



# wwPDB EM Validation Summary Report ⓘ

Jun 30, 2026 – 01:40 PM JST

PDB ID : 9M5A / pdb\_00009m5a  
EMDB ID : EMD-63639  
Title : cryo-EM structure of PSII D1-V185T from *Thermosynechococcus vestitus* BP-1  
Authors : Jiang, H.W.; Nakajima, Y.; Akita, F.; Li, H.J.; Kato, K.; Sugiura, M.; Shen, J.R.  
Deposited on : 2025-03-05  
Resolution : 1.88 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

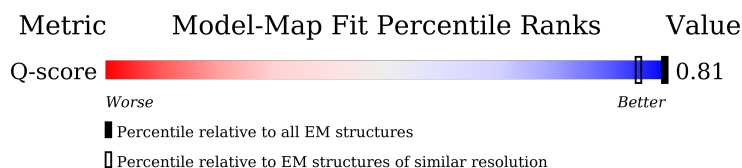
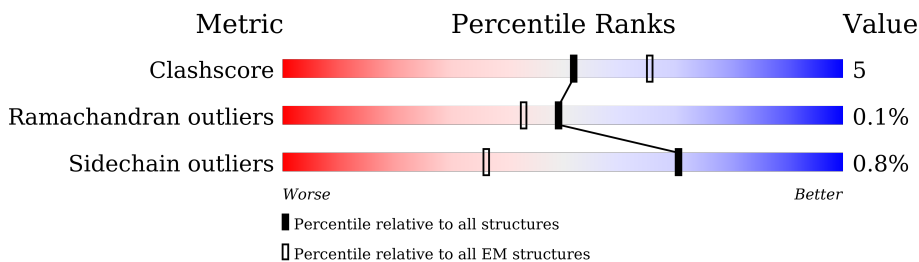
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.88 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.






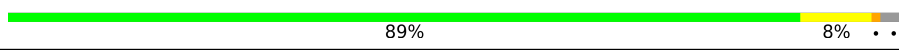
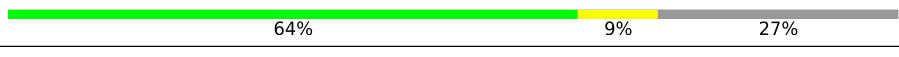

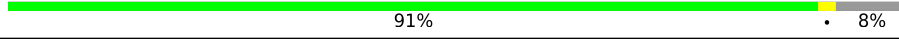
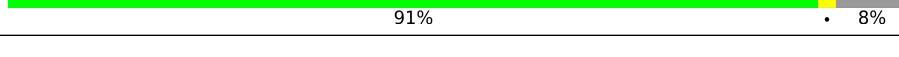
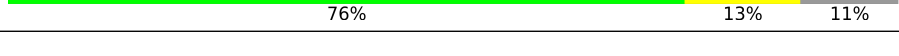
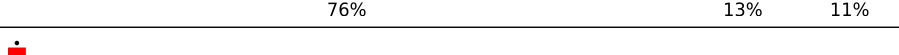
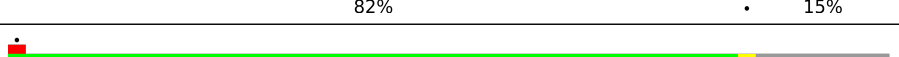
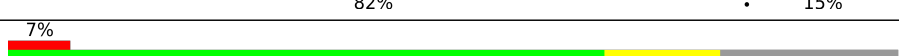

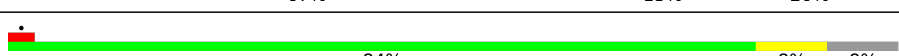
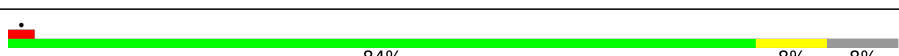
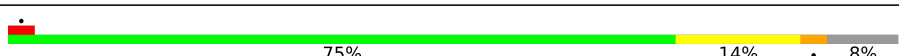





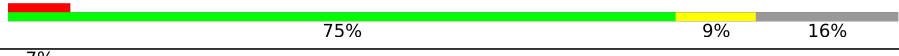

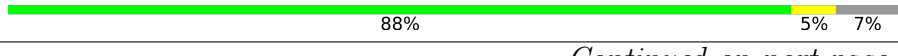

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1004 ( 1.39 - 2.38 )

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  $\geq 3$ , 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	83% 9% 7%
1	a	360	84% 9% 7%
2	B	510	87% 12% .
2	b	510	87% 12% .




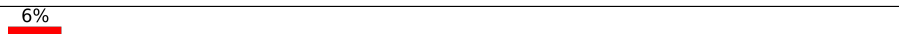
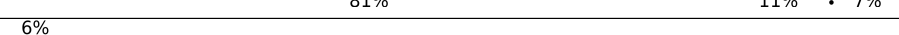




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Mol	Chain	Length	Quality of chain
3	C	461	 89% 8%
3	c	461	 89% 8%
4	D	352	 88% 8%
4	d	352	 89% 8%
5	F	45	 64% 9% 27%
5	f	45	 64% 9% 27%
6	H	66	 91% 8%
6	h	66	 91% 8%
7	I	38	 76% 13% 11%
7	i	38	 76% 13% 11%
8	J	40	 82% 15%
8	j	40	 82% 15%
9	K	46	 7% 67% 13% 20%
9	k	46	 9% 67% 13% 20%
10	L	37	 84% 8% 8%
10	l	37	 84% 8% 8%
11	M	36	 75% 14% 8%
11	m	36	 72% 17% 8%
12	T	32	 88% 9%
12	t	32	 88% 9%
13	U	134	 11% 66% 6% 28%
13	u	134	 11% 66% 5% 28%
14	V	163	 7% 75% 9% 16%
14	v	163	 7% 75% 9% 16%
15	X	41	 88% 5% 7%

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Mol	Chain	Length	Quality of chain
15	x	41	
16	Y	46	
16	y	46	
17	E	84	
17	e	84	
18	O	272	
18	o	272	
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
29	UNL	d	413	-	-	X	-

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 50208 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
			Total	C	N	O	S		
1	A	334	2625	1723	431	457	14	5	1
1	a	334	2625	1723	431	457	14	5	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	THR	VAL	conflict	UNP Q8DIV4
a	185	THR	VAL	conflict	UNP Q8DIV4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	504	3896	2571	646	666	13	1	0
2	b	504	3896	2571	646	666	13	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	450	3451	2264	576	598	13	2	1
3	c	450	3451	2264	576	598	13	2	1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	341	2700	1793	439	456	12	2	1

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	341	2700	1793	439	456	12	2	1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	33	269	184	44	40	1	0	0
5	f	33	269	184	44	40	1	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	61	474	319	73	80	2	0	0
6	h	61	474	319	73	80	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	34	265	182	39	43	1	0	0
7	i	34	265	182	39	43	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	34	243	167	35	40	1	0	0
8	j	34	243	167	35	40	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	K	37	285	199	42	44	0	0
9	k	37	285	199	42	44	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	34	Total	C	N	O	1	0
			278	189	42	47		
10	l	34	Total	C	N	O	1	0
			278	189	42	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	33	Total	C	N	O	S	0	0
			249	168	36	44	1		
11	m	33	Total	C	N	O	S	0	0
			249	168	36	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	29	Total	C	N	O	S	0	0
			241	172	32	35	2		
12	t	29	Total	C	N	O	S	0	0
			241	172	32	35	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	U	96	Total	C	N	O	0	0
			718	463	123	132		
13	u	96	Total	C	N	O	0	0
			718	463	123	132		

- Molecule 14 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	137	Total	C	N	O	S	1	0
			1024	654	169	197	4		
14	v	137	Total	C	N	O	S	1	0
			1024	654	169	197	4		

- Molecule 15 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	38	Total	C	N	O	0	1
			269	180	43	46		
15	x	38	Total	C	N	O	0	1
			269	180	43	46		

- Molecule 16 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0
			199	132	31	33	3		
16	y	29	Total	C	N	O	S	0	0
			199	132	31	33	3		

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	E	78	Total	C	N	O	1	0
			610	404	97	109		
17	e	78	Total	C	N	O	1	0
			610	404	97	109		

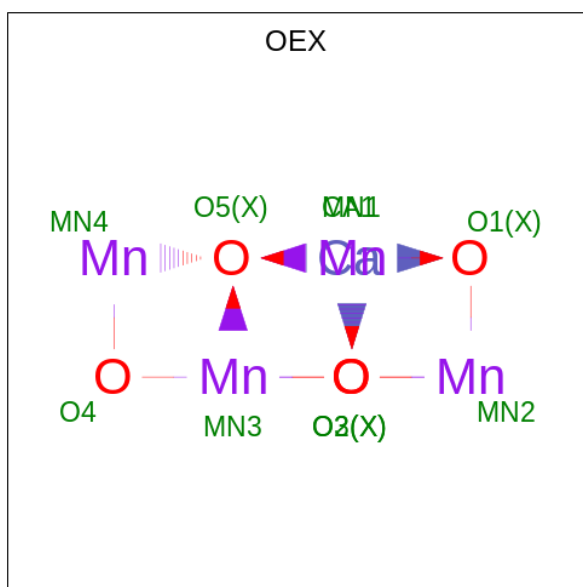
- Molecule 18 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	233	Total	C	N	O	S	3	0
			1676	1066	283	322	5		
18	o	233	Total	C	N	O	S	3	0
			1676	1066	283	322	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	55	Total	C	N	O	S	0	0
			393	270	58	63	2		
19	z	55	Total	C	N	O	S	0	0
			393	270	58	63	2		

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).



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

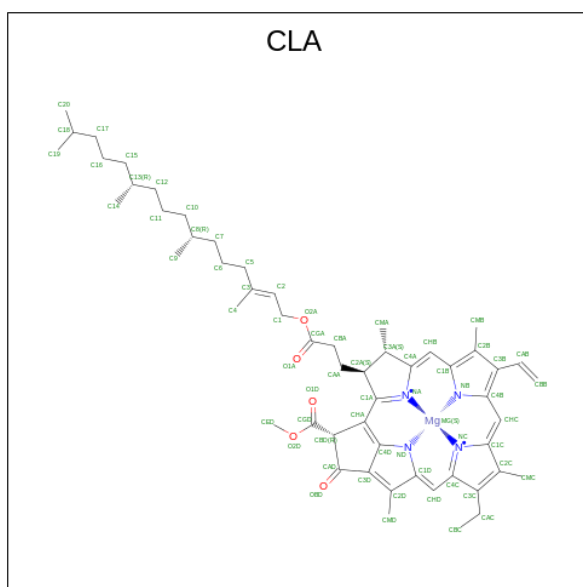
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
23	A	1	65	55	1	4	5	0
23	A	1	56	46	1	4	5	0
23	A	1	52	42	1	4	5	0
23	B	1	58	49	1	4	4	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	B	1	65	55	1	4	5	0
23	B	1	55	45	1	4	5	0
23	B	1	54	44	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	46	36	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	60	50	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	52	42	1	4	5	0
23	C	1	42	34	1	4	3	0
23	D	1	65	55	1	4	5	0
23	D	1	65	55	1	4	5	0
23	D	1	48	38	1	4	5	0

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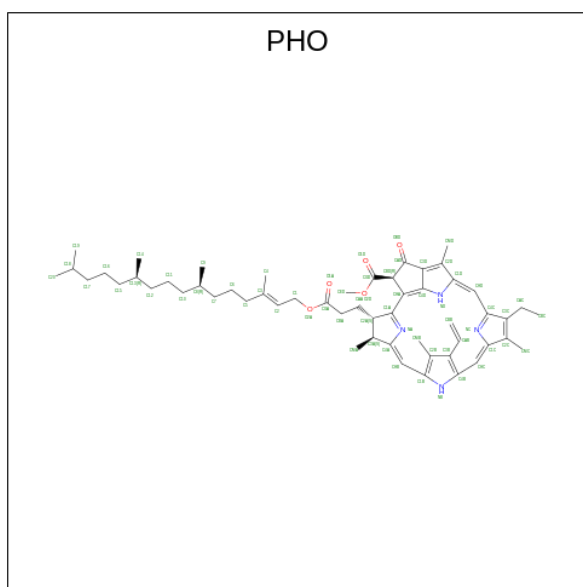
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	a	1	65	55	1	4	5	0
23	a	1	56	46	1	4	5	0
23	a	1	52	42	1	4	5	0
23	b	1	58	49	1	4	4	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	55	45	1	4	5	0
23	b	1	54	44	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0

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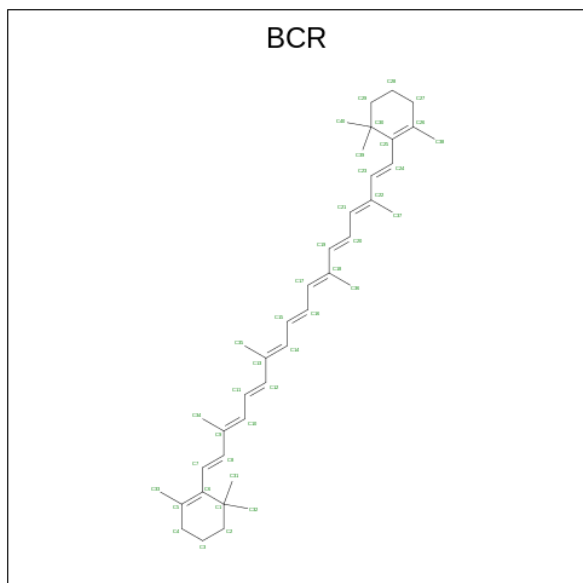
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	46	36	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	60	50	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	52	42	1	4	5	0
23	c	1	42	34	1	4	3	0
23	d	1	65	55	1	4	5	0
23	d	1	65	55	1	4	5	0
23	d	1	48	38	1	4	5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



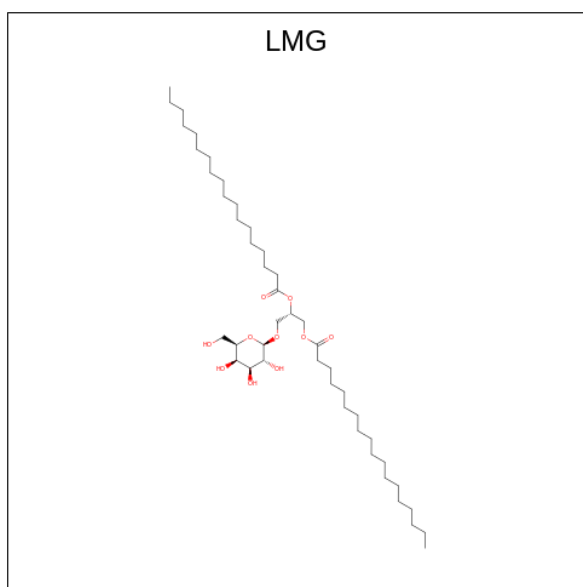
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	A	1	64	55	4	5	0
24	D	1	64	55	4	5	0
24	a	1	64	55	4	5	0
24	d	1	64	55	4	5	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



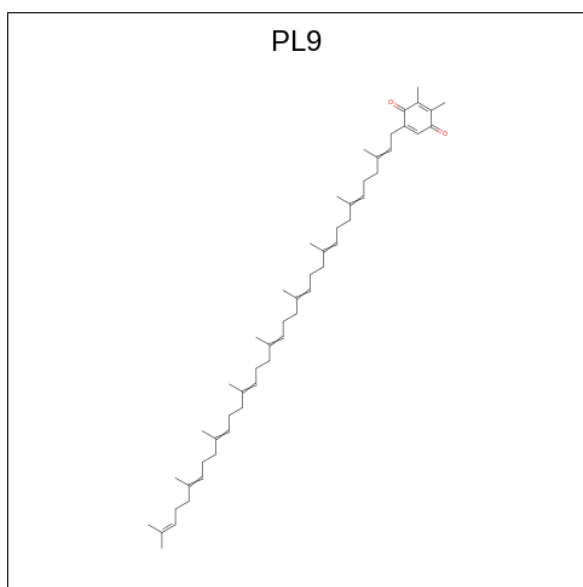
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 37 37	0
25	B	1	Total C 40 40	0
25	C	1	Total C 38 38	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	T	1	Total C 39 39	0
25	Y	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 37 37	0
25	b	1	Total C 40 40	0
25	c	1	Total C 38 38	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	t	1	Total C 39 39	0
25	y	1	Total C 40 40	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



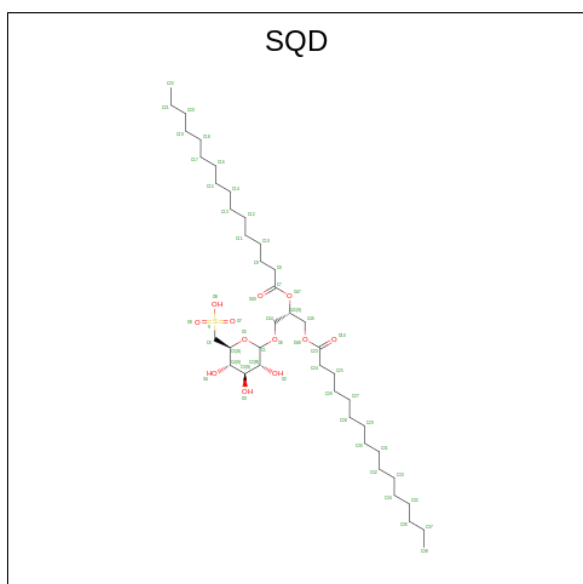
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	A	1	51	41	10	0
26	B	1	47	37	10	0
26	C	1	51	41	10	0
26	C	1	16	16		0
26	D	1	43	33	10	0
26	a	1	51	41	10	0
26	b	1	47	37	10	0
26	c	1	51	41	10	0
26	c	1	16	16		0
26	d	1	43	33	10	0

- Molecule 27 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	42	40	2	0
27	D	1	55	53	2	0
27	a	1	42	40	2	0
27	d	1	55	53	2	0

- Molecule 28 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	
28	A	1	Total	C	O	S	0
			39	26	12	1	
28	C	1	Total	C	O	S	0
			32	19	12	1	
28	D	1	Total	C	O	S	0
			27	15	11	1	
28	T	1	Total	C	O		0
			27	25	2		
28	a	1	Total	C	O	S	0
			39	26	12	1	
28	c	1	Total	C	O	S	0
			32	19	12	1	
28	d	1	Total	C	O	S	0
			27	15	11	1	
28	t	1	Total	C	O		0
			27	25	2		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

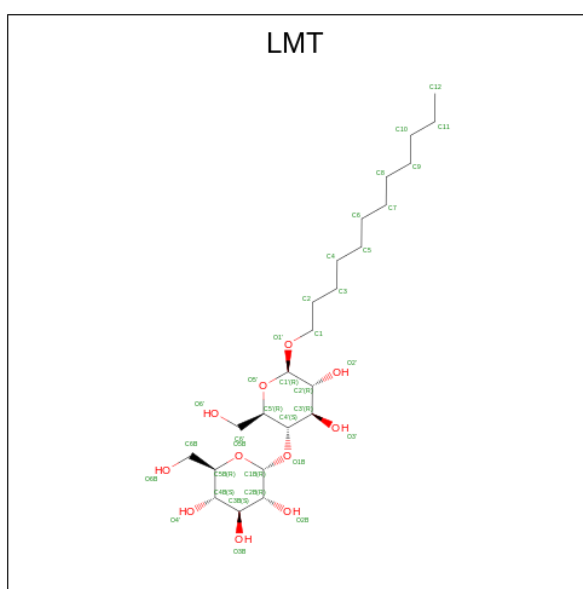
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	C	0
			6	6	
29	B	1	Total	C	0
			14	14	
29	D	3	Total	C	0
			42	42	
29	I	2	Total	C	0
			12	12	
29	K	1	Total	C	0
			15	15	
29	T	1	Total	C	0
			7	7	
29	X	1	Total	C	0
			15	15	
29	a	1	Total	C	0
			6	6	
29	b	1	Total	C	0
			14	14	
29	d	3	Total	C	0
			42	42	
29	i	2	Total	C	0
			12	12	
29	k	1	Total	C	0
			15	15	

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Mol	Chain	Residues	Atoms	AltConf
29	t	1	Total C 7 7	0
29	x	1	Total C 15 15	0
29	E	1	Total C 10 10	0
29	e	1	Total C 10 10	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



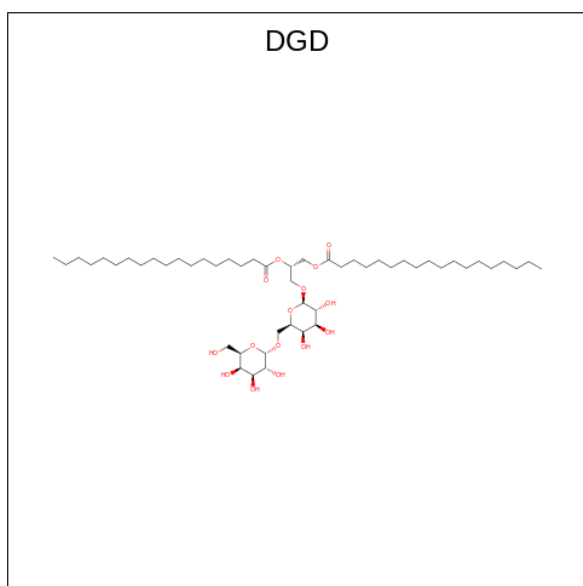
Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C O 35 24 11	0
30	B	1	Total C O 17 16 1	0
30	J	1	Total C O 24 18 6	0
30	M	1	Total C O 35 24 11	0
30	T	1	Total C O 17 16 1	0
30	T	1	Total C O 13 12 1	0
30	b	1	Total C O 35 24 11	0

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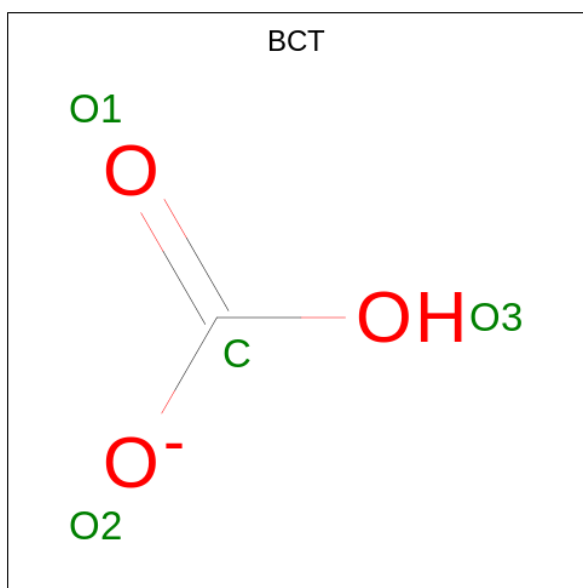
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	j	1	24	18	6	0
30	m	1	35	24	11	0
30	t	1	13	12	1	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



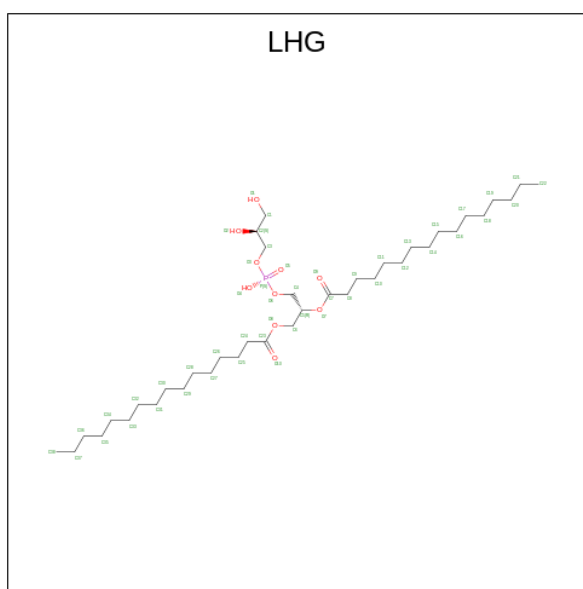
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	C	1	53	38	15	0
31	C	1	52	37	15	0
31	C	1	60	45	15	0
31	H	1	62	47	15	0
31	c	1	53	38	15	0
31	c	1	52	37	15	0
31	c	1	60	45	15	0
31	h	1	62	47	15	0

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



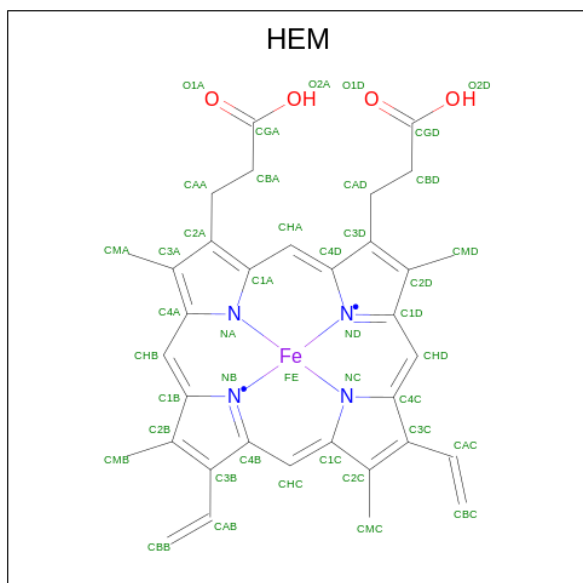
Mol	Chain	Residues	Atoms			AltConf
32	D	1	Total	C	O	1
			4	1	3	
32	d	1	Total	C	O	1
			4	1	3	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).



Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	O	P	0
			43	32	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			45	34	10	1	
33	L	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			43	32	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			45	34	10	1	
33	l	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			35	24	10	1	
33	e	1	Total	C	O	P	0
			35	24	10	1	

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



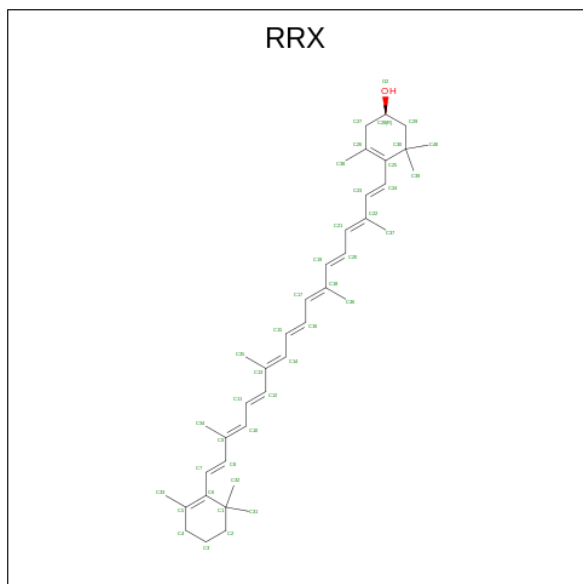
Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	H	1	41	40	1	0
35	h	1	41	40	1	0

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	J	1	1	1	0
36	j	1	1	1	0

- Molecule 37 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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Mol	Chain	Residues	Atoms		AltConf
39	H	42	Total 43	O 43	1
39	I	21	Total 21	O 21	0
39	J	10	Total 10	O 10	0
39	K	3	Total 3	O 3	0
39	L	21	Total 21	O 21	1
39	M	11	Total 11	O 11	0
39	T	16	Total 16	O 16	0
39	U	52	Total 52	O 52	1
39	V	92	Total 93	O 93	1
39	X	10	Total 10	O 10	0
39	Y	3	Total 3	O 3	0
39	a	155	Total 158	O 158	5
39	b	316	Total 321	O 321	5
39	c	239	Total 240	O 240	1
39	d	150	Total 157	O 157	7
39	f	12	Total 12	O 12	0
39	h	42	Total 43	O 43	1
39	i	22	Total 22	O 22	0
39	j	10	Total 10	O 10	0
39	k	4	Total 4	O 4	0
39	l	21	Total 21	O 21	1

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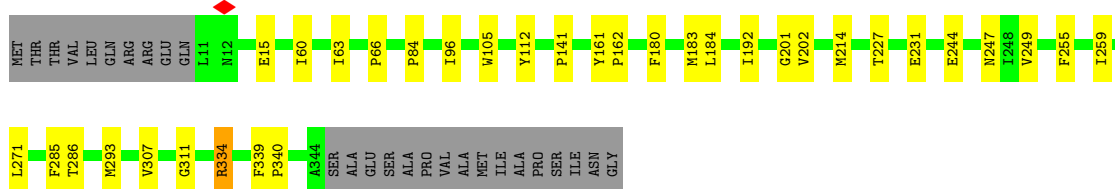
Mol	Chain	Residues	Atoms		AltConf
39	m	11	Total 11	O 11	0
39	t	16	Total 16	O 16	0
39	u	51	Total 51	O 51	1
39	v	92	Total 93	O 93	1
39	x	10	Total 10	O 10	0
39	y	3	Total 3	O 3	0
39	E	20	Total 20	O 20	0
39	O	107	Total 107	O 107	1
39	Z	2	Total 2	O 2	0
39	e	20	Total 20	O 20	0
39	o	106	Total 106	O 106	1
39	z	1	Total 1	O 1	0

### 3 Residue-property plots [i](#)


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

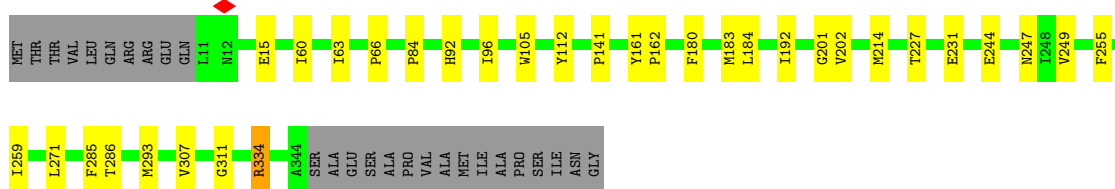
- Molecule 1: Photosystem II protein D1 3

Chain A: 




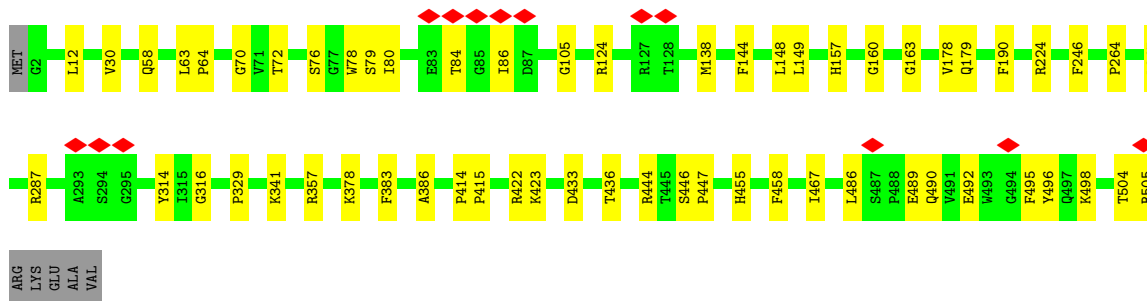
- Molecule 1: Photosystem II protein D1 3

Chain a: 




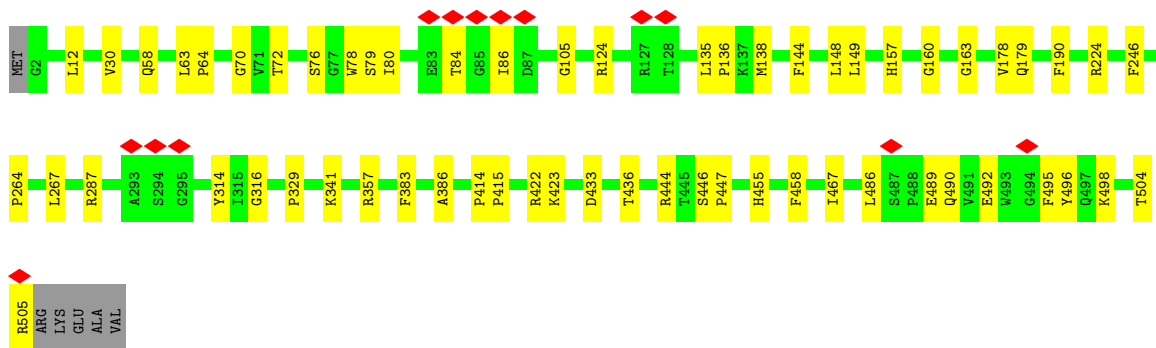
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 




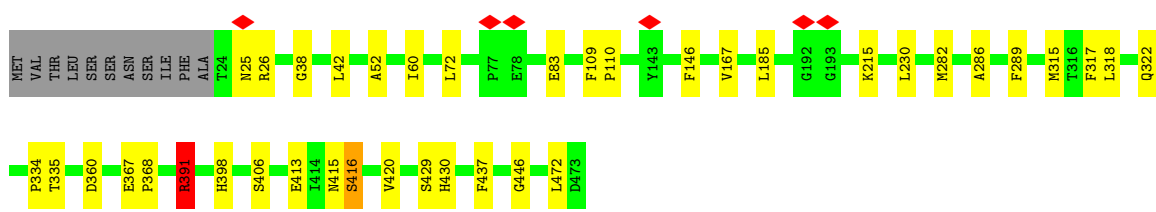
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  87% 12%




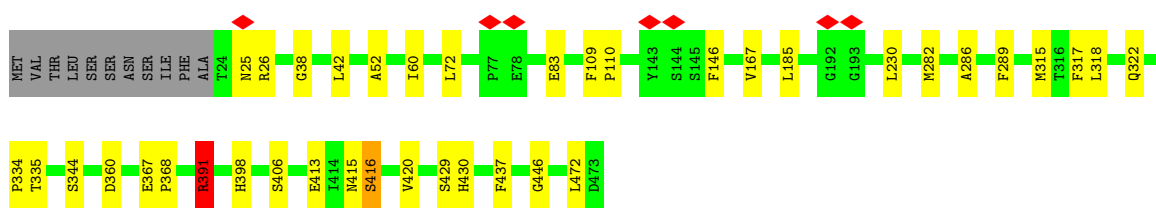
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  89% 8%




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  89% 8%



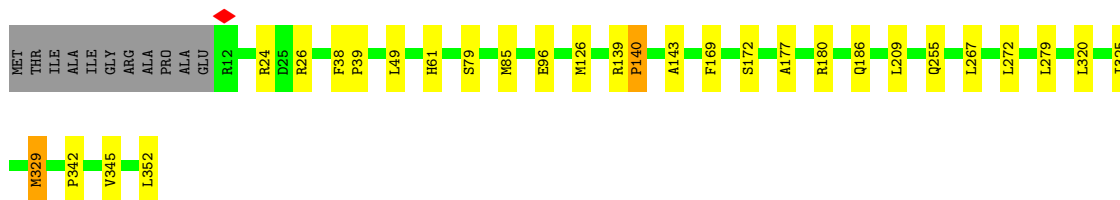
• Molecule 4: Photosystem II D2 protein

Chain D:  88% 8%

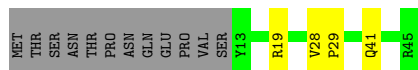


• Molecule 4: Photosystem II D2 protein

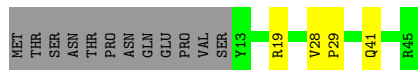
Chain d:  89% 8%



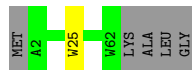
• Molecule 5: Cytochrome b559 subunit beta



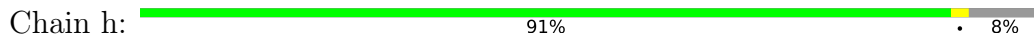
• Molecule 5: Cytochrome b559 subunit beta



• Molecule 6: Photosystem II reaction center protein H



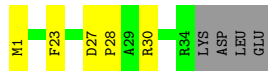
• Molecule 6: Photosystem II reaction center protein H



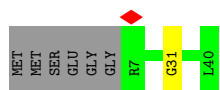
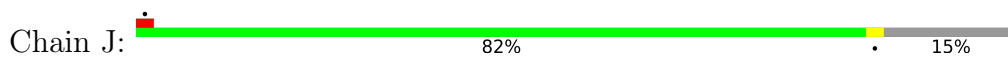
• Molecule 7: Photosystem II reaction center protein I



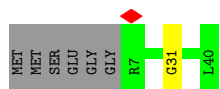
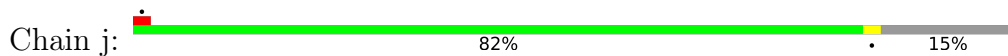
• Molecule 7: Photosystem II reaction center protein I



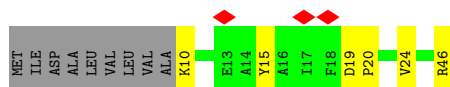
• Molecule 8: Photosystem II reaction center protein J



• Molecule 8: Photosystem II reaction center protein J



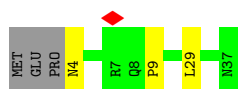
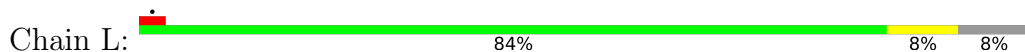
• Molecule 9: Photosystem II reaction center protein K



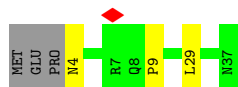
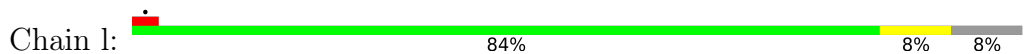
• Molecule 9: Photosystem II reaction center protein K



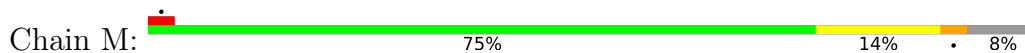
• Molecule 10: Photosystem II reaction center protein L



• Molecule 10: Photosystem II reaction center protein L

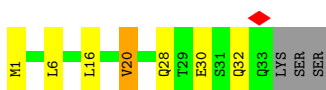


• Molecule 11: Photosystem II reaction center protein M




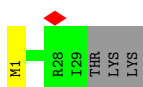
- Molecule 11: Photosystem II reaction center protein M

Chain m:  72% 17% 8%




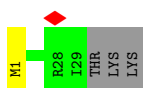
- Molecule 12: Photosystem II reaction center protein T

Chain T:  88% 9%



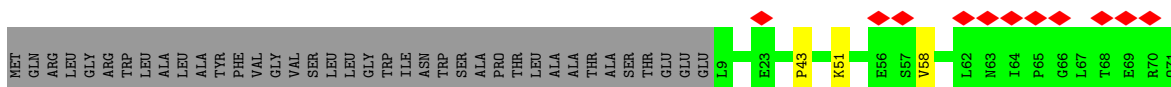
- Molecule 12: Photosystem II reaction center protein T

Chain t:  88% 9%



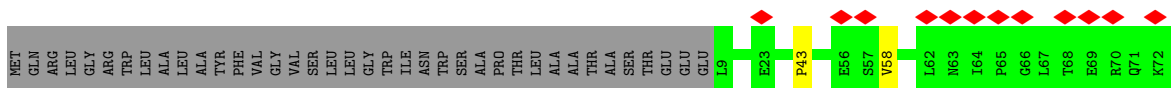
- Molecule 13: Photosystem II extrinsic protein U

Chain U:  66% 11% 6% 28%




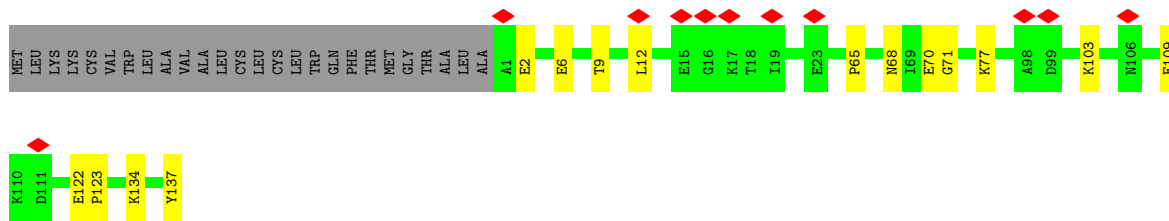
- Molecule 13: Photosystem II extrinsic protein U

Chain u:  66% 11% 5% 28%

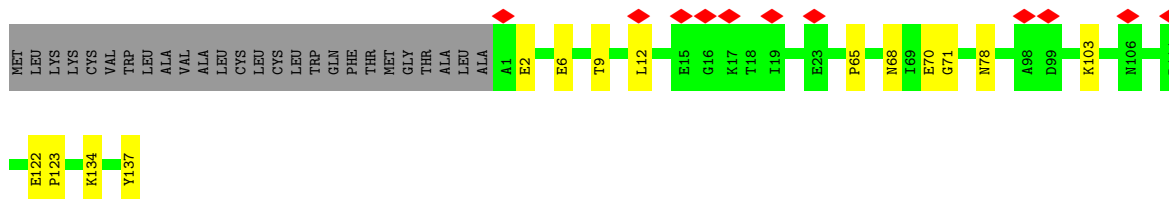
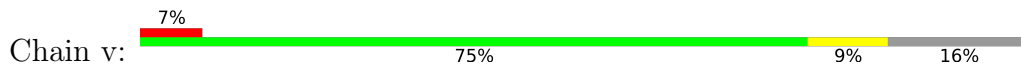


- Molecule 14: Photosystem II extrinsic protein V

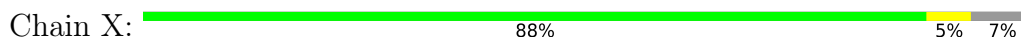
Chain V:  75% 7% 9% 16%



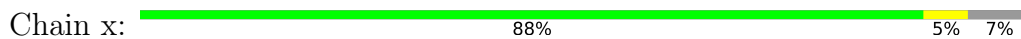
• Molecule 14: Photosystem II extrinsic protein V



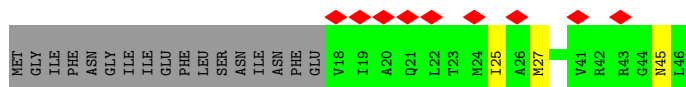
• Molecule 15: Photosystem II reaction center protein X



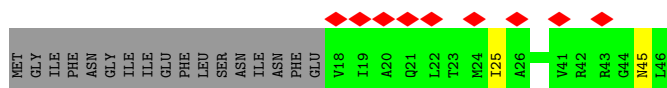
• Molecule 15: Photosystem II reaction center protein X



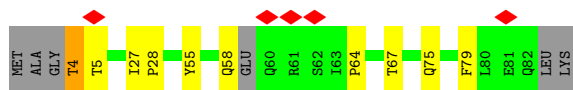
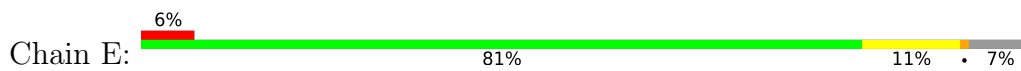
• Molecule 16: Photosystem II reaction center protein Psb30



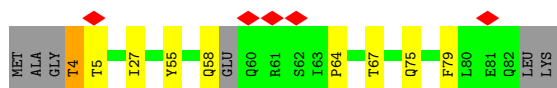
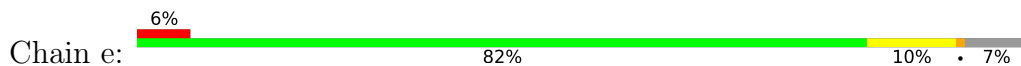
• Molecule 16: Photosystem II reaction center protein Psb30



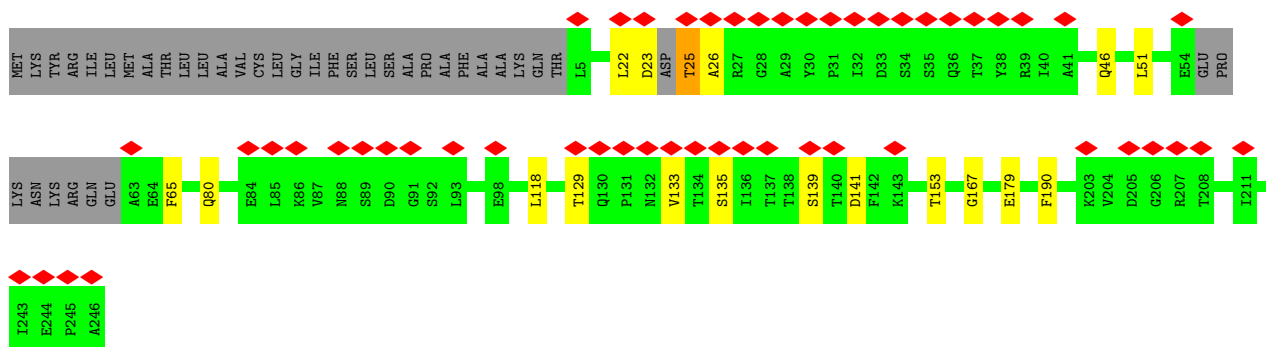
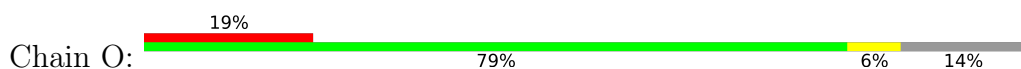
• Molecule 17: Cytochrome b559 subunit alpha



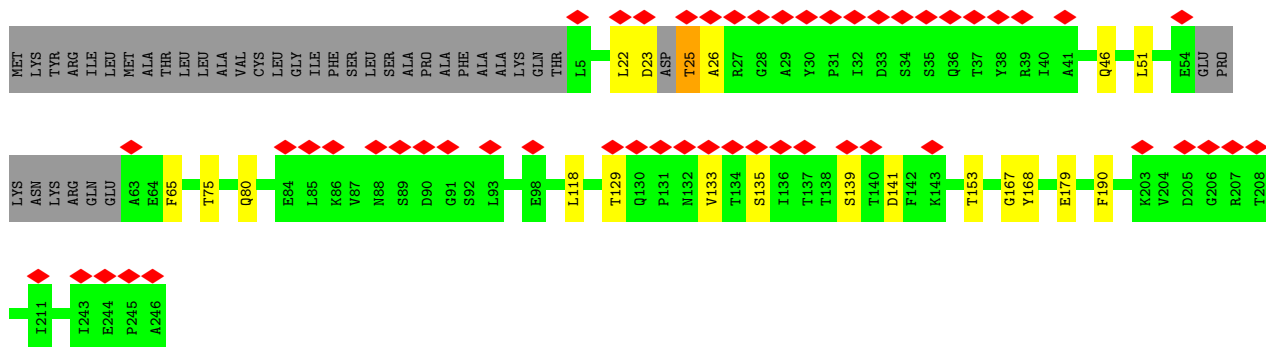
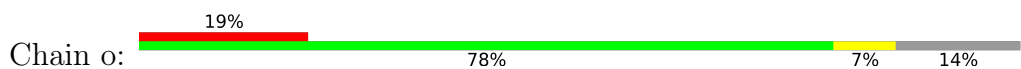
• Molecule 17: Cytochrome b559 subunit alpha



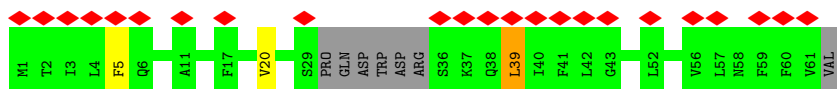
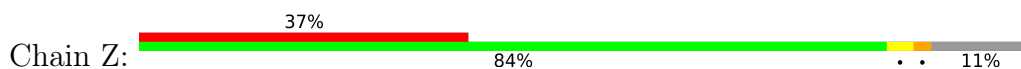
• Molecule 18: Photosystem II extrinsic protein O




• Molecule 18: Photosystem II extrinsic protein O

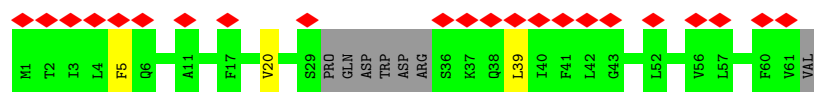


• Molecule 19: Photosystem II reaction center protein Z



## ● Molecule 19: Photosystem II reaction center protein Z

Chain z:  35% 84% 5% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171514	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	0.060	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	290.56, 290.56, 290.56	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.454, 0.454, 0.454	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.58	0/2710	0.91	1/3703 (0.0%)
1	a	0.58	0/2710	0.91	1/3703 (0.0%)
2	B	0.58	0/4036	0.89	3/5511 (0.1%)
2	b	0.58	0/4036	0.89	3/5511 (0.1%)
3	C	0.56	0/3568	0.91	3/4858 (0.1%)
3	c	0.56	0/3568	0.91	3/4858 (0.1%)
4	D	0.58	0/2798	0.91	4/3814 (0.1%)
4	d	0.58	0/2798	0.91	4/3814 (0.1%)
5	F	0.53	0/278	0.87	0/379
5	f	0.53	0/278	0.87	0/379
6	H	0.55	0/487	0.85	0/667
6	h	0.55	0/487	0.85	0/667
7	I	0.53	0/262	0.87	0/358
7	i	0.52	0/262	0.87	0/358
8	J	0.56	0/249	0.84	0/339
8	j	0.56	0/249	0.84	0/339
9	K	0.56	0/295	0.81	0/407
9	k	0.56	0/295	0.81	0/407
10	L	0.58	0/287	0.88	0/390
10	l	0.58	0/287	0.88	0/390
11	M	0.56	0/242	0.79	0/332
11	m	0.56	0/242	0.79	0/332
12	T	0.55	0/240	0.83	0/327
12	t	0.55	0/240	0.83	0/327
13	U	0.46	0/729	0.86	0/992
13	u	0.46	0/729	0.86	0/992
14	V	0.50	0/1045	0.87	0/1427
14	v	0.50	0/1045	0.87	0/1427
15	X	0.52	0/272	0.86	0/367
15	x	0.52	0/272	0.86	0/367
16	Y	0.53	0/200	0.94	0/269

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	y	0.53	0/200	0.94	0/269
17	E	0.54	0/631	0.89	0/864
17	e	0.54	0/631	0.89	0/864
18	O	0.54	0/1712	0.86	0/2327
18	o	0.54	0/1712	0.86	0/2327
19	Z	0.48	0/399	0.87	0/544
19	z	0.48	0/399	0.87	0/544
All	All	0.56	0/40880	0.89	22/55750 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
2	B	0	3
2	b	0	3
3	C	0	1
3	c	0	1
4	D	0	1
4	d	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	317	PHE	CA-CB-CG	-6.99	106.81	113.80
3	c	317	PHE	CA-CB-CG	-6.99	106.81	113.80
3	C	430	HIS	CA-CB-CG	-6.58	107.22	113.80
3	c	430	HIS	CA-CB-CG	-6.58	107.22	113.80
4	D	140	PRO	N-CA-CB	-6.10	96.85	103.25

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ARG	Sidechain
2	B	124	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	357	ARG	Sidechain
2	B	444	ARG	Sidechain
3	C	391	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2625	0	2506	24	0
1	a	2625	0	2506	24	0
2	B	3896	0	3711	40	0
2	b	3896	0	3711	40	0
3	C	3451	0	3355	30	0
3	c	3451	0	3355	30	0
4	D	2700	0	2602	25	0
4	d	2700	0	2602	24	0
5	F	269	0	277	3	0
5	f	269	0	277	3	0
6	H	474	0	480	2	0
6	h	474	0	480	2	0
7	I	265	0	268	4	0
7	i	265	0	268	4	0
8	J	243	0	251	1	0
8	j	243	0	251	1	0
9	K	285	0	287	7	0
9	k	285	0	287	7	0
10	L	278	0	289	4	0
10	l	278	0	289	3	0
11	M	249	0	261	11	0
11	m	249	0	261	12	0
12	T	241	0	236	1	0
12	t	241	0	236	1	0
13	U	718	0	706	6	0
13	u	718	0	706	5	0
14	V	1024	0	997	9	0
14	v	1024	0	997	9	0
15	X	269	0	291	1	0
15	x	269	0	291	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	199	0	211	4	0
16	y	199	0	211	3	0
17	E	610	0	585	9	0
17	e	610	0	585	8	0
18	O	1676	0	1588	14	0
18	o	1676	0	1588	16	0
19	Z	393	0	418	3	0
19	z	393	0	418	2	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	a	2	0	0	1	0
23	A	173	0	166	6	0
23	B	1012	0	1087	23	0
23	C	785	0	814	24	0
23	D	178	0	180	7	0
23	a	173	0	166	6	0
23	b	1012	0	1087	22	0
23	c	785	0	814	21	0
23	d	178	0	180	6	0
24	A	64	0	74	2	0
24	D	64	0	74	3	0
24	a	64	0	74	3	0
24	d	64	0	74	3	0
25	A	40	0	56	1	0
25	B	117	0	159	14	0
25	C	78	0	106	9	0
25	D	40	0	56	3	0
25	K	40	0	56	2	0
25	T	39	0	54	6	0
25	Y	40	0	56	3	0
25	a	40	0	56	1	0
25	b	117	0	159	12	0
25	c	78	0	106	11	0
25	d	40	0	56	2	0
25	k	40	0	56	2	0
25	t	39	0	54	5	0
25	y	40	0	56	4	0
26	A	51	0	72	1	0
26	B	47	0	64	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	67	0	100	0	0
26	D	43	0	56	0	0
26	a	51	0	72	1	0
26	b	47	0	64	0	0
26	c	67	0	100	0	0
26	d	43	0	56	0	0
27	A	42	0	56	2	0
27	D	55	0	80	1	0
27	a	42	0	56	2	0
27	d	55	0	80	1	0
28	A	39	0	47	0	0
28	C	32	0	28	0	0
28	D	27	0	19	0	0
28	T	27	0	40	1	0
28	a	39	0	47	0	0
28	c	32	0	28	0	0
28	d	27	0	19	1	0
28	t	27	0	40	0	0
29	A	6	0	0	0	0
29	B	14	0	0	0	0
29	D	42	0	0	2	0
29	E	10	0	0	0	0
29	I	12	0	0	0	0
29	K	15	0	0	0	0
29	T	7	0	0	0	0
29	X	15	0	0	0	0
29	a	6	0	0	0	0
29	b	14	0	0	0	0
29	d	42	0	0	2	0
29	e	10	0	0	0	0
29	i	12	0	0	0	0
29	k	15	0	0	0	0
29	t	7	0	0	0	0
29	x	15	0	0	0	0
30	B	52	0	71	1	0
30	J	24	0	35	1	0
30	M	35	0	46	1	0
30	T	30	0	50	2	0
30	b	35	0	46	0	0
30	j	24	0	35	1	0
30	m	35	0	46	1	0
30	t	13	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	165	0	204	1	0
31	H	62	0	82	0	0
31	c	165	0	204	1	0
31	h	62	0	82	0	0
32	D	4	0	0	0	0
32	d	4	0	0	0	0
33	D	137	0	191	1	0
33	E	35	0	43	1	0
33	L	49	0	74	0	0
33	d	137	0	191	1	0
33	e	35	0	43	1	0
33	l	49	0	74	0	0
34	F	43	0	30	3	0
34	f	43	0	30	3	0
35	H	41	0	56	1	0
35	h	41	0	56	2	0
36	J	1	0	0	0	0
36	j	1	0	0	0	0
37	V	43	0	30	0	0
37	v	43	0	30	0	0
38	O	1	0	0	0	0
38	o	1	0	0	0	0
39	A	159	0	0	5	0
39	B	322	0	0	11	0
39	C	240	0	0	5	0
39	D	156	0	0	9	0
39	E	20	0	0	2	0
39	F	12	0	0	0	0
39	H	43	0	0	0	0
39	I	21	0	0	1	0
39	J	10	0	0	1	0
39	K	3	0	0	1	0
39	L	21	0	0	2	0
39	M	11	0	0	1	0
39	O	107	0	0	7	0
39	T	16	0	0	0	0
39	U	52	0	0	3	0
39	V	93	0	0	1	0
39	X	10	0	0	0	0
39	Y	3	0	0	0	0
39	Z	2	0	0	0	0
39	a	158	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	b	321	0	0	11	0
39	c	240	0	0	5	0
39	d	157	0	0	10	0
39	e	20	0	0	2	0
39	f	12	0	0	0	0
39	h	43	0	0	0	0
39	i	22	0	0	1	0
39	j	10	0	0	1	0
39	k	4	0	0	1	0
39	l	21	0	0	1	0
39	m	11	0	0	1	0
39	o	106	0	0	7	0
39	t	16	0	0	0	0
39	u	51	0	0	2	0
39	v	93	0	0	2	0
39	x	10	0	0	0	0
39	y	3	0	0	0	0
39	z	1	0	0	0	0
All	All	50208	0	47412	509	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 5.

The worst 5 of 509 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:15:GLU:CG	39:A:645:HOH:O	1.82	1.21
1:a:15:GLU:CG	39:a:644:HOH:O	1.84	1.20
25:T:101:BCR:C25	25:T:101:BCR:C23	2.21	1.19
25:t:103:BCR:C25	25:t:103:BCR:C23	2.21	1.18
4:D:352:LEU:HB2	39:D:505:HOH:O	1.50	1.11

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	337/360 (94%)	334 (99%)	2 (1%)	1 (0%)	36	26
1	a	337/360 (94%)	334 (99%)	2 (1%)	1 (0%)	36	26
2	B	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
3	C	450/461 (98%)	442 (98%)	5 (1%)	3 (1%)	18	7
3	c	450/461 (98%)	442 (98%)	5 (1%)	3 (1%)	18	7
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	F	31/45 (69%)	31 (100%)	0	0	100	100
5	f	31/45 (69%)	31 (100%)	0	0	100	100
6	H	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
6	h	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
7	I	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
7	i	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
8	J	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
8	j	32/40 (80%)	31 (97%)	1 (3%)	0	100	100
9	K	35/46 (76%)	35 (100%)	0	0	100	100
9	k	35/46 (76%)	35 (100%)	0	0	100	100
10	L	33/37 (89%)	33 (100%)	0	0	100	100
10	l	33/37 (89%)	33 (100%)	0	0	100	100
11	M	31/36 (86%)	31 (100%)	0	0	100	100
11	m	31/36 (86%)	31 (100%)	0	0	100	100
12	T	27/32 (84%)	27 (100%)	0	0	100	100
12	t	27/32 (84%)	27 (100%)	0	0	100	100
13	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
13	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
14	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
14	v	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
15	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
15	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Y	27/46 (59%)	27 (100%)	0	0	100	100
16	y	27/46 (59%)	27 (100%)	0	0	100	100
17	E	75/84 (89%)	75 (100%)	0	0	100	100
17	e	75/84 (89%)	75 (100%)	0	0	100	100
18	O	230/272 (85%)	224 (97%)	6 (3%)	0	100	100
18	o	230/272 (85%)	224 (97%)	6 (3%)	0	100	100
19	Z	51/62 (82%)	51 (100%)	0	0	100	100
19	z	51/62 (82%)	51 (100%)	0	0	100	100
All	All	5120/5650 (91%)	5040 (98%)	72 (1%)	8 (0%)	49	34

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	25	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	25	ASN
3	c	416[A]	SER

### 5.3.2 Protein sidechains [i](#)

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	266/291 (91%)	265 (100%)	1 (0%)	84	79
1	a	266/291 (91%)	265 (100%)	1 (0%)	84	79
2	B	380/407 (93%)	379 (100%)	1 (0%)	86	82
2	b	380/407 (93%)	379 (100%)	1 (0%)	86	82
3	C	345/362 (95%)	342 (99%)	3 (1%)	70	63
3	c	345/362 (95%)	342 (99%)	3 (1%)	70	63
4	D	273/283 (96%)	272 (100%)	1 (0%)	84	79
4	d	273/283 (96%)	272 (100%)	1 (0%)	84	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	27/39 (69%)	27 (100%)	0	100	100
5	f	27/39 (69%)	27 (100%)	0	100	100
6	H	50/55 (91%)	50 (100%)	0	100	100
6	h	50/55 (91%)	50 (100%)	0	100	100
7	I	27/34 (79%)	27 (100%)	0	100	100
7	i	27/34 (79%)	27 (100%)	0	100	100
8	J	23/28 (82%)	23 (100%)	0	100	100
8	j	23/28 (82%)	23 (100%)	0	100	100
9	K	27/37 (73%)	27 (100%)	0	100	100
9	k	27/37 (73%)	27 (100%)	0	100	100
10	L	31/35 (89%)	31 (100%)	0	100	100
10	l	31/35 (89%)	31 (100%)	0	100	100
11	M	26/32 (81%)	25 (96%)	1 (4%)	29	13
11	m	26/32 (81%)	25 (96%)	1 (4%)	29	13
12	T	22/28 (79%)	22 (100%)	0	100	100
12	t	22/28 (79%)	22 (100%)	0	100	100
13	U	71/112 (63%)	69 (97%)	2 (3%)	38	22
13	u	71/112 (63%)	69 (97%)	2 (3%)	38	22
14	V	105/138 (76%)	105 (100%)	0	100	100
14	v	105/138 (76%)	105 (100%)	0	100	100
15	X	28/34 (82%)	27 (96%)	1 (4%)	31	14
15	x	28/34 (82%)	27 (96%)	1 (4%)	31	14
16	Y	19/37 (51%)	19 (100%)	0	100	100
16	y	19/37 (51%)	19 (100%)	0	100	100
17	E	63/73 (86%)	62 (98%)	1 (2%)	55	43
17	e	63/73 (86%)	62 (98%)	1 (2%)	55	43
18	O	163/228 (72%)	161 (99%)	2 (1%)	63	53
18	o	163/228 (72%)	161 (99%)	2 (1%)	63	53
19	Z	40/52 (77%)	38 (95%)	2 (5%)	22	7
19	z	40/52 (77%)	38 (95%)	2 (5%)	22	7
All	All	3972/4610 (86%)	3942 (99%)	30 (1%)	70	68

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	391	ARG
18	o	118	LEU
13	u	43	PRO
19	z	39	LEU
19	Z	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	332	GLN
17	E	58	GLN
6	h	59	ASN
14	v	78	ASN
18	O	88	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	T	1	12	8,9,10	0.55	0	7,9,11	1.62	0
7	FME	i	1	7	8,9,10	0.89	0	7,9,11	1.52	2 (28%)
7	FME	I	1	7	8,9,10	0.89	0	7,9,11	1.53	2 (28%)
11	FME	M	1	11	8,9,10	0.69	0	7,9,11	1.49	1 (14%)
11	FME	m	1	11	8,9,10	0.70	0	7,9,11	1.49	1 (14%)
12	FME	t	1	12	8,9,10	0.55	0	7,9,11	1.62	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
12	FME	T	1	12	-	4/7/9/11	-
7	FME	i	1	7	-	1/7/9/11	-
7	FME	I	1	7	-	1/7/9/11	-
11	FME	M	1	11	-	2/7/9/11	-
11	FME	m	1	11	-	2/7/9/11	-
12	FME	t	1	12	-	4/7/9/11	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	1	FME	CA-N-CN	-2.60	118.83	122.82
11	m	1	FME	CA-N-CN	-2.60	118.83	122.82
7	I	1	FME	CA-N-CN	-2.18	119.47	122.82
7	i	1	FME	CA-N-CN	-2.18	119.47	122.82
7	I	1	FME	O1-CN-N	-2.13	119.66	125.27

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	FME	O1-CN-N-CA
11	M	1	FME	O1-CN-N-CA
11	M	1	FME	CB-CA-N-CN
12	T	1	FME	O1-CN-N-CA
12	T	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	1	FME	1	0
12	t	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 10 are monoatomic and 22 are unknown - leaving 154 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
35	RRX	H	101	-	42,42,42	1.60	10 (23%)	57,58,58	1.53	10 (17%)
23	CLA	b	608	2	69,73,73	1.85	18 (26%)	83,113,113	2.65	30 (36%)
25	BCR	K	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.68	12 (21%)
23	CLA	B	611	2	69,73,73	1.98	20 (28%)	83,113,113	3.46	32 (38%)
32	BCT	d	404[A]	21	2,3,3	0.96	0	2,3,3	0.38	0
30	LMT	B	623	-	16,16,36	0.31	0	15,15,47	0.35	0
23	CLA	C	502	3	69,73,73	1.66	17 (24%)	83,113,113	2.77	26 (31%)
25	BCR	k	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.68	12 (21%)
23	CLA	b	614	2	58,62,73	1.97	15 (25%)	69,99,113	3.09	30 (43%)
26	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	C	509	3	64,68,73	1.93	19 (29%)	77,107,113	2.76	29 (37%)
30	LMT	M	101	-	36,36,36	0.45	1 (2%)	47,47,47	0.64	2 (4%)
26	LMG	a	410	-	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
34	HEM	f	101	17,5	50,50,50	1.50	6 (12%)	66,82,82	1.90	13 (19%)
24	PHO	a	407	-	58,69,69	2.22	16 (27%)	56,99,99	3.34	19 (33%)
25	BCR	t	103	-	39,39,41	1.05	3 (7%)	48,52,56	1.55	6 (12%)
25	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	10 (17%)
26	LMG	C	521	-	15,15,55	0.26	0	14,14,63	0.58	0
27	PL9	d	408	-	55,55,55	0.78	2 (3%)	68,69,69	1.56	15 (22%)
33	LHG	E	101	-	34,34,48	0.89	2 (5%)	37,40,54	0.97	2 (5%)
26	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.01	3 (5%)
25	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.72	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	510	3	69,73,73	1.87	18 (26%)	83,113,113	2.73	26 (31%)
33	LHG	d	410	-	48,48,48	0.82	3 (6%)	51,54,54	0.93	1 (1%)
23	CLA	B	608	2	69,73,73	1.85	18 (26%)	83,113,113	2.66	30 (36%)
26	LMG	B	620	-	47,47,55	0.81	2 (4%)	55,55,63	1.33	6 (10%)
23	CLA	D	406	4	52,56,73	2.11	18 (34%)	62,92,113	3.18	29 (46%)
23	CLA	B	610	-	69,73,73	1.80	19 (27%)	83,113,113	2.62	29 (34%)
23	CLA	C	507	3	50,54,73	2.10	19 (38%)	60,90,113	2.99	28 (46%)
26	LMG	d	412	36	43,43,55	0.92	3 (6%)	51,51,63	0.94	4 (7%)
30	LMT	J	102	-	24,24,36	0.23	0	29,29,47	0.49	0
33	LHG	D	409	-	40,40,48	0.93	4 (10%)	41,44,54	0.95	2 (4%)
23	CLA	c	504	3	69,73,73	1.80	17 (24%)	83,113,113	2.54	30 (36%)
26	LMG	D	412	36	43,43,55	0.92	3 (6%)	51,51,63	0.94	4 (7%)
23	CLA	C	513	3	56,60,73	2.01	16 (28%)	67,97,113	3.11	28 (41%)
23	CLA	B	614	2	58,62,73	1.97	15 (25%)	69,99,113	3.09	30 (43%)
23	CLA	a	408	1	56,60,73	1.97	18 (32%)	67,97,113	3.08	31 (46%)
33	LHG	D	411	-	44,44,48	0.81	3 (6%)	47,50,54	0.95	2 (4%)
25	BCR	b	619	-	41,41,41	0.98	2 (4%)	56,56,56	1.49	14 (25%)
25	BCR	A	409	-	41,41,41	0.90	2 (4%)	56,56,56	1.62	9 (16%)
23	CLA	c	509	3	64,68,73	1.93	19 (29%)	77,107,113	2.76	29 (37%)
23	CLA	b	615	2	69,73,73	1.72	15 (21%)	83,113,113	2.57	29 (34%)
23	CLA	B	603	2	69,73,73	1.67	17 (24%)	83,113,113	3.12	31 (37%)
23	CLA	c	502	3	69,73,73	1.66	17 (24%)	83,113,113	2.77	26 (31%)
23	CLA	C	508	-	69,73,73	1.86	17 (24%)	83,113,113	2.68	27 (32%)
31	DGD	h	102	-	63,63,67	0.76	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	C	504	3	69,73,73	1.80	17 (24%)	83,113,113	2.54	30 (36%)
23	CLA	A	405	1	69,73,73	1.83	20 (28%)	83,113,113	2.52	31 (37%)
23	CLA	B	601	-	61,65,73	1.86	17 (27%)	69,99,113	2.87	24 (34%)
25	BCR	B	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.67	11 (19%)
20	OEX	A	401	1,3	0,15,15	-	-	-	-	-
23	CLA	B	607	-	69,73,73	1.85	17 (24%)	83,113,113	2.53	27 (32%)
23	CLA	b	604	2	69,73,73	1.73	23 (33%)	83,113,113	2.77	25 (30%)
31	DGD	c	517	-	54,54,67	0.87	4 (7%)	68,68,81	0.95	3 (4%)
27	PL9	A	411	-	41,41,55	0.78	2 (4%)	49,51,69	1.71	10 (20%)
23	CLA	b	613	2	59,63,73	1.86	16 (27%)	71,101,113	2.69	28 (39%)
25	BCR	B	619	-	41,41,41	0.98	2 (4%)	56,56,56	1.49	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	SQD	a	412	-	38,39,54	1.09	3 (7%)	45,49,65	1.45	8 (17%)
31	DGD	c	518	-	53,53,67	0.89	3 (5%)	67,67,81	0.95	2 (2%)
23	CLA	c	507	3	50,54,73	2.10	19 (38%)	60,90,113	3.00	28 (46%)
23	CLA	c	514	3	46,50,73	2.24	17 (36%)	55,85,113	3.52	28 (50%)
28	SQD	D	415	-	25,26,54	0.85	2 (8%)	32,35,65	2.44	9 (28%)
33	LHG	d	409	-	40,40,48	0.93	4 (10%)	41,44,54	0.95	2 (4%)
26	LMG	b	620	-	47,47,55	0.81	2 (4%)	55,55,63	1.33	6 (10%)
23	CLA	b	602	2	69,73,73	1.77	16 (23%)	83,113,113	2.90	32 (38%)
31	DGD	C	517	-	54,54,67	0.87	4 (7%)	68,68,81	0.96	3 (4%)
33	LHG	L	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.06	3 (5%)
25	BCR	B	618	-	38,38,41	1.15	3 (7%)	47,49,56	1.59	12 (25%)
34	HEM	F	101	17,5	50,50,50	1.50	6 (12%)	66,82,82	1.90	13 (19%)
23	CLA	C	514	3	46,50,73	2.24	17 (36%)	55,85,113	3.52	28 (50%)
23	CLA	B	615	2	69,73,73	1.72	15 (21%)	83,113,113	2.57	29 (34%)
23	CLA	c	503	3	69,73,73	1.64	20 (28%)	83,113,113	2.56	24 (28%)
23	CLA	A	408	1	56,60,73	1.97	18 (32%)	67,97,113	3.08	31 (46%)
24	PHO	D	401	-	58,69,69	2.38	16 (27%)	56,99,99	3.25	16 (28%)
25	BCR	c	515	-	39,39,41	1.05	1 (2%)	50,51,56	2.17	17 (34%)
37	HEC	V	201	14	46,50,50	3.51	23 (50%)	60,82,82	2.62	25 (41%)
23	CLA	B	602	2	69,73,73	1.77	16 (23%)	83,113,113	2.90	32 (38%)
23	CLA	c	510	3	69,73,73	1.87	18 (26%)	83,113,113	2.73	26 (31%)
23	CLA	B	613	2	59,63,73	1.86	16 (27%)	71,101,113	2.70	28 (39%)
25	BCR	b	618	-	38,38,41	1.15	3 (7%)	47,49,56	1.59	12 (25%)
23	CLA	D	405	4	69,73,73	1.73	17 (24%)	83,113,113	2.59	25 (30%)
25	BCR	a	409	-	41,41,41	0.90	2 (4%)	56,56,56	1.62	9 (16%)
23	CLA	c	511	3	69,73,73	1.76	17 (24%)	83,113,113	2.82	31 (37%)
23	CLA	c	508	-	69,73,73	1.86	17 (24%)	83,113,113	2.68	27 (32%)
23	CLA	a	405	1	69,73,73	1.83	20 (28%)	83,113,113	2.52	31 (37%)
23	CLA	A	406	39	60,64,73	1.77	16 (26%)	72,102,113	2.84	27 (37%)
23	CLA	b	601	-	61,65,73	1.86	17 (27%)	69,99,113	2.87	24 (34%)
30	LMT	T	104	-	16,16,36	0.31	0	15,15,47	0.35	0
25	BCR	C	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.72	12 (21%)
30	LMT	T	105	-	12,12,36	0.18	0	11,11,47	0.17	0
33	LHG	l	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.06	3 (5%)
31	DGD	c	519	-	61,61,67	0.79	3 (4%)	75,75,81	0.88	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LMG	c	521	-	15,15,55	0.26	0	14,14,63	0.58	0
25	BCR	T	101	-	39,39,41	1.05	3 (7%)	48,52,56	1.55	6 (12%)
23	CLA	b	612	2	69,73,73	1.73	15 (21%)	83,113,113	2.62	24 (28%)
28	SQD	c	501	-	31,32,54	1.23	4 (12%)	40,43,65	2.30	12 (30%)
35	RRX	h	101	-	42,42,42	1.60	10 (23%)	57,58,58	1.53	10 (17%)
23	CLA	C	503	3	69,73,73	1.64	19 (27%)	83,113,113	2.56	24 (28%)
27	PL9	a	411	-	41,41,55	0.78	2 (4%)	49,51,69	1.71	10 (20%)
23	CLA	d	406	4	52,56,73	2.11	18 (34%)	62,92,113	3.18	29 (46%)
28	SQD	C	501	-	31,32,54	1.23	4 (12%)	40,43,65	2.30	12 (30%)
23	CLA	B	612	2	69,73,73	1.73	15 (21%)	83,113,113	2.62	24 (28%)
26	LMG	A	410	-	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
31	DGD	H	102	-	63,63,67	0.76	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	C	511	3	69,73,73	1.76	17 (24%)	83,113,113	2.82	31 (37%)
24	PHO	A	407	-	58,69,69	2.22	16 (27%)	56,99,99	3.34	19 (33%)
25	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.76	15 (26%)
23	CLA	C	506	3	69,73,73	1.74	18 (26%)	83,113,113	2.53	28 (33%)
23	CLA	d	405	4	69,73,73	1.73	17 (24%)	83,113,113	2.59	25 (30%)
33	LHG	d	411	-	44,44,48	0.81	3 (6%)	47,50,54	0.95	2 (4%)
30	LMT	t	102	-	12,12,36	0.18	0	11,11,47	0.17	0
25	BCR	b	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.67	11 (19%)
31	DGD	C	518	-	53,53,67	0.88	3 (5%)	67,67,81	0.95	2 (2%)
31	DGD	C	519	-	61,61,67	0.79	3 (4%)	75,75,81	0.88	3 (4%)
23	CLA	b	603	2	69,73,73	1.67	17 (24%)	83,113,113	3.12	31 (37%)
23	CLA	b	609	2	69,73,73	1.78	17 (24%)	83,113,113	2.73	29 (34%)
23	CLA	C	505	-	69,73,73	1.79	18 (26%)	83,113,113	3.01	31 (37%)
23	CLA	B	609	2	69,73,73	1.78	17 (24%)	83,113,113	2.73	29 (34%)
23	CLA	b	606	2	69,73,73	1.70	18 (26%)	83,113,113	2.72	31 (37%)
23	CLA	C	512	3	69,73,73	1.81	19 (27%)	83,113,113	2.66	28 (33%)
23	CLA	d	402	39	69,73,73	1.58	15 (21%)	83,113,113	2.65	27 (32%)
28	SQD	d	415	-	25,26,54	0.85	2 (8%)	32,35,65	2.44	9 (28%)
23	CLA	b	605	2	69,73,73	1.67	18 (26%)	83,113,113	2.90	29 (34%)
23	CLA	B	616	2	69,73,73	1.83	18 (26%)	83,113,113	2.78	26 (31%)
23	CLA	D	402	39	69,73,73	1.58	15 (21%)	83,113,113	2.65	27 (32%)
20	OEX	a	401	1,3	0,15,15	-	-	-	-	-
23	CLA	b	610	-	69,73,73	1.80	19 (27%)	83,113,113	2.62	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	506	3	69,73,73	1.74	18 (26%)	83,113,113	2.53	28 (33%)
25	BCR	d	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.76	15 (26%)
23	CLA	a	406	-	60,64,73	1.77	16 (26%)	72,102,113	2.84	27 (37%)
23	CLA	c	505	-	69,73,73	1.79	18 (26%)	83,113,113	3.01	31 (37%)
33	LHG	D	410	-	48,48,48	0.82	3 (6%)	51,54,54	0.93	1 (1%)
24	PHO	d	401	-	58,69,69	2.38	16 (27%)	56,99,99	3.25	16 (28%)
23	CLA	b	607	-	69,73,73	1.84	17 (24%)	83,113,113	2.52	27 (32%)
37	HEC	v	201	14	46,50,50	3.51	23 (50%)	60,82,82	2.62	25 (41%)
23	CLA	c	512	3	69,73,73	1.81	19 (27%)	83,113,113	2.66	28 (33%)
30	LMT	j	102	-	24,24,36	0.23	0	29,29,47	0.49	0
28	SQD	T	103	-	25,25,54	0.84	1 (4%)	24,24,65	0.96	2 (8%)
30	LMT	b	621	-	36,36,36	0.25	0	47,47,47	0.56	1 (2%)
25	BCR	C	515	-	39,39,41	1.05	1 (2%)	50,51,56	2.17	17 (34%)
30	LMT	m	101	-	36,36,36	0.45	1 (2%)	47,47,47	0.64	2 (4%)
32	BCT	D	404[A]	21	2,3,3	0.96	0	2,3,3	0.38	0
23	CLA	c	513	3	56,60,73	2.01	16 (28%)	67,97,113	3.11	28 (41%)
25	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	10 (17%)
23	CLA	b	616	2	69,73,73	1.83	18 (26%)	83,113,113	2.78	26 (31%)
23	CLA	B	606	2	69,73,73	1.70	18 (26%)	83,113,113	2.72	31 (37%)
23	CLA	B	604	2	69,73,73	1.73	23 (33%)	83,113,113	2.77	25 (30%)
33	LHG	e	101	-	34,34,48	0.89	2 (5%)	37,40,54	0.97	2 (5%)
27	PL9	D	408	-	55,55,55	0.78	2 (3%)	68,69,69	1.56	15 (22%)
28	SQD	A	412	-	38,39,54	1.09	3 (7%)	45,49,65	1.45	8 (17%)
28	SQD	t	101	-	25,25,54	0.84	1 (4%)	24,24,65	0.96	2 (8%)
23	CLA	B	605	2	69,73,73	1.67	18 (26%)	83,113,113	2.90	29 (34%)
23	CLA	b	611	2	69,73,73	1.98	20 (28%)	83,113,113	3.46	32 (38%)
30	LMT	B	621	-	36,36,36	0.25	0	47,47,47	0.56	1 (2%)

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
35	RRX	H	101	-	-	4/29/65/65	0/2/2/2
23	CLA	b	608	2	-	1/39/115/115	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	2	-	4/39/115/115	-
30	LMT	B	623	-	-	7/14/14/61	-
23	CLA	C	502	3	-	3/39/115/115	-
25	BCR	k	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	614	2	-	7/26/102/115	-
26	LMG	C	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	509	3	-	7/33/109/115	-
30	LMT	M	101	-	-	1/21/61/61	0/2/2/2
26	LMG	a	410	-	-	19/46/66/70	0/1/1/1
34	HEM	f	101	17,5	-	2/14/54/54	-
24	PHO	a	407	-	-	2/37/103/103	0/5/6/6
25	BCR	t	103	-	-	0/24/53/63	0/2/2/2
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
26	LMG	C	521	-	-	1/13/13/70	-
27	PL9	d	408	-	-	3/53/73/73	0/1/1/1
33	LHG	E	101	-	-	14/38/38/53	-
26	LMG	c	520	-	-	15/46/66/70	0/1/1/1
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	C	510	3	-	5/39/115/115	-
33	LHG	d	410	-	-	9/53/53/53	-
23	CLA	B	608	2	-	1/39/115/115	-
26	LMG	B	620	-	-	8/42/62/70	0/1/1/1
23	CLA	D	406	4	-	2/19/95/115	-
23	CLA	B	610	-	-	3/39/115/115	-
23	CLA	C	507	3	-	3/17/93/115	-
26	LMG	d	412	36	-	5/38/58/70	0/1/1/1
30	LMT	J	102	-	-	5/15/35/61	0/1/1/2
33	LHG	D	409	-	-	4/41/41/53	-
23	CLA	c	504	3	-	3/39/115/115	-
26	LMG	D	412	36	-	5/38/58/70	0/1/1/1
23	CLA	C	513	3	-	9/24/100/115	-
23	CLA	B	614	2	-	7/26/102/115	-
23	CLA	a	408	1	-	4/24/100/115	-
33	LHG	D	411	-	-	6/49/49/53	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	509	3	-	7/33/109/115	-
23	CLA	b	615	2	-	1/39/115/115	-
23	CLA	B	603	2	-	8/39/115/115	-
23	CLA	c	502	3	-	3/39/115/115	-
23	CLA	C	508	-	-	10/39/115/115	-
31	DGD	h	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	504	3	-	3/39/115/115	-
23	CLA	A	405	1	-	3/39/115/115	-
23	CLA	B	601	-	-	11/25/101/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	607	-	-	1/39/115/115	-
23	CLA	b	604	2	-	6/39/115/115	-
31	DGD	c	517	-	-	10/42/82/95	0/2/2/2
27	PL9	A	411	-	-	4/34/54/73	0/1/1/1
23	CLA	b	613	2	-	1/27/103/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
28	SQD	a	412	-	-	14/33/53/69	0/1/1/1
31	DGD	c	518	-	-	10/41/81/95	0/2/2/2
23	CLA	c	507	3	-	3/17/93/115	-
23	CLA	c	514	3	-	0/12/88/115	-
28	SQD	D	415	-	-	4/16/36/69	0/1/1/1
33	LHG	d	409	-	-	4/41/41/53	-
26	LMG	b	620	-	-	8/42/62/70	0/1/1/1
23	CLA	b	602	2	-	4/39/115/115	-
31	DGD	C	517	-	-	10/42/82/95	0/2/2/2
33	LHG	L	101	-	-	17/53/53/53	-
25	BCR	B	618	-	-	2/29/54/63	0/2/2/2
34	HEM	F	101	17,5	-	2/14/54/54	-
23	CLA	C	514	3	-	0/12/88/115	-
23	CLA	B	615	2	-	1/39/115/115	-
23	CLA	c	503	3	-	3/39/115/115	-
23	CLA	A	408	1	-	4/24/100/115	-
24	PHO	D	401	-	-	1/37/103/103	0/5/6/6
25	BCR	c	515	-	-	2/29/57/63	0/2/2/2
37	HEC	V	201	14	-	5/14/54/54	-
23	CLA	B	602	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	510	3	-	5/39/115/115	-
23	CLA	B	613	2	-	1/27/103/115	-
25	BCR	b	618	-	-	2/29/54/63	0/2/2/2
23	CLA	D	405	4	-	3/39/115/115	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
23	CLA	c	511	3	-	4/39/115/115	-
23	CLA	c	508	-	-	10/39/115/115	-
23	CLA	a	405	1	-	3/39/115/115	-
23	CLA	A	406	39	-	6/29/105/115	-
23	CLA	b	601	-	-	11/25/101/115	-
30	LMT	T	104	-	-	7/14/14/61	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
30	LMT	T	105	-	-	3/10/10/61	-
33	LHG	l	101	-	-	17/53/53/53	-
31	DGD	c	519	-	-	7/49/89/95	0/2/2/2
26	LMG	c	521	-	-	1/13/13/70	-
25	BCR	T	101	-	-	0/24/53/63	0/2/2/2
23	CLA	b	612	2	-	5/39/115/115	-
28	SQD	c	501	-	-	4/27/47/69	0/1/1/1
35	RRX	h	101	-	-	4/29/65/65	0/2/2/2
23	CLA	C	503	3	-	3/39/115/115	-
27	PL9	a	411	-	-	4/34/54/73	0/1/1/1
23	CLA	d	406	4	-	2/19/95/115	-
28	SQD	C	501	-	-	4/27/47/69	0/1/1/1
23	CLA	B	612	2	-	5/39/115/115	-
26	LMG	A	410	-	-	19/46/66/70	0/1/1/1
31	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	511	3	-	4/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
25	BCR	D	407	-	-	0/29/63/63	0/2/2/2
23	CLA	C	506	3	-	4/39/115/115	-
23	CLA	d	405	4	-	3/39/115/115	-
33	LHG	d	411	-	-	6/49/49/53	-
30	LMT	t	102	-	-	3/10/10/61	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	C	518	-	-	10/41/81/95	0/2/2/2
31	DGD	C	519	-	-	7/49/89/95	0/2/2/2
23	CLA	b	603	2	-	8/39/115/115	-
23	CLA	b	609	2	-	3/39/115/115	-
23	CLA	C	505	-	-	5/39/115/115	-
23	CLA	B	609	2	-	3/39/115/115	-
23	CLA	b	606	2	-	10/39/115/115	-
23	CLA	C	512	3	-	2/39/115/115	-
23	CLA	d	402	39	-	4/39/115/115	-
28	SQD	d	415	-	-	4/16/36/69	0/1/1/1
23	CLA	b	605	2	-	3/39/115/115	-
23	CLA	B	616	2	-	13/39/115/115	-
23	CLA	D	402	39	-	4/39/115/115	-
23	CLA	b	610	-	-	3/39/115/115	-
23	CLA	c	506	3	-	4/39/115/115	-
25	BCR	d	407	-	-	0/29/63/63	0/2/2/2
23	CLA	a	406	-	-	6/29/105/115	-
23	CLA	c	505	-	-	5/39/115/115	-
33	LHG	D	410	-	-	9/53/53/53	-
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	607	-	-	1/39/115/115	-
37	HEC	v	201	14	-	5/14/54/54	-
23	CLA	c	512	3	-	2/39/115/115	-
30	LMT	j	102	-	-	5/15/35/61	0/1/1/2
28	SQD	T	103	-	-	11/22/22/69	-
30	LMT	b	621	-	-	11/21/61/61	0/2/2/2
25	BCR	C	515	-	-	2/29/57/63	0/2/2/2
30	LMT	m	101	-	-	1/21/61/61	0/2/2/2
23	CLA	c	513	3	-	9/24/100/115	-
25	BCR	y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	b	616	2	-	13/39/115/115	-
23	CLA	B	606	2	-	10/39/115/115	-
23	CLA	B	604	2	-	6/39/115/115	-
33	LHG	e	101	-	-	14/38/38/53	-
27	PL9	D	408	-	-	3/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	412	-	-	14/33/53/69	0/1/1/1
28	SQD	t	101	-	-	11/22/22/69	-
23	CLA	B	605	2	-	3/39/115/115	-
23	CLA	b	611	2	-	4/39/115/115	-
30	LMT	B	621	-	-	11/21/61/61	0/2/2/2

The worst 5 of 1517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	201	HEC	CAB-C3B	13.12	1.51	1.34
37	v	201	HEC	CAB-C3B	13.12	1.51	1.34
37	V	201	HEC	CAC-C3C	12.63	1.50	1.34
37	v	201	HEC	CAC-C3C	12.63	1.50	1.34
24	D	401	PHO	C1B-C2B	8.02	1.48	1.39

The worst 5 of 2580 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C2D-C1D-ND	15.53	120.25	109.53
24	a	407	PHO	C2D-C1D-ND	15.53	120.25	109.53
23	B	611	CLA	C2B-C1B-NB	15.44	120.58	110.23
23	b	611	CLA	C2B-C1B-NB	15.44	120.58	110.23
24	D	401	PHO	C2D-C1D-ND	14.40	119.47	109.53

There are no chirality outliers.

5 of 782 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

106 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	H	101	RRX	1	0
25	K	102	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	611	CLA	2	0
30	B	623	LMT	1	0
23	C	502	CLA	1	0
25	k	102	BCR	2	0
30	M	101	LMT	1	0
26	a	410	LMG	1	0
34	f	101	HEM	3	0
24	a	407	PHO	3	0
25	t	103	BCR	5	0
25	Y	101	BCR	3	0
27	d	408	PL9	1	0
33	E	101	LHG	1	0
25	c	516	BCR	8	0
23	C	510	CLA	2	0
23	D	406	CLA	2	0
23	B	610	CLA	2	0
23	C	507	CLA	1	0
30	J	102	LMT	1	0
23	c	504	CLA	5	0
23	C	513	CLA	5	0
33	D	411	LHG	1	0
25	b	619	BCR	6	0
25	A	409	BCR	1	0
23	b	615	CLA	3	0
23	B	603	CLA	1	0
23	c	502	CLA	1	0
23	C	508	CLA	1	0
23	C	504	CLA	5	0
23	A	405	CLA	3	0
23	B	601	CLA	2	0
25	B	617	BCR	1	0
23	B	607	CLA	1	0
23	b	604	CLA	1	0
27	A	411	PL9	2	0
23	b	613	CLA	2	0
25	B	619	BCR	8	0
31	c	518	DGD	1	0
23	c	514	CLA	2	0
25	B	618	BCR	5	0
34	F	101	HEM	3	0
23	C	514	CLA	2	0
23	B	615	CLA	3	0

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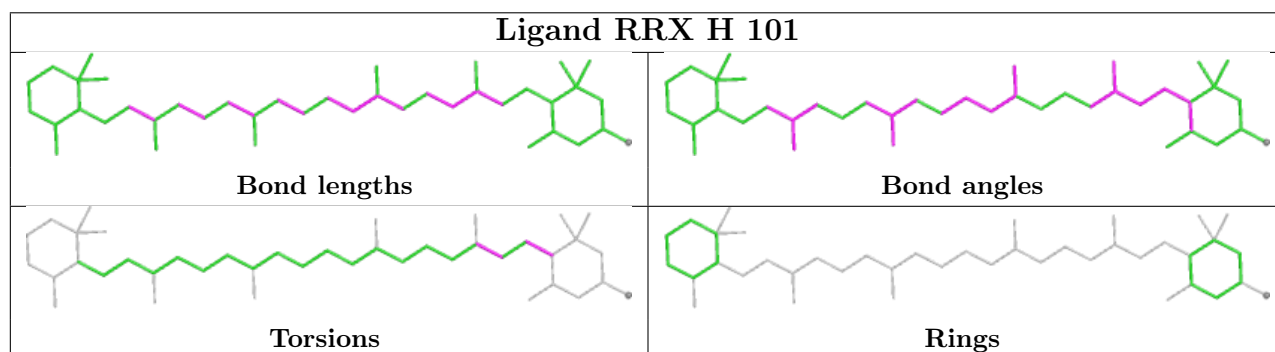
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	503	CLA	2	0
24	D	401	PHO	3	0
25	c	515	BCR	3	0
23	c	510	CLA	2	0
23	B	613	CLA	2	0
25	b	618	BCR	4	0
23	D	405	CLA	2	0
25	a	409	BCR	1	0
23	a	405	CLA	3	0
23	A	406	CLA	3	0
23	b	601	CLA	2	0
30	T	104	LMT	1	0
25	C	516	BCR	6	0
30	T	105	LMT	1	0
25	T	101	BCR	6	0
23	b	612	CLA	2	0
35	h	101	RRX	2	0
23	C	503	CLA	2	0
27	a	411	PL9	2	0
23	d	406	CLA	2	0
23	B	612	CLA	2	0
26	A	410	LMG	1	0
23	C	511	CLA	1	0
24	A	407	PHO	2	0
25	D	407	BCR	3	0
23	C	506	CLA	2	0
23	d	405	CLA	1	0
33	d	411	LHG	1	0
25	b	617	BCR	2	0
31	C	518	DGD	1	0
23	b	603	CLA	1	0
23	b	609	CLA	1	0
23	C	505	CLA	1	0
23	B	609	CLA	1	0
23	b	606	CLA	4	0
23	C	512	CLA	4	0
23	d	402	CLA	3	0
28	d	415	SQD	1	0
23	b	605	CLA	3	0
23	B	616	CLA	2	0
23	D	402	CLA	3	0
23	b	610	CLA	2	0

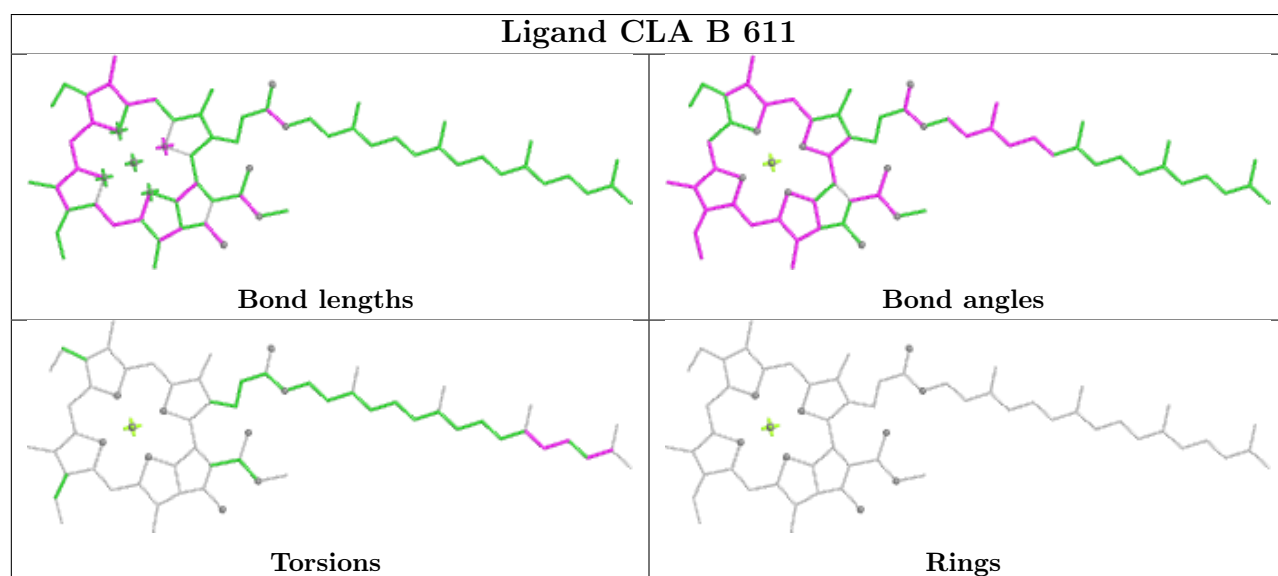
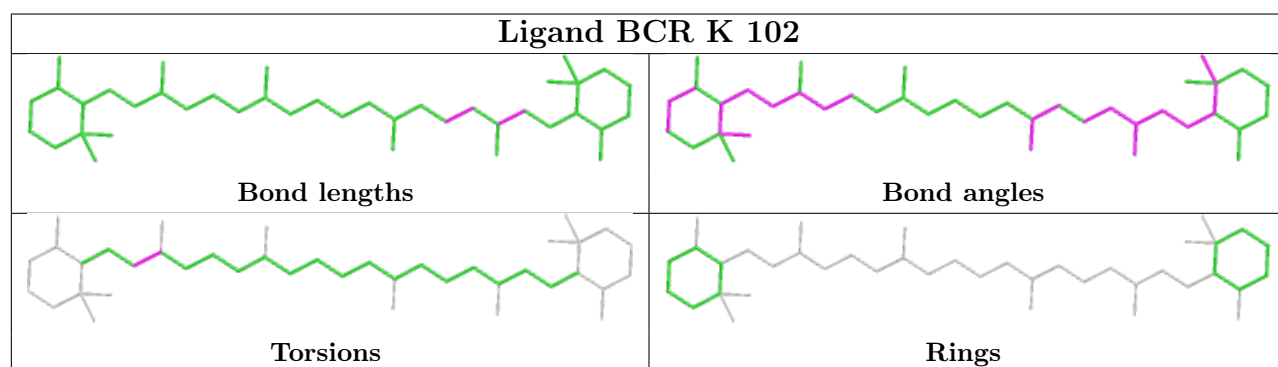
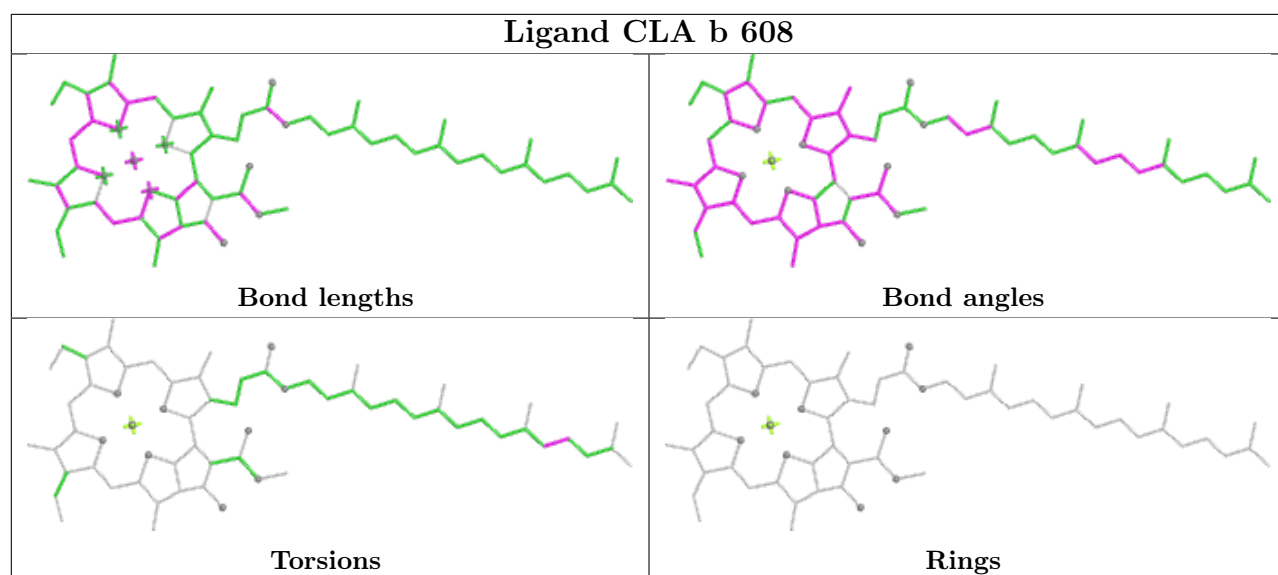
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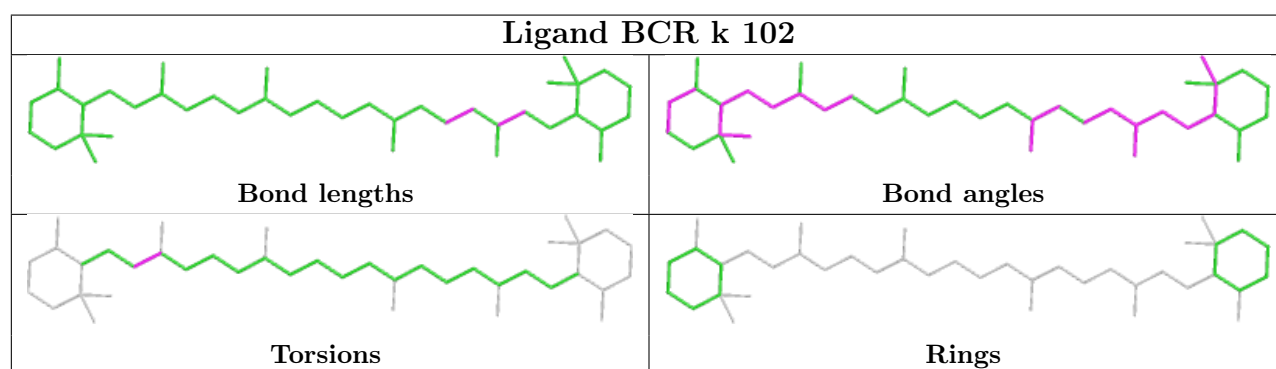
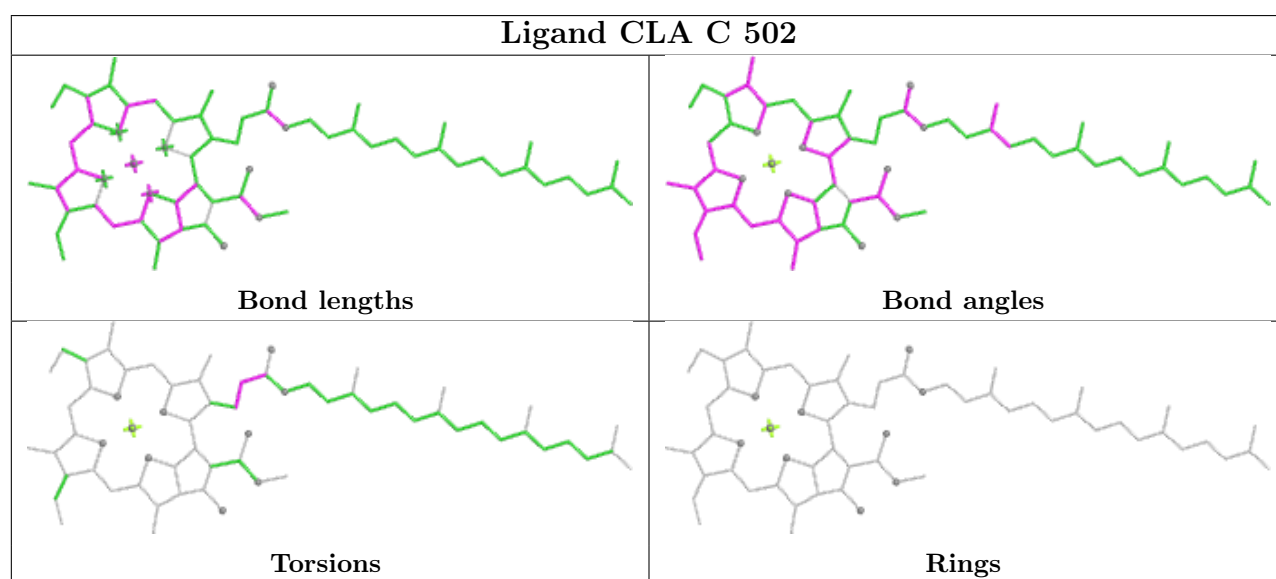
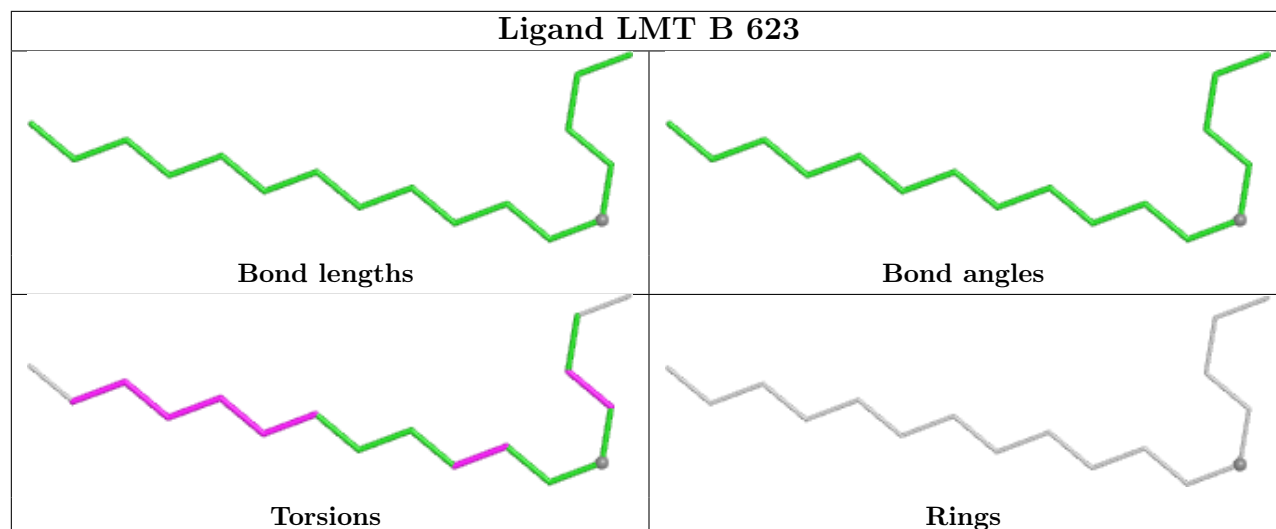
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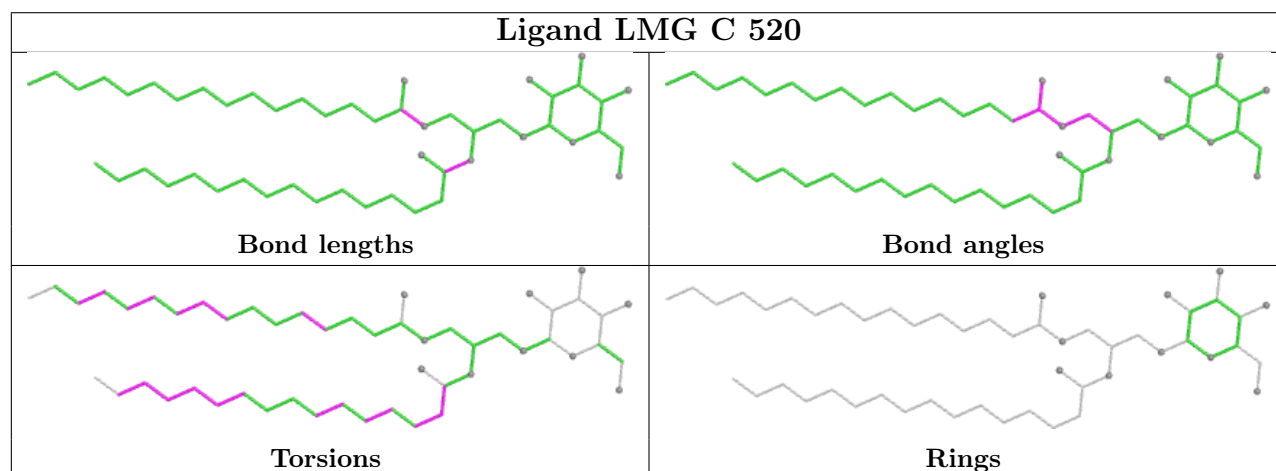
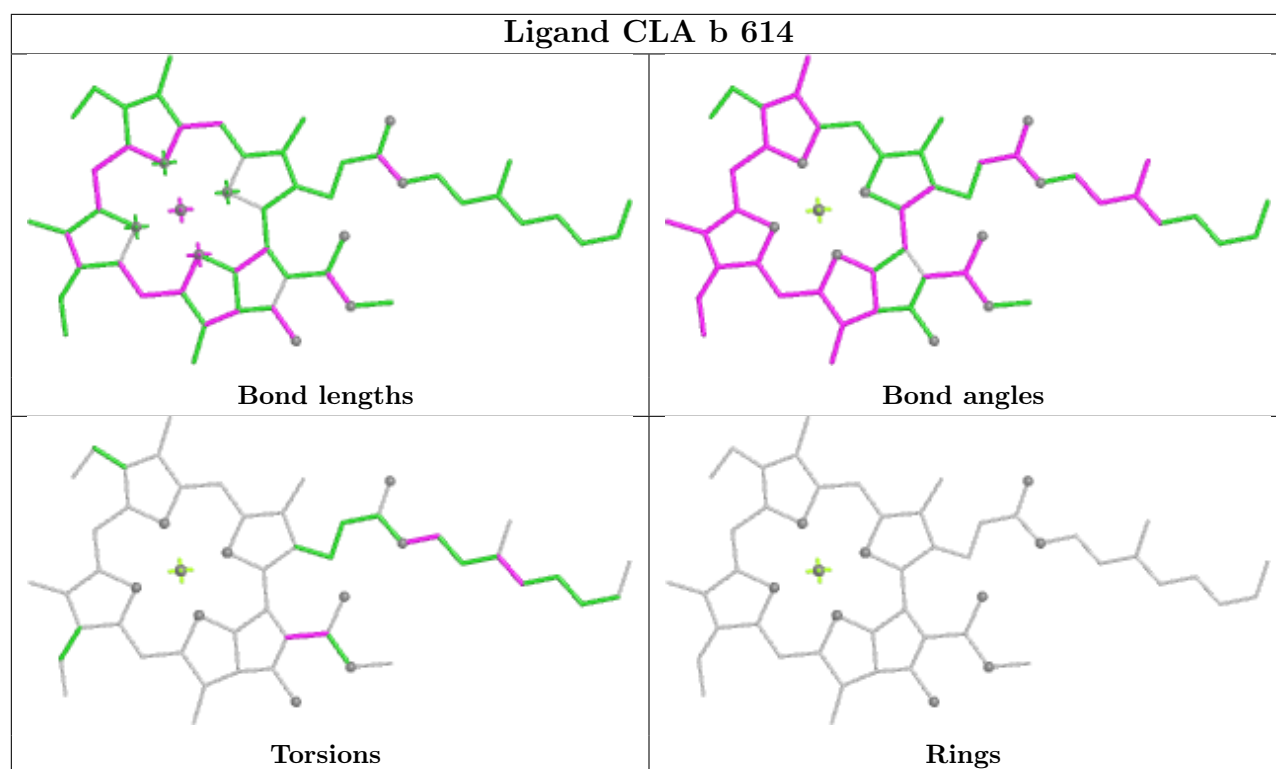
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	506	CLA	2	0
25	d	407	BCR	2	0
23	a	406	CLA	3	0
23	c	505	CLA	1	0
24	d	401	PHO	3	0
23	b	607	CLA	1	0
23	c	512	CLA	4	0
30	j	102	LMT	1	0
28	T	103	SQD	1	0
25	C	515	BCR	3	0
30	m	101	LMT	1	0
23	c	513	CLA	4	0
25	y	101	BCR	4	0
23	b	616	CLA	2	0
23	B	606	CLA	5	0
23	B	604	CLA	1	0
33	e	101	LHG	1	0
27	D	408	PL9	1	0
23	B	605	CLA	3	0
23	b	611	CLA	2	0

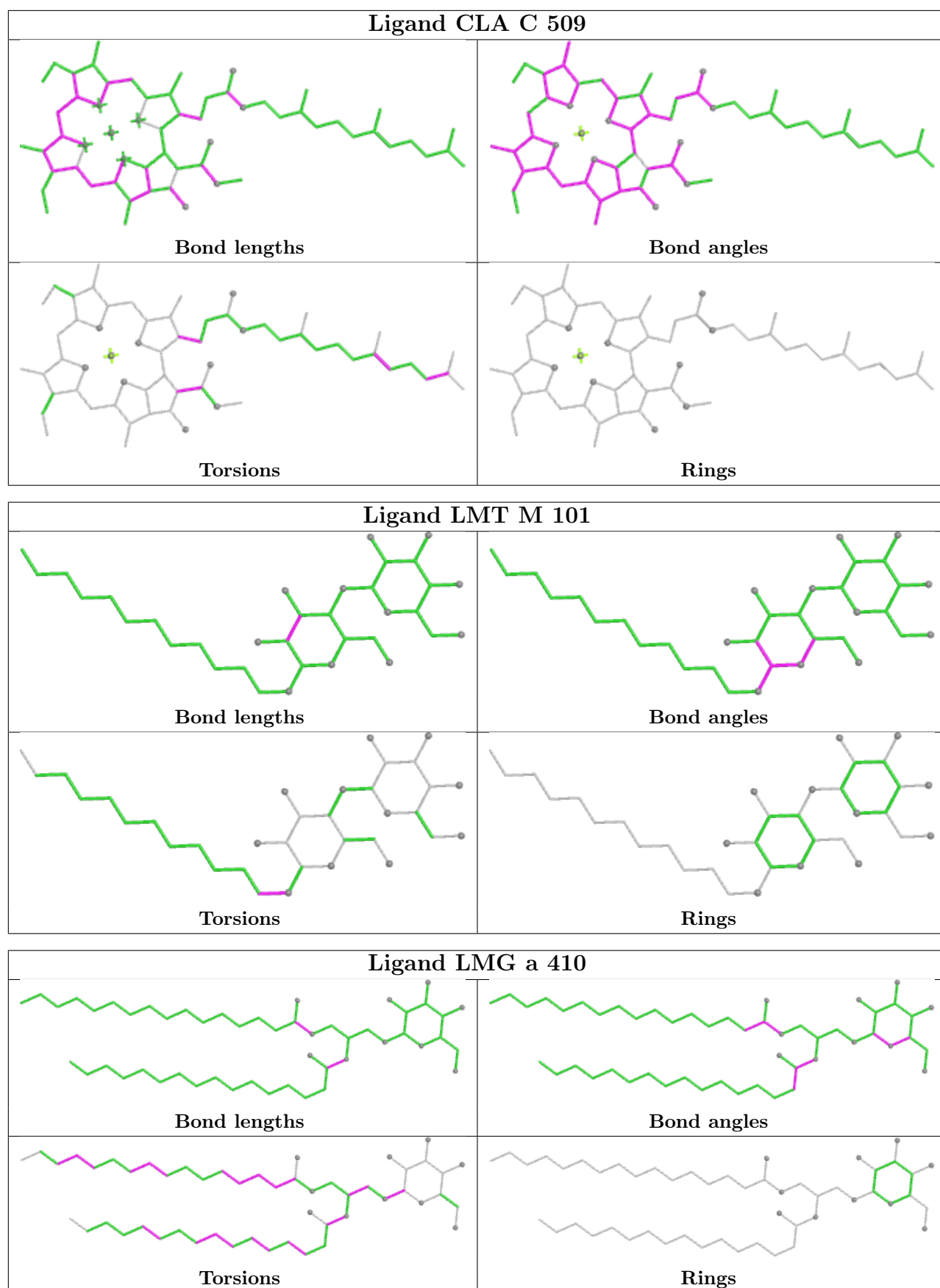
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

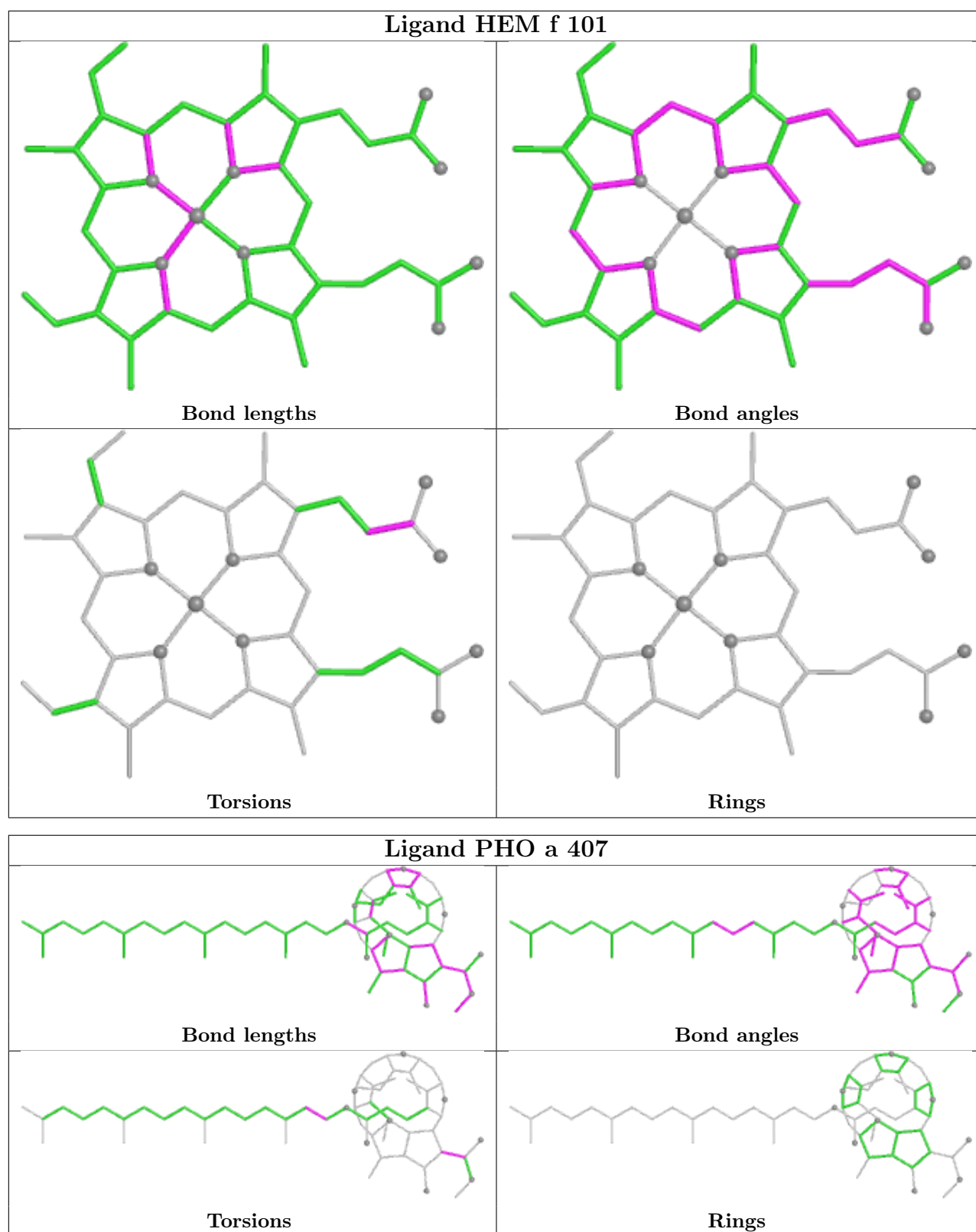


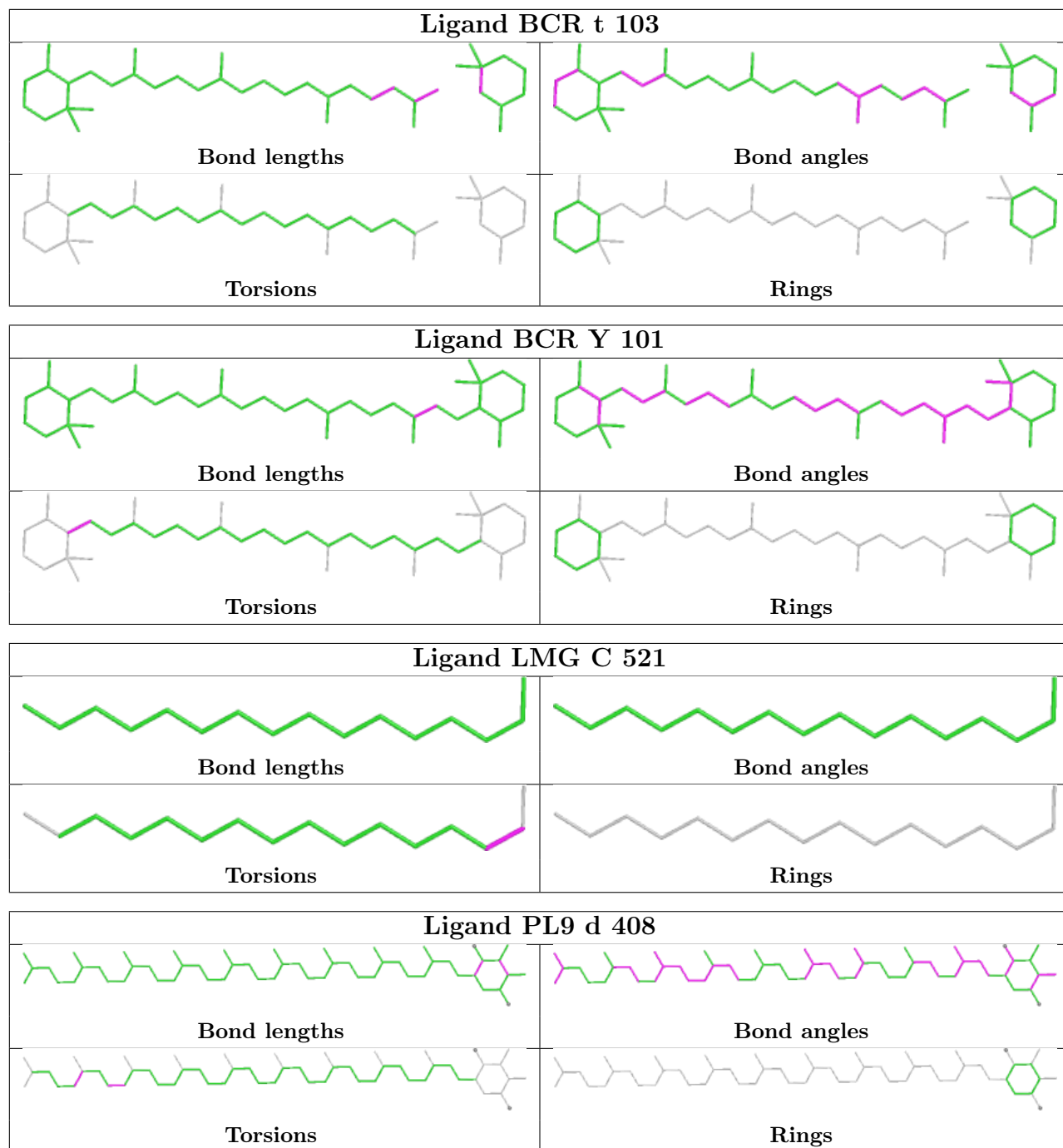


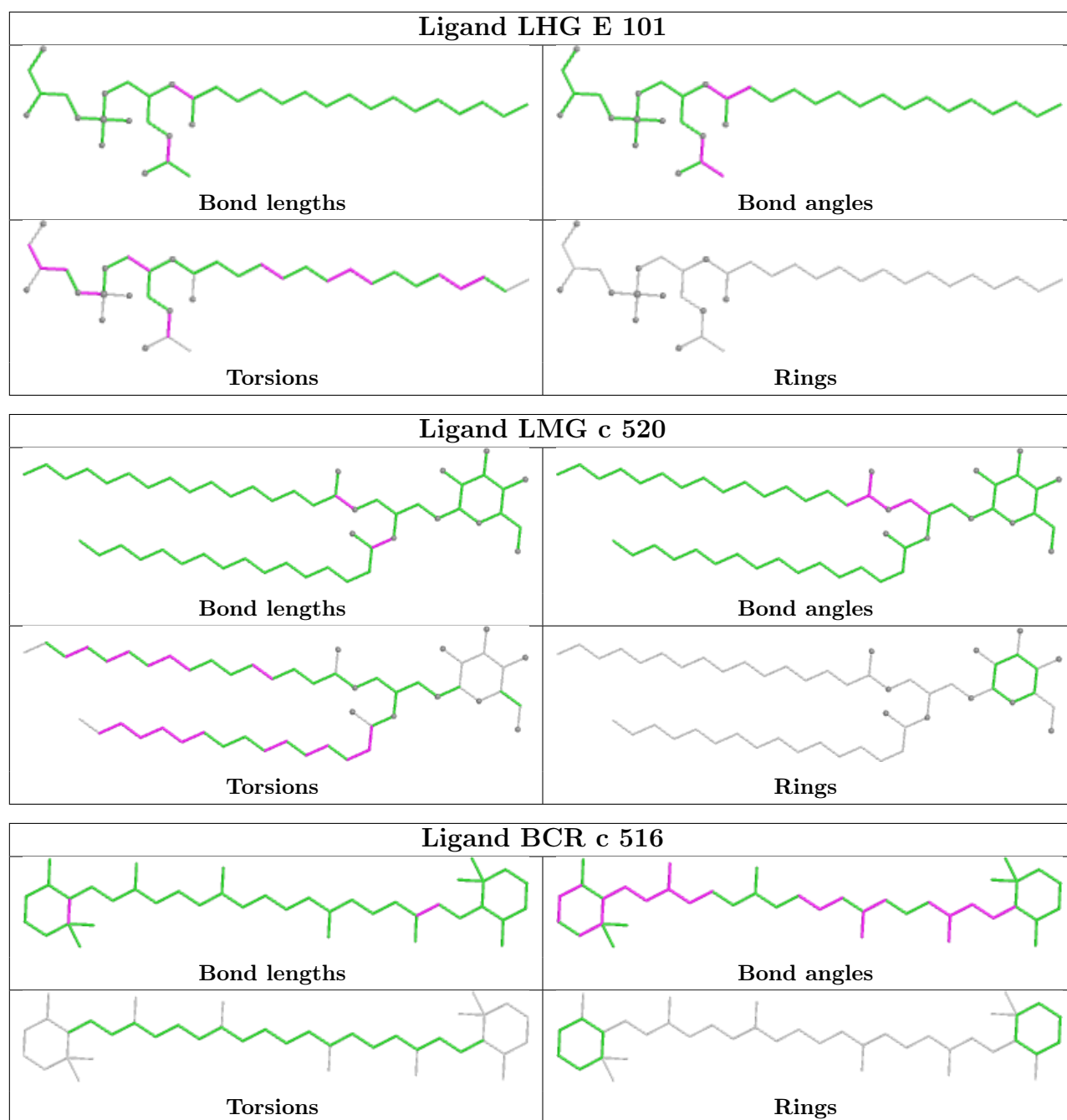


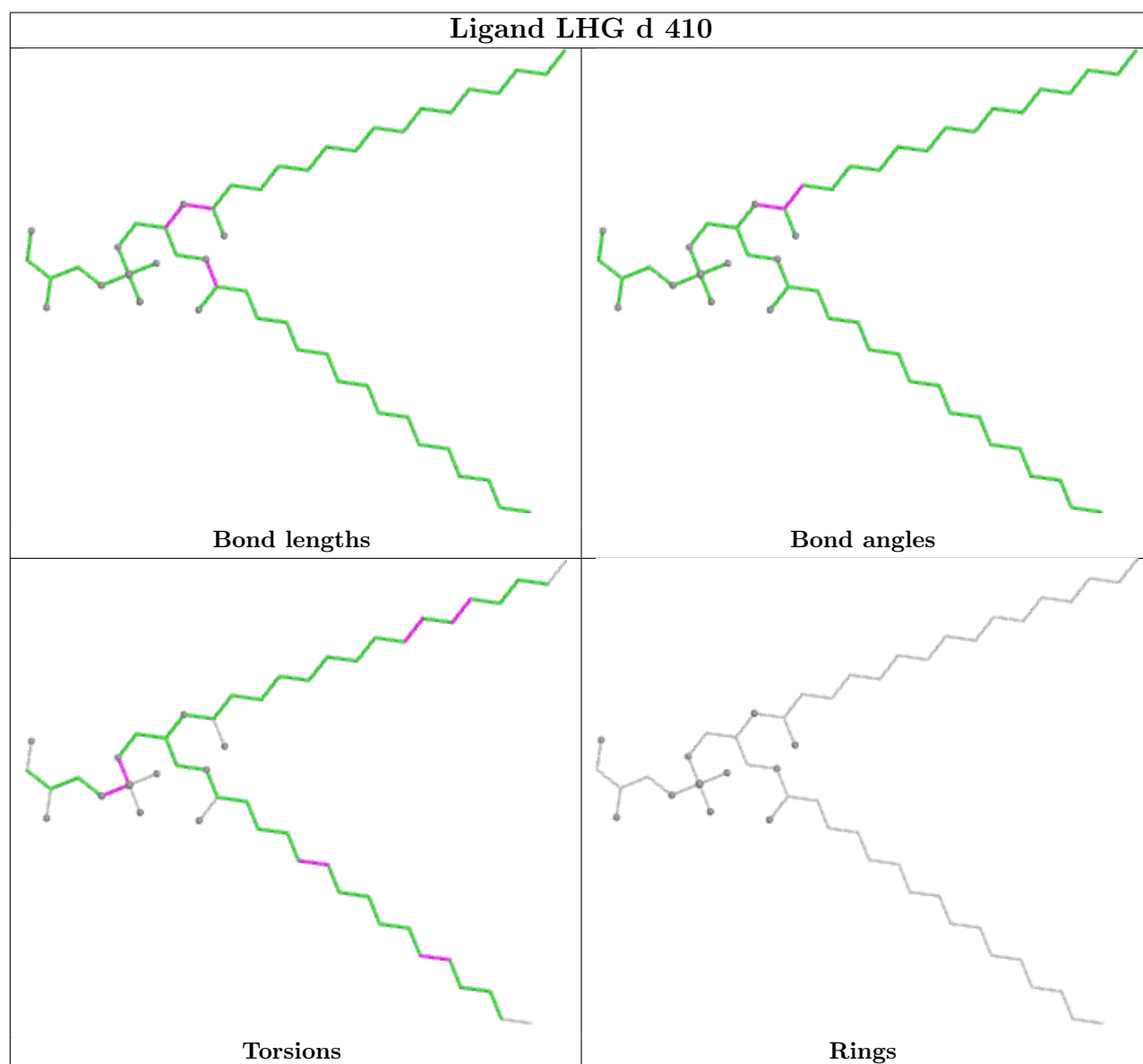
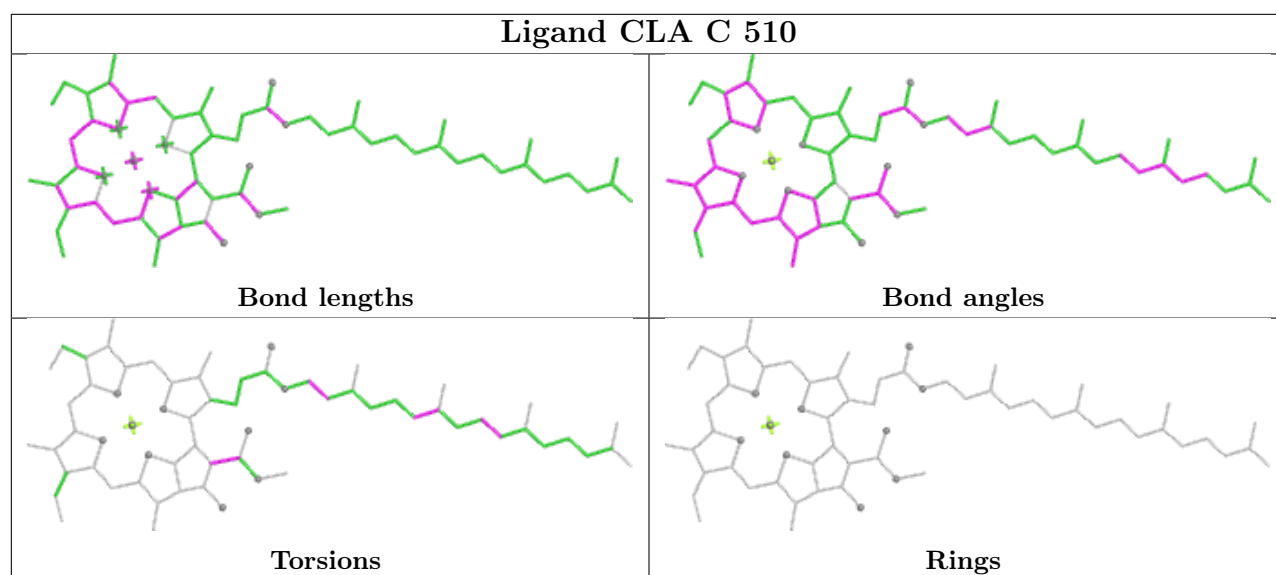


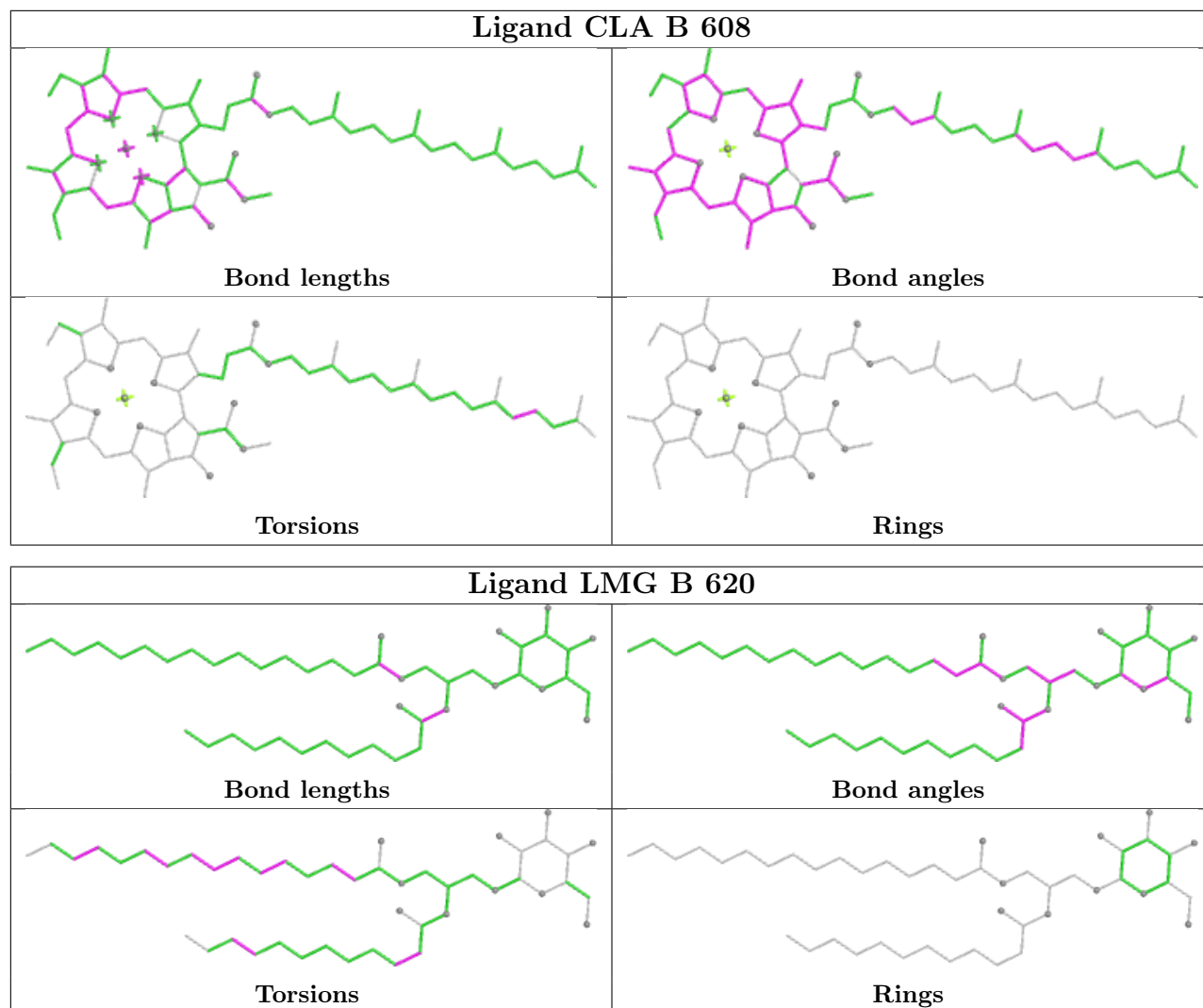


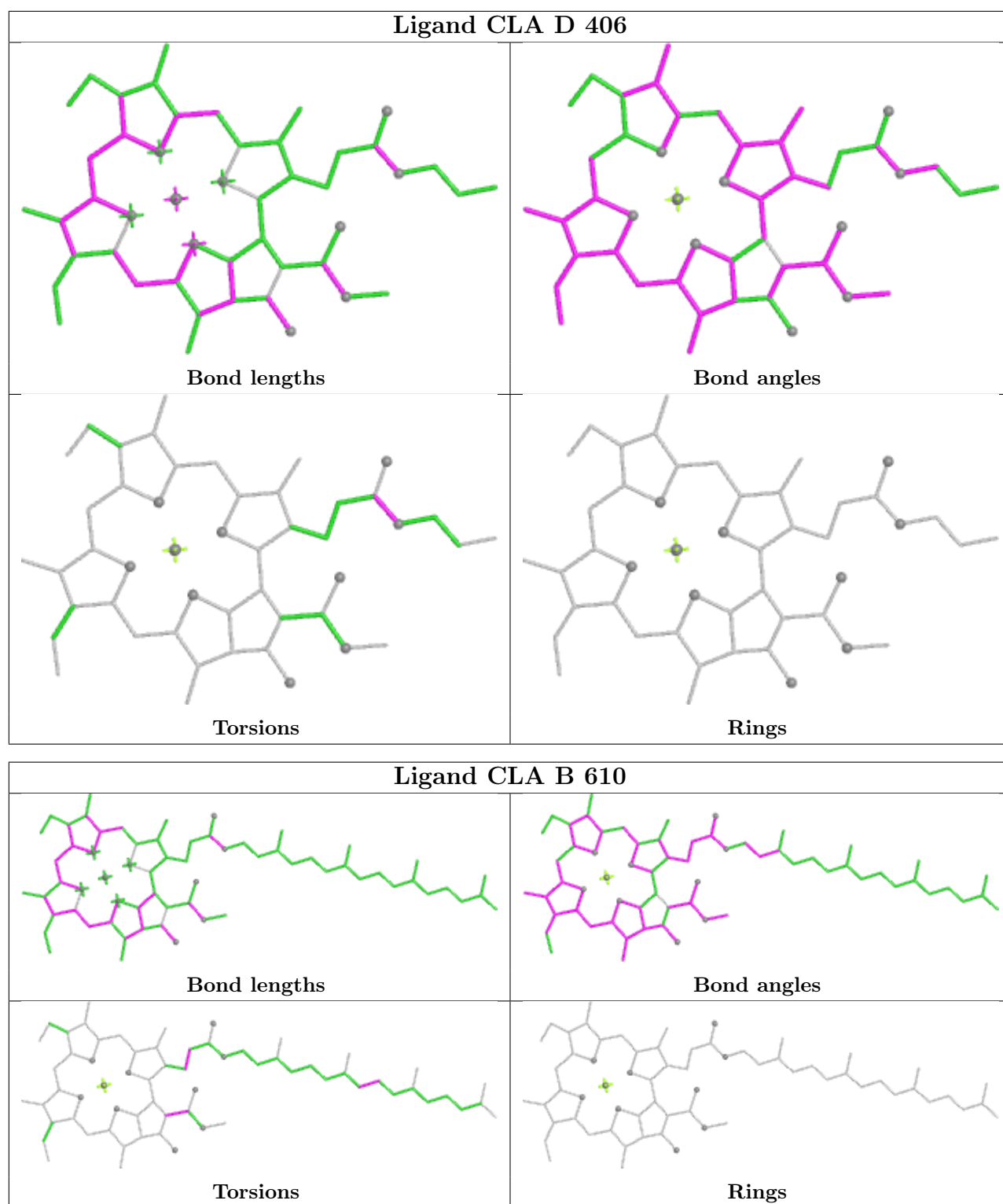


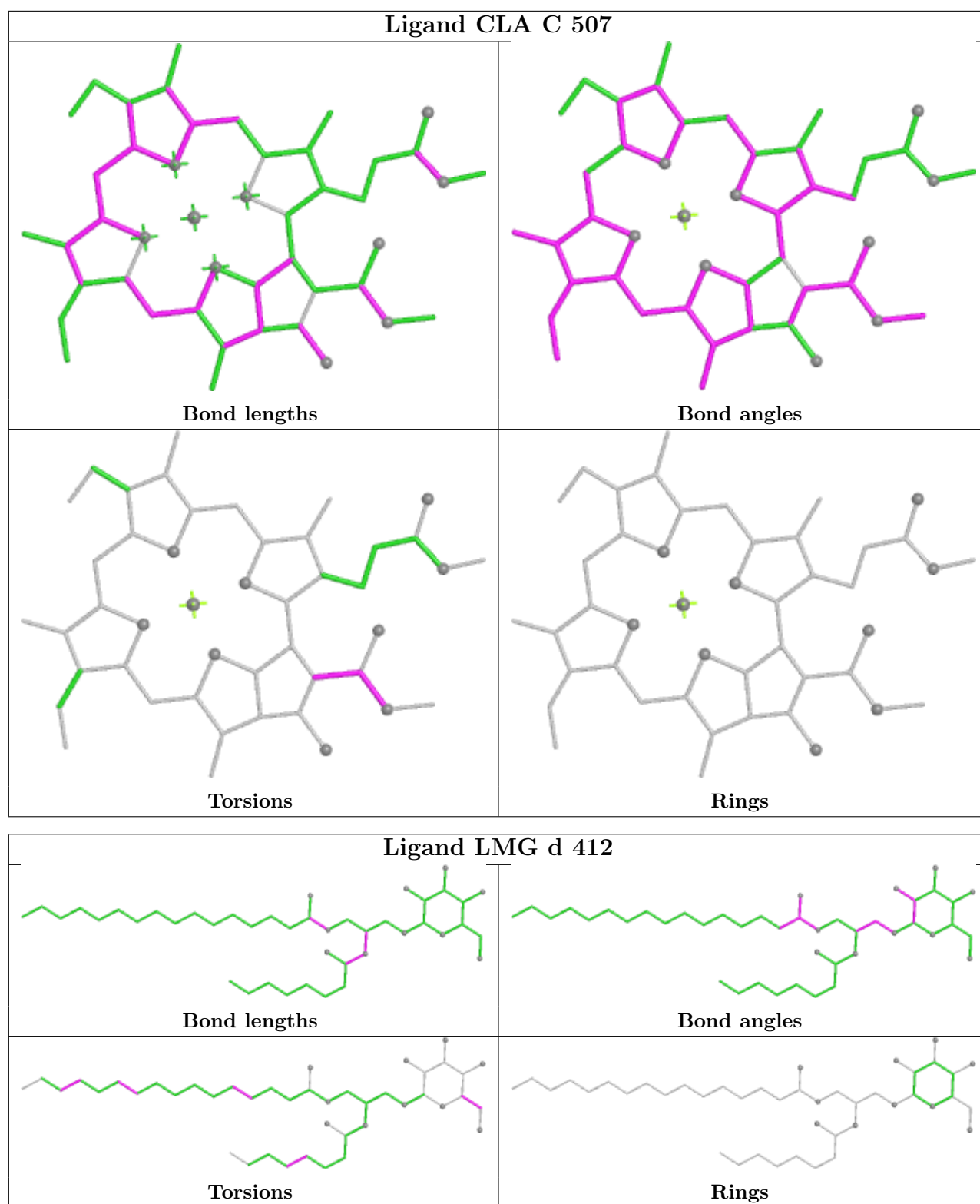


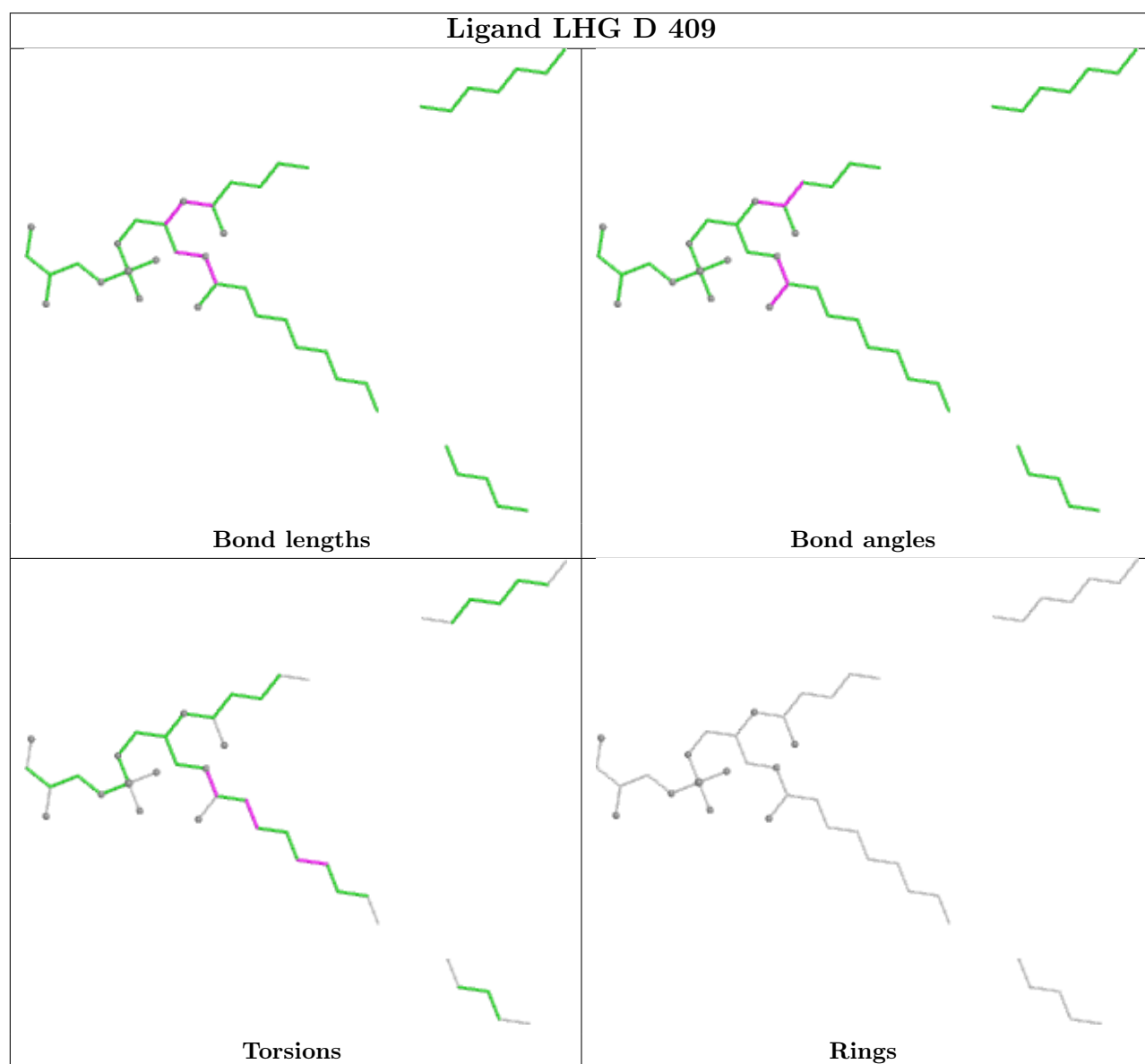
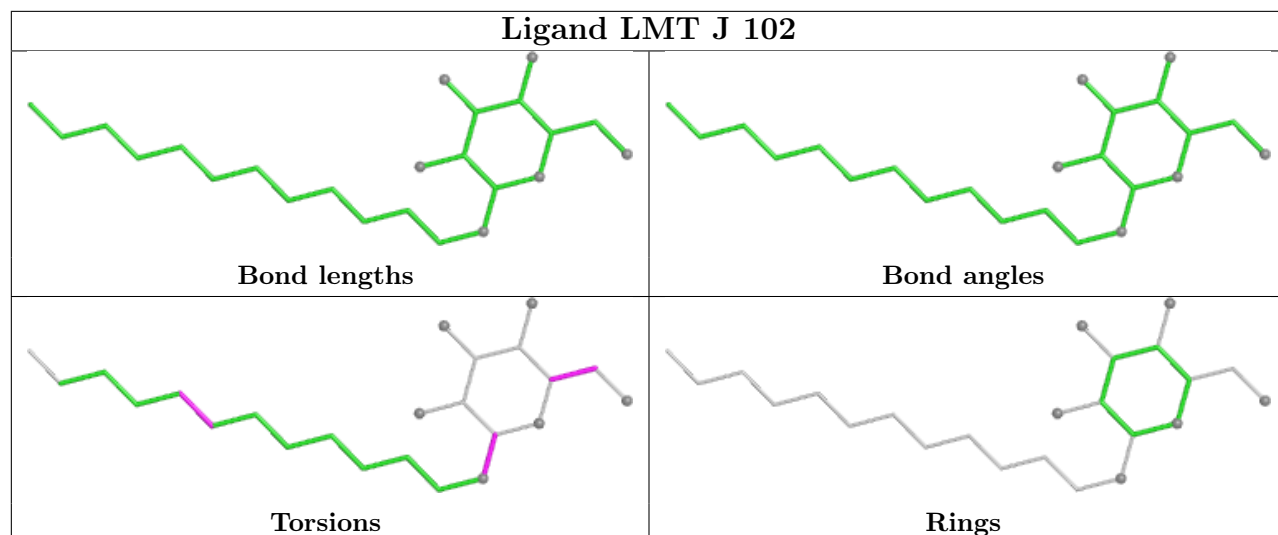


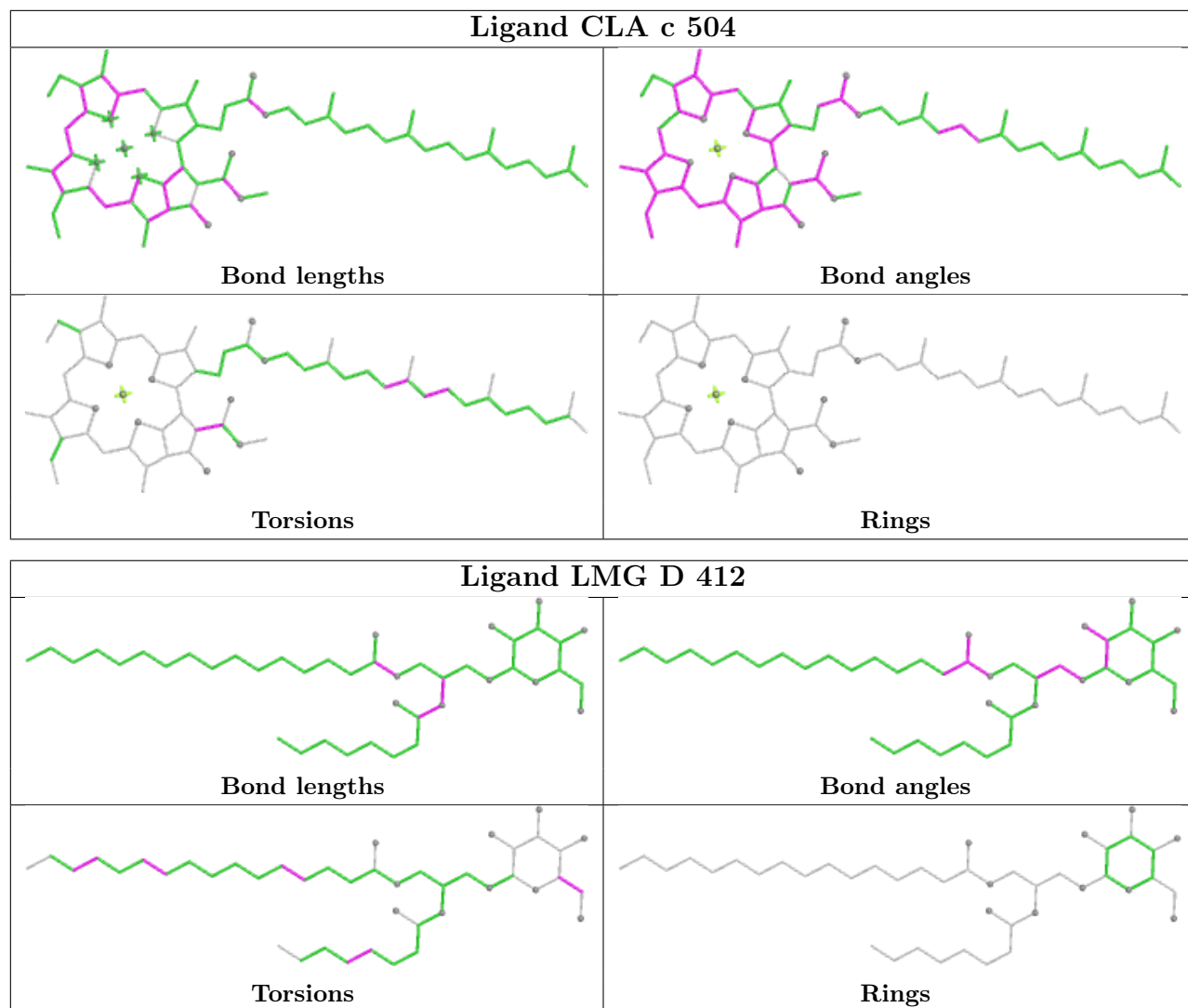


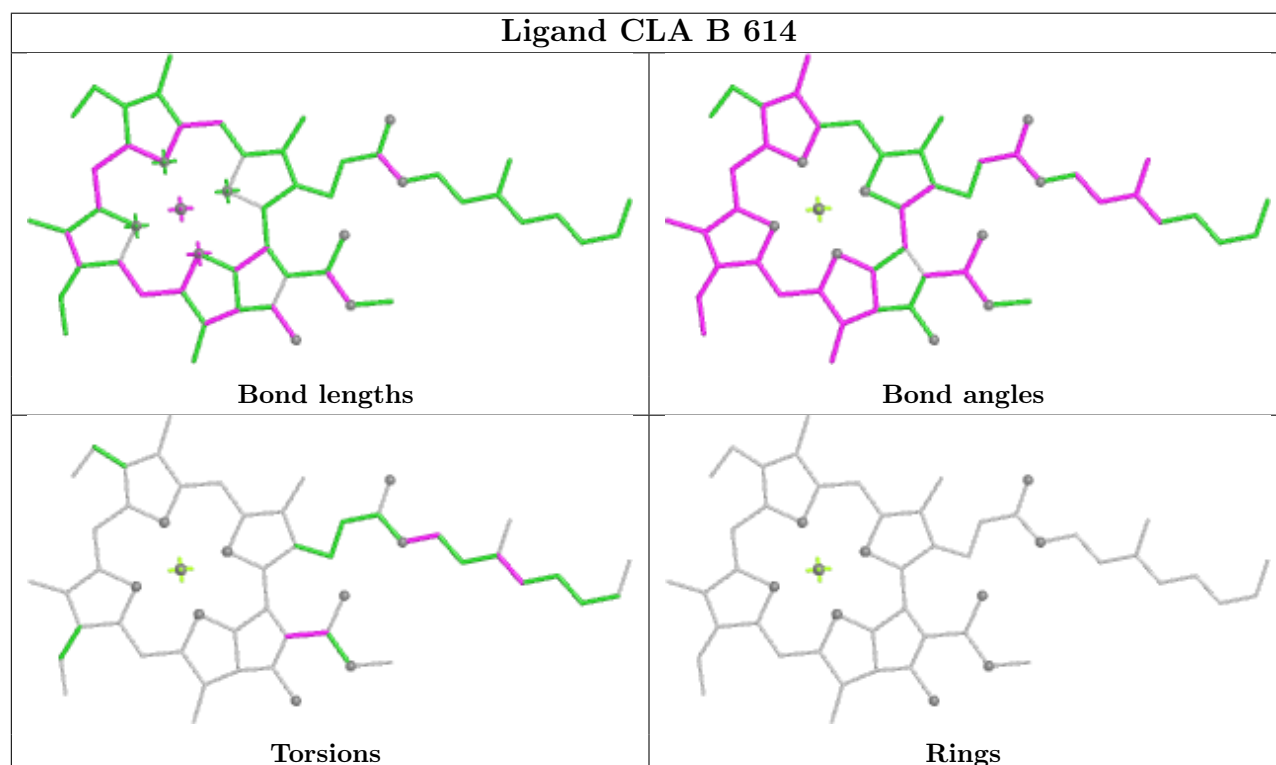
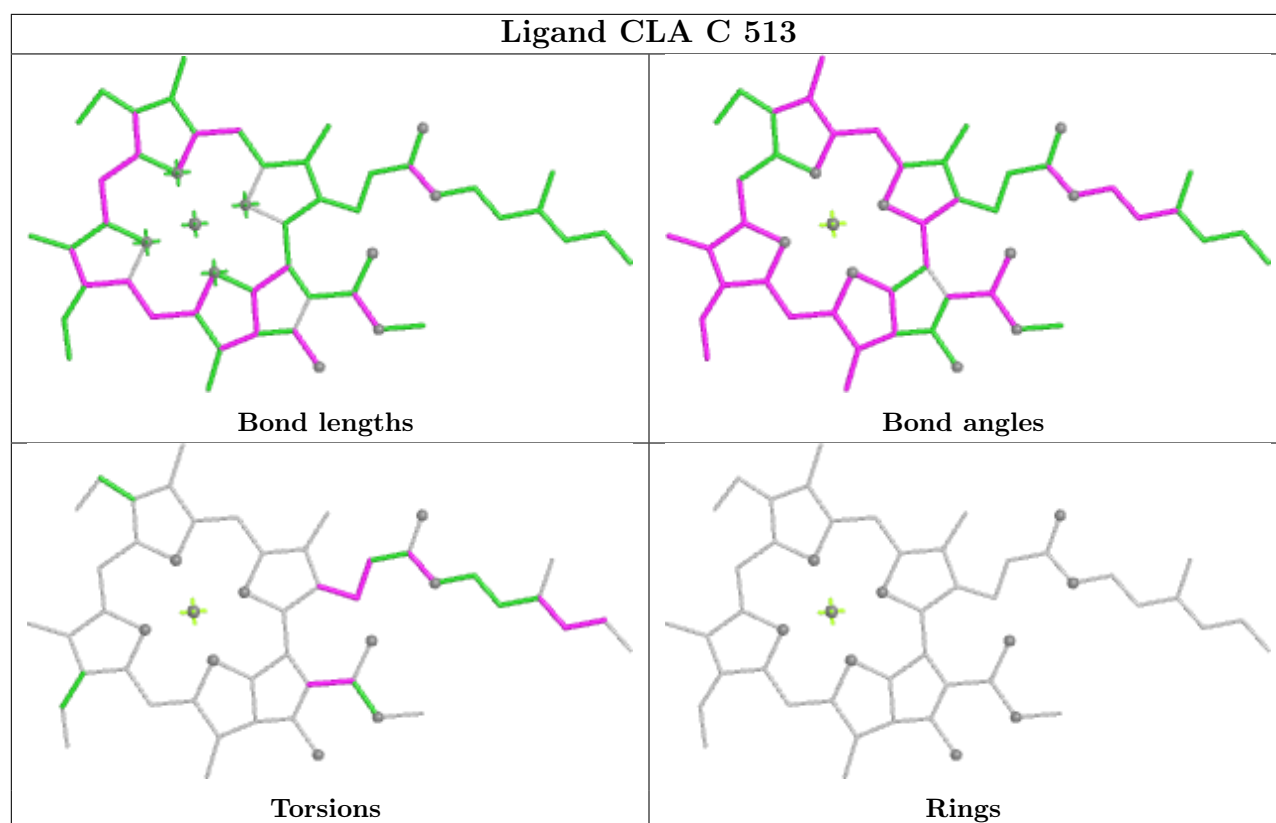


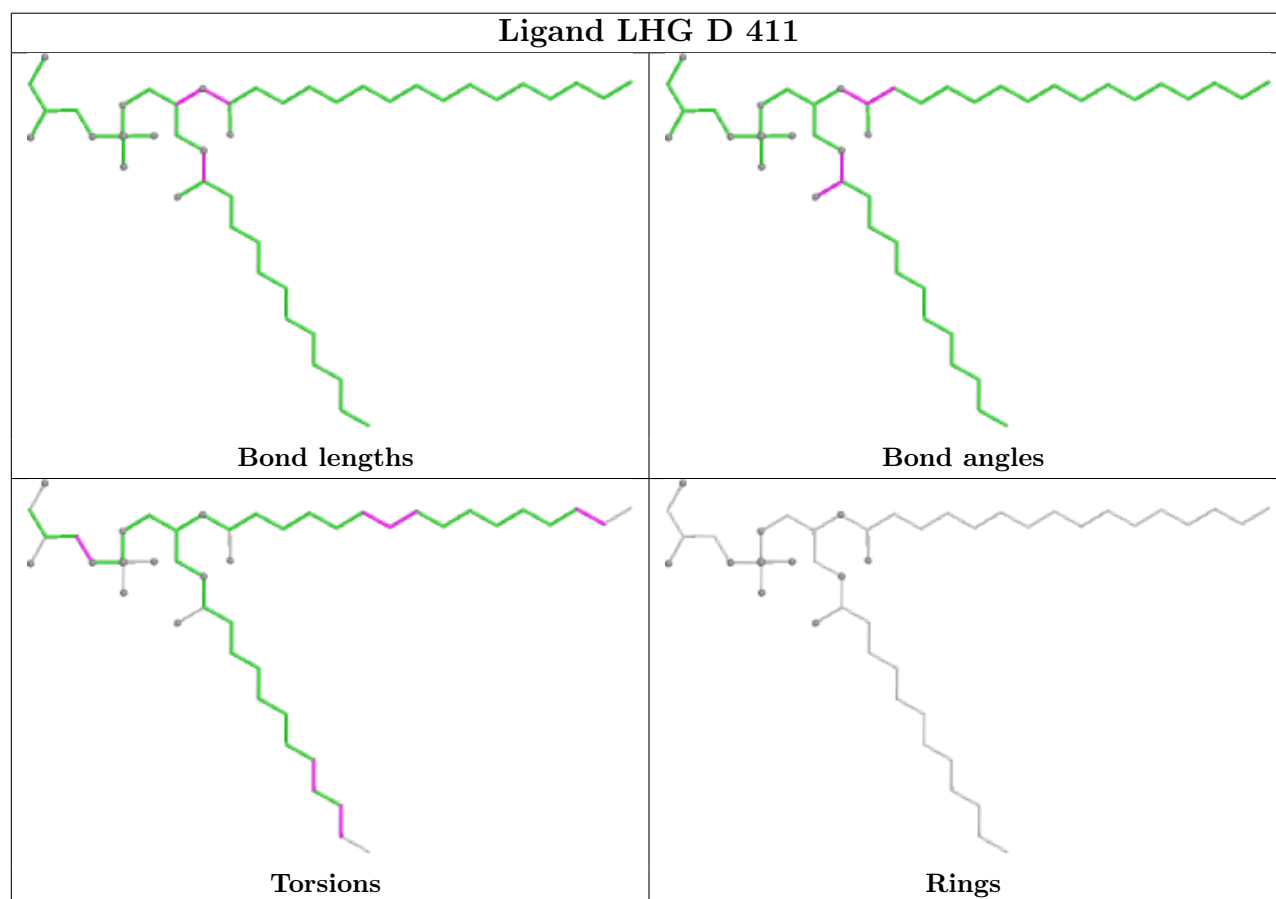
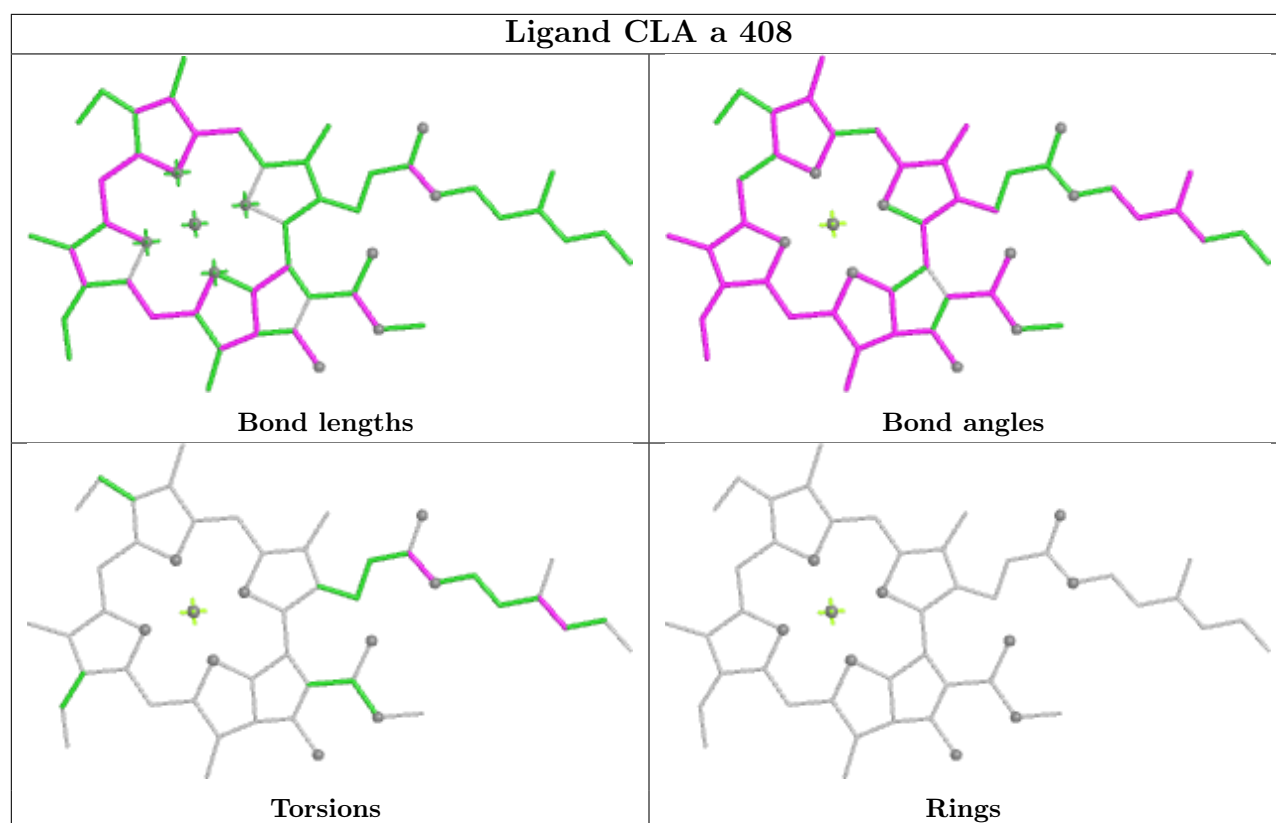


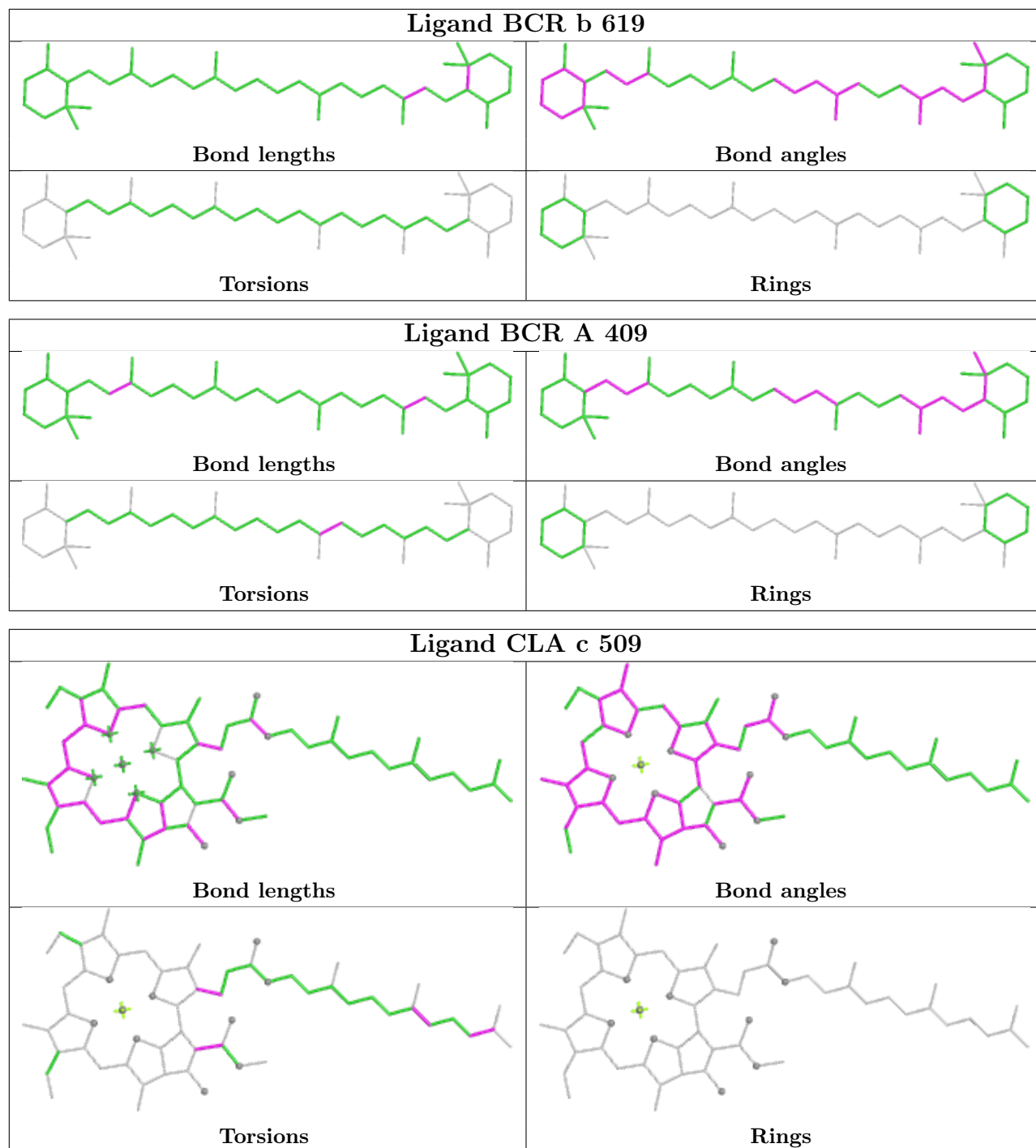


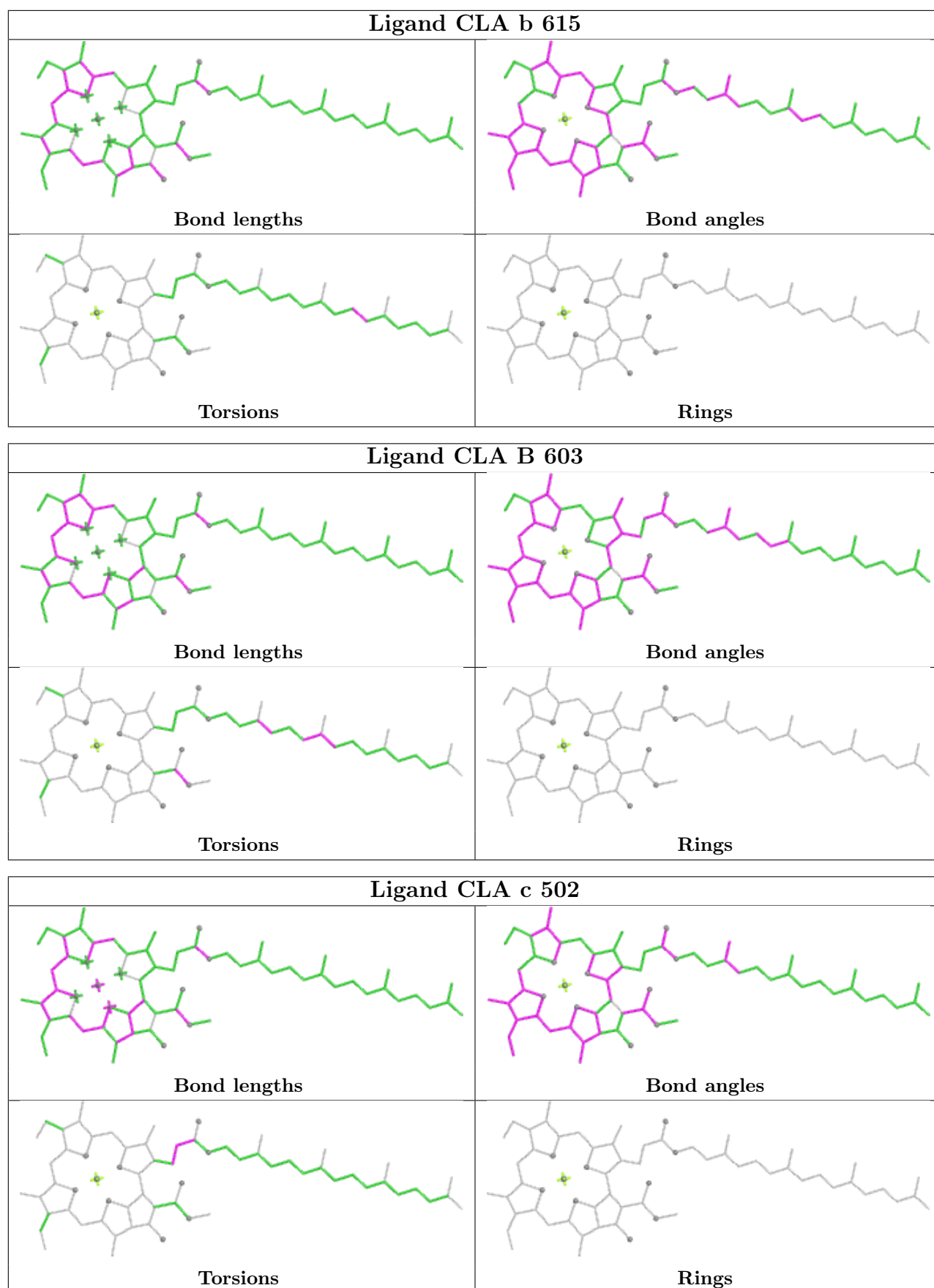


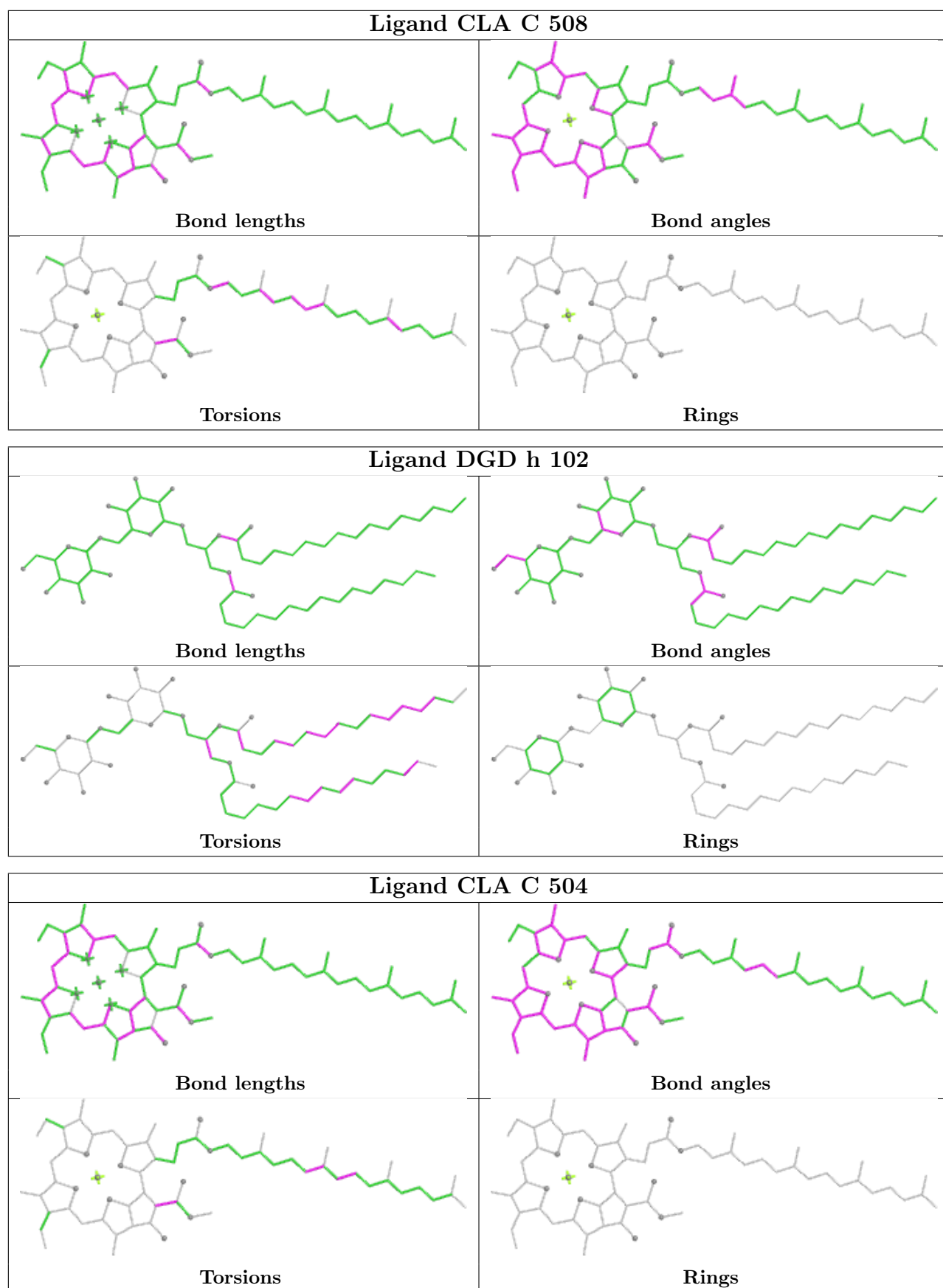


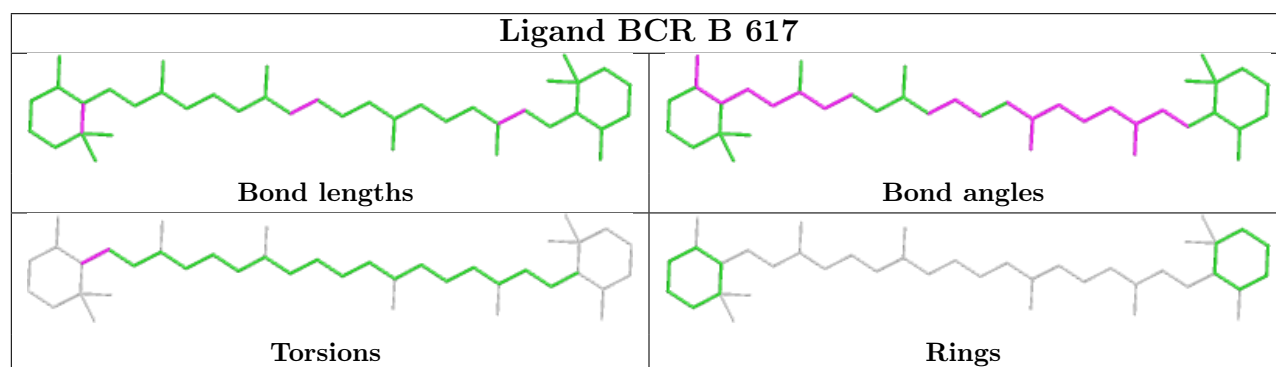
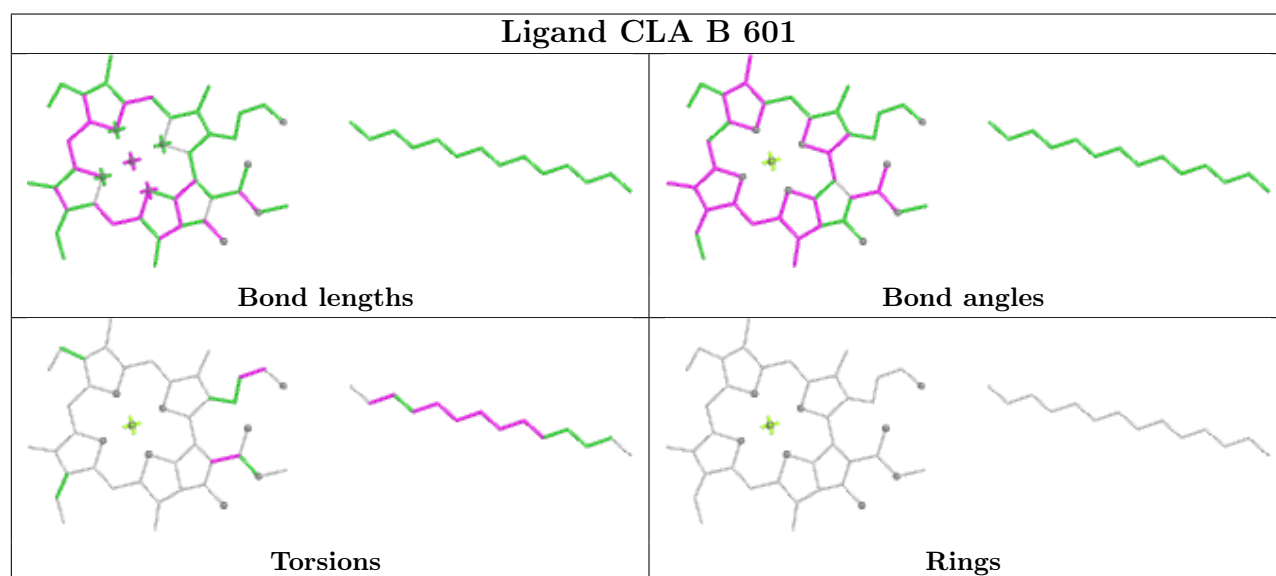
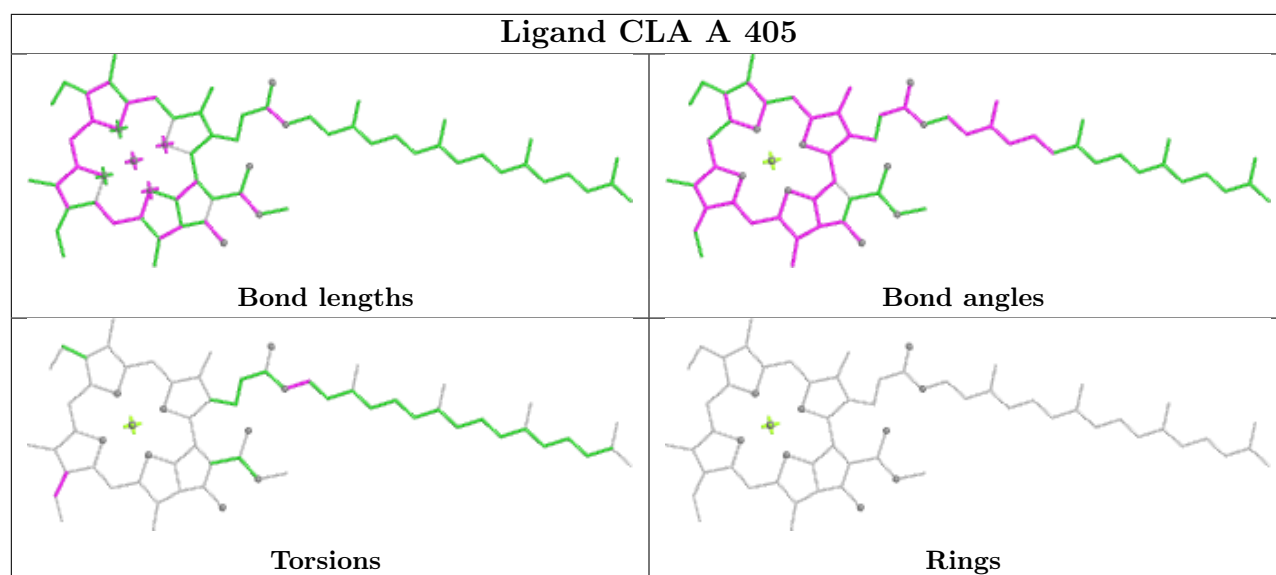


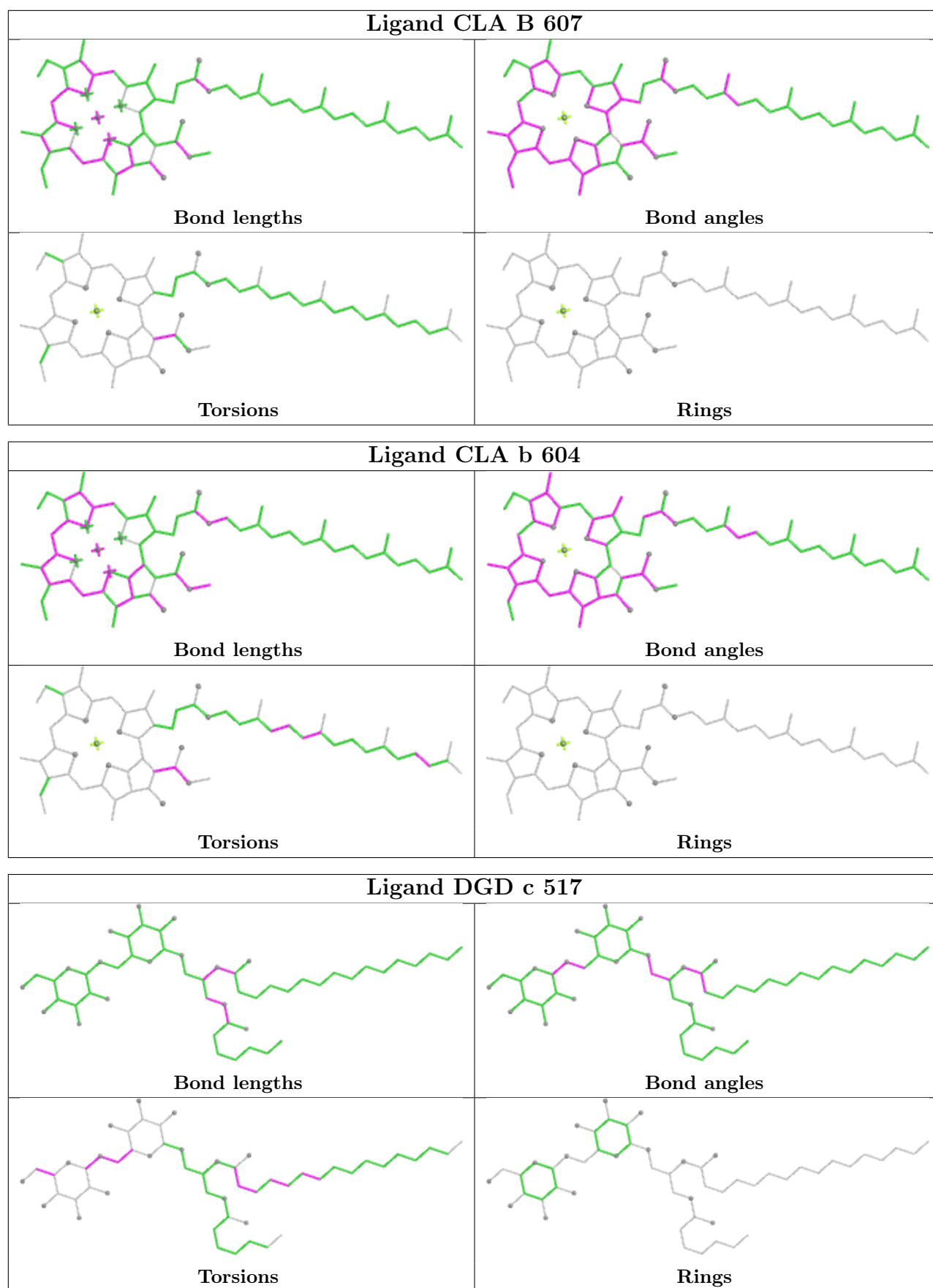


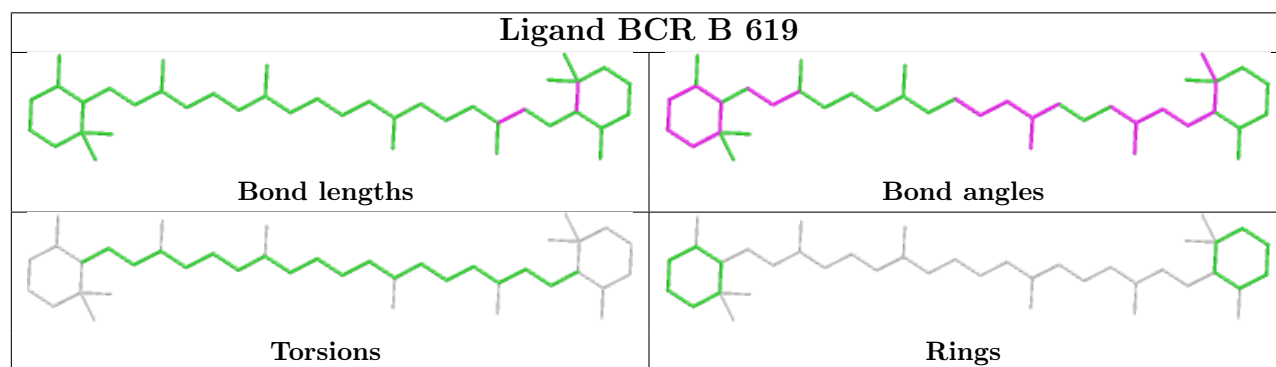
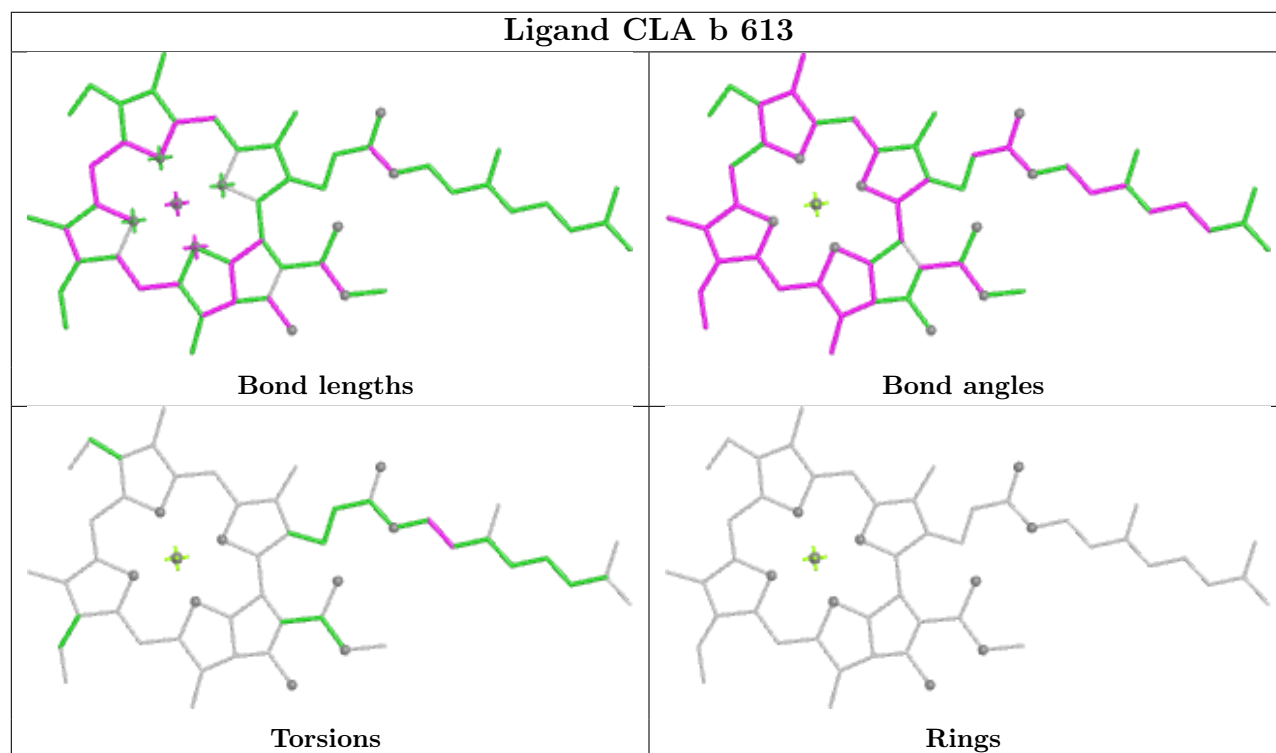
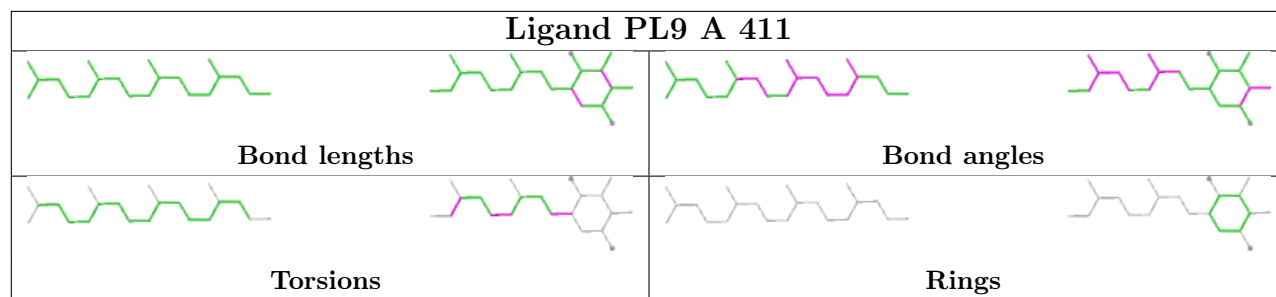


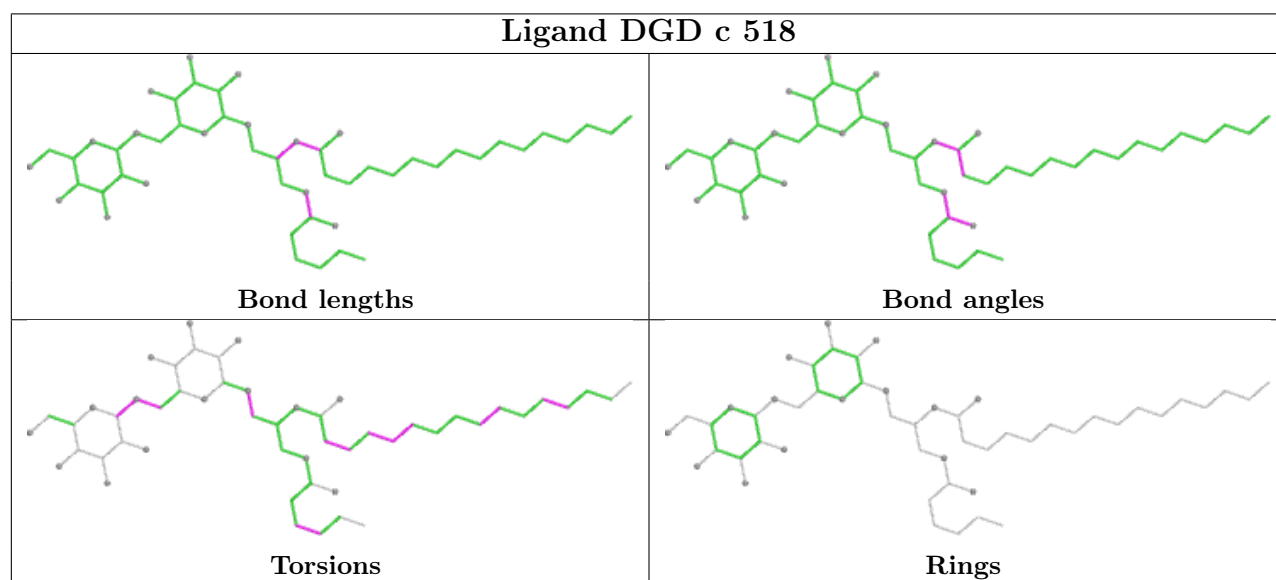
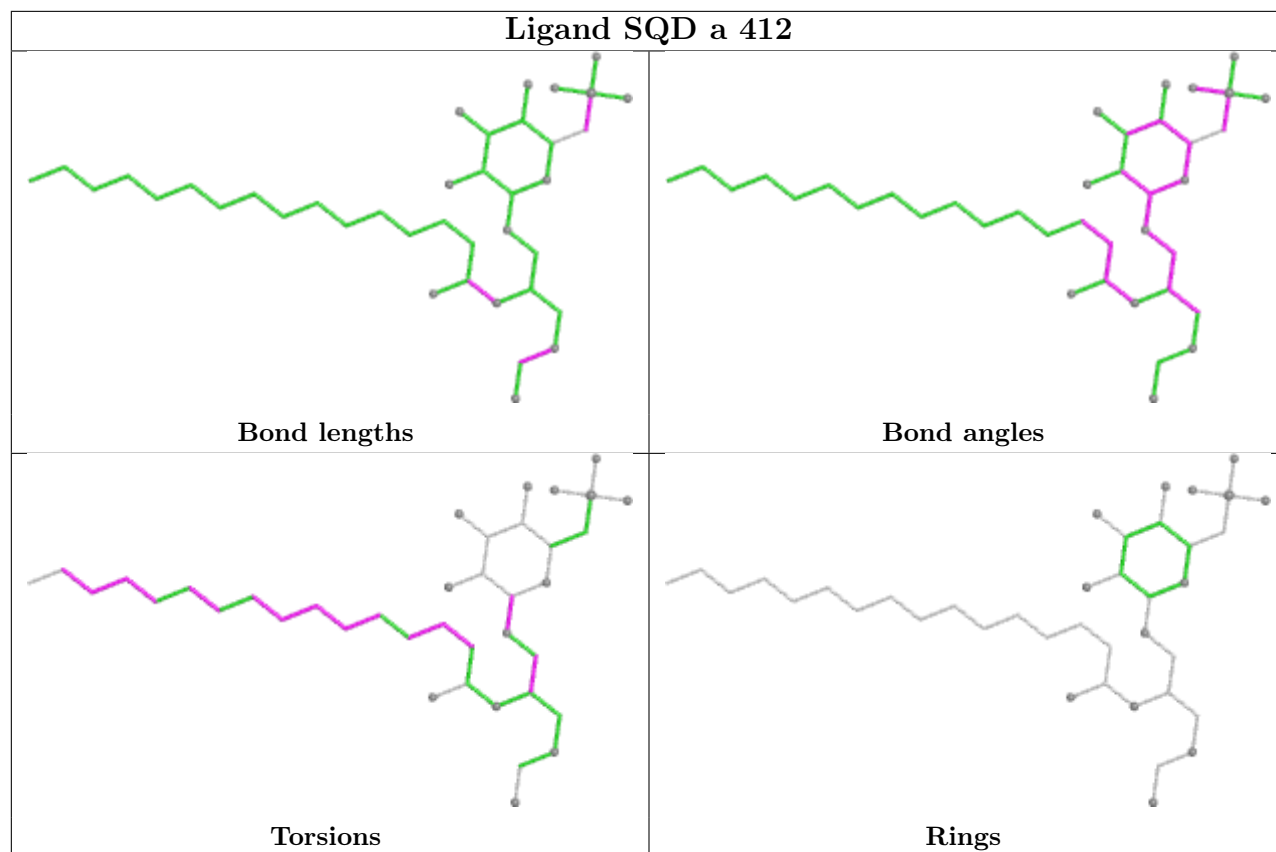


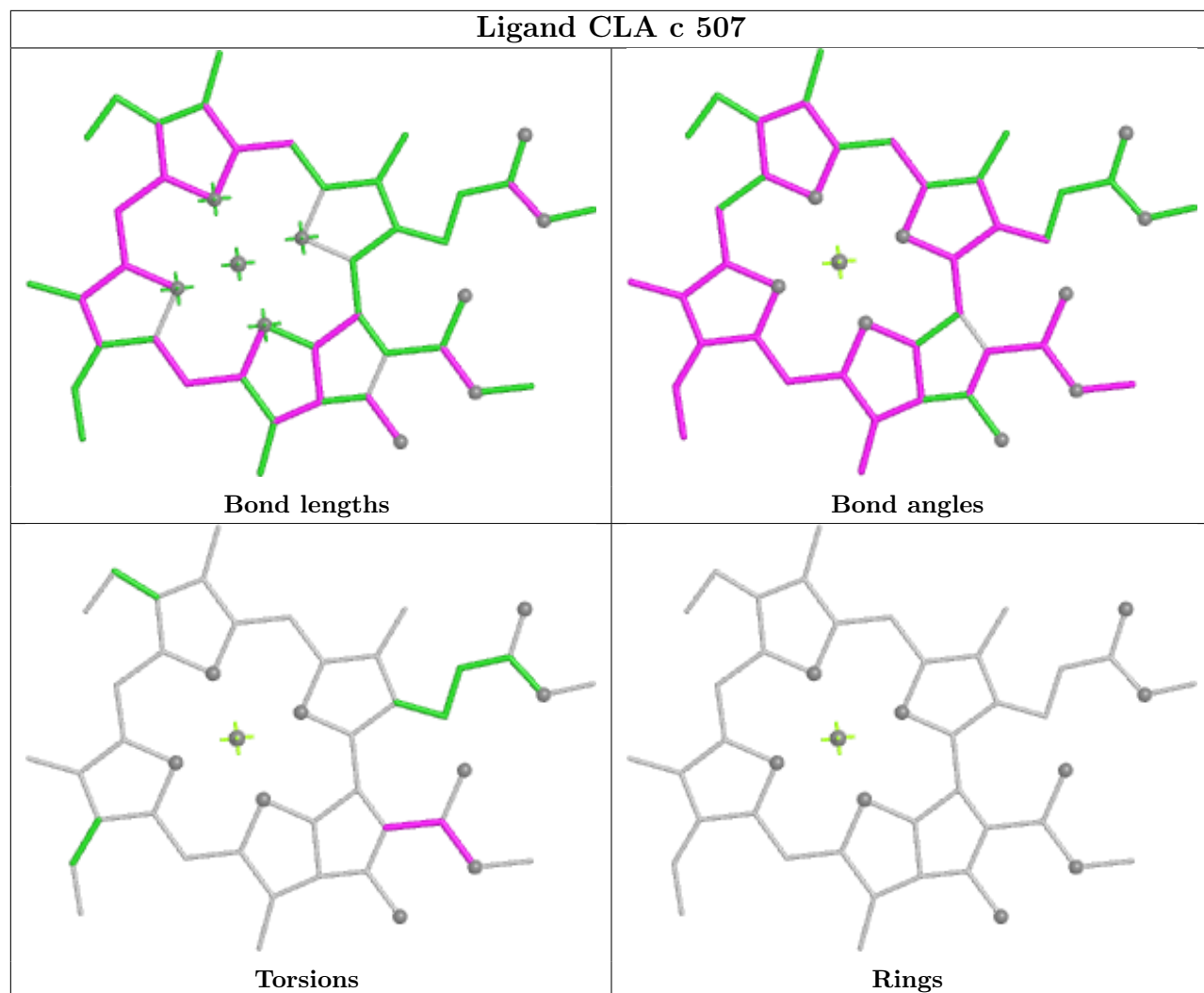


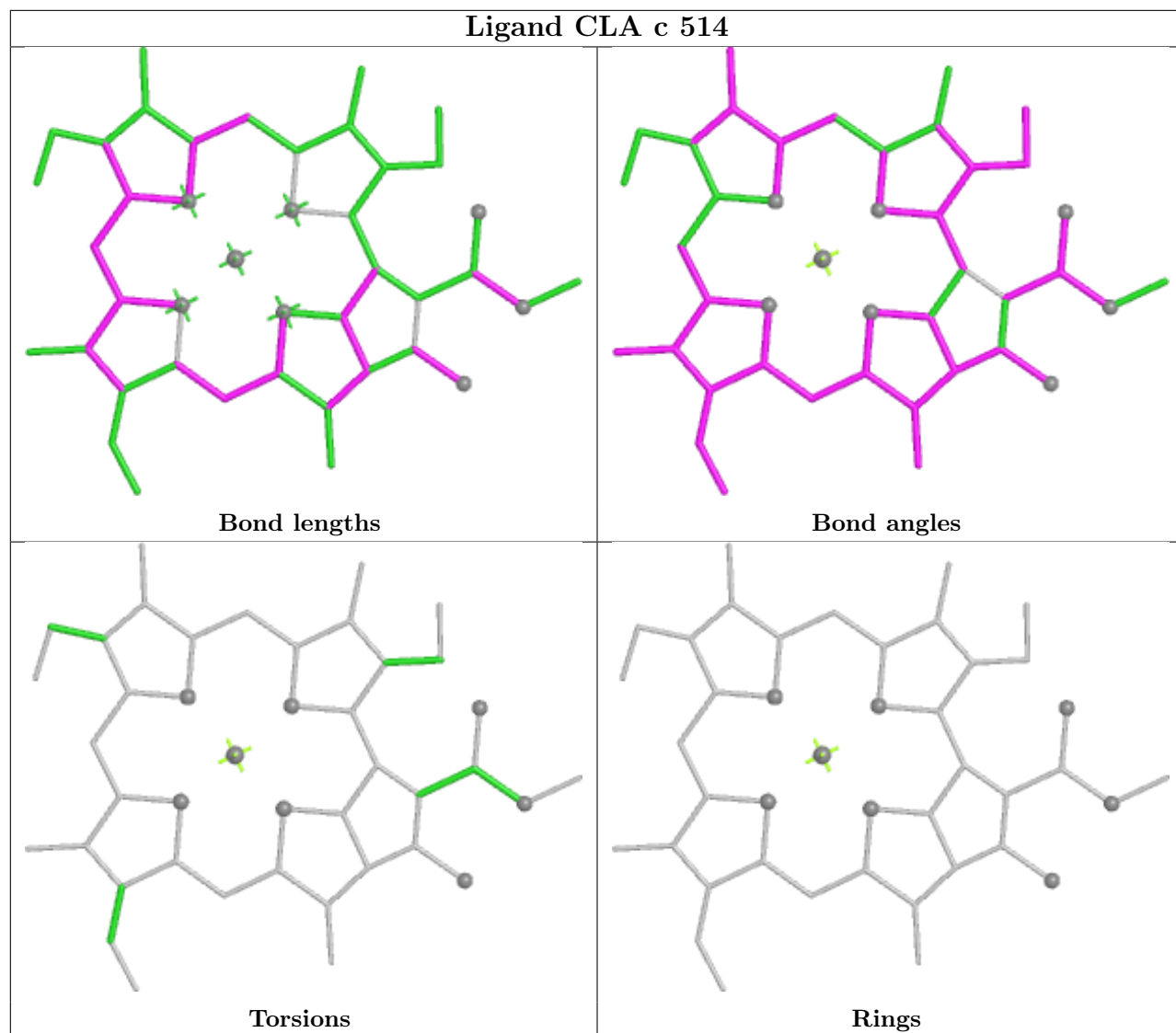


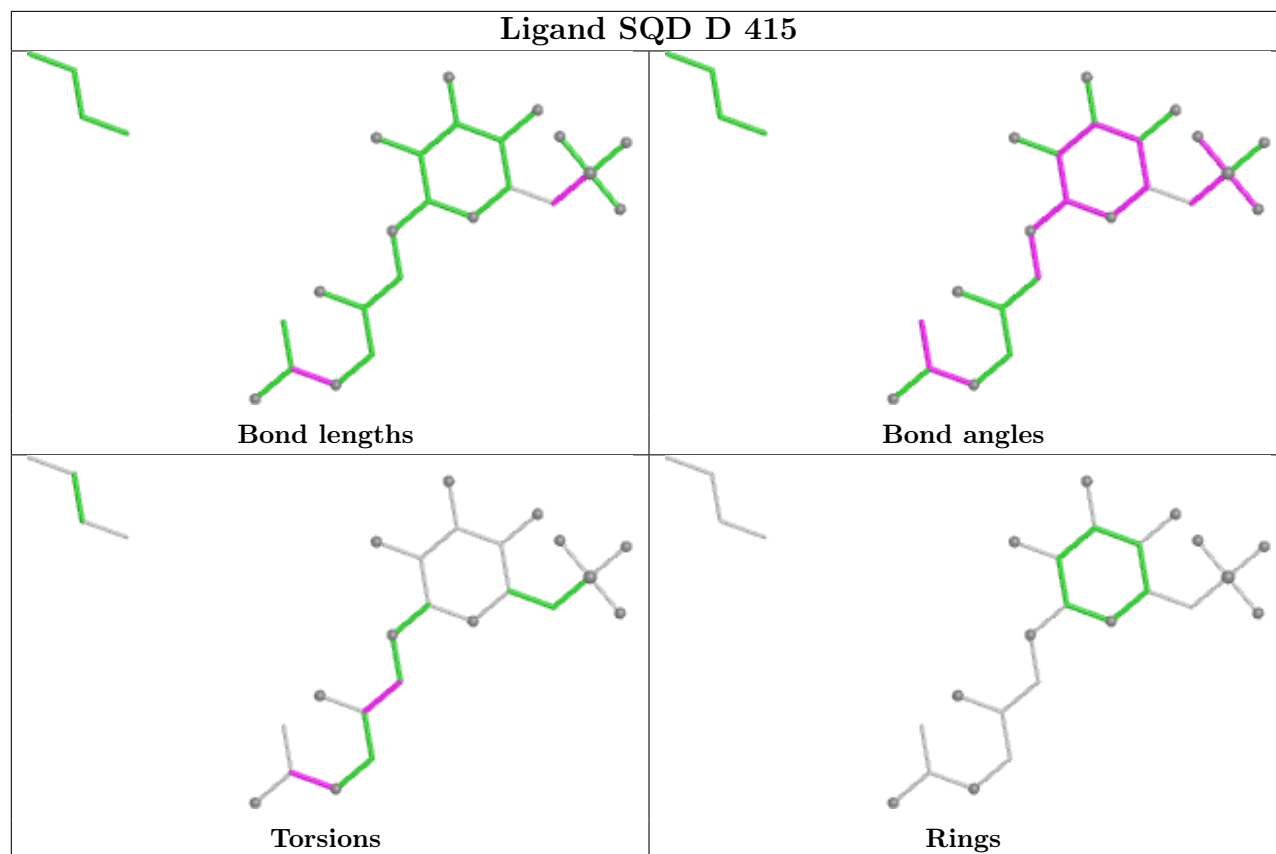


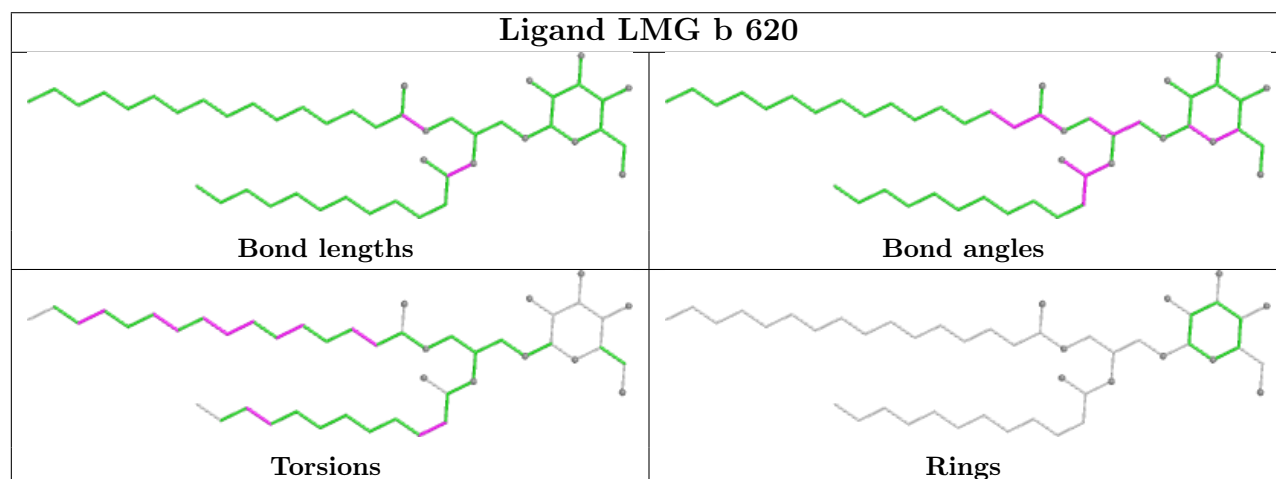
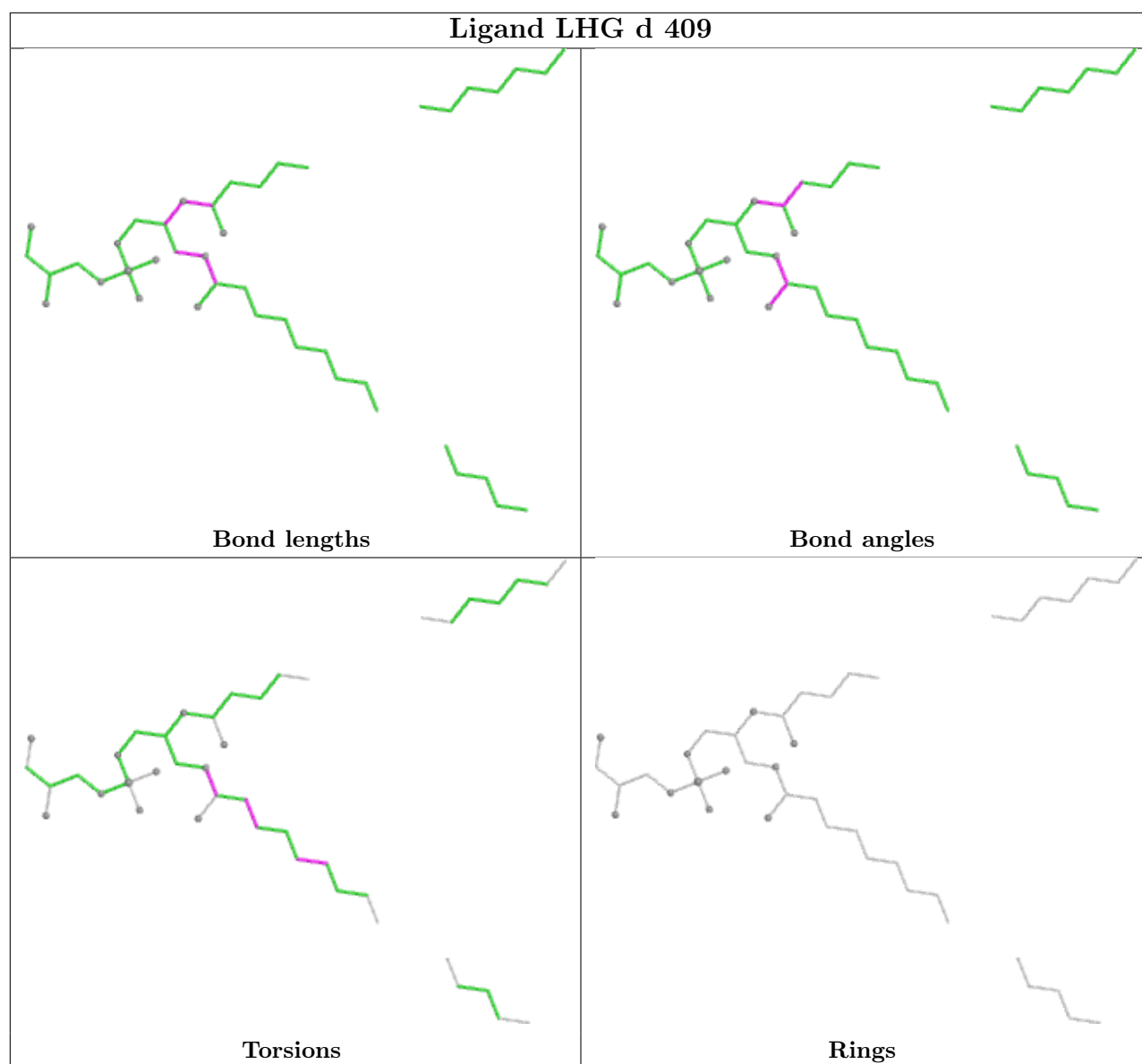


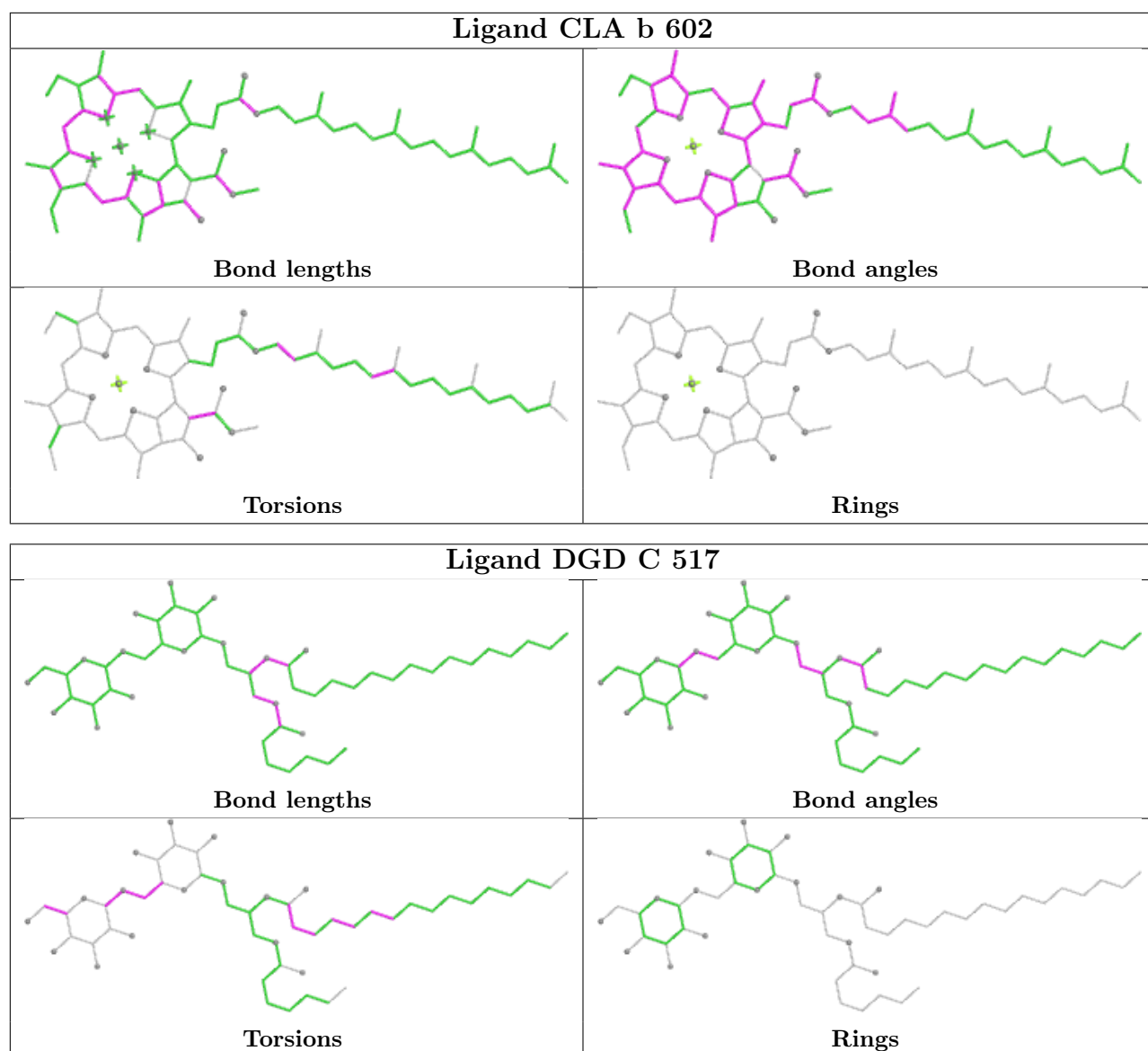


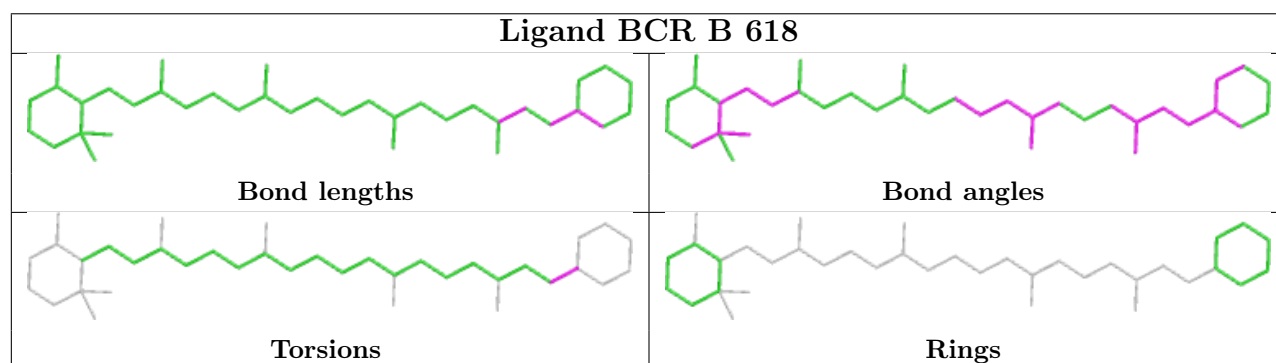
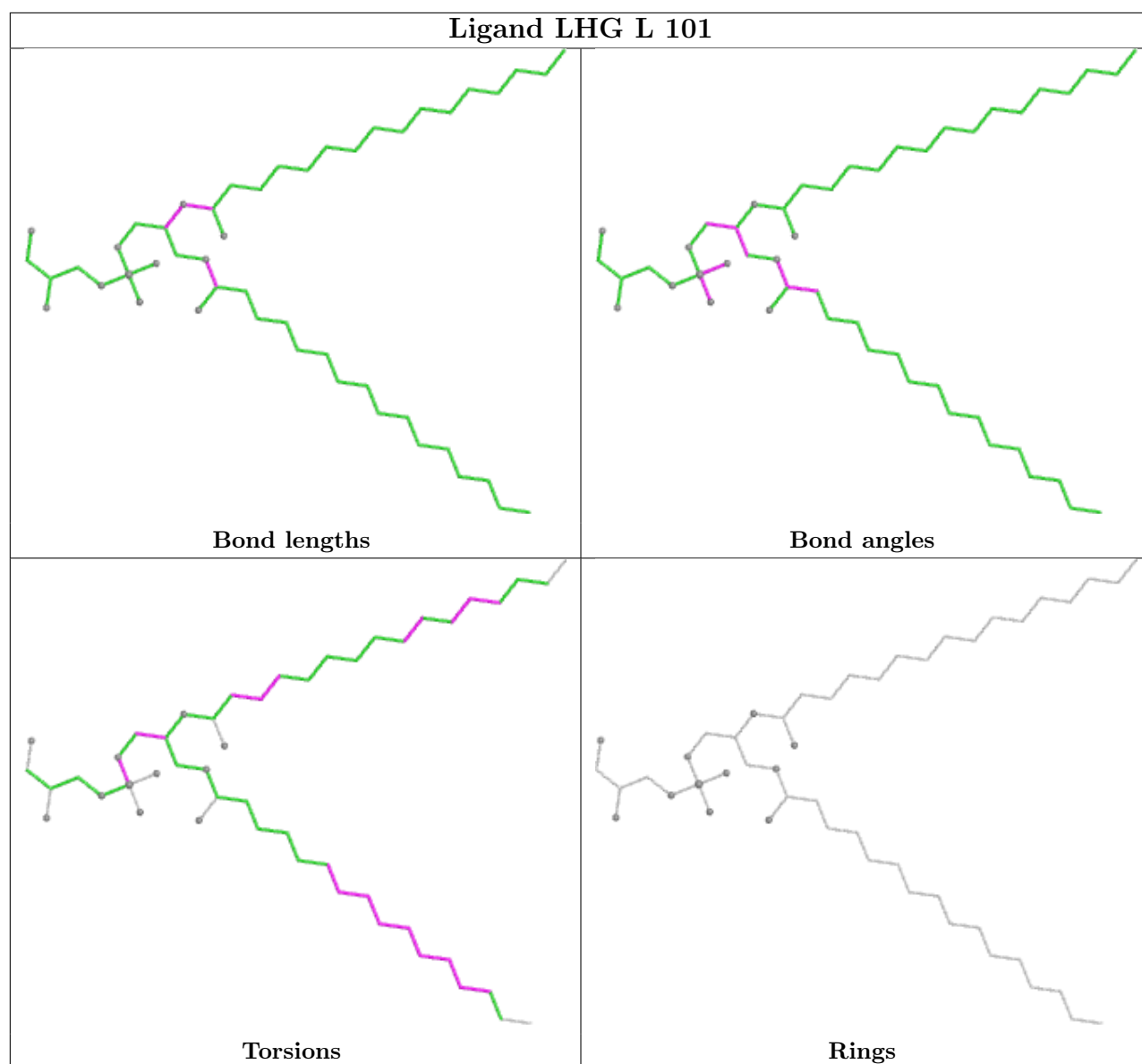


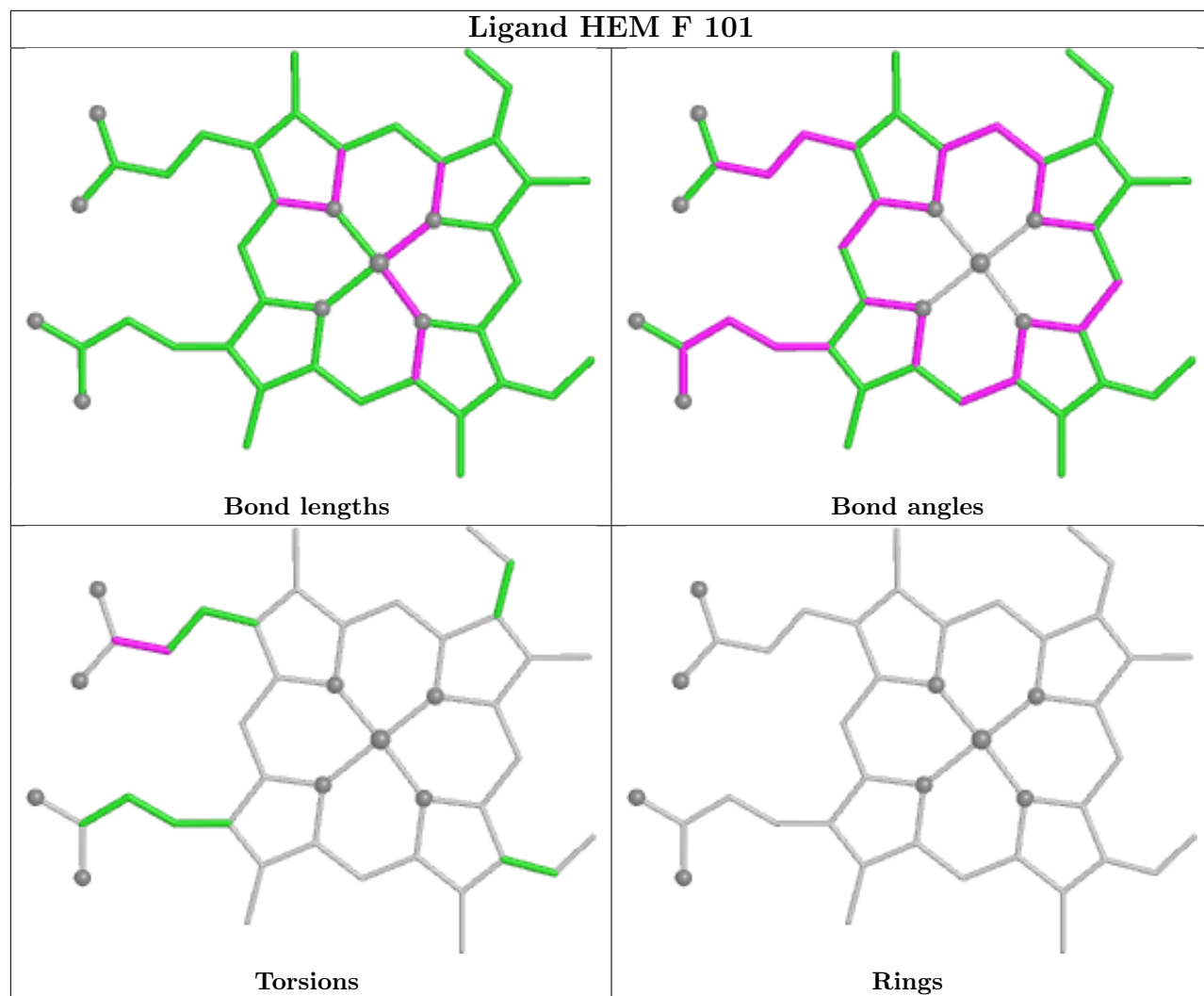


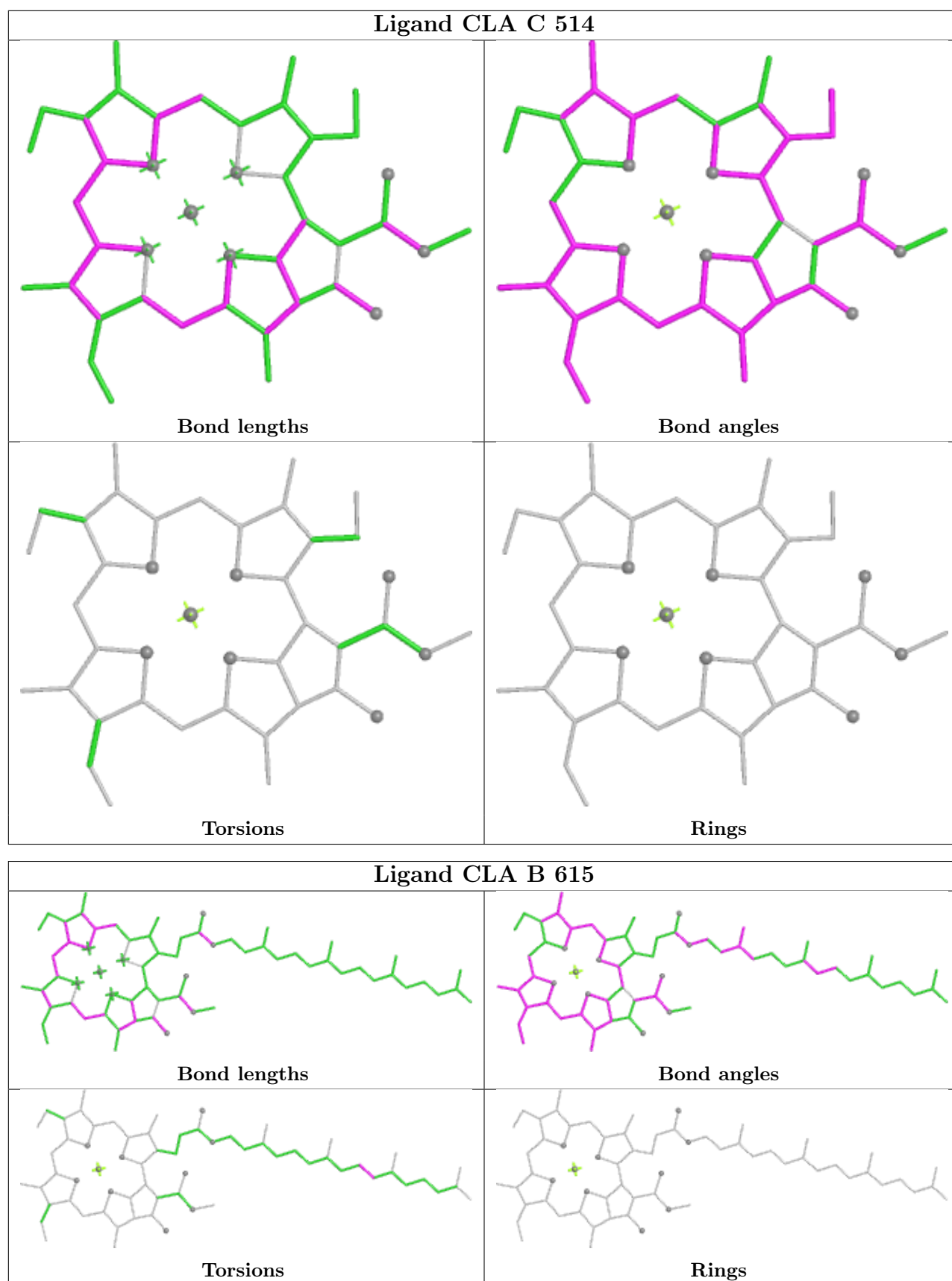


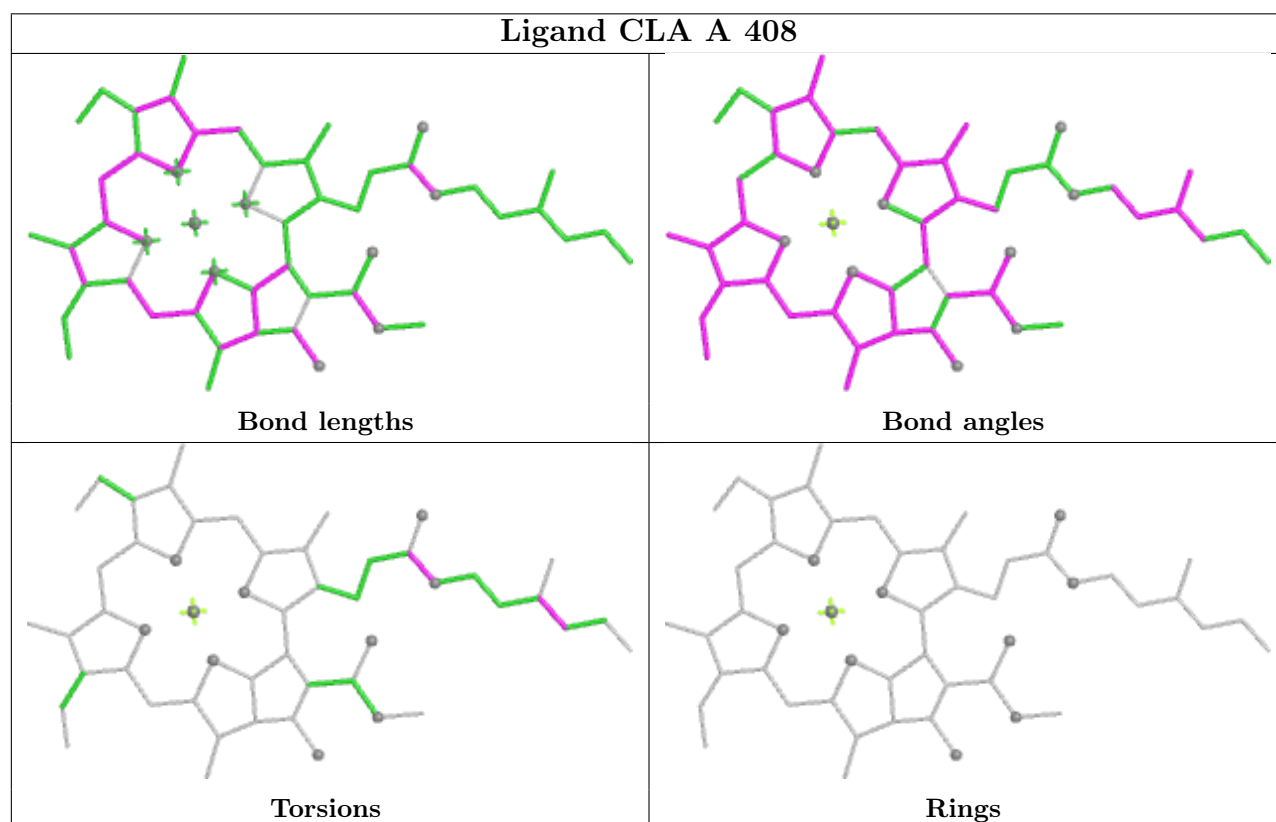
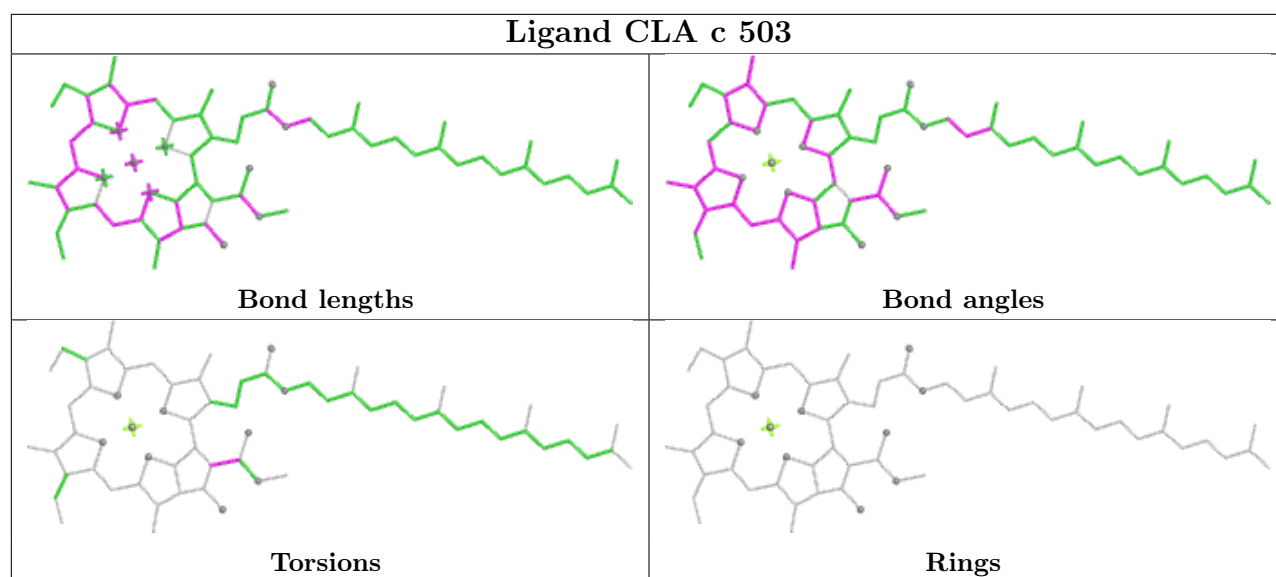


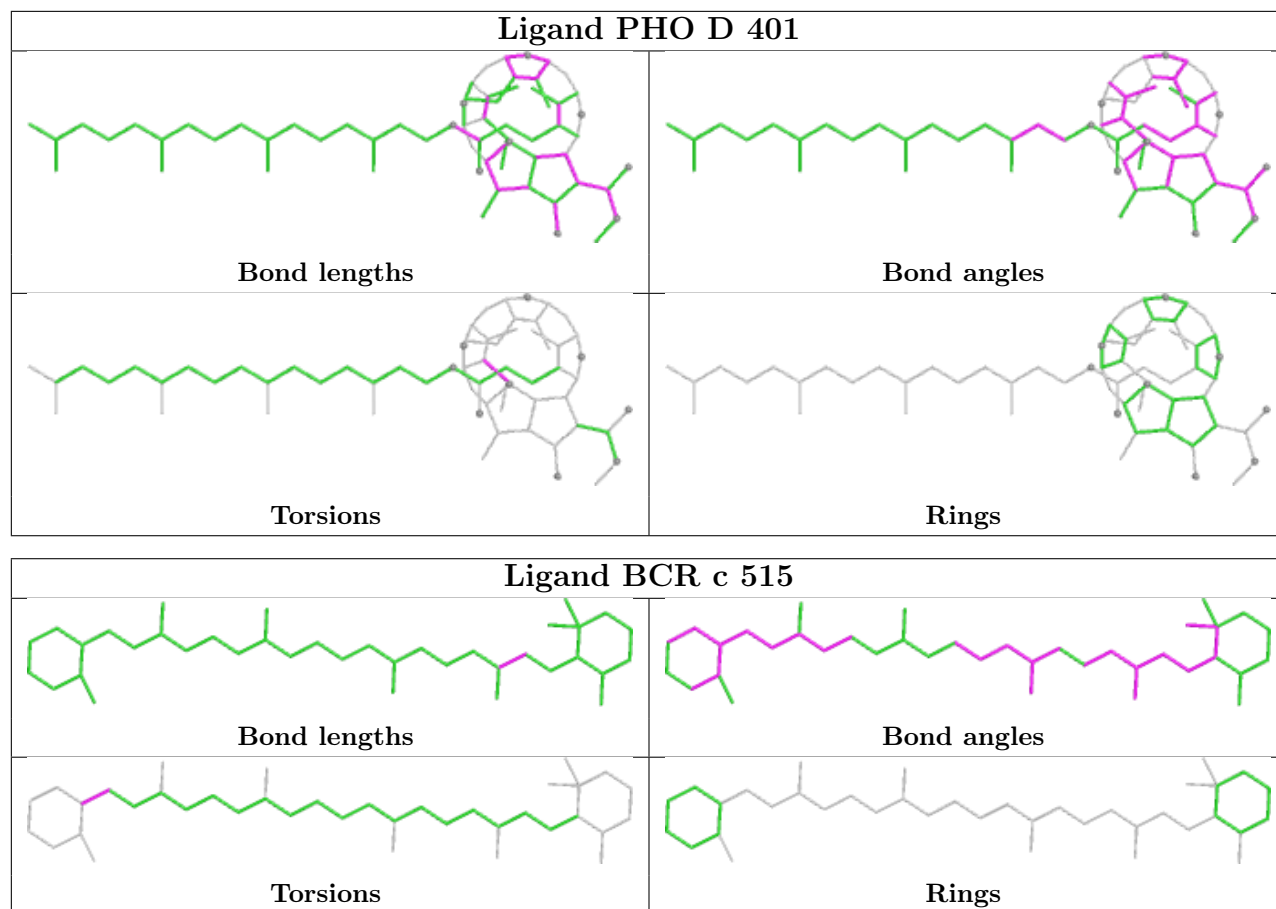


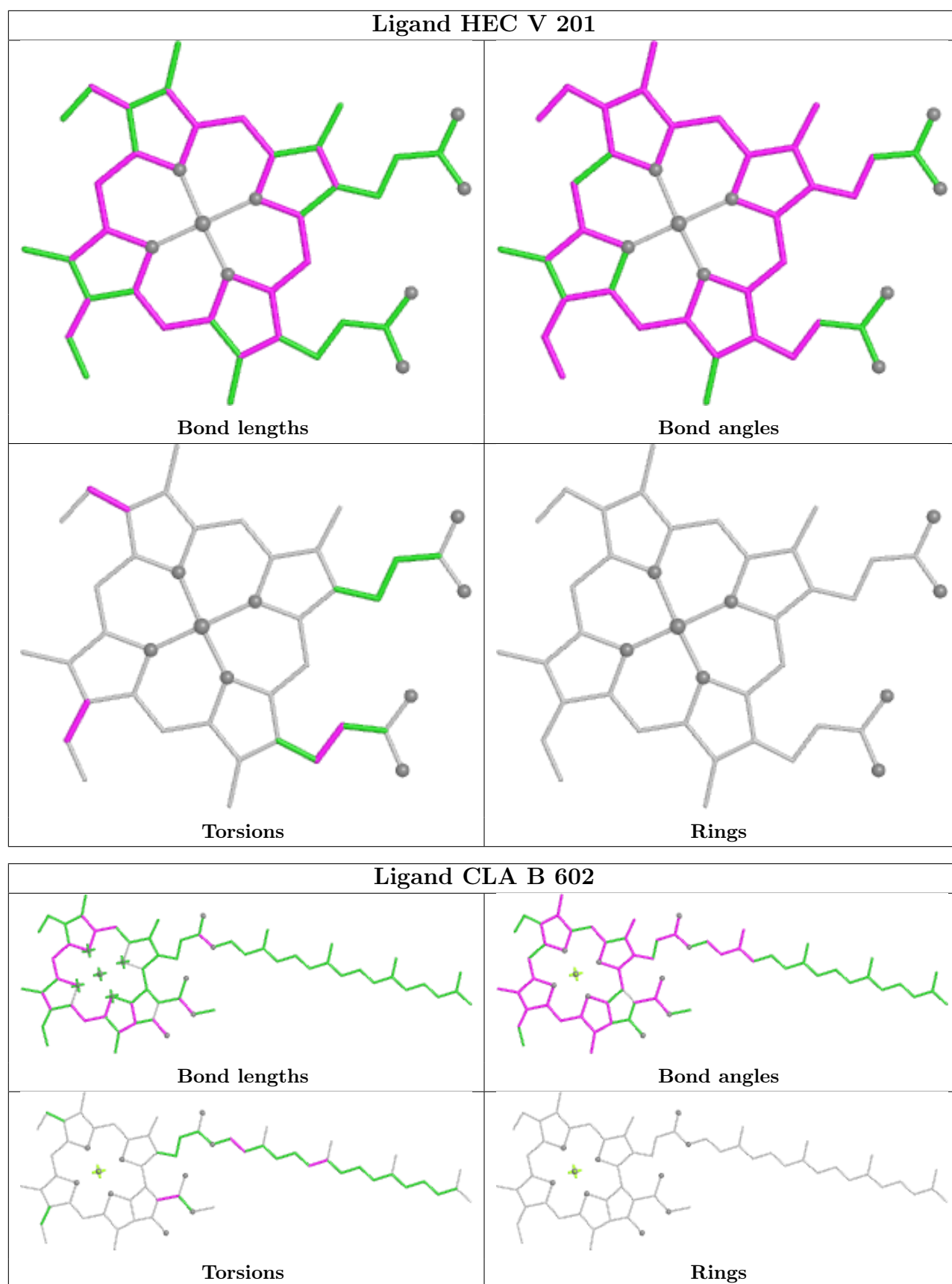


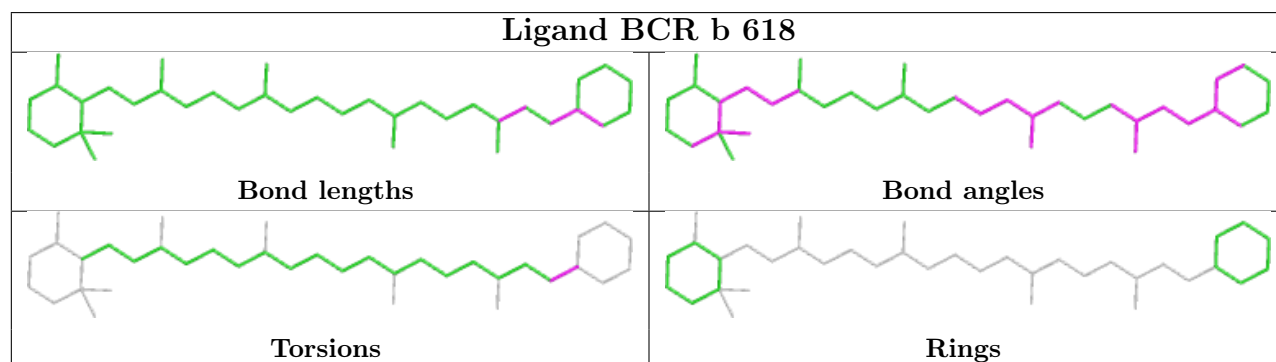
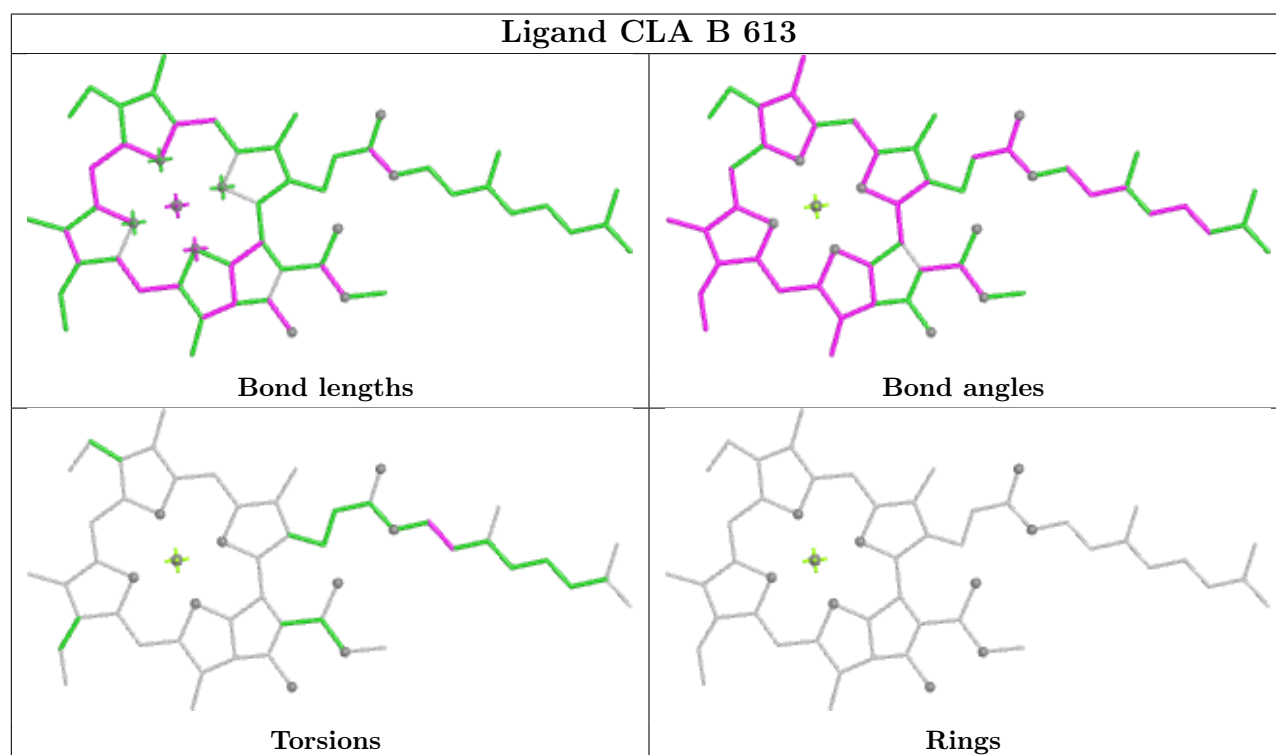
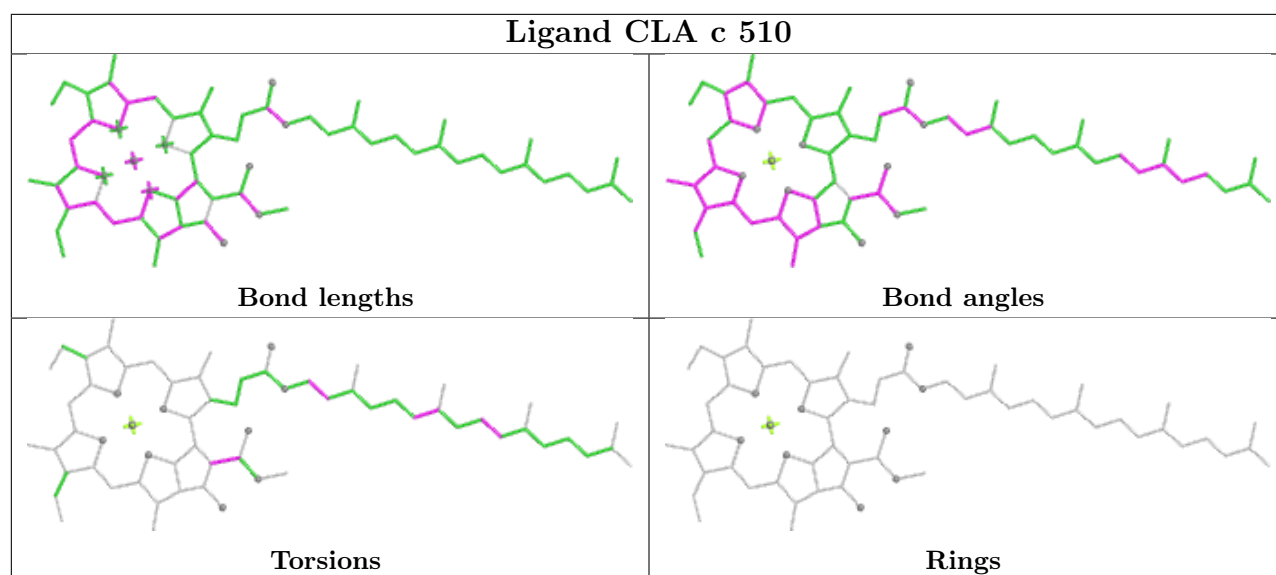


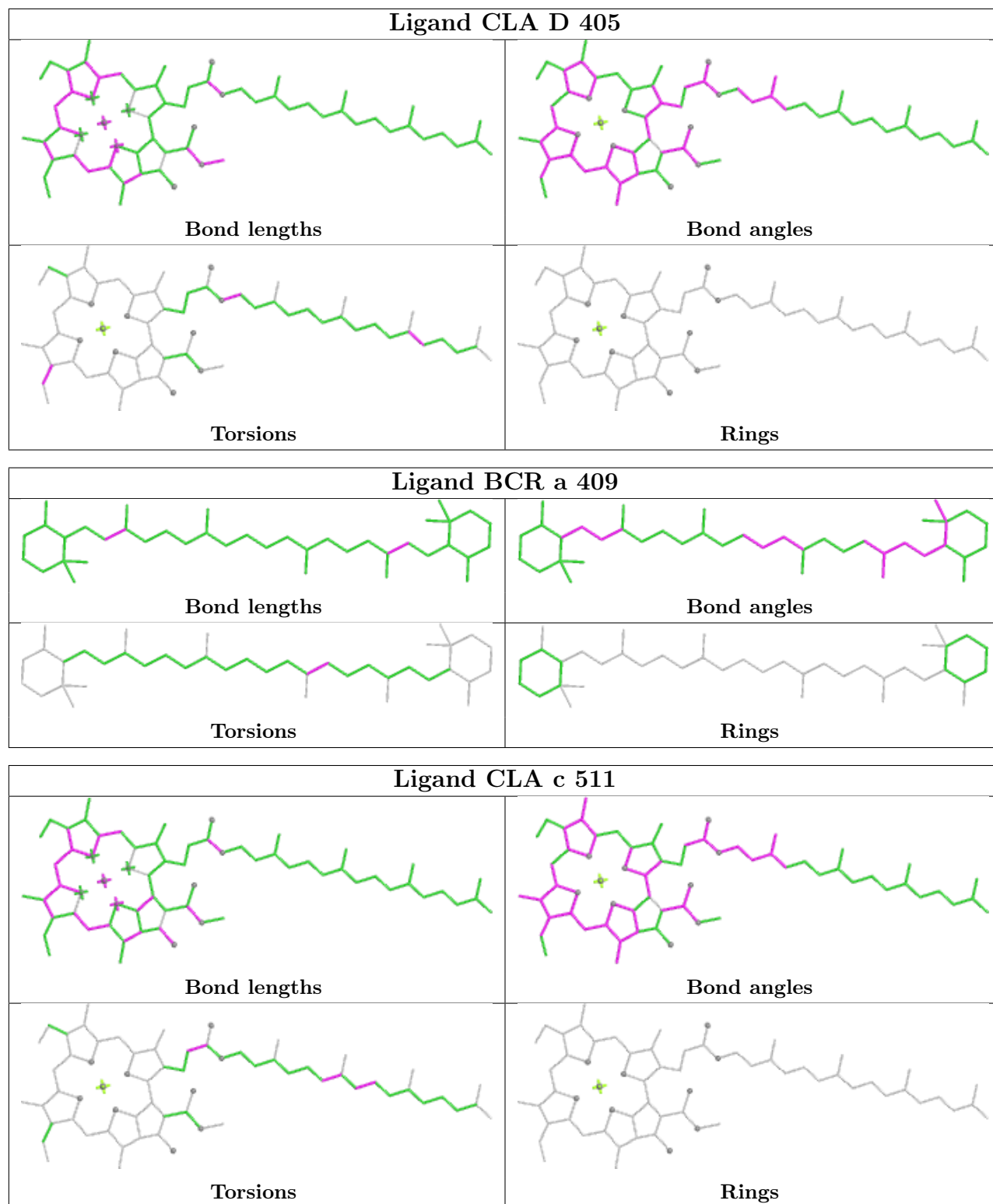


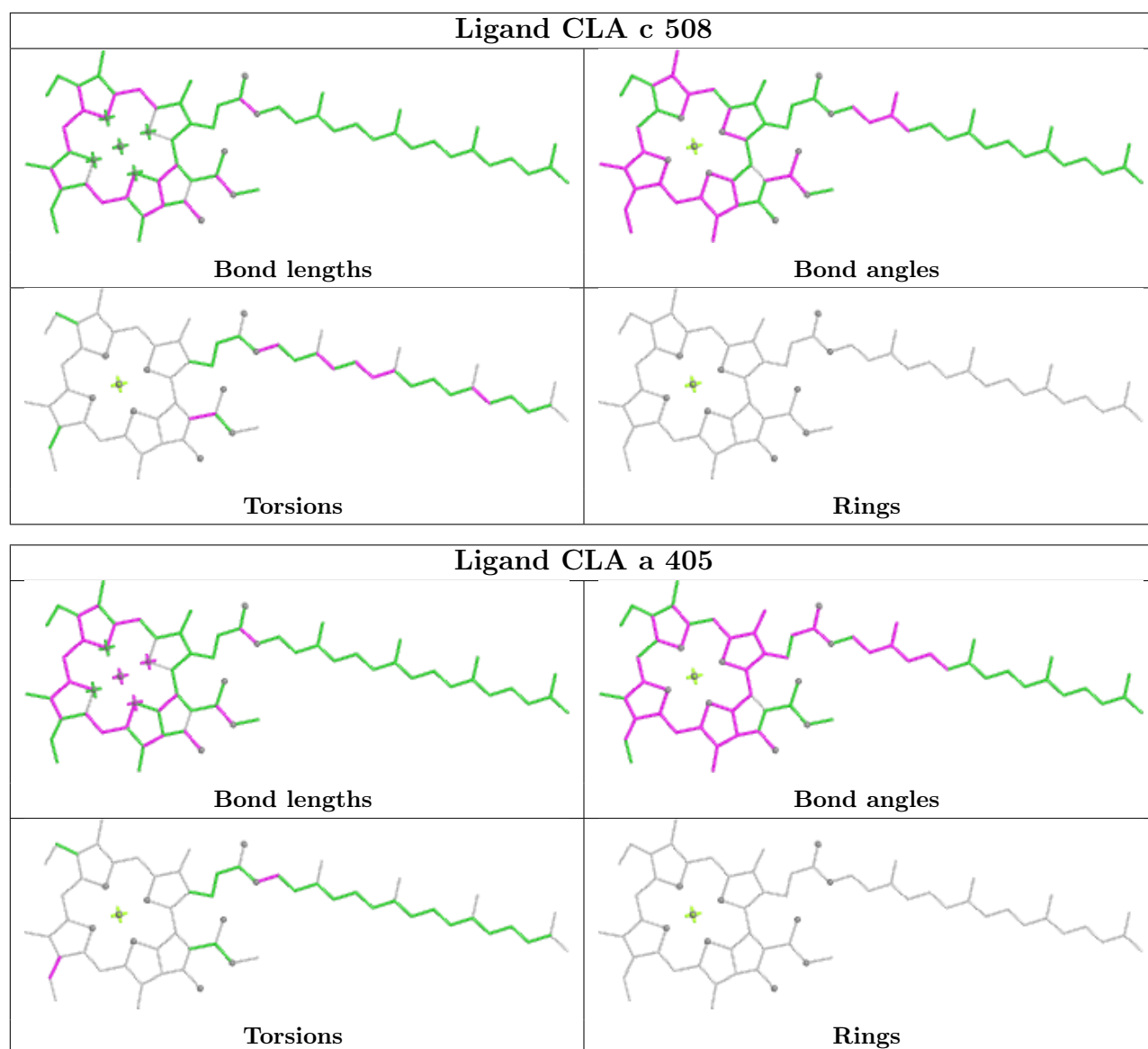


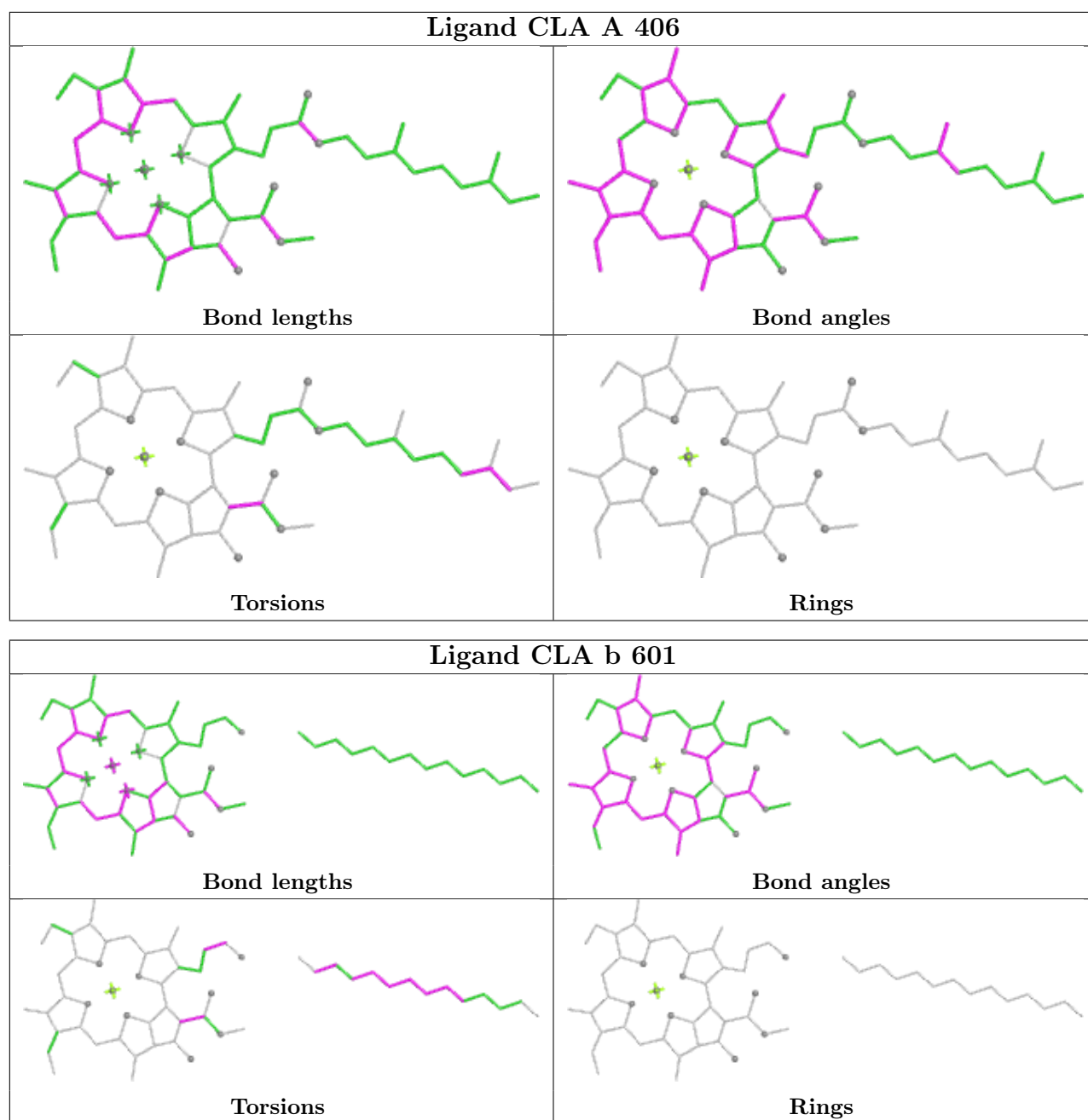


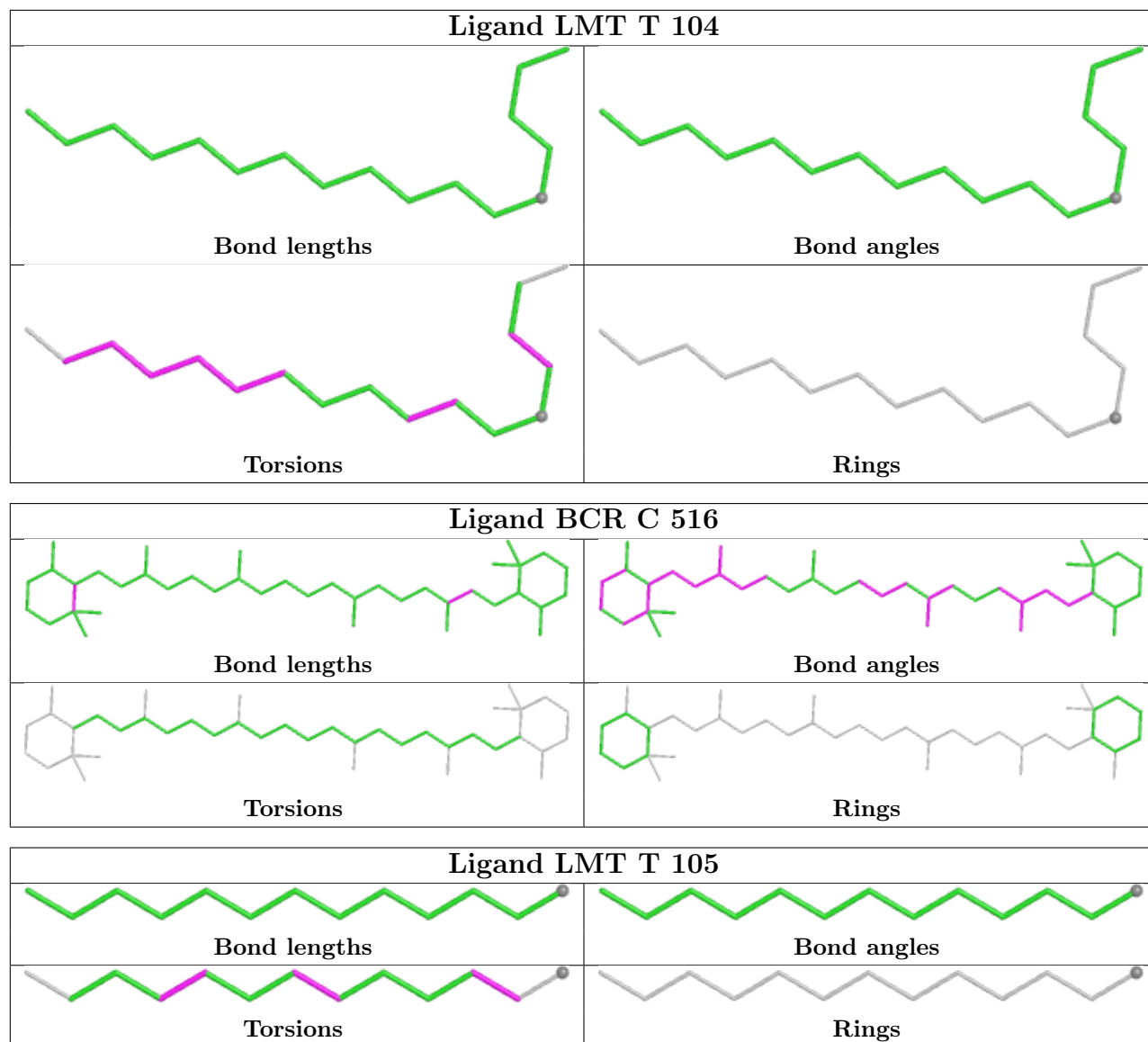


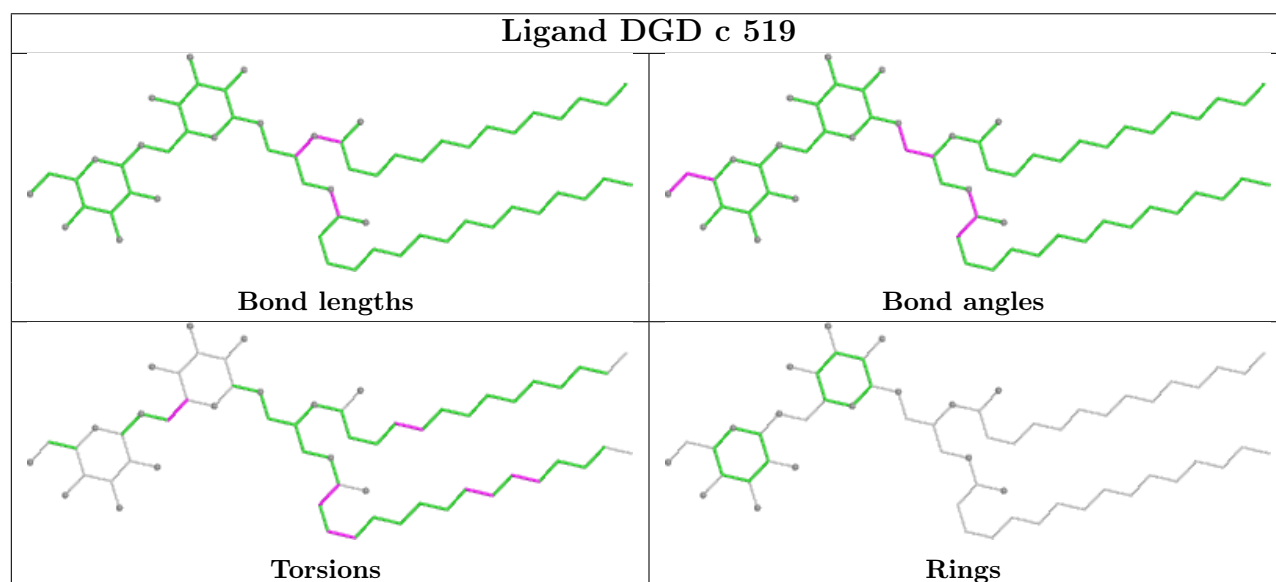
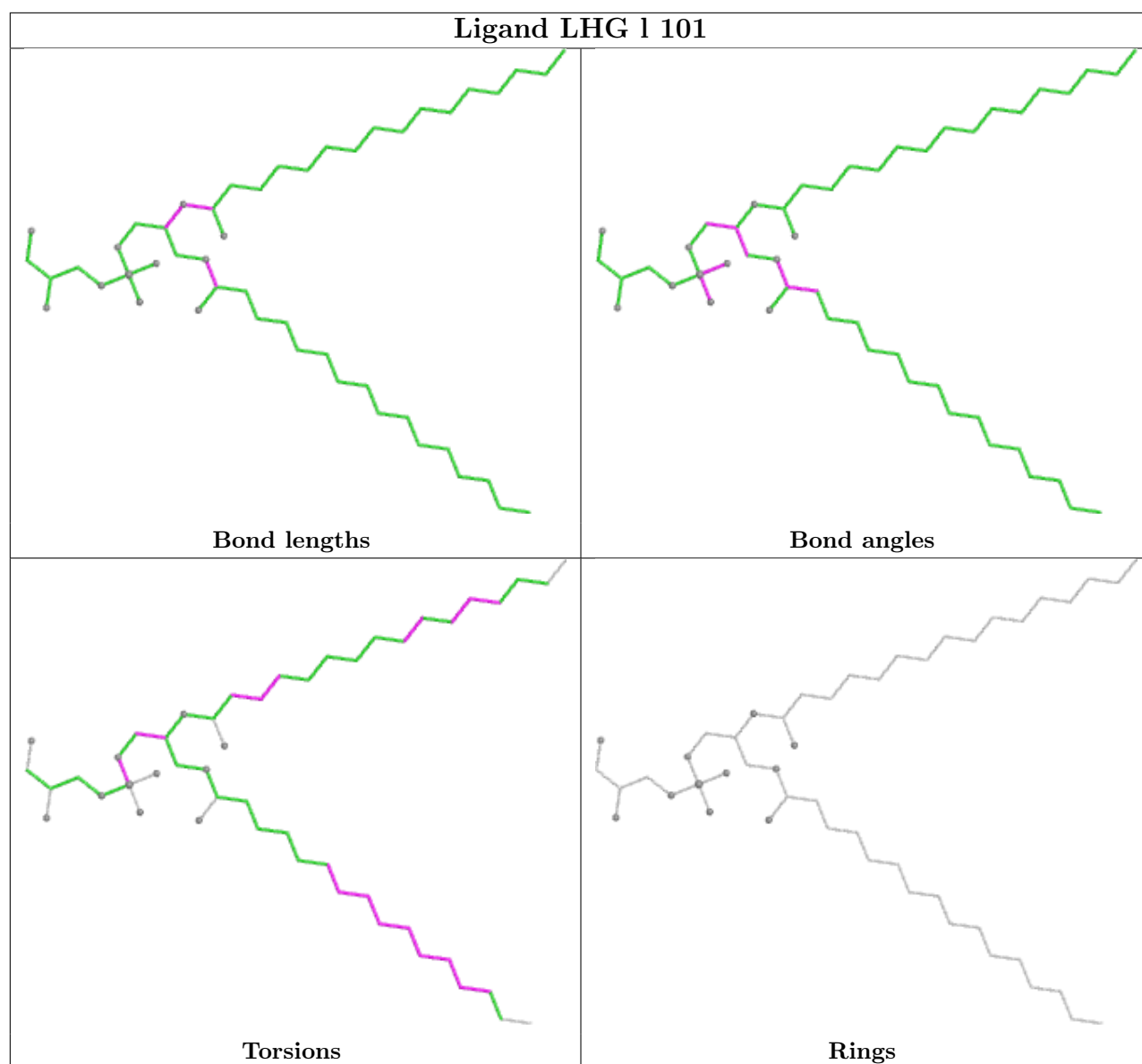


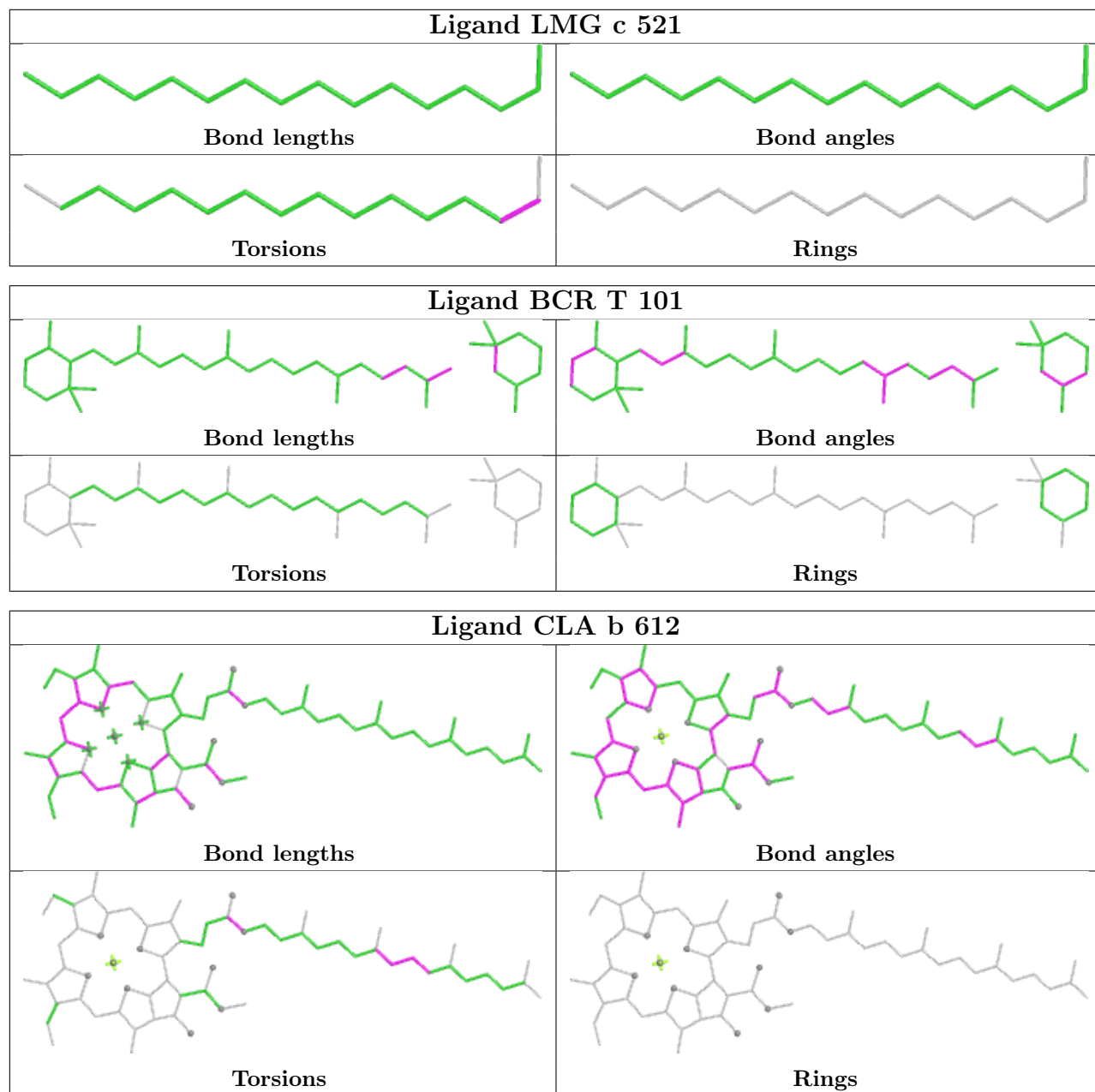


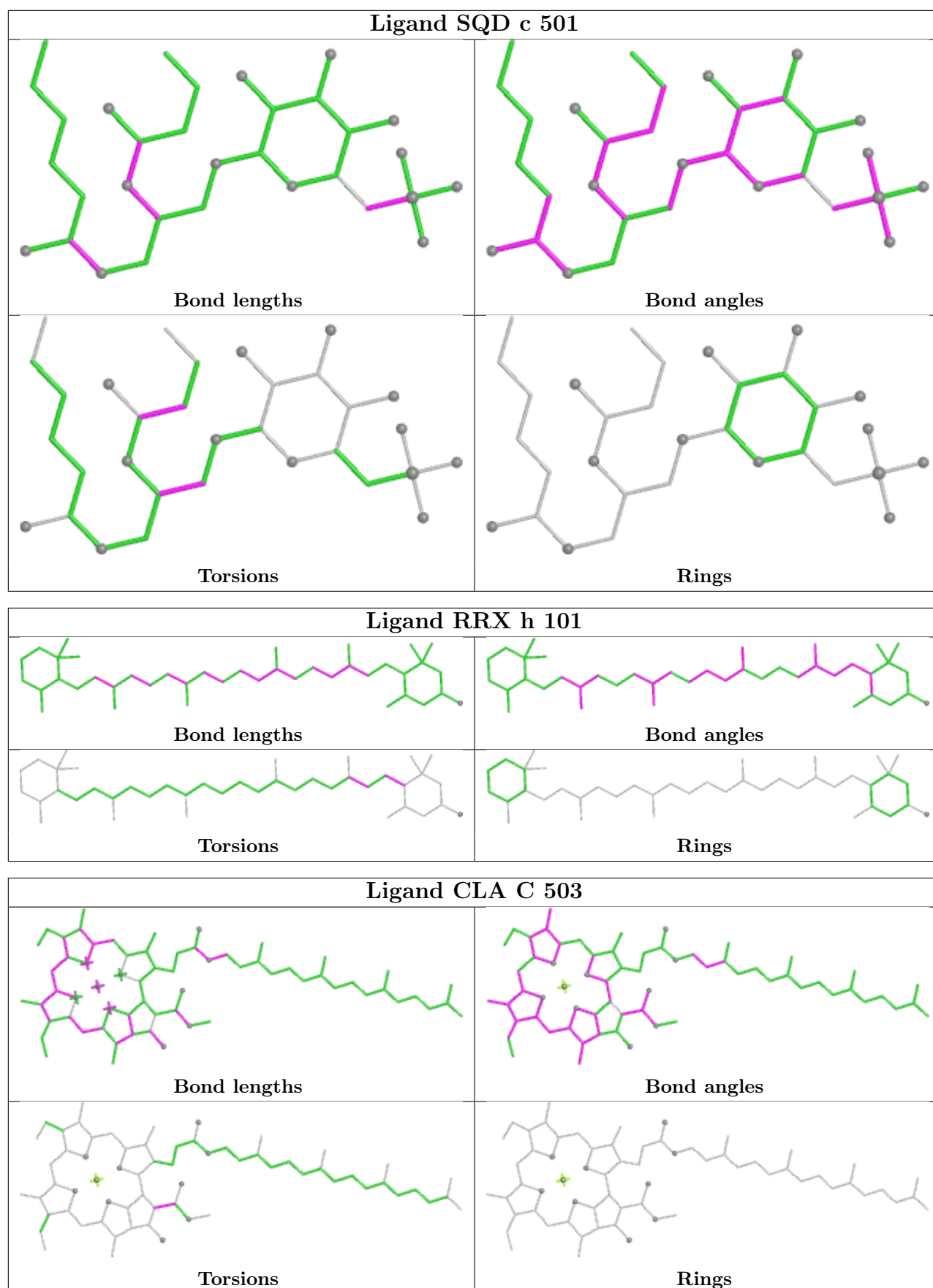


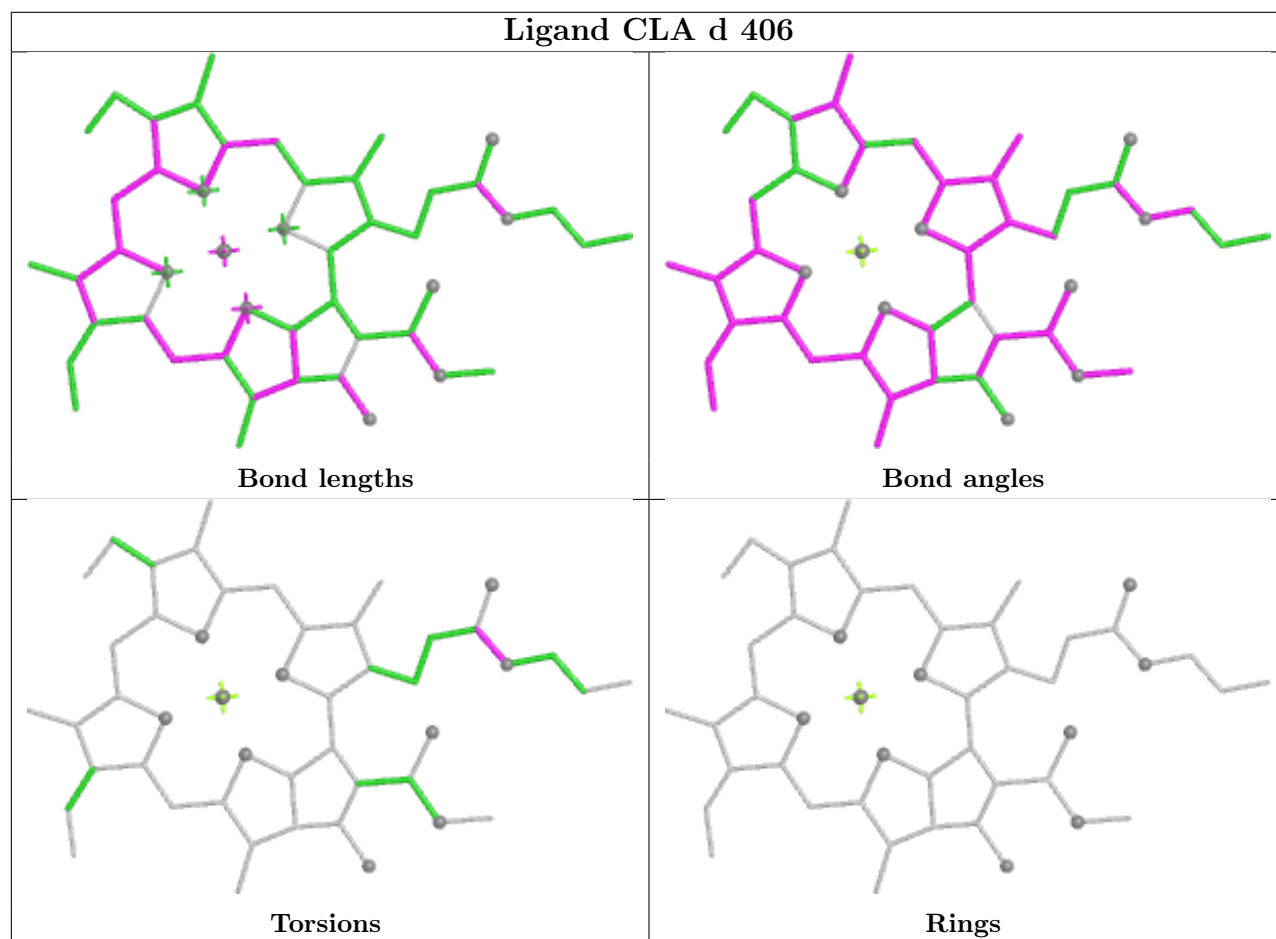
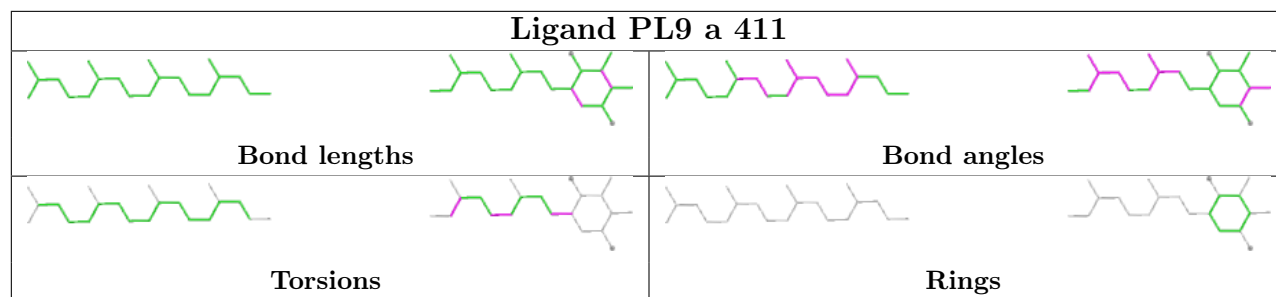


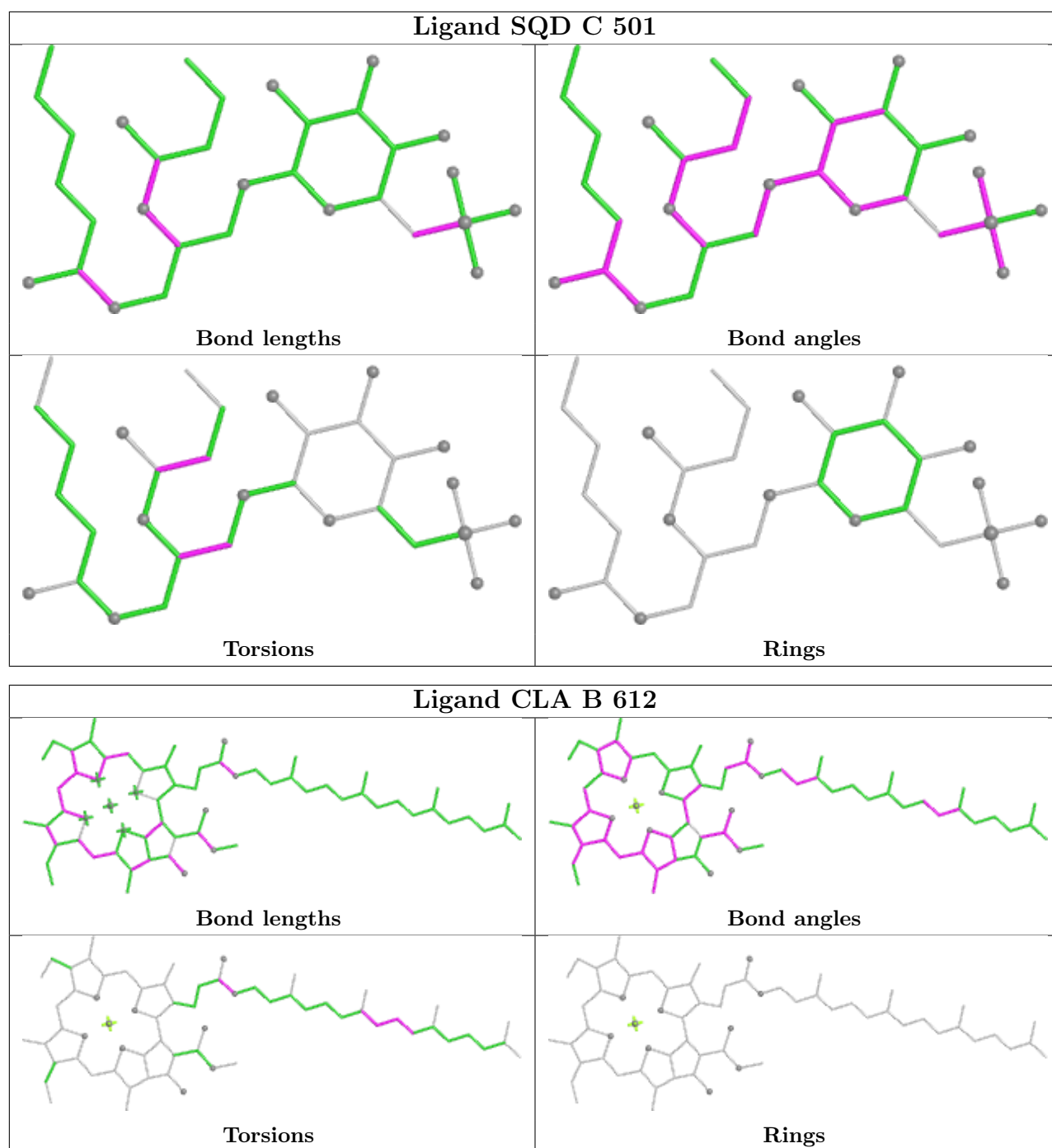


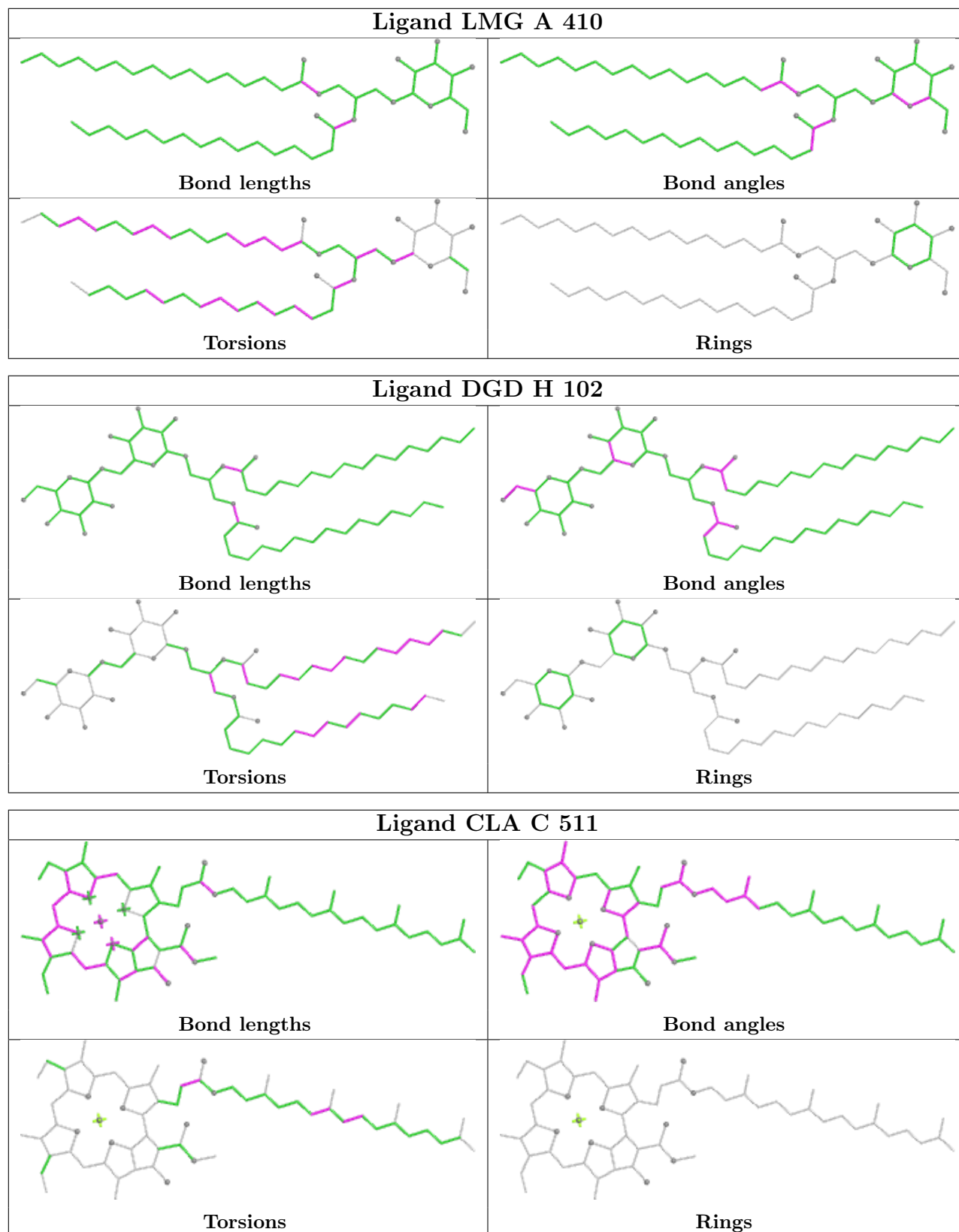


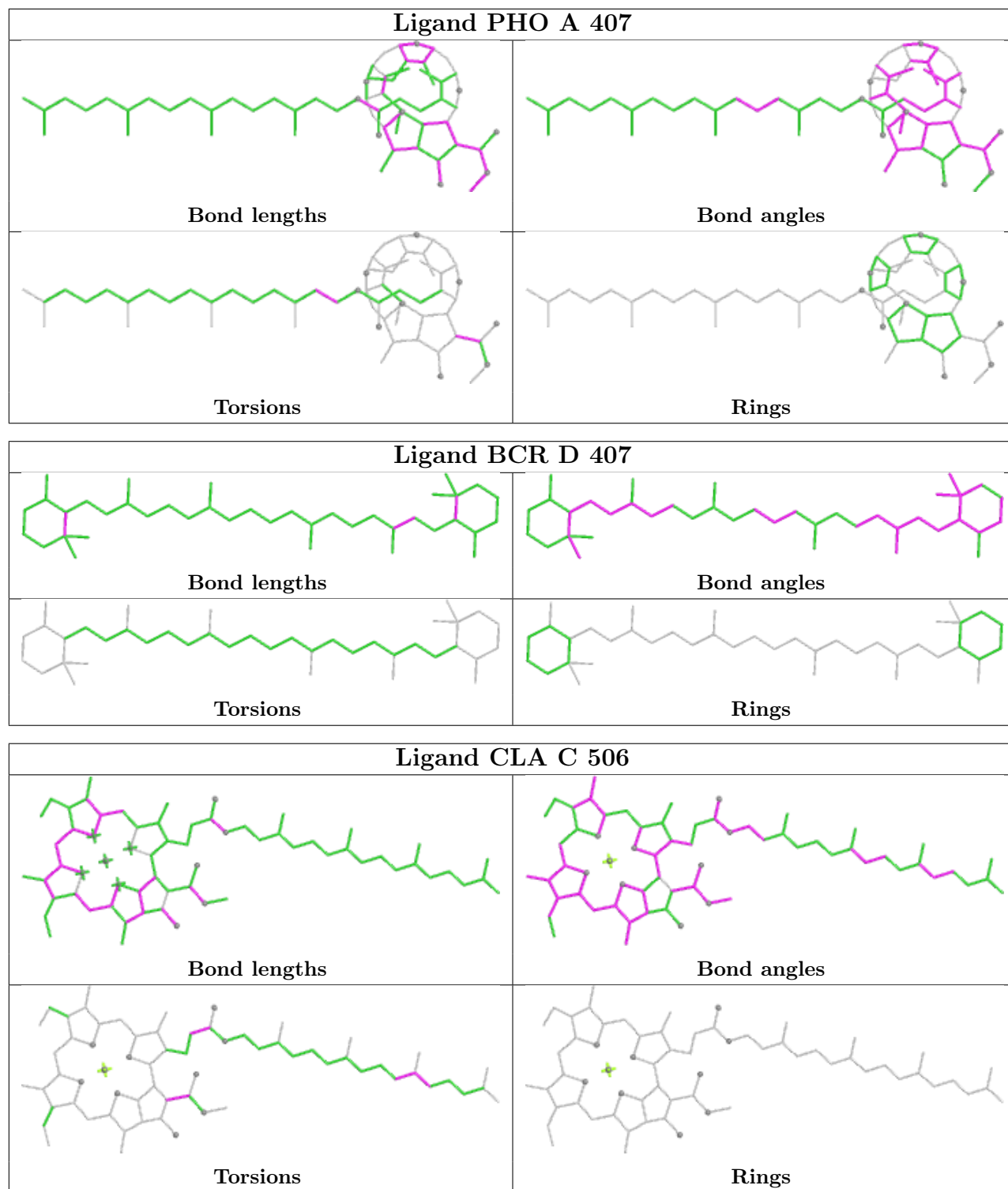


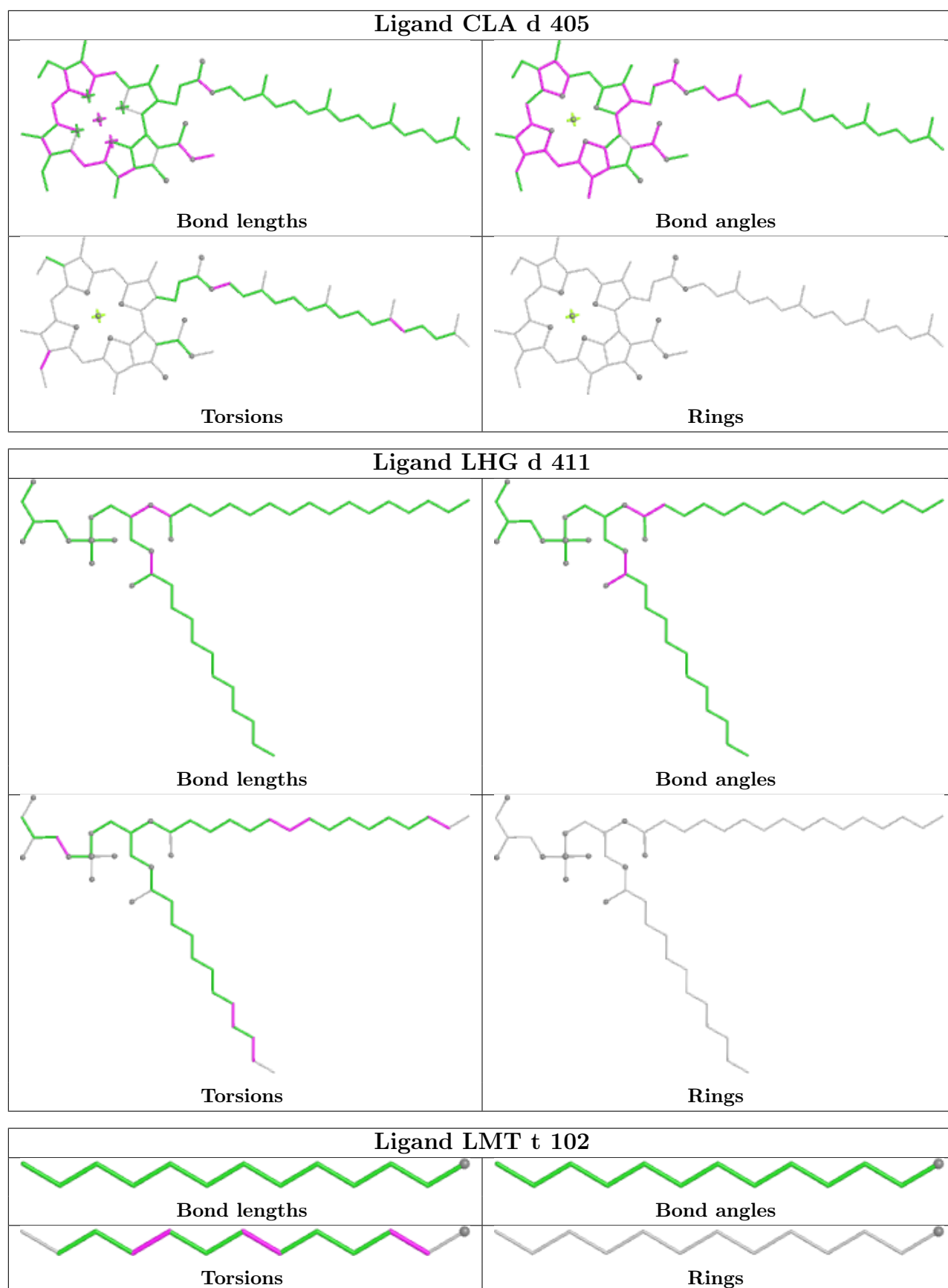


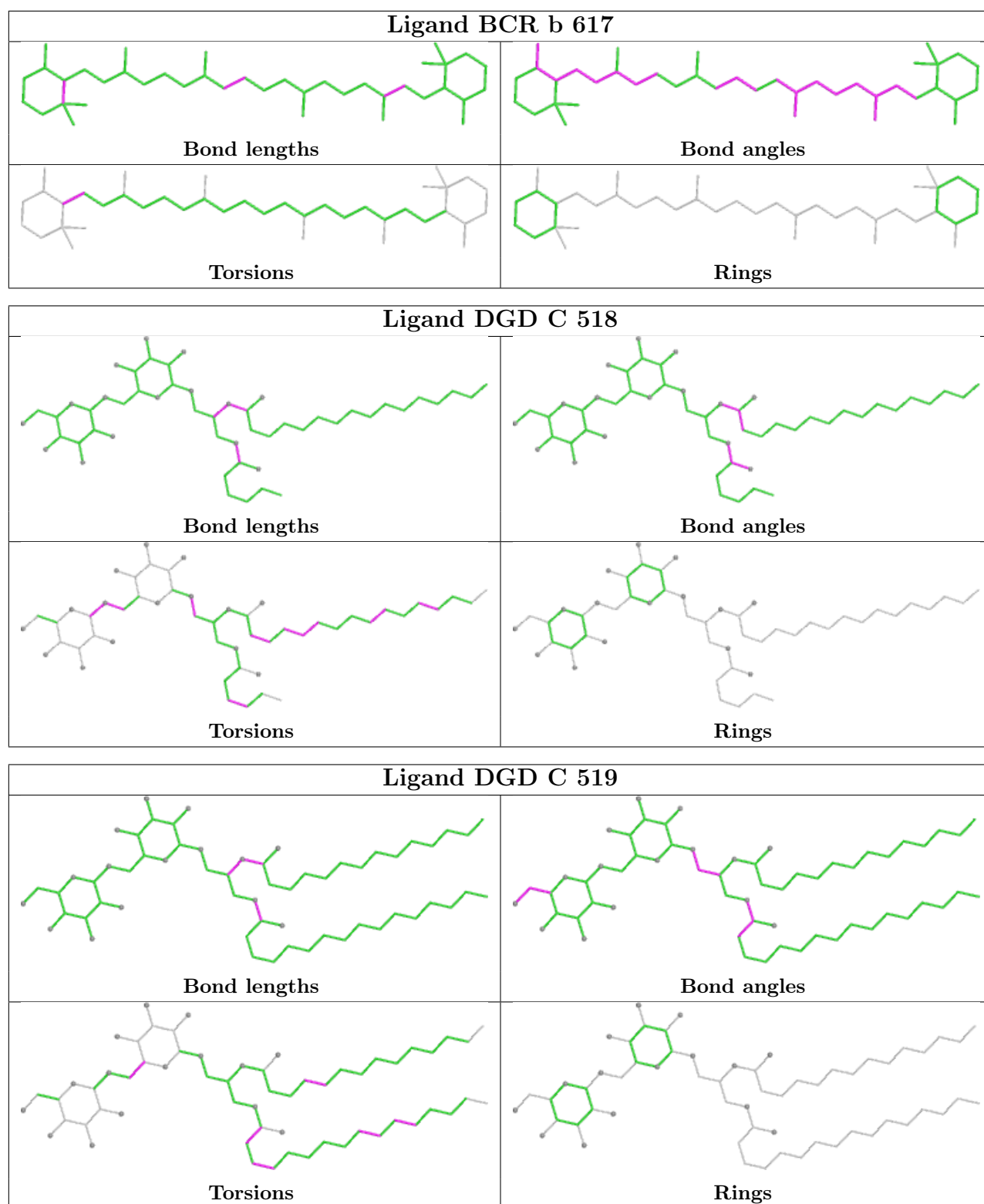


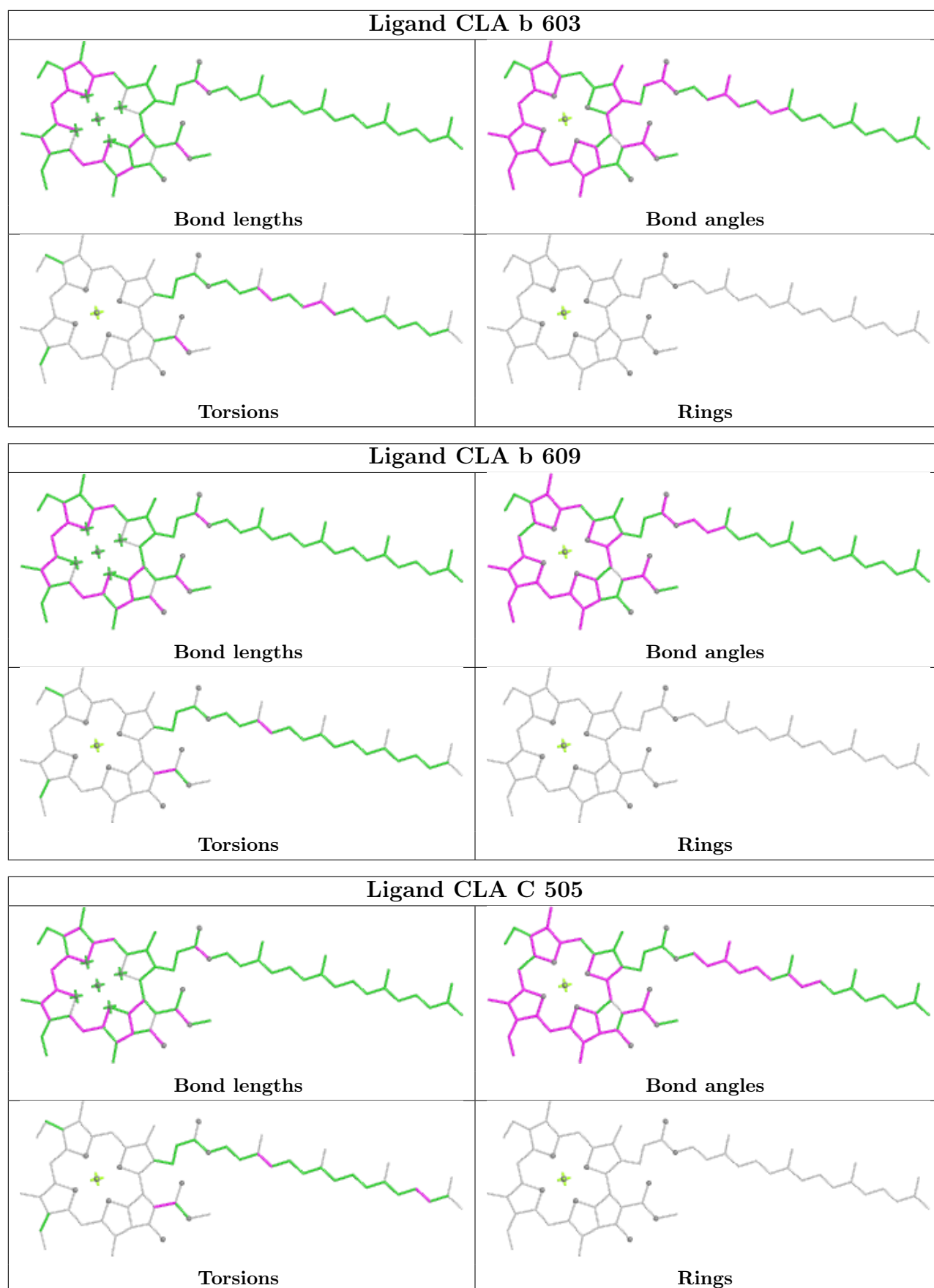


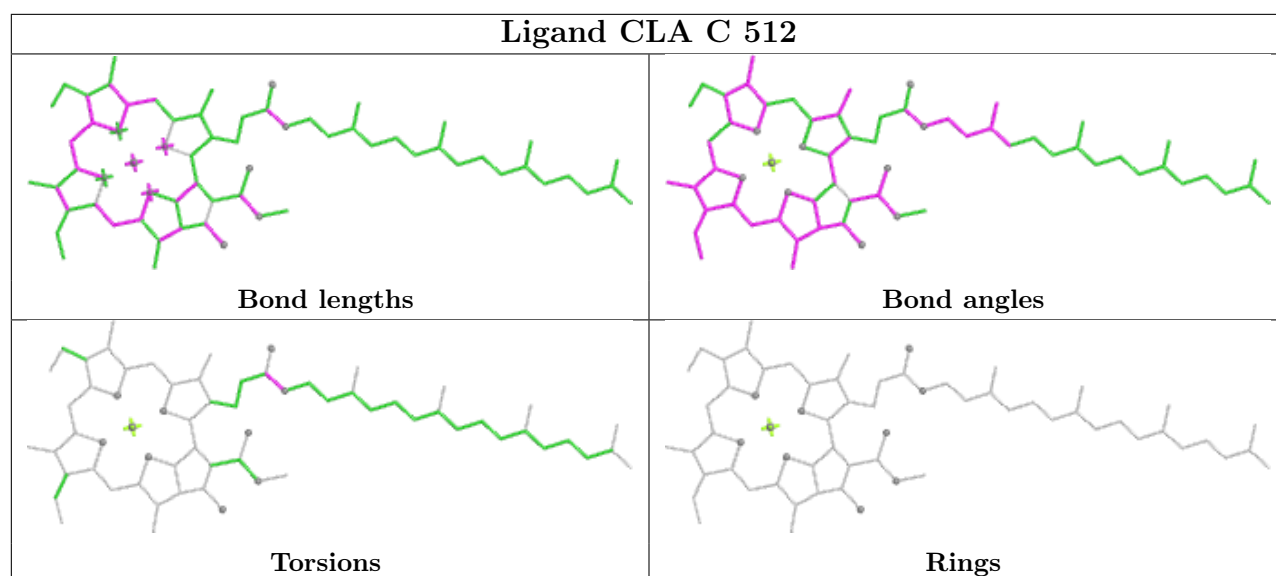
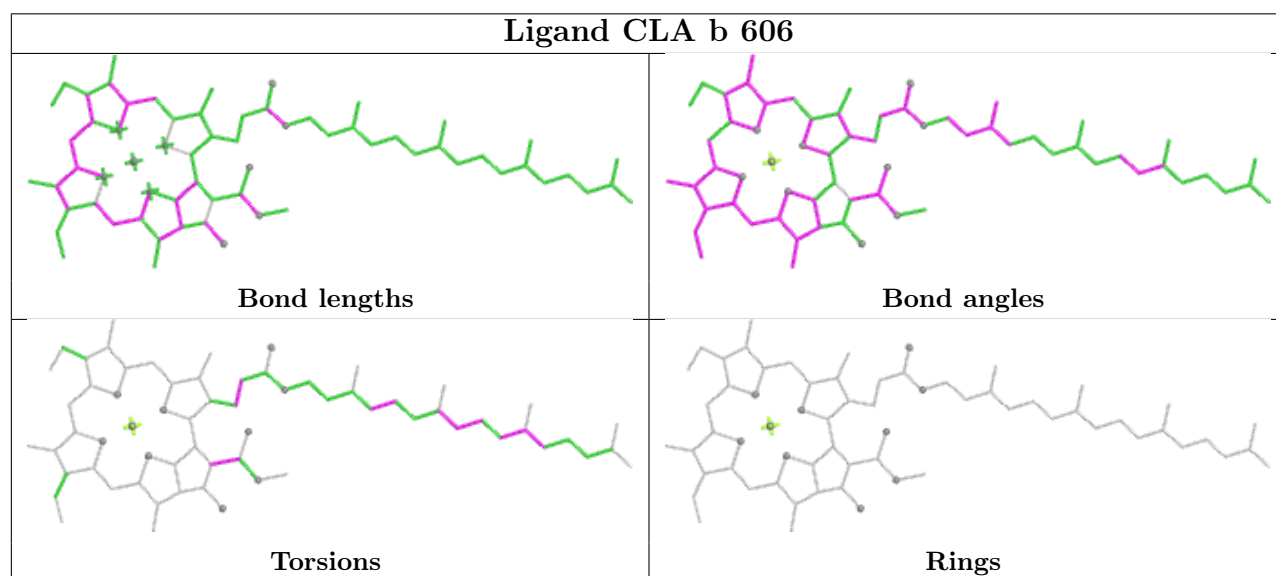
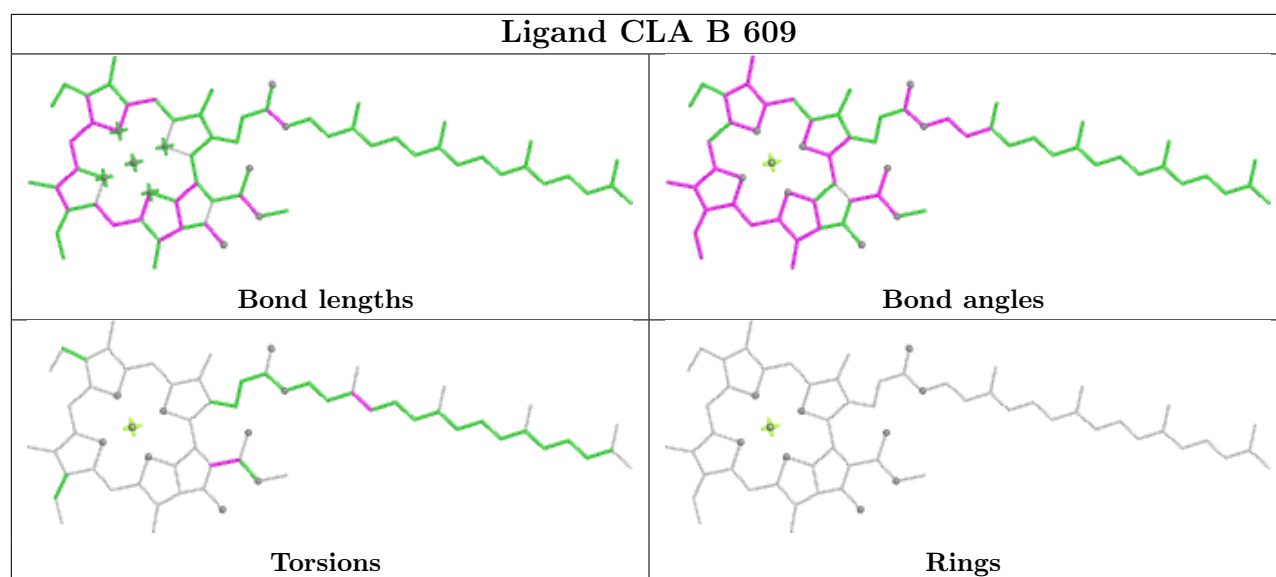


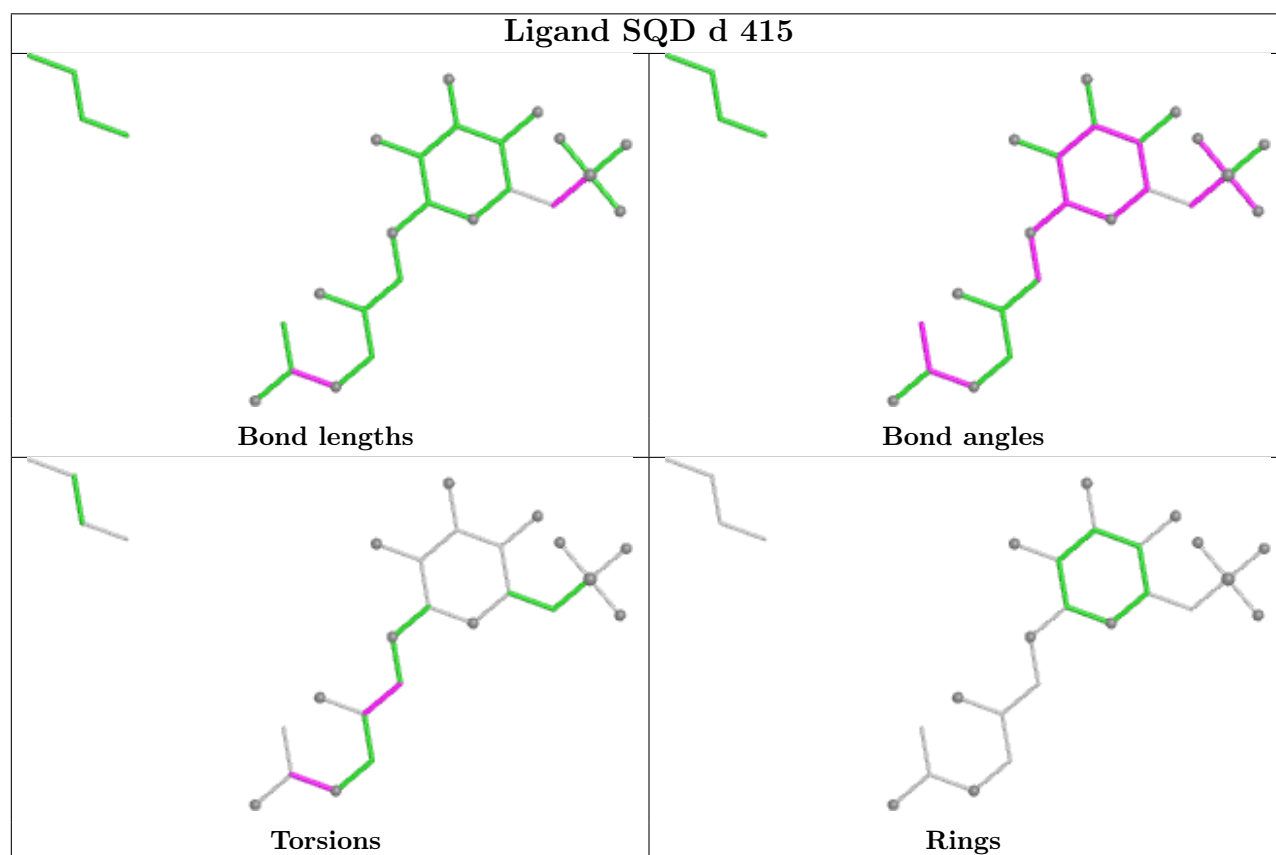
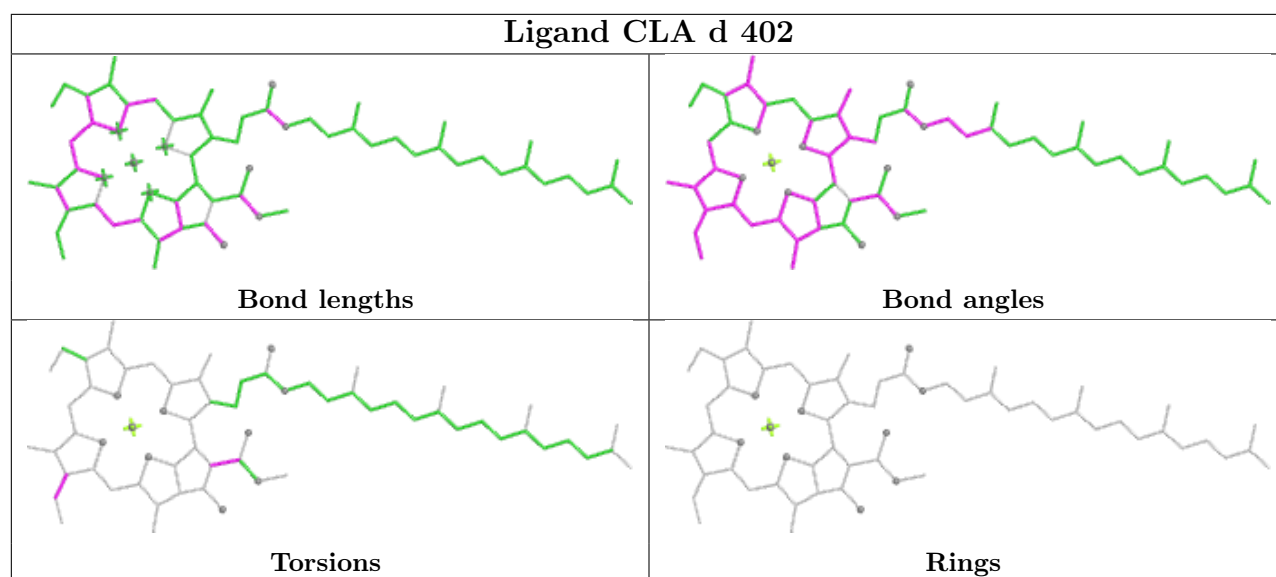


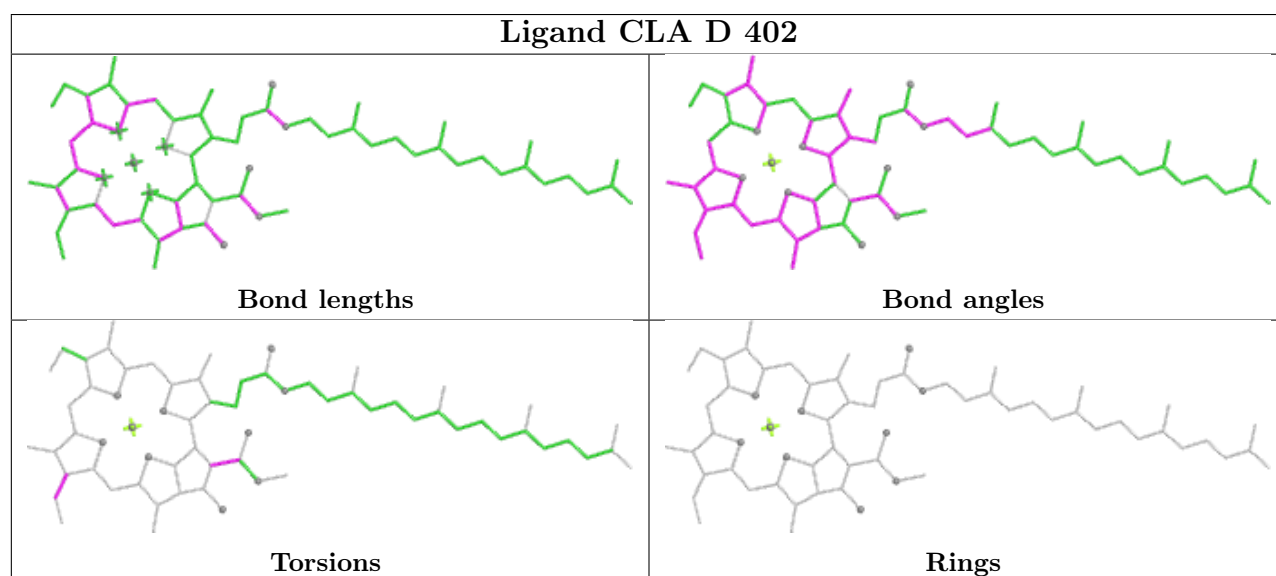
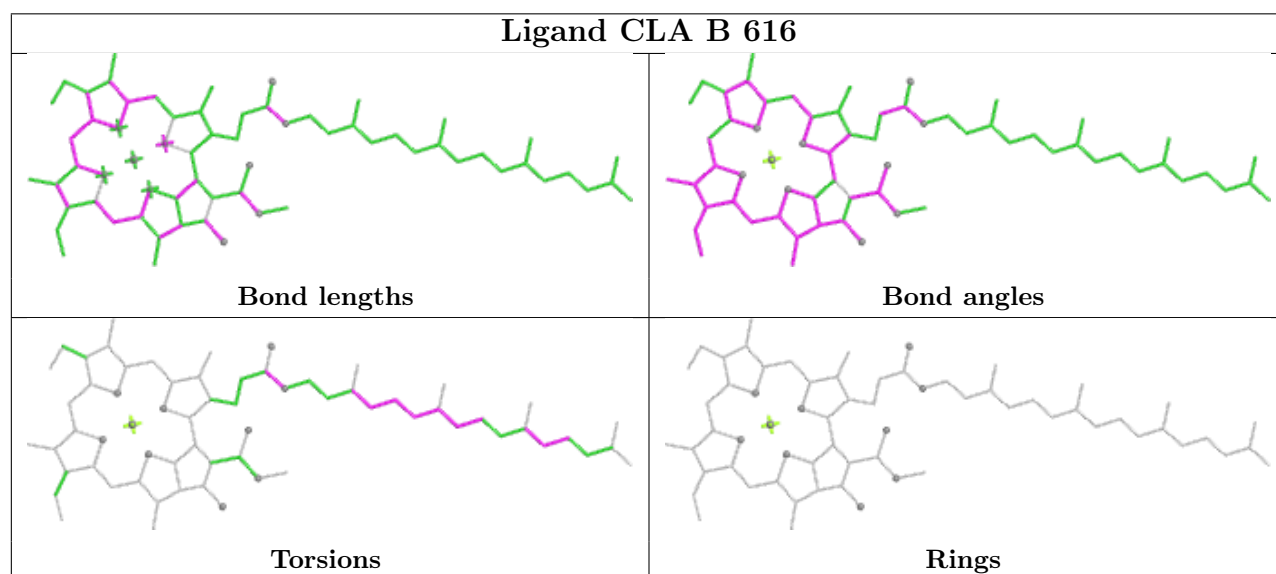
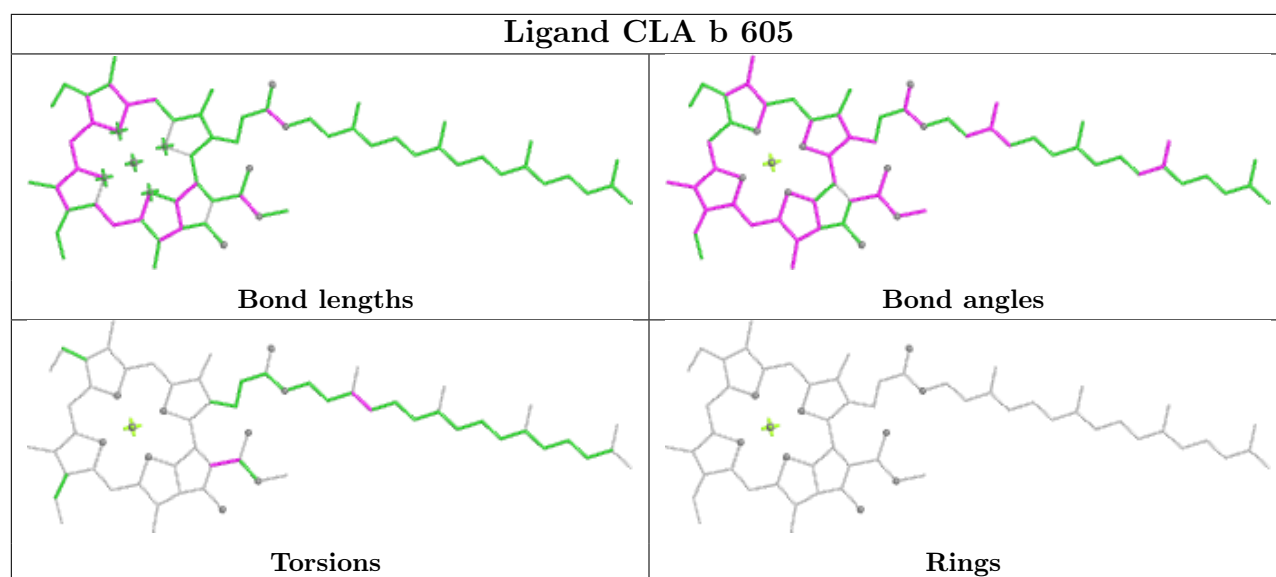


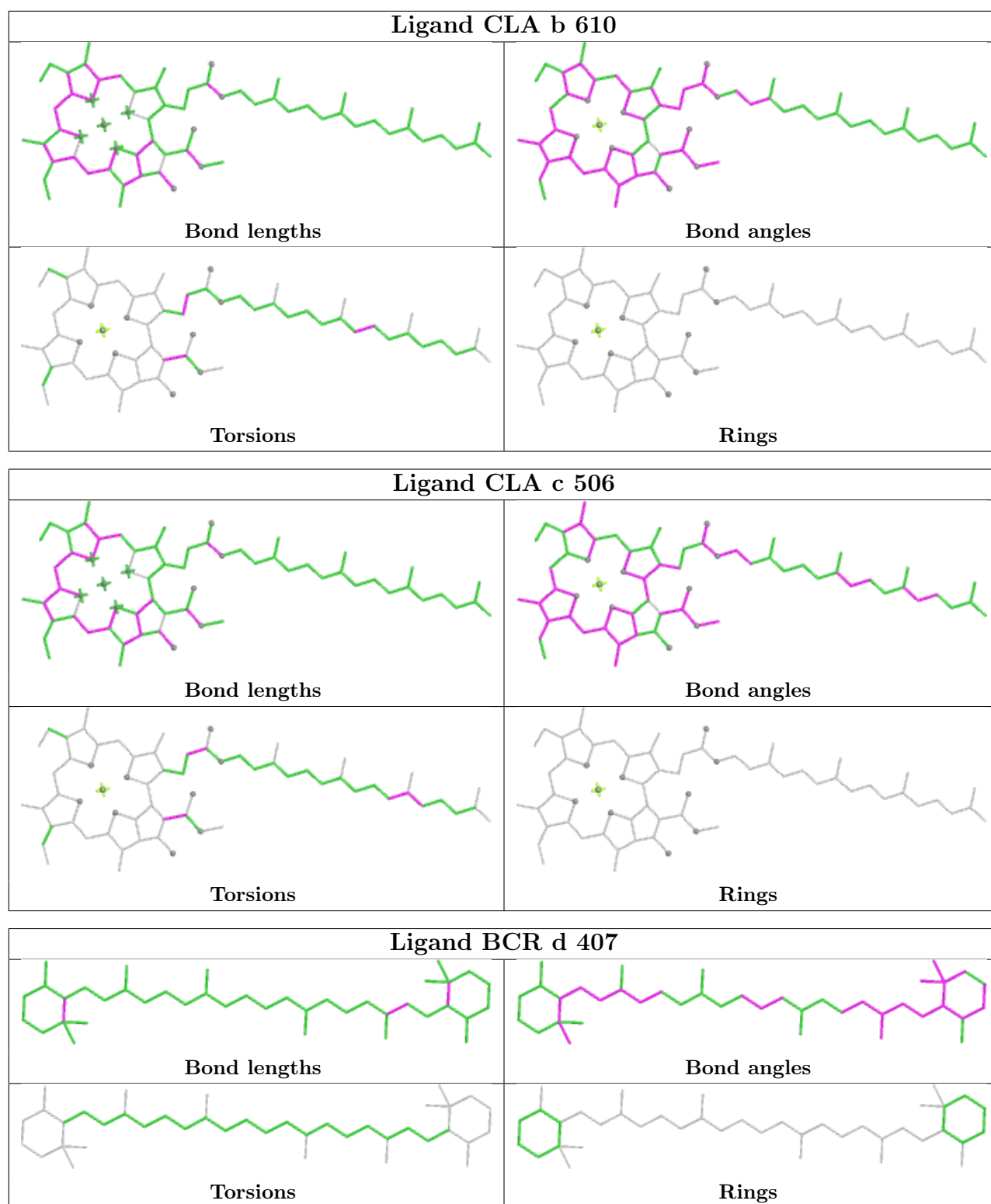


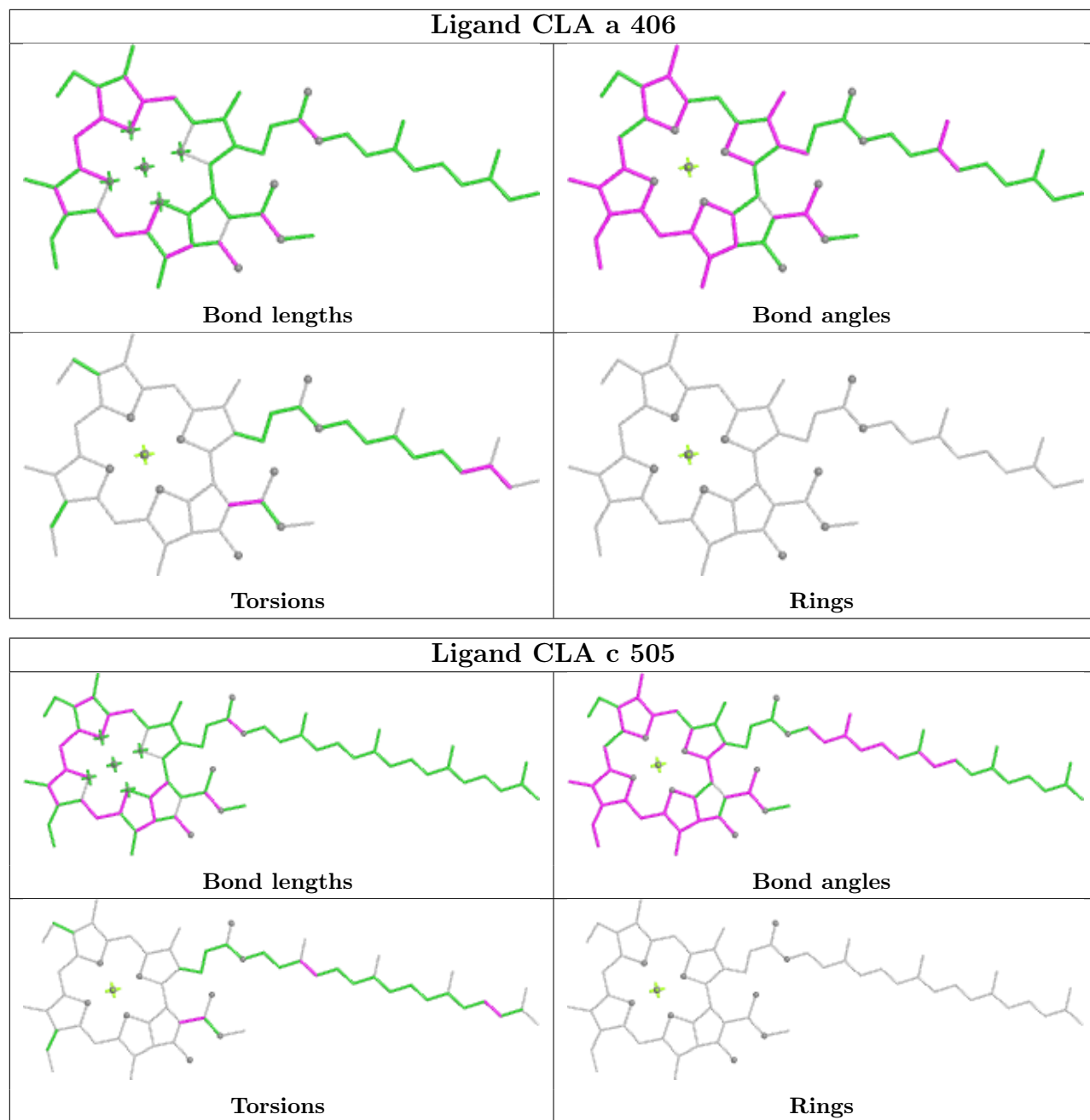


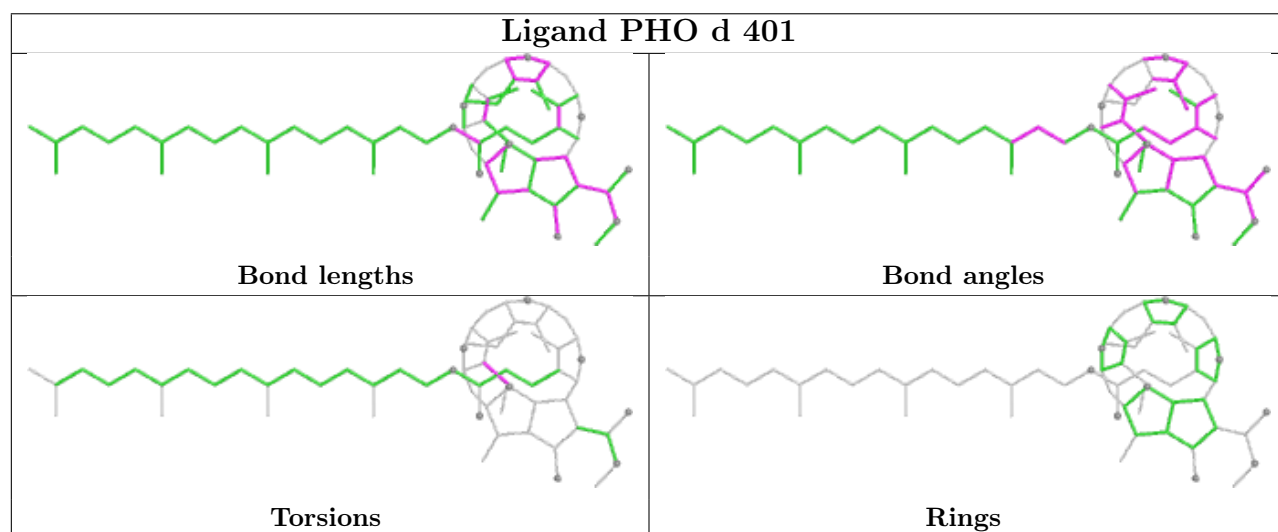
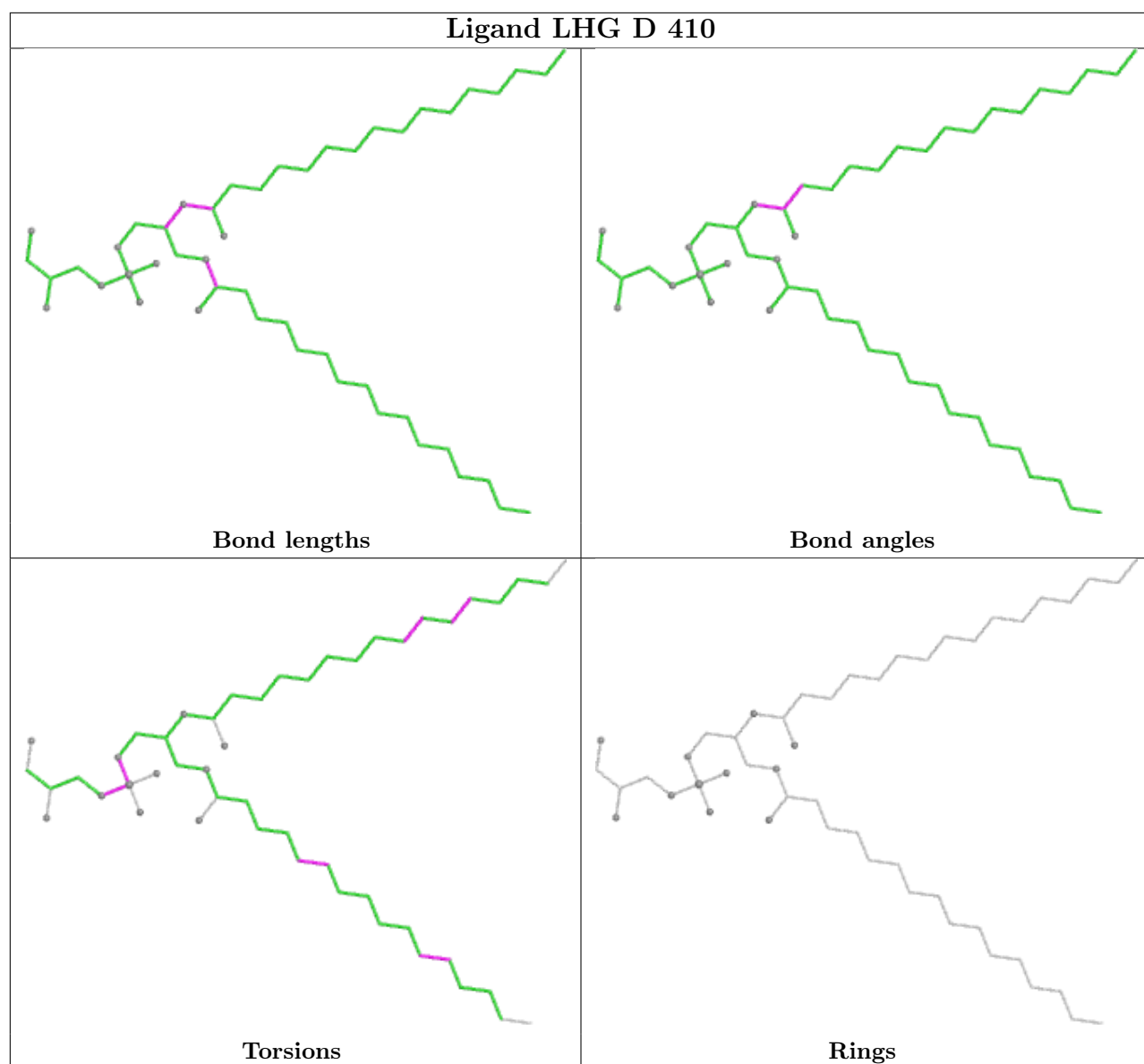


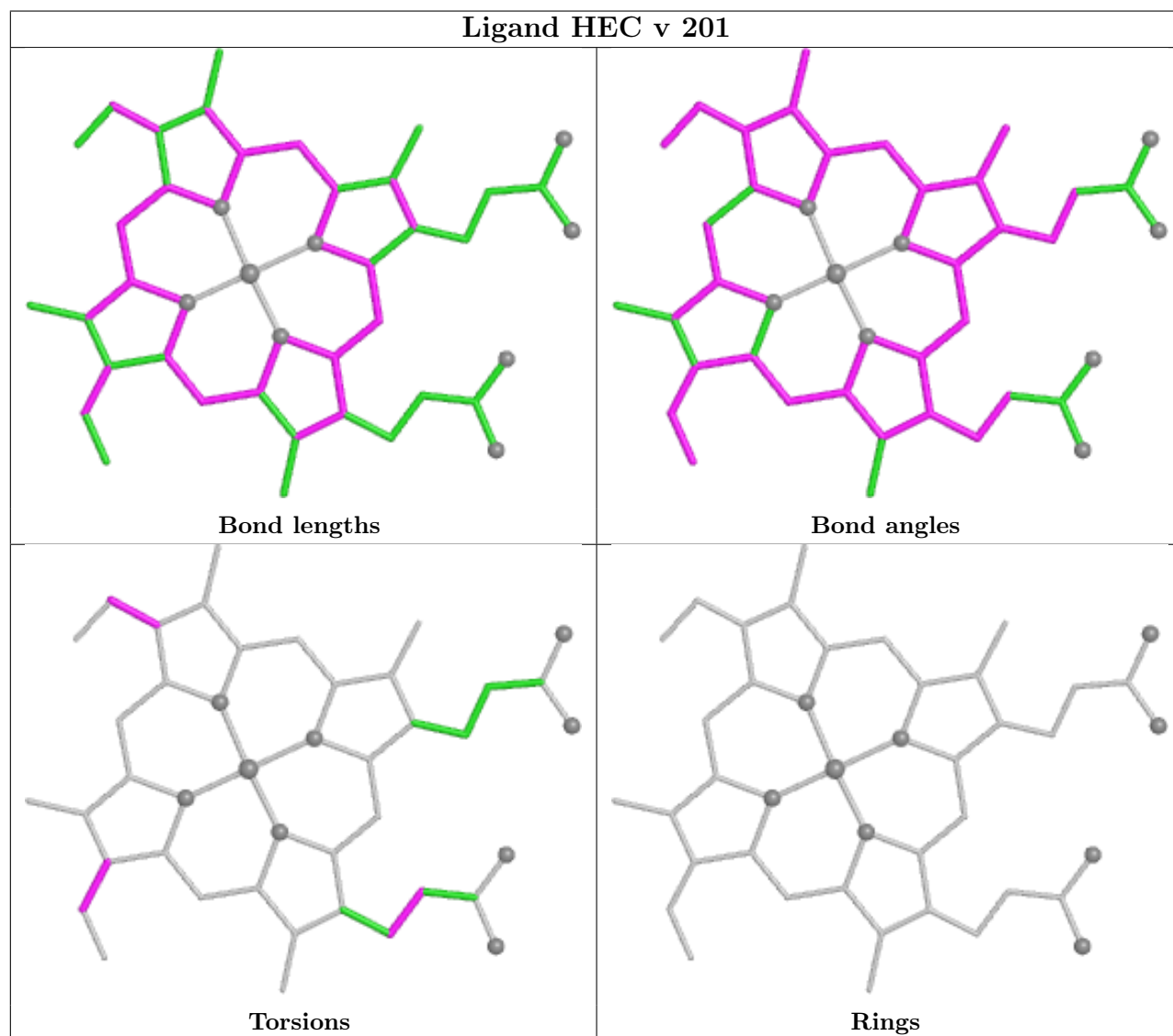
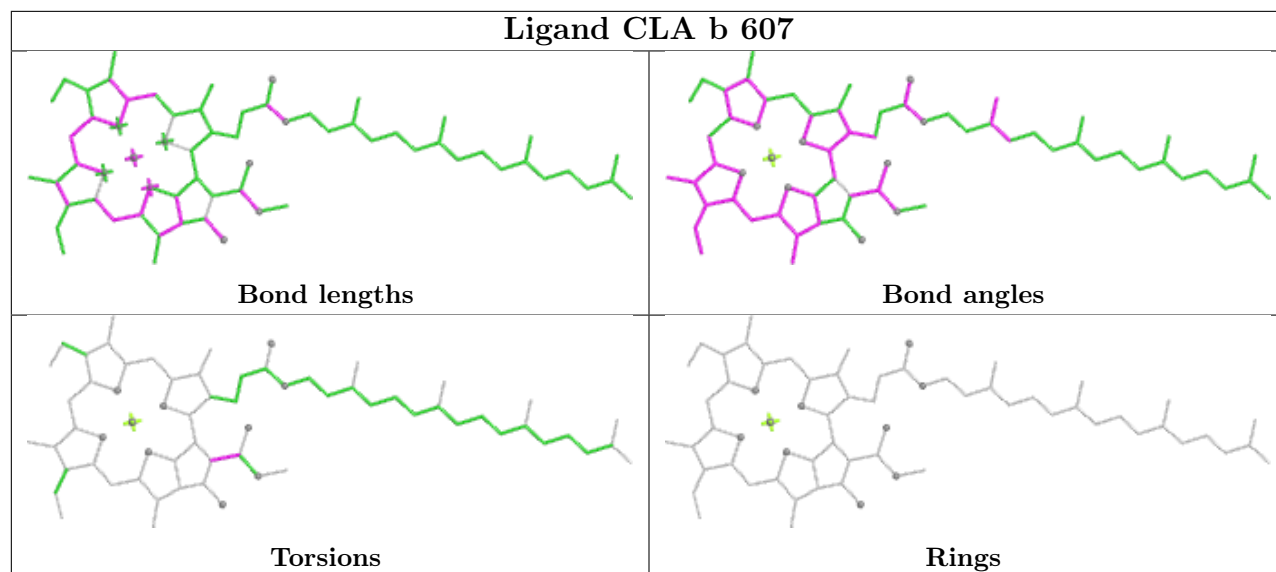


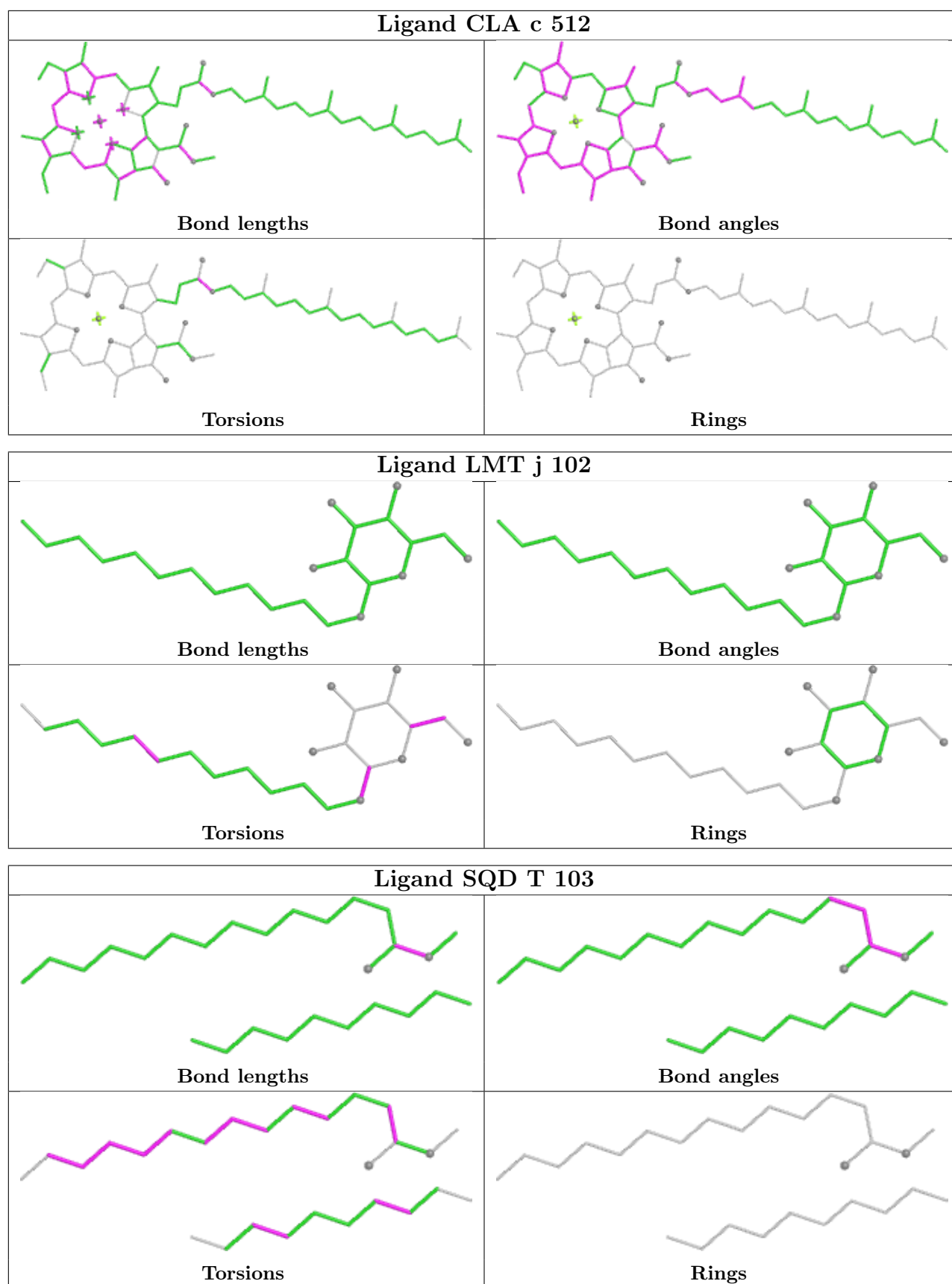


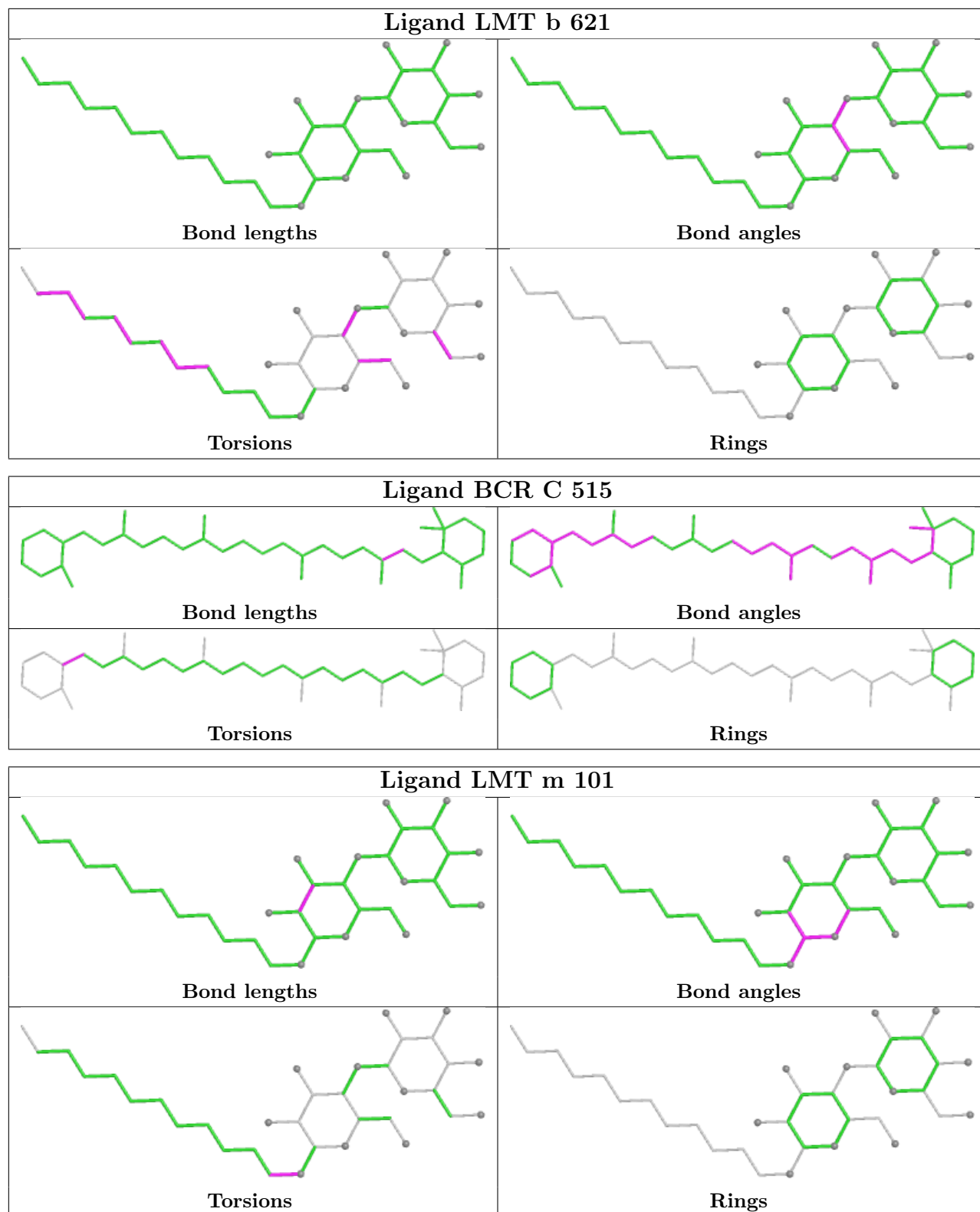


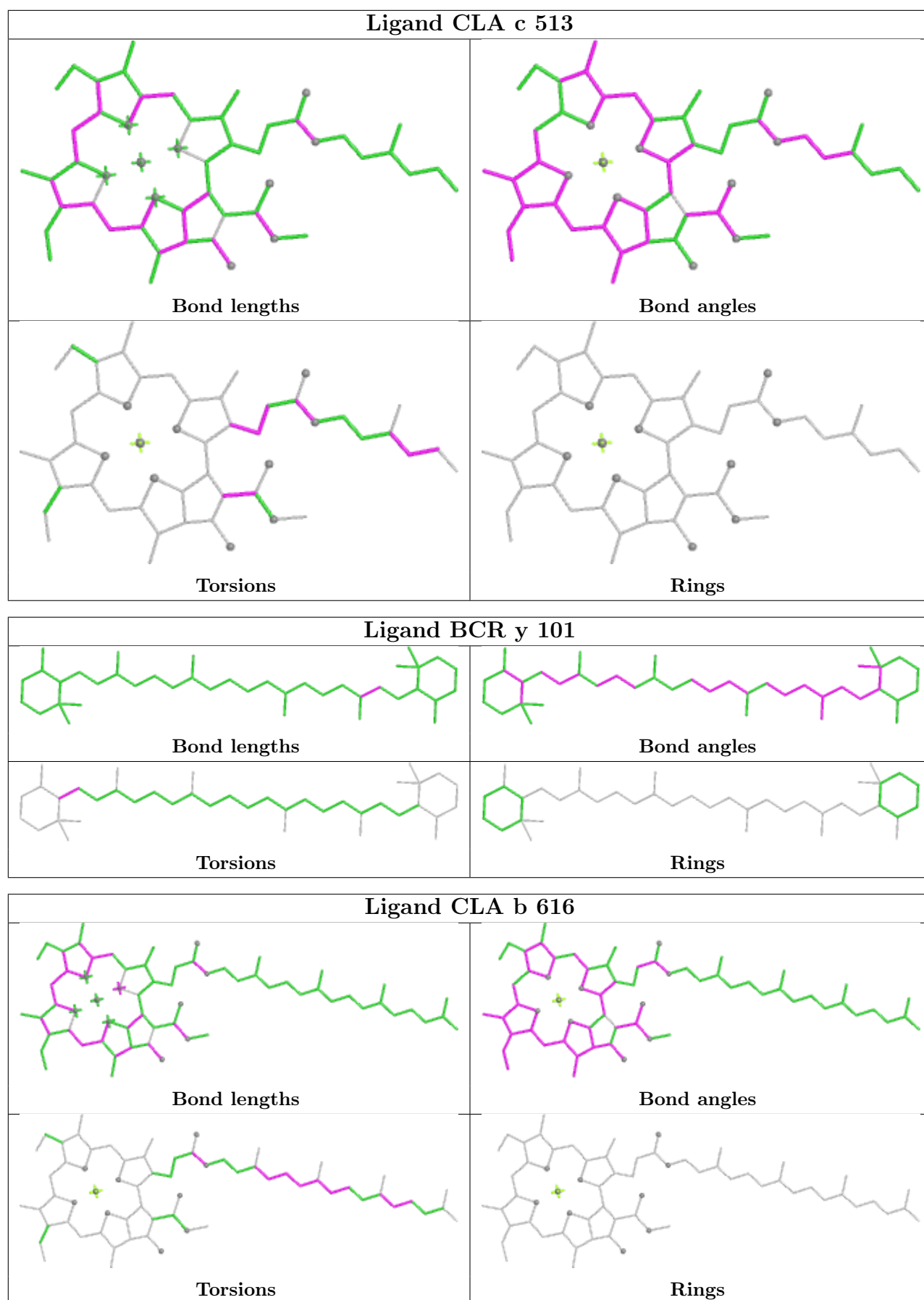


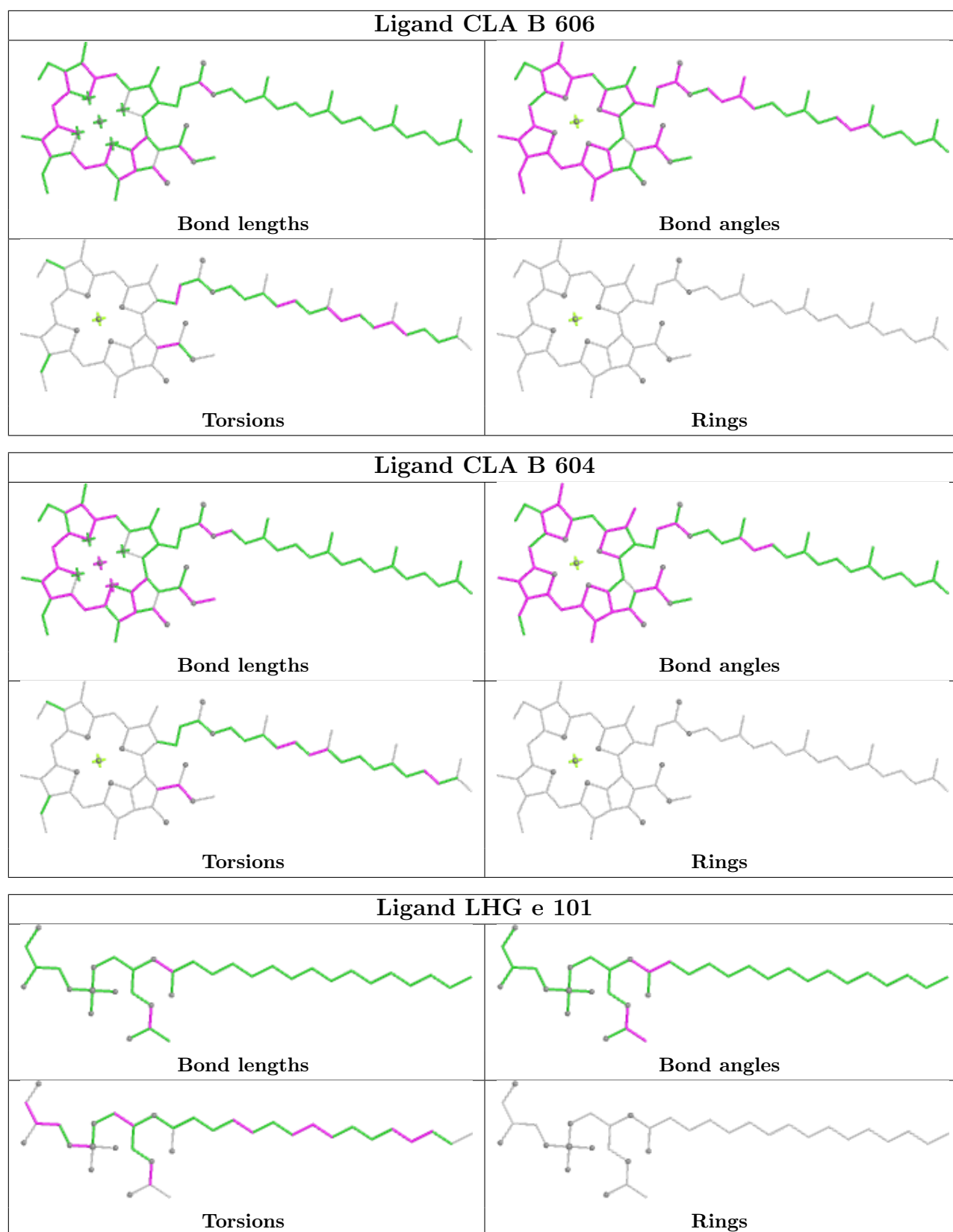


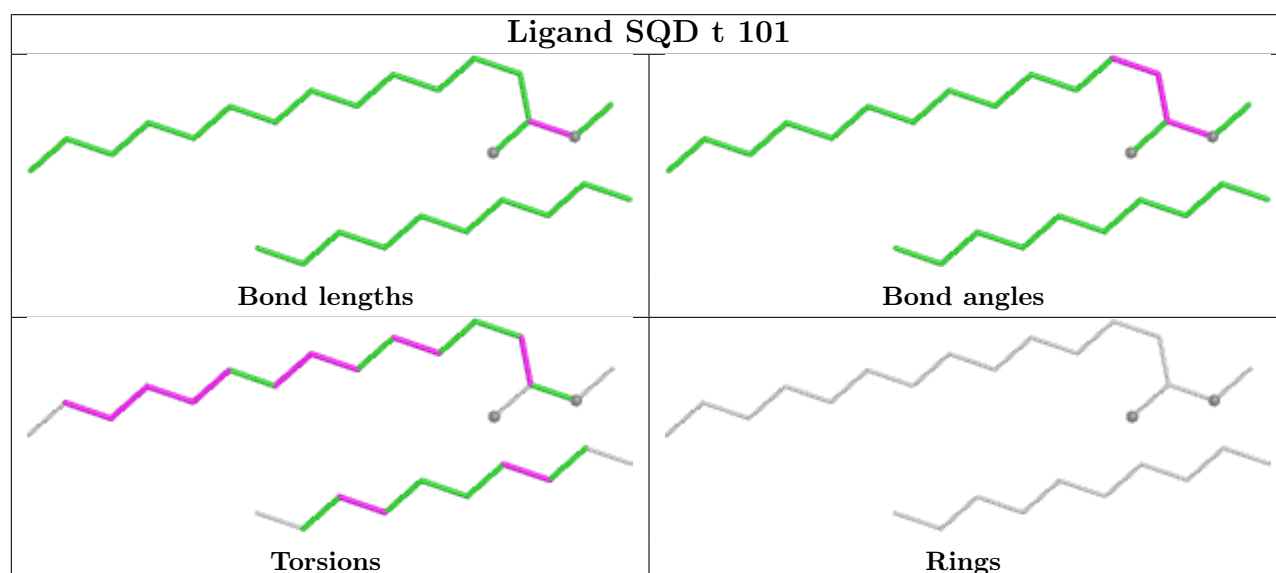
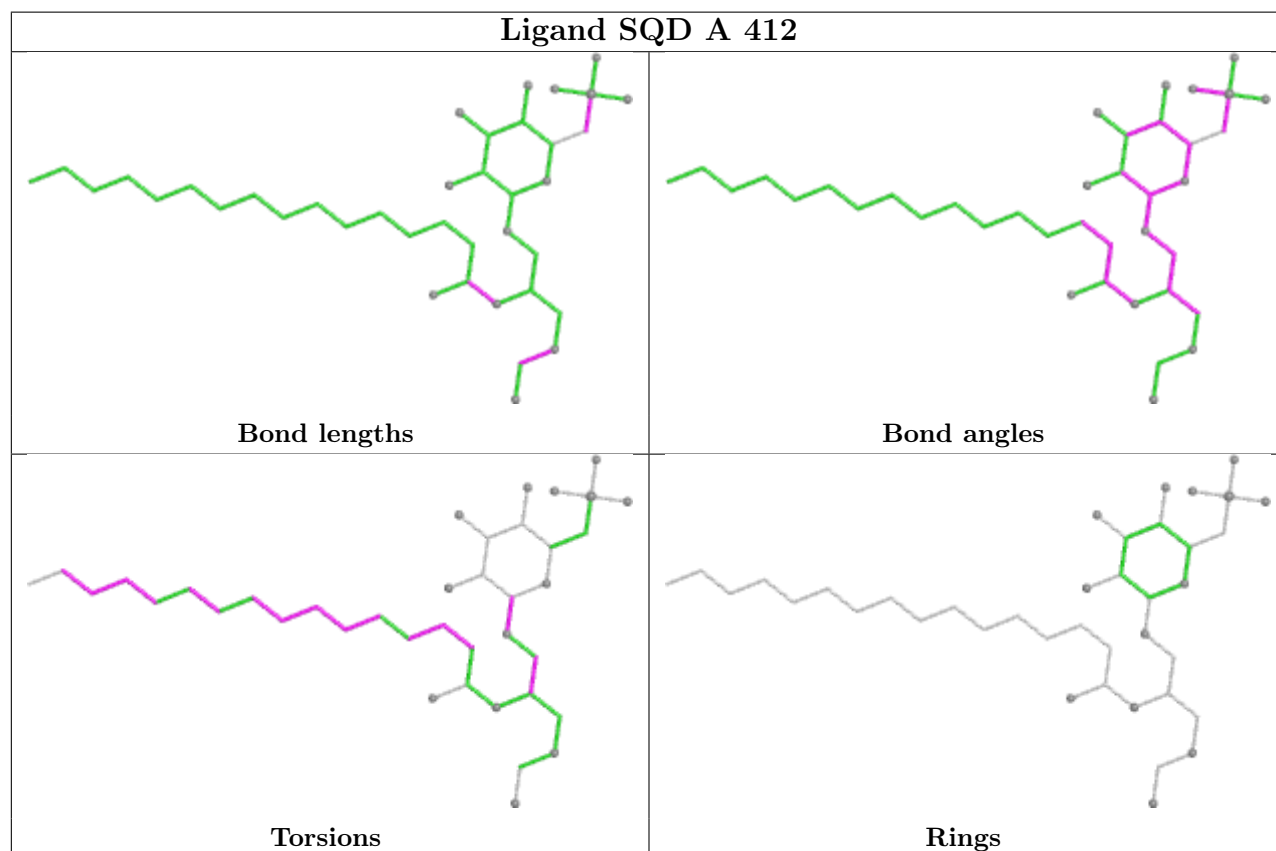
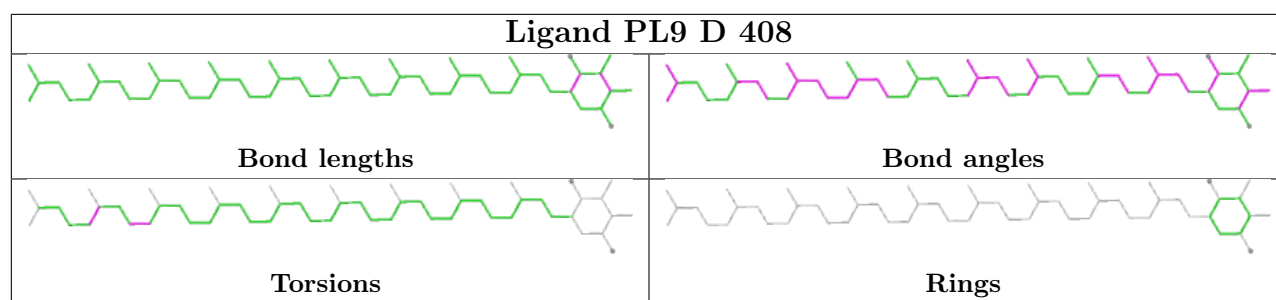


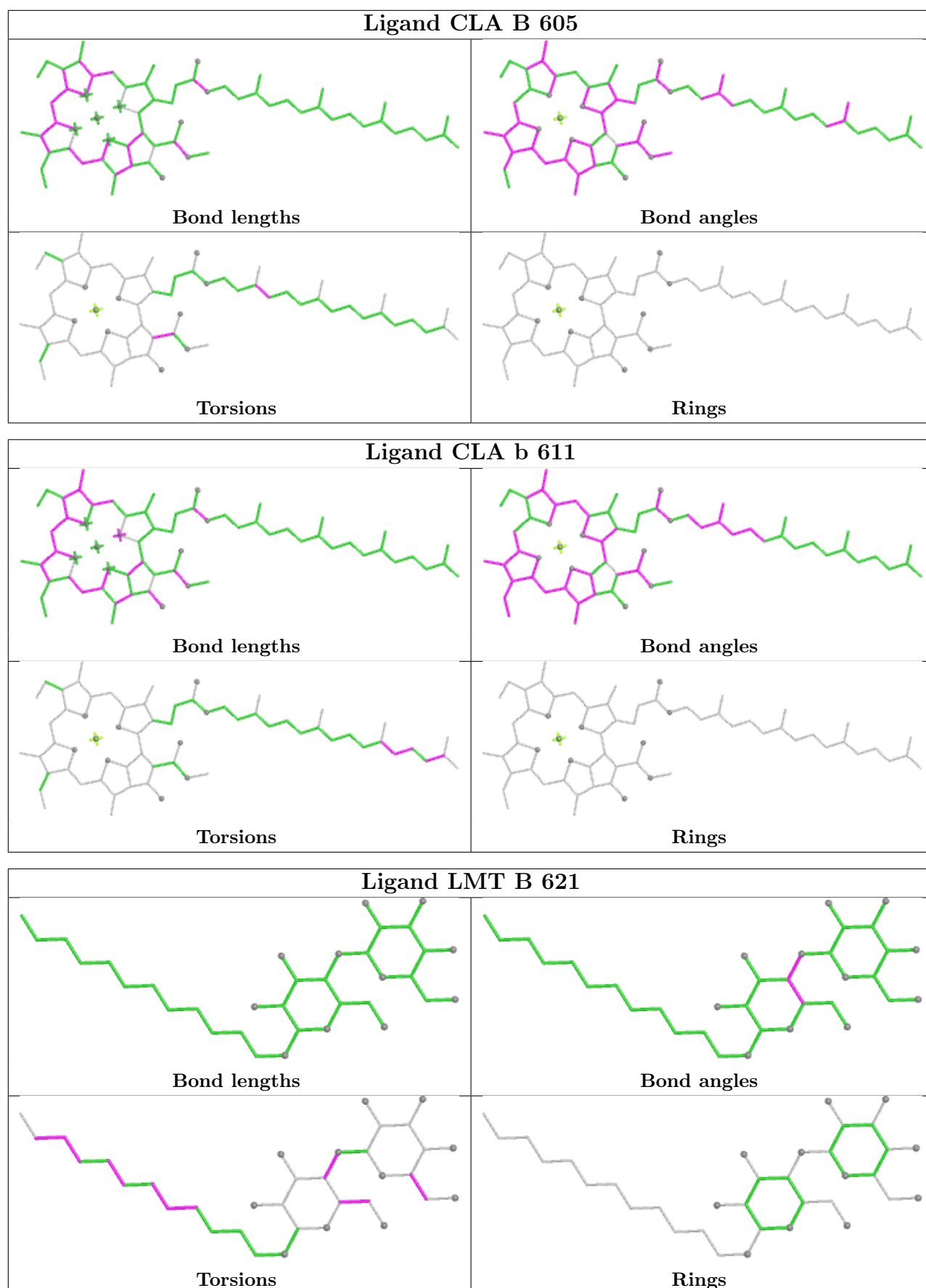












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

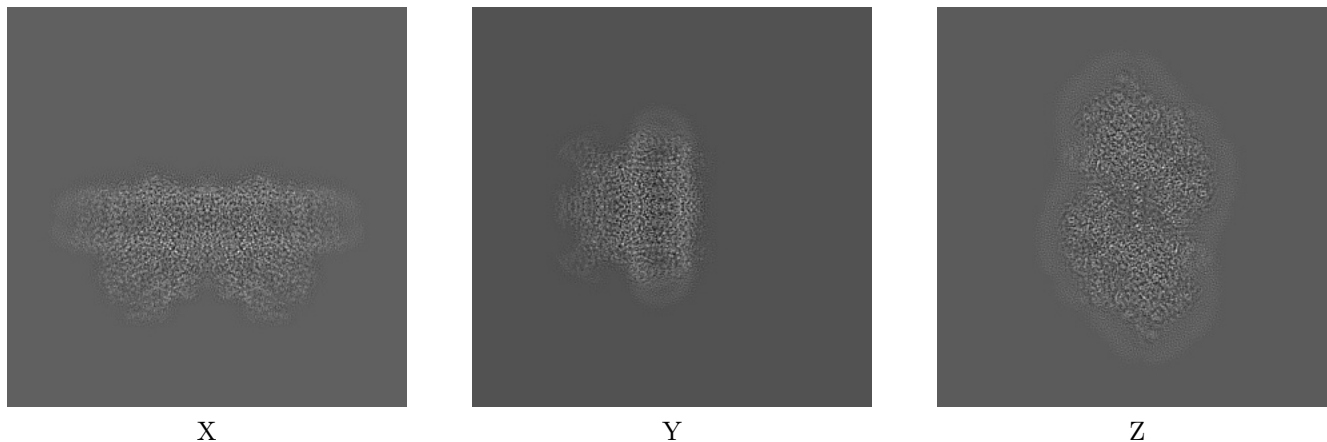
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63639. These allow visual inspection of the internal detail of the map and identification of artifacts.

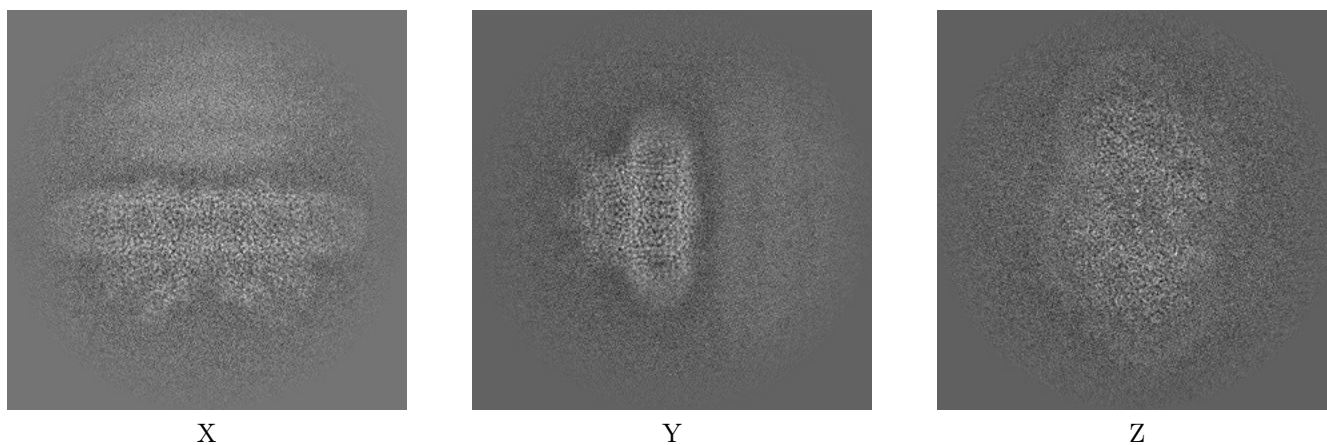
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map



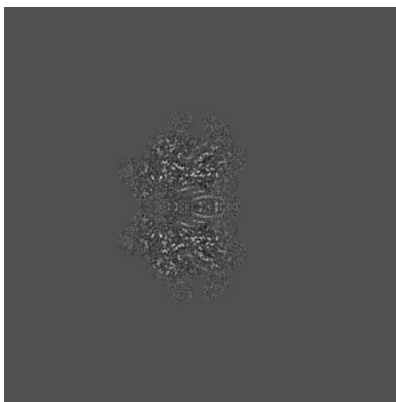
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

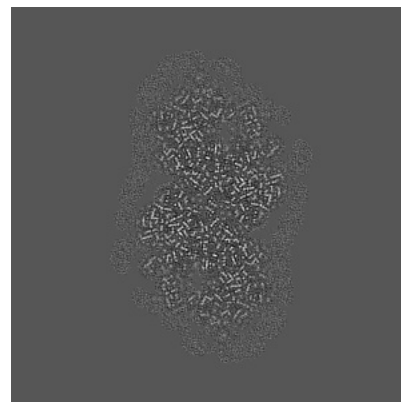
### 6.2.1 Primary map



X Index: 320

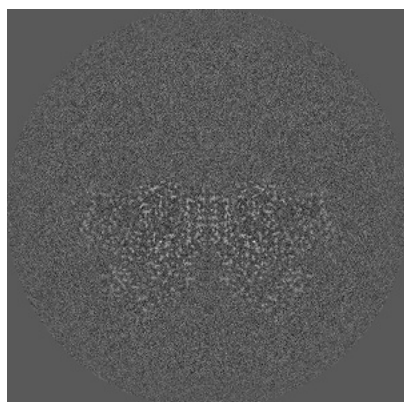


Y Index: 320

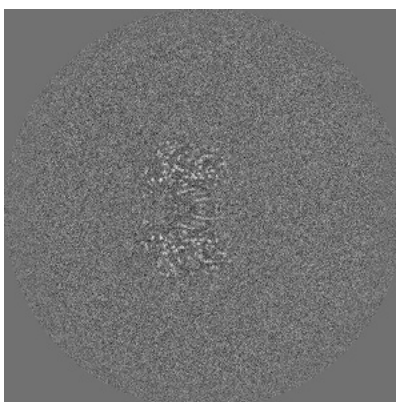


Z Index: 320

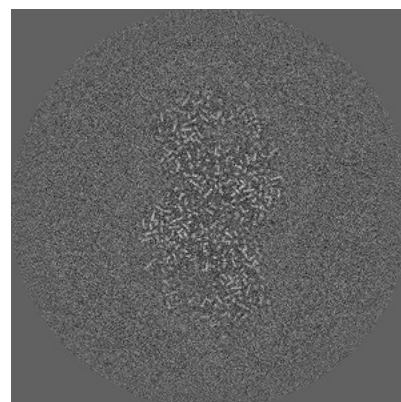
### 6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

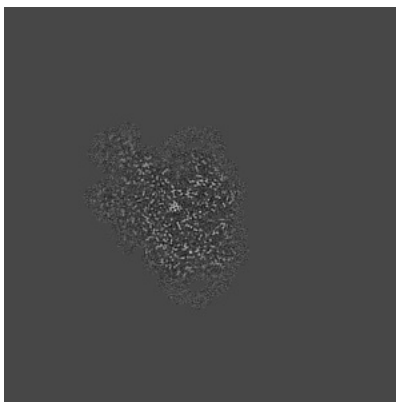
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

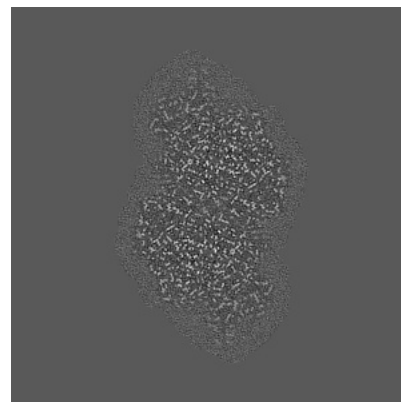
### 6.3.1 Primary map



X Index: 320

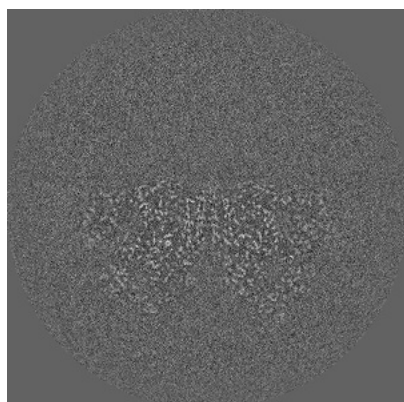


Y Index: 235

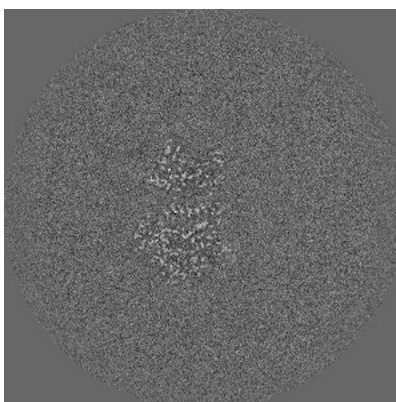


Z Index: 262

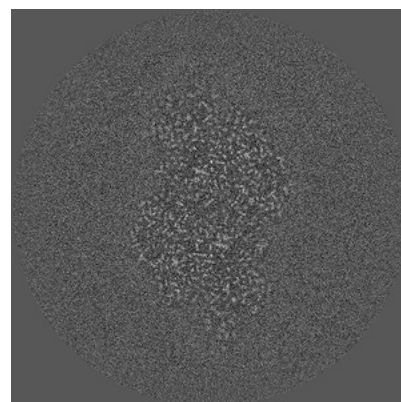
### 6.3.2 Raw map



X Index: 319



Y Index: 312

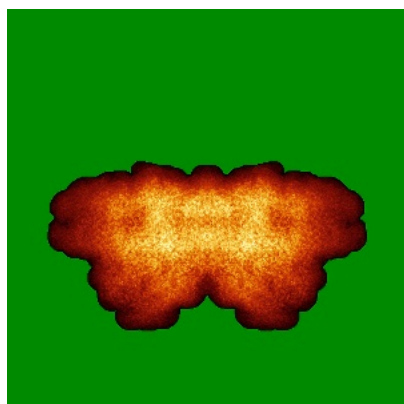


Z Index: 267

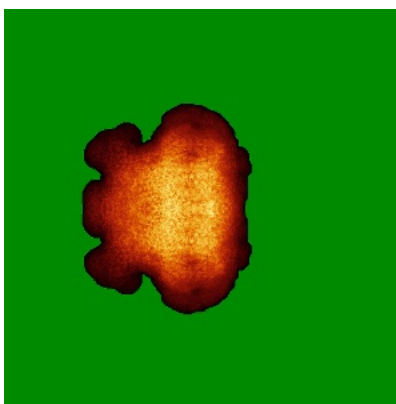
The images above show the largest variance slices of the map in three orthogonal directions.

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

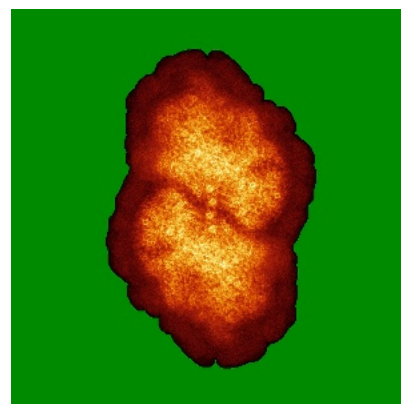
### 6.4.1 Primary map



X

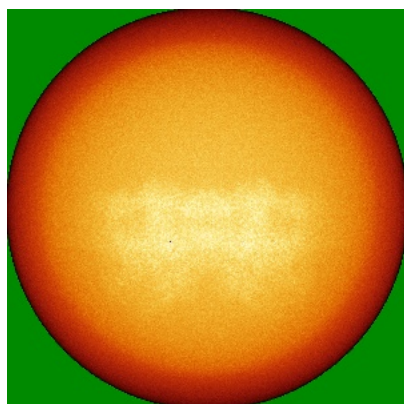


Y

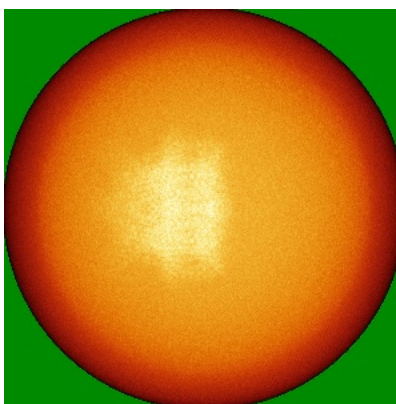


Z

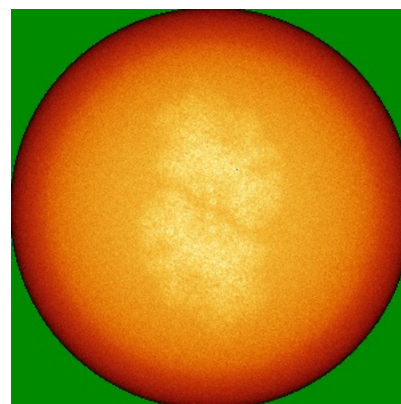
### 6.4.2 Raw map



X



Y

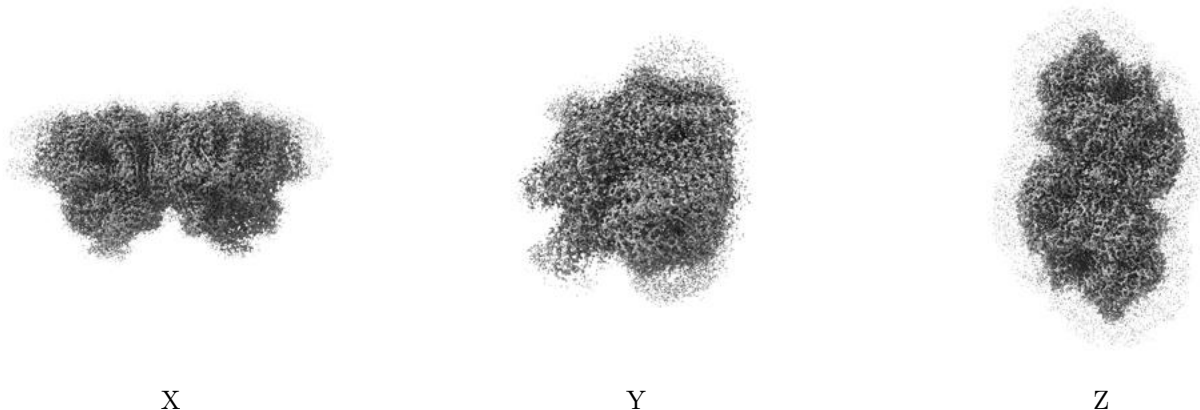


Z

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.

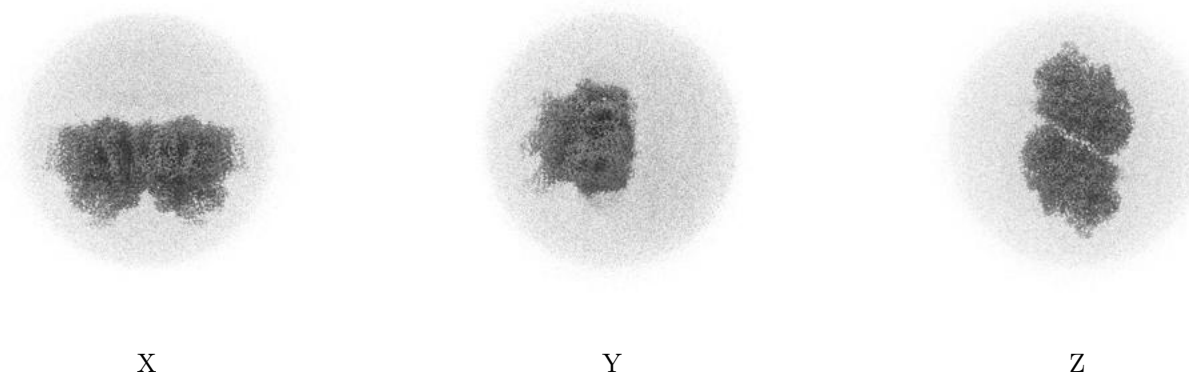
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

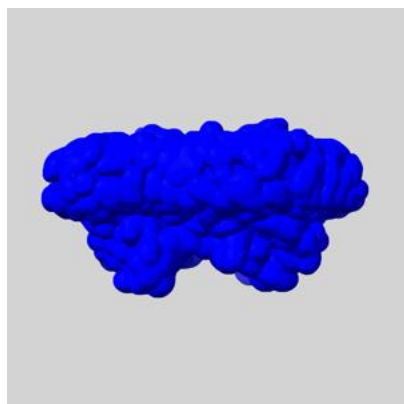
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

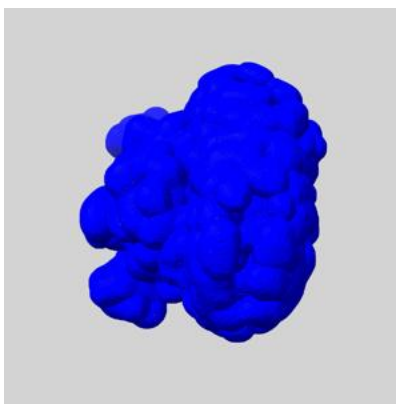
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

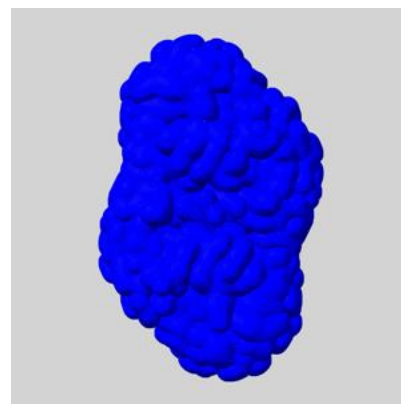
### 6.6.1 emd\_63639\_msk\_1.map [i](#)



X



Y

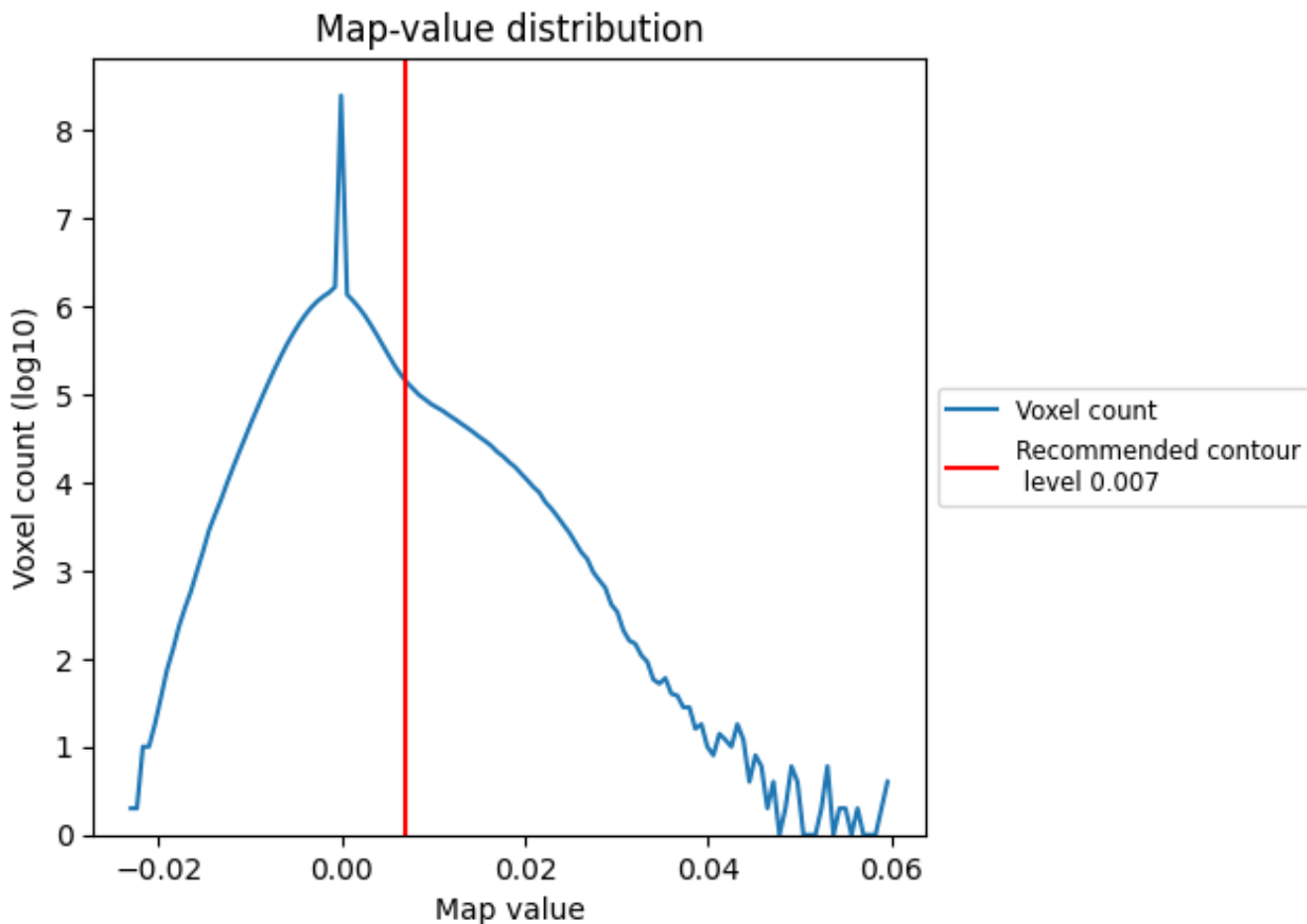


Z

## 7 Map analysis [i](#)

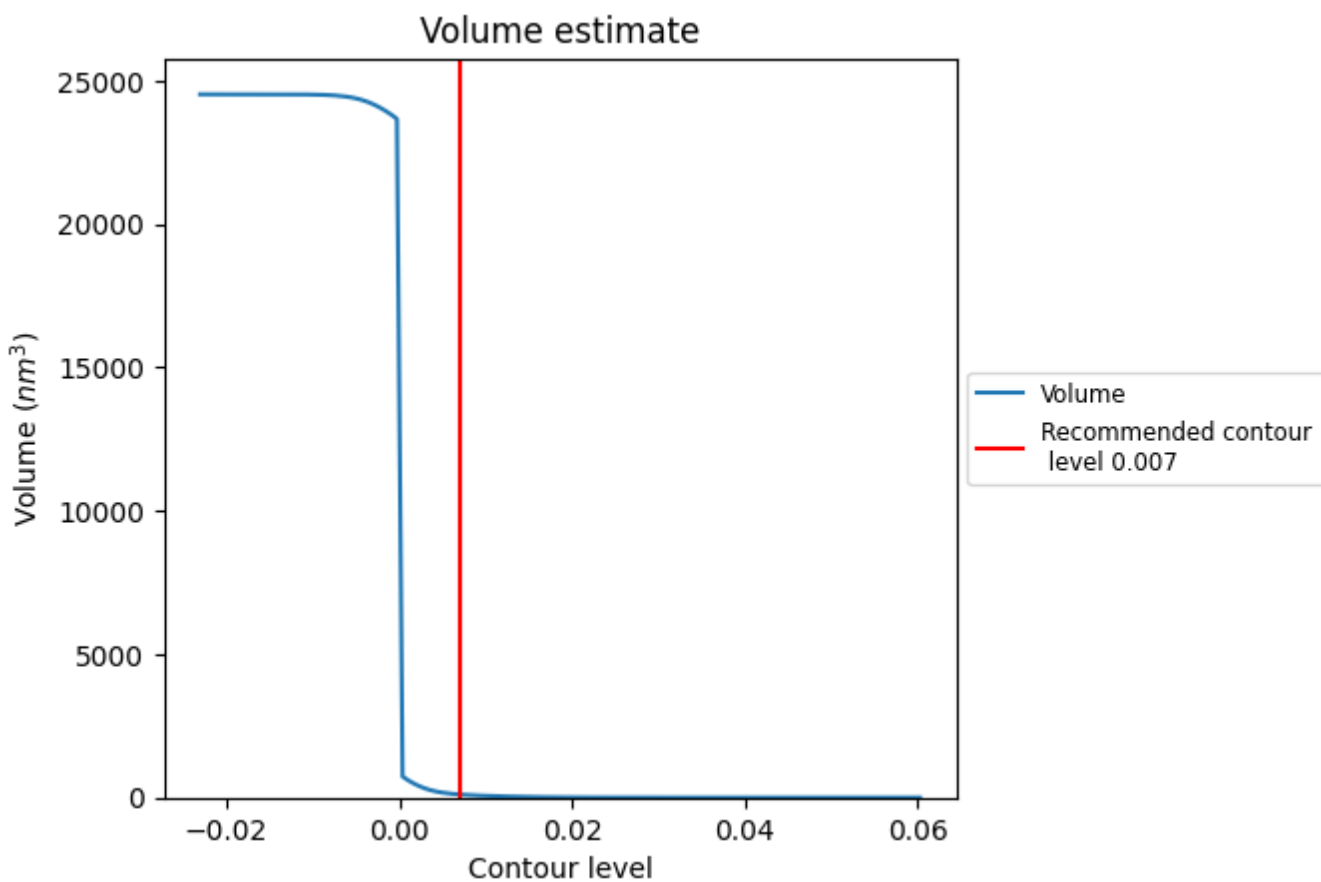
This section contains the results of statistical analysis of the map.

### 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.

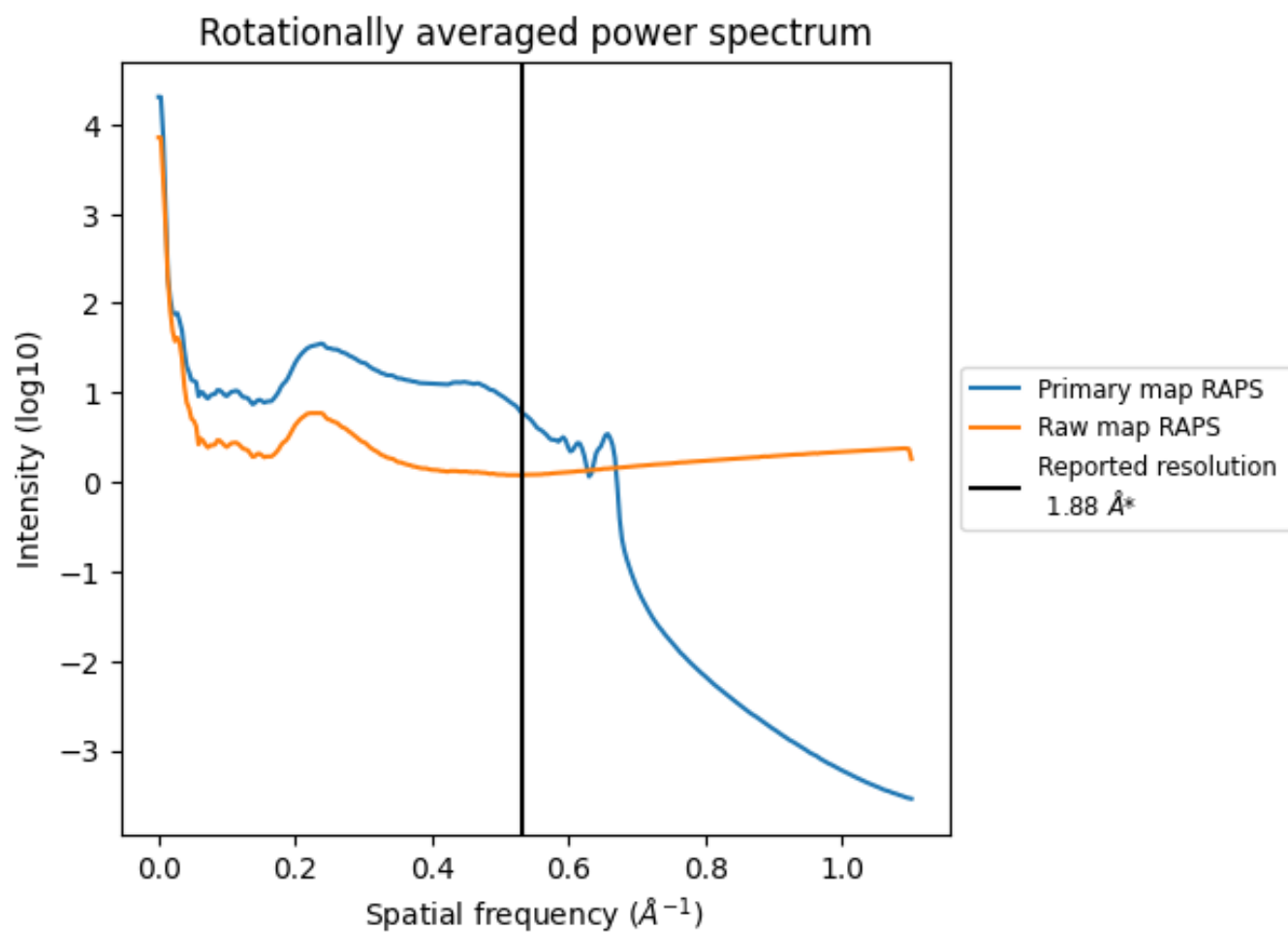
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 107 nm<sup>3</sup>; this corresponds to an approximate mass of 97 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 i

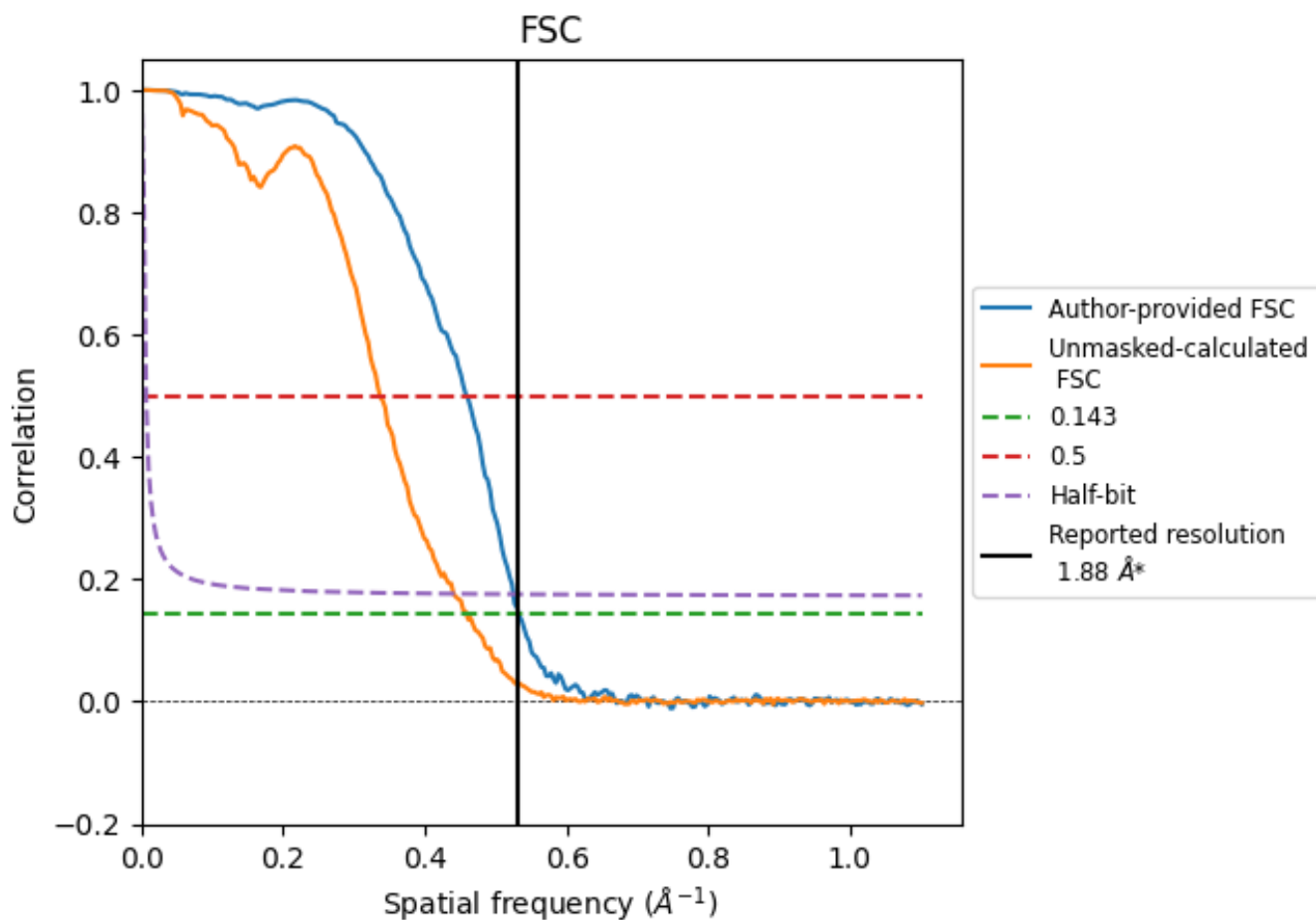


\*Reported resolution corresponds to spatial frequency of 0.532 Å<sup>-1</sup>

## 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 0.532 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

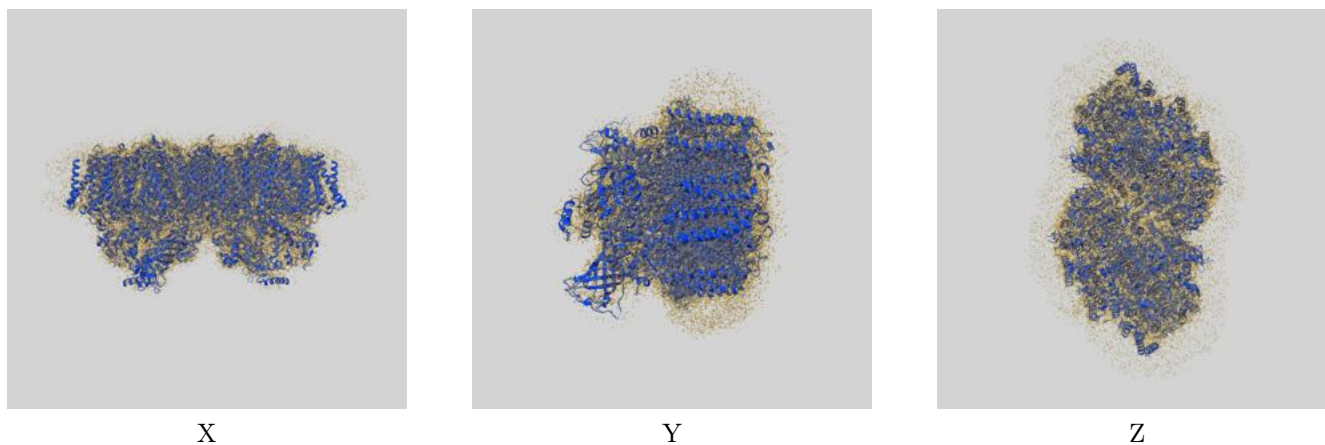
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.88	-	-
Author-provided FSC curve	1.88	2.18	1.91
Unmasked-calculated*	2.18	2.97	2.27

\*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 2.18 differs from the reported value 1.88 by more than 10 %

## 9 Map-model fit [i](#)

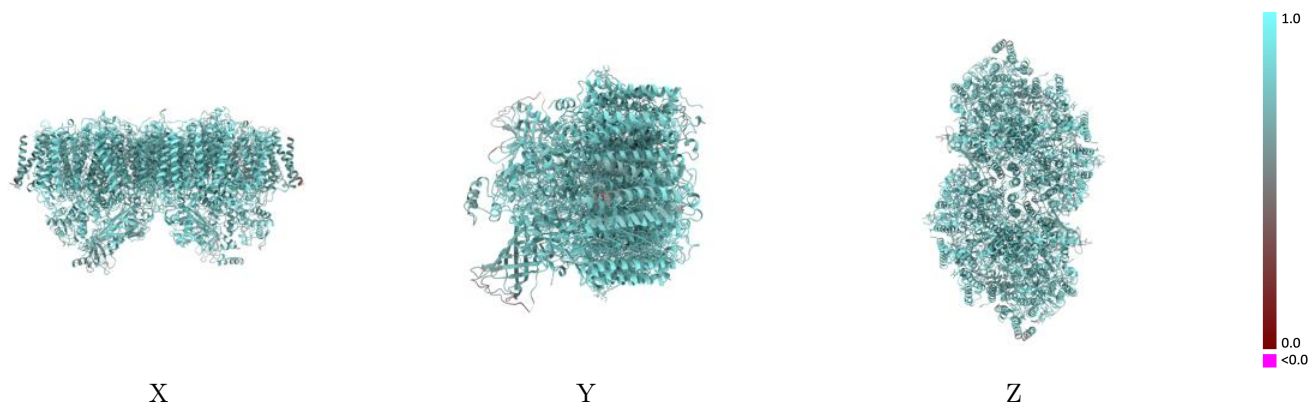
This section contains information regarding the fit between EMDB map EMD-63639 and PDB model 9M5A. Per-residue inclusion information can be found in section 3 on page 27.

### 9.1 Map-model overlay [i](#)



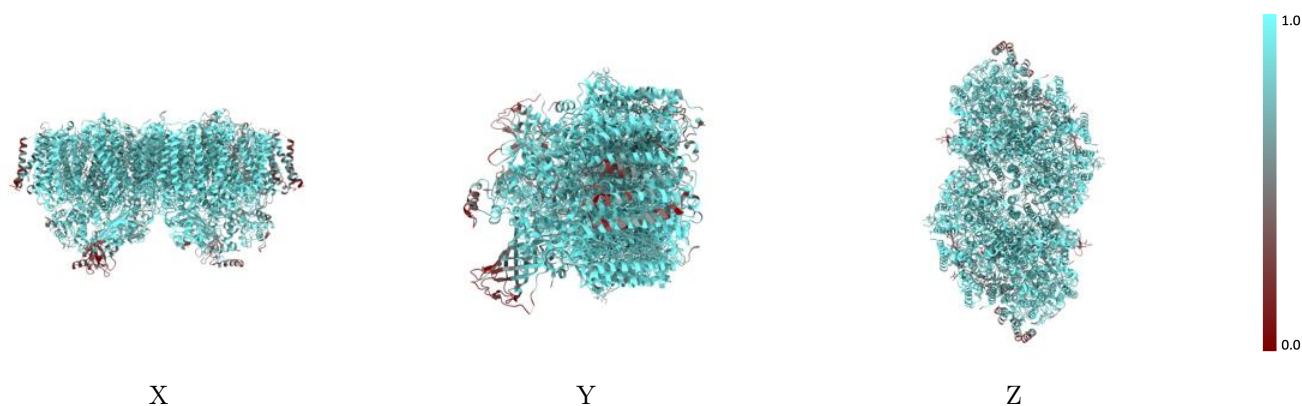
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



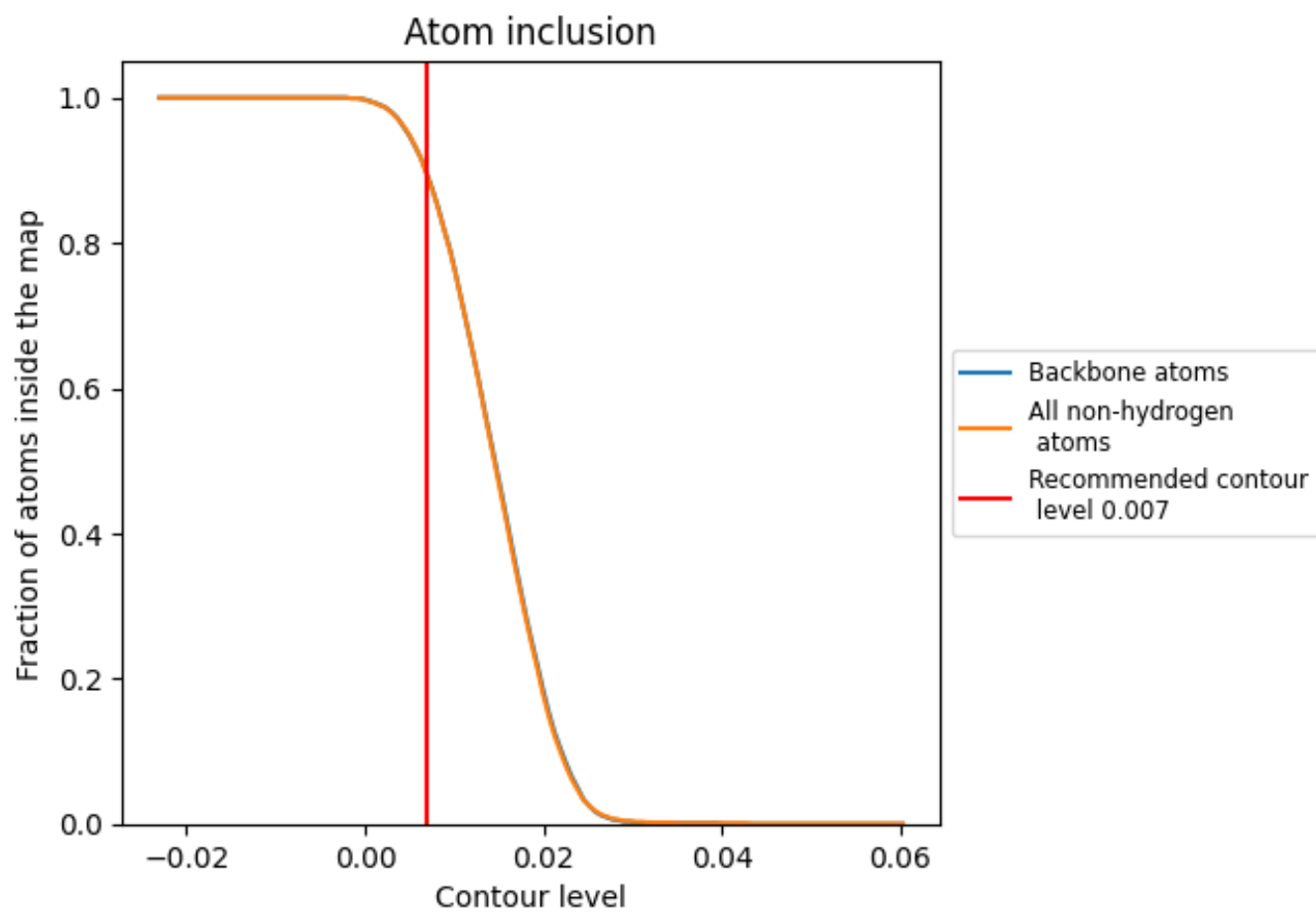
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































## 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.8100
A	 0.9550	 0.8470
B	 0.9320	 0.8240
C	 0.9160	 0.8110
D	 0.9640	 0.8490
E	 0.8090	 0.7600
F	 0.9440	 0.8170
H	 0.9510	 0.8210
I	 0.9420	 0.8210
J	 0.8530	 0.7750
K	 0.8390	 0.7730
L	 0.9310	 0.8420
M	 0.8970	 0.8240
O	 0.7210	 0.7410
T	 0.8910	 0.8050
U	 0.7300	 0.7560
V	 0.7950	 0.7690
X	 0.8330	 0.7830
Y	 0.6190	 0.7240
Z	 0.5010	 0.6690
a	 0.9540	 0.8480
b	 0.9330	 0.8240
c	 0.9150	 0.8100
d	 0.9640	 0.8480
e	 0.8100	 0.7600
f	 0.9440	 0.8180
h	 0.9490	 0.8190
i	 0.9450	 0.8240
j	 0.8530	 0.7750
k	 0.8360	 0.7760
l	 0.9310	 0.8400
m	 0.8970	 0.8250
o	 0.7210	 0.7400
t	 0.9070	 0.8160
u	 0.7300	 0.7550



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*Continued from previous page...*

Chain	Atom inclusion	Q-score
v	 0.7950	 0.7690
x	 0.8330	 0.7860
y	 0.6190	 0.7280
z	 0.5040	 0.6670