



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 07:15 AM JST

PDB ID : 9WQV / pdb_00009wqv
EMDB ID : EMD-66181
Title : Cryo-EM structure of LH1-RC from Rhodovulum sulfidophilum
Authors : Yue, X.-Y.; Wang, G.-L.; Yu, L.-J.
Deposited on : 2025-09-11
Resolution : 1.81 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.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)
Validation Pipeline (wwPDB-VP) : 2.50

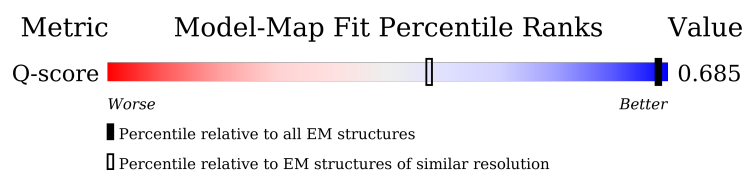
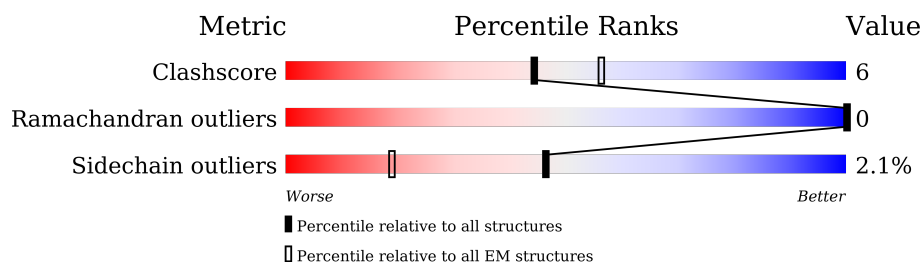
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

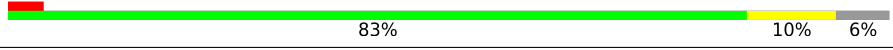
The reported resolution of this entry is 1.81 Å.

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.



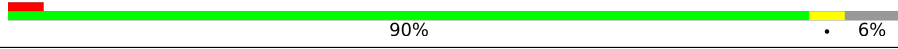
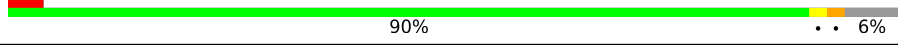
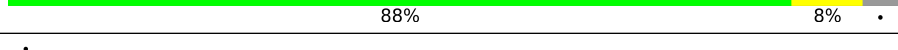
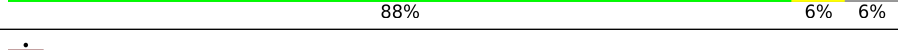
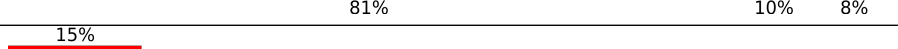
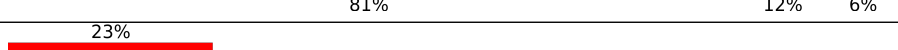
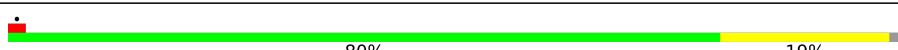
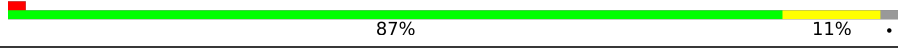
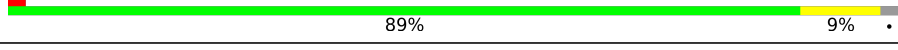
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	869 (1.31 - 2.31)

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	48	
1	2	48	
1	4	48	
1	6	48	

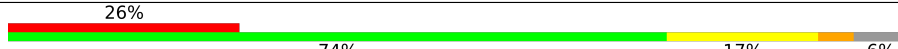
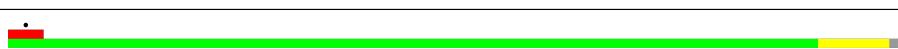
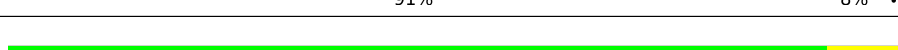
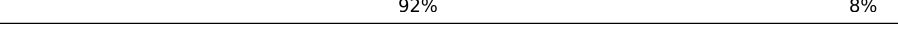
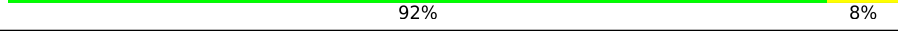
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	48	
1	B	48	
1	E	48	
1	G	48	
1	J	48	
1	N	48	
1	P	48	
1	R	48	
1	T	48	
1	V	48	
1	X	48	
1	Z	48	
2	1	54	
2	3	54	
2	5	54	
2	7	54	
2	9	54	
2	A	54	
2	D	54	
2	F	54	
2	I	54	
2	K	54	
2	O	54	
2	Q	54	
2	S	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	U	54	
2	W	54	
2	Y	54	
3	C	356	
4	H	260	
5	L	284	
6	M	321	
7	a	229	

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
14	HEC	C	401	X	-	-	-
14	HEC	C	402	X	-	-	-
14	HEC	C	403	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 28553 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 pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	2	41	Total	C	N	O	S	0	0
			326	216	53	56	1		
1	4	43	Total	C	N	O	S	0	0
			348	233	55	59	1		
1	6	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	8	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	B	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	E	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	G	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	J	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	N	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	P	46	Total	C	N	O	S	0	0
			371	245	58	67	1		
1	R	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	T	44	Total	C	N	O	S	0	0
			356	237	56	62	1		
1	V	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	X	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	Z	40	Total	C	N	O	S	0	0
			324	216	52	55	1		

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			411	283	64	62	2		
2	3	46	Total	C	N	O	S	0	0
			393	272	60	58	3		
2	5	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	7	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	9	53	Total	C	N	O	S	1	0
			443	302	71	67	3		
2	A	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	D	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	F	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	I	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	K	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	O	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Q	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	S	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	U	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	W	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Y	51	Total	C	N	O	S	0	0
			420	288	66	64	2		

- Molecule 3 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	352	Total	C	N	O	S	0	0
			2715	1701	454	541	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	260	Total	C	N	O	S	0	0
			2026	1303	341	371	11		

- Molecule 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	283	Total	C	N	O	S	0	0
			2241	1505	357	368	11		

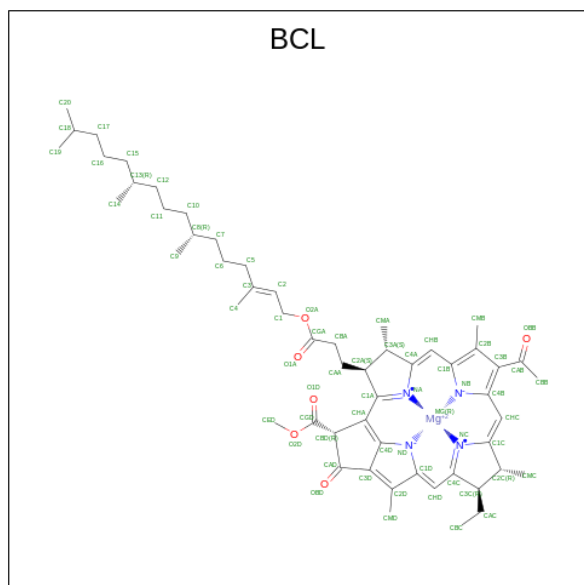
- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	317	Total	C	N	O	S	1	0
			2568	1707	415	431	15		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase 41 kd complex i subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	110	Total	C	N	O	S	0	0
			827	544	143	135	5		

- 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	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
8	4	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	6	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	8	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
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	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	F	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	I	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	K	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	L	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	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	O	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	Q	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	S	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	U	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	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

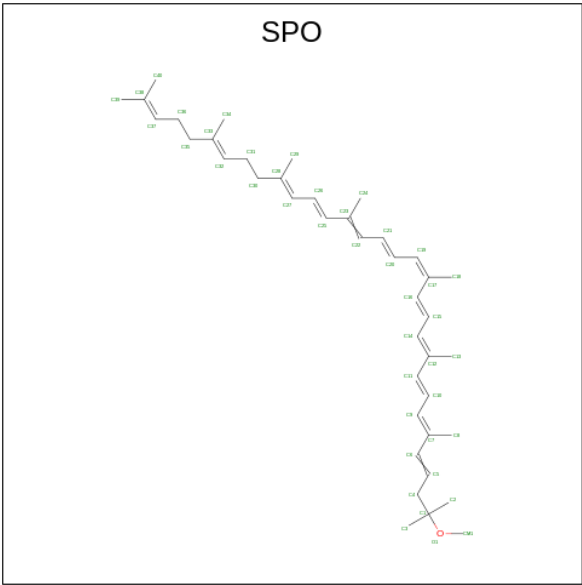
Mol	Chain	Residues	Atoms		AltConf
9	0	1	Total 18	C 18	0
9	6	1	Total 18	C 18	0
9	8	1	Total 18	C 18	0
9	B	1	Total 18	C 18	0
9	D	1	Total 18	C 18	0
9	E	1	Total 18	C 18	0
9	G	1	Total 18	C 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	J	1	Total C 18 18	0
9	N	1	Total C 18 18	0
9	P	1	Total C 18 18	0
9	R	1	Total C 18 18	0
9	T	1	Total C 18 18	0
9	V	1	Total C 18 18	0

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



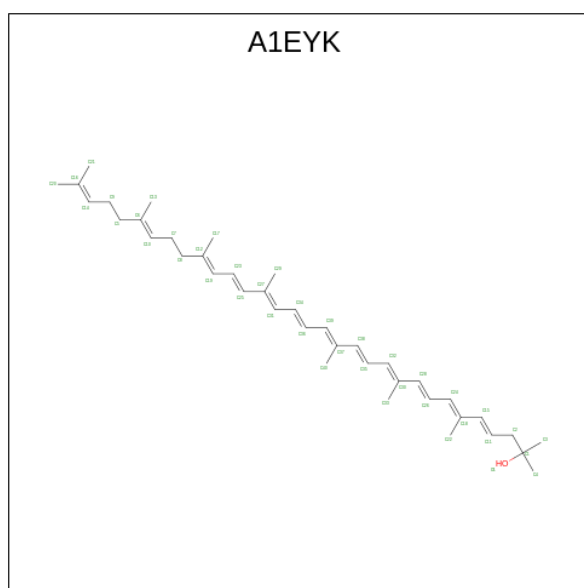
Mol	Chain	Residues	Atoms	AltConf
10	4	1	Total C O 42 41 1	0
10	5	1	Total C O 42 41 1	0
10	7	1	Total C O 42 41 1	0
10	9	1	Total C O 42 41 1	0
10	A	1	Total C O 42 41 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	D	1	Total	C	O	0
			42	41	1	
10	F	1	Total	C	O	0
			42	41	1	
10	I	1	Total	C	O	0
			42	41	1	
10	K	1	Total	C	O	0
			42	41	1	
10	M	1	Total	C	O	0
			42	41	1	
10	O	1	Total	C	O	0
			42	41	1	
10	Q	1	Total	C	O	0
			42	41	1	
10	S	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	Y	1	Total	C	O	0
			42	41	1	

- Molecule 11 is (4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},26 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-2-ol (CCD ID: A1EYK) (formula: C₄₀H₅₈O) (labeled as "Ligand of Interest" by depositor).

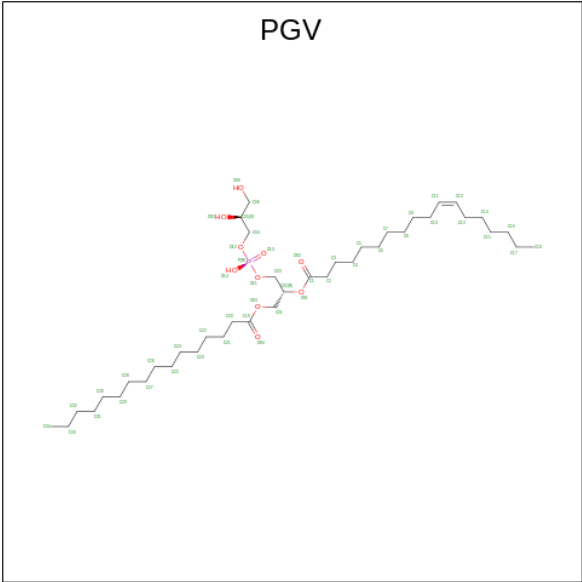


Mol	Chain	Residues	Atoms			AltConf
11	5	1	Total 41	C 40	O 1	0
11	7	1	Total 41	C 40	O 1	0
11	9	1	Total 41	C 40	O 1	0
11	A	1	Total 41	C 40	O 1	0
11	D	1	Total 41	C 40	O 1	0
11	F	1	Total 41	C 40	O 1	0
11	I	1	Total 41	C 40	O 1	0
11	K	1	Total 41	C 40	O 1	0
11	O	1	Total 41	C 40	O 1	0
11	Q	1	Total 41	C 40	O 1	0
11	S	1	Total 41	C 40	O 1	0
11	U	1	Total 41	C 40	O 1	0
11	W	1	Total 41	C 40	O 1	0
11	Z	1	Total 41	C 40	O 1	0

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



- Molecule 13 is (1R)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY](HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			47	36	10	1	
13	D	1	Total	C	O	P	0
			32	23	8	1	
13	F	1	Total	C	O	P	0
			51	40	10	1	
13	H	1	Total	C	O	P	0
			34	23	10	1	
13	H	1	Total	C	O	P	0
			33	22	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			36	27	8	1	
13	L	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			40	31	8	1	
13	M	1	Total	C	O	P	0
			45	34	10	1	
13	M	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of

HEC

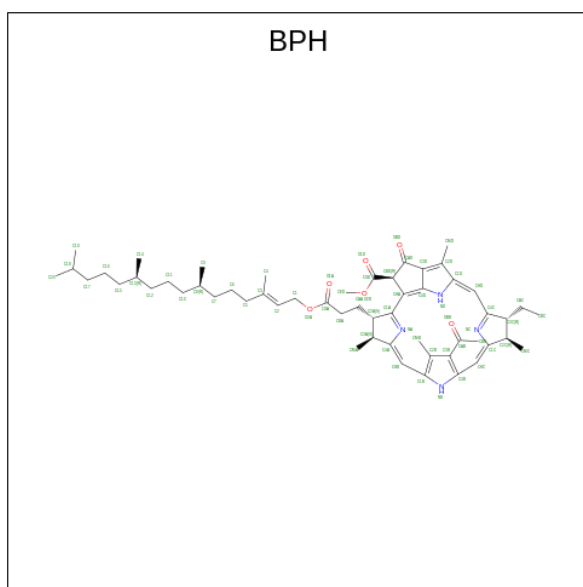
The diagram illustrates the chemical structure of the HEC (Hexaethylcyclotriphosphazene) complex. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various groups, including CMC, CAC, CBB, CMB, CHB, CMA, CAA, CBA, CAD, CBD, CGD, CGA, and CBA. The structure is labeled with various atoms and bonds, including N, Fe, C, H, O, and various substituents like CMC, CAC, CBB, CMB, CHB, CMA, CAA, CBA, CAD, CBD, CGD, CGA, and CBA.

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

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 15 | C | 2 | Total
2 | Mg
2 | 0 |
| 15 | M | 2 | Total
2 | Mg
2 | 0 |

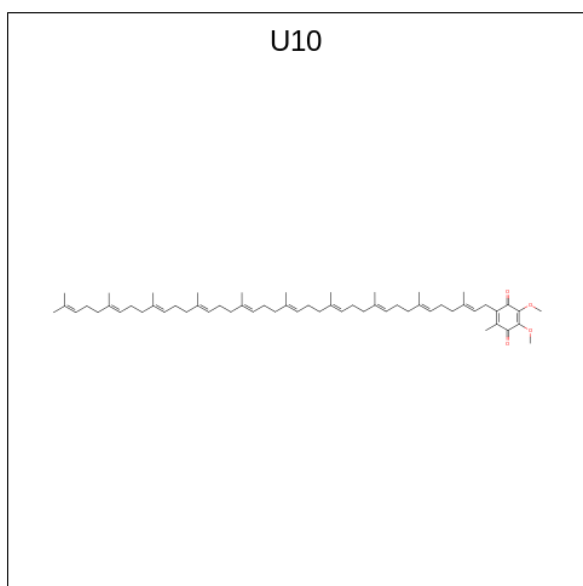
- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 16 | C | 1 | Total Fe
1 1 | 0 |
| 16 | M | 1 | Total Fe
1 1 | 0 |

- 



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

- Molecule 18 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			63	59	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C	O	0
			25	21	4	
18	M	1	Total	C	O	0
			63	59	4	
18	M	1	Total	C	O	0
			28	24	4	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	0	3	Total	O	0
			3	3	
19	6	1	Total	O	0
			1	1	
19	7	3	Total	O	0
			3	3	
19	8	2	Total	O	0
			2	2	
19	9	5	Total	O	0
			5	5	
19	A	12	Total	O	0
			12	12	
19	B	7	Total	O	0
			7	7	
19	C	184	Total	O	0
			184	184	
19	D	5	Total	O	0
			5	5	
19	E	2	Total	O	0
			2	2	
19	F	6	Total	O	0
			6	6	
19	G	2	Total	O	0
			2	2	
19	H	65	Total	O	0
			65	65	
19	I	10	Total	O	0
			10	10	
19	J	4	Total	O	0
			4	4	
19	K	8	Total	O	0
			8	8	

Continued on next page...

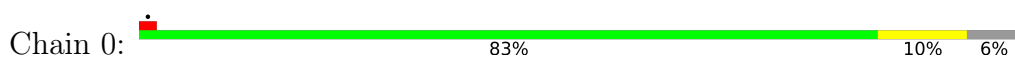
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
19	L	57	Total 57	O 57	0
19	M	76	Total 76	O 76	0
19	N	5	Total 5	O 5	0
19	O	5	Total 5	O 5	0
19	P	3	Total 3	O 3	0
19	Q	11	Total 11	O 11	0
19	R	2	Total 2	O 2	0
19	S	14	Total 14	O 14	0
19	T	2	Total 2	O 2	0
19	U	7	Total 7	O 7	0
19	V	1	Total 1	O 1	0

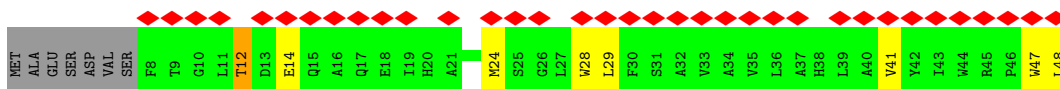
3 Residue-property plots [i](#)

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.

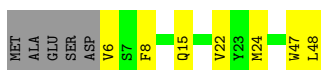
- Molecule 1: Antenna pigment protein beta chain



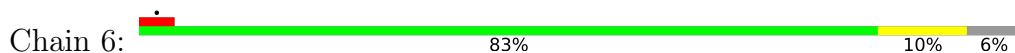
- Molecule 1: Antenna pigment protein beta chain



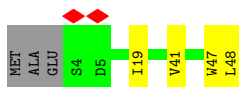
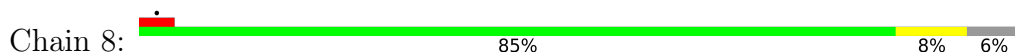
- Molecule 1: Antenna pigment protein beta chain



- Molecule 1: Antenna pigment protein beta chain

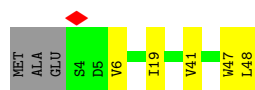


- Molecule 1: Antenna pigment protein beta chain



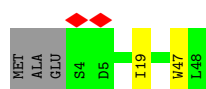
- Molecule 1: Antenna pigment protein beta chain

Chain B:  83% 10% 6%



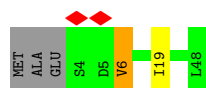
- Molecule 1: Antenna pigment protein beta chain

Chain E:  90% 6% 6%



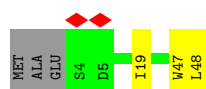
- Molecule 1: Antenna pigment protein beta chain

Chain G:  90% 6% 6%



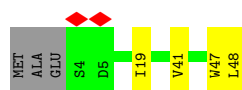
- Molecule 1: Antenna pigment protein beta chain

Chain J:  88% 6% 6%



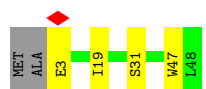
- Molecule 1: Antenna pigment protein beta chain

Chain N:  85% 8% 6%



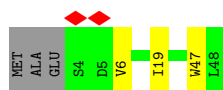
- Molecule 1: Antenna pigment protein beta chain

Chain P:  88% 8% 6%

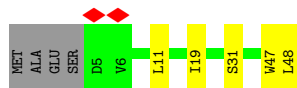
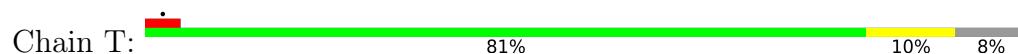


- Molecule 1: Antenna pigment protein beta chain

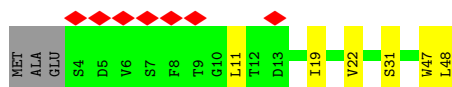
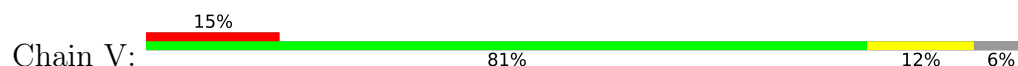
Chain R:  88% 6% 6%



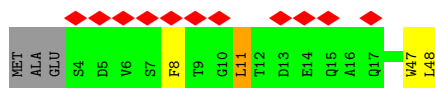
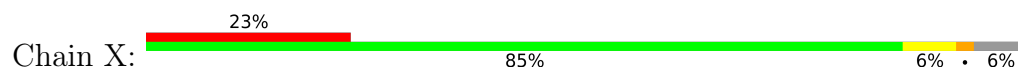
- Molecule 1: Antenna pigment protein beta chain



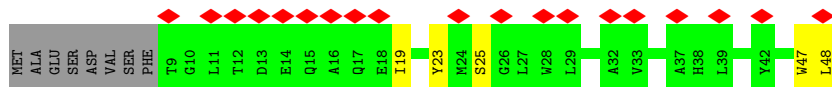
- Molecule 1: Antenna pigment protein beta chain



- Molecule 1: Antenna pigment protein beta chain



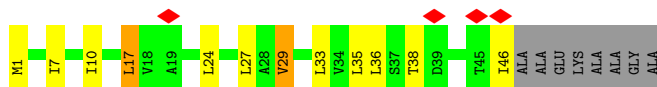
- Molecule 1: Antenna pigment protein beta chain



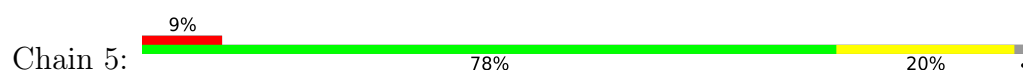
- Molecule 2: Antenna pigment protein alpha chain



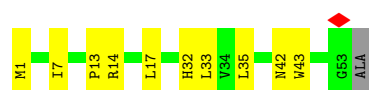
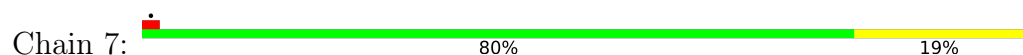
- Molecule 2: Antenna pigment protein alpha chain



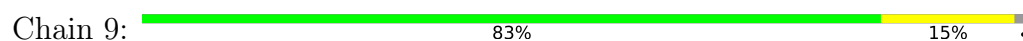
- Molecule 2: Antenna pigment protein alpha chain



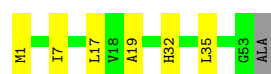
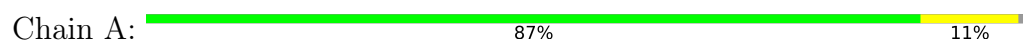
- Molecule 2: Antenna pigment protein alpha chain



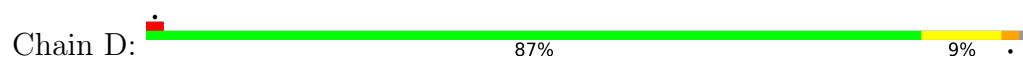
- Molecule 2: Antenna pigment protein alpha chain



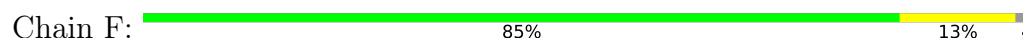
- Molecule 2: Antenna pigment protein alpha chain



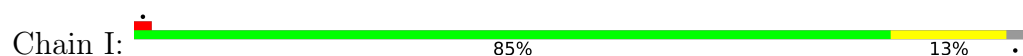
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

Chain K:  87% 11%



- Molecule 2: Antenna pigment protein alpha chain

Chain O:  89% 9%



- Molecule 2: Antenna pigment protein alpha chain

Chain Q:  83% 15%



- Molecule 2: Antenna pigment protein alpha chain

Chain S:  85% 13%



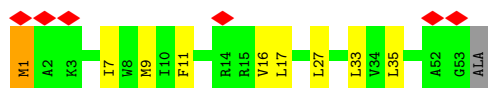
- Molecule 2: Antenna pigment protein alpha chain

Chain U:  85% 11%



- Molecule 2: Antenna pigment protein alpha chain

Chain W:  11% 81% 15%

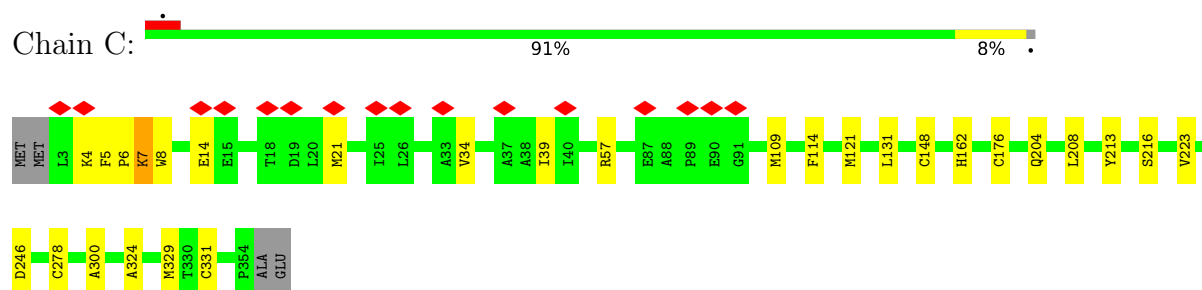


- Molecule 2: Antenna pigment protein alpha chain

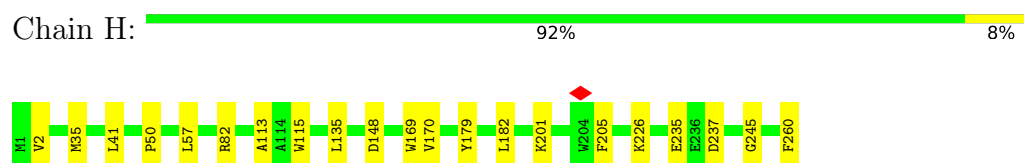
Chain Y:  26% 74% 17% 6%



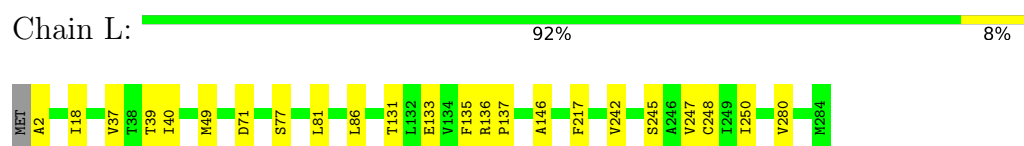
- Molecule 3: Photosynthetic reaction center cytochrome c subunit



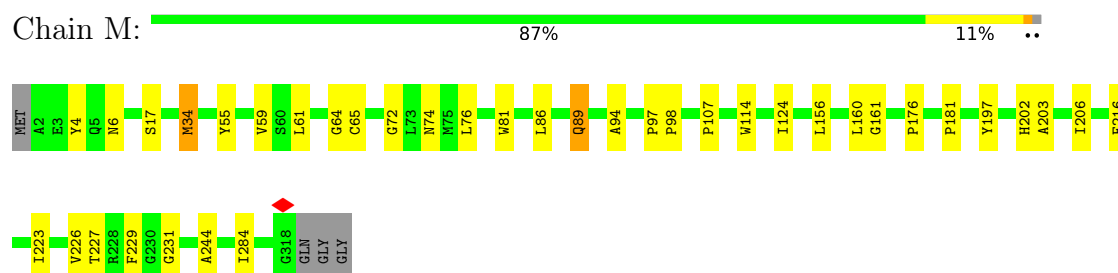
- Molecule 4: photosynthetic reaction center subunit H



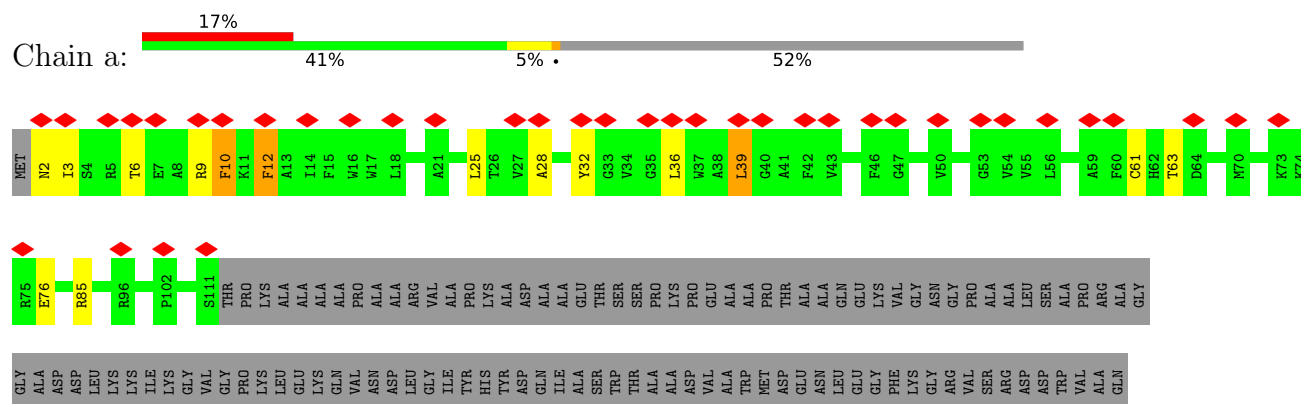
- Molecule 5: Reaction center protein L chain



- Molecule 6: Reaction center protein M chain



- Molecule 7: NADH:ubiquinone oxidoreductase 41 kd complex i subunit



ALA
ARG
ALA
LEU
ALA
LYS
GLU
GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.609	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0519	Depositor
Map size ($\text{\AA}$)	372.224, 372.224, 372.224	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.727, 0.727, 0.727	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: UNL, MG, U10, LMT, FME, BCL, HEC, A1EYK, BPH, FE, SPO, PGV

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	0.09	0/374	0.19	0/512
1	2	0.11	0/337	0.41	0/462
1	4	0.08	0/360	0.23	0/493
1	6	0.08	0/374	0.18	0/512
1	8	0.09	0/374	0.18	0/512
1	B	0.09	0/374	0.19	0/512
1	E	0.09	0/374	0.18	0/512
1	G	0.09	0/374	0.18	0/512
1	J	0.09	0/374	0.18	0/512
1	N	0.09	0/374	0.19	0/512
1	P	0.08	0/383	0.18	0/524
1	R	0.08	0/374	0.18	0/512
1	T	0.10	0/368	0.20	0/504
1	V	0.09	0/374	0.19	0/512
1	X	0.08	0/374	0.21	0/512
1	Z	0.10	0/335	0.29	0/459
2	1	0.09	0/423	0.28	0/574
2	3	0.08	0/395	0.24	0/537
2	5	0.10	0/437	0.21	0/593
2	7	0.09	0/437	0.23	0/593
2	9	0.10	0/448	0.23	0/607
2	A	0.10	0/437	0.22	0/593
2	D	0.10	0/437	0.21	0/593
2	F	0.11	0/437	0.22	0/593
2	I	0.10	0/437	0.20	0/593
2	K	0.10	0/437	0.21	0/593
2	O	0.10	0/437	0.21	0/593
2	Q	0.11	0/437	0.25	0/593
2	S	0.09	0/437	0.22	0/593
2	U	0.08	0/437	0.22	0/593
2	W	0.08	0/437	0.25	0/593
2	Y	0.08	0/432	0.32	0/586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	C	0.12	0/2782	0.30	0/3795
4	H	0.13	0/2084	0.26	0/2827
5	L	0.12	0/2330	0.28	0/3183
6	M	0.13	0/2667	0.29	0/3642
7	a	0.11	0/852	0.31	0/1161
All	All	0.11	0/23554	0.25	0/32102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	362	0	347	4	0
1	2	326	0	308	5	0
1	4	348	0	338	8	0
1	6	362	0	347	5	0
1	8	362	0	347	7	0
1	B	362	0	347	5	0
1	E	362	0	347	3	0
1	G	362	0	347	2	0
1	J	362	0	347	4	0
1	N	362	0	347	4	0
1	P	371	0	353	3	0
1	R	362	0	347	3	0
1	T	356	0	342	5	0
1	V	362	0	347	5	0
1	X	362	0	347	4	0
1	Z	324	0	315	5	0
2	1	411	0	431	11	0
2	3	393	0	413	14	0
2	5	435	0	455	9	0
2	7	435	0	455	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	443	0	468	7	0
2	A	435	0	455	5	0
2	D	435	0	455	5	0
2	F	435	0	455	5	0
2	I	435	0	455	7	0
2	K	435	0	455	7	0
2	O	435	0	455	4	0
2	Q	435	0	455	7	0
2	S	435	0	455	5	0
2	U	435	0	455	6	0
2	W	435	0	455	9	0
2	Y	420	0	439	9	0
3	C	2715	0	2561	24	0
4	H	2026	0	1992	14	0
5	L	2241	0	2176	17	0
6	M	2568	0	2469	28	0
7	a	827	0	841	11	0
8	0	66	0	74	5	0
8	1	66	0	74	7	0
8	2	66	0	74	3	0
8	3	47	0	35	0	0
8	4	66	0	74	5	0
8	5	66	0	74	6	0
8	6	66	0	74	3	0
8	7	66	0	74	2	0
8	8	66	0	74	6	0
8	9	66	0	74	2	0
8	A	66	0	74	3	0
8	B	66	0	74	6	0
8	D	66	0	74	2	0
8	E	66	0	74	5	0
8	F	66	0	74	1	0
8	G	66	0	74	4	0
8	I	66	0	74	0	0
8	J	66	0	74	3	0
8	K	66	0	74	2	0
8	L	198	0	222	7	0
8	M	66	0	74	4	0
8	N	66	0	74	4	0
8	O	66	0	74	2	0
8	P	66	0	74	5	0
8	Q	66	0	74	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	66	0	74	5	0
8	S	66	0	74	1	0
8	T	66	0	74	6	0
8	U	66	0	74	2	0
8	V	66	0	74	5	0
8	W	66	0	74	0	0
8	X	66	0	74	8	0
8	Y	66	0	74	2	0
8	Z	66	0	74	5	0
9	0	18	0	0	0	0
9	6	18	0	0	0	0
9	8	18	0	0	0	0
9	B	18	0	0	0	0
9	D	18	0	0	0	0
9	E	18	0	0	0	0
9	G	18	0	0	0	0
9	J	18	0	0	0	0
9	N	18	0	0	0	0
9	P	18	0	0	0	0
9	R	18	0	0	0	0
9	T	18	0	0	0	0
9	V	18	0	0	0	0
10	4	42	0	60	13	0
10	5	42	0	60	4	0
10	7	42	0	60	6	0
10	9	42	0	60	4	0
10	A	42	0	60	9	0
10	D	42	0	60	7	0
10	F	42	0	60	5	0
10	I	42	0	60	4	0
10	K	42	0	60	5	0
10	M	42	0	60	4	0
10	O	42	0	60	7	0
10	Q	42	0	60	4	0
10	S	42	0	60	5	0
10	U	84	0	120	11	0
10	Y	42	0	60	10	0
11	5	41	0	0	0	0
11	7	41	0	0	0	0
11	9	41	0	0	0	0
11	A	41	0	0	0	0
11	D	41	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	41	0	0	0	0
11	I	41	0	0	0	0
11	K	41	0	0	0	0
11	O	41	0	0	0	0
11	Q	41	0	0	0	0
11	S	41	0	0	0	0
11	U	41	0	0	0	0
11	W	41	0	0	0	0
11	Z	41	0	0	0	0
12	7	27	0	27	4	0
12	9	27	0	27	1	0
12	D	35	0	46	2	0
12	F	28	0	29	0	0
12	K	27	0	27	1	0
12	L	54	0	54	0	0
12	M	53	0	64	0	0
12	O	27	0	27	0	0
13	A	47	0	65	3	0
13	D	32	0	38	1	0
13	F	51	0	76	2	0
13	H	187	0	229	6	0
13	L	43	0	59	2	0
13	M	161	0	200	4	0
14	C	129	0	92	8	0
15	C	2	0	0	0	0
15	M	2	0	0	0	0
16	C	1	0	0	0	0
16	M	1	0	0	0	0
17	L	65	0	76	5	0
17	M	65	0	76	6	0
18	L	63	0	90	4	0
18	M	116	0	148	6	0
19	0	3	0	0	0	0
19	6	1	0	0	0	0
19	7	3	0	0	0	0
19	8	2	0	0	0	0
19	9	5	0	0	0	0
19	A	12	0	0	0	0
19	B	7	0	0	0	0
19	C	184	0	0	1	0
19	D	5	0	0	0	0
19	E	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	F	6	0	0	0	0
19	G	2	0	0	0	0
19	H	65	0	0	0	0
19	I	10	0	0	0	0
19	J	4	0	0	0	0
19	K	8	0	0	0	0
19	L	57	0	0	0	0
19	M	76	0	0	0	0
19	N	5	0	0	0	0
19	O	5	0	0	0	0
19	P	3	0	0	0	0
19	Q	11	0	0	0	0
19	R	2	0	0	0	0
19	S	14	0	0	0	0
19	T	2	0	0	0	0
19	U	7	0	0	0	0
19	V	1	0	0	0	0
All	All	28553	0	27758	357	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 357 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:C:278:CYS:SG	14:C:402:HEC:HAC	1.77	1.24
3:C:278:CYS:SG	14:C:402:HEC:CAC	2.30	1.19
3:C:331:CYS:SG	14:C:403:HEC:CAC	2.50	1.00
3:C:331:CYS:SG	14:C:403:HEC:HAC	2.05	0.95
3:C:204:GLN:OE1	19:C:502:HOH:O	1.89	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	43/48 (90%)	43 (100%)	0	0	100	100
1	2	39/48 (81%)	37 (95%)	2 (5%)	0	100	100
1	4	41/48 (85%)	41 (100%)	0	0	100	100
1	6	43/48 (90%)	43 (100%)	0	0	100	100
1	8	43/48 (90%)	43 (100%)	0	0	100	100
1	B	43/48 (90%)	43 (100%)	0	0	100	100
1	E	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	G	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	J	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	N	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	P	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	R	43/48 (90%)	43 (100%)	0	0	100	100
1	T	42/48 (88%)	42 (100%)	0	0	100	100
1	V	43/48 (90%)	43 (100%)	0	0	100	100
1	X	43/48 (90%)	43 (100%)	0	0	100	100
1	Z	38/48 (79%)	35 (92%)	3 (8%)	0	100	100
2	1	47/54 (87%)	47 (100%)	0	0	100	100
2	3	44/54 (82%)	44 (100%)	0	0	100	100
2	5	51/54 (94%)	51 (100%)	0	0	100	100
2	7	51/54 (94%)	51 (100%)	0	0	100	100
2	9	52/54 (96%)	52 (100%)	0	0	100	100
2	A	51/54 (94%)	51 (100%)	0	0	100	100
2	D	51/54 (94%)	51 (100%)	0	0	100	100
2	F	51/54 (94%)	51 (100%)	0	0	100	100
2	I	51/54 (94%)	51 (100%)	0	0	100	100
2	K	51/54 (94%)	51 (100%)	0	0	100	100
2	O	51/54 (94%)	51 (100%)	0	0	100	100
2	Q	51/54 (94%)	51 (100%)	0	0	100	100
2	S	51/54 (94%)	51 (100%)	0	0	100	100
2	U	51/54 (94%)	51 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	51/54 (94%)	51 (100%)	0	0	100	100
2	Y	49/54 (91%)	49 (100%)	0	0	100	100
3	C	350/356 (98%)	341 (97%)	9 (3%)	0	100	100
4	H	258/260 (99%)	254 (98%)	4 (2%)	0	100	100
5	L	281/284 (99%)	275 (98%)	6 (2%)	0	100	100
6	M	316/321 (98%)	308 (98%)	8 (2%)	0	100	100
7	a	108/229 (47%)	107 (99%)	1 (1%)	0	100	100
All	All	2794/3082 (91%)	2756 (99%)	38 (1%)	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	37/39 (95%)	37 (100%)	0	100	100
1	2	31/39 (80%)	28 (90%)	3 (10%)	8	0
1	4	35/39 (90%)	35 (100%)	0	100	100
1	6	37/39 (95%)	37 (100%)	0	100	100
1	8	37/39 (95%)	37 (100%)	0	100	100
1	B	37/39 (95%)	37 (100%)	0	100	100
1	E	37/39 (95%)	37 (100%)	0	100	100
1	G	37/39 (95%)	36 (97%)	1 (3%)	39	22
1	J	37/39 (95%)	37 (100%)	0	100	100
1	N	37/39 (95%)	37 (100%)	0	100	100
1	P	38/39 (97%)	37 (97%)	1 (3%)	40	23
1	R	37/39 (95%)	36 (97%)	1 (3%)	39	22
1	T	36/39 (92%)	35 (97%)	1 (3%)	38	21
1	V	37/39 (95%)	37 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	37/39 (95%)	36 (97%)	1 (3%)	39	22
1	Z	32/39 (82%)	32 (100%)	0	100	100
2	1	43/43 (100%)	37 (86%)	6 (14%)	3	0
2	3	41/43 (95%)	37 (90%)	4 (10%)	7	0
2	5	43/43 (100%)	42 (98%)	1 (2%)	44	28
2	7	43/43 (100%)	43 (100%)	0	100	100
2	9	44/43 (102%)	43 (98%)	1 (2%)	44	28
2	A	43/43 (100%)	43 (100%)	0	100	100
2	D	43/43 (100%)	42 (98%)	1 (2%)	44	28
2	F	43/43 (100%)	43 (100%)	0	100	100
2	I	43/43 (100%)	43 (100%)	0	100	100
2	K	43/43 (100%)	43 (100%)	0	100	100
2	O	43/43 (100%)	43 (100%)	0	100	100
2	Q	43/43 (100%)	43 (100%)	0	100	100
2	S	43/43 (100%)	42 (98%)	1 (2%)	44	28
2	U	43/43 (100%)	42 (98%)	1 (2%)	44	28
2	W	43/43 (100%)	43 (100%)	0	100	100
2	Y	43/43 (100%)	39 (91%)	4 (9%)	8	1
3	C	295/298 (99%)	289 (98%)	6 (2%)	48	35
4	H	210/210 (100%)	207 (99%)	3 (1%)	59	49
5	L	224/225 (100%)	221 (99%)	3 (1%)	61	50
6	M	256/257 (100%)	252 (98%)	4 (2%)	55	44
7	a	80/162 (49%)	73 (91%)	7 (9%)	9	1
All	All	2331/2464 (95%)	2281 (98%)	50 (2%)	46	32

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	248	CYS
2	S	26	LEU
7	a	76	GLU
6	M	34	MET
6	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	a	2	ASN
1	T	15	GLN
6	M	25	ASN
5	L	240	ASN
6	M	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	5	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	S	1	2	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
2	FME	D	1	2	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
2	FME	9	1	2	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
2	FME	7	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	I	1	2	8,9,10	0.50	0	7,9,11	0.95	1 (14%)
2	FME	F	1	2	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
2	FME	U	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	O	1	2	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
2	FME	Q	1	2	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
2	FME	W	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	K	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	A	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	3	1	2	8,9,10	0.51	0	7,9,11	1.26	1 (14%)

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	1	FME	O-C-CA	-2.57	118.05	124.78
2	Q	1	FME	O-C-CA	-2.56	118.07	124.78
2	W	1	FME	O-C-CA	-2.52	118.18	124.78
2	7	1	FME	O-C-CA	-2.51	118.21	124.78
2	K	1	FME	O-C-CA	-2.50	118.24	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	1	FME	CB-CA-N-CN
2	7	1	FME	O1-CN-N-CA
2	7	1	FME	CB-CA-N-CN
2	9	1	FME	O1-CN-N-CA
2	A	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 13 are unknown and 6 are monoatomic - leaving 98 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	$\# Z > 2$
10	SPO	Y	102	-	40,41,41	0.64	0	47,50,50	1.84	11 (23%)
10	SPO	O	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
8	BCL	6	101	1	69,74,74	1.78	17 (24%)	83,115,115	2.44	26 (31%)
12	LMT	K	104	-	28,28,36	0.45	0	39,39,47	0.79	1 (2%)
12	LMT	F	104	-	29,29,36	0.48	0	40,40,47	1.16	4 (10%)
8	BCL	7	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.50	27 (32%)
10	SPO	U	104	-	40,41,41	0.64	0	47,50,50	1.73	13 (27%)
8	BCL	K	101	2	69,74,74	1.79	17 (24%)	83,115,115	2.57	25 (30%)
8	BCL	T	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.47	25 (30%)
11	A1EYK	F	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.82	1 (2%)
18	U10	M	402	-	25,25,63	0.90	2 (8%)	30,33,79	0.73	0
12	LMT	L	305	-	28,28,36	0.49	0	39,39,47	1.13	5 (12%)
11	A1EYK	5	103	-	39,40,40	1.73	11 (28%)	47,49,49	0.85	0
8	BCL	1	101	2	69,74,74	1.84	17 (24%)	83,115,115	2.38	22 (26%)
8	BCL	F	101	2	69,74,74	1.78	17 (24%)	83,115,115	2.55	27 (32%)
8	BCL	B	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.43	22 (26%)
8	BCL	R	101	1	69,74,74	1.76	17 (24%)	83,115,115	2.43	25 (30%)
11	A1EYK	Z	101	-	39,40,40	1.69	10 (25%)	47,49,49	1.31	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SPO	A	102	-	40,41,41	0.63	0	47,50,50	1.63	10 (21%)
8	BCL	G	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.42	25 (30%)
12	LMT	M	414	-	29,29,36	0.46	0	40,40,47	0.69	1 (2%)
8	BCL	Y	101	2	69,74,74	1.83	17 (24%)	83,115,115	2.45	20 (24%)
8	BCL	D	102	2	69,74,74	1.77	17 (24%)	83,115,115	2.57	28 (33%)
11	A1EYK	W	102	-	39,40,40	1.80	10 (25%)	47,49,49	1.56	6 (12%)
8	BCL	O	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.58	27 (32%)
13	PGV	H	301	-	33,33,50	1.12	2 (6%)	36,39,56	1.19	3 (8%)
11	A1EYK	S	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.83	0
13	PGV	M	407	-	39,39,50	1.06	2 (5%)	43,44,56	1.22	4 (9%)
8	BCL	0	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.43	26 (31%)
8	BCL	E	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.44	23 (27%)
10	SPO	5	102	-	40,41,41	0.63	0	47,50,50	1.71	11 (23%)
17	BPH	M	404	-	59,70,70	0.73	3 (5%)	61,101,101	0.93	3 (4%)
10	SPO	9	102	-	40,41,41	0.62	0	47,50,50	1.66	10 (21%)
18	U10	L	303	-	63,63,63	0.58	2 (3%)	76,79,79	0.50	0
8	BCL	3	101	2	50,55,74	2.22	17 (34%)	60,92,115	2.76	17 (28%)
18	U10	M	405	-	63,63,63	0.61	2 (3%)	76,79,79	0.52	0
13	PGV	H	305	-	35,35,50	1.11	2 (5%)	38,40,56	1.23	4 (10%)
11	A1EYK	U	103	-	39,40,40	1.70	10 (25%)	47,49,49	1.30	5 (10%)
10	SPO	7	102	-	40,41,41	0.62	0	47,50,50	1.70	10 (21%)
12	LMT	D	101	-	36,36,36	0.37	0	47,47,47	0.84	2 (4%)
8	BCL	N	101	1	69,74,74	1.77	16 (23%)	83,115,115	2.48	25 (30%)
13	PGV	D	105	-	31,31,50	1.14	2 (6%)	34,36,56	1.07	3 (8%)
10	SPO	F	102	-	40,41,41	0.61	0	47,50,50	1.65	10 (21%)
10	SPO	M	406	-	40,41,41	0.62	0	47,50,50	1.71	8 (17%)
11	A1EYK	9	103	-	39,40,40	1.73	10 (25%)	47,49,49	1.30	4 (8%)
8	BCL	5	101	2	69,74,74	1.79	17 (24%)	83,115,115	2.43	27 (32%)
12	LMT	O	104	-	28,28,36	0.48	0	39,39,47	0.94	1 (2%)
10	SPO	I	102	-	40,41,41	0.62	0	47,50,50	1.73	11 (23%)
18	U10	M	410	-	28,28,63	0.83	2 (7%)	34,37,79	0.72	0
10	SPO	S	102	-	40,41,41	0.63	0	47,50,50	1.70	10 (21%)
10	SPO	Q	102	-	40,41,41	0.62	0	47,50,50	1.69	10 (21%)
17	BPH	L	302	-	59,70,70	0.75	2 (3%)	61,101,101	0.88	2 (3%)
13	PGV	H	304	-	41,41,50	1.00	2 (4%)	44,47,56	1.16	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	X	101	1	69,74,74	1.80	17 (24%)	83,115,115	2.41	21 (25%)
8	BCL	M	403	6	69,74,74	1.82	17 (24%)	83,115,115	2.57	26 (31%)
8	BCL	L	307	5	69,74,74	1.77	18 (26%)	83,115,115	2.44	24 (28%)
8	BCL	Q	101	2	69,74,74	1.78	18 (26%)	83,115,115	2.64	27 (32%)
8	BCL	S	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.55	27 (32%)
8	BCL	A	101	2	69,74,74	1.78	17 (24%)	83,115,115	2.53	27 (32%)
8	BCL	8	101	1	69,74,74	1.76	17 (24%)	83,115,115	2.47	26 (31%)
14	HEC	C	403	3	50,50,50	1.75	11 (22%)	68,82,82	1.76	15 (22%)
12	LMT	M	413	-	25,25,36	0.44	0	30,30,47	0.56	0
13	PGV	M	408	-	44,44,50	0.96	2 (4%)	47,50,56	1.09	3 (6%)
13	PGV	L	304	-	42,42,50	0.99	2 (4%)	45,48,56	1.04	4 (8%)
13	PGV	F	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.95	2 (3%)
12	LMT	L	306	-	28,28,36	0.44	0	39,39,47	0.75	1 (2%)
11	A1EYK	K	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.80	0
13	PGV	M	411	-	31,31,50	1.15	2 (6%)	33,36,56	1.22	3 (9%)
12	LMT	7	104	-	28,28,36	0.50	0	39,39,47	1.08	2 (5%)
11	A1EYK	O	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.81	0
8	BCL	2	101	1	69,74,74	1.90	17 (24%)	83,115,115	2.33	20 (24%)
8	BCL	9	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.56	27 (32%)
8	BCL	L	301	5	69,74,74	1.78	17 (24%)	83,115,115	2.53	25 (30%)
11	A1EYK	7	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.81	0
8	BCL	4	102	1	69,74,74	1.90	17 (24%)	83,115,115	2.44	22 (26%)
8	BCL	J	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.47	24 (28%)
8	BCL	Z	102	1	69,74,74	1.88	18 (26%)	83,115,115	2.36	24 (28%)
12	LMT	9	104	-	28,28,36	0.51	0	39,39,47	0.98	2 (5%)
8	BCL	V	101	1	69,74,74	1.78	17 (24%)	83,115,115	2.48	25 (30%)
11	A1EYK	I	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.86	2 (4%)
10	SPO	K	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
8	BCL	L	308	6	69,74,74	1.80	17 (24%)	83,115,115	2.48	25 (30%)
10	SPO	D	103	-	40,41,41	0.62	0	47,50,50	1.65	11 (23%)
13	PGV	H	302	-	32,32,50	1.13	2 (6%)	35,38,56	1.14	3 (8%)
14	HEC	C	402	3	50,50,50	1.76	9 (18%)	68,82,82	1.80	17 (25%)
13	PGV	A	104	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	3 (6%)
11	A1EYK	D	104	-	39,40,40	1.71	11 (28%)	47,49,49	0.79	1 (2%)
11	A1EYK	Q	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SPO	U	102	-	40,41,41	0.63	0	47,50,50	1.76	13 (27%)
8	BCL	I	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.59	27 (32%)
13	PGV	H	303	-	41,41,50	1.01	2 (4%)	44,47,56	1.09	3 (6%)
8	BCL	U	101	2	69,74,74	1.78	17 (24%)	83,115,115	2.60	27 (32%)
13	PGV	M	409	-	42,42,50	1.02	2 (4%)	45,48,56	1.01	2 (4%)
10	SPO	4	101	-	40,41,41	0.66	0	47,50,50	2.01	15 (31%)
8	BCL	W	101	2	69,74,74	1.78	18 (26%)	83,115,115	2.61	25 (30%)
11	A1EYK	A	103	-	39,40,40	1.68	11 (28%)	47,49,49	0.81	1 (2%)
14	HEC	C	401	3	50,50,50	1.76	11 (22%)	68,82,82	1.79	17 (25%)
8	BCL	P	101	1	69,74,74	1.77	17 (24%)	83,115,115	2.43	24 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPO	Y	102	-	-	4/47/47/47	-
10	SPO	O	102	-	-	3/47/47/47	-
8	BCL	6	101	1	-	11/41/137/137	-
12	LMT	K	104	-	-	3/13/53/61	0/2/2/2
12	LMT	F	104	-	-	5/14/54/61	0/2/2/2
8	BCL	7	101	2	-	11/41/137/137	-
10	SPO	U	104	-	-	4/47/47/47	-
8	BCL	K	101	2	-	13/41/137/137	-
8	BCL	T	101	1	-	6/41/137/137	-
11	A1EYK	F	103	-	-	1/44/44/44	-
18	U10	M	402	-	-	5/18/42/87	0/1/1/1
12	LMT	L	305	-	-	3/13/53/61	0/2/2/2
11	A1EYK	5	103	-	-	2/44/44/44	-
8	BCL	1	101	2	-	15/41/137/137	-
8	BCL	F	101	2	-	6/41/137/137	-
8	BCL	B	101	1	-	10/41/137/137	-
8	BCL	R	101	1	-	10/41/137/137	-
11	A1EYK	Z	101	-	-	1/44/44/44	-
10	SPO	A	102	-	-	1/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	G	101	1	-	8/41/137/137	-
12	LMT	M	414	-	-	4/14/54/61	0/2/2/2
8	BCL	Y	101	2	-	10/41/137/137	-
8	BCL	D	102	2	-	8/41/137/137	-
11	A1EYK	W	102	-	-	6/44/44/44	-
8	BCL	O	101	2	-	8/41/137/137	-
13	PGV	H	301	-	-	13/38/38/55	-
11	A1EYK	S	103	-	-	2/44/44/44	-
13	PGV	M	407	-	-	4/41/41/55	-
8	BCL	0	101	1	-	9/41/137/137	-
8	BCL	E	101	1	-	9/41/137/137	-
10	SPO	5	102	-	-	3/47/47/47	-
17	BPH	M	404	-	-	6/37/105/105	0/5/6/6
10	SPO	9	102	-	-	3/47/47/47	-
18	U10	L	303	-	-	12/63/87/87	0/1/1/1
8	BCL	3	101	2	-	8/19/115/137	-
18	U10	M	405	-	-	9/63/87/87	0/1/1/1
13	PGV	H	305	-	-	5/37/37/55	-
11	A1EYK	U	103	-	-	4/44/44/44	-
10	SPO	7	102	-	-	2/47/47/47	-
12	LMT	D	101	-	-	3/21/61/61	0/2/2/2
8	BCL	N	101	1	-	6/41/137/137	-
13	PGV	D	105	-	-	9/35/35/55	-
10	SPO	F	102	-	-	3/47/47/47	-
10	SPO	M	406	-	-	5/47/47/47	-
11	A1EYK	9	103	-	-	4/44/44/44	-
8	BCL	5	101	2	-	12/41/137/137	-
12	LMT	O	104	-	-	2/13/53/61	0/2/2/2
10	SPO	I	102	-	-	3/47/47/47	-
18	U10	M	410	-	-	2/21/45/87	0/1/1/1
10	SPO	S	102	-	-	3/47/47/47	-
10	SPO	Q	102	-	-	3/47/47/47	-
17	BPH	L	302	-	-	5/37/105/105	0/5/6/6
13	PGV	H	304	-	-	11/46/46/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	X	101	1	-	14/41/137/137	-
8	BCL	M	403	6	-	11/41/137/137	-
8	BCL	L	307	5	-	8/41/137/137	-
8	BCL	Q	101	2	-	11/41/137/137	-
8	BCL	S	101	2	-	6/41/137/137	-
8	BCL	A	101	2	-	16/41/137/137	-
8	BCL	8	101	1	-	9/41/137/137	-
14	HEC	C	403	3	1/1/3/7	4/14/54/54	-
12	LMT	M	413	-	-	5/17/37/61	0/1/1/2
13	PGV	M	408	-	-	12/49/49/55	-
13	PGV	L	304	-	-	12/47/47/55	-
13	PGV	F	105	-	-	23/55/55/55	-
12	LMT	L	306	-	-	1/13/53/61	0/2/2/2
11	A1EYK	K	103	-	-	1/44/44/44	-
13	PGV	M	411	-	-	10/35/35/55	-
12	LMT	7	104	-	-	4/13/53/61	0/2/2/2
11	A1EYK	O	103	-	-	2/44/44/44	-
8	BCL	2	101	1	-	14/41/137/137	-
8	BCL	9	101	2	-	11/41/137/137	-
8	BCL	L	301	5	-	12/41/137/137	-
11	A1EYK	7	103	-	-	1/44/44/44	-
8	BCL	4	102	1	-	10/41/137/137	-
8	BCL	J	101	1	-	8/41/137/137	-
8	BCL	Z	102	1	-	7/41/137/137	-
12	LMT	9	104	-	-	1/13/53/61	0/2/2/2
8	BCL	V	101	1	-	10/41/137/137	-
11	A1EYK	I	103	-	-	1/44/44/44	-
10	SPO	K	102	-	-	3/47/47/47	-
8	BCL	L	308	6	-	9/41/137/137	-
10	SPO	D	103	-	-	1/47/47/47	-
13	PGV	H	302	-	-	17/37/37/55	-
14	HEC	C	402	3	1/1/3/7	4/14/54/54	-
13	PGV	A	104	-	-	9/51/51/55	-
11	A1EYK	D	104	-	-	2/44/44/44	-
11	A1EYK	Q	103	-	-	2/44/44/44	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPO	U	102	-	-	3/47/47/47	-
8	BCL	I	101	2	-	10/41/137/137	-
13	PGV	H	303	-	-	15/46/46/55	-
8	BCL	U	101	2	-	9/41/137/137	-
13	PGV	M	409	-	-	16/47/47/55	-
10	SPO	4	101	-	-	11/47/47/47	-
8	BCL	W	101	2	-	16/41/137/137	-
11	A1EYK	A	103	-	-	1/44/44/44	-
14	HEC	C	401	3	1/1/3/7	6/14/54/54	-
8	BCL	P	101	1	-	10/41/137/137	-

The worst 5 of 835 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	402	HEC	FE-NB	5.30	2.11	1.94
8	M	403	BCL	O2D-CGD	5.30	1.46	1.33
14	C	403	HEC	FE-NB	5.24	2.11	1.94
8	1	101	BCL	O2D-CGD	5.23	1.46	1.33
14	C	401	HEC	FE-NB	5.23	2.11	1.94

The worst 5 of 1202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C2B-C1B-NB	10.59	117.33	110.23
8	L	301	BCL	C2B-C1B-NB	10.56	117.31	110.23
8	J	101	BCL	C2B-C1B-NB	10.43	117.22	110.23
8	D	102	BCL	C2B-C1B-NB	10.32	117.15	110.23
8	P	101	BCL	C2B-C1B-NB	10.32	117.15	110.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	401	HEC	NA
14	C	402	HEC	NA
14	C	403	HEC	NA

5 of 686 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	0	101	BCL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	1	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C4C-C3C-CAC-CBC
8	1	101	BCL	C2-C3-C5-C6
8	1	101	BCL	C4-C3-C5-C6

There are no ring outliers.

72 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Y	102	SPO	10	0
10	O	102	SPO	7	0
8	6	101	BCL	3	0
12	K	104	LMT	1	0
8	7	101	BCL	2	0
10	U	104	SPO	6	0
8	K	101	BCL	2	0
8	T	101	BCL	6	0
8	1	101	BCL	7	0
8	F	101	BCL	1	0
8	B	101	BCL	6	0
8	R	101	BCL	5	0
10	A	102	SPO	9	0
8	G	101	BCL	4	0
8	Y	101	BCL	2	0
8	D	102	BCL	2	0
8	O	101	BCL	2	0
13	H	301	PGV	1	0
8	0	101	BCL	5	0
8	E	101	BCL	5	0
10	5	102	SPO	4	0
17	M	404	BPH	6	0
10	9	102	SPO	4	0
18	L	303	U10	4	0
18	M	405	U10	5	0
13	H	305	PGV	2	0
10	7	102	SPO	6	0
12	D	101	LMT	2	0
8	N	101	BCL	4	0
13	D	105	PGV	1	0
10	F	102	SPO	5	0
10	M	406	SPO	4	0
8	5	101	BCL	6	0

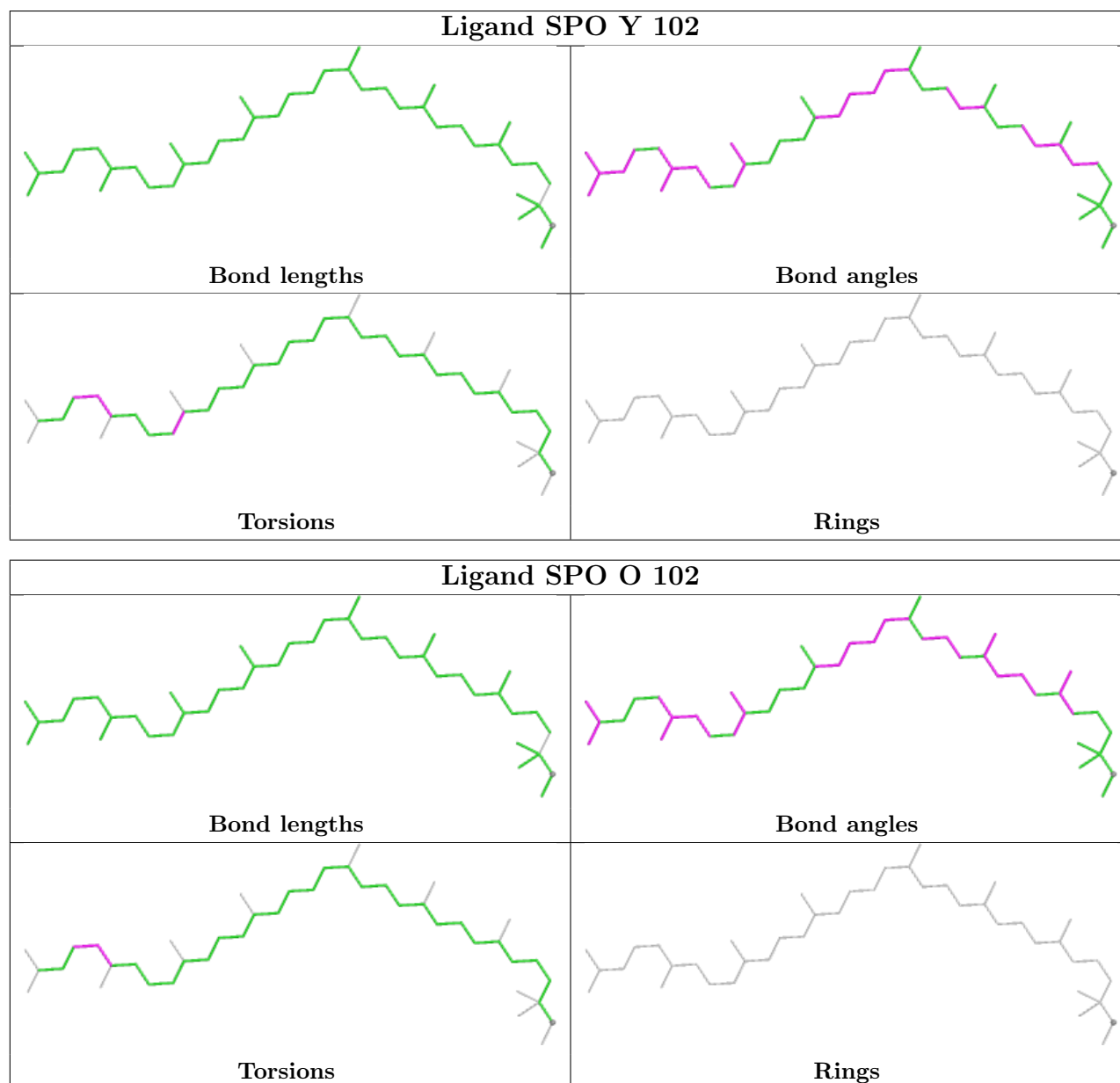
Continued on next page...

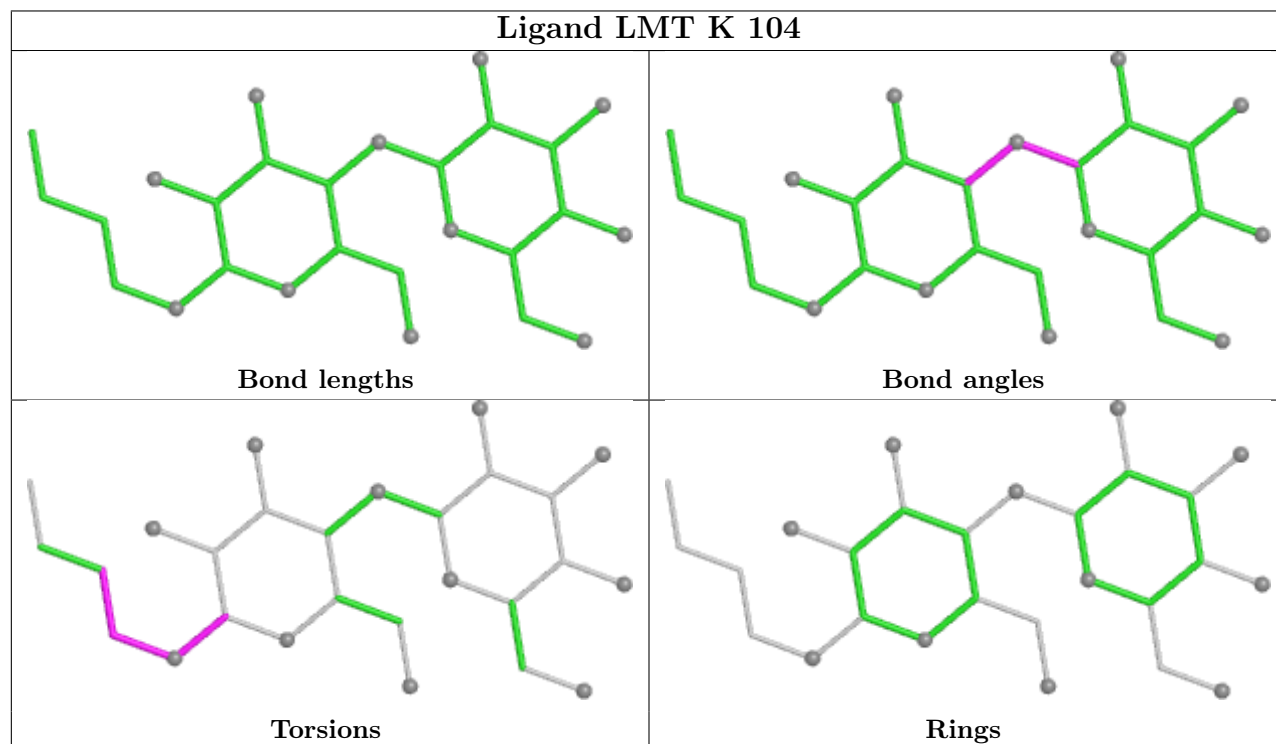
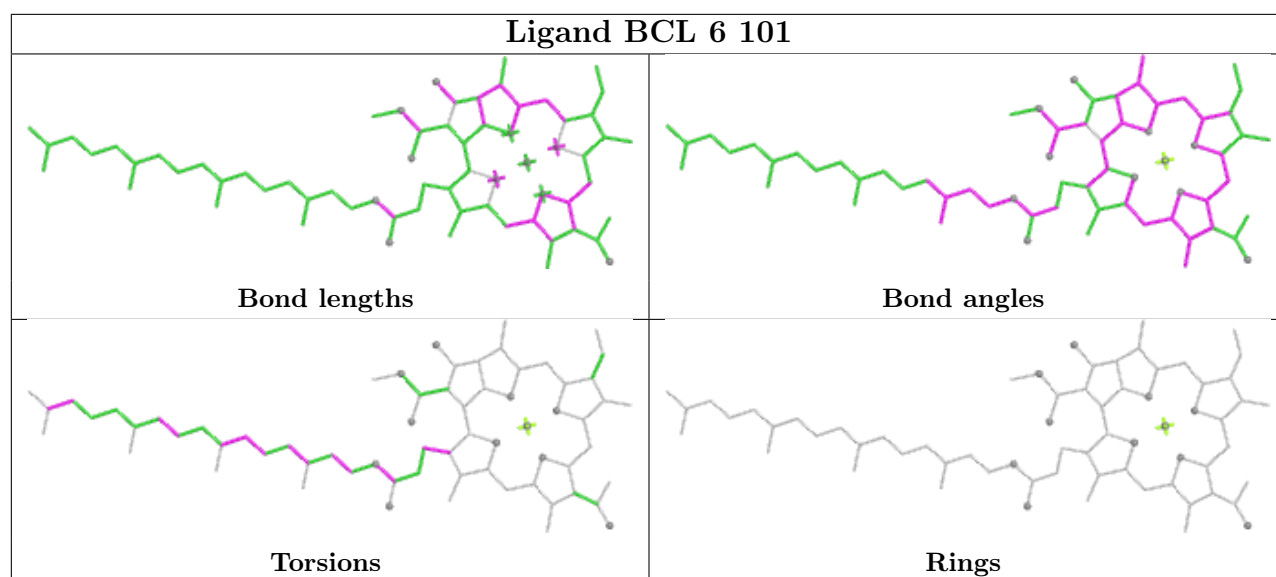
Continued from previous page...

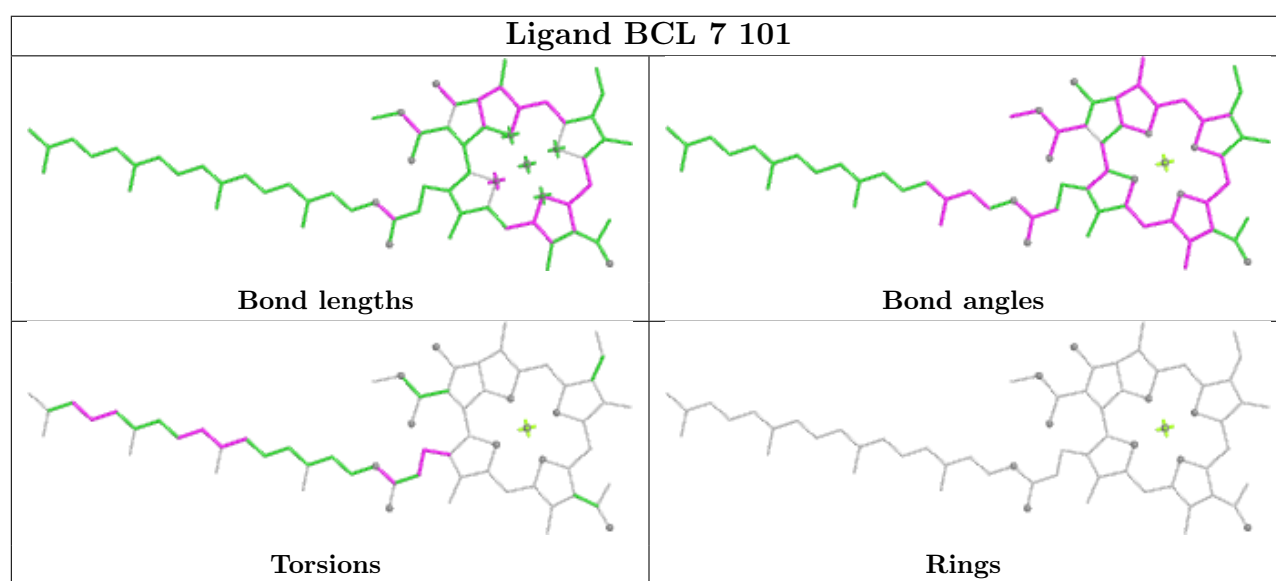
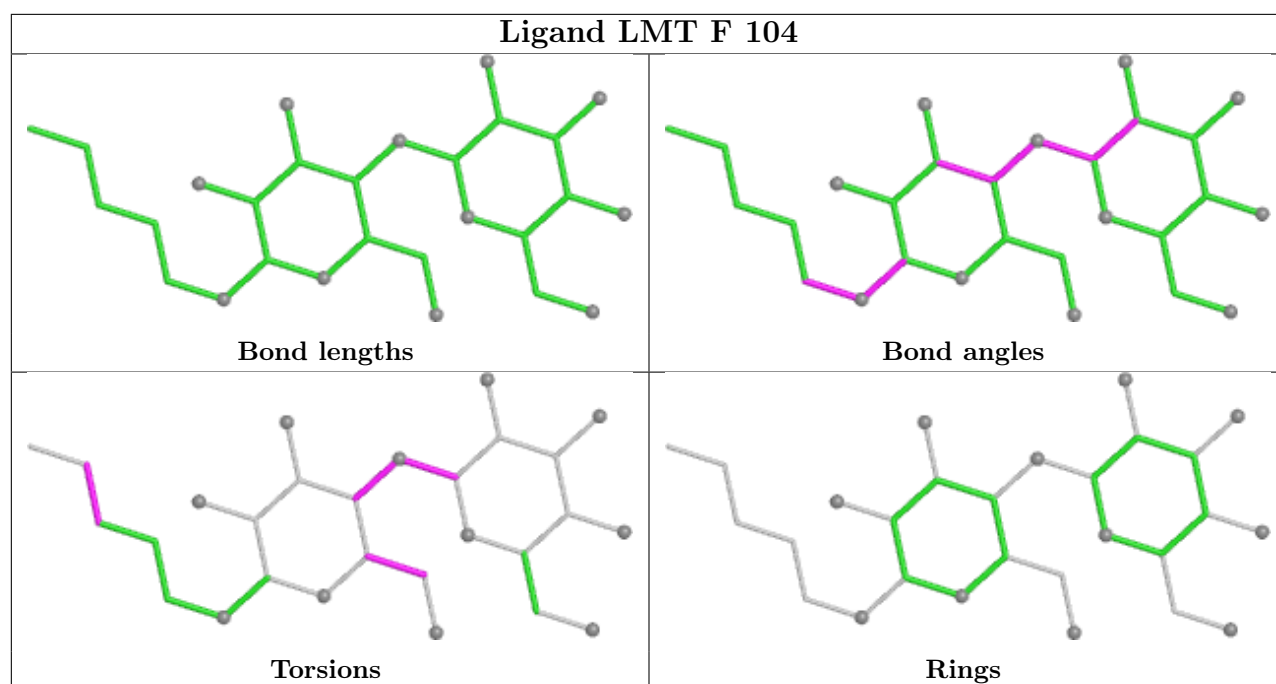
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	102	SPO	4	0
18	M	410	U10	1	0
10	S	102	SPO	5	0
10	Q	102	SPO	4	0
17	L	302	BPH	5	0
13	H	304	PGV	1	0
8	X	101	BCL	8	0
8	M	403	BCL	4	0
8	L	307	BCL	3	0
8	Q	101	BCL	3	0
8	S	101	BCL	1	0
8	A	101	BCL	3	0
8	8	101	BCL	6	0
14	C	403	HEC	2	0
13	M	408	PGV	1	0
13	L	304	PGV	2	0
13	F	105	PGV	2	0
13	M	411	PGV	2	0
12	7	104	LMT	4	0
8	2	101	BCL	3	0
8	9	101	BCL	2	0
8	L	301	BCL	2	0
8	4	102	BCL	5	0
8	J	101	BCL	3	0
8	Z	102	BCL	5	0
12	9	104	LMT	1	0
8	V	101	BCL	5	0
10	K	102	SPO	5	0
8	L	308	BCL	2	0
10	D	103	SPO	7	0
14	C	402	HEC	3	0
13	A	104	PGV	3	0
10	U	102	SPO	5	0
13	H	303	PGV	3	0
8	U	101	BCL	2	0
13	M	409	PGV	1	0
10	4	101	SPO	13	0
14	C	401	HEC	3	0
8	P	101	BCL	5	0

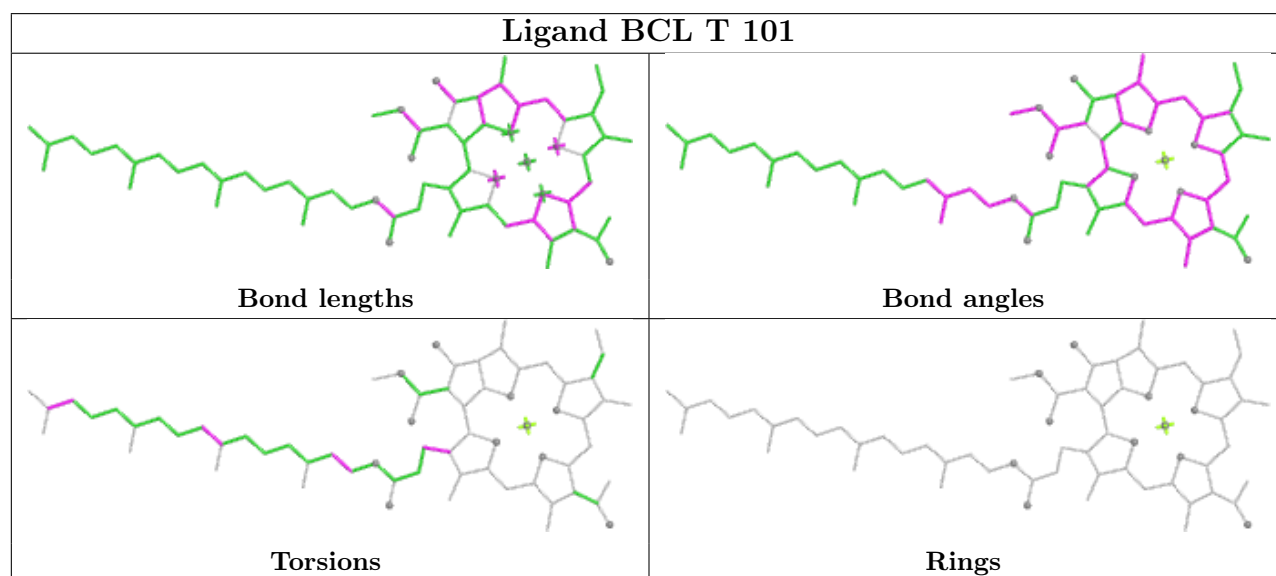
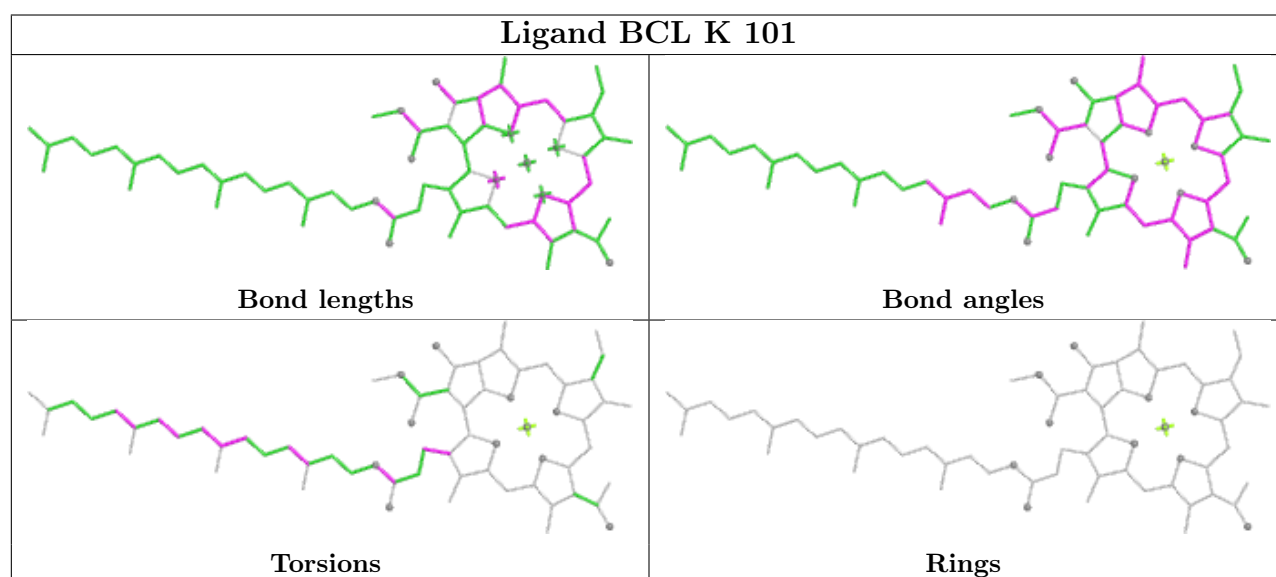
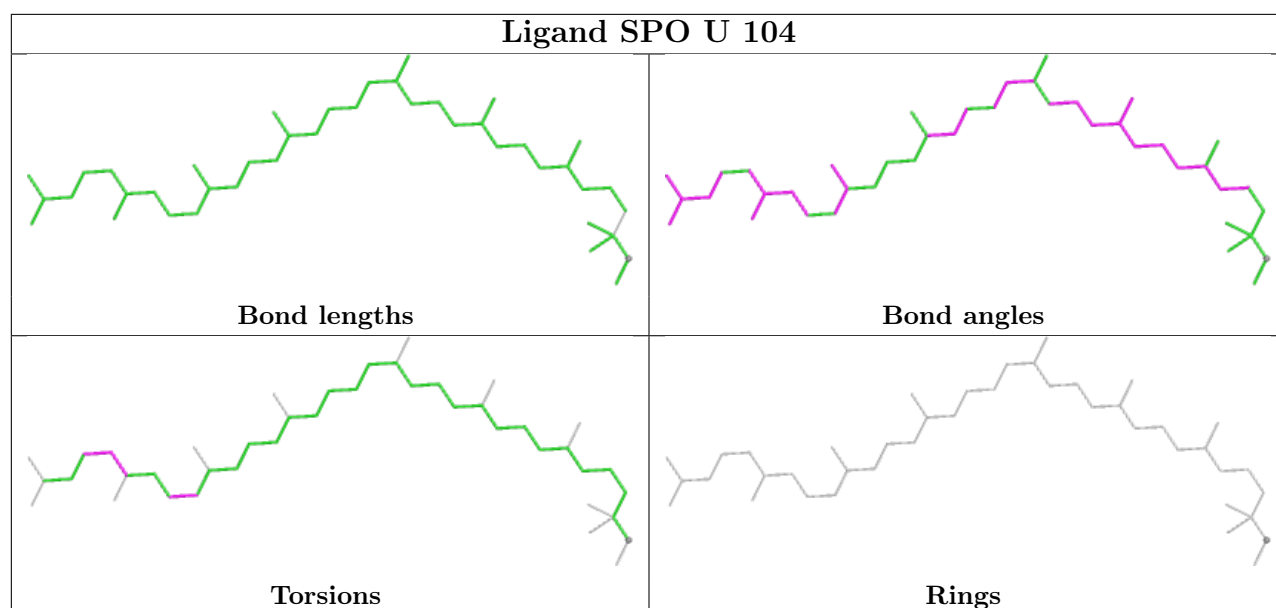
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

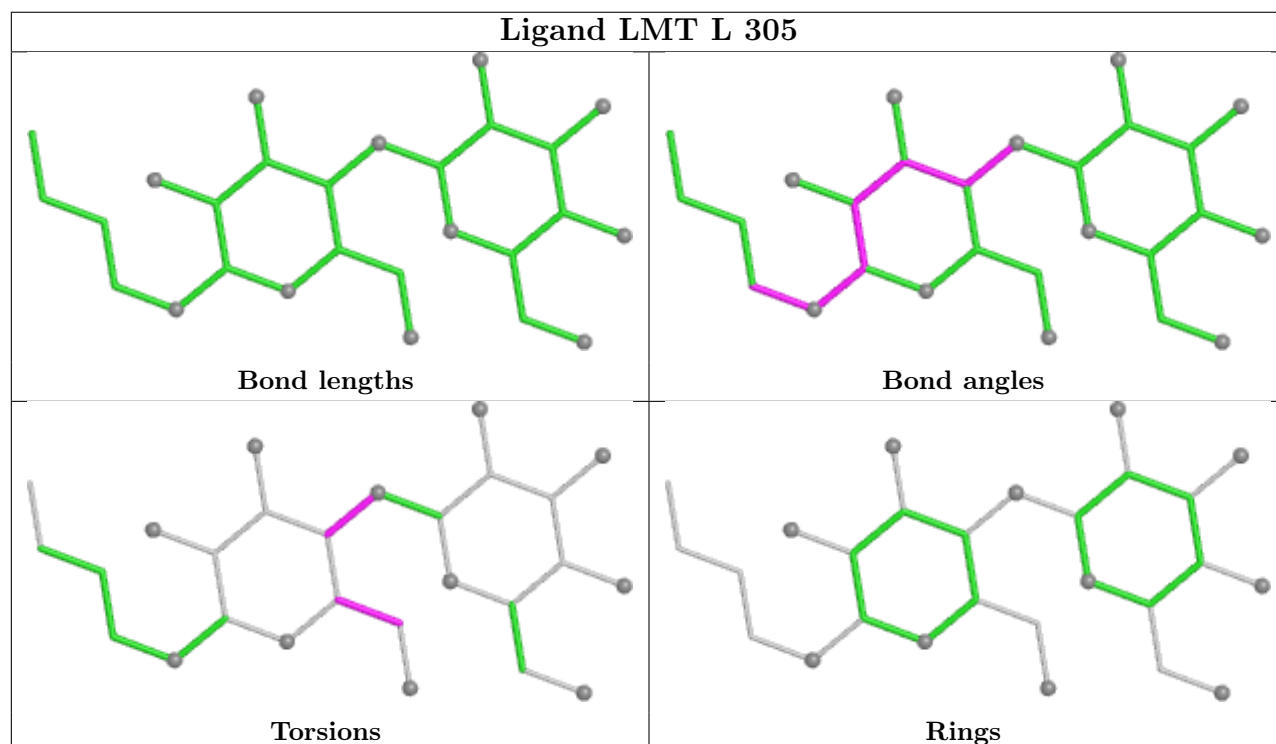
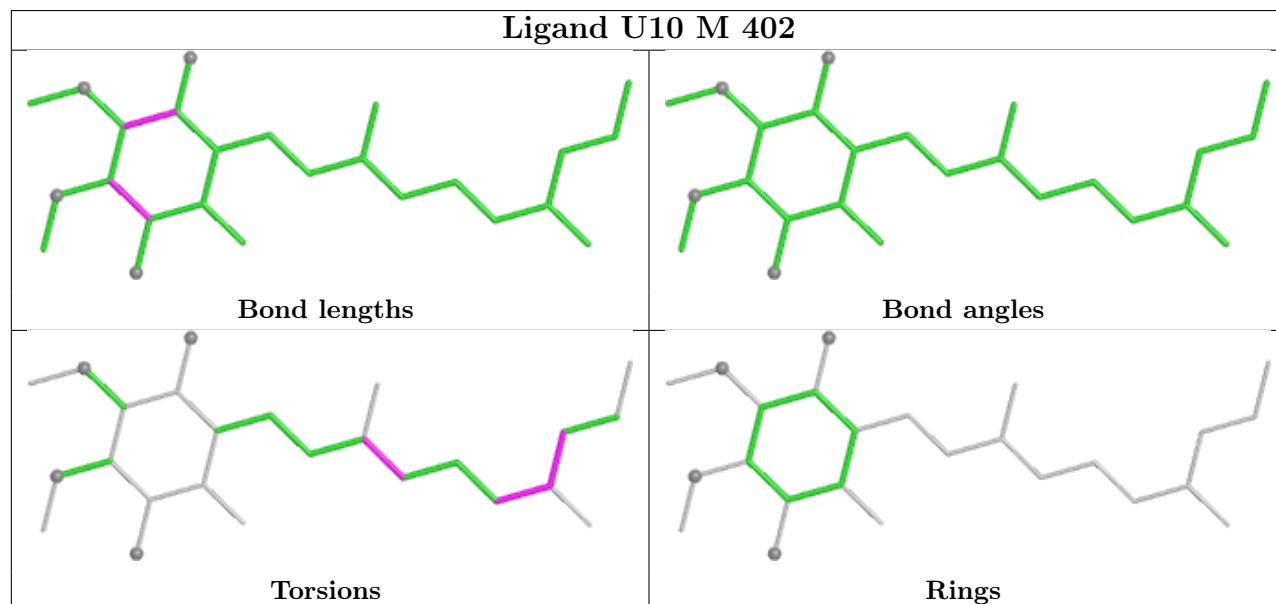
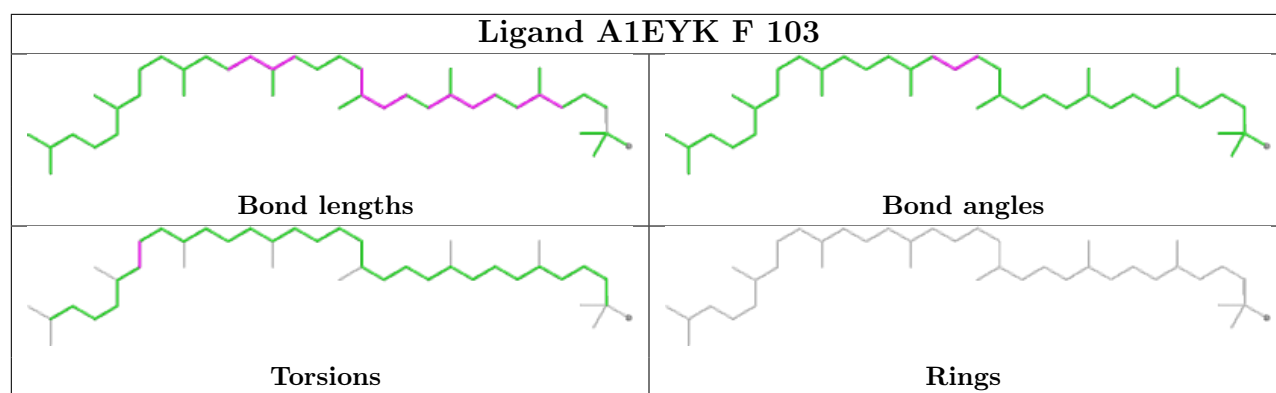
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

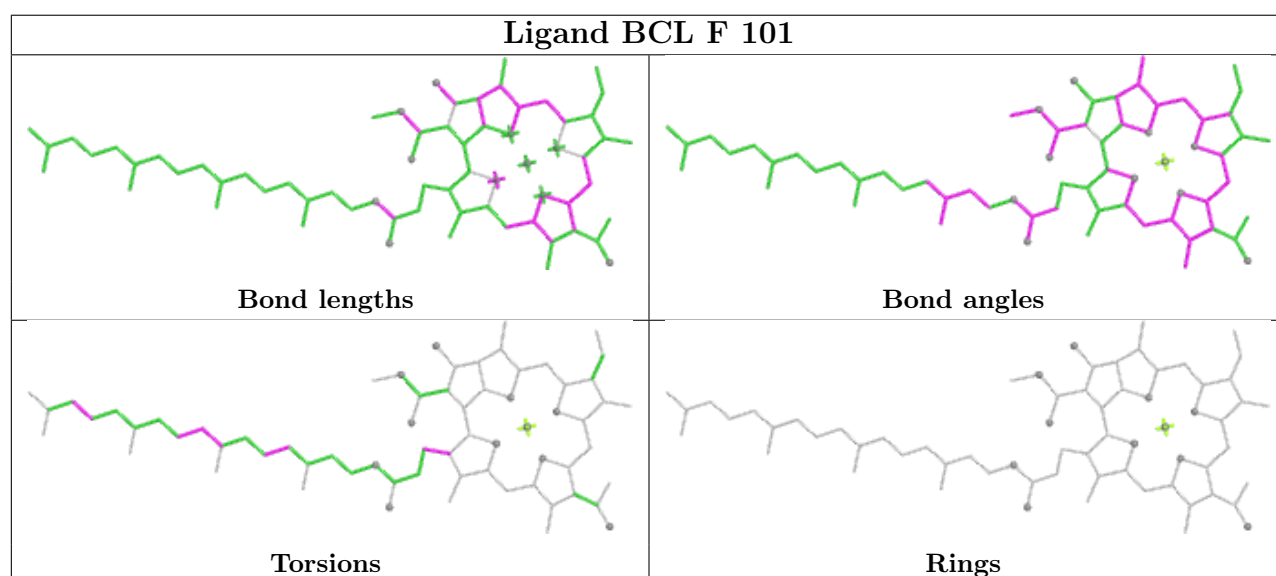
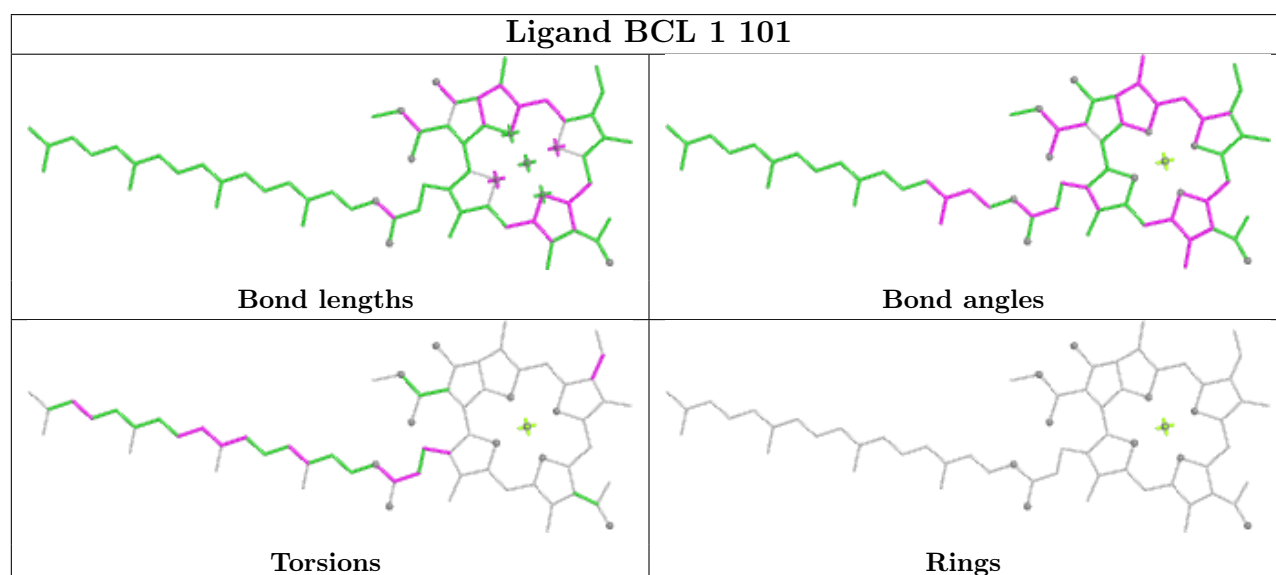
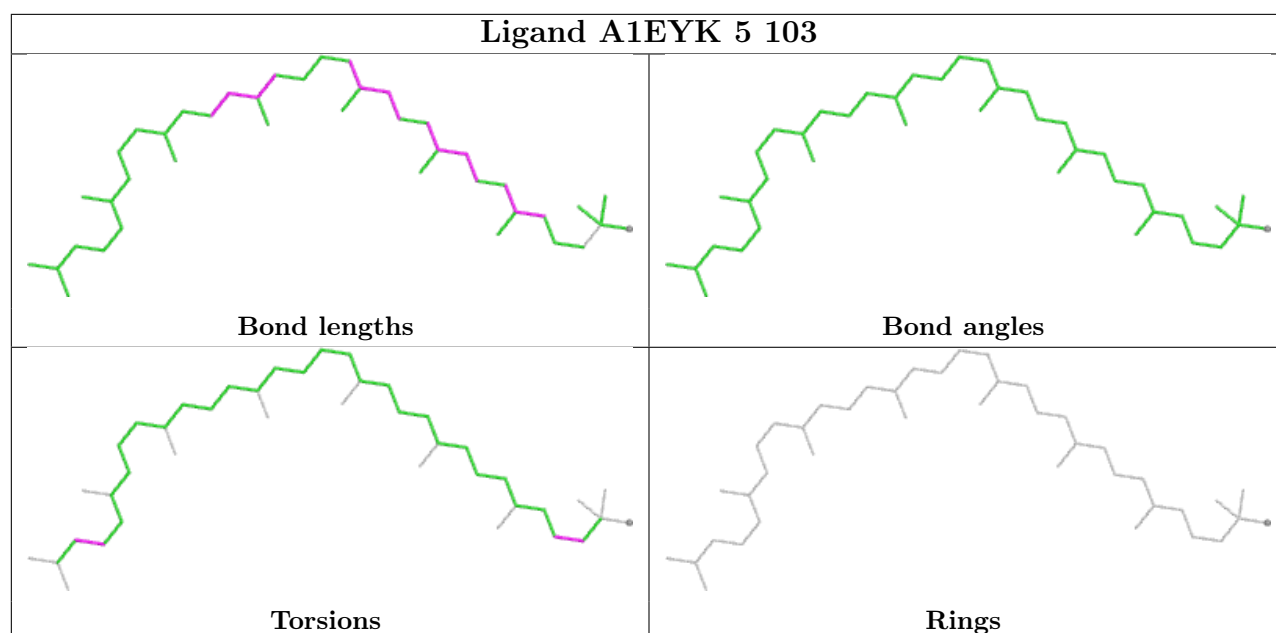


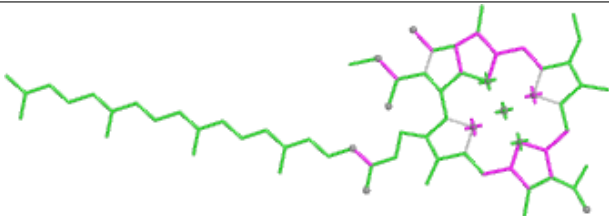
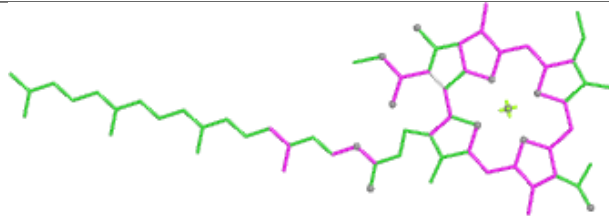
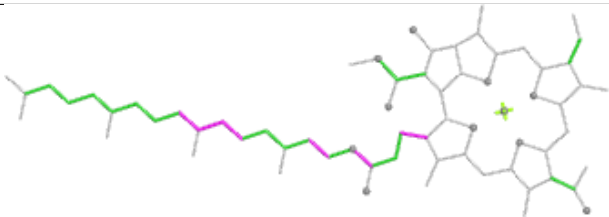
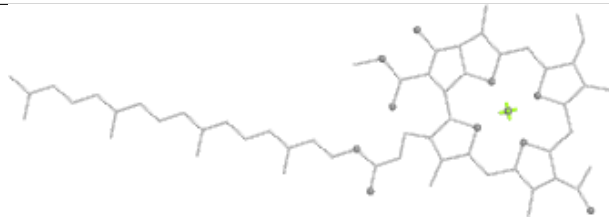


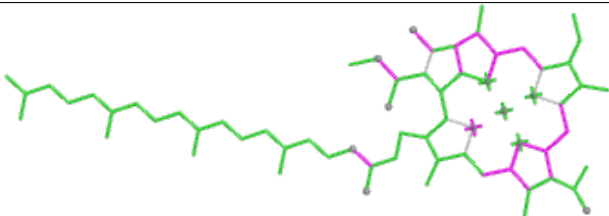
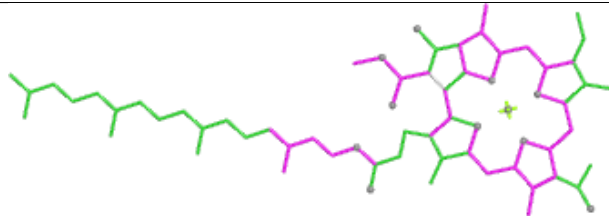
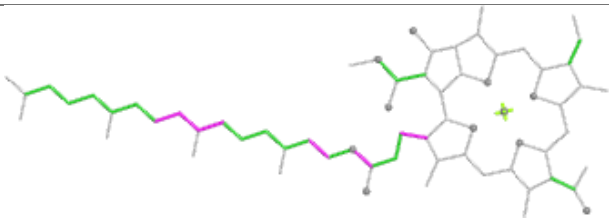
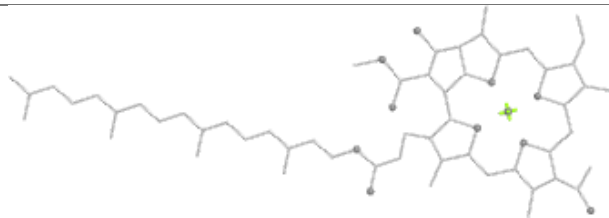


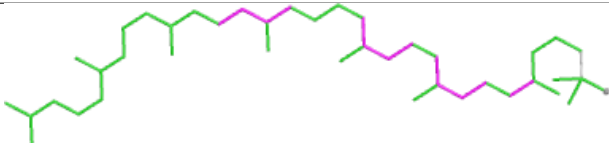
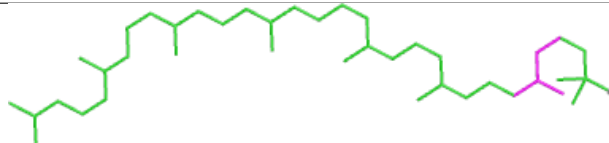
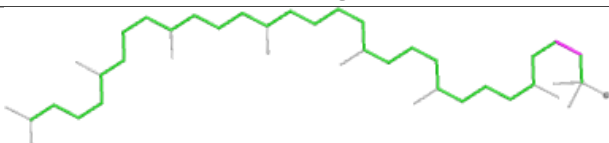
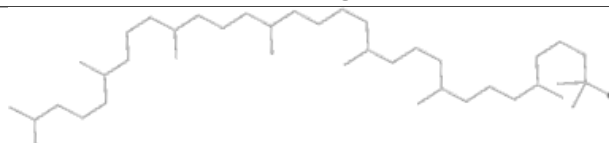


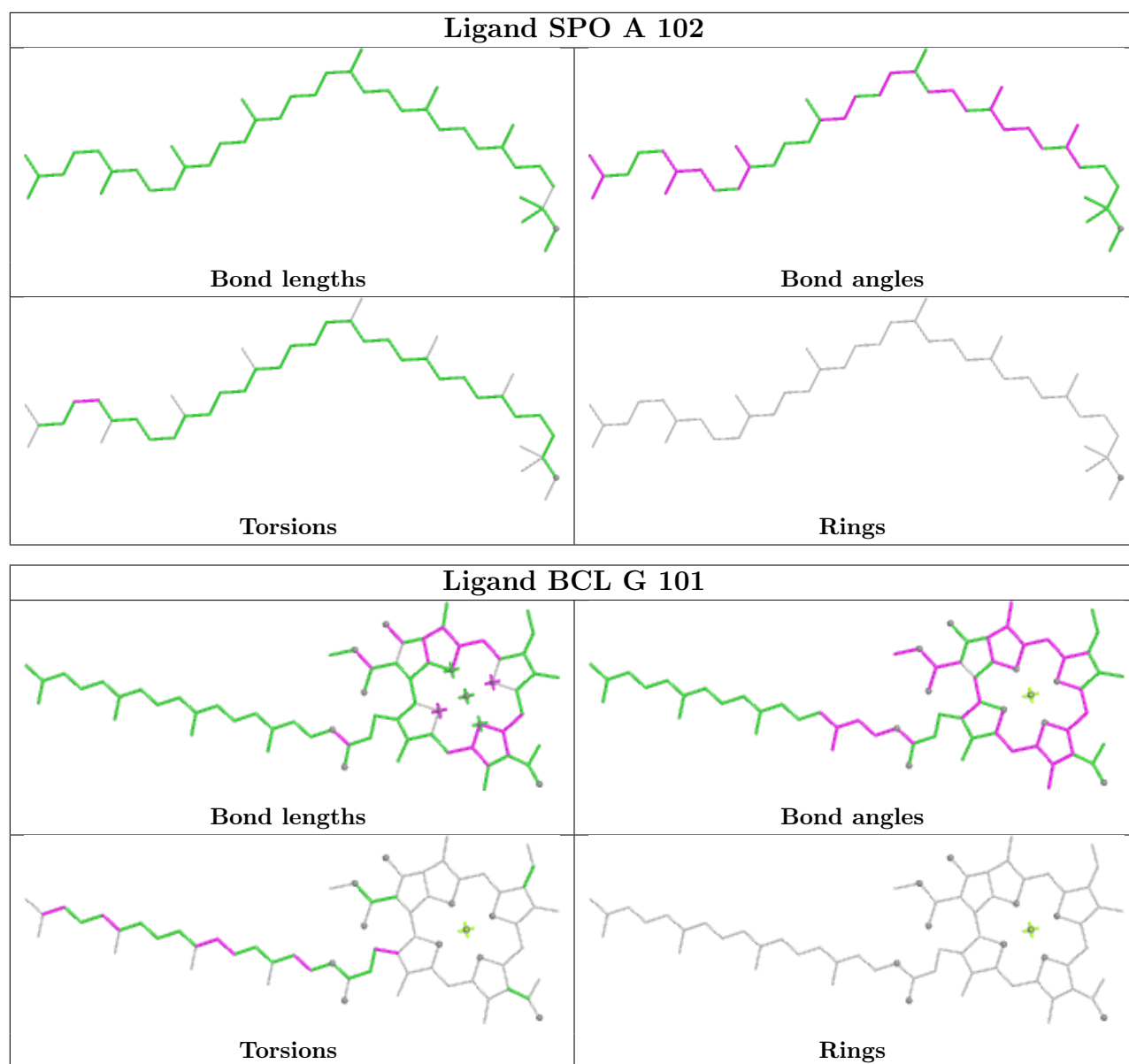


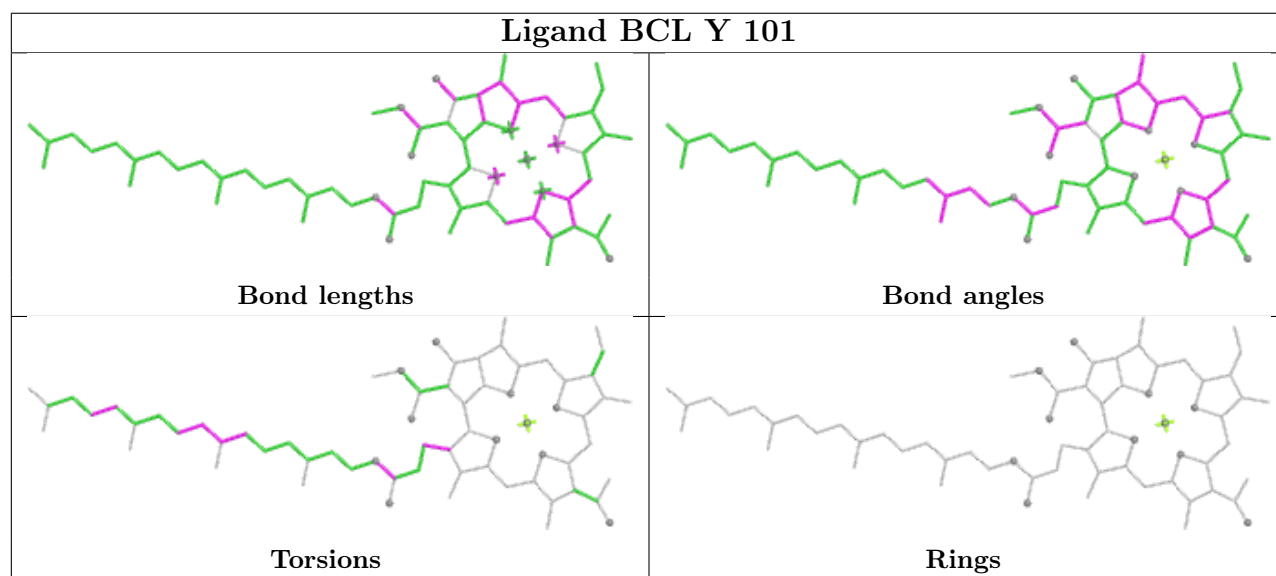
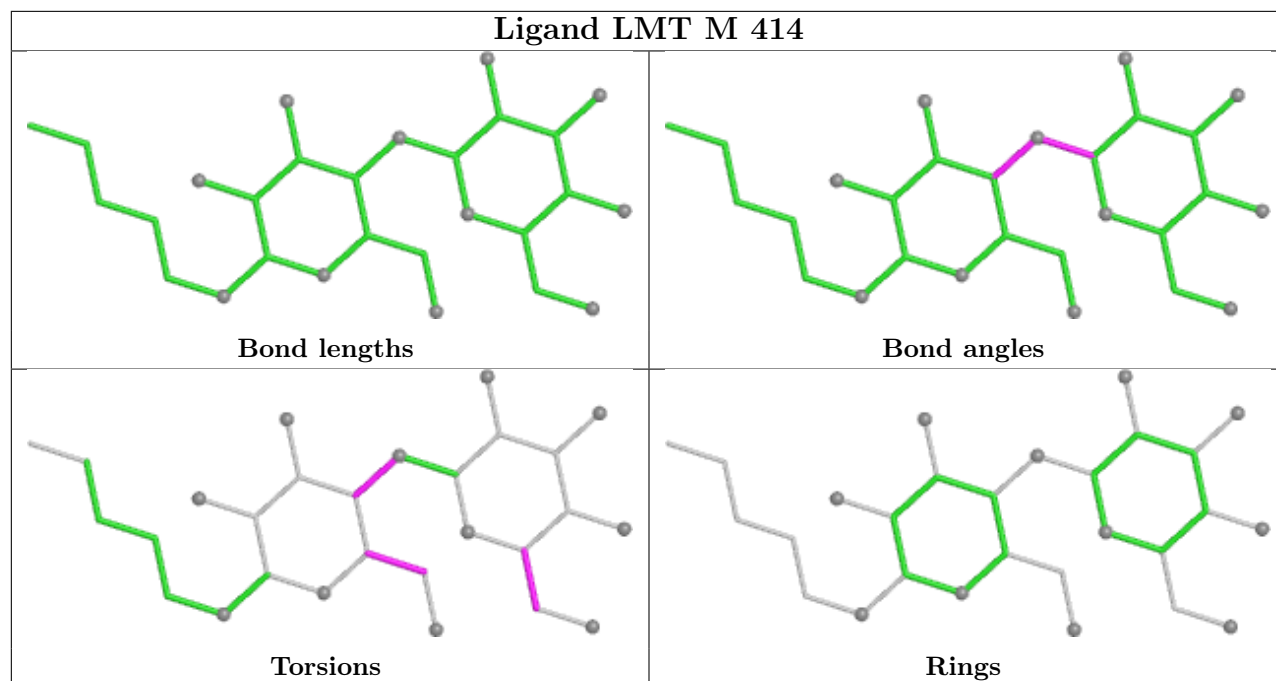


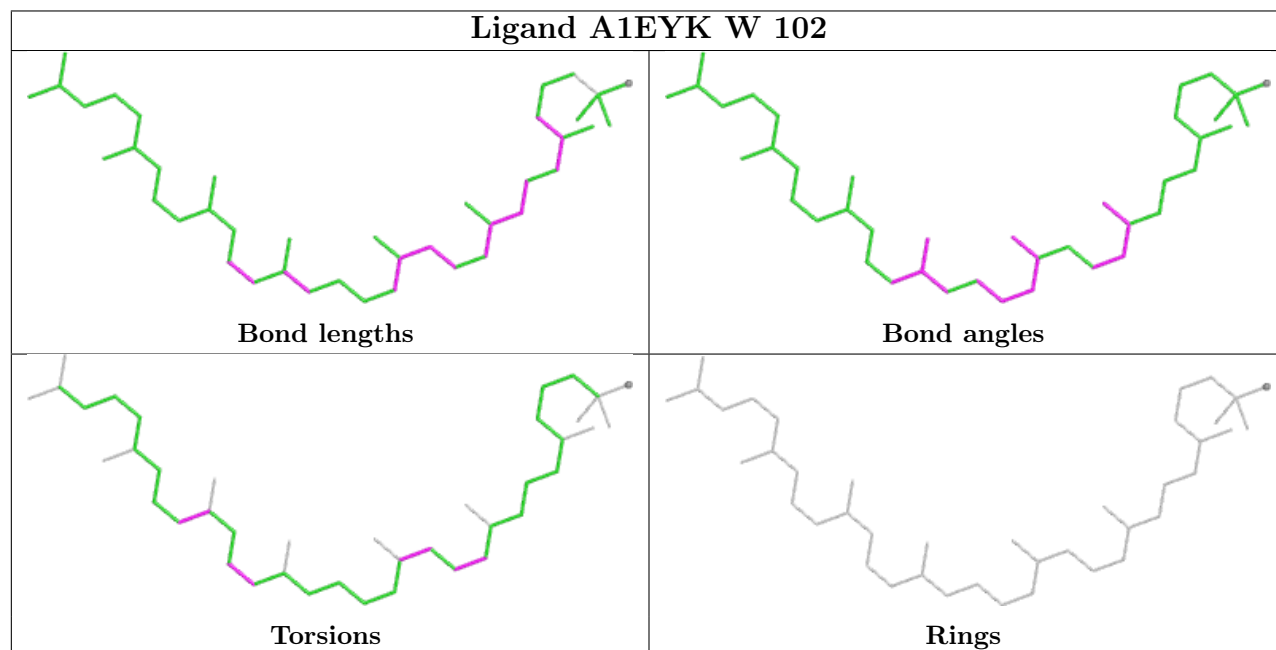
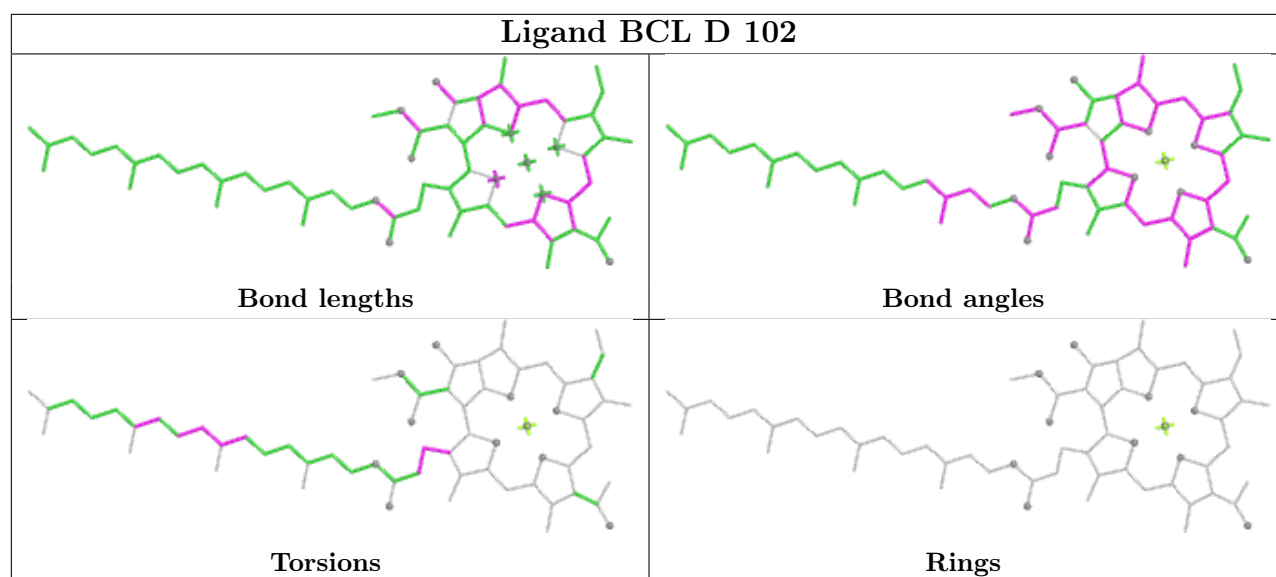
Ligand BCL B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

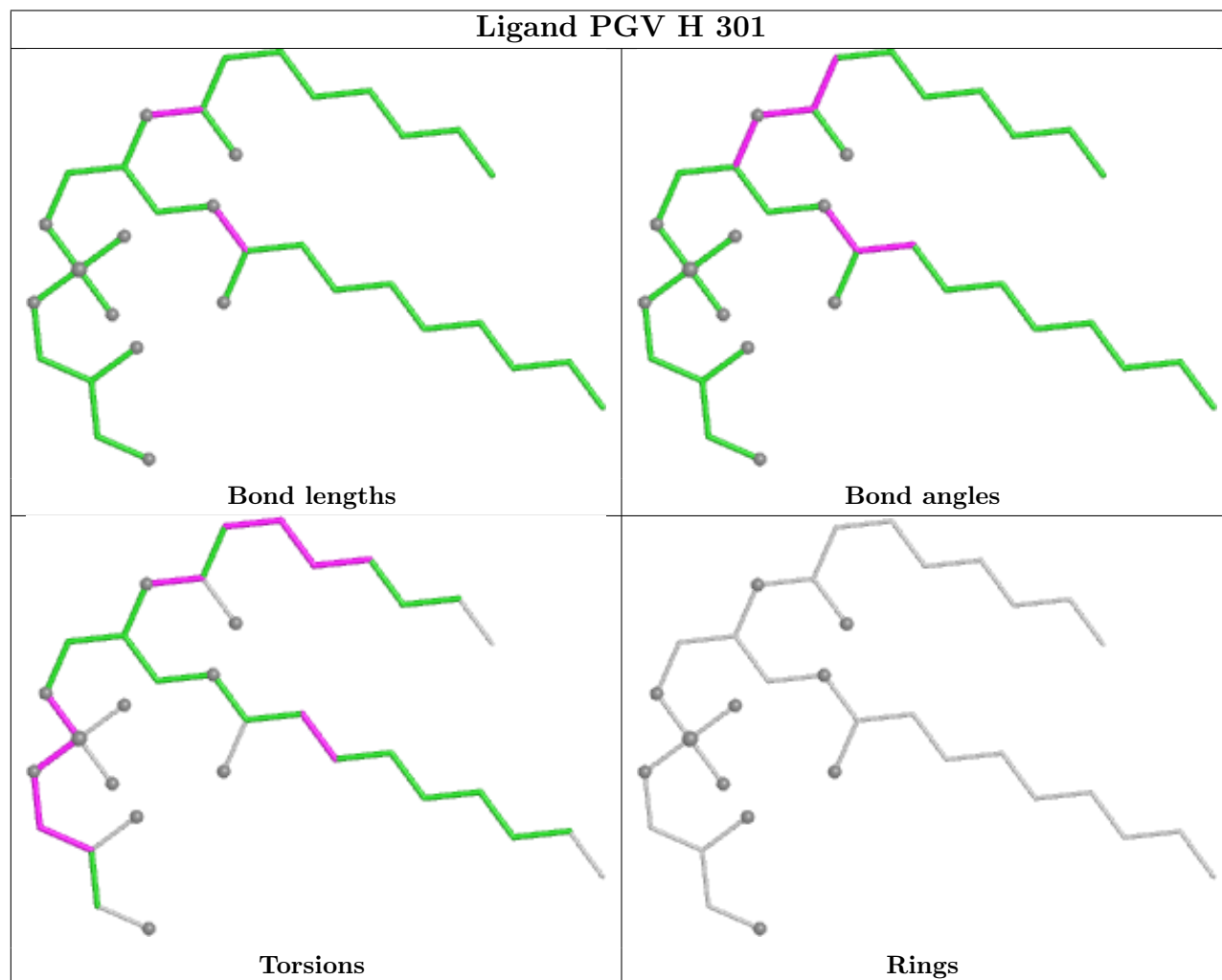
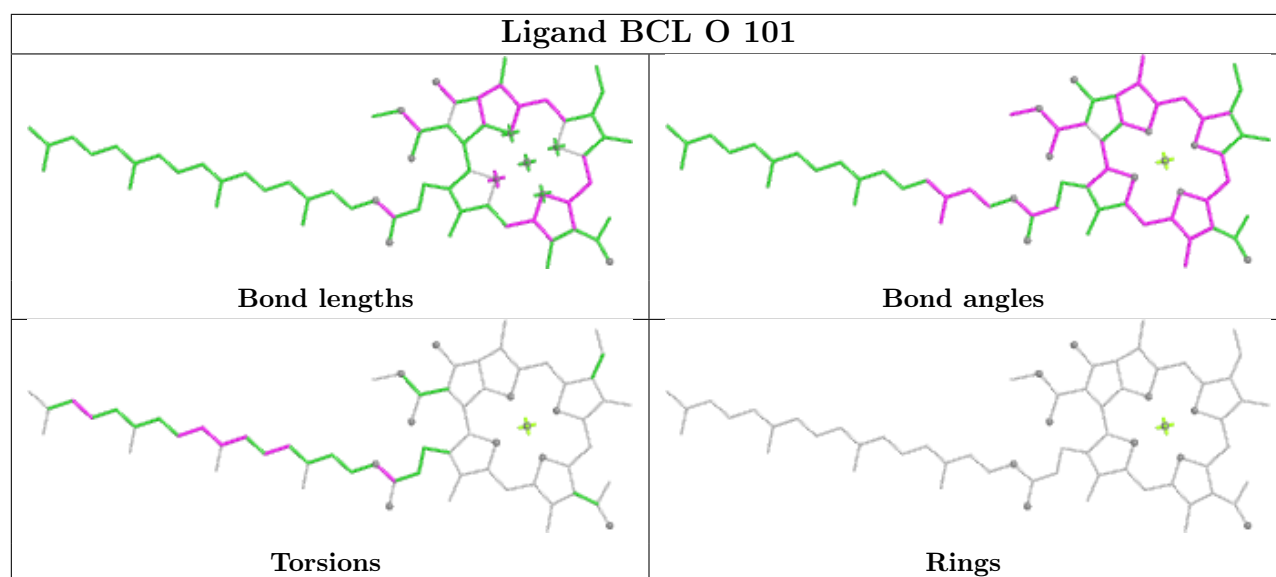
Ligand BCL R 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

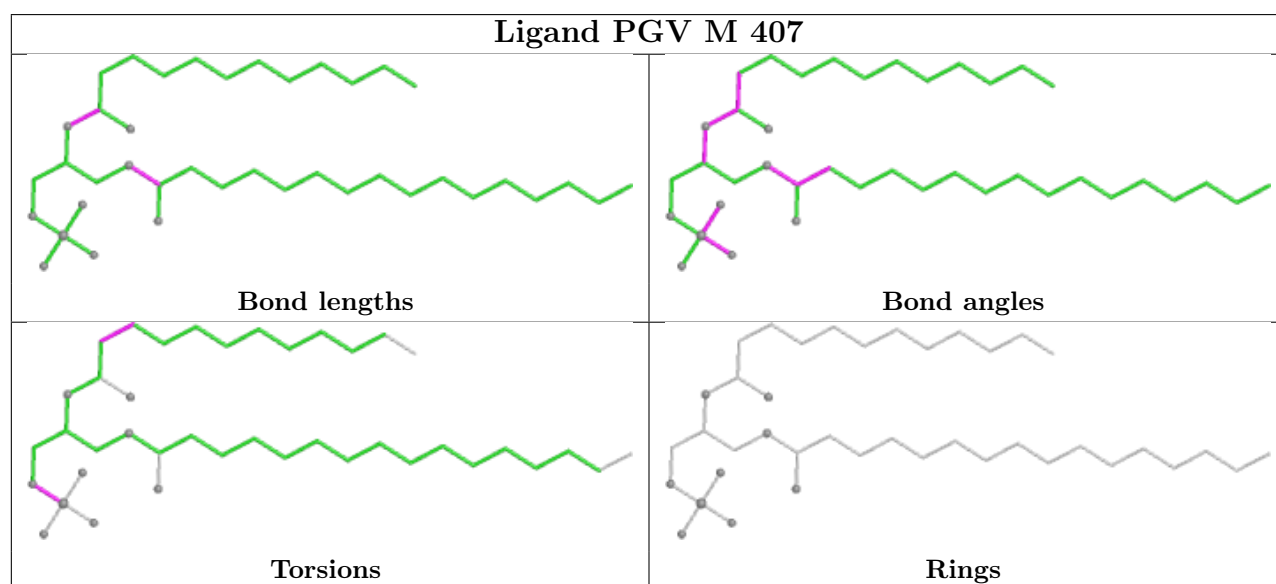
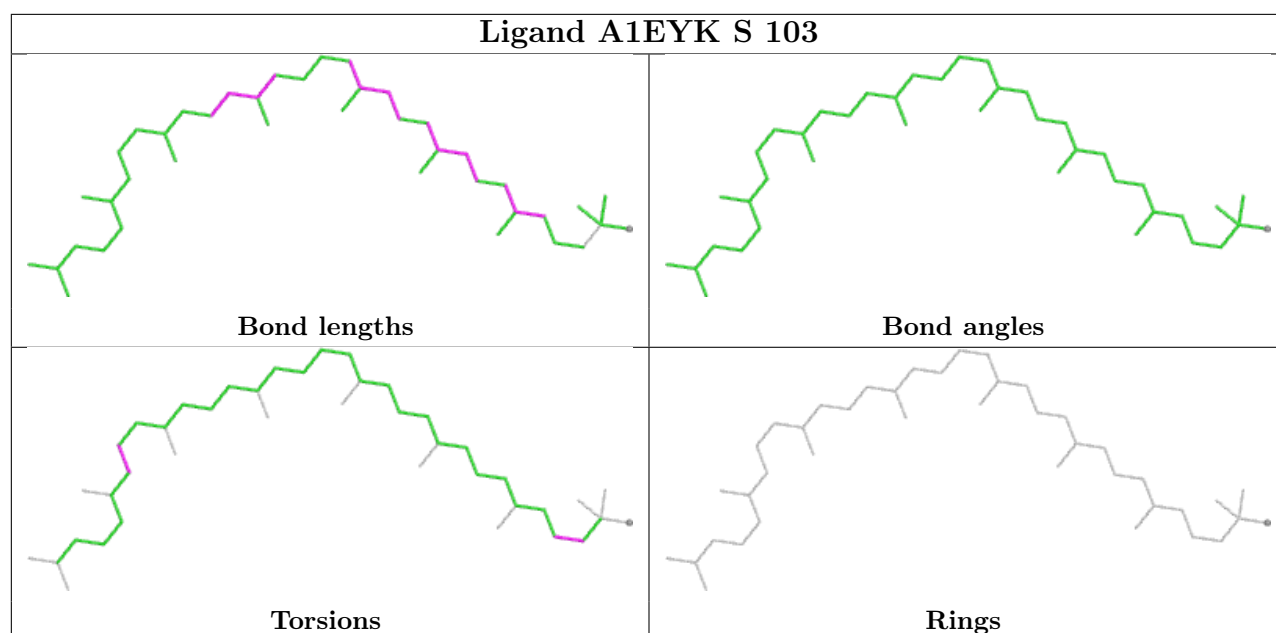
Ligand A1EYK Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

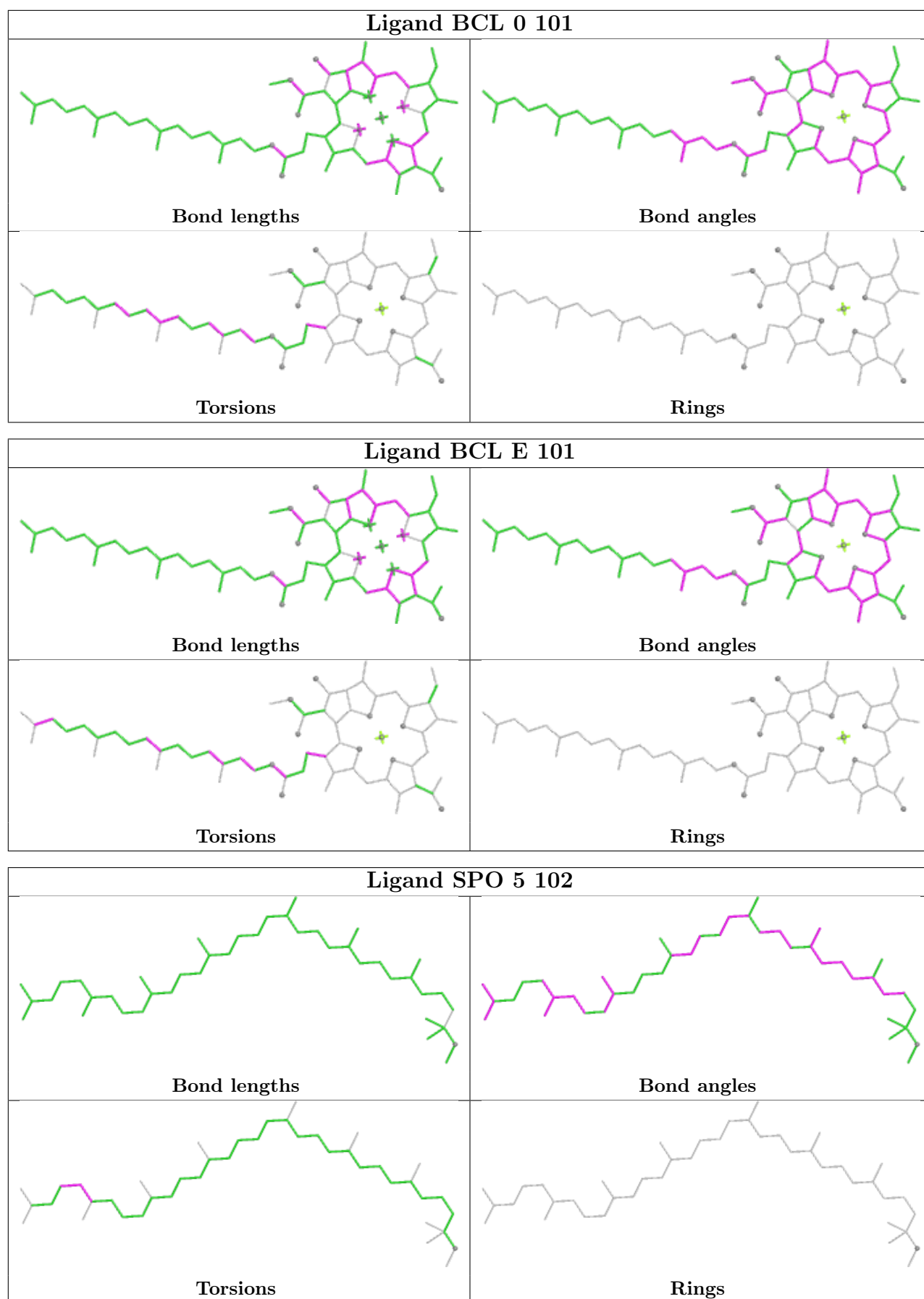


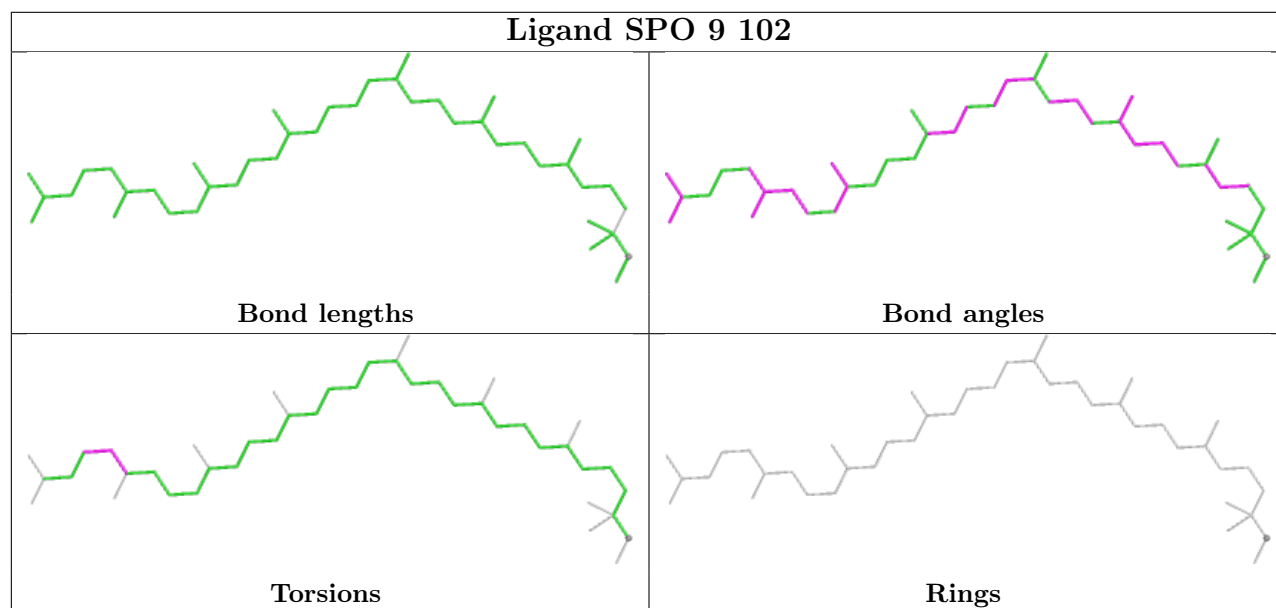
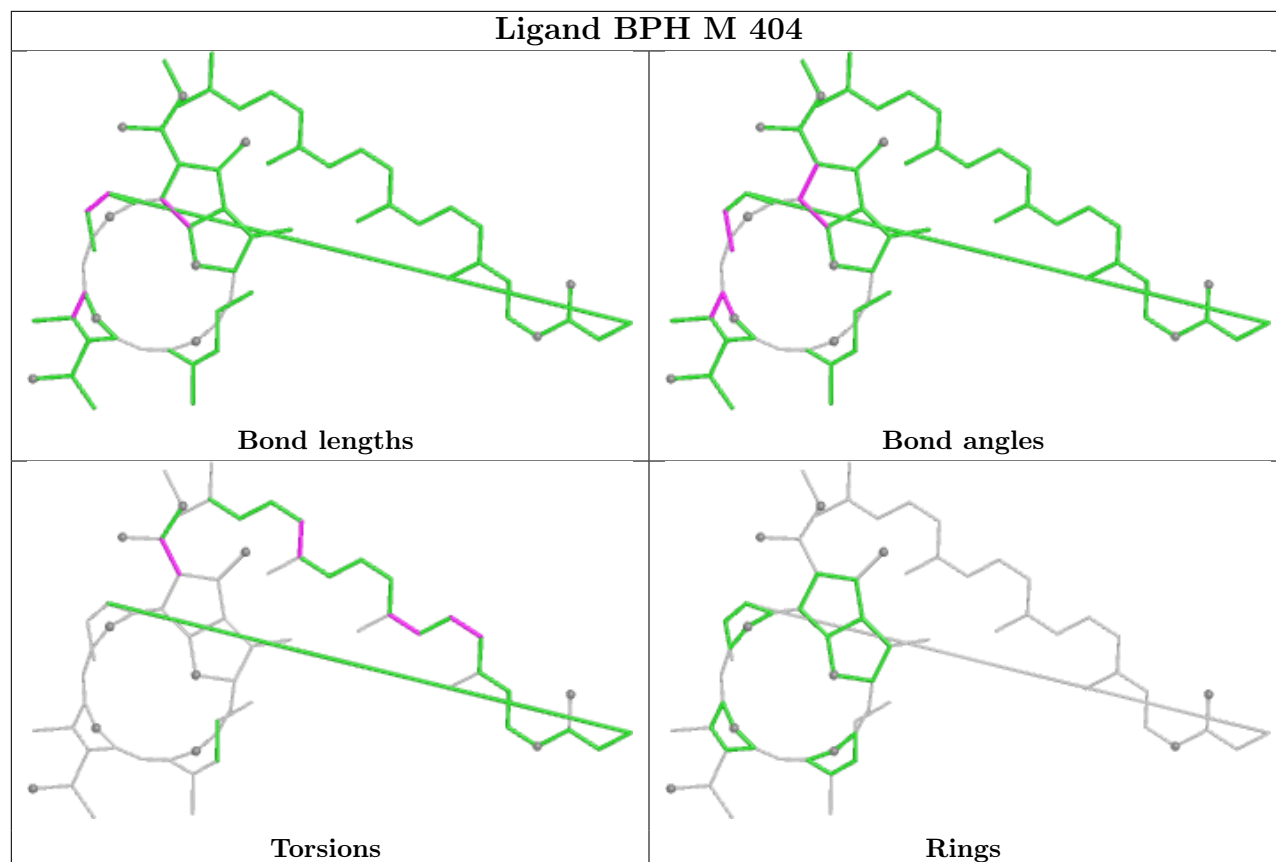


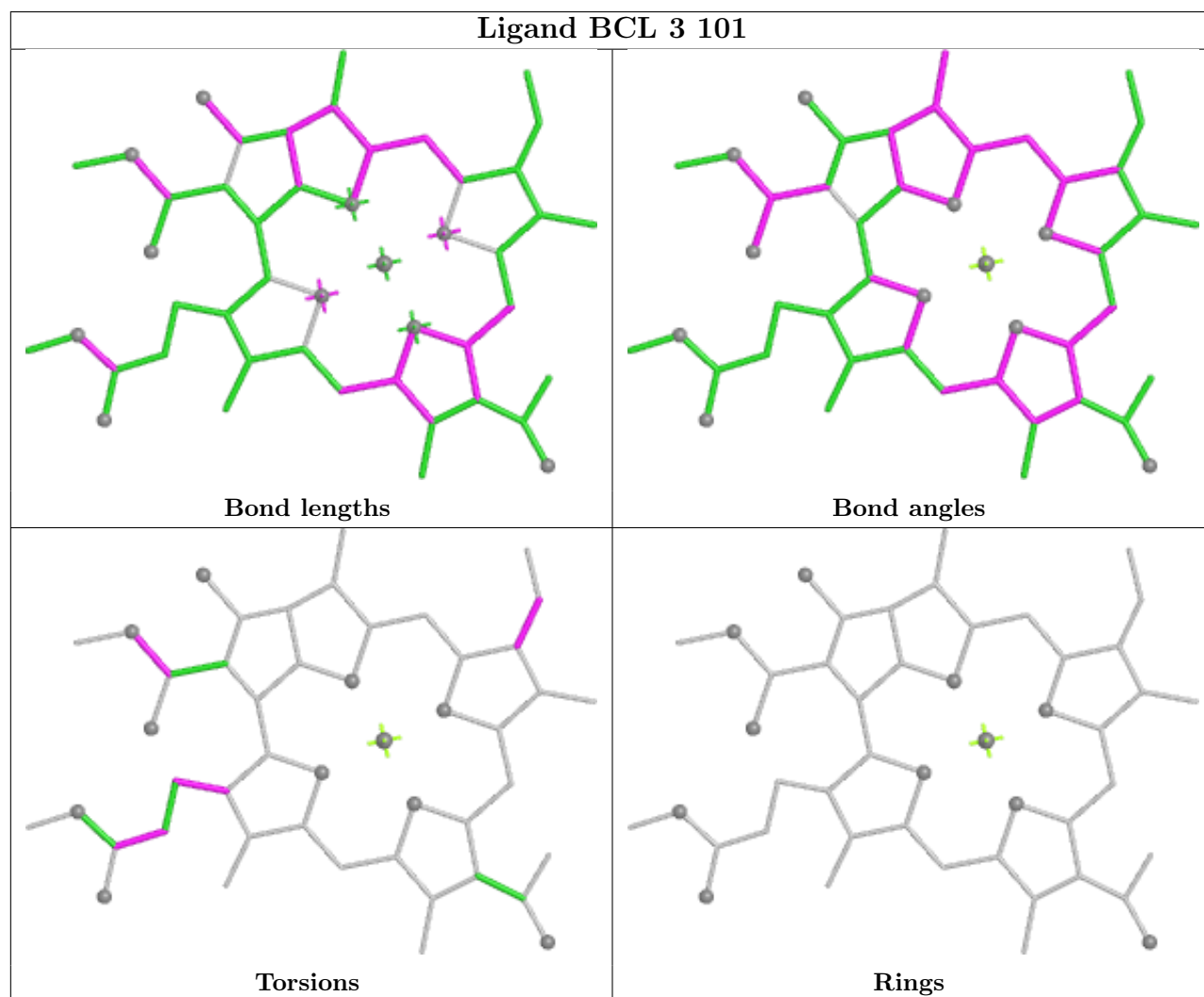
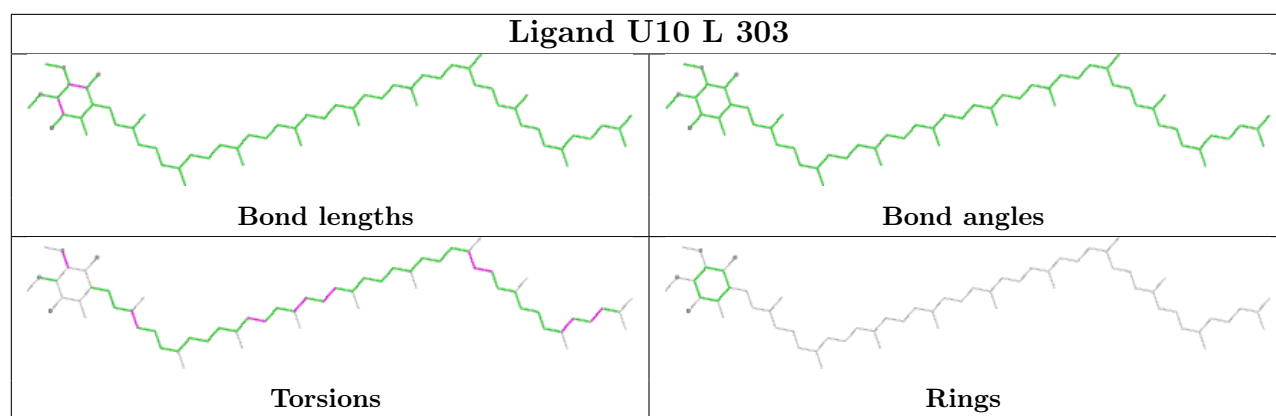


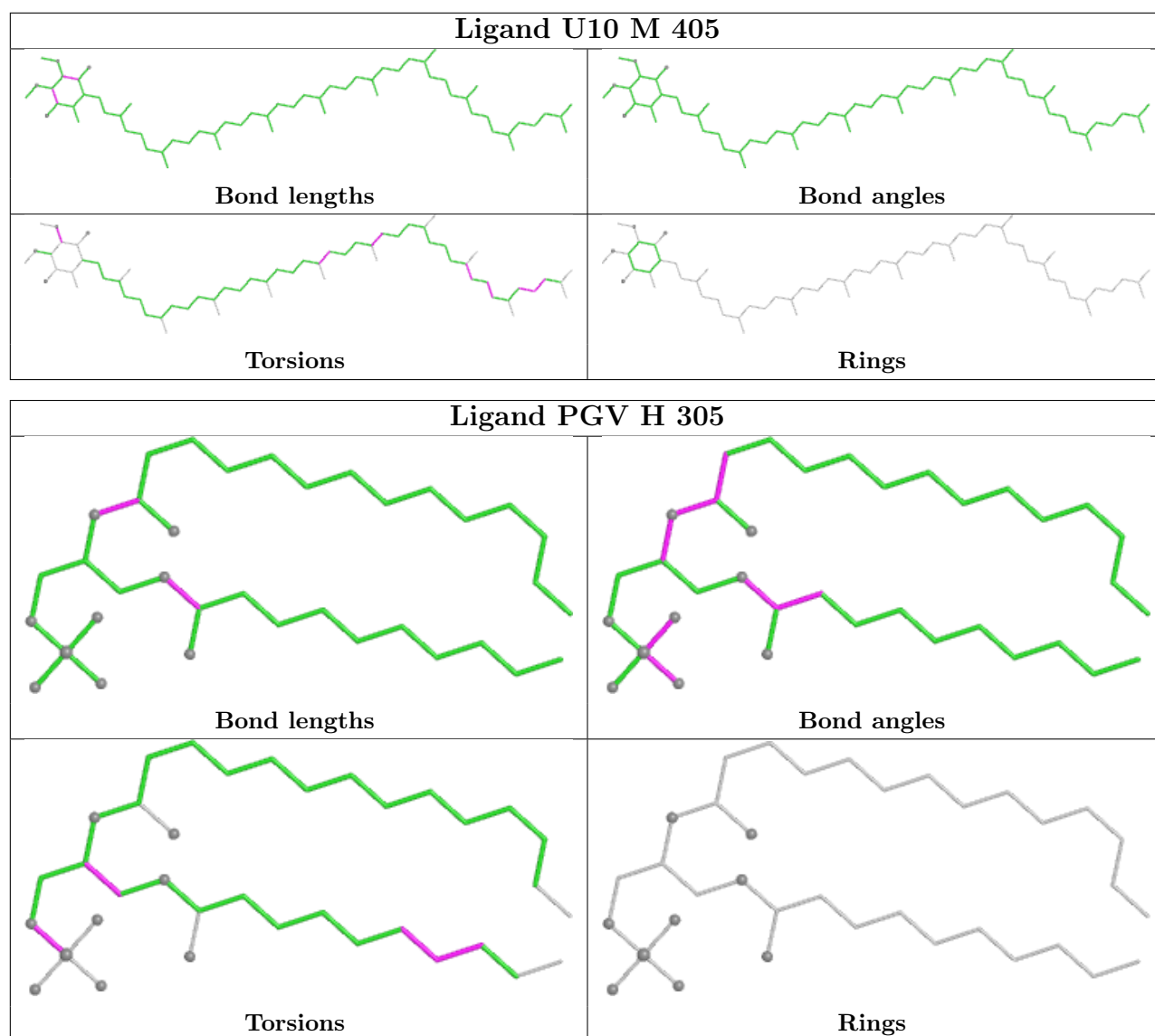


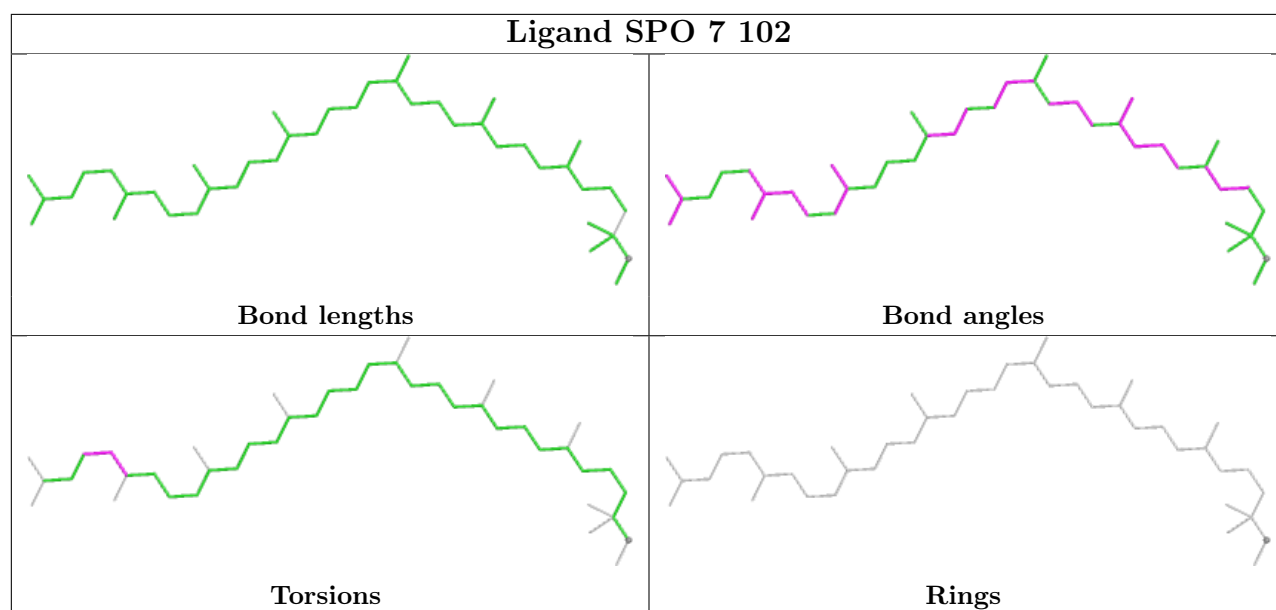
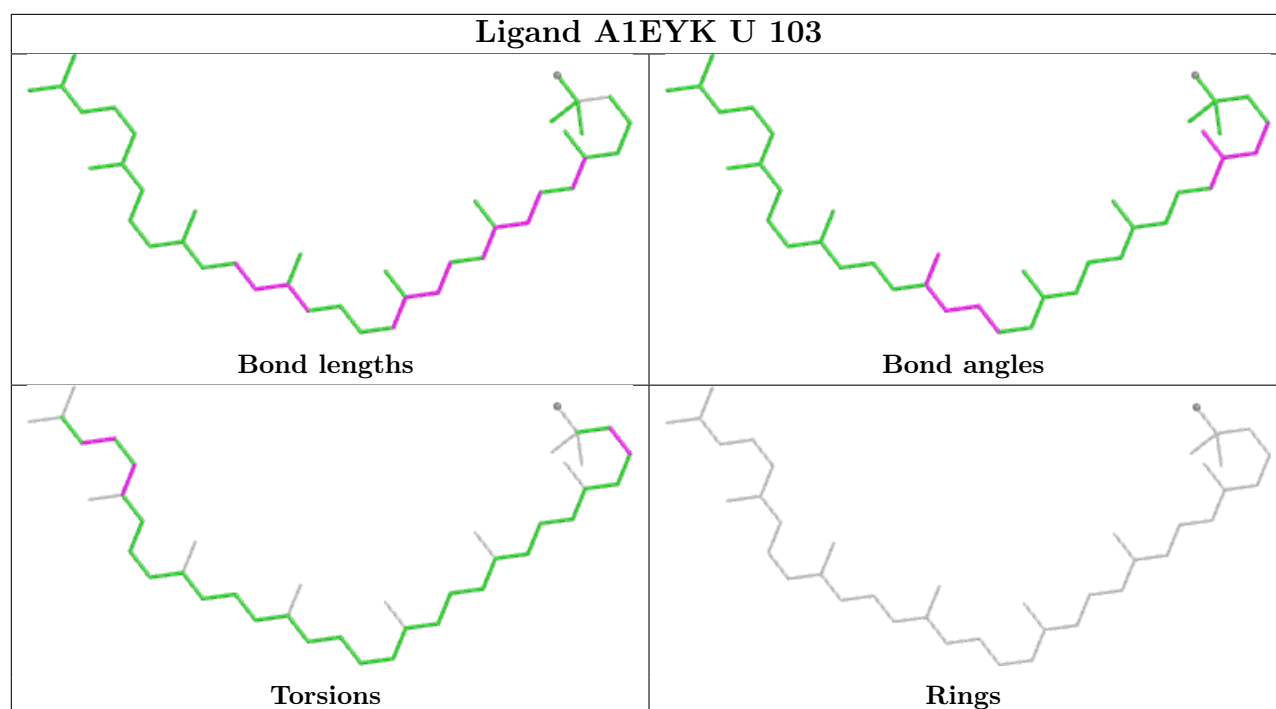


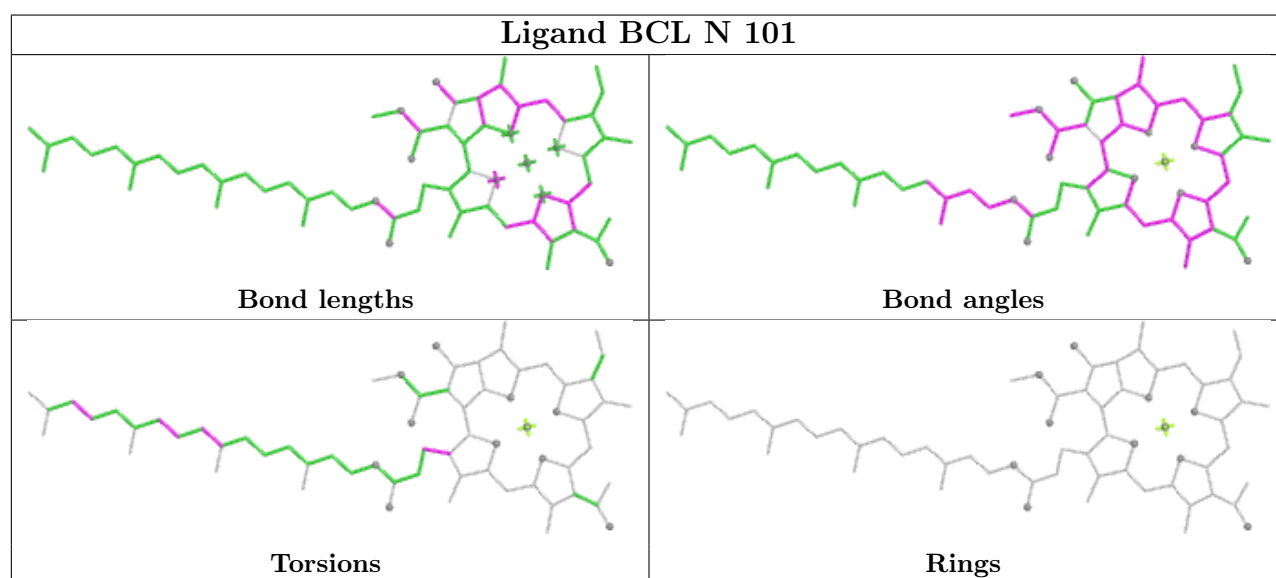
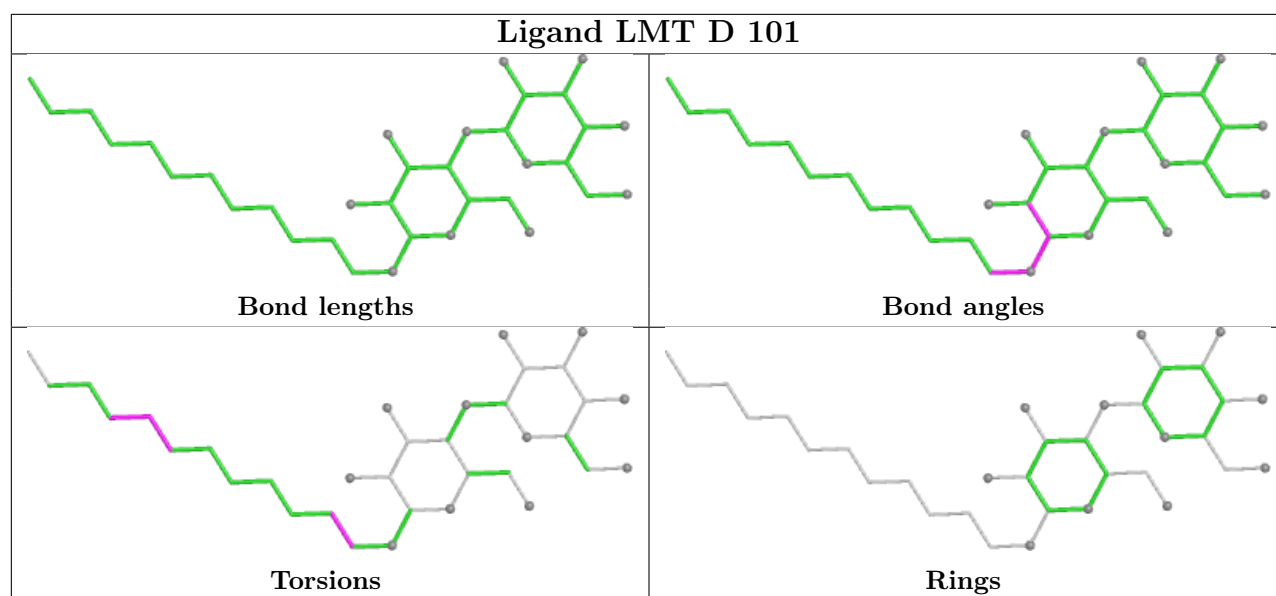


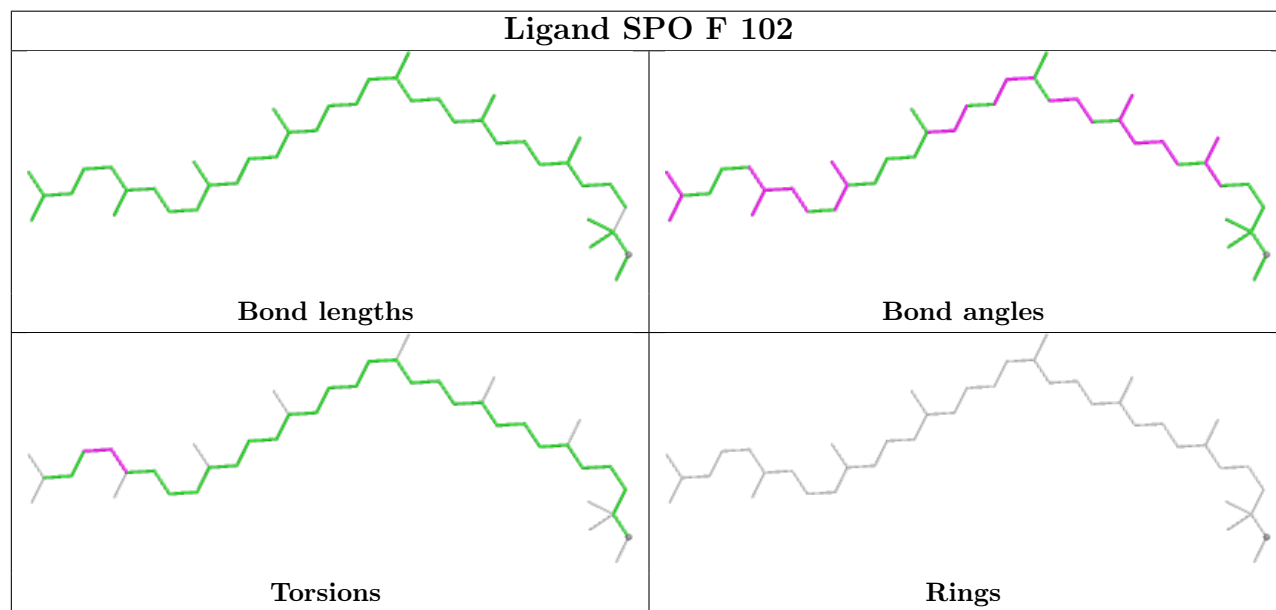
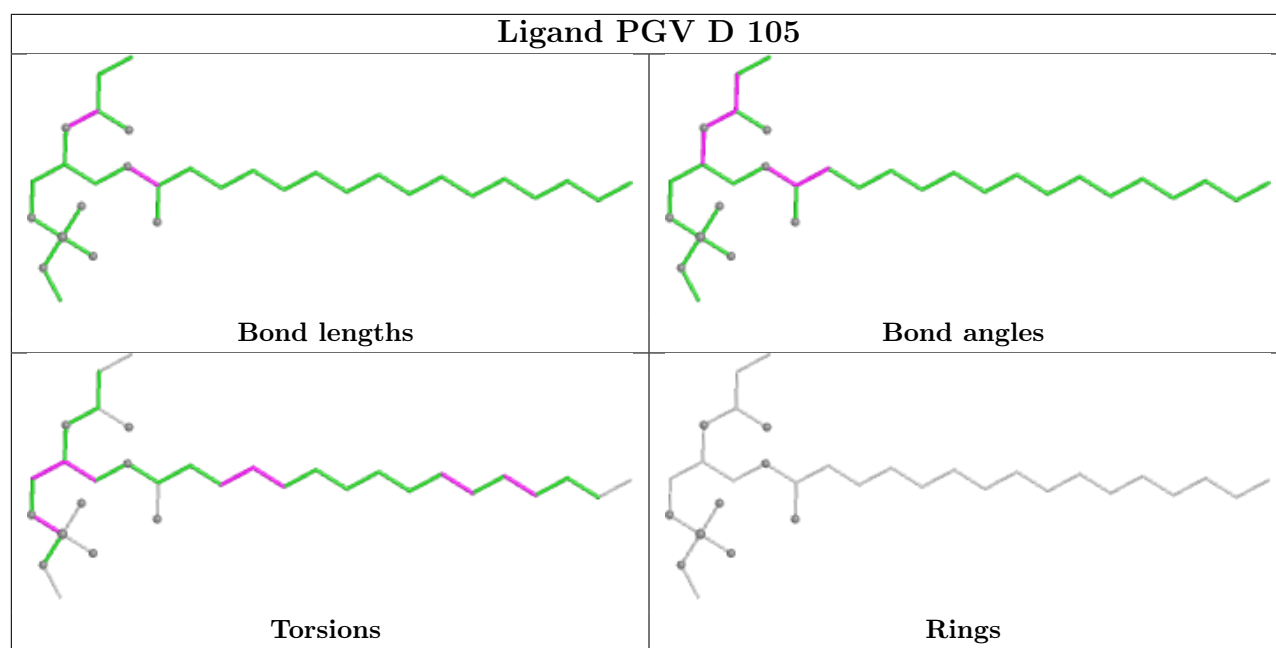


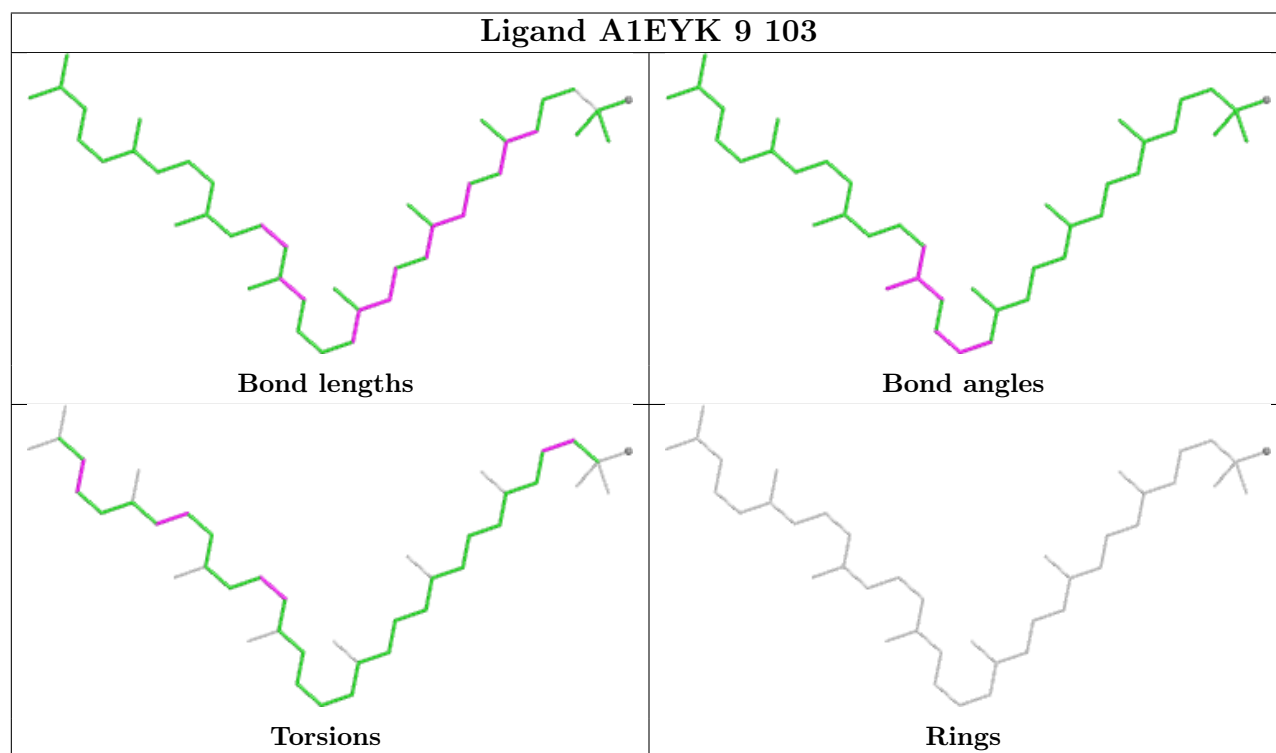
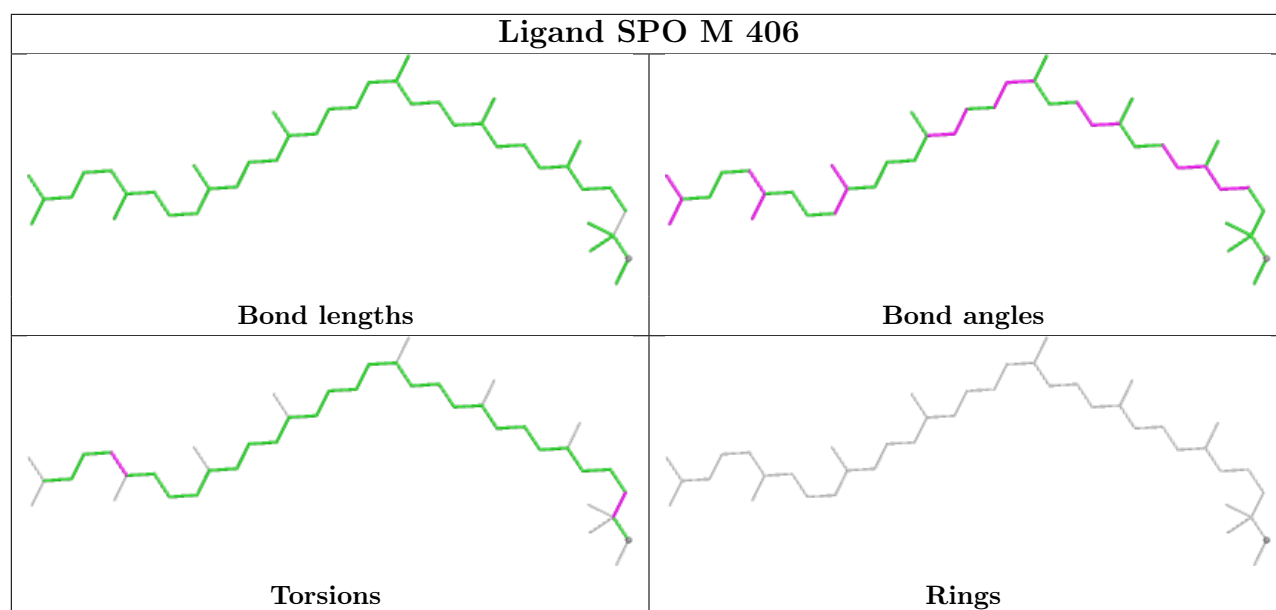


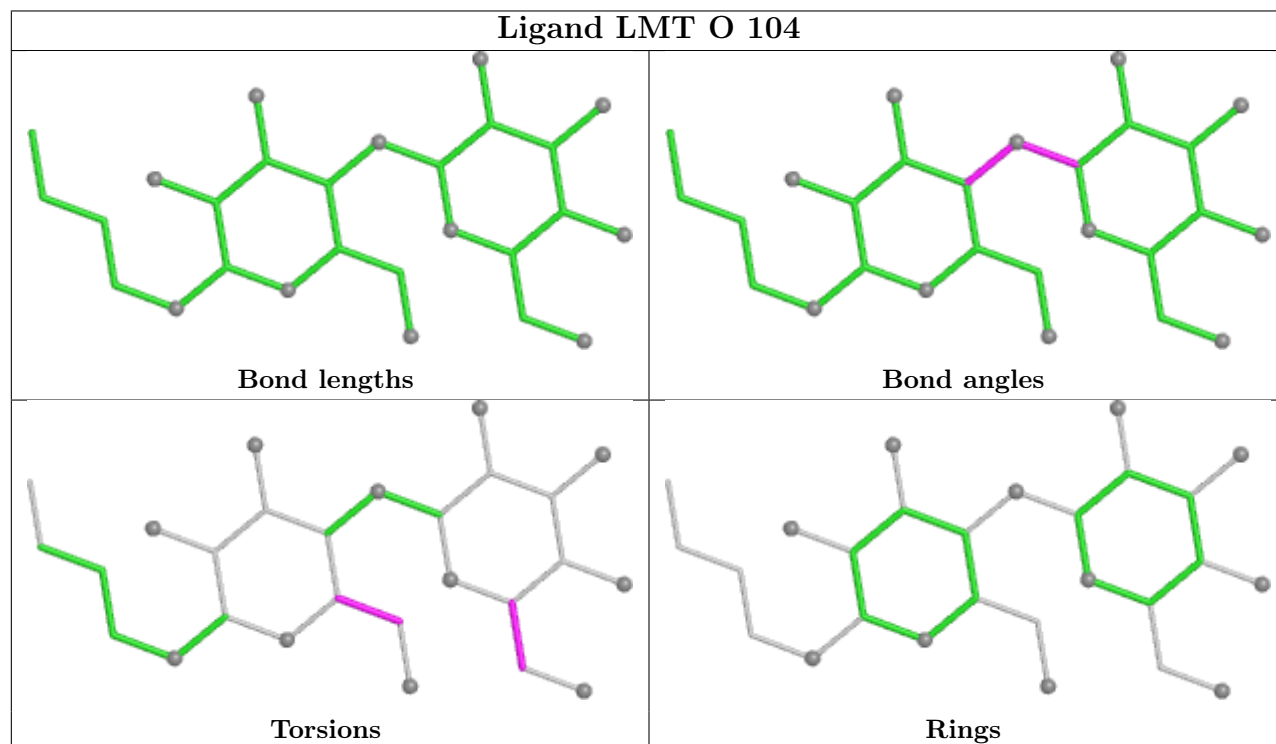
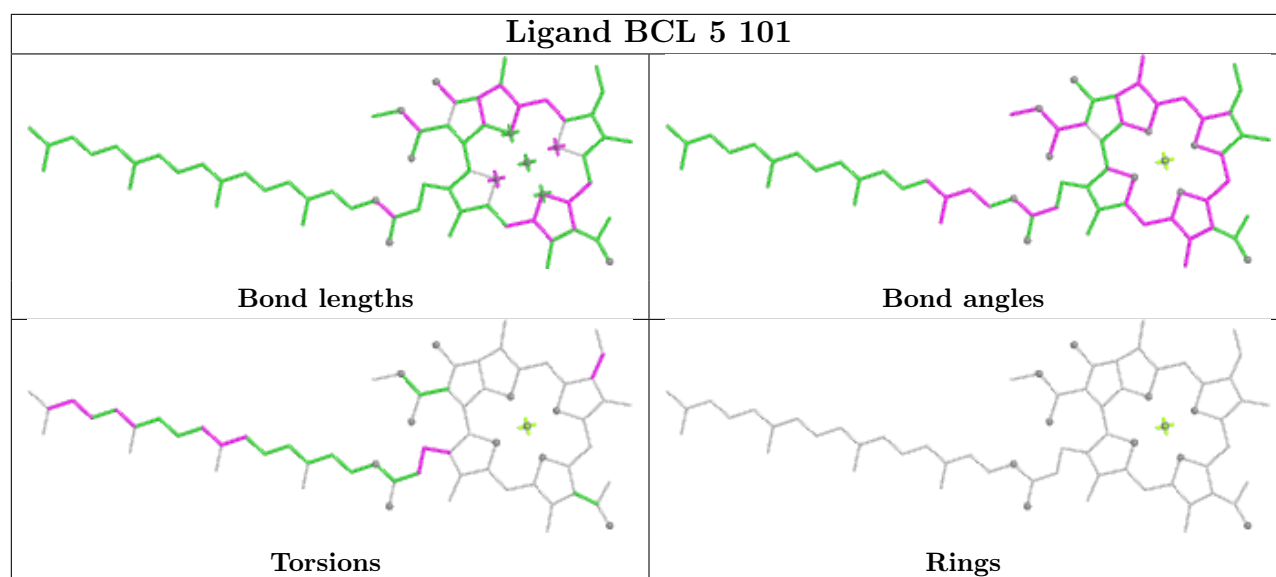


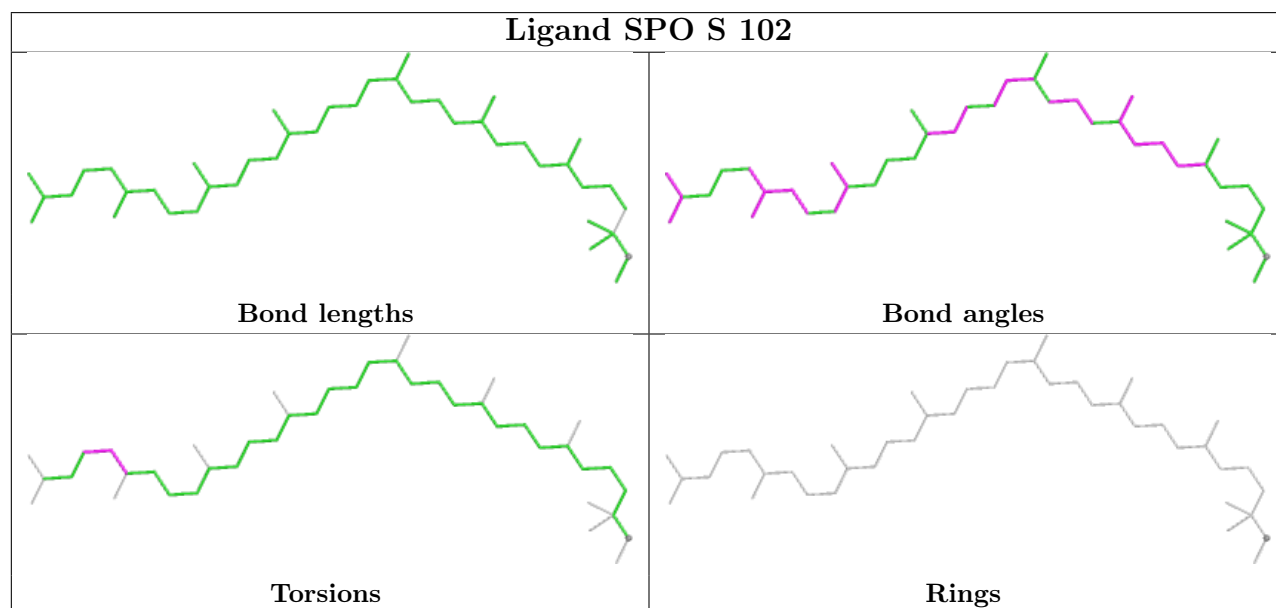
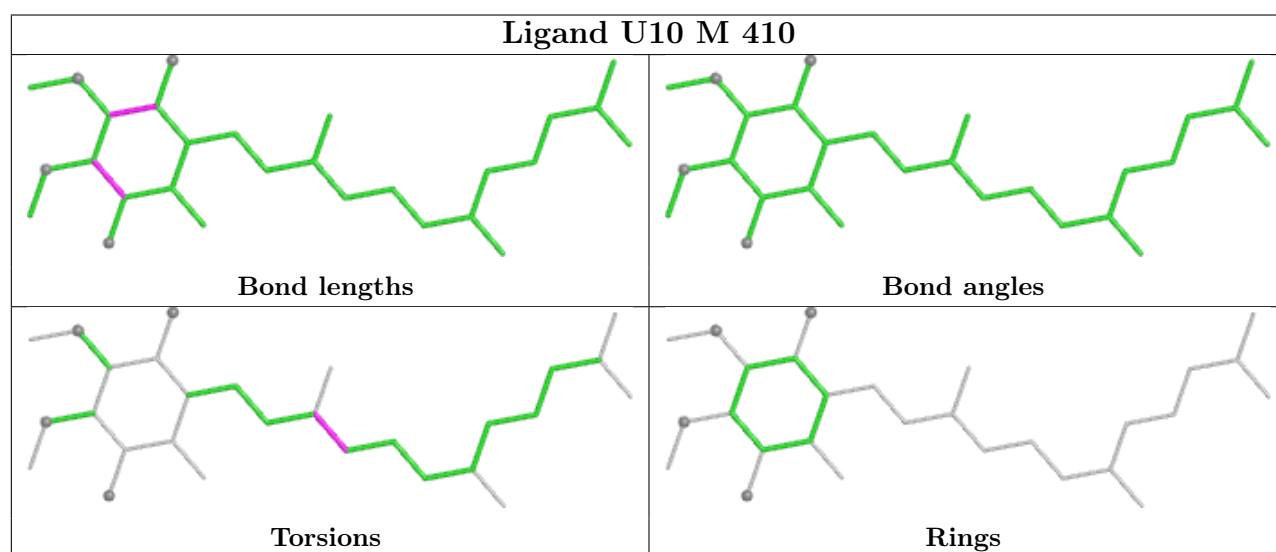
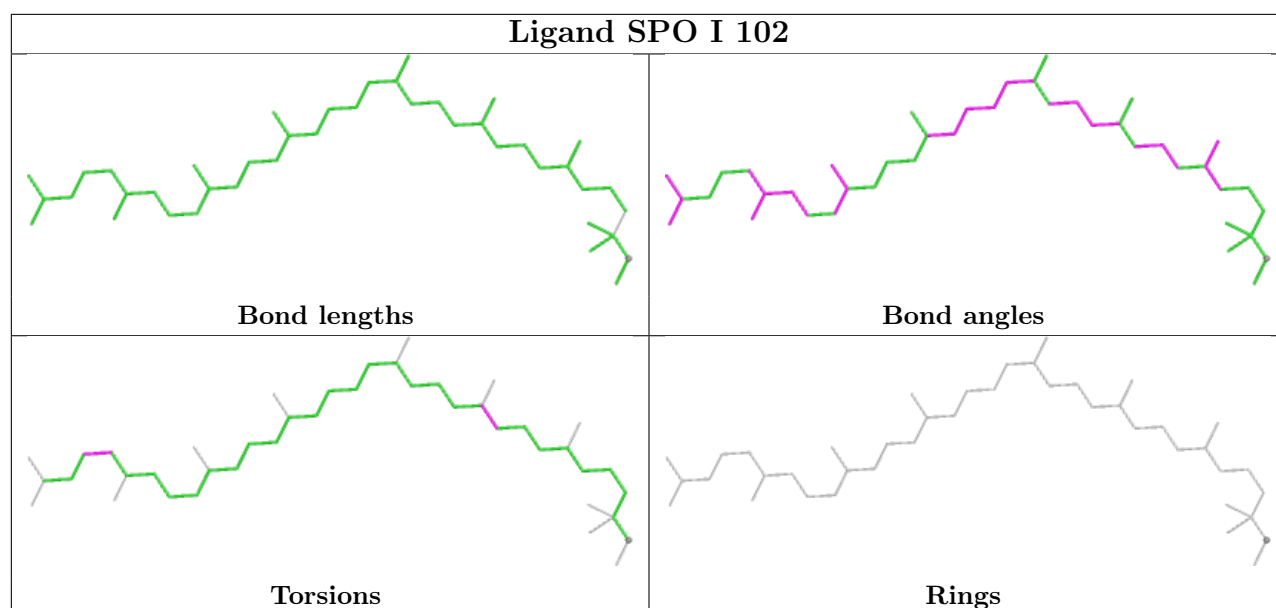


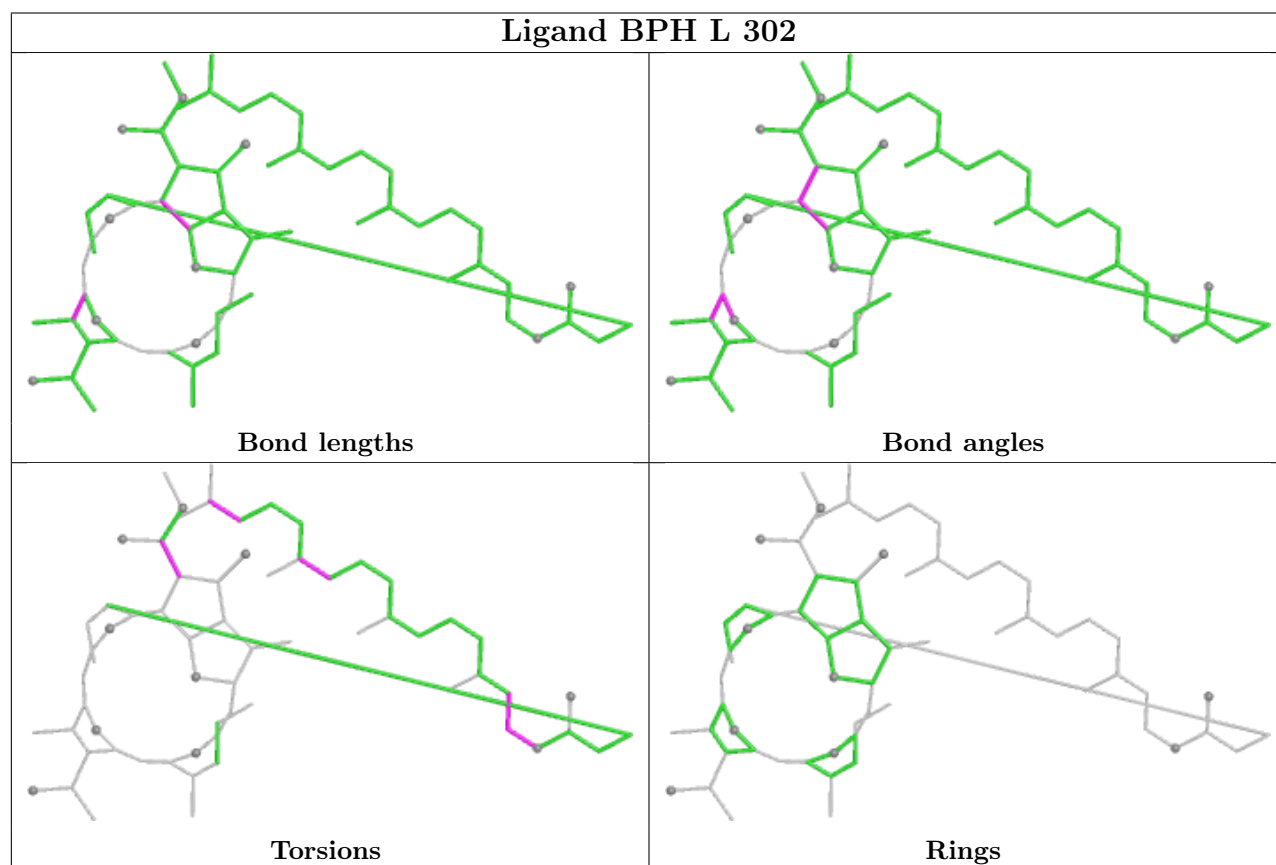
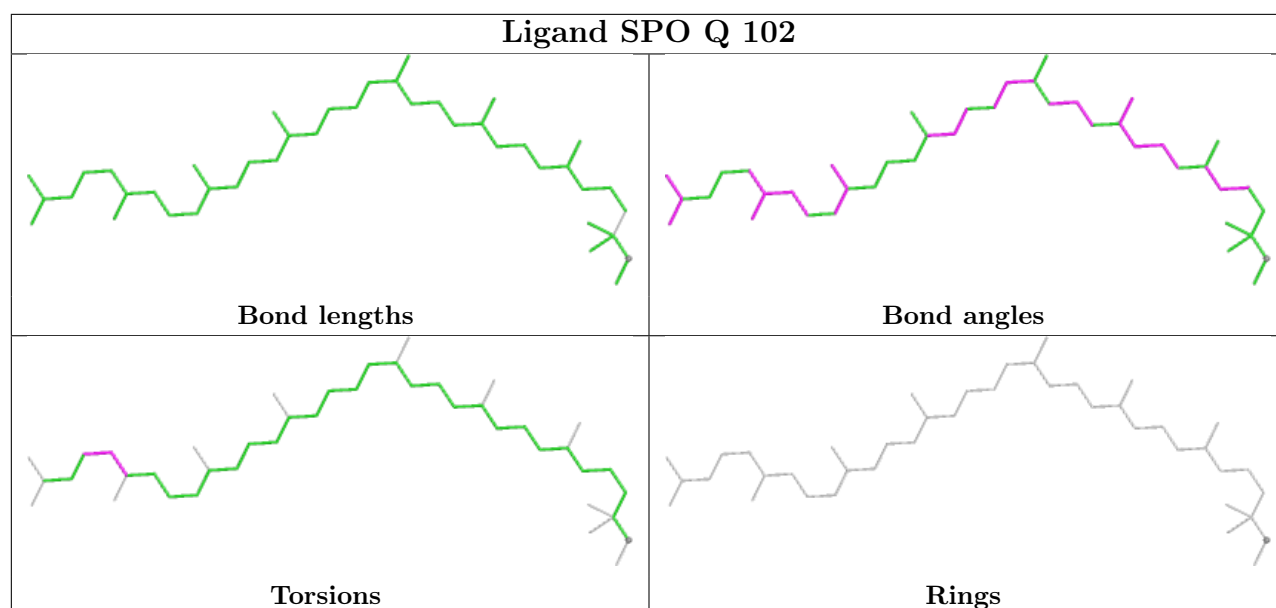


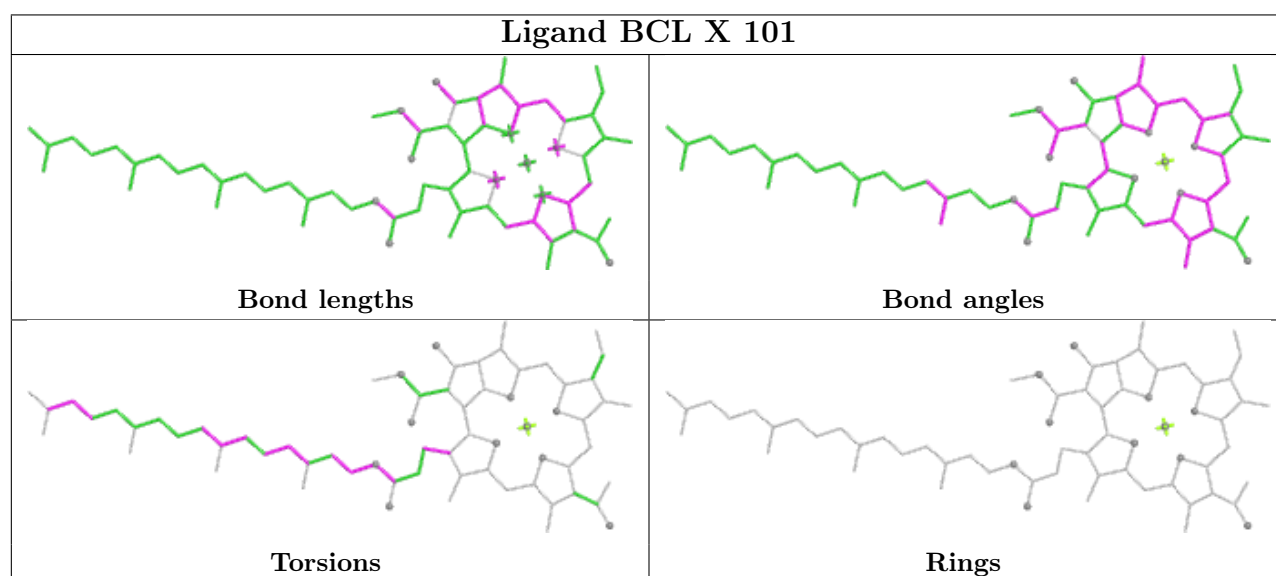
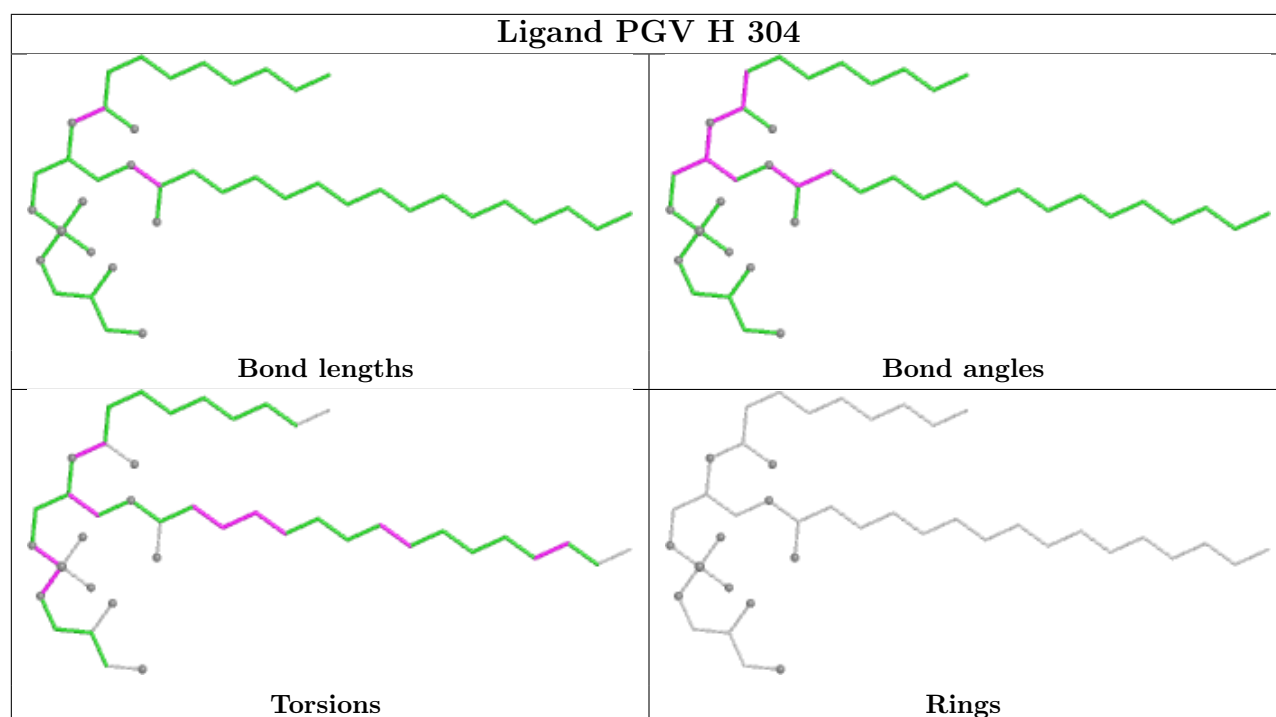


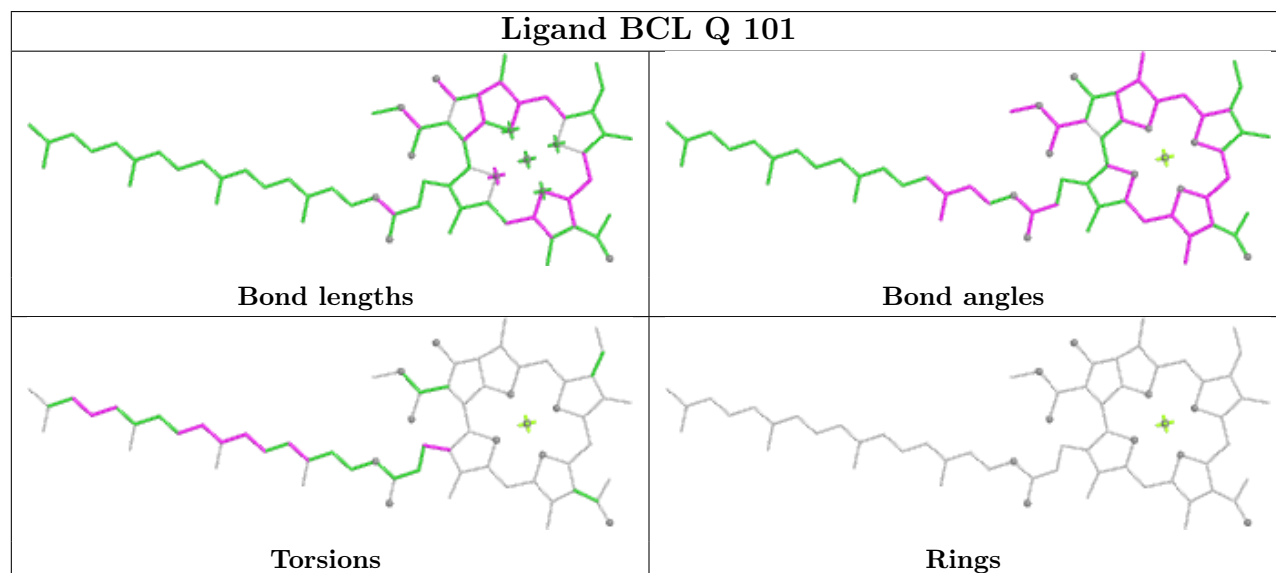
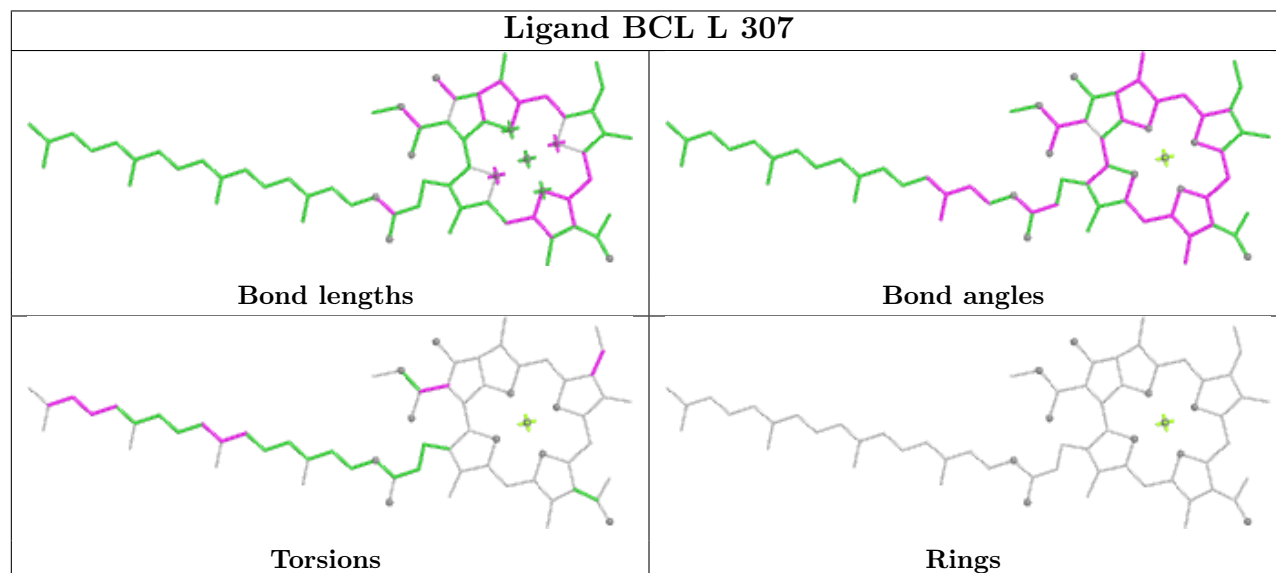
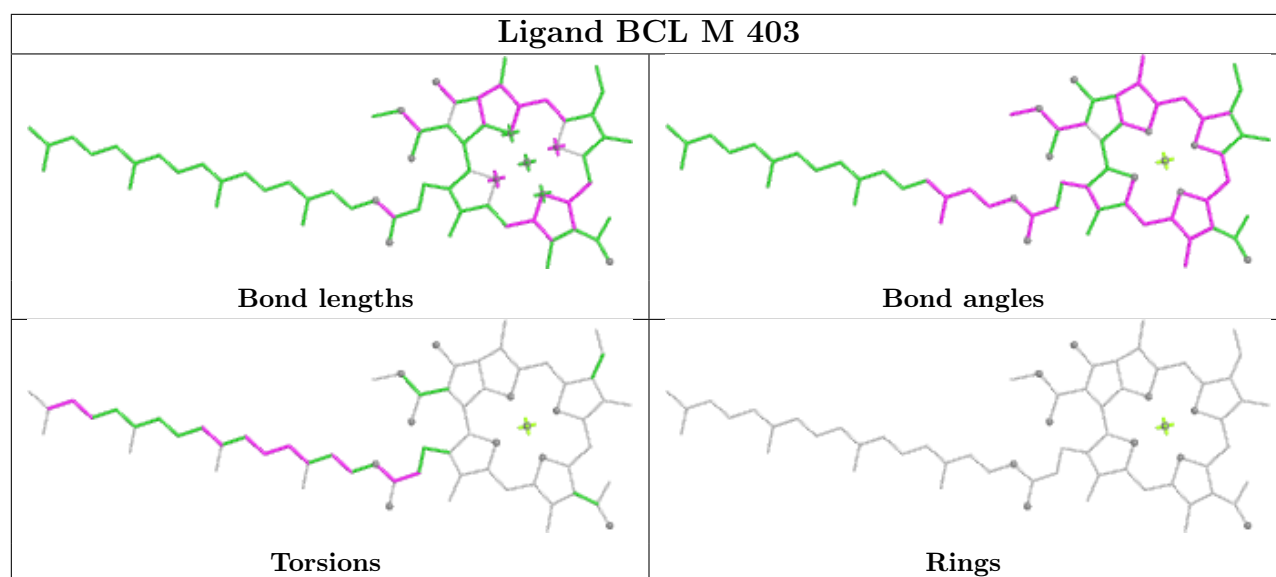


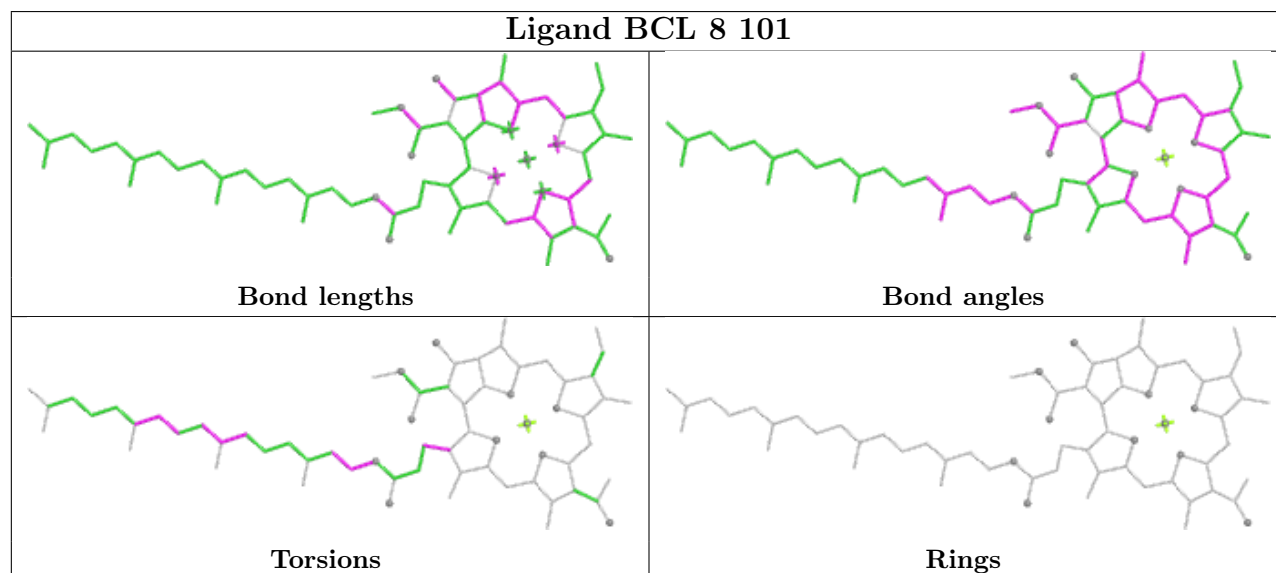
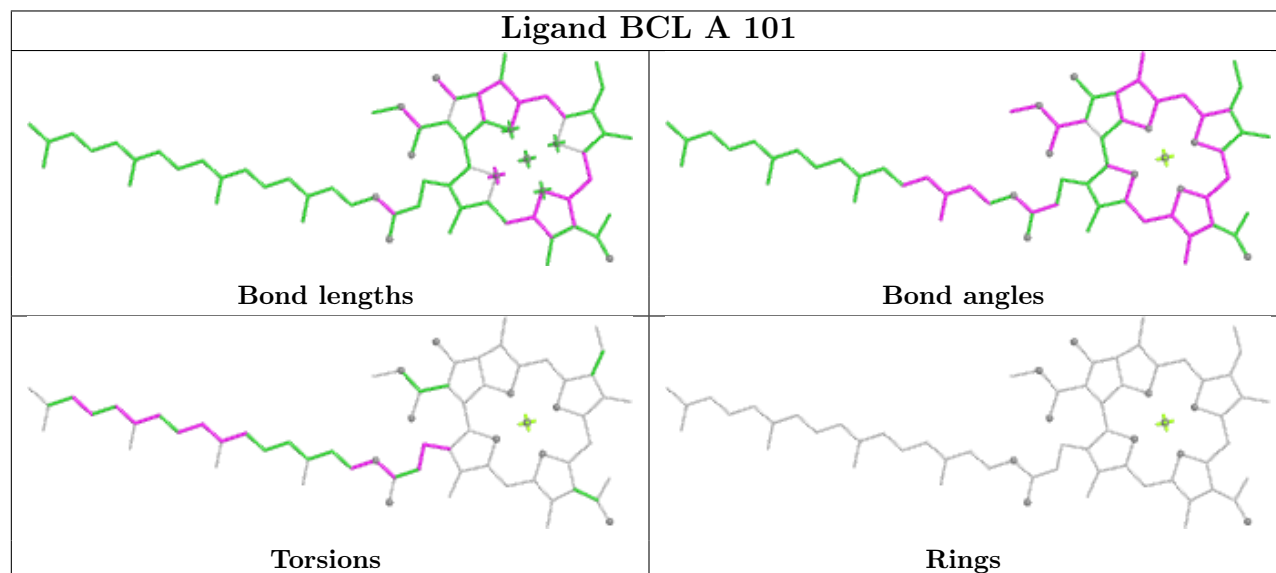
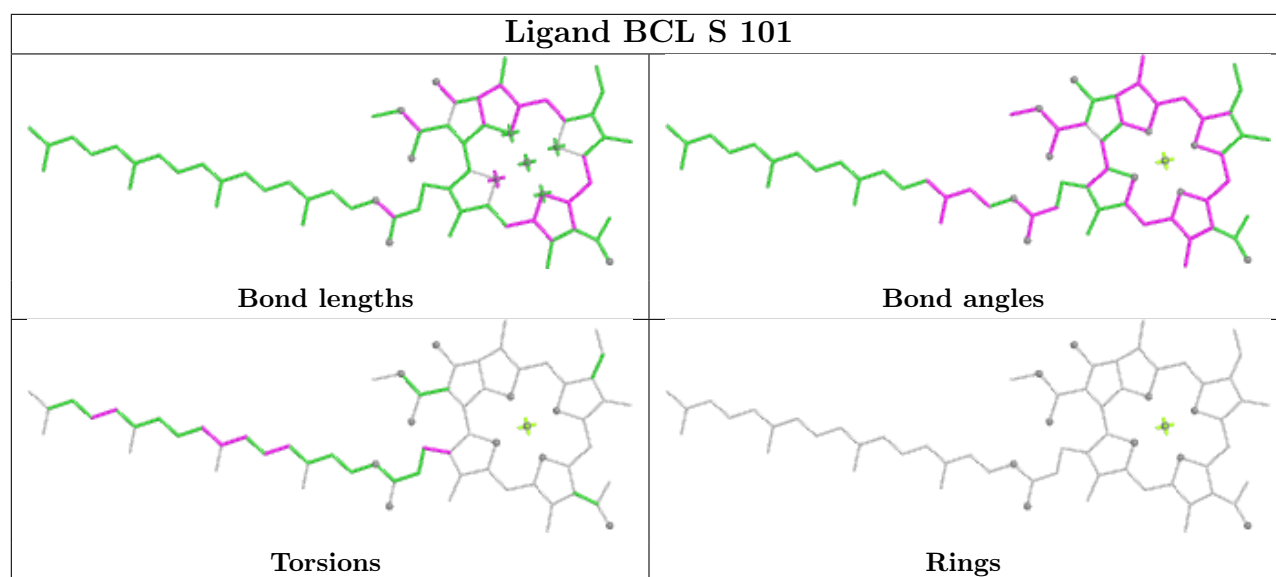


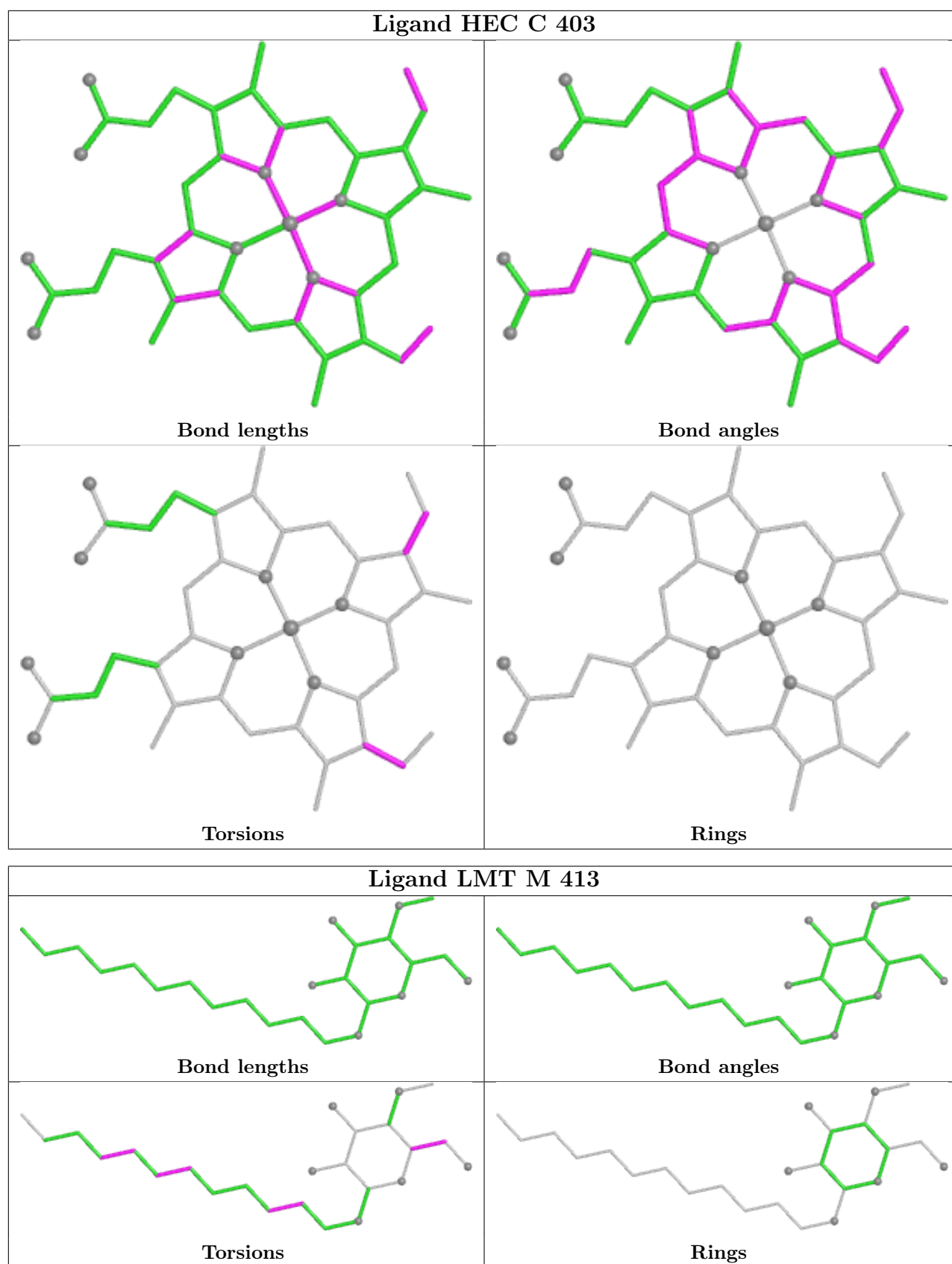


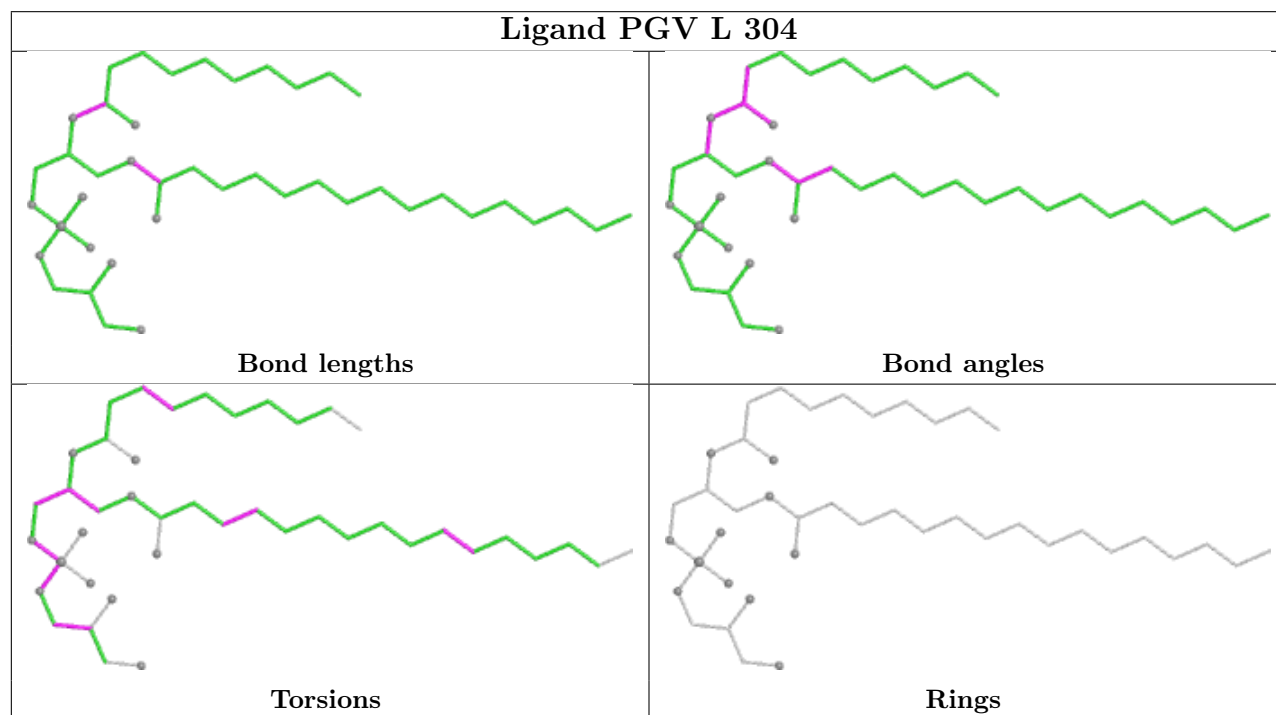
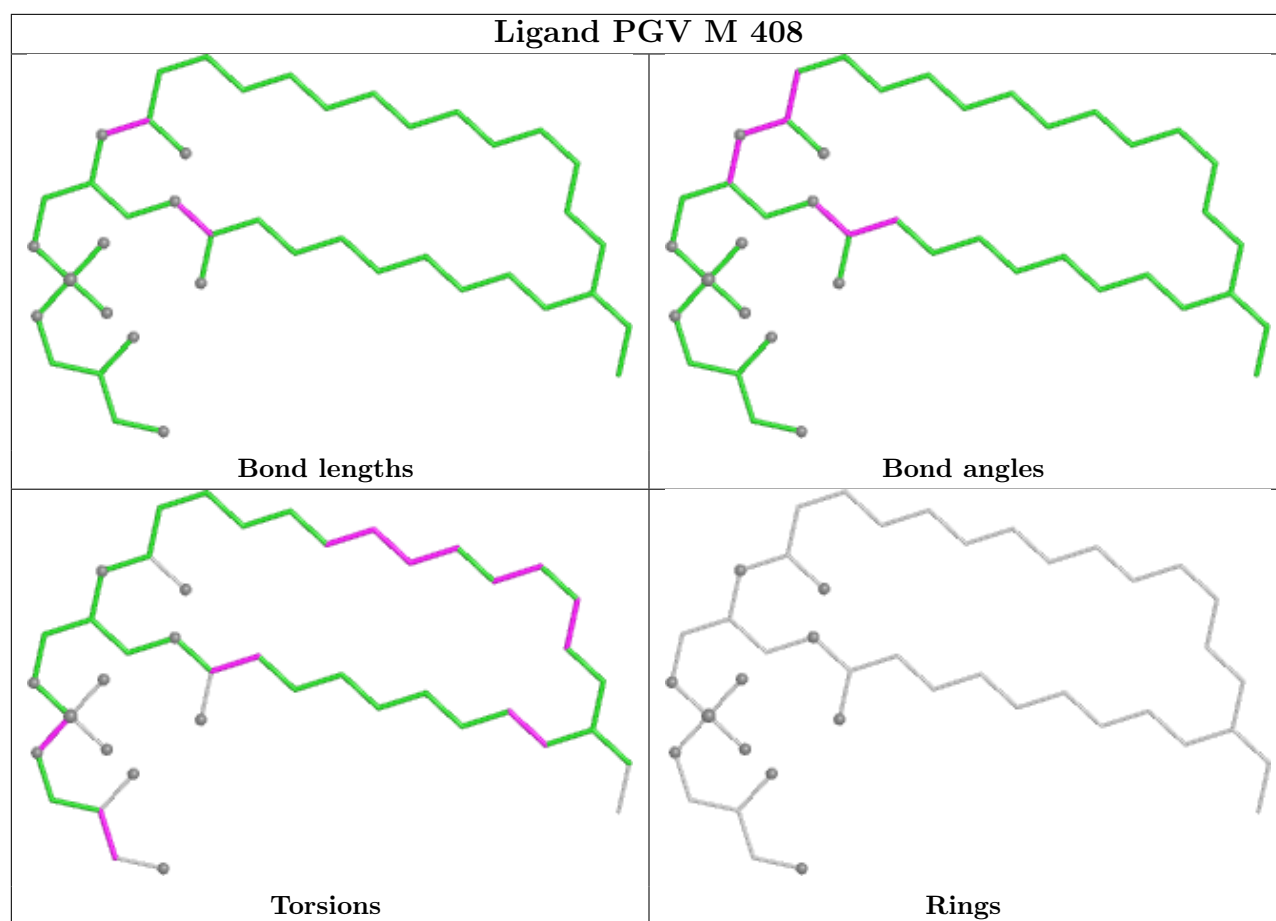


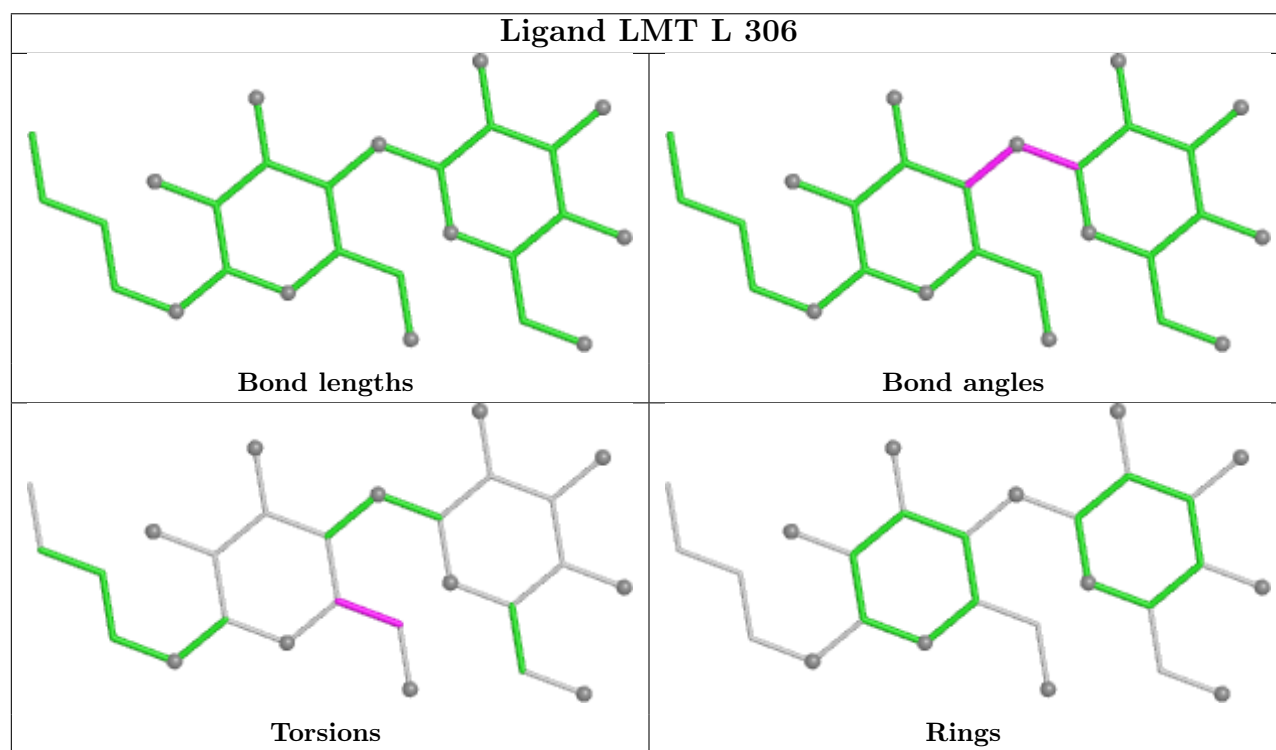
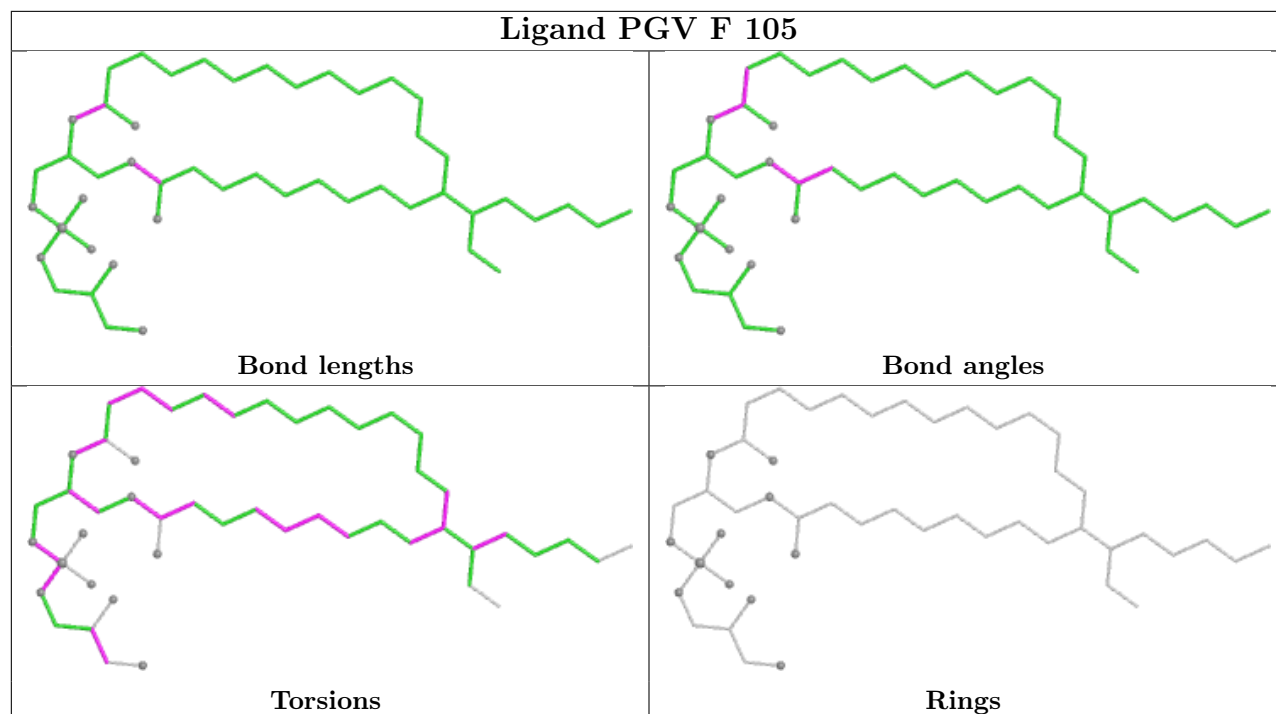


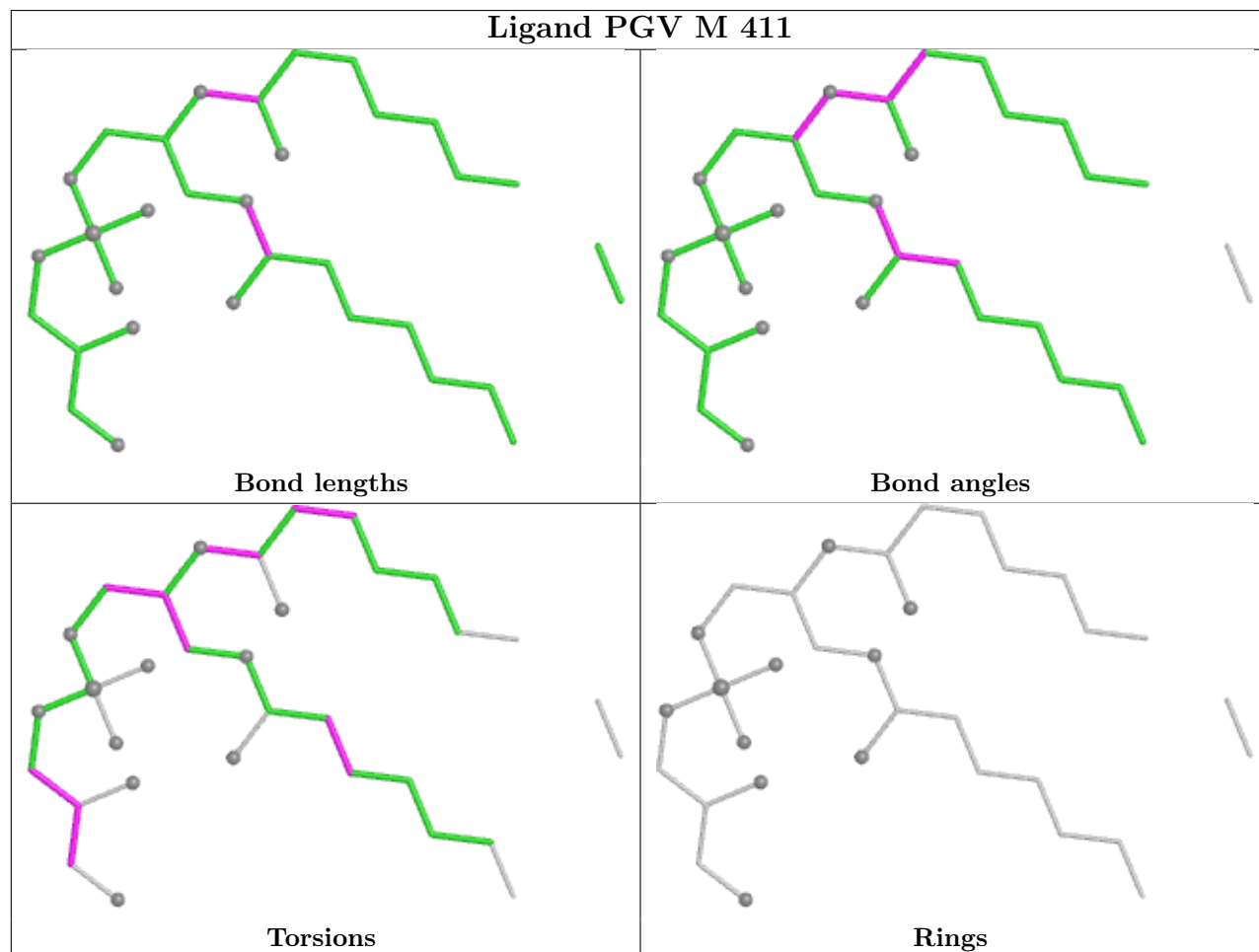
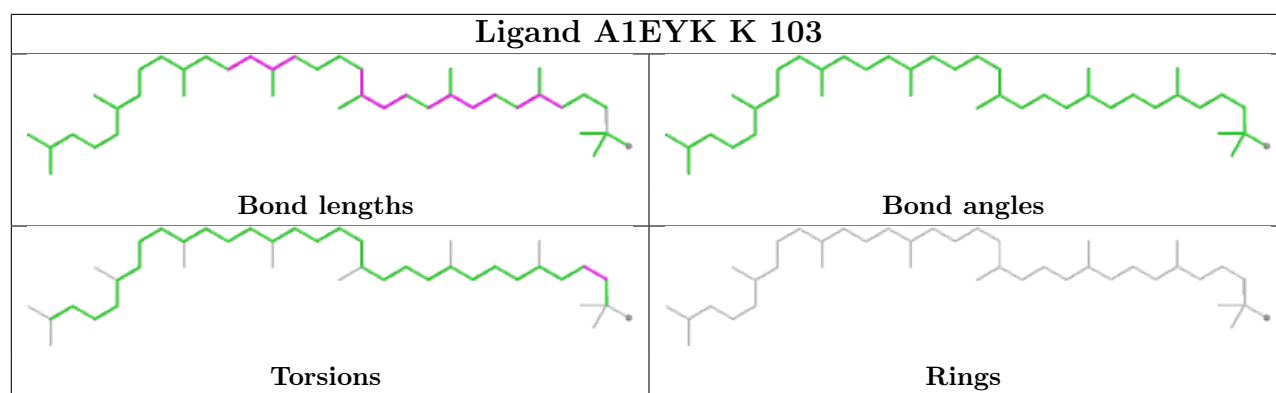


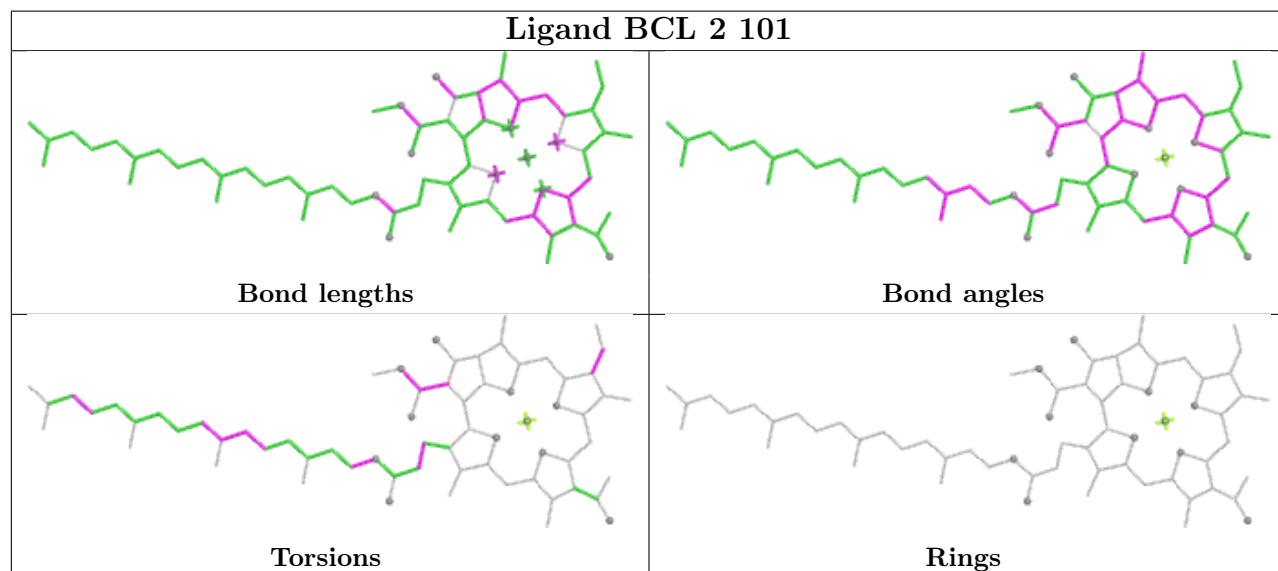
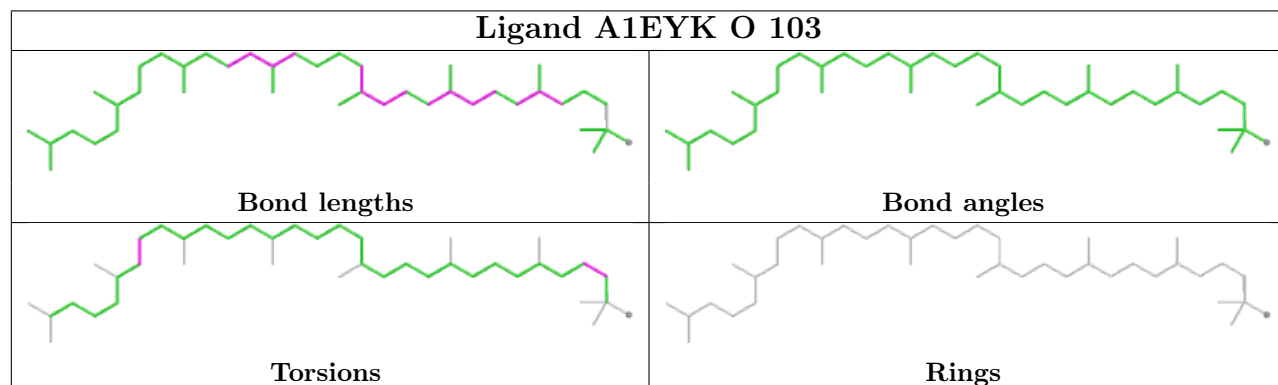
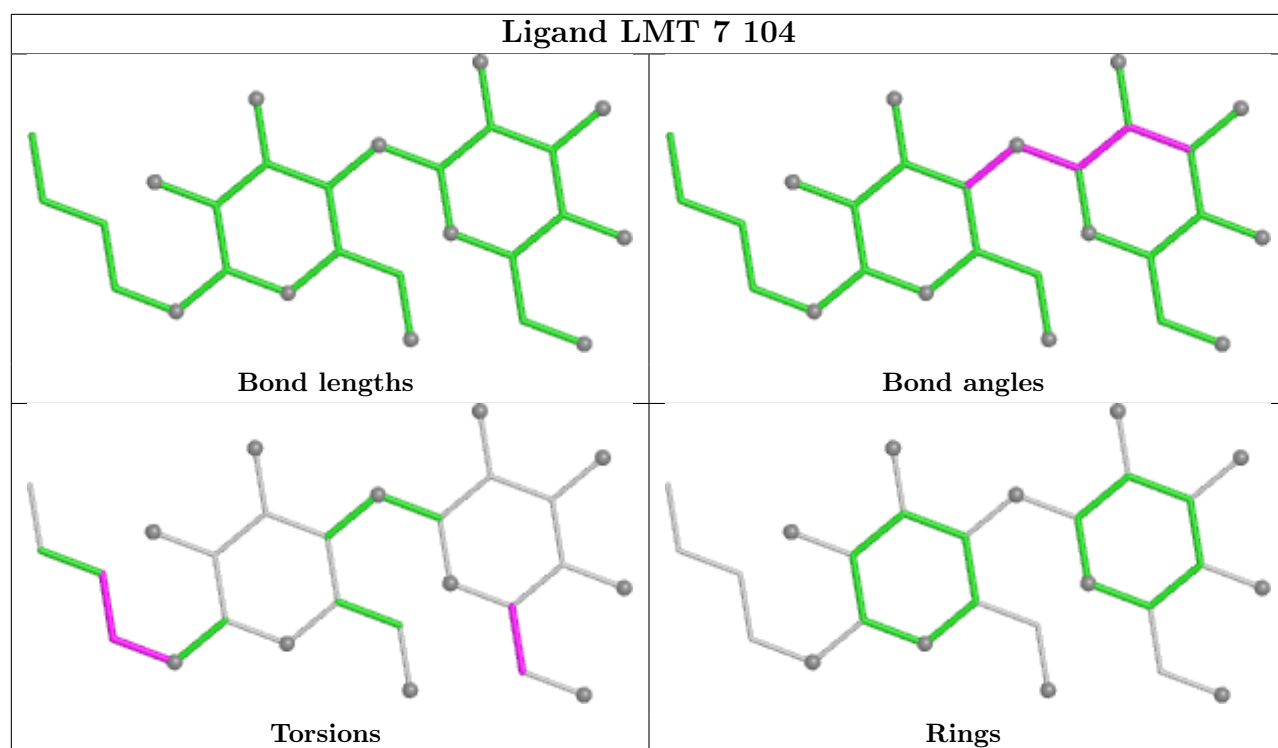


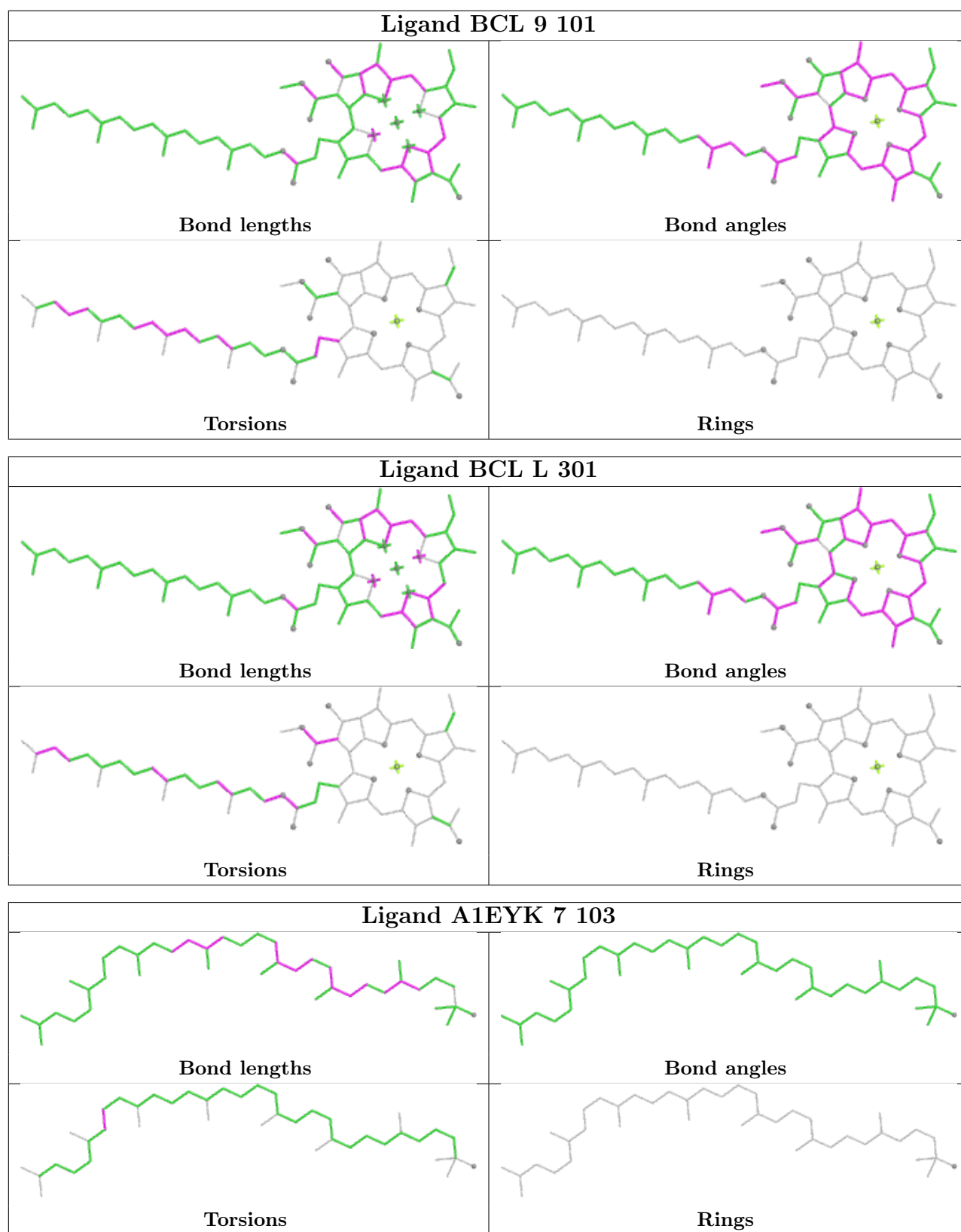


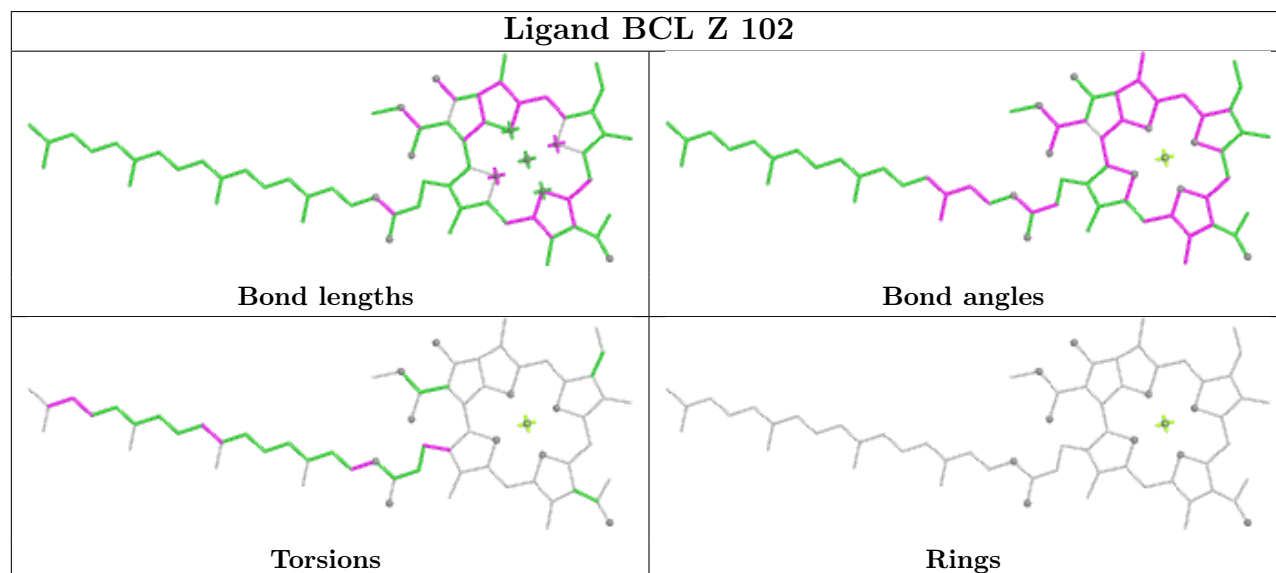
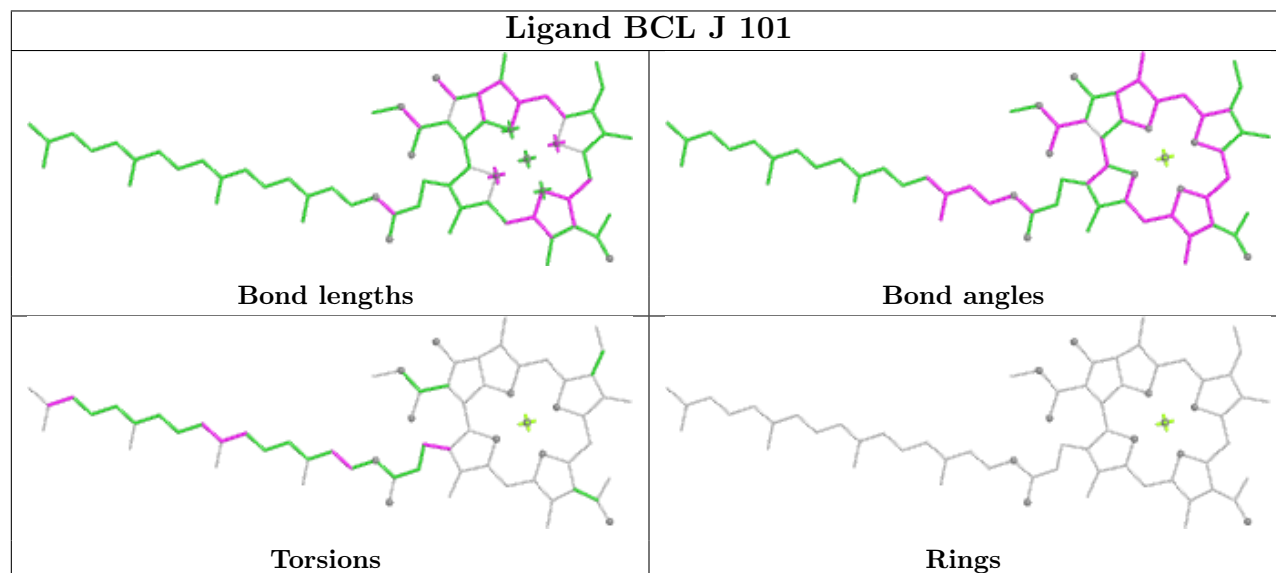
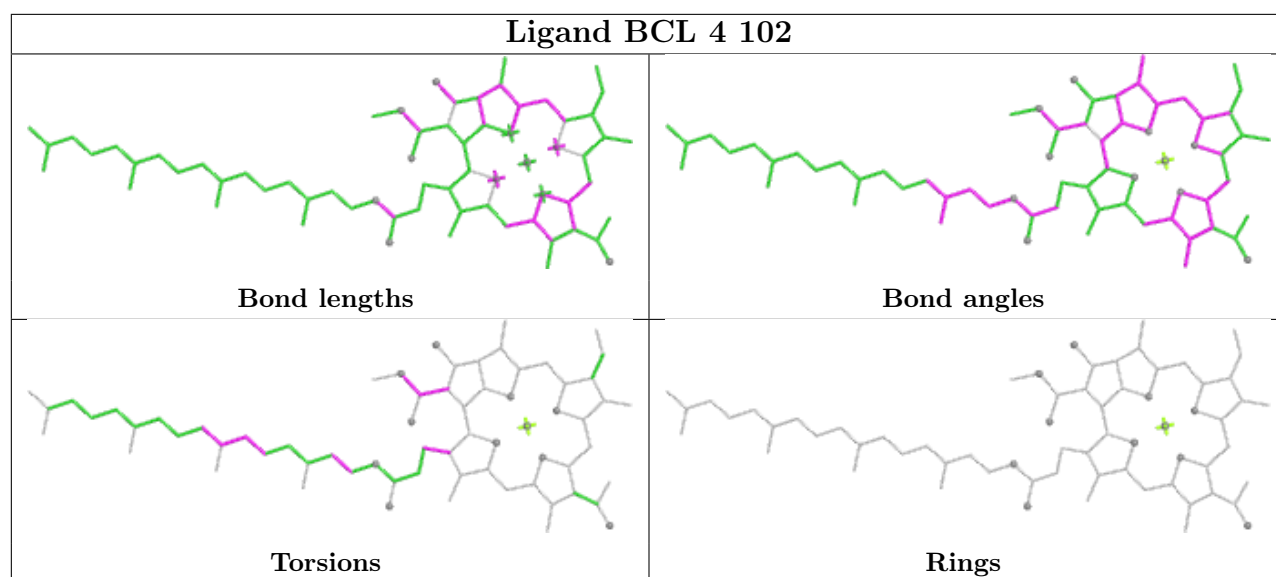


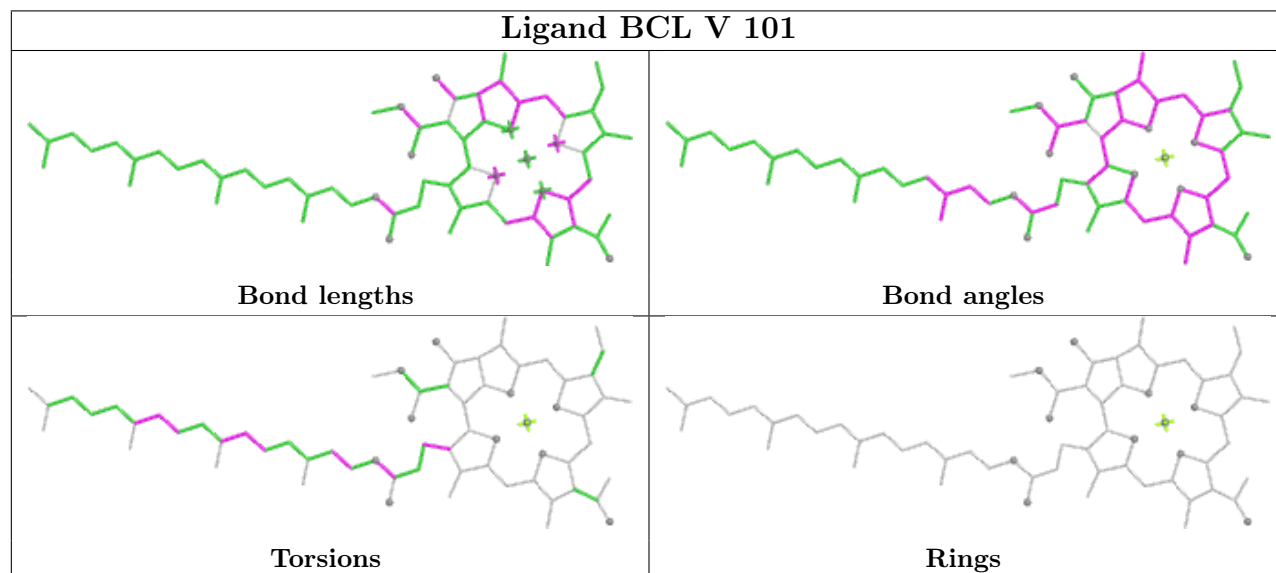
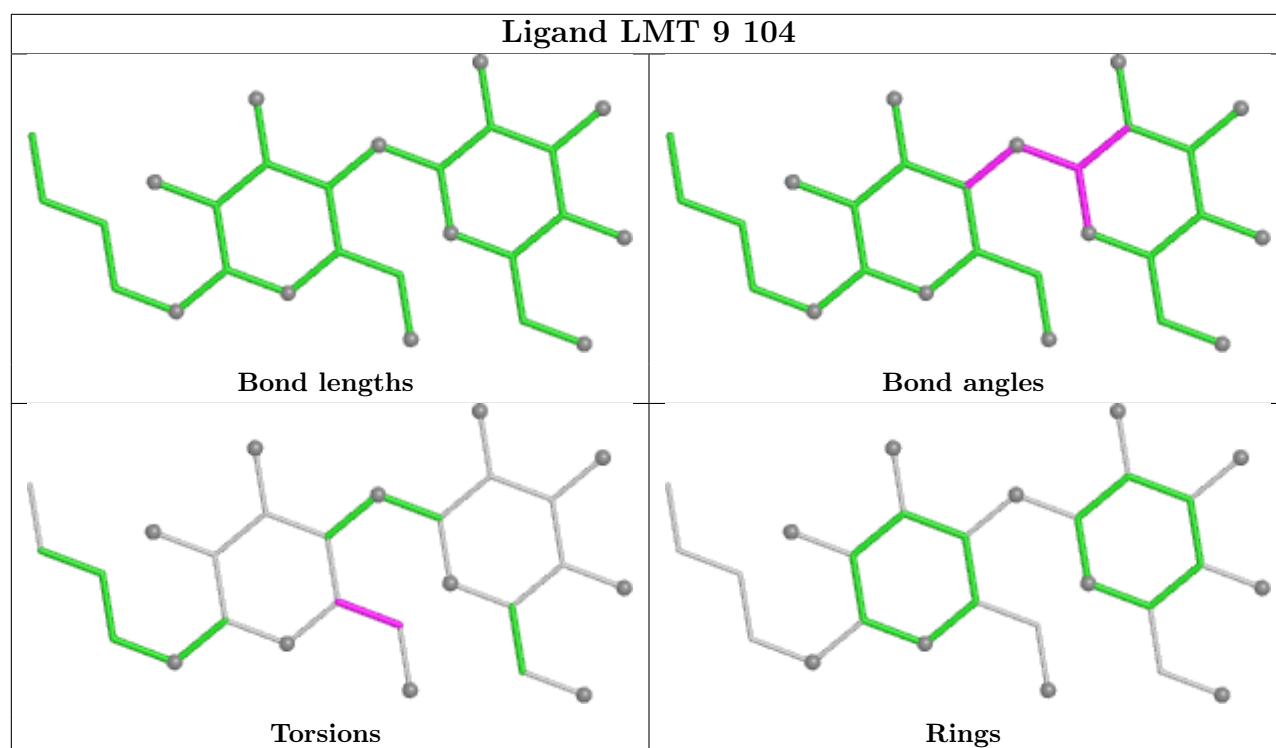


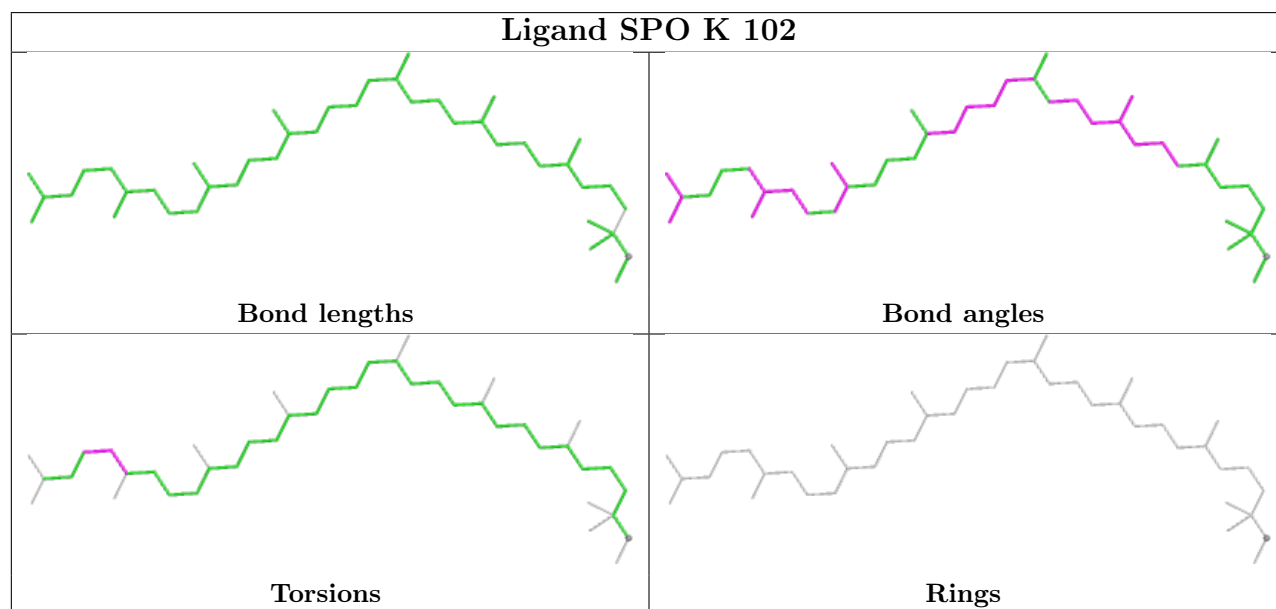
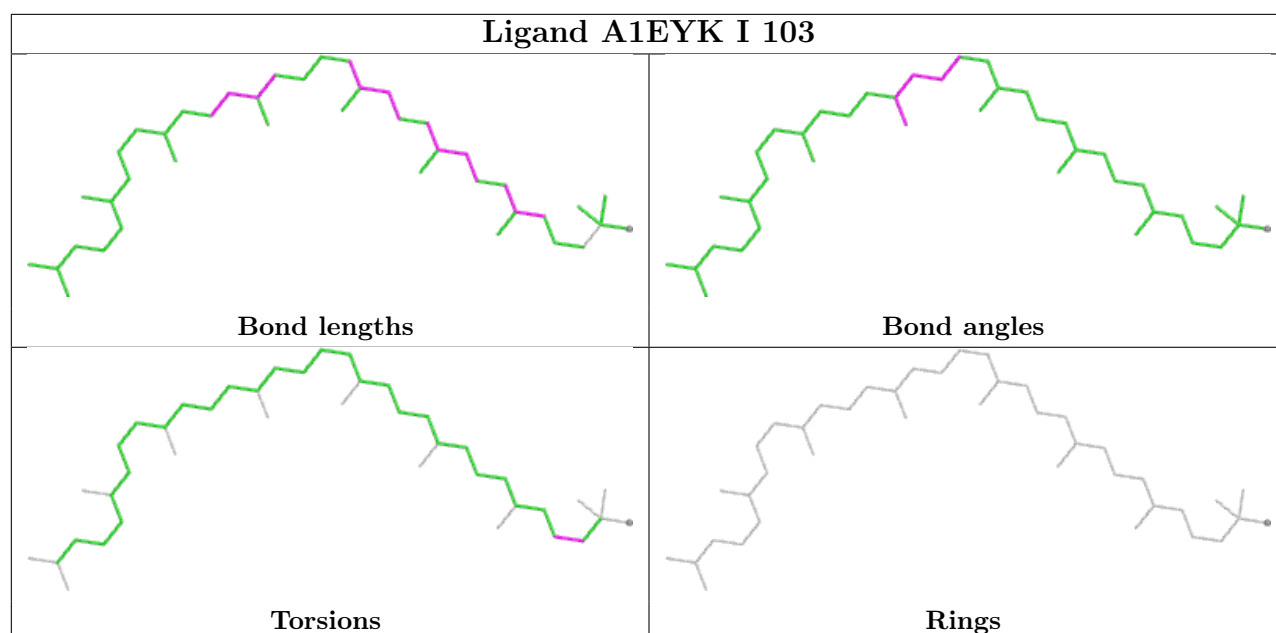


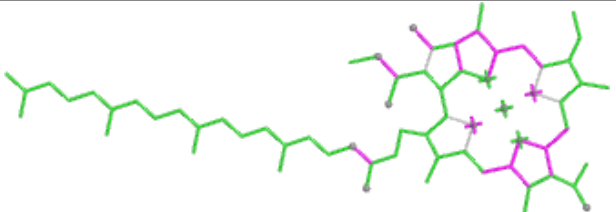
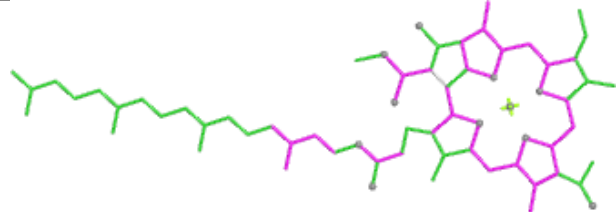
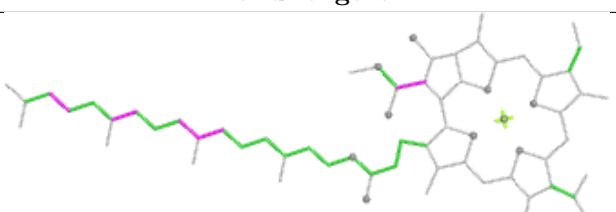
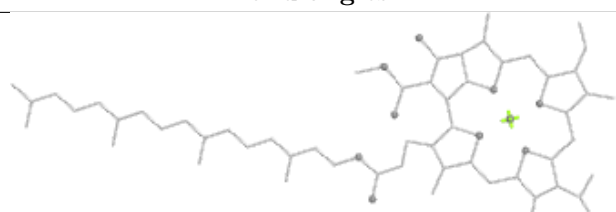


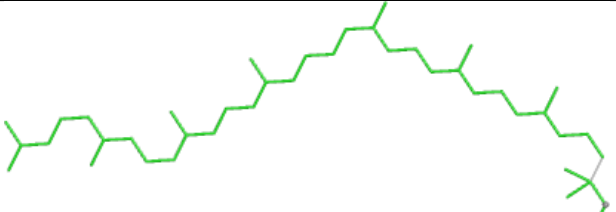
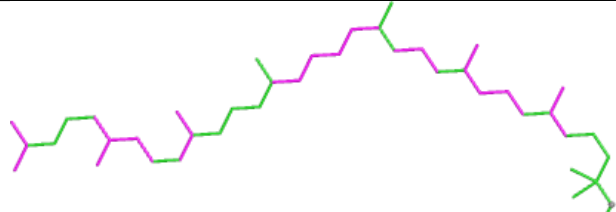
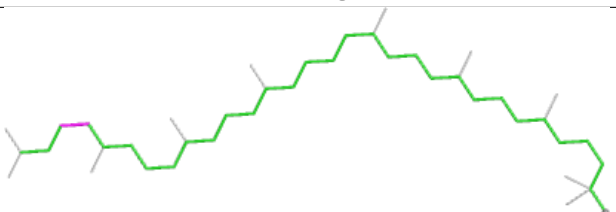


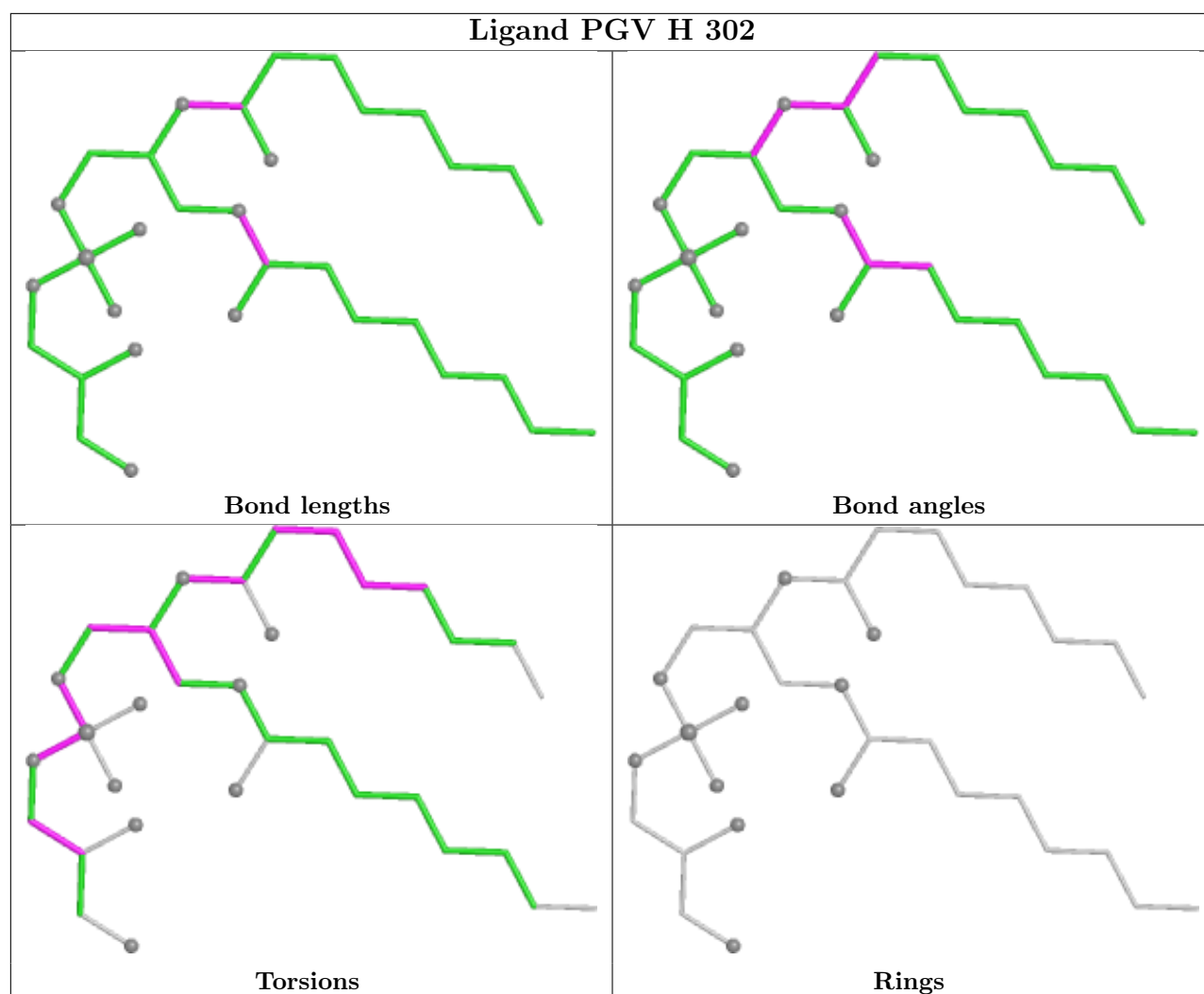


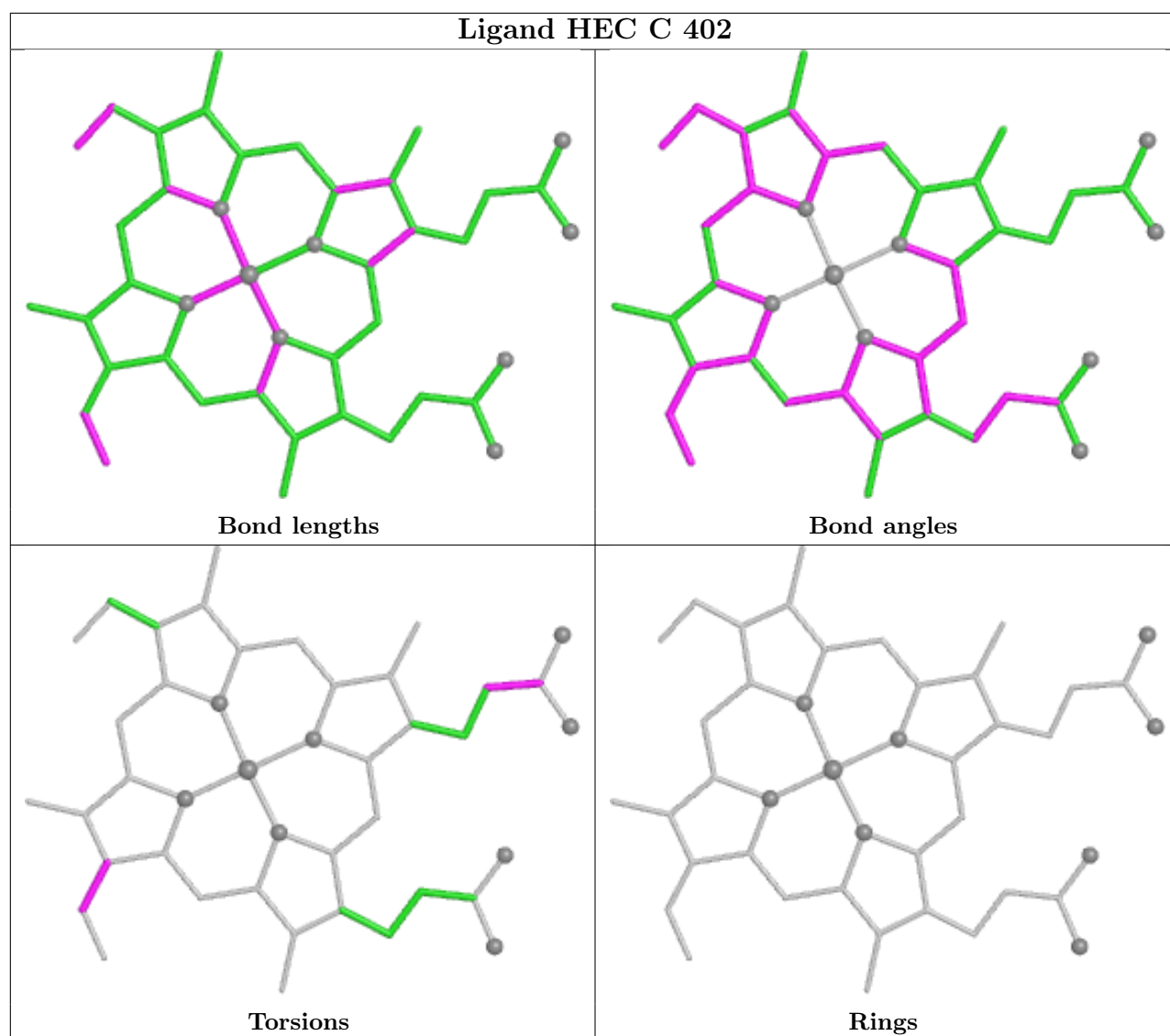


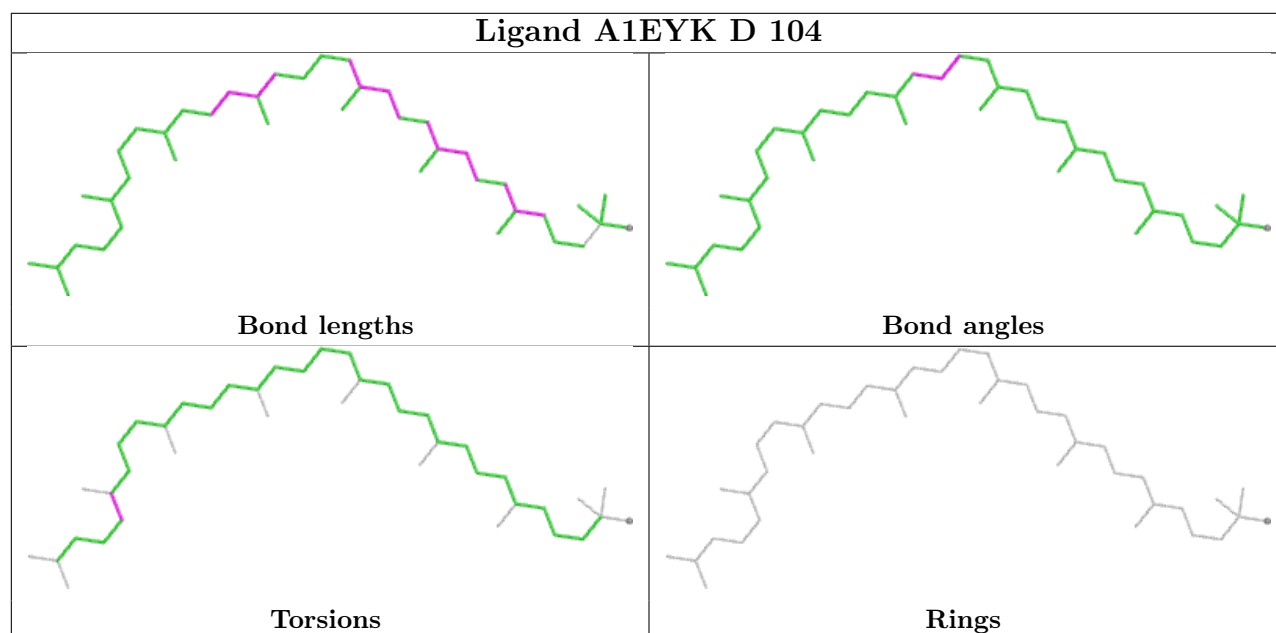
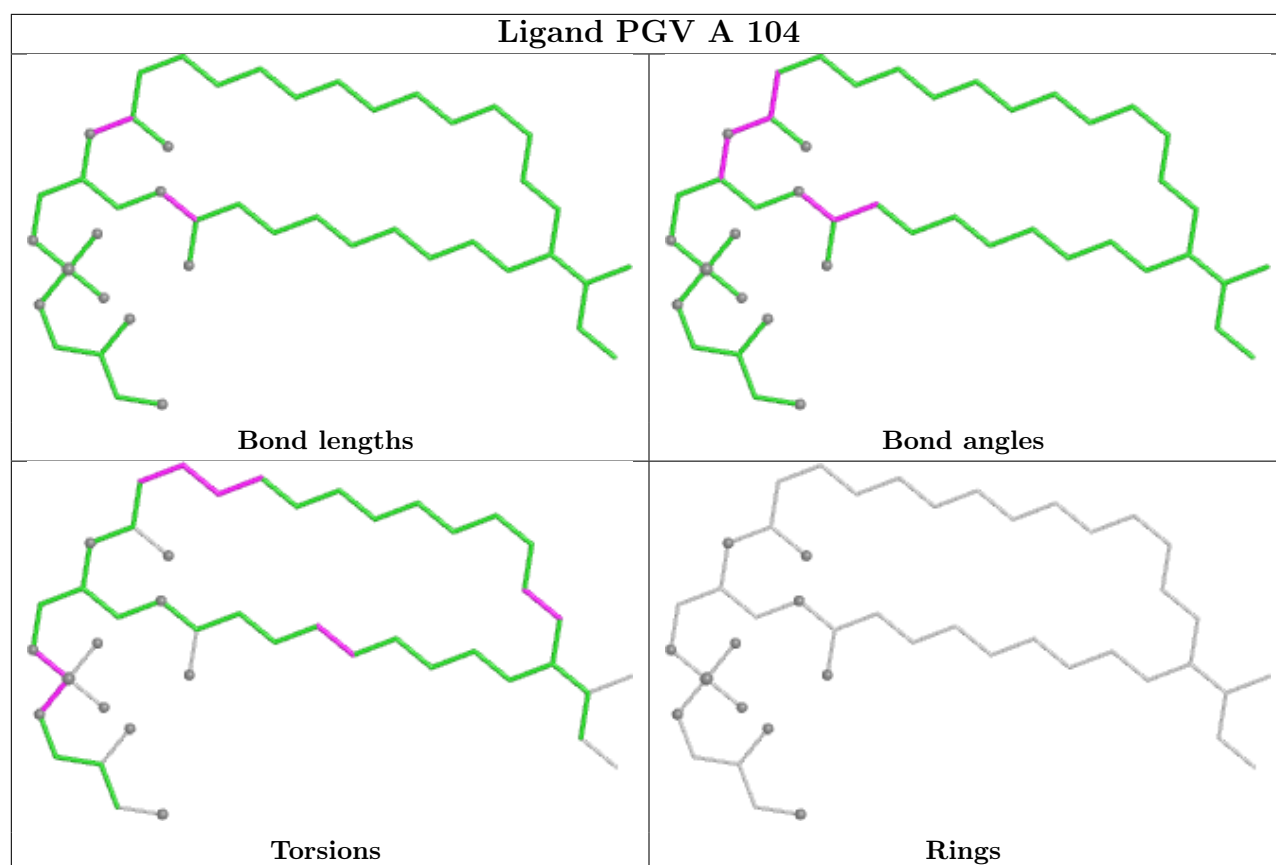


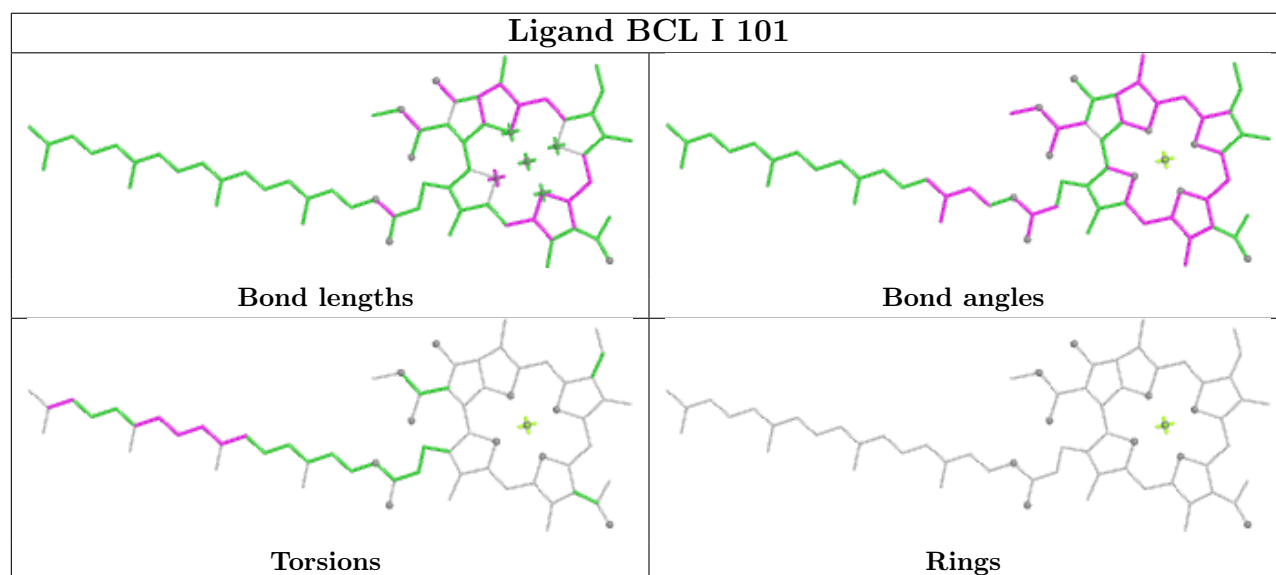
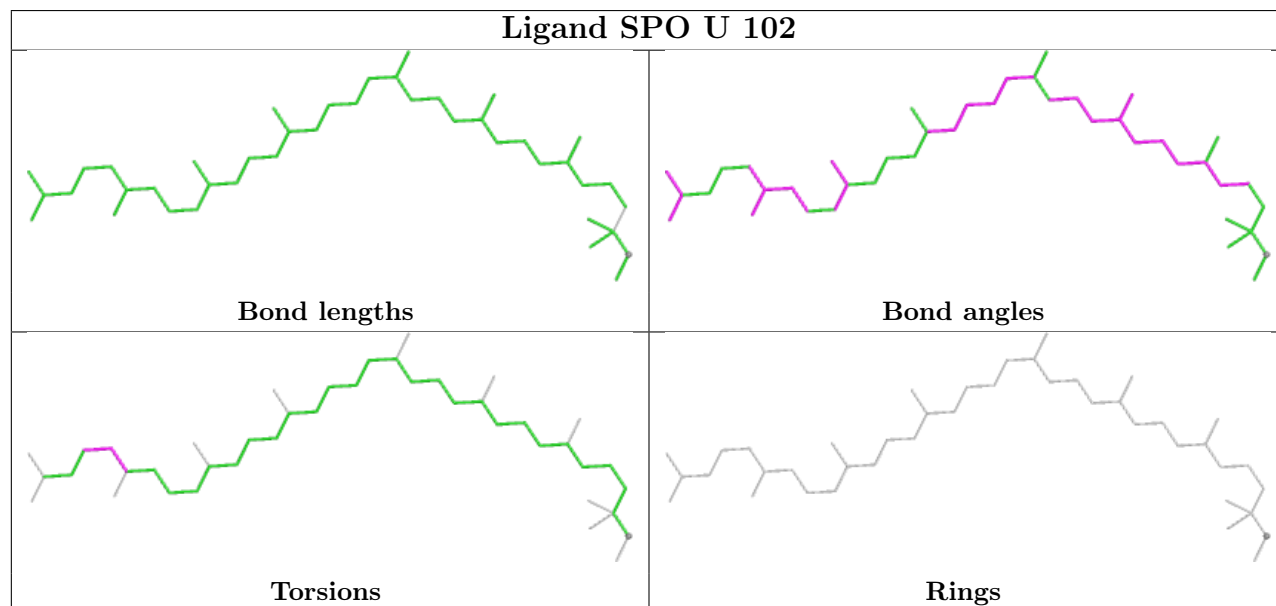
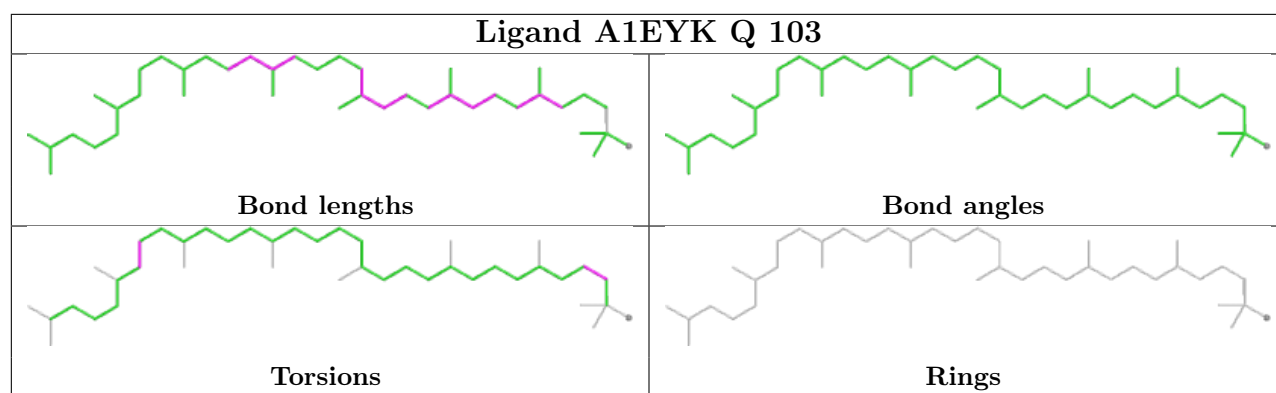
Ligand BCL L 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

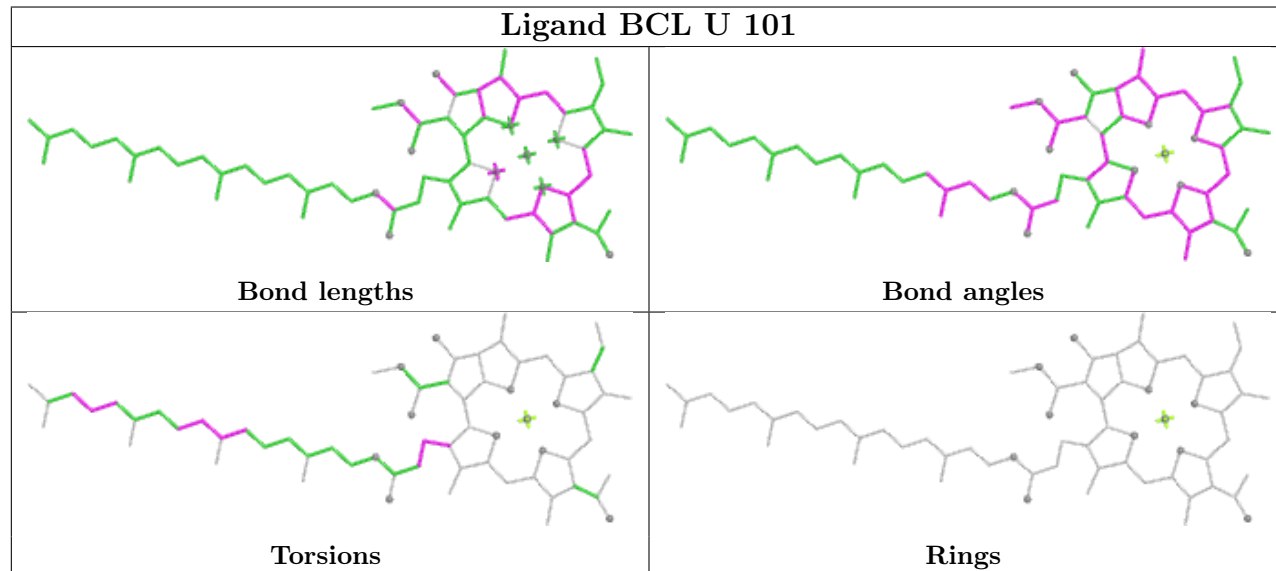
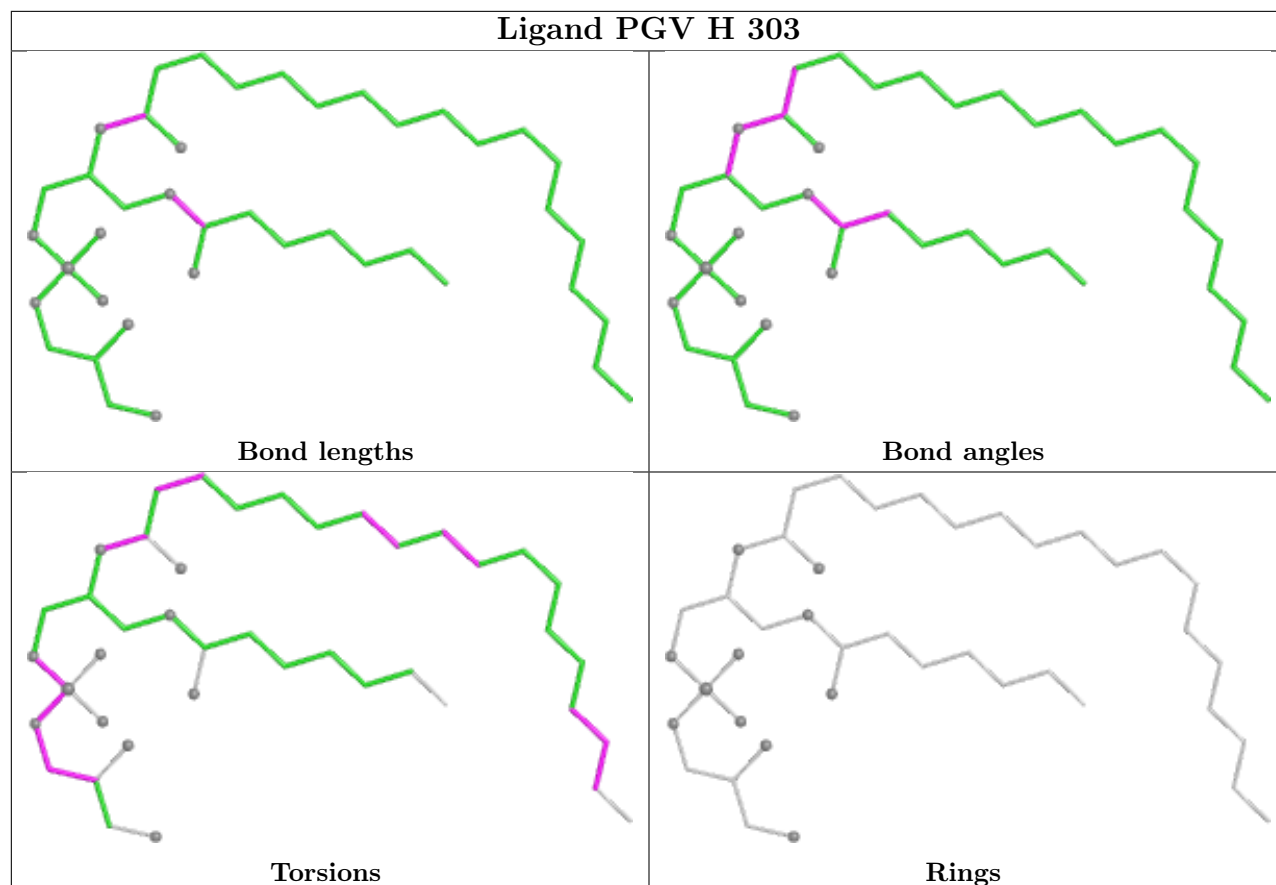
Ligand SPO D 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

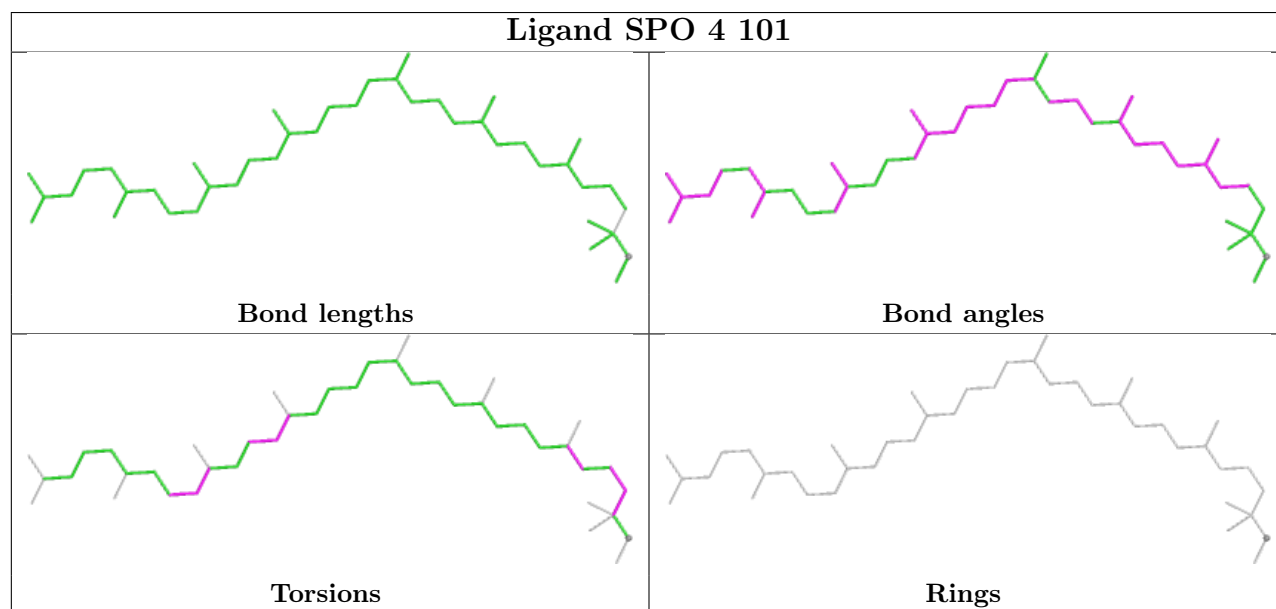
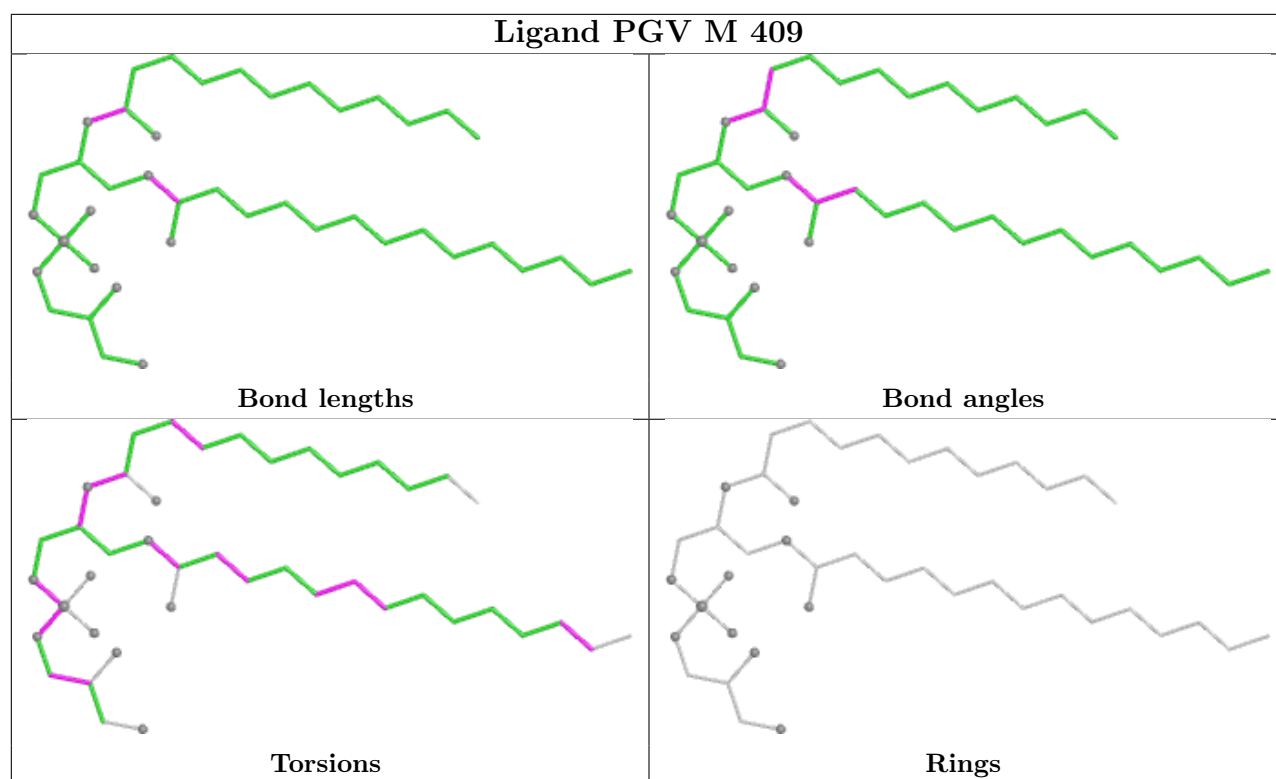


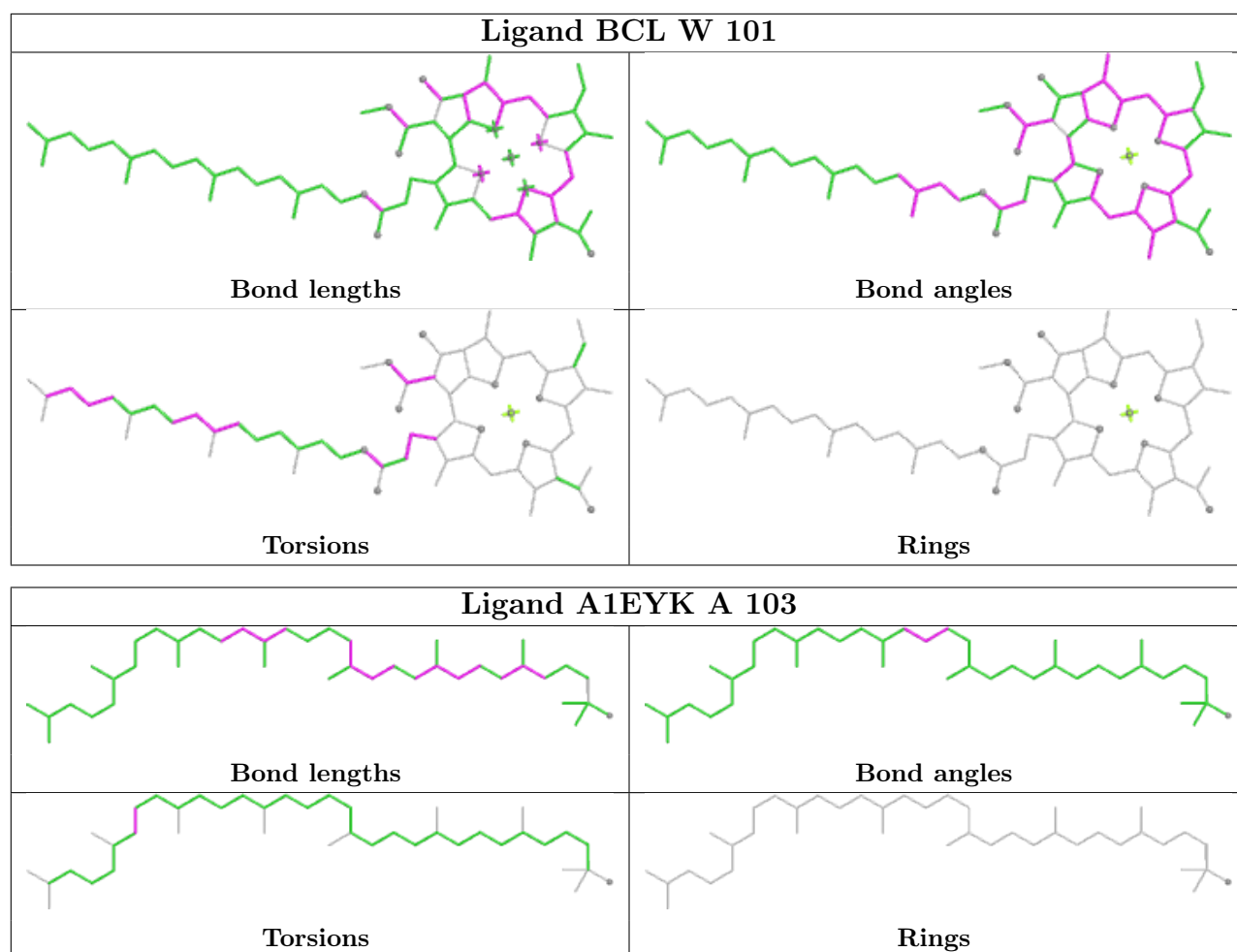


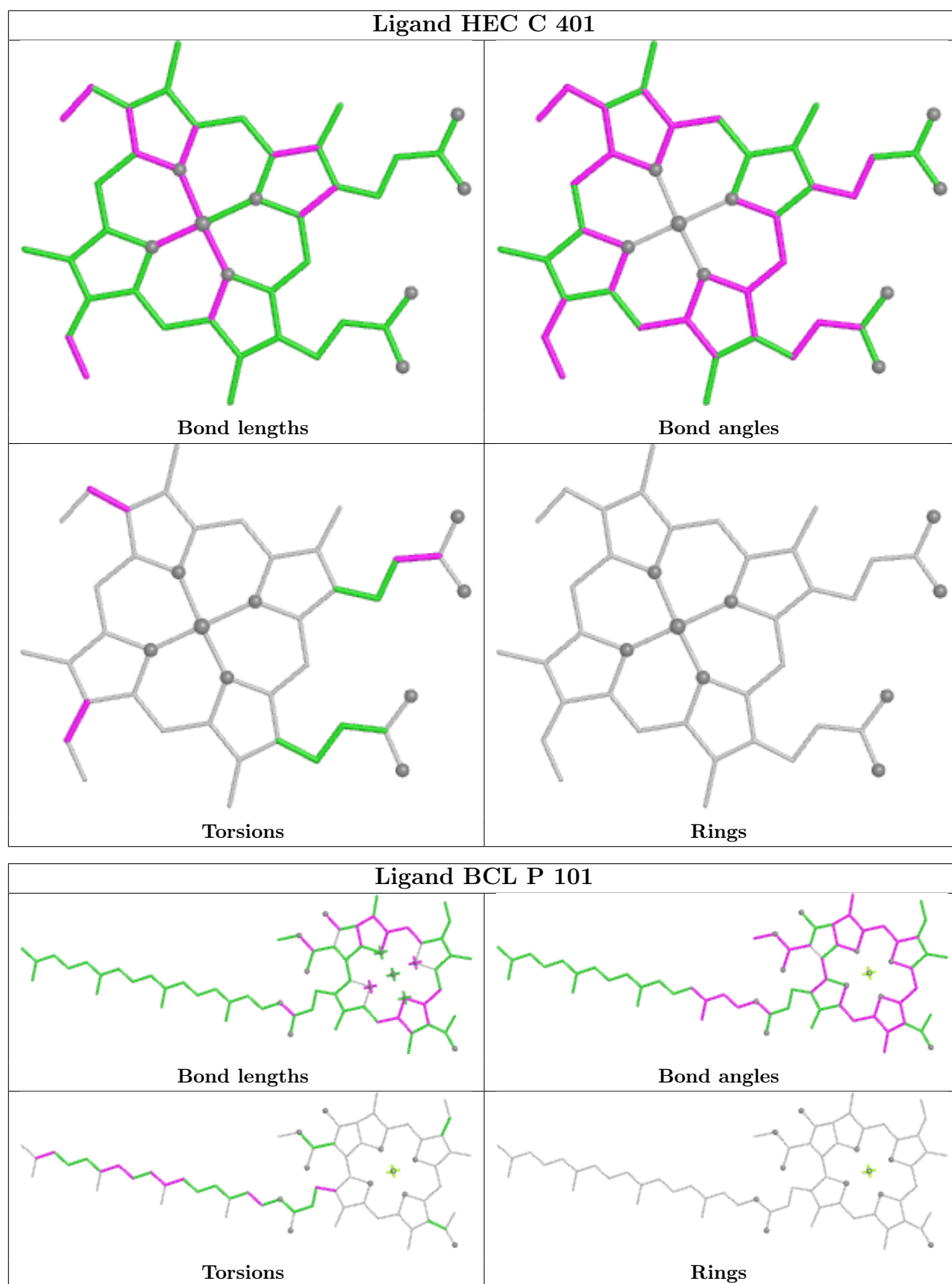












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

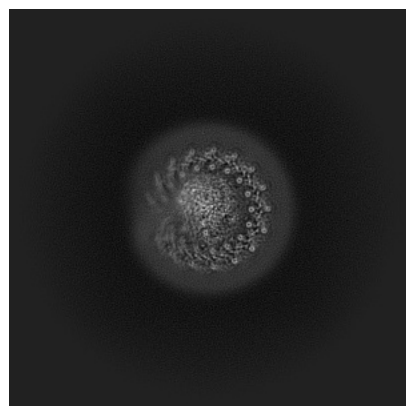
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66181. These allow visual inspection of the internal detail of the map and identification of artifacts.

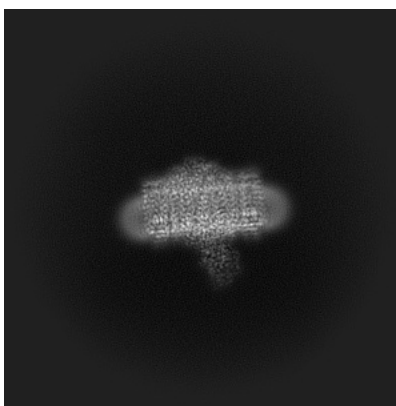
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

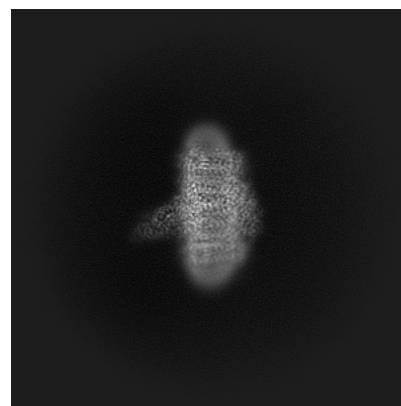
6.1.1 Primary map



X

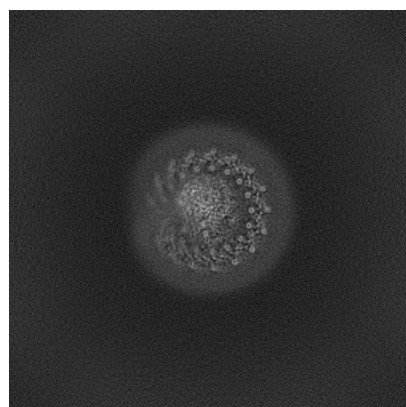


Y

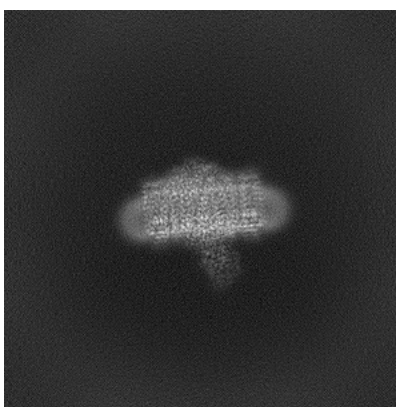


Z

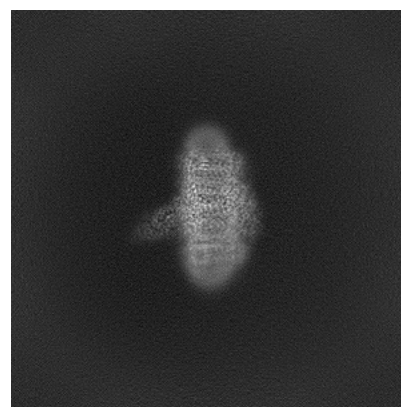
6.1.2 Raw map



X



Y

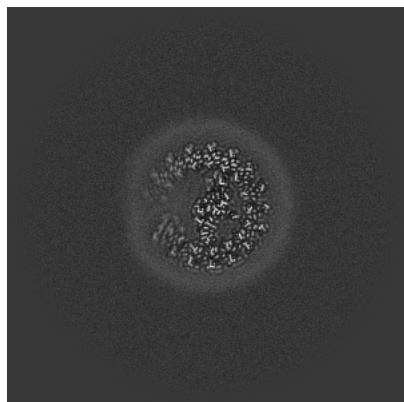


Z

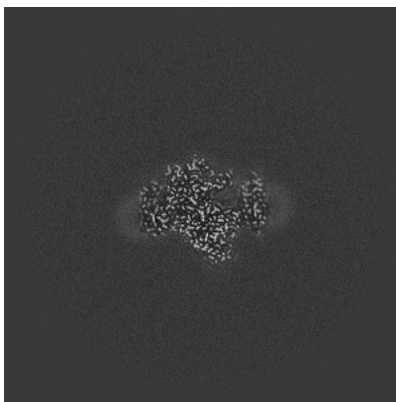
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

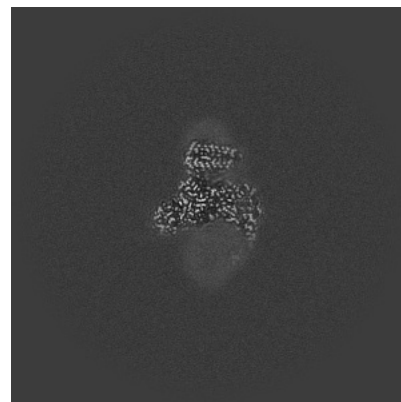
6.2.1 Primary map



X Index: 256

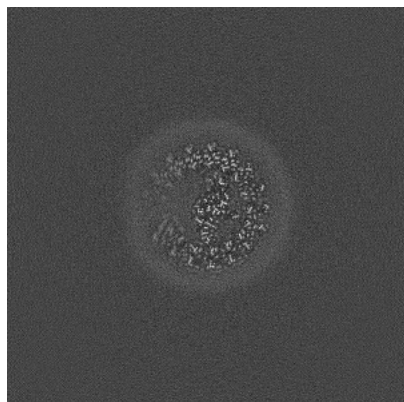


Y Index: 256

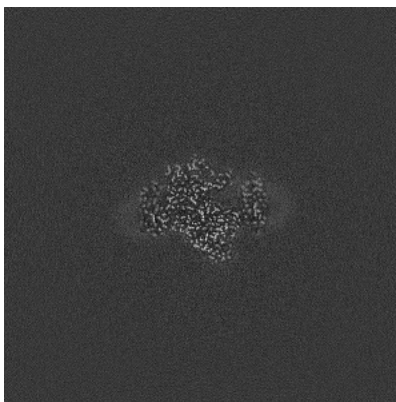


Z Index: 256

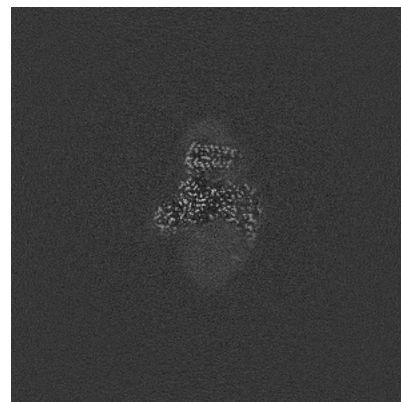
6.2.2 Raw map



X Index: 256



Y Index: 256

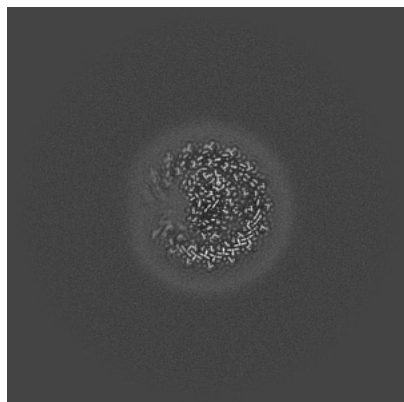


Z Index: 256

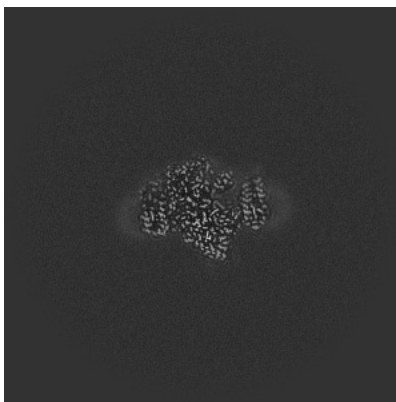
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

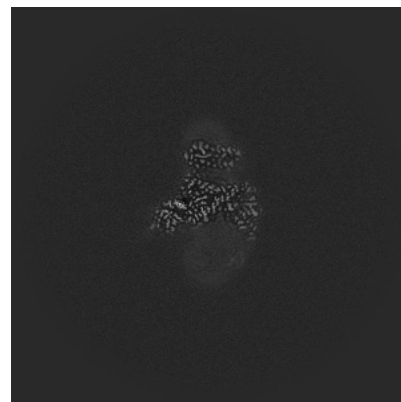
6.3.1 Primary map



X Index: 241

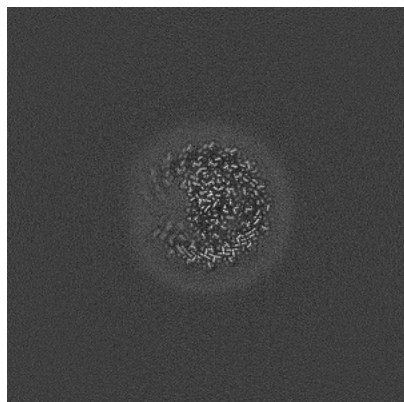


Y Index: 258

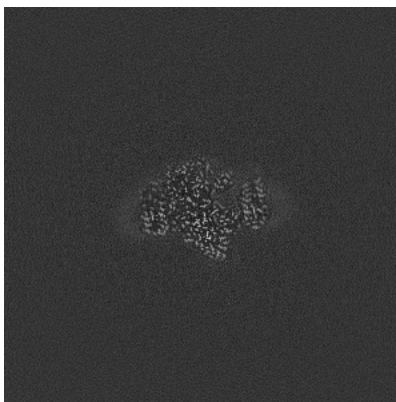


Z Index: 259

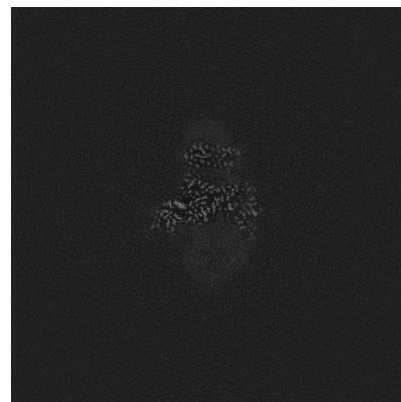
6.3.2 Raw map



X Index: 240



Y Index: 258

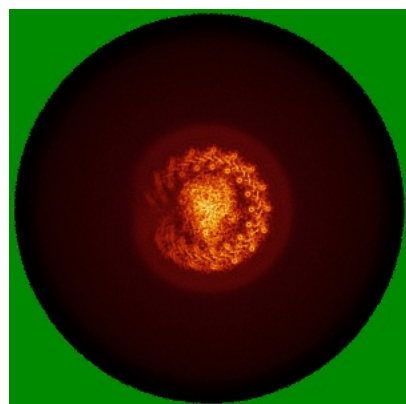


Z Index: 259

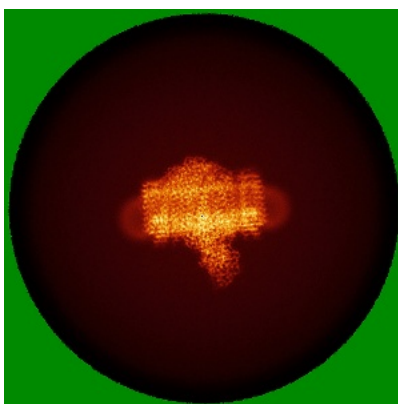
The images above show the largest variance slices of the map in three orthogonal directions.

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

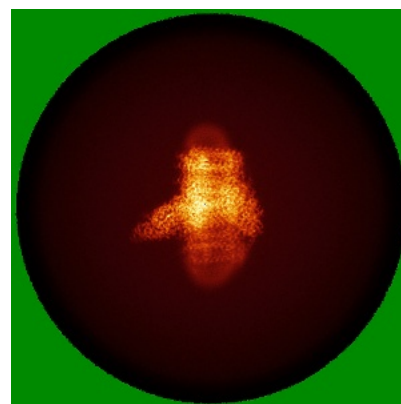
6.4.1 Primary map



X

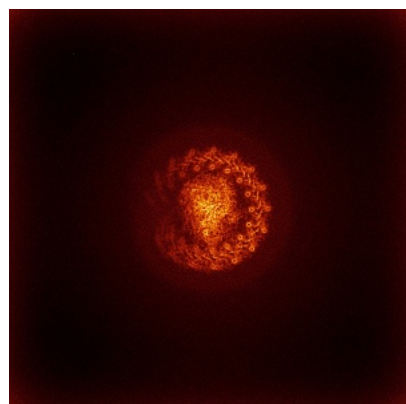


Y

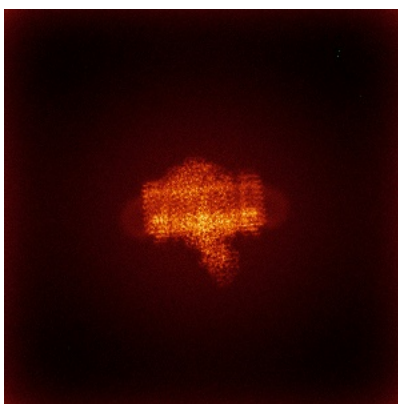


Z

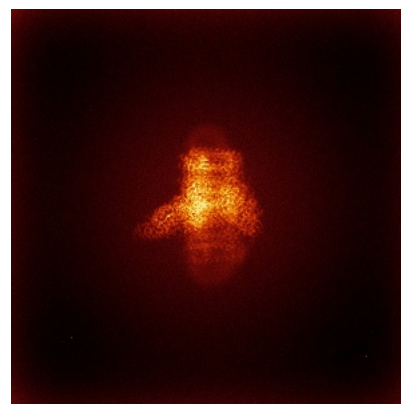
6.4.2 Raw map



X



Y

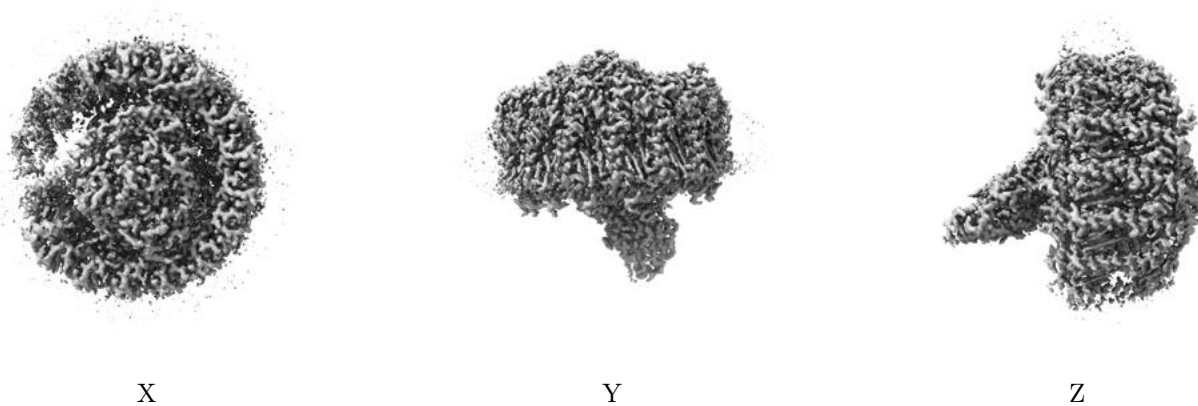


Z

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.

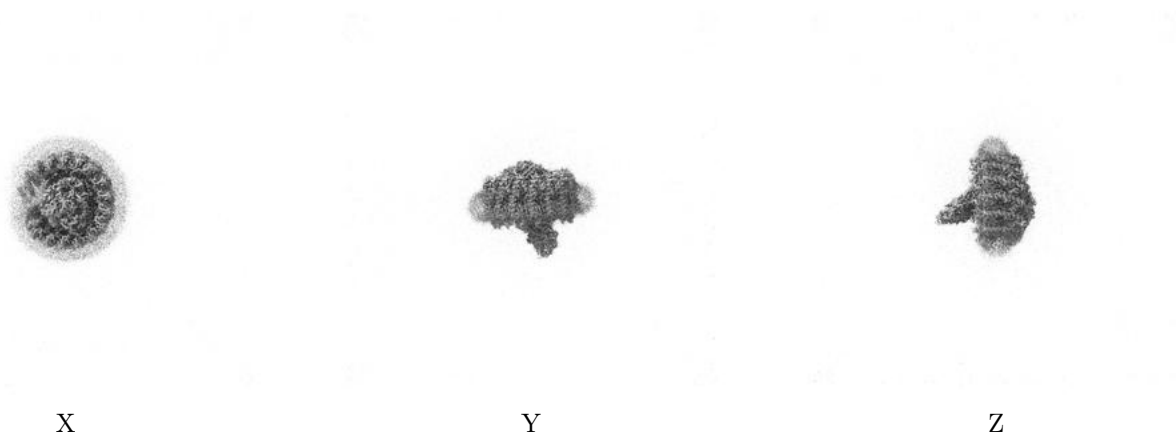
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0519. 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.

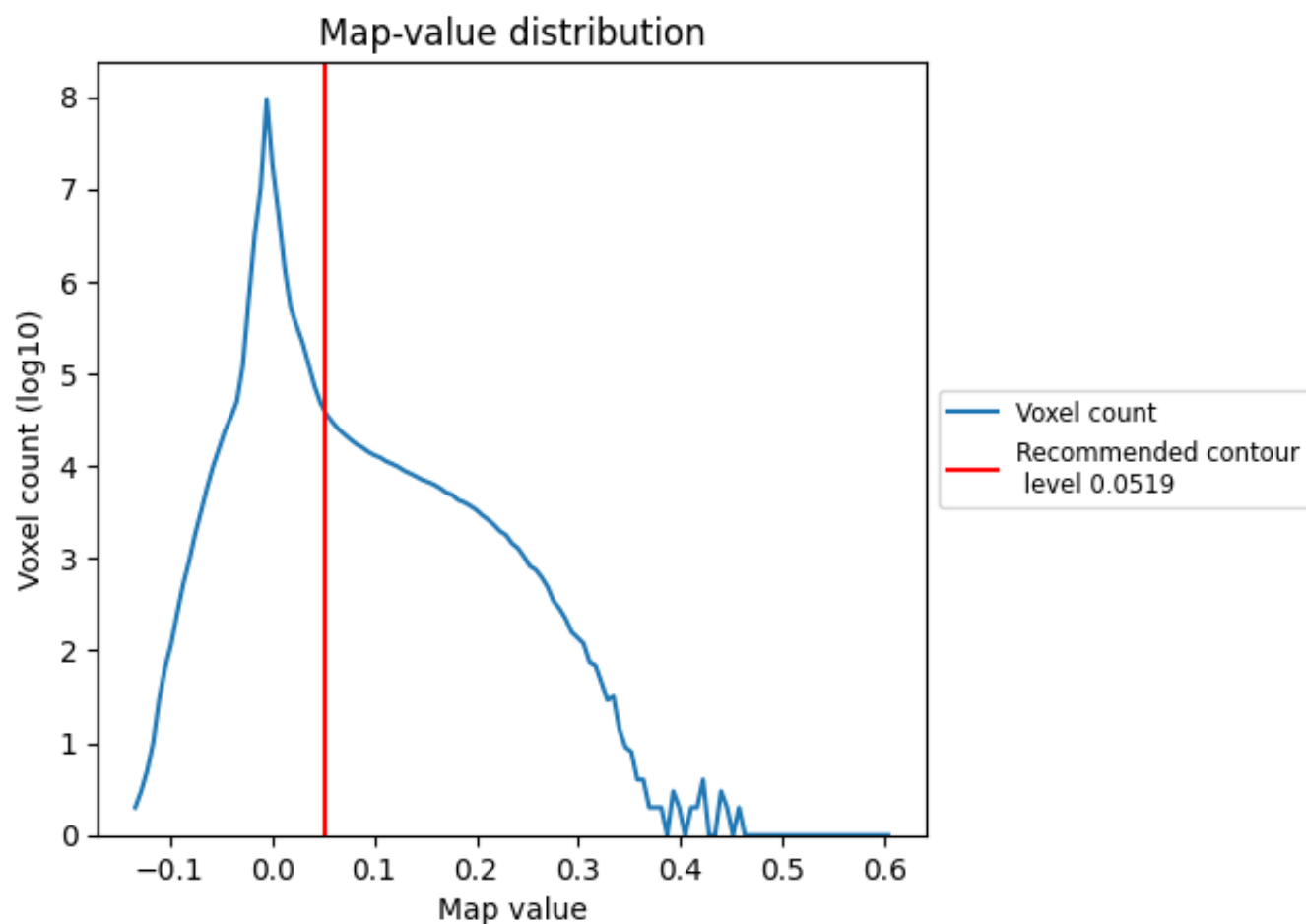
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

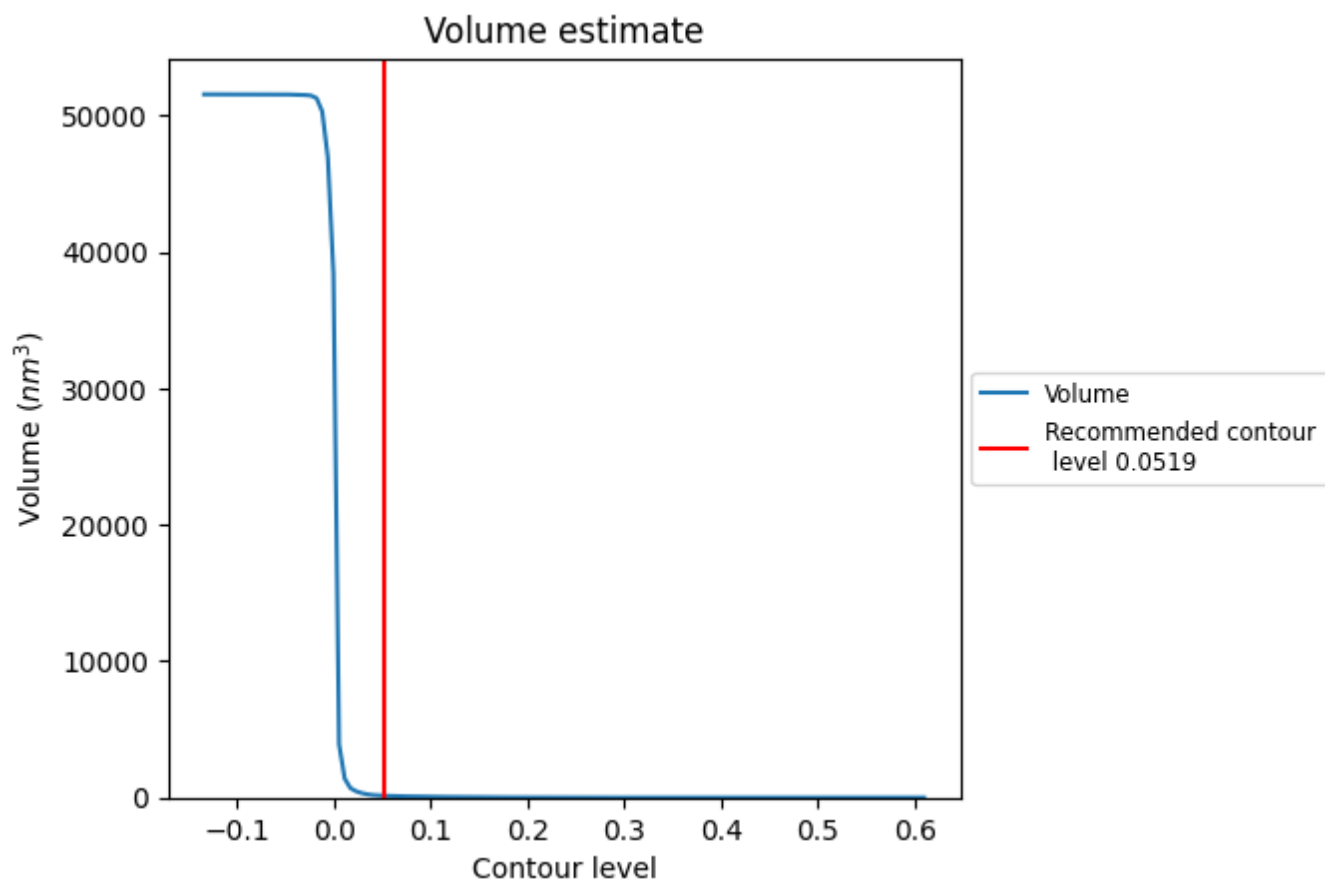
This section contains the results of statistical analysis of the map.

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.

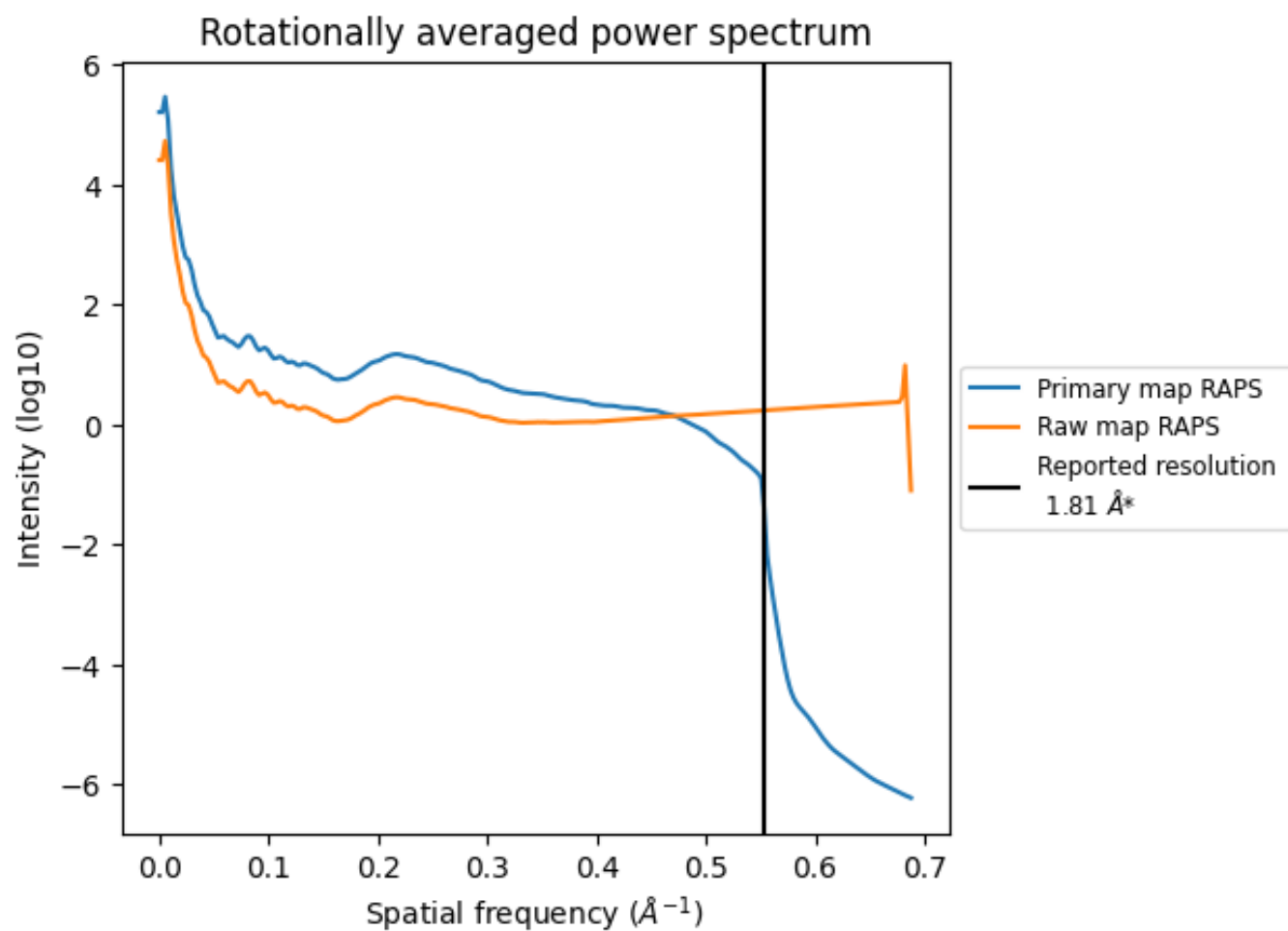
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 ⓘ

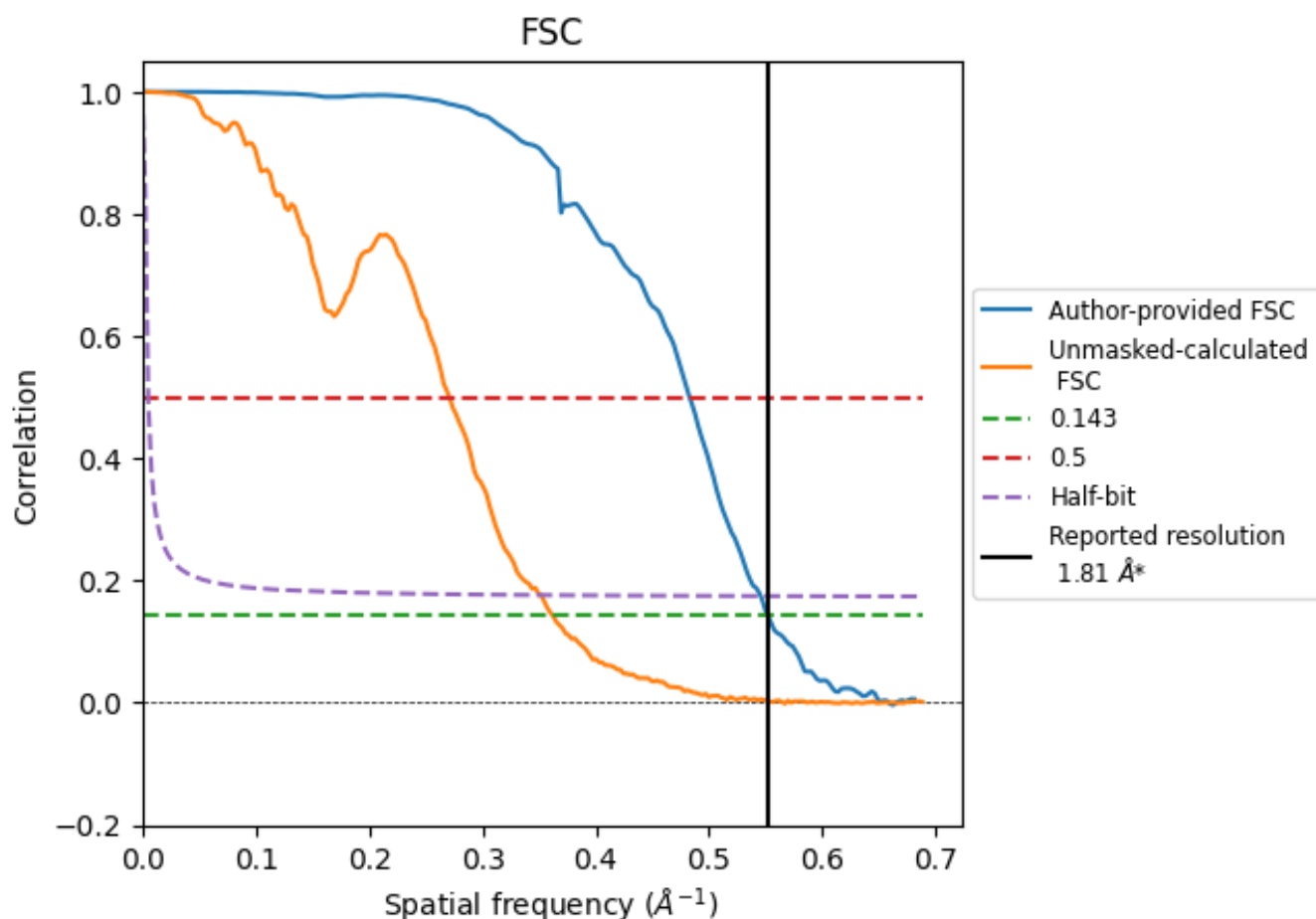


*Reported resolution corresponds to spatial frequency of 0.552 Å⁻¹

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 0.552 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

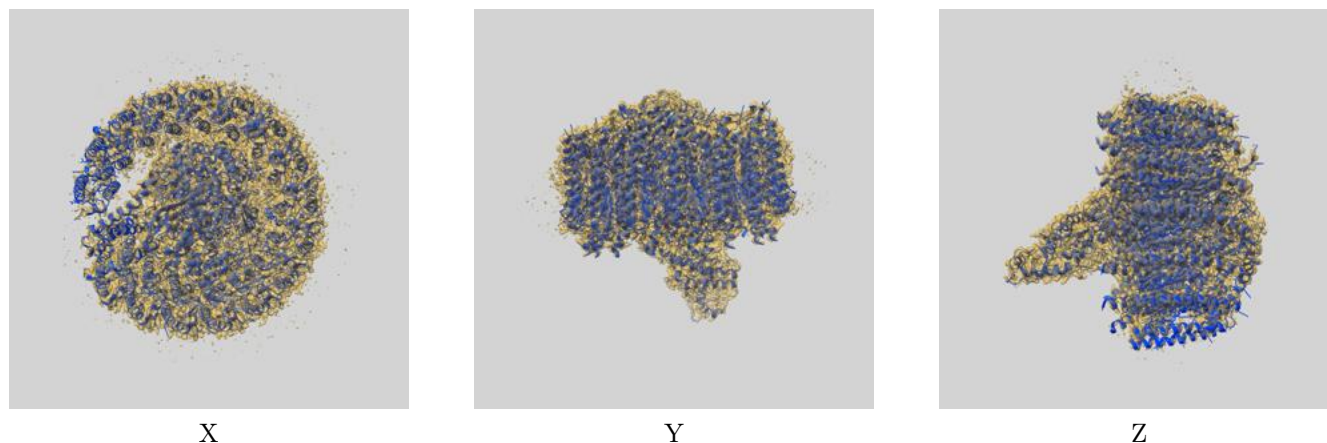
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.81	-	-
Author-provided FSC curve	1.81	2.07	1.83
Unmasked-calculated*	2.76	3.69	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.76 differs from the reported value 1.81 by more than 10 %

9 Map-model fit [i](#)

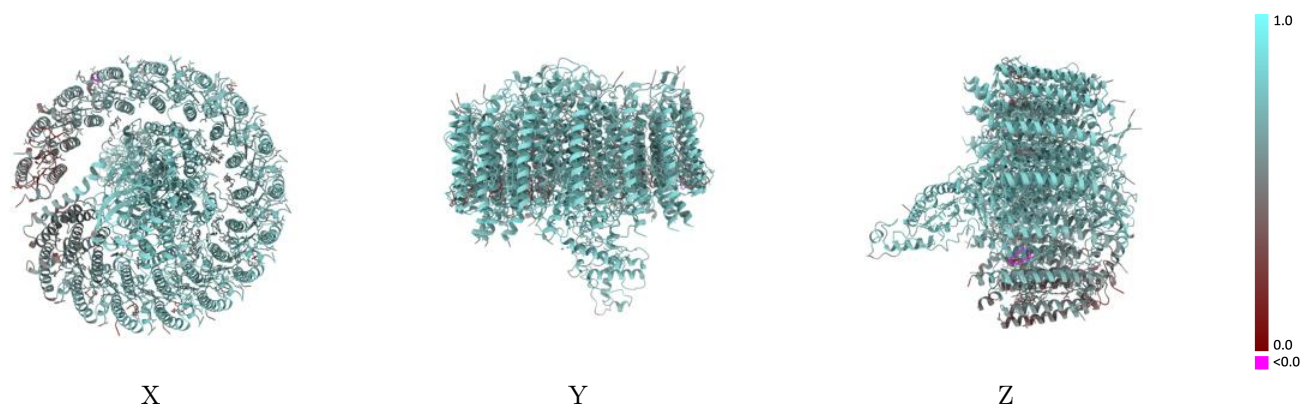
This section contains information regarding the fit between EMDB map EMD-66181 and PDB model 9WQV. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



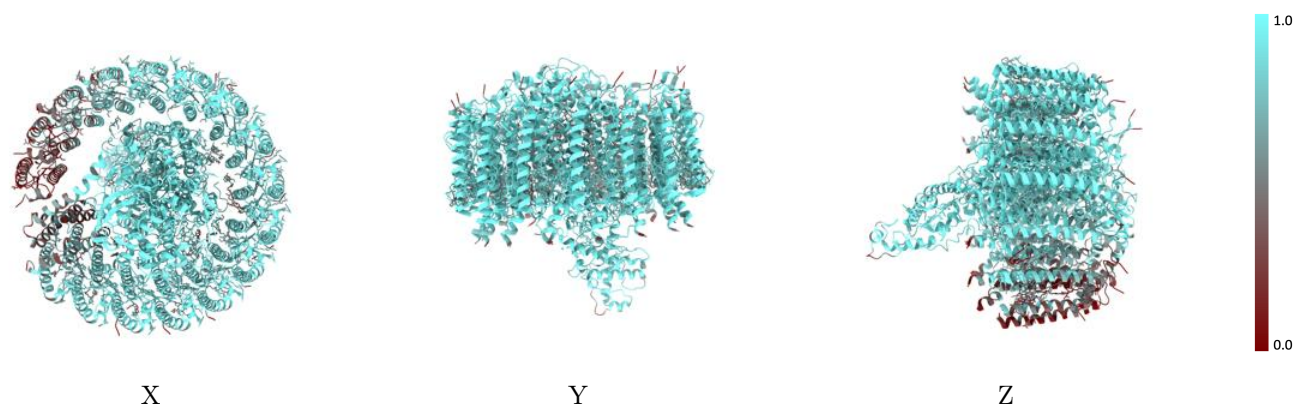
The images above show the 3D surface view of the map at the recommended contour level 0.0519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



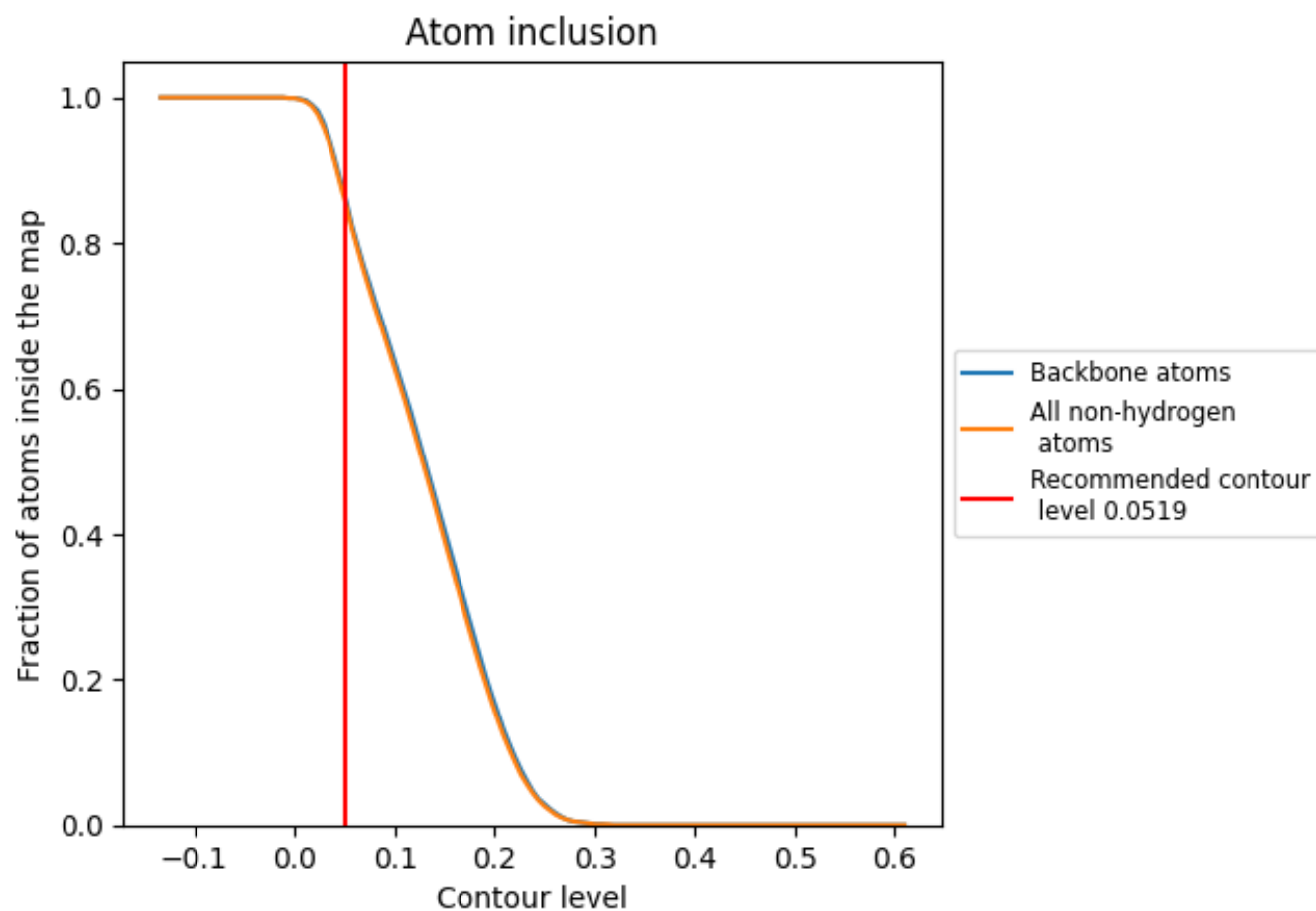
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0519).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.0519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.6850
0	 0.8870	 0.7030
1	 0.2750	 0.4450
2	 0.1780	 0.4040
3	 0.7290	 0.5620
4	 0.6920	 0.5590
5	 0.8410	 0.6340
6	 0.8180	 0.6220
7	 0.9180	 0.7070
8	 0.8760	 0.6670
9	 0.9470	 0.7280
A	 0.9440	 0.7430
B	 0.9030	 0.7050
C	 0.9040	 0.7090
D	 0.9190	 0.7130
E	 0.8920	 0.7000
F	 0.8880	 0.7170
G	 0.8800	 0.6930
H	 0.9370	 0.7280
I	 0.9390	 0.7270
J	 0.8740	 0.6880
K	 0.9300	 0.7130
L	 0.9540	 0.7580
M	 0.9480	 0.7470
N	 0.8740	 0.6760
O	 0.9370	 0.7250
P	 0.8850	 0.6860
Q	 0.9550	 0.7310
R	 0.8780	 0.6810
S	 0.9230	 0.7100
T	 0.8630	 0.6760
U	 0.8210	 0.6700
V	 0.7380	 0.5980
W	 0.7300	 0.6230
X	 0.6430	 0.5580



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.5480	 0.5640
Z	 0.4600	 0.5000
a	 0.5360	 0.5560