



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 11:00 AM JST

PDB ID : 9W5B / pdb_00009w5b
EMDB ID : EMD-65652
Title : cryo-EM structure of PSII D1-S264V from *Thermosynechococcus vestitus* BP-1
Authors : Fan, S.B.; Jiang, H.W.; Kato, K.; Tsai, P.-C.; Jia, A.Q.; Nakajima, Y.; Sug-iura, M.; Shen, J.-R.
Deposited on : 2025-08-01
Resolution : 1.96 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:

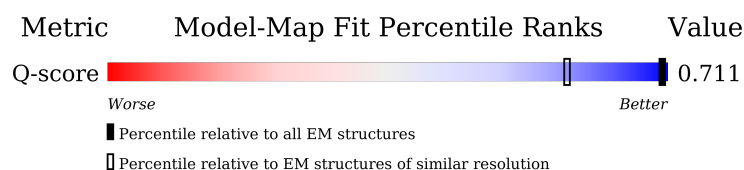
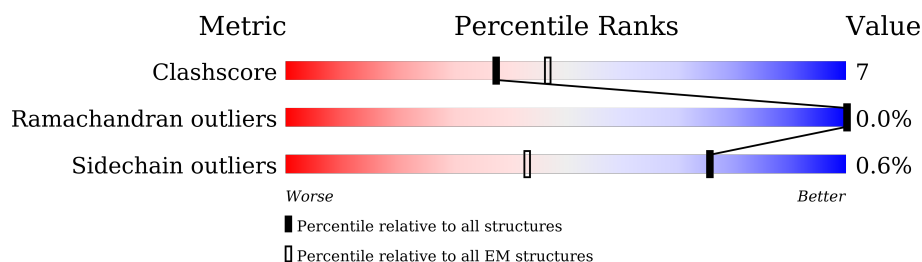
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 1.96 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.



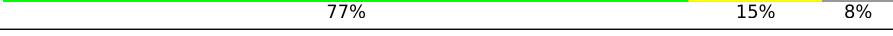
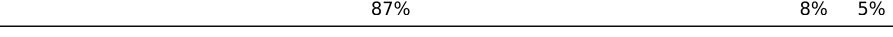
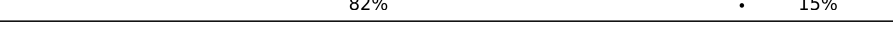
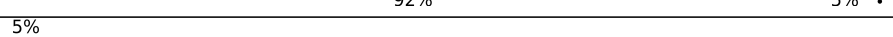
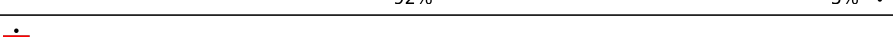
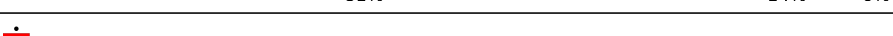
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1340 (1.46 - 2.46)

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	A	360	
1	a	360	
2	B	510	
2	b	510	

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	
19	z	62	

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
20	OEX	A	401	-	-	X	-
20	OEX	a	401	-	-	X	-
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 47744 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 Photosystem II protein D1 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	1
			2575	1694	426	441	14		
1	a	334	Total	C	N	O	S	0	1
			2575	1694	426	441	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	VAL	SER	variant	UNP Q8DIV4
a	264	VAL	SER	variant	UNP Q8DIV4

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	1	0
			3838	2537	645	643	13		
2	b	504	Total	C	N	O	S	1	0
			3838	2537	645	643	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3415	2244	577	581	13		
3	c	450	Total	C	N	O	S	0	0
			3415	2244	577	581	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2686	1786	442	446	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2686	1786	442	446	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	80	Total	C	N	O		0	0
			609	405	99	105			
5	e	80	Total	C	N	O		0	0
			609	405	99	105			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	33	Total	C	N	O	S	0	0
			263	182	43	37	1		
6	f	33	Total	C	N	O	S	0	0
			263	182	43	37	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	61	Total	C	N	O	S	1	0
			495	330	81	82	2		
7	h	61	Total	C	N	O	S	1	0
			495	330	81	82	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			275	188	41	45	1		
8	i	36	Total	C	N	O	S	0	0
			275	188	41	45	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total	C	N	O	S	0	0
			241	166	35	39	1		
9	j	34	Total	C	N	O	S	0	0
			241	166	35	39	1		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			275	193	42	40		
10	k	37	Total	C	N	O	0	0
			275	193	42	40		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	36	Total	C	N	O	1	0
			284	194	44	46		
11	l	36	Total	C	N	O	1	0
			284	194	44	46		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	34	Total	C	N	O	S	0	0
			252	170	37	44	1		
12	m	34	Total	C	N	O	S	0	0
			252	170	37	44	1		

- Molecule 13 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	1	1
			1677	1069	289	314	5		
13	o	243	Total	C	N	O	S	1	1
			1677	1069	289	314	5		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	29	Total	C	N	O	S	0	0
			236	168	32	34	2		
14	t	29	Total	C	N	O	S	0	0
			236	168	32	34	2		

- Molecule 15 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			702	456	123	123		
15	u	97	Total	C	N	O	0	0
			702	456	123	123		

- Molecule 16 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			975	632	168	171	4		
16	v	137	Total	C	N	O	S	0	0
			975	632	168	171	4		

- Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	37	Total	C	N	O	0	0
			248	168	38	42		
17	x	37	Total	C	N	O	0	0
			248	168	38	42		

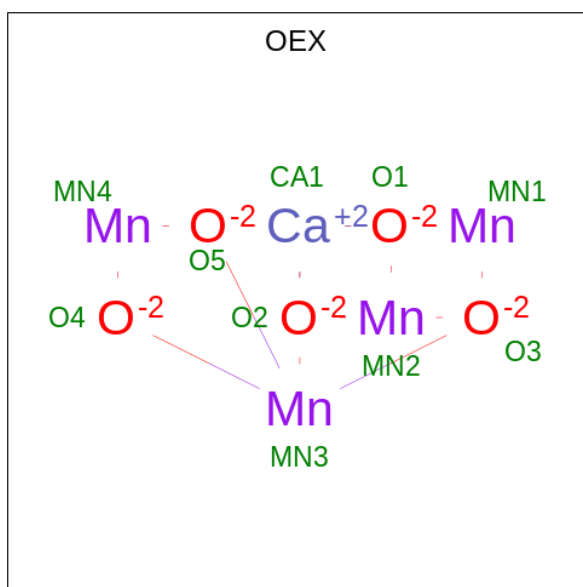
- Molecule 18 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0
			177	118	30	28	1		
18	y	29	Total	C	N	O	S	0	0
			177	118	30	28	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			387	258	63	65	1		
19	z	61	Total	C	N	O	S	0	0
			387	258	63	65	1		

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
20	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

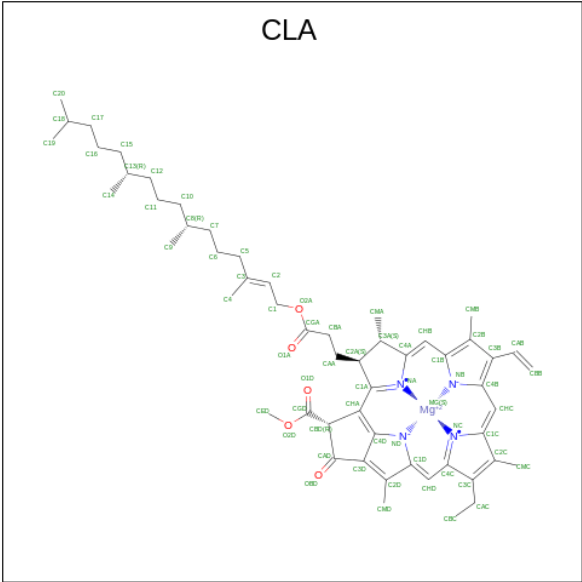
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Fe	0
			1	1	
21	a	1	Total	Fe	0
			1	1	

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Cl	0
			2	2	
22	a	2	Total	Cl	0
			2	2	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 45	C 35	Mg 1	N 4	O 5	0

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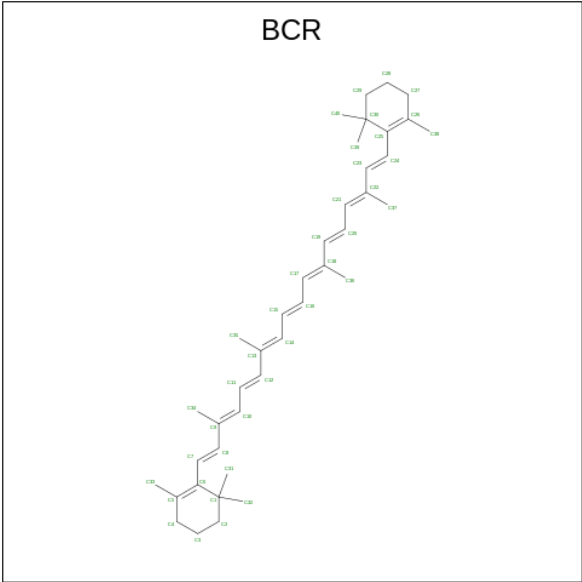
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



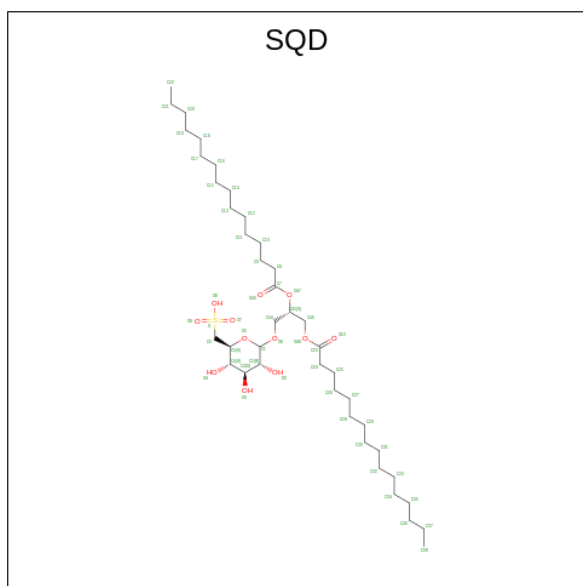
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	C	1	Total	C	0
			40	40	
24	C	1	Total	C	0
			40	40	
24	D	1	Total	C	0
			40	40	
24	K	1	Total	C	0
			40	40	
24	K	1	Total	C	0
			40	40	
24	T	1	Total	C	0
			40	40	
24	a	1	Total	C	0
			40	40	
24	b	1	Total	C	0
			40	40	
24	b	1	Total	C	0
			40	40	
24	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
24	c	1	Total C 40 40	0
24	c	1	Total C 40 40	0
24	d	1	Total C 40 40	0
24	k	1	Total C 40 40	0
24	k	1	Total C 40 40	0
24	t	1	Total C 40 40	0

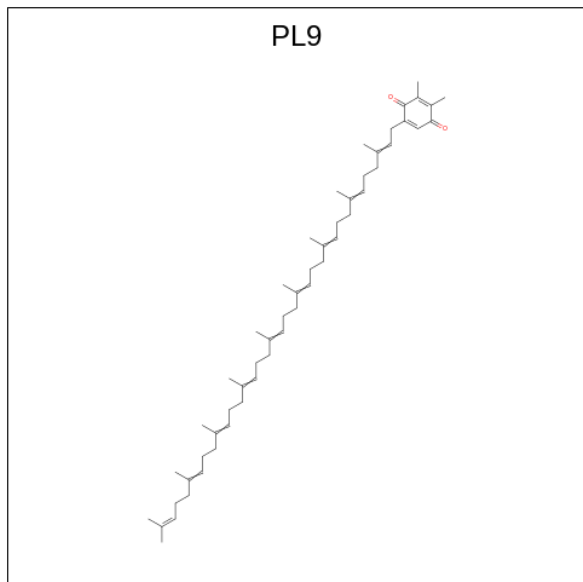
- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O S 32 19 12 1	0
25	F	1	Total C O S 23 11 11 1	0
25	a	1	Total C O S 32 19 12 1	0
25	f	1	Total C O S 23 11 11 1	0

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22

,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			55	53	2	
26	D	1	Total	C	O	0
			55	53	2	
26	a	1	Total	C	O	0
			55	53	2	
26	d	1	Total	C	O	0
			55	53	2	

- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

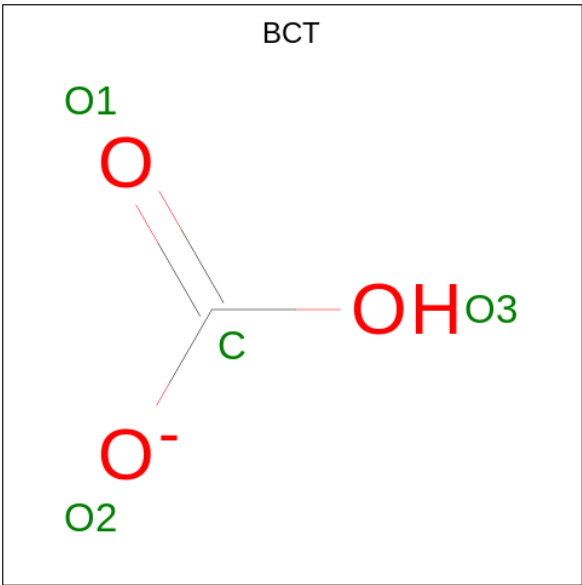
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			8	8	
27	B	2	Total	C	0
			21	21	
27	C	1	Total	C	0
			14	14	
27	D	2	Total	C	0
			19	19	
27	E	1	Total	C	0
			6	6	
27	H	1	Total	C	0
			6	6	

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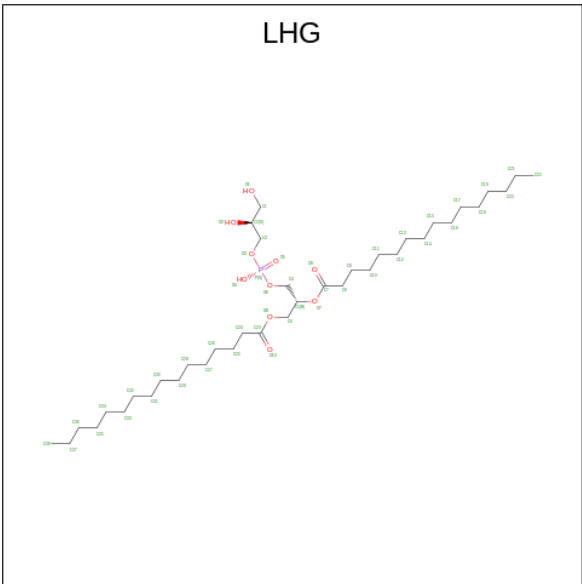
Mol	Chain	Residues	Atoms	AltConf
27	I	1	Total C 6 6	0
27	K	1	Total C 13 13	0
27	T	1	Total C 5 5	0
27	X	1	Total C 9 9	0
27	a	1	Total C 8 8	0
27	b	2	Total C 21 21	0
27	c	1	Total C 14 14	0
27	d	2	Total C 19 19	0
27	e	1	Total C 6 6	0
27	h	1	Total C 6 6	0
27	i	1	Total C 6 6	0
27	k	1	Total C 13 13	0
27	t	1	Total C 5 5	0
27	x	1	Total C 9 9	0

- Molecule 28 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	1
			4	1	3	
28	a	1	Total	C	O	1
			4	1	3	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



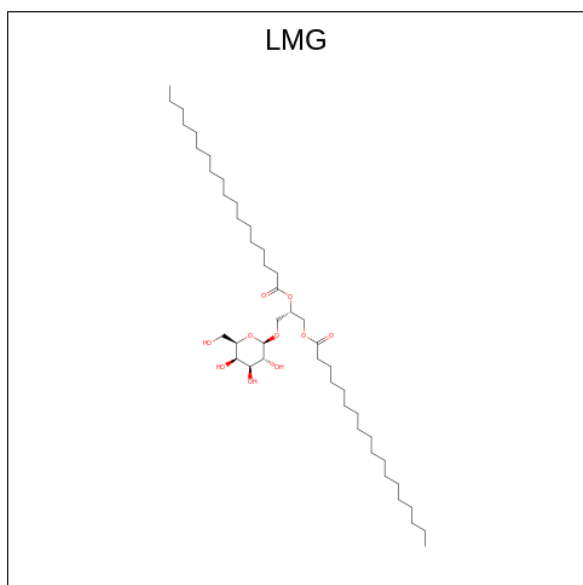
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			39	28	10	1	

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Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			31	22	8	1	
29	B	1	Total	C	O	P	0
			49	38	10	1	
29	D	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	a	1	Total	C	O	P	0
			39	28	10	1	
29	a	1	Total	C	O	P	0
			31	22	8	1	
29	b	1	Total	C	O	P	0
			49	38	10	1	
29	d	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



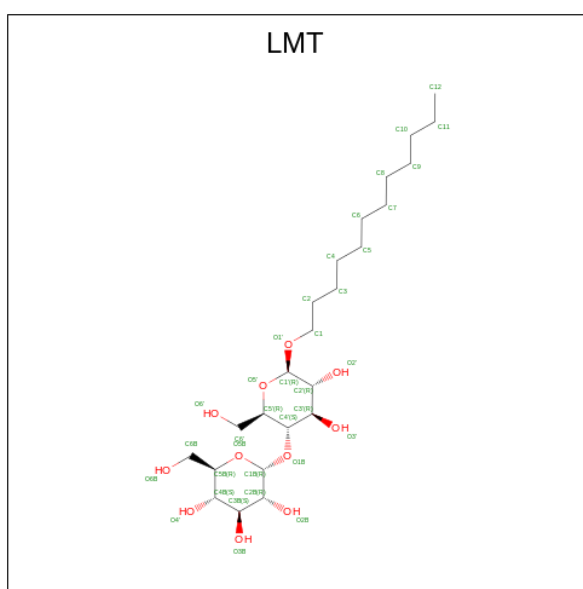
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			45	35	10	
30	C	1	Total	C	O	0
			47	37	10	

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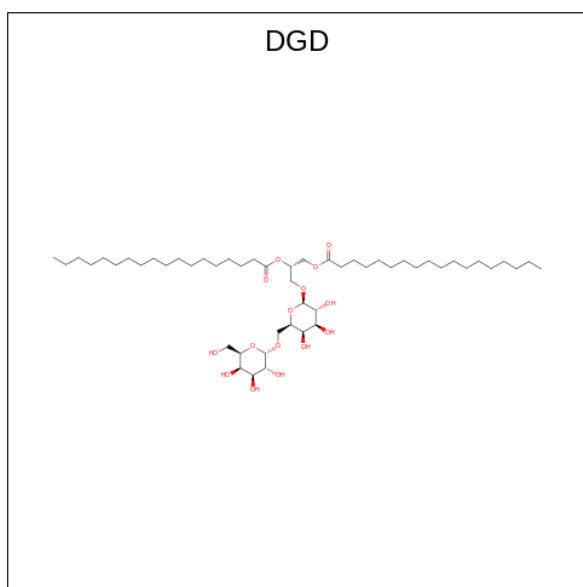
Mol	Chain	Residues	Atoms			AltConf
30	J	1	Total	C	O	0
			38	28	10	
30	b	1	Total	C	O	0
			45	35	10	
30	c	1	Total	C	O	0
			47	37	10	
30	j	1	Total	C	O	0
			38	28	10	

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



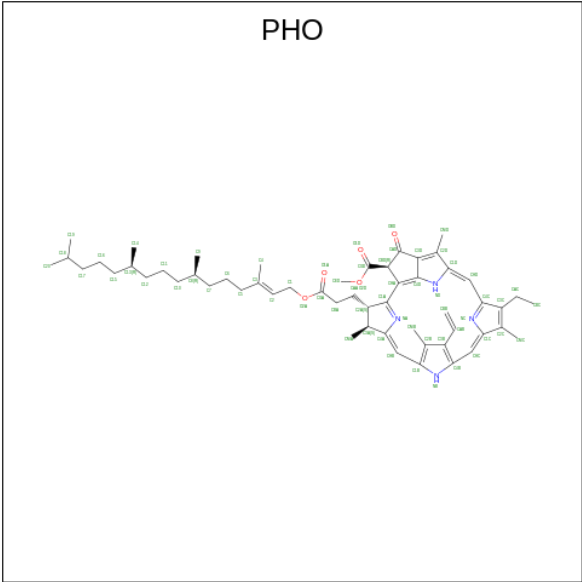
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			35	24	11	
31	J	1	Total	C	O	0
			24	18	6	
31	M	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			35	24	11	
31	j	1	Total	C	O	0
			24	18	6	
31	m	1	Total	C	O	0
			35	24	11	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



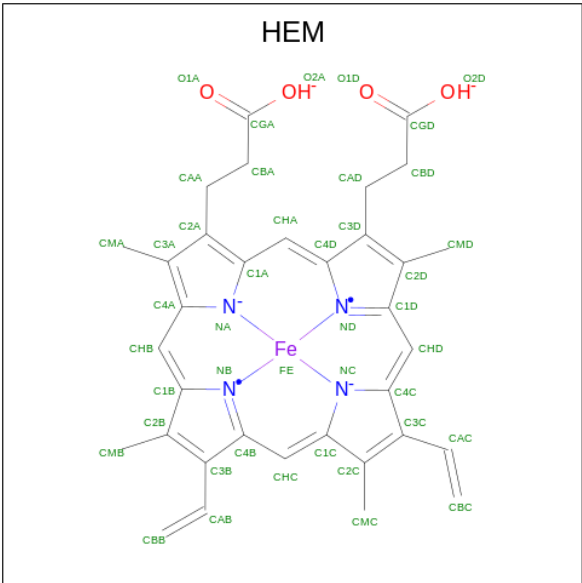
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			52	37	15	
32	C	1	Total	C	O	0
			50	35	15	
32	C	1	Total	C	O	0
			53	38	15	
32	H	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			52	37	15	
32	c	1	Total	C	O	0
			50	35	15	
32	c	1	Total	C	O	0
			53	38	15	
32	h	1	Total	C	O	0
			62	47	15	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	N	O	0
			64	55	4	5	
33	D	1	Total	C	N	O	0
			64	55	4	5	
33	d	1	Total	C	N	O	0
			64	55	4	5	
33	d	1	Total	C	N	O	0
			64	55	4	5	

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

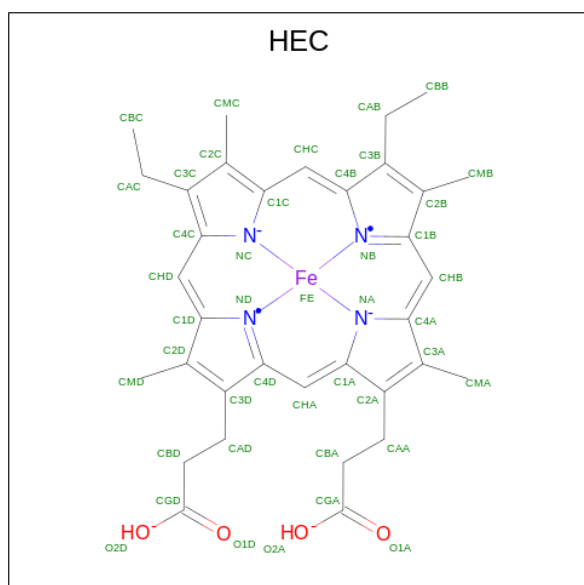


Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

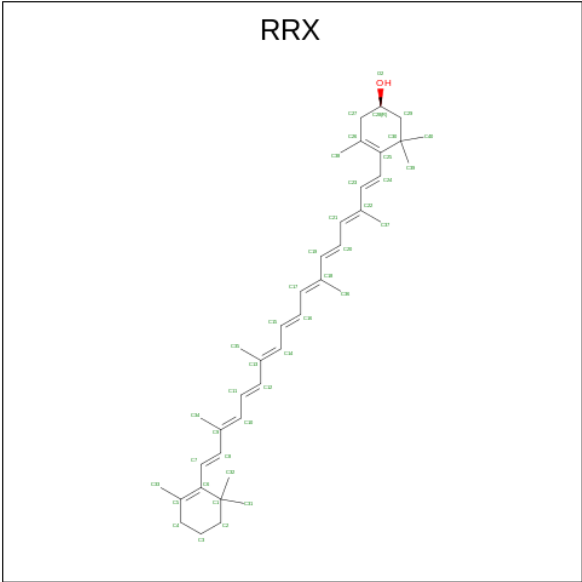
Mol	Chain	Residues	Atoms		AltConf
35	O	1	Total	Ca	0
			1	1	
35	o	1	Total	Ca	0
			1	1	

- Molecule 36 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
36	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
37	X	1	Total	C	O	0
			41	40	1	
37	x	1	Total	C	O	0
			41	40	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	104	Total	O	2
			105	105	
38	B	152	Total	O	1
			153	153	
38	C	89	Total	O	2
			91	91	
38	D	91	Total	O	1
			92	92	
38	E	6	Total	O	0
			6	6	
38	H	16	Total	O	0
			16	16	
38	I	4	Total	O	0
			4	4	
38	J	3	Total	O	0
			3	3	
38	K	2	Total	O	0
			2	2	
38	L	8	Total	O	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
38	M	6	Total 6	O 6	0
38	O	38	Total 38	O 38	1
38	T	4	Total 4	O 4	0
38	U	7	Total 7	O 7	0
38	V	13	Total 13	O 13	0
38	X	4	Total 4	O 4	0
38	a	105	Total 106	O 106	2
38	b	151	Total 152	O 152	1
38	c	89	Total 91	O 91	2
38	d	91	Total 92	O 92	1
38	e	6	Total 6	O 6	0
38	h	16	Total 16	O 16	0
38	i	4	Total 4	O 4	0
38	j	3	Total 3	O 3	0
38	k	2	Total 2	O 2	0
38	l	8	Total 8	O 8	0
38	m	5	Total 5	O 5	0
38	o	38	Total 38	O 38	1
38	t	4	Total 4	O 4	0
38	u	7	Total 7	O 7	0
38	v	12	Total 12	O 12	0

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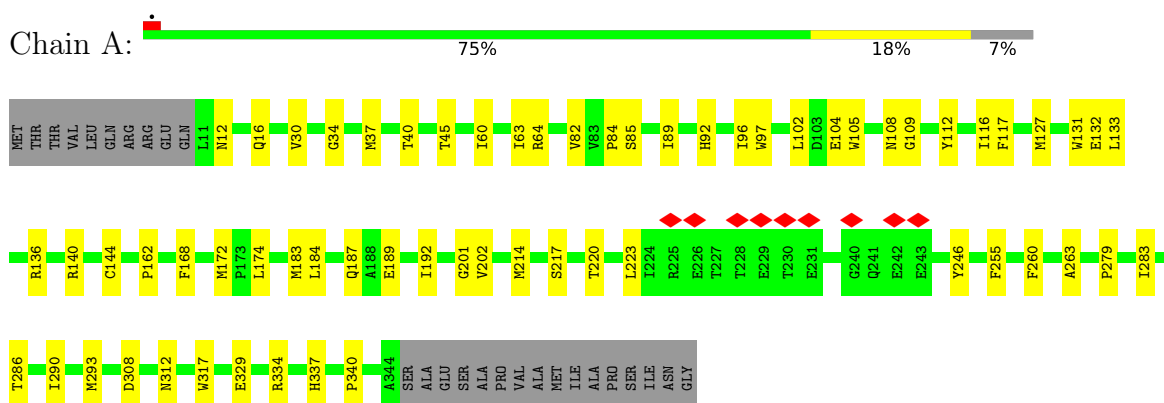
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Mol	Chain	Residues	Atoms		AltConf
38	x	4	Total	O	0
			4	4	

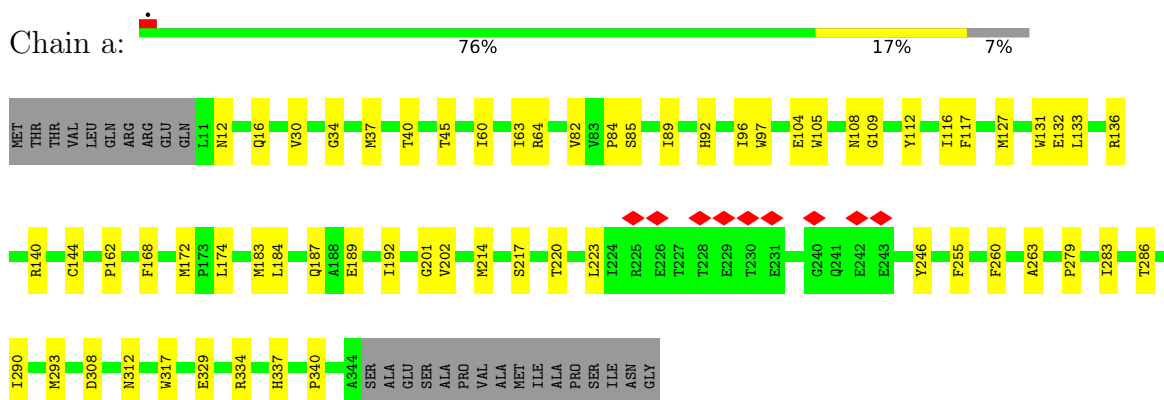
3 Residue-property plots [i](#)

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.

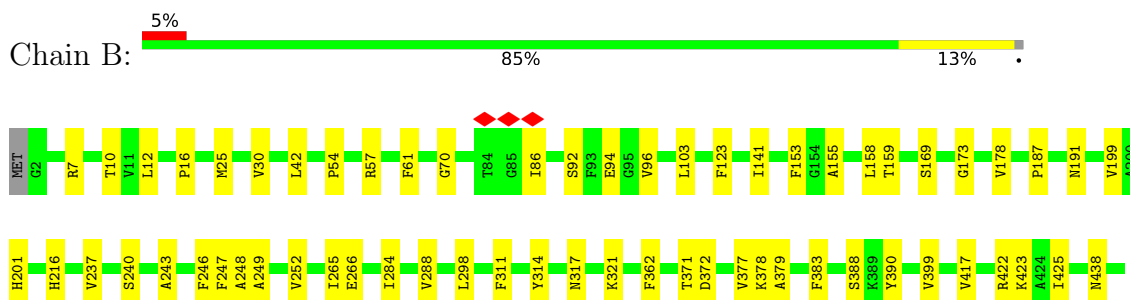
- Molecule 1: Photosystem II protein D1 3

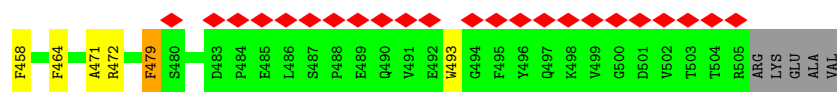


- Molecule 1: Photosystem II protein D1 3

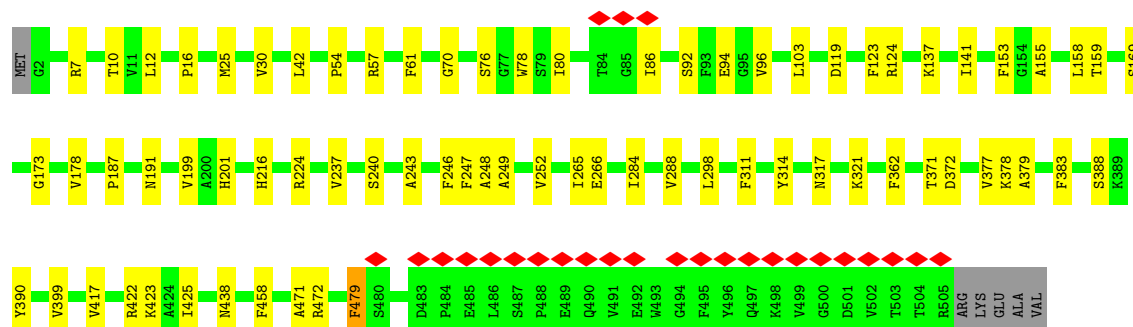
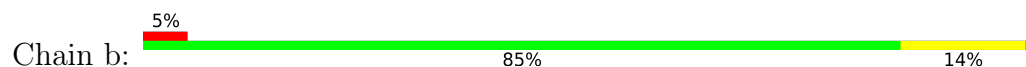


- Molecule 2: Photosystem II CP47 reaction center protein

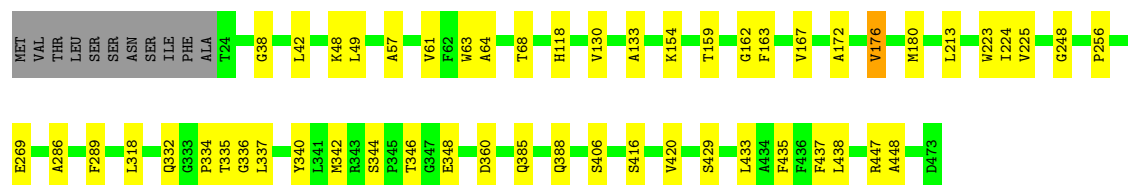
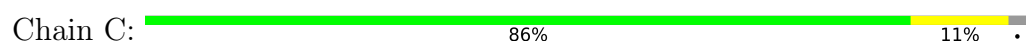




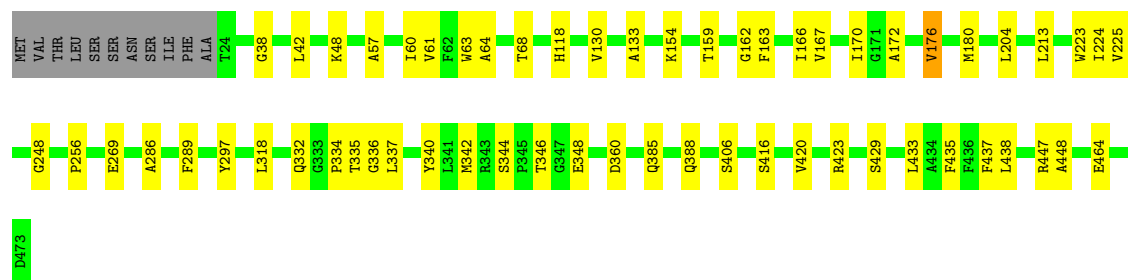
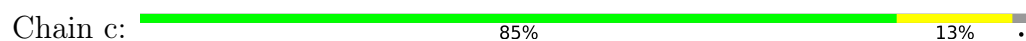
• Molecule 2: Photosystem II CP47 reaction center protein



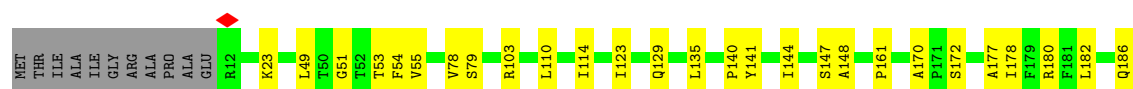
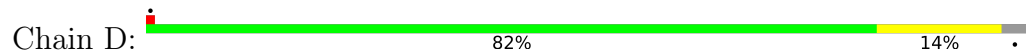
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

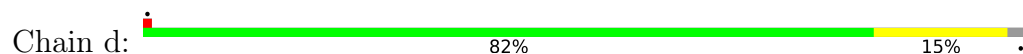


• Molecule 4: Photosystem II D2 protein

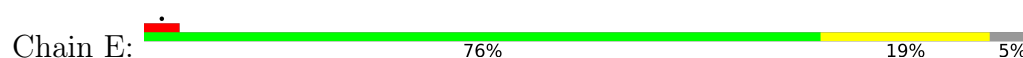




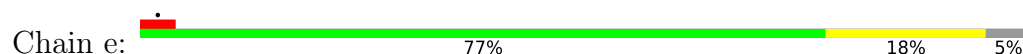
• Molecule 4: Photosystem II D2 protein



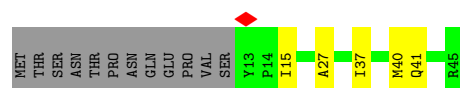
• Molecule 5: Cytochrome b559 subunit alpha



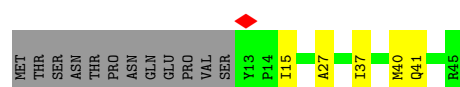
• Molecule 5: Cytochrome b559 subunit alpha



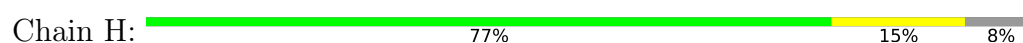
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta

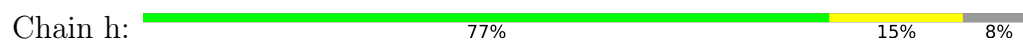


• Molecule 7: Photosystem II reaction center protein H

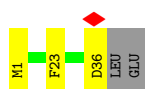
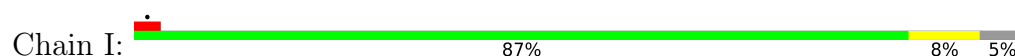




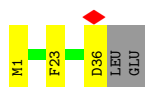
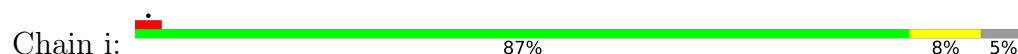
- Molecule 7: Photosystem II reaction center protein H



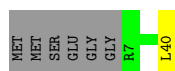
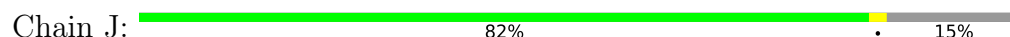
- Molecule 8: Photosystem II reaction center protein I



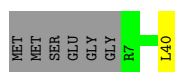
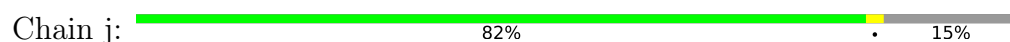
- Molecule 8: Photosystem II reaction center protein I



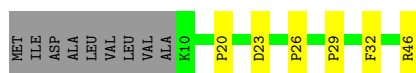
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

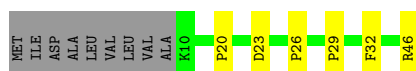


- Molecule 10: Photosystem II reaction center protein K

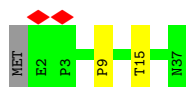
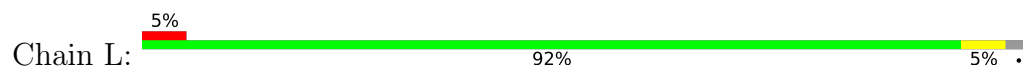


- Molecule 10: Photosystem II reaction center protein K

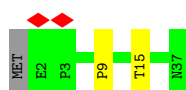
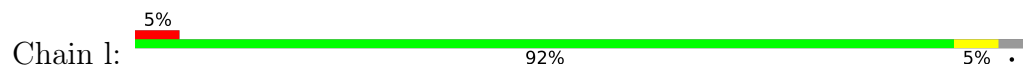




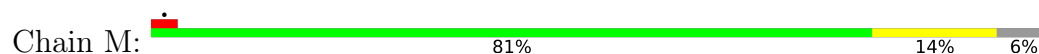
- Molecule 11: Photosystem II reaction center protein L



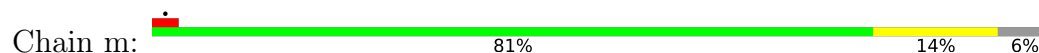
- Molecule 11: Photosystem II reaction center protein L



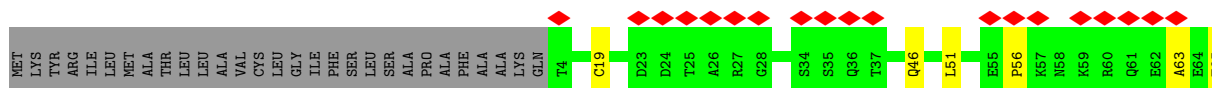
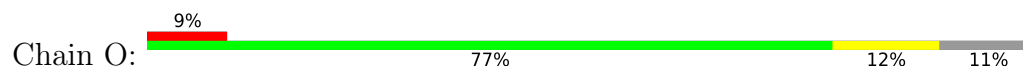
- Molecule 12: Photosystem II reaction center protein M



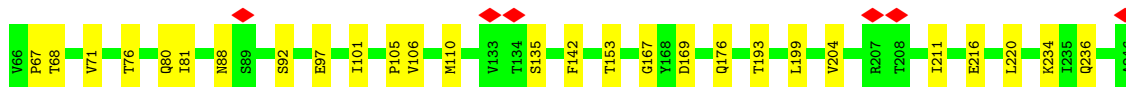
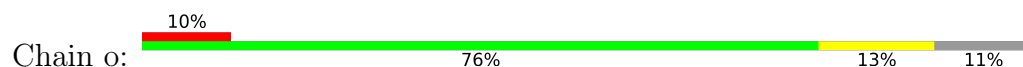
- Molecule 12: Photosystem II reaction center protein M

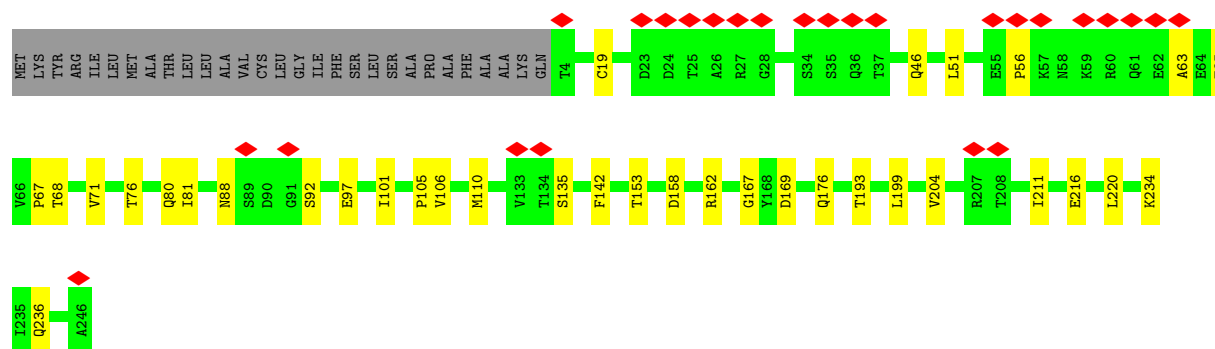


- Molecule 13: Photosystem II extrinsic protein O

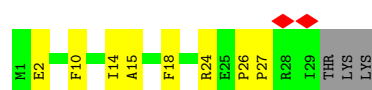


- Molecule 13: Photosystem II extrinsic protein O

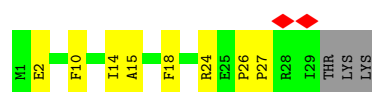




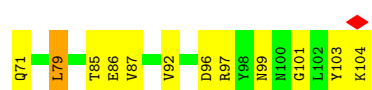
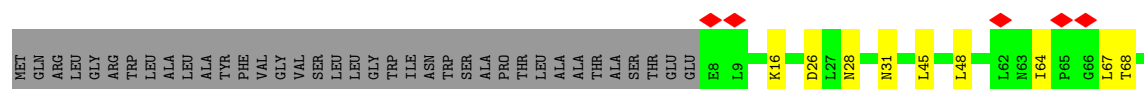
- Molecule 14: Photosystem II reaction center protein T



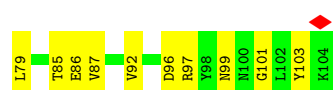
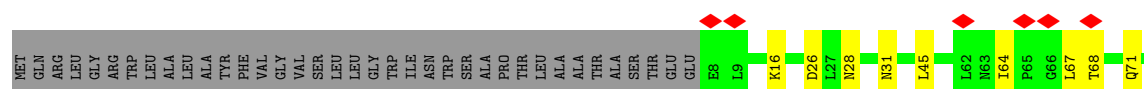
- Molecule 14: Photosystem II reaction center protein T



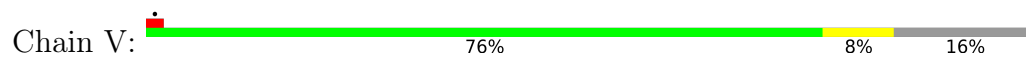
- Molecule 15: Photosystem II extrinsic protein U



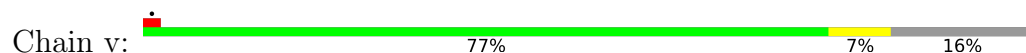
- Molecule 15: Photosystem II extrinsic protein U



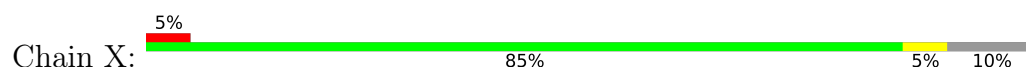
- Molecule 16: Photosystem II extrinsic protein V



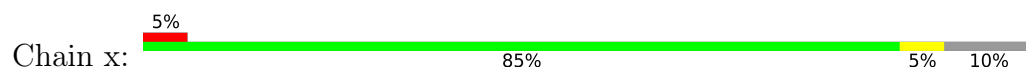
• Molecule 16: Photosystem II extrinsic protein V



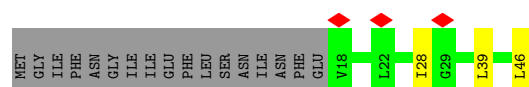
• Molecule 17: Photosystem II reaction center protein X



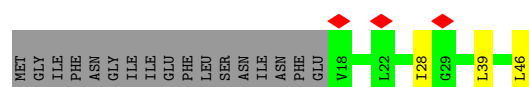
• Molecule 17: Photosystem II reaction center protein X



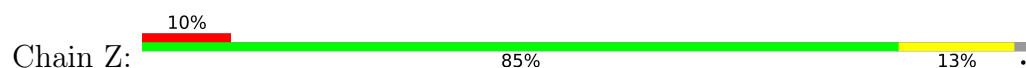
• Molecule 18: Photosystem II reaction center protein Psb30



• Molecule 18: Photosystem II reaction center protein Psb30



• Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  10% 85% 13% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	290.56, 290.56, 290.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5675, 0.5675, 0.5675	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, BCT, CA, PHO, UNL, FE2, HEM, BCR, CL, LMT, HEC, SQD, RRX, LMG, PL9, CLA, OEX, LHG

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	A	0.13	0/2660	0.29	0/3637
1	a	0.13	0/2660	0.29	0/3637
2	B	0.13	0/3981	0.28	0/5440
2	b	0.13	0/3981	0.28	0/5440
3	C	0.12	0/3528	0.28	0/4813
3	c	0.12	0/3528	0.28	0/4813
4	D	0.13	0/2781	0.30	0/3794
4	d	0.13	0/2781	0.30	0/3794
5	E	0.12	0/628	0.27	0/862
5	e	0.12	0/628	0.27	0/862
6	F	0.11	0/272	0.28	0/373
6	f	0.11	0/272	0.28	0/373
7	H	0.12	0/508	0.26	0/693
7	h	0.11	0/508	0.25	0/693
8	I	0.12	0/282	0.26	0/385
8	i	0.12	0/282	0.26	0/385
9	J	0.09	0/247	0.22	0/338
9	j	0.09	0/247	0.22	0/338
10	K	0.15	0/285	0.33	0/395
10	k	0.15	0/285	0.33	0/395
11	L	0.09	0/294	0.23	0/402
11	l	0.10	0/294	0.23	0/402
12	M	0.14	0/255	0.26	0/349
12	m	0.14	0/255	0.27	0/349
13	O	0.11	0/1711	0.30	0/2340
13	o	0.11	0/1711	0.30	0/2340
14	T	0.13	0/245	0.23	0/333
14	t	0.13	0/245	0.23	0/333
15	U	0.09	0/713	0.25	0/974
15	u	0.09	0/713	0.25	0/974
16	V	0.09	0/996	0.29	0/1365

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.09	0/996	0.29	0/1365
17	X	0.11	0/251	0.19	0/341
17	x	0.11	0/251	0.19	0/341
18	Y	0.09	0/178	0.24	0/243
18	y	0.10	0/178	0.24	0/243
19	Z	0.10	0/396	0.25	0/547
19	z	0.10	0/396	0.25	0/547
All	All	0.12	0/40422	0.28	0/55248

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 ⓘ

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	A	2575	0	2451	54	0
1	a	2575	0	2451	52	0
2	B	3838	0	3623	50	0
2	b	3838	0	3623	52	0
3	C	3415	0	3302	38	0
3	c	3415	0	3302	42	0
4	D	2686	0	2586	43	0
4	d	2686	0	2586	45	0
5	E	609	0	580	10	0
5	e	609	0	580	9	0
6	F	263	0	271	6	0
6	f	263	0	271	6	0
7	H	495	0	512	6	0
7	h	495	0	512	7	0
8	I	275	0	275	2	0
8	i	275	0	275	2	0
9	J	241	0	246	1	0
9	j	241	0	246	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	275	0	272	3	0
10	k	275	0	272	3	0
11	L	284	0	295	2	0
11	l	284	0	295	2	0
12	M	252	0	264	5	0
12	m	252	0	264	5	0
13	O	1677	0	1540	23	0
13	o	1677	0	1540	24	0
14	T	236	0	231	10	0
14	t	236	0	231	10	0
15	U	702	0	685	13	0
15	u	702	0	685	10	0
16	V	975	0	956	9	0
16	v	975	0	956	7	0
17	X	248	0	252	1	0
17	x	248	0	252	1	0
18	Y	177	0	164	3	0
18	y	177	0	164	3	0
19	Z	387	0	313	5	0
19	z	387	0	313	6	0
20	A	10	0	0	4	0
20	a	10	0	0	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	237	0	236	14	0
23	B	986	0	1048	45	0
23	C	775	0	791	41	0
23	D	110	0	105	4	0
23	a	237	0	236	14	0
23	b	986	0	1048	45	0
23	c	775	0	791	41	0
23	d	110	0	105	4	0
24	A	40	0	56	0	0
24	B	120	0	168	10	0
24	C	80	0	112	6	0
24	D	40	0	56	3	0
24	K	80	0	112	8	0
24	T	40	0	56	7	0
24	a	40	0	56	3	0
24	b	120	0	168	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	c	80	0	112	7	0
24	d	40	0	56	2	0
24	k	80	0	112	6	0
24	t	40	0	56	8	0
25	A	32	0	28	0	0
25	F	23	0	16	0	0
25	a	32	0	28	0	0
25	f	23	0	16	0	0
26	A	55	0	80	3	0
26	D	55	0	80	3	0
26	a	55	0	80	2	0
26	d	55	0	80	2	0
27	A	8	0	0	0	0
27	B	21	0	0	0	0
27	C	14	0	0	0	0
27	D	19	0	0	0	0
27	E	6	0	0	0	0
27	H	6	0	0	0	0
27	I	6	0	0	0	0
27	K	13	0	0	0	0
27	T	5	0	0	0	0
27	X	9	0	0	0	0
27	a	8	0	0	0	0
27	b	21	0	0	0	0
27	c	14	0	0	0	0
27	d	19	0	0	0	0
27	e	6	0	0	0	0
27	h	6	0	0	0	0
27	i	6	0	0	0	0
27	k	13	0	0	0	0
27	t	5	0	0	0	0
27	x	9	0	0	0	0
28	A	4	0	0	0	0
28	a	4	0	0	0	0
29	A	70	0	84	3	0
29	B	49	0	74	2	0
29	D	49	0	74	1	0
29	L	49	0	74	2	0
29	a	70	0	84	3	0
29	b	49	0	74	3	0
29	d	49	0	74	1	0
29	l	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	45	0	60	0	0
30	C	47	0	64	1	0
30	J	38	0	46	0	0
30	b	45	0	60	0	0
30	c	47	0	64	1	0
30	j	38	0	46	0	0
31	B	35	0	46	1	0
31	J	24	0	35	0	0
31	M	70	0	92	5	0
31	j	24	0	35	0	0
31	m	35	0	46	4	0
32	C	155	0	184	6	0
32	H	62	0	82	1	0
32	c	155	0	184	6	0
32	h	62	0	82	1	0
33	D	128	0	148	4	0
33	d	128	0	148	5	0
34	F	43	0	30	3	0
34	f	43	0	30	3	0
35	O	1	0	0	0	0
35	o	1	0	0	0	0
36	V	43	0	32	0	0
36	v	43	0	32	0	0
37	X	41	0	56	2	0
37	x	41	0	56	0	0
38	A	105	0	0	1	0
38	B	153	0	0	1	0
38	C	91	0	0	0	0
38	D	92	0	0	0	0
38	E	6	0	0	0	0
38	H	16	0	0	0	0
38	I	4	0	0	0	0
38	J	3	0	0	0	0
38	K	2	0	0	0	0
38	L	8	0	0	0	0
38	M	6	0	0	0	0
38	O	38	0	0	0	0
38	T	4	0	0	0	0
38	U	7	0	0	0	0
38	V	13	0	0	0	0
38	X	4	0	0	0	0
38	a	106	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	b	152	0	0	1	0
38	c	91	0	0	0	0
38	d	92	0	0	0	0
38	e	6	0	0	0	0
38	h	16	0	0	0	0
38	i	4	0	0	0	0
38	j	3	0	0	0	0
38	k	2	0	0	0	0
38	l	8	0	0	0	0
38	m	5	0	0	0	0
38	o	38	0	0	0	0
38	t	4	0	0	0	0
38	u	7	0	0	0	0
38	v	12	0	0	0	0
38	x	4	0	0	0	0
All	All	47744	0	45794	691	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 691 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	20:A:401:OEX:O1	1.91	0.87
1:a:189:GLU:OE2	20:a:401:OEX:O1	1.91	0.87
23:A:412:CLA:HHC	23:A:412:CLA:HBB1	1.63	0.81
23:a:412:CLA:HHC	23:a:412:CLA:HBB1	1.63	0.80
5:e:19:TYR:O	5:e:23:HIS:ND1	2.12	0.79

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	A	332/360 (92%)	328 (99%)	4 (1%)	0	100	100
1	a	332/360 (92%)	328 (99%)	4 (1%)	0	100	100
2	B	503/510 (99%)	498 (99%)	4 (1%)	1 (0%)	43	36
2	b	503/510 (99%)	498 (99%)	4 (1%)	1 (0%)	43	36
3	C	448/461 (97%)	441 (98%)	7 (2%)	0	100	100
3	c	448/461 (97%)	441 (98%)	7 (2%)	0	100	100
4	D	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
4	d	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
5	E	78/84 (93%)	78 (100%)	0	0	100	100
5	e	78/84 (93%)	78 (100%)	0	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	60/66 (91%)	59 (98%)	1 (2%)	0	100	100
7	h	60/66 (91%)	59 (98%)	1 (2%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	32/40 (80%)	32 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
13	o	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
14	T	27/32 (84%)	27 (100%)	0	0	100	100
14	t	27/32 (84%)	27 (100%)	0	0	100	100
15	U	95/134 (71%)	94 (99%)	1 (1%)	0	100	100
15	u	95/134 (71%)	94 (99%)	1 (1%)	0	100	100
16	V	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
16	v	135/163 (83%)	134 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	35/41 (85%)	35 (100%)	0	0	100	100
17	x	35/41 (85%)	35 (100%)	0	0	100	100
18	Y	27/46 (59%)	27 (100%)	0	0	100	100
18	y	27/46 (59%)	27 (100%)	0	0	100	100
19	Z	59/62 (95%)	59 (100%)	0	0	100	100
19	z	59/62 (95%)	59 (100%)	0	0	100	100
All	All	5158/5650 (91%)	5076 (98%)	80 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	b	86	ILE

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	A	257/291 (88%)	257 (100%)	0	100	100
1	a	257/291 (88%)	257 (100%)	0	100	100
2	B	364/407 (89%)	360 (99%)	4 (1%)	65	64
2	b	364/407 (89%)	360 (99%)	4 (1%)	65	64
3	C	330/362 (91%)	328 (99%)	2 (1%)	78	79
3	c	330/362 (91%)	328 (99%)	2 (1%)	78	79
4	D	267/283 (94%)	267 (100%)	0	100	100
4	d	267/283 (94%)	267 (100%)	0	100	100
5	E	60/73 (82%)	60 (100%)	0	100	100
5	e	60/73 (82%)	60 (100%)	0	100	100
6	F	26/39 (67%)	26 (100%)	0	100	100
6	f	26/39 (67%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	53/55 (96%)	51 (96%)	2 (4%)	29	19
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	19
8	I	29/35 (83%)	28 (97%)	1 (3%)	32	23
8	i	29/35 (83%)	28 (97%)	1 (3%)	32	23
9	J	22/28 (79%)	22 (100%)	0	100	100
9	j	22/28 (79%)	22 (100%)	0	100	100
10	K	25/37 (68%)	24 (96%)	1 (4%)	28	17
10	k	25/37 (68%)	24 (96%)	1 (4%)	28	17
11	L	32/35 (91%)	32 (100%)	0	100	100
11	l	32/35 (91%)	32 (100%)	0	100	100
12	M	27/33 (82%)	27 (100%)	0	100	100
12	m	27/33 (82%)	27 (100%)	0	100	100
13	O	151/228 (66%)	150 (99%)	1 (1%)	76	76
13	o	151/228 (66%)	150 (99%)	1 (1%)	76	76
14	T	23/29 (79%)	23 (100%)	0	100	100
14	t	23/29 (79%)	23 (100%)	0	100	100
15	U	65/112 (58%)	64 (98%)	1 (2%)	57	54
15	u	65/112 (58%)	64 (98%)	1 (2%)	57	54
16	V	92/138 (67%)	92 (100%)	0	100	100
16	v	92/138 (67%)	92 (100%)	0	100	100
17	X	23/34 (68%)	23 (100%)	0	100	100
17	x	23/34 (68%)	23 (100%)	0	100	100
18	Y	11/37 (30%)	11 (100%)	0	100	100
18	y	11/37 (30%)	11 (100%)	0	100	100
19	Z	24/52 (46%)	24 (100%)	0	100	100
19	z	24/52 (46%)	24 (100%)	0	100	100
All	All	3762/4616 (82%)	3738 (99%)	24 (1%)	76	79

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	388	SER
3	c	346	THR

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Mol	Chain	Res	Type
3	c	176	VAL
7	h	3[A]	ARG
7	H	3[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	231	HIS
15	u	78	ASN
13	O	228	HIS
13	O	46	GLN
15	u	81	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 8 are monoatomic and 24 are unknown - leaving 142 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
23	CLA	b	610	38	69,73,73	2.06	20 (28%)	83,113,113	2.82	29 (34%)
24	BCR	t	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.97	19 (33%)
23	CLA	c	508	3	64,68,73	2.14	20 (31%)	77,107,113	2.93	30 (38%)
26	PL9	D	406	-	55,55,55	0.58	1 (1%)	68,69,69	1.75	19 (27%)
32	DGD	H	101	-	63,63,67	0.85	2 (3%)	77,77,81	0.91	3 (3%)
26	PL9	d	406	-	55,55,55	0.58	1 (1%)	68,69,69	1.75	19 (27%)
23	CLA	C	504	3	69,73,73	2.06	20 (28%)	83,113,113	2.85	28 (33%)
24	BCR	K	102	-	41,41,41	1.10	1 (2%)	56,56,56	1.75	14 (25%)
34	HEM	F	102	5,6	50,50,50	1.53	6 (12%)	66,82,82	1.70	12 (18%)
23	CLA	B	604	2	69,73,73	2.03	19 (27%)	83,113,113	2.78	31 (37%)
23	CLA	c	513	3	46,50,73	2.45	20 (43%)	55,85,113	3.38	27 (49%)
23	CLA	C	519	38	69,73,73	2.07	21 (30%)	83,113,113	2.84	31 (37%)
32	DGD	h	101	-	63,63,67	0.85	2 (3%)	77,77,81	0.91	3 (3%)
24	BCR	C	520	-	41,41,41	1.09	1 (2%)	56,56,56	1.97	19 (33%)
25	SQD	A	409	-	31,32,54	1.29	3 (9%)	40,43,65	1.48	6 (15%)
23	CLA	B	610	38	69,73,73	2.06	20 (28%)	83,113,113	2.82	29 (34%)
23	CLA	b	602	2	69,73,73	2.06	20 (28%)	83,113,113	2.83	31 (37%)
23	CLA	c	502	3	69,73,73	2.07	20 (28%)	83,113,113	2.79	28 (33%)
23	CLA	A	407	1	55,59,73	2.32	20 (36%)	66,96,113	3.18	31 (46%)
30	LMG	B	618	-	45,45,55	0.98	2 (4%)	53,53,63	1.07	3 (5%)
23	CLA	d	403	4	69,73,73	2.02	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	508	3	64,68,73	2.14	20 (31%)	77,107,113	2.93	30 (38%)
23	CLA	B	602	2	69,73,73	2.06	20 (28%)	83,113,113	2.83	31 (37%)
25	SQD	F	101	-	22,23,54	1.02	2 (9%)	30,33,65	1.08	2 (6%)
20	OEX	a	401	38,1,3	0,14,14	-	-	-	-	-
24	BCR	c	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.82	17 (30%)
23	CLA	B	609	2	69,73,73	2.04	20 (28%)	83,113,113	2.82	30 (36%)
29	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
23	CLA	c	519	38	69,73,73	2.07	21 (30%)	83,113,113	2.84	31 (37%)
32	DGD	c	518	-	54,54,67	0.91	2 (3%)	68,68,81	1.03	3 (4%)
30	LMG	C	501	-	47,47,55	0.97	2 (4%)	55,55,63	1.19	5 (9%)
23	CLA	b	601	38	46,50,73	2.45	19 (41%)	55,85,113	3.34	28 (50%)
24	BCR	K	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.99	15 (26%)
20	OEX	A	401	38,1,3	0,14,14	-	-	-	-	-
23	CLA	b	613	2	58,62,73	2.23	20 (34%)	69,99,113	3.05	30 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PL9	A	410	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	21 (30%)
23	CLA	C	513	3	46,50,73	2.45	20 (43%)	55,85,113	3.38	27 (49%)
23	CLA	C	506	3	50,54,73	2.41	21 (42%)	60,90,113	3.18	27 (45%)
24	BCR	b	616	-	41,41,41	1.08	1 (2%)	56,56,56	1.75	12 (21%)
23	CLA	A	405	1	69,73,73	2.04	20 (28%)	83,113,113	2.85	32 (38%)
23	CLA	C	512	3	56,60,73	2.28	20 (35%)	67,97,113	3.13	30 (44%)
23	CLA	C	510	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	31 (37%)
23	CLA	C	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	a	412	38	69,73,73	2.08	21 (30%)	83,113,113	2.84	30 (36%)
23	CLA	c	510	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	31 (37%)
23	CLA	B	601	38	46,50,73	2.45	19 (41%)	55,85,113	3.34	28 (50%)
25	SQD	f	101	-	22,23,54	1.02	2 (9%)	30,33,65	1.08	2 (6%)
29	LHG	b	622	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
29	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
24	BCR	b	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.77	13 (23%)
23	CLA	C	502	3	69,73,73	2.07	20 (28%)	83,113,113	2.79	28 (33%)
24	BCR	T	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.97	19 (33%)
23	CLA	b	606	2	69,73,73	2.06	20 (28%)	83,113,113	2.83	32 (38%)
23	CLA	b	605	2	69,73,73	2.05	20 (28%)	83,113,113	2.86	28 (33%)
33	PHO	D	402	-	58,69,69	2.77	15 (25%)	56,99,99	2.83	15 (26%)
23	CLA	B	607	38	69,73,73	2.05	20 (28%)	83,113,113	2.80	31 (37%)
23	CLA	c	507	38	69,73,73	2.05	20 (28%)	83,113,113	2.81	28 (33%)
31	LMT	M	101	-	36,36,36	0.15	0	47,47,47	0.35	0
37	RRX	X	101	-	42,42,42	1.62	8 (19%)	57,58,58	1.43	10 (17%)
29	LHG	A	414	-	38,38,48	1.05	2 (5%)	41,44,54	1.15	4 (9%)
30	LMG	j	101	-	38,38,55	1.06	2 (5%)	46,46,63	1.12	4 (8%)
23	CLA	c	505	3	59,63,73	2.20	20 (33%)	71,101,113	3.03	30 (42%)
23	CLA	C	509	3	69,73,73	2.08	20 (28%)	83,113,113	2.77	30 (36%)
26	PL9	a	410	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	21 (30%)
37	RRX	x	101	-	42,42,42	1.62	8 (19%)	57,58,58	1.43	10 (17%)
23	CLA	B	606	2	69,73,73	2.06	20 (28%)	83,113,113	2.83	32 (38%)
24	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.82	17 (30%)
36	HEC	v	201	16	50,50,50	1.72	7 (14%)	68,82,82	1.42	5 (7%)
31	LMT	m	101	-	36,36,36	0.15	0	47,47,47	0.35	0
23	CLA	B	614	2	69,73,73	2.06	20 (28%)	83,113,113	2.82	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	A	408	-	41,41,41	1.07	1 (2%)	56,56,56	1.78	15 (26%)
24	BCR	k	102	-	41,41,41	1.10	1 (2%)	56,56,56	1.75	14 (25%)
23	CLA	a	406	38	60,64,73	2.23	21 (35%)	72,102,113	3.01	31 (43%)
23	CLA	a	407	1	55,59,73	2.32	20 (36%)	66,96,113	3.18	31 (46%)
30	LMG	c	501	-	47,47,55	0.97	2 (4%)	55,55,63	1.19	5 (9%)
23	CLA	d	404	4	49,53,73	2.45	20 (40%)	59,89,113	3.25	27 (45%)
23	CLA	B	615	2	49,53,73	2.43	20 (40%)	59,89,113	3.25	25 (42%)
23	CLA	B	608	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	28 (33%)
31	LMT	J	102	-	24,24,36	0.15	0	29,29,47	0.29	0
32	DGD	C	515	-	53,53,67	0.92	2 (3%)	67,67,81	1.03	3 (4%)
23	CLA	B	611	2	69,73,73	2.05	20 (28%)	83,113,113	2.84	28 (33%)
23	CLA	b	609	2	69,73,73	2.04	20 (28%)	83,113,113	2.83	30 (36%)
32	DGD	c	516	-	51,51,67	0.94	2 (3%)	65,65,81	1.08	4 (6%)
23	CLA	b	607	38	69,73,73	2.05	20 (28%)	83,113,113	2.80	31 (37%)
23	CLA	D	404	4	49,53,73	2.45	20 (40%)	59,89,113	3.25	27 (45%)
28	BCT	a	413[A]	21	2,3,3	0.70	0	2,3,3	0.67	0
23	CLA	B	613	2	58,62,73	2.23	20 (34%)	69,99,113	3.05	30 (43%)
24	BCR	D	405	-	41,41,41	1.08	1 (2%)	56,56,56	2.02	11 (19%)
23	CLA	a	405	1	69,73,73	2.04	20 (28%)	83,113,113	2.85	32 (38%)
23	CLA	b	612	2	69,73,73	2.04	19 (27%)	83,113,113	2.75	29 (34%)
23	CLA	b	615	2	49,53,73	2.43	20 (40%)	59,89,113	3.25	25 (42%)
23	CLA	b	608	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	28 (33%)
24	BCR	B	616	-	41,41,41	1.08	1 (2%)	56,56,56	1.75	12 (21%)
24	BCR	d	405	-	41,41,41	1.08	1 (2%)	56,56,56	2.02	11 (19%)
23	CLA	A	406	38	60,64,73	2.23	21 (35%)	72,102,113	3.01	31 (43%)
33	PHO	D	401	-	58,69,69	2.74	15 (25%)	56,99,99	2.86	17 (30%)
33	PHO	d	401	-	58,69,69	2.74	15 (25%)	56,99,99	2.86	17 (30%)
29	LHG	a	414	-	38,38,48	1.05	2 (5%)	41,44,54	1.15	4 (9%)
32	DGD	C	518	-	54,54,67	0.91	2 (3%)	68,68,81	1.03	3 (4%)
23	CLA	D	403	4	69,73,73	2.02	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	B	605	2	69,73,73	2.05	20 (28%)	83,113,113	2.86	28 (33%)
23	CLA	C	507	38	69,73,73	2.05	20 (28%)	83,113,113	2.81	28 (33%)
28	BCT	A	413[A]	21	2,3,3	0.70	0	2,3,3	0.67	0
29	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	B	603	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	509	3	69,73,73	2.08	20 (28%)	83,113,113	2.77	30 (36%)
24	BCR	a	408	-	41,41,41	1.07	1 (2%)	56,56,56	1.78	15 (26%)
23	CLA	b	604	2	69,73,73	2.03	19 (27%)	83,113,113	2.78	31 (37%)
24	BCR	c	520	-	41,41,41	1.09	1 (2%)	56,56,56	1.97	19 (33%)
25	SQD	a	409	-	31,32,54	1.29	3 (9%)	40,43,65	1.48	6 (15%)
24	BCR	B	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	13 (23%)
29	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
24	BCR	k	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.99	15 (26%)
23	CLA	C	511	3	69,73,73	2.05	20 (28%)	83,113,113	2.81	28 (33%)
23	CLA	c	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	B	621	2	69,73,73	2.04	20 (28%)	83,113,113	2.77	29 (34%)
32	DGD	C	516	-	51,51,67	0.94	2 (3%)	65,65,81	1.08	4 (6%)
30	LMG	J	101	-	38,38,55	1.06	2 (5%)	46,46,63	1.12	4 (8%)
23	CLA	c	511	3	69,73,73	2.05	20 (28%)	83,113,113	2.81	28 (33%)
23	CLA	b	614	2	69,73,73	2.05	20 (28%)	83,113,113	2.82	29 (34%)
36	HEC	V	201	16	50,50,50	1.72	6 (12%)	68,82,82	1.42	5 (7%)
30	LMG	b	618	-	45,45,55	0.98	2 (4%)	53,53,63	1.07	3 (5%)
23	CLA	c	512	3	56,60,73	2.28	20 (35%)	67,97,113	3.13	30 (44%)
34	HEM	f	102	5,6	50,50,50	1.53	6 (12%)	66,82,82	1.70	12 (18%)
33	PHO	d	402	-	58,69,69	2.77	15 (25%)	56,99,99	2.83	15 (26%)
23	CLA	c	504	3	69,73,73	2.06	20 (28%)	83,113,113	2.85	28 (33%)
32	DGD	c	515	-	53,53,67	0.92	2 (3%)	67,67,81	1.03	3 (4%)
23	CLA	b	603	2	69,73,73	2.05	20 (28%)	83,113,113	2.80	32 (38%)
24	BCR	b	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	13 (23%)
23	CLA	b	611	2	69,73,73	2.05	20 (28%)	83,113,113	2.84	28 (33%)
23	CLA	A	412	38	69,73,73	2.07	21 (30%)	83,113,113	2.84	30 (36%)
23	CLA	C	505	3	59,63,73	2.20	20 (33%)	71,101,113	3.03	30 (42%)
24	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	14 (25%)
23	CLA	B	612	2	69,73,73	2.04	19 (27%)	83,113,113	2.75	28 (33%)
29	LHG	A	415	-	30,30,48	0.99	2 (6%)	33,35,54	1.15	2 (6%)
31	LMT	M	102	-	36,36,36	0.15	0	47,47,47	0.29	0
29	LHG	B	622	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
31	LMT	j	102	-	24,24,36	0.15	0	29,29,47	0.29	0
23	CLA	b	621	2	69,73,73	2.04	20 (28%)	83,113,113	2.77	28 (33%)
29	LHG	a	415	-	30,30,48	0.99	2 (6%)	33,35,54	1.15	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	506	3	50,54,73	2.41	21 (42%)	60,90,113	3.18	27 (45%)
31	LMT	B	623	-	36,36,36	0.15	0	47,47,47	0.29	0

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
23	CLA	b	610	38	-	4/39/115/115	-
24	BCR	t	102	-	-	7/29/63/63	0/2/2/2
23	CLA	c	508	3	-	8/33/109/115	-
26	PL9	D	406	-	-	14/53/73/73	0/1/1/1
32	DGD	H	101	-	-	6/51/91/95	0/2/2/2
26	PL9	d	406	-	-	14/53/73/73	0/1/1/1
23	CLA	C	504	3	-	2/39/115/115	-
24	BCR	K	102	-	-	5/29/63/63	0/2/2/2
34	HEM	F	102	5,6	-	8/14/54/54	-
23	CLA	B	604	2	-	8/39/115/115	-
23	CLA	c	513	3	-	0/12/88/115	-
23	CLA	C	519	38	-	12/39/115/115	-
32	DGD	h	101	-	-	6/51/91/95	0/2/2/2
24	BCR	C	520	-	-	2/29/63/63	0/2/2/2
25	SQD	A	409	-	-	3/27/47/69	0/1/1/1
23	CLA	B	610	38	-	4/39/115/115	-
23	CLA	b	602	2	-	5/39/115/115	-
23	CLA	c	502	3	-	7/39/115/115	-
23	CLA	A	407	1	-	4/23/99/115	-
30	LMG	B	618	-	-	2/40/60/70	0/1/1/1
23	CLA	d	403	4	-	2/39/115/115	-
23	CLA	C	508	3	-	8/33/109/115	-
23	CLA	B	602	2	-	5/39/115/115	-
25	SQD	F	101	-	-	2/15/35/69	0/1/1/1
24	BCR	c	514	-	-	2/29/63/63	0/2/2/2
23	CLA	B	609	2	-	4/39/115/115	-
29	LHG	D	407	-	-	10/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	519	38	-	12/39/115/115	-
32	DGD	c	518	-	-	3/42/82/95	0/2/2/2
30	LMG	C	501	-	-	5/42/62/70	0/1/1/1
23	CLA	b	601	38	-	3/12/88/115	-
24	BCR	K	103	-	-	0/29/63/63	0/2/2/2
23	CLA	b	613	2	-	12/26/102/115	-
26	PL9	A	410	-	-	14/53/73/73	0/1/1/1
23	CLA	C	513	3	-	0/12/88/115	-
23	CLA	C	506	3	-	6/17/93/115	-
24	BCR	b	616	-	-	2/29/63/63	0/2/2/2
23	CLA	A	405	1	-	5/39/115/115	-
23	CLA	C	512	3	-	10/24/100/115	-
23	CLA	C	510	3	-	8/39/115/115	-
23	CLA	C	503	3	-	7/39/115/115	-
23	CLA	a	412	38	-	7/39/115/115	-
23	CLA	c	510	3	-	8/39/115/115	-
23	CLA	B	601	38	-	3/12/88/115	-
25	SQD	f	101	-	-	2/15/35/69	0/1/1/1
29	LHG	b	622	-	-	22/53/53/53	-
29	LHG	d	407	-	-	10/53/53/53	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
23	CLA	C	502	3	-	7/39/115/115	-
24	BCR	T	102	-	-	7/29/63/63	0/2/2/2
23	CLA	b	606	2	-	10/39/115/115	-
23	CLA	b	605	2	-	6/39/115/115	-
33	PHO	D	402	-	-	0/37/103/103	0/5/6/6
23	CLA	B	607	38	-	13/39/115/115	-
23	CLA	c	507	38	-	9/39/115/115	-
31	LMT	M	101	-	-	1/21/61/61	0/2/2/2
37	RRX	X	101	-	-	9/29/65/65	0/2/2/2
29	LHG	A	414	-	-	10/43/43/53	-
30	LMG	j	101	-	-	3/33/53/70	0/1/1/1
23	CLA	c	505	3	-	9/27/103/115	-
23	CLA	C	509	3	-	10/39/115/115	-
26	PL9	a	410	-	-	14/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	RRX	x	101	-	-	9/29/65/65	0/2/2/2
23	CLA	B	606	2	-	10/39/115/115	-
24	BCR	C	514	-	-	2/29/63/63	0/2/2/2
36	HEC	v	201	16	1/1/3/7	2/14/54/54	-
31	LMT	m	101	-	-	1/21/61/61	0/2/2/2
23	CLA	B	614	2	-	9/39/115/115	-
24	BCR	A	408	-	-	3/29/63/63	0/2/2/2
24	BCR	k	102	-	-	5/29/63/63	0/2/2/2
23	CLA	a	406	38	-	2/29/105/115	-
23	CLA	a	407	1	-	4/23/99/115	-
30	LMG	c	501	-	-	5/42/62/70	0/1/1/1
23	CLA	d	404	4	-	0/15/91/115	-
23	CLA	B	615	2	-	3/15/91/115	-
23	CLA	B	608	2	-	4/39/115/115	-
31	LMT	J	102	-	-	0/15/35/61	0/1/1/2
32	DGD	C	515	-	-	9/41/81/95	0/2/2/2
23	CLA	B	611	2	-	7/39/115/115	-
23	CLA	b	609	2	-	4/39/115/115	-
32	DGD	c	516	-	-	6/39/79/95	0/2/2/2
23	CLA	b	607	38	-	13/39/115/115	-
23	CLA	D	404	4	-	0/15/91/115	-
23	CLA	B	613	2	-	12/26/102/115	-
24	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	a	405	1	-	5/39/115/115	-
23	CLA	b	612	2	-	10/39/115/115	-
23	CLA	b	615	2	-	3/15/91/115	-
23	CLA	b	608	2	-	4/39/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
24	BCR	d	405	-	-	8/29/63/63	0/2/2/2
23	CLA	A	406	38	-	2/29/105/115	-
33	PHO	D	401	-	-	6/37/103/103	0/5/6/6
33	PHO	d	401	-	-	6/37/103/103	0/5/6/6
29	LHG	a	414	-	-	10/43/43/53	-
32	DGD	C	518	-	-	3/42/82/95	0/2/2/2
23	CLA	D	403	4	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	605	2	-	6/39/115/115	-
23	CLA	C	507	38	-	9/39/115/115	-
29	LHG	L	101	-	-	14/53/53/53	-
23	CLA	B	603	2	-	7/39/115/115	-
23	CLA	c	509	3	-	10/39/115/115	-
24	BCR	a	408	-	-	4/29/63/63	0/2/2/2
23	CLA	b	604	2	-	8/39/115/115	-
24	BCR	c	520	-	-	2/29/63/63	0/2/2/2
25	SQD	a	409	-	-	3/27/47/69	0/1/1/1
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LHG	l	101	-	-	14/53/53/53	-
24	BCR	k	103	-	-	0/29/63/63	0/2/2/2
23	CLA	C	511	3	-	5/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	B	621	2	-	5/39/115/115	-
32	DGD	C	516	-	-	6/39/79/95	0/2/2/2
30	LMG	J	101	-	-	3/33/53/70	0/1/1/1
36	HEC	V	201	16	1/1/3/7	2/14/54/54	-
23	CLA	b	614	2	-	9/39/115/115	-
23	CLA	c	511	3	-	5/39/115/115	-
30	LMG	b	618	-	-	2/40/60/70	0/1/1/1
23	CLA	c	512	3	-	10/24/100/115	-
34	HEM	f	102	5,6	-	8/14/54/54	-
33	PHO	d	402	-	-	0/37/103/103	0/5/6/6
23	CLA	c	504	3	-	2/39/115/115	-
32	DGD	c	515	-	-	9/41/81/95	0/2/2/2
23	CLA	b	603	2	-	7/39/115/115	-
24	BCR	b	617	-	-	4/29/63/63	0/2/2/2
23	CLA	b	611	2	-	7/39/115/115	-
23	CLA	A	412	38	-	7/39/115/115	-
23	CLA	C	505	3	-	9/27/103/115	-
24	BCR	B	617	-	-	4/29/63/63	0/2/2/2
23	CLA	B	612	2	-	10/39/115/115	-
29	LHG	A	415	-	-	7/33/33/53	-
31	LMT	M	102	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	B	622	-	-	22/53/53/53	-
31	LMT	j	102	-	-	0/15/35/61	0/1/1/2
23	CLA	b	621	2	-	5/39/115/115	-
29	LHG	a	415	-	-	7/33/33/53	-
23	CLA	c	506	3	-	6/17/93/115	-
31	LMT	B	623	-	-	2/21/61/61	0/2/2/2

The worst 5 of 1585 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	402	PHO	C1D-C2D	8.79	1.49	1.39
33	d	402	PHO	C1D-C2D	8.79	1.49	1.39
33	D	401	PHO	C1D-C2D	8.74	1.49	1.39
33	d	401	PHO	C1D-C2D	8.74	1.49	1.39
33	D	401	PHO	C1B-C2B	8.71	1.49	1.39

The worst 5 of 2645 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	401	PHO	C2D-C1D-ND	11.32	117.34	109.53
33	d	401	PHO	C2D-C1D-ND	11.32	117.34	109.53
33	D	402	PHO	C2D-C1D-ND	11.29	117.32	109.53
33	d	402	PHO	C2D-C1D-ND	11.29	117.32	109.53
23	B	605	CLA	C1D-ND-C4D	-9.84	99.35	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	V	201	HEC	NA
36	v	201	HEC	NA

5 of 829 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C2B-C3B-CAB-CBB
23	A	407	CLA	C4B-C3B-CAB-CBB
23	A	412	CLA	CHA-CBD-CGD-O1D
23	A	412	CLA	CHA-CBD-CGD-O2D
23	B	604	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

124 monomers are involved in 327 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	610	CLA	2	0
24	t	102	BCR	8	0
23	c	508	CLA	4	0
26	D	406	PL9	3	0
32	H	101	DGD	1	0
26	d	406	PL9	2	0
23	C	504	CLA	3	0
24	K	102	BCR	3	0
34	F	102	HEM	3	0
23	B	604	CLA	4	0
23	c	513	CLA	2	0
23	C	519	CLA	5	0
32	h	101	DGD	1	0
24	C	520	BCR	3	0
23	B	610	CLA	2	0
23	b	602	CLA	4	0
23	c	502	CLA	6	0
23	A	407	CLA	1	0
23	d	403	CLA	4	0
23	C	508	CLA	4	0
23	B	602	CLA	5	0
20	a	401	OEX	4	0
24	c	514	BCR	4	0
23	B	609	CLA	4	0
29	D	407	LHG	1	0
23	c	519	CLA	4	0
32	c	518	DGD	2	0
30	C	501	LMG	1	0
23	b	601	CLA	1	0
24	K	103	BCR	5	0
20	A	401	OEX	4	0
23	b	613	CLA	4	0
26	A	410	PL9	3	0
23	C	513	CLA	2	0
23	C	506	CLA	3	0
24	b	616	BCR	4	0
23	A	405	CLA	7	0
23	C	512	CLA	2	0
23	C	510	CLA	4	0
23	C	503	CLA	5	0
23	a	412	CLA	5	0
23	c	510	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	601	CLA	1	0
29	b	622	LHG	3	0
29	d	407	LHG	1	0
24	b	620	BCR	6	0
23	C	502	CLA	5	0
24	T	102	BCR	7	0
23	b	606	CLA	4	0
23	b	605	CLA	7	0
33	D	402	PHO	3	0
23	B	607	CLA	2	0
23	c	507	CLA	10	0
31	M	101	LMT	4	0
37	X	101	RRX	2	0
29	A	414	LHG	2	0
23	c	505	CLA	5	0
23	C	509	CLA	3	0
26	a	410	PL9	2	0
23	B	606	CLA	4	0
24	C	514	BCR	3	0
31	m	101	LMT	4	0
23	B	614	CLA	5	0
24	k	102	BCR	2	0
23	a	406	CLA	2	0
23	a	407	CLA	1	0
30	c	501	LMG	1	0
23	B	615	CLA	1	0
23	B	608	CLA	2	0
32	C	515	DGD	3	0
23	B	611	CLA	3	0
23	b	609	CLA	4	0
32	c	516	DGD	1	0
23	b	607	CLA	2	0
23	B	613	CLA	3	0
24	D	405	BCR	3	0
23	a	405	CLA	6	0
23	b	612	CLA	4	0
23	b	615	CLA	1	0
23	b	608	CLA	3	0
24	B	616	BCR	3	0
24	d	405	BCR	2	0
23	A	406	CLA	2	0
33	D	401	PHO	1	0

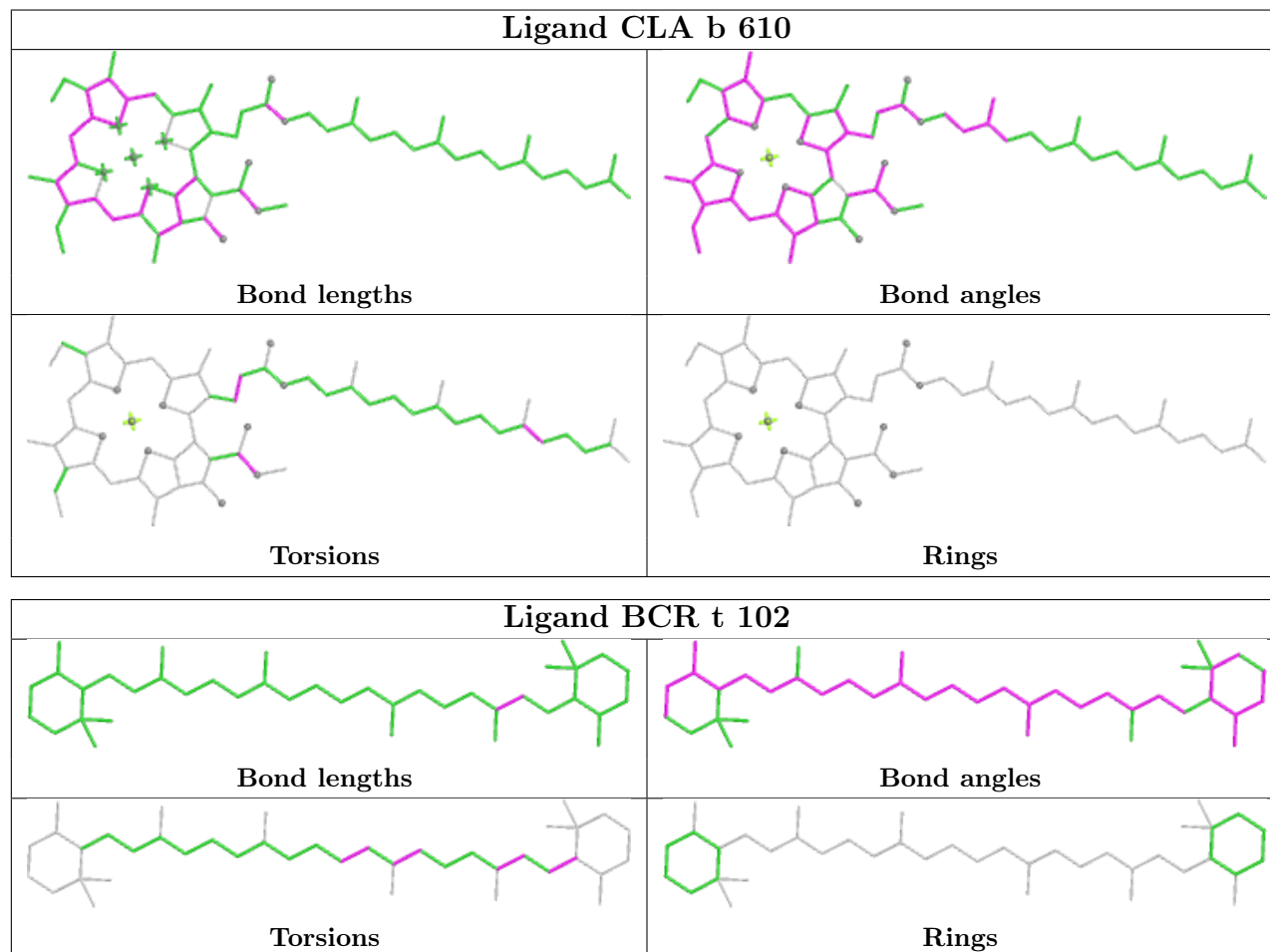
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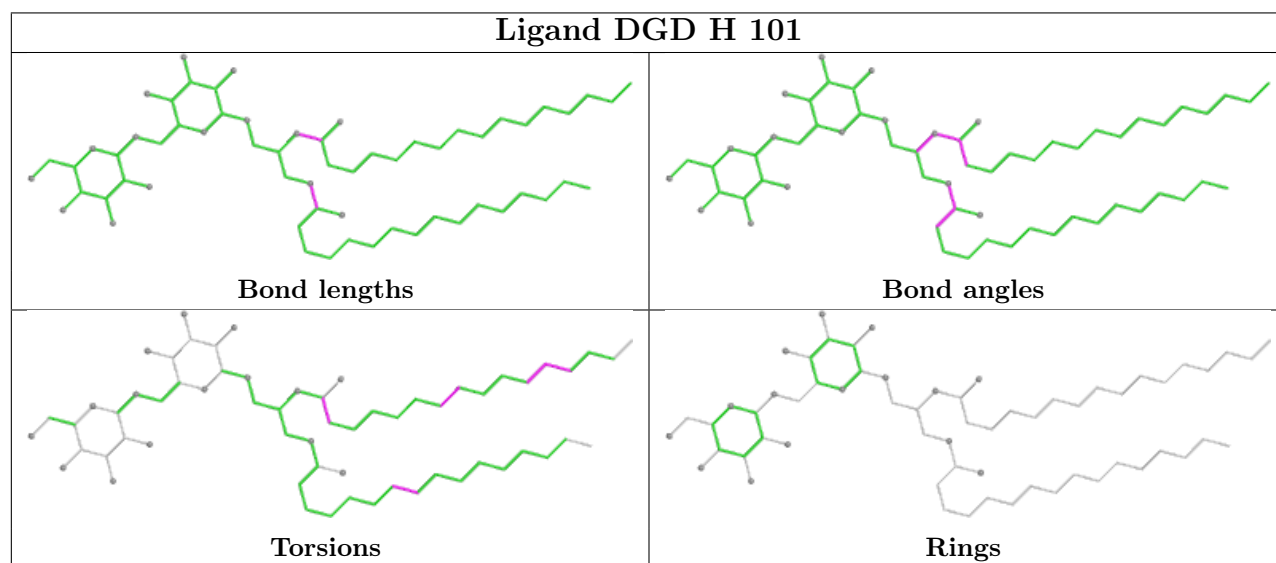
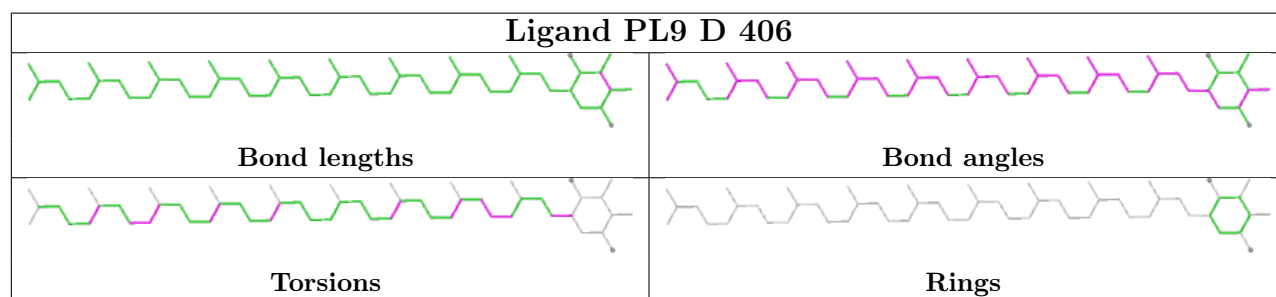
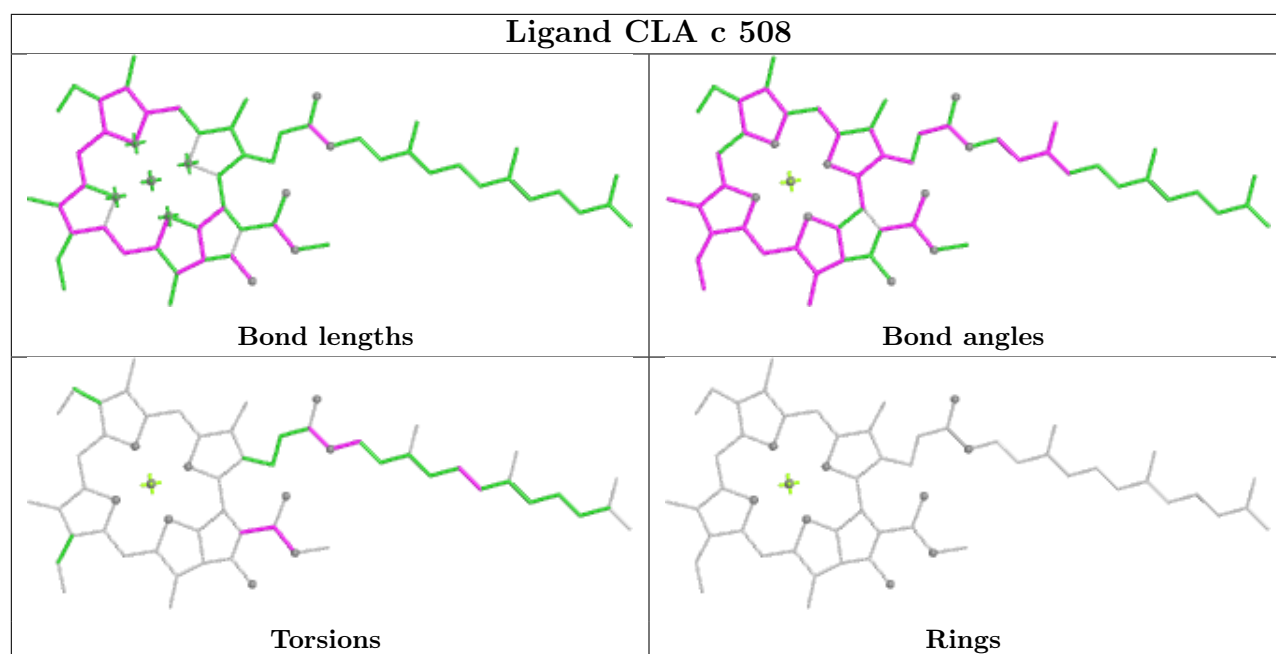
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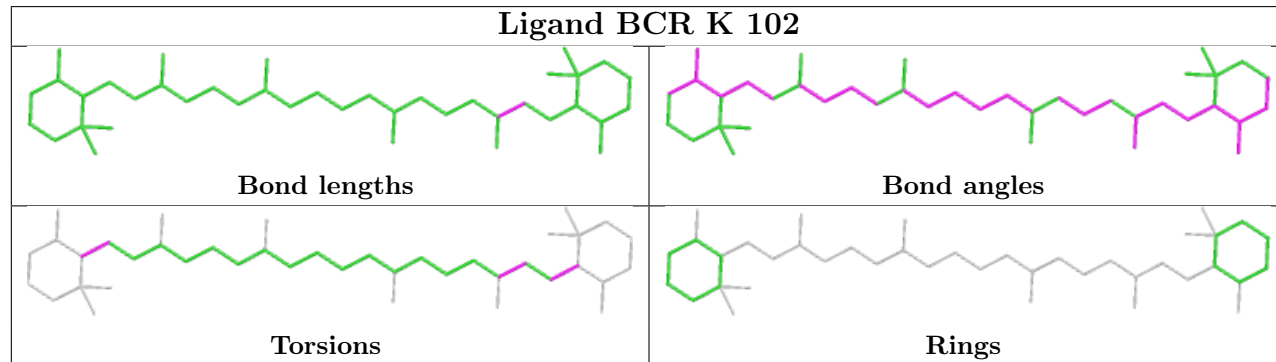
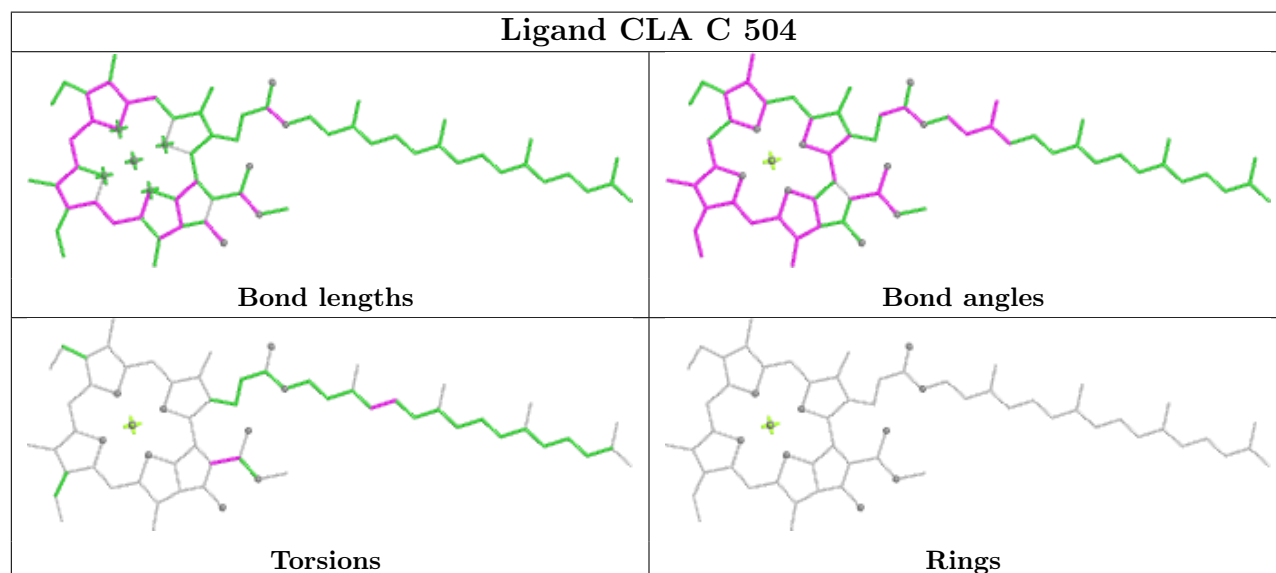
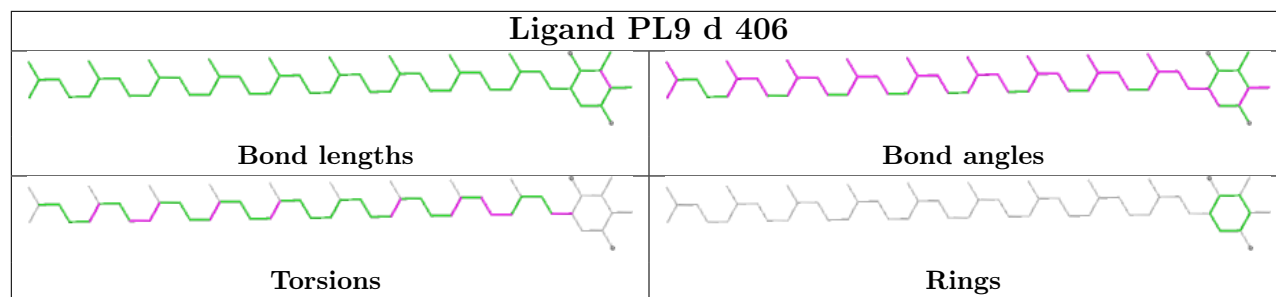
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	401	PHO	2	0
29	a	414	LHG	2	0
32	C	518	DGD	2	0
23	D	403	CLA	4	0
23	B	605	CLA	7	0
23	C	507	CLA	9	0
29	L	101	LHG	2	0
23	B	603	CLA	2	0
23	c	509	CLA	2	0
24	a	408	BCR	3	0
23	b	604	CLA	4	0
24	c	520	BCR	3	0
24	B	620	BCR	5	0
29	l	101	LHG	2	0
24	k	103	BCR	4	0
23	C	511	CLA	7	0
23	c	503	CLA	5	0
23	B	621	CLA	4	0
32	C	516	DGD	1	0
23	c	511	CLA	7	0
23	b	614	CLA	5	0
23	c	512	CLA	1	0
34	f	102	HEM	3	0
33	d	402	PHO	3	0
23	c	504	CLA	4	0
32	c	515	DGD	3	0
23	b	603	CLA	3	0
24	b	617	BCR	1	0
23	b	611	CLA	2	0
23	A	412	CLA	5	0
23	C	505	CLA	5	0
24	B	617	BCR	2	0
23	B	612	CLA	4	0
29	A	415	LHG	1	0
31	M	102	LMT	1	0
29	B	622	LHG	2	0
23	b	621	CLA	3	0
29	a	415	LHG	1	0
23	c	506	CLA	3	0
31	B	623	LMT	1	0

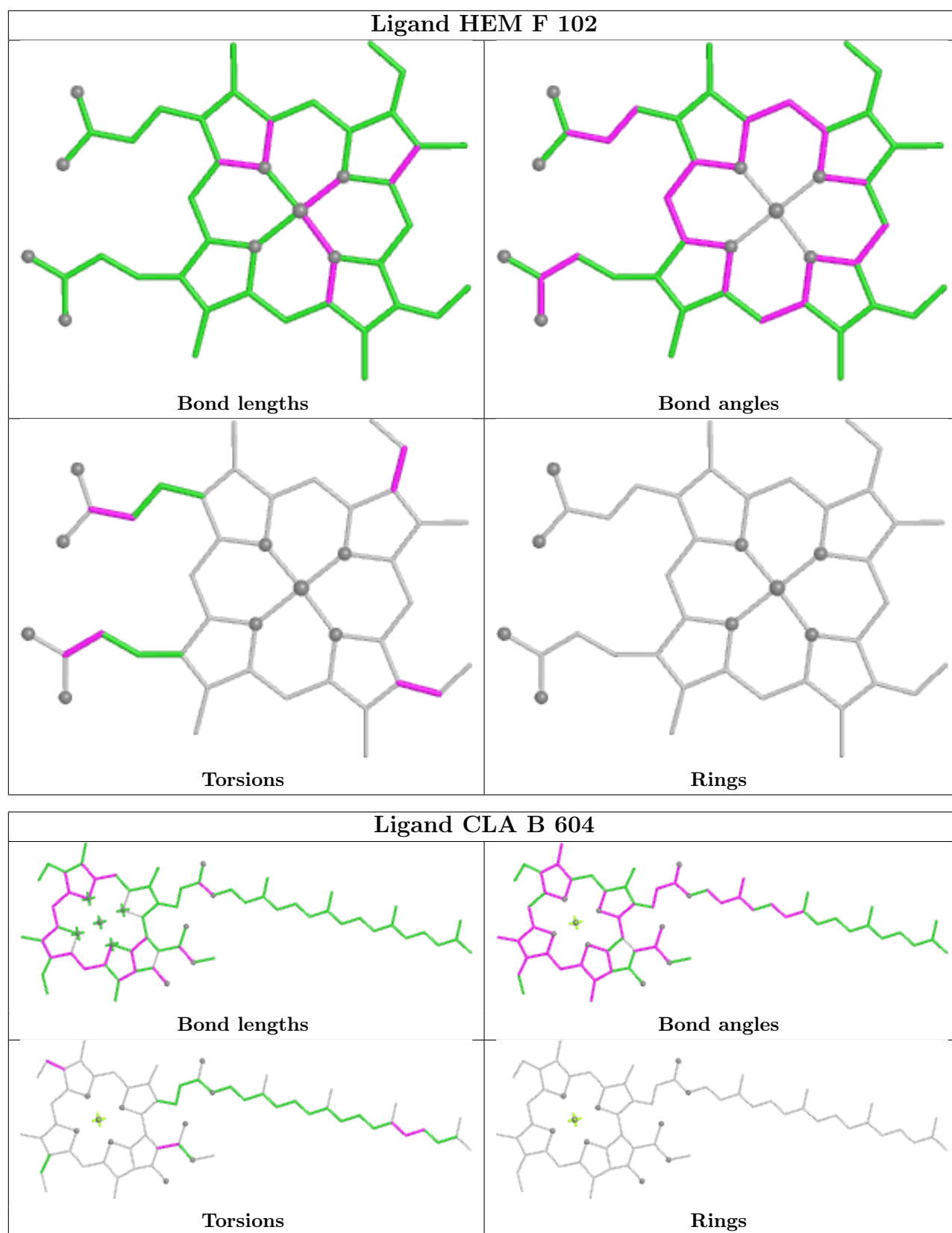
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

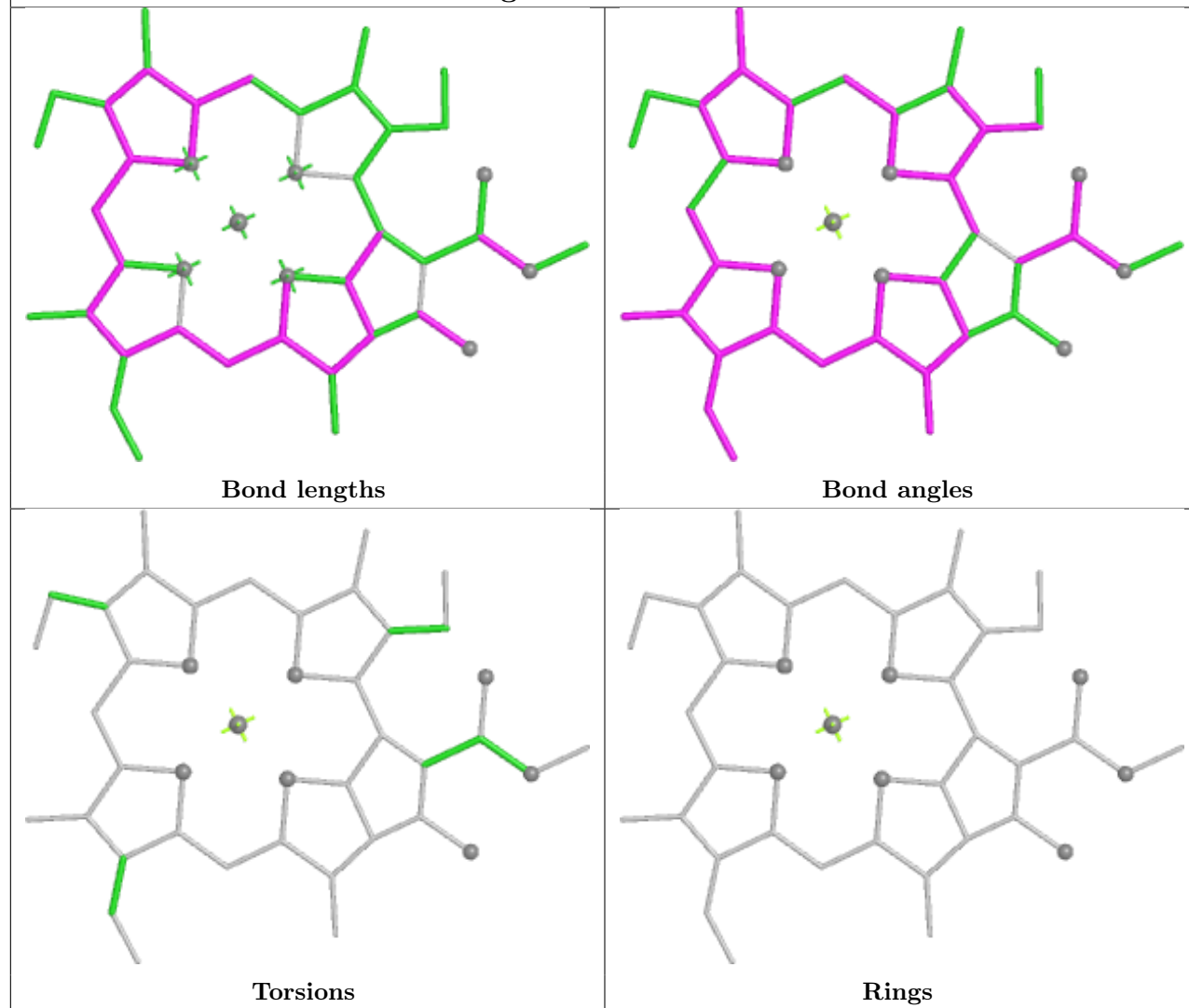




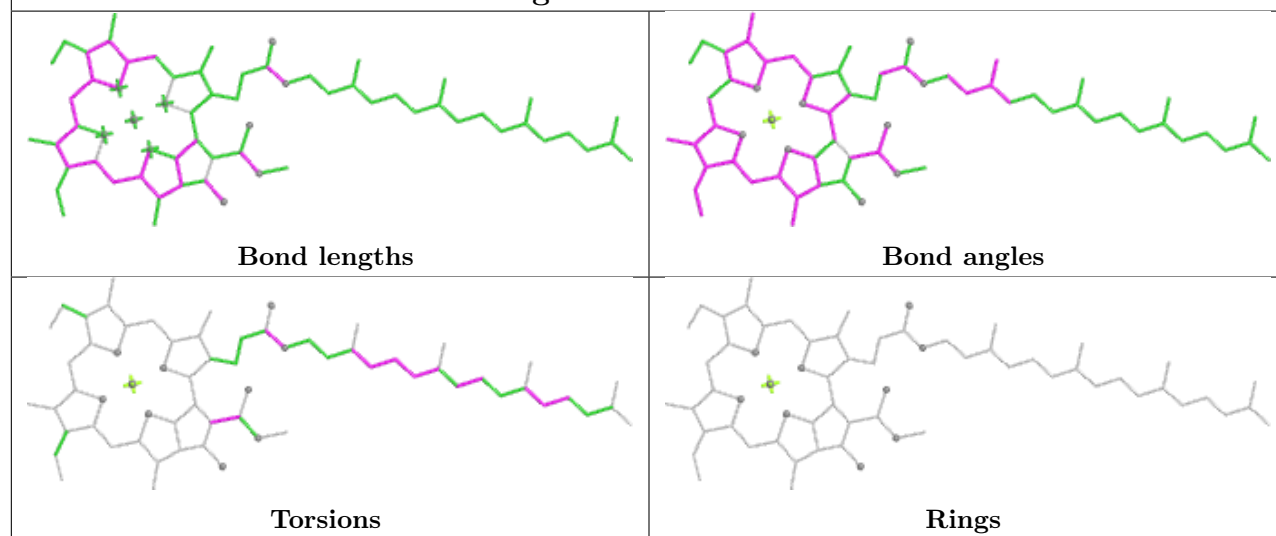


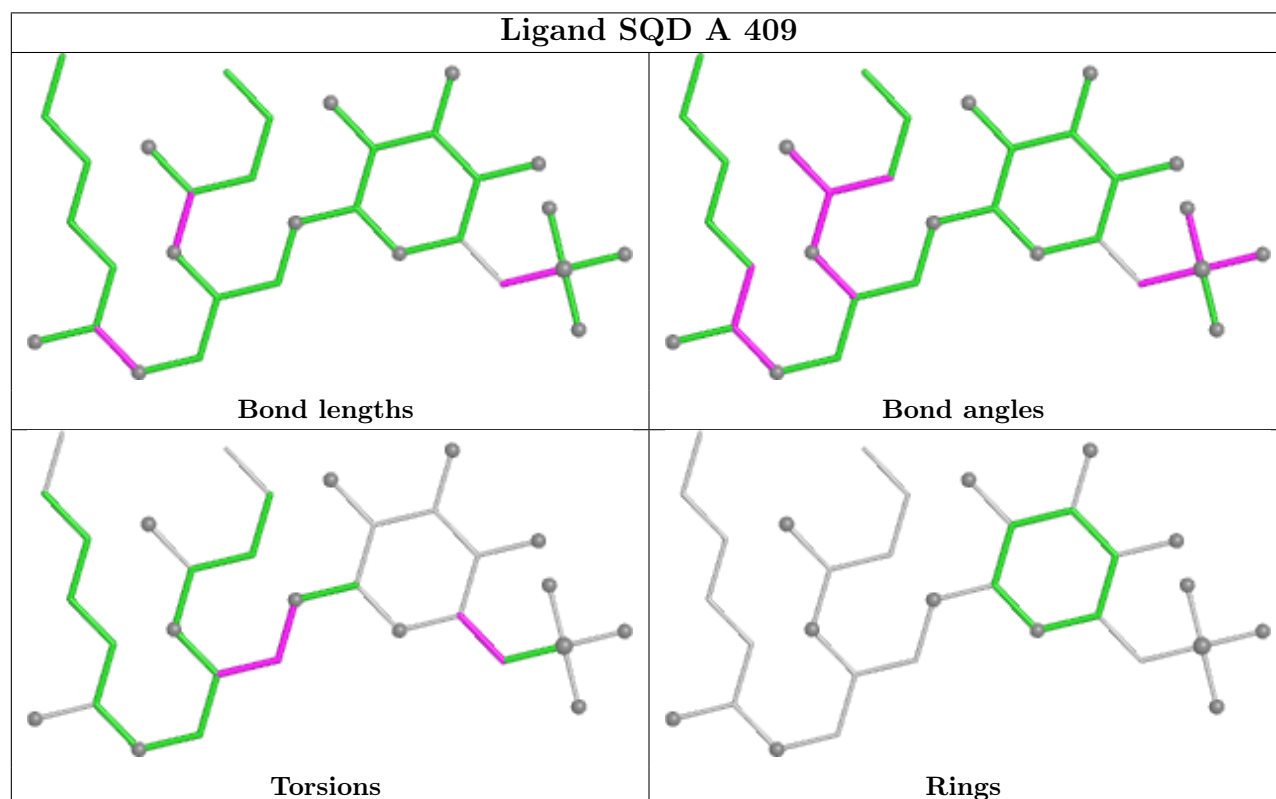
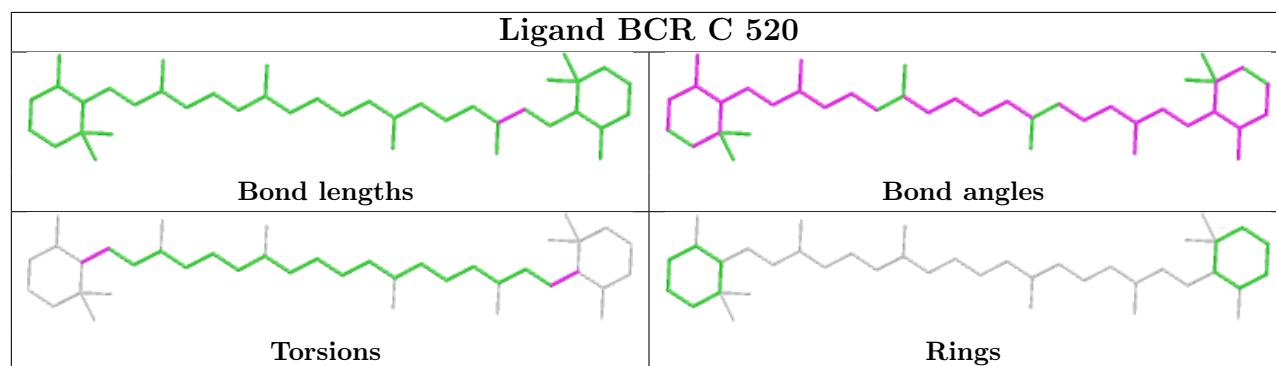
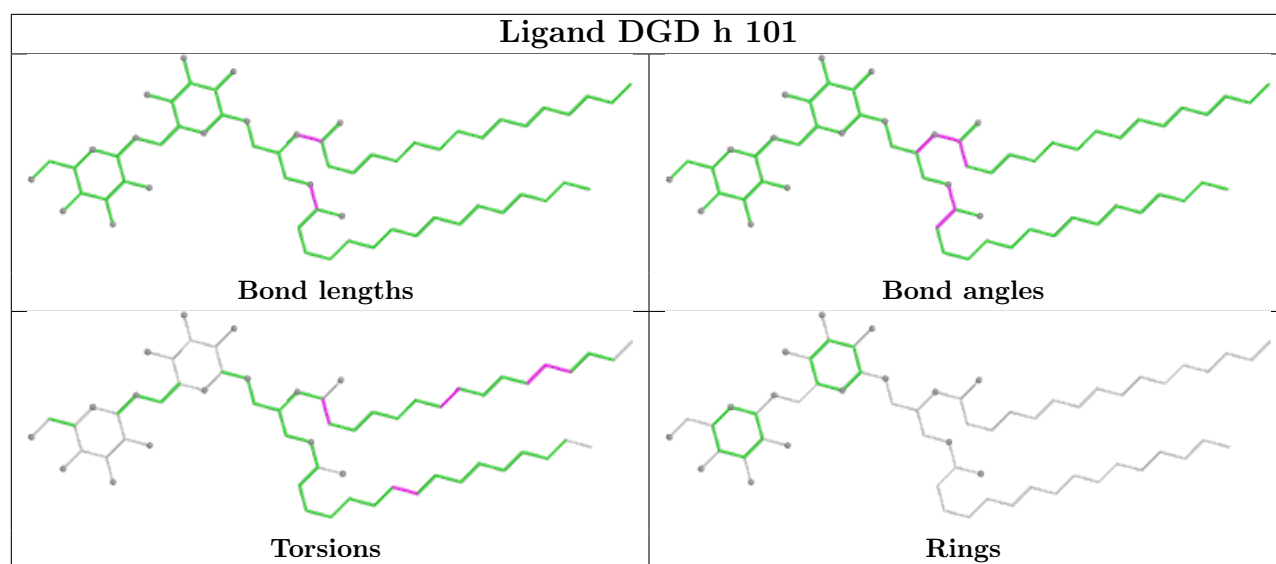


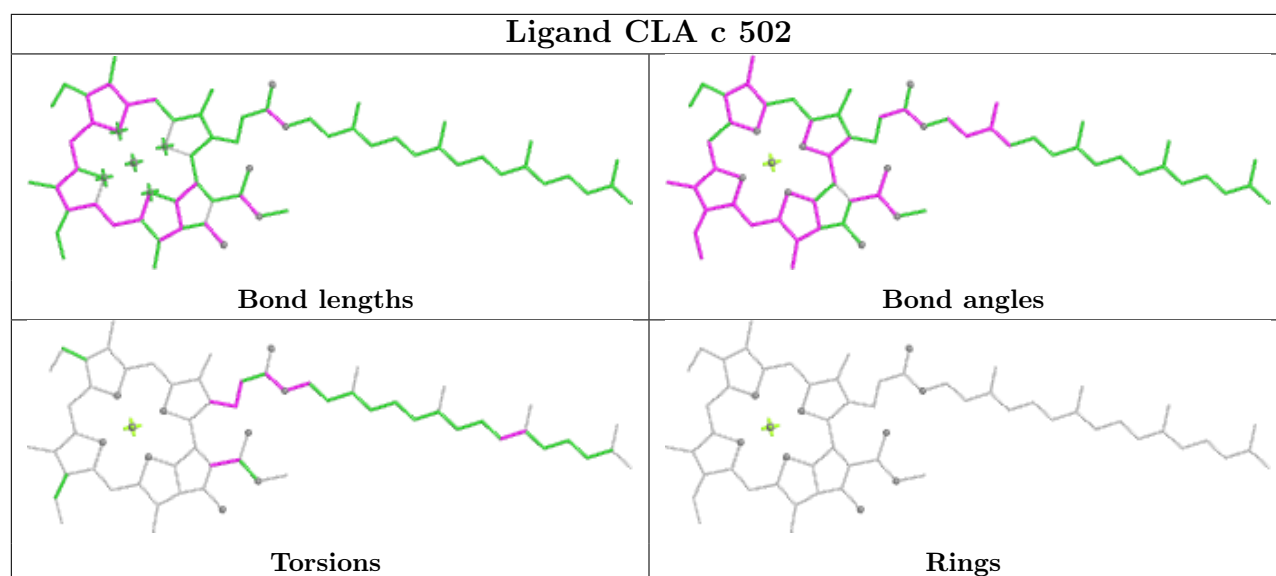
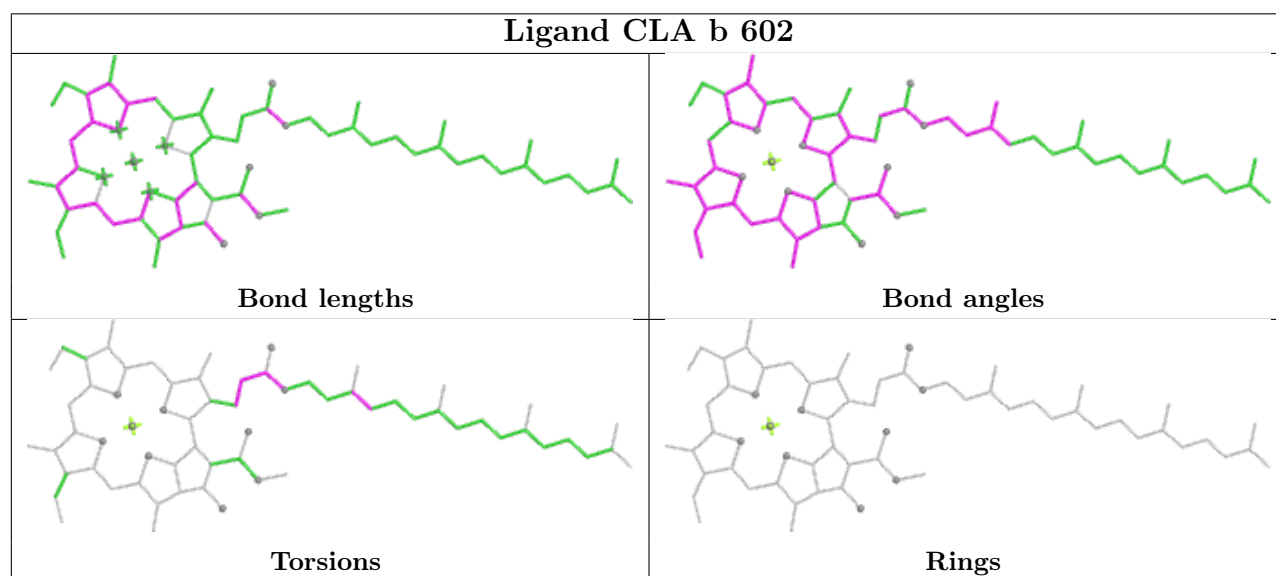
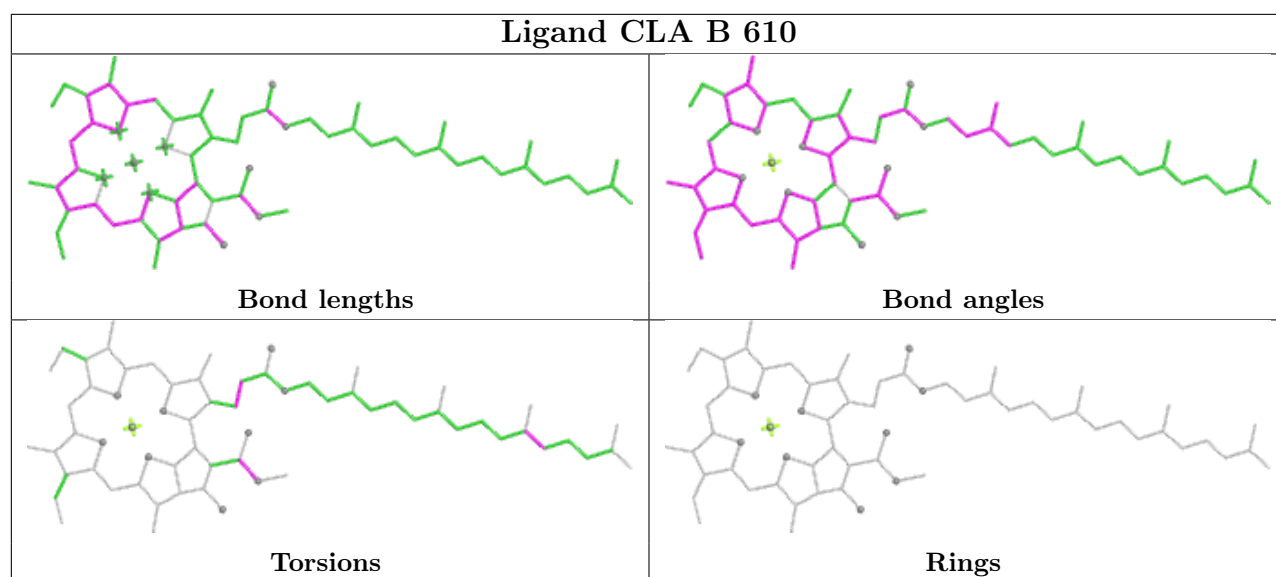
Ligand CLA c 513

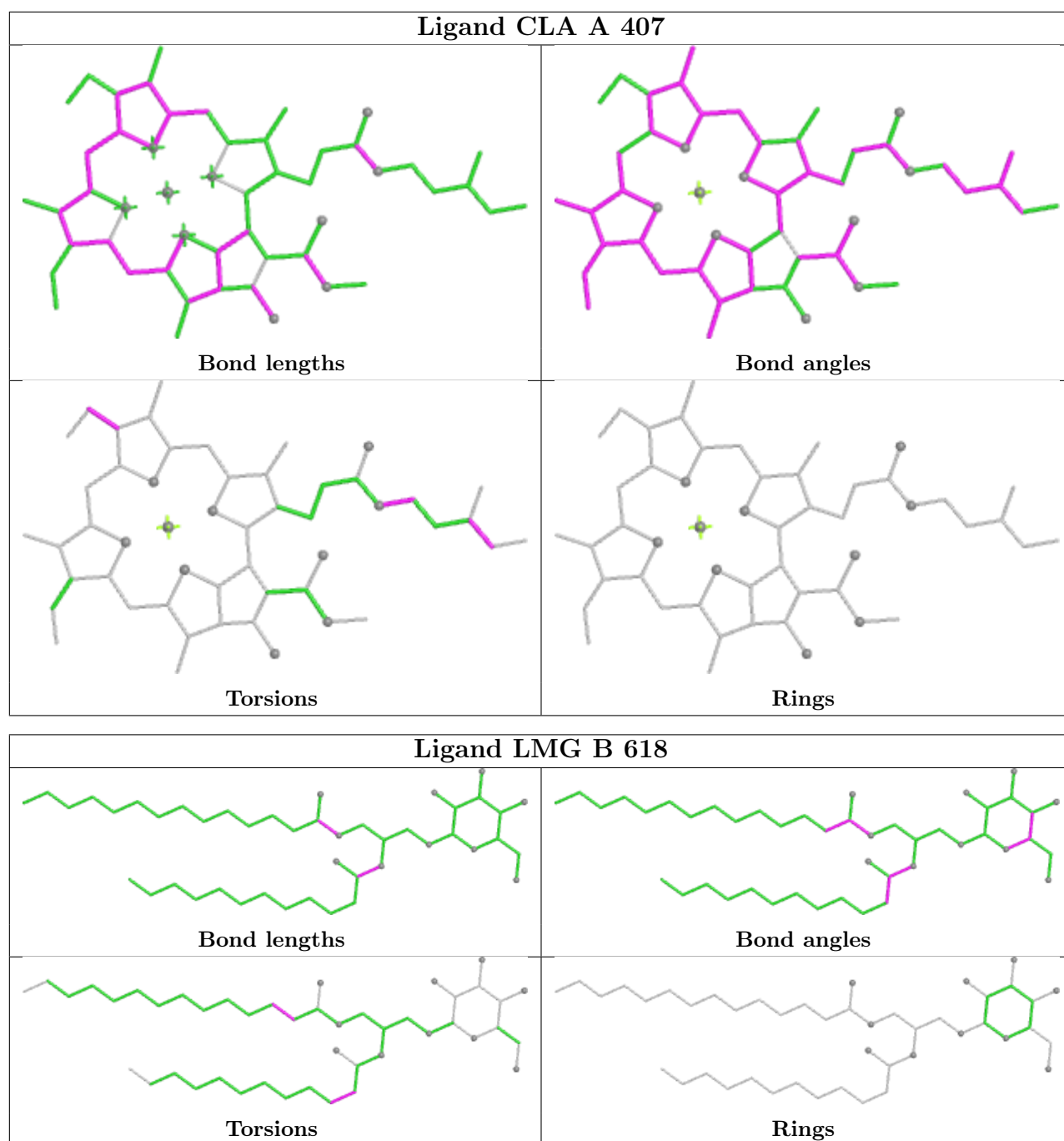


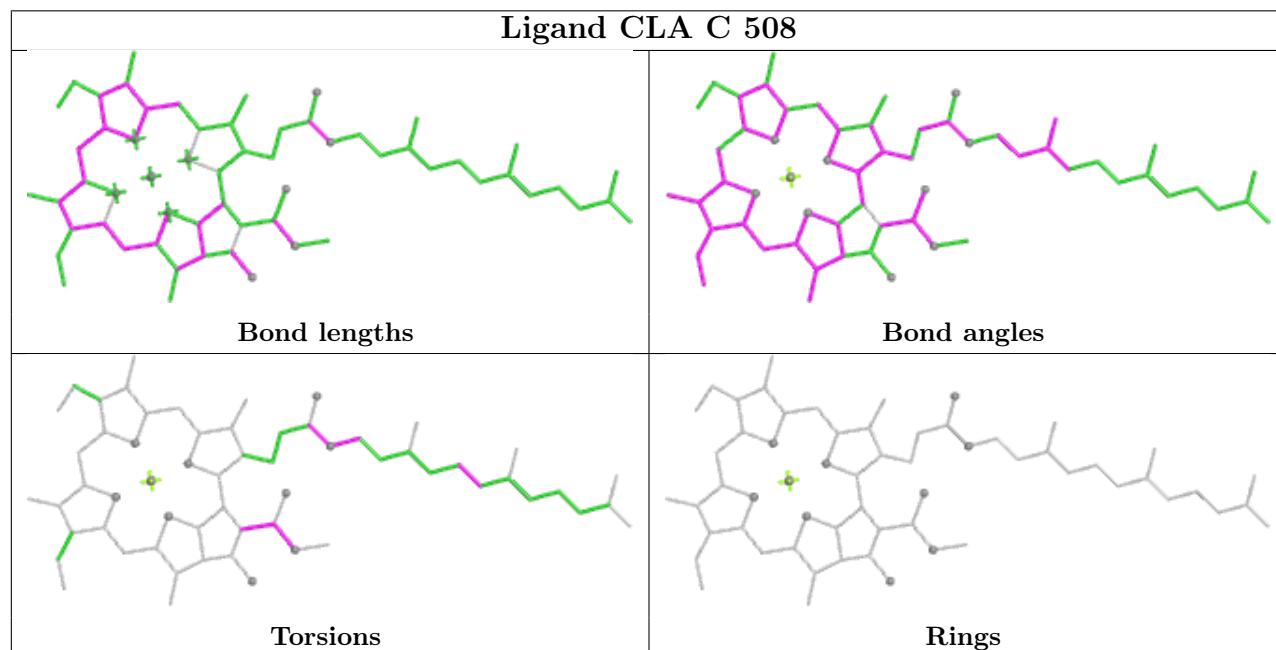
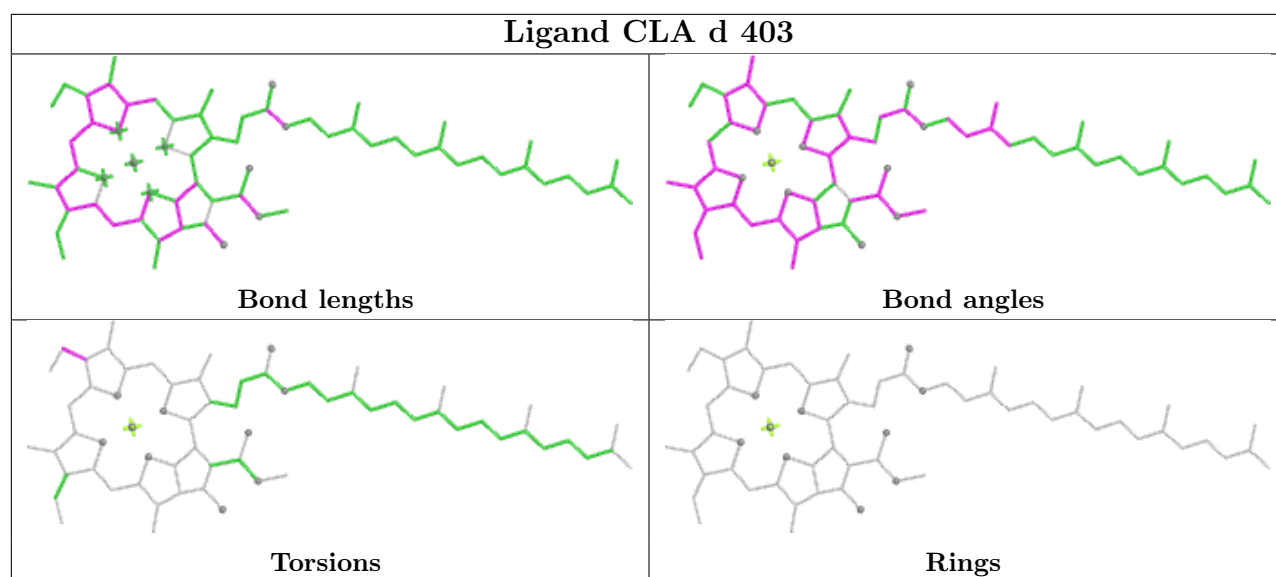
Ligand CLA C 519

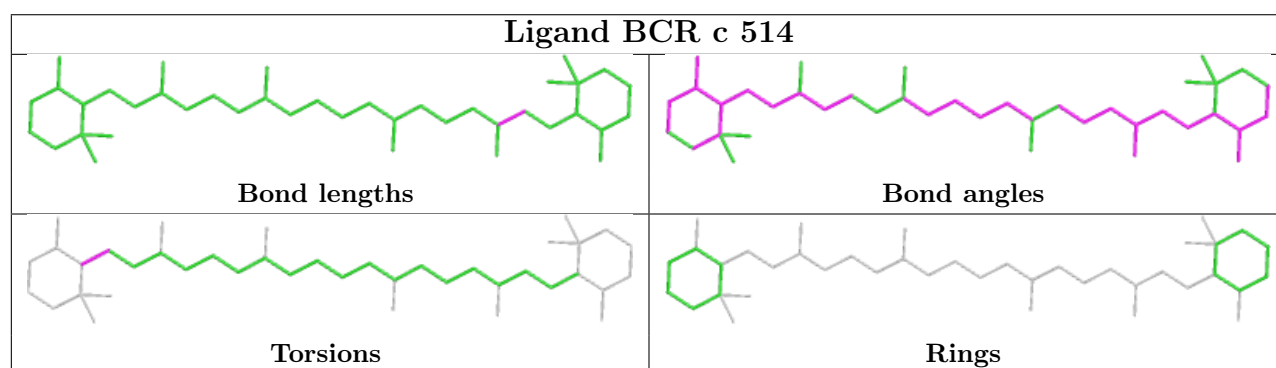
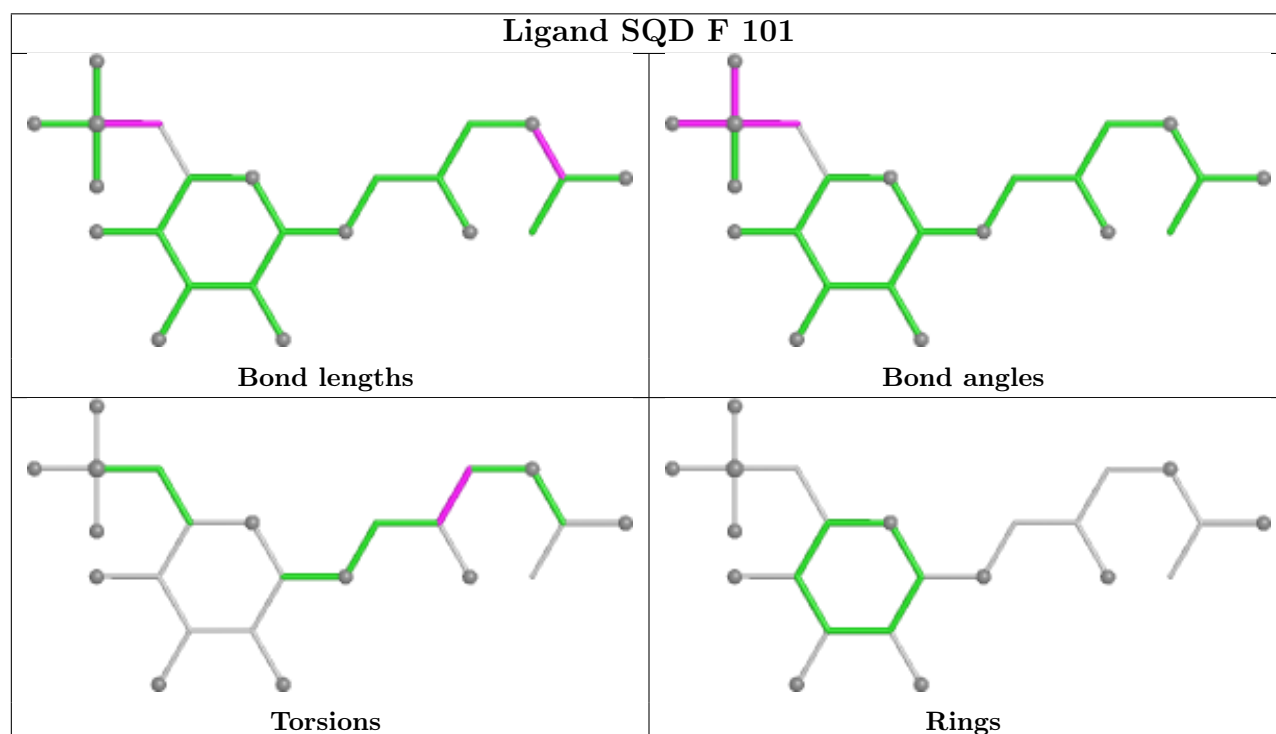
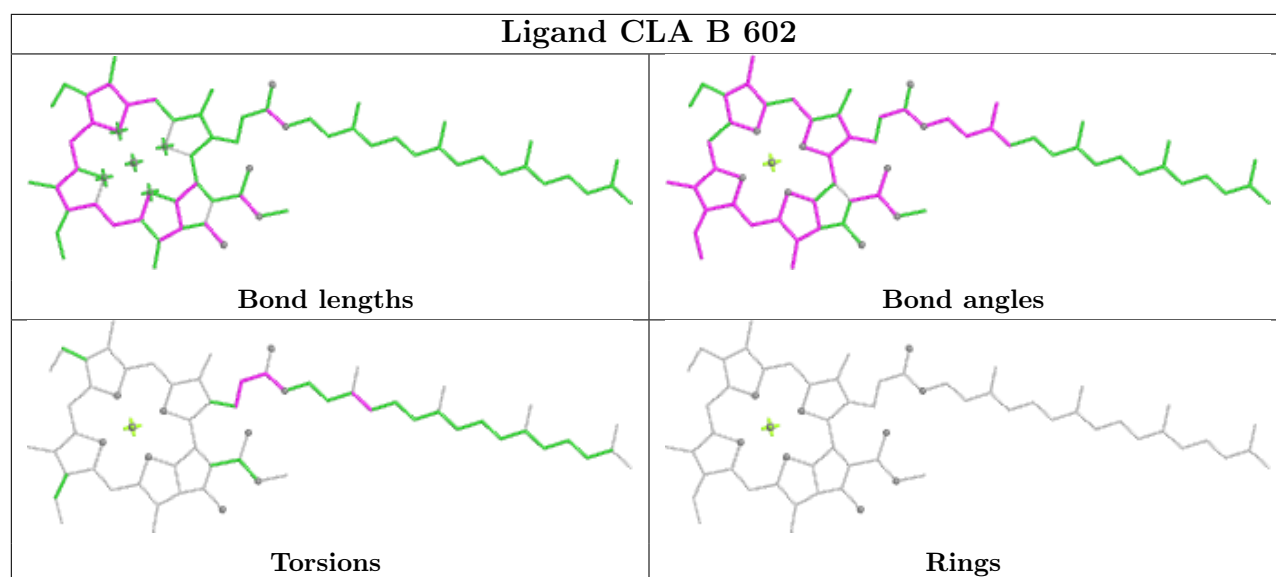


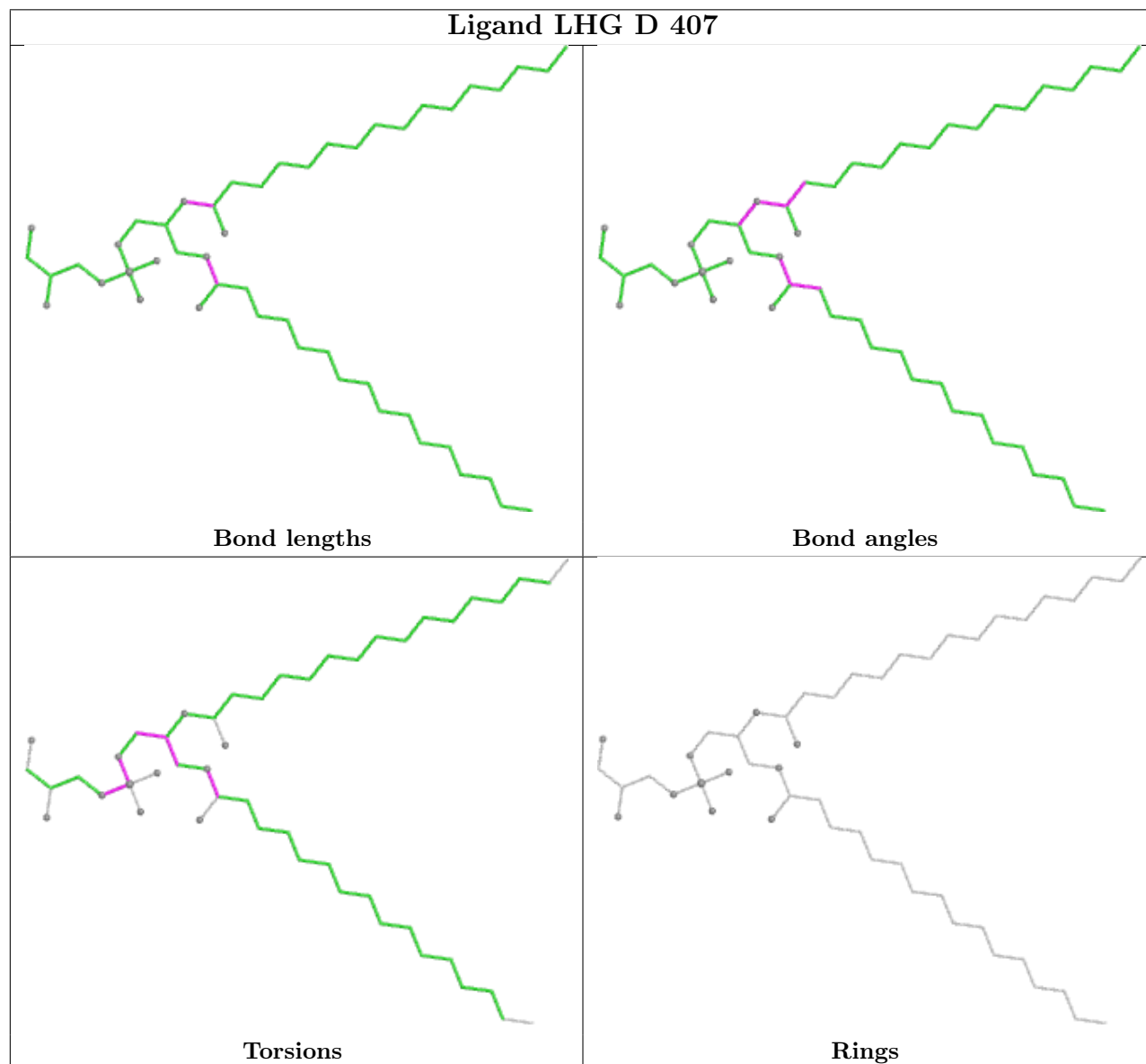
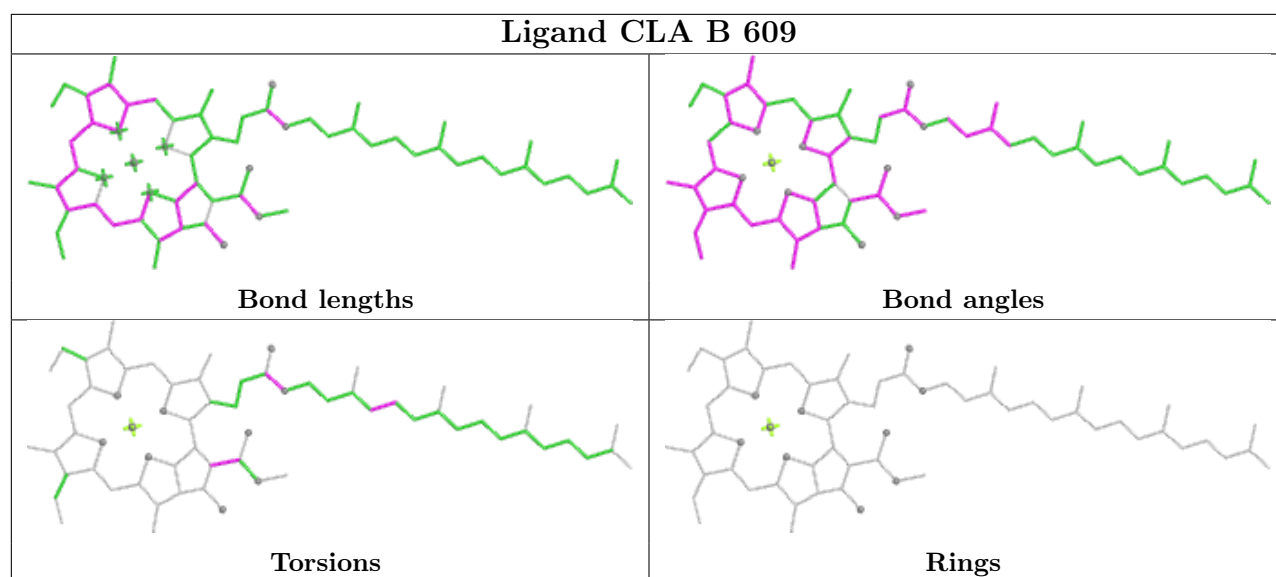


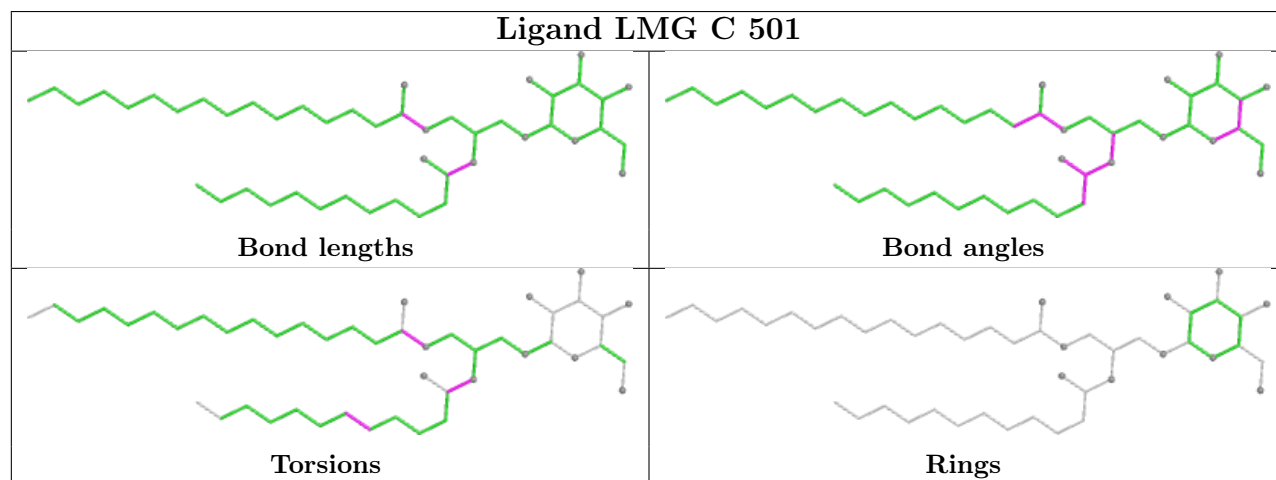
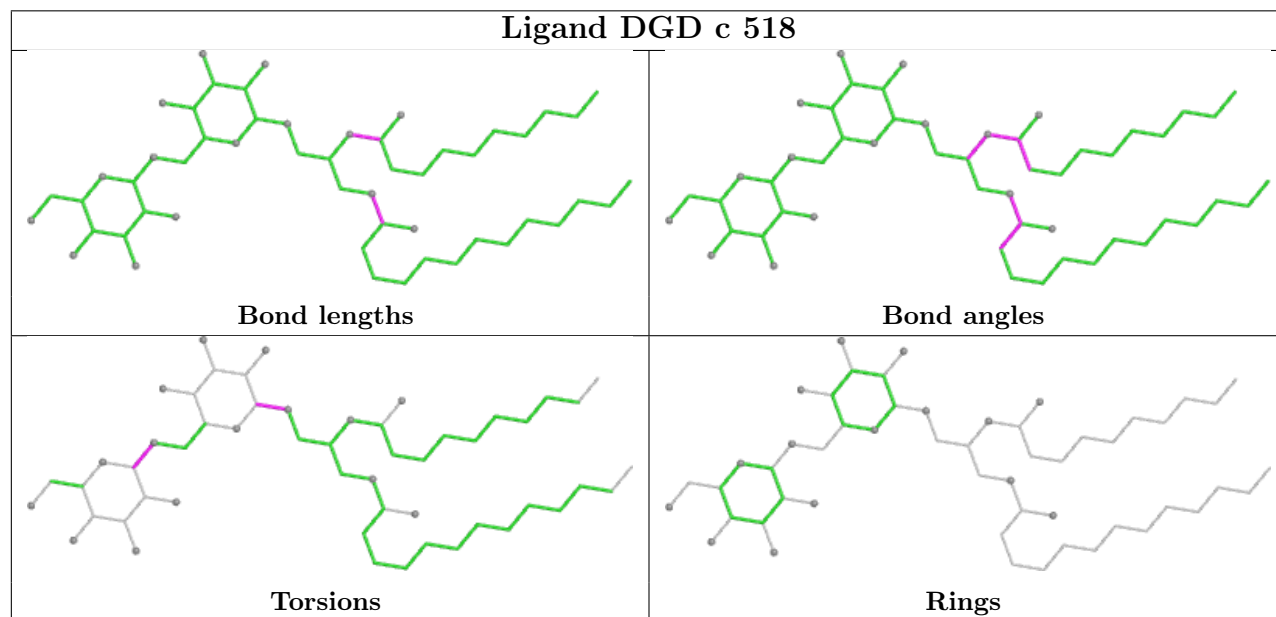
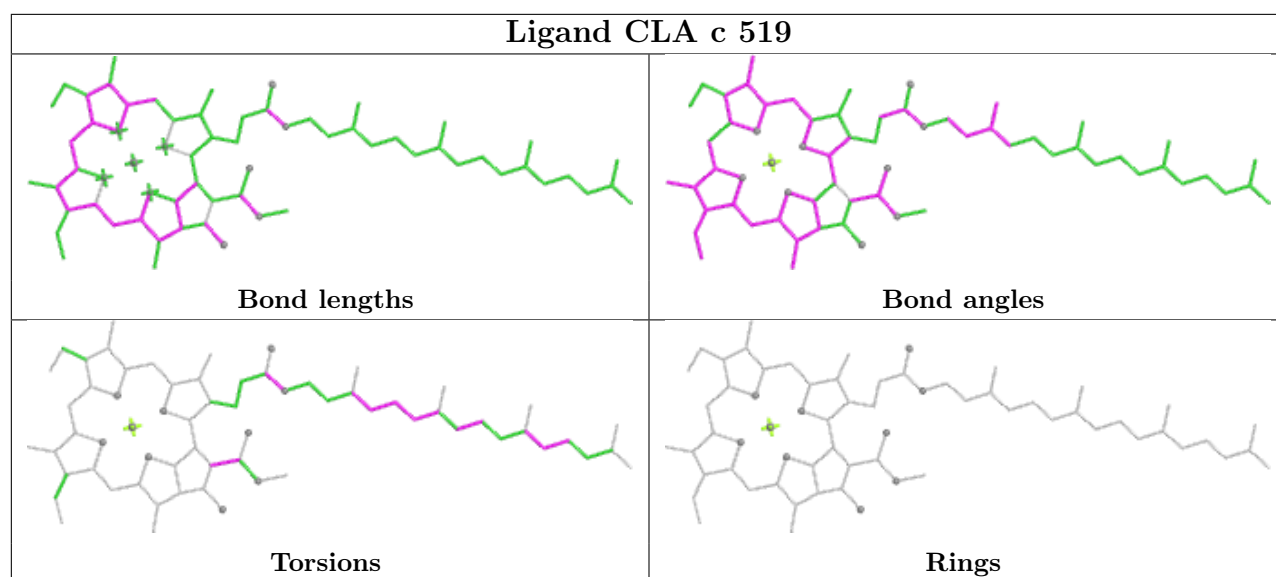




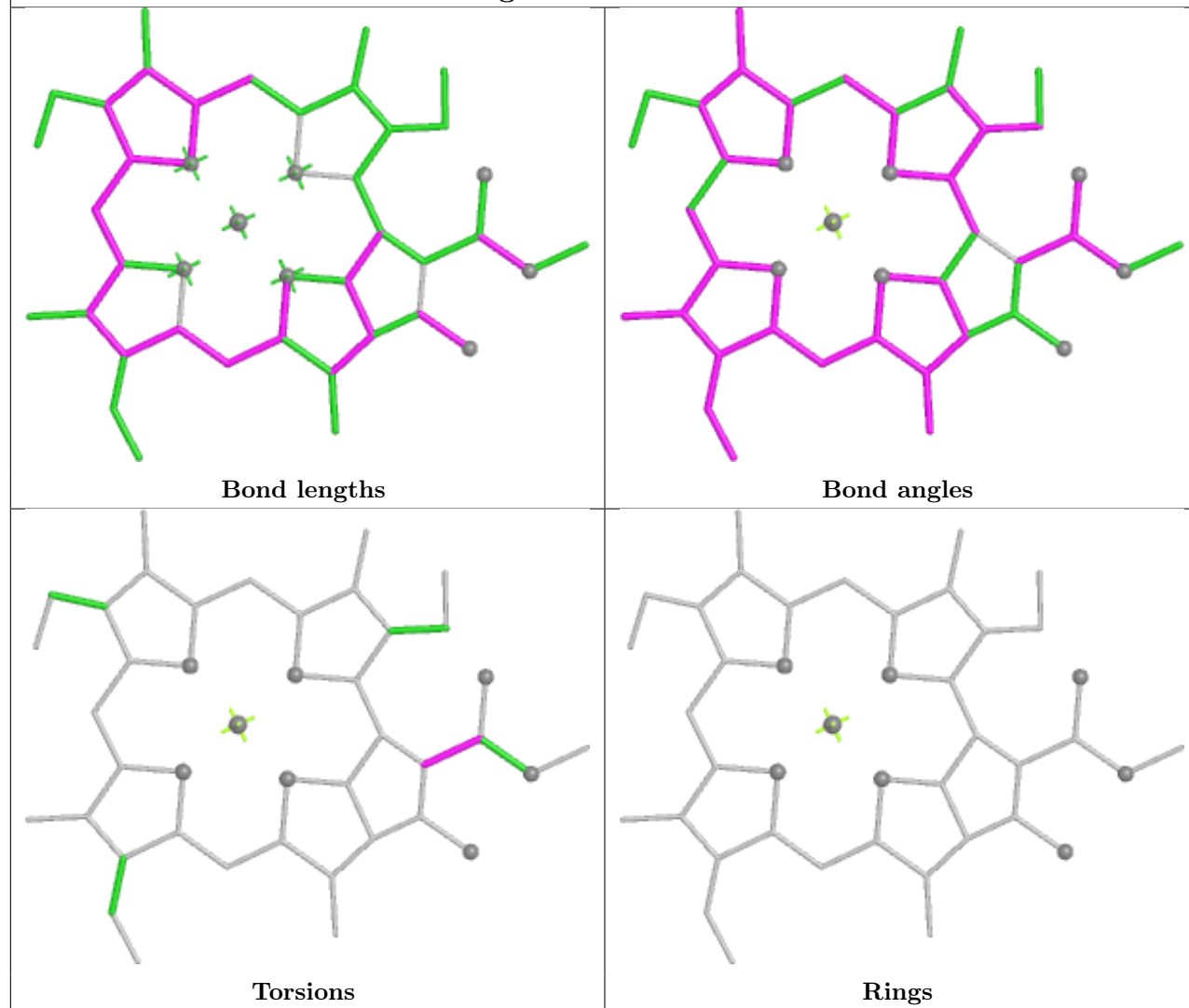




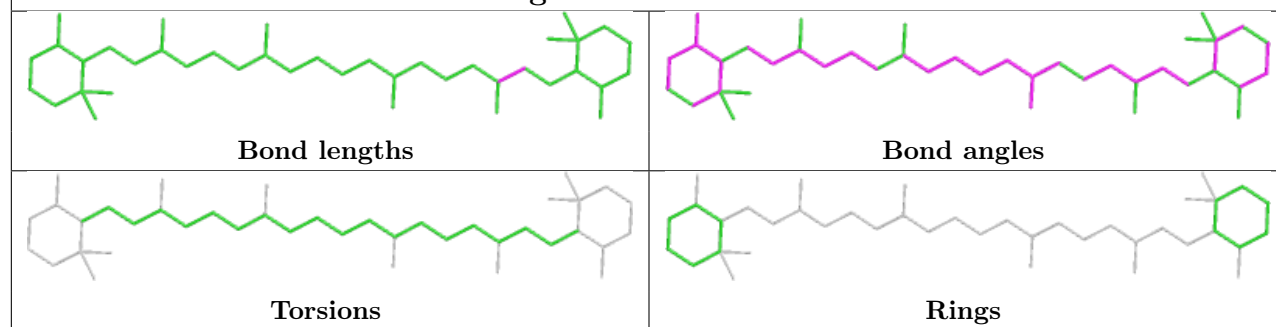


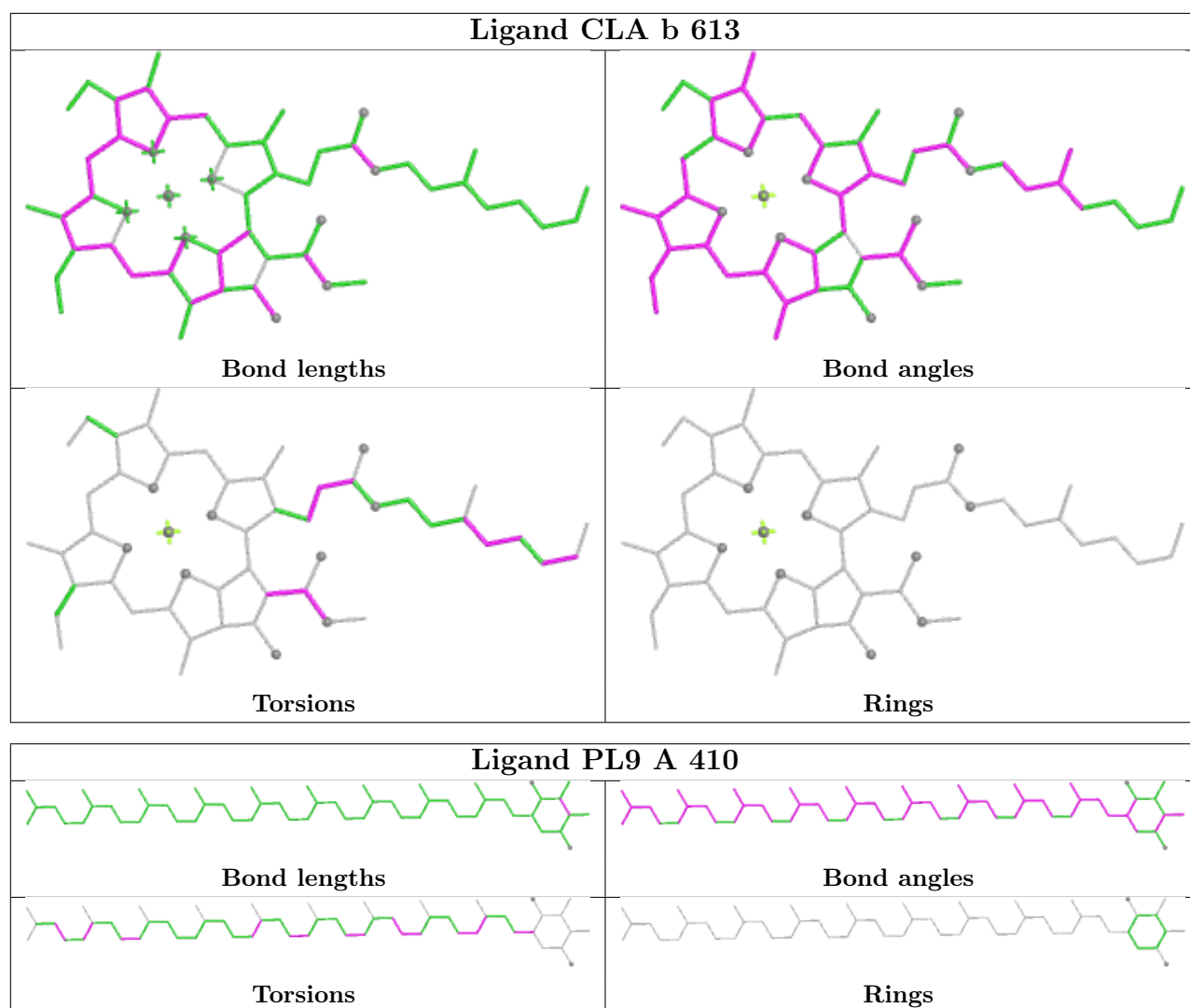


Ligand CLA b 601

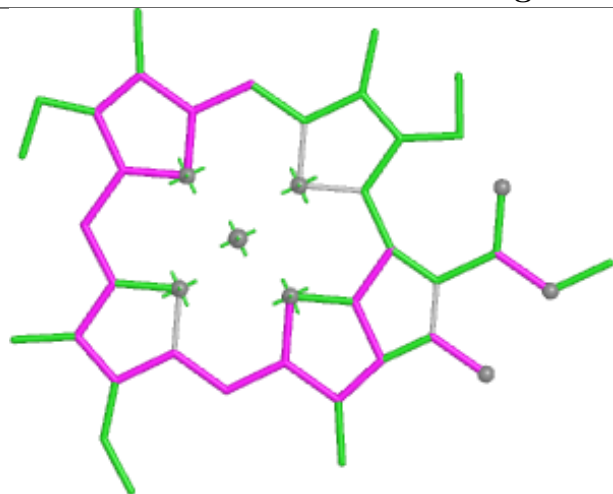


Ligand BCR K 103

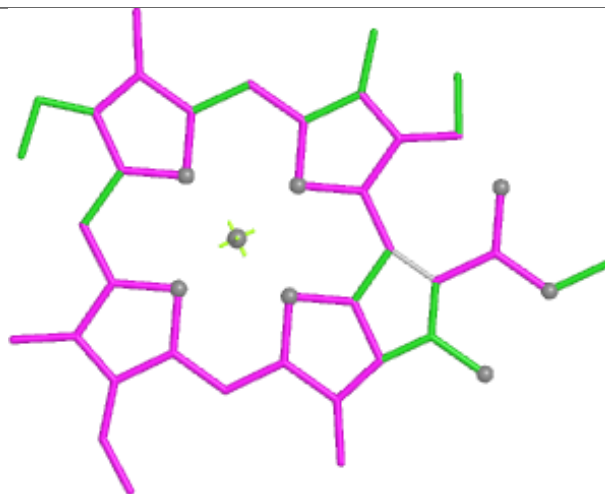




Ligand CLA C 513



Bond lengths



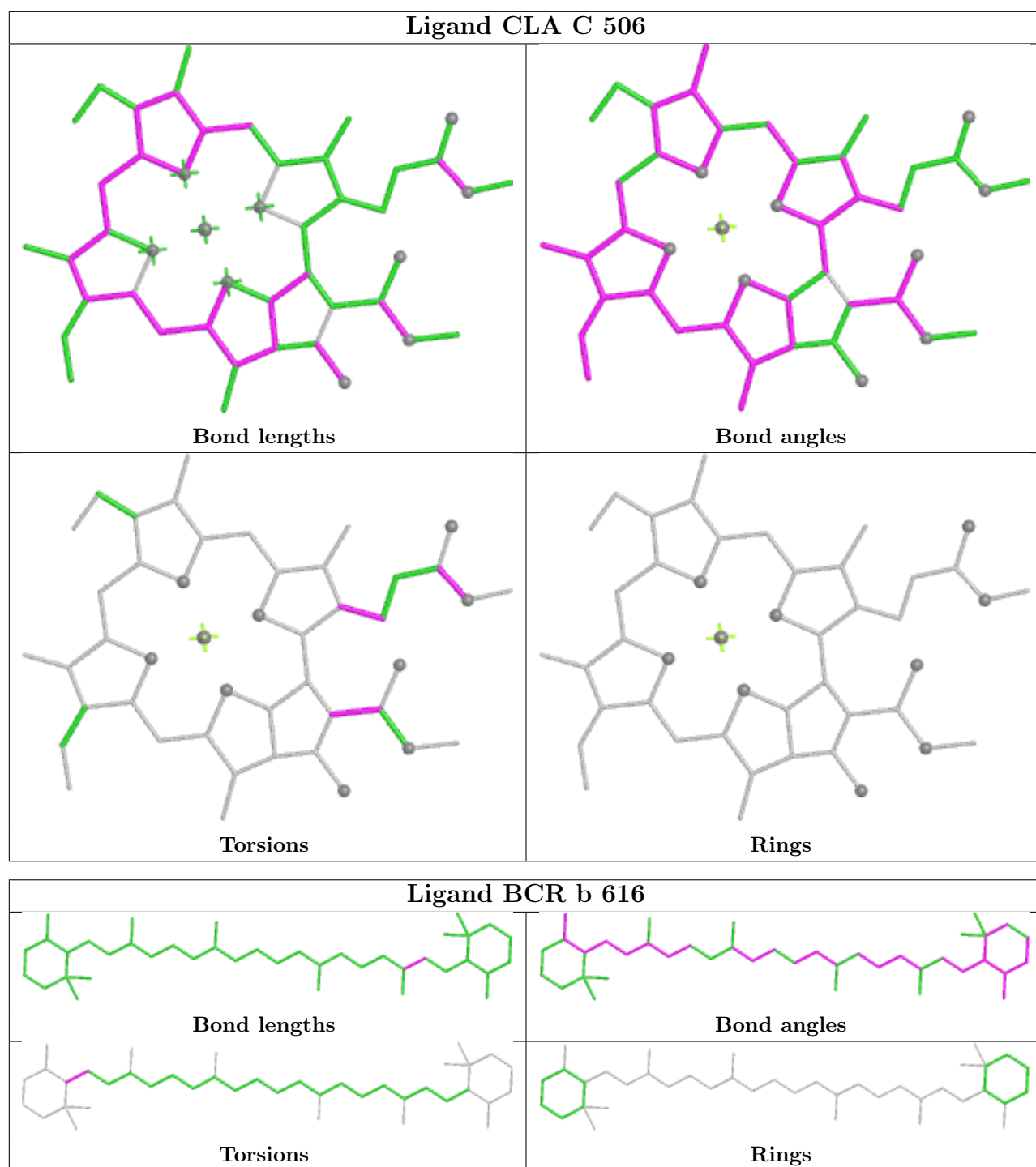
Bond angles

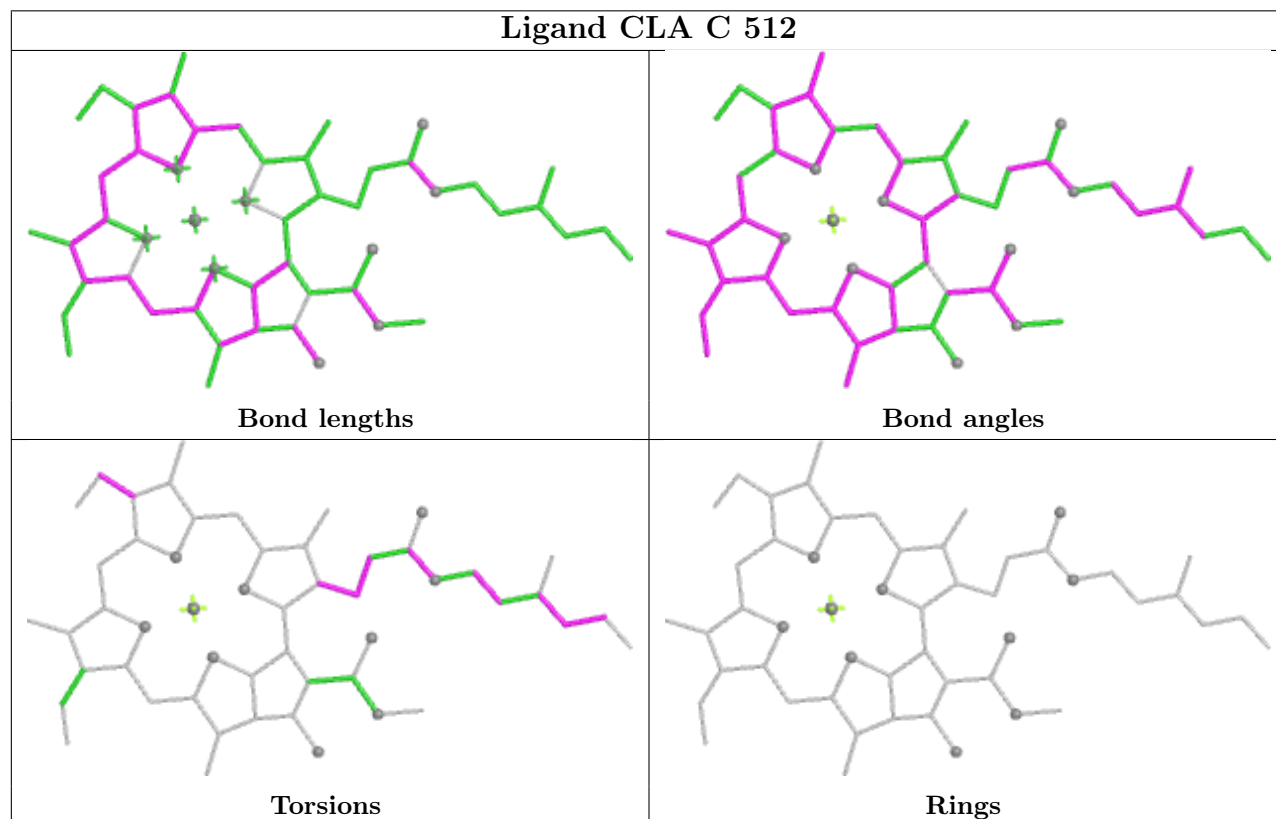
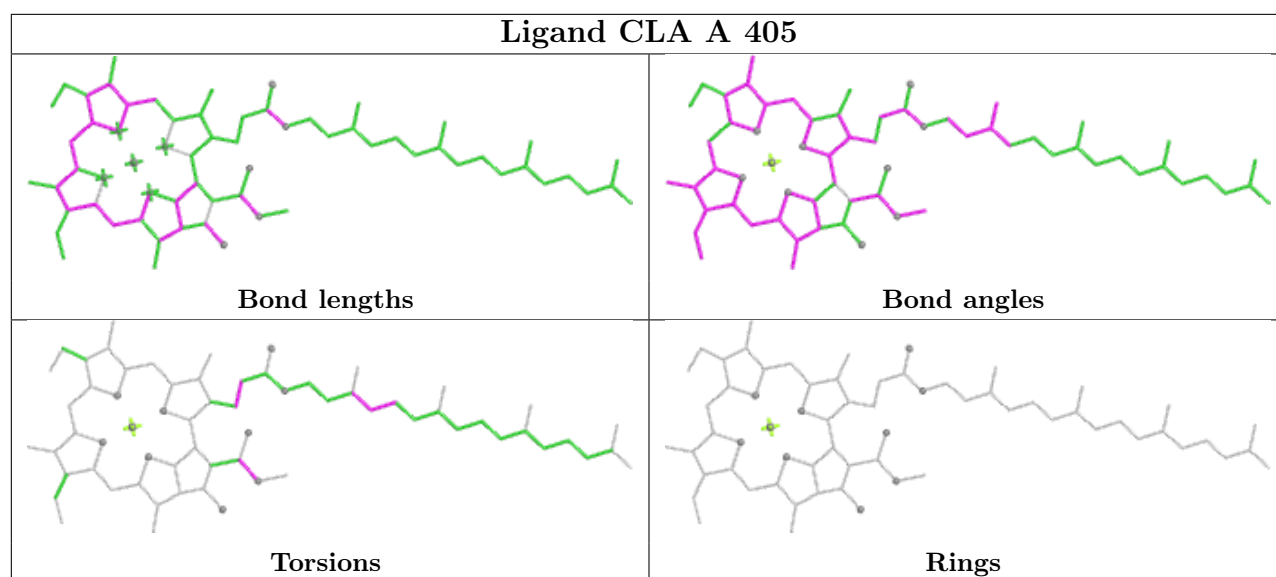


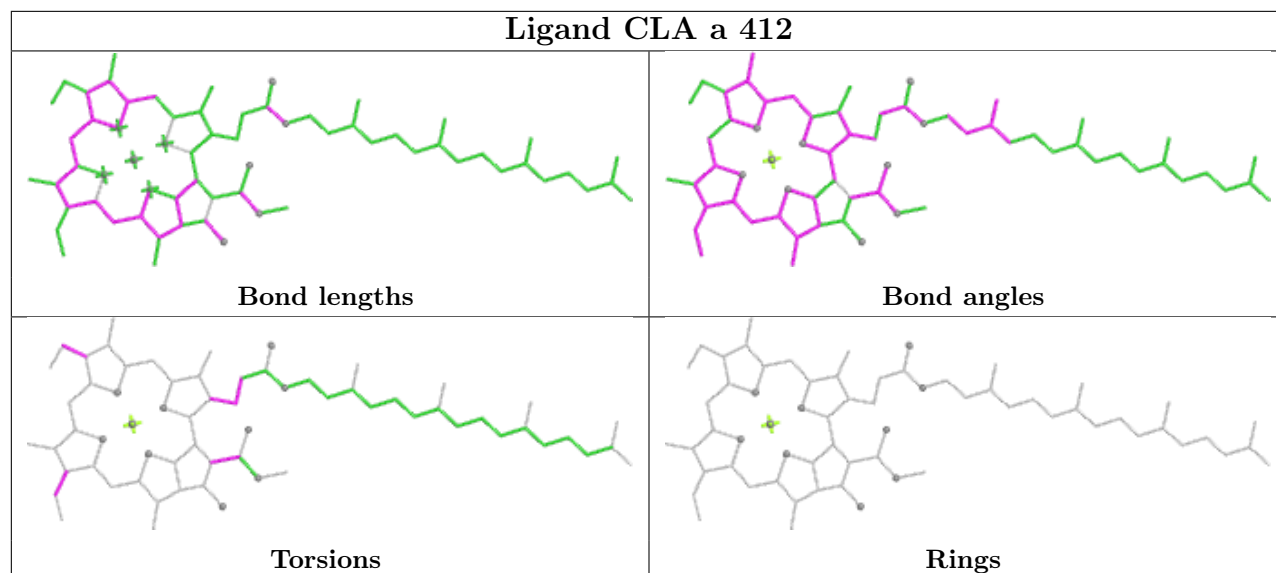
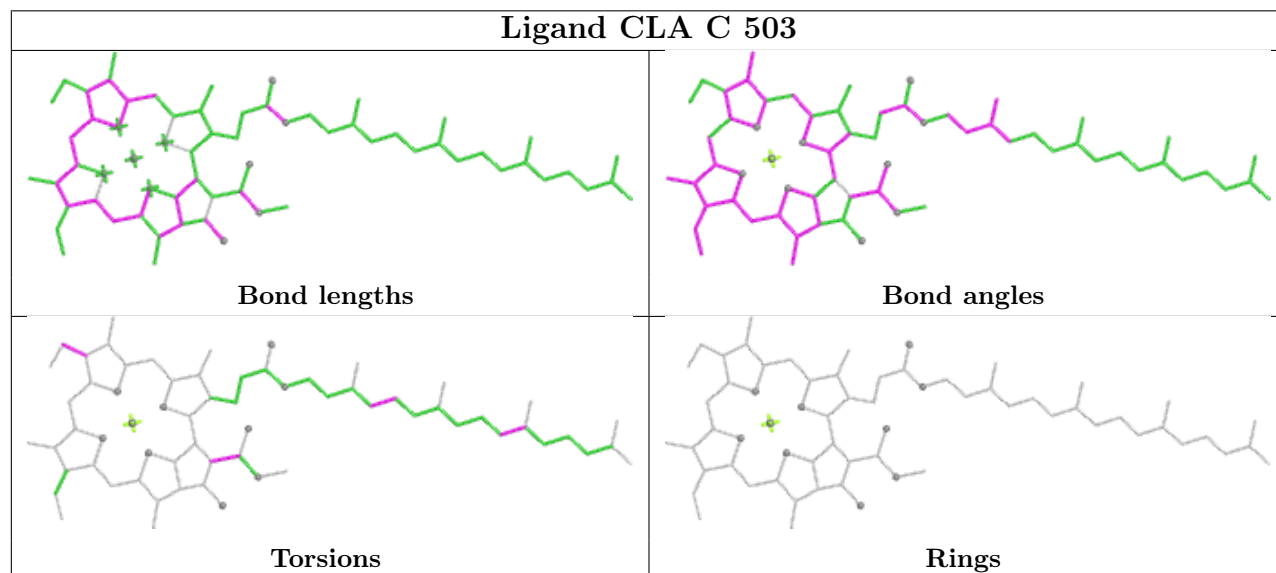
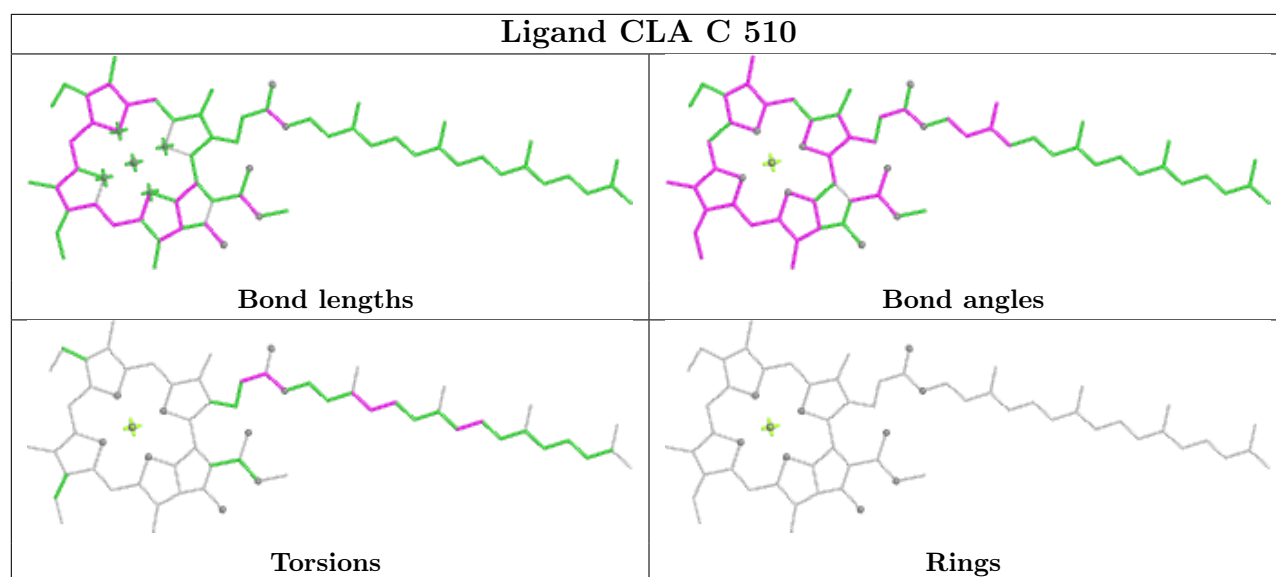
Torsions



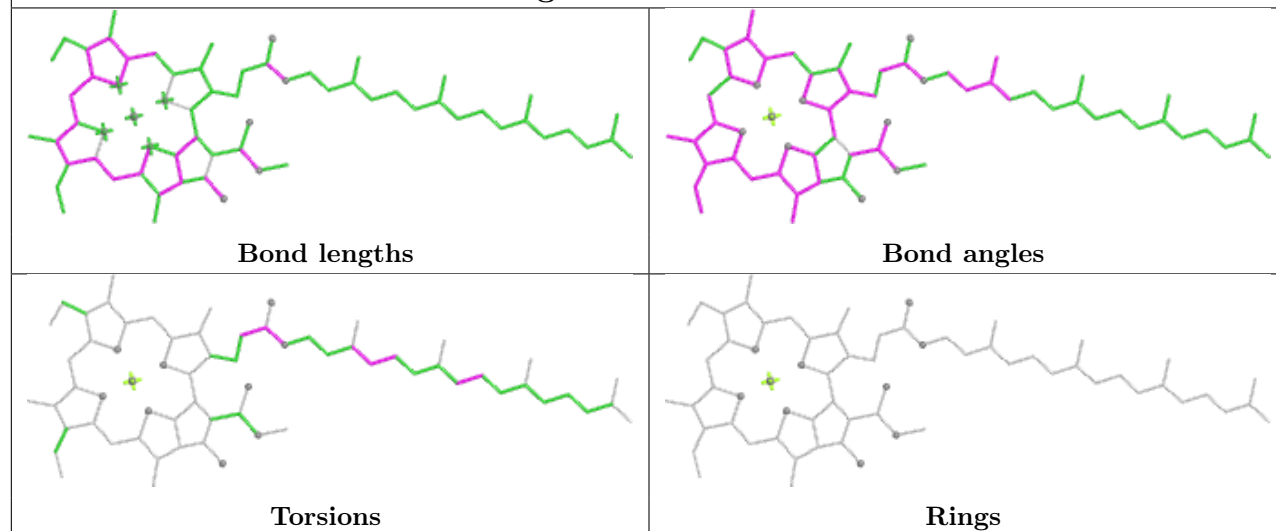
Rings



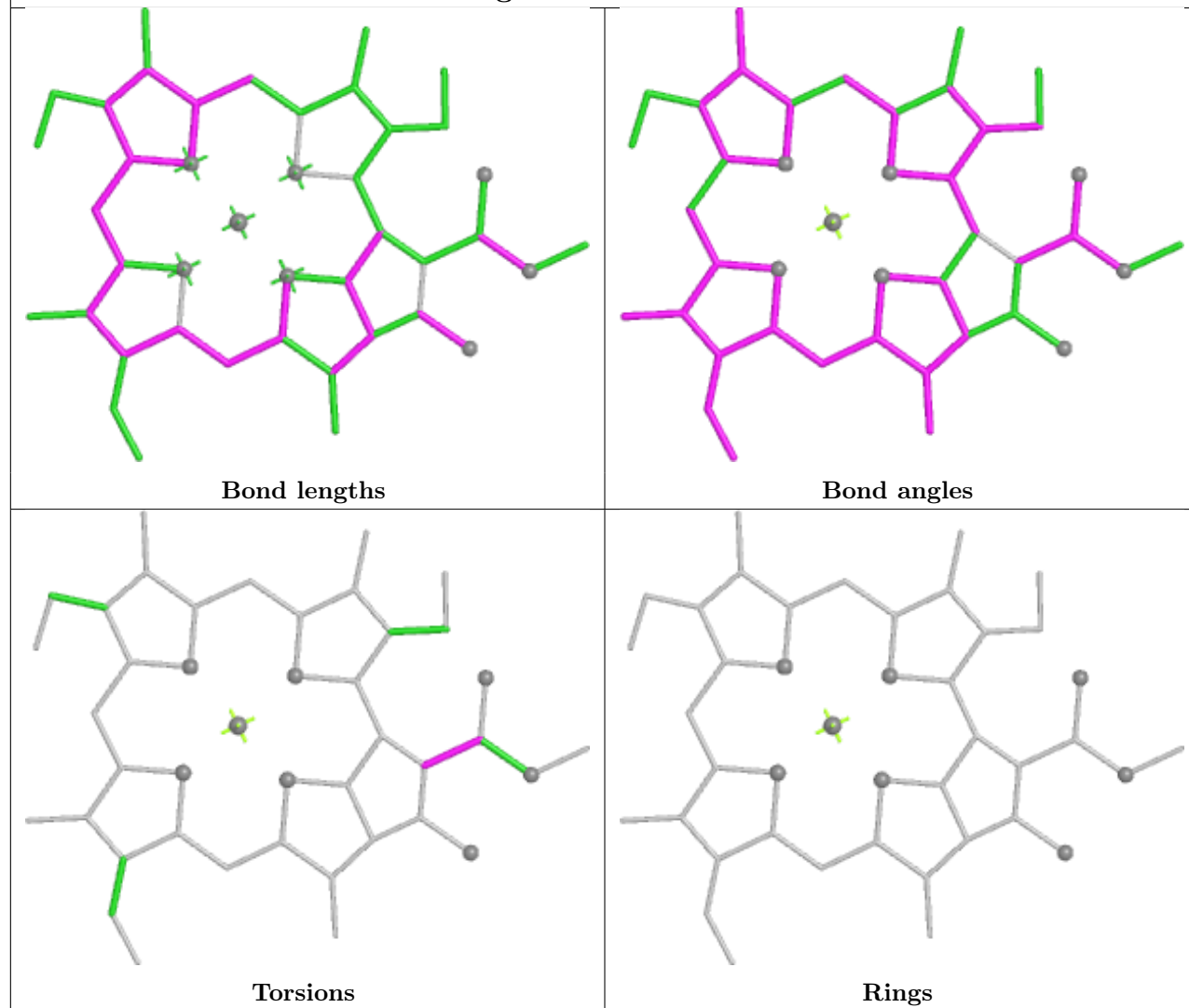


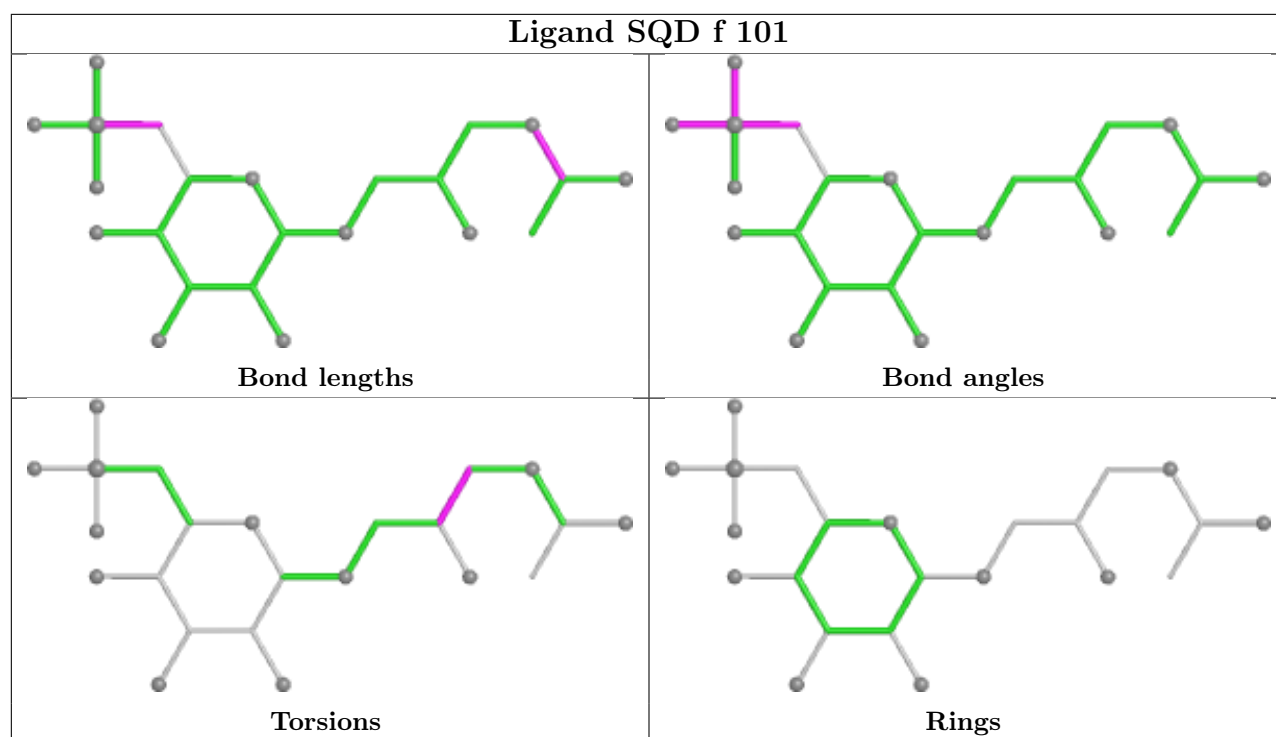


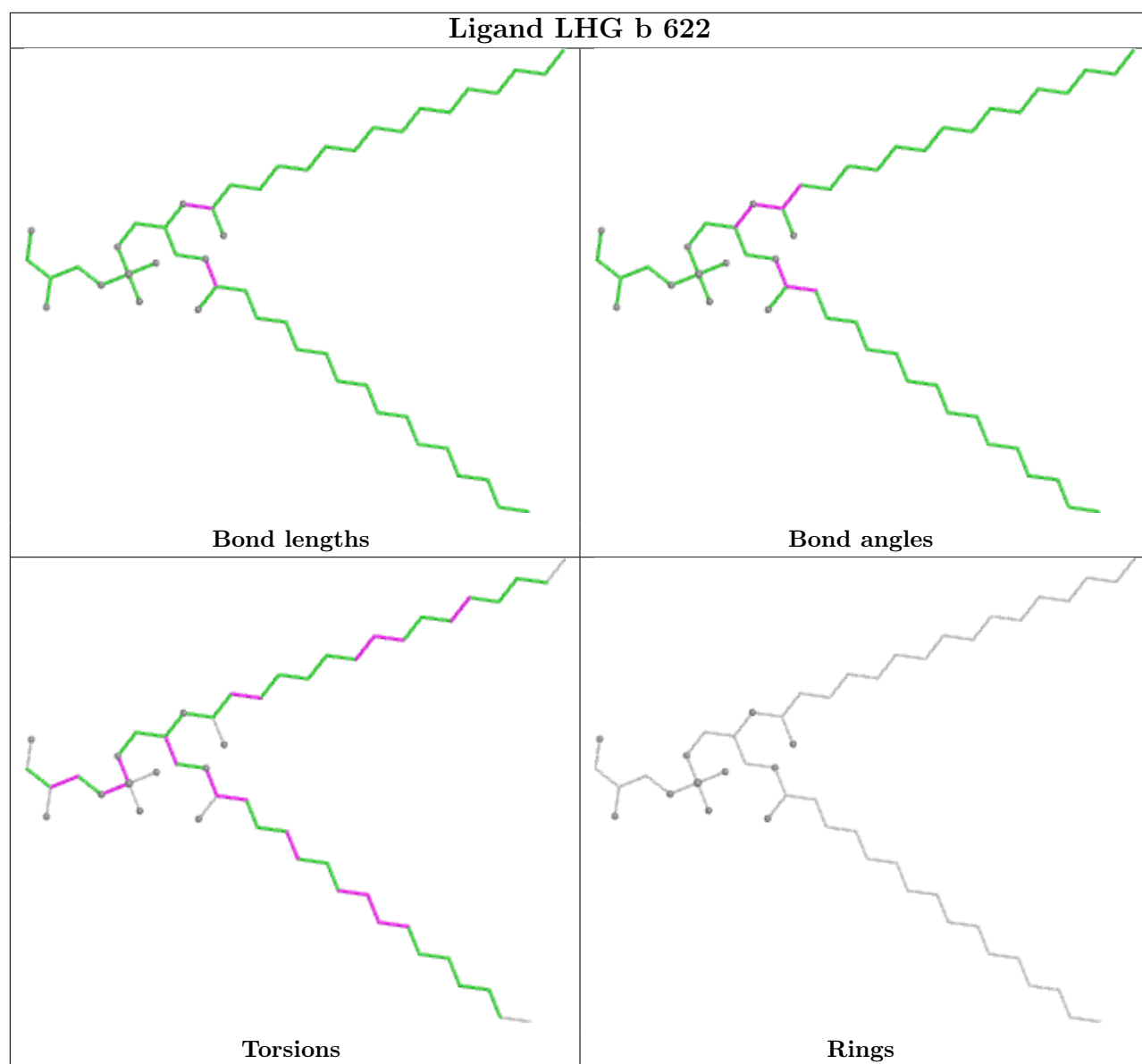
Ligand CLA c 510

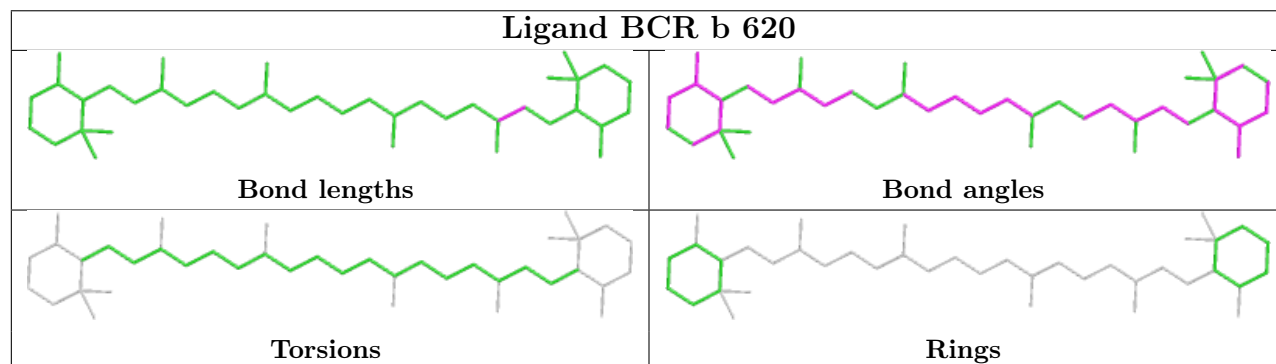
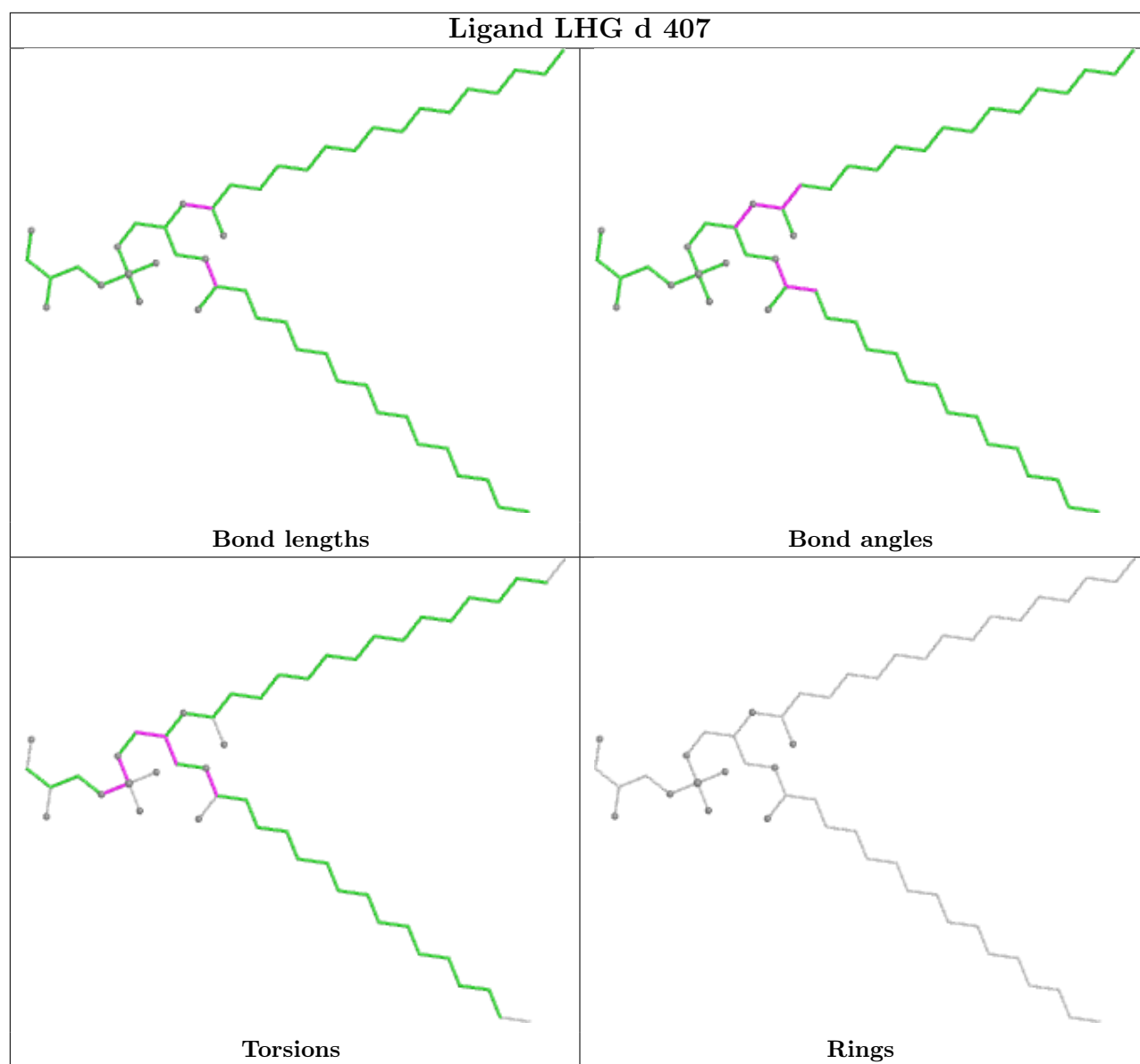


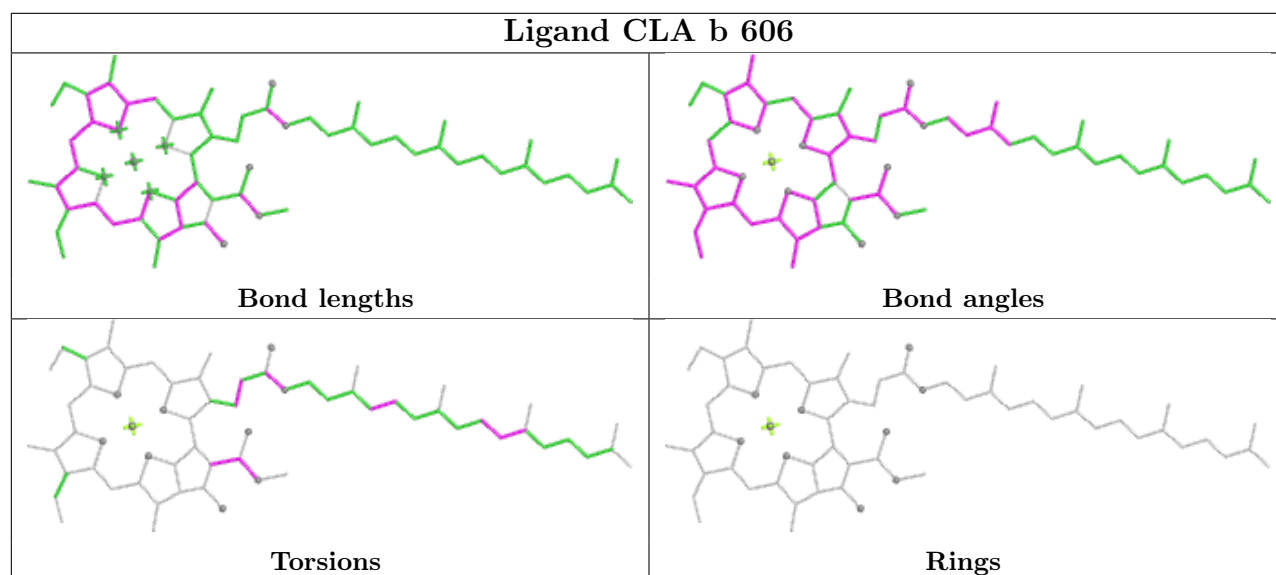
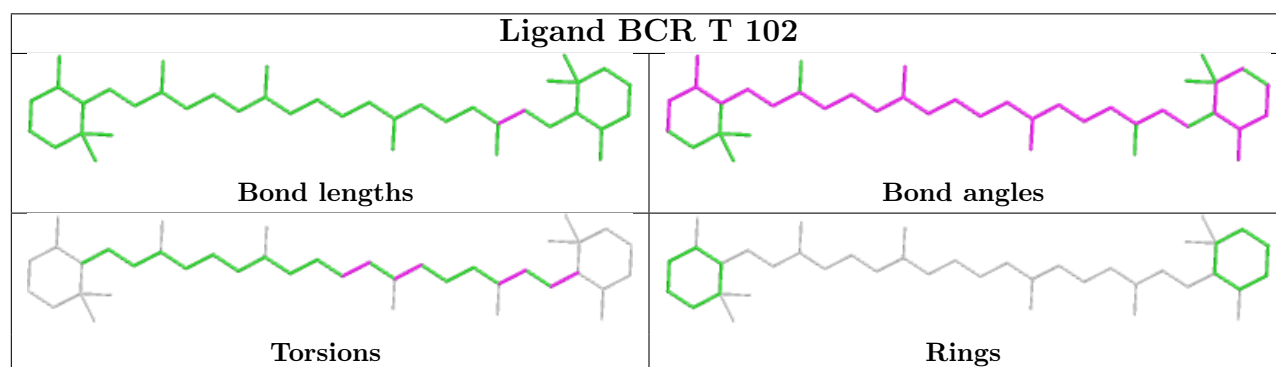
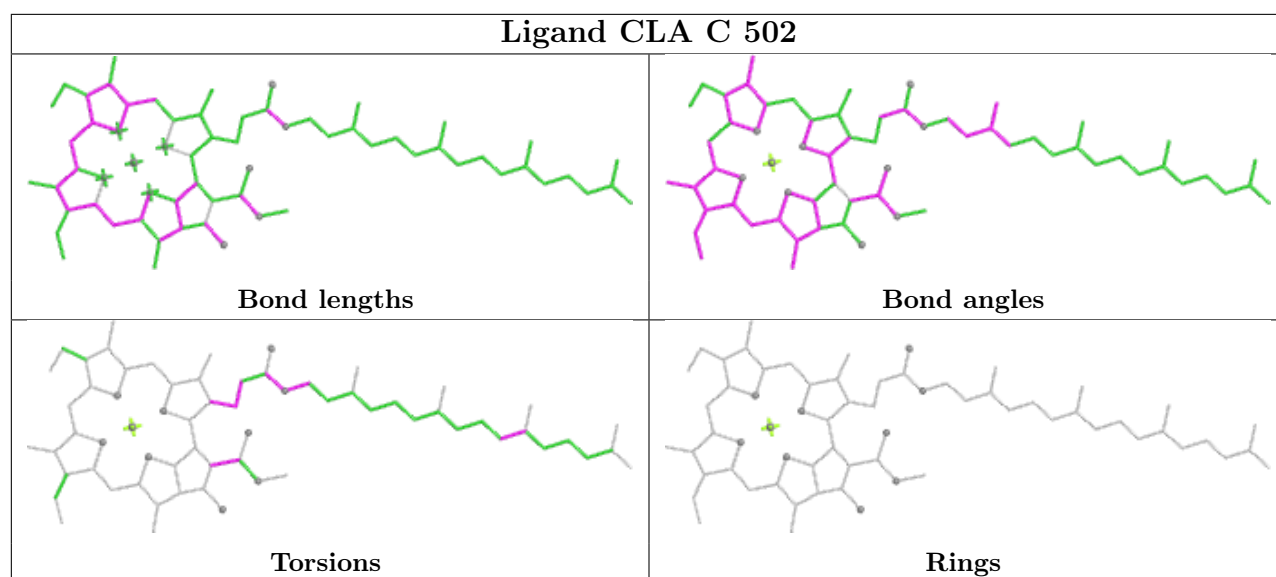
Ligand CLA B 601

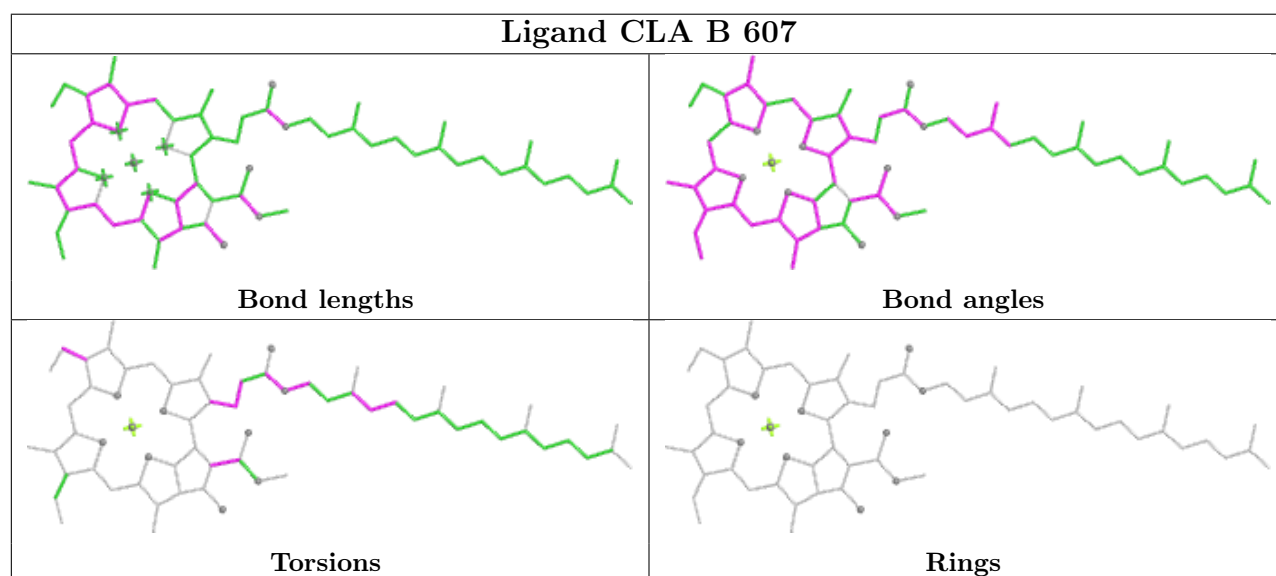
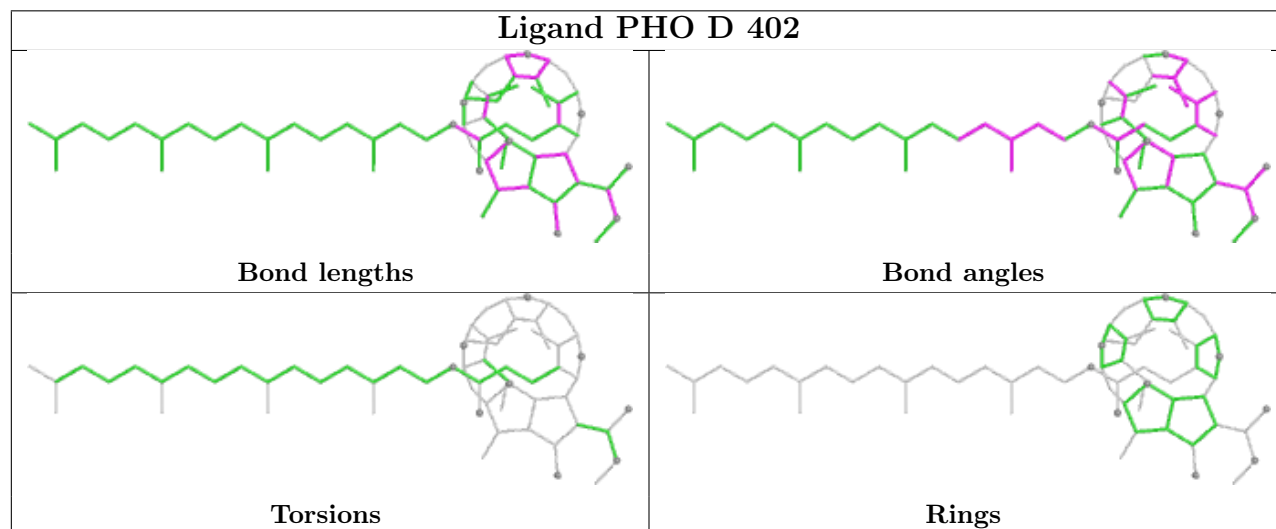
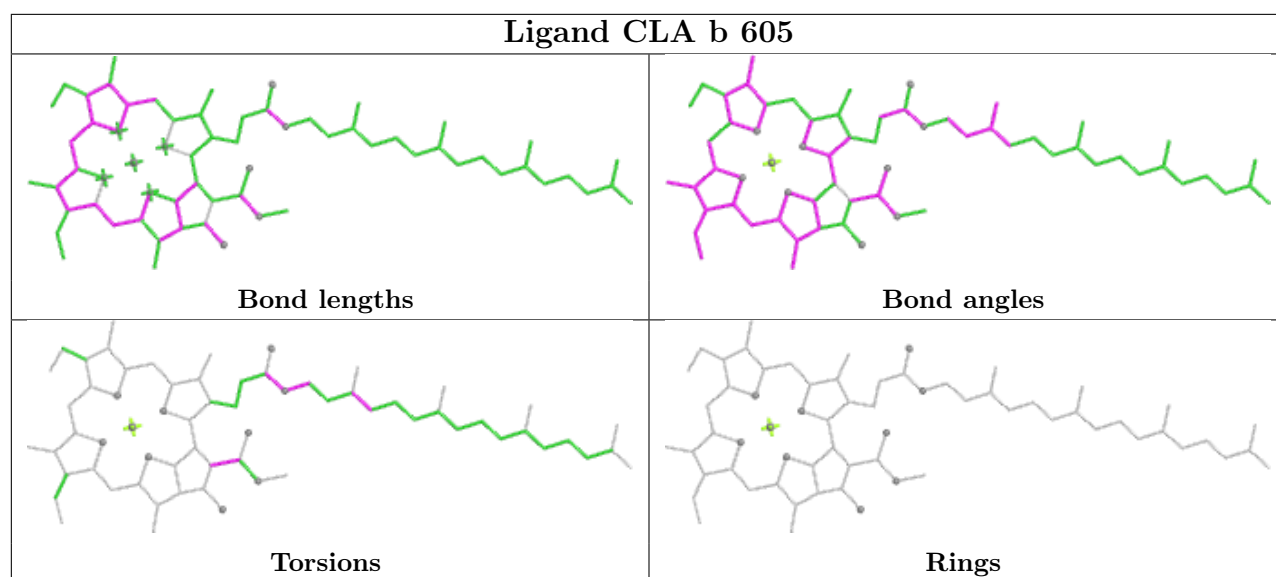


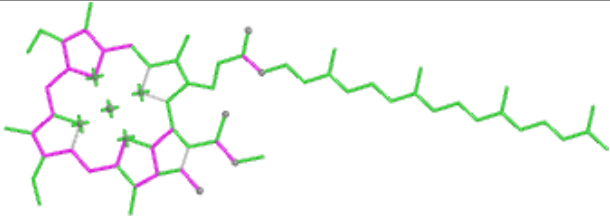
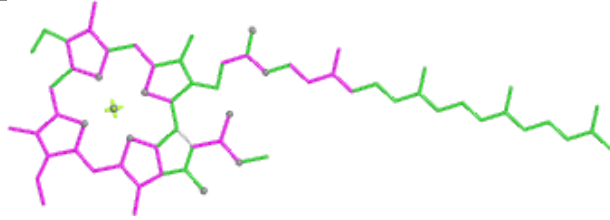
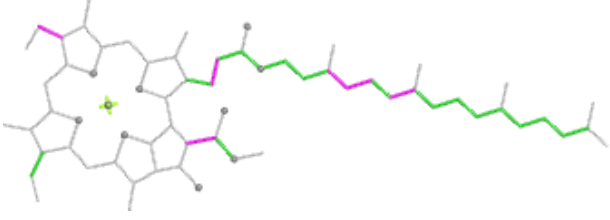
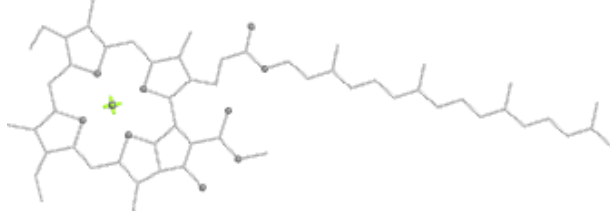
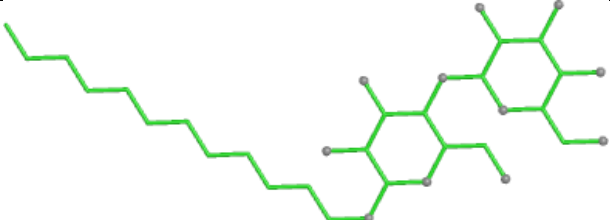
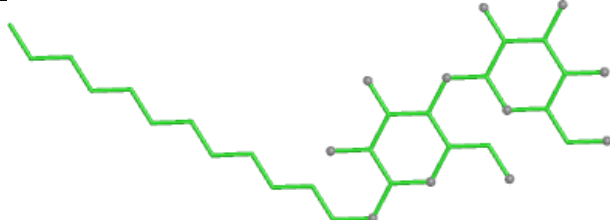
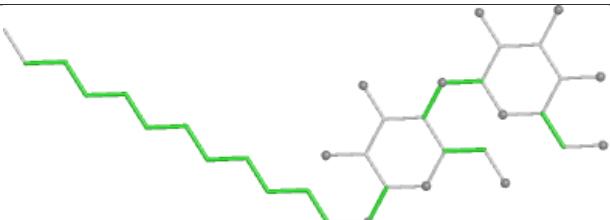
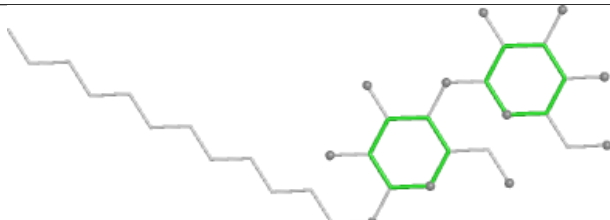
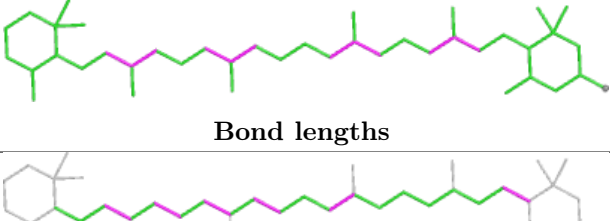
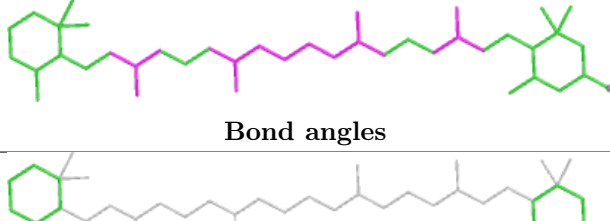
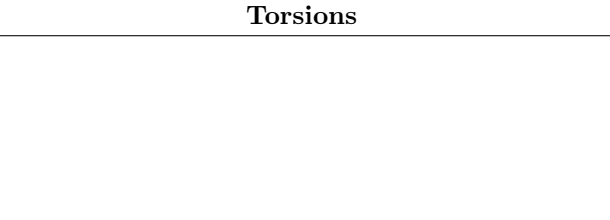
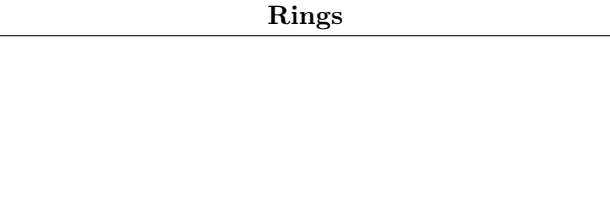


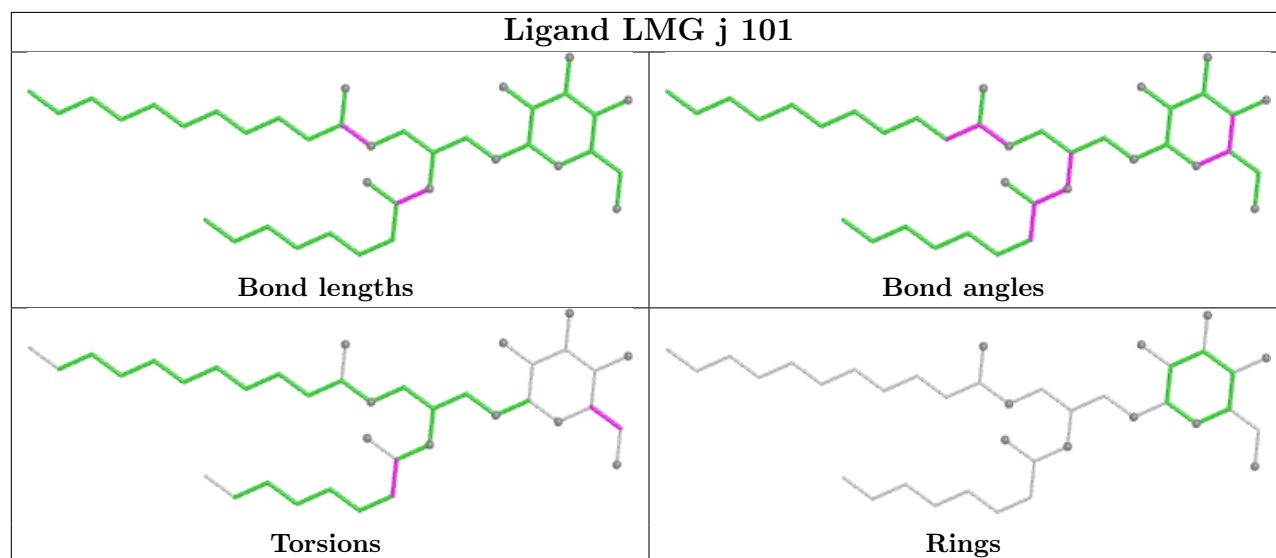
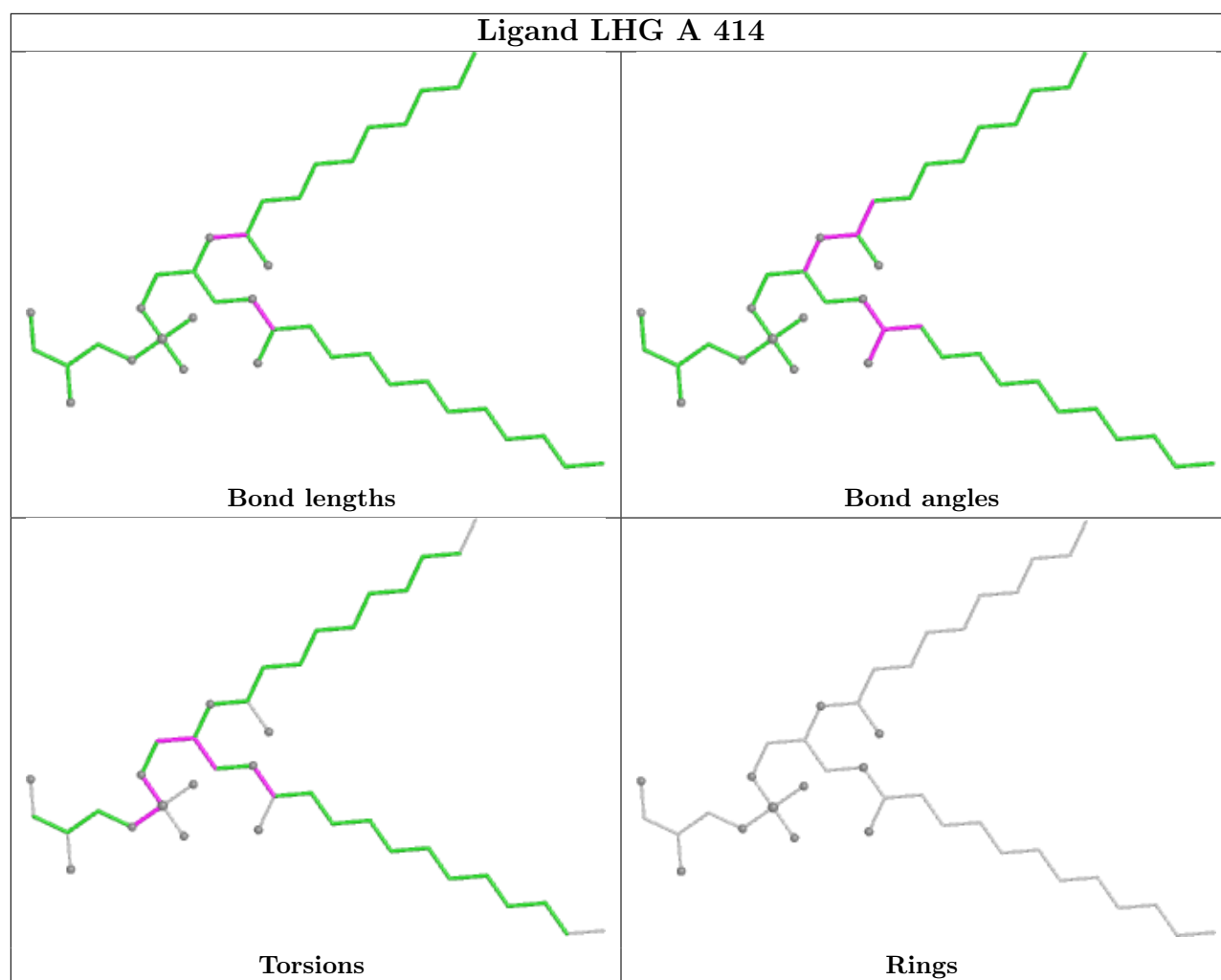


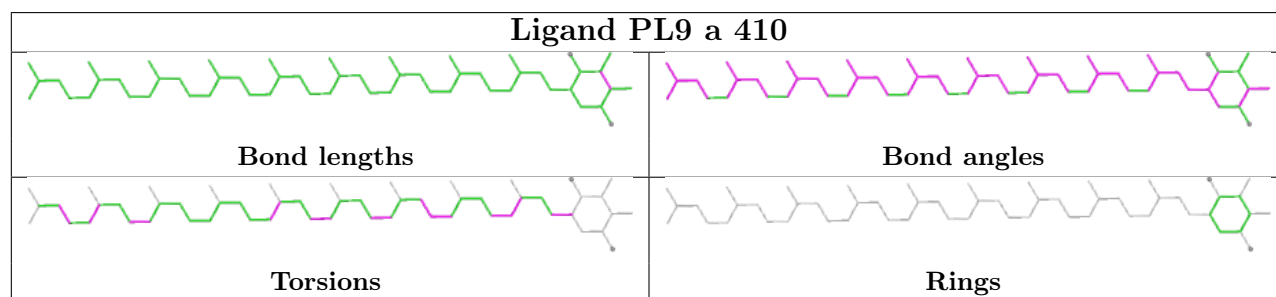
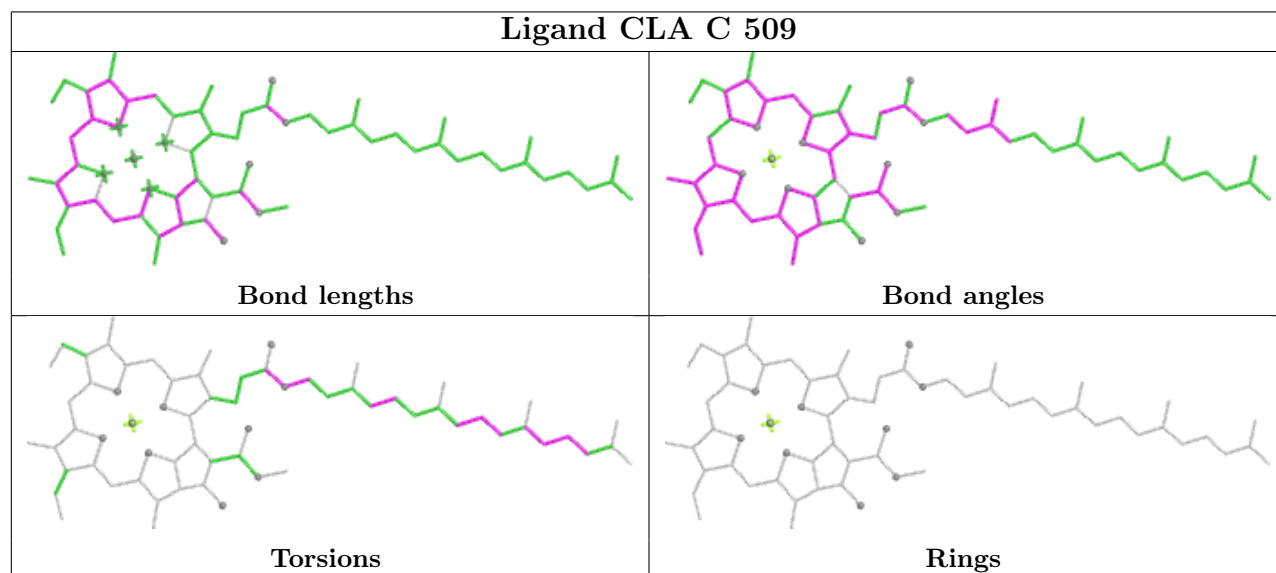
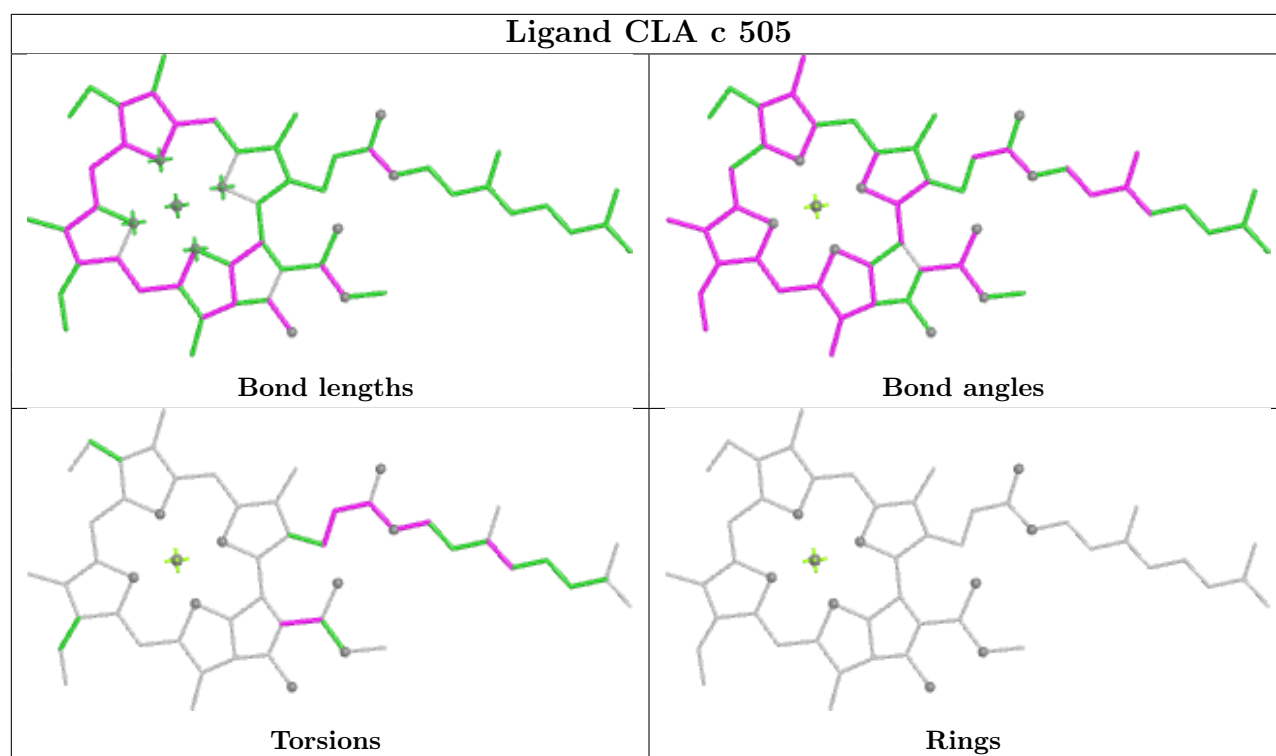


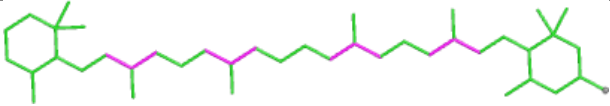
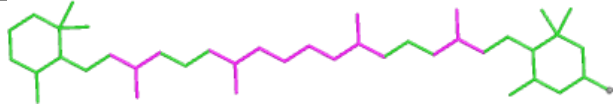
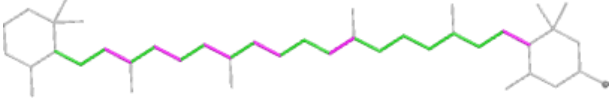
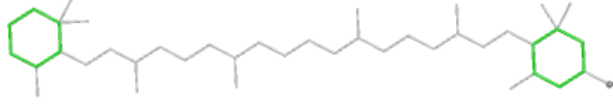
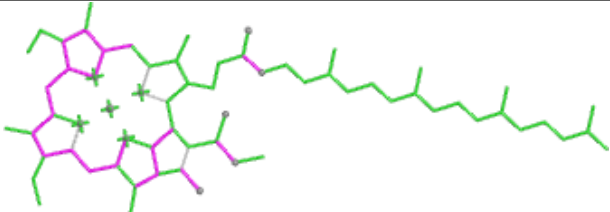
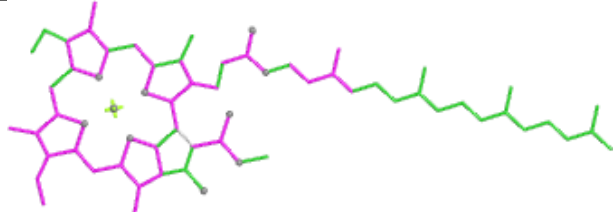
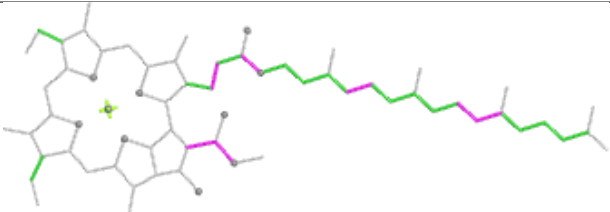
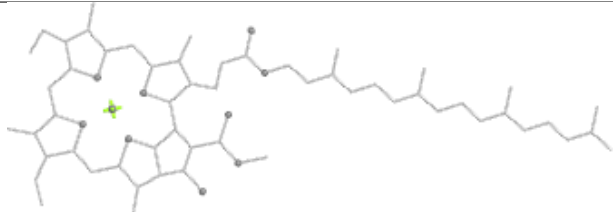
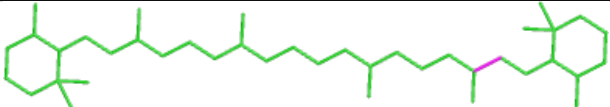
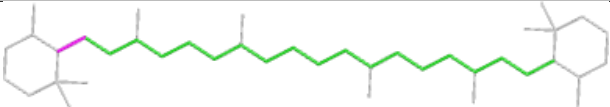
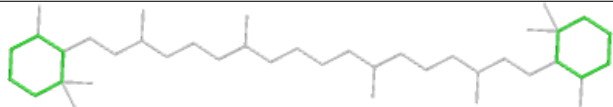




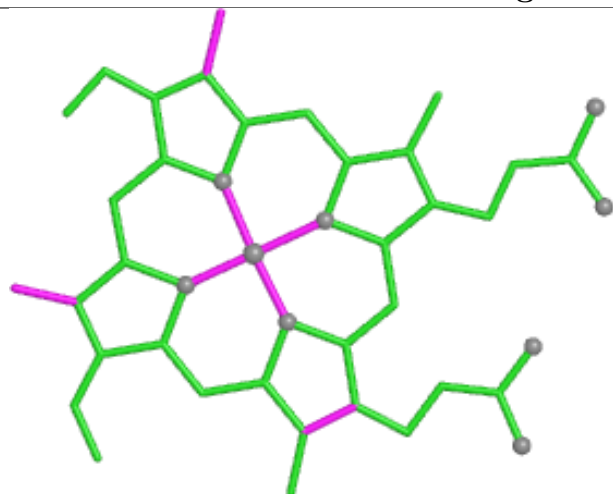
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



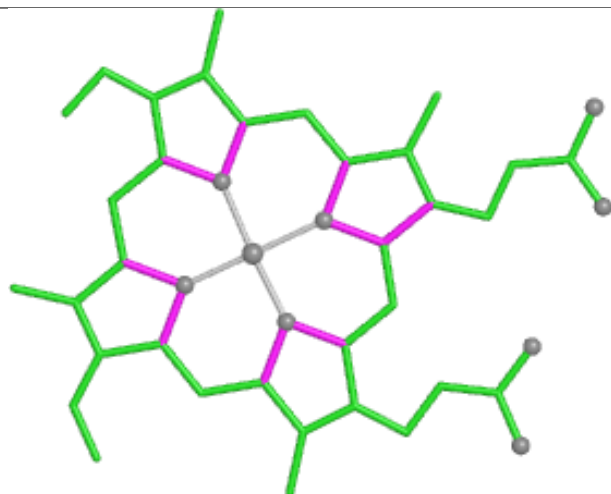


Ligand RRX x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

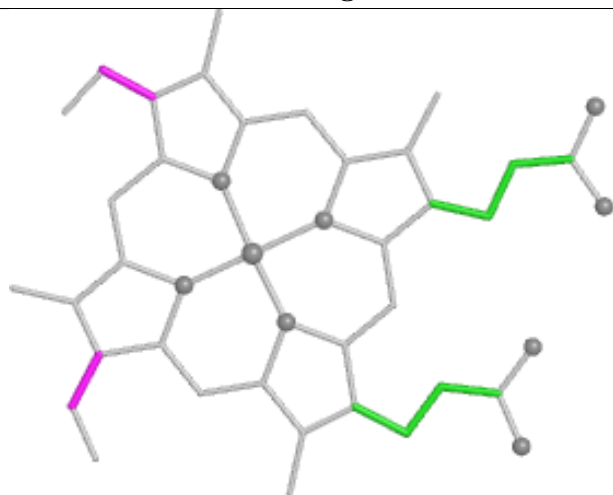
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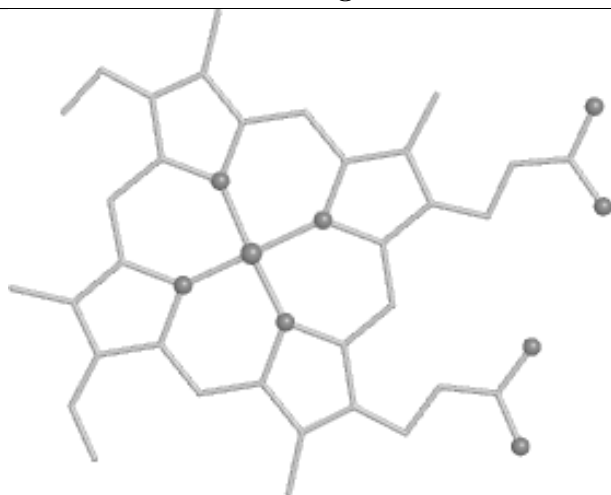
Bond lengths



Bond angles

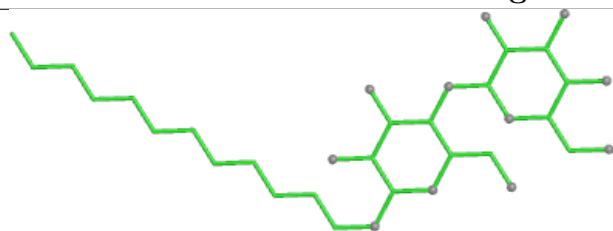


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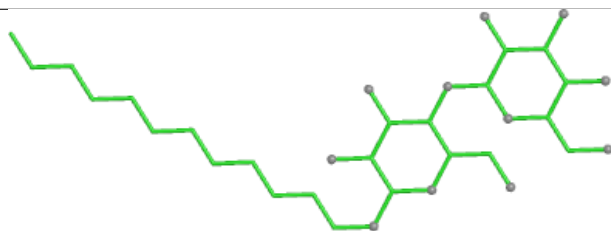


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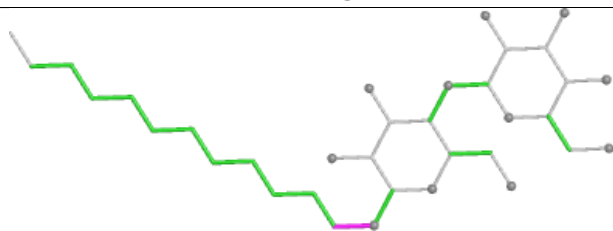
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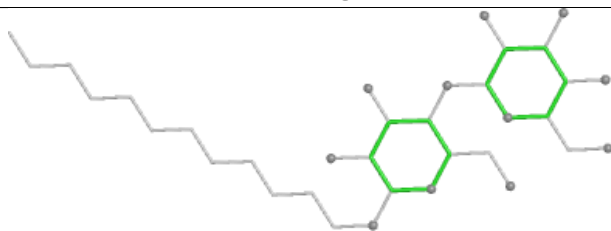
Bond lengths



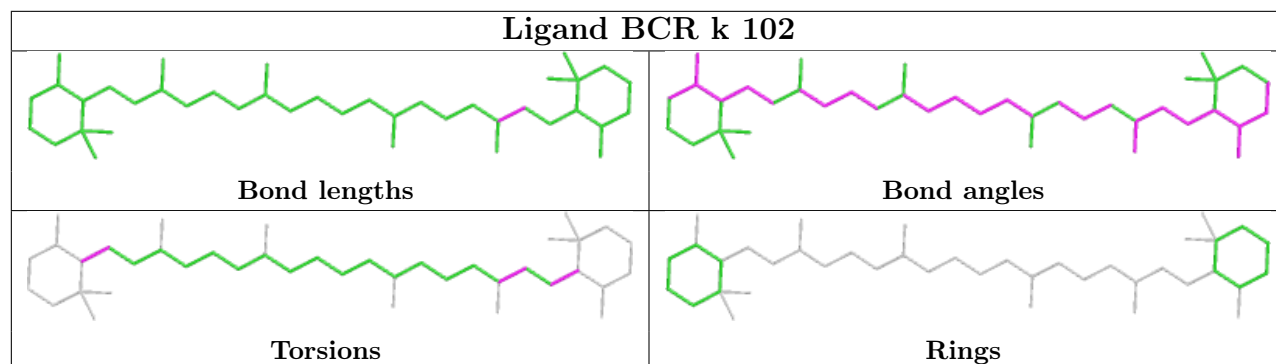
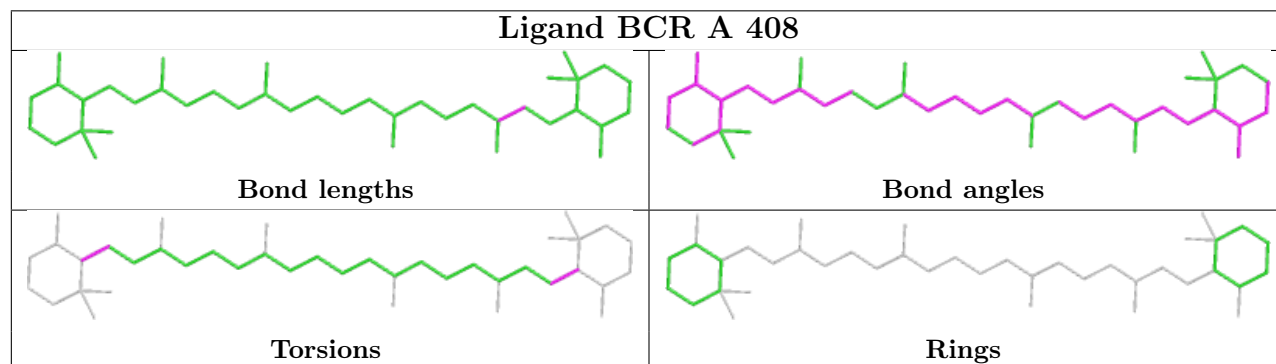
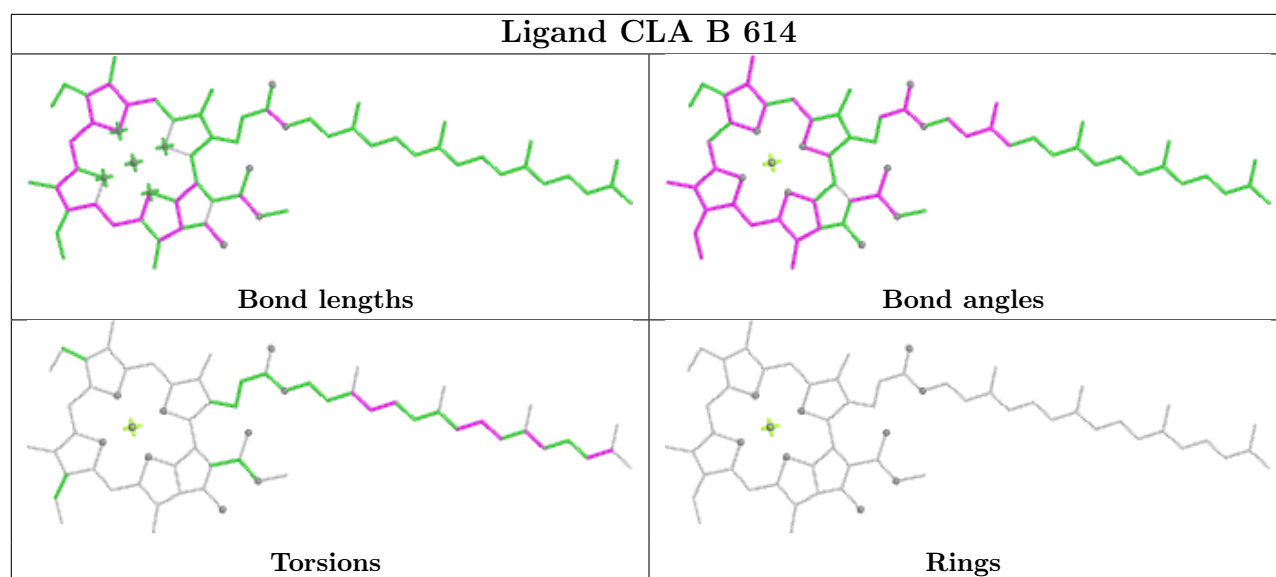
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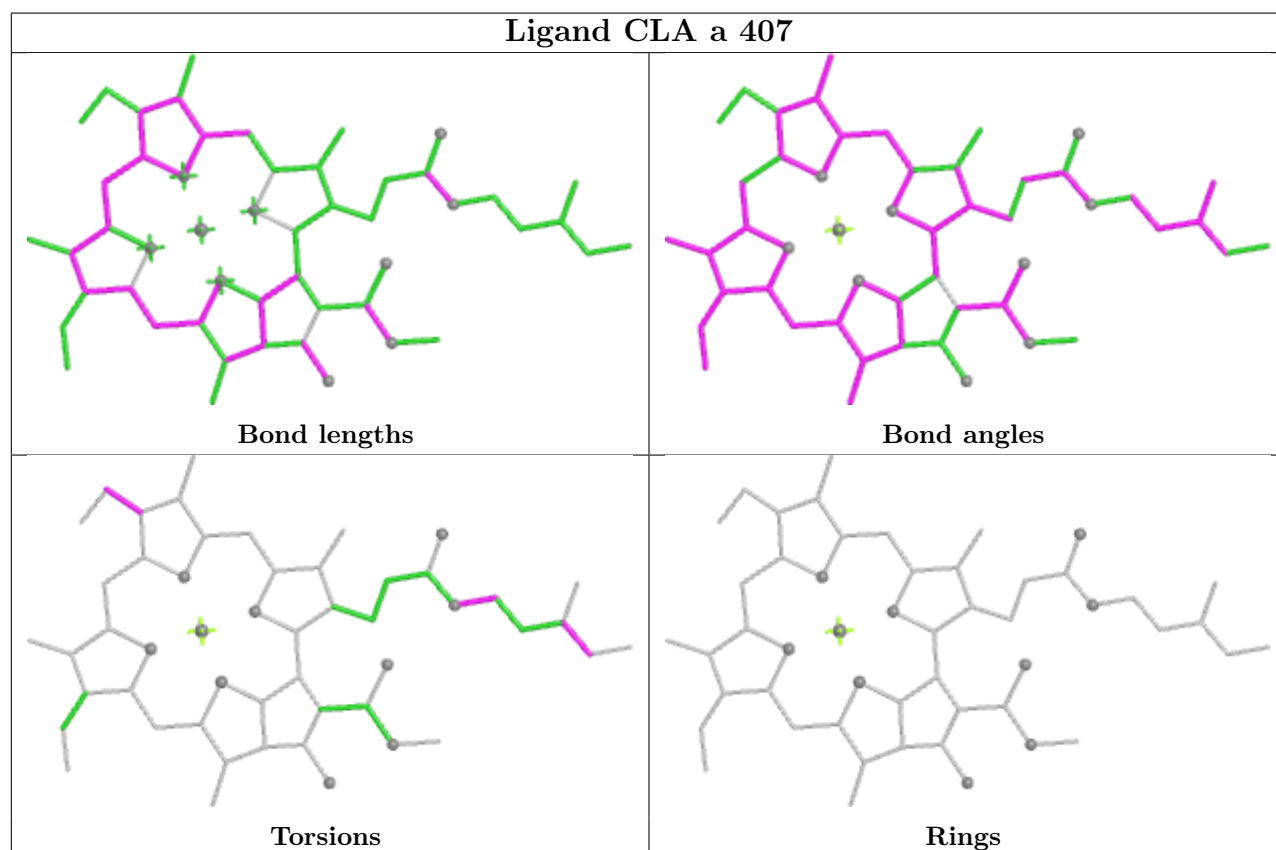
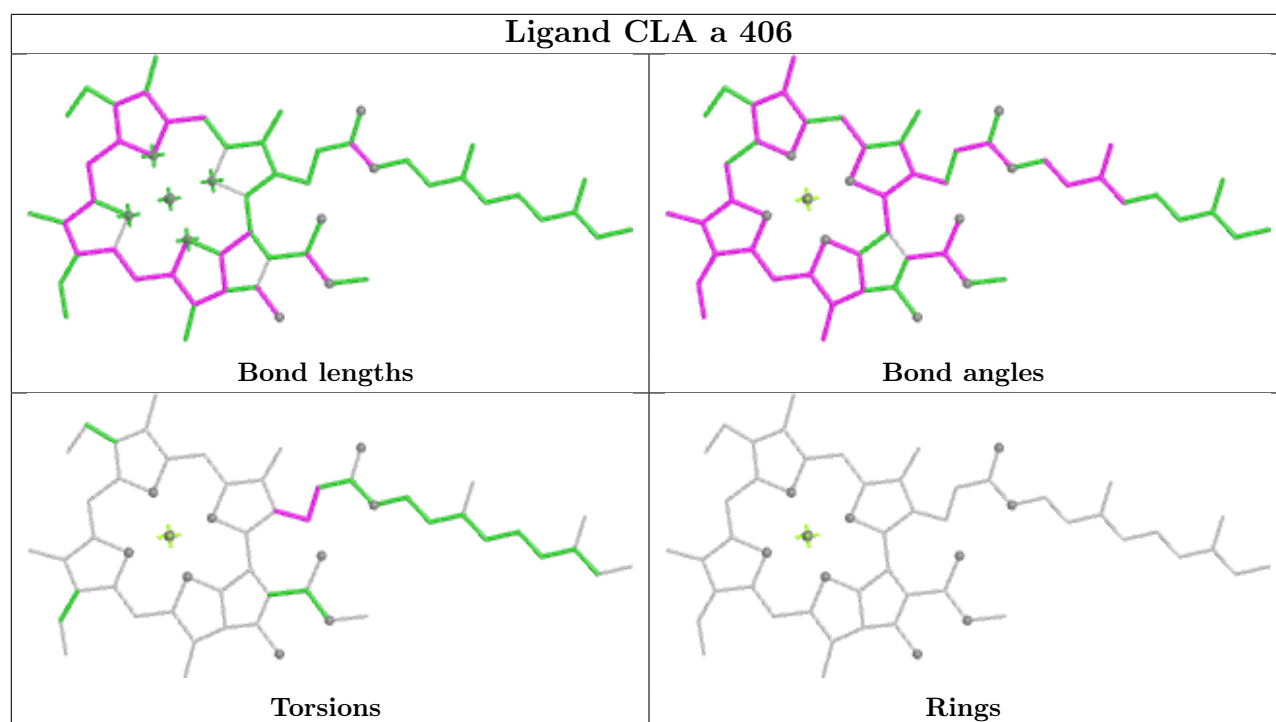


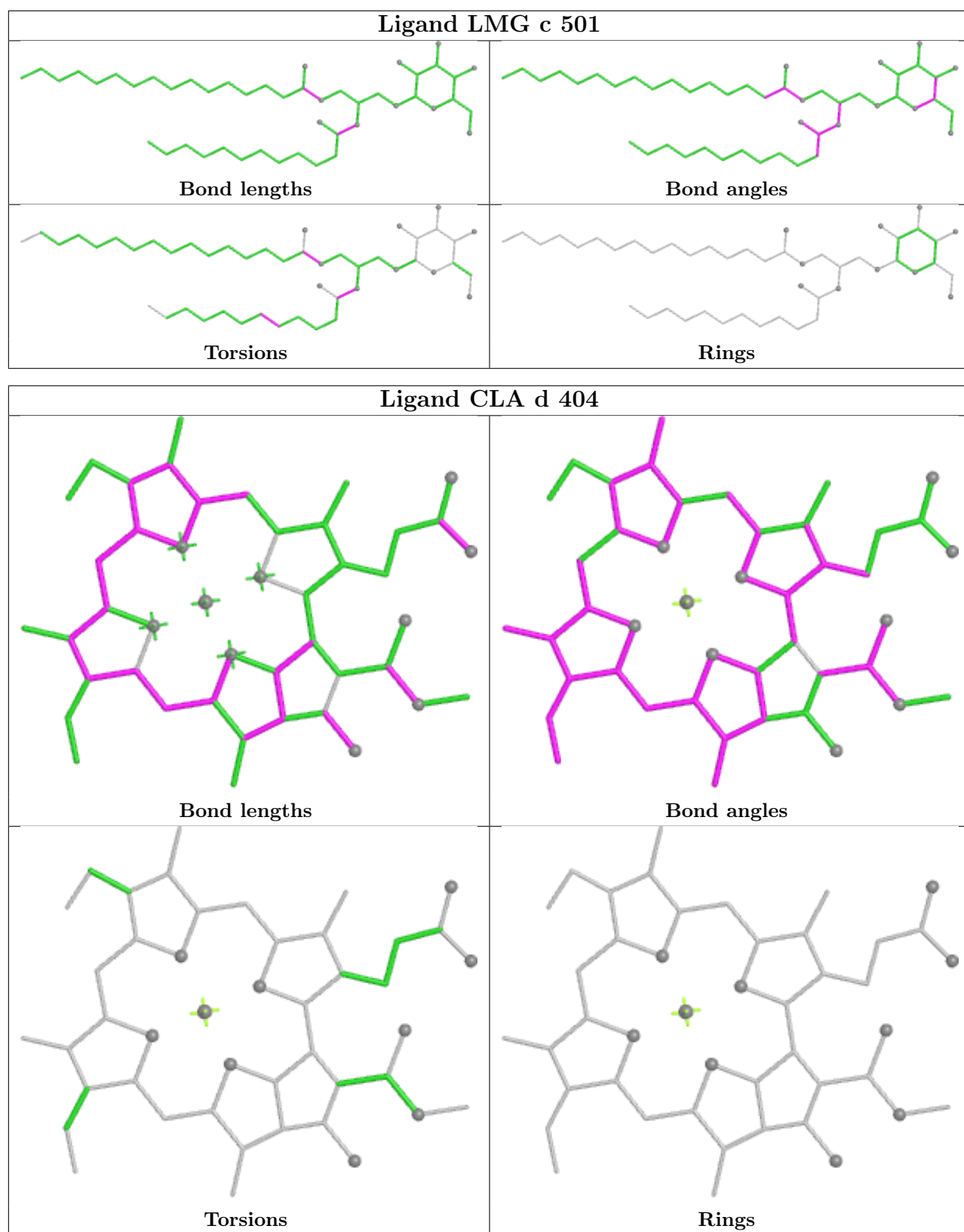
Torsions



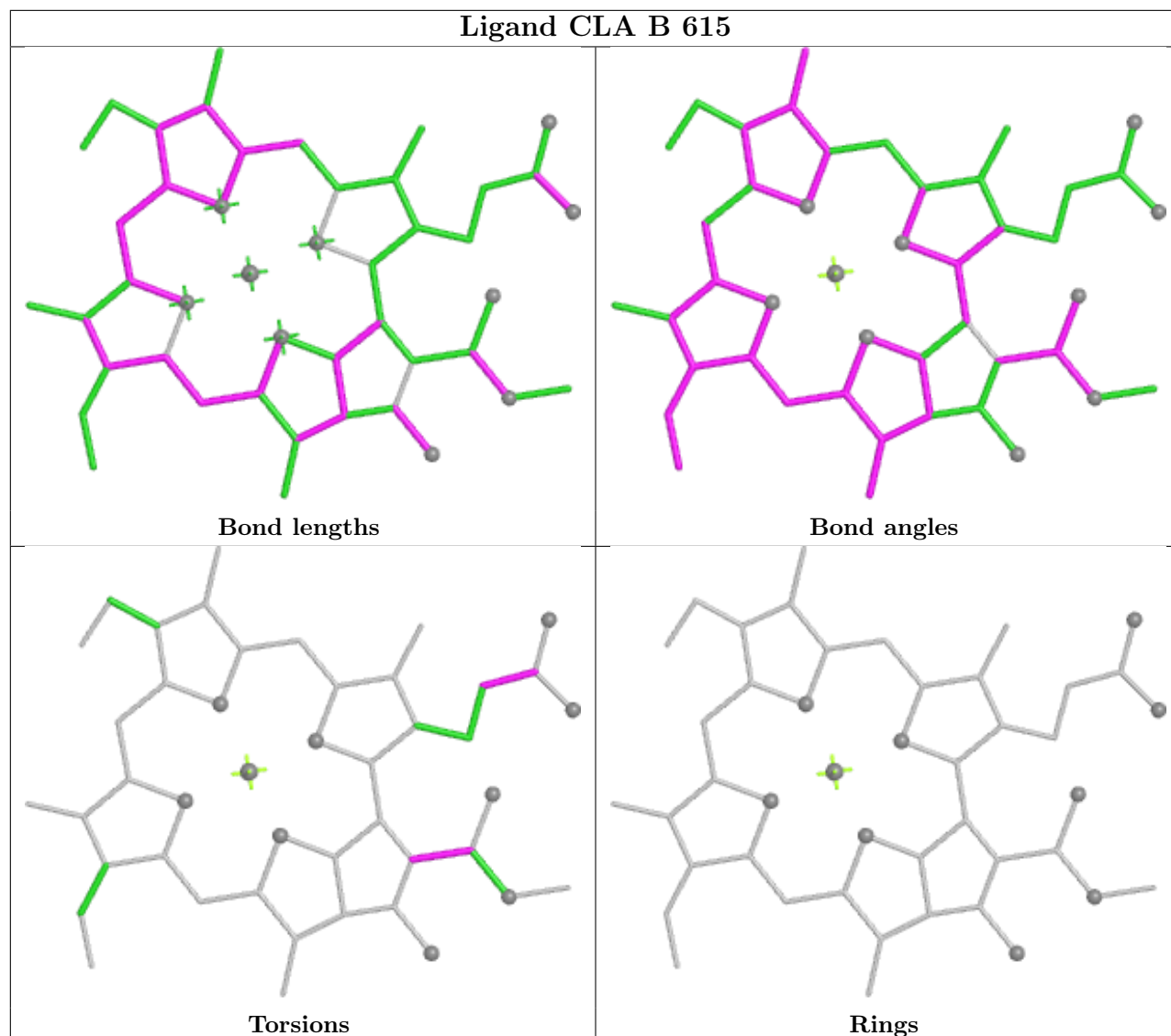
Rings



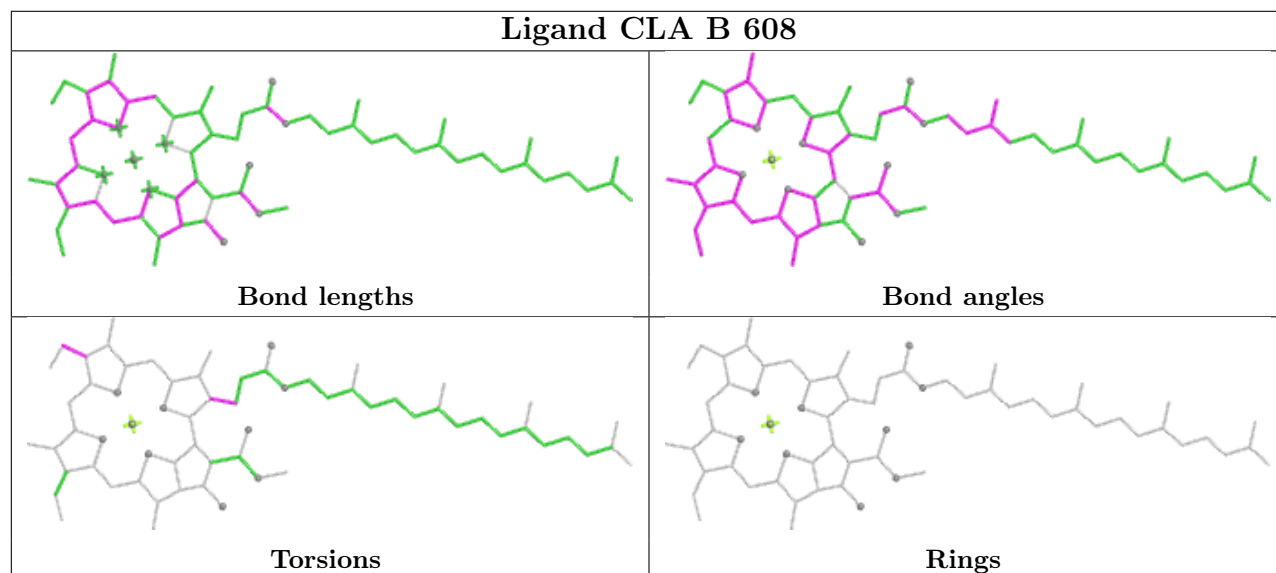


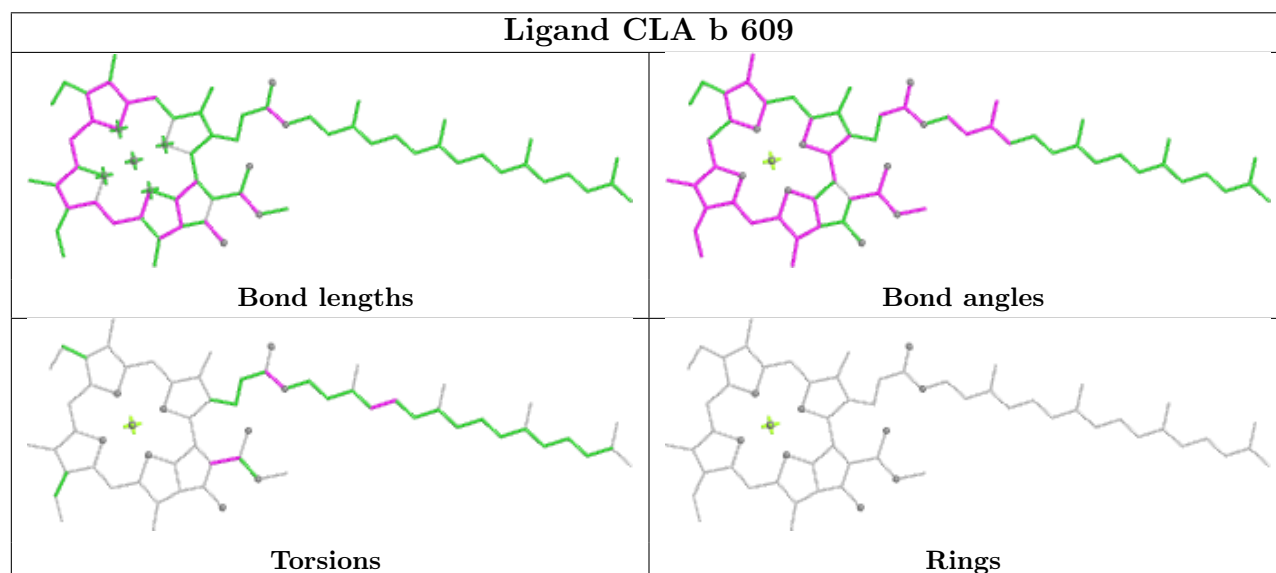
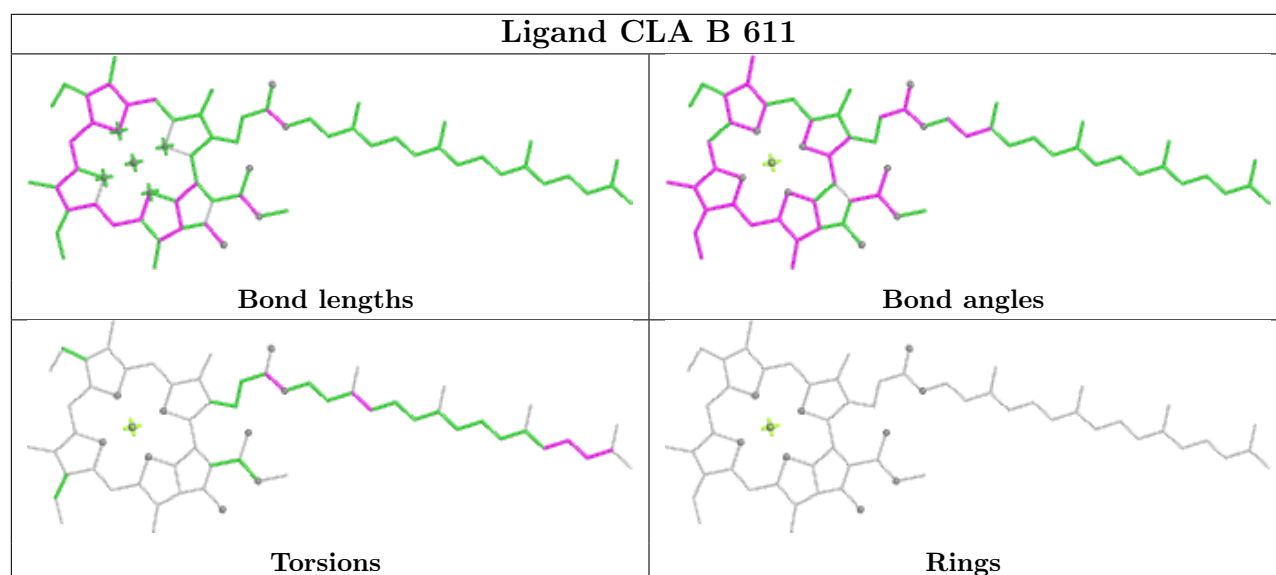
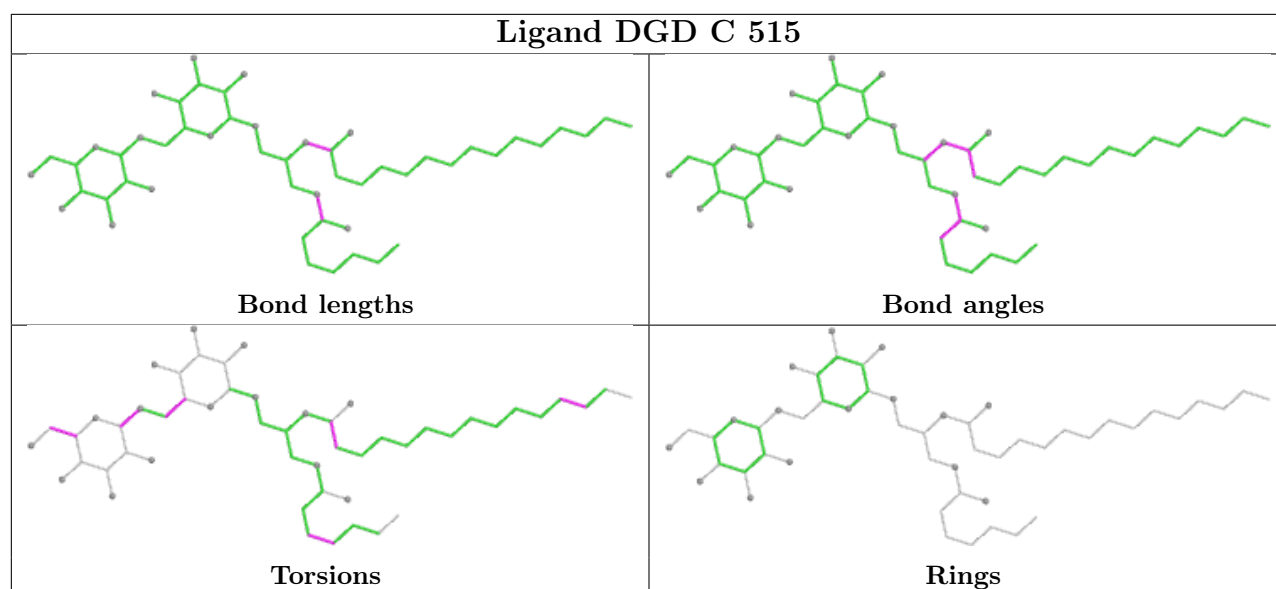


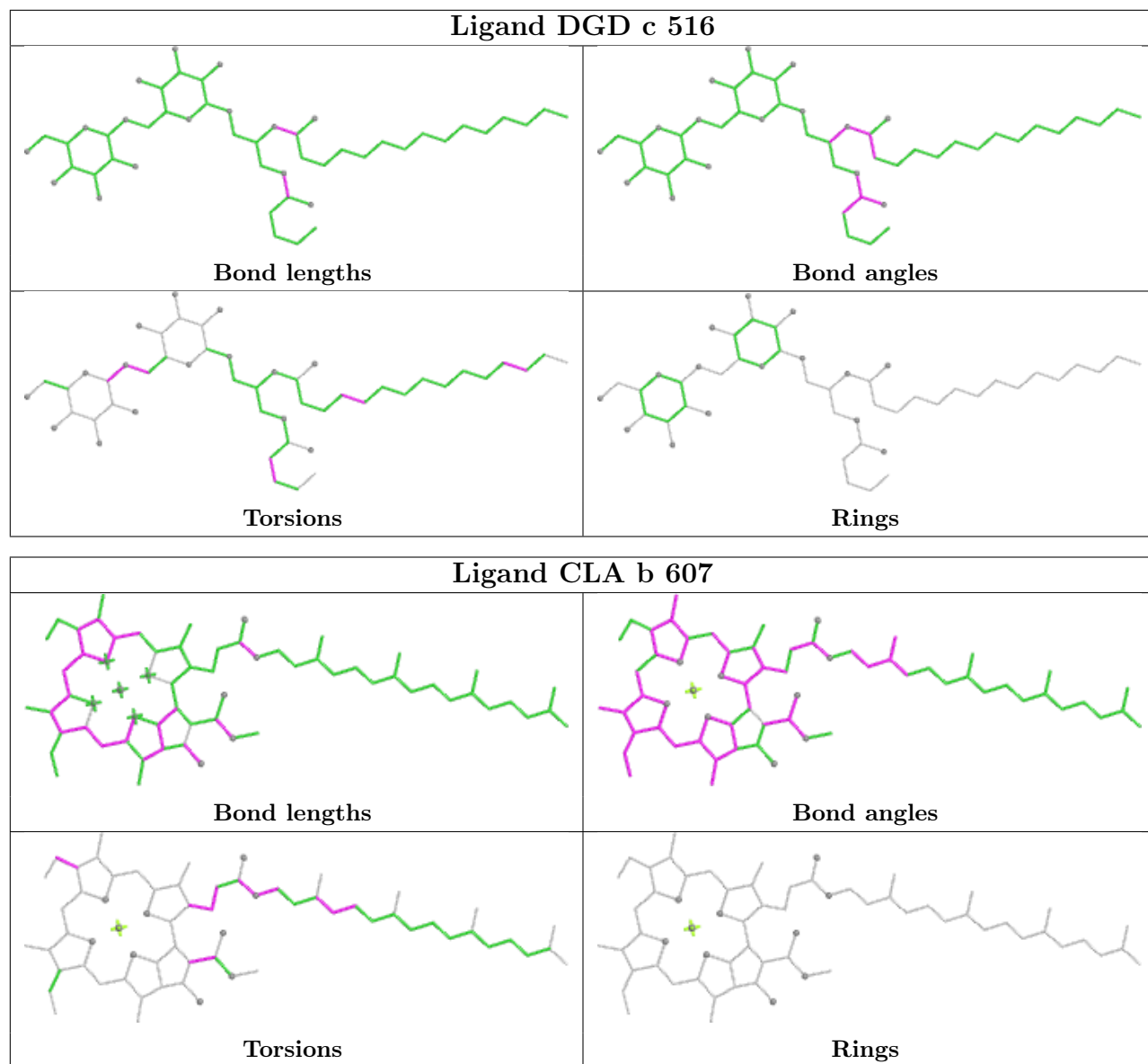
Ligand CLA B 615

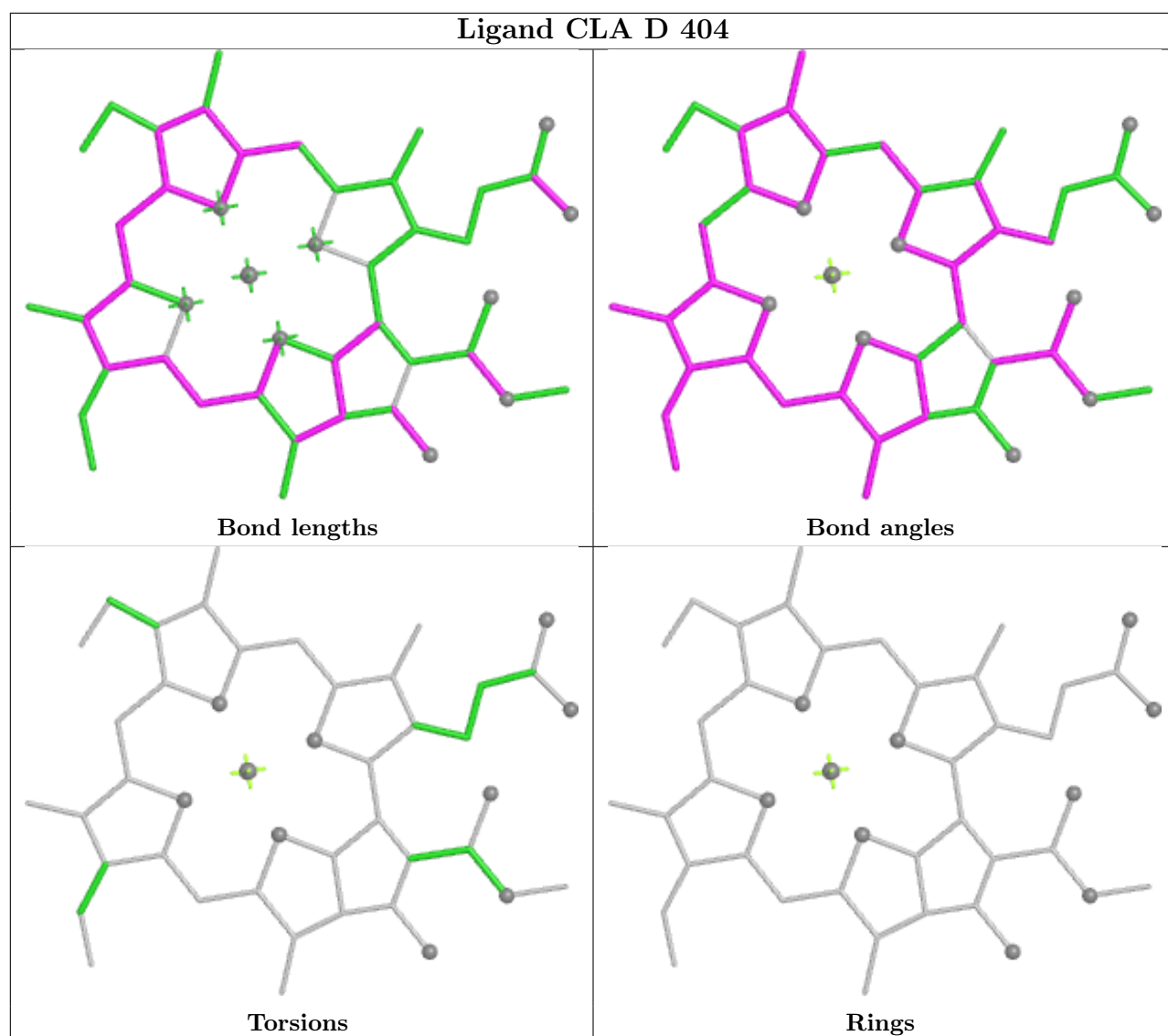


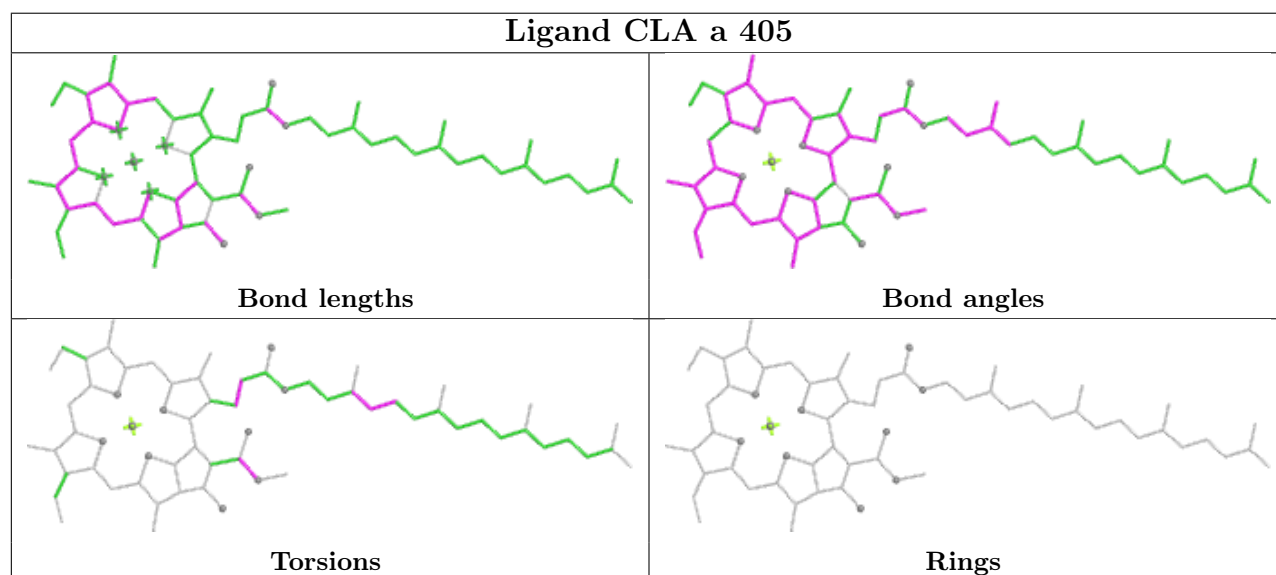
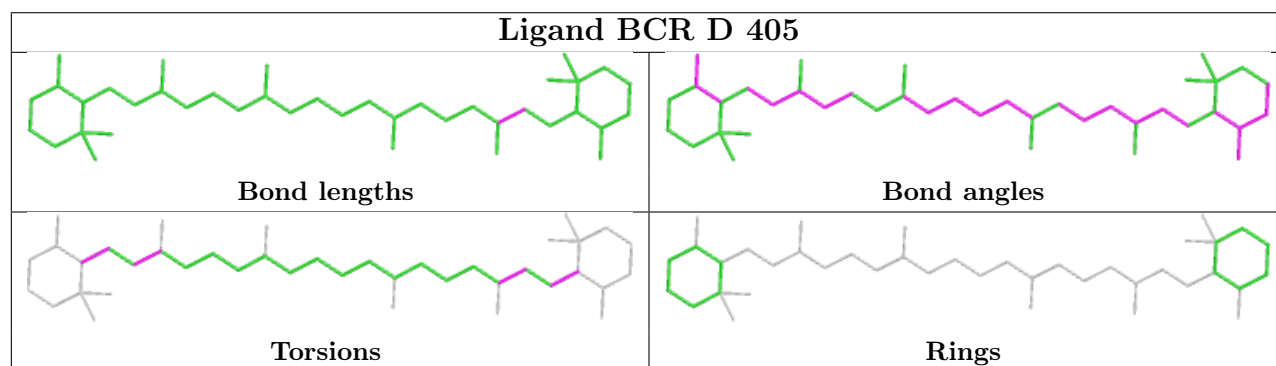
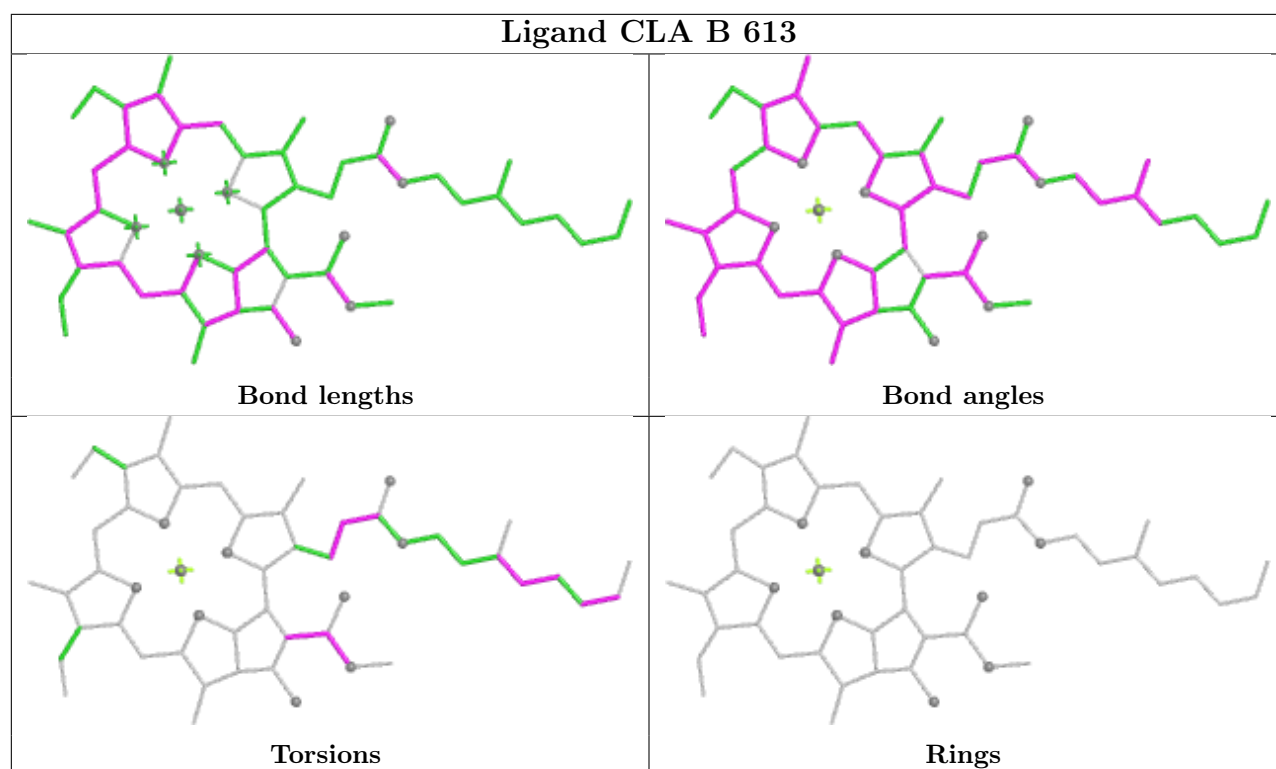
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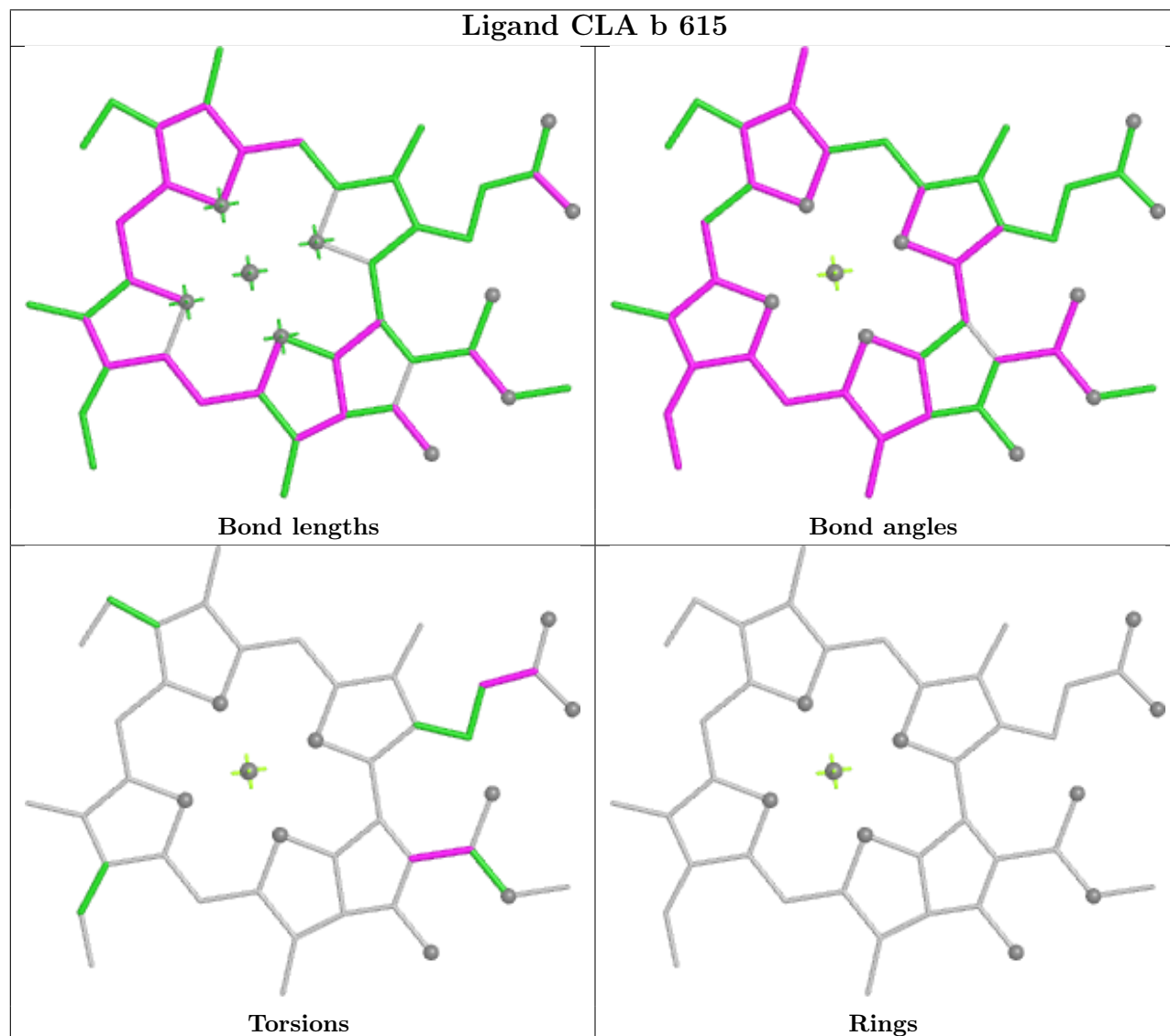
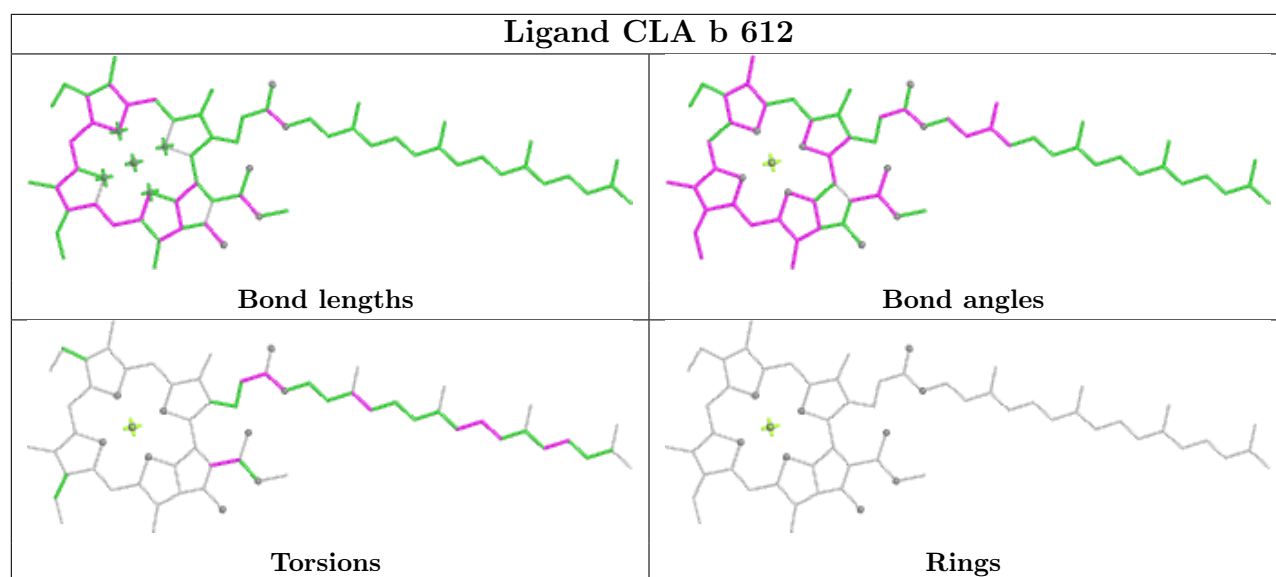


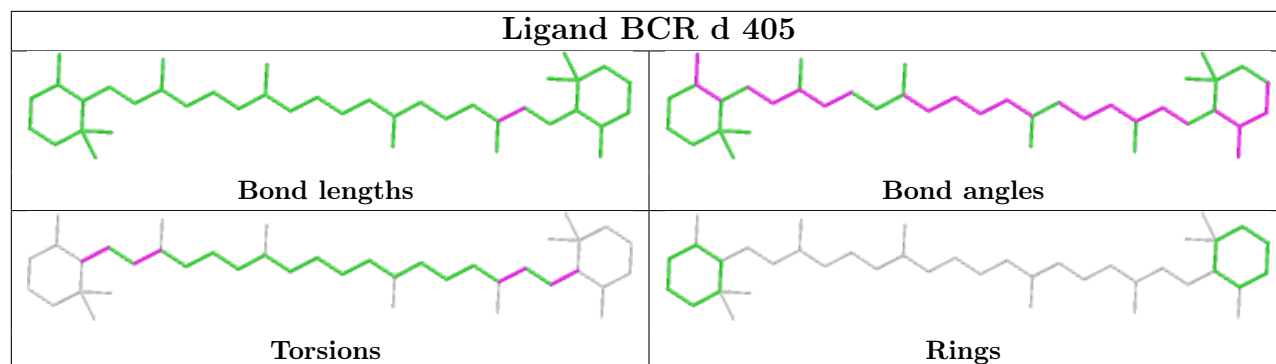
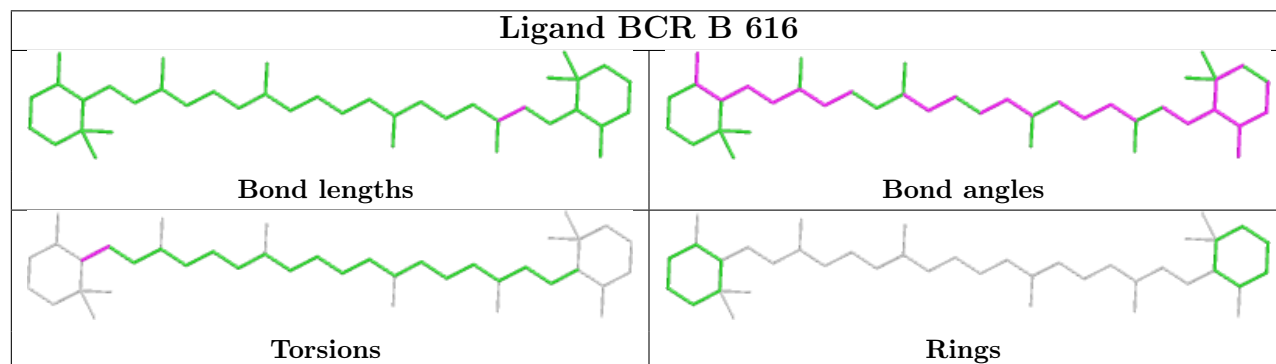
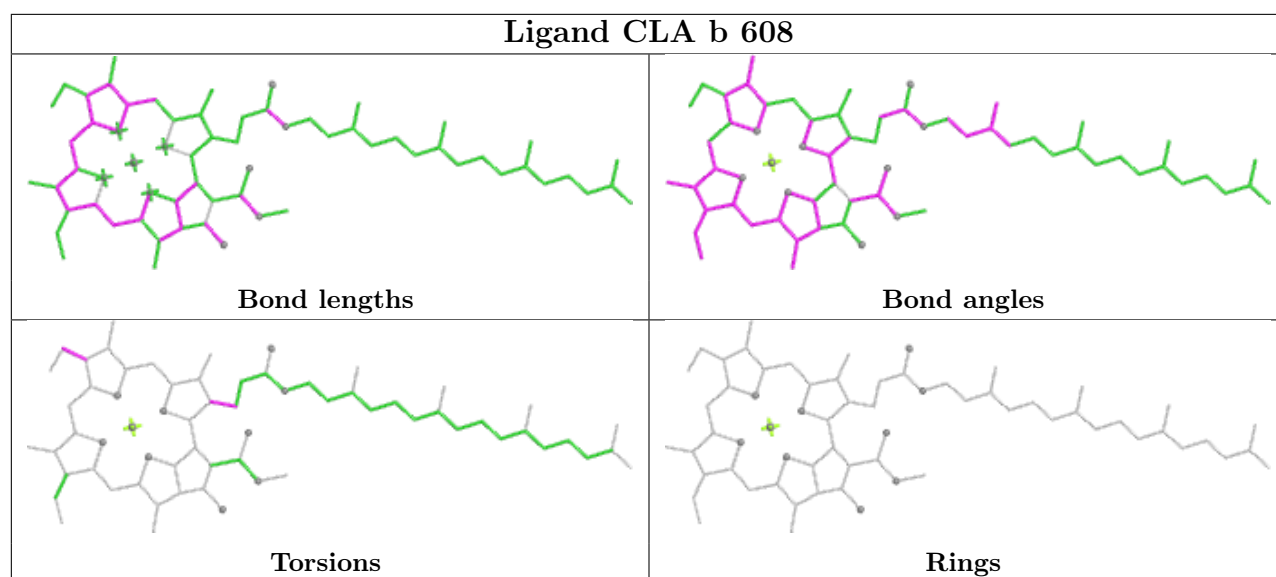


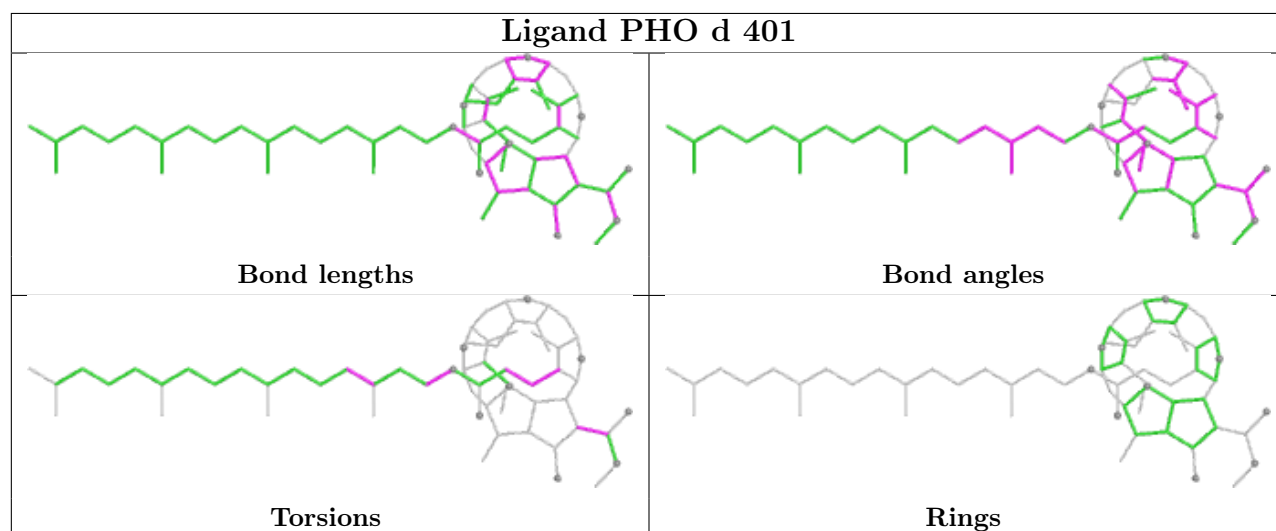
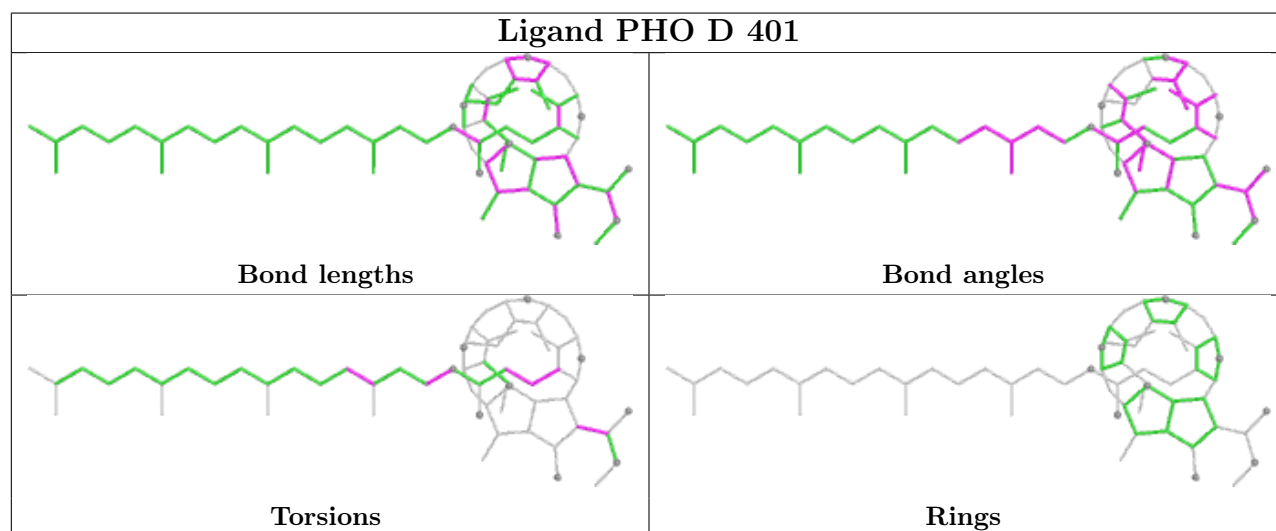
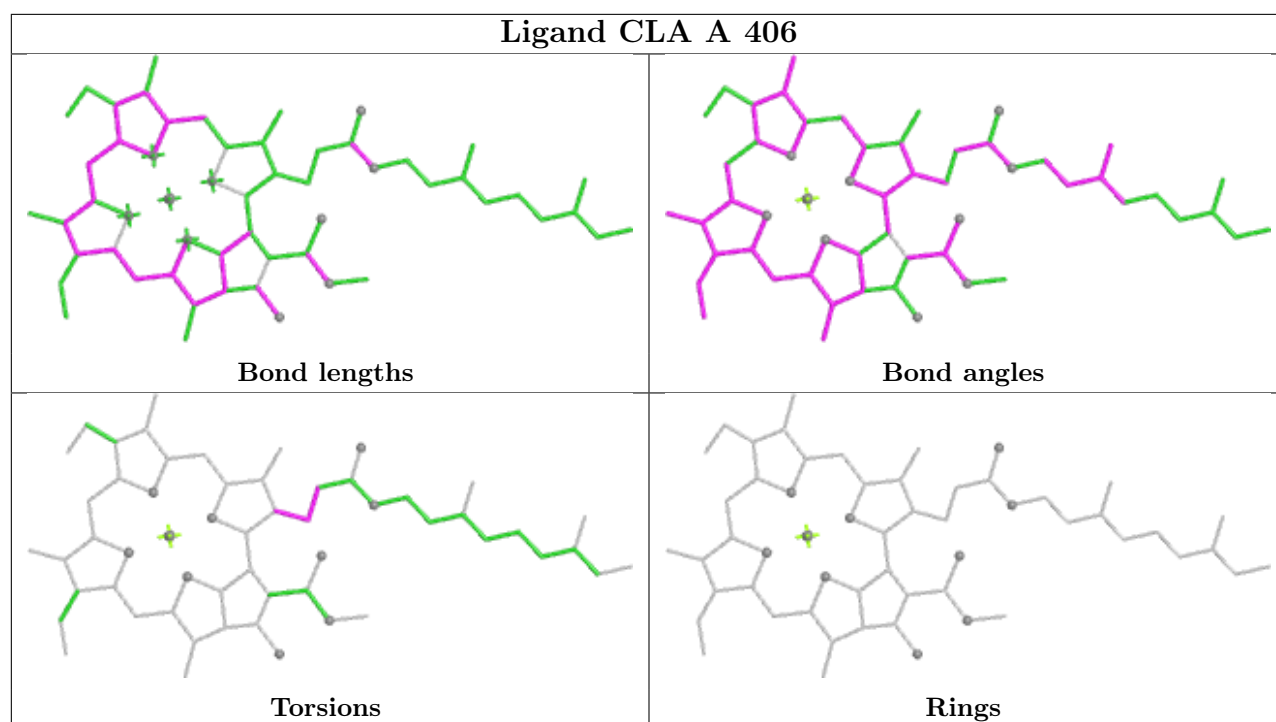


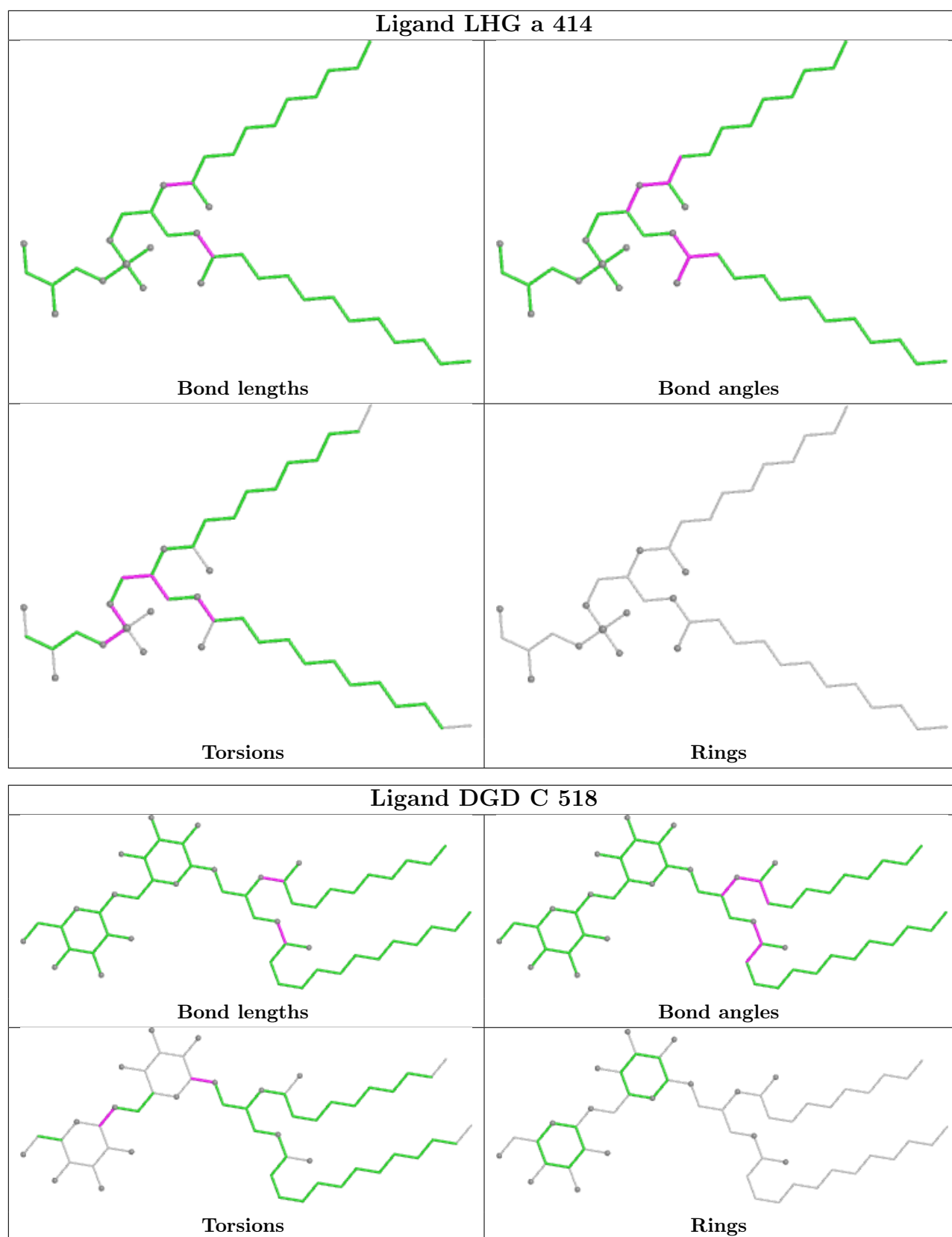


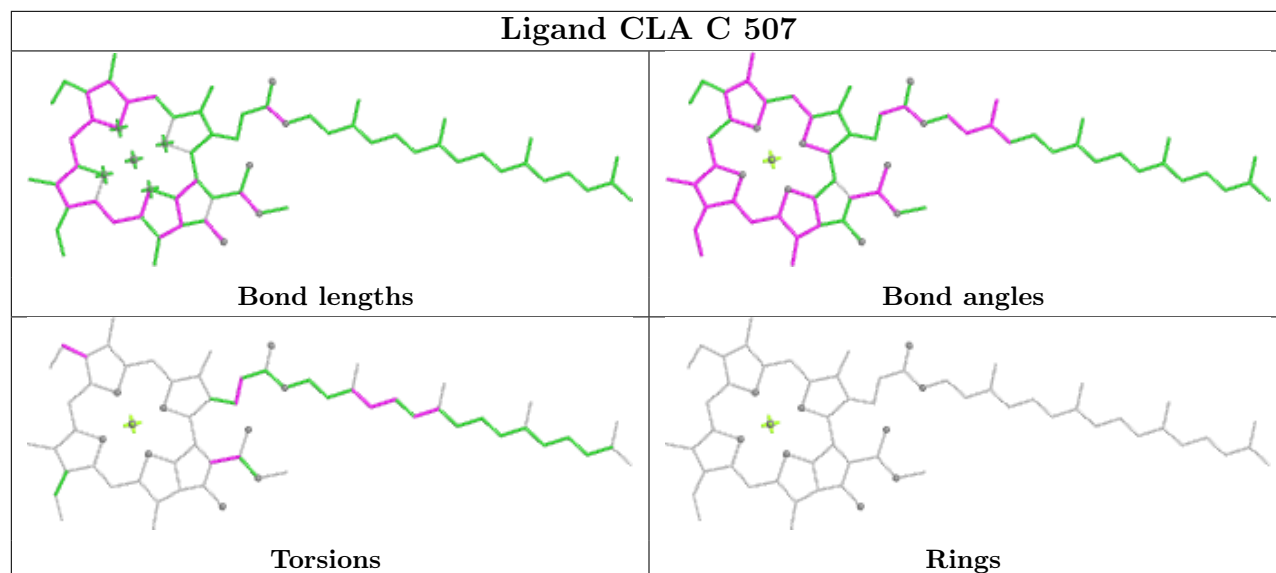
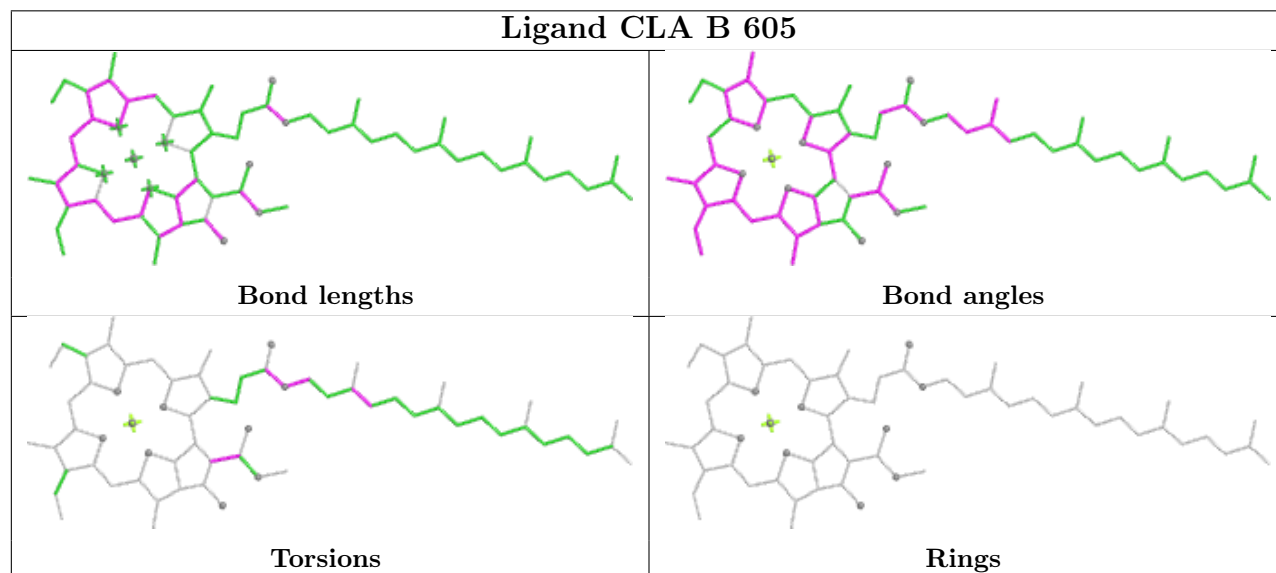
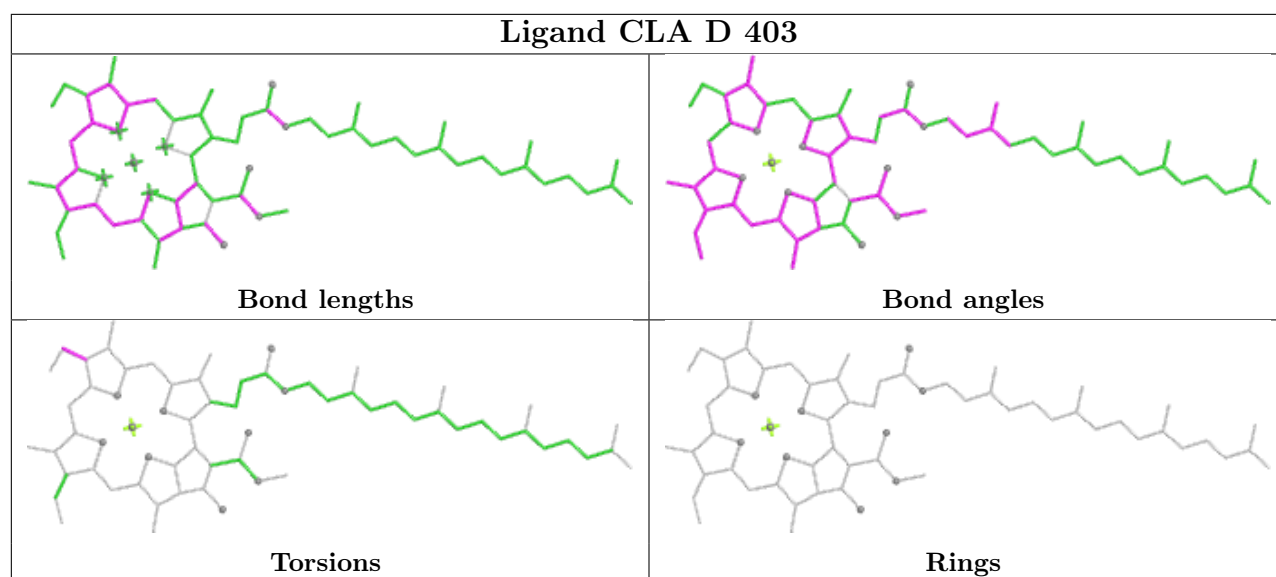


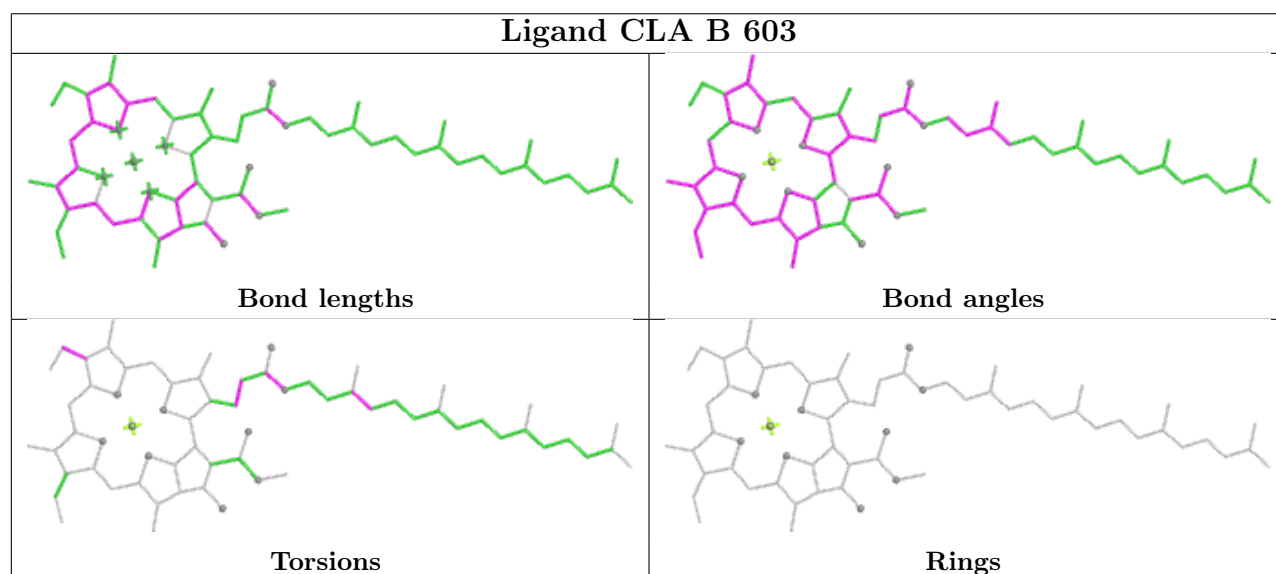
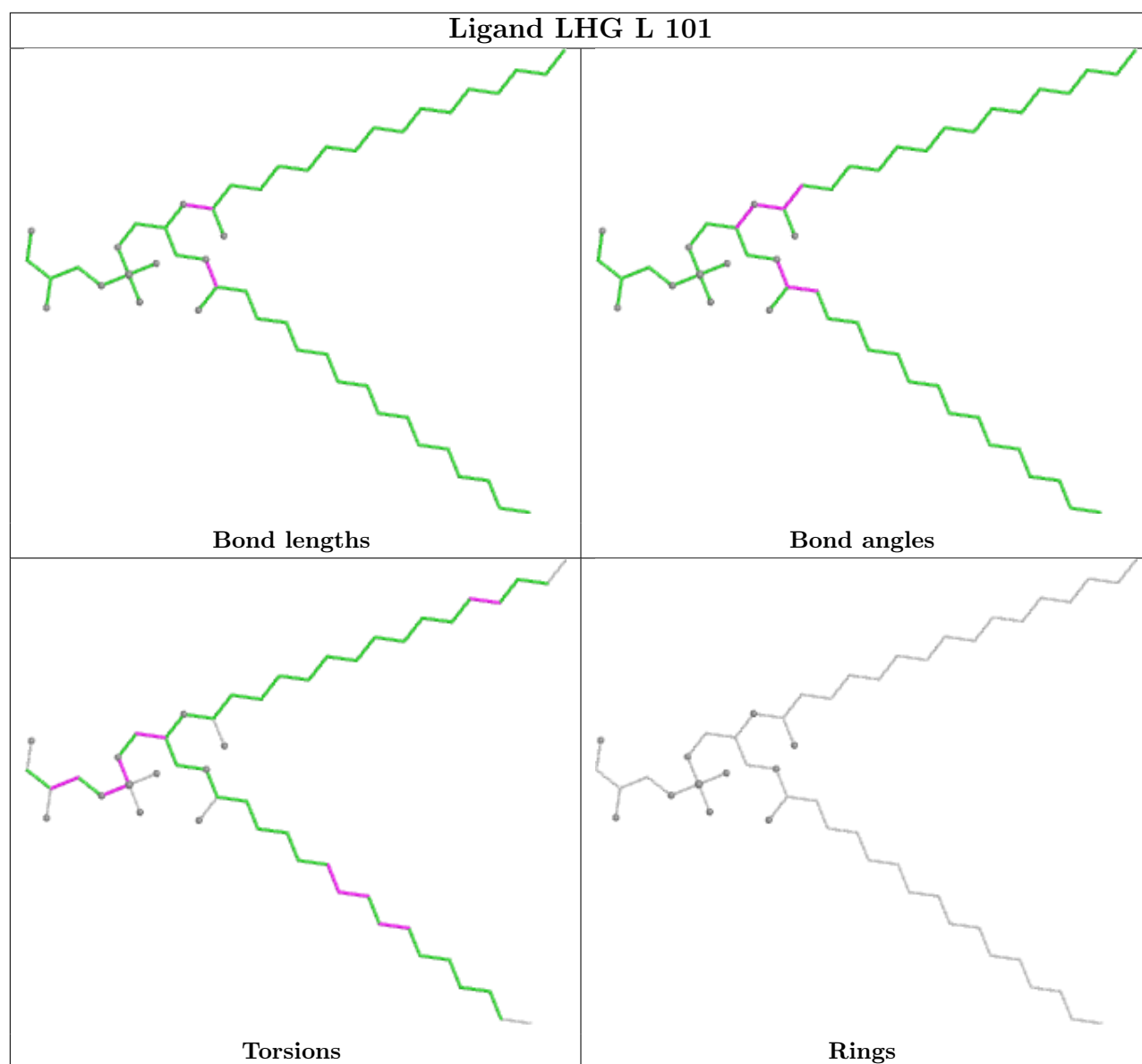


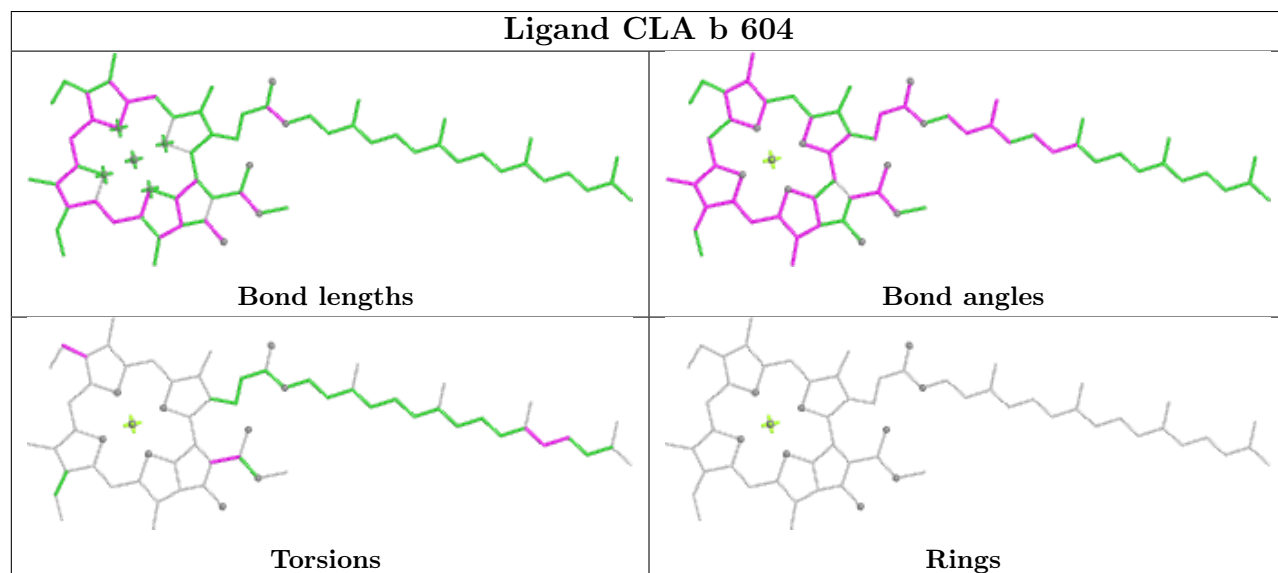
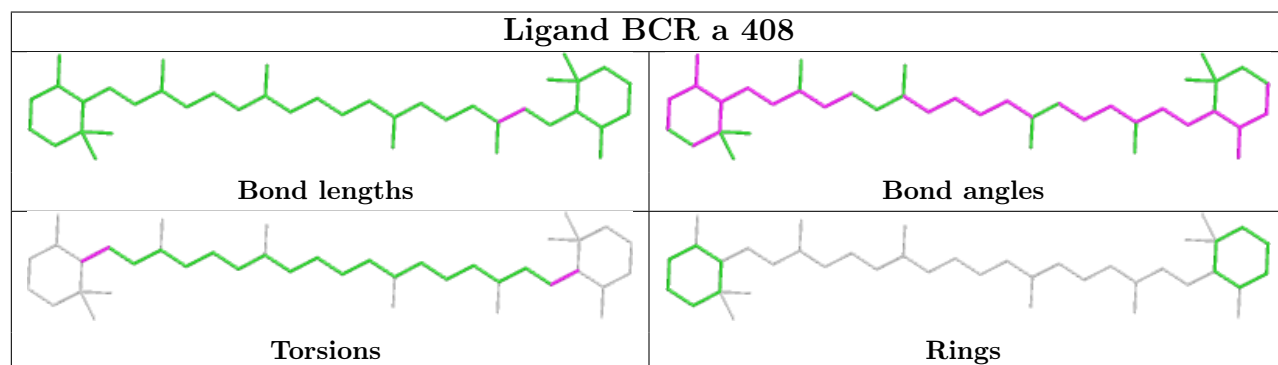
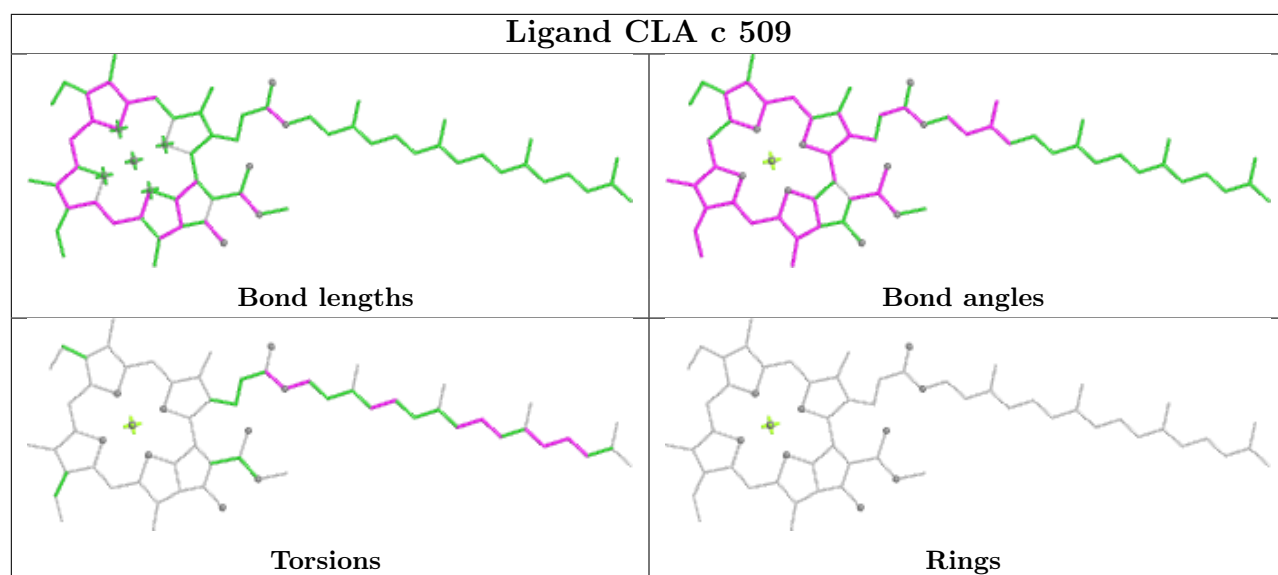


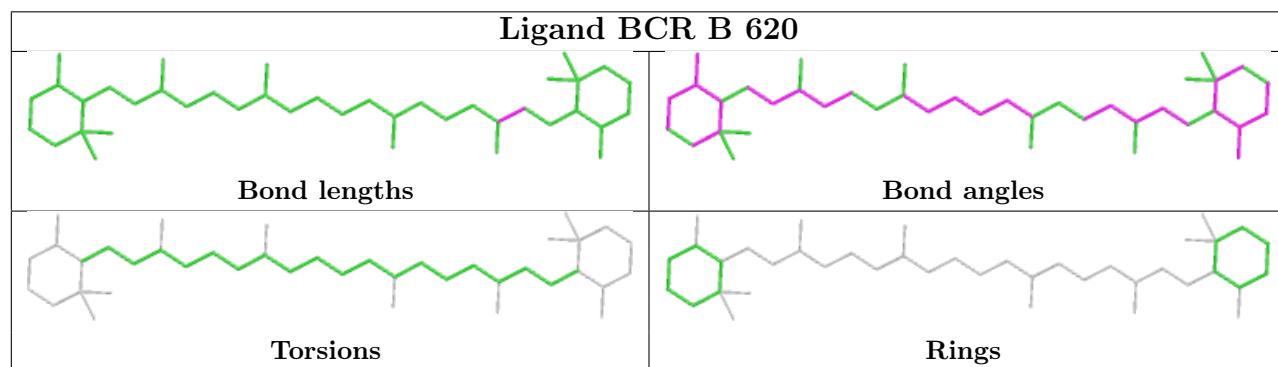
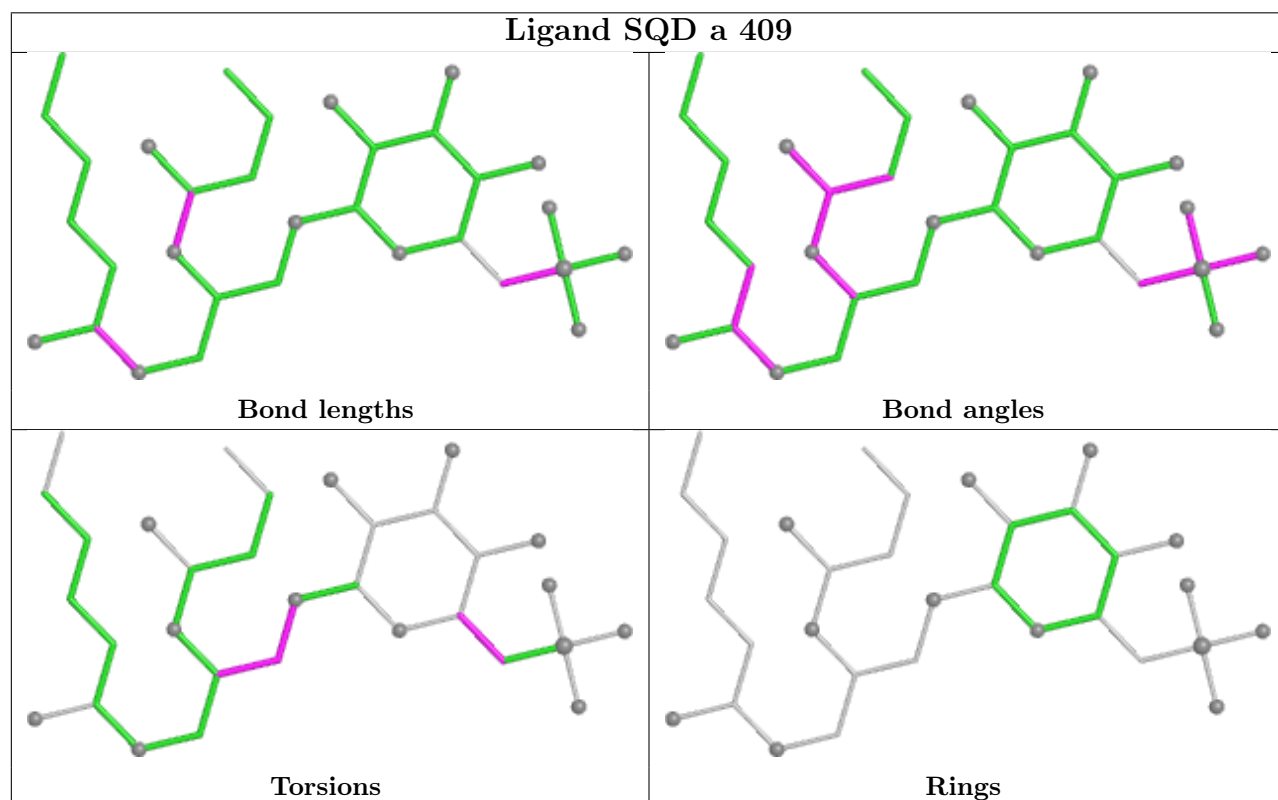
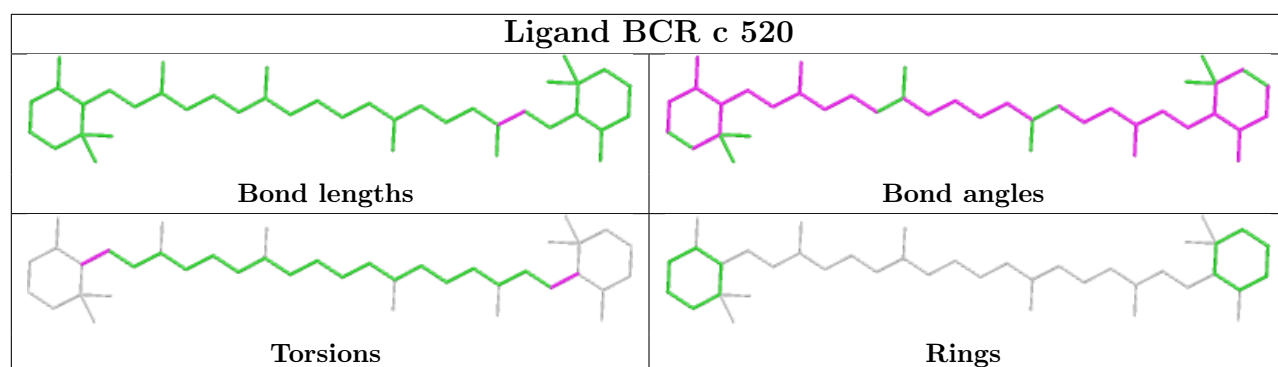


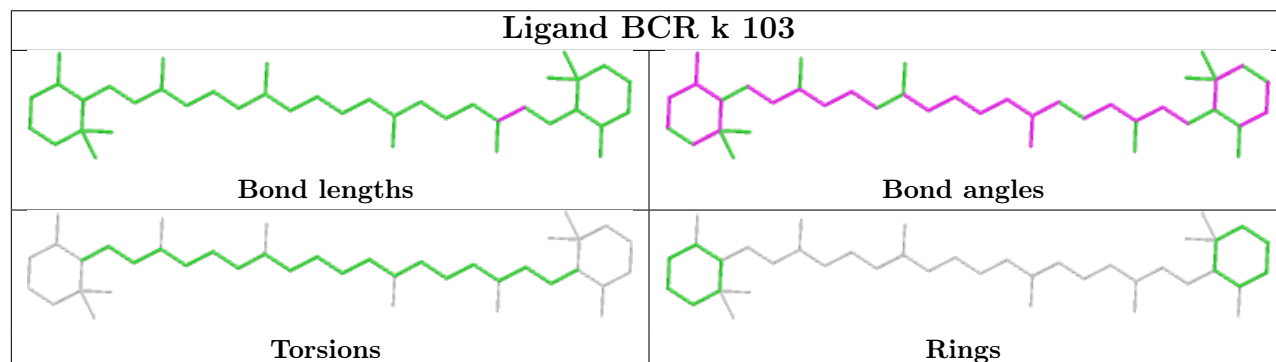
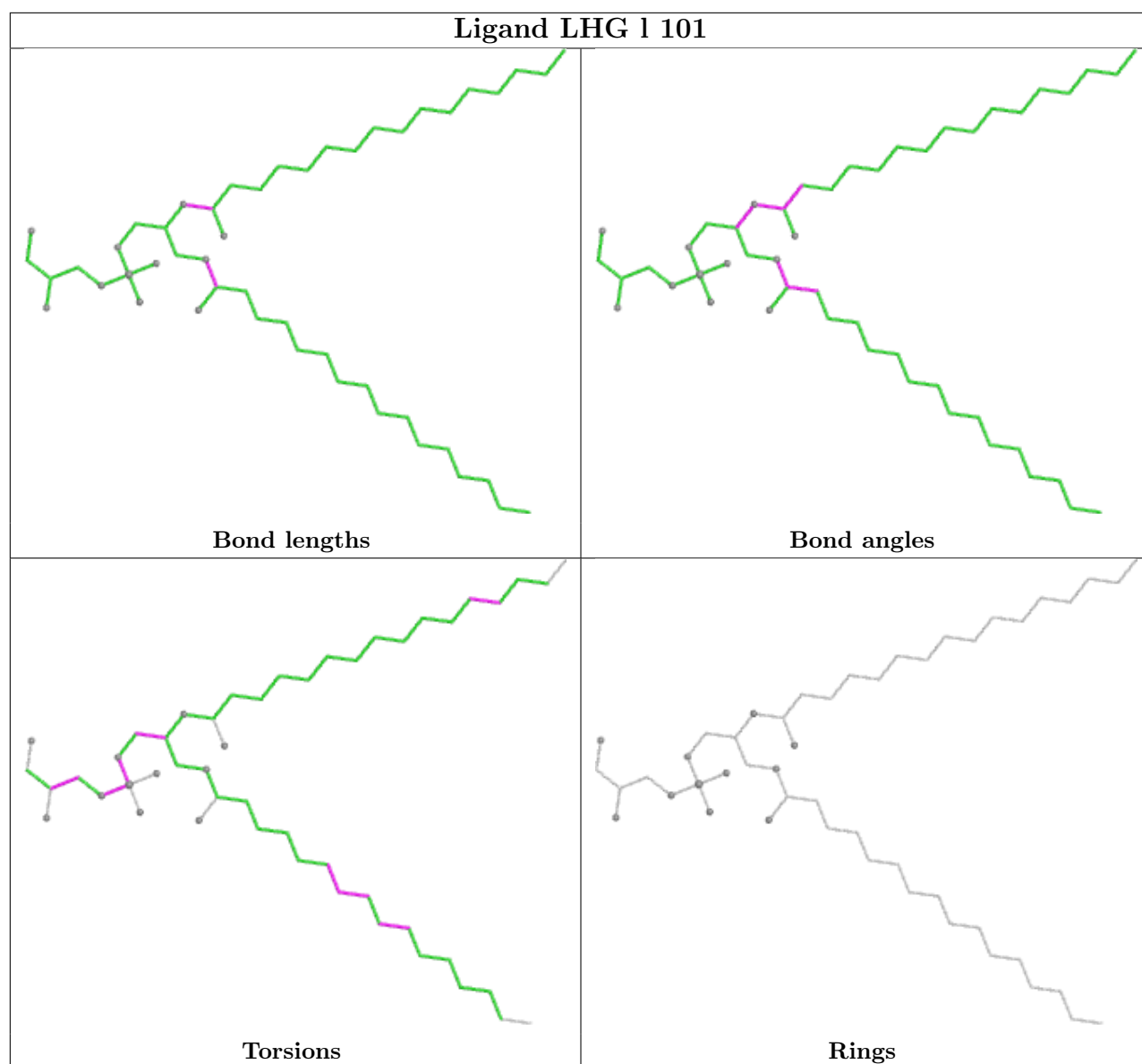


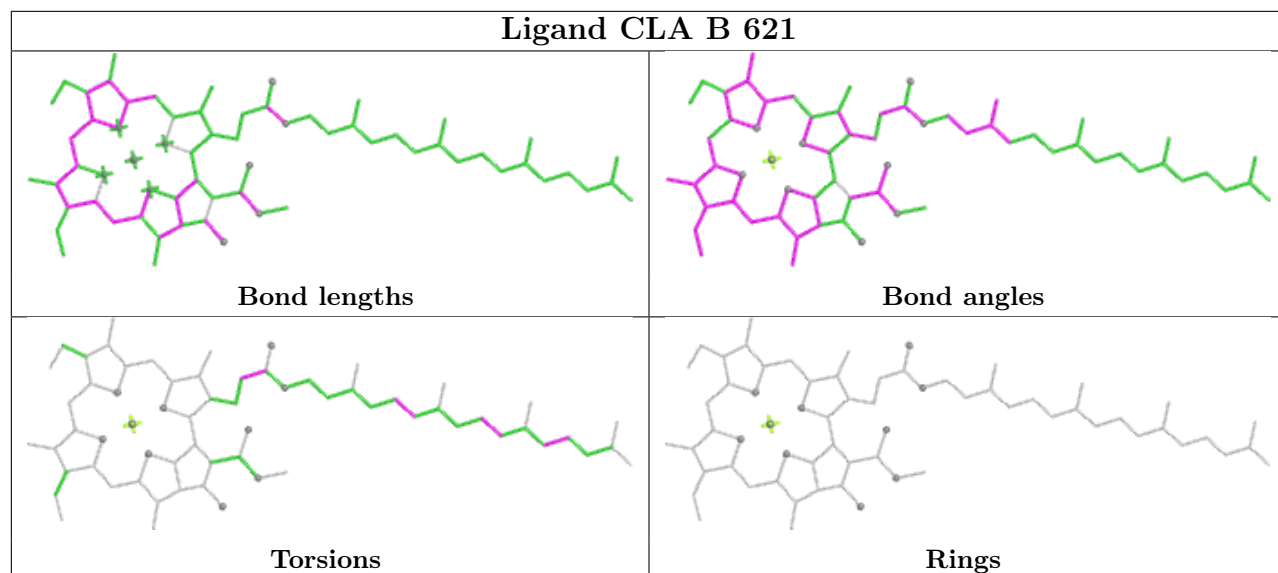
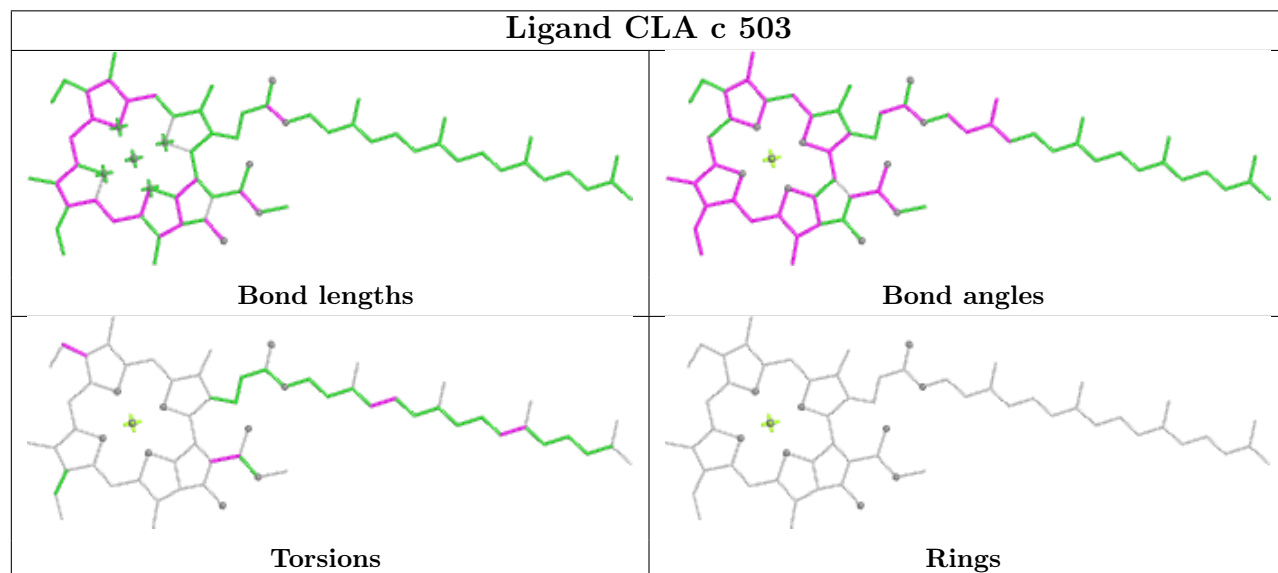
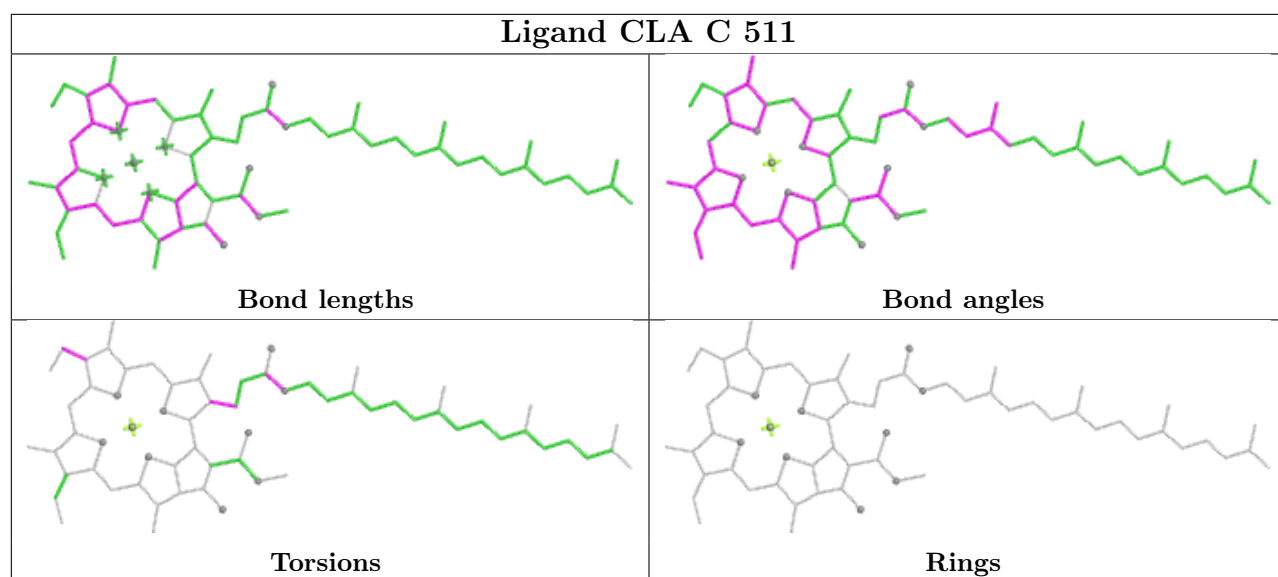


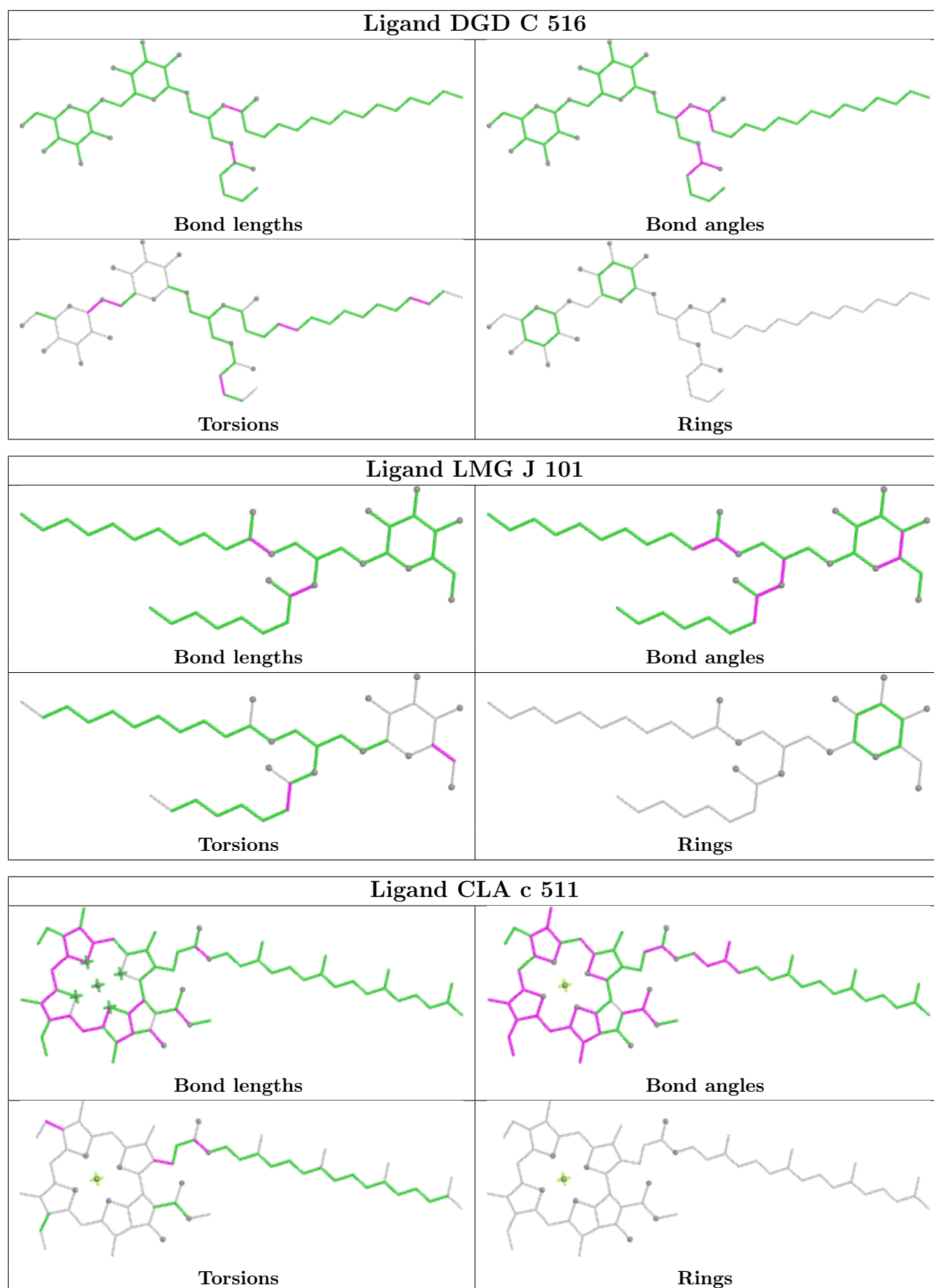




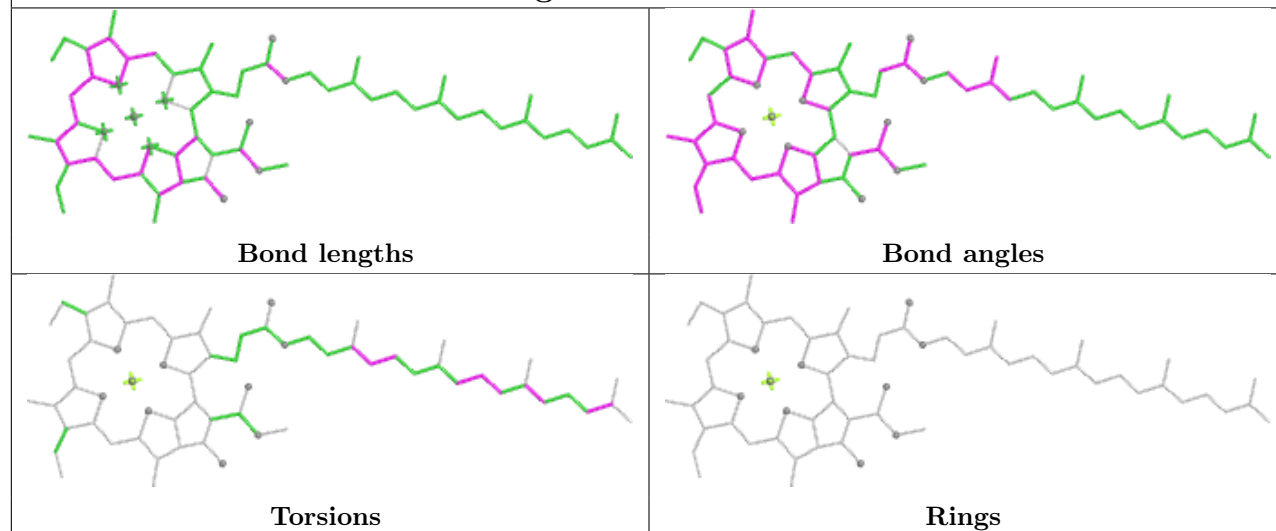




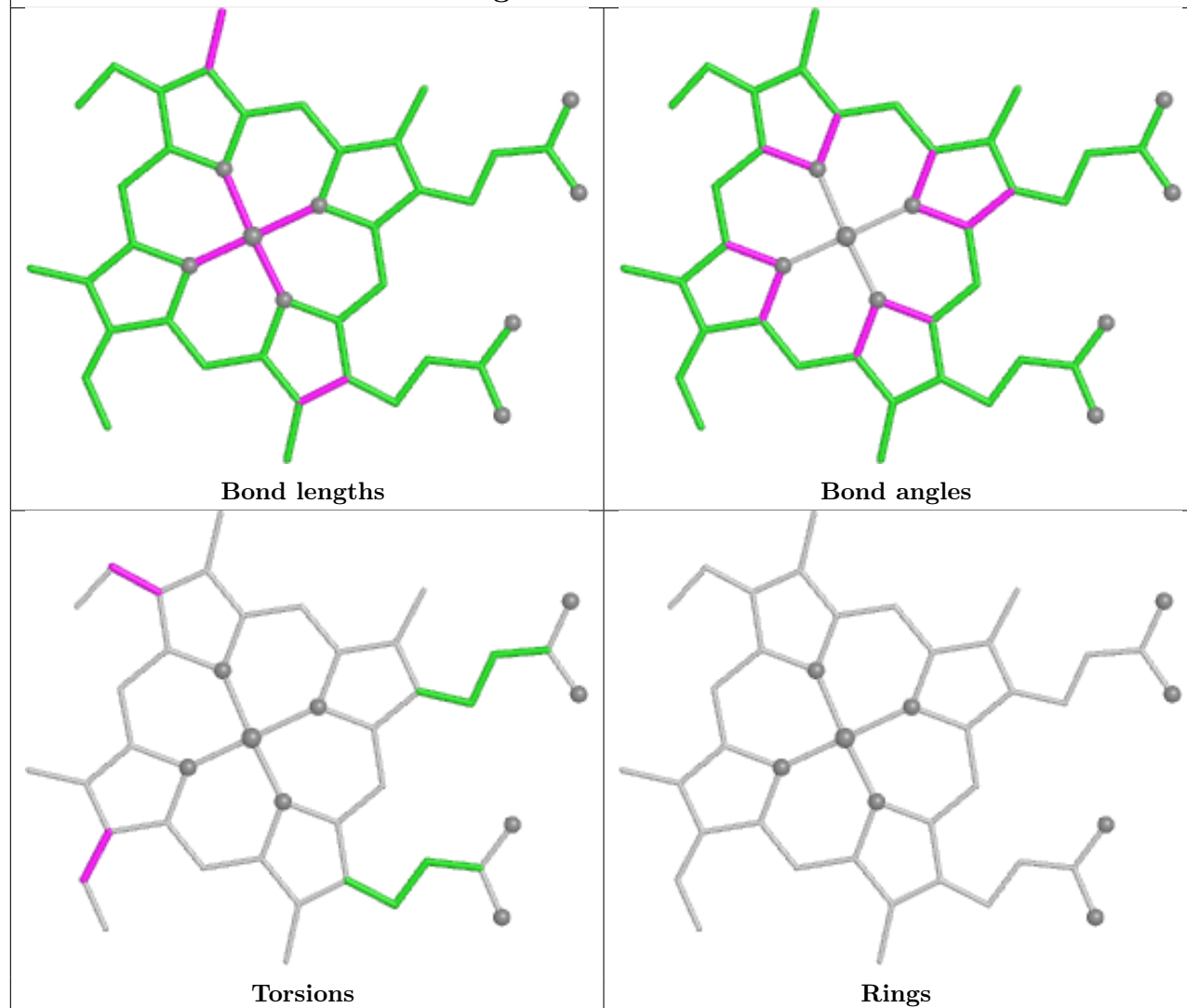


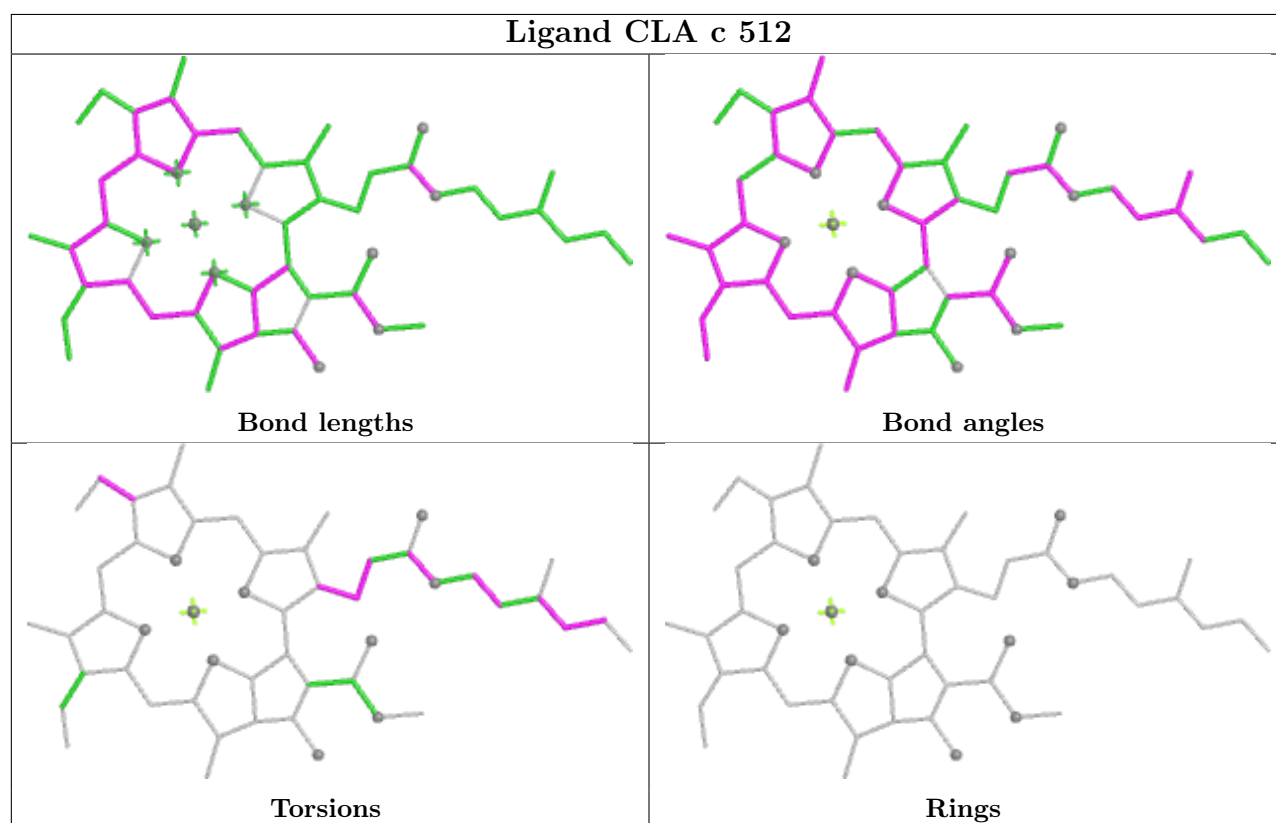
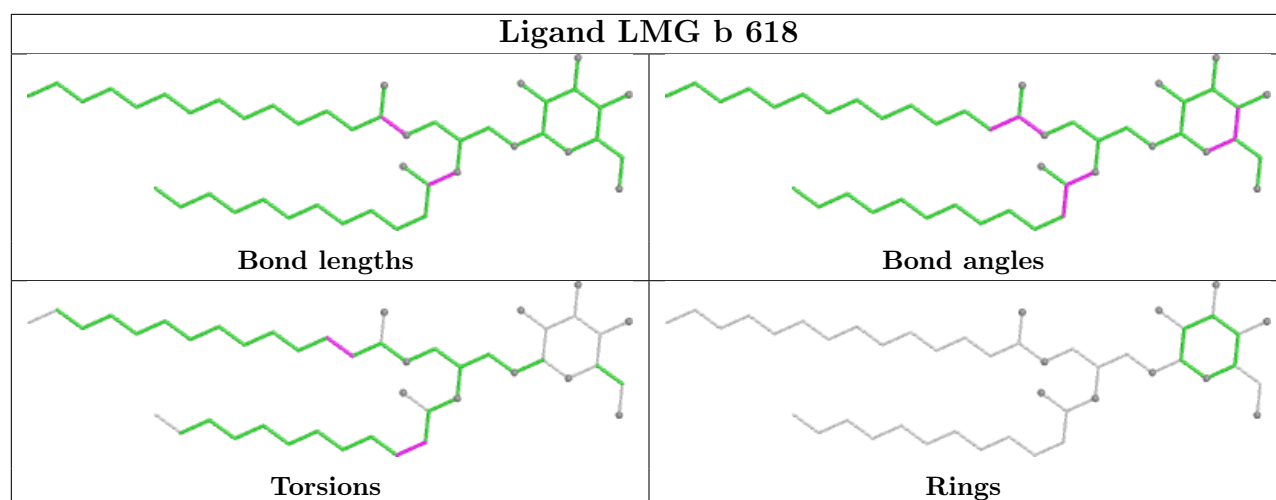


Ligand CLA b 614

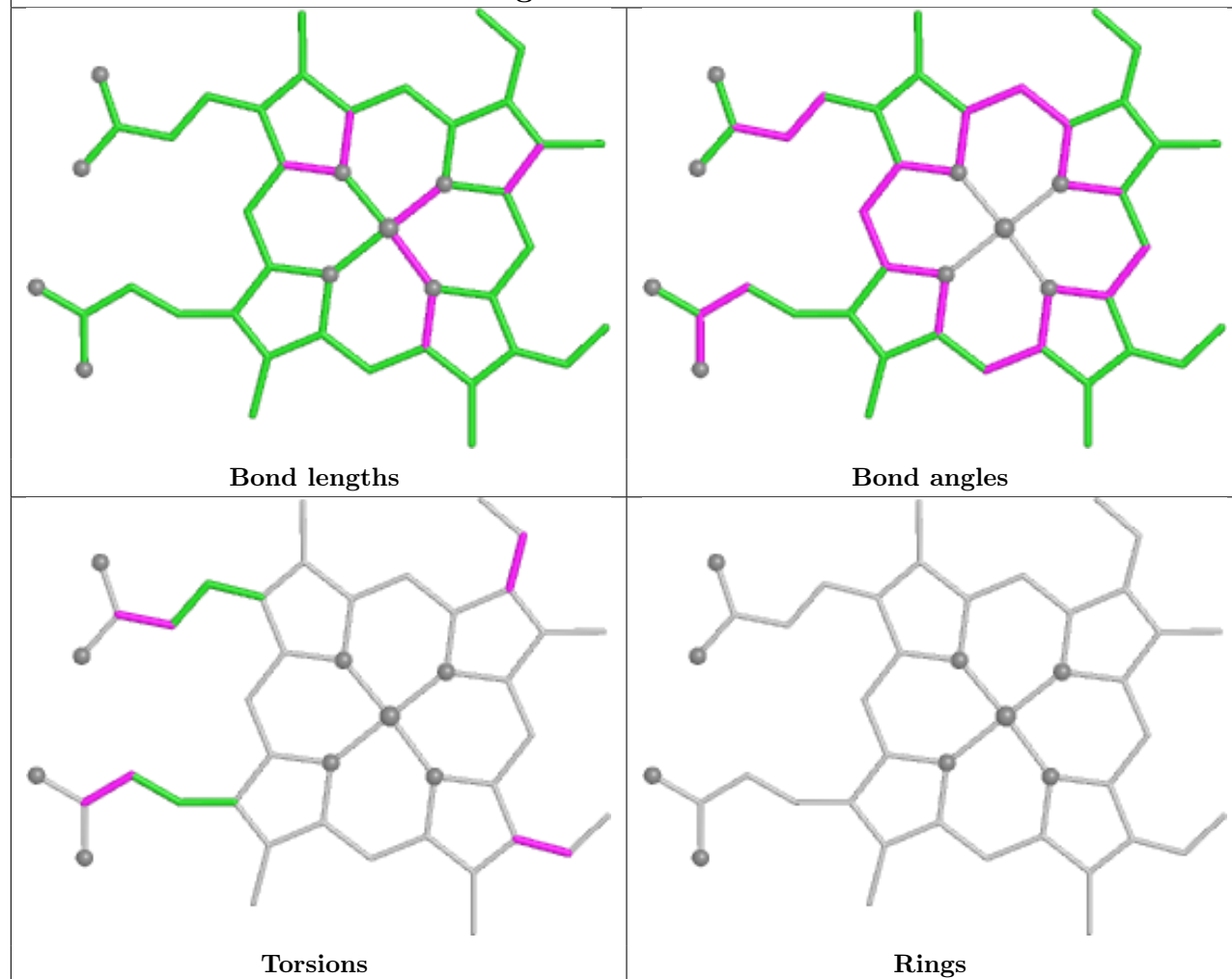


Ligand HEC V 201

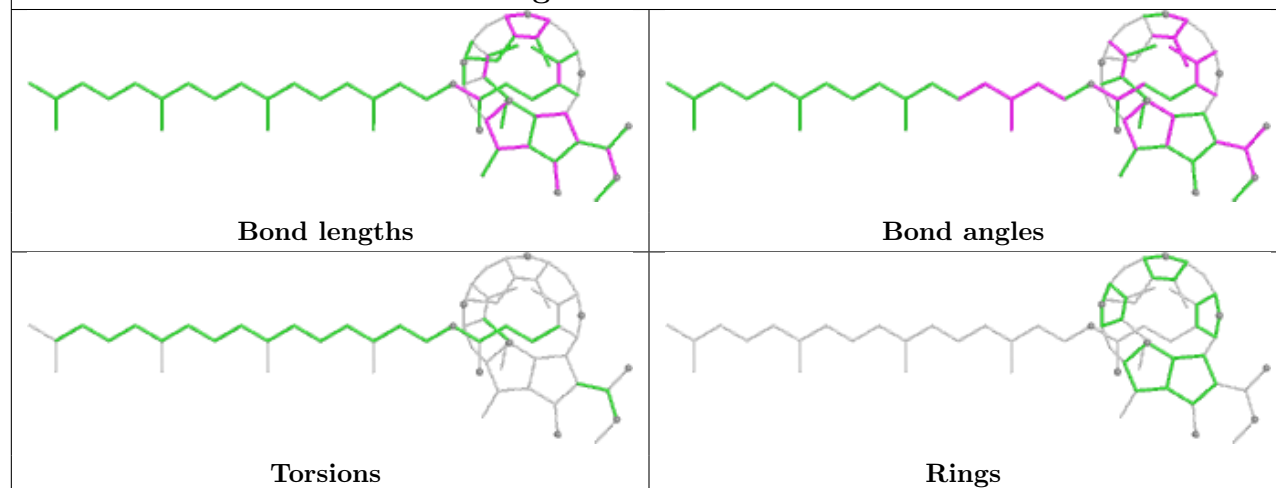


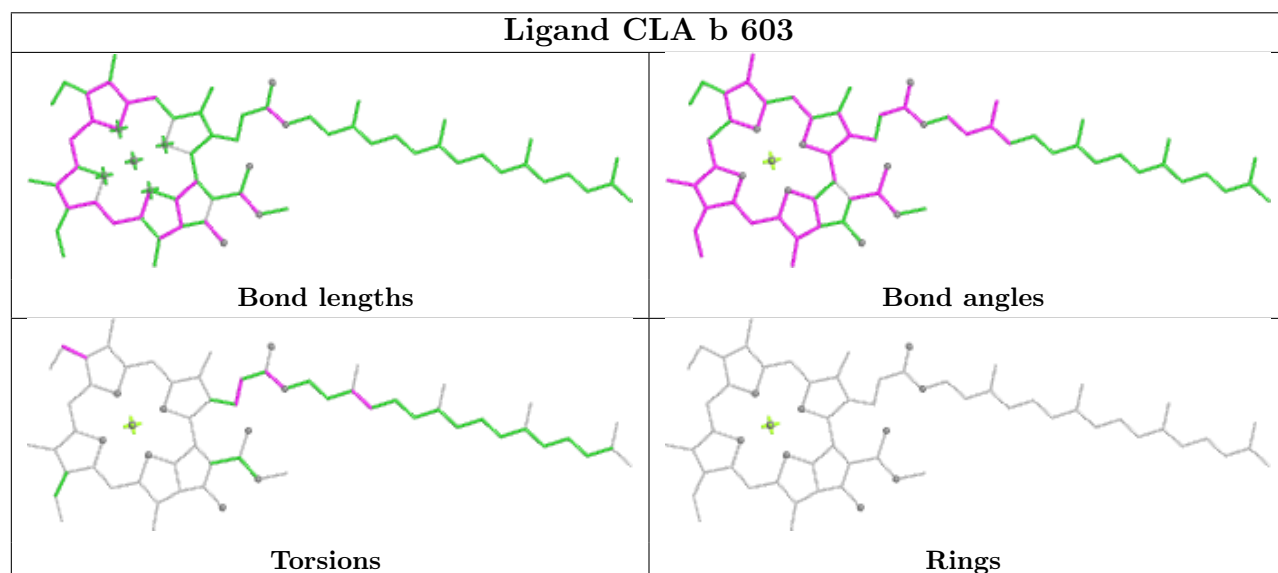
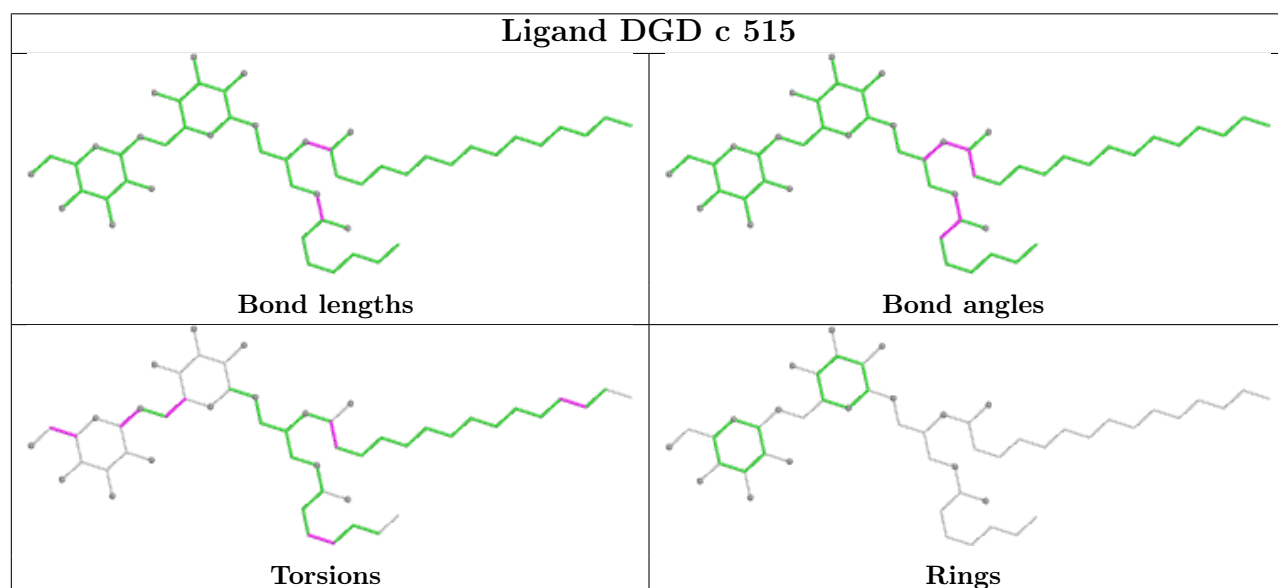
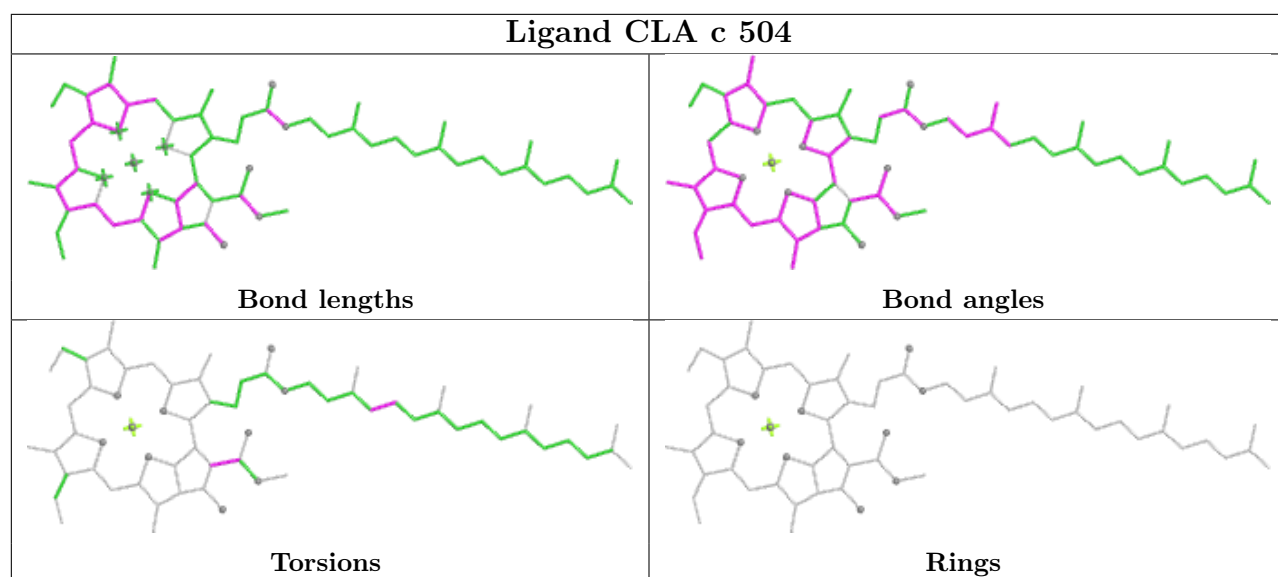


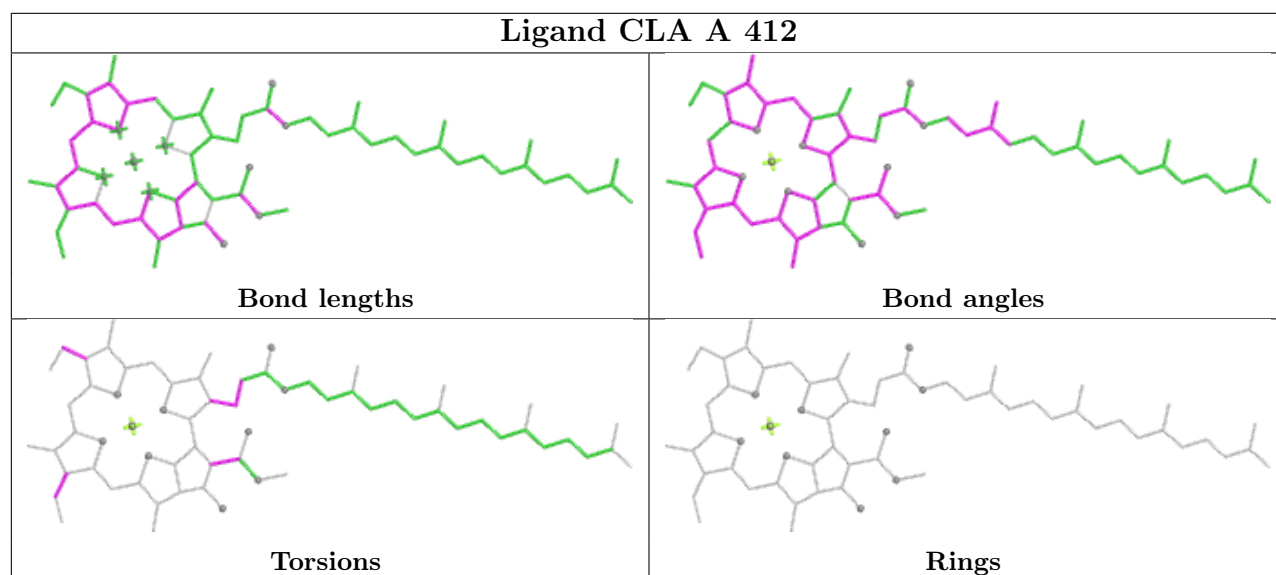
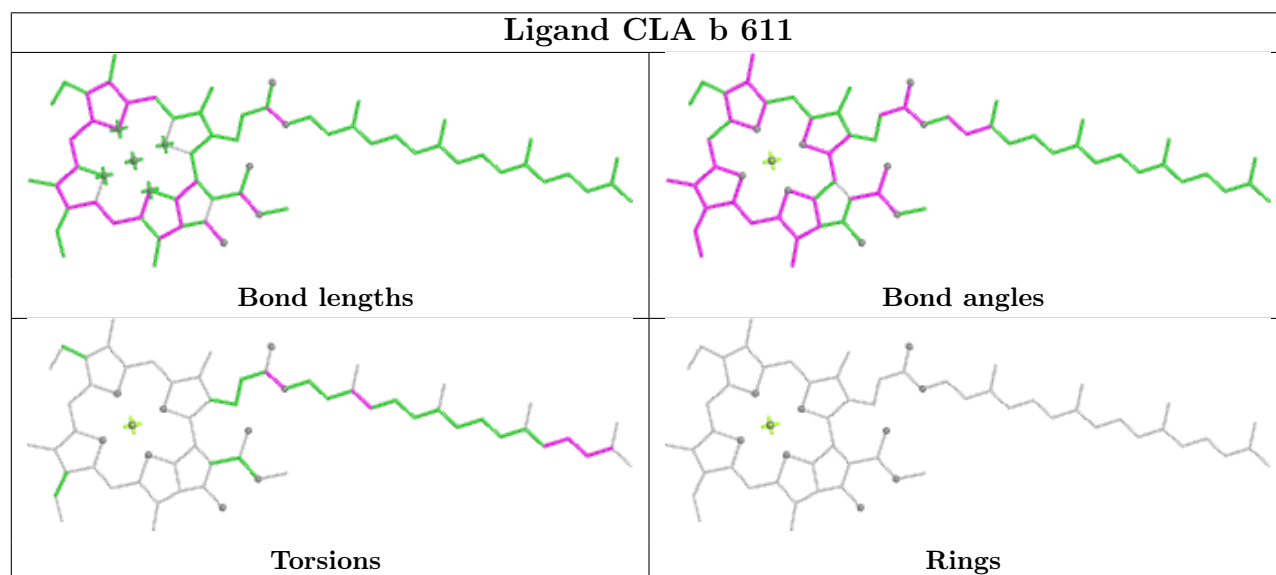
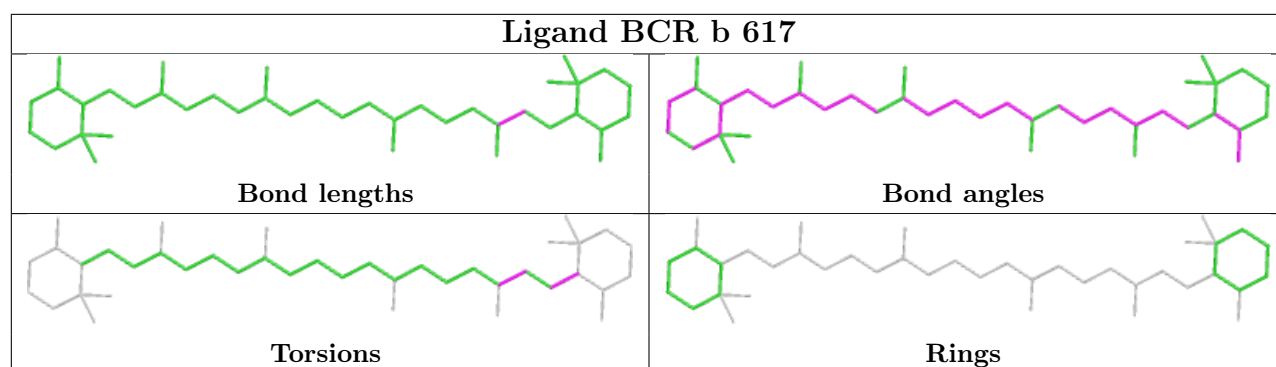
Ligand HEM f 102

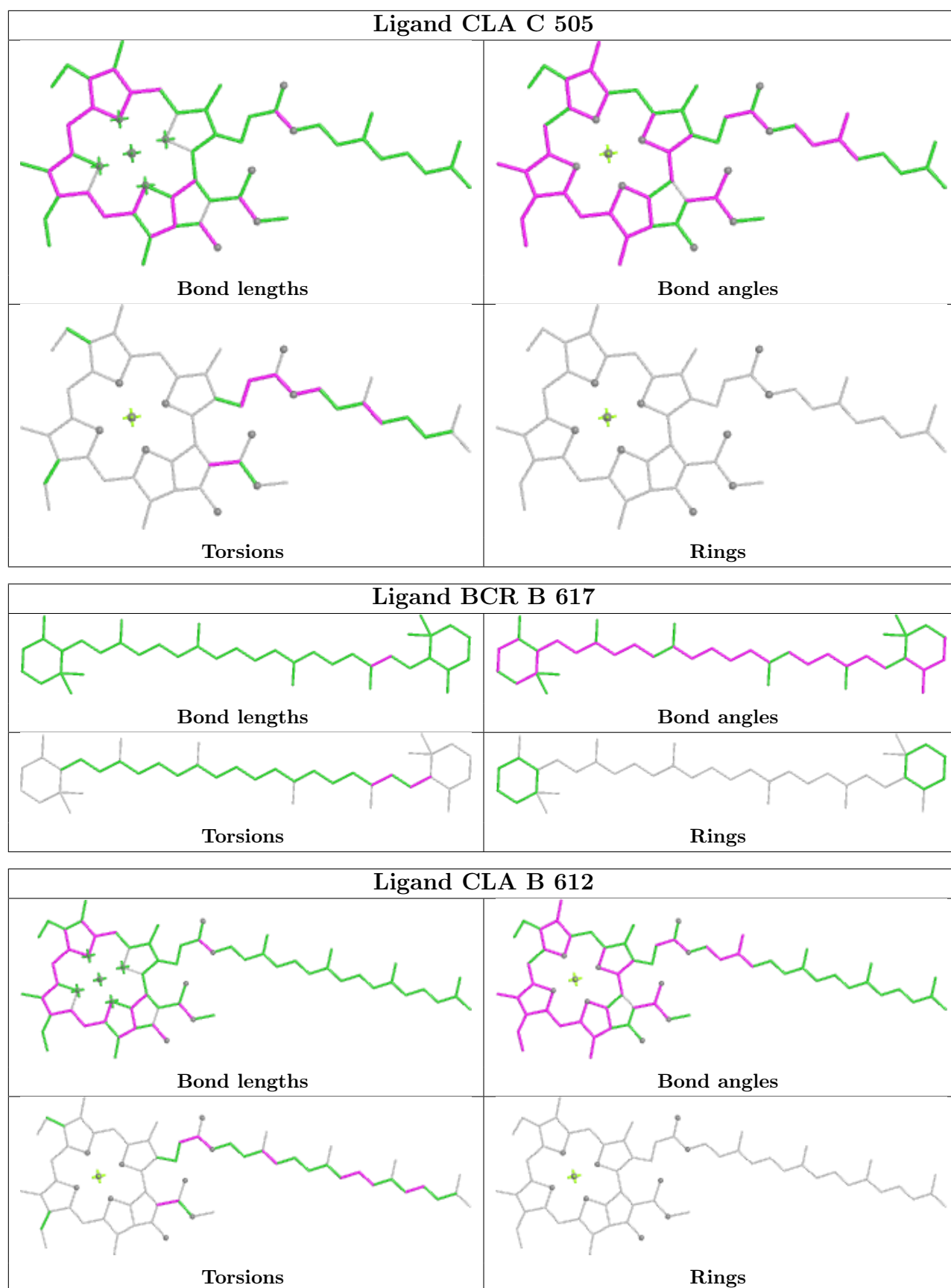


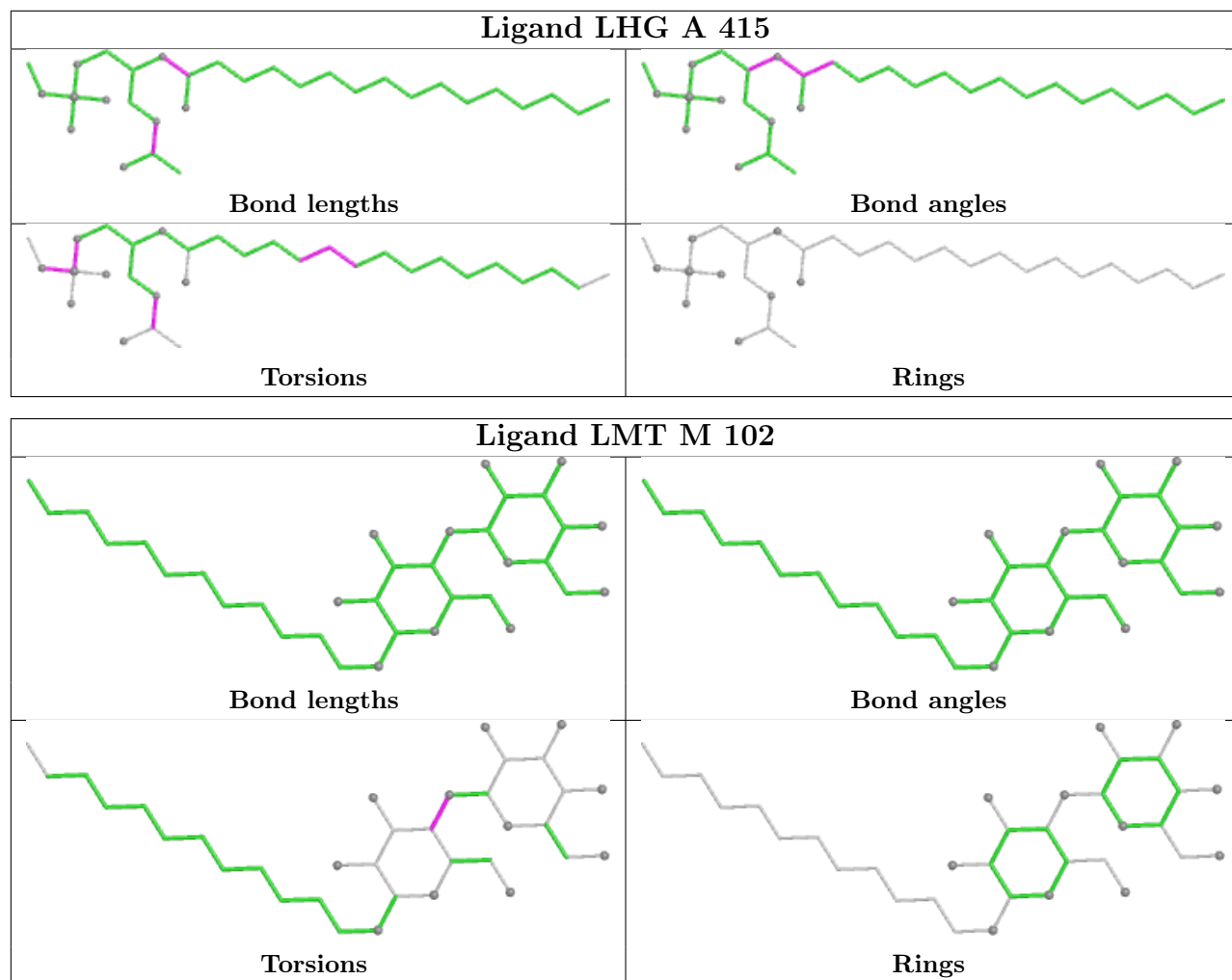
Ligand PHO d 402

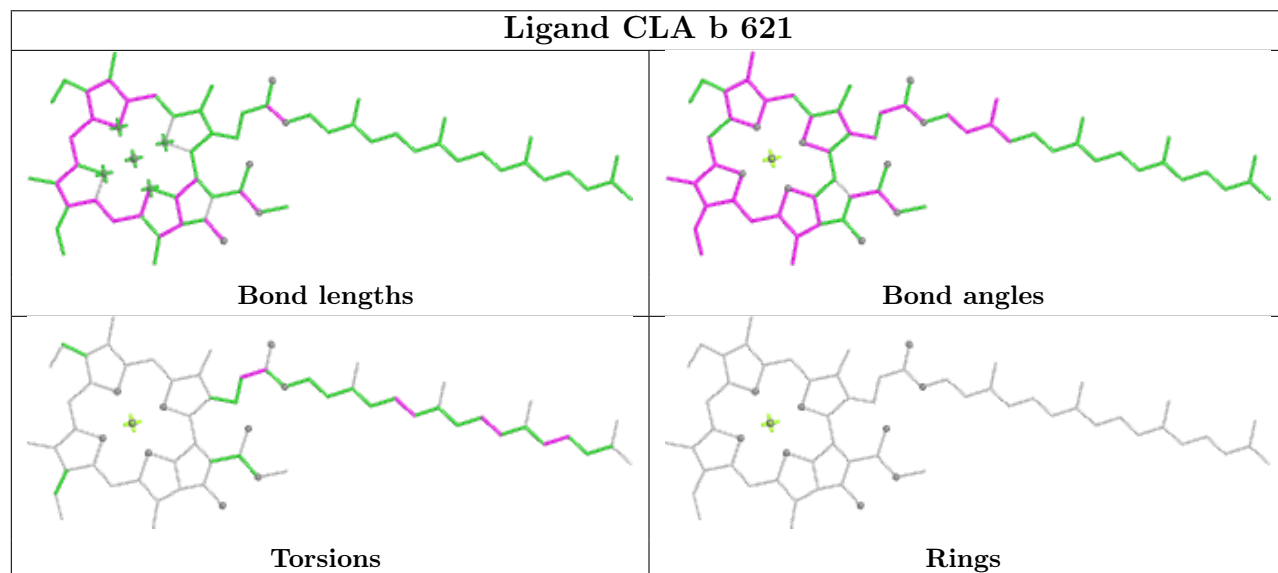
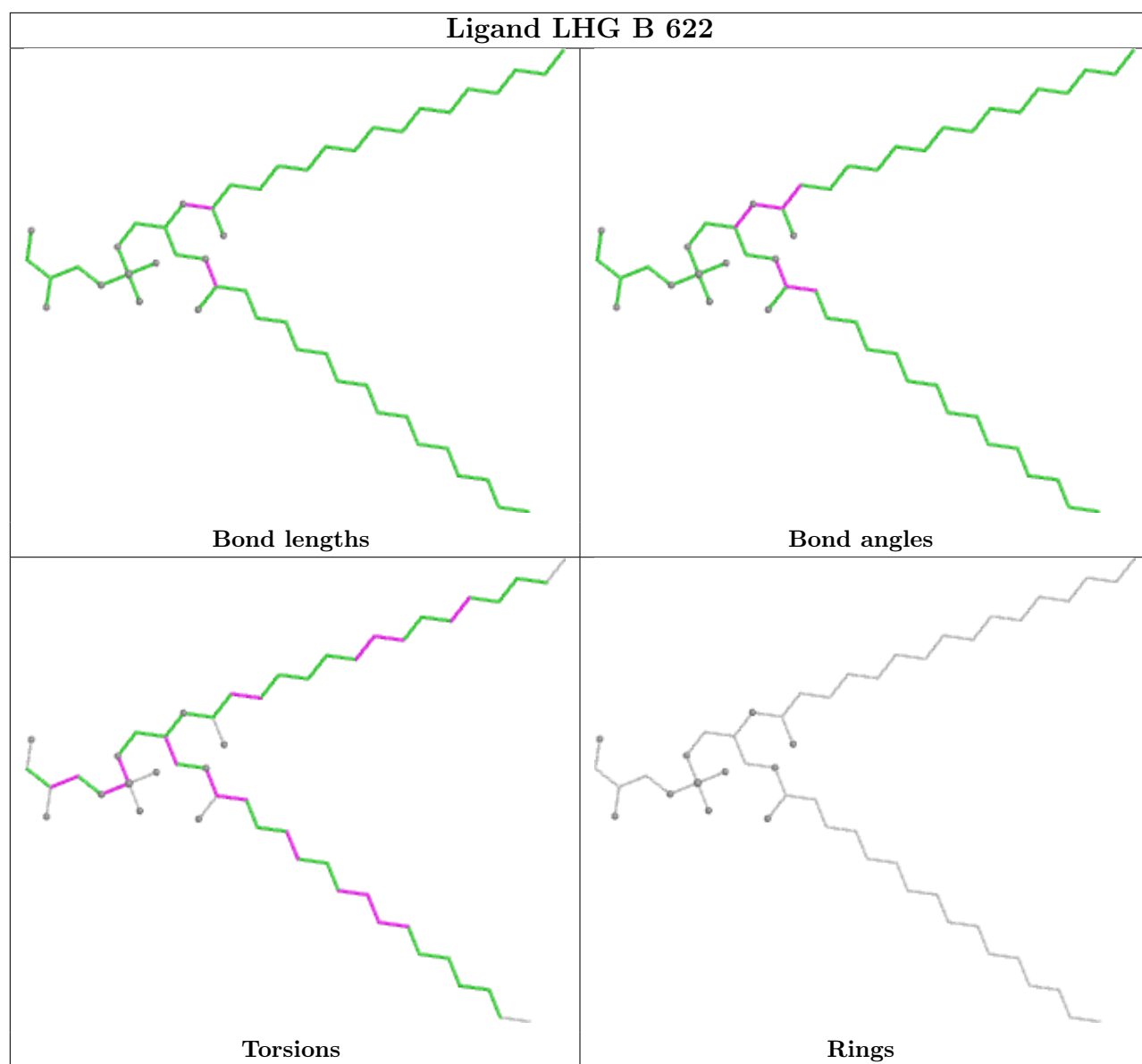


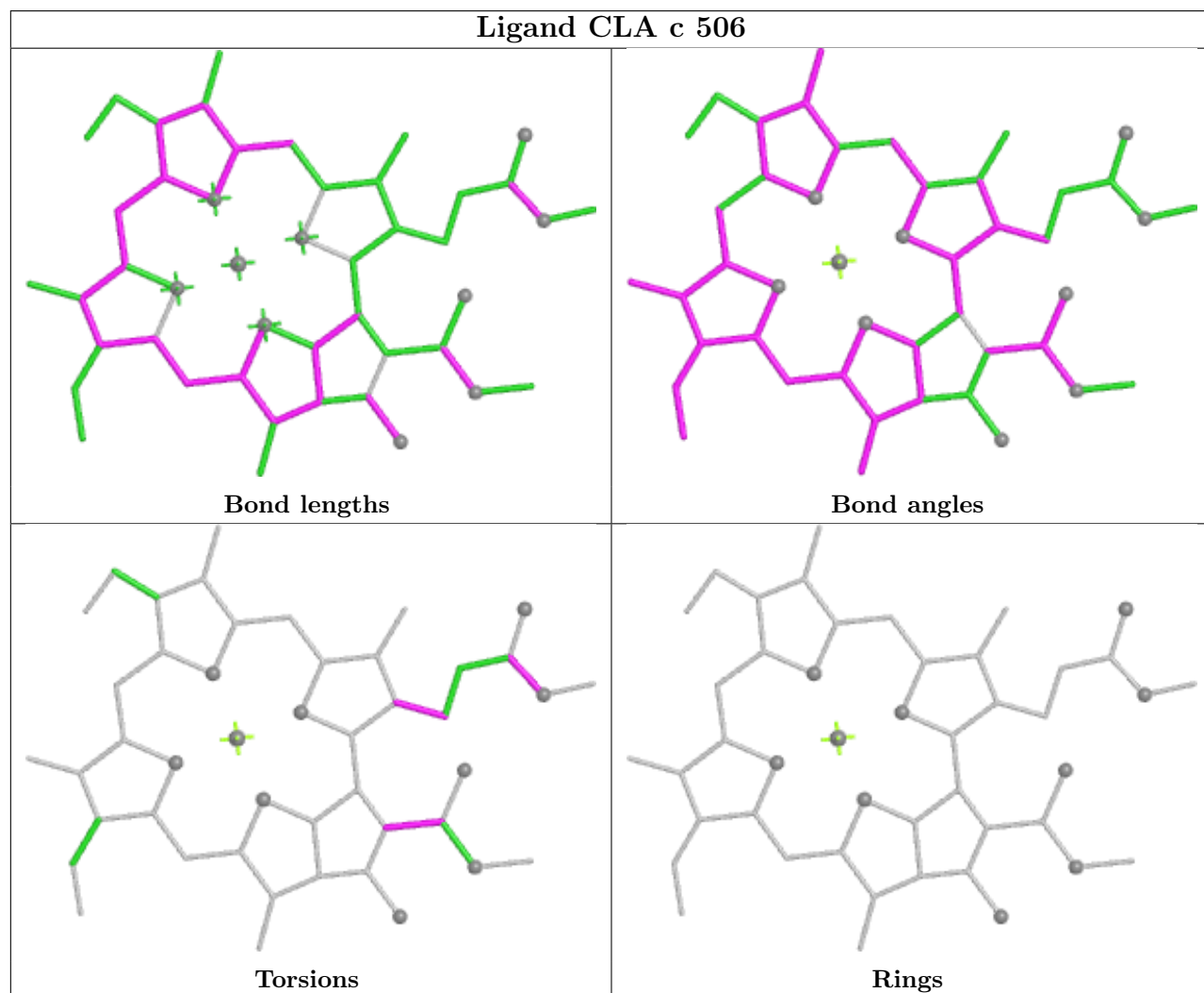
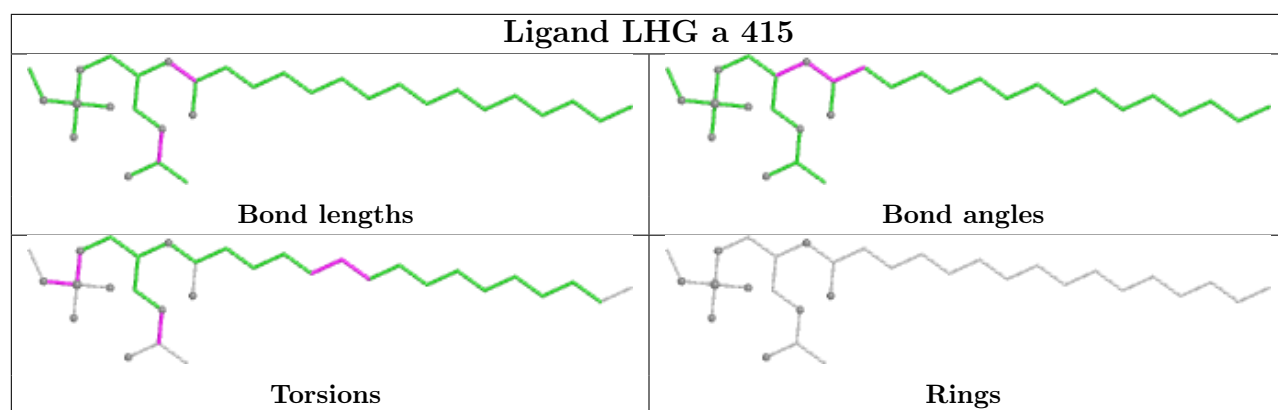


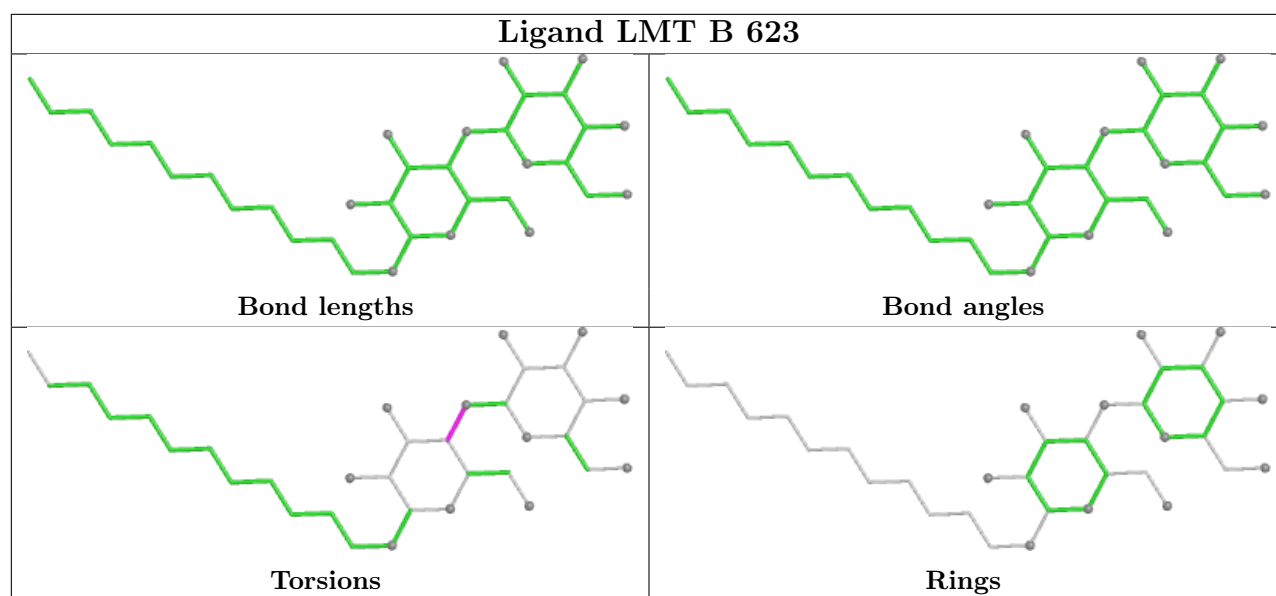












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

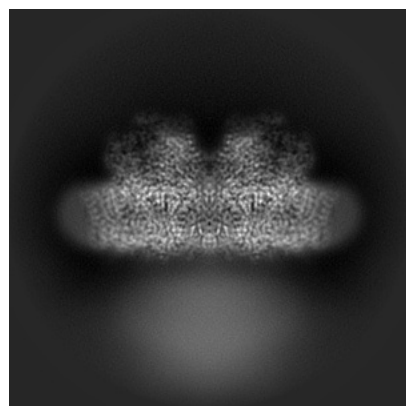
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65652. These allow visual inspection of the internal detail of the map and identification of artifacts.

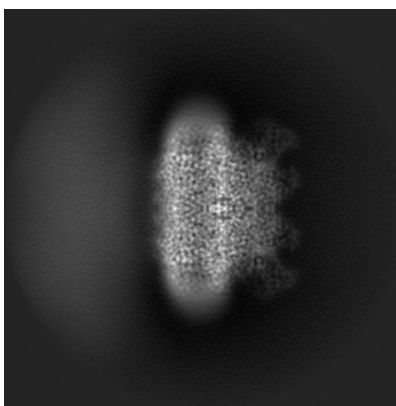
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

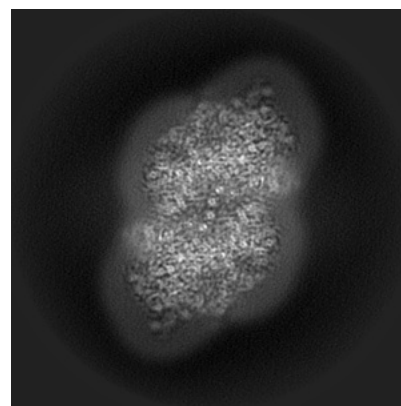
6.1.1 Primary map



X

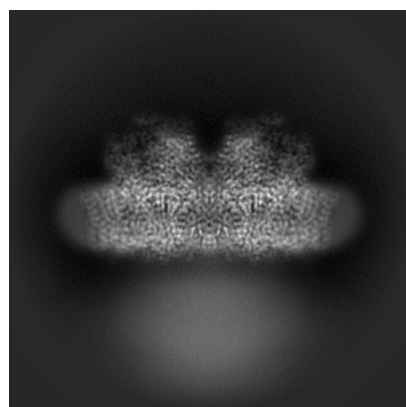


Y

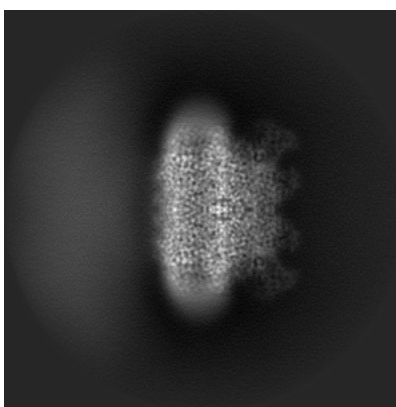


Z

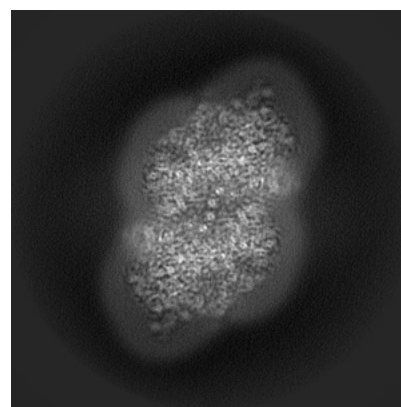
6.1.2 Raw map



X



Y

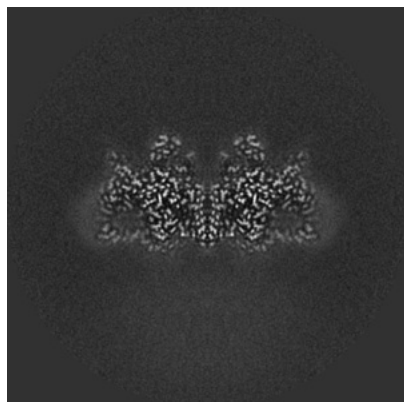


Z

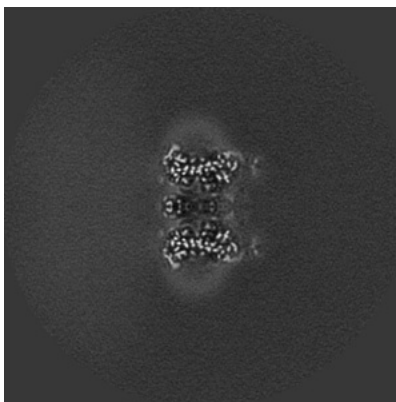
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

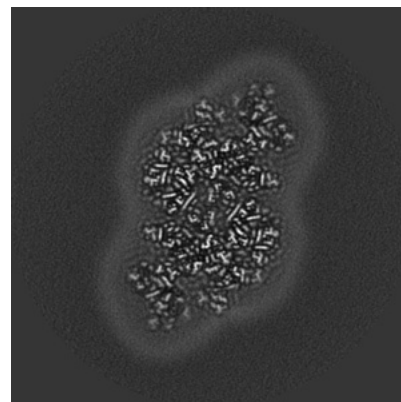
6.2.1 Primary map



X Index: 256

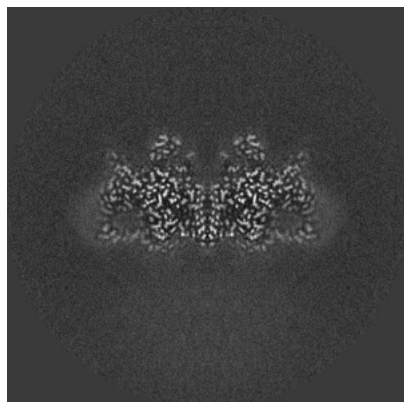


Y Index: 256

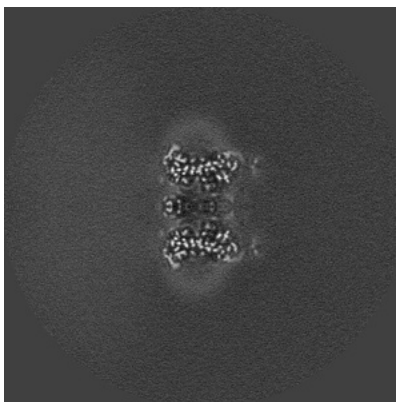


Z Index: 256

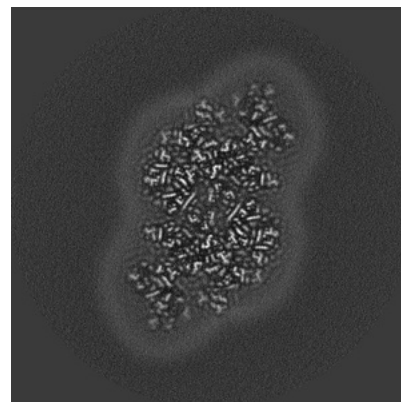
6.2.2 Raw map



X Index: 256



Y Index: 256

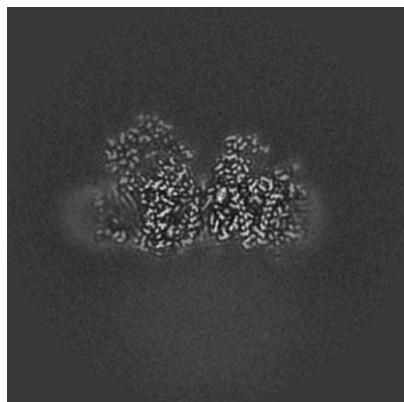


Z Index: 256

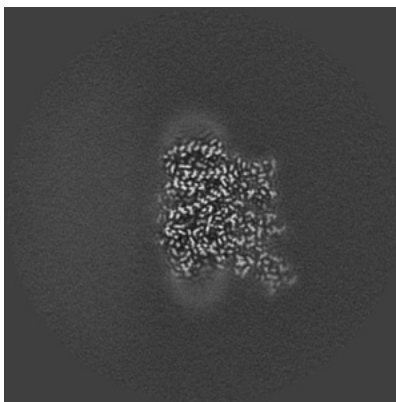
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

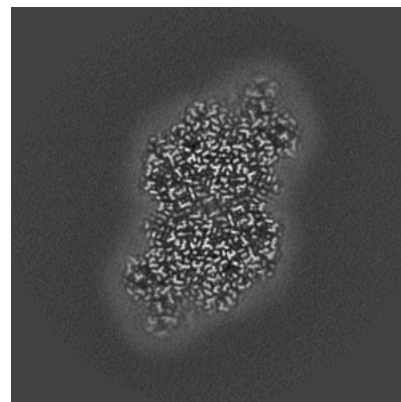
6.3.1 Primary map



X Index: 230

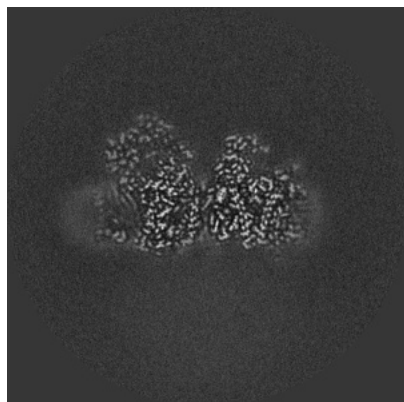


Y Index: 209

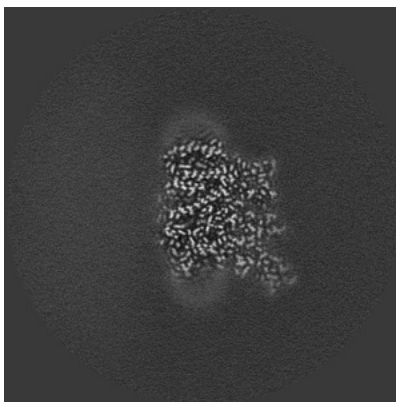


Z Index: 275

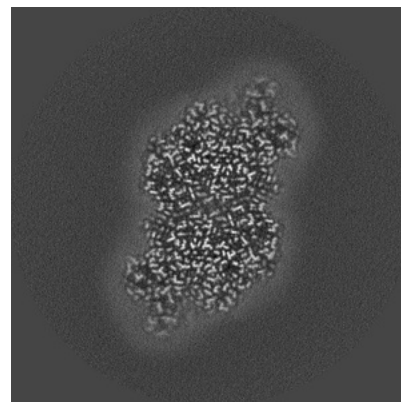
6.3.2 Raw map



X Index: 230



Y Index: 209

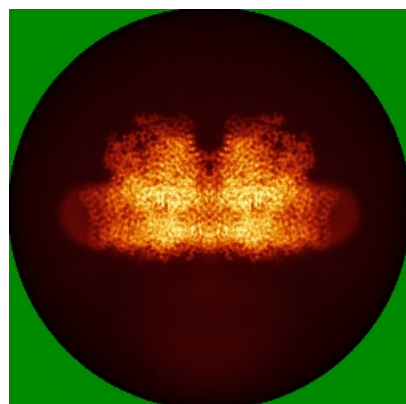


Z Index: 275

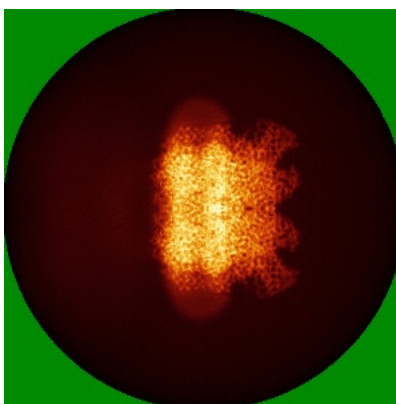
The images above show the largest variance slices of the map in three orthogonal directions.

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

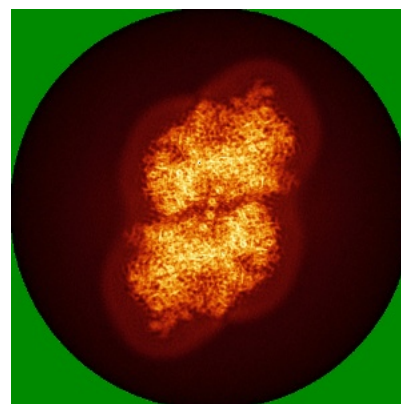
6.4.1 Primary map



X

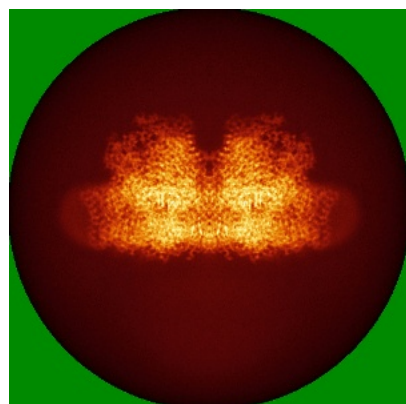


Y

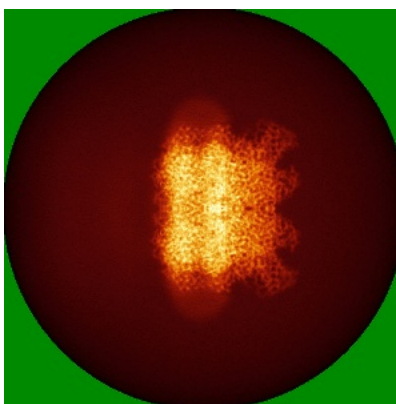


Z

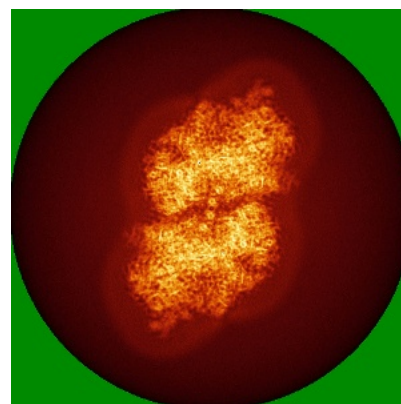
6.4.2 Raw map



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.

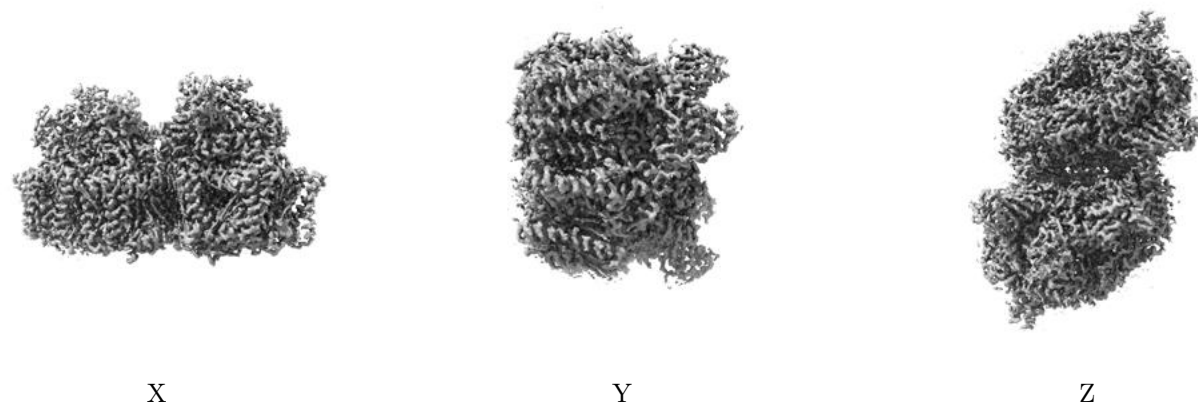
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

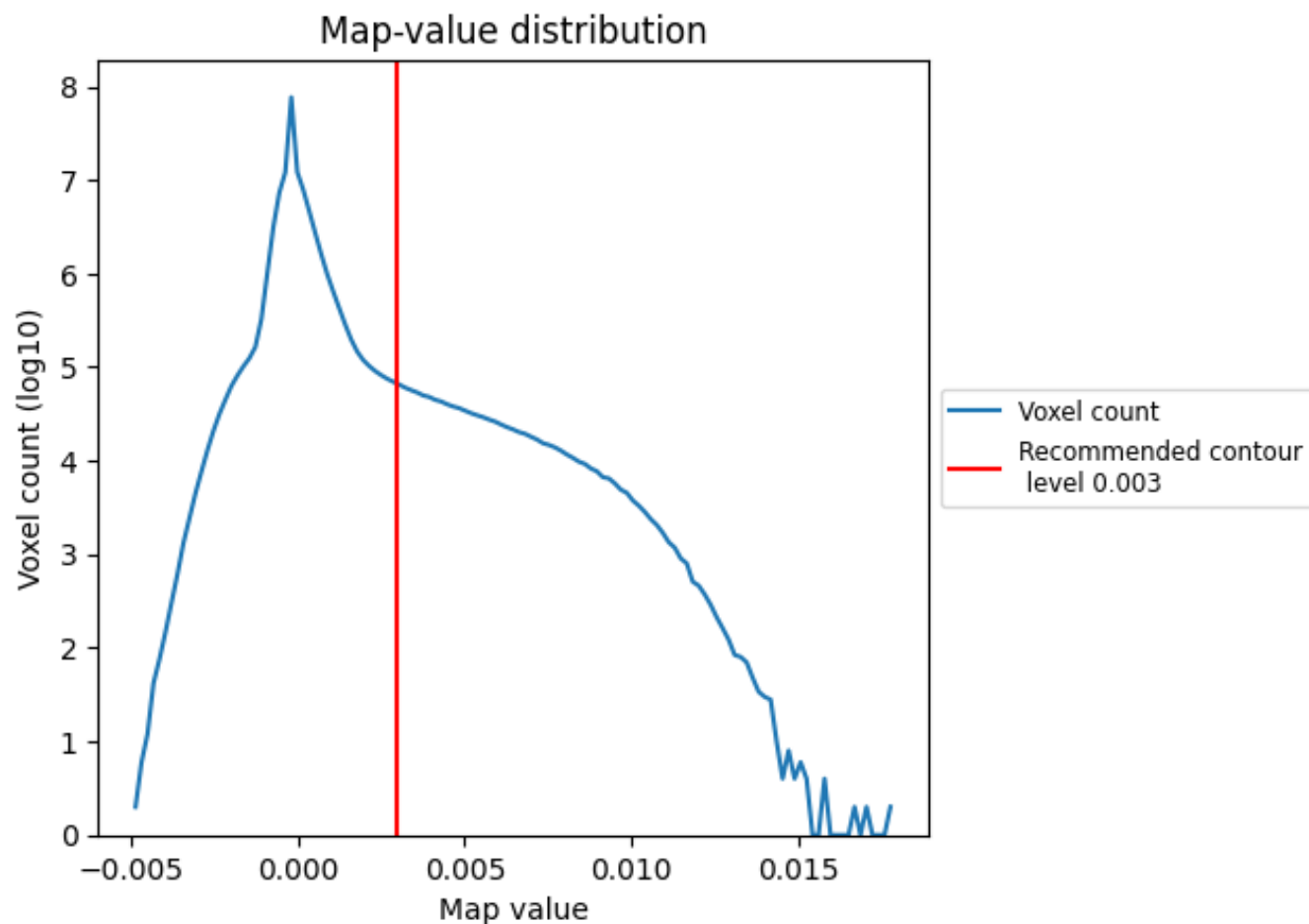
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

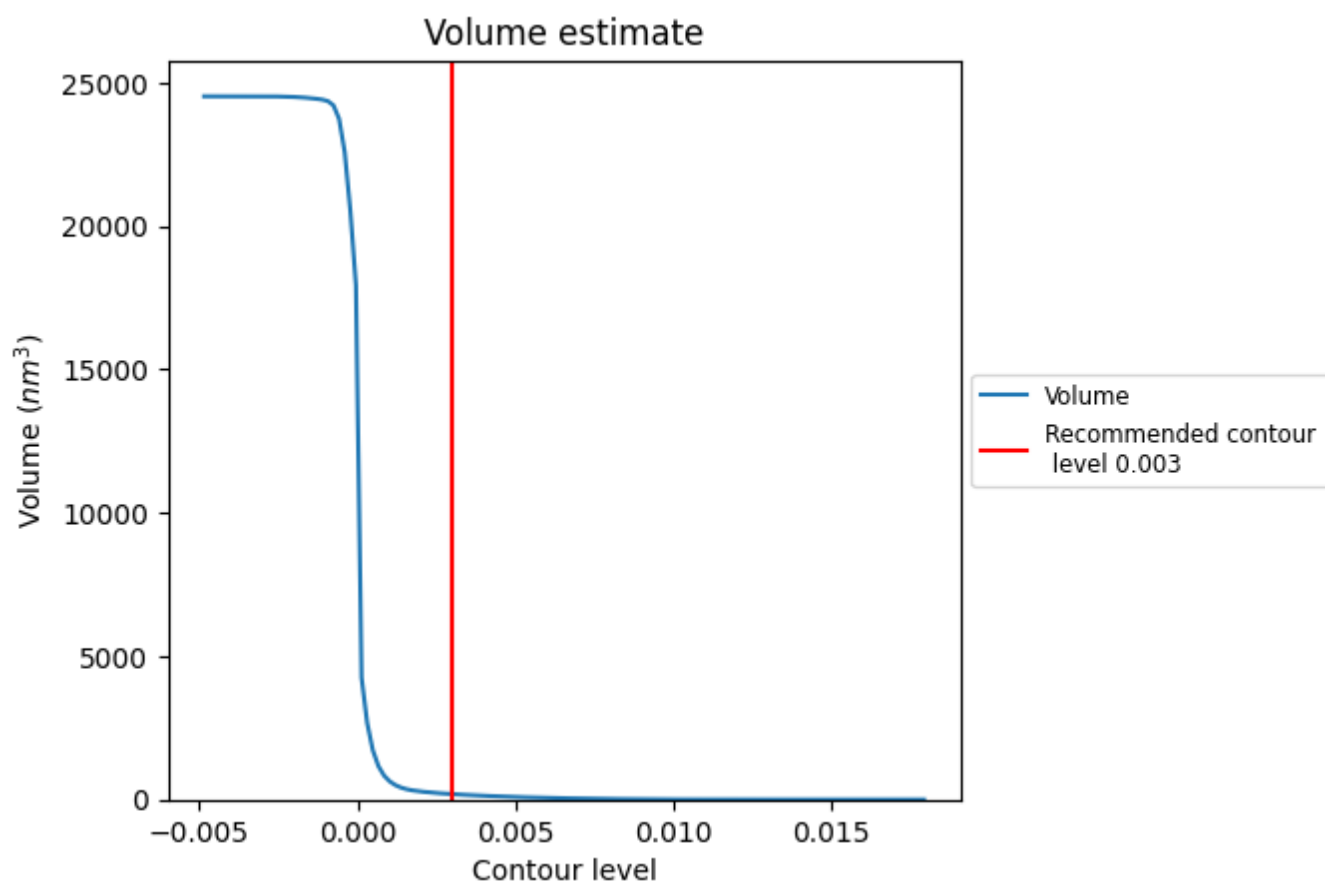
This section contains the results of statistical analysis of the map.

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.

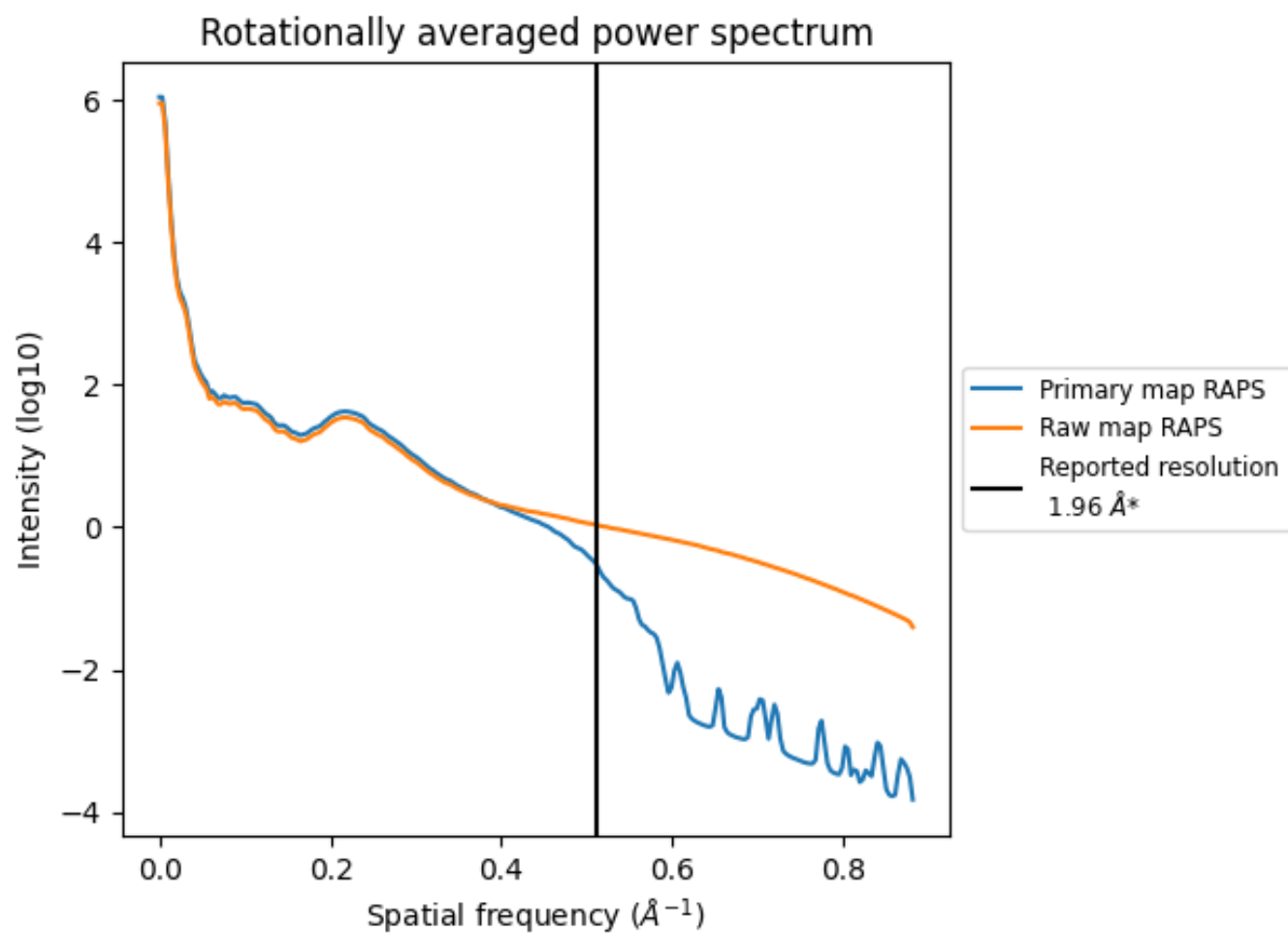
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 172 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 ⓘ

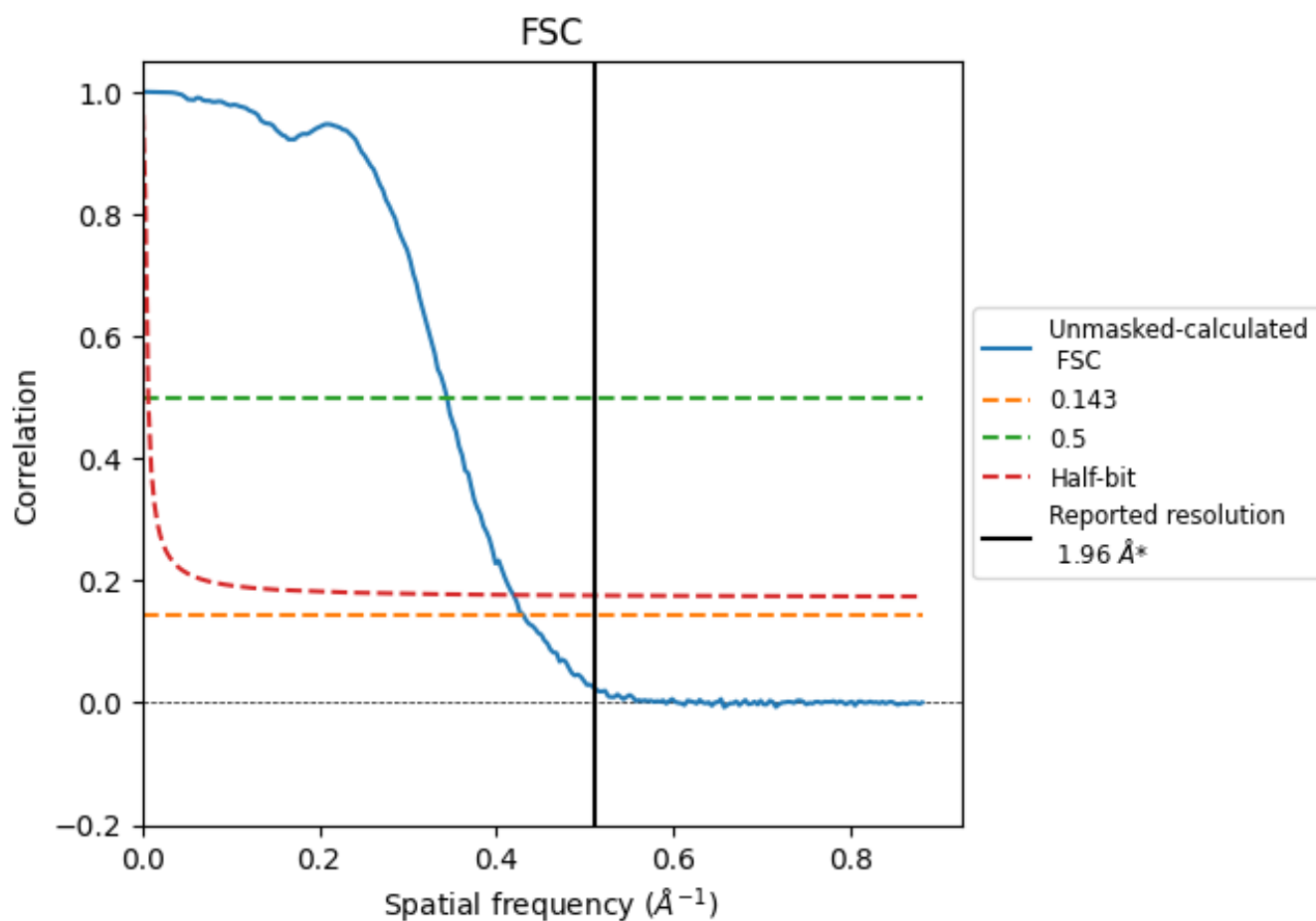


*Reported resolution corresponds to spatial frequency of 0.510 Å⁻¹

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 0.510 Å⁻¹

8.2 Resolution estimates [i](#)

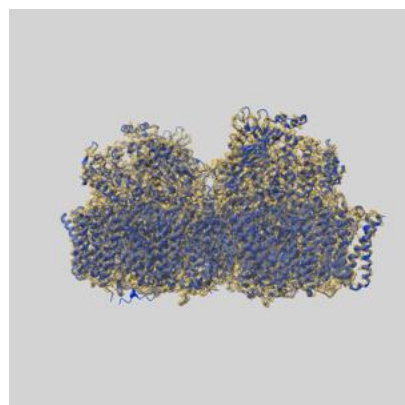
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.32	2.91	2.38

*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 2.32 differs from the reported value 1.96 by more than 10 %

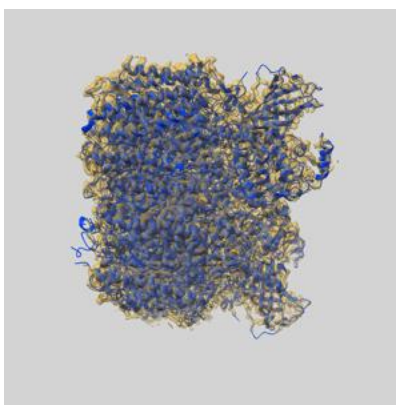
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65652 and PDB model 9W5B. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

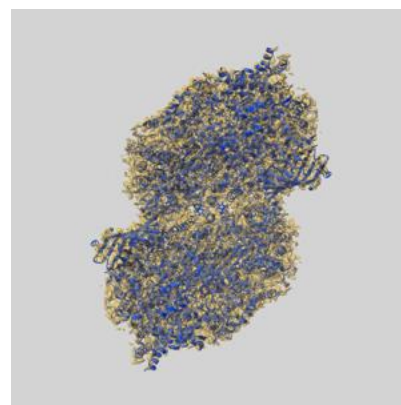
9.1 Map-model overlay [i](#)



X



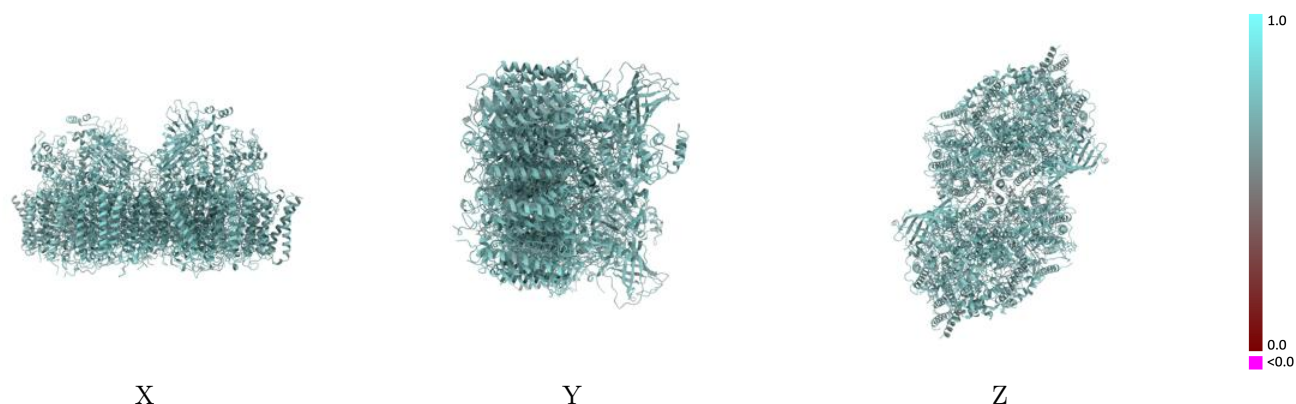
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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](#)



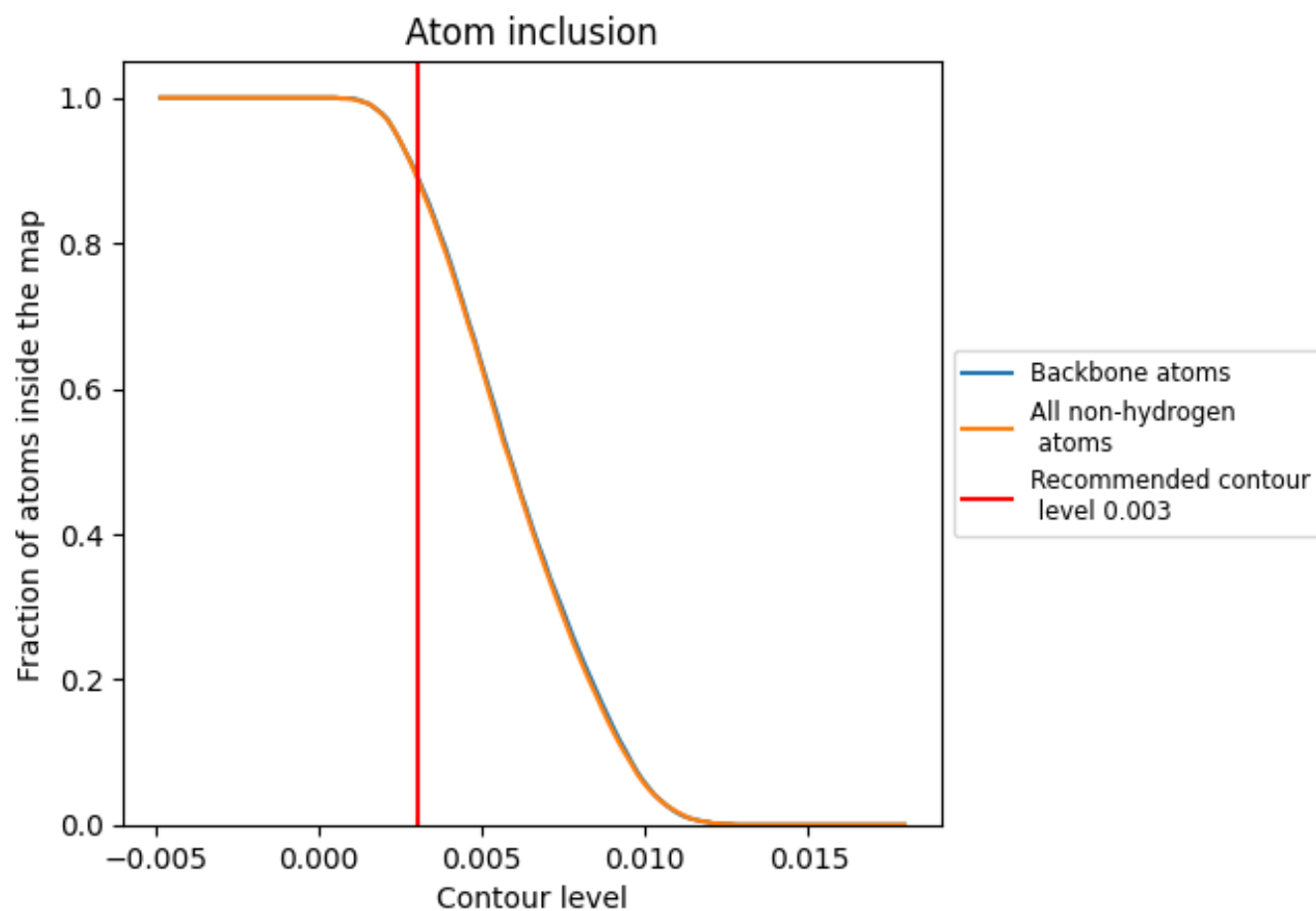
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.7110
A	 0.9260	 0.7300
B	 0.9260	 0.7230
C	 0.9170	 0.7020
D	 0.9650	 0.7370
E	 0.8250	 0.6820
F	 0.8310	 0.6800
H	 0.9480	 0.7110
I	 0.9320	 0.6960
J	 0.7870	 0.6860
K	 0.8540	 0.6750
L	 0.9230	 0.7380
M	 0.8440	 0.6980
O	 0.8020	 0.6910
T	 0.9390	 0.7370
U	 0.7170	 0.6950
V	 0.7730	 0.6860
X	 0.8420	 0.6920
Y	 0.6550	 0.6500
Z	 0.6520	 0.6290
a	 0.9260	 0.7300
b	 0.9300	 0.7240
c	 0.9170	 0.7020
d	 0.9650	 0.7360
e	 0.8250	 0.6820
f	 0.8310	 0.6760
h	 0.9480	 0.7090
i	 0.9320	 0.7010
j	 0.7870	 0.6870
k	 0.8540	 0.6820
l	 0.9230	 0.7380
m	 0.9130	 0.7210
o	 0.8020	 0.6910
t	 0.9390	 0.7350
u	 0.7160	 0.6930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
v	 0.7730	 0.6860
x	 0.8420	 0.6910
y	 0.6550	 0.6480
z	 0.6520	 0.6290