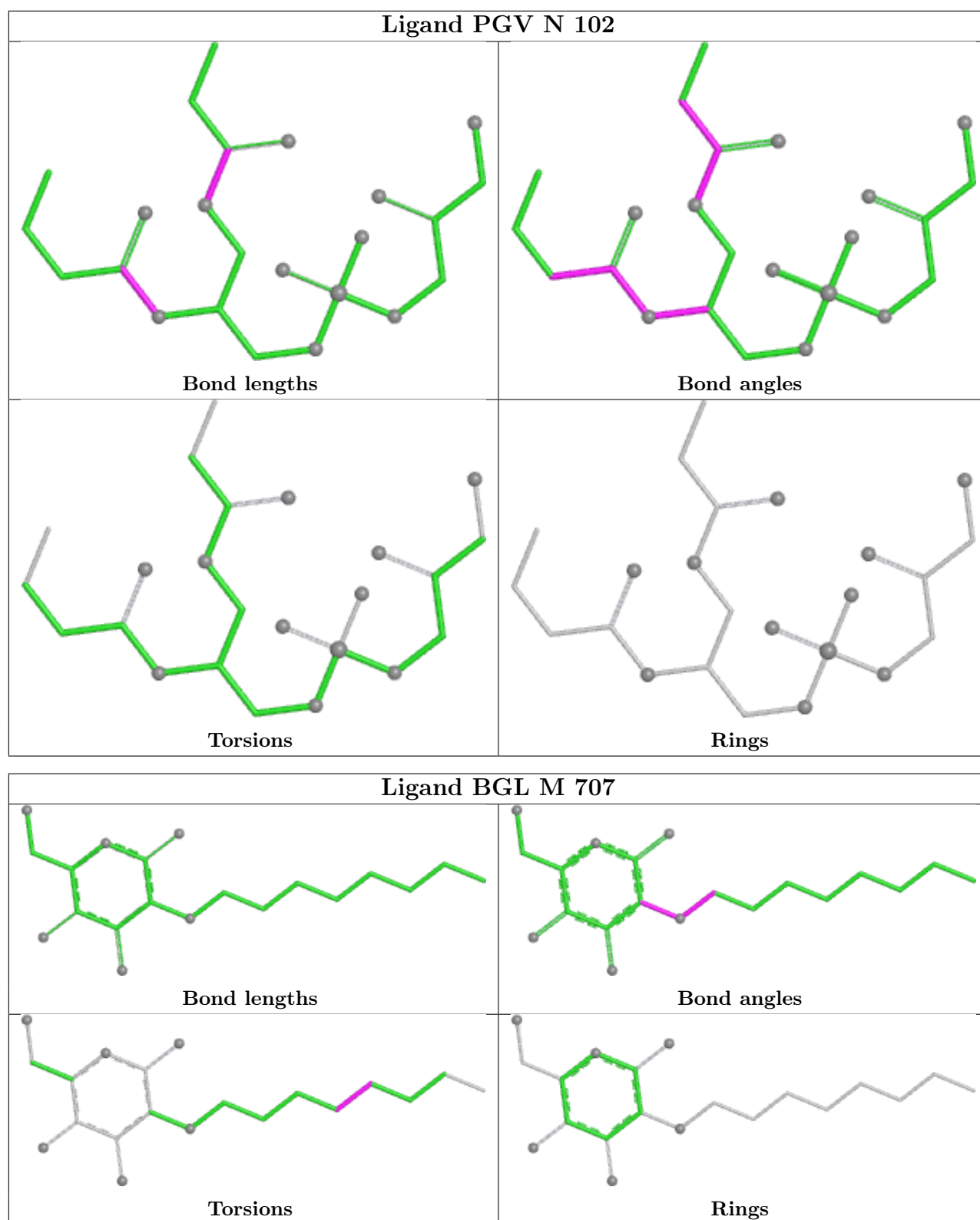


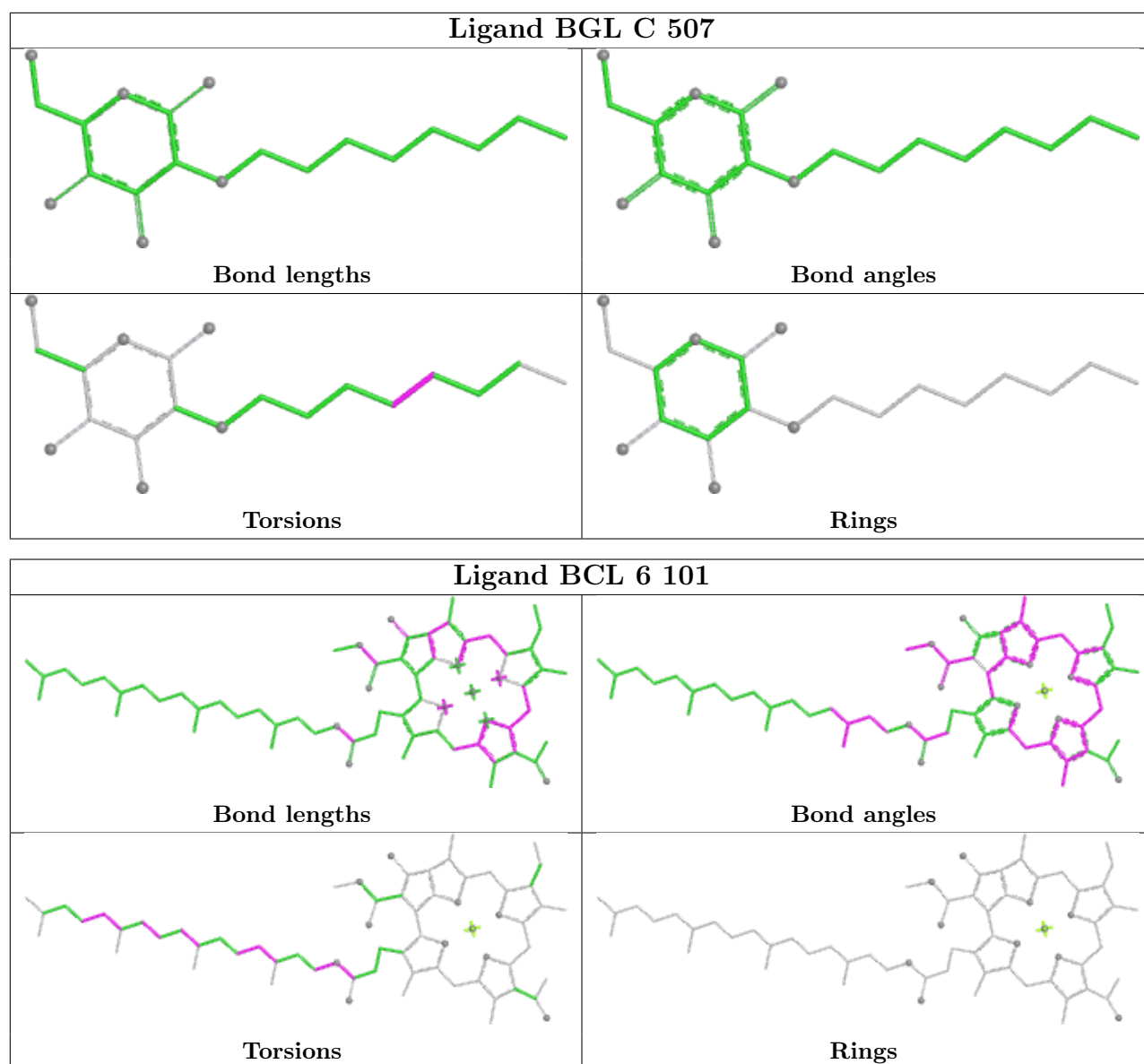
Torsions

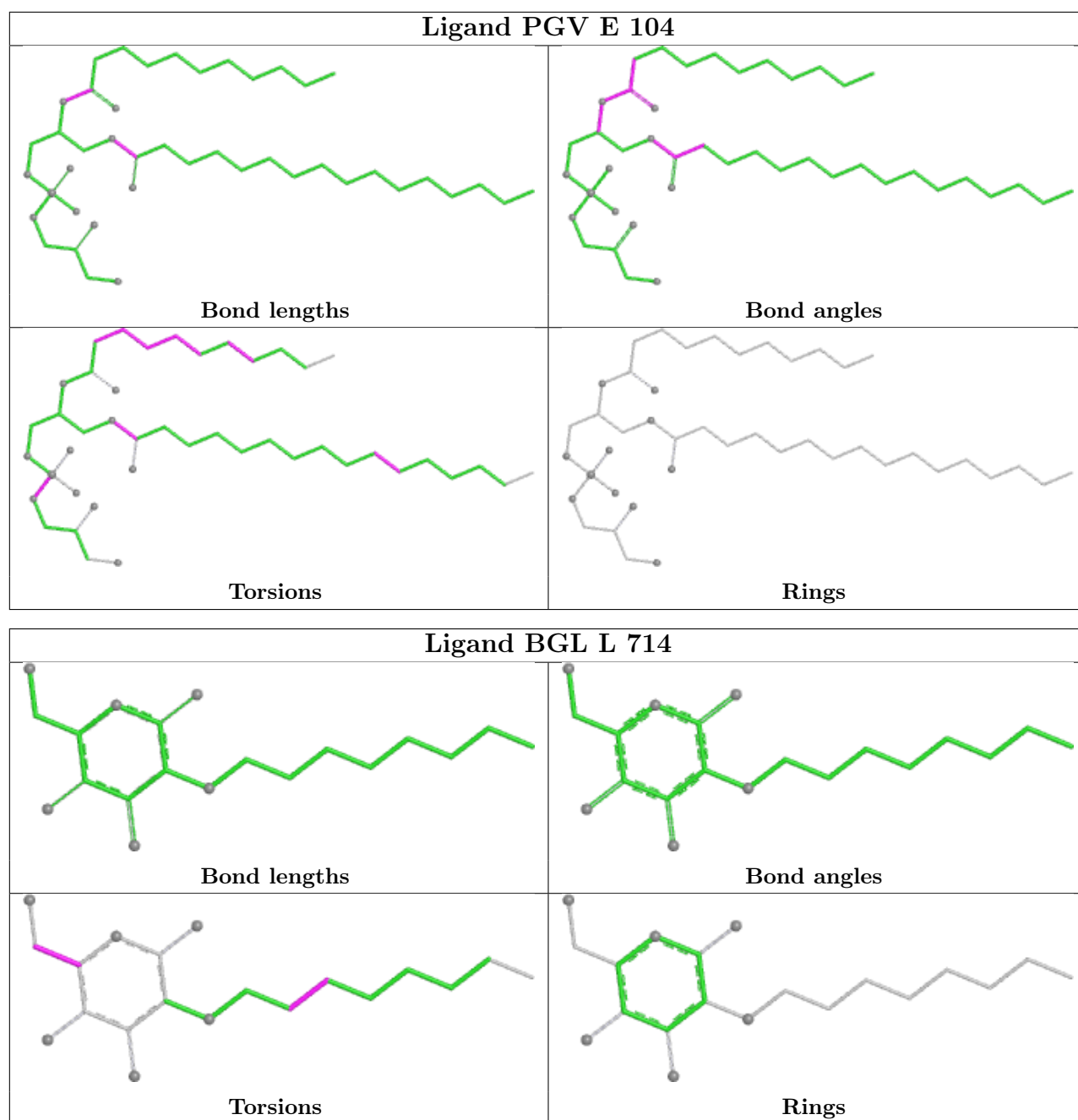


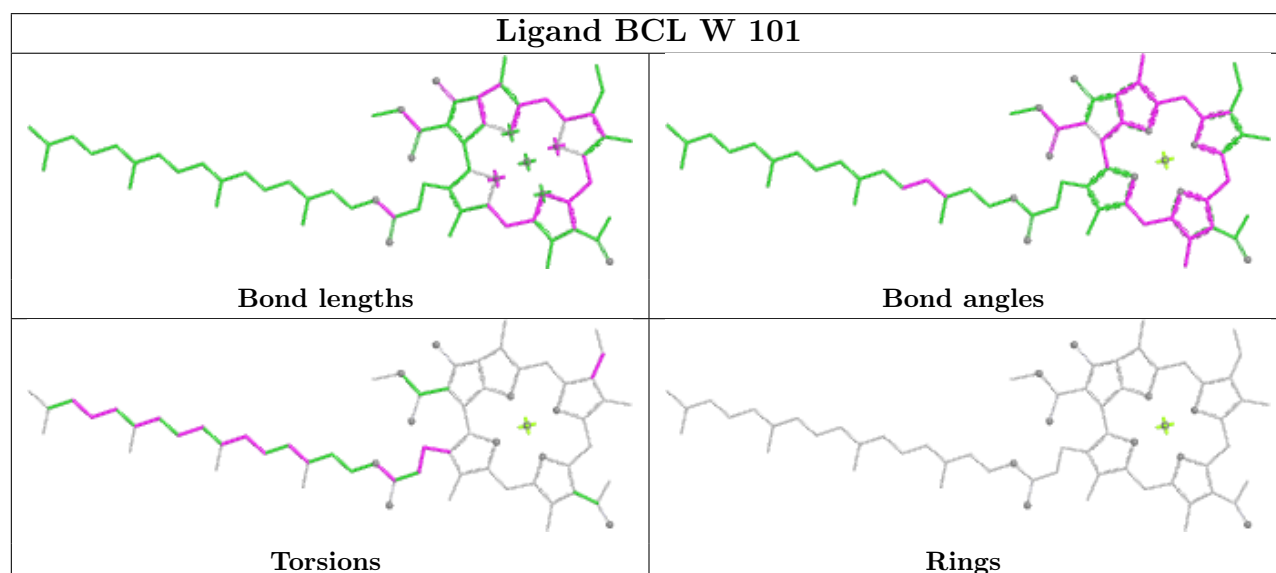
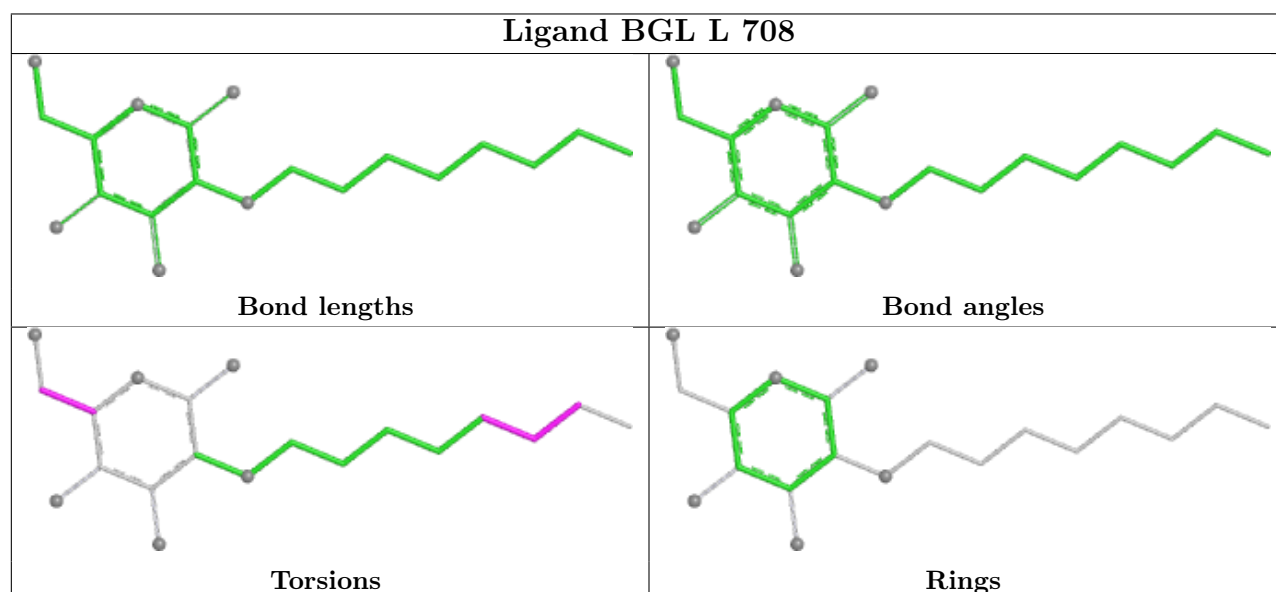
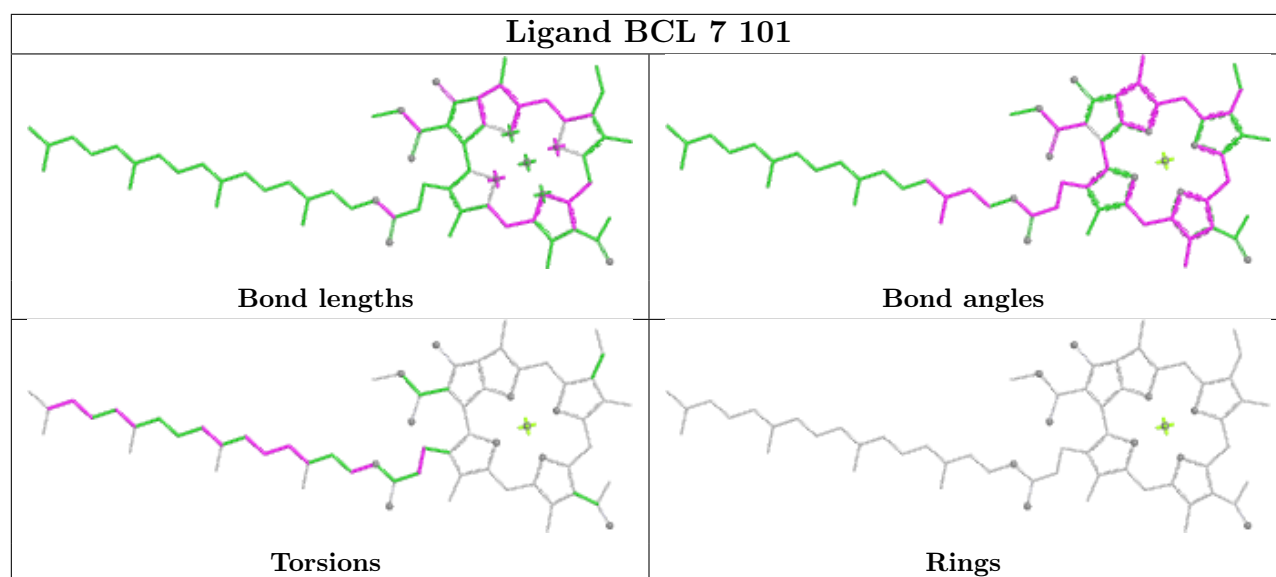
Rings

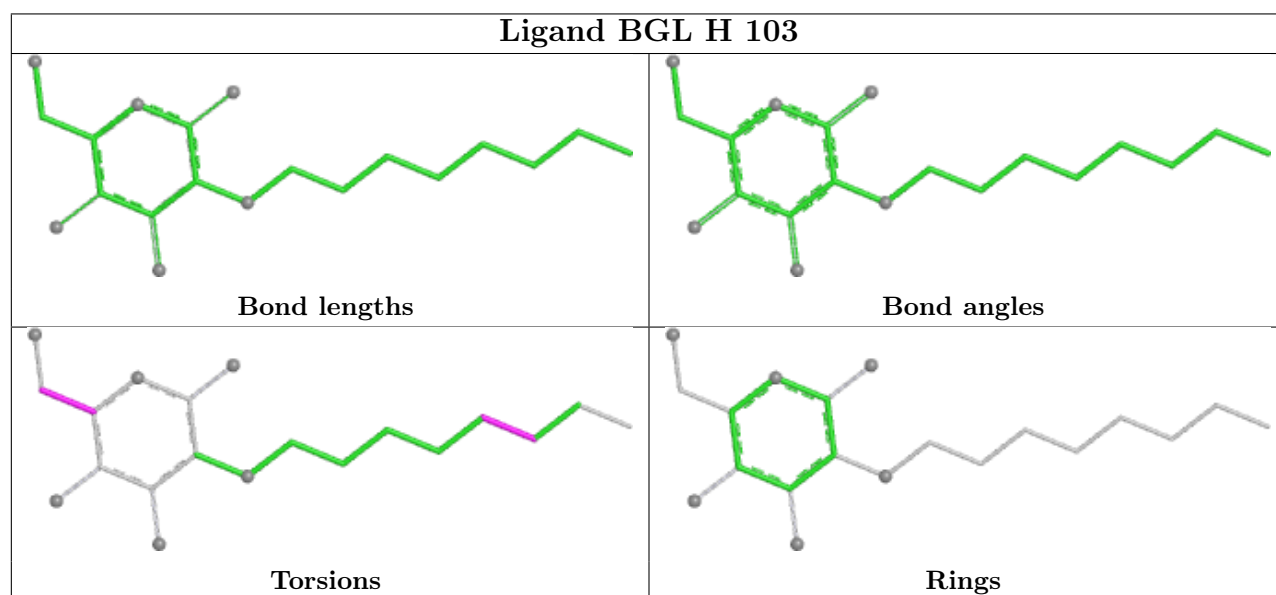
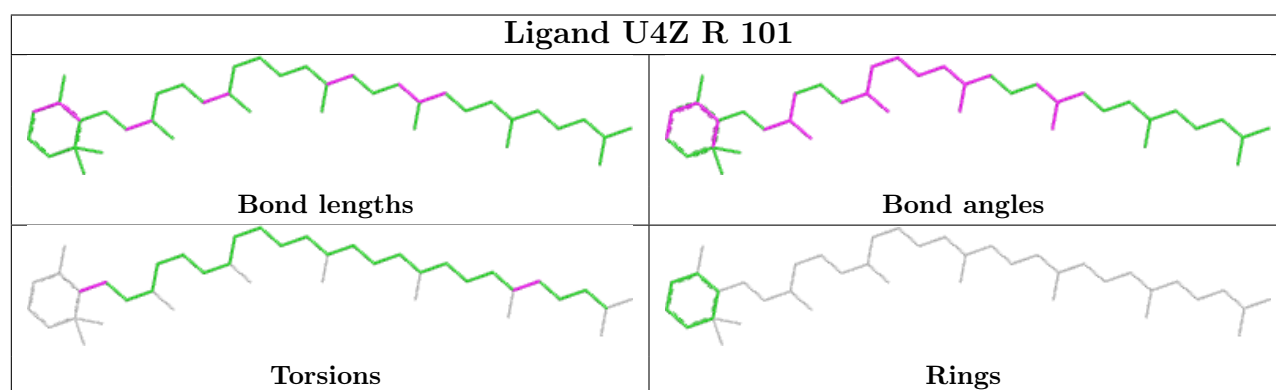
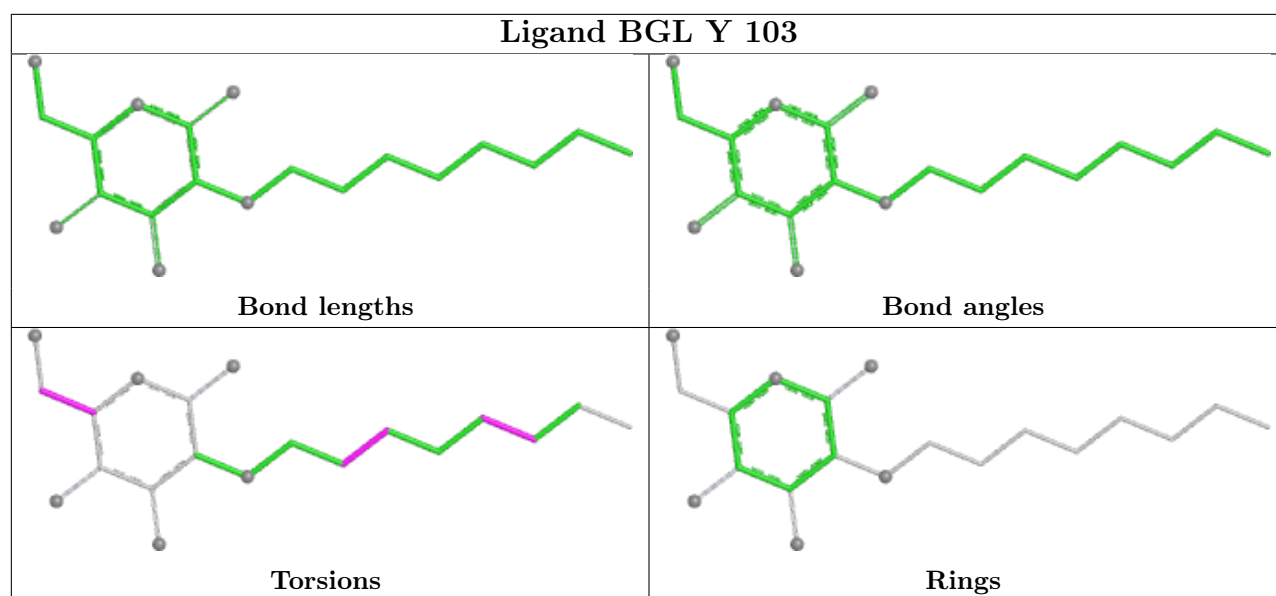


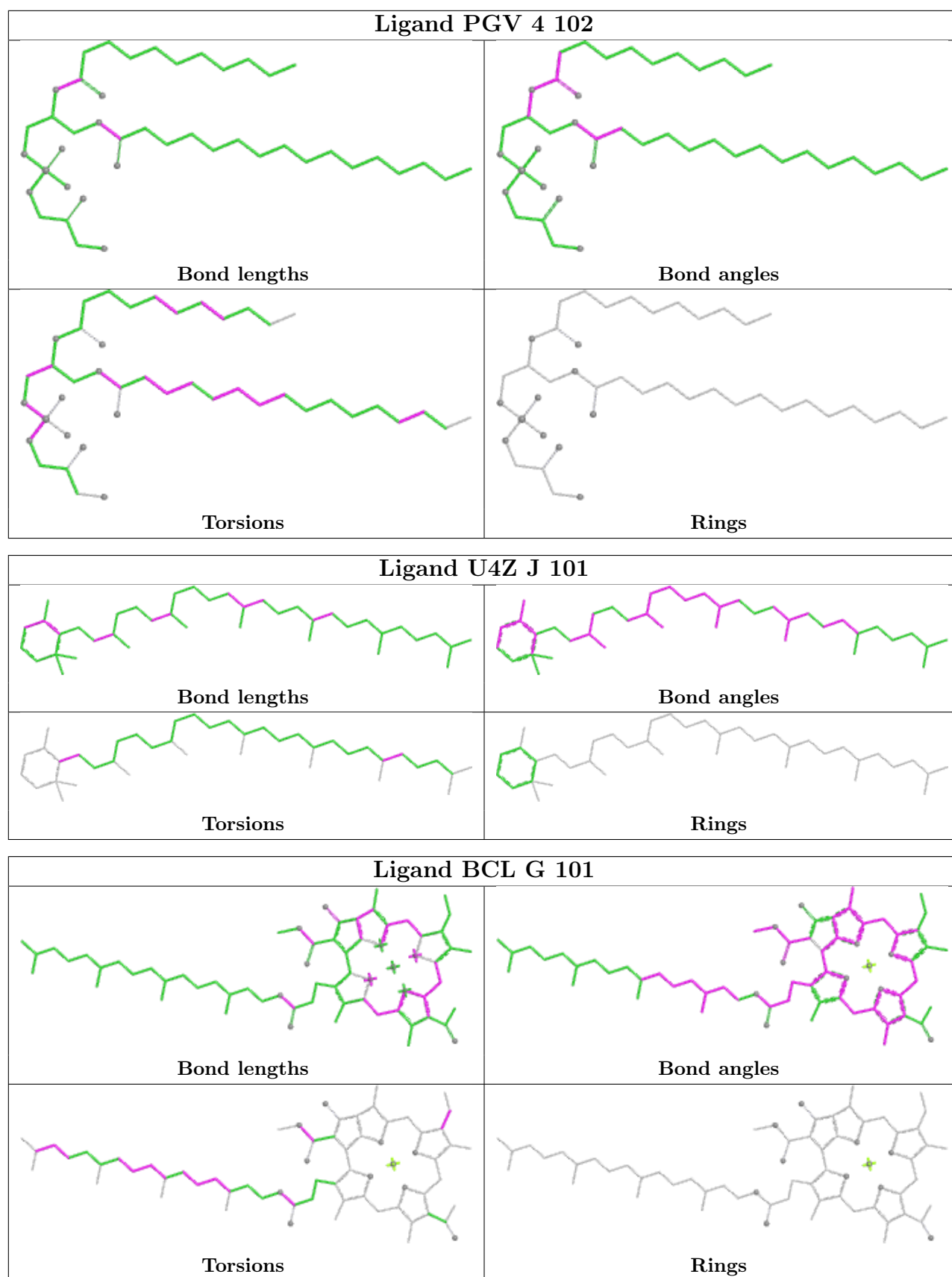


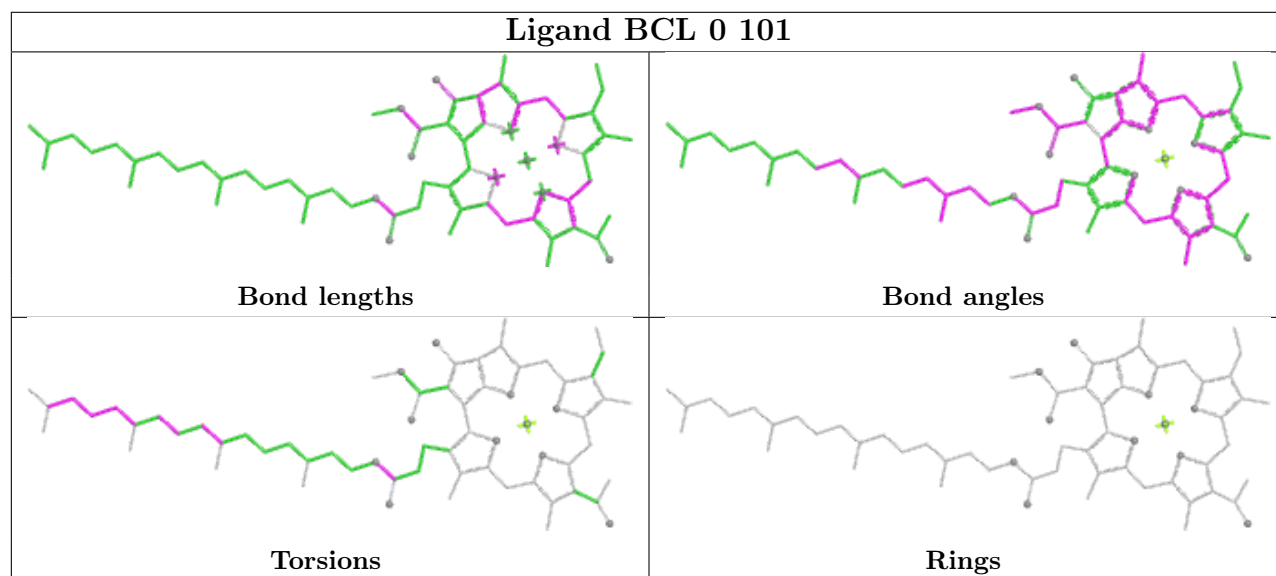
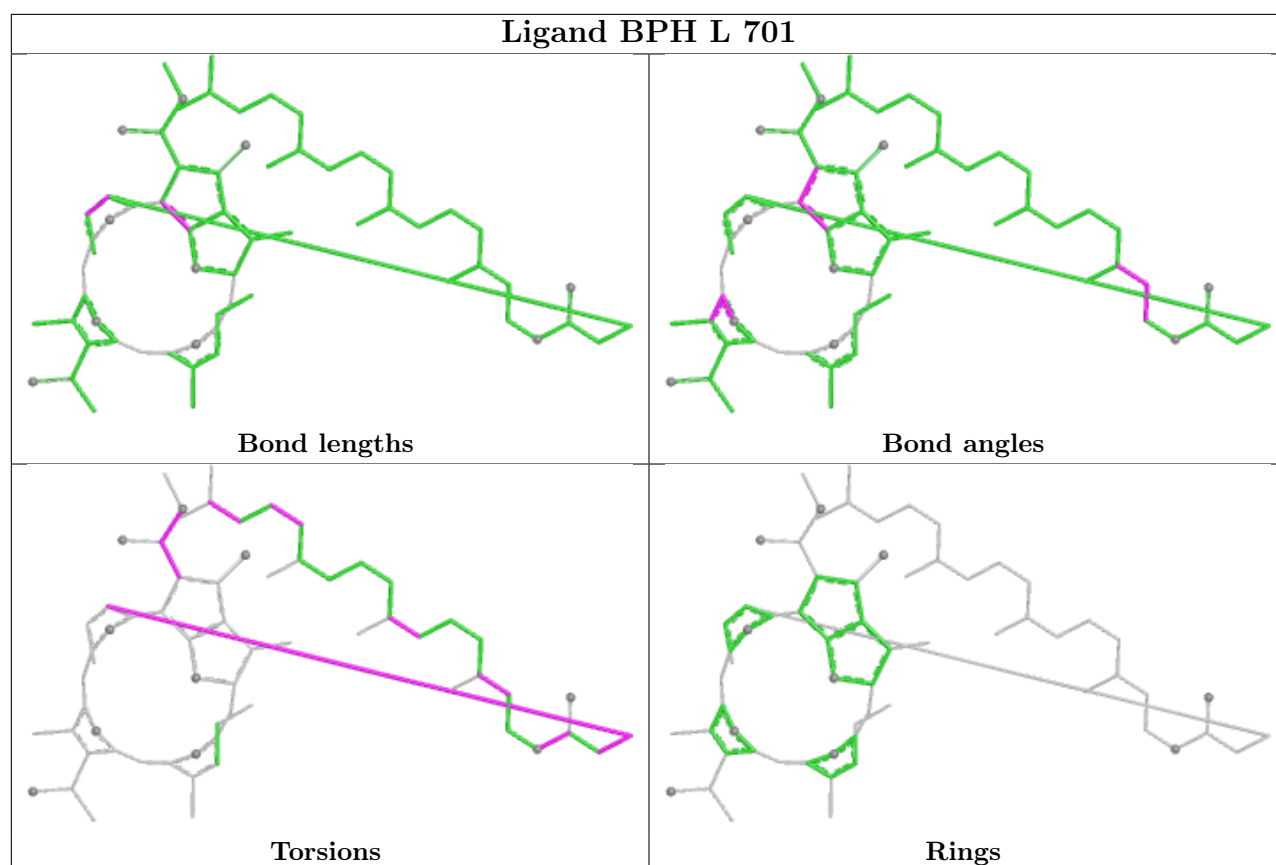


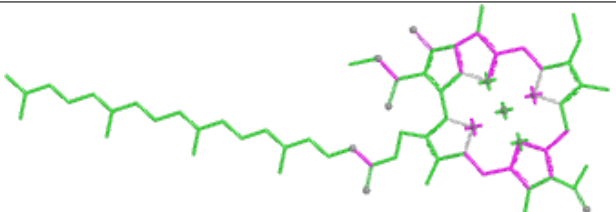
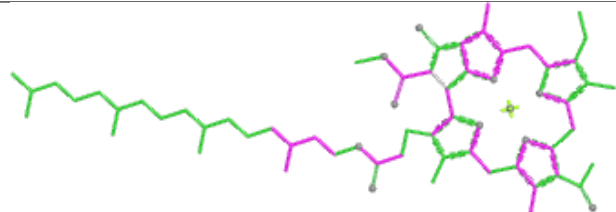
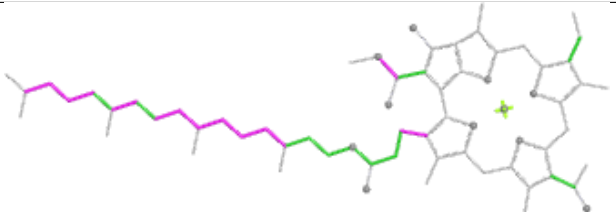
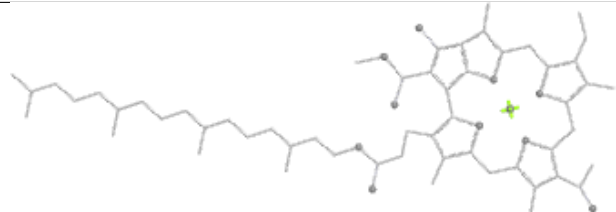


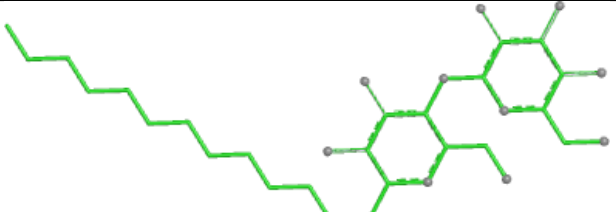
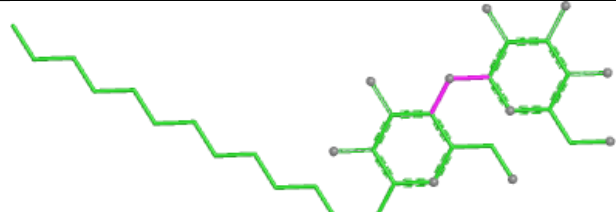
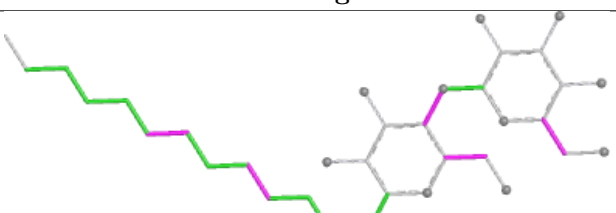
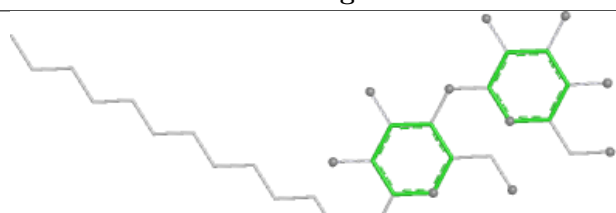


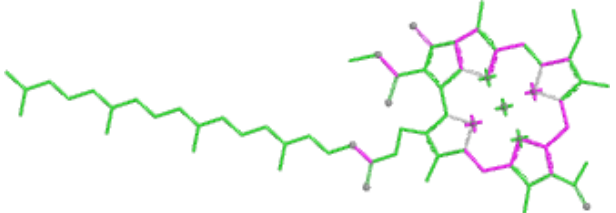
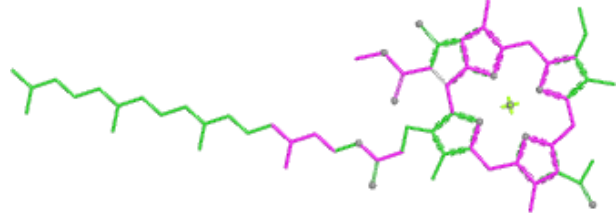
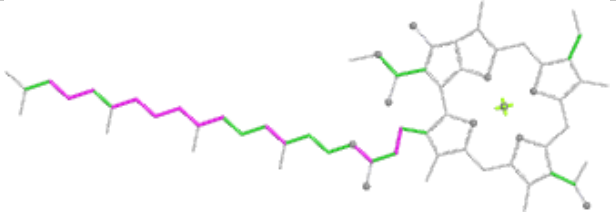
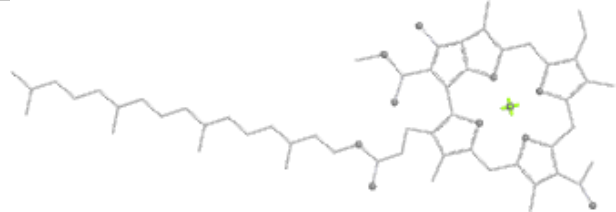


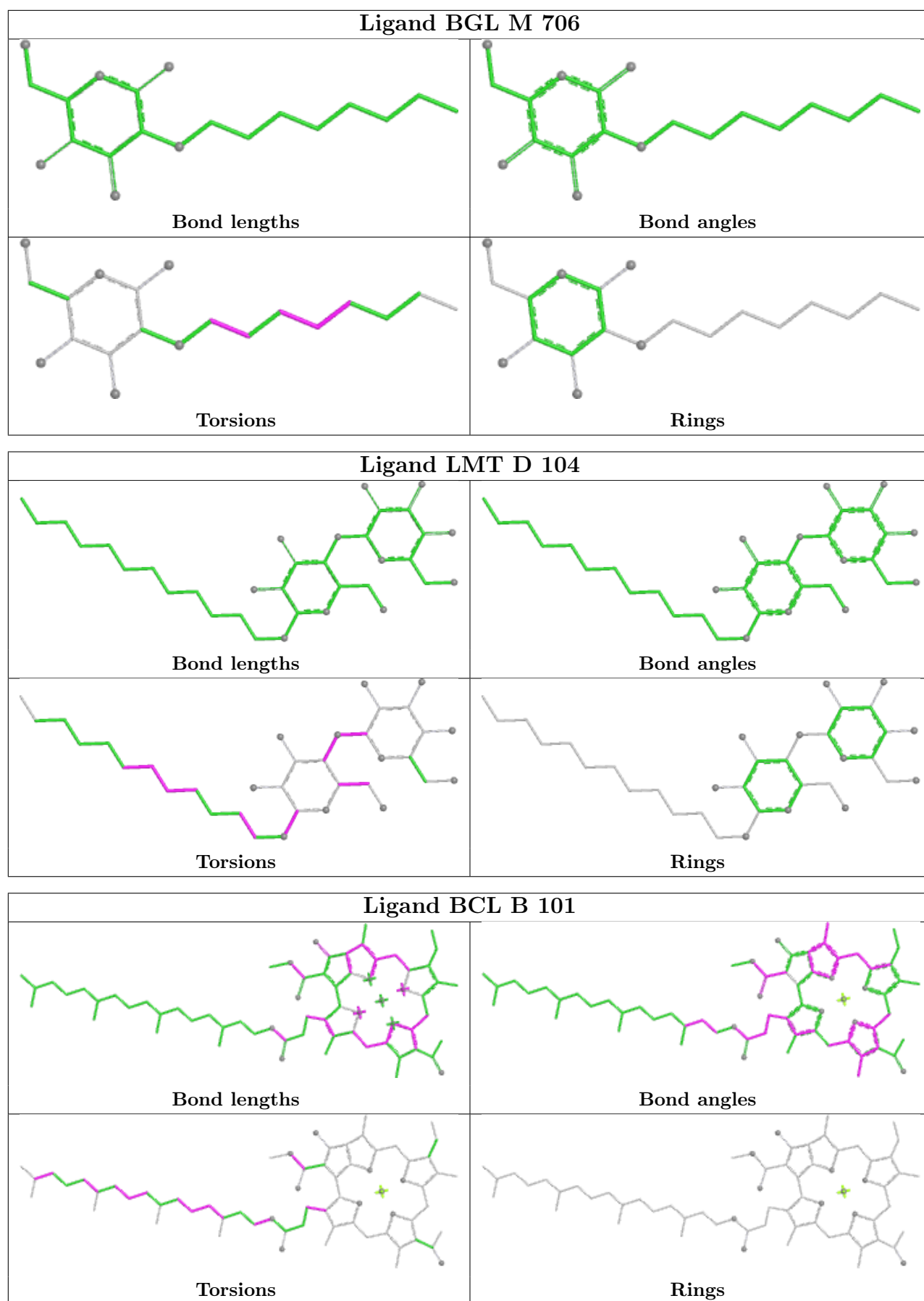


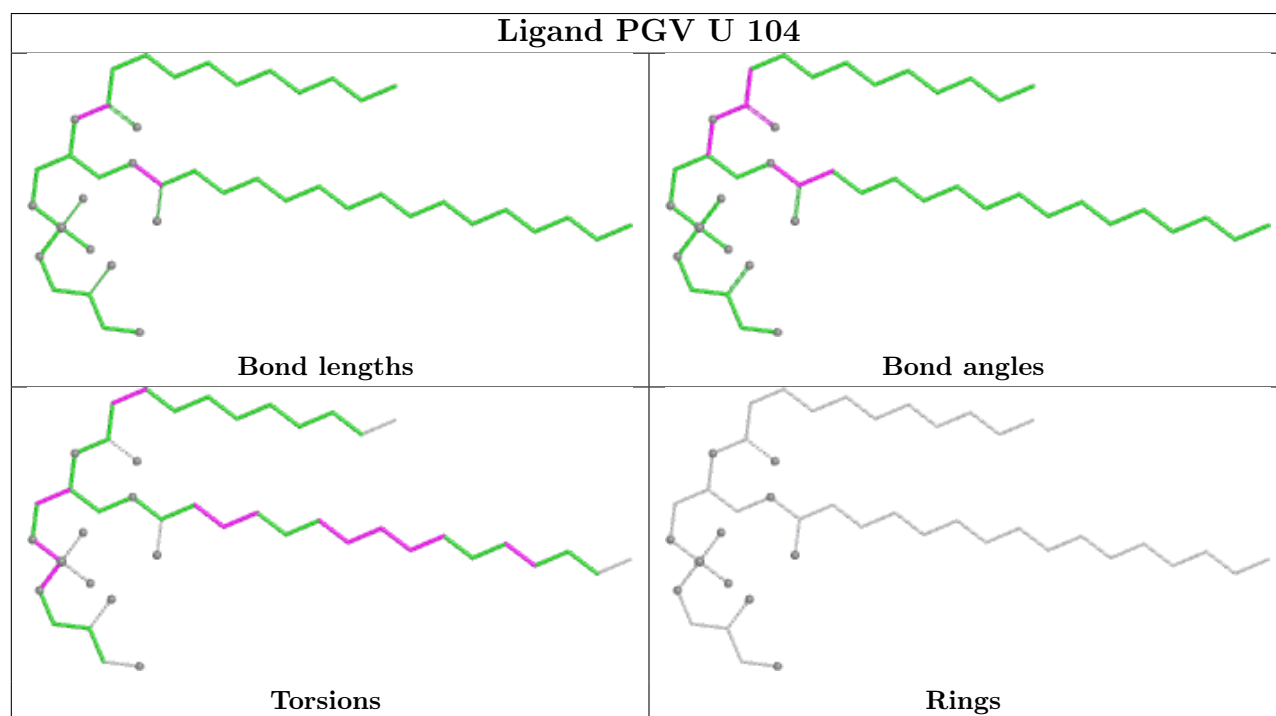
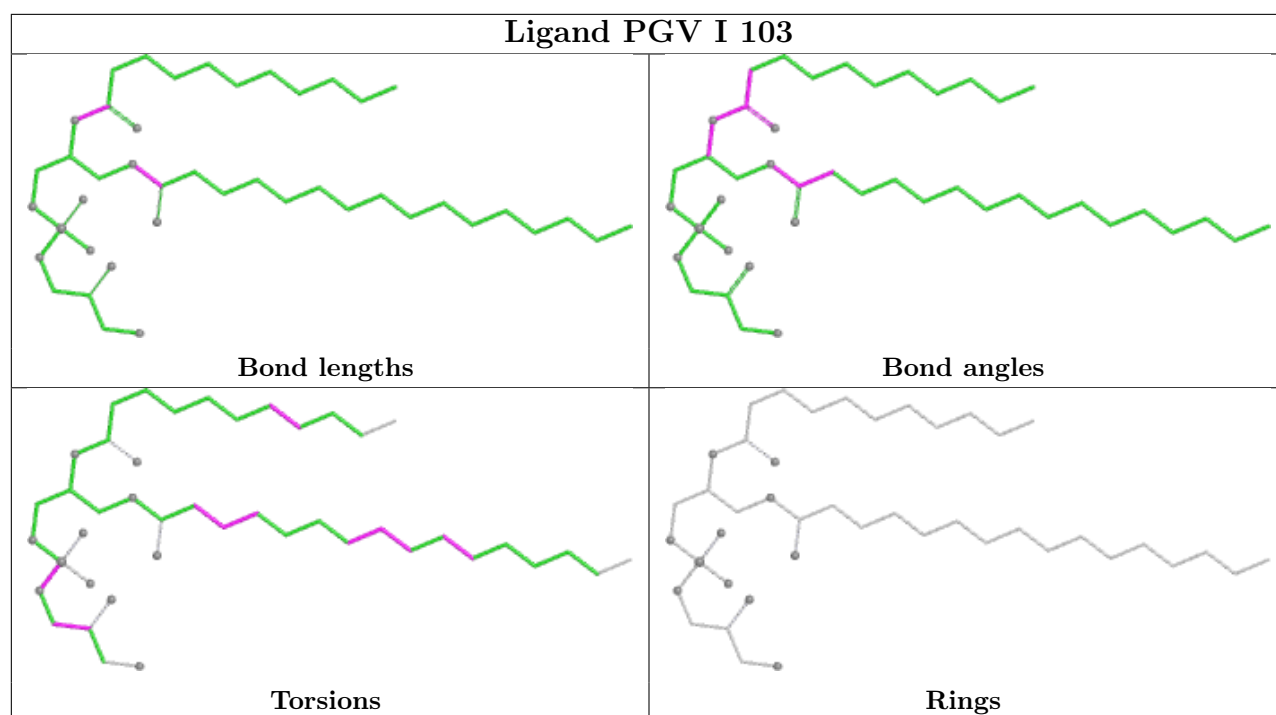


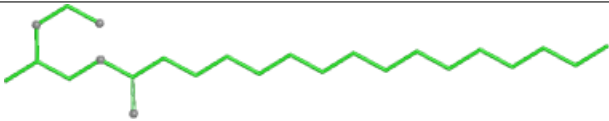
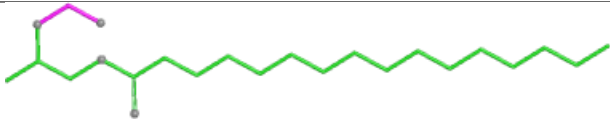
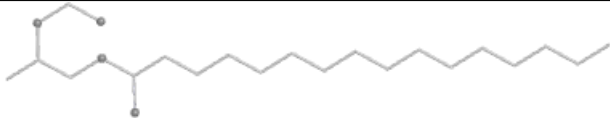
Ligand BCL V 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

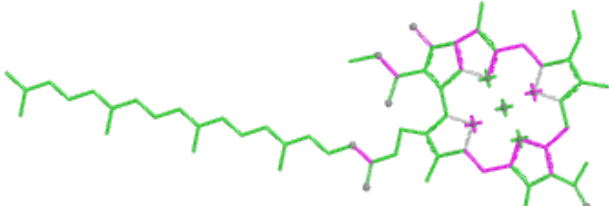
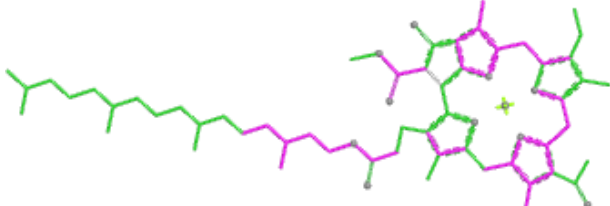
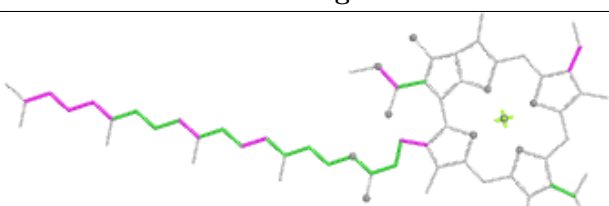
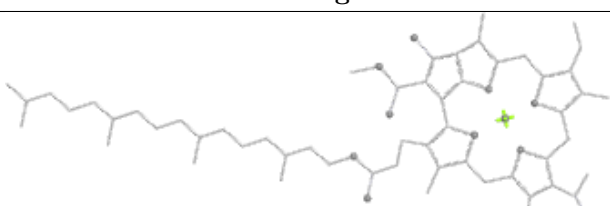
Ligand LMT H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

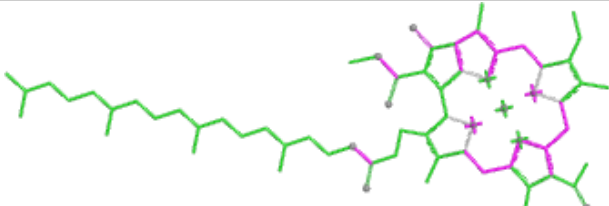
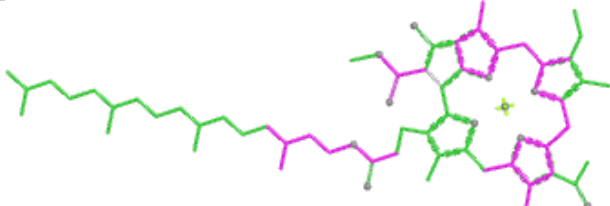
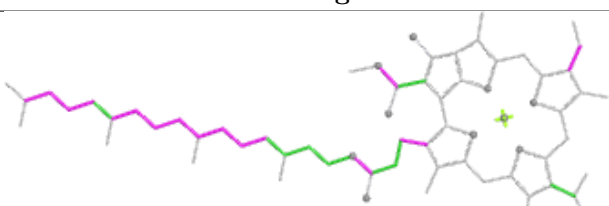
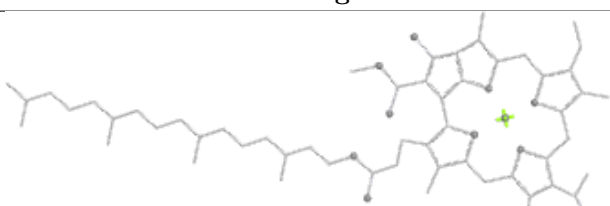
Ligand BCL 8 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

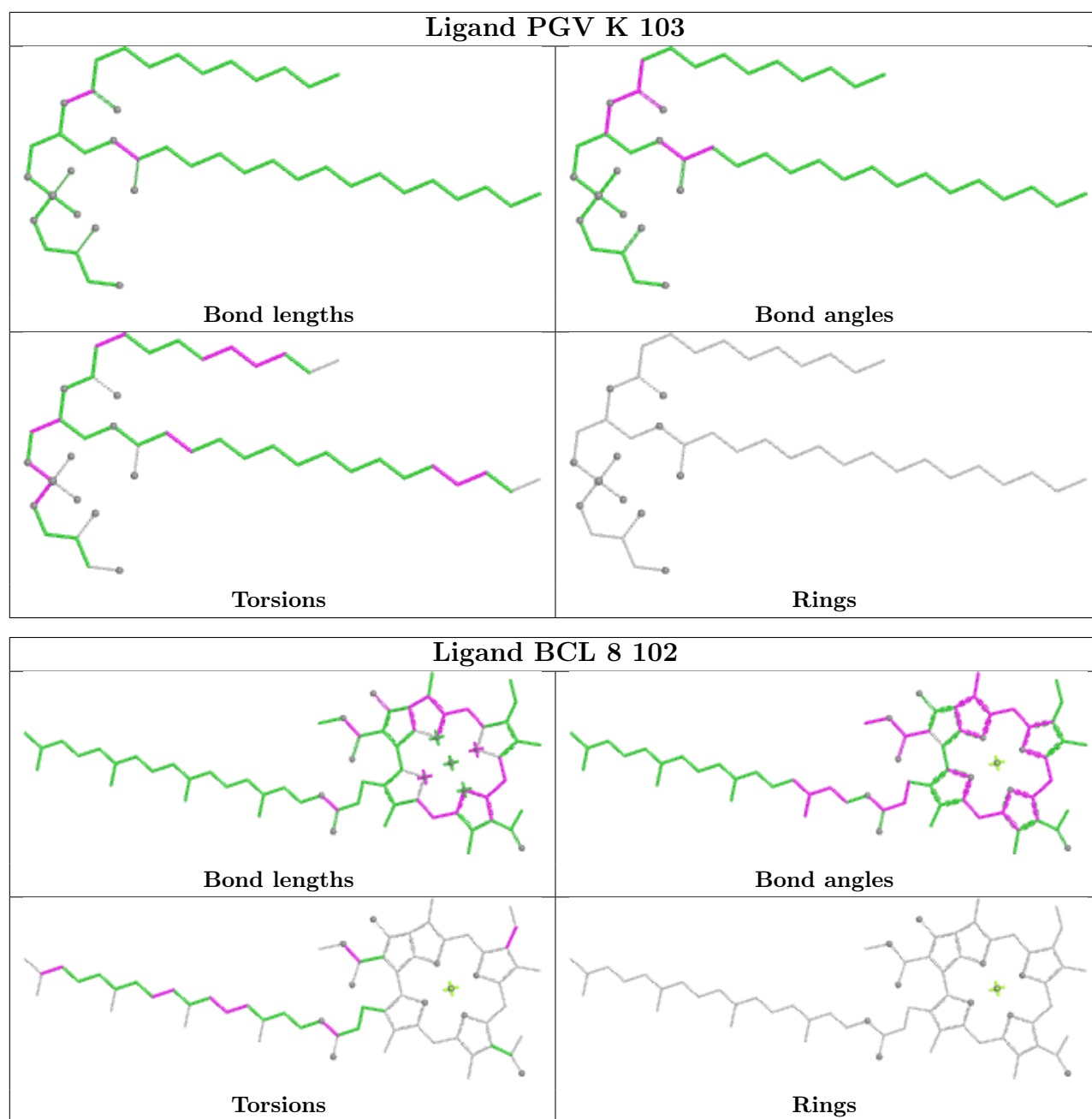


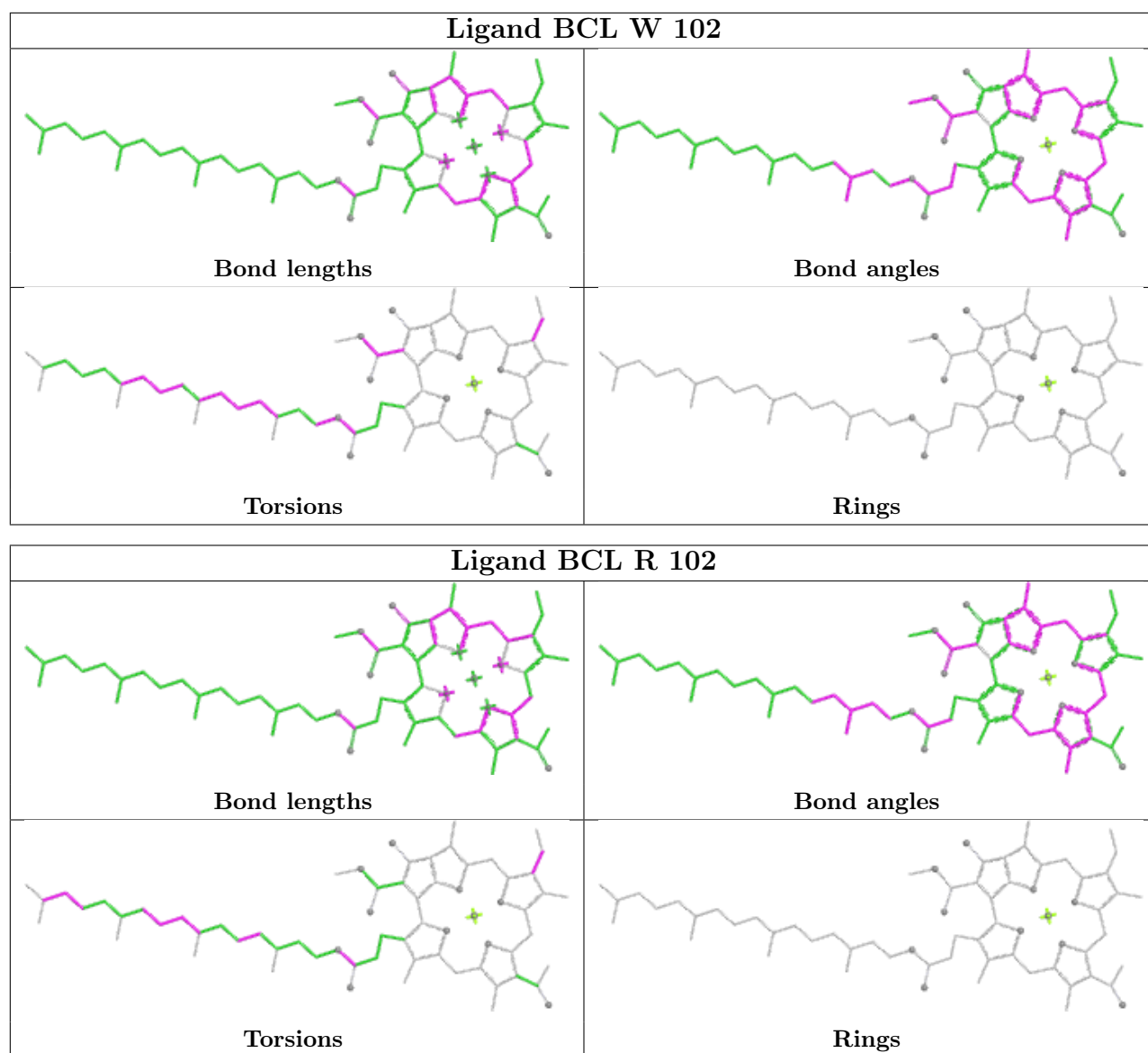


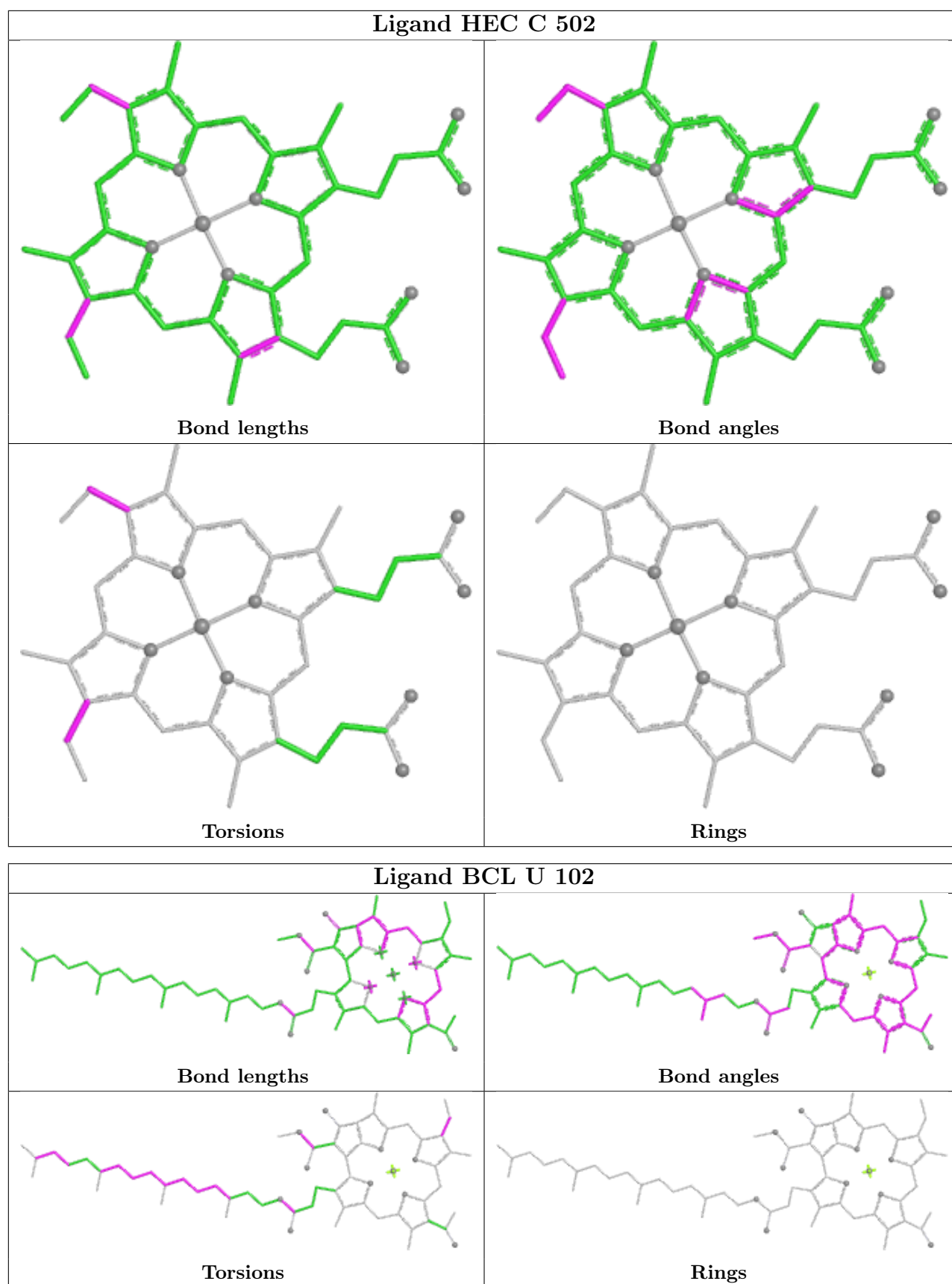
Ligand LHG h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

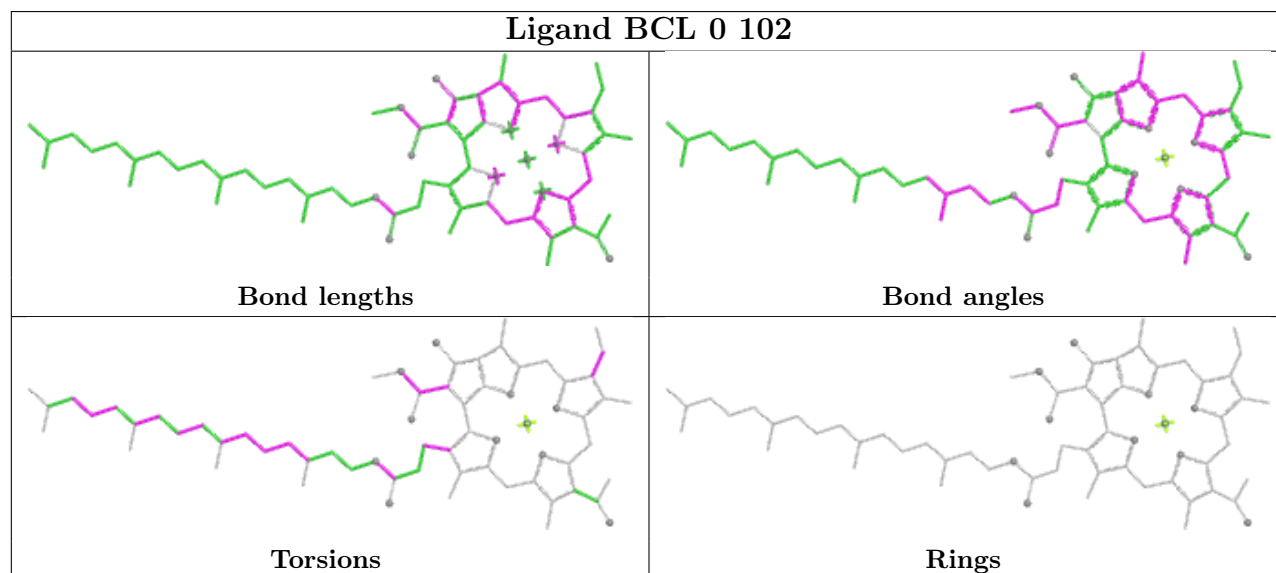
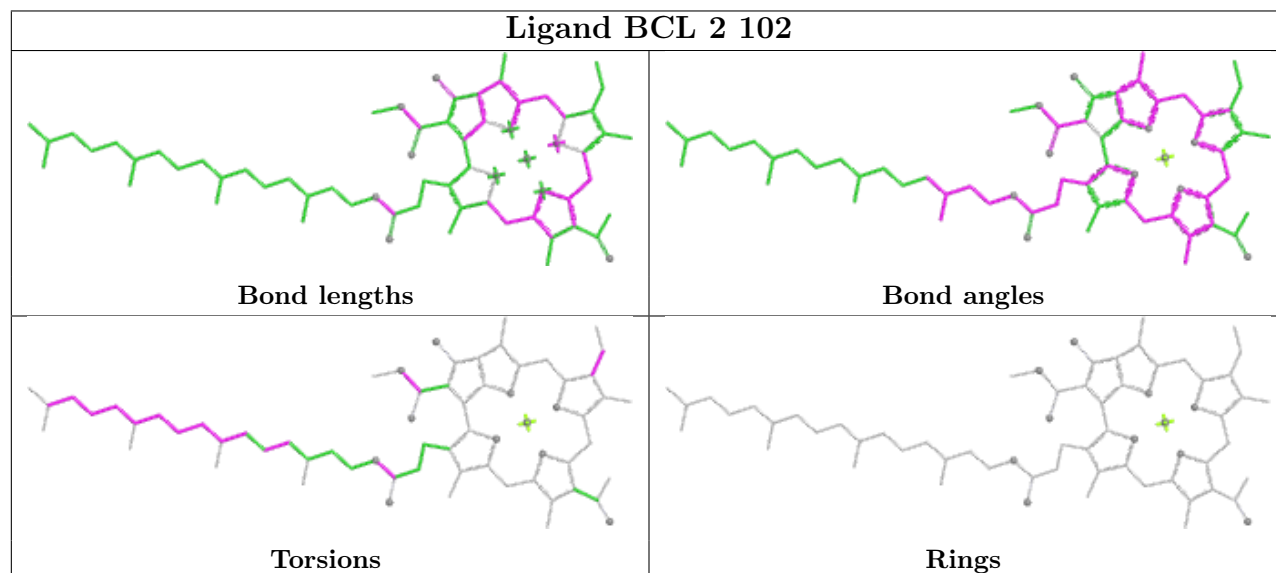
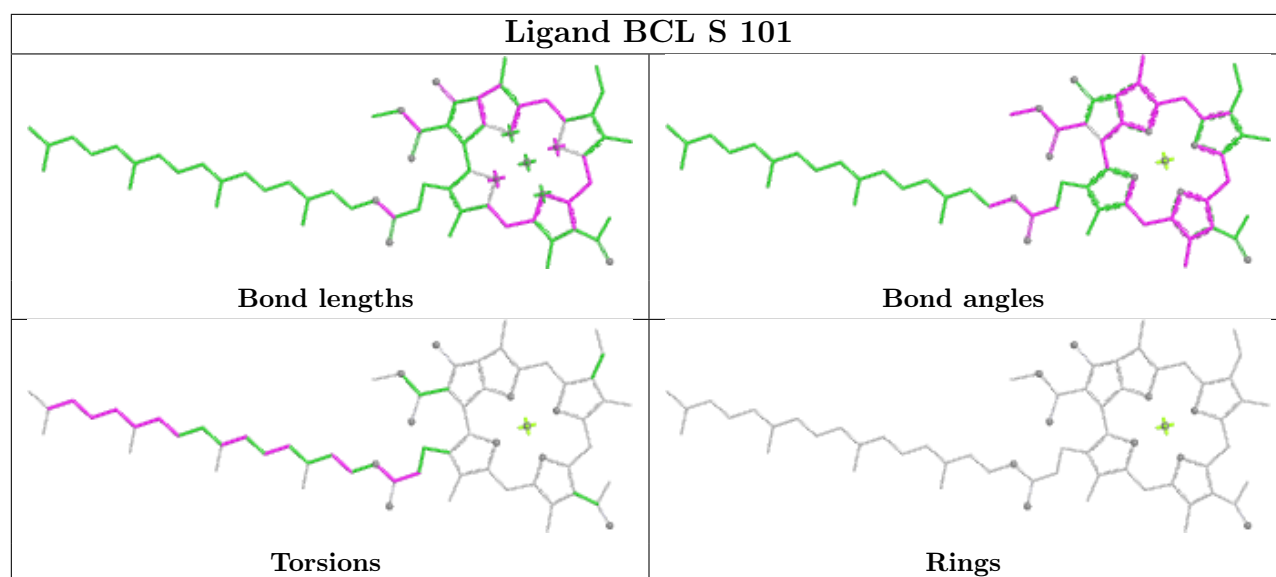
Ligand BCL L 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

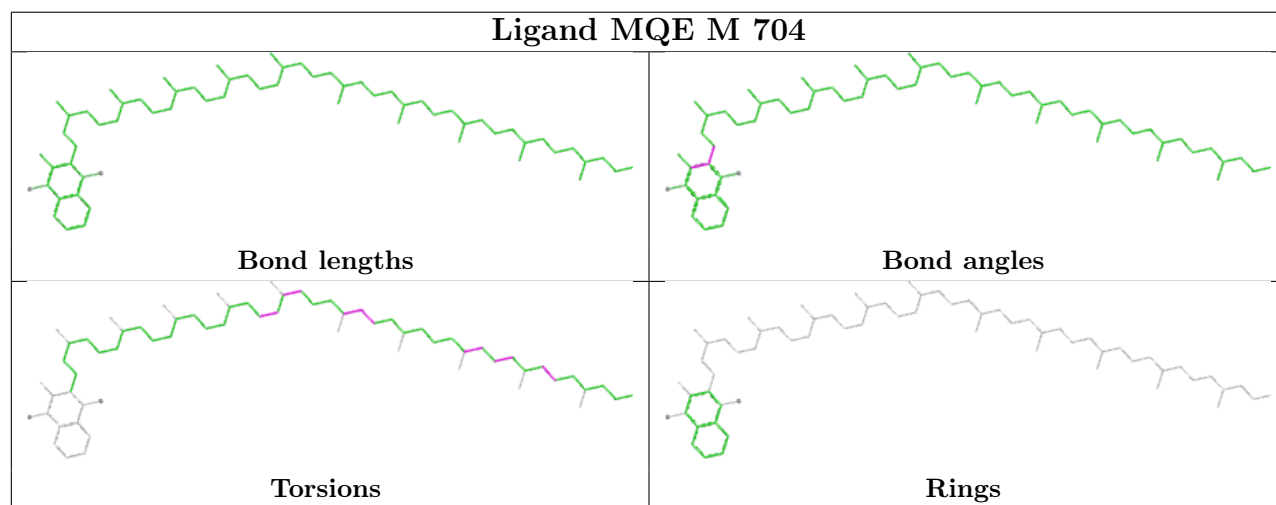
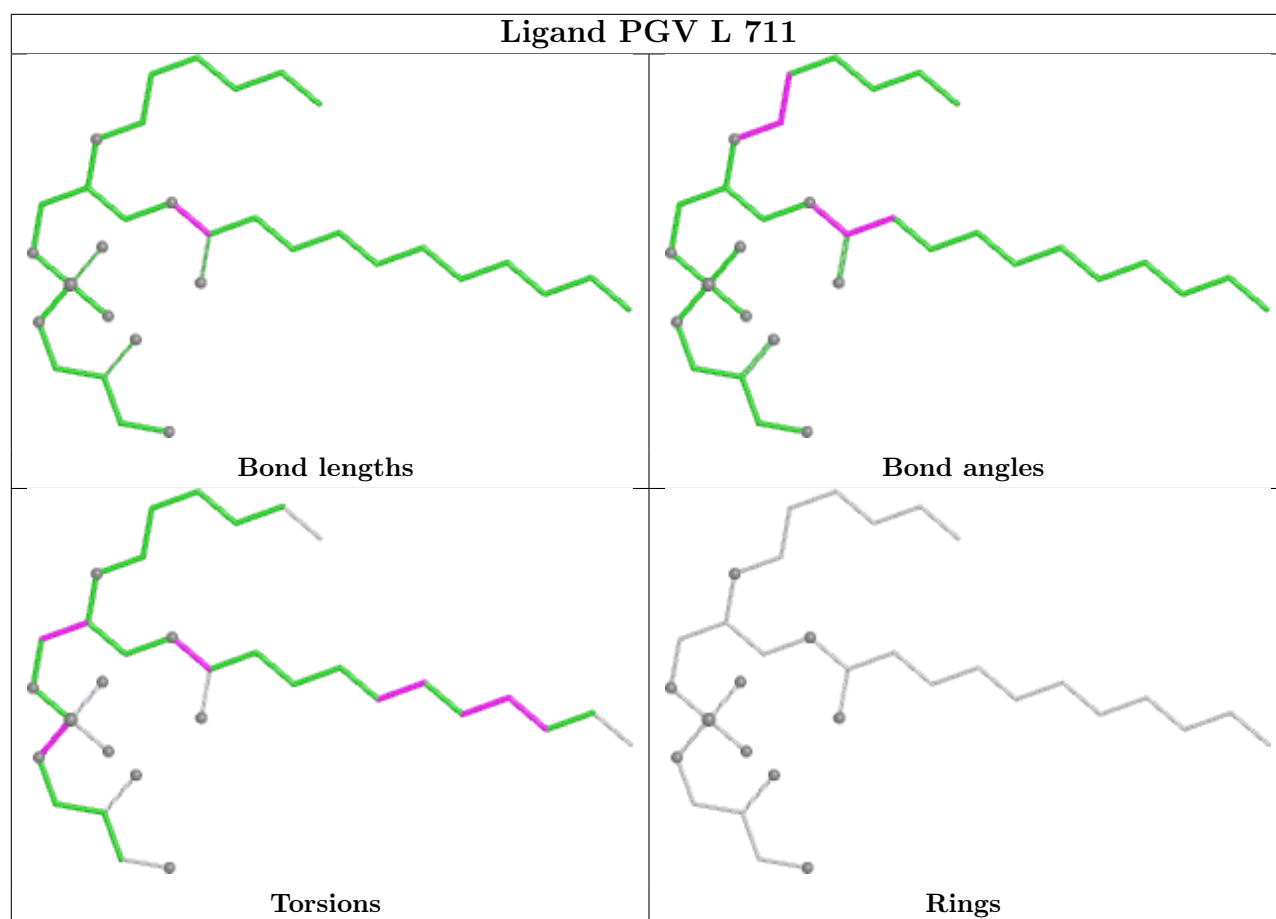
Ligand BCL Q 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

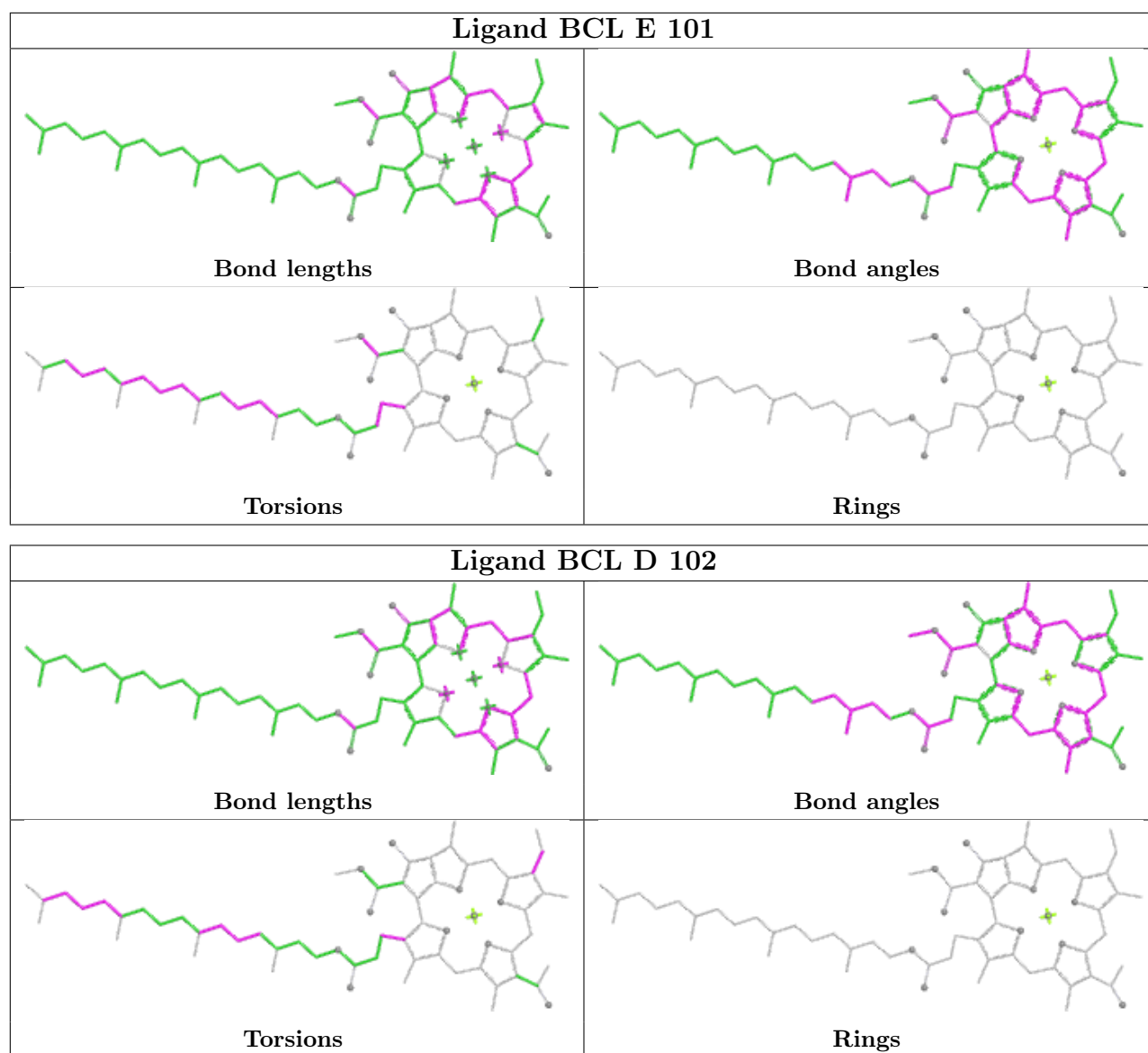


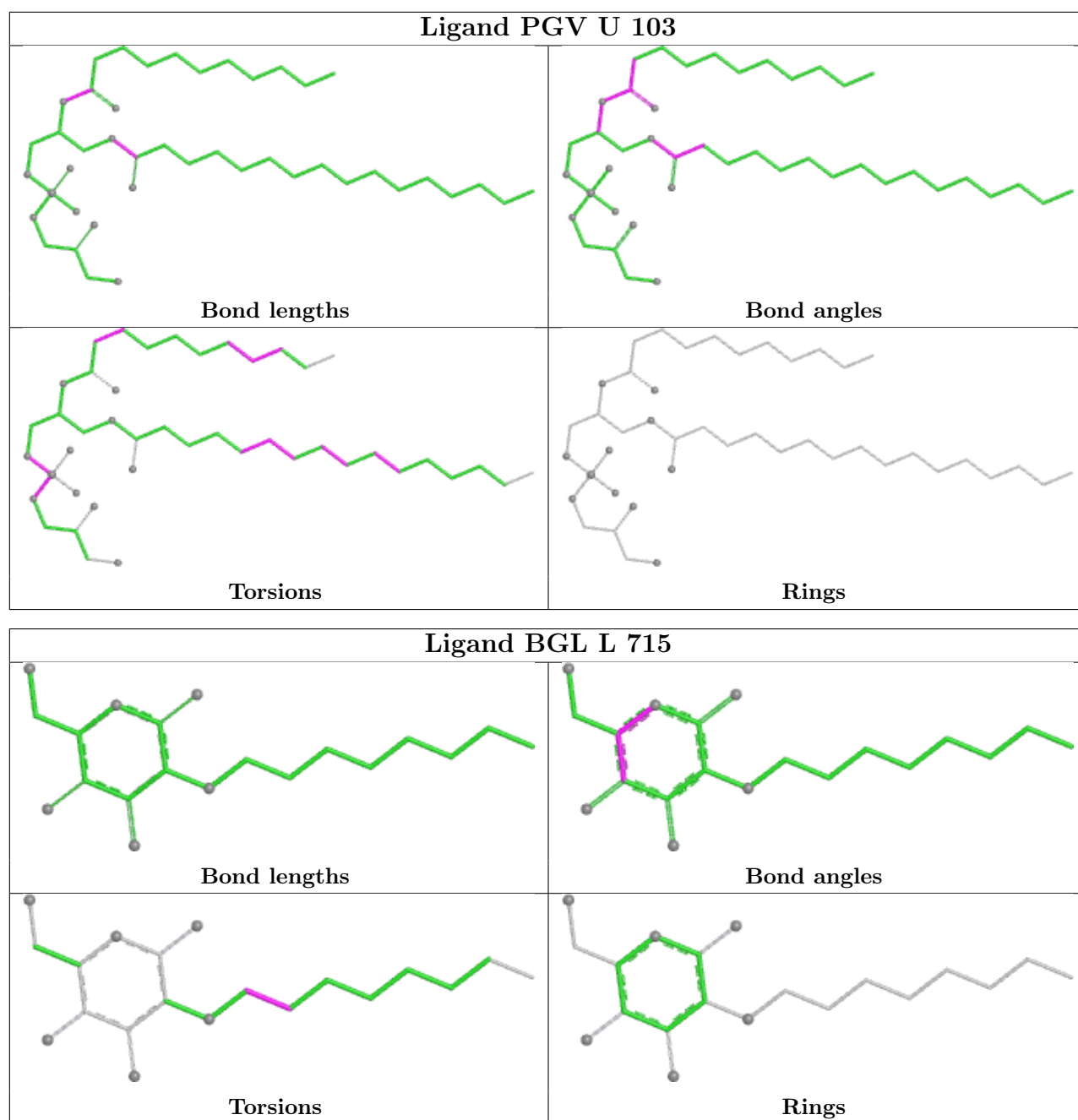


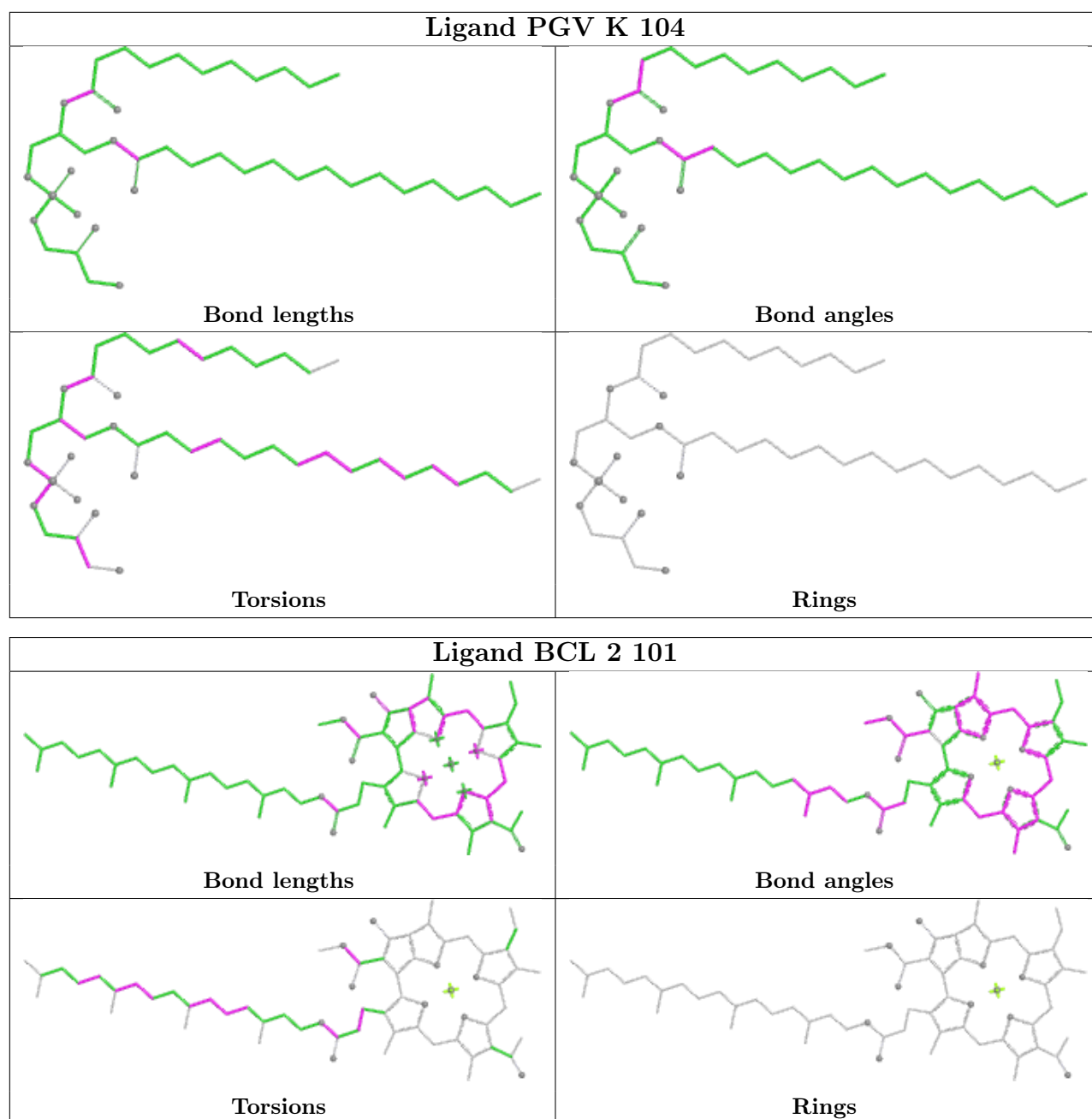


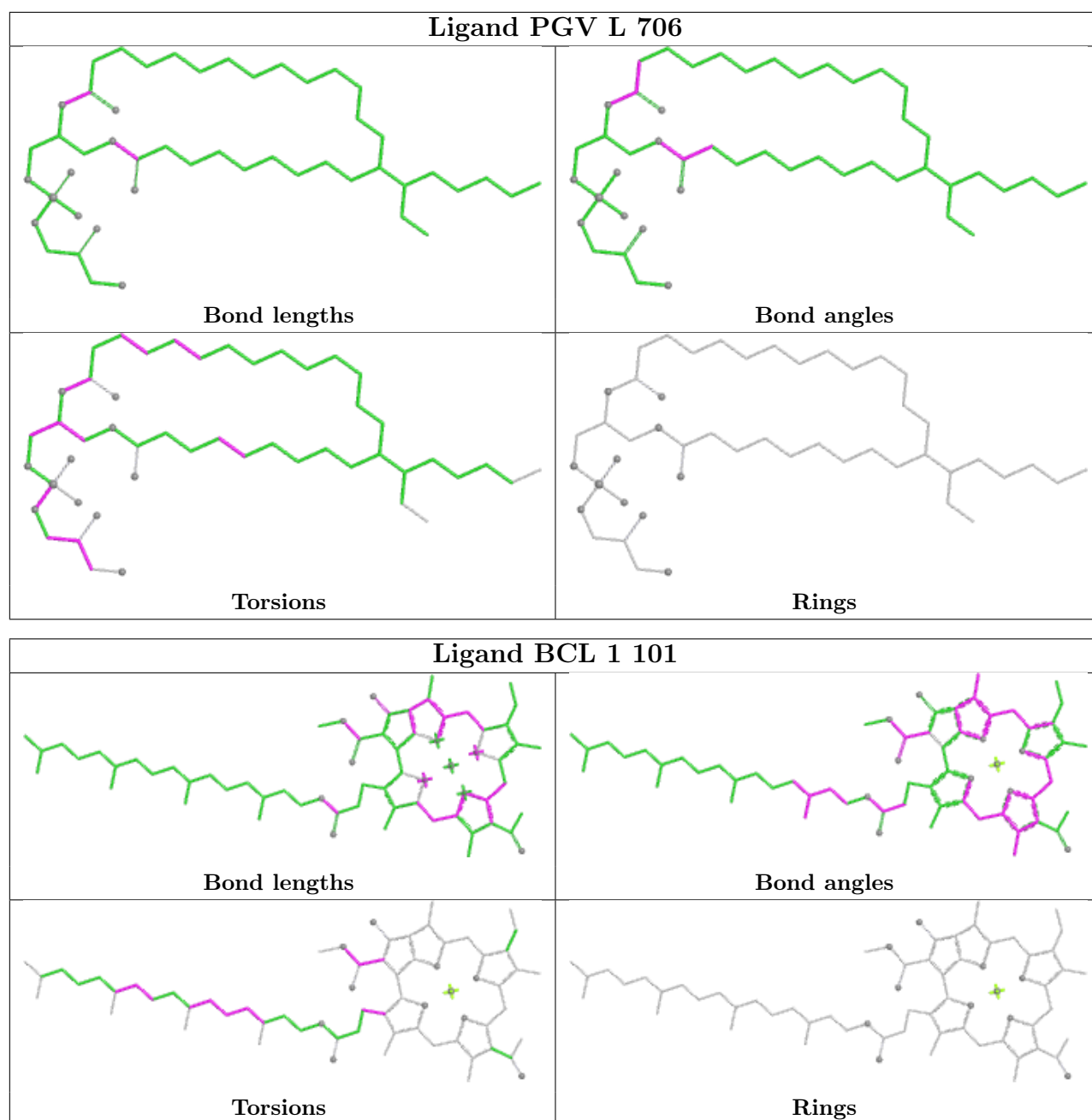


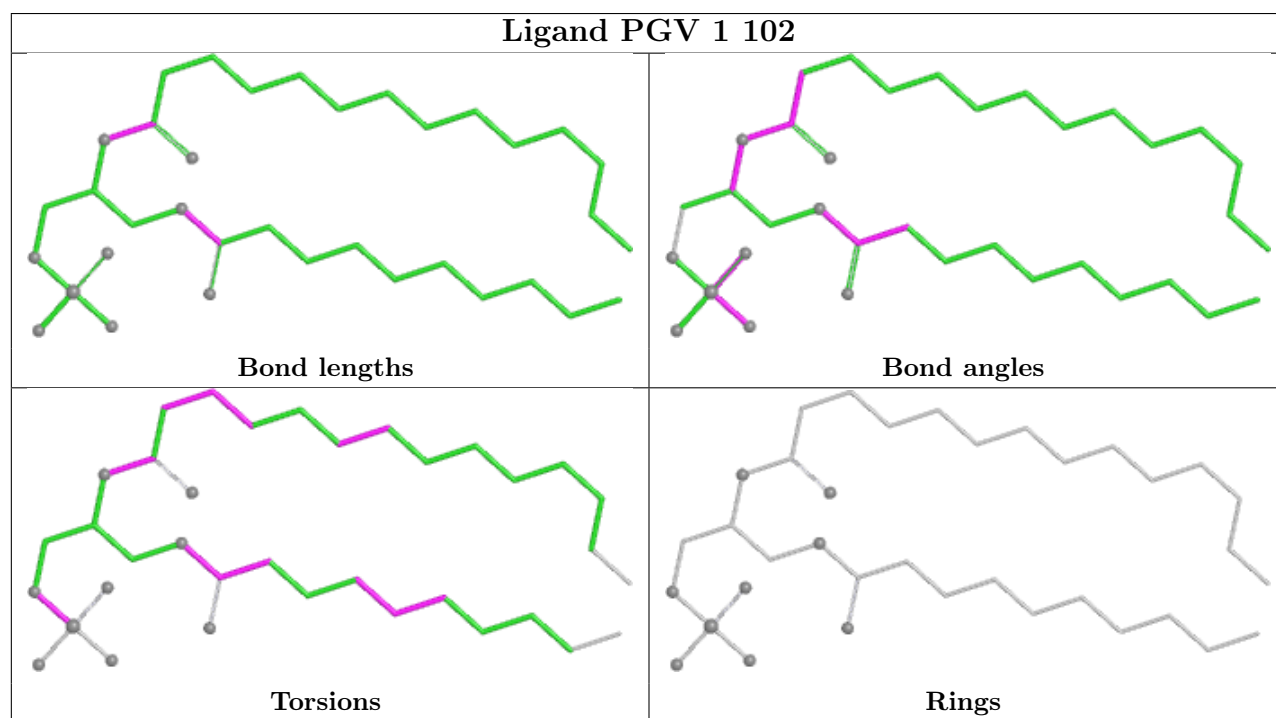
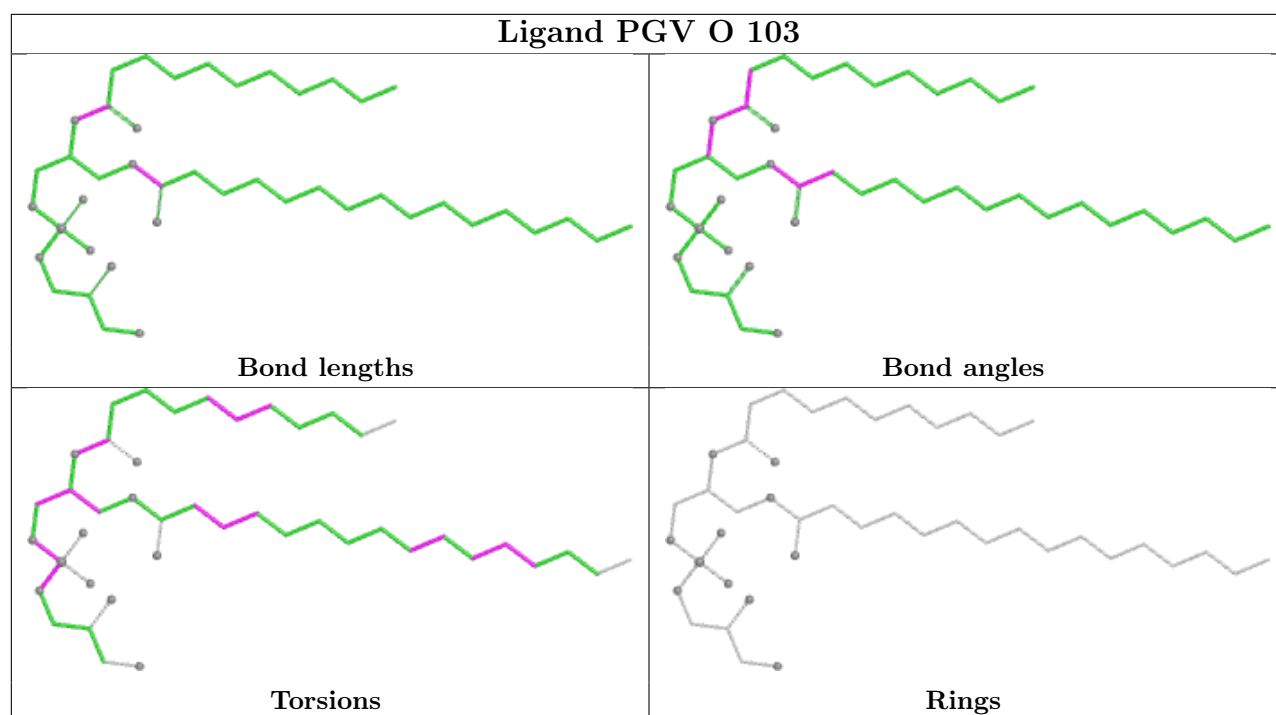


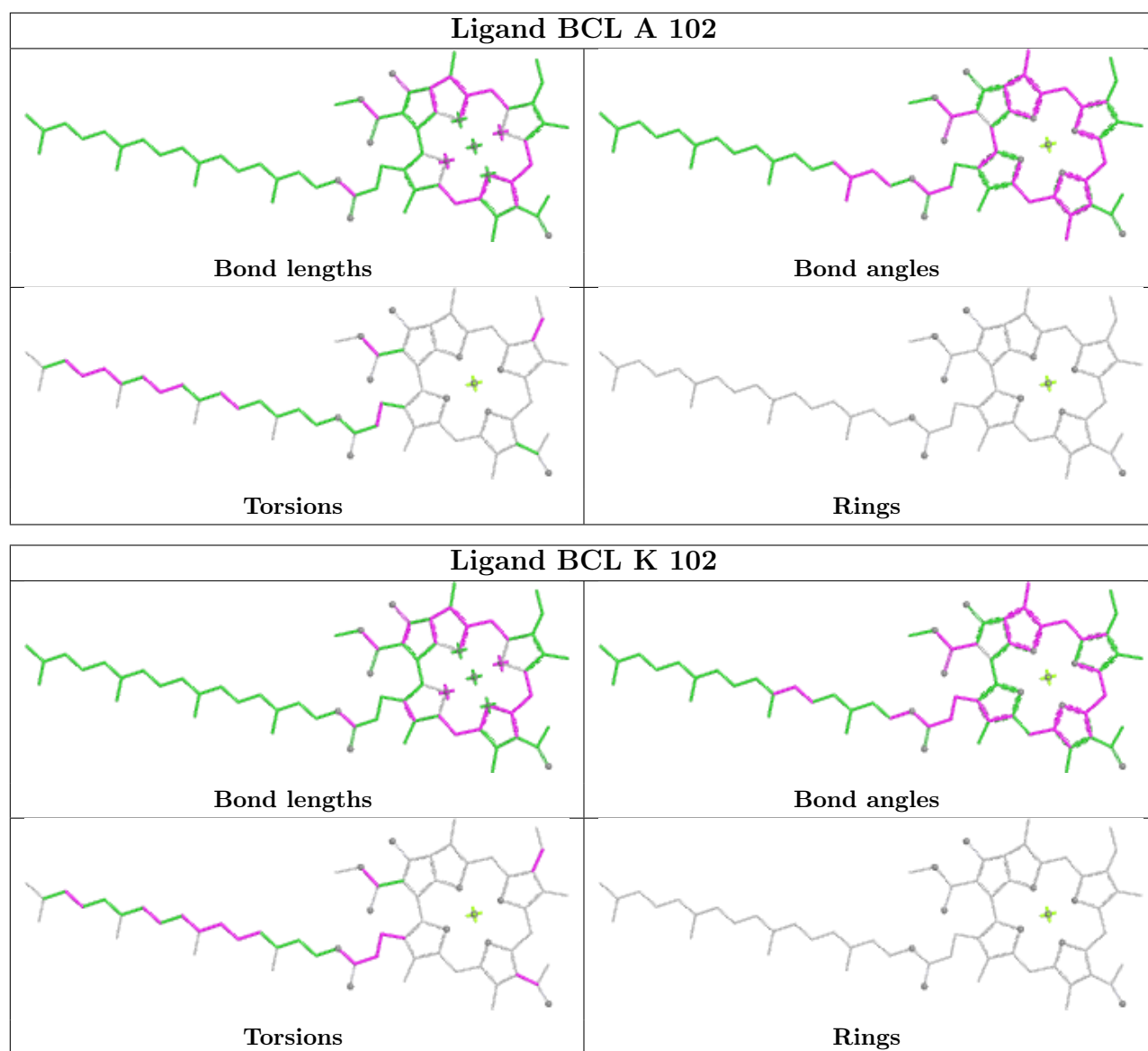


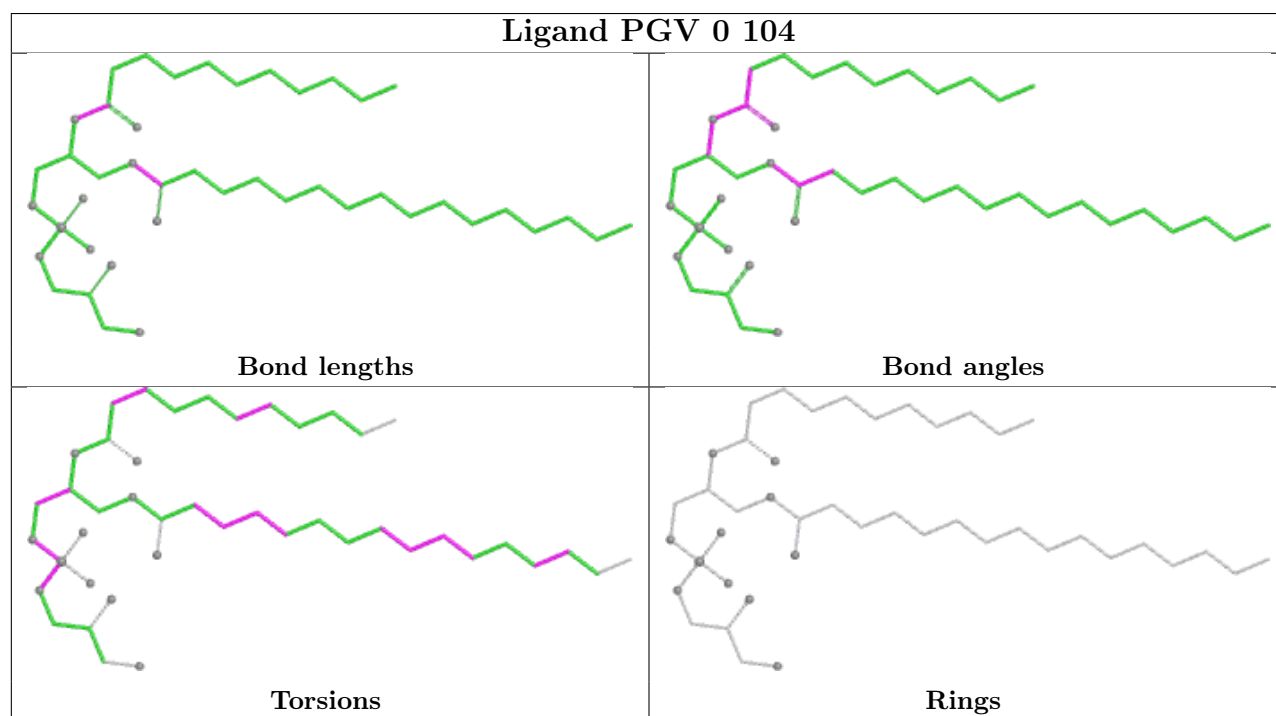
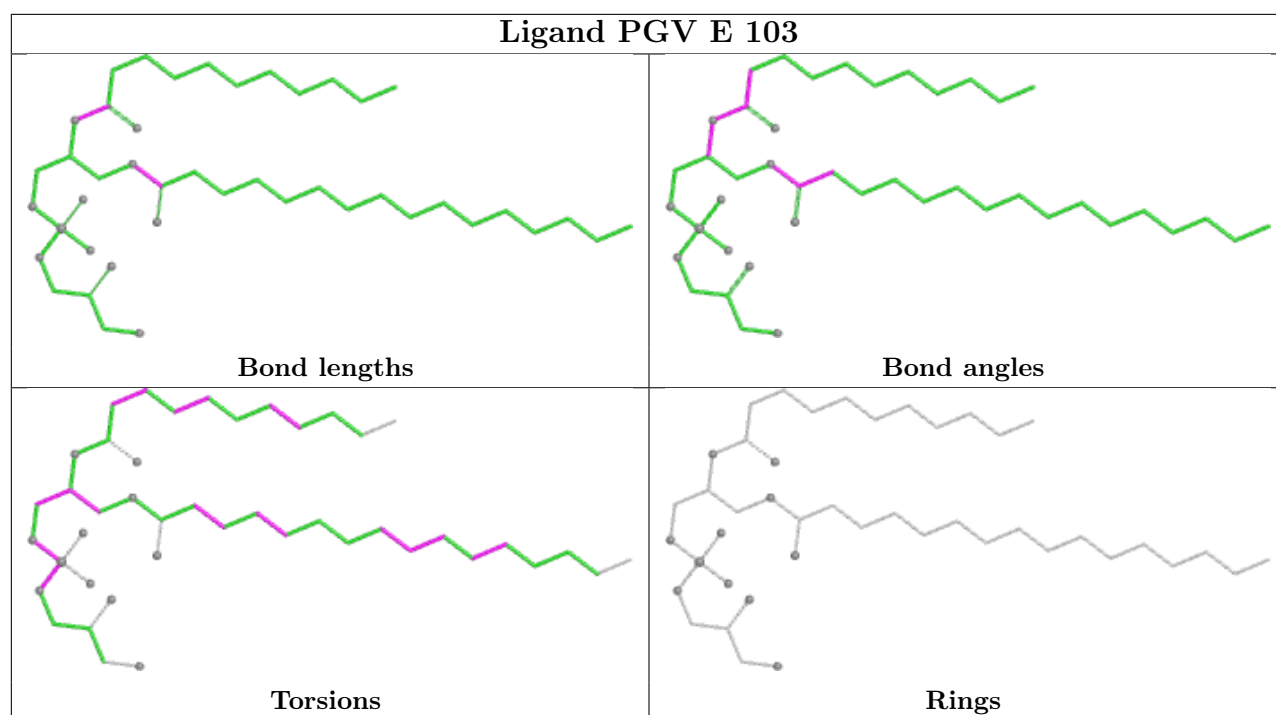


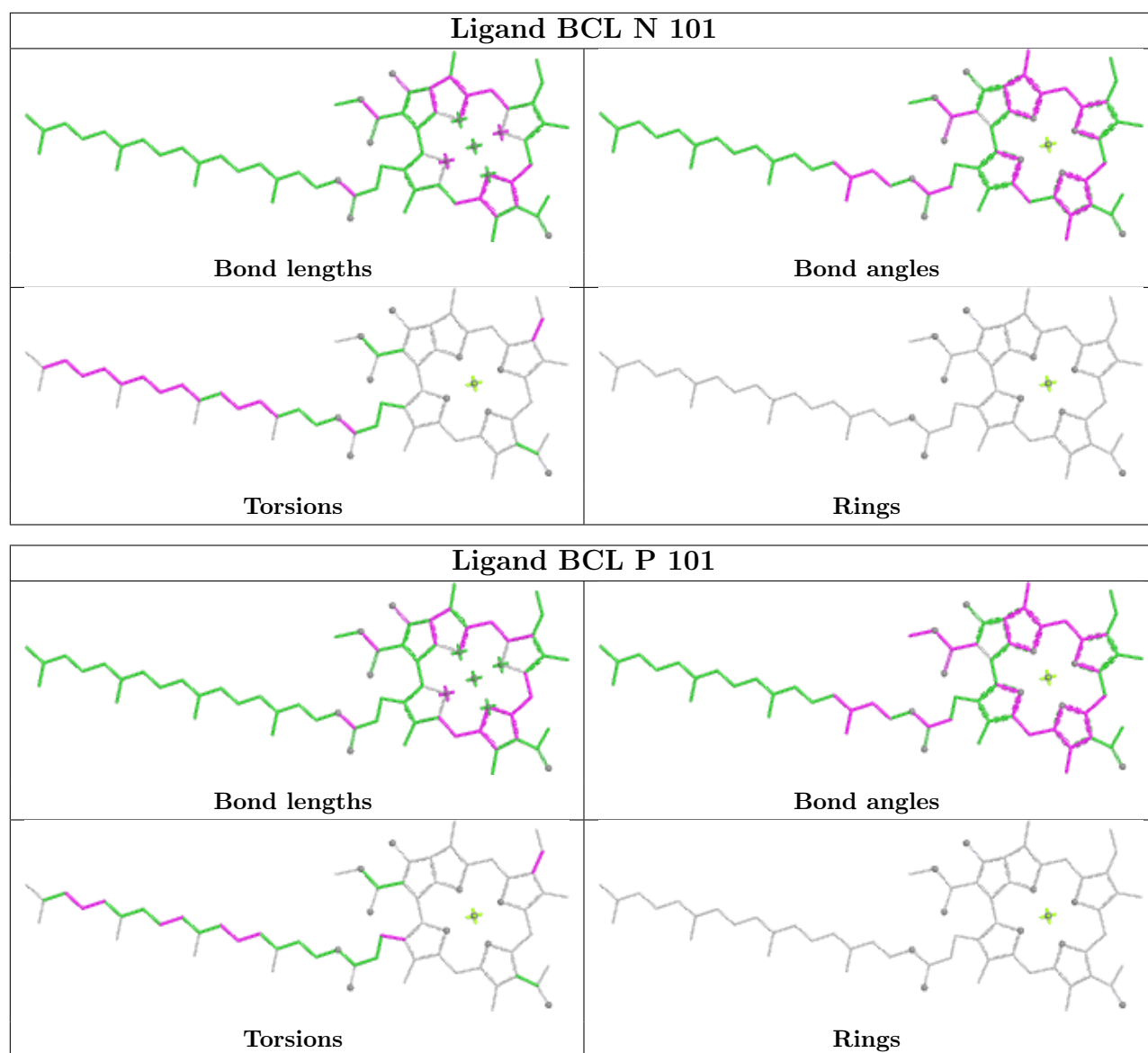


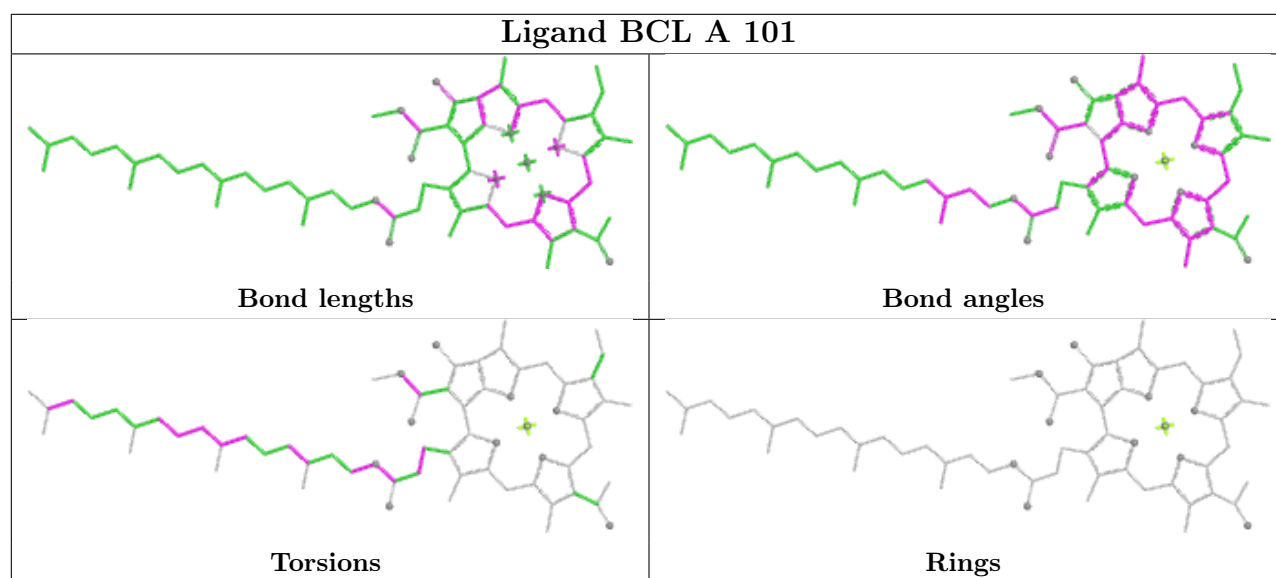
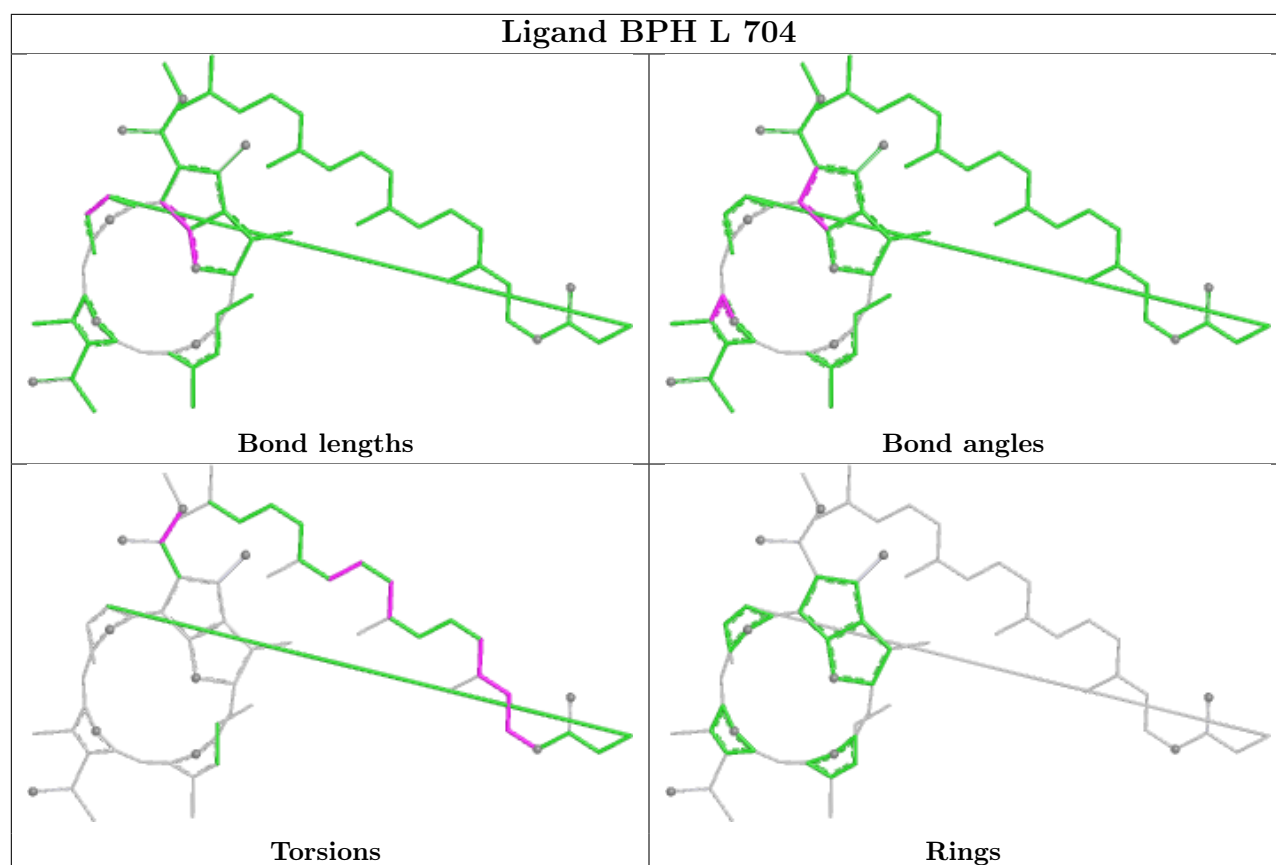




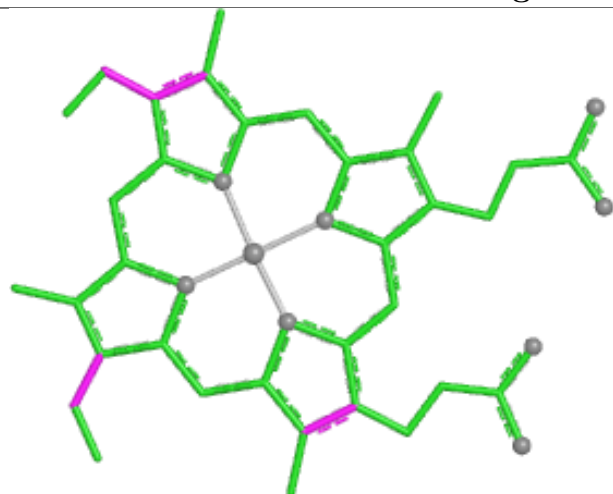




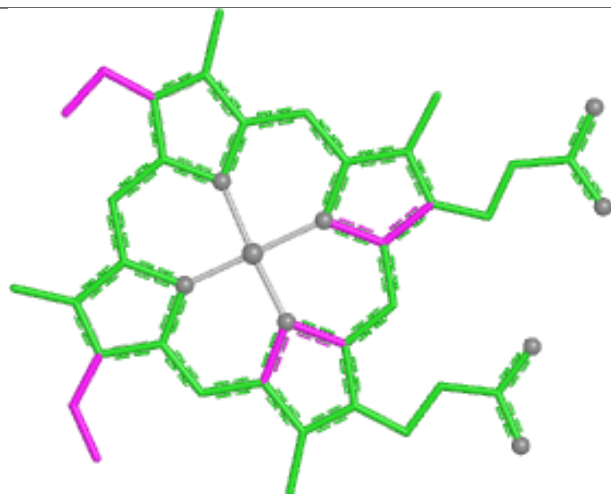




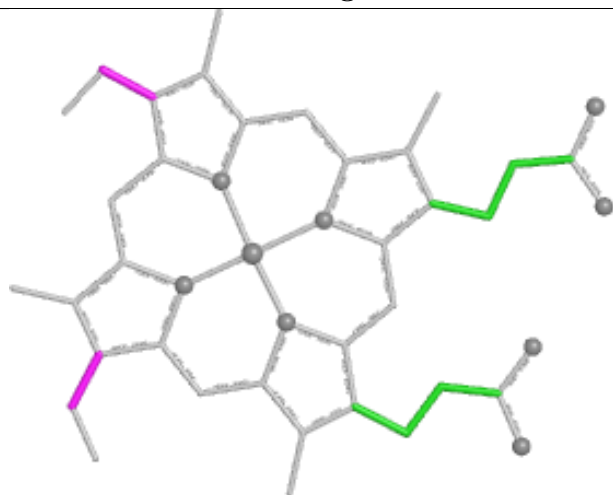
Ligand HEC C 503



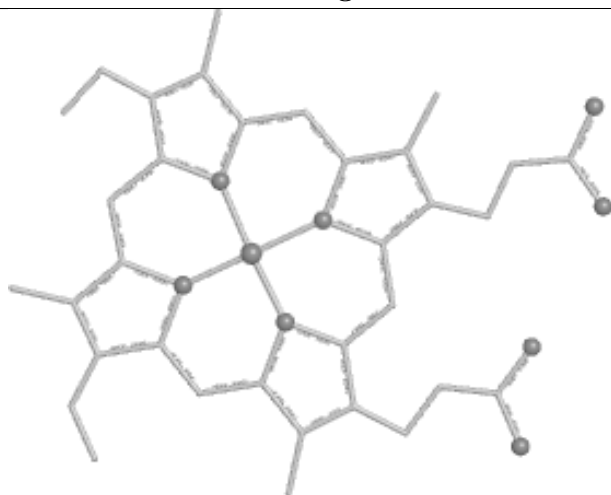
Bond lengths



Bond angles

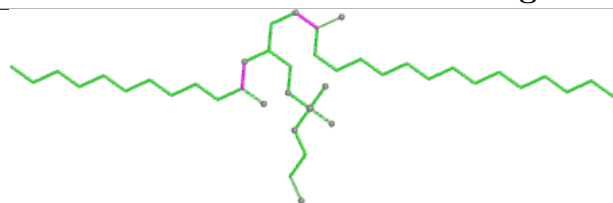


Torsions

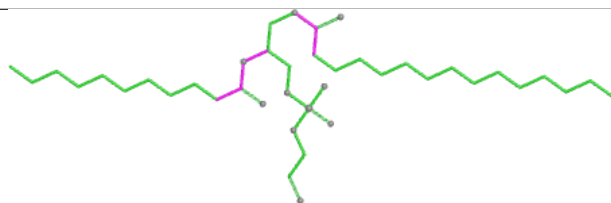


Rings

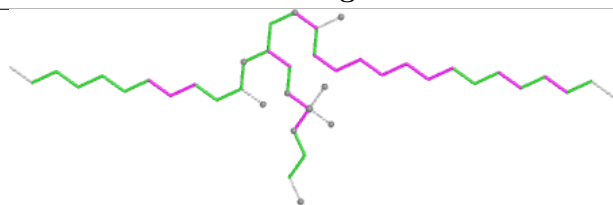
Ligand PEF h 103



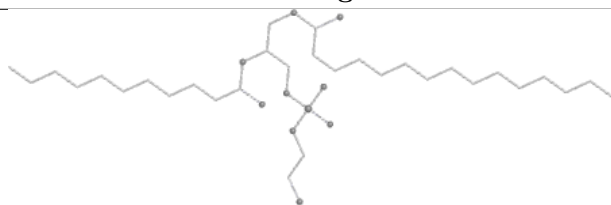
Bond lengths



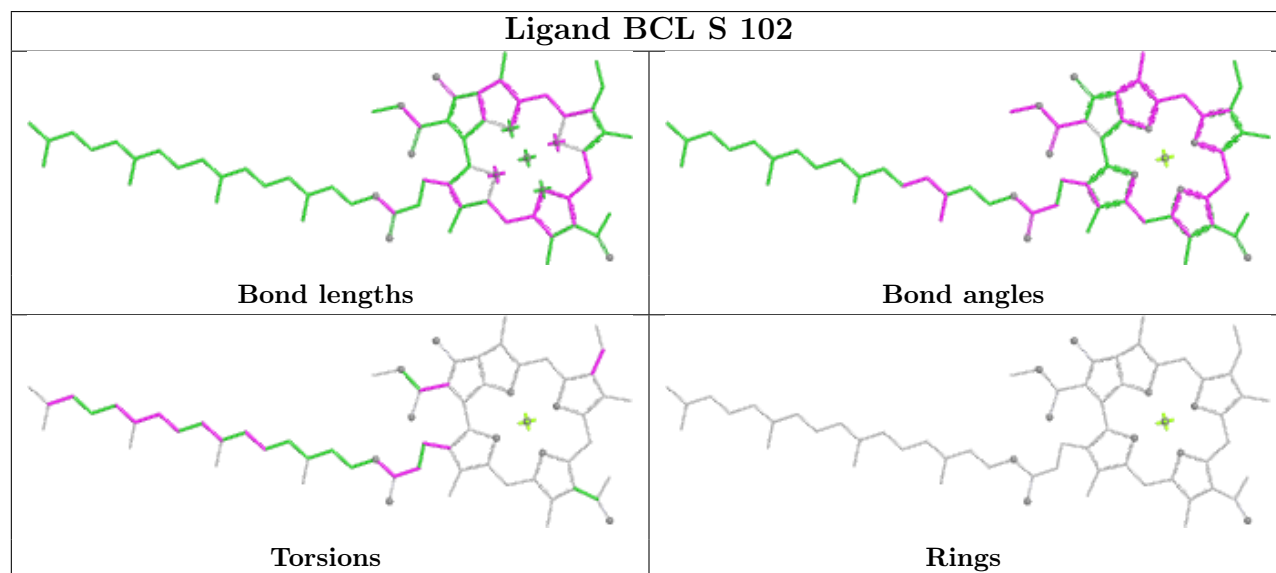
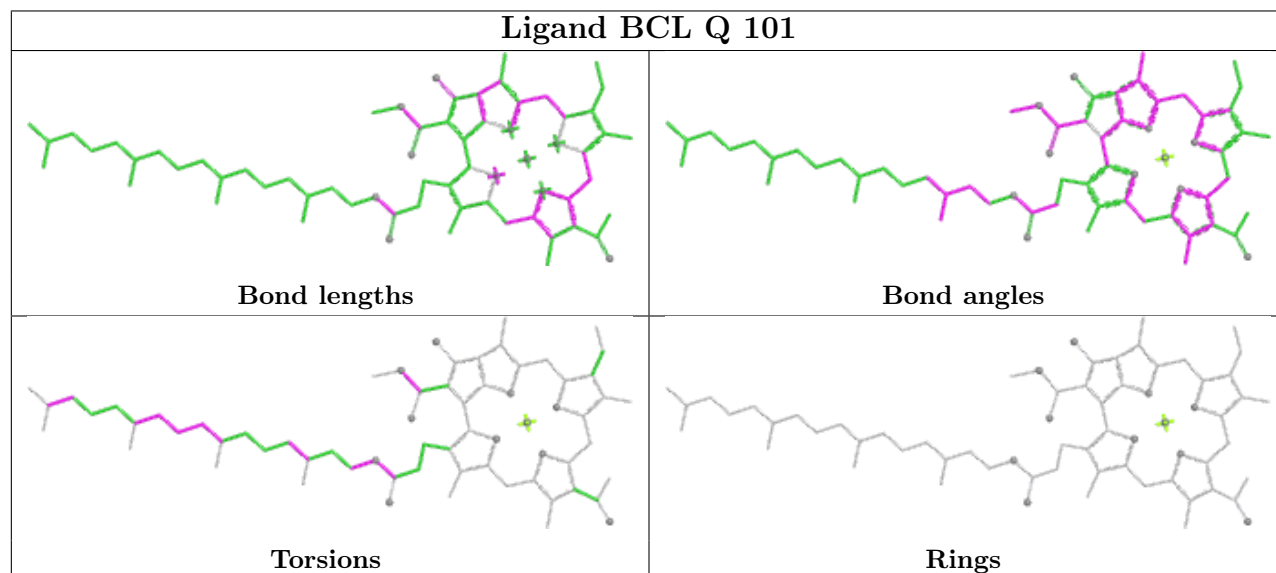
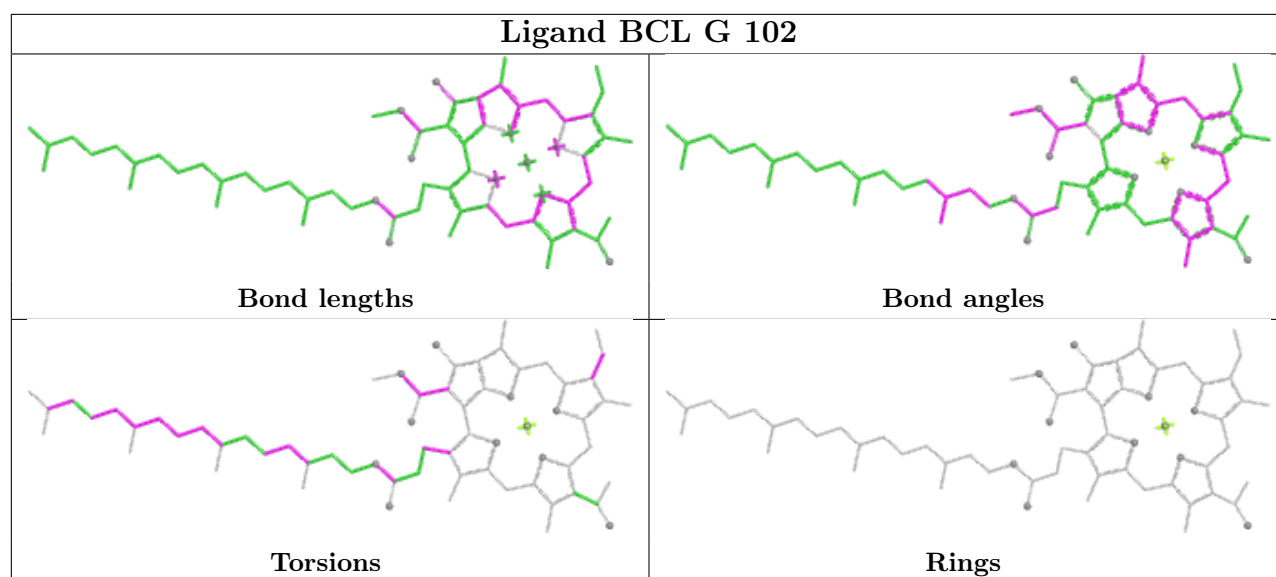
Bond angles

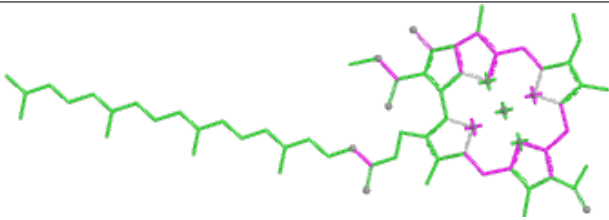
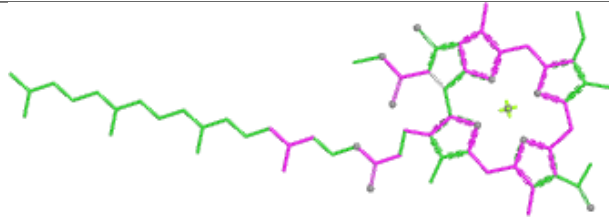
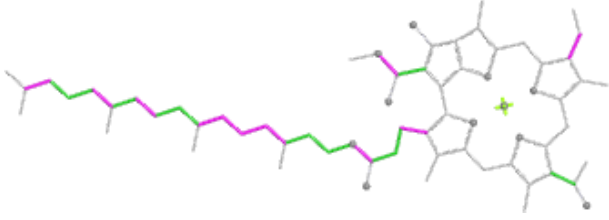
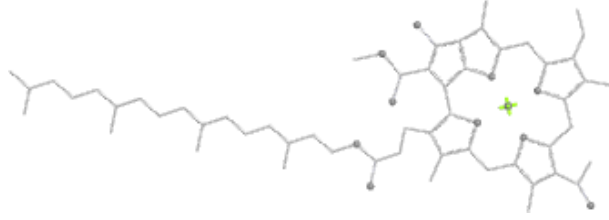


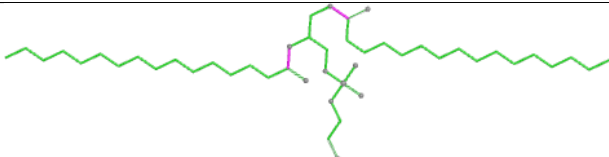
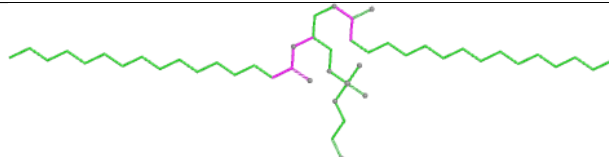
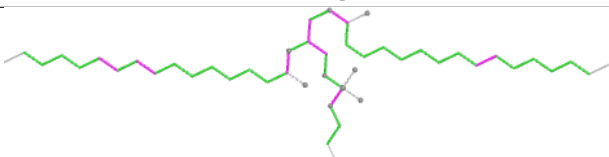
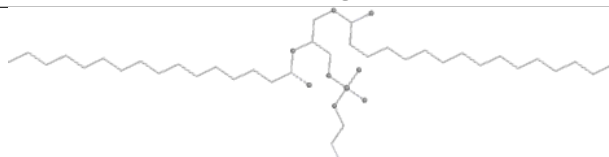
Torsions

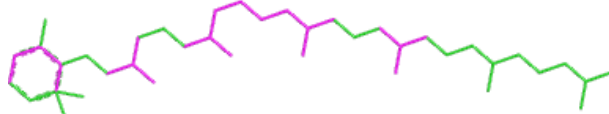
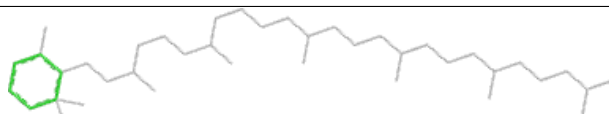


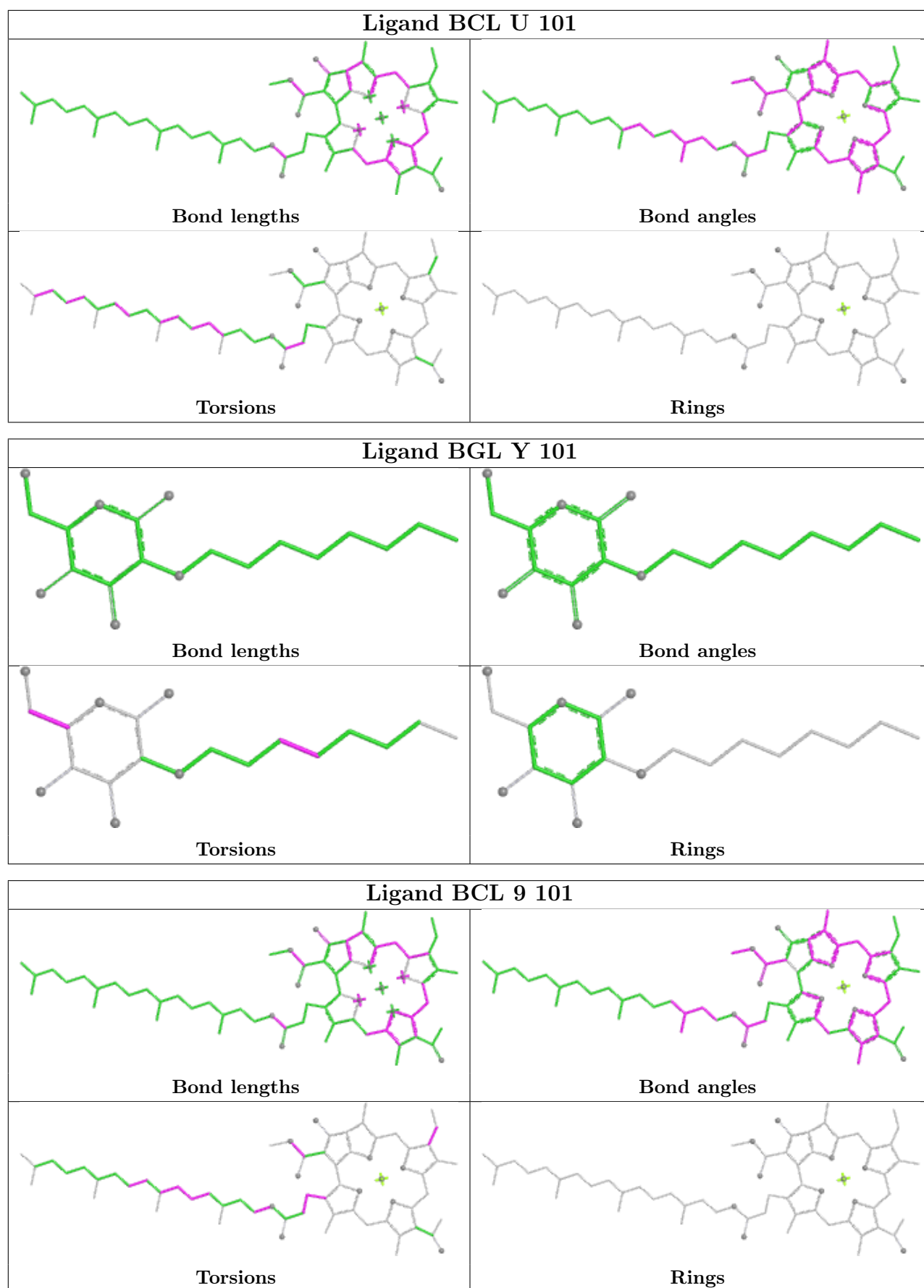
Rings

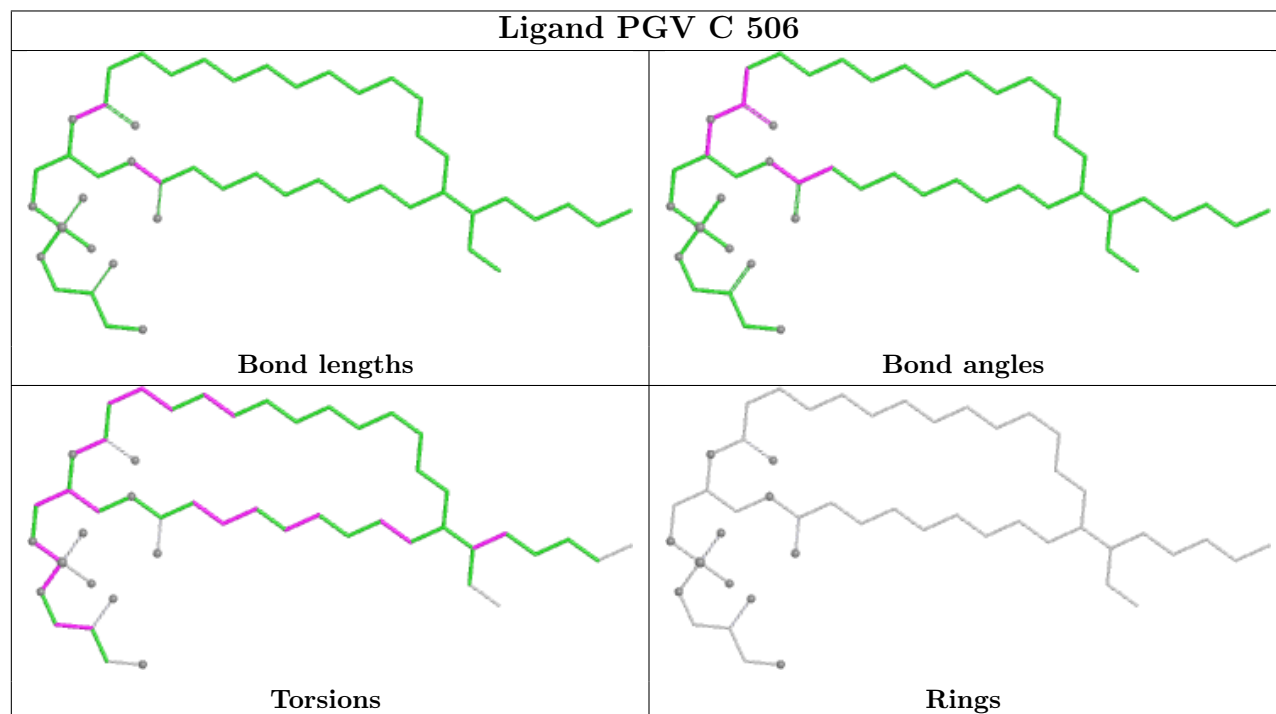
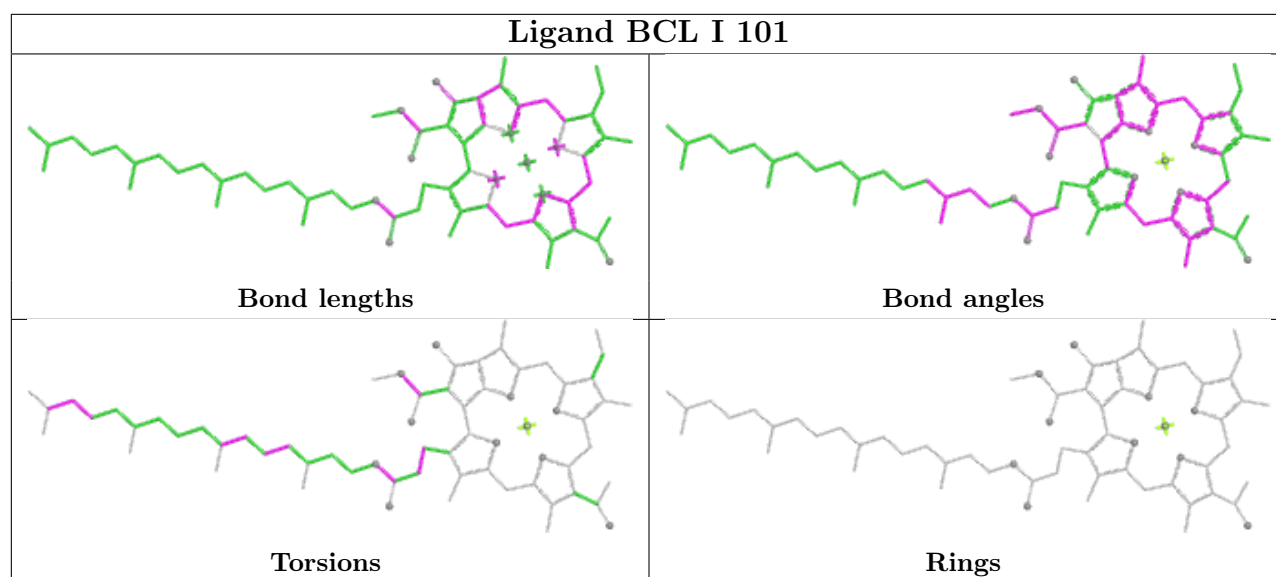


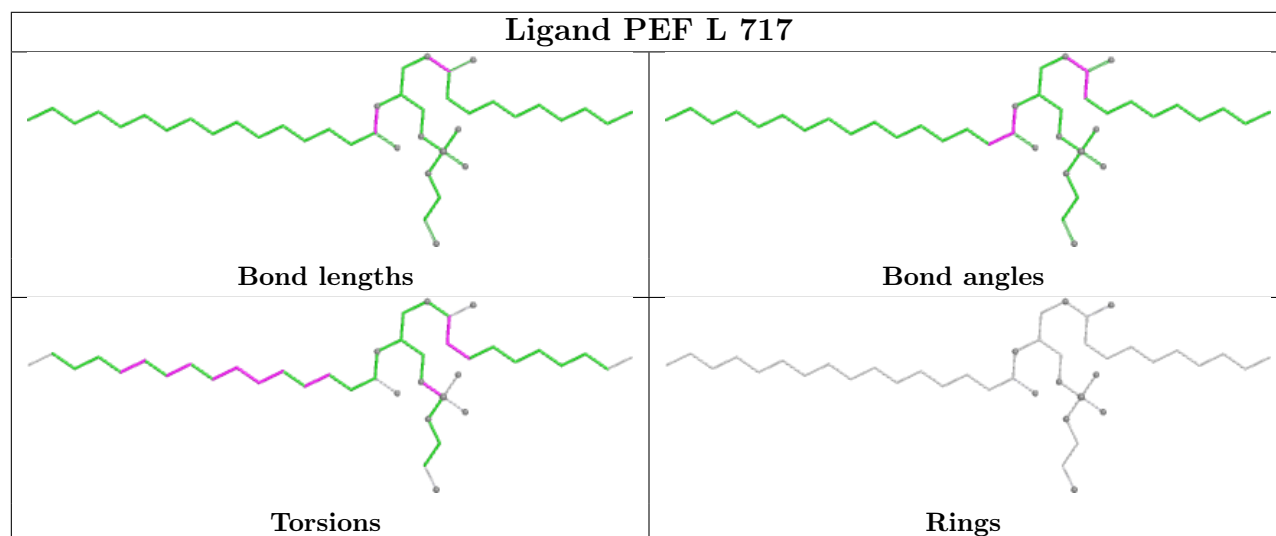
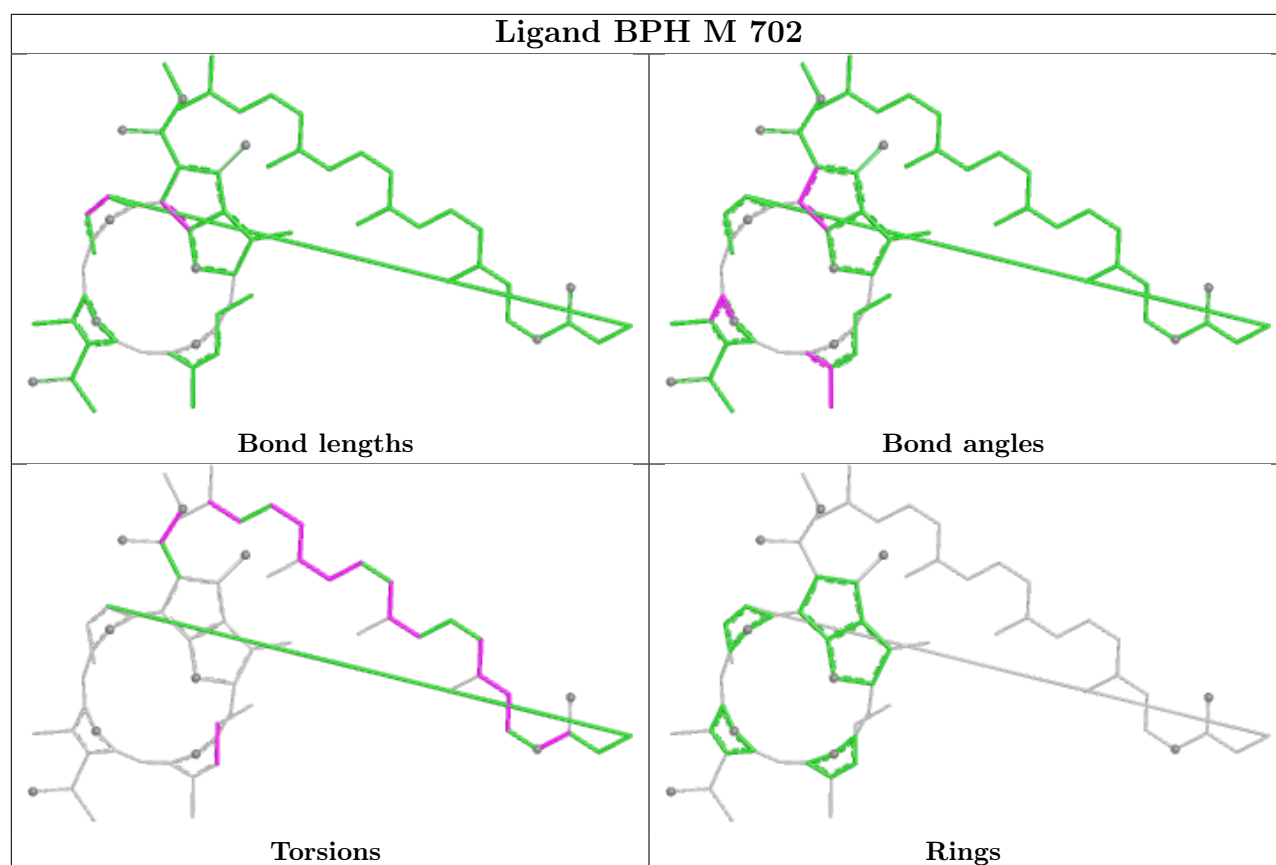
Ligand BCL O 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

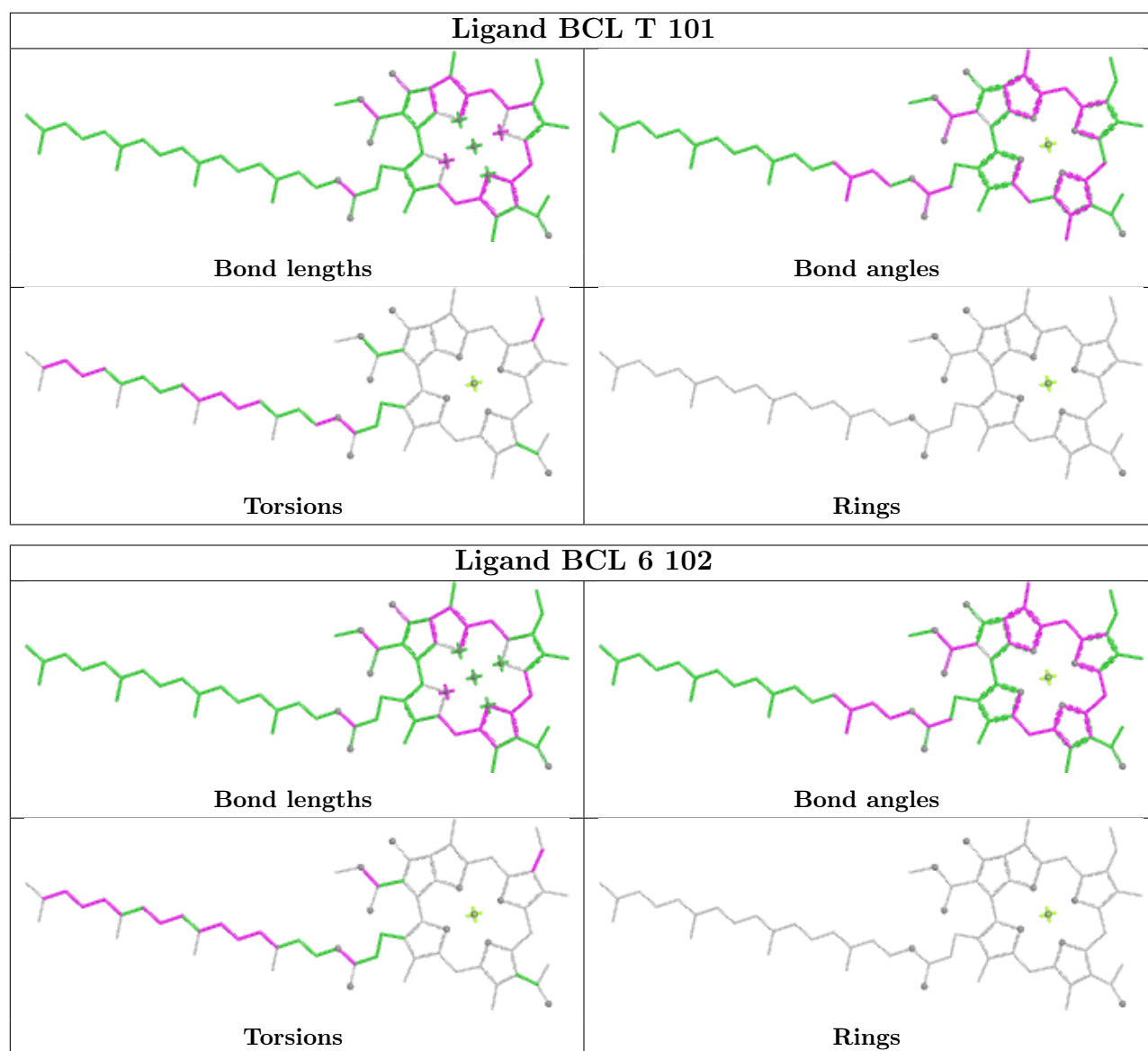
Ligand PEF L 713	
	
Bond lengths	Bond angles
	
Torsions	Rings

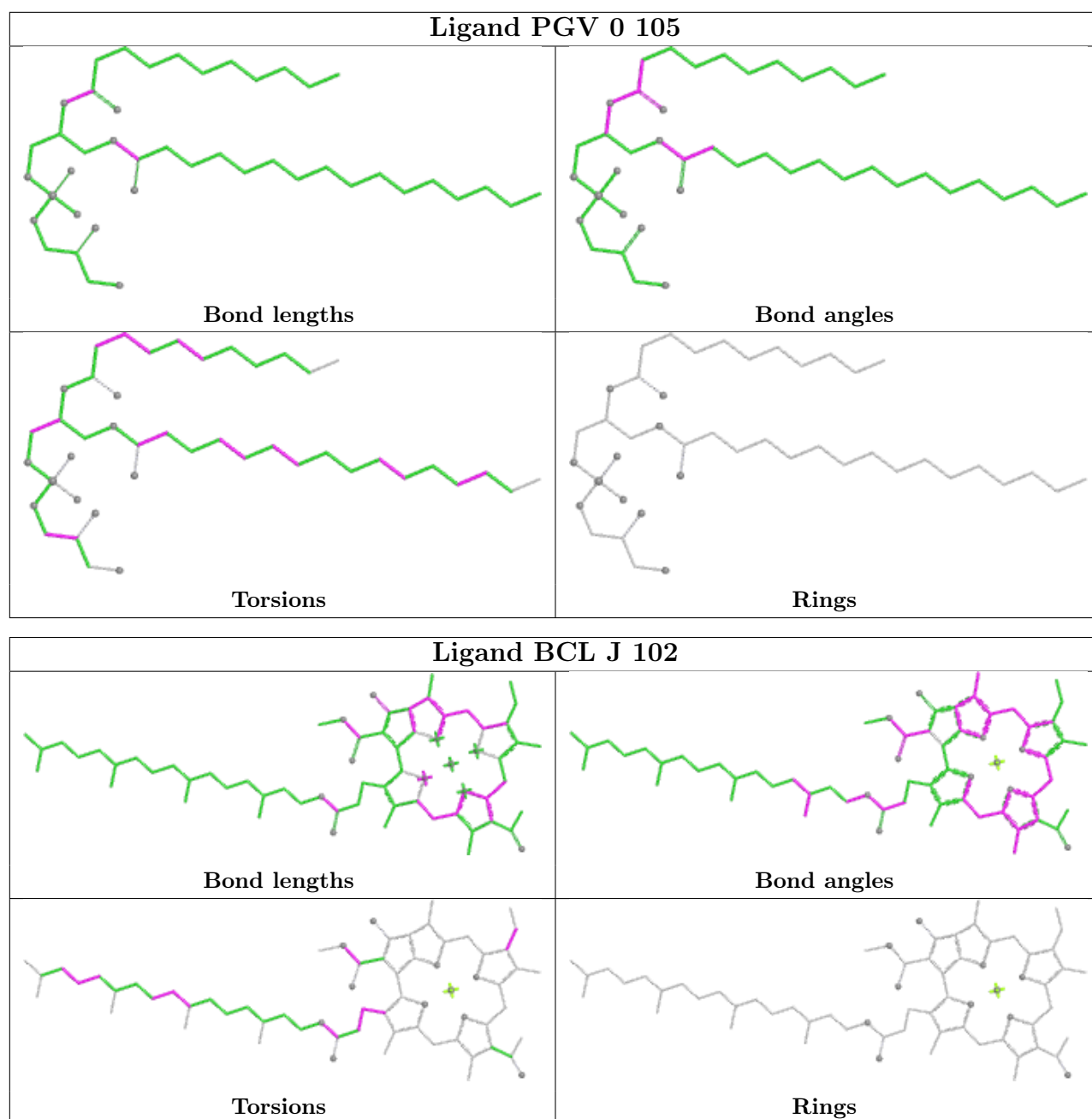
Ligand U4Z O 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

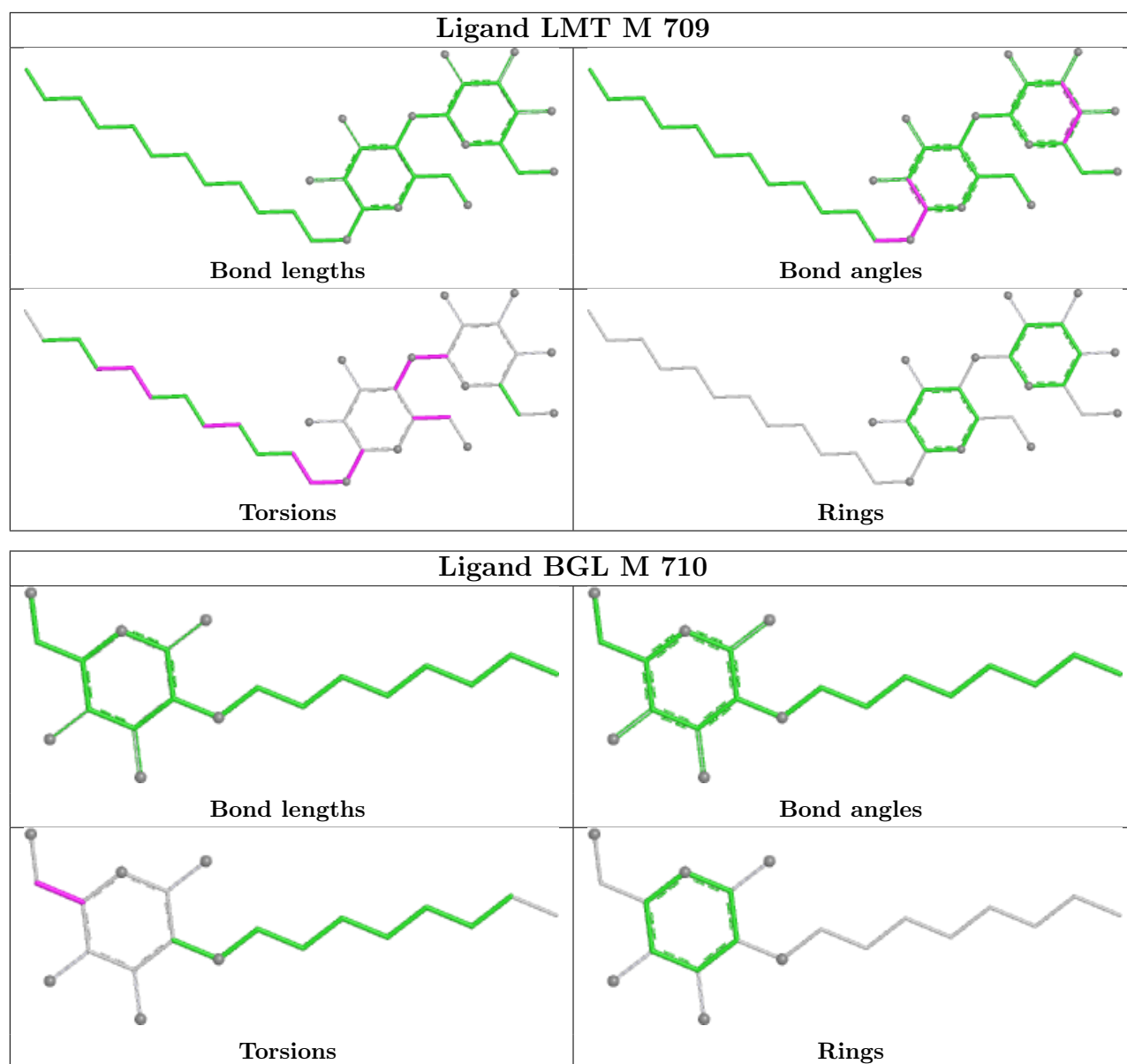


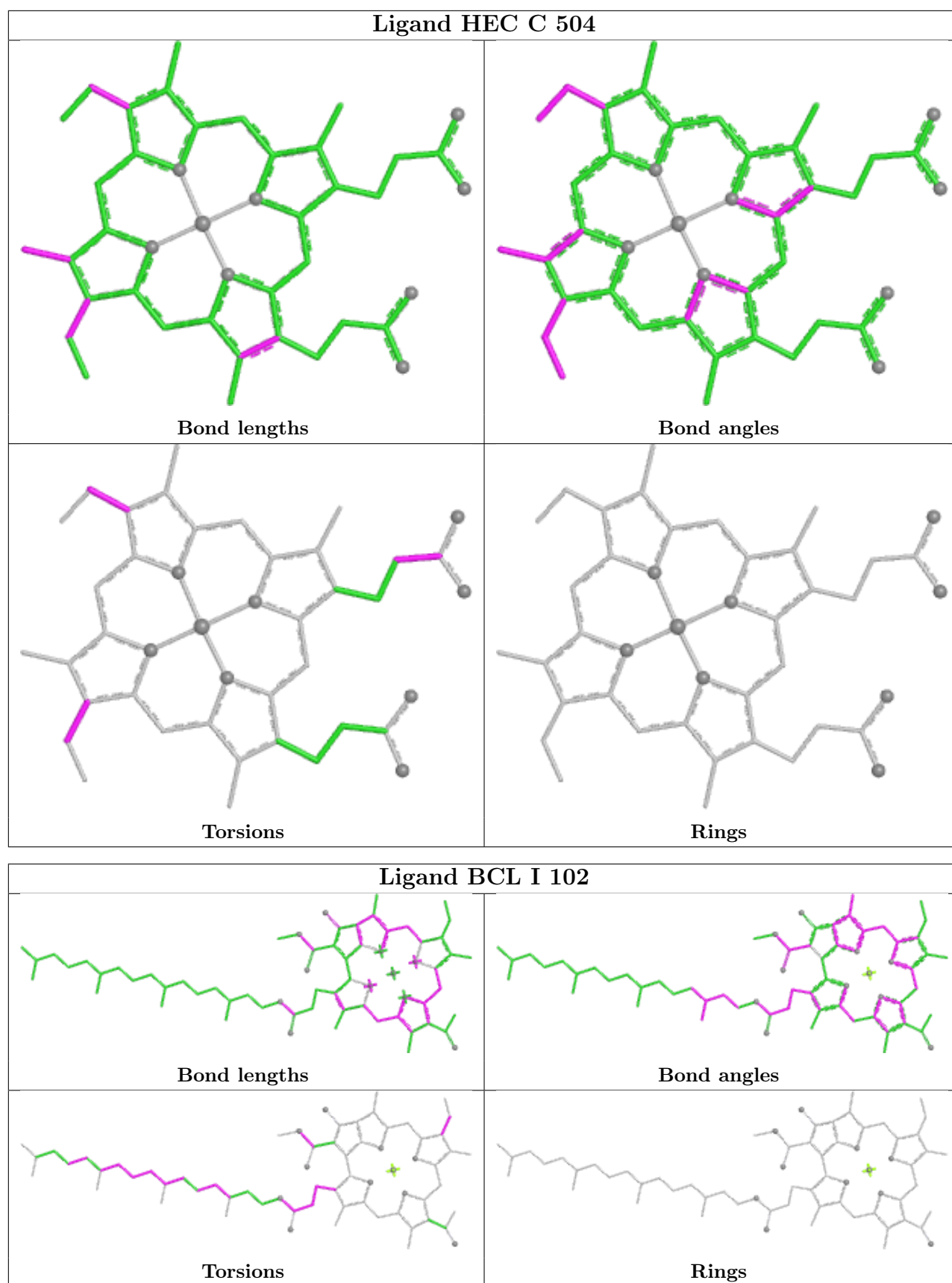


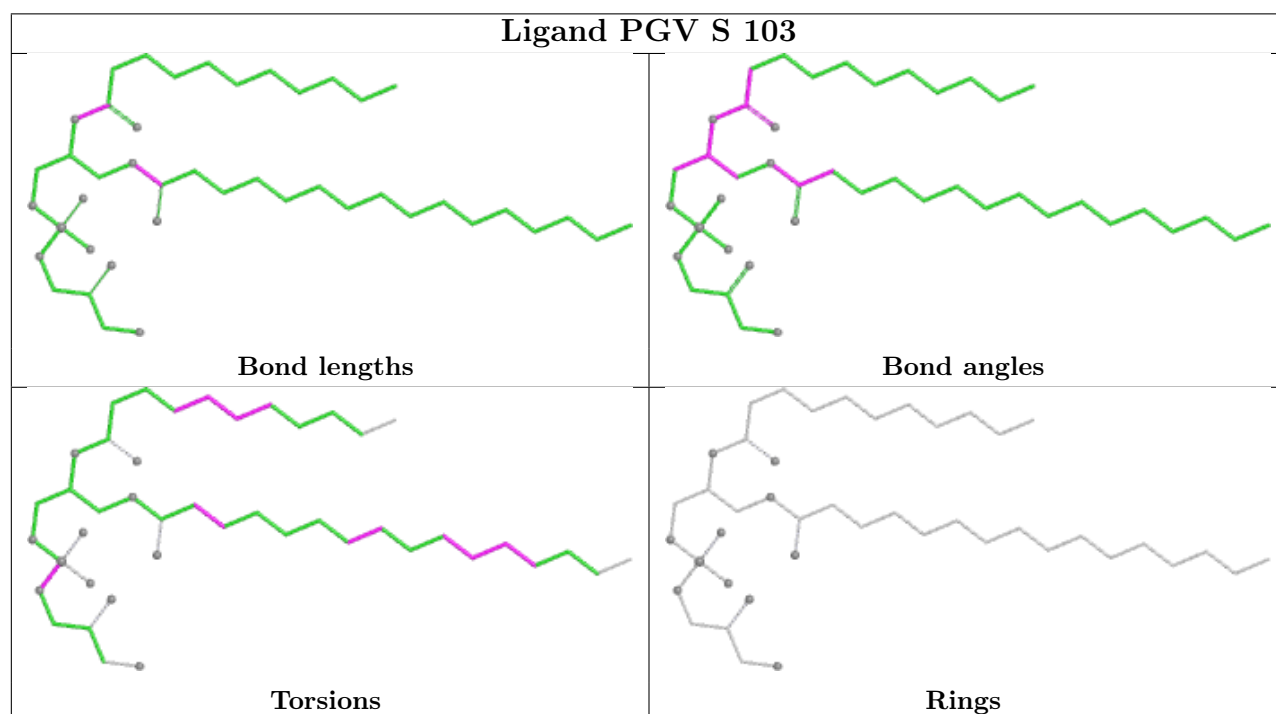
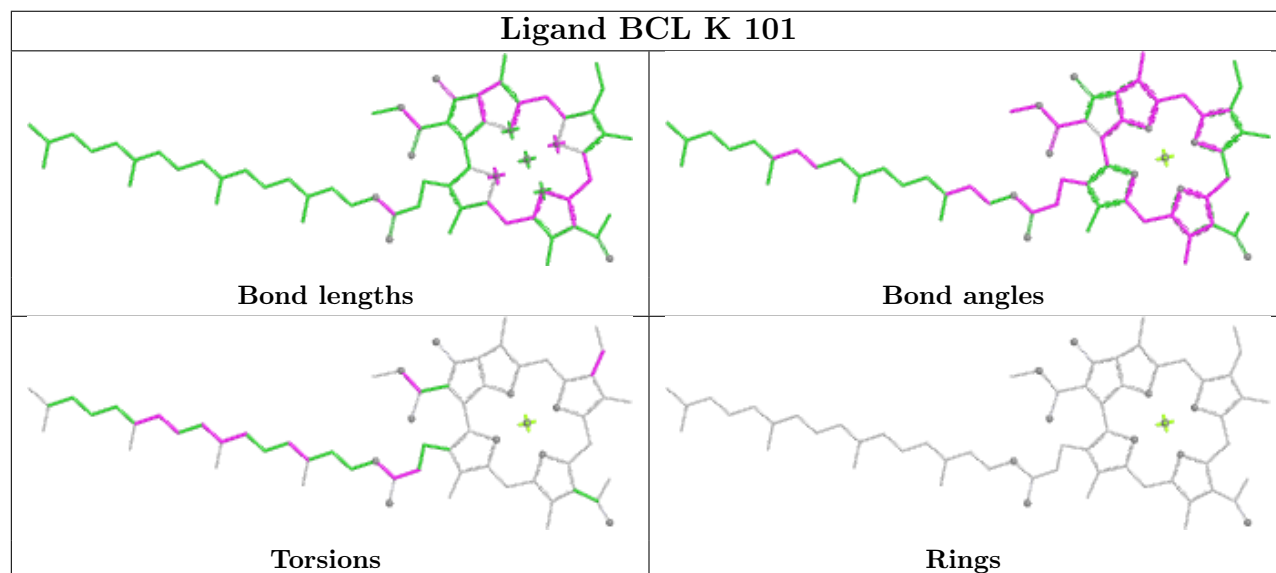
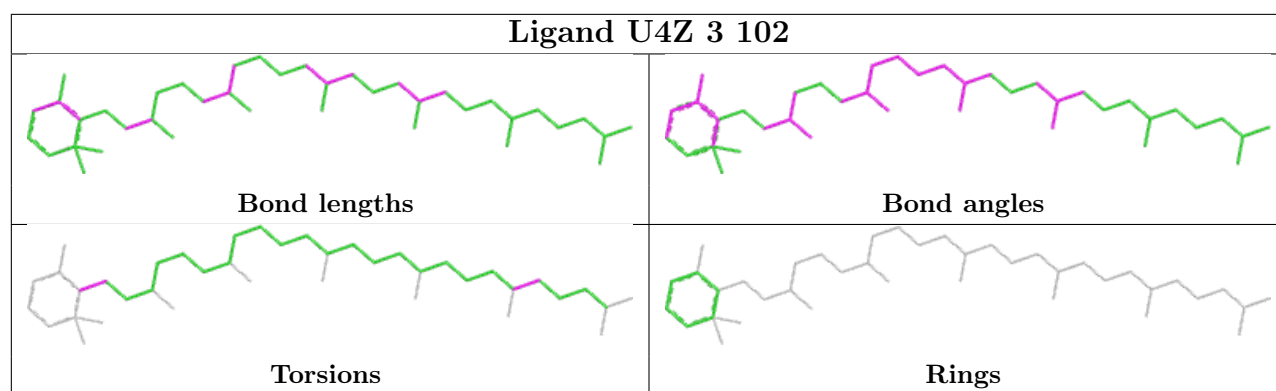


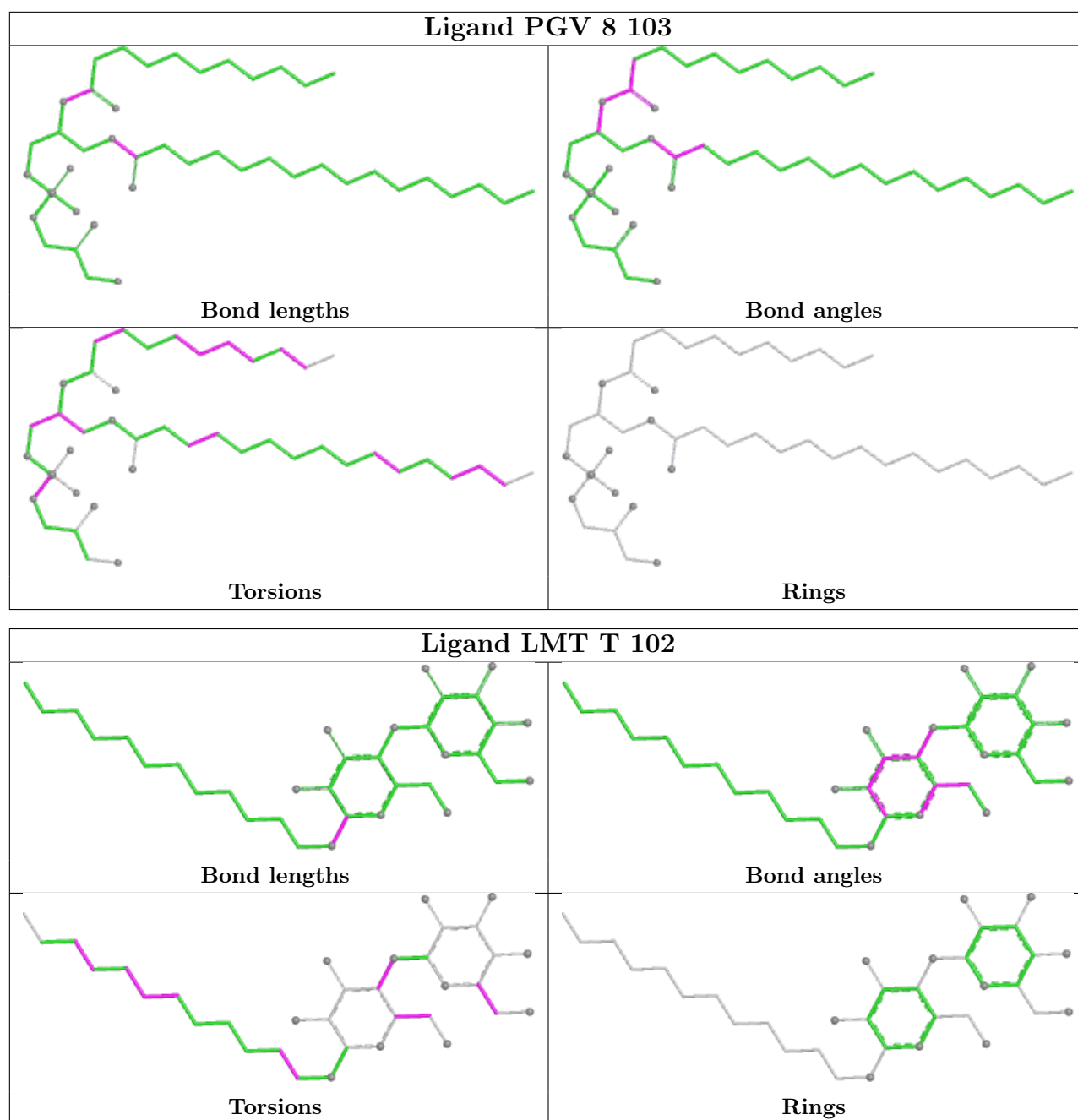


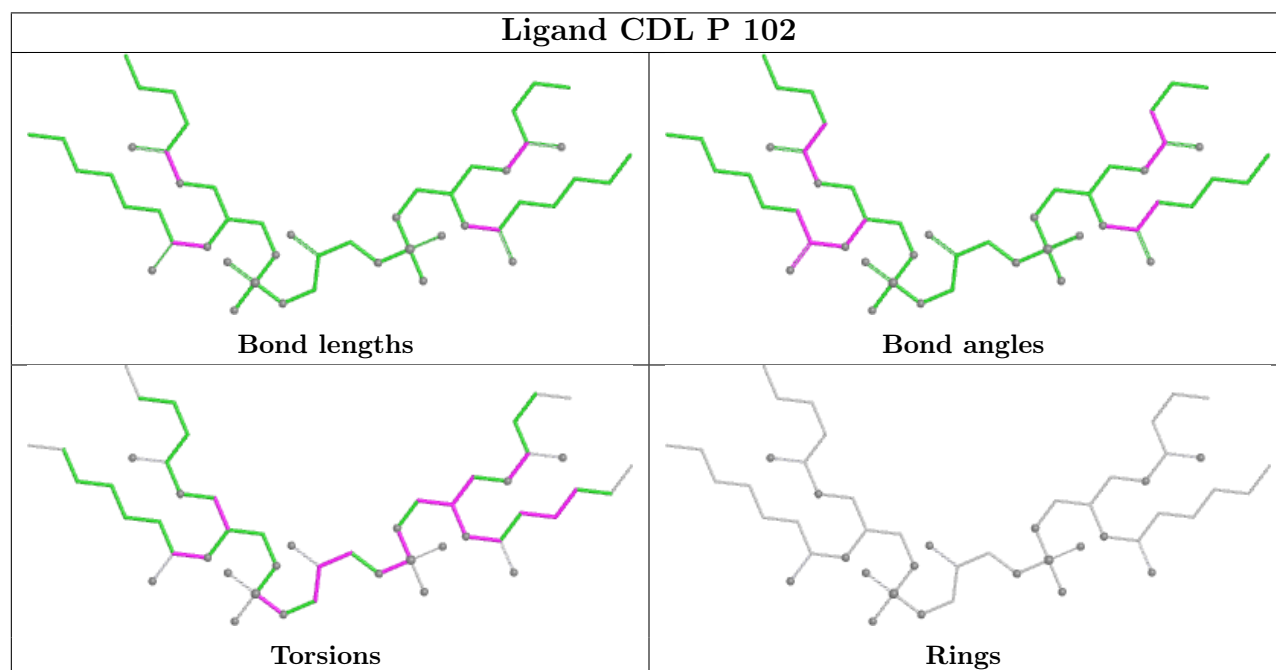
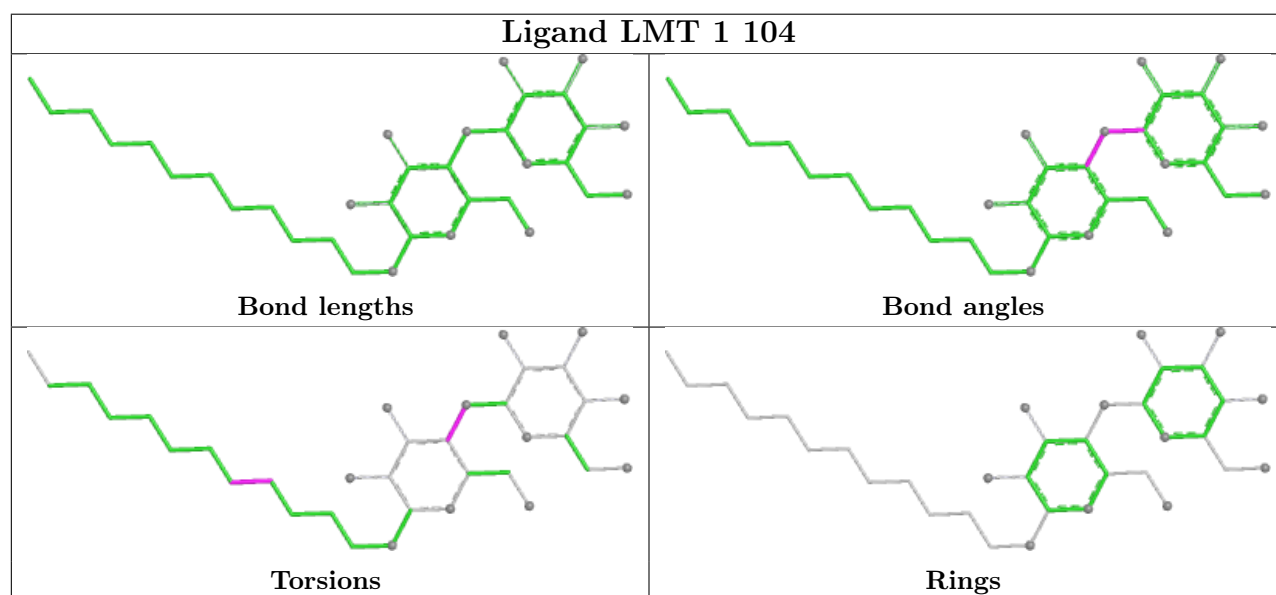
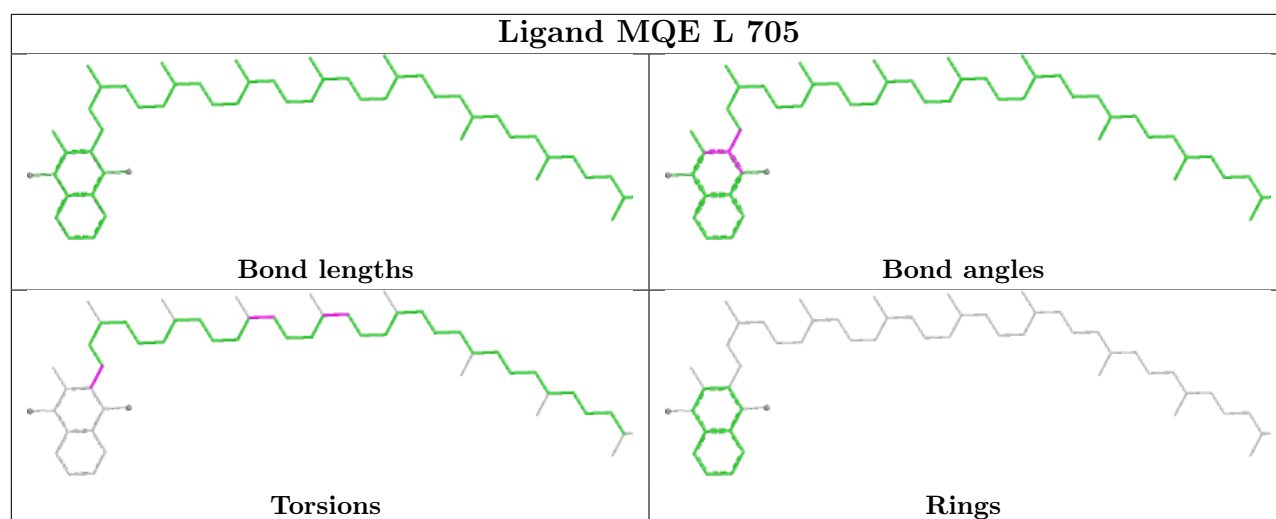


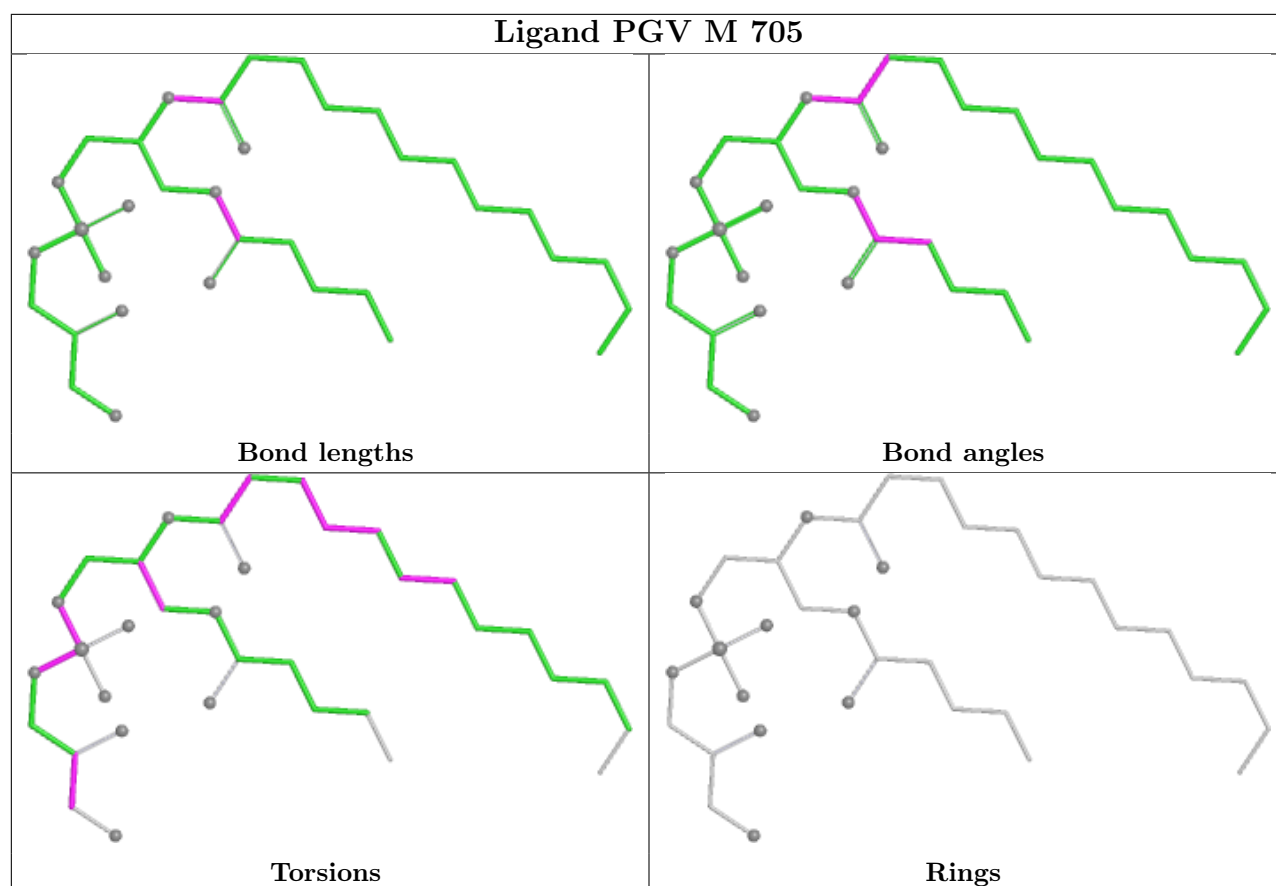












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

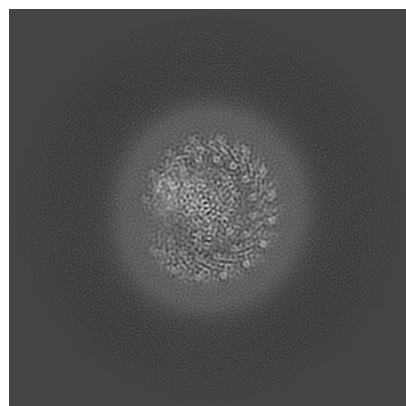
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35727. These allow visual inspection of the internal detail of the map and identification of artifacts.

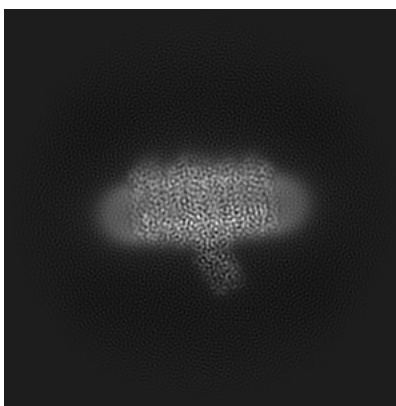
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

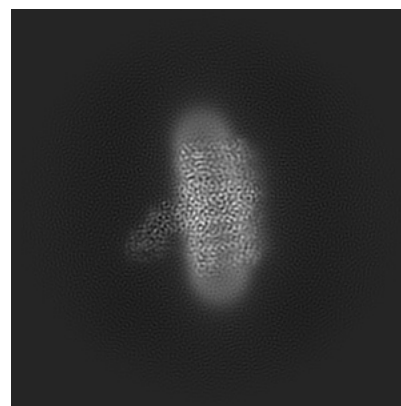
6.1.1 Primary map



X

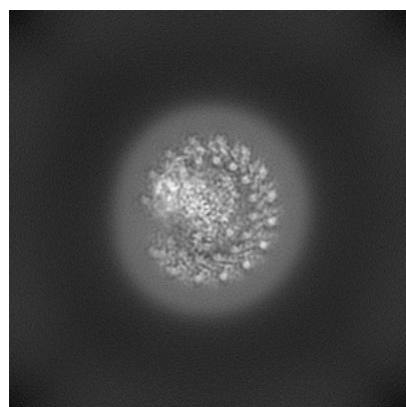


Y

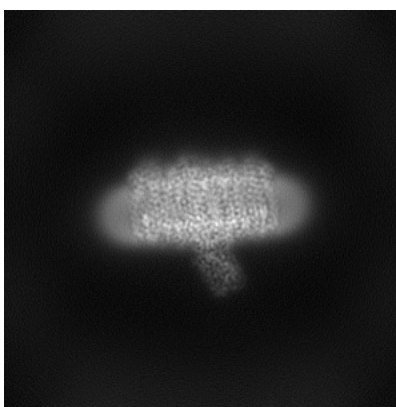


Z

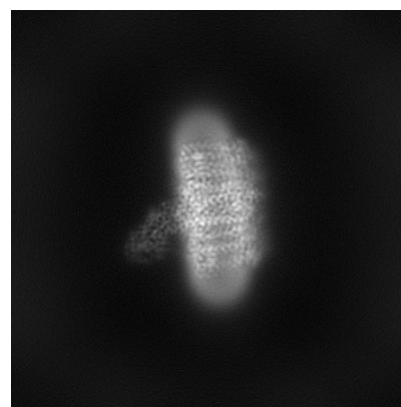
6.1.2 Raw map



X



Y

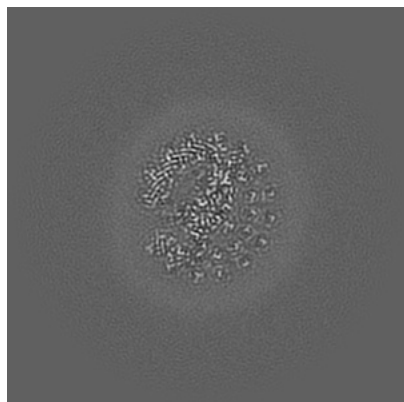


Z

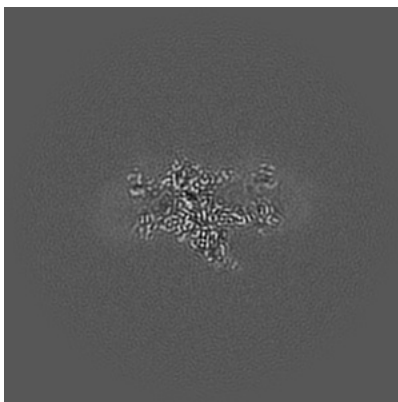
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

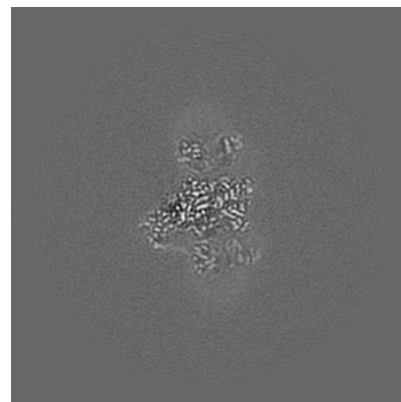
6.2.1 Primary map



X Index: 180

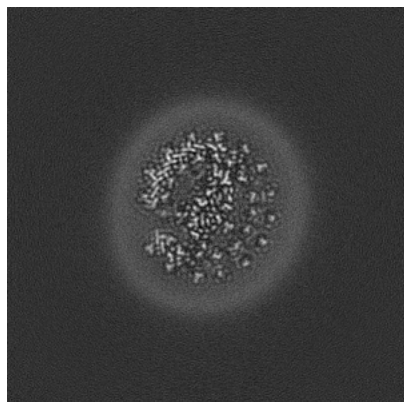


Y Index: 180

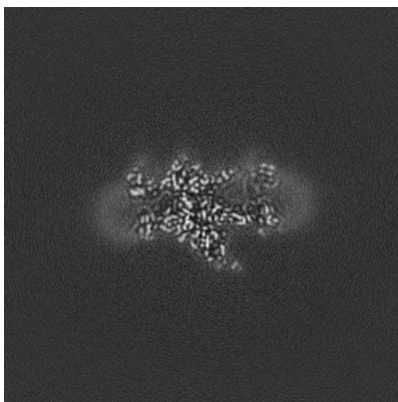


Z Index: 180

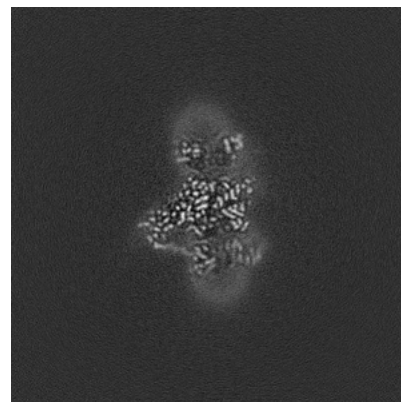
6.2.2 Raw map



X Index: 180



Y Index: 180

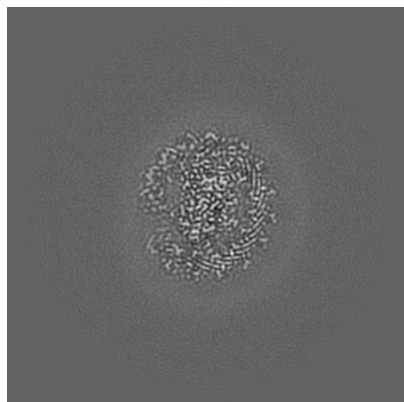


Z Index: 180

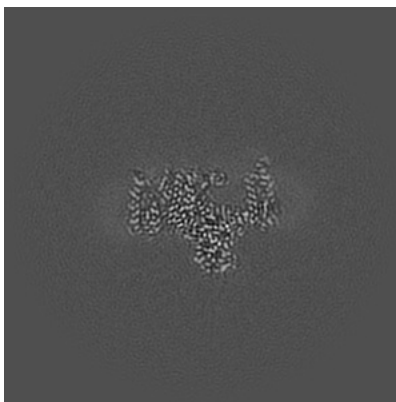
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

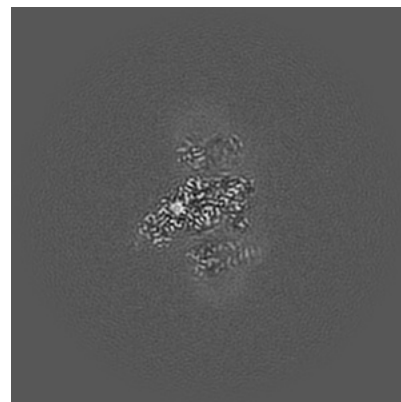
6.3.1 Primary map



X Index: 168

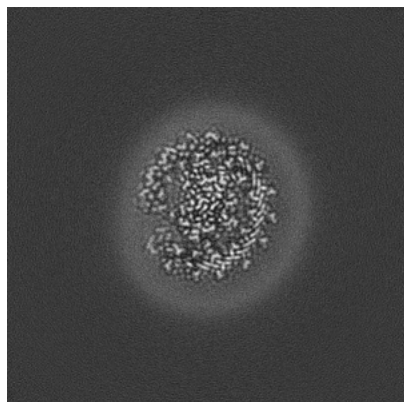


Y Index: 170

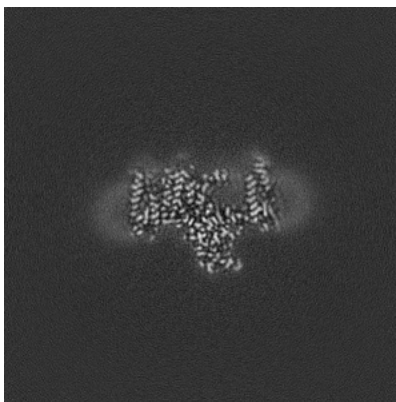


Z Index: 183

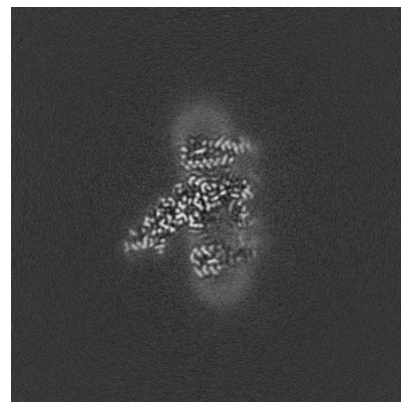
6.3.2 Raw map



X Index: 168



Y Index: 172

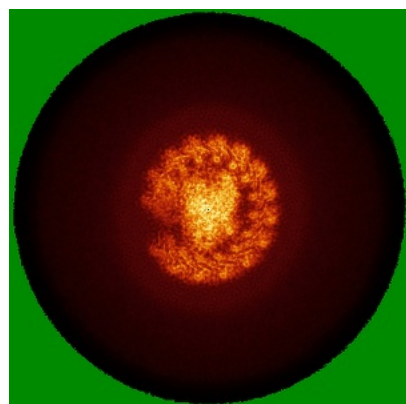


Z Index: 190

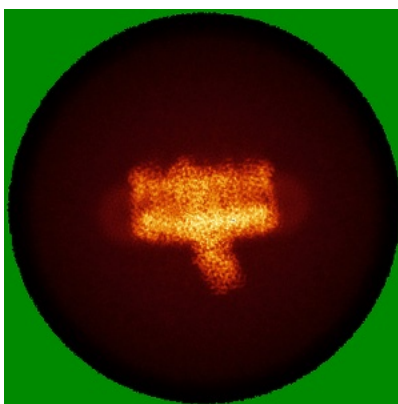
The images above show the largest variance slices of the map in three orthogonal directions.

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

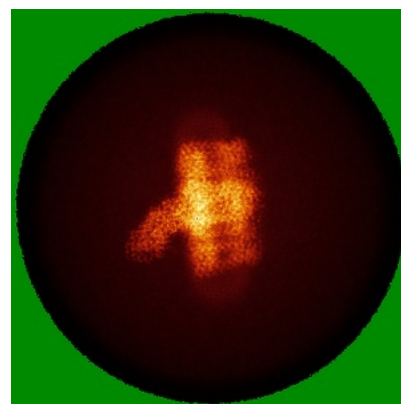
6.4.1 Primary map



X

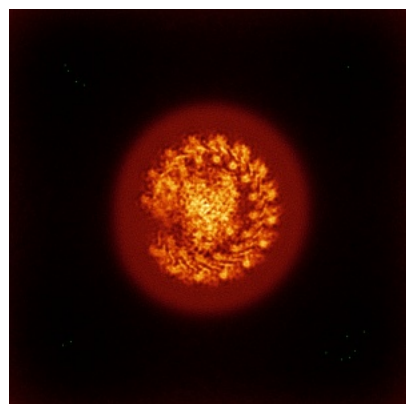


Y

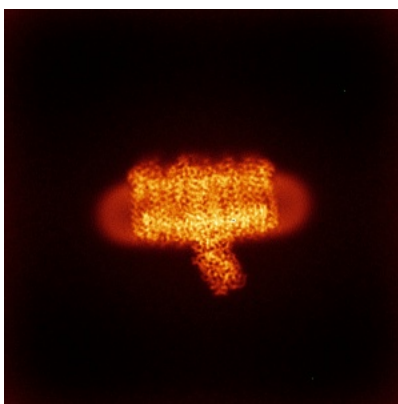


Z

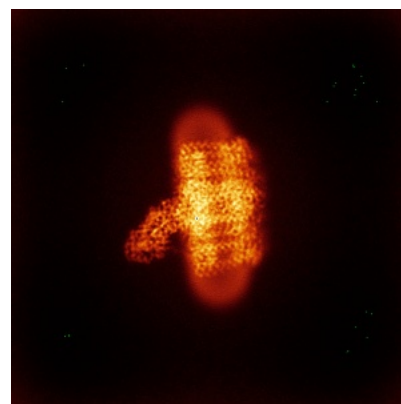
6.4.2 Raw map



X



Y

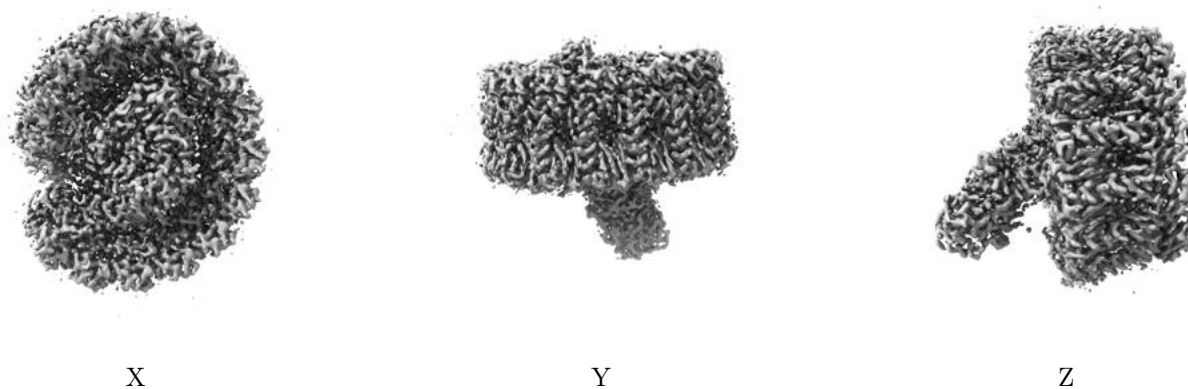


Z

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.

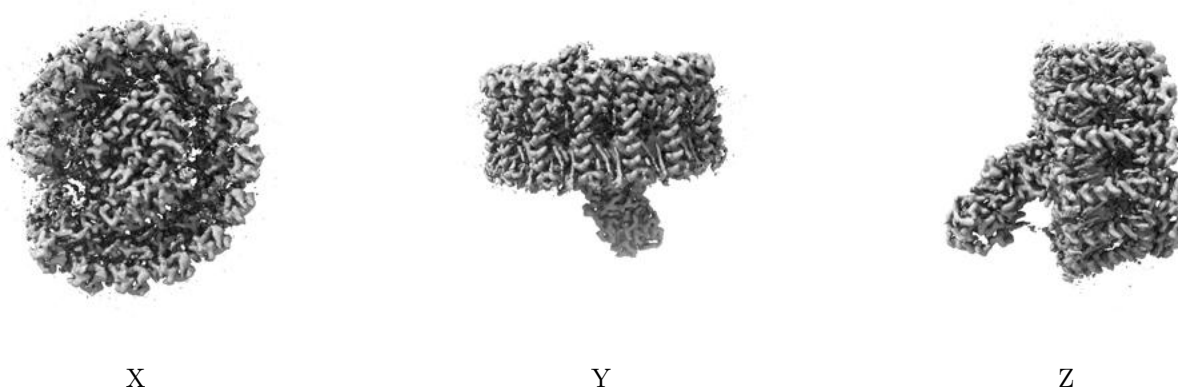
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.307. 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.

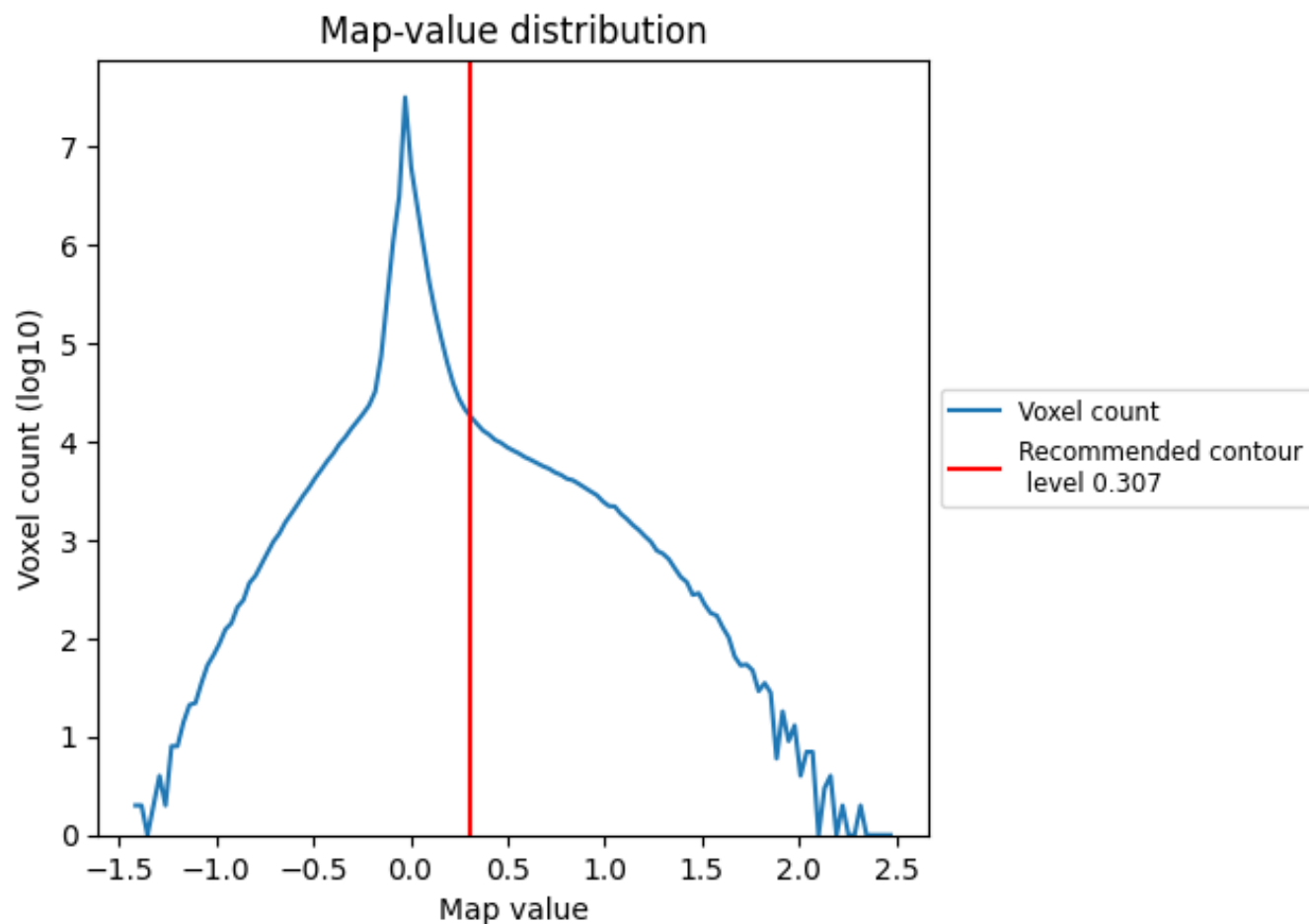
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

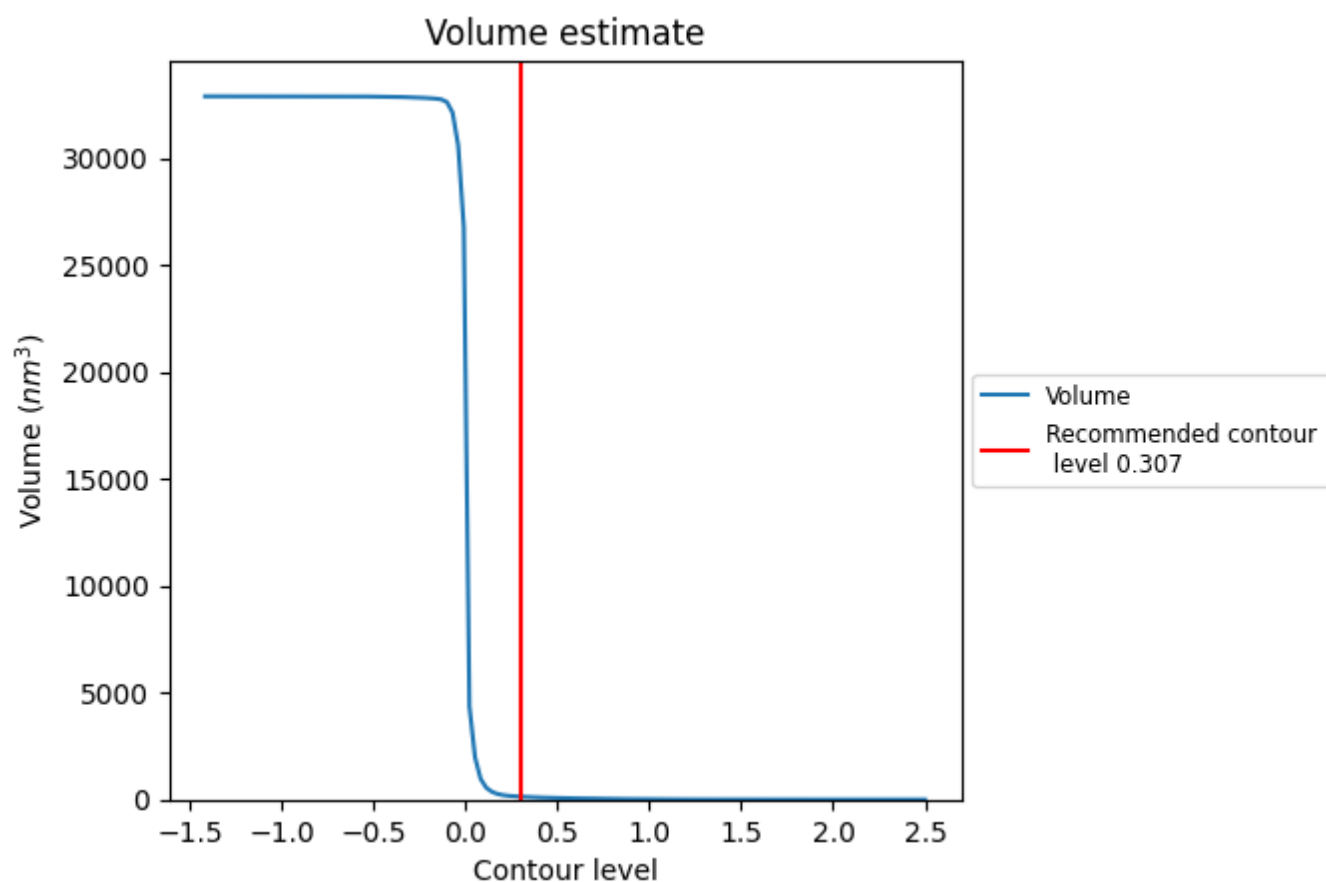
This section contains the results of statistical analysis of the map.

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.

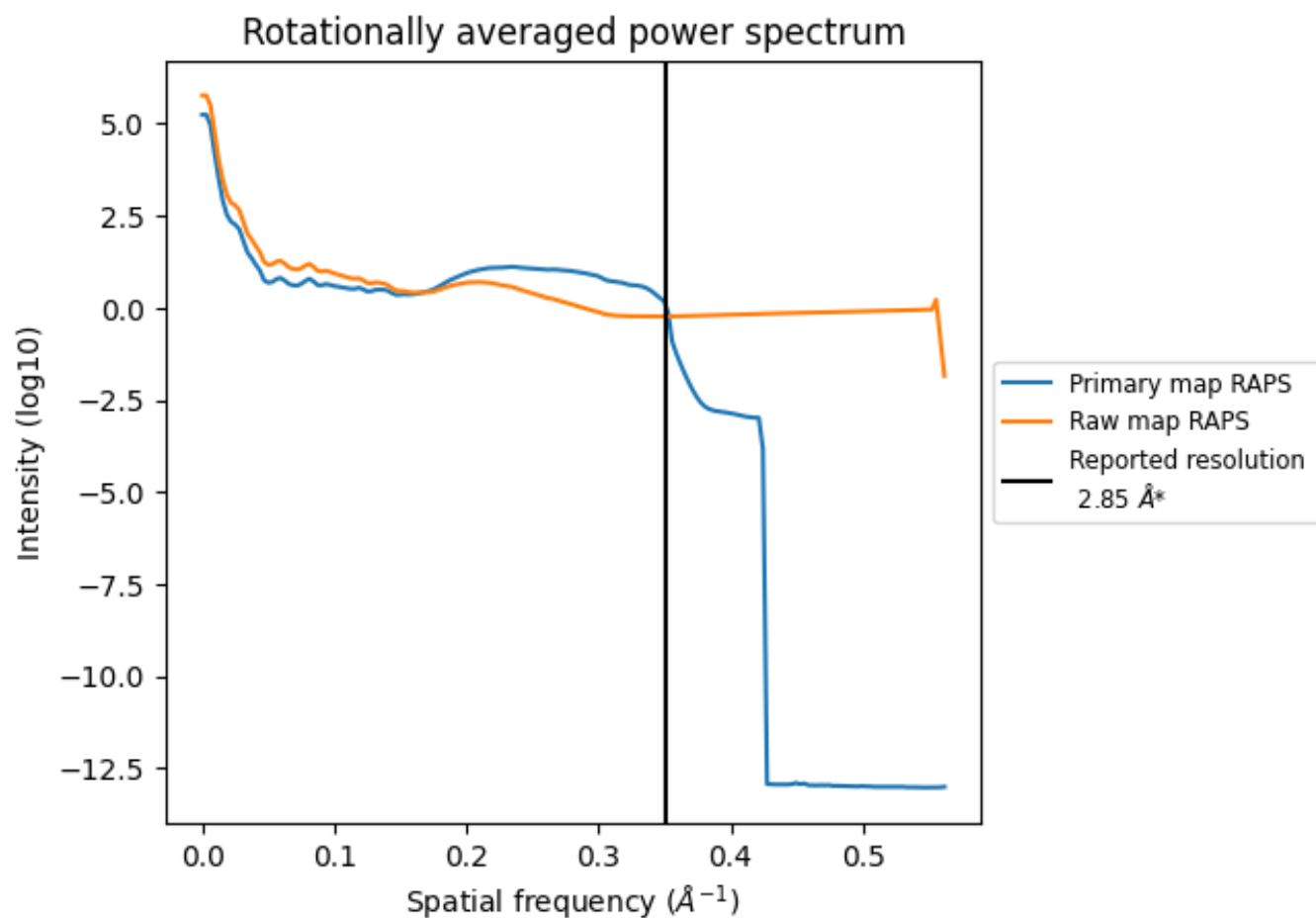
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 118 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 ⓘ

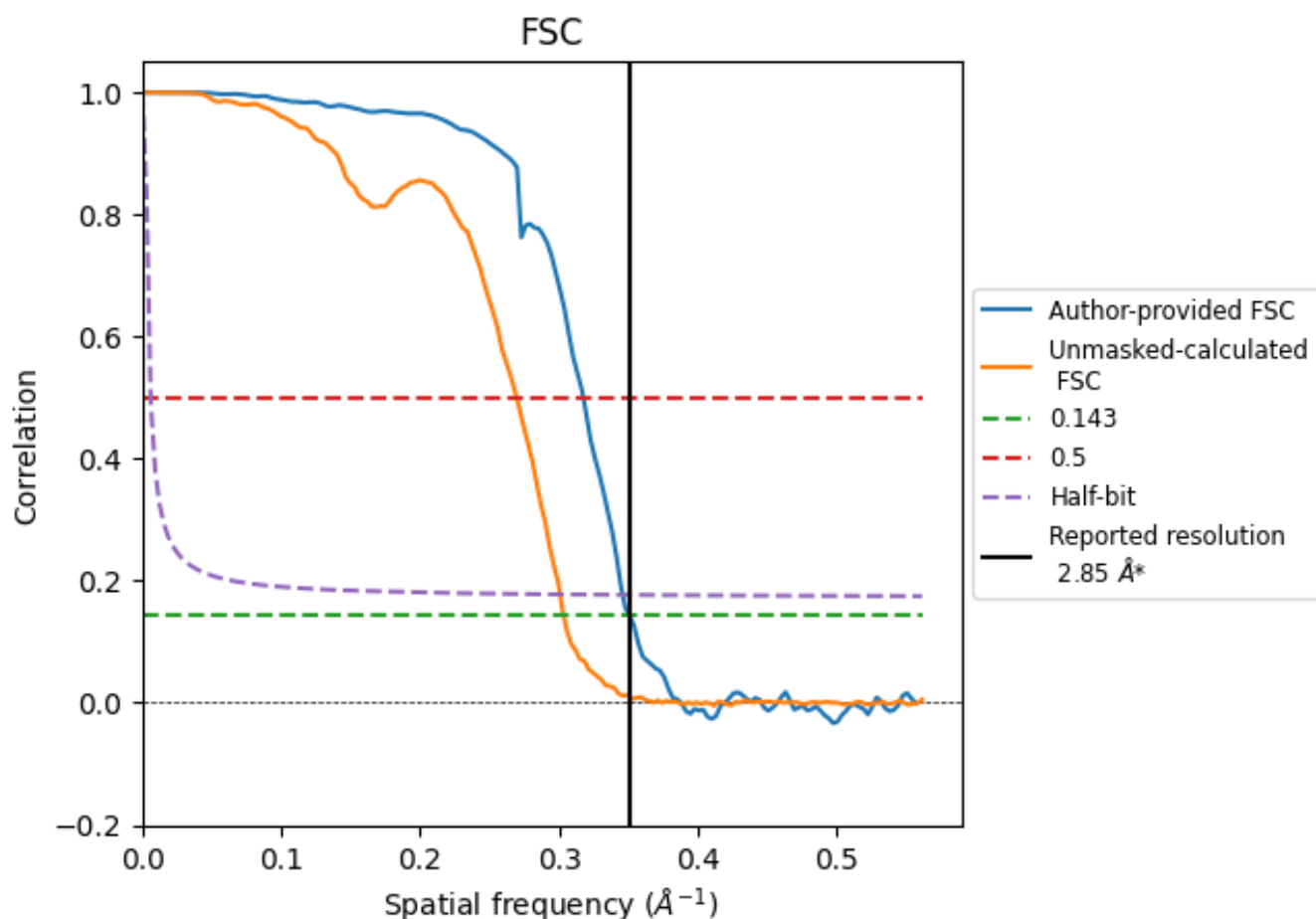


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 $0.351 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

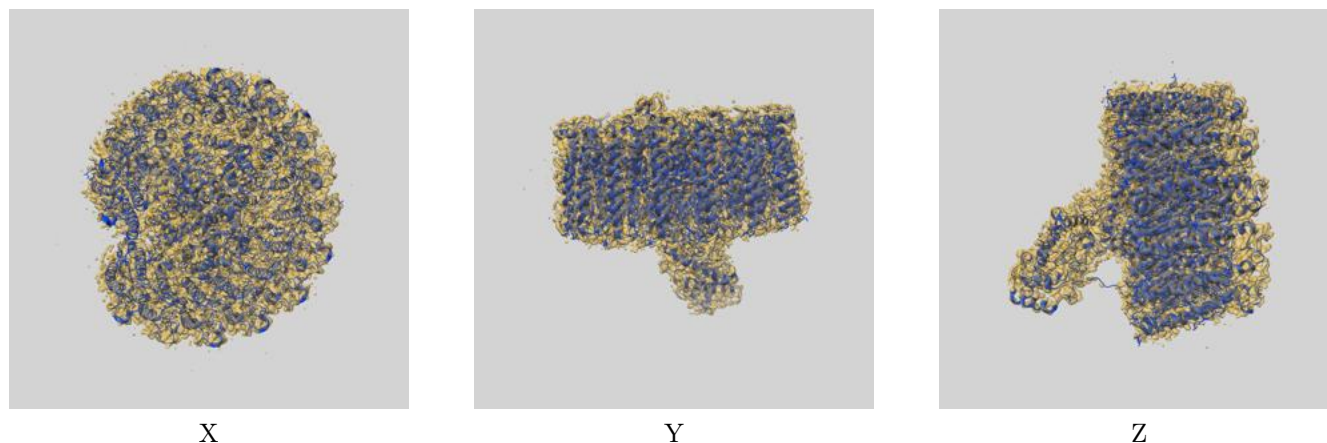
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.15	2.89
Unmasked-calculated*	3.29	3.71	3.32

*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 3.29 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

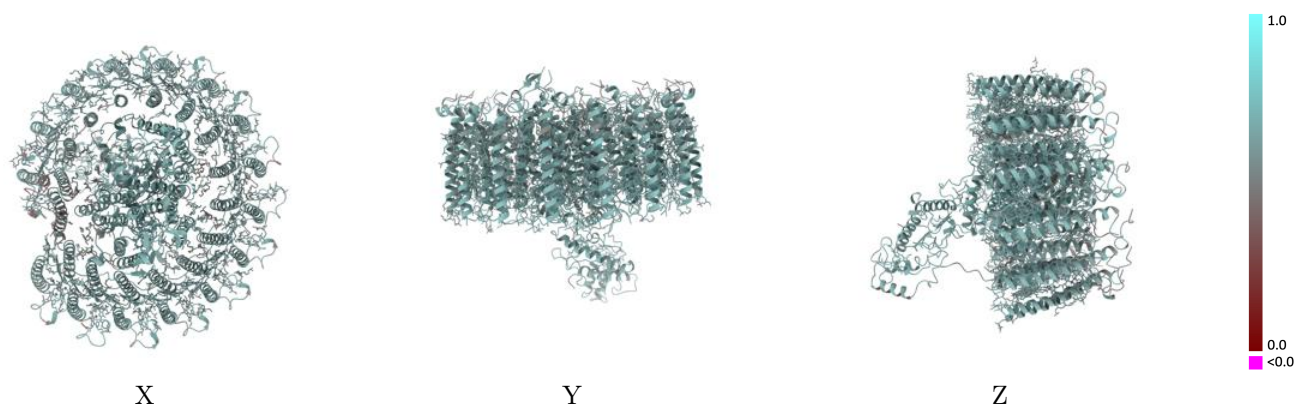
This section contains information regarding the fit between EMDB map EMD-35727 and PDB model 8IUN. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



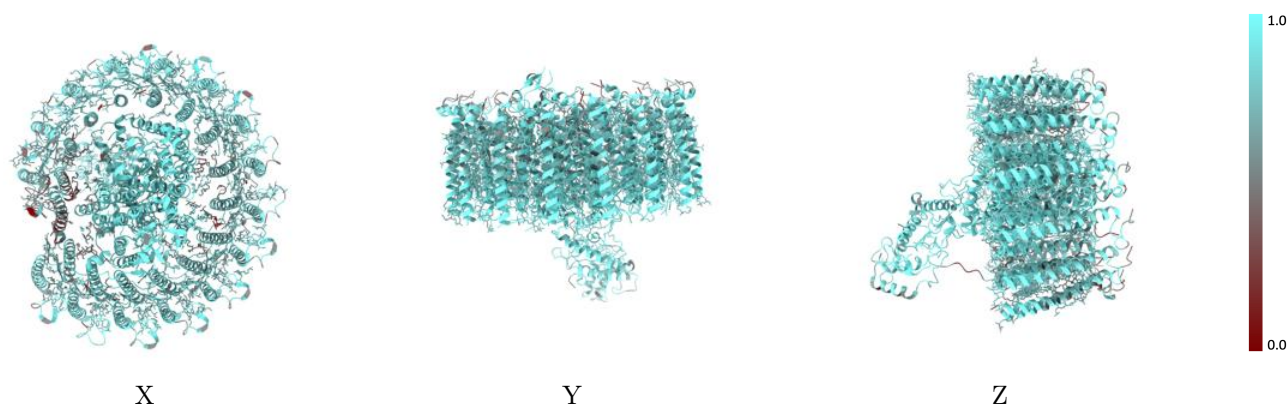
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



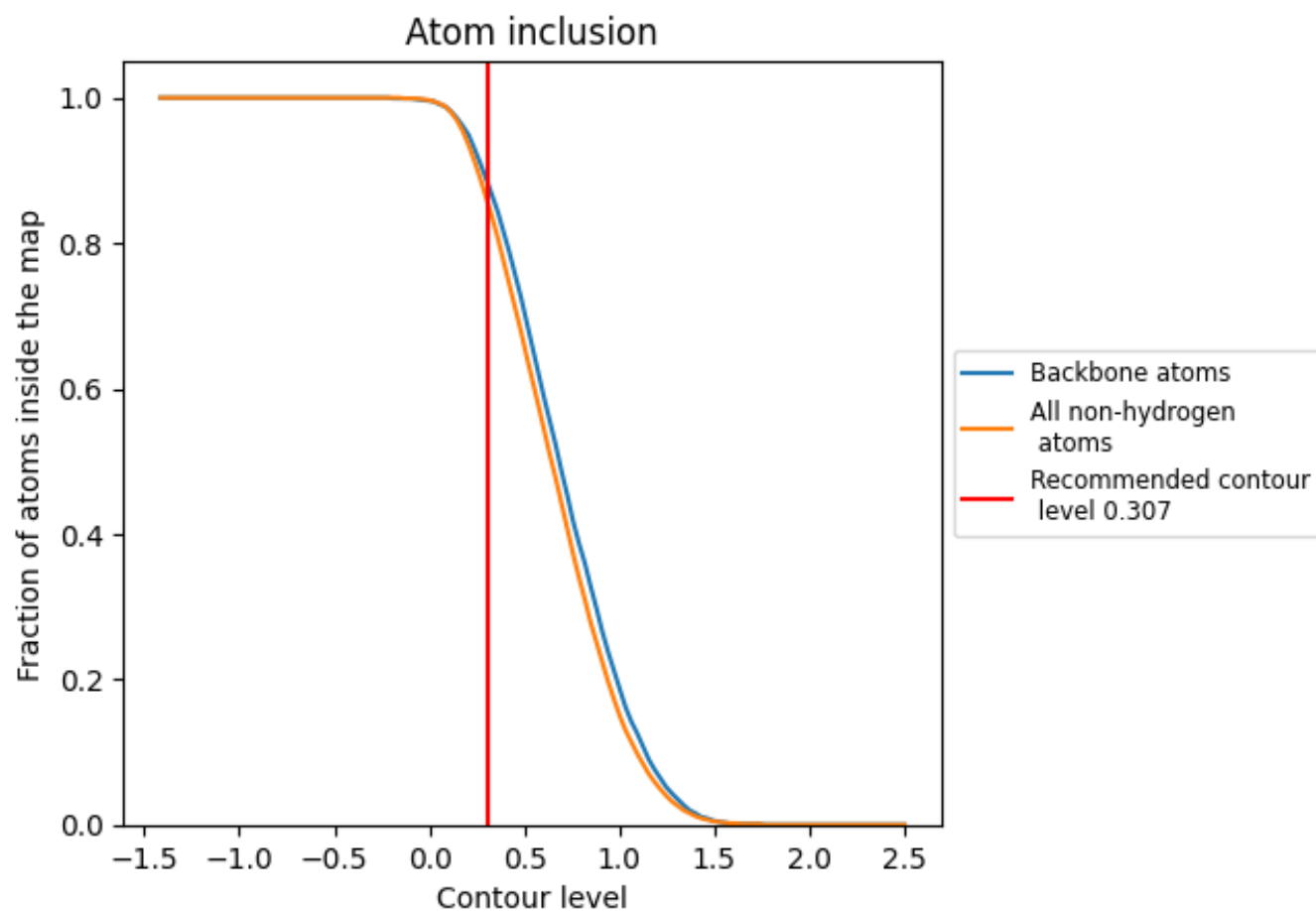
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.307).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.6130
0	 0.8280	 0.6020
1	 0.6870	 0.5670
2	 0.6600	 0.5410
3	 0.7690	 0.5950
4	 0.7800	 0.5820
5	 0.8130	 0.5950
6	 0.8250	 0.6050
7	 0.8320	 0.6040
8	 0.8370	 0.6020
9	 0.8410	 0.5980
A	 0.9260	 0.6340
B	 0.8940	 0.6170
C	 0.8680	 0.6150
D	 0.8570	 0.6190
E	 0.8290	 0.6040
F	 0.8300	 0.6040
G	 0.8440	 0.6080
H	 0.7660	 0.5880
I	 0.8210	 0.5970
J	 0.8530	 0.6170
K	 0.8160	 0.6020
L	 0.9320	 0.6380
M	 0.9460	 0.6440
N	 0.8450	 0.6170
O	 0.8350	 0.6090
P	 0.8690	 0.6180
Q	 0.8500	 0.6080
R	 0.8900	 0.6280
S	 0.8440	 0.6070
T	 0.8620	 0.6050
U	 0.8240	 0.6010
V	 0.7400	 0.5740
W	 0.7860	 0.5940
Y	 0.8450	 0.6080



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Chain	Atom inclusion	Q-score
Z	 0.9610	 0.6370
h	 0.8750	 0.6210