



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 11:02 PM BST

PDB ID : 4FBY
Title : fs X-ray diffraction of Photosystem II
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2012-05-23
Resolution : 6.56 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](#) ①) 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	:	2.13
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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

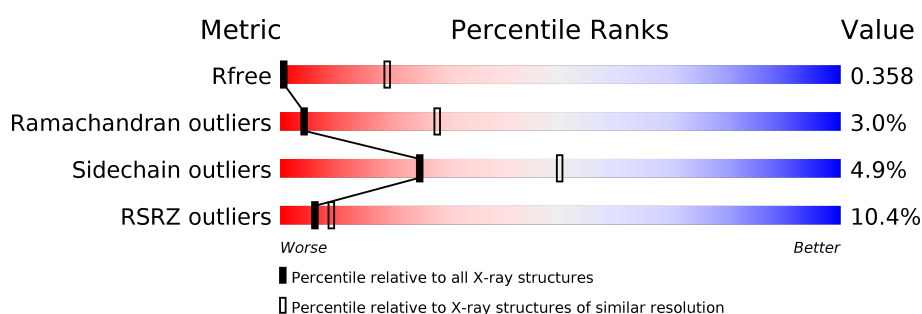
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.56 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	1000 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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	<div> <div>8%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	G	344	<div> <div>6%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
2	B	510	<div> <div>11%</div> <div>91%</div> <div>.</div> <div>.</div> <div>.</div> </div>
2	N	510	<div> <div>13%</div> <div>91%</div> <div>.</div> <div>.</div> <div>.</div> </div>
3	C	461	<div> <div>5%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
3	P	461	<div> <div>15%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
4	D	352	<div> <div>7%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	Q	352	
5	E	83	
5	R	83	
6	F	44	
6	S	44	
7	H	65	
7	W	65	
8	I	38	
8	a	38	
9	J	39	
9	b	39	
10	K	37	
10	c	37	
11	L	37	
11	d	37	
12	M	36	
12	e	36	
13	O	246	
13	f	246	
14	T	32	
14	g	32	
15	U	104	
15	h	104	
16	V	137	
16	i	137	

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Mol	Chain	Length	Quality of chain
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	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
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	X
21	CLA	B	601	X	-	-	X
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	X
21	CLA	B	605	X	-	-	X
21	CLA	B	606	X	-	-	-
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	X
21	CLA	B	609	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	611	X	-	-	-
21	CLA	B	612	X	-	-	X
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	X
21	CLA	B	616	X	-	-	X
21	CLA	C	501	X	-	-	X
21	CLA	C	502	X	-	-	X
21	CLA	C	503	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	X
21	CLA	C	506	X	-	-	X
21	CLA	C	507	X	-	-	X
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	X
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	X
21	CLA	C	512	X	-	-	X
21	CLA	C	513	X	-	-	X
21	CLA	D	401	X	-	-	X
21	CLA	D	403	X	-	-	-
21	CLA	G	402	X	-	-	-
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	X
21	CLA	N	605	X	-	-	X
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	X
21	CLA	N	608	X	-	-	X
21	CLA	N	609	X	-	-	X
21	CLA	N	610	X	-	-	X
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	-
21	CLA	N	613	X	-	-	X
21	CLA	N	614	X	-	-	-
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	X
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	X
21	CLA	N	620	X	-	-	X
21	CLA	P	501	X	-	-	-
21	CLA	P	502	X	-	-	X
21	CLA	P	503	X	-	-	X
21	CLA	P	504	X	-	-	-
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	-
21	CLA	P	507	X	-	-	X
21	CLA	P	508	X	-	-	-
21	CLA	P	509	X	-	-	X
21	CLA	P	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	511	X	-	-	X
21	CLA	P	512	X	-	-	-
21	CLA	P	513	X	-	-	X
21	CLA	Q	402	X	-	-	X
21	CLA	Q	404	X	-	-	-
22	PHO	D	402	-	-	-	X
23	PL9	G	407	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	b	101	-	-	-	X
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	X
24	DGD	B	628	X	-	-	X
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	X
24	DGD	G	408	X	-	-	X
24	DGD	N	602	X	-	-	X
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	-
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	X
24	DGD	W	102	X	-	-	-
25	LHG	A	411	-	-	-	X
25	LHG	G	412	-	-	-	X
26	SQD	A	414	-	-	-	X
26	SQD	B	624	-	-	-	X
26	SQD	B	627	-	-	-	X
26	SQD	F	101	-	-	-	X
26	SQD	N	601	-	-	-	X
26	SQD	Q	408	-	-	-	X
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	X
27	LMG	D	406	X	-	-	-
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	X
27	LMG	E	102	X	-	-	X
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	X
27	LMG	P	521	X	-	-	X
27	LMG	Q	401	X	-	-	X
27	LMG	Q	406	X	-	-	-
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	X
27	LMG	a	102	X	-	-	X
27	LMG	e	102	X	-	-	-
30	BCR	B	620	-	-	-	X
30	BCR	C	514	-	-	-	X
30	BCR	C	515	-	-	-	X
30	BCR	D	405	-	-	-	X
30	BCR	H	101	-	-	-	X
30	BCR	I	101	-	-	-	X
30	BCR	J	102	-	-	-	X
30	BCR	K	101	-	-	-	X
30	BCR	P	514	-	-	-	X
30	BCR	P	516	-	-	-	X
30	BCR	T	103	-	-	-	X
30	BCR	W	101	-	-	-	X
30	BCR	a	101	-	-	-	X
30	BCR	b	102	-	-	-	X
30	BCR	c	101	-	-	-	X
31	LMT	B	625	-	-	-	X
31	LMT	B	626	-	-	-	X
31	LMT	B	629	-	-	-	X
31	LMT	B	630	-	-	-	X
31	LMT	D	409	-	-	-	X
31	LMT	I	103	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	N	603	-	-	-	X
31	LMT	N	604	-	-	-	X
31	LMT	N	624	-	-	-	X
31	LMT	N	625	-	-	-	X
31	LMT	Q	410	-	-	-	X
31	LMT	a	103	-	-	-	X
31	LMT	e	101	-	-	-	X
33	CL	D	411	-	-	-	X
35	CA	O	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CA	f	301	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 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	G	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	N	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	P	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	Q	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	R	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	S	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	W	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	a	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	b	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	c	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	d	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	e	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	f	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	g	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	h	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	i	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	m	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

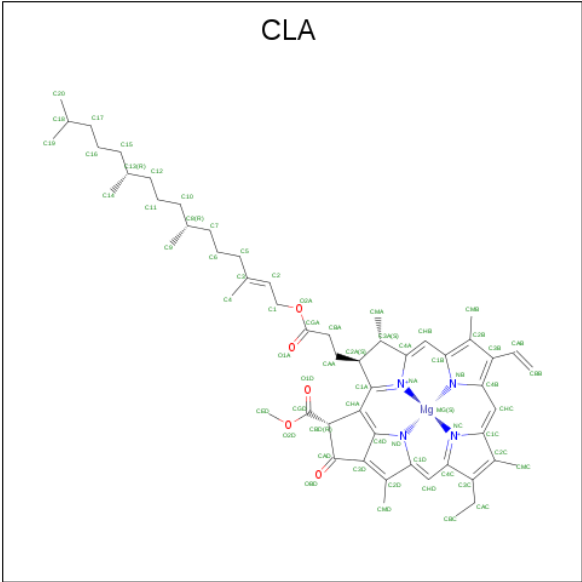
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	k	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	l	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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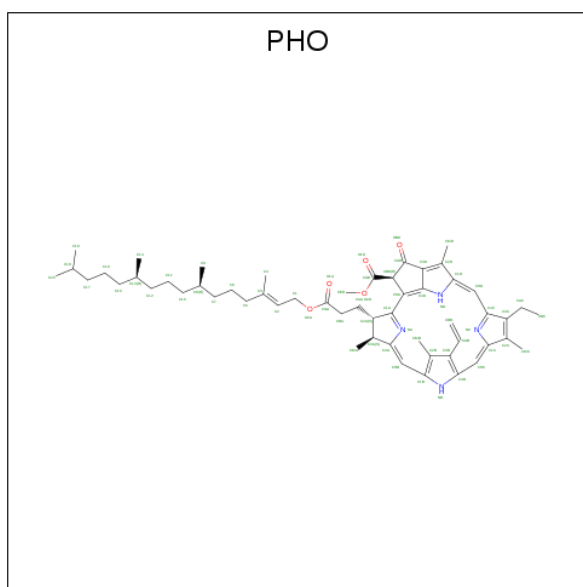
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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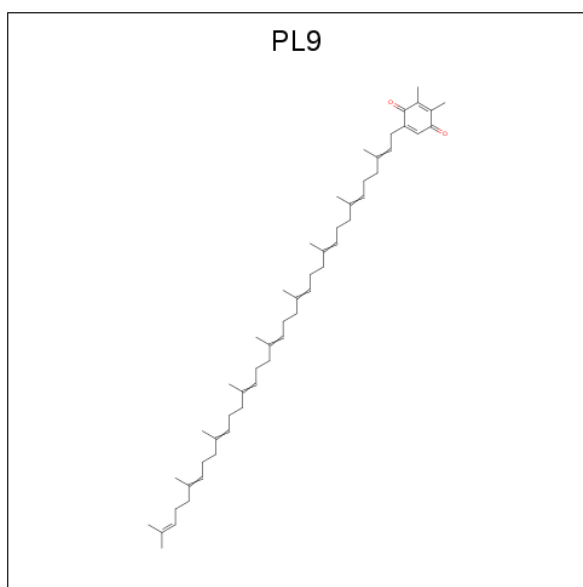
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



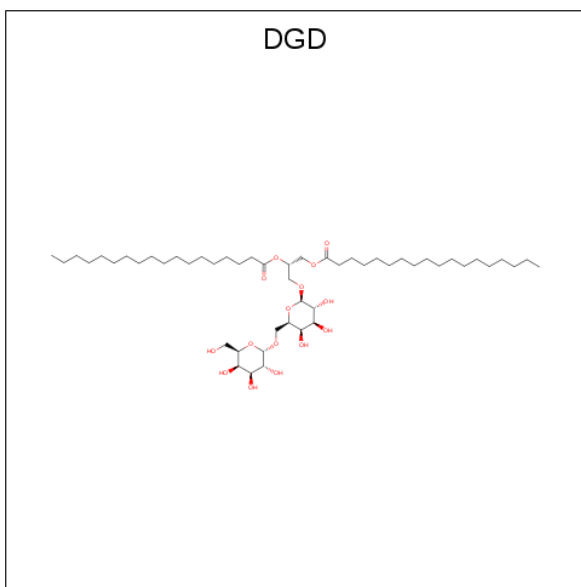
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		
22	G	1	Total	C	N	O	0	0
			64	55	4	5		
22	Q	1	Total	C	N	O	0	0
			64	55	4	5		

- 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).



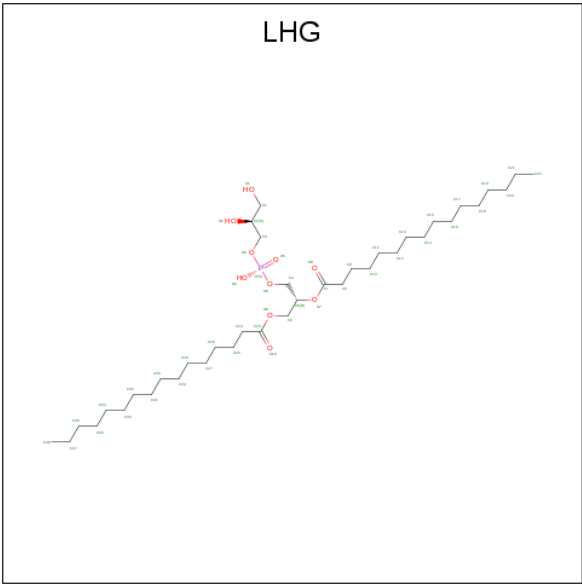
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



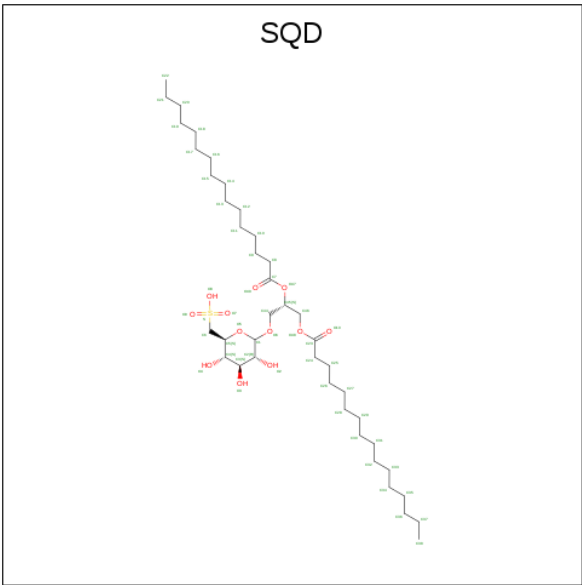
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



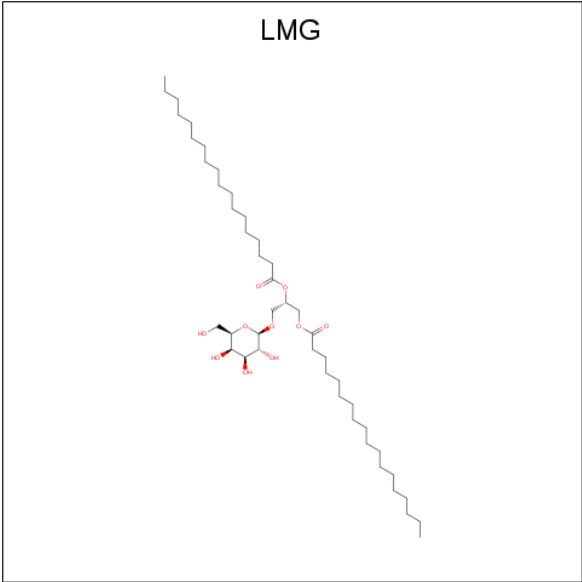
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		
25	G	1	Total	C	O	P	0	0
			39	28	10	1		
25	G	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			51	38	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			43	30	12	1		
26	B	1	Total	C	O	S	0	0
			47	34	12	1		
26	F	1	Total	C	O	S	0	0
			45	32	12	1		
26	G	1	Total	C	O	S	0	0
			54	41	12	1		
26	G	1	Total	C	O	S	0	0
			51	38	12	1		
26	N	1	Total	C	O	S	0	0
			47	34	12	1		
26	Q	1	Total	C	O	S	0	0
			43	30	12	1		
26	S	1	Total	C	O	S	0	0
			45	32	12	1		

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



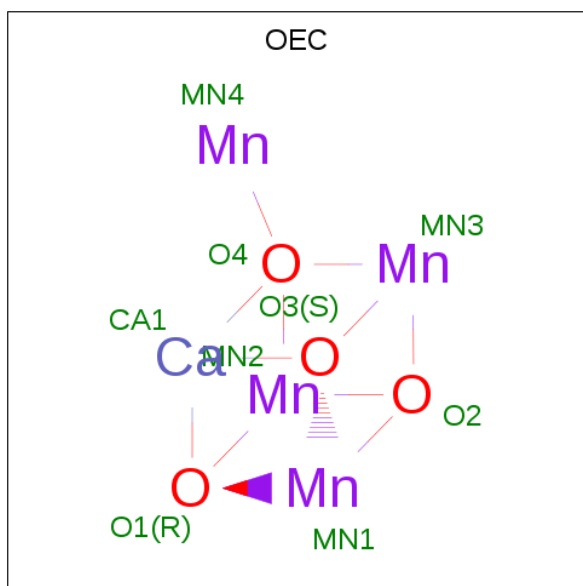
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			42	32	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	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

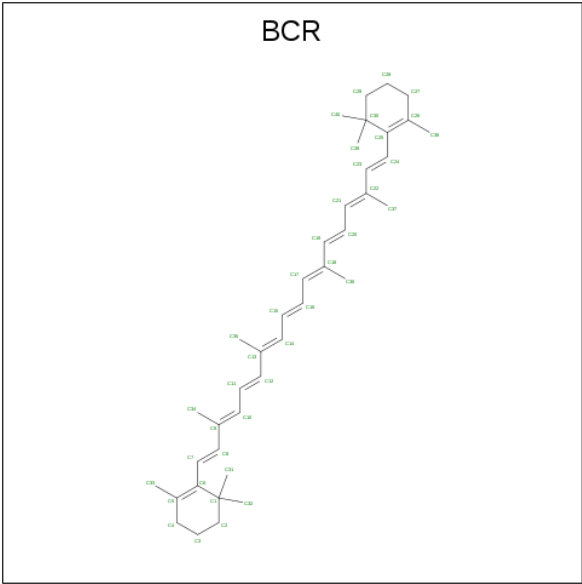


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total Fe 1 1	0	0
29	A	1	Total Fe 1 1	0	0

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



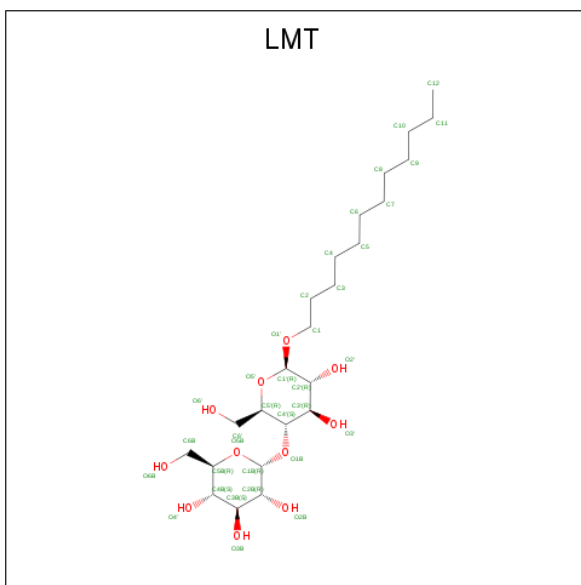
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0

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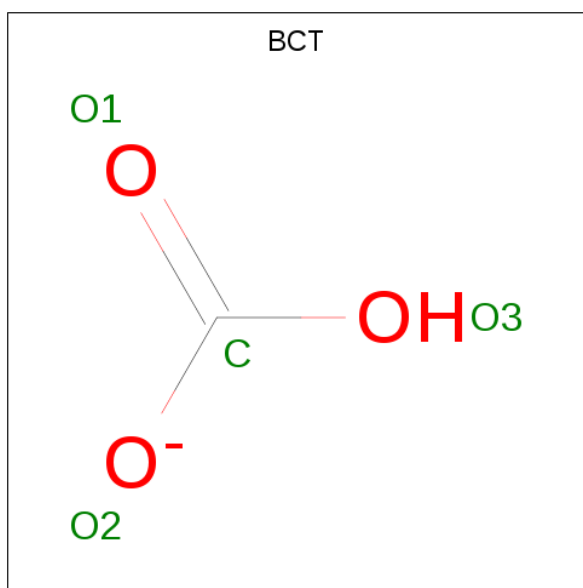
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	D	1	Total 31	C 20	O 11	0	0
31	I	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	Q	1	Total 31	C 20	O 11	0	0
31	a	1	Total 35	C 24	O 11	0	0
31	e	1	Total 35	C 24	O 11	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

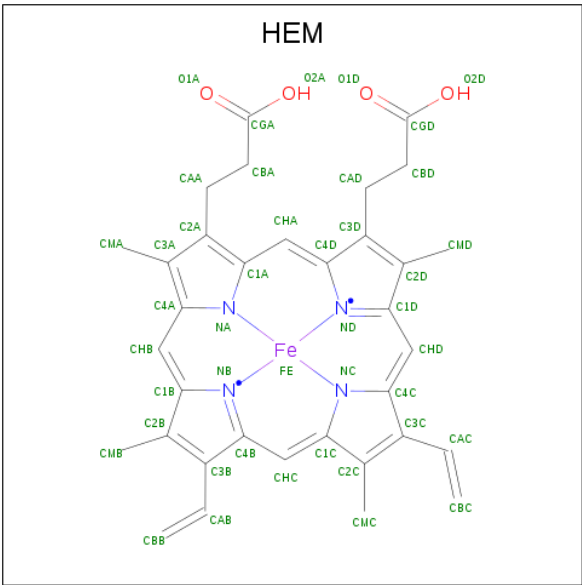


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	G	1	Total	Cl	0	0
			1	1		
33	D	1	Total	Cl	0	0
			1	1		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	R	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	i	1	Total	C	Fe	N	O	
			43	34	1	4	4	

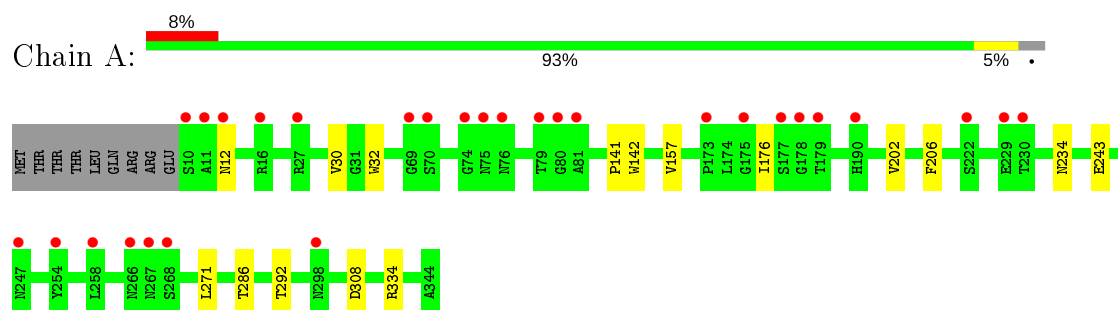
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total	Ca		
			1	1	0	0
35	f	1	Total	Ca		
			1	1	0	0

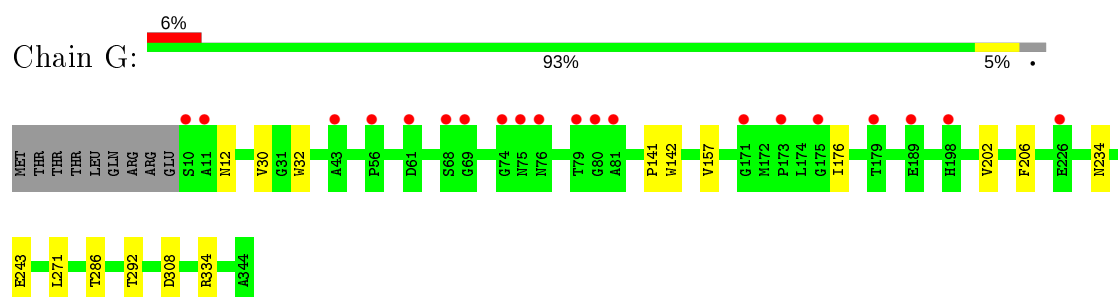
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

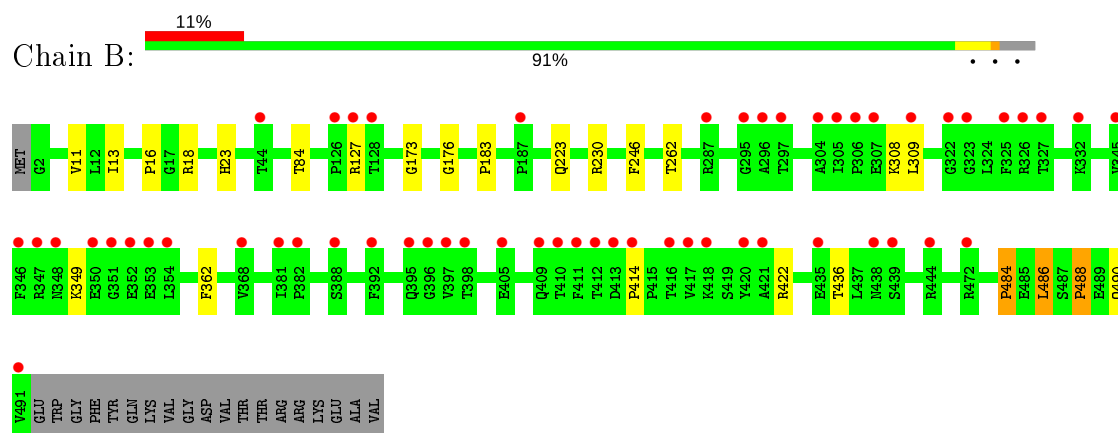
- Molecule 1: Photosystem Q(B) protein 1



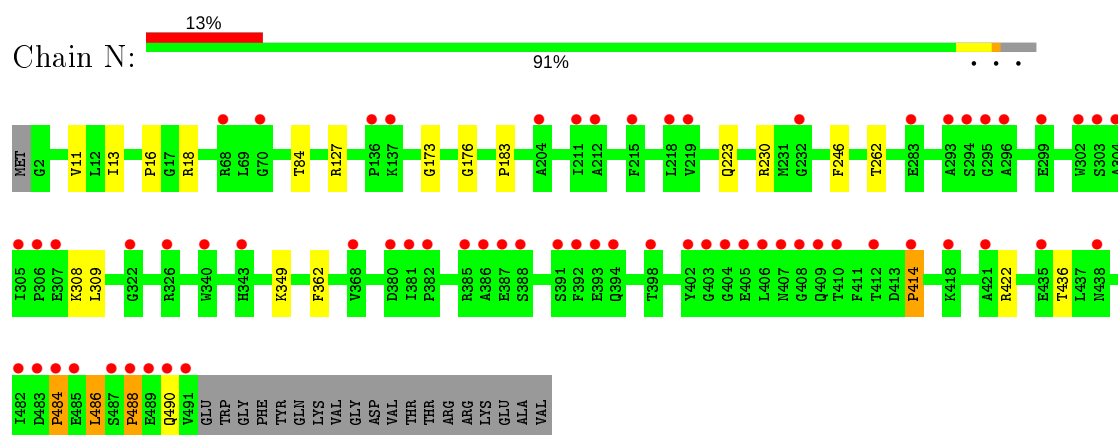
- Molecule 1: Photosystem Q(B) protein 1



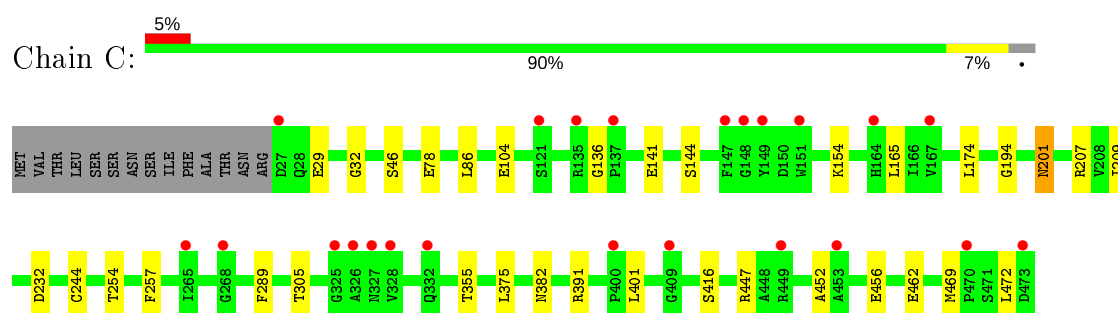
- Molecule 2: Photosystem II core light harvesting protein



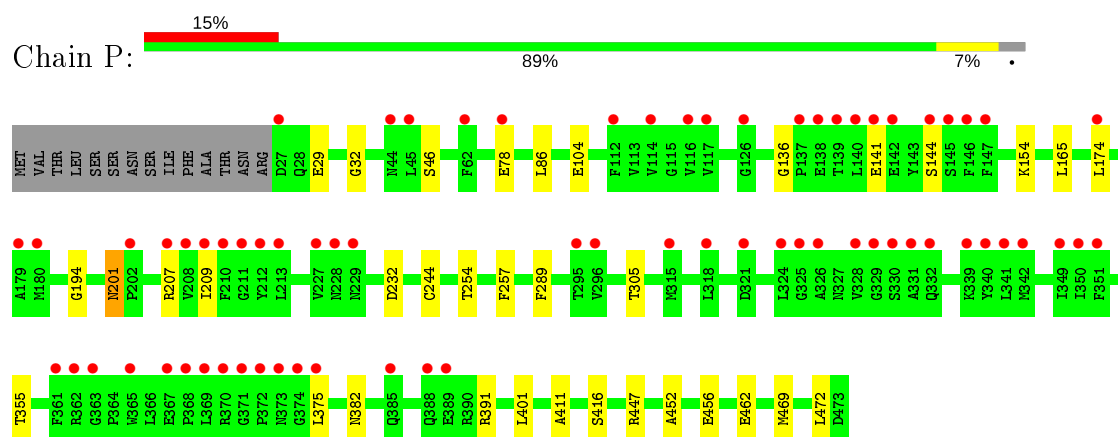
- Molecule 2: Photosystem II core light harvesting protein



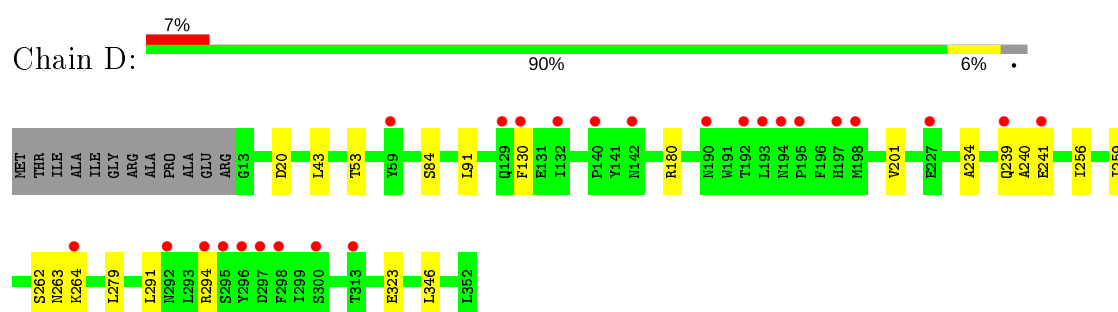
- Molecule 3: Photosystem II CP43 protein



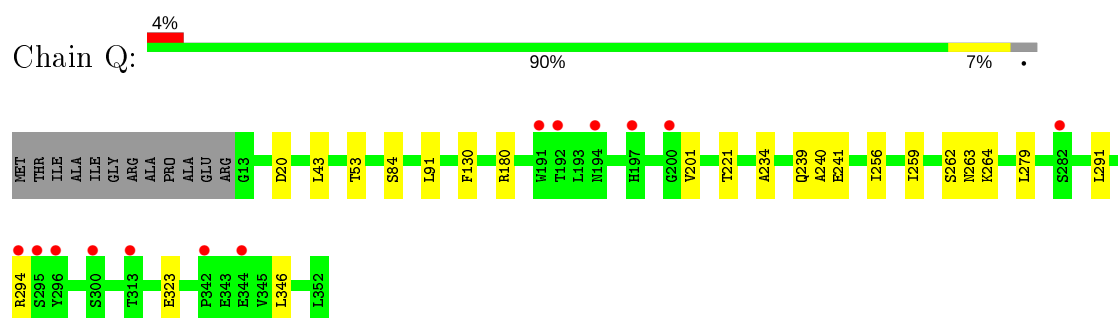
- Molecule 3: Photosystem II CP43 protein



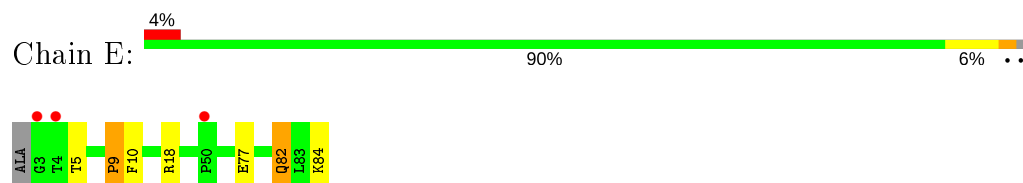
- Molecule 4: Photosystem II D2 protein



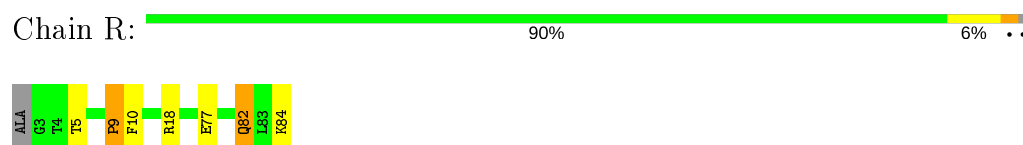
- Molecule 4: Photosystem II D2 protein



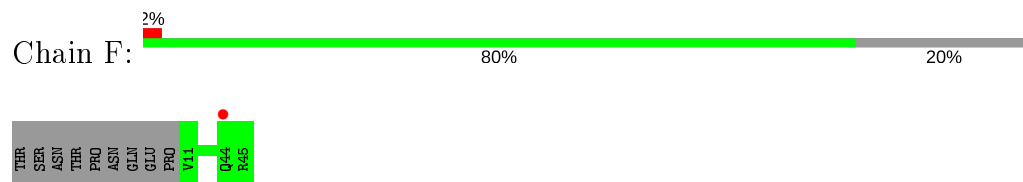
- Molecule 5: Cytochrome b559 subunit alpha



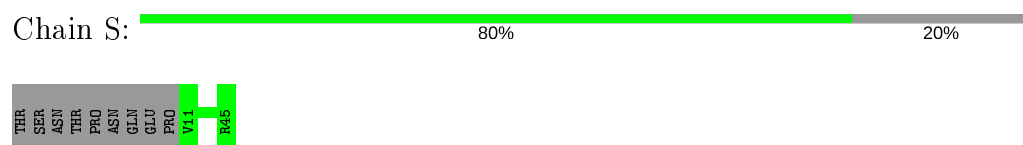
- Molecule 5: Cytochrome b559 subunit alpha



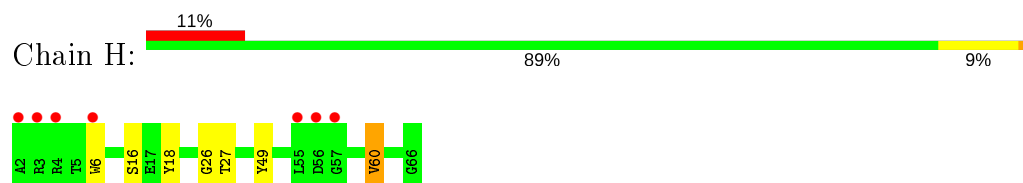
- Molecule 6: Cytochrome b559 subunit beta



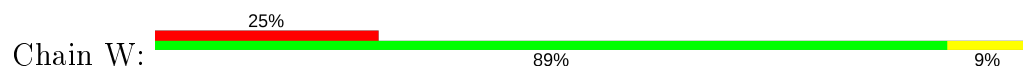
- Molecule 6: Cytochrome b559 subunit beta

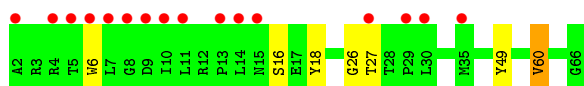


- Molecule 7: Photosystem II reaction center protein H

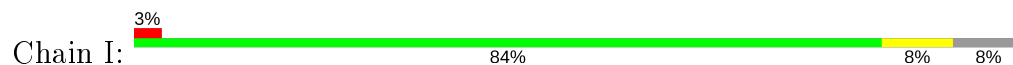


- Molecule 7: Photosystem II reaction center protein H

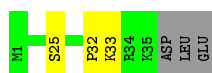
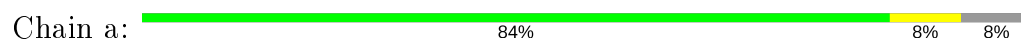




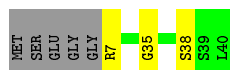
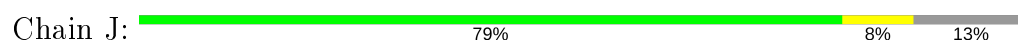
- Molecule 8: Photosystem II reaction center protein I



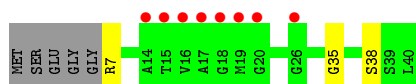
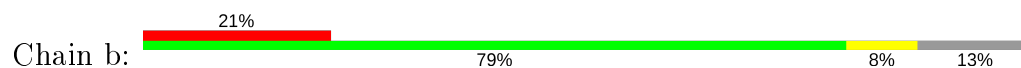
- Molecule 8: Photosystem II reaction center protein I



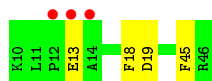
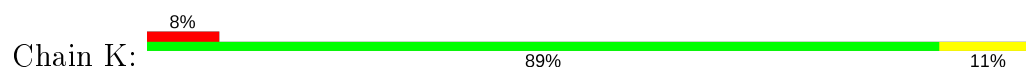
- Molecule 9: Photosystem II reaction center protein J



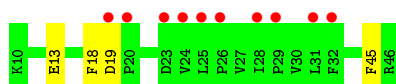
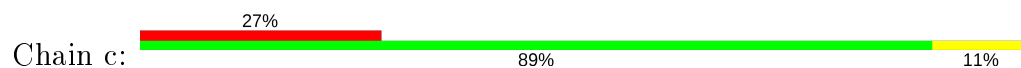
- Molecule 9: Photosystem II reaction center protein J



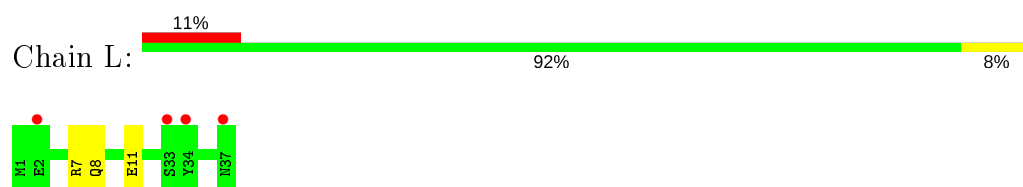
- Molecule 10: Photosystem II reaction center protein K



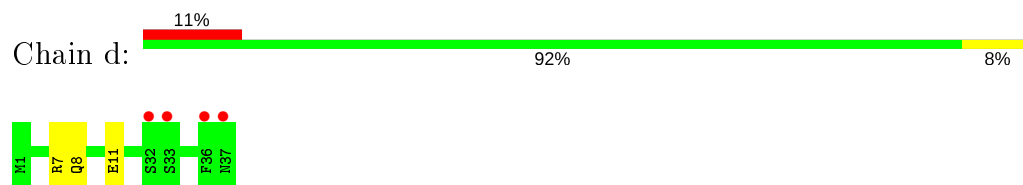
- Molecule 10: Photosystem II reaction center protein K



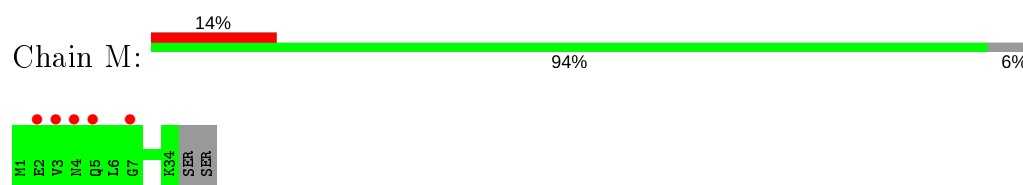
- Molecule 11: Photosystem II reaction center protein L



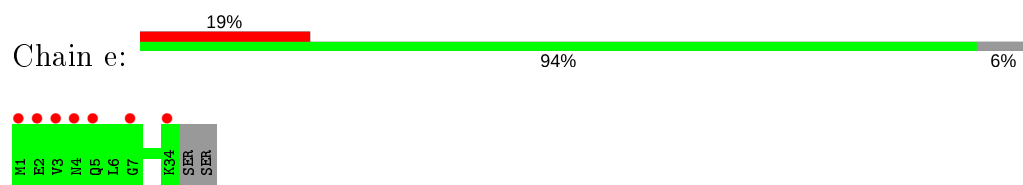
- Molecule 11: Photosystem II reaction center protein L



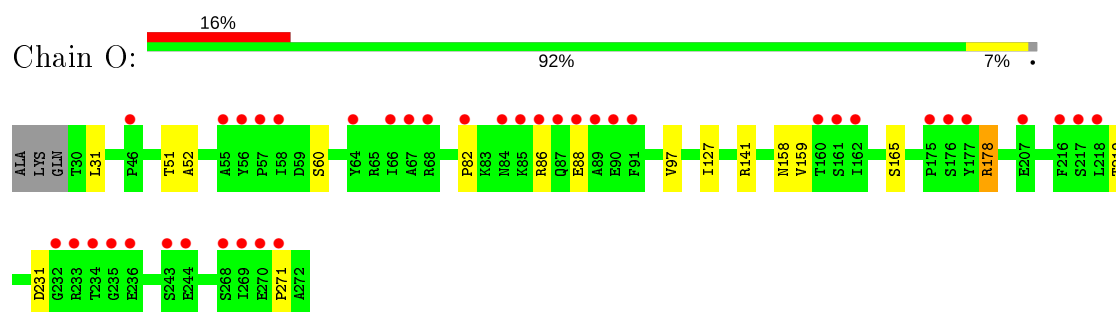
- Molecule 12: Photosystem II reaction center protein M



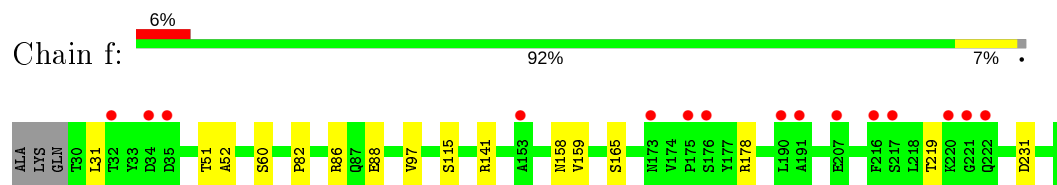
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

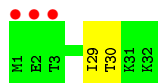


- Molecule 14: Photosystem II reaction center protein T

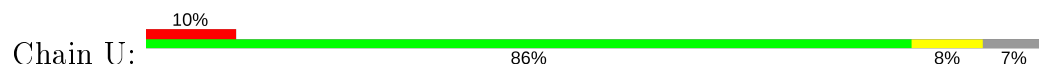




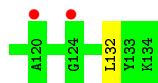
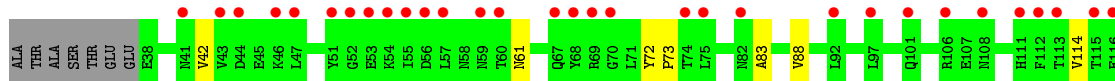
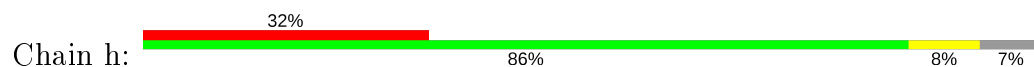
- Molecule 14: Photosystem II reaction center protein T



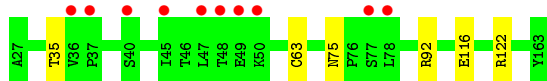
- Molecule 15: Photosystem II 12 kDa extrinsic protein



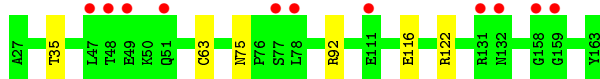
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

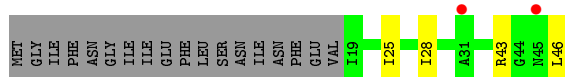


- Molecule 16: Cytochrome c-550

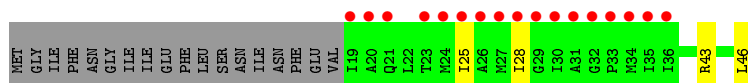


- Molecule 17: Photosystem II reaction center protein ycf12

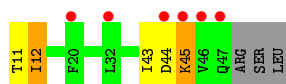




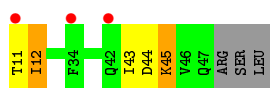
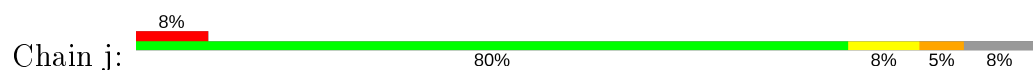
- Molecule 17: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Y



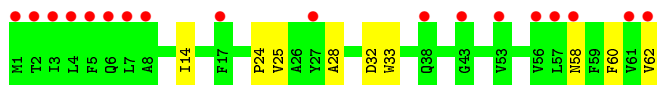
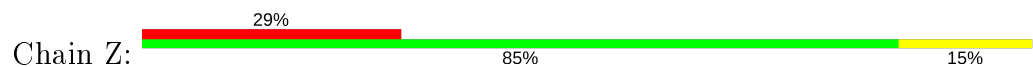
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

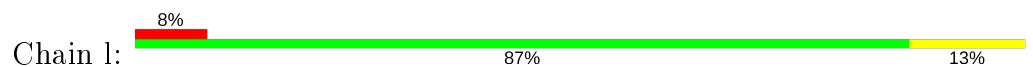


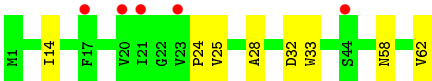
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.78 Å 227.76 Å 308.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.88 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.8 (85.88-6.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 6.72 Å)	Xtriage
Refinement program	PHENIX 1.7.3	Depositor
R, R_{free}	0.366 , 0.385 0.342 , 0.358	Depositor DCC
R_{free} test set	895 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	6.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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	0.26	0/2713	0.55	0/3700
1	G	0.26	0/2713	0.54	0/3700
2	B	0.26	0/3986	0.55	2/5433 (0.0%)
2	N	0.27	0/3986	0.56	2/5433 (0.0%)
3	C	0.25	0/3556	0.56	0/4842
3	P	0.25	0/3556	0.56	0/4842
4	D	0.26	0/2801	0.55	0/3818
4	Q	0.26	0/2801	0.54	0/3818
5	E	0.27	0/685	0.58	0/933
5	R	0.27	0/685	0.58	0/933
6	F	0.25	0/291	0.49	0/397
6	S	0.23	0/291	0.48	0/397
7	H	0.27	0/520	0.61	0/709
7	W	0.28	0/520	0.61	0/709
8	I	0.26	0/293	0.53	0/395
8	a	0.27	0/293	0.53	0/395
9	J	0.24	0/255	0.56	0/346
9	b	0.24	0/255	0.57	0/346
10	K	0.30	0/303	0.59	0/416
10	c	0.30	0/303	0.59	0/416
11	L	0.25	0/311	0.52	0/422
11	d	0.26	0/311	0.52	0/422
12	M	0.28	0/270	0.58	0/367
12	e	0.29	0/270	0.57	0/367
13	O	0.26	0/1876	0.60	1/2548 (0.0%)
13	f	0.26	0/1876	0.61	0/2548
14	T	0.27	0/284	0.53	0/381
14	g	0.27	0/284	0.53	0/381
15	U	0.27	0/785	0.61	0/1064
15	h	0.27	0/785	0.62	0/1064
16	V	0.24	0/1081	0.54	0/1468
16	i	0.24	0/1081	0.53	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.27	0/202	0.68	0/272
17	y	0.30	0/202	0.69	0/272
18	X	0.32	0/273	0.59	0/370
18	j	0.32	0/273	0.59	0/370
20	Z	0.28	0/490	0.62	0/669
20	l	0.28	0/490	0.62	0/669
All	All	0.26	0/41950	0.56	5/57100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	7.03	131.46	115.30
2	N	486	LEU	CA-CB-CG	6.79	130.91	115.30
2	N	484	PRO	N-CA-C	5.16	125.51	112.10
2	B	484	PRO	N-CA-C	5.05	125.24	112.10
13	O	178	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	297 (89%)	31 (9%)	5 (2%)	10	46
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	10	46
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	5	32
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	5	32
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	3	26
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	3	25
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	8	40
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	8	40
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	3	24
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	3	24
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	13
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	13
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	1	17
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	1	17
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	16
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	16
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	18
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	3	24
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	26
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	26
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	22
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	22
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	22	63
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	22	63
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	13
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	13
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	7
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	7
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	20
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	20
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	4	28

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO

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%)	260 (96%)	11 (4%)	30	55
1	G	271/280 (97%)	260 (96%)	11 (4%)	30	55
2	B	390/407 (96%)	377 (97%)	13 (3%)	38	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	390/407 (96%)	376 (96%)	14 (4%)	35	59
3	C	347/362 (96%)	327 (94%)	20 (6%)	20	45
3	P	347/362 (96%)	327 (94%)	20 (6%)	20	45
4	D	275/283 (97%)	259 (94%)	16 (6%)	20	45
4	Q	275/283 (97%)	258 (94%)	17 (6%)	18	43
5	E	72/72 (100%)	66 (92%)	6 (8%)	11	34
5	R	72/72 (100%)	66 (92%)	6 (8%)	11	34
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	20	45
7	W	53/54 (98%)	50 (94%)	3 (6%)	20	45
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	a	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/27 (89%)	23 (96%)	1 (4%)	30	54
9	b	24/27 (89%)	23 (96%)	1 (4%)	30	54
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	41
10	c	30/30 (100%)	28 (93%)	2 (7%)	16	41
11	L	35/35 (100%)	32 (91%)	3 (9%)	10	32
11	d	35/35 (100%)	32 (91%)	3 (9%)	10	32
12	M	31/33 (94%)	31 (100%)	0	100	100
12	e	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	196 (97%)	6 (3%)	41	63
13	f	202/208 (97%)	196 (97%)	6 (3%)	41	63
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	g	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	51
15	h	84/89 (94%)	80 (95%)	4 (5%)	25	51
16	V	116/117 (99%)	111 (96%)	5 (4%)	29	53
16	i	116/117 (99%)	111 (96%)	5 (4%)	29	53
17	m	20/37 (54%)	18 (90%)	2 (10%)	7	26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	30/33 (91%)	27 (90%)	3 (10%)	7	26
18	j	30/33 (91%)	27 (90%)	3 (10%)	7	26
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	27
20	l	52/52 (100%)	47 (90%)	5 (10%)	8	27
All	All	4244/4442 (96%)	4038 (95%)	206 (5%)	25	50

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	46	LEU
2	N	84	THR
15	h	132	LEU
18	X	12	ILE
1	G	157	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	234	ASN
1	G	241	GLN
4	Q	250	ASN
11	L	8	GLN
4	Q	129	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 182 ligands modelled in this entry, 6 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
24	DGD	B	628	-	53,53,67	1.02	3 (5%)	67,67,81	1.53	11 (16%)
21	CLA	B	615	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	11 (16%)
21	CLA	Q	404	-	59,73,73	1.41	12 (20%)	67,113,113	2.08	9 (13%)
30	BCR	J	102	-	41,41,41	0.79	0	56,56,56	3.06	21 (37%)
31	LMT	B	625	-	36,36,36	0.41	0	47,47,47	0.70	0
27	LMG	I	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.31	5 (9%)
31	LMT	B	630	-	36,36,36	0.39	0	47,47,47	0.62	0
31	LMT	N	604	-	36,36,36	0.42	0	47,47,47	0.62	0
30	BCR	K	101	-	41,41,41	0.79	0	56,56,56	1.62	12 (21%)
21	CLA	P	512	-	59,73,73	1.41	12 (20%)	67,113,113	2.07	10 (14%)
24	DGD	A	407	-	57,57,67	0.99	4 (7%)	71,71,81	1.48	8 (11%)
22	PHO	D	402	-	67,69,69	2.15	18 (26%)	85,99,99	1.84	19 (22%)
24	DGD	B	621	-	59,59,67	0.95	3 (5%)	73,73,81	1.39	9 (12%)
27	LMG	D	412	-	42,42,55	1.04	2 (4%)	50,50,63	1.26	5 (10%)
27	LMG	D	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.34	7 (12%)
21	CLA	B	603	-	59,73,73	1.43	14 (23%)	67,113,113	2.07	10 (14%)
21	CLA	B	609	-	59,73,73	1.41	12 (20%)	67,113,113	2.04	8 (11%)
21	CLA	P	502	-	59,73,73	1.41	13 (22%)	67,113,113	2.06	9 (13%)
30	BCR	H	101	-	41,41,41	0.76	0	56,56,56	1.46	11 (19%)
27	LMG	G	411	-	51,51,55	0.96	2 (3%)	59,59,63	1.23	4 (6%)
21	CLA	C	506	-	59,73,73	1.42	14 (23%)	67,113,113	2.05	10 (14%)
23	PL9	b	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.59	10 (22%)
21	CLA	C	503	-	59,73,73	1.40	12 (20%)	67,113,113	2.06	10 (14%)
30	BCR	Z	101	-	41,41,41	0.67	0	56,56,56	1.62	12 (21%)
27	LMG	N	622	-	49,49,55	0.93	2 (4%)	57,57,63	1.36	7 (12%)
21	CLA	N	605	-	59,73,73	1.38	14 (23%)	67,113,113	2.07	10 (14%)
28	OEC	G	413	1	0,0,13	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	D	401	-	59,73,73	1.42	10 (16%)	67,113,113	2.04	11 (16%)
30	BCR	b	102	-	41,41,41	0.78	0	56,56,56	3.10	20 (35%)
21	CLA	G	404	-	59,73,73	1.39	13 (22%)	67,113,113	2.06	10 (14%)
21	CLA	B	611	-	59,73,73	1.41	14 (23%)	67,113,113	2.12	12 (17%)
26	SQD	B	627	-	46,47,54	1.28	5 (10%)	55,58,65	1.47	9 (16%)
31	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
30	BCR	T	102	-	41,41,41	0.69	0	56,56,56	1.86	15 (26%)
28	OEC	A	412	1,3	0,0,13	0.00	-	-		
30	BCR	P	514	-	41,41,41	0.70	0	56,56,56	2.37	18 (32%)
21	CLA	N	614	-	59,73,73	1.41	13 (22%)	67,113,113	2.03	10 (14%)
34	HEM	R	101	5,6	27,50,50	2.14	5 (18%)	17,82,82	2.25	3 (17%)
23	PL9	D	404	-	55,55,55	1.24	8 (14%)	68,69,69	1.64	19 (27%)
26	SQD	F	101	-	44,45,54	1.30	4 (9%)	53,56,65	1.22	8 (15%)
27	LMG	R	102	-	44,44,55	1.00	2 (4%)	52,52,63	1.12	5 (9%)
30	BCR	c	101	-	41,41,41	0.78	0	56,56,56	1.57	11 (19%)
21	CLA	N	608	-	59,73,73	1.41	13 (22%)	67,113,113	2.07	10 (14%)
21	CLA	P	511	3	59,73,73	1.40	12 (20%)	67,113,113	2.07	10 (14%)
21	CLA	N	609	-	59,73,73	1.40	13 (22%)	67,113,113	2.13	12 (17%)
22	PHO	Q	403	-	67,69,69	2.15	18 (26%)	85,99,99	1.82	19 (22%)
21	CLA	C	505	-	59,73,73	1.40	12 (20%)	67,113,113	2.12	10 (14%)
27	LMG	P	520	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	6 (10%)
27	LMG	A	410	-	51,51,55	0.95	2 (3%)	59,59,63	1.26	4 (6%)
31	LMT	N	624	-	36,36,36	0.41	0	47,47,47	0.67	0
21	CLA	C	511	3	59,73,73	1.40	13 (22%)	67,113,113	2.11	10 (14%)
27	LMG	e	102	-	42,42,55	1.03	2 (4%)	50,50,63	1.32	6 (12%)
27	LMG	Q	401	-	42,42,55	1.04	2 (4%)	50,50,63	1.23	5 (10%)
21	CLA	P	510	-	59,73,73	1.41	13 (22%)	67,113,113	2.05	9 (13%)
21	CLA	A	405	-	59,73,73	1.40	13 (22%)	67,113,113	2.08	11 (16%)
21	CLA	B	607	-	59,73,73	1.42	12 (20%)	67,113,113	2.06	9 (13%)
34	HEM	V	201	16	27,50,50	2.15	5 (18%)	17,82,82	1.95	3 (17%)
21	CLA	N	610	-	59,73,73	1.42	12 (20%)	67,113,113	2.06	11 (16%)
24	DGD	P	517	-	54,54,67	0.99	3 (5%)	68,68,81	1.55	10 (14%)
27	LMG	P	521	-	45,45,55	1.03	2 (4%)	53,53,63	1.22	5 (9%)
21	CLA	P	501	-	59,73,73	1.41	12 (20%)	67,113,113	2.08	9 (13%)
21	CLA	C	501	-	59,73,73	1.41	12 (20%)	67,113,113	2.06	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	B	619	-	41,41,41	0.74	0	56,56,56	1.52	10 (17%)
21	CLA	N	607	-	59,73,73	1.43	13 (22%)	67,113,113	2.04	12 (17%)
23	PL9	A	406	-	45,45,55	1.23	7 (15%)	56,57,69	1.71	18 (32%)
27	LMG	Q	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	5 (8%)
30	BCR	B	620	-	41,41,41	0.71	0	56,56,56	1.61	10 (17%)
21	CLA	B	608	-	59,73,73	1.42	14 (23%)	67,113,113	2.03	8 (11%)
30	BCR	D	405	-	41,41,41	0.70	0	56,56,56	1.72	10 (17%)
30	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.60	11 (19%)
21	CLA	Q	402	-	59,73,73	1.41	10 (16%)	67,113,113	2.03	11 (16%)
21	CLA	C	512	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	10 (14%)
30	BCR	N	621	-	41,41,41	0.73	0	56,56,56	1.55	13 (23%)
30	BCR	P	516	-	41,41,41	0.75	0	56,56,56	1.69	15 (26%)
26	SQD	B	624	-	42,43,54	1.34	5 (11%)	51,54,65	1.45	7 (13%)
31	LMT	D	409	-	32,32,36	0.47	0	43,43,47	0.65	1 (2%)
21	CLA	C	502	-	59,73,73	1.40	13 (22%)	67,113,113	2.05	7 (10%)
21	CLA	B	614	-	59,73,73	1.42	11 (18%)	67,113,113	2.03	10 (14%)
31	LMT	e	101	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
21	CLA	B	604	-	59,73,73	1.41	12 (20%)	67,113,113	2.05	11 (16%)
21	CLA	P	505	-	59,73,73	1.40	12 (20%)	67,113,113	2.11	8 (11%)
21	CLA	N	606	-	59,73,73	1.42	13 (22%)	67,113,113	2.08	10 (14%)
31	LMT	Q	410	-	32,32,36	0.47	0	43,43,47	0.64	1 (2%)
30	BCR	B	618	-	41,41,41	0.70	0	56,56,56	1.88	15 (26%)
24	DGD	P	519	-	67,67,67	0.90	4 (5%)	81,81,81	1.28	7 (8%)
21	CLA	P	503	-	59,73,73	1.40	11 (18%)	67,113,113	2.02	10 (14%)
27	LMG	D	407	-	48,48,55	0.95	2 (4%)	56,56,63	1.28	5 (8%)
26	SQD	Q	408	-	42,43,54	1.35	5 (11%)	51,54,65	1.45	6 (11%)
34	HEM	i	201	16	27,50,50	2.15	6 (22%)	17,82,82	1.94	5 (29%)
25	LHG	G	409	-	38,38,48	1.07	2 (5%)	41,44,54	0.95	2 (4%)
30	BCR	I	101	-	41,41,41	0.69	0	56,56,56	1.58	12 (21%)
24	DGD	G	408	-	57,57,67	0.98	4 (7%)	71,71,81	1.47	8 (11%)
21	CLA	G	403	-	59,73,73	1.40	13 (22%)	67,113,113	2.05	12 (17%)
25	LHG	G	412	-	36,36,48	1.09	2 (5%)	39,42,54	1.05	2 (5%)
21	CLA	D	403	-	59,73,73	1.40	12 (20%)	67,113,113	2.08	9 (13%)
21	CLA	B	612	-	59,73,73	1.42	14 (23%)	67,113,113	2.04	10 (14%)
21	CLA	A	401	-	59,73,73	1.42	13 (22%)	67,113,113	1.98	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	Q	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.30	4 (7%)
32	BCT	Q	411	29	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	A	403	-	59,73,73	1.41	13 (22%)	67,113,113	2.01	9 (13%)
21	CLA	N	615	-	59,73,73	1.41	14 (23%)	67,113,113	2.07	11 (16%)
31	LMT	N	625	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
27	LMG	M	101	-	42,42,55	1.03	2 (4%)	50,50,63	1.30	6 (12%)
30	BCR	W	101	-	41,41,41	0.76	0	56,56,56	1.46	8 (14%)
23	PL9	J	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.57	9 (20%)
27	LMG	B	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.28	6 (10%)
21	CLA	P	506	-	59,73,73	1.42	14 (23%)	67,113,113	2.04	10 (14%)
24	DGD	Q	409	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
21	CLA	C	509	-	59,73,73	1.42	14 (23%)	67,113,113	1.99	10 (14%)
31	LMT	B	629	-	36,36,36	0.45	0	47,47,47	0.76	1 (2%)
24	DGD	W	102	-	59,59,67	0.95	3 (5%)	73,73,81	1.41	9 (12%)
21	CLA	G	406	-	59,73,73	1.39	13 (22%)	67,113,113	2.08	10 (14%)
21	CLA	C	507	-	59,73,73	1.39	13 (22%)	67,113,113	2.05	7 (10%)
21	CLA	P	507	-	59,73,73	1.39	13 (22%)	67,113,113	2.03	8 (11%)
21	CLA	P	508	-	59,73,73	1.41	13 (22%)	67,113,113	2.12	11 (16%)
26	SQD	S	102	-	44,45,54	1.31	5 (11%)	53,56,65	1.22	7 (13%)
27	LMG	C	519	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	6 (10%)
24	DGD	N	602	-	53,53,67	1.02	3 (5%)	67,67,81	1.53	9 (13%)
21	CLA	N	620	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	10 (14%)
22	PHO	G	405	-	67,69,69	2.13	18 (26%)	85,99,99	1.94	23 (27%)
24	DGD	C	518	-	67,67,67	0.92	4 (5%)	81,81,81	1.33	8 (9%)
25	LHG	A	411	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
24	DGD	P	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.51	13 (16%)
21	CLA	N	611	-	59,73,73	1.43	12 (20%)	67,113,113	2.03	8 (11%)
27	LMG	N	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.24	8 (14%)
23	PL9	G	407	-	45,45,55	1.23	7 (15%)	56,57,69	1.72	17 (30%)
21	CLA	N	613	-	59,73,73	1.40	12 (20%)	67,113,113	2.06	9 (13%)
24	DGD	C	516	-	54,54,67	0.98	3 (5%)	68,68,81	1.52	10 (14%)
21	CLA	P	504	-	59,73,73	1.42	13 (22%)	67,113,113	2.00	8 (11%)
30	BCR	S	101	-	41,41,41	0.71	0	56,56,56	1.74	11 (19%)
21	CLA	B	610	-	59,73,73	1.41	12 (20%)	67,113,113	2.07	10 (14%)
21	CLA	B	602	-	59,73,73	1.41	12 (20%)	67,113,113	2.03	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	C	510	-	59,73,73	1.41	14 (23%)	67,113,113	2.02	9 (13%)
21	CLA	A	402	-	59,73,73	1.41	13 (22%)	67,113,113	2.08	11 (16%)
26	SQD	G	401	-	53,54,54	1.18	4 (7%)	62,65,65	1.06	4 (6%)
31	LMT	I	103	-	36,36,36	0.47	1 (2%)	47,47,47	0.70	1 (2%)
30	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.69	12 (21%)
27	LMG	B	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.26	8 (14%)
21	CLA	B	601	-	59,73,73	1.39	13 (22%)	67,113,113	2.11	10 (14%)
23	PL9	Q	405	-	55,55,55	1.25	9 (16%)	68,69,69	1.66	19 (27%)
22	PHO	A	404	-	67,69,69	2.14	18 (26%)	85,99,99	1.92	21 (24%)
21	CLA	G	402	-	59,73,73	1.42	13 (22%)	67,113,113	2.04	10 (14%)
30	BCR	P	515	-	41,41,41	0.68	0	56,56,56	1.57	12 (21%)
27	LMG	E	102	-	44,44,55	1.02	2 (4%)	52,52,63	1.11	5 (9%)
24	DGD	C	517	-	63,63,67	0.92	3 (4%)	77,77,81	1.51	13 (16%)
30	BCR	C	514	-	41,41,41	0.72	0	56,56,56	2.34	18 (32%)
26	SQD	N	601	-	46,47,54	1.28	5 (10%)	55,58,65	1.54	10 (18%)
21	CLA	C	504	-	59,73,73	1.42	13 (22%)	67,113,113	2.03	7 (10%)
21	CLA	N	617	-	59,73,73	1.43	14 (23%)	67,113,113	2.03	7 (10%)
21	CLA	N	616	-	59,73,73	1.44	13 (22%)	67,113,113	2.11	9 (13%)
30	BCR	T	103	-	41,41,41	0.69	0	56,56,56	1.63	11 (19%)
26	SQD	G	410	-	50,51,54	1.21	4 (8%)	59,62,65	1.46	9 (15%)
26	SQD	A	414	-	53,54,54	1.17	4 (7%)	62,65,65	1.08	4 (6%)
31	LMT	N	603	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
27	LMG	C	520	-	45,45,55	1.04	2 (4%)	53,53,63	1.26	6 (11%)
21	CLA	P	513	-	59,73,73	1.42	13 (22%)	67,113,113	2.02	10 (14%)
21	CLA	B	606	-	59,73,73	1.40	12 (20%)	67,113,113	2.04	12 (17%)
31	LMT	a	103	-	36,36,36	0.46	0	47,47,47	0.69	1 (2%)
30	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.59	11 (19%)
21	CLA	P	509	-	59,73,73	1.41	14 (23%)	67,113,113	2.02	10 (14%)
24	DGD	D	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.32	9 (11%)
25	LHG	A	408	-	38,38,48	1.07	2 (5%)	41,44,54	0.95	2 (4%)
26	SQD	A	409	-	50,51,54	1.21	4 (8%)	59,62,65	1.44	9 (15%)
21	CLA	B	605	-	59,73,73	1.41	13 (22%)	67,113,113	2.09	12 (17%)
31	LMT	B	626	-	36,36,36	0.44	0	47,47,47	0.66	1 (2%)
27	LMG	a	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.33	6 (11%)
21	CLA	N	619	-	59,73,73	1.38	12 (20%)	67,113,113	2.11	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	N	618	-	59,73,73	1.42	12 (20%)	67,113,113	2.01	10 (14%)
21	CLA	B	613	-	59,73,73	1.41	14 (23%)	67,113,113	2.03	8 (11%)
21	CLA	C	508	-	59,73,73	1.41	12 (20%)	67,113,113	2.09	13 (19%)
34	HEM	E	101	5,6	27,50,50	2.13	5 (18%)	17,82,82	2.06	4 (23%)
30	BCR	a	101	-	41,41,41	0.69	0	56,56,56	1.59	11 (19%)
21	CLA	C	513	-	59,73,73	1.41	13 (22%)	67,113,113	2.04	9 (13%)
21	CLA	B	616	-	59,73,73	1.40	13 (22%)	67,113,113	2.08	10 (14%)
32	BCT	D	410	29	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	N	612	-	59,73,73	1.42	13 (22%)	67,113,113	2.00	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
24	DGD	B	628	-	3/3/13/13	22/41/81/95	0/2/2/2
21	CLA	B	615	-	3/3/20/25	9/37/135/135	-
21	CLA	Q	404	-	3/3/20/25	4/37/135/135	-
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
31	LMT	B	625	-	-	3/21/61/61	0/2/2/2
27	LMG	I	102	-	2/2/8/8	18/38/58/70	0/1/1/1
31	LMT	B	630	-	-	5/21/61/61	0/2/2/2
31	LMT	N	604	-	-	5/21/61/61	0/2/2/2
30	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	CLA	P	512	-	3/3/20/25	19/37/135/135	-
24	DGD	A	407	-	3/3/13/13	14/45/85/95	0/2/2/2
22	PHO	D	402	-	-	15/53/103/103	0/5/6/6
24	DGD	B	621	-	3/3/13/13	16/47/87/95	0/2/2/2
27	LMG	D	412	-	2/2/8/8	15/37/57/70	0/1/1/1
21	CLA	B	603	-	3/3/20/25	14/37/135/135	-
21	CLA	B	609	-	3/3/20/25	8/37/135/135	-
21	CLA	P	502	-	3/3/20/25	10/37/135/135	-
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	LMG	G	411	-	2/2/8/8	22/46/66/70	0/1/1/1
21	CLA	C	506	-	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PL9	b	101	-	-	11/29/49/73	0/1/1/1
21	CLA	C	503	-	3/3/20/25	14/37/135/135	-
30	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
27	LMG	N	622	-	2/2/8/8	22/44/64/70	0/1/1/1
26	SQD	B	624	-	-	10/38/58/69	0/1/1/1
21	CLA	N	605	-	3/3/20/25	21/37/135/135	-
21	CLA	D	401	-	3/3/20/25	15/37/135/135	-
30	BCR	b	102	-	-	2/29/63/63	0/2/2/2
21	CLA	G	404	-	3/3/20/25	12/37/135/135	-
21	CLA	B	611	-	3/3/20/25	14/37/135/135	-
26	SQD	B	627	-	-	14/42/62/69	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
28	OEC	A	412	1,3	-	-	0/1/0/5
30	BCR	P	514	-	-	5/29/63/63	0/2/2/2
21	CLA	N	614	-	3/3/20/25	17/37/135/135	-
30	BCR	T	102	-	-	4/29/63/63	0/2/2/2
23	PL9	D	404	-	-	16/53/73/73	0/1/1/1
26	SQD	F	101	-	-	14/40/60/69	0/1/1/1
27	LMG	R	102	-	2/2/8/8	16/39/59/70	0/1/1/1
30	BCR	c	101	-	-	6/29/63/63	0/2/2/2
21	CLA	N	608	-	3/3/20/25	9/37/135/135	-
21	CLA	P	511	3	3/3/20/25	16/37/135/135	-
21	CLA	N	609	-	3/3/20/25	20/37/135/135	-
22	PHO	Q	403	-	-	15/53/103/103	0/5/6/6
21	CLA	C	505	-	3/3/20/25	19/37/135/135	-
27	LMG	P	520	-	2/2/8/8	20/43/63/70	0/1/1/1
27	LMG	A	410	-	2/2/8/8	22/46/66/70	0/1/1/1
34	HEM	R	101	5,6	-	1/6/54/54	-
31	LMT	N	624	-	-	3/21/61/61	0/2/2/2
21	CLA	C	511	3	3/3/20/25	17/37/135/135	-
27	LMG	e	102	-	2/2/8/8	12/37/57/70	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	15/37/57/70	0/1/1/1
21	CLA	P	510	-	3/3/20/25	13/37/135/135	-
21	CLA	A	405	-	3/3/20/25	11/37/135/135	-
21	CLA	B	607	-	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEM	V	201	16	-	0/6/54/54	-
21	CLA	N	610	-	3/3/20/25	14/37/135/135	-
24	DGD	P	517	-	3/3/13/13	17/42/82/95	0/2/2/2
27	LMG	P	521	-	2/2/8/8	19/40/60/70	0/1/1/1
21	CLA	P	501	-	3/3/20/25	12/37/135/135	-
21	CLA	C	501	-	3/3/20/25	13/37/135/135	-
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
21	CLA	N	607	-	3/3/20/25	13/37/135/135	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
27	LMG	Q	407	-	2/2/8/8	18/43/63/70	0/1/1/1
30	BCR	B	620	-	-	4/29/63/63	0/2/2/2
21	CLA	B	608	-	3/3/20/25	17/37/135/135	-
30	BCR	D	405	-	-	8/29/63/63	0/2/2/2
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
21	CLA	Q	402	-	3/3/20/25	15/37/135/135	-
21	CLA	C	512	-	3/3/20/25	20/37/135/135	-
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
30	BCR	P	516	-	-	8/29/63/63	0/2/2/2
27	LMG	D	406	-	2/2/8/8	12/41/61/70	0/1/1/1
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
21	CLA	C	502	-	3/3/20/25	10/37/135/135	-
21	CLA	B	614	-	3/3/20/25	20/37/135/135	-
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
21	CLA	B	604	-	3/3/20/25	9/37/135/135	-
21	CLA	P	505	-	3/3/20/25	19/37/135/135	-
21	CLA	N	606	-	3/3/20/25	21/37/135/135	-
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
24	DGD	P	519	-	3/3/13/13	20/55/95/95	0/2/2/2
21	CLA	P	503	-	3/3/20/25	14/37/135/135	-
27	LMG	D	407	-	2/2/8/8	20/43/63/70	0/1/1/1
26	SQD	Q	408	-	-	10/38/58/69	0/1/1/1
34	HEM	i	201	16	-	0/6/54/54	-
25	LHG	G	409	-	-	14/43/43/53	-
30	BCR	I	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DGD	G	408	-	3/3/13/13	14/45/85/95	0/2/2/2
21	CLA	G	403	-	3/3/20/25	16/37/135/135	-
25	LHG	G	412	-	-	14/41/41/53	-
21	CLA	D	403	-	3/3/20/25	6/37/135/135	-
21	CLA	B	612	-	3/3/20/25	10/37/135/135	-
21	CLA	A	401	-	3/3/20/25	9/37/135/135	-
27	LMG	Q	406	-	2/2/8/8	14/41/61/70	0/1/1/1
21	CLA	A	403	-	3/3/20/25	13/37/135/135	-
21	CLA	N	615	-	3/3/20/25	13/37/135/135	-
31	LMT	N	625	-	-	2/21/61/61	0/2/2/2
27	LMG	M	101	-	2/2/8/8	14/37/57/70	0/1/1/1
30	BCR	W	101	-	-	2/29/63/63	0/2/2/2
23	PL9	J	101	-	-	11/29/49/73	0/1/1/1
27	LMG	B	622	-	2/2/8/8	23/44/64/70	0/1/1/1
21	CLA	P	506	-	3/3/20/25	17/37/135/135	-
24	DGD	Q	409	-	3/3/13/13	32/52/92/95	0/2/2/2
21	CLA	C	509	-	3/3/20/25	10/37/135/135	-
31	LMT	B	629	-	-	3/21/61/61	0/2/2/2
24	DGD	W	102	-	3/3/13/13	16/47/87/95	0/2/2/2
21	CLA	G	406	-	3/3/20/25	11/37/135/135	-
21	CLA	C	507	-	3/3/20/25	15/37/135/135	-
21	CLA	P	507	-	3/3/20/25	12/37/135/135	-
21	CLA	P	508	-	3/3/20/25	11/37/135/135	-
26	SQD	S	102	-	-	13/40/60/69	0/1/1/1
27	LMG	C	519	-	2/2/8/8	20/43/63/70	0/1/1/1
24	DGD	N	602	-	3/3/13/13	22/41/81/95	0/2/2/2
21	CLA	N	620	-	3/3/20/25	19/37/135/135	-
22	PHO	G	405	-	-	12/53/103/103	0/5/6/6
24	DGD	C	518	-	3/3/13/13	21/55/95/95	0/2/2/2
25	LHG	A	411	-	-	12/41/41/53	-
24	DGD	P	518	-	3/3/13/13	19/51/91/95	0/2/2/2
21	CLA	N	611	-	3/3/20/25	10/37/135/135	-
27	LMG	N	623	-	2/2/8/8	17/44/64/70	0/1/1/1
23	PL9	G	407	-	-	18/41/61/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	N	613	-	3/3/20/25	7/37/135/135	-
24	DGD	C	516	-	3/3/13/13	18/42/82/95	0/2/2/2
21	CLA	P	504	-	3/3/20/25	10/37/135/135	-
30	BCR	S	101	-	-	7/29/63/63	0/2/2/2
21	CLA	B	610	-	3/3/20/25	17/37/135/135	-
21	CLA	B	602	-	3/3/20/25	19/37/135/135	-
21	CLA	C	510	-	3/3/20/25	17/37/135/135	-
21	CLA	A	402	-	3/3/20/25	17/37/135/135	-
26	SQD	G	401	-	-	16/49/69/69	0/1/1/1
31	LMT	I	103	-	-	4/21/61/61	0/2/2/2
30	BCR	C	515	-	-	8/29/63/63	0/2/2/2
27	LMG	B	623	-	2/2/8/8	15/44/64/70	0/1/1/1
21	CLA	B	601	-	3/3/20/25	18/37/135/135	-
23	PL9	Q	405	-	-	17/53/73/73	0/1/1/1
22	PHO	A	404	-	-	12/53/103/103	0/5/6/6
21	CLA	G	402	-	3/3/20/25	8/37/135/135	-
30	BCR	P	515	-	-	4/29/63/63	0/2/2/2
27	LMG	E	102	-	2/2/8/8	14/39/59/70	0/1/1/1
24	DGD	C	517	-	3/3/13/13	19/51/91/95	0/2/2/2
30	BCR	C	514	-	-	4/29/63/63	0/2/2/2
26	SQD	N	601	-	-	13/42/62/69	0/1/1/1
21	CLA	C	504	-	3/3/20/25	10/37/135/135	-
21	CLA	N	617	-	3/3/20/25	19/37/135/135	-
21	CLA	N	616	-	3/3/20/25	11/37/135/135	-
30	BCR	T	103	-	-	4/29/63/63	0/2/2/2
26	SQD	G	410	-	-	15/46/66/69	0/1/1/1
26	SQD	A	414	-	-	17/49/69/69	0/1/1/1
31	LMT	N	603	-	-	3/21/61/61	0/2/2/2
27	LMG	C	520	-	2/2/8/8	17/40/60/70	0/1/1/1
21	CLA	P	513	-	3/3/20/25	20/37/135/135	-
21	CLA	B	606	-	3/3/20/25	14/37/135/135	-
31	LMT	a	103	-	-	4/21/61/61	0/2/2/2
30	BCR	T	101	-	-	2/29/63/63	0/2/2/2
21	CLA	P	509	-	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DGD	D	408	-	3/3/13/13	32/52/92/95	0/2/2/2
25	LHG	A	408	-	-	13/43/43/53	-
26	SQD	A	409	-	-	16/46/66/69	0/1/1/1
21	CLA	B	605	-	3/3/20/25	19/37/135/135	-
31	LMT	B	626	-	-	2/21/61/61	0/2/2/2
27	LMG	a	102	-	2/2/8/8	20/38/58/70	0/1/1/1
21	CLA	N	619	-	3/3/20/25	9/37/135/135	-
21	CLA	N	618	-	3/3/20/25	19/37/135/135	-
21	CLA	B	613	-	3/3/20/25	17/37/135/135	-
21	CLA	C	508	-	3/3/20/25	11/37/135/135	-
34	HEM	E	101	5,6	-	1/6/54/54	-
30	BCR	a	101	-	-	4/29/63/63	0/2/2/2
21	CLA	C	513	-	3/3/20/25	20/37/135/135	-
21	CLA	B	616	-	3/3/20/25	19/37/135/135	-
21	CLA	N	612	-	3/3/20/25	16/37/135/135	-

The worst 5 of 1165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	PHO	CHB-C1B	5.79	1.49	1.38
22	G	405	PHO	CHB-C1B	5.69	1.49	1.38
22	D	402	PHO	CHB-C1B	5.65	1.49	1.38
22	Q	403	PHO	CHB-C1B	5.64	1.49	1.38
34	i	201	HEM	C3D-C2D	5.46	1.53	1.37

The worst 5 of 1536 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-13.47	88.45	110.30
30	J	102	BCR	C32-C1-C6	-13.40	88.56	110.30
21	C	505	CLA	C4A-NA-C1A	13.25	112.67	106.71
21	P	505	CLA	C4A-NA-C1A	13.10	112.60	106.71
21	B	611	CLA	C4A-NA-C1A	12.83	112.47	106.71

5 of 296 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	628	DGD	C2D
24	B	628	DGD	C5D

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Mol	Chain	Res	Type	Atom
24	B	628	DGD	C5E
21	B	615	CLA	NC
21	B	615	CLA	ND

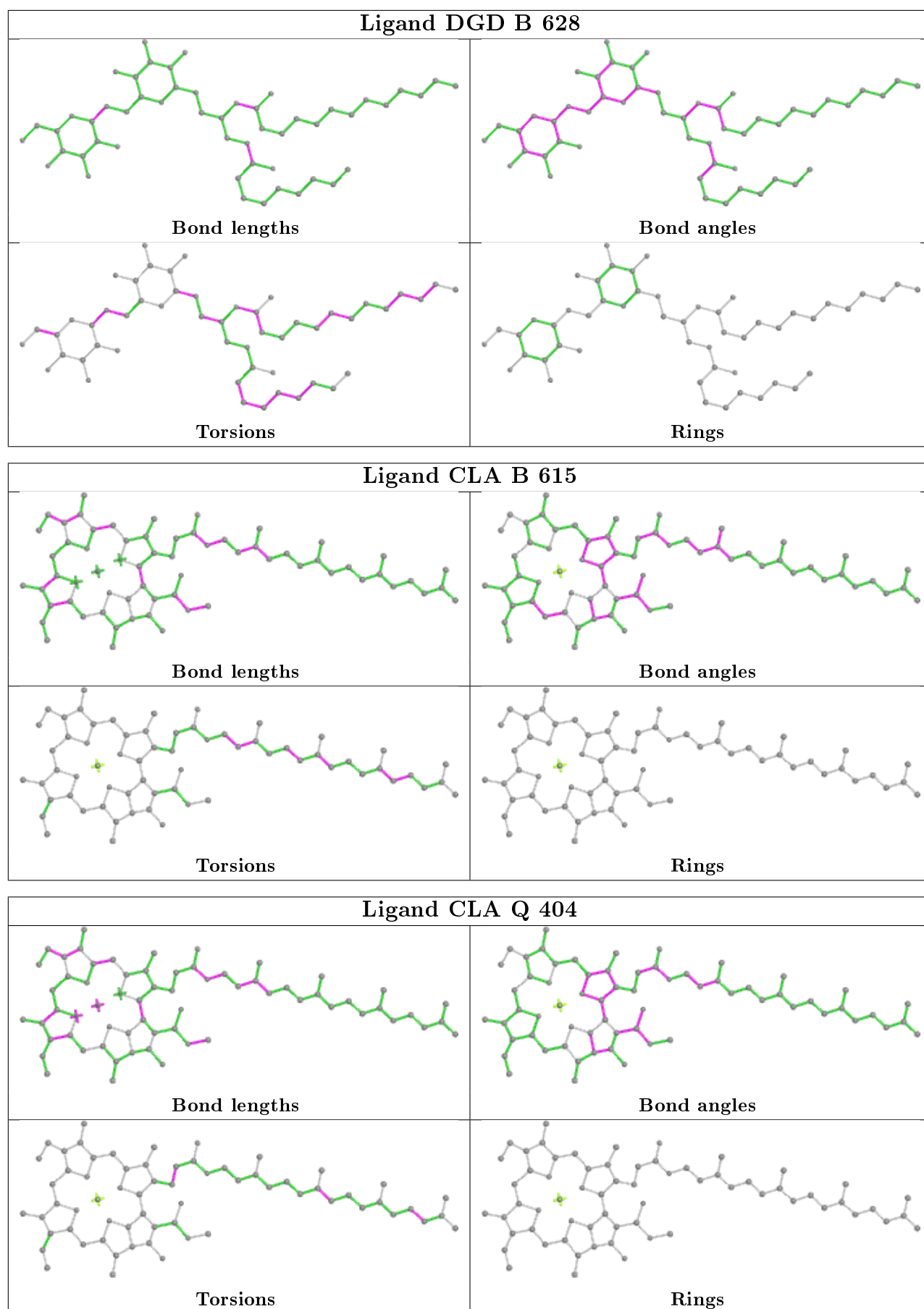
5 of 2119 torsion outliers are listed below:

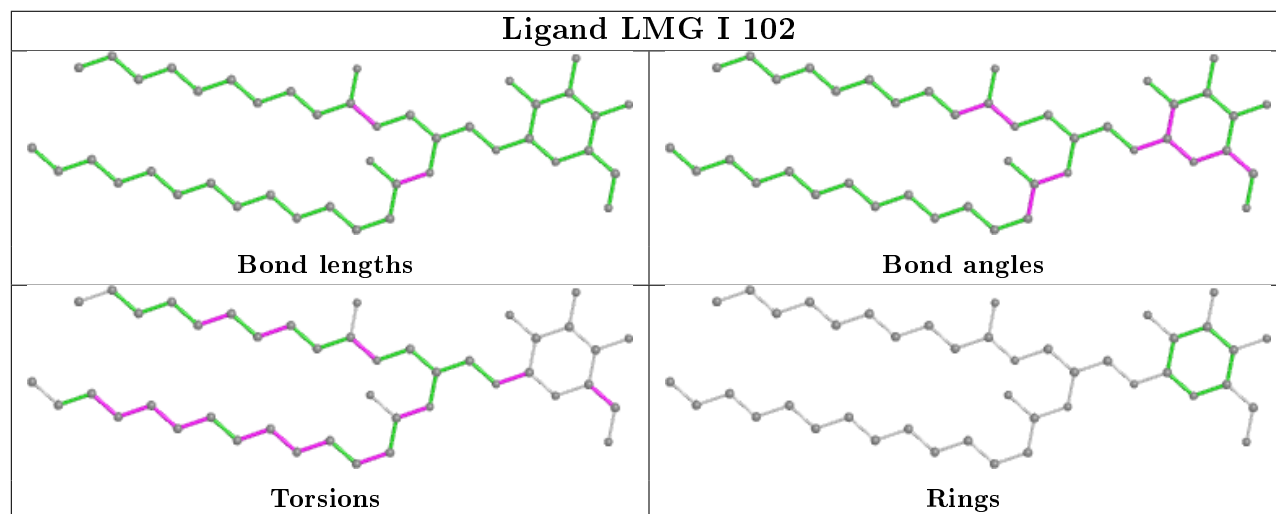
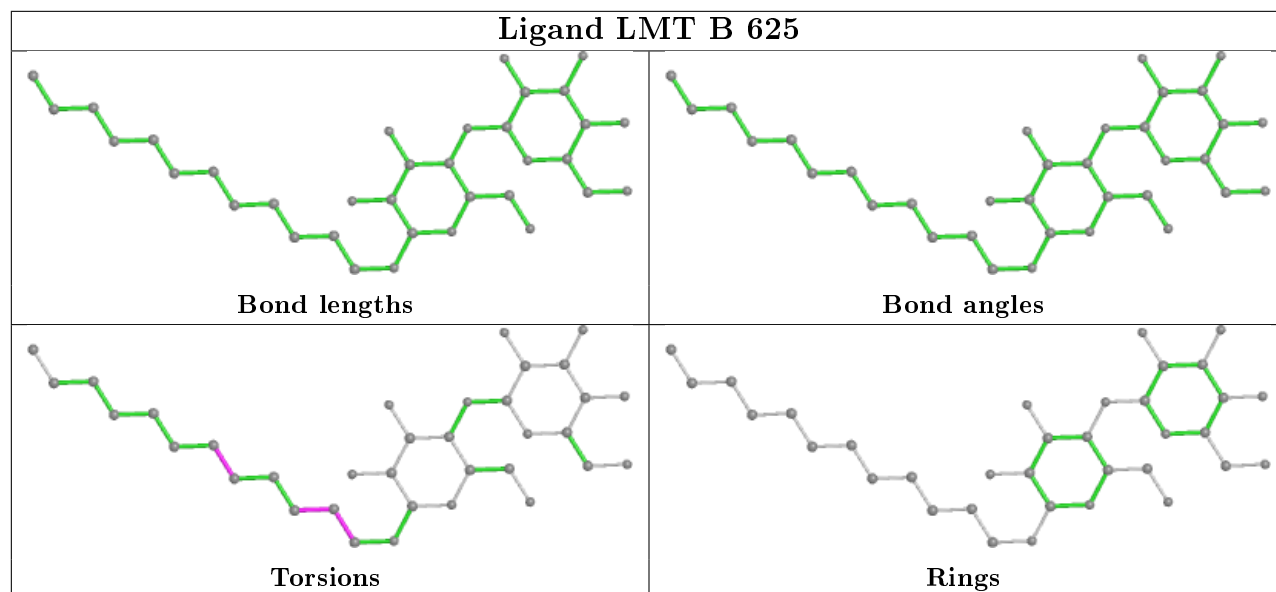
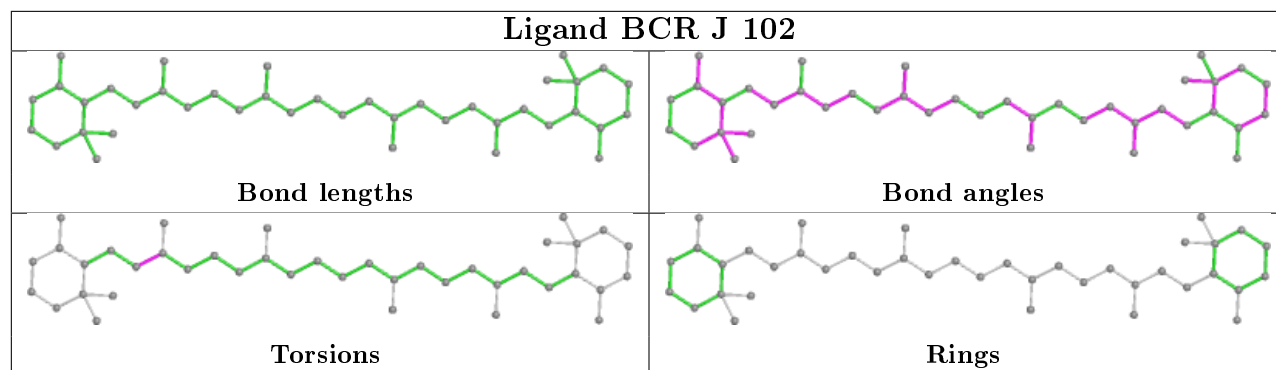
Mol	Chain	Res	Type	Atoms
24	B	628	DGD	O1B-C1B-O2G-C2G
24	B	628	DGD	O2G-C2G-C3G-O3G
24	B	628	DGD	C2D-C1D-O3G-C3G
24	B	628	DGD	O6D-C1D-O3G-C3G
24	B	628	DGD	C5D-C6D-O5D-C1E

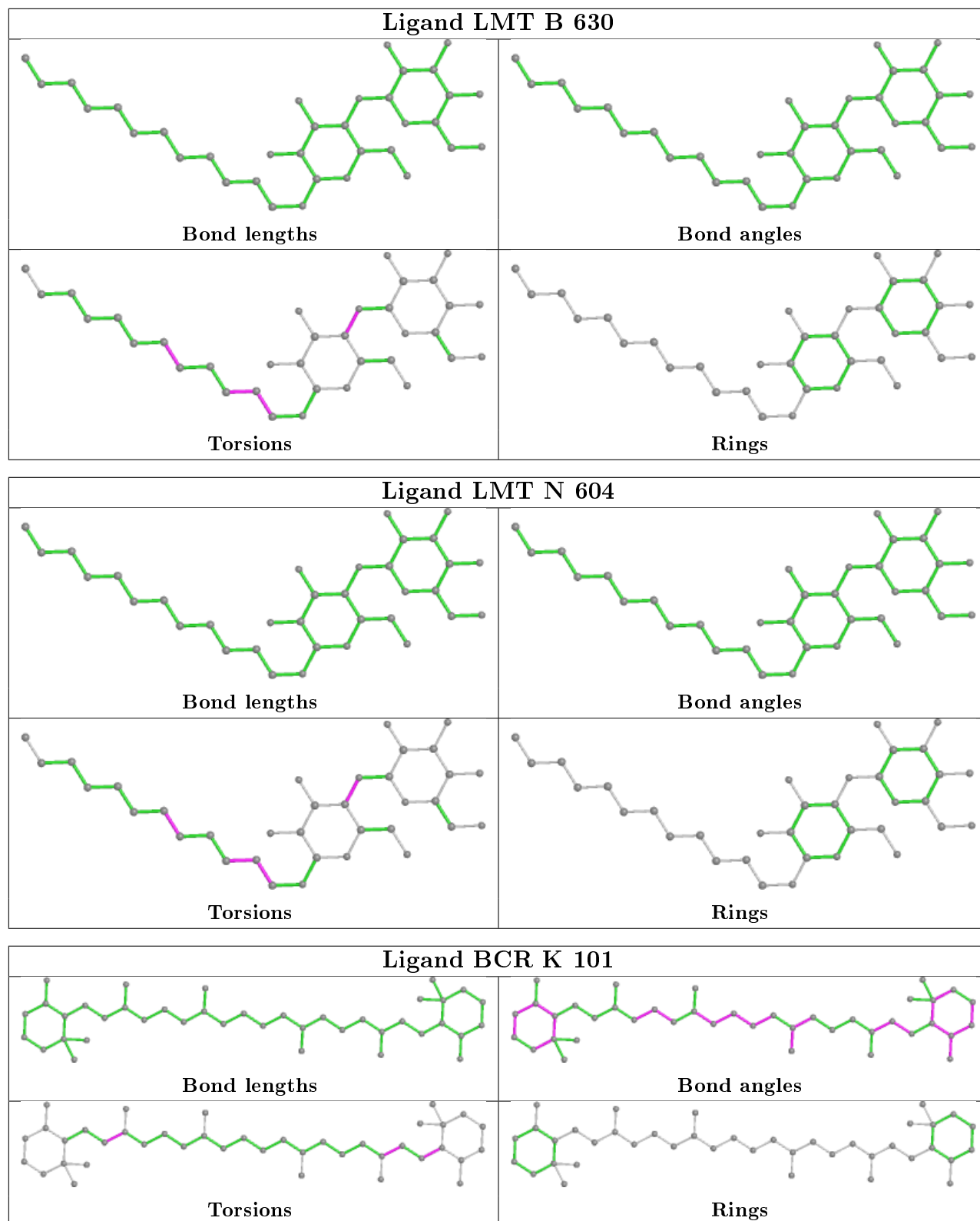
There are no ring outliers.

No monomer is involved in short contacts.

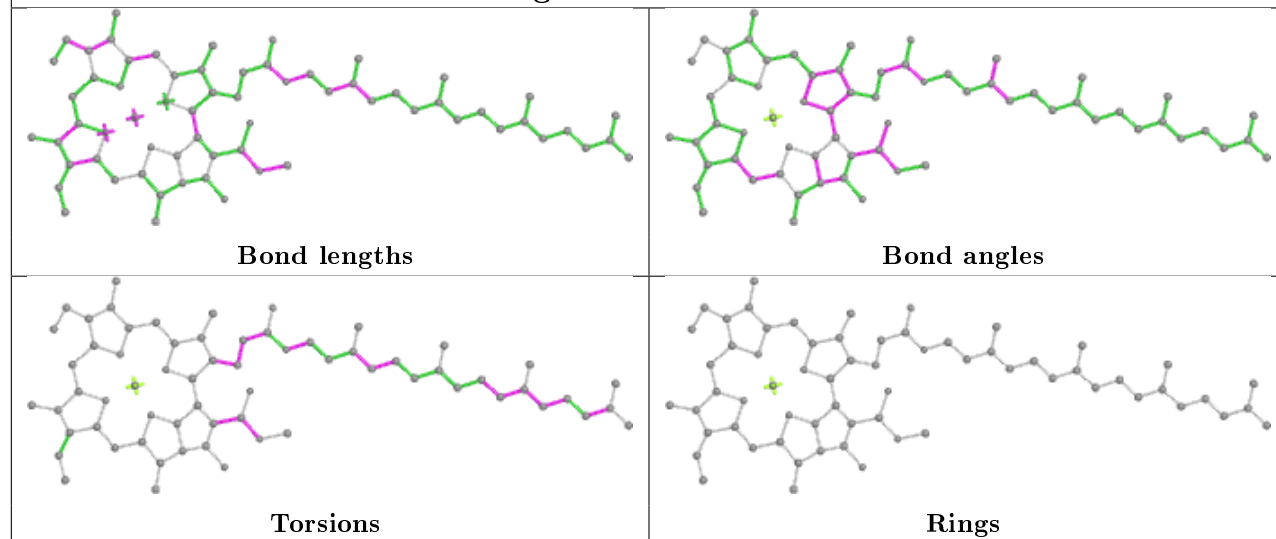
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



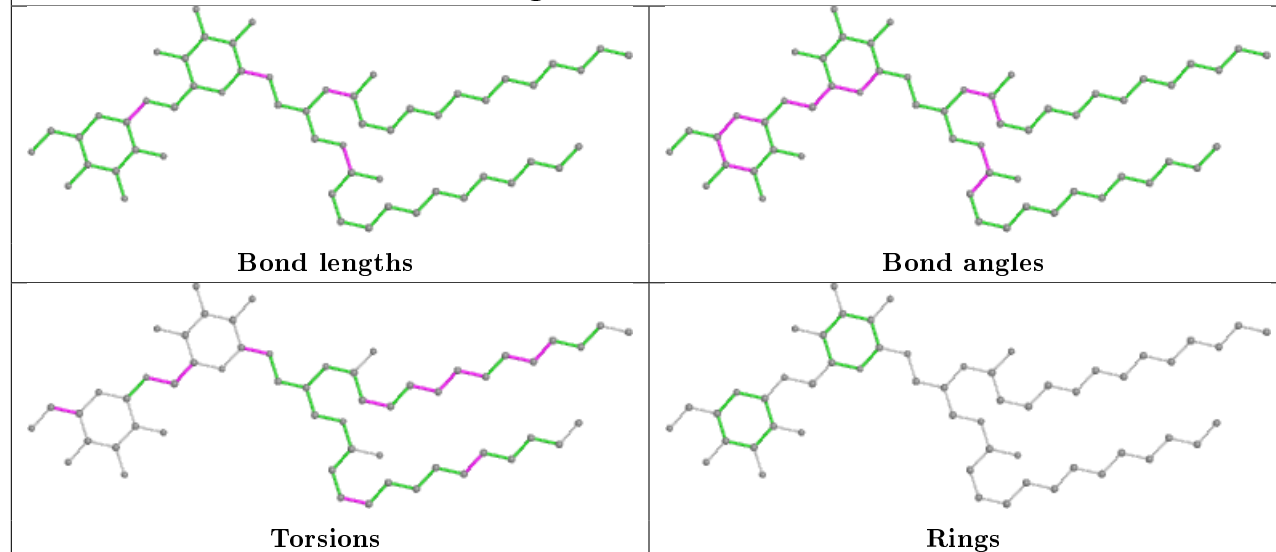




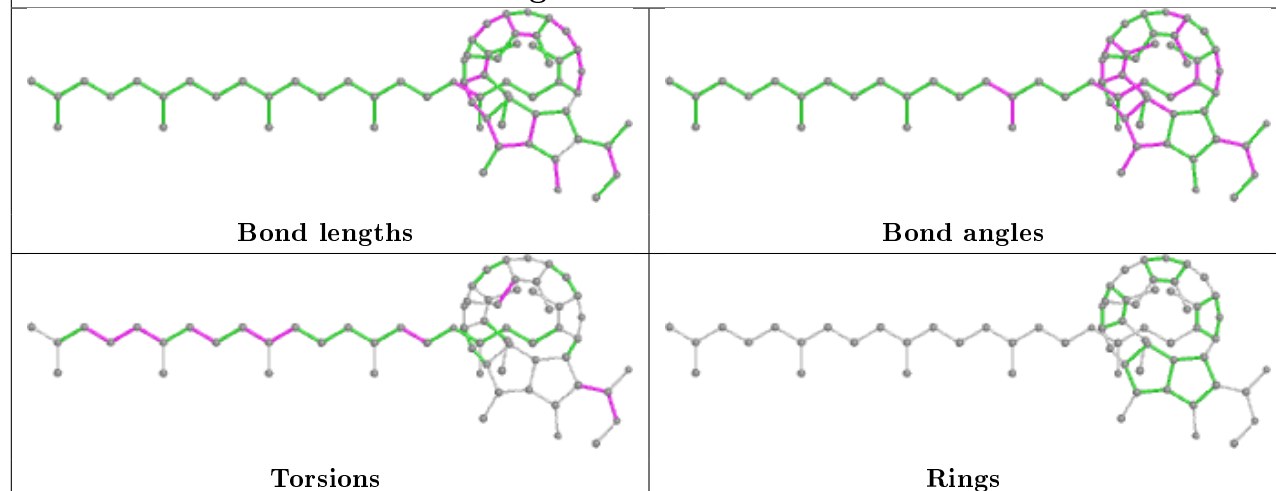
Ligand CLA P 512

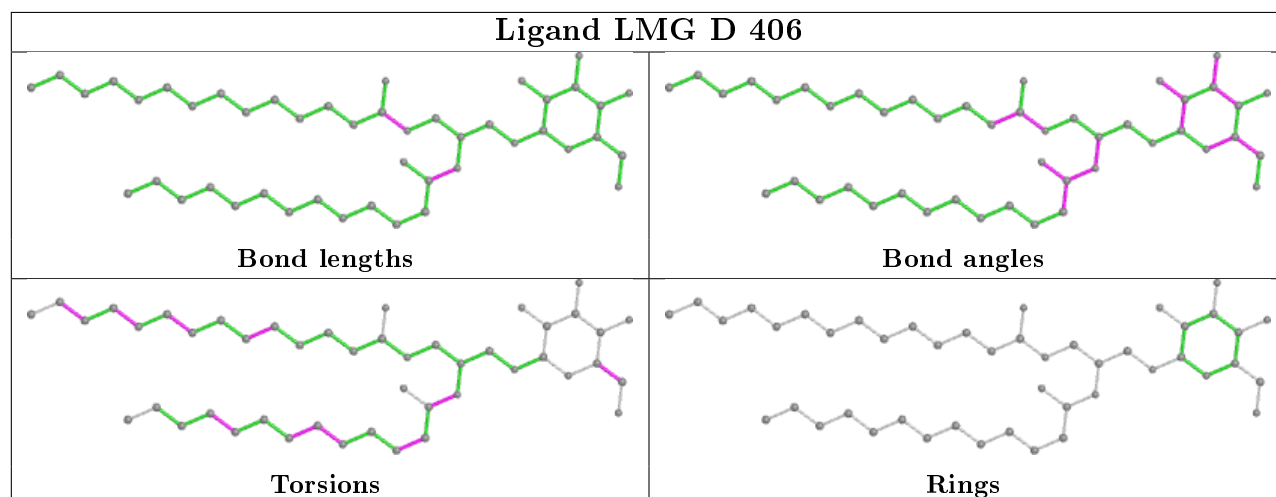
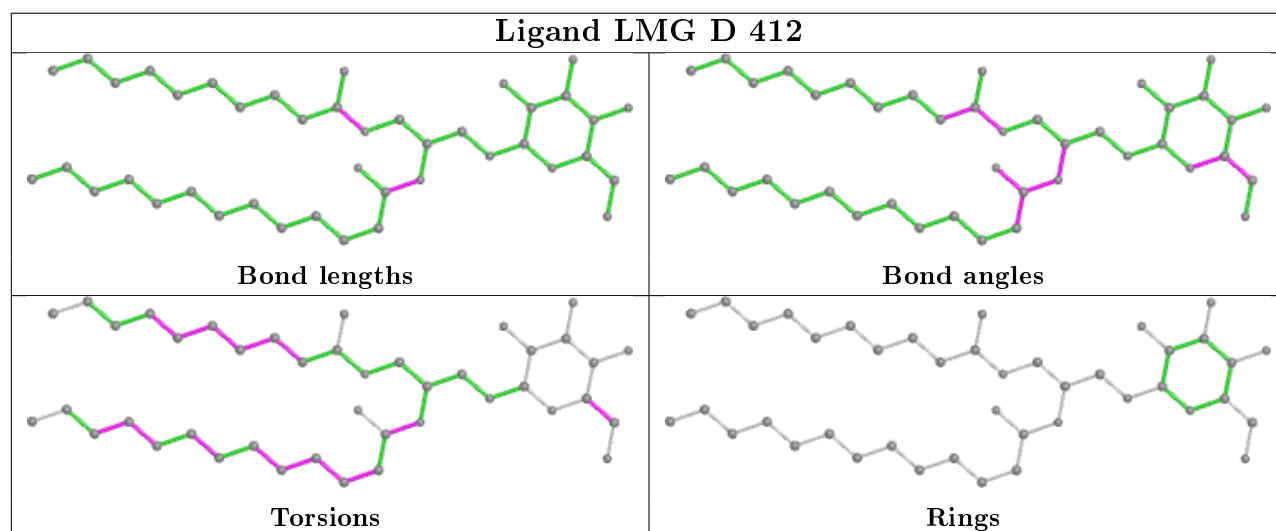
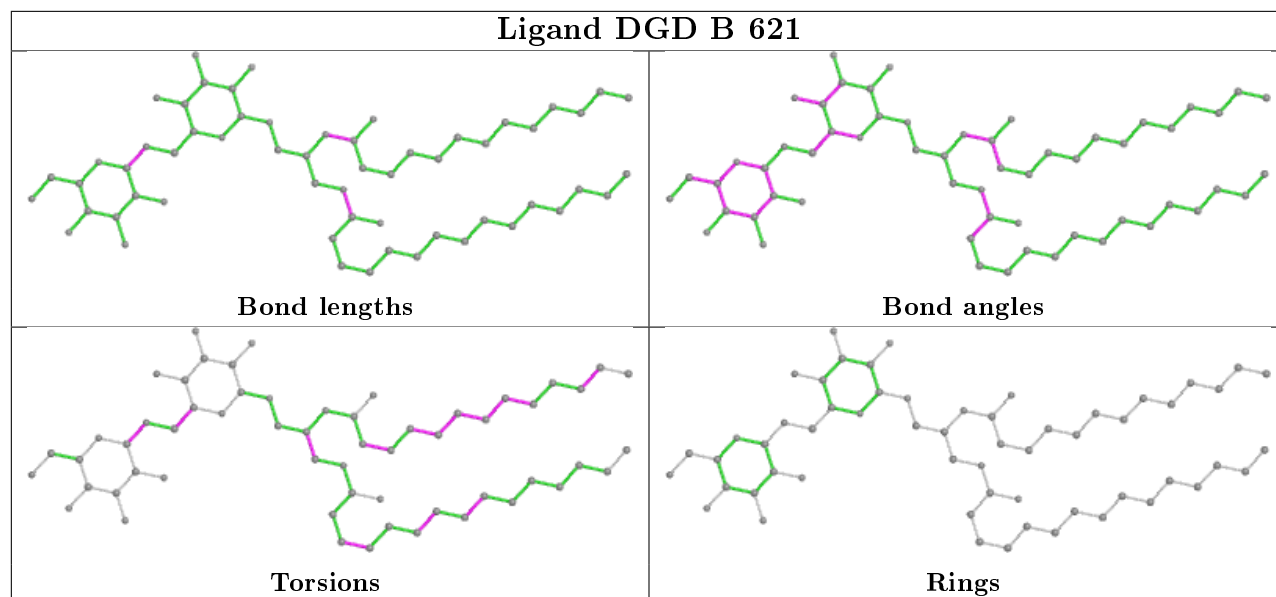


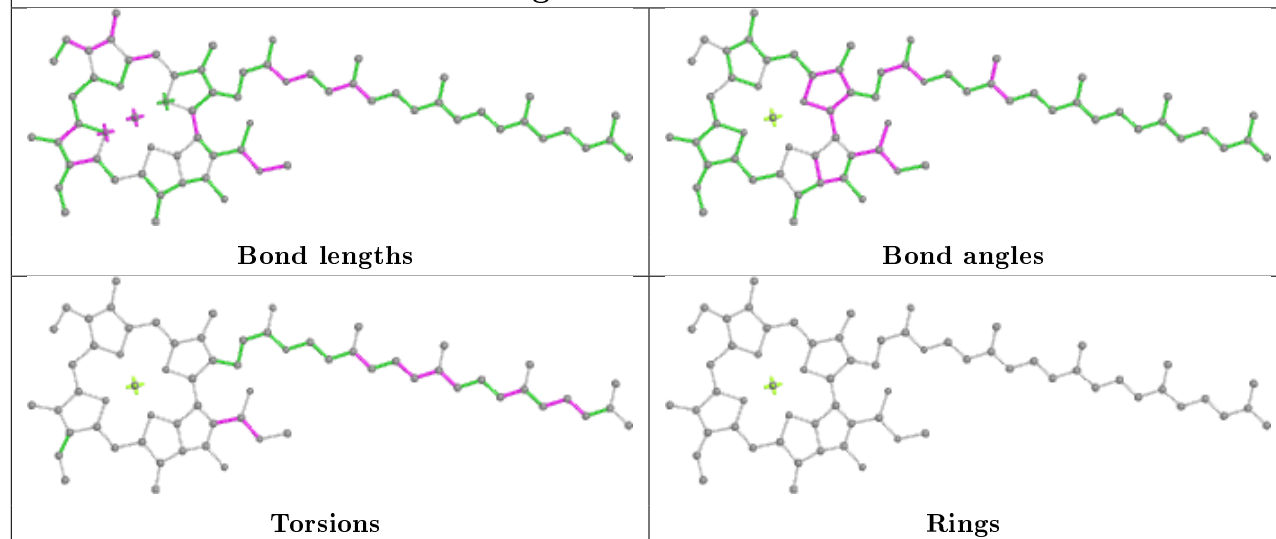
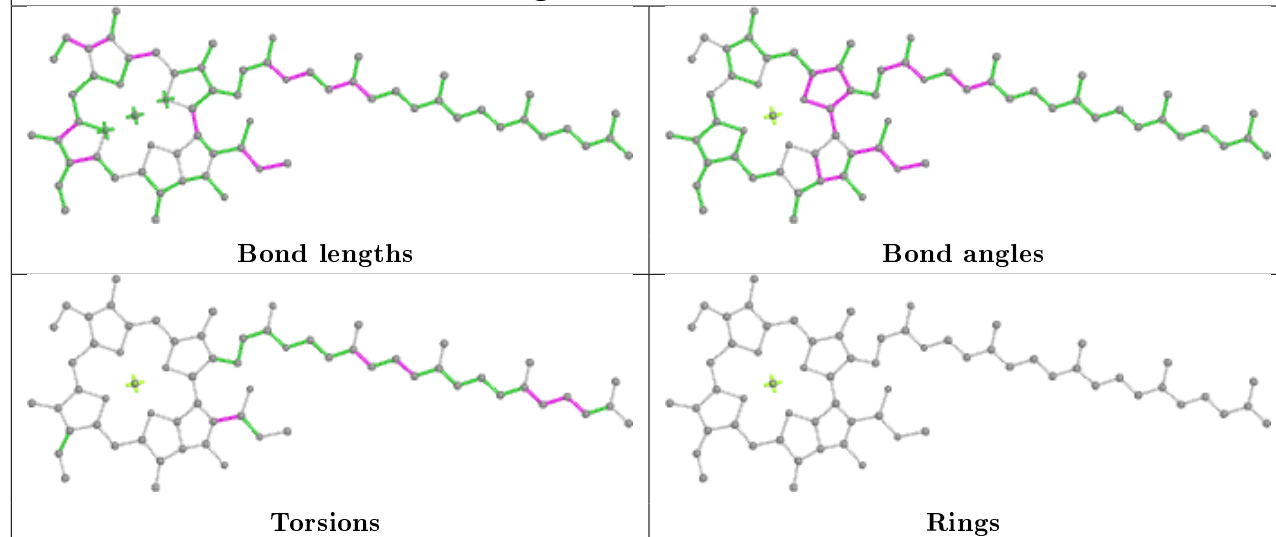
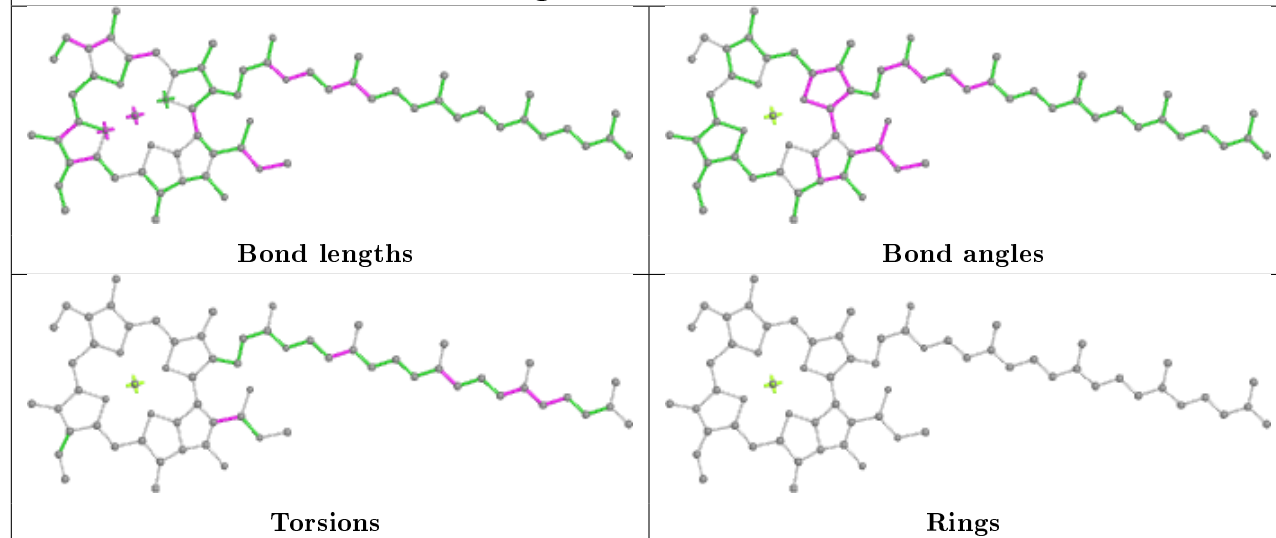
Ligand DGD A 407

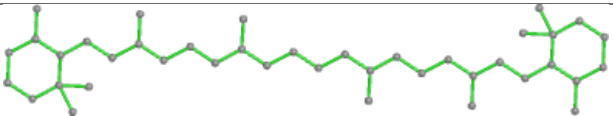
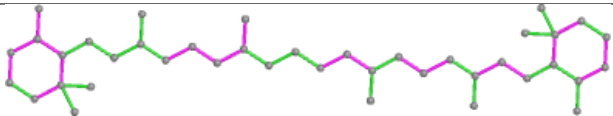
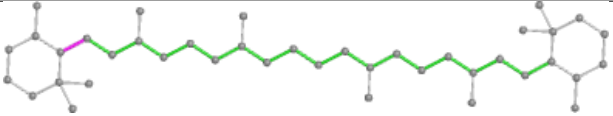
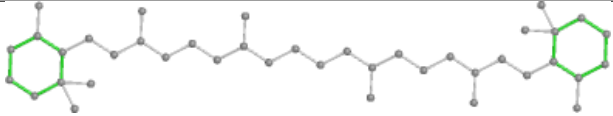


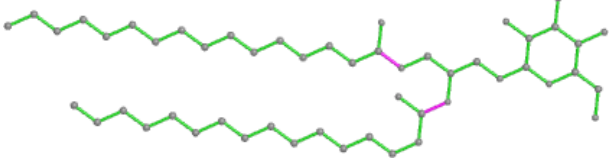
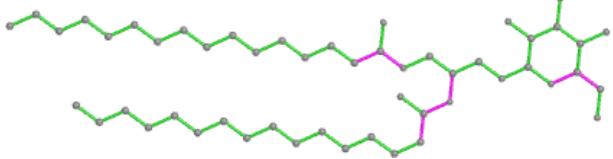
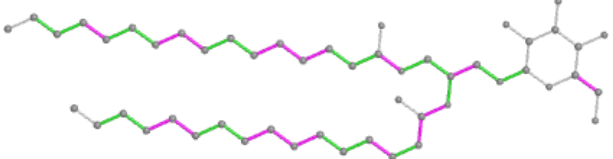
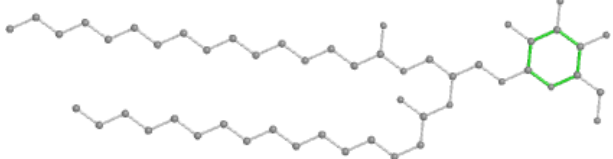
Ligand PHO D 402

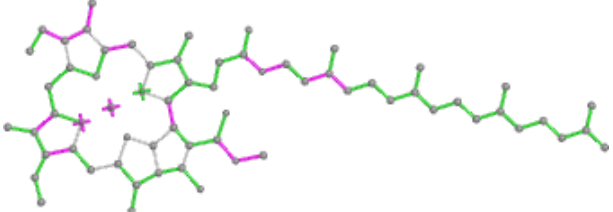
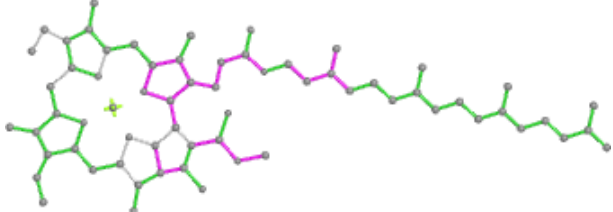
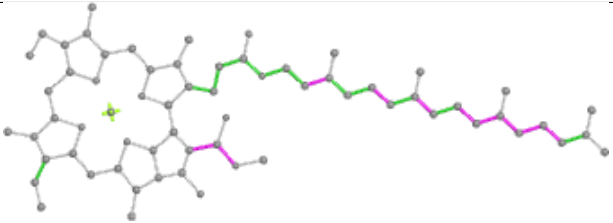
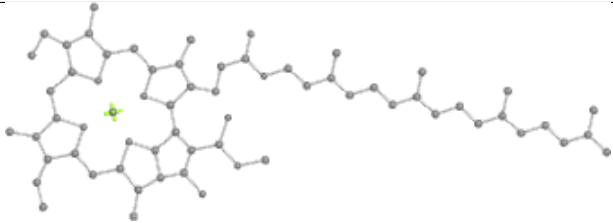


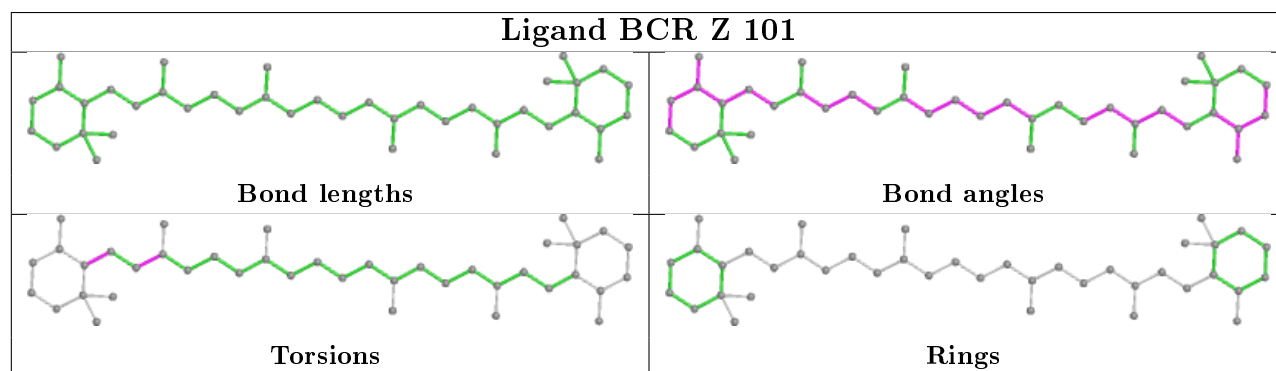
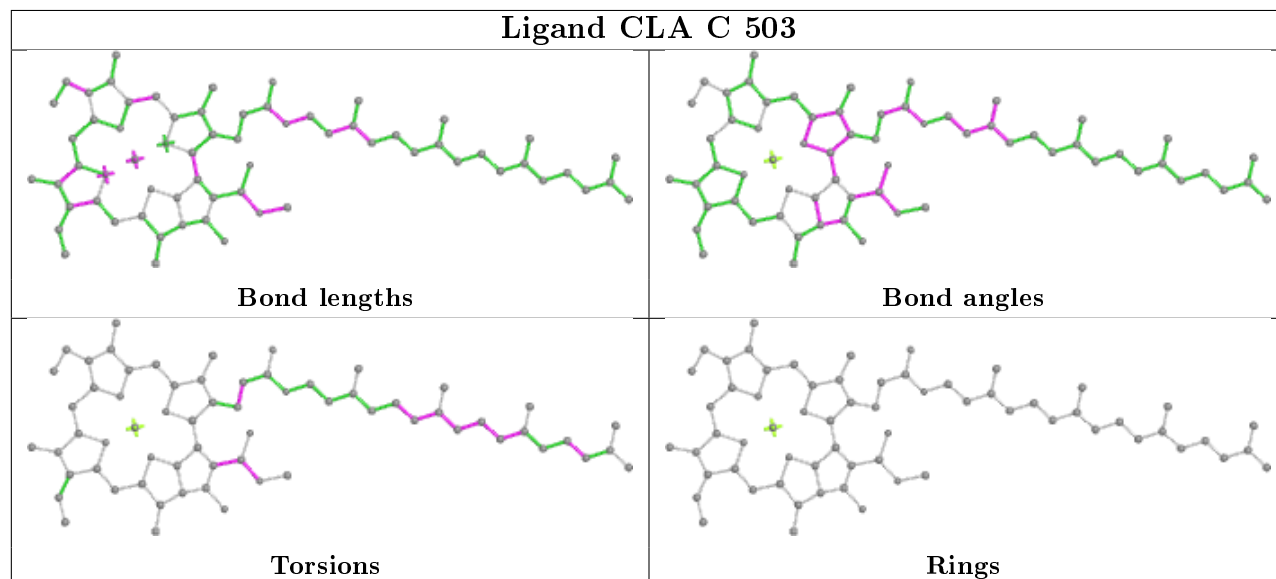
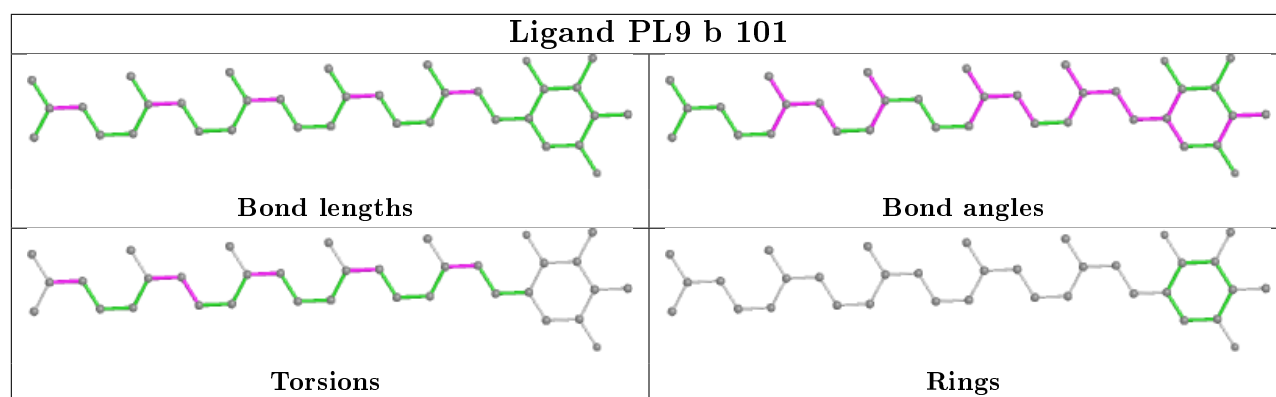


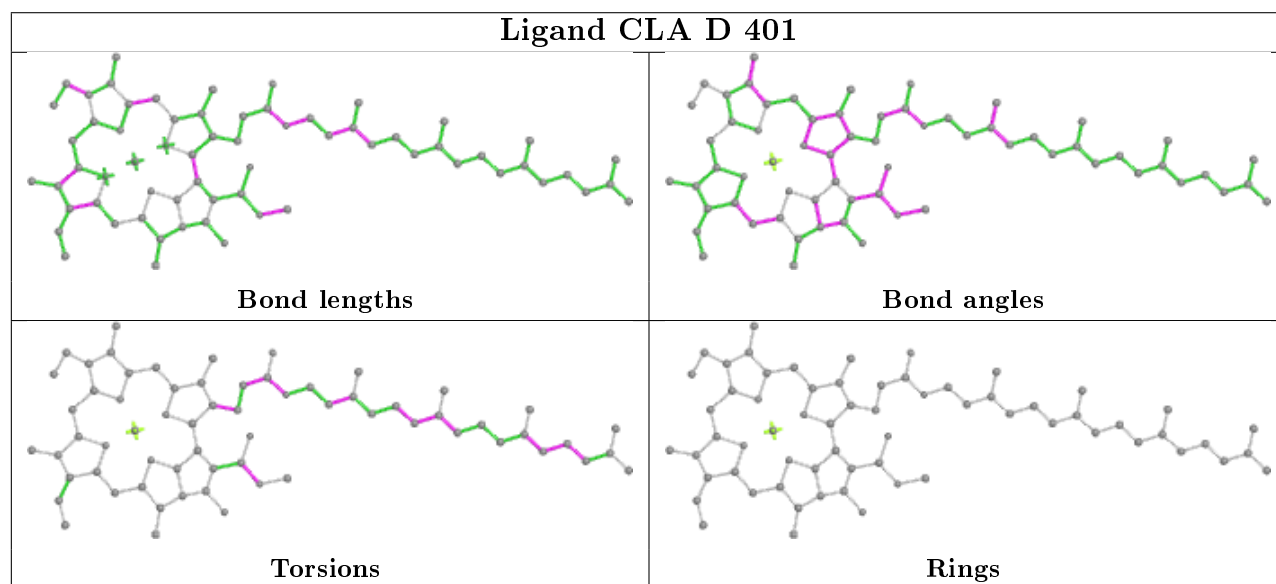
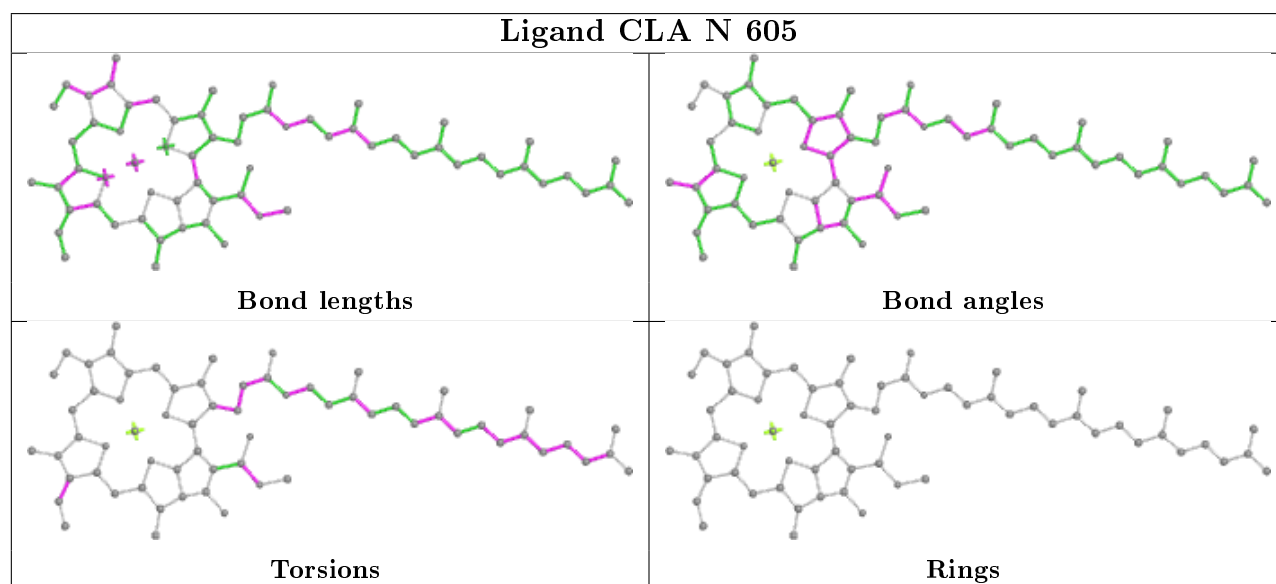
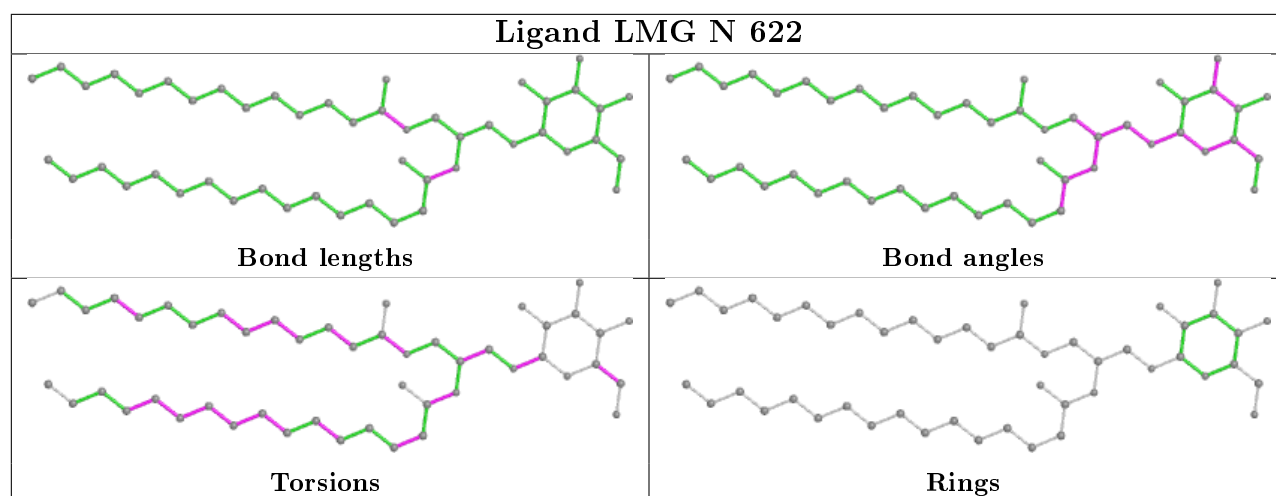
Ligand CLA B 603**Ligand CLA B 609****Ligand CLA P 502**

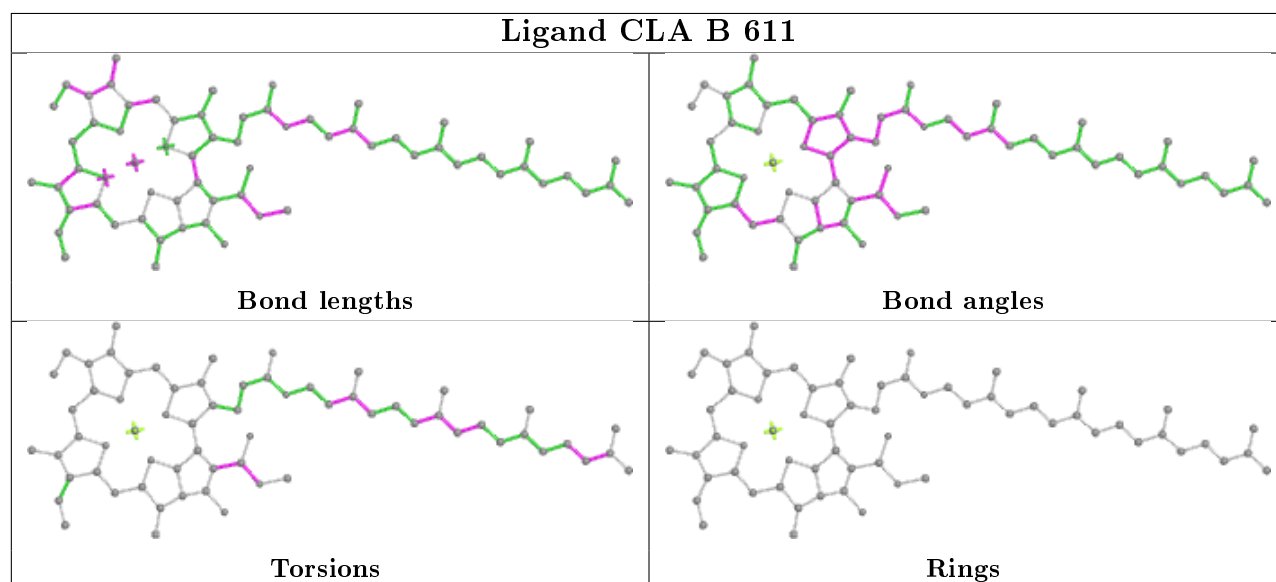
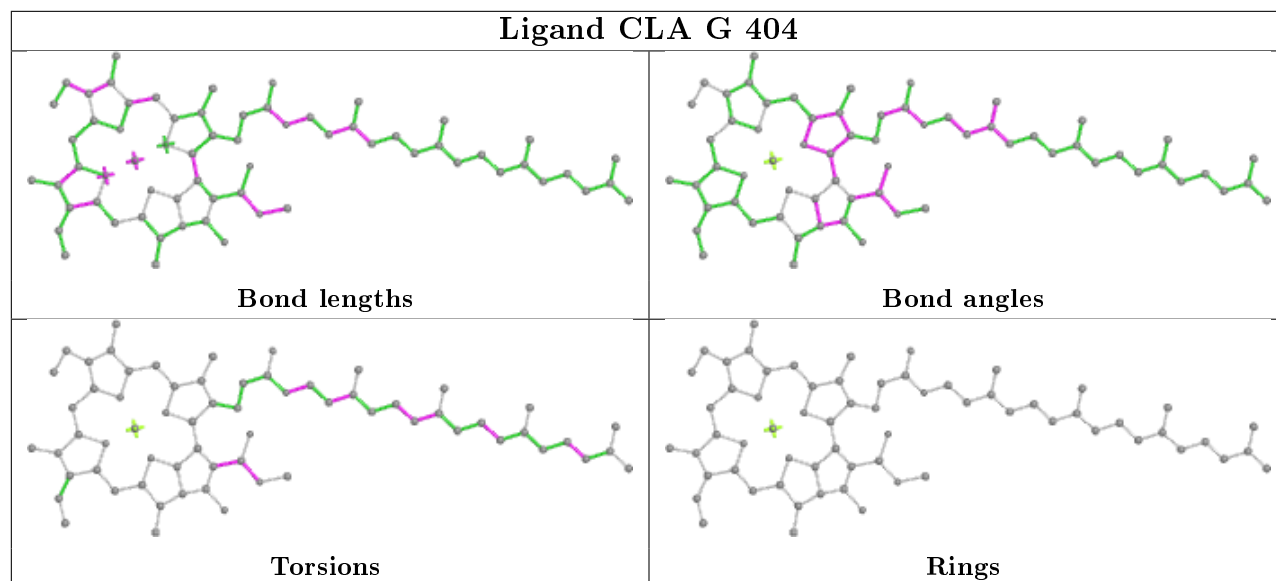
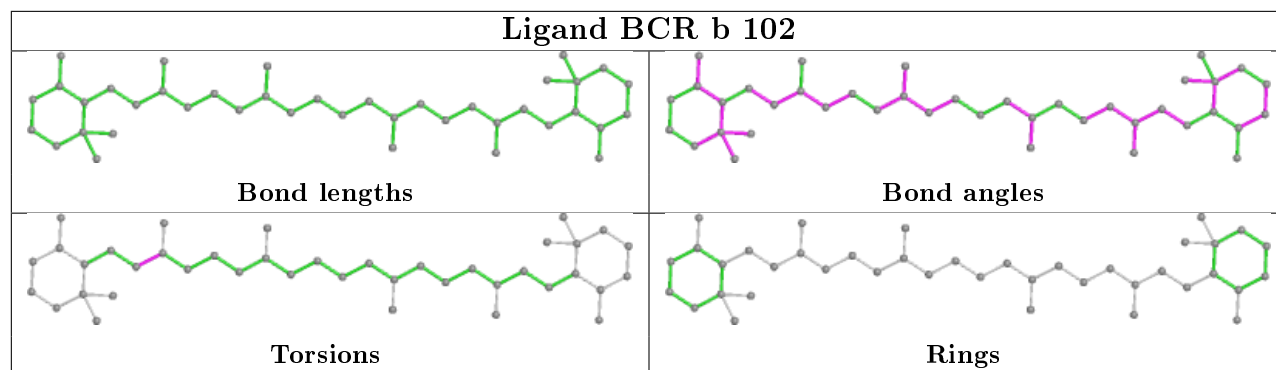
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

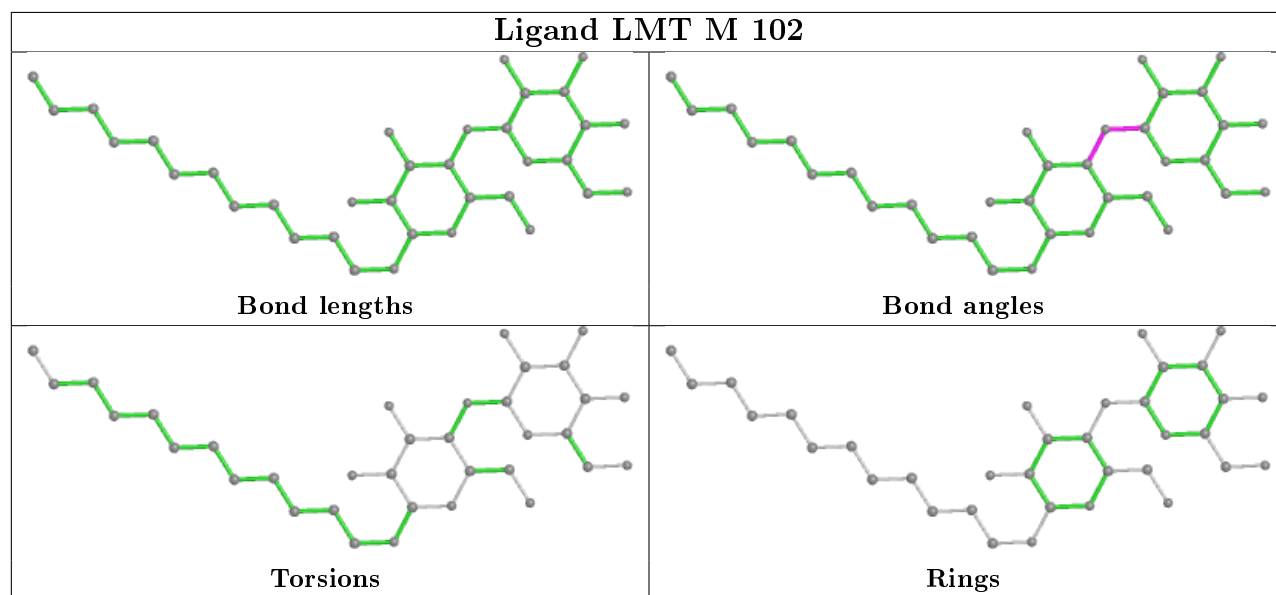
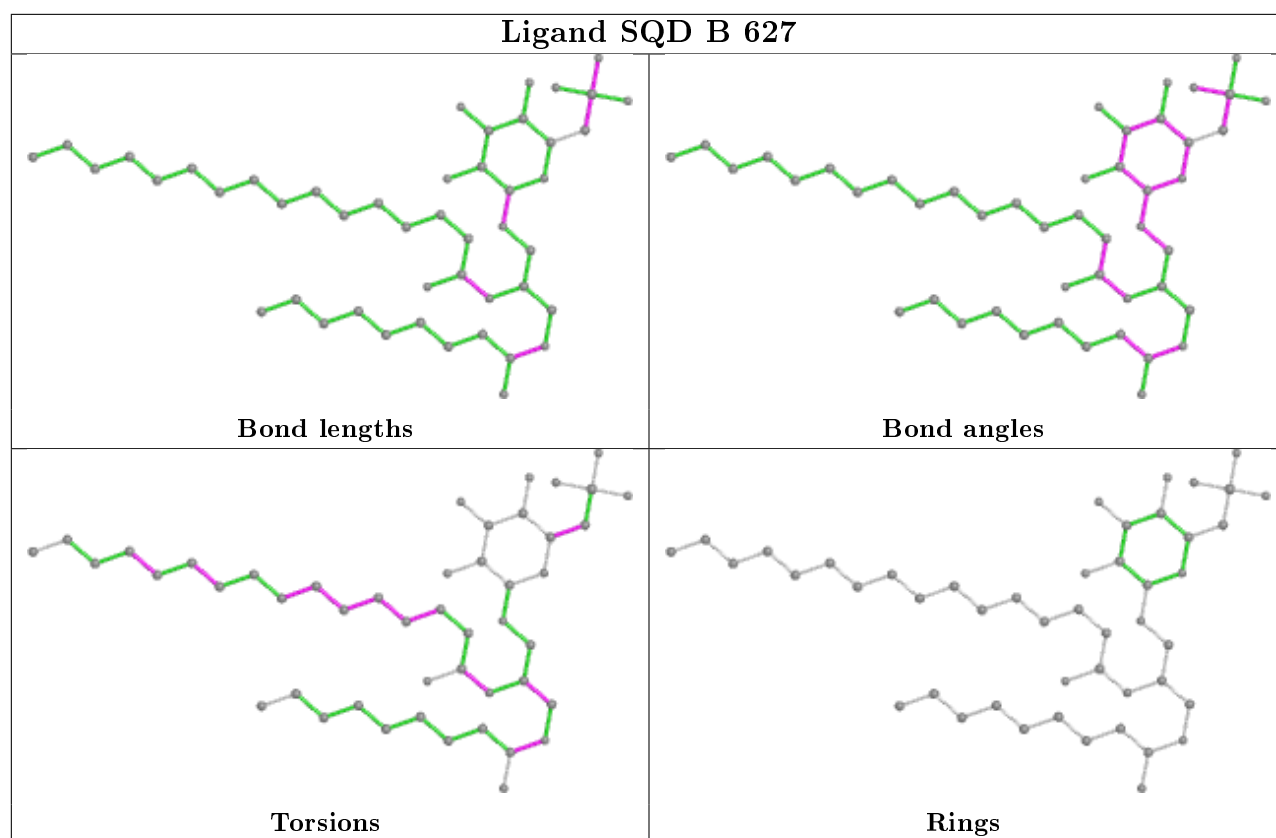
Ligand LMG G 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

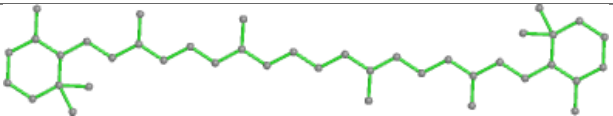
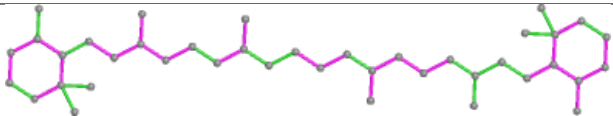
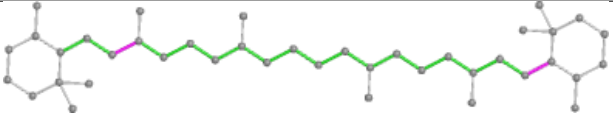
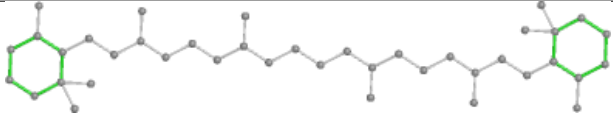
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

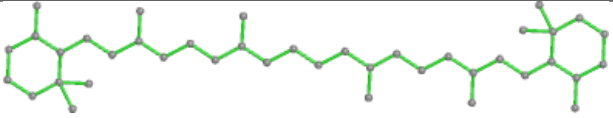
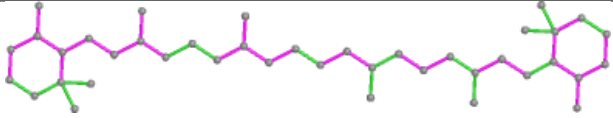
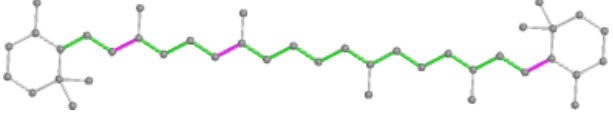
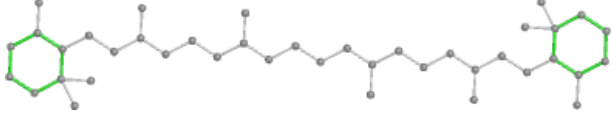


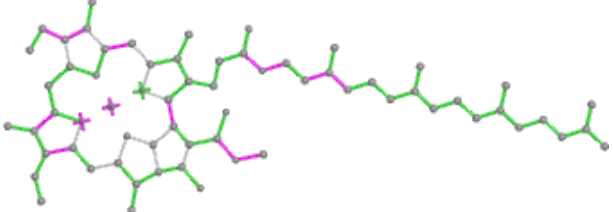
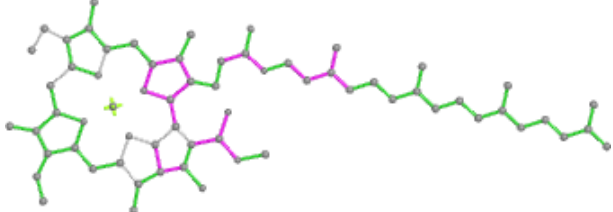
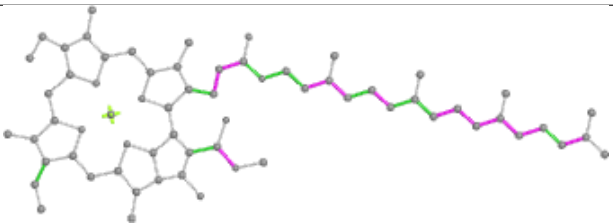
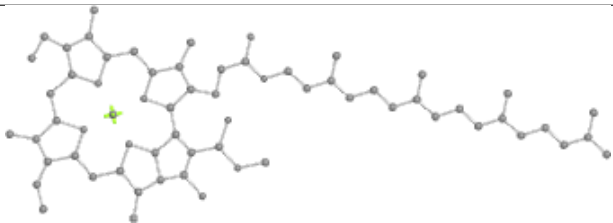


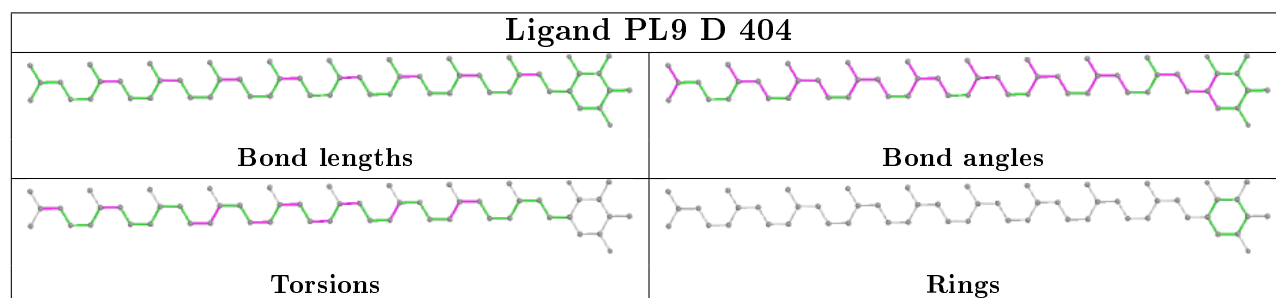
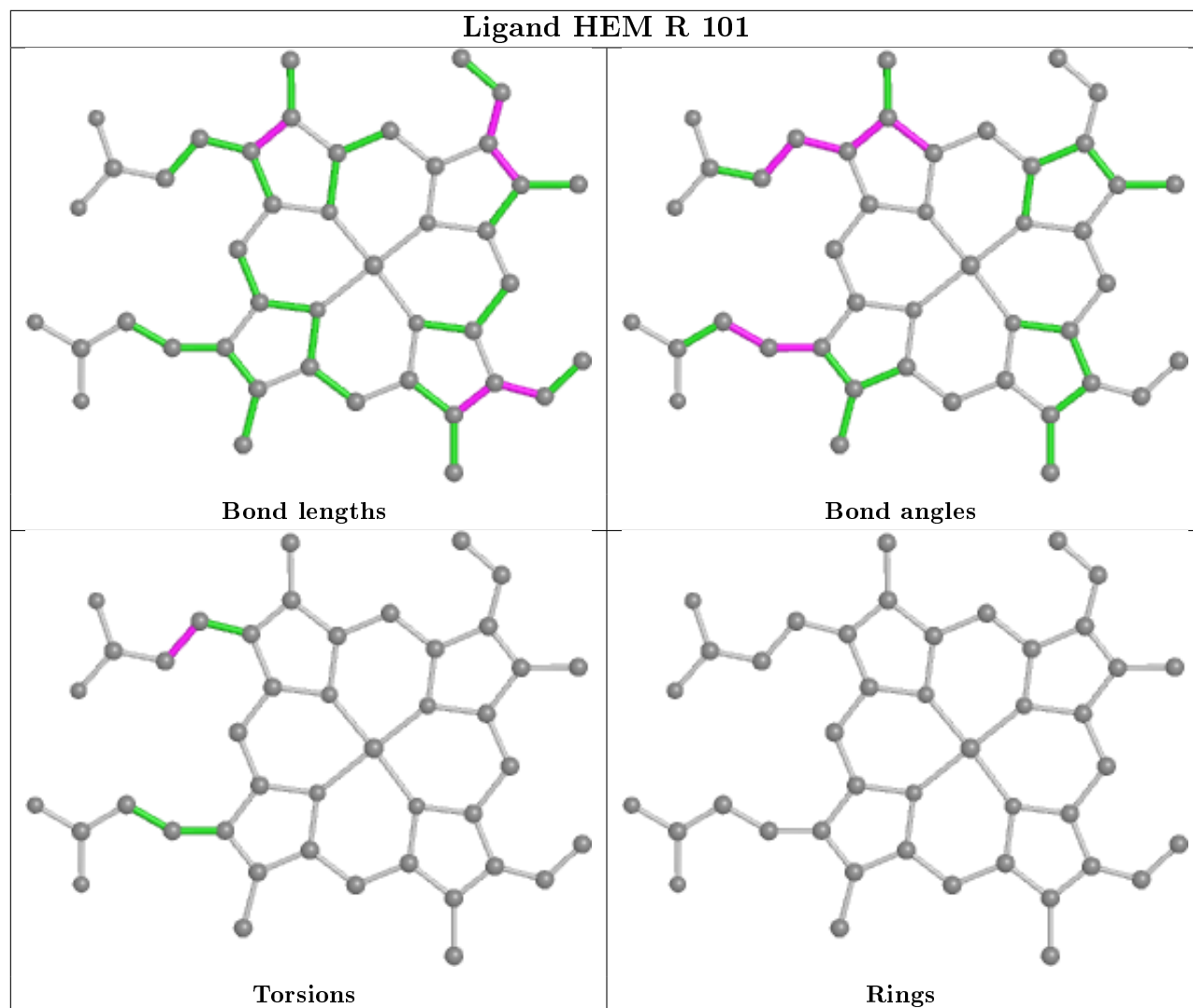




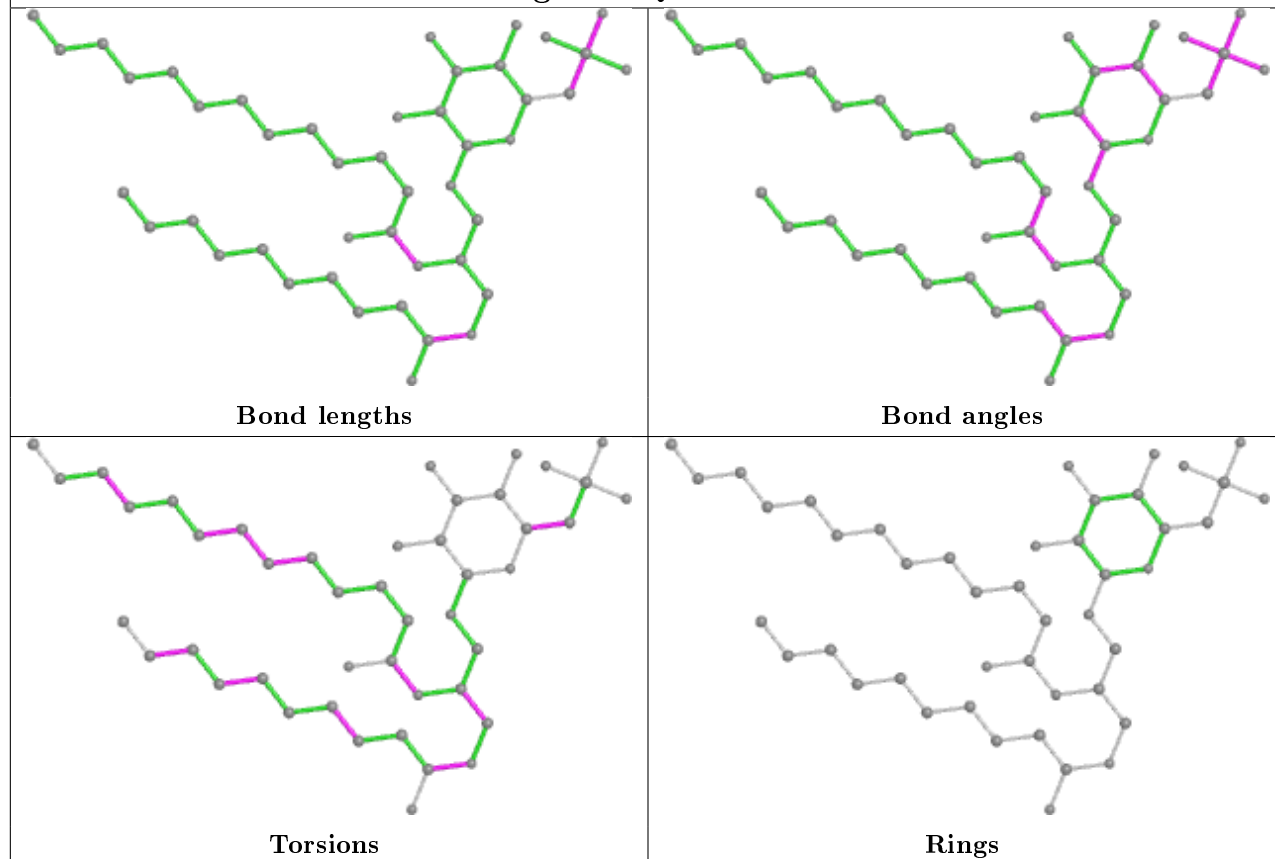
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR P 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

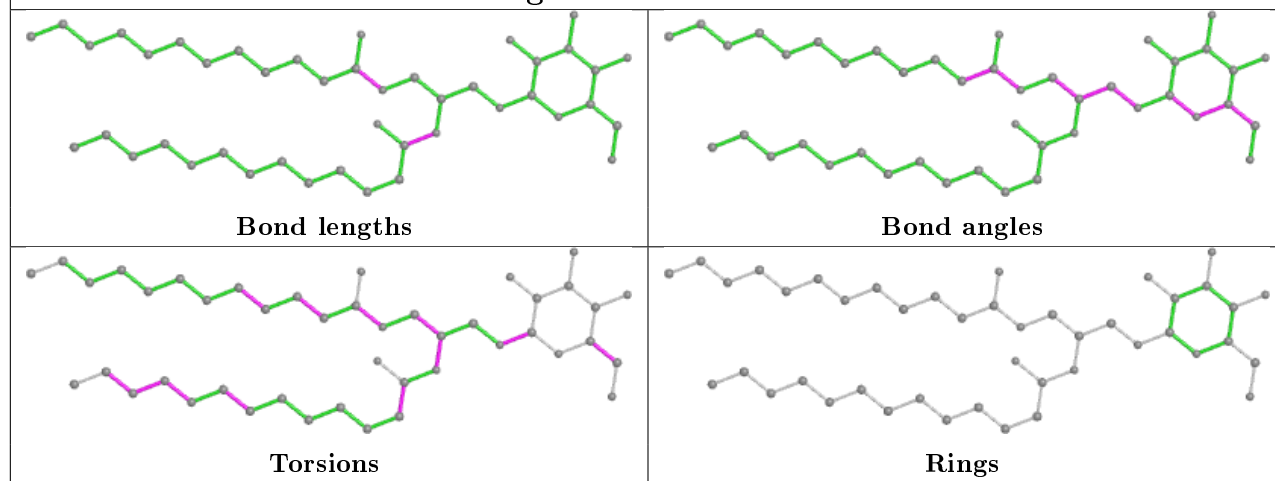
Ligand CLA N 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

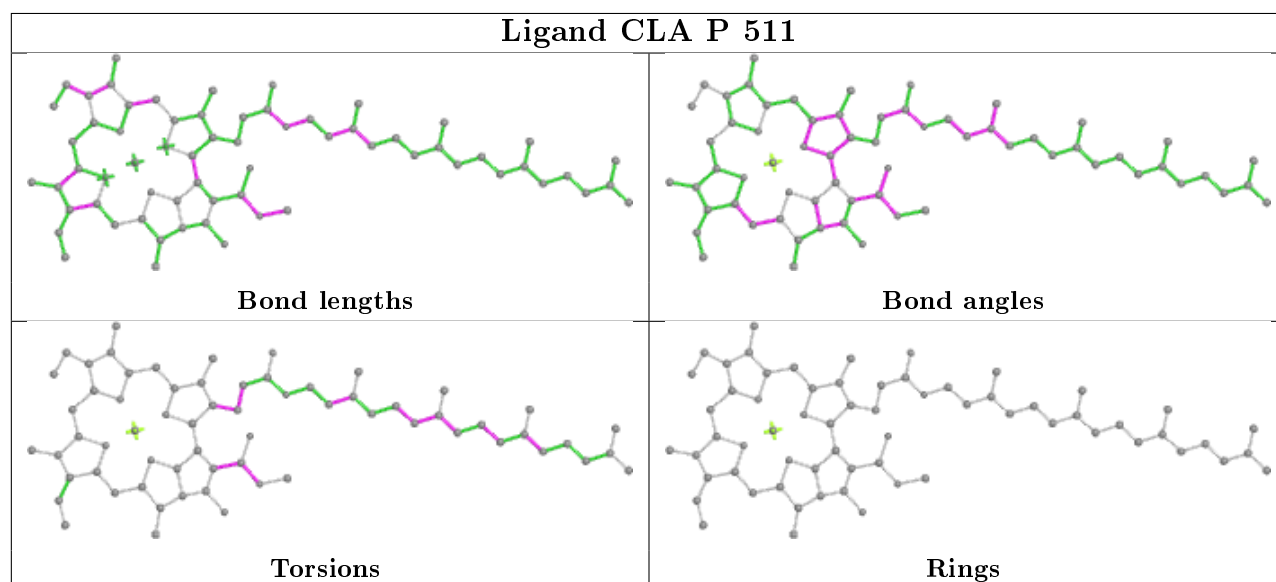
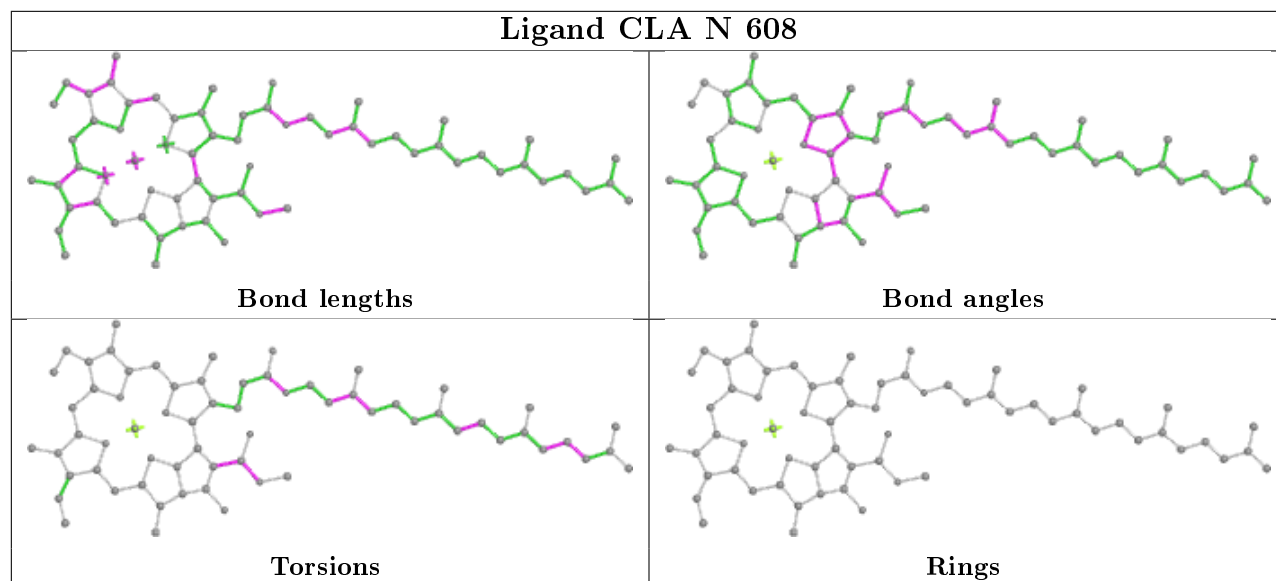
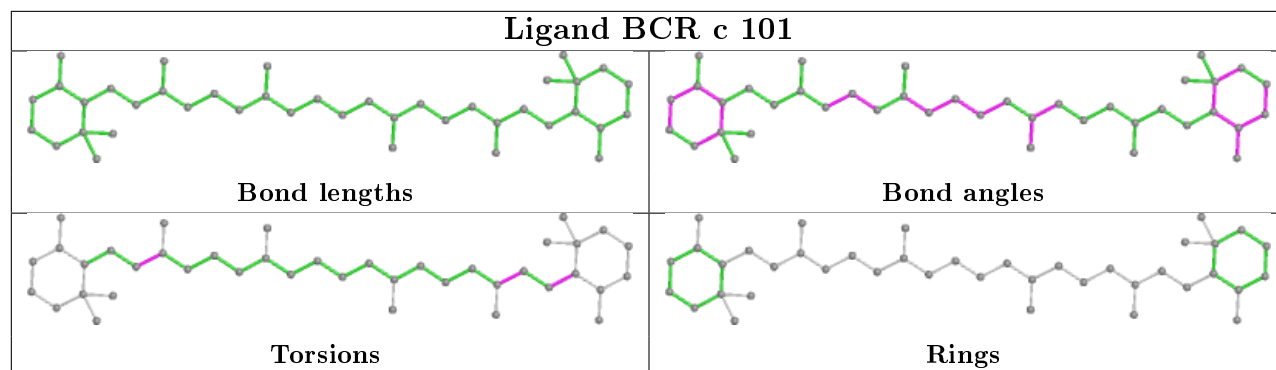


Ligand SQD F 101

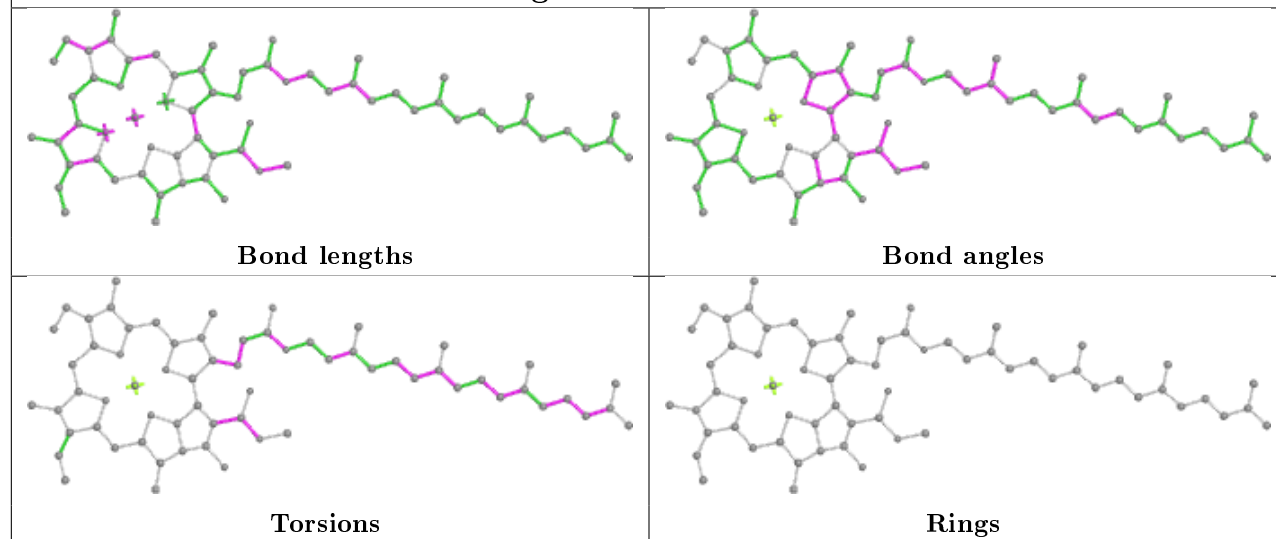


Ligand LMG R 102

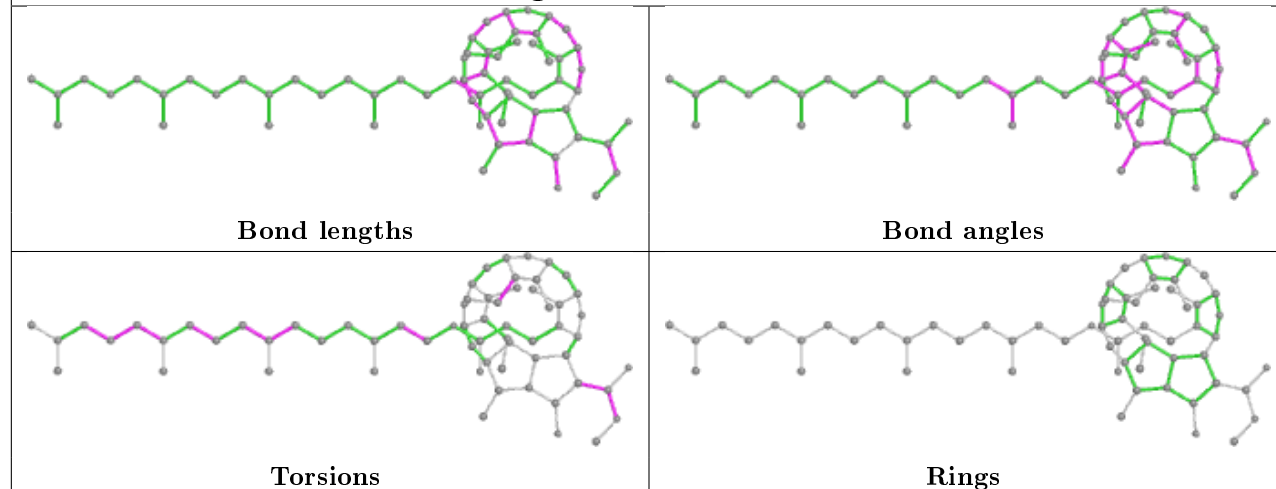




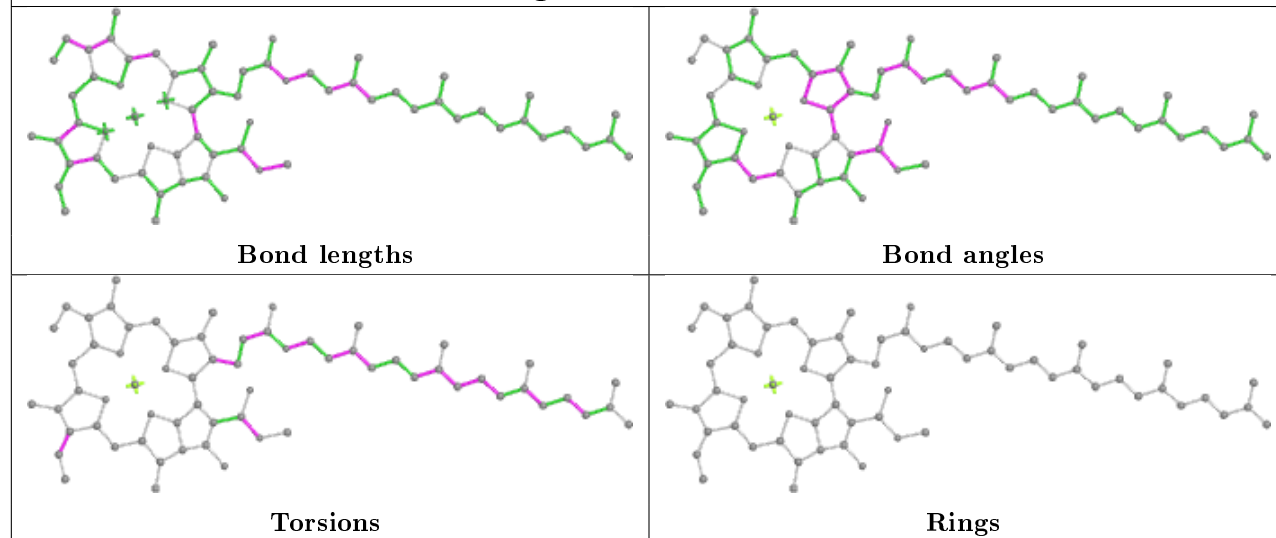
Ligand CLA N 609

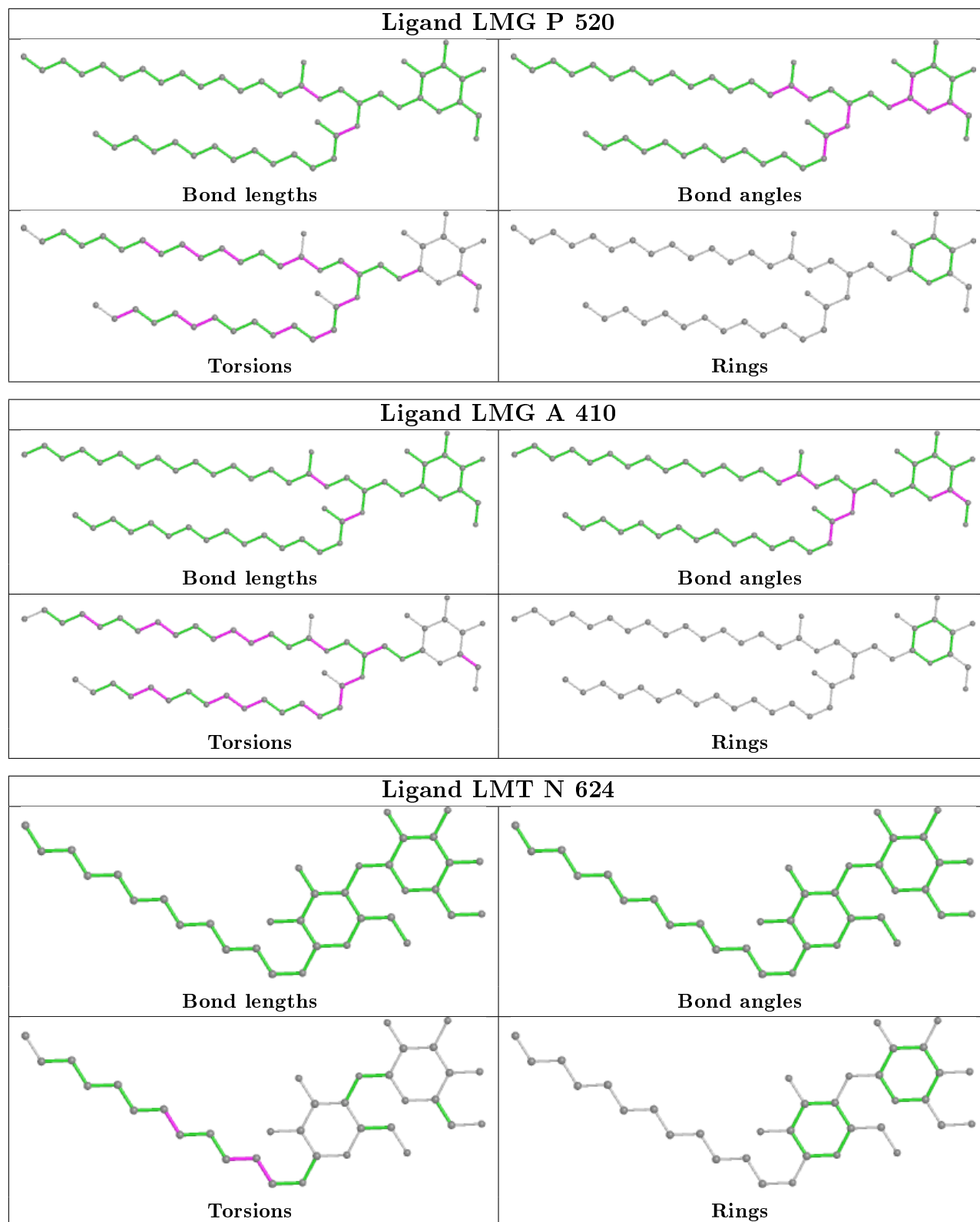


Ligand PHO Q 403

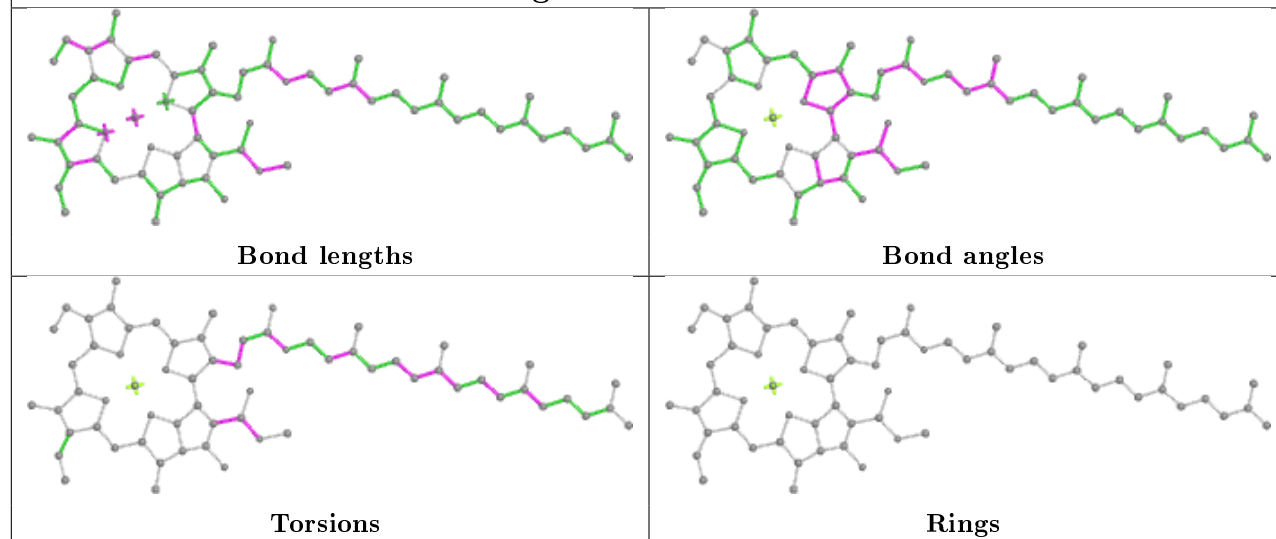


Ligand CLA C 505

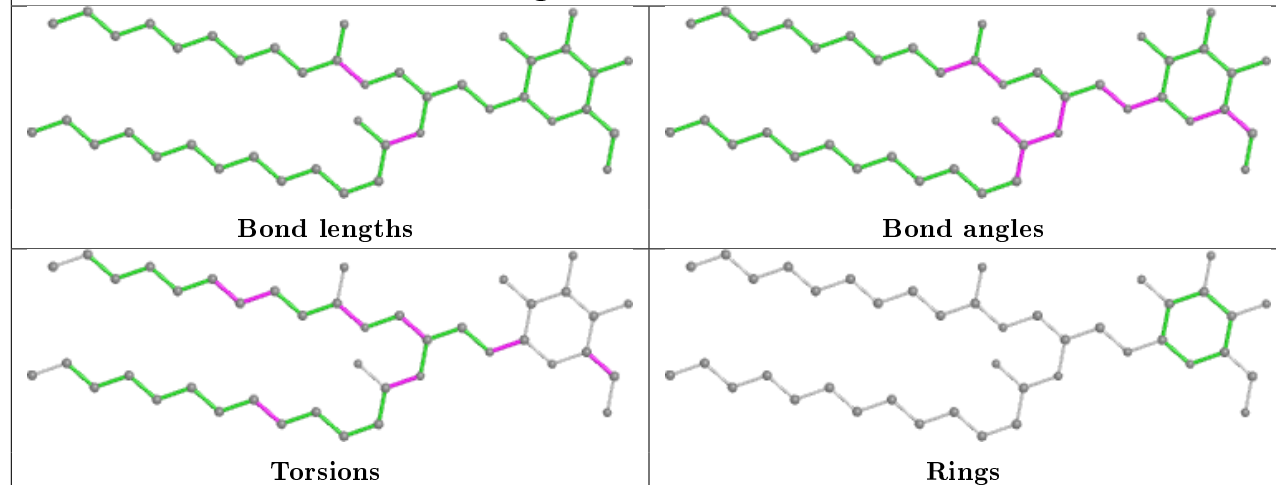




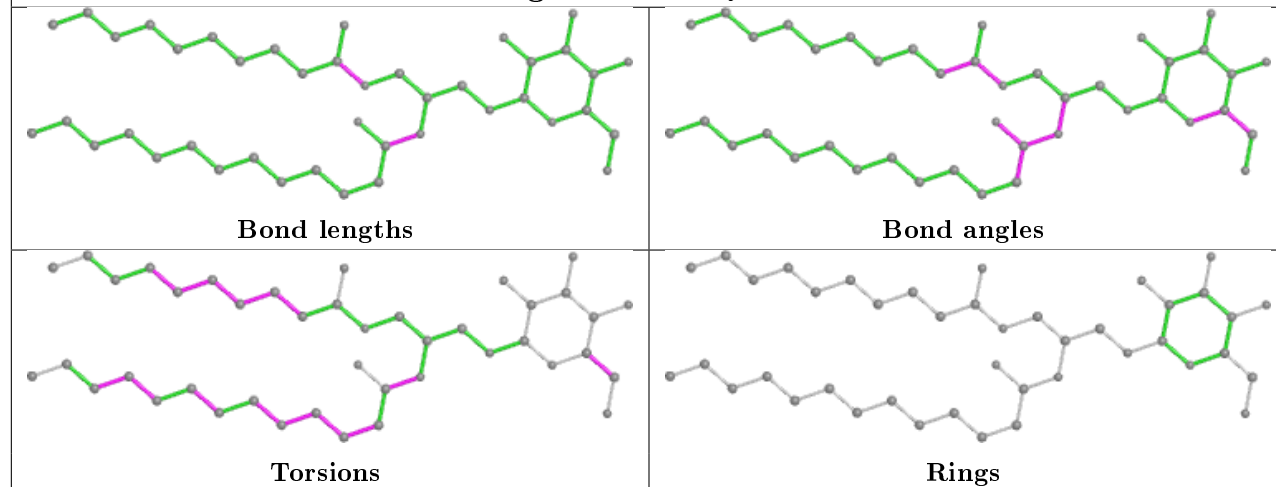
Ligand CLA C 511



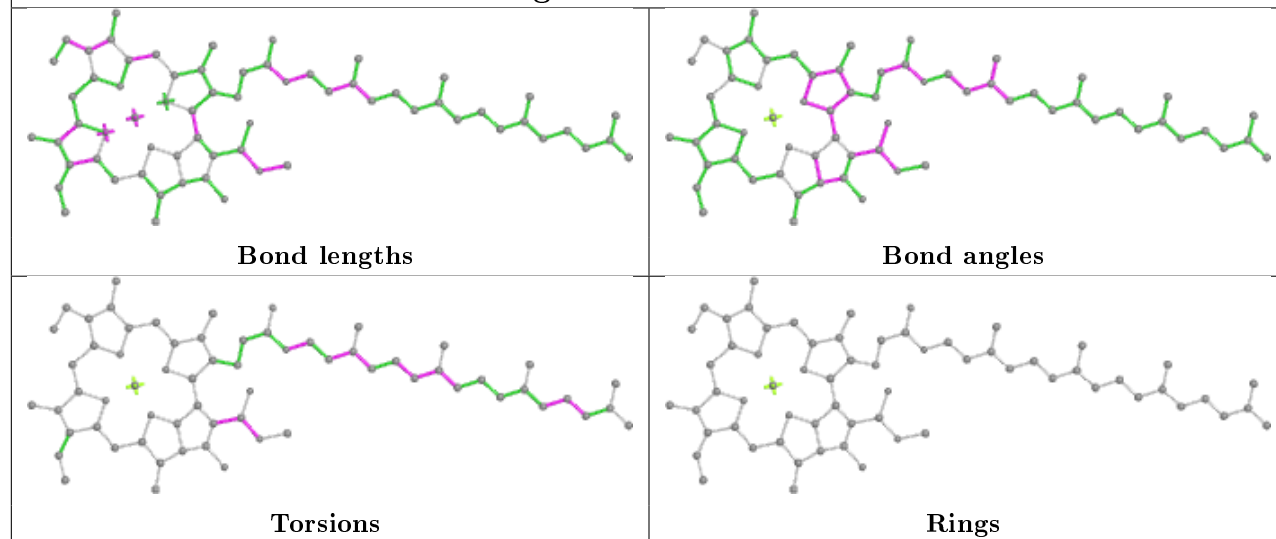
Ligand LMG e 102



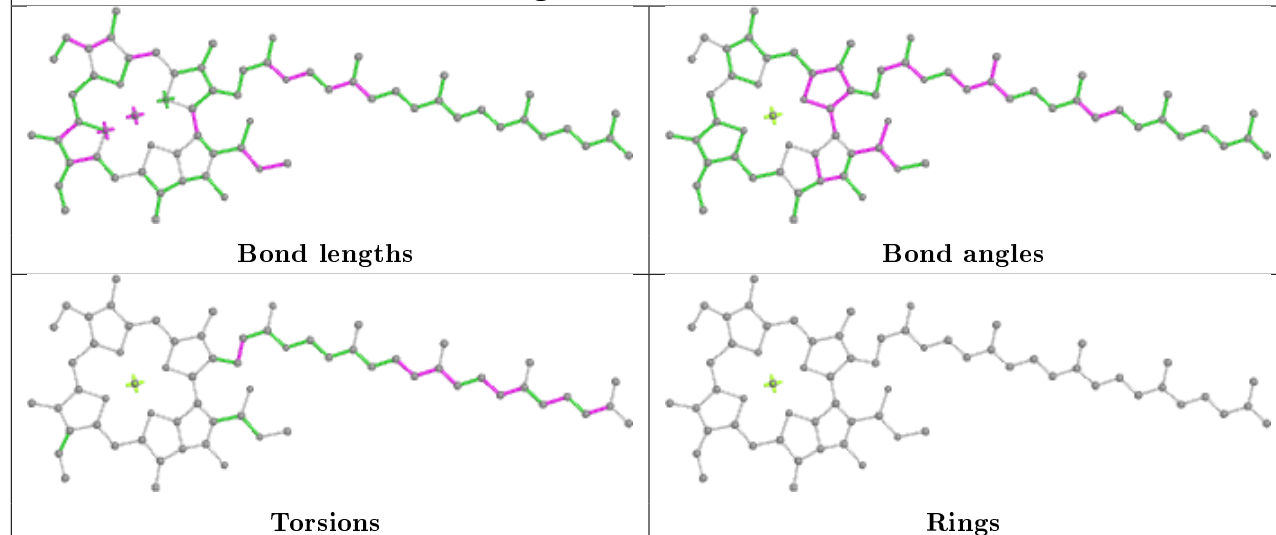
Ligand LMG Q 401



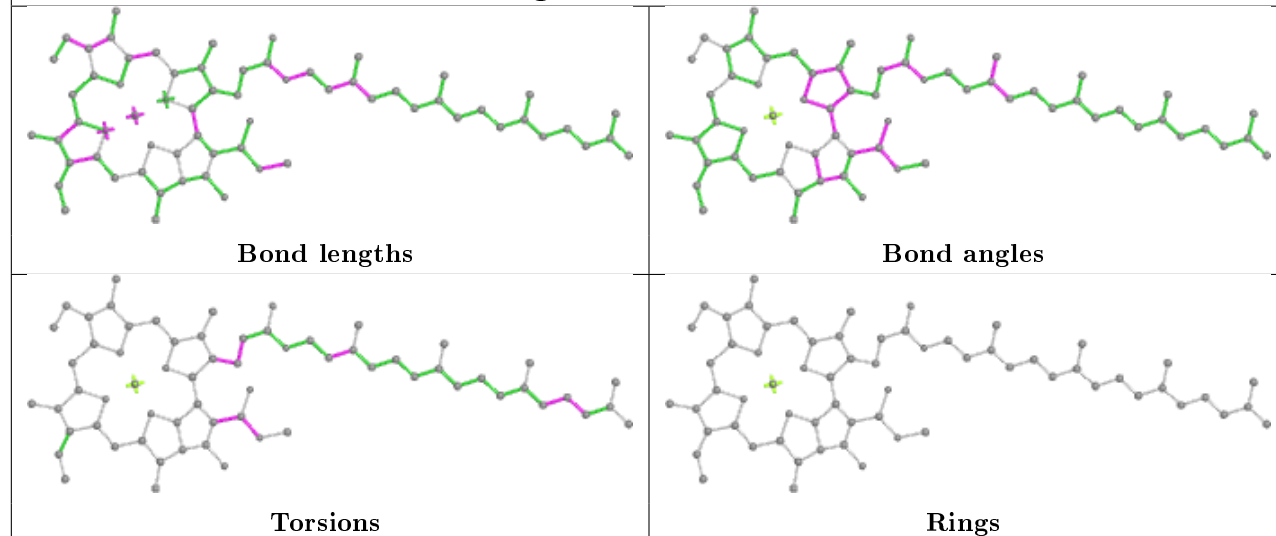
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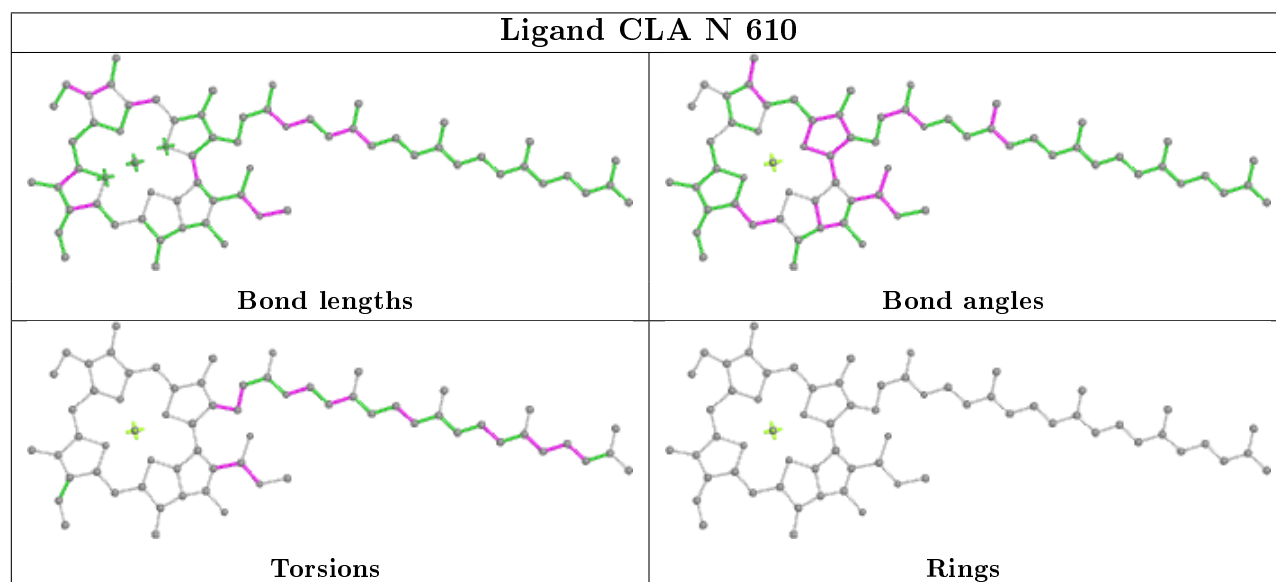
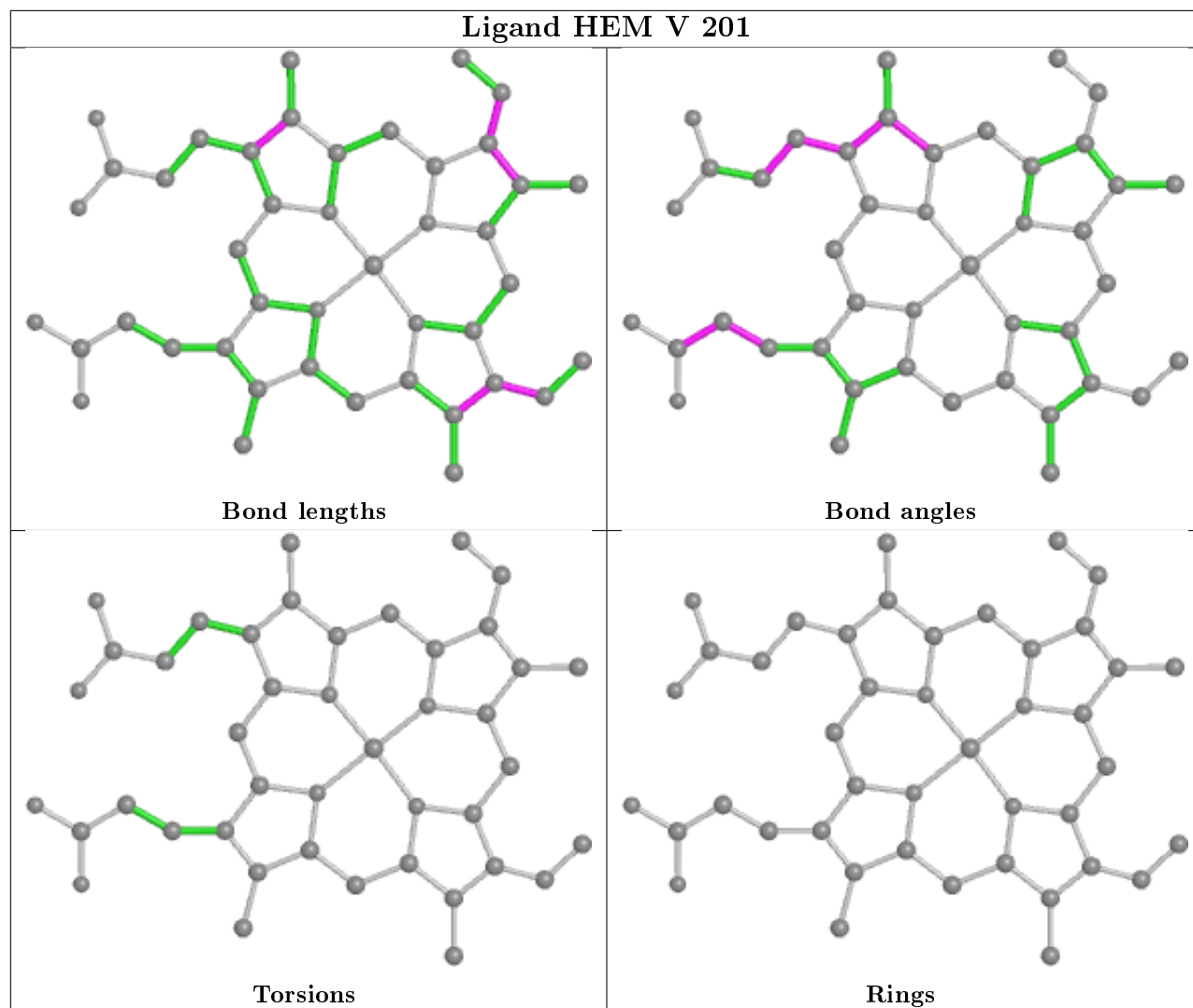


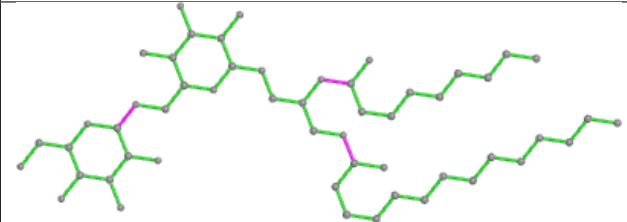
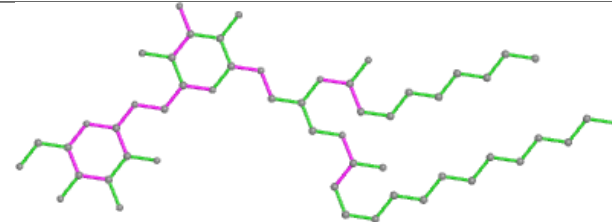
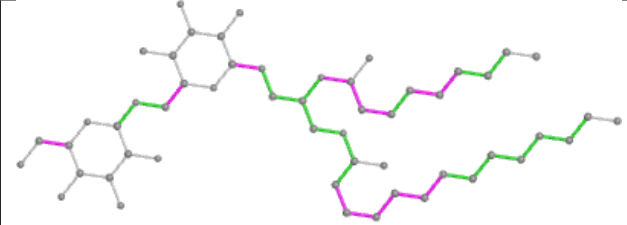
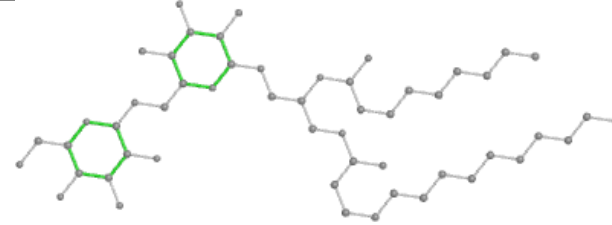
Ligand CLA A 405

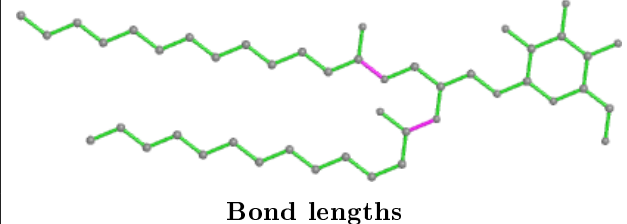
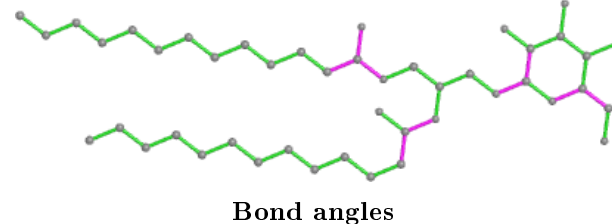
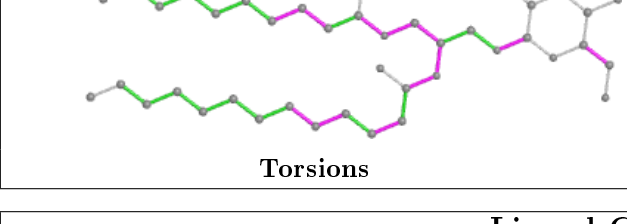
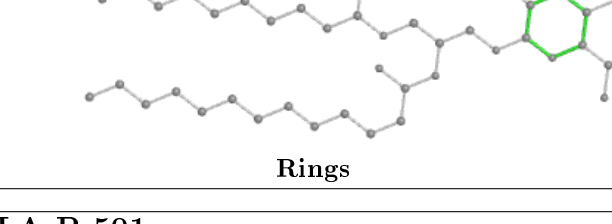


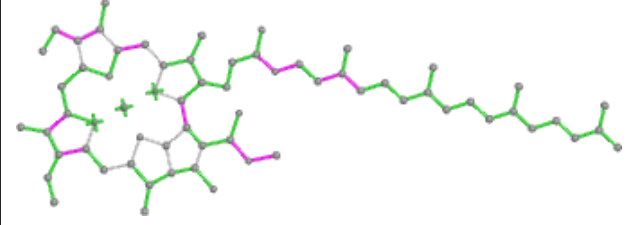
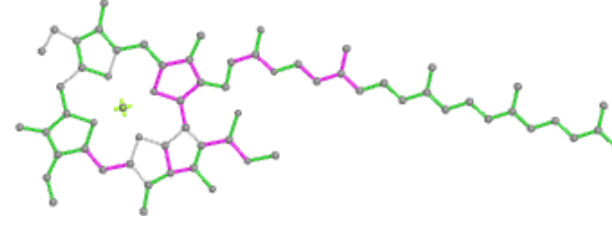
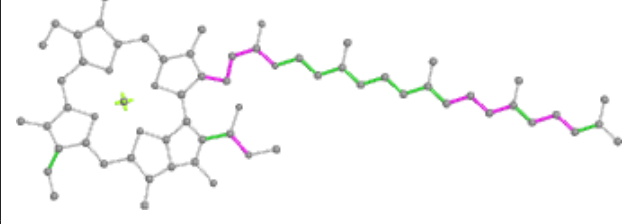
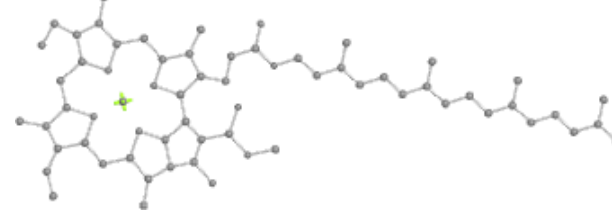
Ligand CLA B 607

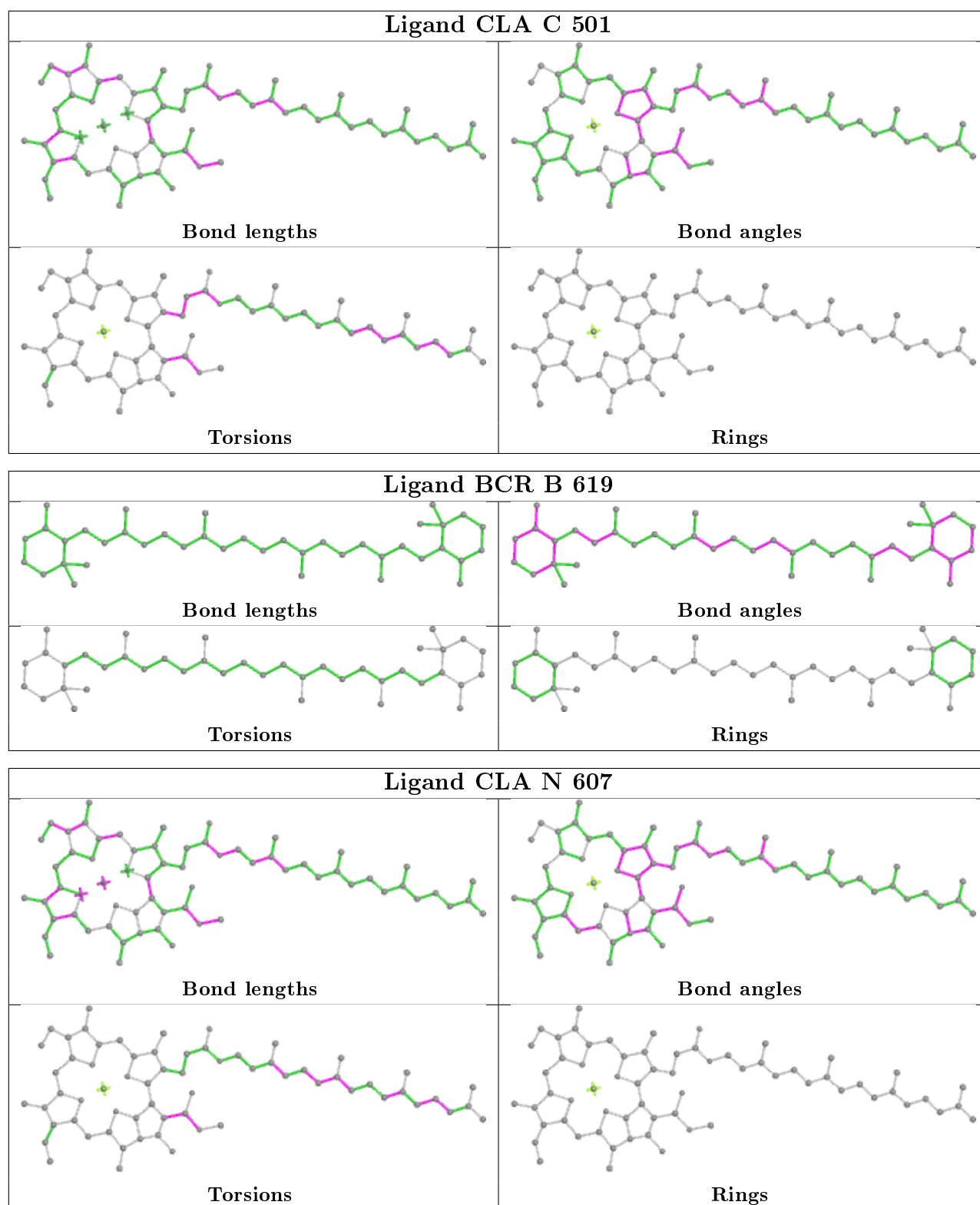


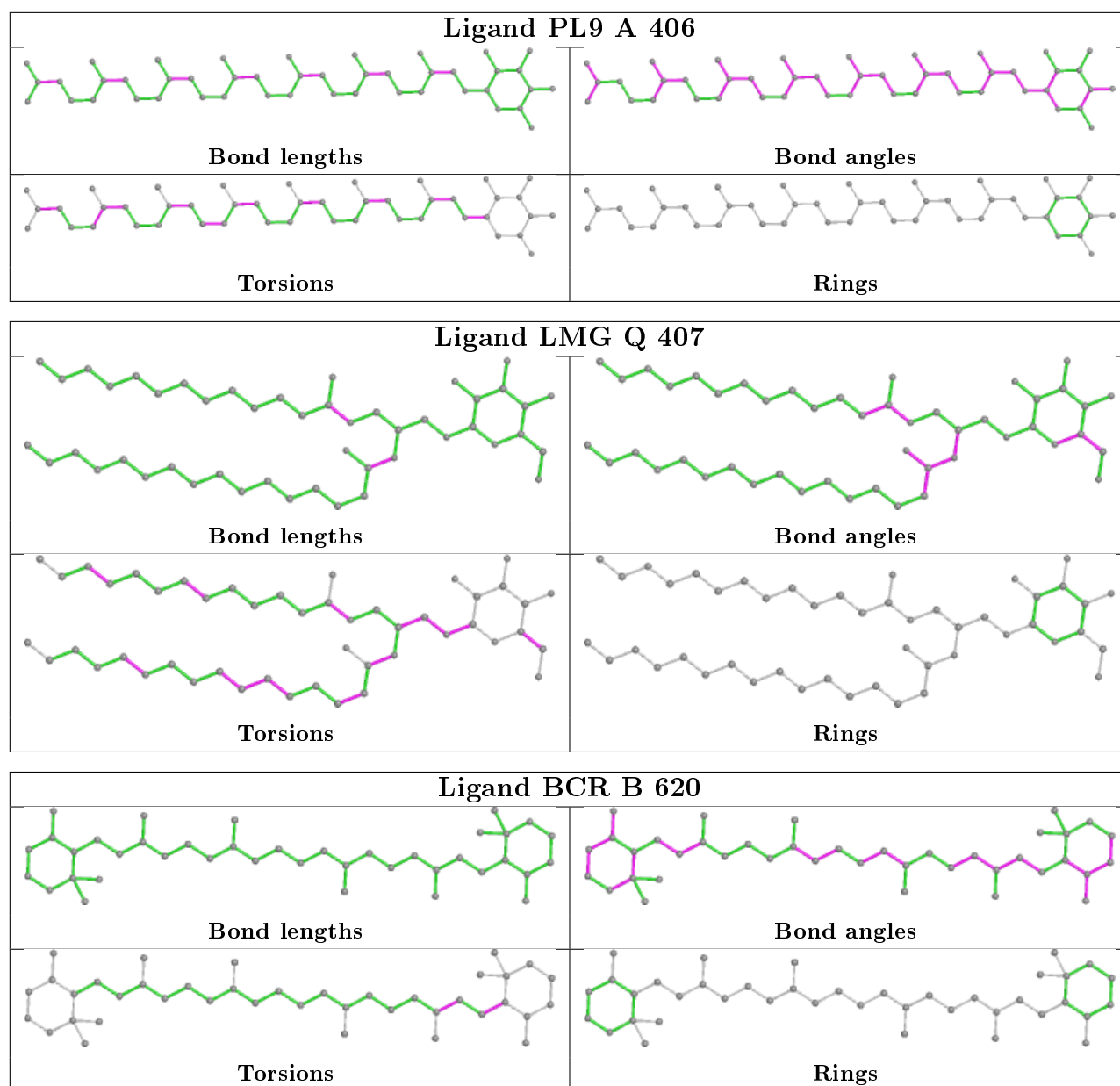


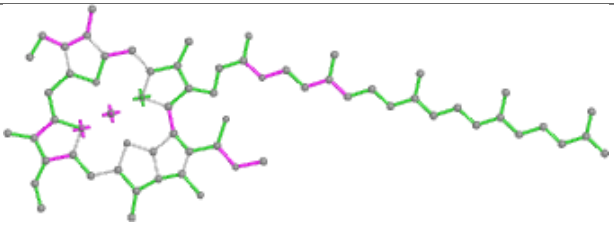
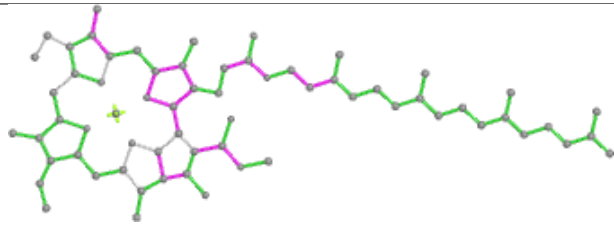
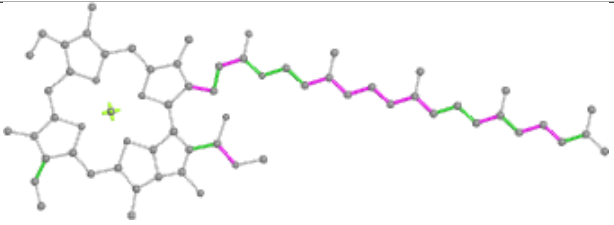
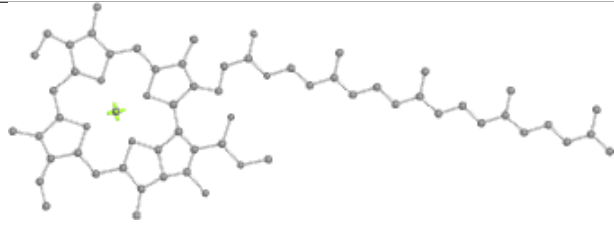
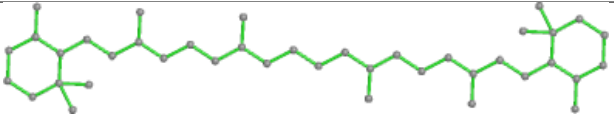
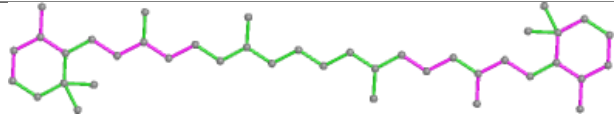
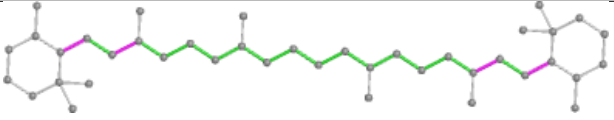
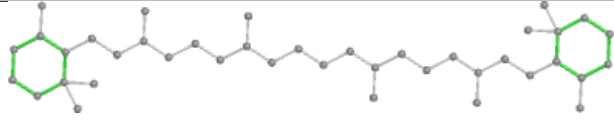
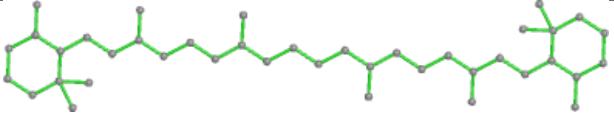
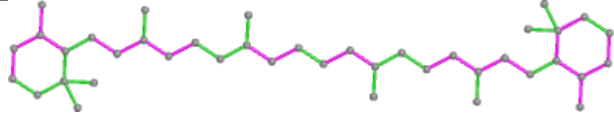
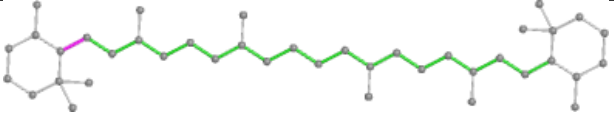
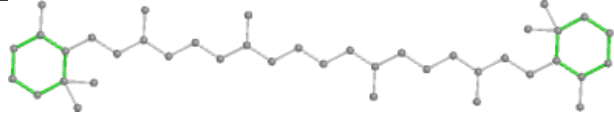
Ligand DGD P 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG P 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

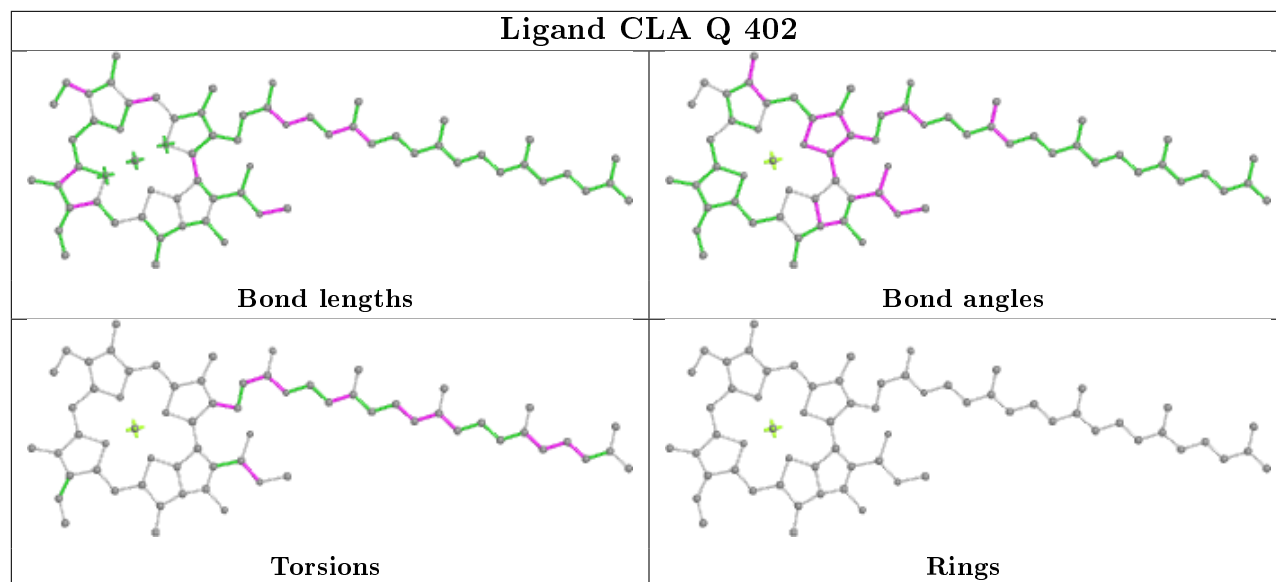
Ligand CLA P 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



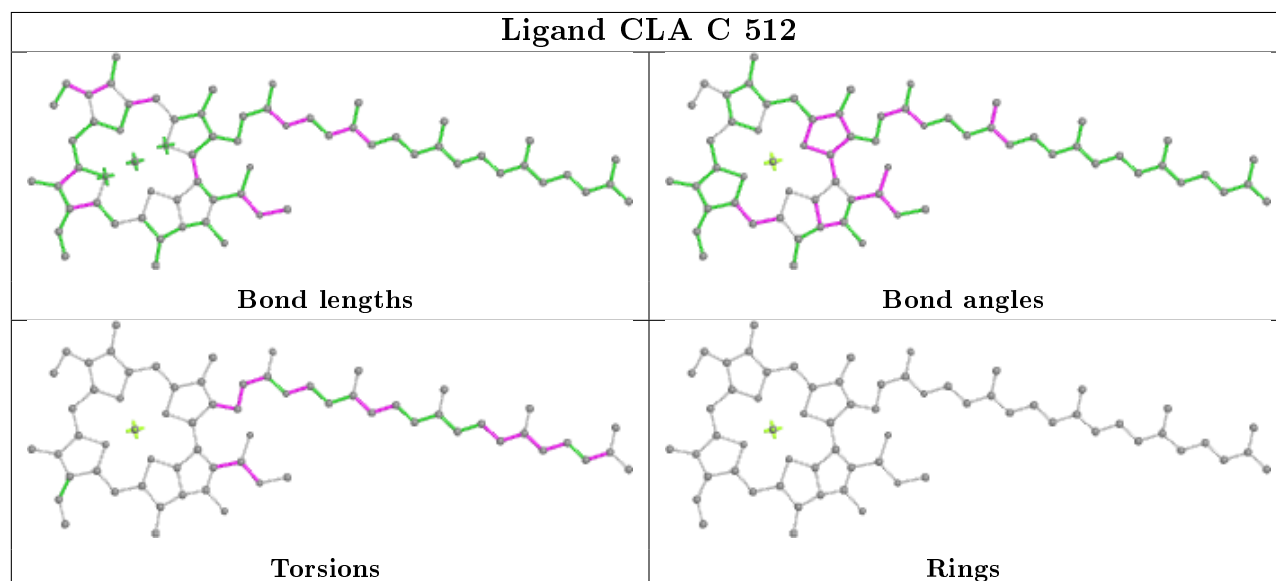


Ligand CLA B 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR D 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

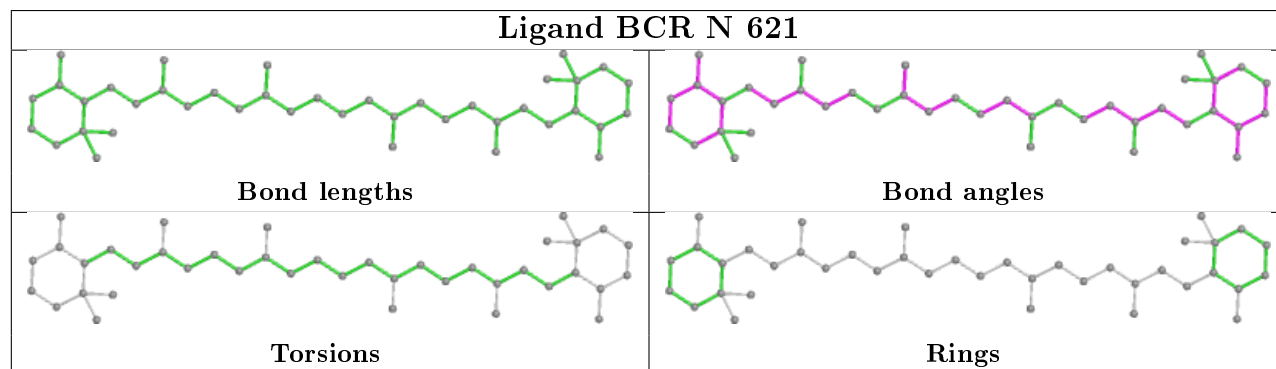
Ligand CLA Q 402

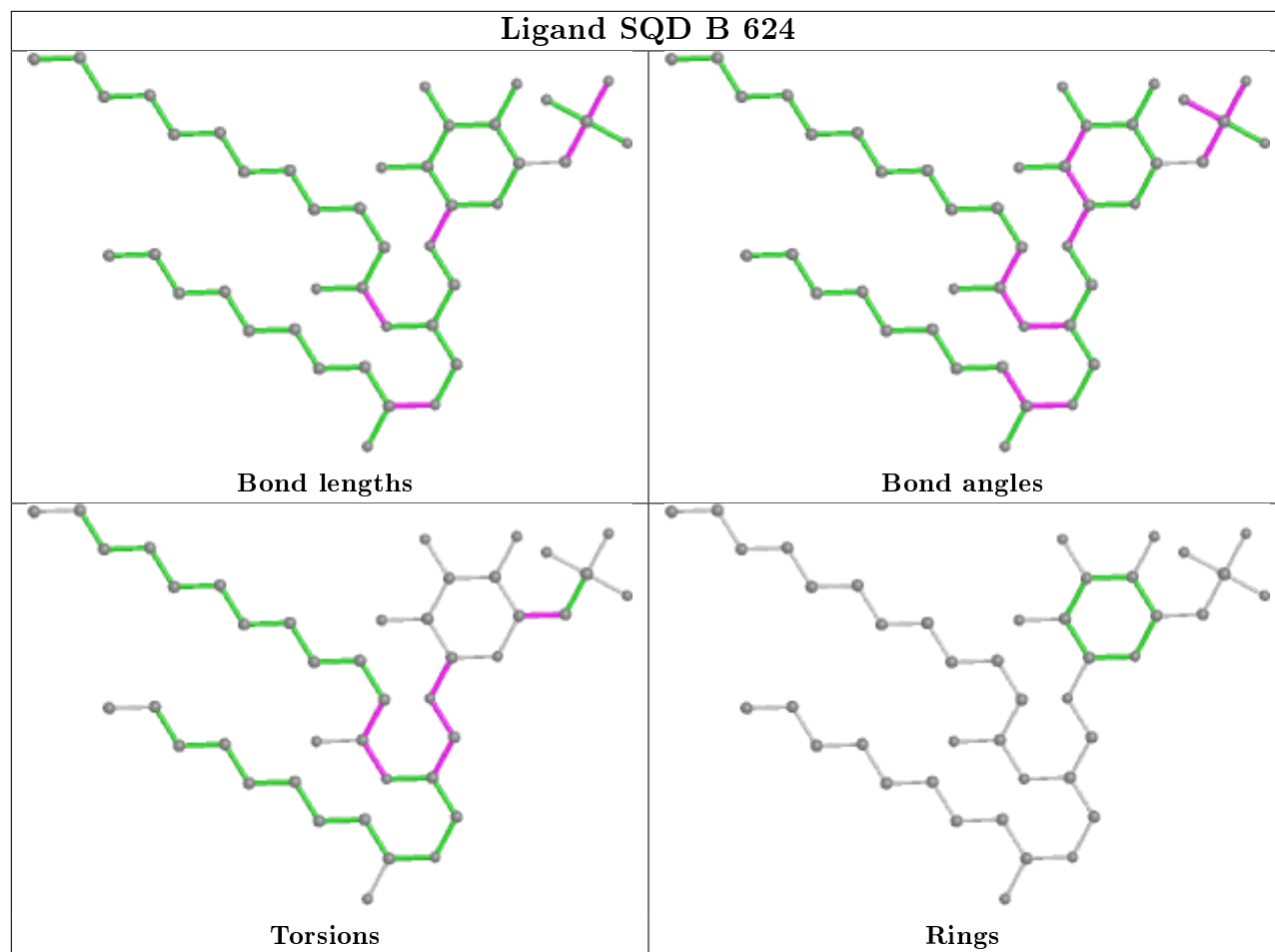
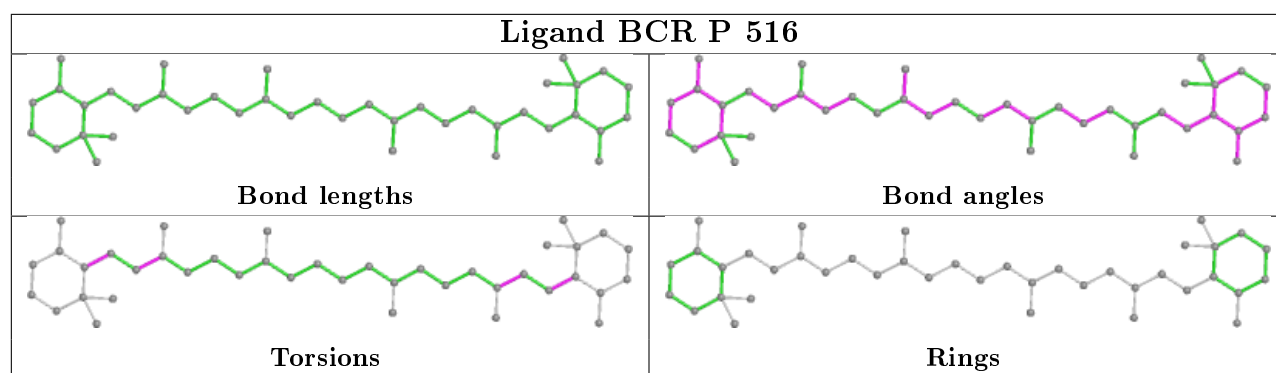


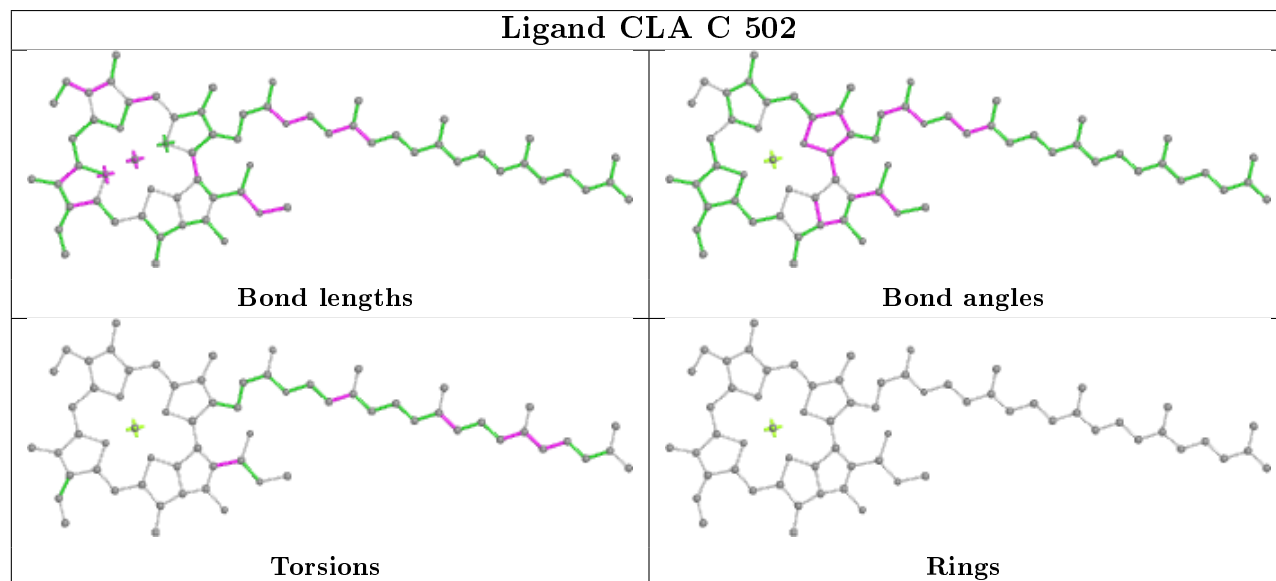
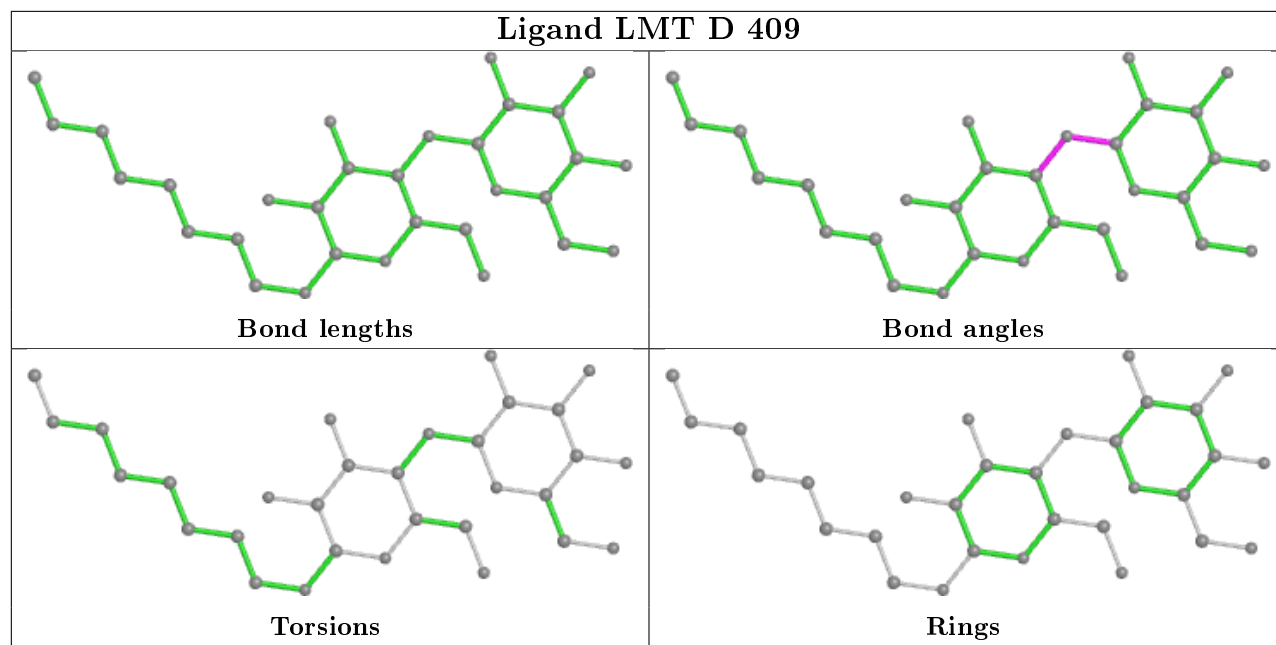
Ligand CLA C 512



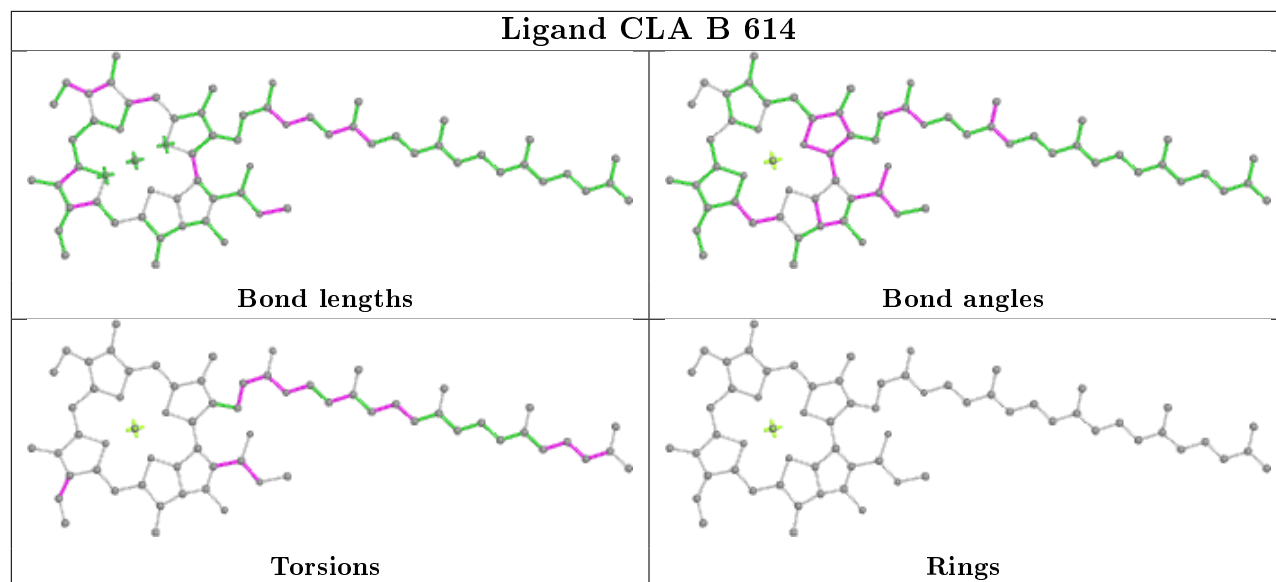
Ligand BCR N 621



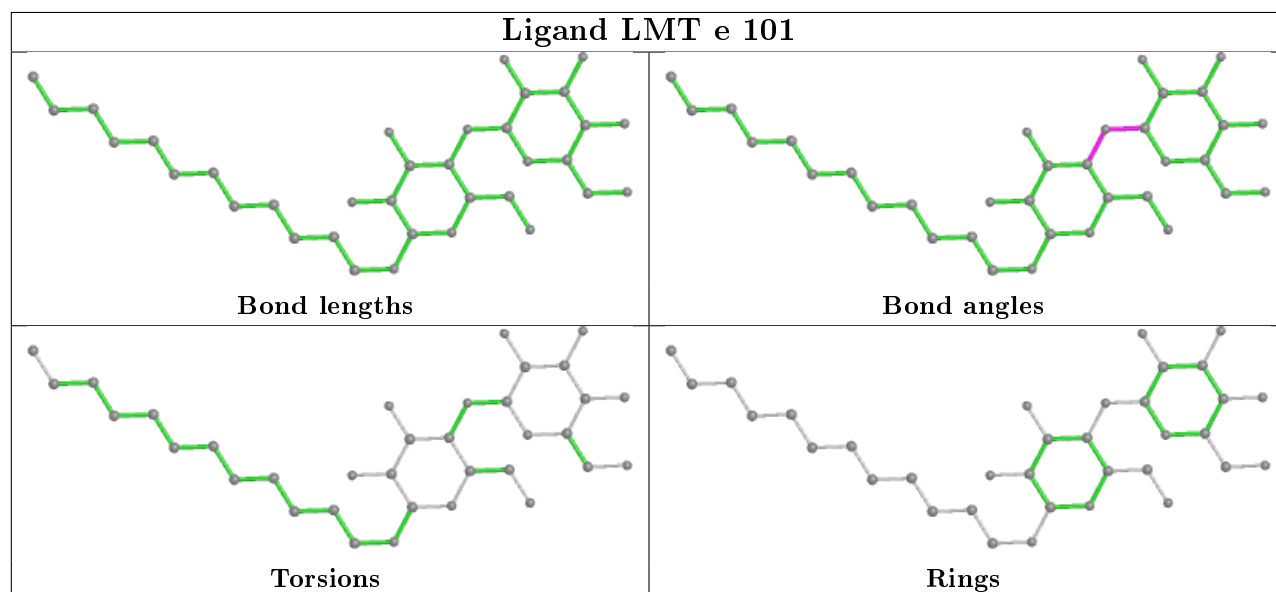




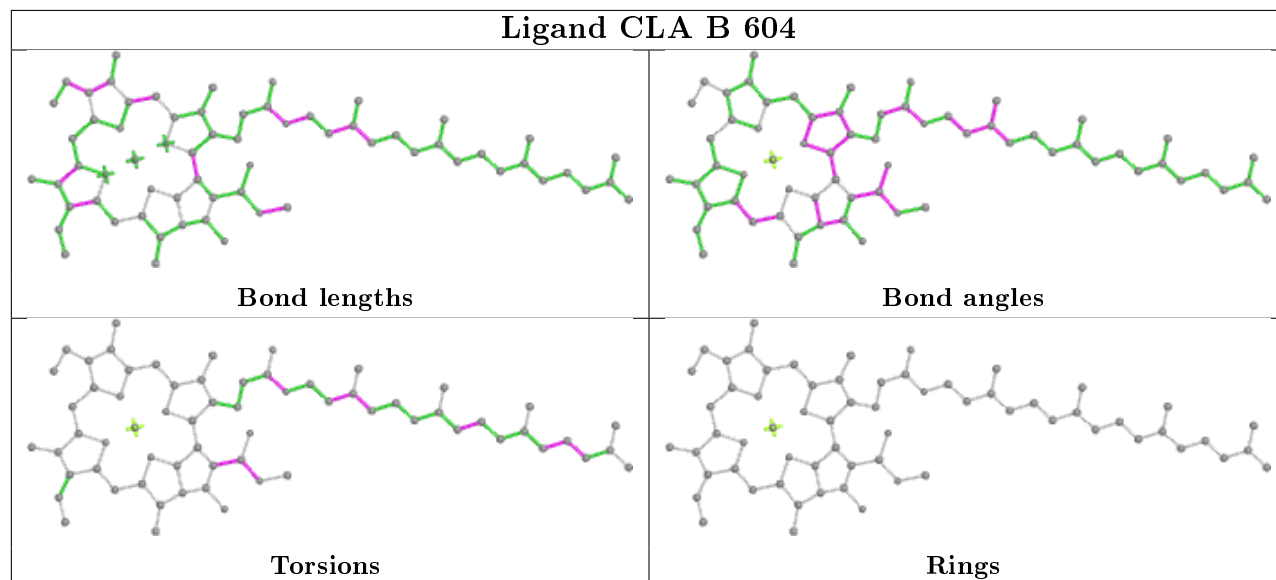
Ligand CLA B 614



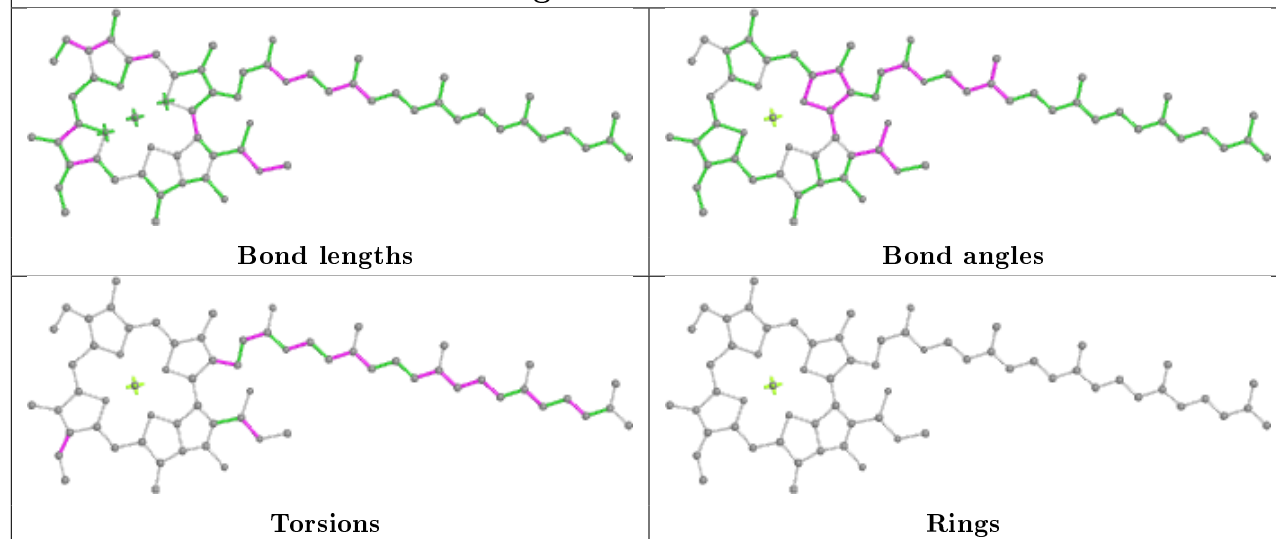
Ligand LMT e 101



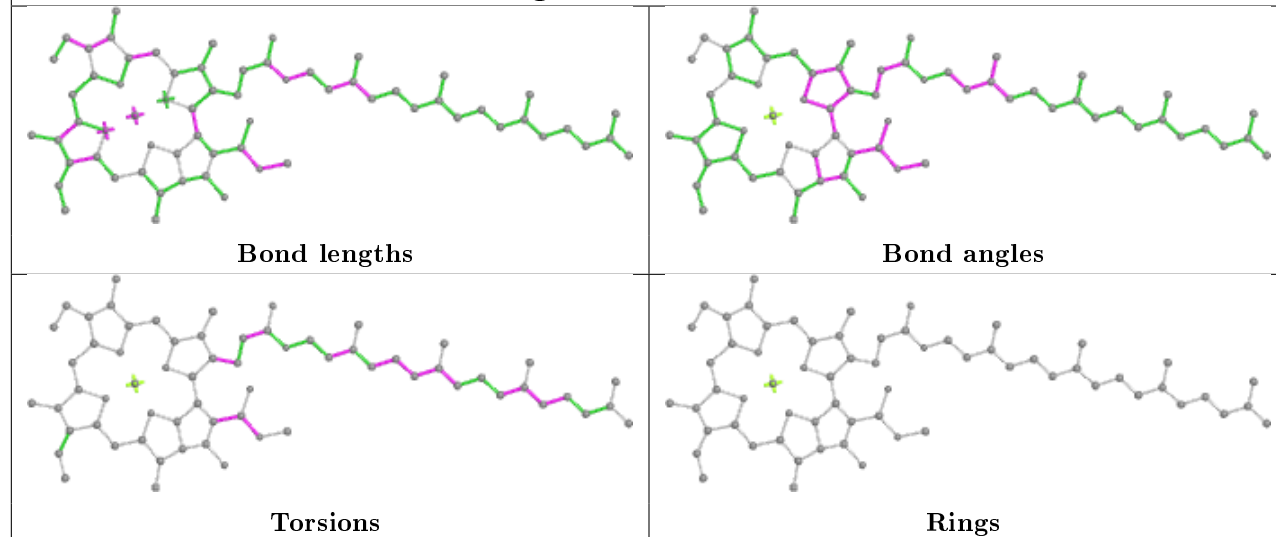
Ligand CLA B 604

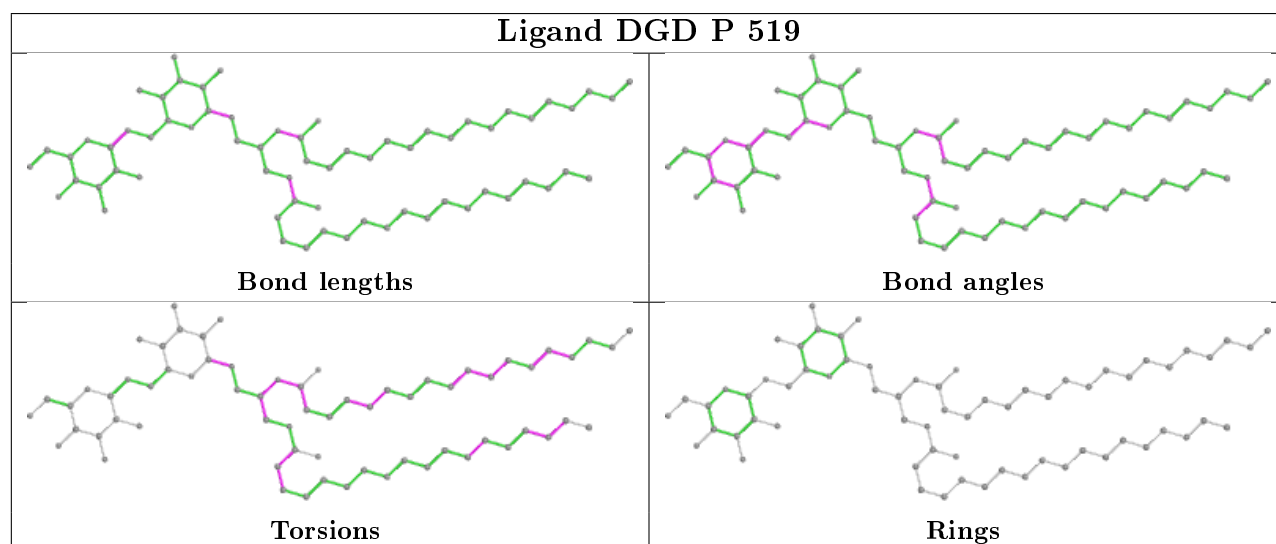
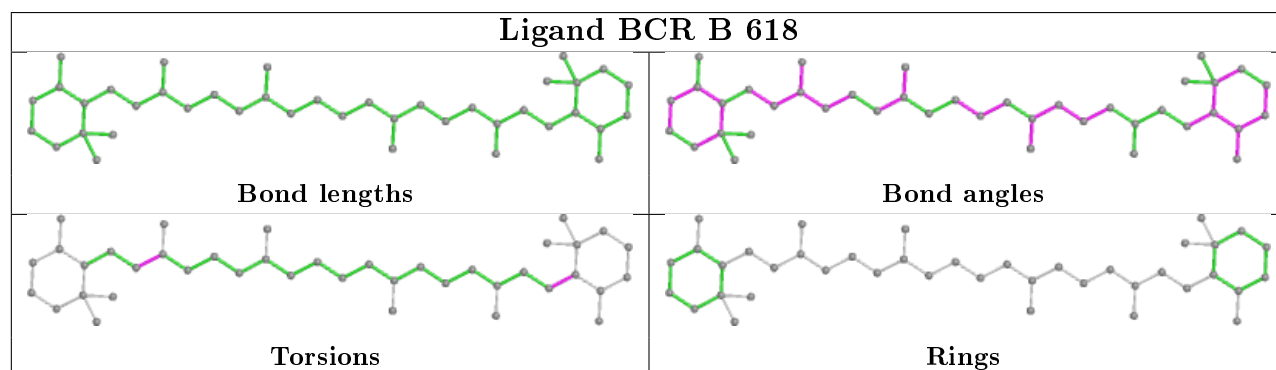
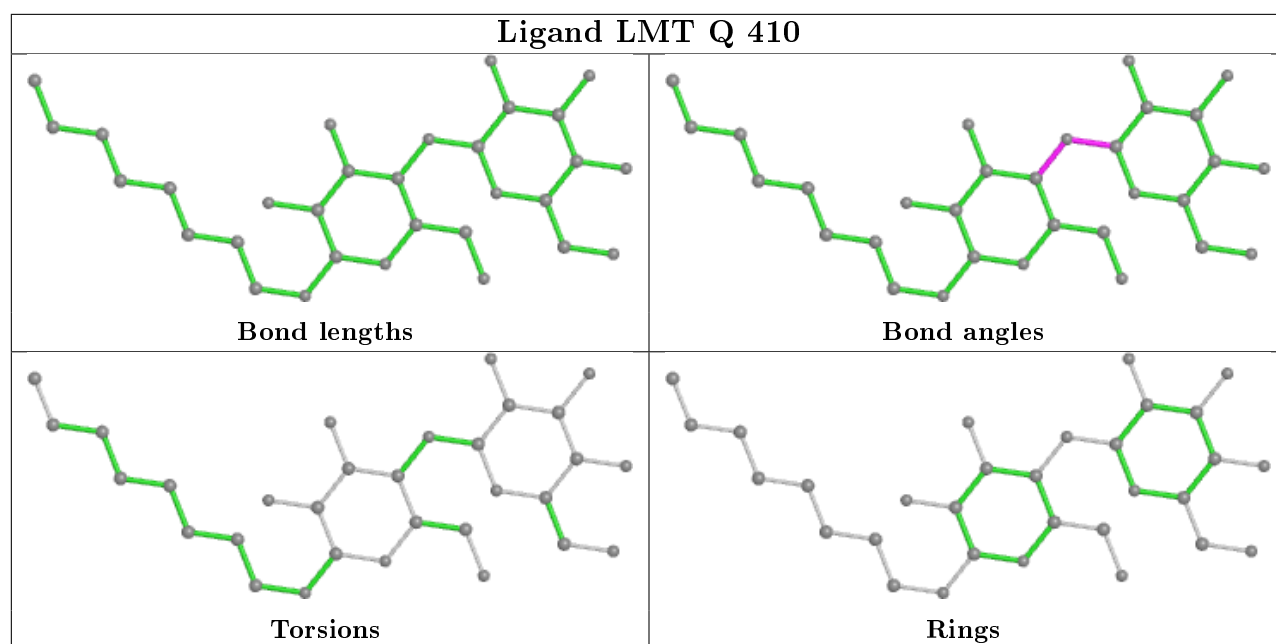


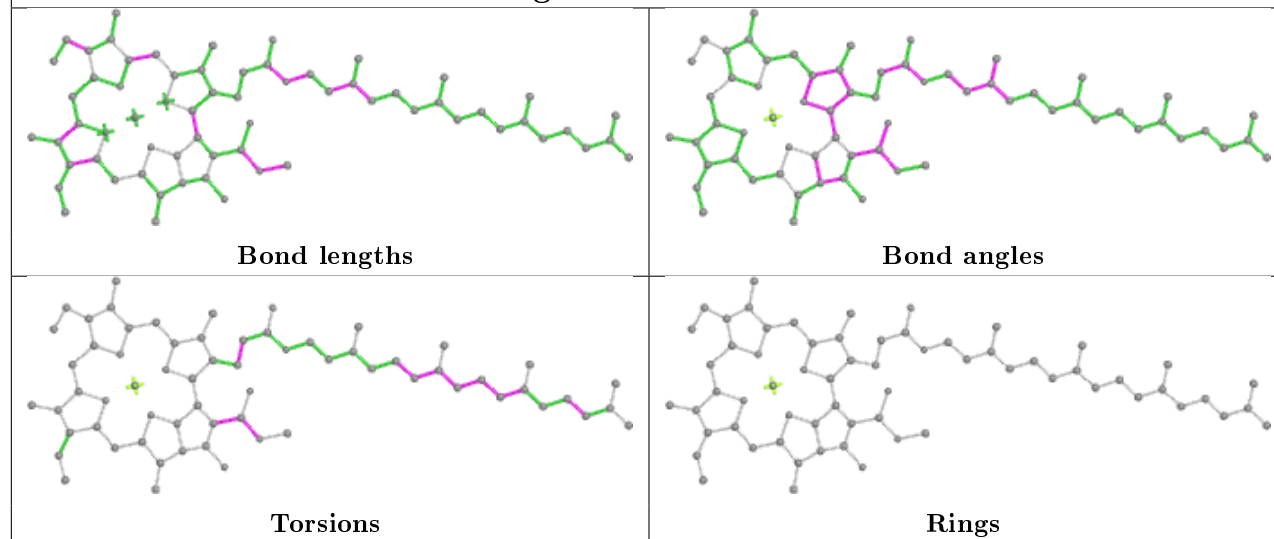
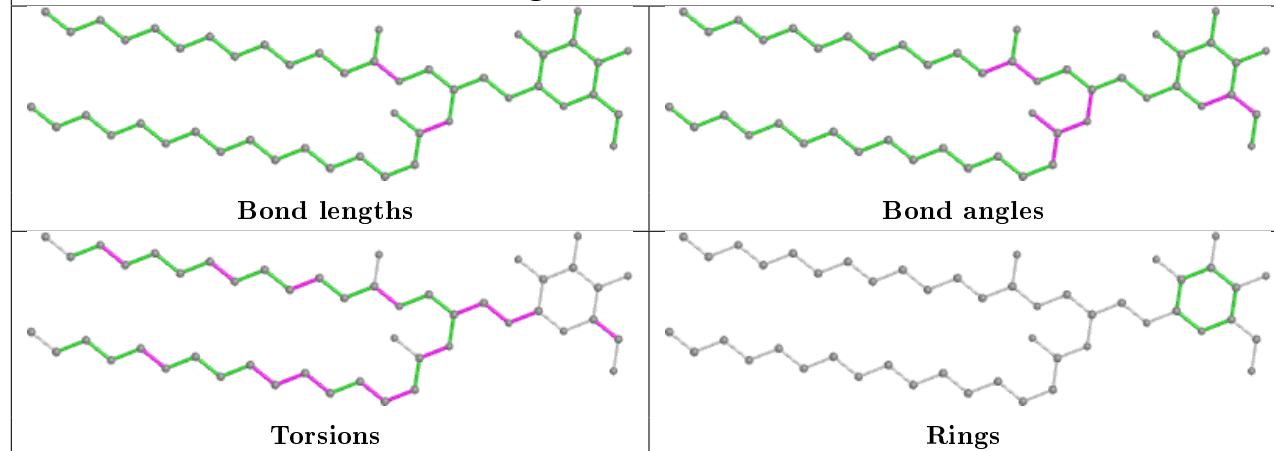
Ligand CLA P 505

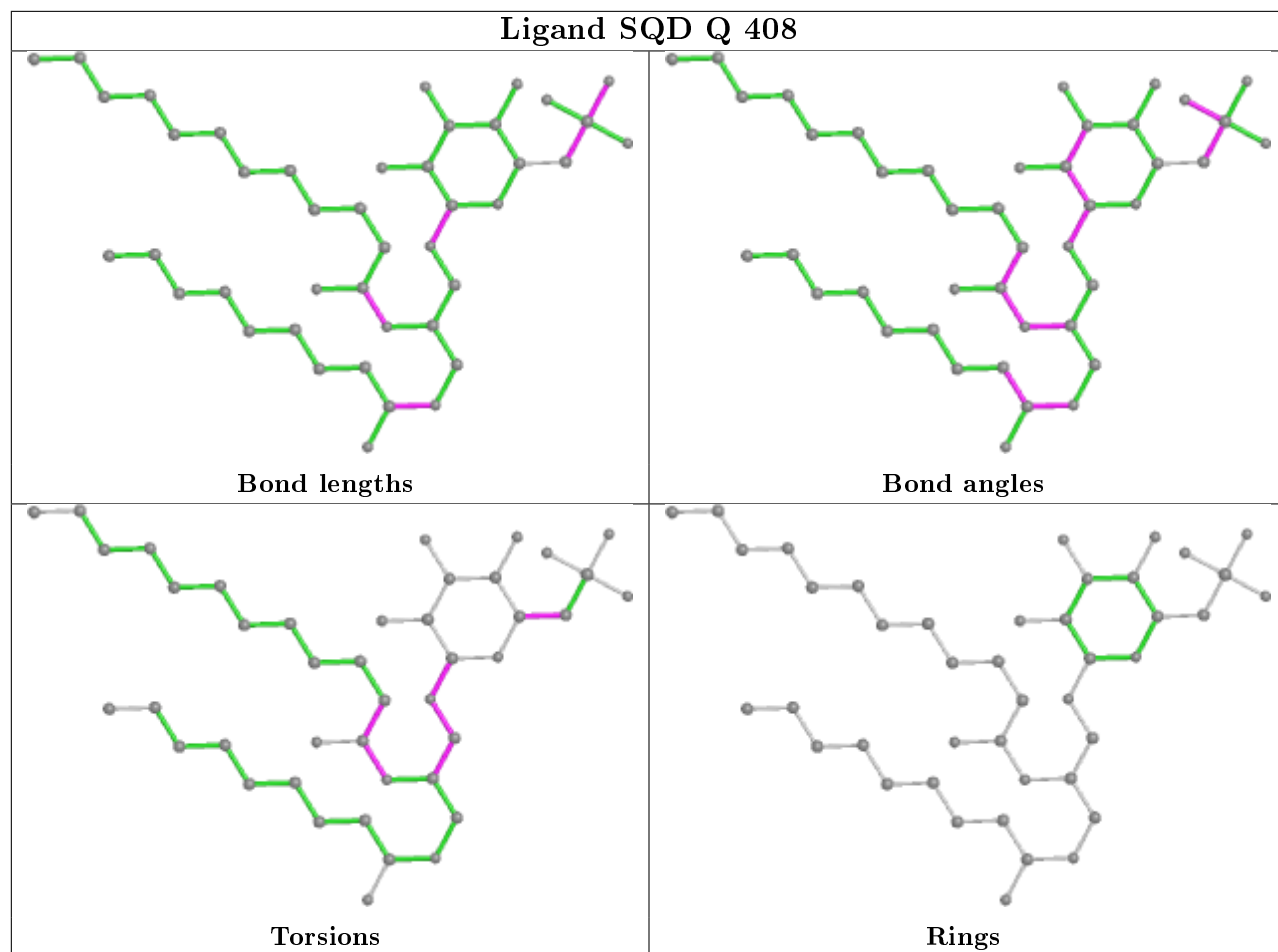


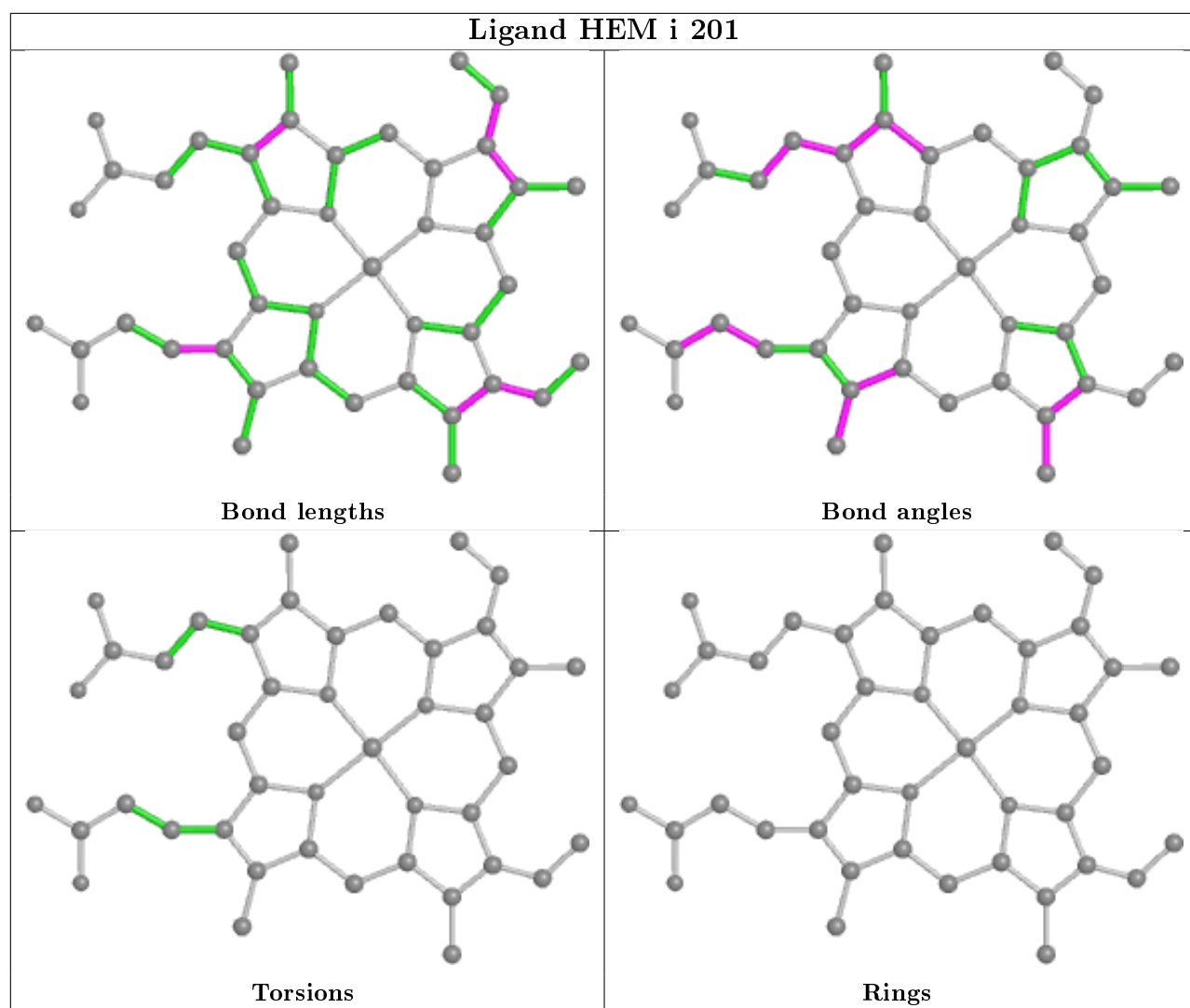
Ligand CLA N 606

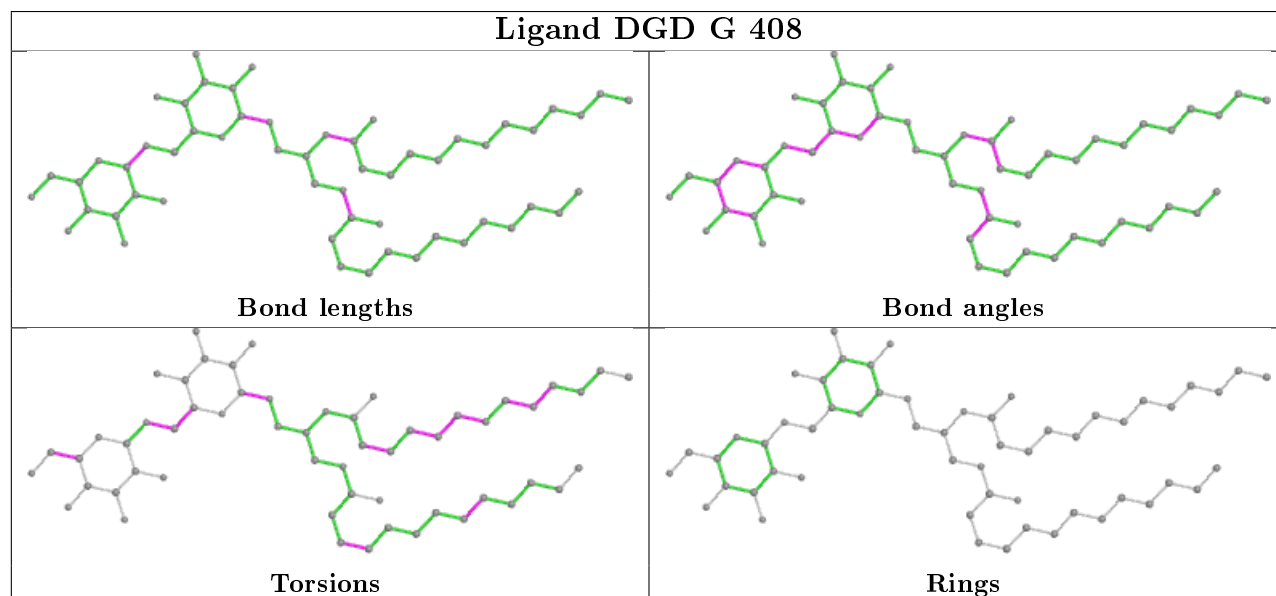
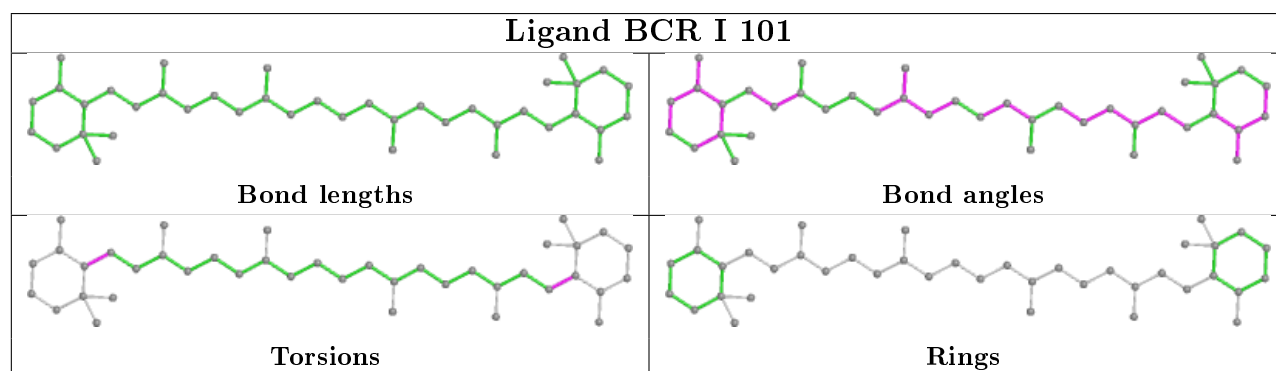
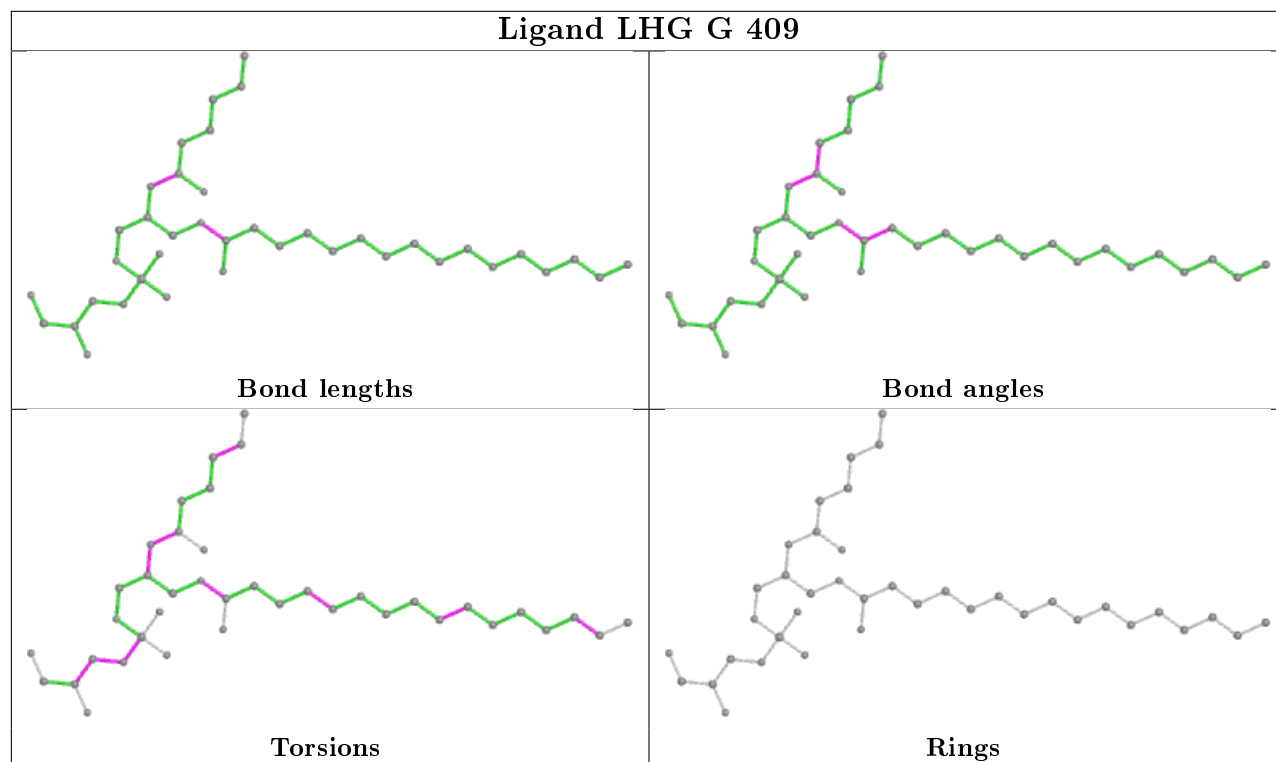


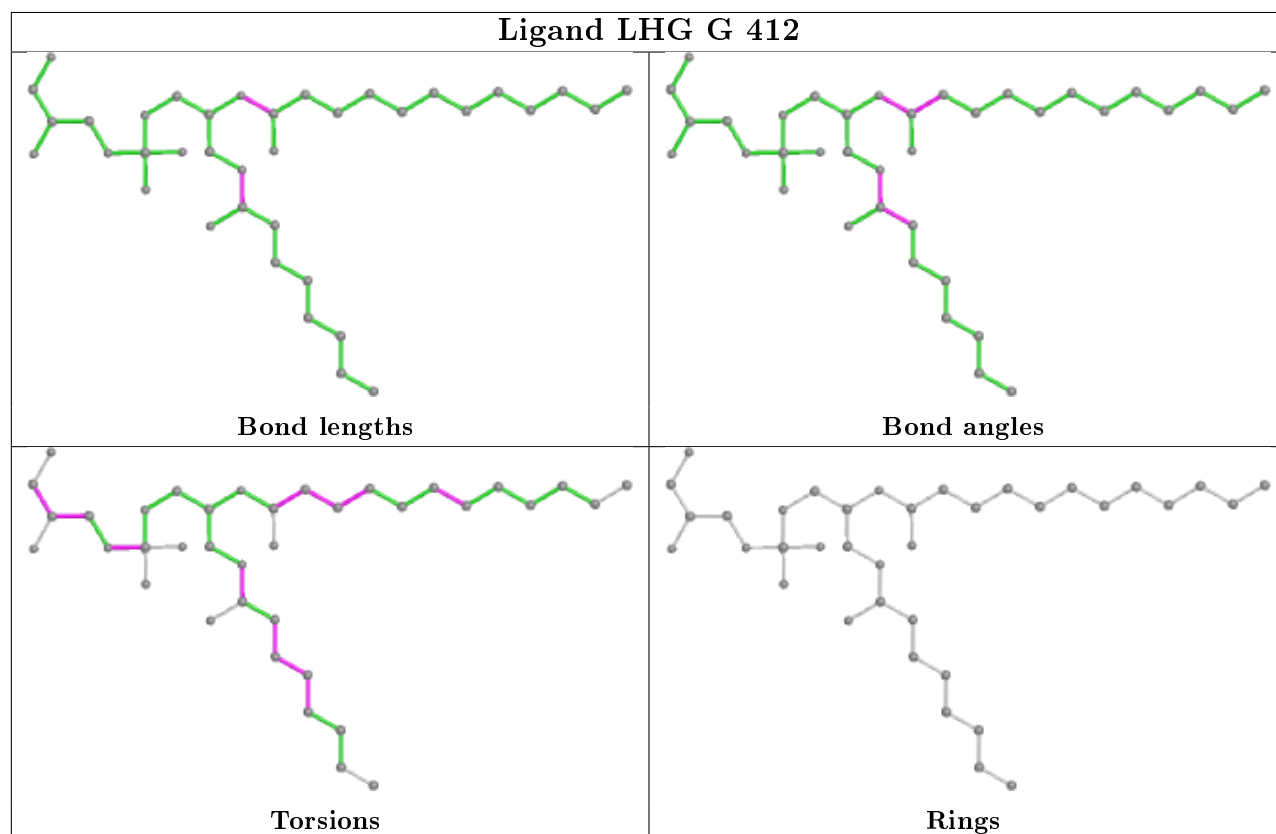
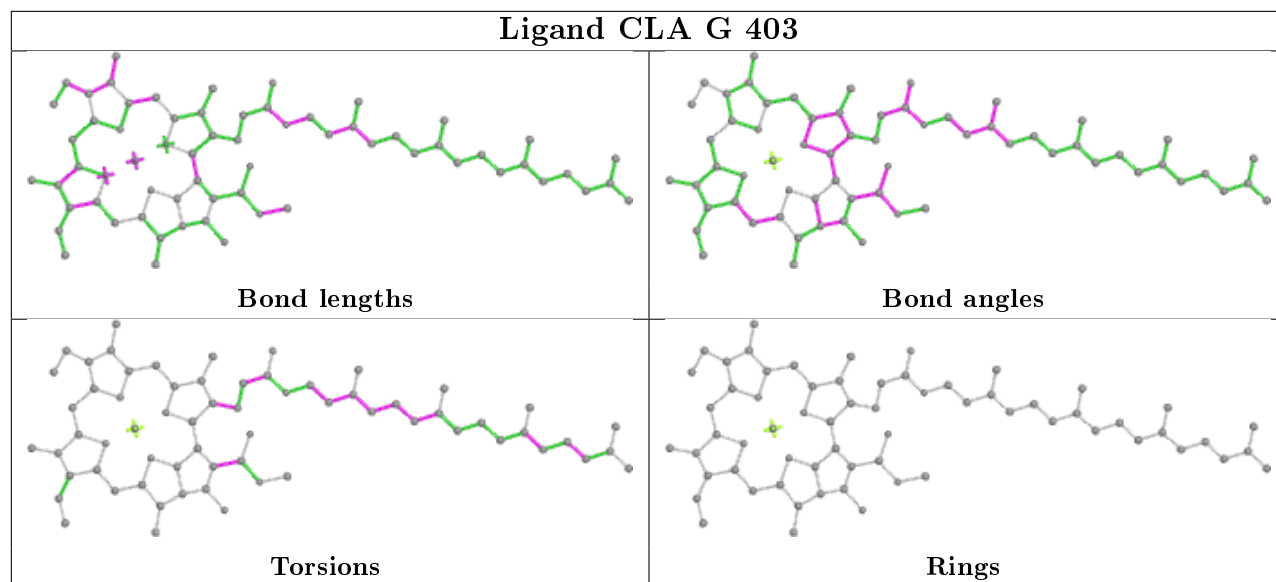


Ligand CLA P 503**Ligand LMG D 407**

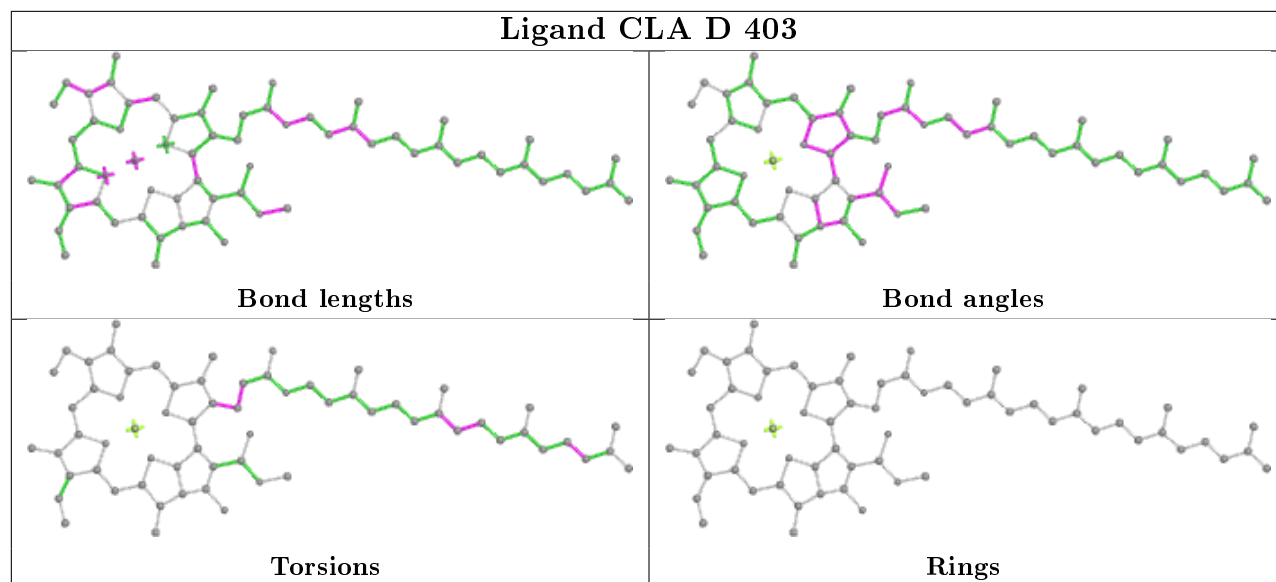




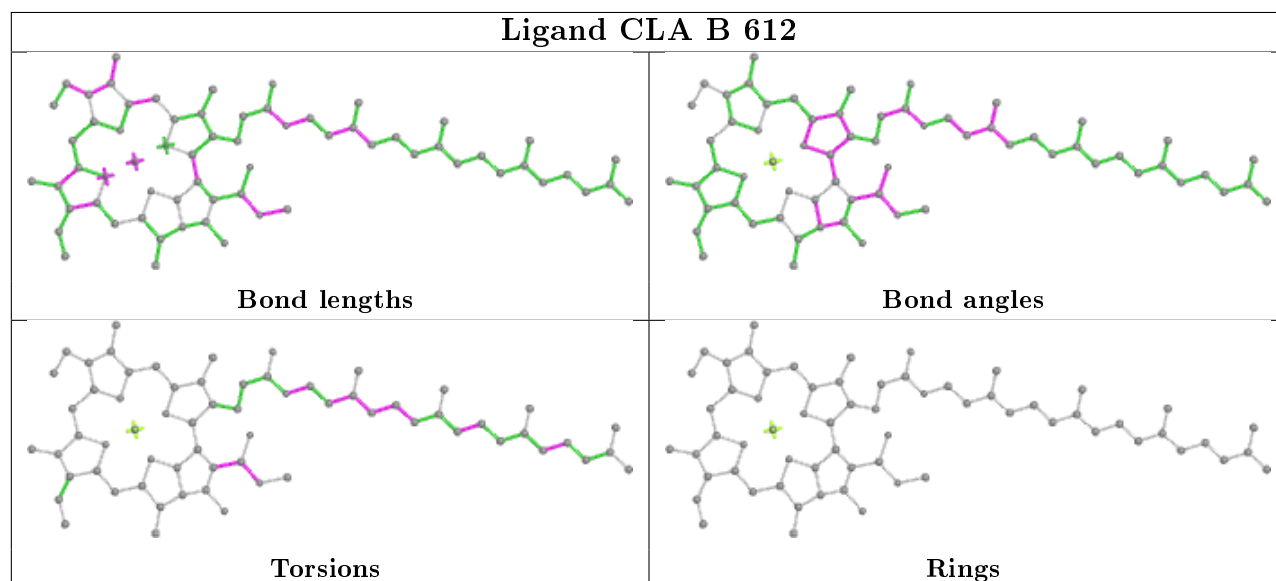




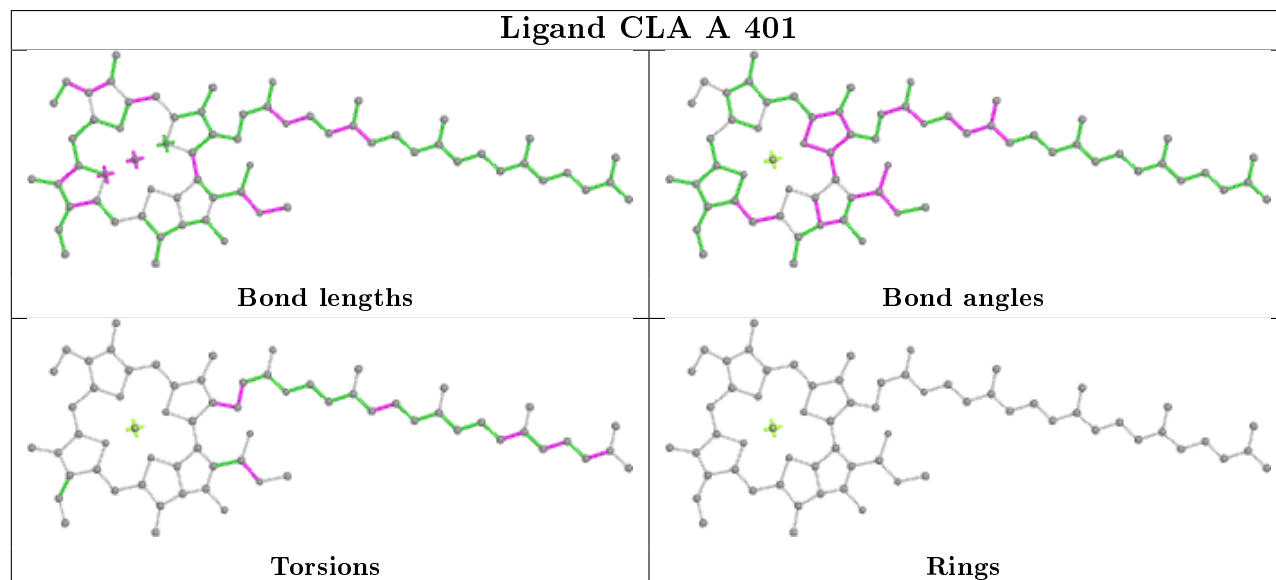
Ligand CLA D 403

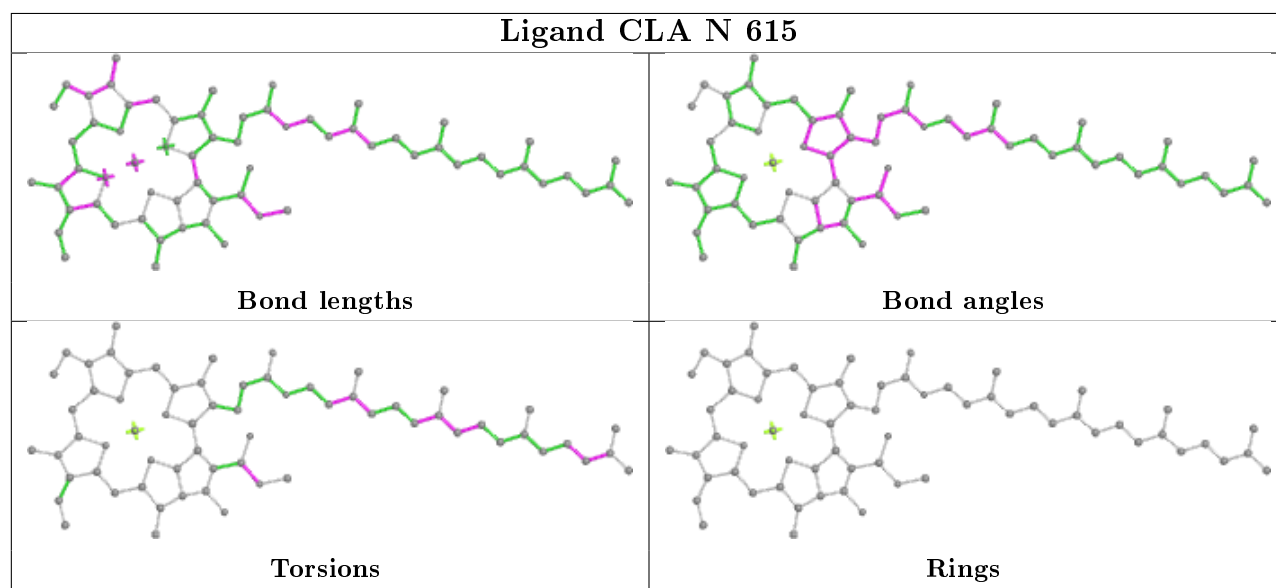
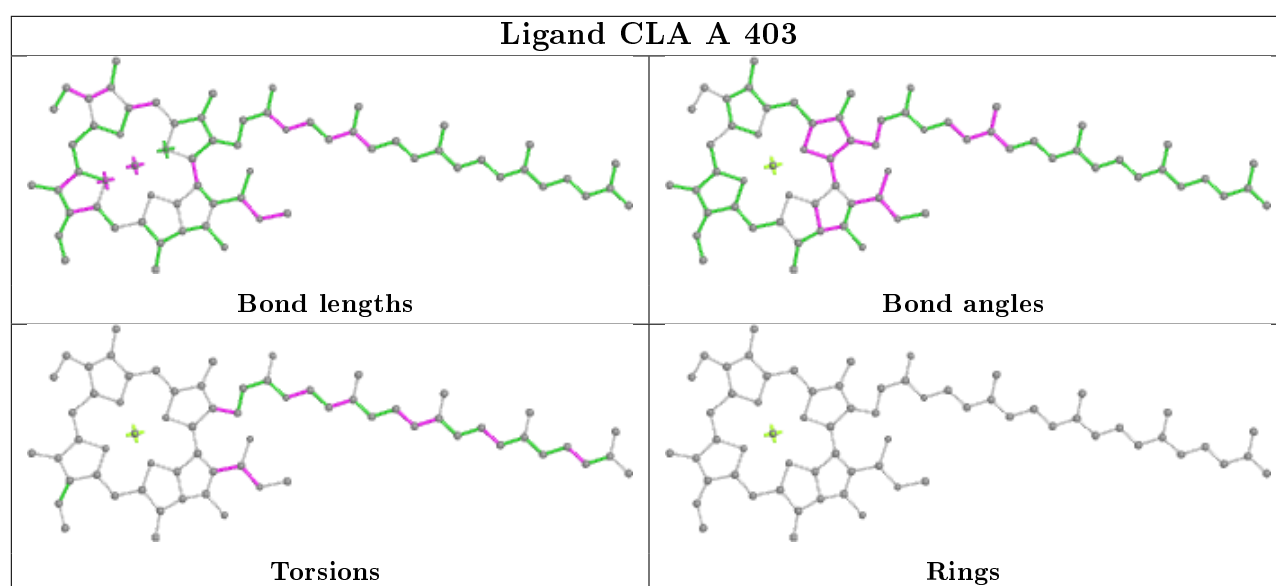
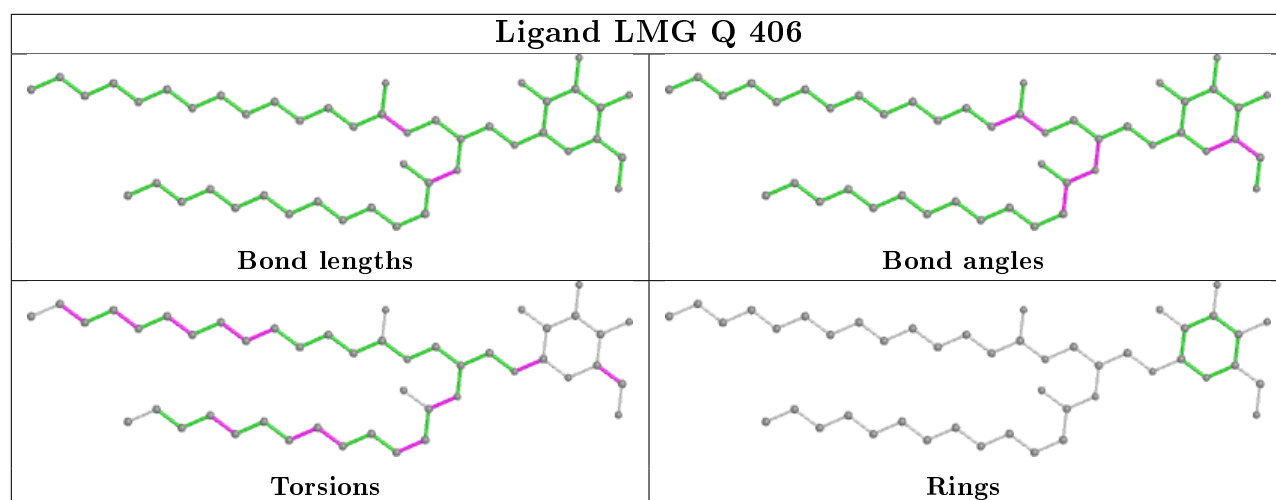


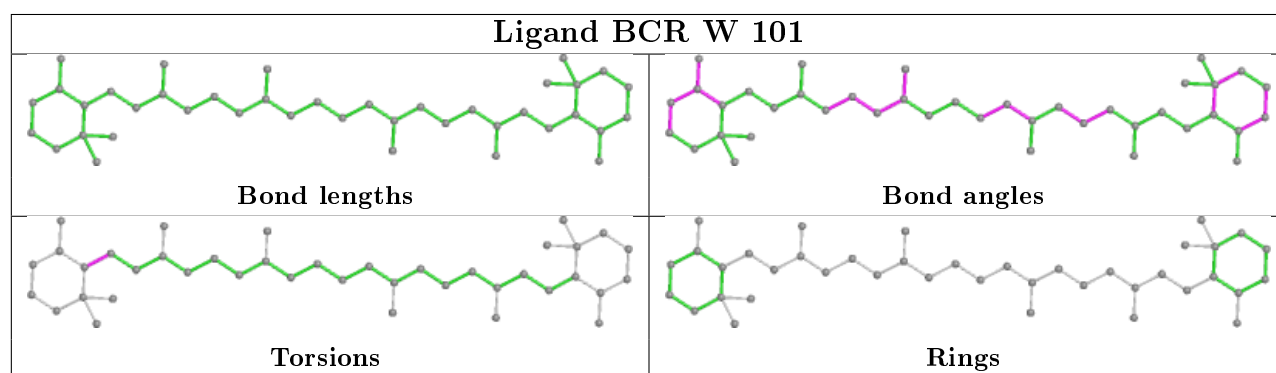
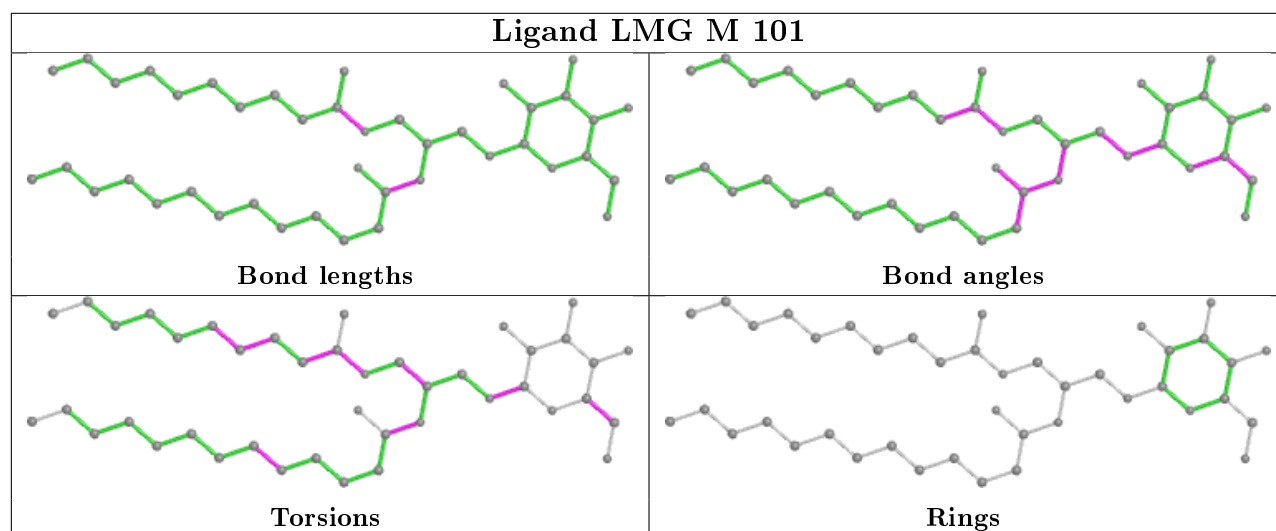
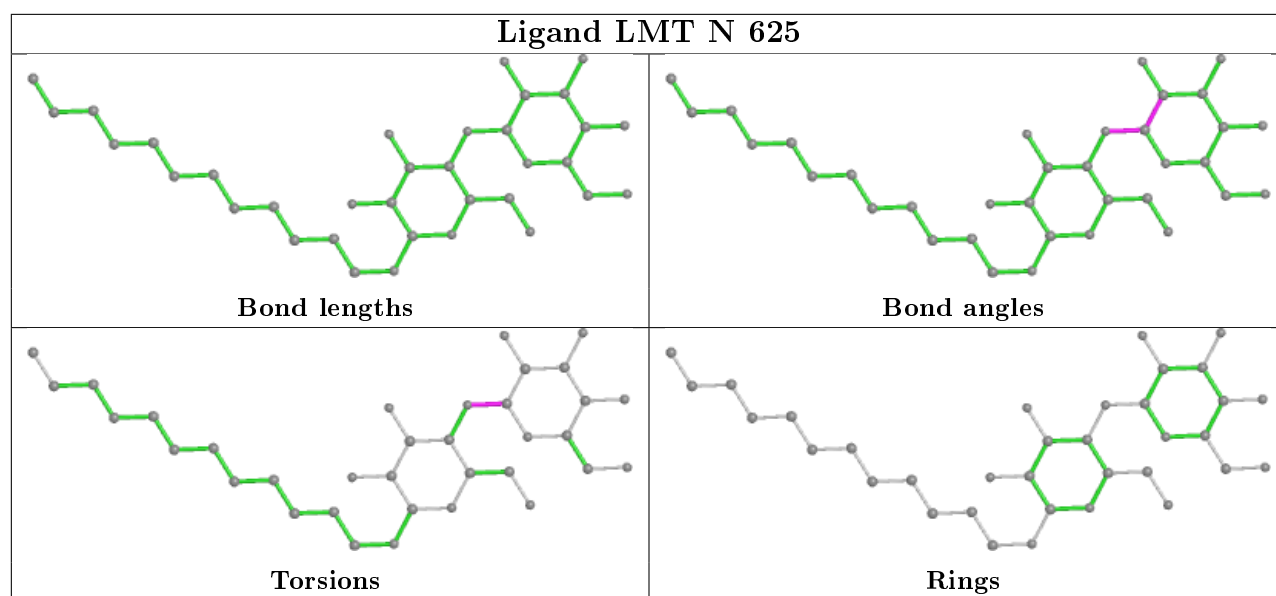
Ligand CLA B 612

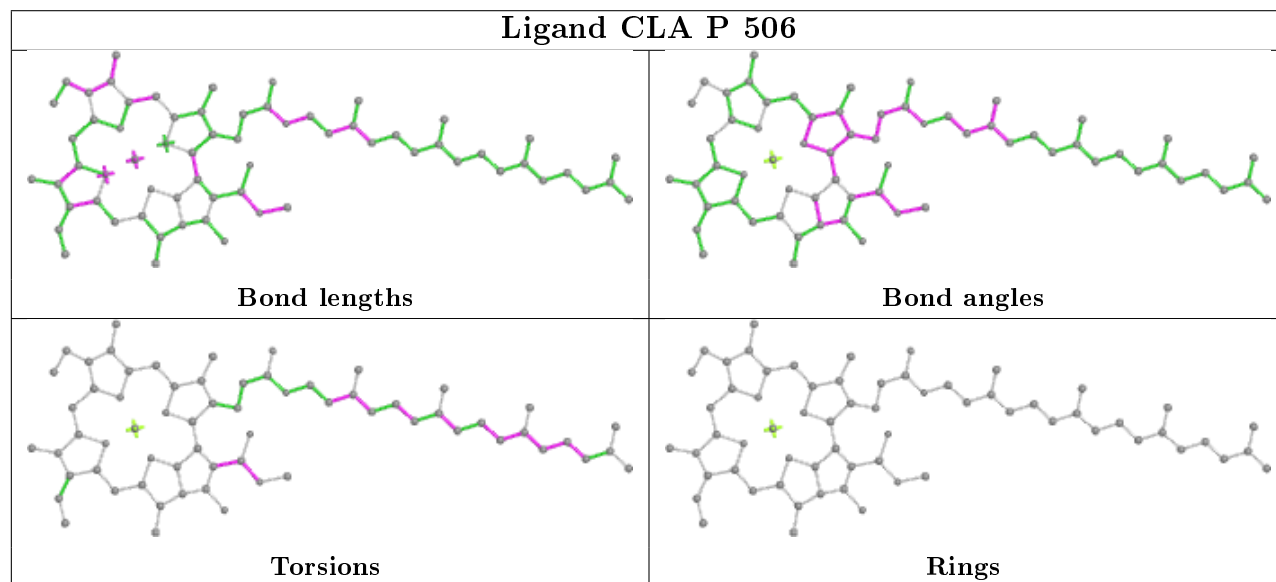
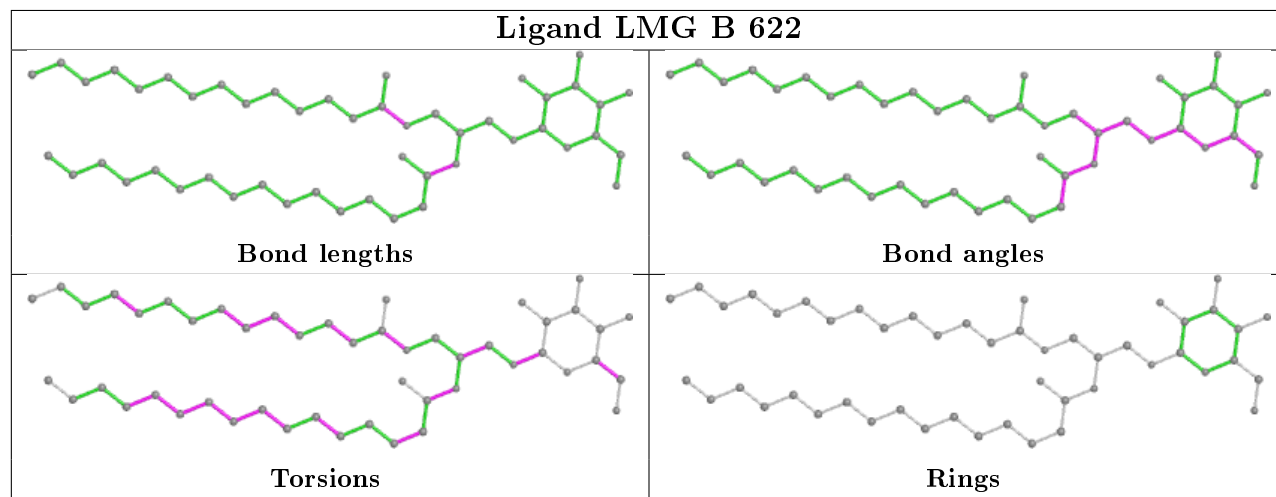
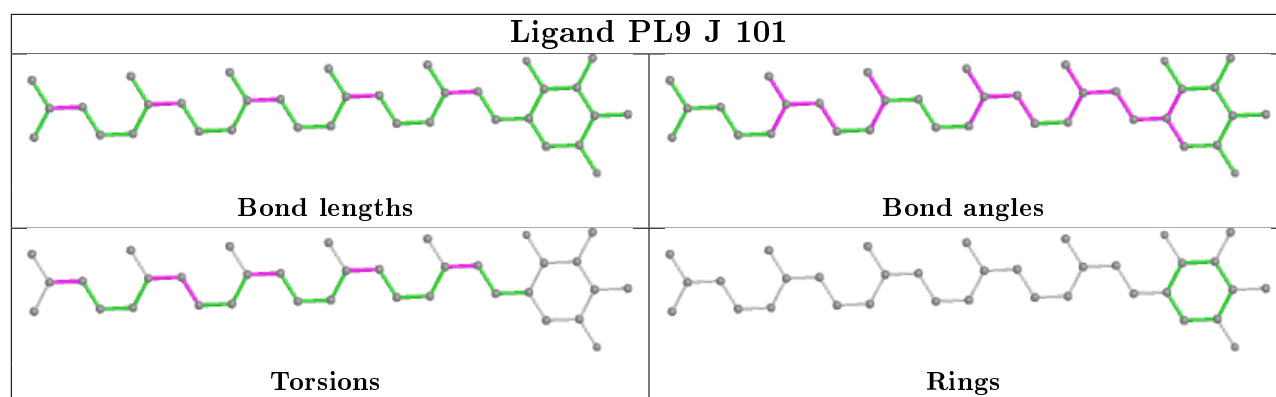


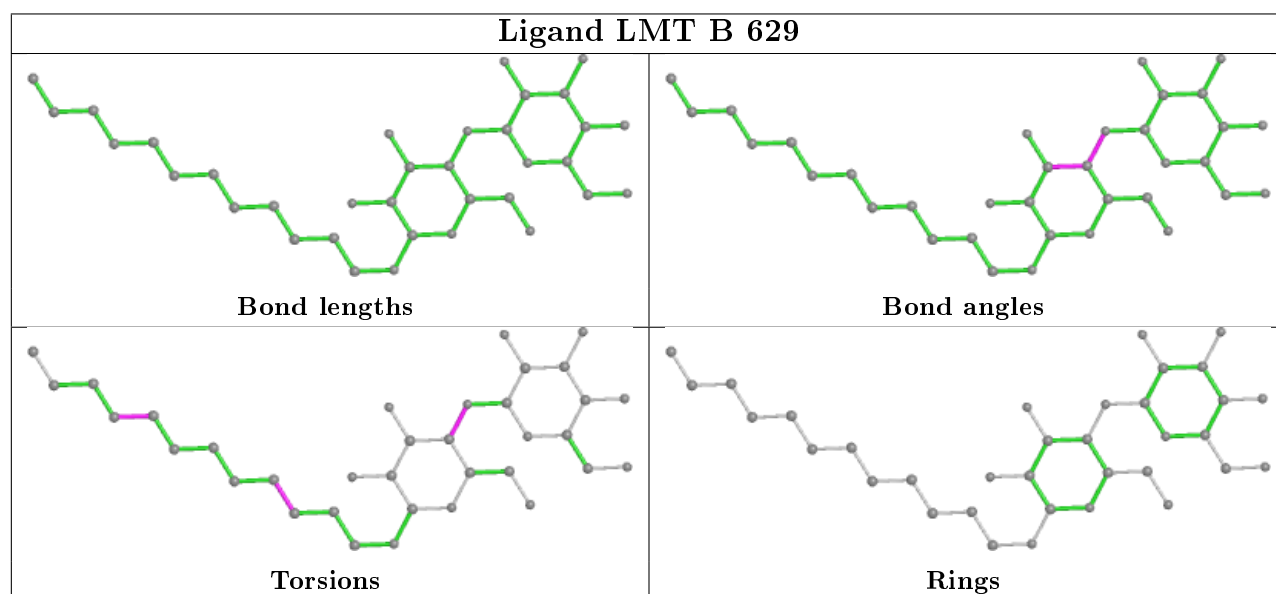
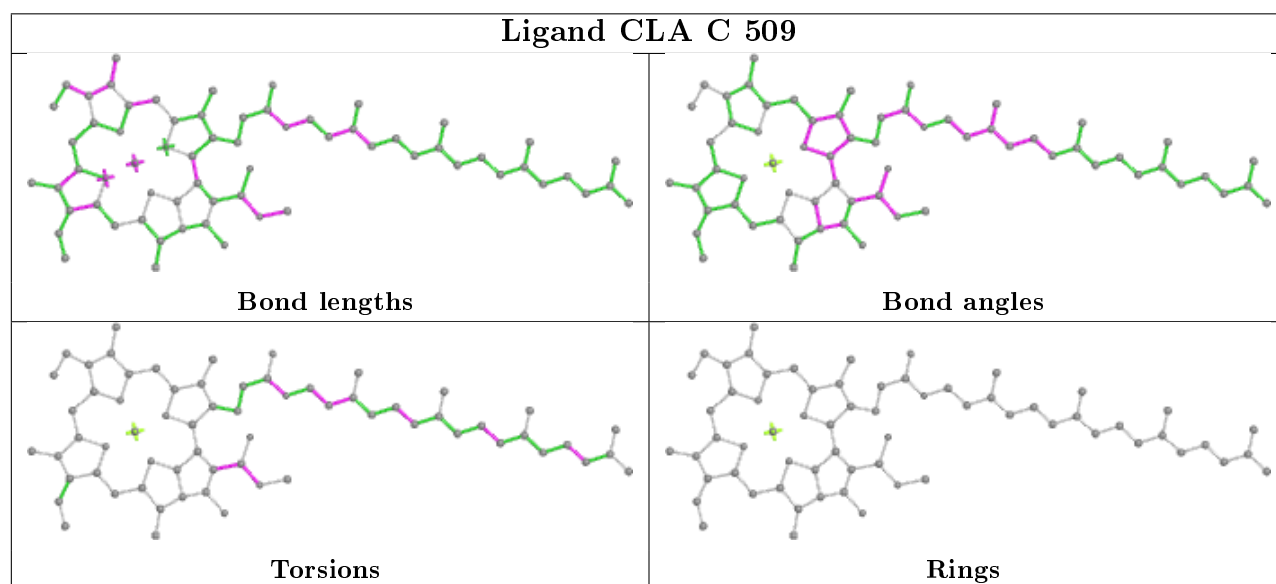
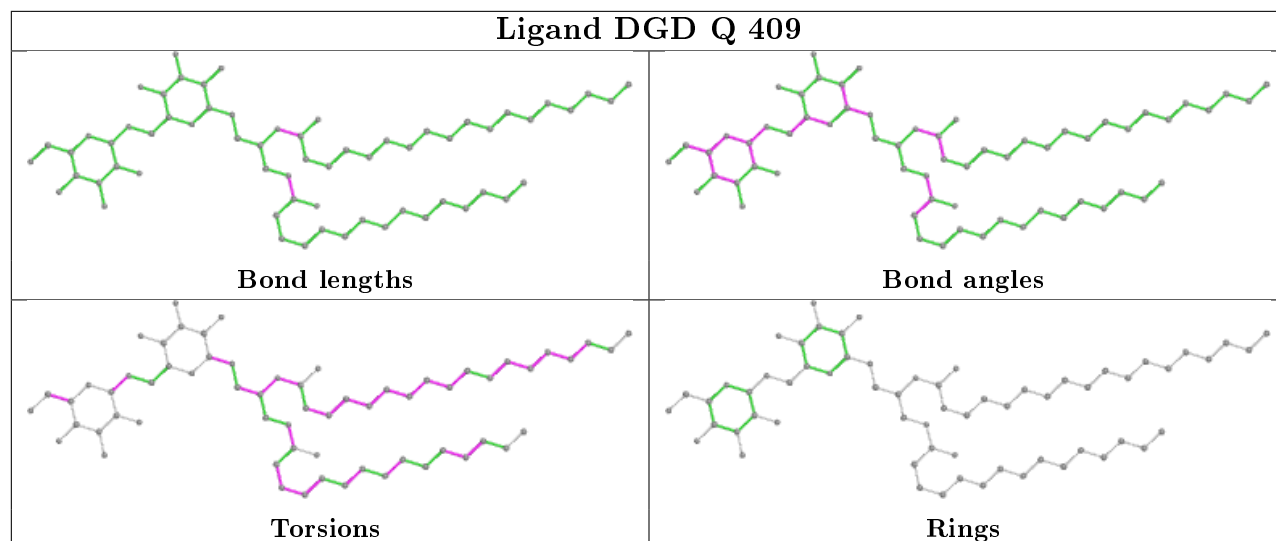
Ligand CLA A 401

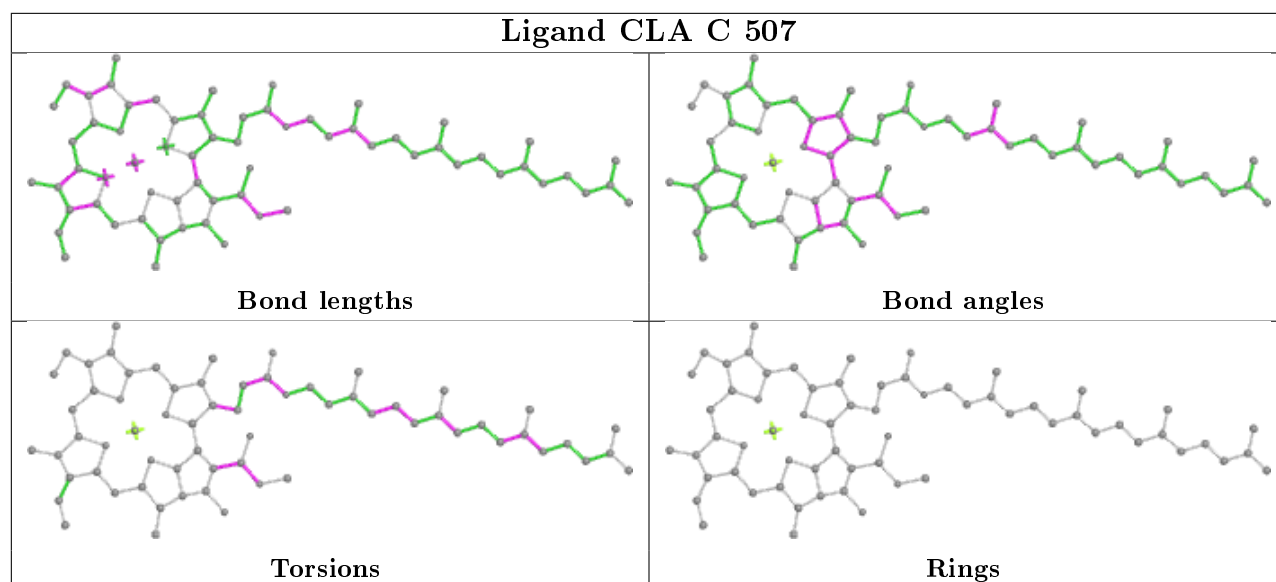
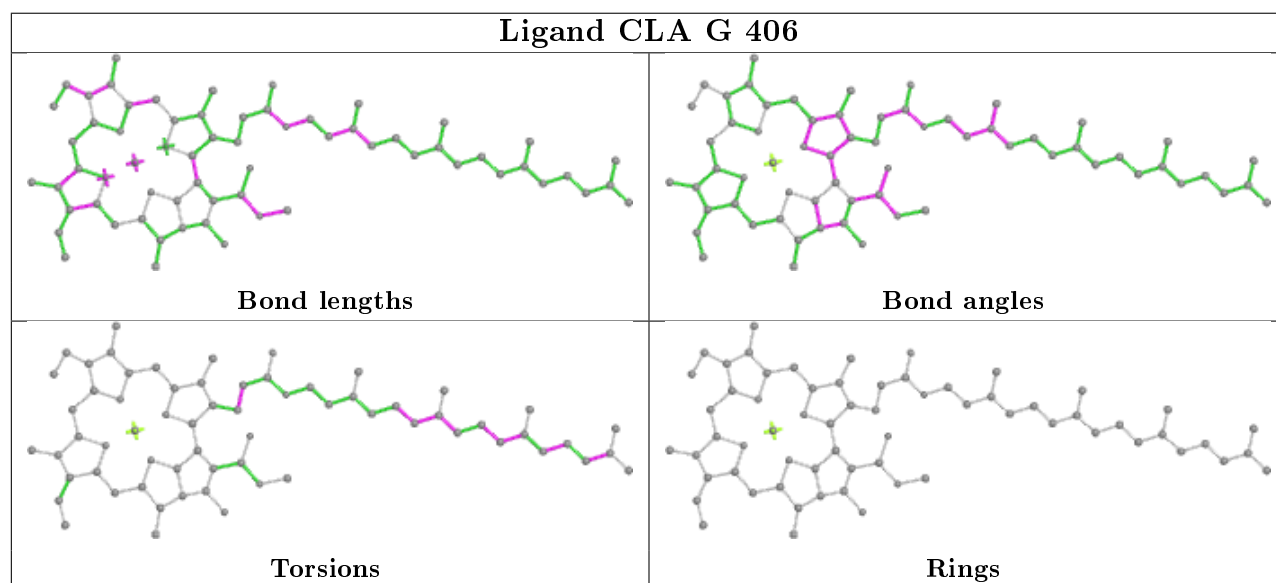
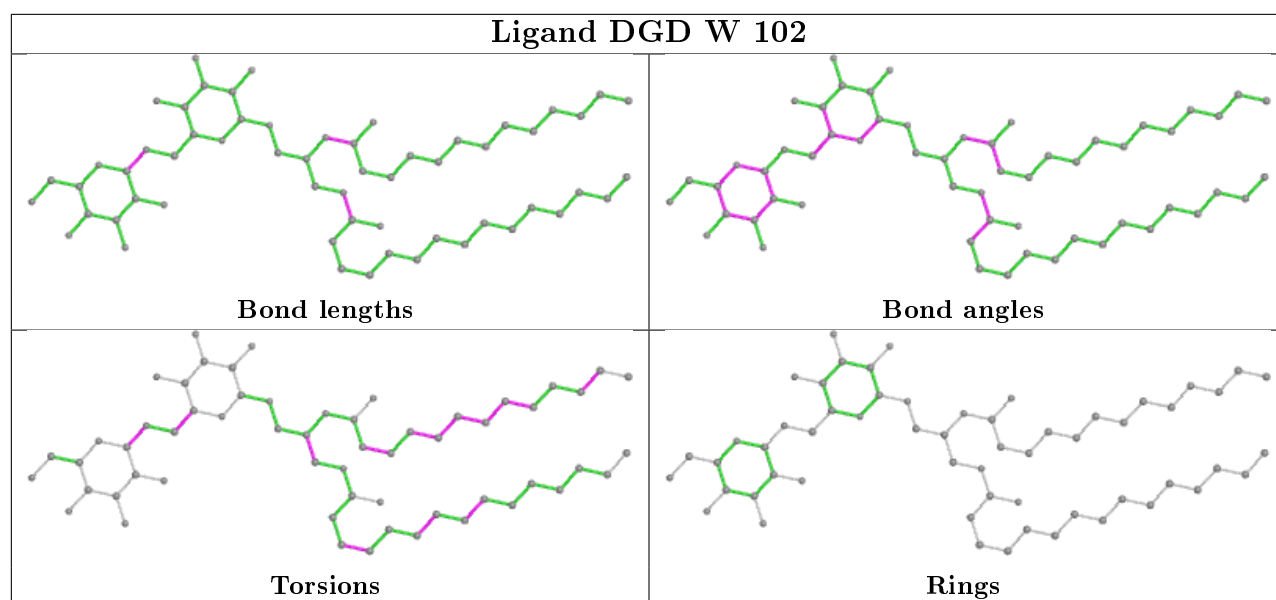




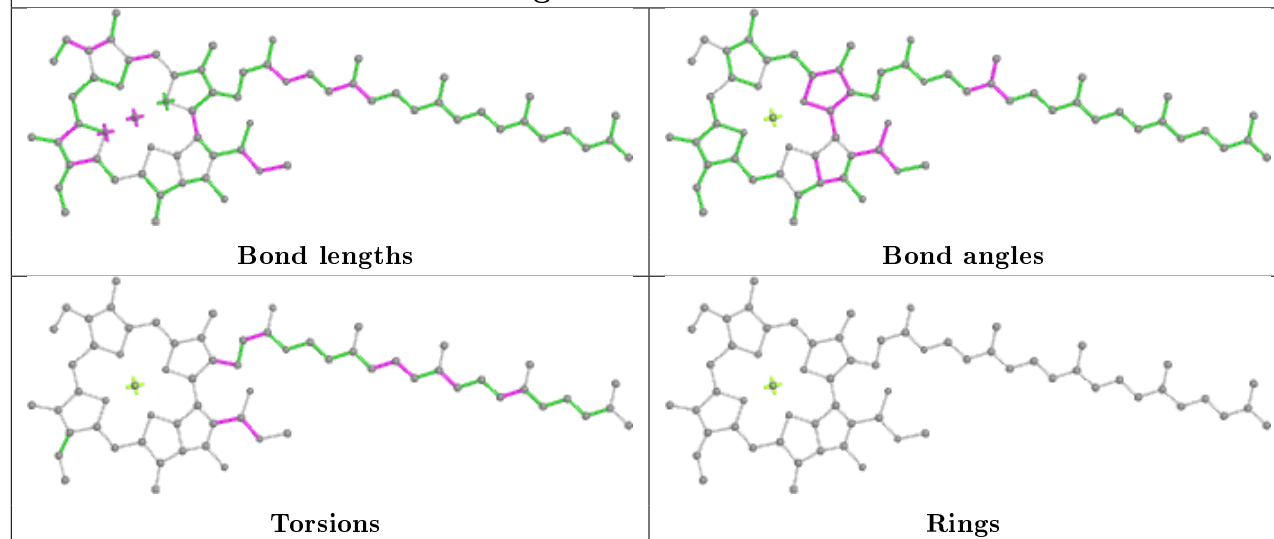




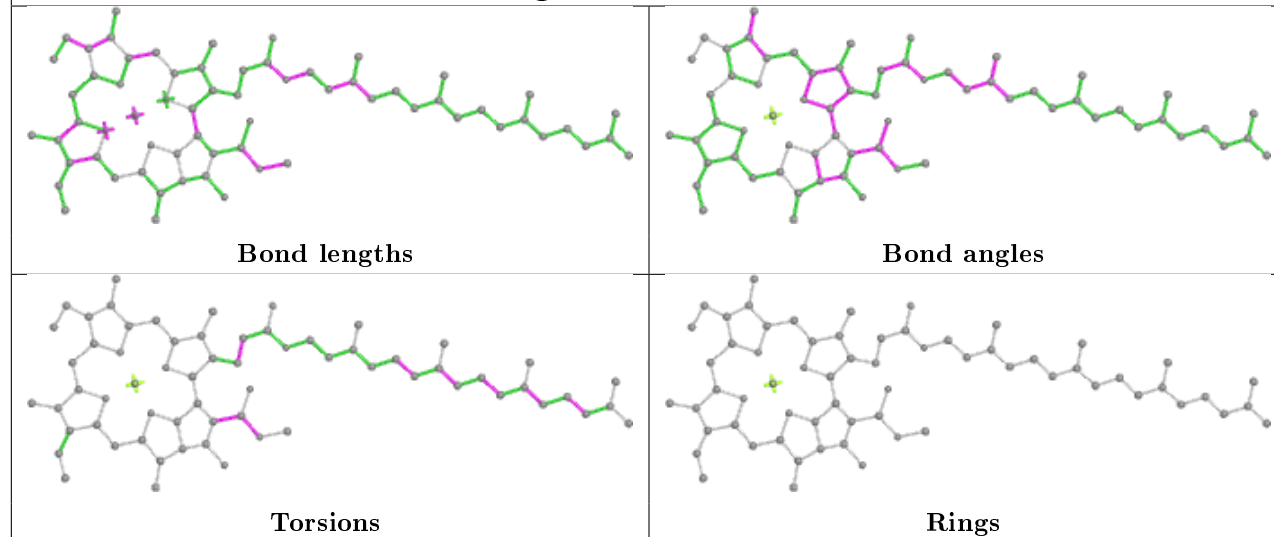




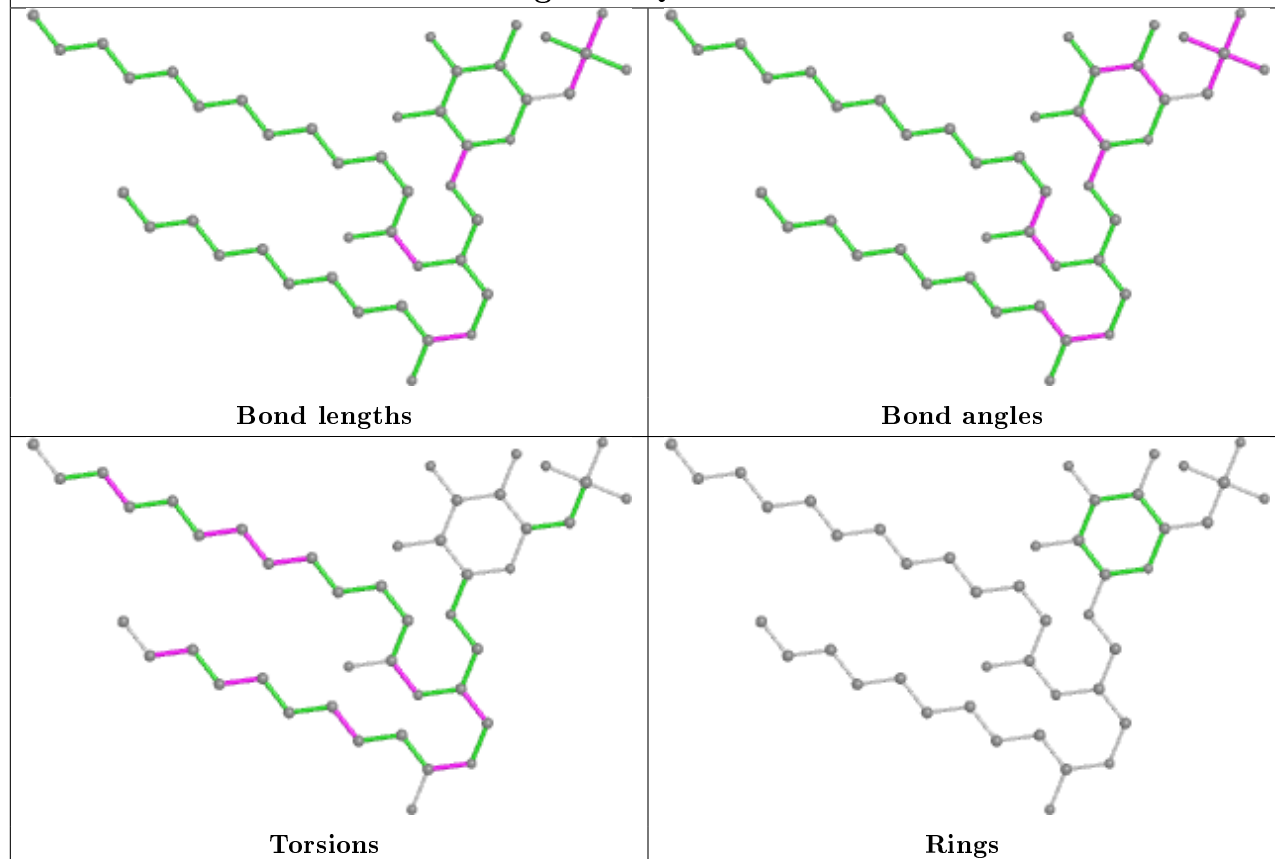
Ligand CLA P 507



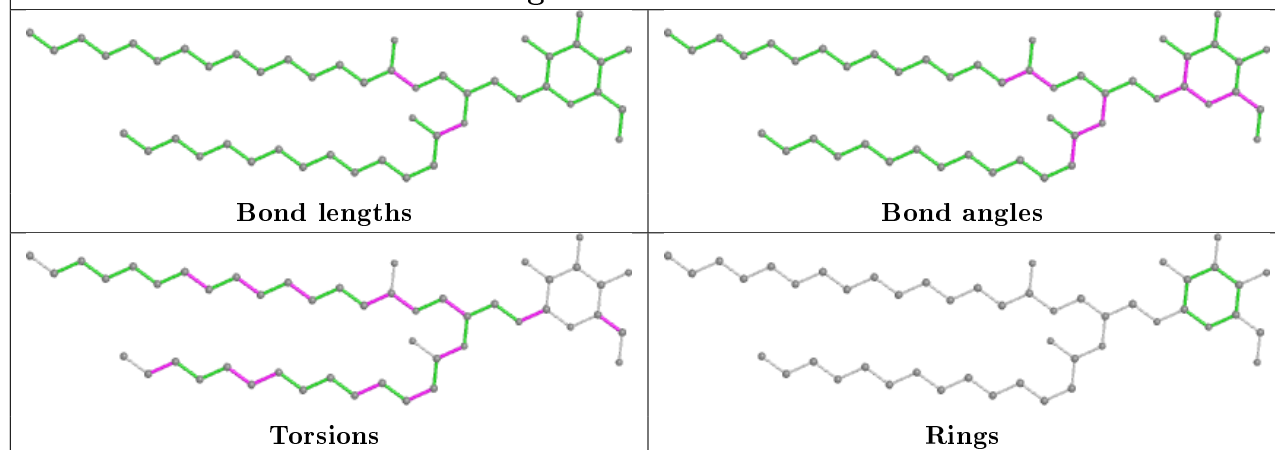
Ligand CLA P 508

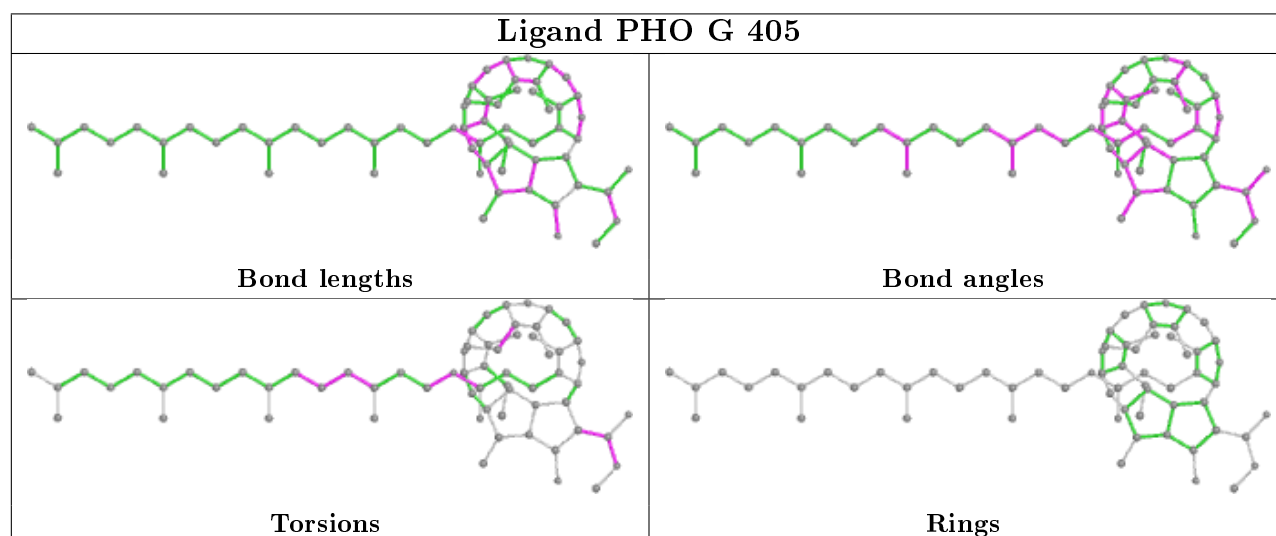
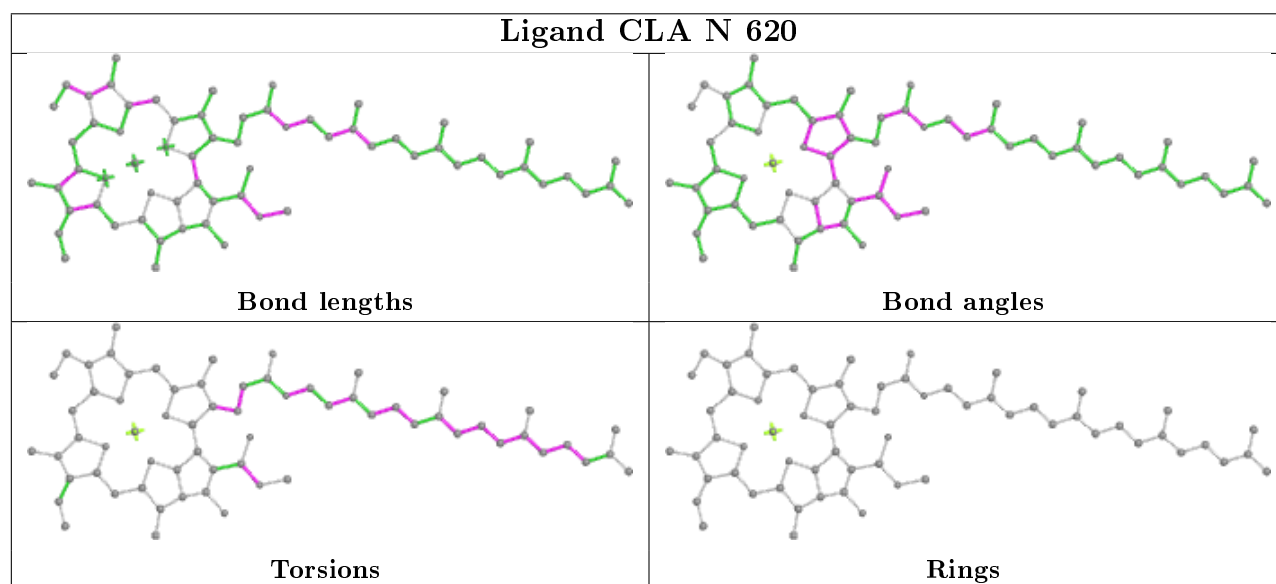
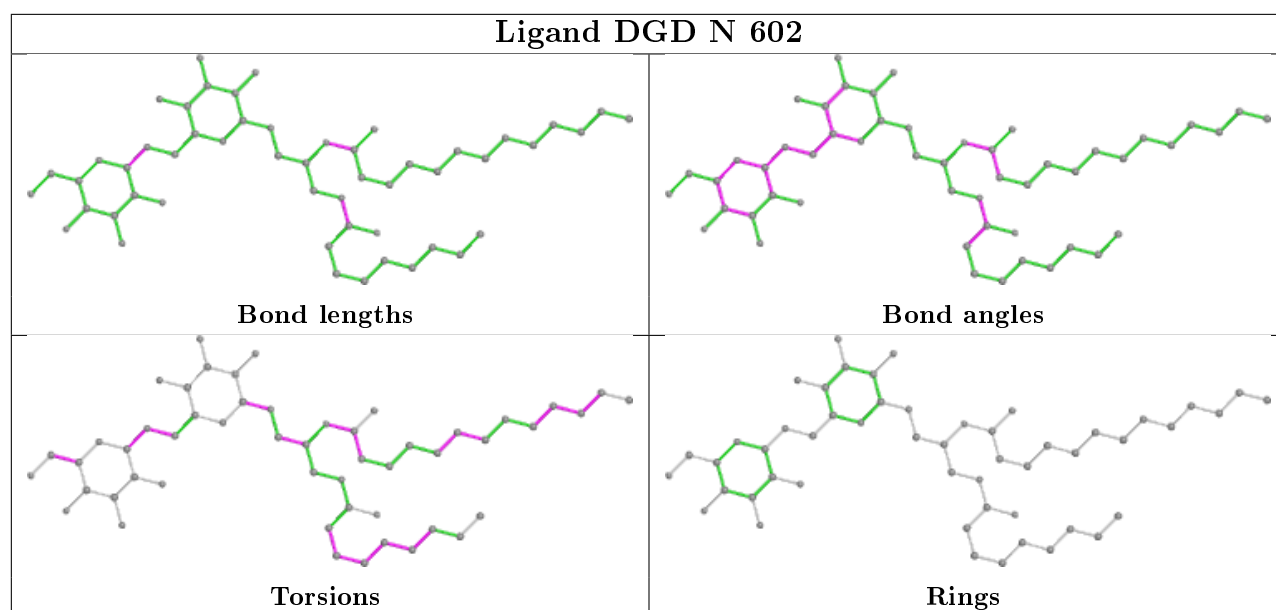


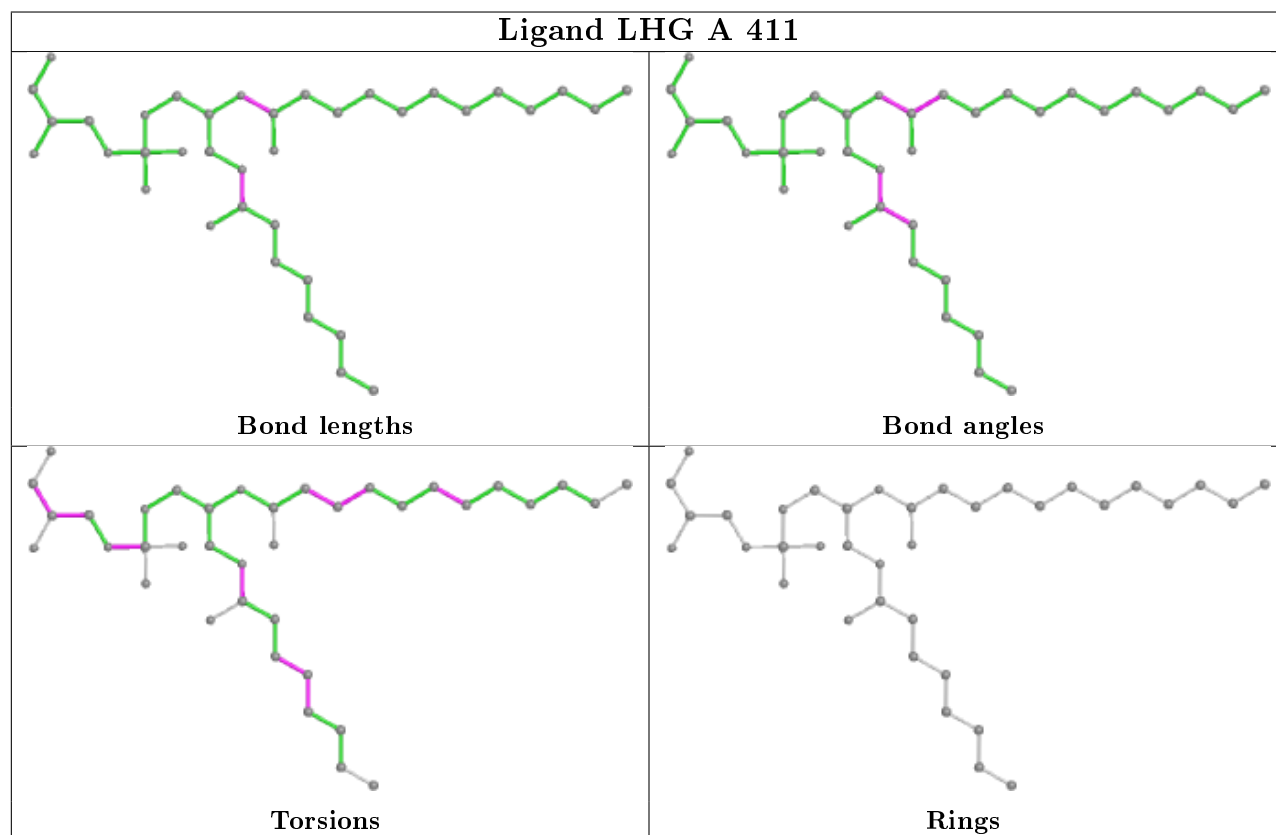
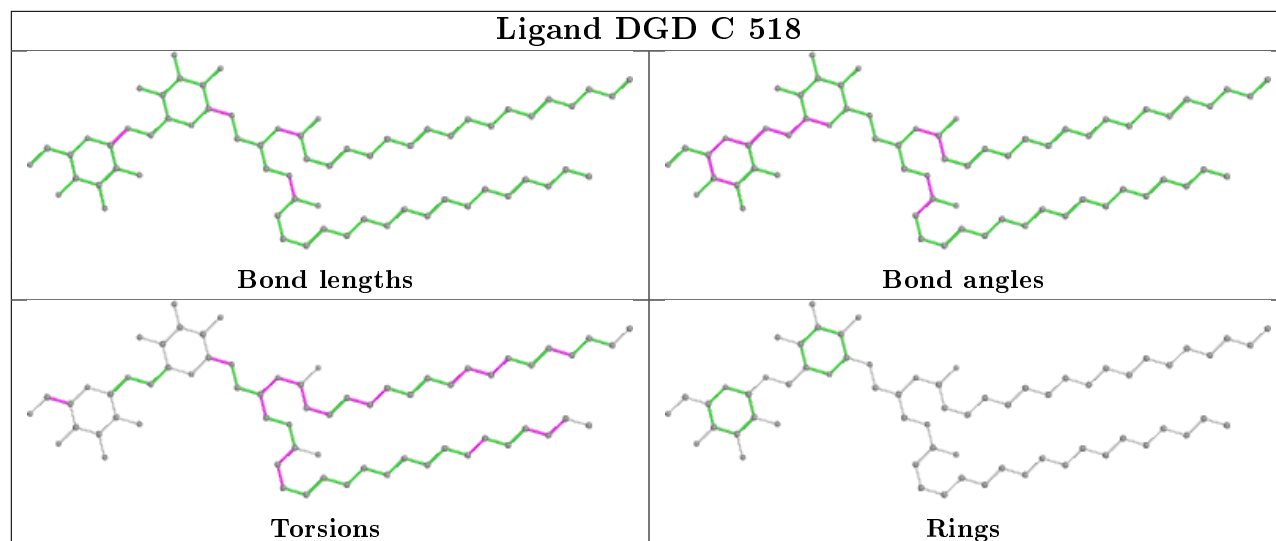
Ligand SQD S 102

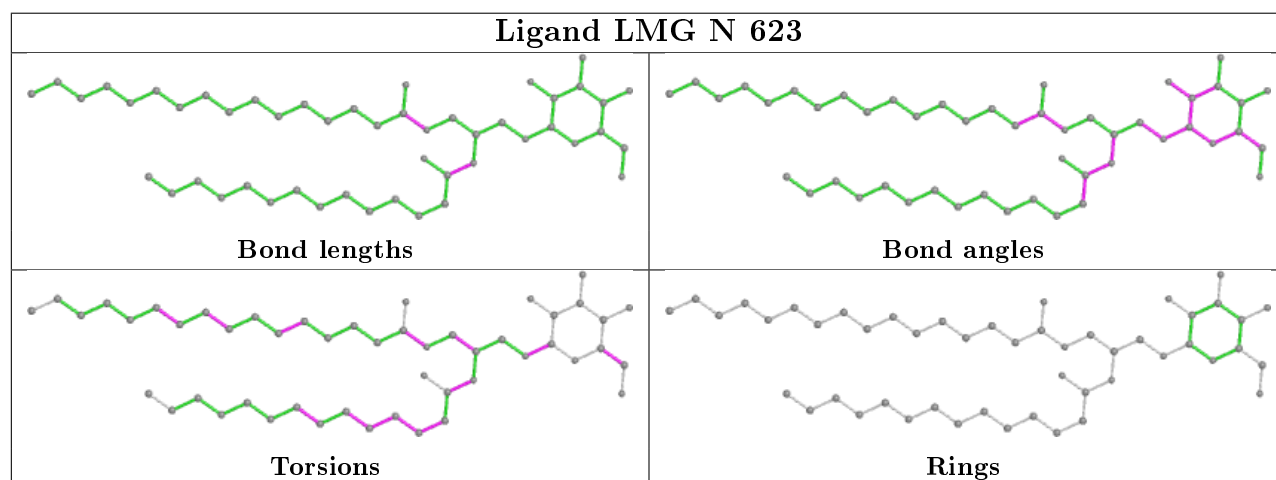
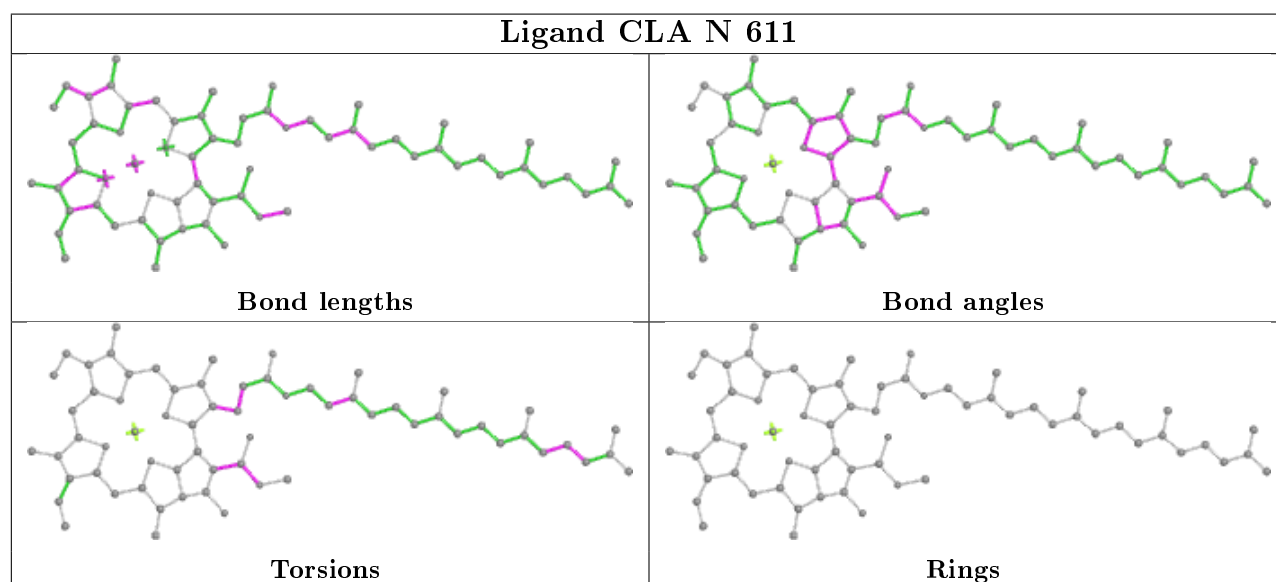
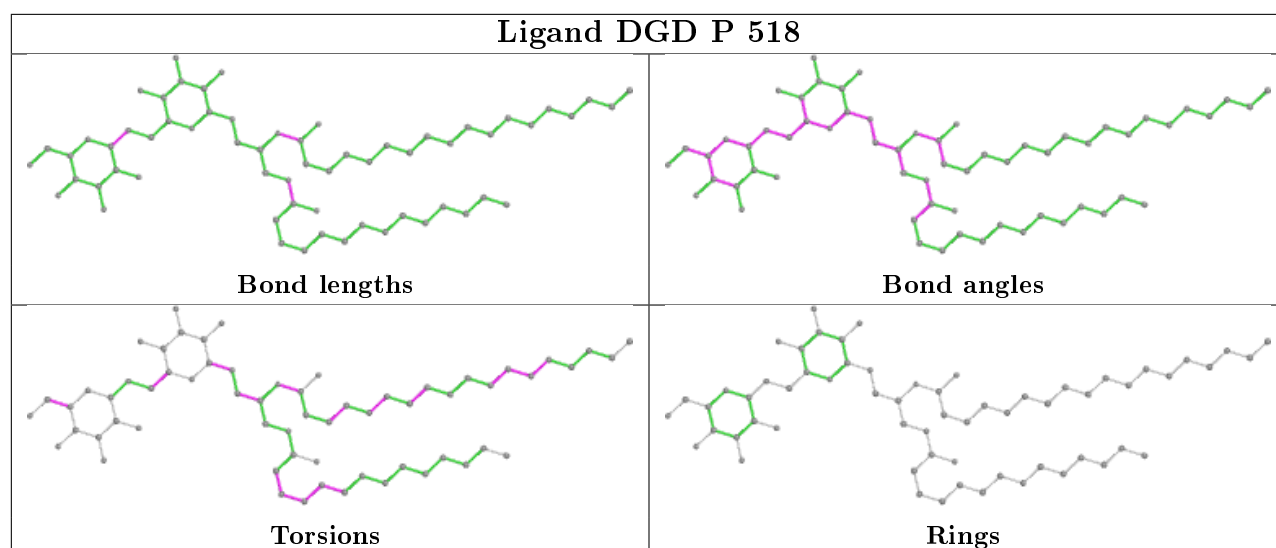


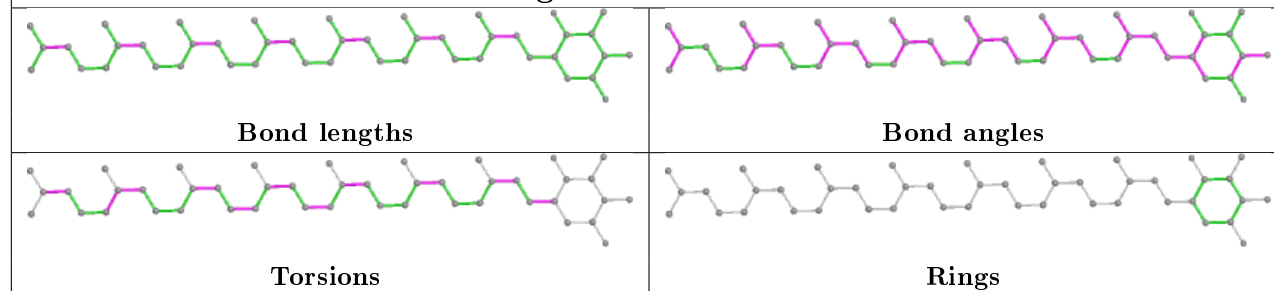
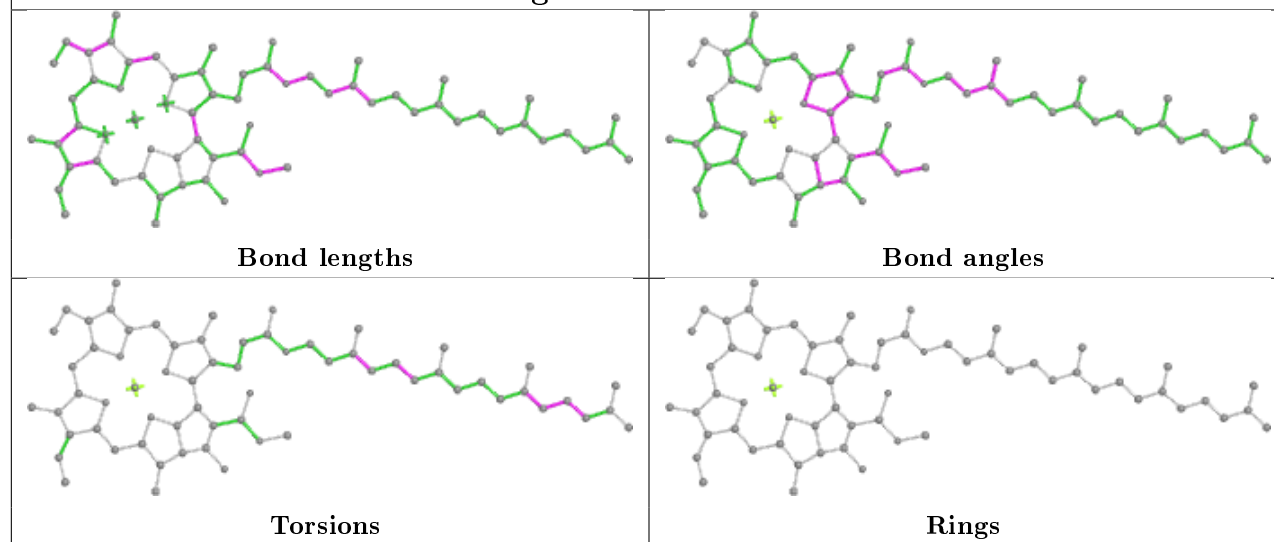
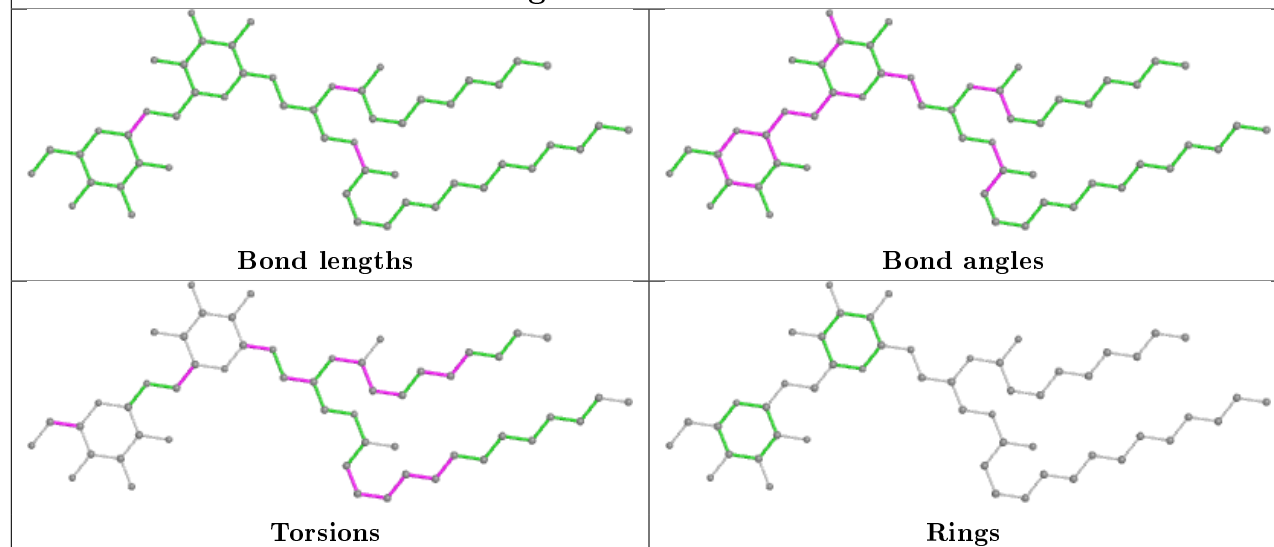
Ligand LMG C 519

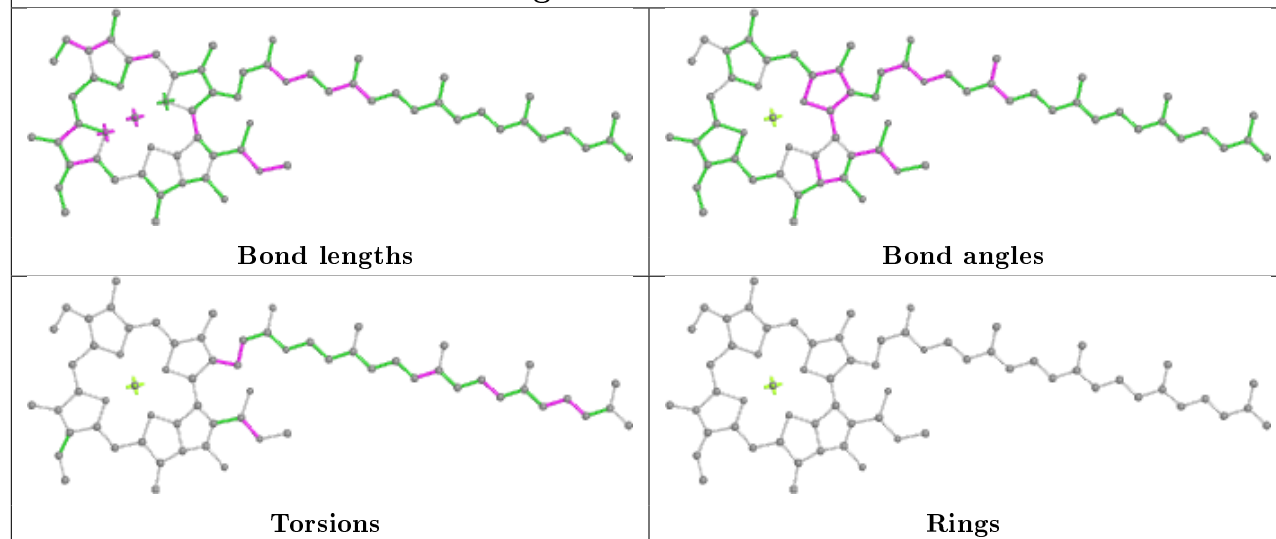
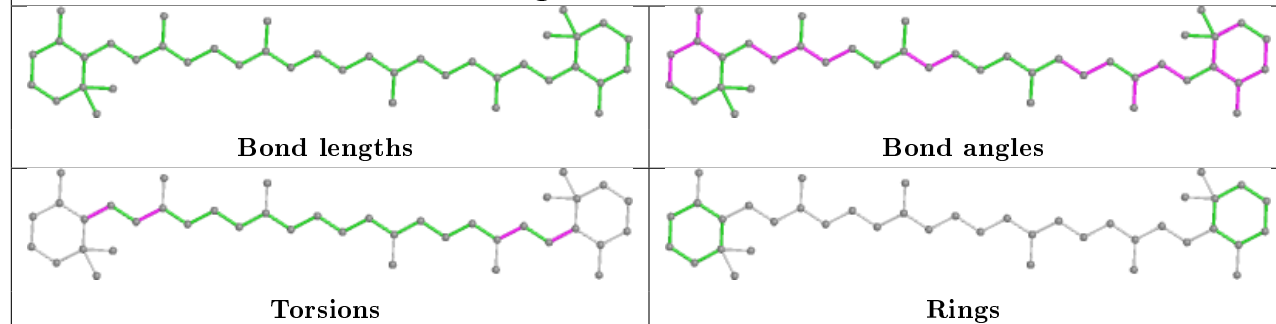
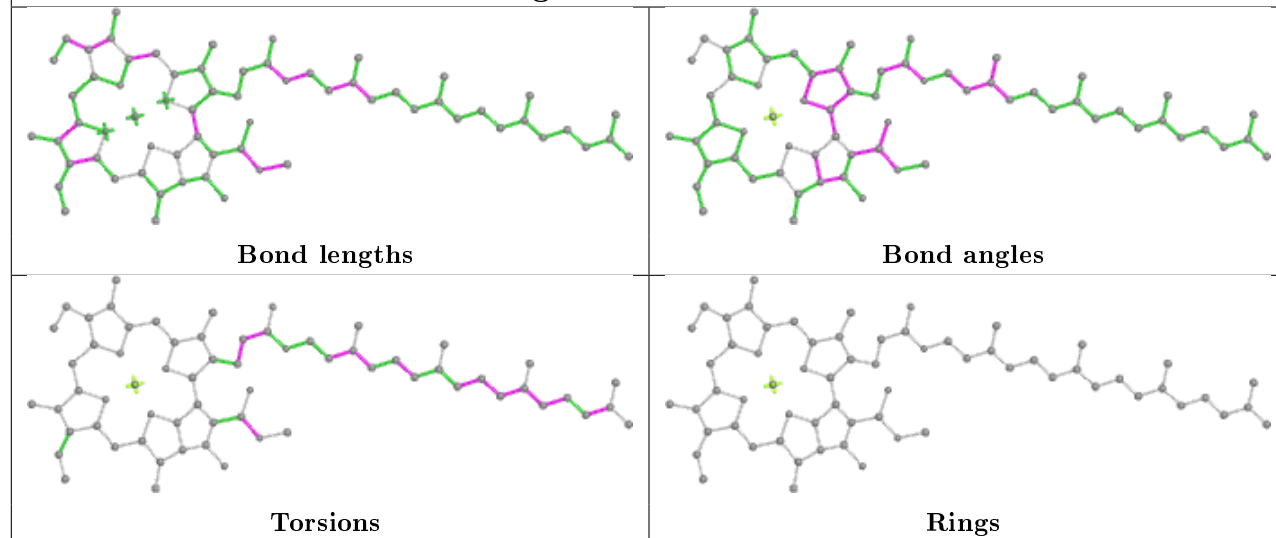


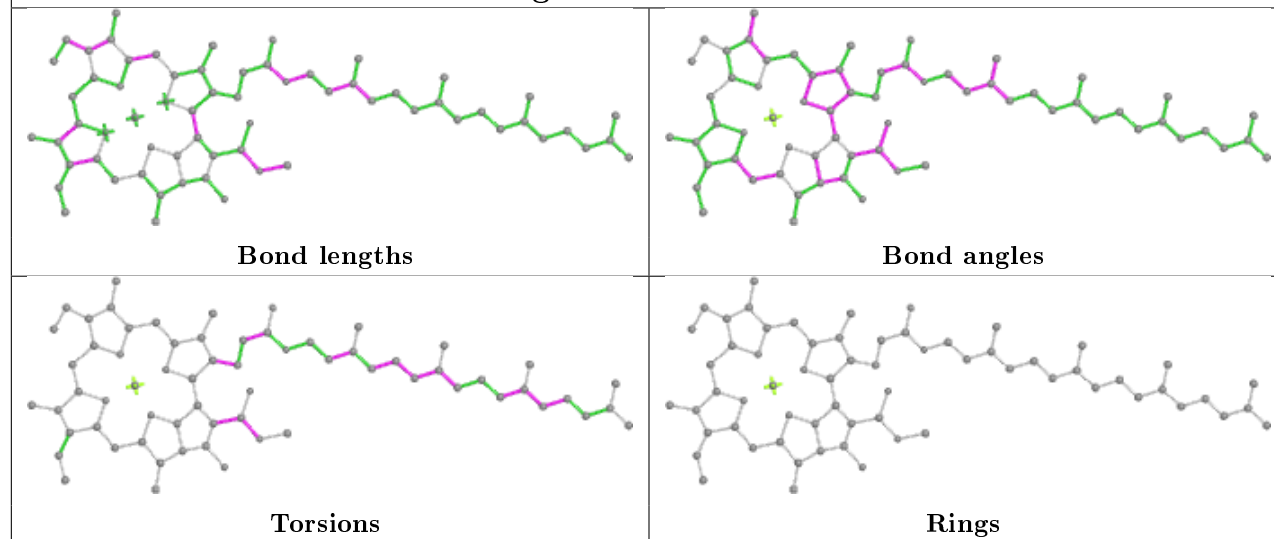
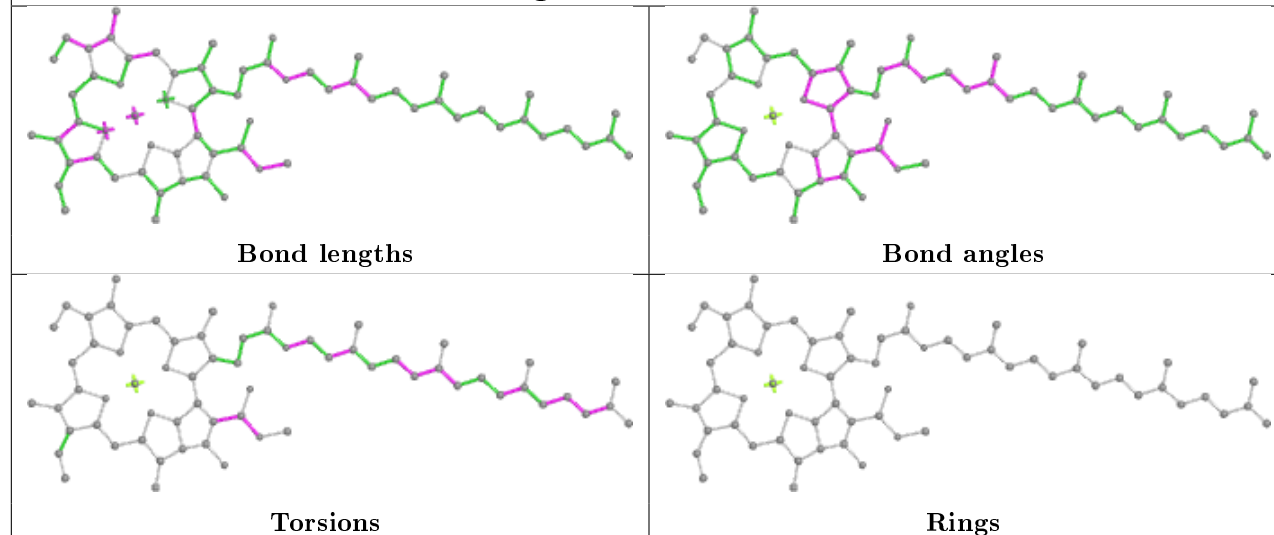
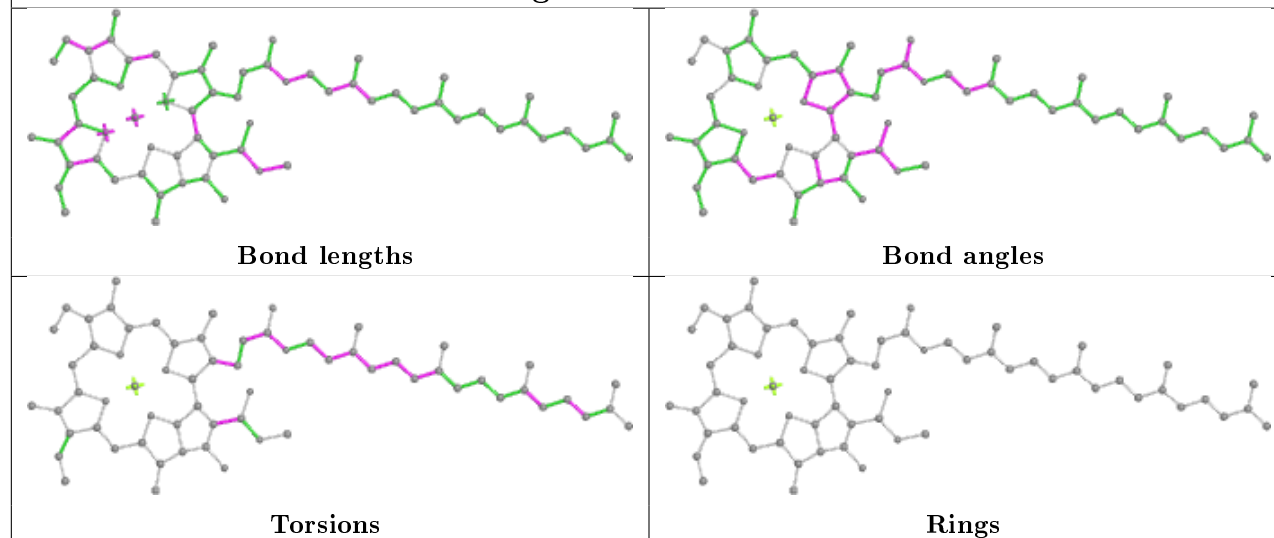


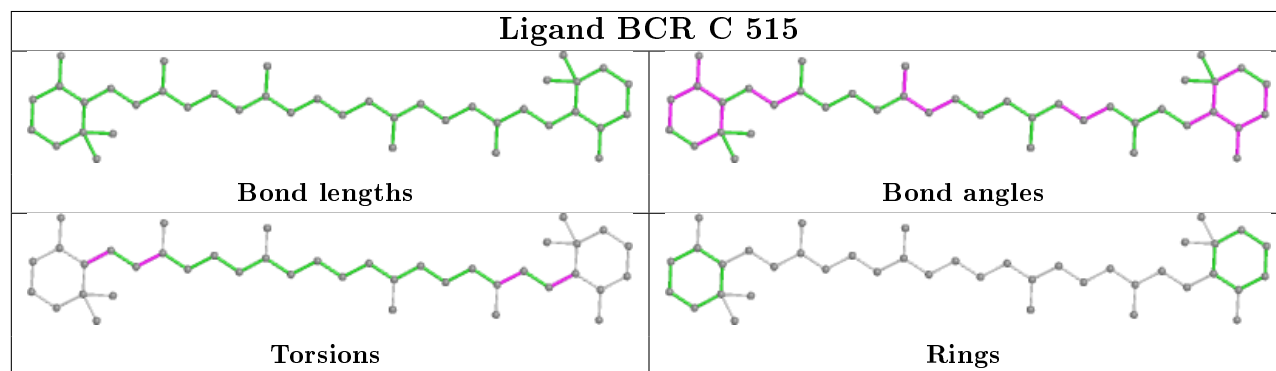
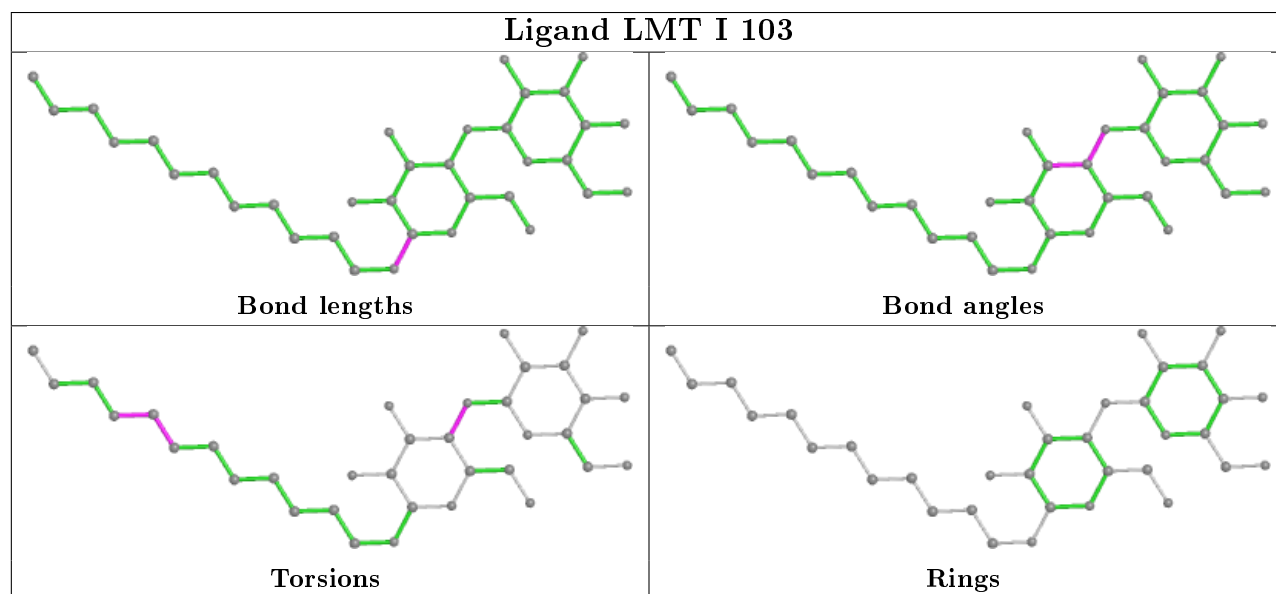
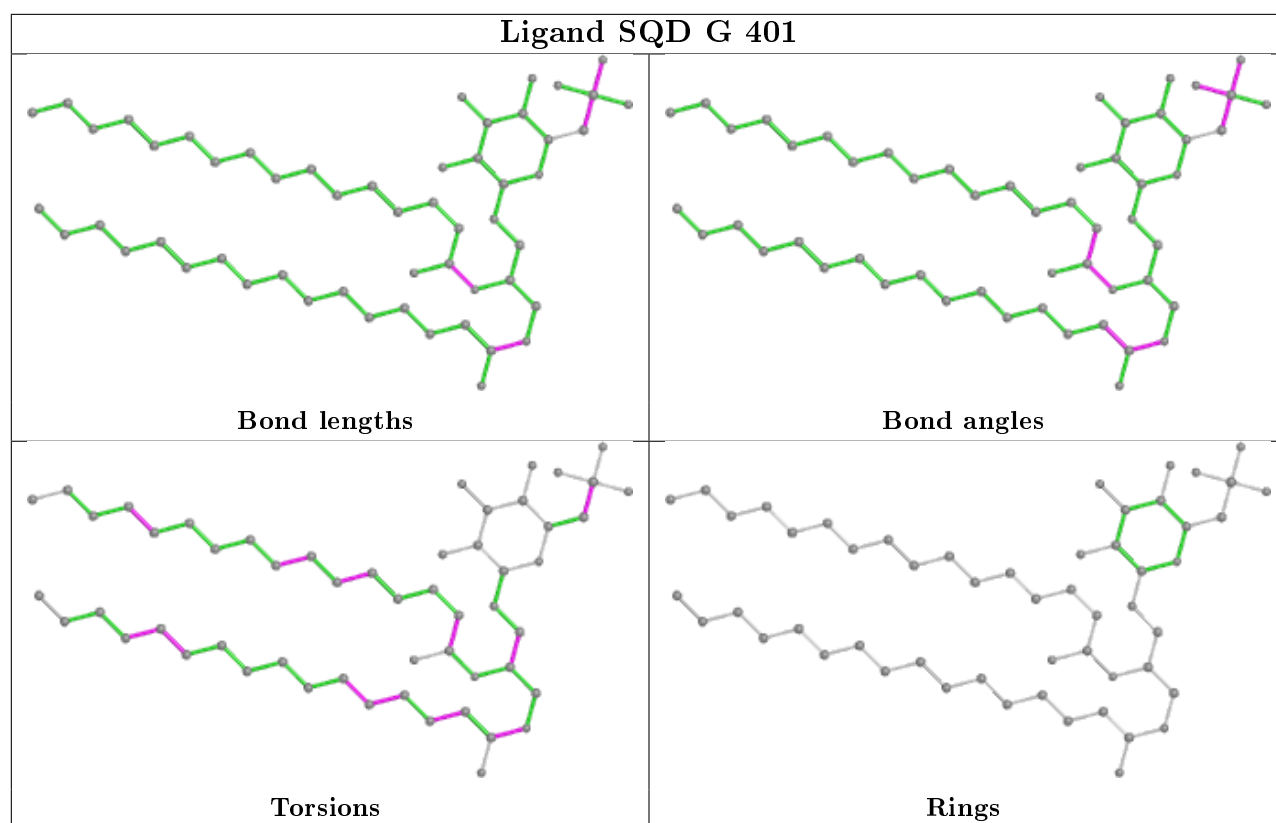


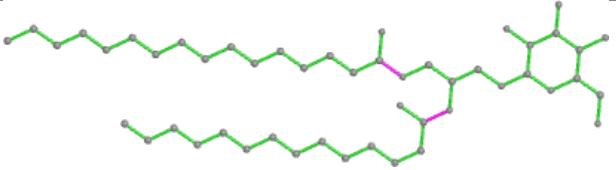
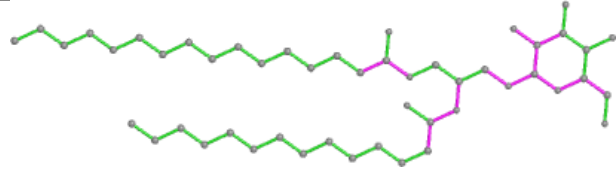
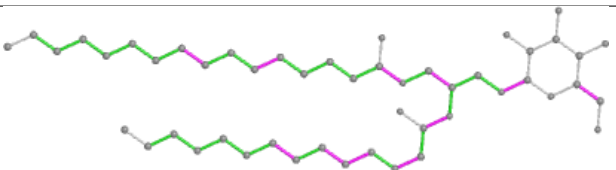
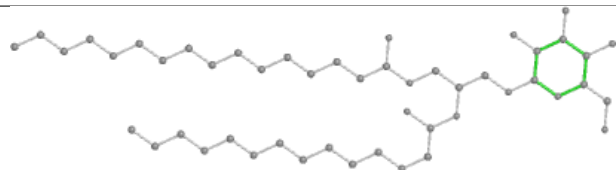


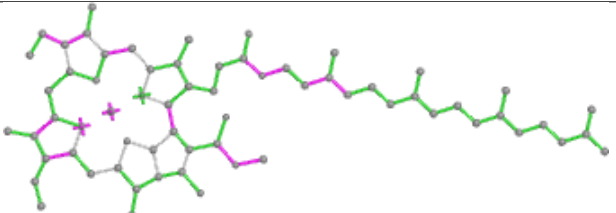
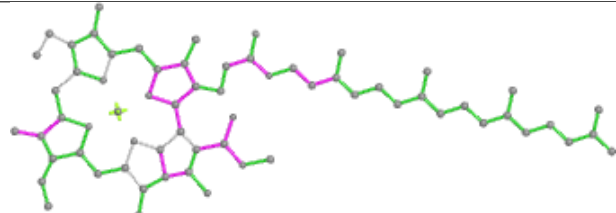
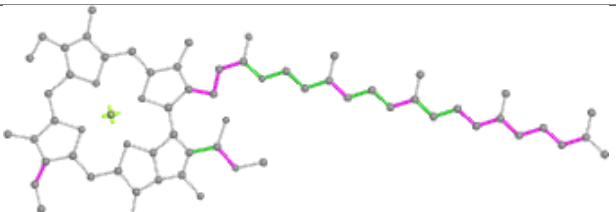
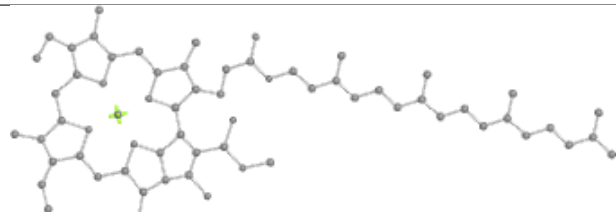
Ligand PL9 G 407**Ligand CLA N 613****Ligand DGD C 516**

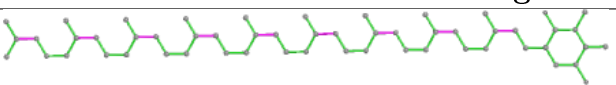
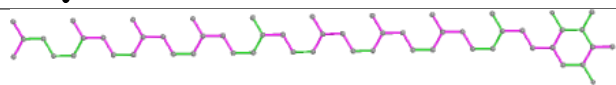
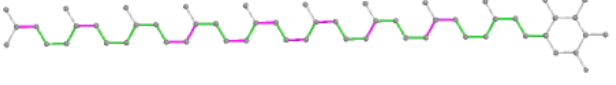
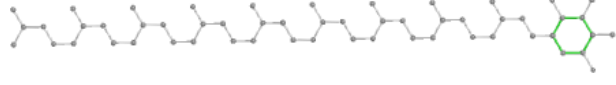
Ligand CLA P 504**Ligand BCR S 101****Ligand CLA B 610**

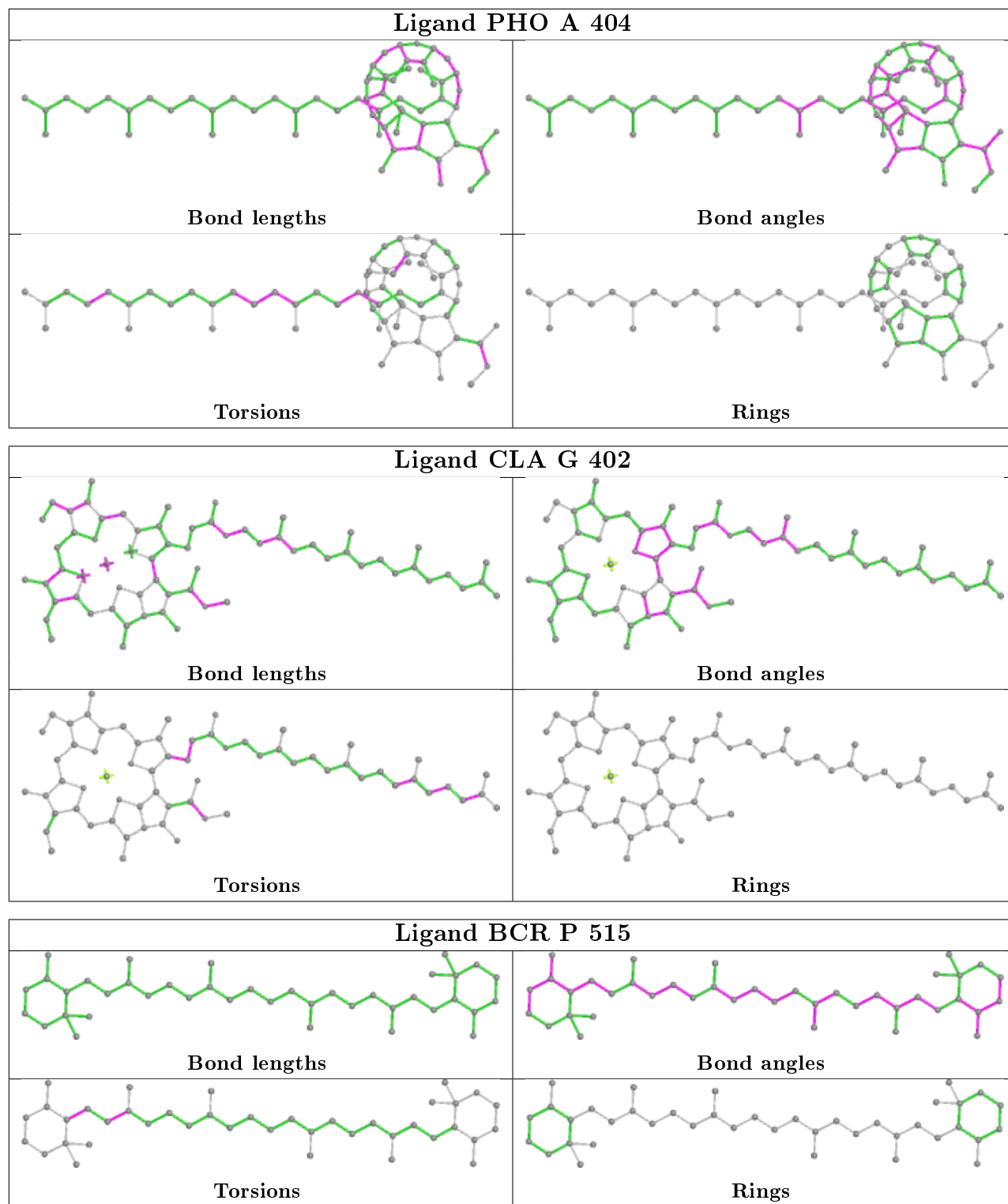
Ligand CLA B 602**Ligand CLA C 510****Ligand CLA A 402**

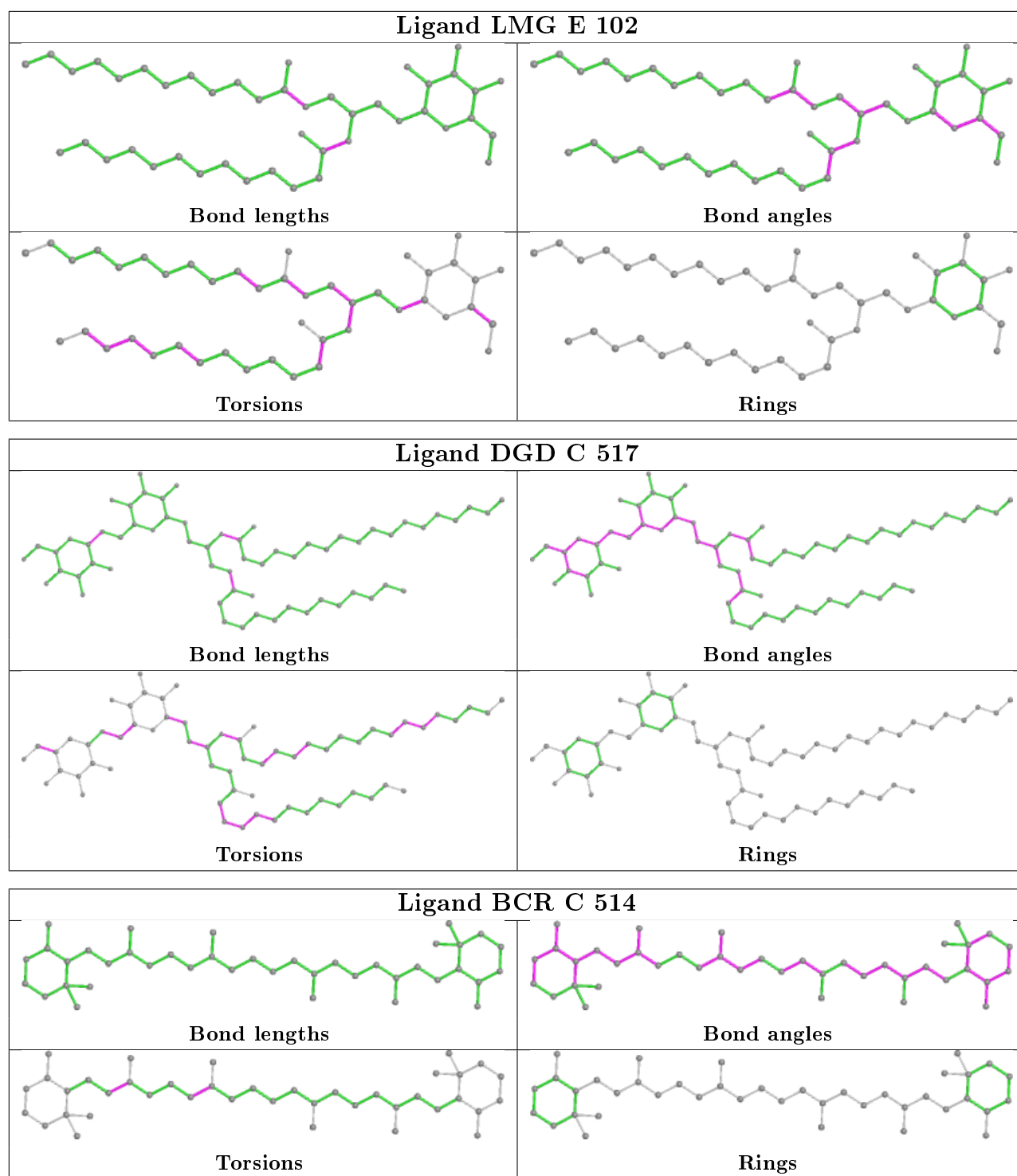


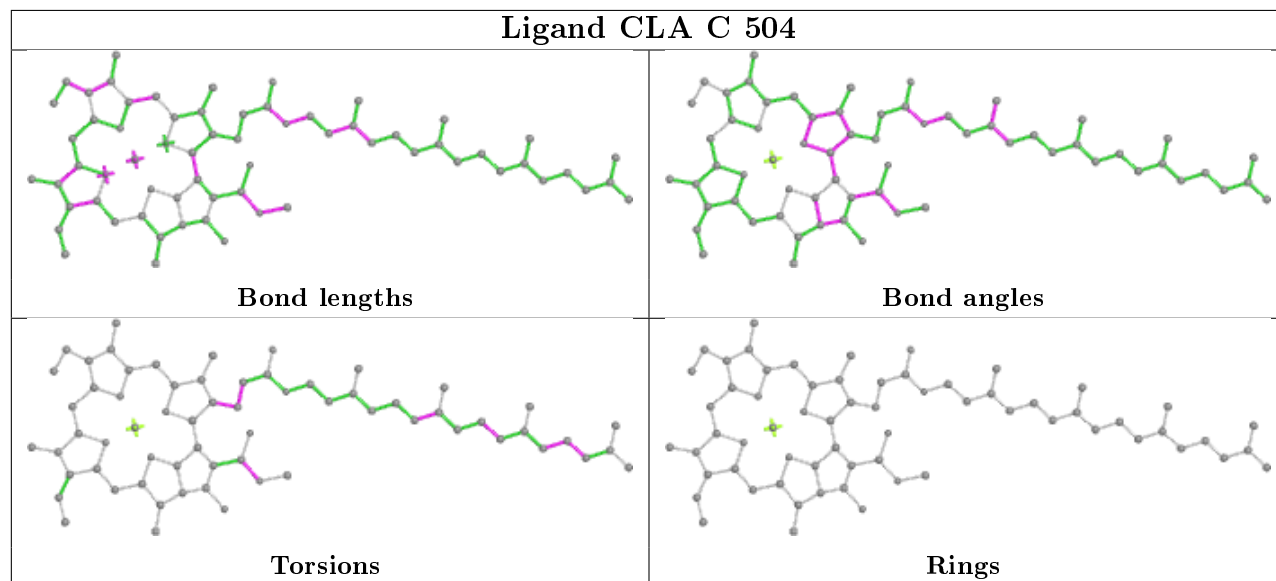
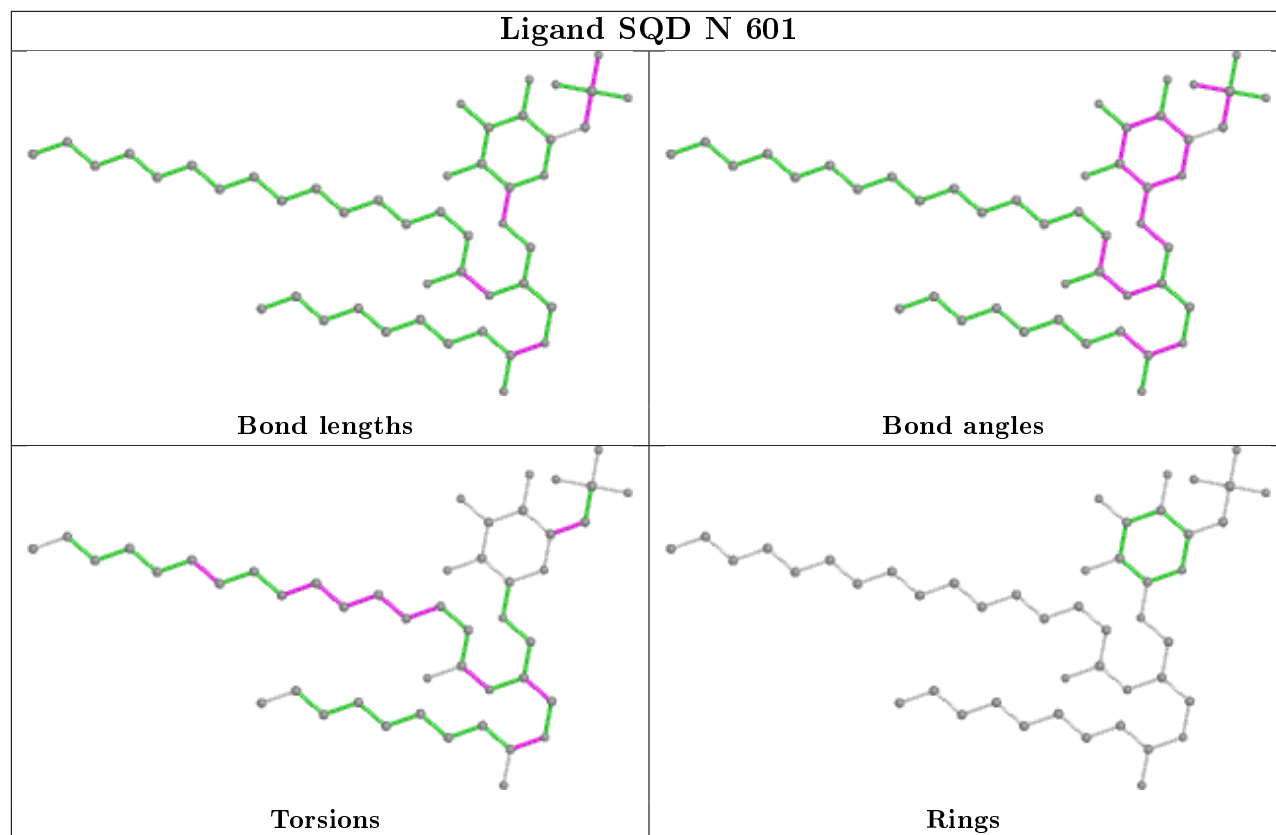
Ligand LMG B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

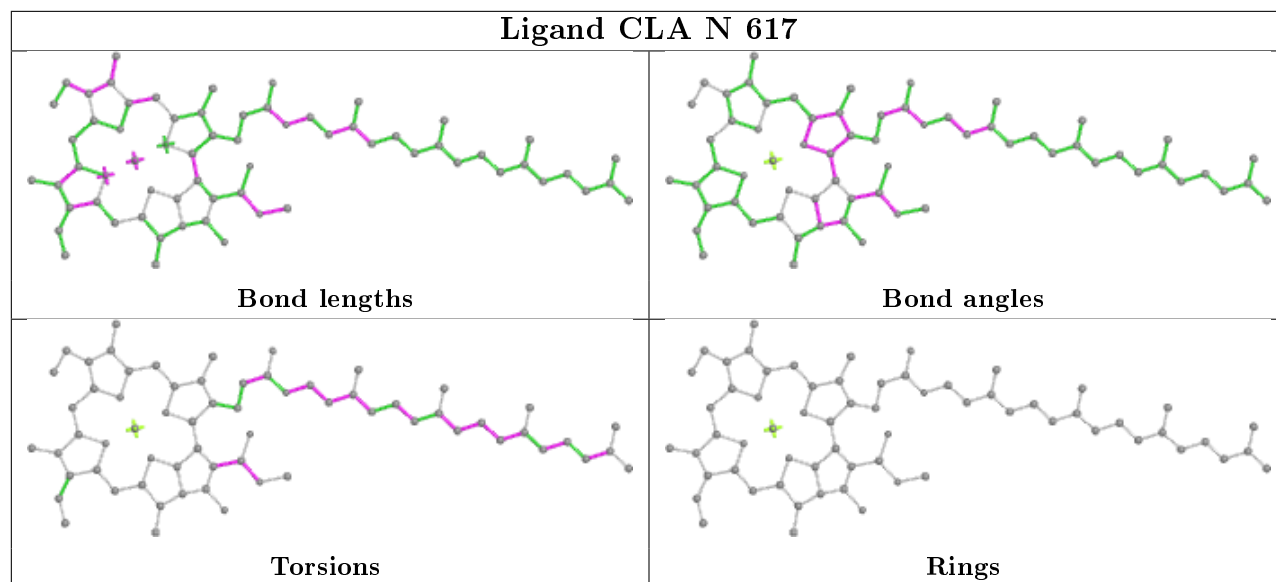
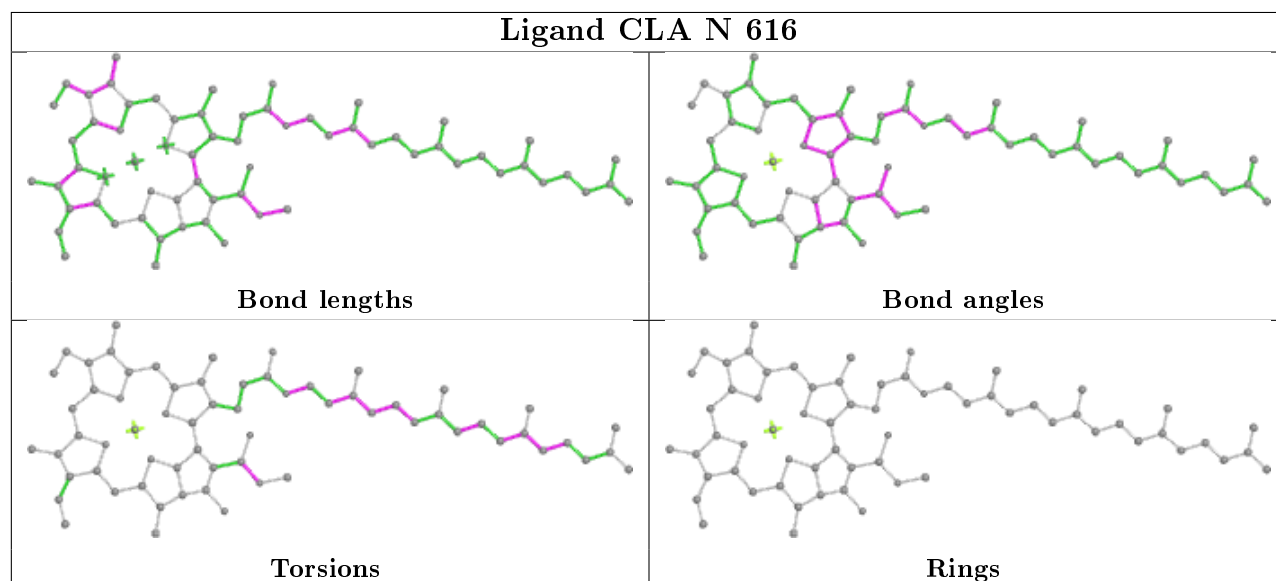
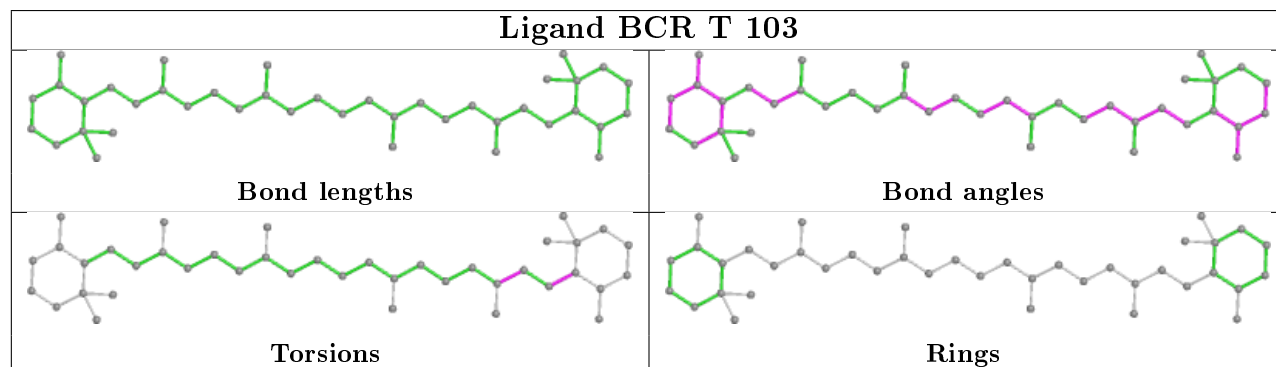
Ligand CLA B 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

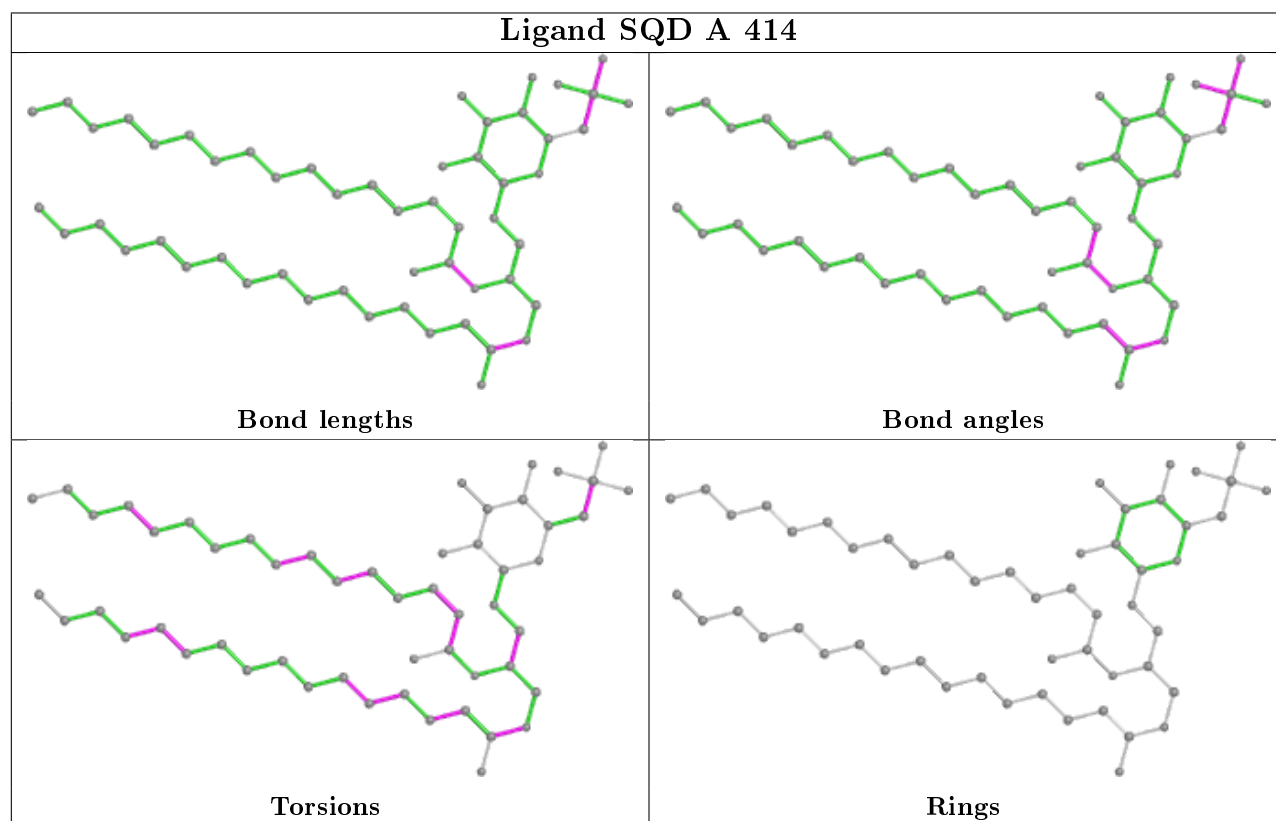
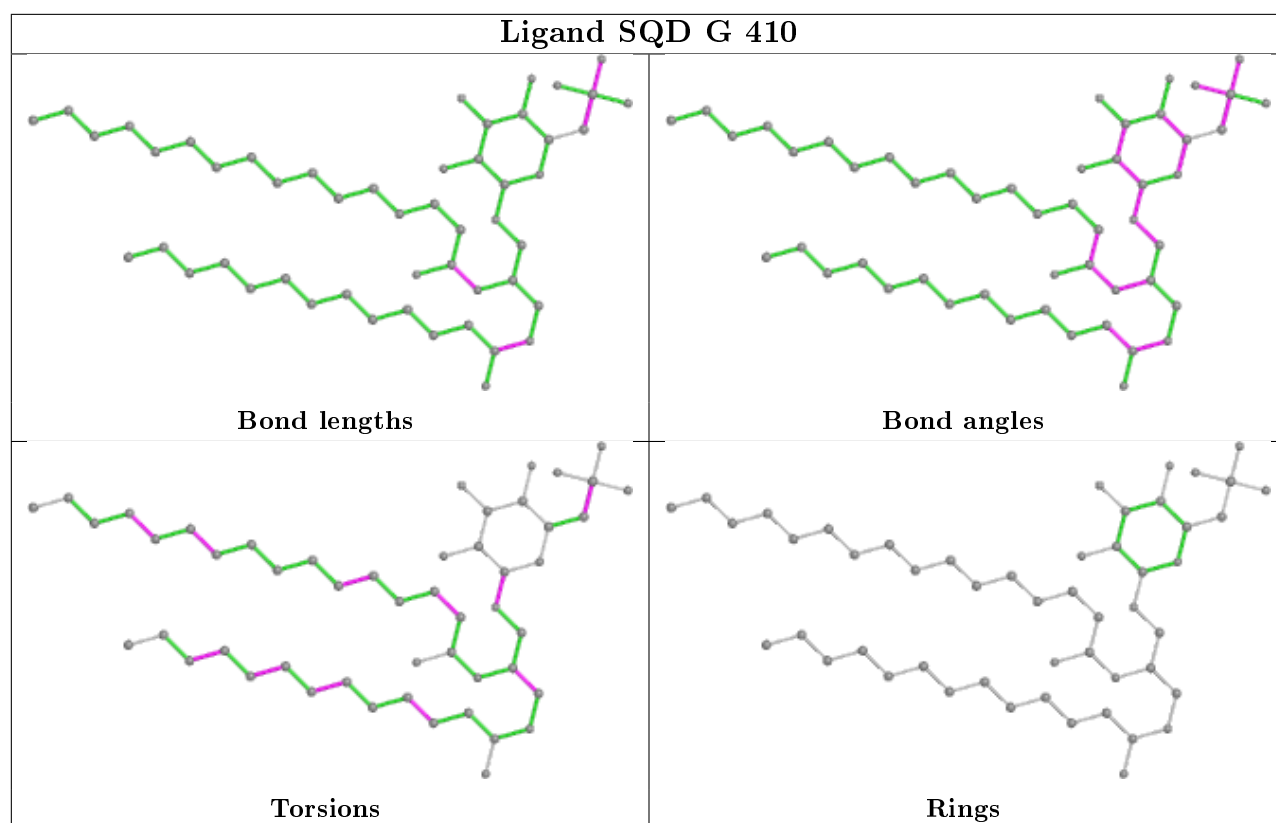
Ligand PL9 Q 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

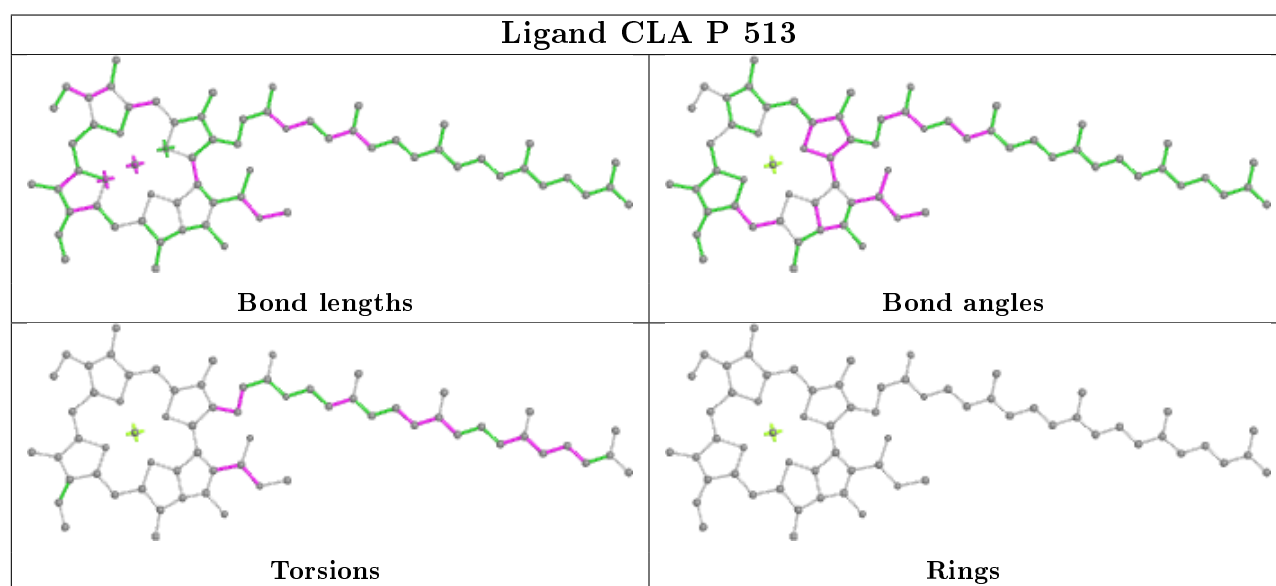
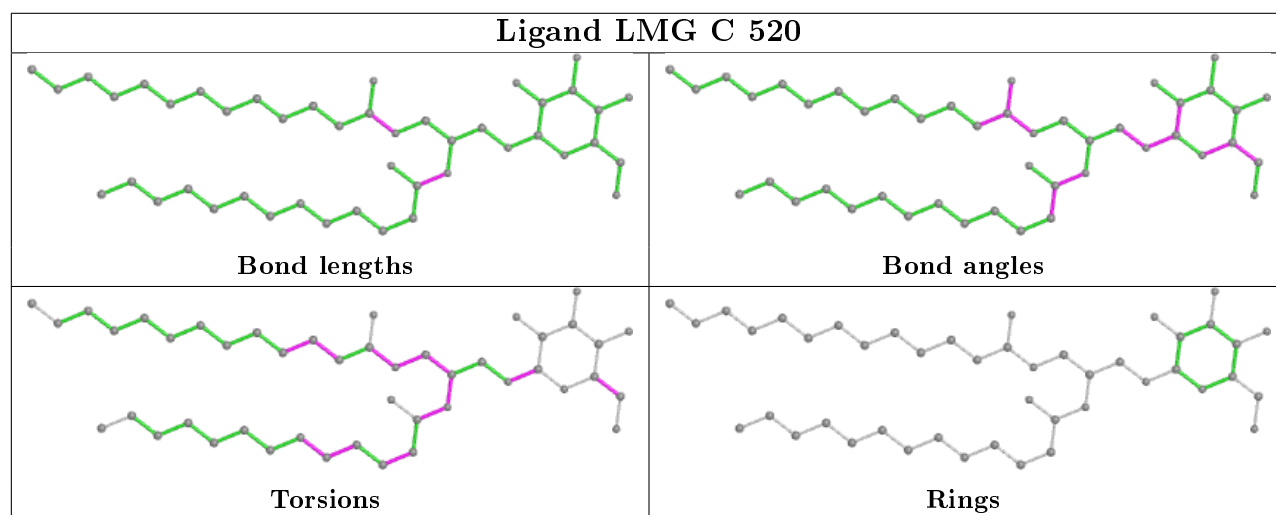
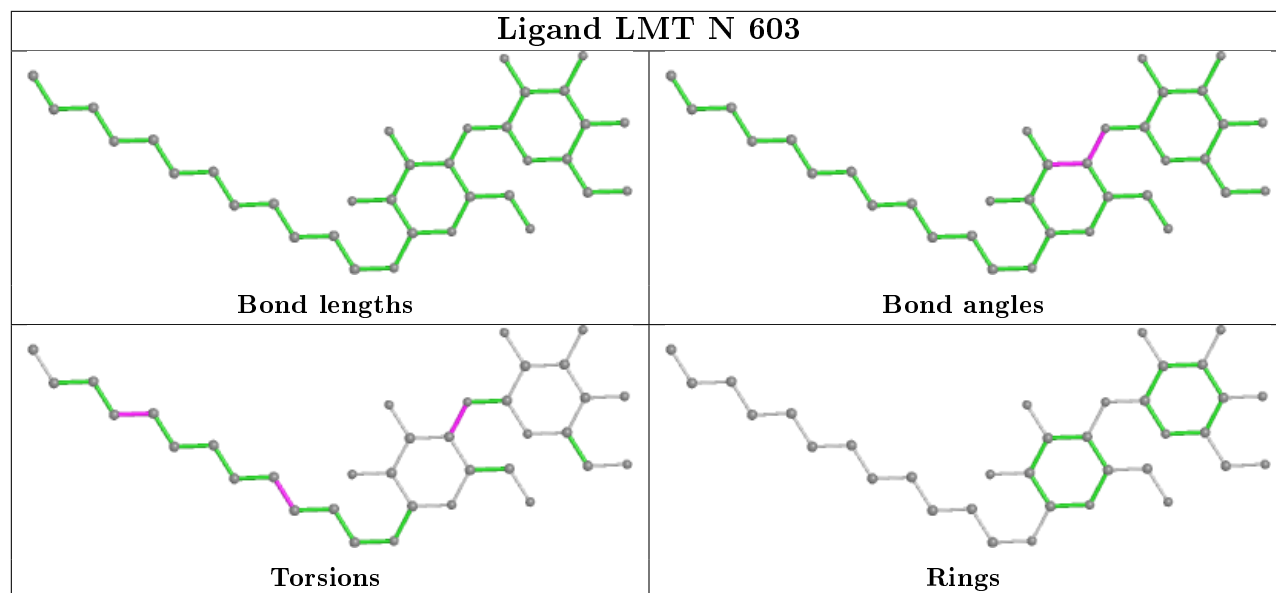


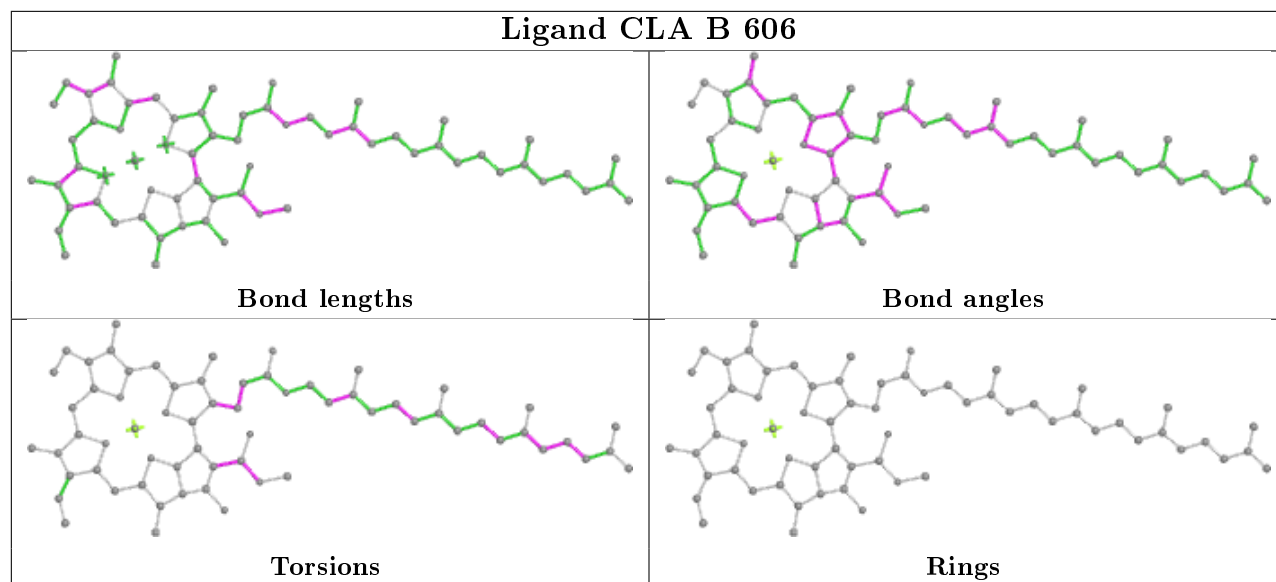
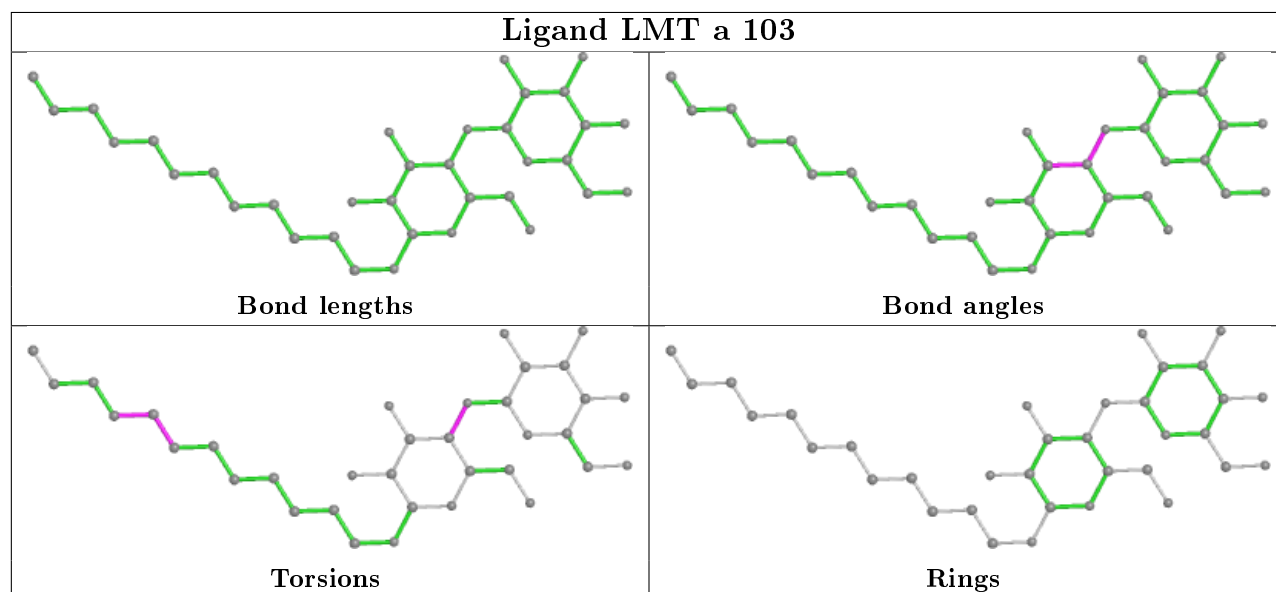
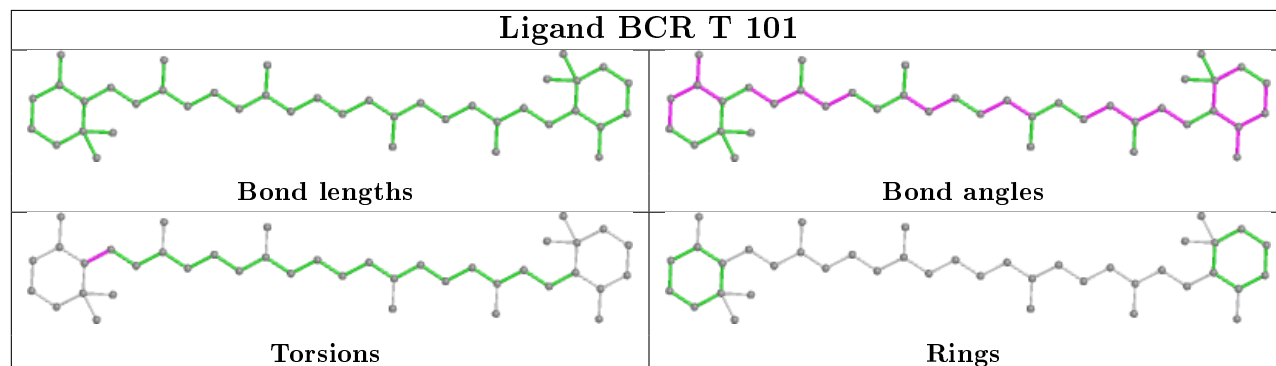


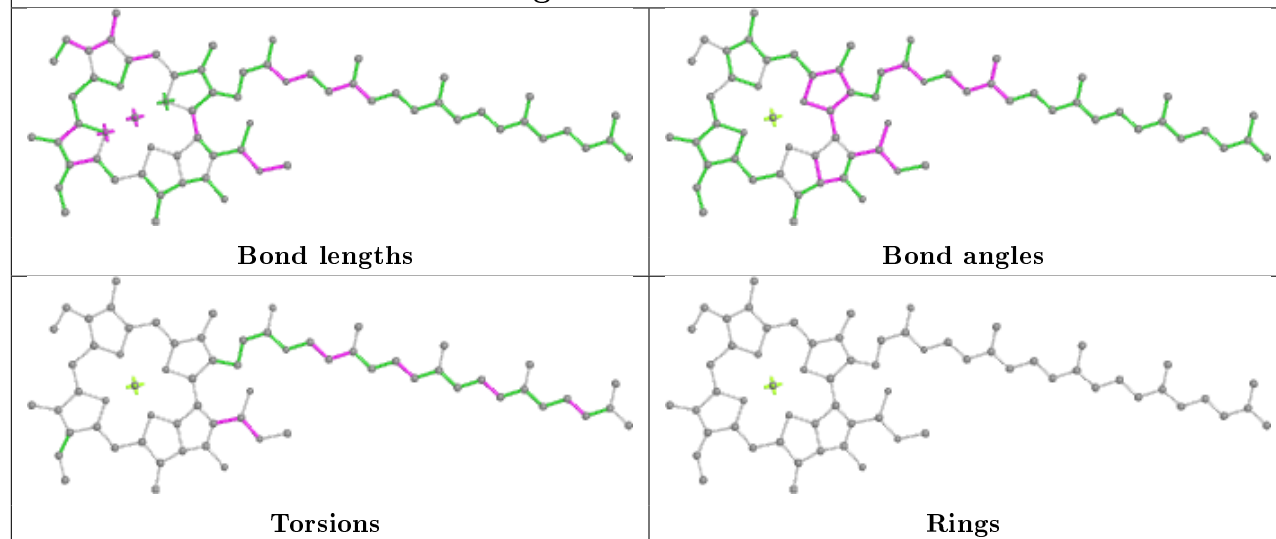
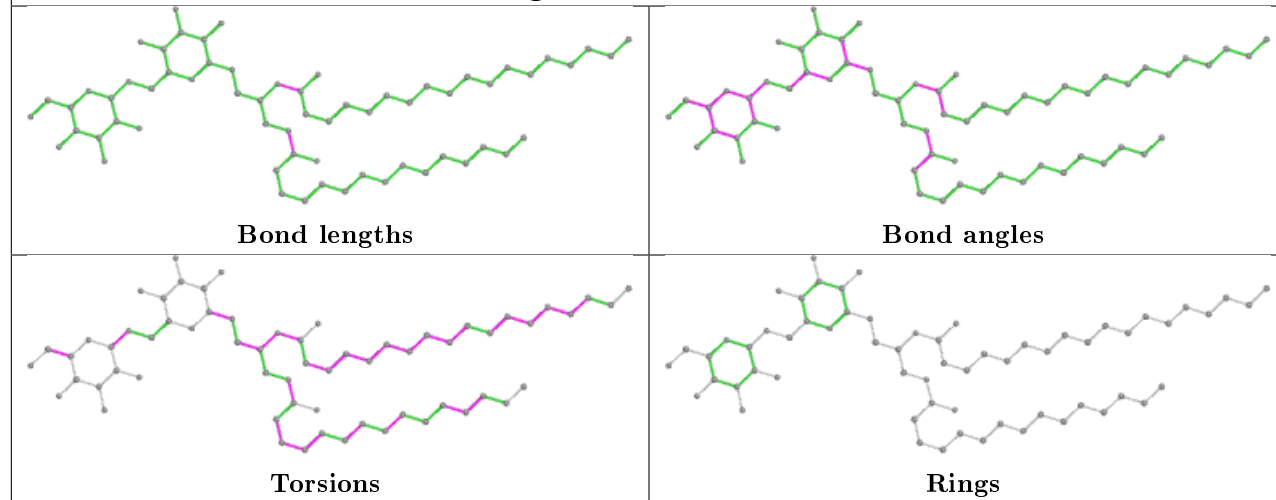


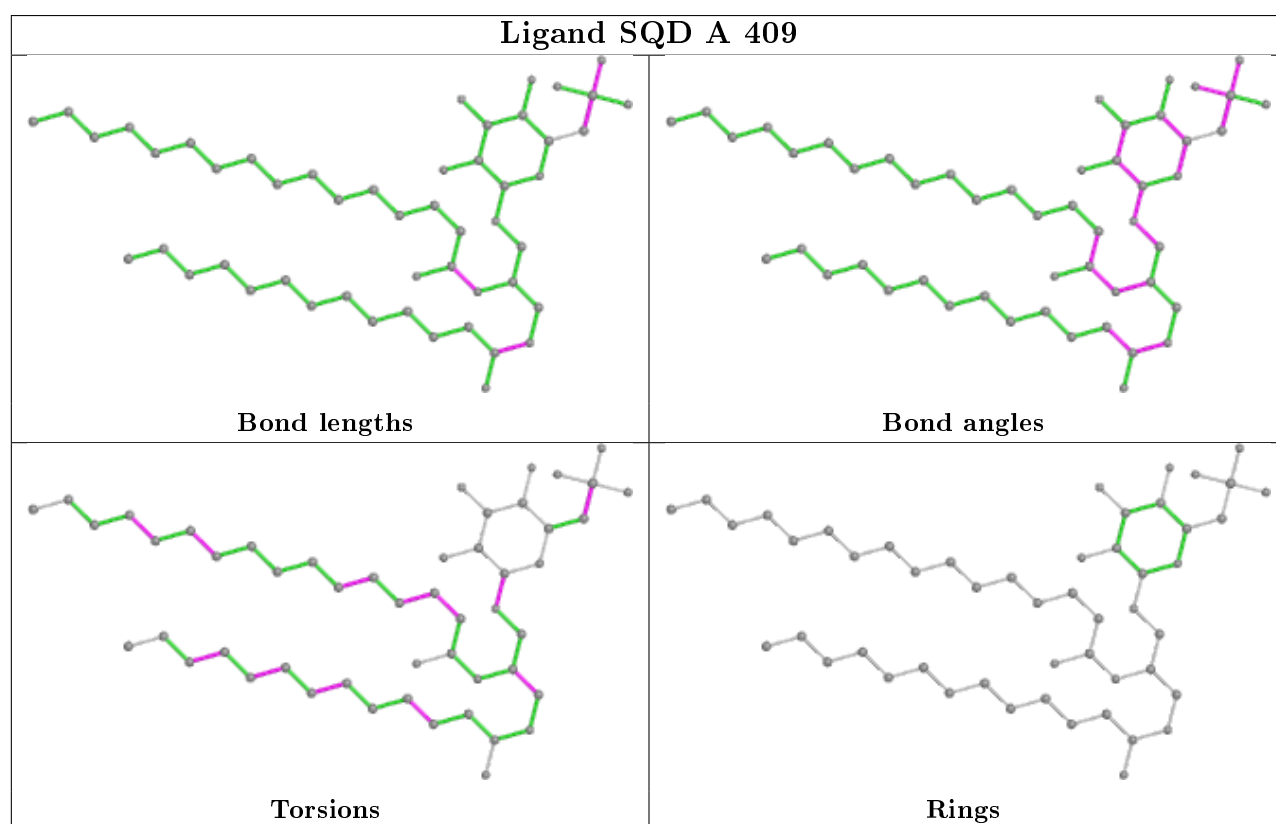
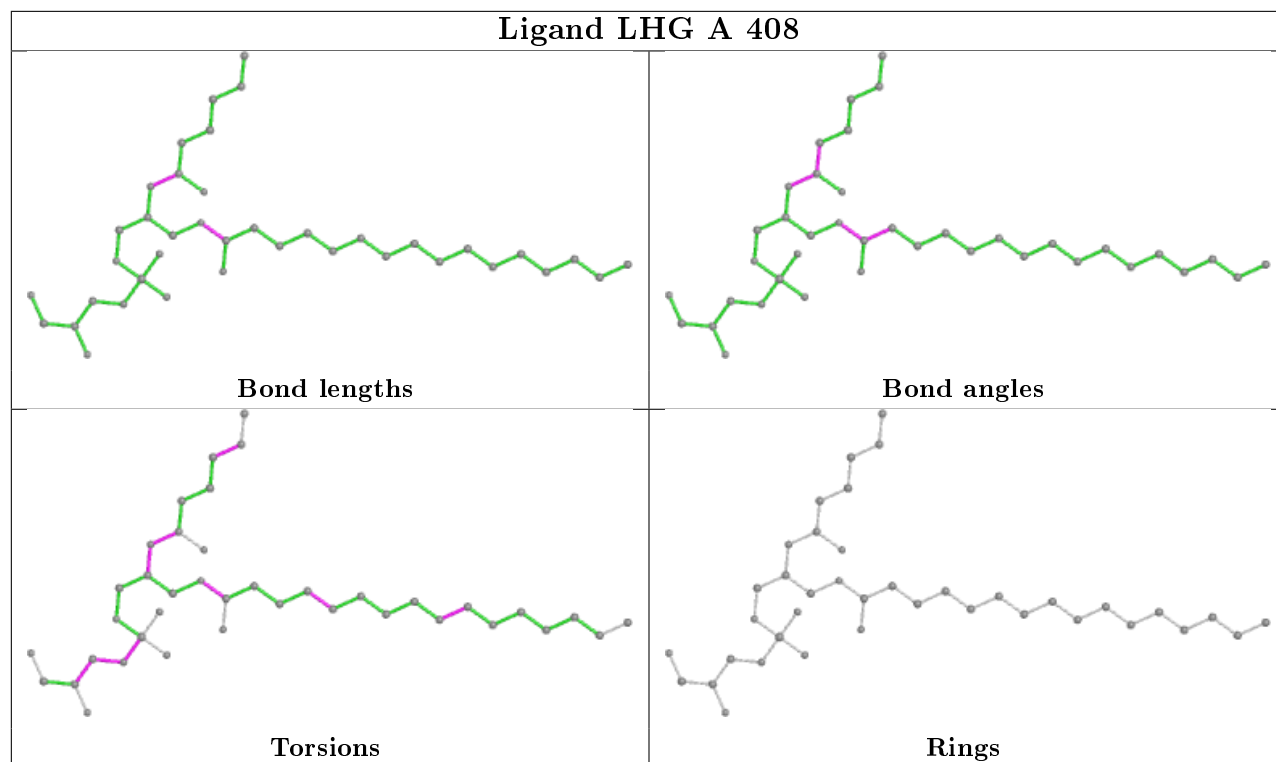
Ligand CLA N 617**Ligand CLA N 616****Ligand BCR T 103**



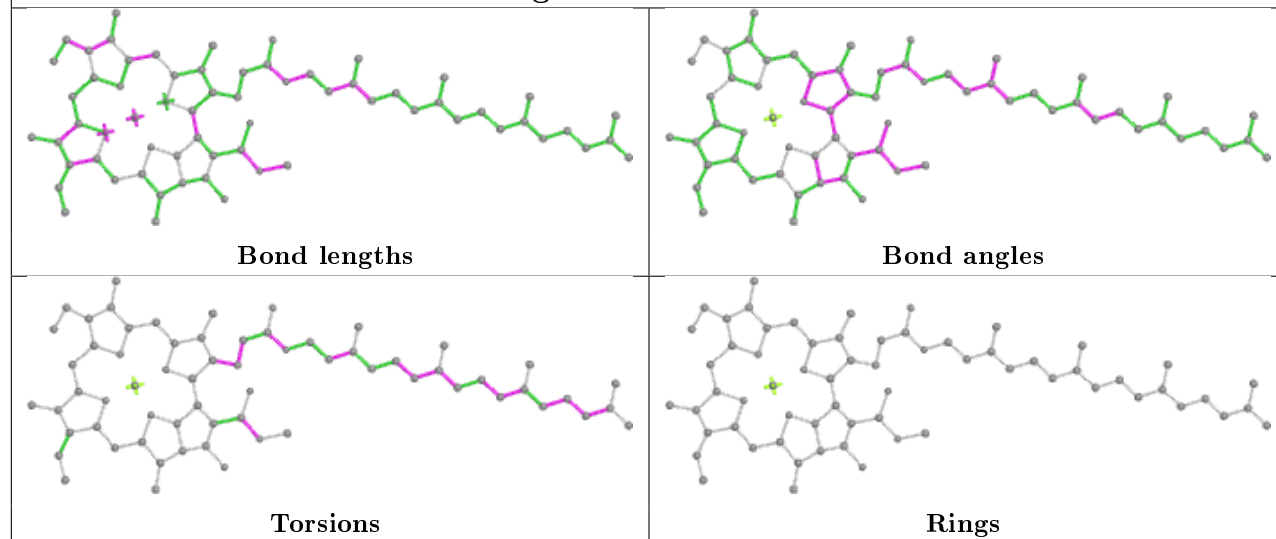


Ligand CLA B 606**Ligand LMT a 103****Ligand BCR T 101**

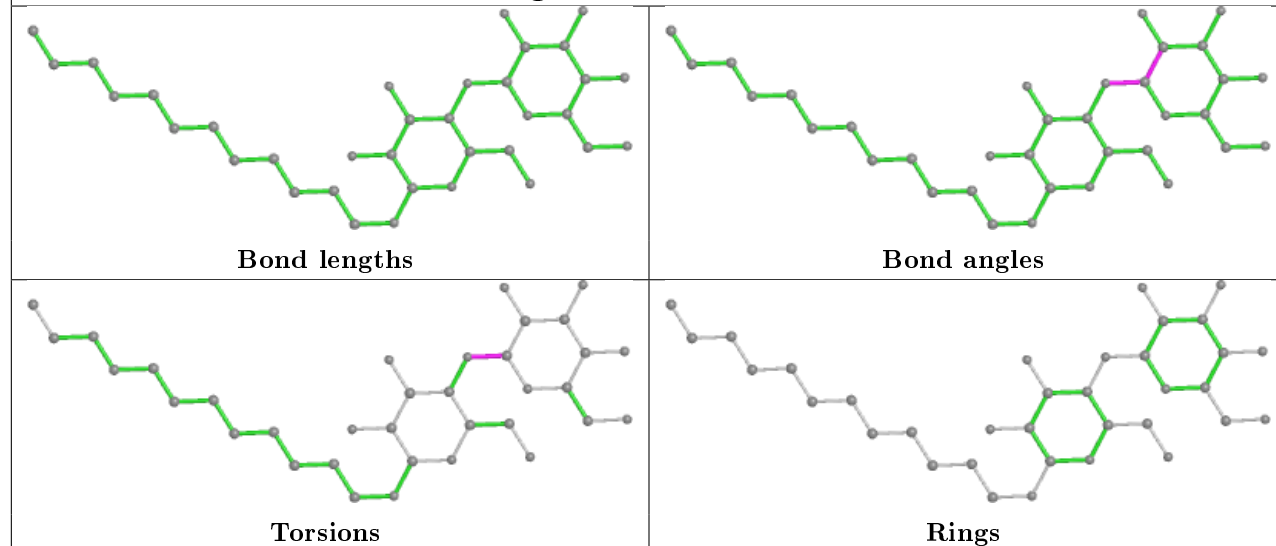
Ligand CLA P 509**Ligand DGD D 408**



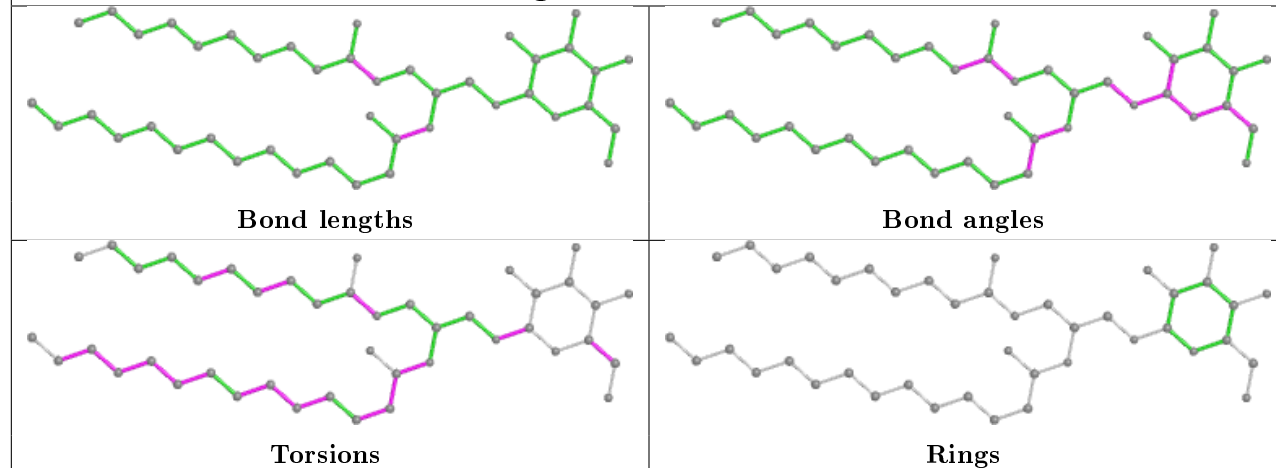
Ligand CLA B 605

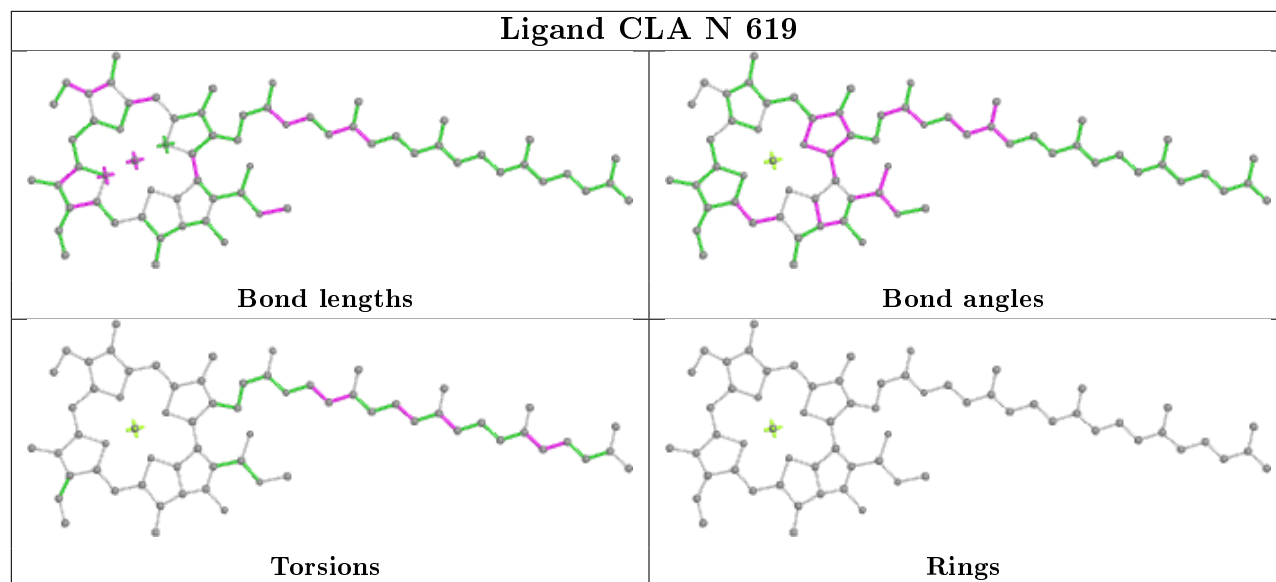
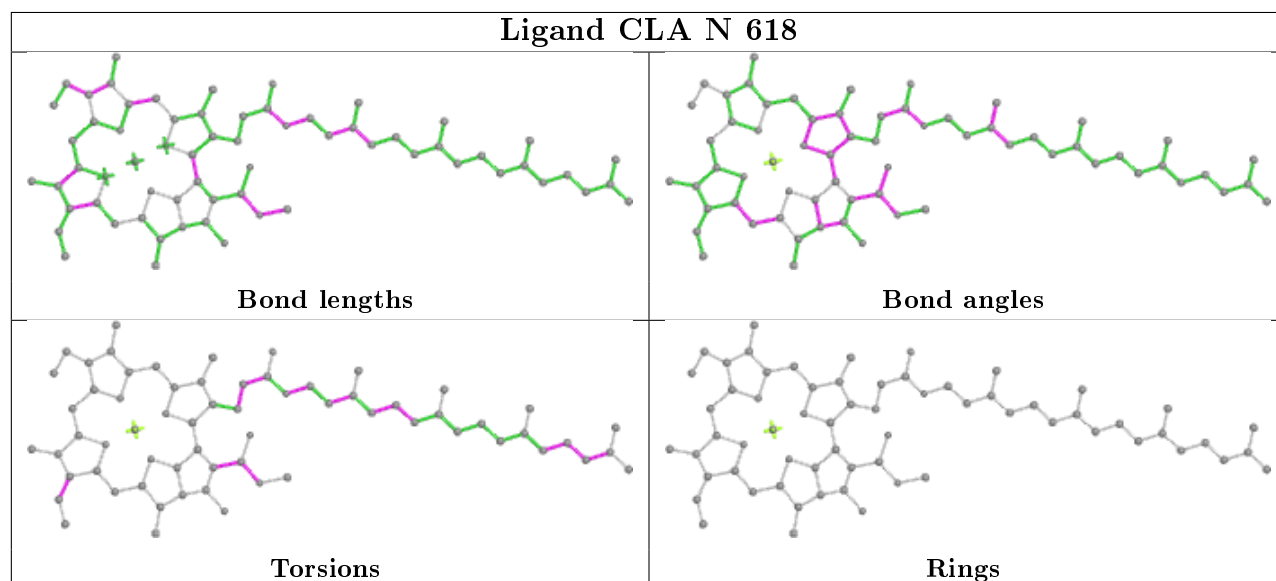
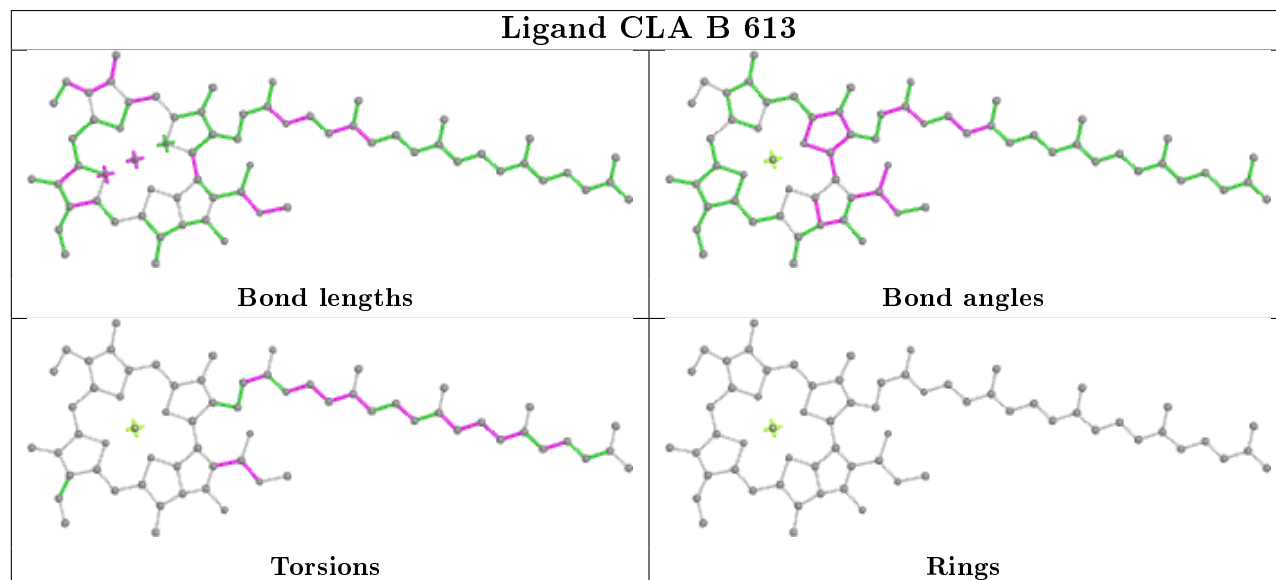


Ligand LMT B 626

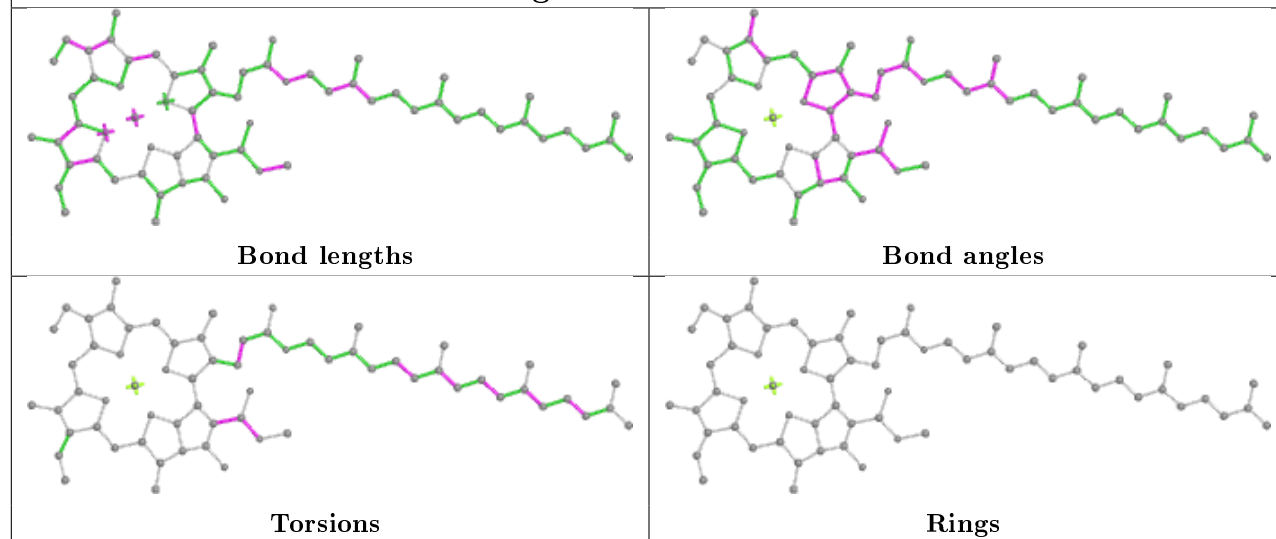


Ligand LMG a 102

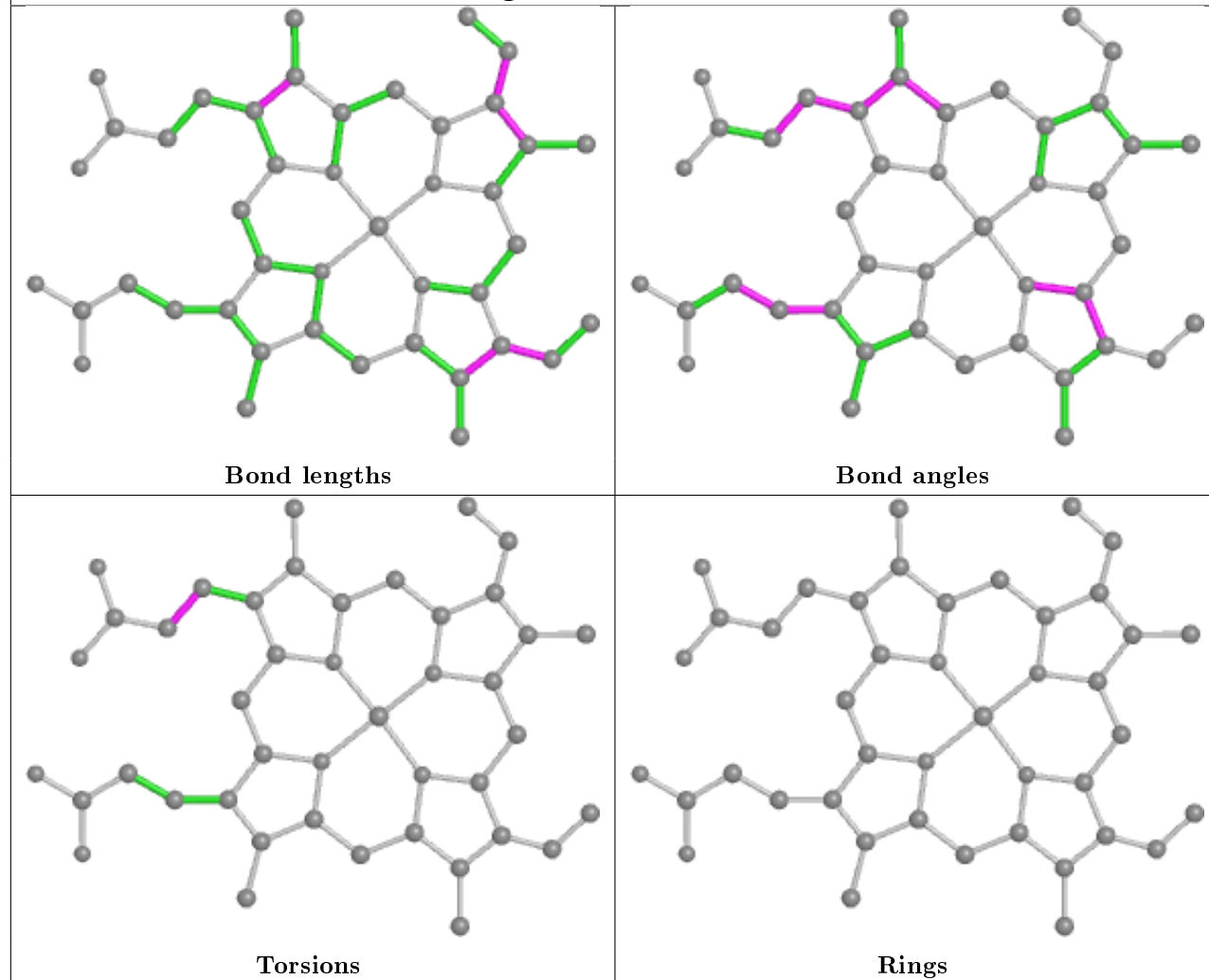


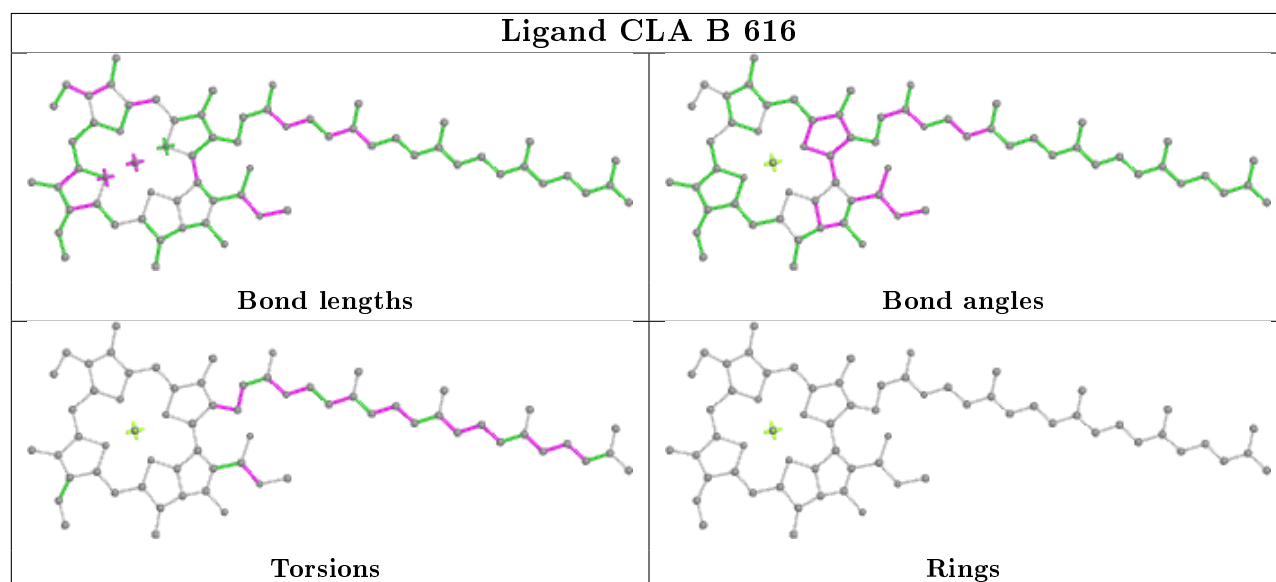
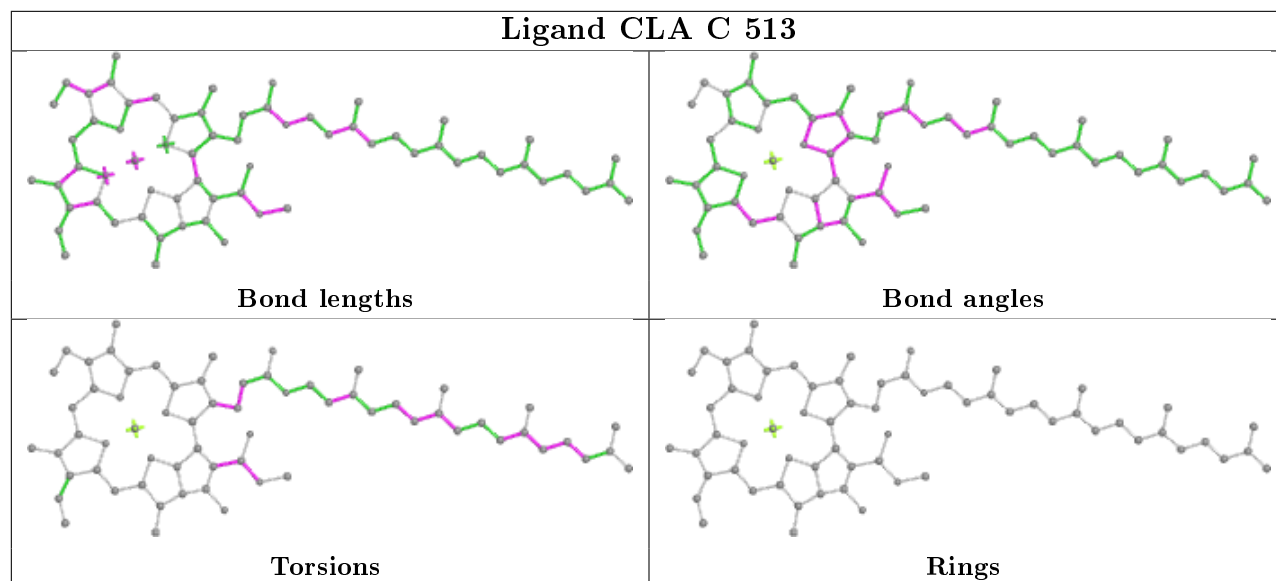
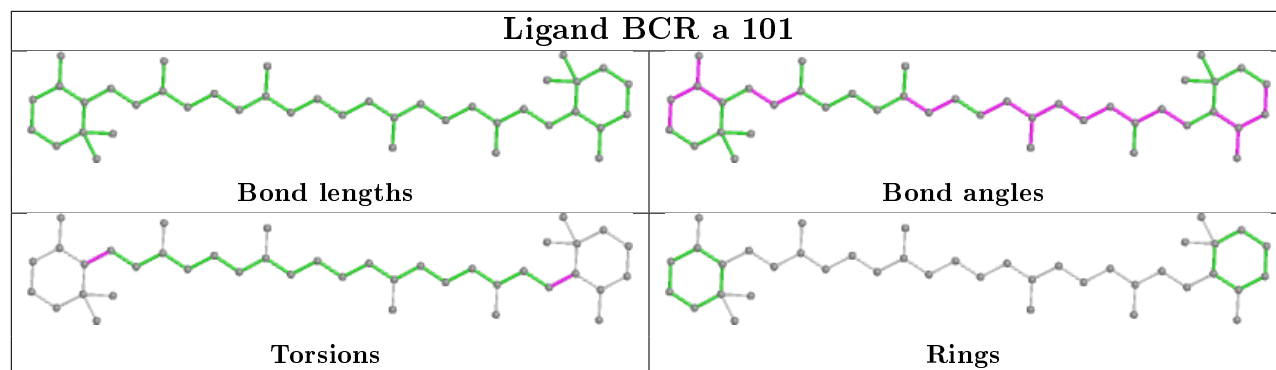
Ligand CLA N 619**Ligand CLA N 618****Ligand CLA B 613**

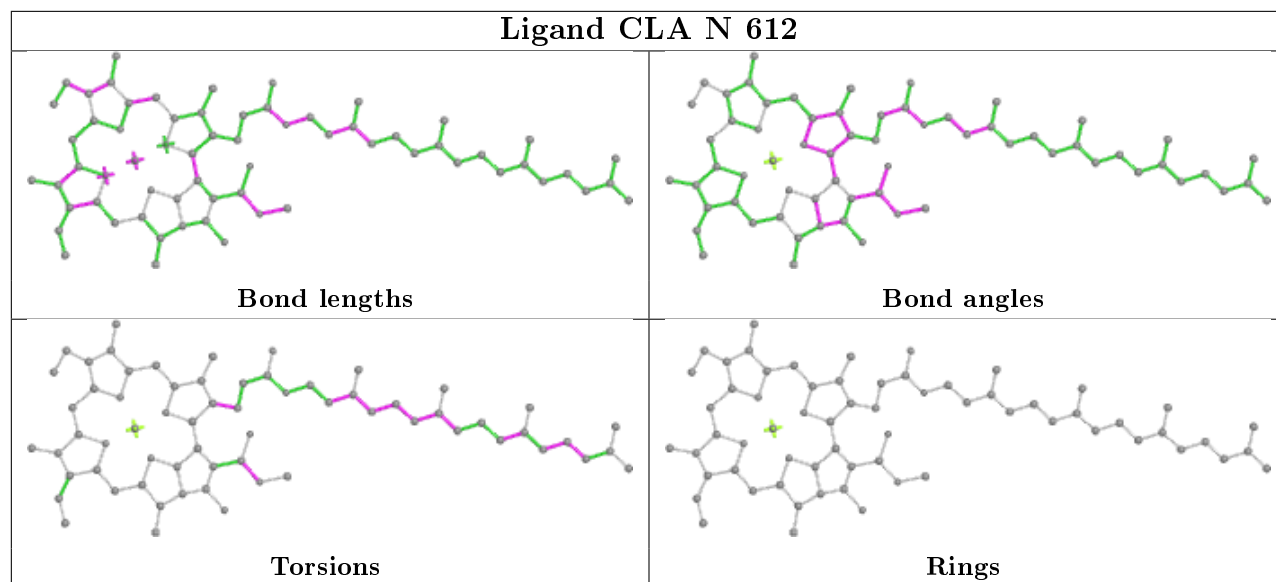
Ligand CLA C 508



Ligand HEM E 101







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%)	0.46	29 (8%) 10 12	131, 152, 182, 204	0
1	G	335/344 (97%)	0.29	20 (5%) 21 21	128, 156, 184, 213	0
2	B	490/510 (96%)	0.58	56 (11%) 5 8	128, 158, 178, 195	0
2	N	490/510 (96%)	0.63	64 (13%) 3 7	129, 160, 180, 207	0
3	C	447/461 (96%)	0.30	23 (5%) 28 27	129, 164, 183, 211	0
3	P	447/461 (96%)	0.66	70 (15%) 2 5	139, 165, 183, 197	0
4	D	340/352 (96%)	0.33	25 (7%) 14 15	125, 152, 176, 198	0
4	Q	340/352 (96%)	0.18	13 (3%) 40 36	130, 155, 175, 184	0
5	E	82/83 (98%)	0.17	3 (3%) 41 37	148, 171, 188, 198	0
5	R	82/83 (98%)	-0.15	0 100 100	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.18	1 (2%) 51 44	140, 168, 185, 199	0
6	S	35/44 (79%)	0.37	0 100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	0.78	7 (10%) 5 9	154, 172, 189, 195	0
7	W	65/65 (100%)	0.86	16 (24%) 0 2	154, 173, 188, 196	0
8	I	35/38 (92%)	0.20	1 (2%) 51 44	147, 163, 174, 178	0
8	a	35/38 (92%)	0.03	0 100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	0.03	0 100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	1.19	8 (23%) 0 2	156, 176, 190, 190	0
10	K	37/37 (100%)	0.21	3 (8%) 12 14	158, 170, 181, 185	0
10	c	37/37 (100%)	1.36	10 (27%) 0 2	152, 171, 187, 195	0
11	L	37/37 (100%)	0.27	4 (10%) 5 9	137, 155, 186, 190	0
11	d	37/37 (100%)	0.26	4 (10%) 5 9	143, 158, 194, 201	0
12	M	34/36 (94%)	0.38	5 (14%) 2 5	147, 163, 179, 195	0
12	e	34/36 (94%)	0.45	7 (20%) 1 3	147, 159, 176, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/246 (98%)	0.84	39 (16%) 1 4	132, 162, 190, 201	0
13	f	243/246 (98%)	0.55	15 (6%) 20 20	127, 164, 191, 211	0
14	T	32/32 (100%)	0.21	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	0.28	3 (9%) 8 11	145, 158, 179, 198	0
15	U	97/104 (93%)	0.88	10 (10%) 6 9	136, 154, 173, 177	0
15	h	97/104 (93%)	1.74	33 (34%) 0 2	140, 154, 165, 174	0
16	V	137/137 (100%)	0.45	10 (7%) 15 16	135, 156, 170, 180	0
16	i	137/137 (100%)	0.54	11 (8%) 12 14	131, 158, 176, 185	0
17	m	28/46 (60%)	2.12	17 (60%) 0 0	167, 183, 198, 205	0
17	y	28/46 (60%)	0.46	2 (7%) 16 16	164, 182, 197, 201	0
18	X	37/40 (92%)	1.21	6 (16%) 1 4	158, 173, 188, 190	0
18	j	37/40 (92%)	0.77	3 (8%) 12 14	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	1.56	18 (29%) 0 2	159, 178, 198, 208	0
20	l	62/62 (100%)	0.97	5 (8%) 12 14	164, 178, 199, 208	0
All	All	5214/5482 (95%)	0.53	541 (10%) 6 9	125, 161, 185, 213	0

The worst 5 of 541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	295	SER	7.7
12	M	2	GLU	6.5
16	i	132	ASN	6.3
15	U	123	GLU	6.3
2	N	393	GLU	6.1

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 monosaccharides 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	0.05	0.78	138,138,138,138	0
23	PL9	b	101	35/55	0.28	0.47	168,188,199,208	0
35	CA	f	301	1/1	0.28	0.81	210,210,210,210	0
27	LMG	C	520	45/55	0.29	1.14	164,178,186,187	0
31	LMT	I	103	35/35	0.31	1.02	153,189,201,206	0
31	LMT	Q	410	31/35	0.39	0.73	165,182,193,197	0
30	BCR	a	101	40/40	0.39	0.56	139,159,176,181	0
30	BCR	c	101	40/40	0.40	1.10	151,171,188,190	0
27	LMG	P	521	45/55	0.43	1.10	149,175,191,198	0
31	LMT	N	624	35/35	0.44	0.92	166,201,210,213	0
21	CLA	N	605	65/65	0.46	0.79	170,189,202,205	0
23	PL9	J	101	35/55	0.46	0.49	177,190,200,204	0
30	BCR	I	101	40/40	0.47	0.54	143,155,171,183	0
31	LMT	a	103	35/35	0.48	0.86	169,180,206,216	0
30	BCR	T	103	40/40	0.49	0.88	155,168,181,184	0
21	CLA	B	601	65/65	0.49	1.00	167,188,199,203	0
30	BCR	J	102	40/40	0.50	0.47	167,182,207,208	0
31	LMT	B	625	35/35	0.50	0.89	163,196,218,227	0
31	LMT	N	603	35/35	0.53	0.61	153,179,189,190	0
27	LMG	D	412	42/55	0.53	0.42	147,178,195,199	0
31	LMT	D	409	31/35	0.56	1.06	162,187,202,208	0
31	LMT	B	629	35/35	0.57	0.74	153,166,181,185	0
24	DGD	D	408	63/66	0.58	0.78	167,181,198,212	0
31	LMT	N	625	35/35	0.59	0.87	165,184,206,216	0
25	LHG	G	412	37/49	0.59	0.52	147,176,193,204	0
31	LMT	N	604	35/35	0.59	0.51	145,180,209,212	0
27	LMG	I	102	43/55	0.60	0.79	152,184,203,207	0
30	BCR	B	620	40/40	0.61	0.76	161,168,186,196	0
27	LMG	Q	401	42/55	0.61	0.65	131,168,174,183	0
30	BCR	H	101	40/40	0.62	0.96	165,178,188,190	0
21	CLA	N	608	65/65	0.63	0.59	146,158,176,191	0
26	SQD	A	414	54/54	0.63	0.57	139,173,190,200	0
30	BCR	b	102	40/40	0.63	0.54	158,178,202,203	0
26	SQD	Q	408	43/54	0.64	0.59	143,180,193,194	0
31	LMT	e	101	35/35	0.65	0.52	164,176,191,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	P	502	65/65	0.65	0.87	146,161,175,182	0
30	BCR	D	405	40/40	0.65	0.69	145,161,176,179	0
31	LMT	B	630	35/35	0.65	0.53	157,169,199,220	0
21	CLA	N	620	65/65	0.65	0.79	156,175,192,194	0
21	CLA	C	513	65/65	0.66	1.15	173,193,206,213	0
27	LMG	R	102	44/55	0.67	0.42	161,177,189,192	0
21	CLA	P	513	65/65	0.67	1.02	168,182,207,216	0
24	DGD	Q	409	63/66	0.67	0.54	157,183,208,238	0
21	CLA	C	502	65/65	0.68	0.51	142,157,179,185	0
21	CLA	N	609	65/65	0.68	0.68	148,165,174,178	0
21	CLA	C	507	65/65	0.68	0.82	159,172,185,187	0
21	CLA	C	505	65/65	0.68	0.50	147,172,186,188	0
26	SQD	B	627	47/54	0.68	0.41	143,179,209,227	0
26	SQD	B	624	43/54	0.68	0.45	150,181,199,206	0
21	CLA	A	403	65/65	0.68	0.40	142,161,183,185	0
21	CLA	D	401	65/65	0.68	0.42	137,149,176,181	0
31	LMT	M	102	35/35	0.69	0.59	134,165,196,205	0
21	CLA	B	604	65/65	0.69	0.69	148,158,172,182	0
21	CLA	N	607	65/65	0.69	0.71	133,163,170,175	0
27	LMG	C	519	48/55	0.69	0.39	132,169,183,188	0
30	BCR	P	516	40/40	0.69	0.85	164,173,180,187	0
25	LHG	A	411	37/49	0.69	0.41	156,178,214,232	0
21	CLA	N	610	65/65	0.70	0.77	152,178,191,194	0
21	CLA	G	406	65/65	0.70	0.61	145,159,181,186	0
31	LMT	B	626	35/35	0.70	0.41	163,194,202,213	0
21	CLA	C	509	65/65	0.70	0.80	145,170,180,183	0
26	SQD	N	601	47/54	0.70	0.44	141,176,198,202	0
33	CL	D	411	1/1	0.71	0.86	121,121,121,121	0
30	BCR	B	618	40/40	0.71	0.30	149,162,168,169	0
24	DGD	C	518	66/66	0.71	0.34	139,157,179,185	0
22	PHO	D	402	64/64	0.72	0.49	135,155,161,168	0
23	PL9	G	407	45/55	0.72	0.44	148,160,183,188	0
27	LMG	a	102	43/55	0.72	0.64	160,179,196,200	0
21	CLA	P	511	65/65	0.72	1.03	156,174,184,187	0
30	BCR	P	514	40/40	0.72	1.53	139,152,173,175	0
24	DGD	B	628	52/66	0.73	0.47	148,173,194,200	0
22	PHO	A	404	64/64	0.73	0.32	129,151,167,177	0
21	CLA	C	503	65/65	0.74	0.54	155,171,181,183	0
30	BCR	T	101	40/40	0.74	0.29	144,167,181,184	0
24	DGD	N	602	52/66	0.74	0.46	154,176,204,206	0
27	LMG	B	623	49/55	0.74	0.36	128,147,164,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	DGD	B	621	58/66	0.74	0.49	142,158,168,171	0
24	DGD	G	408	56/66	0.74	0.42	163,179,188,193	0
21	CLA	G	404	65/65	0.74	0.36	141,159,179,181	0
21	CLA	P	509	65/65	0.75	0.84	152,174,181,184	0
22	PHO	G	405	64/64	0.75	0.37	131,149,159,162	0
21	CLA	B	605	65/65	0.75	0.76	156,167,176,179	0
21	CLA	A	405	65/65	0.75	0.51	144,155,176,187	0
30	BCR	C	514	40/40	0.75	0.84	153,160,171,173	0
21	CLA	N	619	65/65	0.75	0.86	158,180,190,193	0
30	BCR	B	617	40/40	0.75	0.28	151,158,176,180	0
24	DGD	A	407	56/66	0.75	0.35	147,171,188,195	0
21	CLA	C	512	65/65	0.76	1.23	173,183,196,199	0
30	BCR	K	101	40/40	0.76	0.81	154,167,176,181	0
21	CLA	N	613	65/65	0.76	0.78	160,170,177,182	0
21	CLA	P	507	65/65	0.76	0.66	162,172,191,194	0
21	CLA	C	501	65/65	0.76	0.55	160,174,184,185	0
26	SQD	F	101	45/54	0.77	0.61	157,176,196,198	0
27	LMG	E	102	44/55	0.77	0.44	168,188,198,203	0
26	SQD	G	410	51/54	0.77	0.39	161,172,184,190	0
21	CLA	Q	402	65/65	0.77	0.50	136,144,158,169	0
21	CLA	C	506	65/65	0.78	0.45	159,175,202,211	0
27	LMG	B	622	49/55	0.78	0.36	148,163,174,176	0
24	DGD	C	517	62/66	0.78	0.35	145,169,193,200	0
21	CLA	B	607	65/65	0.78	0.30	135,152,161,165	0
21	CLA	P	503	65/65	0.78	1.06	144,174,187,195	0
21	CLA	N	616	65/65	0.78	0.57	156,167,181,184	0
30	BCR	W	101	40/40	0.78	0.79	164,176,182,186	0
30	BCR	B	619	40/40	0.79	0.25	140,156,169,178	0
27	LMG	P	520	48/55	0.79	0.58	147,168,177,184	0
30	BCR	C	515	40/40	0.79	0.66	139,164,177,180	0
21	CLA	B	608	65/65	0.79	0.72	147,165,180,186	0
21	CLA	C	511	65/65	0.79	0.47	155,172,181,184	0
21	CLA	G	403	65/65	0.79	0.32	123,139,149,162	0
30	BCR	N	621	40/40	0.79	0.21	132,154,165,172	0
26	SQD	G	401	54/54	0.80	0.37	158,176,209,210	0
26	SQD	A	409	51/54	0.80	0.35	156,178,191,194	0
21	CLA	B	615	65/65	0.80	0.67	162,178,191,194	0
21	CLA	N	614	65/65	0.80	0.75	150,162,173,178	0
23	PL9	Q	405	55/55	0.80	0.22	137,146,166,170	0
21	CLA	B	612	65/65	0.80	0.55	152,163,174,176	0
30	BCR	T	102	40/40	0.80	0.30	143,167,176,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	PHO	Q	403	64/64	0.80	0.37	144,155,164,168	0
21	CLA	B	616	65/65	0.80	0.46	155,166,199,214	0
21	CLA	Q	404	65/65	0.81	0.60	152,162,187,194	0
21	CLA	P	501	65/65	0.81	0.96	149,170,185,188	0
21	CLA	P	512	65/65	0.81	1.30	172,184,194,199	0
34	HEM	V	201	43/43	0.81	0.43	139,151,166,173	0
21	CLA	A	402	65/65	0.81	0.25	139,147,158,164	0
27	LMG	Q	407	48/55	0.82	0.25	142,156,168,176	0
21	CLA	B	603	65/65	0.82	1.03	147,166,178,179	0
27	LMG	N	623	49/55	0.82	0.27	139,152,164,171	0
26	SQD	S	102	45/54	0.82	0.58	160,188,201,203	0
27	LMG	D	407	48/55	0.82	0.32	145,159,169,175	0
21	CLA	B	610	65/65	0.82	0.58	146,163,174,176	0
21	CLA	P	505	65/65	0.82	0.37	134,164,180,183	0
21	CLA	B	606	65/65	0.82	0.55	156,173,194,204	0
21	CLA	B	609	65/65	0.82	0.79	162,177,185,186	0
21	CLA	P	510	65/65	0.82	0.69	145,161,170,178	0
21	CLA	B	614	65/65	0.83	0.28	157,172,181,184	0
24	DGD	C	516	53/66	0.83	0.34	141,158,168,170	0
21	CLA	P	504	65/65	0.83	0.46	155,169,181,186	0
24	DGD	P	519	66/66	0.83	0.32	142,157,177,186	0
24	DGD	P	518	62/66	0.83	0.44	144,168,195,200	0
21	CLA	D	403	65/65	0.83	0.89	153,160,181,189	0
34	HEM	i	201	43/43	0.83	0.49	131,158,169,172	0
25	LHG	A	408	39/49	0.83	0.35	146,167,179,179	0
24	DGD	W	102	58/66	0.84	0.34	145,157,168,172	0
21	CLA	G	402	65/65	0.84	0.43	136,148,155,166	0
30	BCR	P	515	40/40	0.84	1.38	165,176,185,189	0
30	BCR	S	101	40/40	0.84	0.63	145,159,176,178	0
27	LMG	M	101	42/55	0.84	0.32	166,174,184,188	0
27	LMG	Q	406	46/55	0.84	0.41	135,162,171,180	0
21	CLA	P	506	65/65	0.84	0.43	159,176,194,202	0
21	CLA	N	612	65/65	0.84	0.50	151,164,181,190	0
27	LMG	G	411	51/55	0.85	0.24	152,164,177,178	0
21	CLA	B	602	65/65	0.85	0.72	152,172,182,185	0
21	CLA	N	618	65/65	0.85	0.31	153,171,180,185	0
34	HEM	E	101	43/43	0.85	0.36	166,179,188,190	0
21	CLA	C	504	65/65	0.85	0.29	153,172,198,204	0
30	BCR	Z	101	40/40	0.85	1.17	163,178,192,197	0
27	LMG	e	102	42/55	0.85	0.30	155,166,183,191	0
24	DGD	P	517	53/66	0.85	0.33	141,160,173,176	0
21	CLA	A	401	65/65	0.86	0.27	138,146,156,160	0

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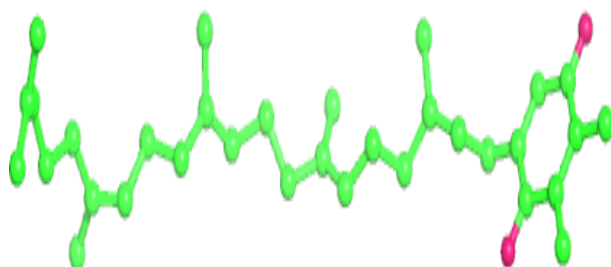
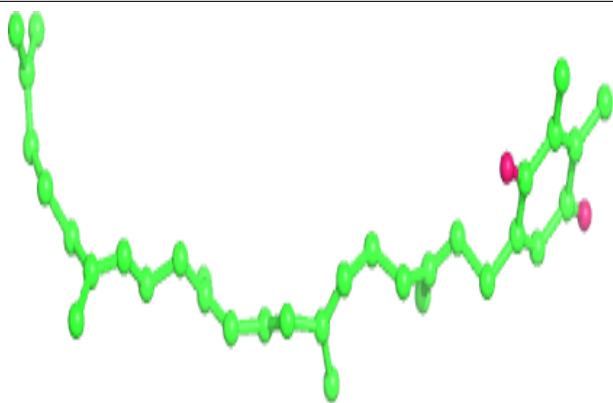
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	PL9	D	404	55/55	0.86	0.23	129,150,158,160	0
21	CLA	N	606	65/65	0.86	0.37	152,172,178,182	0
33	CL	G	415	1/1	0.86	0.89	122,122,122,122	0
32	BCT	D	410	4/4	0.87	0.35	166,167,167,169	0
27	LMG	A	410	51/55	0.87	0.30	138,157,168,171	0
23	PL9	A	406	45/55	0.88	0.51	152,174,185,188	0
21	CLA	N	611	65/65	0.88	0.29	145,156,164,166	0
25	LHG	G	409	39/49	0.88	0.39	156,168,188,191	0
27	LMG	N	622	49/55	0.88	0.28	145,154,172,174	0
21	CLA	N	615	65/65	0.88	0.30	152,158,168,173	0
21	CLA	B	613	65/65	0.88	0.30	148,160,171,175	0
32	BCT	Q	411	4/4	0.89	0.41	164,166,168,173	0
27	LMG	D	406	46/55	0.89	0.36	140,153,176,181	0
21	CLA	N	617	65/65	0.89	0.29	149,168,182,188	0
21	CLA	C	510	65/65	0.89	0.28	149,161,171,178	0
29	FE2	A	413	1/1	0.89	0.17	166,166,166,166	0
21	CLA	B	611	65/65	0.89	0.32	149,160,167,169	0
21	CLA	P	508	65/65	0.89	0.43	157,168,182,193	0
28	OEC	G	413	5/9	0.90	0.47	91,102,115,124	0
34	HEM	R	101	43/43	0.90	0.50	164,184,192,199	0
21	CLA	C	508	65/65	0.90	0.34	154,170,194,203	0
29	FE2	G	414	1/1	0.92	0.16	149,149,149,149	0
28	OEC	A	412	5/9	0.96	0.47	122,122,126,129	0

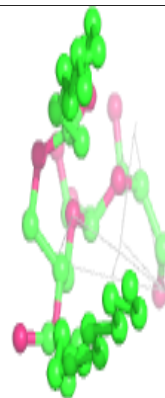
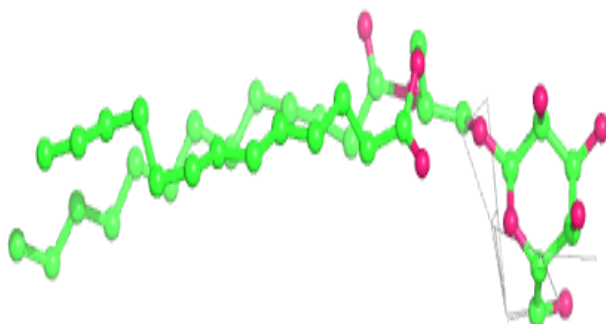
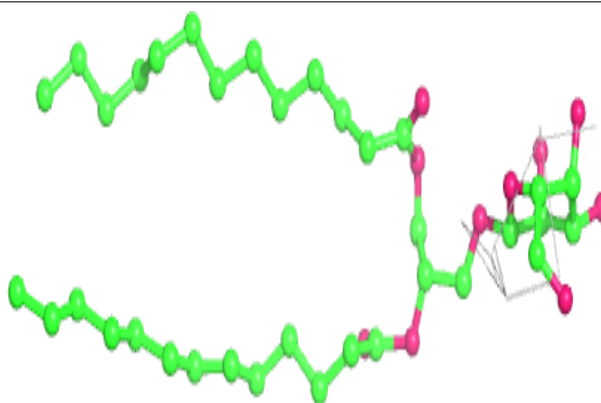
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PL9 b 101:

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

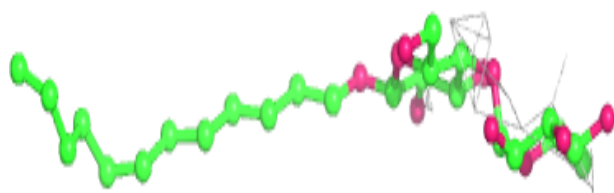
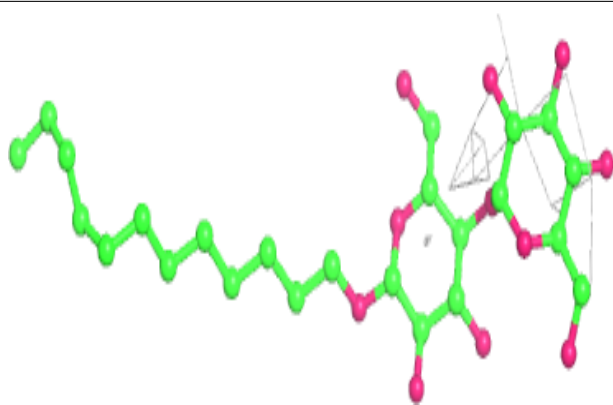
**Electron density around LMG C 520:**

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

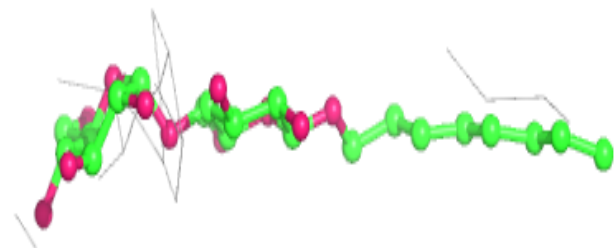
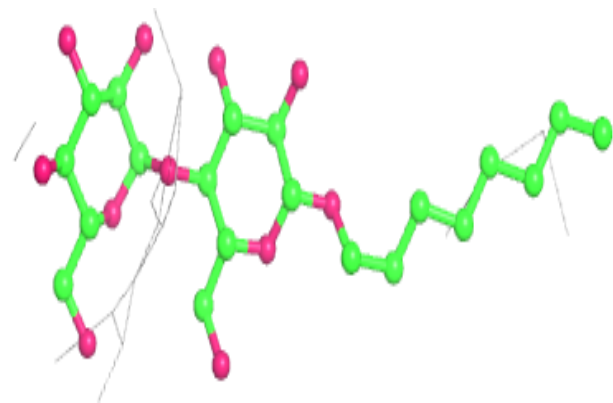


Electron density around LMT I 103:

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

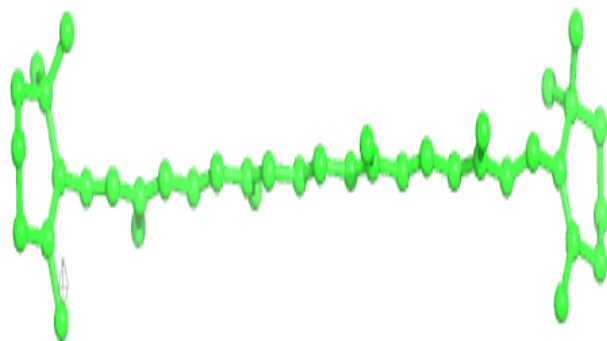
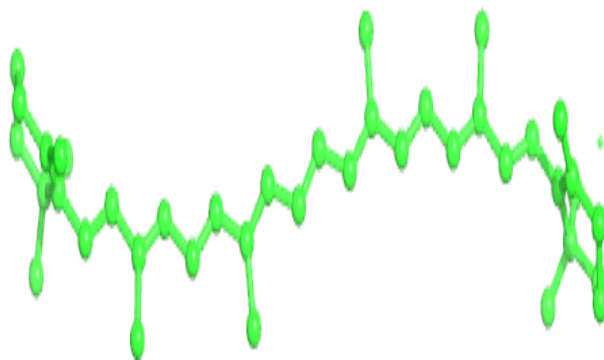
**Electron density around LMT Q 410:**

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

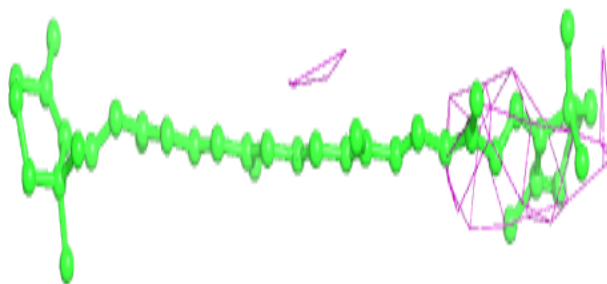
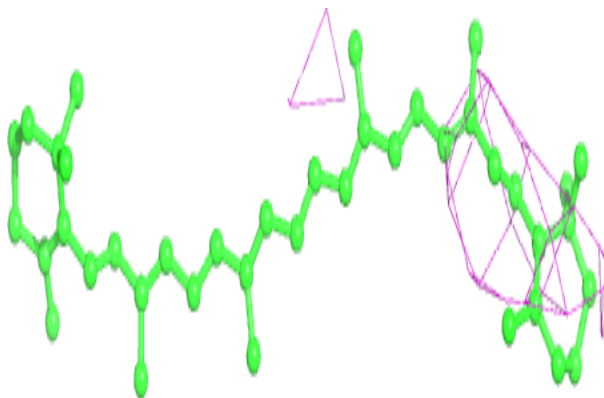


Electron density around BCR a 101:

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

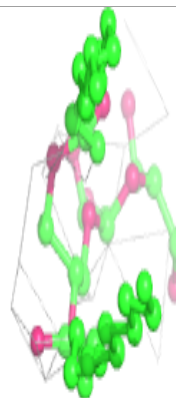
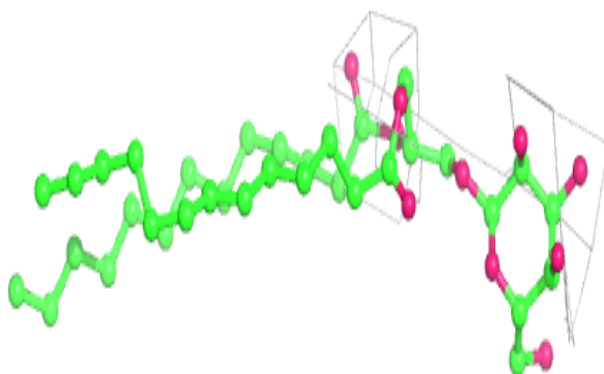
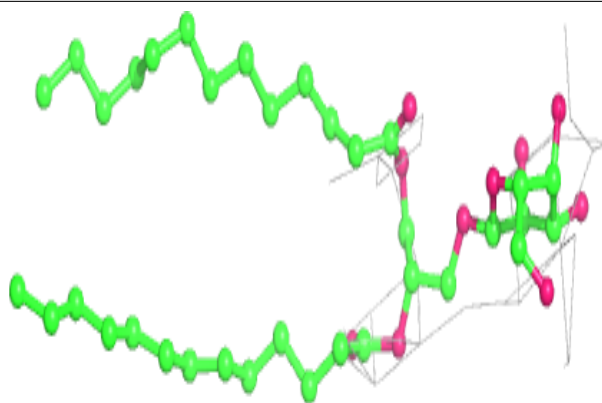
**Electron density around BCR c 101:**

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

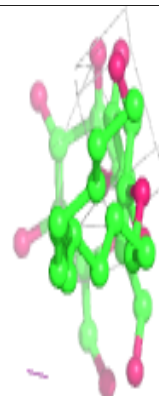
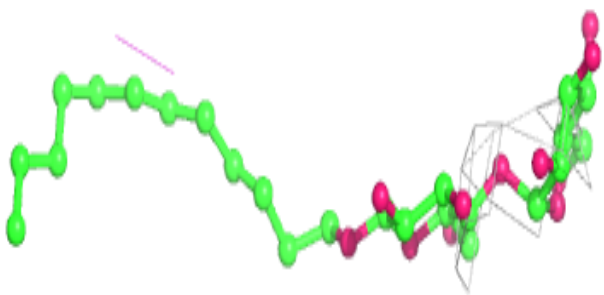
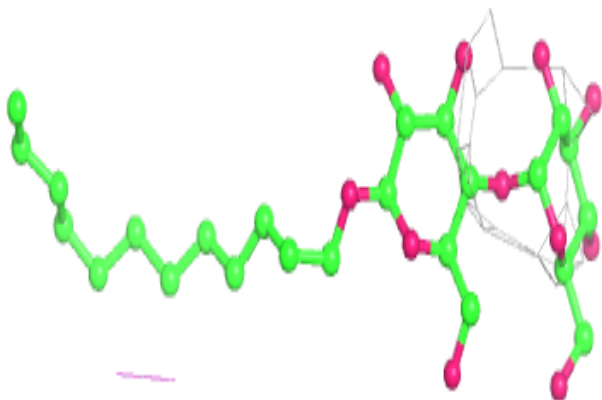


Electron density around LMG P 521:

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

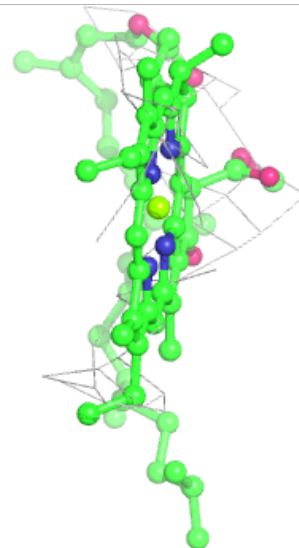
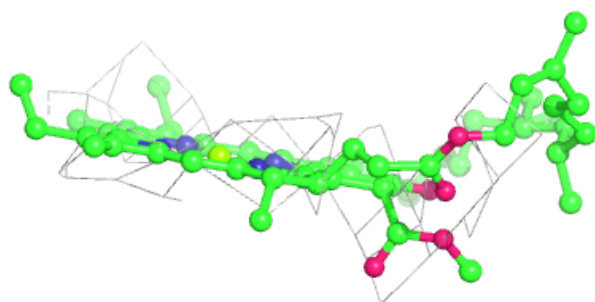
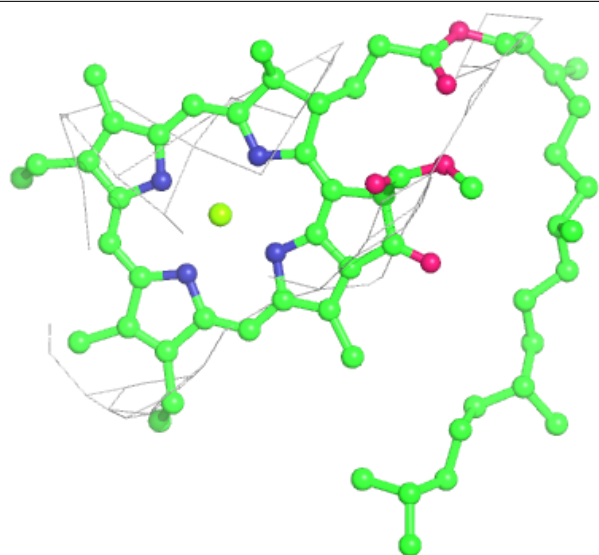
**Electron density around LMT N 624:**

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



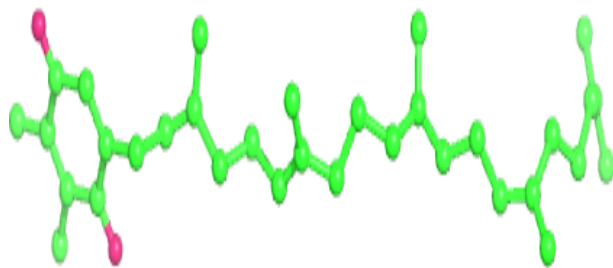
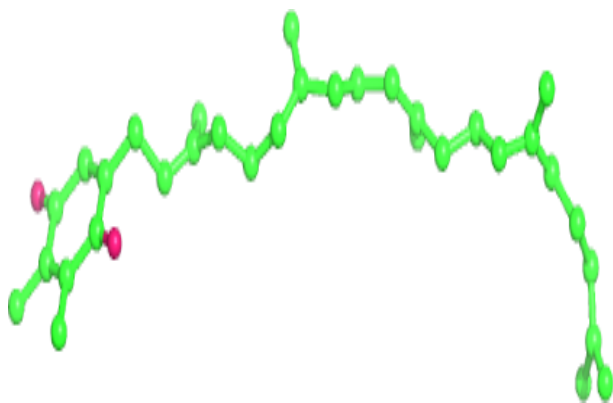
Electron density around CLA N 605:

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

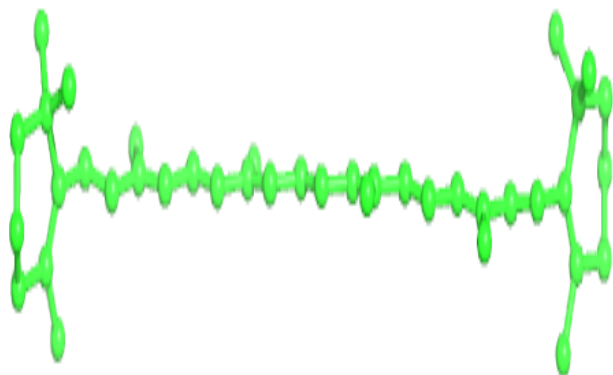
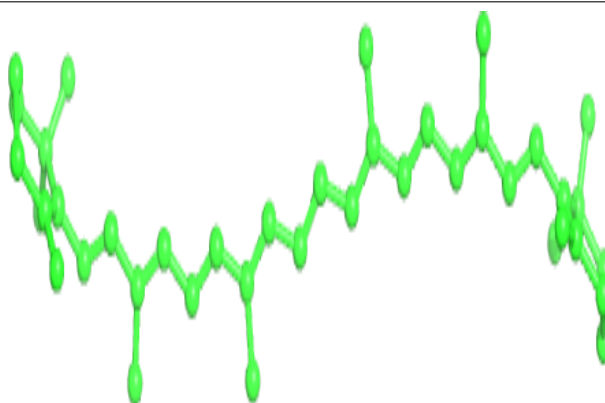


Electron density around PL9 J 101:

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

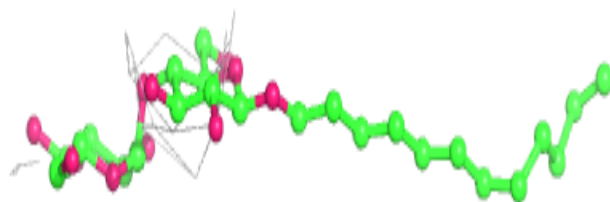
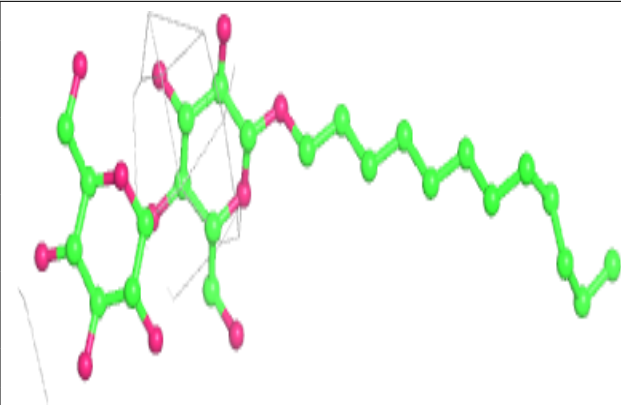
**Electron density around BCR I 101:**

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

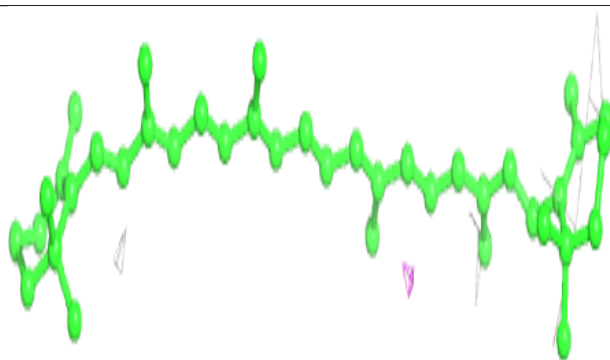
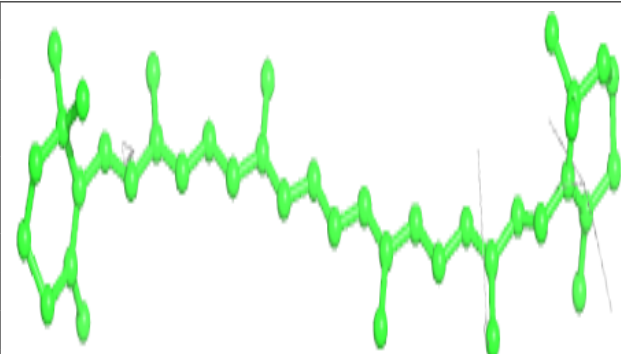


Electron density around LMT a 103:

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

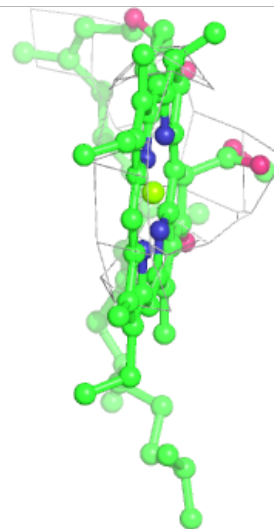
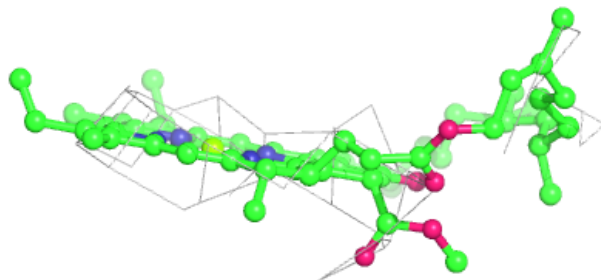
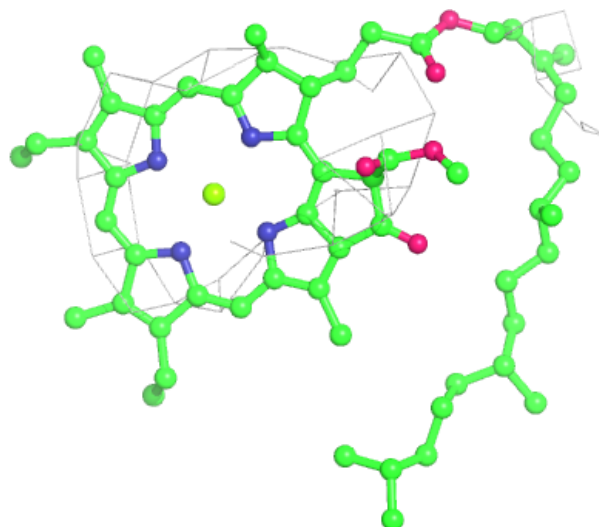
**Electron density around BCR T 103:**

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



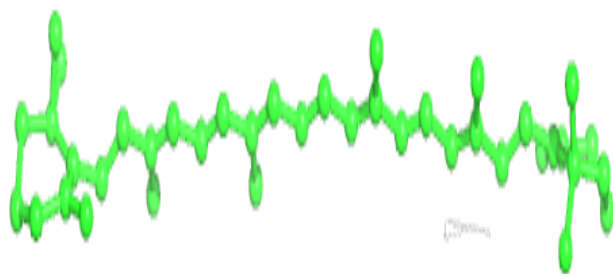
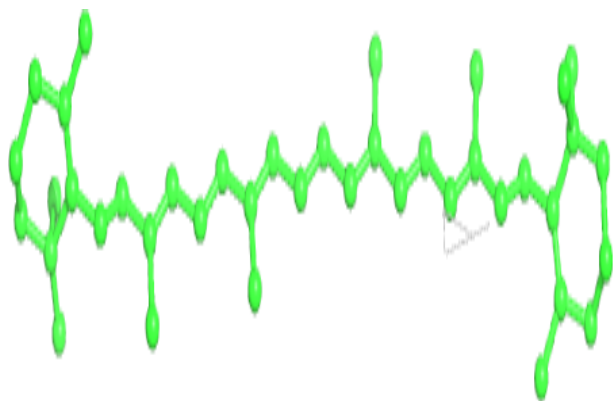
Electron density around CLA B 601:

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

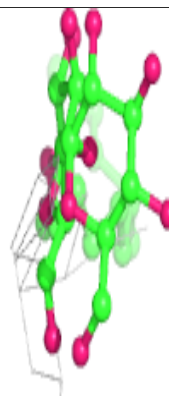
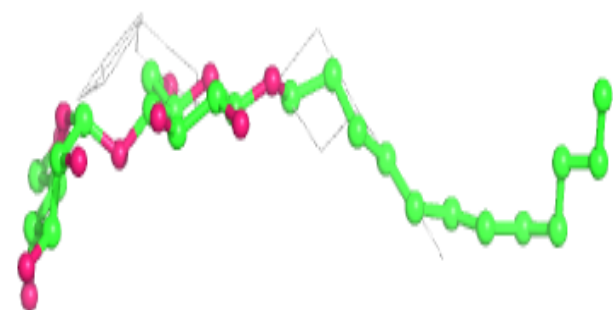
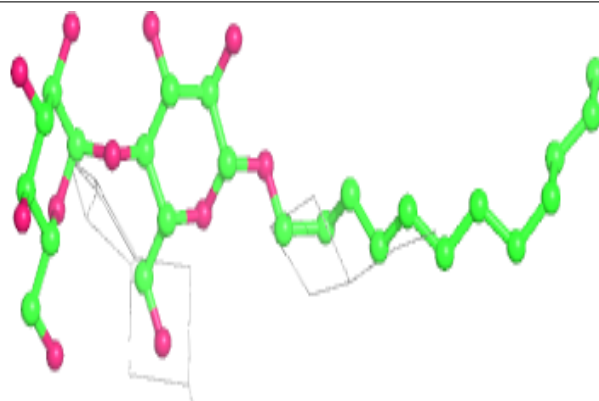


Electron density around BCR J 102:

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

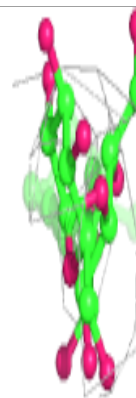
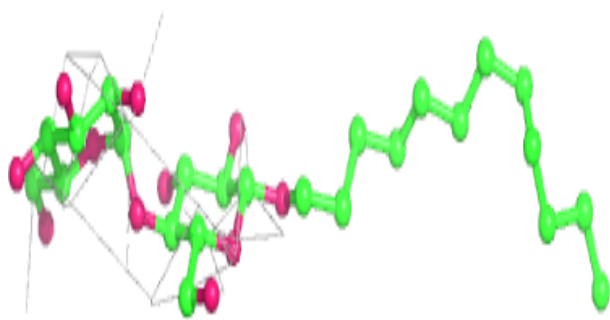
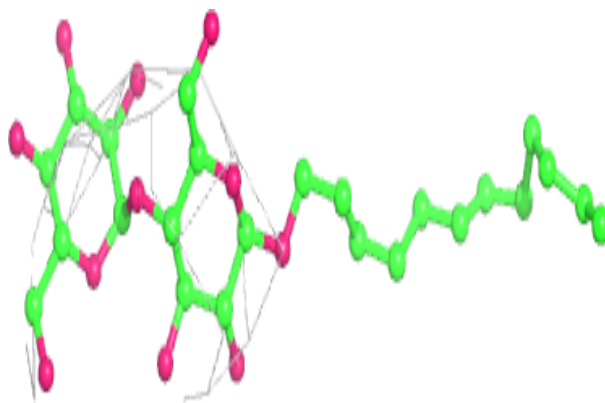
**Electron density around LMT B 625:**

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

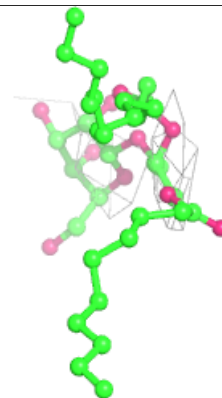
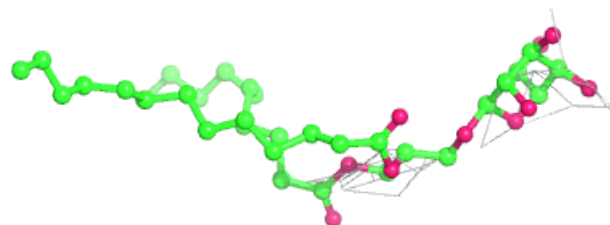
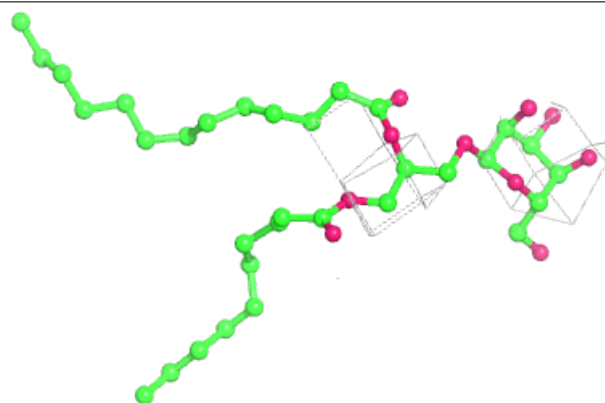


Electron density around LMT N 603:

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

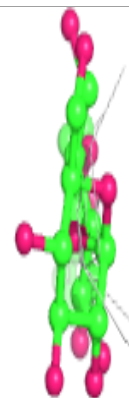
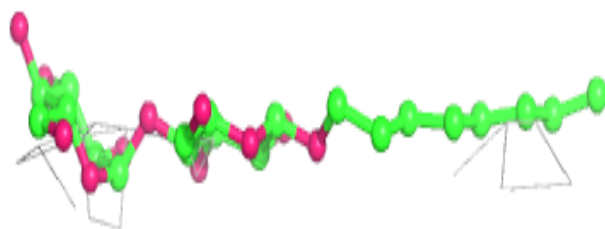
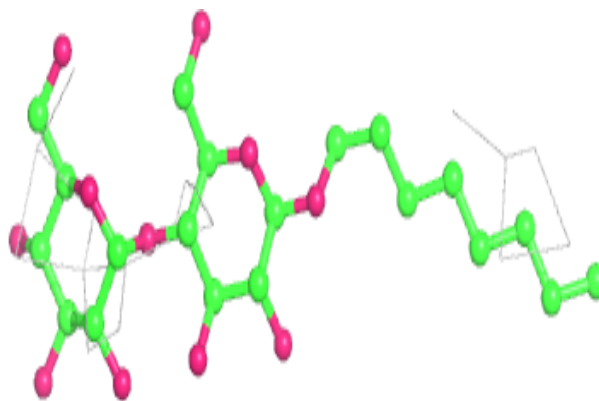
**Electron density around LMG D 412:**

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

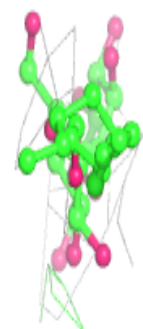
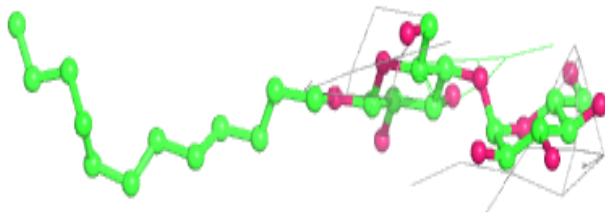
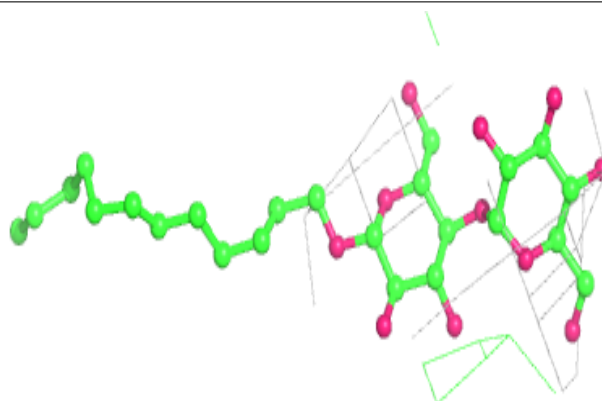


Electron density around LMT D 409:

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

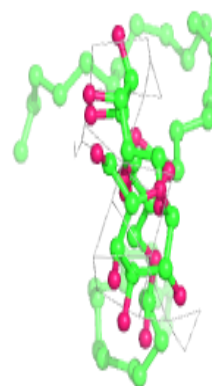
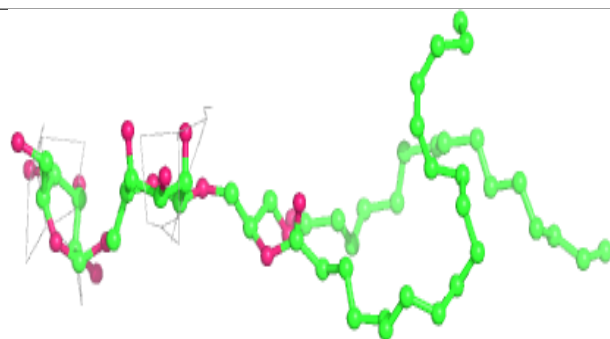
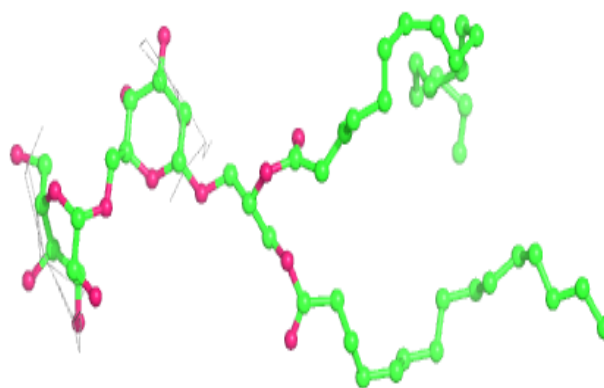
**Electron density around LMT B 629:**

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

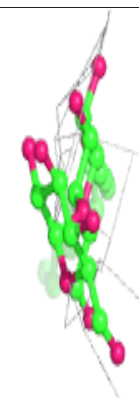
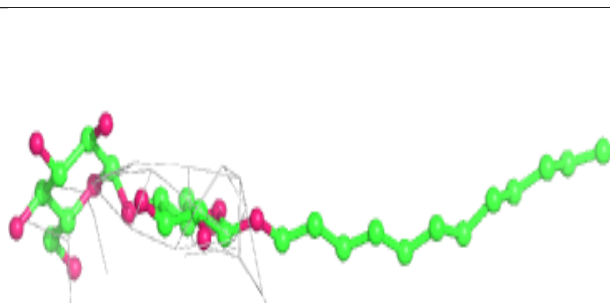
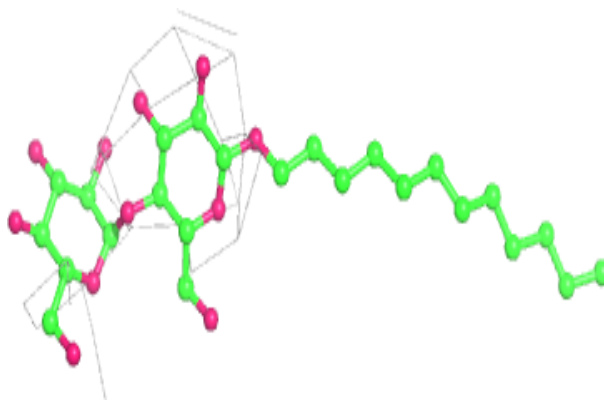


Electron density around DGD D 408:

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

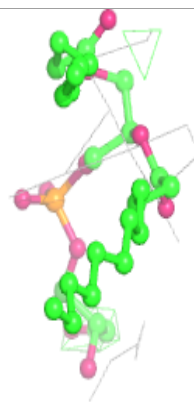
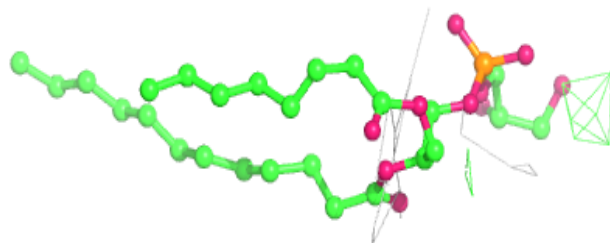
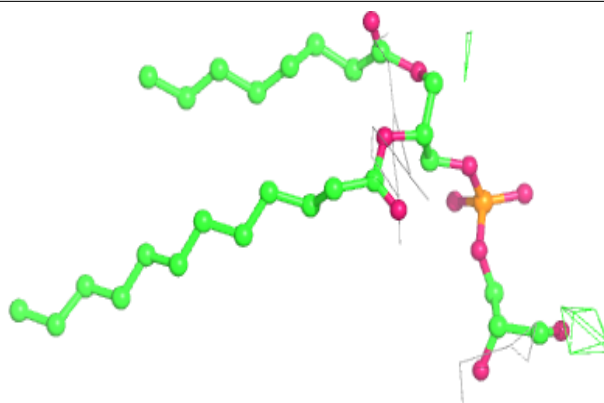
**Electron density around LMT N 625:**

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

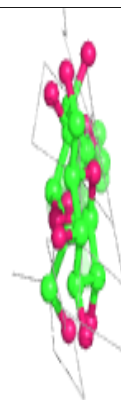
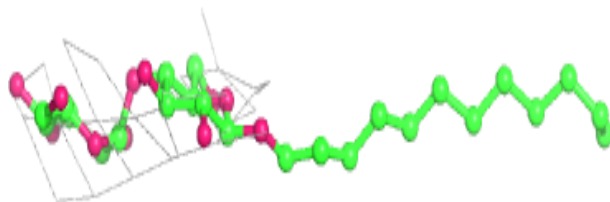
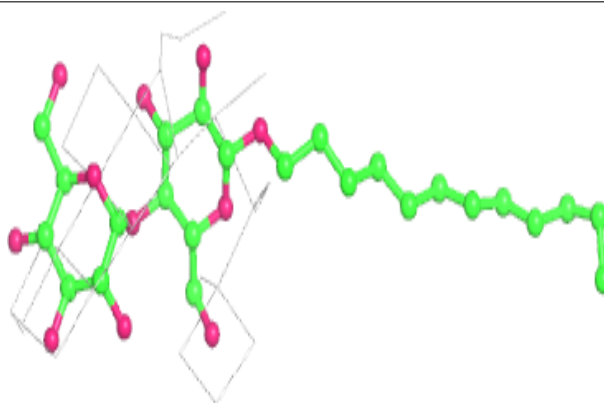


Electron density around LHG G 412:

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

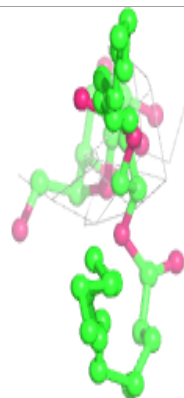
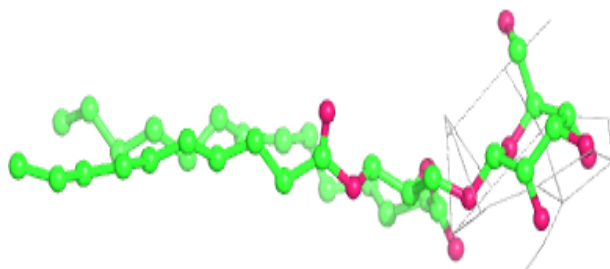
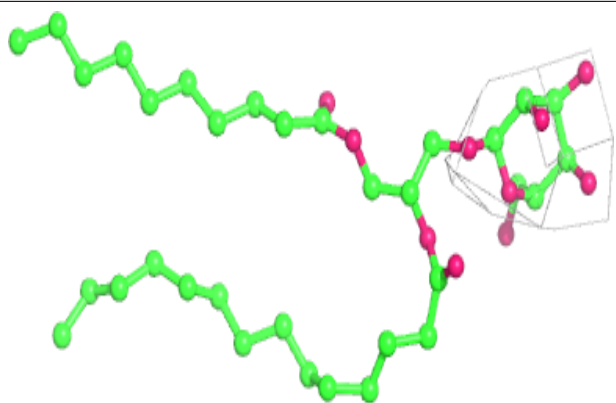
**Electron density around LMT N 604:**

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

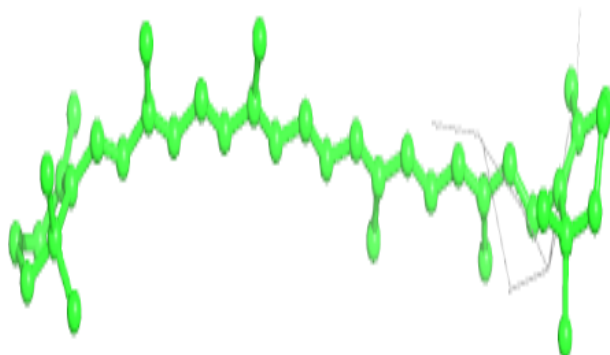
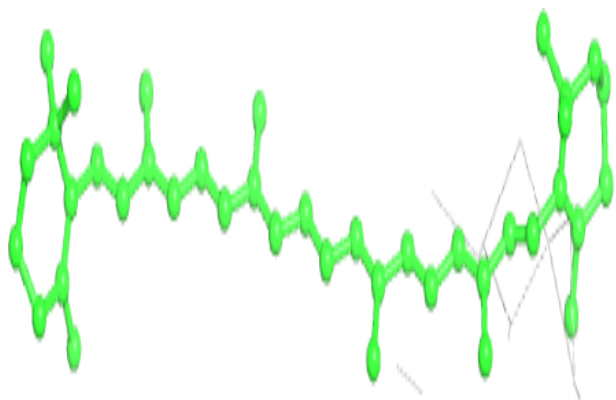


Electron density around LMG I 102:

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

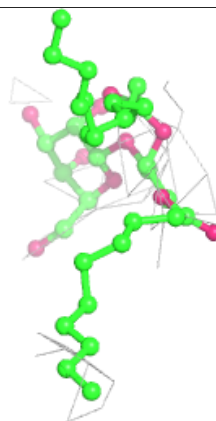
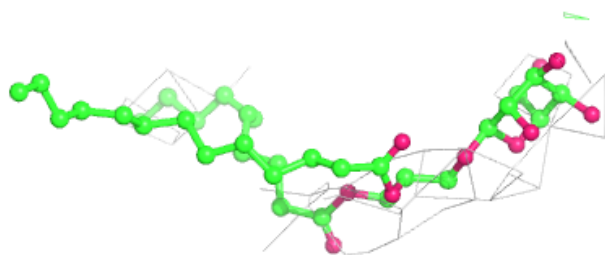
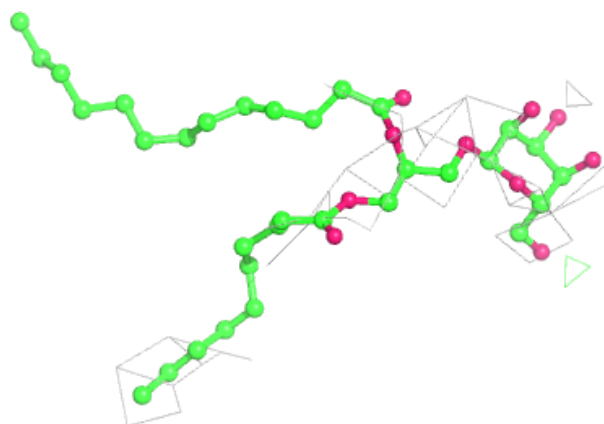
**Electron density around BCR B 620:**

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

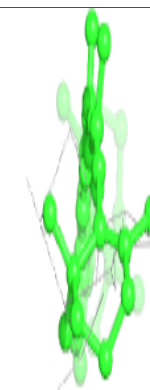
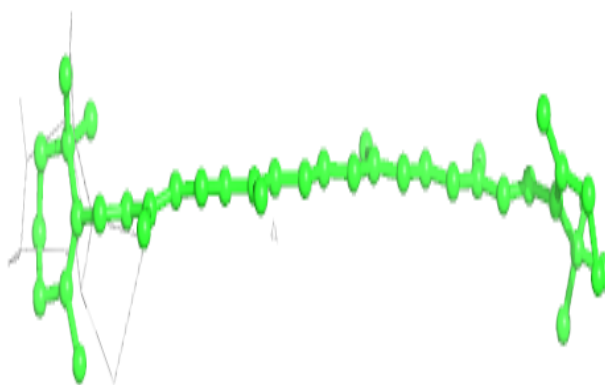
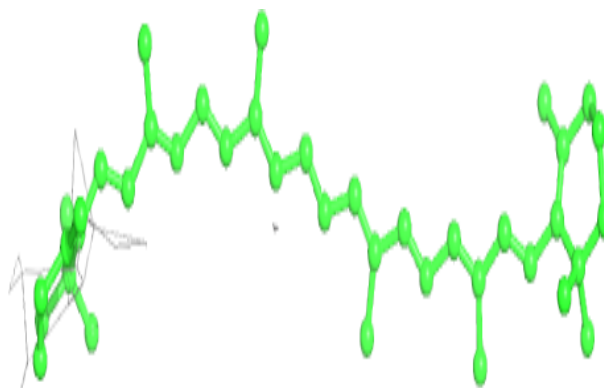


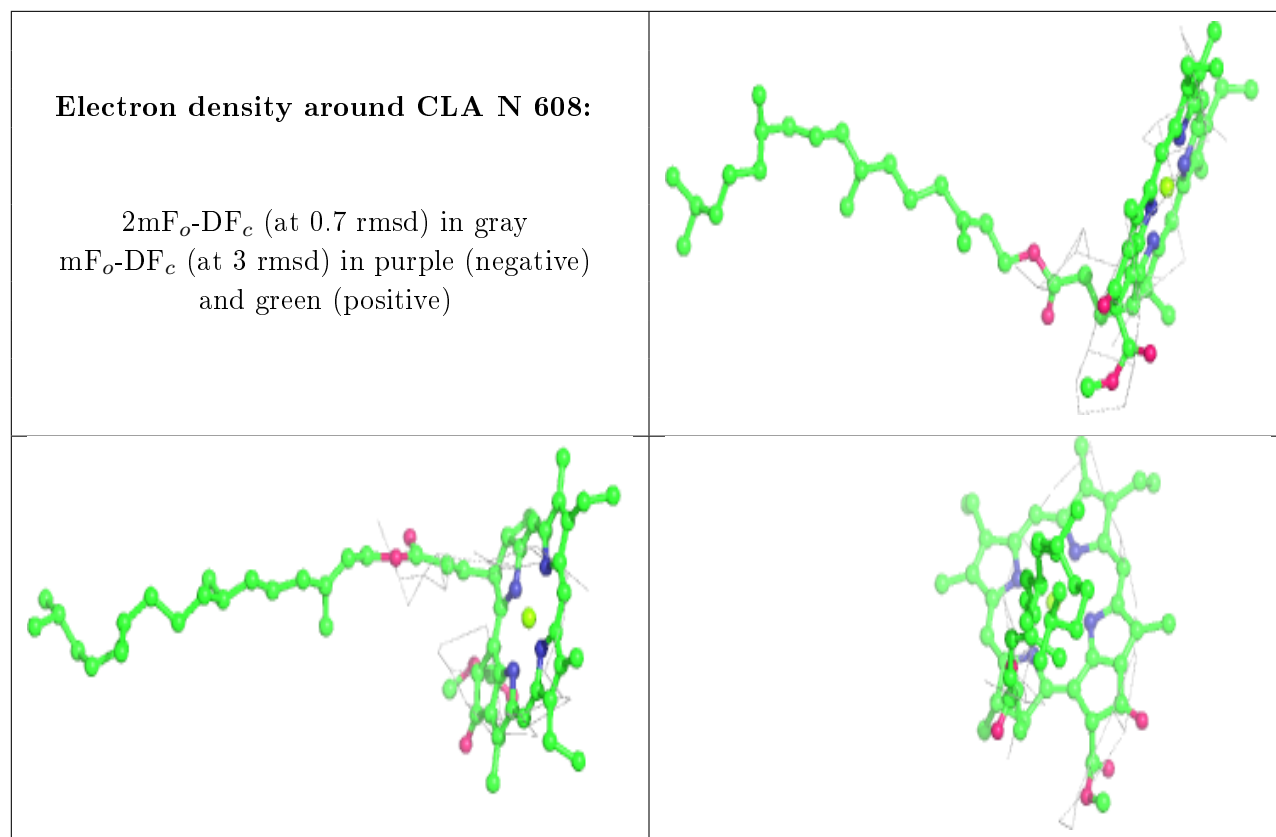
Electron density around LMG Q 401:

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

**Electron density around BCR H 101:**

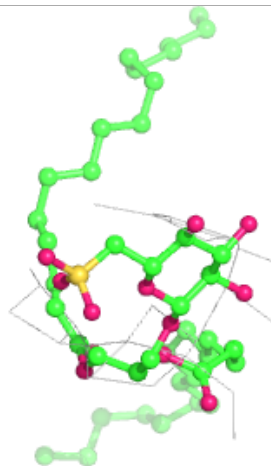
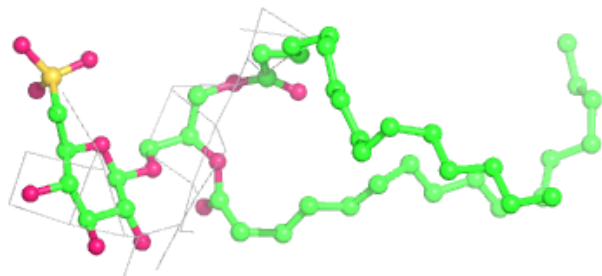
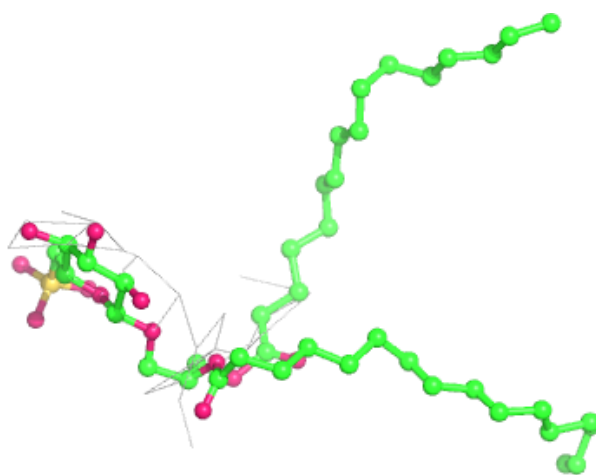
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





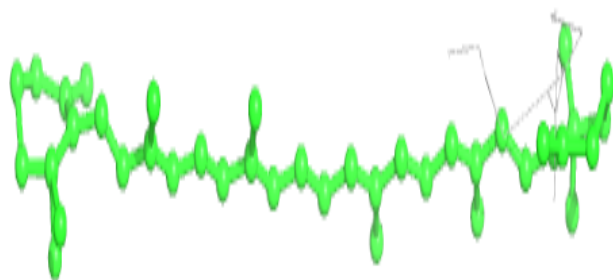
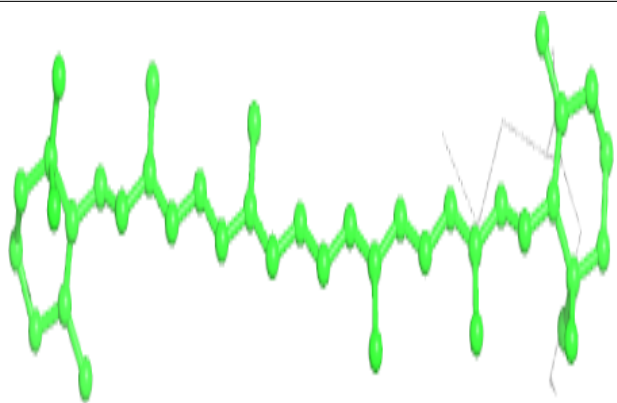
Electron density around SQD A 414:

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

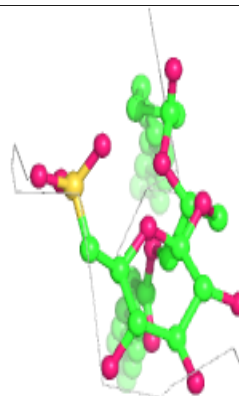
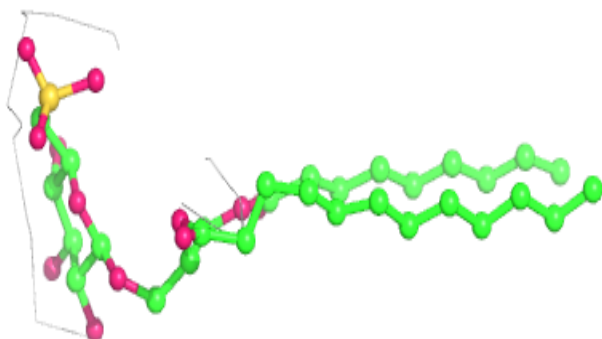
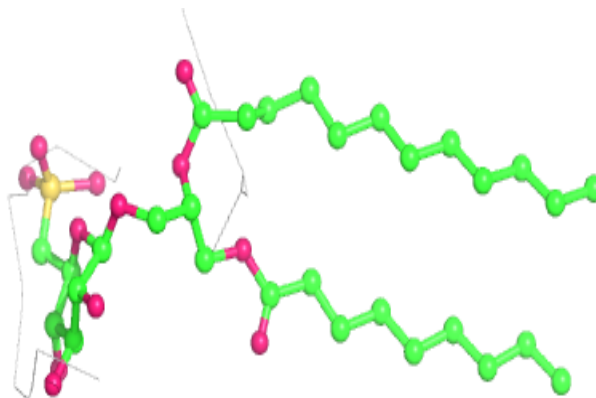


Electron density around BCR b 102:

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

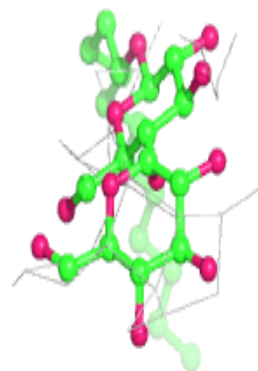
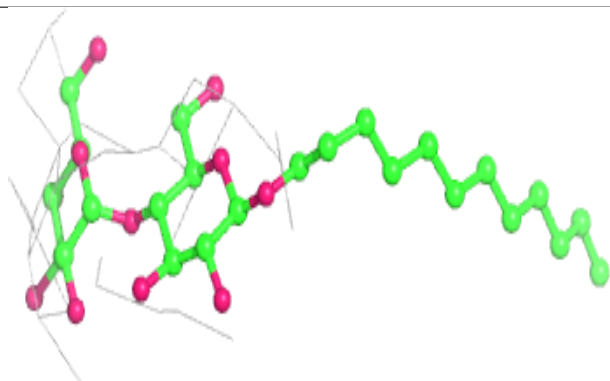
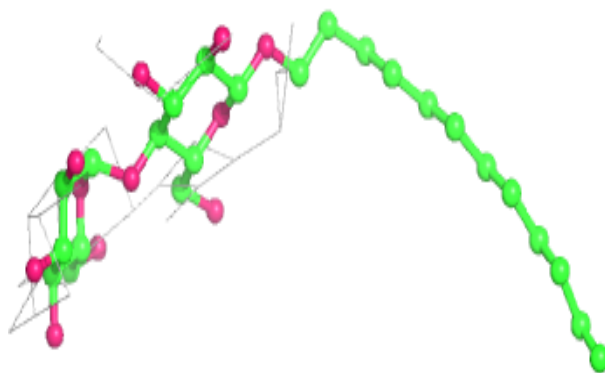
**Electron density around SQD Q 408:**

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

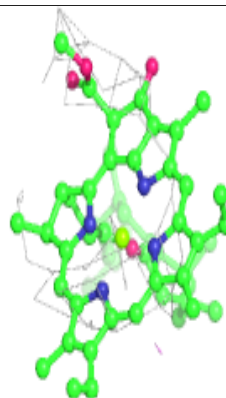
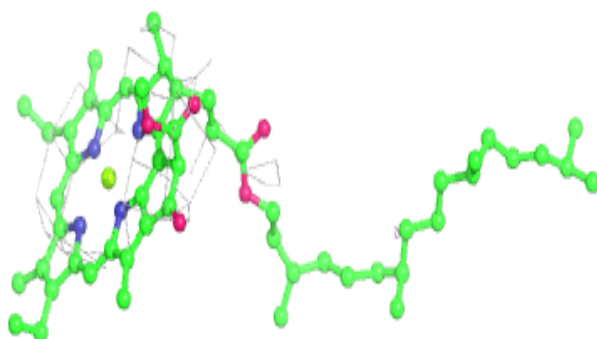
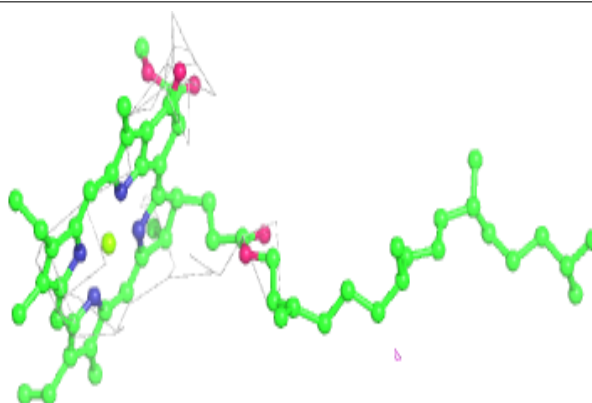


Electron density around LMT e 101:

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

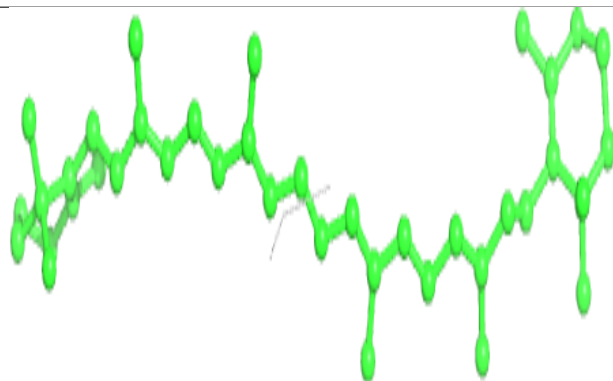
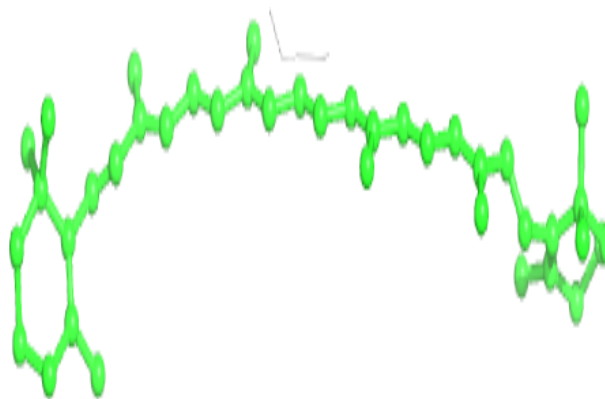
**Electron density around CLA P 502:**

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

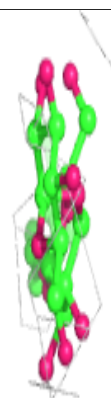
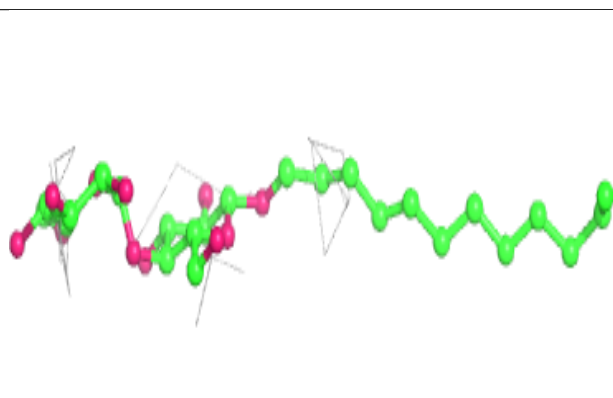
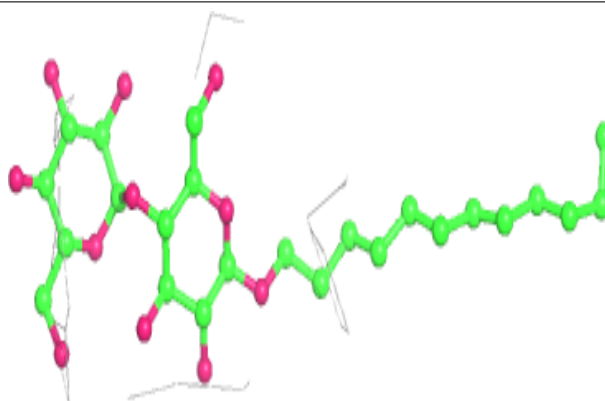


Electron density around BCR D 405:

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

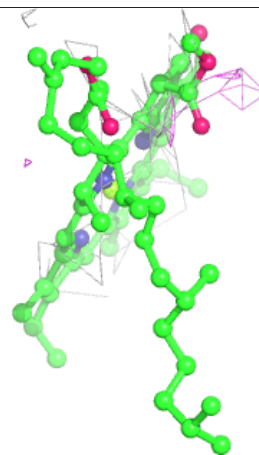
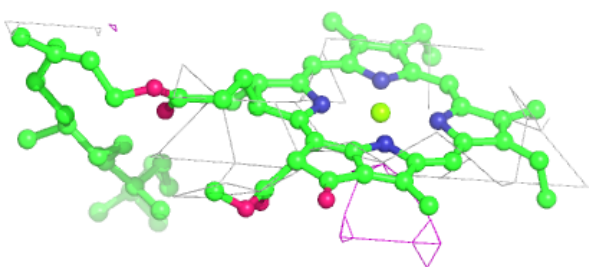
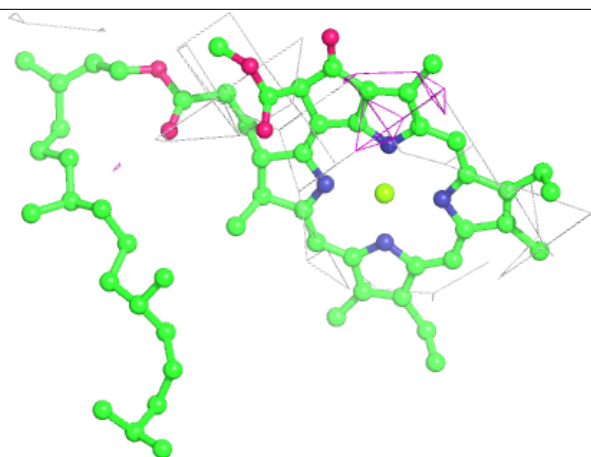
**Electron density around LMT B 630:**

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

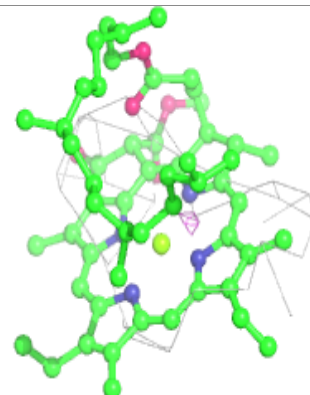
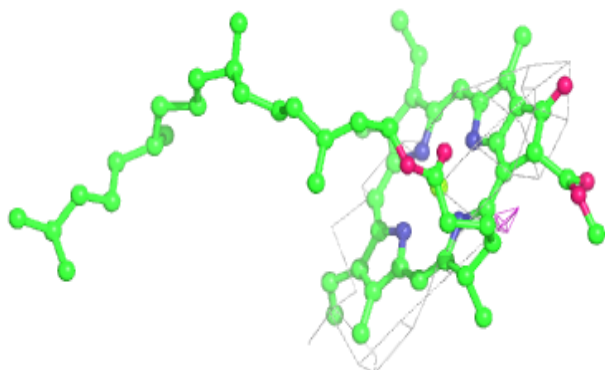
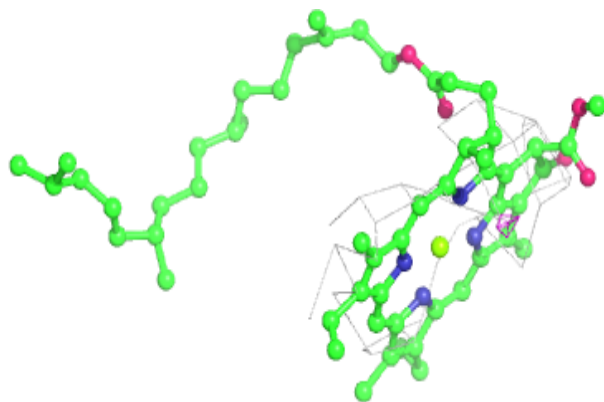


Electron density around CLA N 620:

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

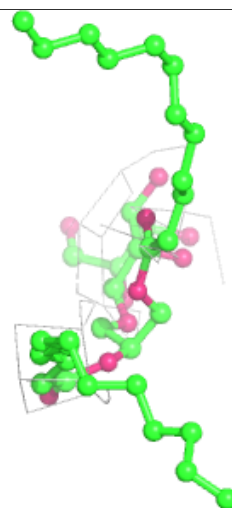
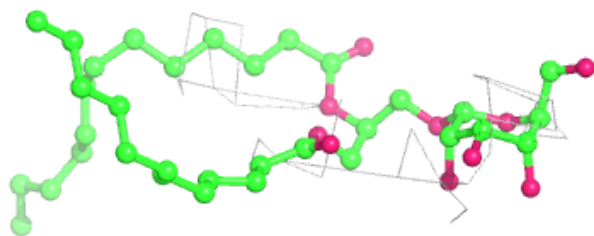
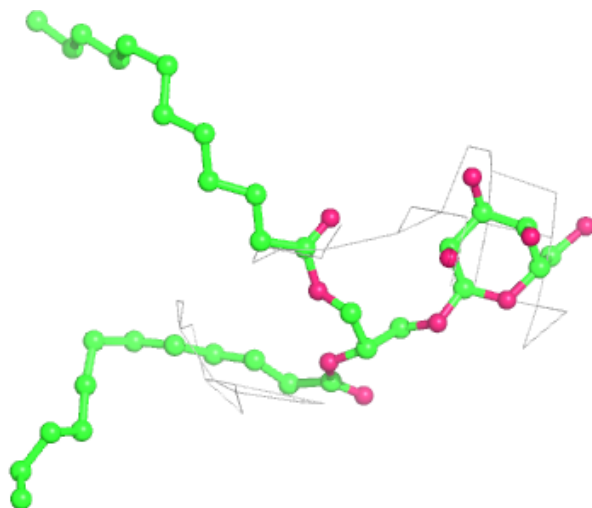
**Electron density around CLA C 513:**

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



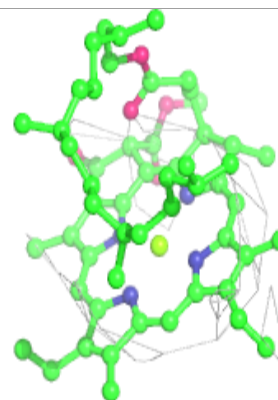
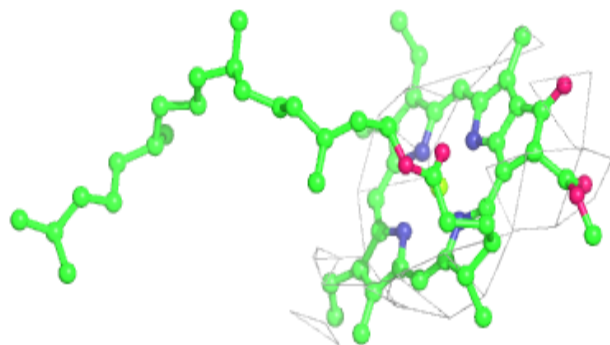
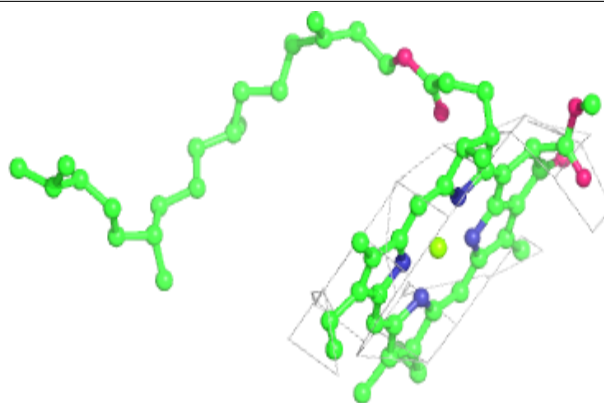
Electron density around LMG R 102:

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

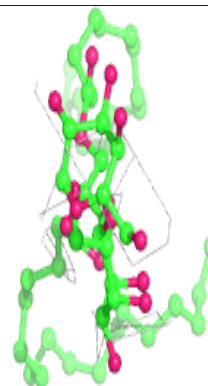
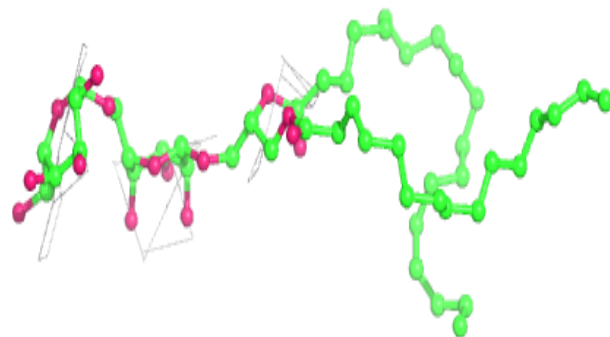
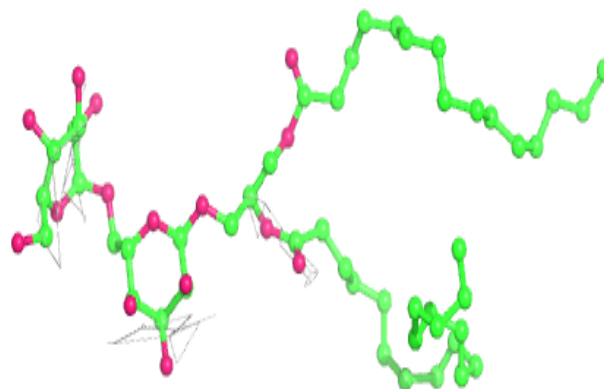


Electron density around CLA P 513:

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

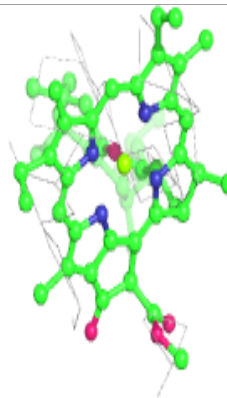
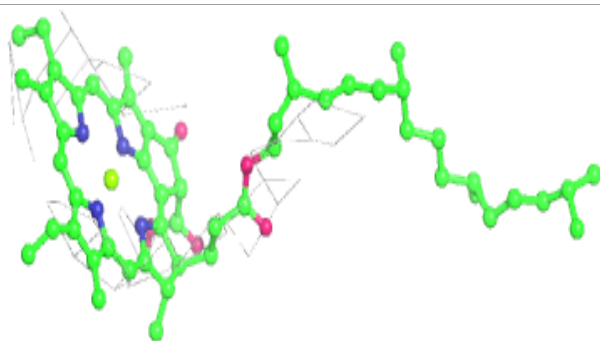
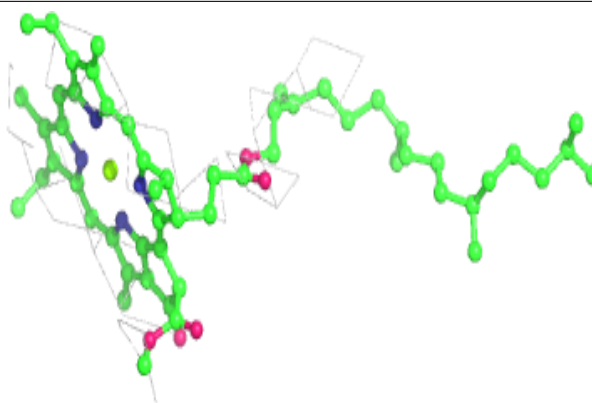
**Electron density around DGD Q 409:**

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

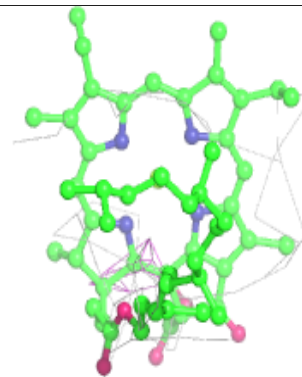
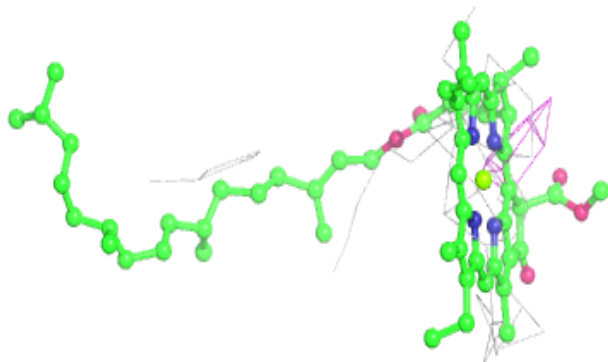
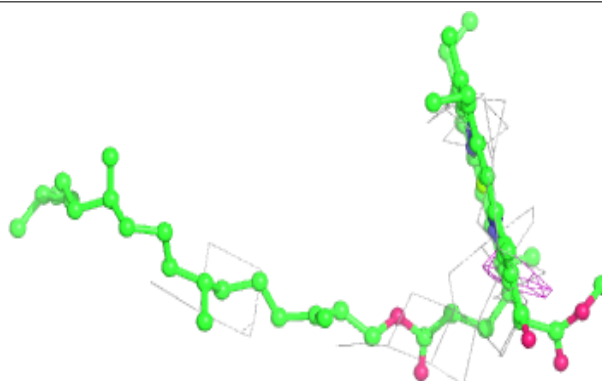


Electron density around CLA C 502:

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

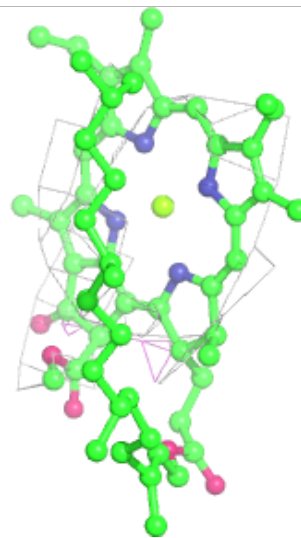
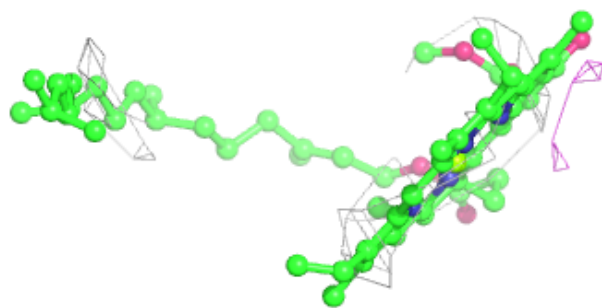
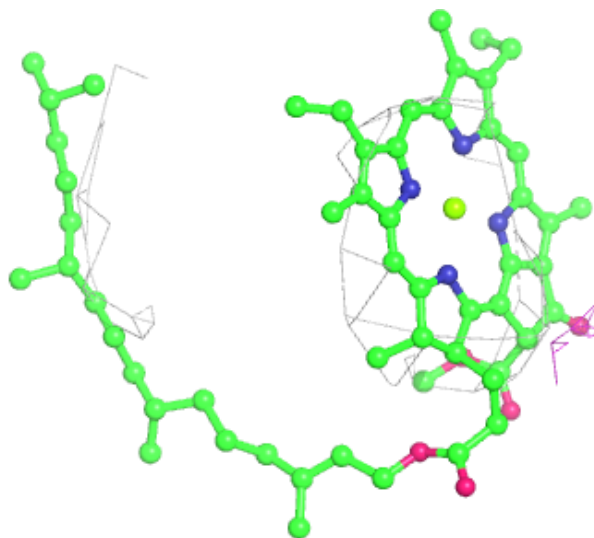
**Electron density around CLA N 609:**

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



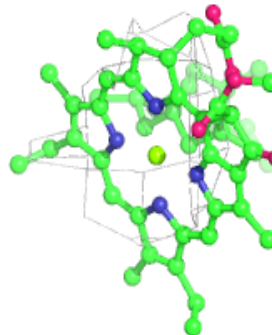
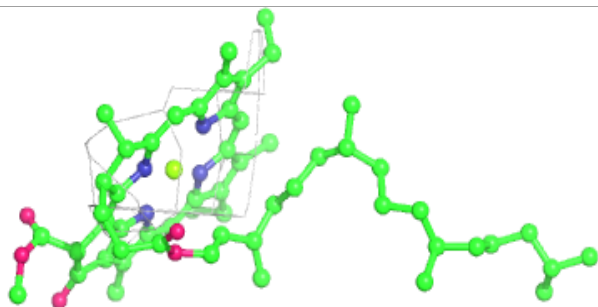
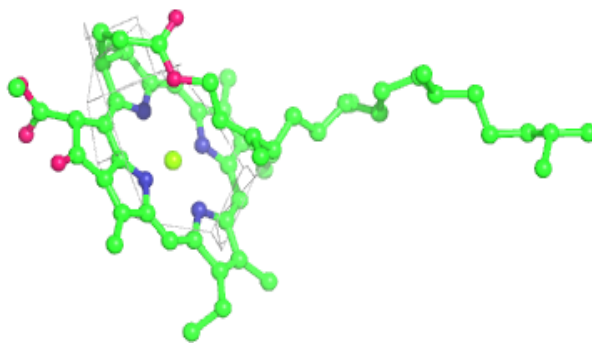
Electron density around CLA C 507:

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

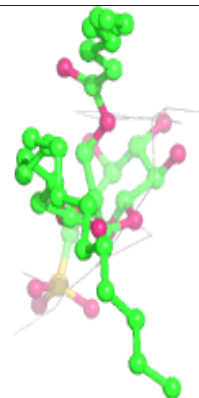
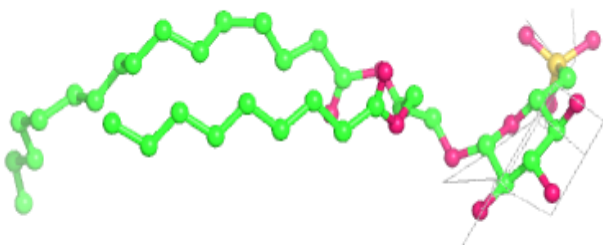
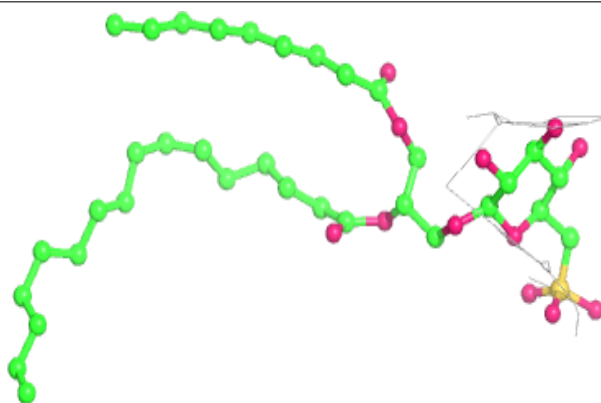


Electron density around CLA C 505:

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

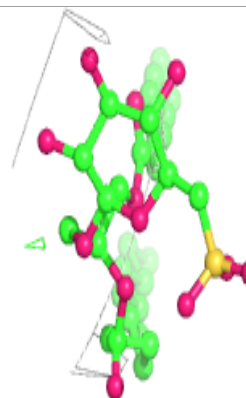
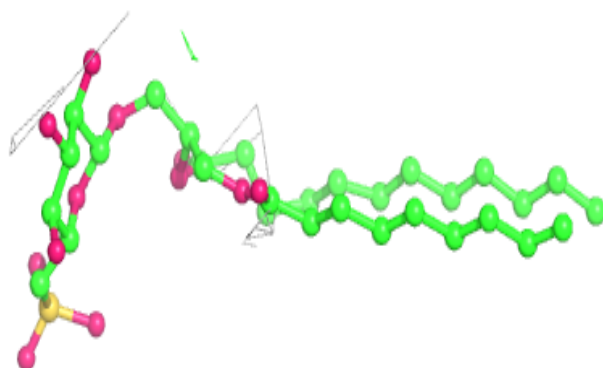
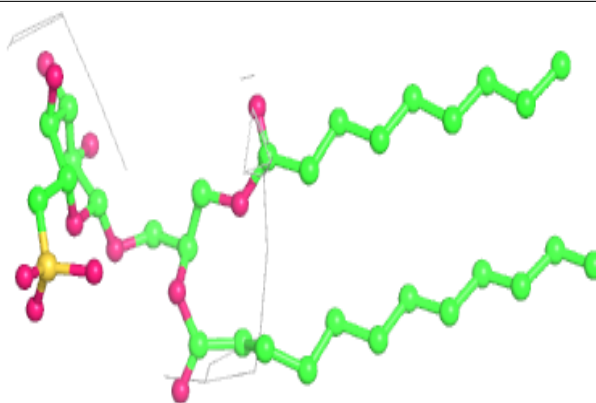
**Electron density around SQD B 627:**

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

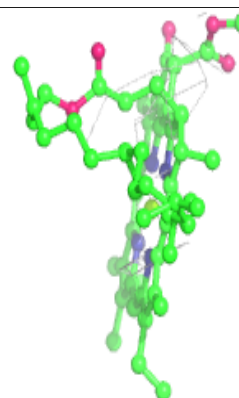
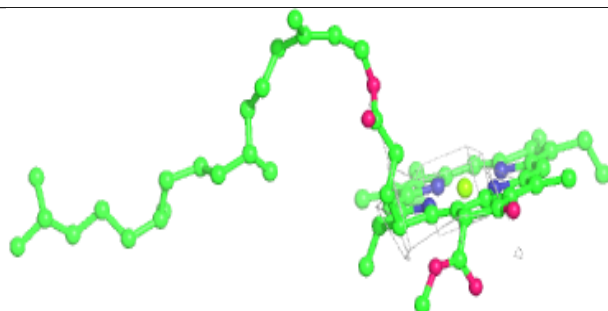
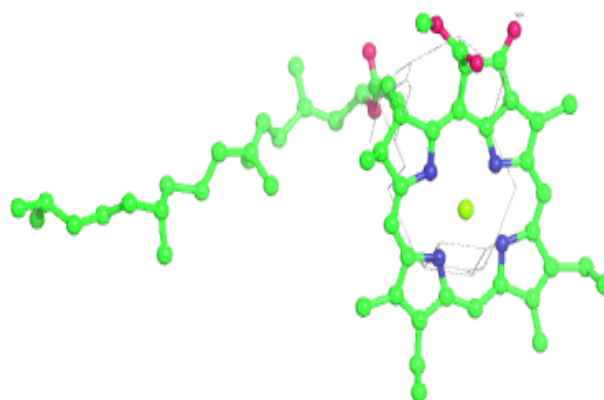


Electron density around SQD B 624:

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

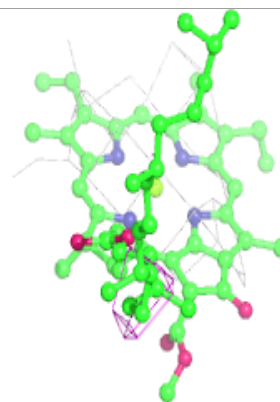
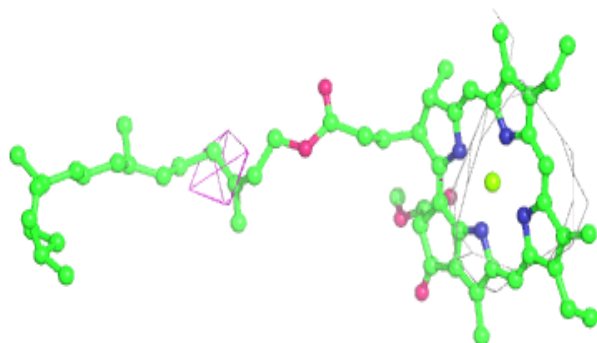
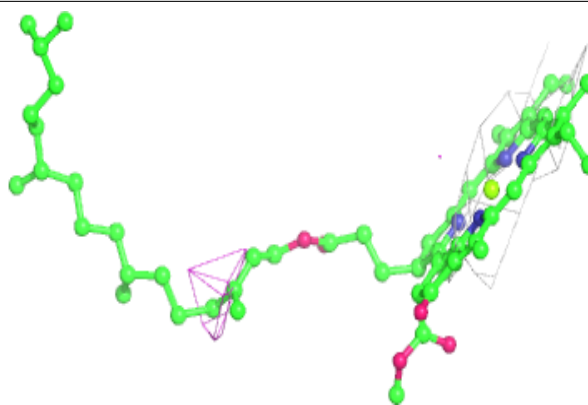
**Electron density around CLA A 403:**

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

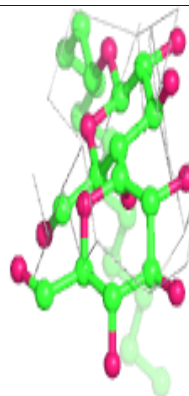
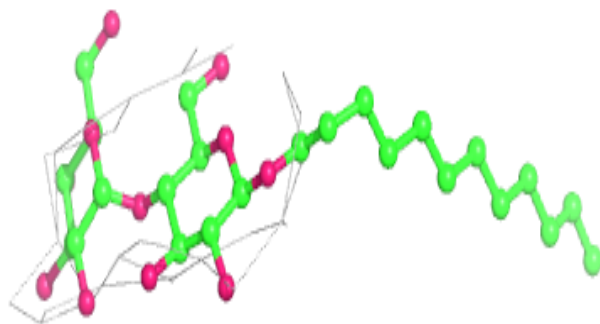
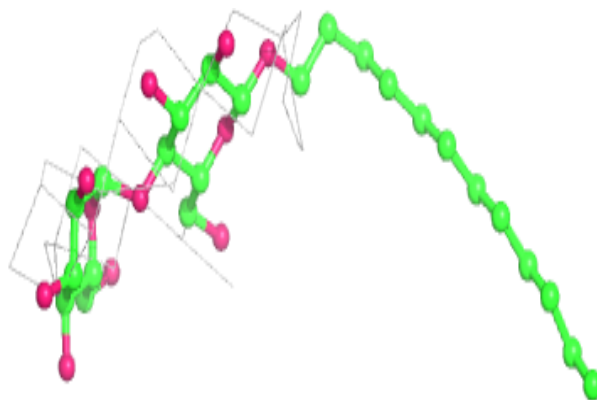


Electron density around CLA D 401:

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

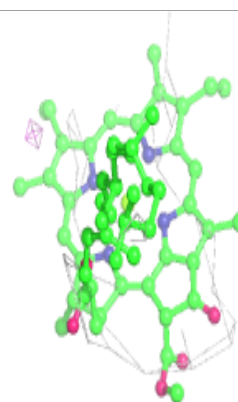
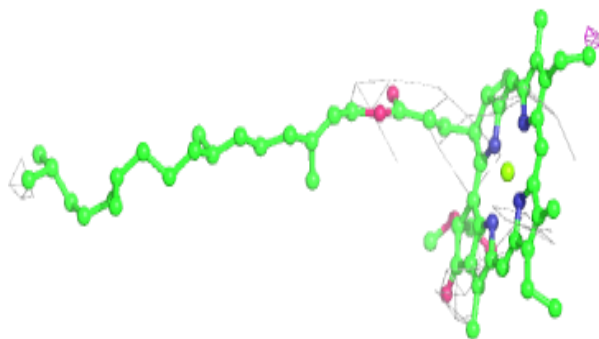
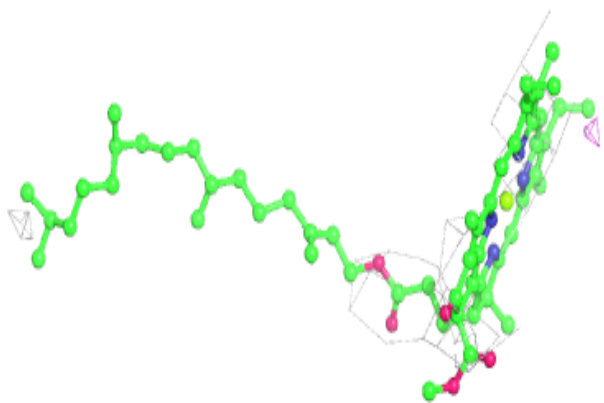
**Electron density around LMT M 102:**

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

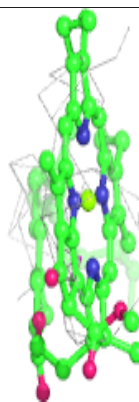
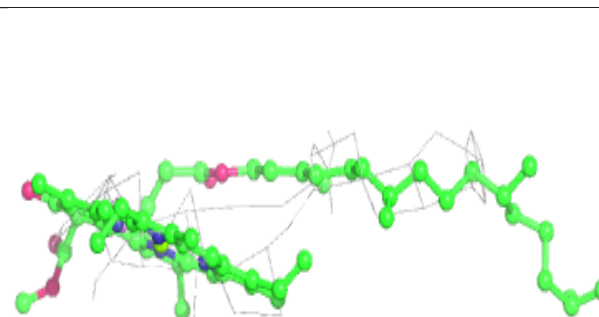
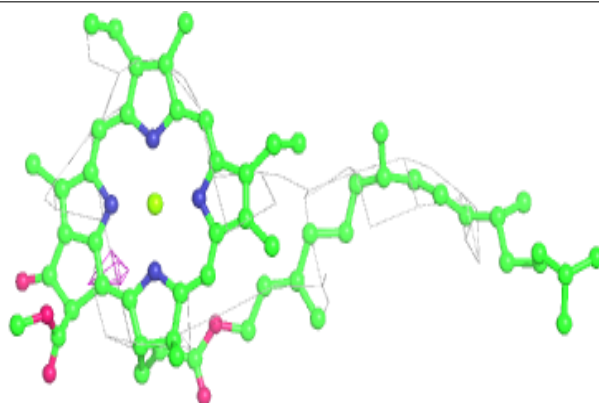


Electron density around CLA B 604:

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

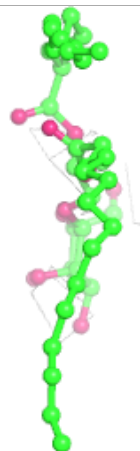
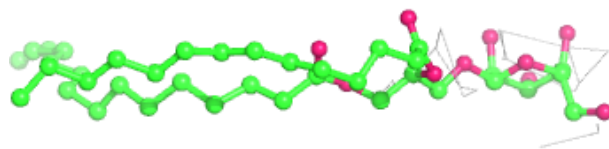
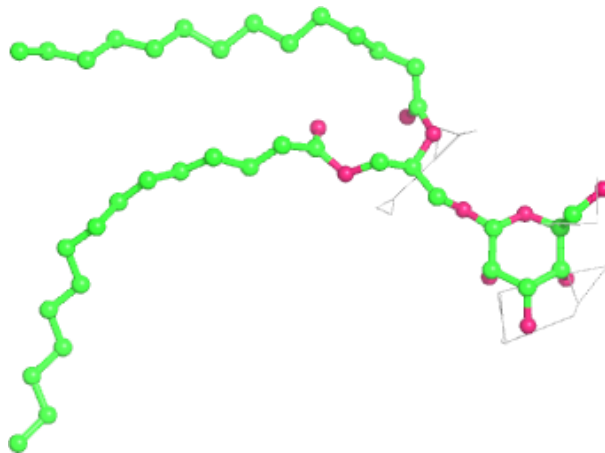
**Electron density around CLA N 607:**

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



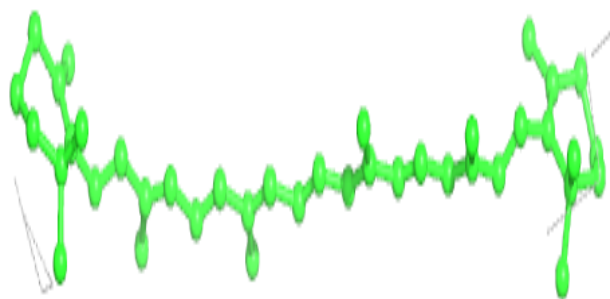
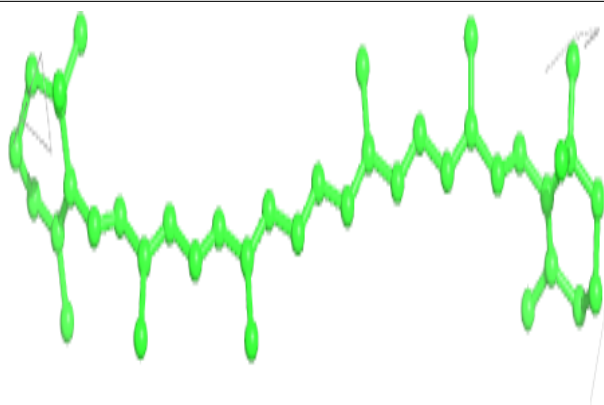
Electron density around LMG C 519:

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

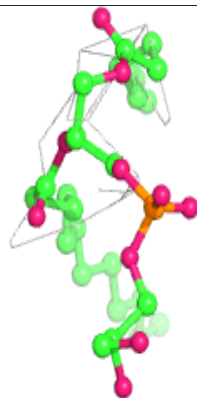
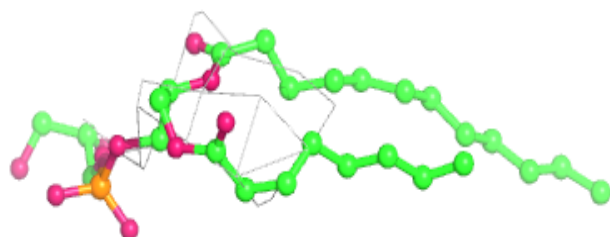
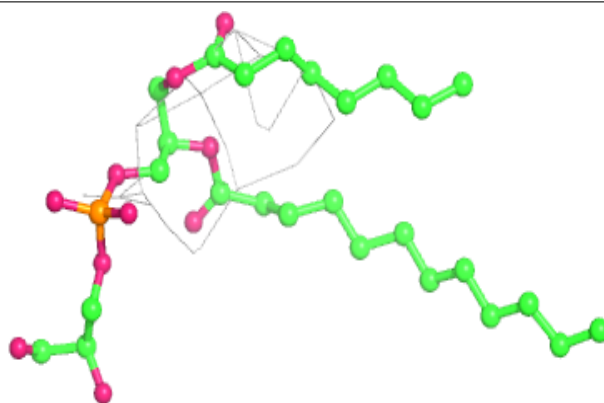


Electron density around BCR P 516:

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

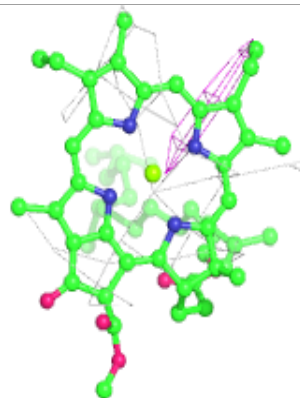
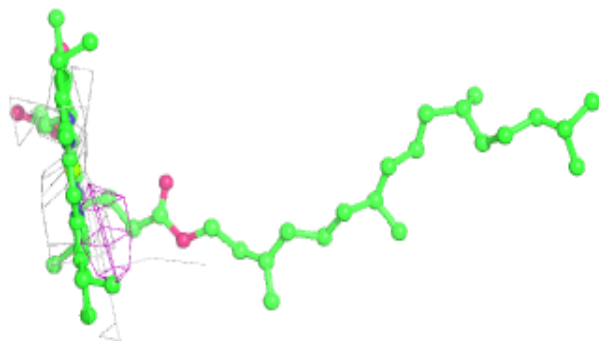
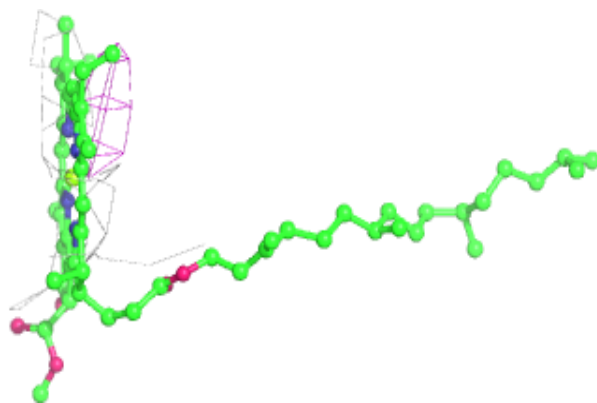
**Electron density around LHG A 411:**

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

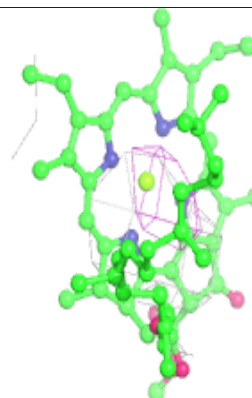
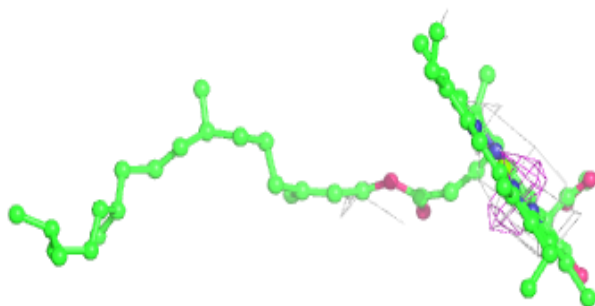
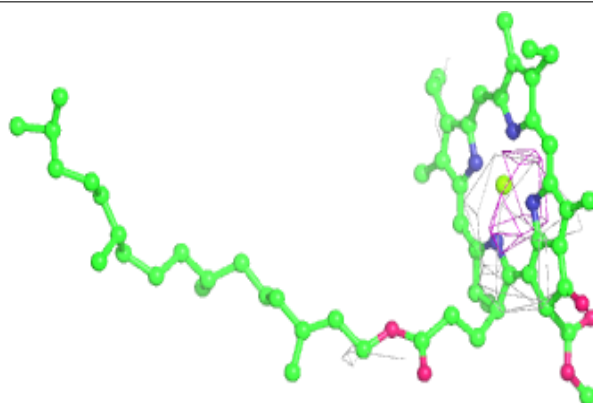


Electron density around CLA N 610:

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

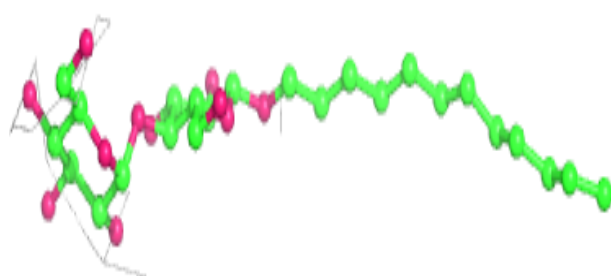
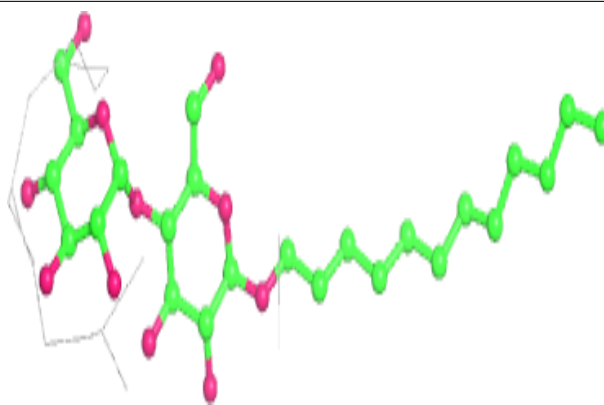
**Electron density around CLA G 406:**

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

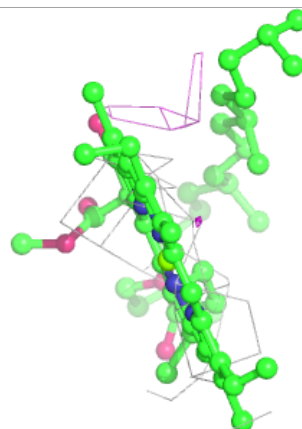
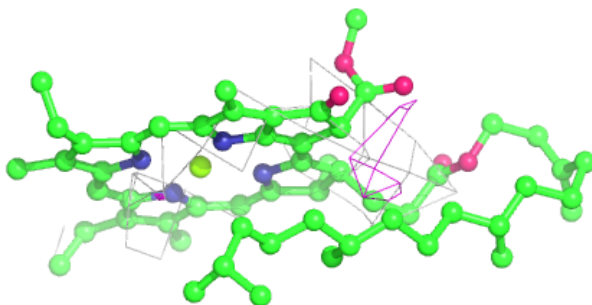
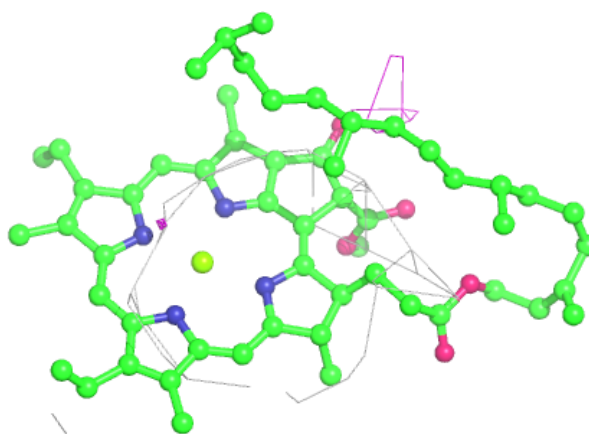


Electron density around LMT B 626:

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

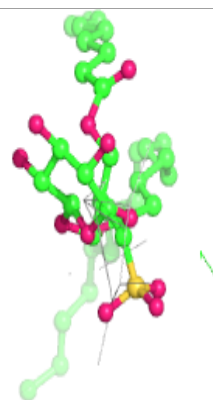
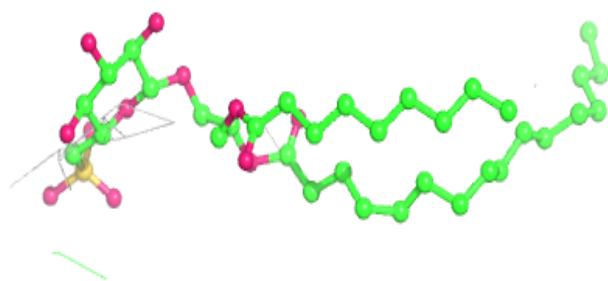
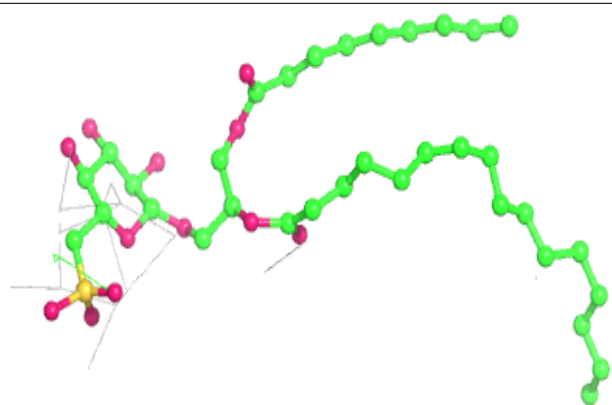
**Electron density around CLA C 509:**

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

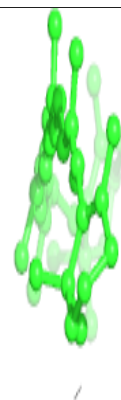
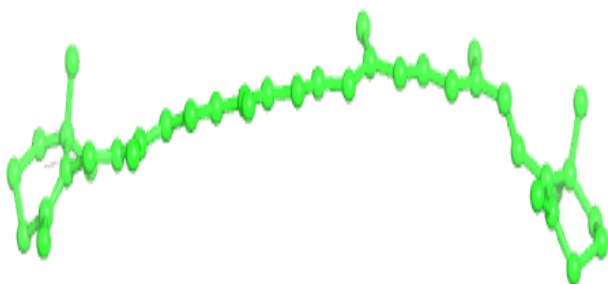
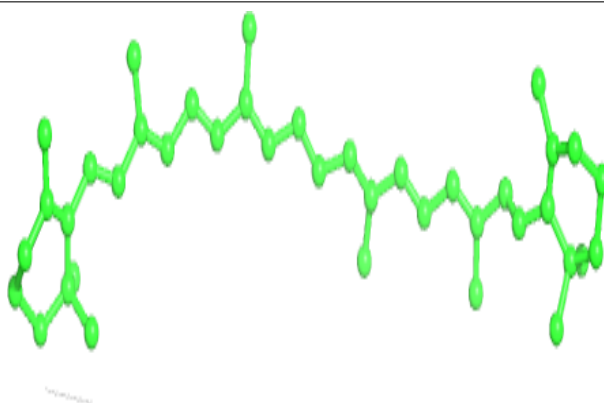


Electron density around SQD N 601:

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

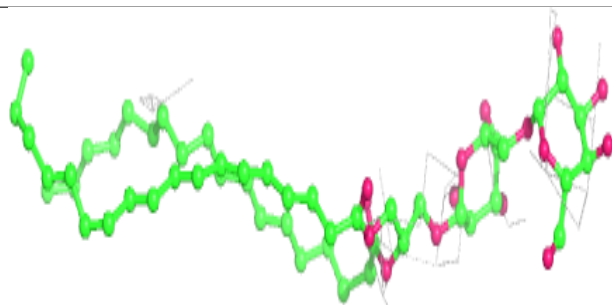
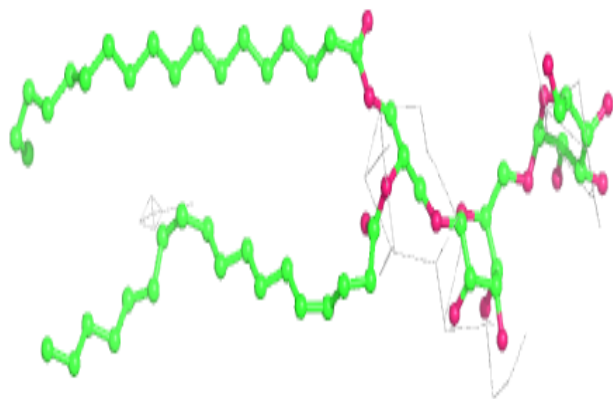
**Electron density around BCR B 618:**

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



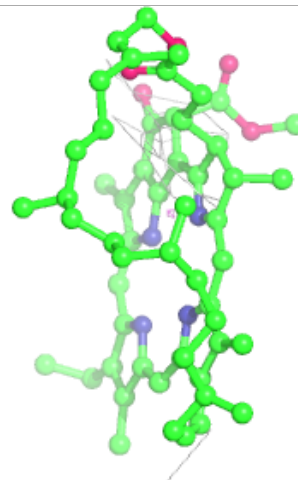
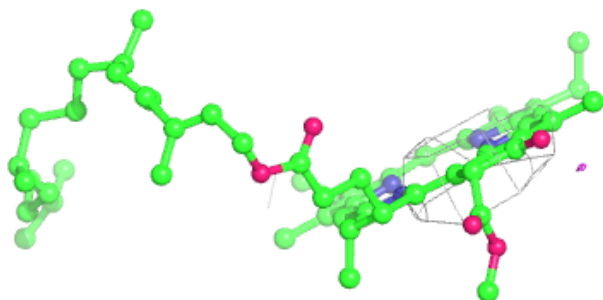
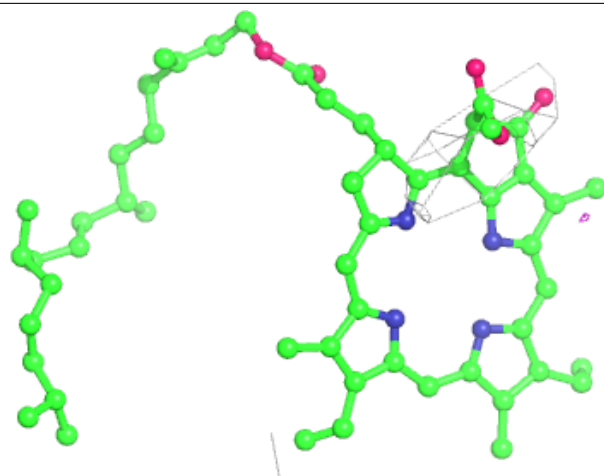
Electron density around DGD C 518:

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



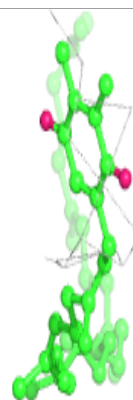
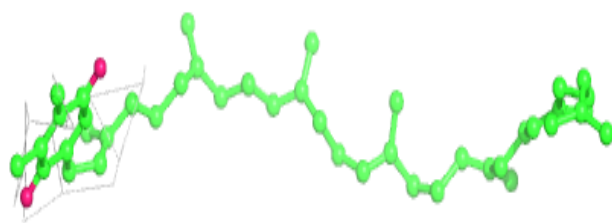
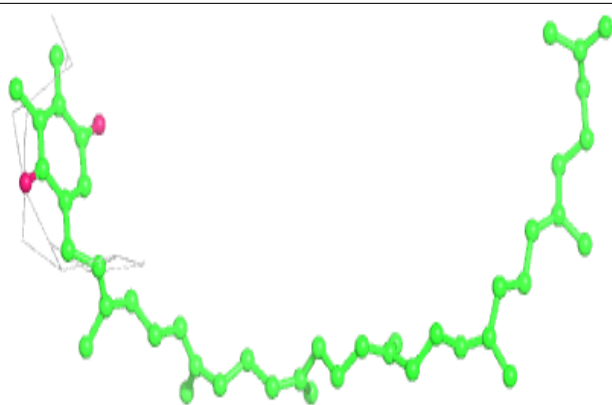
Electron density around PHO D 402:

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

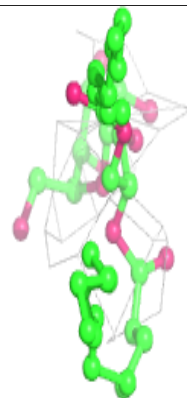
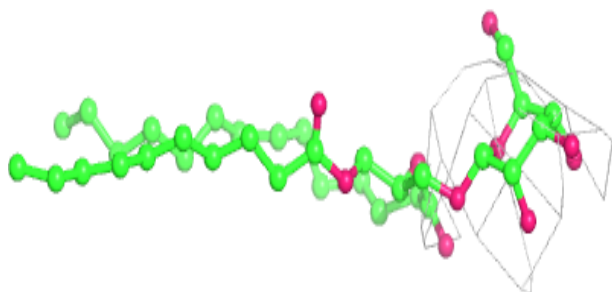
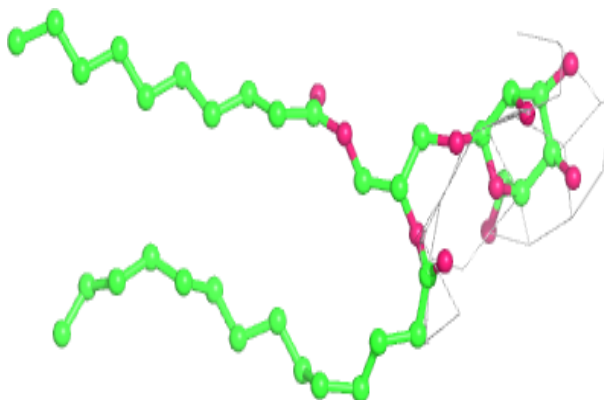


Electron density around PL9 G 407:

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

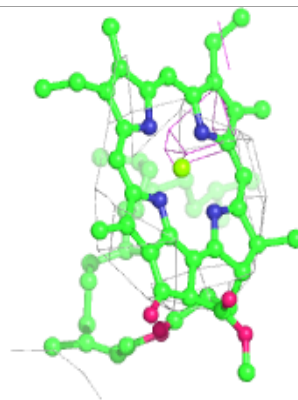
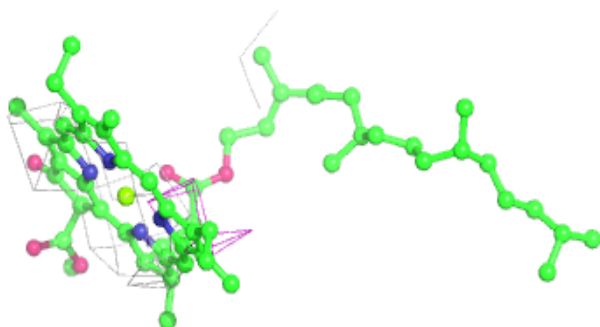
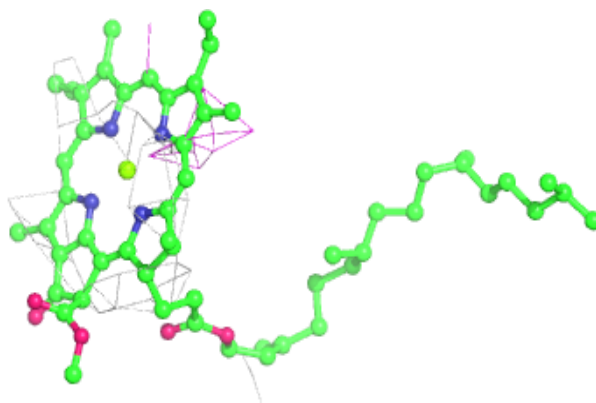
**Electron density around LMG a 102:**

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

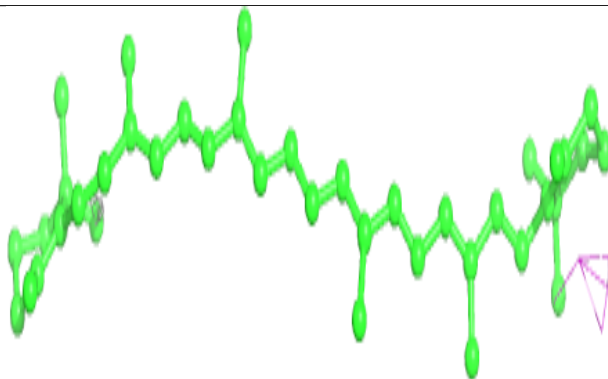
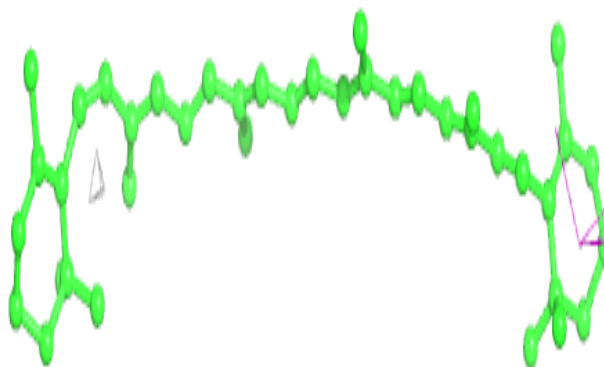


Electron density around CLA P 511:

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

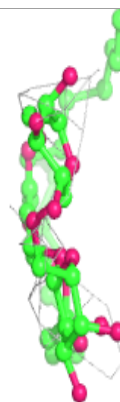
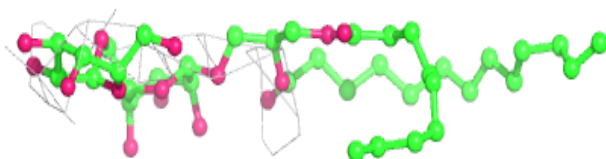
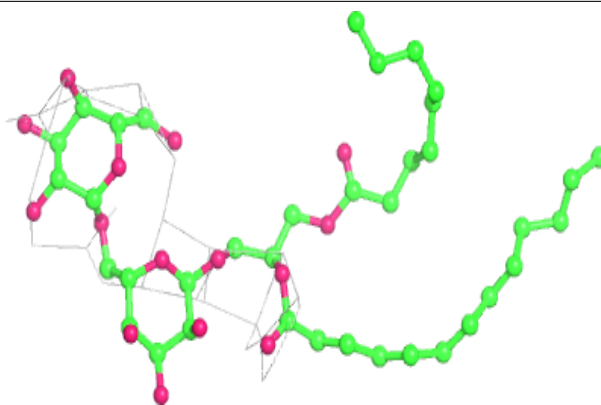
**Electron density around BCR P 514:**

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

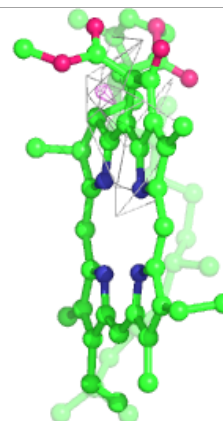
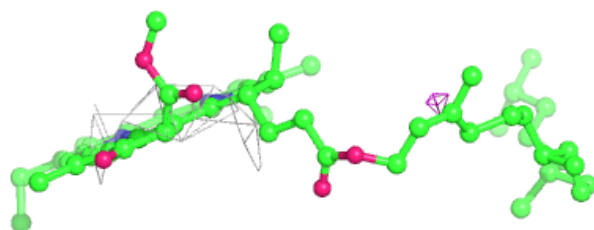
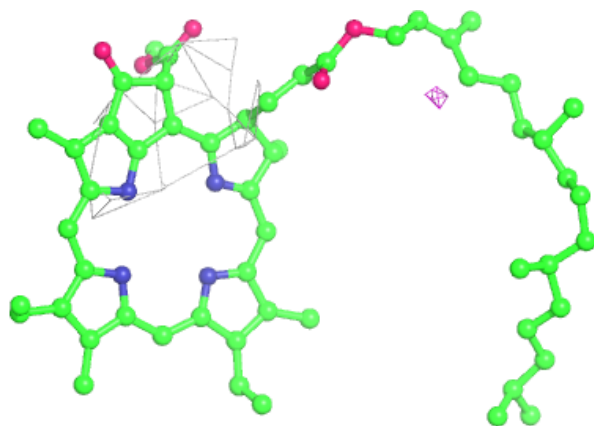


Electron density around DGD B 628:

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

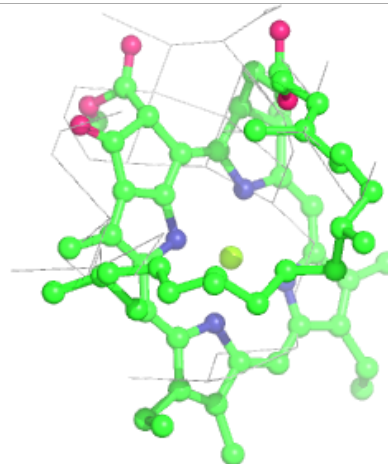
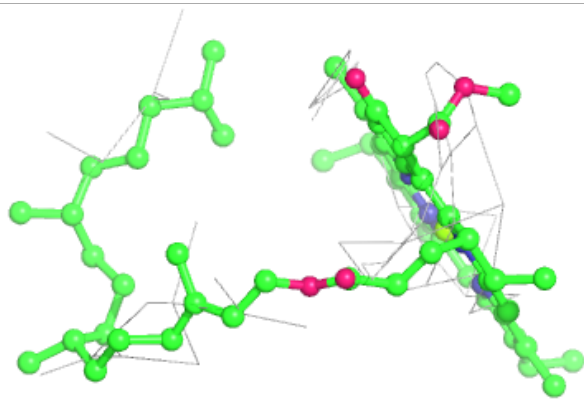
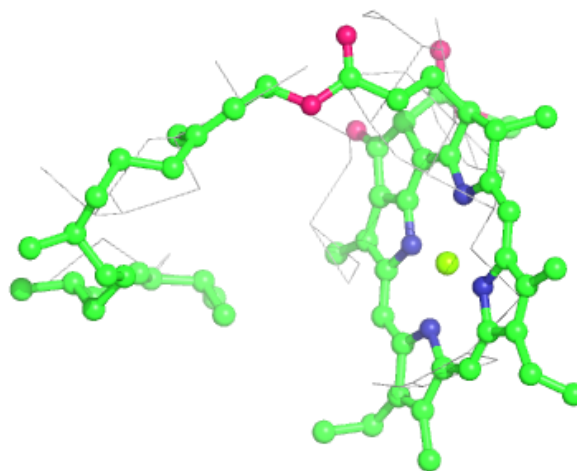
**Electron density around PHO A 404:**

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



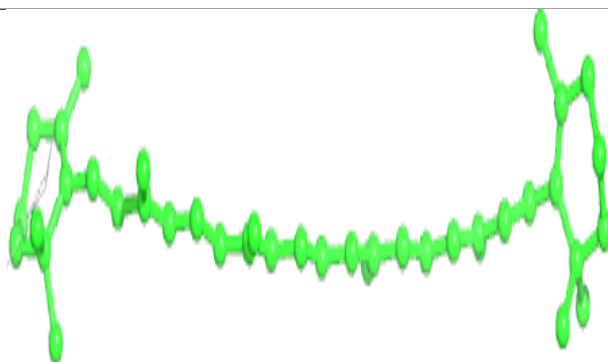
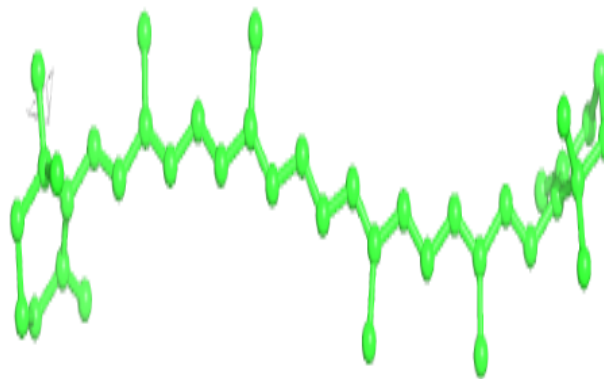
Electron density around CLA C 503:

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

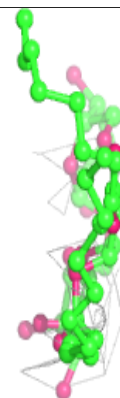
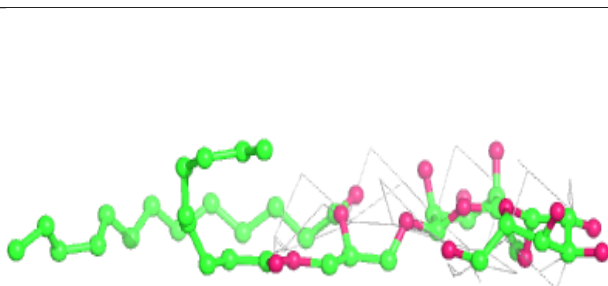
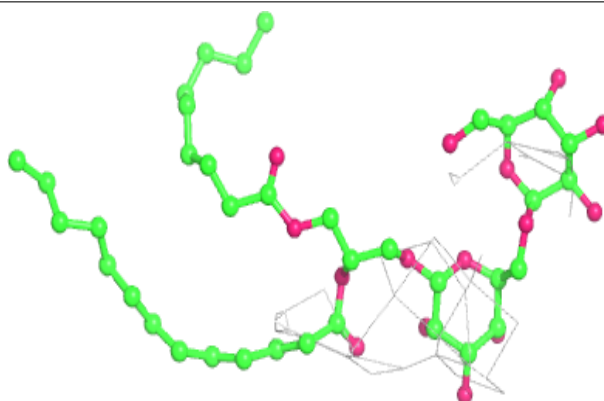


Electron density around BCR T 101:

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

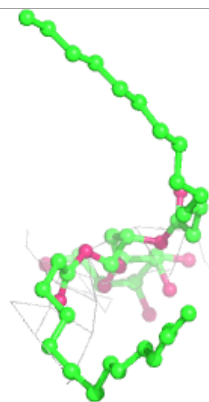
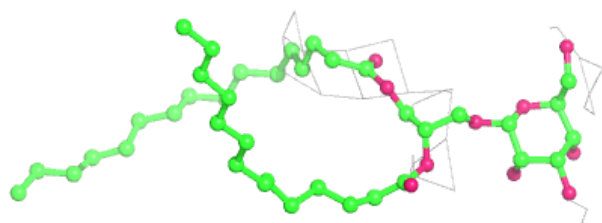
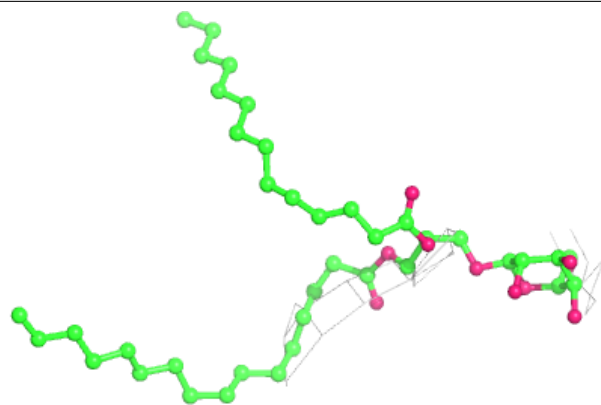
**Electron density around DGD N 602:**

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

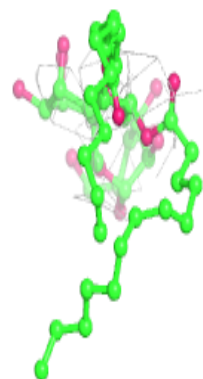
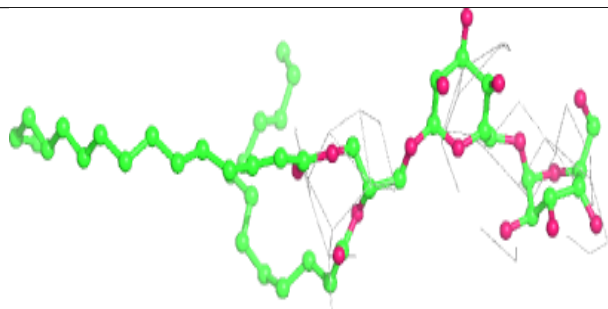
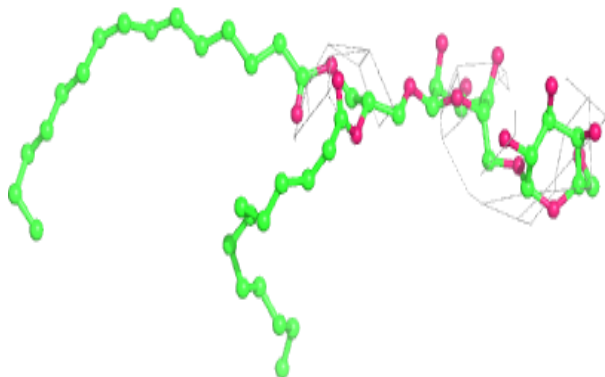


Electron density around LMG B 623:

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

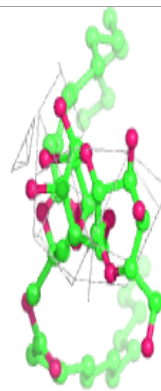
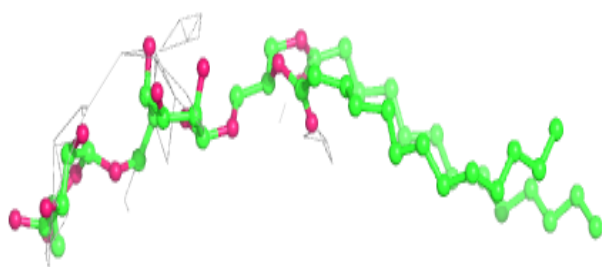
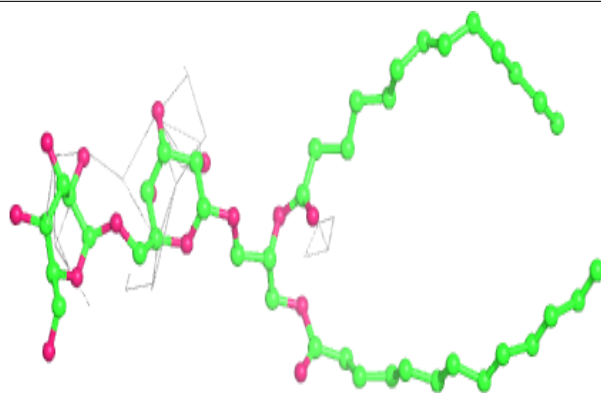
**Electron density around DGD B 621:**

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

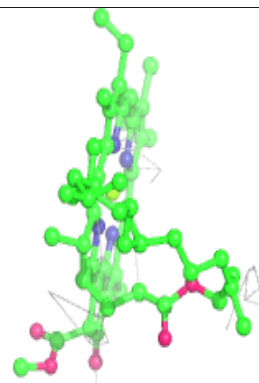
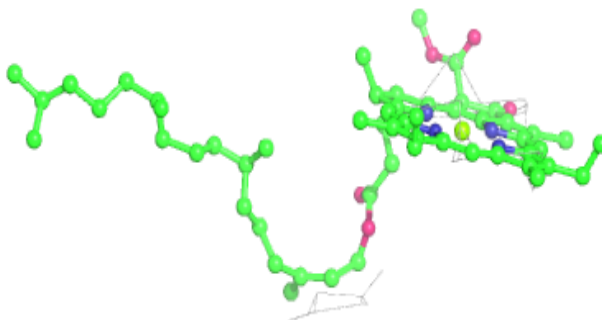
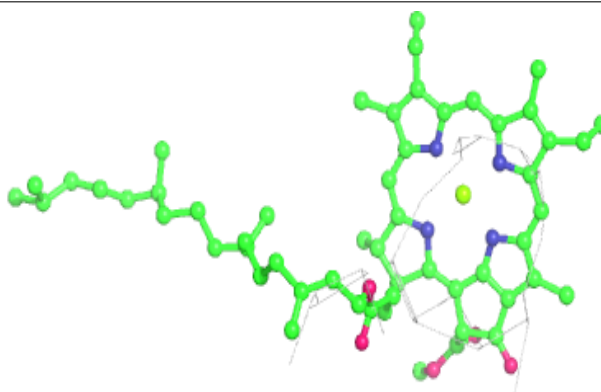


Electron density around DGD G 408:

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

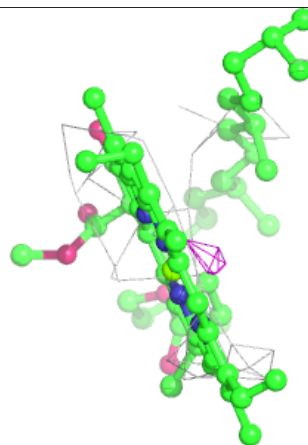
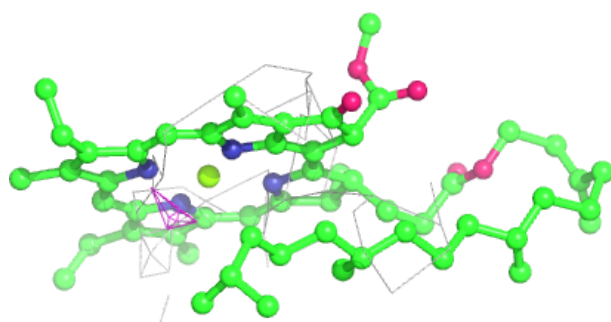
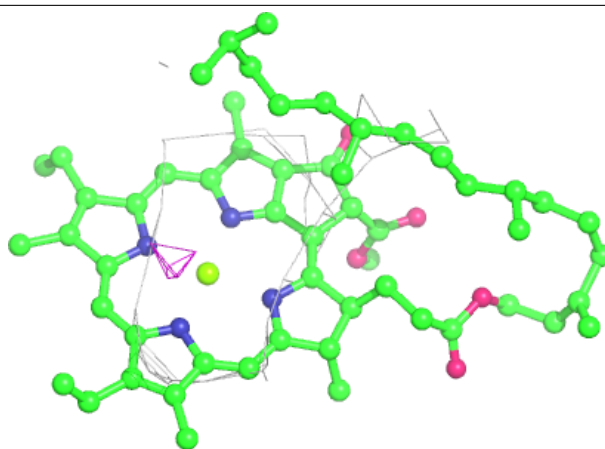
**Electron density around CLA G 404:**

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



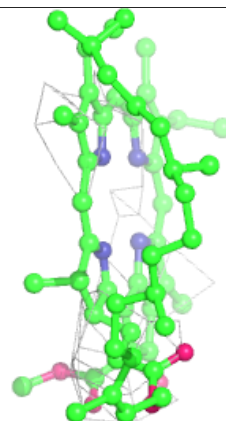
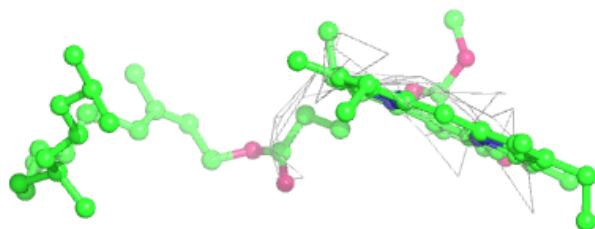
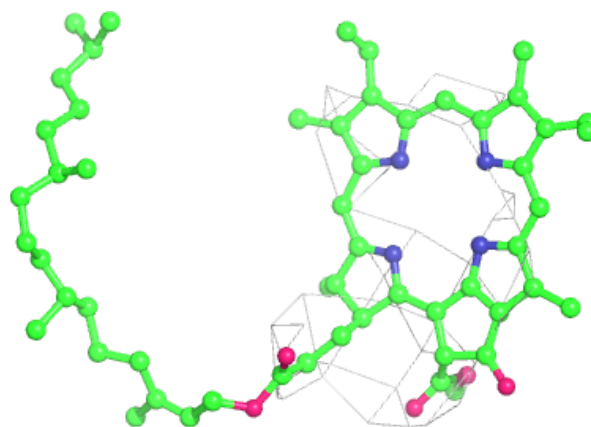
Electron density around CLA P 509:

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

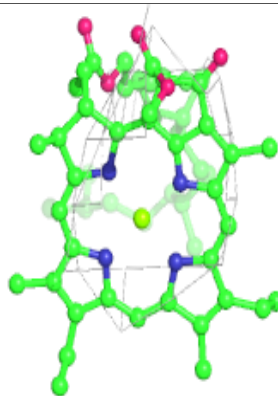
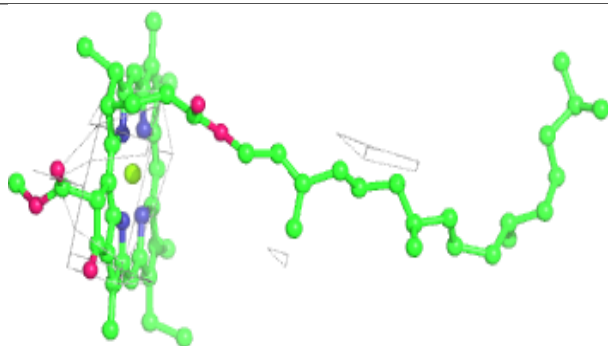
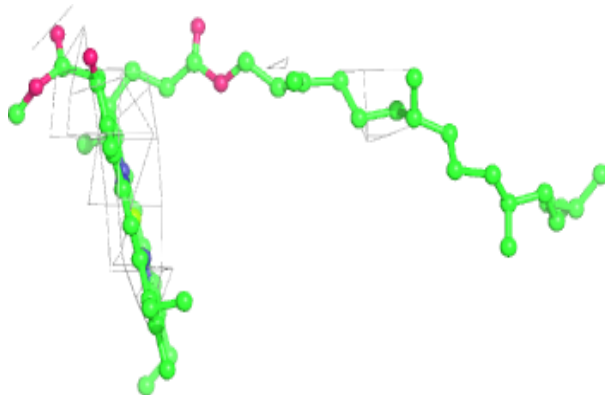


Electron density around PHO G 405:

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

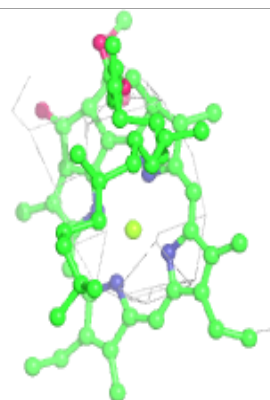
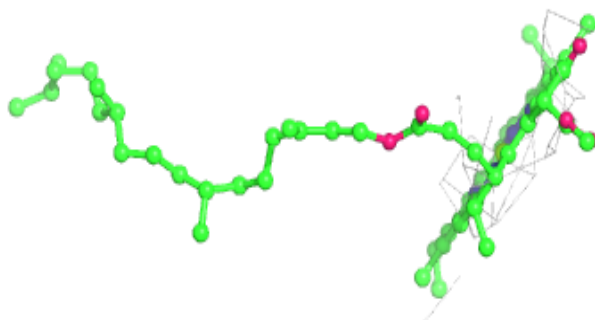
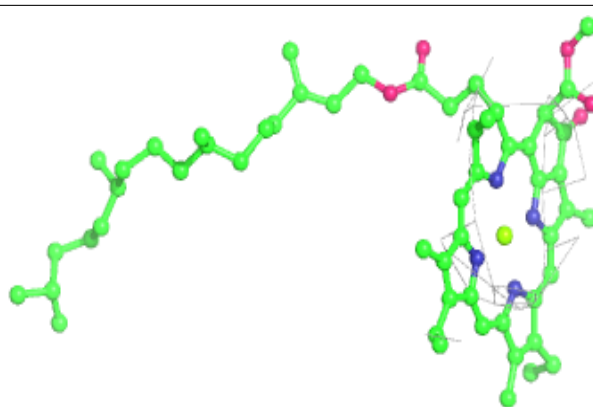
**Electron density around CLA B 605:**

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

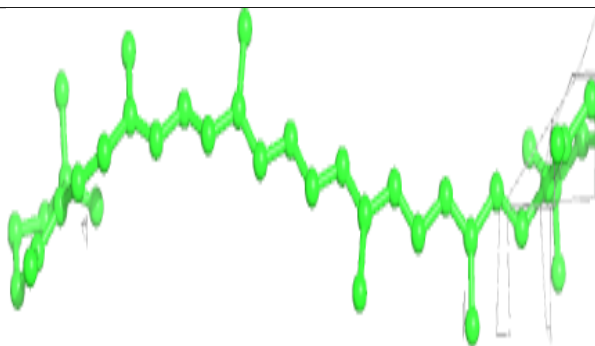
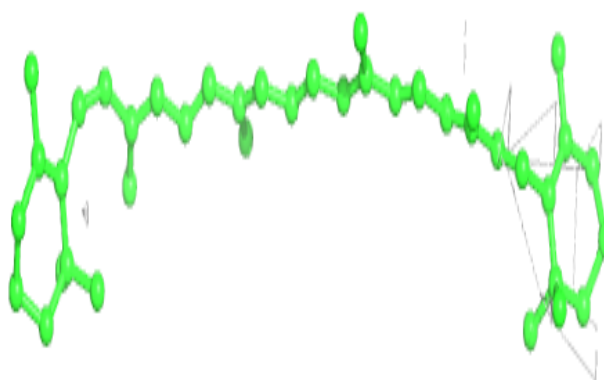


Electron density around CLA A 405:

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

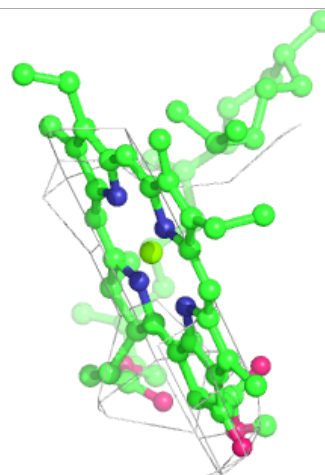
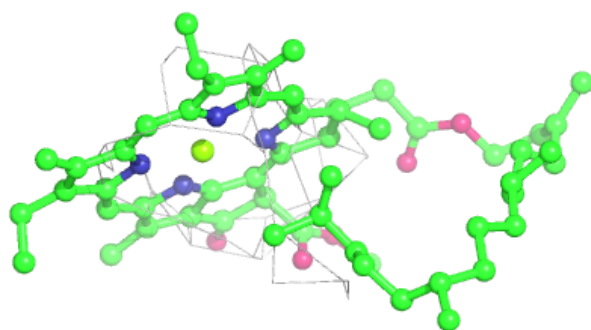
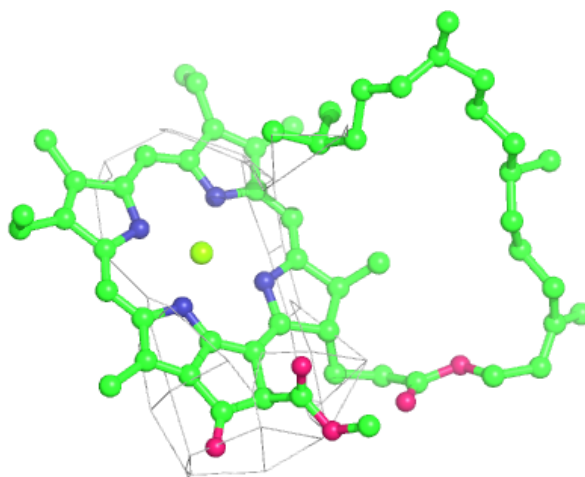
**Electron density around BCR C 514:**

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



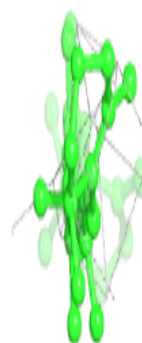
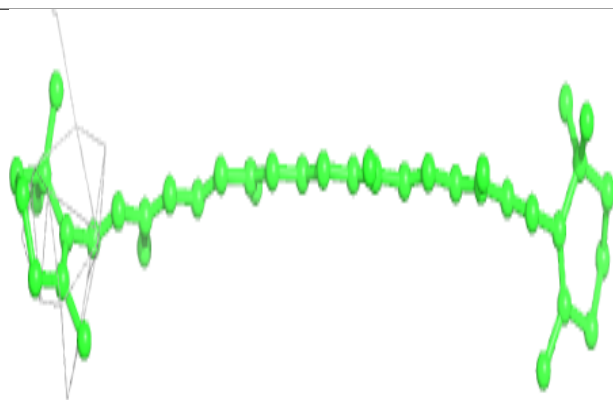
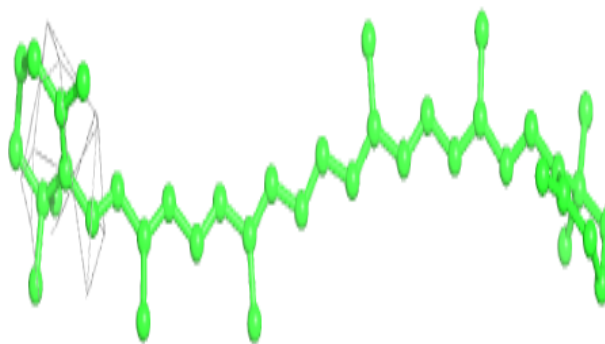
Electron density around CLA N 619:

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

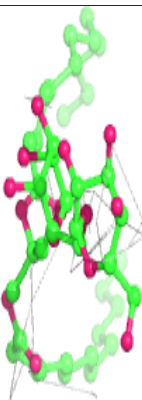
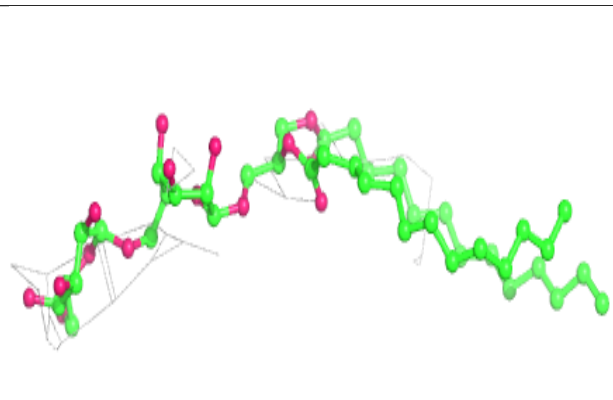
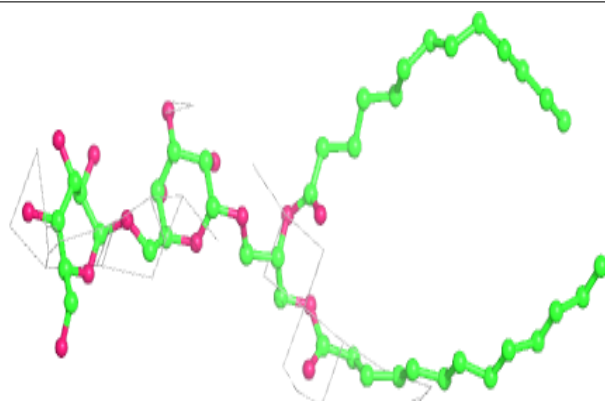


Electron density around BCR B 617:

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

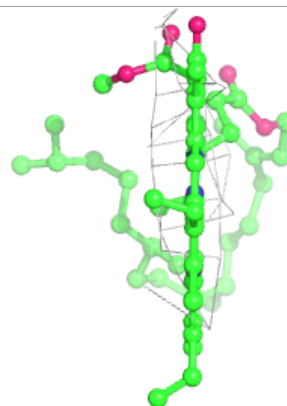
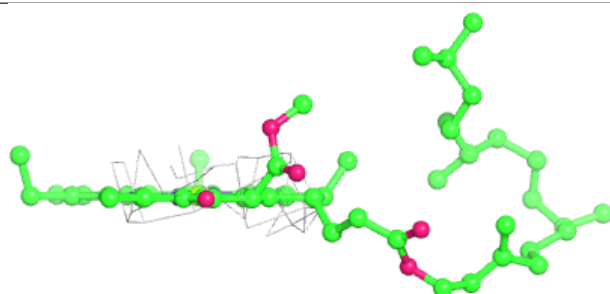
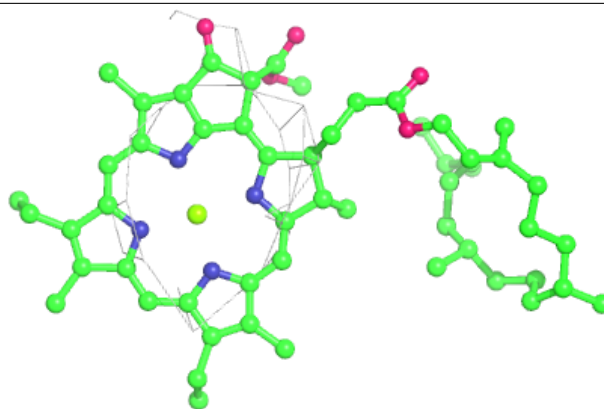
**Electron density around DGD A 407:**

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

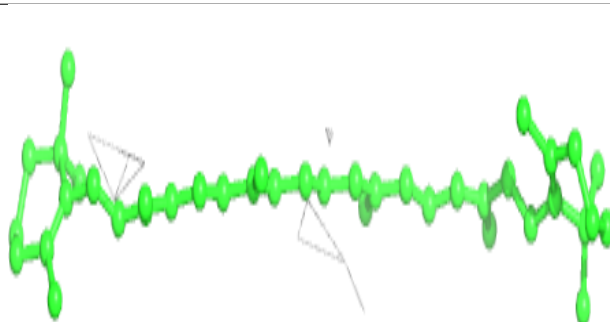
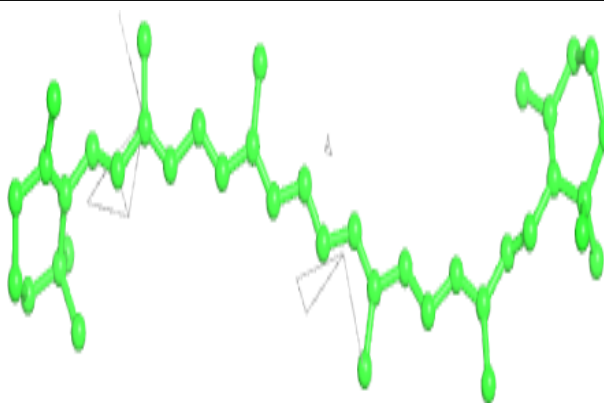


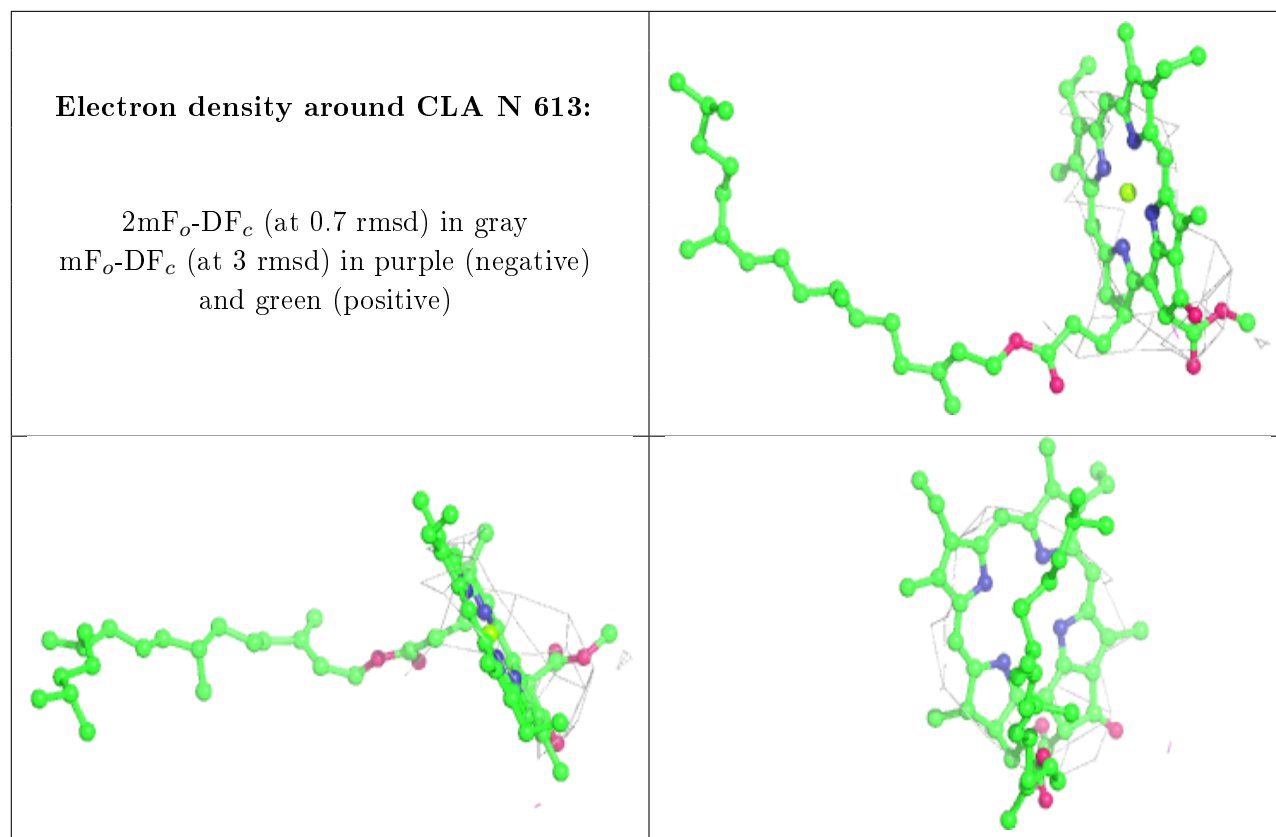
Electron density around CLA C 512:

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

**Electron density around BCR K 101:**

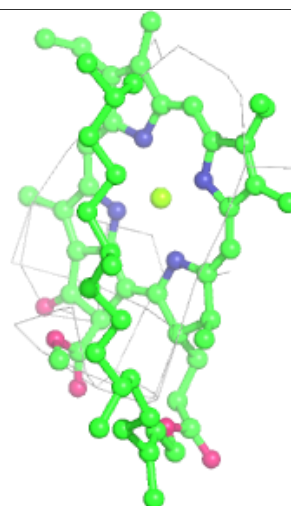
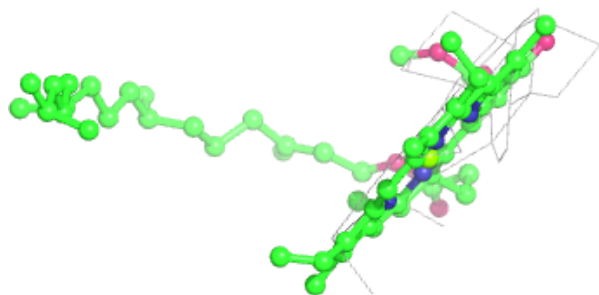
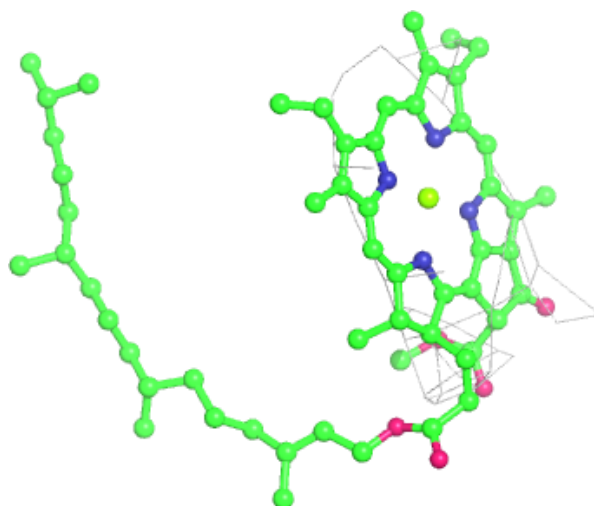
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





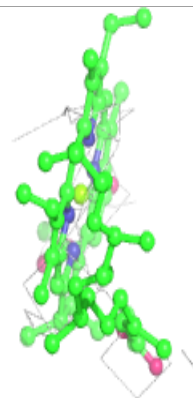
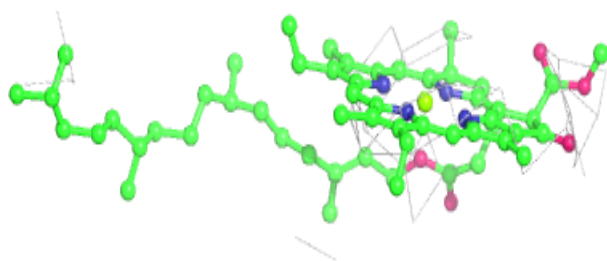
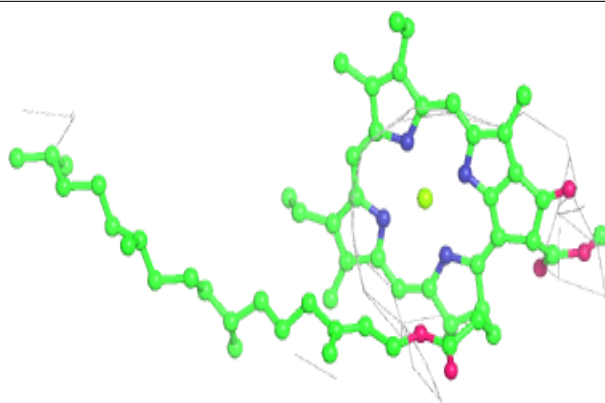
Electron density around CLA P 507:

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

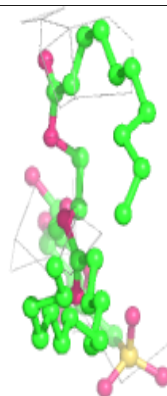
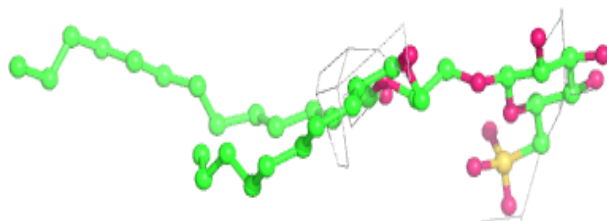
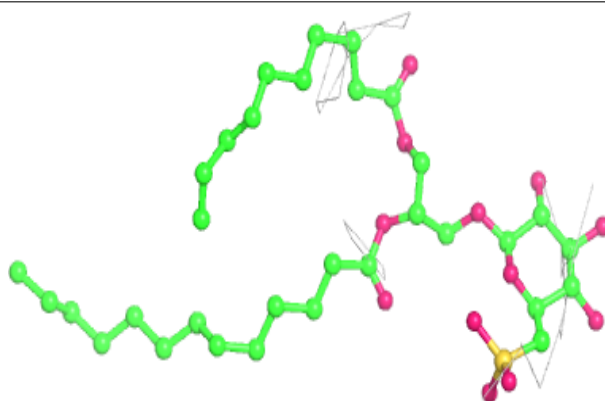


Electron density around CLA C 501:

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

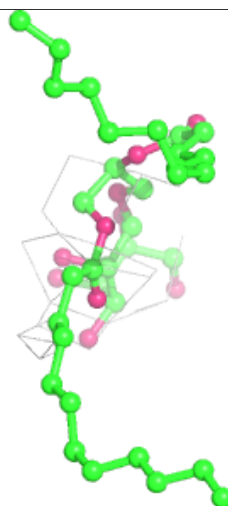
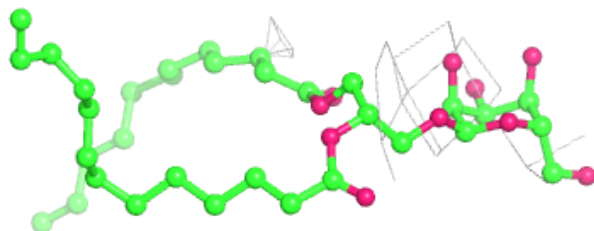
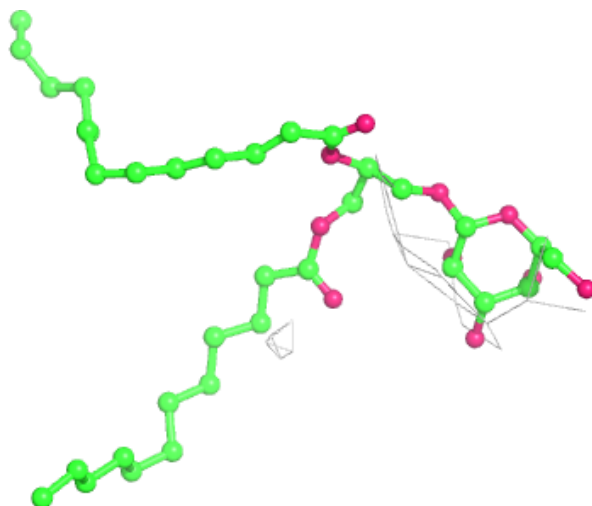
**Electron density around SQD F 101:**

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



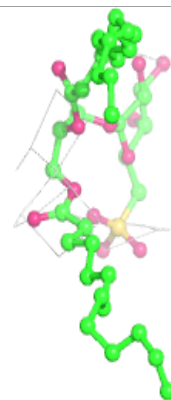
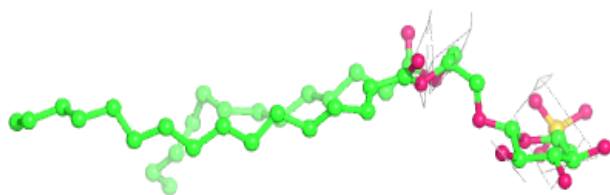
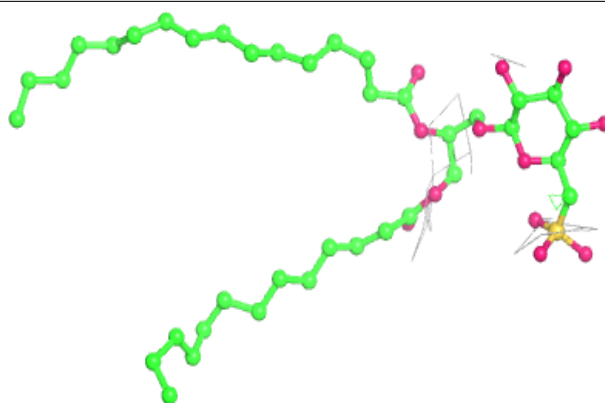
Electron density around LMG E 102:

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

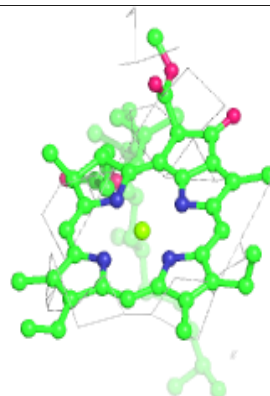
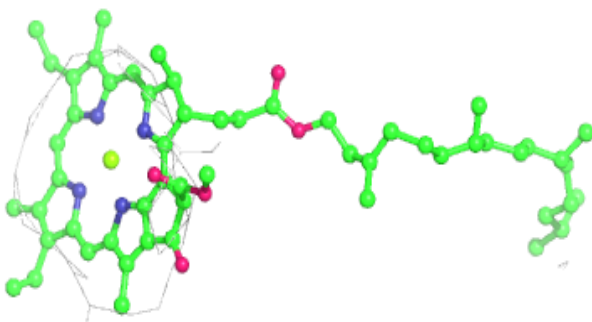
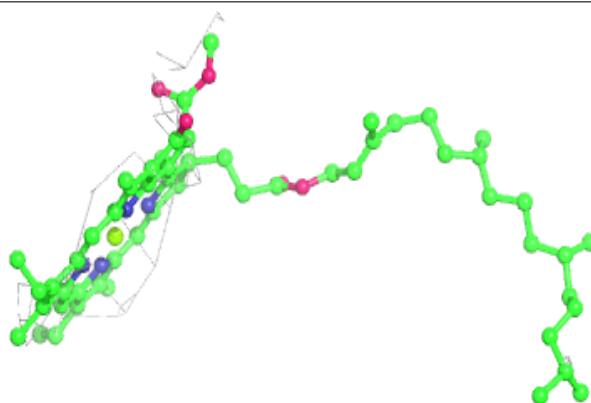


Electron density around SQD G 410:

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

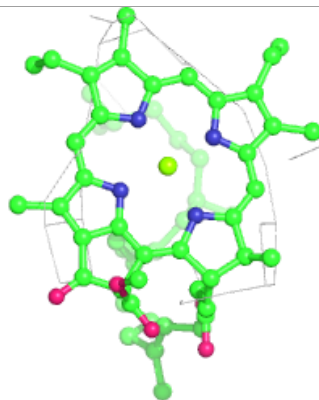
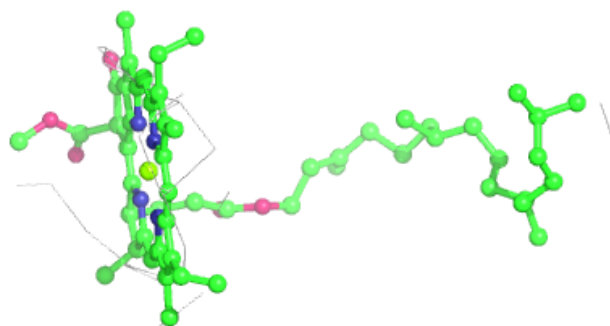
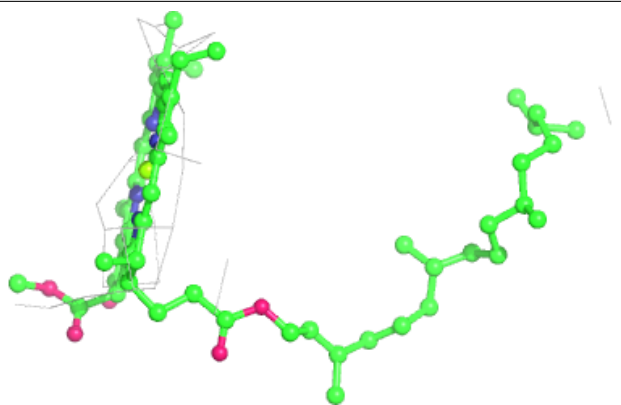
**Electron density around CLA Q 402:**

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

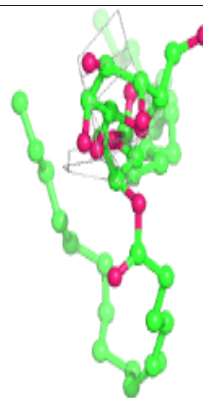
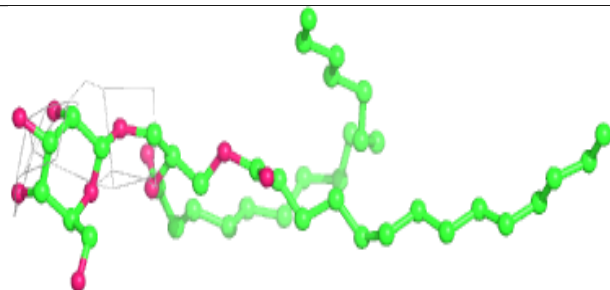
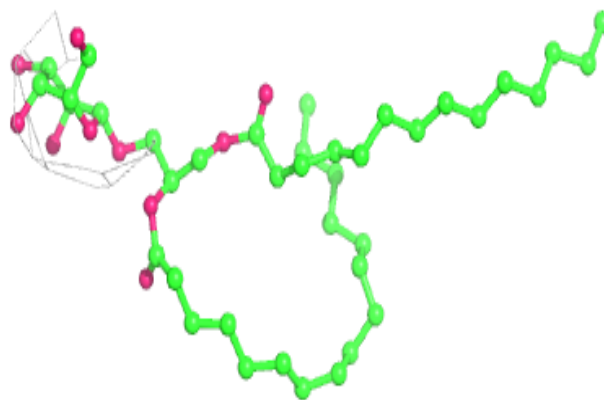


Electron density around CLA C 506:

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

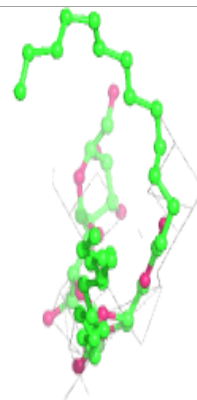
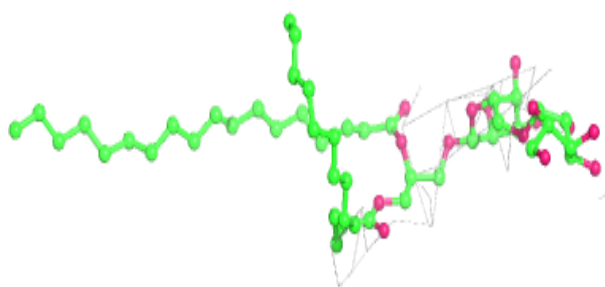
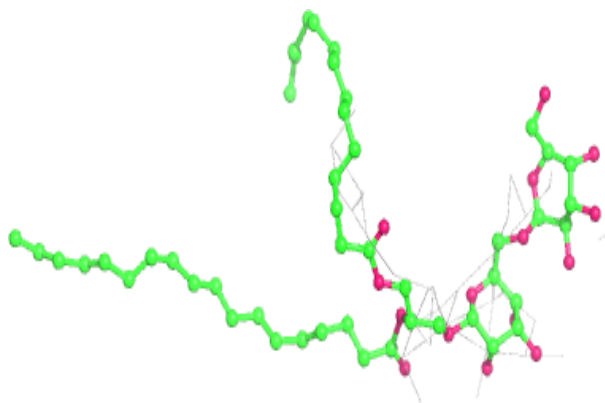
**Electron density around LMG B 622:**

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

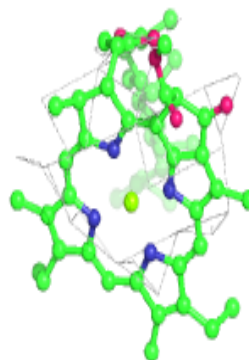
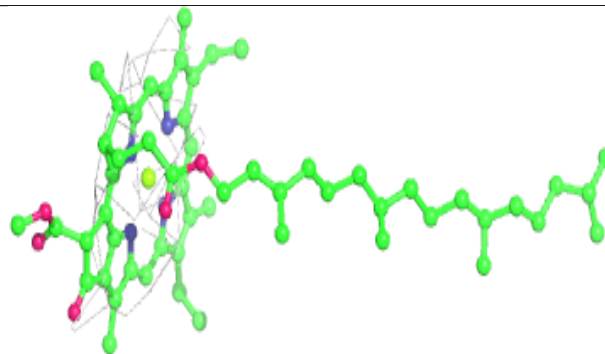
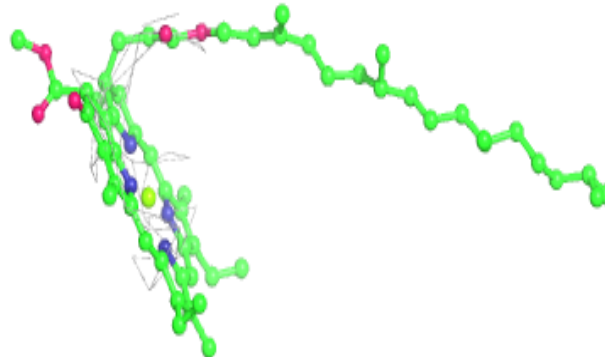


Electron density around DGD C 517:

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

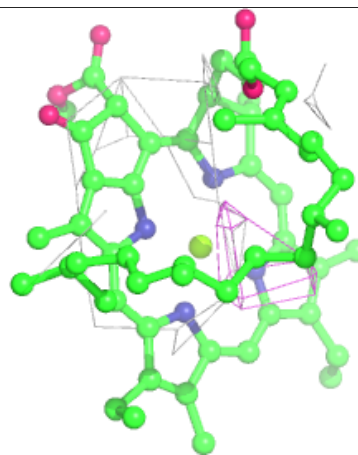
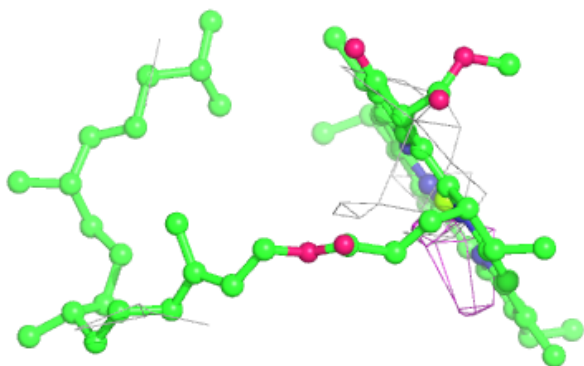
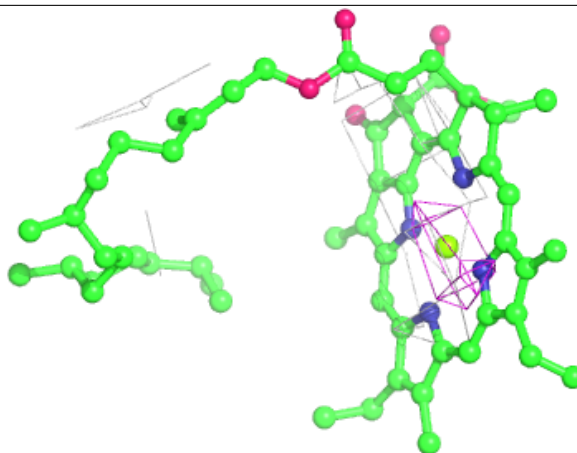
**Electron density around CLA B 607:**

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

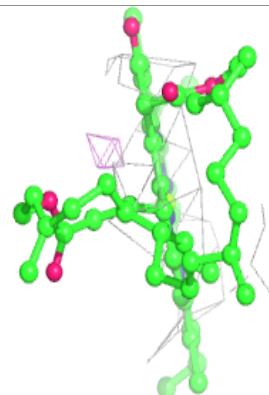
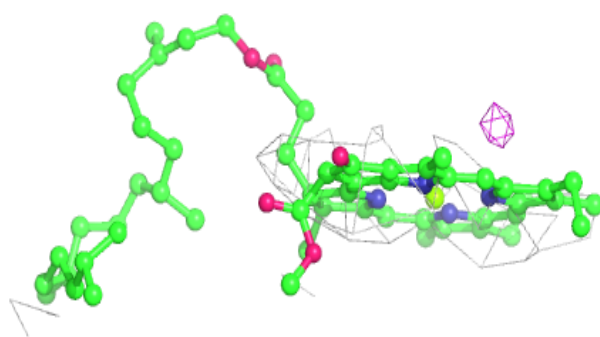
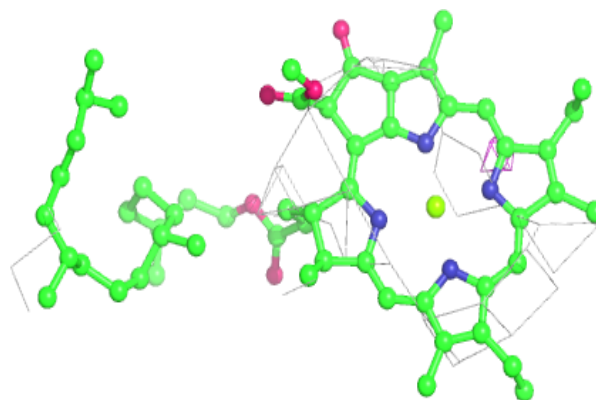


Electron density around CLA P 503:

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

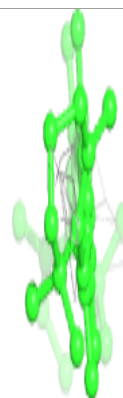
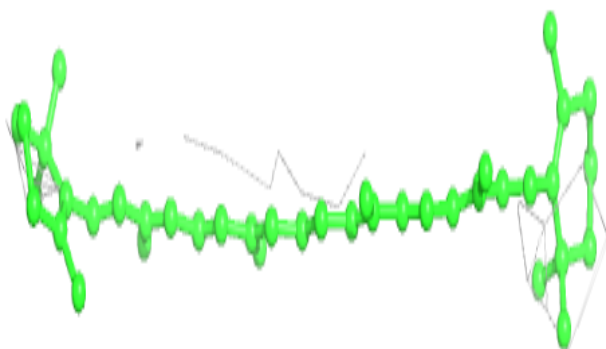
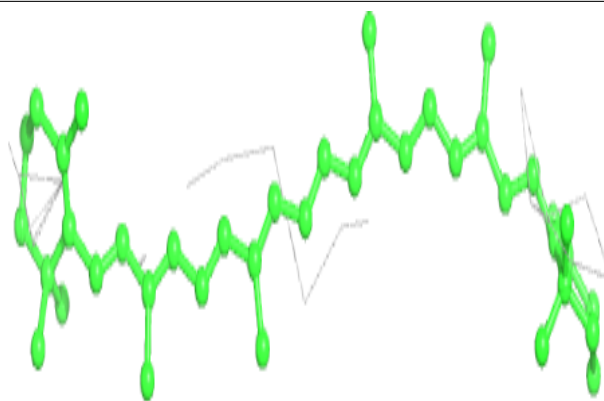
**Electron density around CLA N 616:**

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

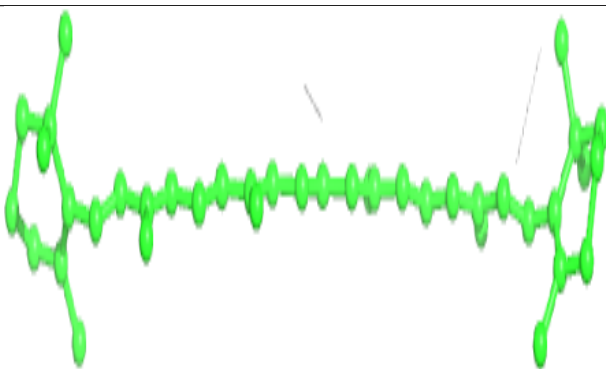
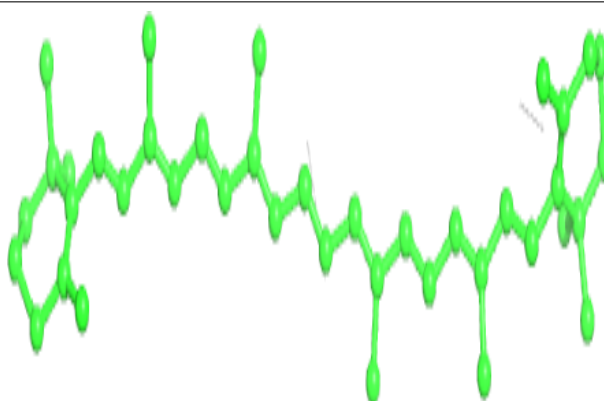


Electron density around BCR W 101:

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

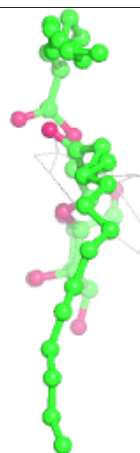
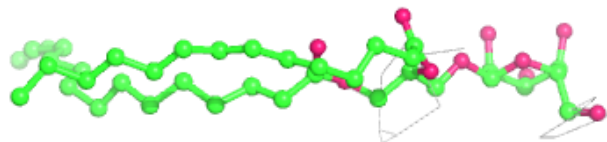
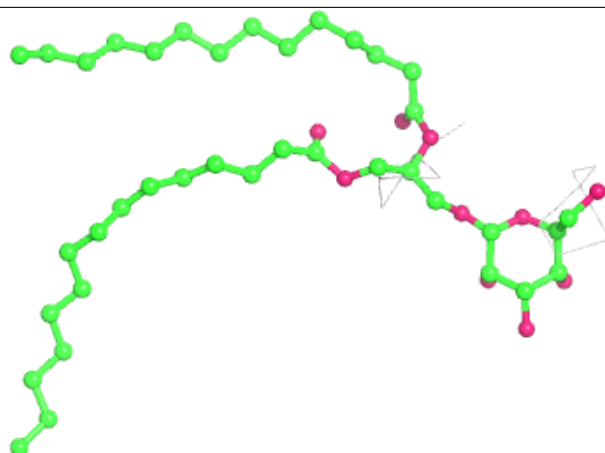
**Electron density around BCR B 619:**

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

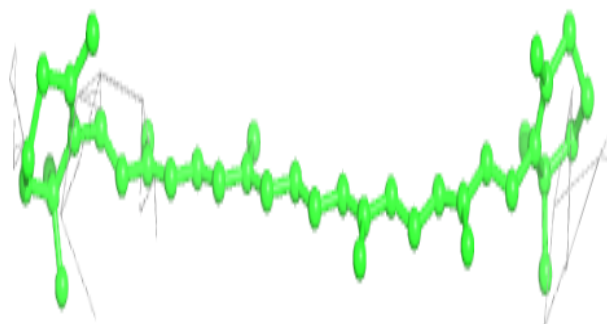
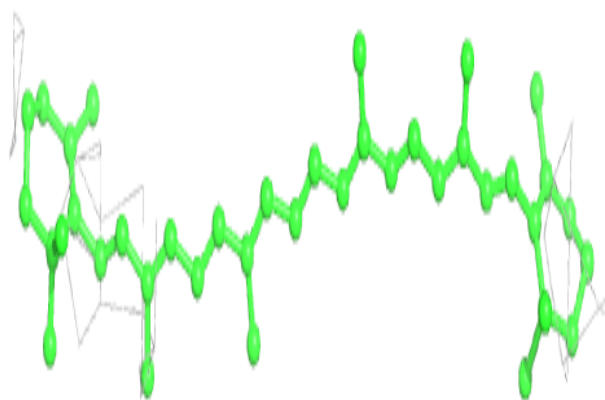


Electron density around LMG P 520:

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

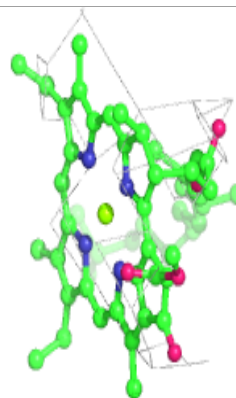
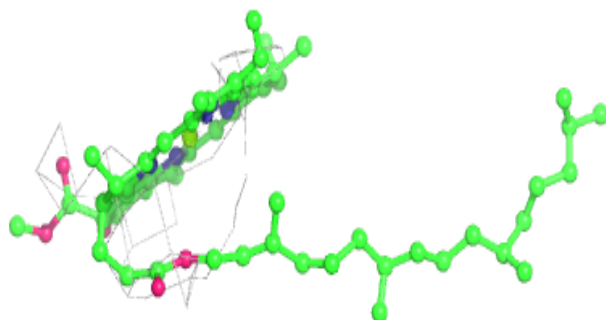
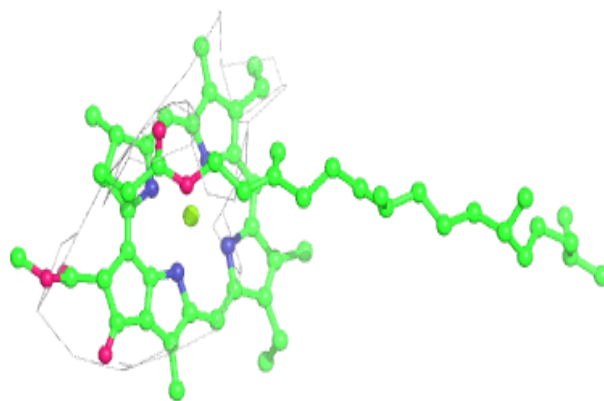
**Electron density around BCR C 515:**

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

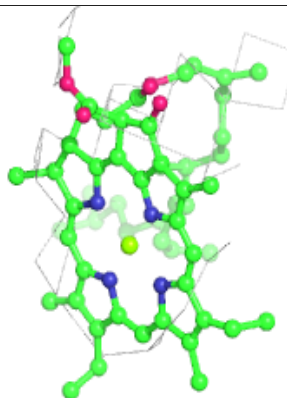
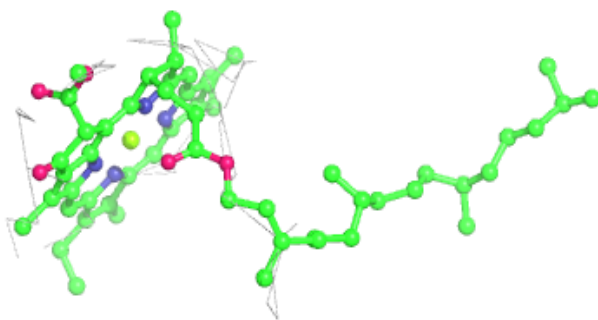
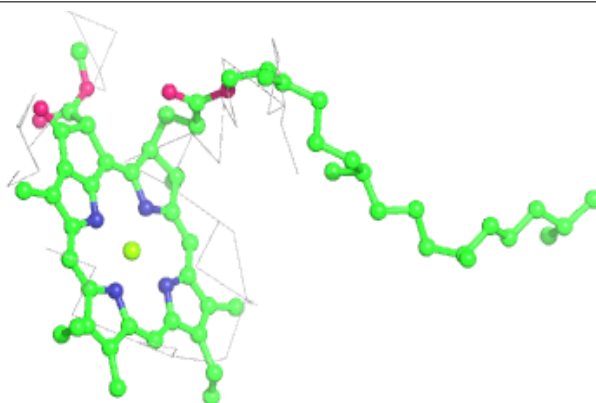


Electron density around CLA B 608:

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

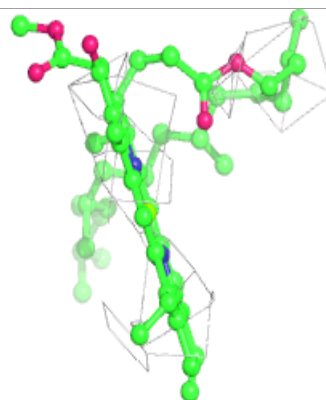
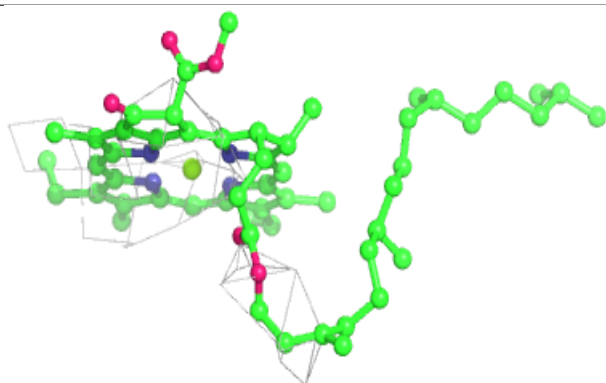
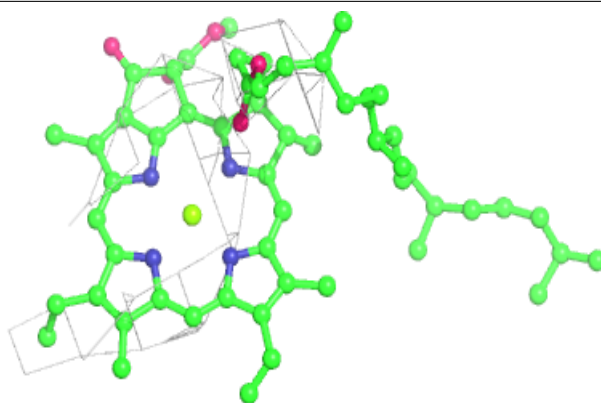
**Electron density around CLA C 511:**

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

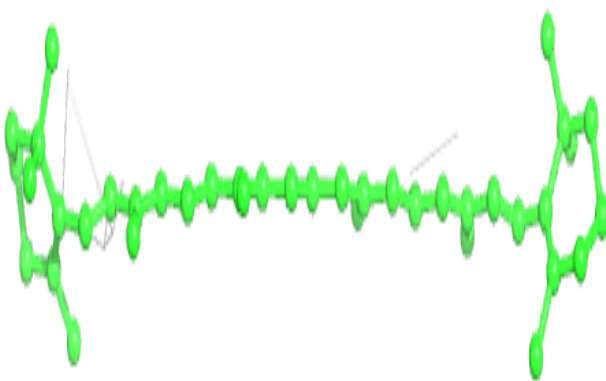
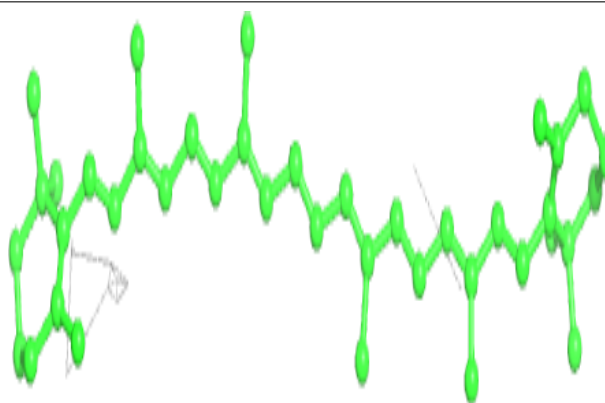


Electron density around CLA G 403:

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

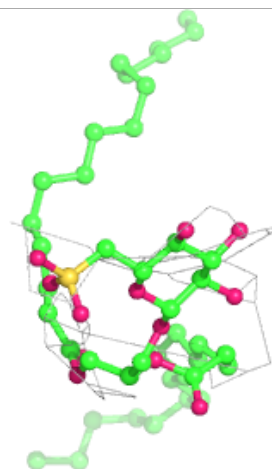
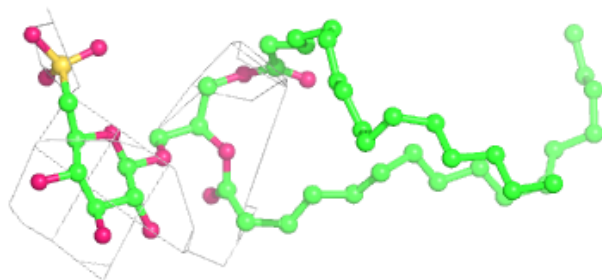
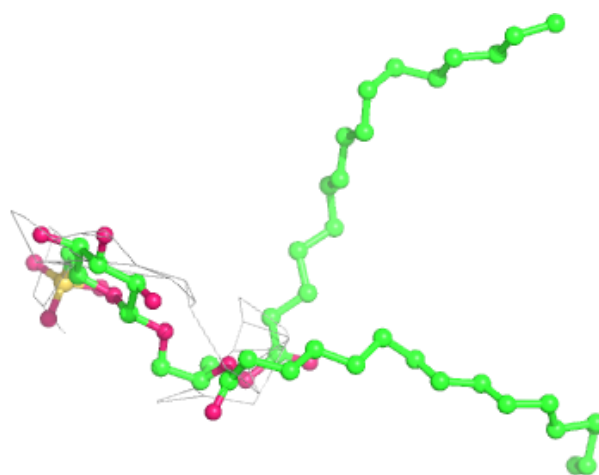
**Electron density around BCR N 621:**

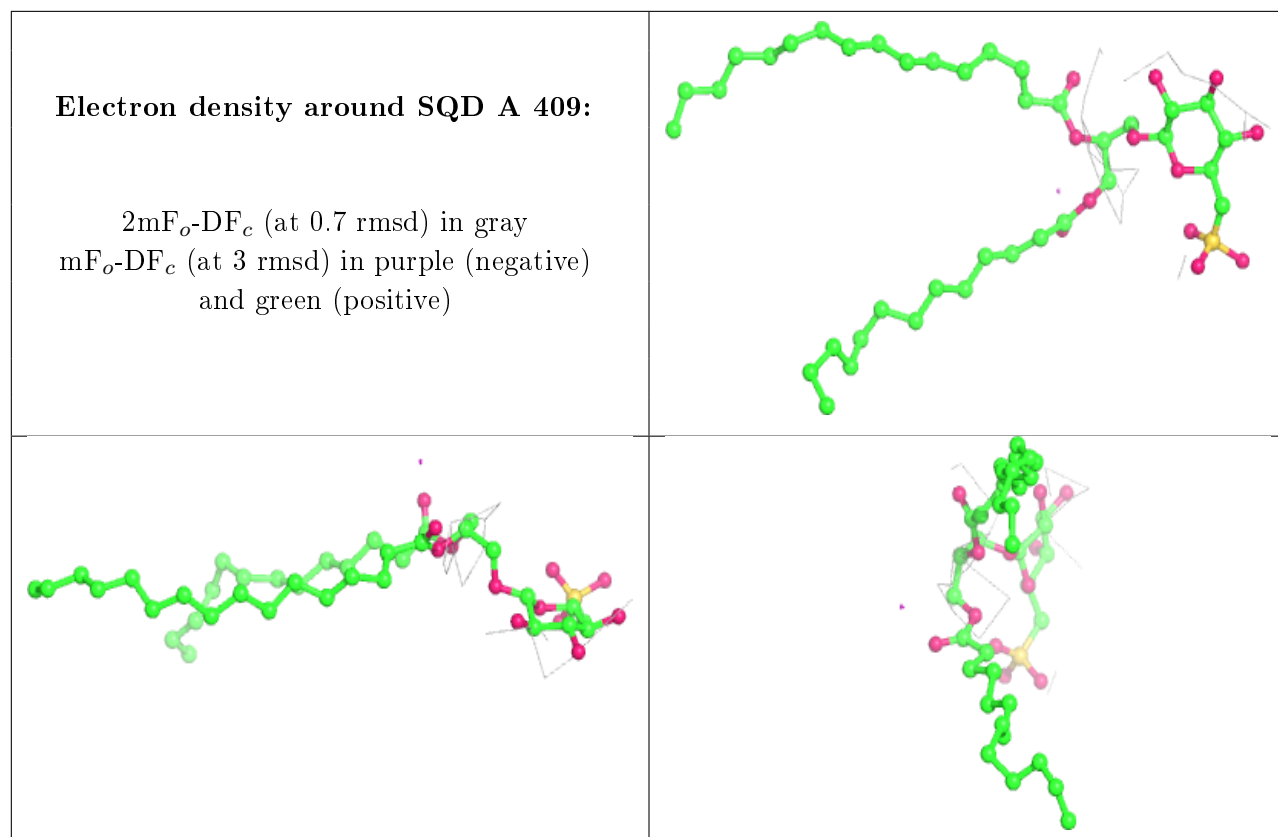
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD G 401:

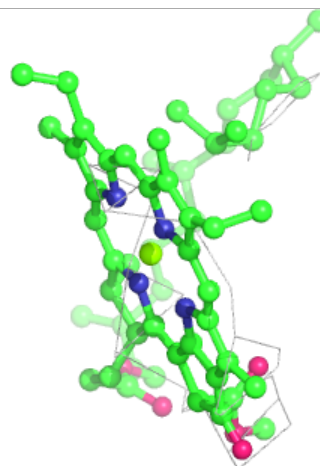
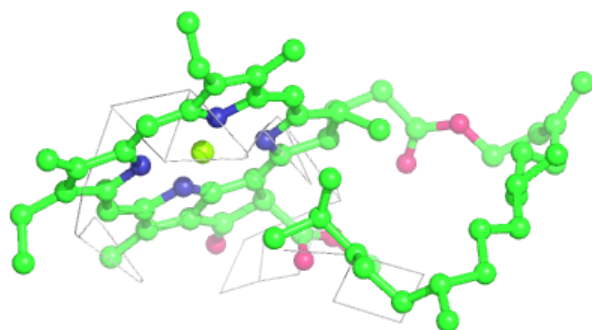
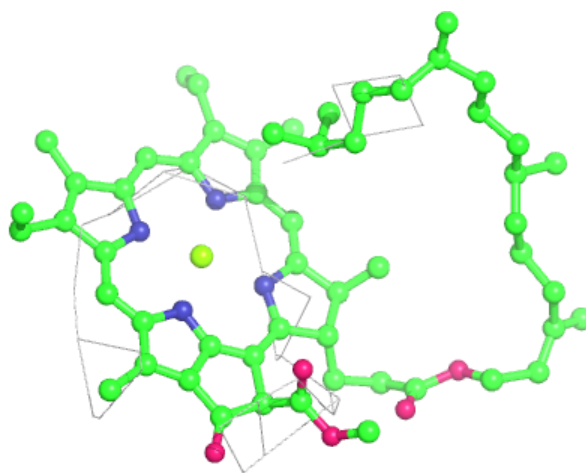
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





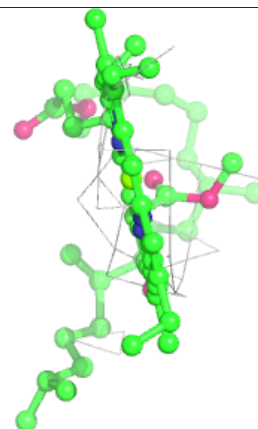
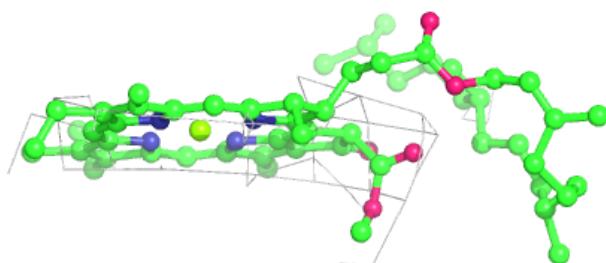
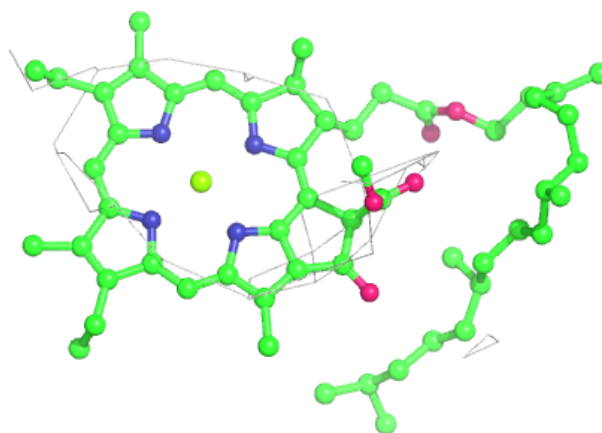
Electron density around CLA B 615:

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

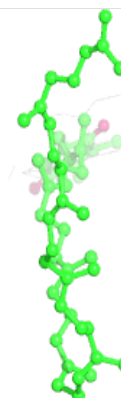
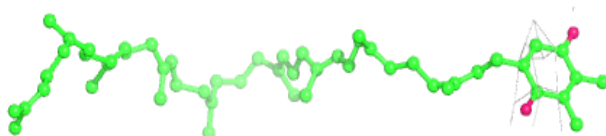
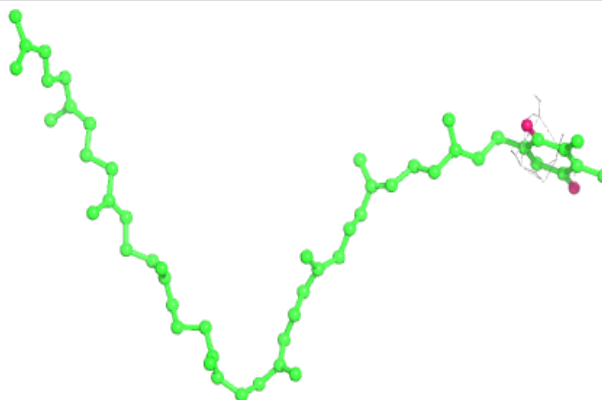


Electron density around CLA N 614:

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

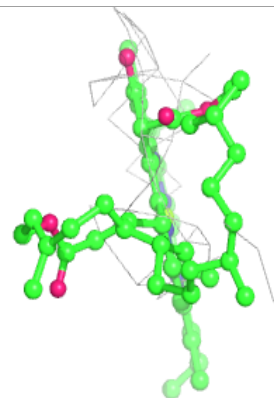
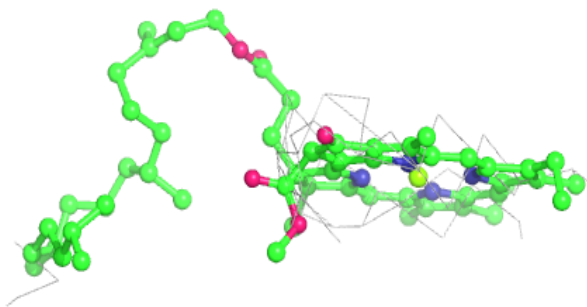
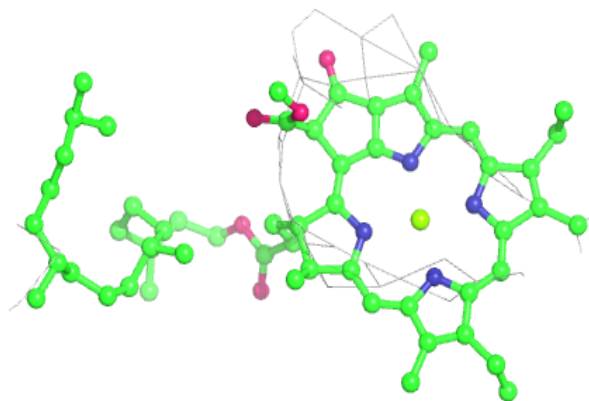
**Electron density around PL9 Q 405:**

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

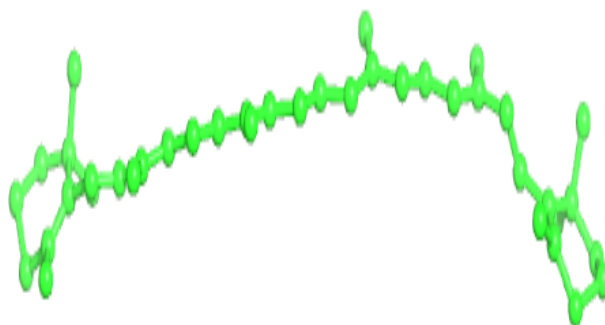
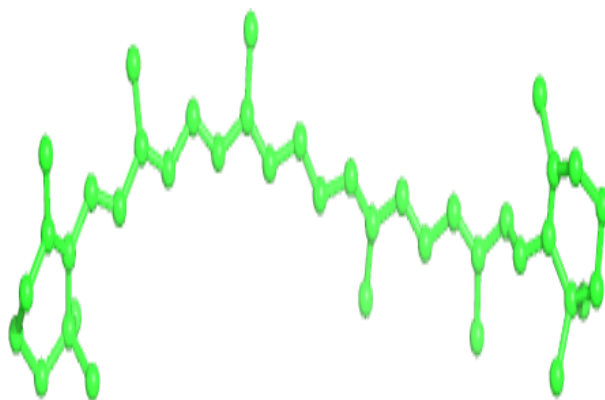


Electron density around CLA B 612:

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

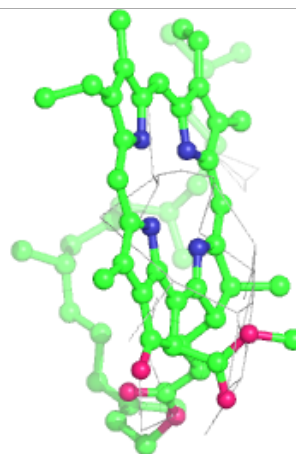
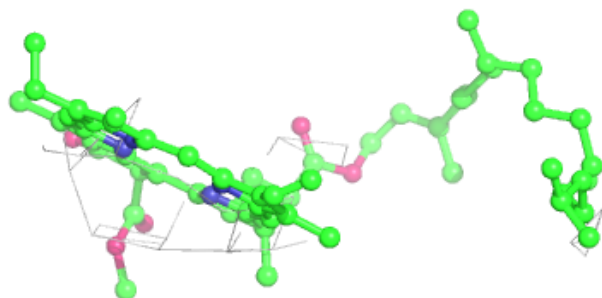
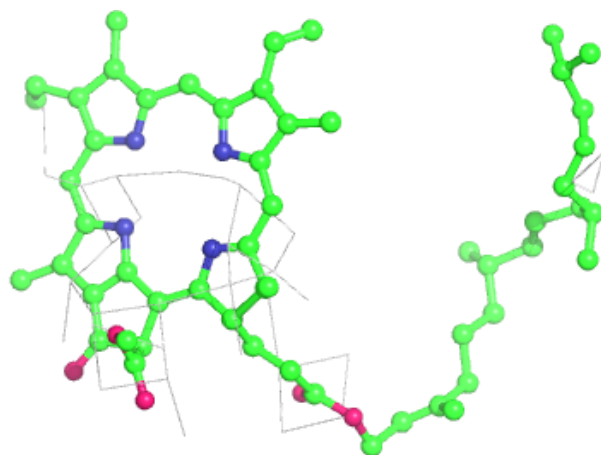
**Electron density around BCR T 102:**

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



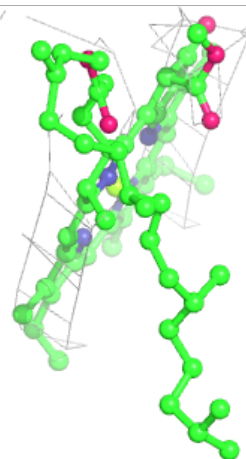
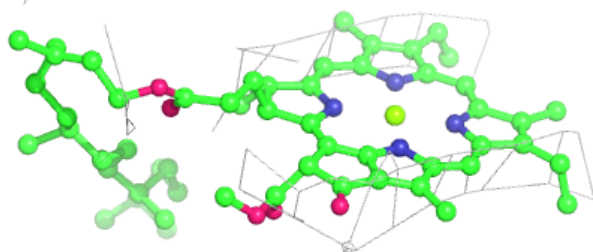
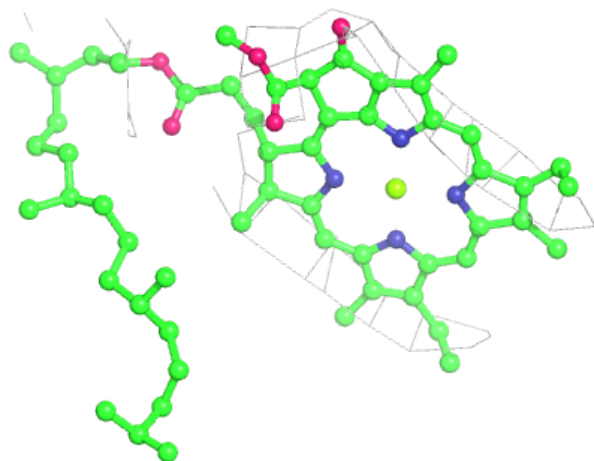
Electron density around PHO Q 403:

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



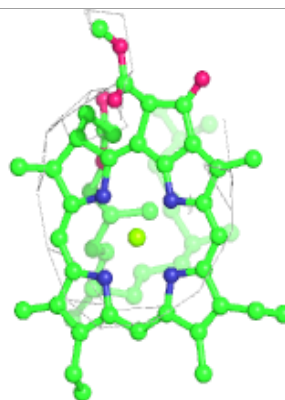
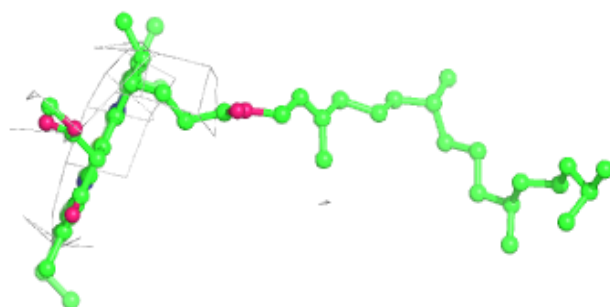
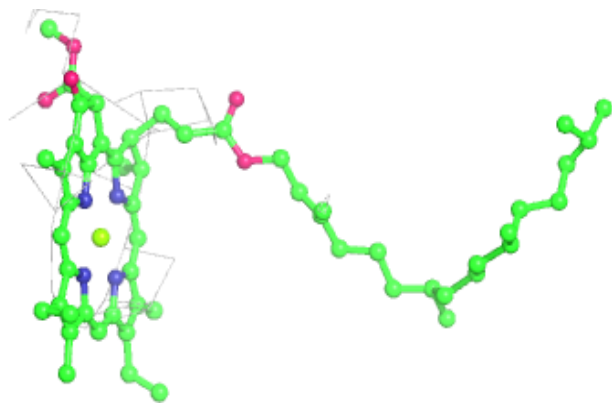
Electron density around CLA B 616:

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

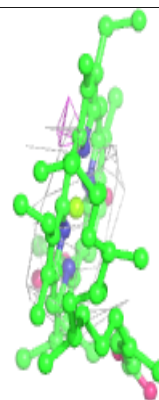
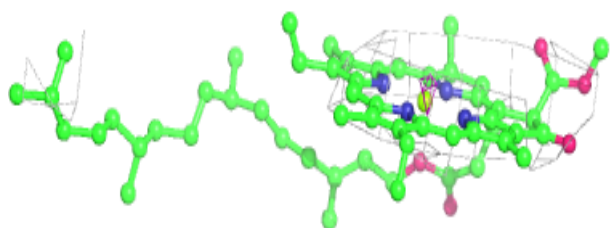
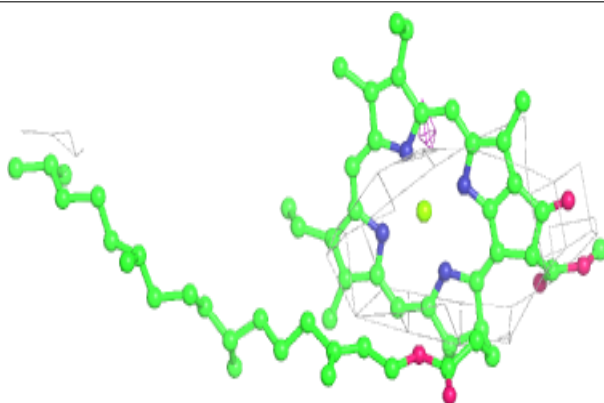


Electron density around CLA Q 404:

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

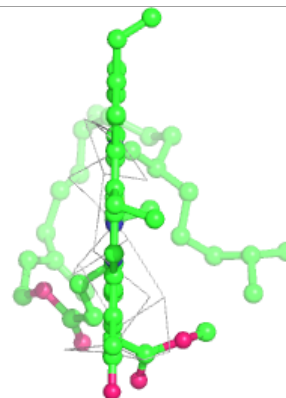
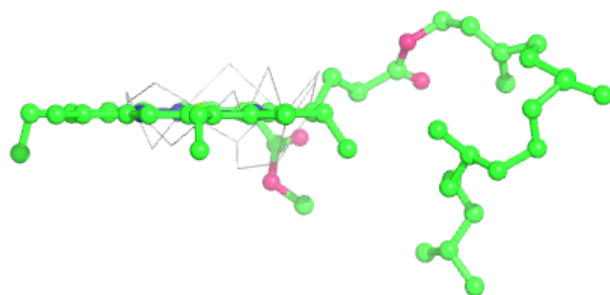
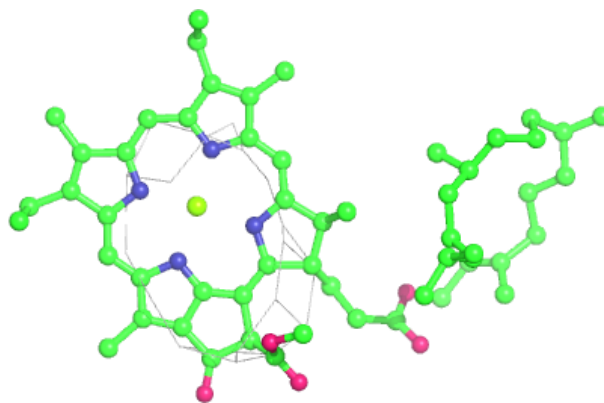
**Electron density around CLA P 501:**

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



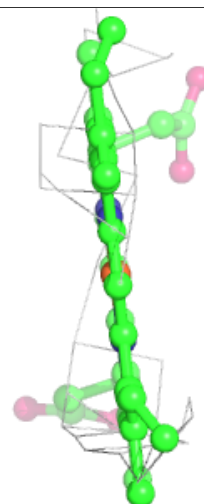
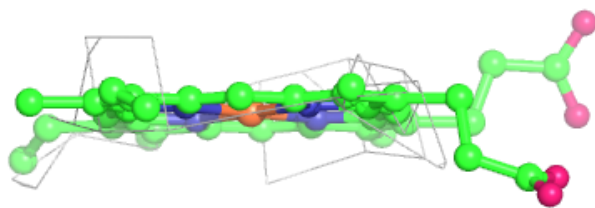
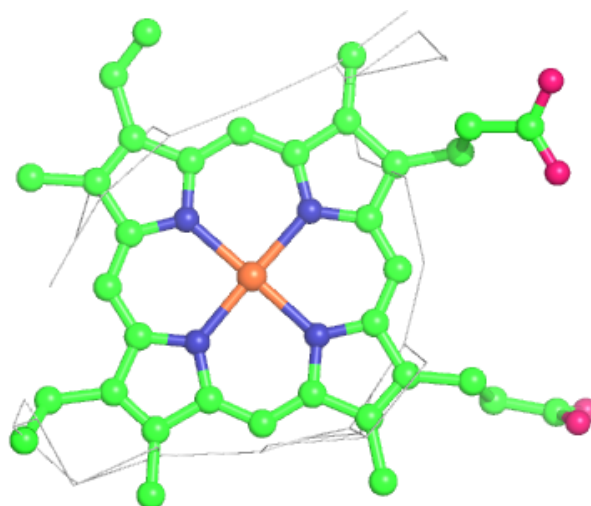
Electron density around CLA P 512:

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



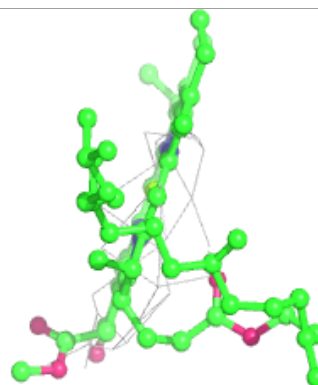
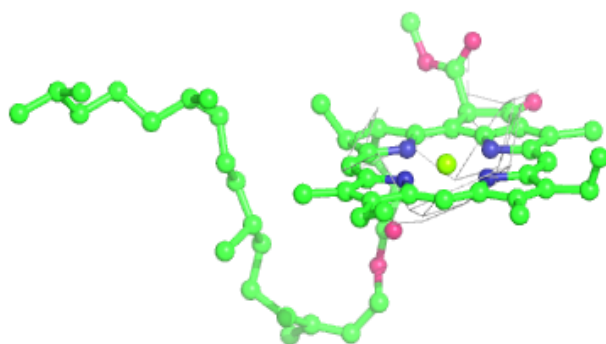
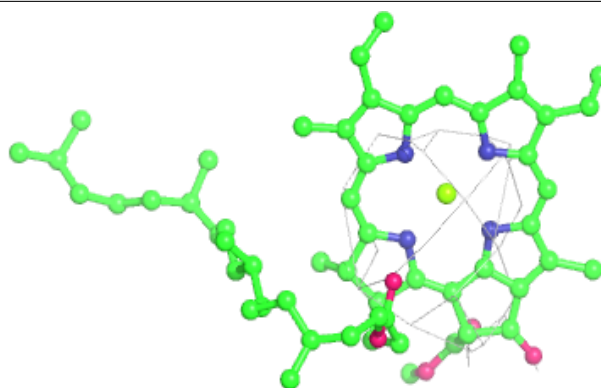
Electron density around HEM V 201:

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

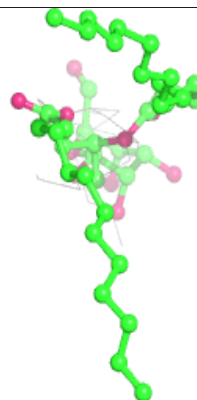
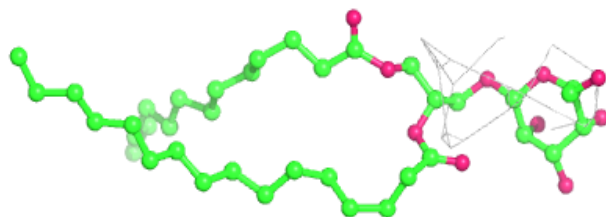
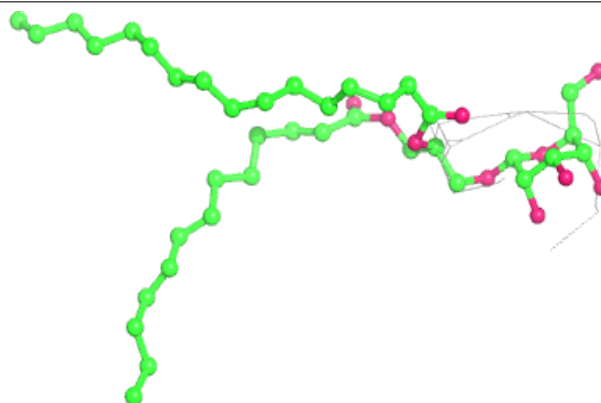


Electron density around CLA A 402:

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

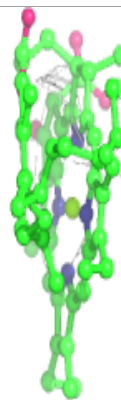
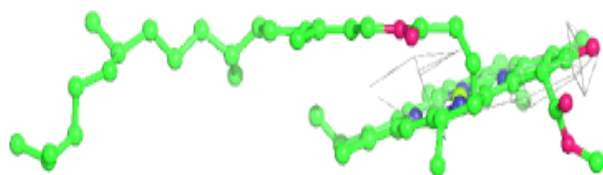
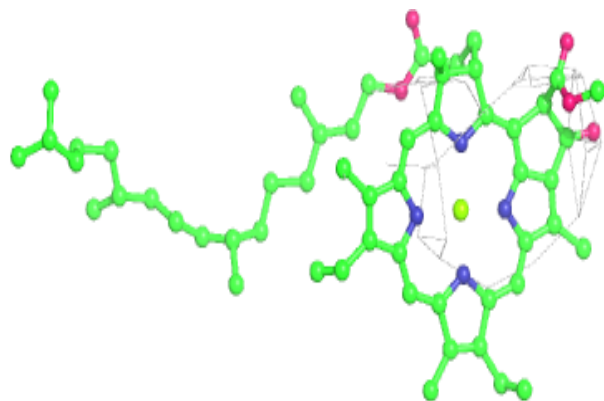
**Electron density around LMG Q 407:**

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

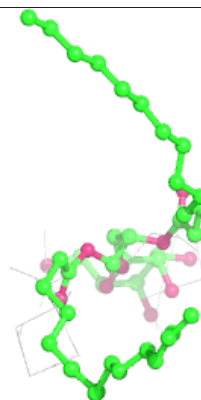
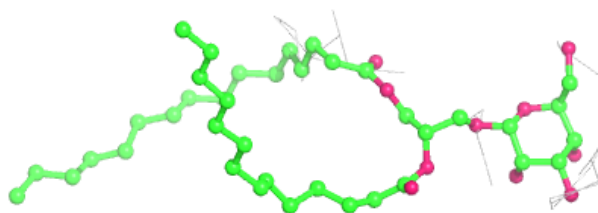
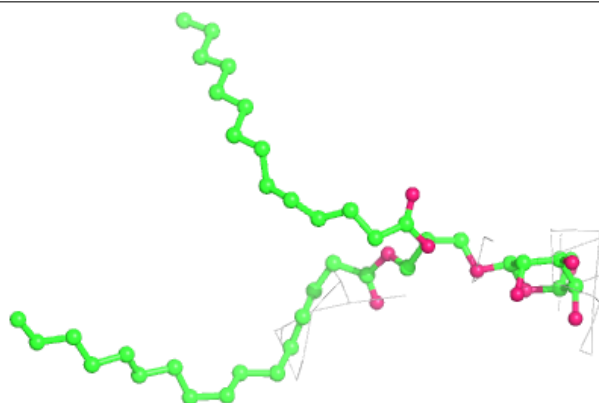


Electron density around CLA B 603:

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

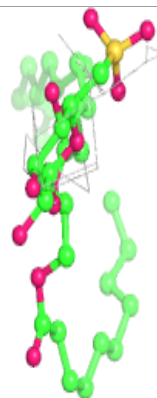
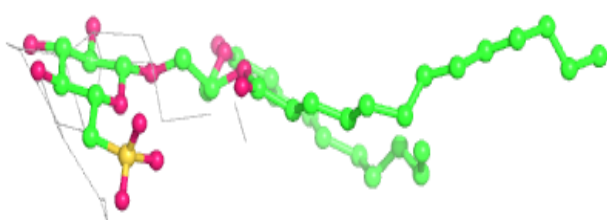
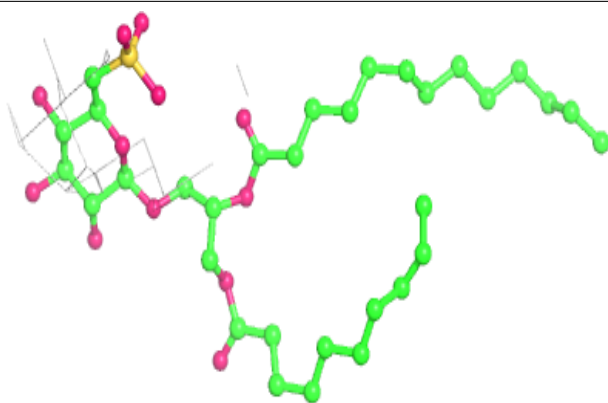
**Electron density around LMG N 623:**

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

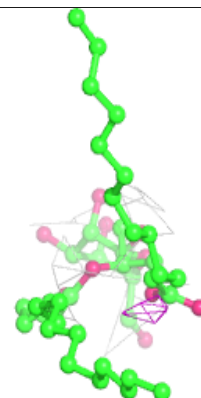
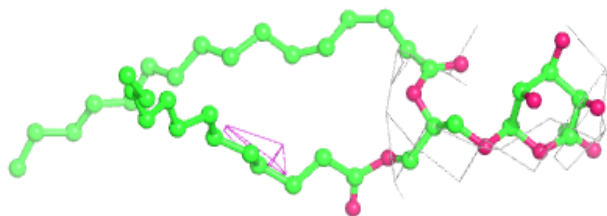
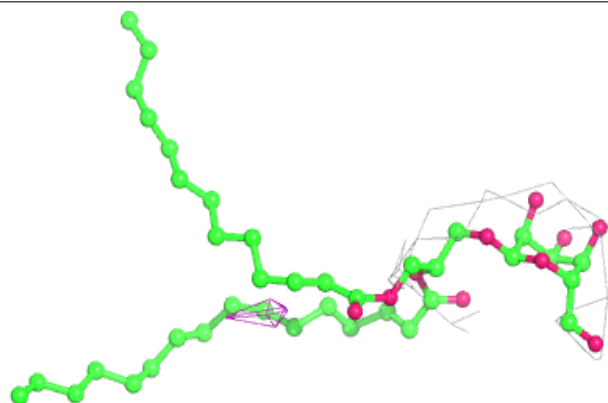


Electron density around SQD S 102:

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

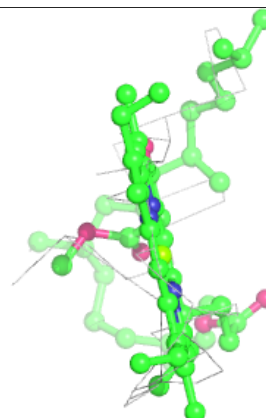
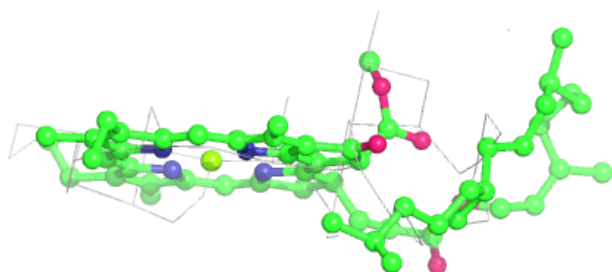
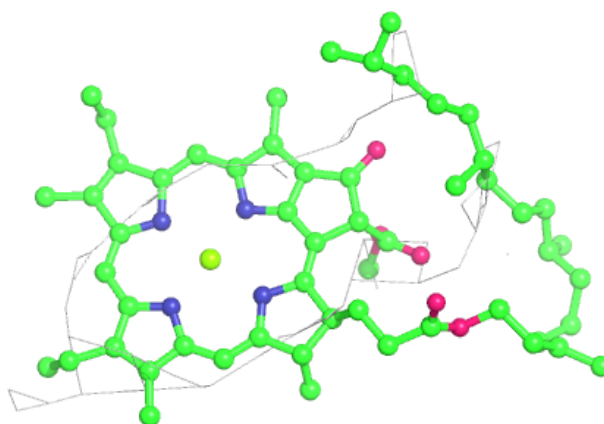
**Electron density around LMG D 407:**

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

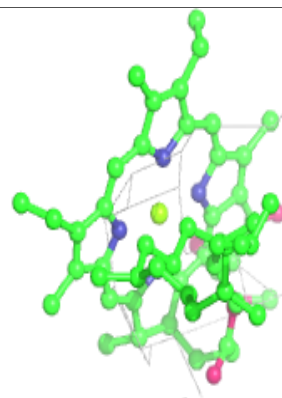
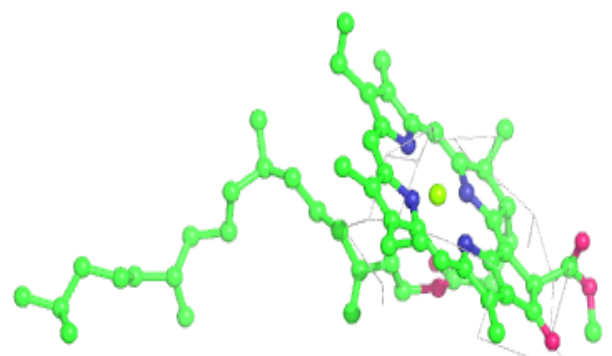
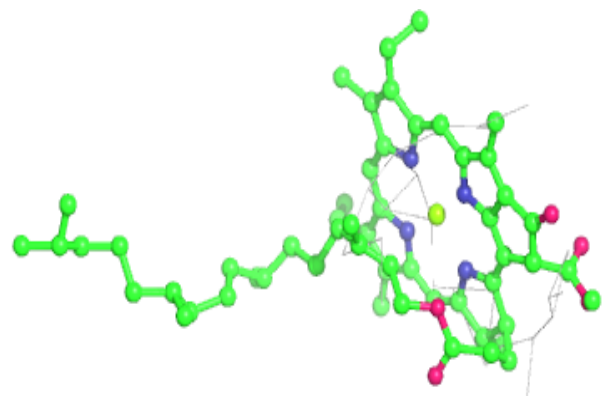


Electron density around CLA B 610:

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

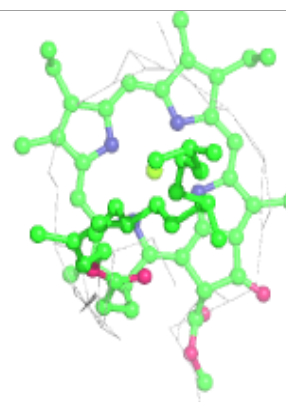
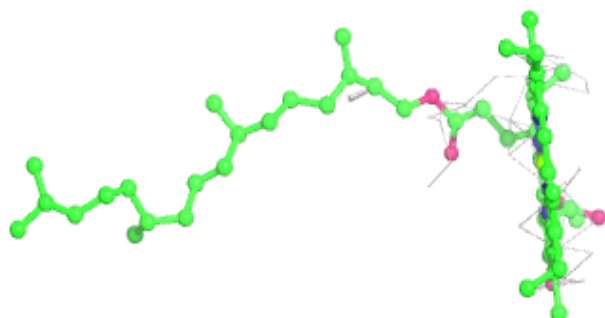
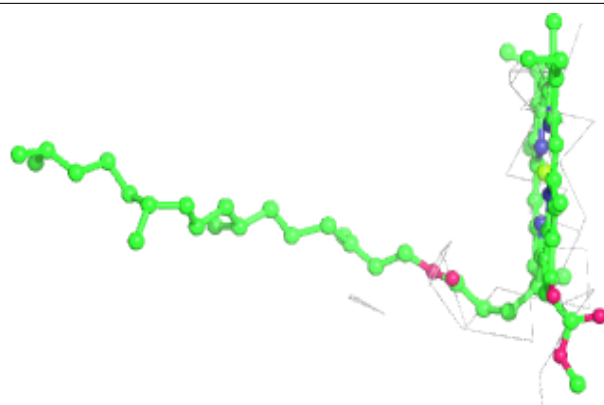
**Electron density around CLA P 505:**

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

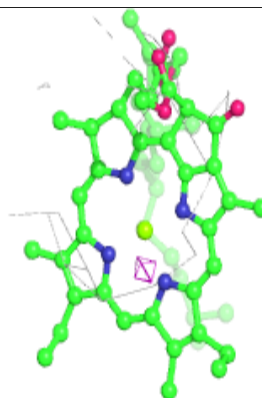
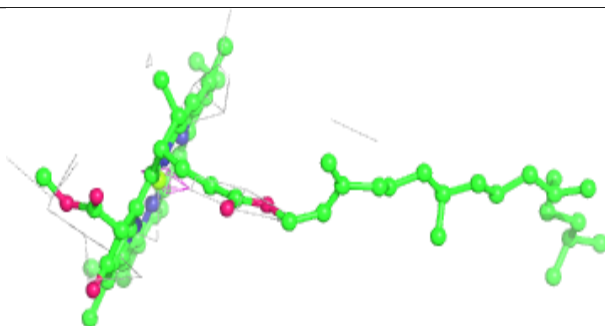
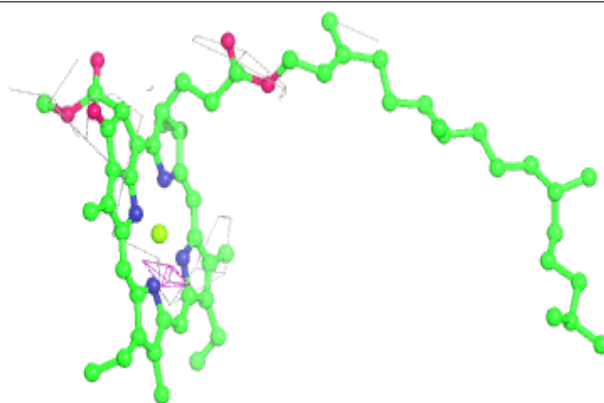


Electron density around CLA B 606:

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

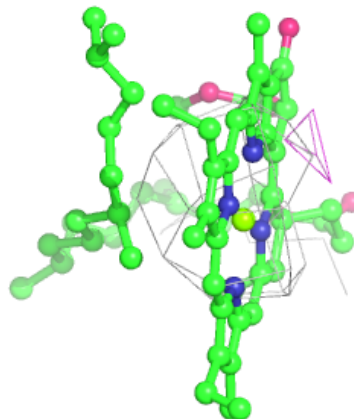
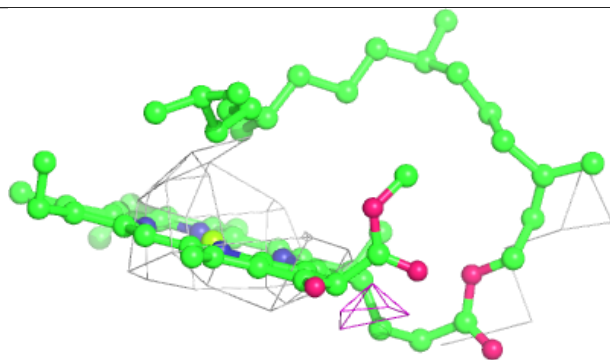
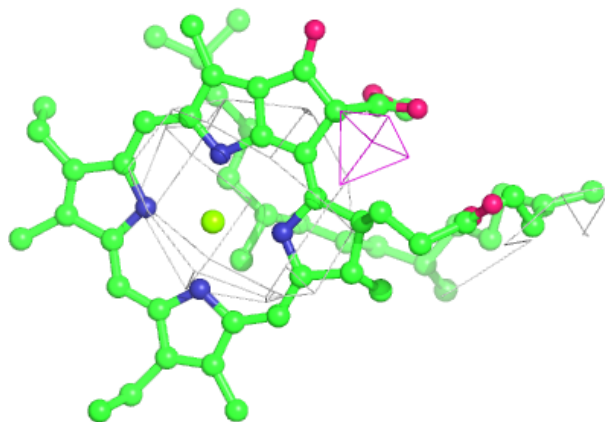
**Electron density around CLA B 609:**

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

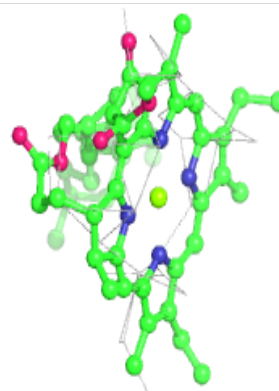
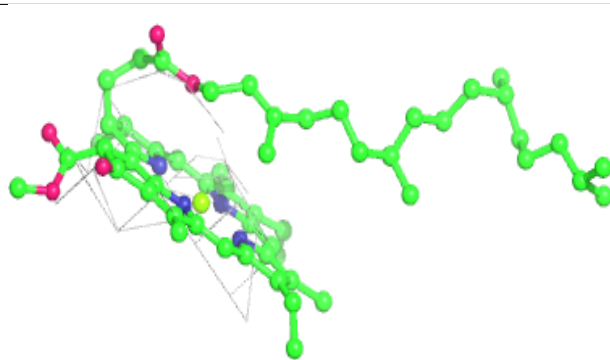
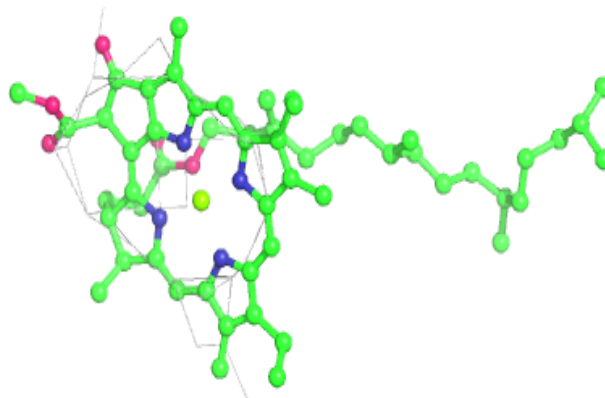


Electron density around CLA P 510:

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

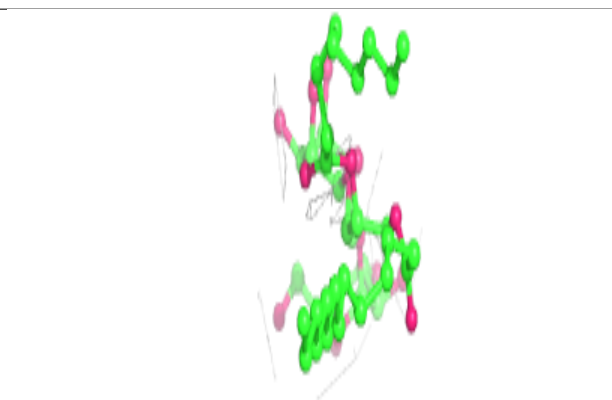
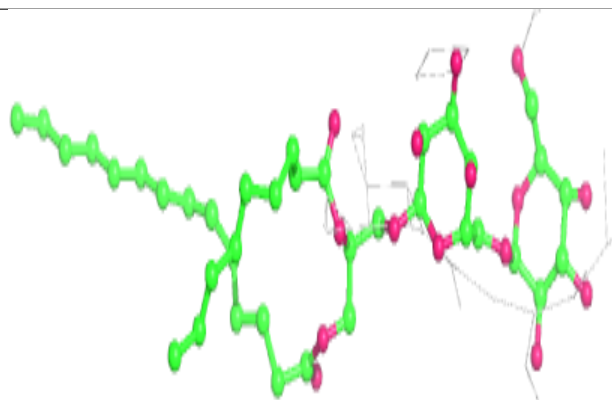
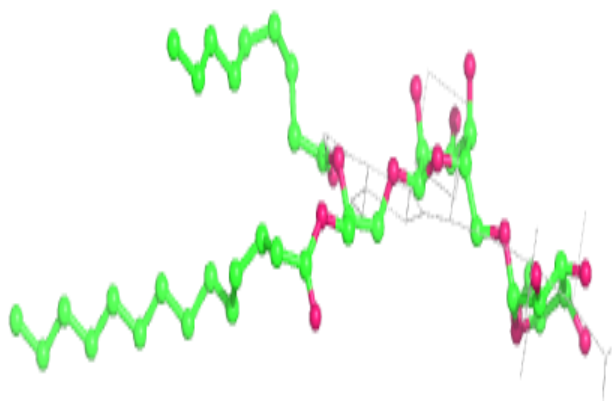
**Electron density around CLA B 614:**

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

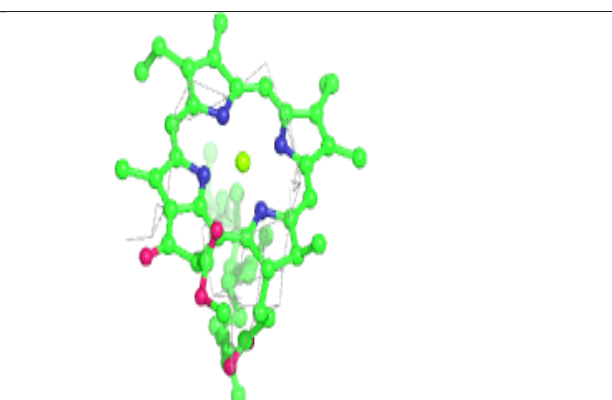
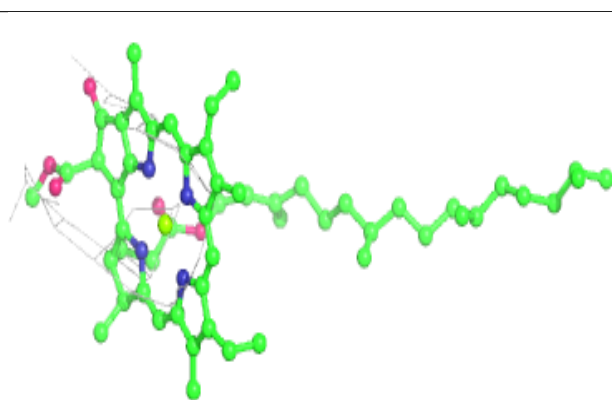
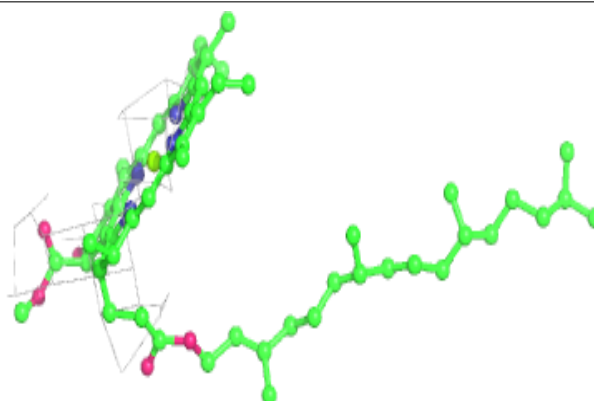


Electron density around DGD C 516:

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

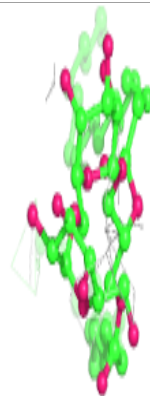
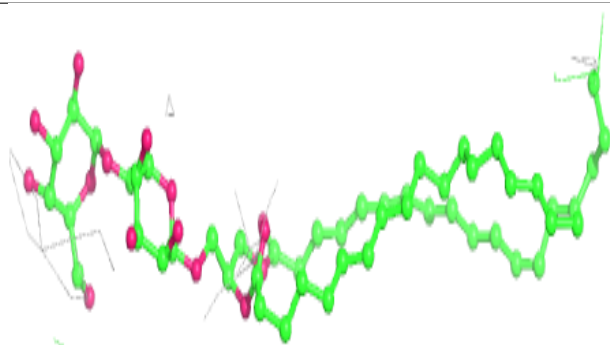
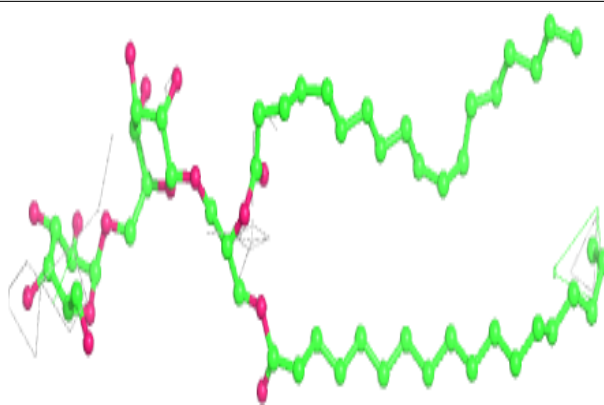
**Electron density around CLA P 504:**

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

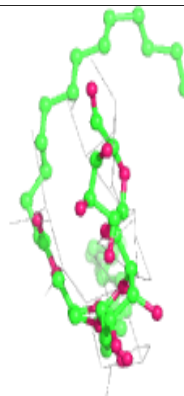
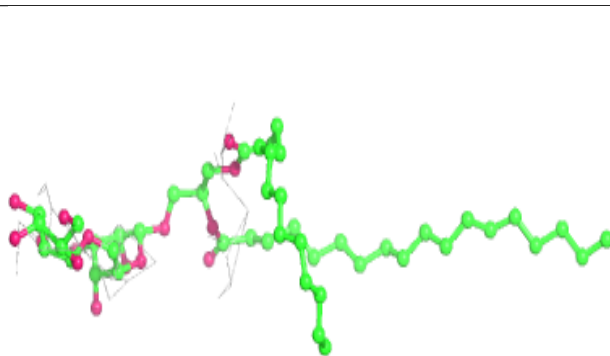
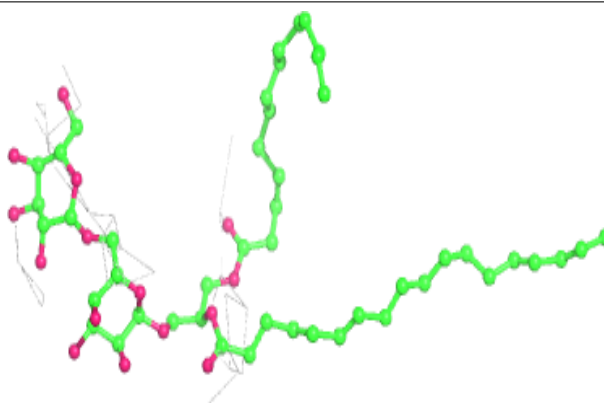


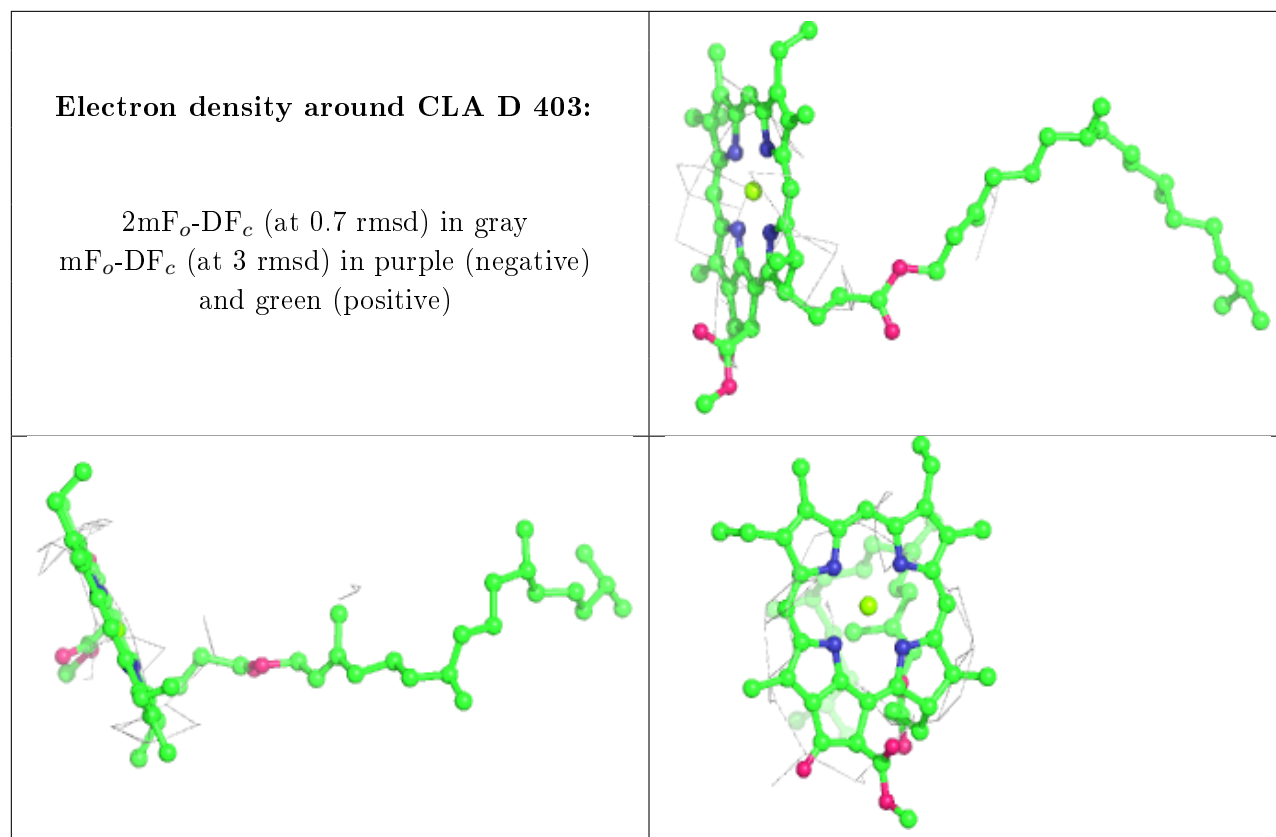
Electron density around DGD P 519:

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

**Electron density around DGD P 518:**

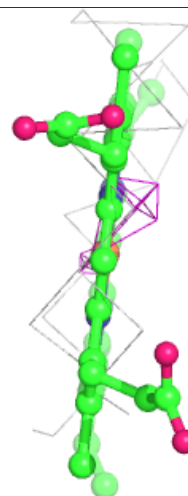
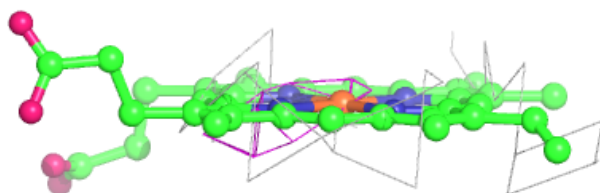
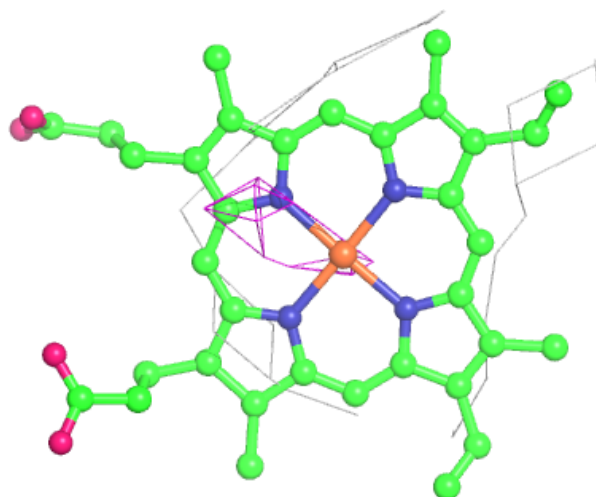
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





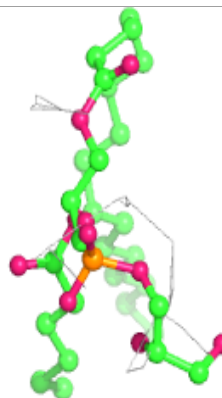
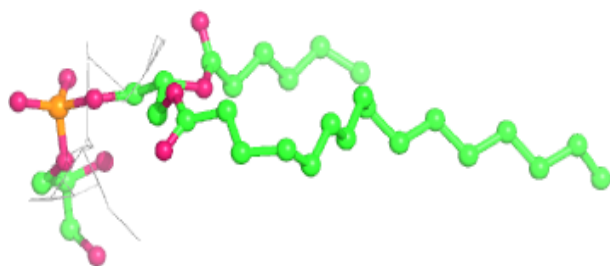
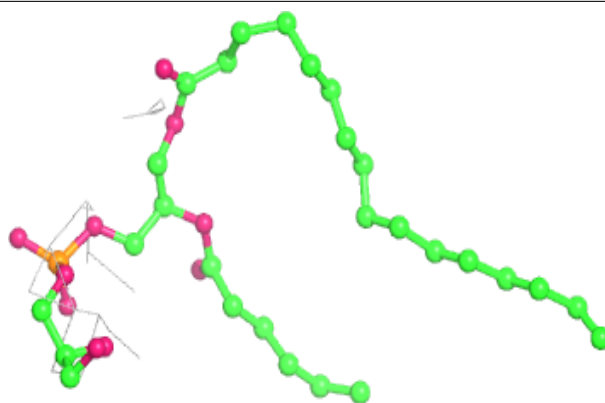
Electron density around HEM i 201:

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

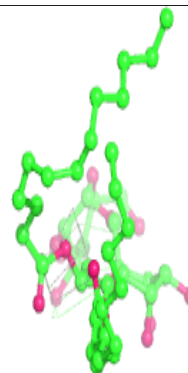
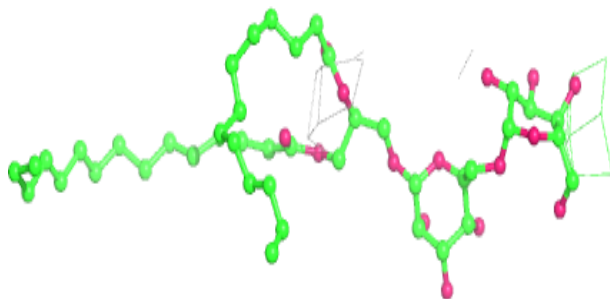
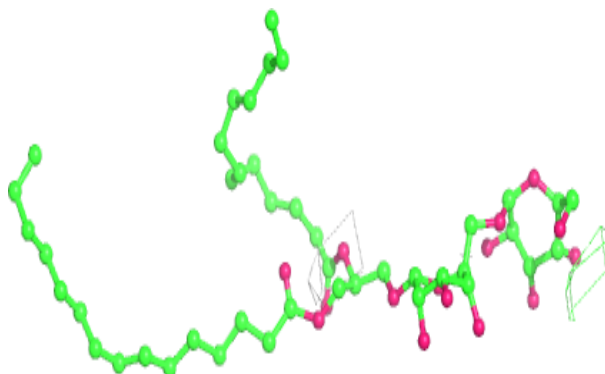


Electron density around LHG A 408:

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

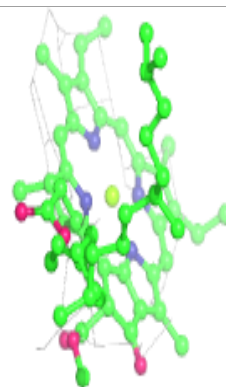
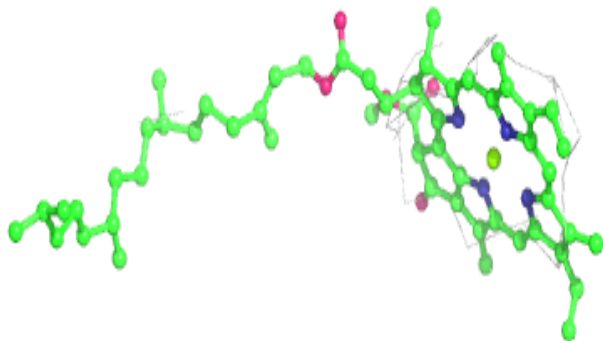
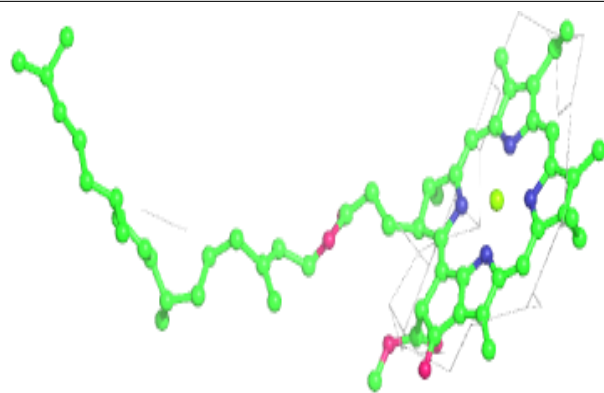
**Electron density around DGD W 102:**

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

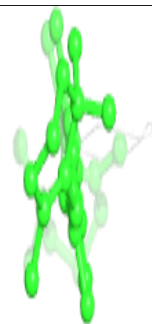
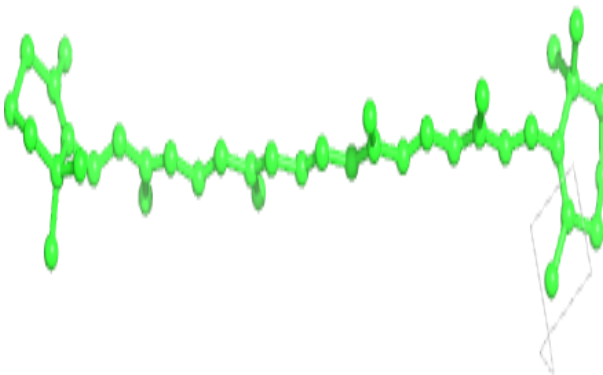
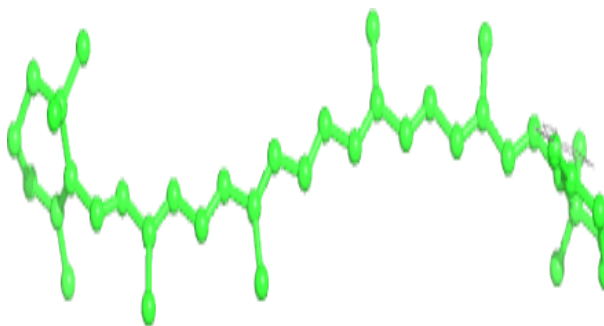


Electron density around CLA G 402:

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

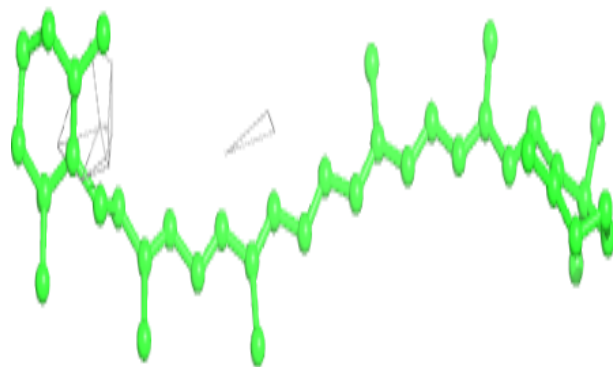
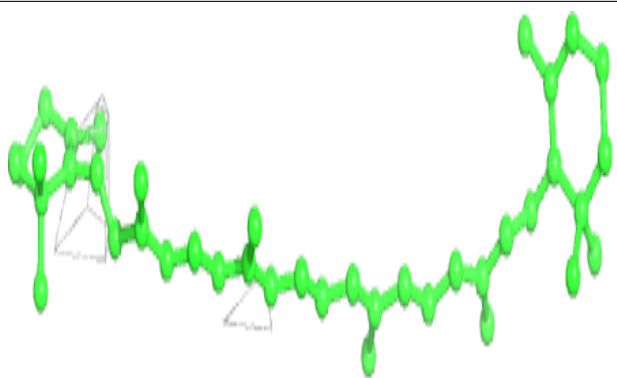
**Electron density around BCR P 515:**

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

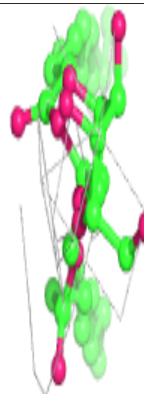
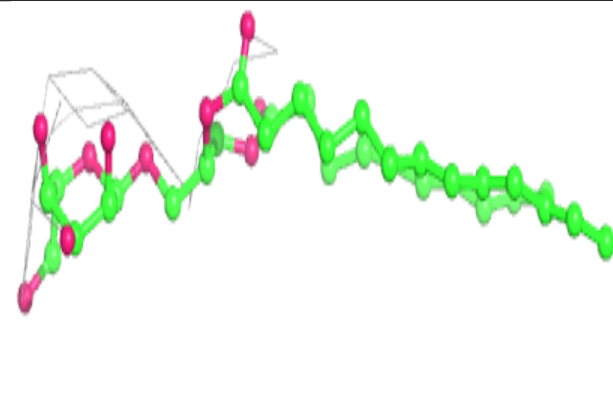
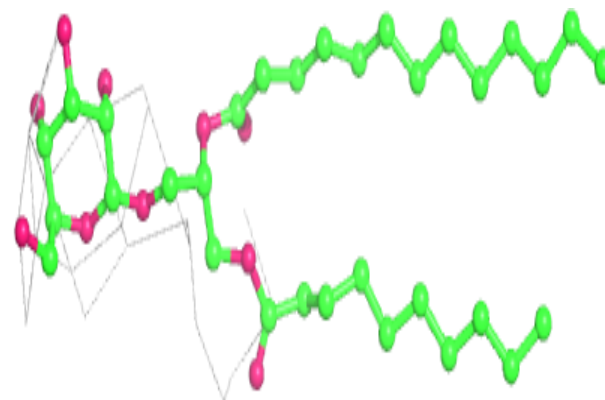


Electron density around BCR S 101:

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

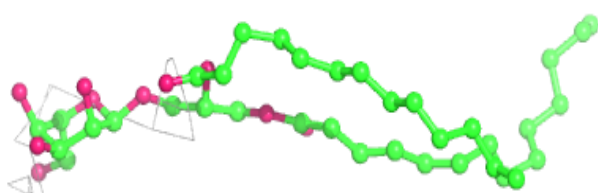
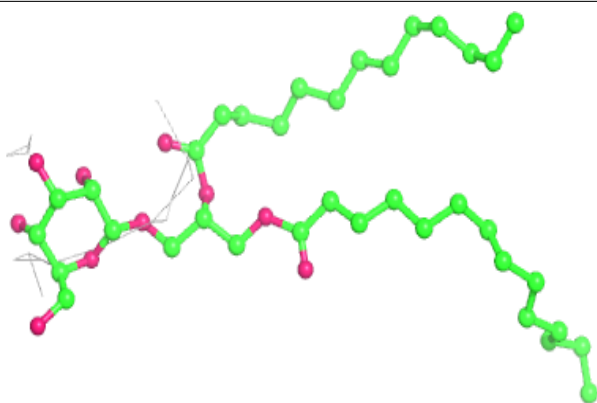
**Electron density around LMG M 101:**

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

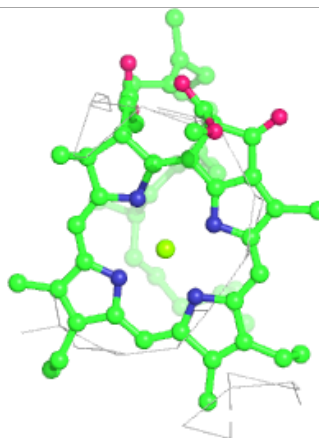
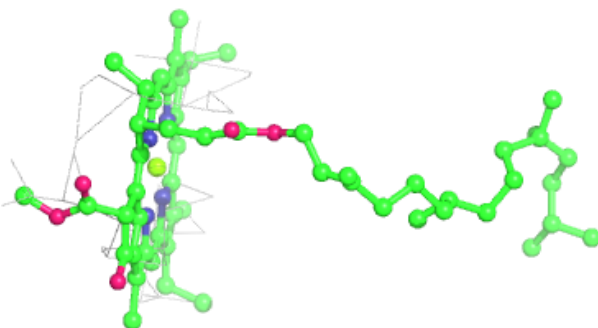
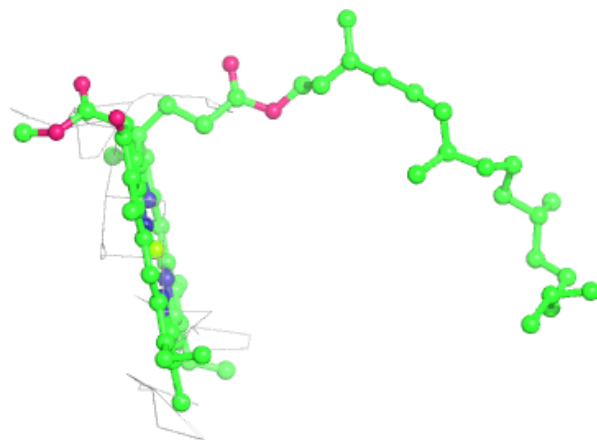


Electron density around LMG Q 406:

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

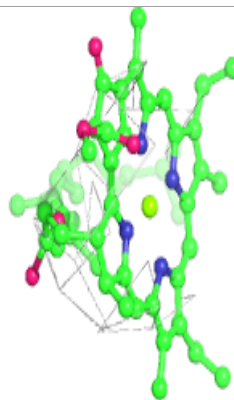
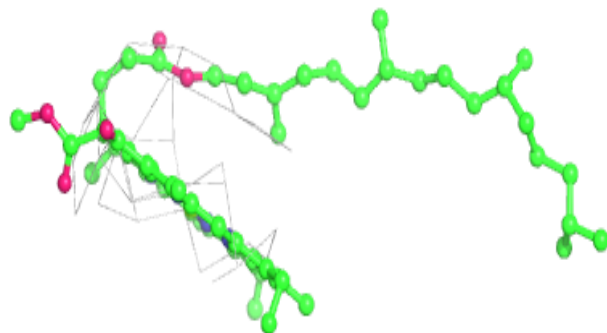
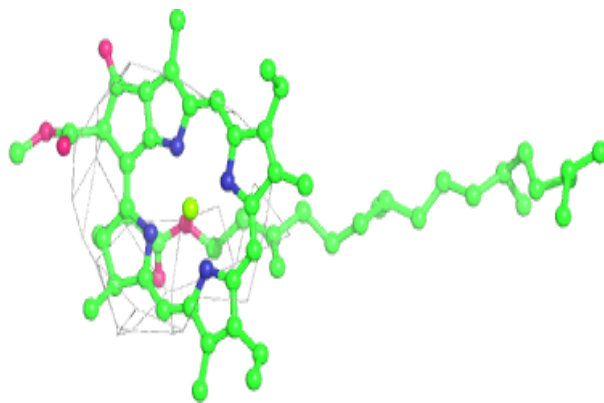
**Electron density around CLA P 506:**

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



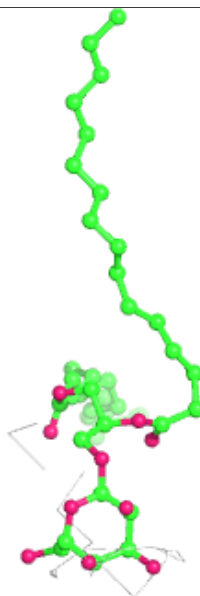
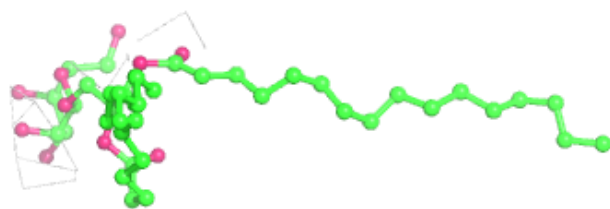
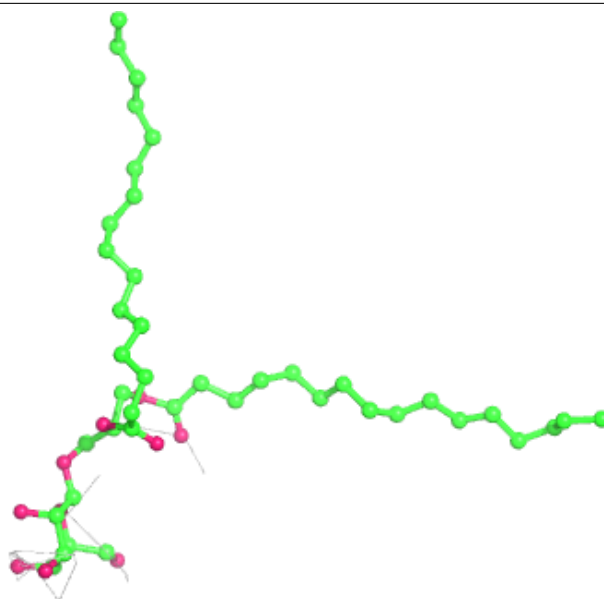
Electron density around CLA N 612:

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



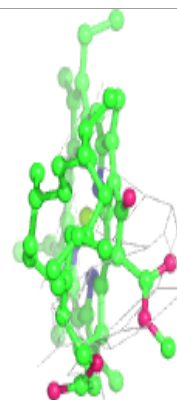
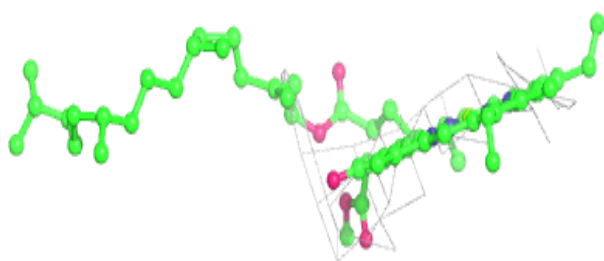
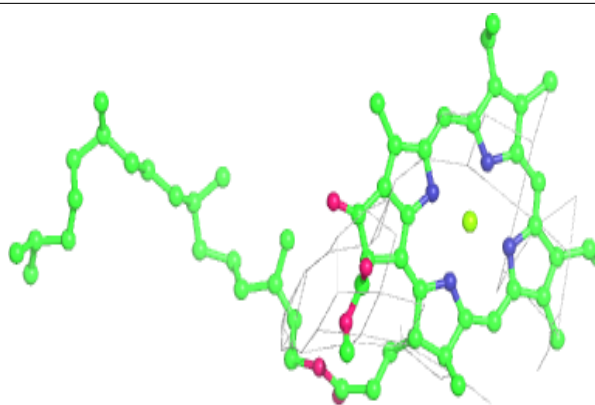
Electron density around LMG G 411:

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

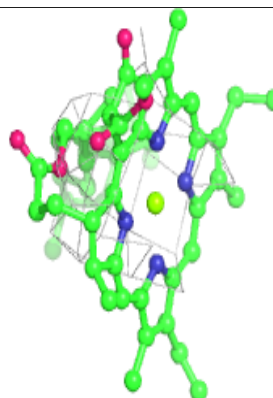
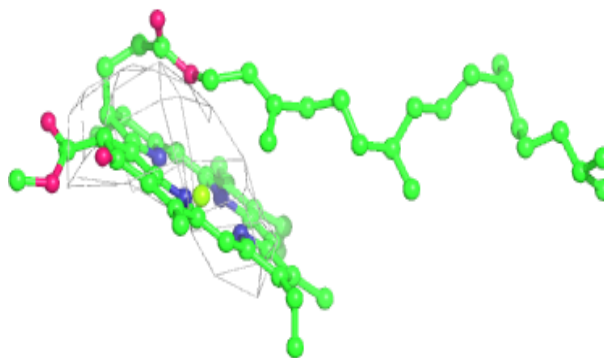
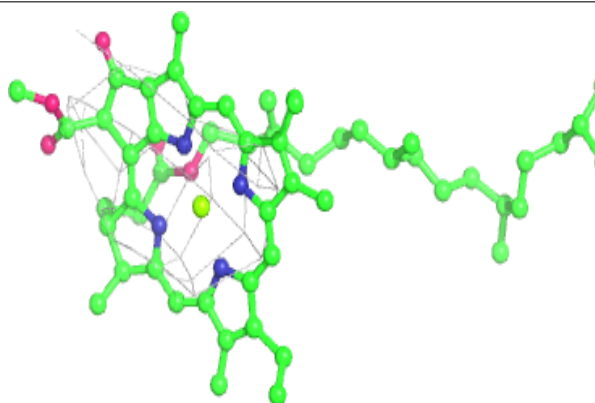


Electron density around CLA B 602:

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

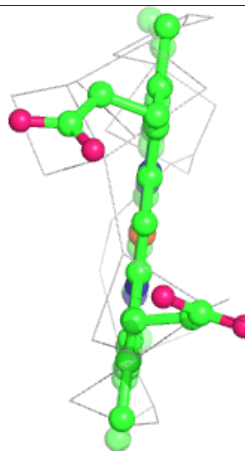
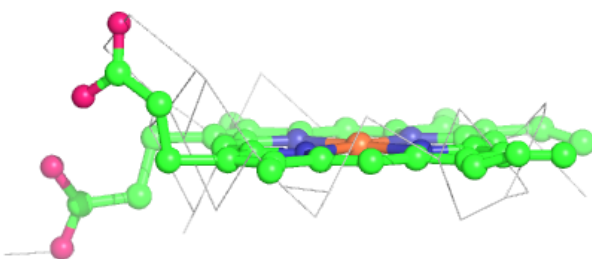
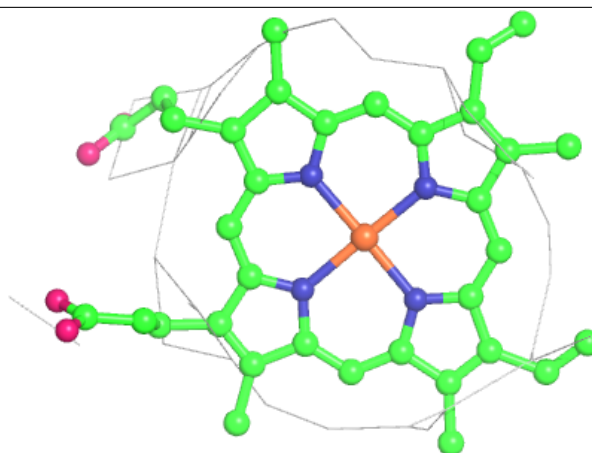
**Electron density around CLA N 618:**

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

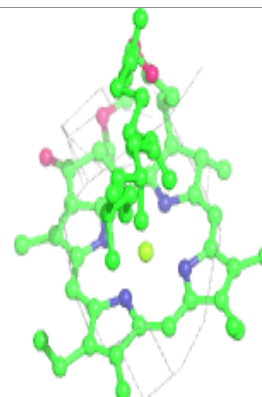
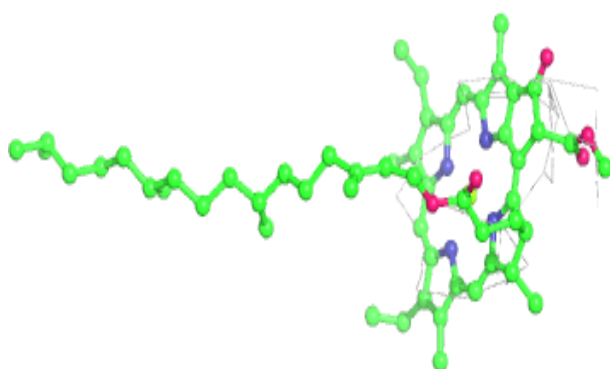
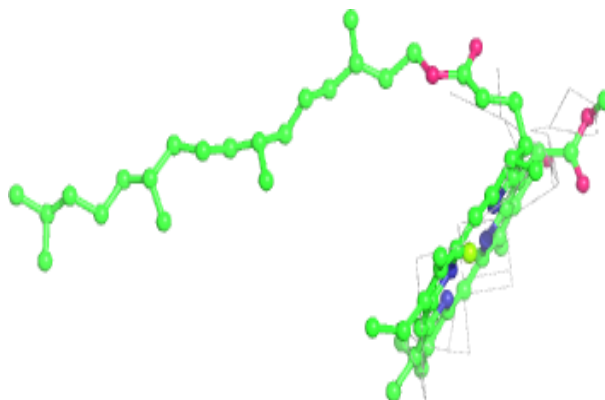


Electron density around HEM E 101:

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

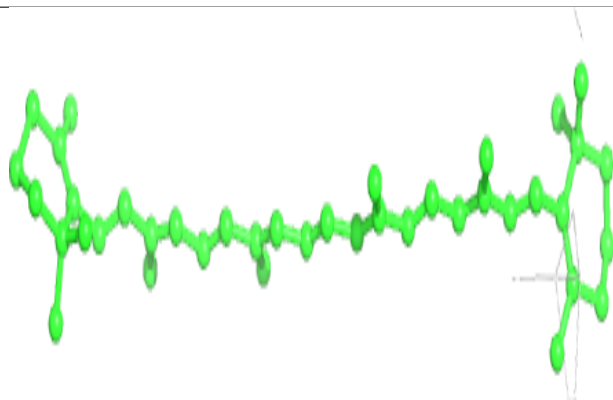
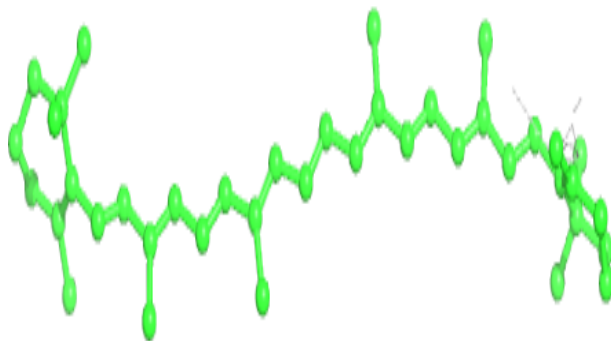
**Electron density around CLA C 504:**

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

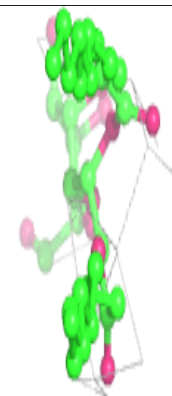
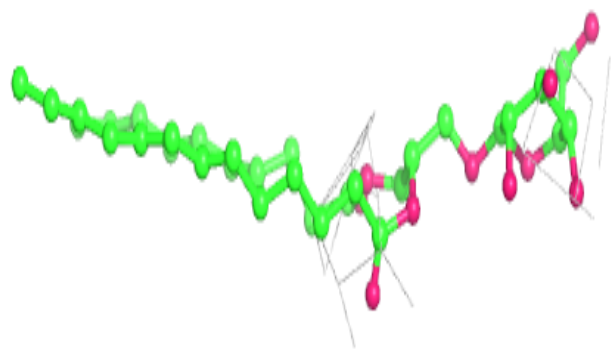
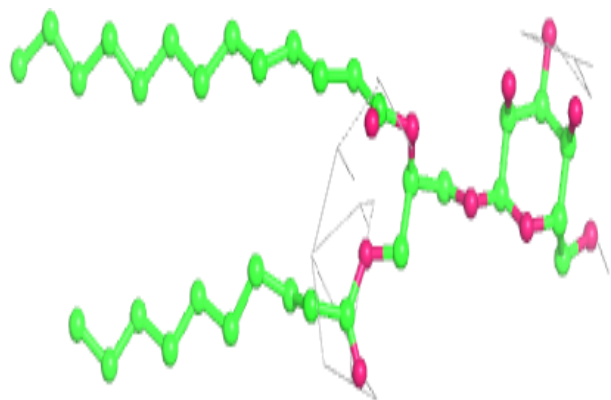


Electron density around BCR Z 101:

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

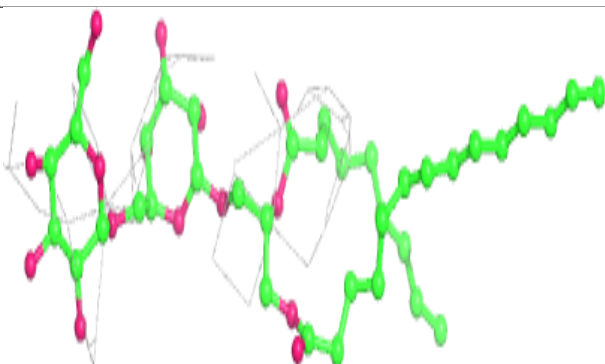
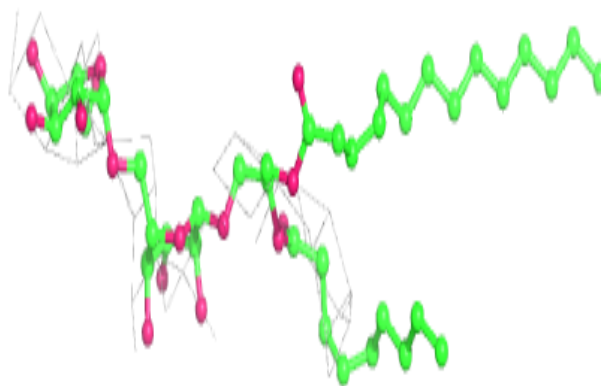
**Electron density around LMG e 102:**

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

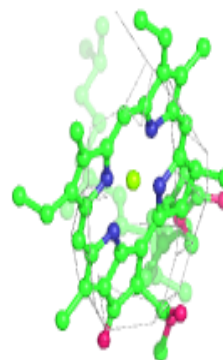
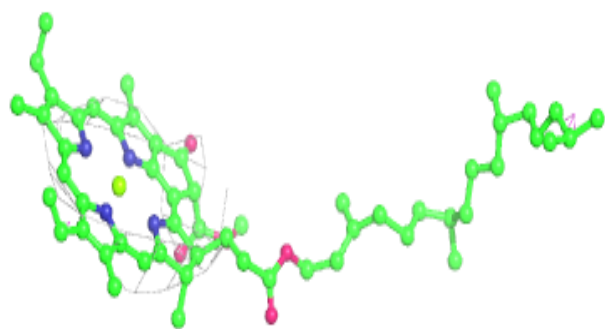
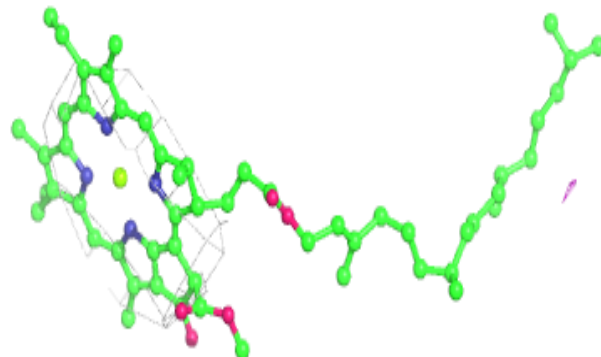


Electron density around DGD P 517:

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

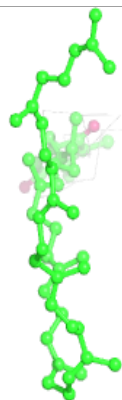
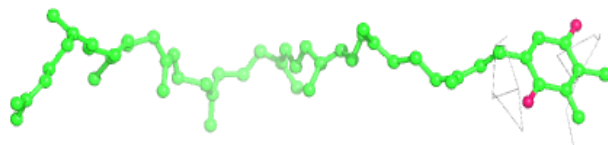
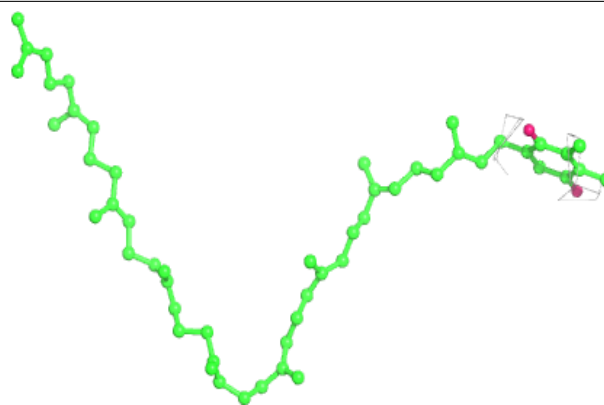
**Electron density around CLA A 401:**

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

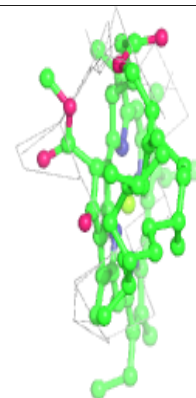
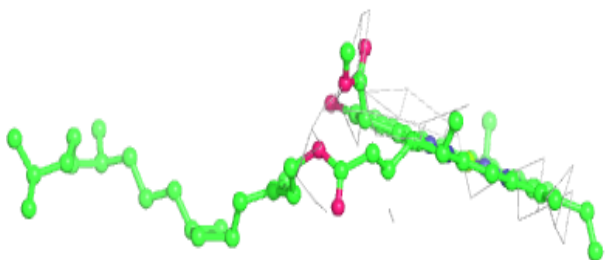
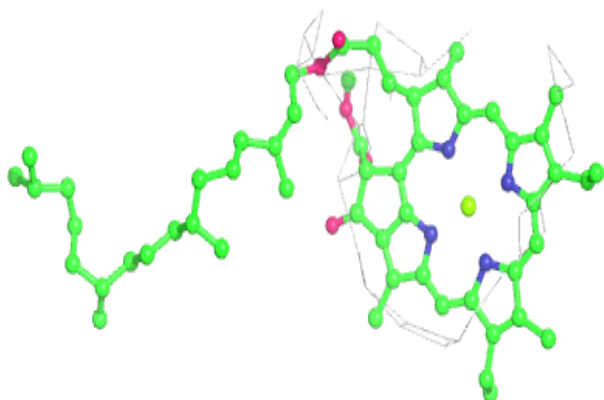


Electron density around PL9 D 404:

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

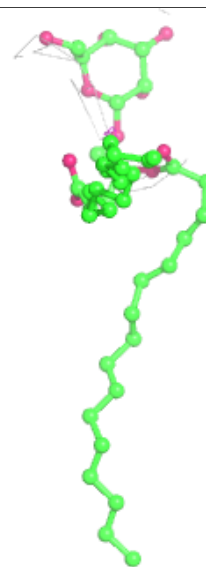
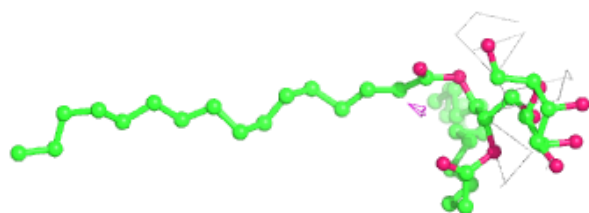
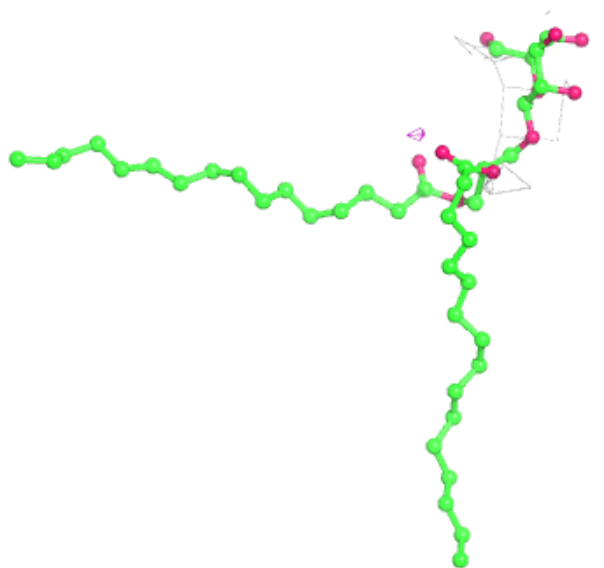
**Electron density around CLA N 606:**

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



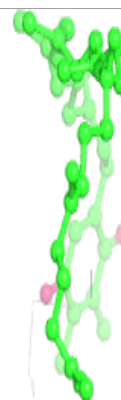
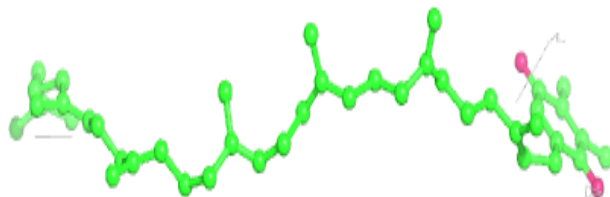
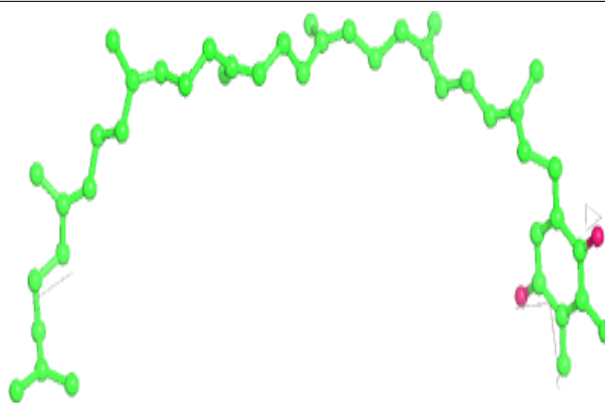
Electron density around LMG A 410:

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

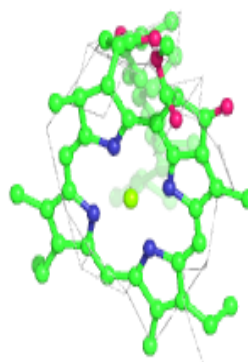
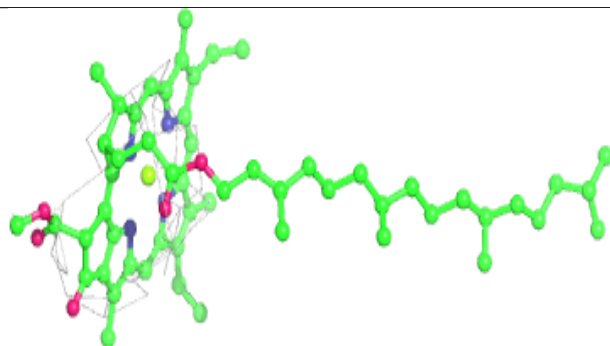
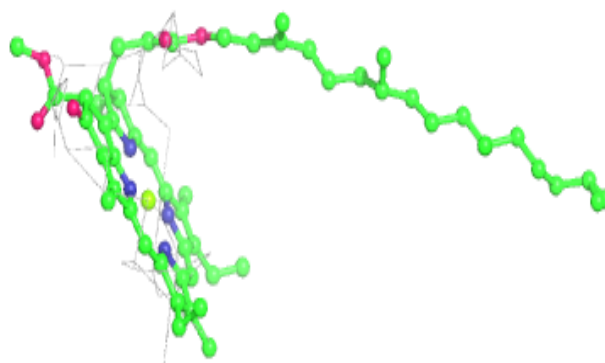


Electron density around PL9 A 406:

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

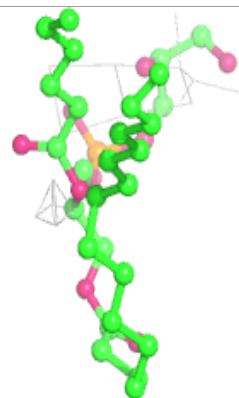
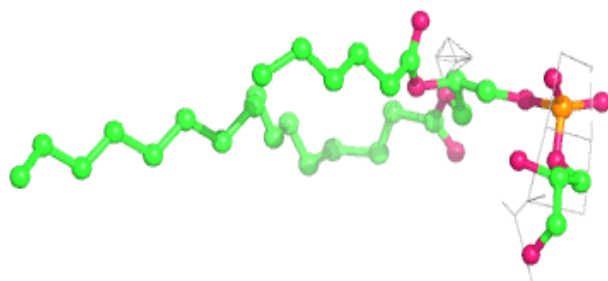
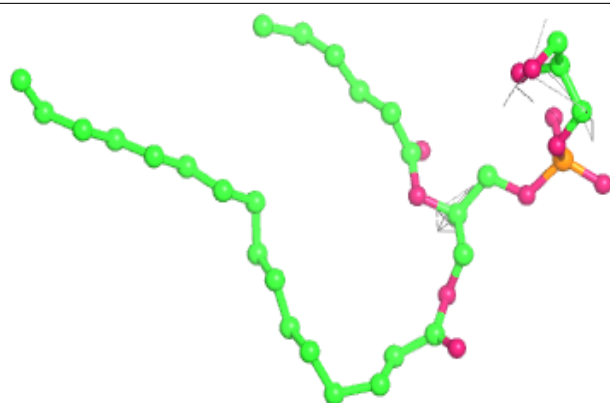
**Electron density around CLA N 611:**

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

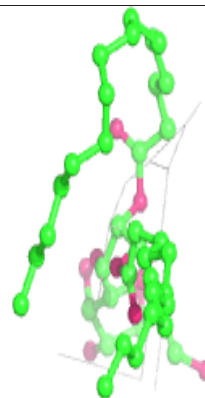
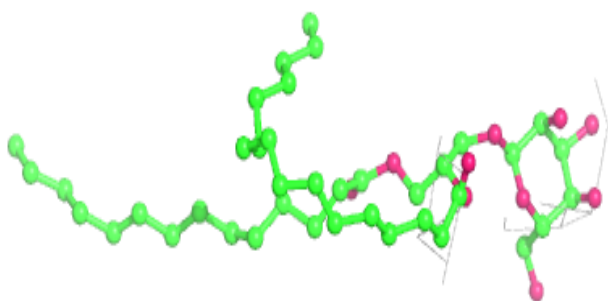
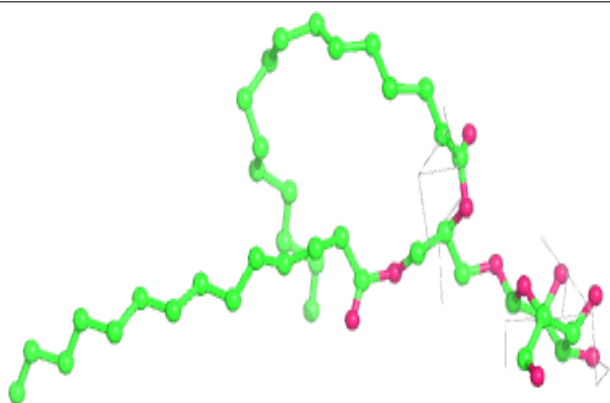


Electron density around LHG G 409:

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

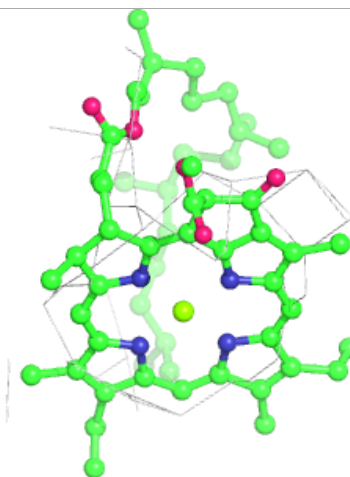
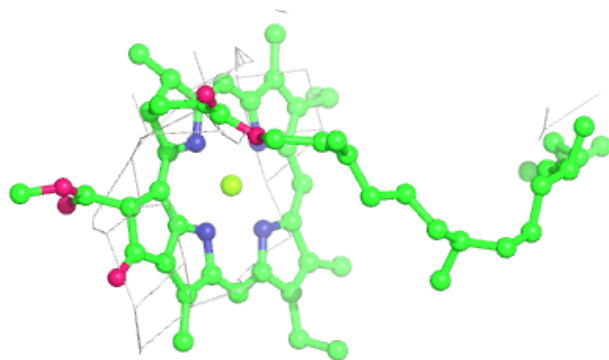
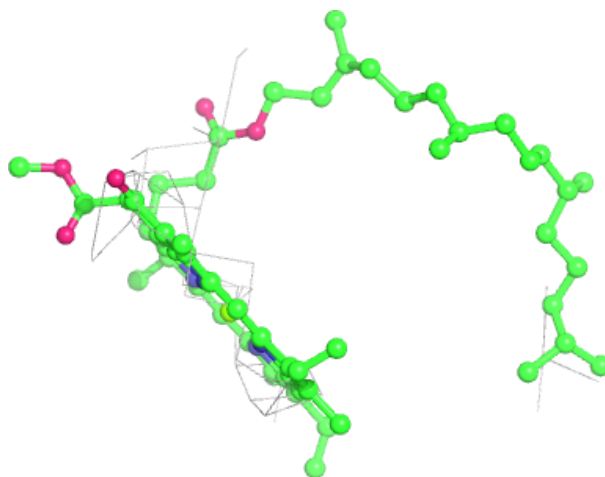
**Electron density around LMG N 622:**

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



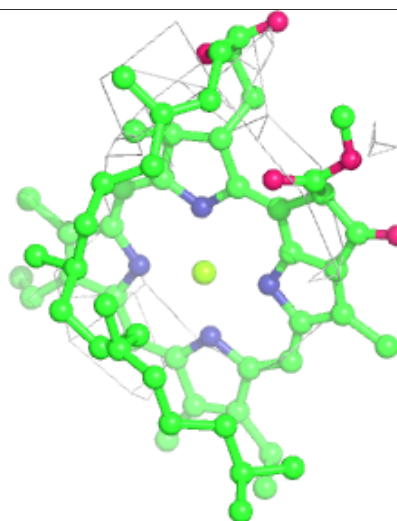
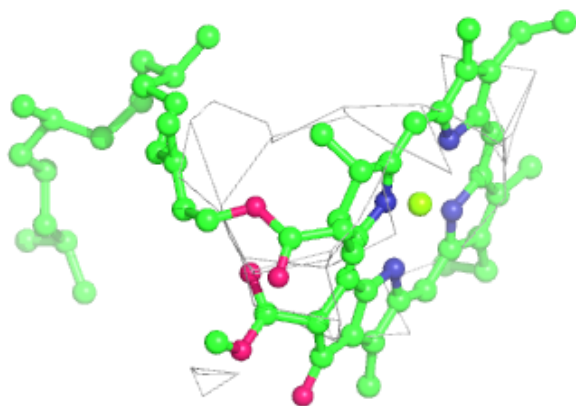
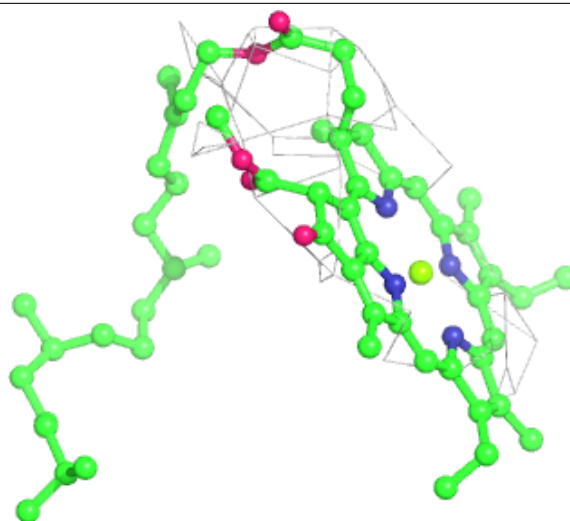
Electron density around CLA N 615:

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



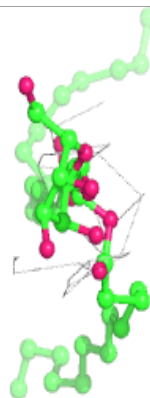
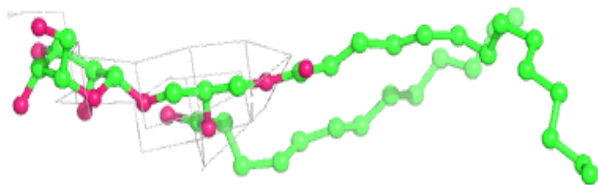
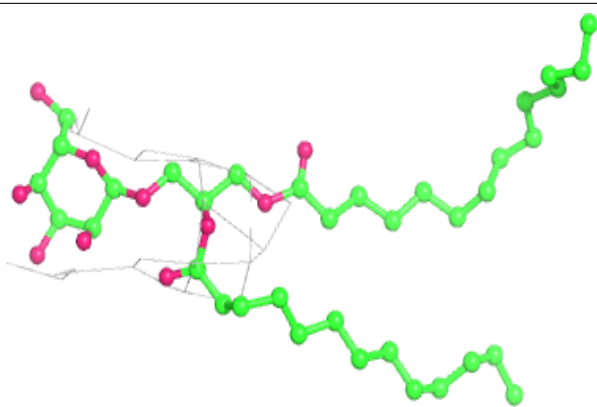
Electron density around CLA B 613:

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



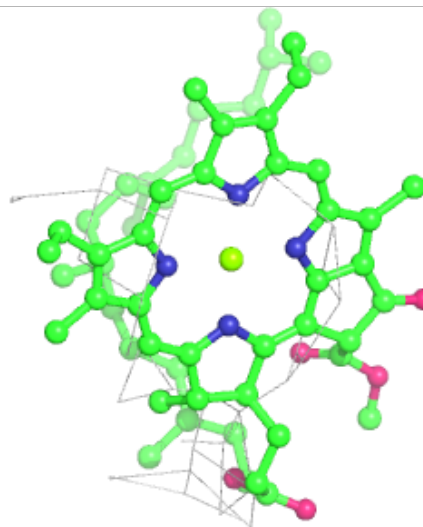
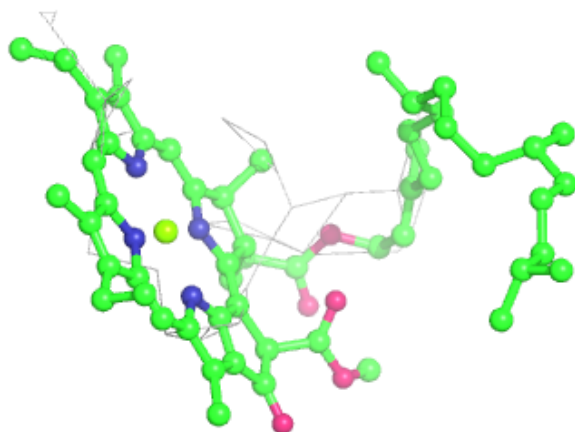
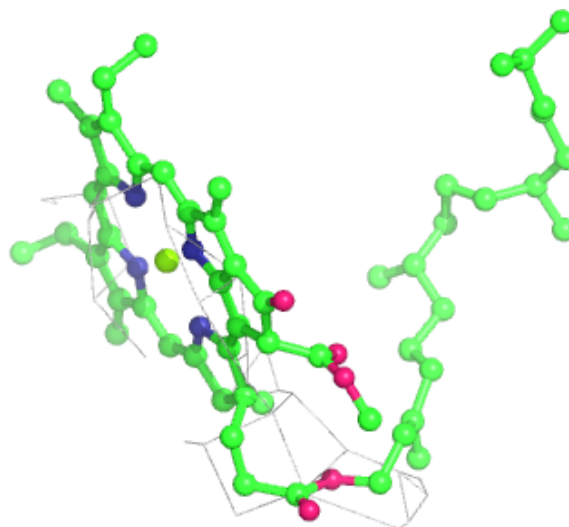
Electron density around LMG D 406:

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



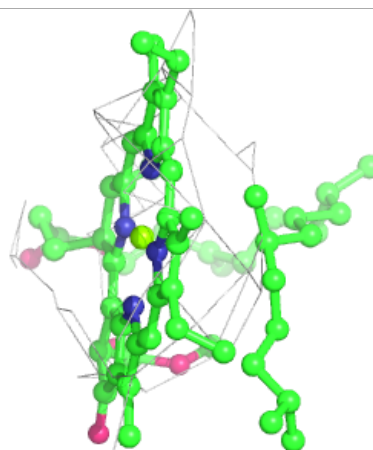
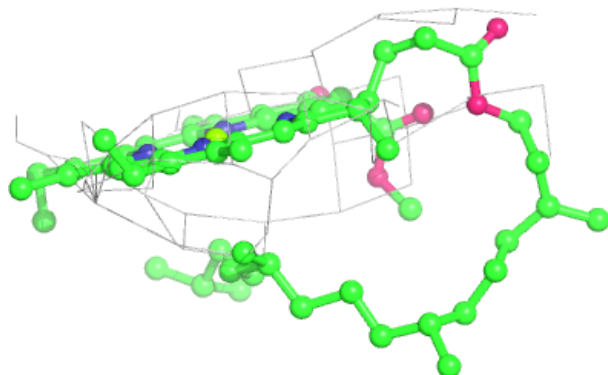
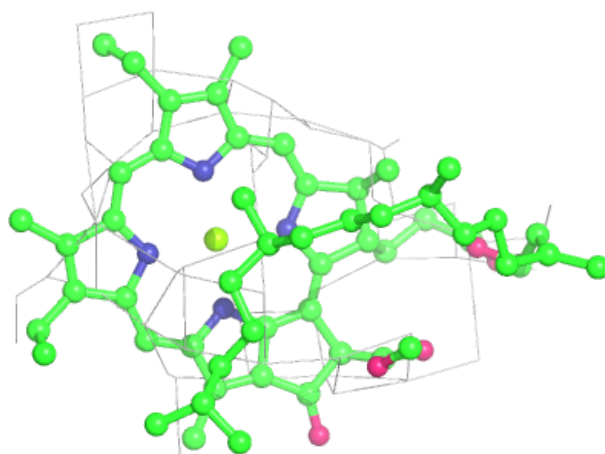
Electron density around CLA N 617:

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



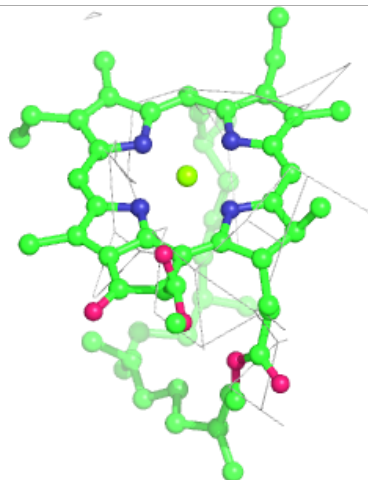
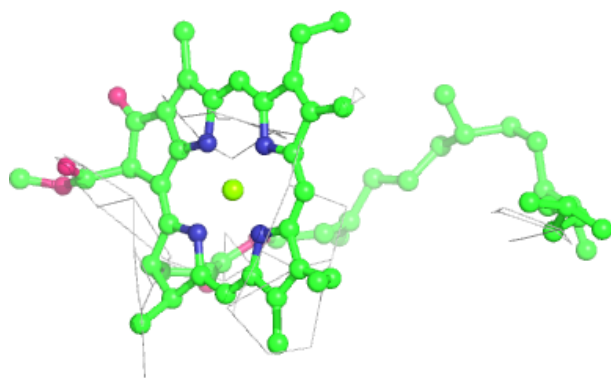
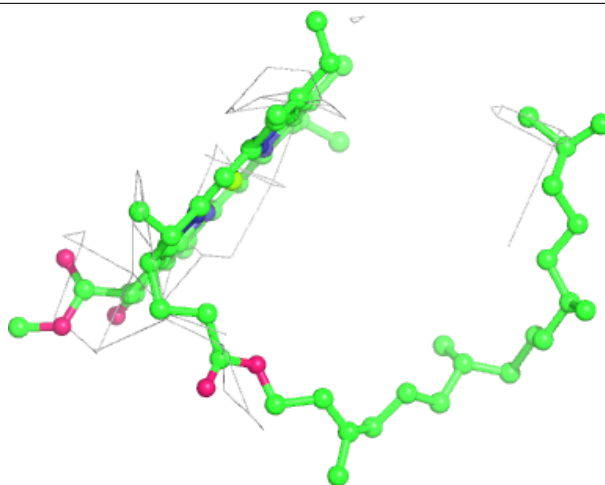
Electron density around CLA C 510:

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



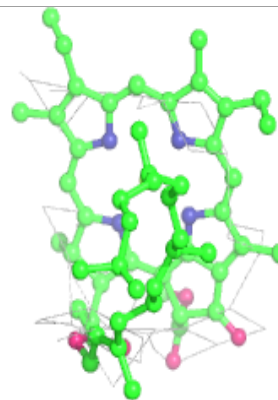
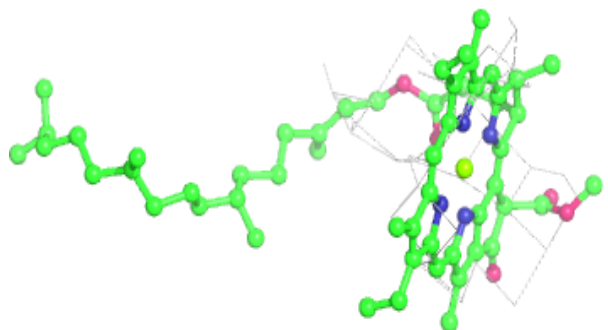
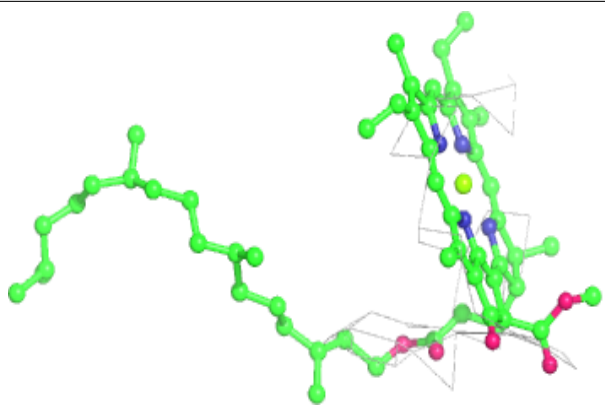
Electron density around CLA B 611:

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



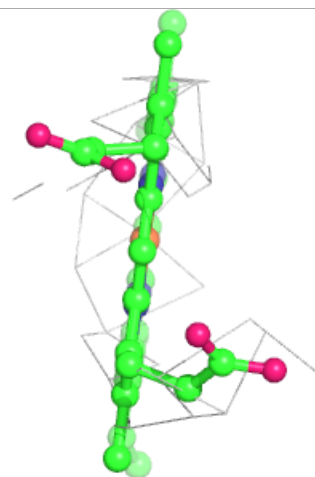
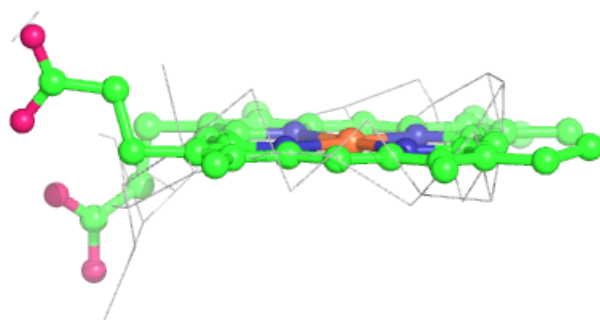
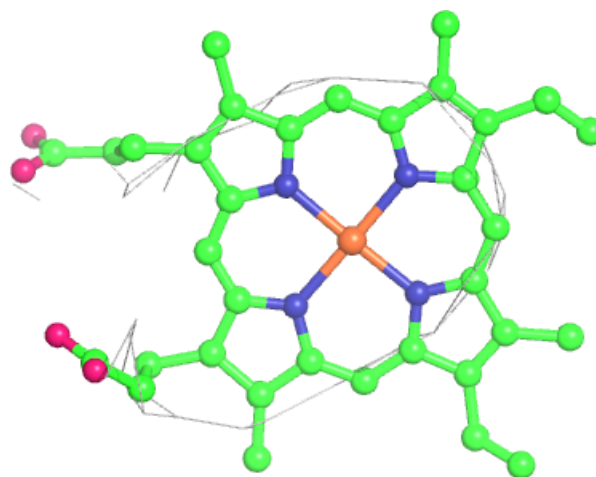
Electron density around CLA P 508:

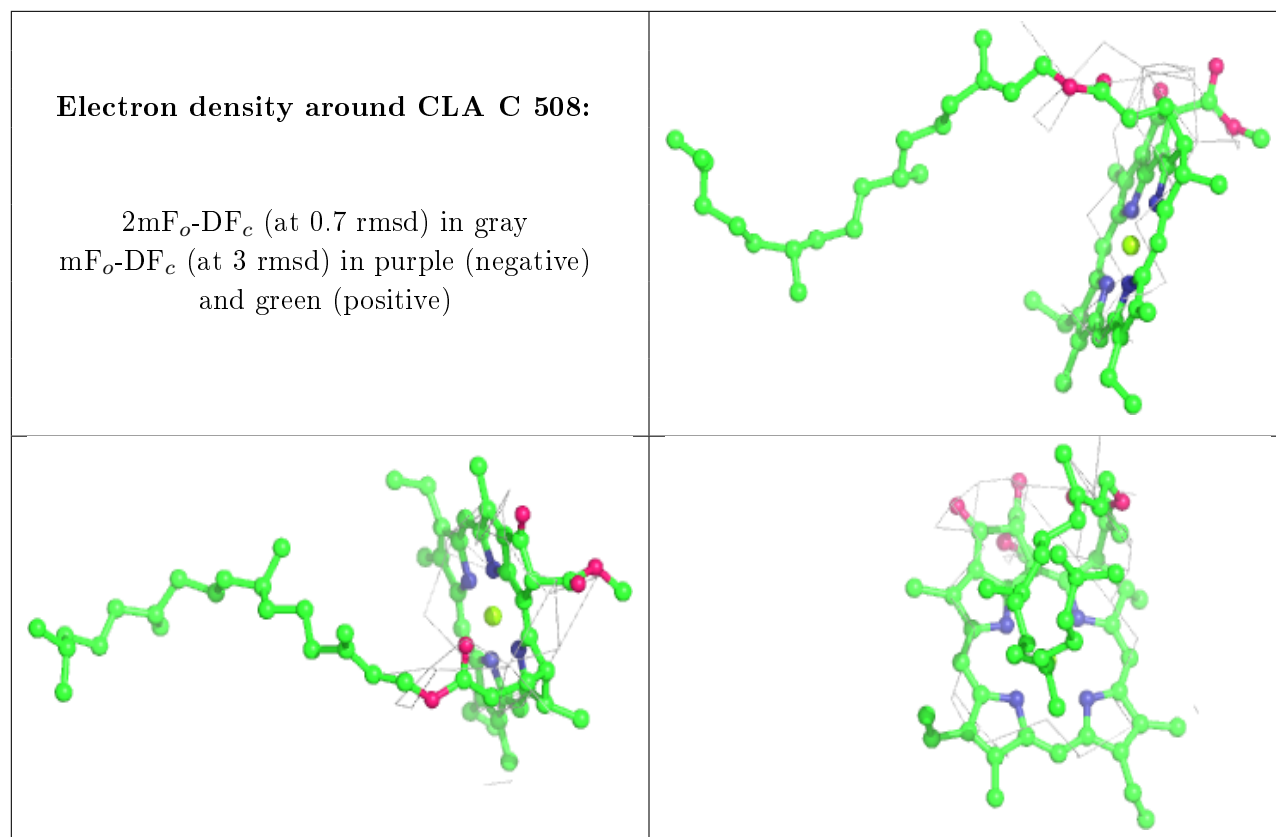
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM R 101:

$2mF_o-DF_c$ (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.