



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 11:21 pm BST

PDB ID : 4TNJ
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

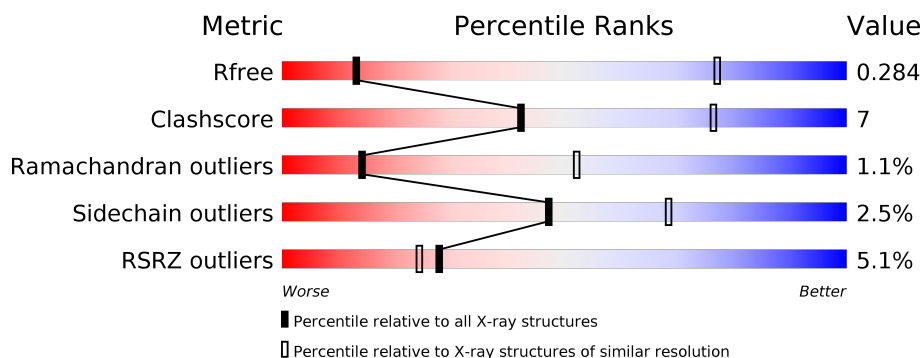
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	

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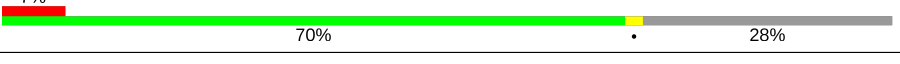
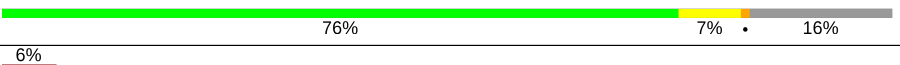

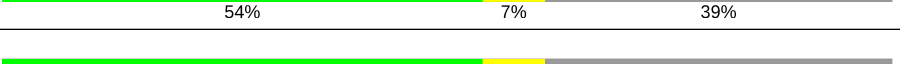
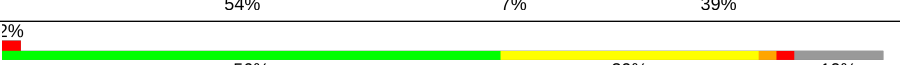
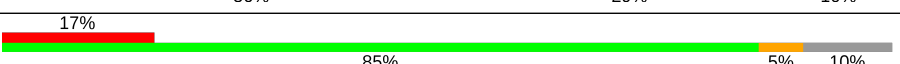
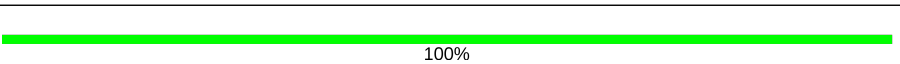
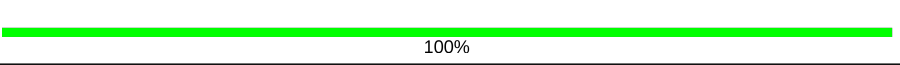

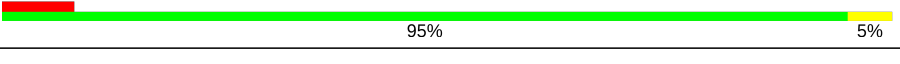

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	

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Mol	Chain	Length	Quality of chain
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X
27	LMG	M	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	a	402	-	-	-	X
27	LMG	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	622	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

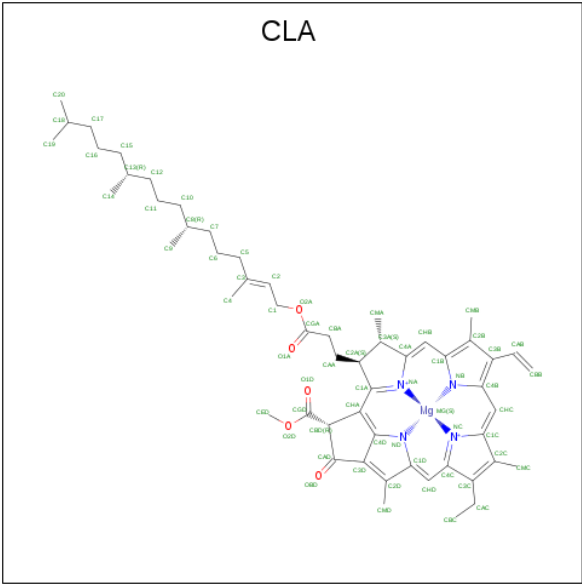
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	A	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0
22	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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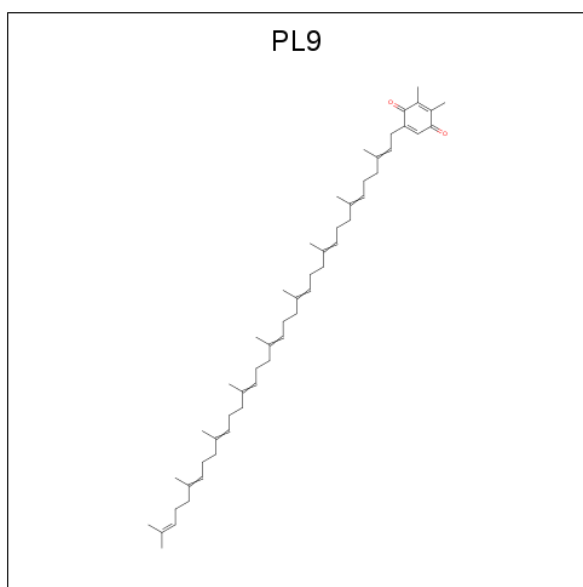
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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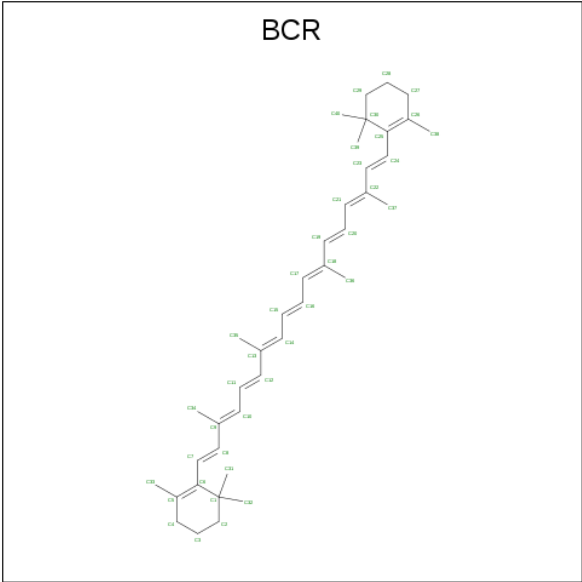
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 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 (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



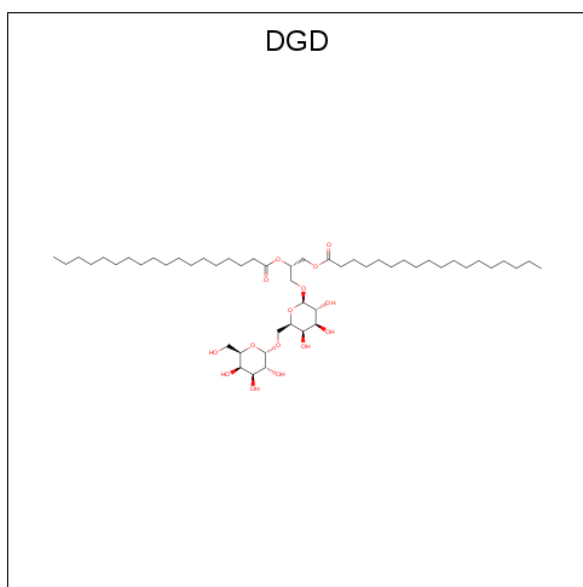
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



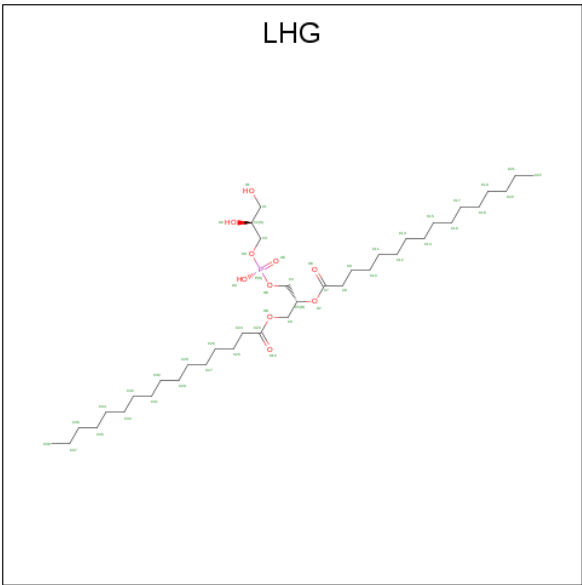
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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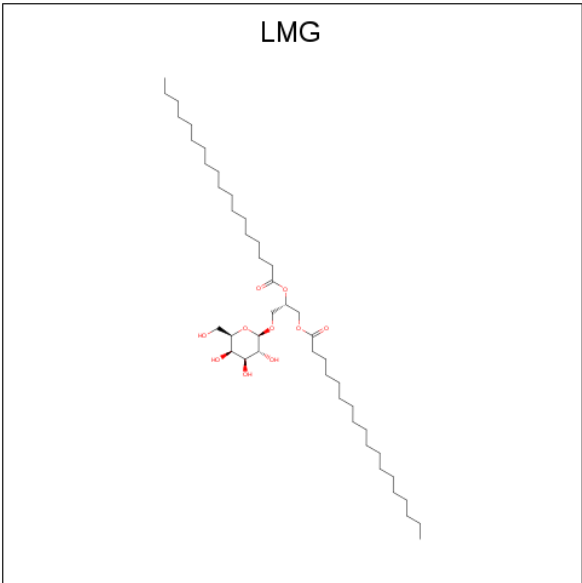
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	C	O	0	0
			52	37	15		
25	b	1	Total	C	O	0	0
			58	43	15		
25	c	1	Total	C	O	0	0
			53	38	15		
25	c	1	Total	C	O	0	0
			62	47	15		
25	c	1	Total	C	O	0	0
			66	51	15		
25	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).

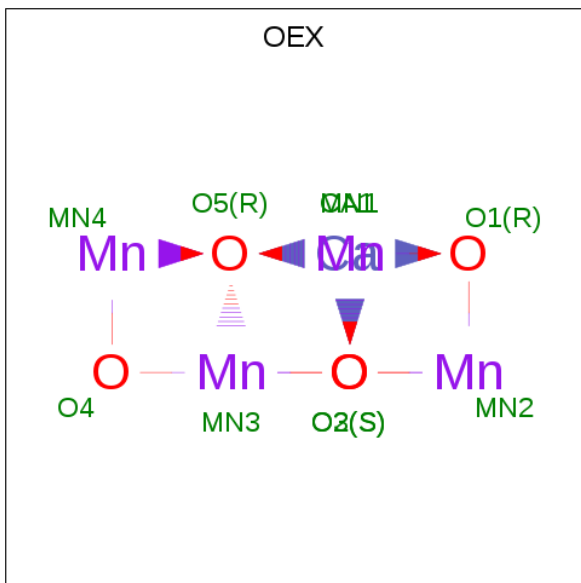


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	c	1	Total	C	O	0	0
			45	35	10		
27	c	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			46	36	10		
27	e	1	Total	C	O	0	0
			44	34	10		
27	i	1	Total	C	O	0	0
			43	33	10		
27	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

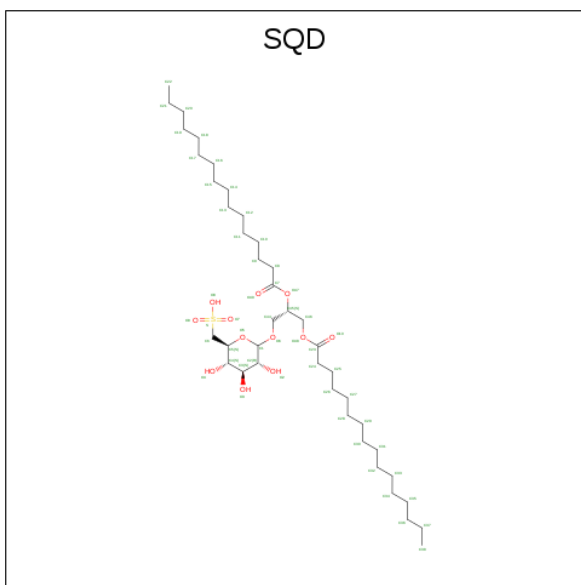
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



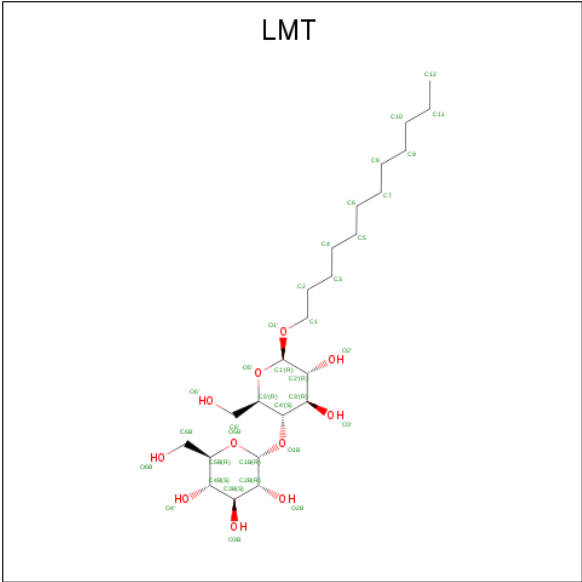
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



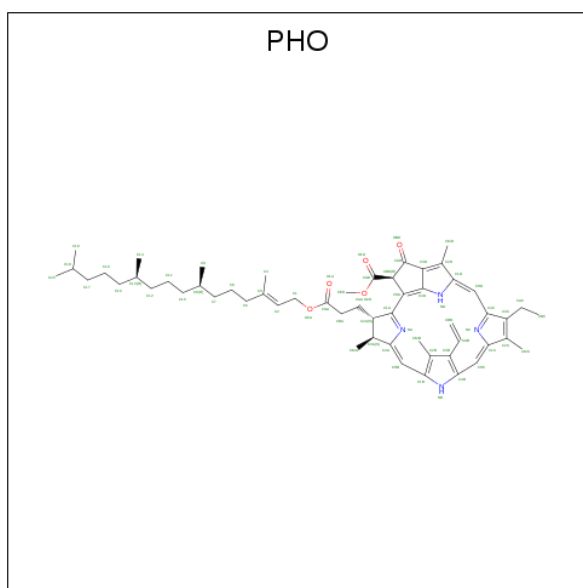
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

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



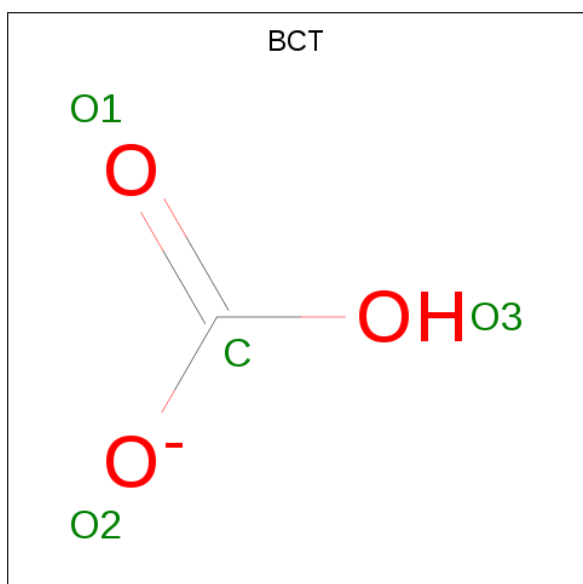
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	d	1	Total	C	O	0	0
			31	20	11		
31	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



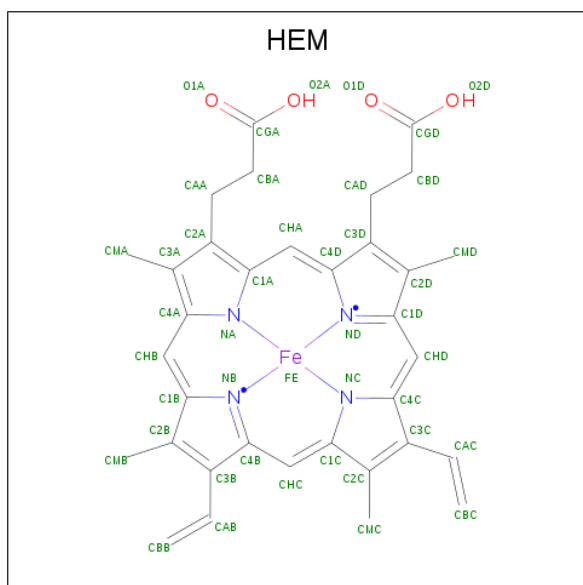
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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



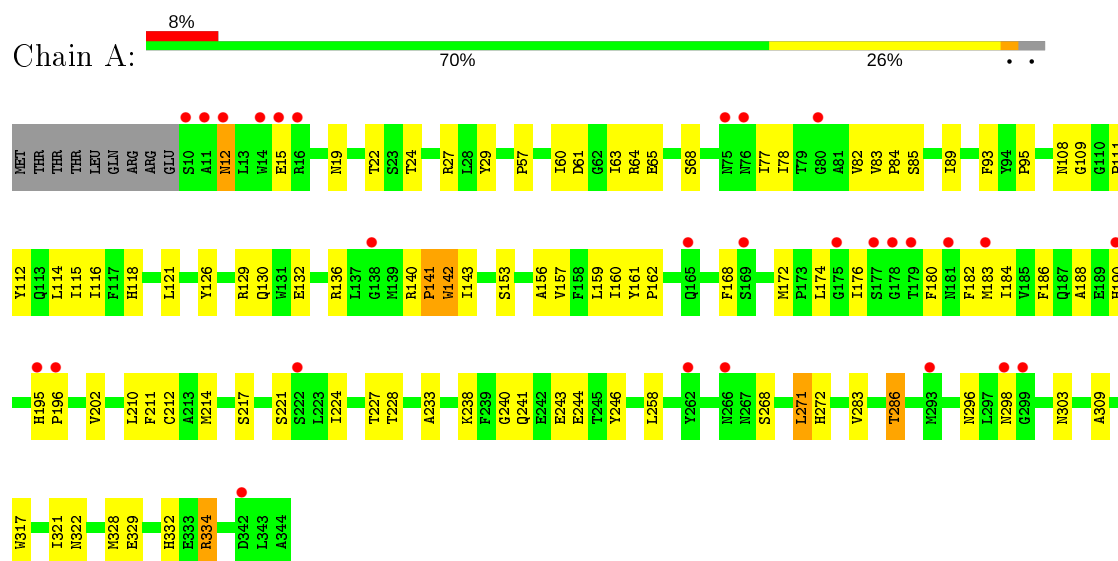
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	k	1	Total	Ca	0	0
			1	1		

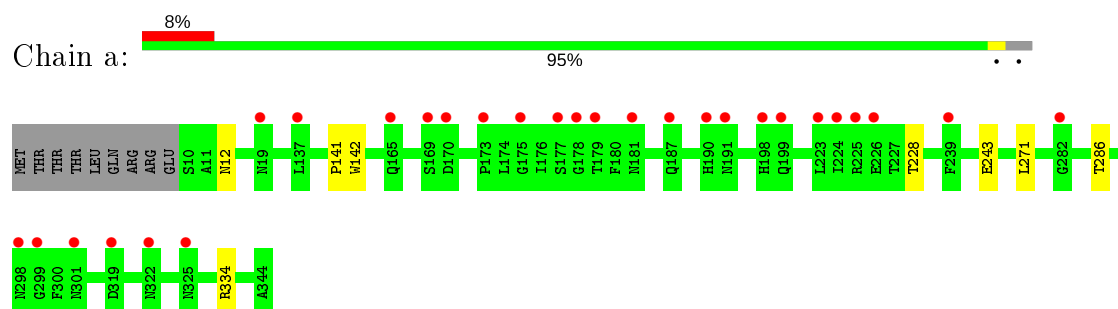
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

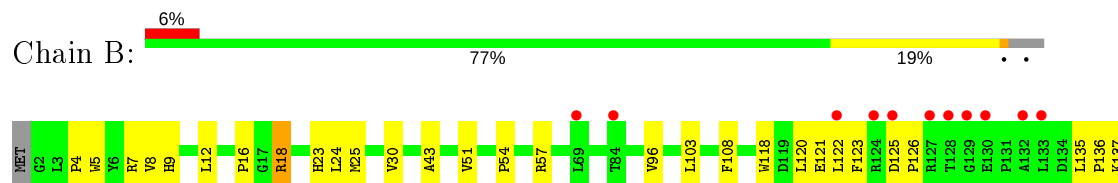
• Molecule 1: Photosystem Q(B) protein 1

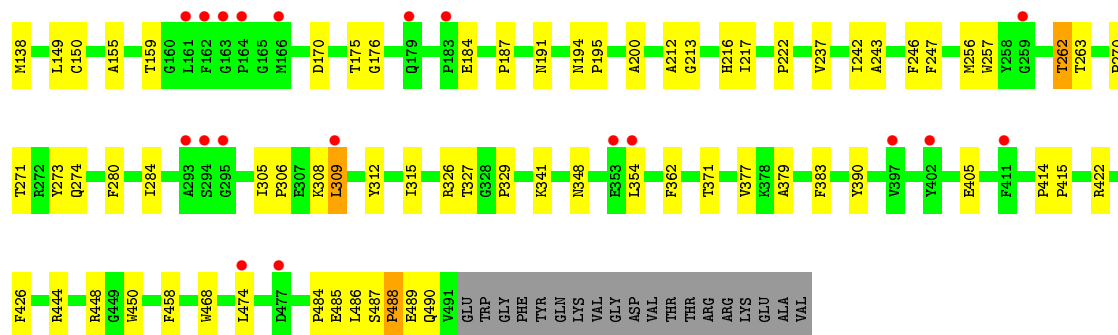


• Molecule 1: Photosystem Q(B) protein 1

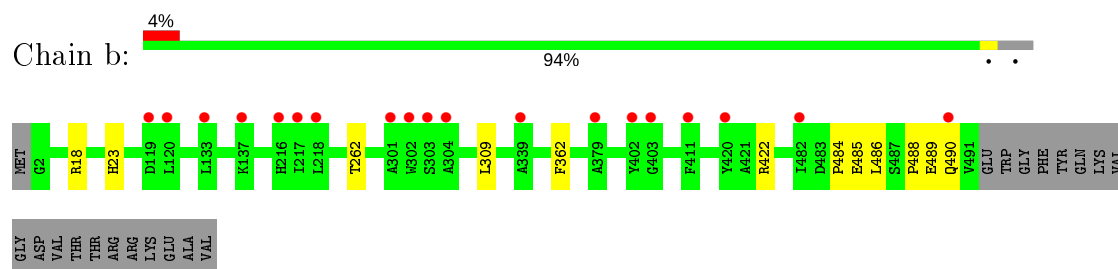


• Molecule 2: Photosystem II core light harvesting protein

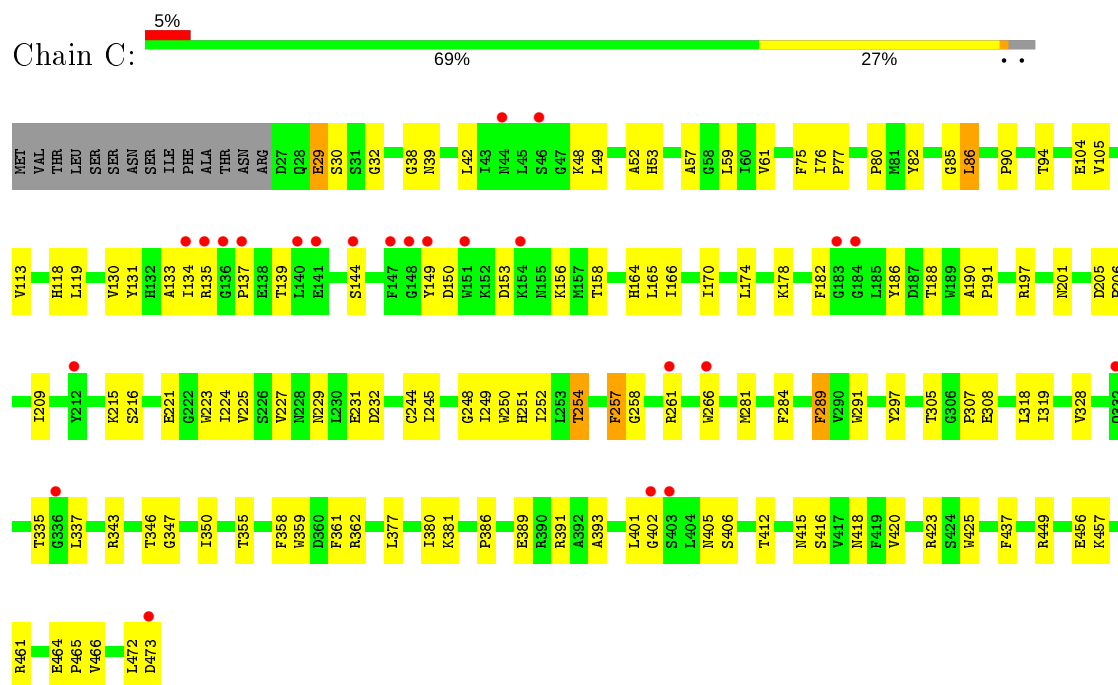




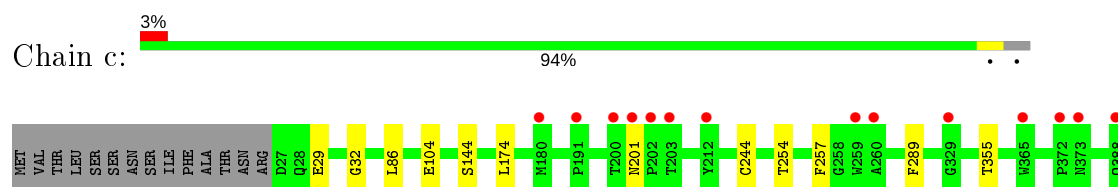
• Molecule 2: Photosystem II core light harvesting protein

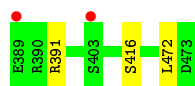


• Molecule 3: Photosystem II CP43 protein

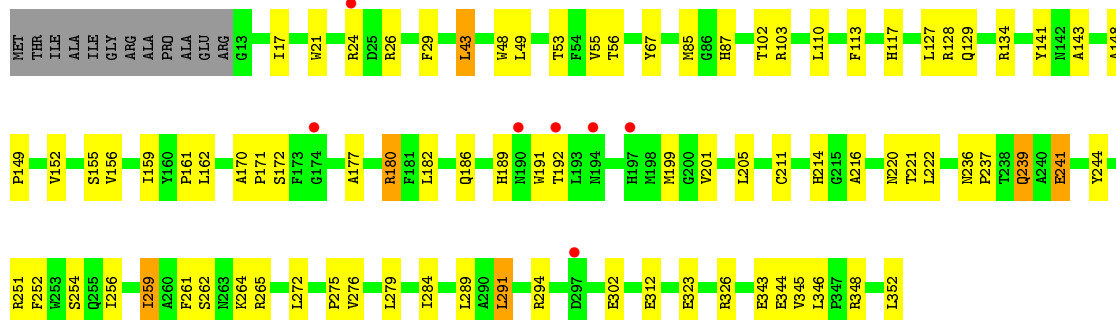
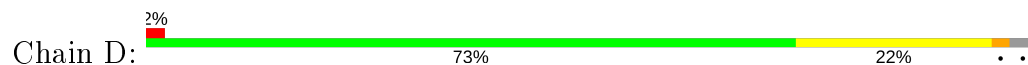


• Molecule 3: Photosystem II CP43 protein

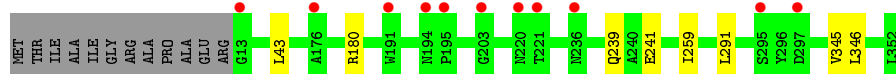




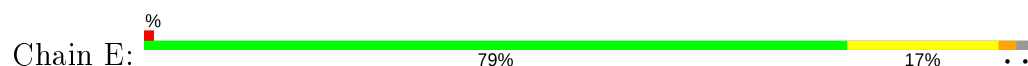
• Molecule 4: Photosystem II D2 protein



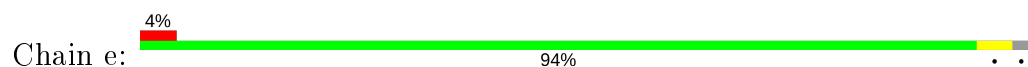
• Molecule 4: Photosystem II D2 protein



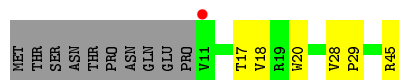
• Molecule 5: Cytochrome b559 subunit alpha




• Molecule 5: Cytochrome b559 subunit alpha

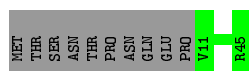


• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta

Chain f:  78% 22%




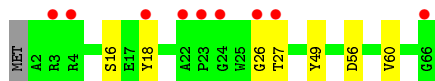
- Molecule 7: Photosystem II reaction center protein H

Chain H:  11% 70% 27% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  14% 88% 11% .




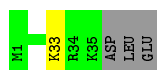
- Molecule 8: Photosystem II reaction center protein I

Chain I:  76% 16% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  89% . 8%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 25% . 15%



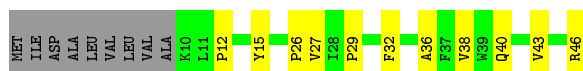
- Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




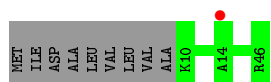
- Molecule 10: Photosystem II reaction center protein K

Chain K:  57% 24% 20%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  2% 80% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 81% 19%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  97% 3%



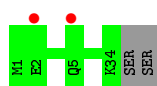
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 78% 17% 6%



- Molecule 12: Photosystem II reaction center protein M

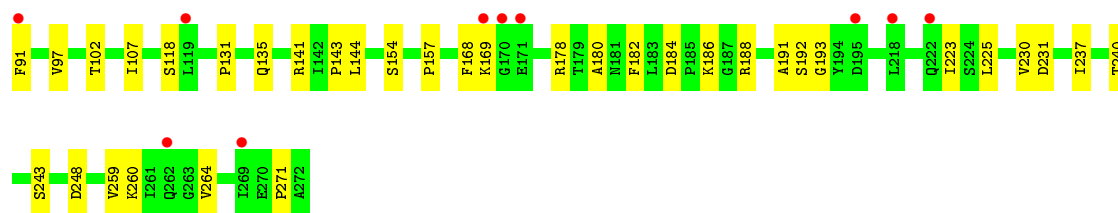
Chain m:  6% 94% 6%



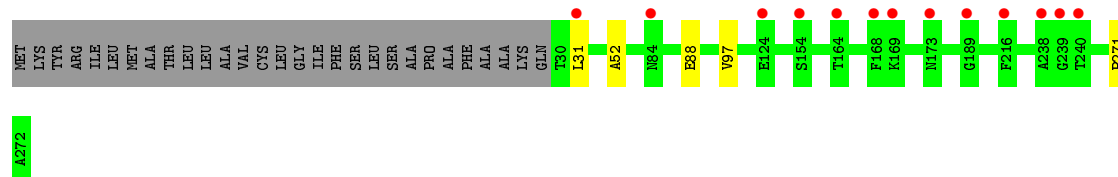
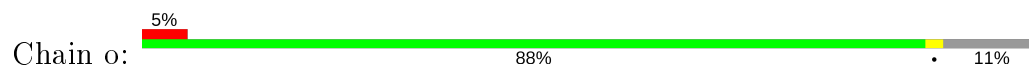
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  6% 72% 18% 11%

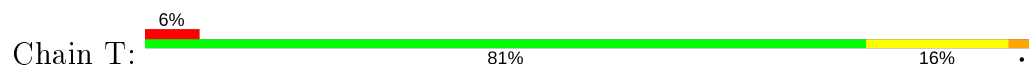




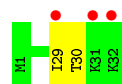
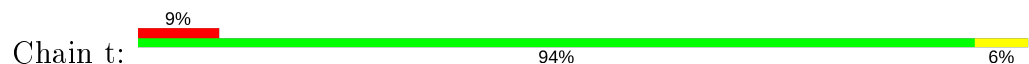
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



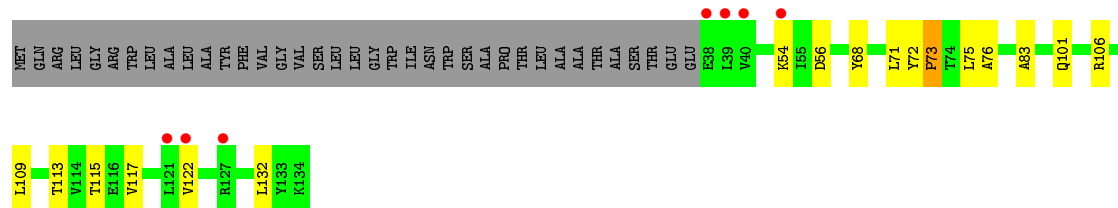
- Molecule 14: Photosystem II reaction center protein T



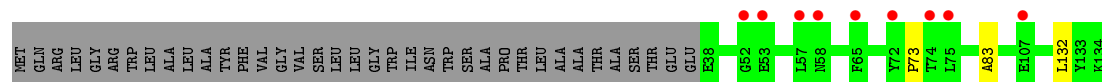
- Molecule 14: Photosystem II reaction center protein T




- Molecule 15: Photosystem II 12 kDa extrinsic protein

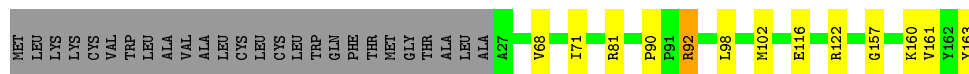


- Molecule 15: Photosystem II 12 kDa extrinsic protein




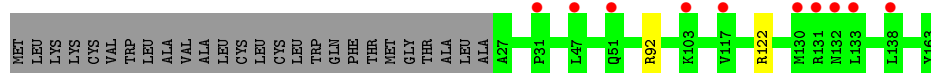
- Molecule 16: Cytochrome c-550

Chain V:  76% 7% 16%



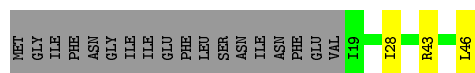
- Molecule 16: Cytochrome c-550

Chain v:  6% 83% 16%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  54% 7% 39%



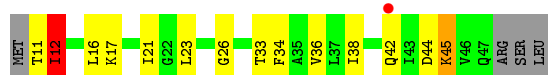
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:  2% 54% 7% 39%




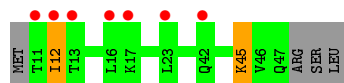
- Molecule 18: Photosystem II reaction center X protein

Chain X:  2% 56% 29% 10%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  17% 85% 5% 10%



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%


There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

Chain G:  100%

There are no outlier residues recorded for this chain.

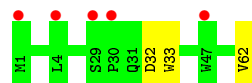
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  2% 84% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  8% 95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.277 , 0.284	Depositor DCC
R_{free} test set	2668 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	79	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	87	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	18	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	267	0	289	6	0
12	m	267	0	289	0	0
13	O	1845	0	1801	29	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	13	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	92	0
22	C	845	0	936	49	0
22	D	130	0	144	14	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	3	0
23	D	55	0	80	8	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	11	0
24	C	120	0	168	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	98	0	136	6	0
27	C	93	0	126	7	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	0	0
27	b	98	0	136	0	0
27	c	93	0	126	0	0
27	d	94	0	128	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	16	0
32	a	64	0	74	0	0
32	d	64	0	74	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	586	0

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

The worst 5 of 586 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.87
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.50	0.80
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.77

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 X-ray entries followed by that with respect to entries of similar resolution.

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	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	27
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	27
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
All	All	5138/5618 (92%)	4673 (91%)	410 (8%)	55 (1%)	14	52

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	271/280 (97%)	267 (98%)	4 (2%)	65	80
1	a	271/280 (97%)	267 (98%)	4 (2%)	65	80
2	B	390/407 (96%)	381 (98%)	9 (2%)	50	70
2	b	390/407 (96%)	381 (98%)	9 (2%)	50	70
3	C	347/362 (96%)	336 (97%)	11 (3%)	39	62
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	62
4	D	275/283 (97%)	268 (98%)	7 (2%)	47	68
4	d	275/283 (97%)	268 (98%)	7 (2%)	47	68
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	65
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	65
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	40
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	63
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	63
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	55
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	55
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	61
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	61
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	28
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	28
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	43
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	43
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	58
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	47	68

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	46	LEU
2	b	262	THR
16	v	92	ARG
18	X	12	ILE
1	a	228	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\# Z > 2$
29	OEX	a	414	1,3	0,15,15	0.00	-	-		
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
31	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
27	LMG	d	407	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.64	10 (18%)
22	CLA	b	605	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	7 (10%)
30	SQD	f	103	-	44,45,54	1.04	4 (9%)	53,56,65	1.63	11 (20%)
25	DGD	c	516	-	63,63,67	0.92	1 (1%)	77,77,81	1.45	12 (15%)
22	CLA	A	404	-	59,73,73	1.41	5 (8%)	67,113,113	1.44	7 (10%)
22	CLA	c	510	3	59,73,73	1.42	5 (8%)	67,113,113	1.50	7 (10%)
22	CLA	C	511	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	b	610	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	9 (13%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
22	CLA	D	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	B	615	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	d	404	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
27	LMG	a	413	-	51,51,55	0.74	1 (1%)	59,59,63	1.34	7 (11%)
27	LMG	d	410	-	46,46,55	0.80	1 (2%)	54,54,63	1.31	4 (7%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
31	LMT	D	410	-	32,32,36	1.18	5 (15%)	43,43,47	1.00	2 (4%)
22	CLA	B	614	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	c	520	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.24	4 (8%)
29	OEX	A	412	1,3	0,15,15	0.00	-	-		
30	SQD	a	401	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
27	LMG	b	625	-	49,49,55	0.78	1 (2%)	57,57,63	1.31	6 (10%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.79	10 (19%)
22	CLA	b	606	-	59,73,73	1.40	5 (8%)	67,113,113	1.46	9 (13%)
31	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.02	1 (2%)
31	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.94	1 (2%)
24	BCR	x	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	2 (3%)
23	PL9	j	101	-	35,35,55	1.00	1 (2%)	44,45,69	1.56	7 (15%)
24	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
23	PL9	D	407	-	55,55,55	1.03	3 (5%)	68,69,69	1.52	13 (19%)
22	CLA	b	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.52	10 (14%)
31	LMT	I	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	c	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	9 (16%)
22	CLA	c	512	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	9 (13%)
31	LMT	M	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
34	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.44	3 (17%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.41	7 (9%)
22	CLA	D	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.43	8 (11%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	6 (8%)
31	LMT	b	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
22	CLA	B	608	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
25	DGD	C	515	-	54,54,67	0.98	2 (3%)	68,68,81	1.27	6 (8%)
22	CLA	C	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
22	CLA	b	619	-	59,73,73	1.44	6 (10%)	67,113,113	1.43	7 (10%)
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
24	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
34	HEM	V	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.45	2 (11%)
22	CLA	b	612	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	8 (11%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
22	CLA	c	509	-	59,73,73	1.44	5 (8%)	67,113,113	1.41	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.50	8 (11%)
24	BCR	D	411	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	b	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	7 (10%)
22	CLA	C	507	-	59,73,73	1.43	5 (8%)	67,113,113	1.51	9 (13%)
22	CLA	B	611	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	C	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.41	7 (10%)
22	CLA	C	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)
27	LMG	D	412	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	4 (7%)
24	BCR	c	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	12 (21%)
24	BCR	g	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	b	618	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
23	PL9	A	406	-	45,45,55	0.98	4 (8%)	56,57,69	1.56	10 (17%)
22	CLA	c	503	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	8 (11%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	10 (17%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.79	10 (18%)
25	DGD	d	408	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	b	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
24	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	A	403	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	8 (11%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
22	CLA	c	504	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	b	609	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	H	101	-	59,73,73	1.43	5 (8%)	67,113,113	1.44	8 (11%)
26	LHG	C	519	-	36,36,48	0.71	0	39,42,54	1.25	4 (10%)
25	DGD	D	409	-	64,64,67	0.91	0	78,78,81	1.33	9 (11%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.74	10 (16%)
22	CLA	A	402	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	7 (10%)
34	HEM	v	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.42	2 (11%)
32	PHO	a	407	-	67,69,69	1.26	8 (11%)	85,99,99	1.00	5 (5%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	41,44,54	1.19	3 (7%)
27	LMG	B	624	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
22	CLA	a	408	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	b	615	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	623	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	B	607	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
30	SQD	D	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.78	10 (19%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
22	CLA	a	406	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
31	LMT	i	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.41	10 (12%)
22	CLA	C	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	B	605	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	8 (11%)
25	DGD	b	601	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
22	CLA	d	405	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	12 (15%)
22	CLA	b	616	-	59,73,73	1.40	5 (8%)	67,113,113	1.51	9 (13%)
23	PL9	a	409	-	45,45,55	1.02	3 (6%)	56,57,69	1.55	10 (17%)
31	LMT	d	409	-	32,32,36	1.18	5 (15%)	43,43,47	0.98	2 (4%)
22	CLA	B	603	-	59,73,73	1.41	5 (8%)	67,113,113	1.54	10 (14%)
24	BCR	C	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	C	503	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	7 (10%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
32	PHO	D	402	-	67,69,69	1.27	10 (14%)	85,99,99	1.01	5 (5%)
31	LMT	b	626	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
30	SQD	A	414	-	53,54,54	0.96	5 (9%)	62,65,65	1.57	9 (14%)
22	CLA	C	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	8 (11%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	8 (10%)
22	CLA	B	612	-	59,73,73	1.40	5 (8%)	67,113,113	1.50	8 (11%)
31	LMT	B	622	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
23	PL9	d	406	-	55,55,55	1.02	2 (3%)	68,69,69	1.53	14 (20%)
22	CLA	c	507	-	59,73,73	1.43	5 (8%)	67,113,113	1.53	10 (14%)
24	BCR	B	616	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	8 (14%)
22	CLA	c	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	8 (11%)
22	CLA	c	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)
31	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	C	520	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	504	-	59,73,73	1.42	5 (8%)	67,113,113	1.52	8 (11%)
34	HEM	f	101	5,6	27,50,50	2.16	5 (18%)	17,82,82	1.46	3 (17%)
22	CLA	c	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.44	8 (11%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	601	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	8 (11%)
26	LHG	A	409	-	38,38,48	0.69	0	41,44,54	1.18	3 (7%)
22	CLA	b	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	C	510	3	59,73,73	1.42	5 (8%)	67,113,113	1.53	7 (10%)
22	CLA	B	606	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	10 (14%)
27	LMG	a	402	-	42,42,55	0.84	0	50,50,63	1.25	3 (6%)
22	CLA	B	602	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	9 (13%)
23	PL9	J	101	-	35,35,55	1.02	1 (2%)	44,45,69	1.56	7 (15%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
32	PHO	D	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.01	5 (5%)
24	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	3 (5%)
22	CLA	C	509	-	59,73,73	1.45	5 (8%)	67,113,113	1.41	8 (11%)
22	CLA	A	405	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	B	609	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	8 (11%)
25	DGD	a	411	-	57,57,67	0.94	1 (1%)	71,71,81	1.39	7 (9%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
22	CLA	h	101	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	7 (10%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.26	4 (10%)
24	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	b	614	-	59,73,73	1.48	5 (8%)	67,113,113	1.50	9 (13%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.33	6 (8%)
27	LMG	b	628	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	12 (21%)
22	CLA	a	404	-	59,73,73	1.45	5 (8%)	67,113,113	1.44	8 (11%)
31	LMT	B	623	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	613	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	9 (13%)
24	BCR	b	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	B	610	-	59,73,73	1.47	5 (8%)	67,113,113	1.50	10 (14%)
22	CLA	c	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	7 (10%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
22	CLA	B	604	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
32	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.03	6 (7%)
30	SQD	A	413	-	50,51,54	0.97	4 (8%)	59,62,65	1.72	10 (16%)
22	CLA	B	613	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	7 (10%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
27	LMG	C	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
31	LMT	B	628	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	1 (2%)
22	CLA	C	512	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)

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
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	DGD	c	517	-	-	21/55/95/95	0/2/2/2
22	CLA	B	614	-	3/3/20/25	10/37/135/135	-
22	CLA	b	605	-	3/3/20/25	14/37/135/135	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	A	404	-	3/3/20/25	10/37/135/135	-
22	CLA	c	510	3	3/3/20/25	17/37/135/135	-
22	CLA	C	511	-	3/3/20/25	19/37/135/135	-
22	CLA	b	610	-	3/3/20/25	9/37/135/135	-
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
22	CLA	D	406	-	2/2/20/25	6/37/135/135	-
22	CLA	B	615	-	3/3/20/25	18/37/135/135	-
22	CLA	d	404	-	3/3/20/25	12/37/135/135	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
22	CLA	c	520	-	3/3/20/25	10/37/135/135	-
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
30	SQD	d	402	-	-	13/38/58/69	0/1/1/1
22	CLA	b	606	-	3/3/20/25	13/37/135/135	-
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
24	BCR	f	102	-	-	7/29/63/63	0/2/2/2
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	607	-	3/3/20/25	7/37/135/135	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
22	CLA	c	506	-	3/3/20/25	13/37/135/135	-
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	c	512	-	3/3/20/25	21/37/135/135	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	B	611	-	3/3/20/25	13/37/135/135	-
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	D	405	-	3/3/20/25	14/37/135/135	-
25	DGD	c	515	-	-	20/42/82/95	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
22	CLA	B	608	-	3/3/20/25	11/37/135/135	-
24	BCR	D	411	-	-	6/29/63/63	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
22	CLA	b	619	-	3/3/20/25	19/37/135/135	-
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
22	CLA	C	520	-	3/3/20/25	12/37/135/135	-
34	HEM	V	201	16	-	2/6/54/54	-
22	CLA	b	612	-	3/3/20/25	11/37/135/135	-
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
22	CLA	c	509	-	3/3/20/25	16/37/135/135	-
22	CLA	a	405	-	3/3/20/25	14/37/135/135	-
22	CLA	b	618	-	3/3/20/25	9/37/135/135	-
22	CLA	b	617	-	3/3/20/25	15/37/135/135	-
22	CLA	C	507	-	3/3/20/25	15/37/135/135	-
22	CLA	C	508	-	3/3/20/25	16/37/135/135	-
22	CLA	C	502	-	3/3/20/25	9/37/135/135	-
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
22	CLA	c	503	-	3/3/20/25	14/37/135/135	-
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
30	SQD	b	602	-	-	15/42/62/69	0/1/1/1
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
22	CLA	b	611	-	3/3/20/25	12/37/135/135	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
22	CLA	A	403	-	3/3/20/25	14/37/135/135	-
27	LMG	I	101	-	-	17/38/58/70	0/1/1/1
22	CLA	c	504	-	3/3/20/25	19/37/135/135	-
22	CLA	b	609	-	3/3/20/25	15/37/135/135	-
22	CLA	H	101	-	3/3/20/25	19/37/135/135	-
26	LHG	C	519	-	-	16/41/41/53	-
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
22	CLA	A	402	-	3/3/20/25	8/37/135/135	-
34	HEM	v	201	16	-	2/6/54/54	-
32	PHO	a	407	-	-	12/53/103/103	0/5/6/6
26	LHG	a	412	-	-	12/43/43/53	-
27	LMG	B	624	-	-	24/44/64/70	0/1/1/1
22	CLA	a	408	-	3/3/20/25	8/37/135/135	-
22	CLA	b	615	-	3/3/20/25	13/37/135/135	-
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2
24	BCR	B	617	-	-	9/29/63/63	0/2/2/2
22	CLA	B	607	-	3/3/20/25	12/37/135/135	-
30	SQD	D	403	-	-	13/38/58/69	0/1/1/1
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	a	406	-	3/3/20/25	9/37/135/135	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
25	DGD	C	517	-	-	22/55/95/95	0/2/2/2
22	CLA	C	505	-	3/3/20/25	17/37/135/135	-
22	CLA	B	605	-	3/3/20/25	12/37/135/135	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
22	CLA	d	405	-	3/3/20/25	6/37/135/135	-
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	b	616	-	3/3/20/25	15/37/135/135	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
22	CLA	B	603	-	3/3/20/25	7/37/135/135	-
22	CLA	c	511	-	3/3/20/25	19/37/135/135	-
22	CLA	C	503	-	3/3/20/25	15/37/135/135	-
27	LMG	C	518	-	-	21/40/60/70	0/1/1/1
32	PHO	D	402	-	-	12/53/103/103	0/5/6/6
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
22	CLA	C	501	-	3/3/20/25	15/37/135/135	-
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	612	-	3/3/20/25	15/37/135/135	-
22	CLA	C	504	-	3/3/20/25	19/37/135/135	-
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
22	CLA	c	507	-	3/3/20/25	14/37/135/135	-
22	CLA	C	506	-	3/3/20/25	13/37/135/135	-
22	CLA	c	508	-	3/3/20/25	15/37/135/135	-
22	CLA	c	502	-	3/3/20/25	11/37/135/135	-
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	BCR	C	521	-	-	6/29/63/63	0/2/2/2
34	HEM	f	101	5,6	-	0/6/54/54	-
22	CLA	c	501	-	3/3/20/25	13/37/135/135	-
22	CLA	B	601	-	3/3/20/25	16/37/135/135	-
26	LHG	A	409	-	-	14/43/43/53	-
22	CLA	b	608	-	3/3/20/25	15/37/135/135	-
22	CLA	C	510	3	3/3/20/25	15/37/135/135	-
27	LMG	C	522	-	-	20/43/63/70	0/1/1/1
22	CLA	B	606	-	3/3/20/25	9/37/135/135	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	B	602	-	3/3/20/25	15/37/135/135	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
32	PHO	D	401	-	-	13/53/103/103	0/5/6/6
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	509	-	3/3/20/25	16/37/135/135	-
22	CLA	A	405	-	3/3/20/25	8/37/135/135	-
22	CLA	B	609	-	3/3/20/25	18/37/135/135	-
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	b	621	-	-	9/29/63/63	0/2/2/2
22	CLA	b	614	-	3/3/20/25	9/37/135/135	-
27	LMG	a	413	-	-	25/46/66/70	0/1/1/1
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
34	HEM	F	101	5,6	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	404	-	3/3/20/25	8/37/135/135	-
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	b	613	-	3/3/20/25	18/37/135/135	-
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	B	610	-	3/3/20/25	10/37/135/135	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	3/3/20/25	17/37/135/135	-
27	LMG	B	621	-	-	16/44/64/70	0/1/1/1
22	CLA	B	604	-	3/3/20/25	14/37/135/135	-
32	PHO	d	401	-	-	14/53/103/103	0/5/6/6
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
22	CLA	B	613	-	3/3/20/25	16/37/135/135	-
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
22	CLA	h	101	-	3/3/20/25	19/37/135/135	-
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
22	CLA	C	512	-	3/3/20/25	17/37/135/135	-

The worst 5 of 606 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C4B-NB	7.79	1.42	1.35
22	B	601	CLA	C4B-NB	7.74	1.42	1.35
22	a	404	CLA	C4B-NB	7.74	1.42	1.35
22	b	605	CLA	C4B-NB	7.74	1.42	1.35
22	c	508	CLA	C4B-NB	7.72	1.42	1.35

The worst 5 of 1197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	c	504	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	B	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	611	CLA	C4A-NA-C1A	7.06	109.88	106.71

5 of 209 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND

5 of 2136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	m	101	LMG	O9-C10-O7-C8
27	e	101	LMG	C2-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
27	d	407	LMG	C2-C1-O1-C7
27	d	407	LMG	O6-C1-O1-C7

There are no ring outliers.

80 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	627	LMT	2	0
24	B	618	BCR	3	0
30	F	102	SQD	2	0
22	A	404	CLA	16	0
22	C	511	CLA	1	0
27	A	415	LMG	1	0
22	D	406	CLA	3	0
22	B	615	CLA	6	0
24	A	407	BCR	2	0
22	B	614	CLA	2	0
27	E	101	LMG	1	0
27	A	410	LMG	2	0
27	M	101	LMG	1	0
23	D	407	PL9	8	0
31	I	102	LMT	1	0
34	F	101	HEM	4	0
25	A	408	DGD	1	0
22	D	405	CLA	11	0
22	B	608	CLA	14	0
25	C	515	DGD	3	0
22	C	506	CLA	6	0
34	V	201	HEM	3	0
30	B	626	SQD	3	0
24	D	411	BCR	3	0

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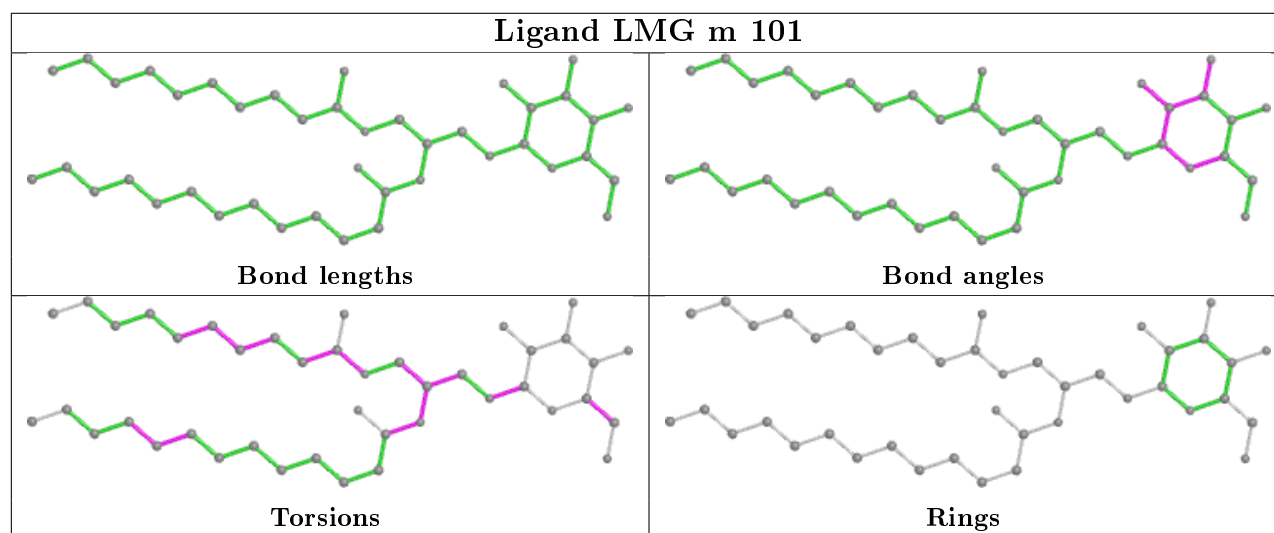
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	507	CLA	4	0
22	B	611	CLA	10	0
22	C	508	CLA	4	0
27	D	412	LMG	1	0
23	A	406	PL9	3	0
22	A	403	CLA	12	0
27	I	101	LMG	1	0
22	H	101	CLA	11	0
26	C	519	LHG	2	0
25	D	409	DGD	2	0
22	A	402	CLA	11	0
27	B	624	LMG	3	0
24	B	617	BCR	1	0
22	B	607	CLA	10	0
30	D	403	SQD	3	0
24	C	513	BCR	8	0
25	C	517	DGD	5	0
22	C	505	CLA	2	0
22	B	605	CLA	6	0
25	C	516	DGD	4	0
22	B	603	CLA	3	0
24	C	521	BCR	5	0
22	C	503	CLA	5	0
27	C	518	LMG	4	0
32	D	402	PHO	5	0
30	A	414	SQD	3	0
22	C	501	CLA	6	0
25	B	620	DGD	2	0
22	B	612	CLA	10	0
31	B	622	LMT	2	0
24	B	616	BCR	6	0
22	C	520	CLA	5	0
22	C	504	CLA	4	0
22	B	601	CLA	1	0
26	A	409	LHG	3	0
22	C	510	CLA	10	0
22	B	606	CLA	16	0
22	B	602	CLA	11	0
32	D	401	PHO	11	0
24	H	102	BCR	1	0
22	C	509	CLA	6	0
22	A	405	CLA	8	0

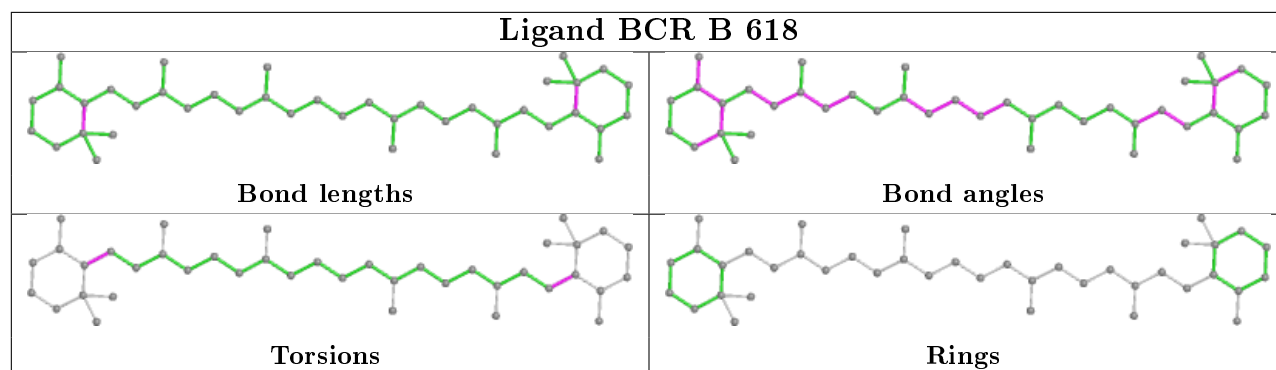
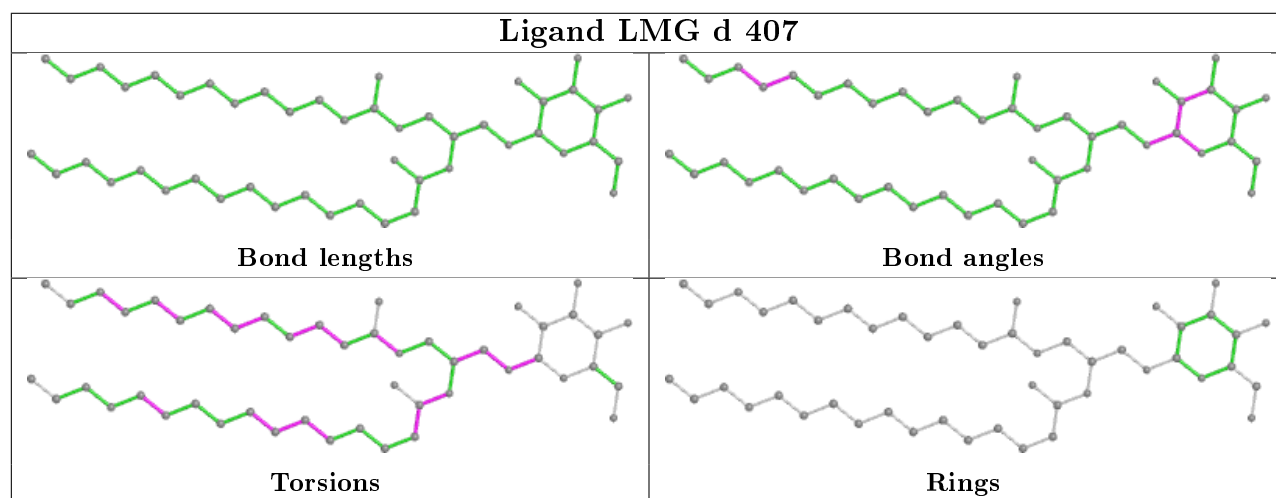
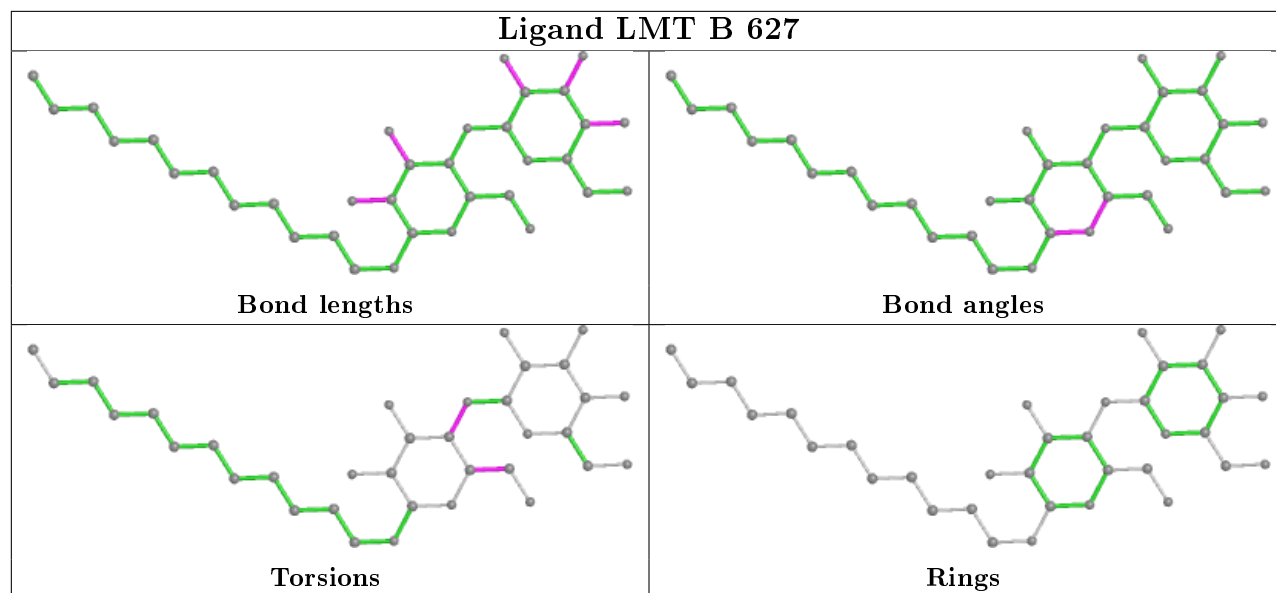
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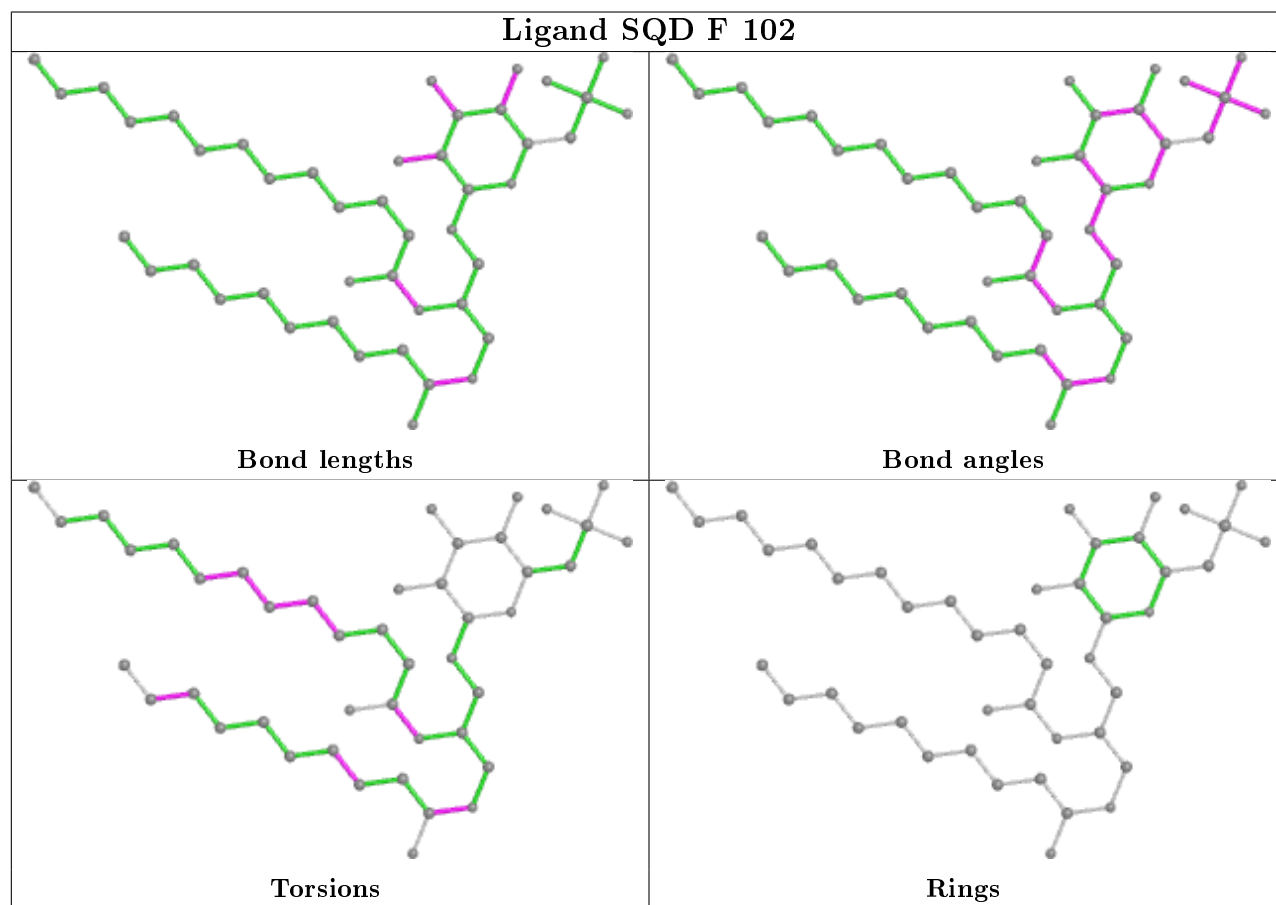
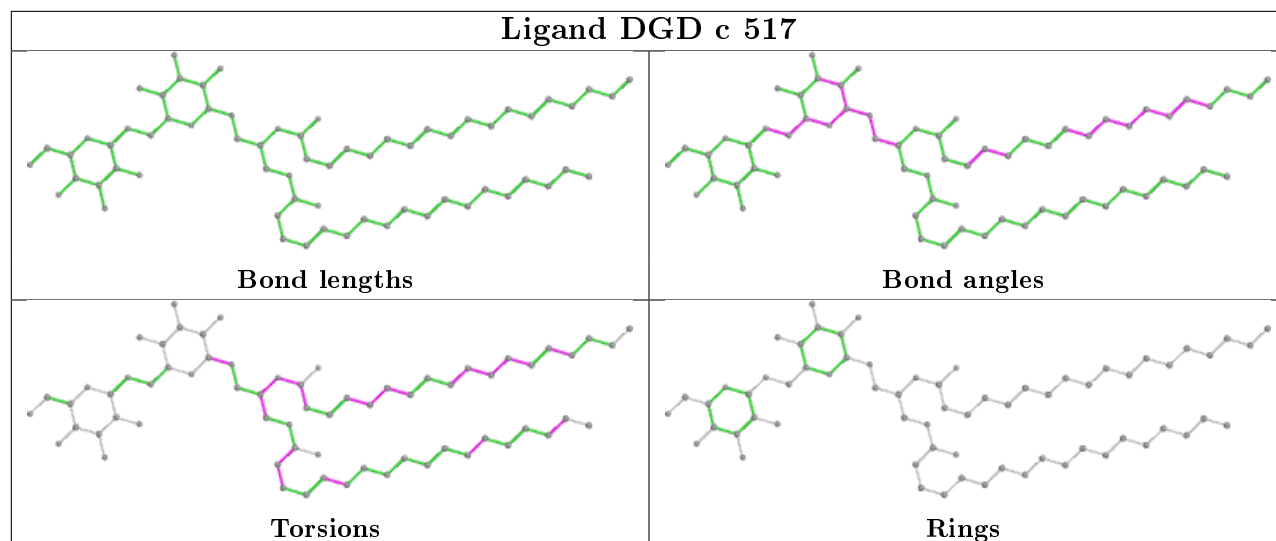
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	609	CLA	3	0
24	B	619	BCR	2	0
25	B	625	DGD	2	0
24	J	102	BCR	2	0
22	B	610	CLA	6	0
24	C	514	BCR	7	0
27	B	621	LMG	3	0
22	B	604	CLA	10	0
30	A	413	SQD	3	0
22	B	613	CLA	4	0
27	D	408	LMG	6	0
27	C	522	LMG	3	0
31	B	628	LMT	2	0
22	C	512	CLA	3	0

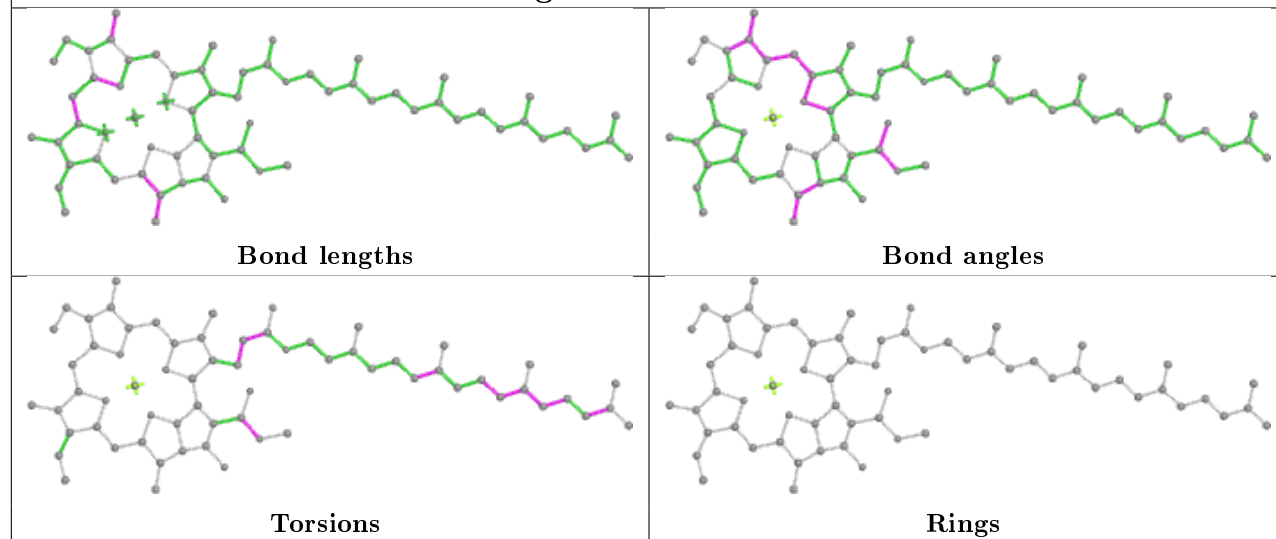
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



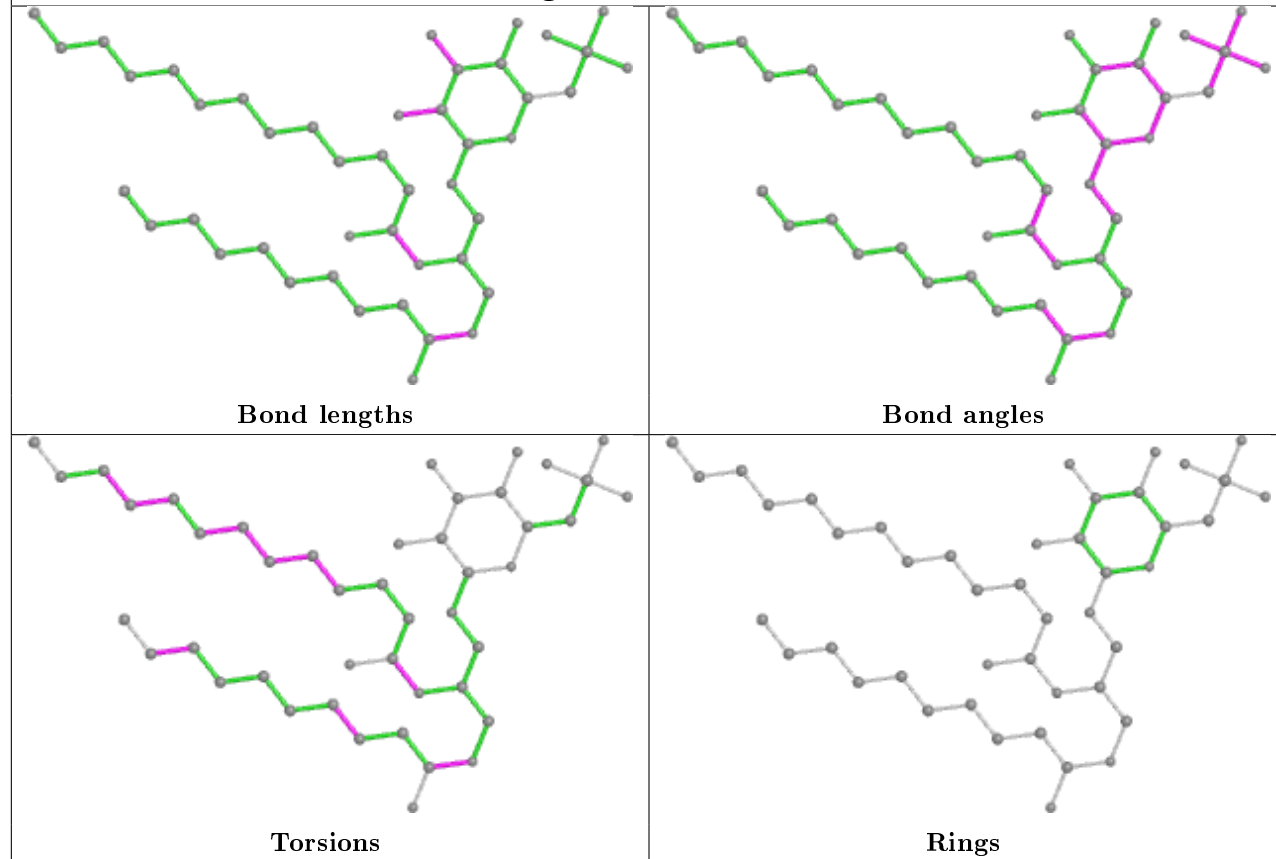


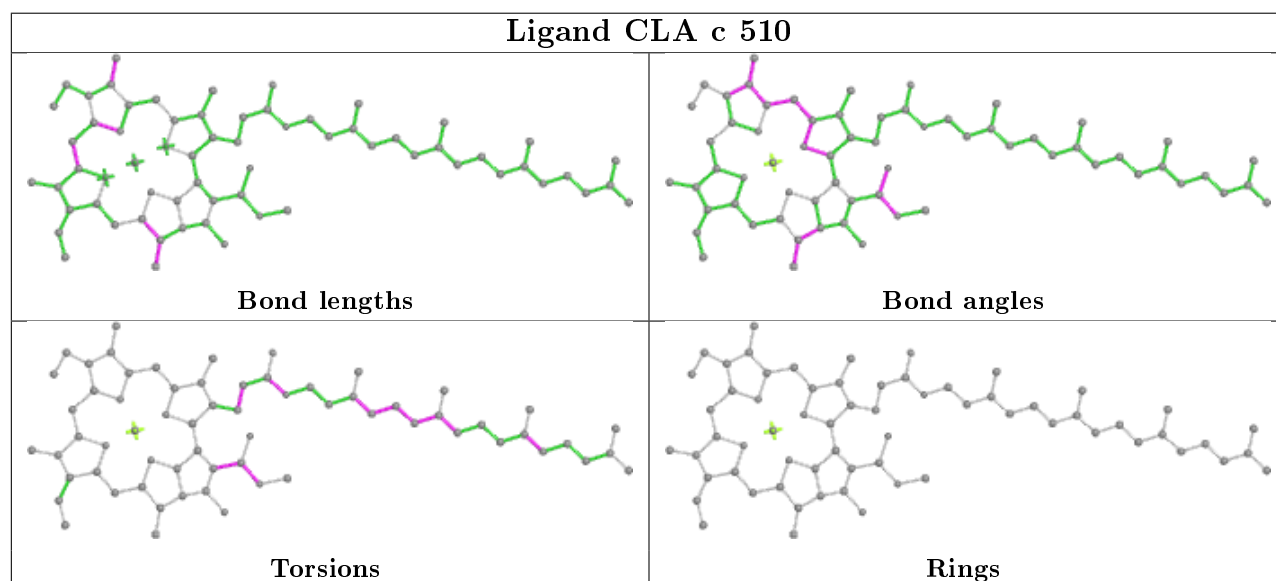
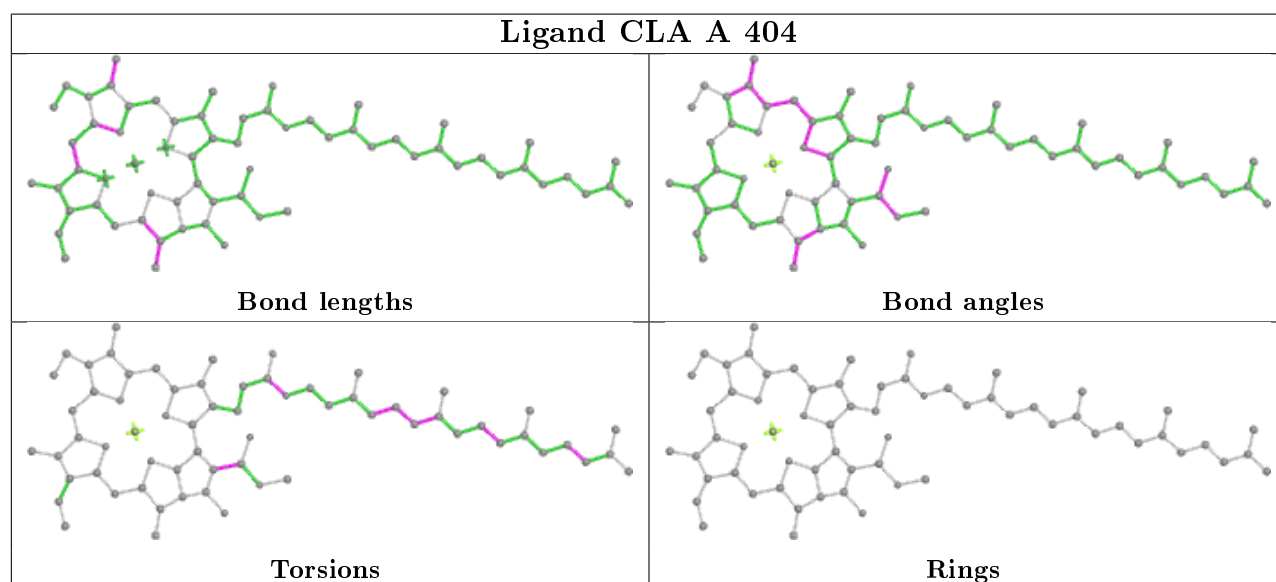
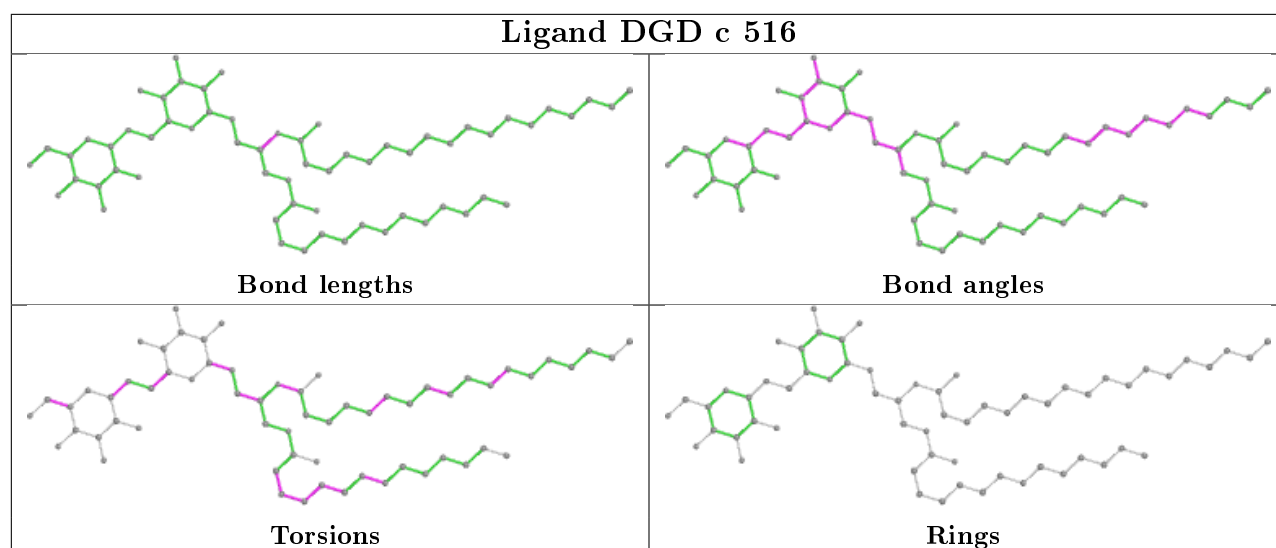


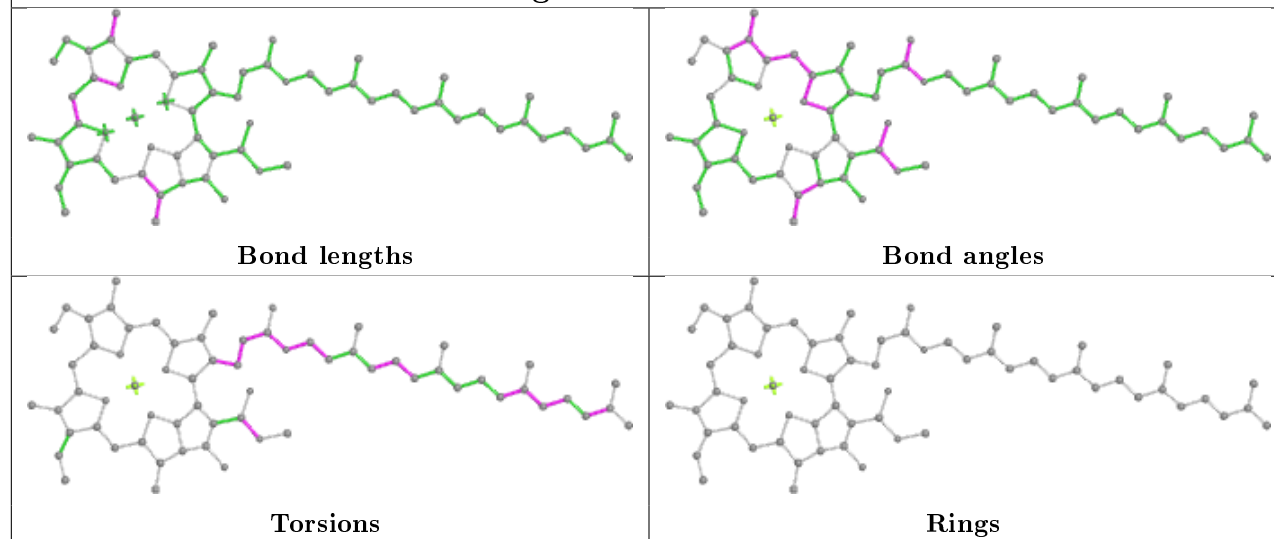
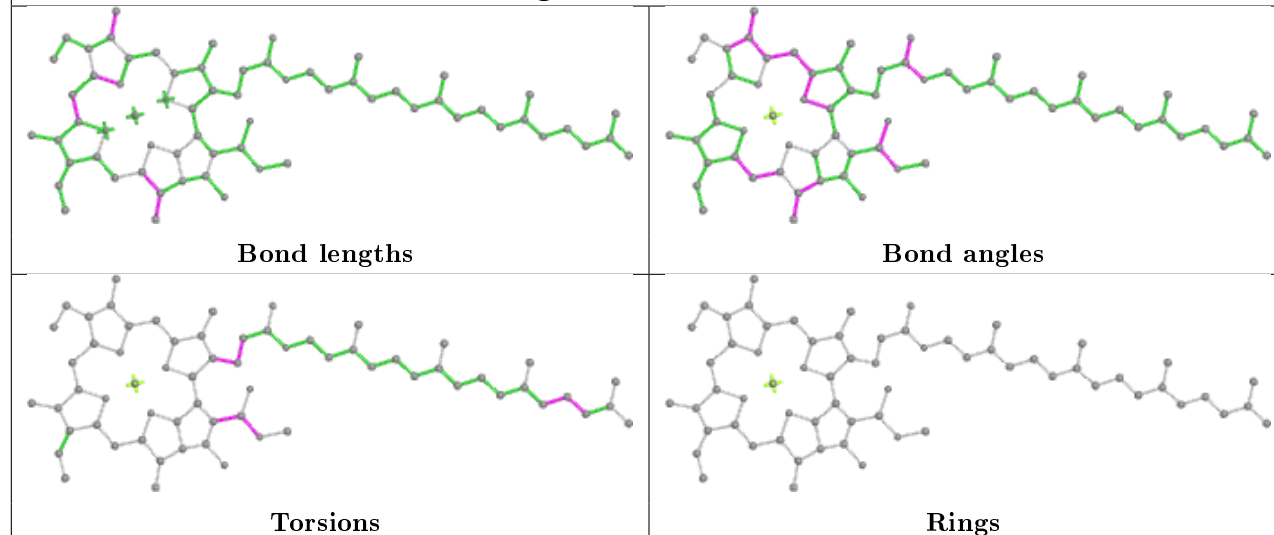
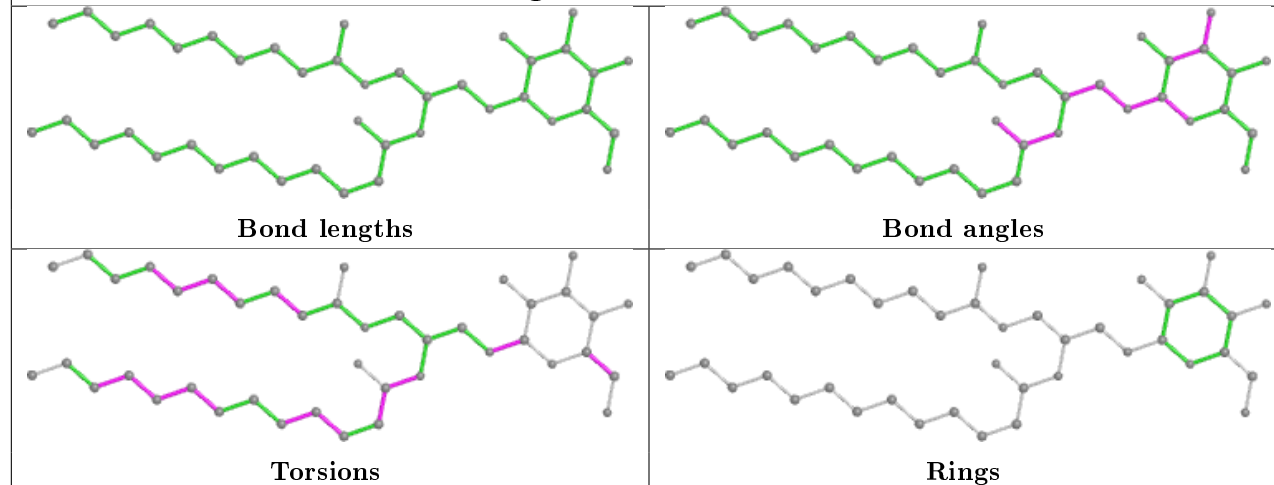
Ligand CLA b 605

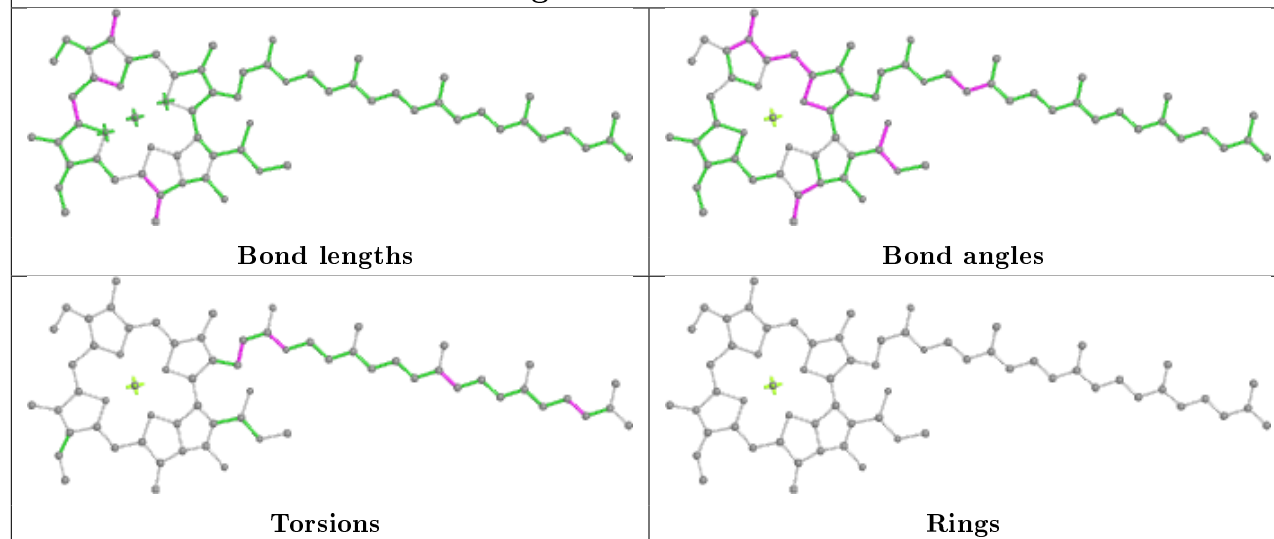
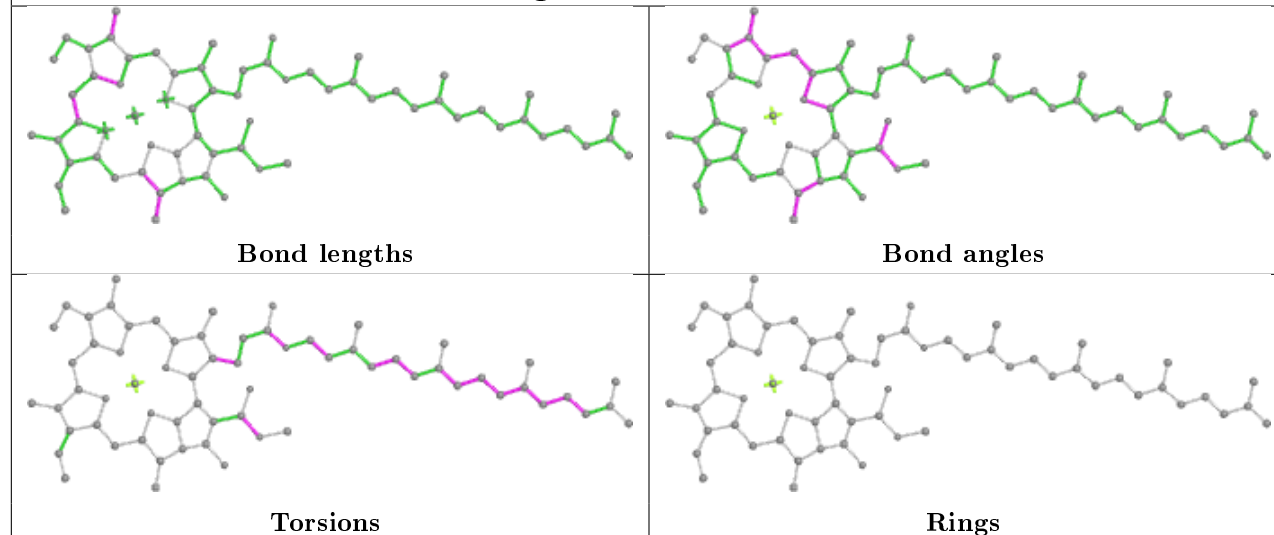
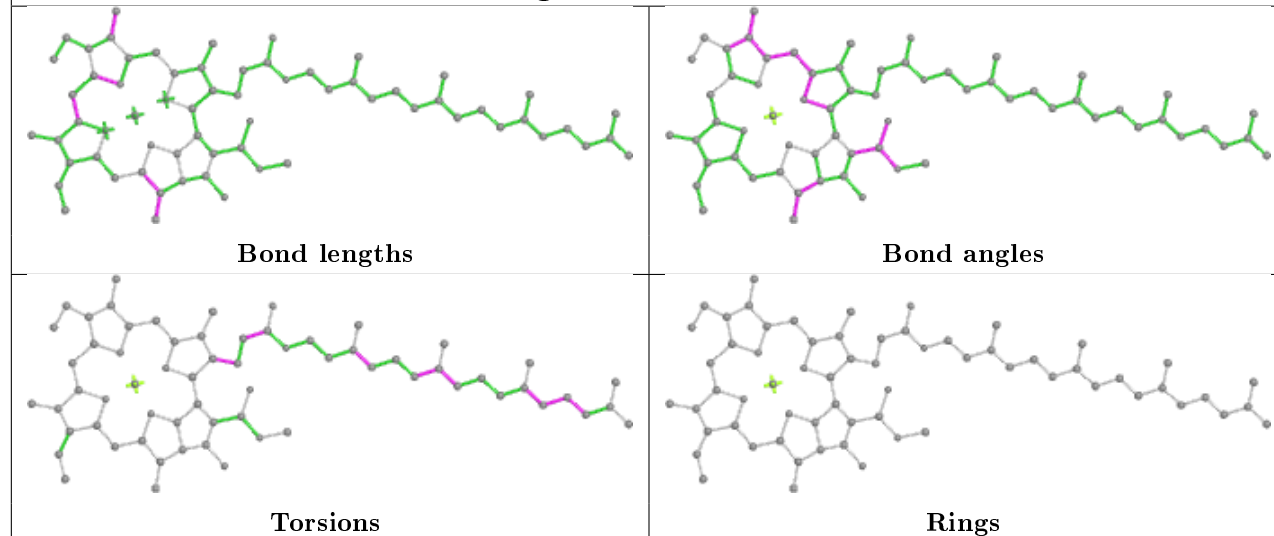


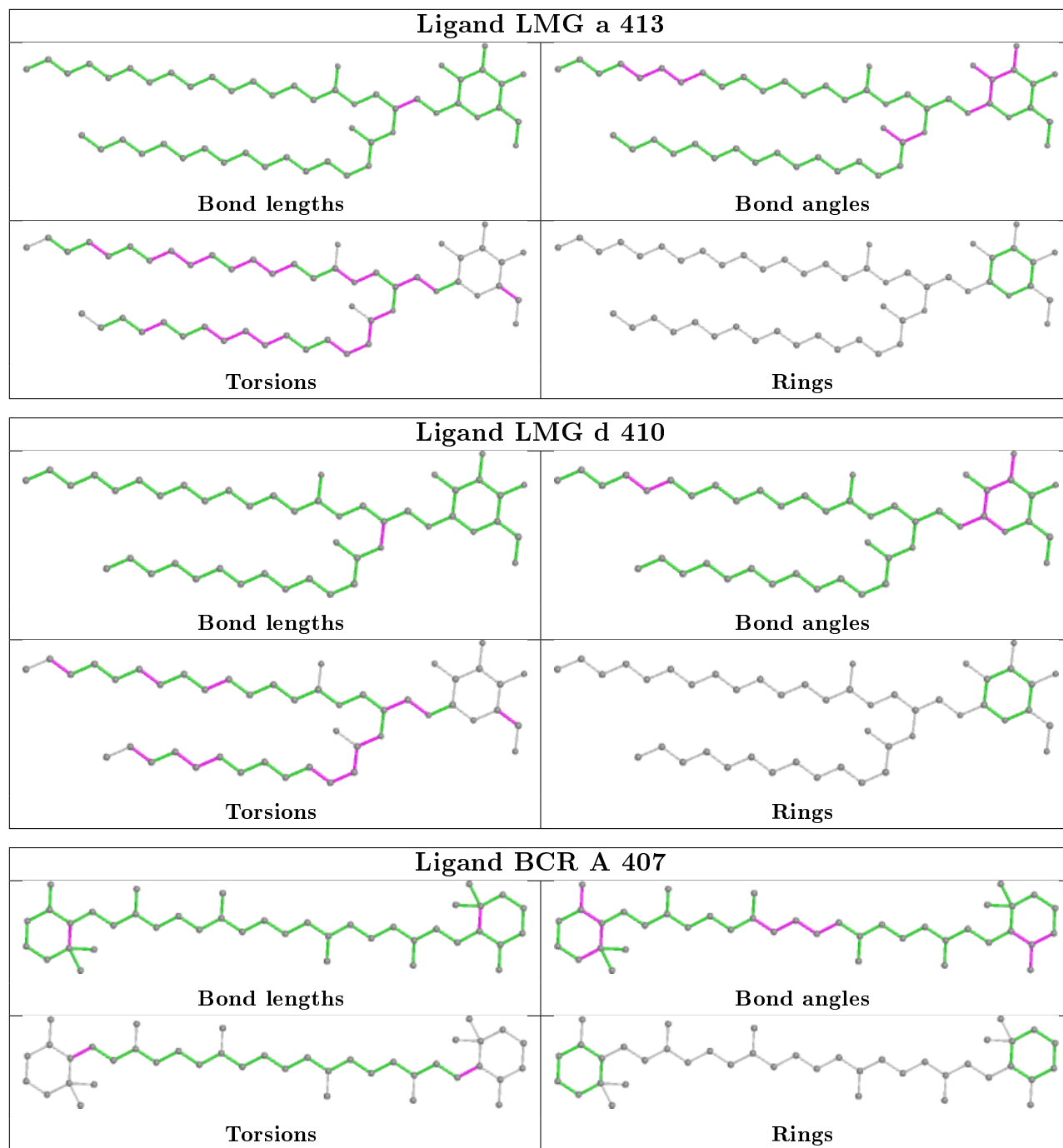
Ligand SQD f 103

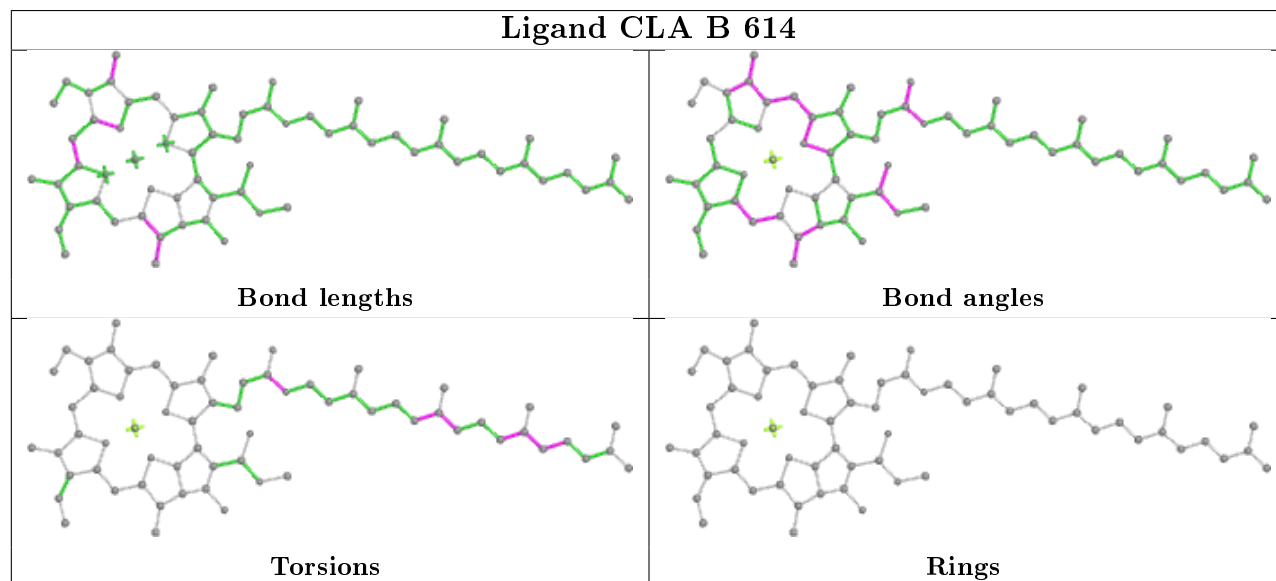
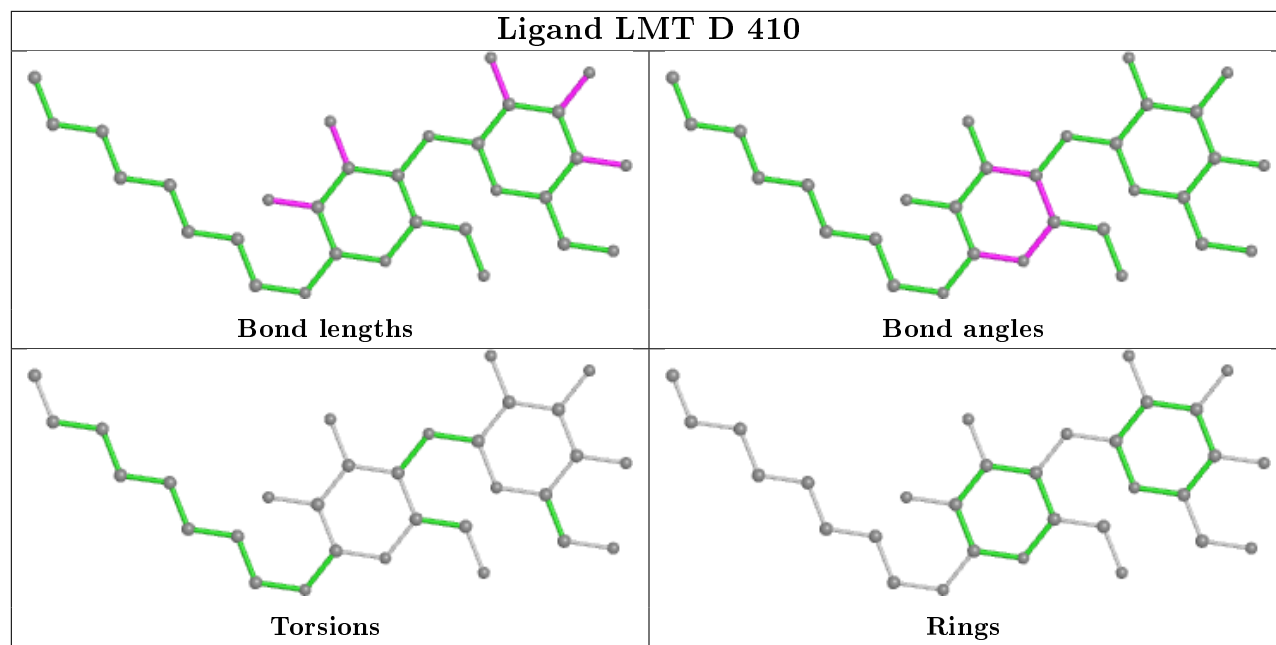




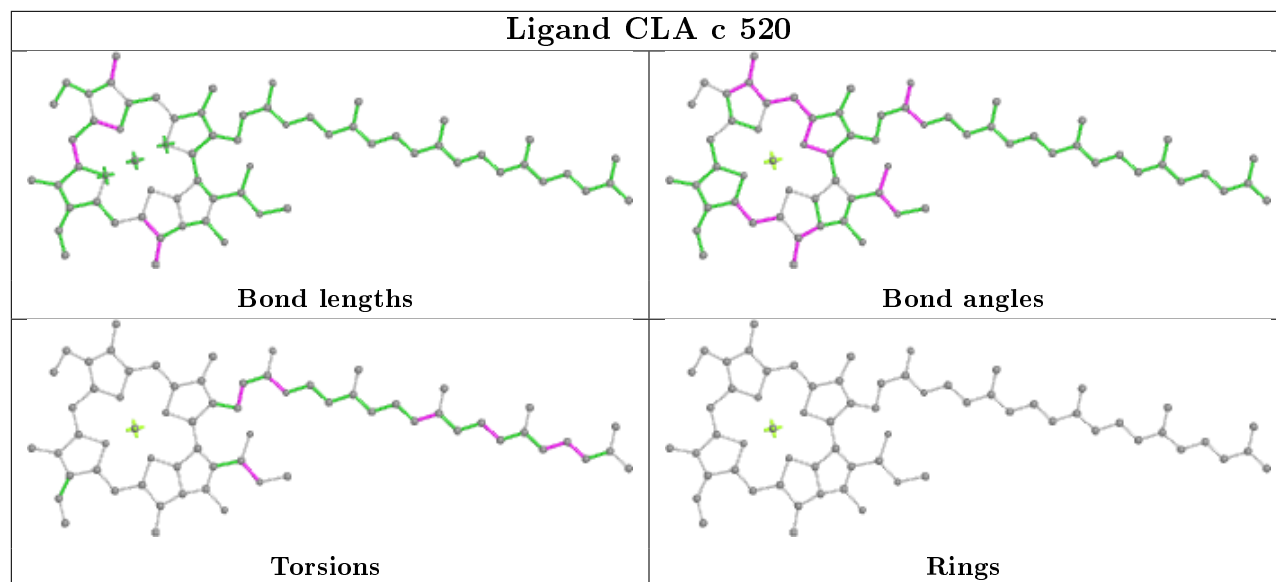
Ligand CLA C 511**Ligand CLA b 610****Ligand LMG A 415**

Ligand CLA D 406**Ligand CLA B 615****Ligand CLA d 404**

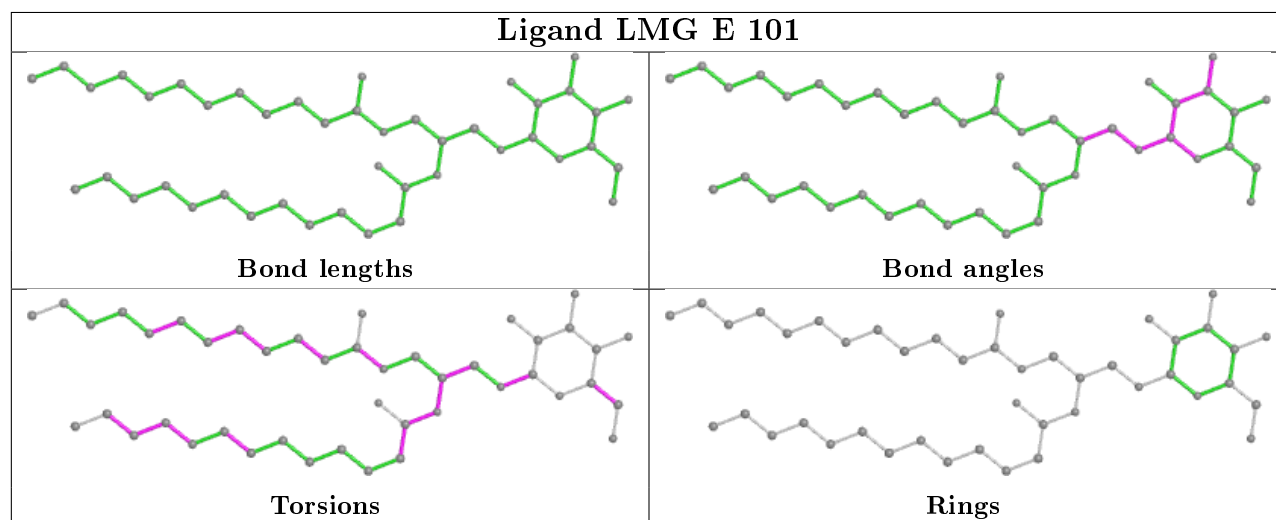




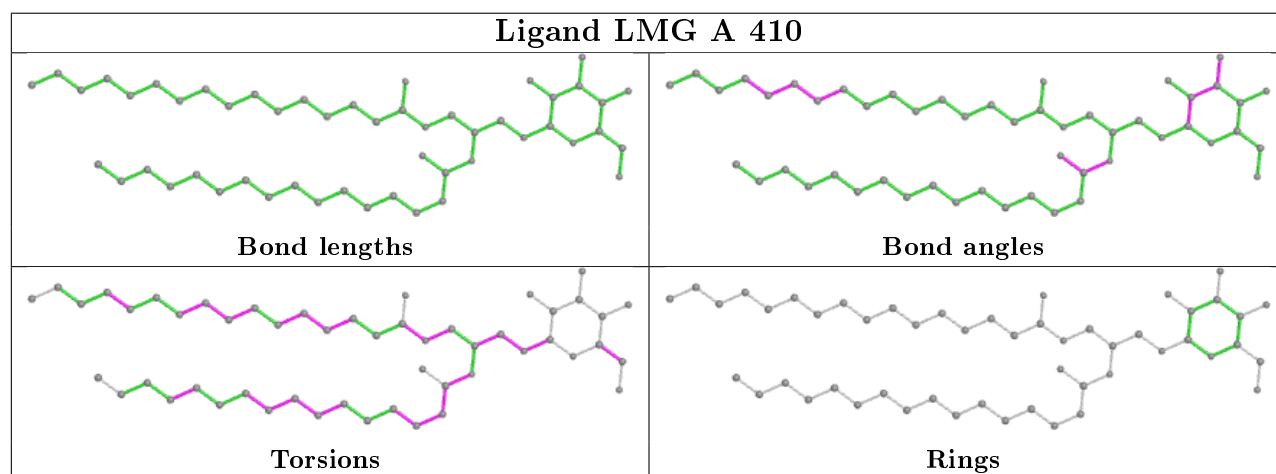
Ligand CLA c 520

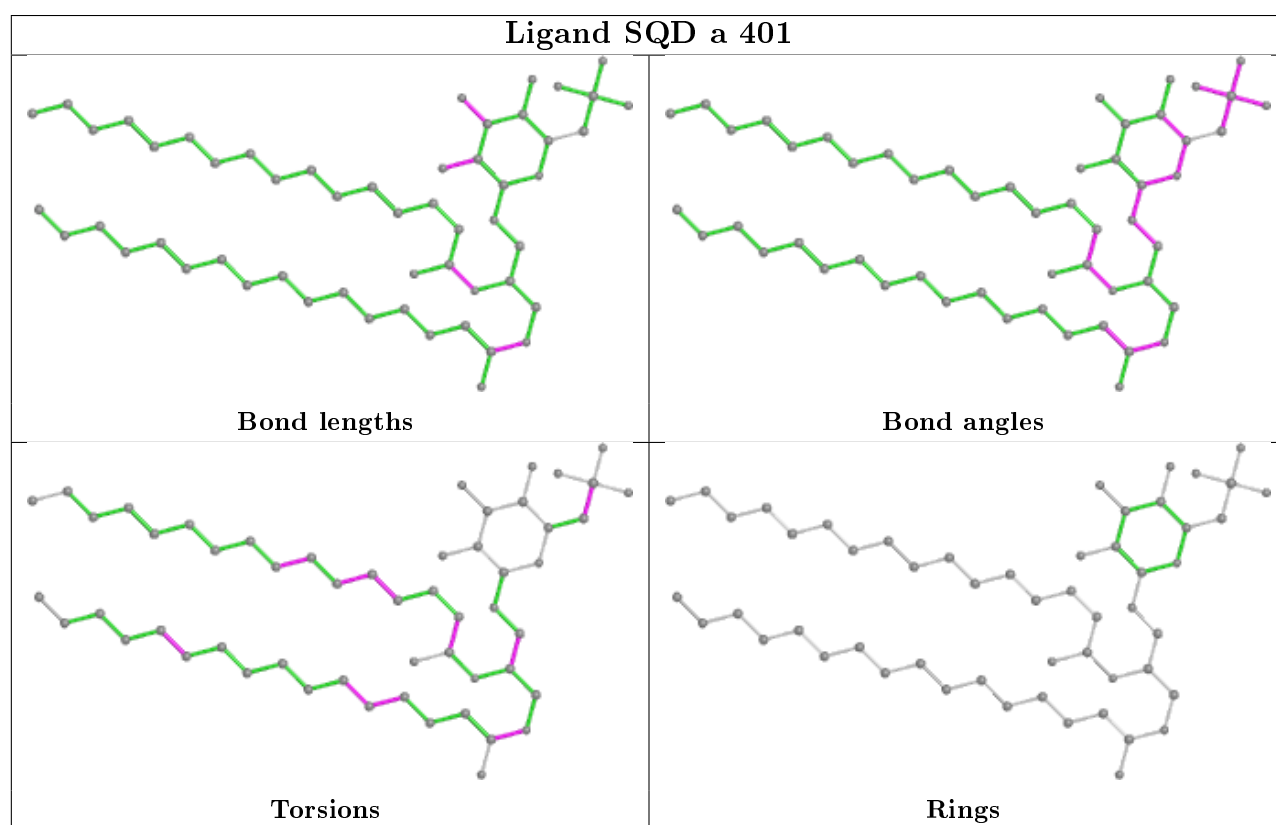
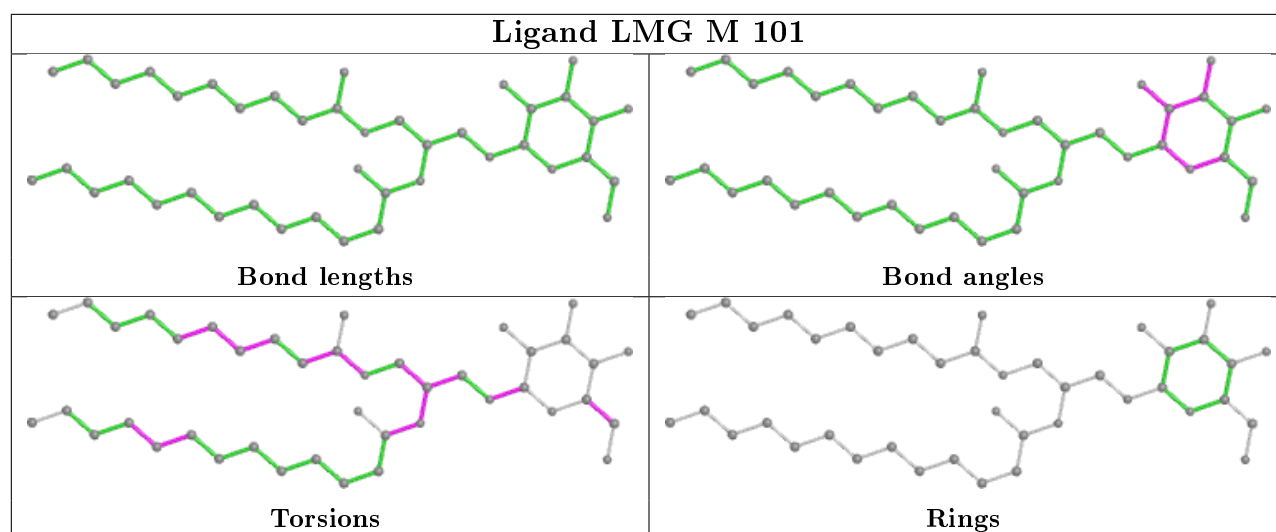


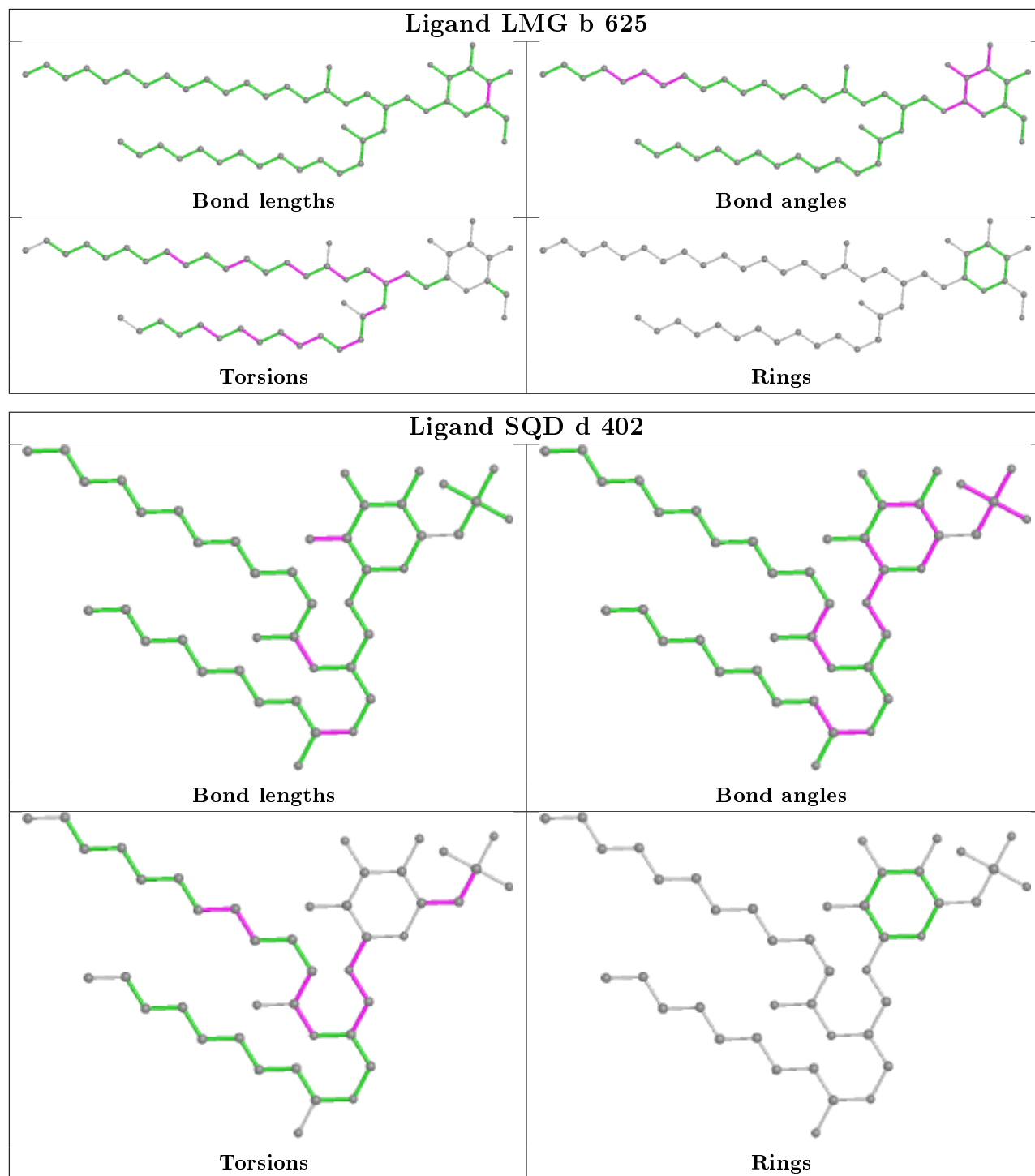
Ligand LMG E 101



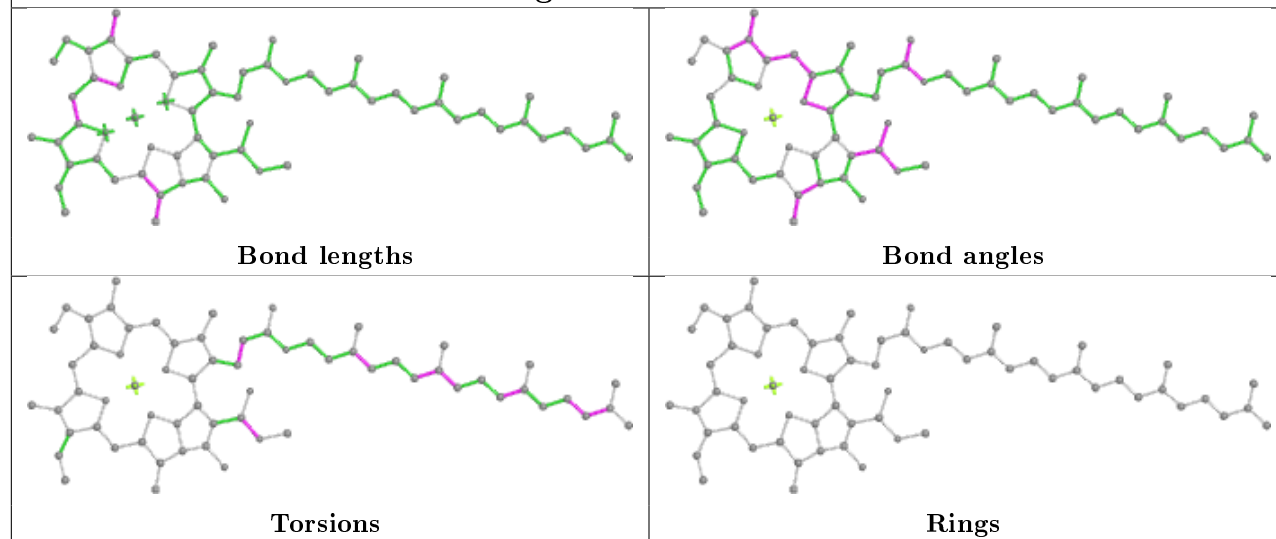
Ligand LMG A 410



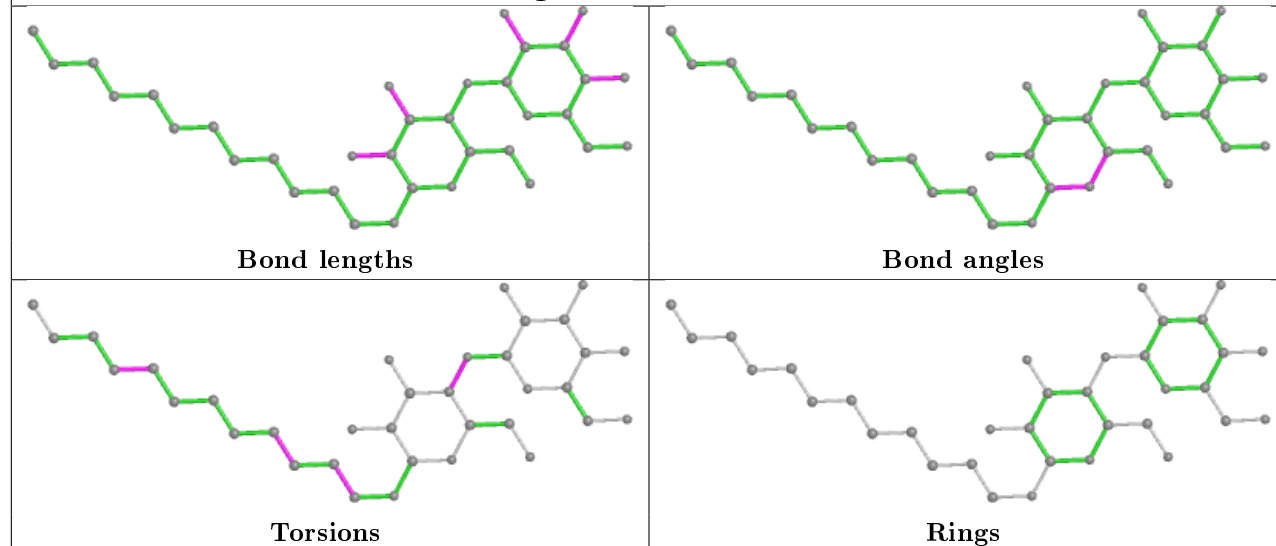




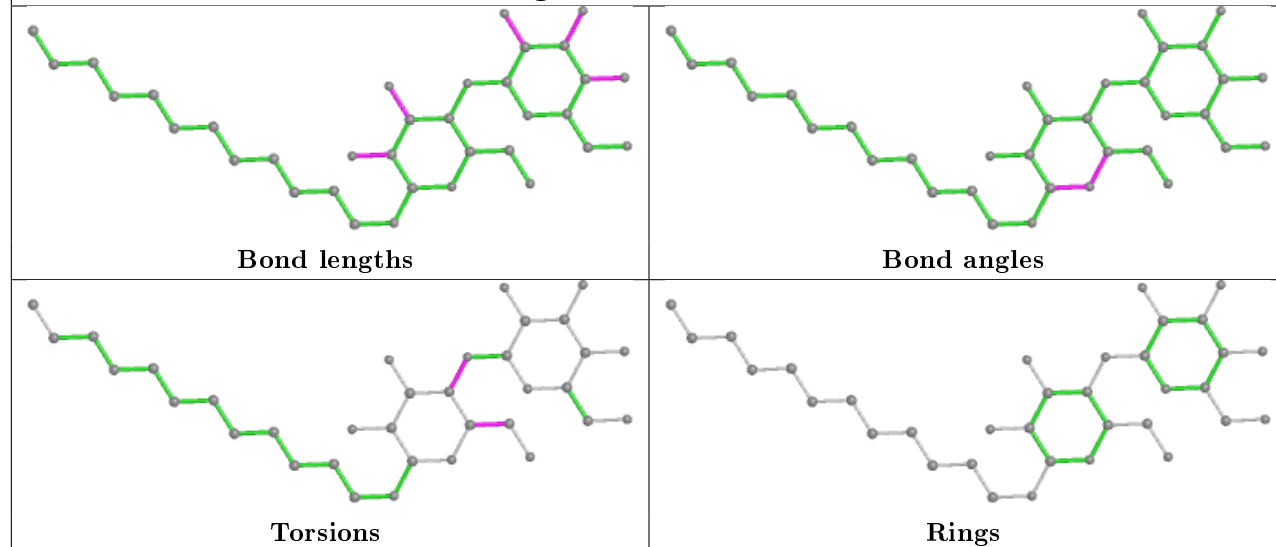
Ligand CLA b 606

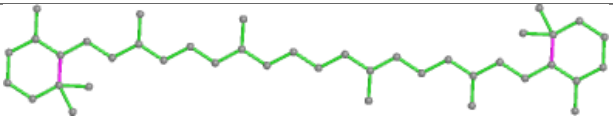
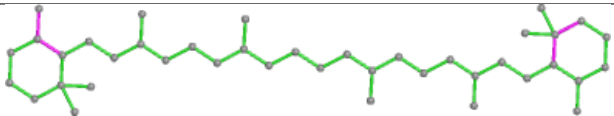
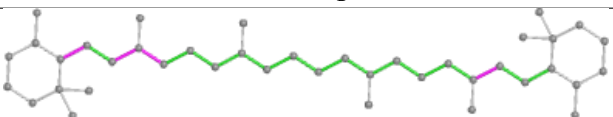
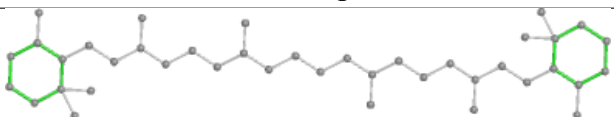


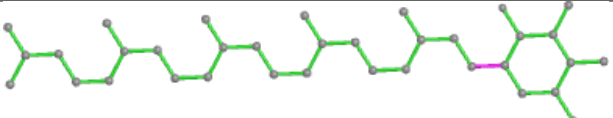
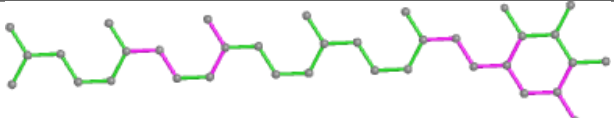
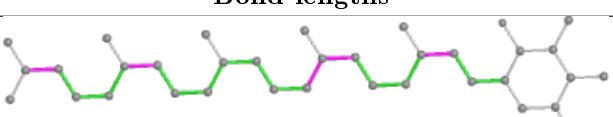
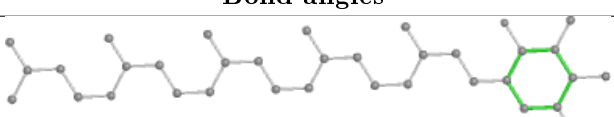
Ligand LMT b 604

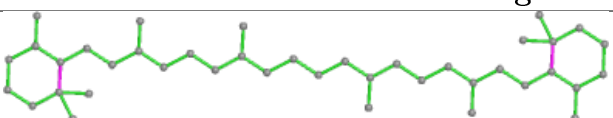
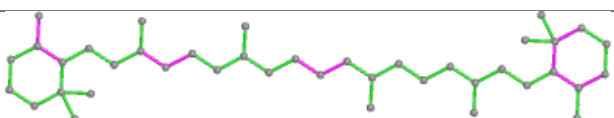
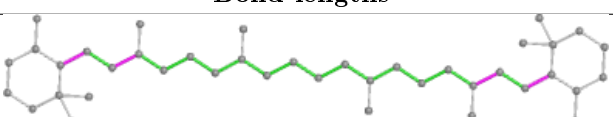
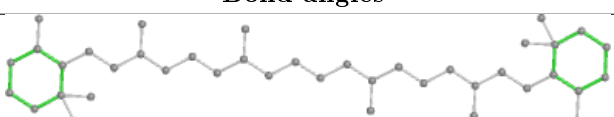


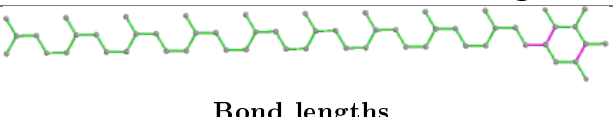
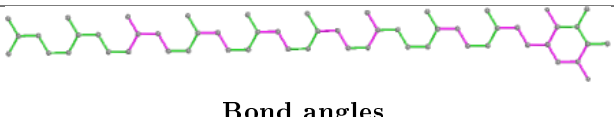
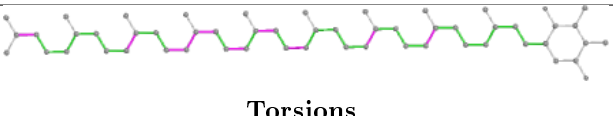
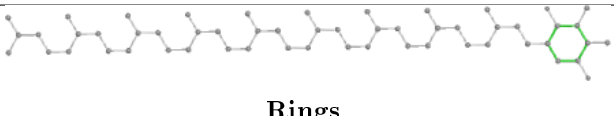
Ligand LMT b 603



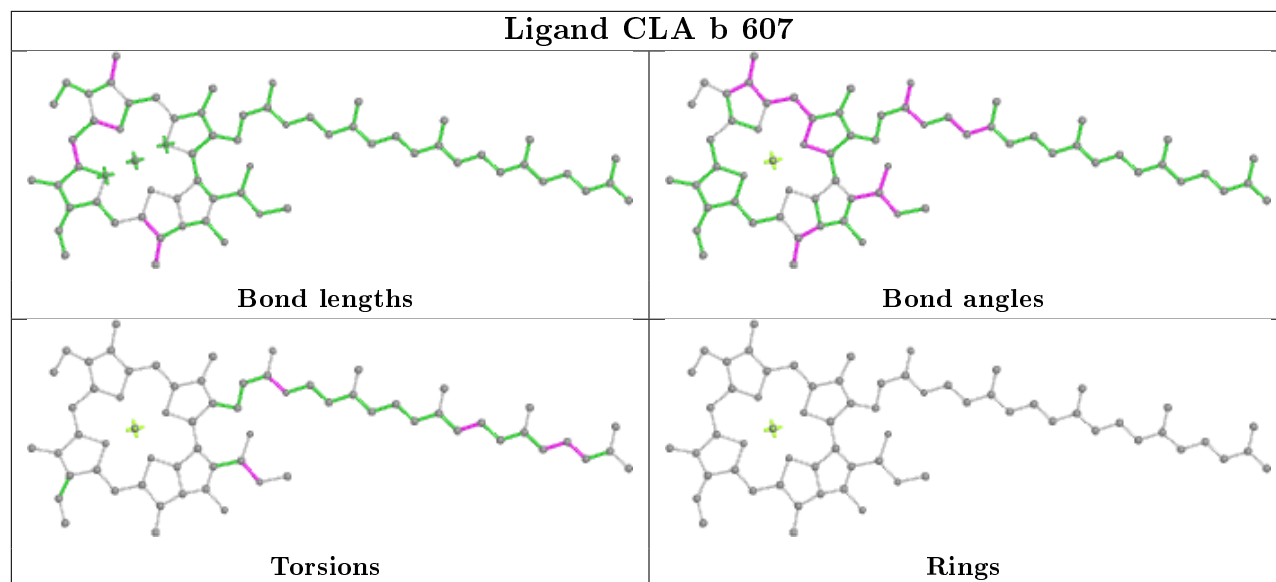
Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

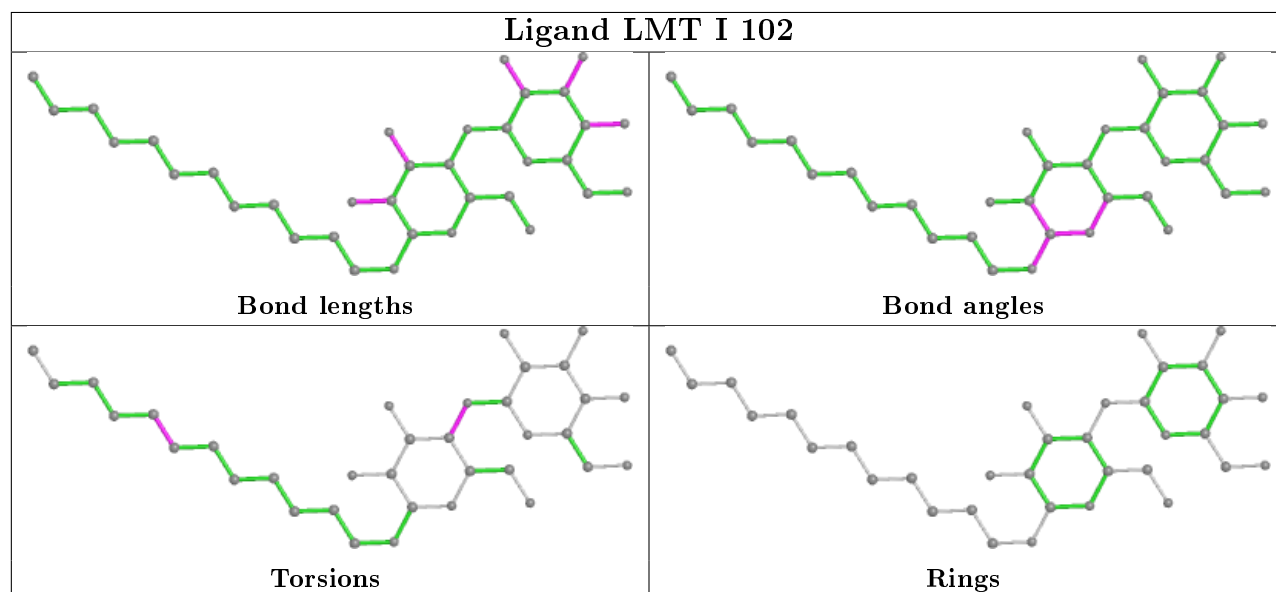
Ligand BCR f 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

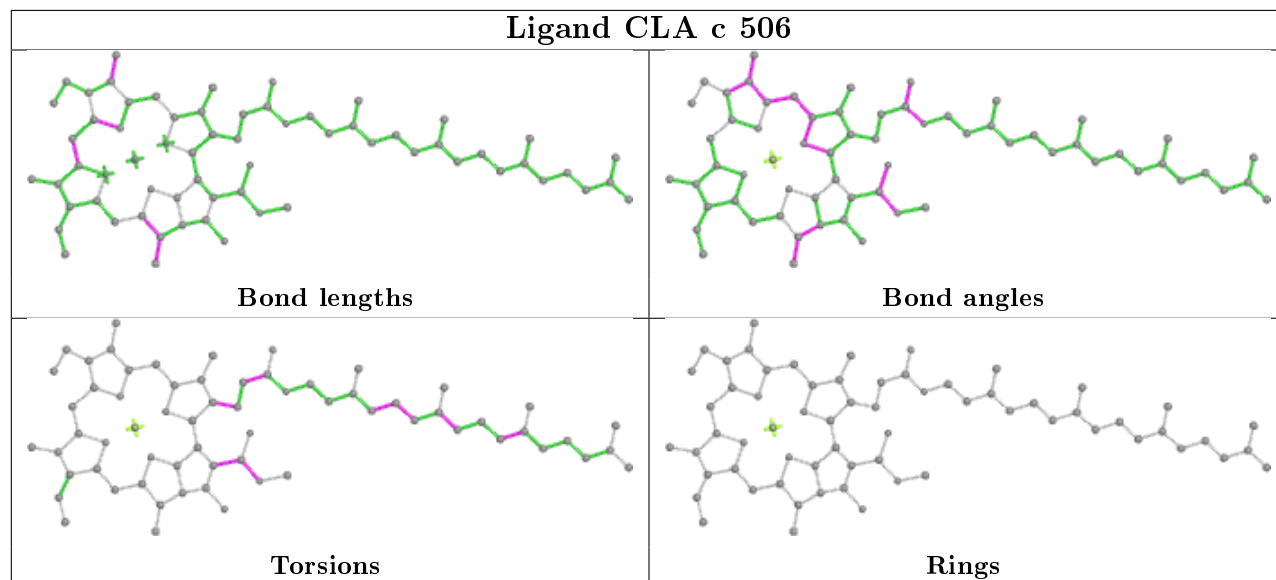
Ligand CLA b 607

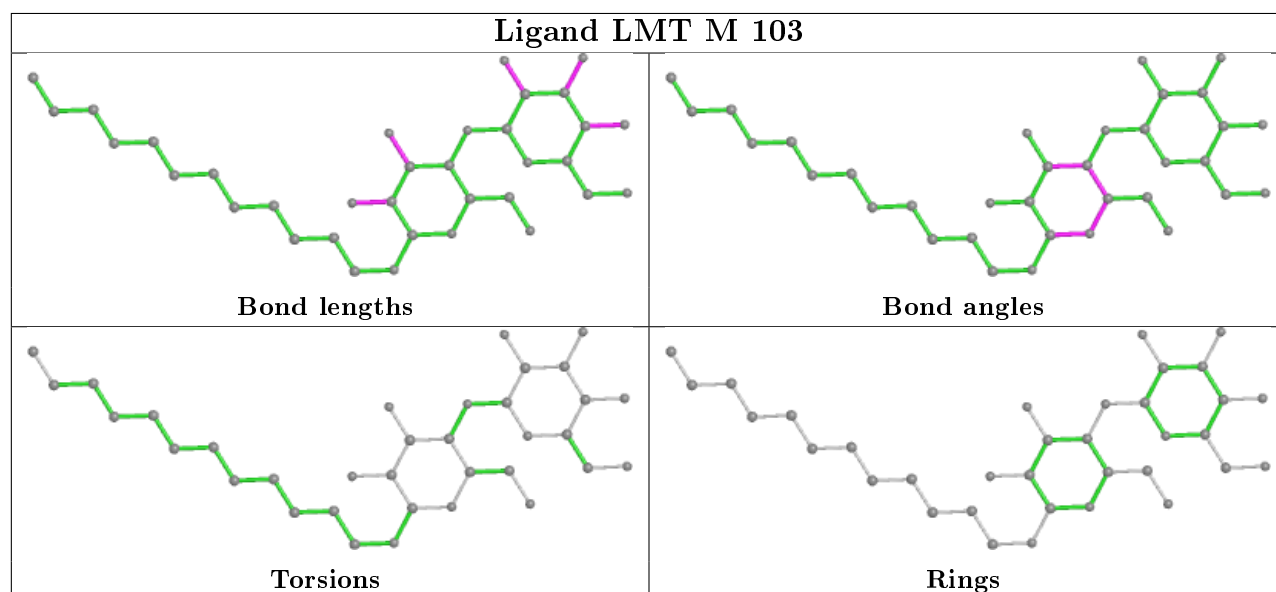
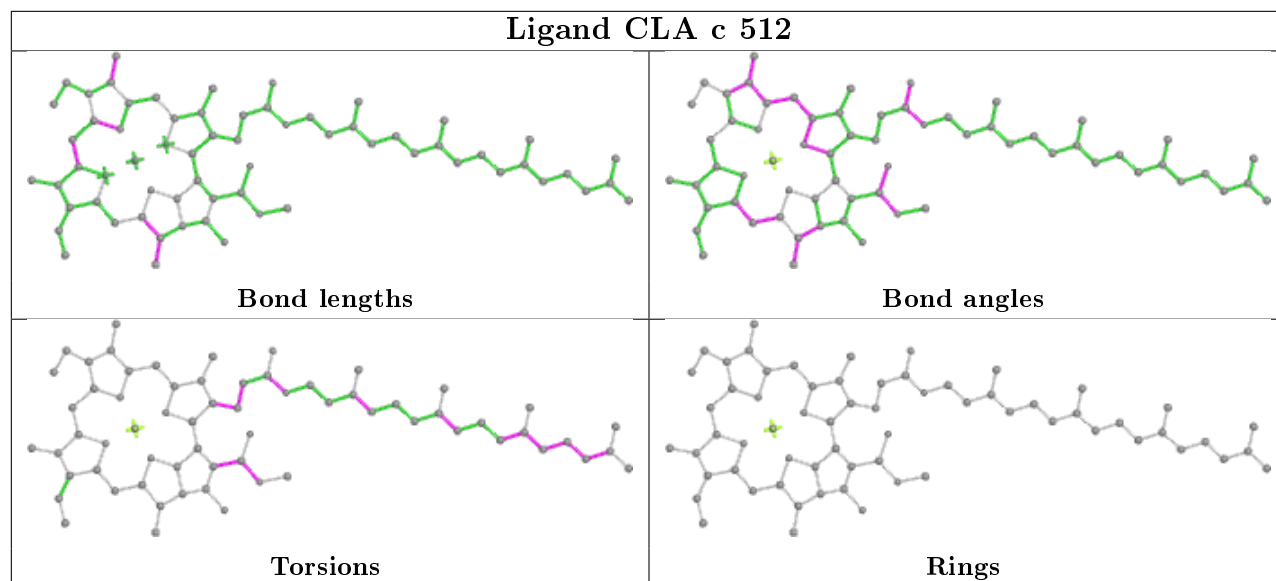
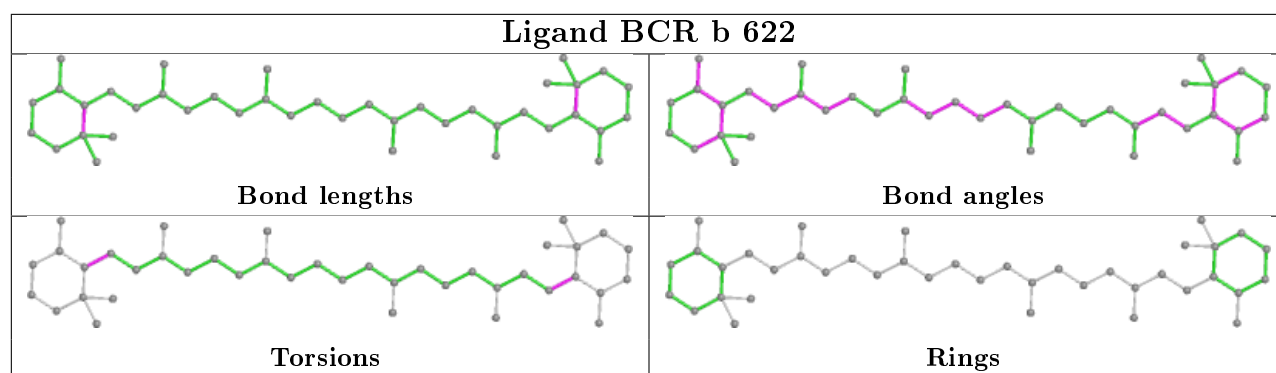


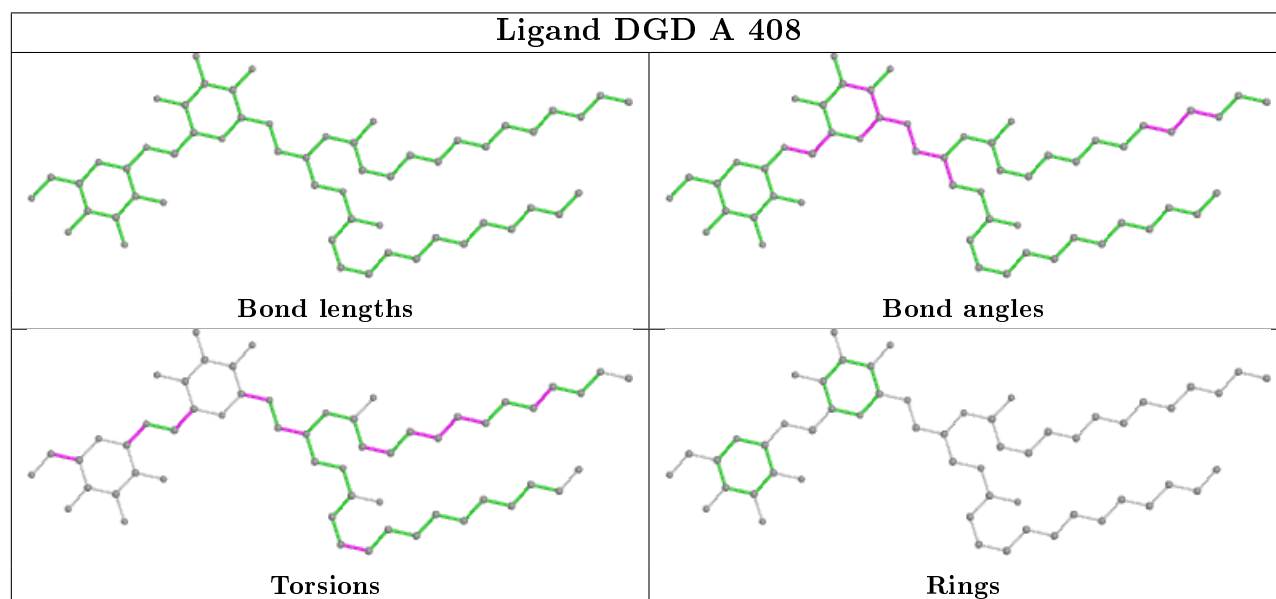
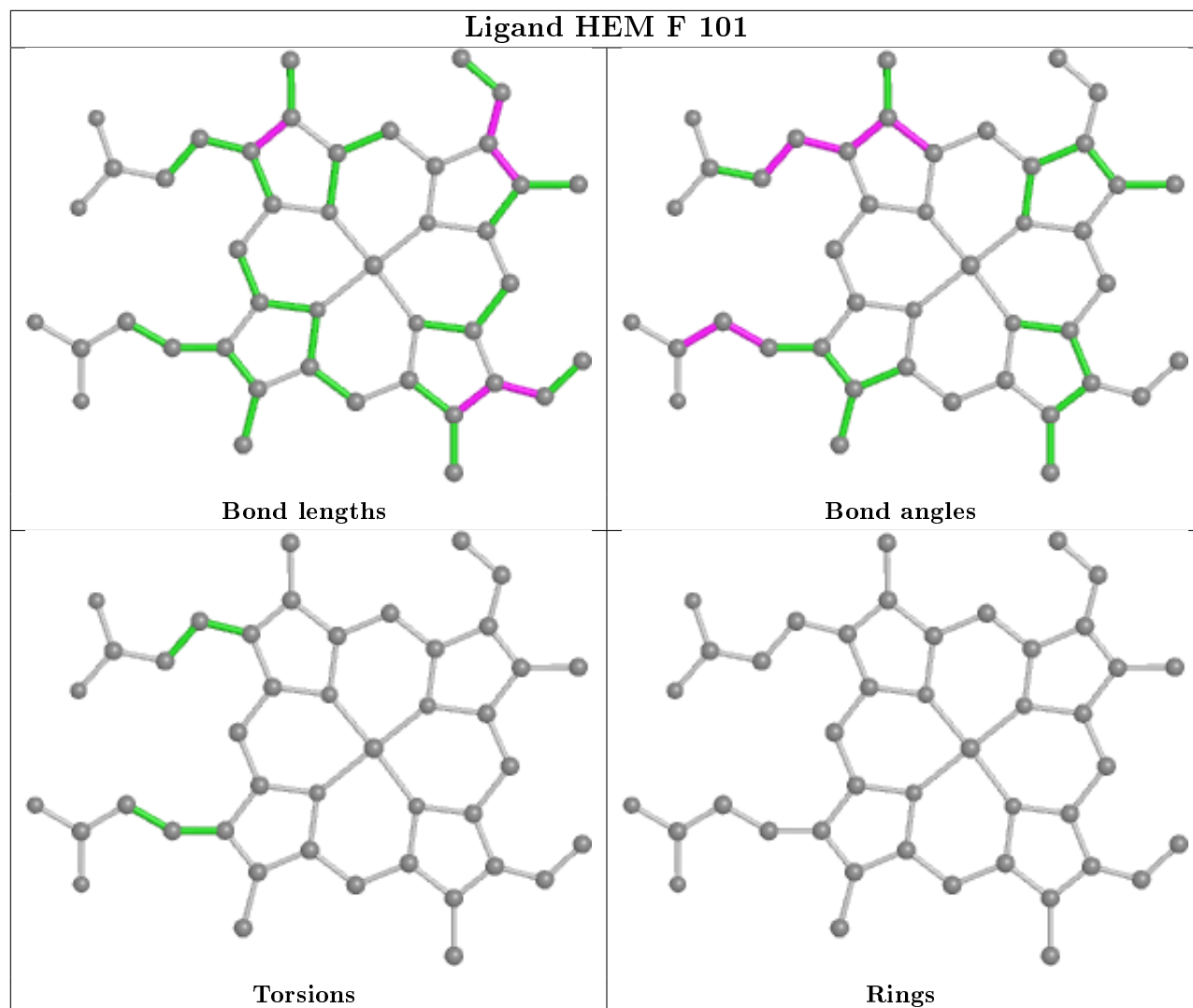
Ligand LMT I 102



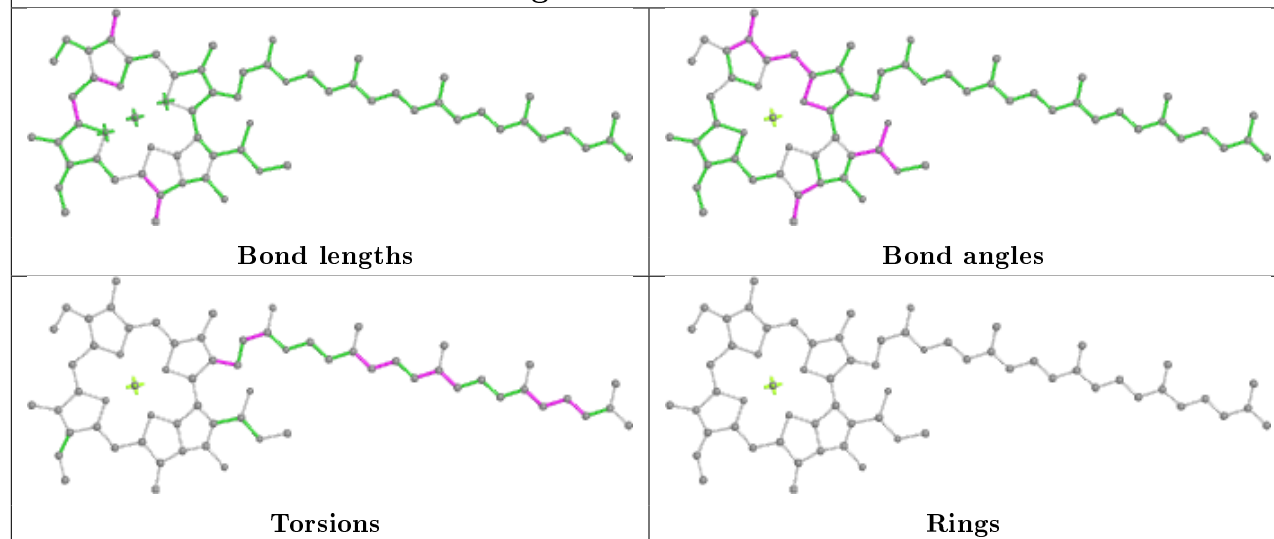
Ligand CLA c 506



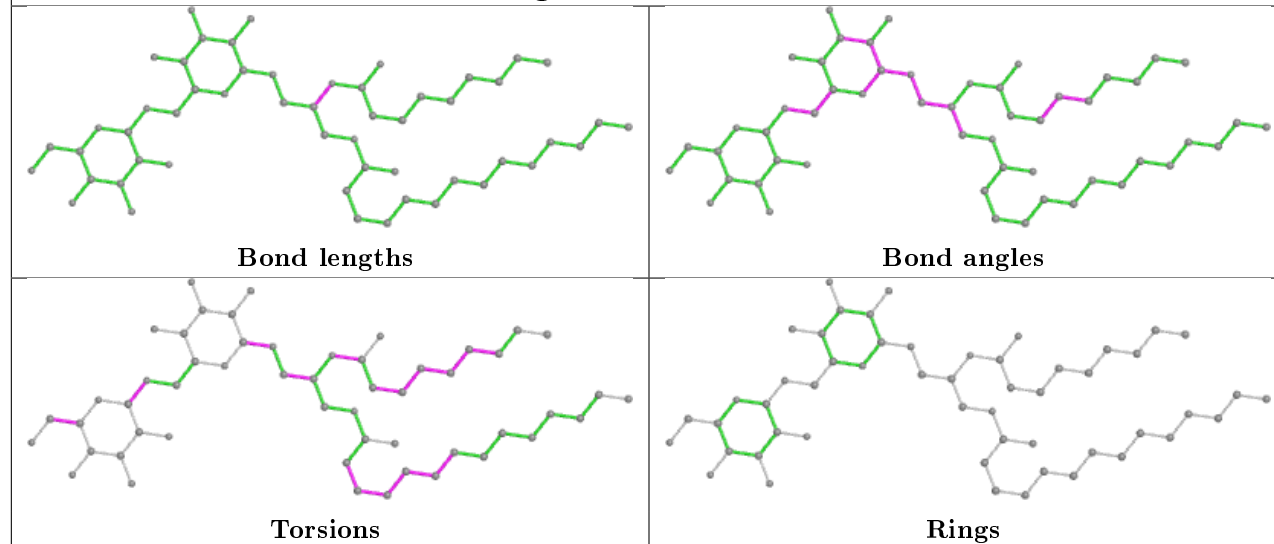




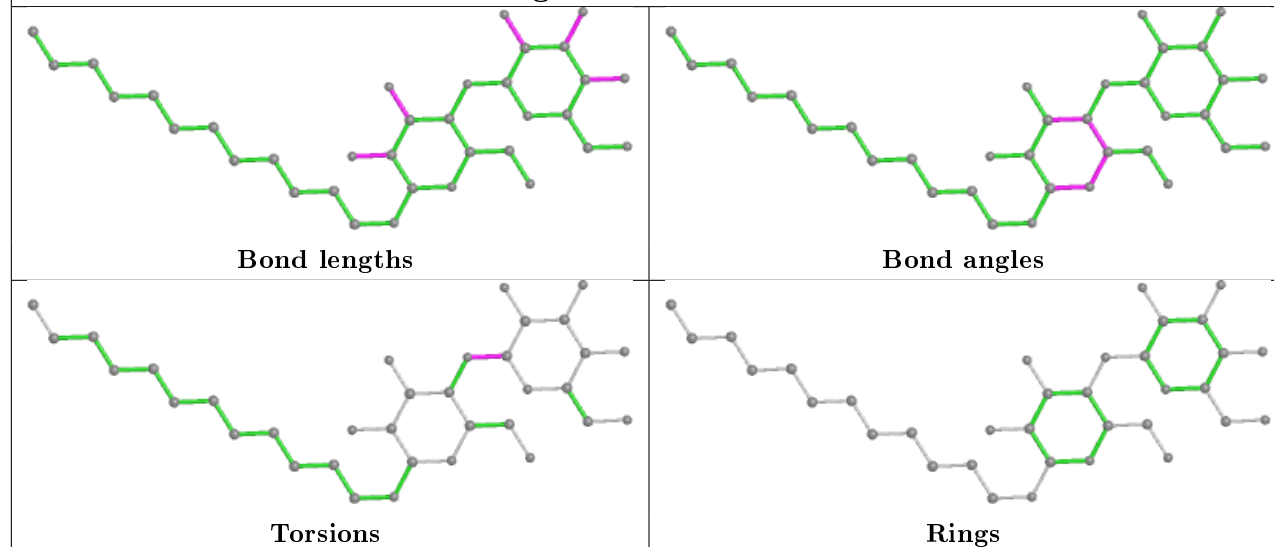
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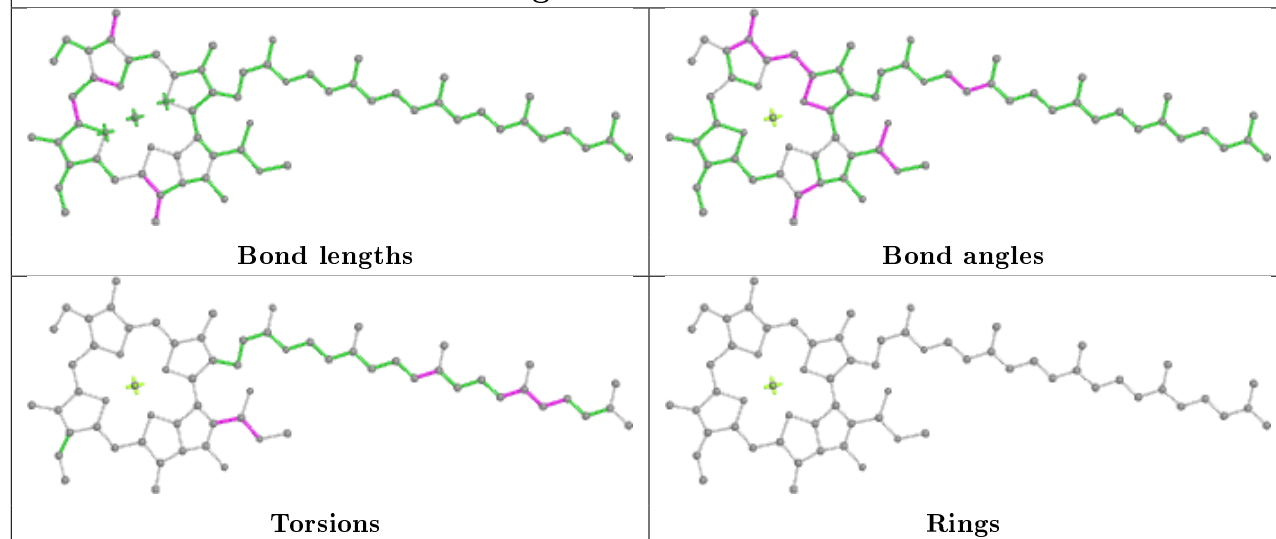
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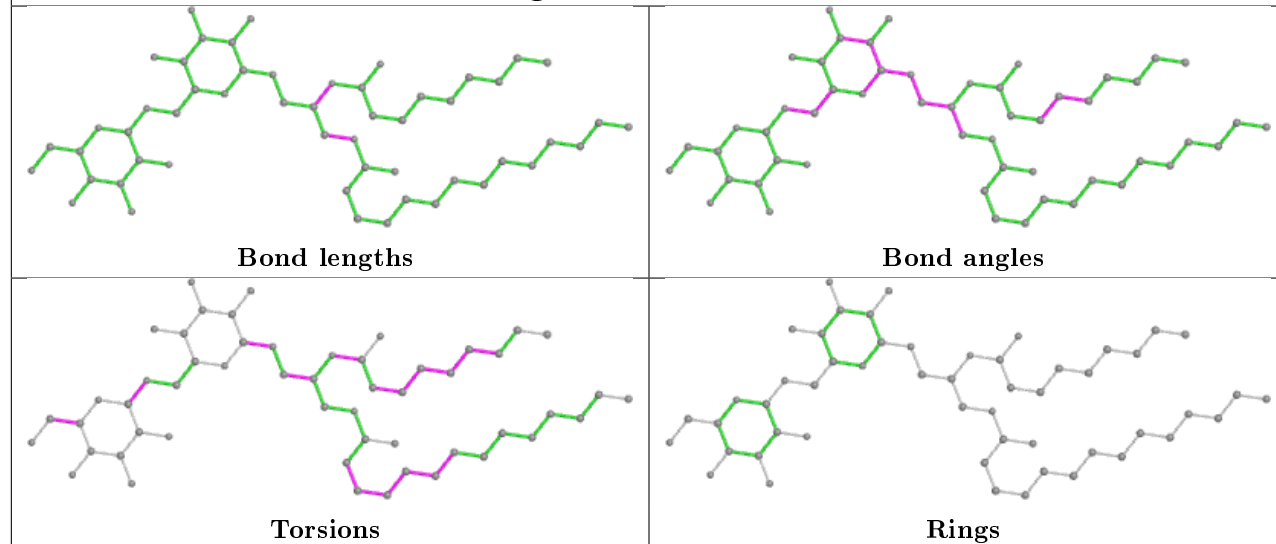
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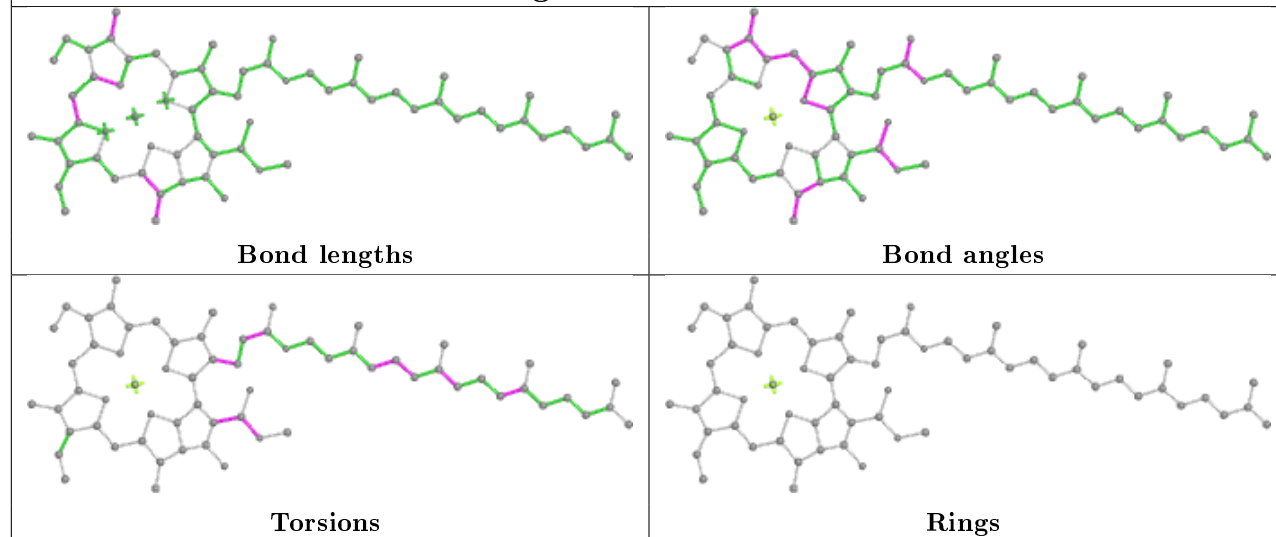
Ligand CLA B 608

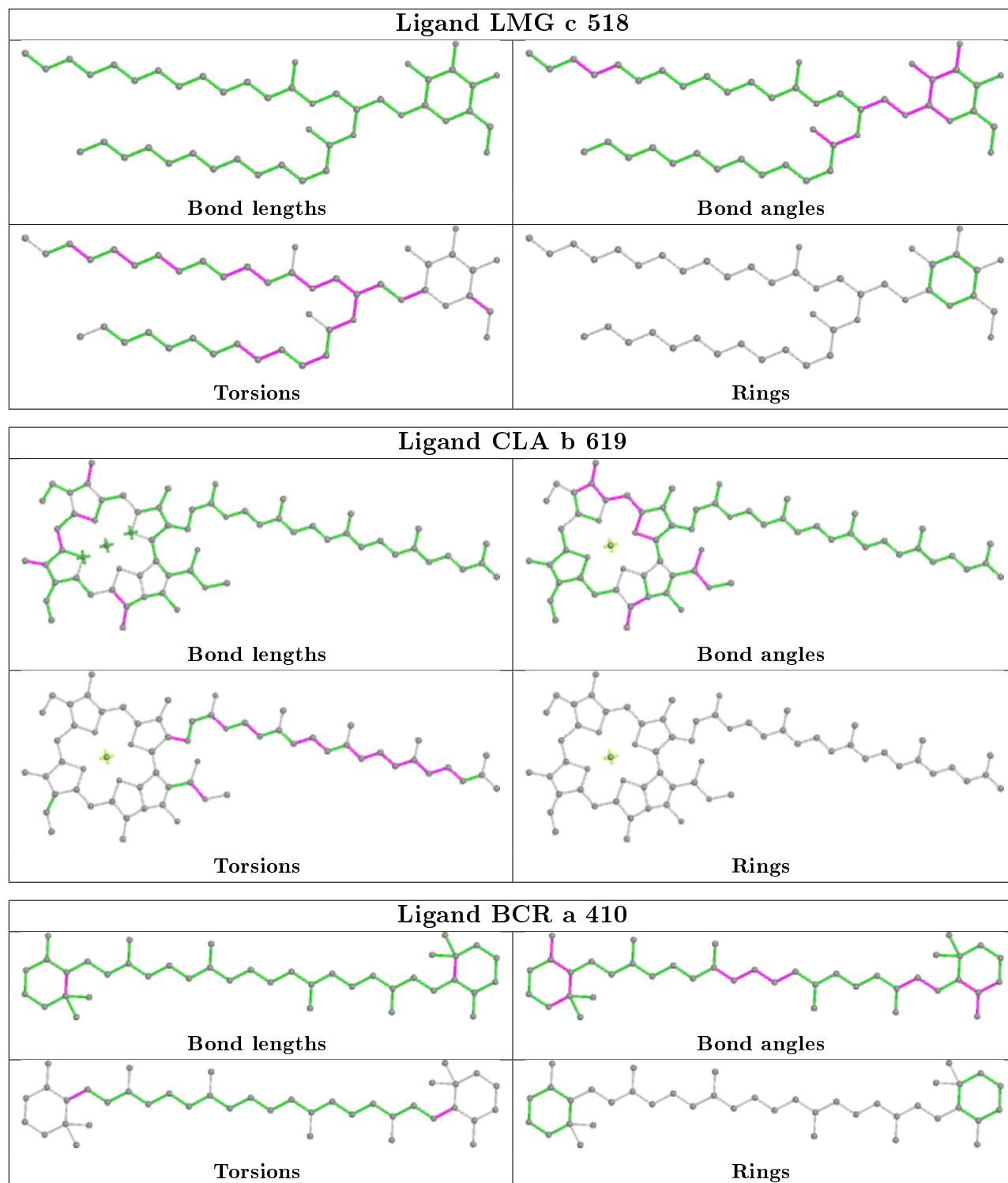


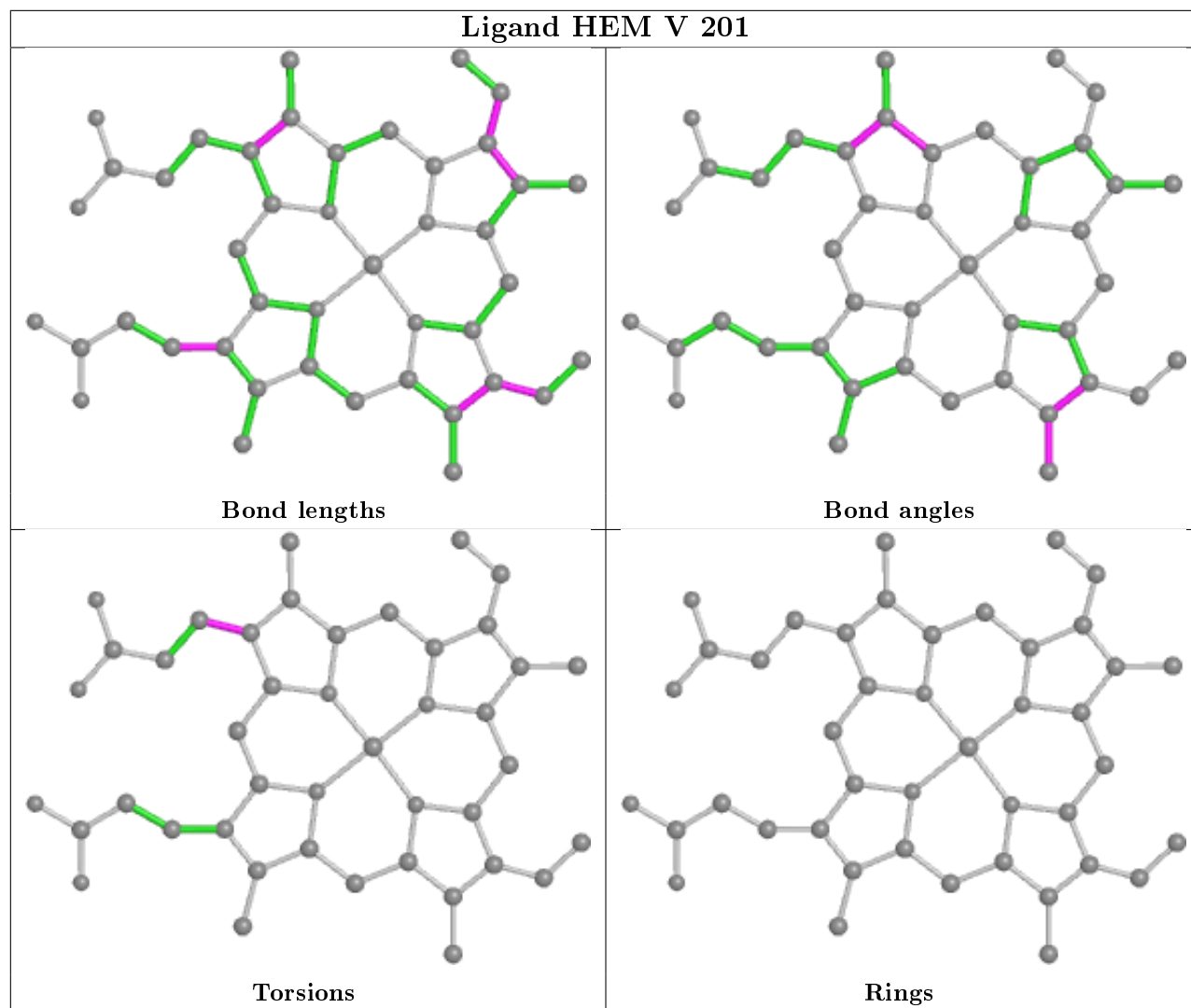
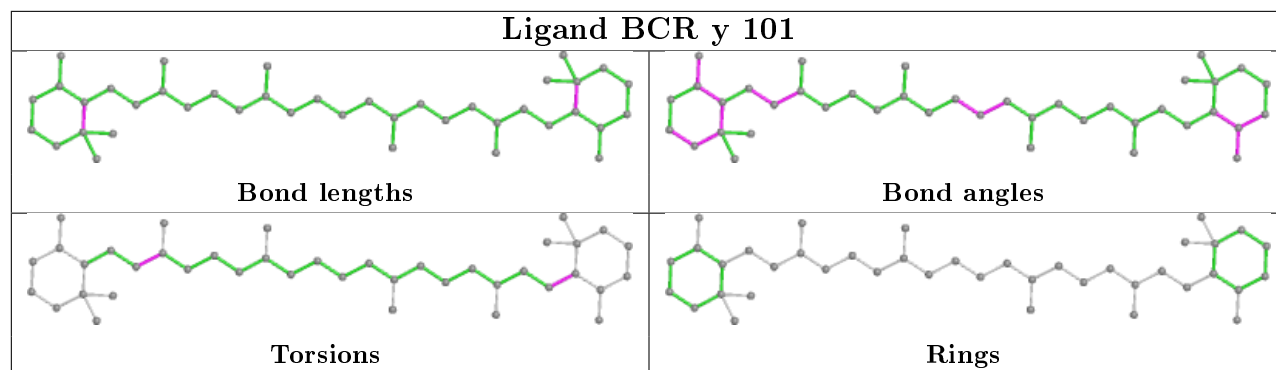
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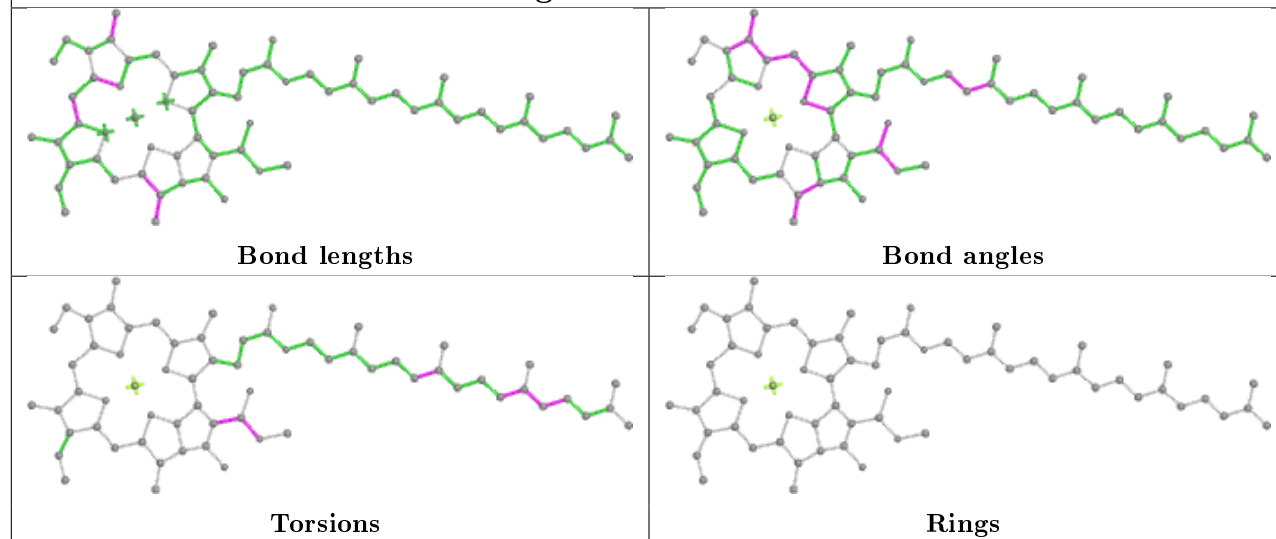
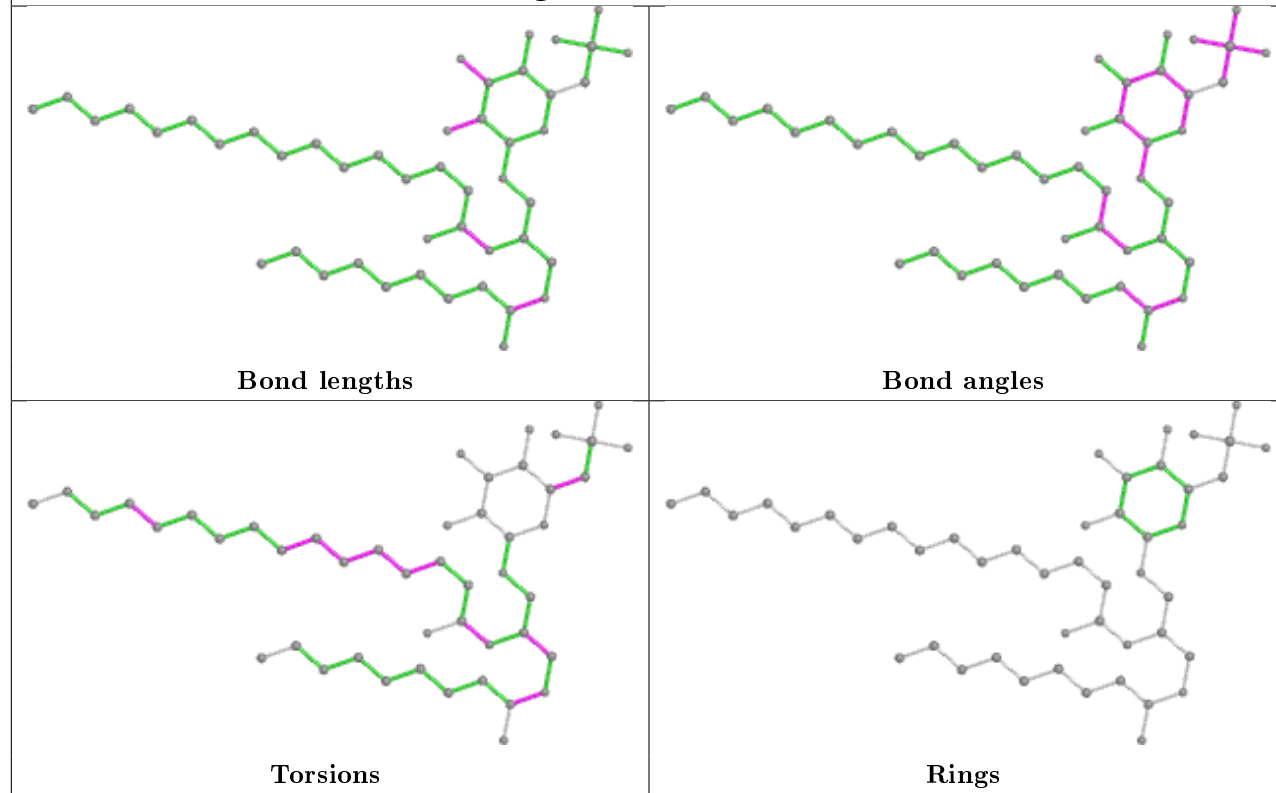


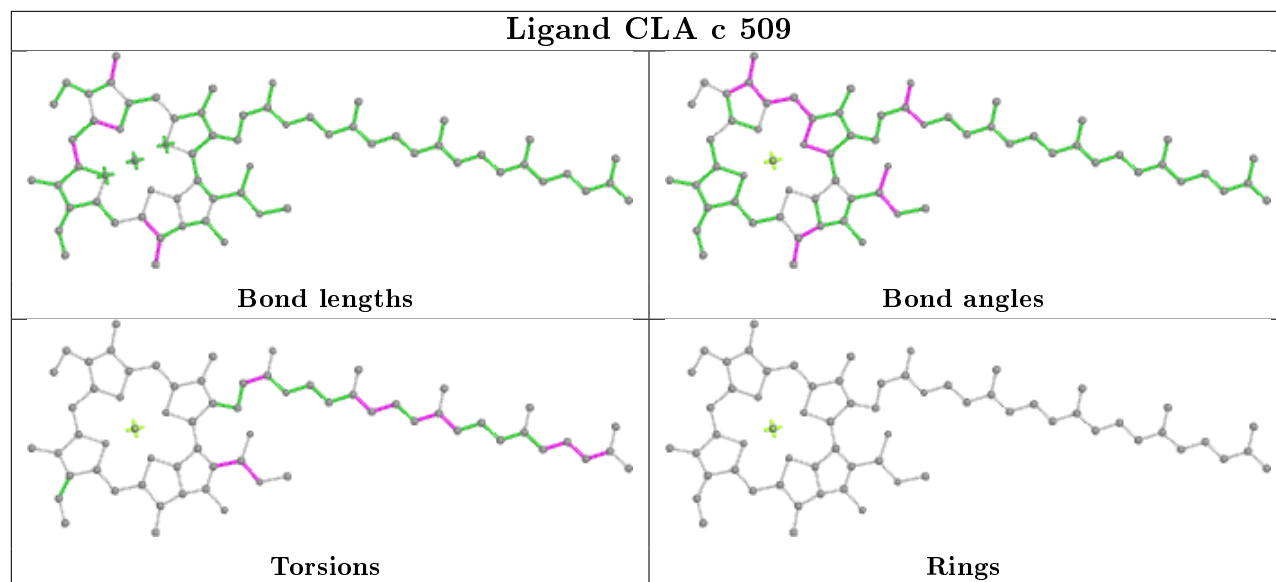
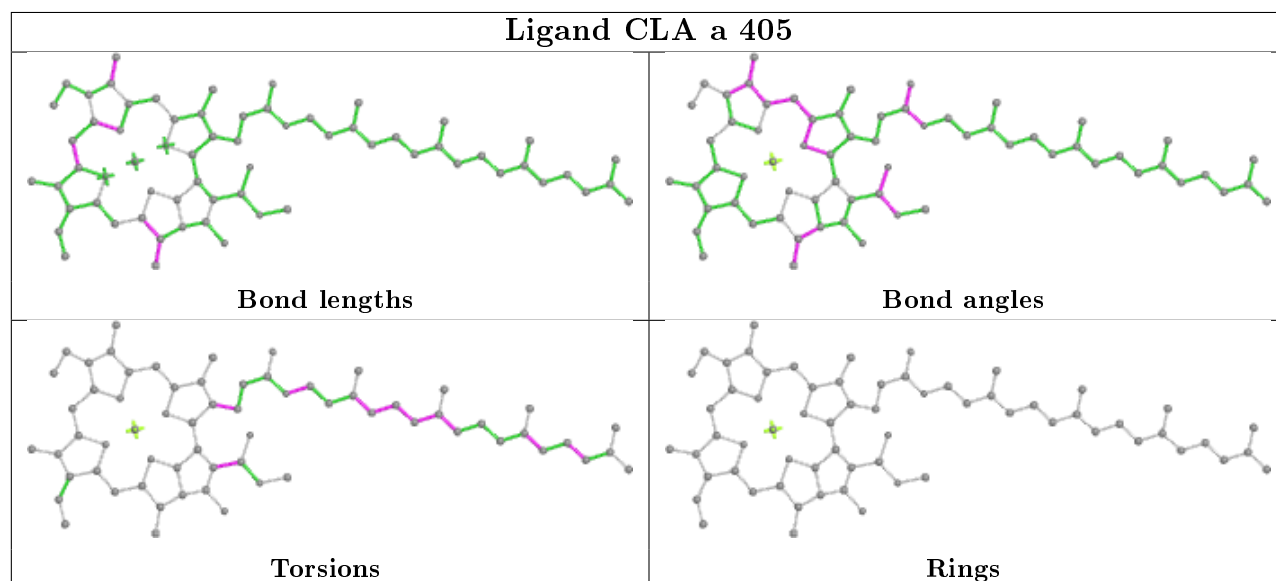
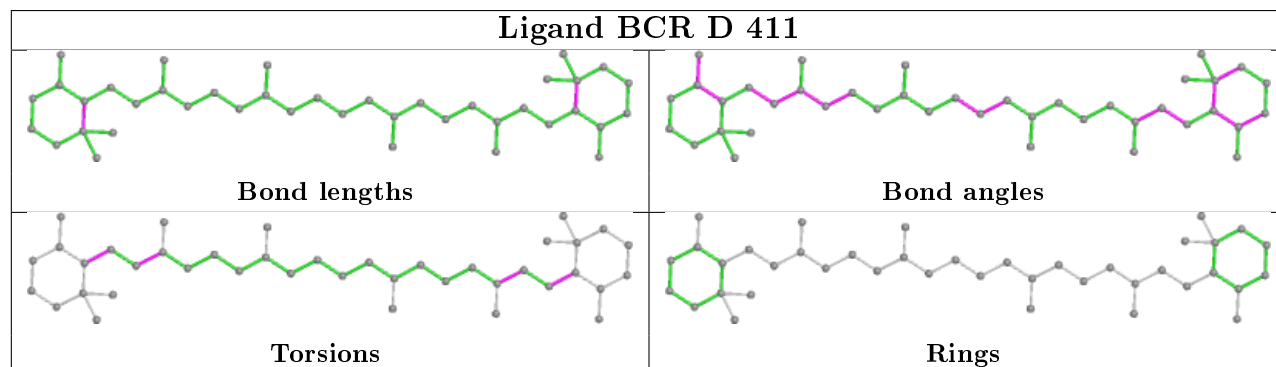
Ligand CLA C 506



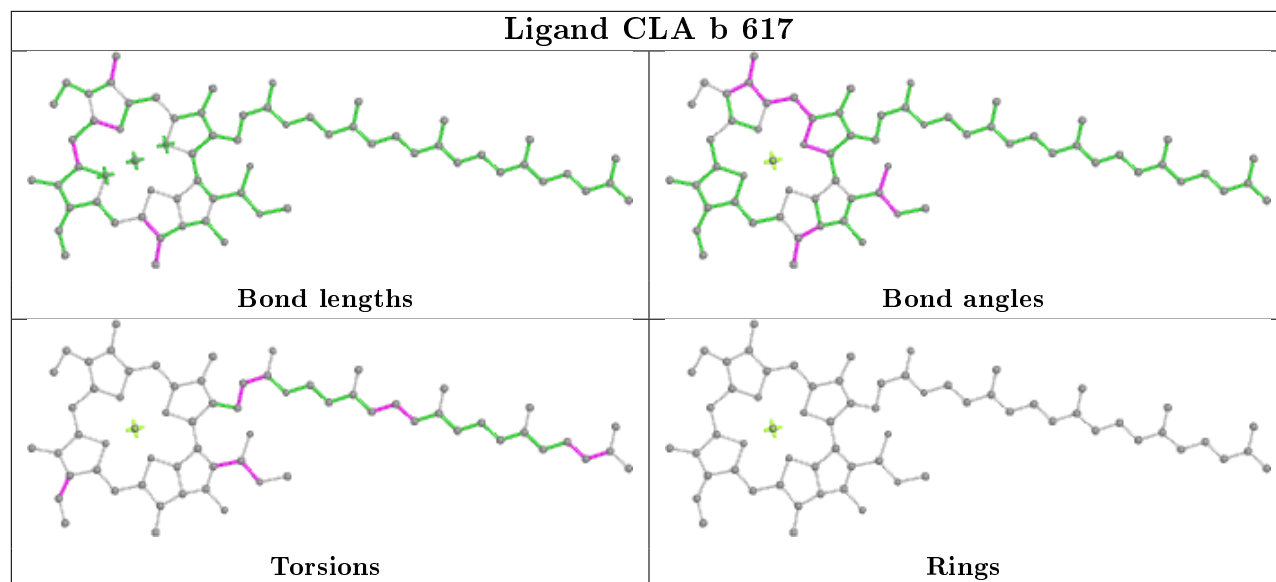




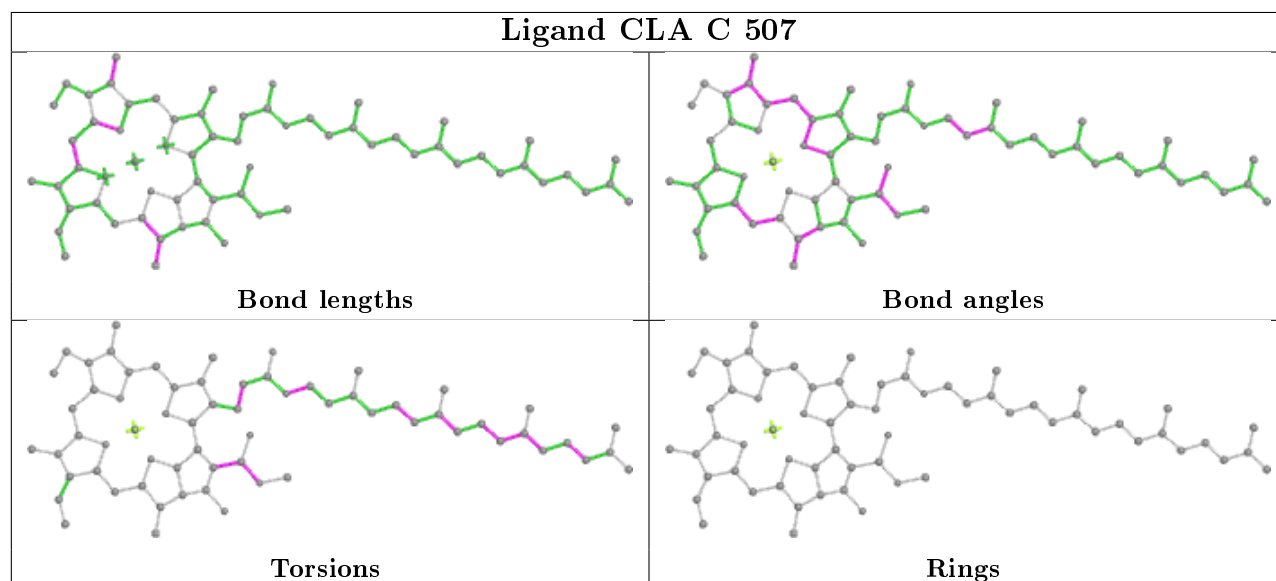
Ligand CLA b 612**Ligand SQD B 626**

Ligand CLA c 509**Ligand CLA a 405****Ligand BCR D 411**

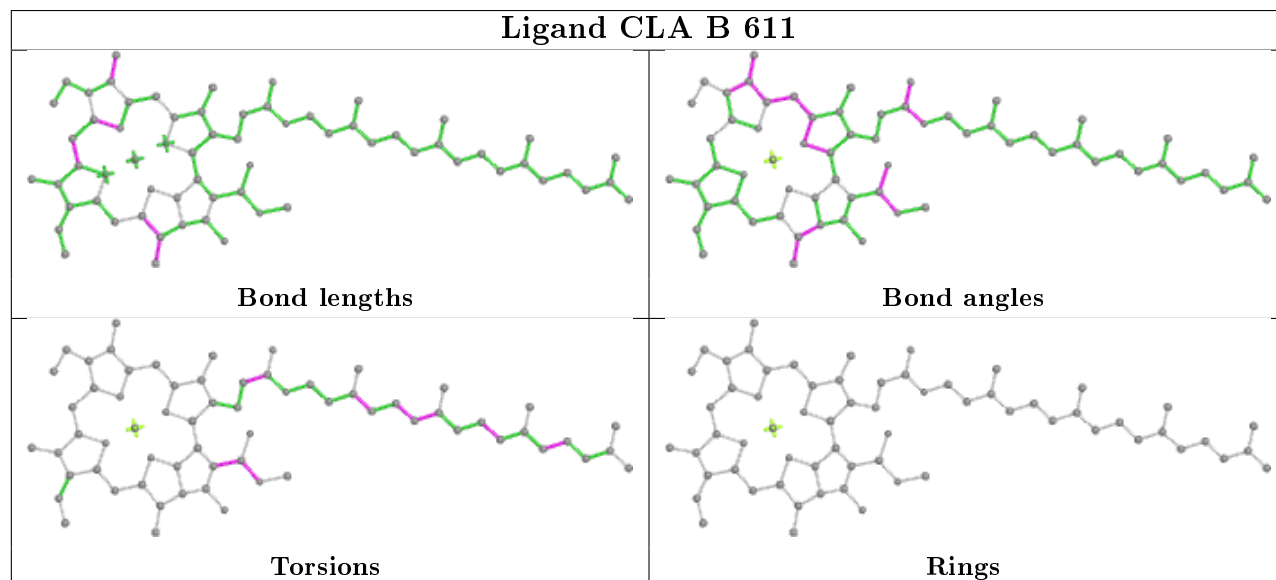
Ligand CLA b 617



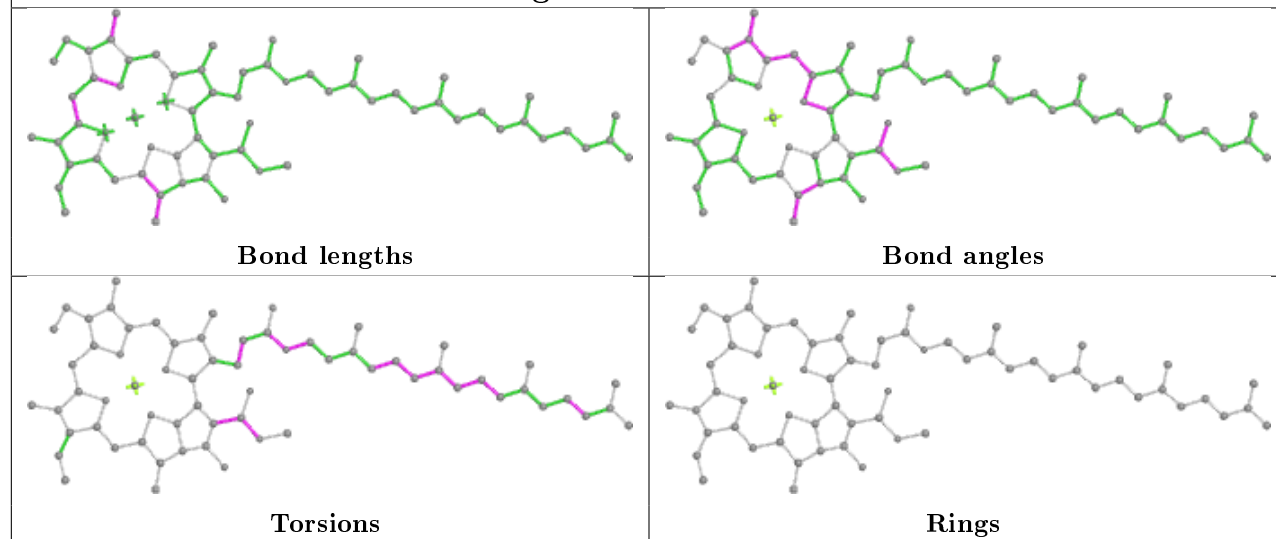
Ligand CLA C 507



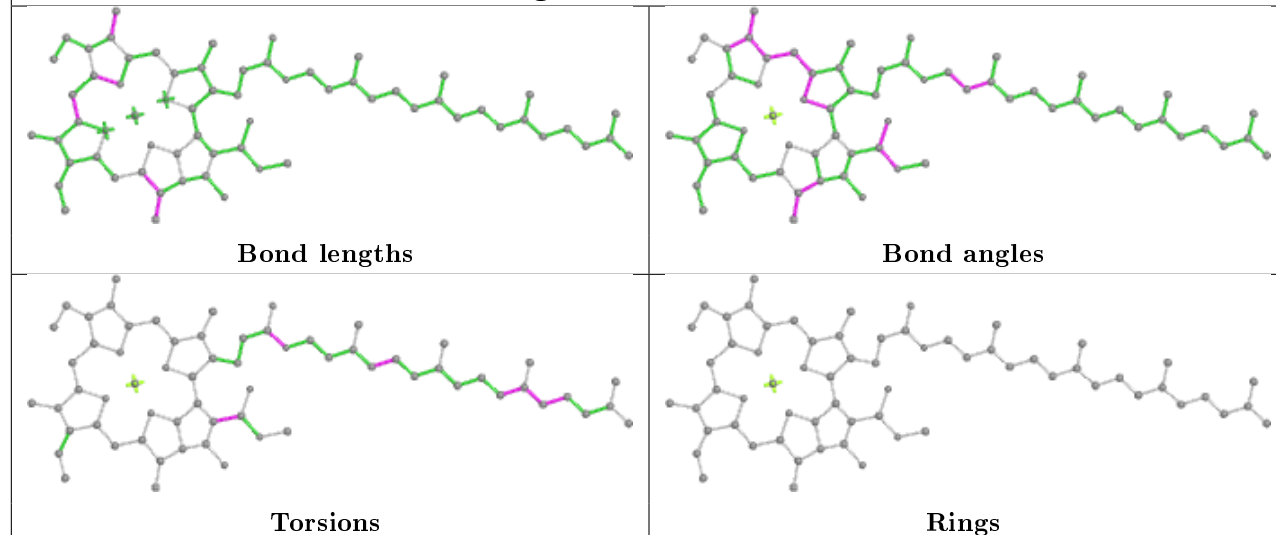
Ligand CLA B 611



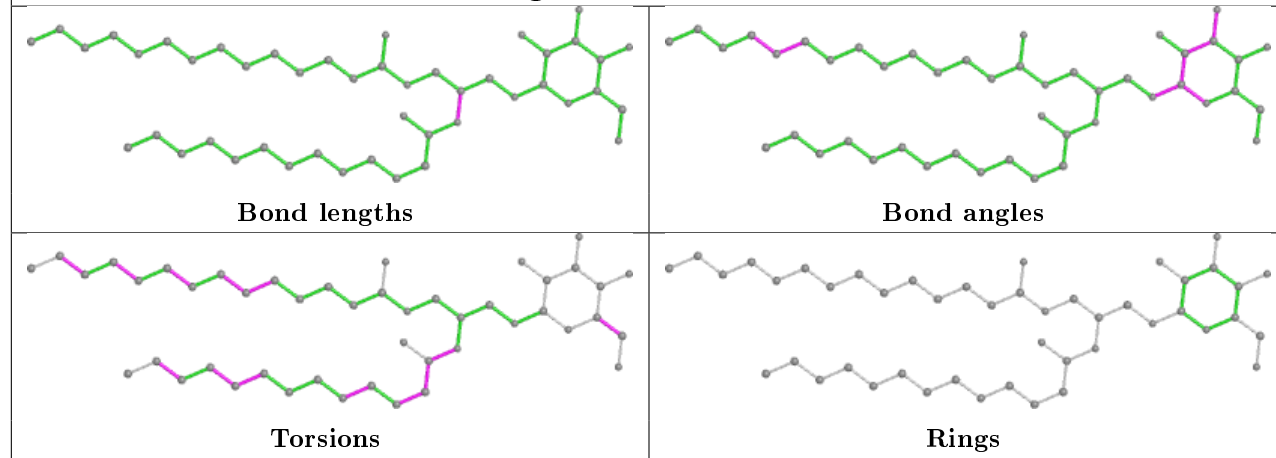
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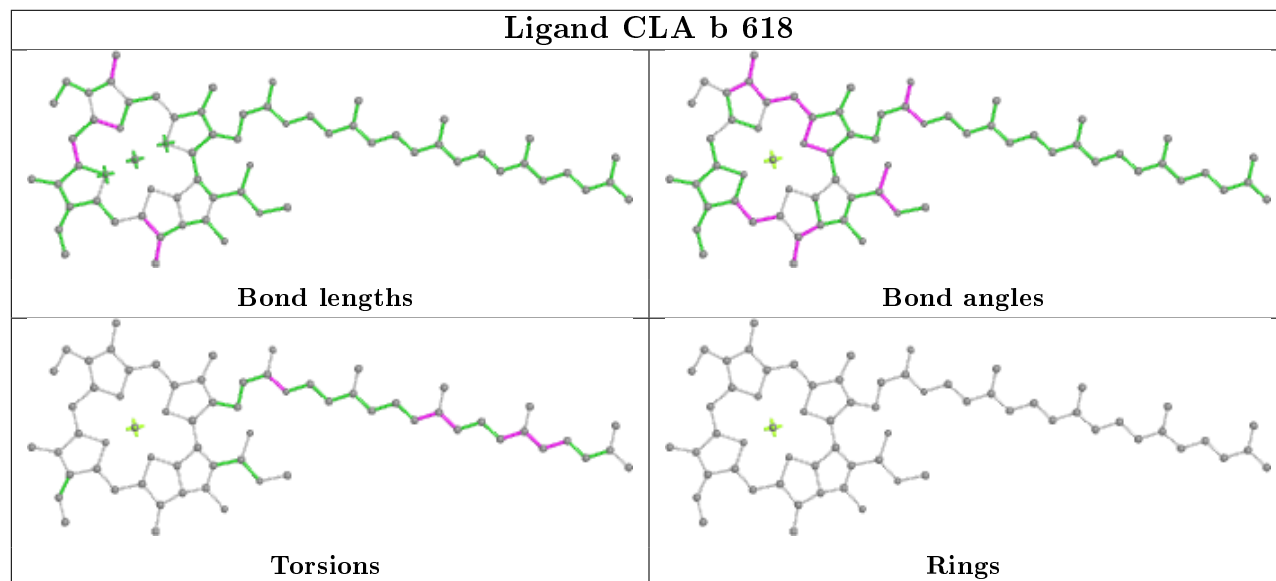
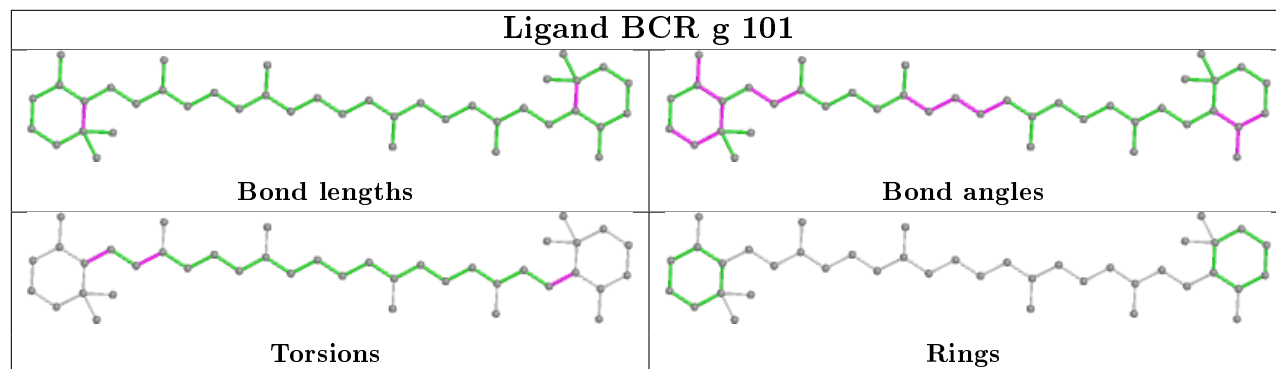
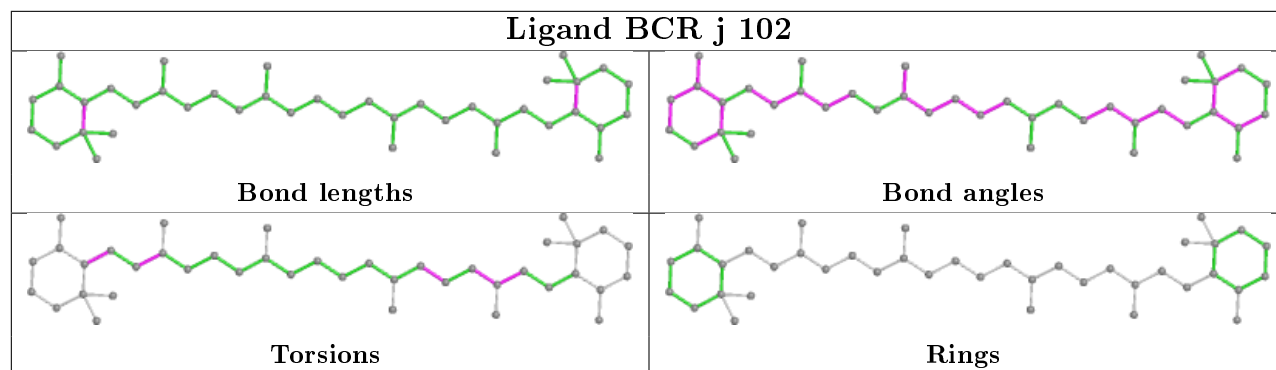
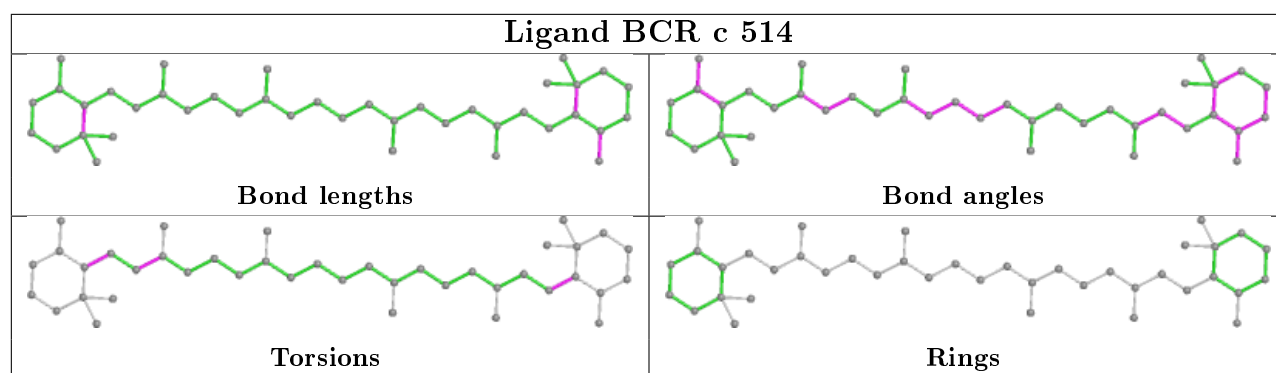


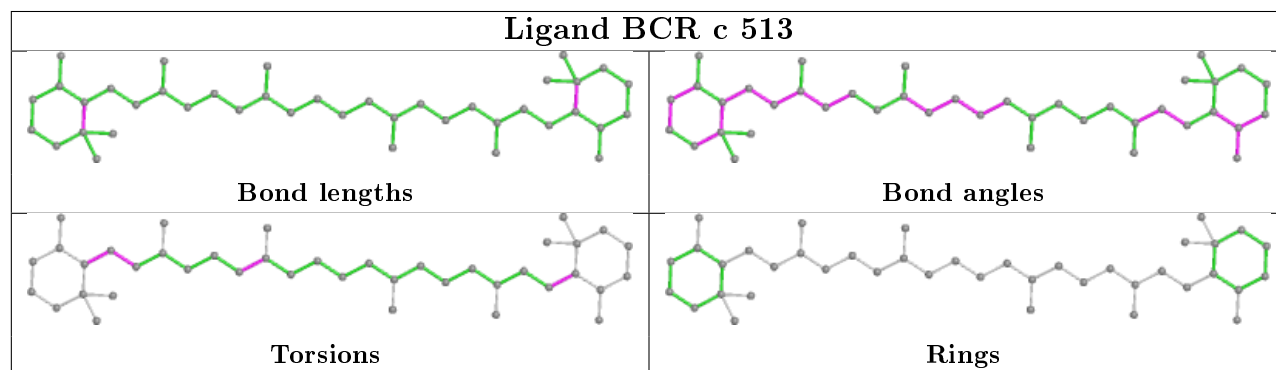
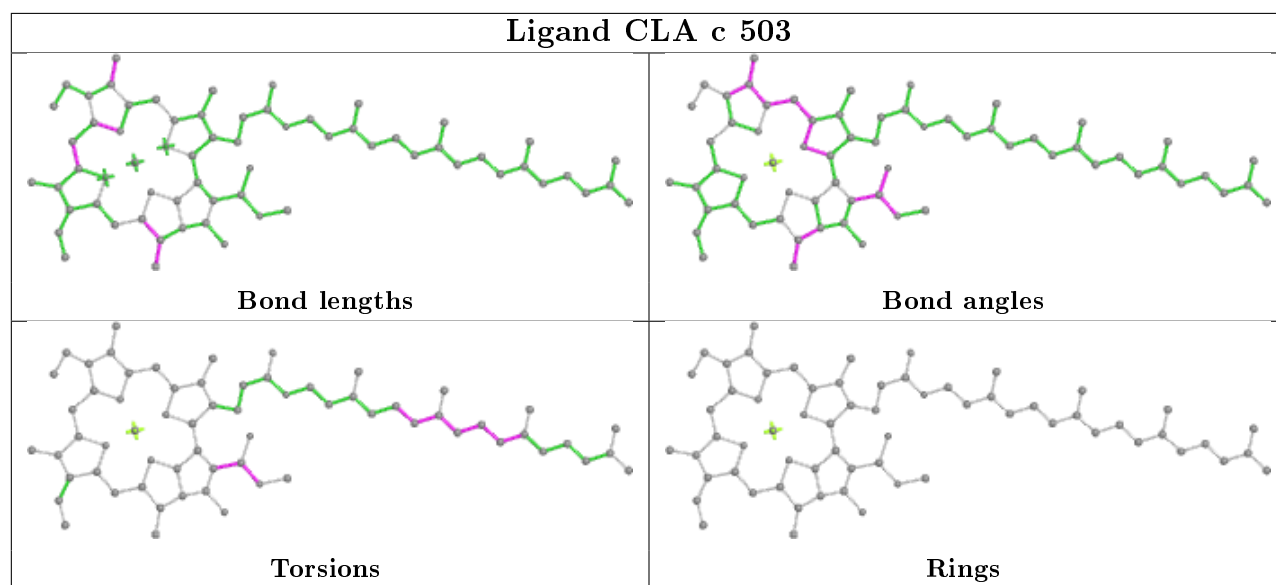
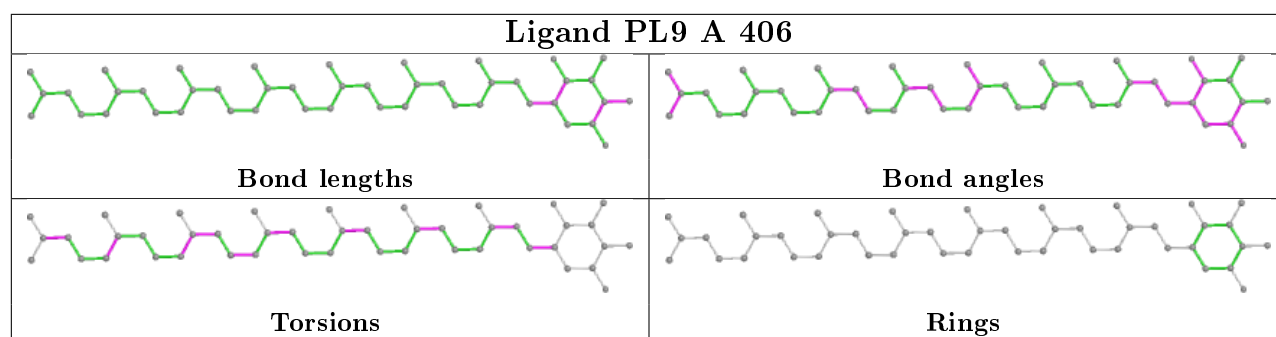
Ligand CLA C 502

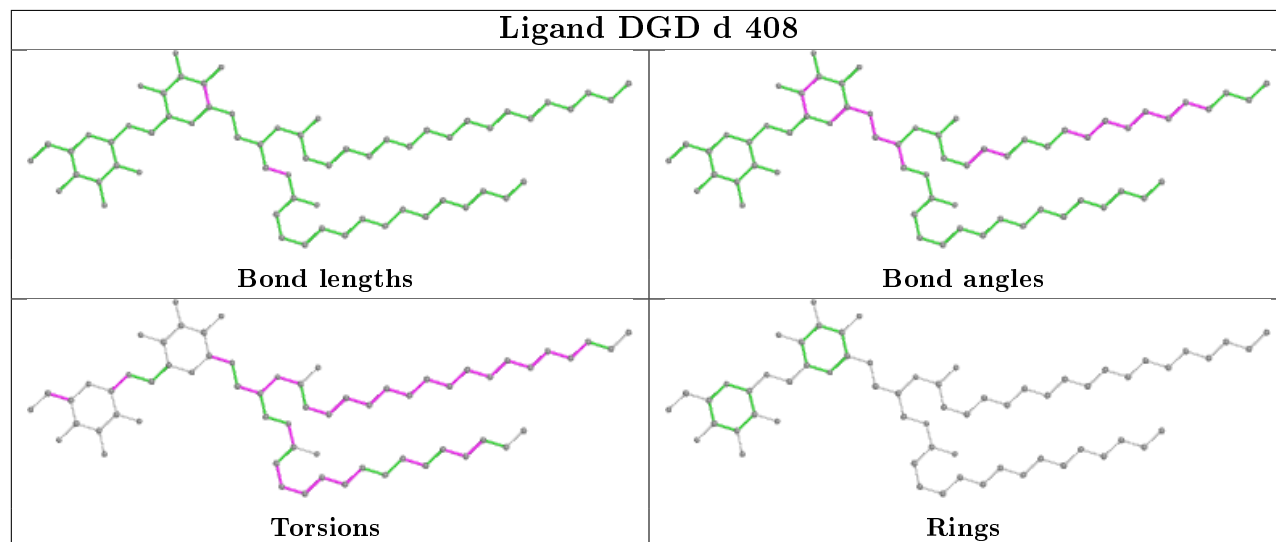
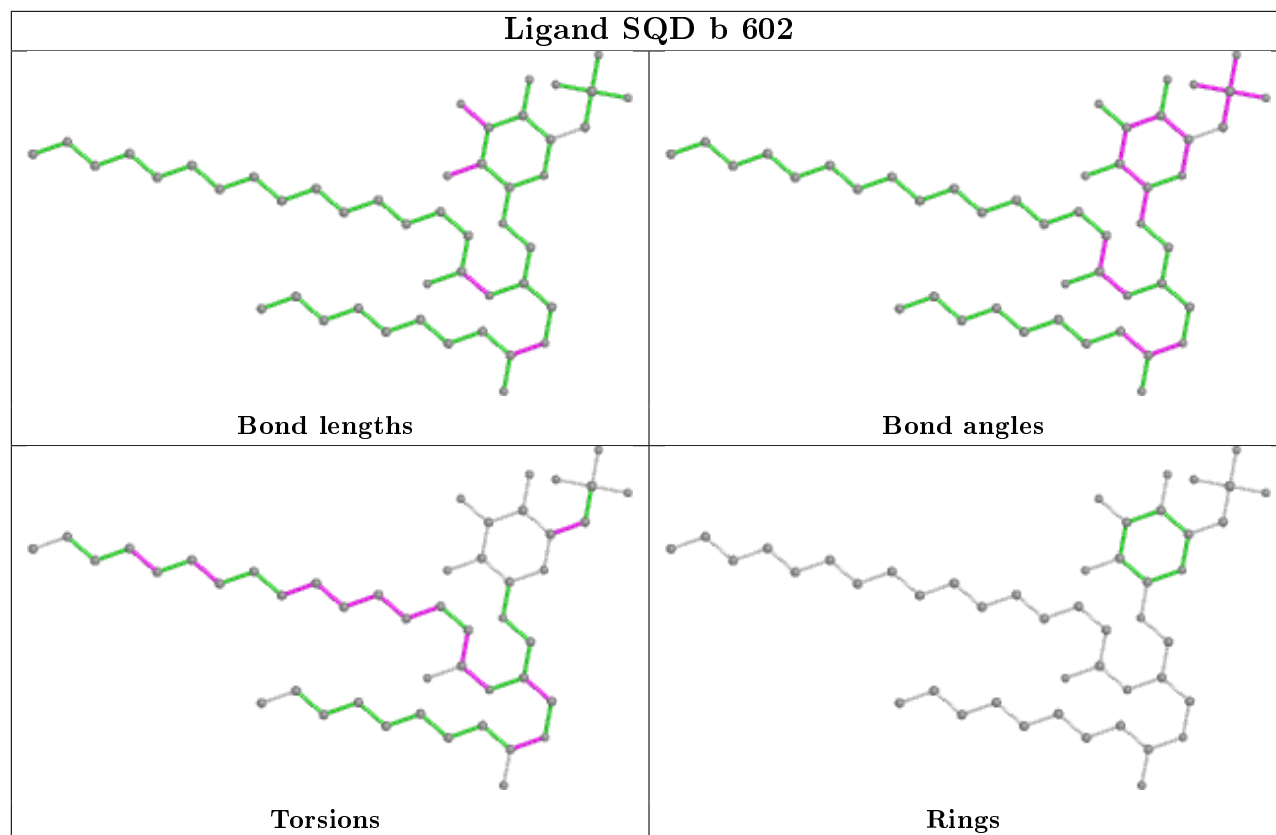


Ligand LMG D 412

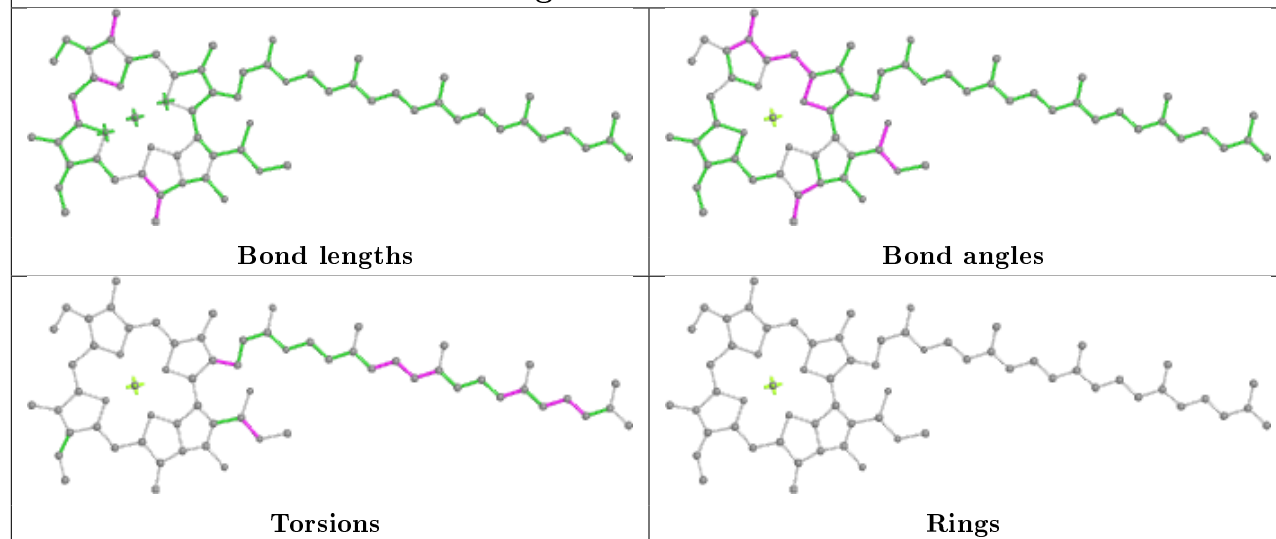




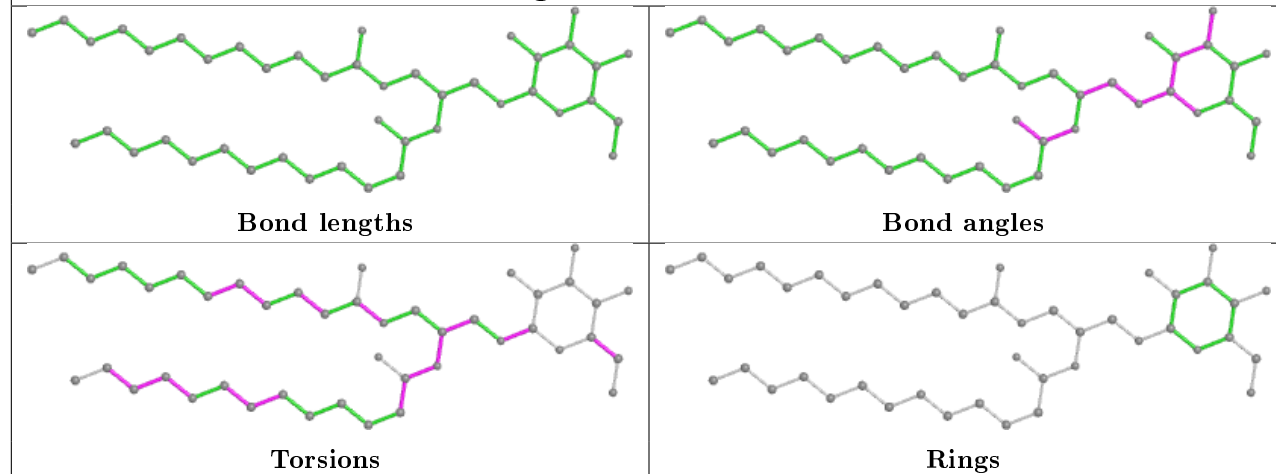




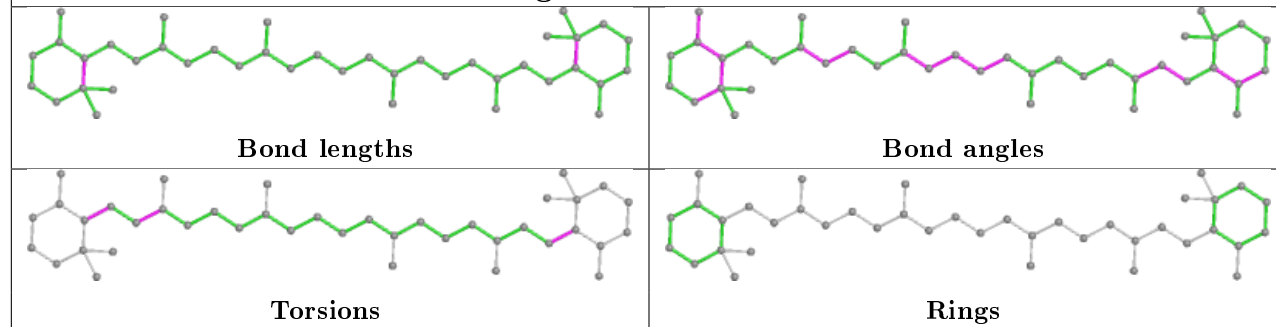
Ligand CLA b 611



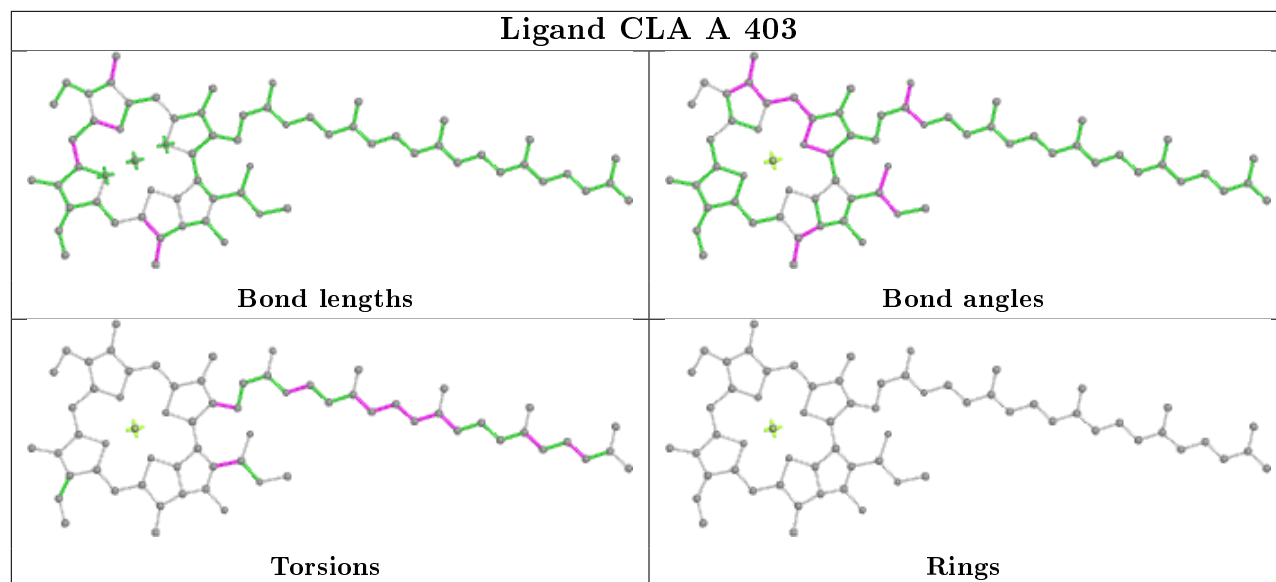
Ligand LMG e 101



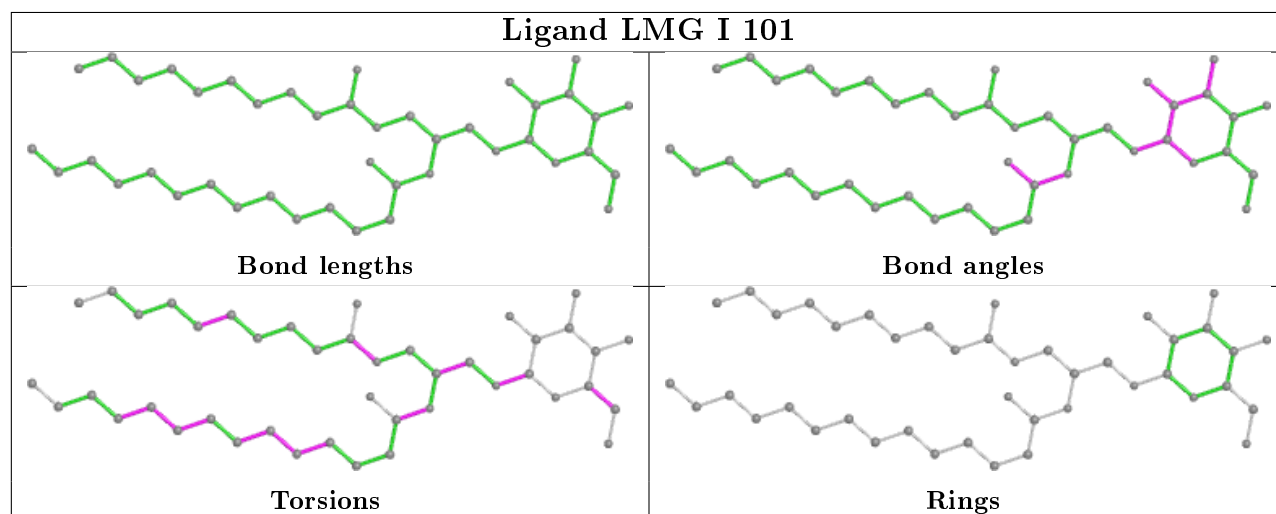
Ligand BCR c 521



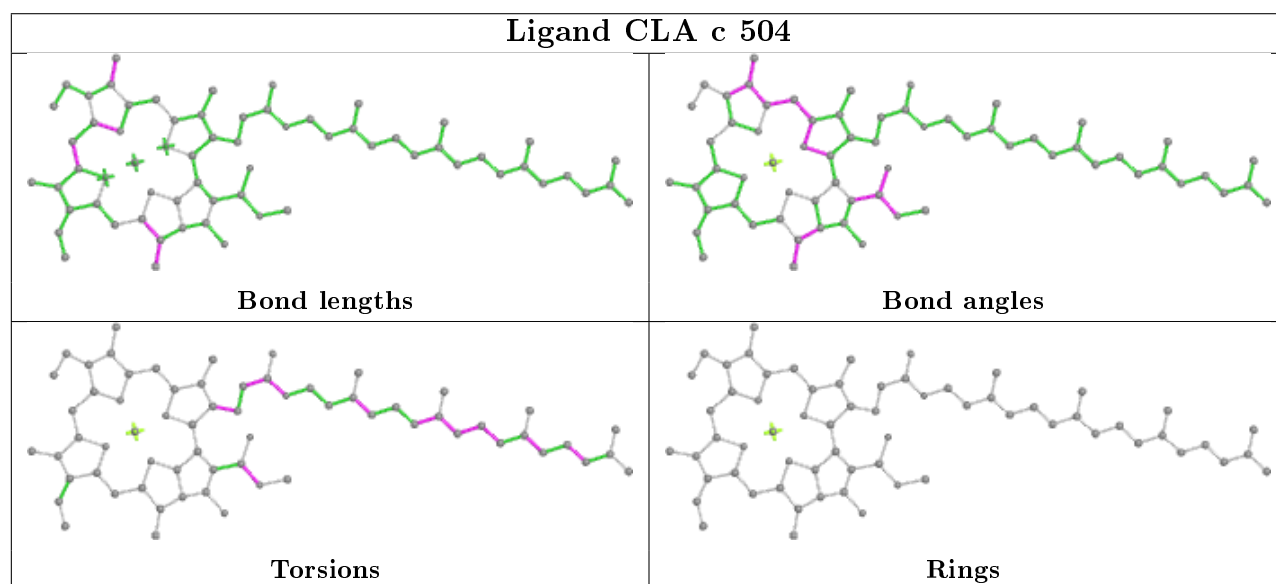
Ligand CLA A 403

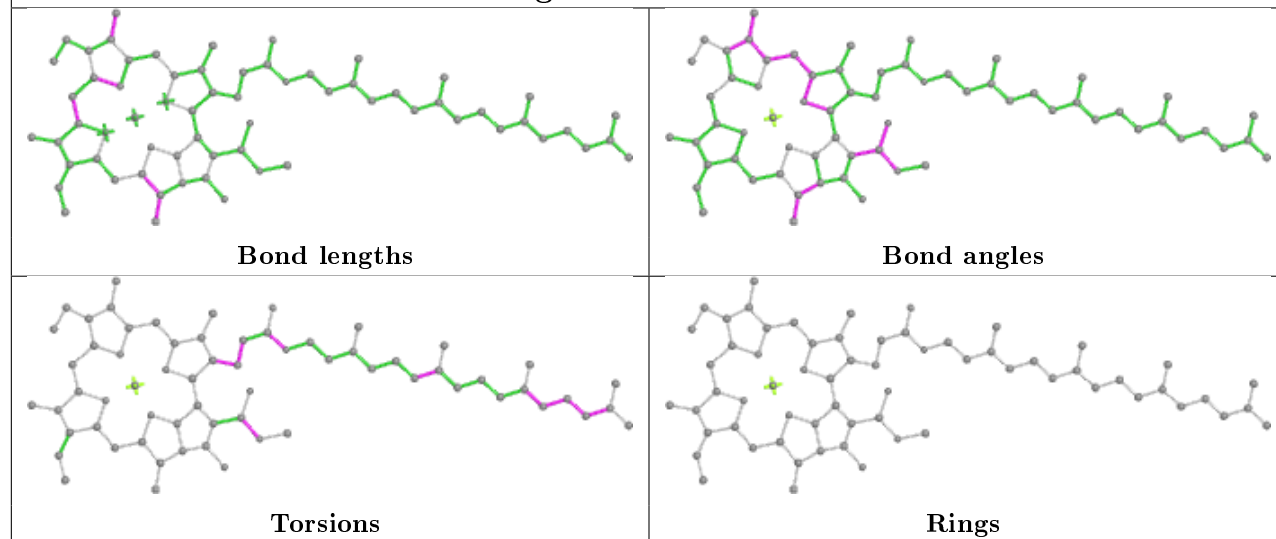
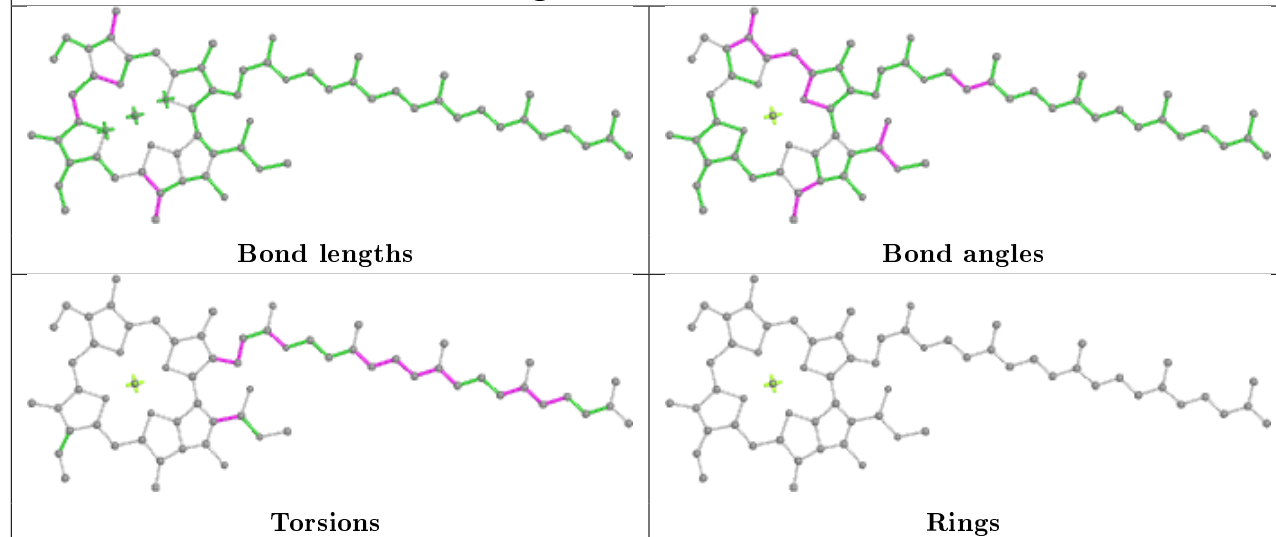


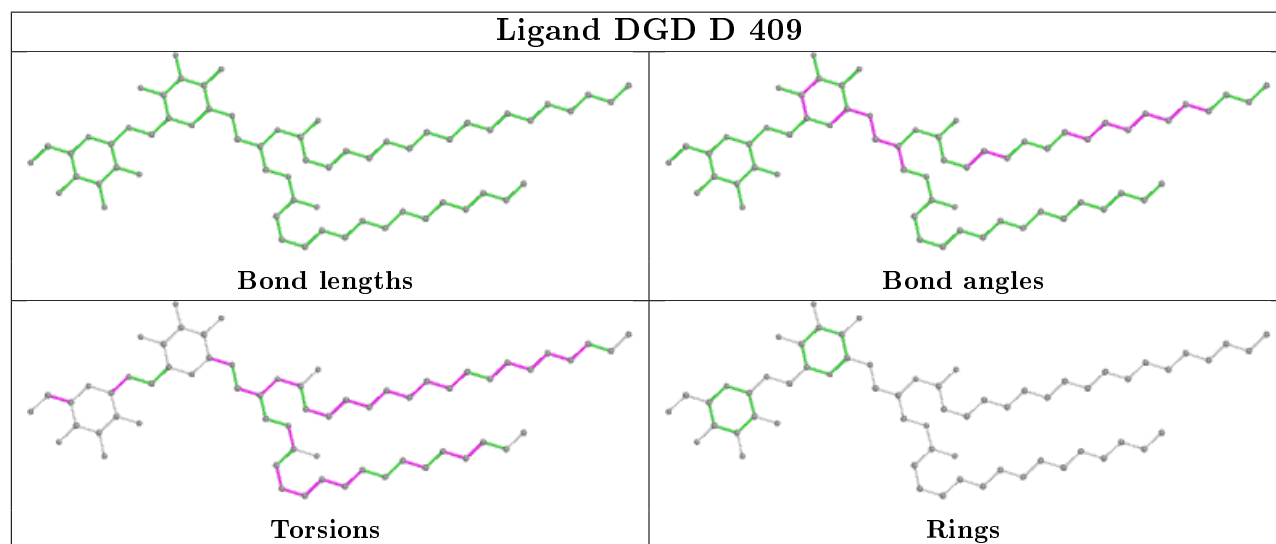
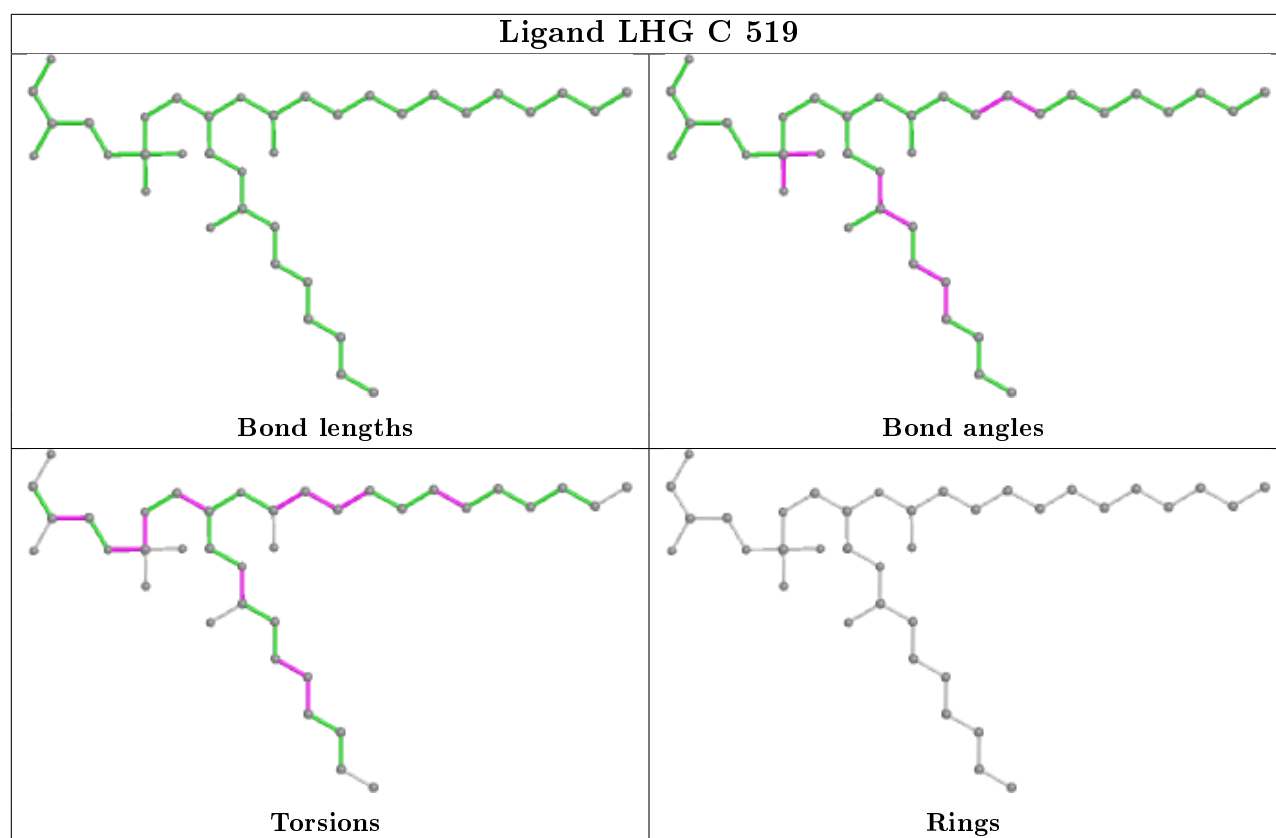
Ligand LMG I 101

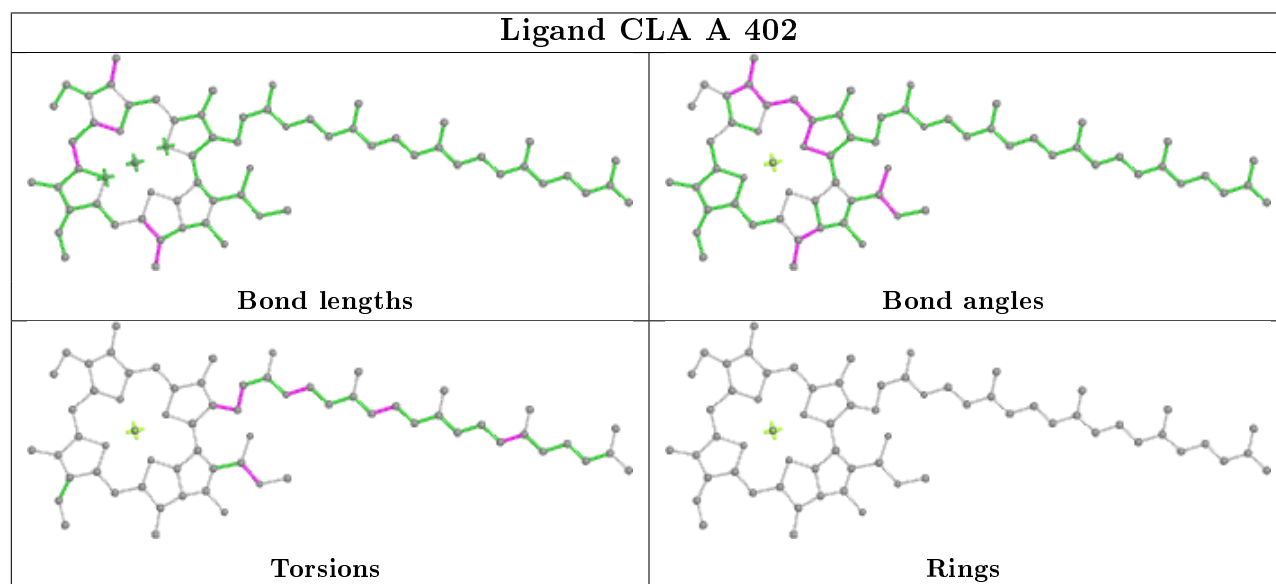
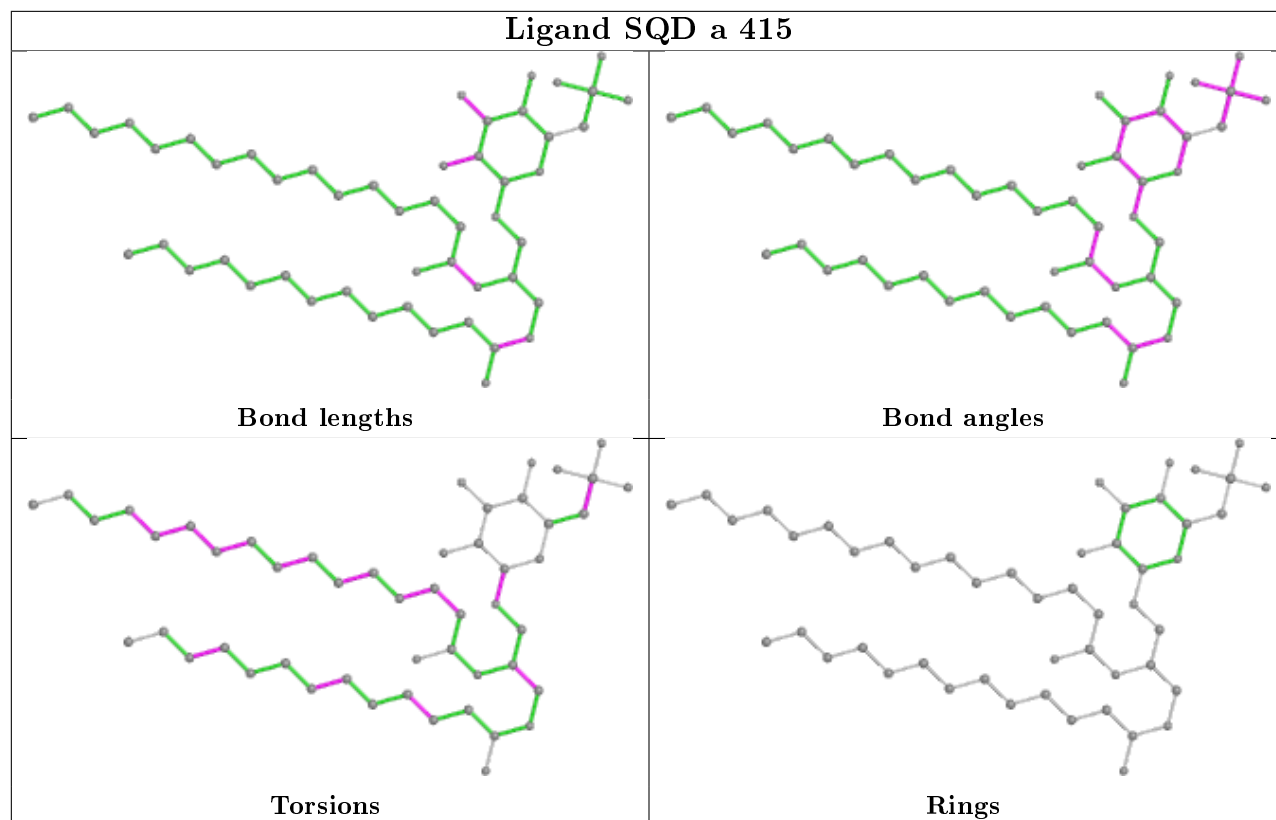


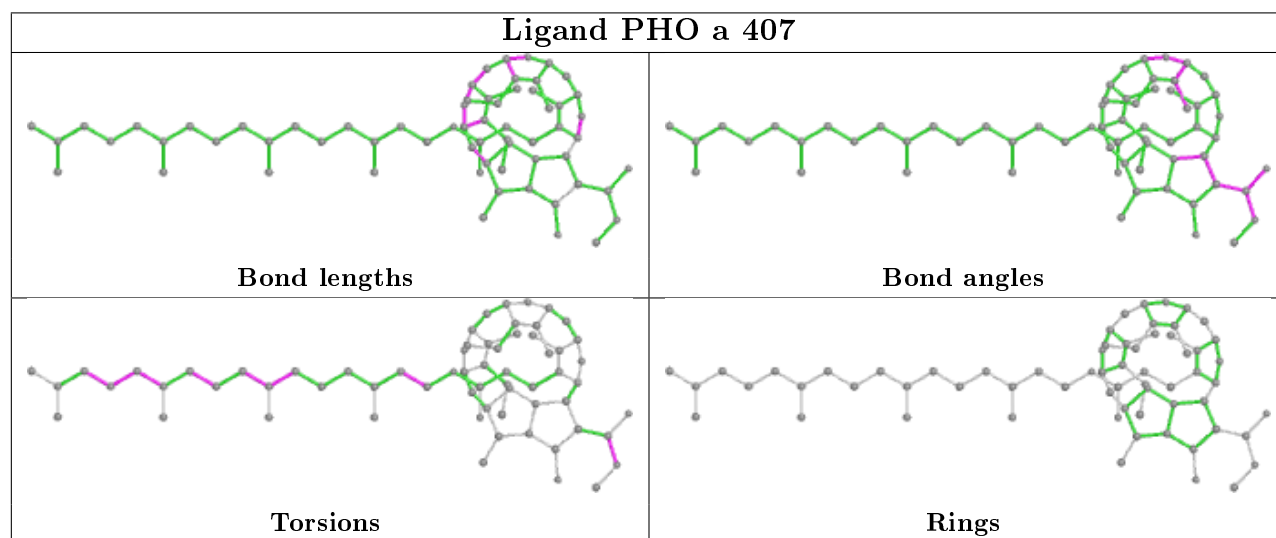
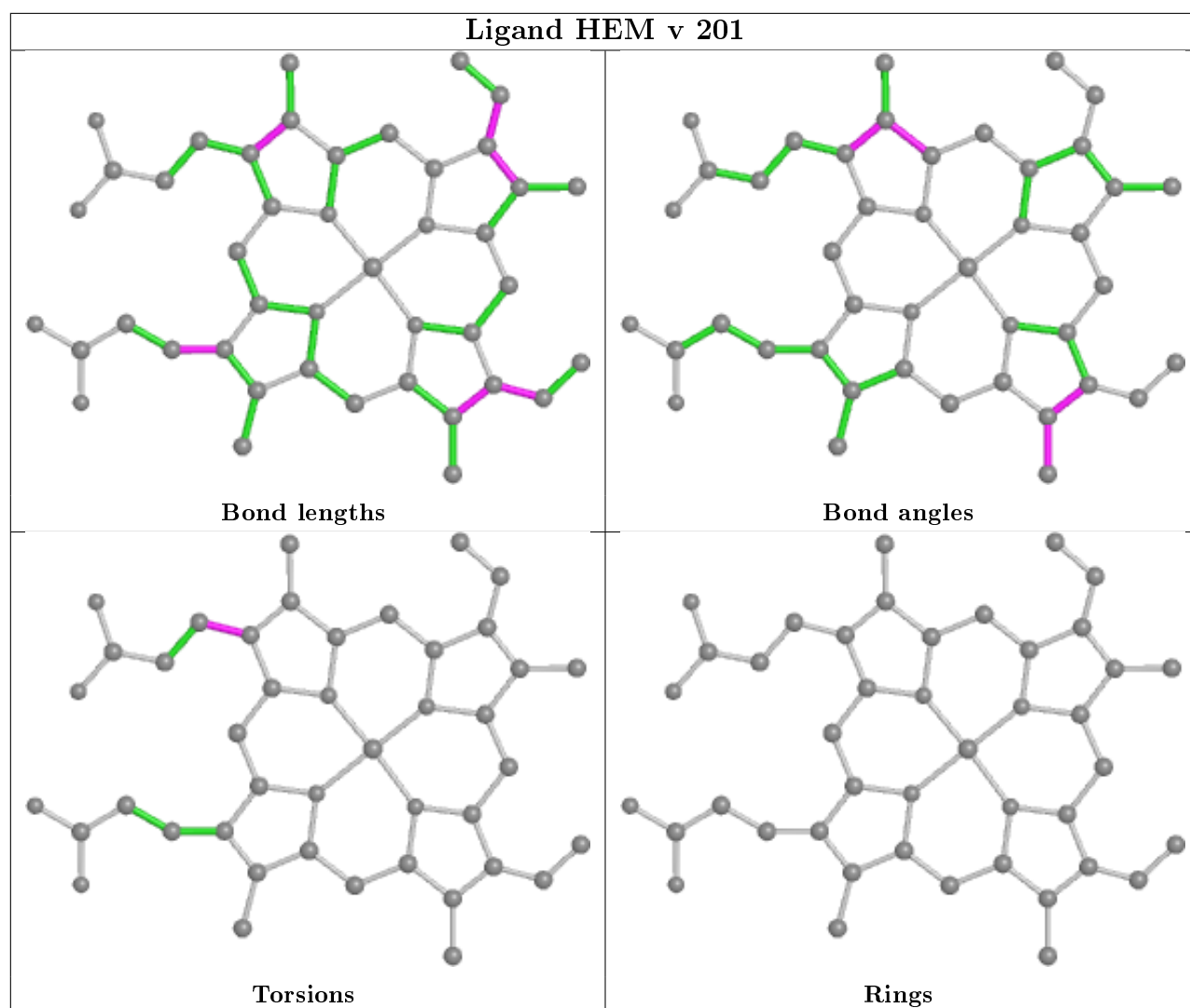
Ligand CLA c 504

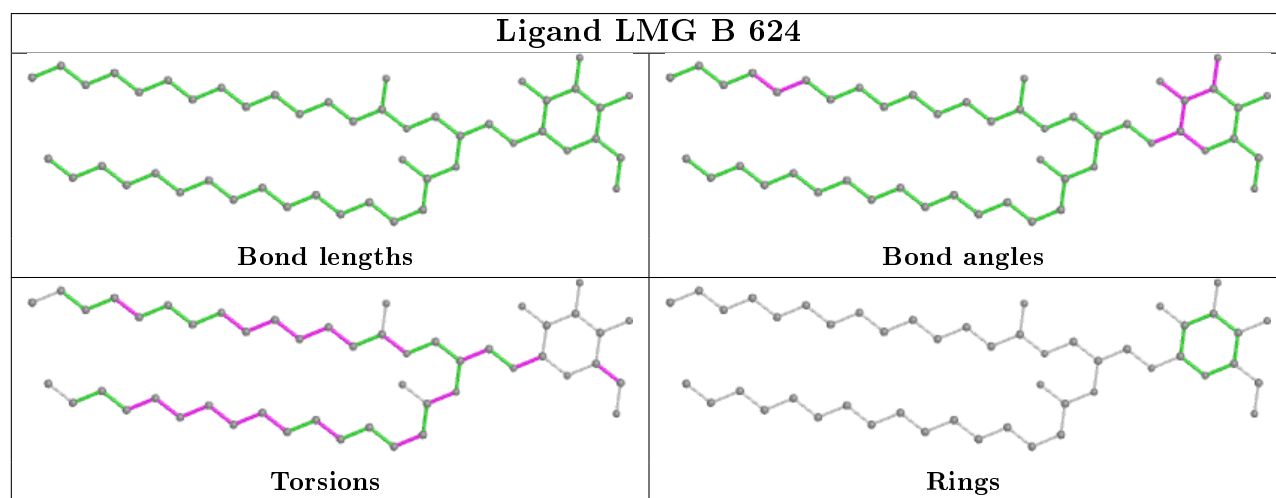
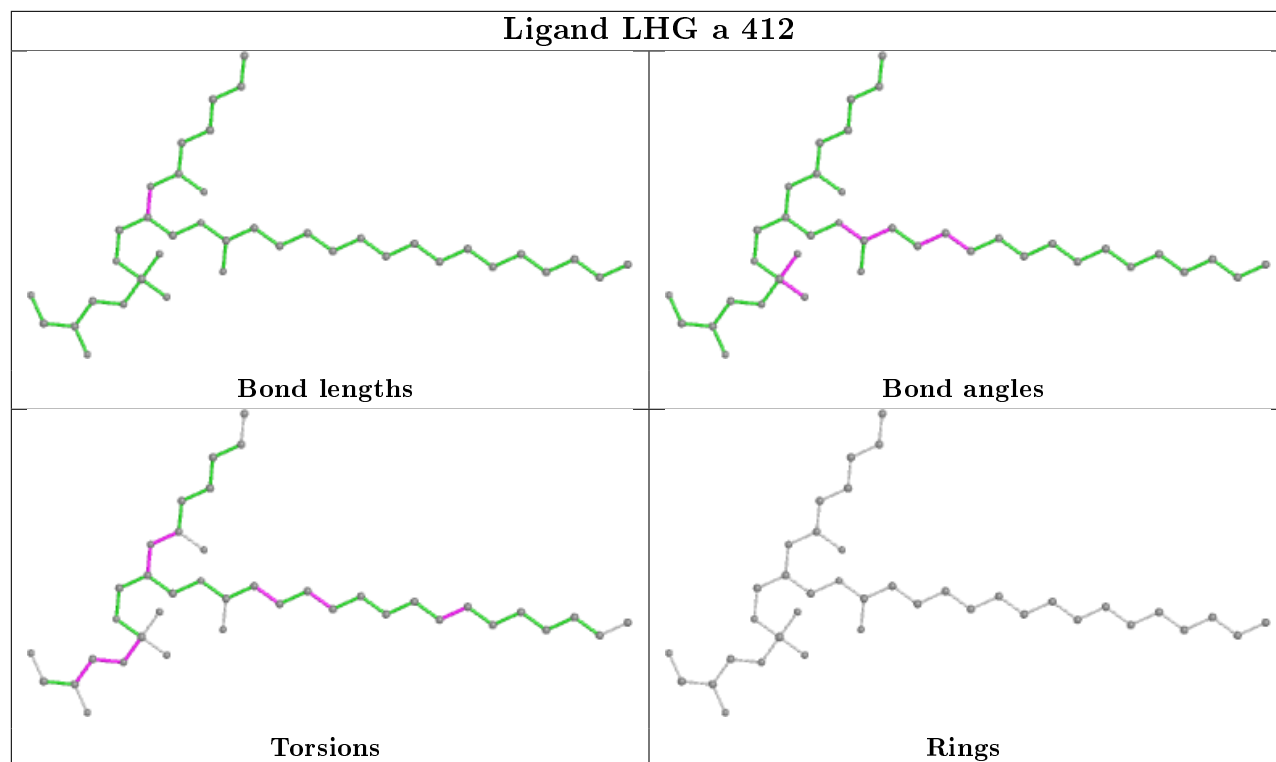


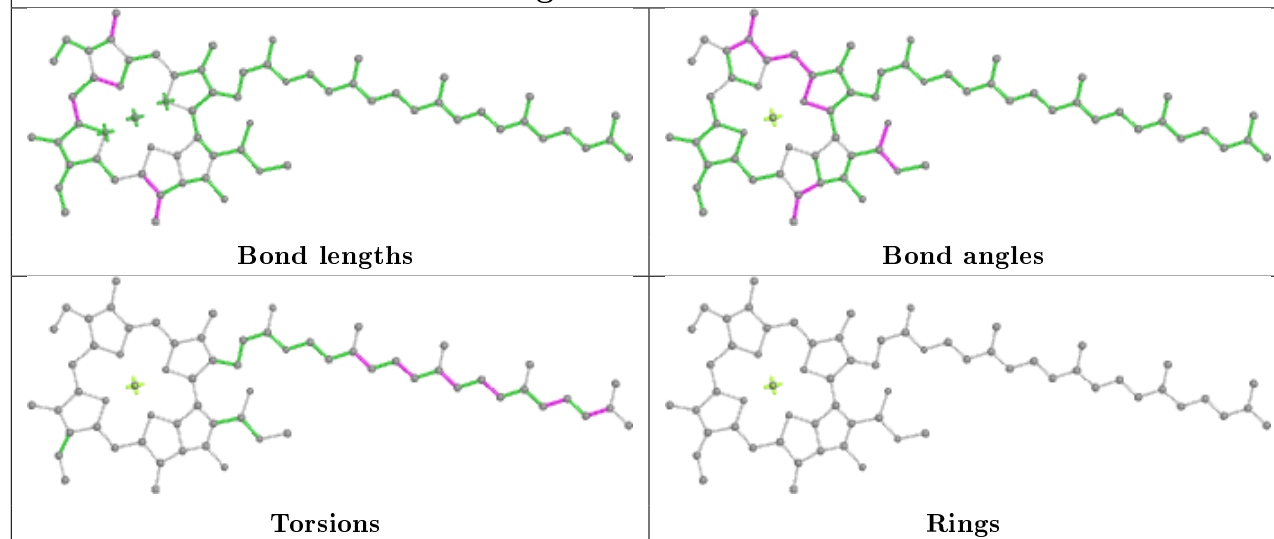
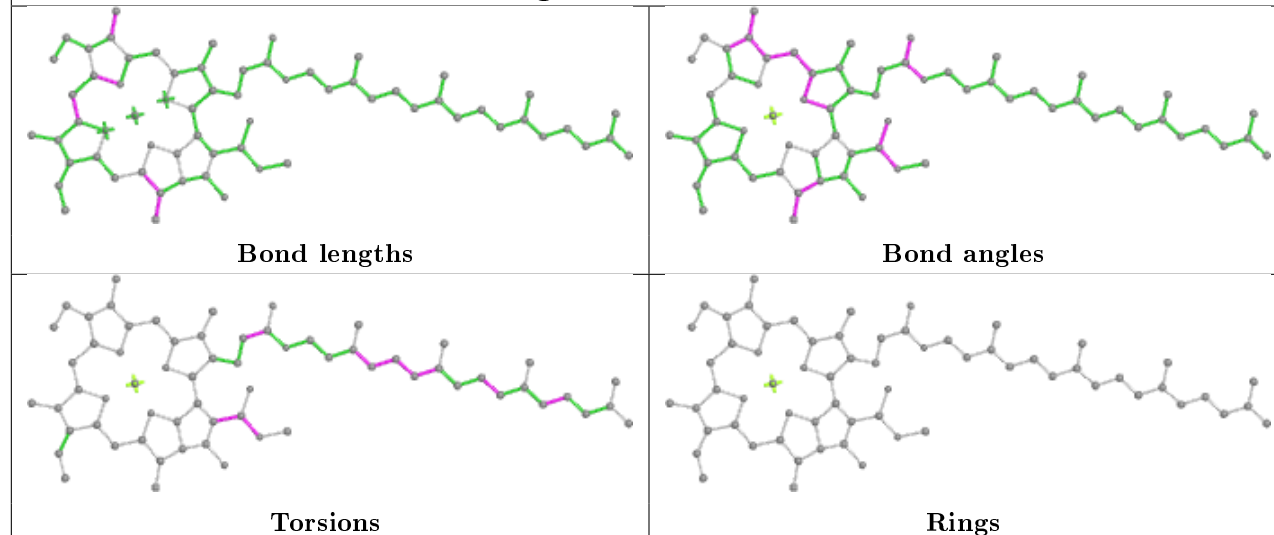
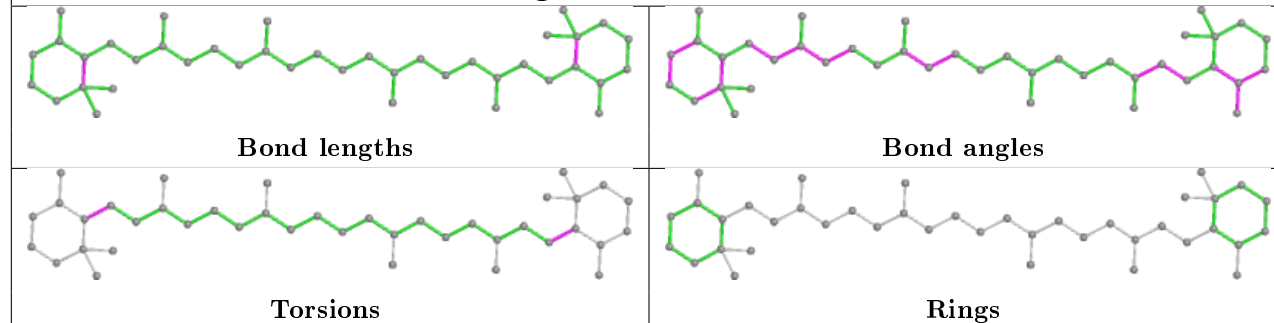
Ligand CLA b 609**Ligand CLA H 101**

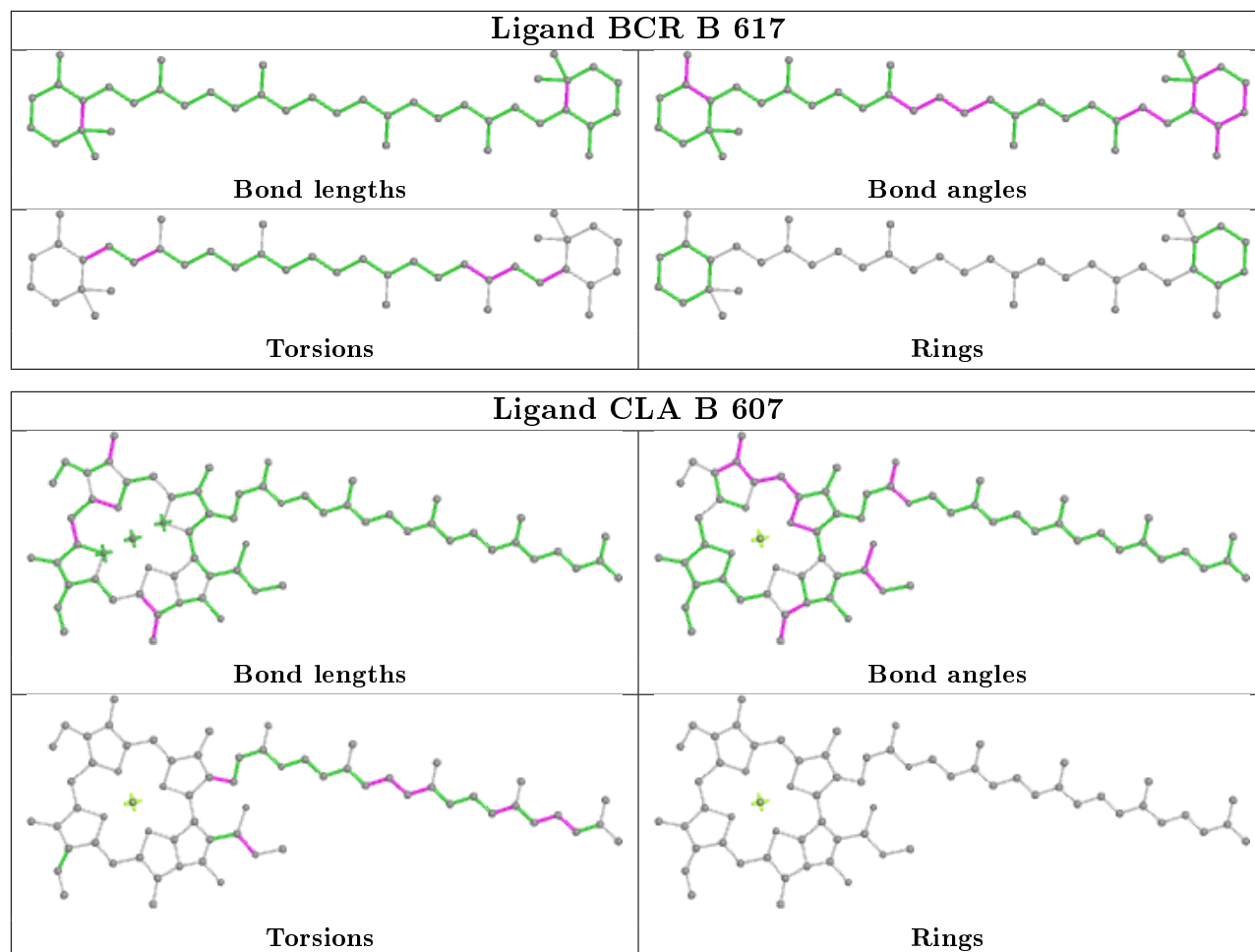


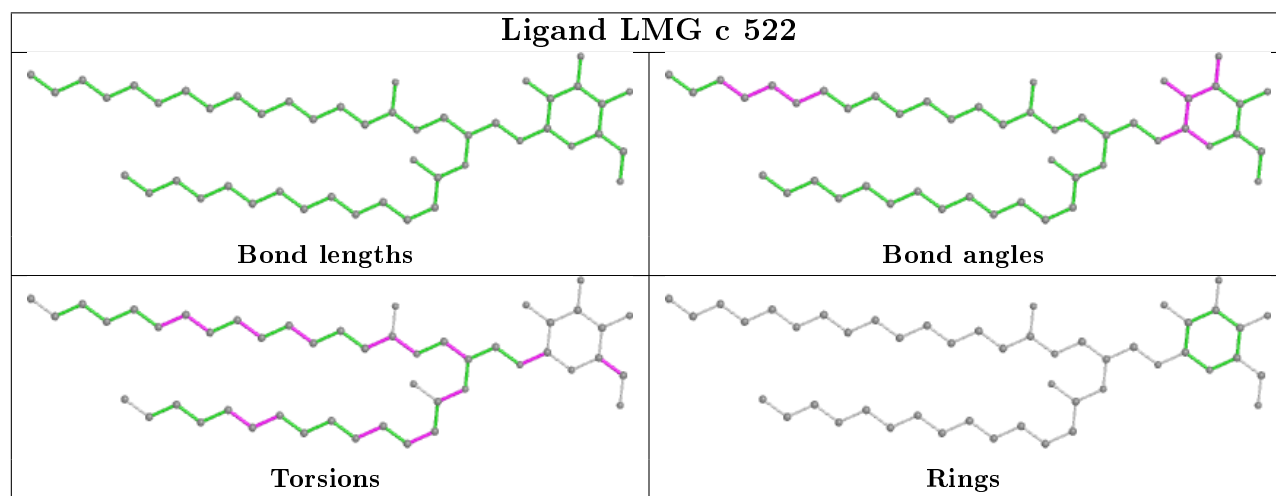
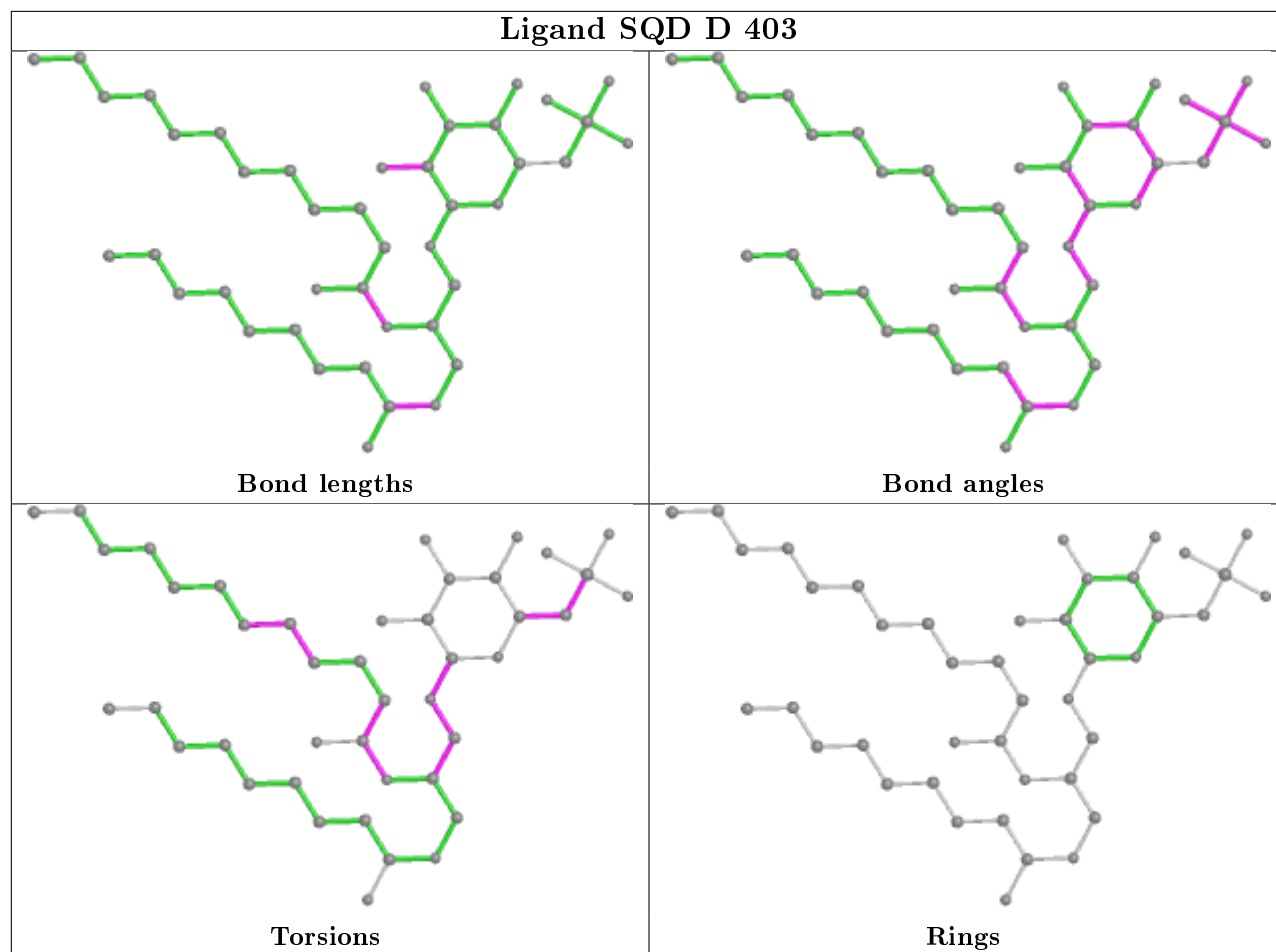


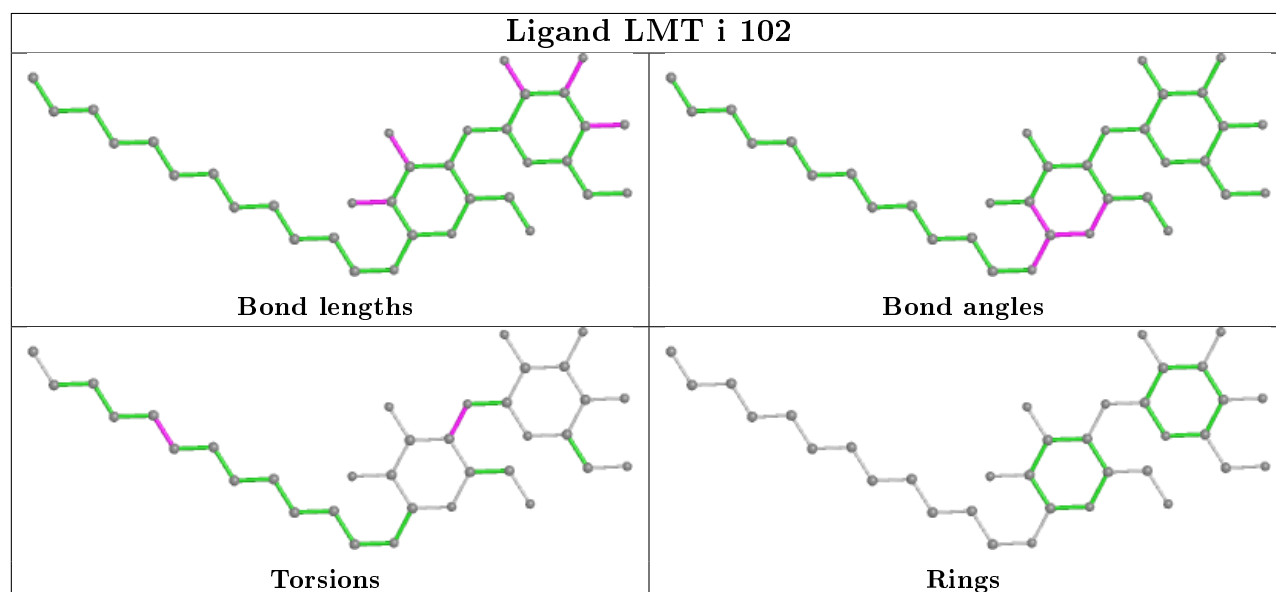
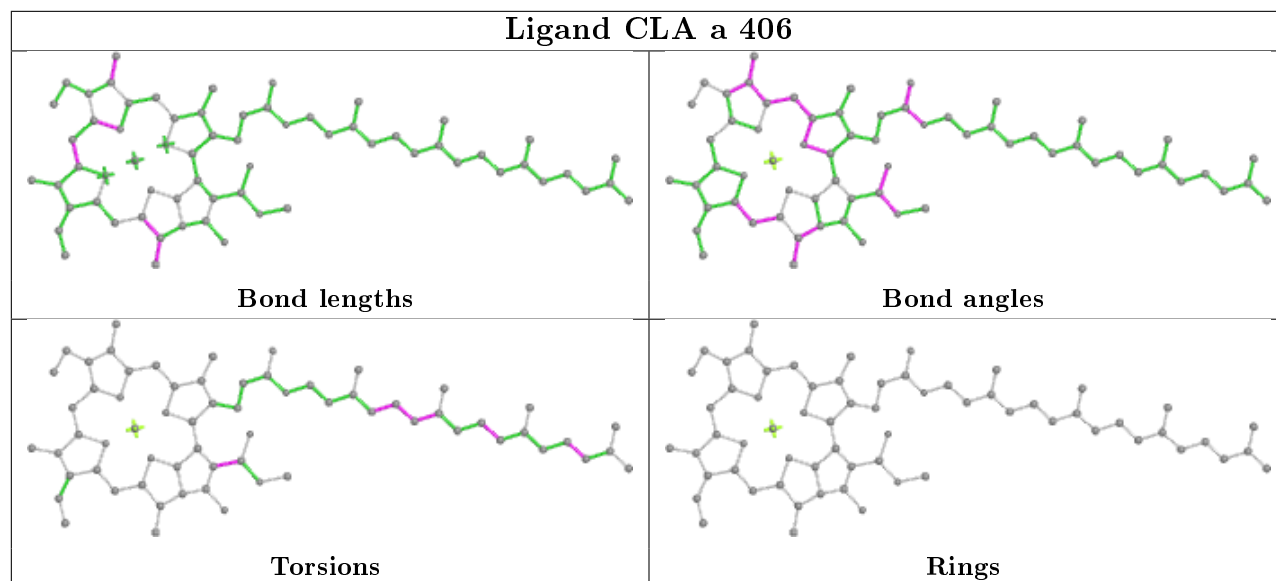
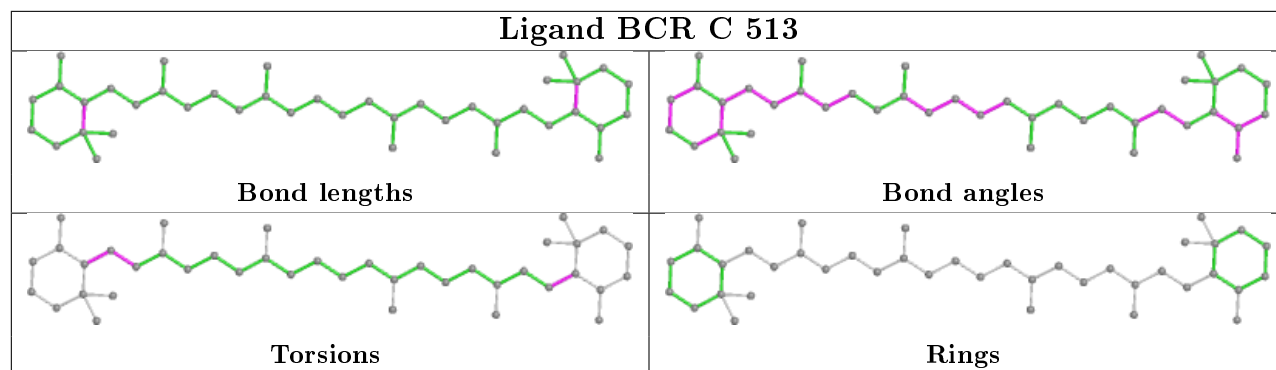


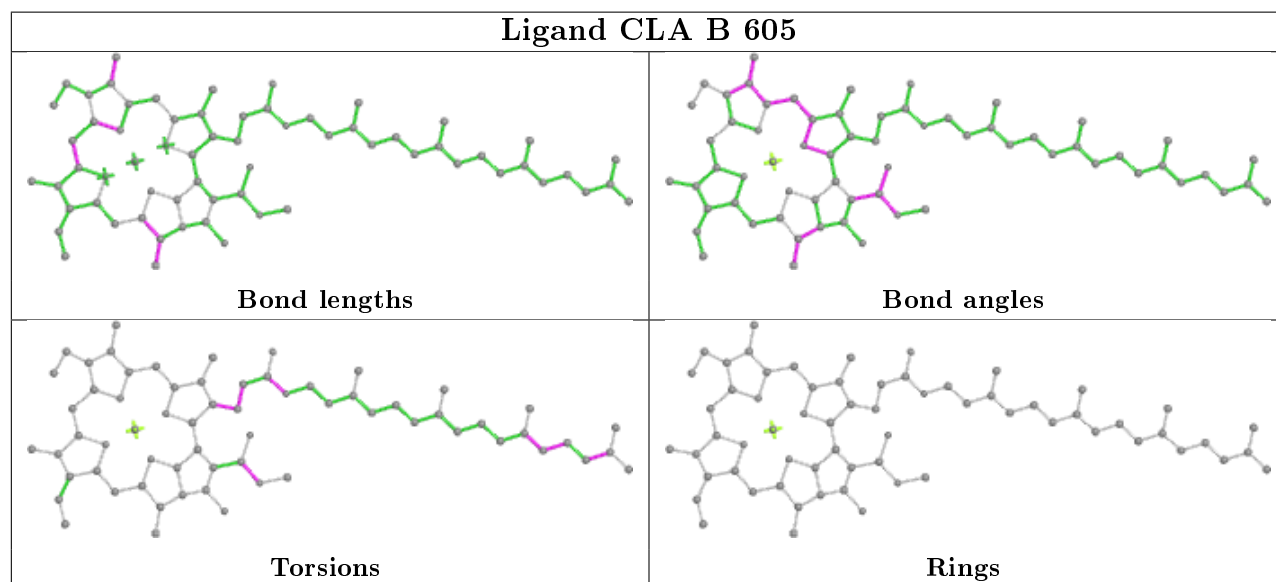
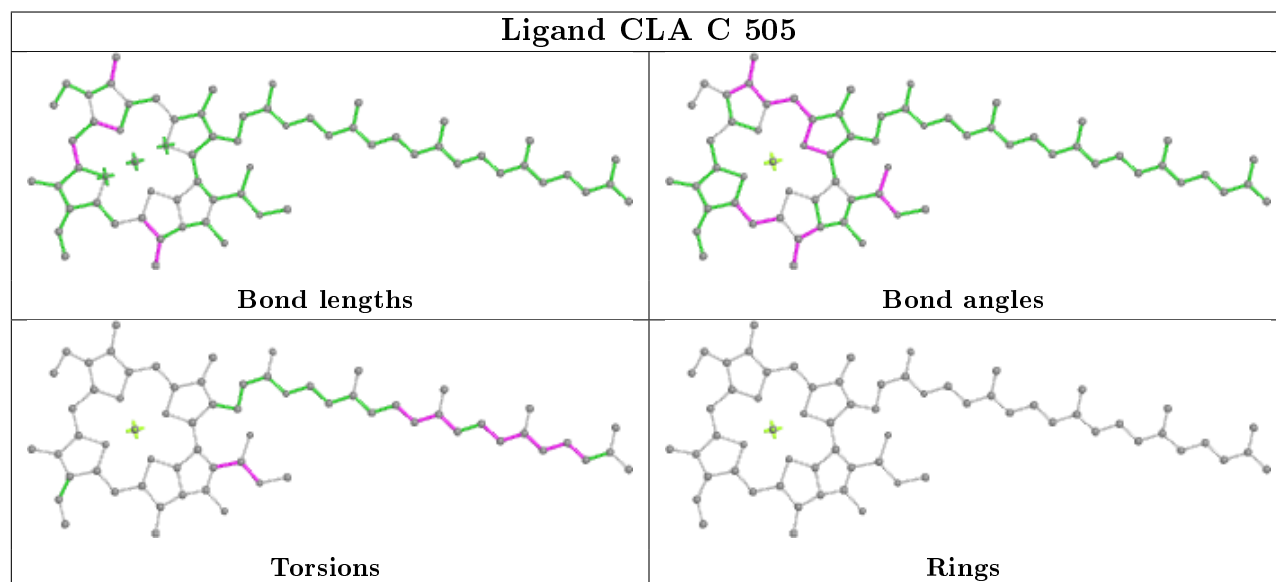
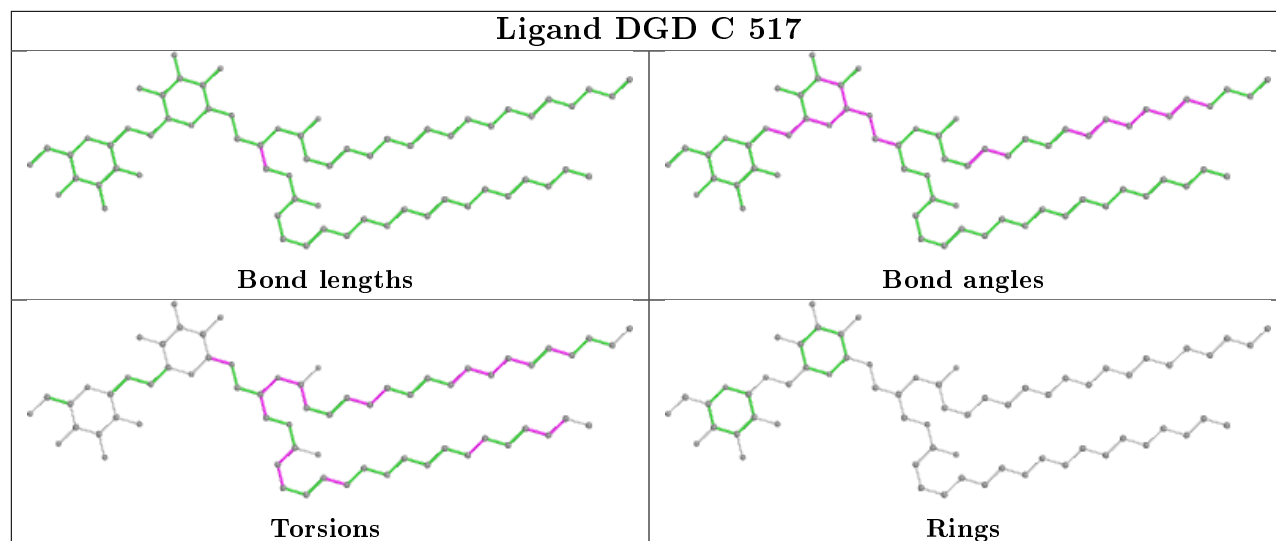


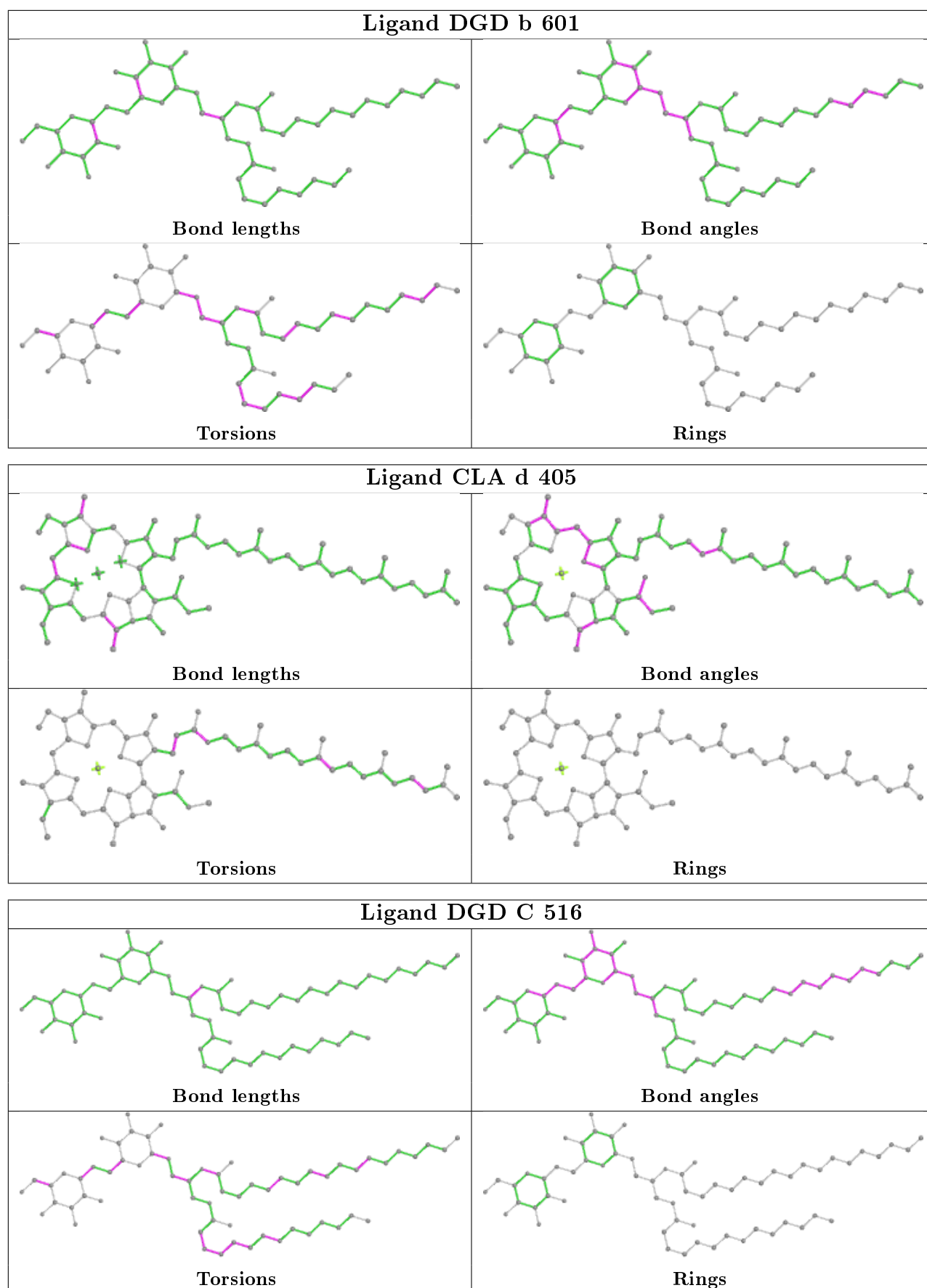
Ligand CLA a 408**Ligand CLA b 615****Ligand BCR b 623**

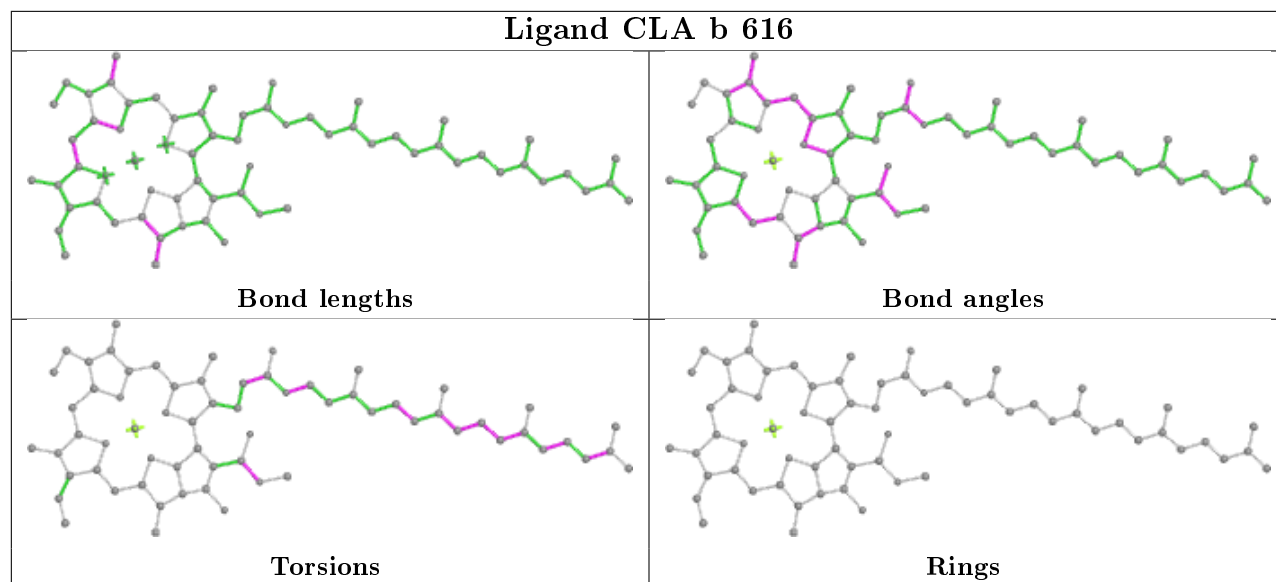
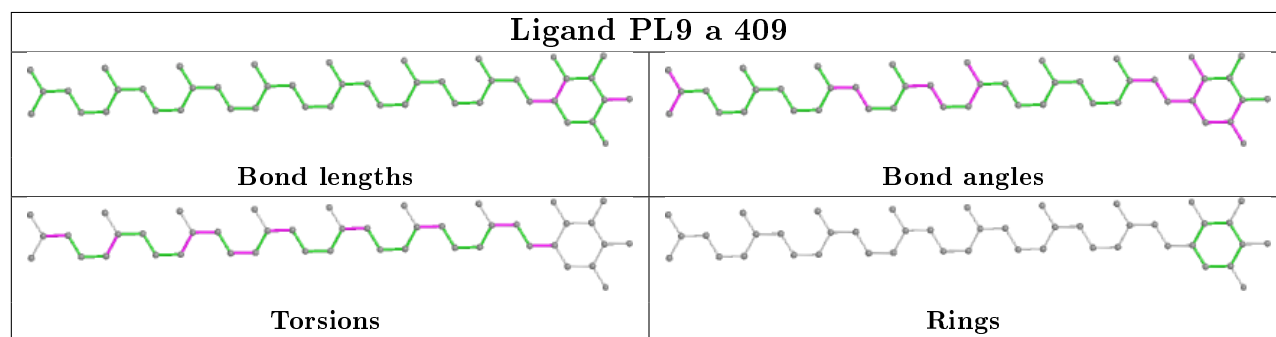
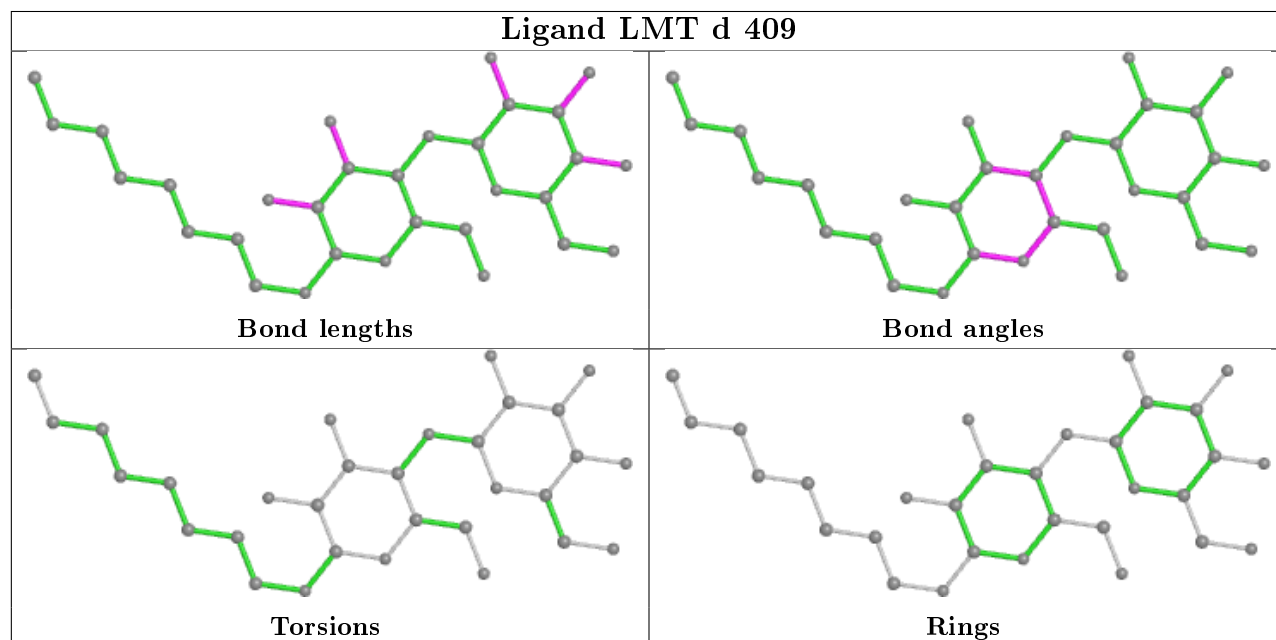


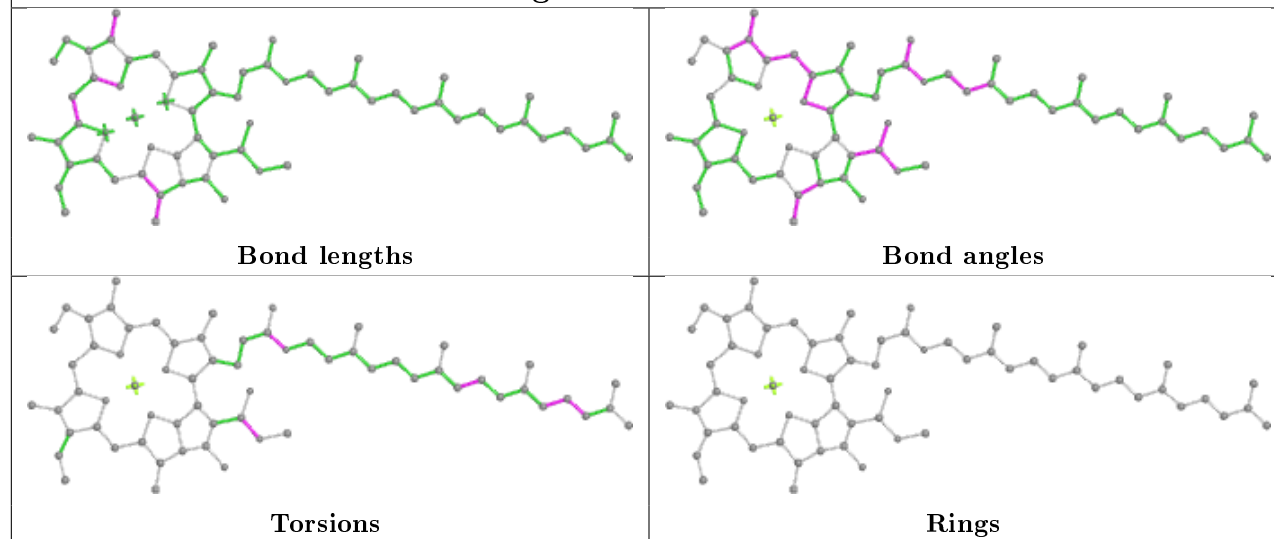
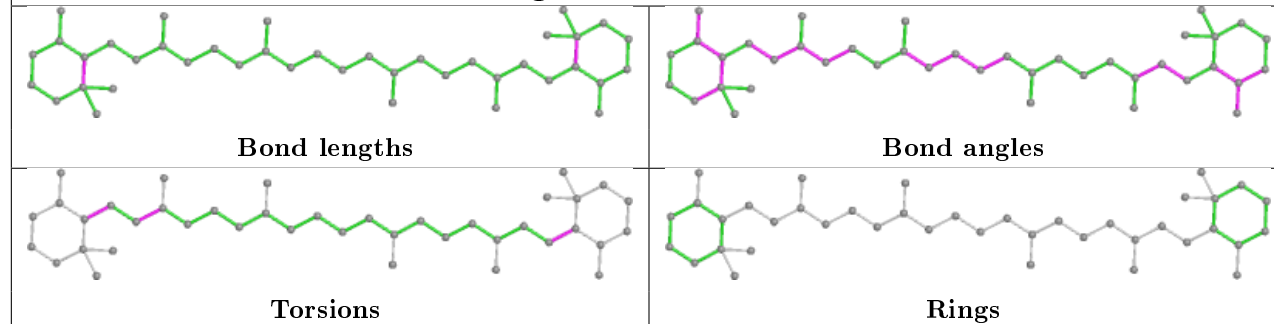
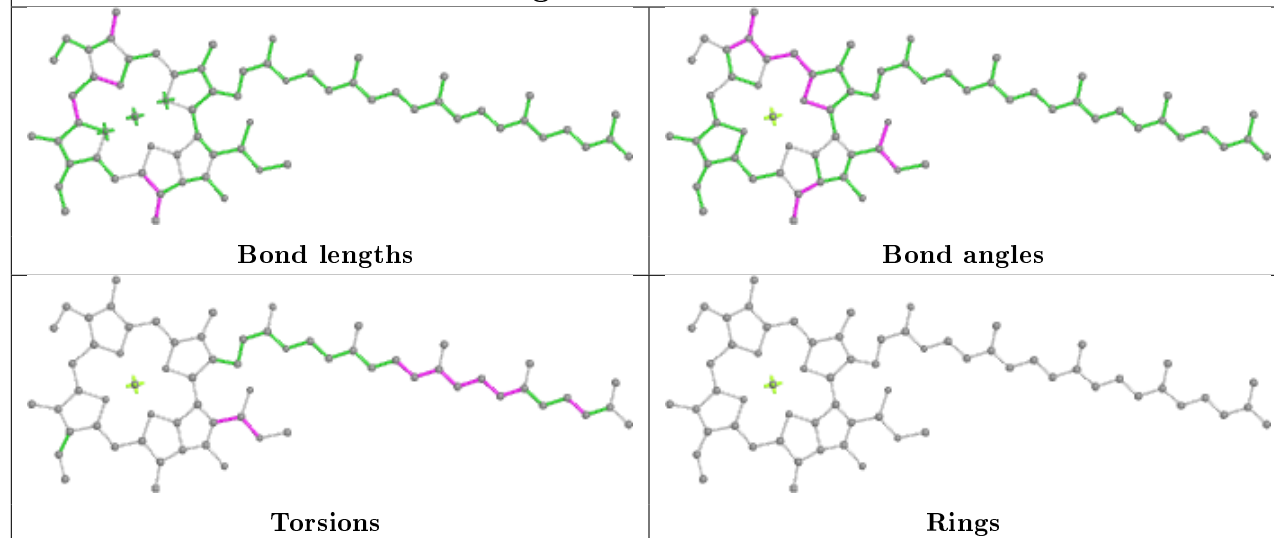


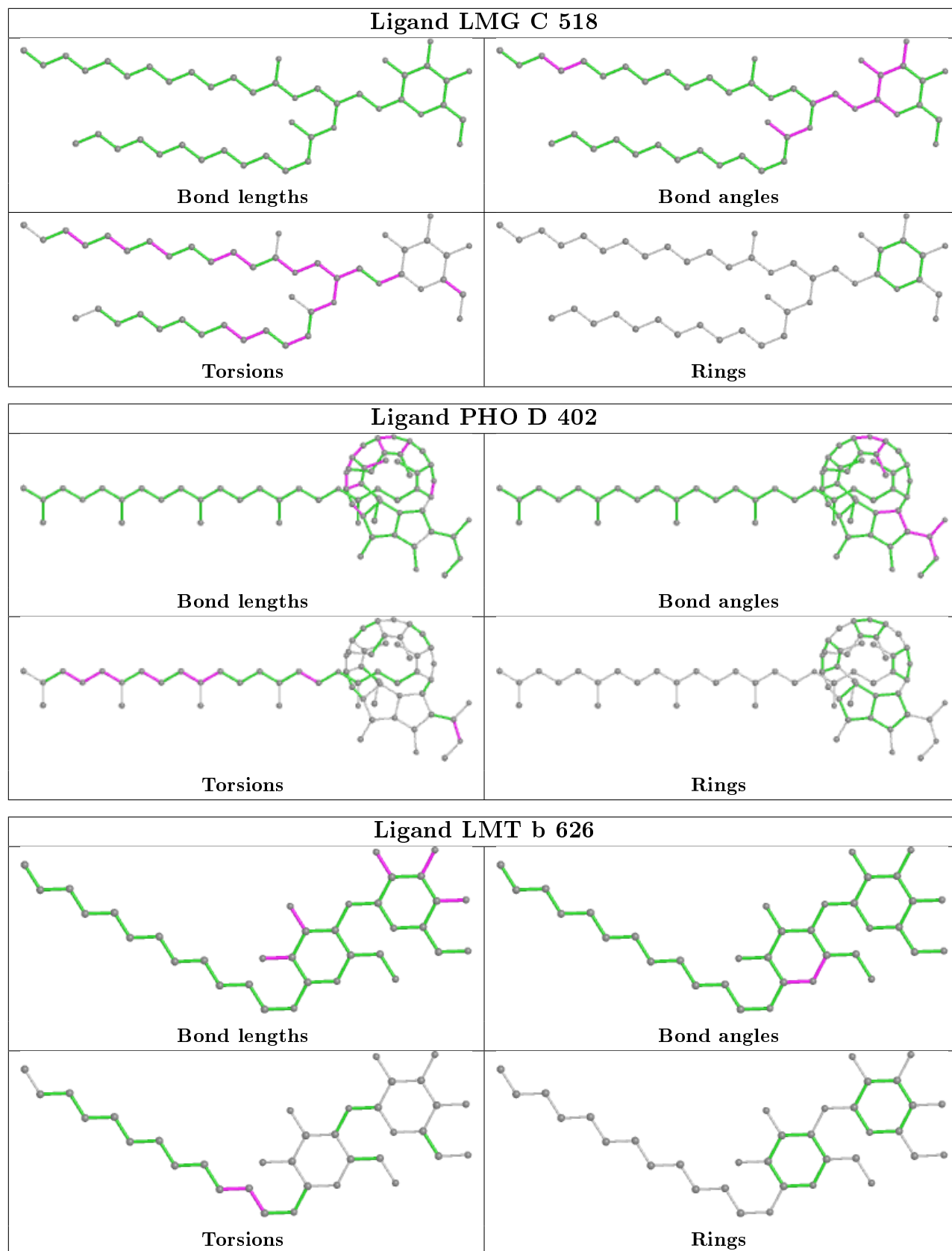


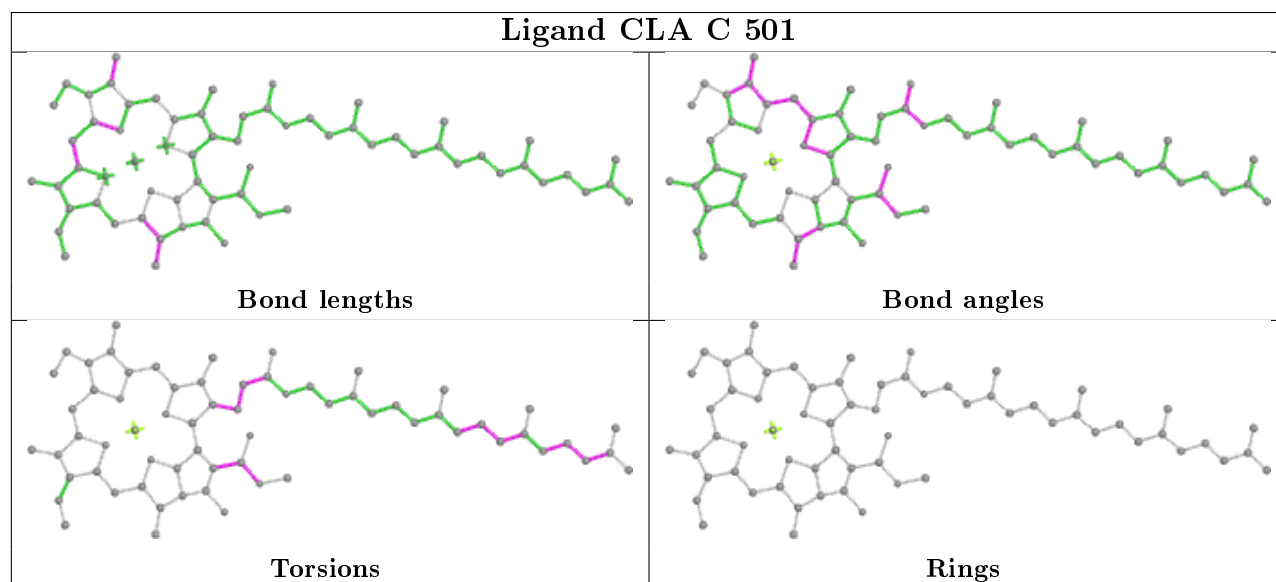
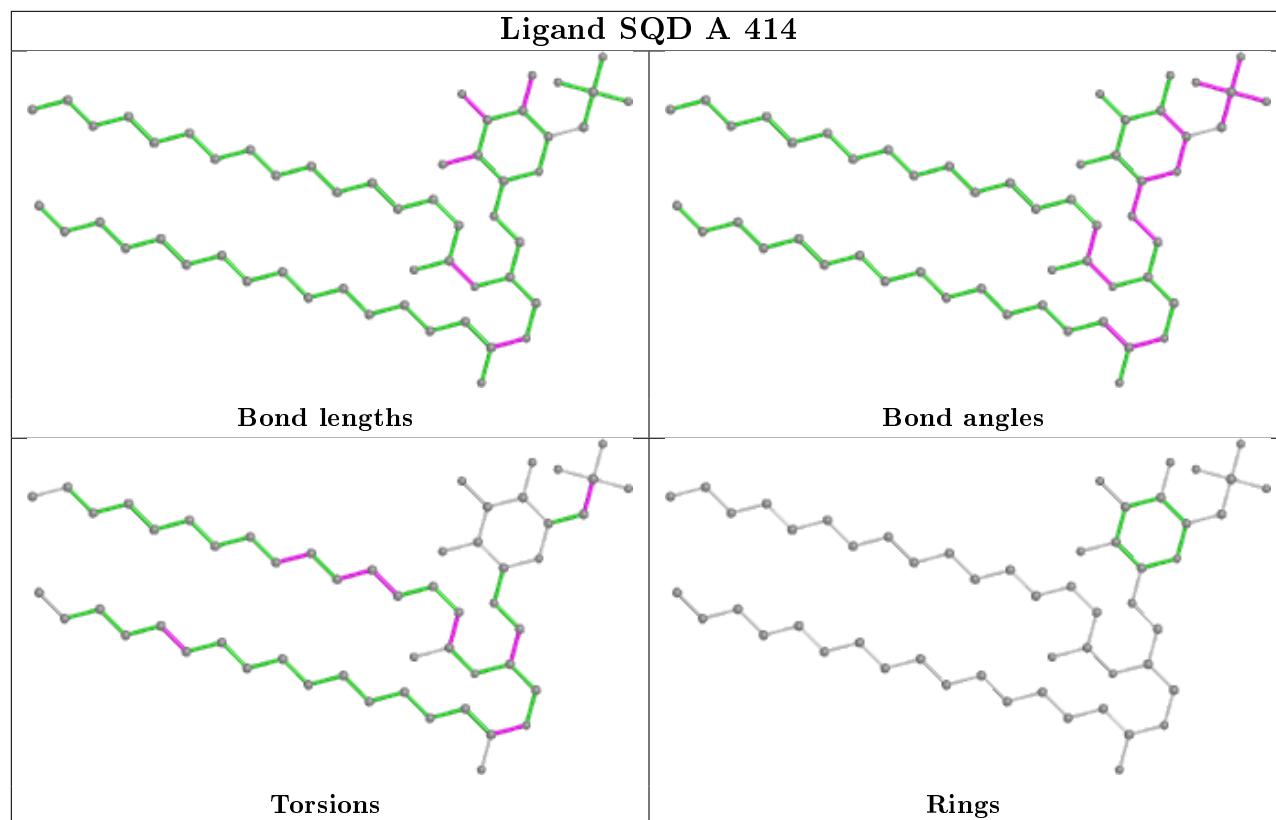


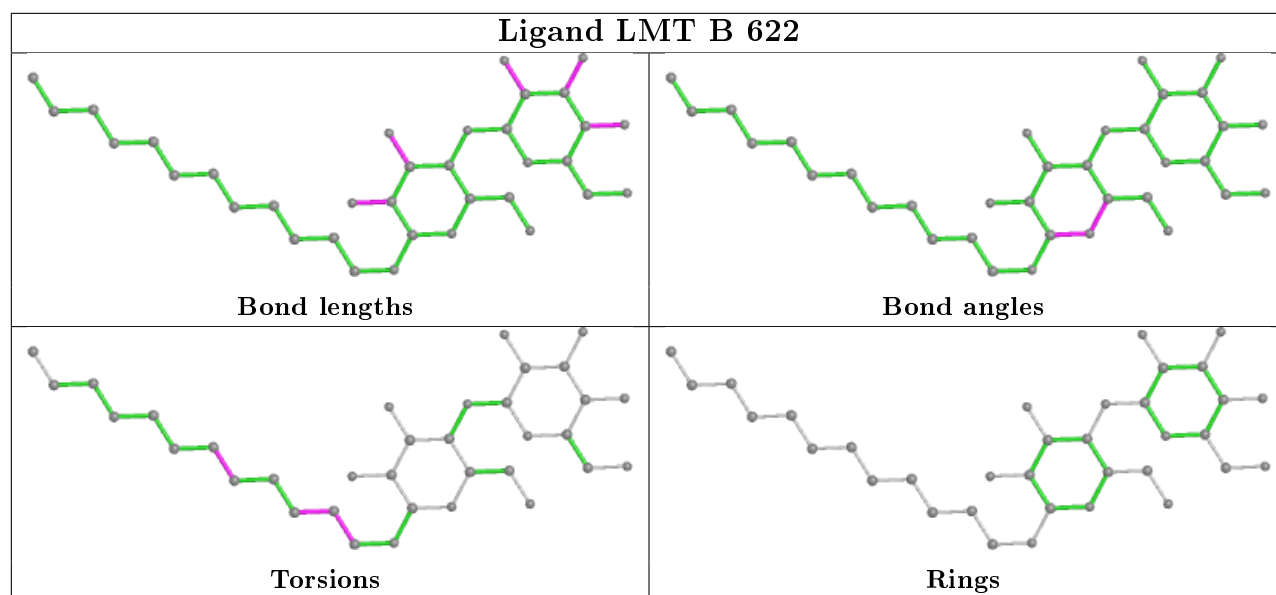
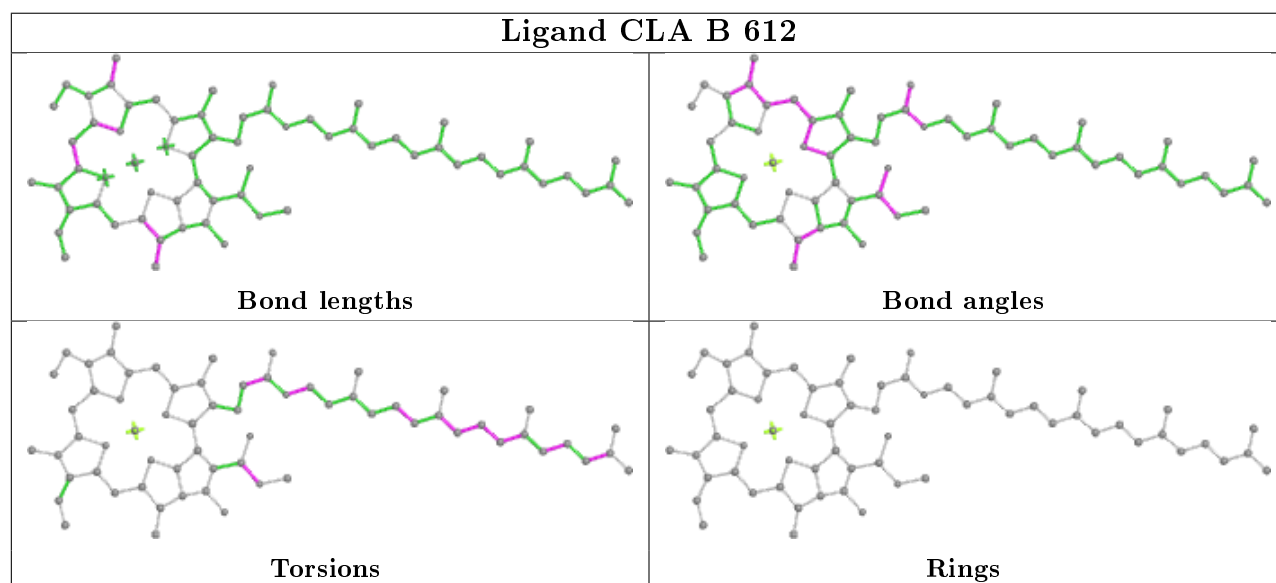
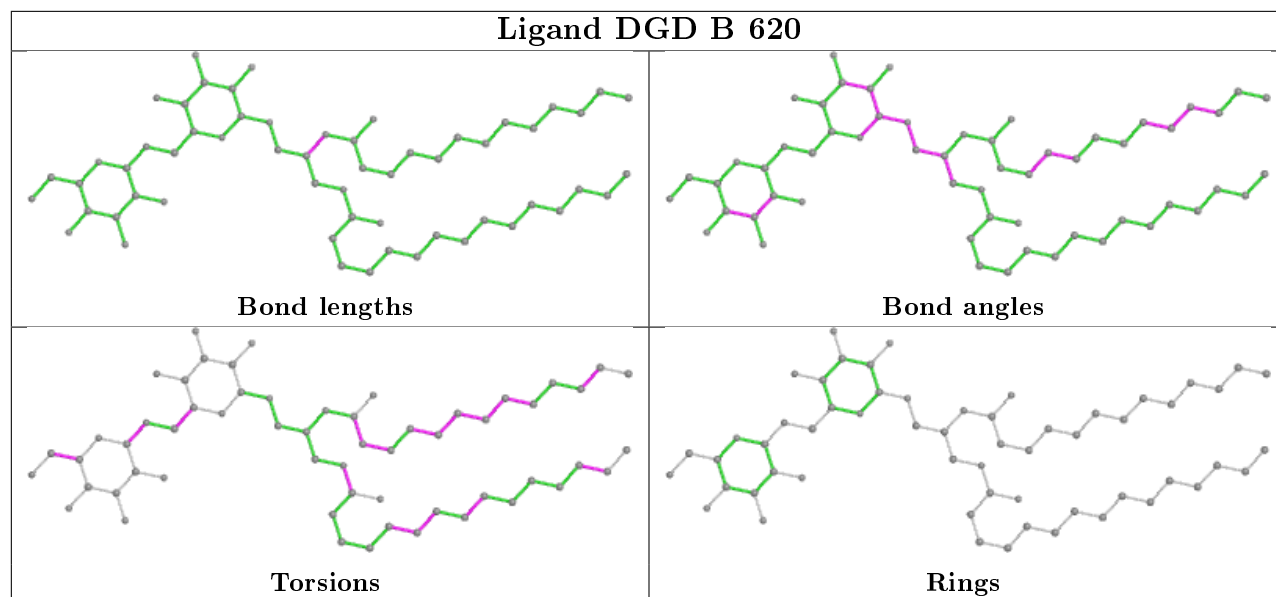


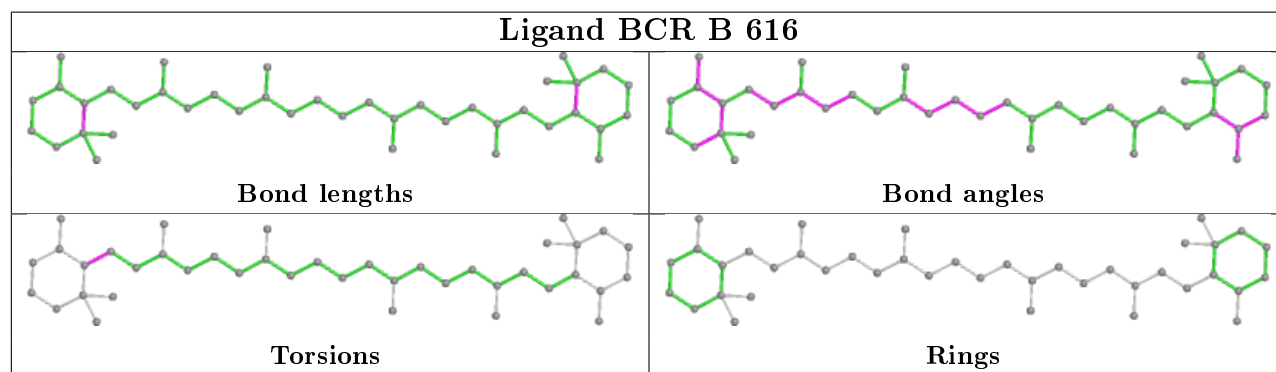
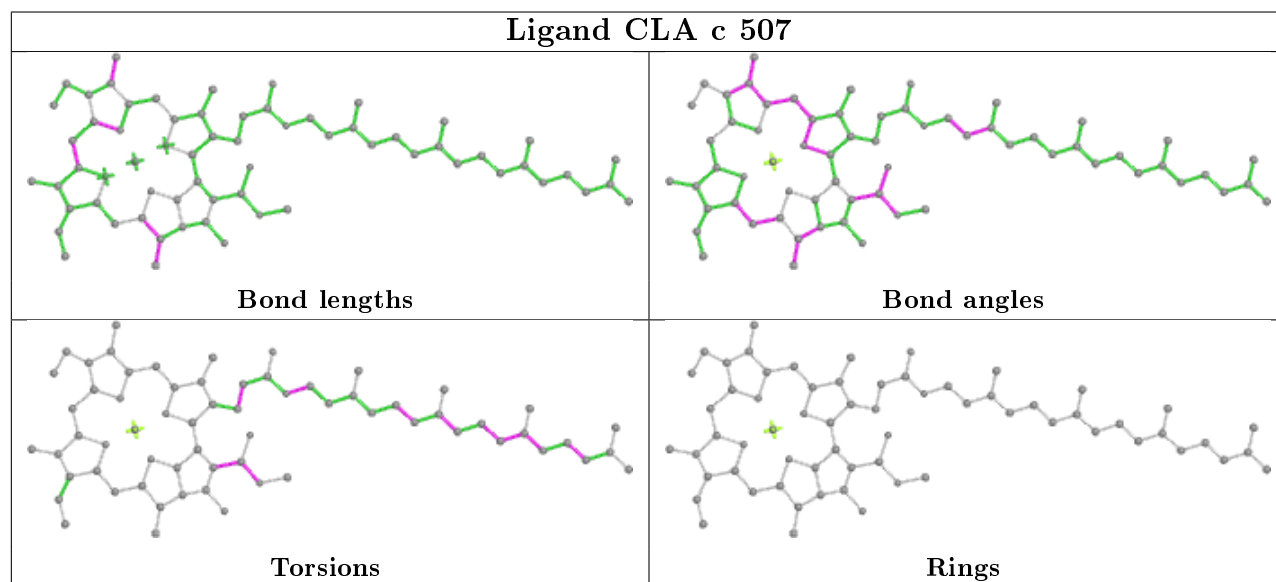
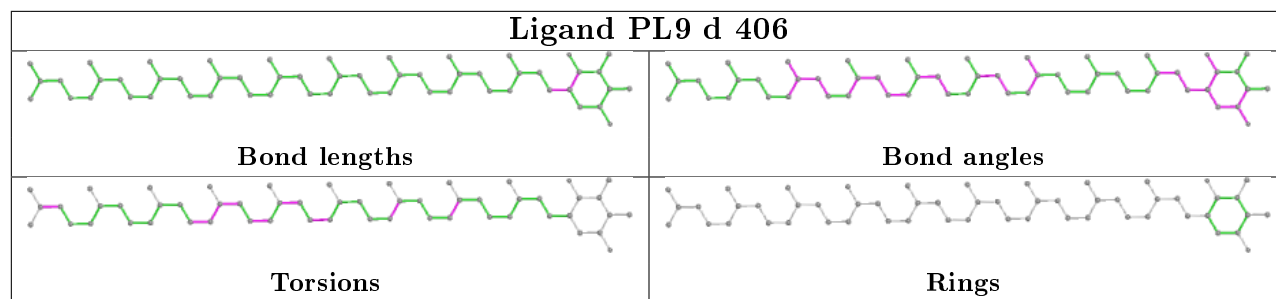
Ligand CLA b 616**Ligand PL9 a 409****Ligand LMT d 409**

Ligand CLA B 603**Ligand BCR C 521****Ligand CLA C 503**

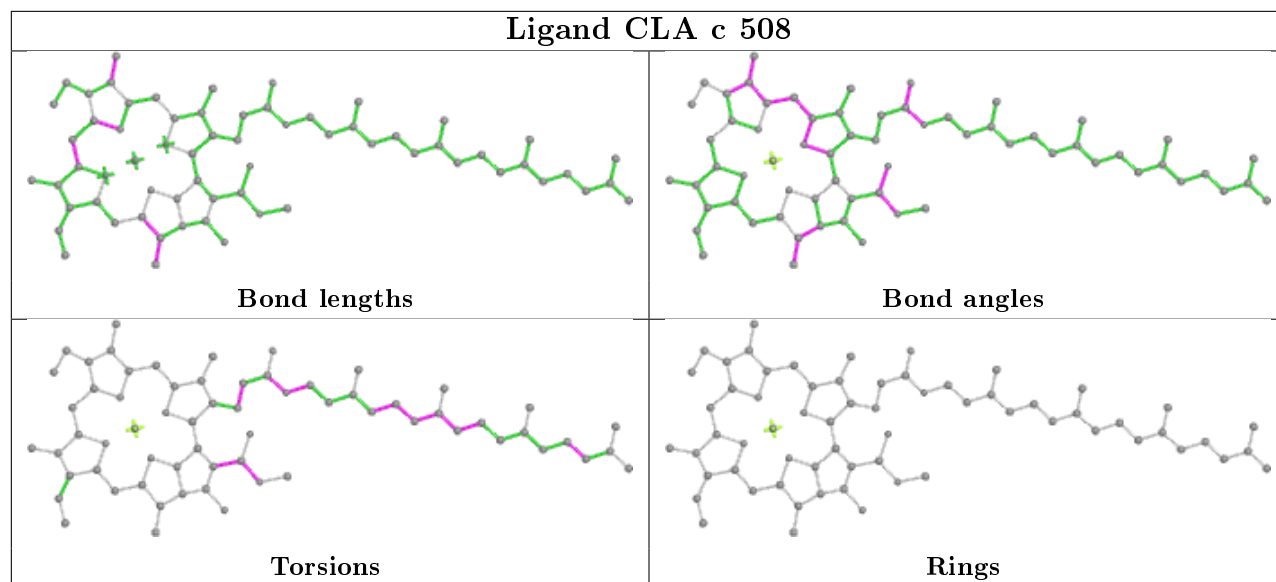




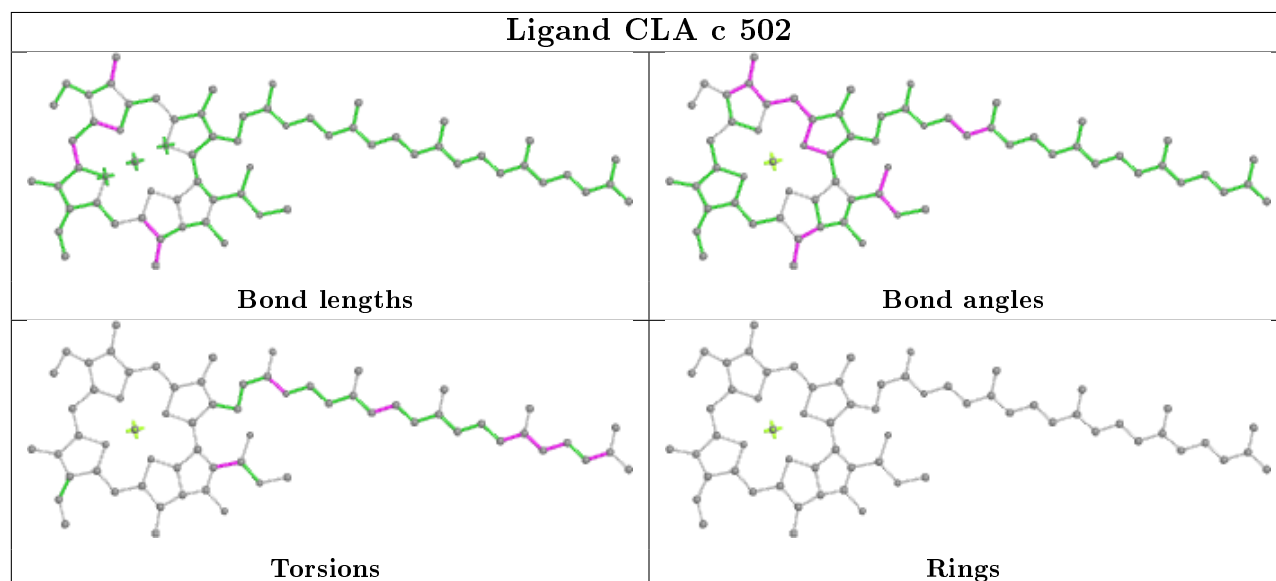




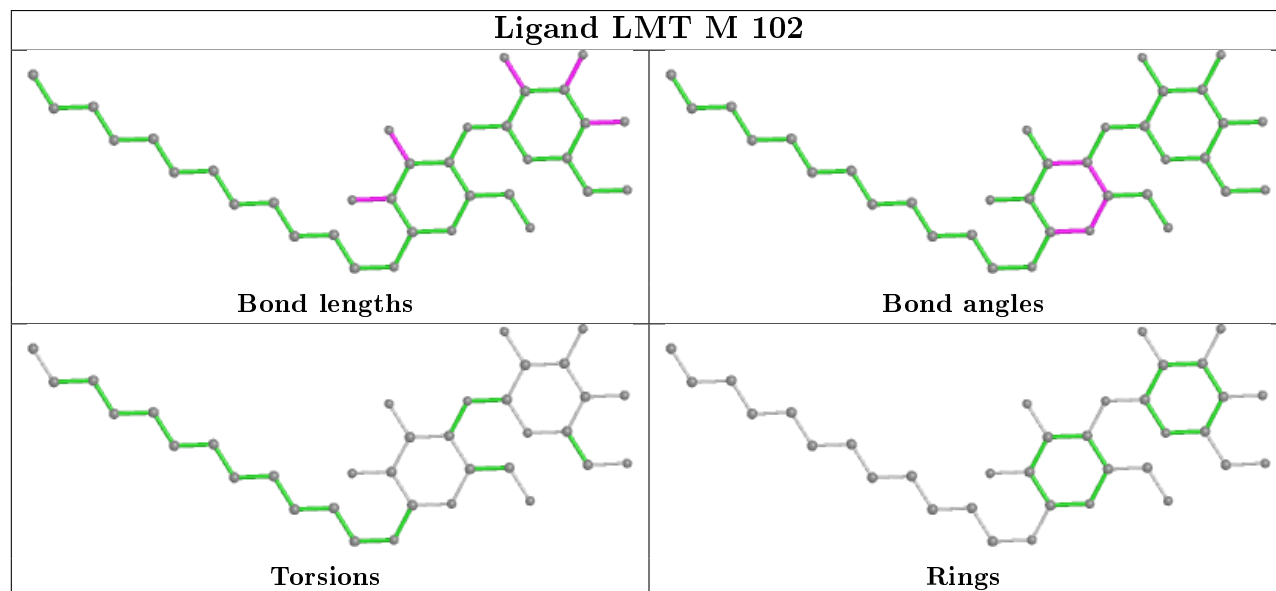
Ligand CLA c 508

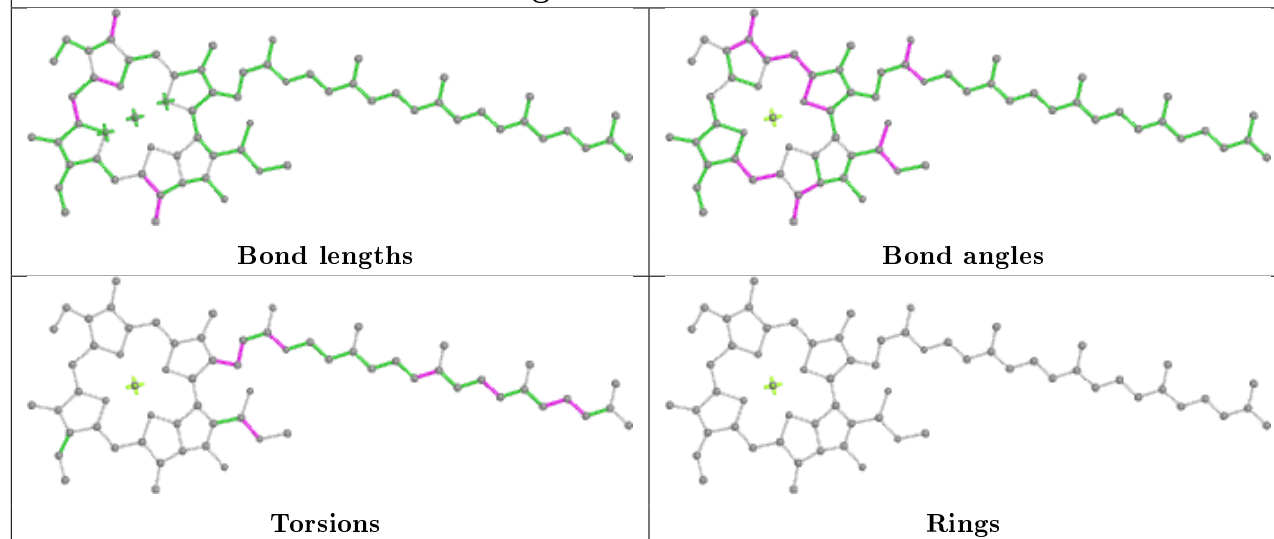
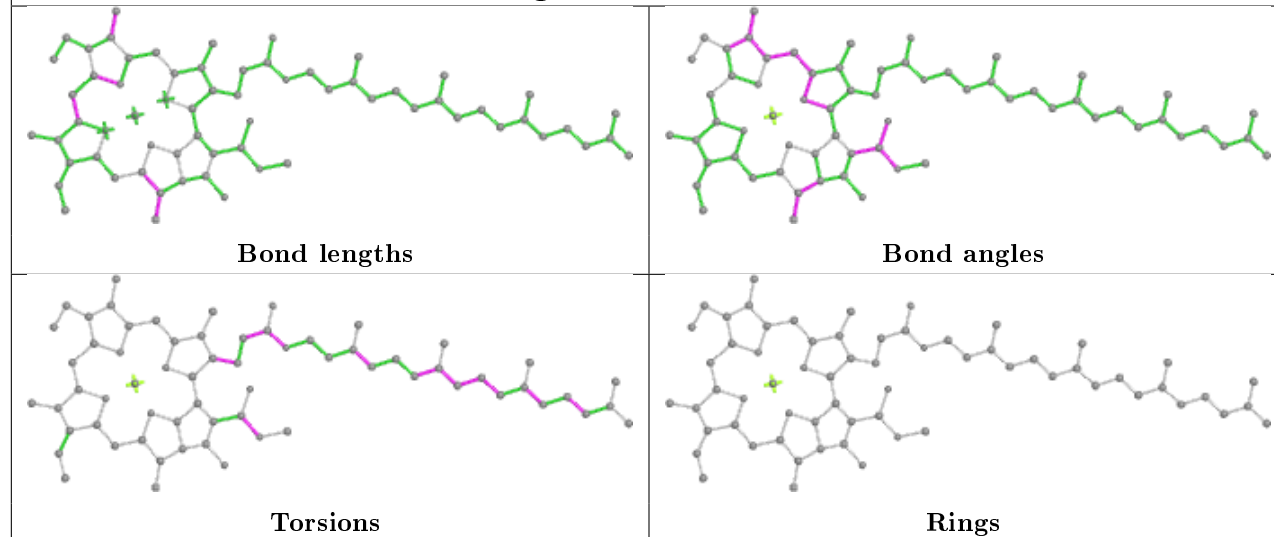


Ligand CLA c 502

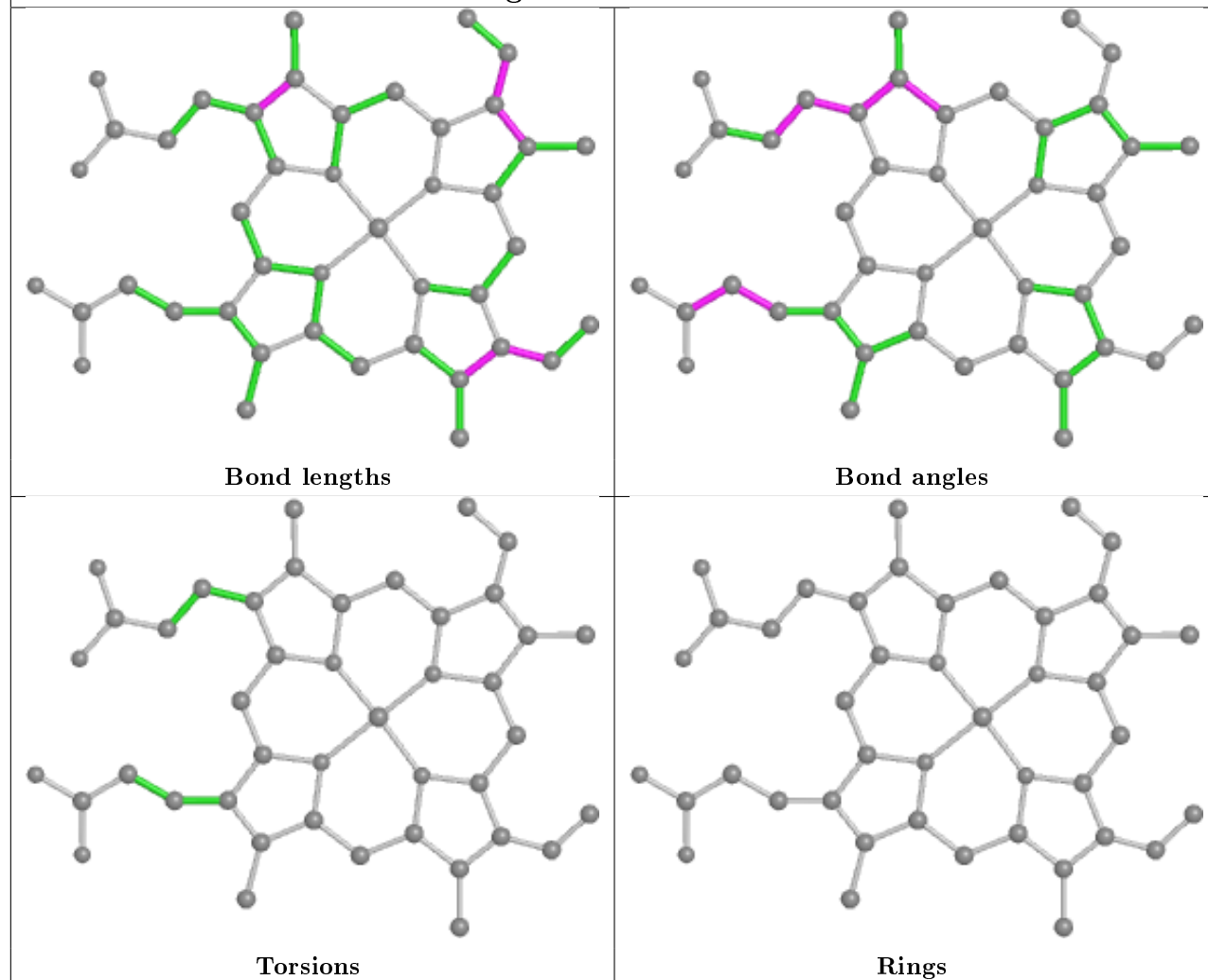


Ligand LMT M 102

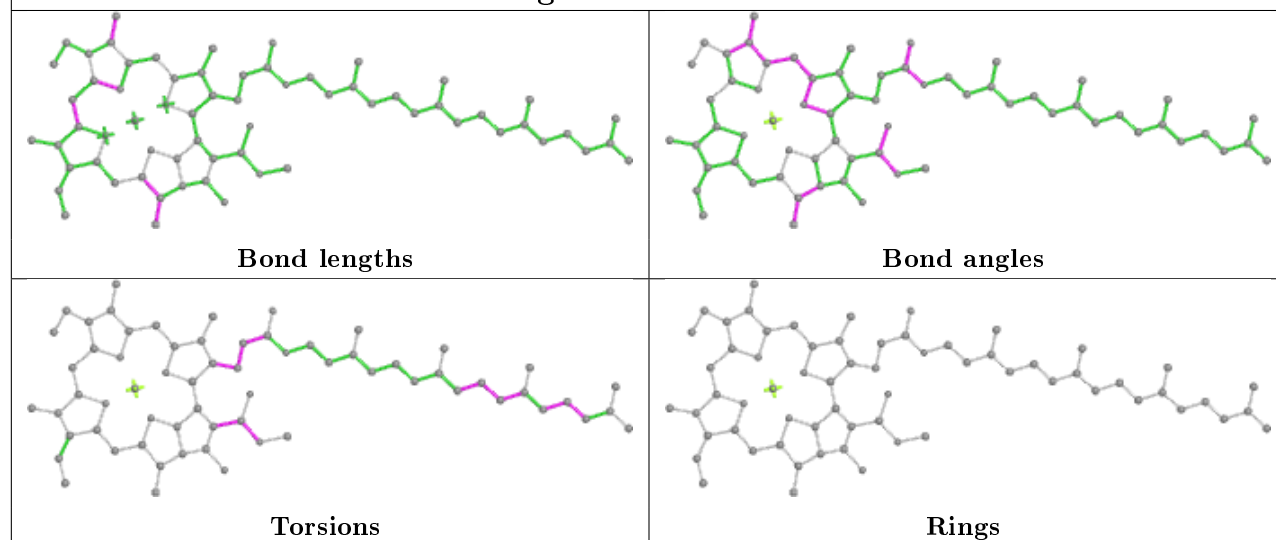


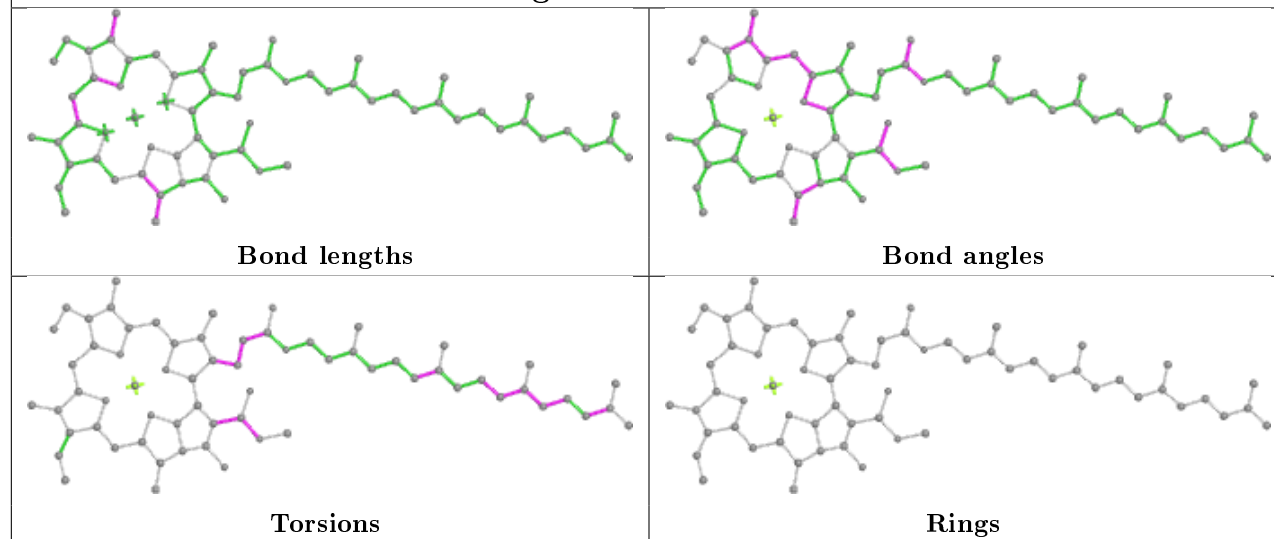
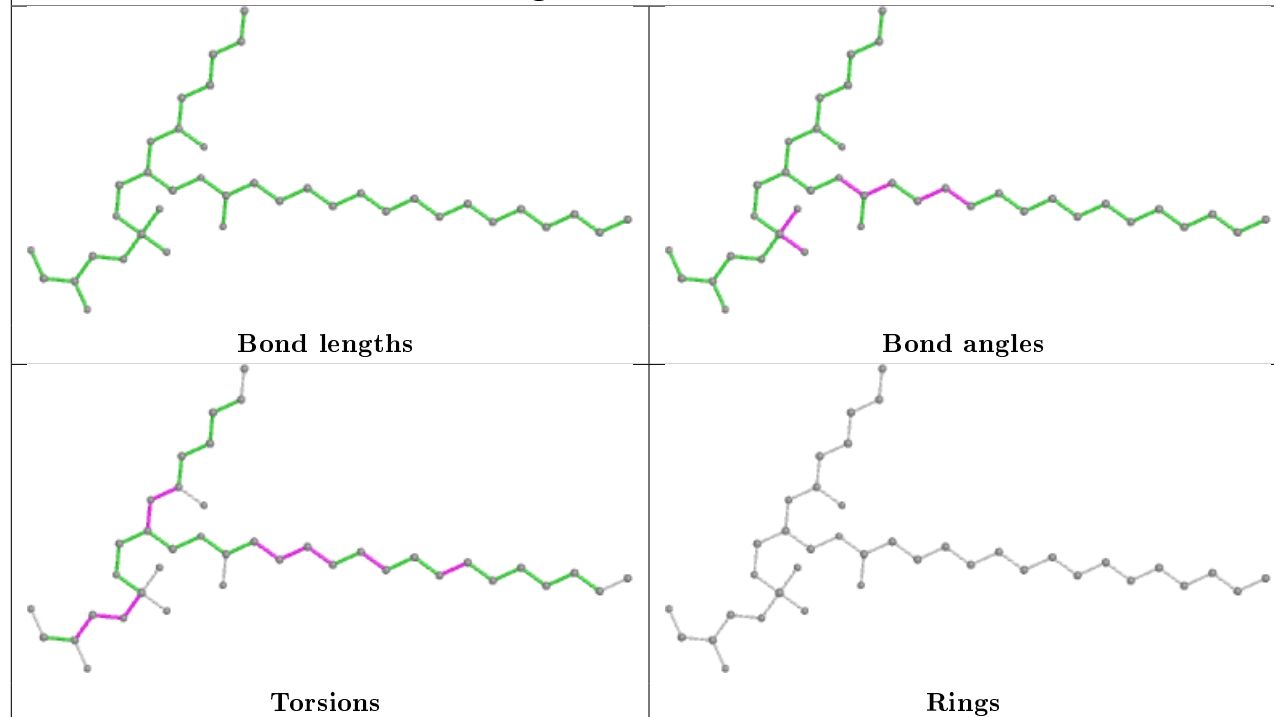
Ligand CLA C 520**Ligand CLA C 504**

Ligand HEM f 101

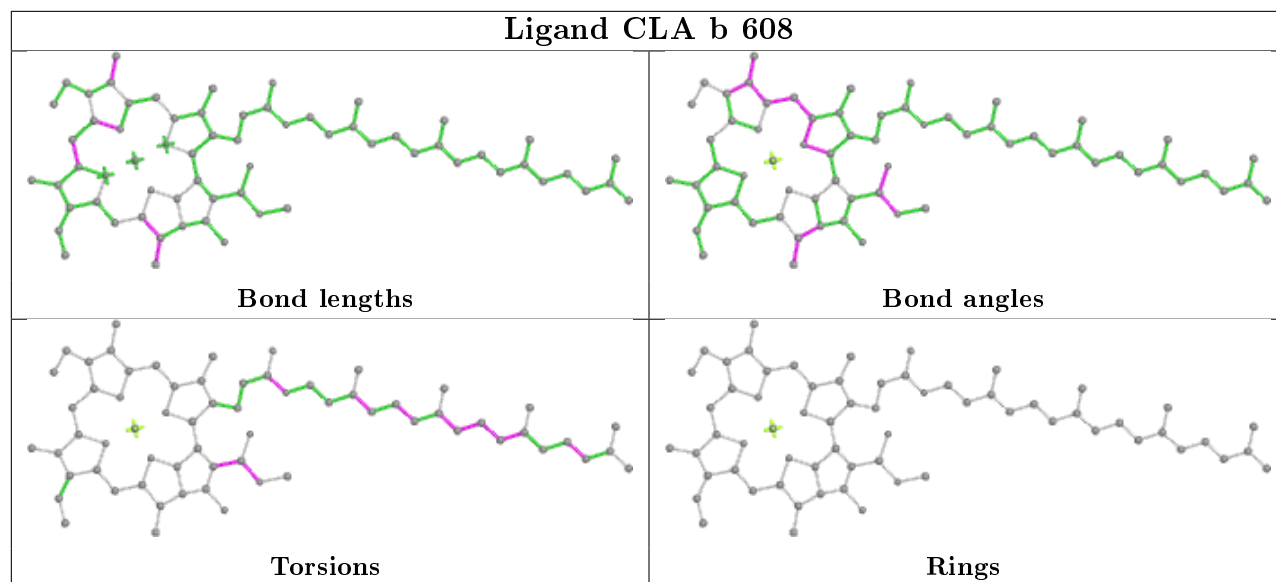


Ligand CLA c 501

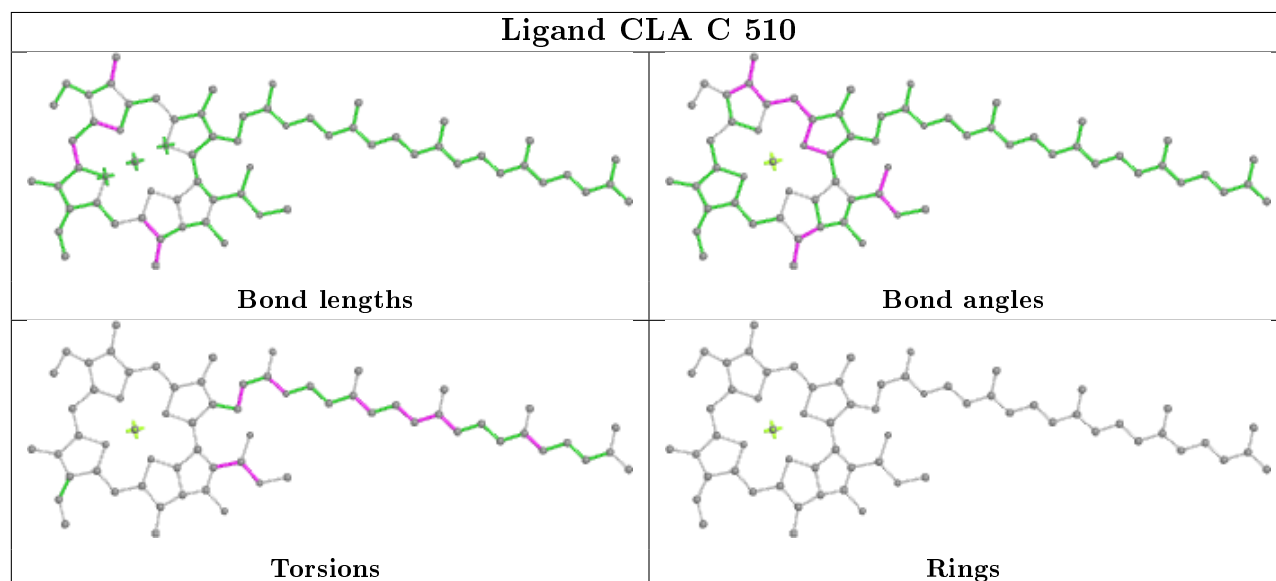


Ligand CLA B 601**Ligand LHG A 409**

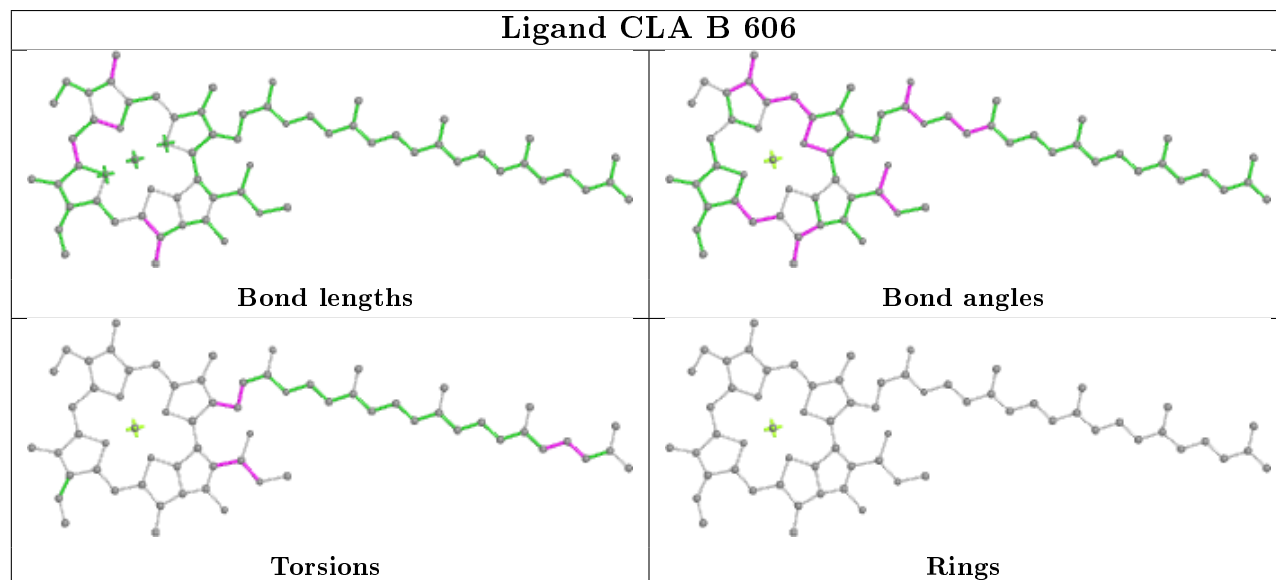
Ligand CLA b 608

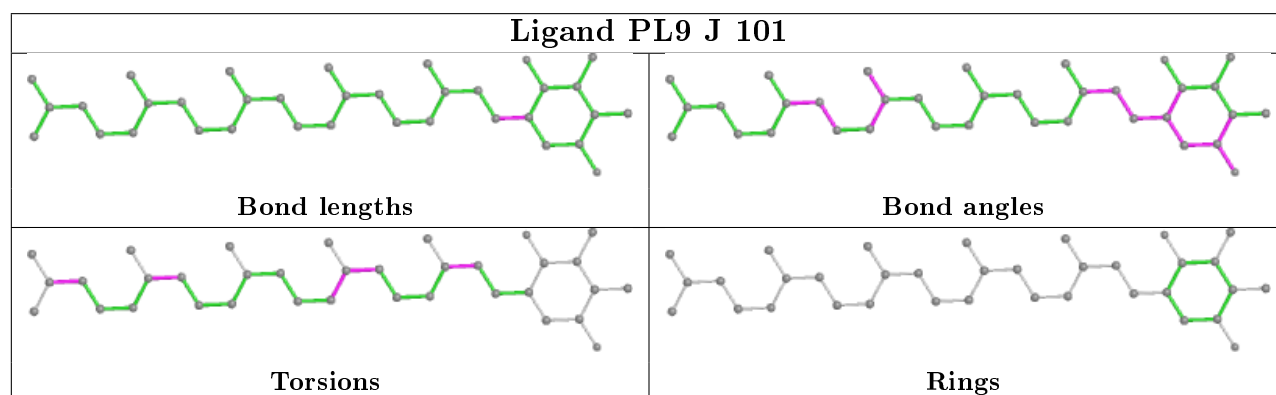
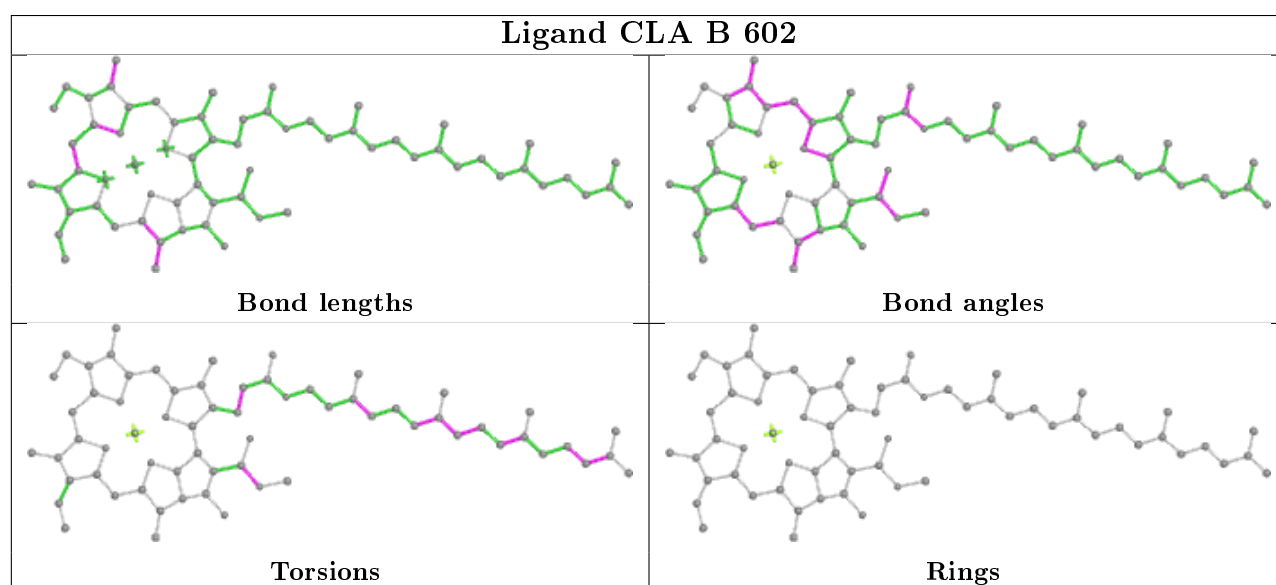
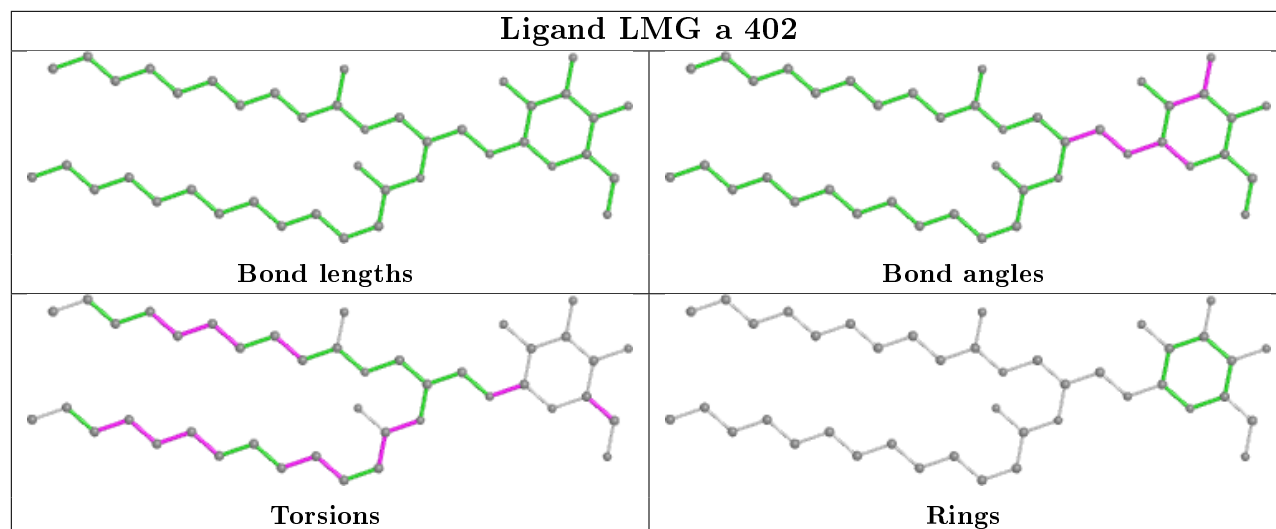


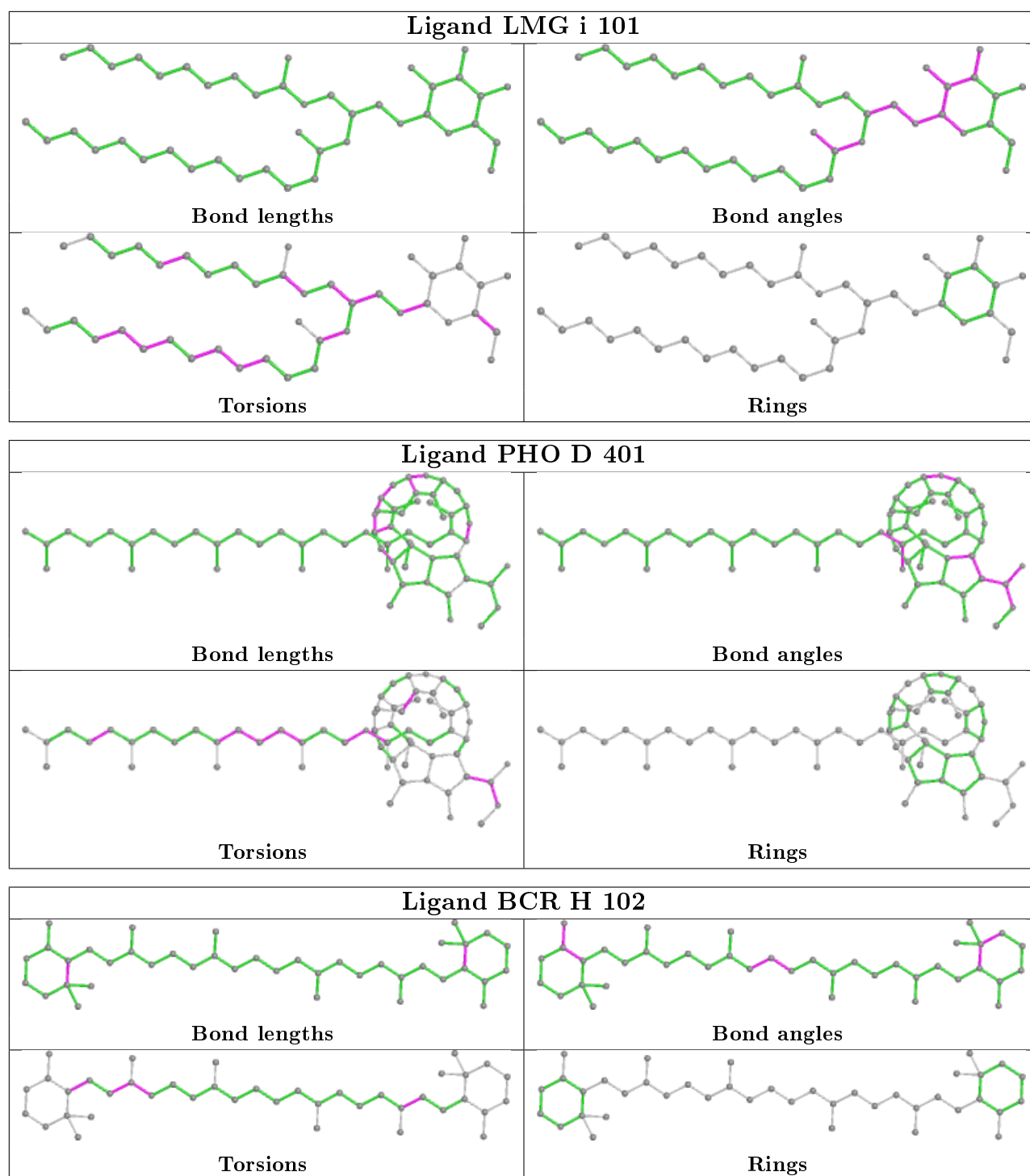
Ligand CLA C 510

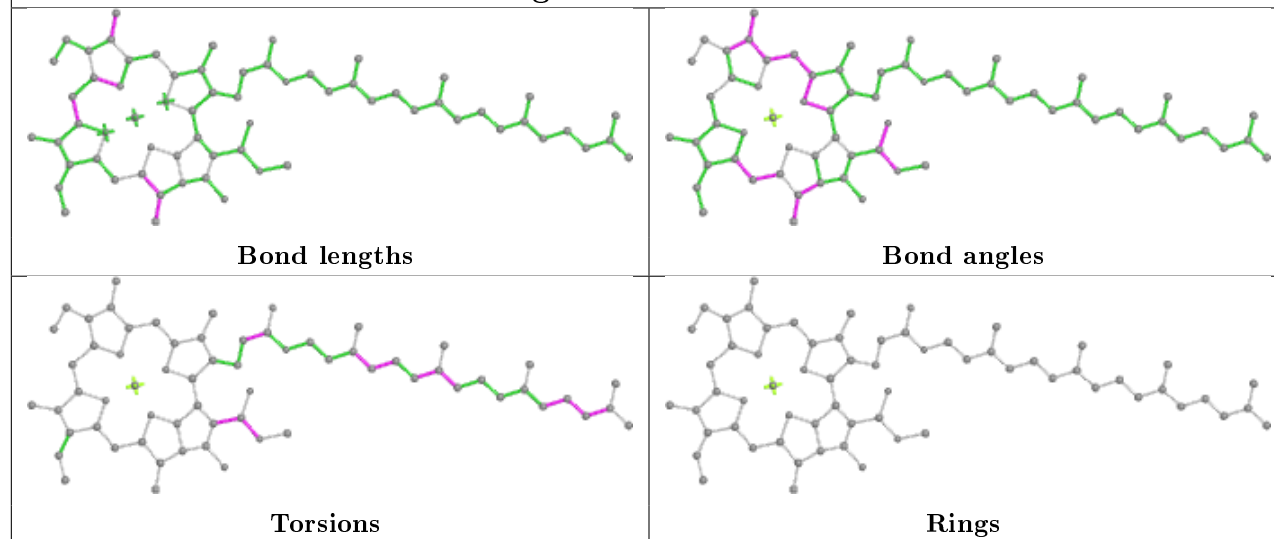
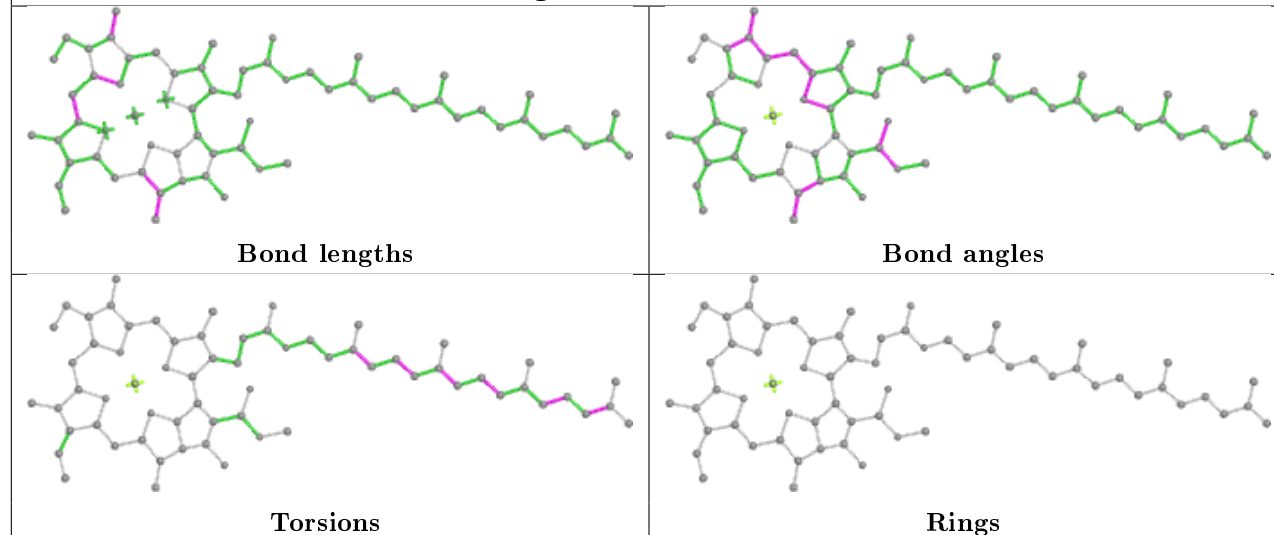
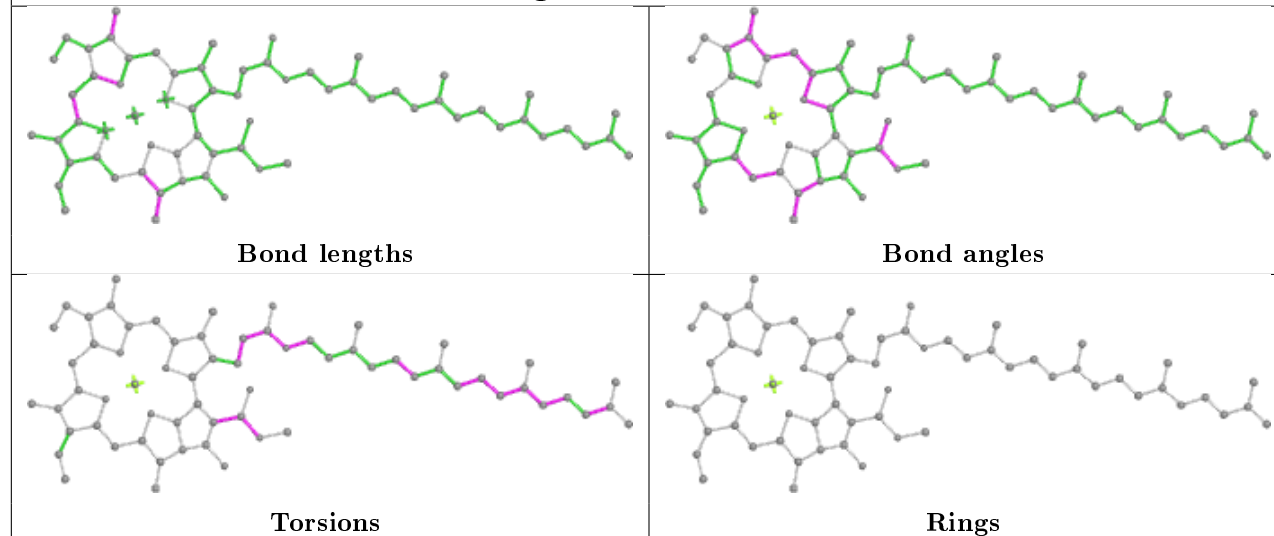


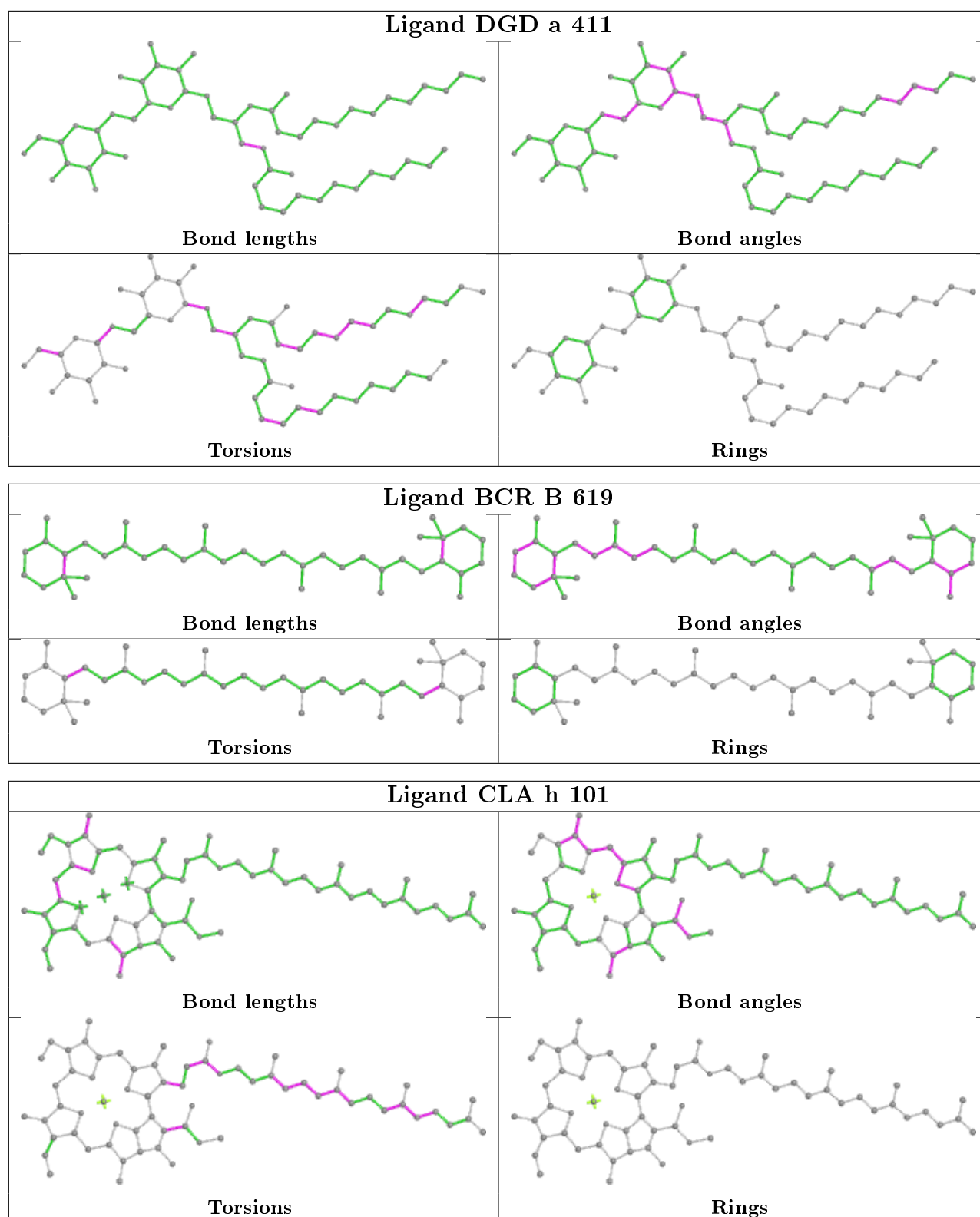
Ligand CLA B 606

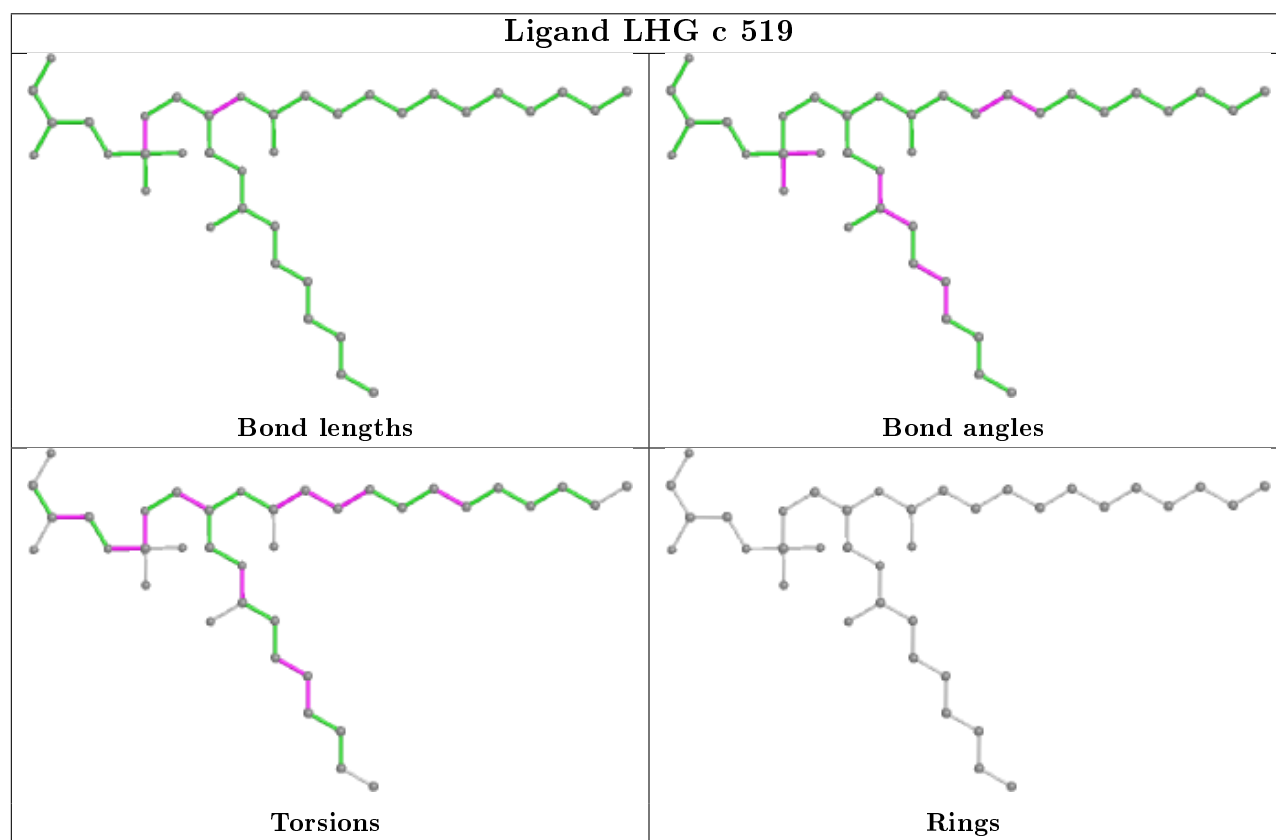
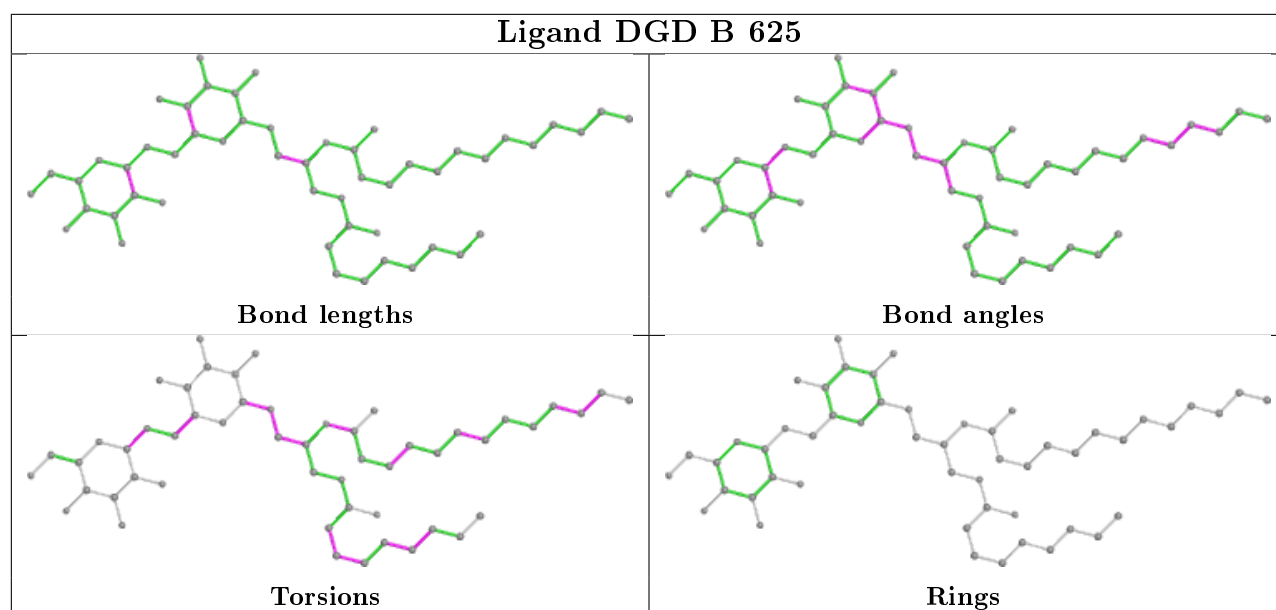


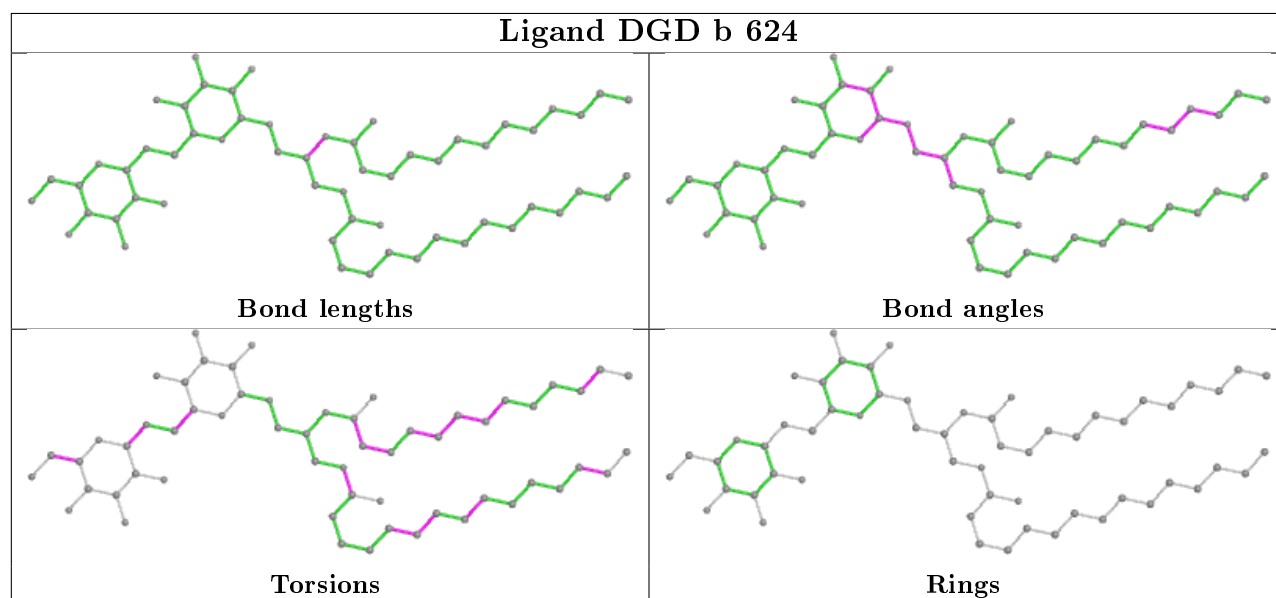
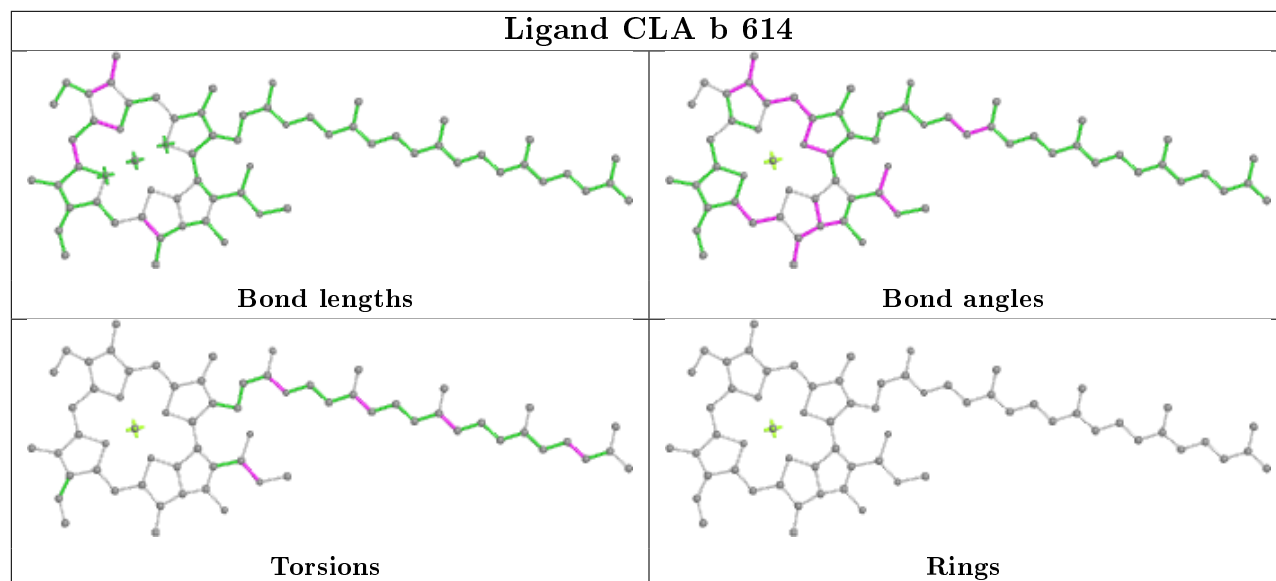
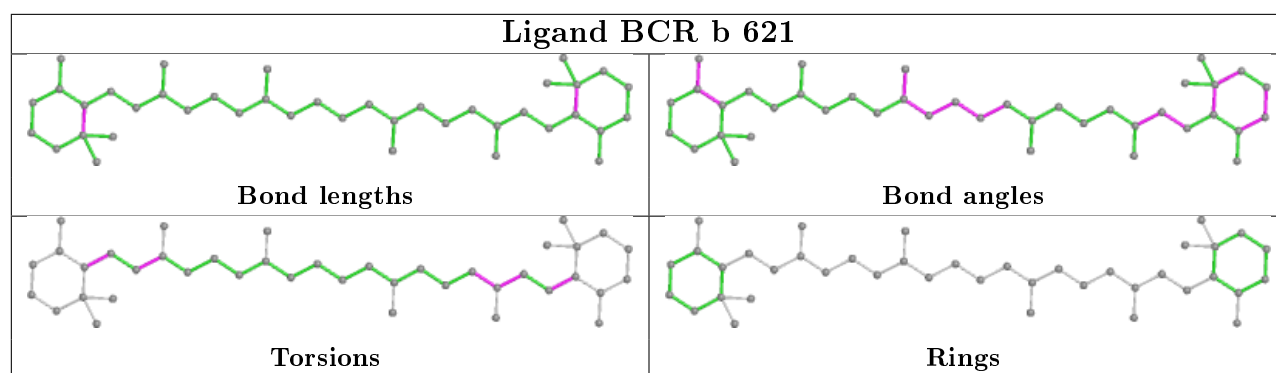


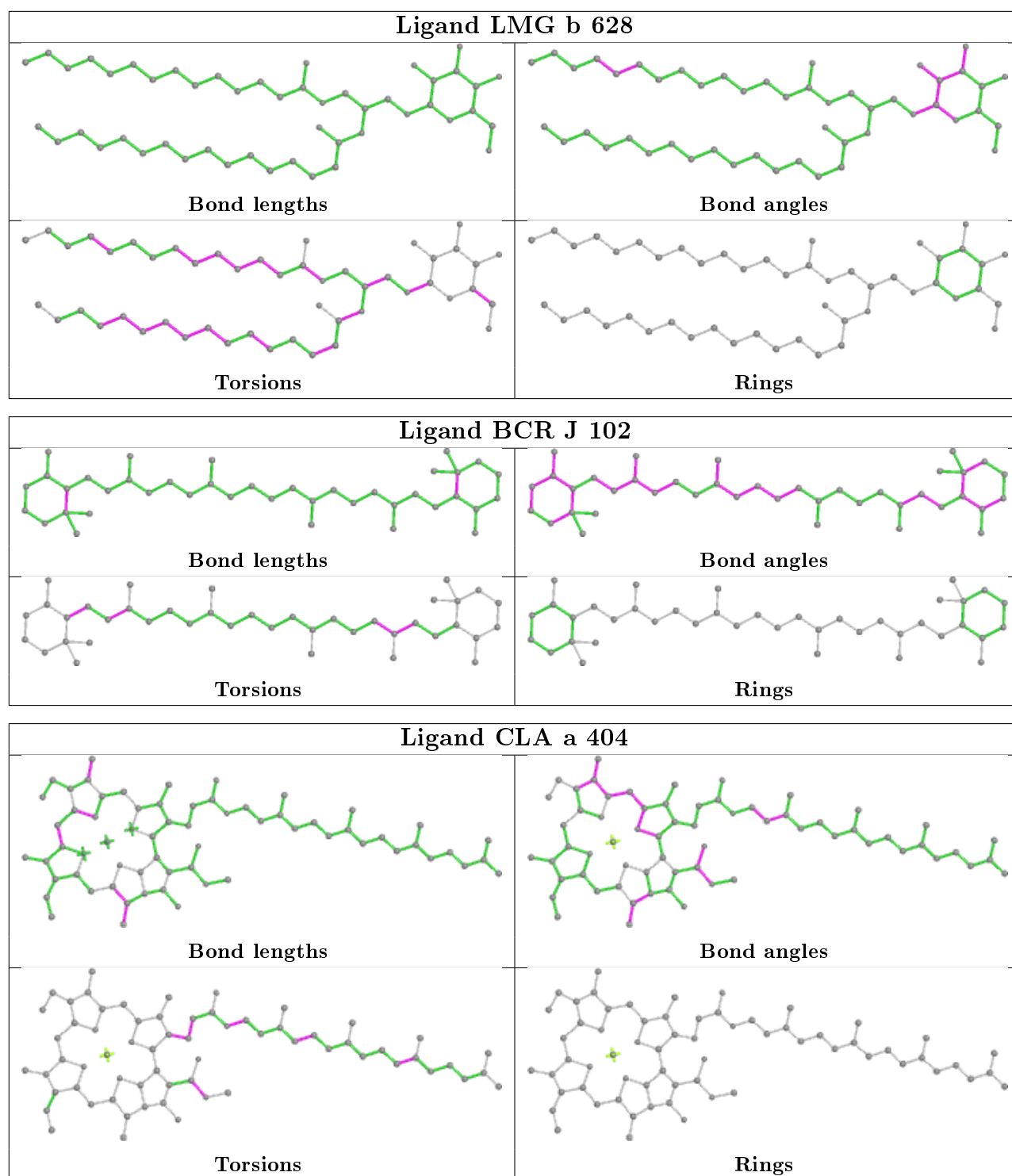


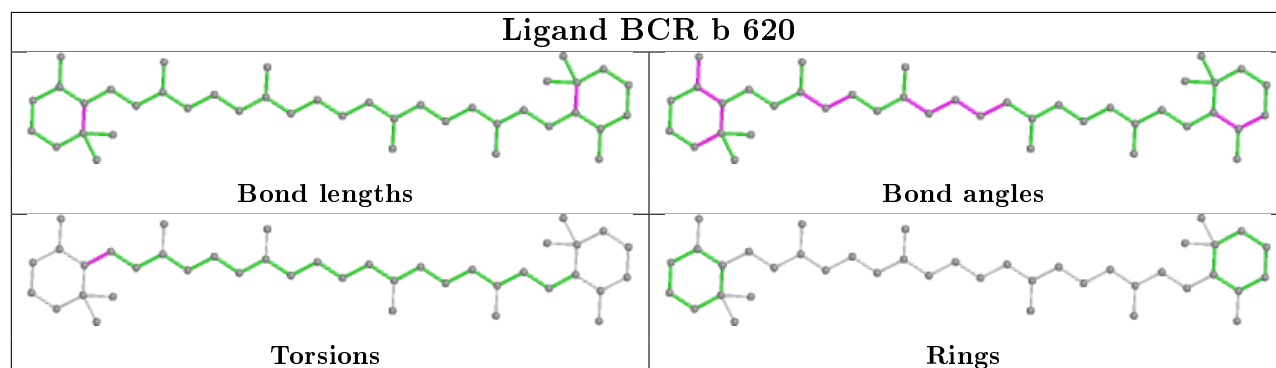
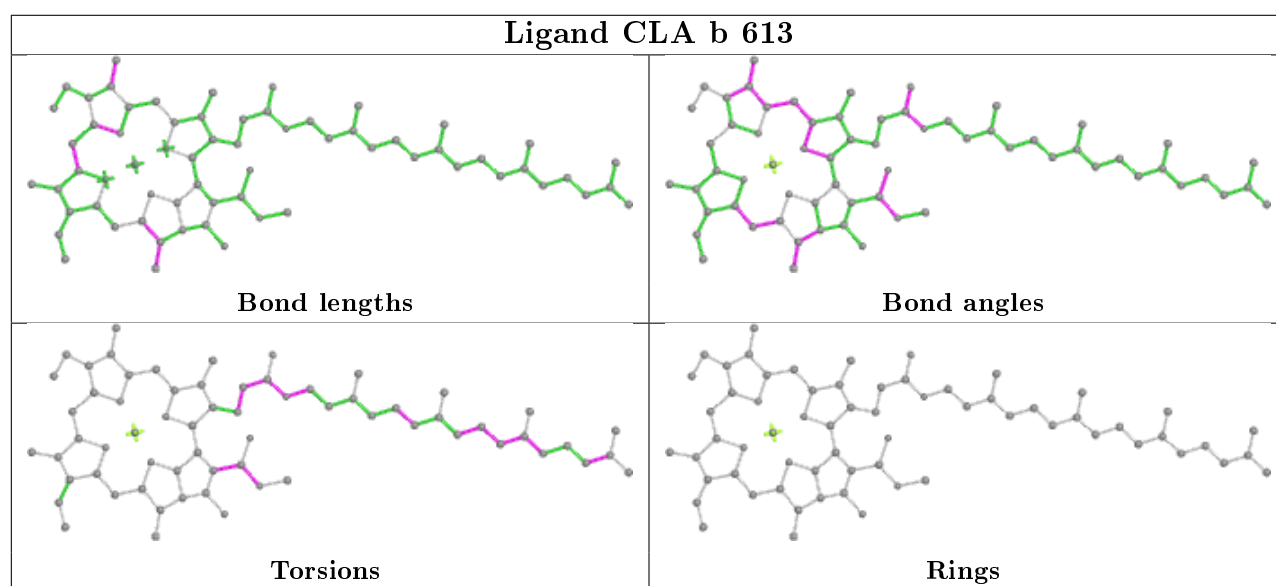
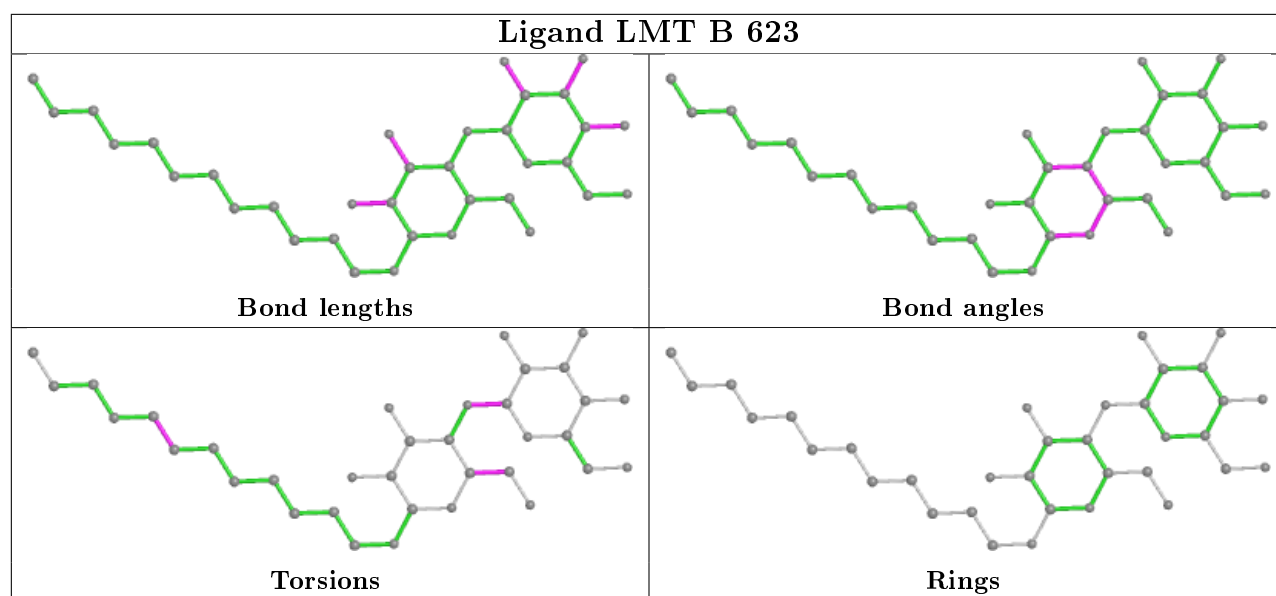
Ligand CLA C 509**Ligand CLA A 405****Ligand CLA B 609**

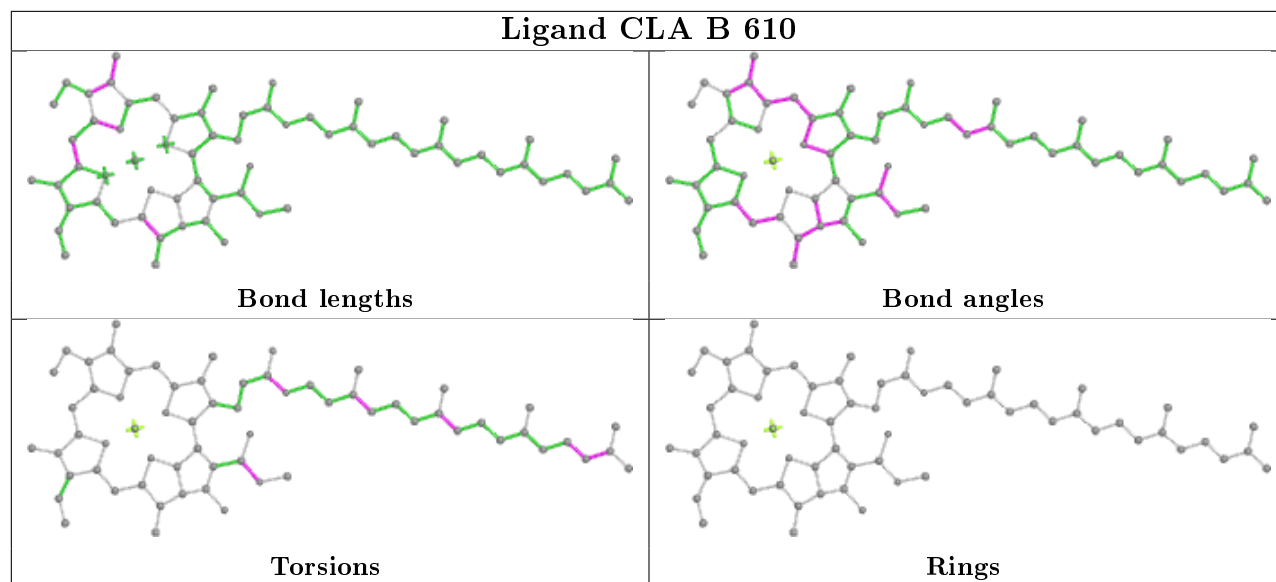
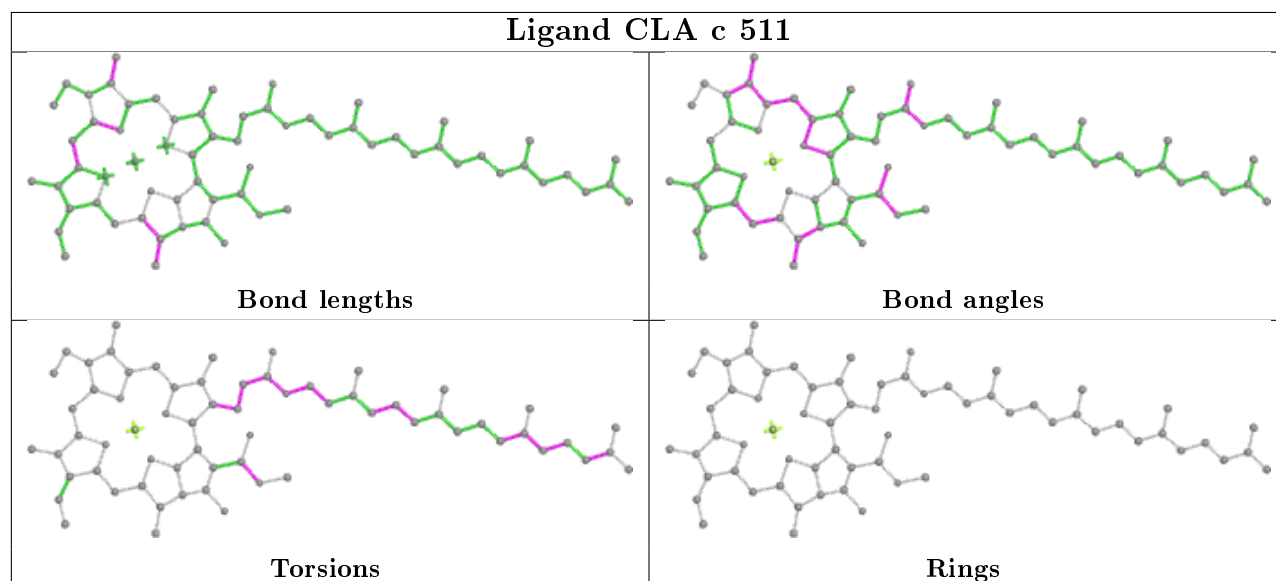
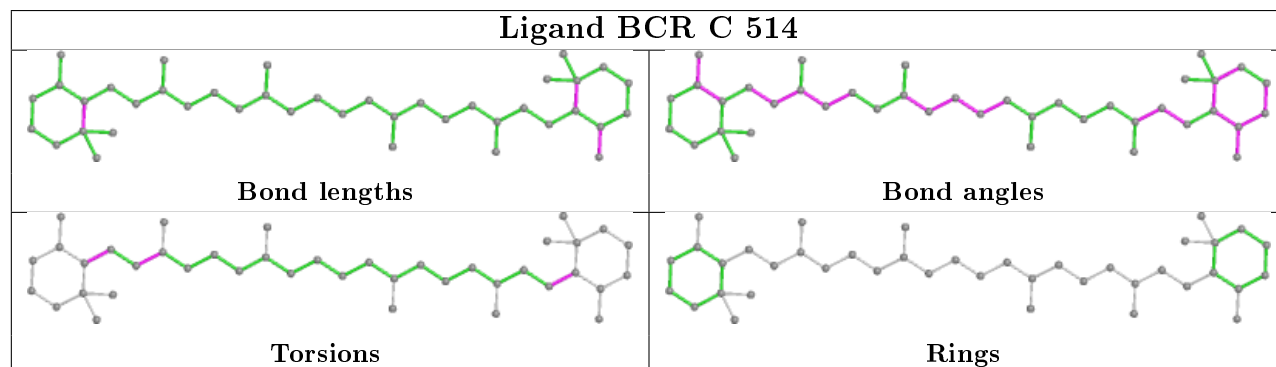


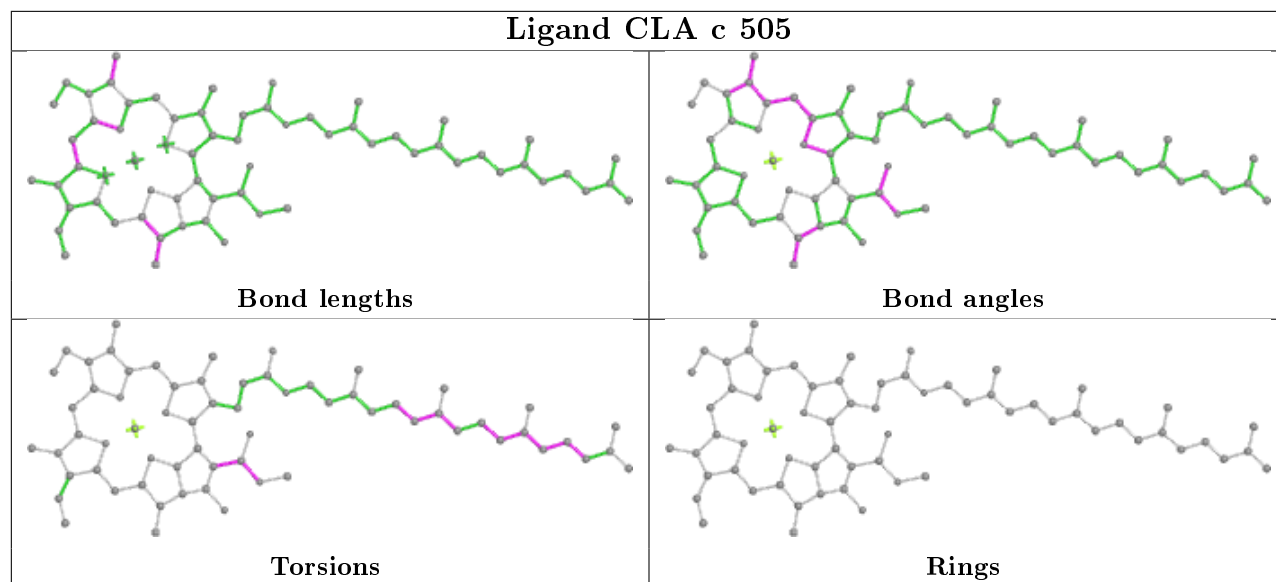
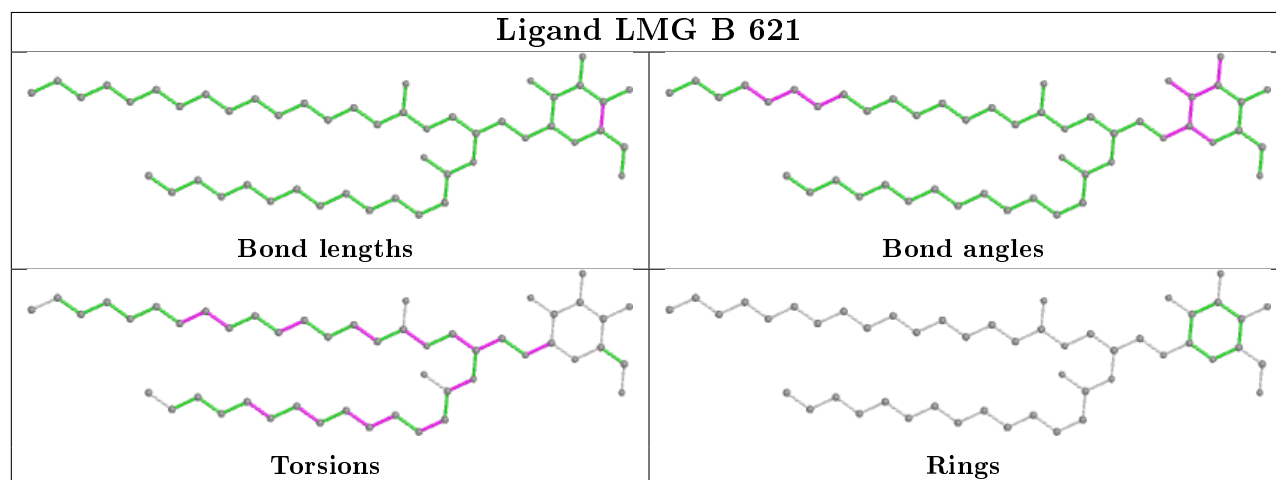
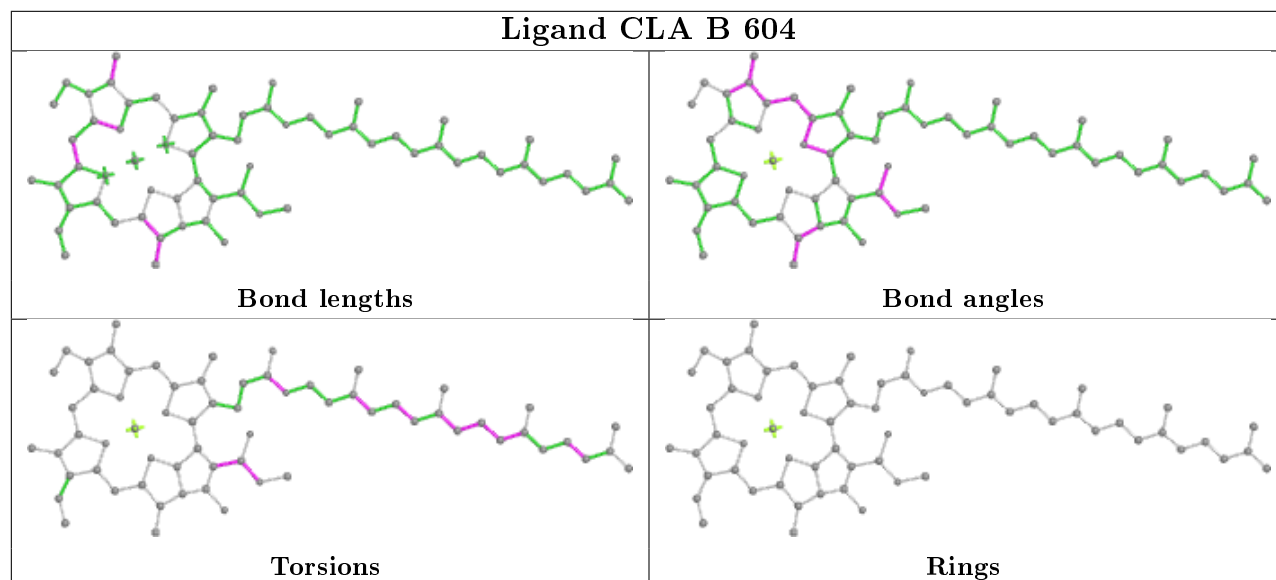


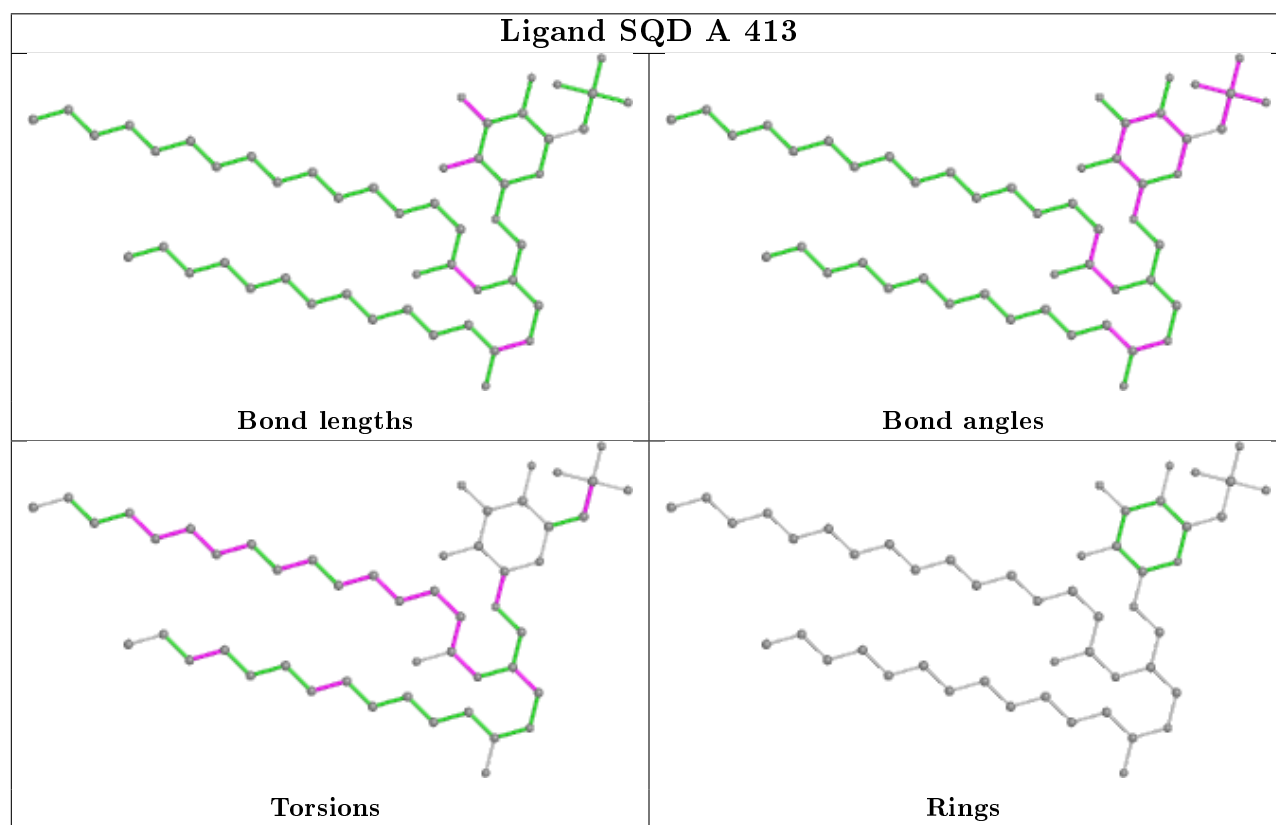
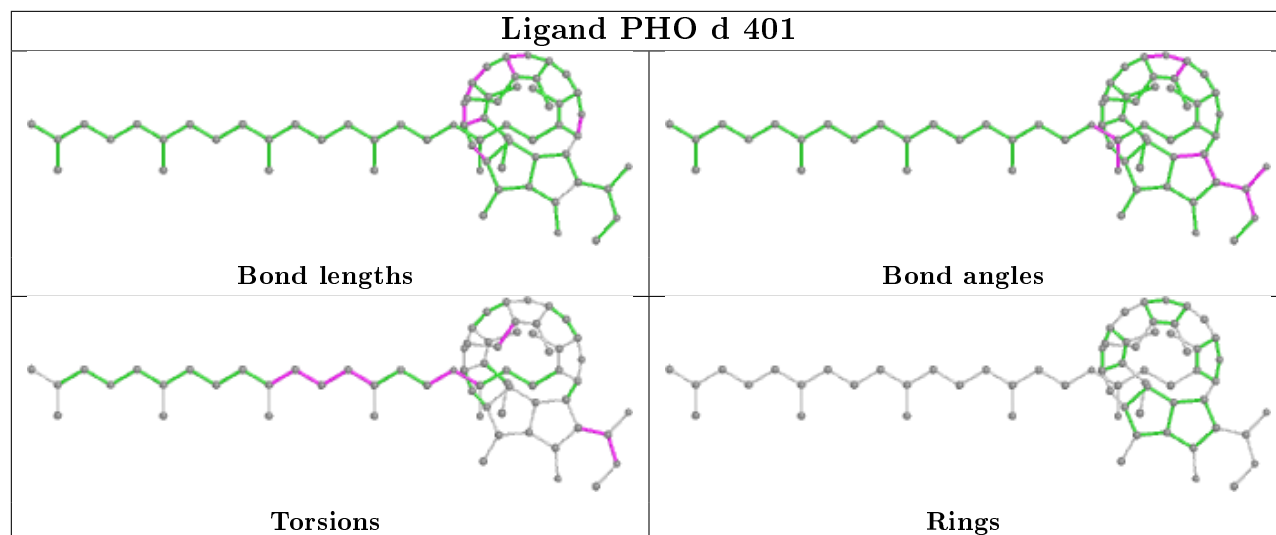


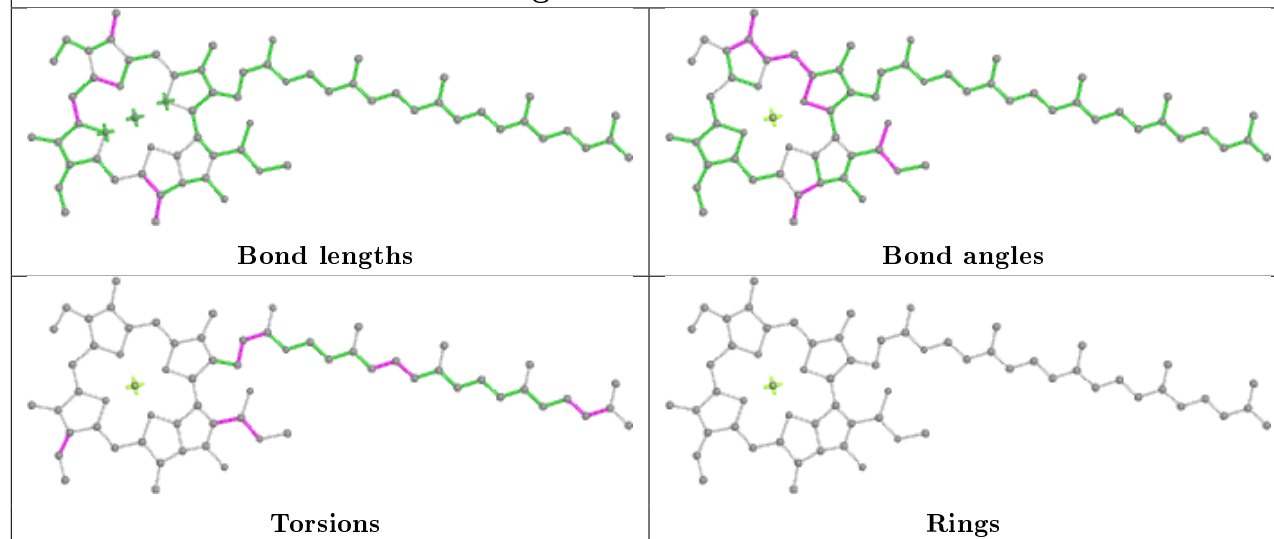
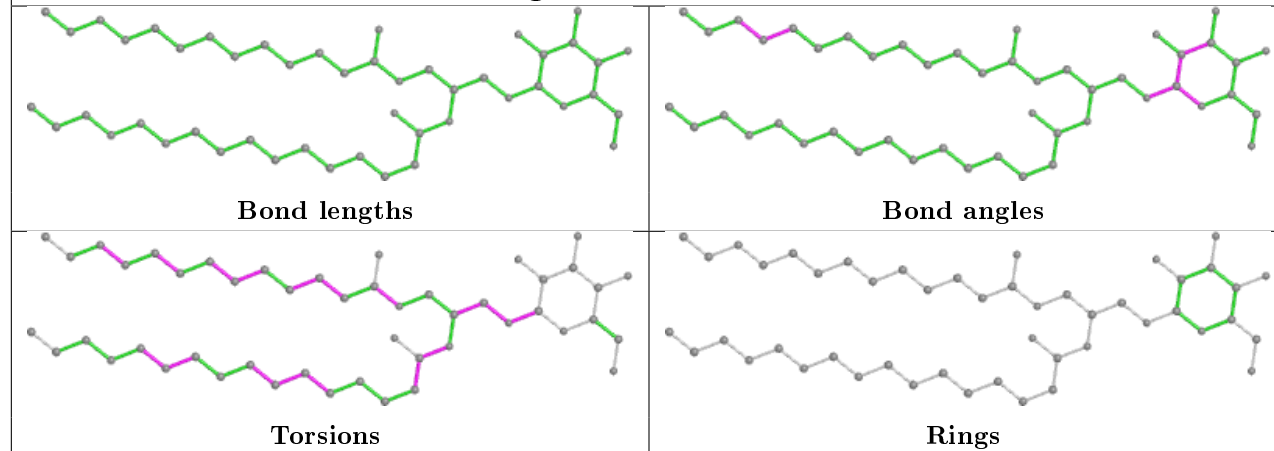
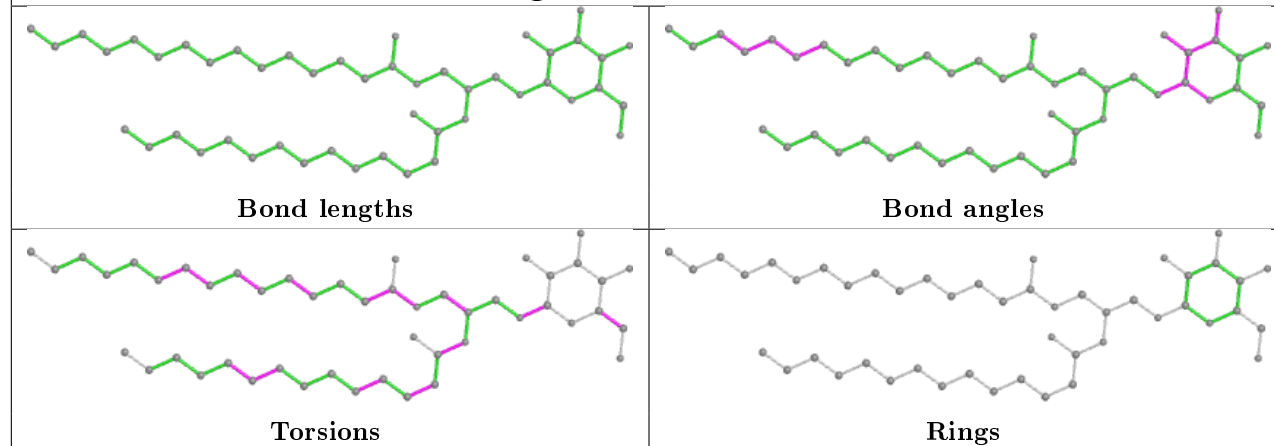


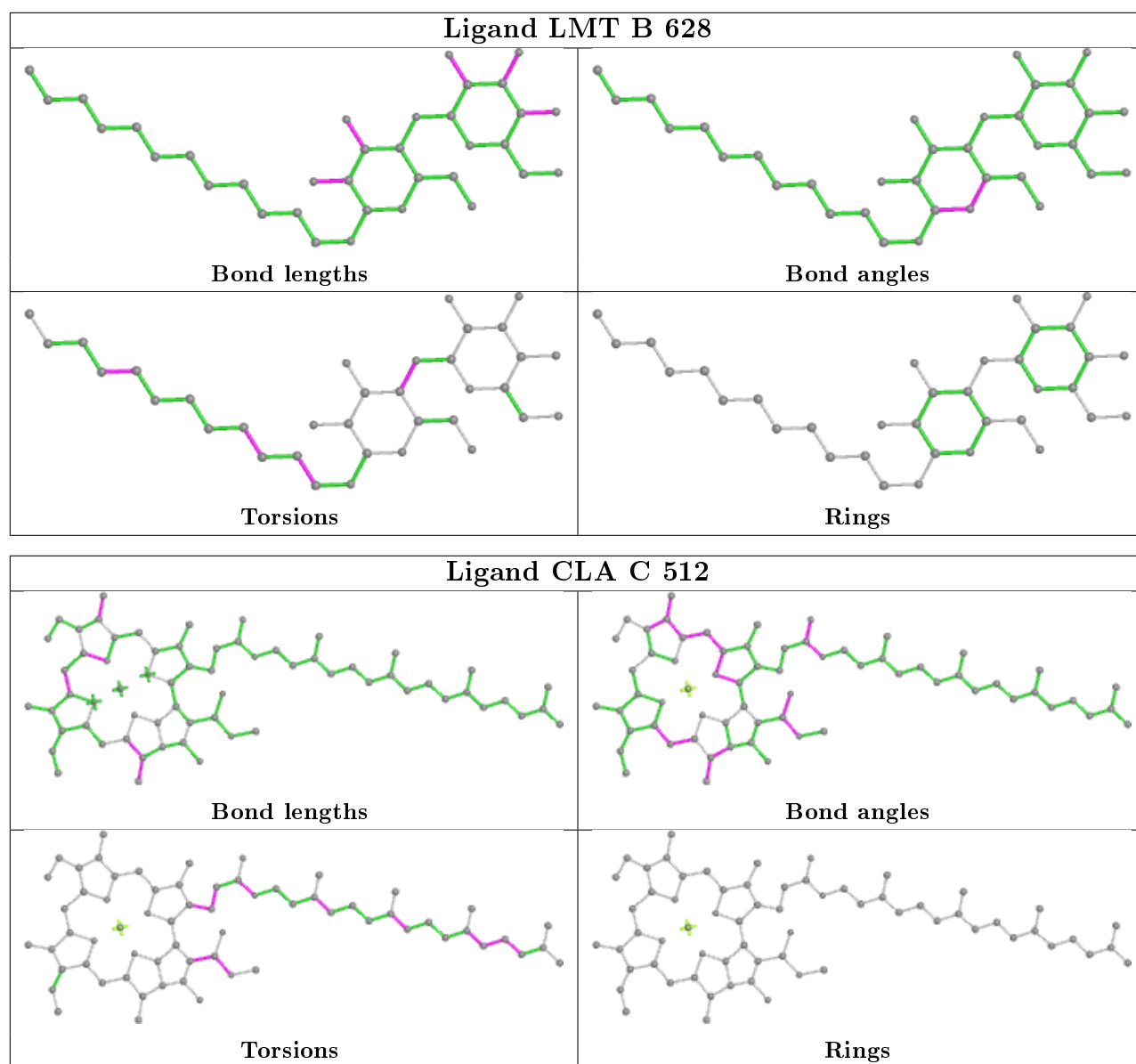


Ligand CLA B 610**Ligand CLA c 511****Ligand BCR C 514**

Ligand CLA c 505**Ligand LMG B 621****Ligand CLA B 604**



Ligand CLA B 613**Ligand LMG D 408****Ligand LMG C 522**



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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.43	28 (8%) 11 10	172, 174, 175, 176	0
1	a	335/344 (97%)	0.45	28 (8%) 11 10	172, 174, 175, 176	0
2	B	490/510 (96%)	0.22	30 (6%) 21 17	172, 174, 175, 176	0
2	b	490/510 (96%)	0.27	19 (3%) 39 31	172, 174, 175, 176	0
3	C	447/461 (96%)	0.25	24 (5%) 25 22	172, 174, 175, 176	0
3	c	447/461 (96%)	0.13	16 (3%) 42 35	173, 174, 175, 176	0
4	D	340/352 (96%)	0.17	7 (2%) 63 54	171, 174, 175, 176	0
4	d	340/352 (96%)	0.17	11 (3%) 47 38	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.07	1 (1%) 79 70	172, 174, 175, 175	0
5	e	82/84 (97%)	0.03	3 (3%) 41 33	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.14	1 (2%) 51 41	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.45	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.42	7 (10%) 5 6	173, 174, 175, 176	0
7	h	65/66 (98%)	0.71	9 (13%) 2 3	173, 174, 175, 176	0
8	I	35/38 (92%)	0.24	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.12	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.11	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.43	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.31	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.15	1 (2%) 54 45	174, 174, 175, 176	0
11	L	37/37 (100%)	0.35	1 (2%) 54 45	172, 174, 175, 175	0
11	l	37/37 (100%)	0.16	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.21	1 (2%) 51 41	172, 174, 174, 176	0
12	m	34/36 (94%)	0.11	2 (5%) 22 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.47	16 (6%) 18 15	172, 174, 175, 176	0
13	o	243/272 (89%)	0.47	13 (5%) 26 23	172, 174, 175, 176	0
14	T	32/32 (100%)	0.27	2 (6%) 20 16	173, 174, 176, 176	0
14	t	32/32 (100%)	0.34	3 (9%) 8 8	173, 174, 175, 176	0
15	U	97/134 (72%)	0.46	7 (7%) 15 13	172, 174, 174, 175	0
15	u	97/134 (72%)	0.63	9 (9%) 8 8	173, 174, 175, 175	0
16	V	137/163 (84%)	0.05	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.49	10 (7%) 15 12	173, 174, 175, 176	0
17	g	28/46 (60%)	0.32	1 (3%) 42 35	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.06	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.31	1 (2%) 54 45	173, 174, 175, 176	0
18	x	37/41 (90%)	0.84	7 (18%) 1 2	173, 175, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.26	1 (1%) 72 62	173, 174, 175, 176	0
20	z	62/62 (100%)	0.88	5 (8%) 12 11	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.27	264 (5%) 28 24	171, 174, 175, 177	0

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.6
1	a	224	ILE	5.2
5	e	84	LYS	5.0
15	U	38	GLU	4.9
3	C	135	ARG	4.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	CA	o	301	1/1	0.32	0.68	180,180,180,180	0
31	LMT	I	102	35/35	0.40	0.94	173,175,176,178	0
23	PL9	J	101	35/55	0.43	0.54	172,175,176,176	0
23	PL9	j	101	35/55	0.49	0.37	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	172,174,176,177	0
31	LMT	i	102	35/35	0.52	1.29	173,175,176,177	0
31	LMT	d	409	31/35	0.53	0.66	172,175,177,177	0
35	CA	O	301	1/1	0.53	0.38	177,177,177,177	0
31	LMT	b	627	35/35	0.54	1.22	173,175,177,177	0
31	LMT	b	626	35/35	0.59	0.69	172,175,176,177	0
22	CLA	b	605	65/65	0.61	1.14	172,175,176,176	0
27	LMG	A	415	42/55	0.62	0.53	171,174,176,177	0
22	CLA	B	601	65/65	0.62	0.85	172,175,176,177	0
27	LMG	C	518	45/55	0.62	1.09	171,174,175,175	0
27	LMG	E	101	44/55	0.63	0.56	170,174,176,177	0
24	BCR	f	102	40/40	0.63	0.47	171,173,175,175	0
24	BCR	j	102	40/40	0.63	0.34	173,175,177,178	0
24	BCR	g	101	40/40	0.64	0.78	173,174,175,175	0
31	LMT	D	410	31/35	0.64	0.93	174,175,176,176	0
22	CLA	b	619	65/65	0.65	0.77	172,174,175,175	0
27	LMG	a	402	42/55	0.65	0.49	171,174,176,176	0
26	LHG	C	519	37/49	0.65	0.48	172,174,179,183	0
27	LMG	I	101	43/55	0.66	1.04	172,174,177,177	0
25	DGD	d	408	63/66	0.66	0.77	172,175,177,178	0
31	LMT	B	628	35/35	0.66	0.46	172,174,177,178	0
22	CLA	c	502	65/65	0.66	0.54	173,174,175,175	0
24	BCR	c	514	40/40	0.67	0.71	172,173,175,175	0
24	BCR	D	411	40/40	0.67	0.44	171,173,174,175	0
31	LMT	B	622	35/35	0.67	0.88	171,175,177,177	0
23	PL9	D	407	55/55	0.68	0.39	171,173,174,175	0
23	PL9	d	406	55/55	0.68	0.39	172,173,175,175	0
23	PL9	A	406	45/55	0.69	0.43	172,174,175,175	0
24	BCR	H	102	40/40	0.69	0.94	173,174,175,176	0
27	LMG	a	413	51/55	0.69	0.42	172,173,175,176	0
25	DGD	D	409	63/66	0.70	0.81	172,174,176,178	0
31	LMT	b	604	35/35	0.70	0.47	172,174,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	502	65/65	0.70	0.53	173,174,174,175	0
27	LMG	c	518	45/55	0.71	1.01	172,174,176,176	0
24	BCR	x	101	40/40	0.71	0.86	173,174,175,175	0
25	DGD	A	408	56/66	0.71	0.45	172,174,175,176	0
25	DGD	b	601	52/66	0.72	0.47	172,174,176,177	0
32	PHO	d	401	64/64	0.72	0.42	172,173,174,174	0
24	BCR	B	616	40/40	0.72	0.43	172,173,174,175	0
27	LMG	C	522	48/55	0.73	0.36	172,174,174,175	0
27	LMG	M	101	42/55	0.73	0.53	173,174,176,176	0
25	DGD	a	411	56/66	0.73	0.44	173,174,175,176	0
30	SQD	A	413	51/54	0.73	0.37	172,174,175,176	0
24	BCR	a	410	40/40	0.73	0.68	172,173,174,175	0
22	CLA	a	408	65/65	0.74	0.82	173,174,175,175	0
27	LMG	i	101	43/55	0.74	0.80	172,174,177,178	0
26	LHG	c	519	37/49	0.74	0.35	172,174,178,181	0
30	SQD	d	402	43/54	0.75	0.83	172,174,176,178	0
24	BCR	B	617	40/40	0.75	0.44	172,173,174,174	0
27	LMG	e	101	44/55	0.75	0.39	171,174,175,176	0
23	PL9	a	409	45/55	0.76	0.38	171,173,174,175	0
31	LMT	B	627	35/35	0.76	0.55	172,175,177,177	0
28	CL	A	411	1/1	0.76	0.42	172,172,172,172	0
31	LMT	M	103	35/35	0.76	0.47	172,173,175,176	0
25	DGD	B	625	52/66	0.76	0.56	172,175,177,177	0
22	CLA	B	613	65/65	0.76	0.46	172,174,174,175	0
25	DGD	b	624	58/66	0.76	0.40	171,173,174,175	0
22	CLA	C	507	65/65	0.77	0.40	173,174,175,177	0
31	LMT	M	102	35/35	0.77	0.46	172,174,175,175	0
35	CA	k	101	1/1	0.77	0.20	172,172,172,172	0
25	DGD	C	517	66/66	0.77	0.34	172,173,174,175	0
22	CLA	C	506	65/65	0.77	0.73	172,174,175,175	0
24	BCR	y	101	40/40	0.77	1.00	173,173,174,175	0
27	LMG	B	624	49/55	0.78	0.31	171,173,174,175	0
27	LMG	D	412	46/55	0.78	0.40	172,174,175,175	0
24	BCR	C	514	40/40	0.78	0.83	172,173,175,175	0
22	CLA	c	512	65/65	0.78	0.68	172,174,176,176	0
27	LMG	m	101	42/55	0.78	0.45	170,174,175,175	0
27	LMG	b	625	49/55	0.78	0.34	172,174,175,175	0
22	CLA	h	101	65/65	0.78	0.53	171,174,175,175	0
24	BCR	b	622	40/40	0.78	0.36	171,172,173,173	0
24	BCR	A	407	40/40	0.79	0.48	171,173,174,174	0
32	PHO	D	402	64/64	0.79	0.37	171,173,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	C	521	40/40	0.79	0.82	172,174,175,176	0
22	CLA	C	505	65/65	0.79	0.45	172,174,175,176	0
27	LMG	A	410	51/55	0.79	0.35	171,173,174,175	0
30	SQD	F	102	45/54	0.79	0.69	172,175,177,178	0
30	SQD	B	626	47/54	0.79	0.46	170,174,176,178	0
31	LMT	B	623	35/35	0.79	0.50	173,174,177,177	0
25	DGD	c	517	66/66	0.80	0.35	172,173,175,176	0
24	BCR	b	623	40/40	0.80	0.76	171,173,174,174	0
24	BCR	B	619	40/40	0.80	0.83	172,173,174,175	0
30	SQD	b	602	47/54	0.80	0.38	171,174,176,178	0
27	LMG	c	522	48/55	0.81	0.29	172,174,175,176	0
31	LMT	b	603	35/35	0.81	0.44	172,174,175,176	0
22	CLA	B	603	65/65	0.81	0.49	171,173,175,175	0
22	CLA	b	609	65/65	0.81	0.55	172,174,175,175	0
35	CA	K	101	1/1	0.81	0.35	177,177,177,177	0
22	CLA	b	613	65/65	0.81	0.67	172,174,175,175	0
24	BCR	c	521	40/40	0.81	1.26	172,174,175,175	0
22	CLA	b	618	65/65	0.82	0.66	172,174,175,175	0
22	CLA	c	503	65/65	0.82	0.57	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	173,173,175,176	0
22	CLA	C	520	65/65	0.82	0.33	172,174,175,176	0
30	SQD	D	403	43/54	0.82	0.41	172,174,177,180	0
22	CLA	b	607	65/65	0.82	0.43	172,173,175,176	0
25	DGD	C	515	53/66	0.83	0.36	172,173,174,174	0
24	BCR	c	513	40/40	0.83	0.87	172,173,175,175	0
26	LHG	a	412	39/49	0.83	0.28	171,174,176,177	0
24	BCR	B	618	40/40	0.83	0.32	171,172,174,174	0
22	CLA	A	405	65/65	0.83	0.62	172,174,175,176	0
22	CLA	C	510	65/65	0.83	0.46	172,173,175,175	0
22	CLA	C	512	65/65	0.83	0.88	172,174,176,177	0
22	CLA	a	405	65/65	0.83	0.58	170,172,174,175	0
25	DGD	C	516	62/66	0.84	0.29	171,174,175,176	0
22	CLA	B	610	65/65	0.84	0.34	172,174,174,175	0
30	SQD	f	103	45/54	0.84	0.52	172,174,176,178	0
25	DGD	B	620	58/66	0.84	0.33	171,173,175,176	0
22	CLA	C	504	65/65	0.84	0.41	171,173,175,175	0
22	CLA	d	404	65/65	0.84	0.45	172,173,174,174	0
30	SQD	a	401	54/54	0.84	0.58	172,174,176,178	0
22	CLA	c	508	65/65	0.84	0.56	172,174,175,175	0
32	PHO	D	401	64/64	0.84	0.40	171,173,174,175	0
22	CLA	b	612	65/65	0.84	0.66	171,174,175,176	0
22	CLA	a	406	65/65	0.85	0.36	172,174,175,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	607	65/65	0.85	0.42	172,174,174,175	0
22	CLA	c	505	65/65	0.85	0.45	172,174,175,175	0
22	CLA	c	501	65/65	0.85	0.45	172,174,175,175	0
24	BCR	b	621	40/40	0.85	0.33	171,173,174,174	0
30	SQD	a	415	51/54	0.85	0.29	173,174,175,176	0
26	LHG	A	409	39/49	0.85	0.28	172,173,175,176	0
22	CLA	C	509	65/65	0.85	0.34	173,173,174,174	0
22	CLA	b	606	65/65	0.85	0.61	172,173,174,174	0
30	SQD	A	414	54/54	0.85	0.40	171,174,176,179	0
22	CLA	d	405	65/65	0.86	0.45	172,174,175,175	0
27	LMG	d	407	48/55	0.86	0.28	171,173,175,175	0
22	CLA	B	615	65/65	0.86	0.66	172,174,175,175	0
32	PHO	a	407	64/64	0.86	0.26	173,174,175,175	0
24	BCR	C	513	40/40	0.86	0.77	172,173,174,174	0
22	CLA	B	609	65/65	0.86	0.53	172,174,175,175	0
22	CLA	C	503	65/65	0.86	0.41	172,174,175,176	0
21	FE2	a	403	1/1	0.86	0.18	175,175,175,175	0
22	CLA	c	510	65/65	0.86	0.53	173,174,175,176	0
22	CLA	c	506	65/65	0.86	0.55	173,174,175,175	0
22	CLA	H	101	65/65	0.86	0.35	172,174,175,175	0
22	CLA	B	605	65/65	0.86	0.72	172,173,175,176	0
25	DGD	c	515	53/66	0.86	0.36	171,174,175,177	0
22	CLA	C	508	65/65	0.87	0.86	172,174,175,175	0
22	CLA	c	509	65/65	0.87	0.32	172,173,175,175	0
22	CLA	D	406	65/65	0.87	0.64	172,174,175,176	0
22	CLA	c	520	65/65	0.87	0.36	173,174,174,175	0
22	CLA	B	604	65/65	0.87	0.67	172,173,175,175	0
27	LMG	D	408	48/55	0.87	0.28	170,173,175,175	0
25	DGD	c	516	62/66	0.87	0.30	172,174,175,175	0
22	CLA	A	404	65/65	0.87	0.47	170,173,174,175	0
22	CLA	C	501	65/65	0.87	0.40	172,174,174,175	0
22	CLA	b	608	65/65	0.88	0.51	172,173,175,176	0
22	CLA	a	404	65/65	0.88	0.54	172,173,174,176	0
34	HEM	V	201	43/43	0.88	0.45	172,173,175,175	0
27	LMG	B	621	49/55	0.88	0.26	172,173,174,174	0
22	CLA	b	614	65/65	0.88	0.30	172,173,174,175	0
22	CLA	B	606	65/65	0.88	0.34	172,173,174,175	0
22	CLA	D	405	65/65	0.89	0.36	172,173,174,175	0
22	CLA	B	614	65/65	0.89	0.62	172,174,175,175	0
22	CLA	c	504	65/65	0.89	0.33	172,174,175,175	0
22	CLA	c	511	65/65	0.89	0.62	172,174,175,176	0
22	CLA	C	511	65/65	0.90	0.92	172,174,175,175	0

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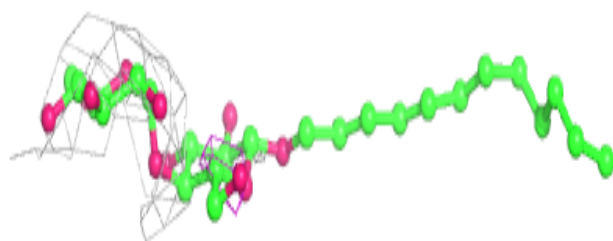
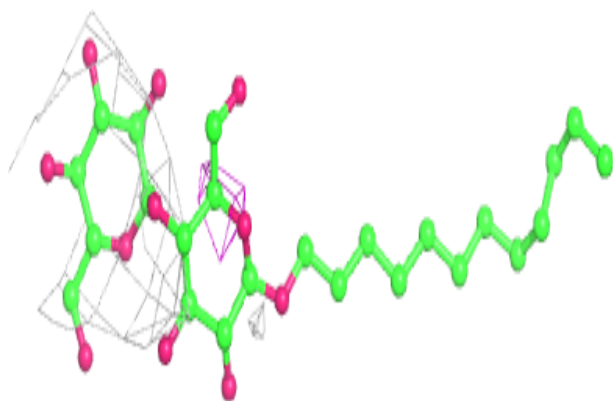
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	A	402	65/65	0.90	0.42	172,173,174,175	0
22	CLA	B	612	65/65	0.90	0.28	171,173,175,175	0
34	HEM	v	201	43/43	0.90	0.55	171,174,175,175	0
24	BCR	b	620	40/40	0.90	0.32	172,173,174,175	0
22	CLA	B	608	65/65	0.90	0.50	172,174,175,175	0
22	CLA	b	610	65/65	0.90	0.33	172,173,175,175	0
27	LMG	d	410	46/55	0.91	0.23	172,173,175,175	0
34	HEM	F	101	43/43	0.91	0.48	173,174,175,176	0
33	BCT	d	403	4/4	0.91	0.92	174,174,175,176	0
28	CL	a	416	1/1	0.91	0.33	173,173,173,173	0
22	CLA	c	507	65/65	0.91	0.24	172,174,175,176	0
21	FE2	A	401	1/1	0.92	0.18	170,170,170,170	0
22	CLA	b	615	65/65	0.92	0.40	172,173,174,175	0
22	CLA	b	611	65/65	0.92	0.31	172,174,175,175	0
22	CLA	B	611	65/65	0.92	0.36	171,173,174,174	0
22	CLA	B	602	65/65	0.92	0.52	171,173,174,175	0
27	LMG	b	628	49/55	0.93	0.23	172,174,175,175	0
22	CLA	A	403	65/65	0.93	0.54	171,173,174,175	0
34	HEM	f	101	43/43	0.93	0.34	173,174,175,175	0
29	OEX	A	412	10/10	0.93	0.42	165,169,172,173	0
22	CLA	b	616	65/65	0.95	0.29	171,173,174,175	0
33	BCT	D	404	4/4	0.95	0.25	173,174,174,174	0
29	OEX	a	414	10/10	0.96	0.45	168,171,173,177	0

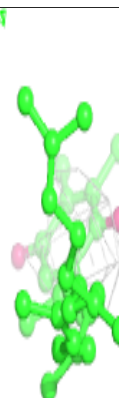
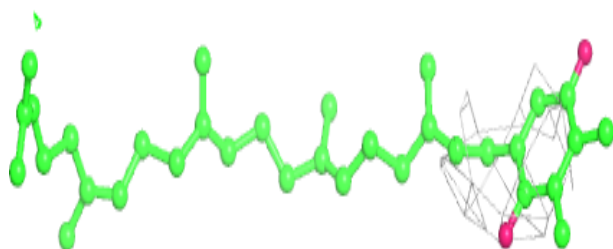
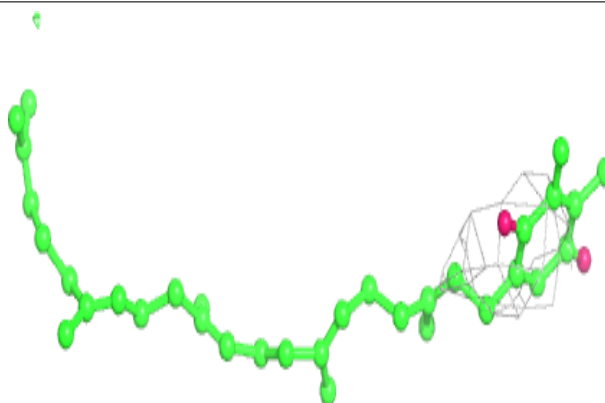
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT I 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

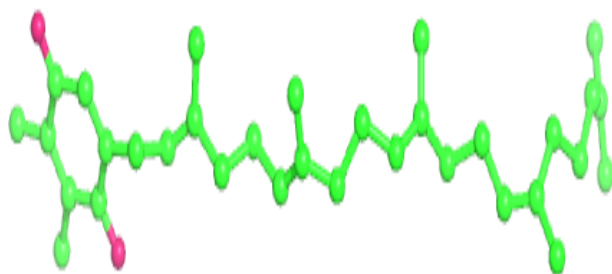
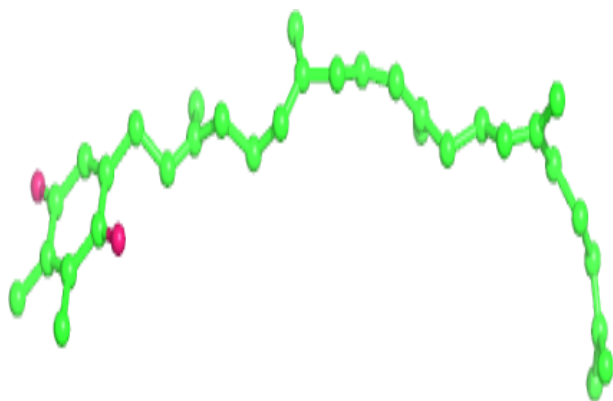
**Electron density around PL9 J 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

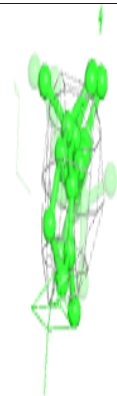
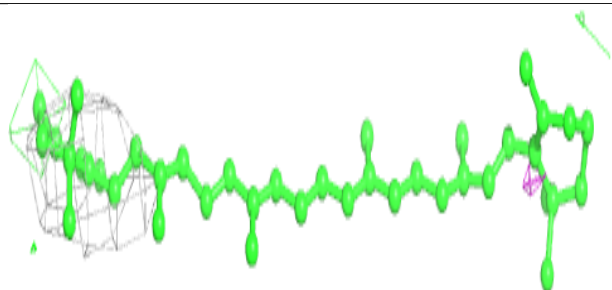
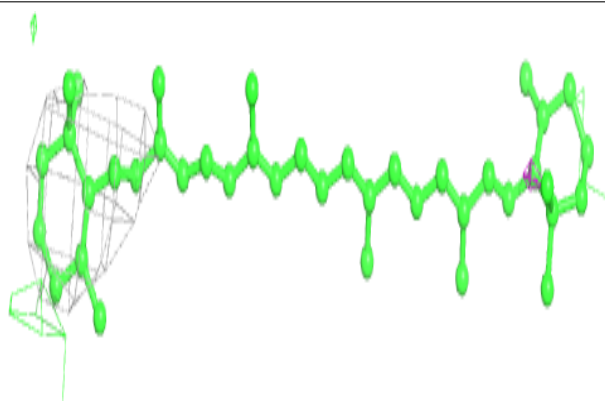


Electron density around PL9 j 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

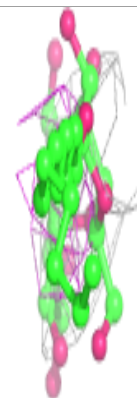
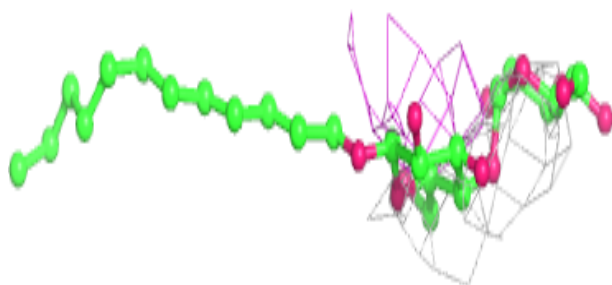
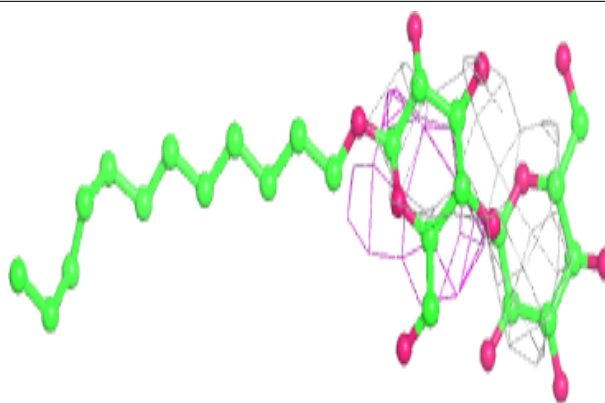
**Electron density around BCR J 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

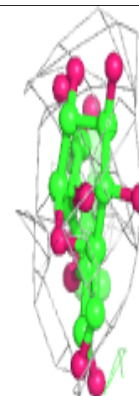
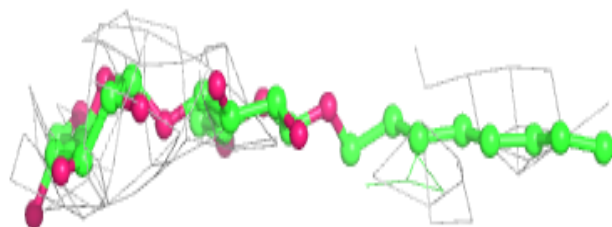
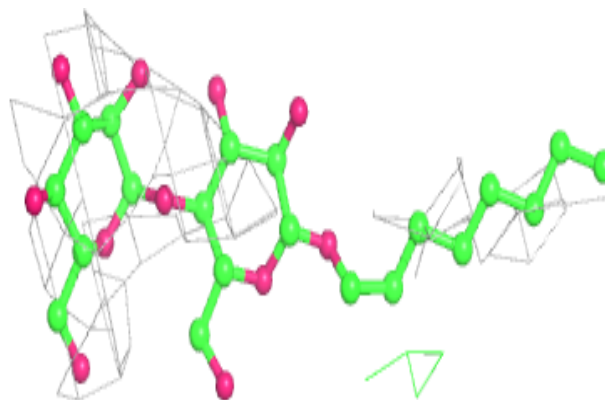


Electron density around LMT i 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

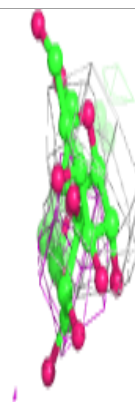
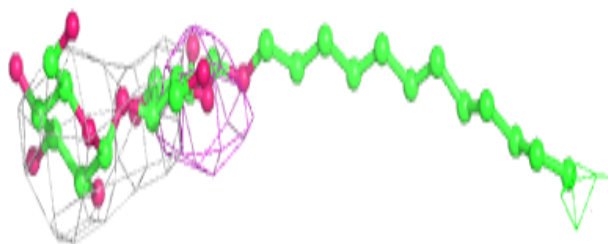
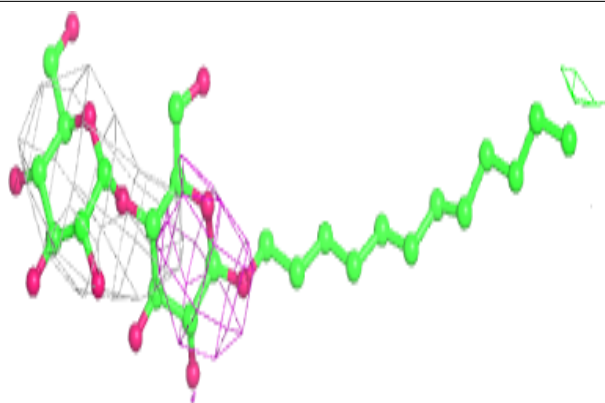
**Electron density around LMT d 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

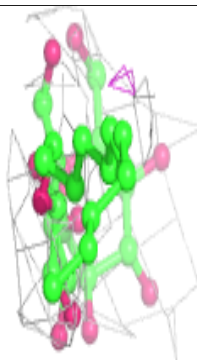
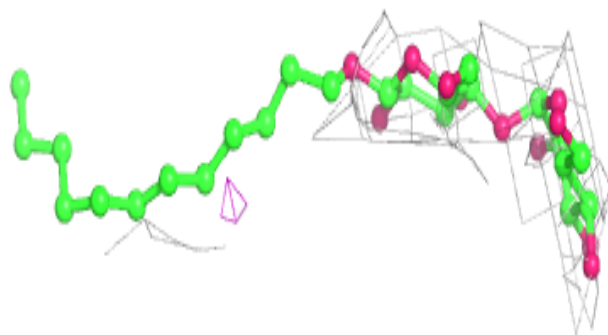
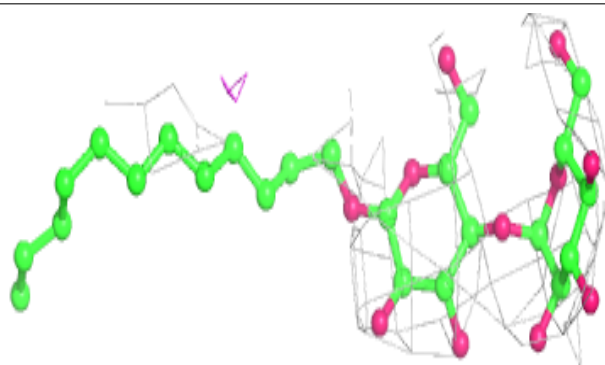


Electron density around LMT b 627:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

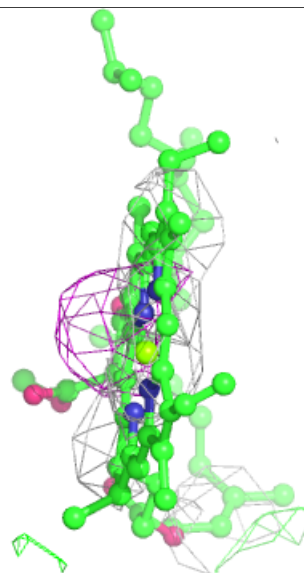
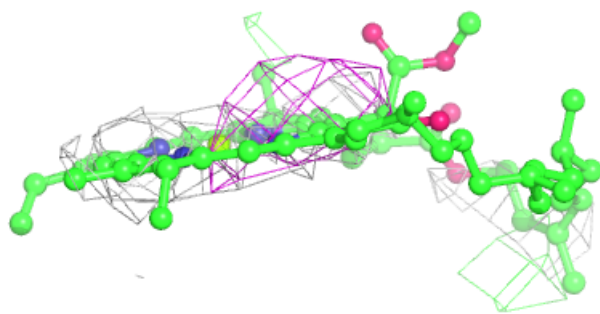
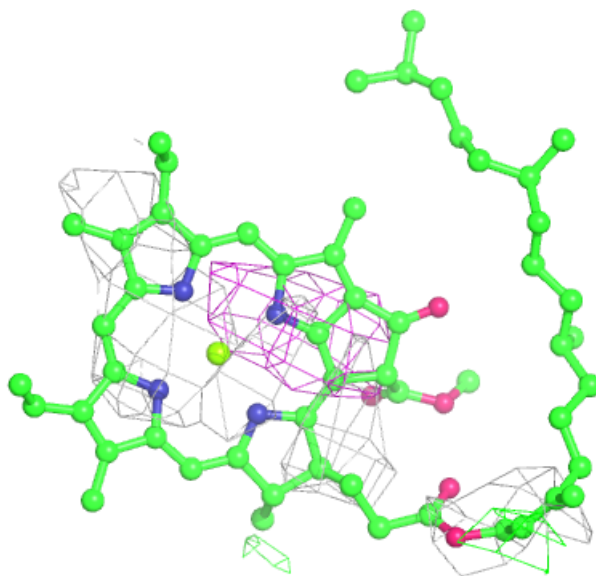
**Electron density around LMT b 626:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



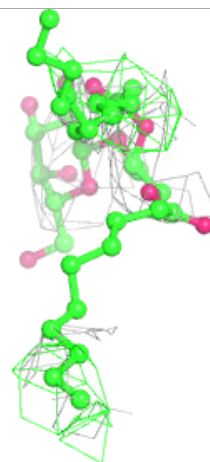
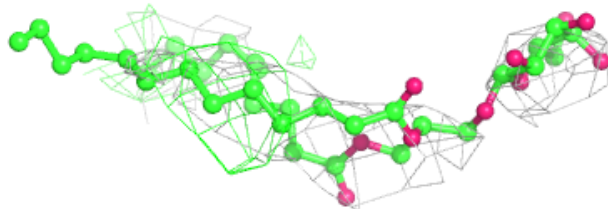
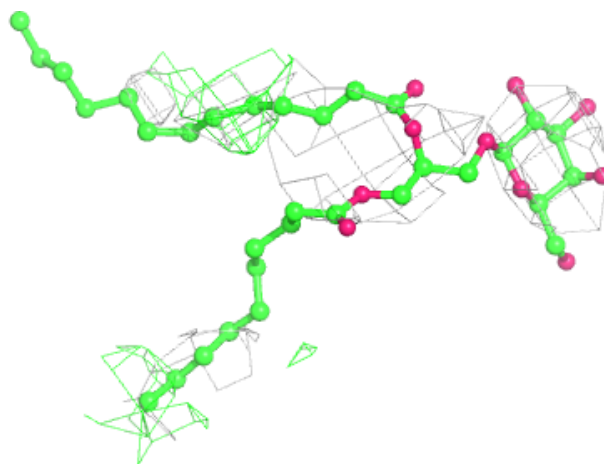
Electron density around CLA b 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



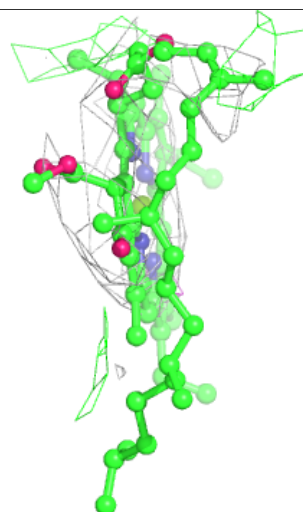
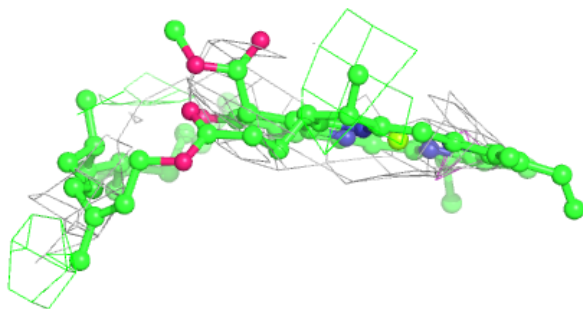
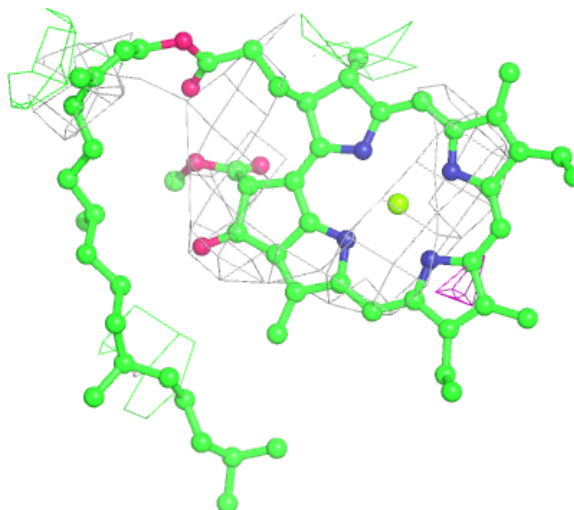
Electron density around LMG A 415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



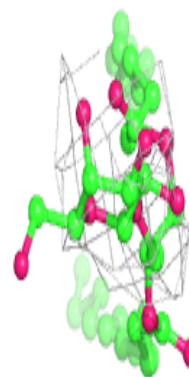
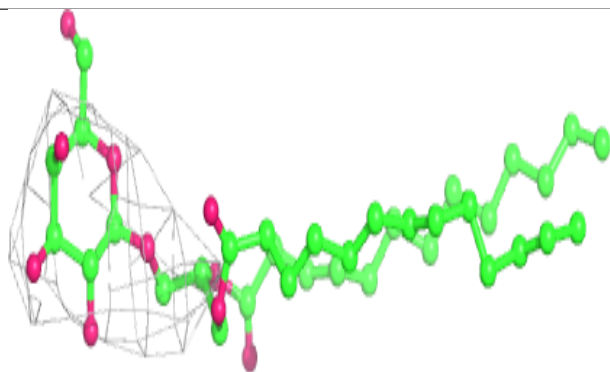
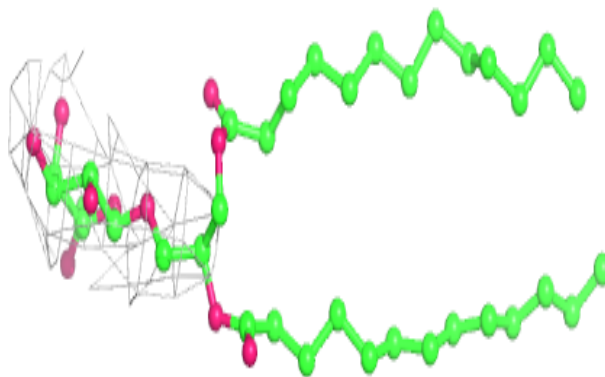
Electron density around CLA B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



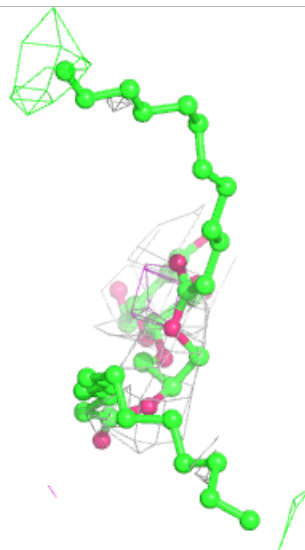
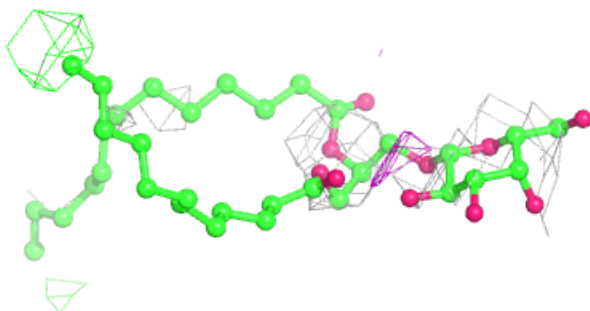
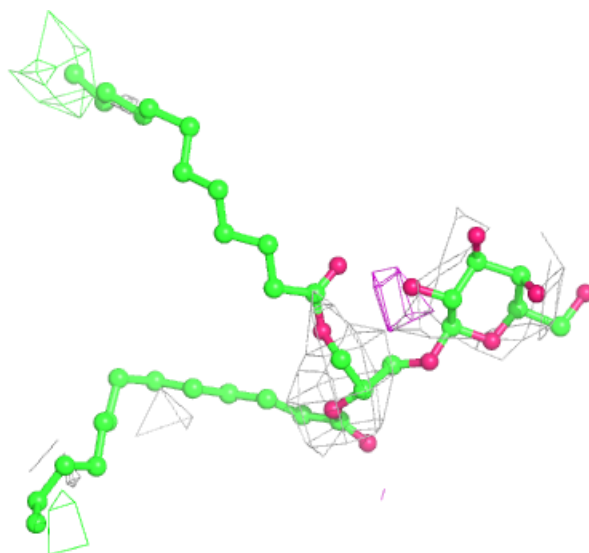
Electron density around LMG C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



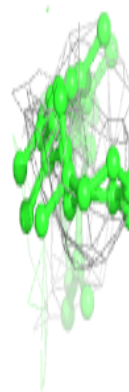
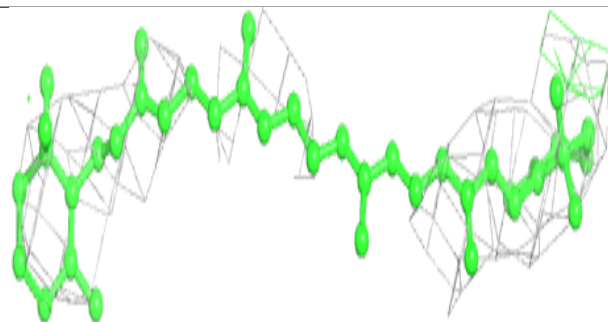
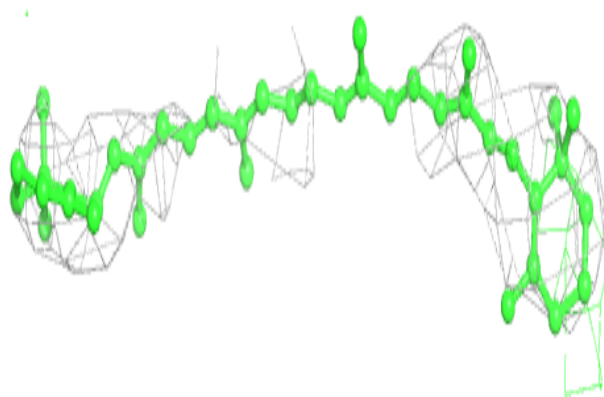
Electron density around LMG E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

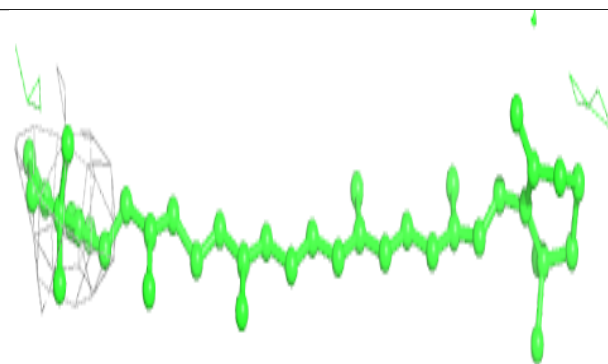
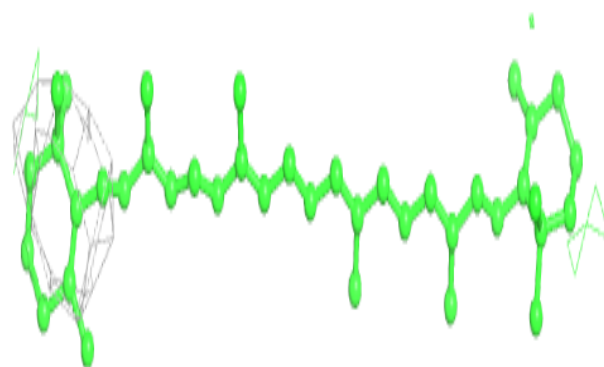


Electron density around BCR f 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

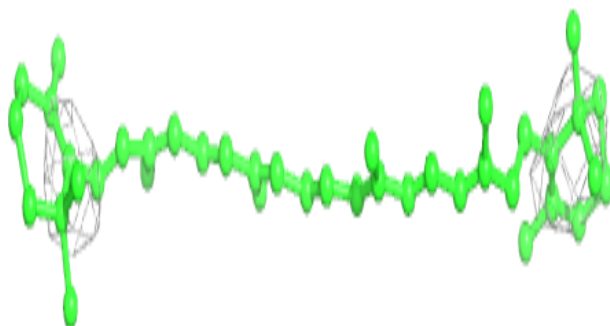
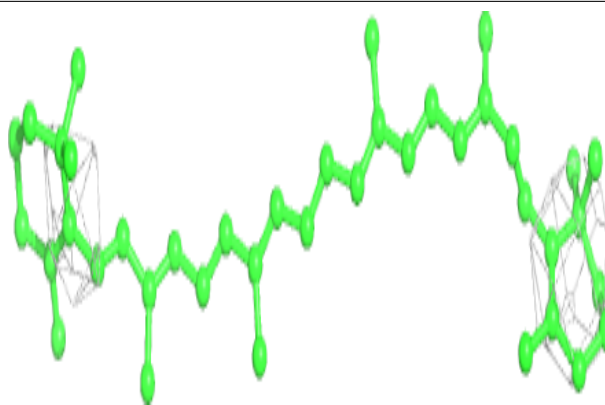
**Electron density around BCR j 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

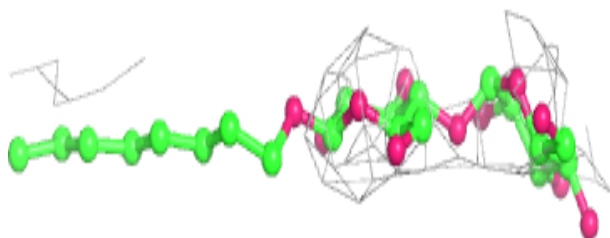
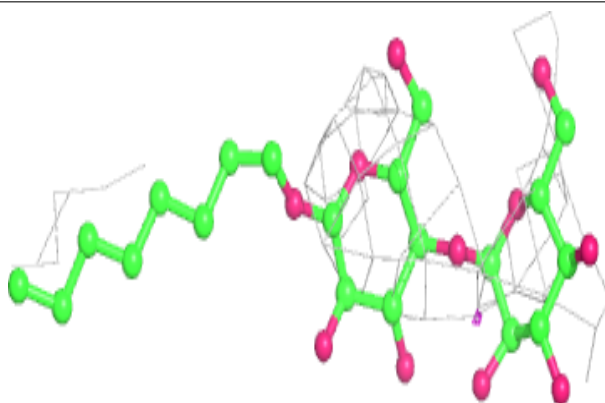


Electron density around BCR g 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

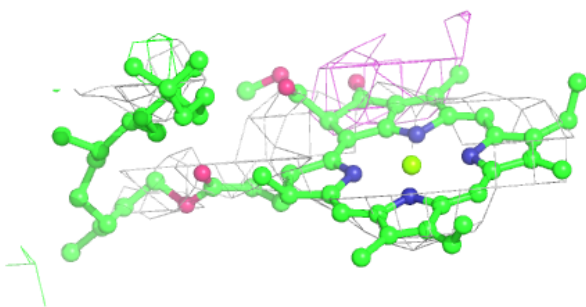
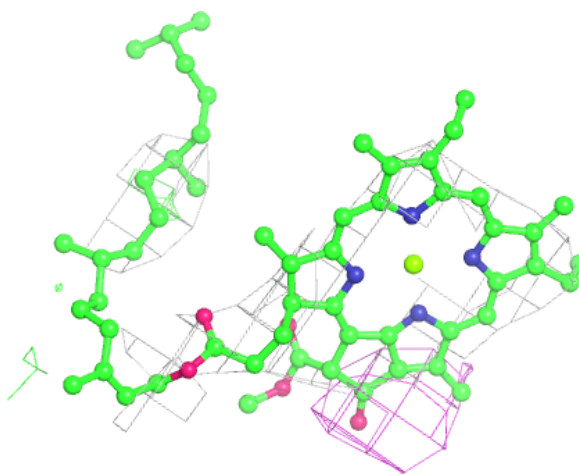
**Electron density around LMT D 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



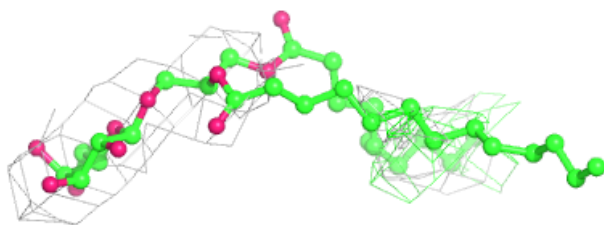
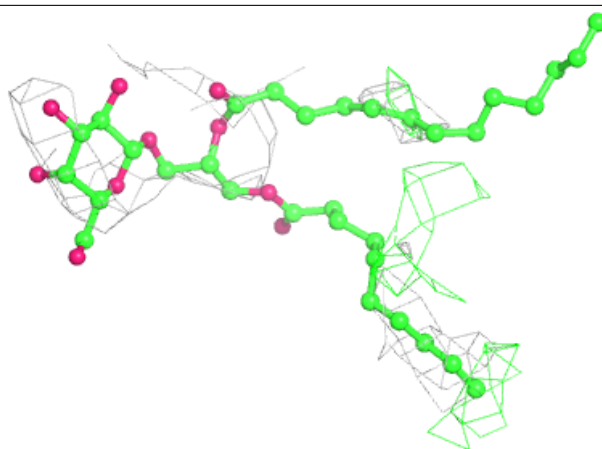
Electron density around CLA b 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

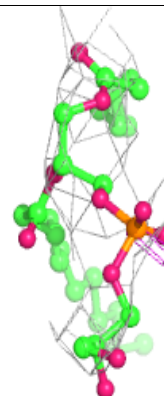
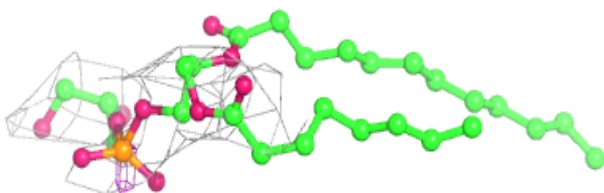
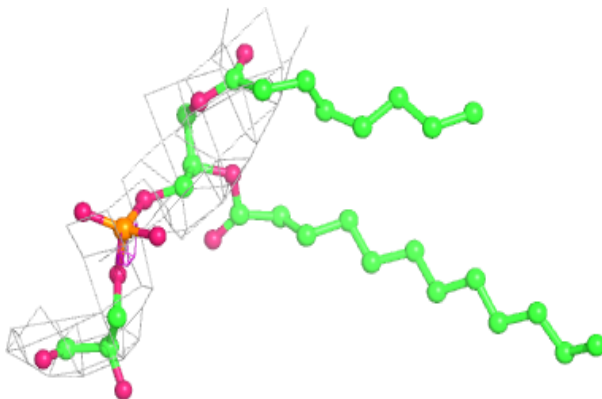


Electron density around LMG a 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

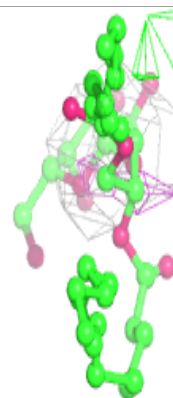
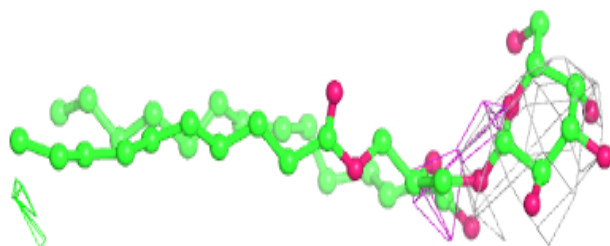
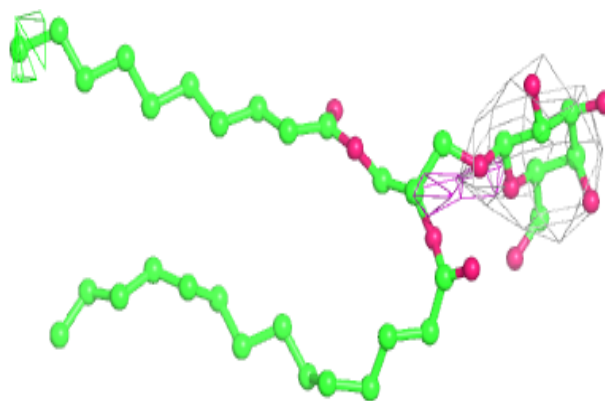
**Electron density around LHG C 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

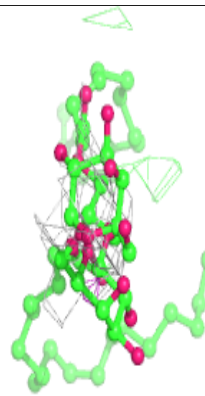
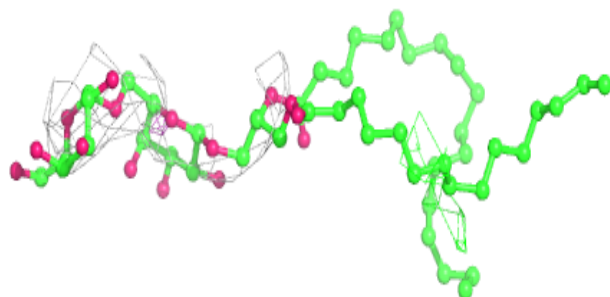
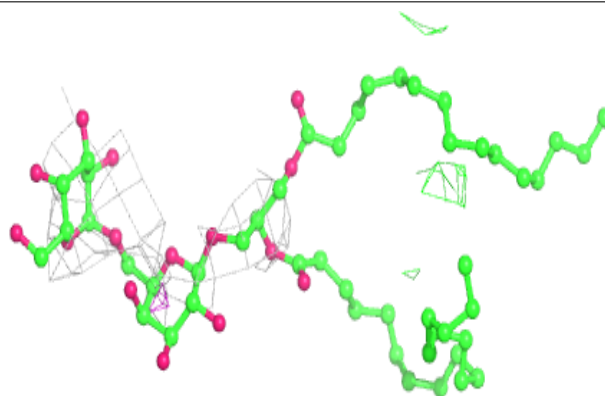


Electron density around LMG I 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

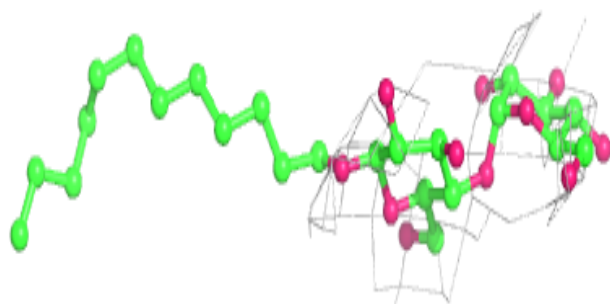
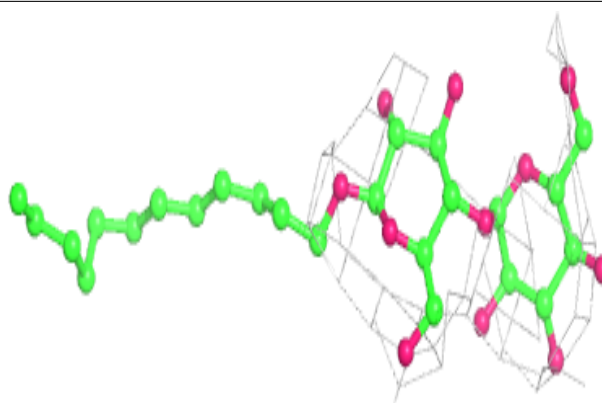
**Electron density around DGD d 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

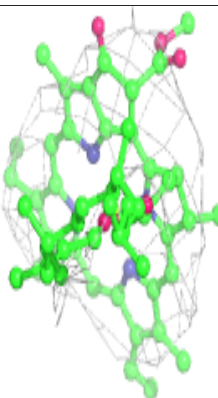
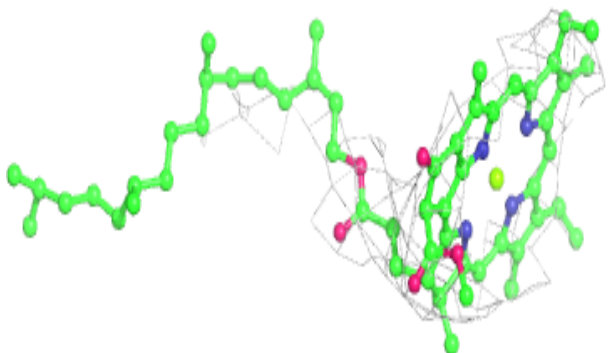
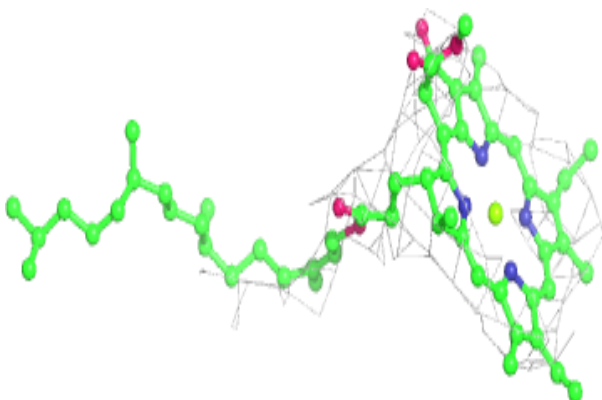


Electron density around LMT B 628:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

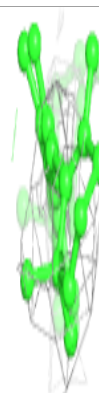
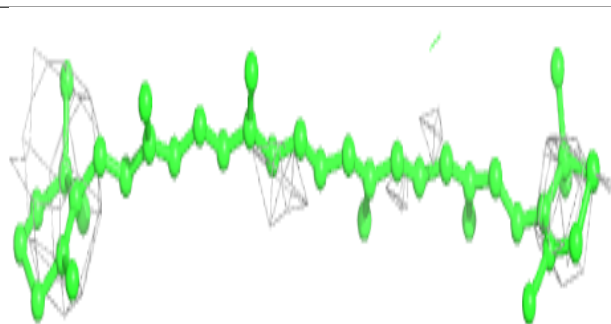
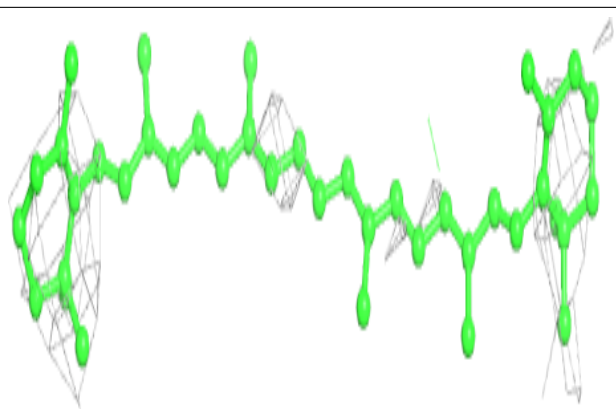
**Electron density around CLA c 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

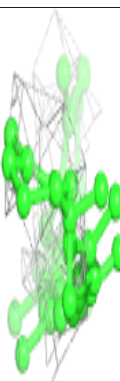
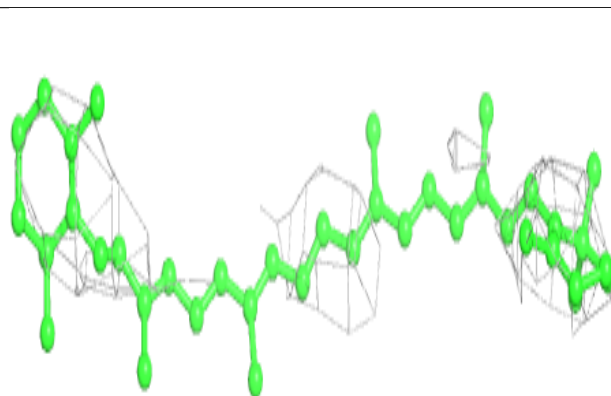
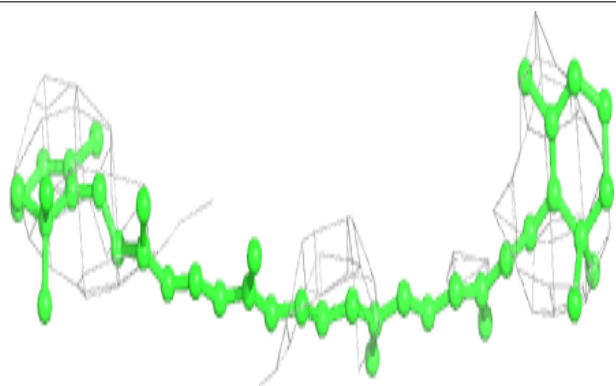


Electron density around BCR c 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

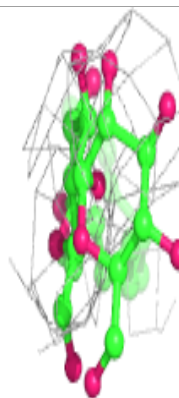
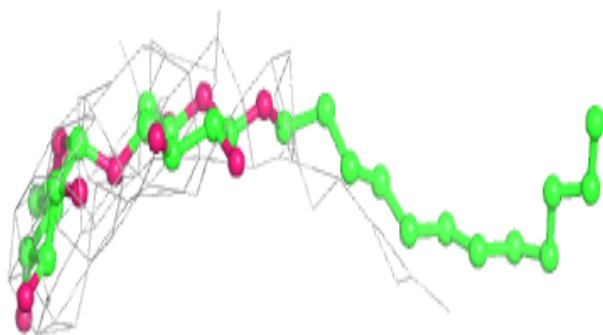
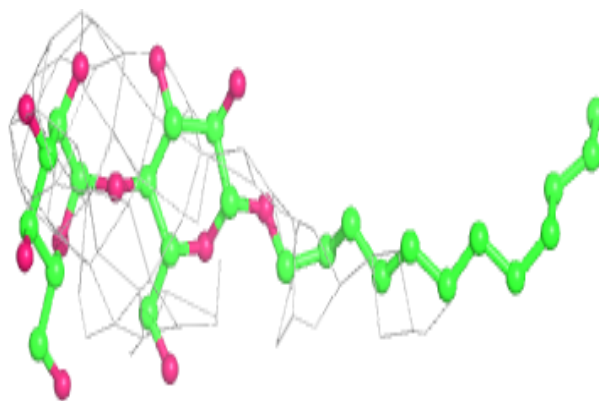
**Electron density around BCR D 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

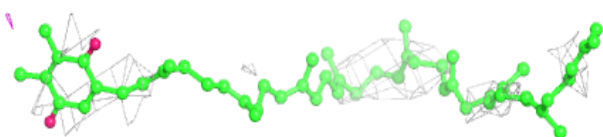
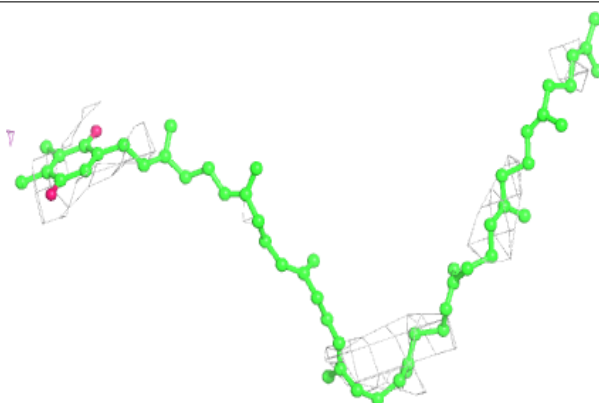


Electron density around LMT B 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

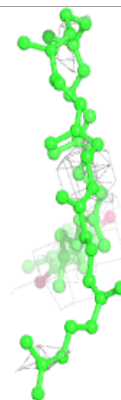
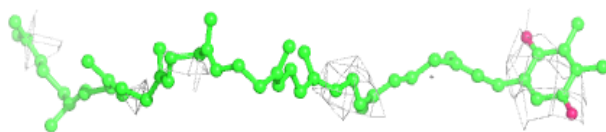
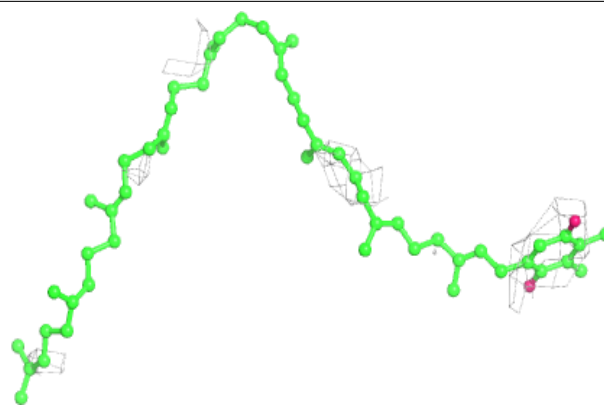
**Electron density around PL9 D 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

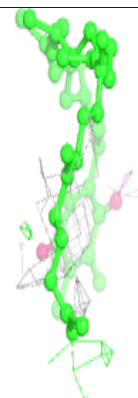
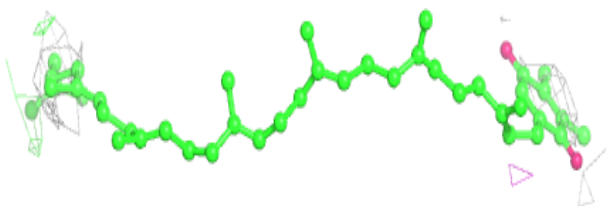
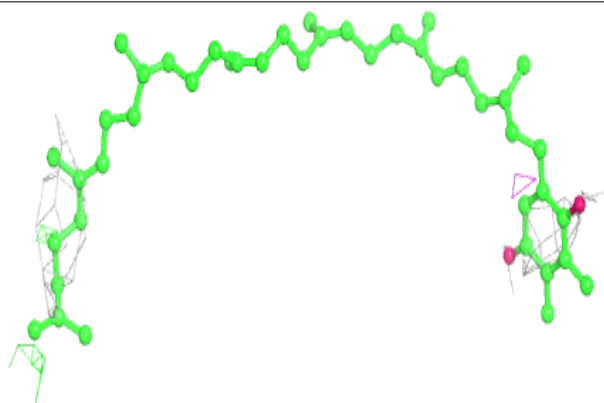


Electron density around PL9 d 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

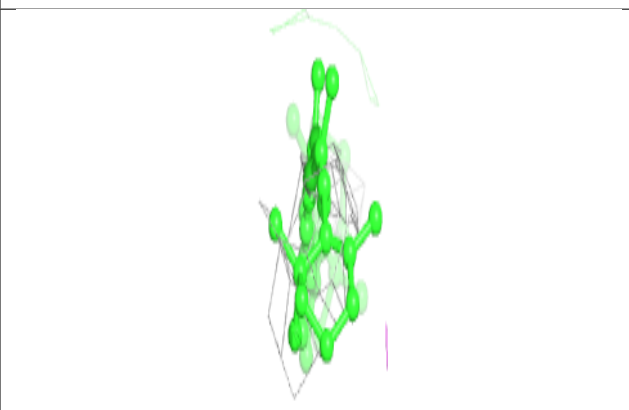
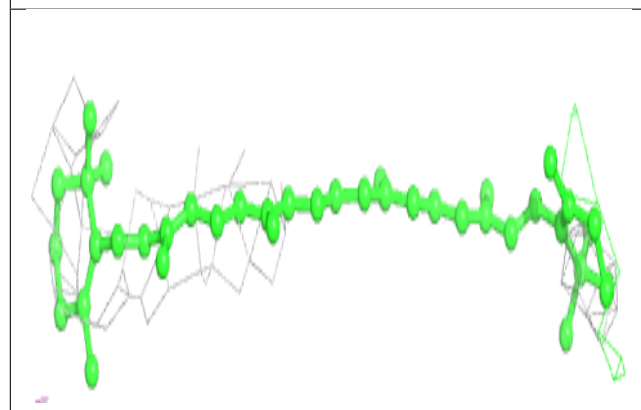
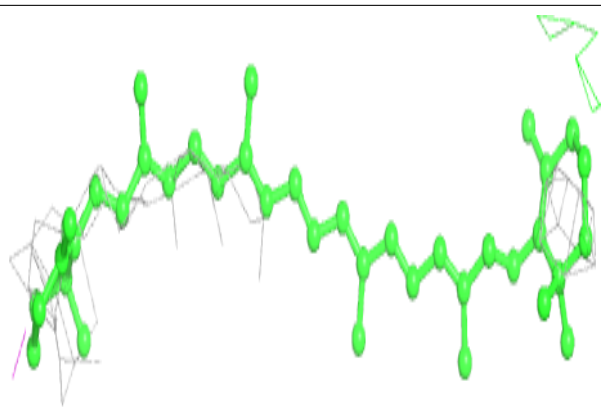
**Electron density around PL9 A 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



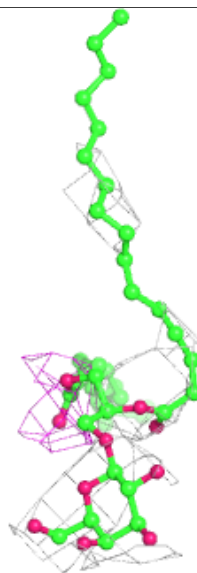
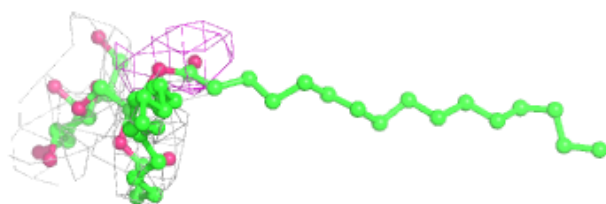
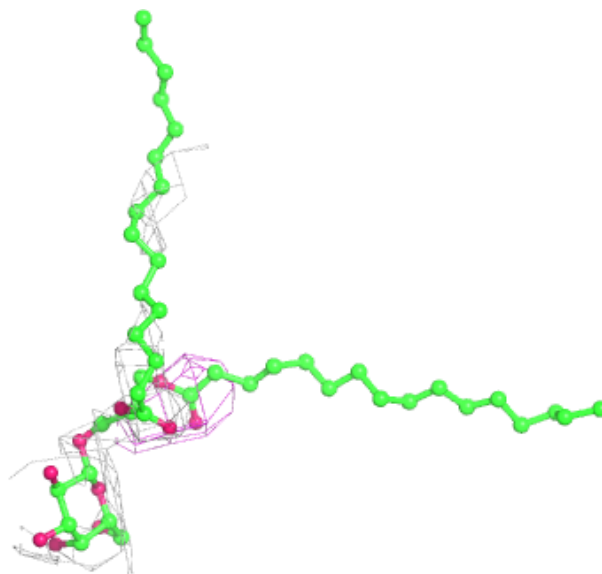
Electron density around BCR H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



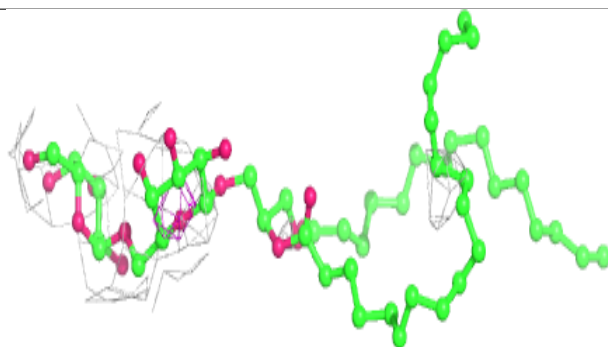
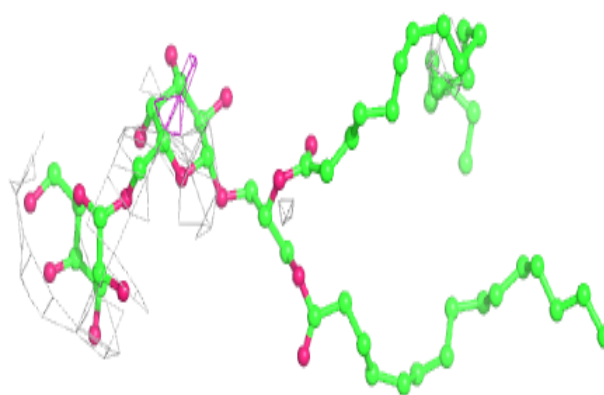
Electron density around LMG a 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

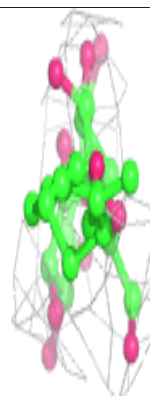
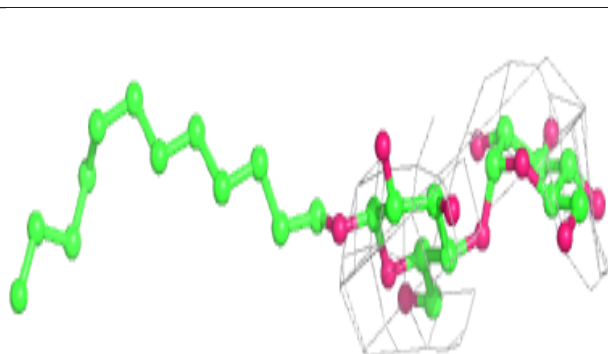
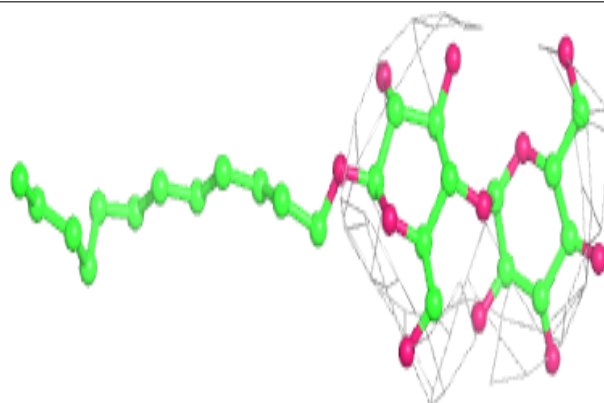


Electron density around DGD D 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

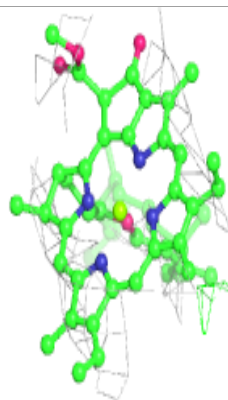
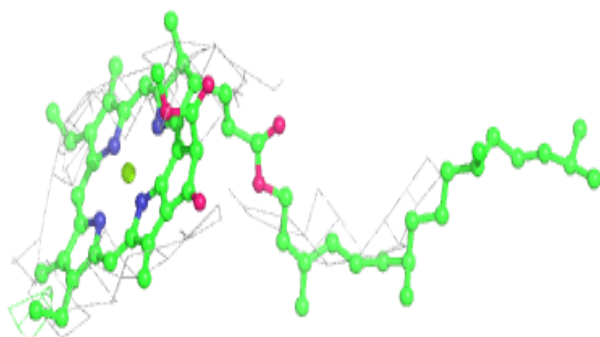
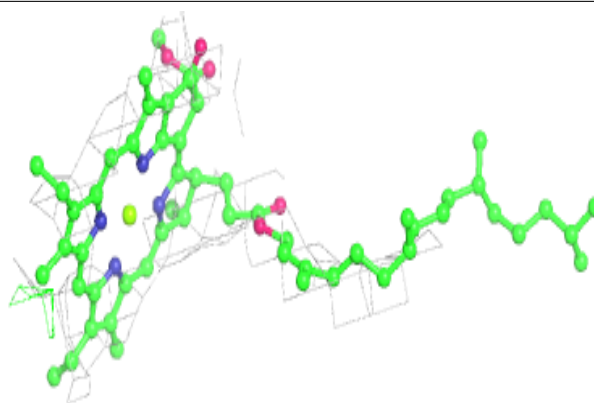
**Electron density around LMT b 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

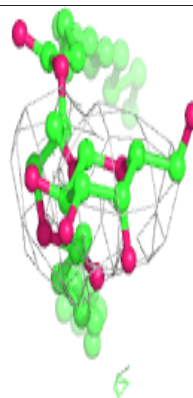
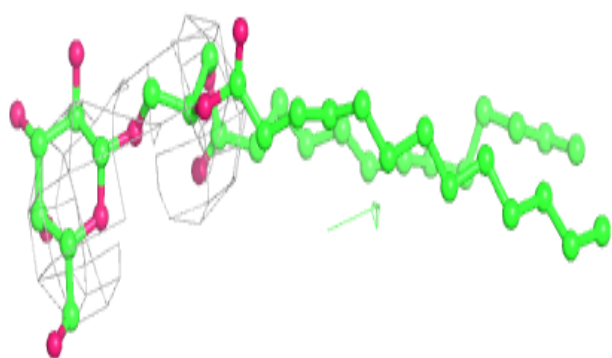
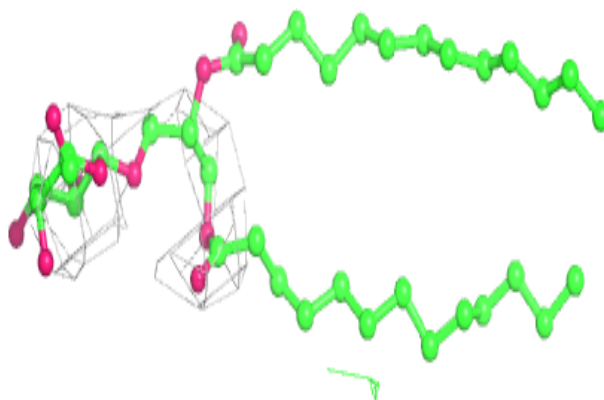


Electron density around CLA C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

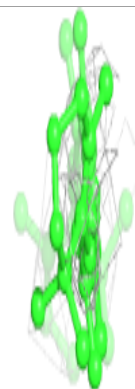
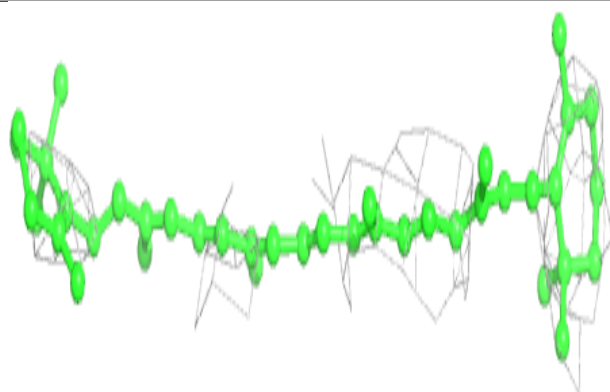
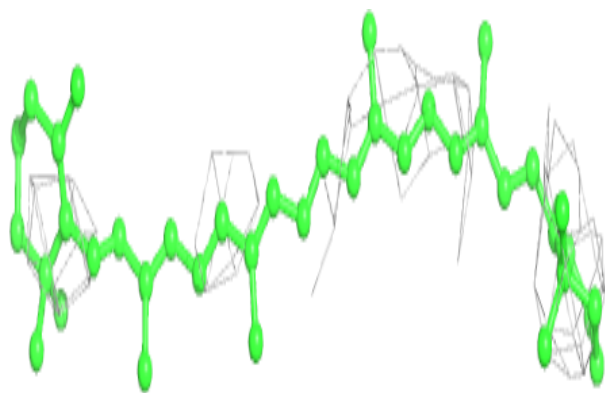
**Electron density around LMG c 518:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

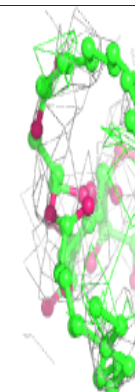
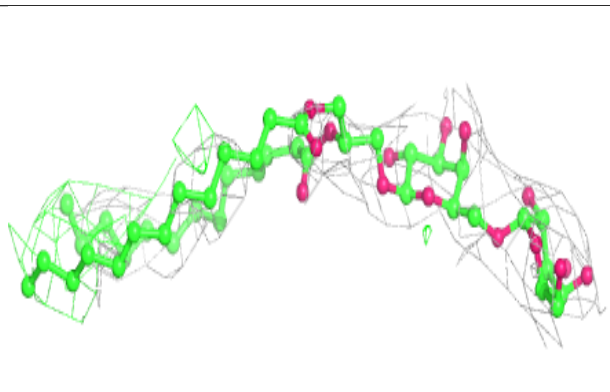
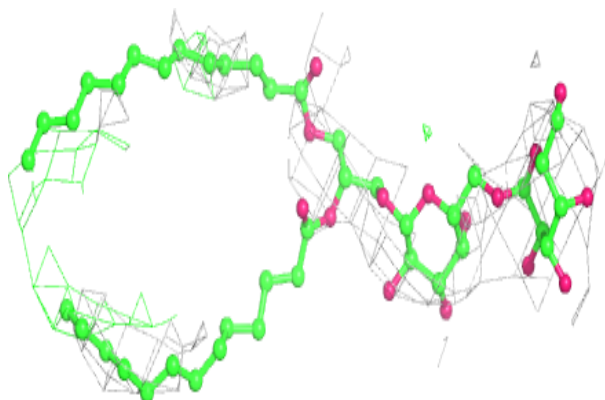


Electron density around BCR x 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

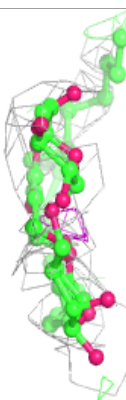
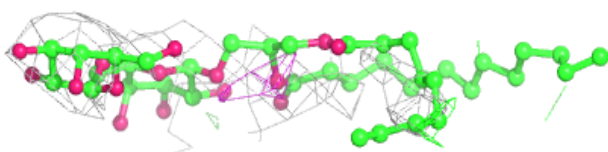
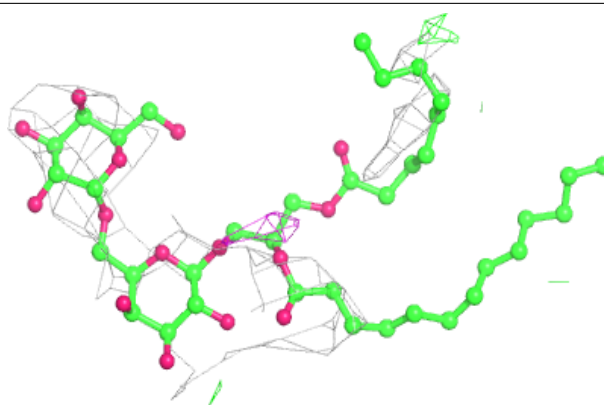
**Electron density around DGD A 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

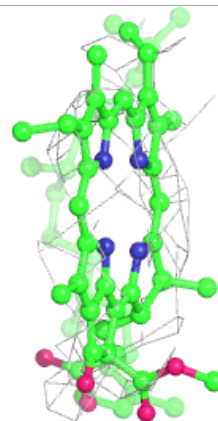
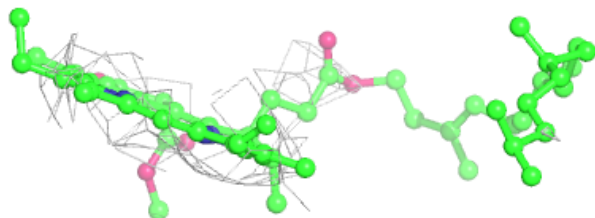
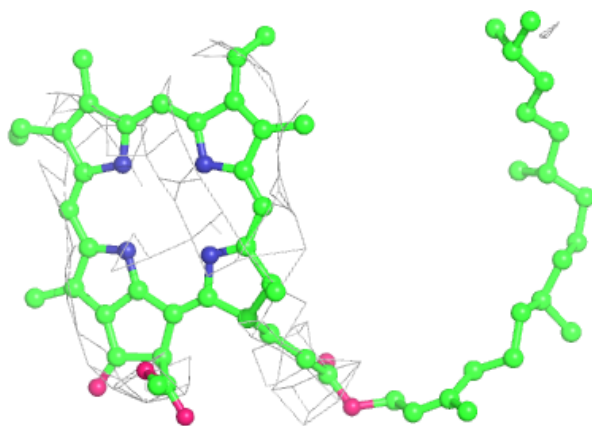


Electron density around DGD b 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

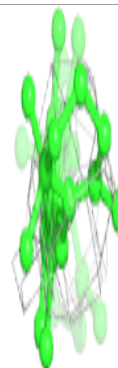
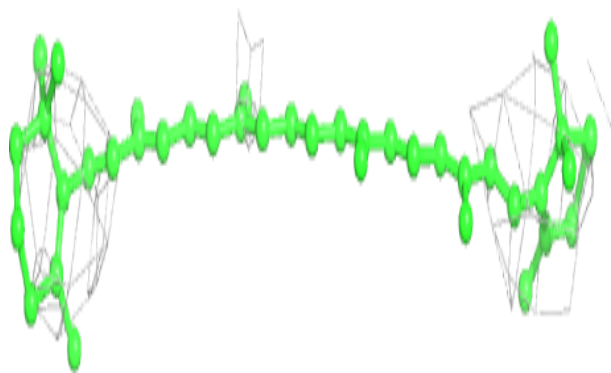
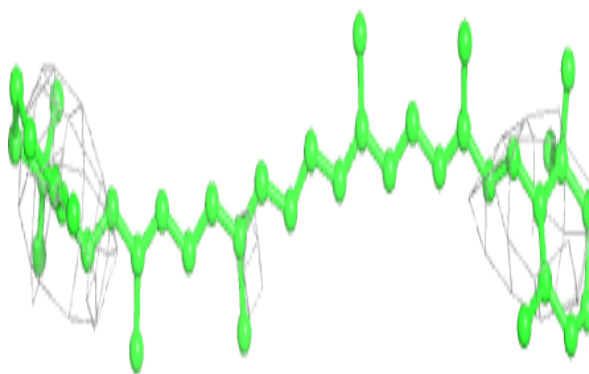
**Electron density around PHO d 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

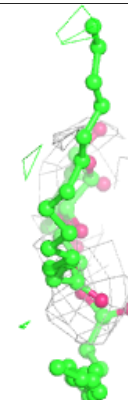
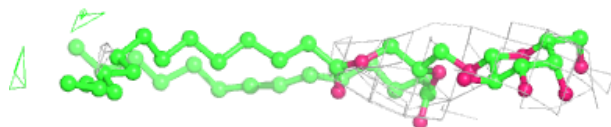
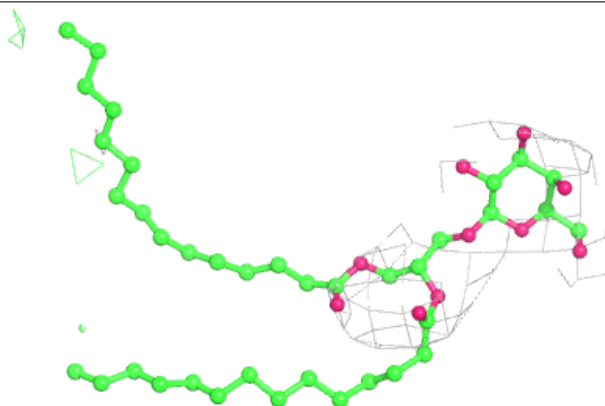


Electron density around BCR B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

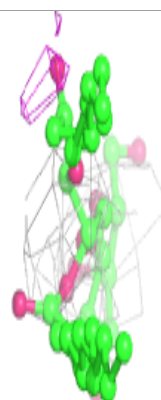
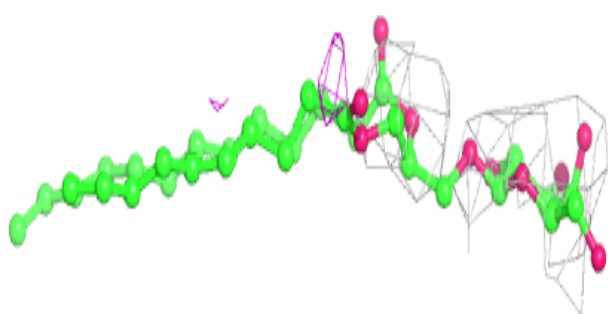
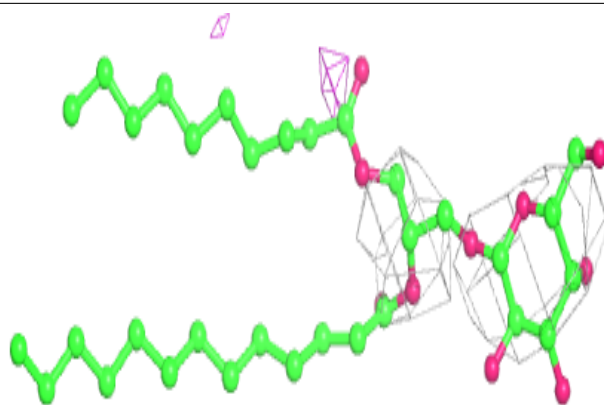
**Electron density around LMG C 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

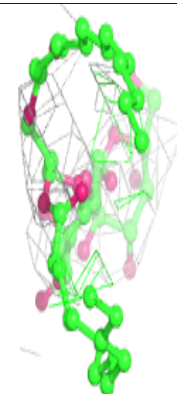
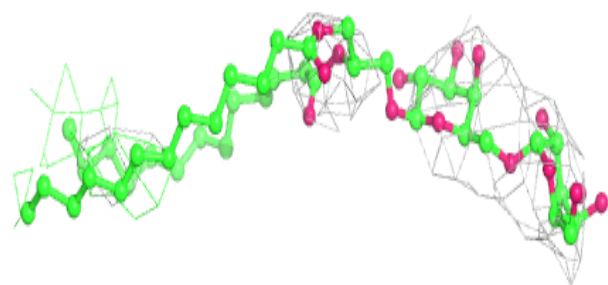
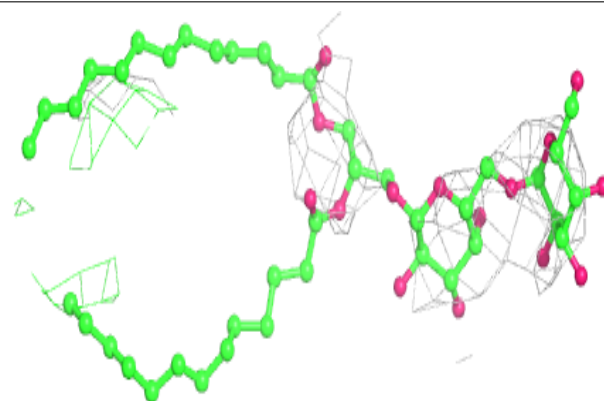


Electron density around LMG M 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

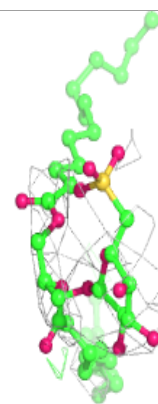
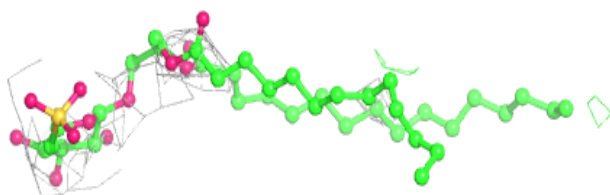
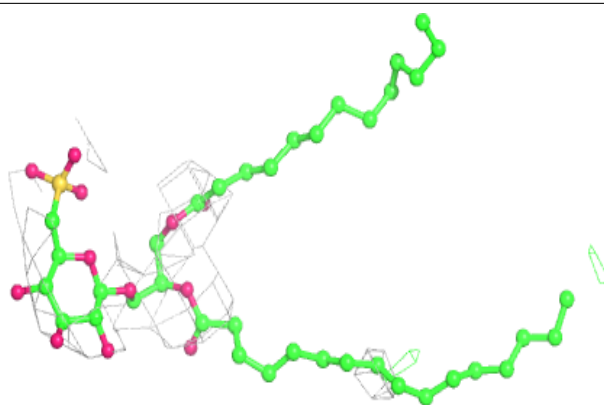
**Electron density around DGD a 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

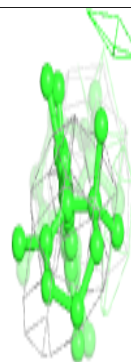
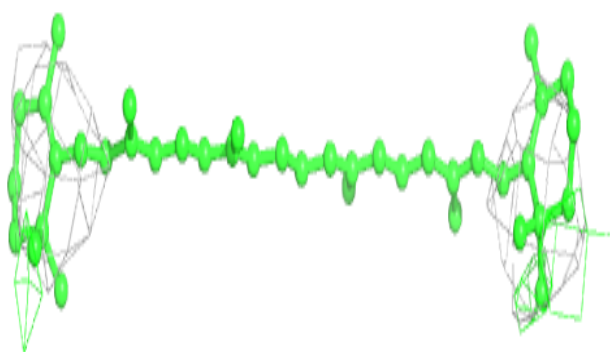
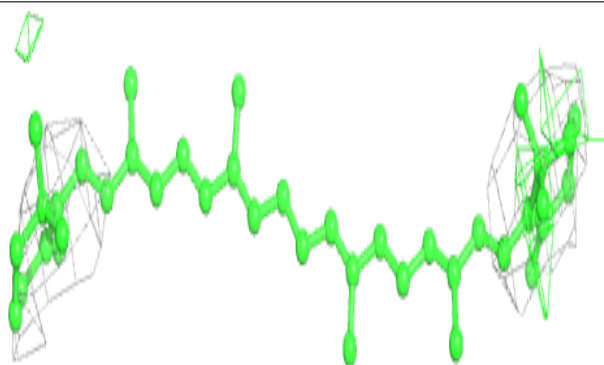


Electron density around SQD A 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

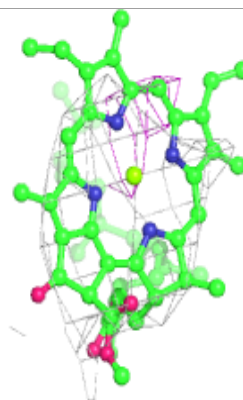
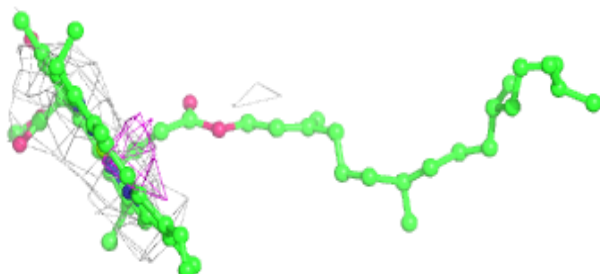
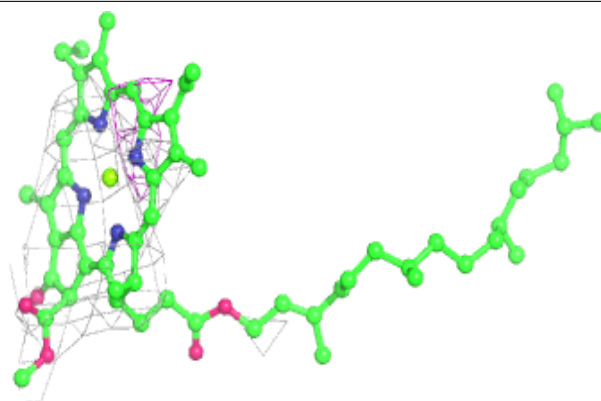
**Electron density around BCR a 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

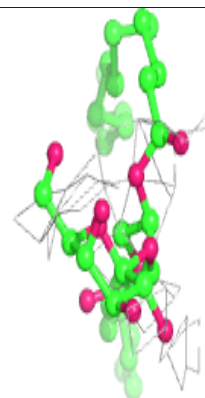
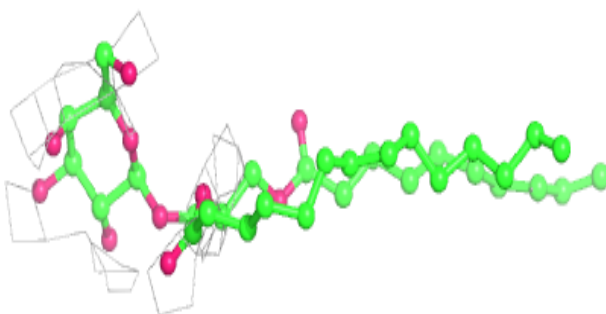
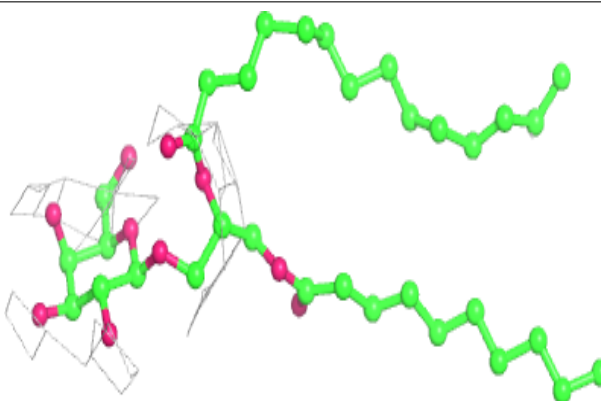


Electron density around CLA a 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

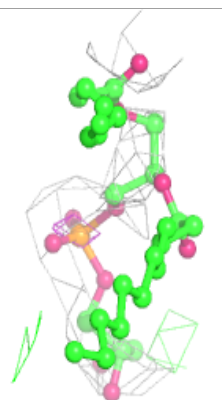
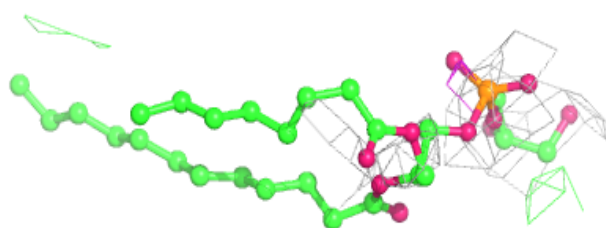
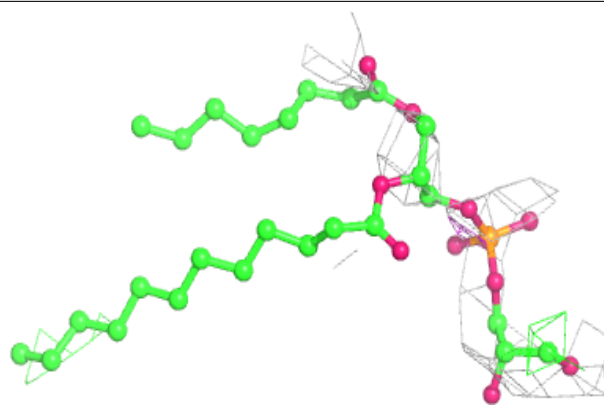
**Electron density around LMG i 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

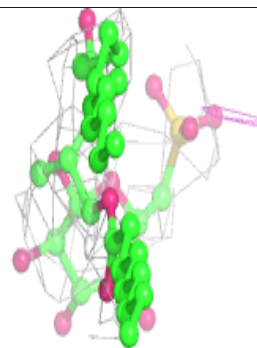
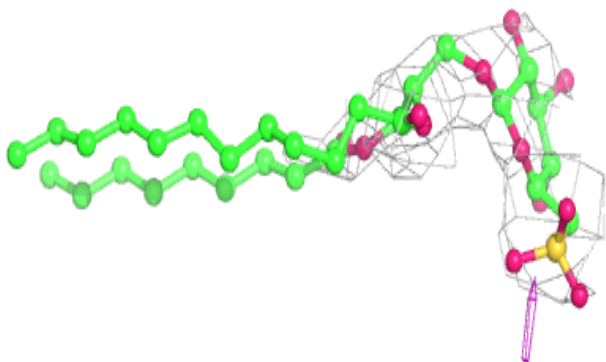
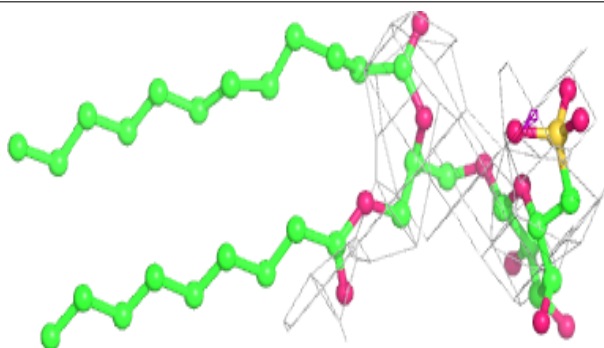


Electron density around LHG c 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

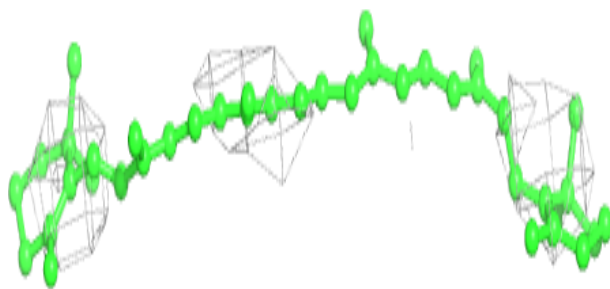
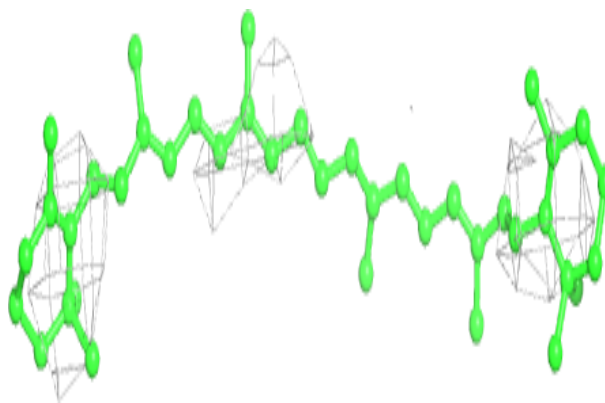
**Electron density around SQD d 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



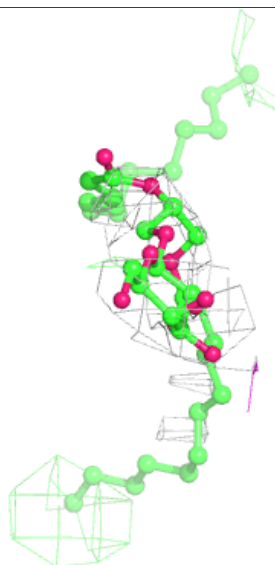
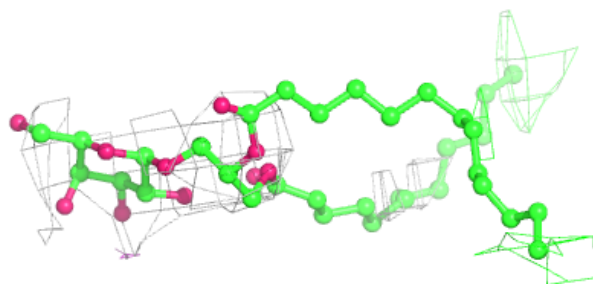
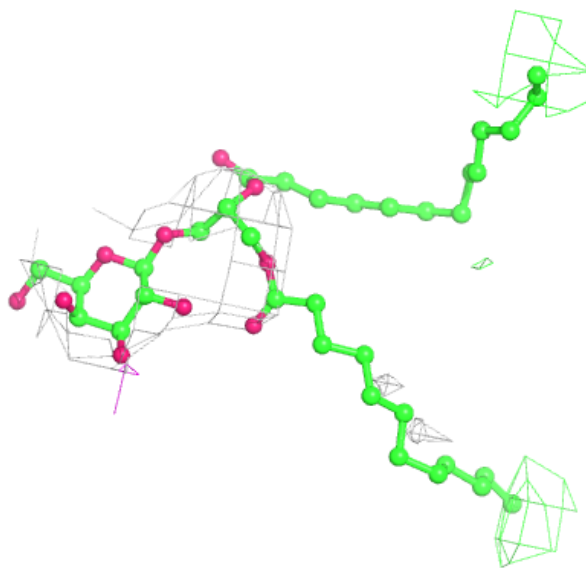
Electron density around BCR B 617:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



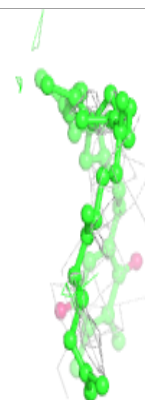
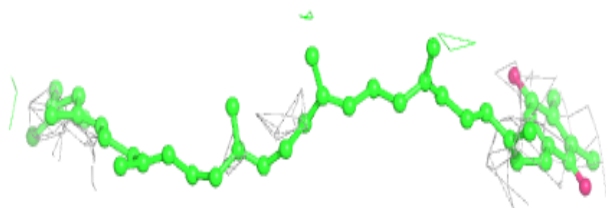
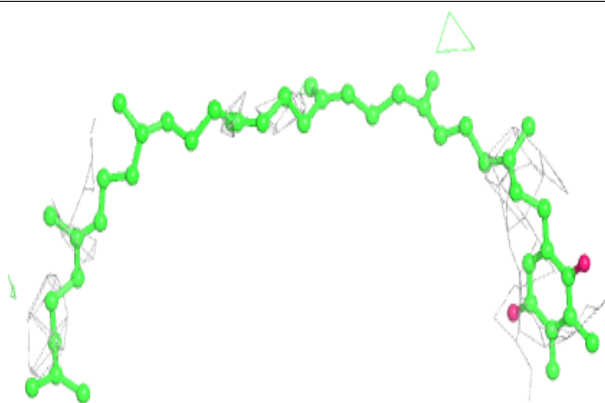
Electron density around LMG e 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

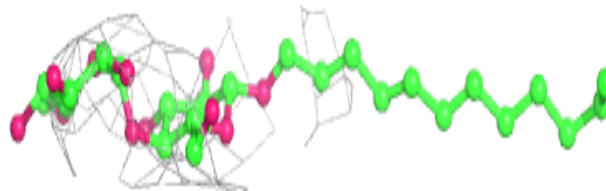
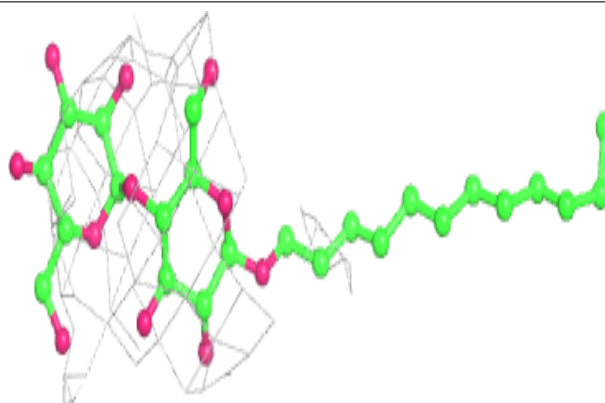


Electron density around PL9 a 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

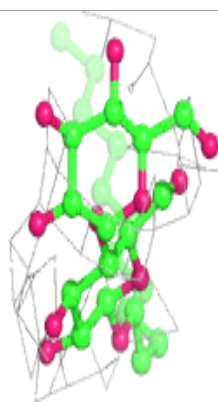
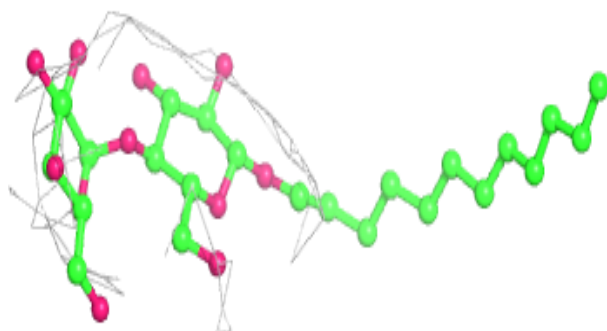
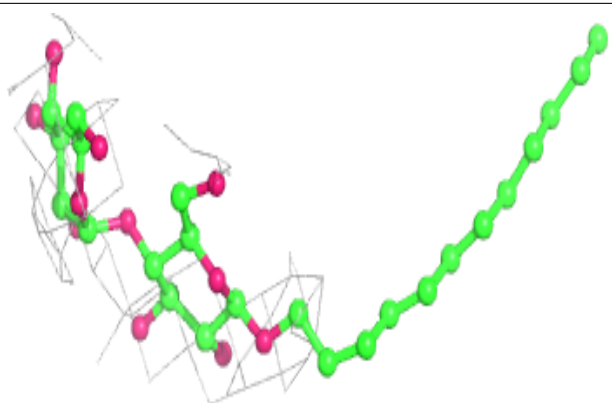
**Electron density around LMT B 627:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

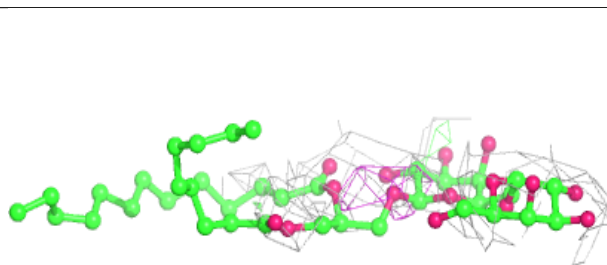
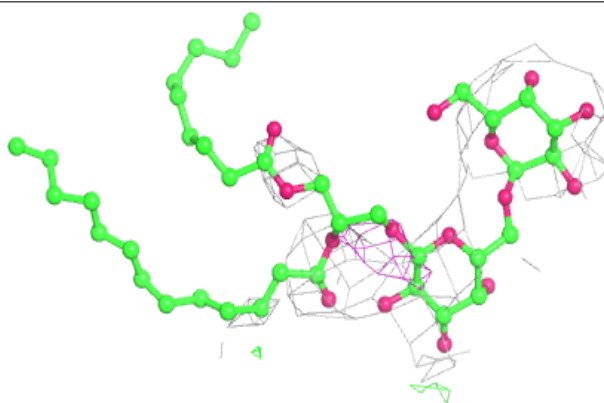


Electron density around LMT M 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

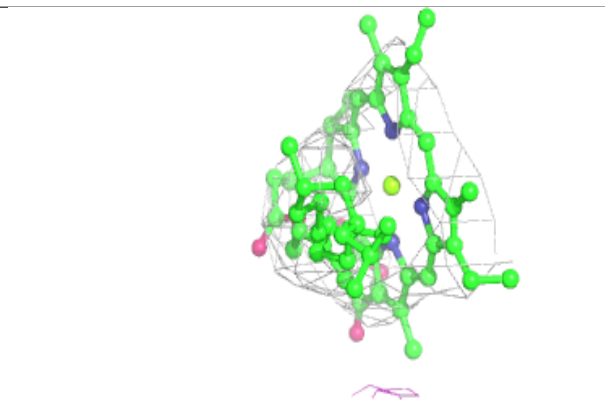
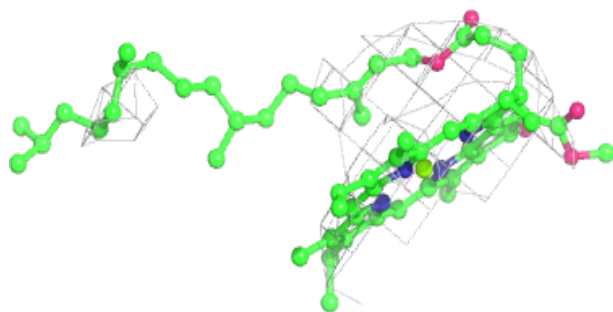
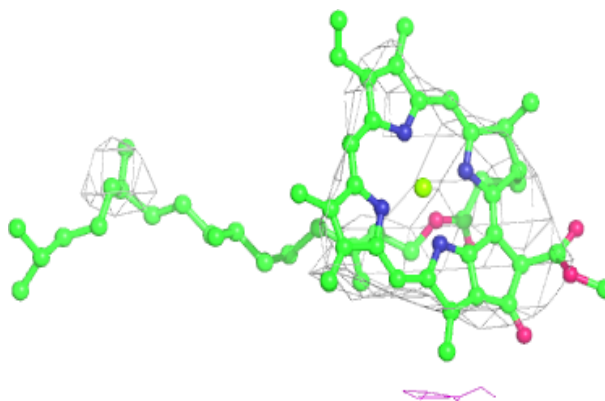
**Electron density around DGD B 625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

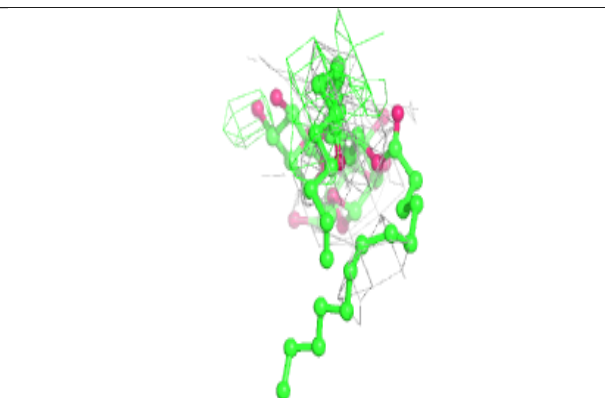
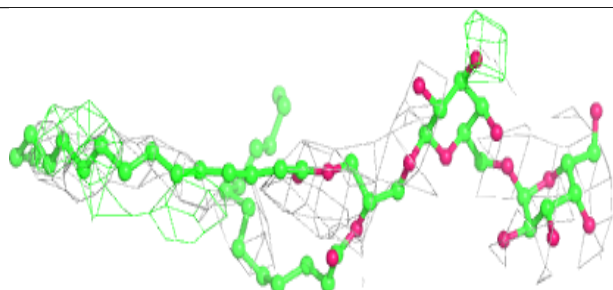
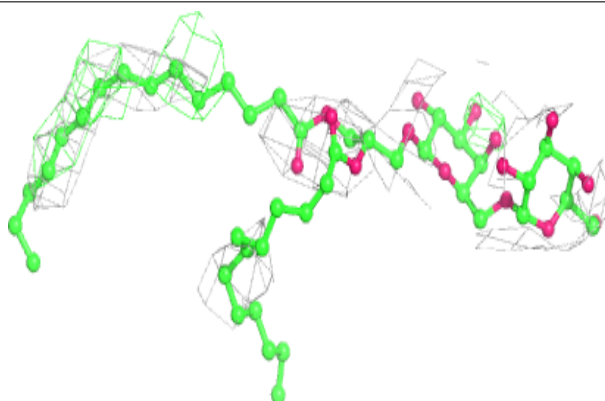


Electron density around CLA B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

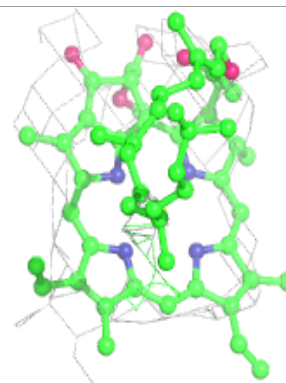
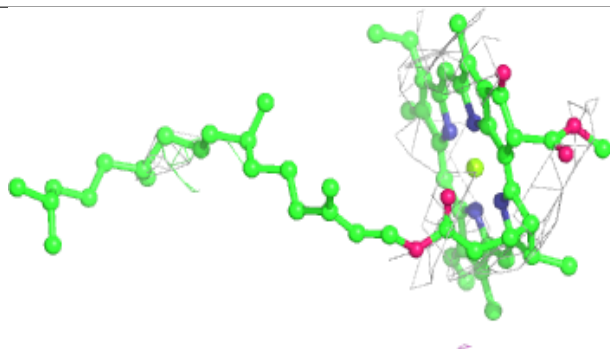
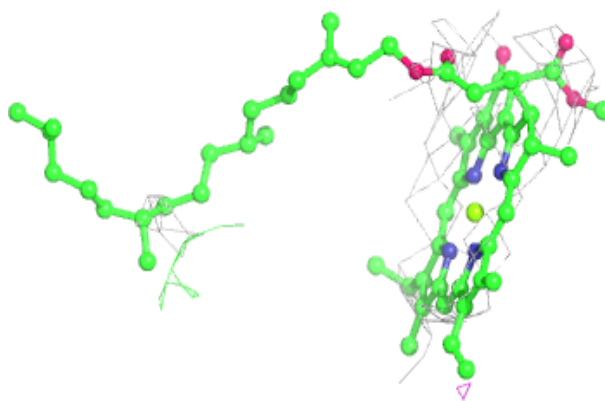
**Electron density around DGD b 624:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

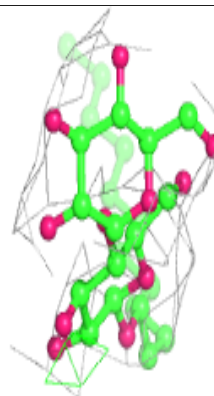
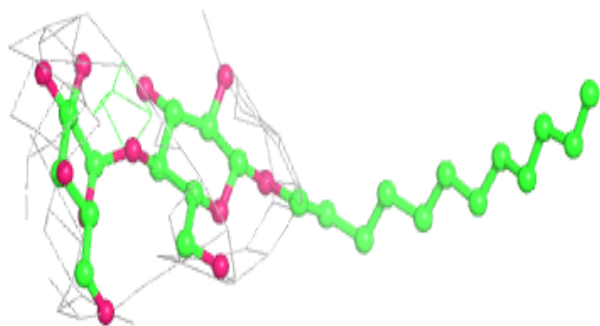
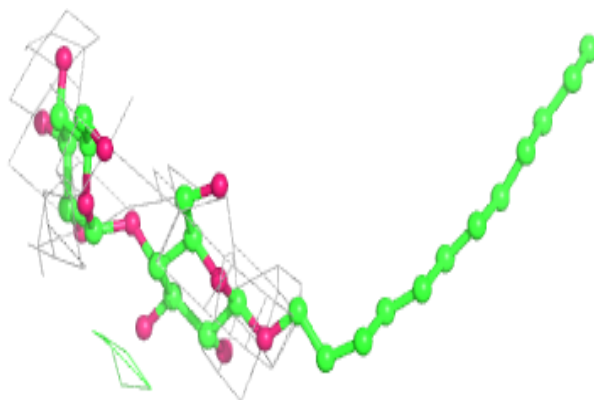


Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

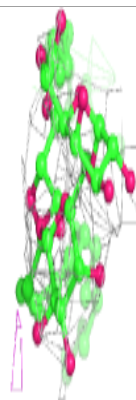
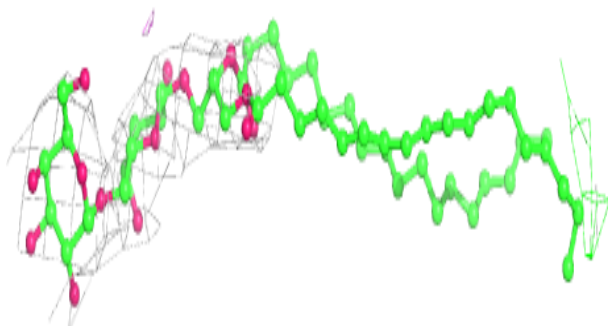
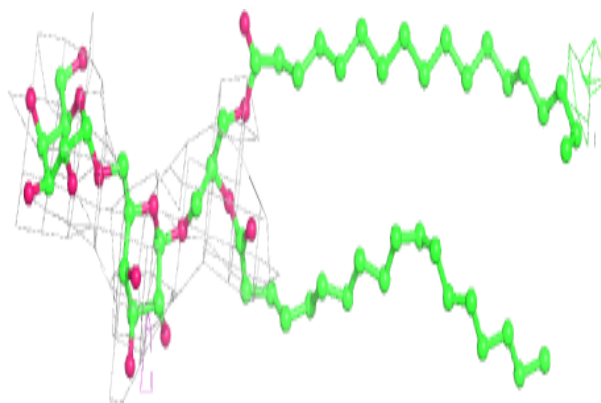
**Electron density around LMT M 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



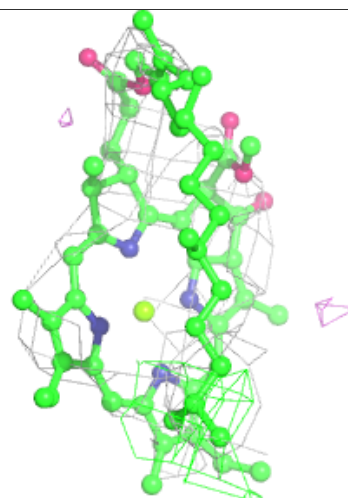
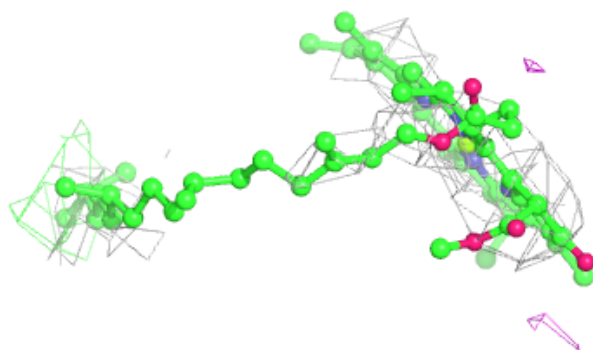
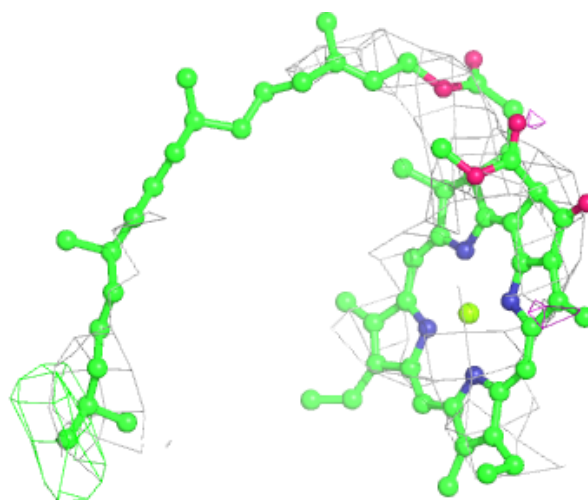
Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



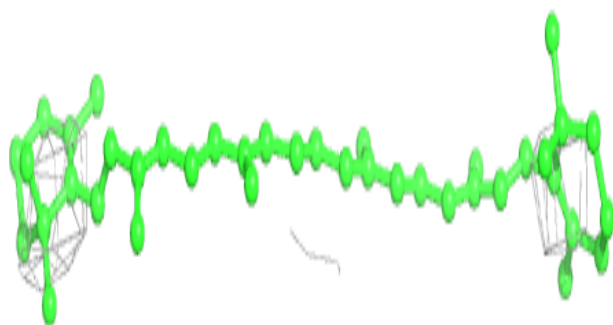
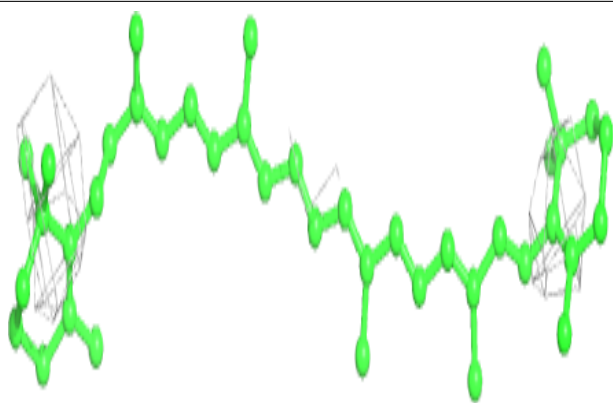
Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

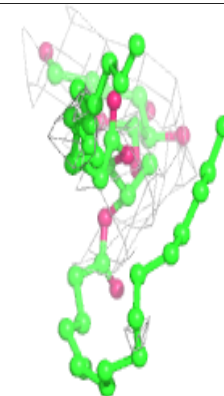
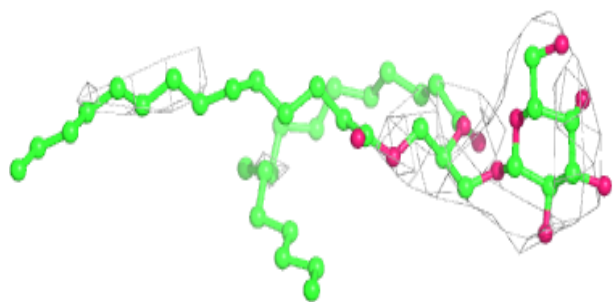
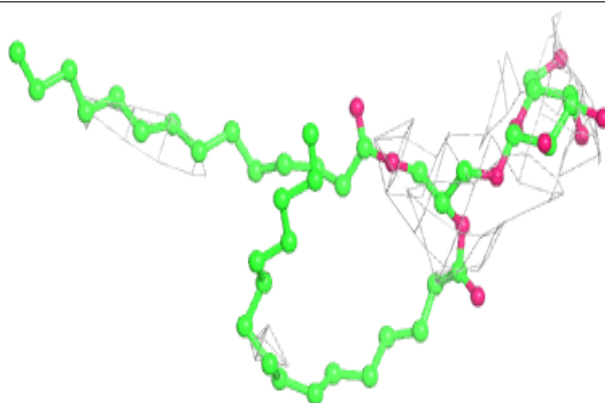


Electron density around BCR y 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

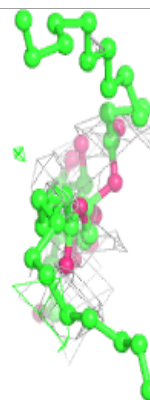
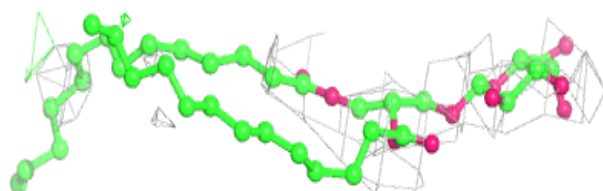
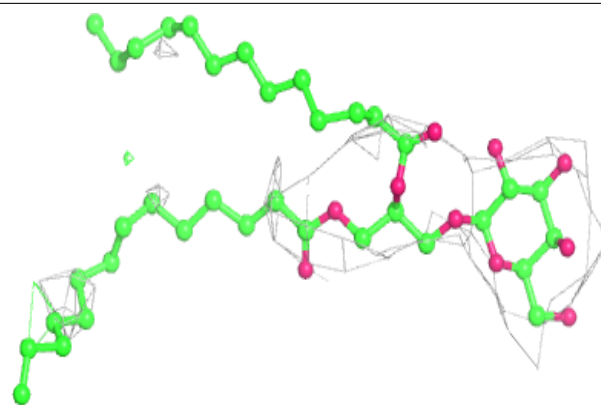
**Electron density around LMG B 624:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

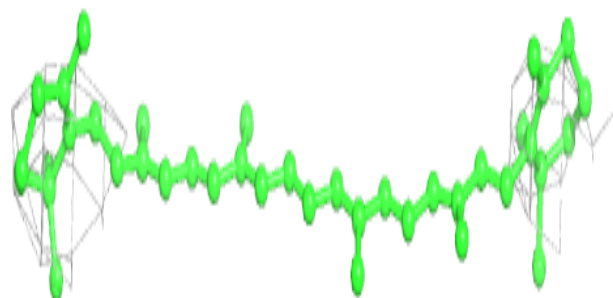
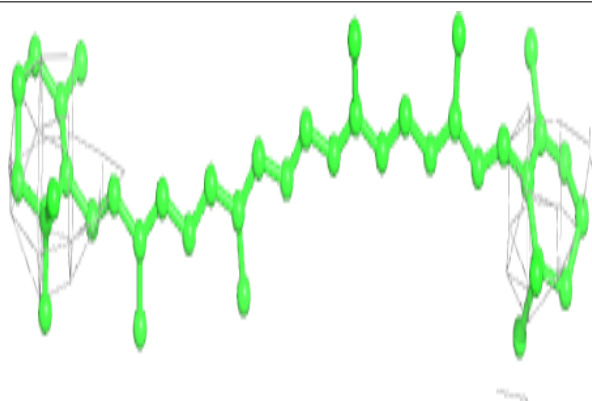


Electron density around LMG D 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

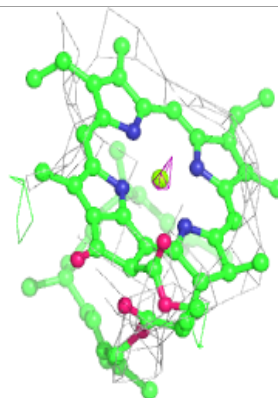
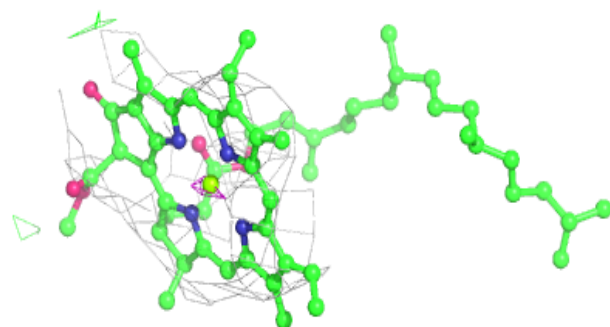
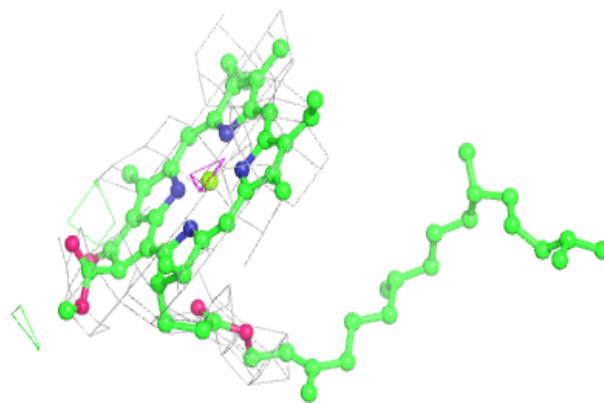
**Electron density around BCR C 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

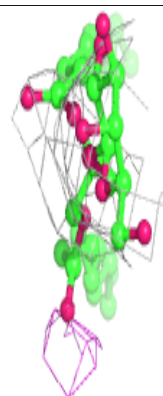
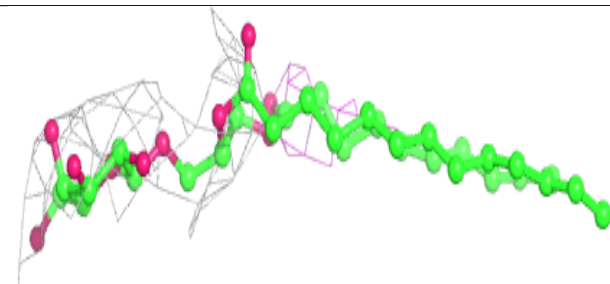
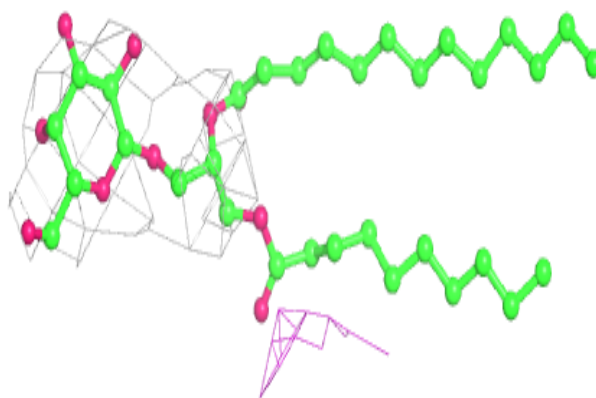


Electron density around CLA c 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

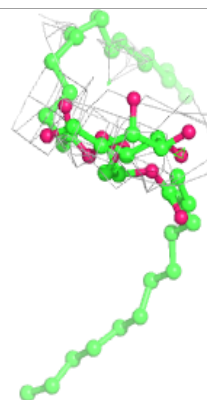
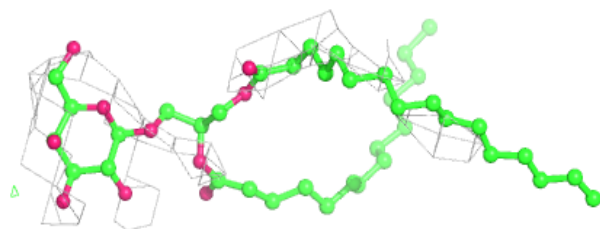
**Electron density around LMG m 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

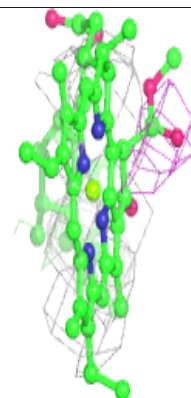
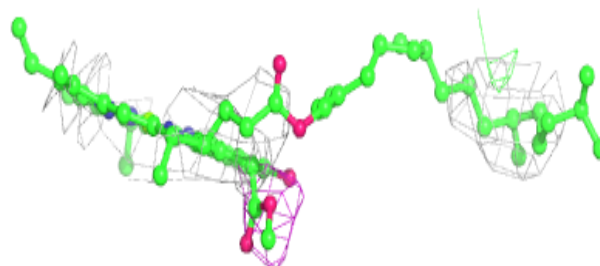
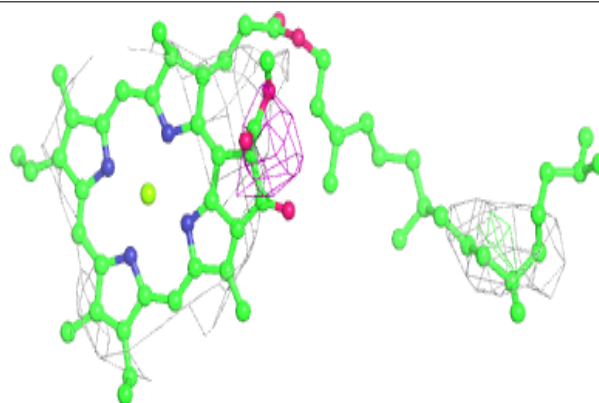


Electron density around LMG b 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

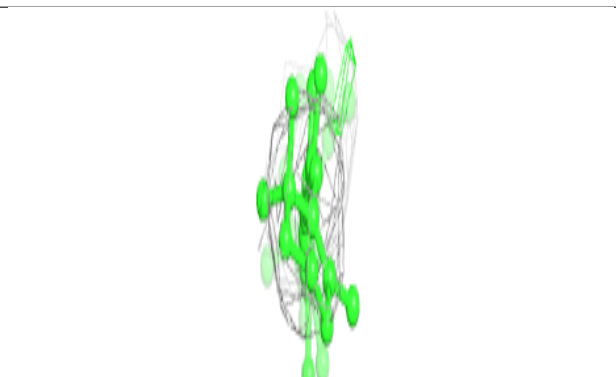
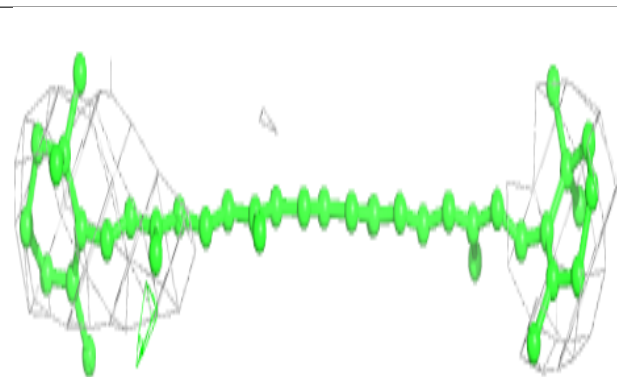
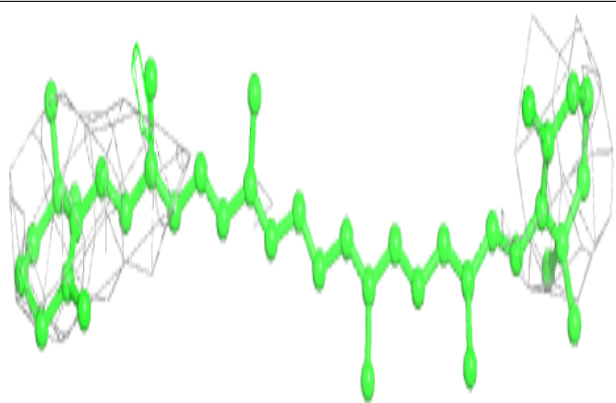
**Electron density around CLA h 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

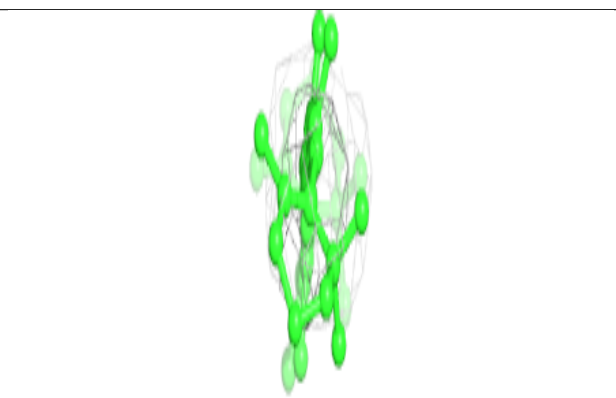
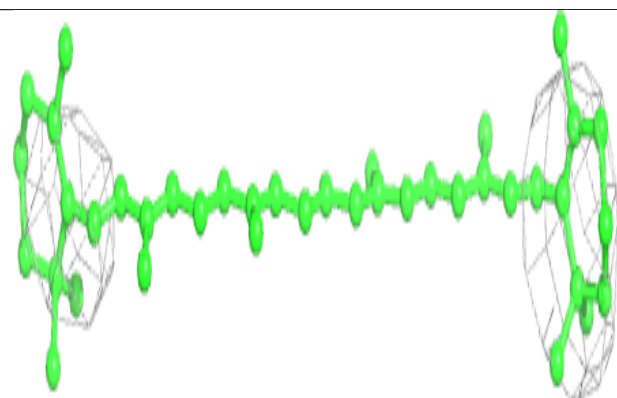
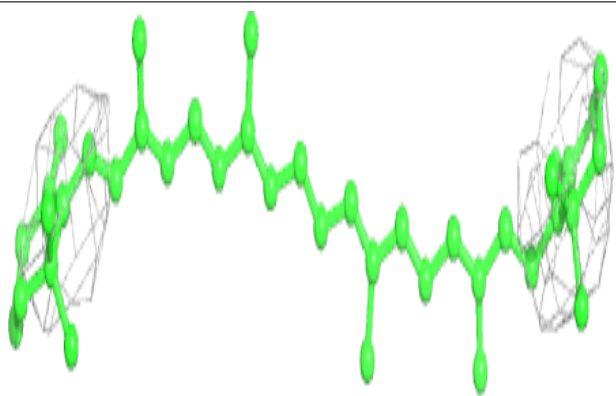


Electron density around BCR b 622:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

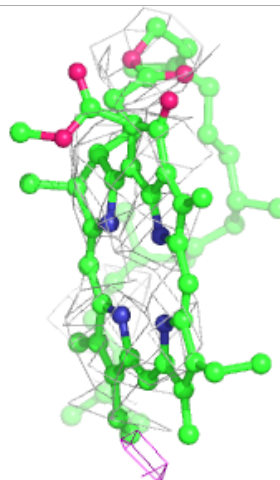
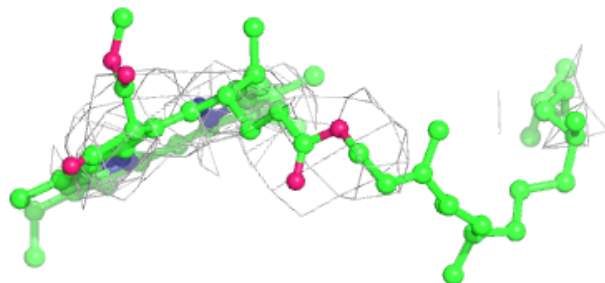
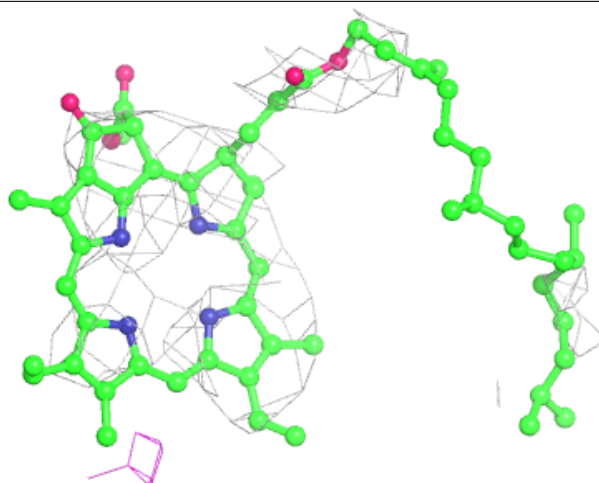
**Electron density around BCR A 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



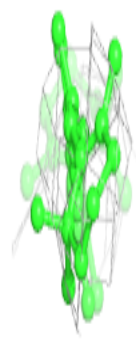
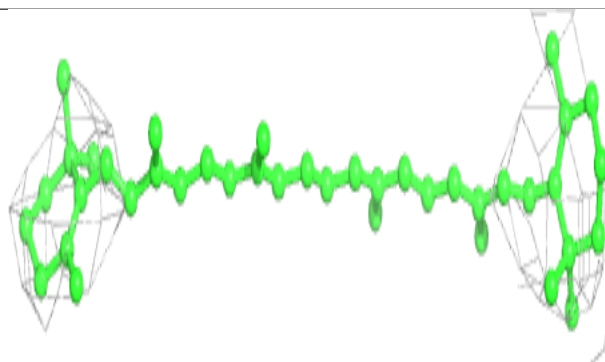
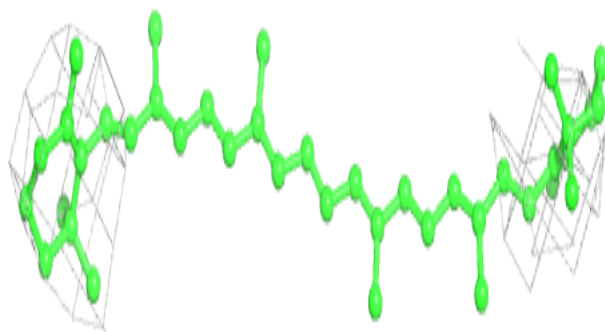
Electron density around PHO D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

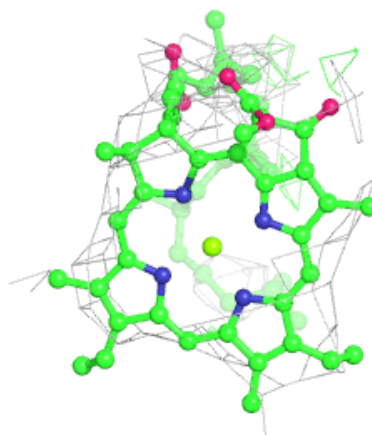
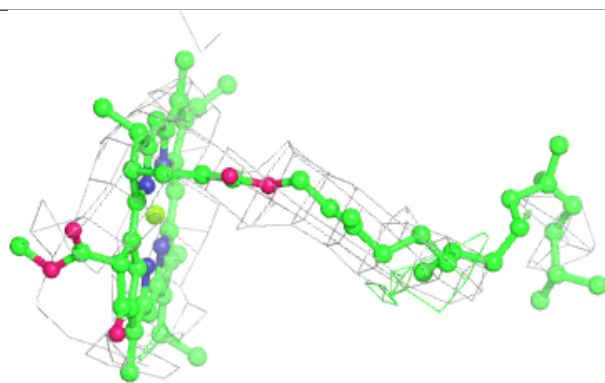
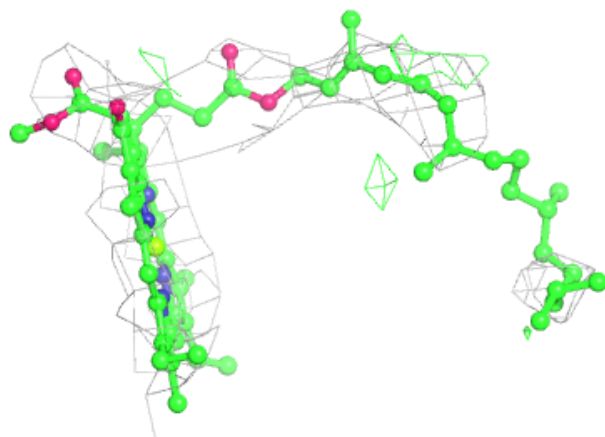


Electron density around BCR C 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

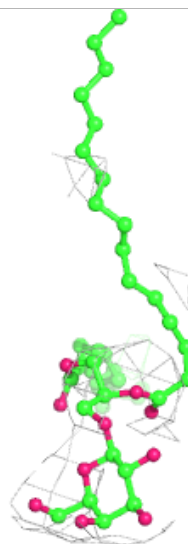
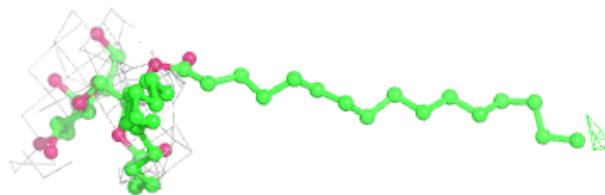
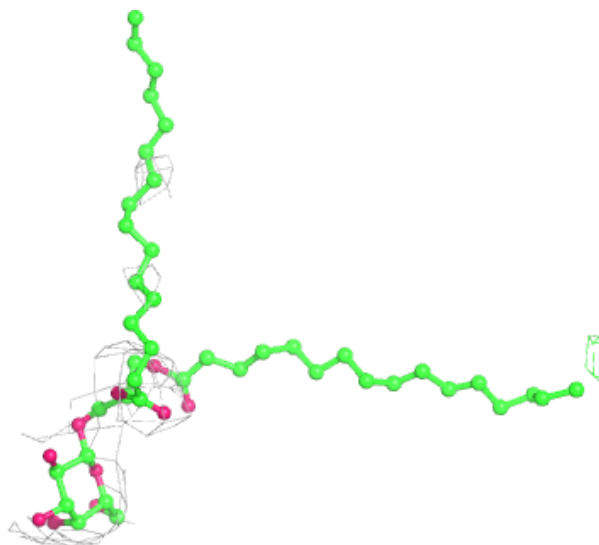
**Electron density around CLA C 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



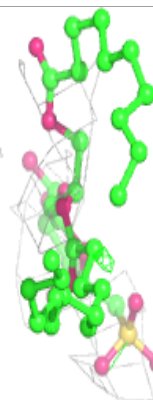
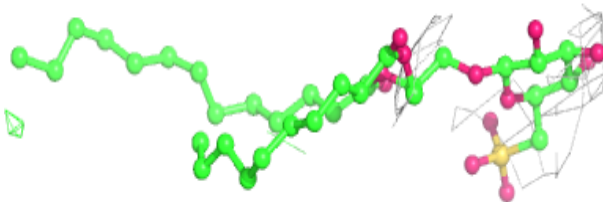
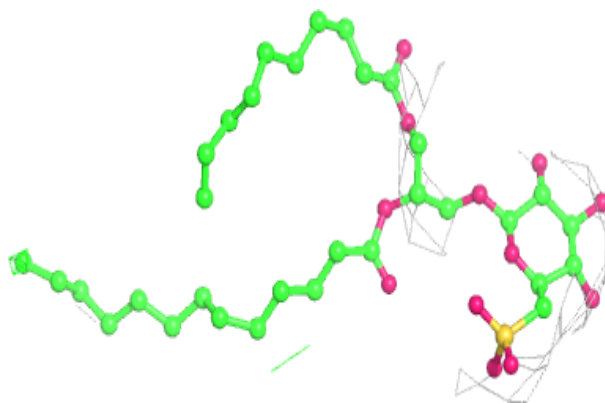
Electron density around LMG A 410:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

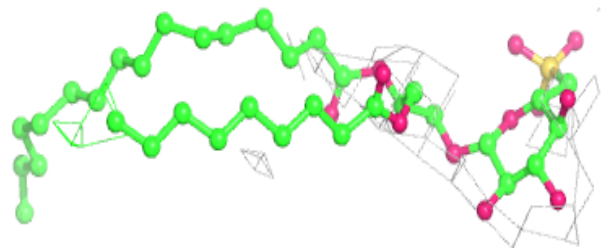
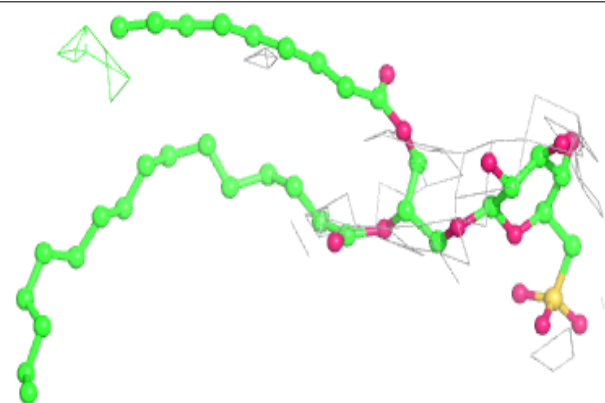


Electron density around SQD F 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

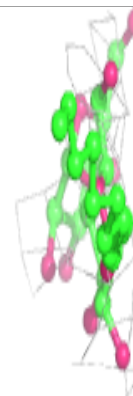
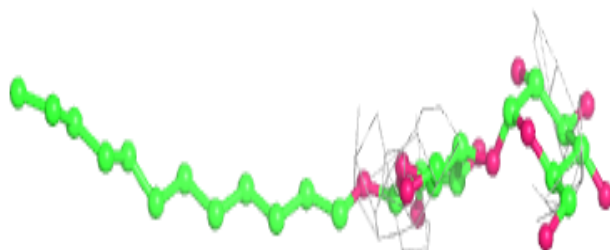
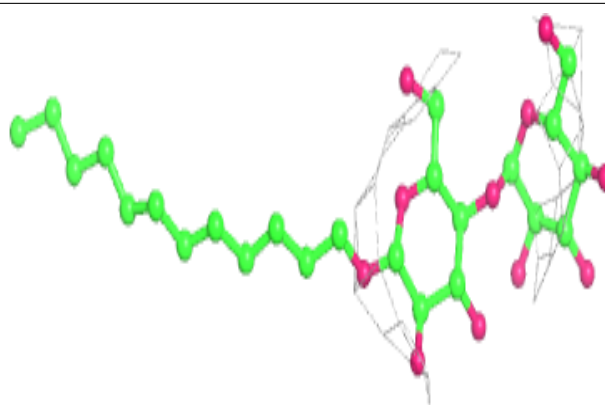
**Electron density around SQD B 626:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

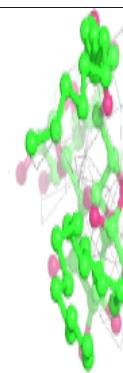
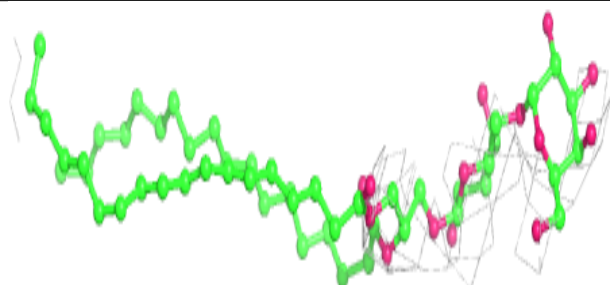
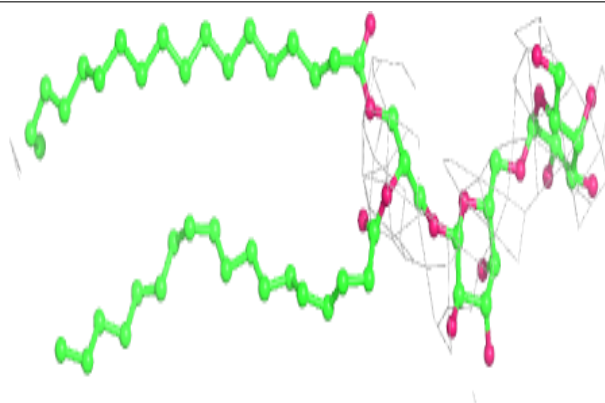


Electron density around LMT B 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

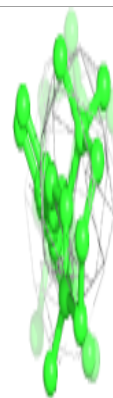
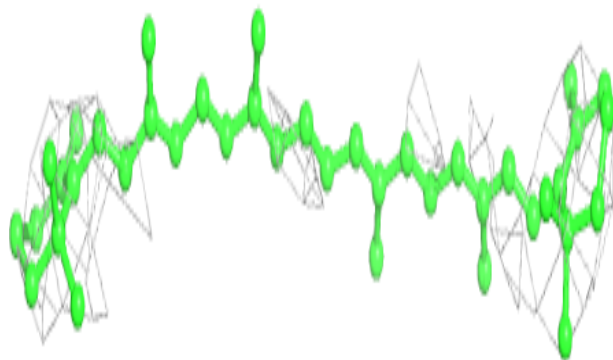
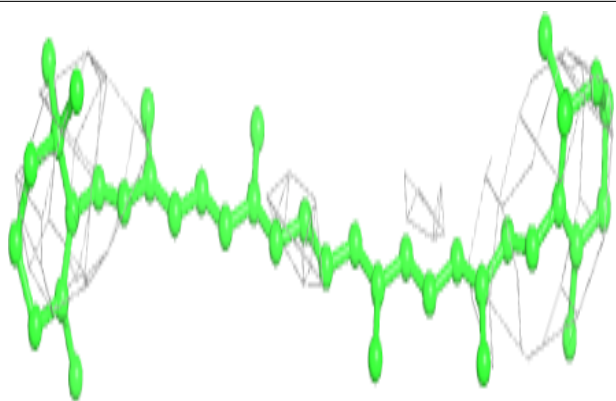
**Electron density around DGD c 517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

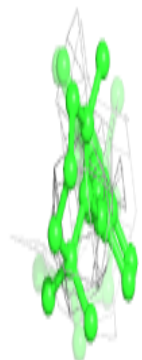
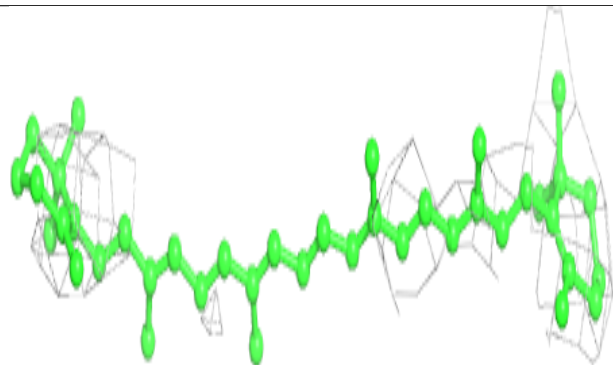
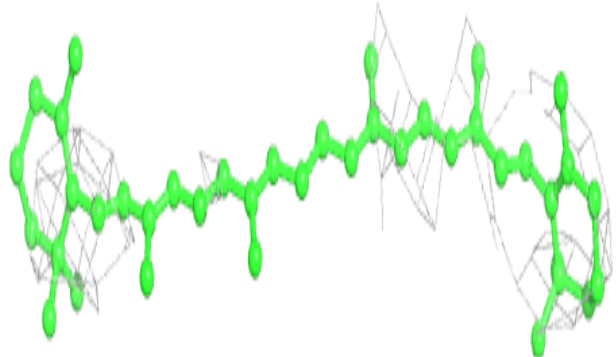


Electron density around BCR b 623:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

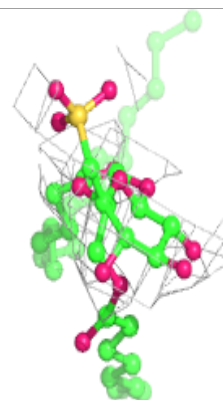
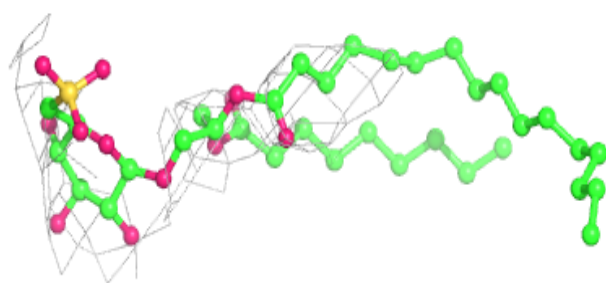
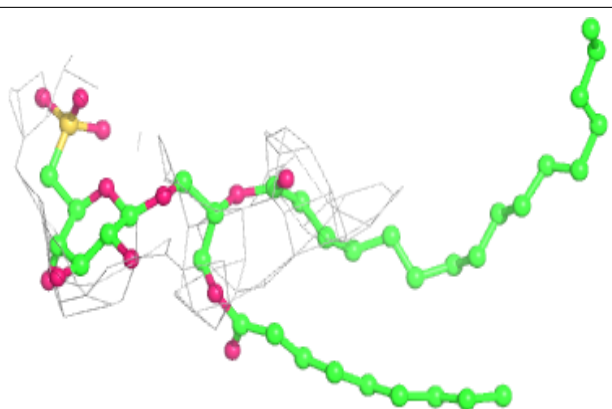
**Electron density around BCR B 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

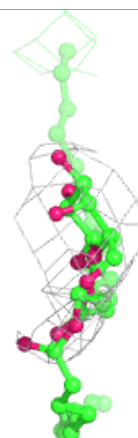
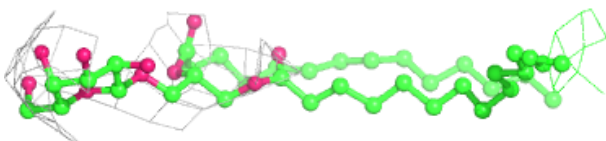
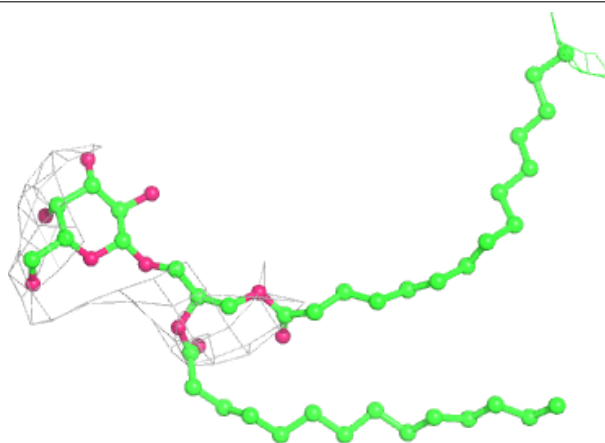


Electron density around SQD b 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

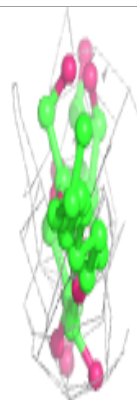
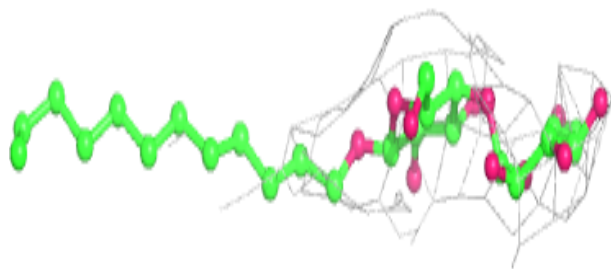
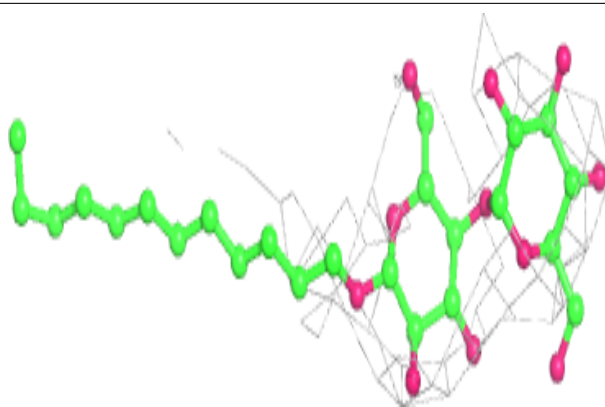
**Electron density around LMG c 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

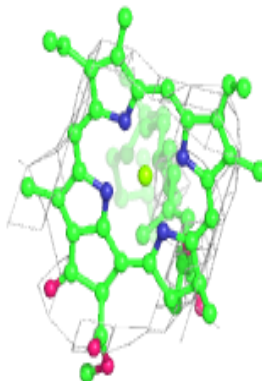
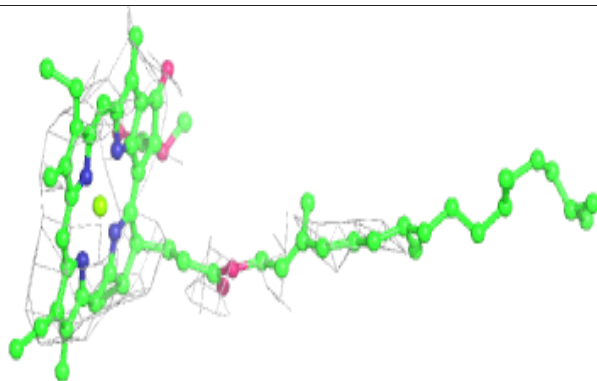
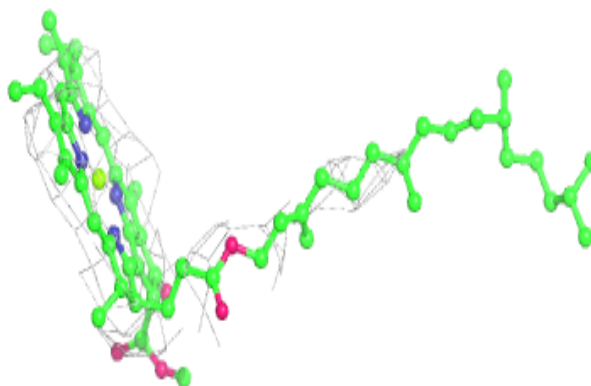


Electron density around LMT b 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

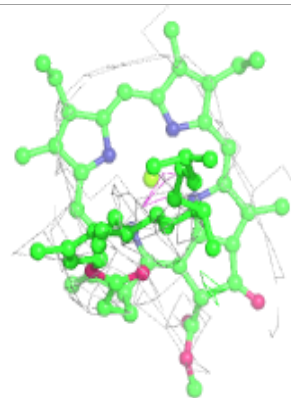
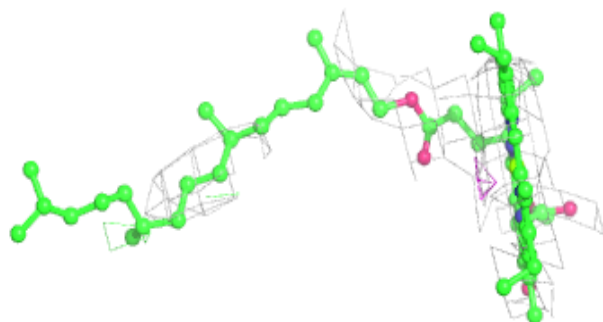
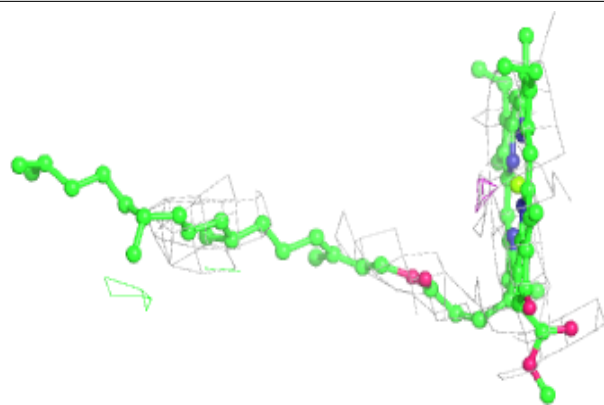
**Electron density around CLA B 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

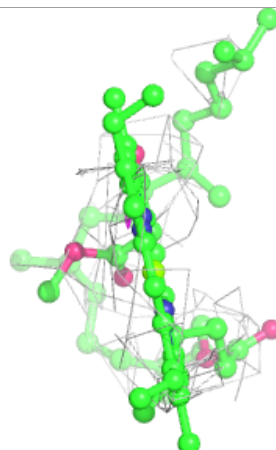
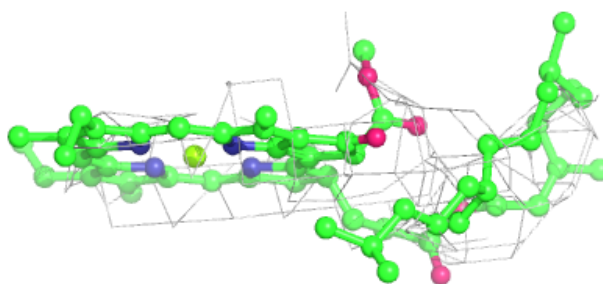
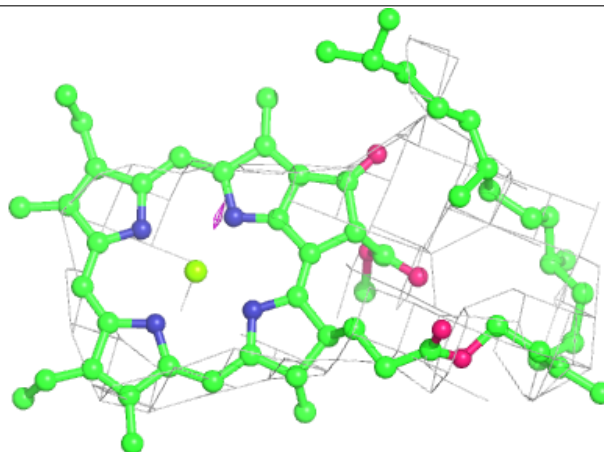


Electron density around CLA b 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

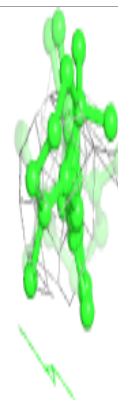
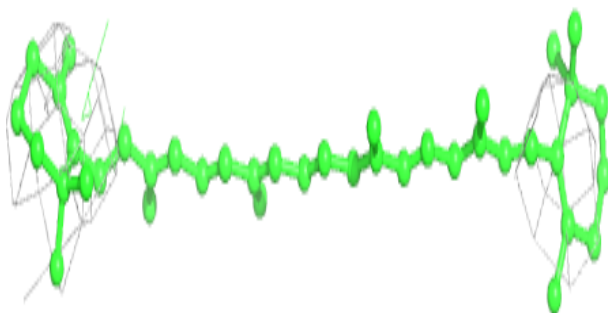
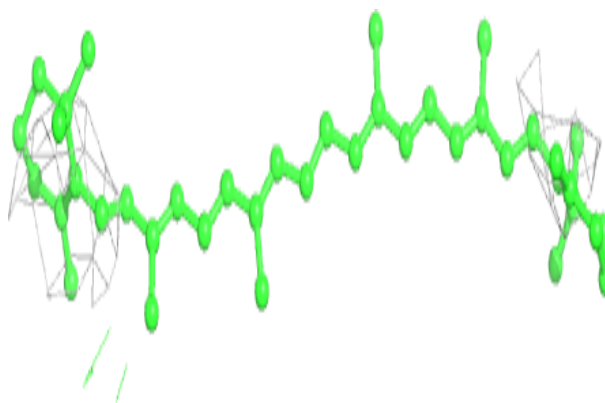
**Electron density around CLA b 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



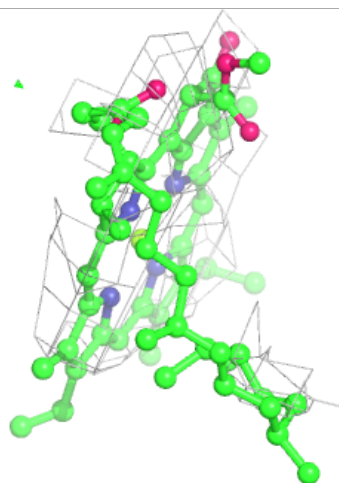
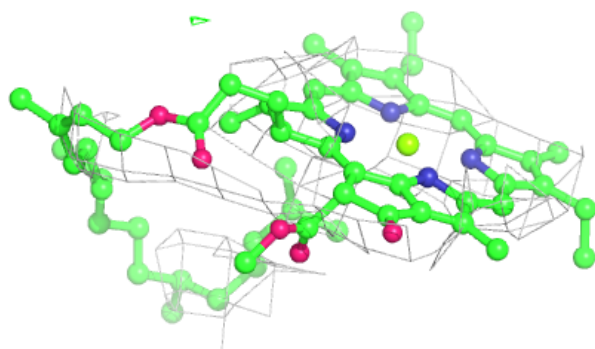
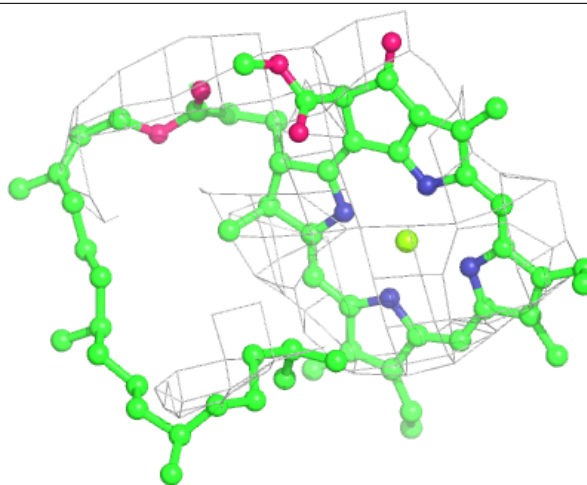
Electron density around BCR c 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



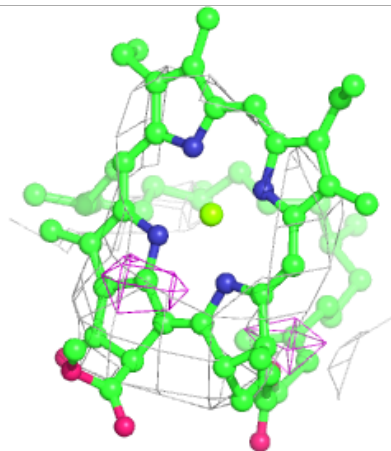
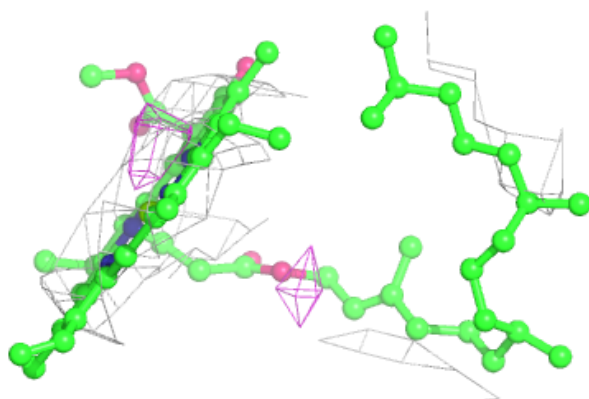
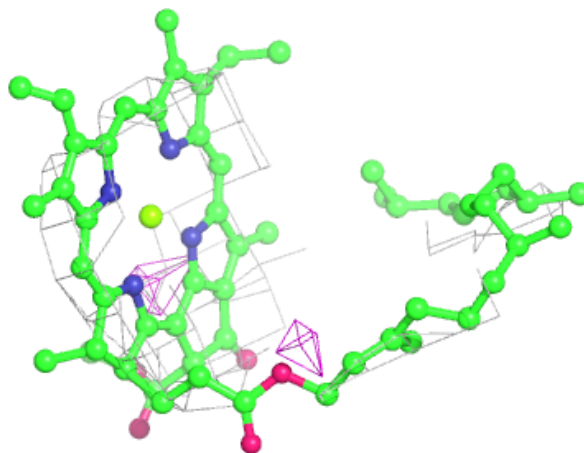
Electron density around CLA b 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



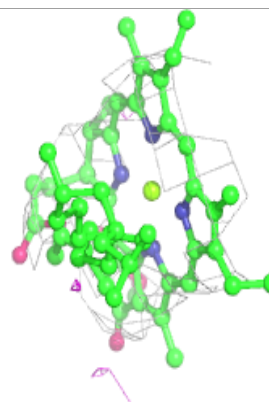
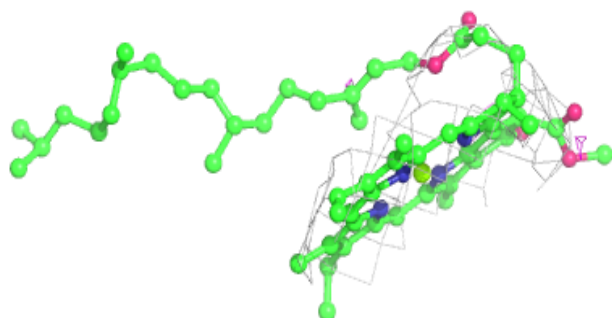
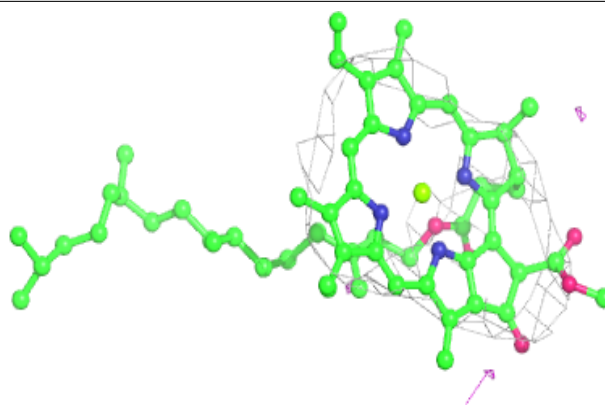
Electron density around CLA c 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

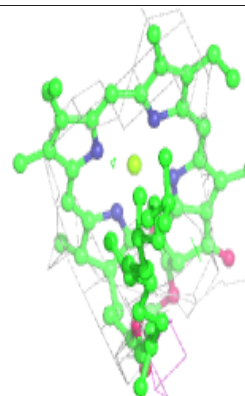
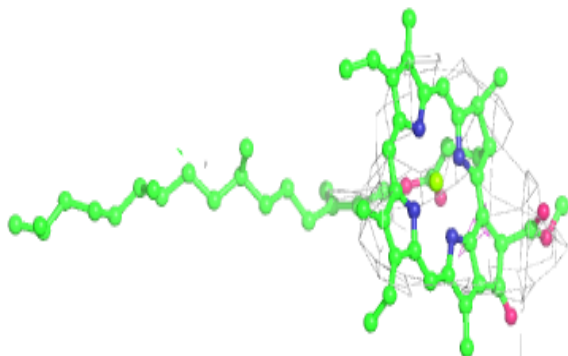
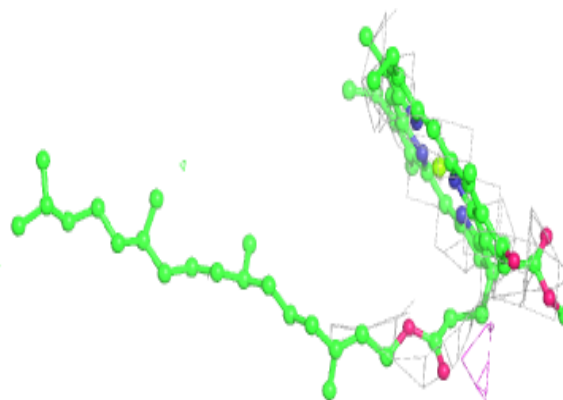


Electron density around CLA b 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

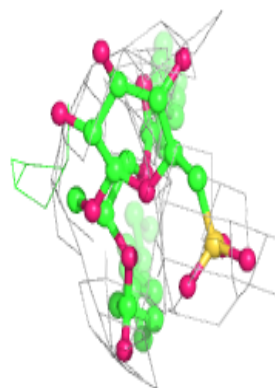
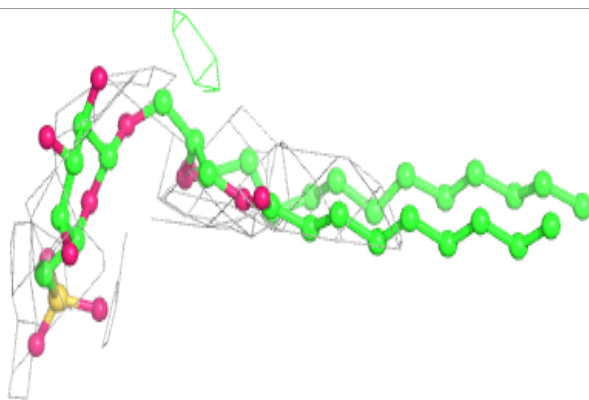
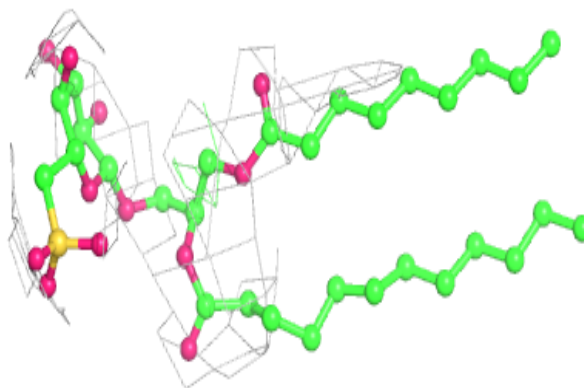
**Electron density around CLA C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

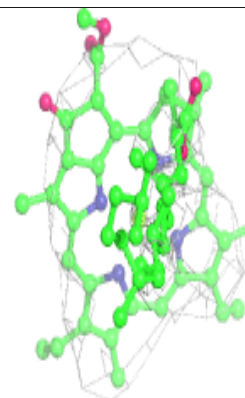
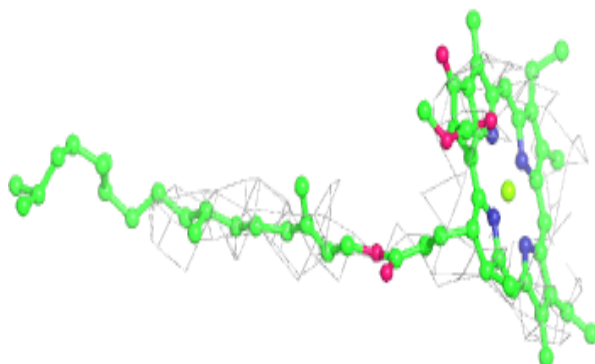
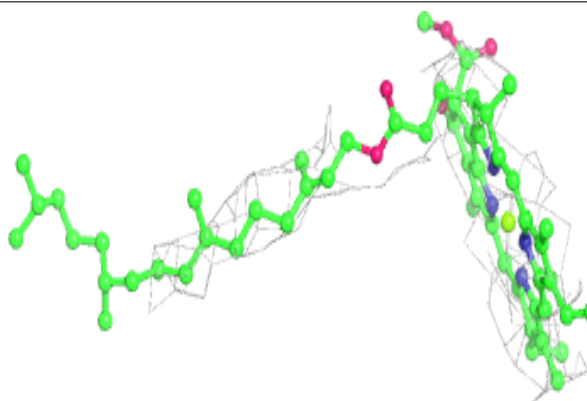


Electron density around SQD D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

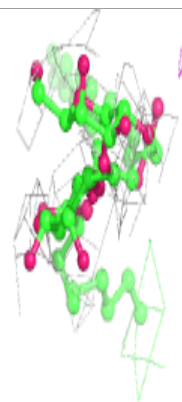
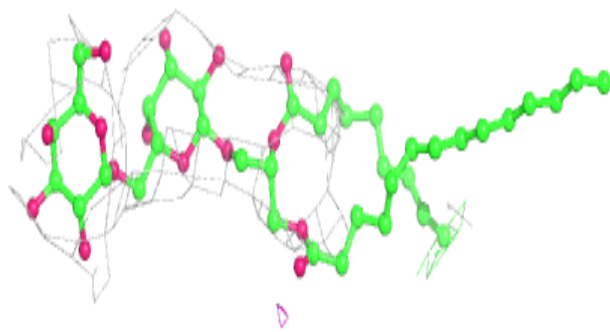
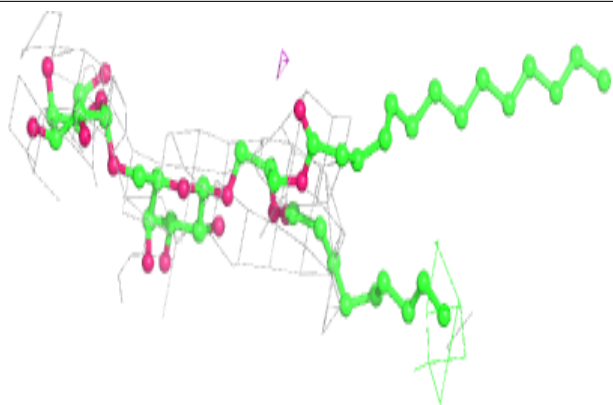
**Electron density around CLA b 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

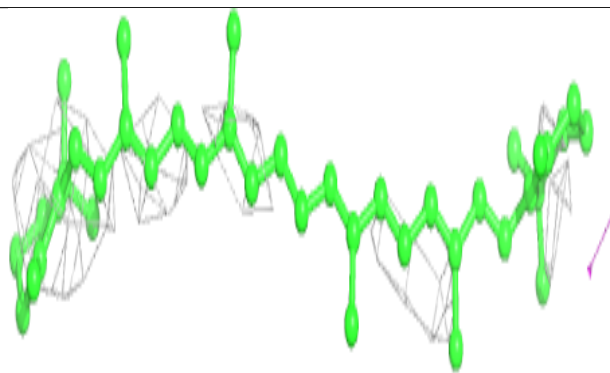
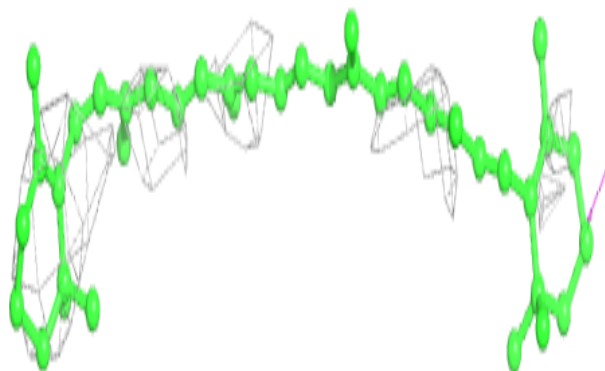


Electron density around DGD C 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

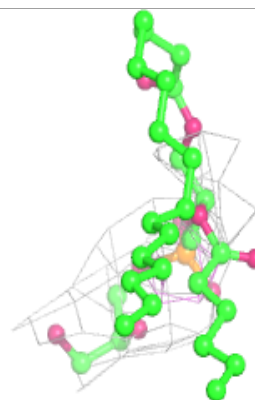
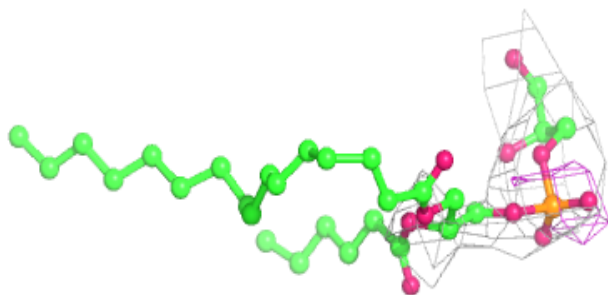
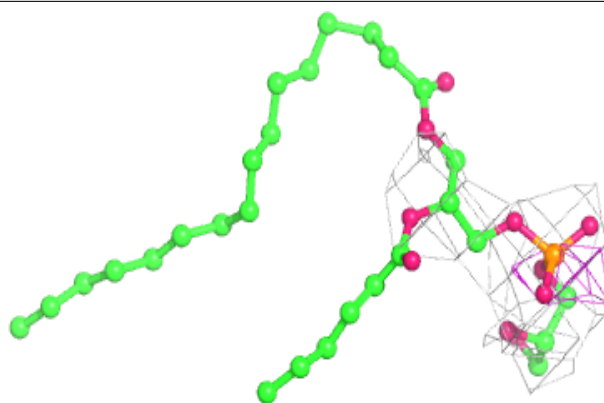
**Electron density around BCR c 513:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

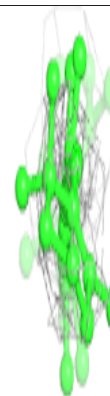
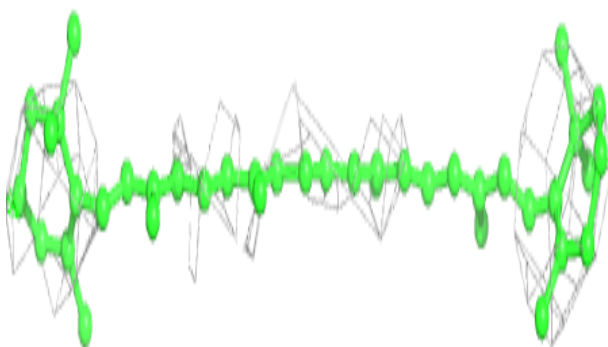
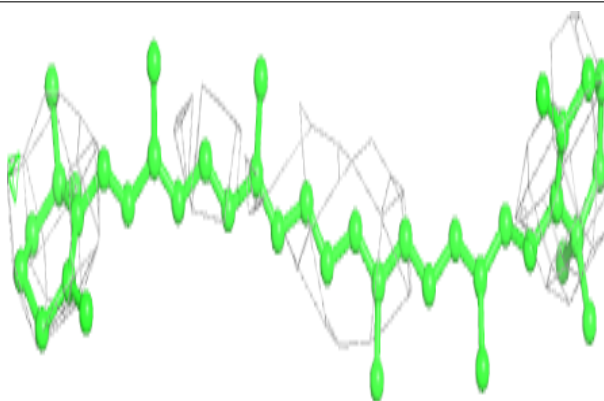


Electron density around LHG a 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

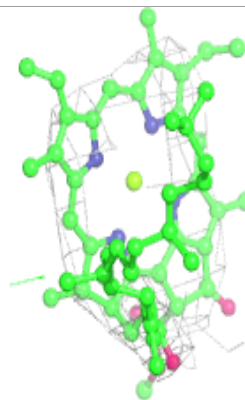
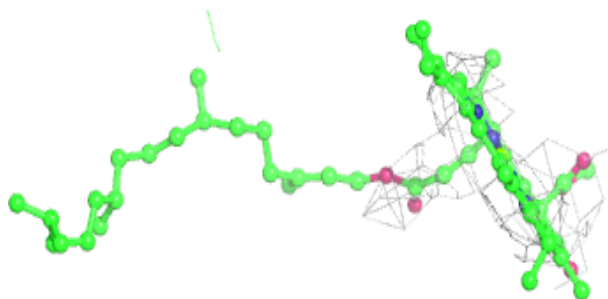
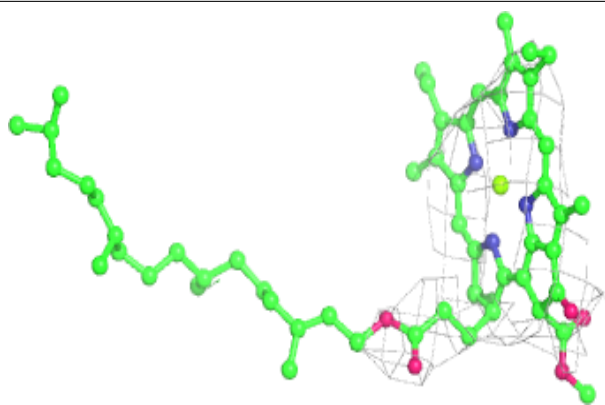
**Electron density around BCR B 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

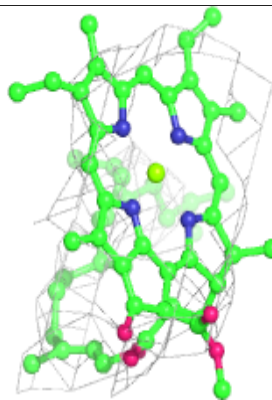
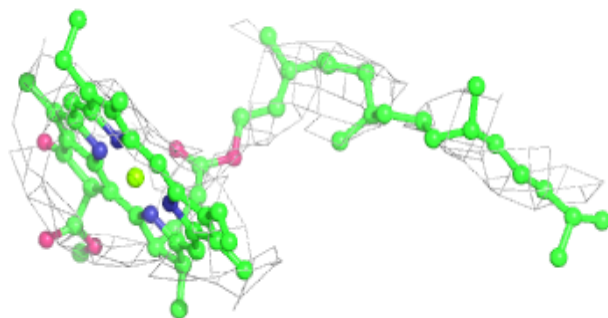
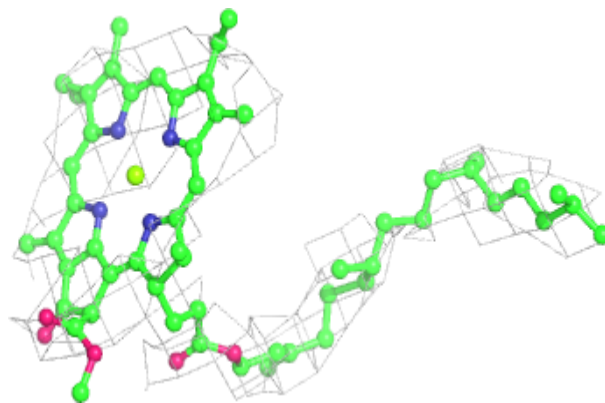


Electron density around CLA A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

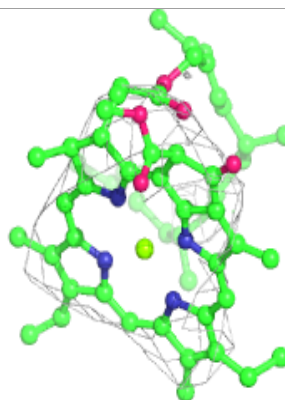
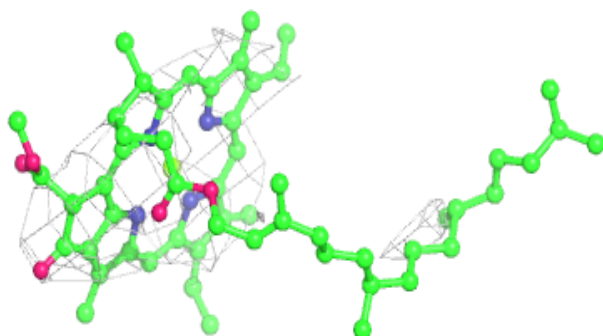
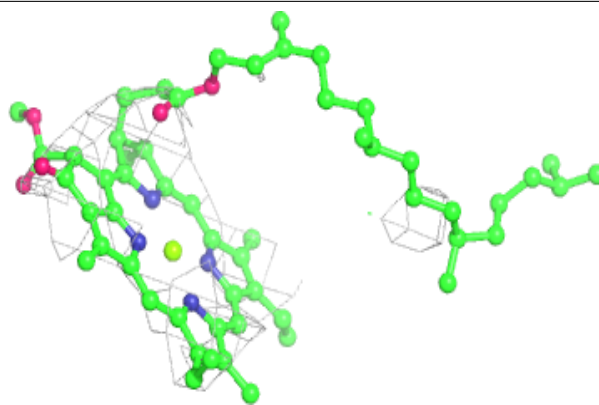
**Electron density around CLA C 510:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

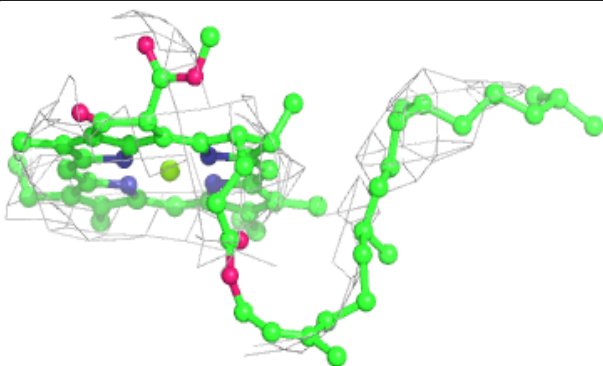
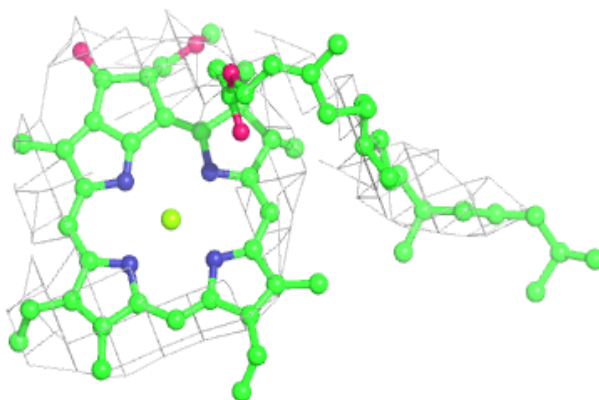


Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

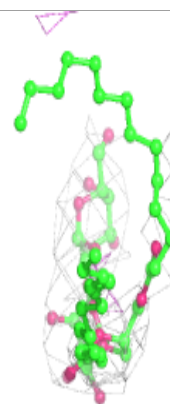
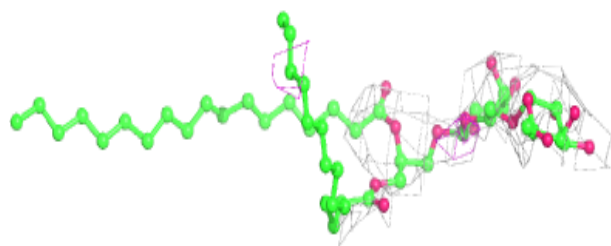
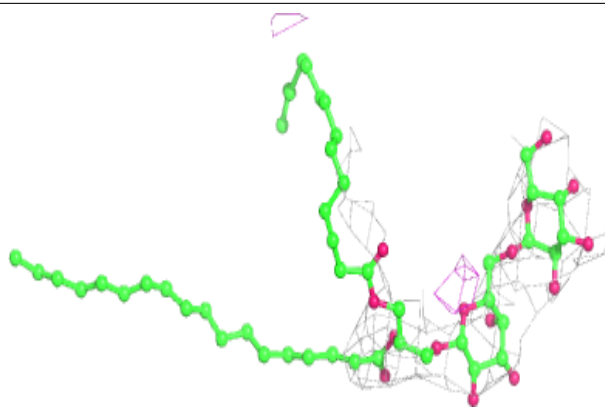
**Electron density around CLA a 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



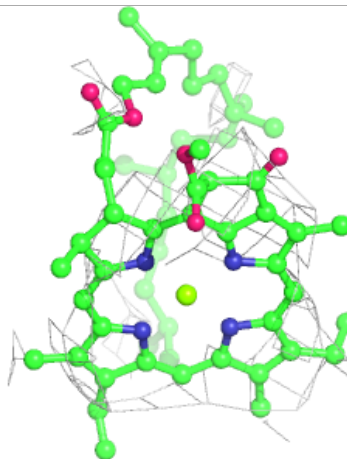
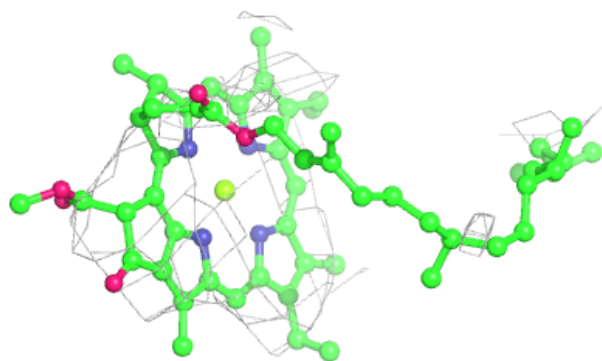
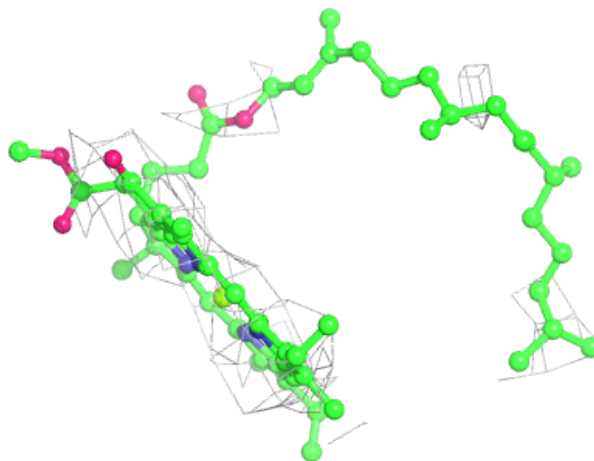
Electron density around DGD C 516:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



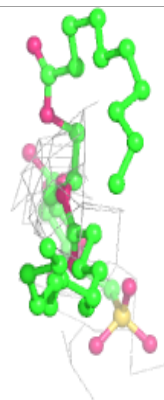
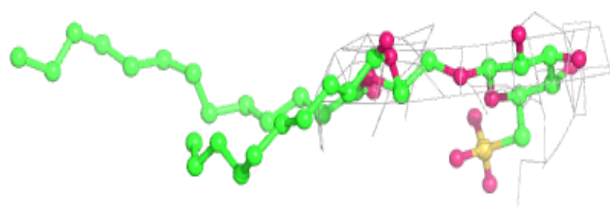
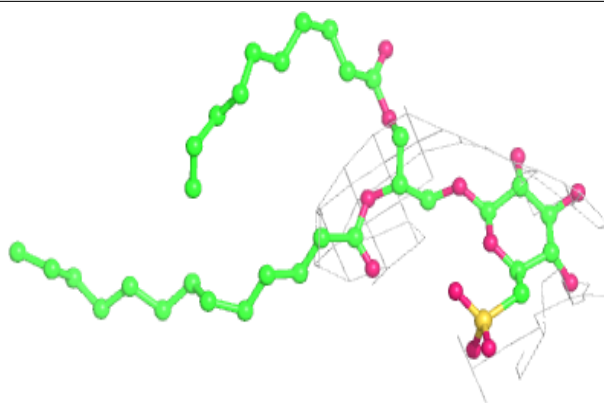
Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

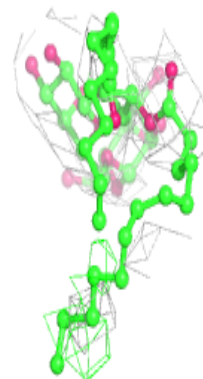
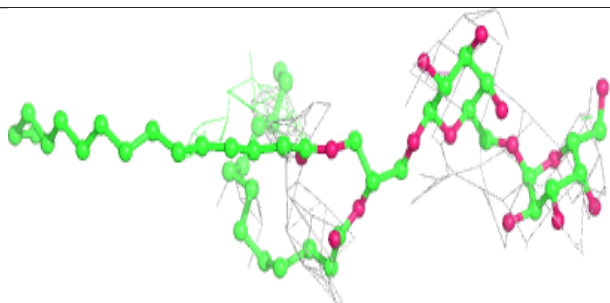
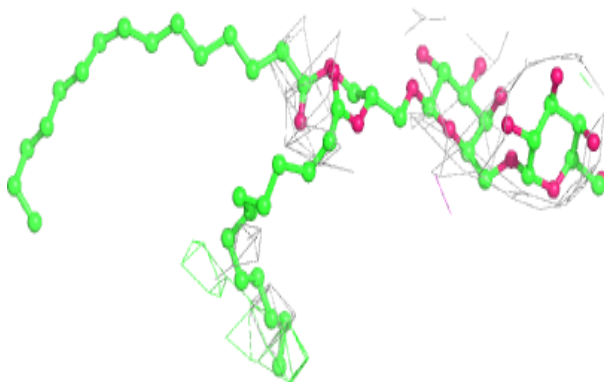


Electron density around SQD f 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

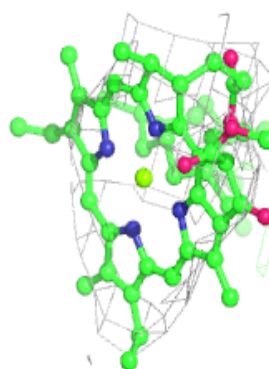
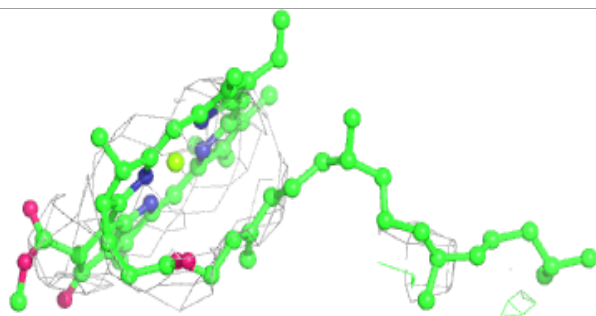
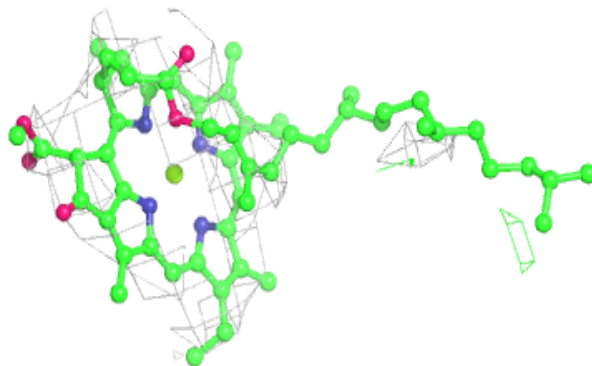
**Electron density around DGD B 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

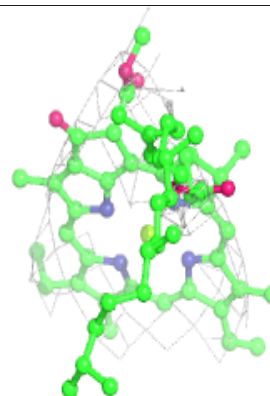
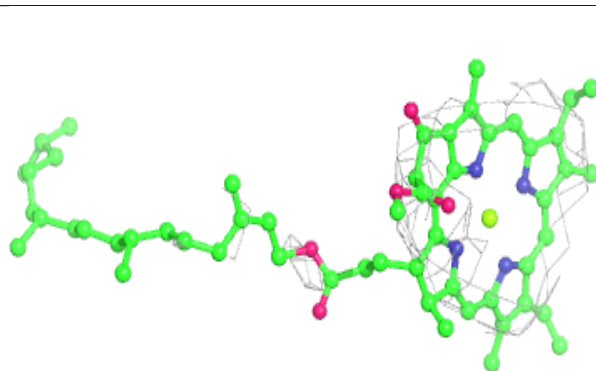
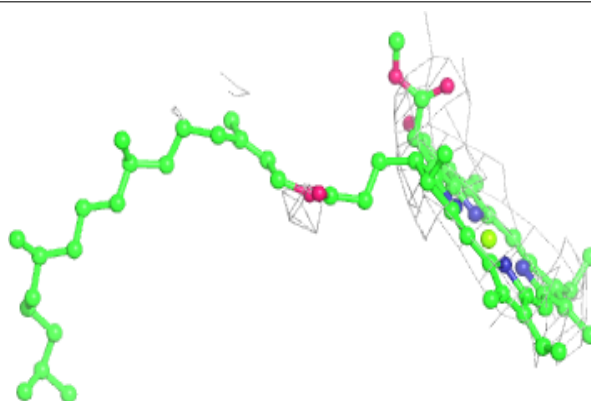


Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

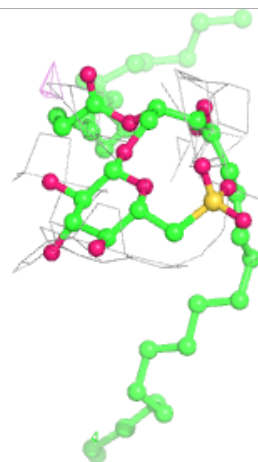
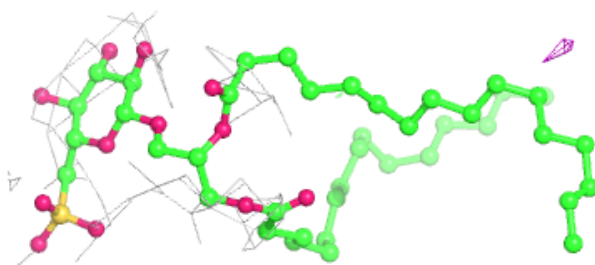
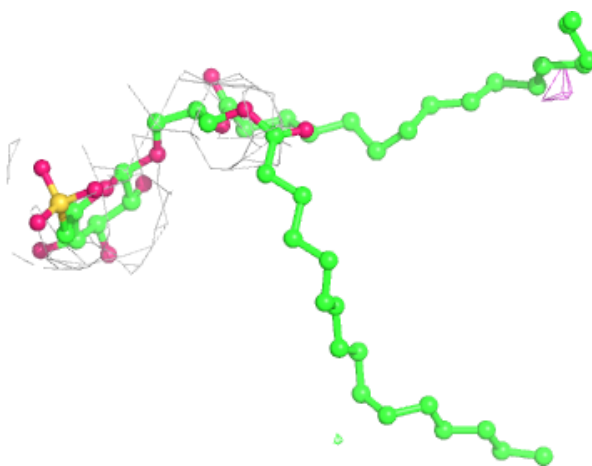
**Electron density around CLA d 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



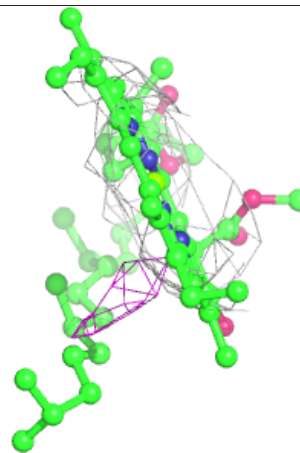
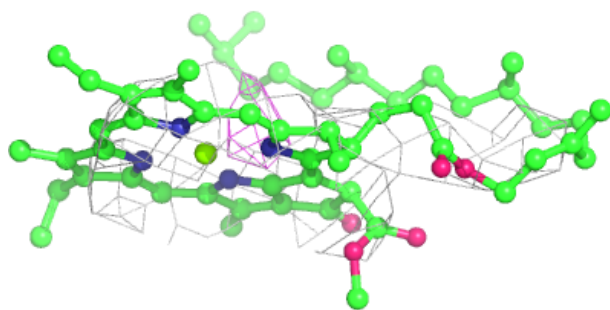
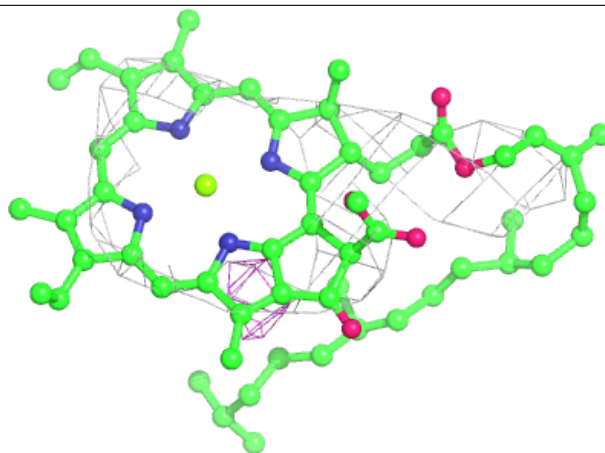
Electron density around SQD a 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



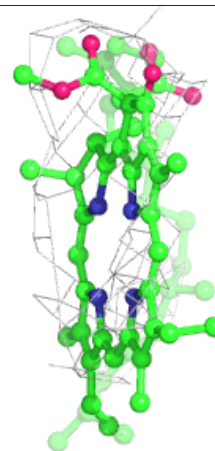
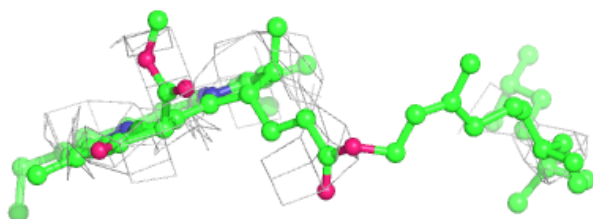
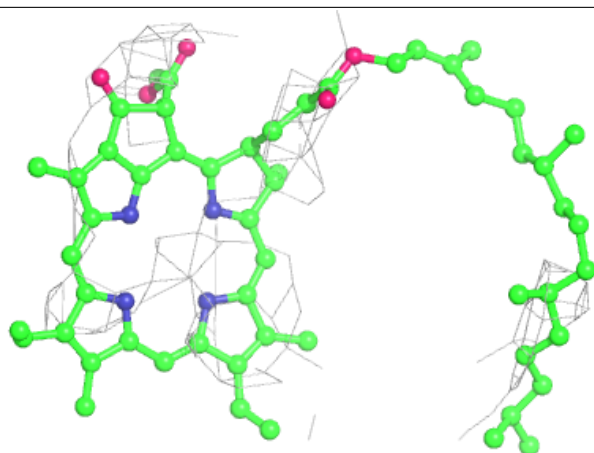
Electron density around CLA c 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

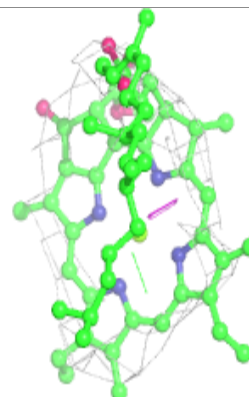
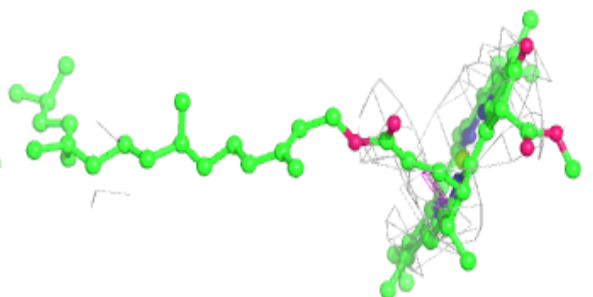
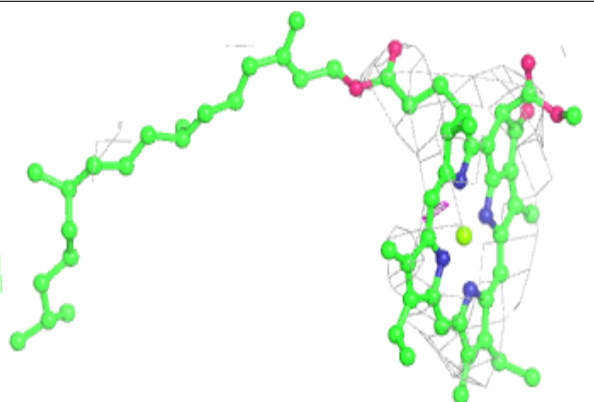


Electron density around PHO D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

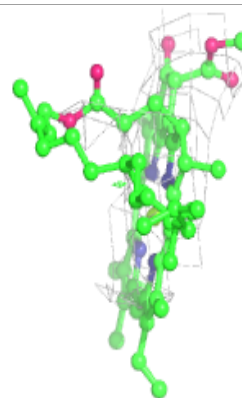
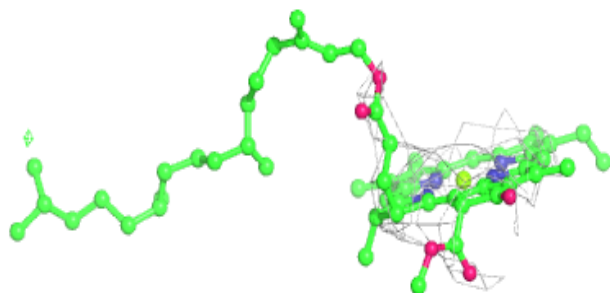
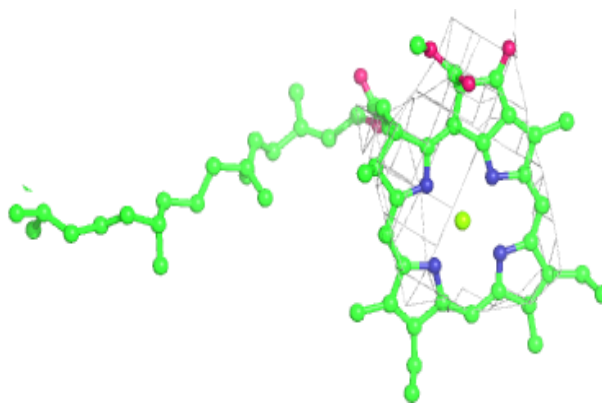
**Electron density around CLA b 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

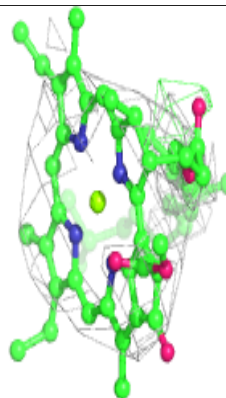
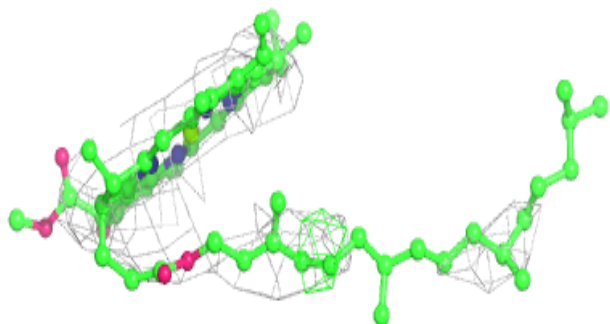
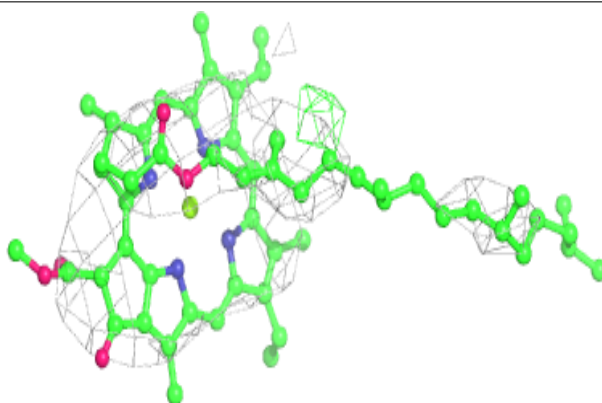


Electron density around CLA a 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

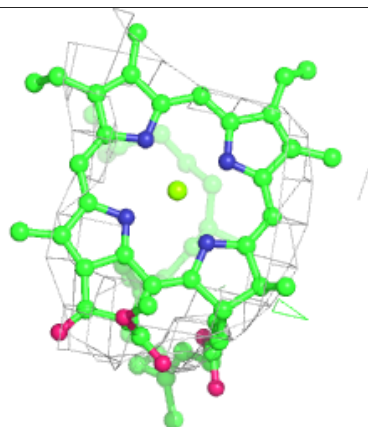
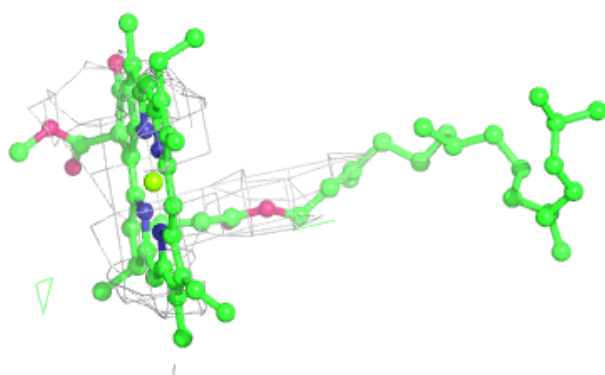
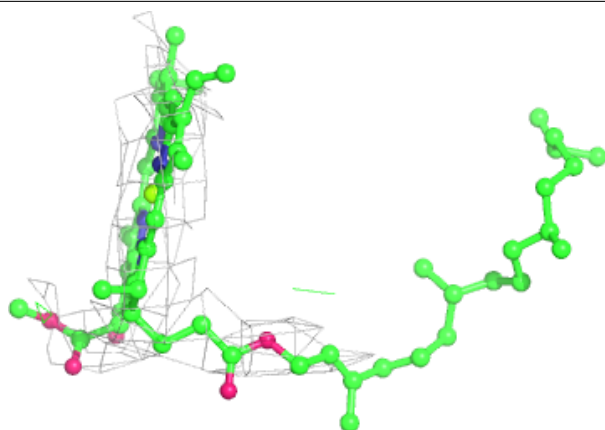
**Electron density around CLA B 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

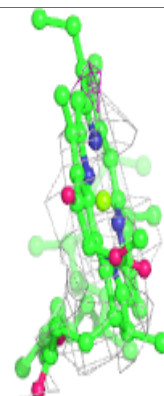
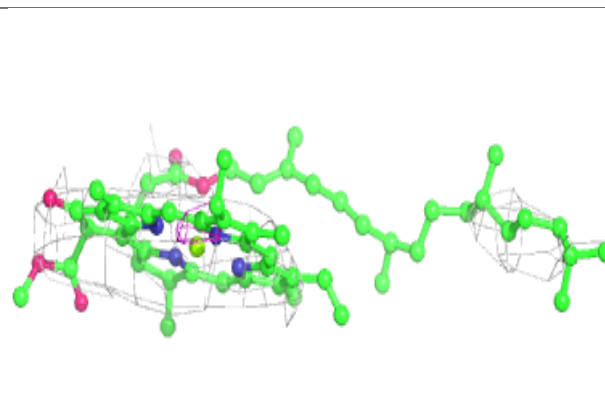
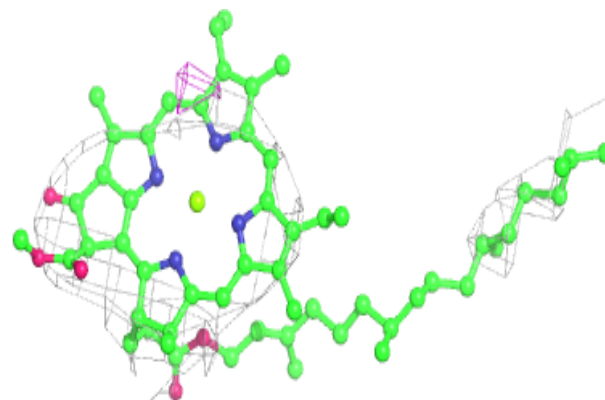


Electron density around CLA c 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

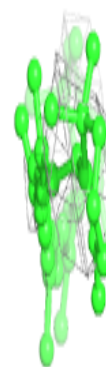
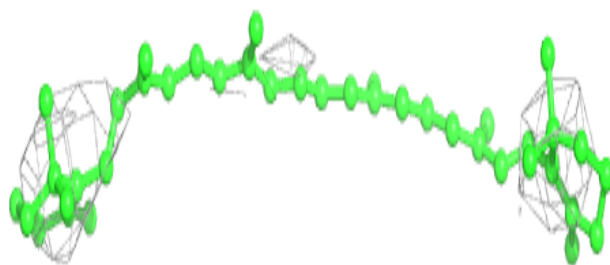
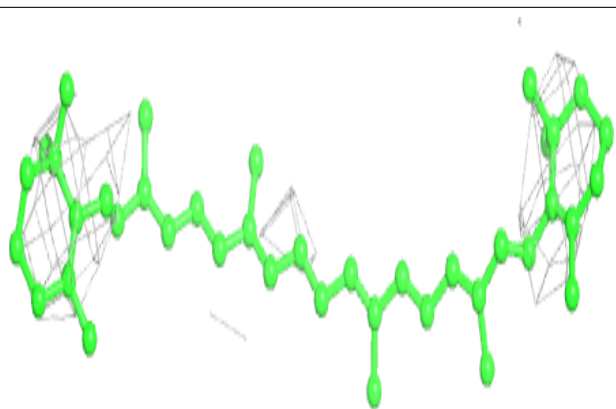
**Electron density around CLA c 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

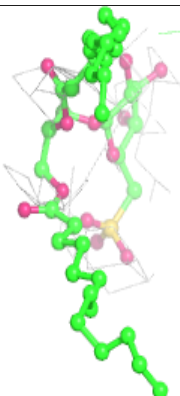
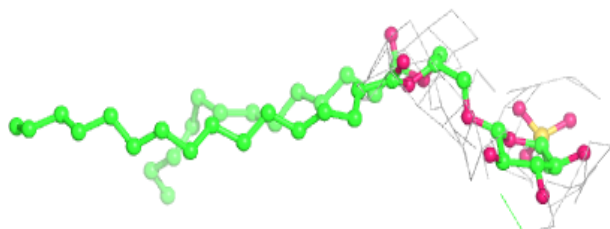
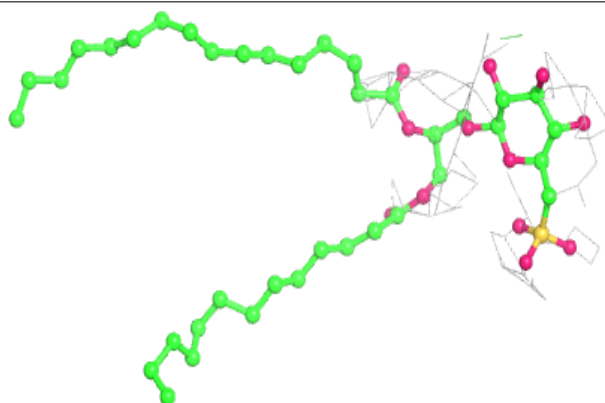


Electron density around BCR b 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

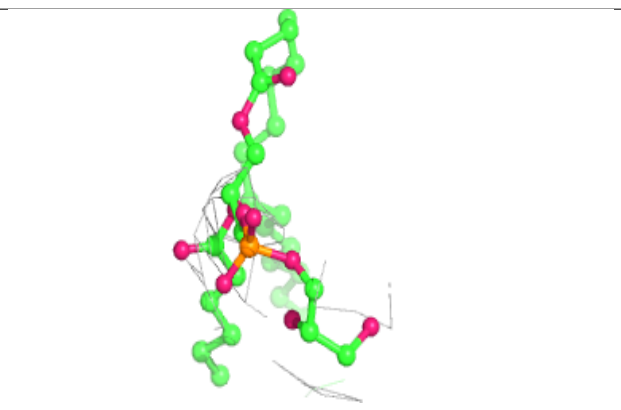
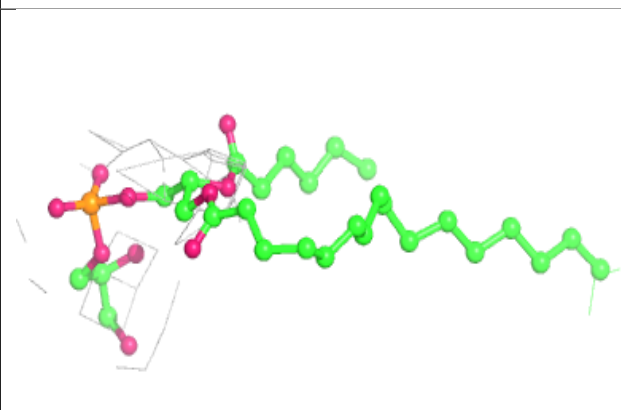
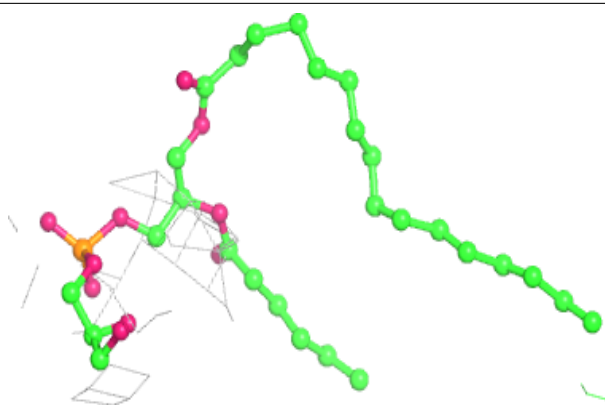
**Electron density around SQD a 415:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



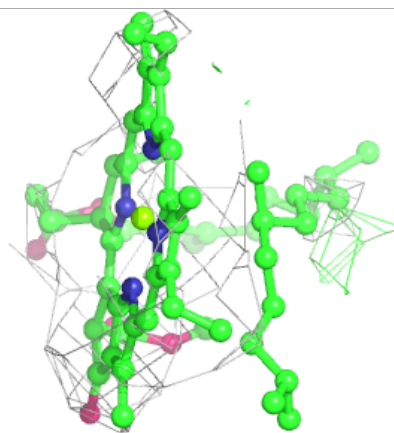
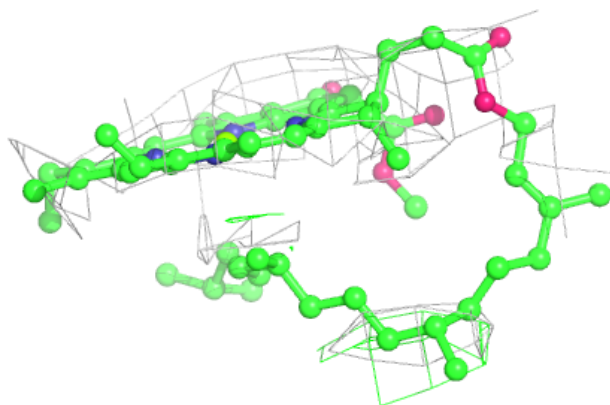
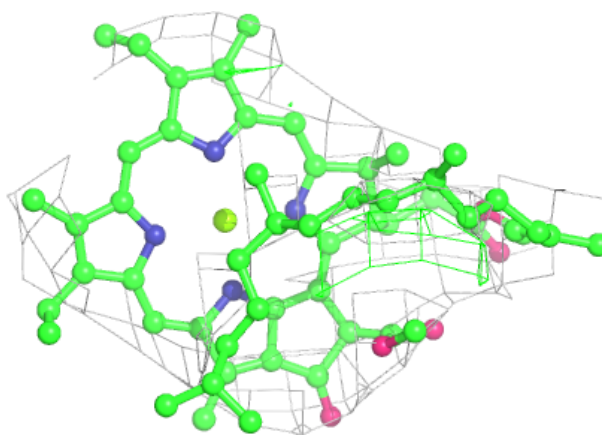
Electron density around LHG A 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



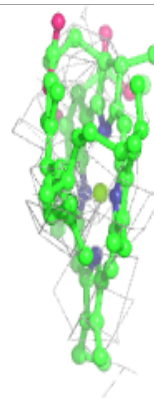
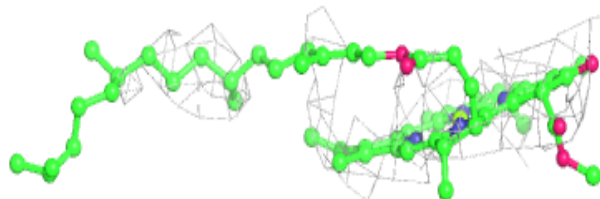
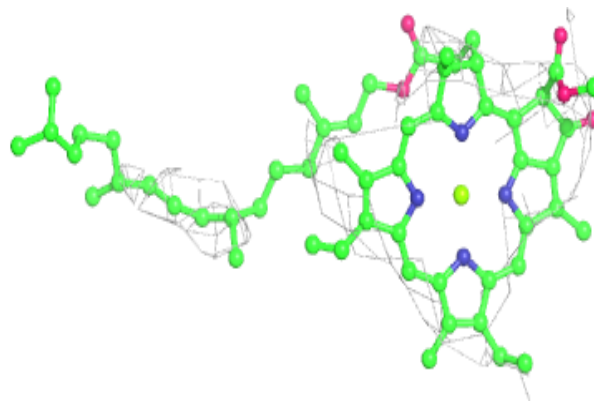
Electron density around CLA C 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

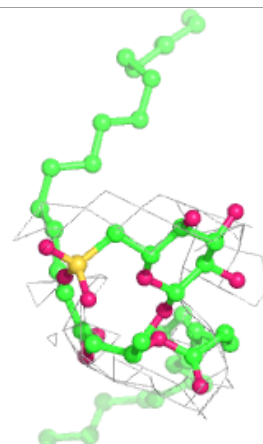
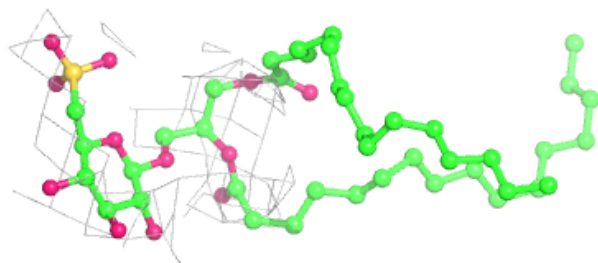
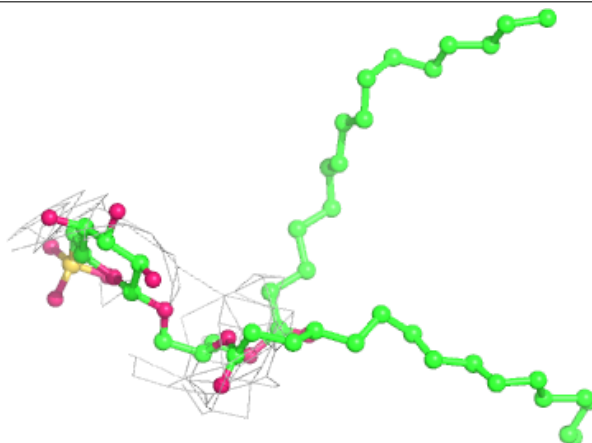


Electron density around CLA b 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

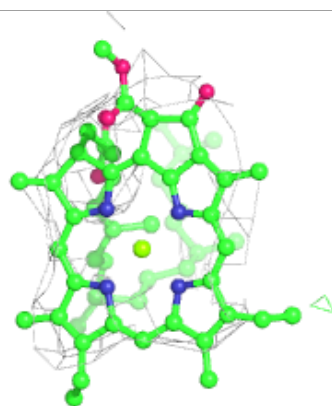
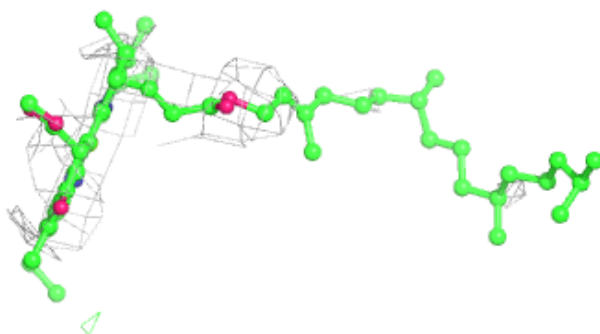
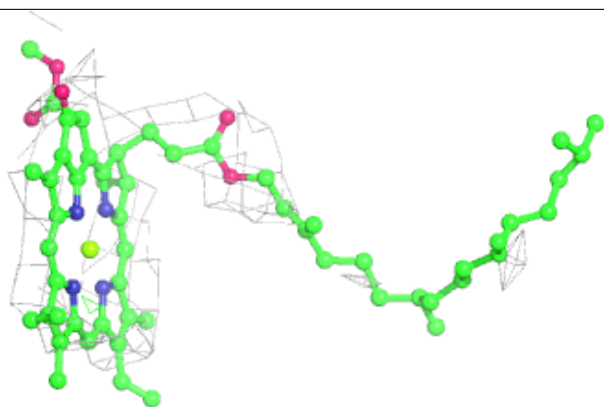
**Electron density around SQD A 414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

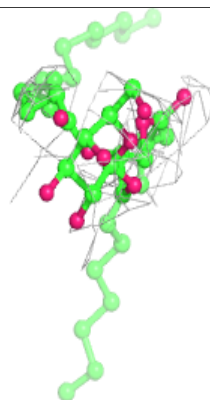
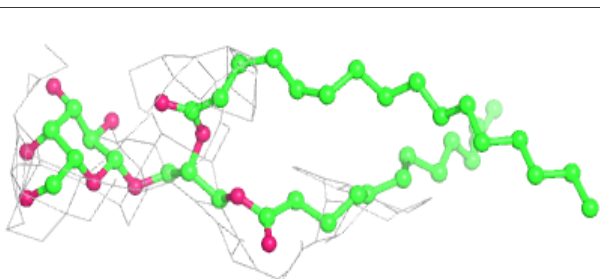
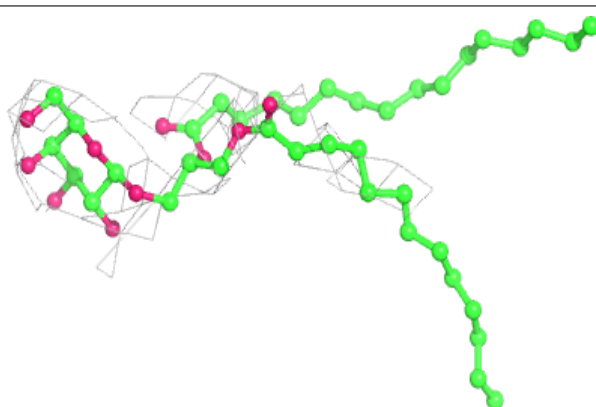


Electron density around CLA d 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

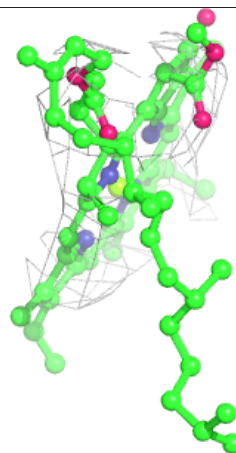
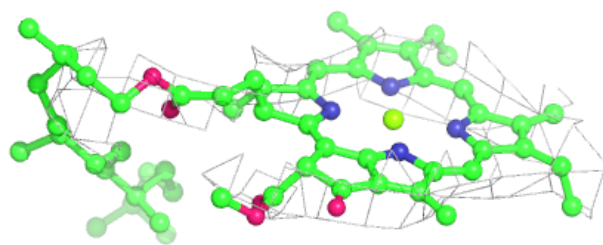
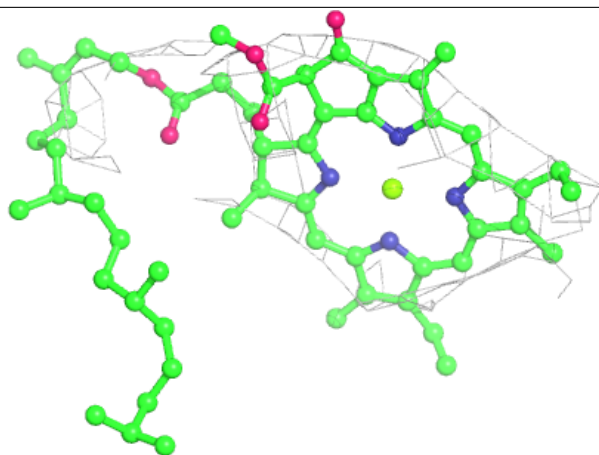
**Electron density around LMG d 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



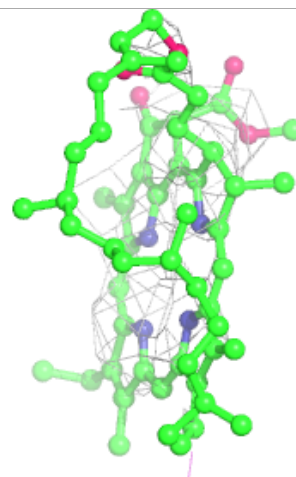
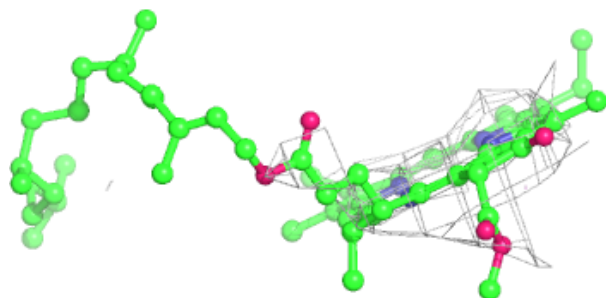
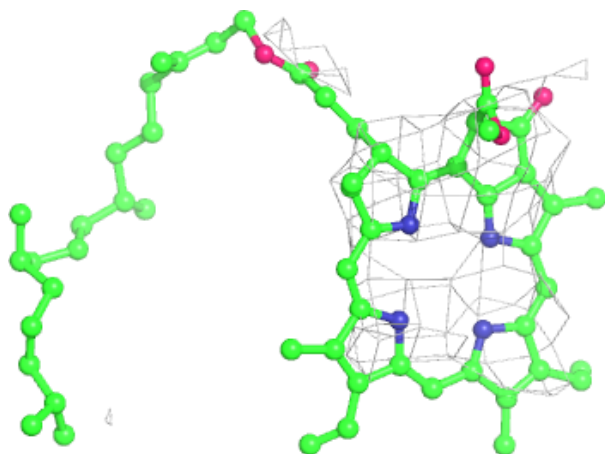
Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



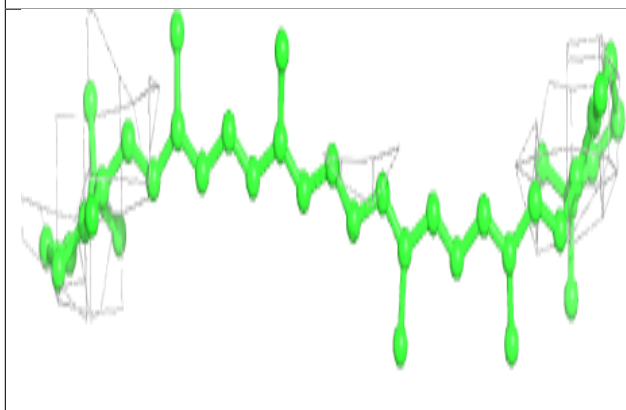
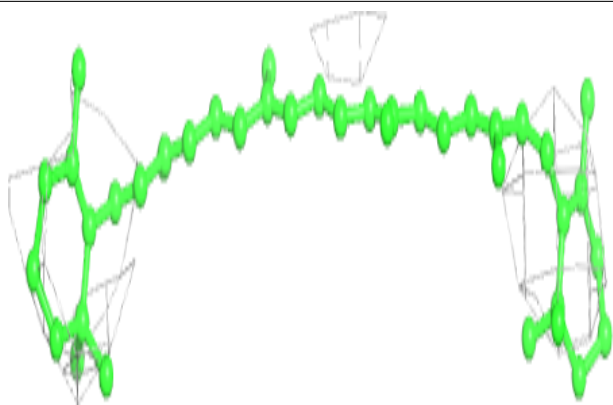
Electron density around PHO a 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



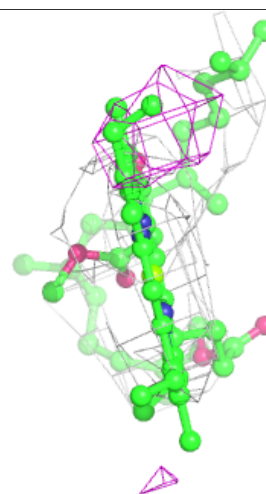
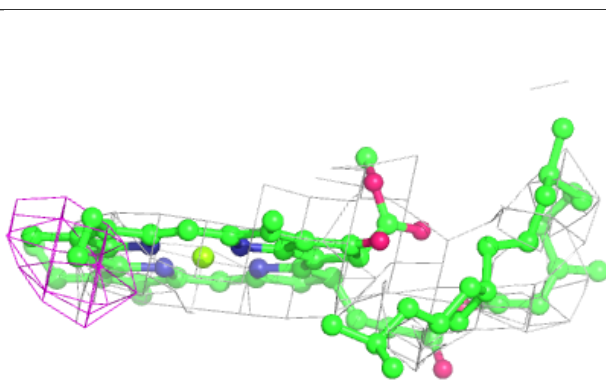
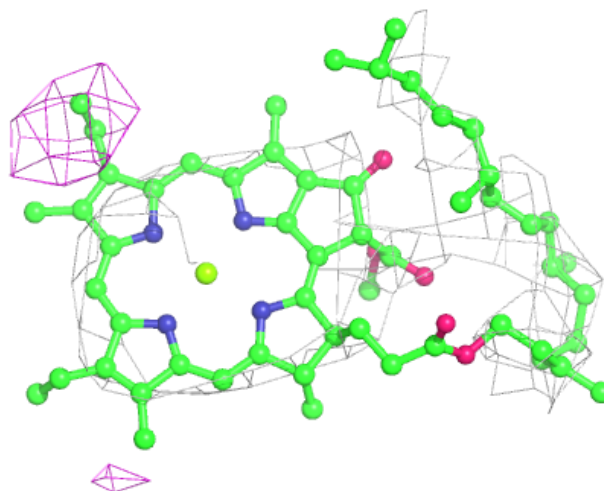
Electron density around BCR C 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



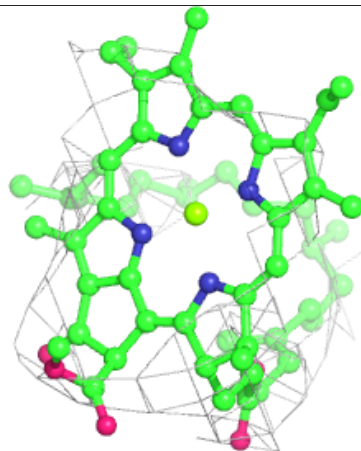
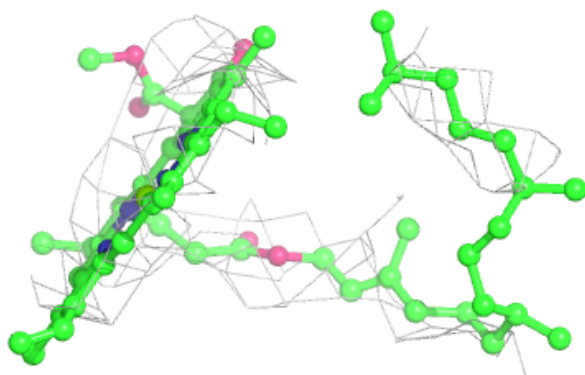
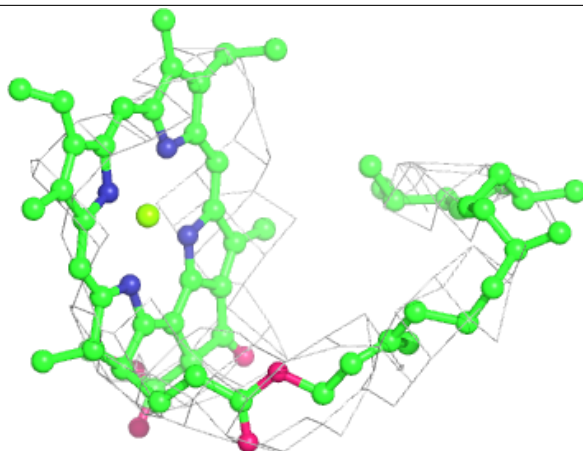
Electron density around CLA B 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

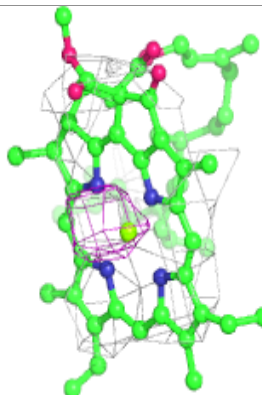
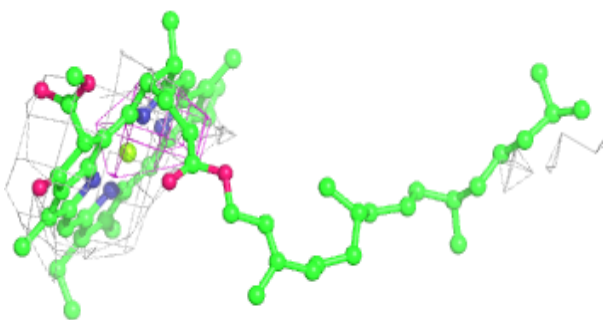
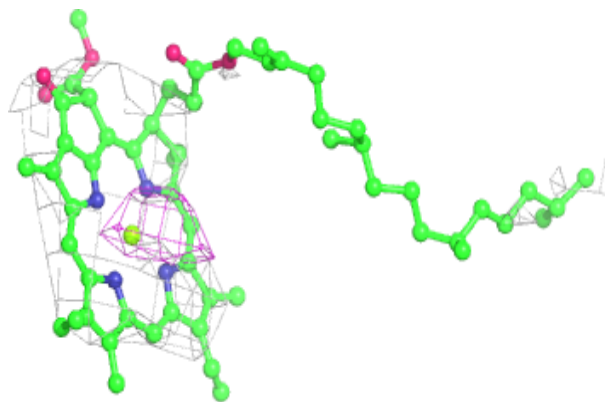


Electron density around CLA C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

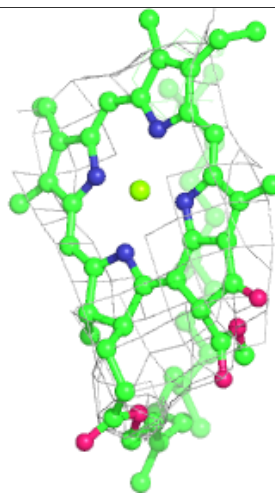
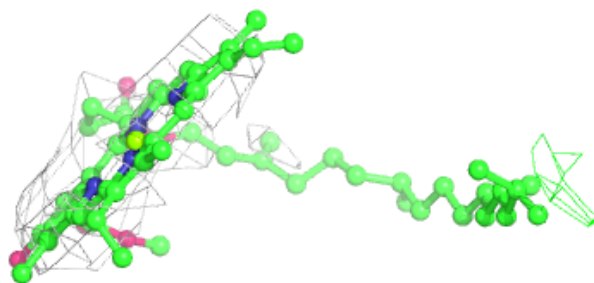
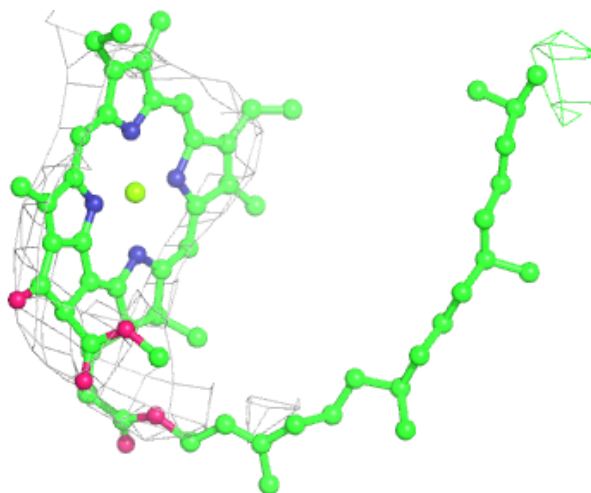
**Electron density around CLA c 510:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



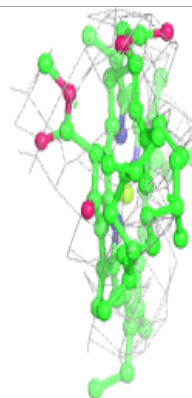
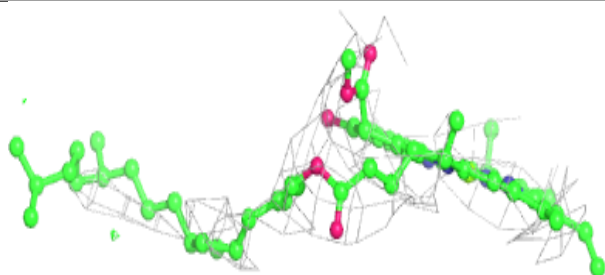
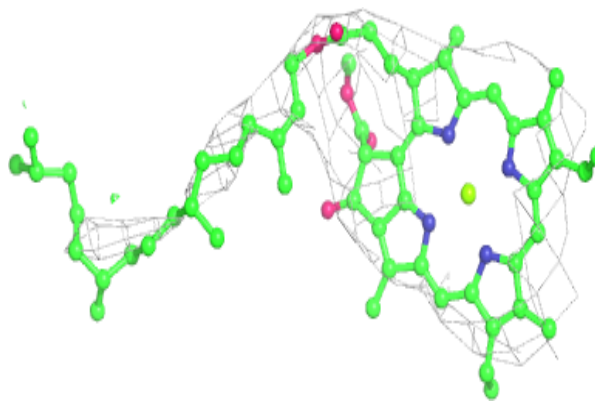
Electron density around CLA c 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

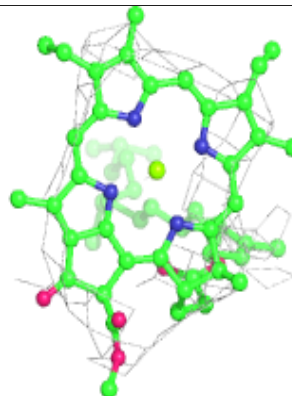
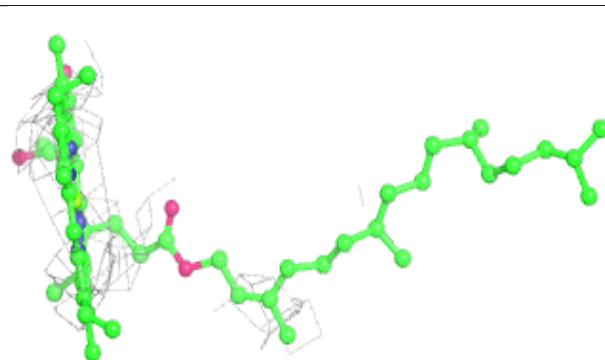
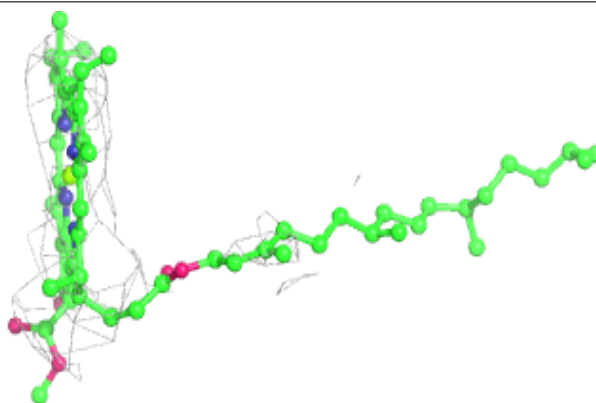


Electron density around CLA H 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

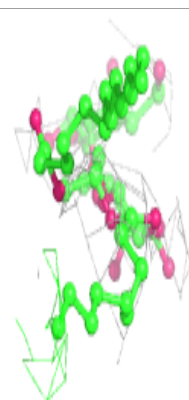
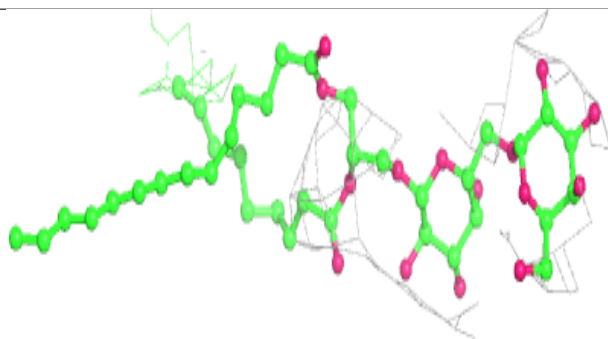
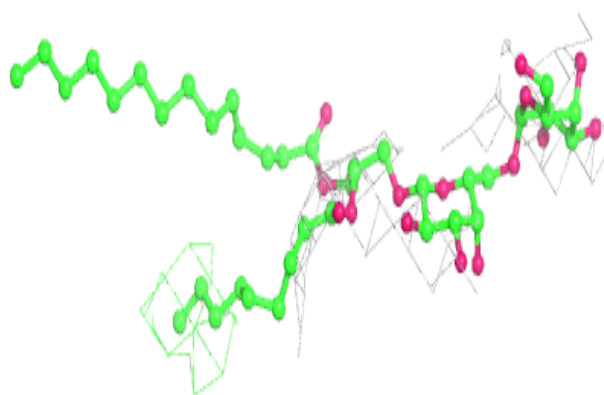
**Electron density around CLA B 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

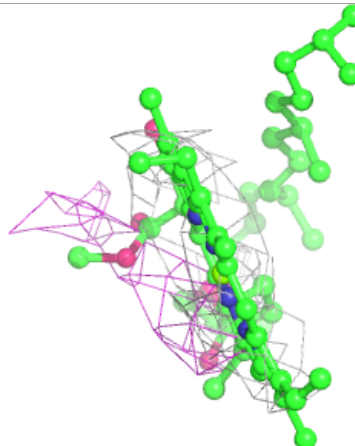
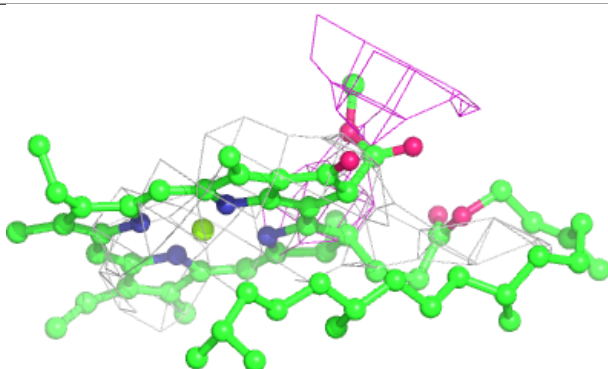
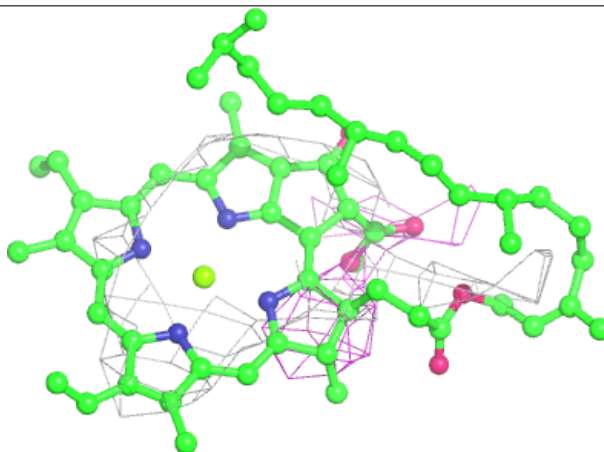


Electron density around DGD c 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

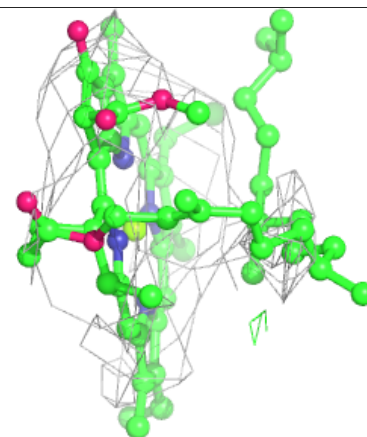
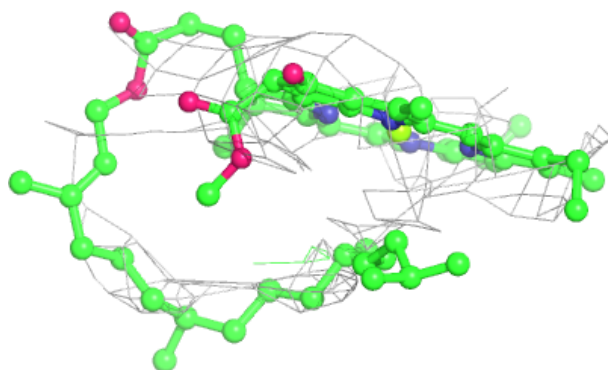
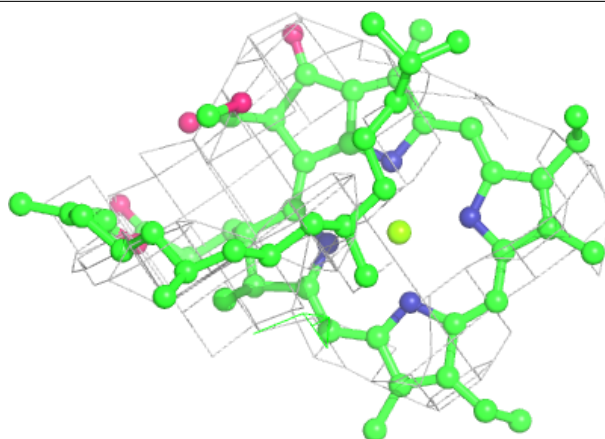
**Electron density around CLA C 508:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

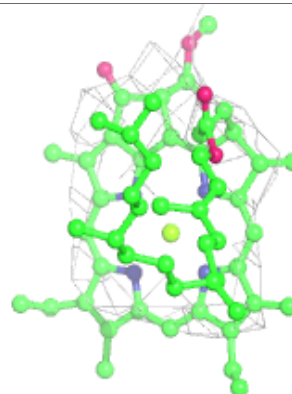
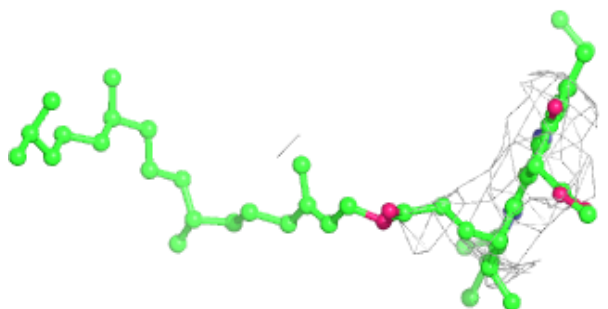
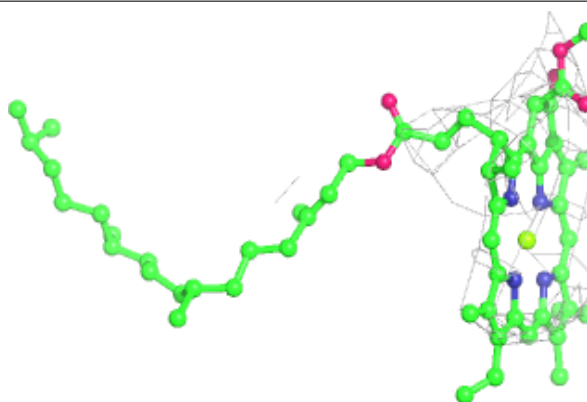


Electron density around CLA c 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

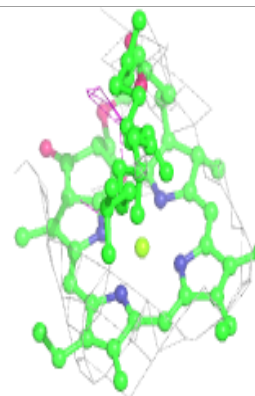
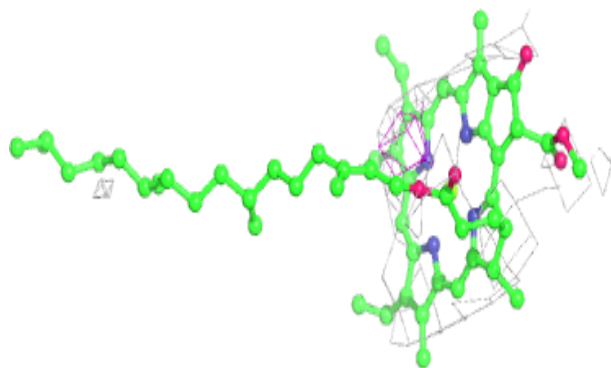
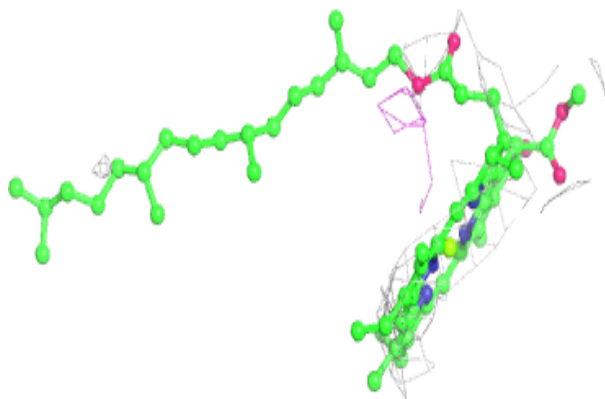
**Electron density around CLA D 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

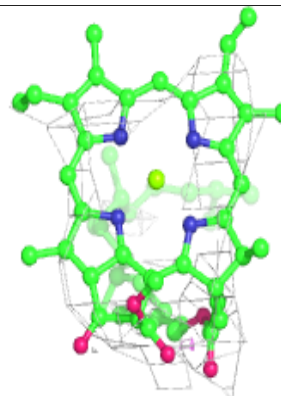
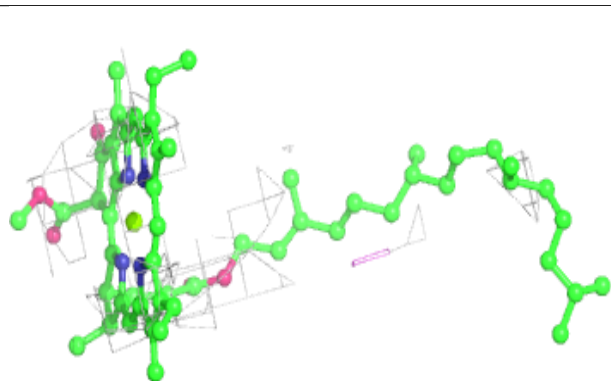
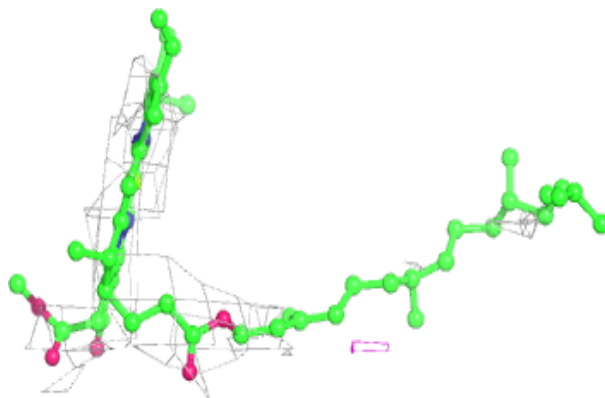


Electron density around CLA c 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

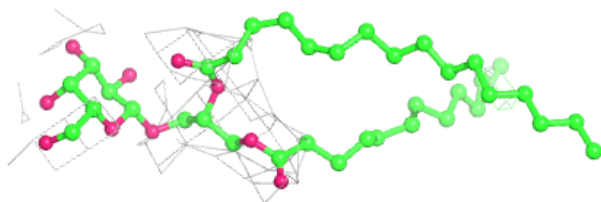
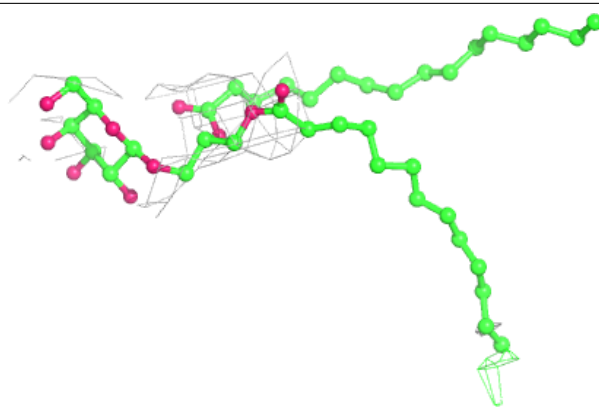
**Electron density around CLA B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

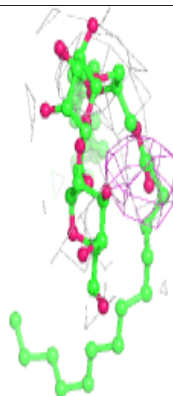
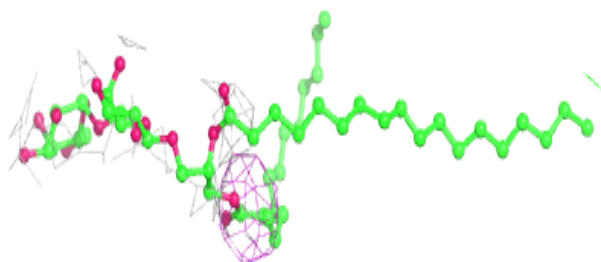
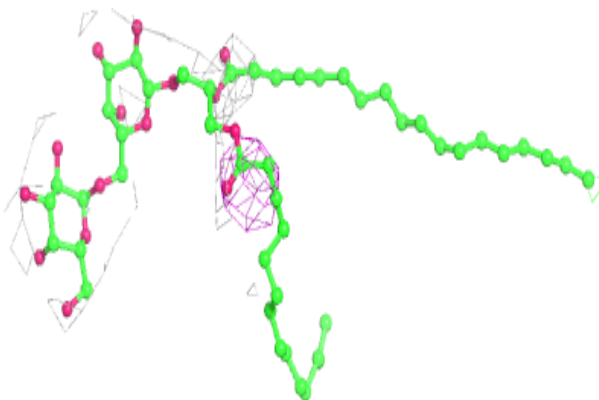


Electron density around LMG D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

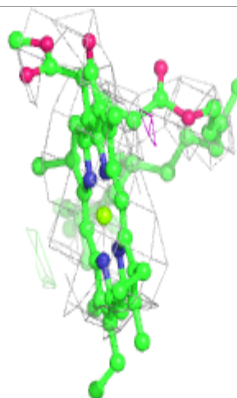
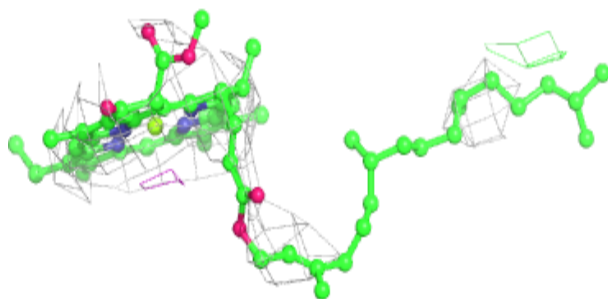
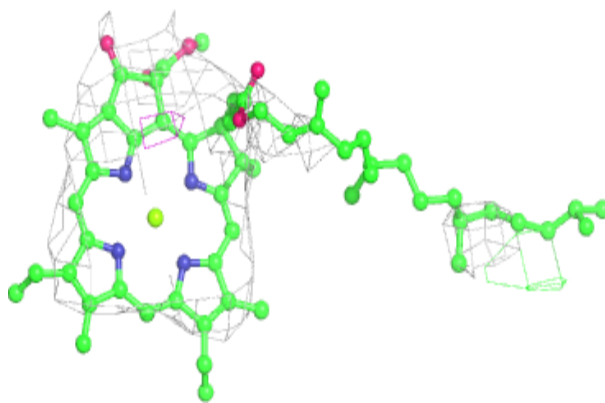
**Electron density around DGD c 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

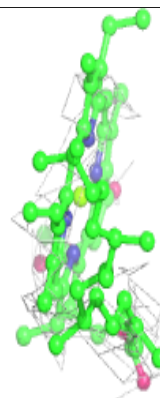
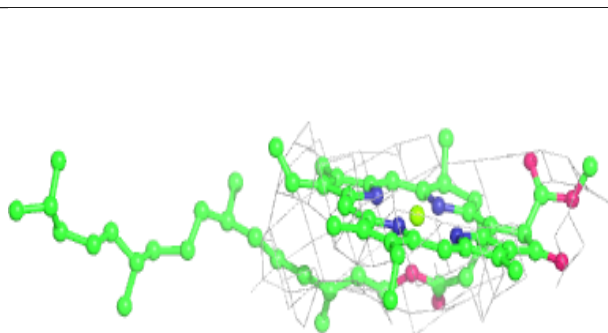
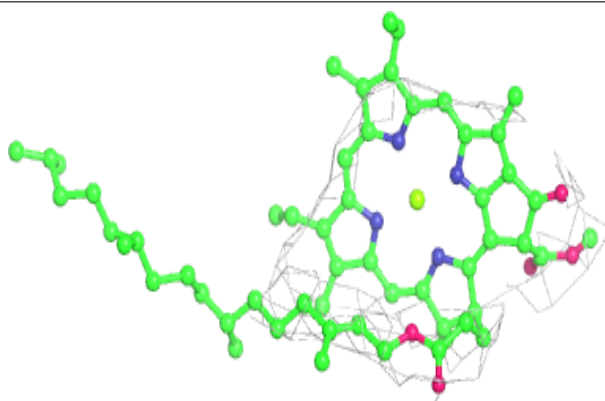


Electron density around CLA A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

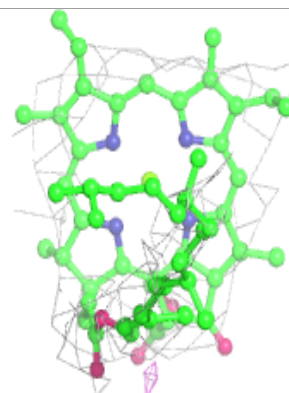
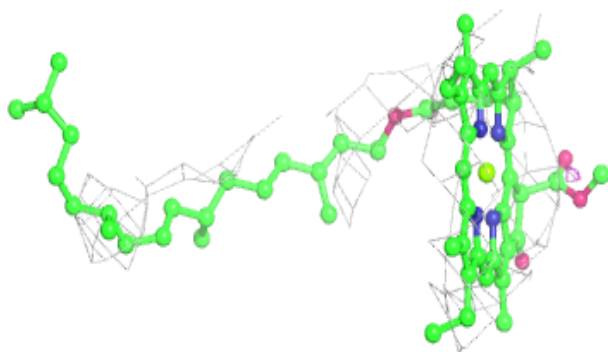
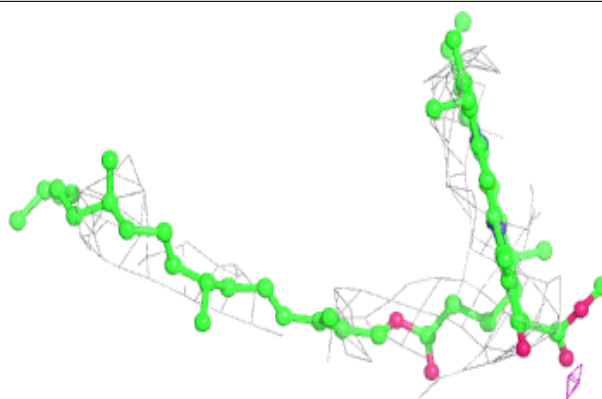
**Electron density around CLA C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

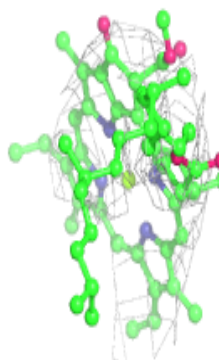
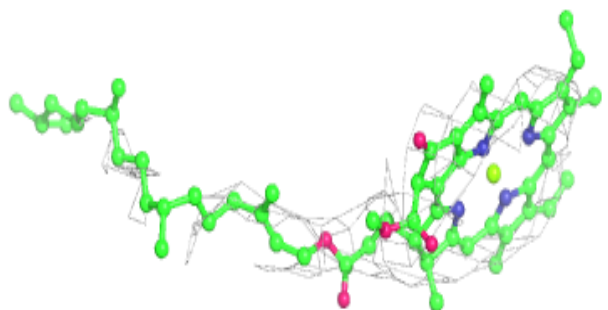
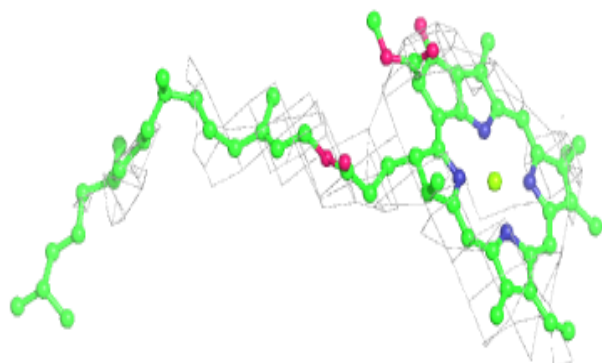


Electron density around CLA b 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

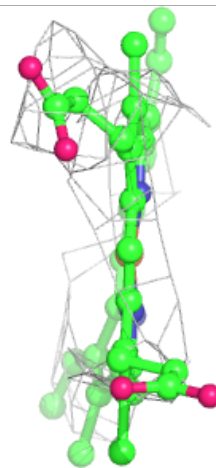
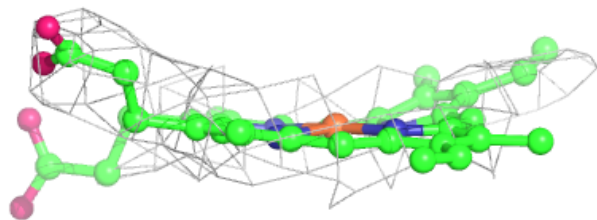
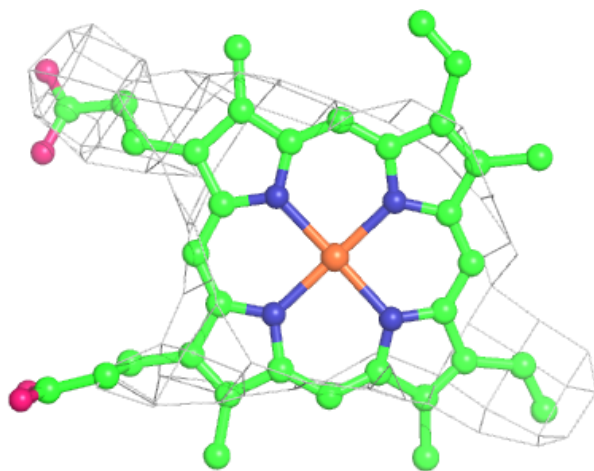
**Electron density around CLA a 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



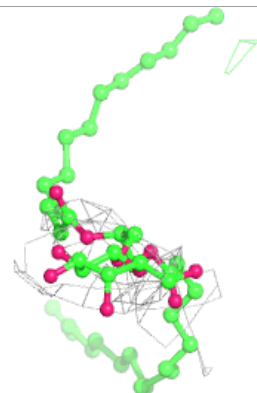
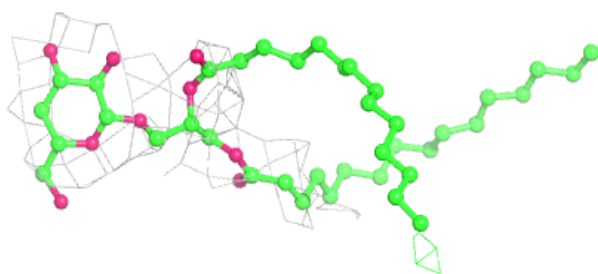
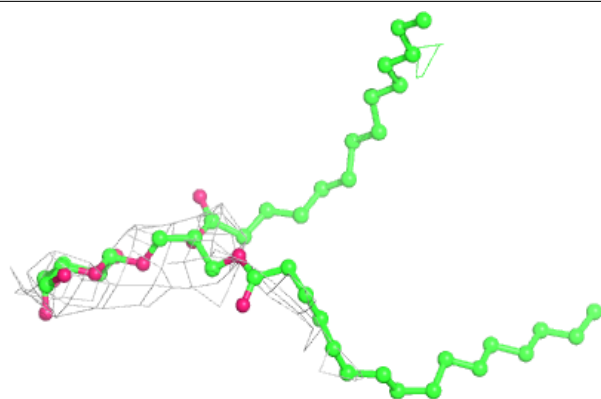
Electron density around HEM V 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



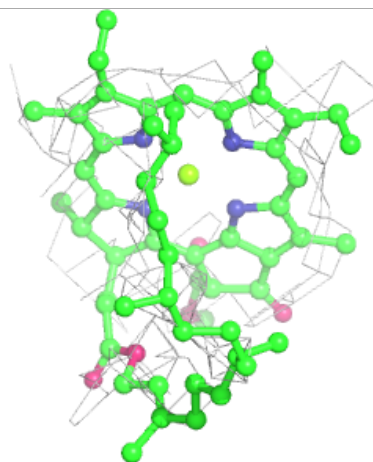
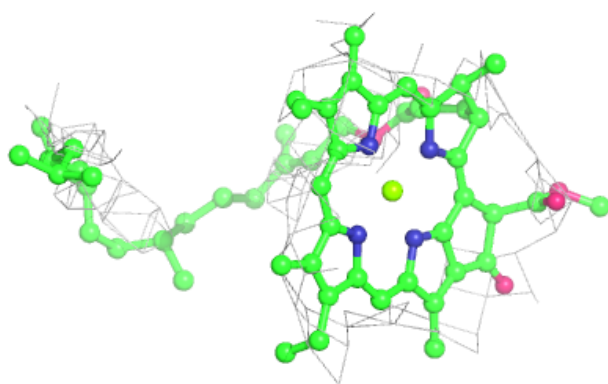
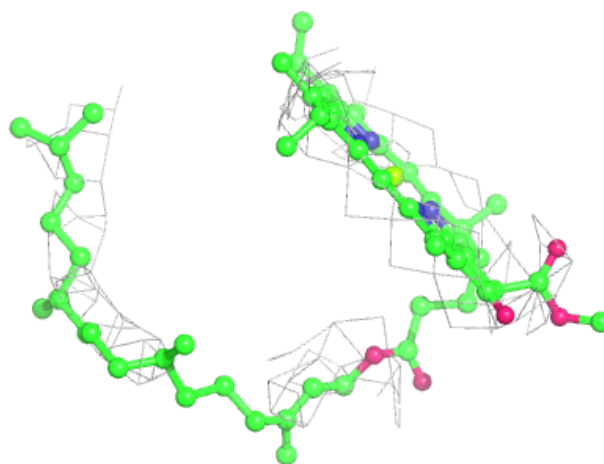
Electron density around LMG B 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



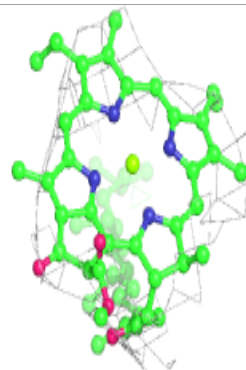
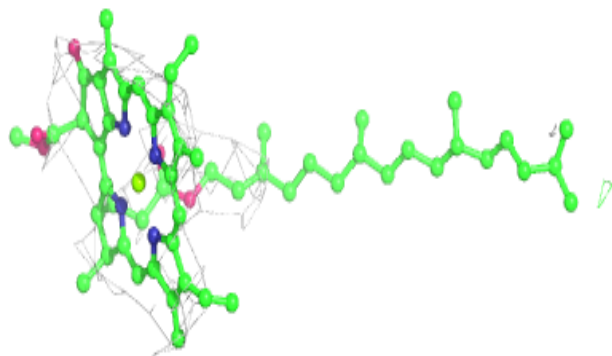
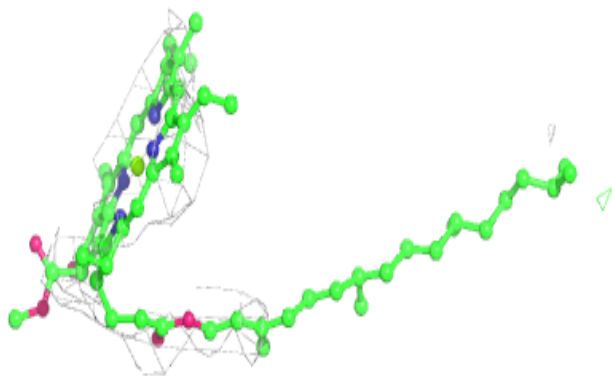
Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

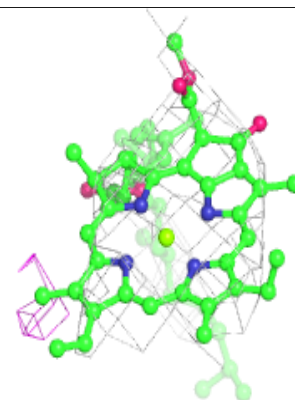
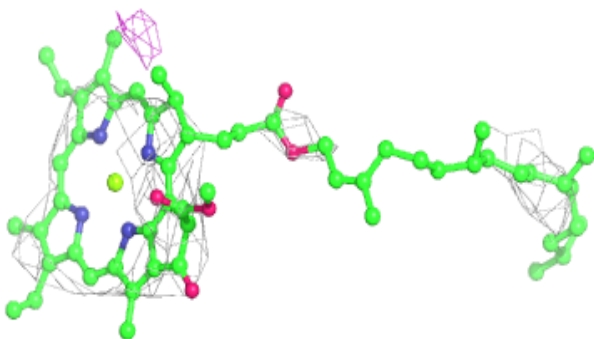
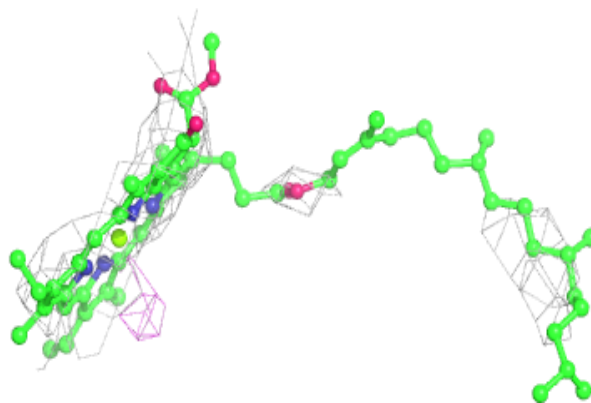


Electron density around CLA B 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

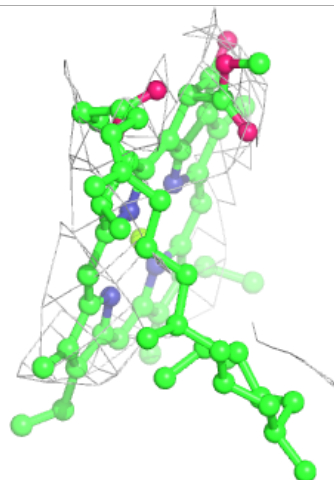
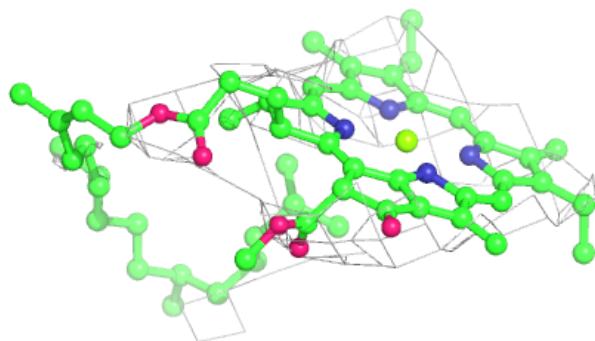
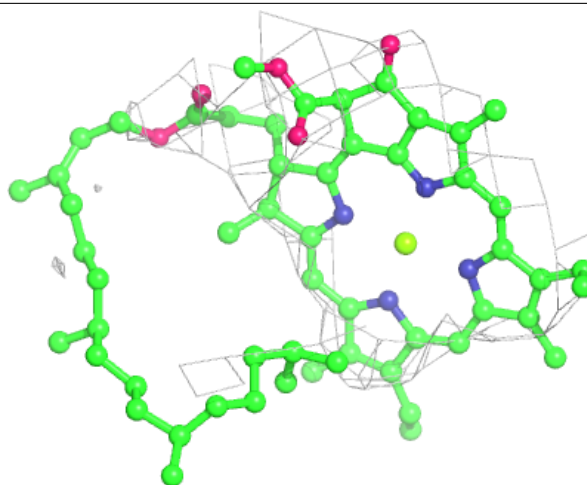
**Electron density around CLA D 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



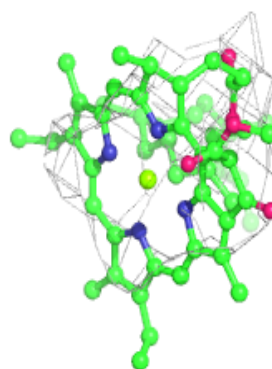
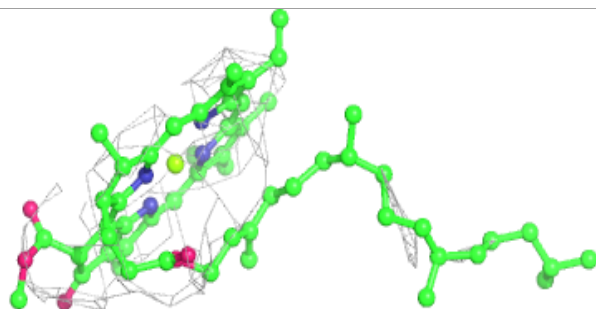
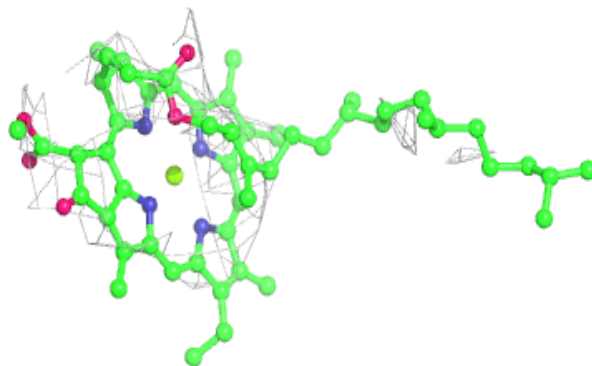
Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

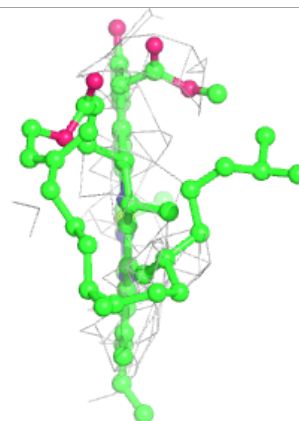
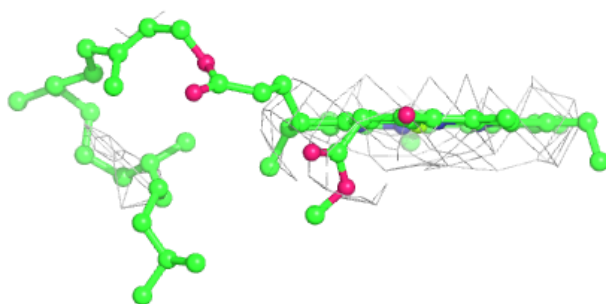
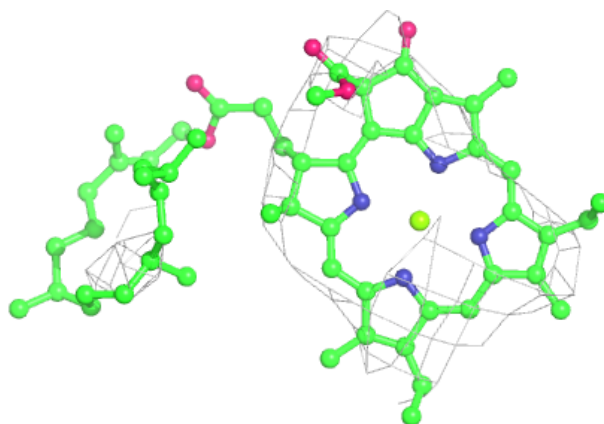


Electron density around CLA c 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

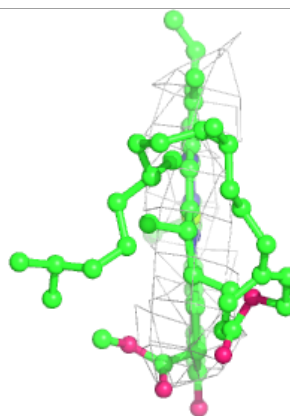
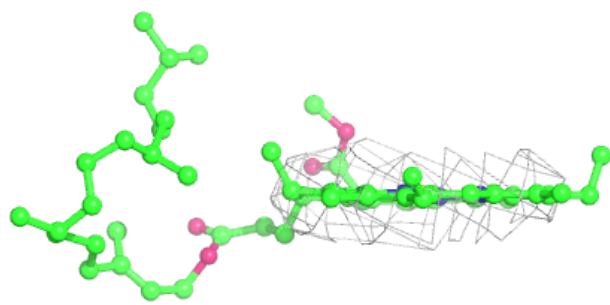
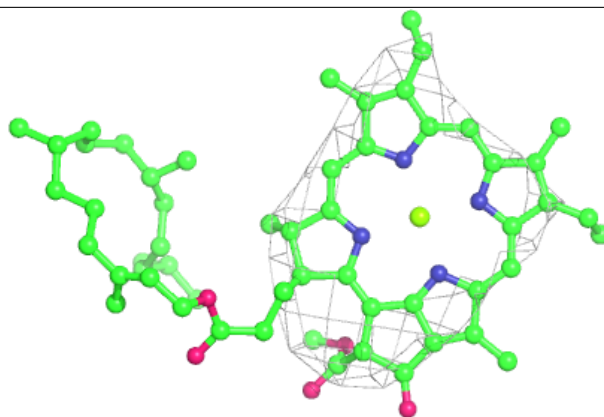
**Electron density around CLA c 511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

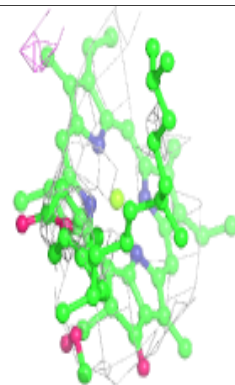
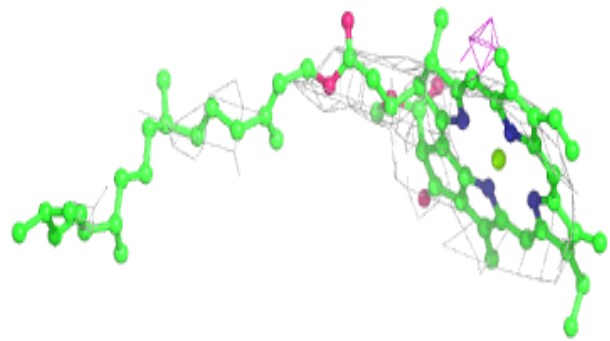
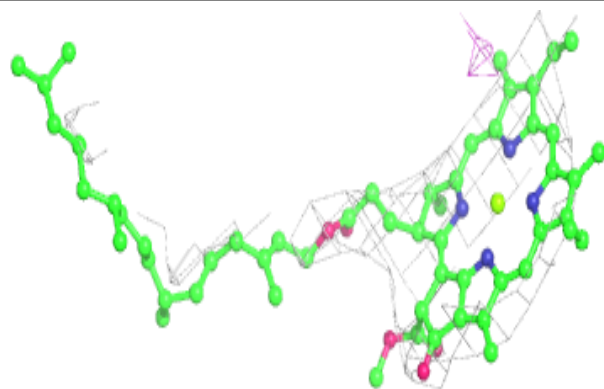


Electron density around CLA C 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

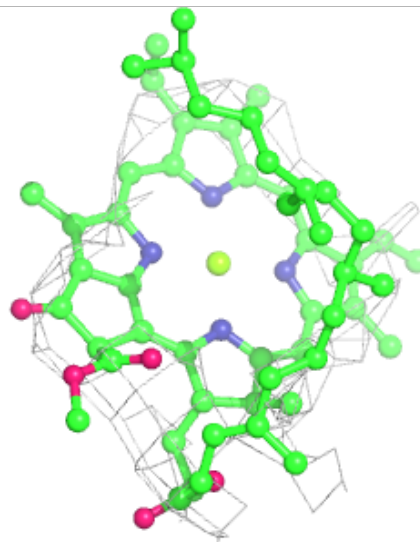
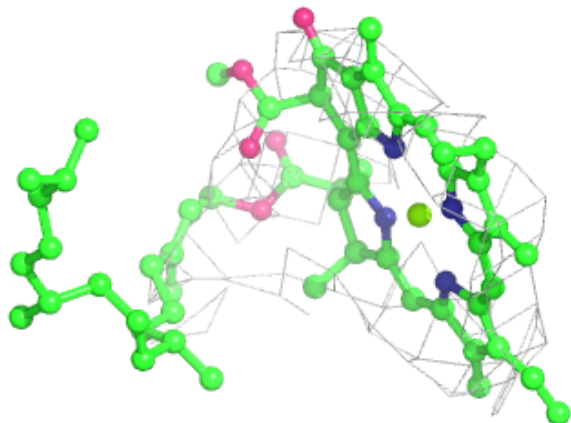
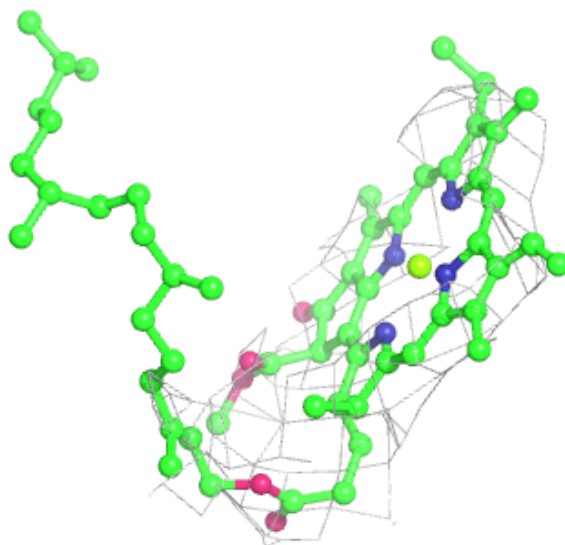
**Electron density around CLA A 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



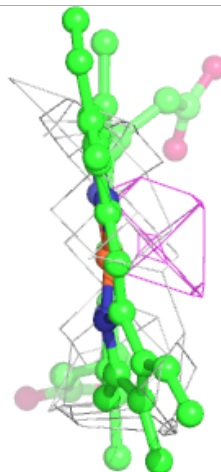
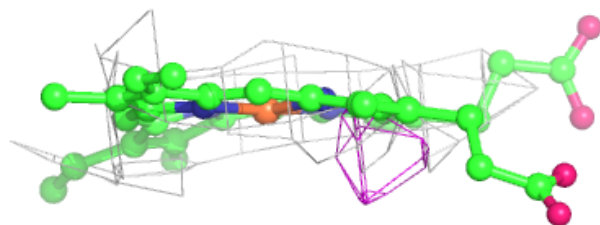
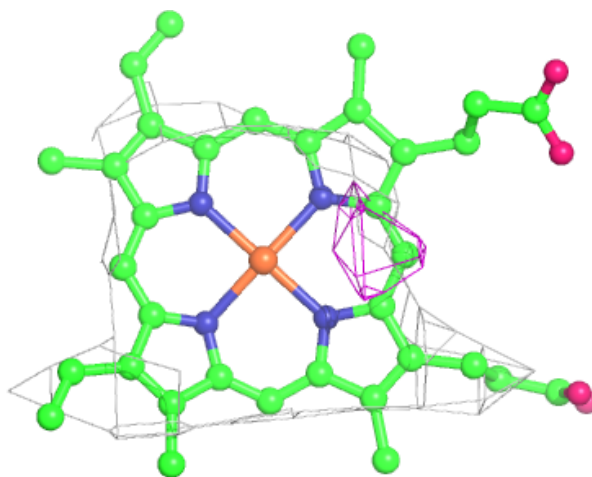
Electron density around CLA B 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



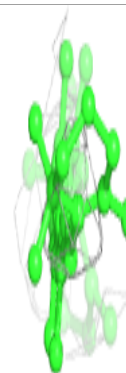
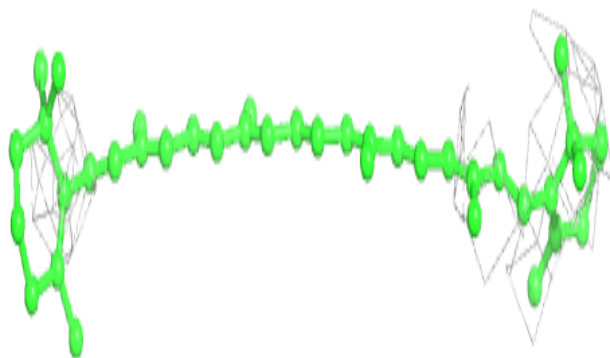
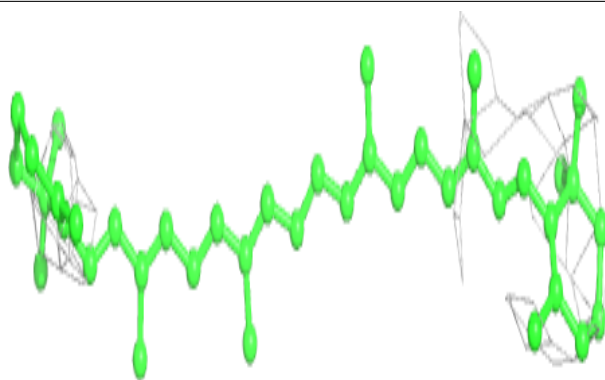
Electron density around HEM v 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

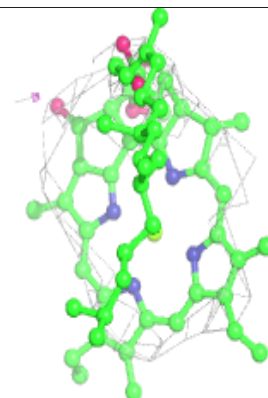
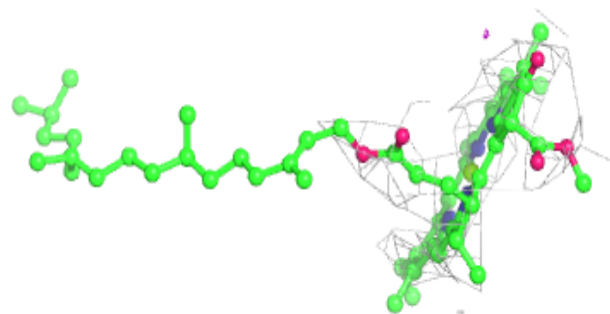
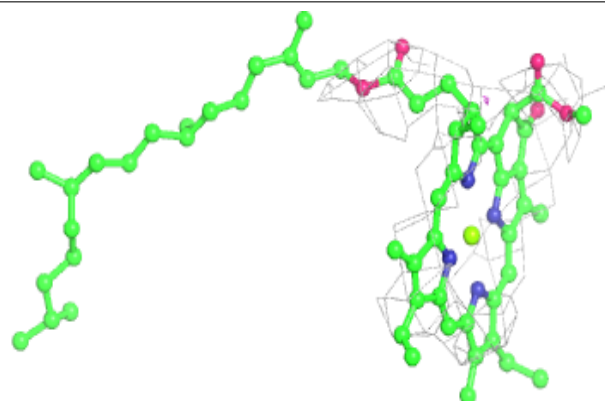


Electron density around BCR b 620:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

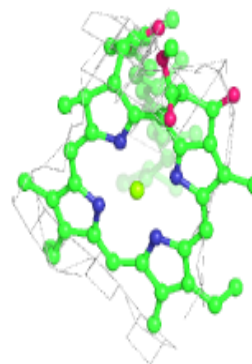
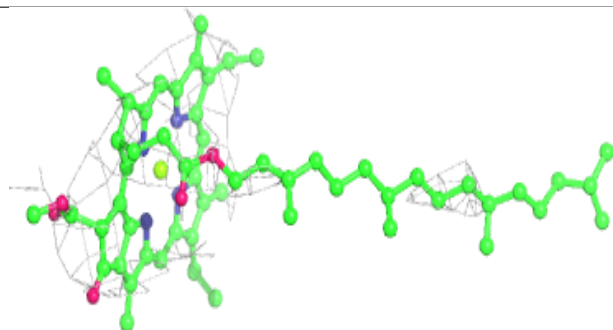
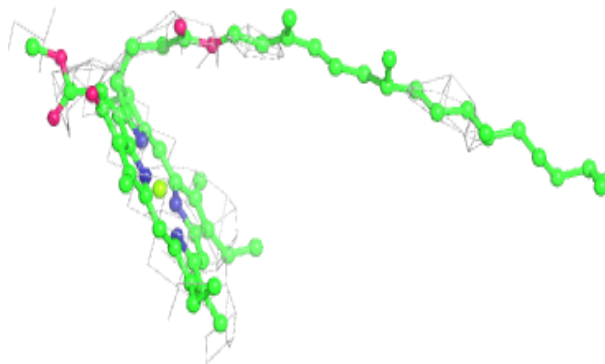
**Electron density around CLA B 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

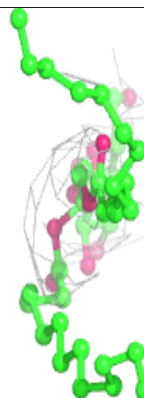
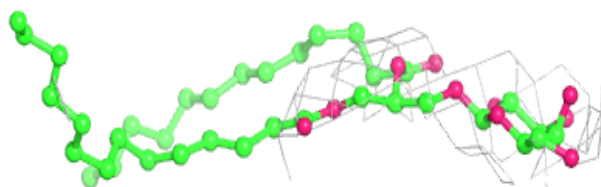
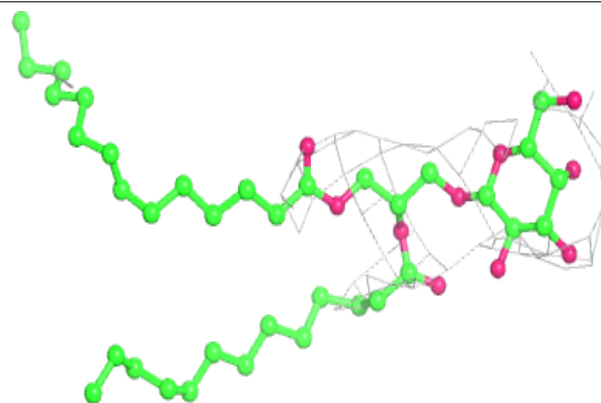


Electron density around CLA b 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

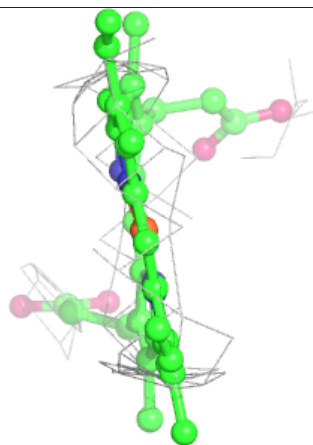
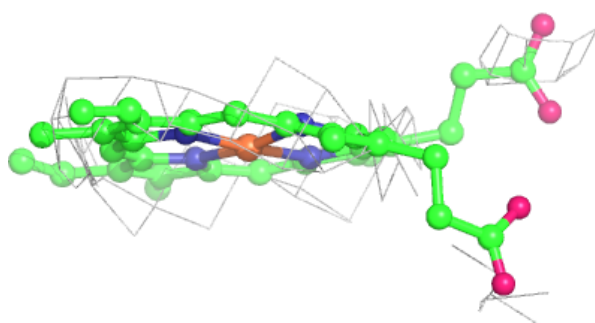
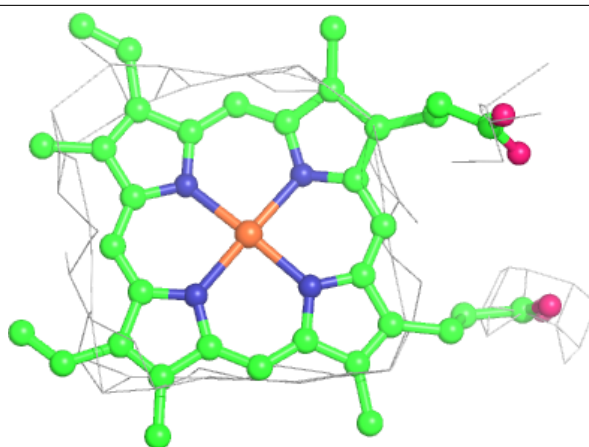
**Electron density around LMG d 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

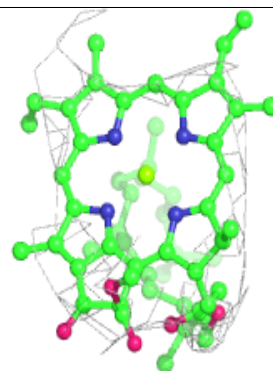
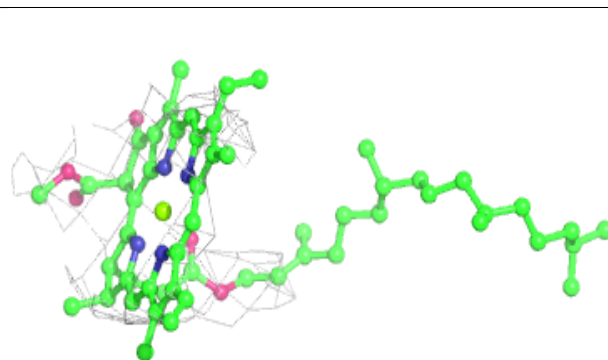
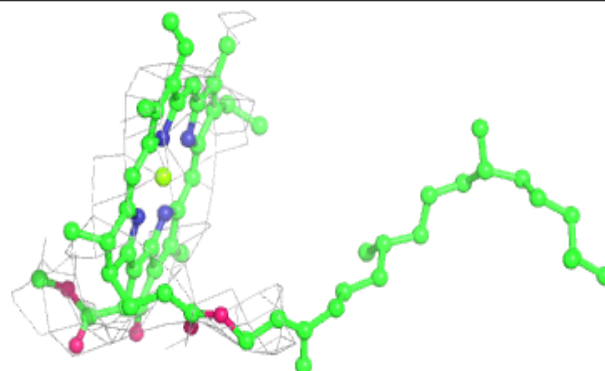


Electron density around HEM F 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

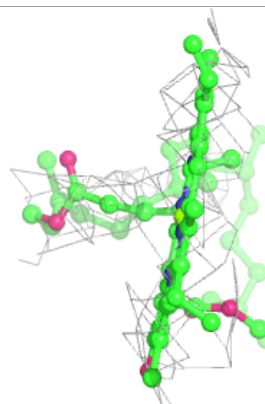
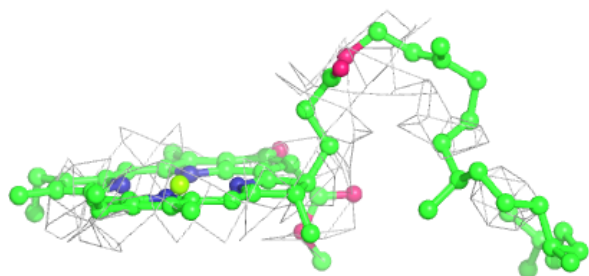
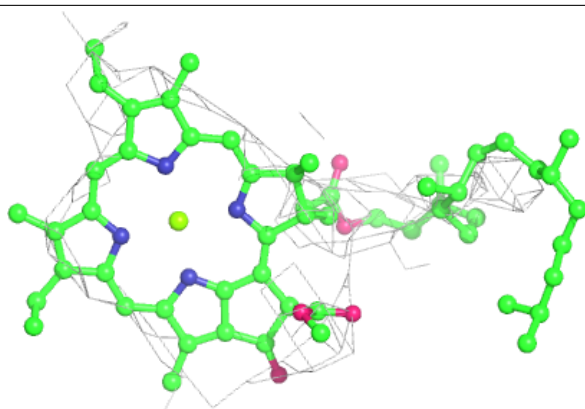
**Electron density around CLA c 507:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

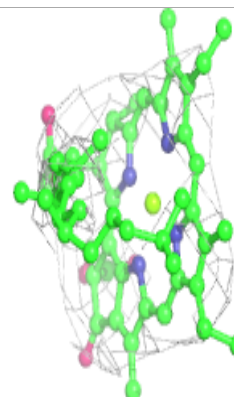
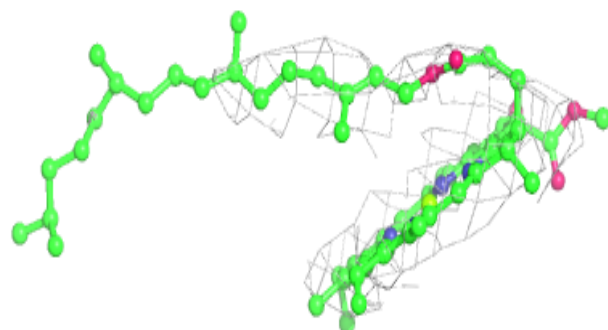
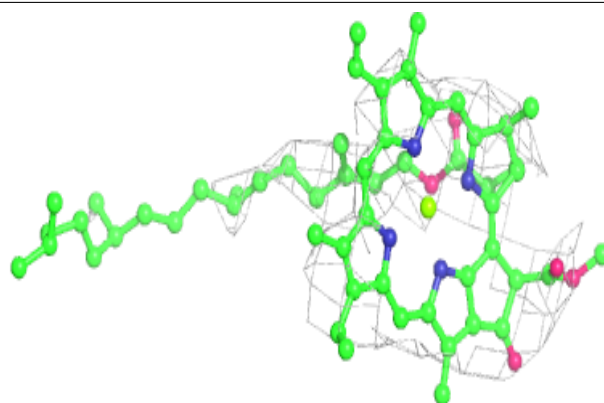


Electron density around CLA b 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

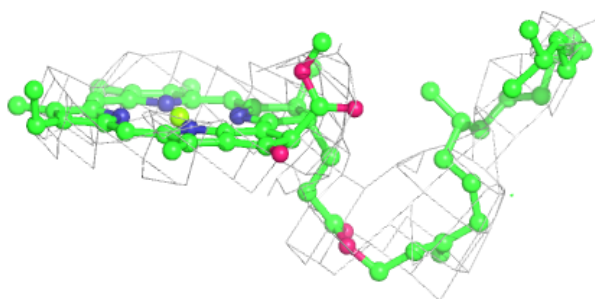
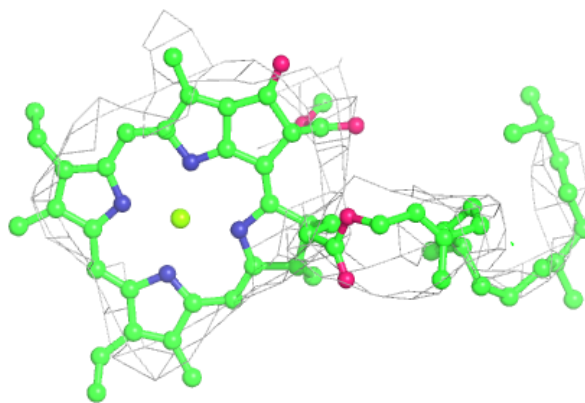
**Electron density around CLA b 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

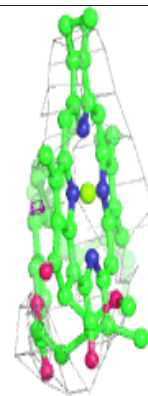
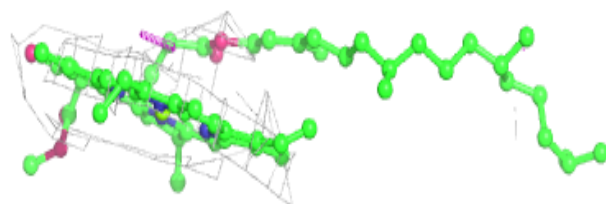
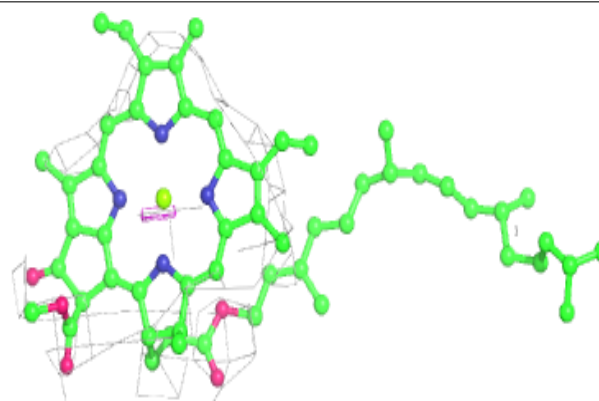


Electron density around CLA B 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

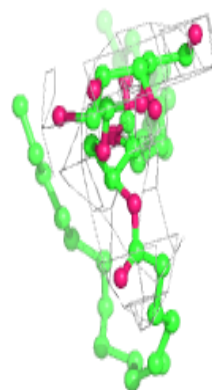
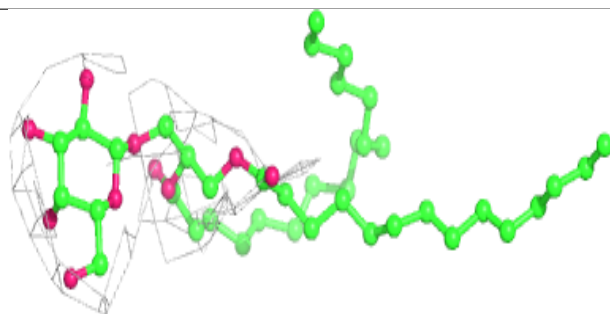
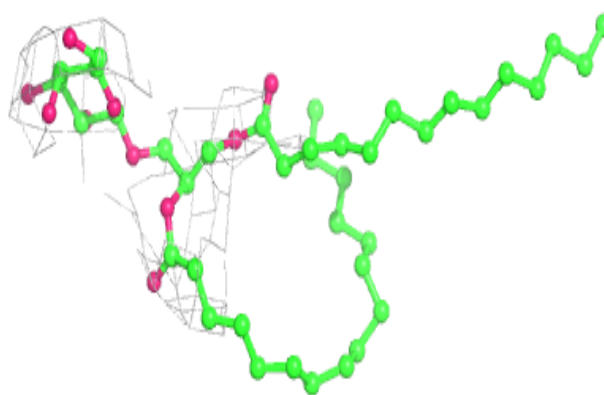
**Electron density around CLA B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

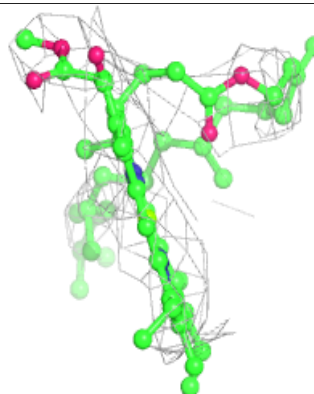
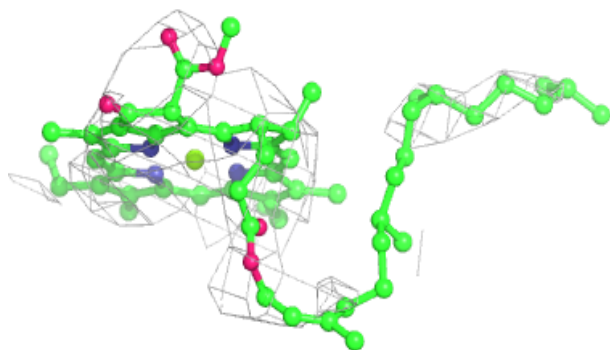
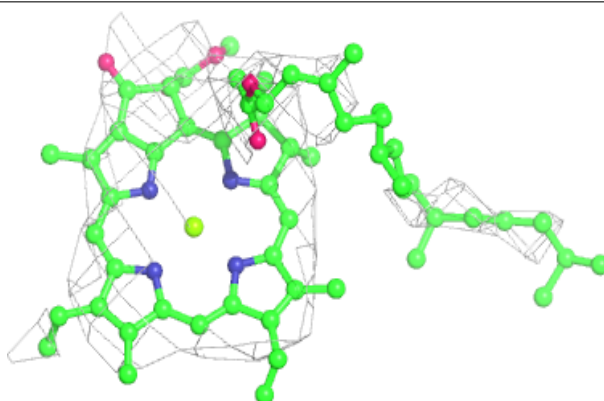


Electron density around LMG b 628:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

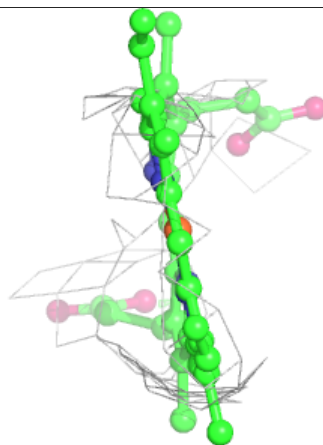
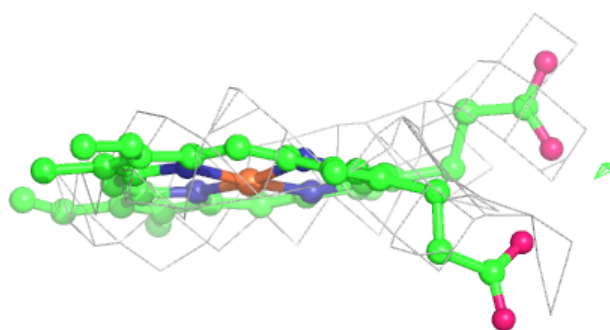
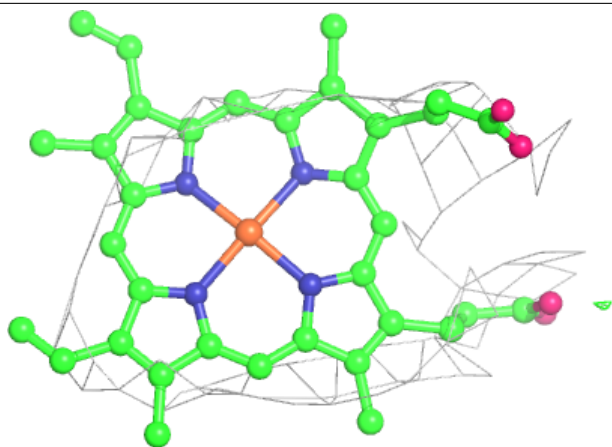
**Electron density around CLA A 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



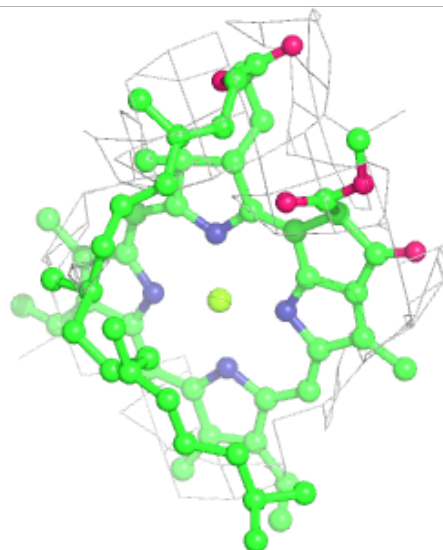
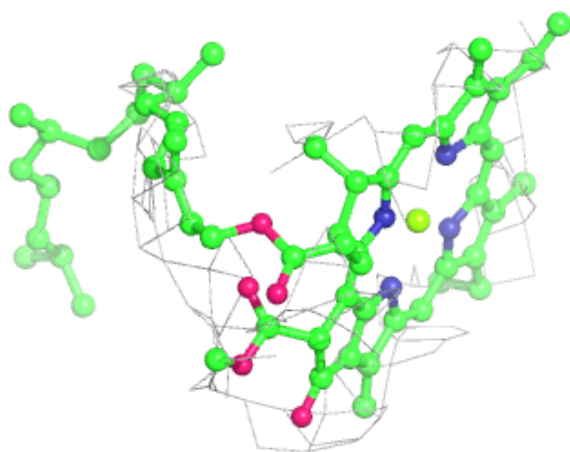
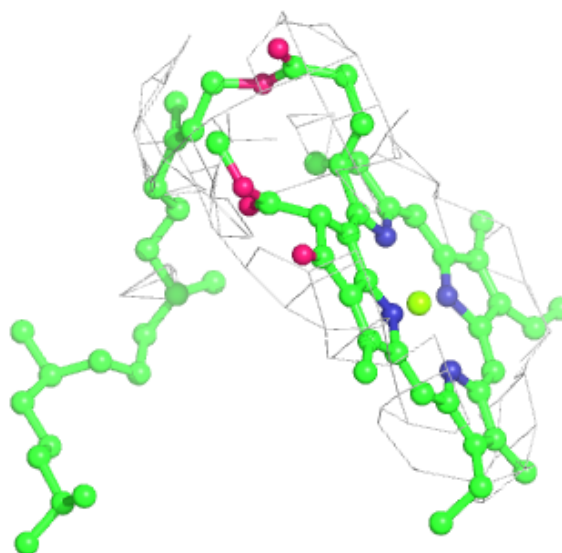
Electron density around HEM f 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.