



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:33 PM BST

PDB ID : 6W1O  
Title : RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.08 Angstrom resolution  
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2020-03-04  
Resolution : 2.08 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)

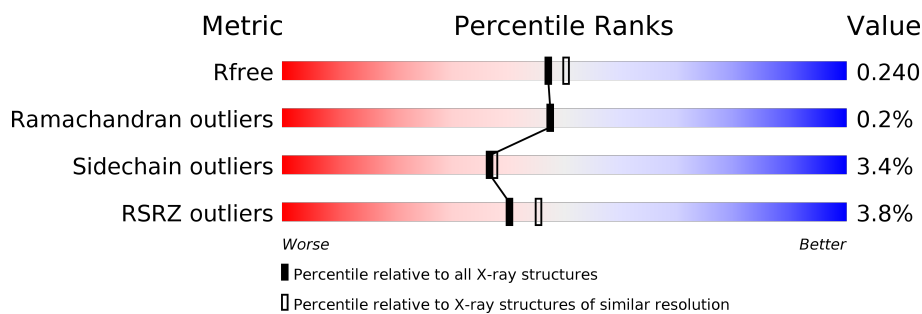
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	
1	a	334	
2	B	506	
2	b	506	
3	C	461	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

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Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	40	
14	r	40	
15	T	30	
15	t	30	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	410	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
31	STE	E	102	-	-	-	X

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 103895 atoms, of which 51610 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 II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6768	2249	3342	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

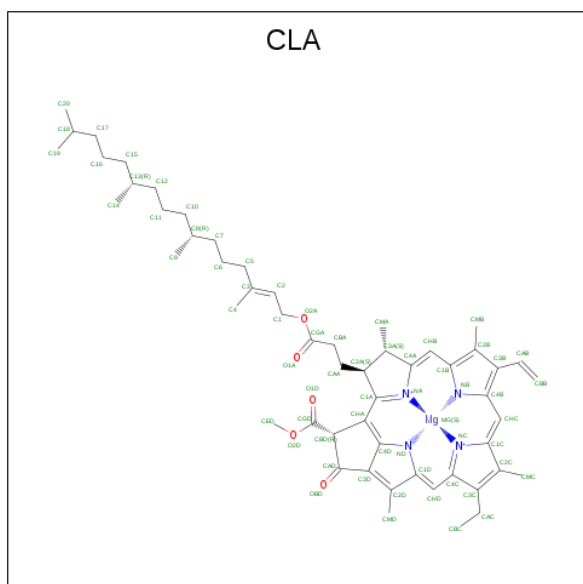
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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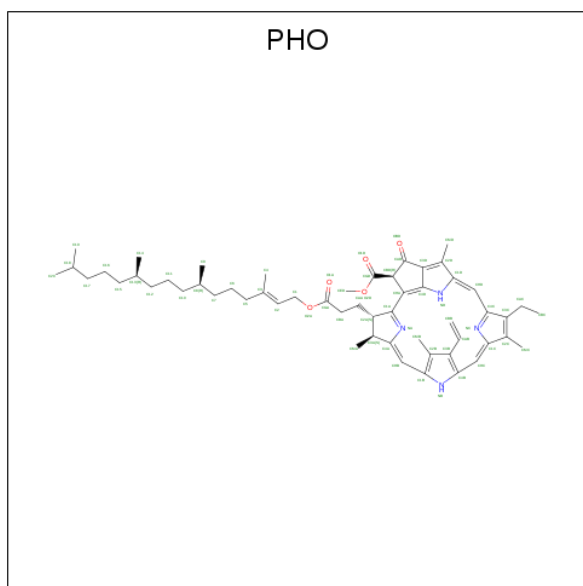
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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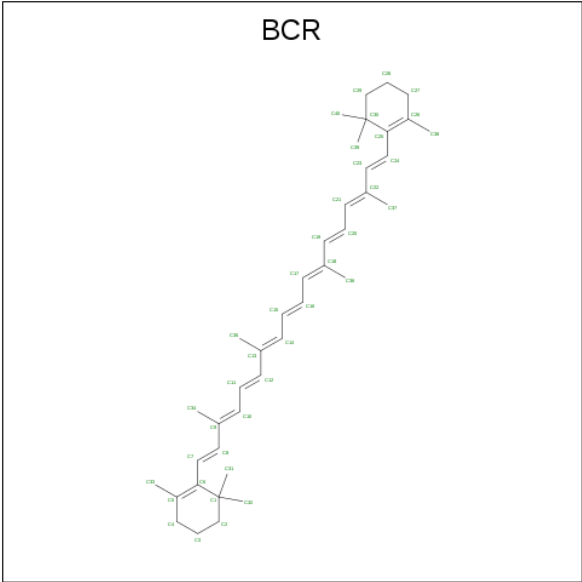
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	D	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	F	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	a	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		

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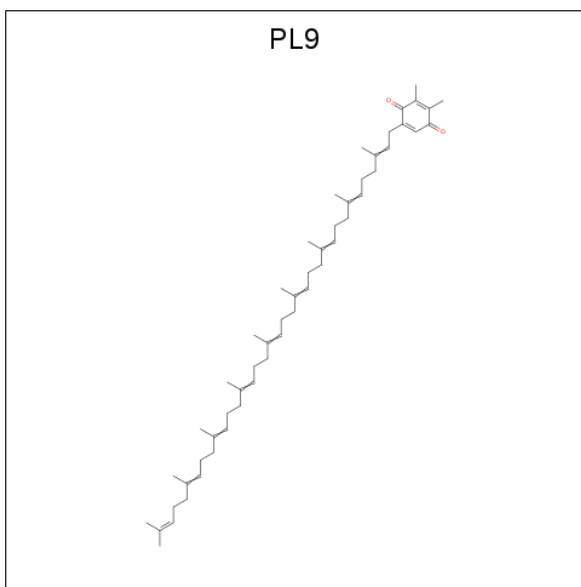
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

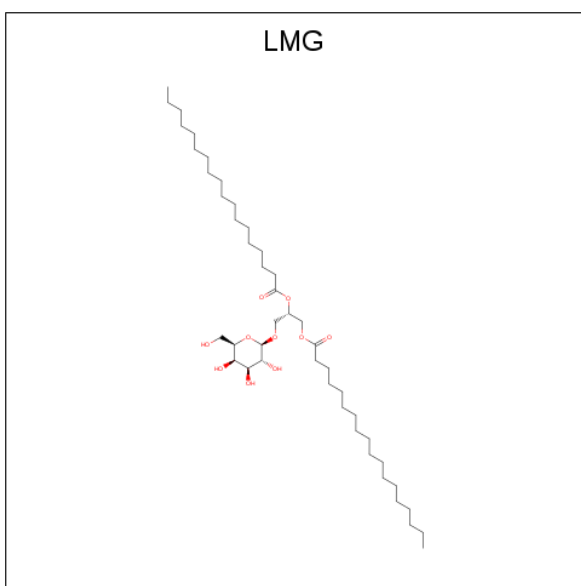
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



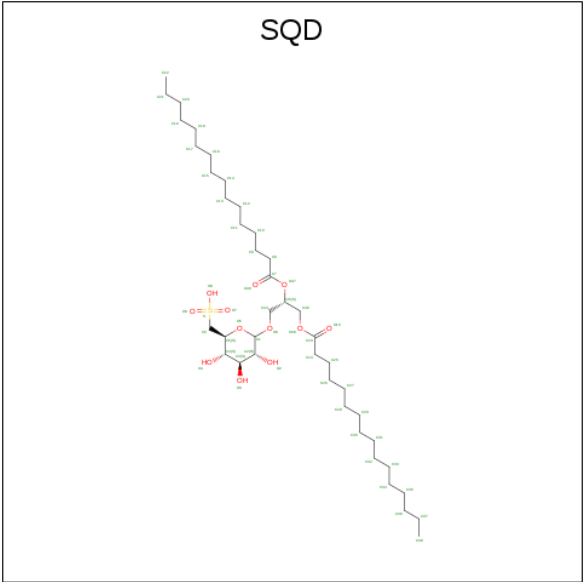
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



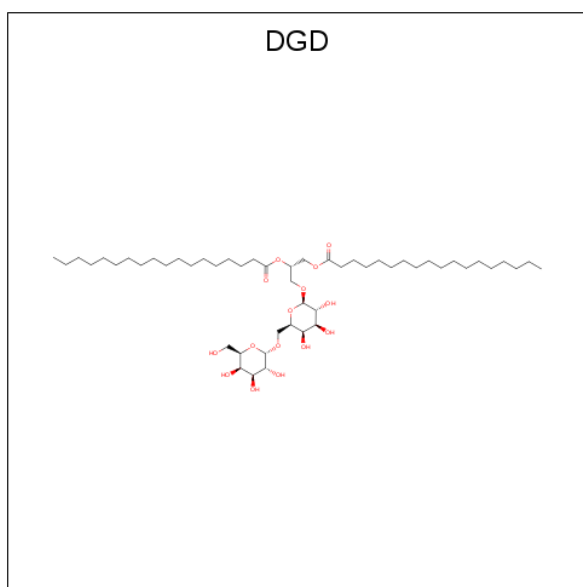
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



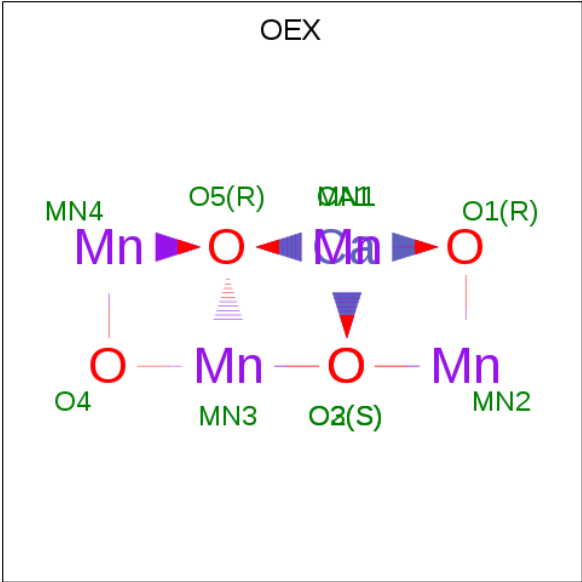
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



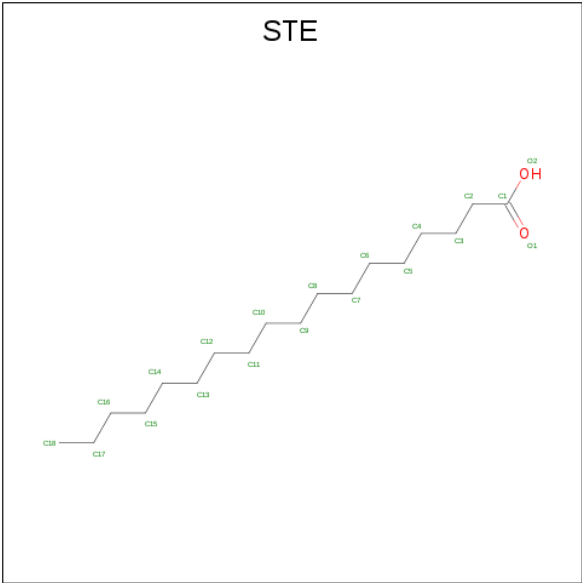
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			43	15	26	2		

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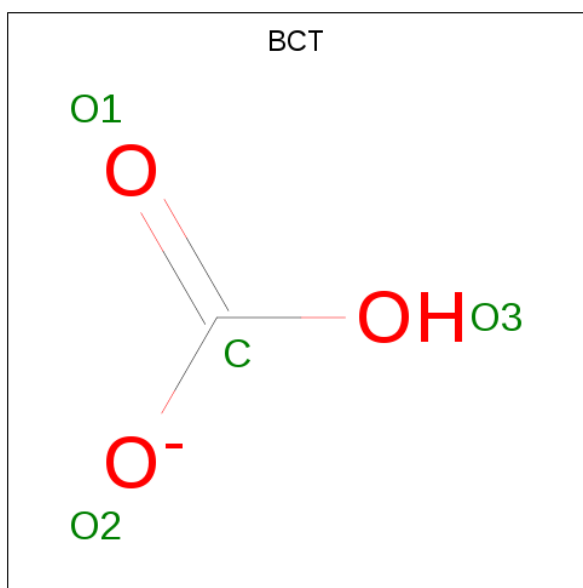
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			34	12	20	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		
31	B	1	Total	C	H		0	0
			47	16	31			
31	B	1	Total	C	H		0	0
			41	15	26			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	C	1	Total	C	H		0	0
			47	16	31			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	D	1	Total	C	H	O	0	0
			55	18	35	2		
31	E	1	Total	C	H	O	0	0
			28	10	16	2		
31	H	1	Total	C	H		0	0
			53	18	35			
31	I	1	Total	C	H		0	0
			41	15	26			
31	J	1	Total	C	H	O	0	0
			28	10	16	2		
31	M	1	Total	C	H	O	0	0
			37	13	22	2		
31	M	1	Total	C	H		0	0
			26	10	16			
31	T	1	Total	C	H		0	0
			44	15	29			
31	Z	1	Total	C	H		0	0
			20	8	12			
31	a	1	Total	C	H		0	0
			26	10	16			
31	a	1	Total	C	H	O	0	0
			28	10	16	2		
31	b	1	Total	C	H		0	0
			47	16	31			
31	b	1	Total	C	H	O	0	0
			55	18	35	2		

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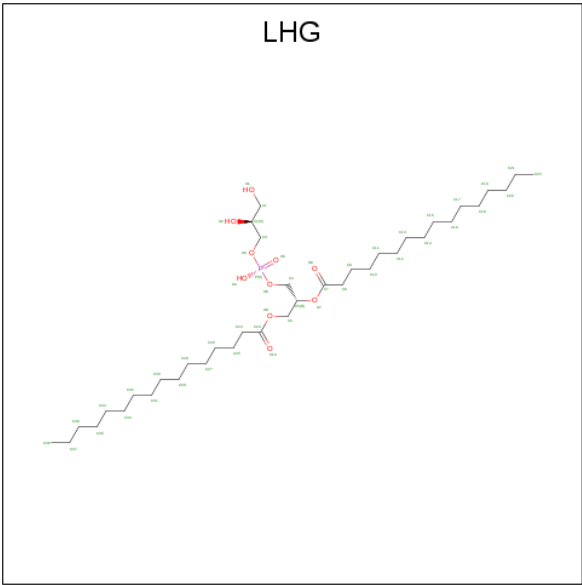
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 28 10 16 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 40 14 24 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	m	1	Total C H 53 18 35	0	0
31	m	1	Total C H O 28 10 16 2	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	H	O	0	0
			5	1	1	3		
32	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



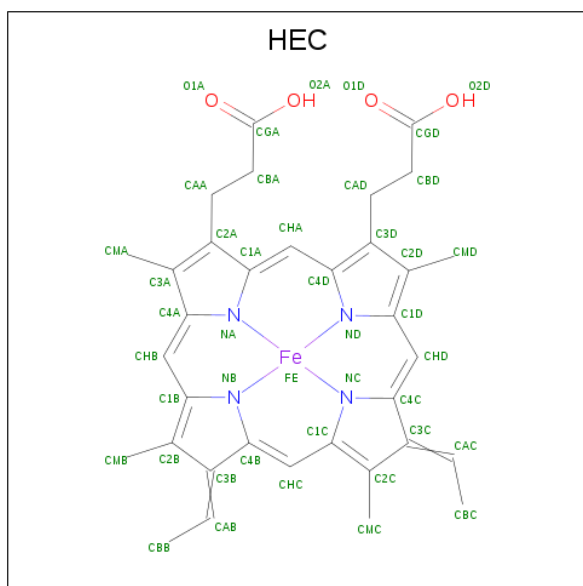
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	1	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	142	Total O 142 142	0	0
35	B	212	Total O 212 212	0	0
35	C	184	Total O 184 184	0	0
35	D	138	Total O 138 138	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	E	36	Total 36	O 36	0	0
35	F	8	Total 8	O 8	0	0
35	H	40	Total 40	O 40	0	0
35	I	24	Total 24	O 24	0	0
35	J	15	Total 15	O 15	0	0
35	K	7	Total 7	O 7	0	0
35	L	9	Total 9	O 9	0	0
35	M	11	Total 11	O 11	0	0
35	O	104	Total 104	O 104	0	0
35	R	4	Total 4	O 4	0	0
35	T	10	Total 10	O 10	0	0
35	U	52	Total 52	O 52	0	0
35	V	59	Total 59	O 59	0	0
35	X	15	Total 15	O 15	0	0
35	Y	5	Total 5	O 5	0	0
35	Z	6	Total 6	O 6	0	0
35	a	116	Total 116	O 116	0	0
35	b	201	Total 201	O 201	0	0
35	c	187	Total 187	O 187	0	0
35	d	115	Total 115	O 115	0	0
35	e	21	Total 21	O 21	0	0

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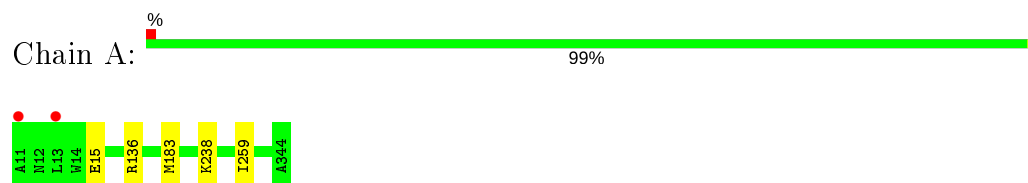
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	f	6	Total 6	O 6	0	0
35	h	31	Total 31	O 31	0	0
35	i	12	Total 12	O 12	0	0
35	j	6	Total 6	O 6	0	0
35	k	7	Total 7	O 7	0	0
35	l	5	Total 5	O 5	0	0
35	m	10	Total 10	O 10	0	0
35	o	86	Total 86	O 86	0	0
35	r	6	Total 6	O 6	0	0
35	t	9	Total 9	O 9	0	0
35	u	53	Total 53	O 53	0	0
35	v	62	Total 62	O 62	0	0
35	x	8	Total 8	O 8	0	0
35	y	4	Total 4	O 4	0	0
35	z	11	Total 11	O 11	0	0

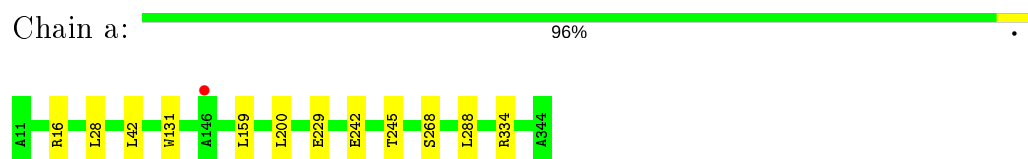
### 3 Residue-property plots [i](#)

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.

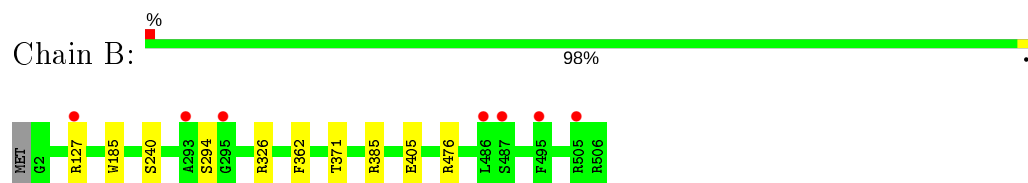
- Molecule 1: Photosystem II protein D1 1



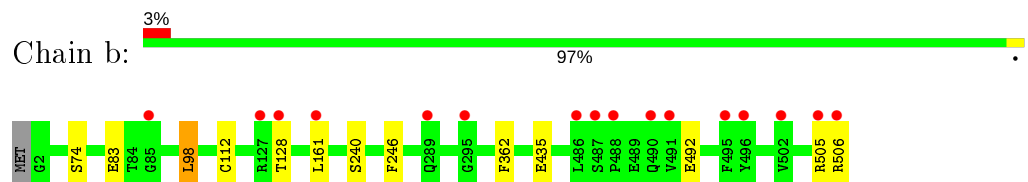
- Molecule 1: Photosystem II protein D1 1



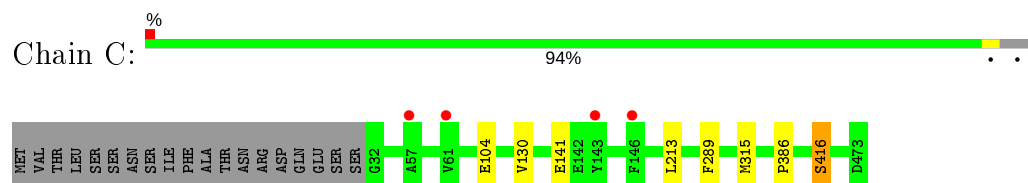
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



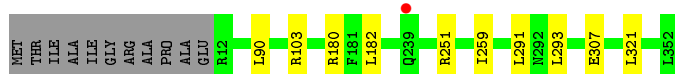
- Molecule 3: Photosystem II CP43 reaction center protein



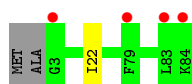
- Molecule 4: Photosystem II D2 protein



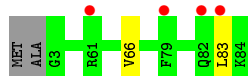
- Molecule 4: Photosystem II D2 protein



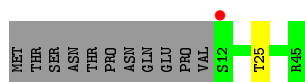
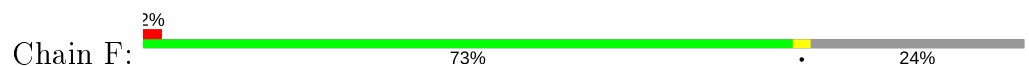
- Molecule 5: Cytochrome b559 subunit alpha



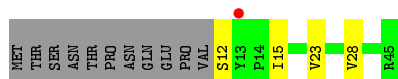
- Molecule 5: Cytochrome b559 subunit alpha



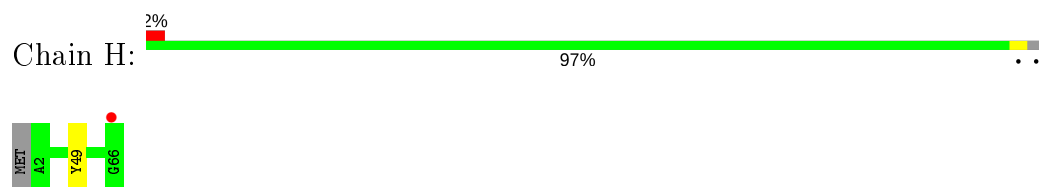
- Molecule 6: Cytochrome b559 subunit beta



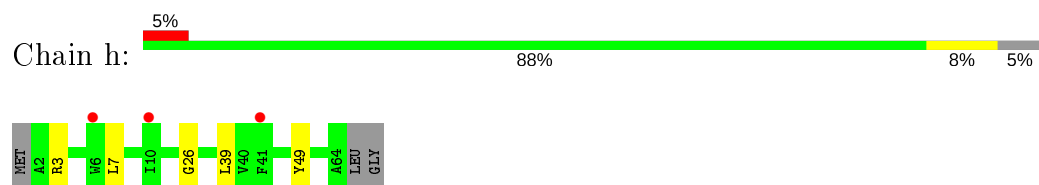
- Molecule 6: Cytochrome b559 subunit beta



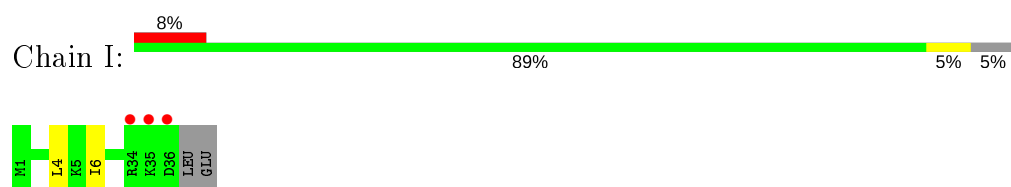
- Molecule 7: Photosystem II reaction center protein H



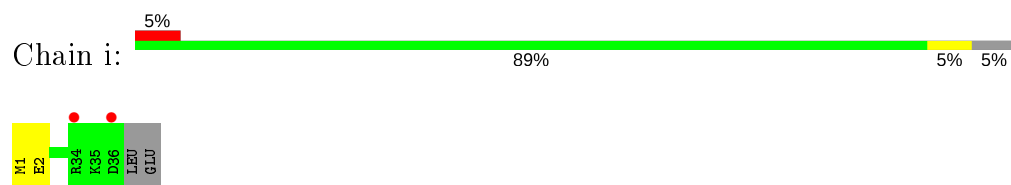
- Molecule 7: Photosystem II reaction center protein H



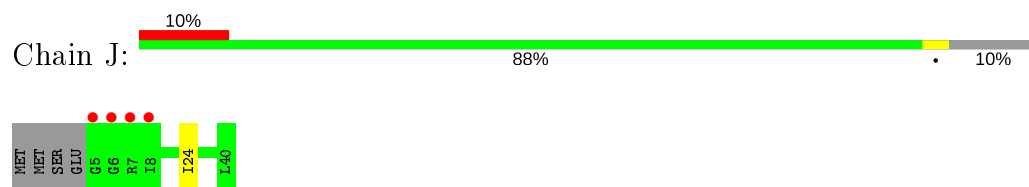
- Molecule 8: Photosystem II reaction center protein I



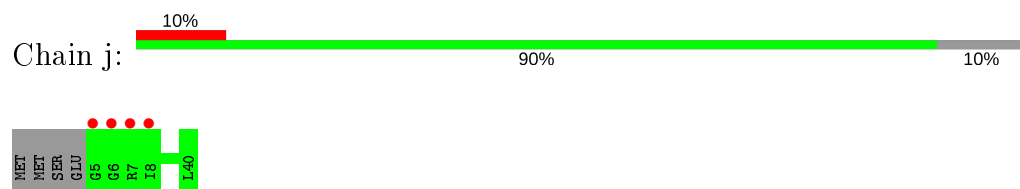
- Molecule 8: Photosystem II reaction center protein I



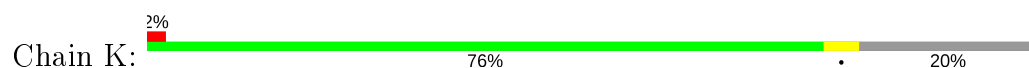
- Molecule 9: Photosystem II reaction center protein J

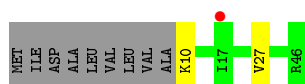


- Molecule 9: Photosystem II reaction center protein J

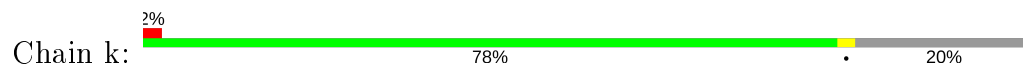


- Molecule 10: Photosystem II reaction center protein K

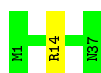




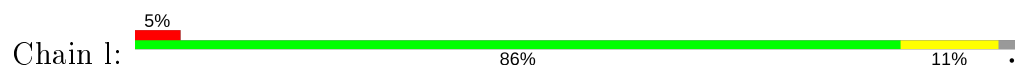
- Molecule 10: Photosystem II reaction center protein K



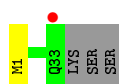
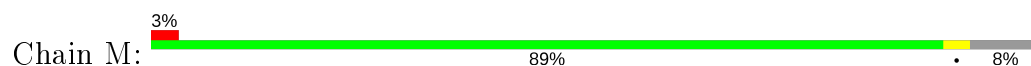
- Molecule 11: Photosystem II reaction center protein L



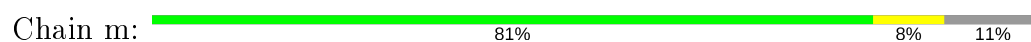
- Molecule 11: Photosystem II reaction center protein L



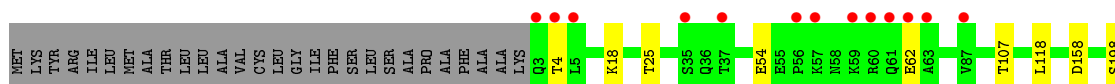
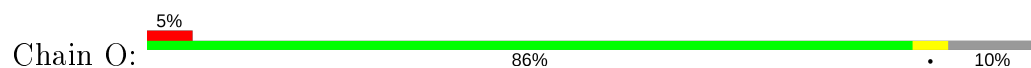
- Molecule 12: Photosystem II reaction center protein M



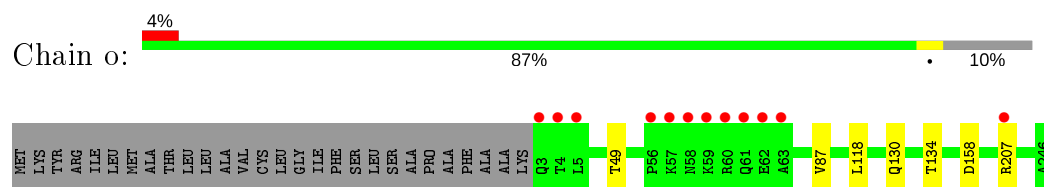
- Molecule 12: Photosystem II reaction center protein M



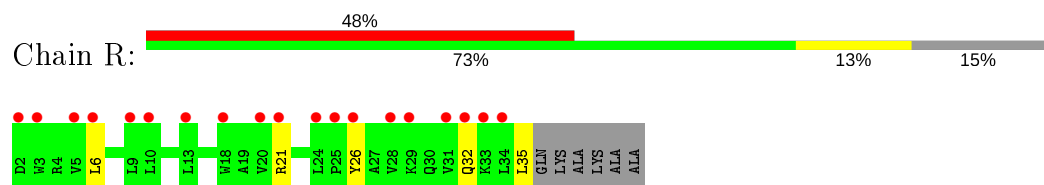
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



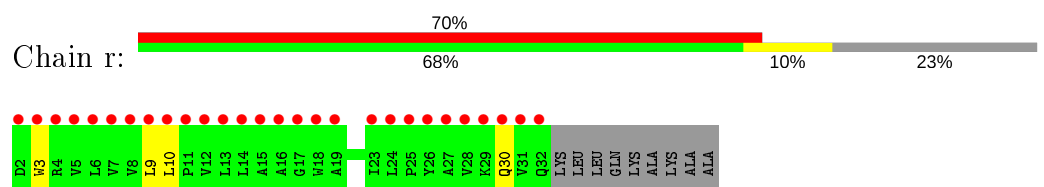
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



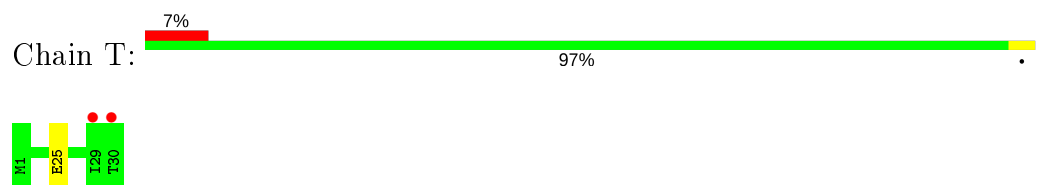
- Molecule 14: Photosystem II protein Y



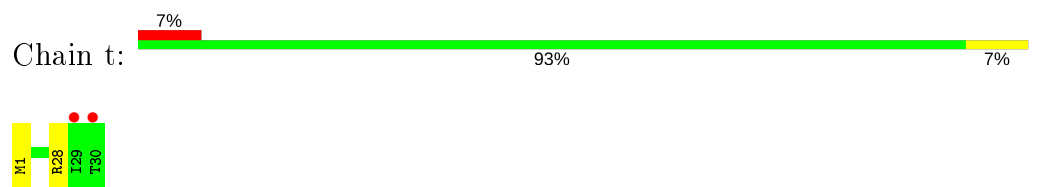
- Molecule 14: Photosystem II protein Y



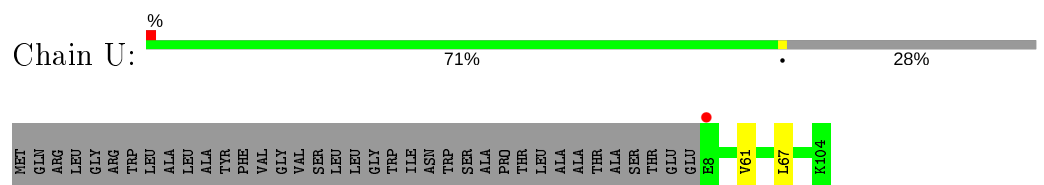
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

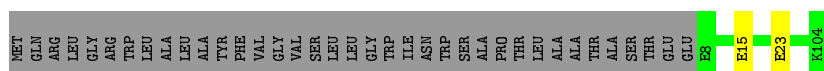


- Molecule 16: Photosystem II 12 kDa extrinsic protein

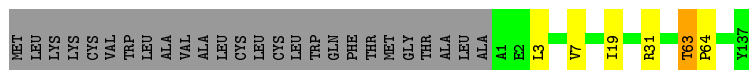
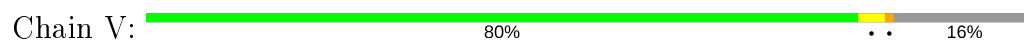


- Molecule 16: Photosystem II 12 kDa extrinsic protein

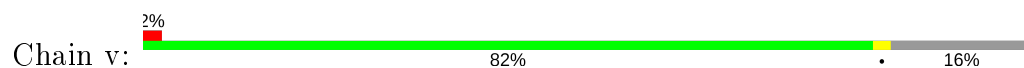




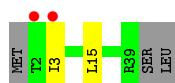
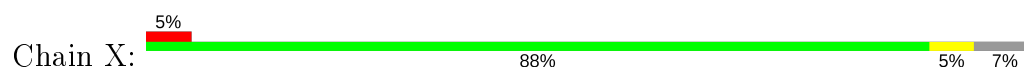
- Molecule 17: Cytochrome c-550



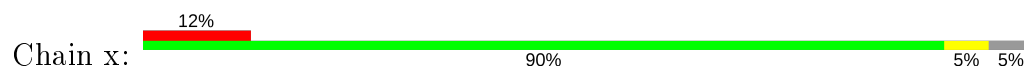
- Molecule 17: Cytochrome c-550



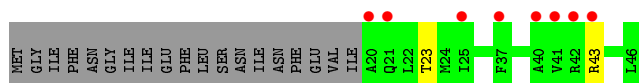
- Molecule 18: Photosystem II reaction center X protein



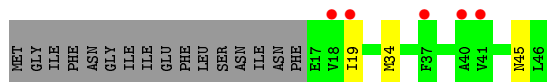
- Molecule 18: Photosystem II reaction center X protein



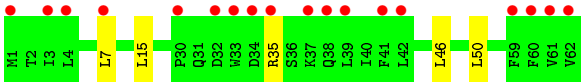
- Molecule 19: Photosystem II reaction center protein Ycf12



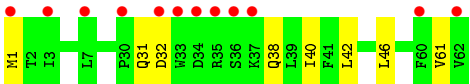
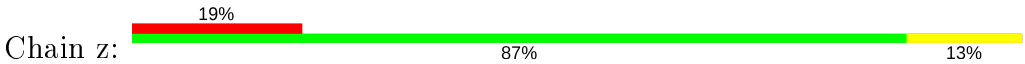
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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, $\alpha$ , $\beta$ , $\gamma$	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.1 (33.64-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.181 , 0.240 0.181 , 0.240	Depositor DCC
$R_{free}$ test set	4226 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	103895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, STE, OEX, PHO, DGD, CL, CLA, PL9, LMG, FE2, HEC, BCT, FME, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.67	0/2707	0.70	2/3692 (0.1%)
1	a	0.66	0/2704	0.71	2/3688 (0.1%)
2	B	0.65	1/4161 (0.0%)	0.68	1/5669 (0.0%)
2	b	0.63	1/4118 (0.0%)	0.68	1/5611 (0.0%)
3	C	0.62	0/3547	0.68	0/4830
3	c	0.59	0/3619	0.66	0/4926
4	D	0.66	1/2812 (0.0%)	0.69	1/3832 (0.0%)
4	d	0.64	0/2821	0.69	1/3844 (0.0%)
5	E	0.55	0/688	0.62	0/940
5	e	0.50	0/683	0.59	0/932
6	F	0.55	0/284	0.56	0/387
6	f	0.46	0/284	0.60	0/387
7	H	0.63	0/523	0.69	0/713
7	h	0.58	0/511	0.67	0/697
8	I	0.61	0/293	0.65	0/396
8	i	0.69	0/293	0.71	0/396
9	J	0.54	0/263	0.64	0/356
9	j	0.50	0/263	0.62	0/356
10	K	0.51	0/303	0.62	0/416
10	k	0.55	0/303	0.65	0/416
11	L	0.70	0/311	0.73	1/422 (0.2%)
11	l	0.71	0/303	0.70	0/412
12	M	0.71	0/249	0.77	0/341
12	m	0.65	0/244	0.76	0/334
13	O	0.62	0/1904	0.73	1/2585 (0.0%)
13	o	0.60	0/1905	0.75	1/2583 (0.0%)
14	R	0.45	0/277	0.53	0/380
14	r	0.43	0/246	0.52	0/339
15	T	0.68	0/257	0.69	0/349
15	t	0.69	0/255	0.63	0/346
16	U	0.54	0/785	0.69	0/1064
16	u	0.64	0/785	0.74	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	V	0.60	0/1085	0.72	1/1473 (0.1%)
17	v	0.55	0/1085	0.64	0/1473
18	X	0.51	0/284	0.63	0/384
18	x	0.39	0/289	0.55	0/391
19	Y	0.45	0/197	0.63	0/264
19	y	0.39	0/219	0.54	0/294
20	Z	0.46	0/490	0.55	0/669
20	z	0.45	0/488	0.55	0/666
All	All	0.62	3/42838 (0.0%)	0.68	12/58317 (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
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	211	CYS	CB-SG	-5.77	1.72	1.81
2	B	185	TRP	CB-CG	-5.58	1.40	1.50
2	b	112	CYS	CB-SG	-5.16	1.73	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	334	ARG	NE-CZ-NH1	6.96	123.78	120.30
17	V	63	THR	C-N-CD	-6.82	105.61	120.60
13	o	158	ASP	CB-CG-OD1	6.30	123.97	118.30
2	B	326	ARG	NE-CZ-NH2	-5.80	117.40	120.30
4	d	251	ARG	NE-CZ-NH2	-5.76	117.42	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	39
1	a	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	B	508/506 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/506 (99%)	490 (97%)	13 (3%)	0	100	100
3	C	442/461 (96%)	433 (98%)	8 (2%)	1 (0%)	47	47
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	47	47
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	9	4
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	30 (88%)	4 (12%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	224 (92%)	18 (7%)	1 (0%)	34	31
13	o	242/272 (89%)	230 (95%)	12 (5%)	0	100	100
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	17
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	4
All	All	5240/5666 (92%)	5072 (97%)	159 (3%)	9 (0%)	47	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
19	Y	43	ARG

### 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	270/270 (100%)	268 (99%)	2 (1%)	84	87
1	a	269/270 (100%)	259 (96%)	10 (4%)	34	34
2	B	408/404 (101%)	400 (98%)	8 (2%)	55	59
2	b	402/404 (100%)	390 (97%)	12 (3%)	41	43
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	53
3	c	354/362 (98%)	342 (97%)	12 (3%)	37	37
4	D	276/283 (98%)	270 (98%)	6 (2%)	52	55
4	d	277/283 (98%)	268 (97%)	9 (3%)	39	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	46
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	46
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	35
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	41
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	29
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	12
10	k	30/37 (81%)	29 (97%)	1 (3%)	38	39
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	32
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	44
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	1
14	r	23/32 (72%)	20 (87%)	3 (13%)	4	2
15	T	26/26 (100%)	25 (96%)	1 (4%)	33	33
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	52
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	52
17	V	117/138 (85%)	113 (97%)	4 (3%)	37	37
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	49
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	13
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	13
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	20
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	1
All	All	4328/4622 (94%)	4179 (97%)	149 (3%)	37	37

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	242	GLU
3	c	24	THR
18	x	2	THR
1	a	268	SER
2	b	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
20	Z	6	GLN
20	Z	31	GLN
3	c	373	ASN
13	O	88	ASN
3	c	28	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	M	1	12	8,9,10	1.07	1 (12%)	7,9,11	0.79	0
15	FME	T	1	15	8,9,10	1.18	0	7,9,11	0.65	0
15	FME	t	1	15	8,9,10	1.06	0	7,9,11	1.26	1 (14%)
12	FME	m	1	12	8,9,10	1.12	1 (12%)	7,9,11	0.44	0
8	FME	i	1	8	8,9,10	1.20	1 (12%)	7,9,11	1.20	1 (14%)
8	FME	I	1	8	8,9,10	1.01	0	7,9,11	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.76	1.42	1.46
12	m	1	FME	CA-N	-2.32	1.43	1.46
12	M	1	FME	CA-N	-2.05	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.41	119.12	122.82
15	t	1	FME	C-CA-N	2.40	114.06	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
15	T	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	DGD	A	413	-	67,67,67	1.31	10 (14%)	81,81,81	1.53	13 (16%)
34	HEC	v	201	17	26,50,50	2.35	4 (15%)	18,82,82	1.95	4 (22%)
28	SQD	L	101	-	48,49,54	0.94	2 (4%)	57,60,65	2.40	16 (28%)
22	CLA	B	605	-	59,73,73	1.29	8 (13%)	67,113,113	1.91	15 (22%)
24	BCR	a	406	-	41,41,41	1.22	3 (7%)	56,56,56	1.22	6 (10%)
27	LMG	c	520	-	37,37,55	1.17	4 (10%)	45,45,63	1.27	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	STE	B	601	-	8,11,19	0.36	0	7,11,19	0.97	0
27	LMG	d	410	-	44,44,55	1.15	4 (9%)	52,52,63	1.31	5 (9%)
27	LMG	c	523	-	49,49,55	1.04	5 (10%)	57,57,63	1.30	5 (8%)
22	CLA	C	512	-	59,73,73	1.36	6 (10%)	67,113,113	1.45	13 (19%)
31	STE	C	518	-	8,11,19	0.46	0	7,11,19	0.66	0
24	BCR	t	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.47	12 (21%)
31	STE	b	620	-	15,15,19	0.43	0	14,14,19	0.82	0
28	SQD	B	622	-	53,54,54	1.00	3 (5%)	62,65,65	1.87	13 (20%)
31	STE	b	625	-	9,9,19	0.50	0	8,8,19	0.54	0
22	CLA	C	507	35	59,73,73	1.47	6 (10%)	67,113,113	1.84	12 (17%)
22	CLA	c	502	-	59,73,73	1.42	8 (13%)	67,113,113	1.74	9 (13%)
24	BCR	k	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.10	3 (5%)
22	CLA	b	613	-	59,73,73	1.35	8 (13%)	67,113,113	1.68	14 (20%)
31	STE	m	101	-	17,17,19	0.42	0	16,16,19	0.80	0
31	STE	b	627	-	16,19,19	0.32	0	15,19,19	1.01	0
22	CLA	a	405	-	59,73,73	1.34	6 (10%)	67,113,113	1.63	14 (20%)
32	BCT	D	402	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	c	510	-	59,73,73	1.26	6 (10%)	67,113,113	1.87	12 (17%)
22	CLA	C	509	-	59,73,73	1.45	10 (16%)	67,113,113	1.41	9 (13%)
34	HEC	V	201	17	26,50,50	2.27	4 (15%)	18,82,82	1.86	5 (27%)
24	BCR	c	515	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	2 (3%)
22	CLA	B	608	-	59,73,73	1.76	8 (13%)	67,113,113	1.66	10 (14%)
26	PL9	d	406	-	55,55,55	1.54	10 (18%)	68,69,69	1.84	16 (23%)
30	OEX	A	414	1,3,35	0,15,15	0.00	-	-	-	-
24	BCR	F	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	5 (8%)
29	DGD	c	519	-	63,63,67	1.22	8 (12%)	77,77,81	1.41	8 (10%)
22	CLA	A	405	-	48,62,73	1.80	9 (18%)	53,99,113	1.73	12 (22%)
24	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	10 (17%)
22	CLA	C	508	-	59,73,73	1.61	6 (10%)	67,113,113	1.70	9 (13%)
27	LMG	D	407	-	51,51,55	0.91	2 (3%)	59,59,63	1.37	8 (13%)
29	DGD	c	518	-	63,63,67	1.15	6 (9%)	77,77,81	1.41	11 (14%)
23	PHO	a	404	-	67,69,69	1.05	5 (7%)	85,99,99	1.18	8 (9%)
22	CLA	C	506	-	59,73,73	1.62	6 (10%)	67,113,113	1.51	10 (14%)
22	CLA	c	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.65	11 (16%)
22	CLA	b	610	35	59,73,73	1.30	9 (15%)	67,113,113	1.57	17 (25%)
22	CLA	C	510	-	59,73,73	1.30	8 (13%)	67,113,113	1.40	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	STE	J	101	-	8,11,19	0.30	0	7,11,19	0.95	0
22	CLA	c	508	35	59,73,73	1.33	7 (11%)	67,113,113	1.45	8 (11%)
26	PL9	D	406	-	55,55,55	1.35	6 (10%)	68,69,69	1.64	14 (20%)
22	CLA	C	504	35	53,67,73	1.53	7 (13%)	59,105,113	1.64	14 (23%)
31	STE	H	104	-	17,17,19	0.40	0	16,16,19	0.88	0
22	CLA	d	403	-	59,73,73	1.48	8 (13%)	67,113,113	1.31	7 (10%)
22	CLA	B	615	-	59,73,73	1.61	10 (16%)	67,113,113	1.41	8 (11%)
31	STE	a	413	-	9,9,19	0.53	0	8,8,19	0.56	0
22	CLA	b	604	-	59,73,73	1.85	6 (10%)	67,113,113	1.99	13 (19%)
22	CLA	D	405	-	59,73,73	1.32	7 (11%)	67,113,113	1.26	8 (11%)
22	CLA	B	613	-	59,73,73	1.65	10 (16%)	67,113,113	1.57	12 (17%)
26	PL9	a	409	-	55,55,55	1.07	4 (7%)	68,69,69	1.61	11 (16%)
31	STE	j	101	-	8,11,19	0.61	0	7,11,19	0.62	0
31	STE	d	412	-	13,16,19	0.37	0	12,16,19	0.72	0
27	LMG	A	410	-	48,48,55	0.99	2 (4%)	56,56,63	1.43	7 (12%)
22	CLA	B	616	-	54,68,73	1.72	8 (14%)	61,107,113	1.84	15 (24%)
23	PHO	D	401	-	67,69,69	1.23	9 (13%)	85,99,99	1.10	6 (7%)
31	STE	B	627	-	14,14,19	0.51	0	13,13,19	0.64	0
24	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.36	7 (12%)
22	CLA	b	611	-	59,73,73	1.27	7 (11%)	67,113,113	1.88	10 (14%)
27	LMG	B	621	-	20,26,55	0.53	0	18,26,63	1.11	0
23	PHO	A	404	-	67,69,69	1.25	10 (14%)	85,99,99	1.03	4 (4%)
28	SQD	a	412	-	35,35,54	1.19	2 (5%)	37,37,65	1.46	4 (10%)
24	BCR	K	102	-	41,41,41	0.99	3 (7%)	56,56,56	1.26	5 (8%)
22	CLA	c	511	-	59,73,73	1.38	7 (11%)	67,113,113	1.64	11 (16%)
34	HEC	f	101	5,6	26,50,50	2.55	5 (19%)	18,82,82	2.33	5 (27%)
26	PL9	A	409	-	55,55,55	0.95	1 (1%)	68,69,69	1.60	14 (20%)
31	STE	m	102	-	8,11,19	0.46	0	7,11,19	0.79	0
28	SQD	A	411	-	51,52,54	1.11	5 (9%)	60,63,65	1.70	11 (18%)
29	DGD	C	517	-	63,63,67	1.16	7 (11%)	77,77,81	1.47	12 (15%)
31	STE	B	624	-	8,11,19	0.39	0	7,11,19	0.97	0
22	CLA	c	505	35	54,68,73	1.55	6 (11%)	61,107,113	1.71	14 (22%)
33	LHG	E	101	-	48,48,48	0.86	3 (6%)	51,54,54	1.20	6 (11%)
22	CLA	B	603	-	59,73,73	1.23	5 (8%)	67,113,113	1.61	11 (16%)
24	BCR	k	102	-	41,41,41	0.94	2 (4%)	56,56,56	1.20	5 (8%)
22	CLA	H	101	35	59,73,73	1.72	9 (15%)	67,113,113	1.57	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	610	35	59,73,73	1.50	10 (16%)	67,113,113	1.52	12 (17%)
22	CLA	C	502	-	59,73,73	1.46	6 (10%)	67,113,113	1.44	11 (16%)
31	STE	E	102	-	8,11,19	0.54	0	7,11,19	0.40	0
22	CLA	b	601	35	59,73,73	1.68	7 (11%)	67,113,113	1.47	10 (14%)
22	CLA	c	504	-	59,73,73	1.43	9 (15%)	67,113,113	1.78	14 (20%)
24	BCR	T	101	-	41,41,41	1.18	4 (9%)	56,56,56	1.19	4 (7%)
29	DGD	c	517	-	63,63,67	1.37	7 (11%)	77,77,81	1.34	8 (10%)
22	CLA	b	607	35	59,73,73	1.48	6 (10%)	67,113,113	1.44	11 (16%)
22	CLA	C	501	-	59,73,73	1.60	8 (13%)	67,113,113	1.57	10 (14%)
22	CLA	B	614	-	59,73,73	1.46	7 (11%)	67,113,113	1.48	13 (19%)
28	SQD	D	408	-	35,36,54	0.94	2 (5%)	42,45,65	1.87	9 (21%)
24	BCR	h	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.38	9 (16%)
22	CLA	b	608	-	59,73,73	1.61	7 (11%)	67,113,113	1.58	14 (20%)
24	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	5 (8%)
24	BCR	c	516	-	41,41,41	1.21	4 (9%)	56,56,56	1.29	6 (10%)
22	CLA	c	512	3	59,73,73	1.73	7 (11%)	67,113,113	1.65	8 (11%)
31	STE	C	520	-	8,11,19	0.33	0	7,11,19	1.20	0
31	STE	B	625	-	14,17,19	0.41	0	13,17,19	0.83	0
22	CLA	c	507	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	13 (19%)
22	CLA	b	614	-	59,73,73	1.43	8 (13%)	67,113,113	1.32	7 (10%)
24	BCR	K	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.44	9 (16%)
22	CLA	A	403	35	59,73,73	1.54	8 (13%)	67,113,113	1.46	11 (16%)
22	CLA	c	513	-	59,73,73	1.42	7 (11%)	67,113,113	1.53	10 (14%)
27	LMG	a	415	-	55,55,55	1.42	7 (12%)	63,63,63	1.46	6 (9%)
27	LMG	D	411	-	31,31,55	1.11	3 (9%)	33,33,63	1.15	2 (6%)
22	CLA	a	402	-	59,73,73	1.62	5 (8%)	67,113,113	1.67	15 (22%)
31	STE	C	519	-	15,15,19	0.56	0	14,14,19	0.50	0
22	CLA	b	615	-	59,73,73	1.95	6 (10%)	67,113,113	1.53	10 (14%)
27	LMG	c	522	-	48,48,55	1.12	5 (10%)	56,56,63	1.19	3 (5%)
22	CLA	b	605	-	59,73,73	1.28	4 (6%)	67,113,113	1.76	17 (25%)
22	CLA	c	509	-	58,72,73	1.44	9 (15%)	65,111,113	1.54	12 (18%)
24	BCR	A	406	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	c	503	-	59,73,73	1.27	8 (13%)	67,113,113	1.54	10 (14%)
31	STE	T	102	-	14,14,19	0.42	0	13,13,19	0.85	0
31	STE	I	101	-	14,14,19	0.53	0	13,13,19	0.45	0
27	LMG	M	101	-	51,51,55	1.13	3 (5%)	59,59,63	1.48	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	B	619	-	41,41,41	1.11	1 (2%)	56,56,56	1.47	9 (16%)
31	STE	B	620	-	13,16,19	0.59	0	12,16,19	0.57	0
32	BCT	d	402	21	0,3,3	0.00	-	0,3,3	0.00	-
29	DGD	h	102	-	63,63,67	1.16	10 (15%)	77,77,81	1.38	10 (12%)
31	STE	c	521	-	16,19,19	0.37	0	15,19,19	0.72	0
31	STE	d	413	-	16,19,19	0.41	0	15,19,19	0.65	0
33	LHG	d	408	-	48,48,48	0.98	1 (2%)	51,54,54	1.15	3 (5%)
24	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.40	9 (16%)
33	LHG	L	102	-	48,48,48	0.79	2 (4%)	51,54,54	1.18	3 (5%)
28	SQD	A	412	-	38,38,54	1.03	3 (7%)	40,40,65	1.30	4 (10%)
34	HEC	F	102	5,6	26,50,50	2.57	5 (19%)	18,82,82	2.22	6 (33%)
22	CLA	B	604	-	59,73,73	1.31	7 (11%)	67,113,113	1.91	19 (28%)
29	DGD	C	515	-	63,63,67	1.44	11 (17%)	77,77,81	1.46	12 (15%)
22	CLA	c	514	-	59,73,73	1.73	9 (15%)	67,113,113	1.38	11 (16%)
31	STE	b	626	-	13,13,19	0.40	0	12,12,19	0.77	0
31	STE	b	622	-	16,19,19	0.39	0	15,19,19	0.81	0
22	CLA	b	606	-	59,73,73	1.70	9 (15%)	67,113,113	1.70	9 (13%)
33	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.14	4 (7%)
22	CLA	B	602	-	59,73,73	1.51	6 (10%)	67,113,113	1.61	12 (17%)
27	LMG	b	621	-	51,51,55	1.00	4 (7%)	59,59,63	1.42	10 (16%)
22	CLA	a	403	35	59,73,73	1.53	7 (11%)	67,113,113	1.62	12 (17%)
24	BCR	C	514	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	8 (14%)
31	STE	c	501	-	8,11,19	0.39	0	7,11,19	0.84	0
30	OEX	a	416	1,3,35	0,15,15	0.00	-	-	-	-
22	CLA	D	404	35	59,73,73	1.61	8 (13%)	67,113,113	1.49	8 (11%)
27	LMG	b	623	-	55,55,55	0.87	3 (5%)	63,63,63	1.60	11 (17%)
22	CLA	B	612	-	59,73,73	1.30	6 (10%)	67,113,113	1.67	13 (19%)
31	STE	M	102	-	11,14,19	0.57	0	10,14,19	0.39	0
29	DGD	H	103	-	63,63,67	1.32	8 (12%)	77,77,81	1.53	14 (18%)
22	CLA	b	602	-	59,73,73	1.65	10 (16%)	67,113,113	1.44	10 (14%)
24	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	5 (8%)
31	STE	B	623	-	10,13,19	0.49	0	9,13,19	0.74	0
22	CLA	D	403	-	59,73,73	1.34	4 (6%)	67,113,113	1.64	12 (17%)
31	STE	Z	101	-	7,7,19	0.42	0	6,6,19	0.55	0
33	LHG	d	409	-	38,38,48	0.99	1 (2%)	41,44,54	1.06	2 (4%)
22	CLA	a	410	35	59,73,73	1.49	7 (11%)	67,113,113	1.58	13 (19%)
22	CLA	b	612	-	59,73,73	1.21	4 (6%)	67,113,113	1.70	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	513	-	59,73,73	1.38	9 (15%)	67,113,113	1.66	13 (19%)
22	CLA	b	616	-	54,68,73	1.38	8 (14%)	61,107,113	1.92	11 (18%)
23	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.29	9 (10%)
24	BCR	b	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.38	11 (19%)
22	CLA	A	402	-	59,73,73	1.40	8 (13%)	67,113,113	1.47	7 (10%)
33	LHG	d	407	-	48,48,48	1.00	2 (4%)	51,54,54	1.44	5 (9%)
22	CLA	B	607	35	59,73,73	1.19	8 (13%)	67,113,113	1.57	10 (14%)
31	STE	d	411	-	12,15,19	0.46	0	11,15,19	0.58	0
22	CLA	C	511	3	59,73,73	1.45	8 (13%)	67,113,113	1.37	6 (8%)
28	SQD	f	102	-	40,41,54	1.11	4 (10%)	49,52,65	1.91	10 (20%)
33	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.28	6 (11%)
22	CLA	C	503	-	59,73,73	1.67	10 (16%)	67,113,113	1.60	11 (16%)
31	STE	B	626	-	15,15,19	0.45	0	14,14,19	0.71	0
33	LHG	D	412	-	48,48,48	0.76	1 (2%)	51,54,54	1.32	5 (9%)
22	CLA	B	609	-	59,73,73	1.45	8 (13%)	67,113,113	1.56	12 (17%)
28	SQD	a	411	-	53,54,54	1.02	5 (9%)	62,65,65	2.18	16 (25%)
31	STE	b	624	-	16,19,19	0.46	0	15,19,19	0.69	0
31	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.72	0
22	CLA	B	606	-	59,73,73	1.77	9 (15%)	67,113,113	1.60	9 (13%)
22	CLA	C	505	-	59,73,73	1.56	7 (11%)	67,113,113	1.59	12 (17%)
33	LHG	D	410	-	46,46,48	1.03	3 (6%)	49,52,54	1.21	4 (8%)
22	CLA	b	603	-	59,73,73	1.47	8 (13%)	67,113,113	1.64	11 (16%)
33	LHG	e	101	-	41,41,48	0.91	1 (2%)	44,47,54	1.22	4 (9%)
24	BCR	d	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	5 (8%)
31	STE	a	414	-	8,11,19	0.40	0	7,11,19	0.81	0
22	CLA	d	404	-	59,73,73	1.40	7 (11%)	67,113,113	1.42	10 (14%)
27	LMG	Y	101	-	48,48,55	0.96	2 (4%)	56,56,63	1.35	6 (10%)
31	STE	D	413	-	16,19,19	0.31	0	15,19,19	0.92	0
22	CLA	b	609	-	59,73,73	1.72	8 (13%)	67,113,113	1.49	12 (17%)
24	BCR	K	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	8 (14%)
22	CLA	B	611	-	59,73,73	1.47	8 (13%)	67,113,113	1.79	16 (23%)
29	DGD	C	516	-	63,63,67	1.20	9 (14%)	77,77,81	1.40	11 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	A	413	-	-	30/55/95/95	0/2/2/2
34	HEC	v	201	17	-	0/6/54/54	-
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
22	CLA	B	605	-	3/3/25/25	9/37/135/135	-
24	BCR	a	406	-	-	3/29/63/63	0/2/2/2
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
31	STE	B	601	-	-	4/7/9/17	-
31	STE	d	412	-	-	5/12/14/17	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
22	CLA	C	512	-	3/3/25/25	15/37/135/135	-
31	STE	C	518	-	-	4/7/9/17	-
22	CLA	C	508	-	1/1/25/25	9/37/135/135	-
28	SQD	B	622	-	-	19/49/69/69	0/1/1/1
31	STE	b	625	-	-	6/7/7/17	-
22	CLA	C	507	35	3/3/25/25	5/37/135/135	-
22	CLA	c	502	-	3/3/25/25	1/37/135/135	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
22	CLA	b	613	-	3/3/25/25	7/37/135/135	-
31	STE	m	101	-	-	7/15/15/17	-
31	STE	b	627	-	-	9/15/17/17	-
22	CLA	a	405	-	3/3/25/25	7/37/135/135	-
22	CLA	c	510	-	3/3/25/25	15/37/135/135	-
22	CLA	C	509	-	3/3/25/25	11/37/135/135	-
22	CLA	b	610	35	3/3/25/25	3/37/135/135	-
24	BCR	c	515	-	-	10/29/63/63	0/2/2/2
22	CLA	B	608	-	2/2/25/25	4/37/135/135	-
26	PL9	d	406	-	-	15/53/73/73	0/1/1/1
24	BCR	F	101	-	-	5/29/63/63	0/2/2/2
29	DGD	c	519	-	-	18/51/91/95	0/2/2/2
22	CLA	A	405	-	3/3/22/25	3/24/122/135	-
24	BCR	b	619	-	-	8/29/63/63	0/2/2/2
31	STE	b	620	-	-	7/13/13/17	-
27	LMG	D	407	-	-	16/46/66/70	0/1/1/1
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
31	STE	d	411	-	-	7/11/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	506	-	2/2/25/25	10/37/135/135	-
34	HEC	V	201	17	-	0/6/54/54	-
22	CLA	C	510	-	3/3/25/25	8/37/135/135	-
31	STE	J	101	-	-	3/7/9/17	-
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1
22	CLA	C	504	35	3/3/23/25	8/30/128/135	-
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	d	403	-	1/1/25/25	10/37/135/135	-
22	CLA	B	615	-	3/3/25/25	9/37/135/135	-
31	STE	a	413	-	-	5/7/7/17	-
22	CLA	b	604	-	3/3/25/25	7/37/135/135	-
22	CLA	D	405	-	3/3/25/25	7/37/135/135	-
22	CLA	B	613	-	3/3/25/25	13/37/135/135	-
26	PL9	a	409	-	-	21/53/73/73	0/1/1/1
31	STE	j	101	-	-	4/7/9/17	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
27	LMG	A	410	-	-	18/43/63/70	0/1/1/1
22	CLA	B	616	-	3/3/24/25	10/31/129/135	-
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
31	STE	B	627	-	-	5/12/12/17	-
24	BCR	H	102	-	-	6/29/63/63	0/2/2/2
22	CLA	b	611	-	2/2/25/25	7/37/135/135	-
27	LMG	B	621	-	-	9/18/22/70	-
23	PHO	A	404	-	-	4/53/103/103	0/5/6/6
28	SQD	a	412	-	-	15/37/37/69	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	c	511	-	3/3/25/25	7/37/135/135	-
34	HEC	f	101	5,6	-	1/6/54/54	-
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
31	STE	m	102	-	-	4/7/9/17	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
28	SQD	A	411	-	-	9/47/67/69	0/1/1/1
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
31	STE	B	624	-	-	3/7/9/17	-
22	CLA	c	505	35	3/3/24/25	7/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	E	101	-	-	31/53/53/53	-
22	CLA	B	603	-	3/3/25/25	14/37/135/135	-
24	BCR	k	102	-	-	6/29/63/63	0/2/2/2
22	CLA	H	101	35	2/2/25/25	20/37/135/135	-
22	CLA	B	610	35	3/3/25/25	6/37/135/135	-
22	CLA	C	502	-	3/3/25/25	10/37/135/135	-
31	STE	E	102	-	-	5/7/9/17	-
22	CLA	b	601	35	2/2/25/25	16/37/135/135	-
22	CLA	c	504	-	2/2/25/25	11/37/135/135	-
23	PHO	a	404	-	-	6/53/103/103	0/5/6/6
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
29	DGD	c	517	-	-	24/51/91/95	0/2/2/2
22	CLA	b	607	35	3/3/25/25	15/37/135/135	-
22	CLA	C	501	-	3/3/25/25	3/37/135/135	-
22	CLA	B	614	-	3/3/25/25	10/37/135/135	-
28	SQD	D	408	-	-	13/28/48/69	0/1/1/1
24	BCR	h	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/25/25	5/37/135/135	-
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
24	BCR	c	516	-	-	6/29/63/63	0/2/2/2
22	CLA	c	512	3	3/3/25/25	11/37/135/135	-
31	STE	C	520	-	-	2/7/9/17	-
31	STE	B	625	-	-	12/13/15/17	-
22	CLA	c	507	-	3/3/25/25	16/37/135/135	-
22	CLA	b	614	-	3/3/25/25	16/37/135/135	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
22	CLA	A	403	35	1/1/25/25	14/37/135/135	-
22	CLA	c	513	-	3/3/25/25	19/37/135/135	-
27	LMG	a	415	-	-	31/50/70/70	0/1/1/1
27	LMG	D	411	-	-	15/33/33/70	-
22	CLA	a	402	-	3/3/25/25	7/37/135/135	-
31	STE	C	519	-	-	5/13/13/17	-
22	CLA	b	615	-	3/3/25/25	8/37/135/135	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
22	CLA	b	605	-	3/3/25/25	8/37/135/135	-
22	CLA	c	509	-	2/2/24/25	7/36/134/135	-
24	BCR	A	406	-	-	11/29/63/63	0/2/2/2
22	CLA	c	503	-	2/2/25/25	8/37/135/135	-
31	STE	T	102	-	-	7/12/12/17	-
31	STE	I	101	-	-	7/12/12/17	-
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
24	BCR	B	619	-	-	5/29/63/63	0/2/2/2
31	STE	B	620	-	-	8/12/14/17	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
29	DGD	h	102	-	-	18/51/91/95	0/2/2/2
33	LHG	D	412	-	-	20/53/53/53	-
31	STE	c	521	-	-	9/15/17/17	-
31	STE	d	413	-	-	9/15/17/17	-
33	LHG	d	408	-	-	20/53/53/53	-
24	BCR	B	618	-	-	9/29/63/63	0/2/2/2
33	LHG	L	102	-	-	20/53/53/53	-
28	SQD	A	412	-	-	17/39/39/69	-
34	HEC	F	102	5,6	-	0/6/54/54	-
22	CLA	B	604	-	3/3/25/25	12/37/135/135	-
29	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	c	514	-	3/3/25/25	10/37/135/135	-
31	STE	b	626	-	-	5/11/11/17	-
31	STE	b	622	-	-	6/15/17/17	-
22	CLA	b	606	-	3/3/25/25	7/37/135/135	-
33	LHG	l	101	-	-	17/53/53/53	-
22	CLA	B	602	-	3/3/25/25	8/37/135/135	-
27	LMG	b	621	-	-	14/46/66/70	0/1/1/1
22	CLA	C	506	-	2/2/25/25	8/37/135/135	-
31	STE	c	501	-	-	3/7/9/17	-
22	CLA	D	404	35	1/1/25/25	10/37/135/135	-
27	LMG	b	623	-	-	26/50/70/70	0/1/1/1
22	CLA	B	612	-	3/3/25/25	12/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	M	102	-	-	5/10/12/17	-
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
22	CLA	b	602	-	1/1/25/25	6/37/135/135	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
31	STE	B	623	-	-	3/9/11/17	-
22	CLA	D	403	-	1/1/25/25	5/37/135/135	-
31	STE	Z	101	-	-	2/5/5/17	-
33	LHG	d	409	-	-	12/43/43/53	-
22	CLA	a	410	35	1/1/25/25	6/37/135/135	-
22	CLA	b	612	-	3/3/25/25	8/37/135/135	-
22	CLA	C	513	-	3/3/25/25	17/37/135/135	-
22	CLA	b	616	-	3/3/24/25	10/31/129/135	-
23	PHO	d	401	-	-	5/53/103/103	0/5/6/6
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
22	CLA	A	402	-	3/3/25/25	5/37/135/135	-
33	LHG	d	407	-	-	14/53/53/53	-
22	CLA	B	607	35	3/3/25/25	7/37/135/135	-
22	CLA	c	508	35	3/3/25/25	8/37/135/135	-
22	CLA	C	511	3	3/3/25/25	9/37/135/135	-
28	SQD	f	102	-	-	15/36/56/69	0/1/1/1
33	LHG	D	409	-	-	28/53/53/53	-
22	CLA	C	503	-	3/3/25/25	5/37/135/135	-
31	STE	B	626	-	-	8/13/13/17	-
22	CLA	B	606	-	3/3/25/25	13/37/135/135	-
22	CLA	B	609	-	1/1/25/25	8/37/135/135	-
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
31	STE	b	624	-	-	8/15/17/17	-
31	STE	M	103	-	-	3/7/7/17	-
22	CLA	C	505	-	2/2/25/25	12/37/135/135	-
33	LHG	D	410	-	-	22/51/51/53	-
22	CLA	b	603	-	3/3/25/25	10/37/135/135	-
33	LHG	e	101	-	-	23/46/46/53	-
24	BCR	d	405	-	-	8/29/63/63	0/2/2/2
31	STE	a	414	-	-	2/7/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	404	-	2/2/25/25	5/37/135/135	-
22	CLA	a	403	35	2/2/25/25	11/37/135/135	-
31	STE	D	413	-	-	7/15/17/17	-
22	CLA	b	609	-	1/1/25/25	8/37/135/135	-
24	BCR	K	103	-	-	7/29/63/63	0/2/2/2
22	CLA	B	611	-	3/3/25/25	2/37/135/135	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2

The worst 5 of 799 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	C4B-NB	9.07	1.43	1.35
22	b	615	CLA	MG-NA	8.66	2.26	2.06
22	b	615	CLA	C4B-NB	8.52	1.42	1.35
22	A	405	CLA	C4B-NB	8.31	1.42	1.35
22	c	505	CLA	C4B-NB	8.28	1.42	1.35

The worst 5 of 1351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O6-C1-C2	10.32	124.41	108.30
28	a	411	SQD	O6-C1-C2	9.80	123.61	108.30
22	b	604	CLA	C4A-NA-C1A	9.48	110.97	106.71
22	b	611	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	c	510	CLA	C4A-NA-C1A	9.26	110.87	106.71

5 of 178 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND

5 of 1855 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	413	DGD	C2B-C1B-O2G-C2G
29	A	413	DGD	O1B-C1B-O2G-C2G

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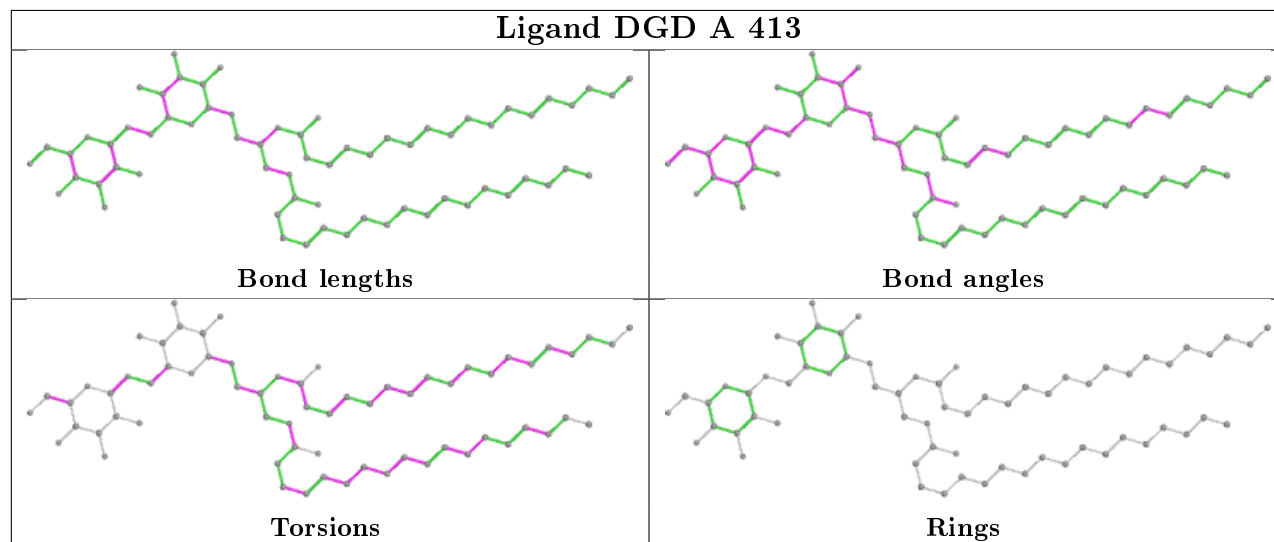
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Mol	Chain	Res	Type	Atoms
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O10-C23-O48-C46
28	L	101	SQD	C24-C23-O48-C46

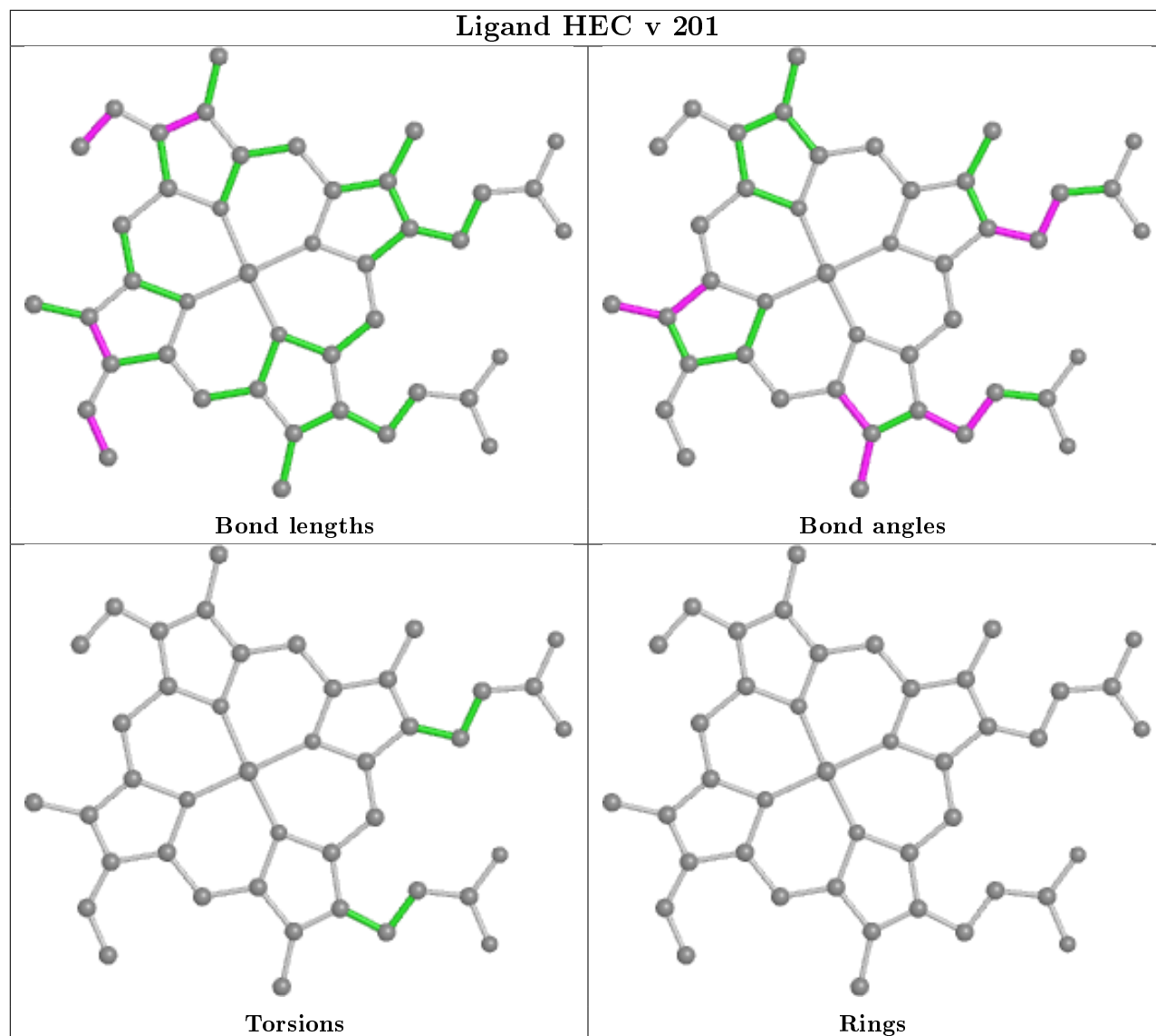
There are no ring outliers.

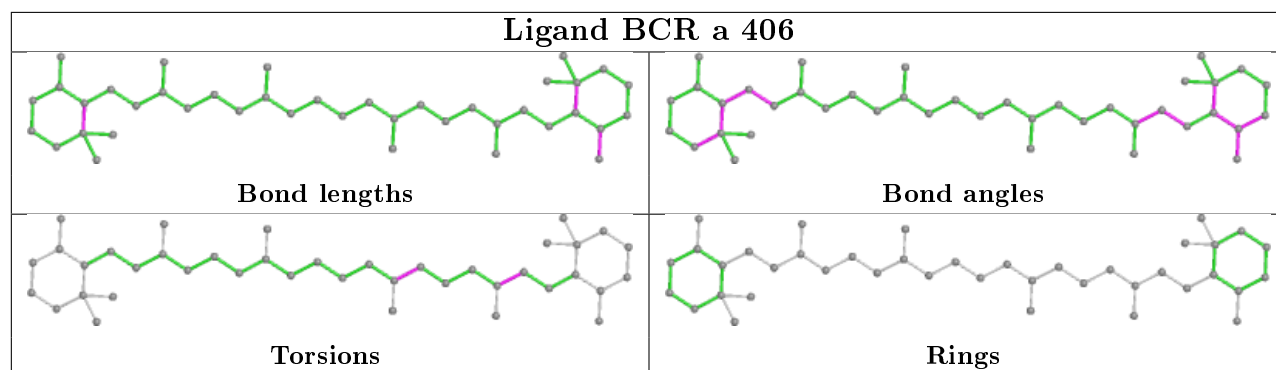
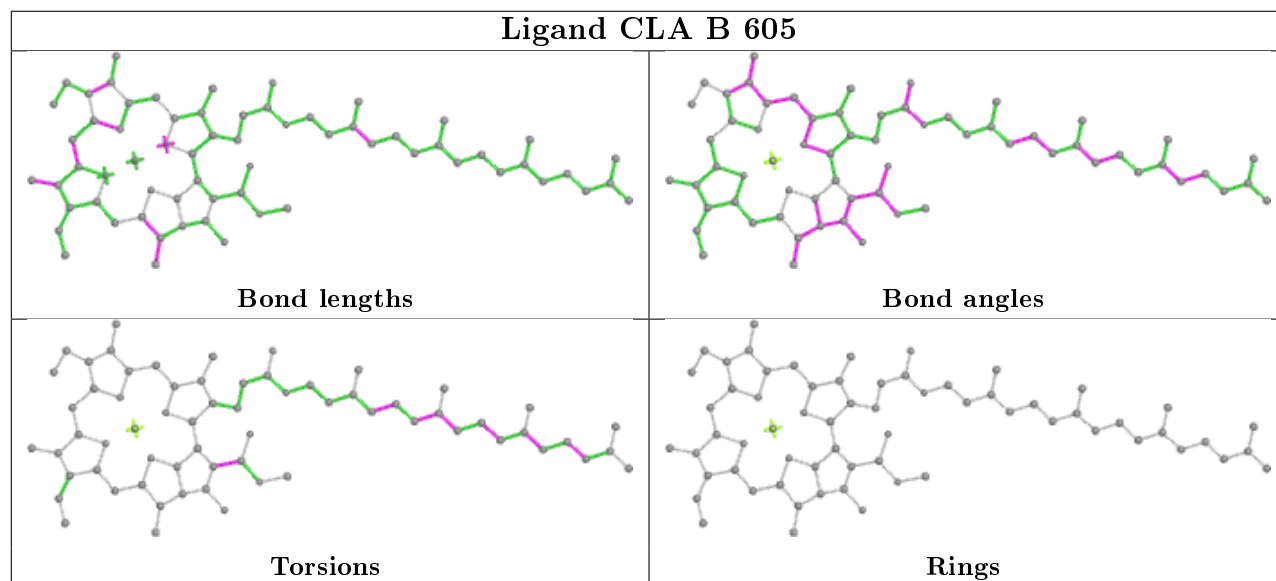
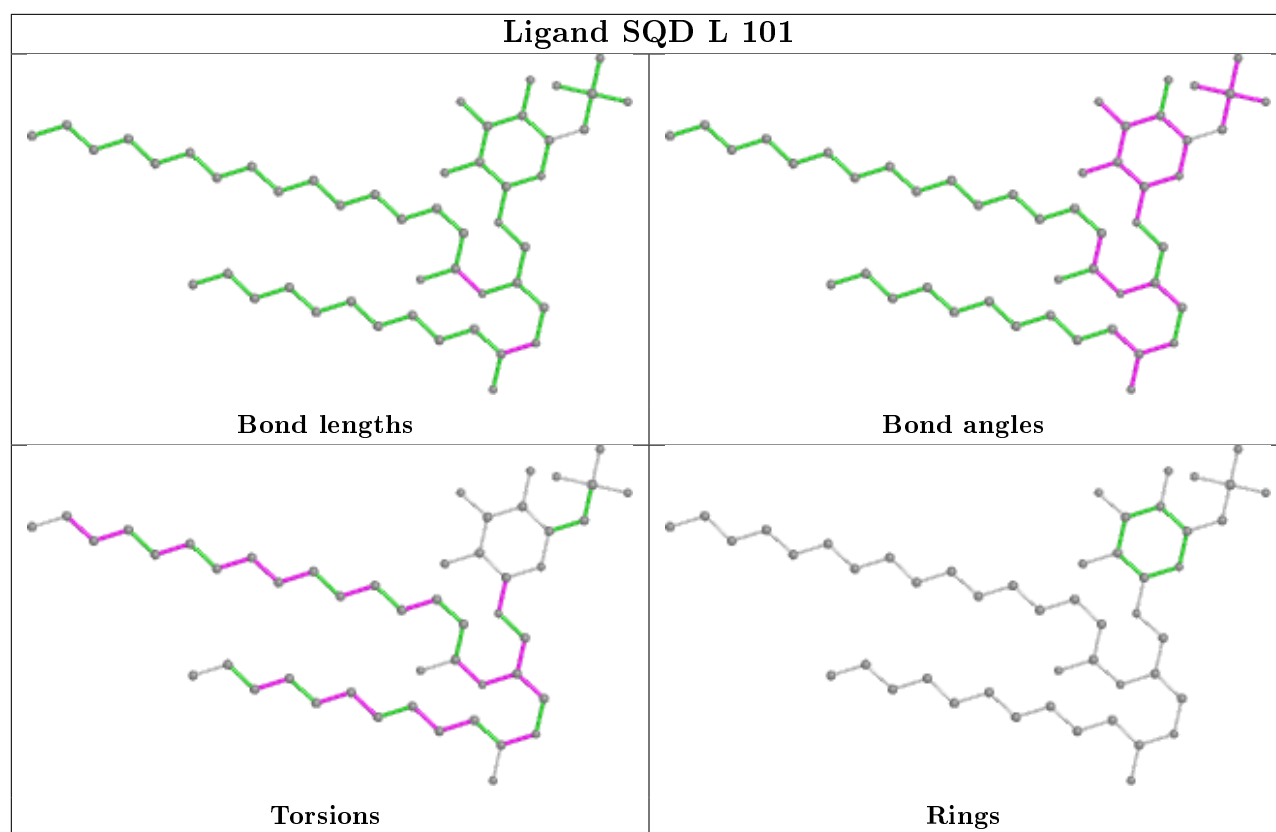
No monomer is involved in short contacts.

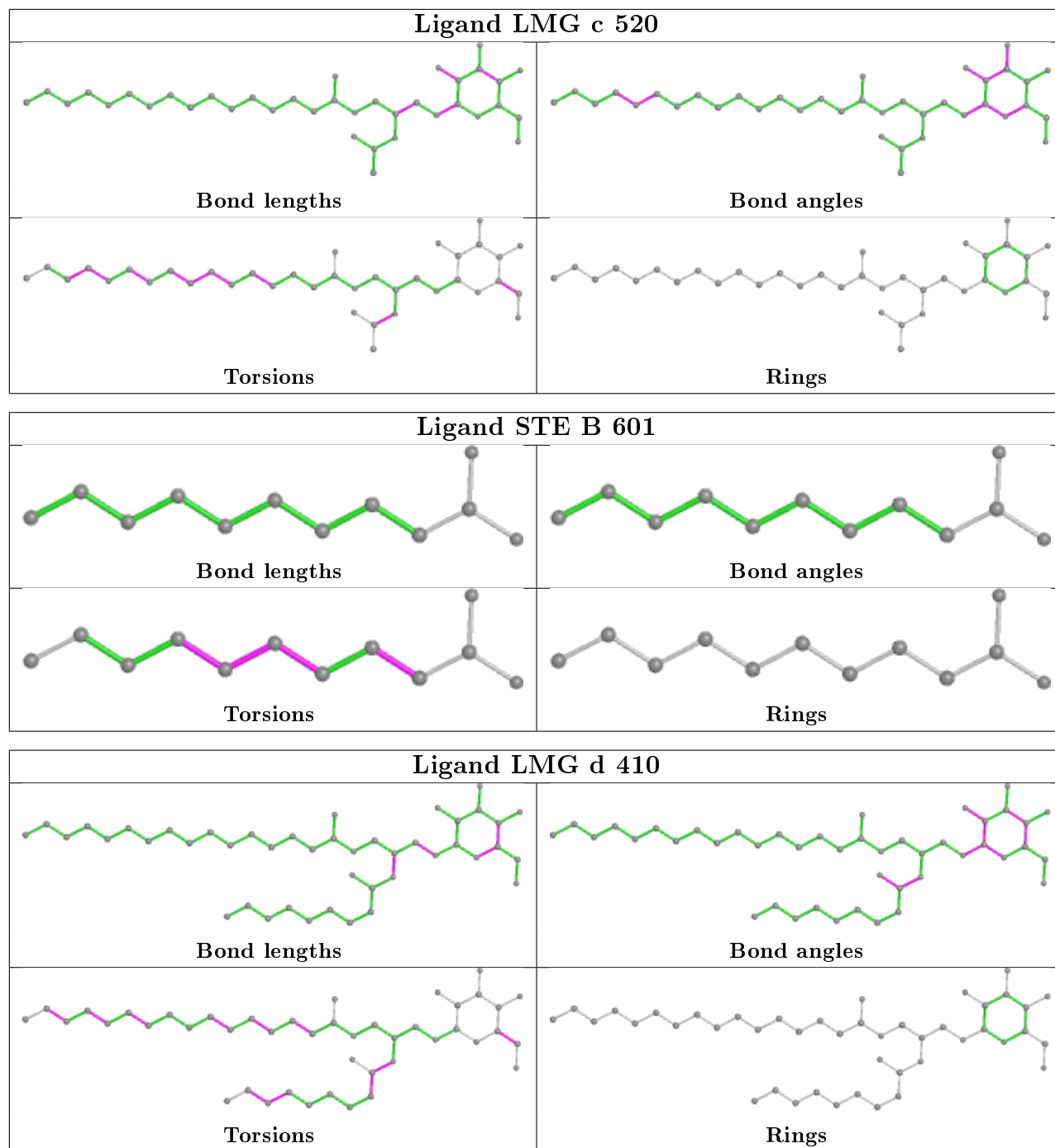
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

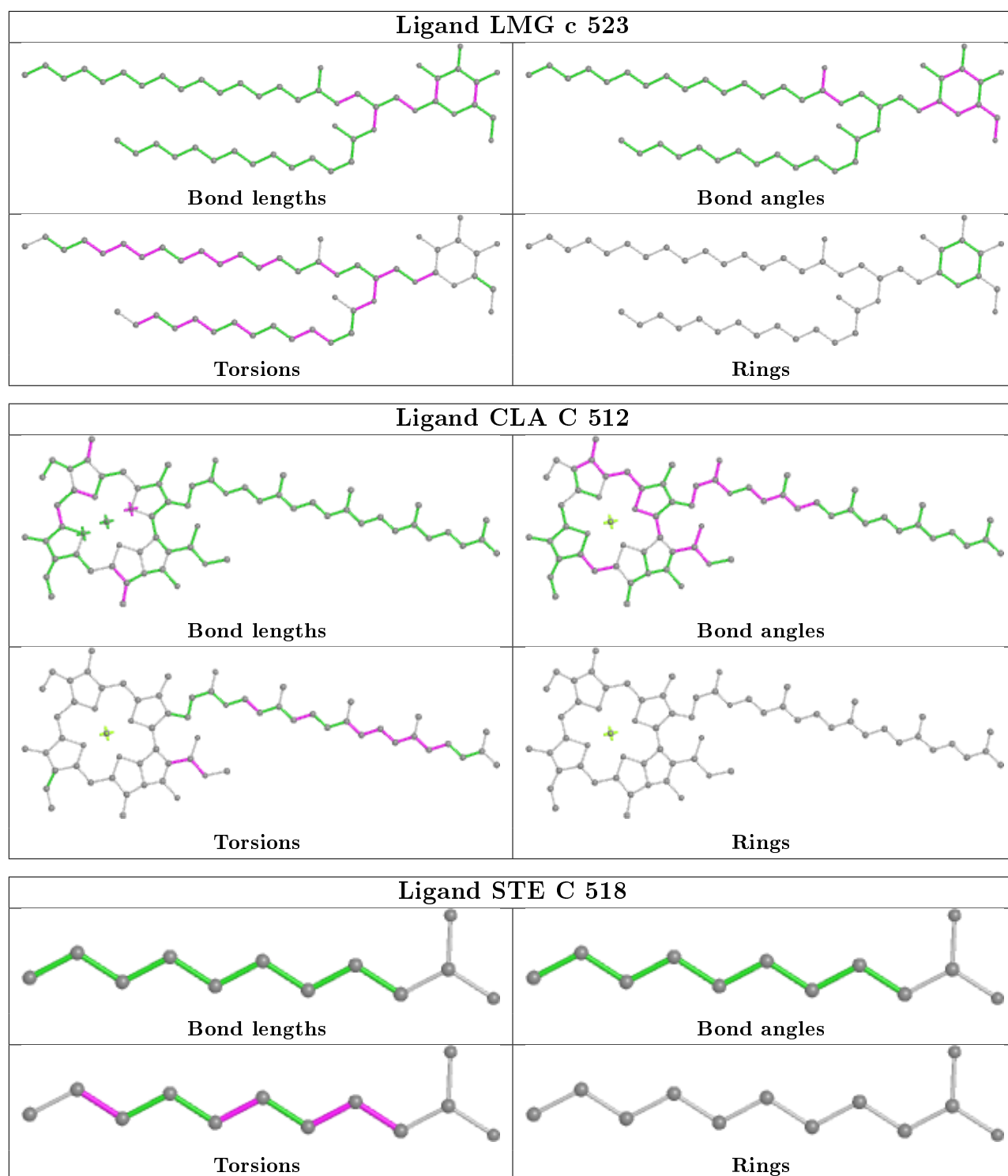


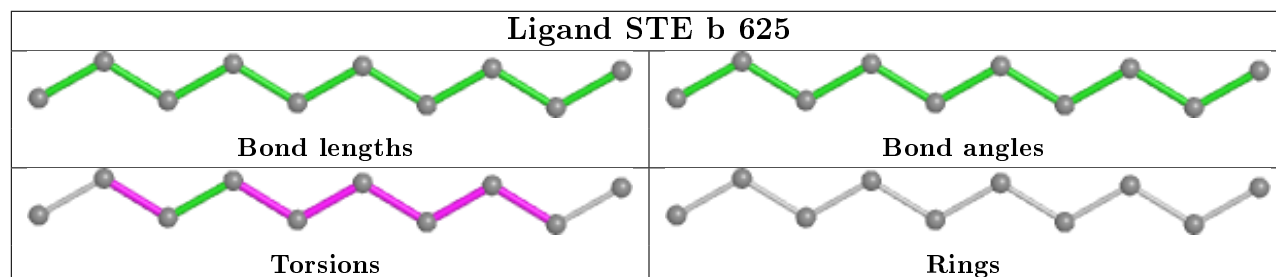
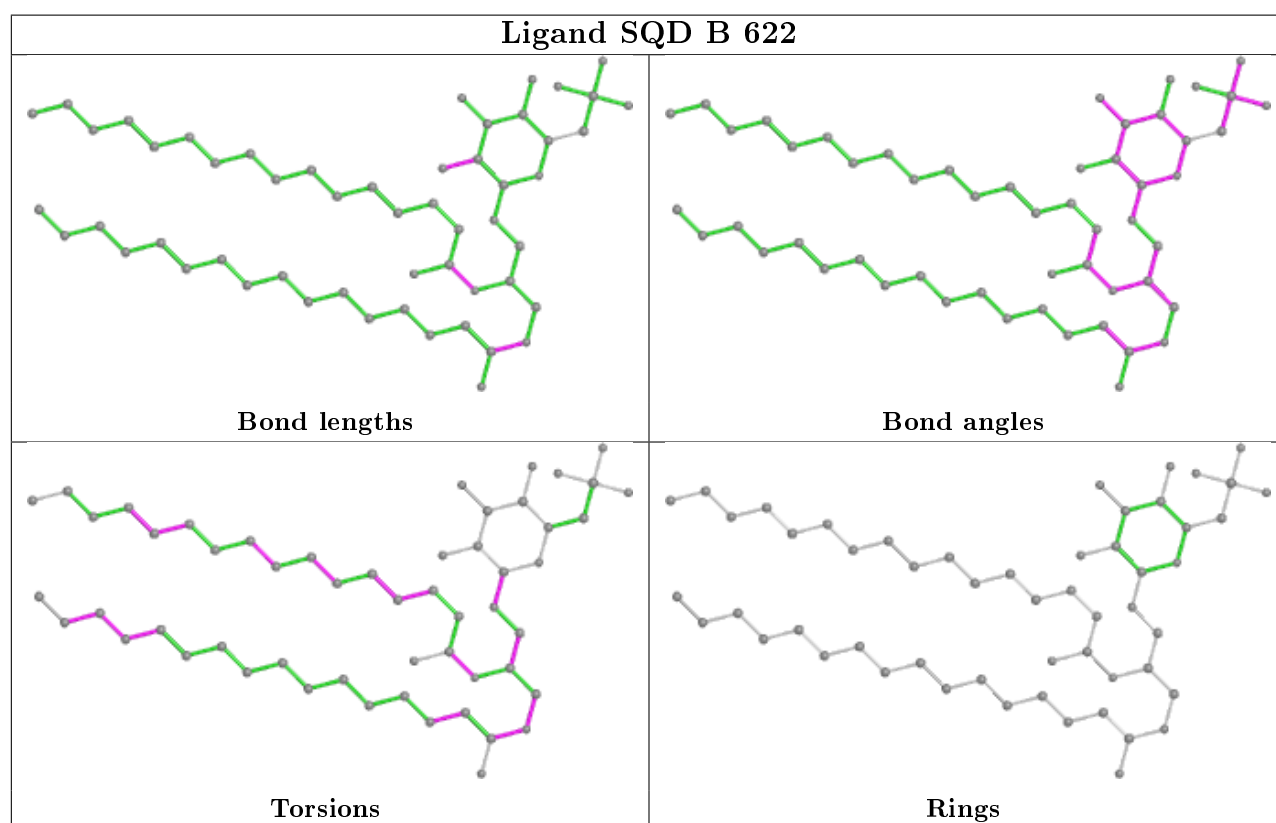
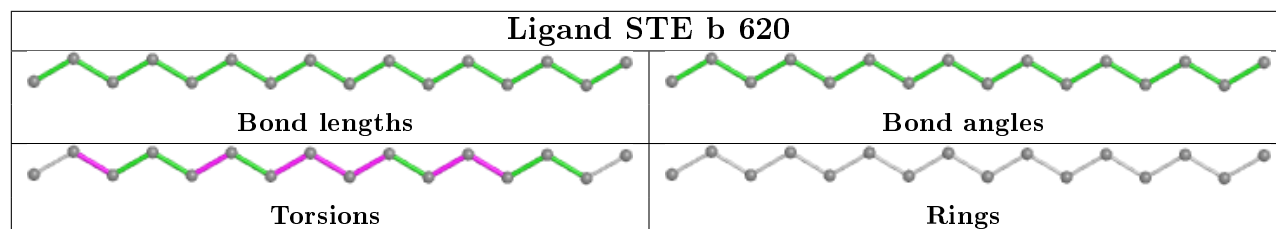
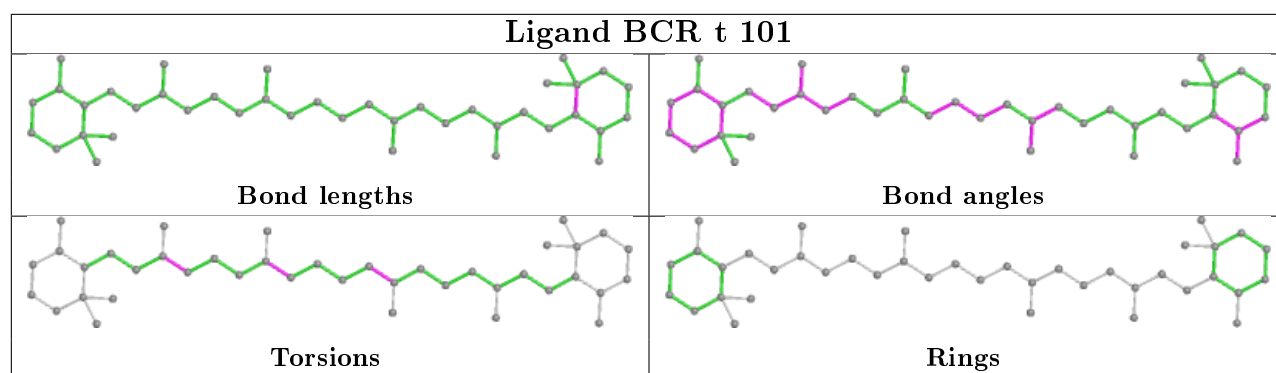
## Ligand HEC v 201



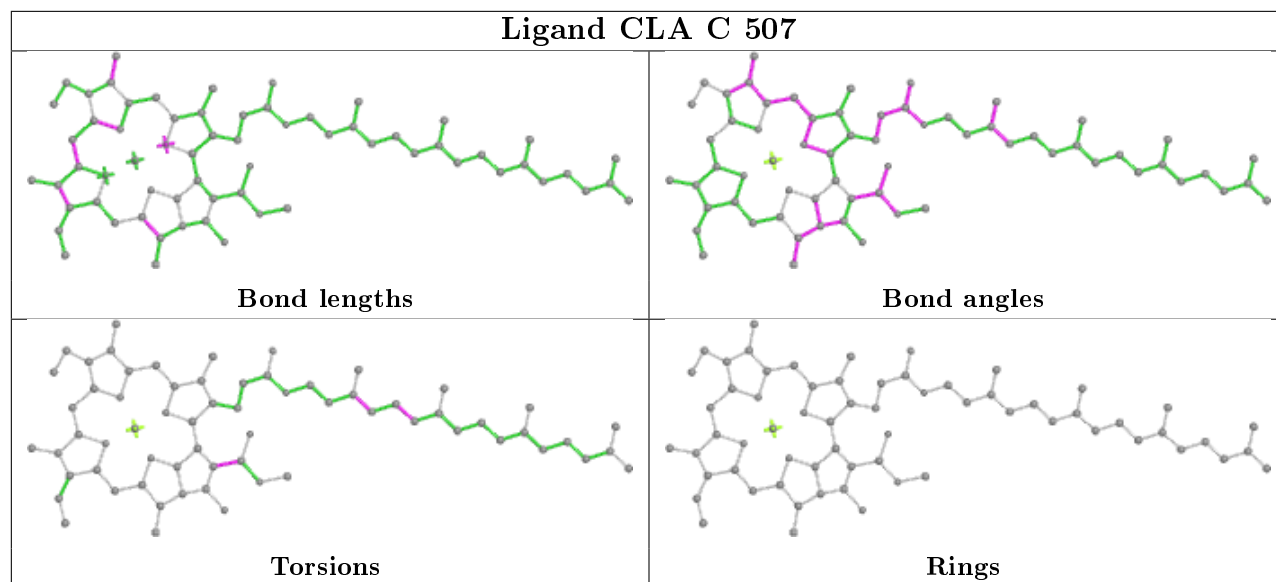




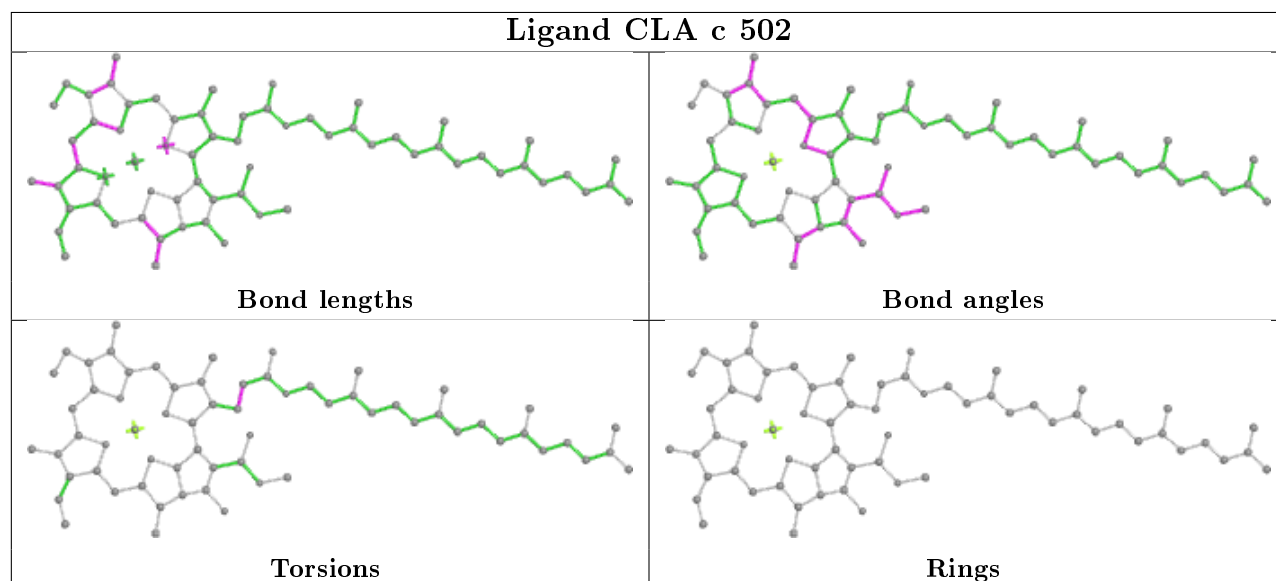




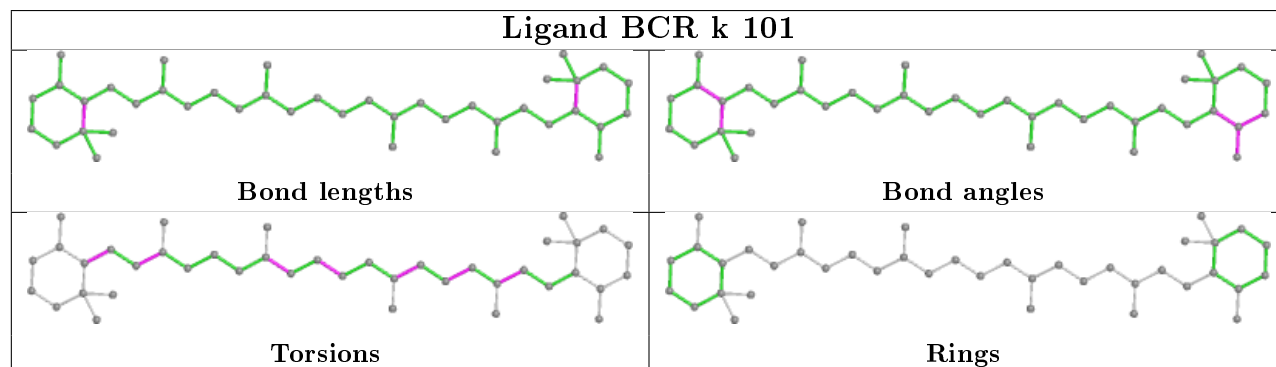
## Ligand CLA C 507

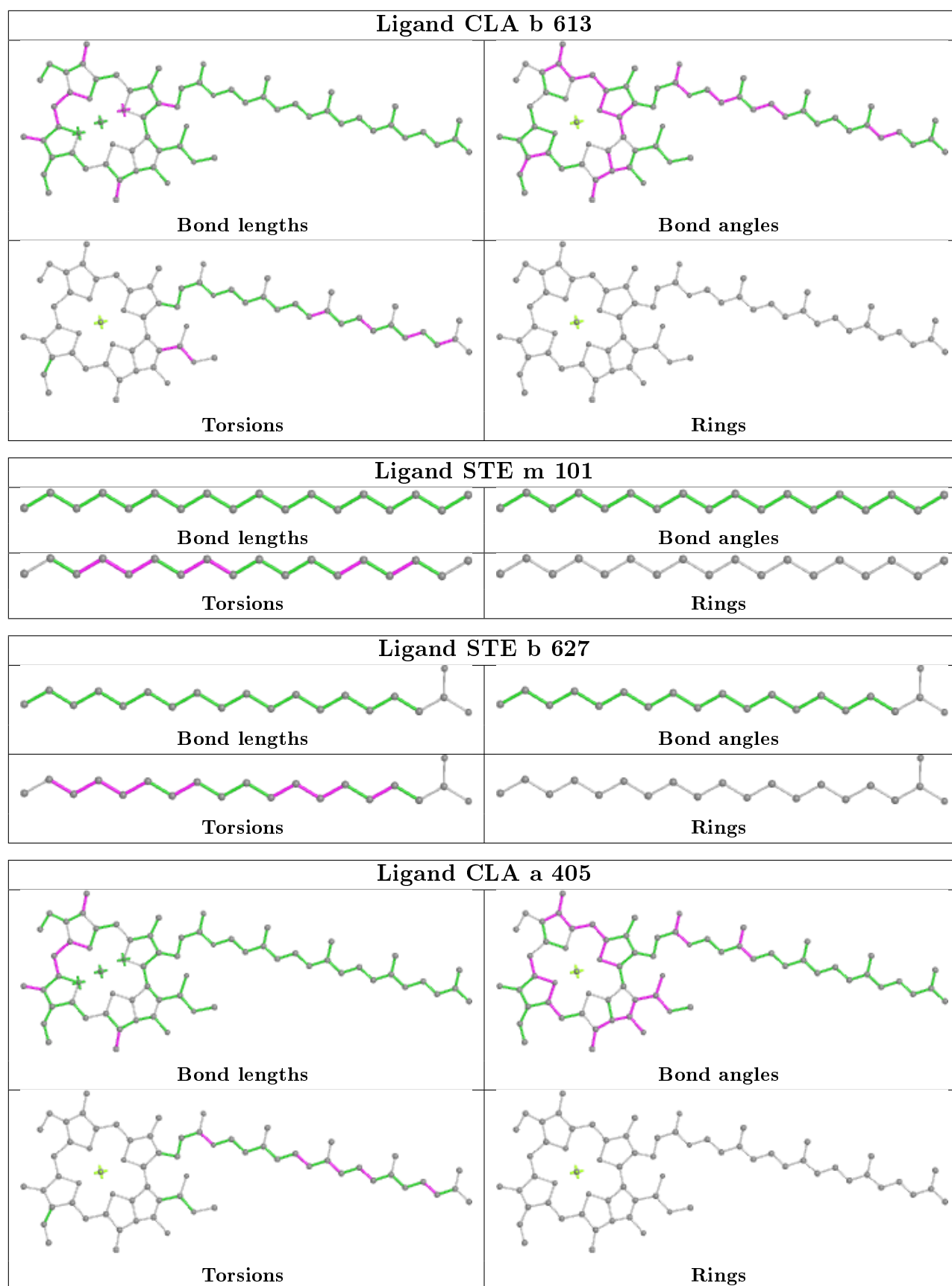


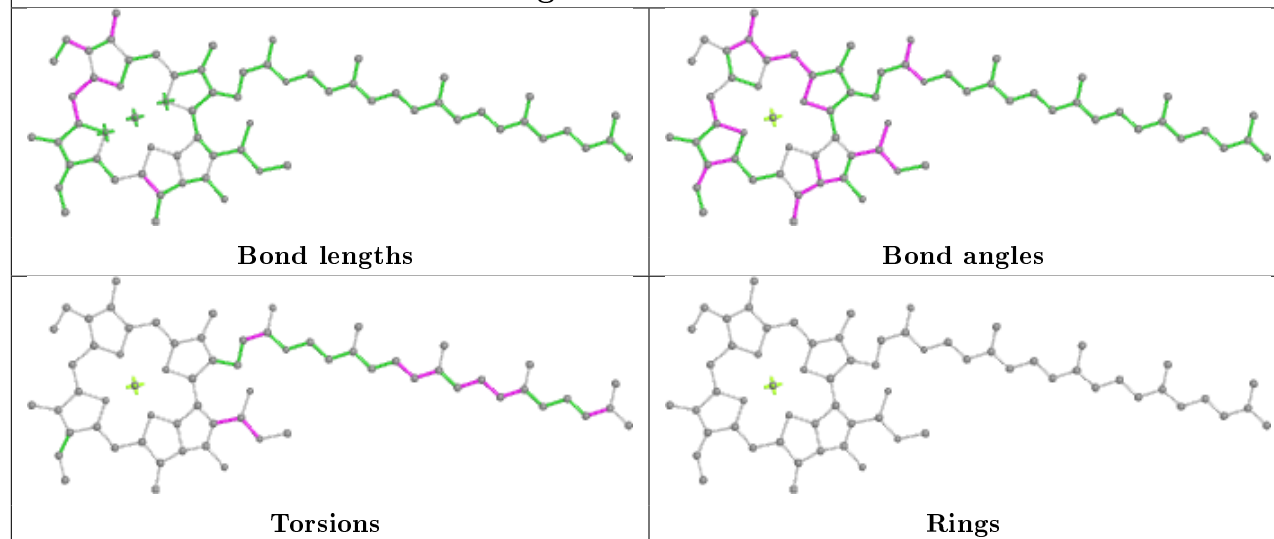
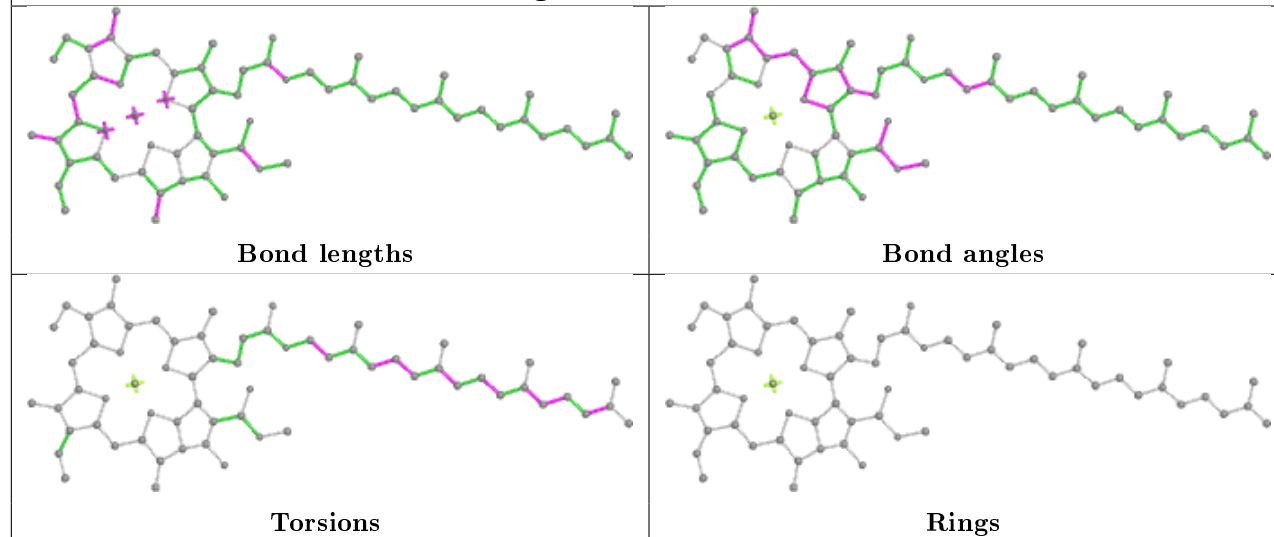
## Ligand CLA c 502



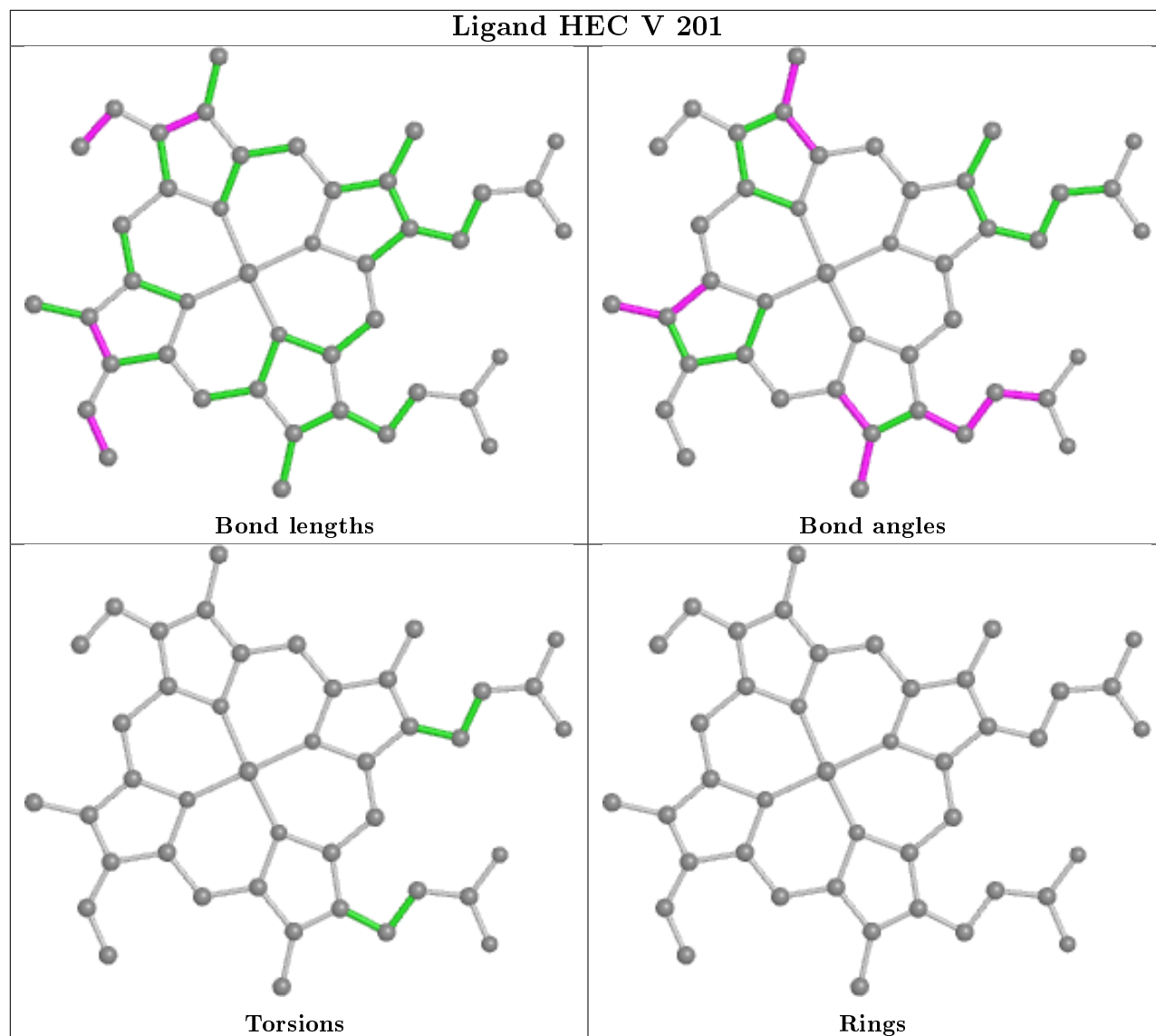
## Ligand BCR k 101



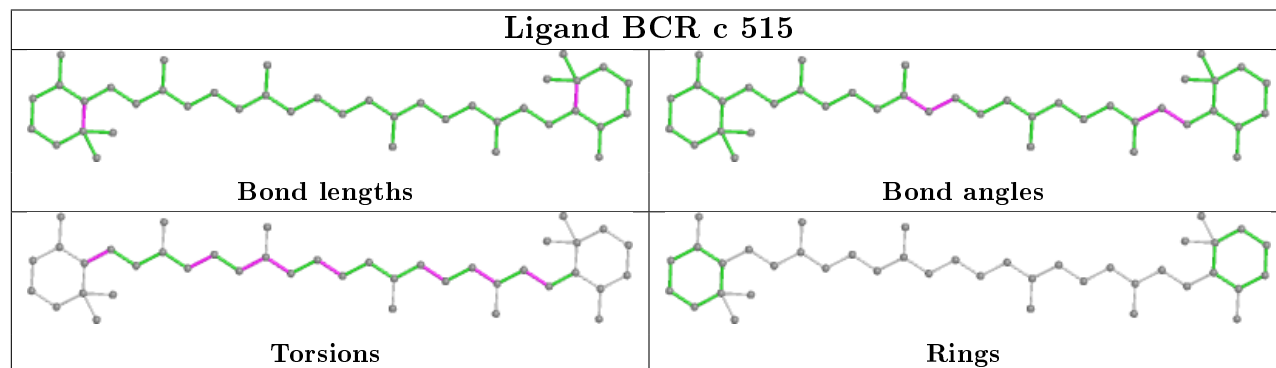


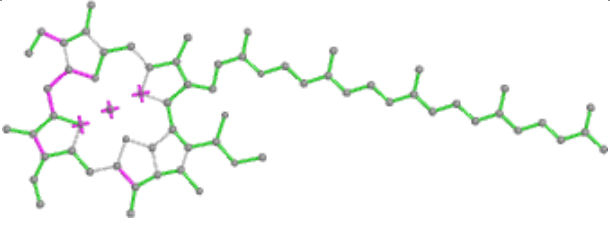
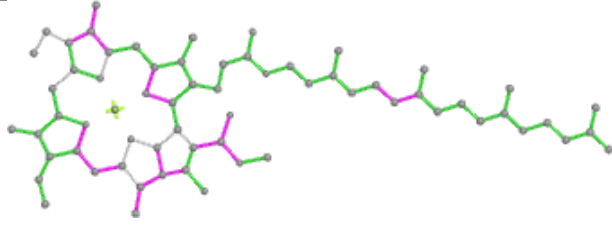
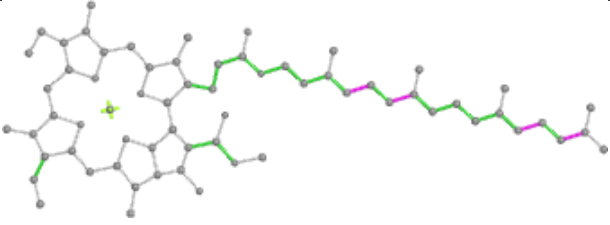
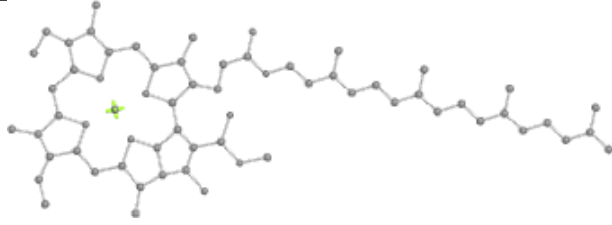
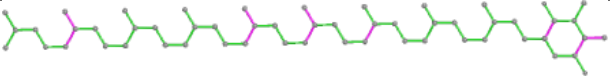
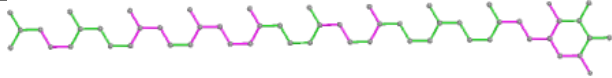
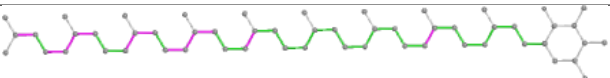
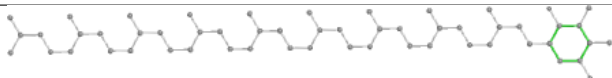
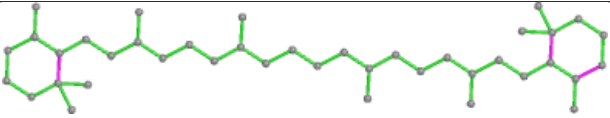
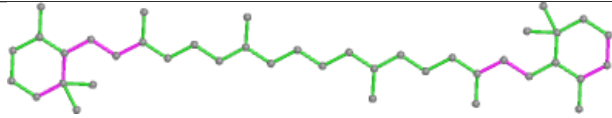
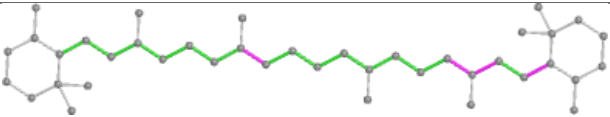
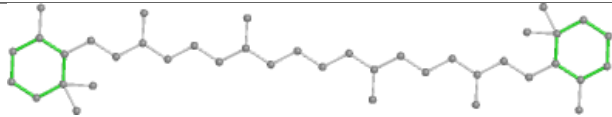
**Ligand CLA c 510****Ligand CLA C 509**

## Ligand HEC V 201

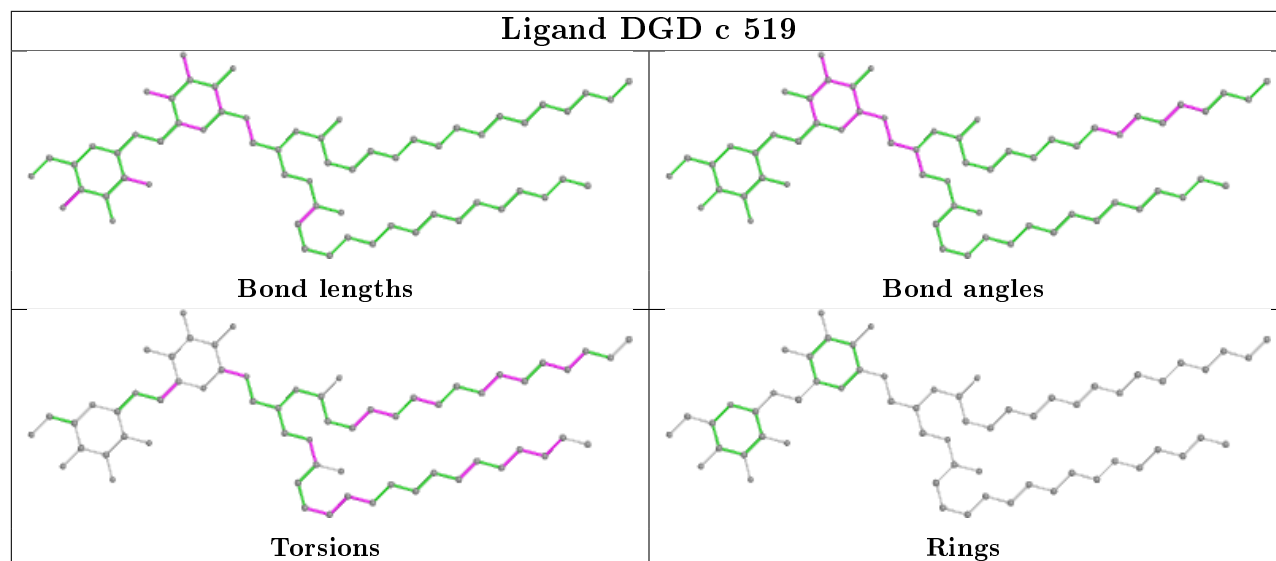


## Ligand BCR c 515

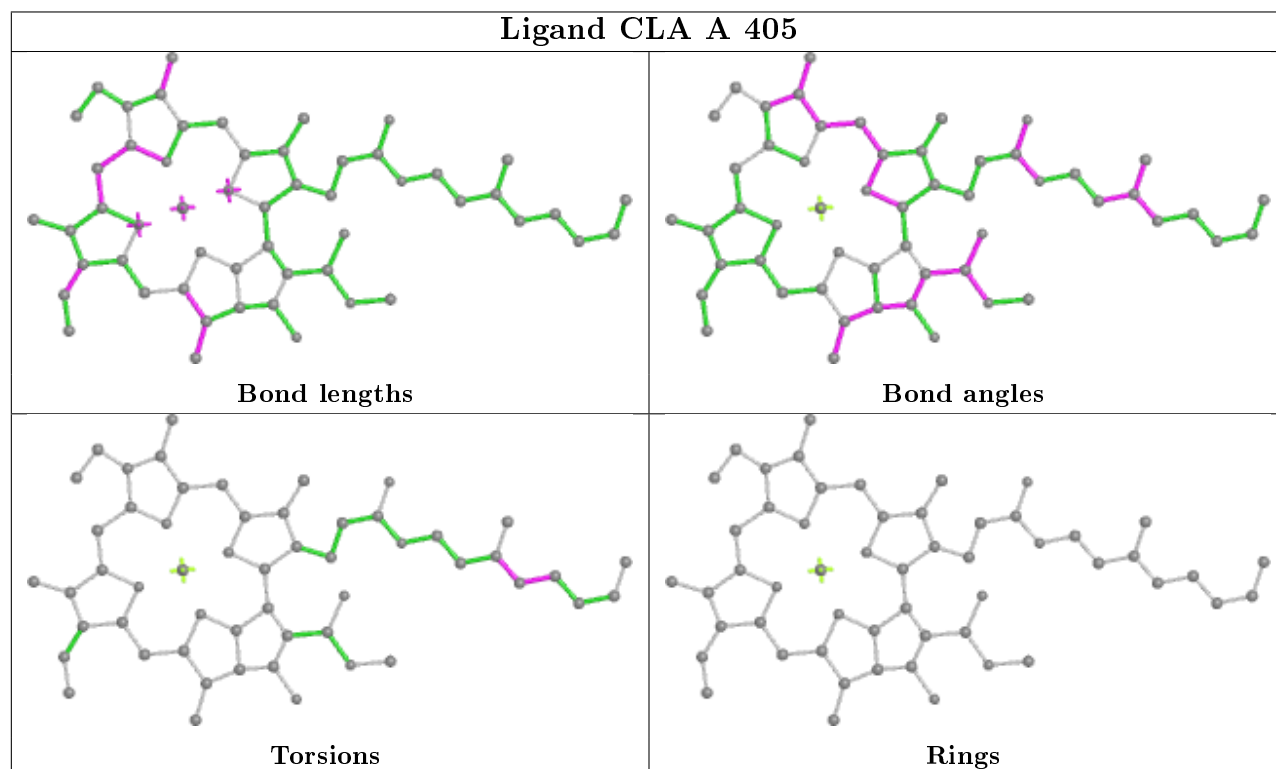


Ligand CLA B 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR F 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

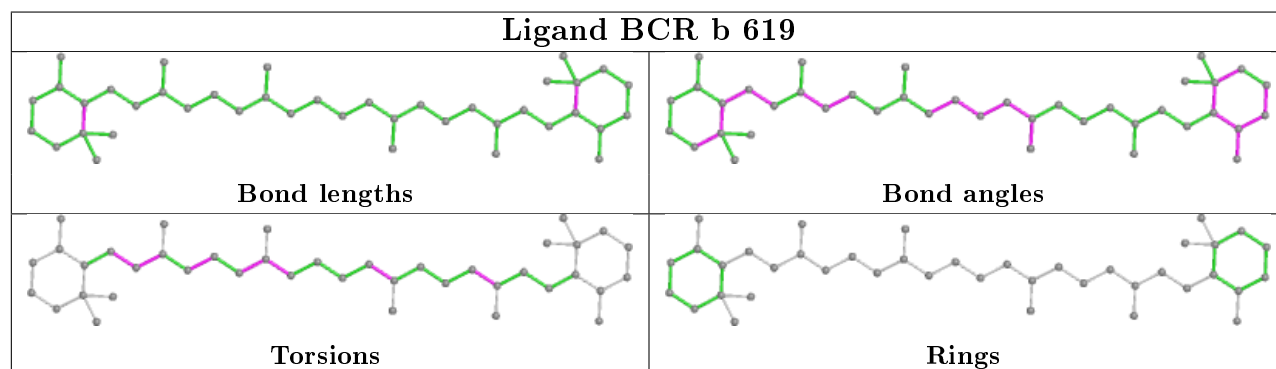
## Ligand DGD c 519

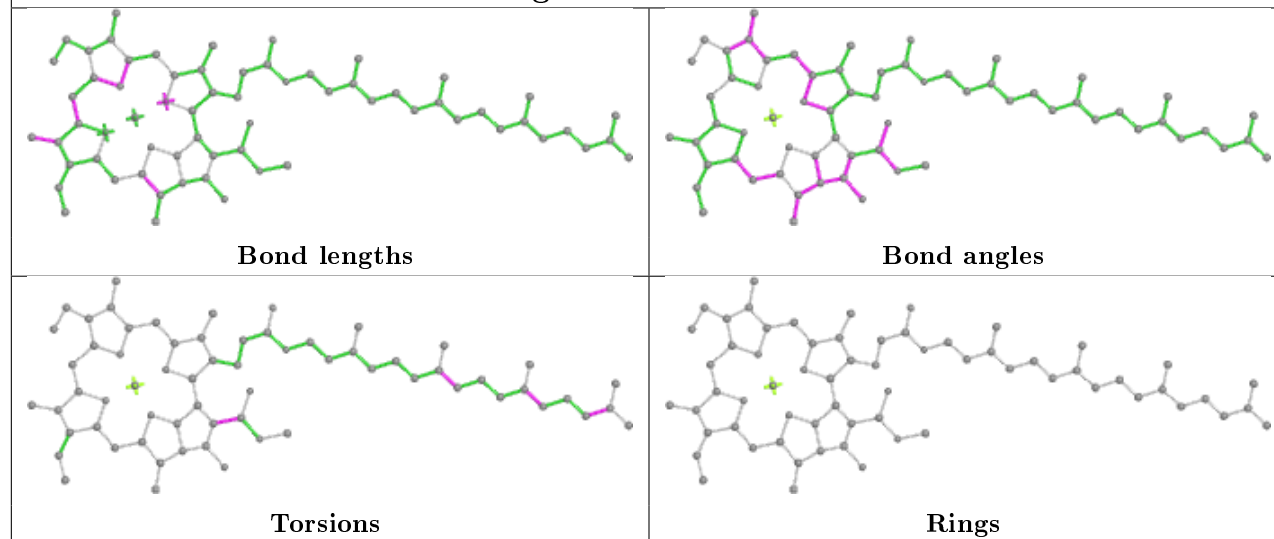
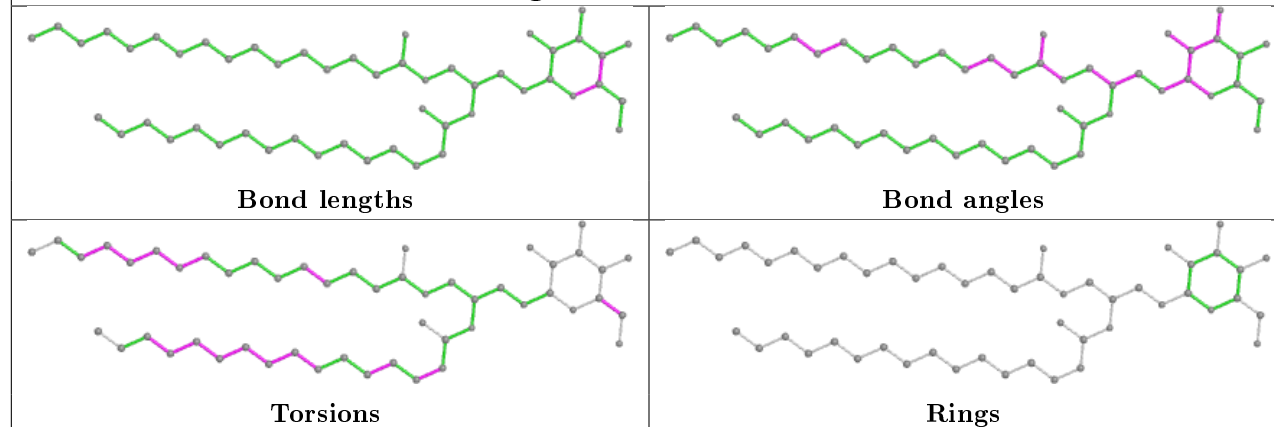
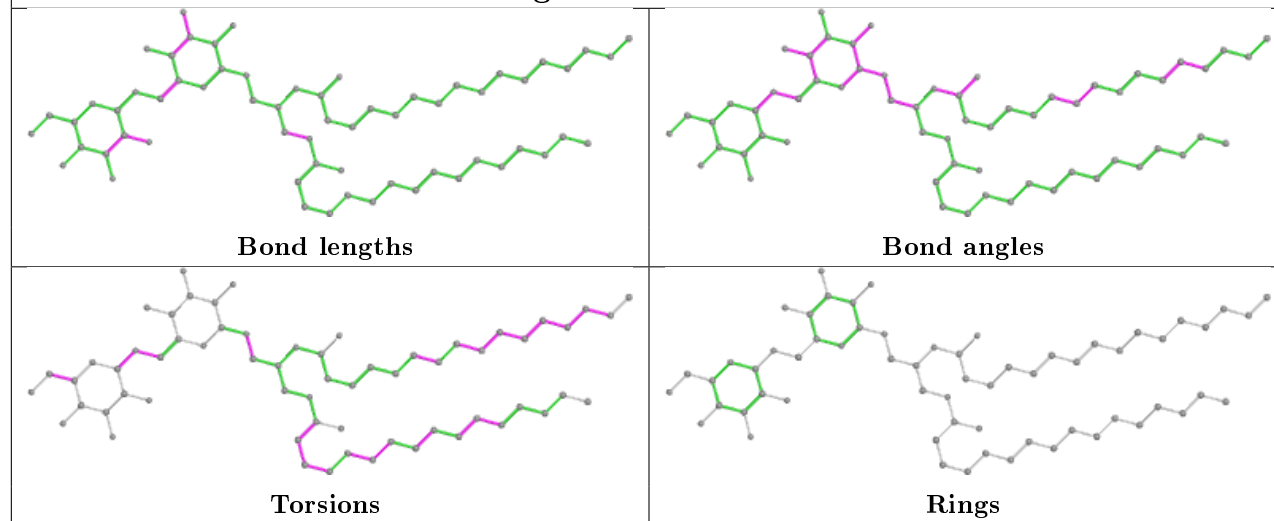


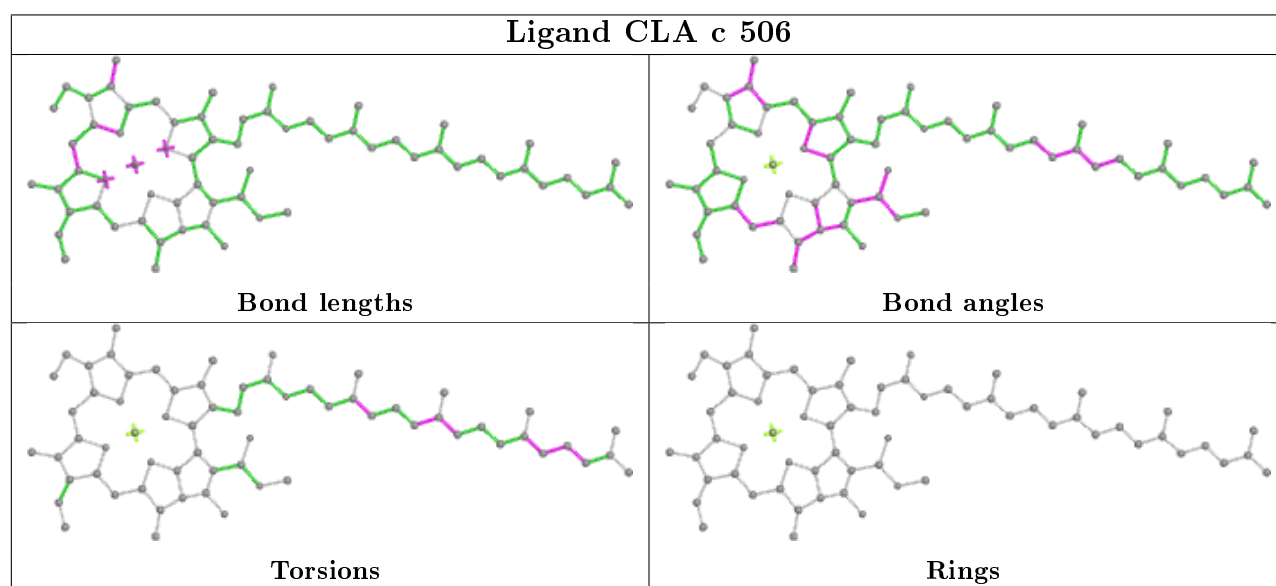
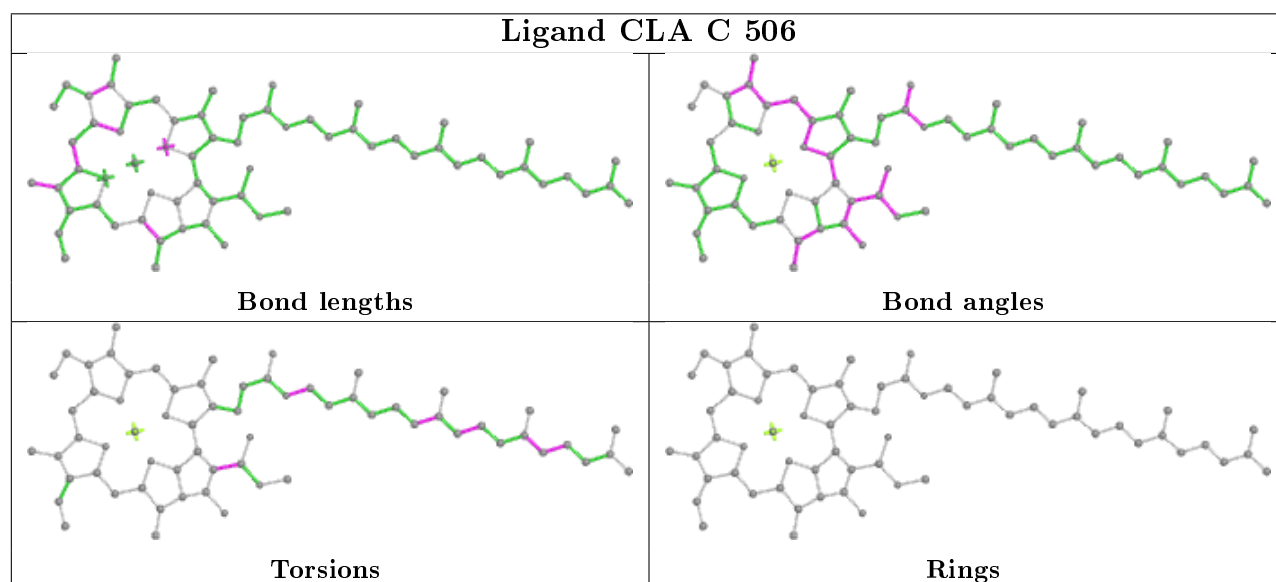
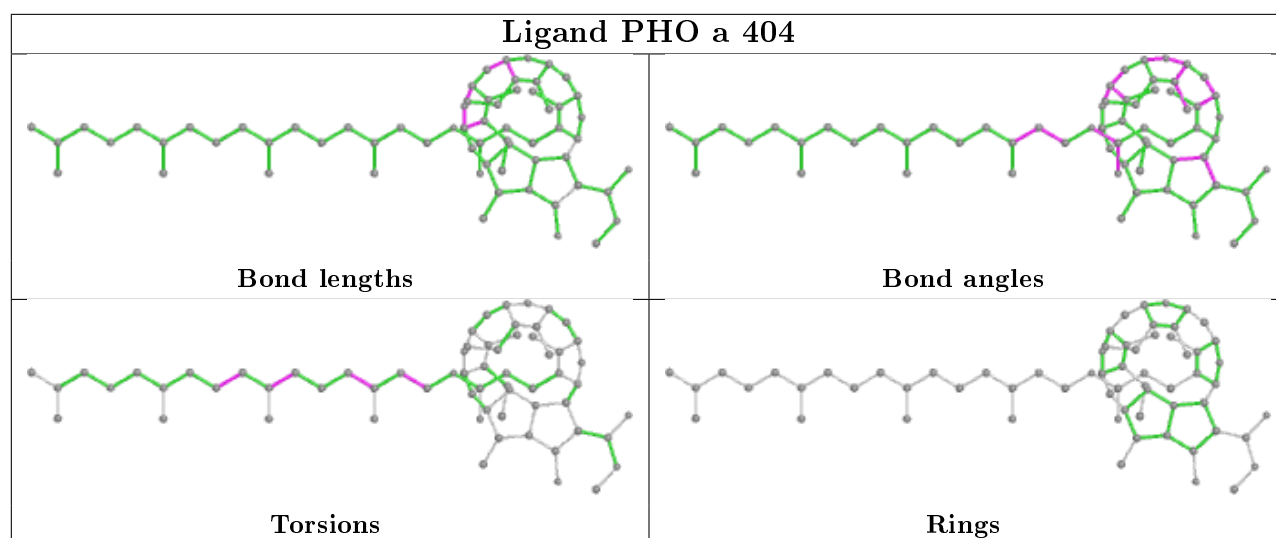
## Ligand CLA A 405



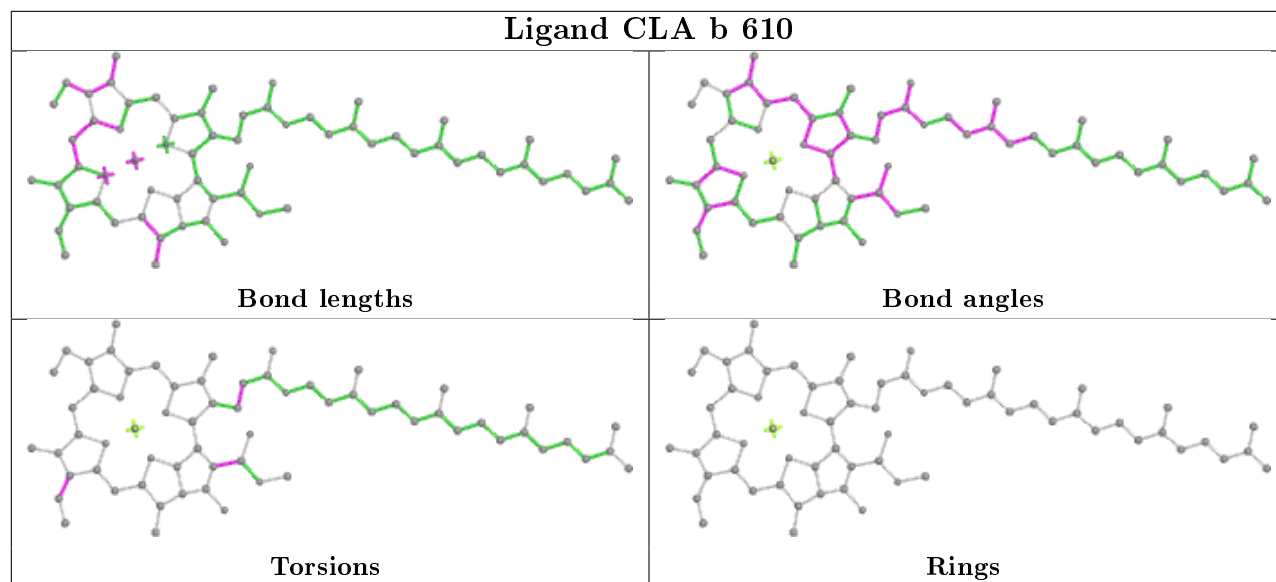
## Ligand BCR b 619



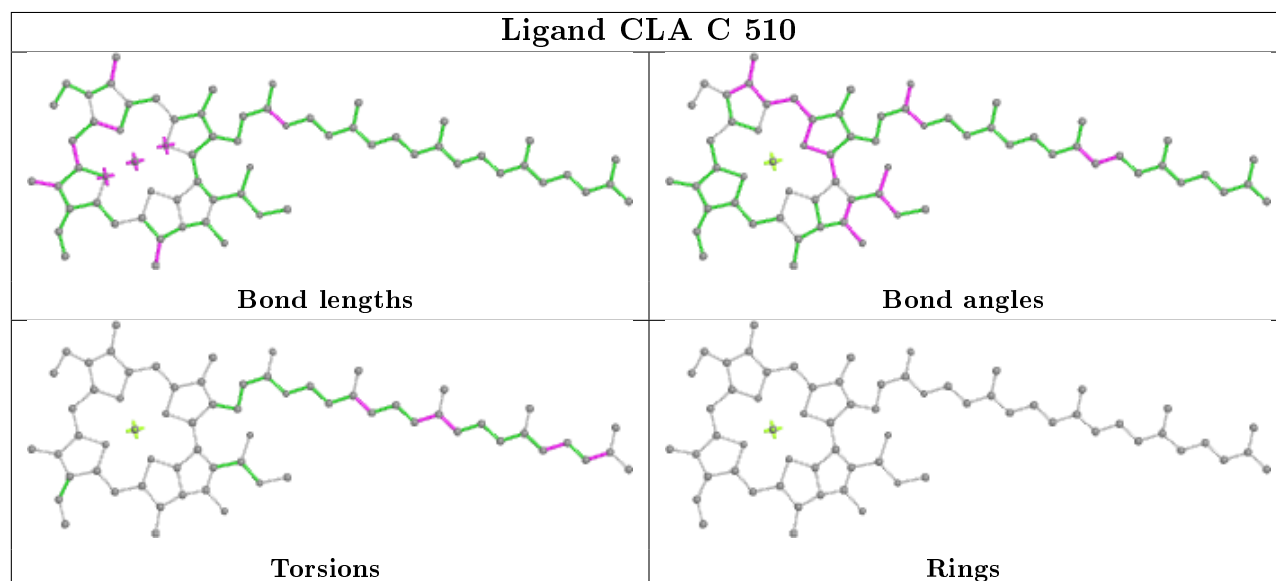
**Ligand CLA C 508****Ligand LMG D 407****Ligand DGD c 518**



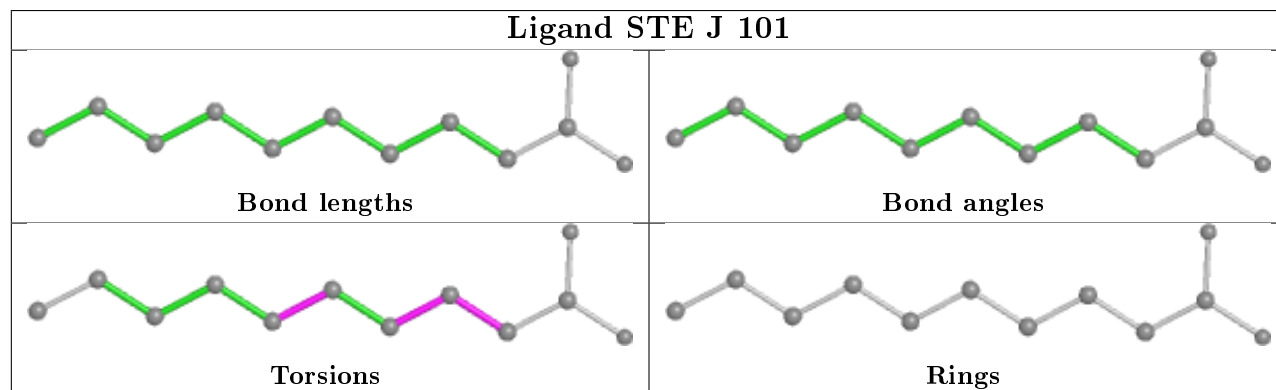
## Ligand CLA b 610



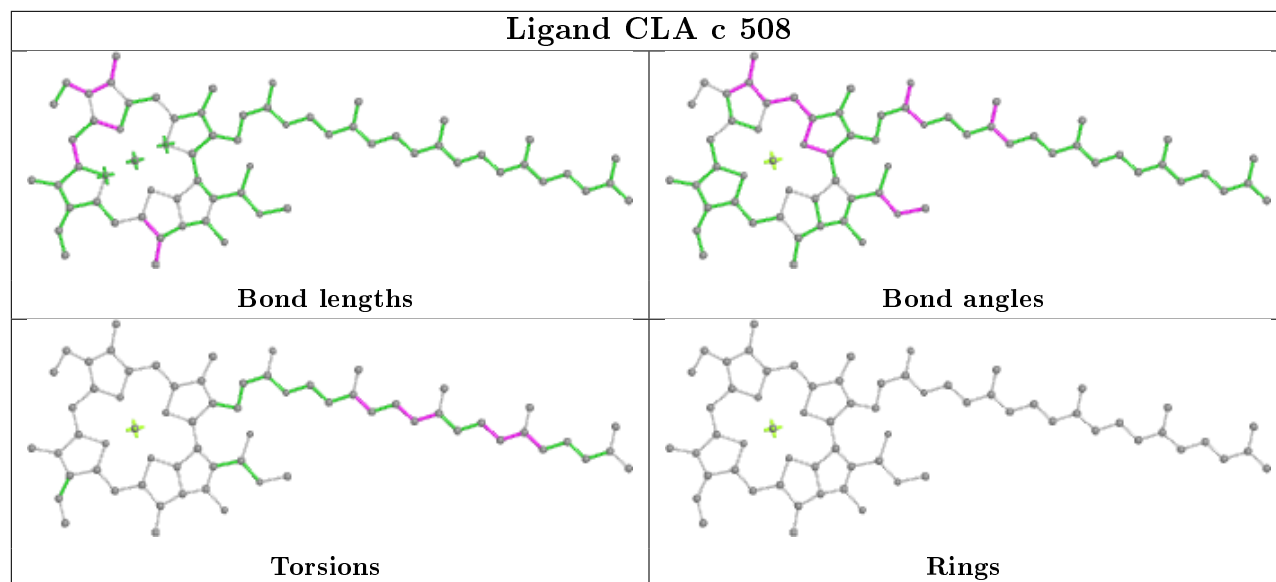
## Ligand CLA C 510



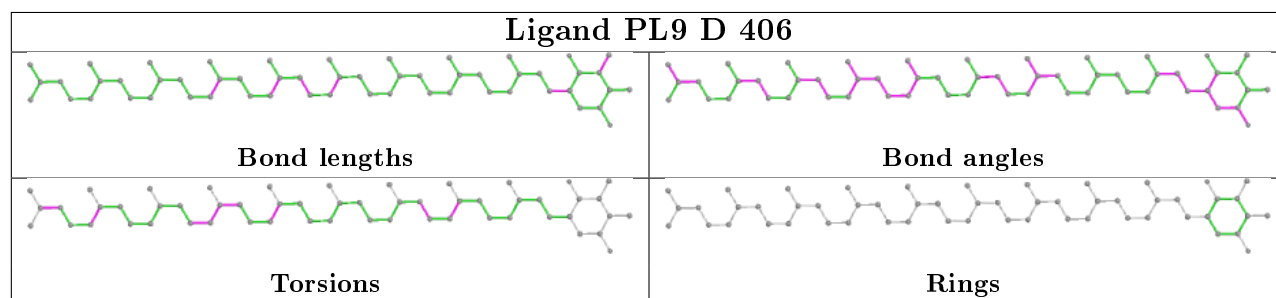
## Ligand STE J 101



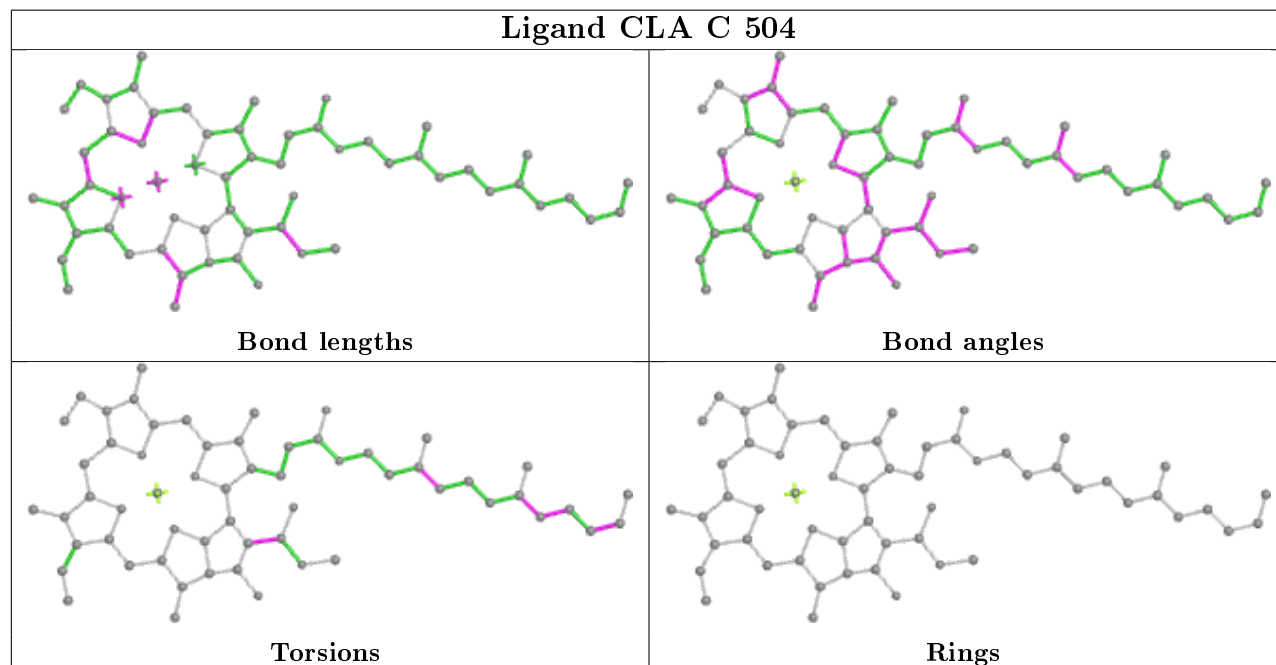
## Ligand CLA c 508

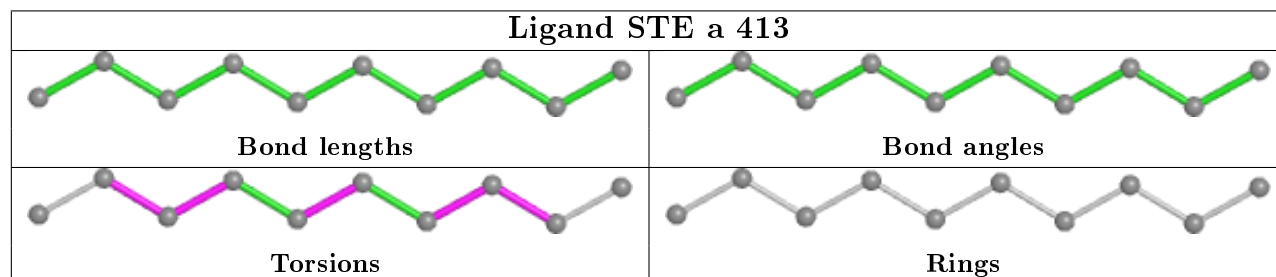
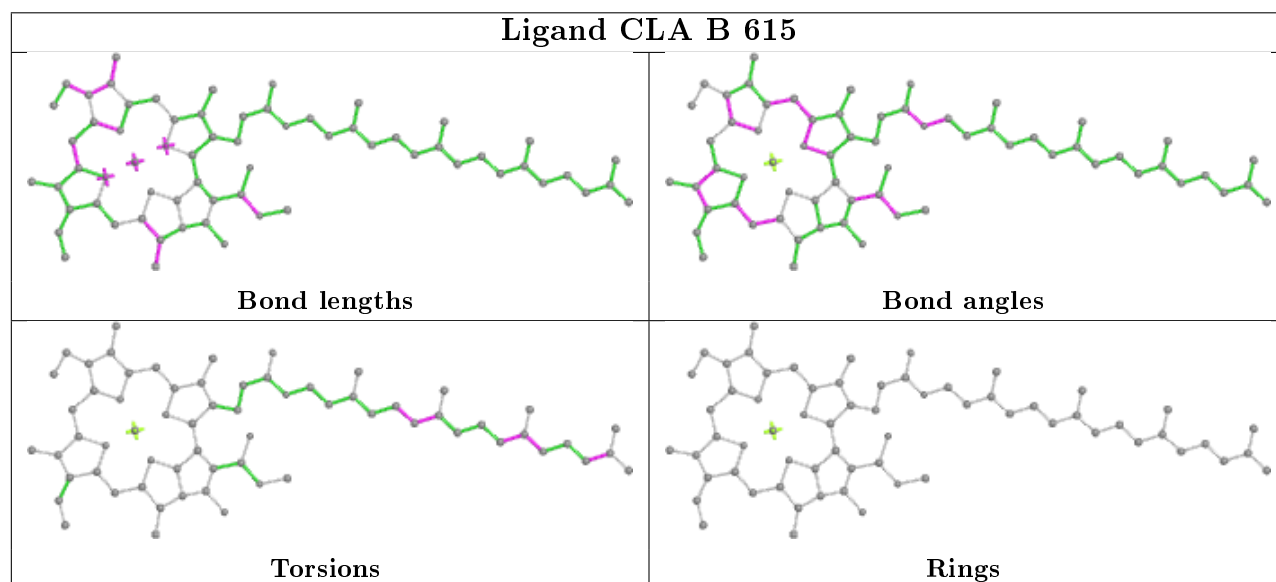
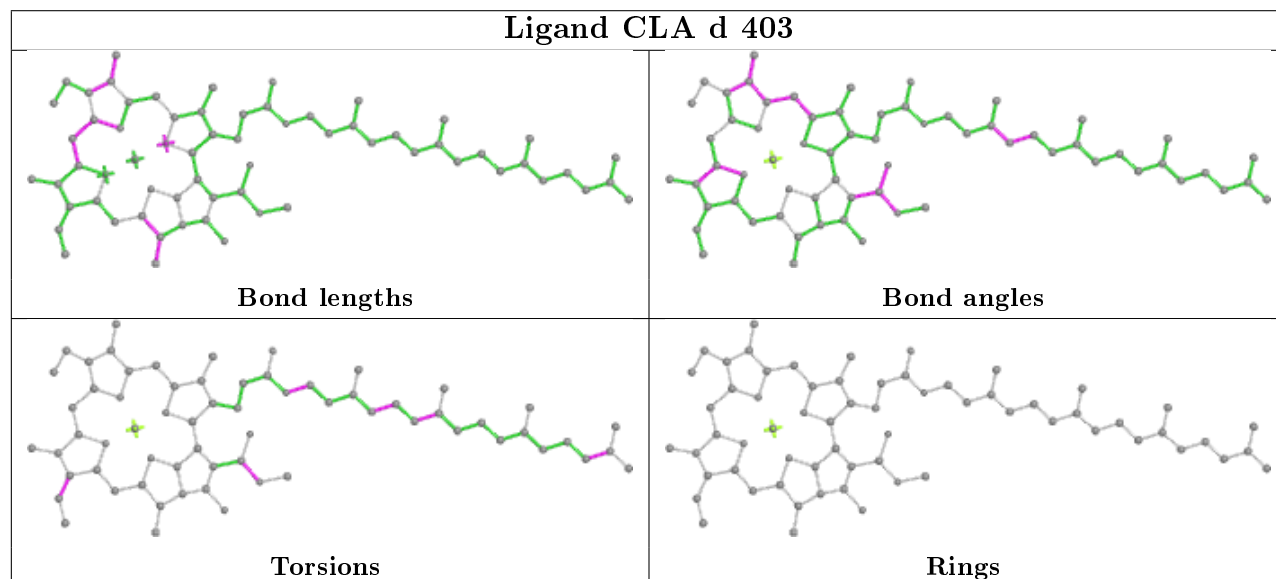
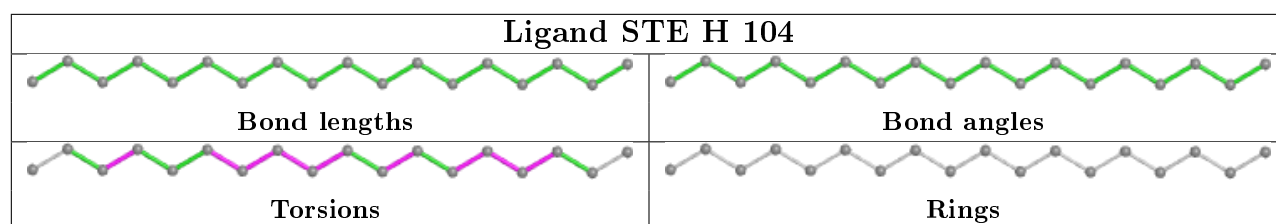


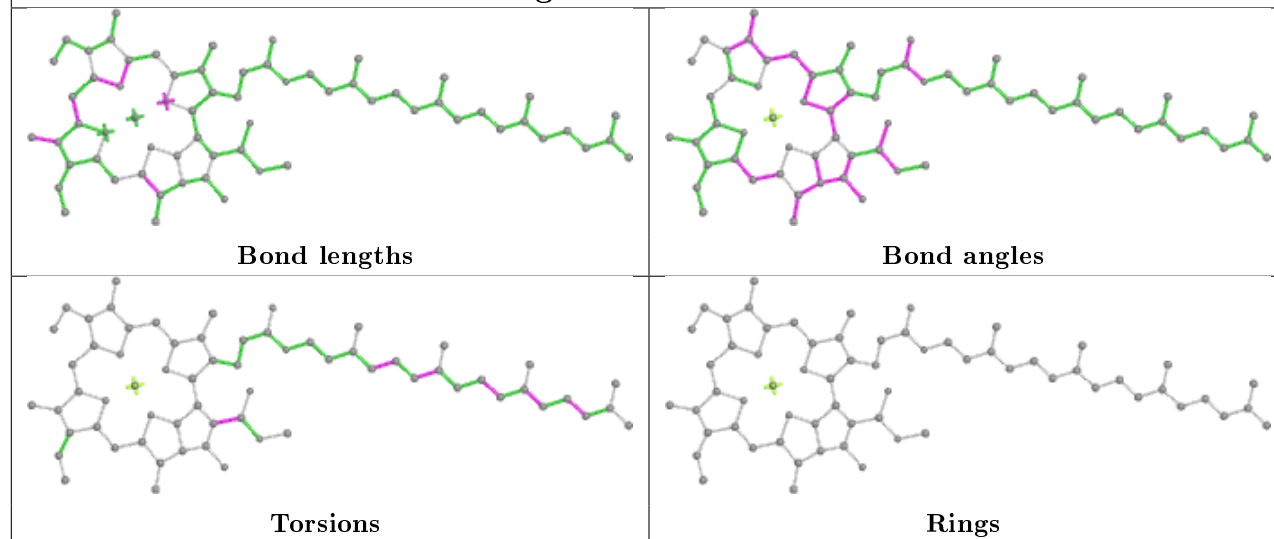
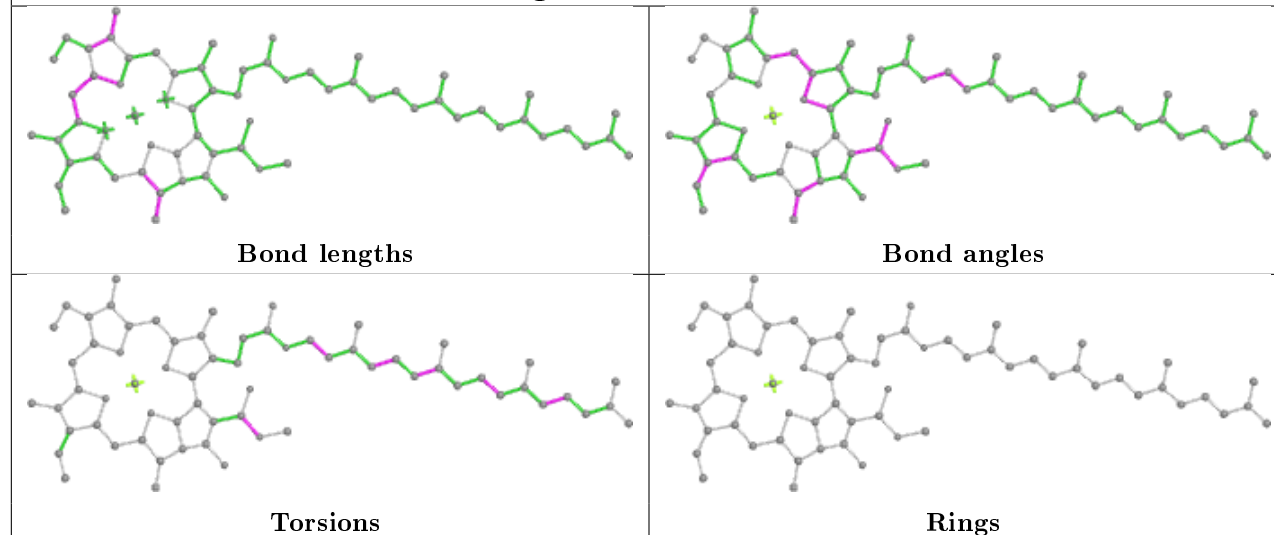
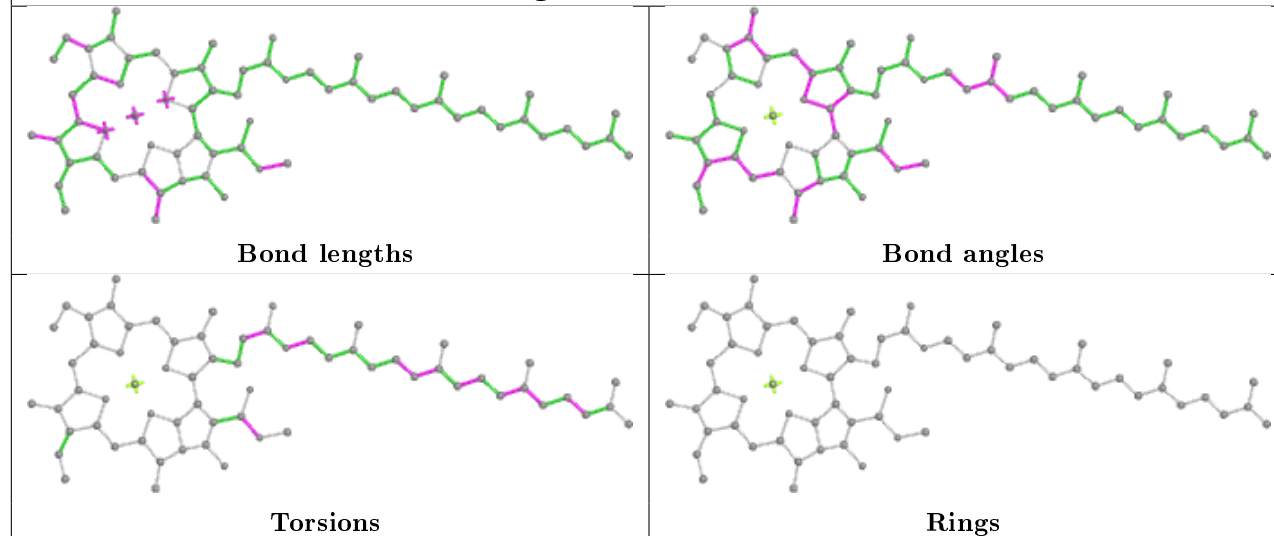
## Ligand PL9 D 406

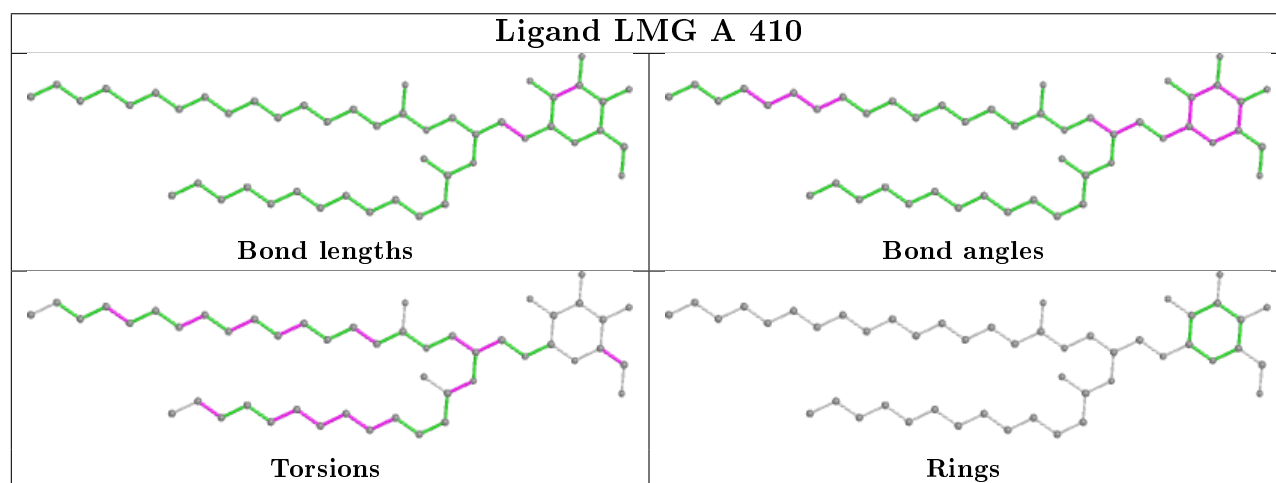
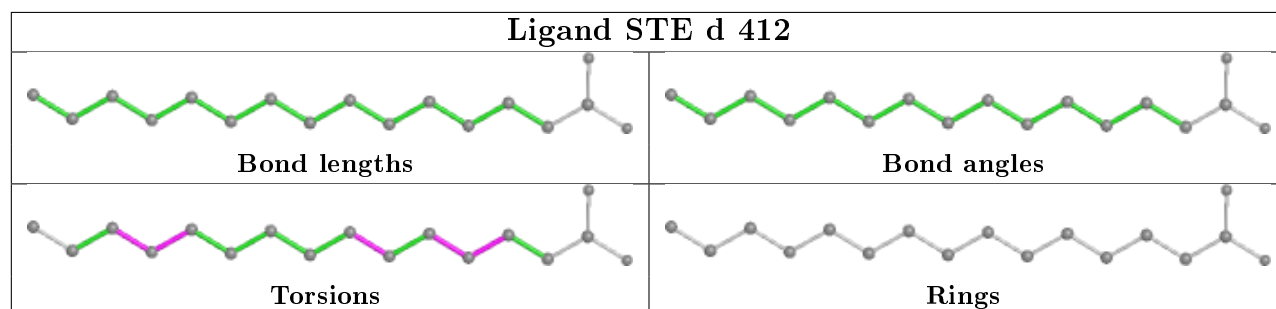
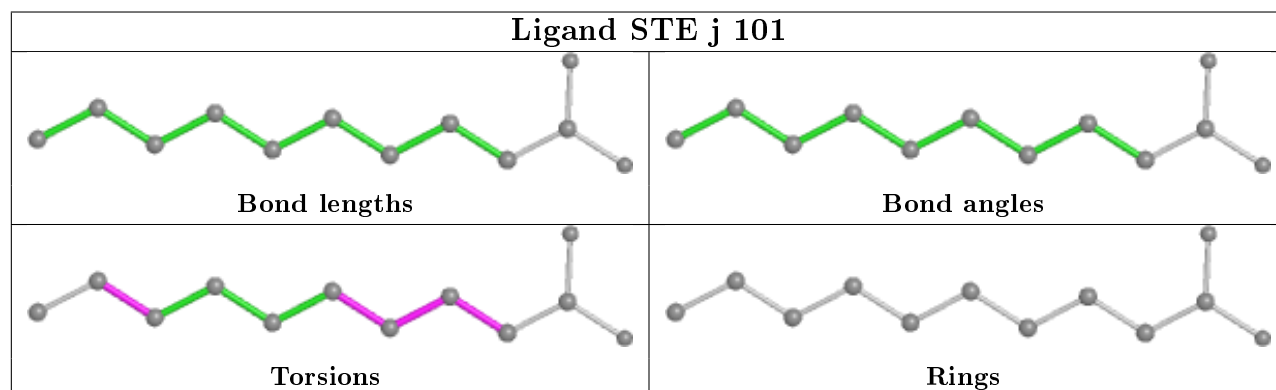
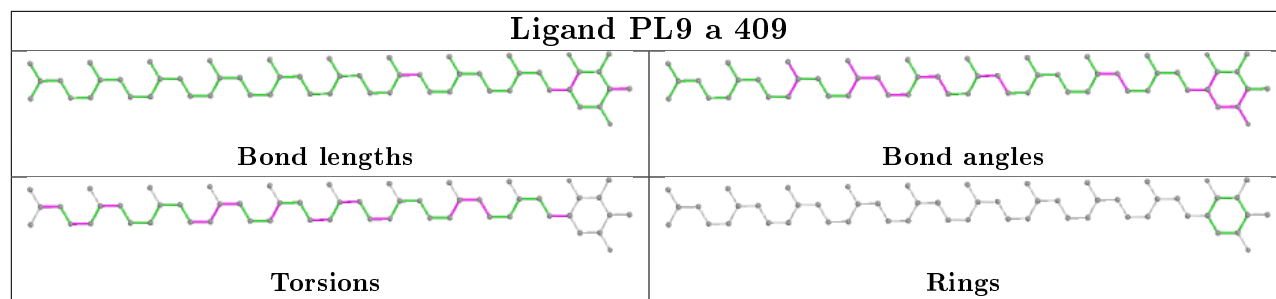


## Ligand CLA C 504

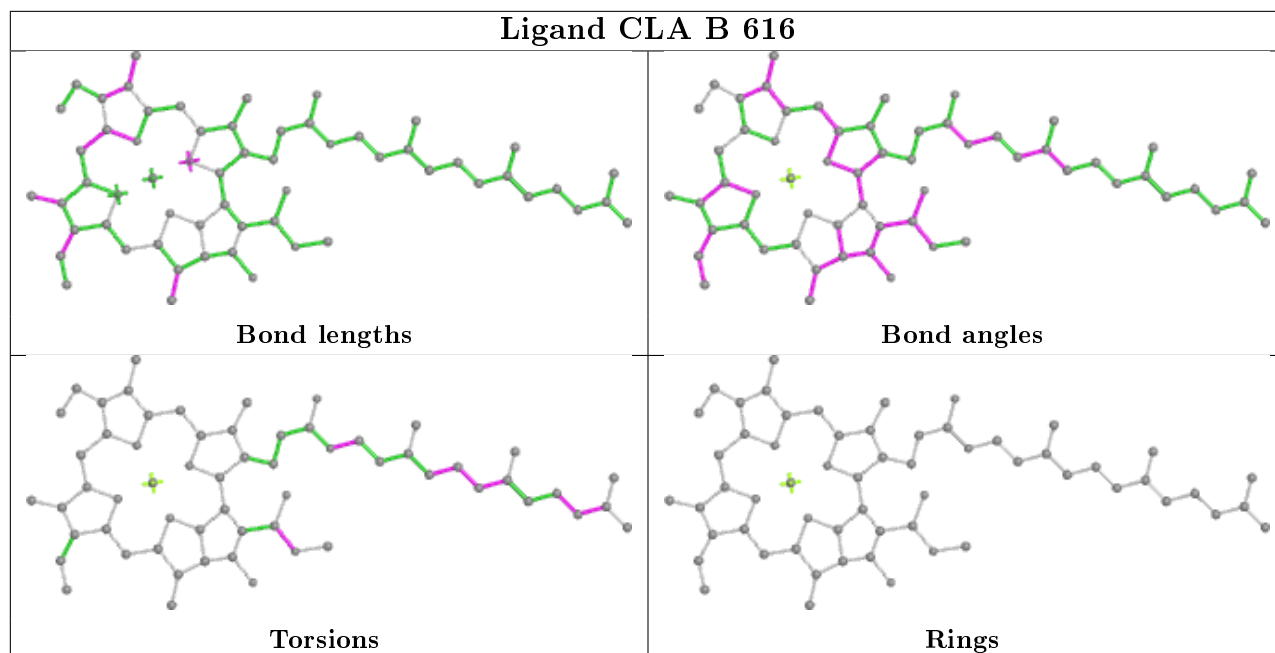




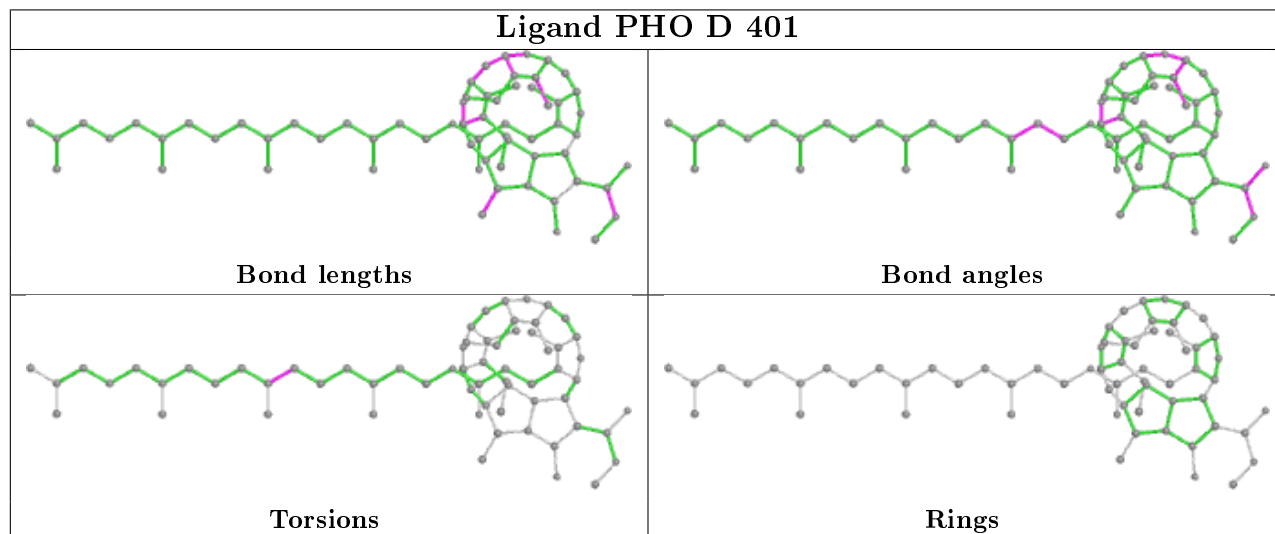
**Ligand CLA b 604****Ligand CLA D 405****Ligand CLA B 613**



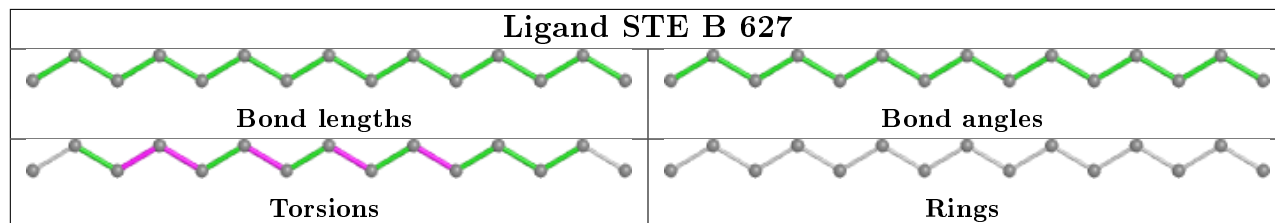
## Ligand CLA B 616

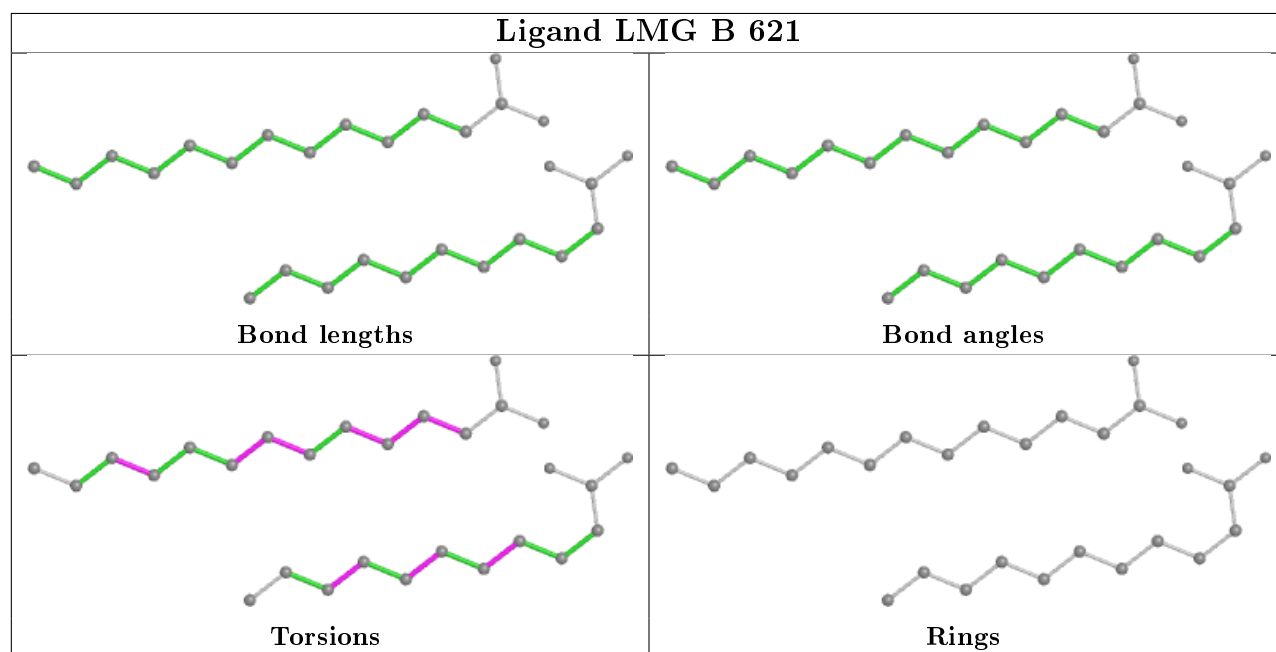
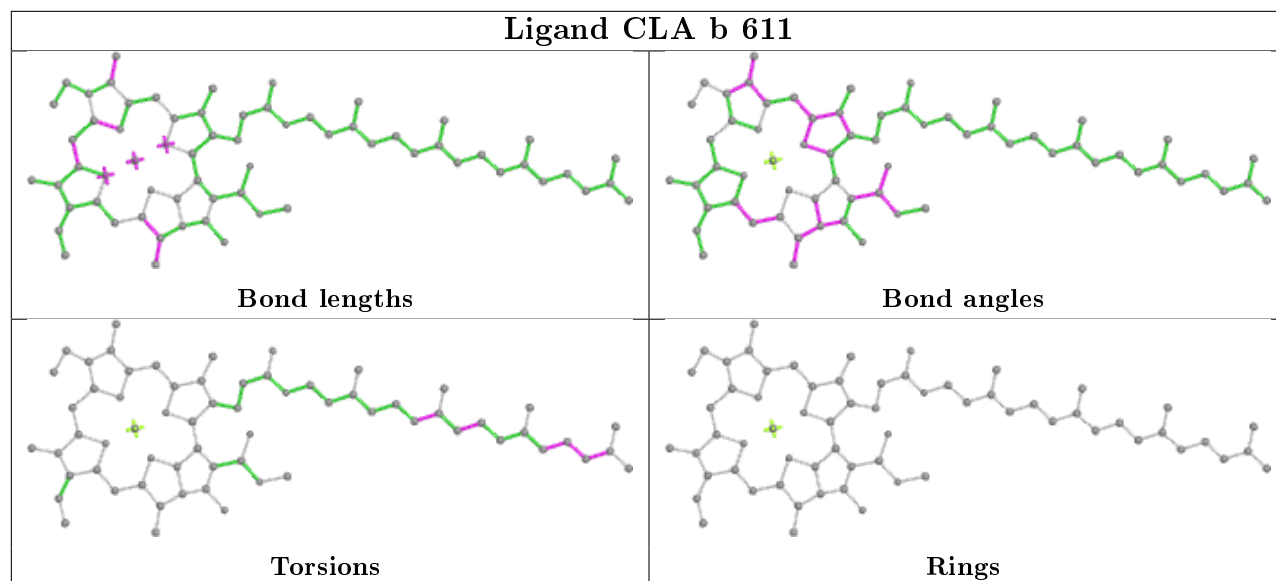
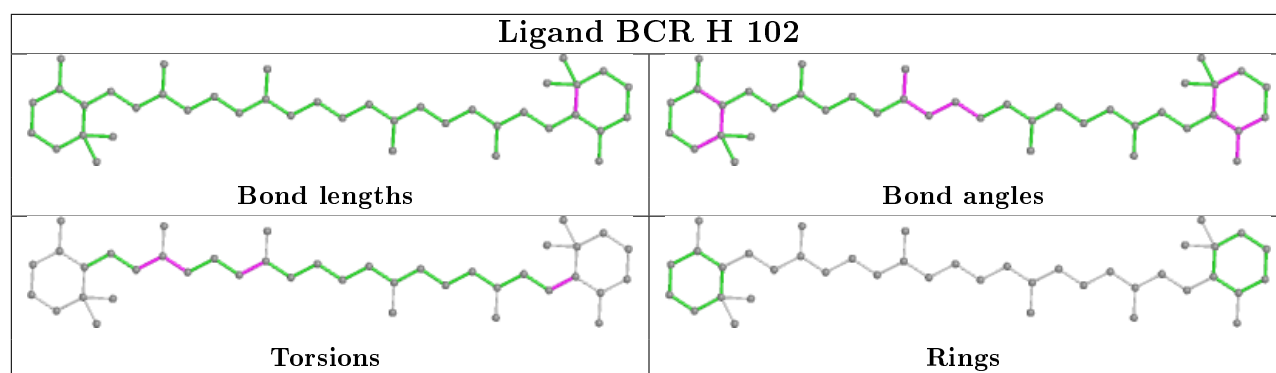


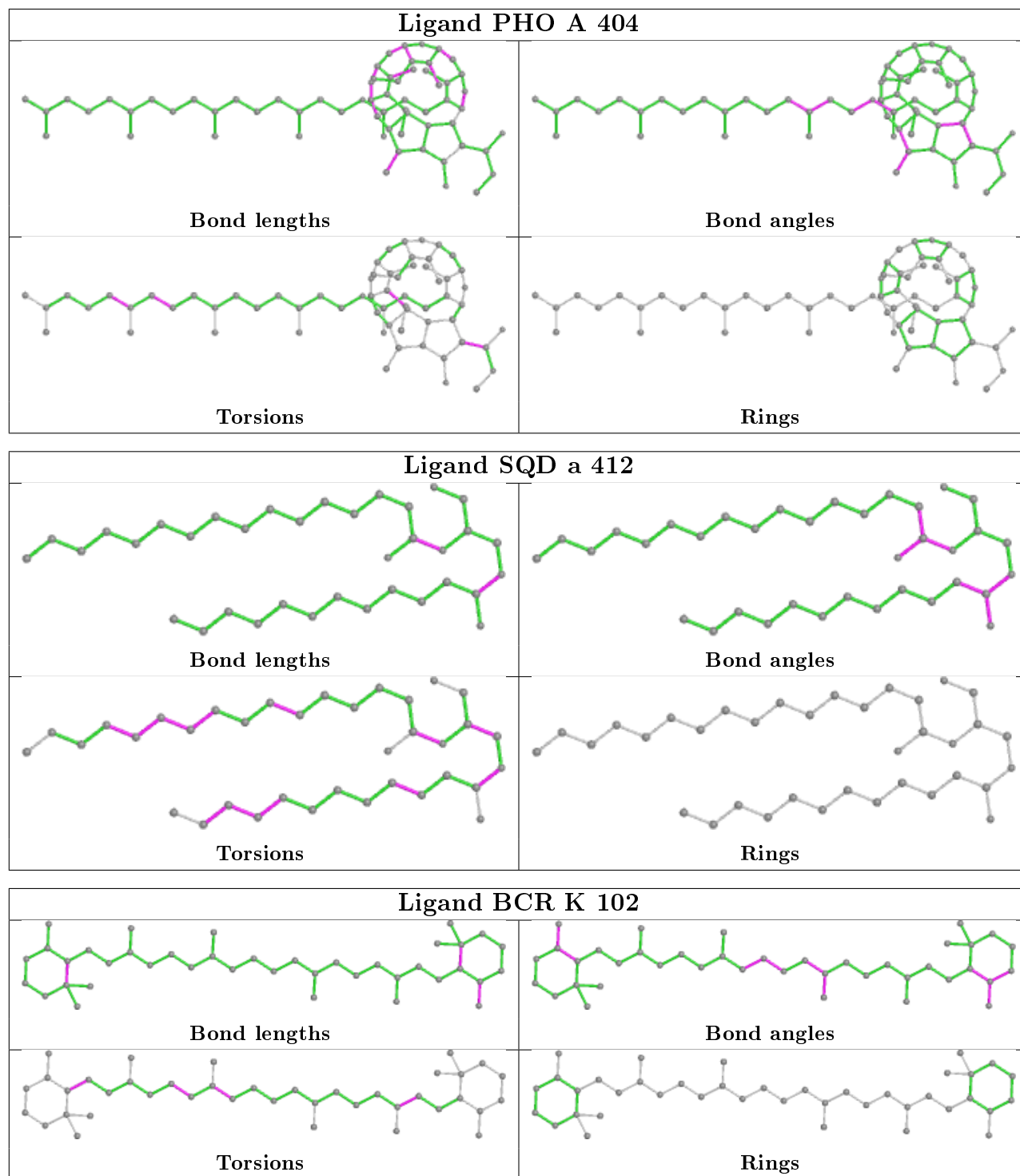
## Ligand PHO D 401



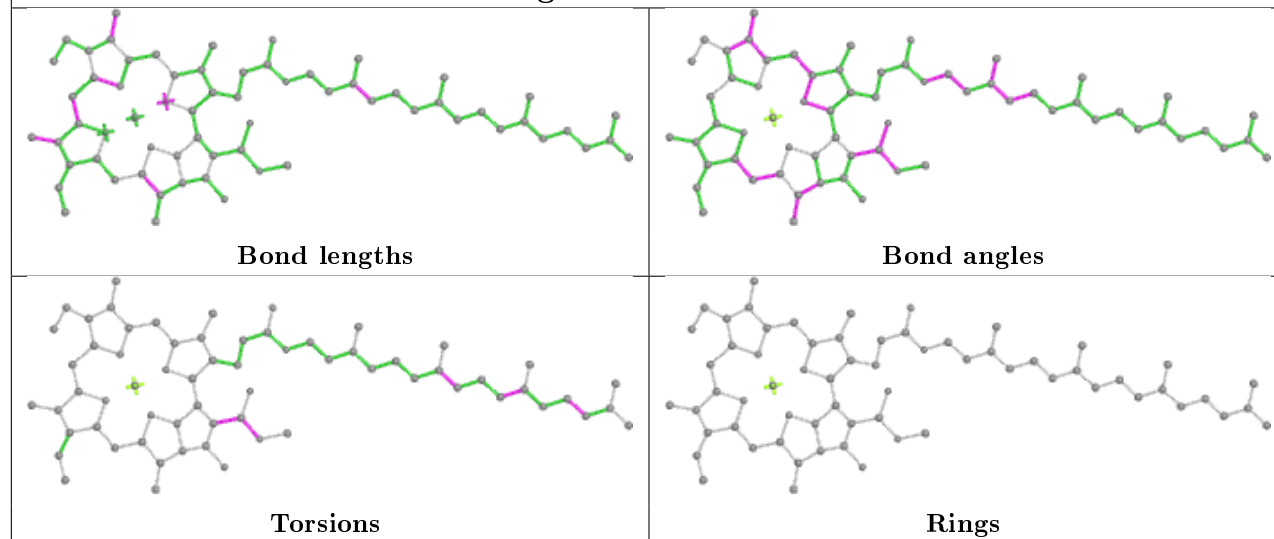
## Ligand STE B 627



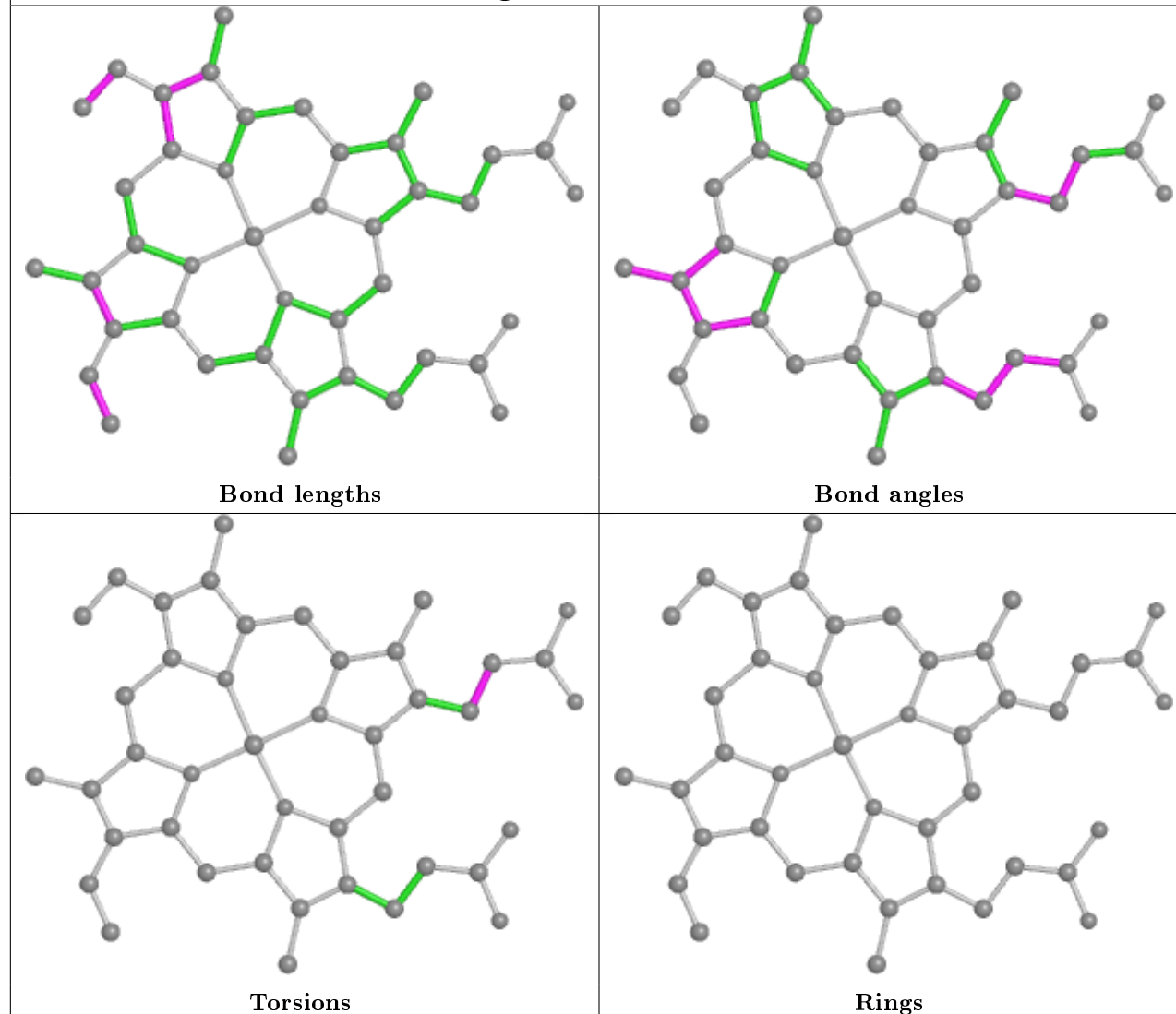


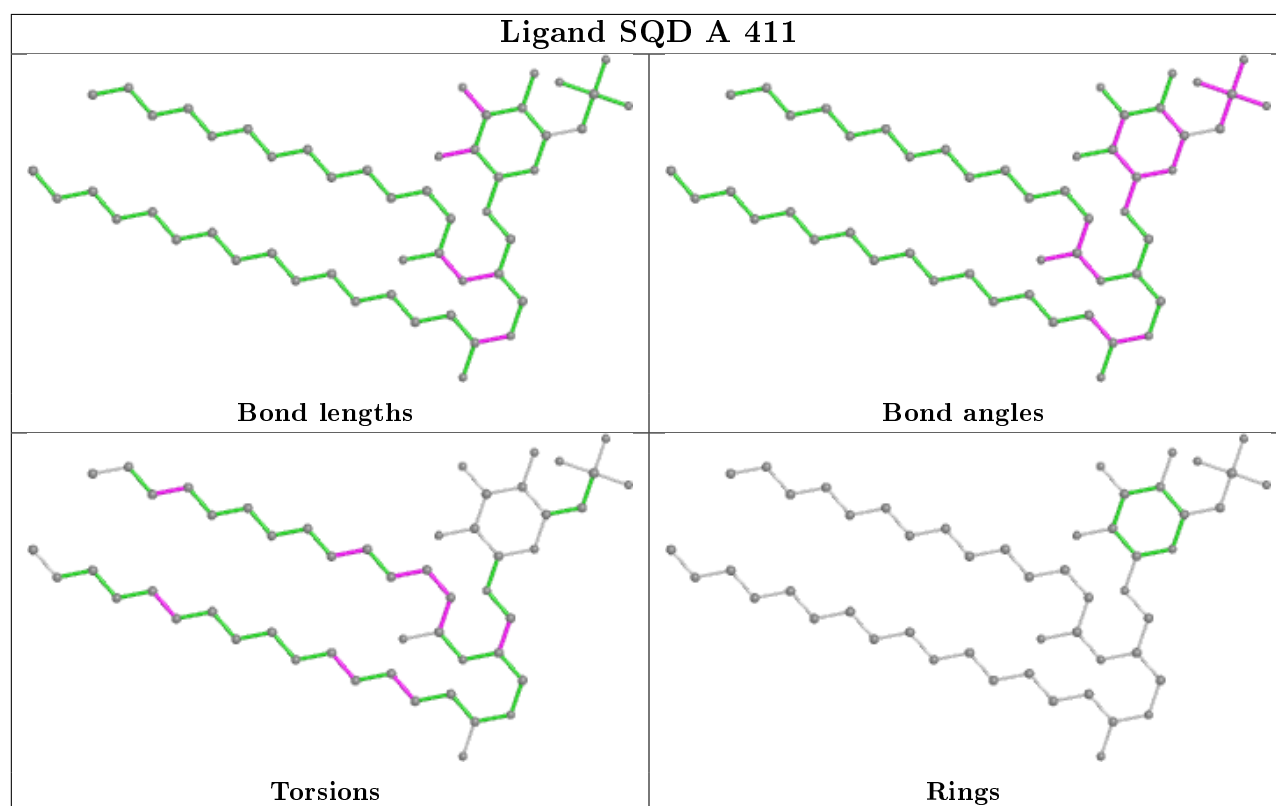
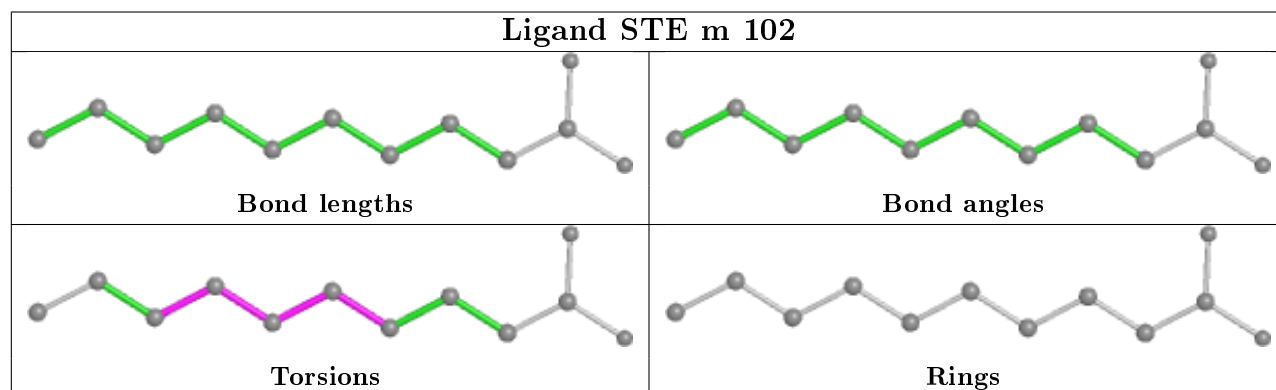
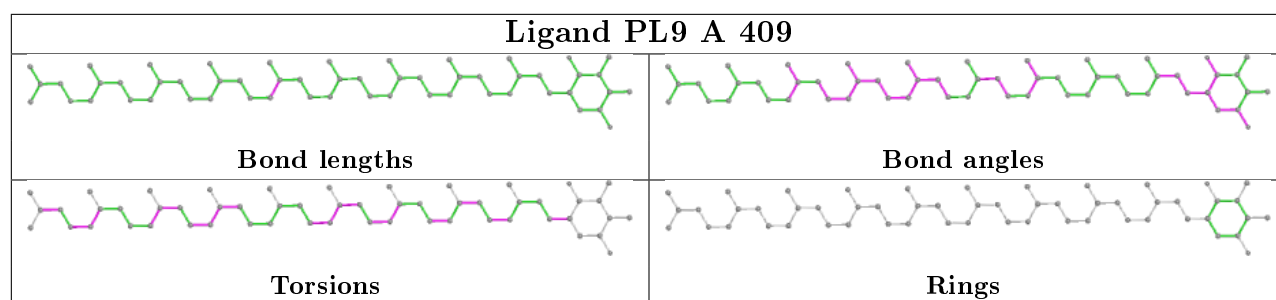


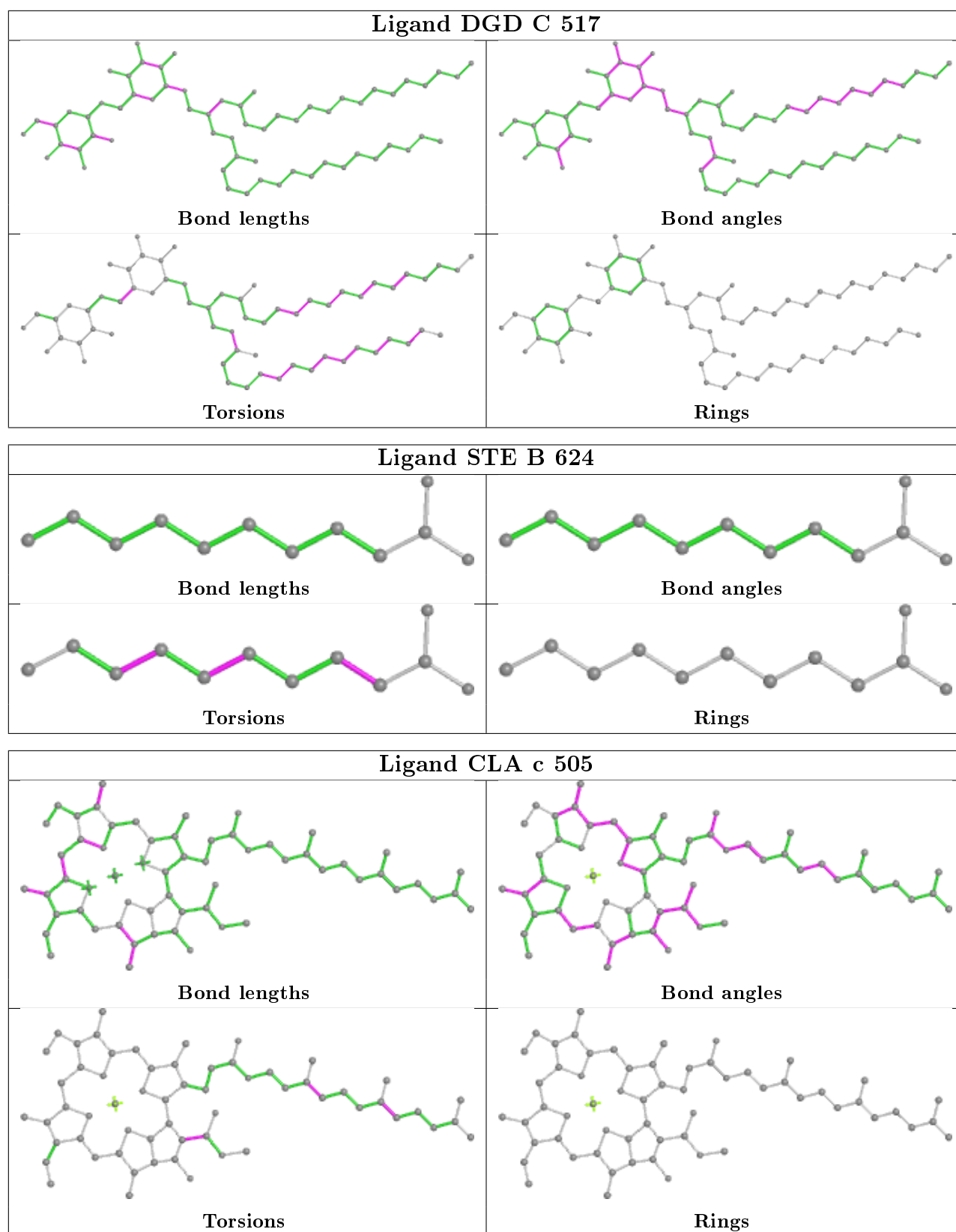
## Ligand CLA c 511

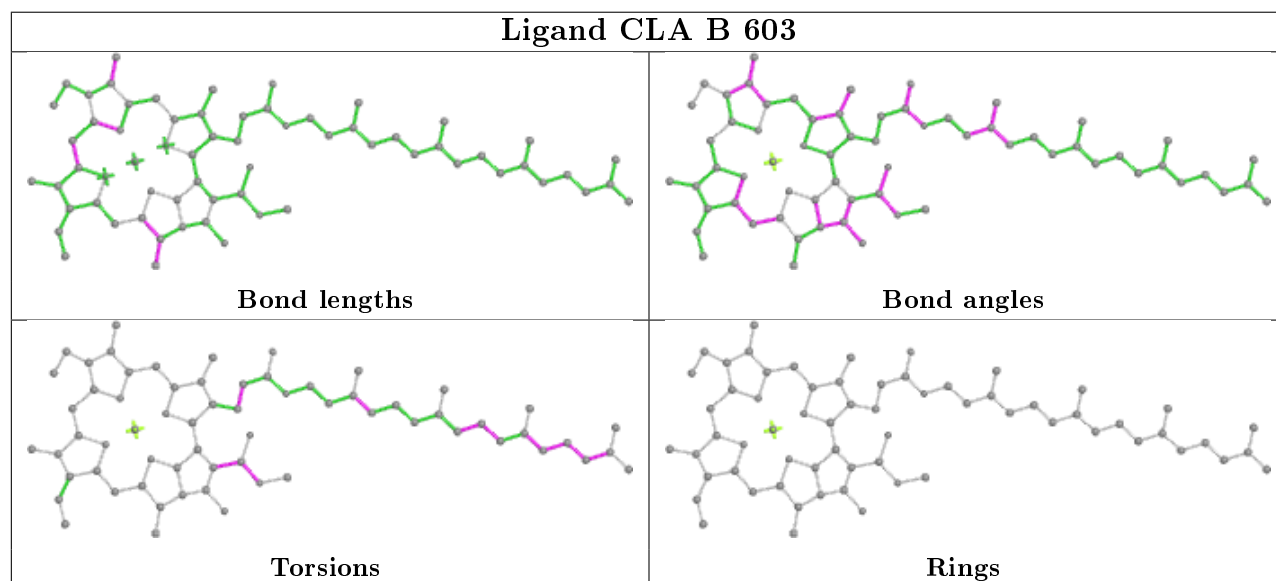
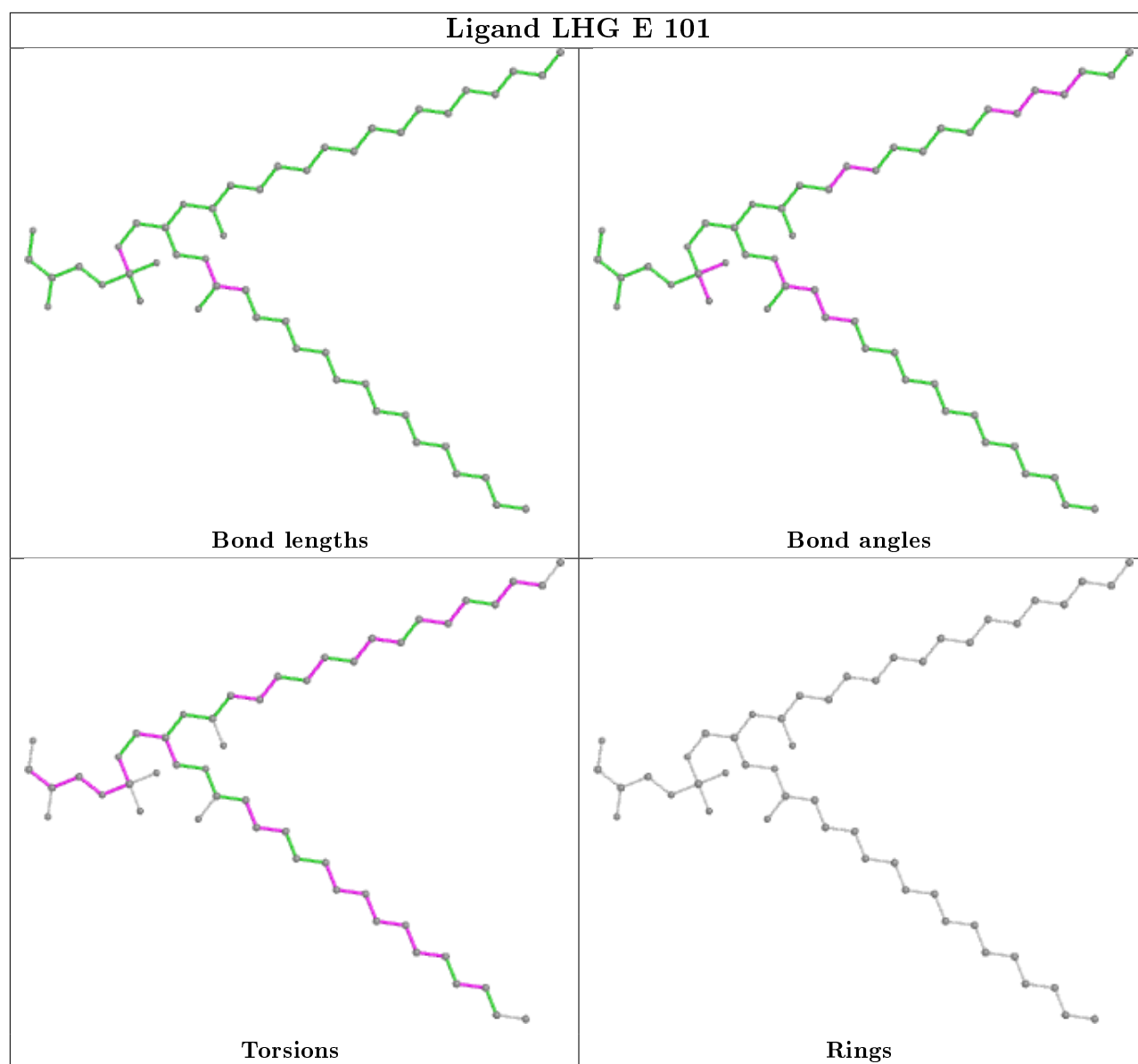


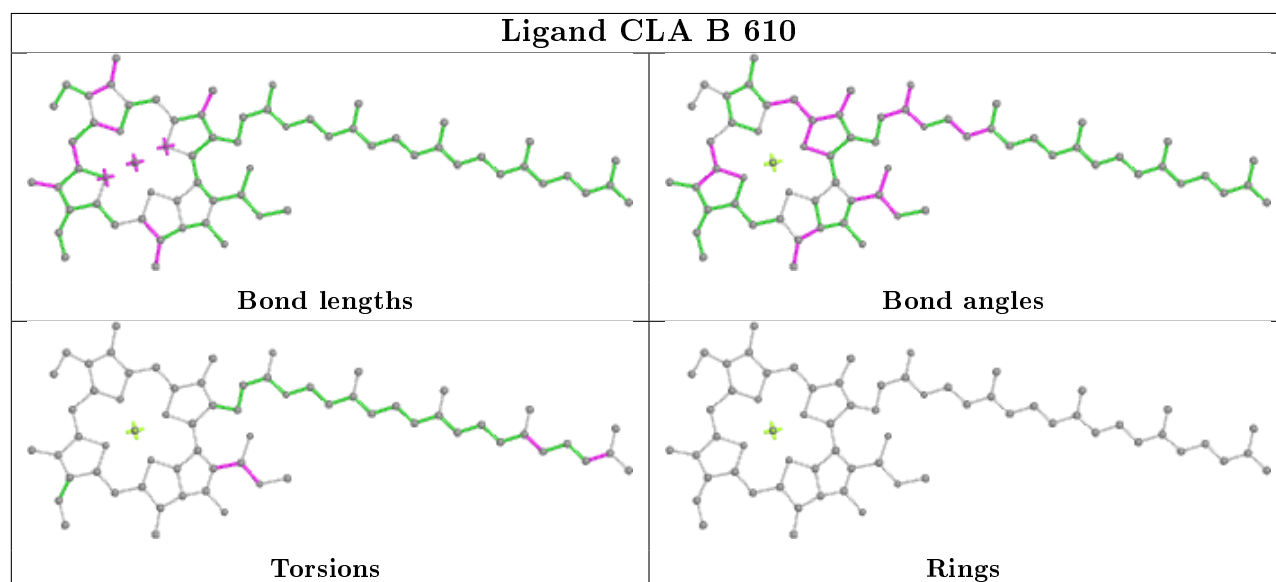
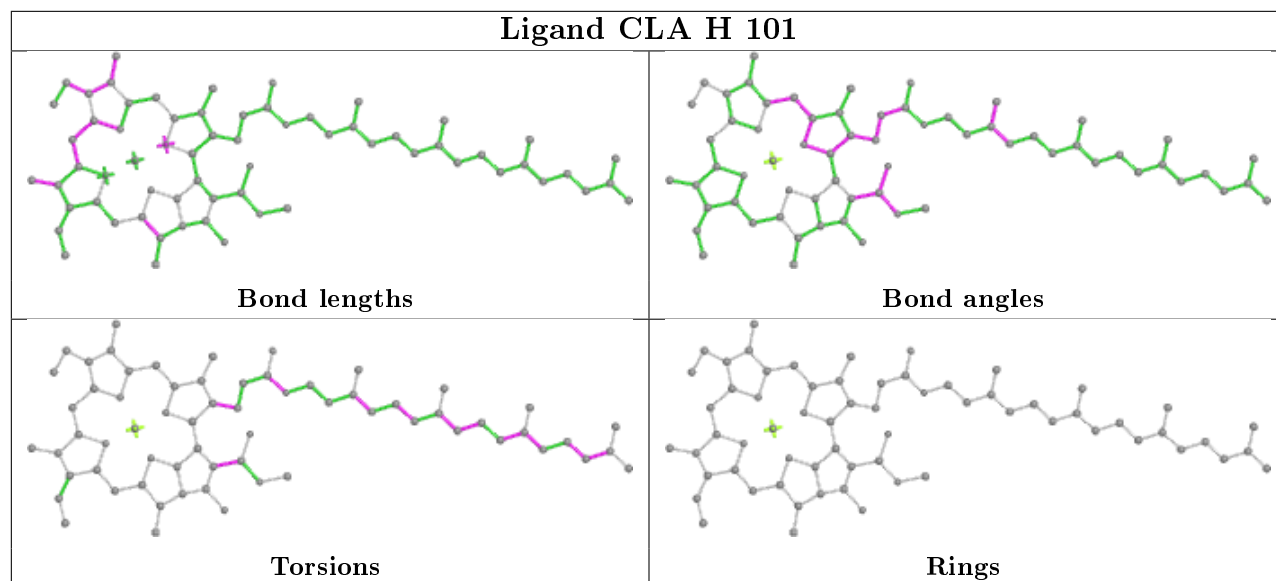
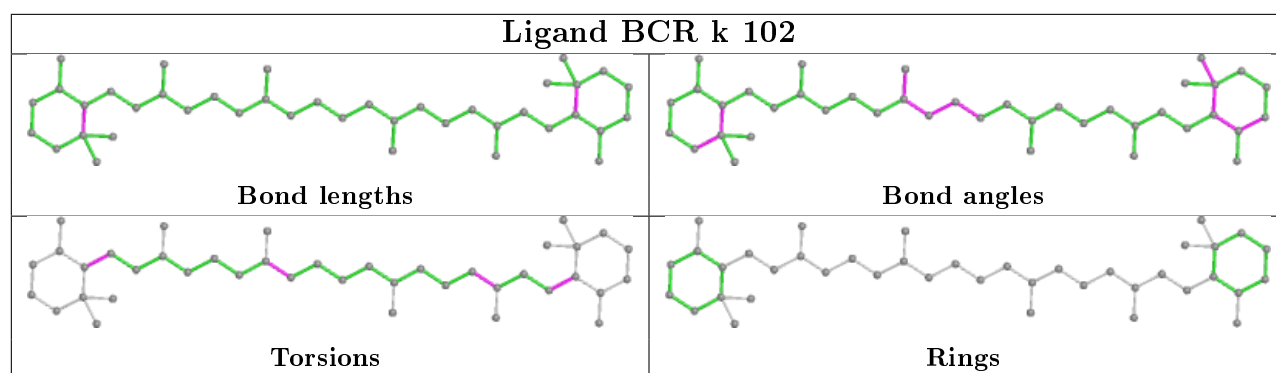
## Ligand HEC f 101



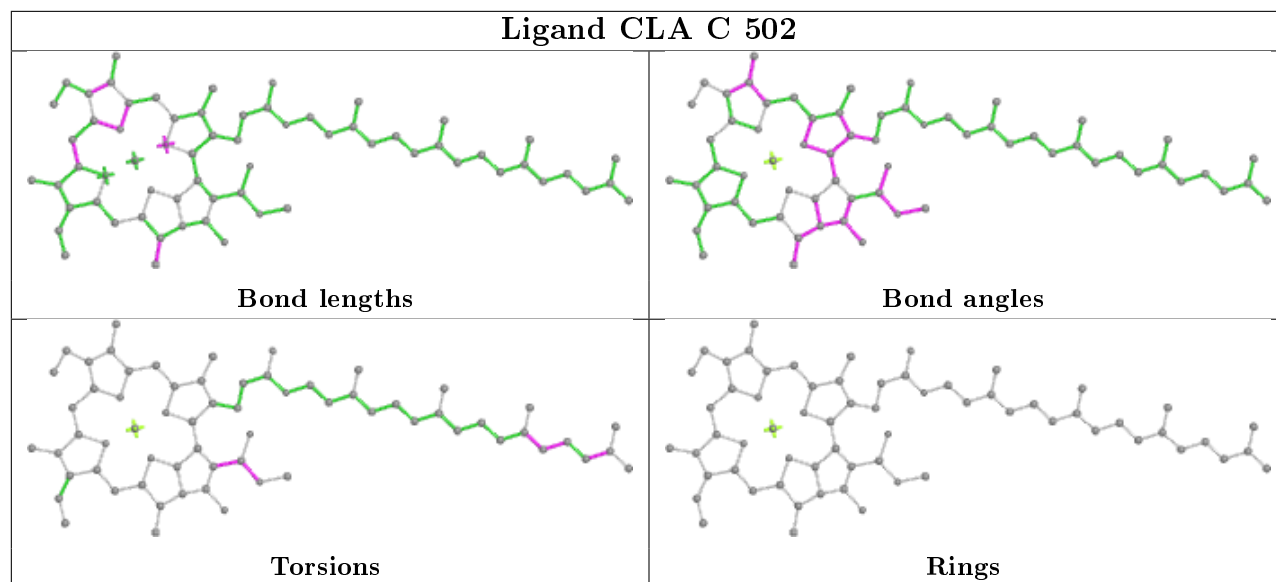




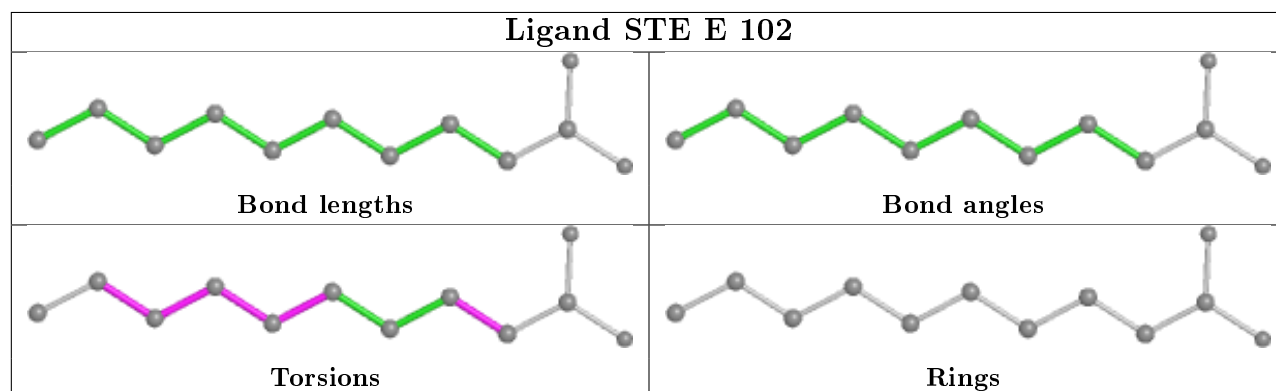




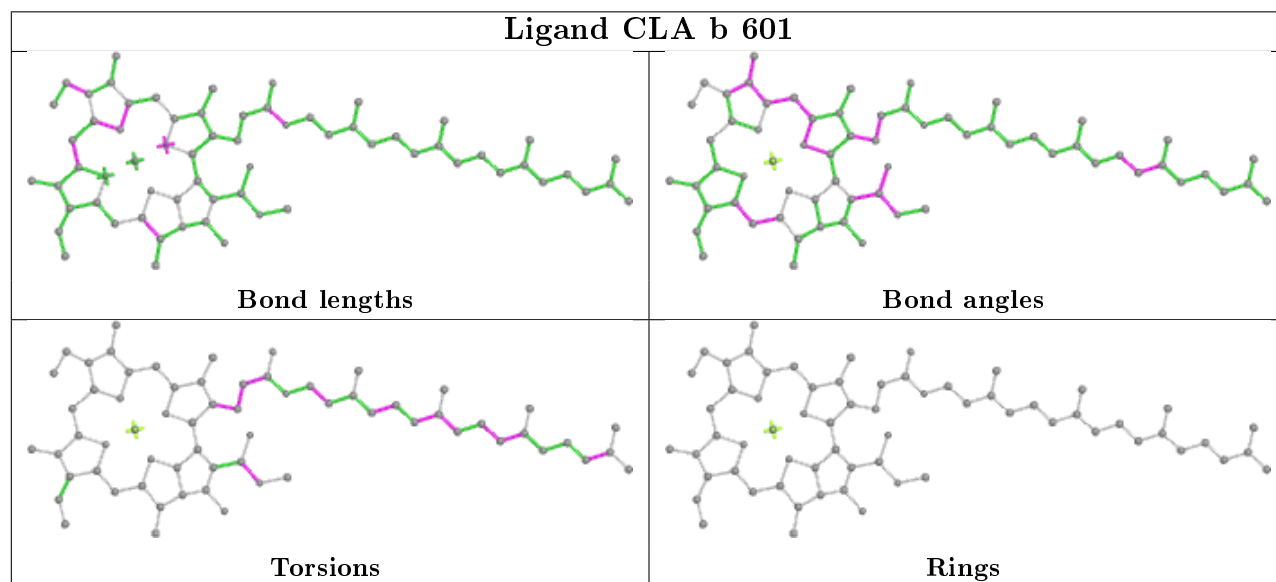
## Ligand CLA C 502

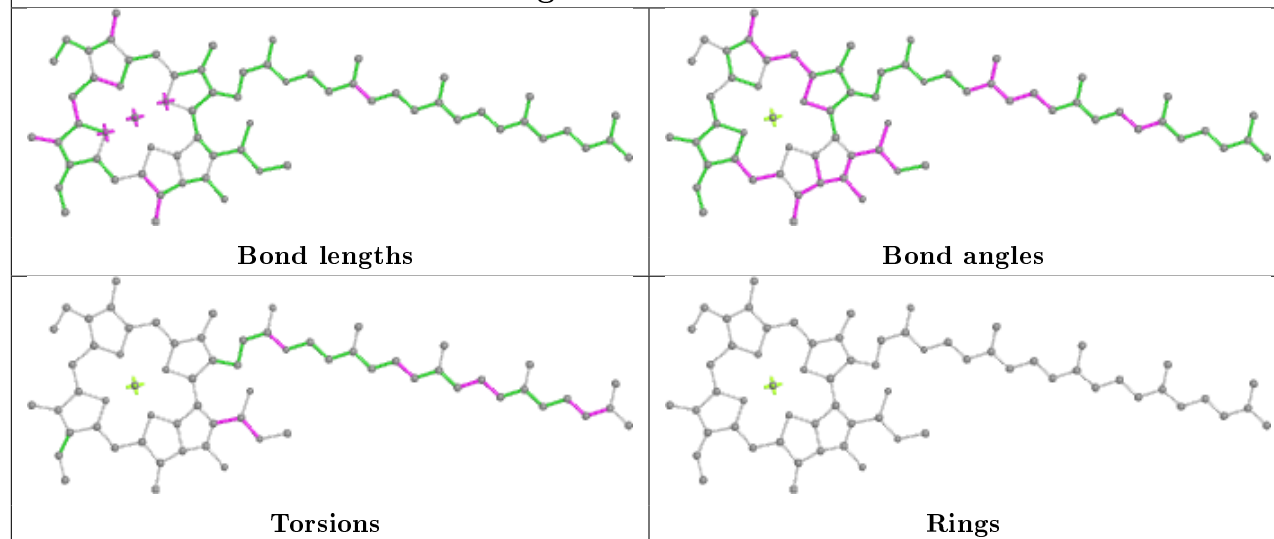
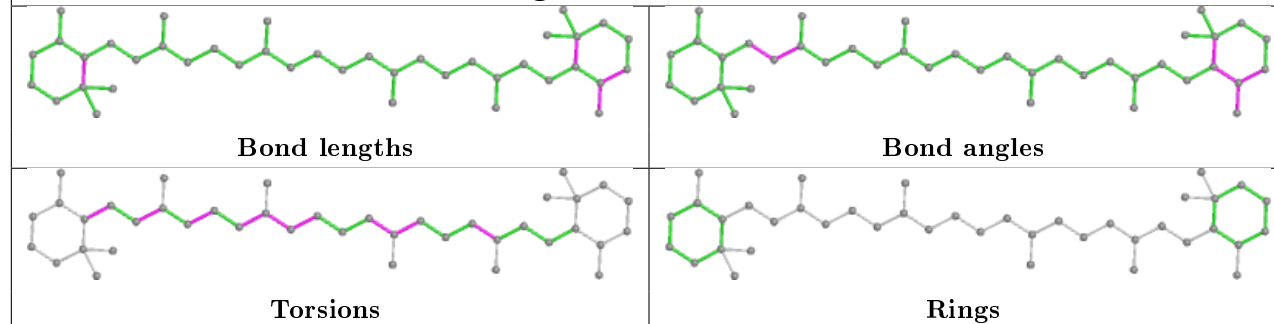
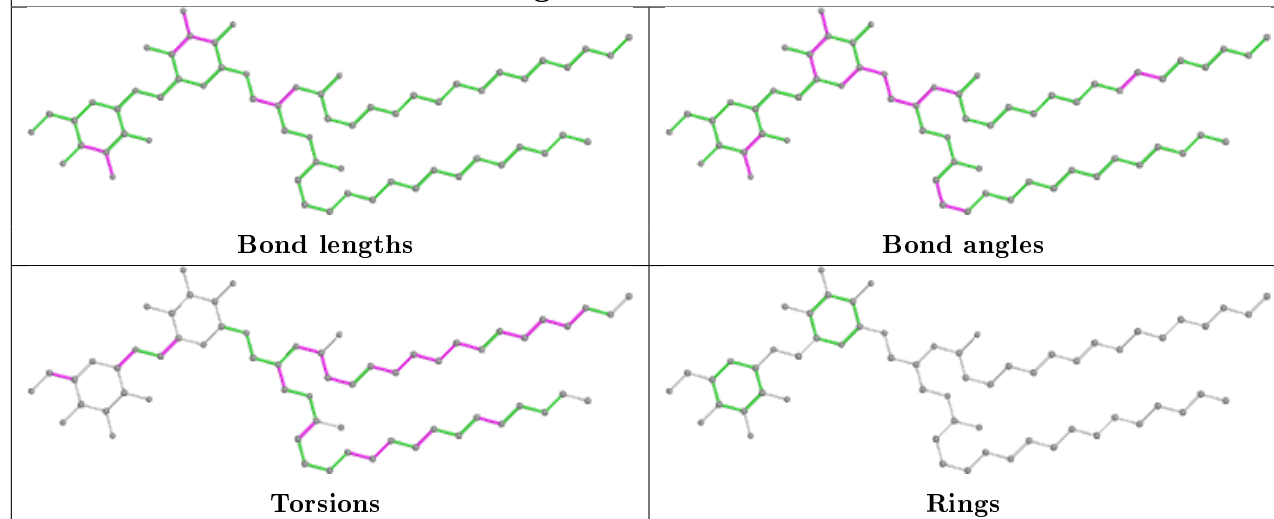


## Ligand STE E 102

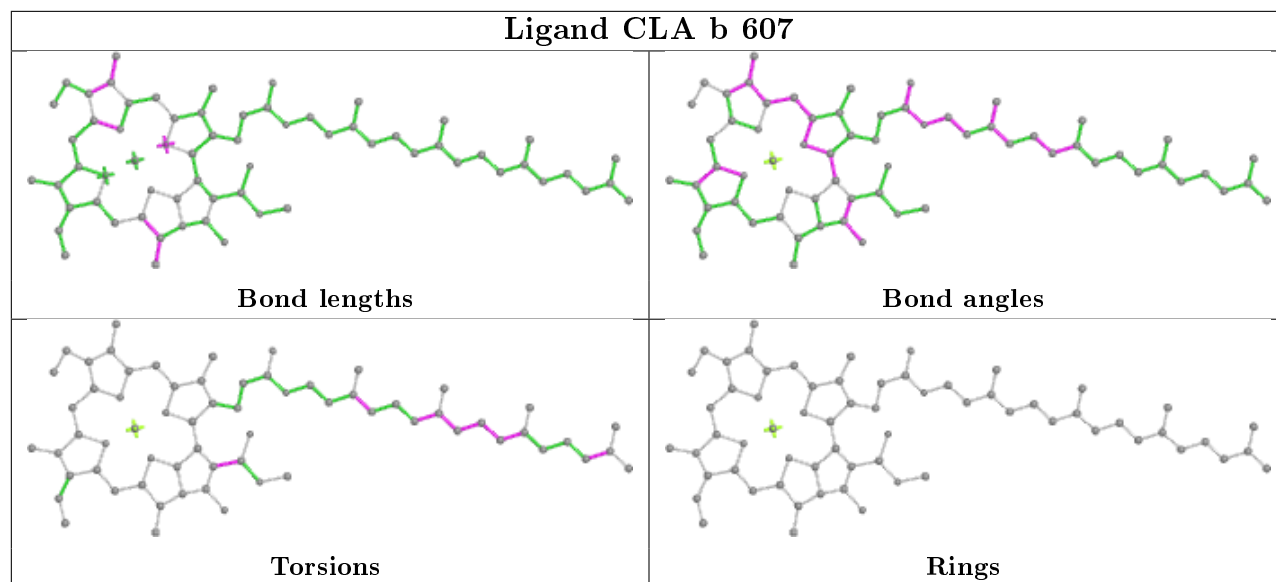


## Ligand CLA b 601

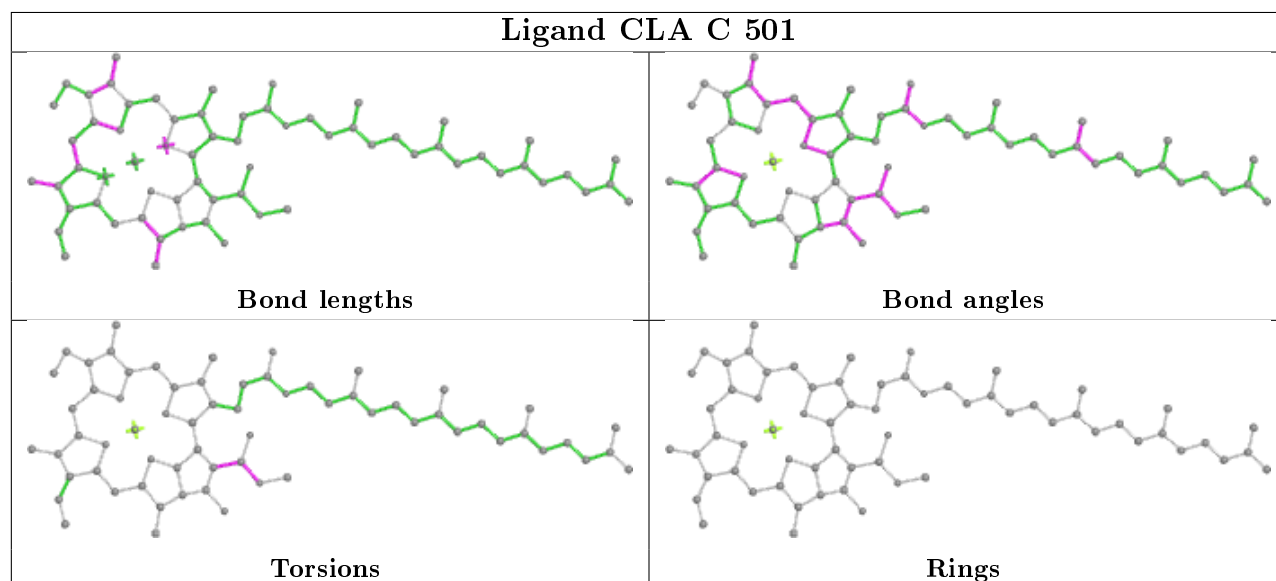


**Ligand CLA c 504****Ligand BCR T 101****Ligand DGD c 517**

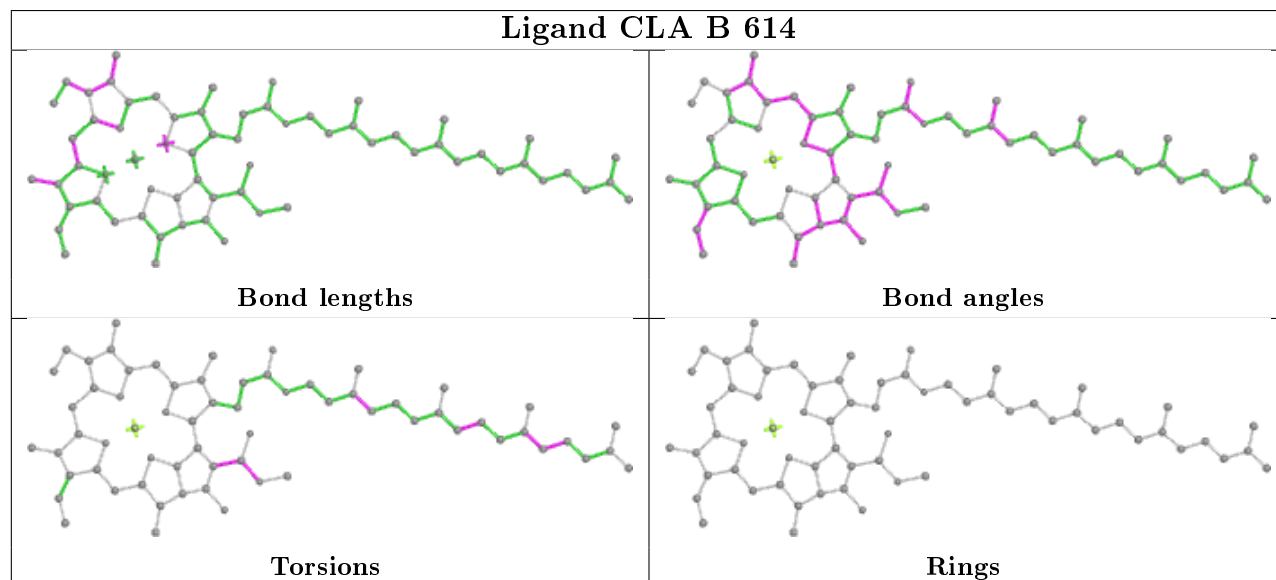
## Ligand CLA b 607

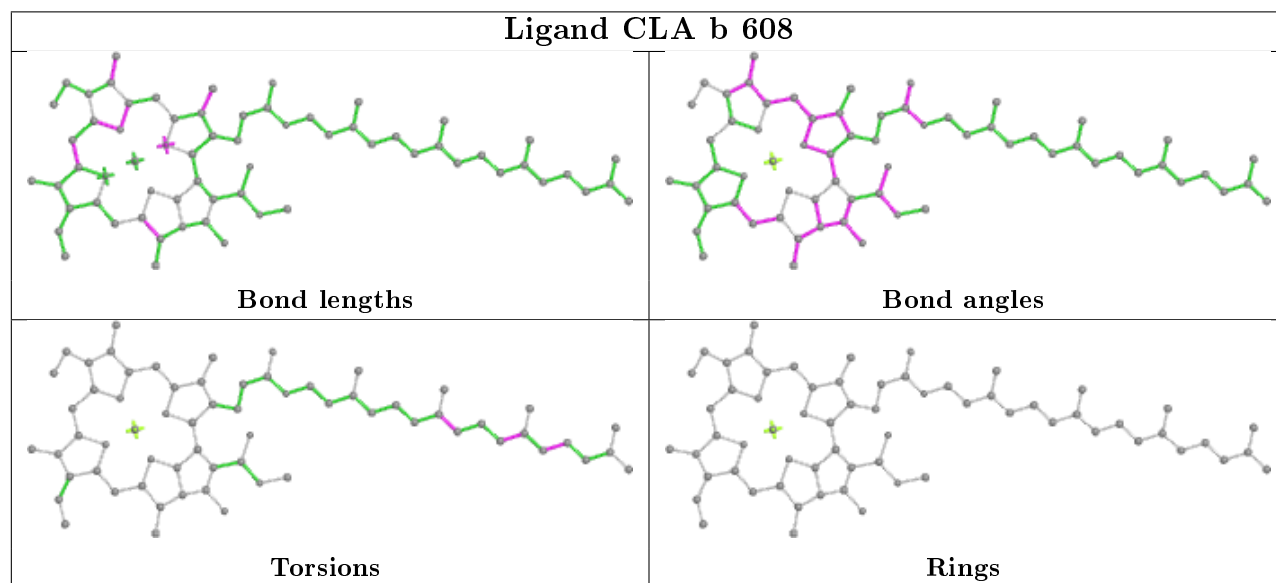
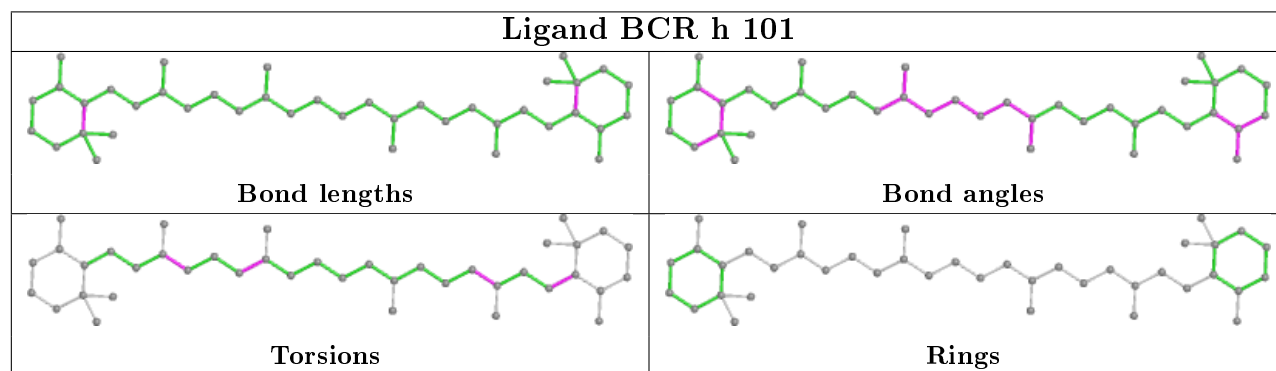
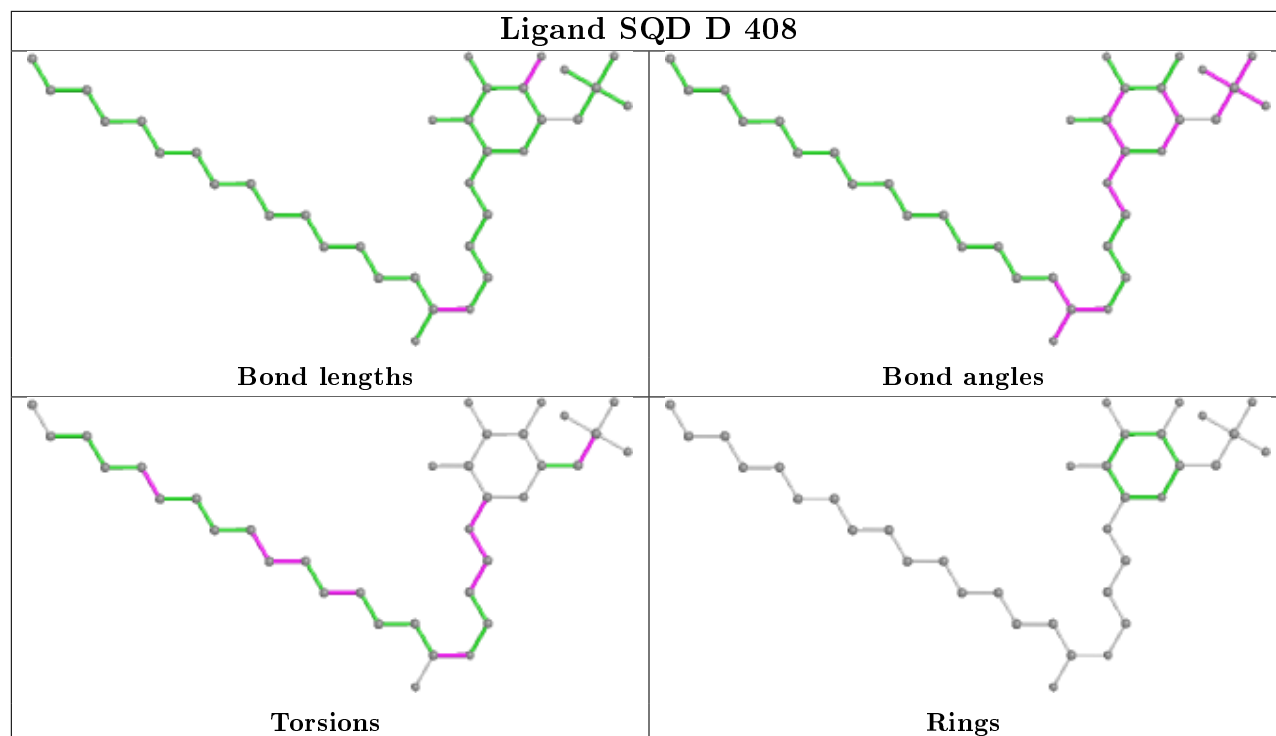


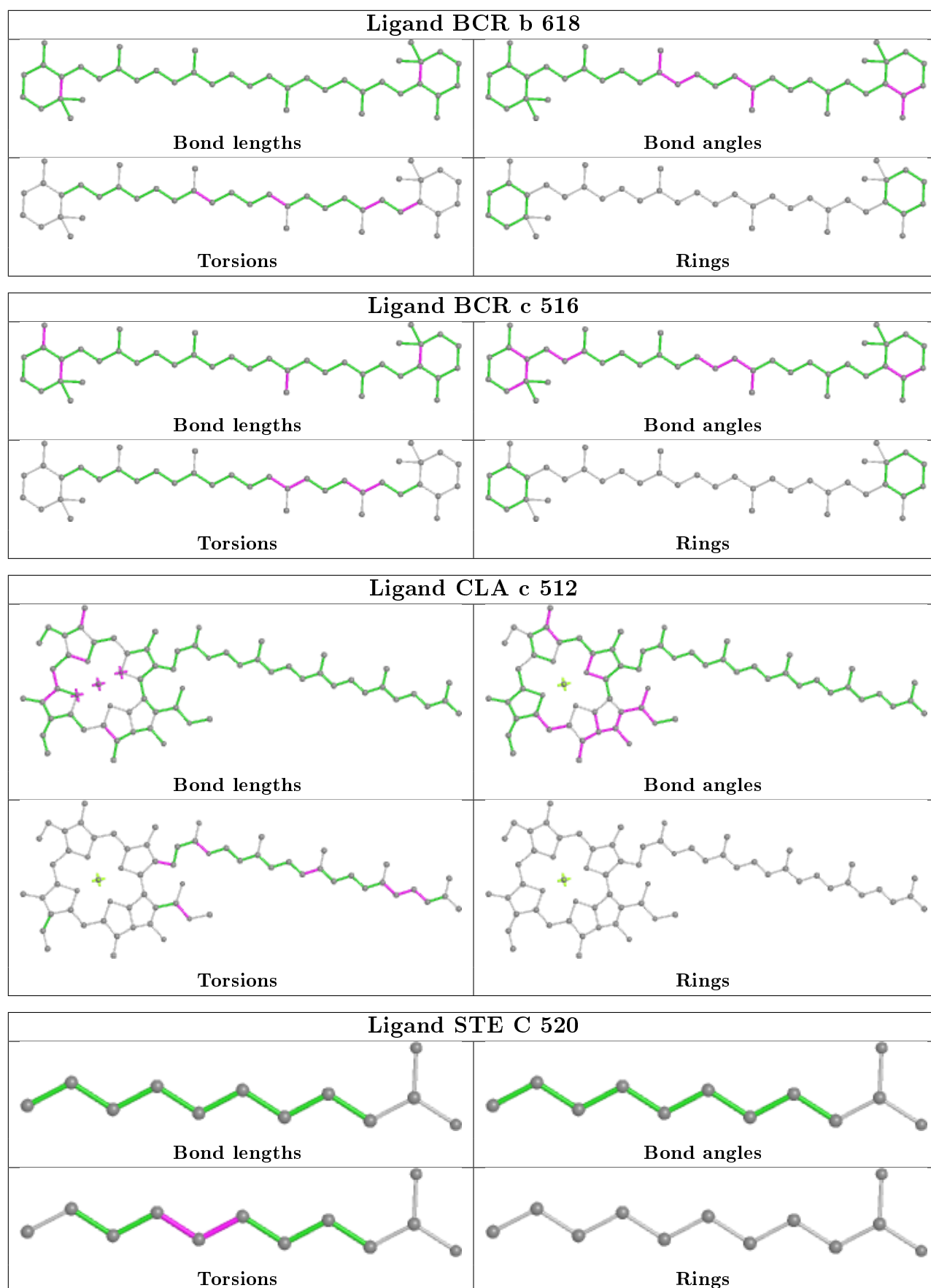
## Ligand CLA C 501

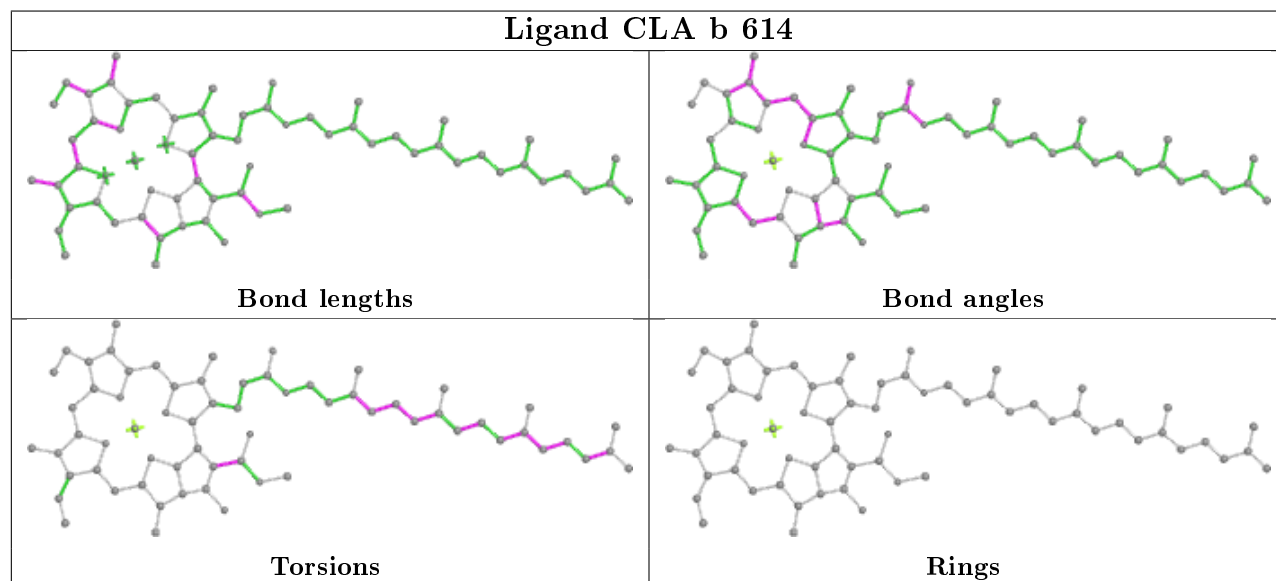
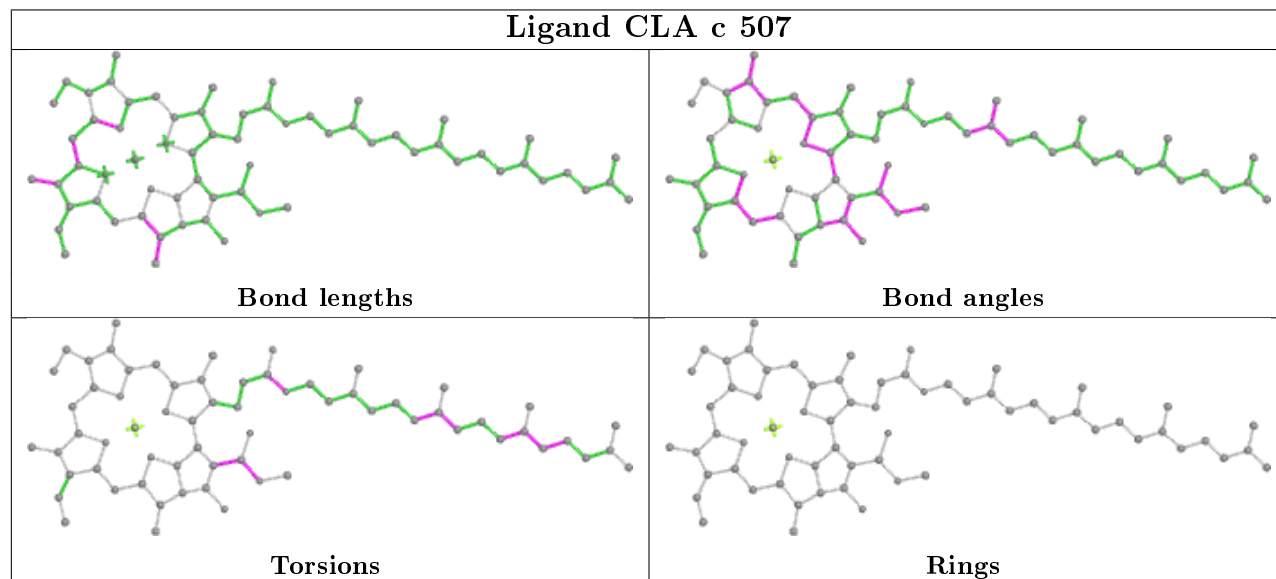
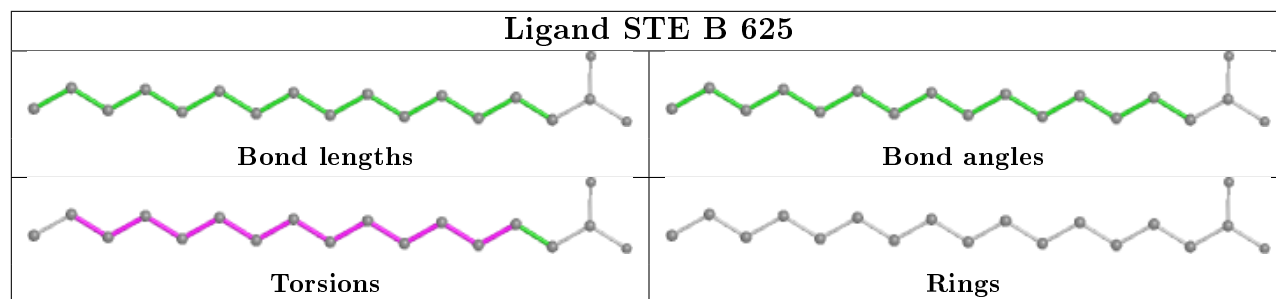


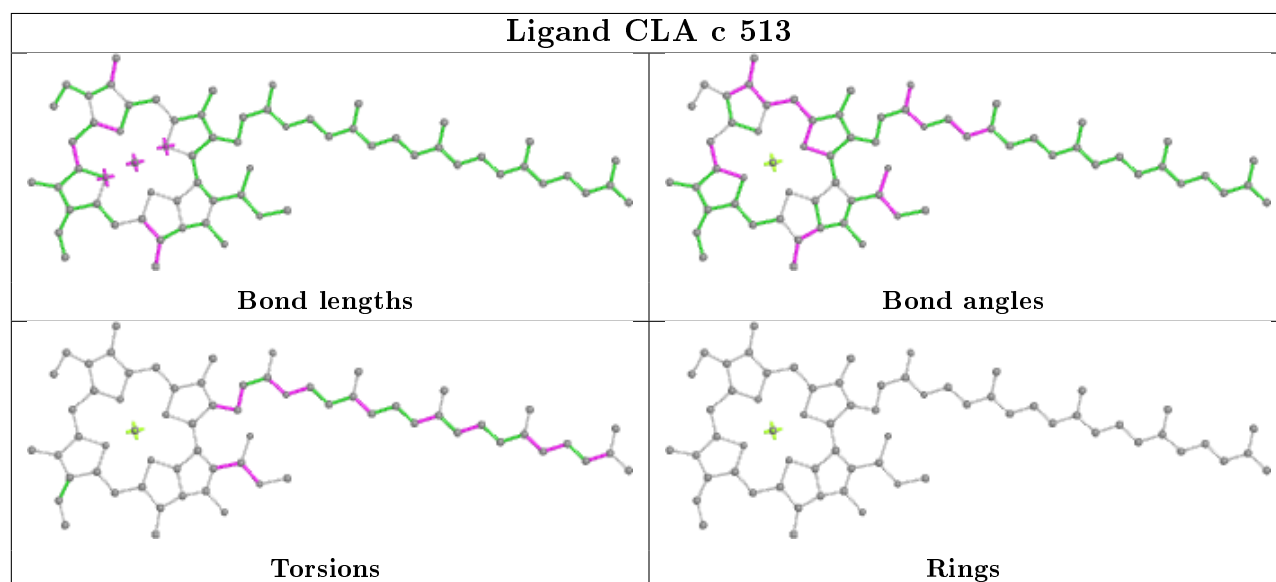
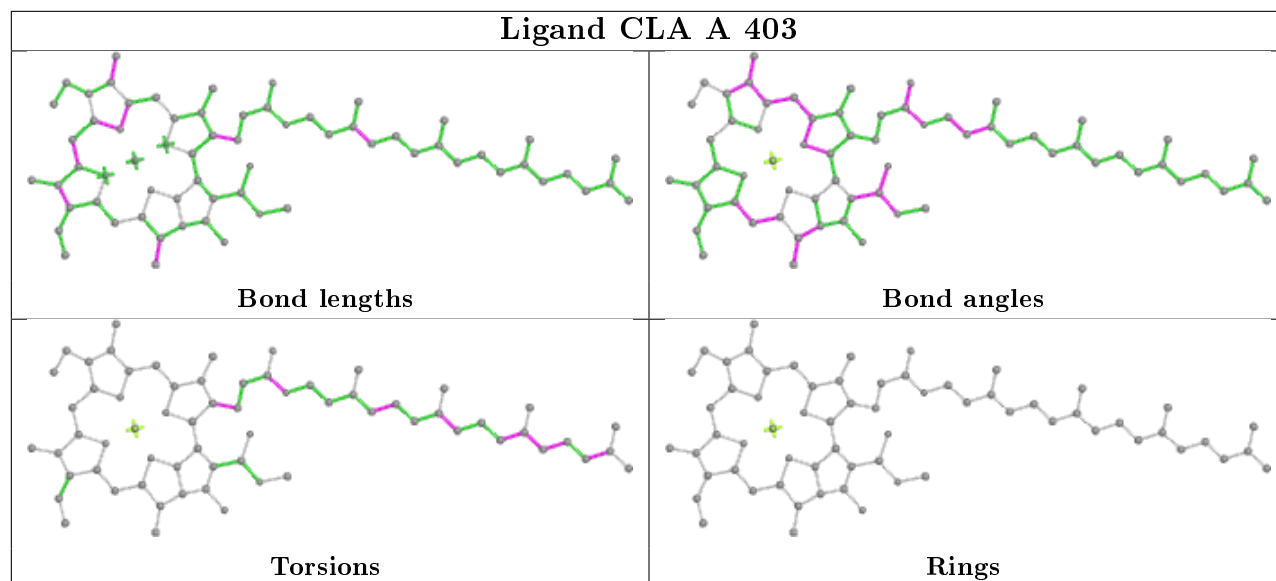
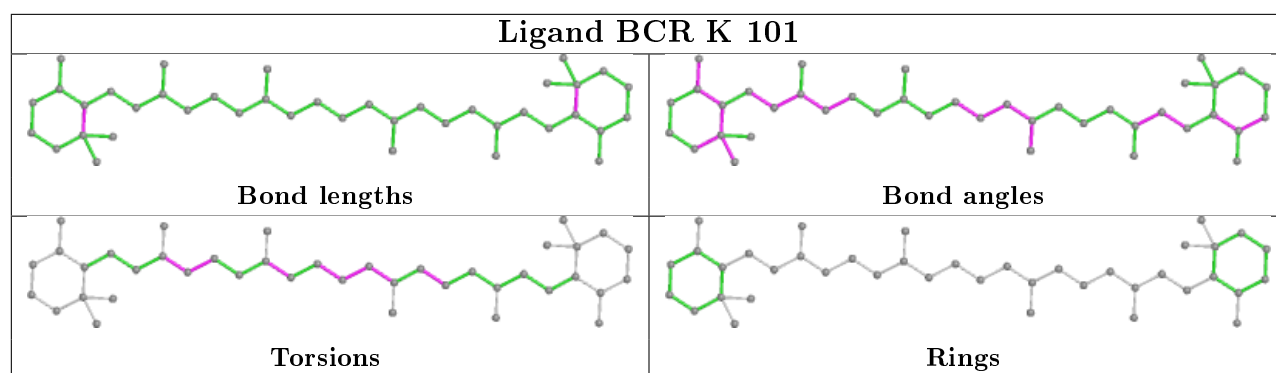
## Ligand CLA B 614

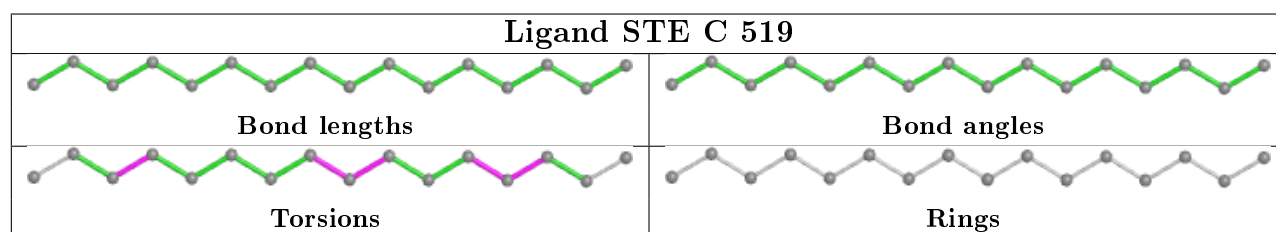
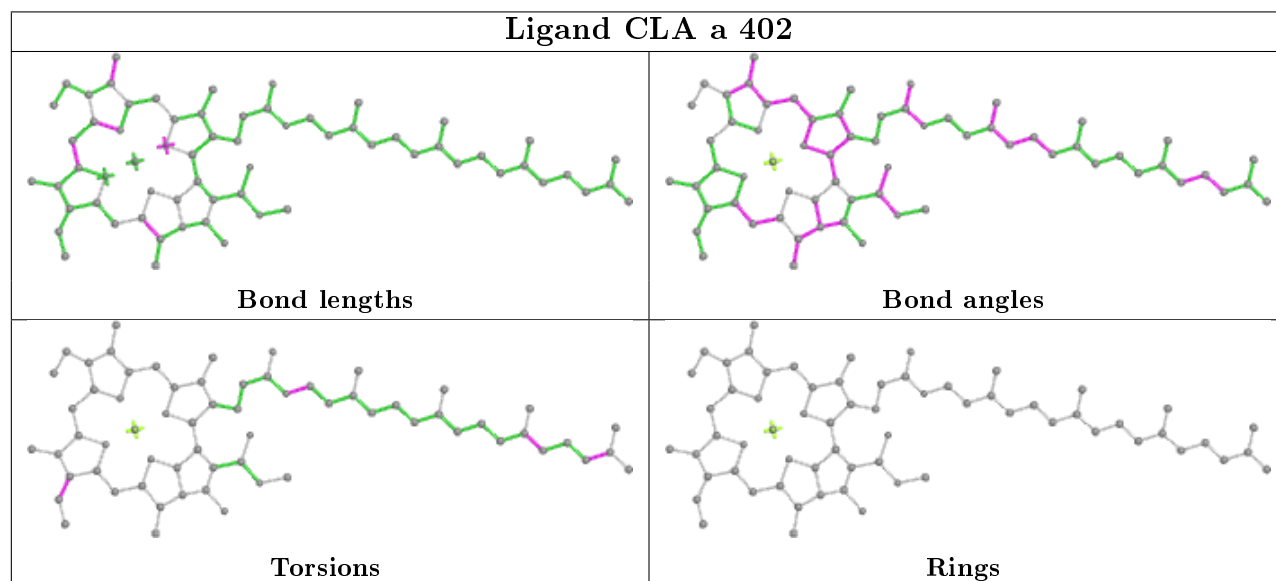
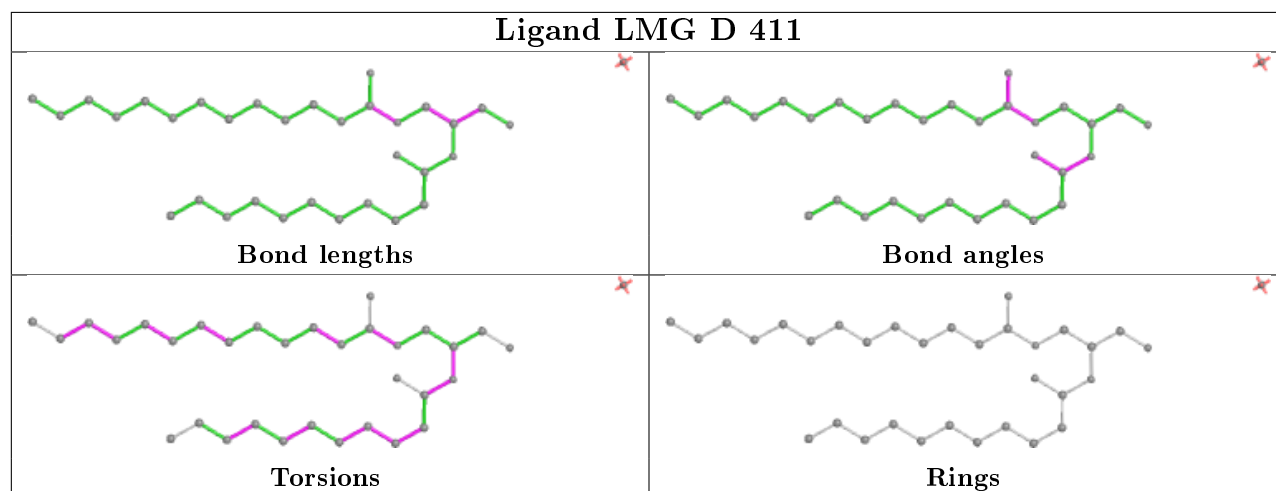
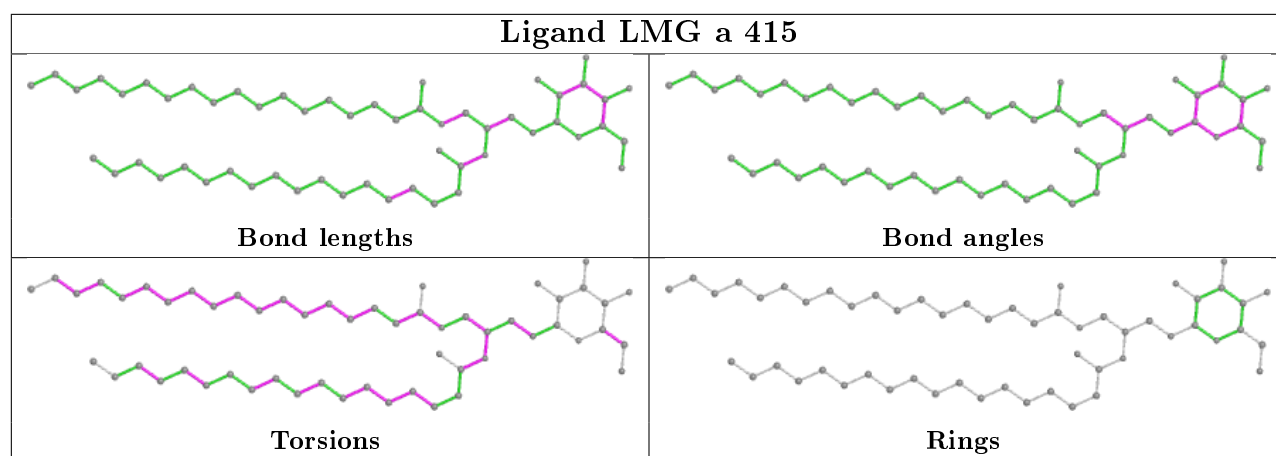


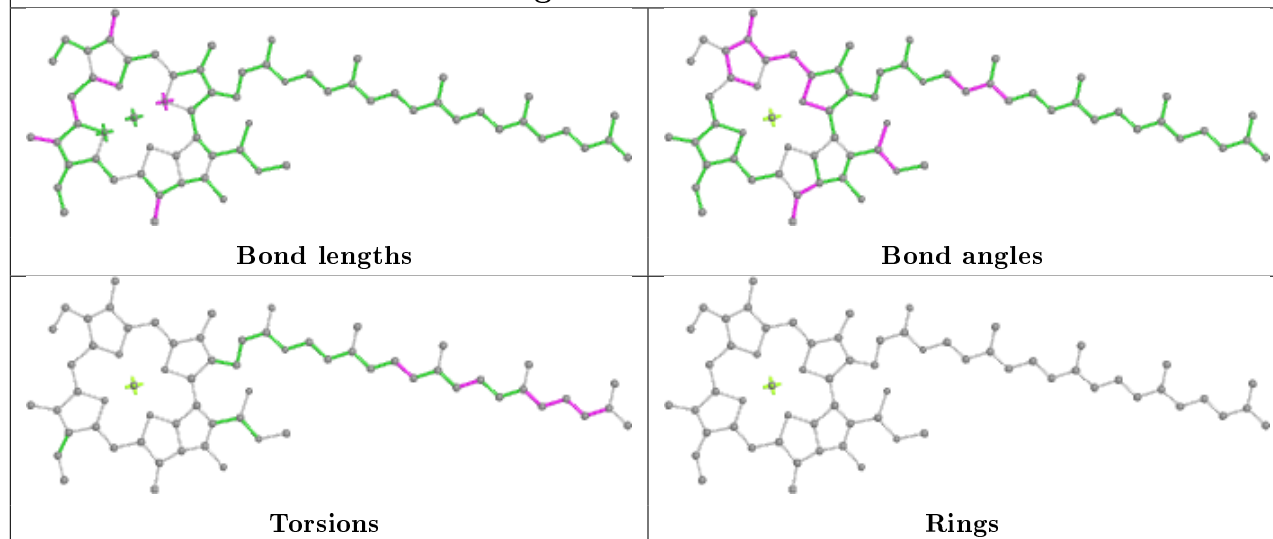
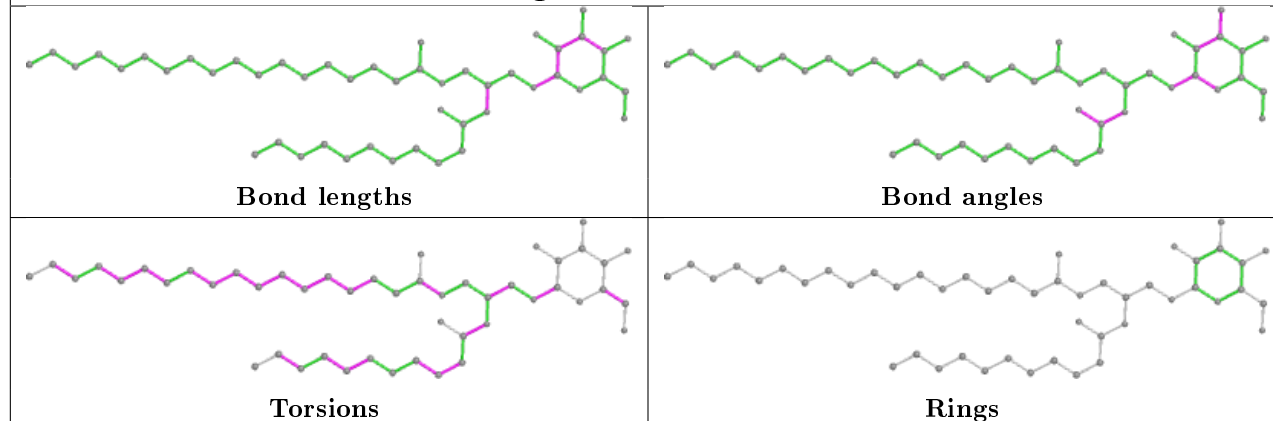
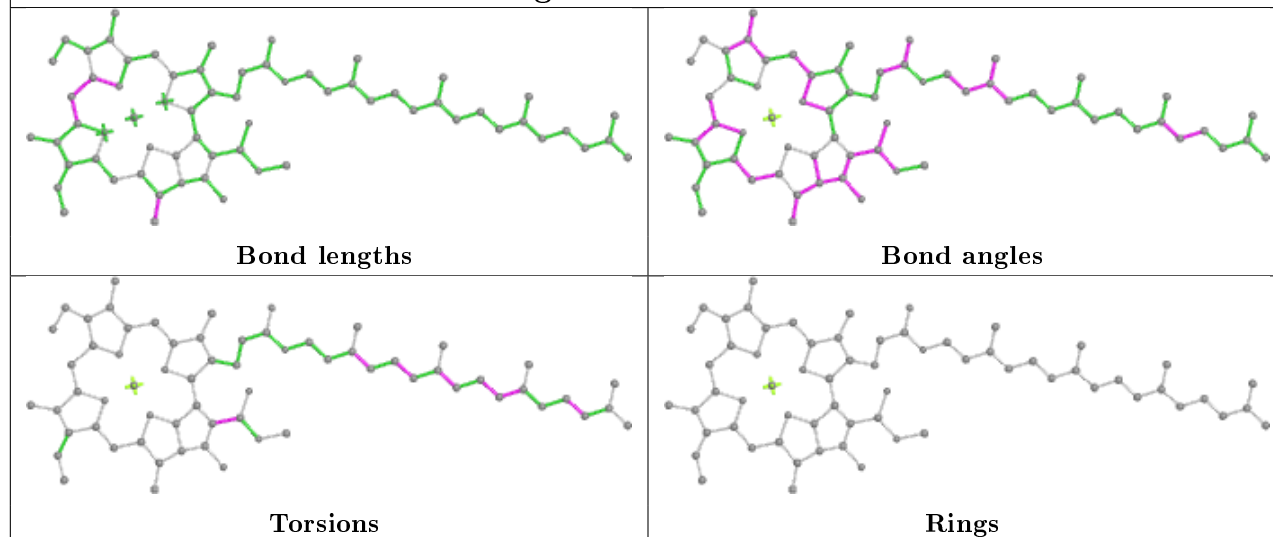


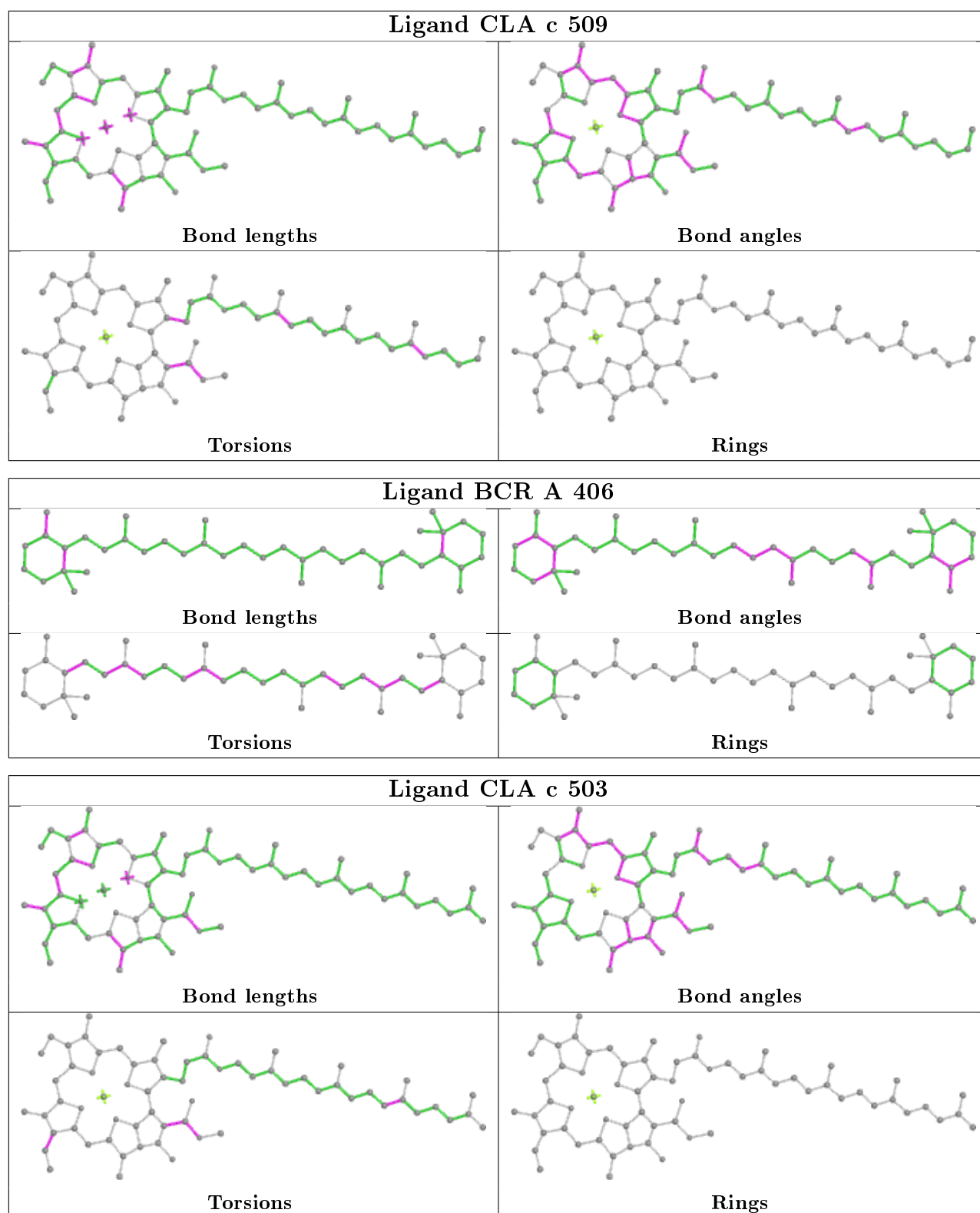


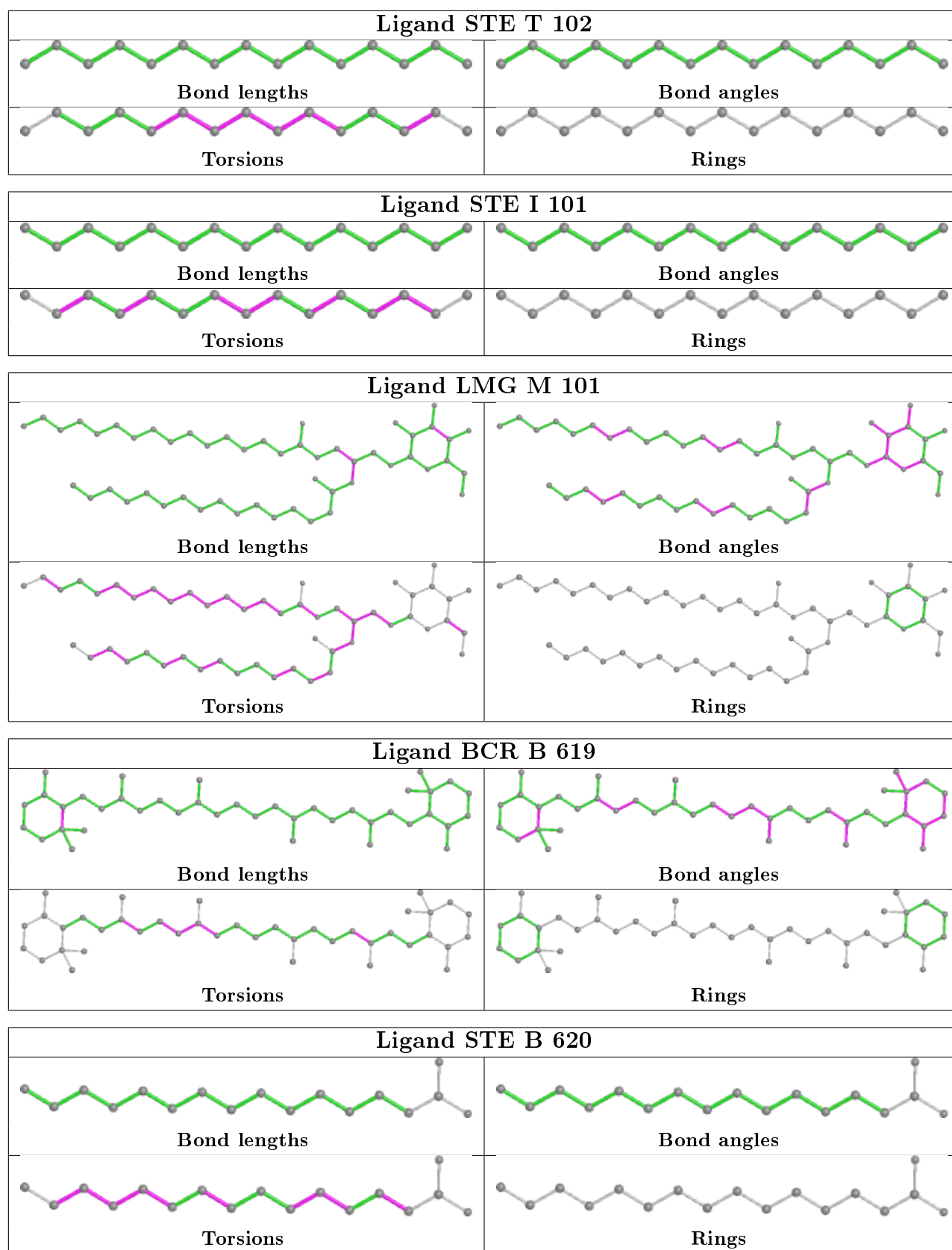


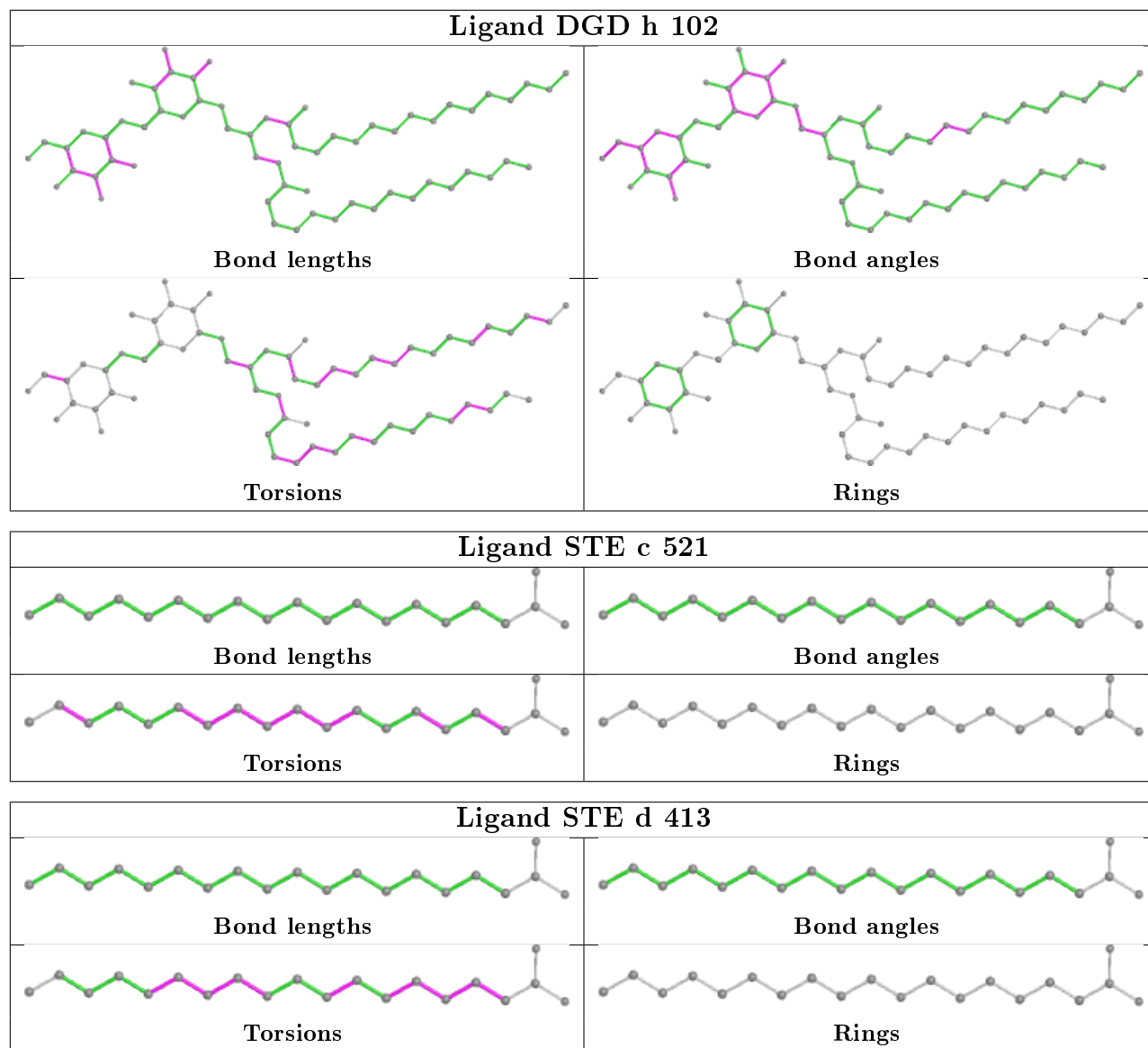




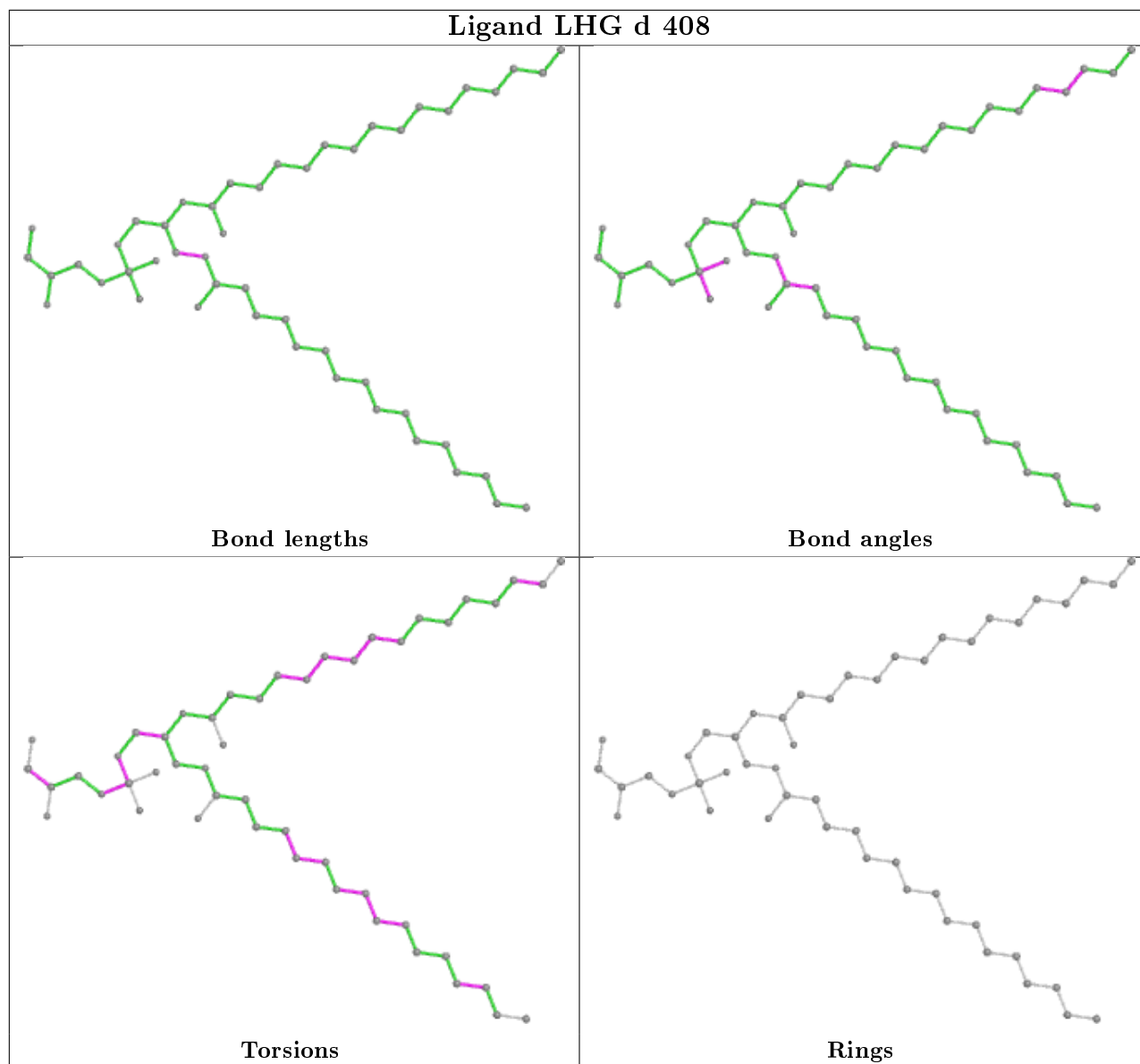
**Ligand CLA b 615****Ligand LMG c 522****Ligand CLA b 605**



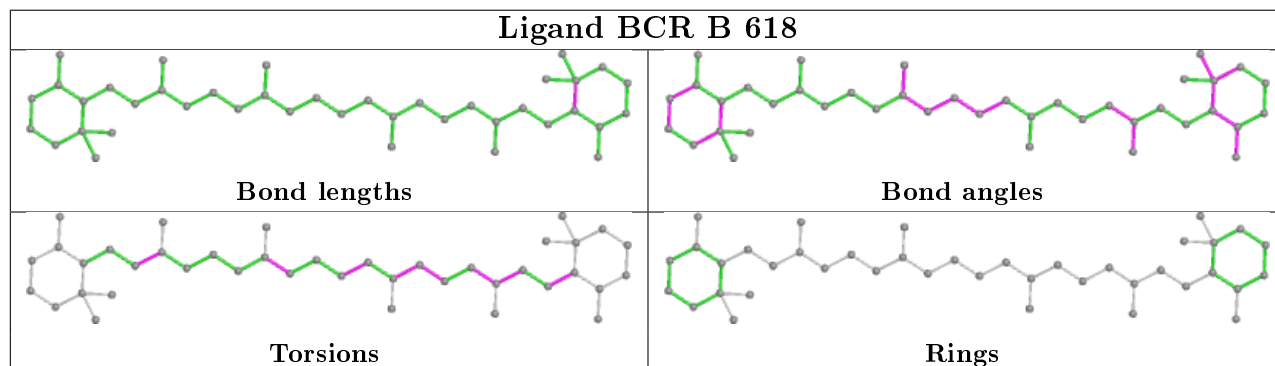


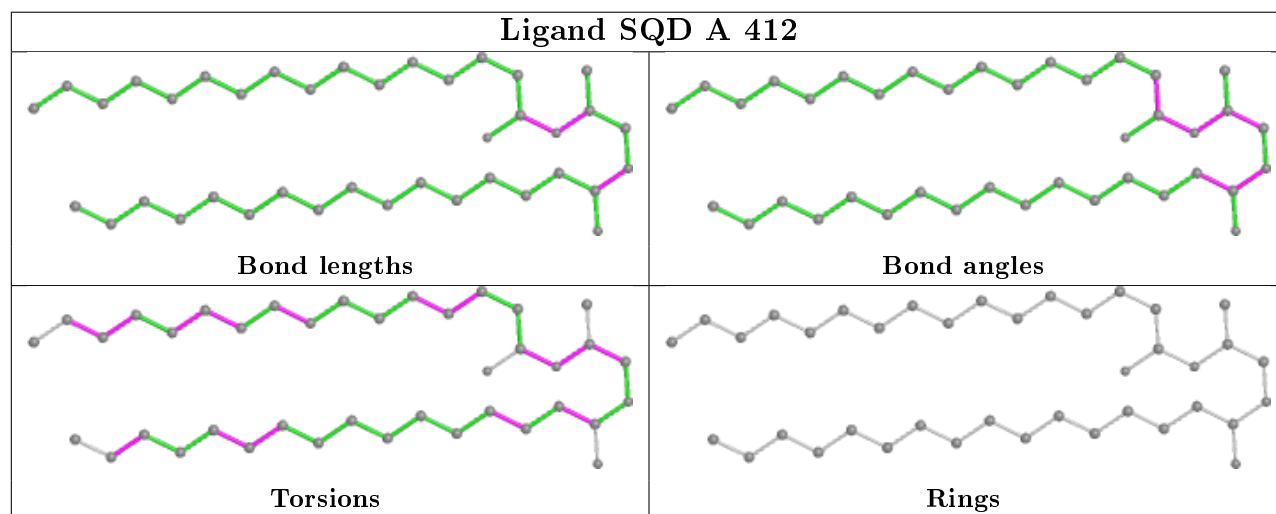
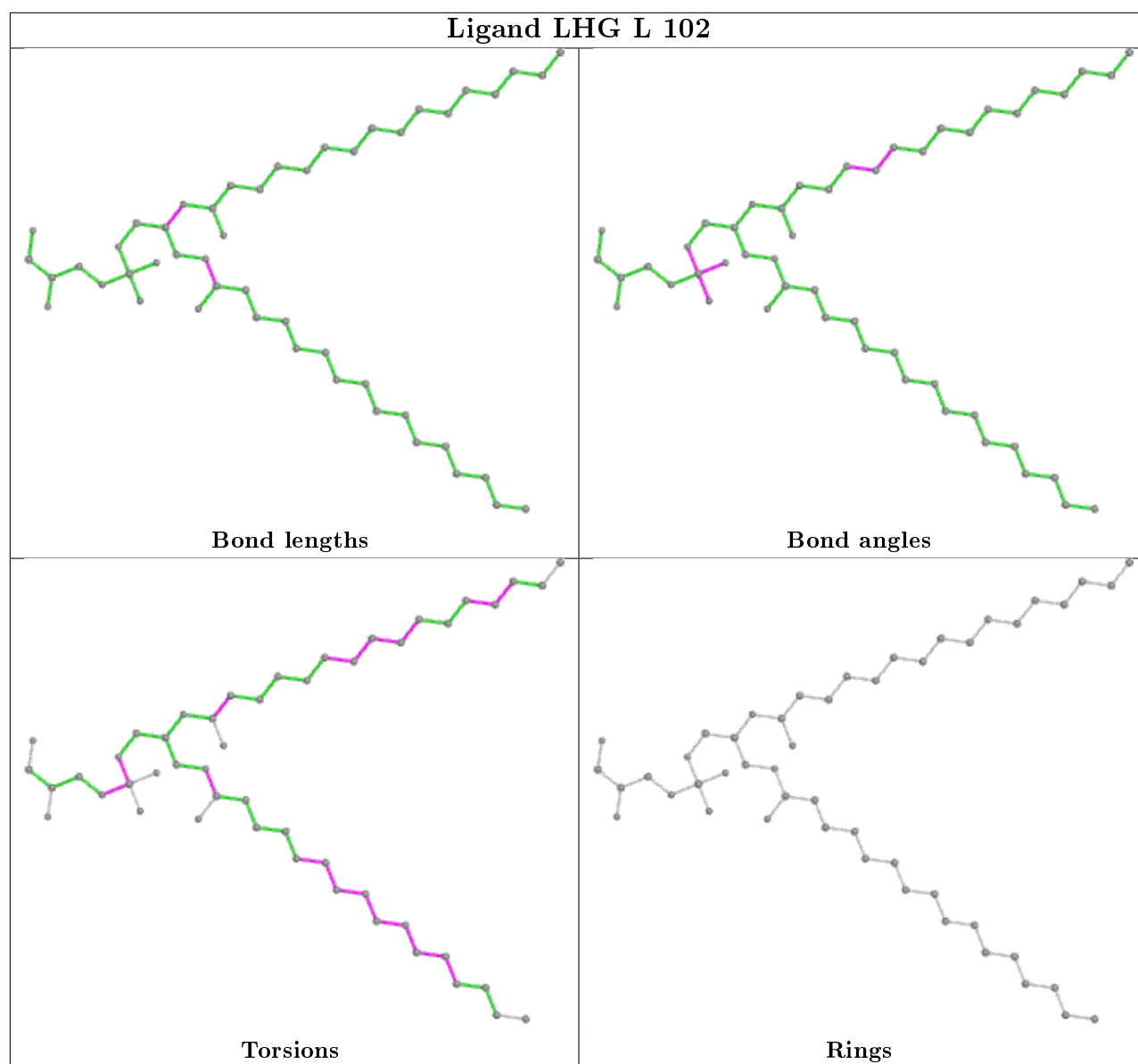


## Ligand LHG d 408

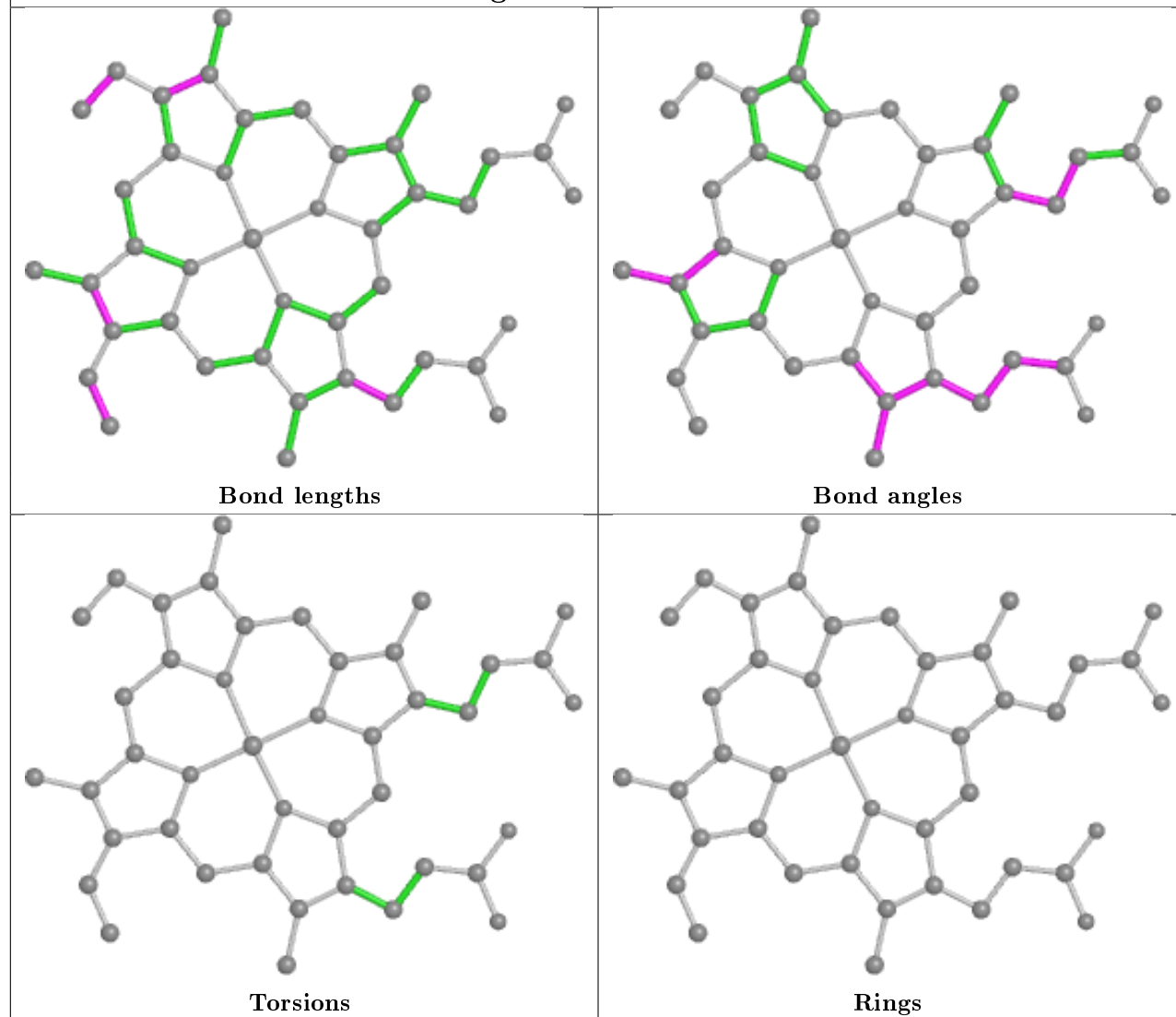


## Ligand BCR B 618

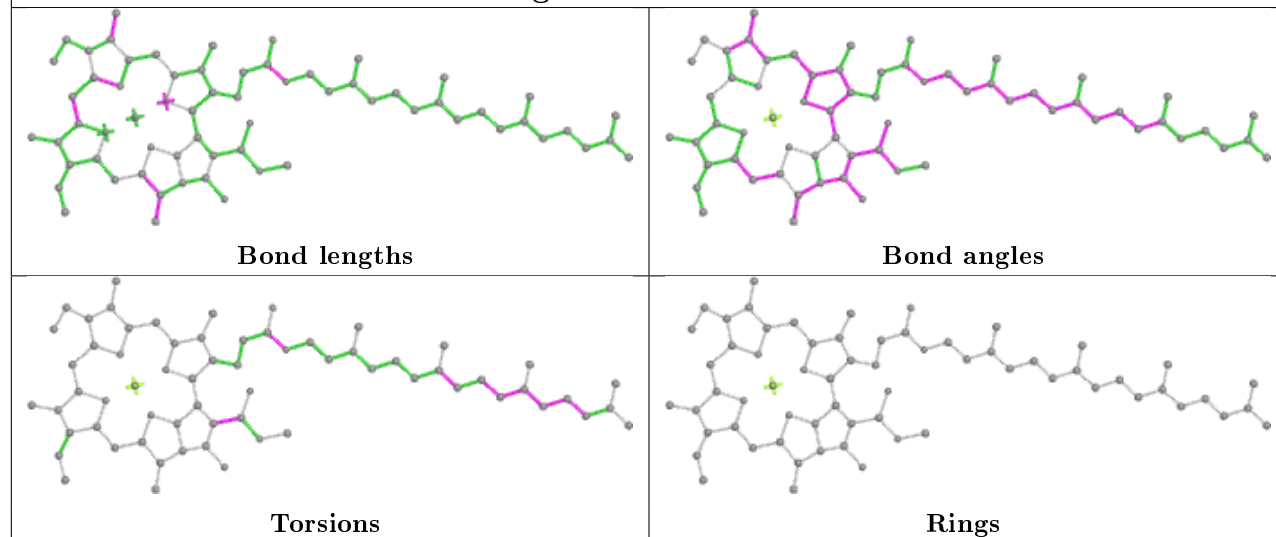


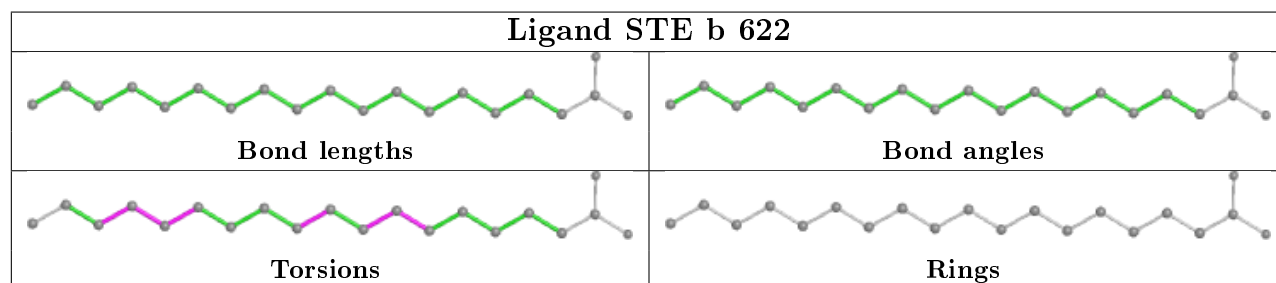
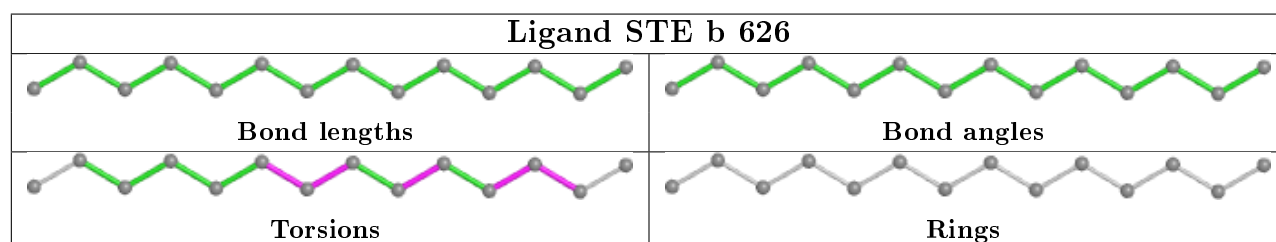
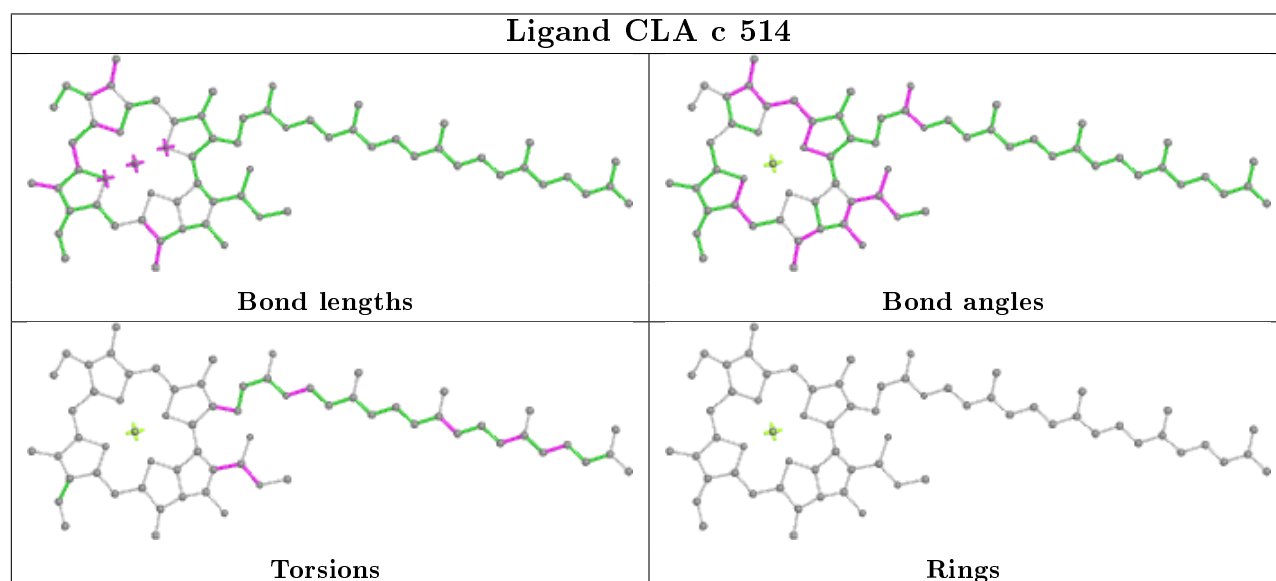
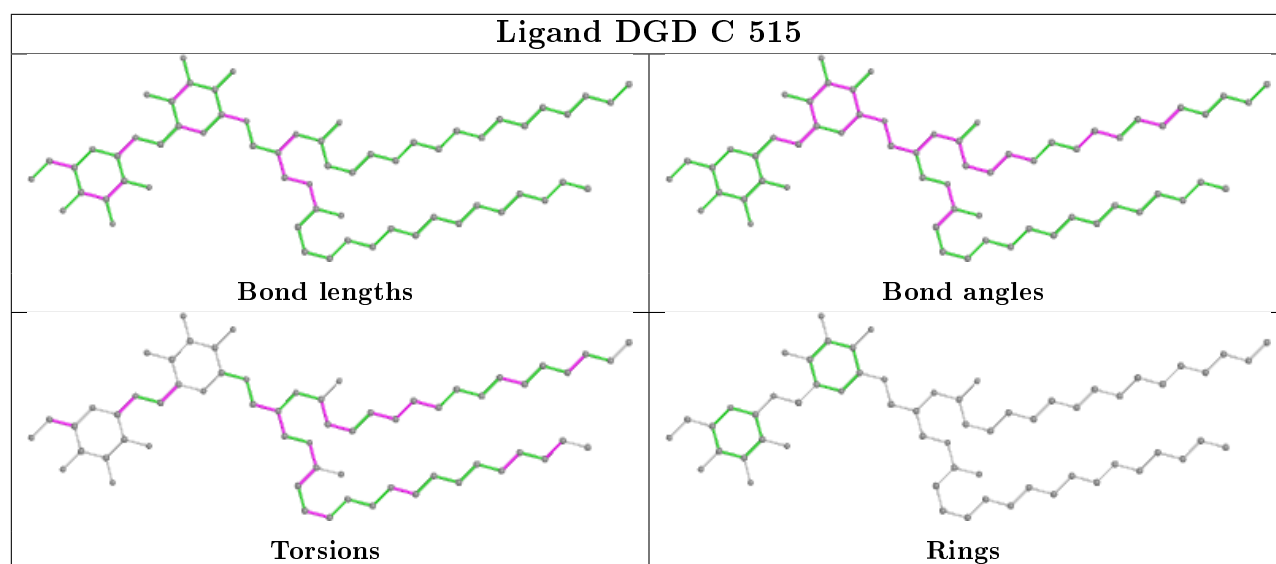


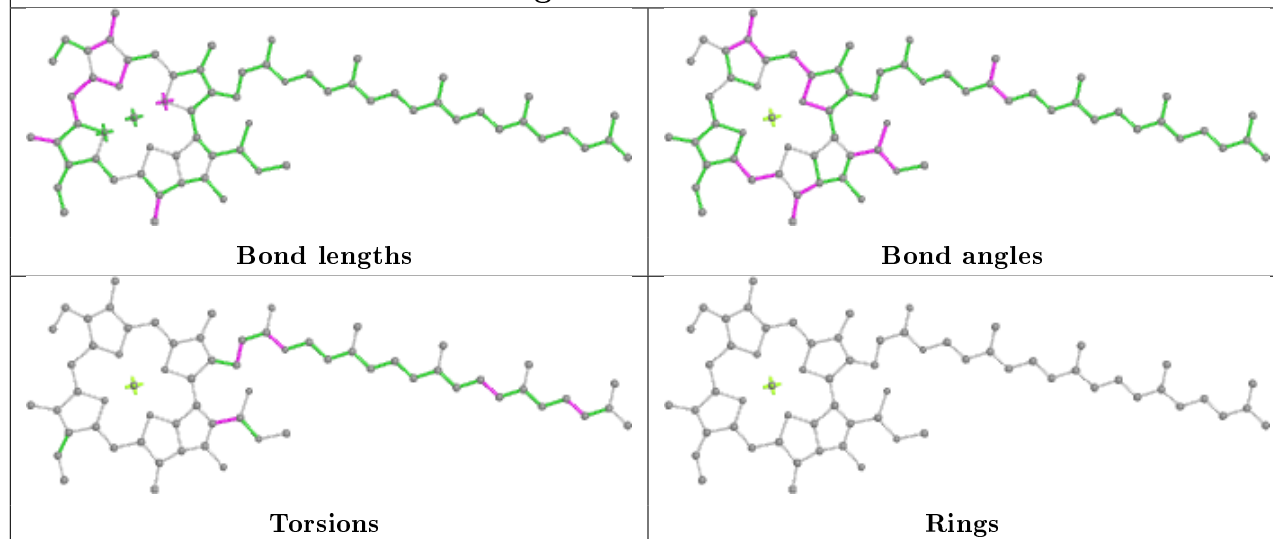
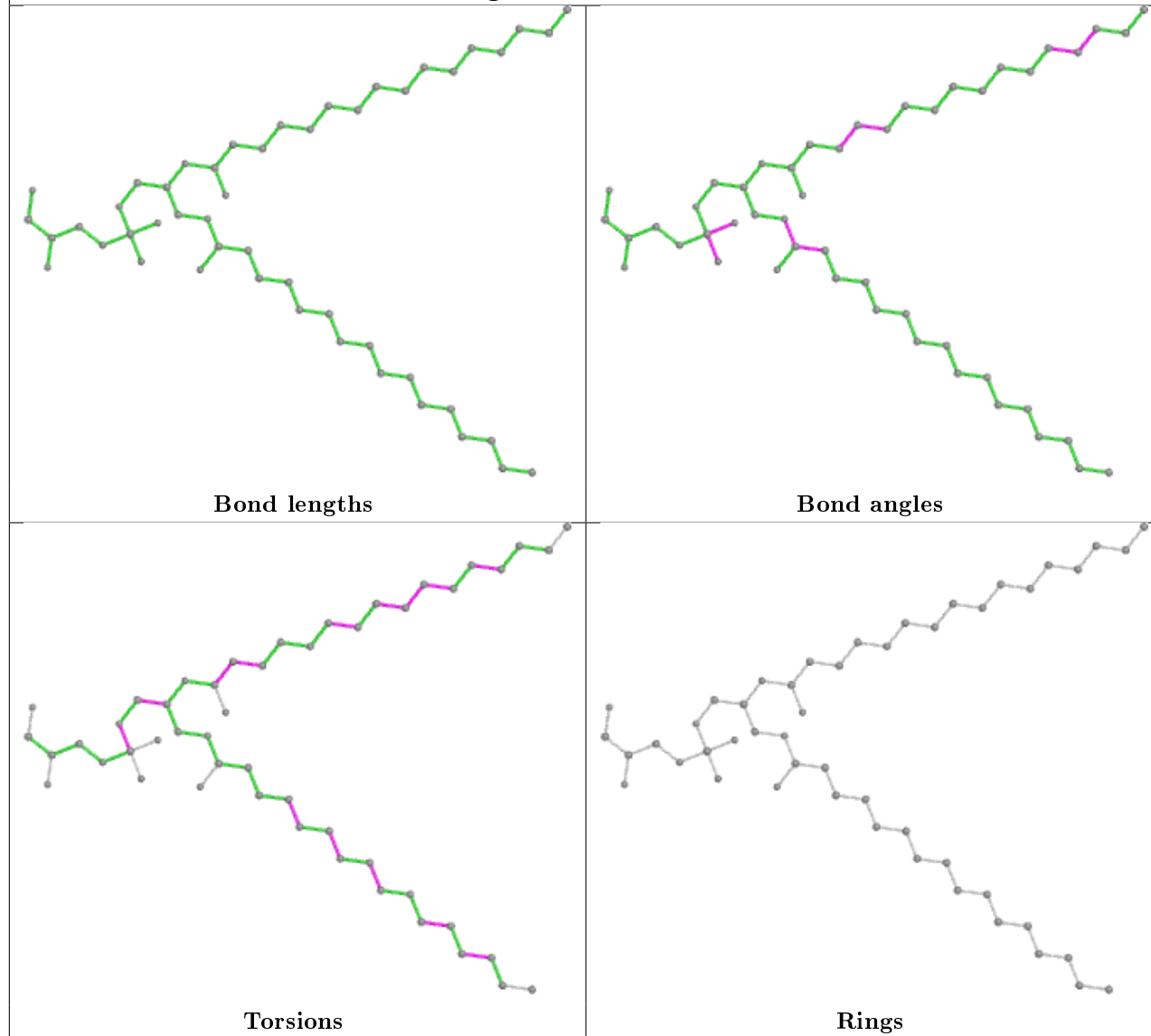
## Ligand HEC F 102

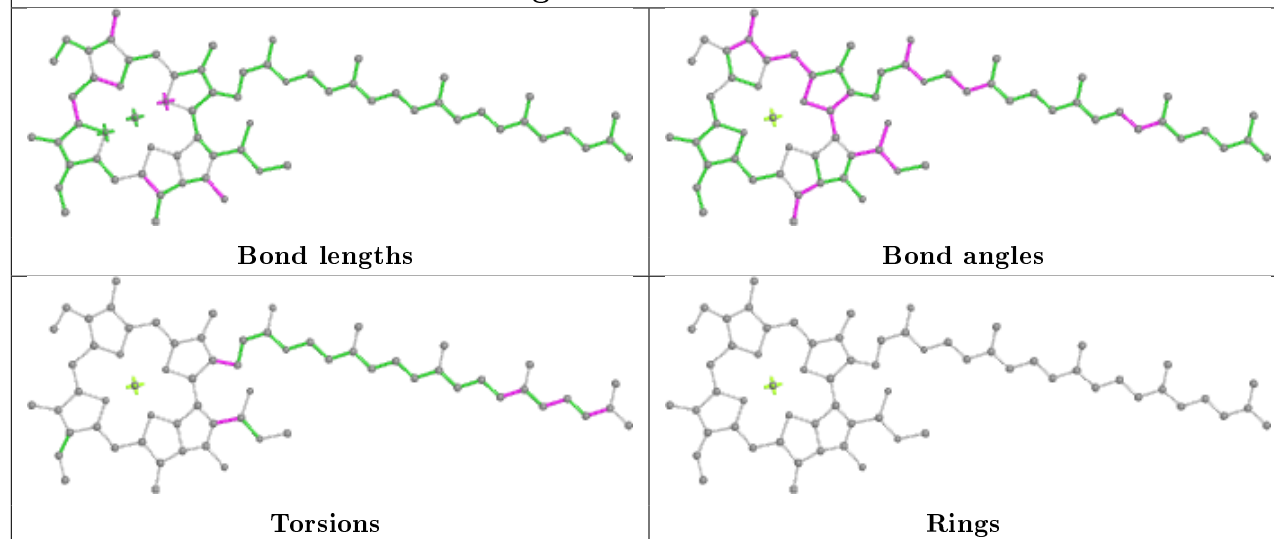
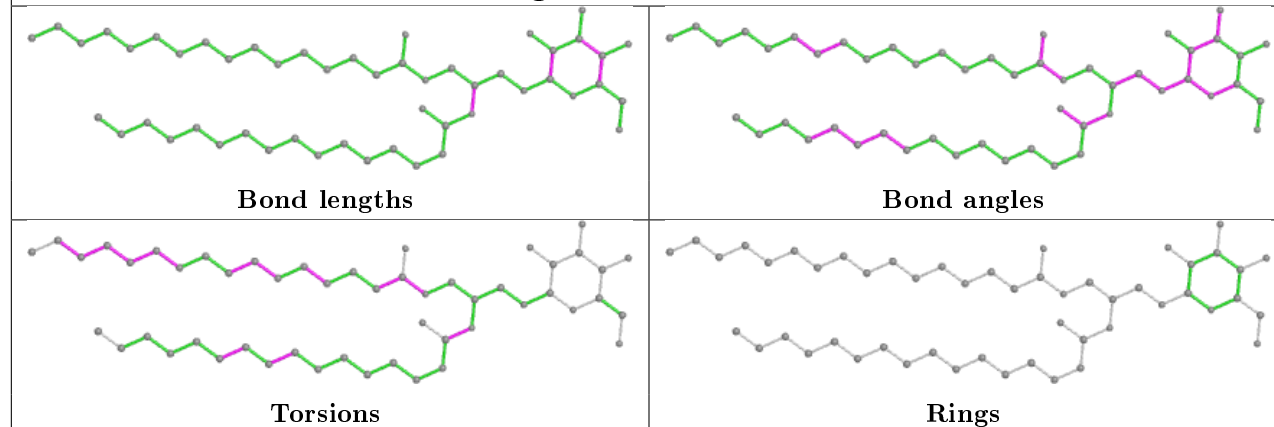
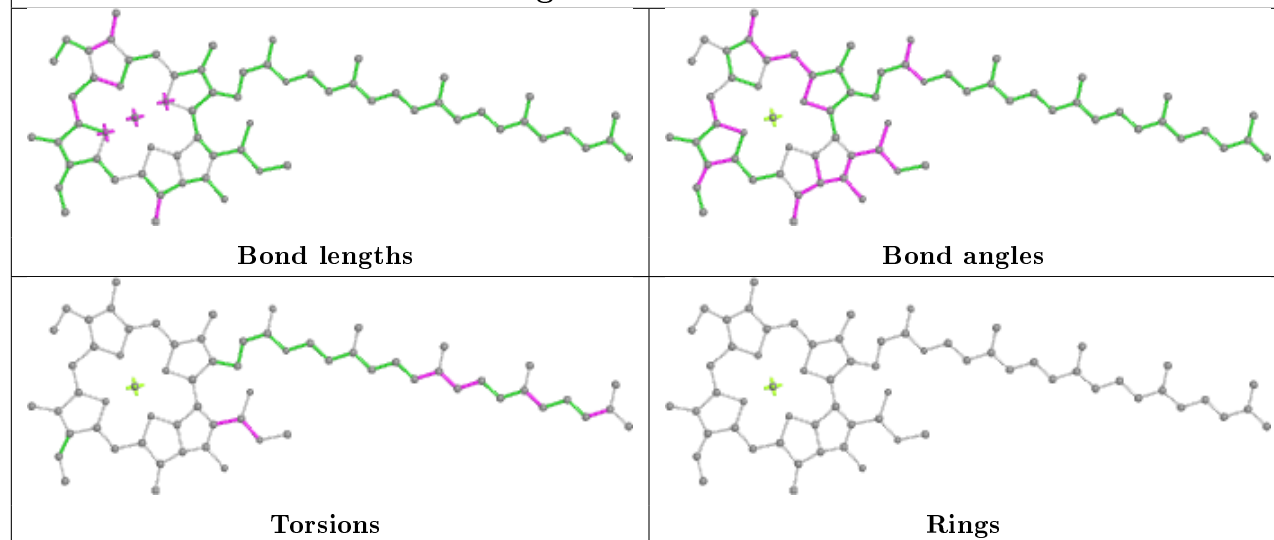


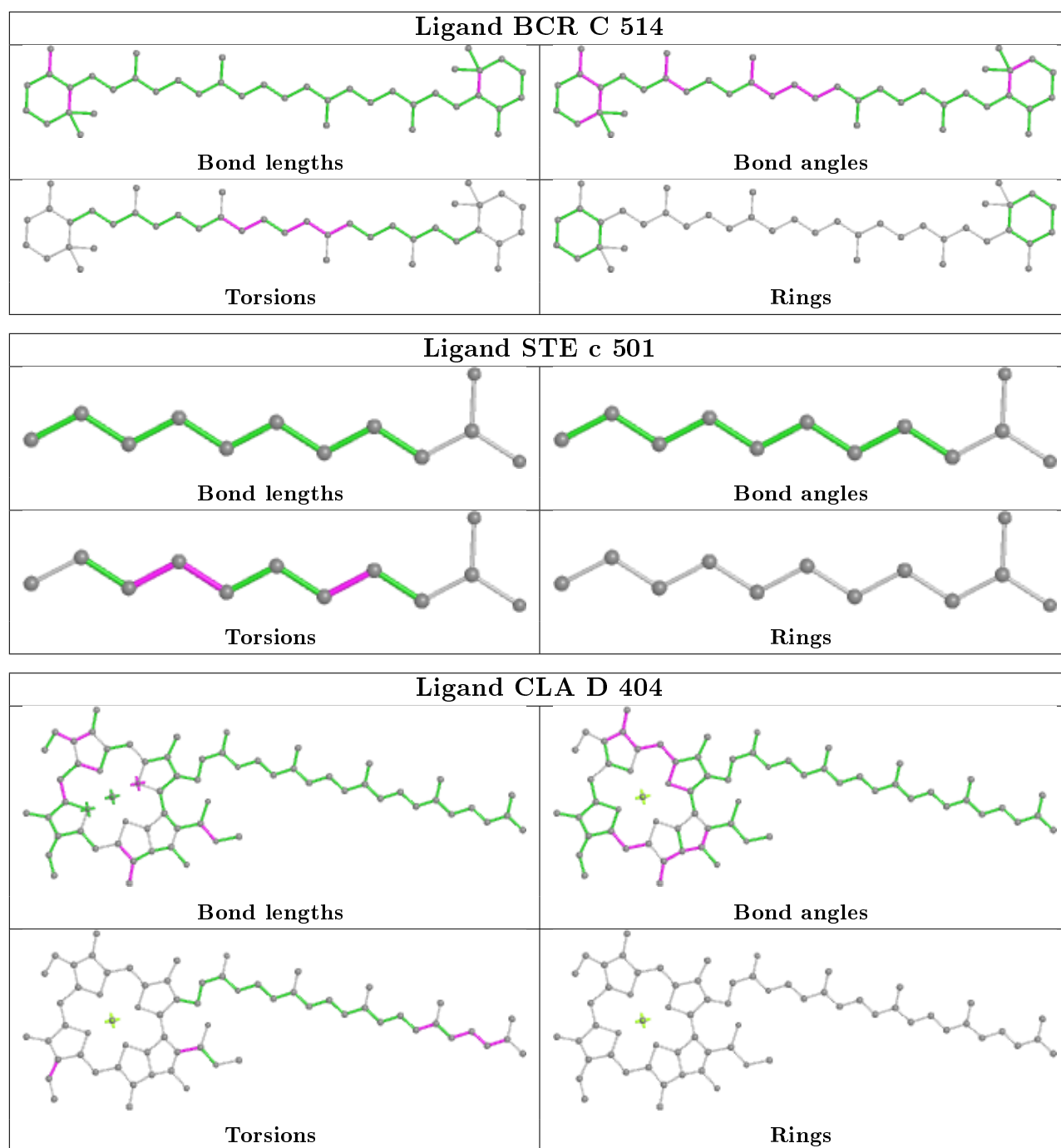
## Ligand CLA B 604

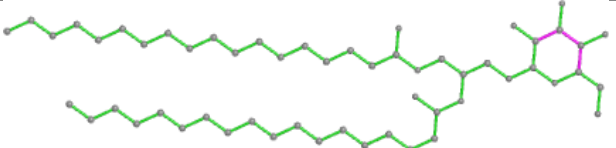
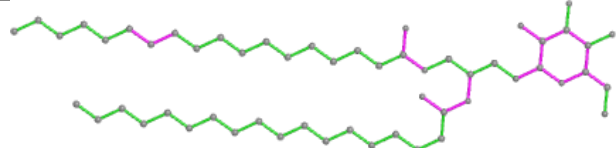
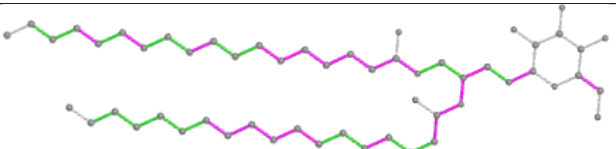
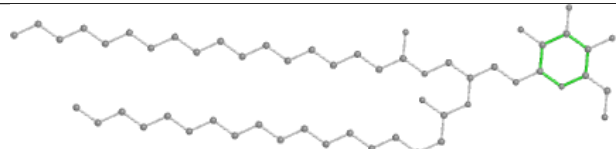


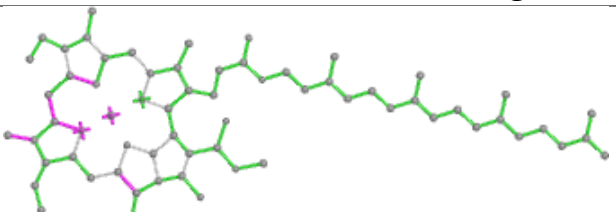
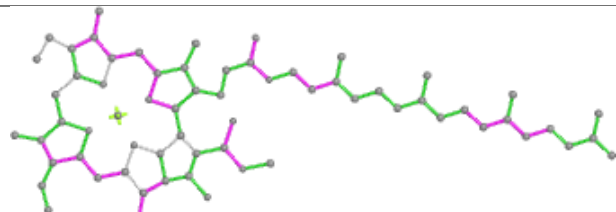
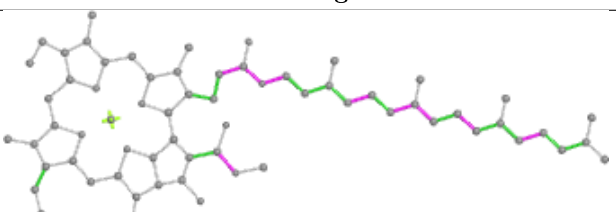
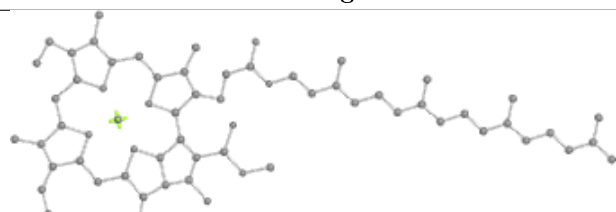


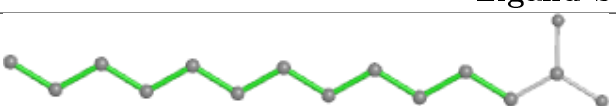
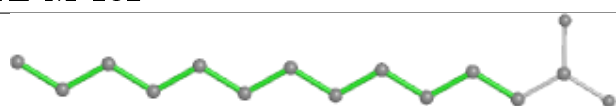
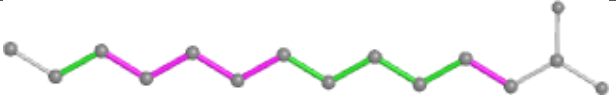
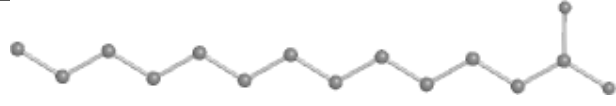
**Ligand CLA b 606****Ligand LHG 1 101**

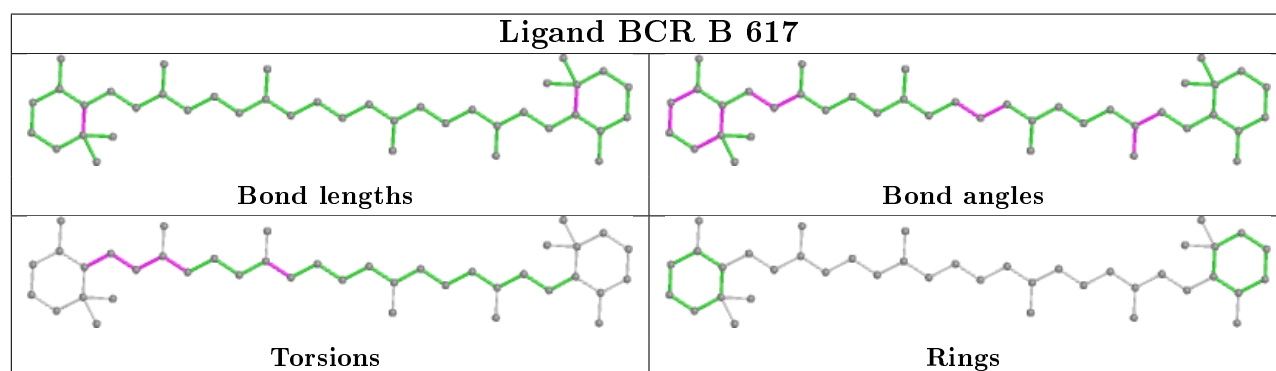
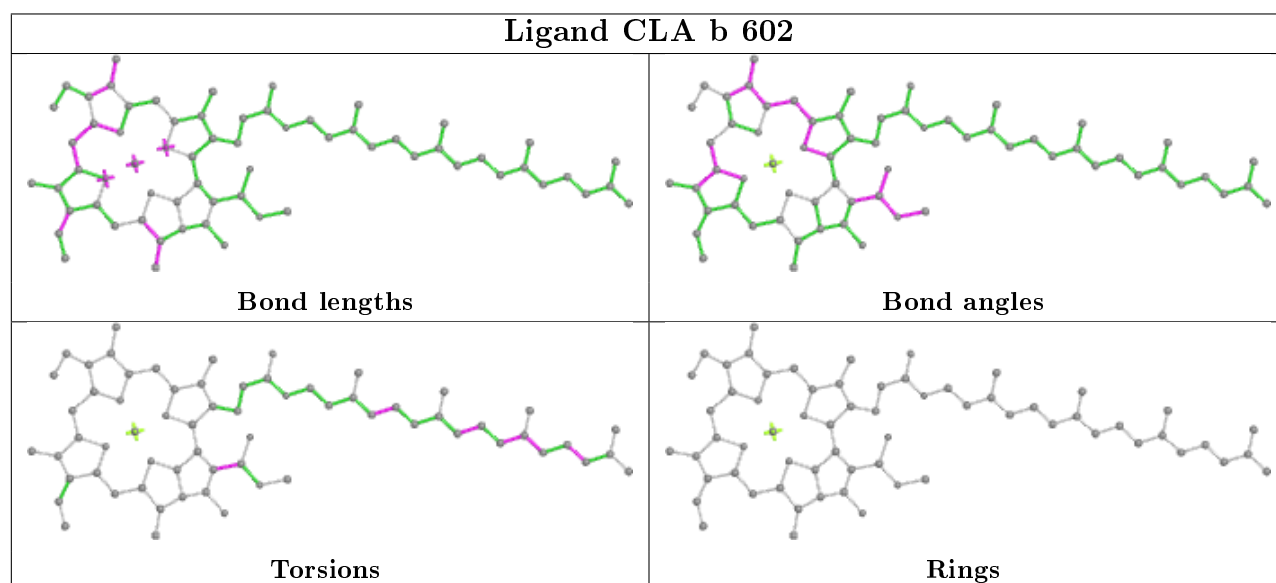
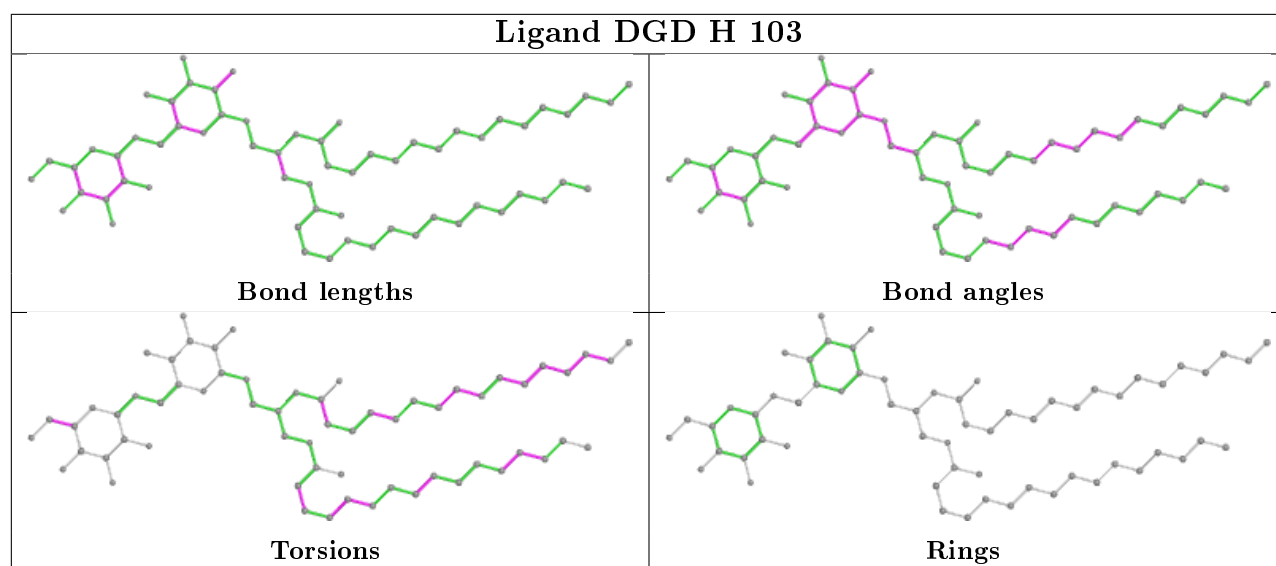
**Ligand CLA B 602****Ligand LMG b 621****Ligand CLA a 403**

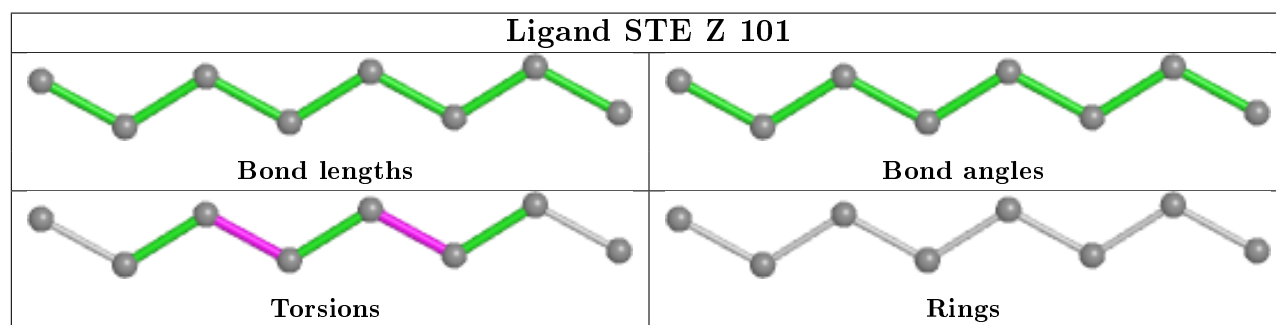
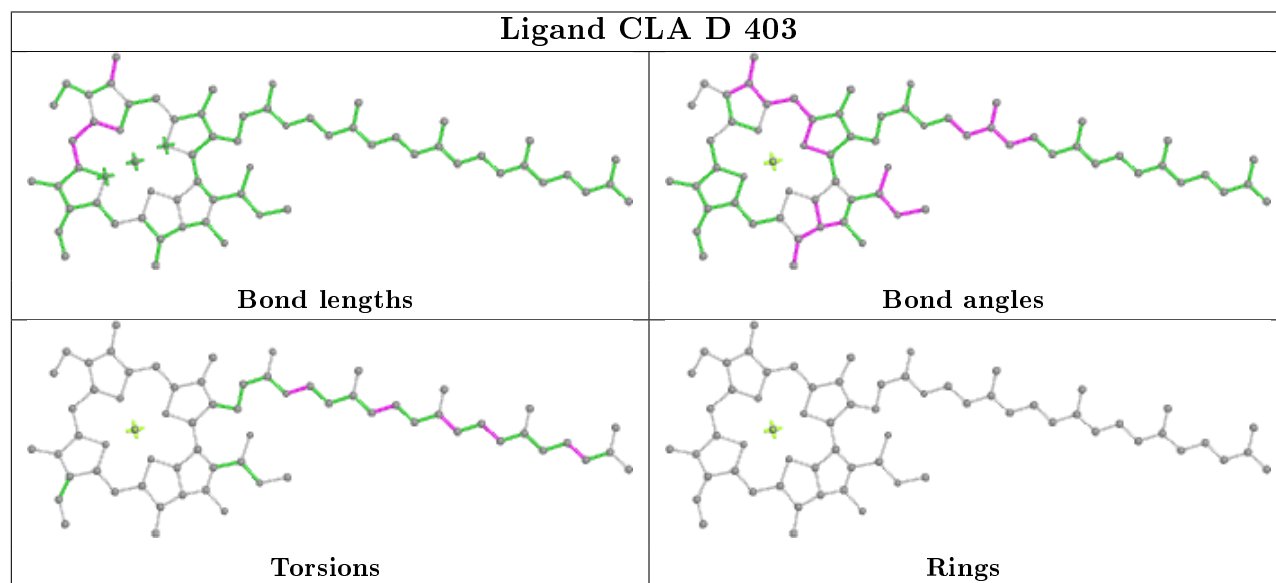
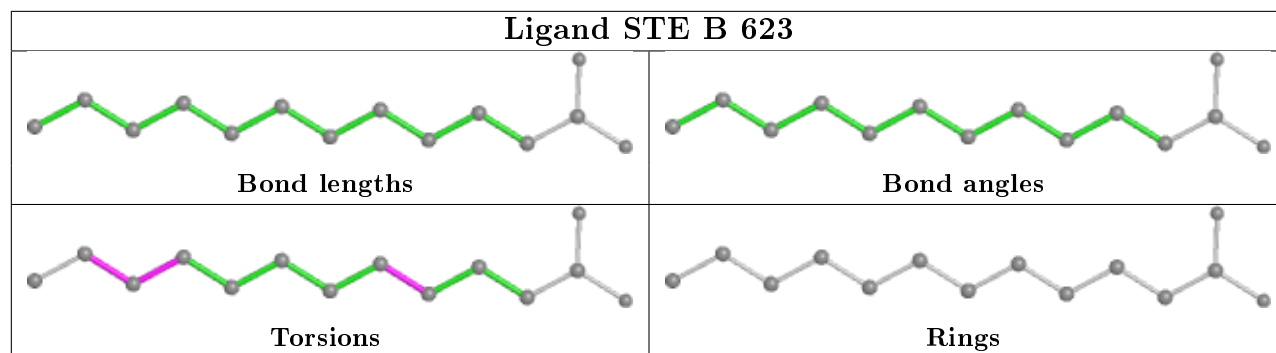


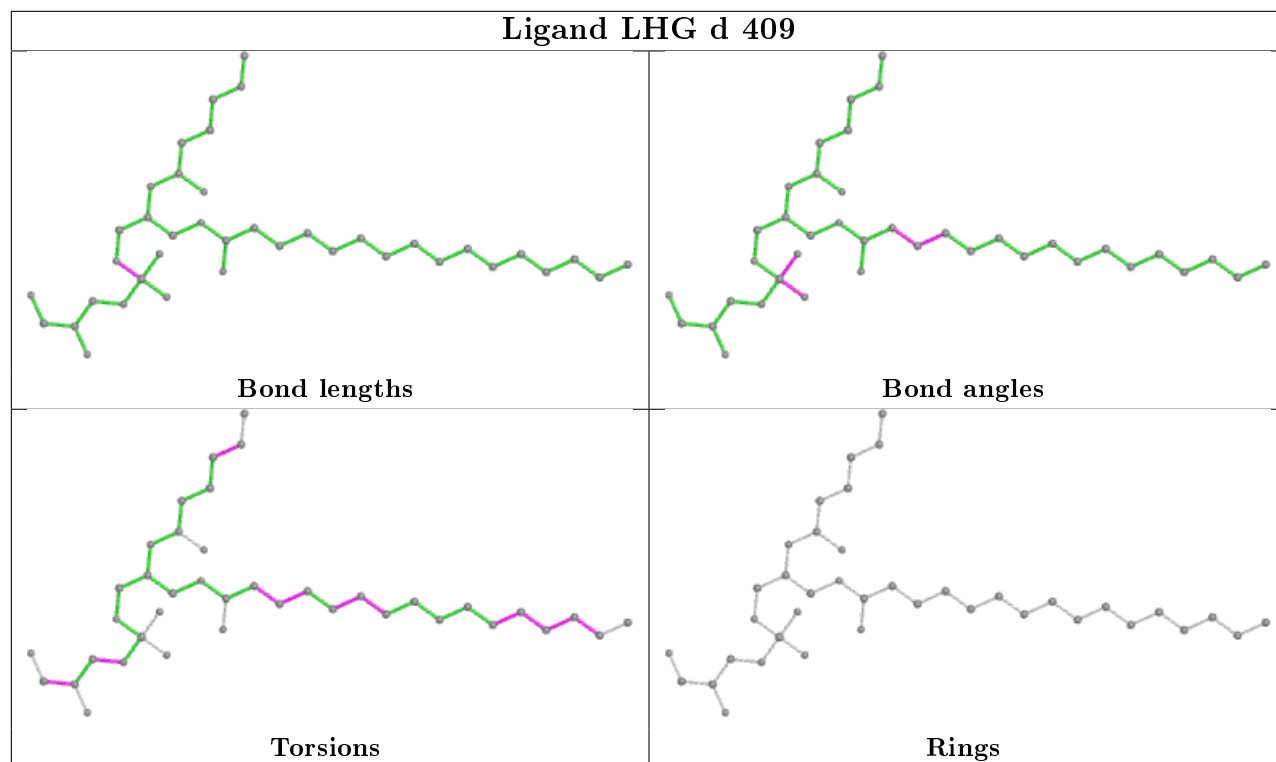
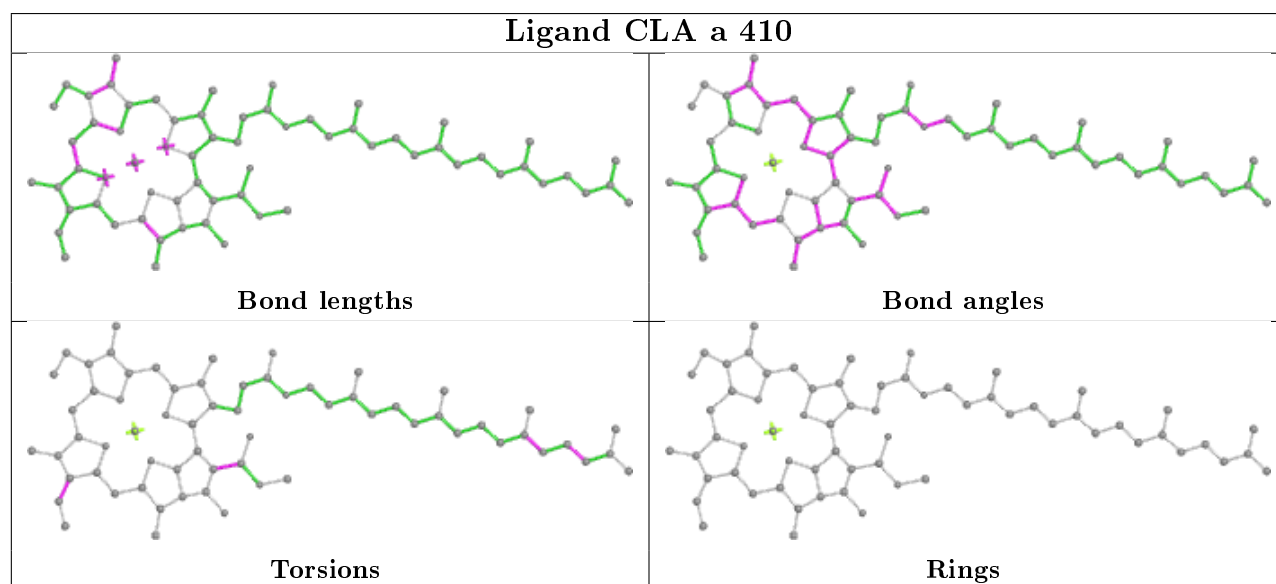
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

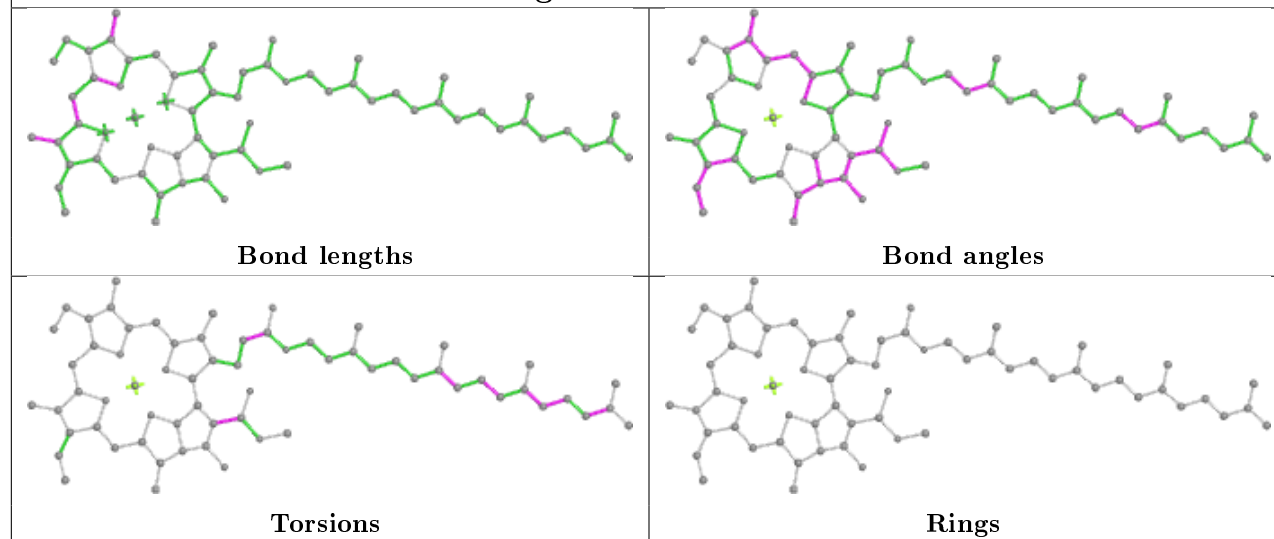
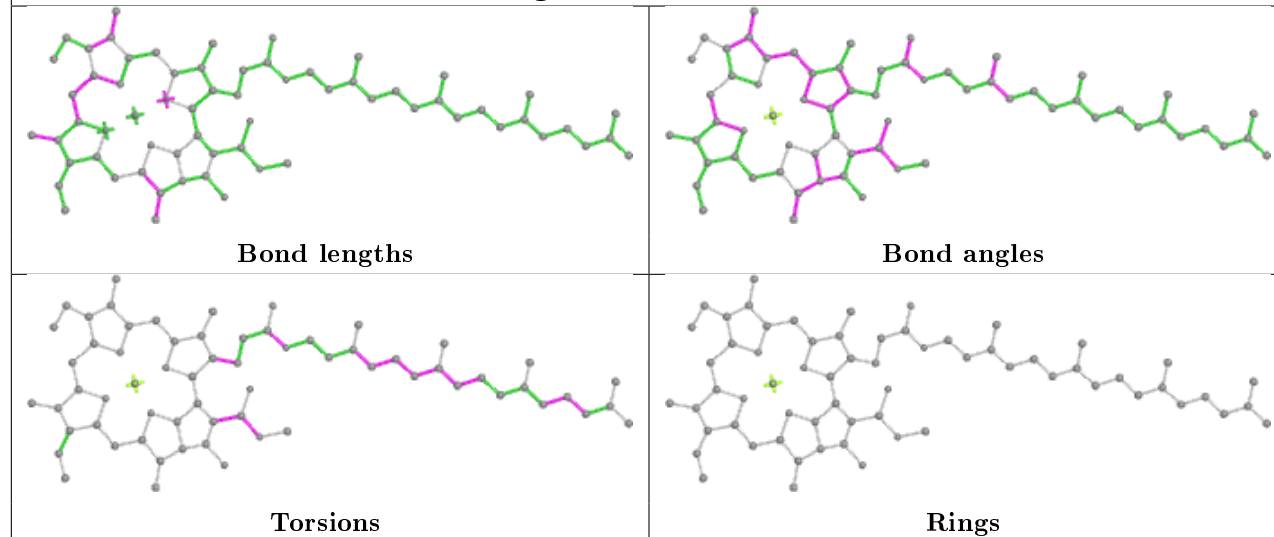
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

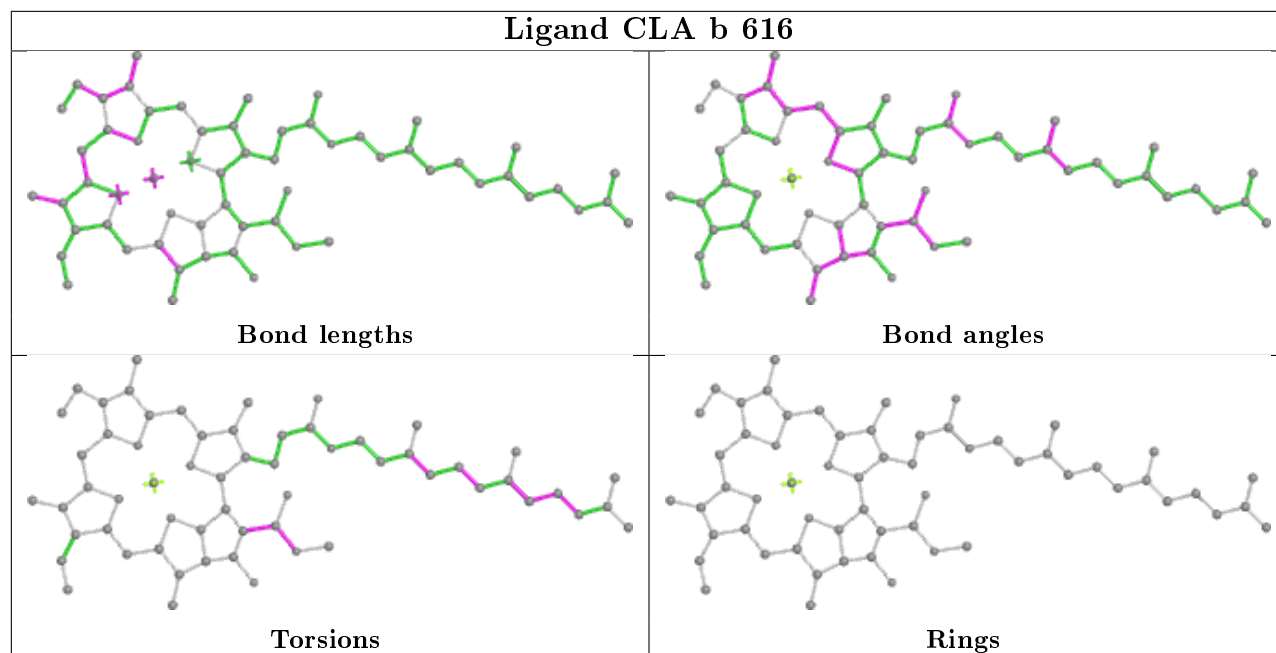
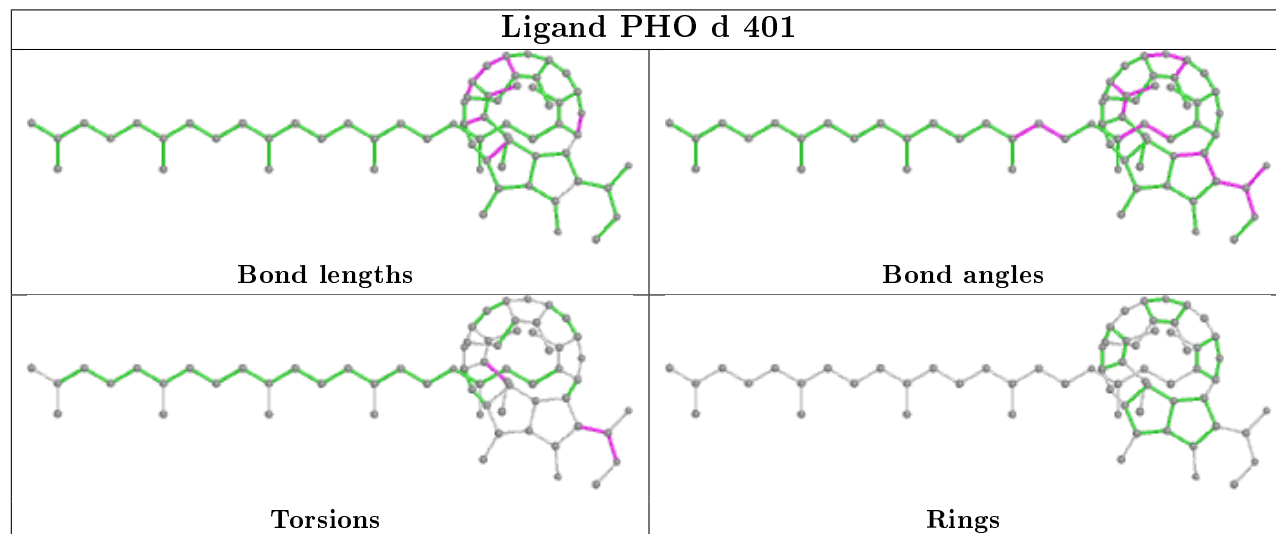
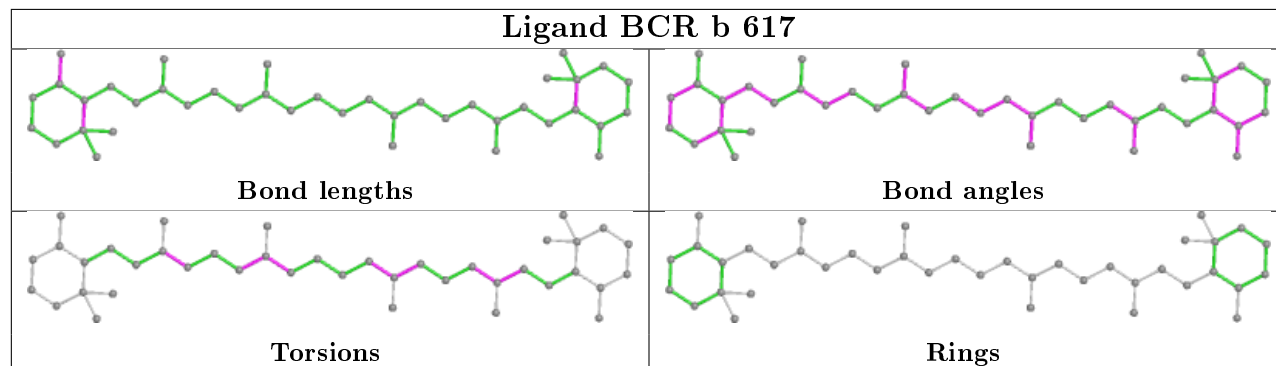
Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

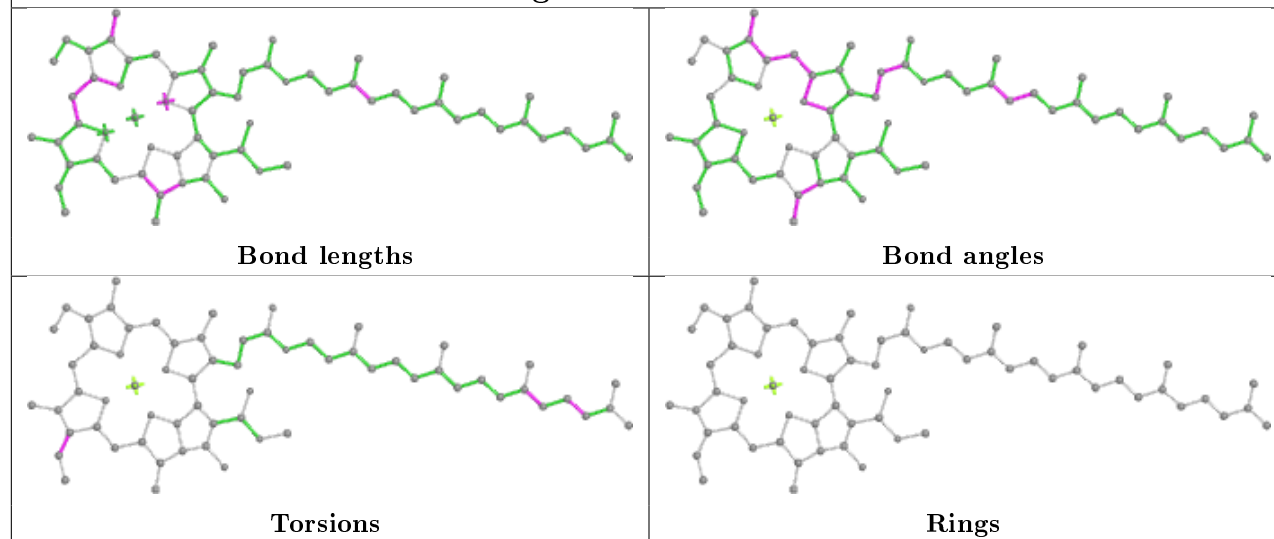
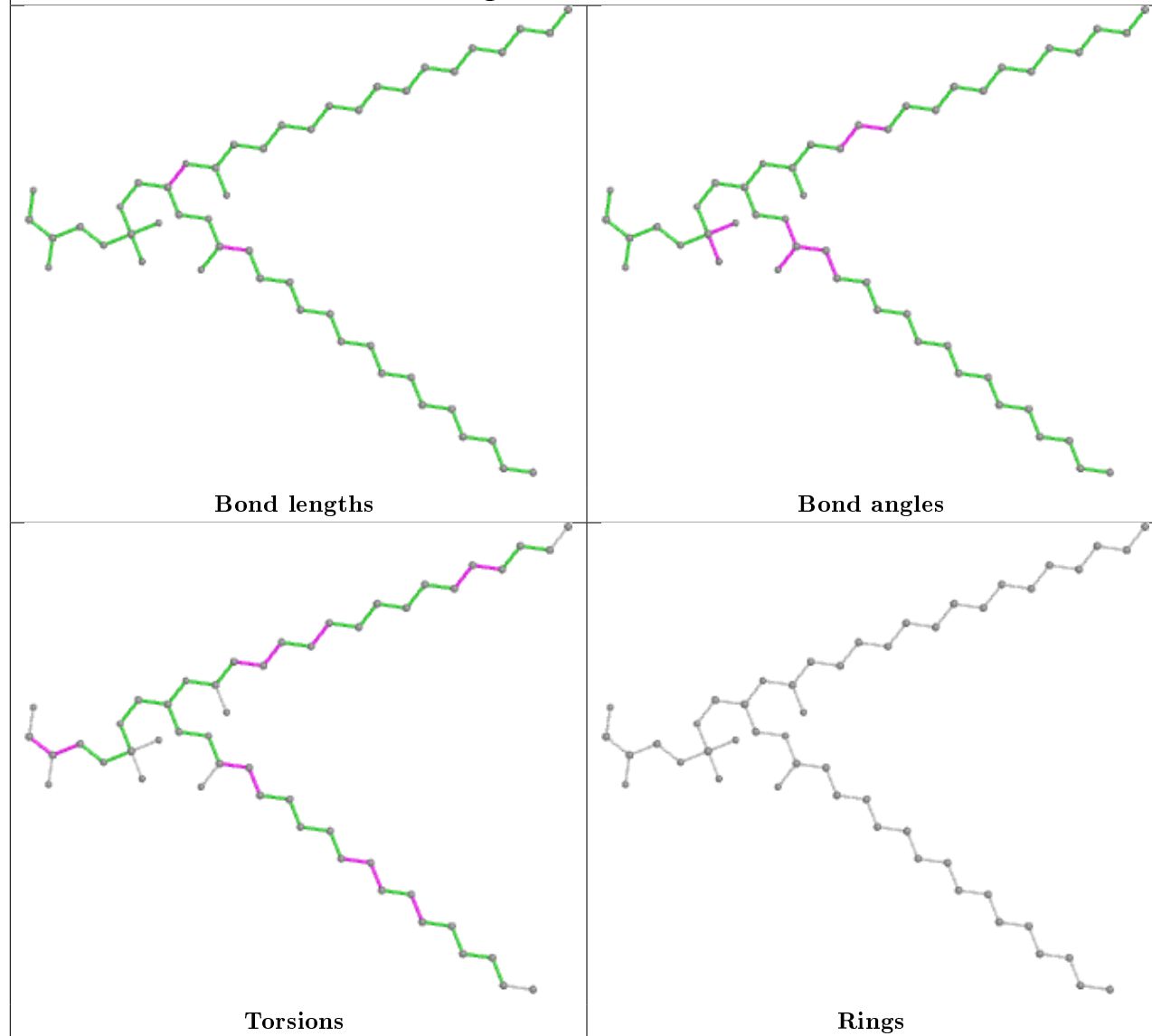




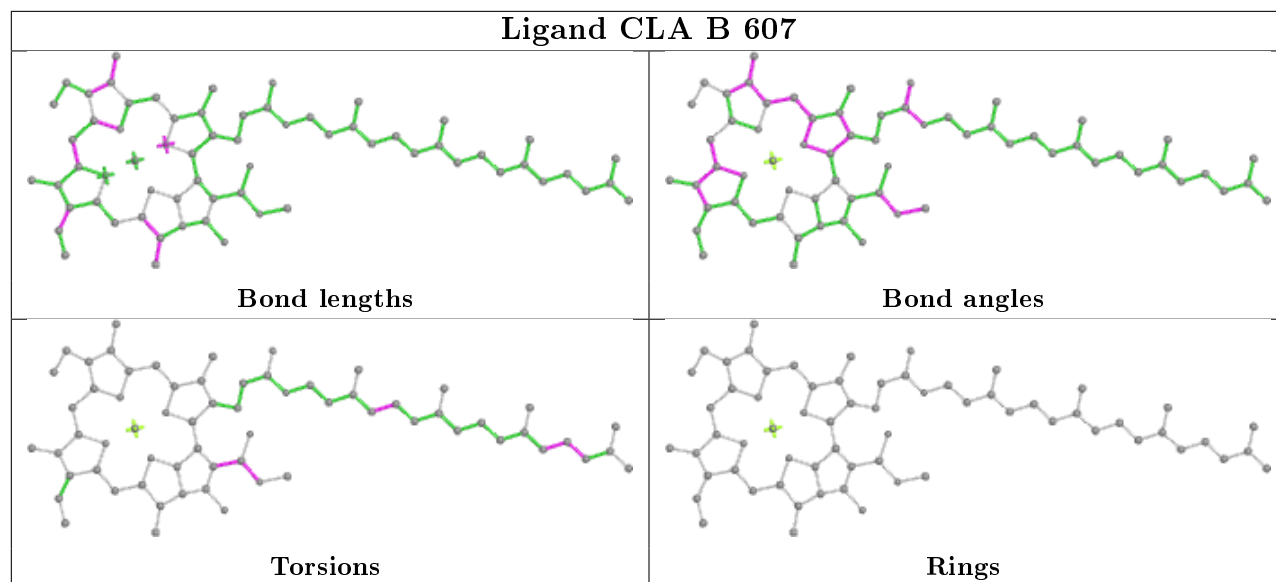
**Ligand LHG d 409****Ligand CLA a 410**

**Ligand CLA b 612****Ligand CLA C 513**

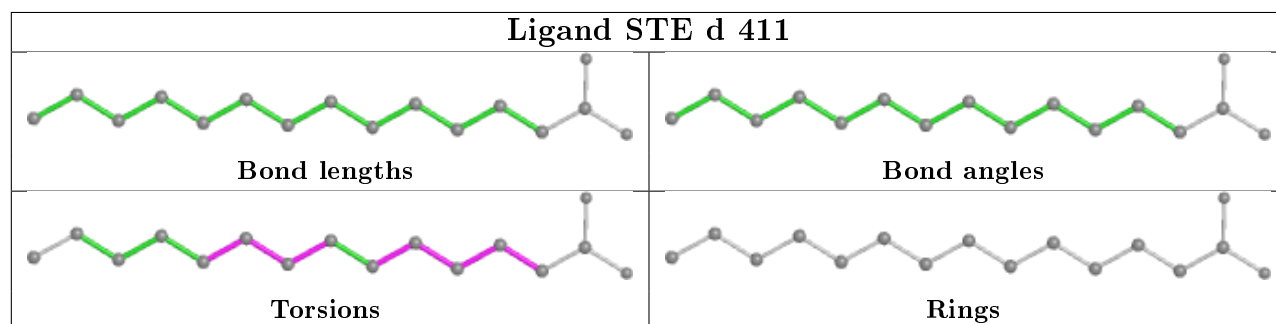
**Ligand CLA b 616****Ligand PHO d 401****Ligand BCR b 617**

**Ligand CLA A 402****Ligand LHG d 407**

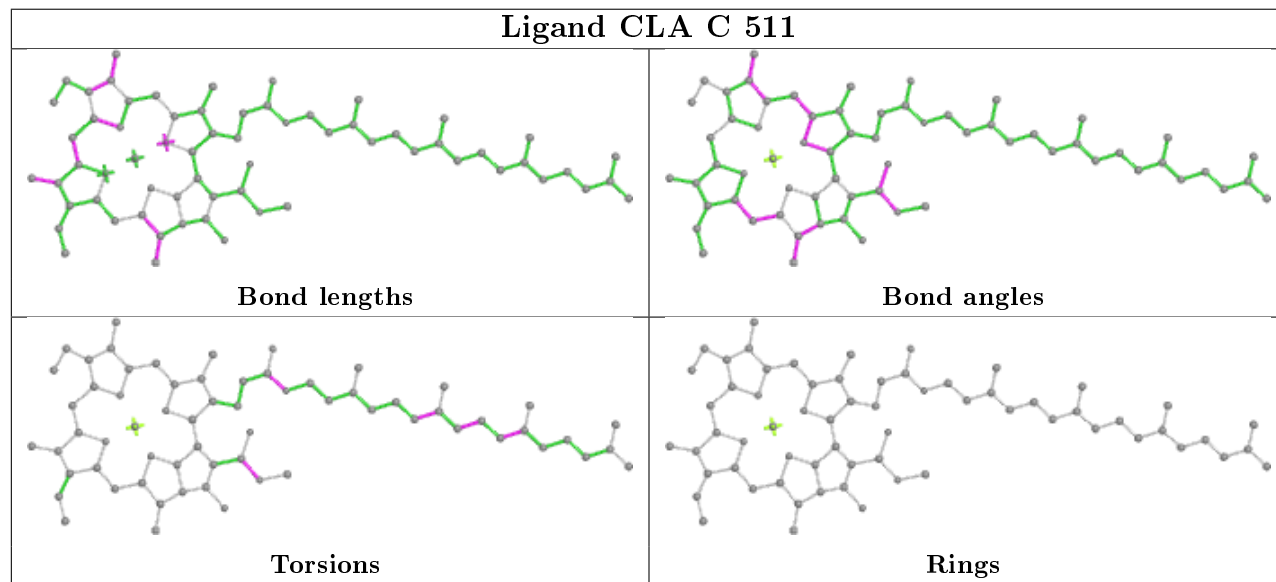
## Ligand CLA B 607

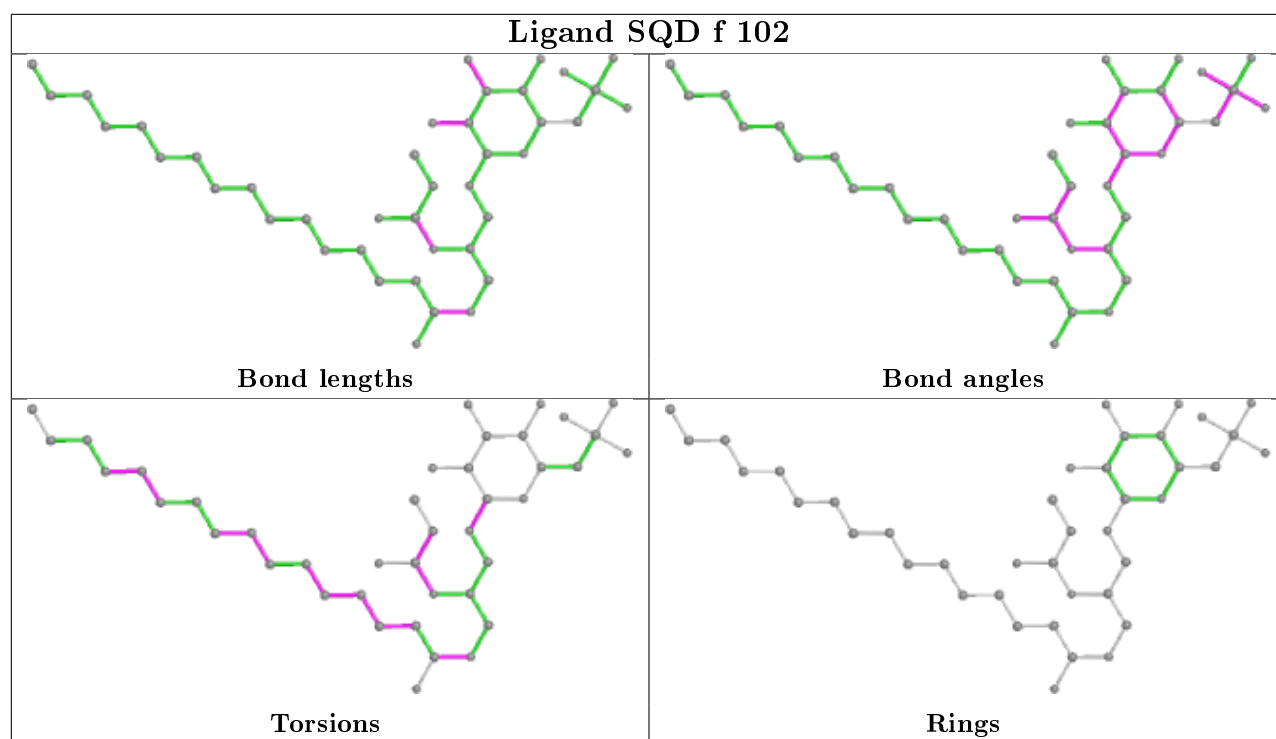


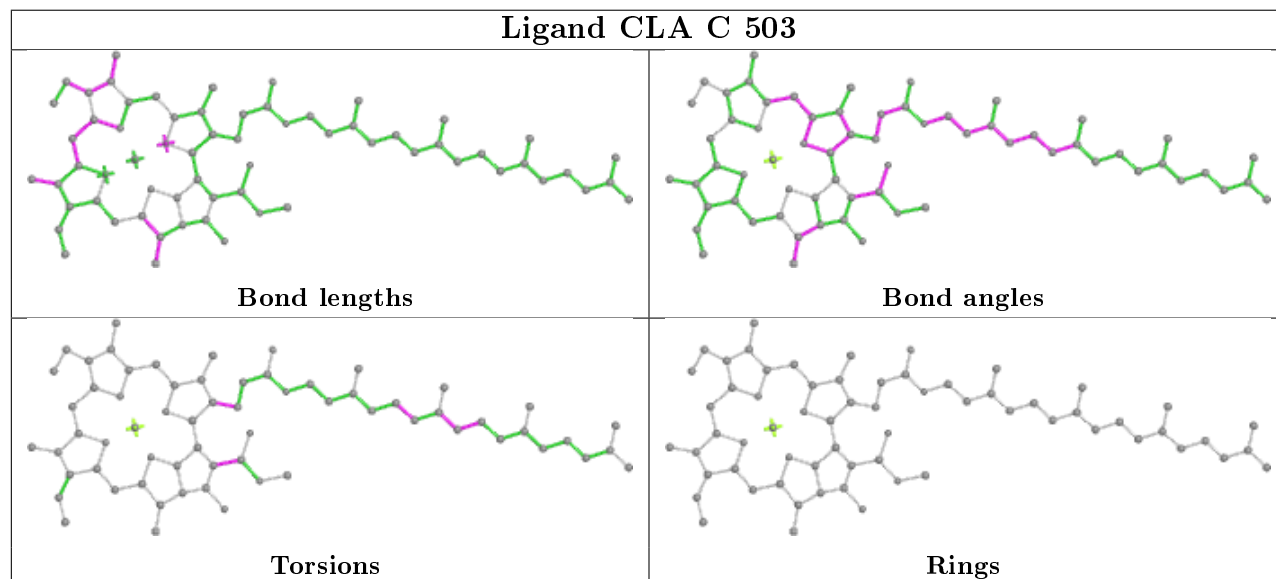
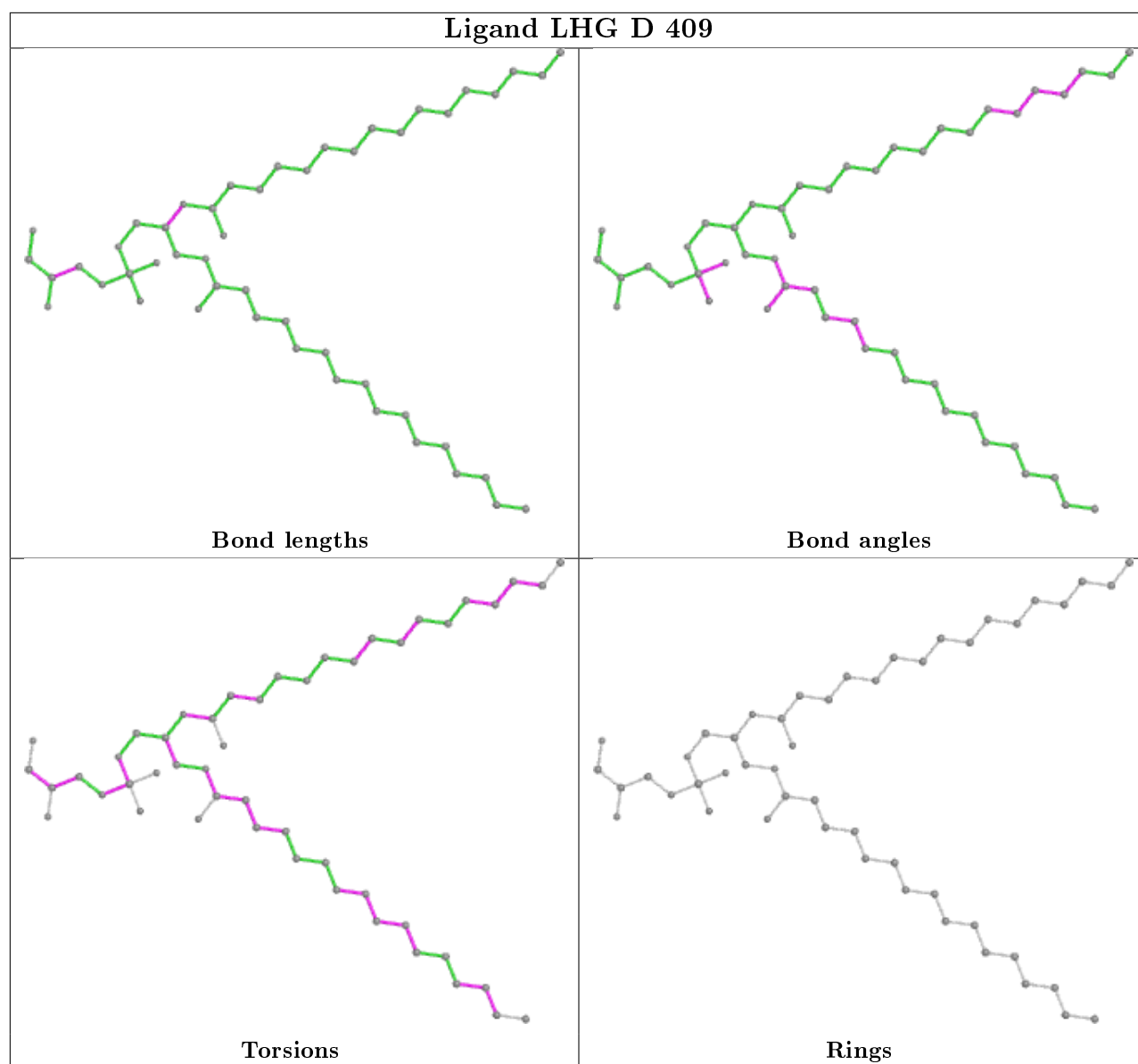
## Ligand STE d 411

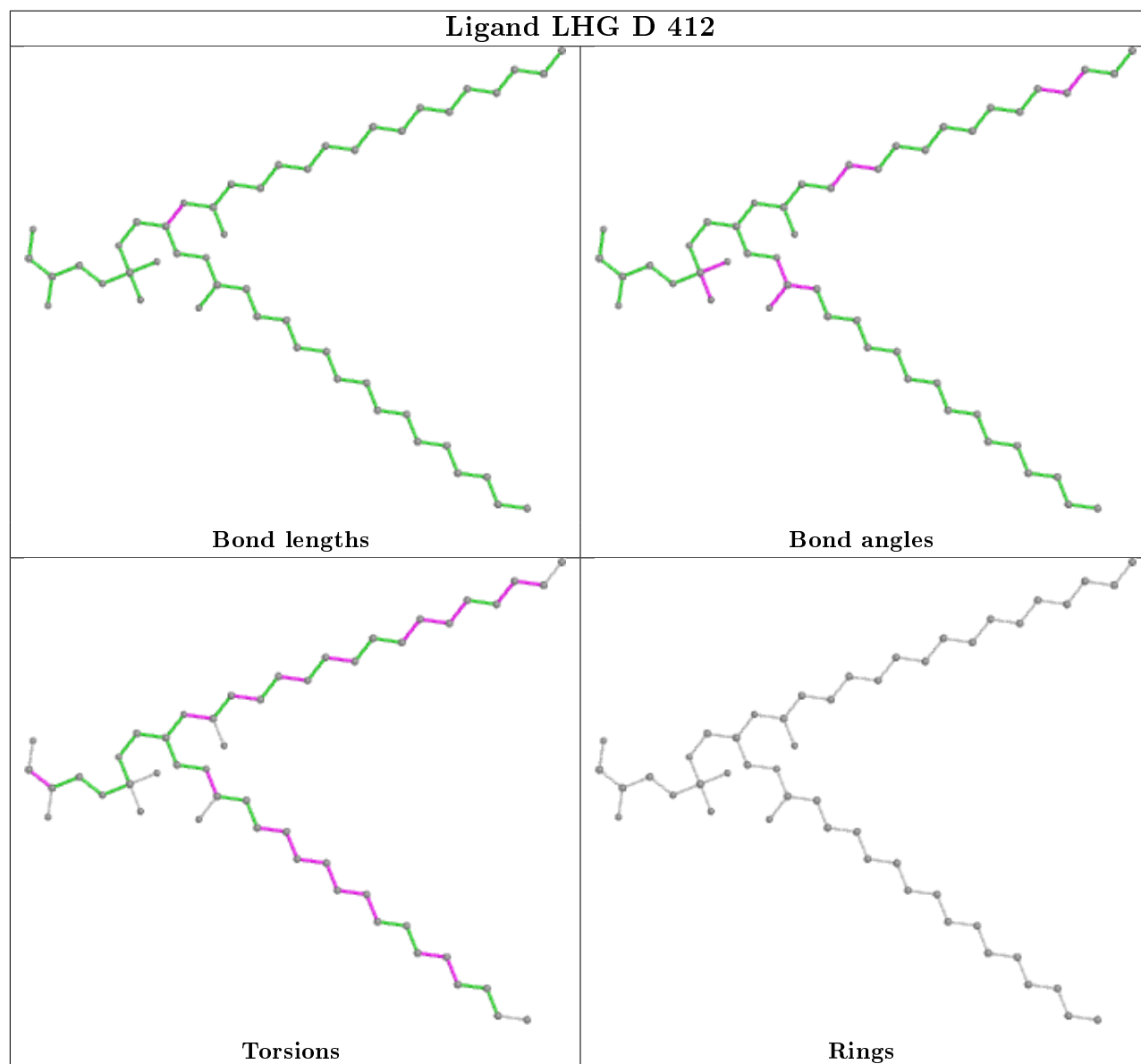
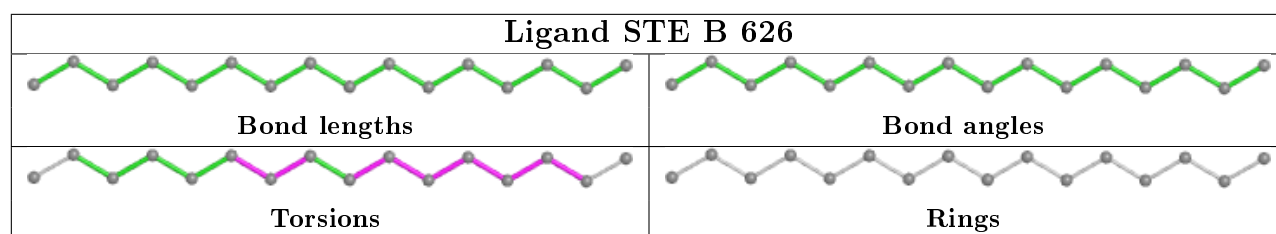


## Ligand CLA C 511

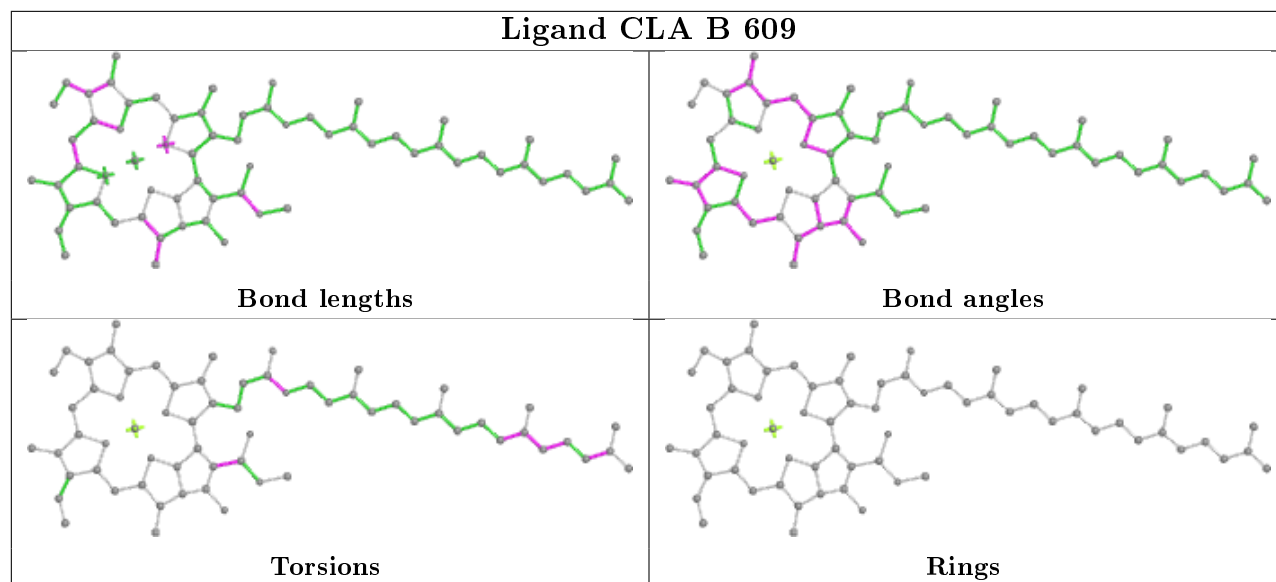




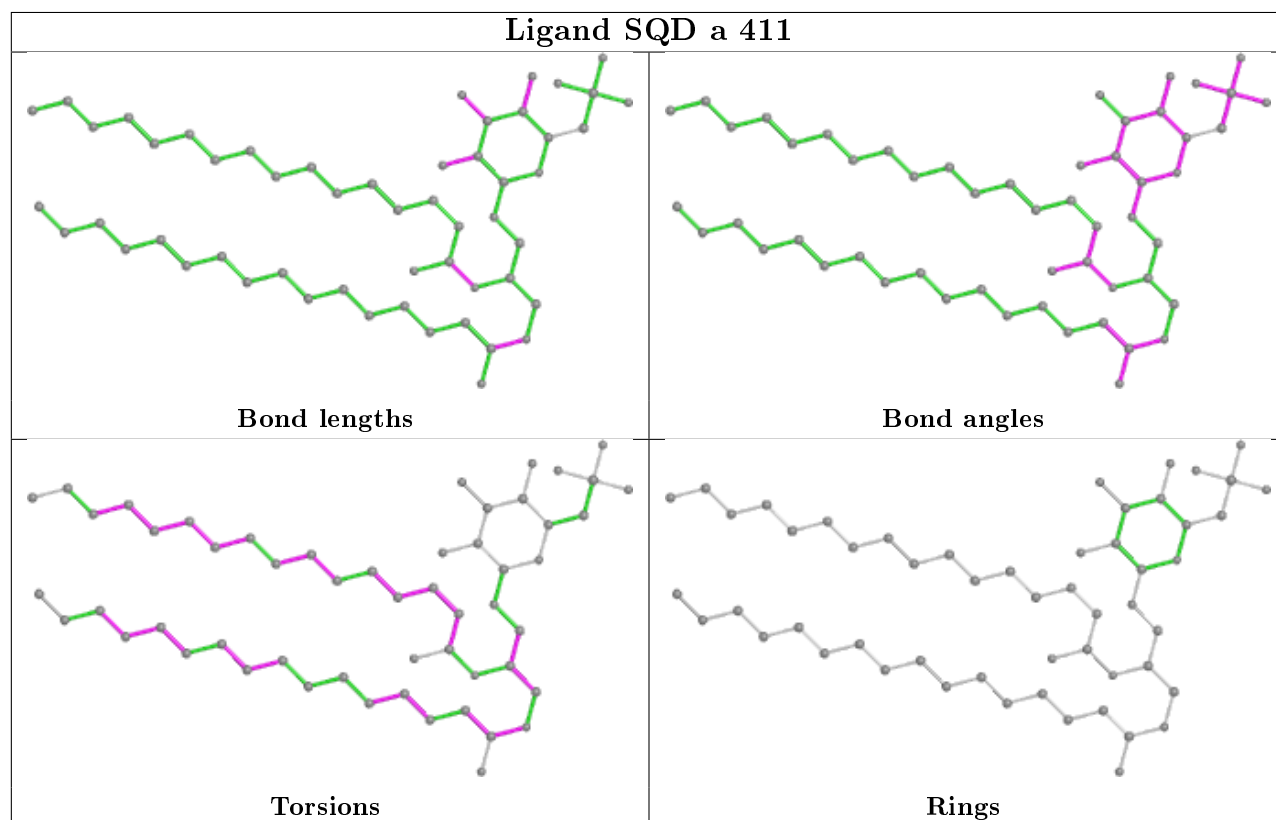




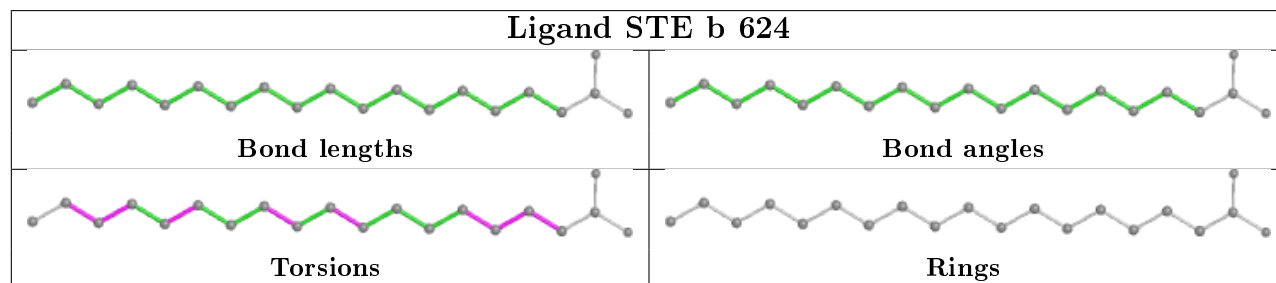
## Ligand CLA B 609

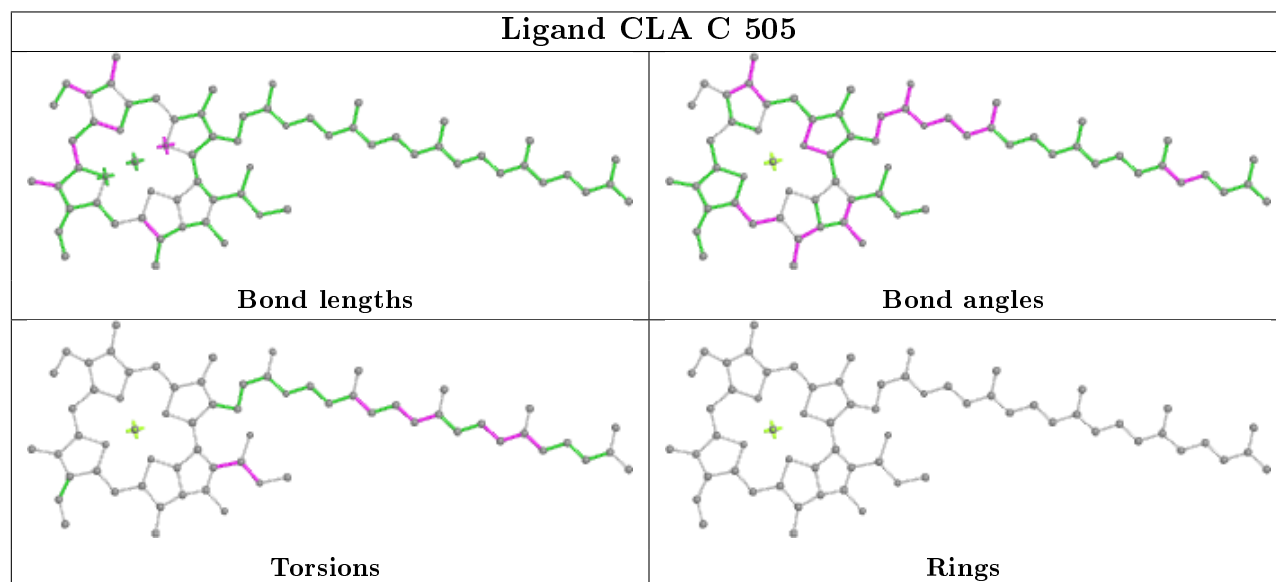
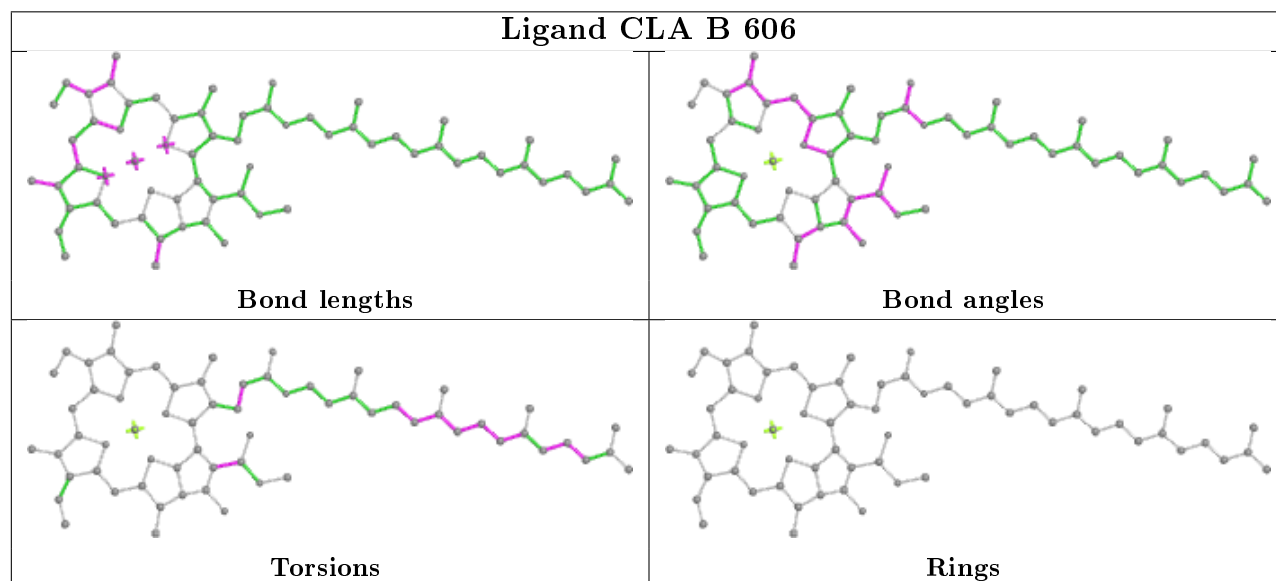
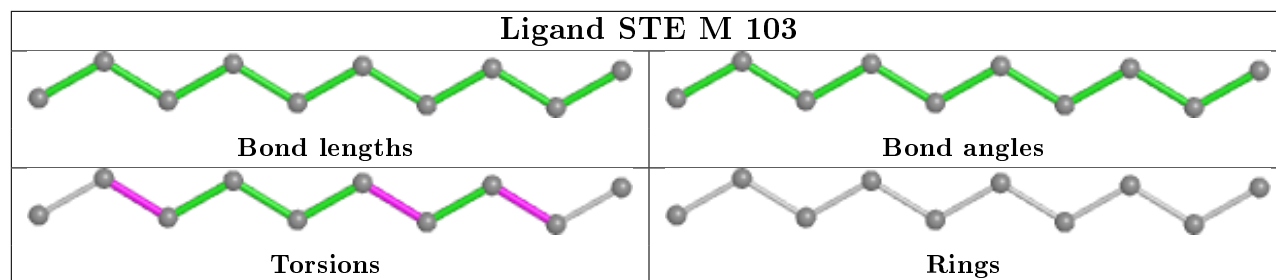


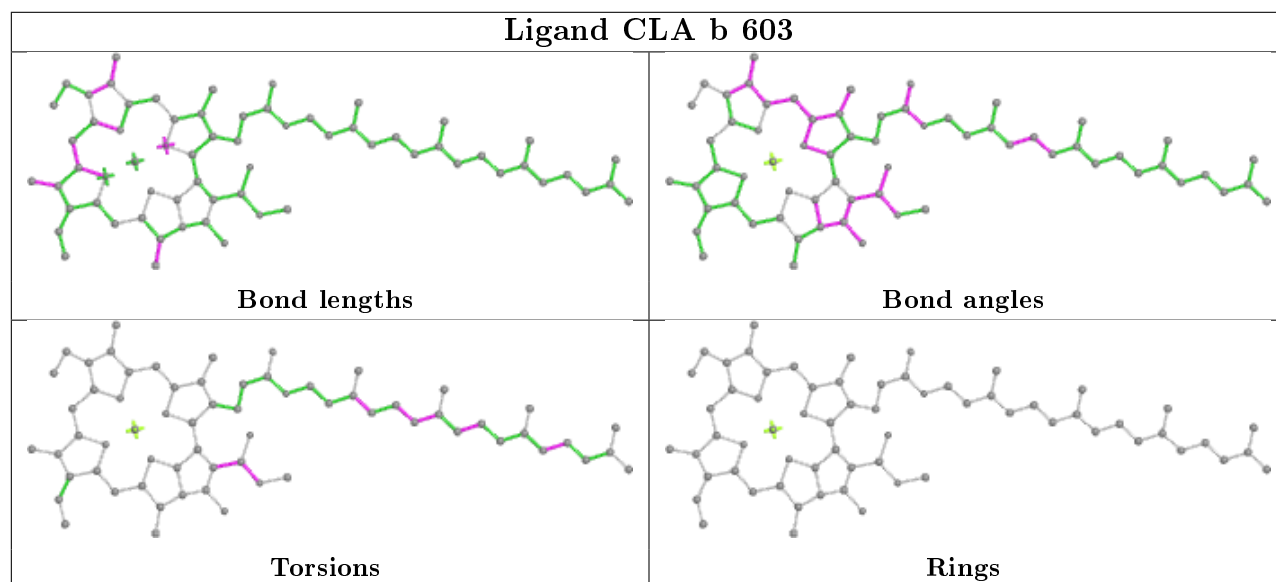
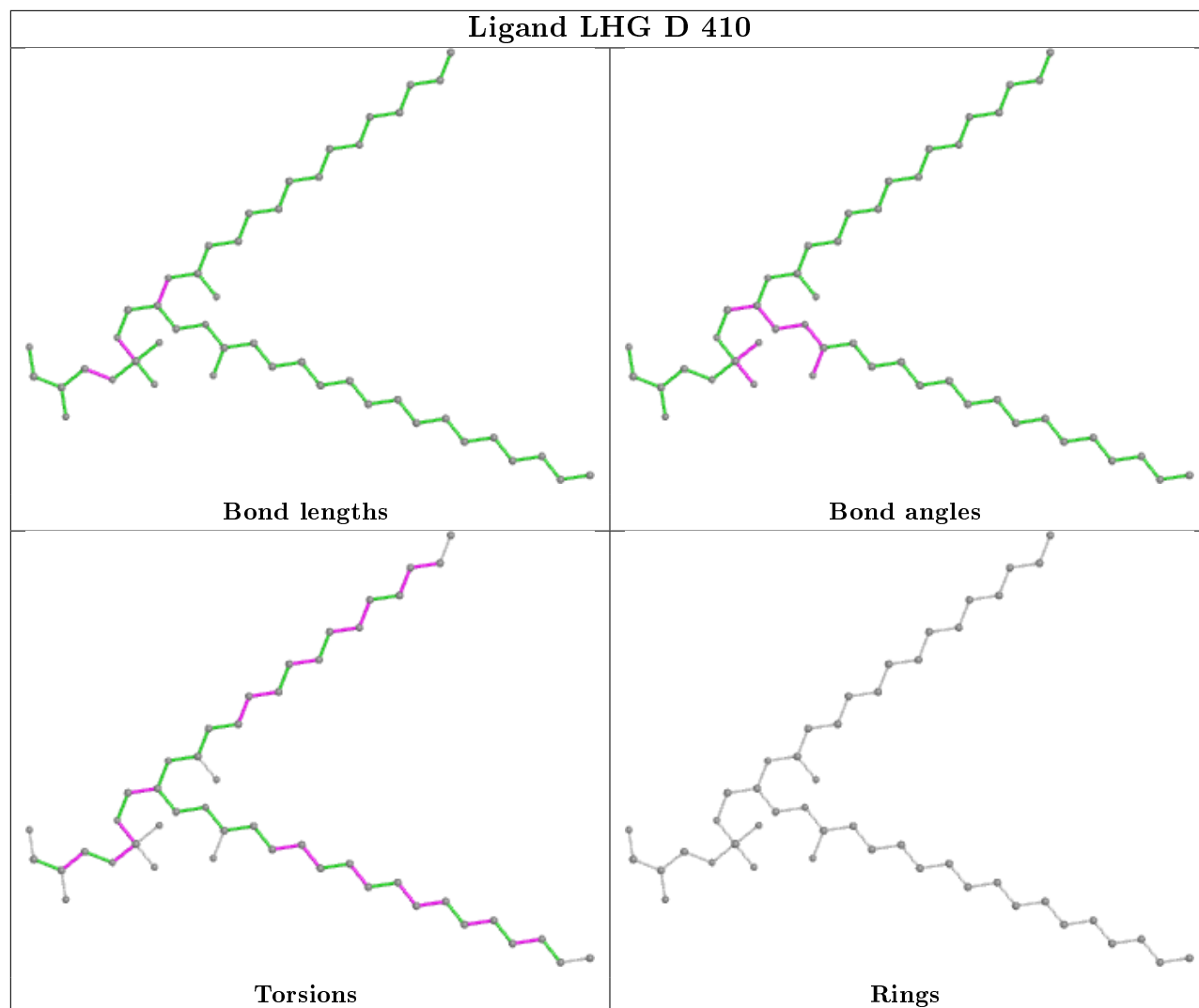
## Ligand SQD a 411

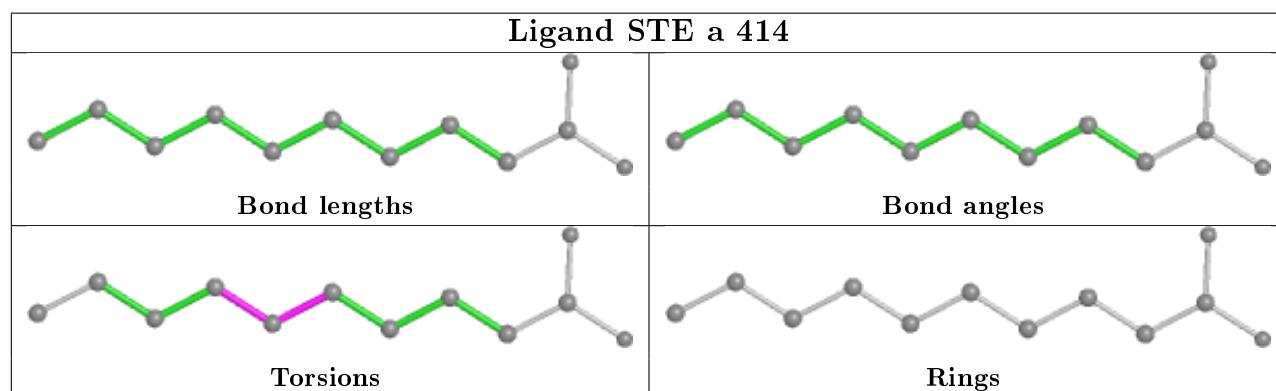
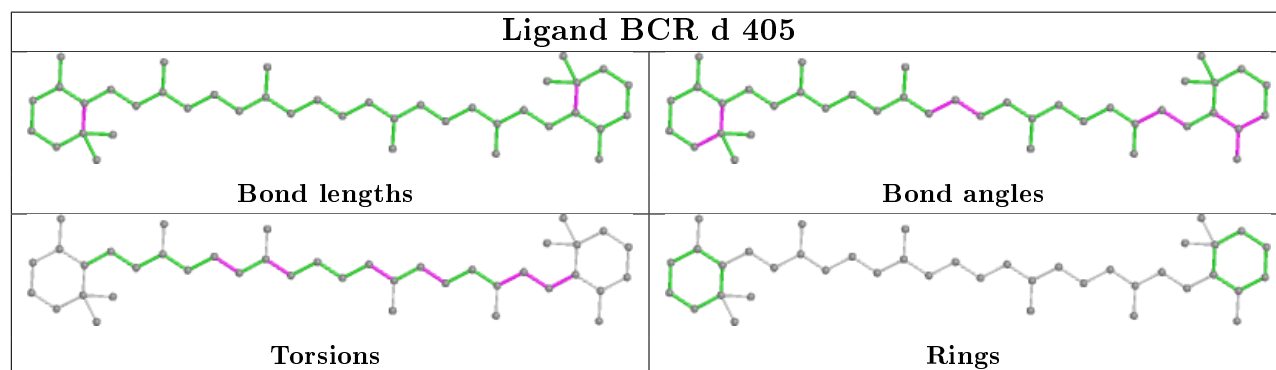
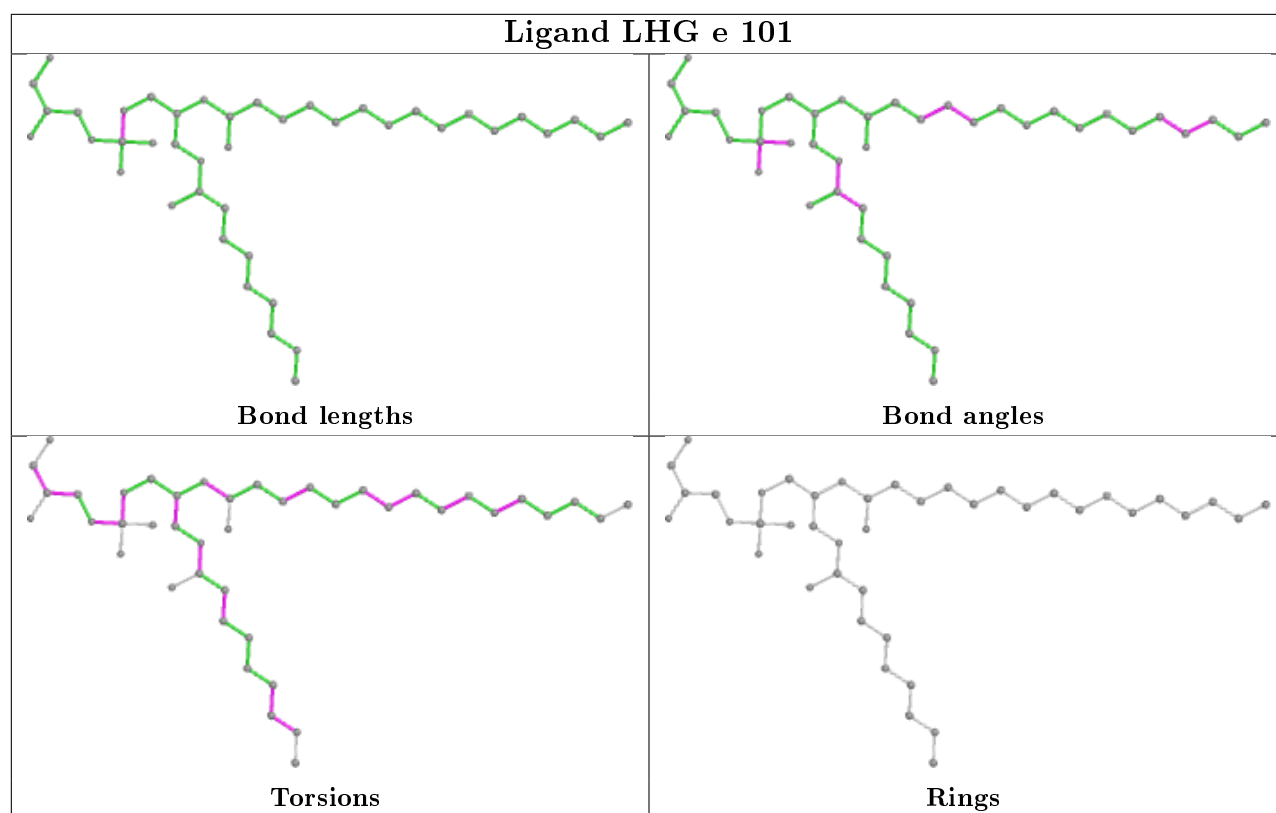


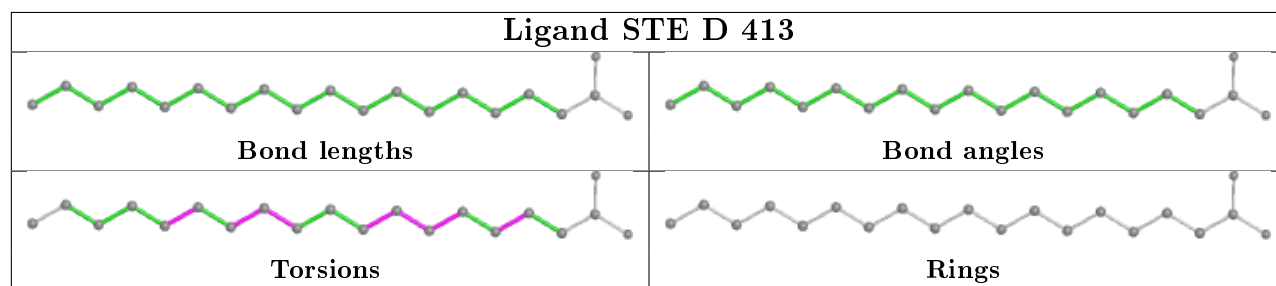
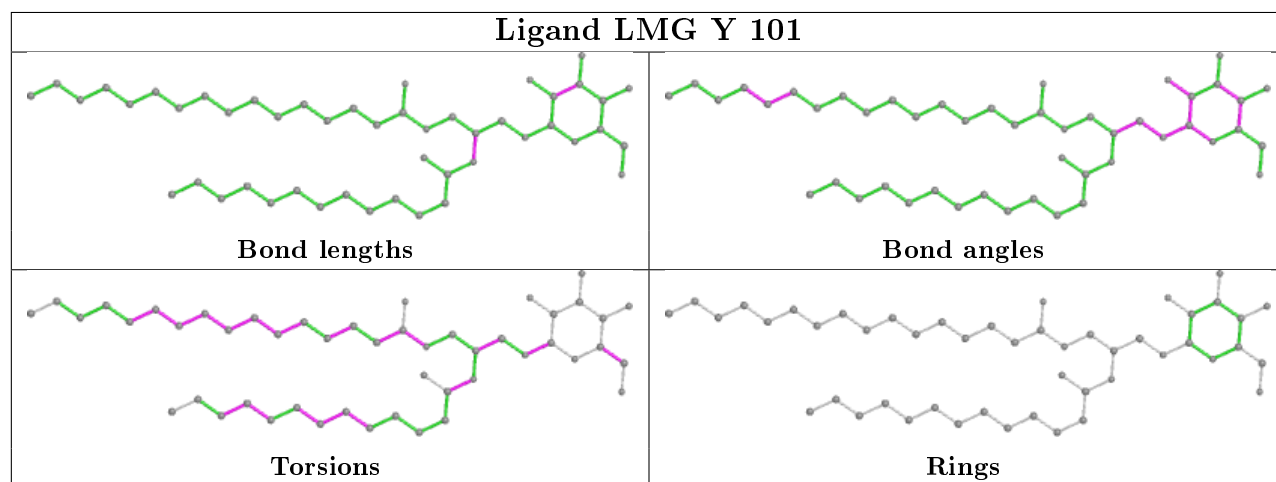
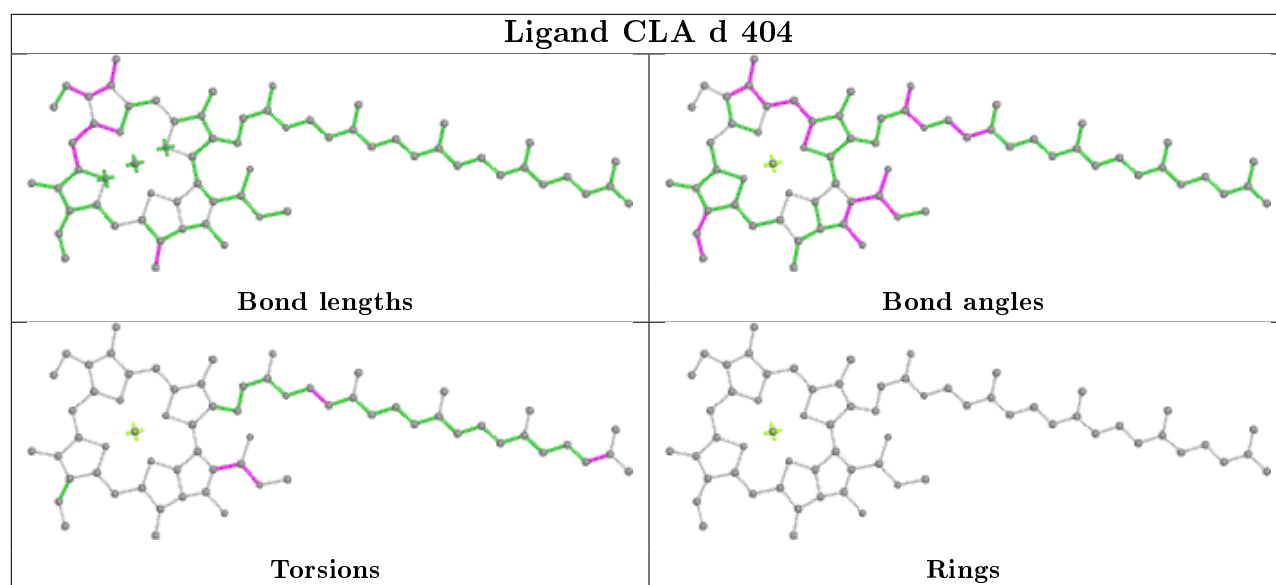
## Ligand STE b 624

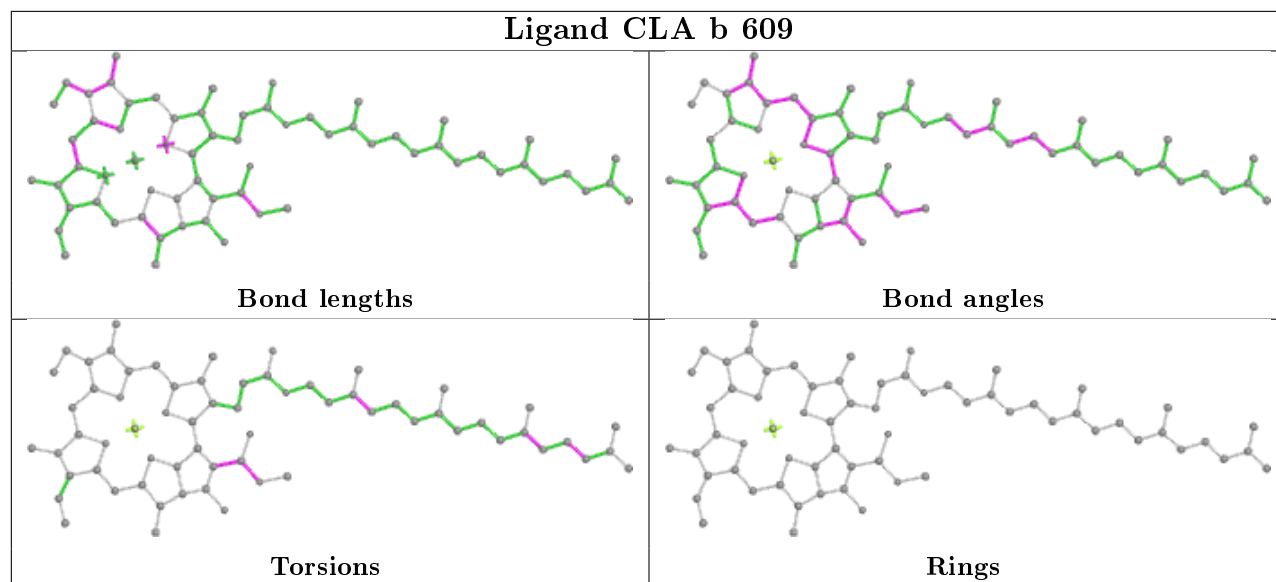
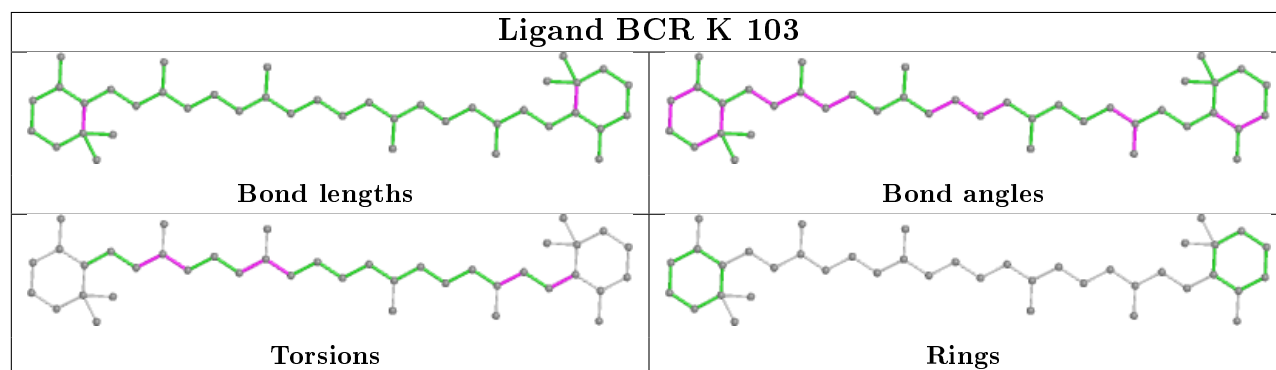
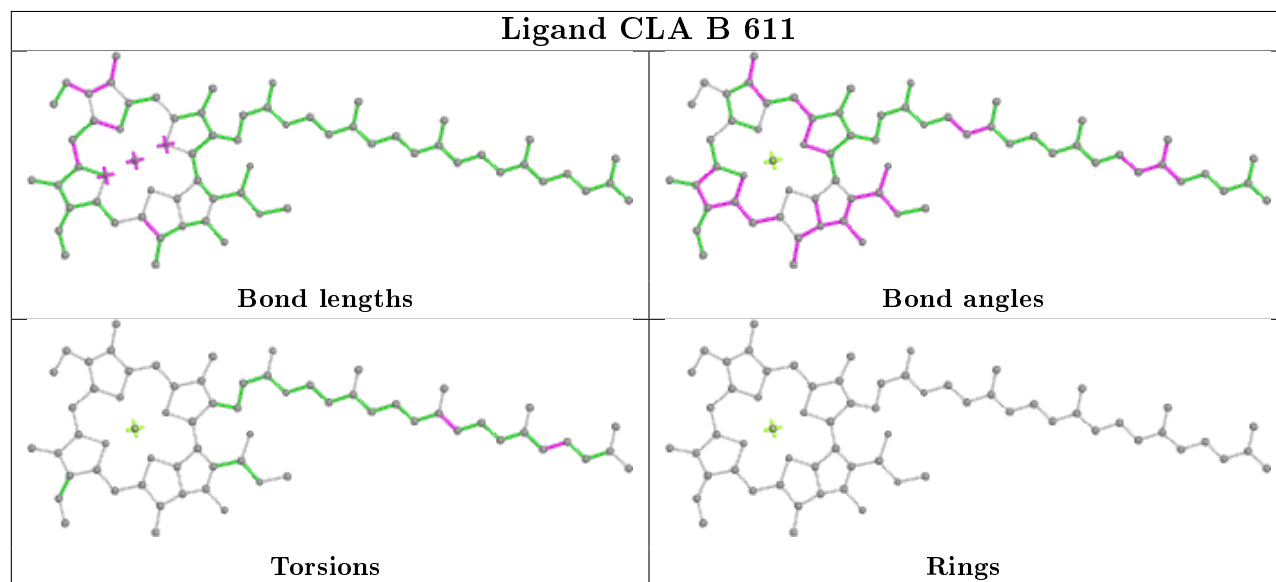


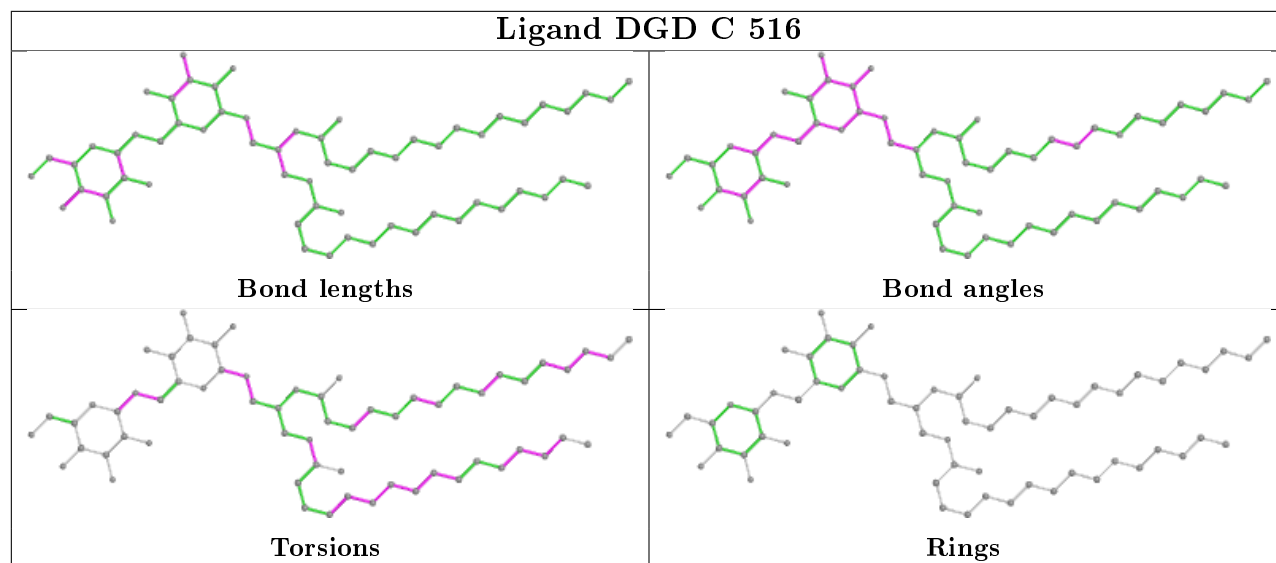








**Ligand CLA b 609****Ligand BCR K 103****Ligand CLA B 611**



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	-0.35	2 (0%) 89 91	21, 28, 49, 74	0
1	a	334/334 (100%)	-0.36	1 (0%) 94 94	22, 30, 56, 74	0
2	B	505/506 (99%)	-0.30	7 (1%) 75 78	22, 32, 61, 88	0
2	b	505/506 (99%)	-0.14	16 (3%) 47 53	21, 35, 69, 101	0
3	C	442/461 (95%)	-0.24	4 (0%) 84 86	23, 35, 51, 73	0
3	c	451/461 (97%)	-0.16	7 (1%) 72 75	25, 38, 59, 88	0
4	D	341/352 (96%)	-0.30	1 (0%) 94 94	20, 29, 48, 78	0
4	d	341/352 (96%)	-0.23	1 (0%) 94 94	22, 33, 55, 76	0
5	E	82/84 (97%)	0.05	4 (4%) 29 34	32, 50, 69, 76	0
5	e	82/84 (97%)	0.21	4 (4%) 29 34	38, 56, 76, 83	0
6	F	34/45 (75%)	-0.26	1 (2%) 51 56	34, 41, 62, 87	0
6	f	34/45 (75%)	-0.22	1 (2%) 51 56	41, 47, 75, 86	0
7	H	65/66 (98%)	-0.07	1 (1%) 73 76	30, 39, 57, 67	0
7	h	63/66 (95%)	0.22	3 (4%) 30 35	40, 48, 59, 71	0
8	I	35/38 (92%)	-0.09	3 (8%) 10 12	29, 37, 68, 80	0
8	i	35/38 (92%)	-0.24	2 (5%) 23 28	30, 39, 73, 77	0
9	J	36/40 (90%)	0.13	4 (11%) 5 6	33, 48, 73, 87	0
9	j	36/40 (90%)	0.21	4 (11%) 5 6	38, 50, 79, 91	0
10	K	37/46 (80%)	0.25	1 (2%) 54 59	42, 50, 66, 73	0
10	k	37/46 (80%)	0.08	1 (2%) 54 59	48, 54, 65, 75	0
11	L	37/37 (100%)	-0.44	0 100 100	23, 29, 59, 67	0
11	l	36/37 (97%)	-0.23	2 (5%) 24 28	24, 29, 69, 80	0
12	M	32/36 (88%)	-0.09	1 (3%) 49 54	26, 31, 56, 65	0
12	m	31/36 (86%)	-0.15	0 100 100	25, 32, 50, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.03	14 (5%) 23 28	25, 39, 76, 124	0
13	o	244/272 (89%)	-0.12	12 (4%) 29 34	23, 38, 72, 104	0
14	R	34/40 (85%)	2.46	19 (55%) 0 0	63, 73, 90, 102	0
14	r	31/40 (77%)	4.42	28 (90%) 0 0	70, 93, 109, 116	0
15	T	29/30 (96%)	-0.47	2 (6%) 16 20	24, 29, 58, 75	0
15	t	29/30 (96%)	-0.21	2 (6%) 16 20	25, 31, 72, 88	0
16	U	97/134 (72%)	-0.26	1 (1%) 82 84	30, 42, 64, 84	0
16	u	97/134 (72%)	-0.42	0 100 100	29, 38, 56, 78	0
17	V	137/163 (84%)	-0.45	0 100 100	29, 39, 55, 76	0
17	v	137/163 (84%)	-0.14	3 (2%) 62 66	30, 45, 65, 85	0
18	X	38/41 (92%)	-0.03	2 (5%) 26 31	38, 49, 71, 78	0
18	x	39/41 (95%)	0.54	5 (12%) 3 4	46, 57, 87, 100	0
19	Y	27/46 (58%)	1.31	8 (29%) 0 0	50, 69, 85, 92	0
19	y	30/46 (65%)	0.57	5 (16%) 1 1	58, 69, 81, 88	0
20	Z	62/62 (100%)	1.06	18 (29%) 0 0	53, 66, 109, 121	0
20	z	62/62 (100%)	0.95	12 (19%) 1 1	56, 67, 101, 116	0
All	All	5302/5666 (93%)	-0.11	202 (3%) 40 45	20, 36, 71, 124	0

The worst 5 of 202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	9.0
2	b	495	PHE	7.7
13	o	58	ASN	7.4
14	r	9	LEU	7.2
20	z	33	TRP	7.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.95	0.12	40,53,69,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	FME	T	1	10/11	0.95	0.09	29,44,67,67	0
12	FME	m	1	10/11	0.95	0.10	33,47,65,76	0
8	FME	I	1	10/11	0.95	0.12	40,48,64,66	0
8	FME	i	1	10/11	0.96	0.18	40,50,65,66	0
15	FME	t	1	10/11	0.96	0.09	28,43,73,73	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
31	STE	E	102	12/20	0.68	0.42	46,78,92,94	0
31	STE	a	414	12/20	0.71	0.26	40,65,71,75	0
31	STE	b	624	20/20	0.75	0.21	41,60,75,89	0
31	STE	B	627	15/20	0.76	0.16	36,61,74,77	0
31	STE	B	626	16/20	0.76	0.29	35,58,78,79	0
31	STE	H	104	18/20	0.77	0.27	44,73,89,94	0
26	PL9	A	409	55/55	0.78	0.31	47,68,94,97	0
31	STE	j	101	12/20	0.78	0.17	42,56,74,75	0
31	STE	c	501	12/20	0.79	0.19	54,68,87,89	0
26	PL9	a	409	55/55	0.79	0.25	47,74,93,96	0
24	BCR	H	102	40/40	0.80	0.16	30,50,66,75	0
31	STE	C	519	16/20	0.80	0.17	42,58,73,77	0
27	LMG	c	522	48/55	0.80	0.23	46,80,104,108	0
31	STE	b	625	10/20	0.81	0.22	44,53,61,73	0
33	LHG	E	101	49/49	0.81	0.25	50,83,110,126	0
28	SQD	a	412	36/54	0.81	0.19	29,63,90,97	0
33	LHG	e	101	42/49	0.81	0.27	65,87,116,127	0
27	LMG	D	411	33/55	0.81	0.19	34,56,84,89	0
31	STE	I	101	15/20	0.82	0.17	37,55,73,76	0
27	LMG	a	415	55/55	0.82	0.17	34,58,80,92	0
31	STE	B	620	17/20	0.82	0.16	32,50,63,71	0
22	CLA	b	601	65/65	0.82	0.17	43,68,89,92	0
24	BCR	h	101	40/40	0.82	0.15	35,54,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	STE	m	101	18/20	0.83	0.13	34,51,78,79	0
31	STE	a	413	10/20	0.83	0.20	38,61,67,68	0
27	LMG	b	623	55/55	0.84	0.27	42,70,95,101	0
31	STE	d	413	20/20	0.84	0.21	42,57,76,84	0
22	CLA	C	512	65/65	0.84	0.17	35,55,82,95	0
31	STE	B	624	12/20	0.84	0.11	32,48,63,76	0
29	DGD	A	413	66/66	0.84	0.18	44,62,78,99	0
31	STE	c	521	20/20	0.85	0.20	37,55,93,103	0
31	STE	m	102	12/20	0.85	0.19	46,61,76,76	0
22	CLA	c	514	65/65	0.85	0.20	39,67,109,116	0
31	STE	b	626	14/20	0.85	0.22	51,65,84,88	0
31	STE	T	102	15/20	0.85	0.20	44,59,83,85	0
24	BCR	K	102	40/40	0.85	0.13	33,53,68,74	0
31	STE	B	623	14/20	0.86	0.13	36,47,56,62	0
22	CLA	c	513	65/65	0.86	0.16	38,56,91,106	0
28	SQD	A	412	39/54	0.86	0.19	42,61,90,93	0
22	CLA	H	101	65/65	0.86	0.16	33,63,91,110	0
31	STE	b	627	20/20	0.86	0.16	38,64,84,90	0
28	SQD	L	101	49/54	0.87	0.14	38,60,89,107	0
24	BCR	K	101	40/40	0.87	0.16	40,58,75,82	0
28	SQD	B	622	54/54	0.87	0.14	37,61,91,101	0
31	STE	d	411	16/20	0.87	0.16	45,62,78,83	0
31	STE	Z	101	8/20	0.88	0.14	50,61,70,70	0
22	CLA	C	513	65/65	0.88	0.18	38,64,97,109	0
31	STE	b	622	20/20	0.88	0.24	36,54,79,85	0
31	STE	B	625	18/20	0.88	0.11	40,58,76,83	0
31	STE	M	102	15/20	0.88	0.17	32,48,69,74	0
24	BCR	k	102	40/40	0.88	0.18	40,55,67,68	0
31	STE	D	413	20/20	0.88	0.15	34,54,71,79	0
31	STE	J	101	12/20	0.89	0.11	45,59,69,77	0
28	SQD	f	102	41/54	0.89	0.20	55,91,113,119	0
31	STE	d	412	17/20	0.89	0.14	41,56,67,74	0
31	STE	B	601	12/20	0.89	0.49	51,67,78,86	0
27	LMG	Y	101	48/55	0.89	0.14	34,68,86,99	0
27	LMG	c	523	49/55	0.89	0.14	30,56,82,98	0
24	BCR	k	101	40/40	0.89	0.13	42,60,81,85	0
22	CLA	c	503	65/65	0.90	0.16	29,41,62,66	0
27	LMG	A	410	48/55	0.90	0.14	38,57,72,87	0
31	STE	b	620	16/20	0.90	0.14	35,46,64,71	0
31	STE	M	103	10/20	0.90	0.13	34,47,64,70	0
31	STE	C	520	12/20	0.90	0.10	34,46,57,58	0
22	CLA	C	502	65/65	0.90	0.14	26,42,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	d	404	65/65	0.90	0.17	32,49,89,106	0
27	LMG	c	520	37/55	0.90	0.16	40,67,80,83	0
22	CLA	c	509	64/65	0.91	0.14	27,46,86,103	0
24	BCR	F	101	40/40	0.91	0.12	21,44,82,90	0
22	CLA	b	616	60/65	0.91	0.12	24,42,86,88	0
22	CLA	C	507	65/65	0.91	0.14	20,40,56,66	0
31	STE	C	518	12/20	0.91	0.10	41,55,62,66	0
27	LMG	M	101	51/55	0.91	0.12	31,48,72,90	0
27	LMG	b	621	51/55	0.91	0.12	32,53,76,97	0
22	CLA	a	405	65/65	0.91	0.14	18,35,82,91	0
24	BCR	d	405	40/40	0.91	0.12	28,54,85,95	0
22	CLA	D	405	65/65	0.91	0.13	22,42,107,119	0
24	BCR	c	515	40/40	0.91	0.15	41,62,76,77	0
24	BCR	C	514	40/40	0.91	0.11	23,38,55,63	0
29	DGD	C	516	62/66	0.91	0.13	34,51,97,119	0
24	BCR	B	619	40/40	0.92	0.09	25,42,61,72	0
22	CLA	b	615	65/65	0.92	0.13	24,39,59,63	0
22	CLA	c	506	65/65	0.92	0.16	24,40,64,70	0
24	BCR	b	619	40/40	0.92	0.11	31,47,63,67	0
27	LMG	B	621	28/55	0.92	0.14	35,51,65,73	0
22	CLA	b	602	65/65	0.92	0.15	26,44,65,72	0
27	LMG	D	407	51/55	0.92	0.16	27,56,86,93	0
28	SQD	D	408	36/54	0.92	0.17	46,75,89,100	0
22	CLA	B	616	60/65	0.92	0.15	25,39,94,110	0
24	BCR	K	103	40/40	0.92	0.17	36,54,67,69	0
22	CLA	c	512	65/65	0.92	0.12	39,52,65,74	0
29	DGD	c	518	62/66	0.93	0.11	33,50,90,96	0
22	CLA	c	508	65/65	0.93	0.14	28,44,59,63	0
22	CLA	c	504	65/65	0.93	0.14	28,41,54,58	0
29	DGD	h	102	62/66	0.93	0.11	29,48,65,68	0
28	SQD	a	411	54/54	0.93	0.15	39,62,94,96	0
22	CLA	C	506	65/65	0.93	0.12	28,45,83,99	0
22	CLA	c	507	65/65	0.93	0.13	29,48,102,109	0
22	CLA	C	505	65/65	0.93	0.16	19,39,71,77	0
24	BCR	T	101	40/40	0.93	0.10	23,39,52,52	0
24	BCR	B	618	40/40	0.93	0.10	23,39,50,52	0
29	DGD	H	103	62/66	0.93	0.11	29,46,61,73	0
22	CLA	C	510	65/65	0.93	0.14	27,46,62,66	0
22	CLA	B	615	65/65	0.93	0.12	21,38,60,69	0
22	CLA	b	609	65/65	0.93	0.13	27,43,64,74	0
24	BCR	c	516	40/40	0.93	0.11	22,44,60,72	0
22	CLA	c	511	65/65	0.93	0.15	29,47,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	B	614	65/65	0.94	0.15	20,36,75,87	0
22	CLA	c	510	65/65	0.94	0.17	33,47,70,77	0
24	BCR	A	406	40/40	0.94	0.09	23,35,43,47	0
22	CLA	B	613	65/65	0.94	0.14	17,31,71,73	0
22	CLA	b	608	65/65	0.94	0.15	25,42,60,69	0
24	BCR	b	618	40/40	0.94	0.10	22,38,51,52	0
22	CLA	C	509	65/65	0.94	0.17	25,46,62,69	0
29	DGD	C	517	62/66	0.94	0.11	26,46,77,87	0
22	CLA	a	410	65/65	0.94	0.12	17,29,48,54	0
22	CLA	b	612	65/65	0.94	0.17	15,33,48,57	0
27	LMG	d	410	44/55	0.94	0.13	31,51,89,104	0
24	BCR	t	101	40/40	0.94	0.09	23,38,51,52	0
24	BCR	b	617	40/40	0.94	0.11	25,41,54,59	0
22	CLA	c	505	60/65	0.94	0.11	32,45,76,89	0
22	CLA	C	511	65/65	0.94	0.11	27,49,66,77	0
22	CLA	b	610	65/65	0.94	0.18	23,36,50,56	0
22	CLA	C	503	65/65	0.94	0.13	32,42,51,61	0
22	CLA	b	614	65/65	0.94	0.12	21,38,78,86	0
22	CLA	B	606	65/65	0.94	0.10	23,36,69,86	0
22	CLA	B	609	65/65	0.94	0.13	24,39,57,69	0
24	BCR	a	406	40/40	0.94	0.09	19,32,50,55	0
22	CLA	A	403	65/65	0.94	0.14	21,34,97,110	0
29	DGD	c	519	62/66	0.94	0.13	28,54,83,91	0
22	CLA	B	604	65/65	0.94	0.12	19,32,79,84	0
29	DGD	C	515	62/66	0.94	0.12	21,40,73,87	0
26	PL9	D	406	55/55	0.94	0.10	21,34,49,54	0
22	CLA	C	504	59/65	0.94	0.12	27,41,81,83	0
22	CLA	A	405	54/65	0.94	0.11	18,31,66,72	0
22	CLA	a	403	65/65	0.94	0.14	25,40,97,106	0
22	CLA	b	606	65/65	0.94	0.11	22,37,73,77	0
22	CLA	B	602	65/65	0.94	0.15	20,36,55,66	0
22	CLA	b	613	65/65	0.94	0.14	17,34,73,87	0
22	CLA	C	508	65/65	0.94	0.11	25,42,97,107	0
26	PL9	d	406	55/55	0.95	0.10	22,33,42,53	0
33	LHG	d	407	49/49	0.95	0.12	33,49,76,80	0
29	DGD	c	517	62/66	0.95	0.11	24,42,84,94	0
22	CLA	C	501	65/65	0.95	0.12	19,36,51,56	0
22	CLA	b	611	65/65	0.95	0.13	19,34,53,61	0
22	CLA	B	605	65/65	0.95	0.14	19,31,47,52	0
23	PHO	A	404	64/64	0.95	0.10	18,28,40,48	0
22	CLA	D	404	65/65	0.95	0.10	19,28,52,62	0
22	CLA	B	603	65/65	0.95	0.14	15,32,63,67	0

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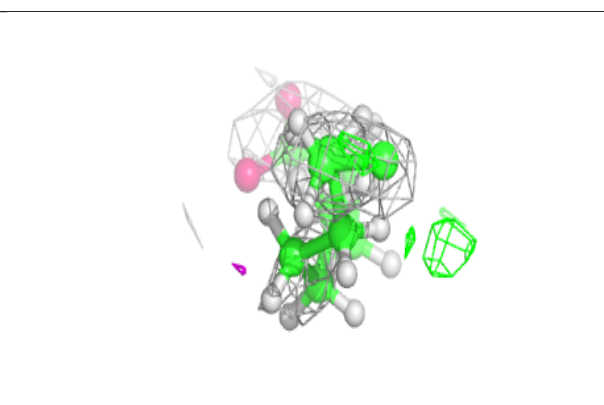
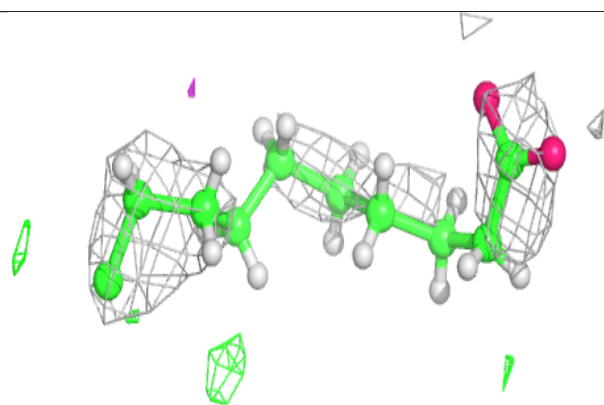
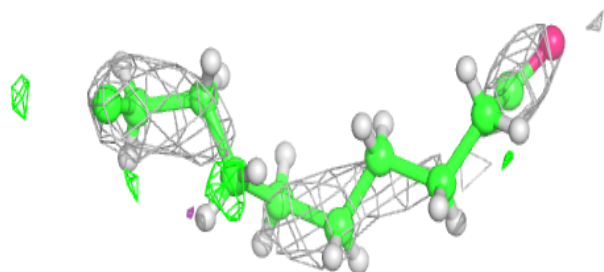
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	B	612	65/65	0.95	0.14	19,31,47,56	0
22	CLA	d	403	65/65	0.95	0.11	19,34,54,65	0
22	CLA	c	502	65/65	0.95	0.13	26,41,53,57	0
22	CLA	b	605	65/65	0.95	0.11	21,34,49,53	0
33	LHG	D	410	47/49	0.95	0.12	24,46,82,99	0
24	BCR	B	617	40/40	0.95	0.11	24,38,59,60	0
34	HEC	F	102	43/43	0.95	0.12	37,48,64,66	0
22	CLA	D	403	65/65	0.95	0.12	15,29,52,61	0
22	CLA	B	610	65/65	0.95	0.15	18,33,46,50	0
33	LHG	d	409	39/49	0.95	0.10	29,45,72,80	0
22	CLA	B	608	65/65	0.95	0.12	20,34,56,61	0
22	CLA	b	604	65/65	0.95	0.12	20,33,81,91	0
23	PHO	a	404	64/64	0.95	0.13	19,29,40,44	0
22	CLA	B	611	65/65	0.95	0.13	19,30,46,50	0
28	SQD	A	411	52/54	0.95	0.14	34,59,84,88	0
22	CLA	b	603	65/65	0.96	0.12	18,36,65,76	0
23	PHO	D	401	64/64	0.96	0.13	21,32,44,48	0
33	LHG	L	102	49/49	0.96	0.10	26,41,53,60	0
33	LHG	D	412	49/49	0.96	0.11	30,44,65,76	0
23	PHO	d	401	64/64	0.96	0.11	20,37,47,61	0
33	LHG	l	101	49/49	0.96	0.10	26,45,55,64	0
22	CLA	A	402	65/65	0.96	0.10	16,26,46,49	0
22	CLA	a	402	65/65	0.96	0.10	19,29,46,56	0
22	CLA	B	607	65/65	0.96	0.10	14,34,62,66	0
22	CLA	b	607	65/65	0.96	0.12	18,35,69,78	0
34	HEC	f	101	43/43	0.96	0.12	42,58,81,84	0
34	HEC	v	201	43/43	0.97	0.12	27,37,50,51	0
34	HEC	V	201	43/43	0.97	0.13	19,35,43,44	0
33	LHG	d	408	49/49	0.97	0.09	23,42,57,68	0
33	LHG	D	409	49/49	0.97	0.09	26,41,53,56	0
25	CL	A	407	1/1	0.98	0.06	29,29,29,29	0
32	BCT	d	402	4/4	0.98	0.17	31,35,44,53	0
32	BCT	D	402	4/4	0.98	0.17	22,26,32,36	0
21	FE2	A	401	1/1	0.99	0.10	26,26,26,26	0
30	OEX	A	414	10/10	0.99	0.11	22,26,28,29	0
25	CL	A	408	1/1	0.99	0.03	30,30,30,30	0
30	OEX	a	416	10/10	0.99	0.12	23,26,30,31	0
25	CL	a	408	1/1	0.99	0.05	28,28,28,28	0
21	FE2	a	401	1/1	0.99	0.08	34,34,34,34	0
25	CL	a	407	1/1	0.99	0.02	28,28,28,28	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.

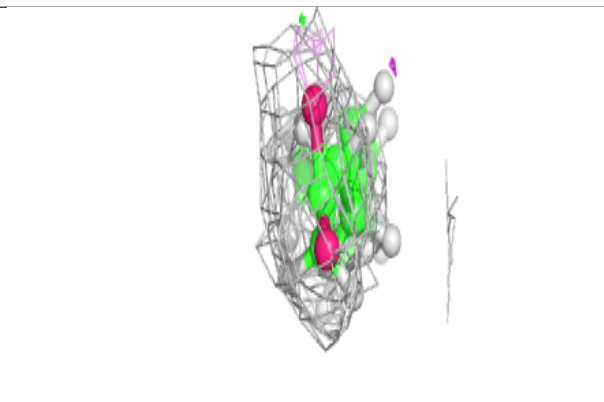
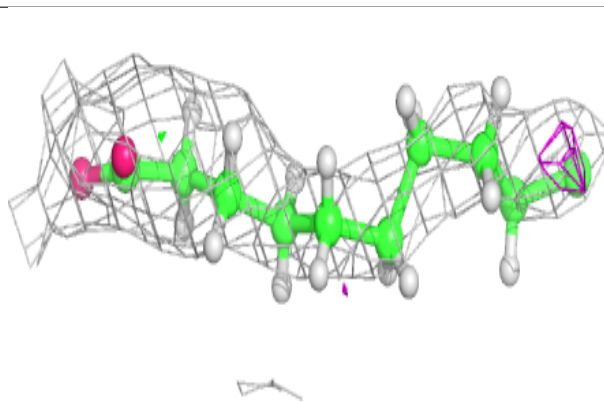
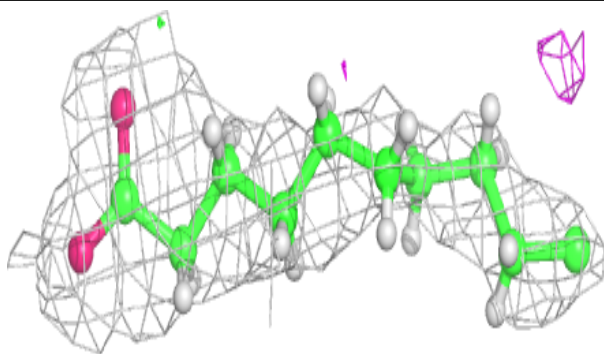
**Electron density around STE E 102:**

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



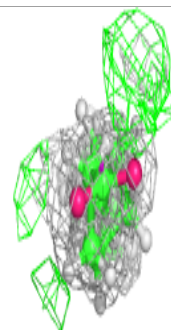
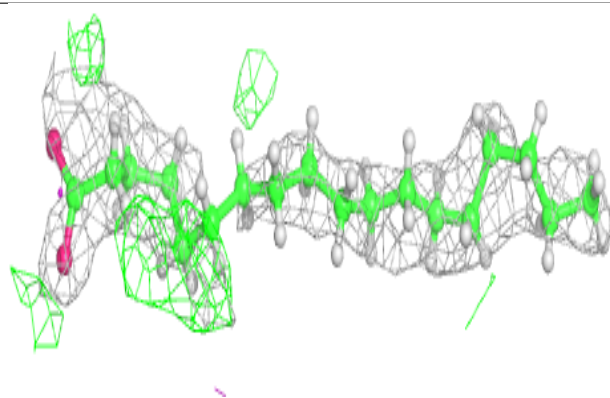
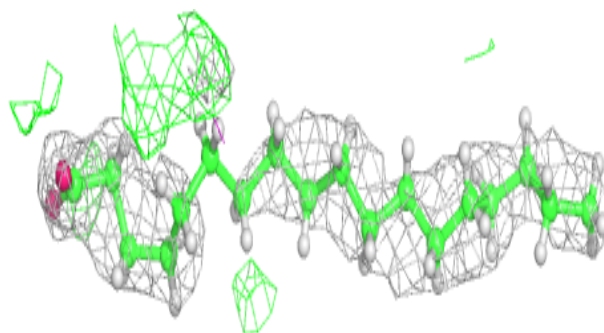
**Electron density around STE a 414:**

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

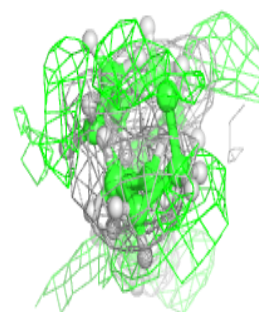
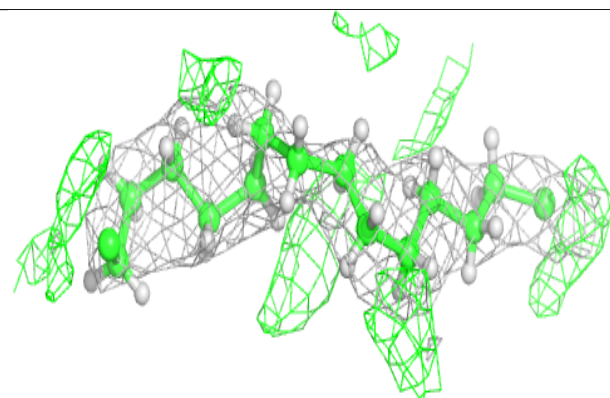
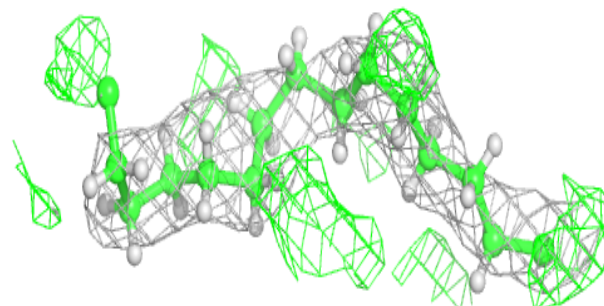


**Electron density around STE b 624:**

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

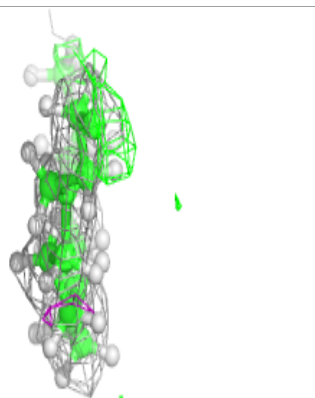
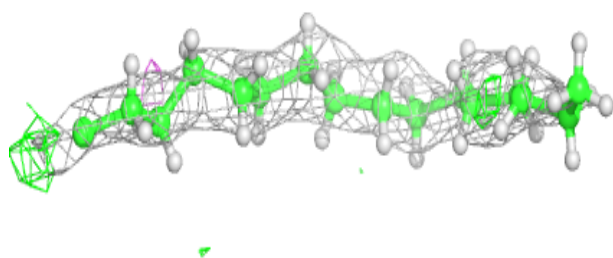
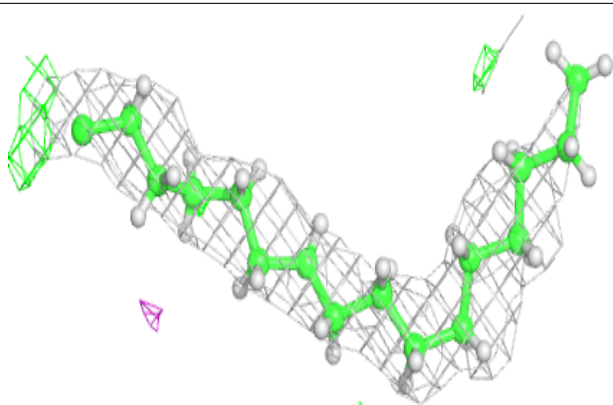
**Electron density around STE B 627:**

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

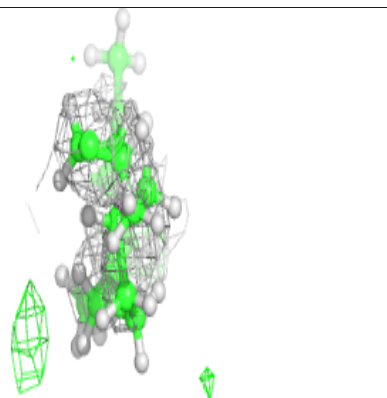
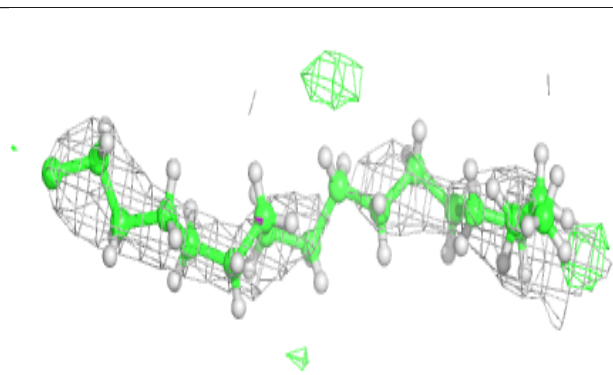
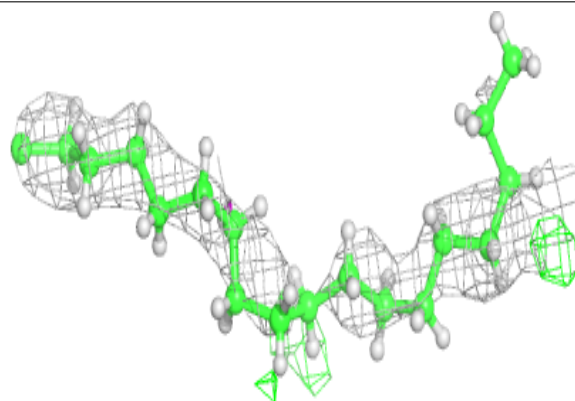


**Electron density around STE B 626:**

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

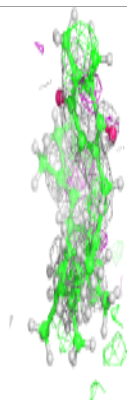
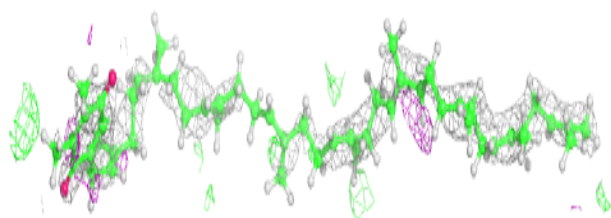
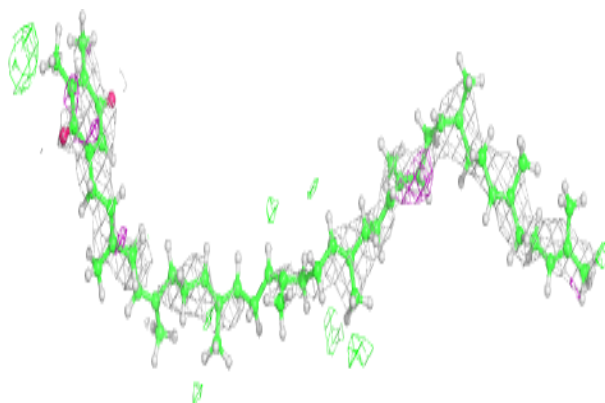
**Electron density around STE H 104:**

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

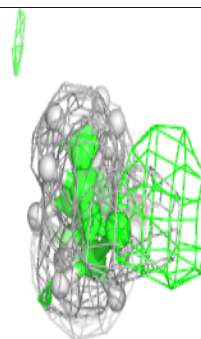
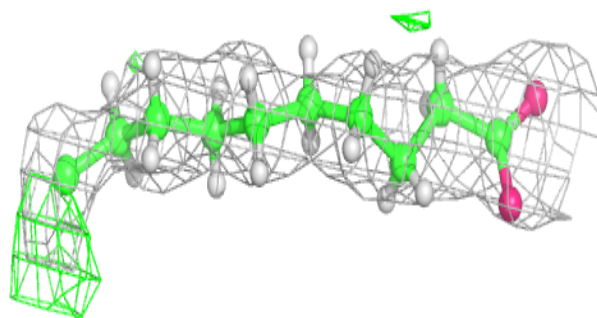
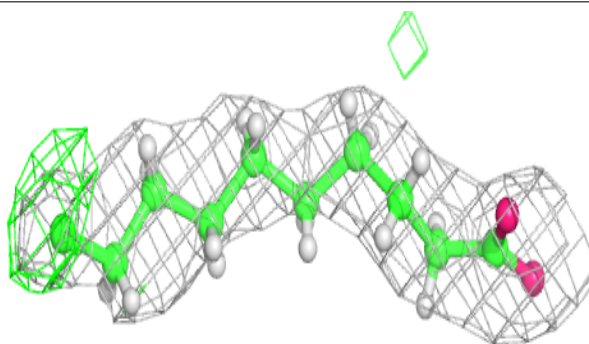


**Electron density around PL9 A 409:**

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

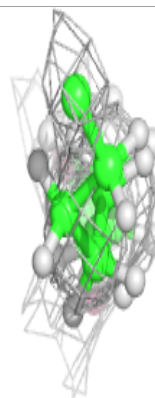
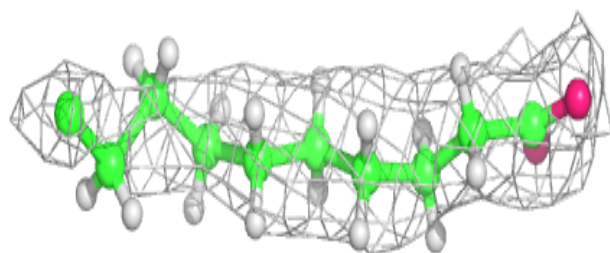
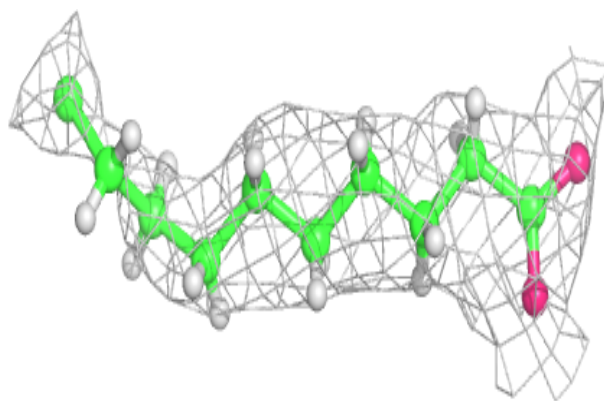
**Electron density around STE j 101:**

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

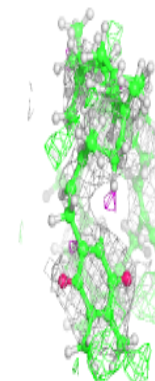
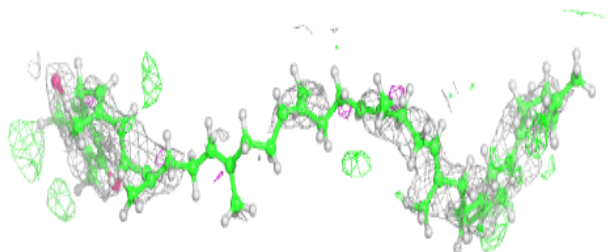
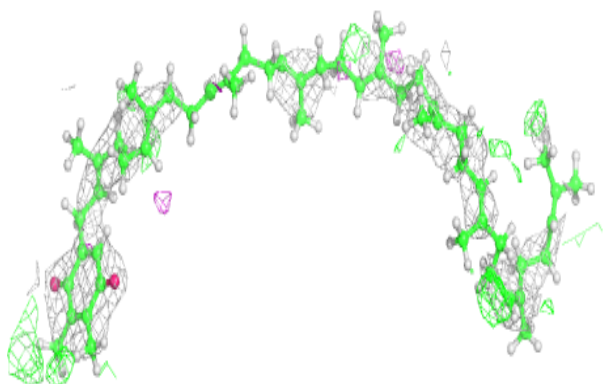


**Electron density around STE c 501:**

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

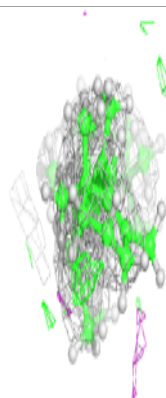
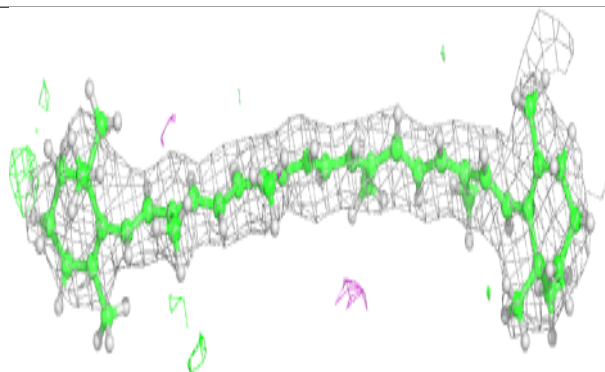
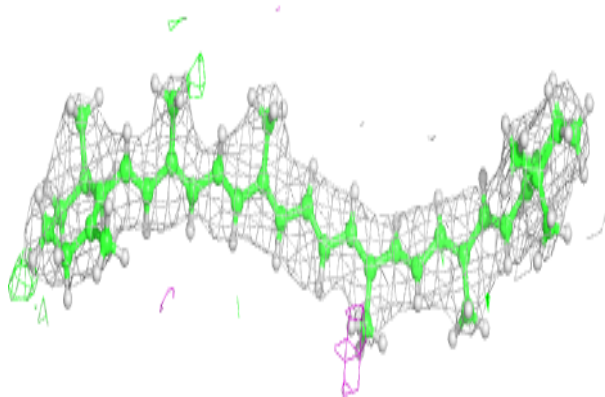
**Electron density around PL9 a 409:**

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

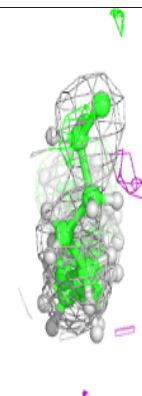
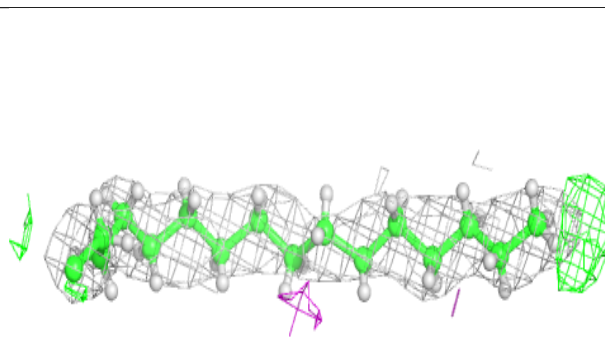
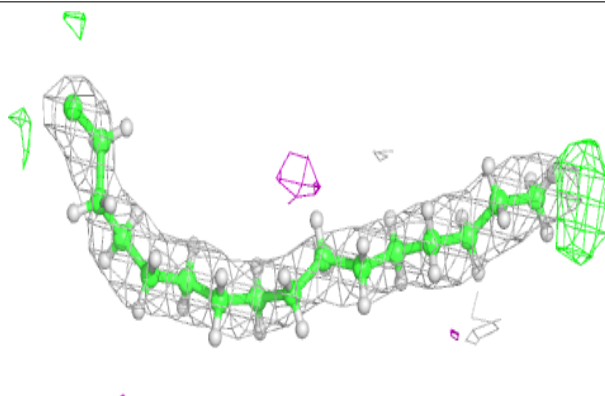


**Electron density around BCR H 102:**

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

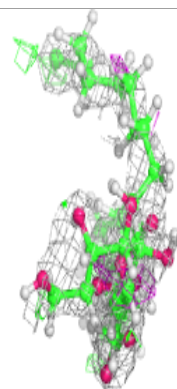
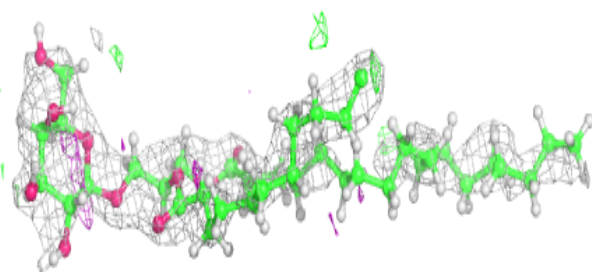
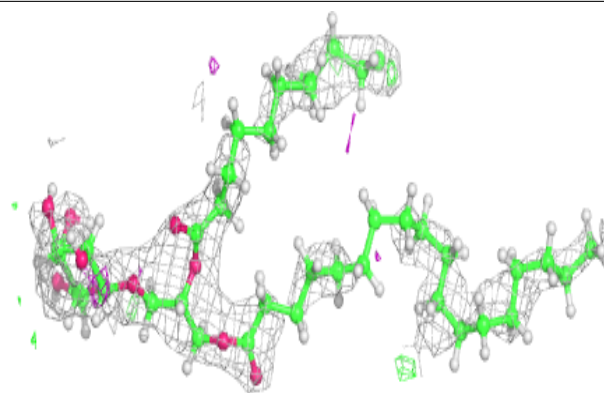
**Electron density around STE C 519:**

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

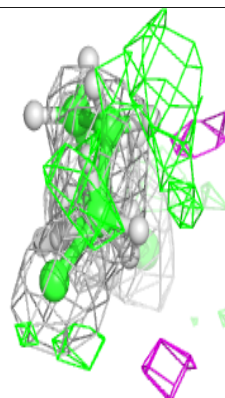
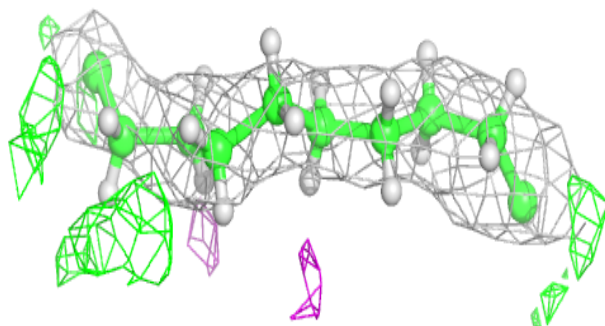
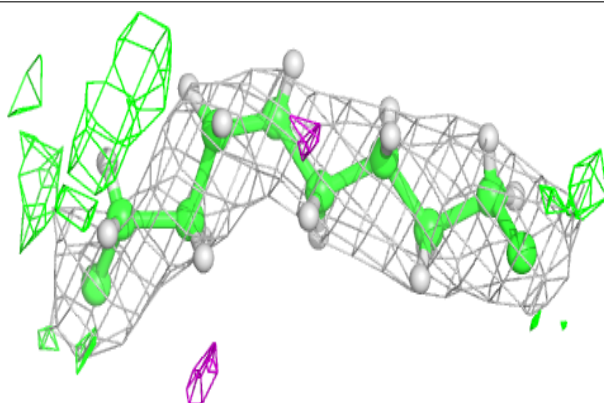


**Electron density around LMG c 522:**

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

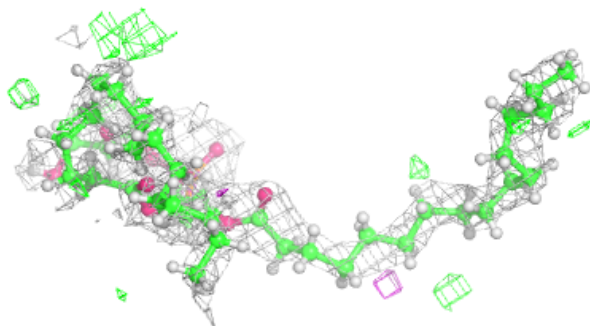
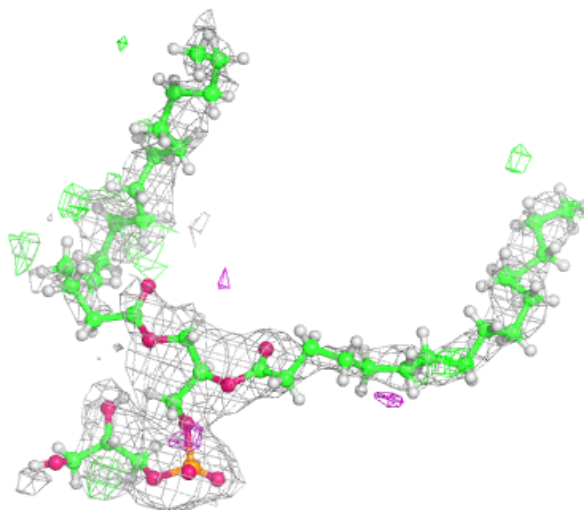
**Electron density around STE b 625:**

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



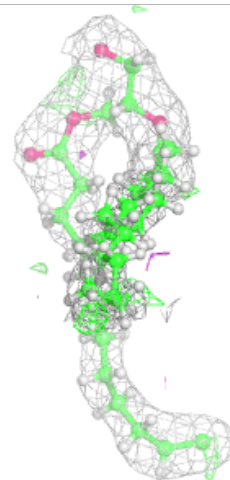
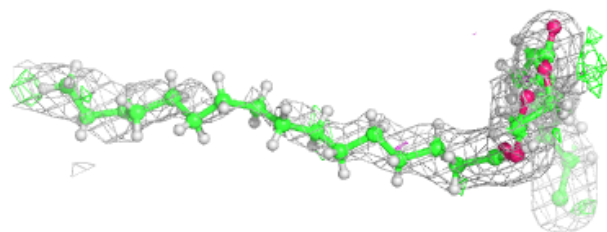
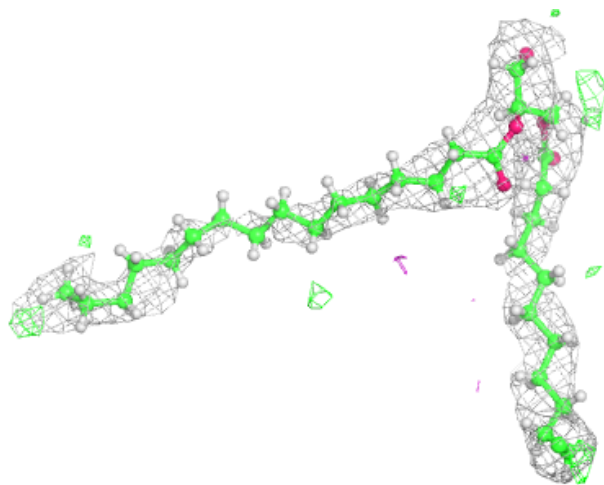
**Electron density around LHG E 101:**

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



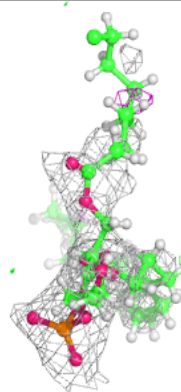
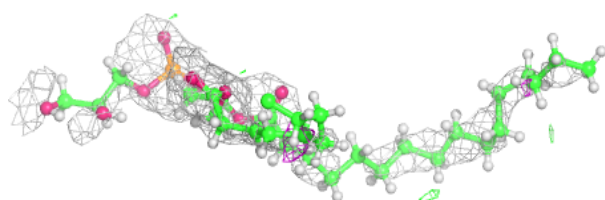
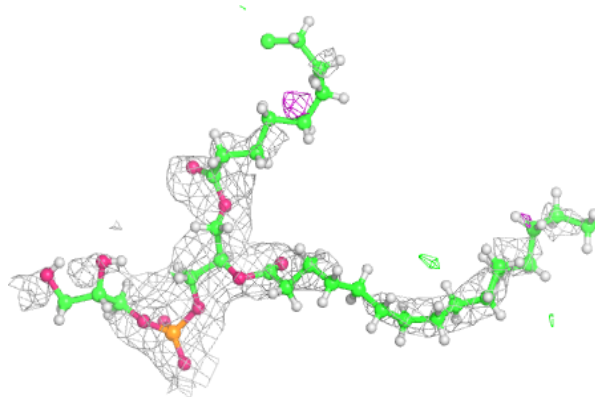
**Electron density around SQD a 412:**

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

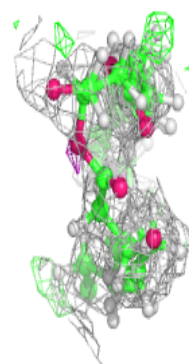
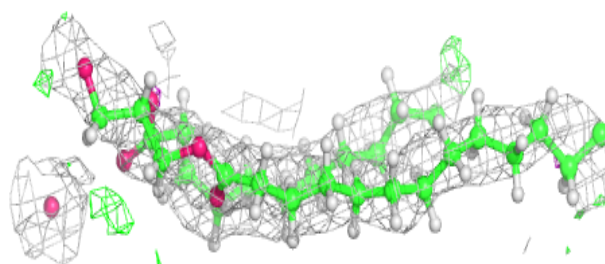
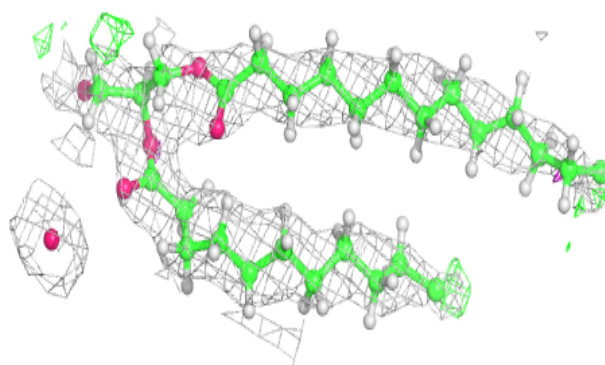


**Electron density around LHG e 101:**

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

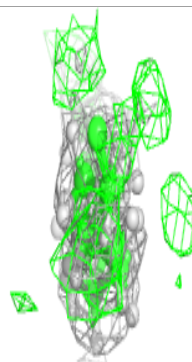
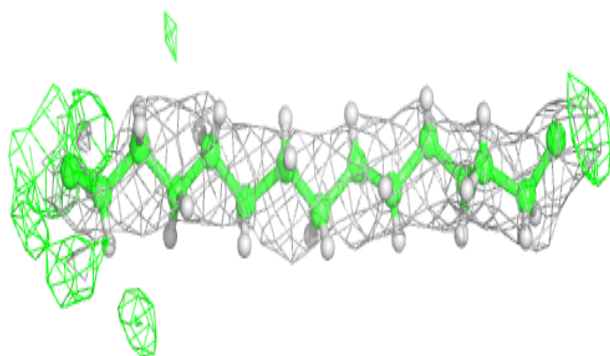
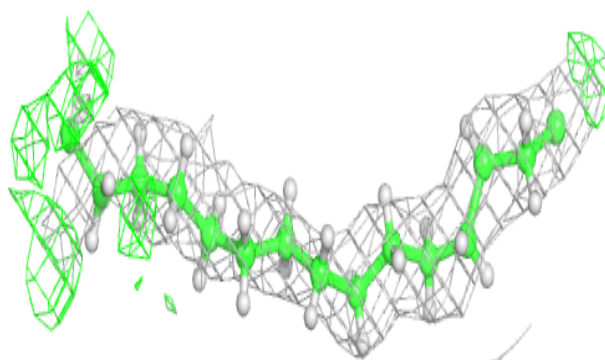
**Electron density around LMG D 411:**

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

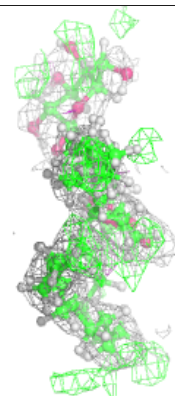
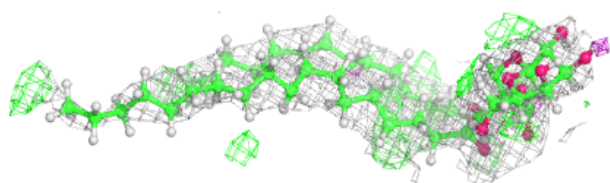
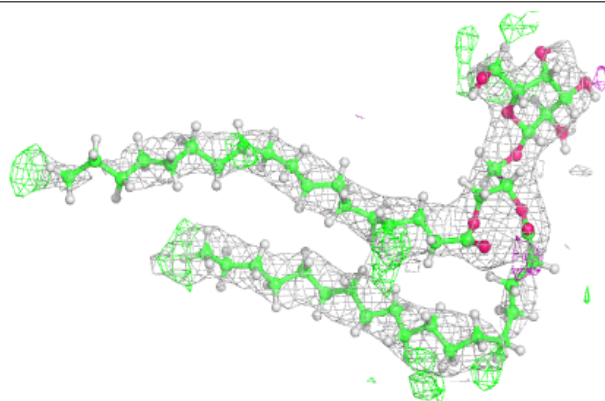


**Electron density around STE I 101:**

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

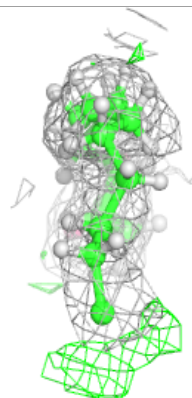
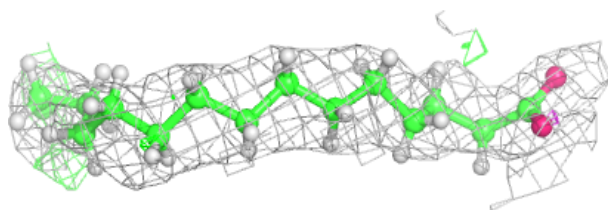
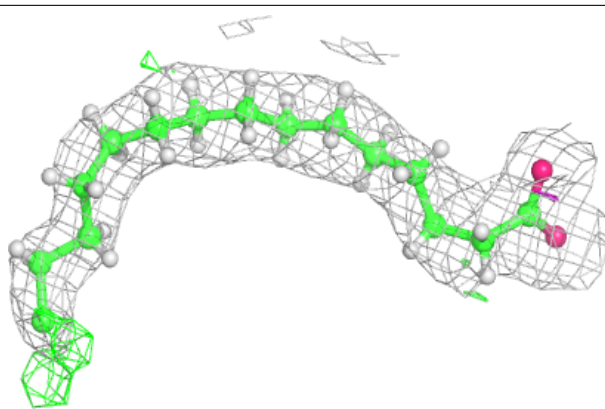
**Electron density around LMG a 415:**

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

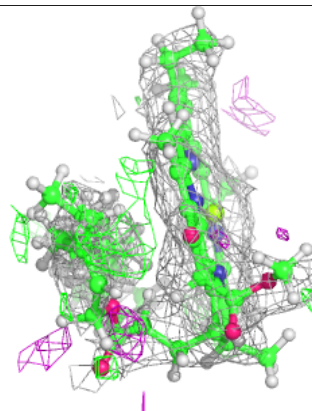
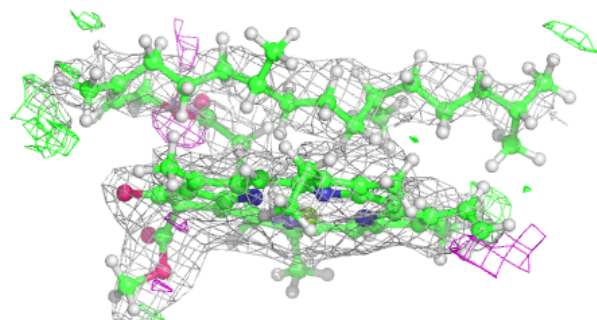
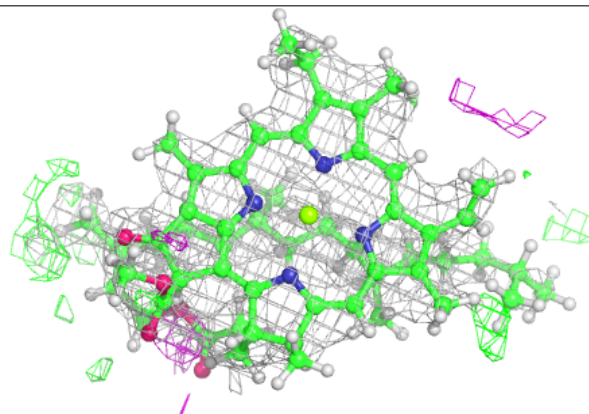


**Electron density around STE B 620:**

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

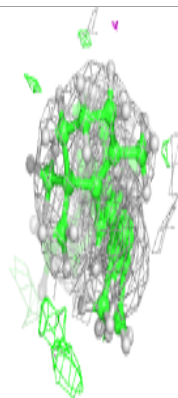
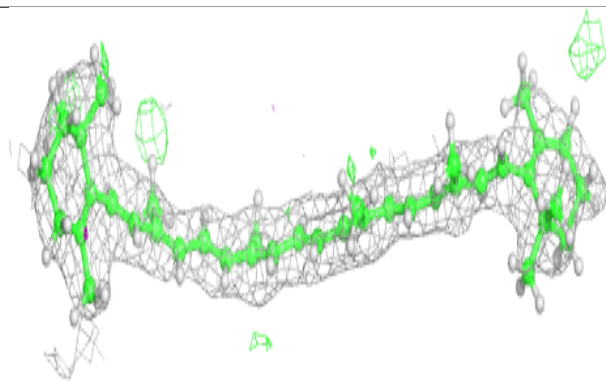
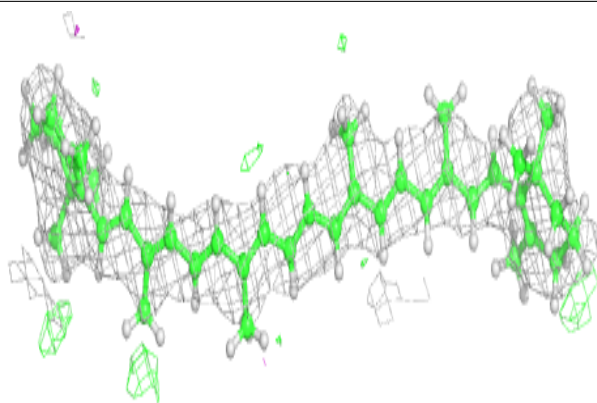
**Electron density around CLA b 601:**

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

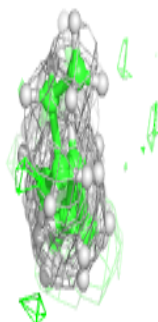
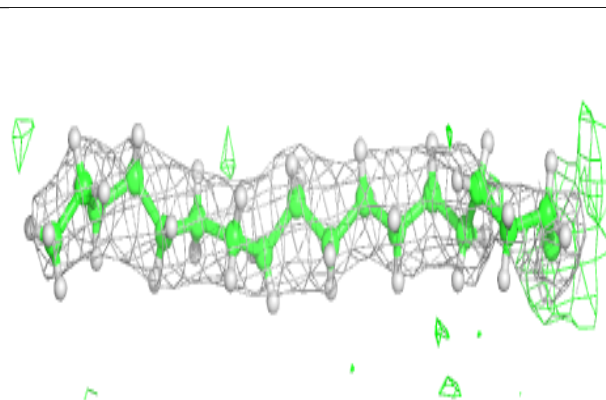
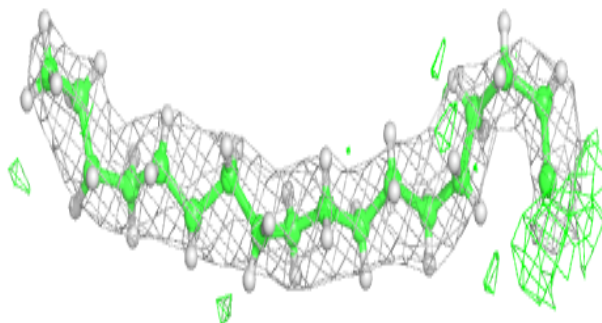


**Electron density around BCR h 101:**

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

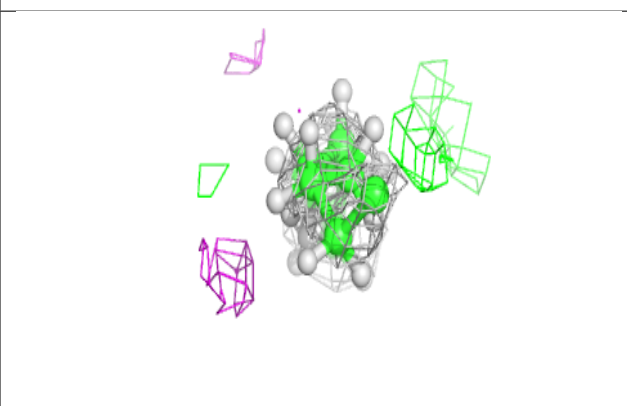
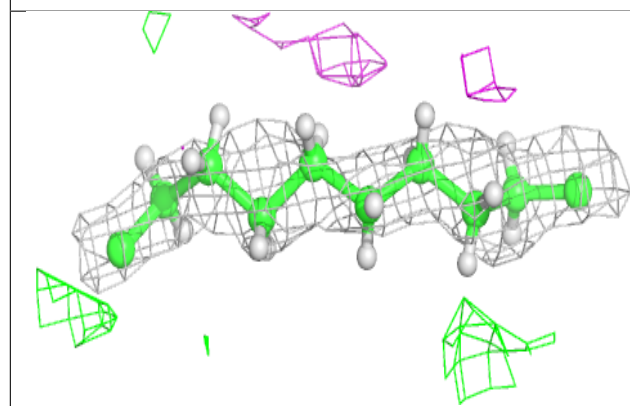
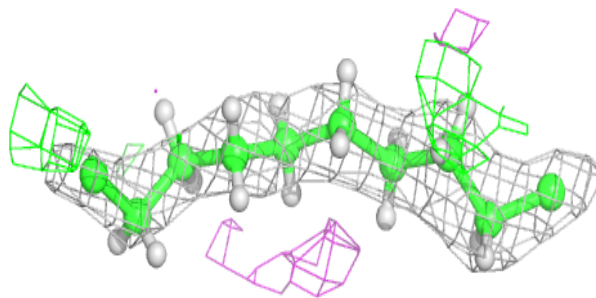
**Electron density around STE m 101:**

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

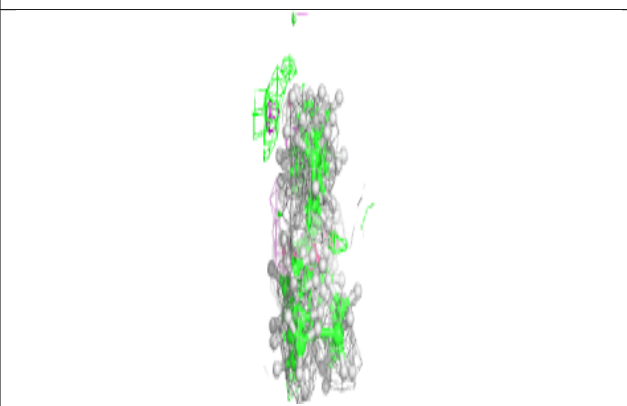
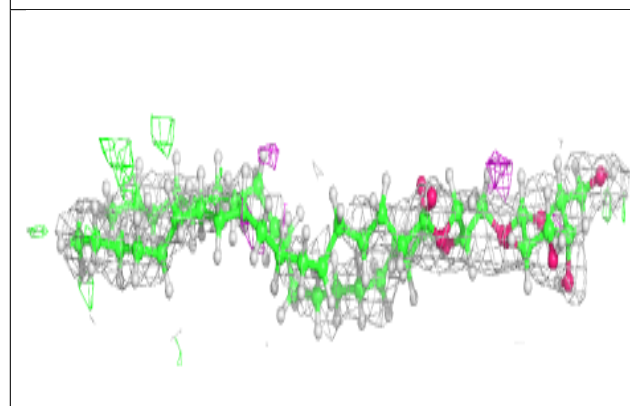
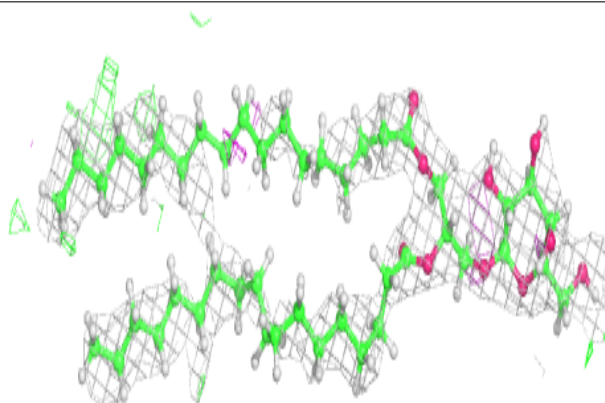


**Electron density around STE a 413:**

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

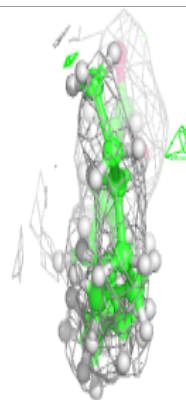
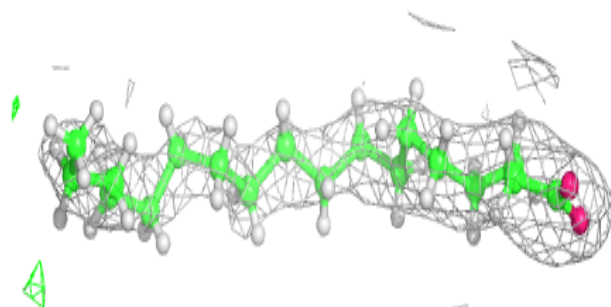
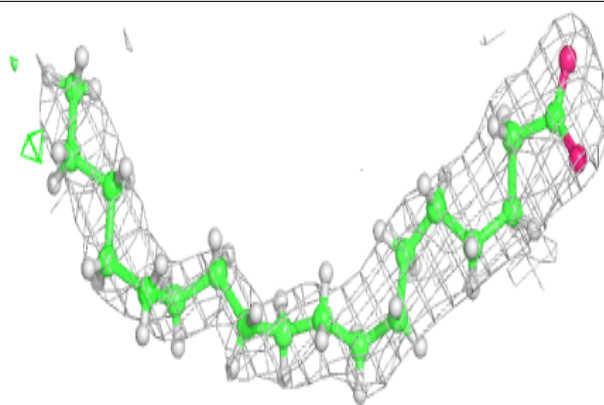
**Electron density around LMG b 623:**

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



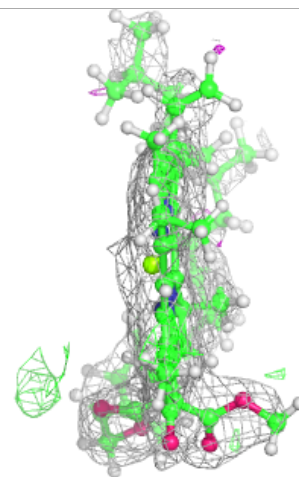
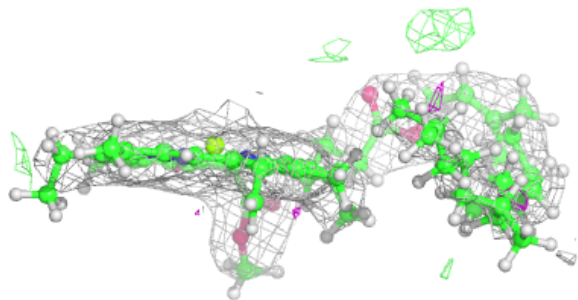
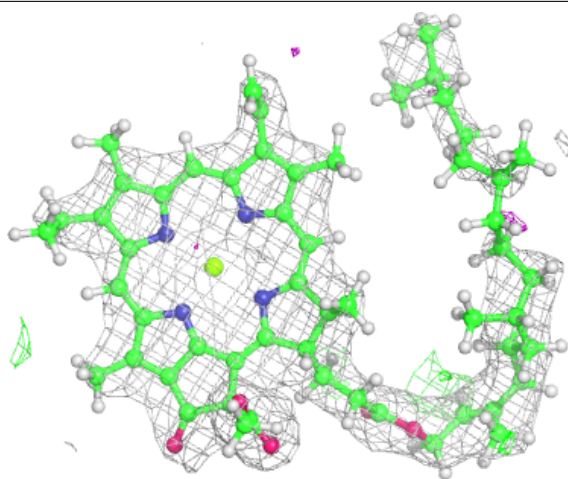
**Electron density around STE d 413:**

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



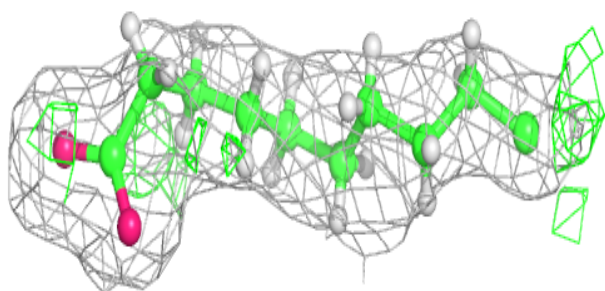
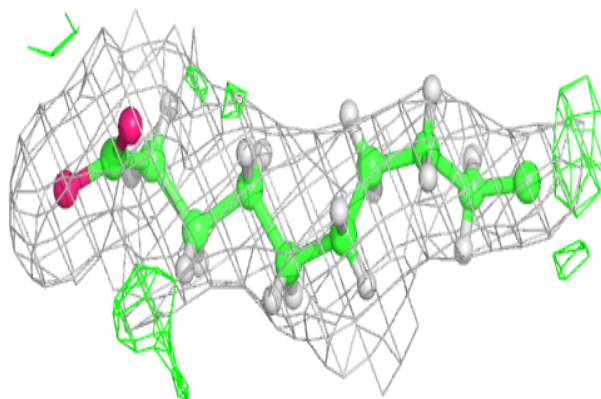
**Electron density around CLA C 512:**

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

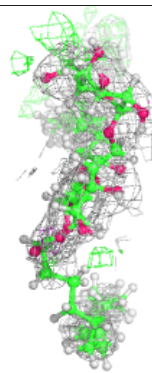
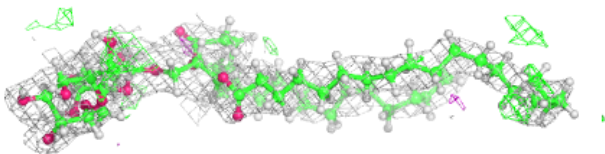
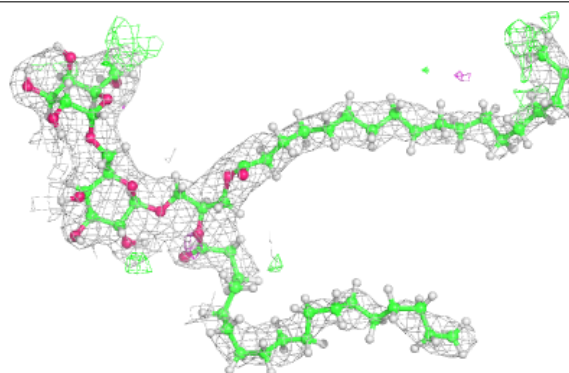


**Electron density around STE B 624:**

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

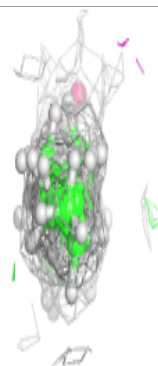
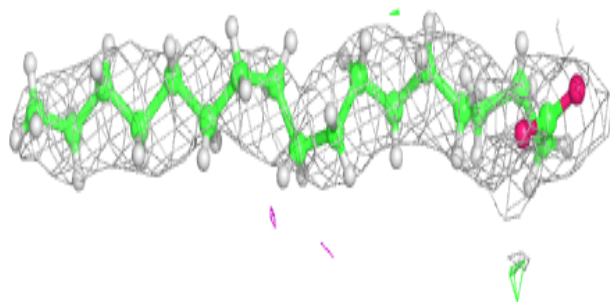
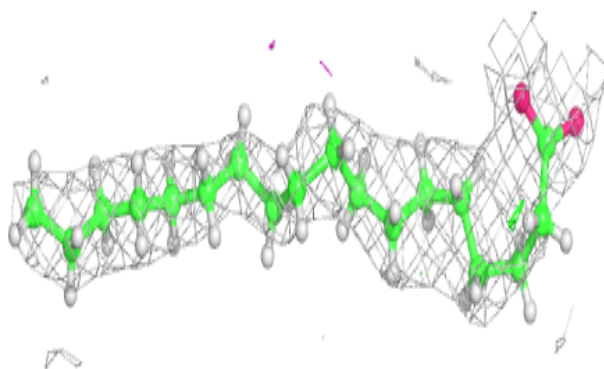
**Electron density around DGD A 413:**

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

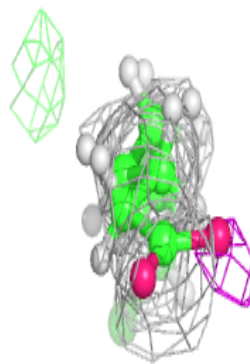
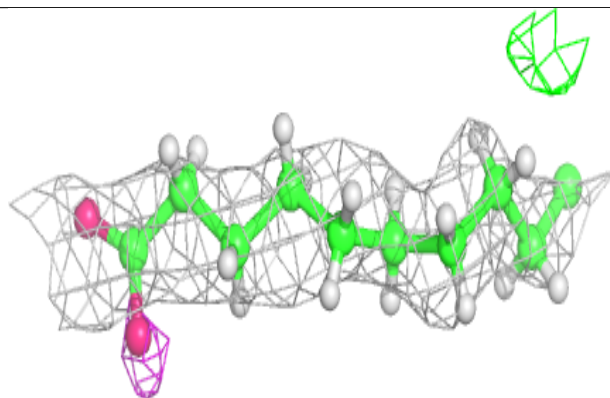
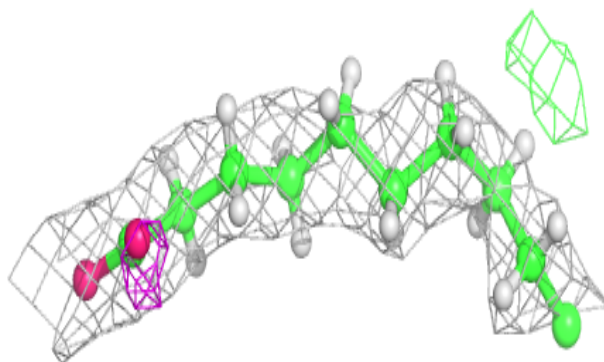


**Electron density around STE c 521:**

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

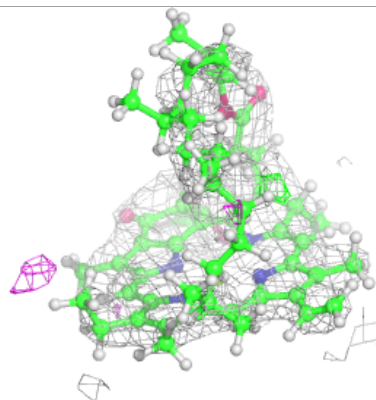
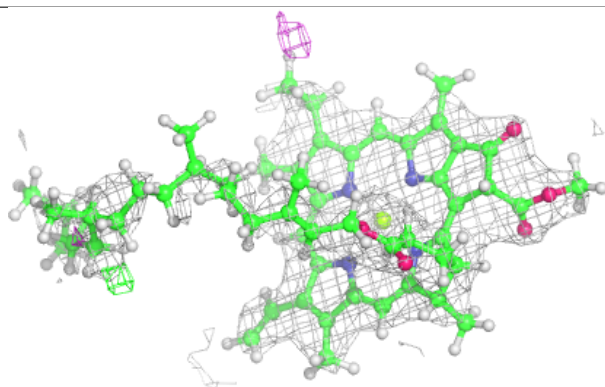
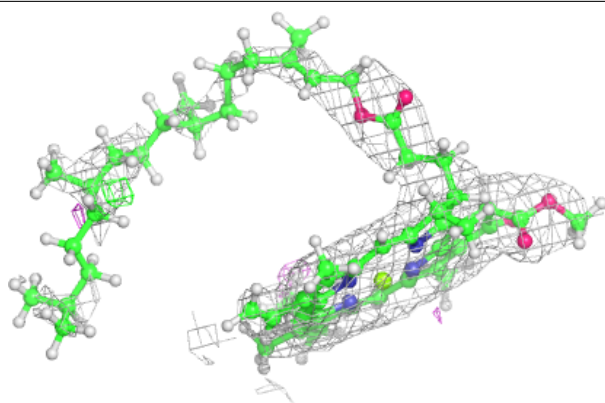
**Electron density around STE m 102:**

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

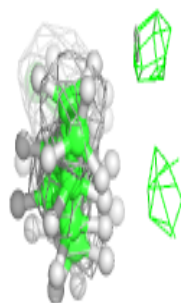
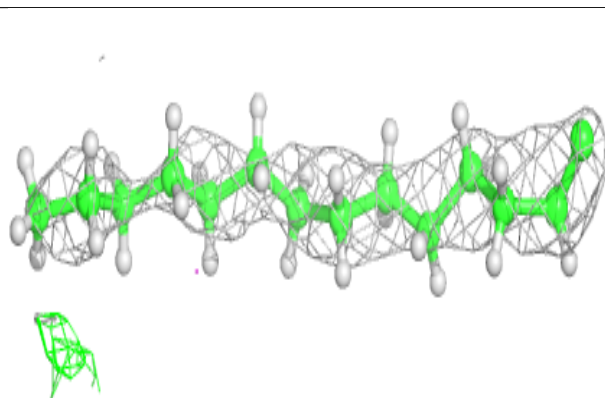
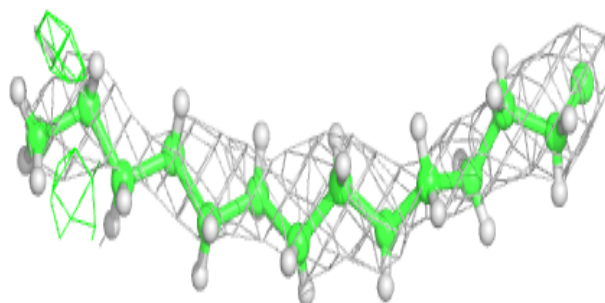


**Electron density around CLA c 514:**

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

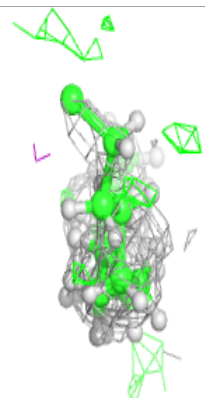
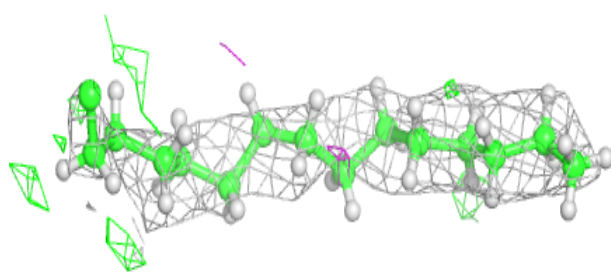
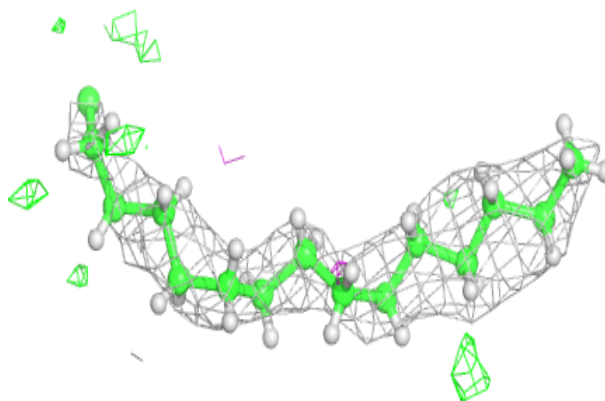
**Electron density around STE b 626:**

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

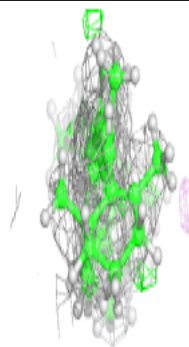
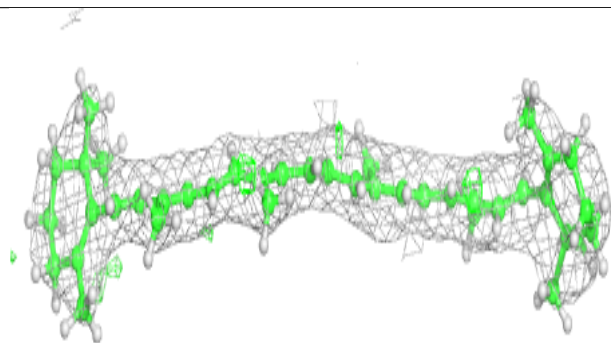
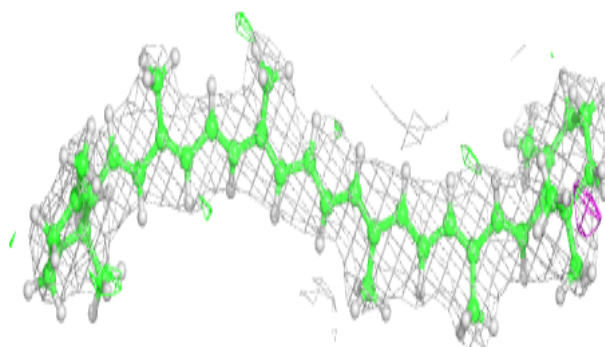


**Electron density around STE T 102:**

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

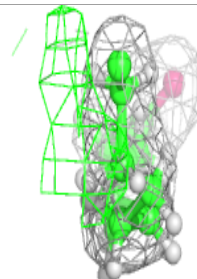
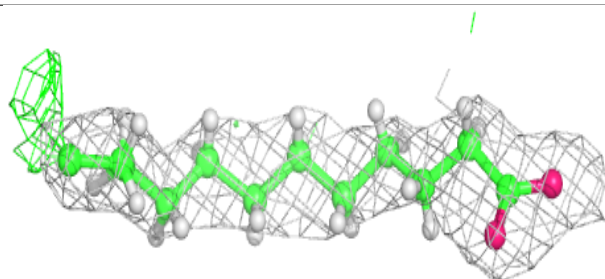
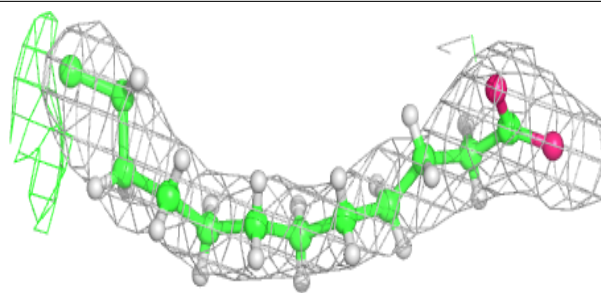
**Electron density around BCR K 102:**

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



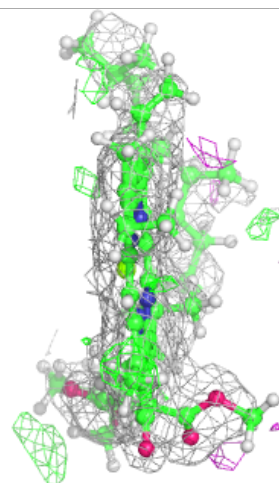
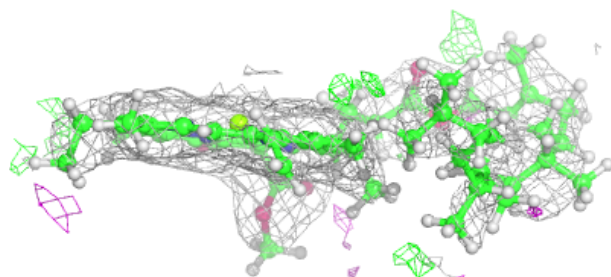
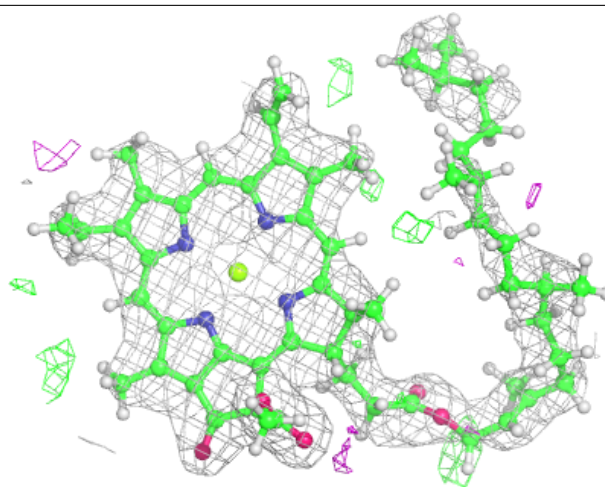
**Electron density around STE B 623:**

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



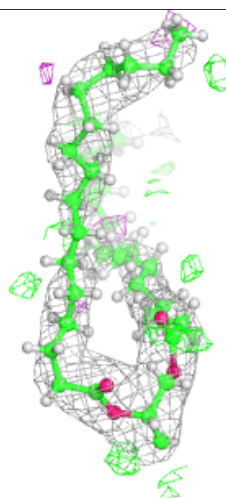
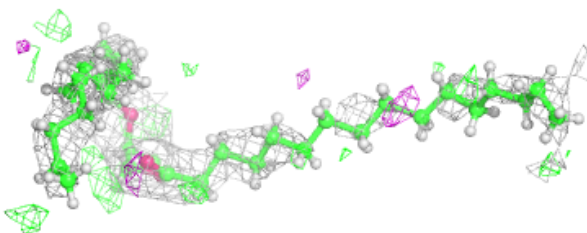
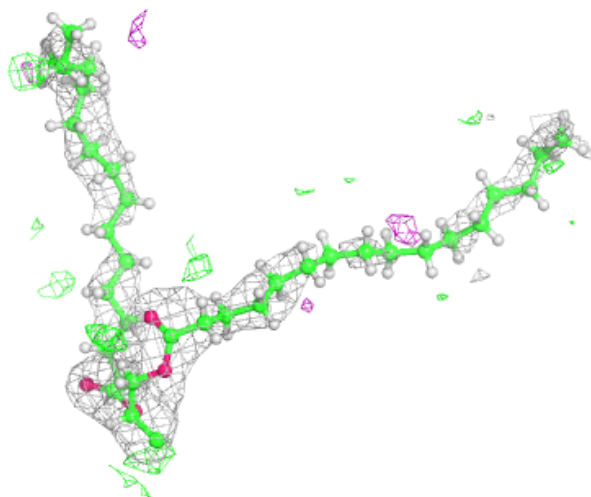
**Electron density around CLA c 513:**

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



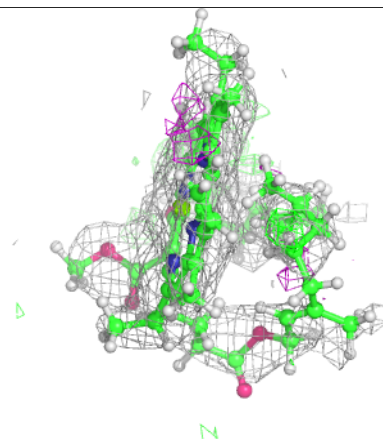
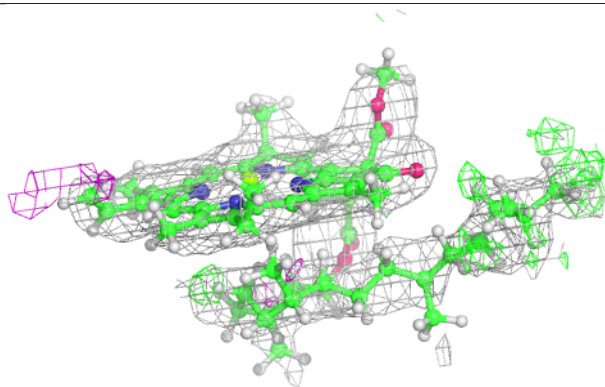
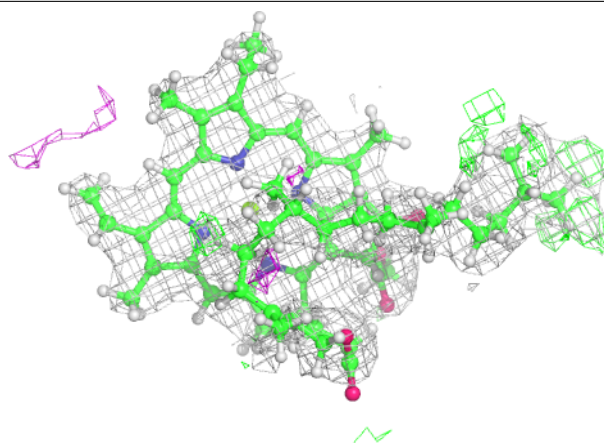
**Electron density around SQD A 412:**

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

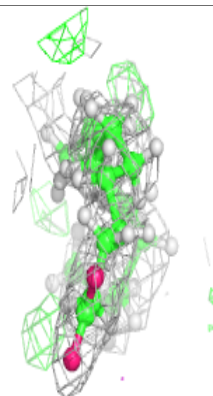
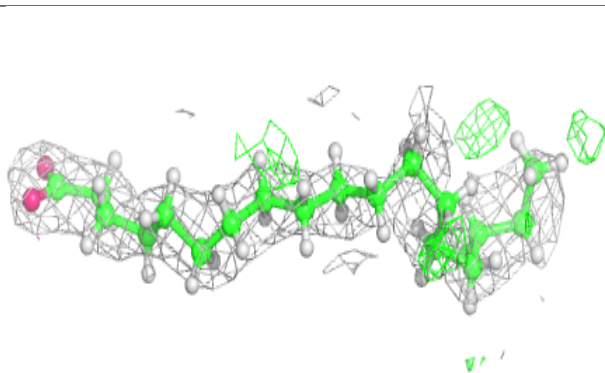
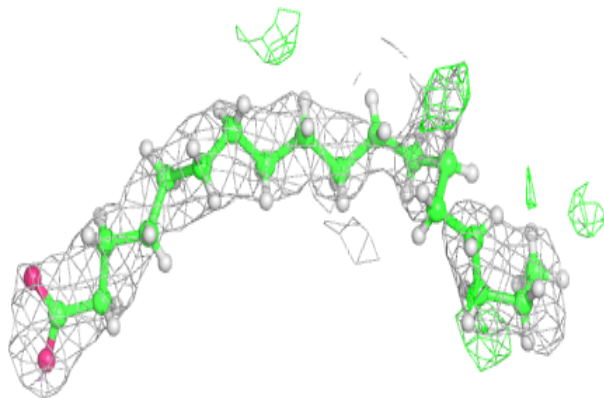


**Electron density around CLA H 101:**

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

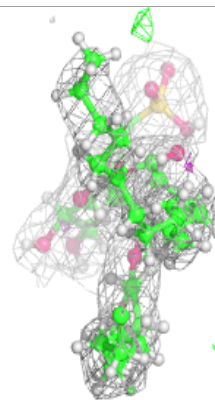
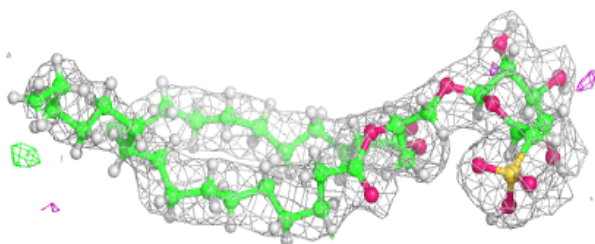
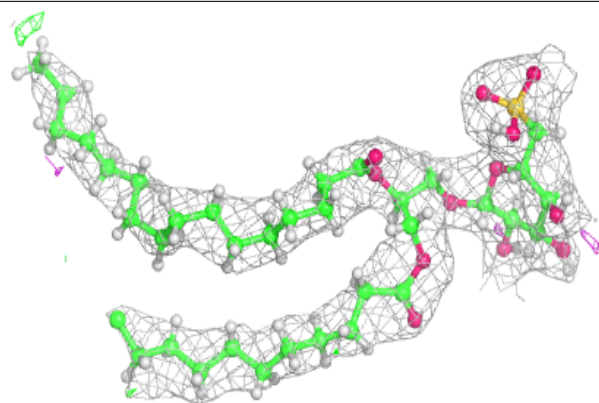
**Electron density around STE b 627:**

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

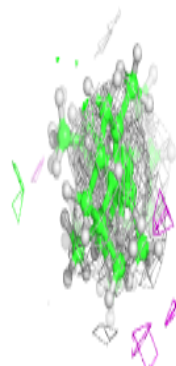
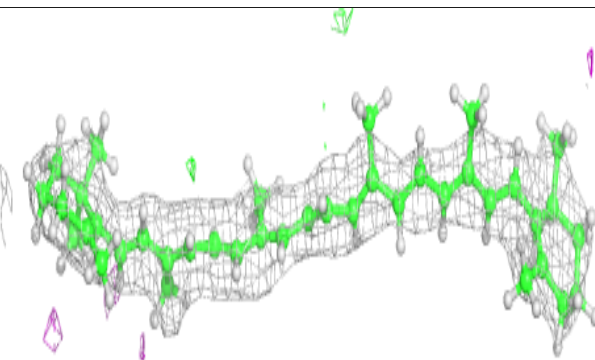
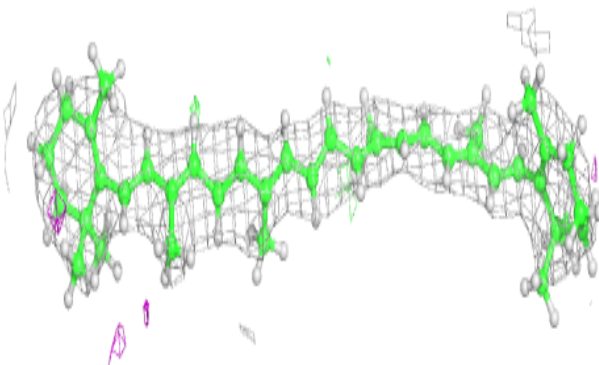


**Electron density around SQD L 101:**

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

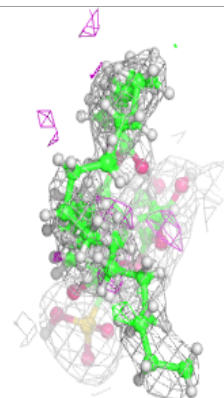
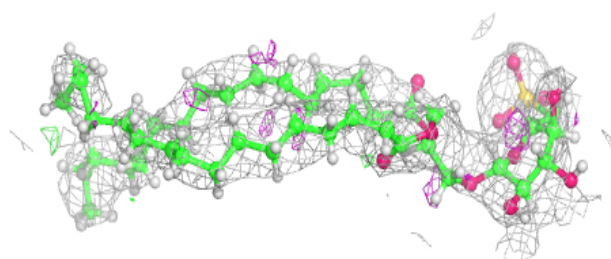
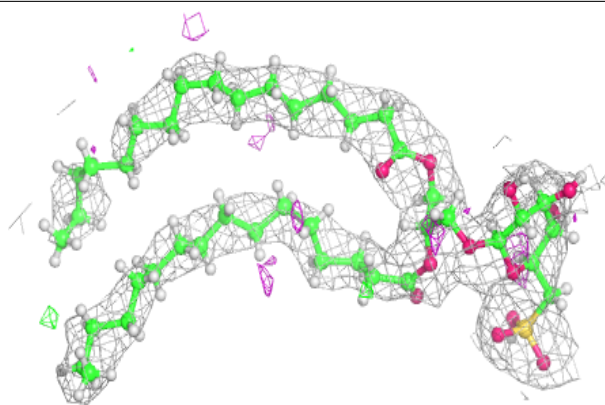
**Electron density around BCR K 101:**

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

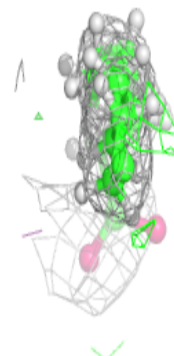
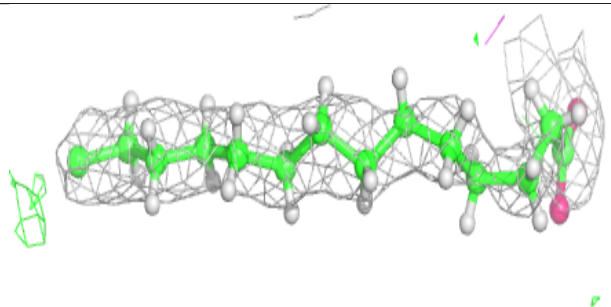
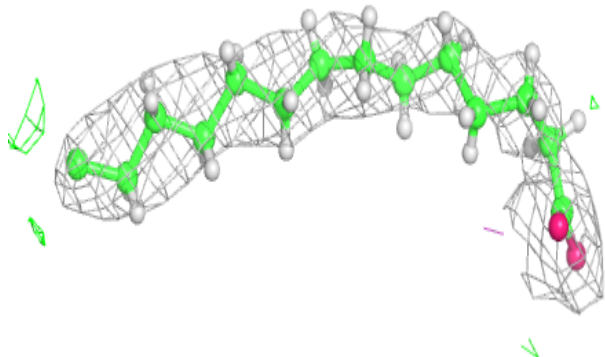


**Electron density around SQD B 622:**

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

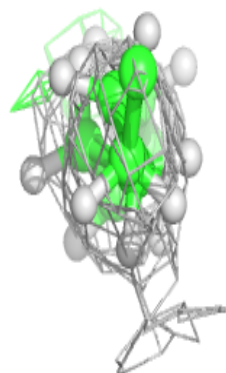
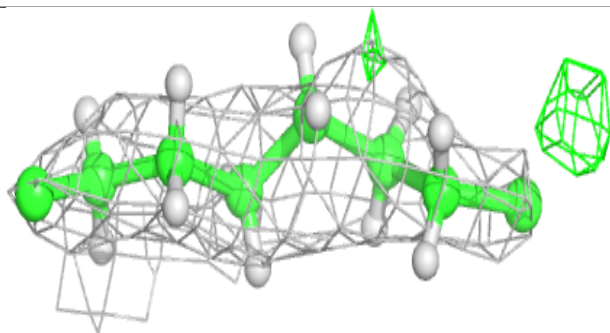
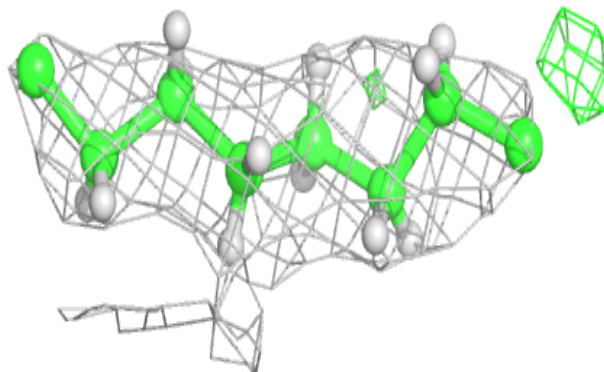
**Electron density around STE d 411:**

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

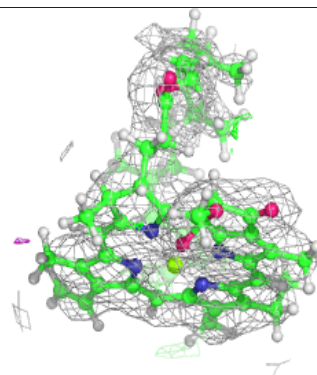
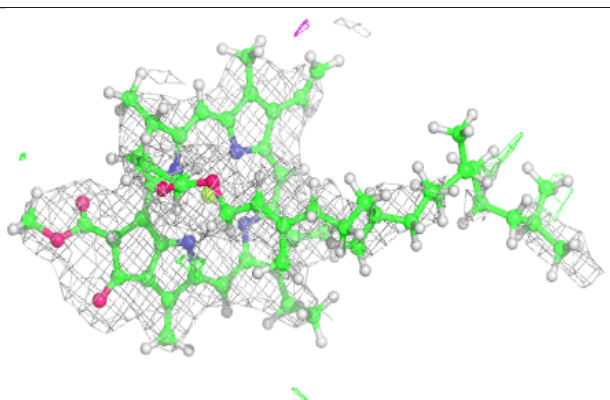
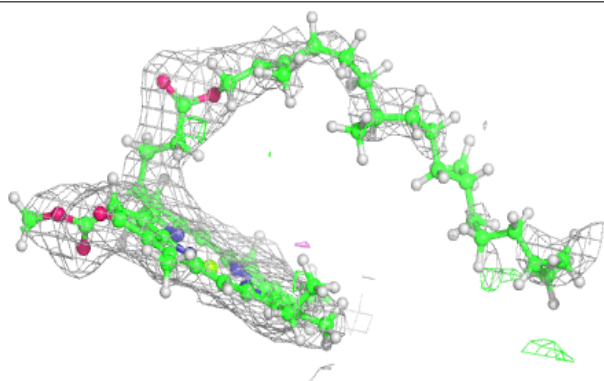


**Electron density around STE Z 101:**

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

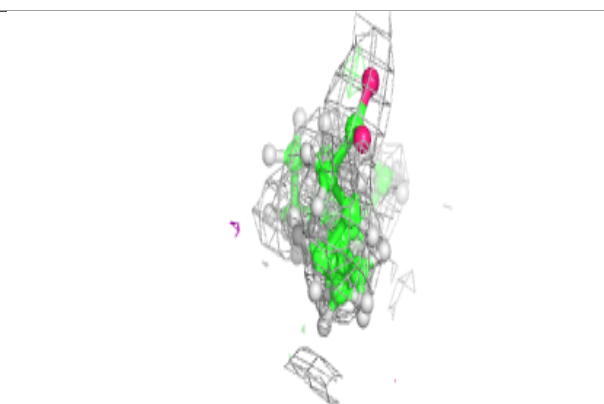
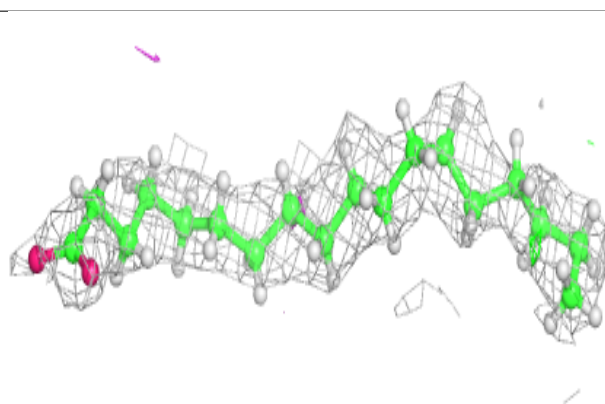
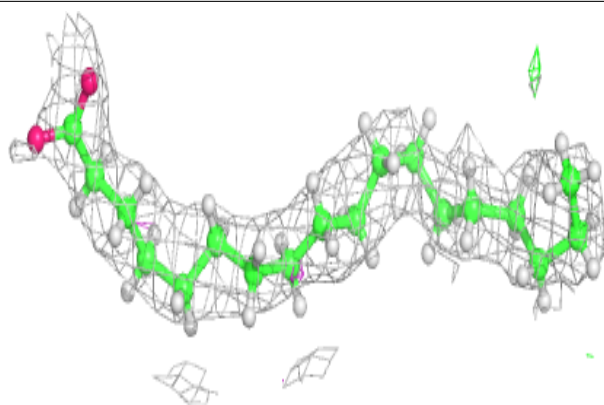
**Electron density around CLA C 513:**

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

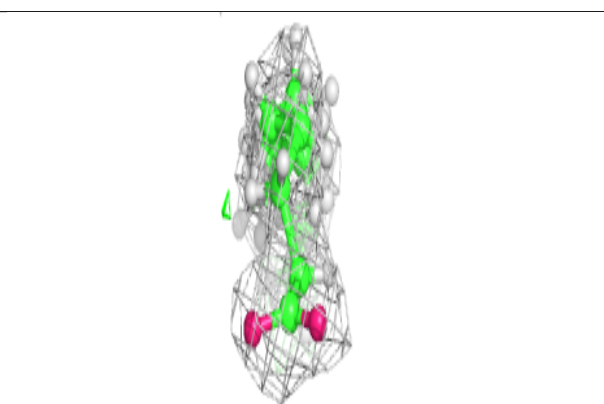
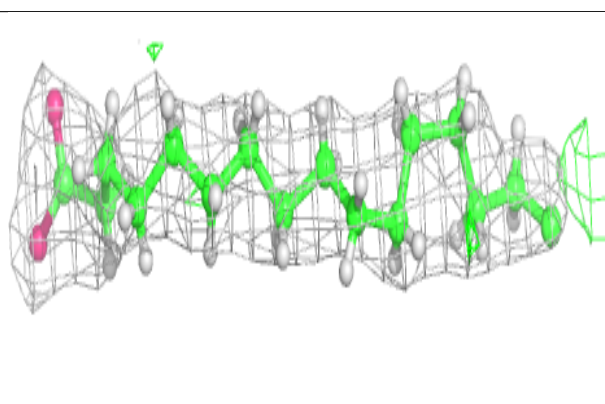
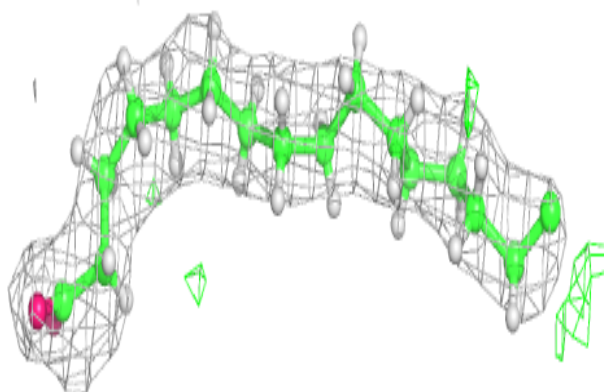


**Electron density around STE b 622:**

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

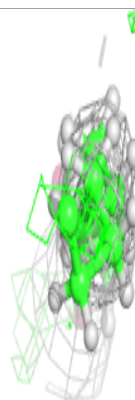
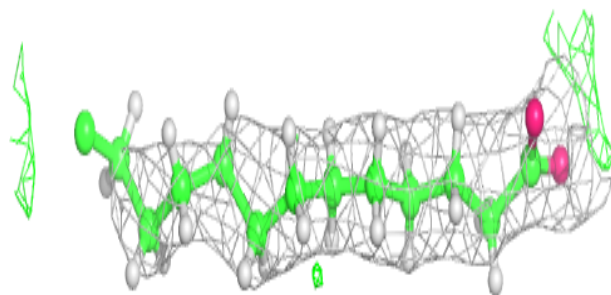
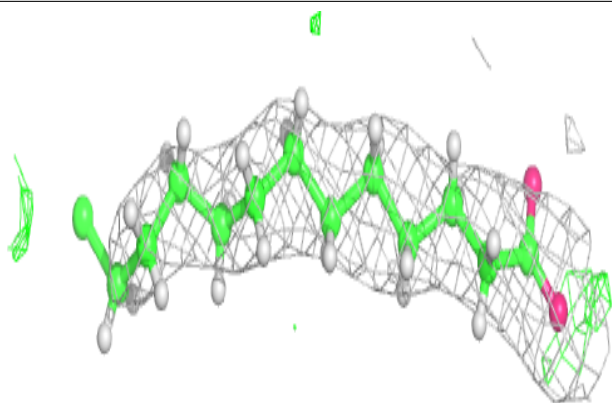
**Electron density around STE B 625:**

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

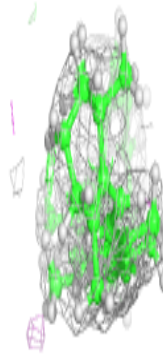
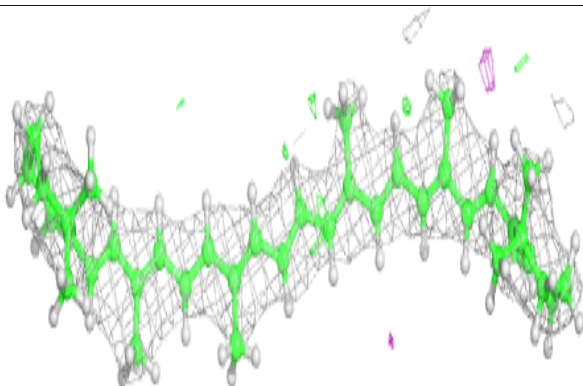
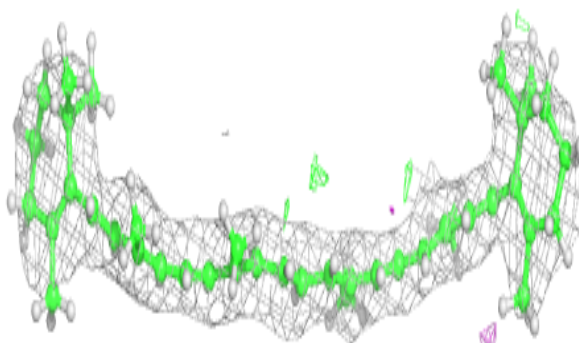


**Electron density around STE M 102:**

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

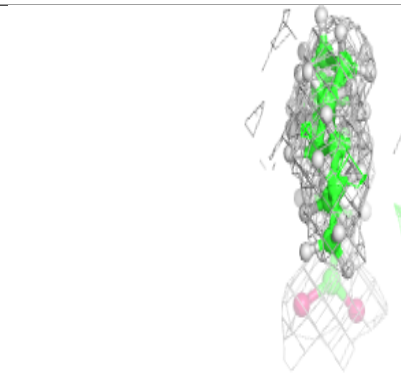
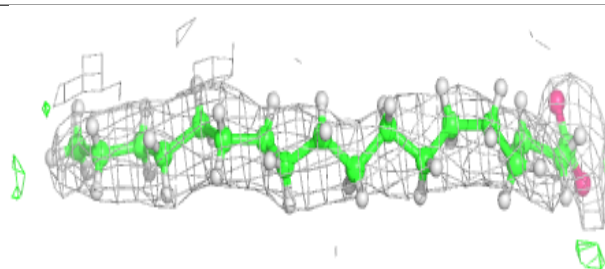
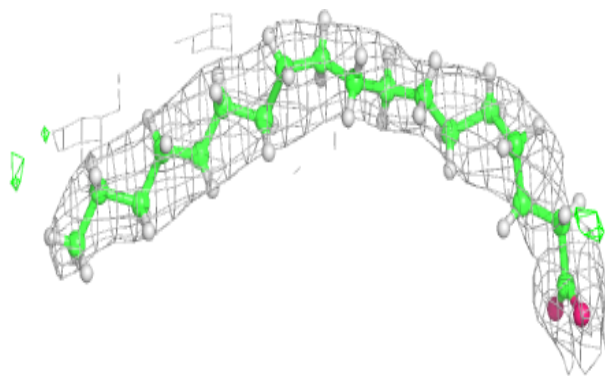
**Electron density around BCR k 102:**

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

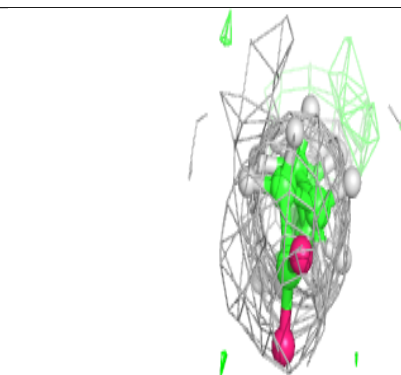
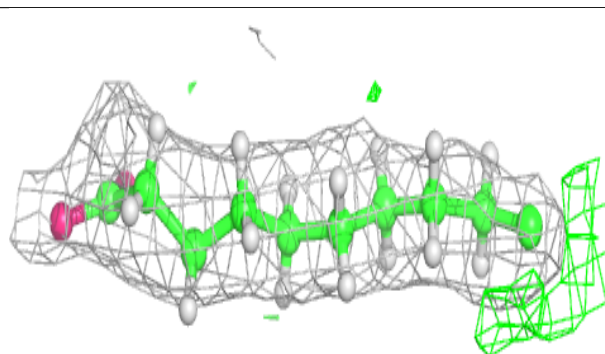
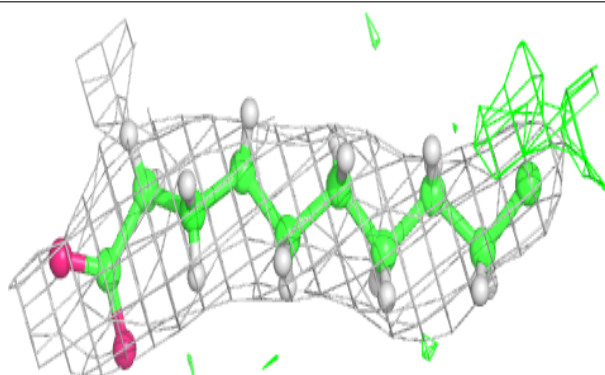


**Electron density around STE D 413:**

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

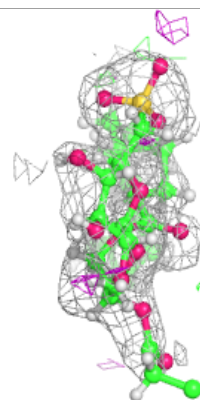
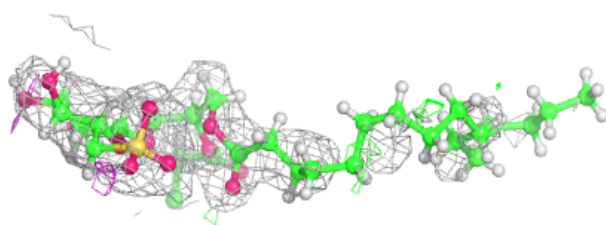
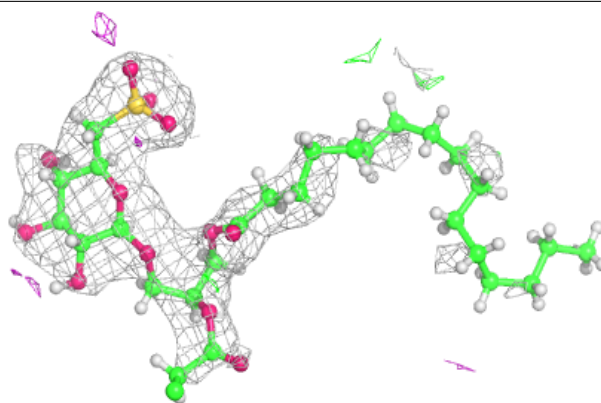
**Electron density around STE J 101:**

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

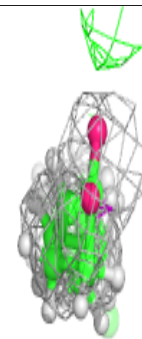
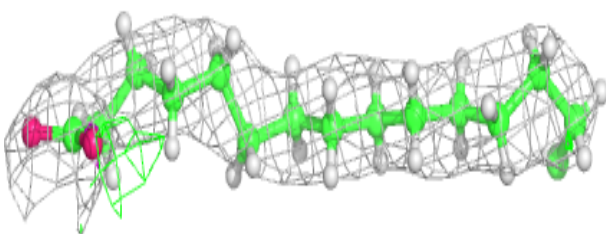
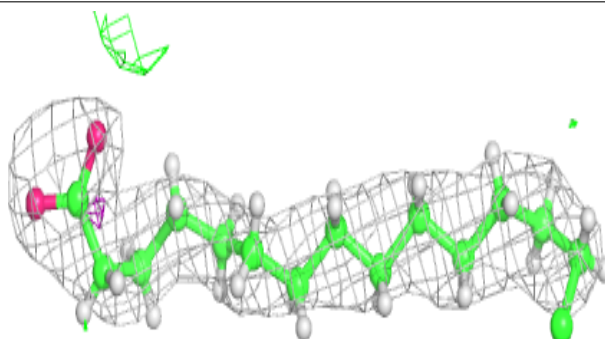


**Electron density around SQD f 102:**

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

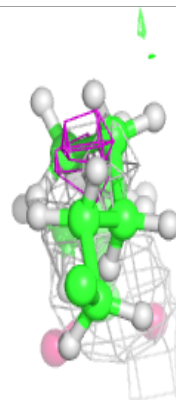
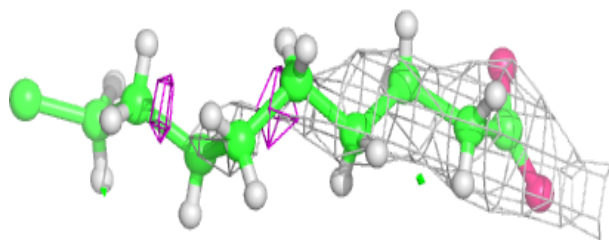
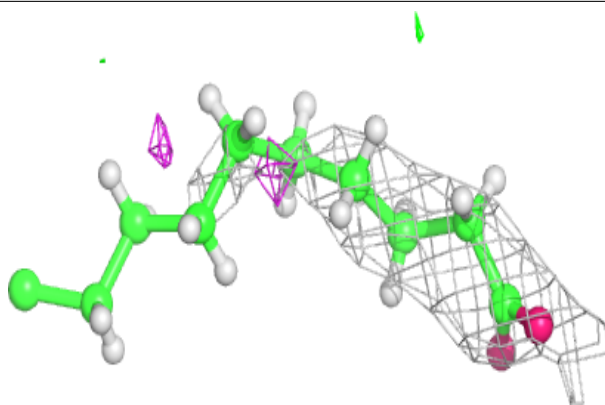
**Electron density around STE d 412:**

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



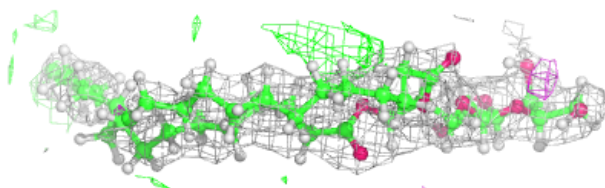
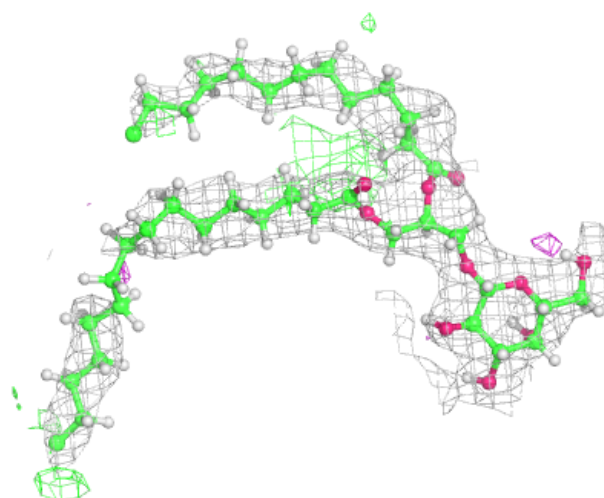
**Electron density around STE B 601:**

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



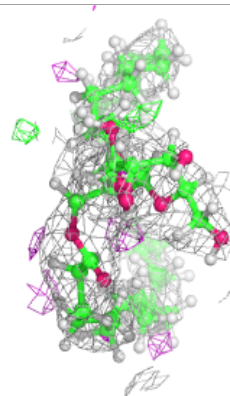
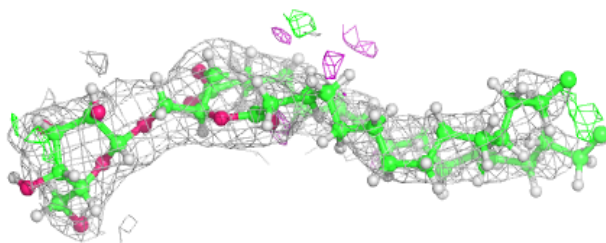
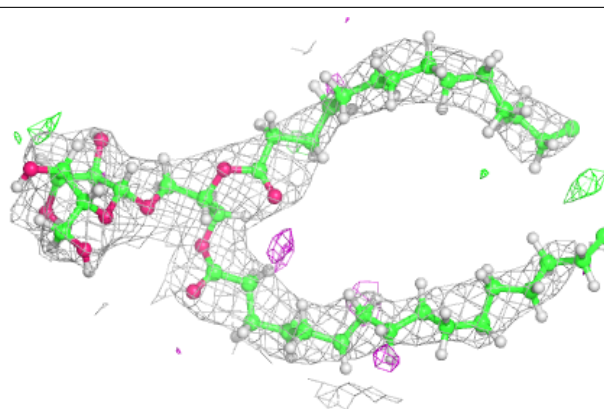
**Electron density around LMG Y 101:**

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

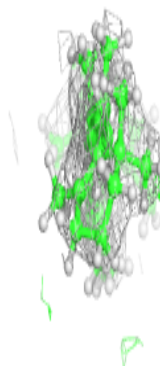
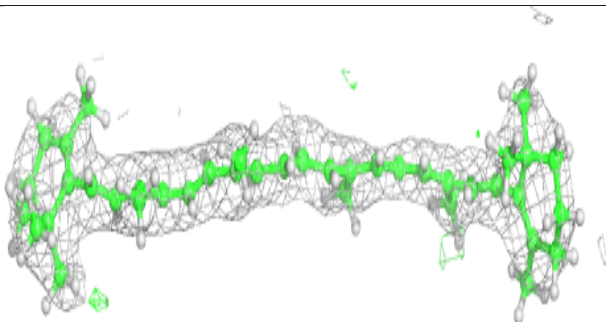
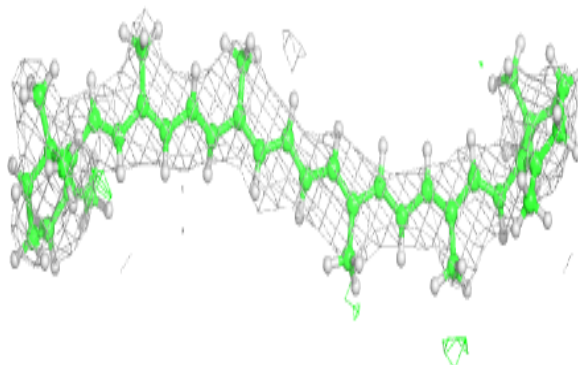


**Electron density around LMG c 523:**

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

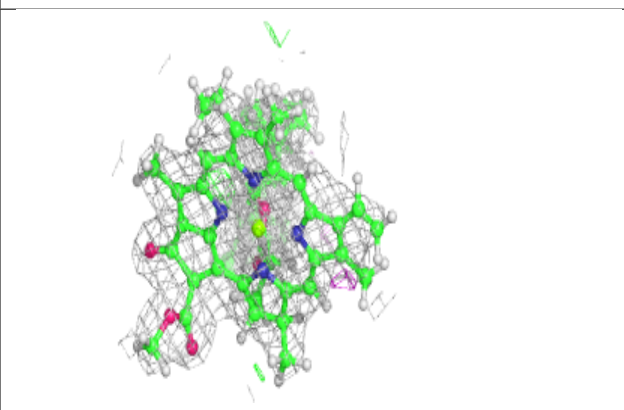
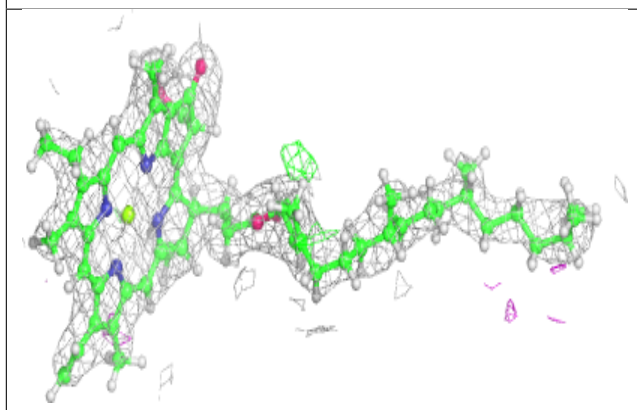
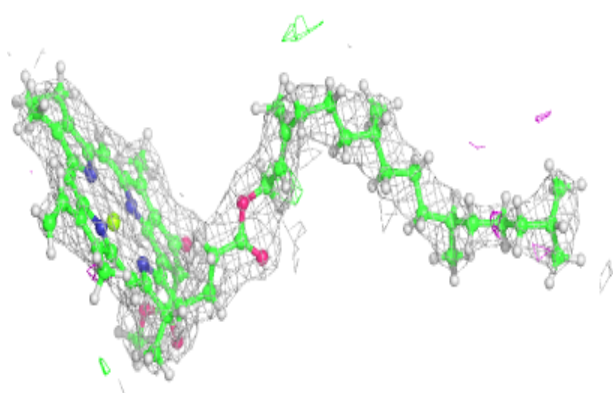
**Electron density around BCR k 101:**

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

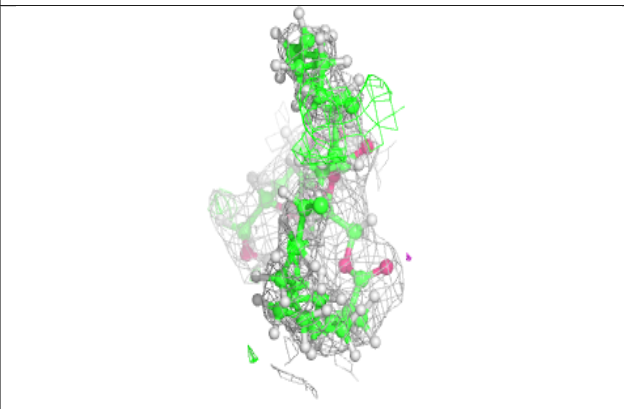
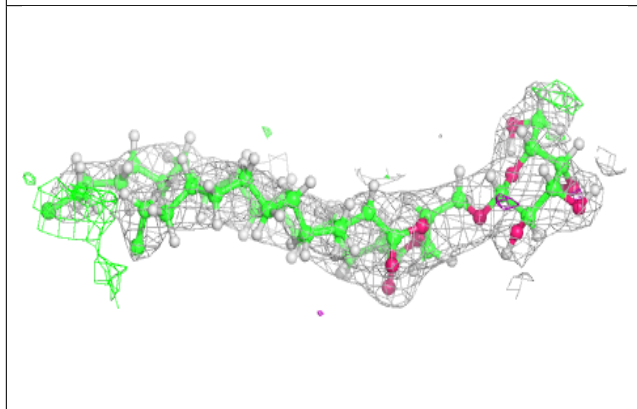
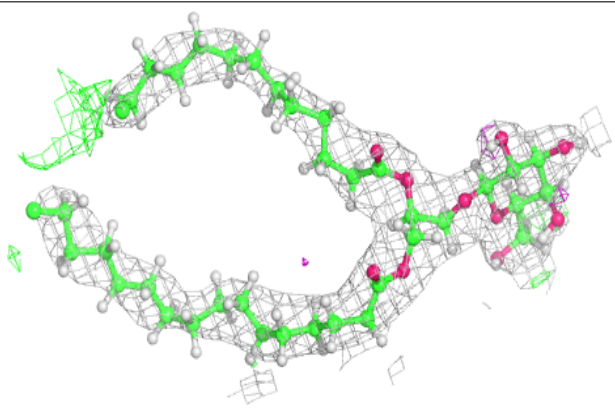


**Electron density around CLA c 503:**

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

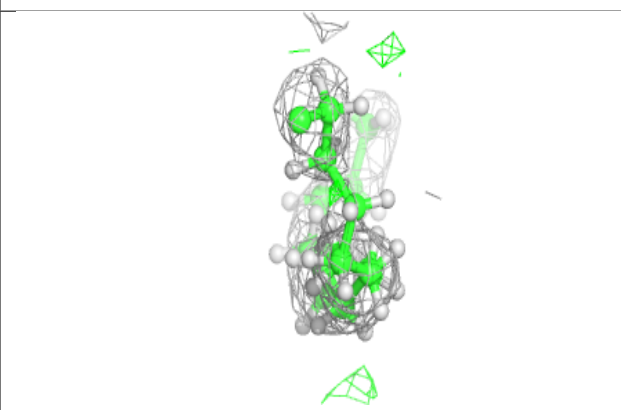
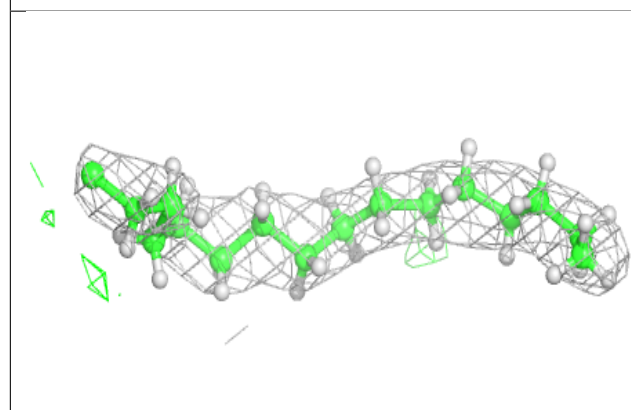
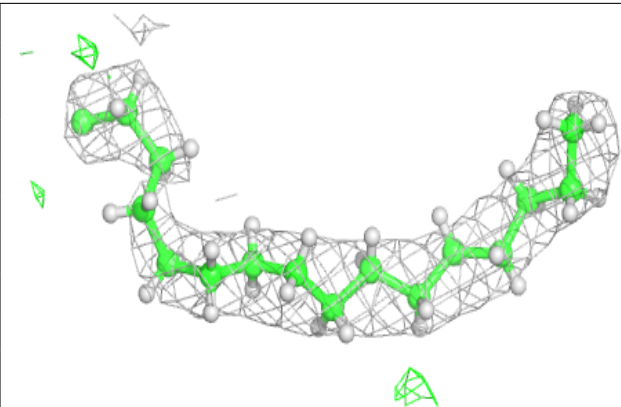
**Electron density around LMG A 410:**

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

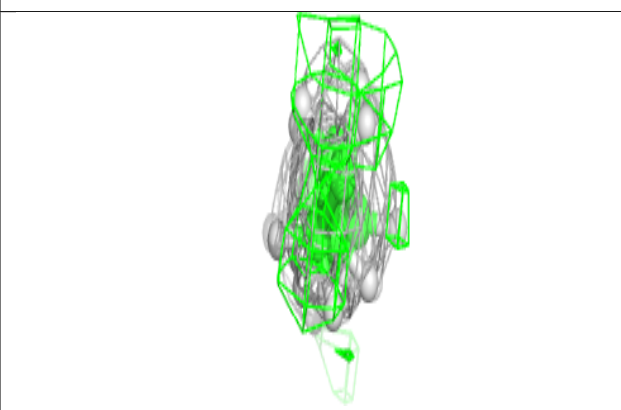
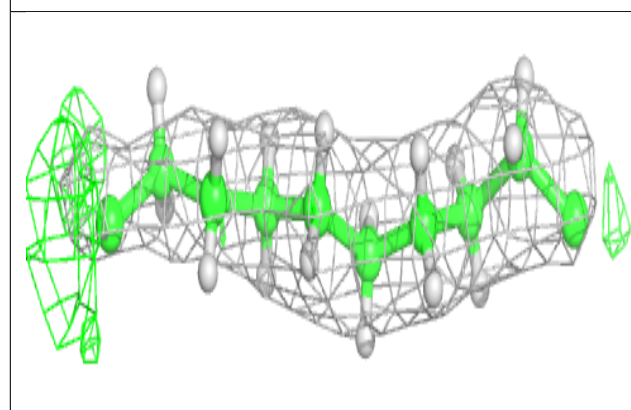
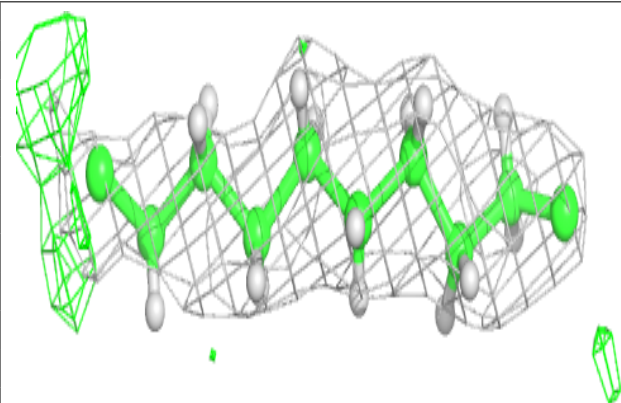


**Electron density around STE b 620:**

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

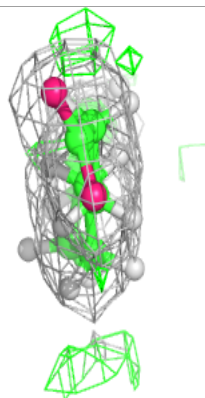
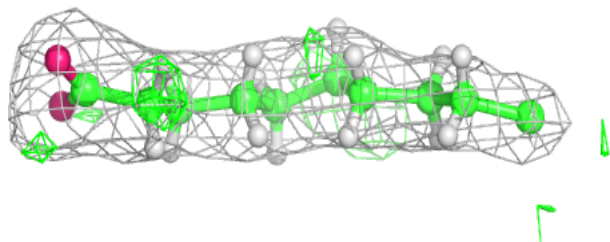
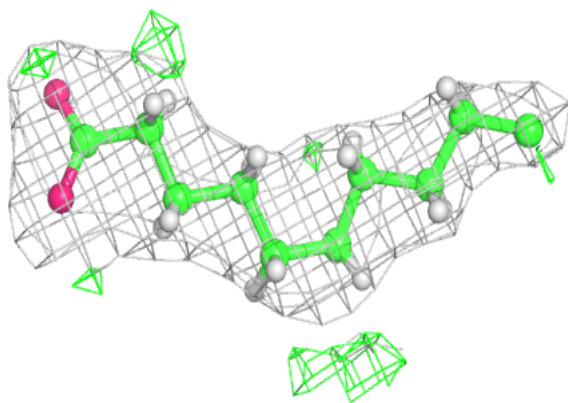
**Electron density around STE M 103:**

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

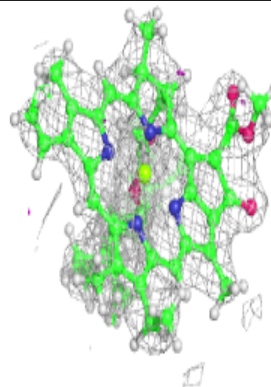
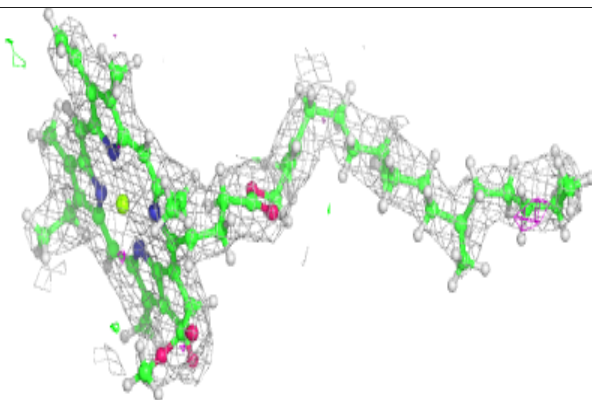
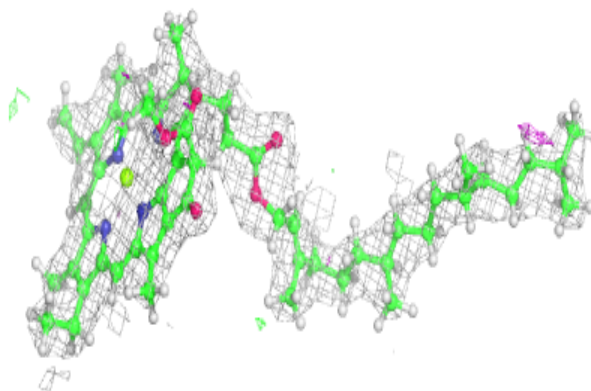


**Electron density around STE C 520:**

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

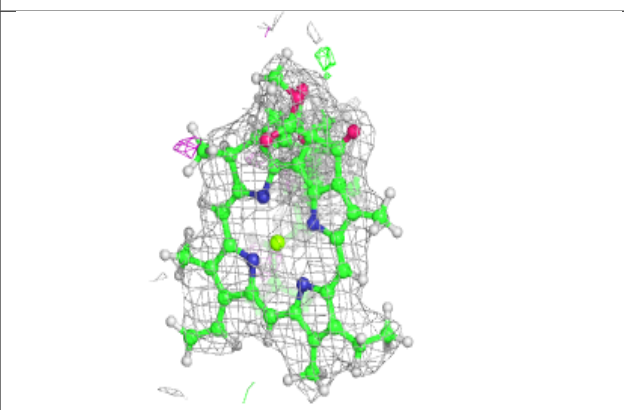
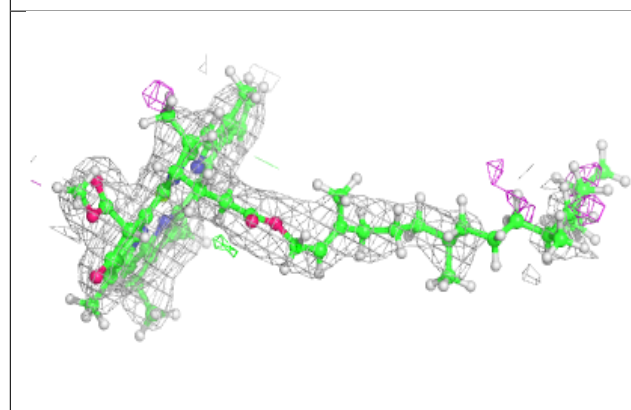
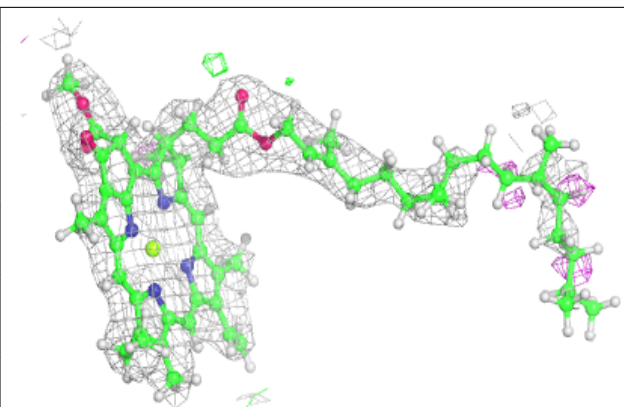
**Electron density around CLA C 502:**

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

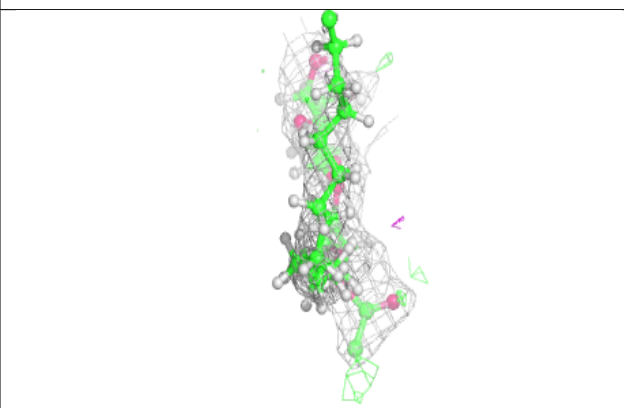
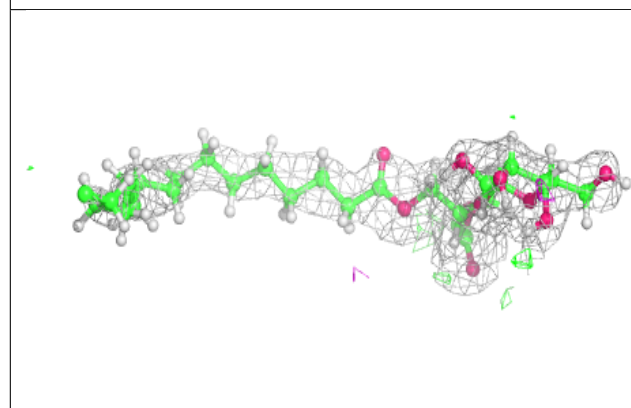
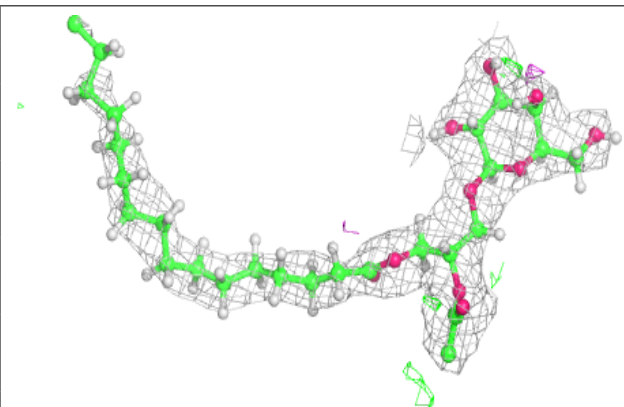


**Electron density around CLA d 404:**

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

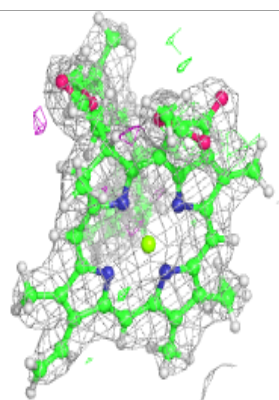
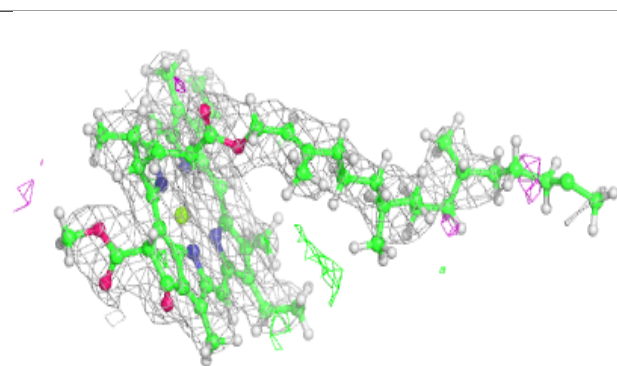
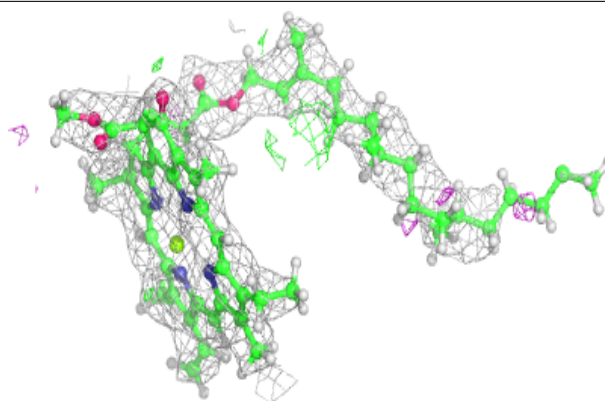
**Electron density around LMG c 520:**

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

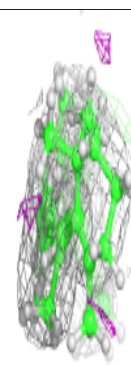
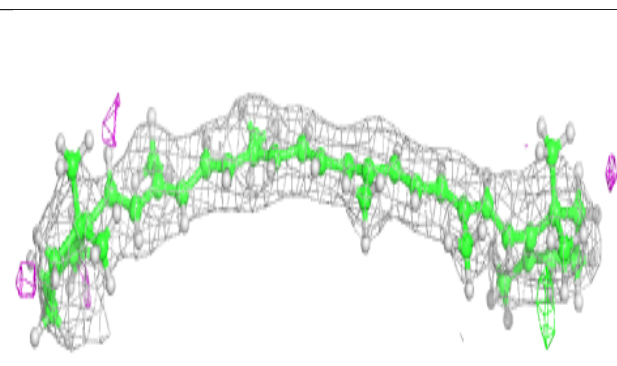
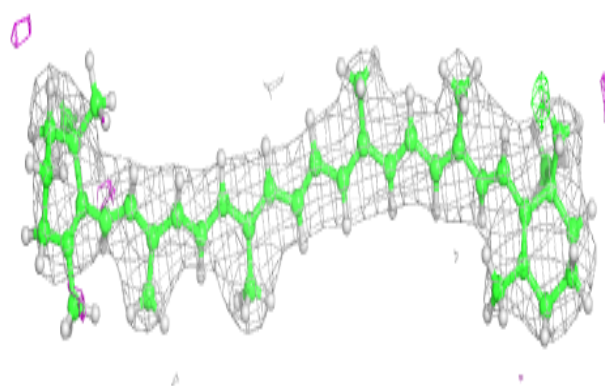


**Electron density around CLA c 509:**

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

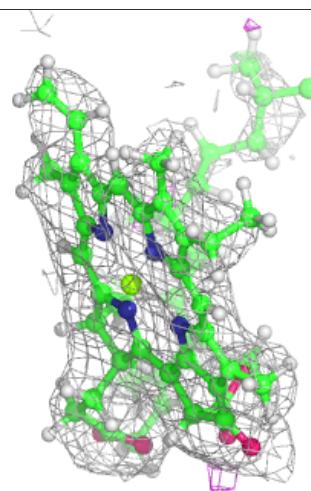
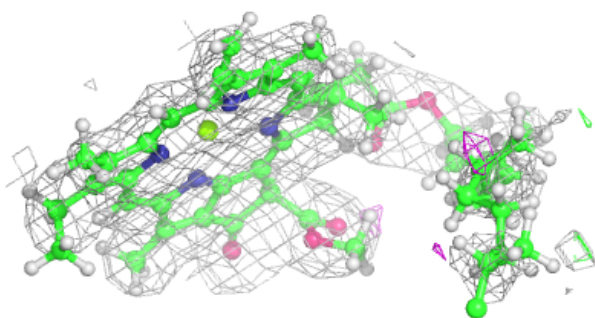
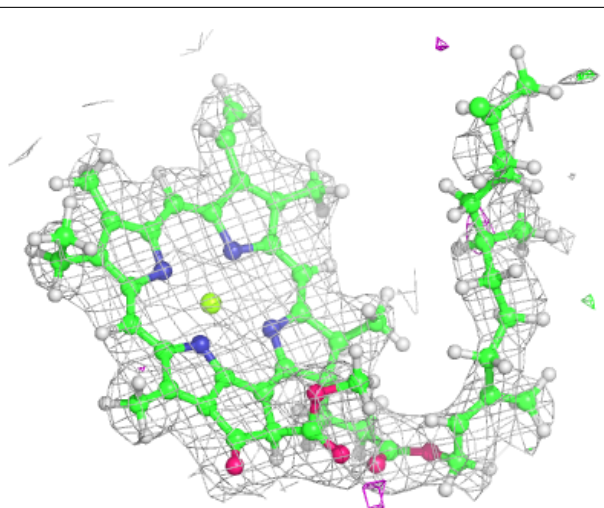
**Electron density around BCR F 101:**

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



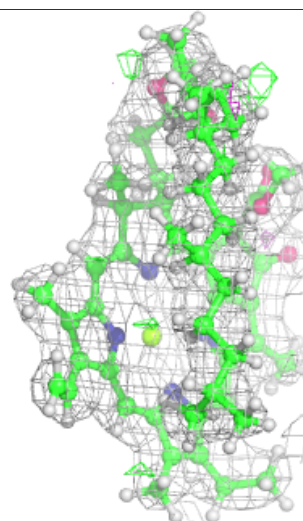
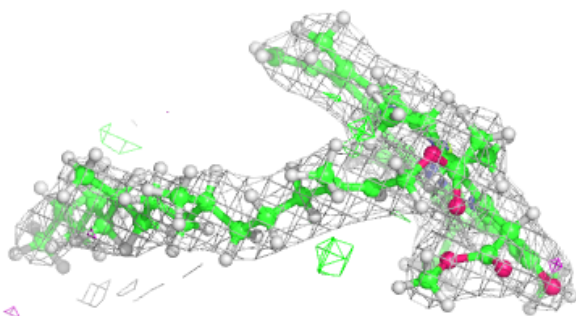
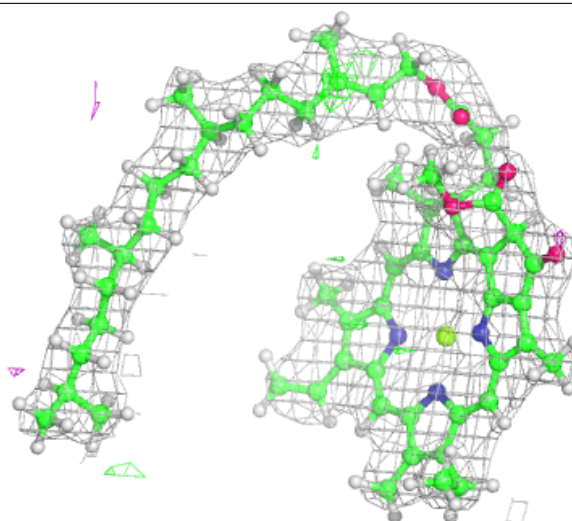
**Electron density around CLA b 616:**

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



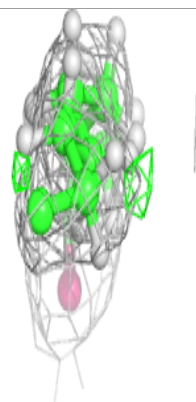
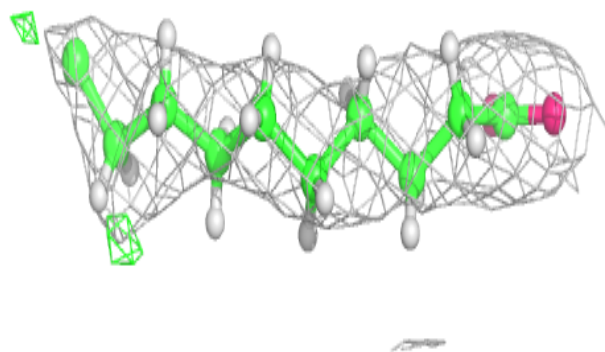
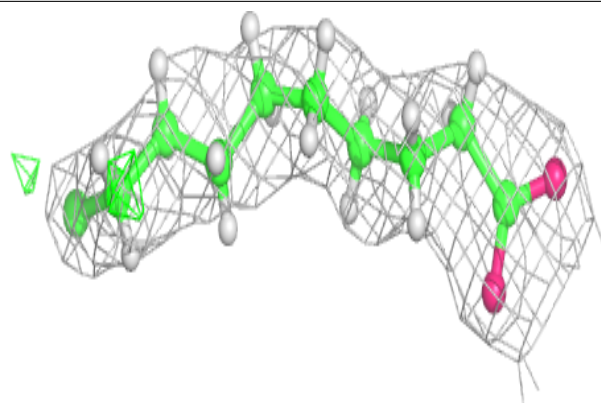
**Electron density around CLA C 507:**

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

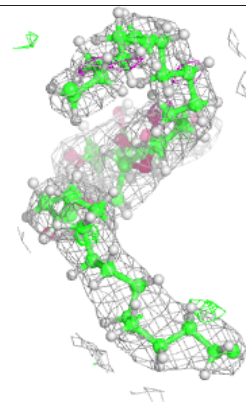
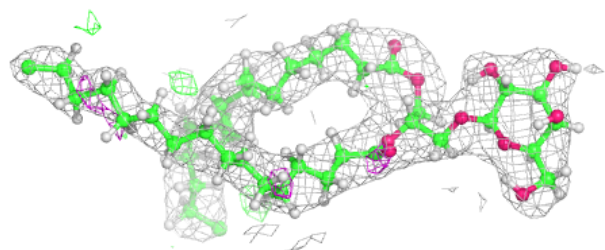
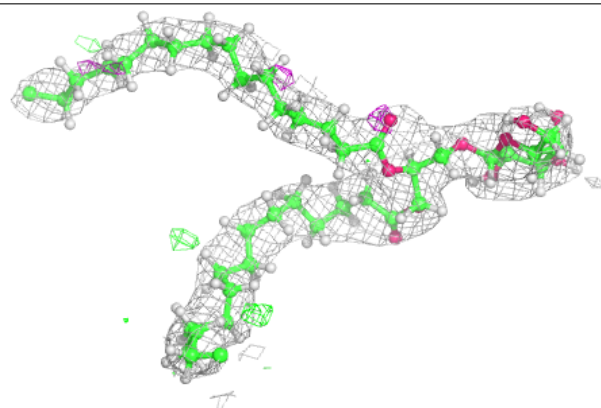


**Electron density around STE C 518:**

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

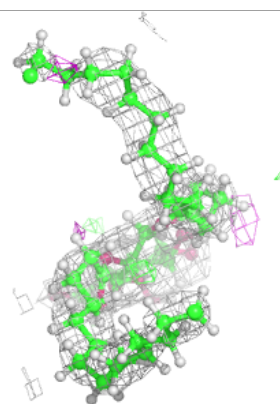
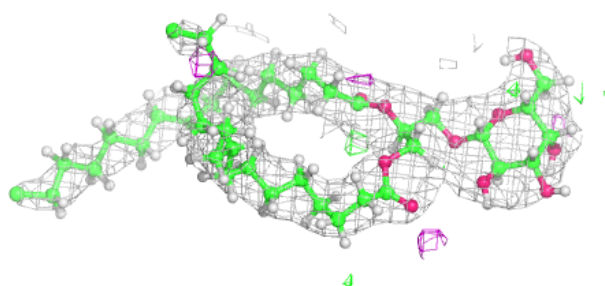
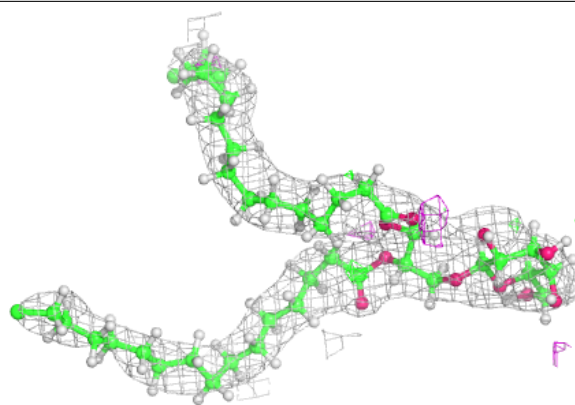
**Electron density around LMG M 101:**

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



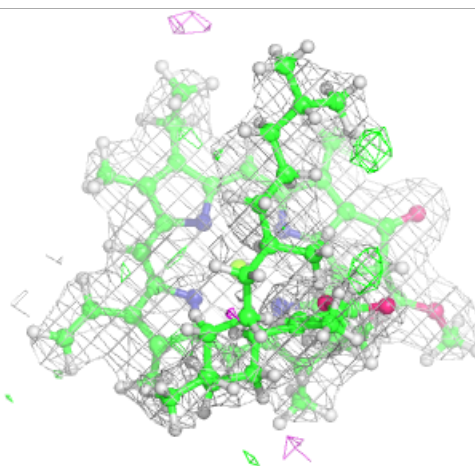
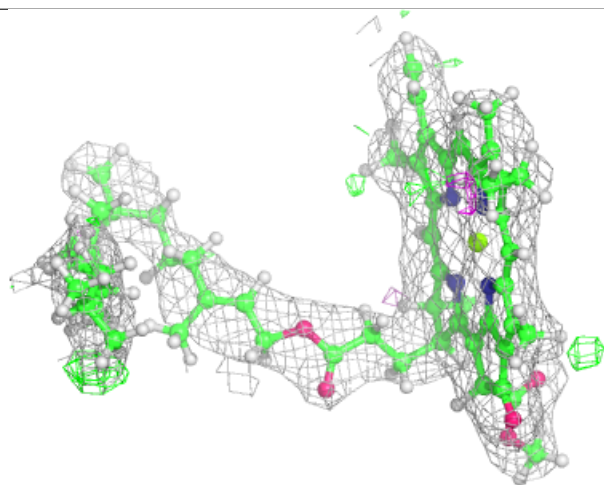
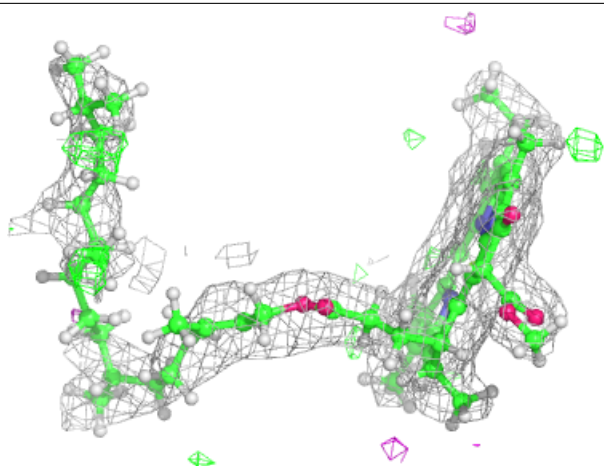
**Electron density around LMG b 621:**

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



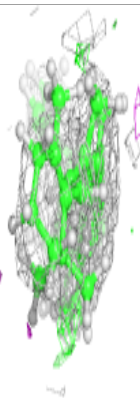
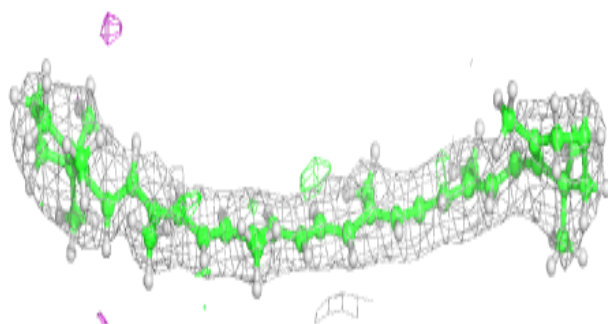
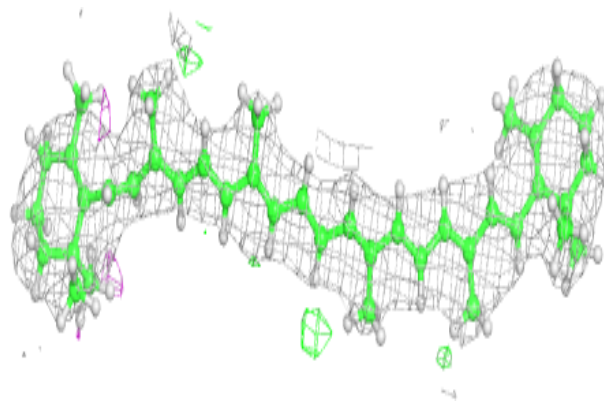
**Electron density around CLA a 405:**

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

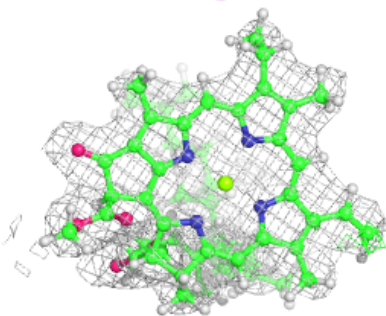
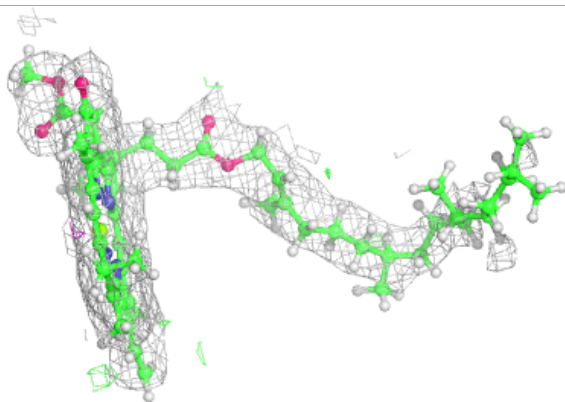
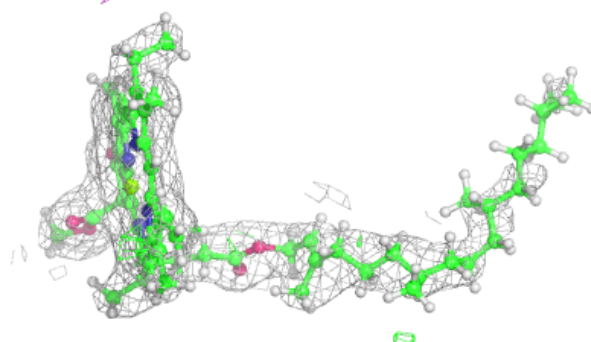


**Electron density around BCR d 405:**

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

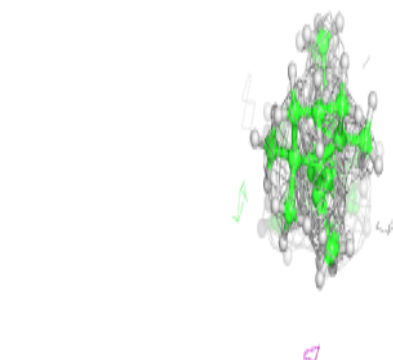
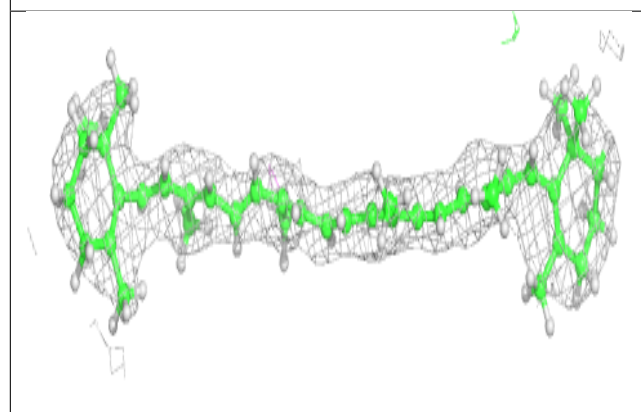
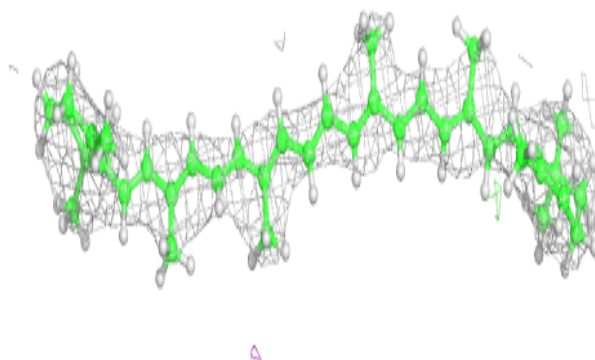
**Electron density around CLA D 405:**

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

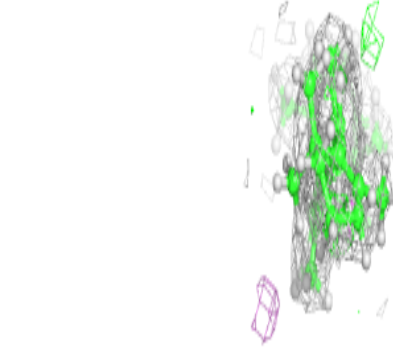
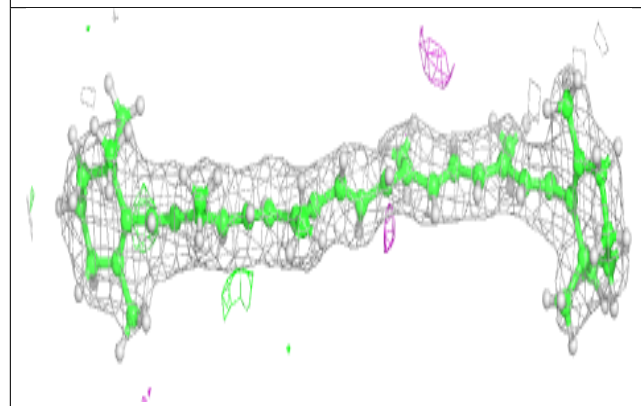
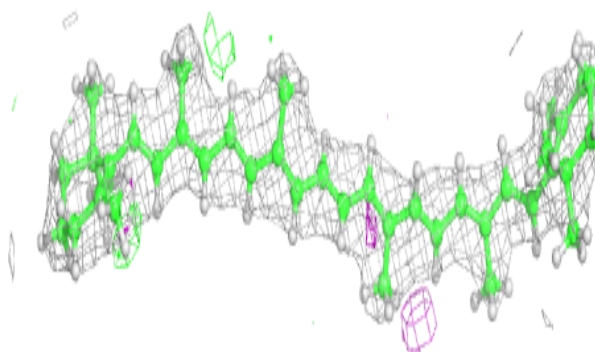


**Electron density around BCR c 515:**

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

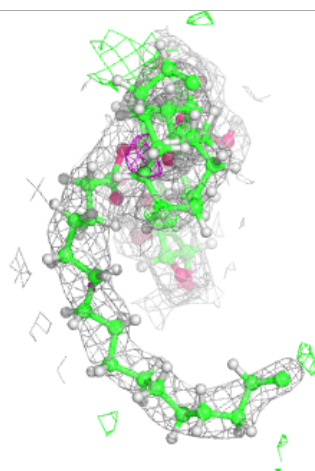
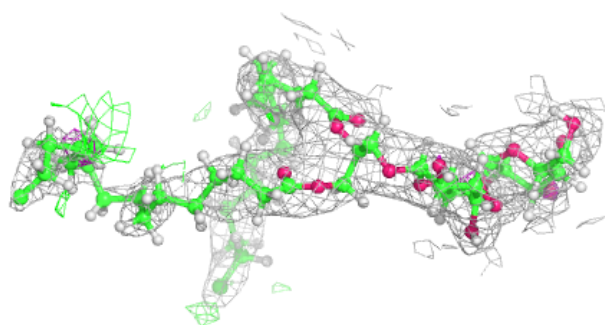
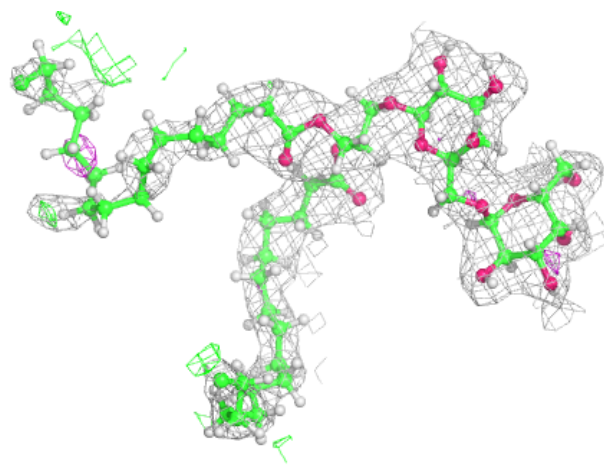
**Electron density around BCR C 514:**

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



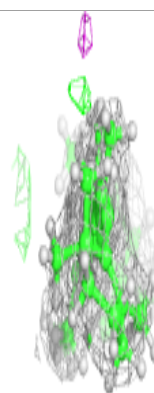
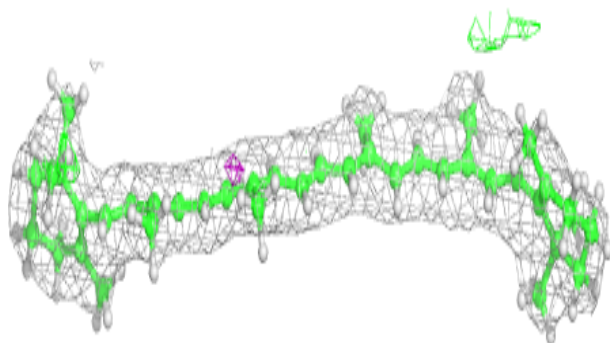
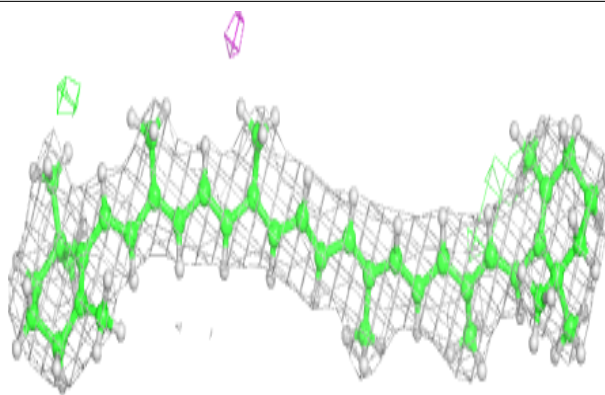
**Electron density around DGD C 516:**

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



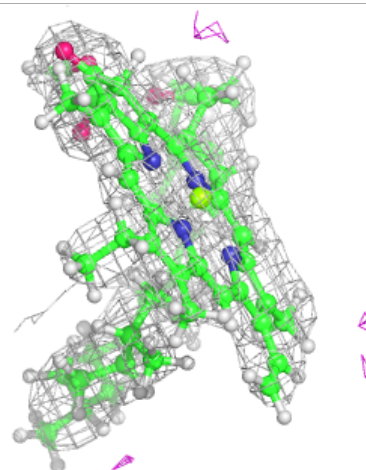
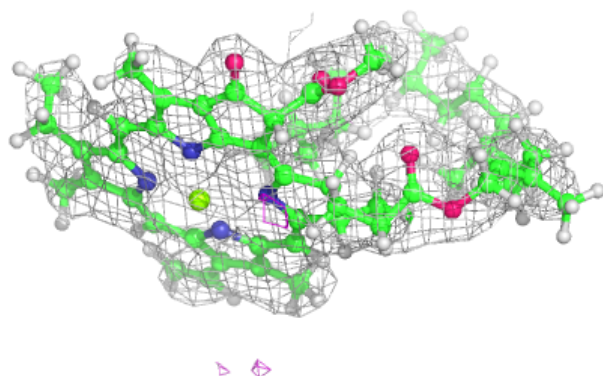
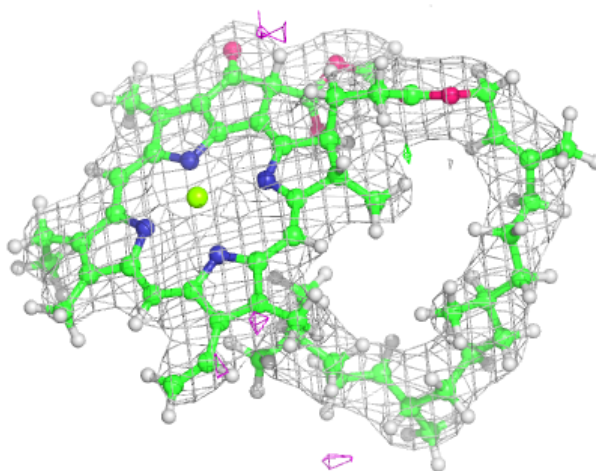
**Electron density around BCR B 619:**

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



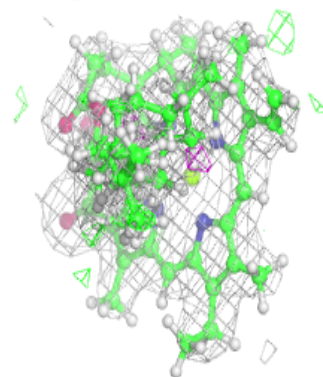
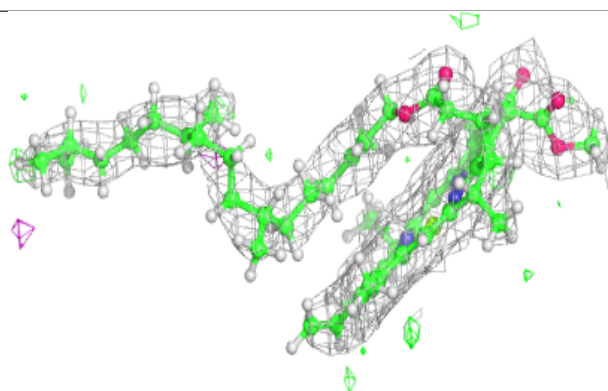
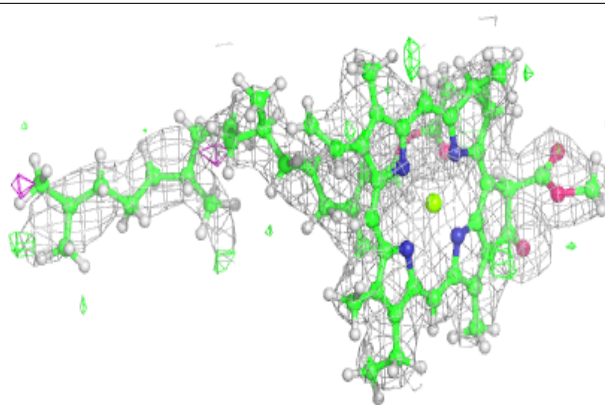
**Electron density around CLA b 615:**

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

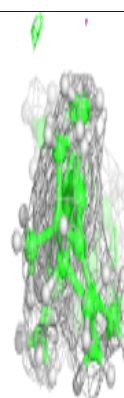
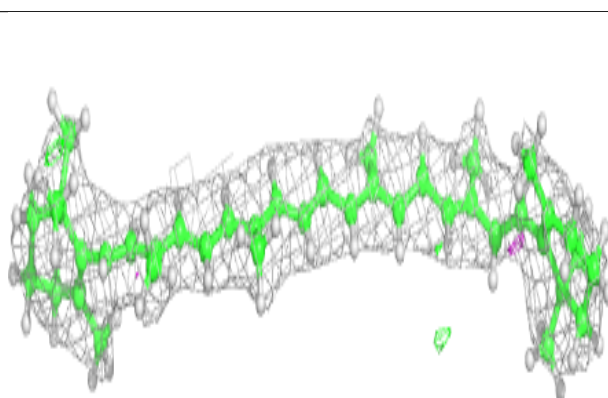
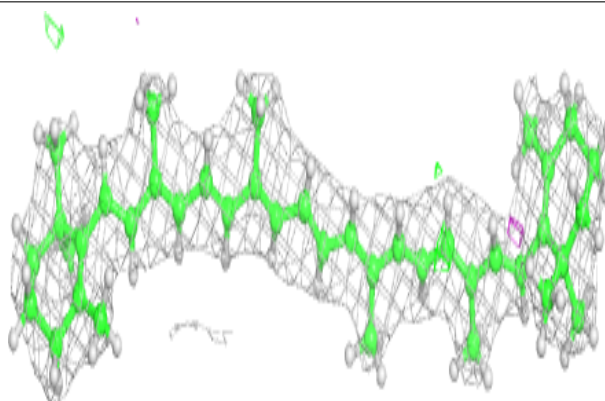


**Electron density around CLA c 506:**

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

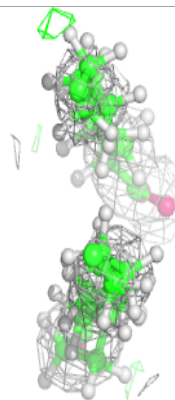
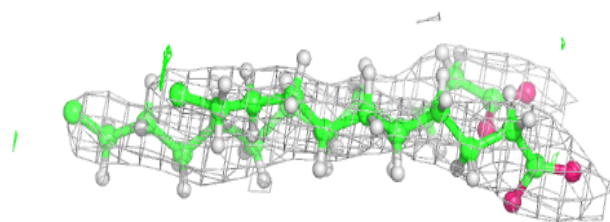
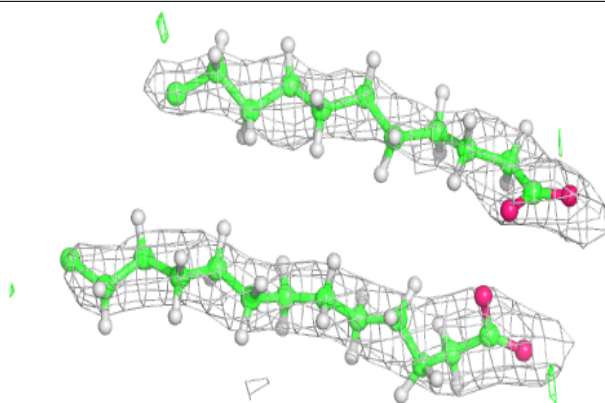
**Electron density around BCR b 619:**

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

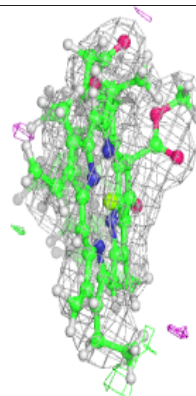
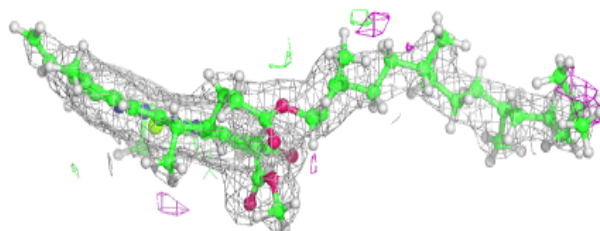
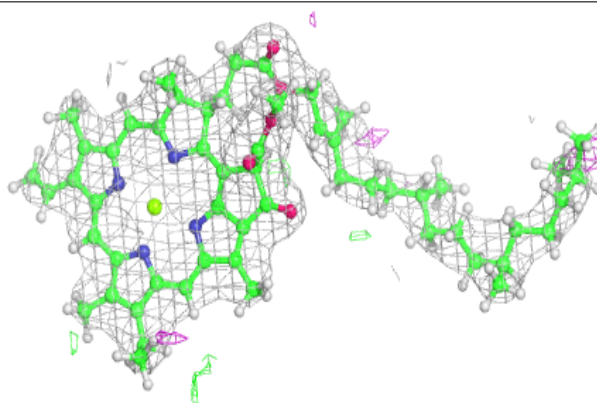


**Electron density around LMG B 621:**

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

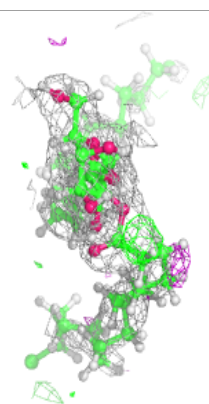
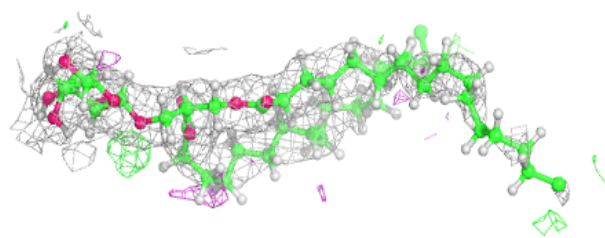
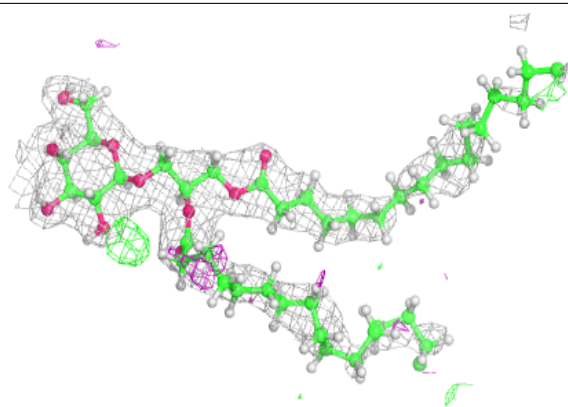
**Electron density around CLA b 602:**

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

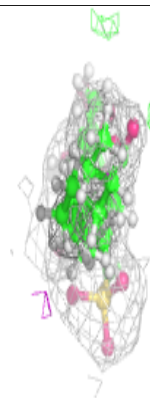
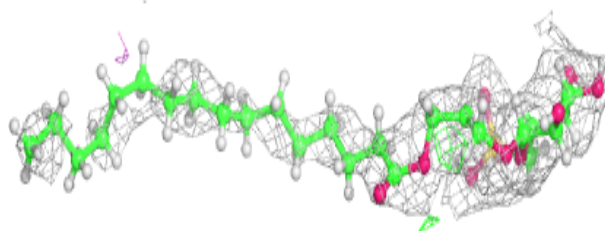
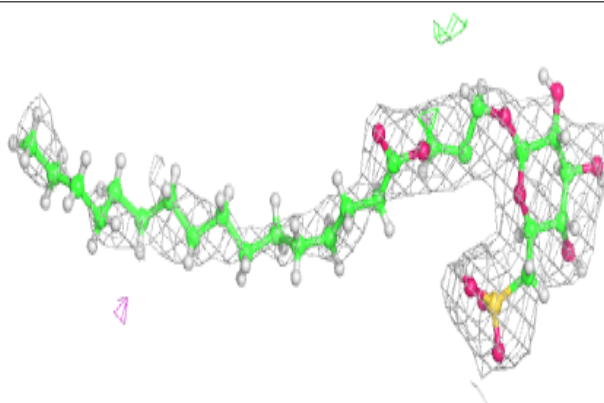


**Electron density around LMG D 407:**

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

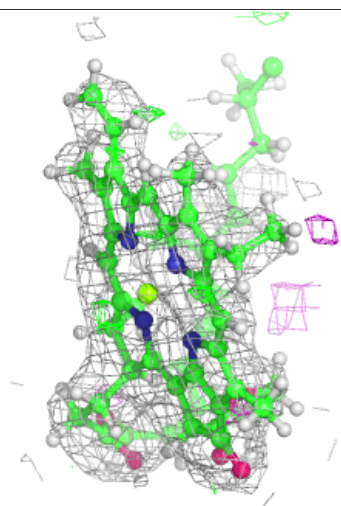
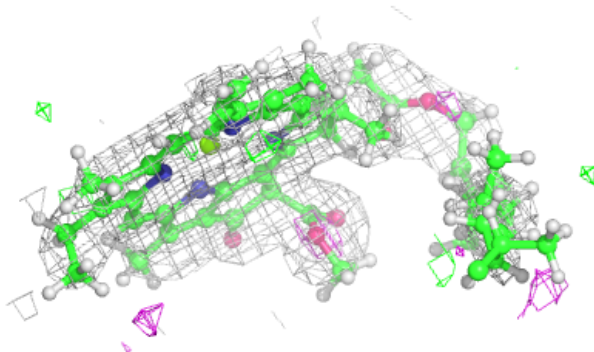
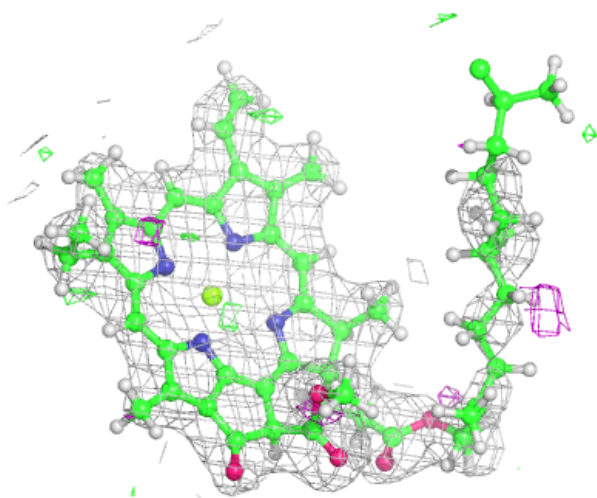
**Electron density around SQD D 408:**

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



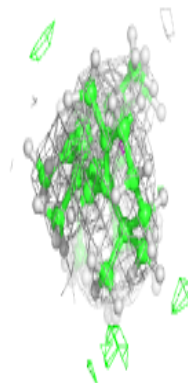
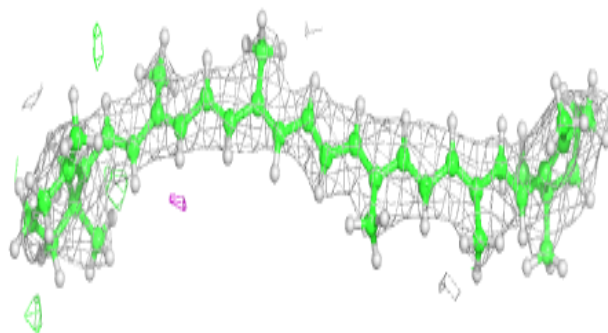
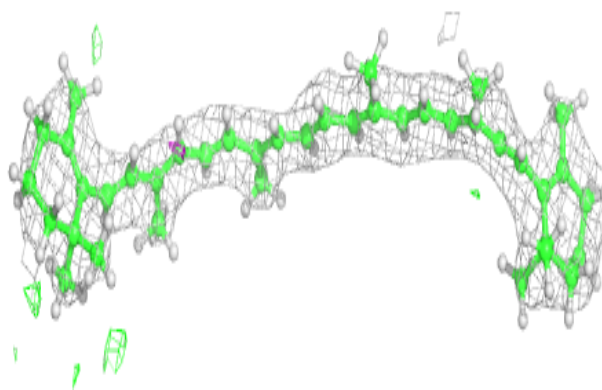
**Electron density around CLA B 616:**

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

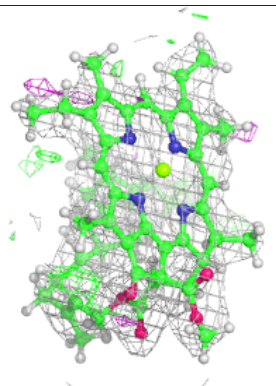
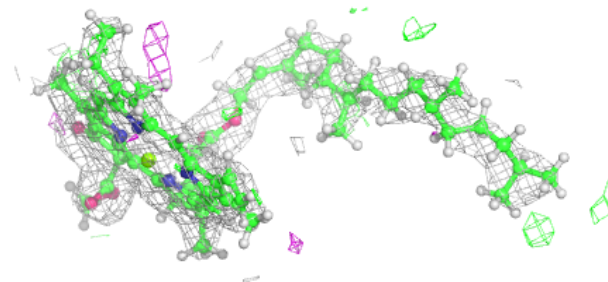
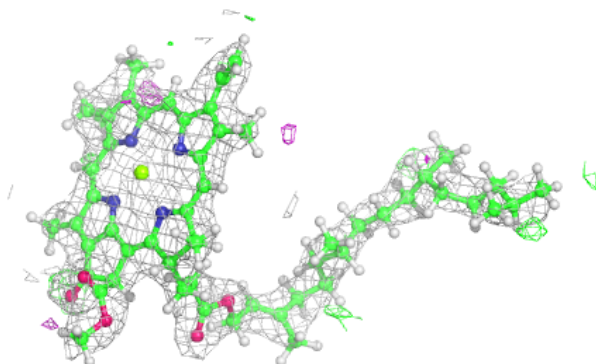


**Electron density around BCR K 103:**

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

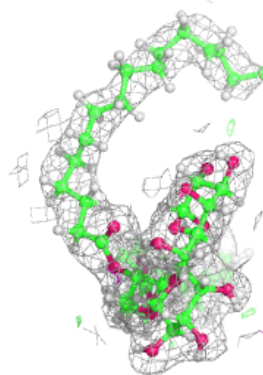
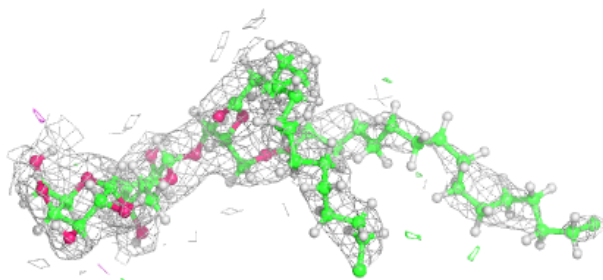
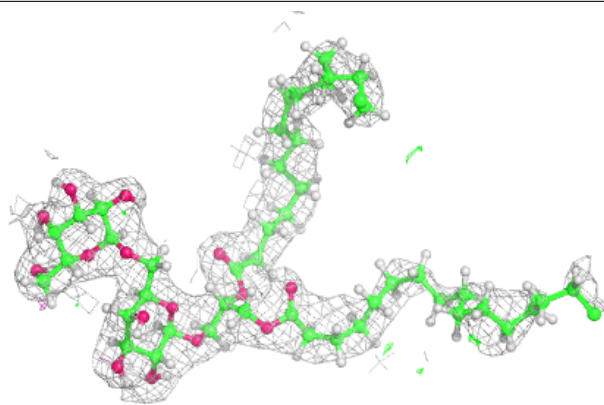
**Electron density around CLA c 512:**

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



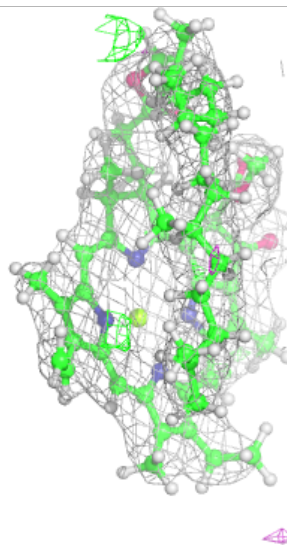
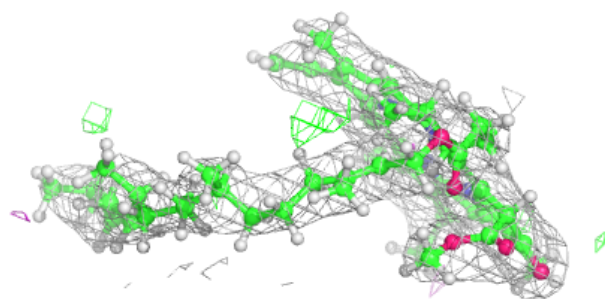
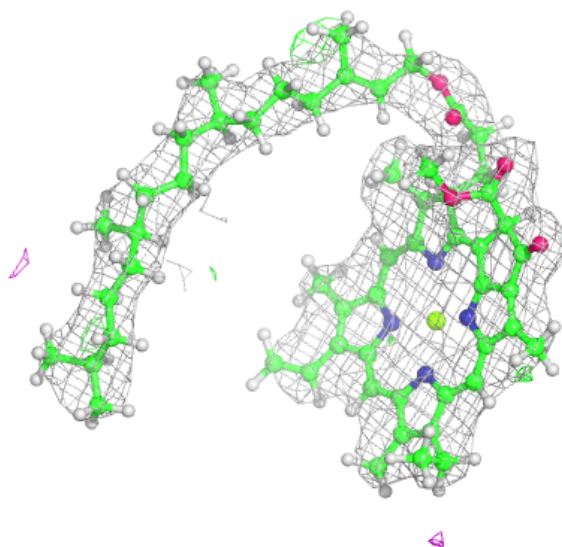
**Electron density around DGD c 518:**

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



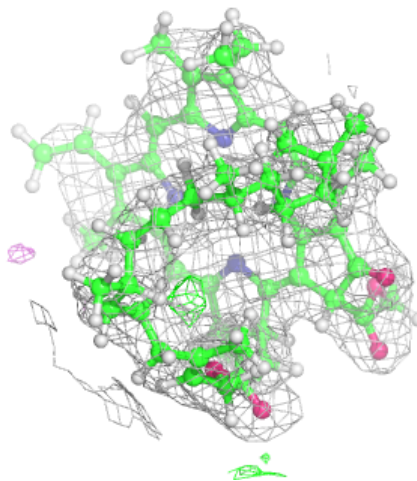
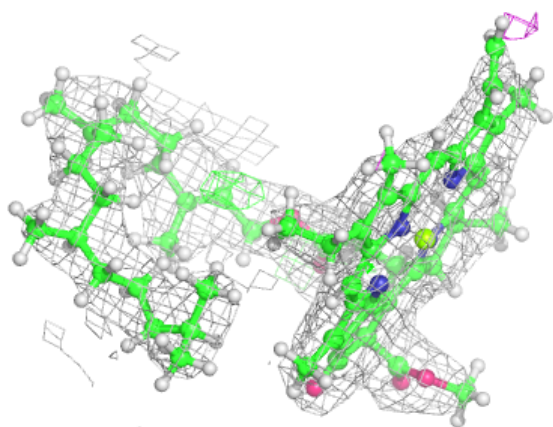
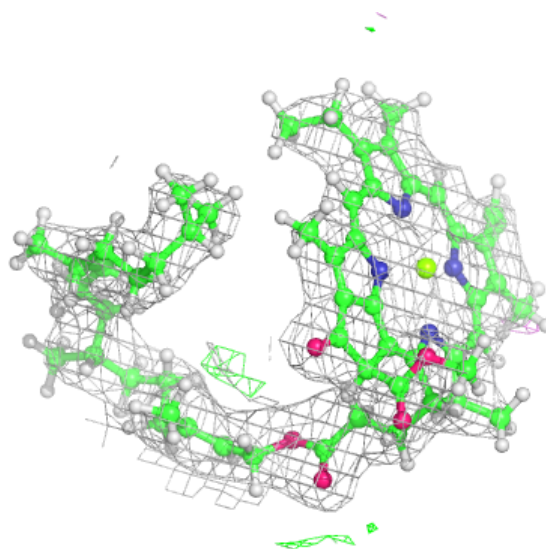
**Electron density around CLA c 508:**

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



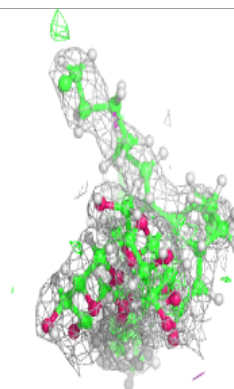
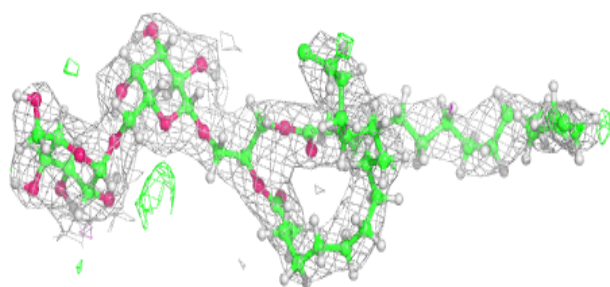
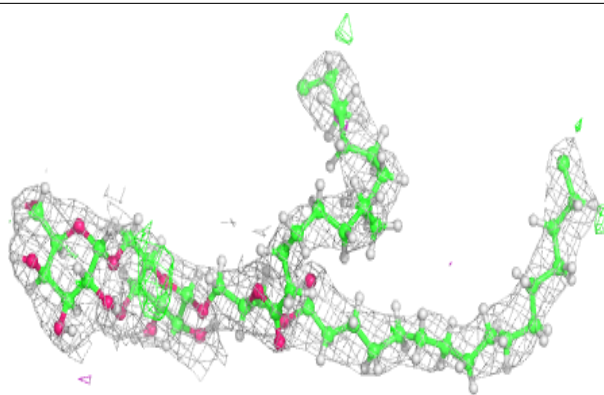
**Electron density around CLA c 504:**

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



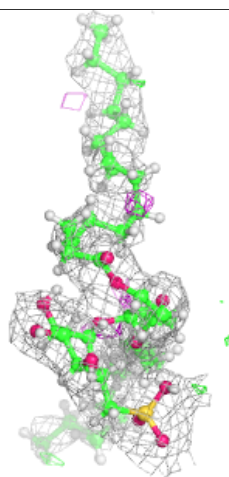
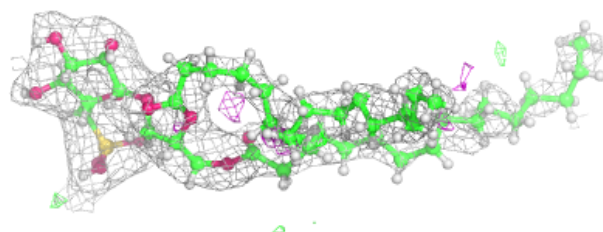
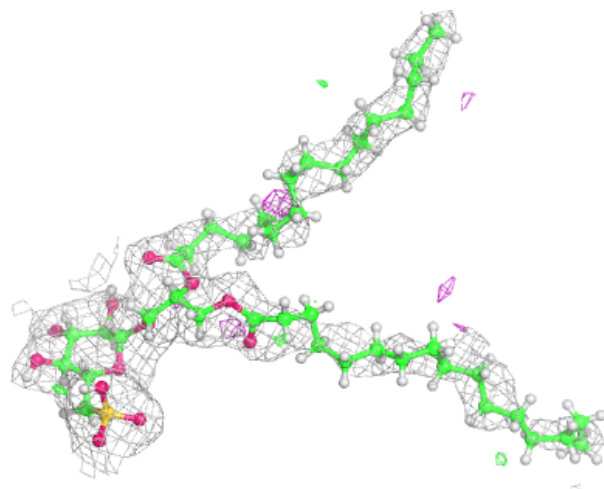
**Electron density around DGD h 102:**

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



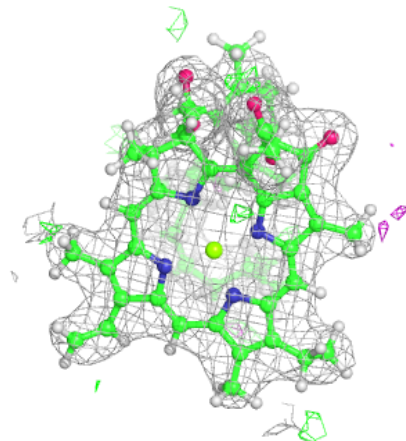
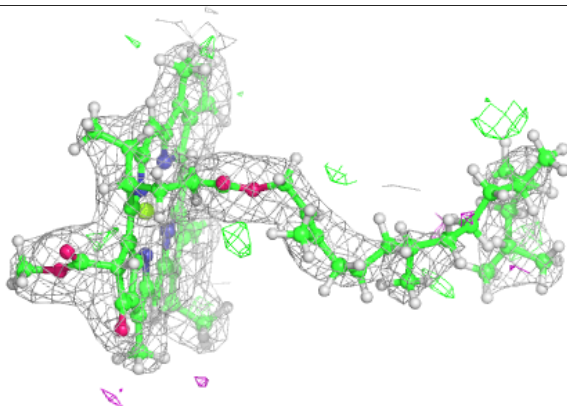
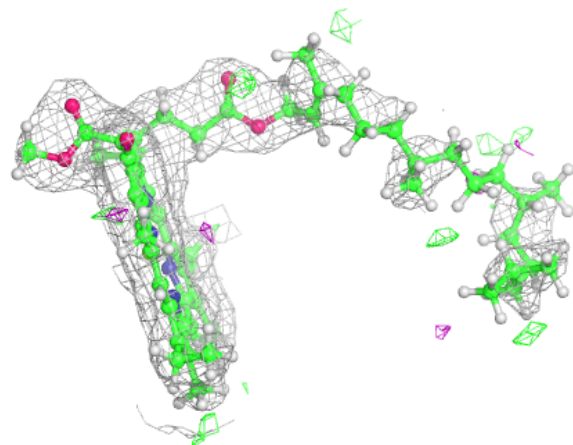
**Electron density around SQD a 411:**

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



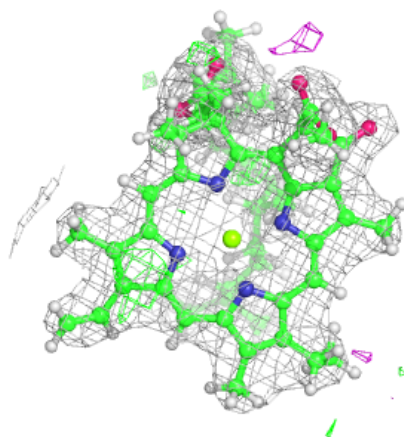
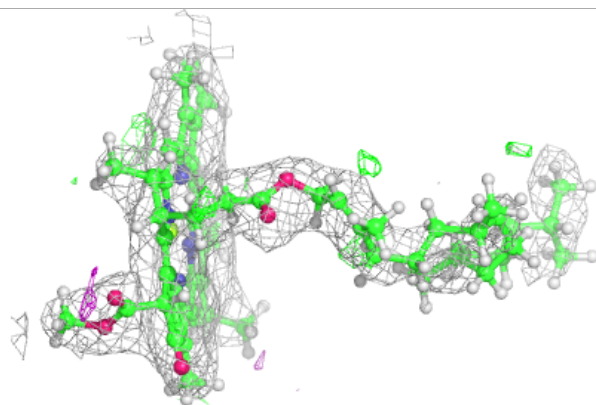
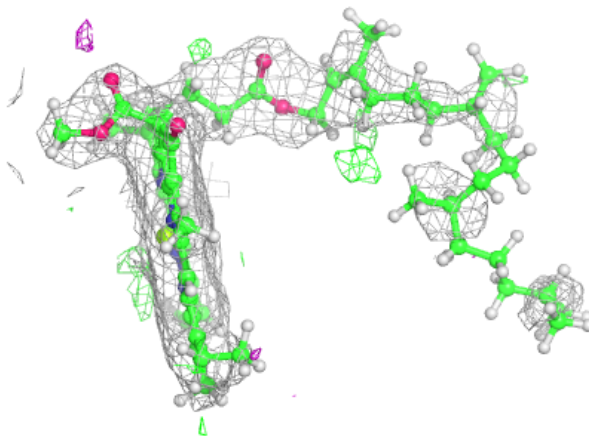
**Electron density around CLA C 506:**

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



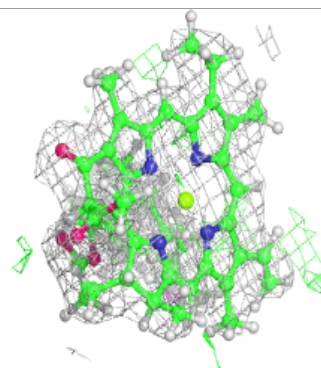
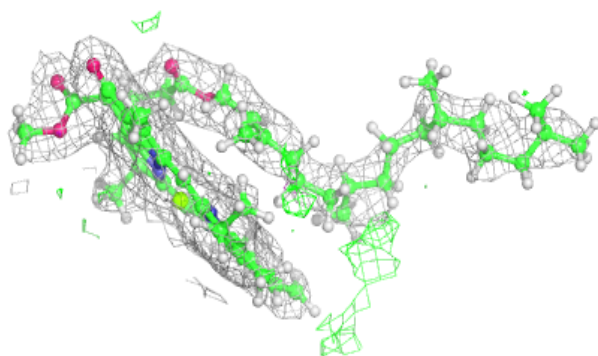
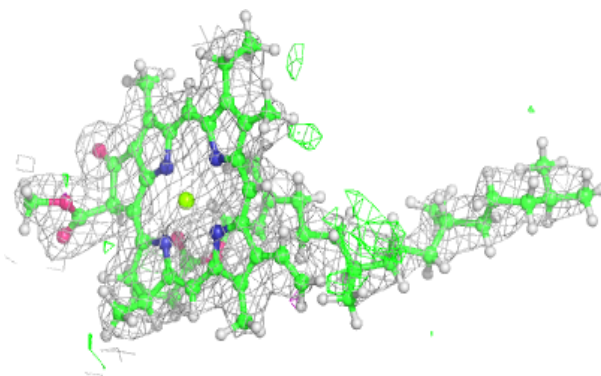
**Electron density around CLA c 507:**

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

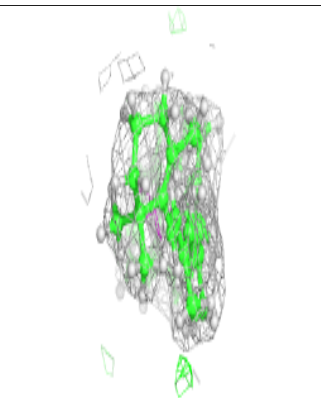
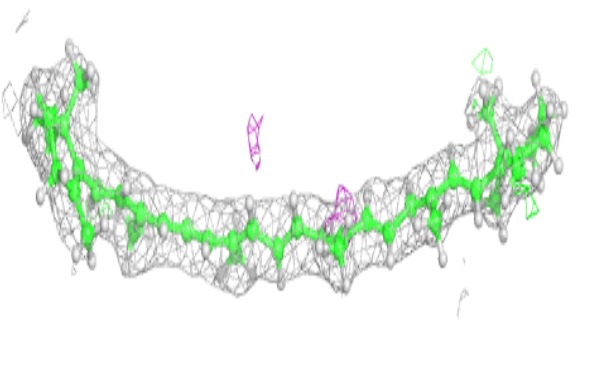
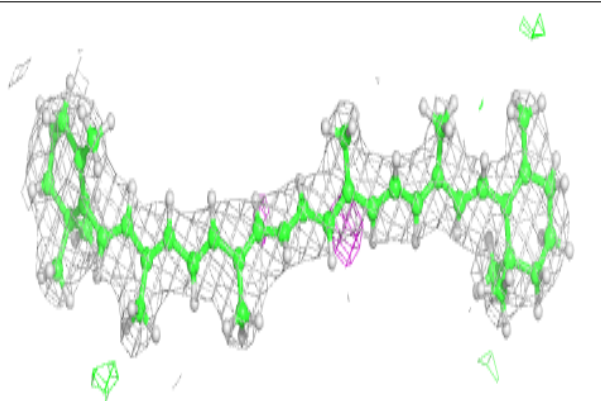


**Electron density around CLA C 505:**

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

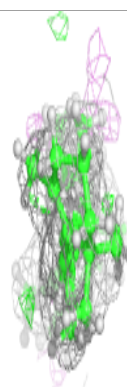
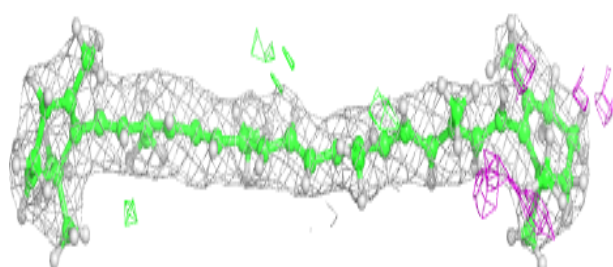
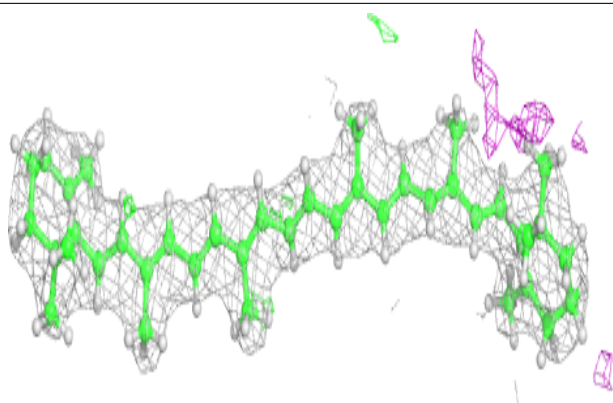
**Electron density around BCR T 101:**

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

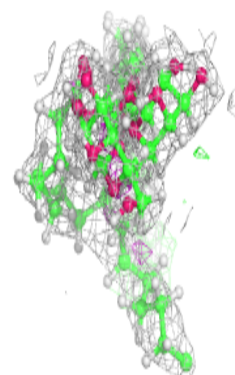
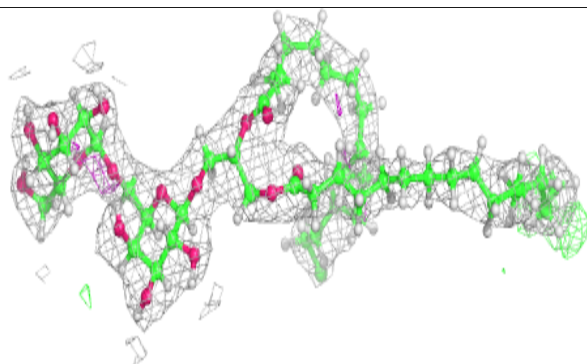
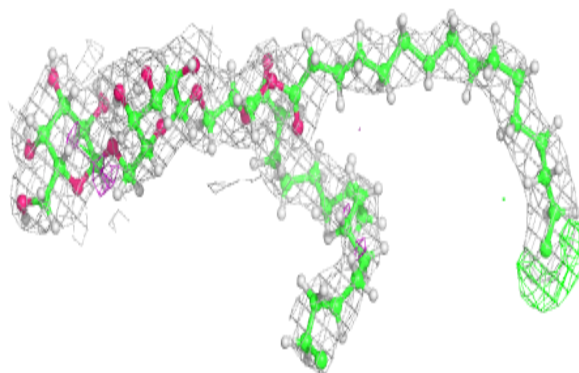


**Electron density around BCR B 618:**

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

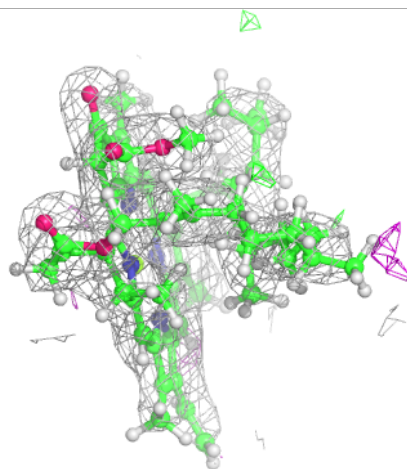
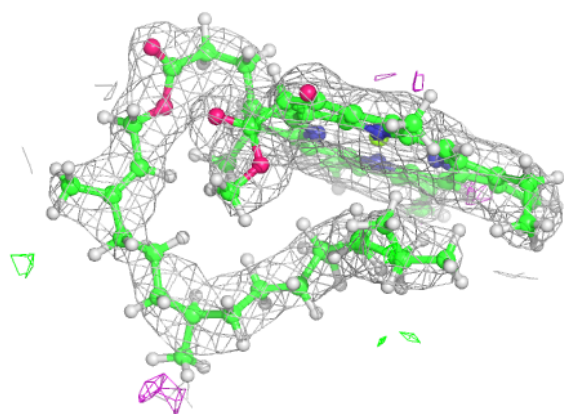
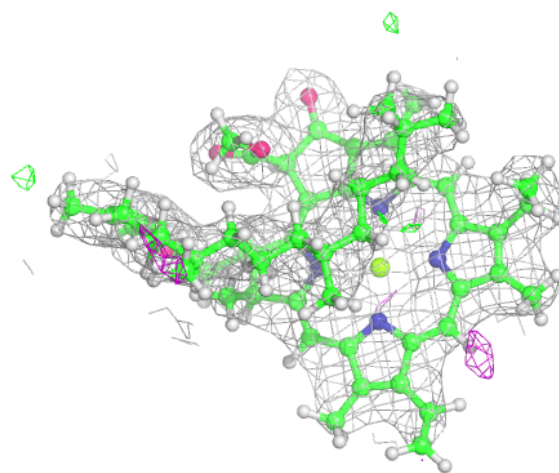
**Electron density around DGD H 103:**

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



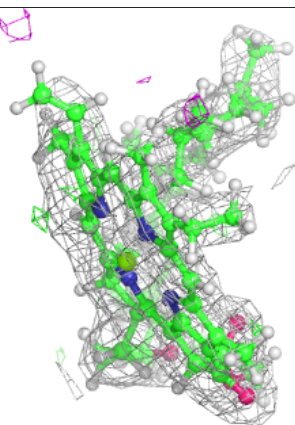
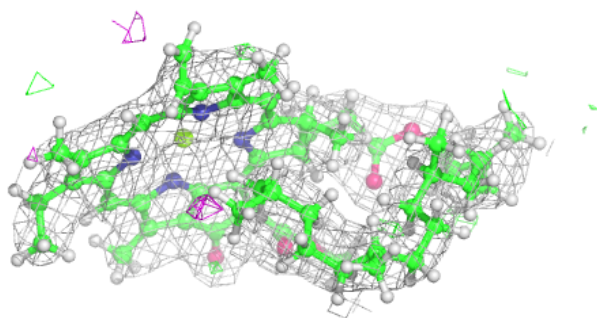
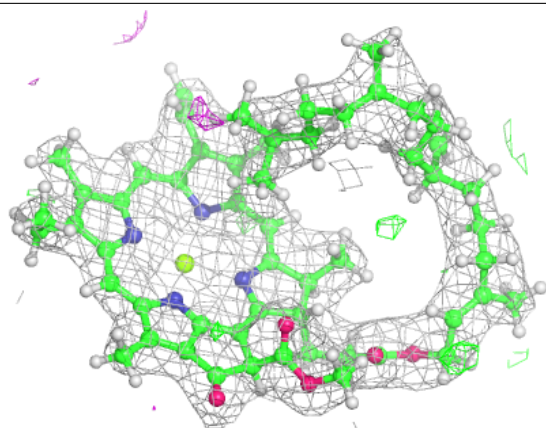
**Electron density around CLA C 510:**

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

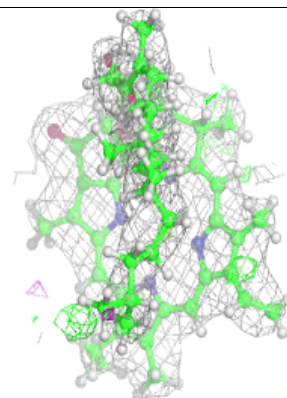
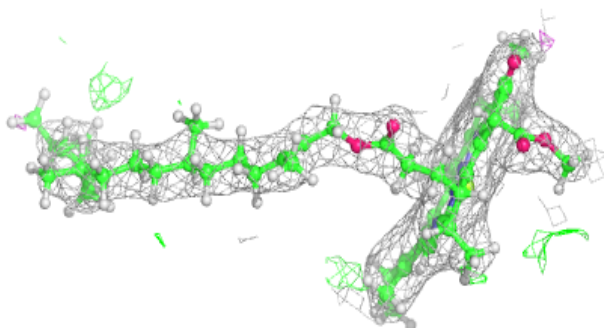
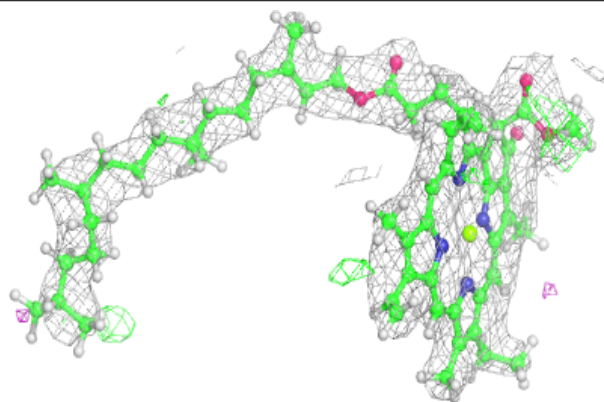


**Electron density around CLA B 615:**

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

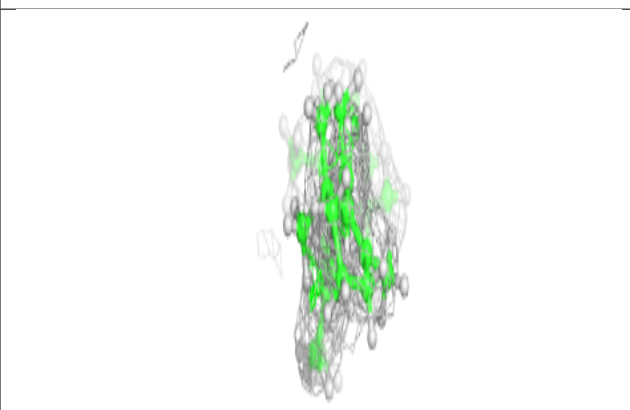
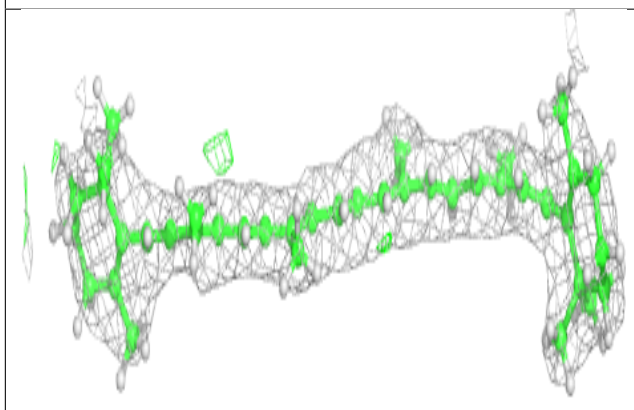
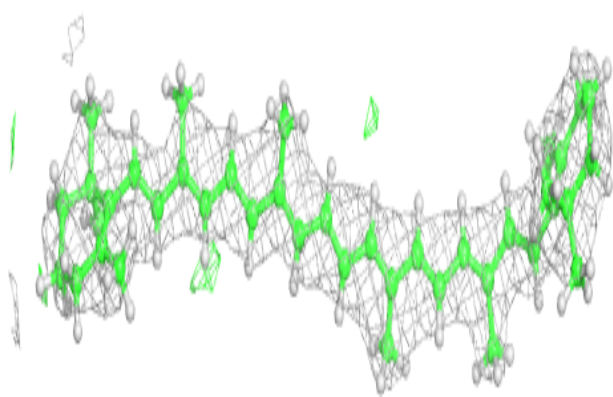
**Electron density around CLA b 609:**

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

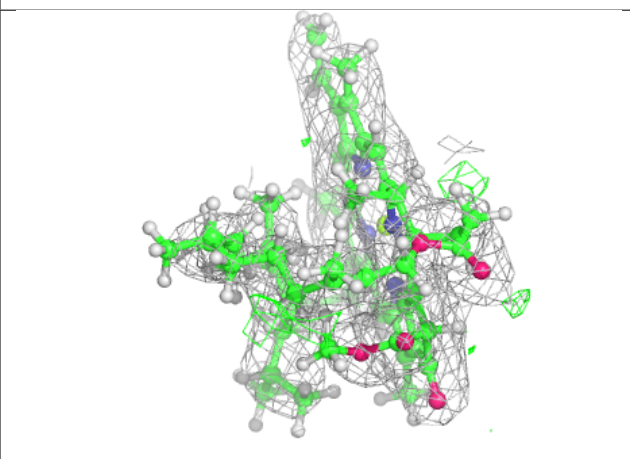
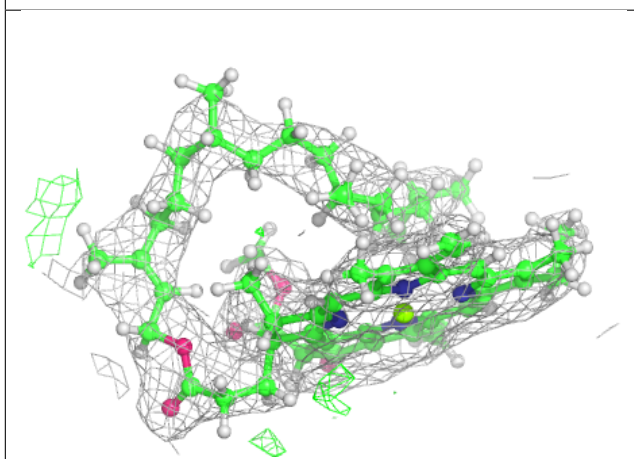
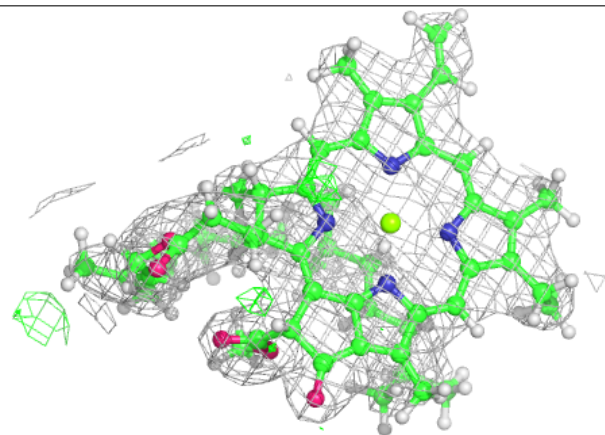


**Electron density around BCR c 516:**

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

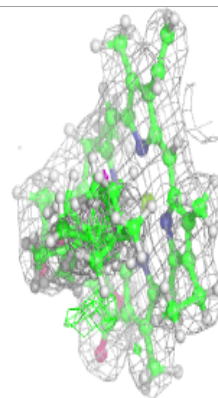
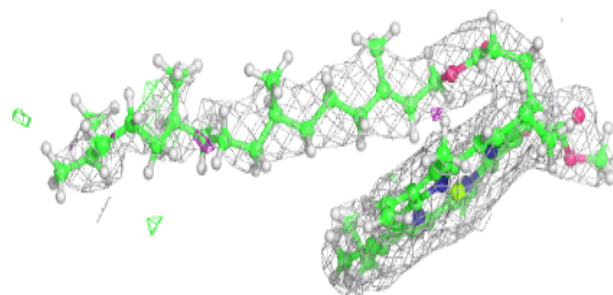
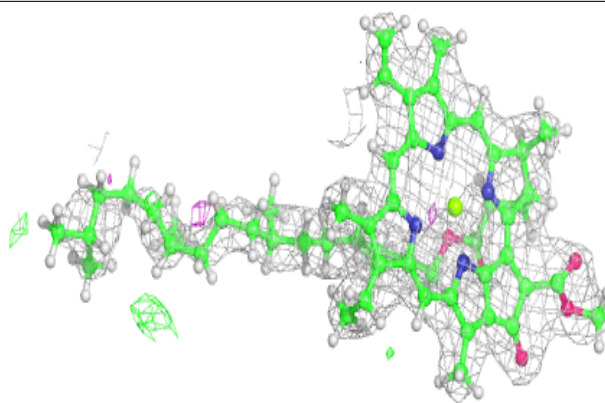
**Electron density around CLA c 511:**

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



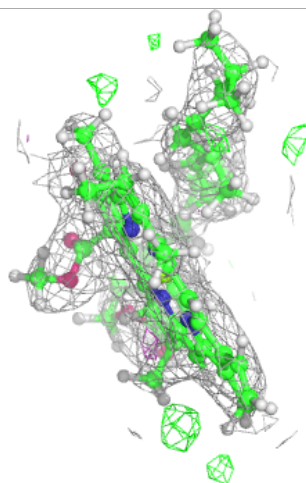
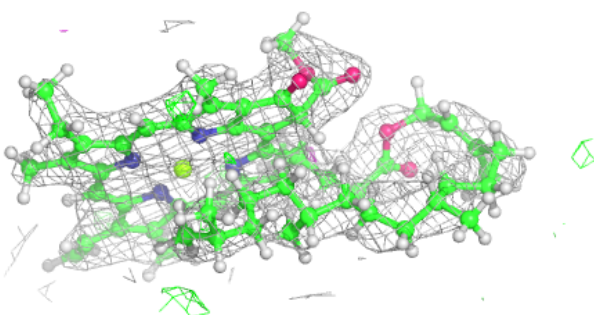
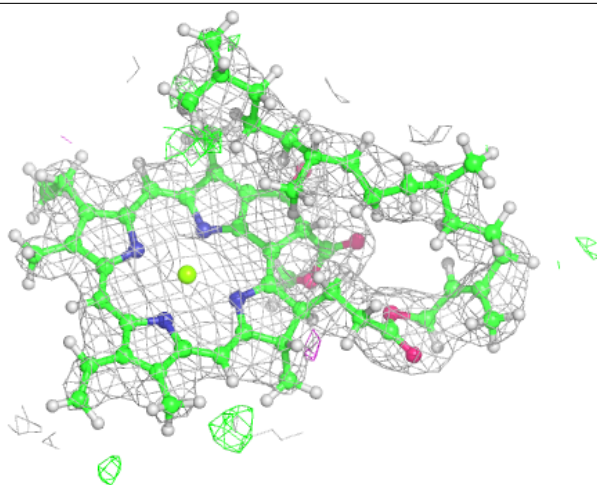
**Electron density around CLA B 614:**

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



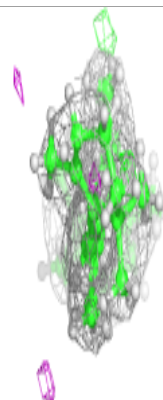
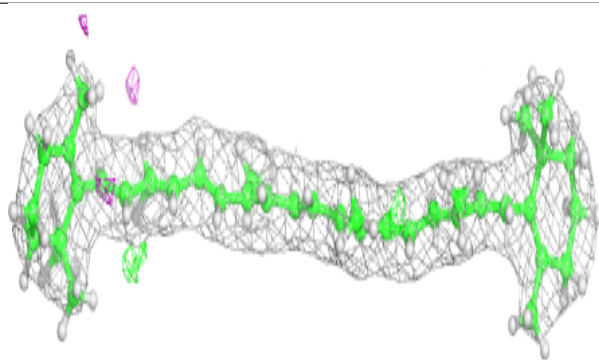
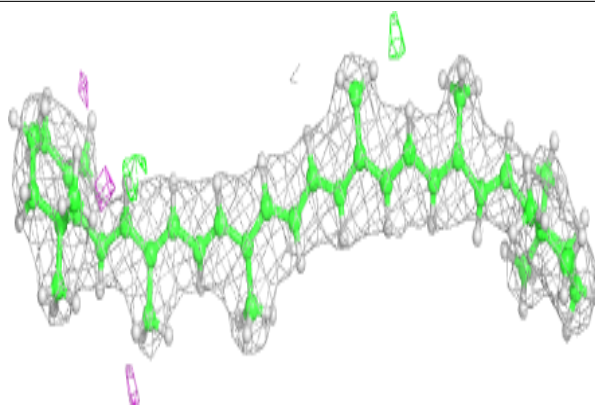
**Electron density around CLA c 510:**

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



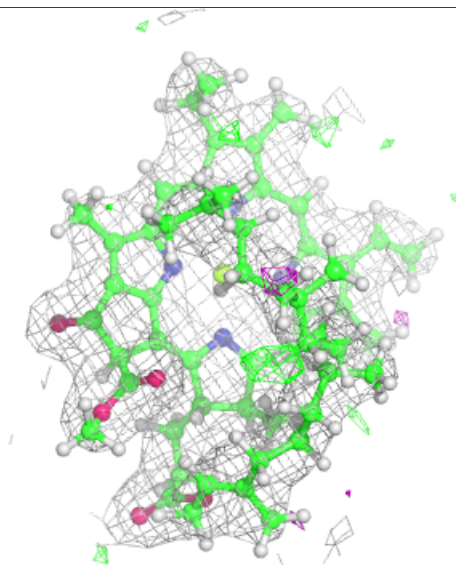
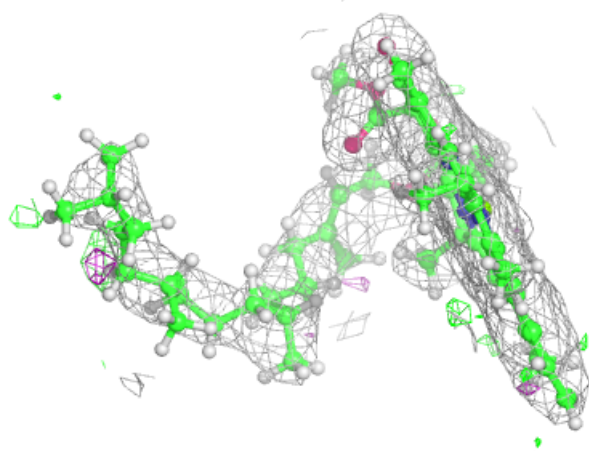
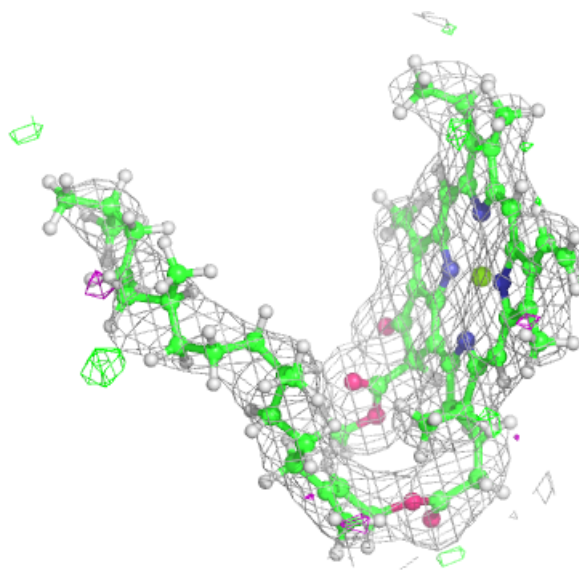
**Electron density around BCR A 406:**

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



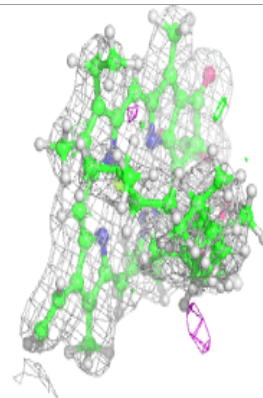
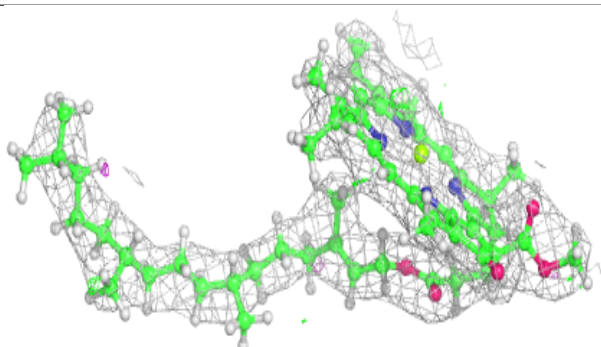
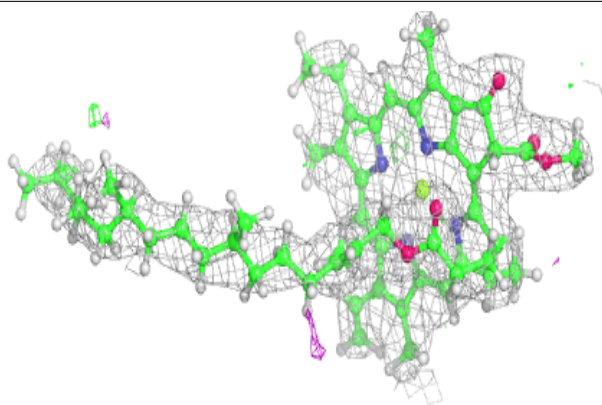
**Electron density around CLA B 613:**

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

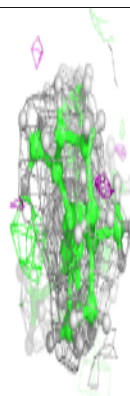
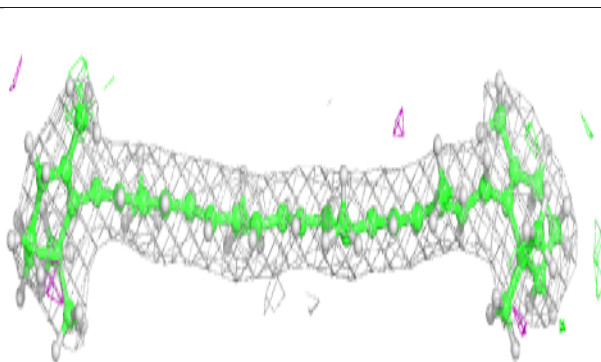
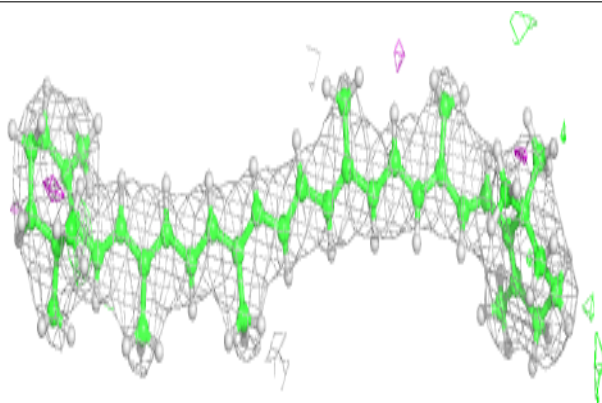


**Electron density around CLA b 608:**

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

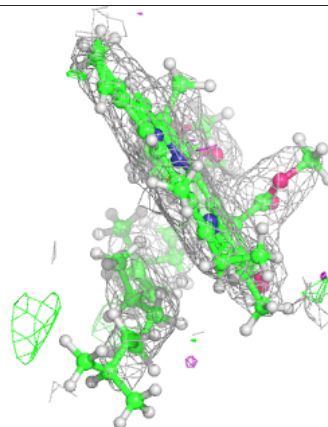
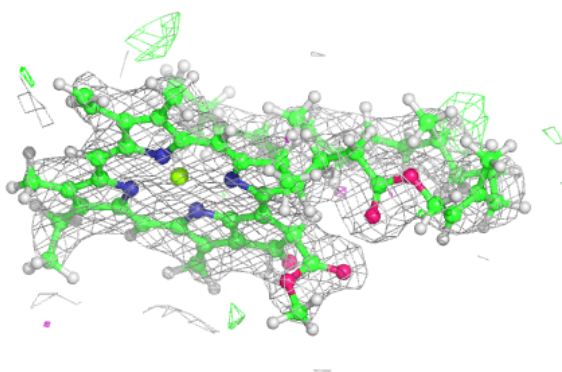
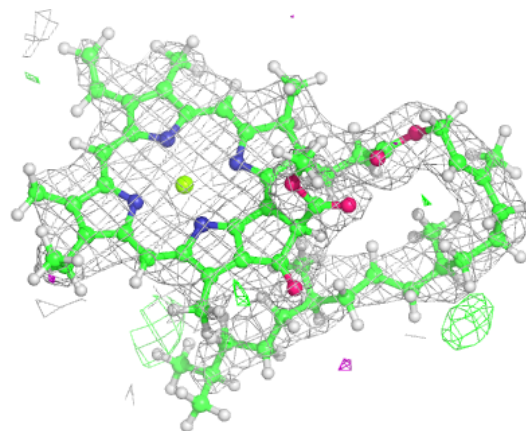
**Electron density around BCR b 618:**

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

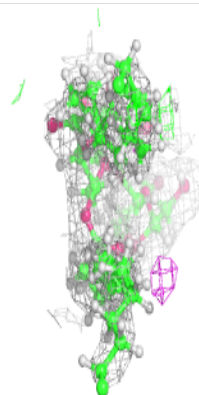
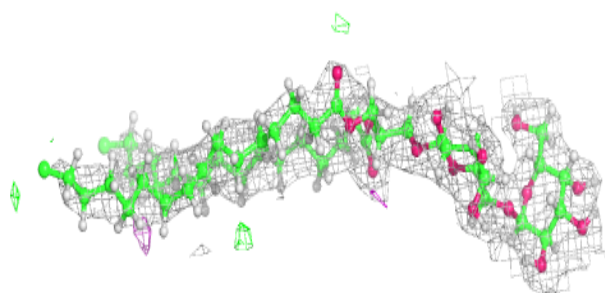
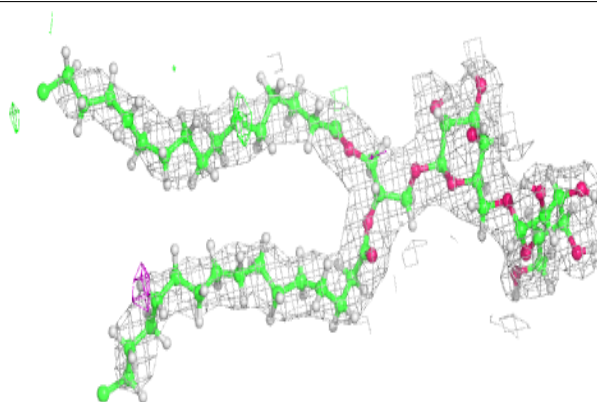


**Electron density around CLA C 509:**

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

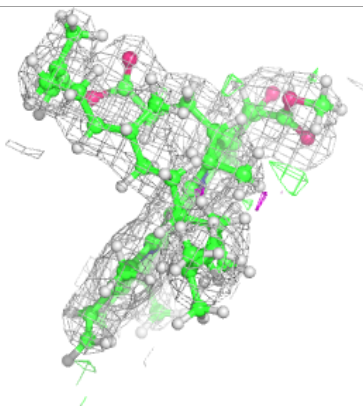
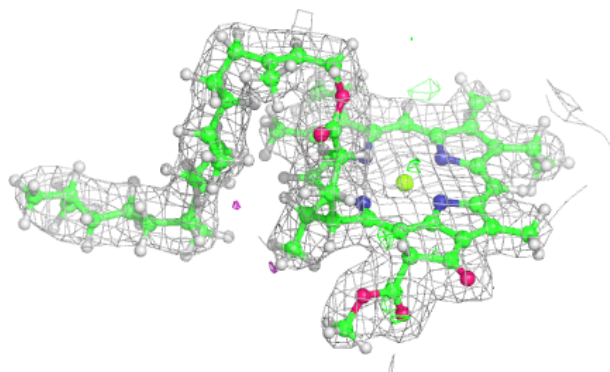
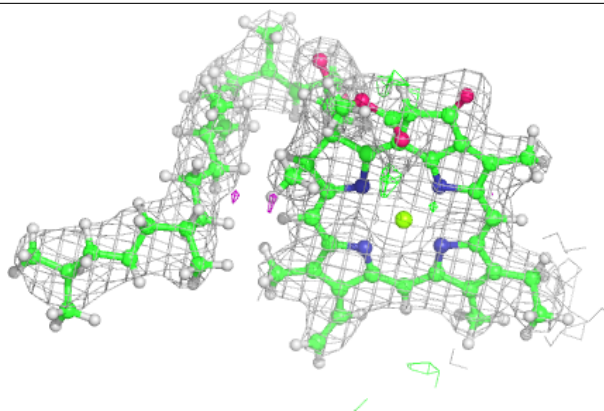
**Electron density around DGD C 517:**

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

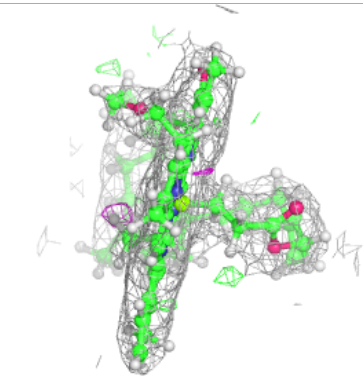
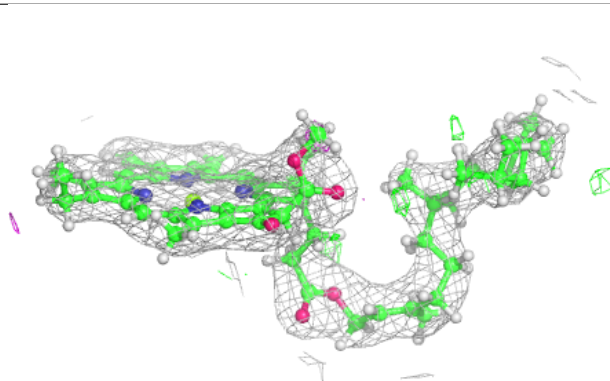
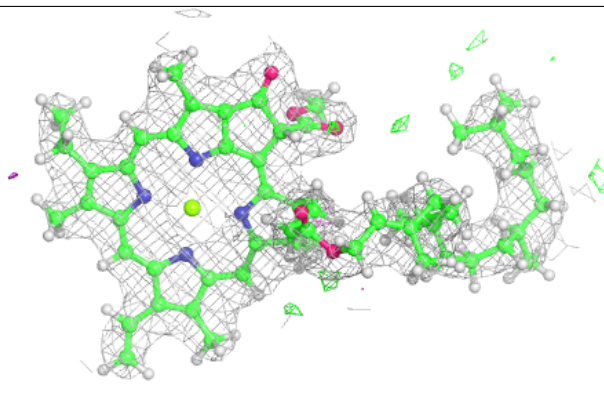


**Electron density around CLA a 410:**

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

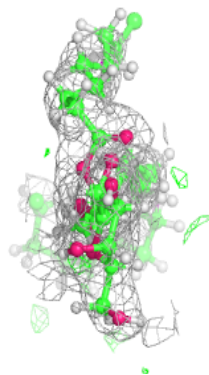
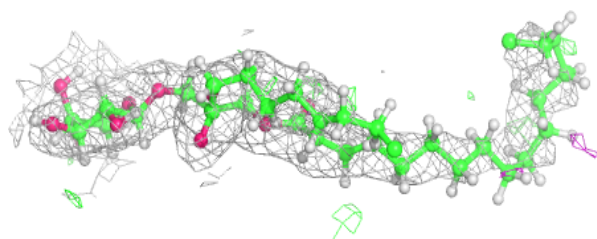
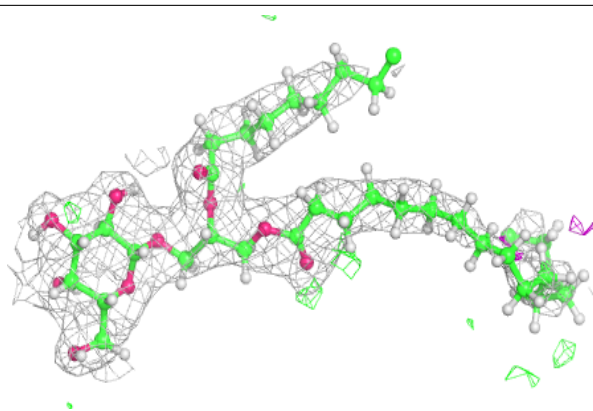
**Electron density around CLA b 612:**

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

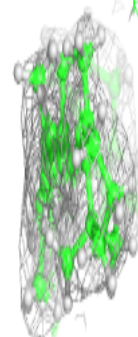
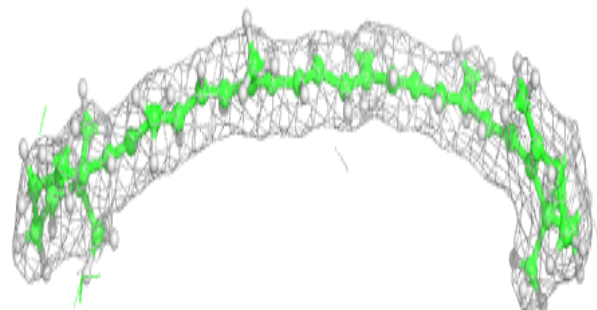
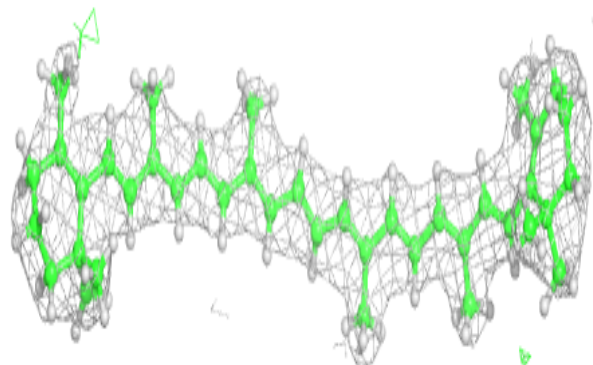


**Electron density around LMG d 410:**

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

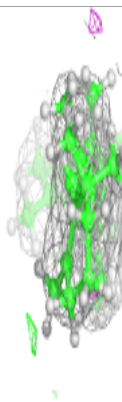
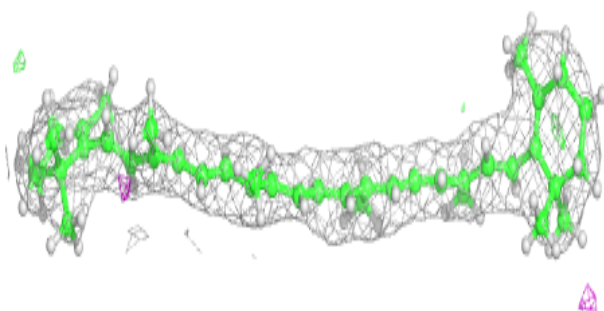
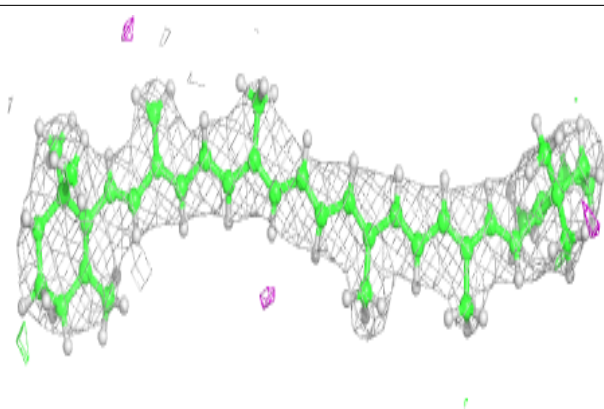
**Electron density around BCR t 101:**

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

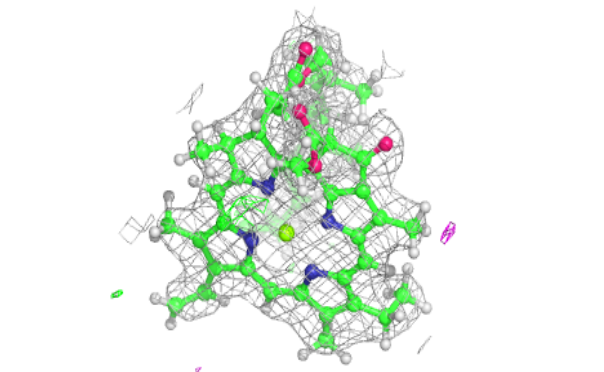
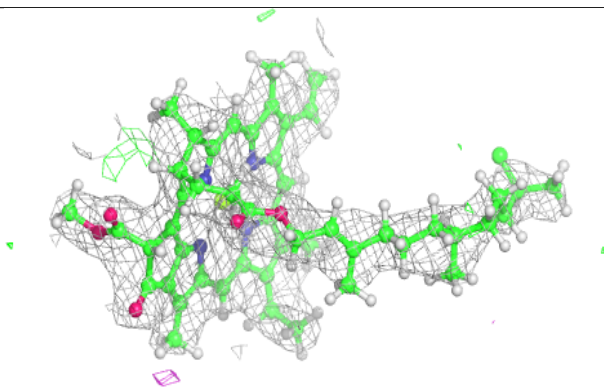
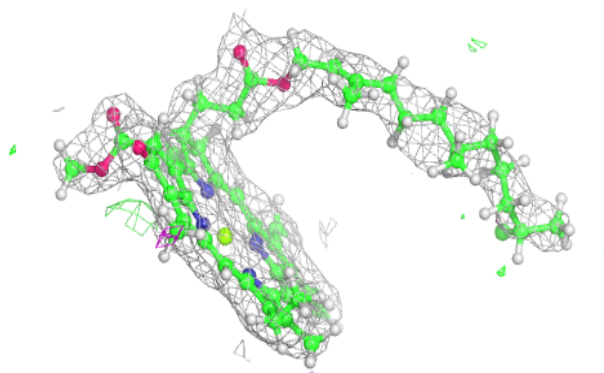


**Electron density around BCR b 617:**

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

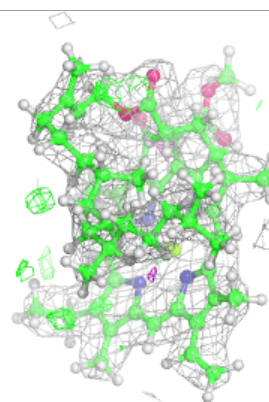
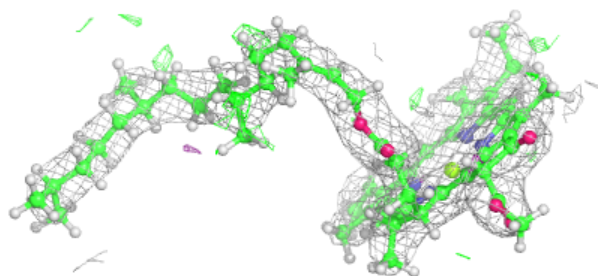
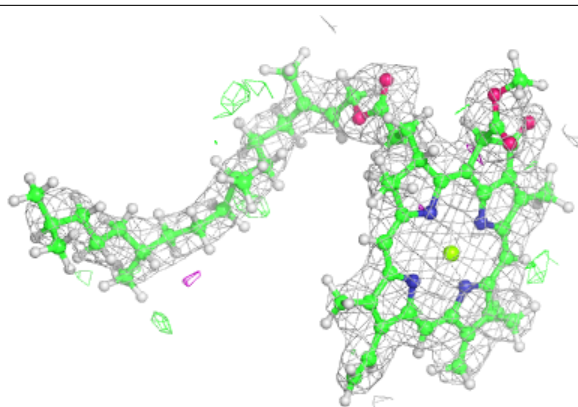
**Electron density around CLA c 505:**

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



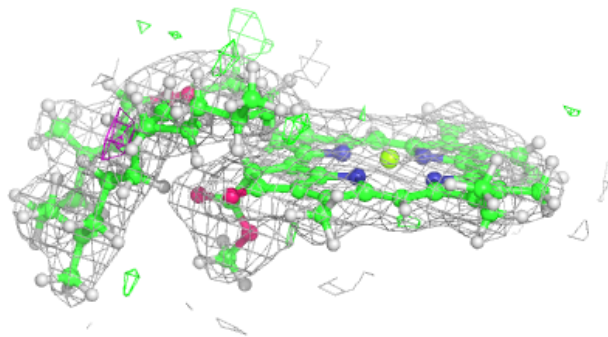
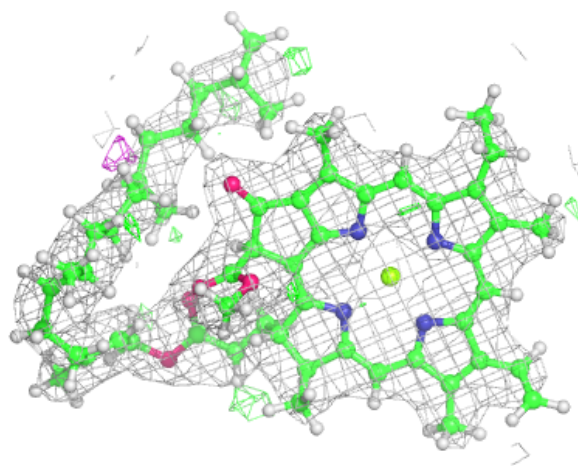
**Electron density around CLA C 511:**

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



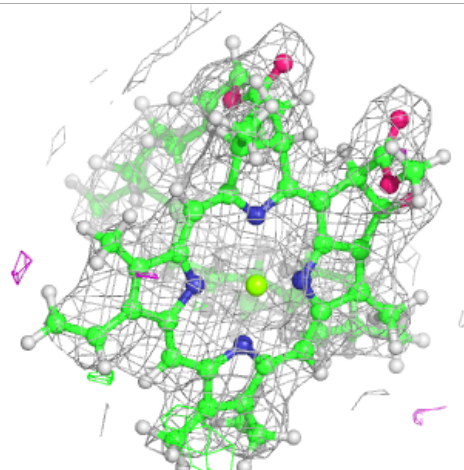
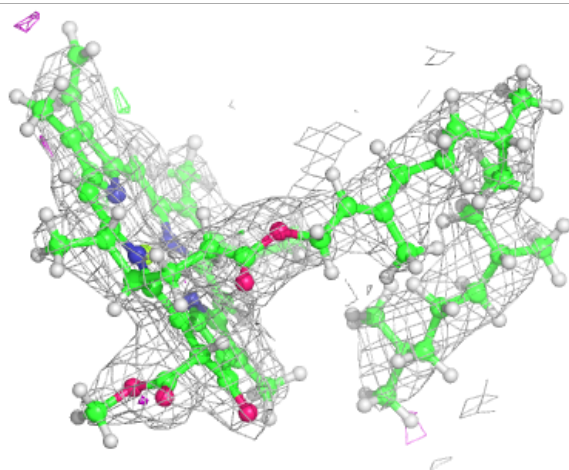
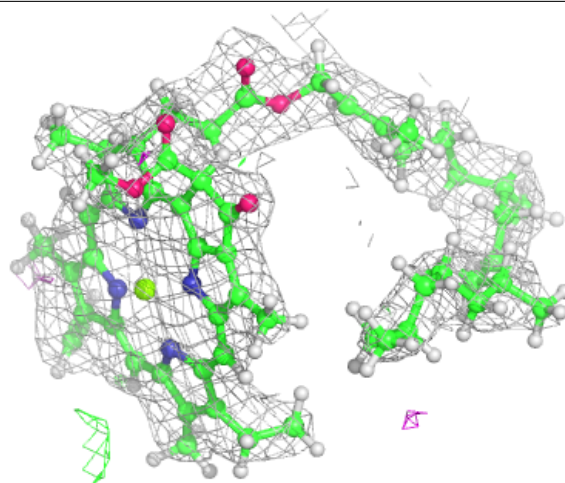
**Electron density around CLA b 610:**

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



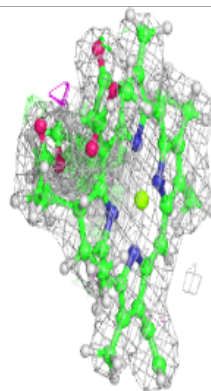
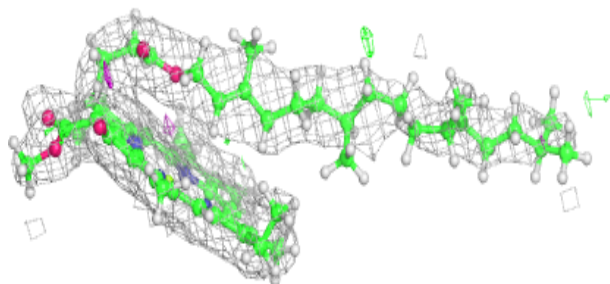
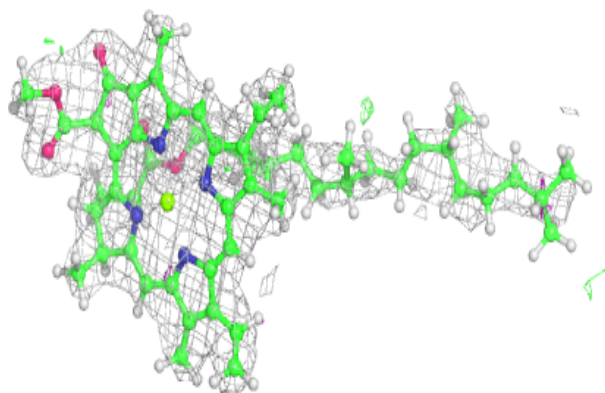
**Electron density around CLA C 503:**

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

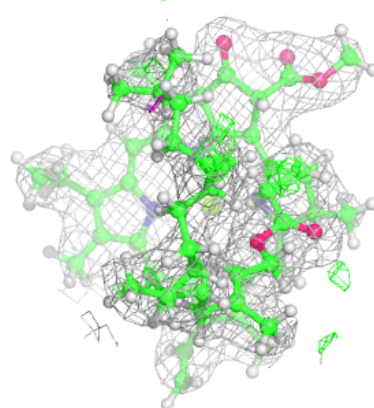
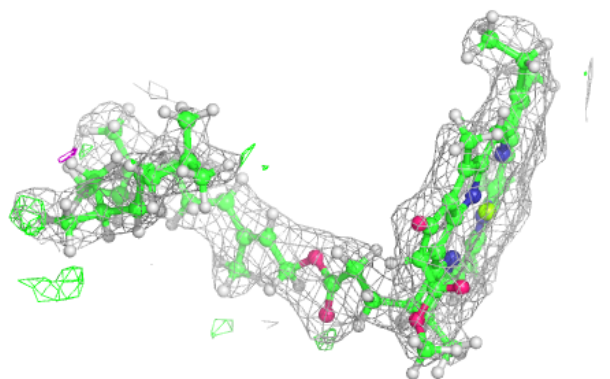
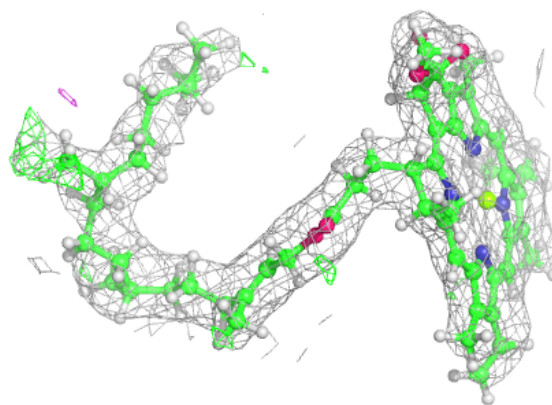


**Electron density around CLA b 614:**

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

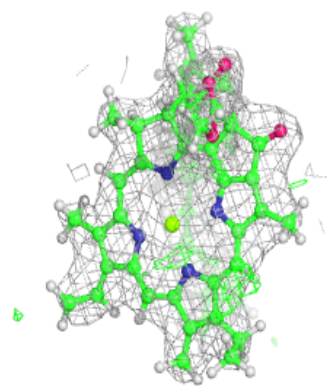
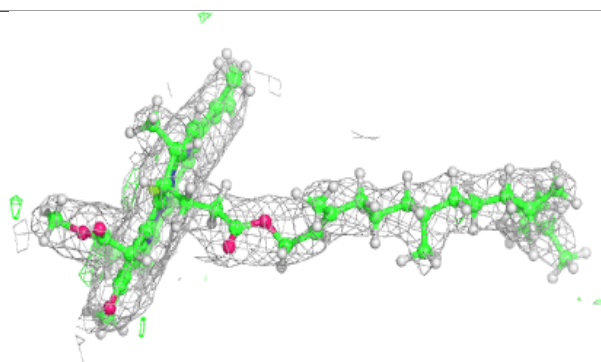
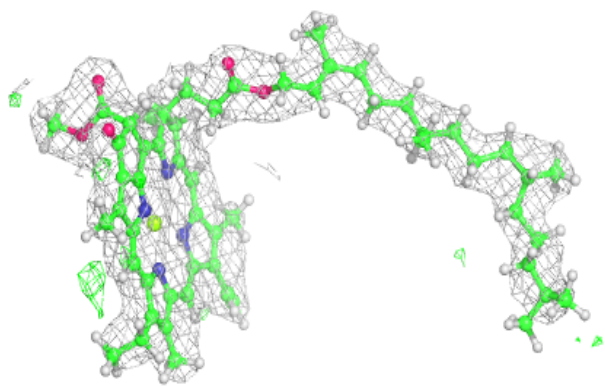
**Electron density around CLA B 606:**

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

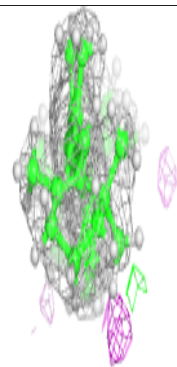
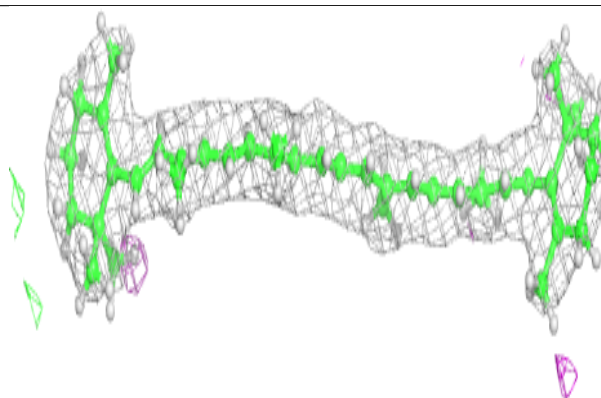
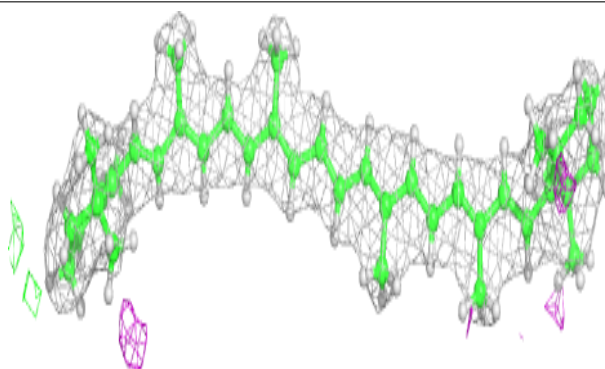


**Electron density around CLA B 609:**

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

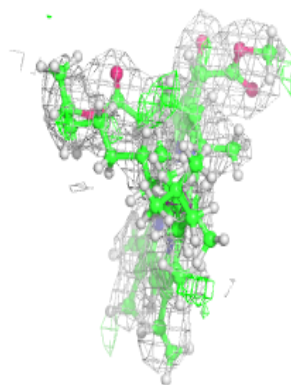
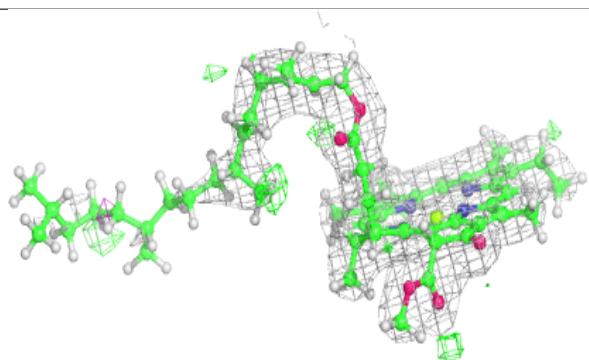
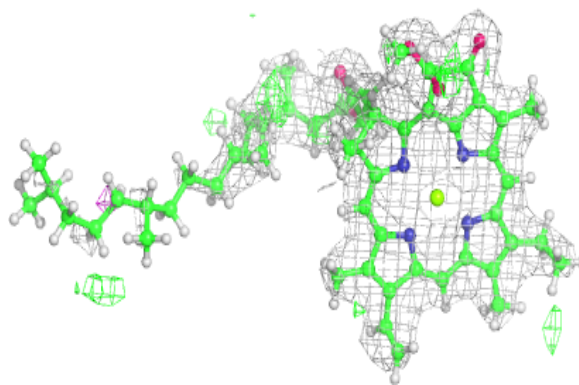
**Electron density around BCR a 406:**

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

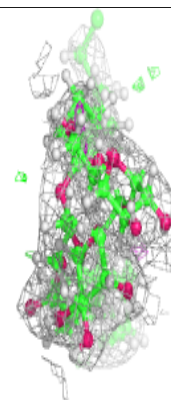
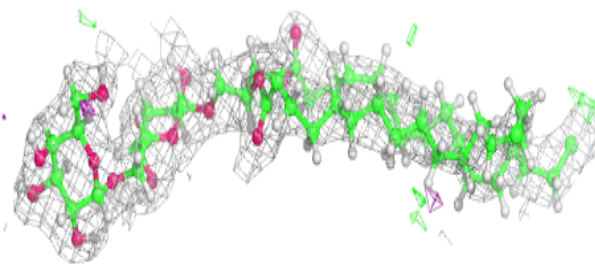
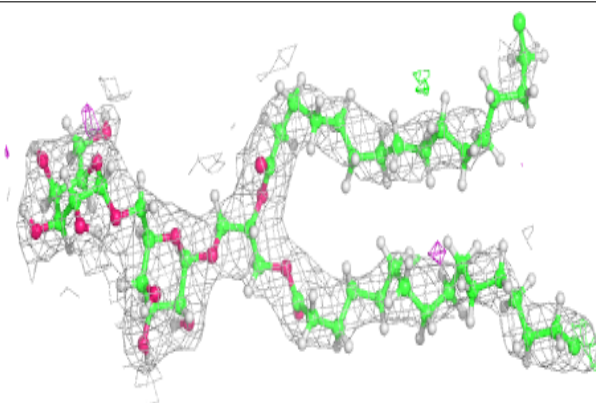


**Electron density around CLA A 403:**

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

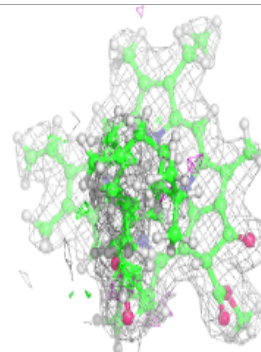
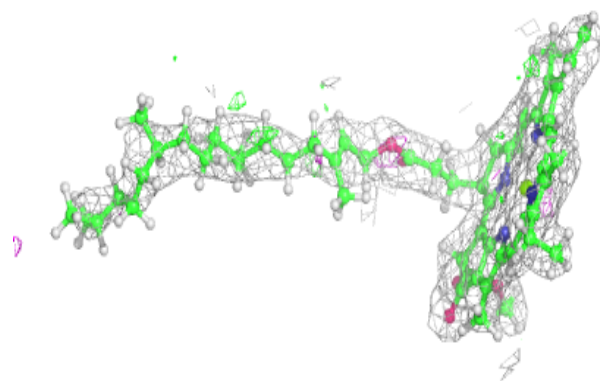
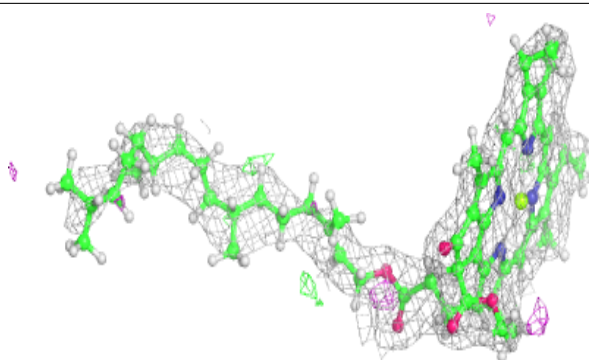
**Electron density around DGD c 519:**

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

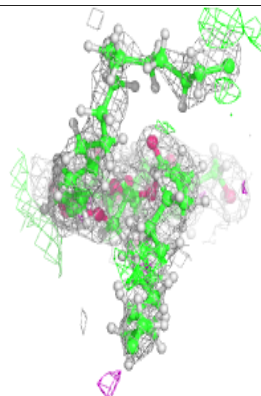
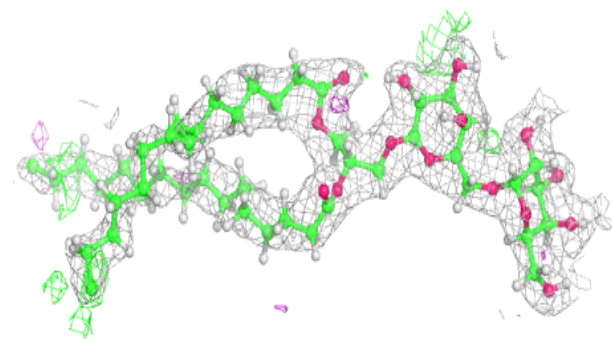
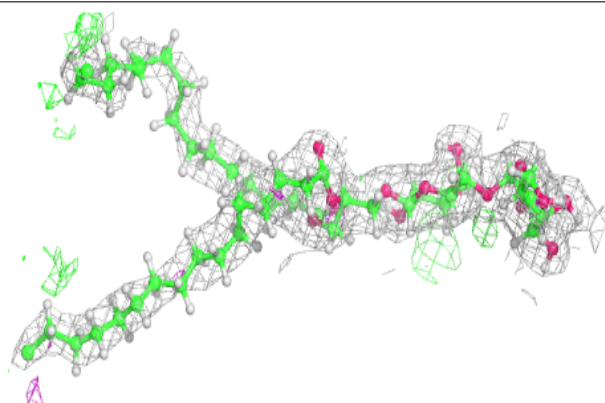


**Electron density around CLA B 604:**

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

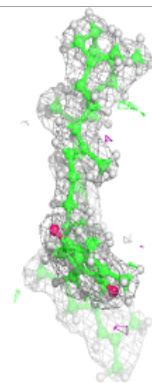
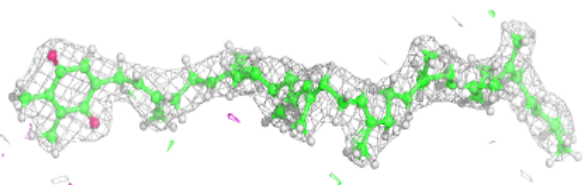
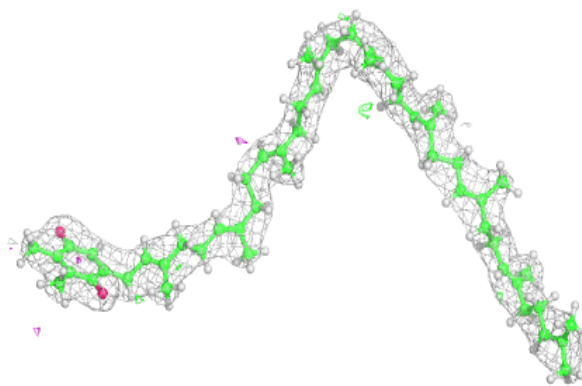
**Electron density around DGD C 515:**

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

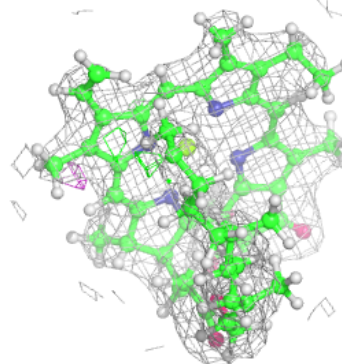
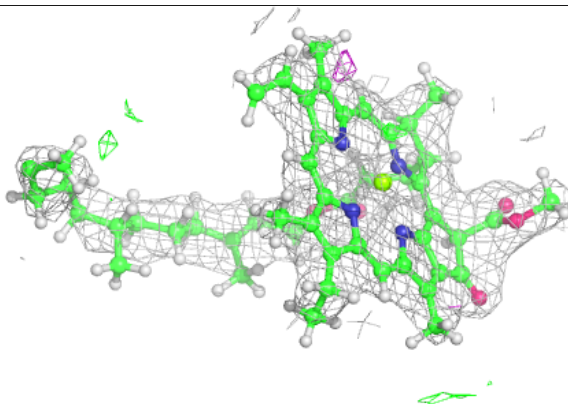
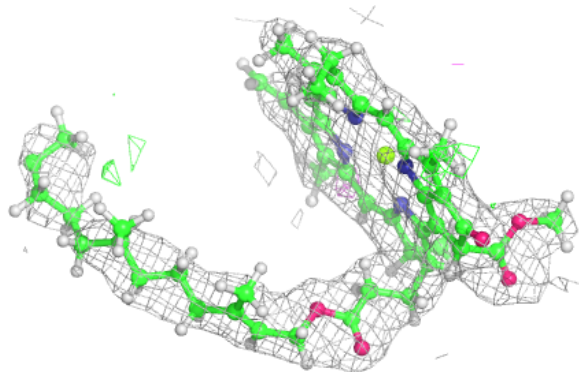


**Electron density around PL9 D 406:**

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

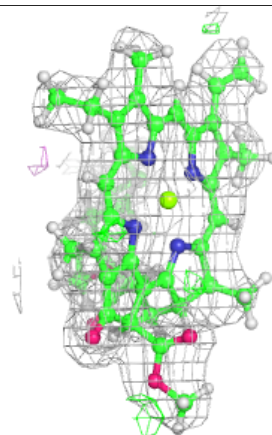
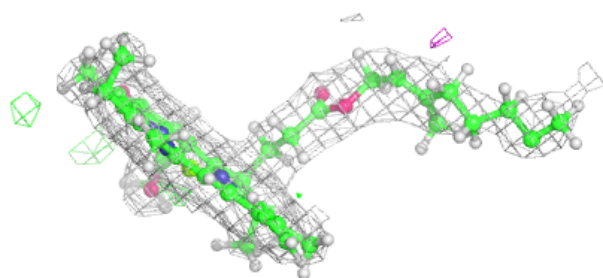
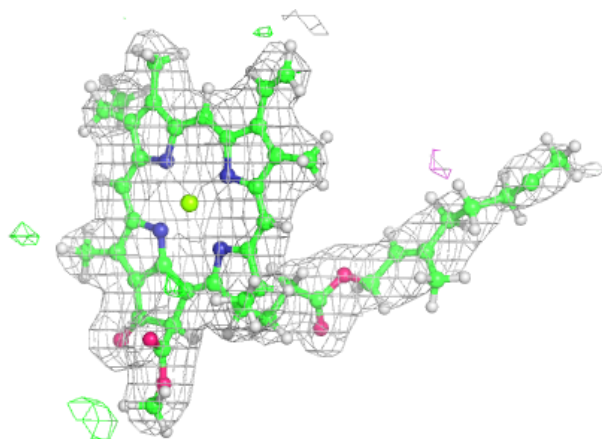
**Electron density around CLA C 504:**

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

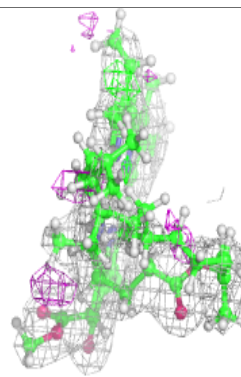
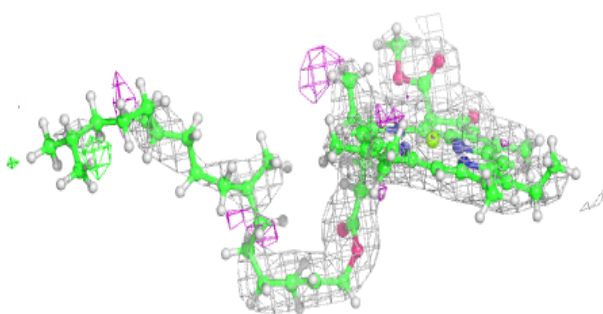
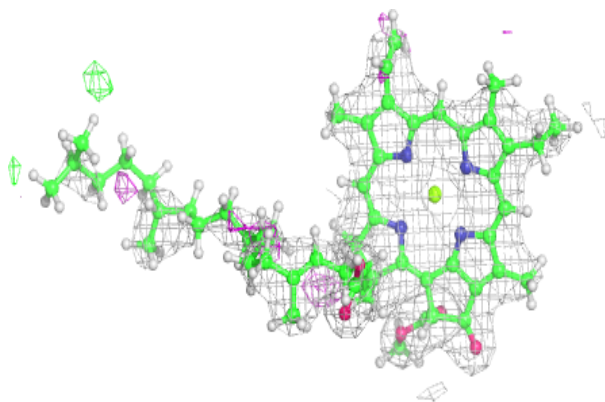


**Electron density around CLA A 405:**

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

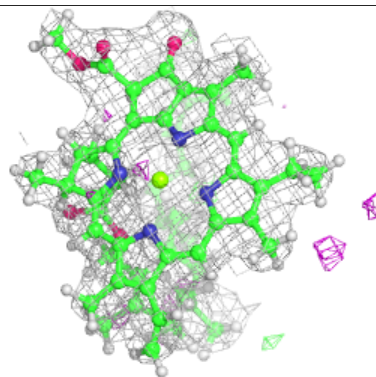
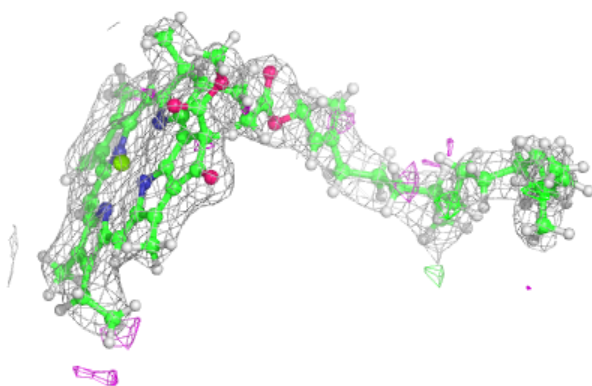
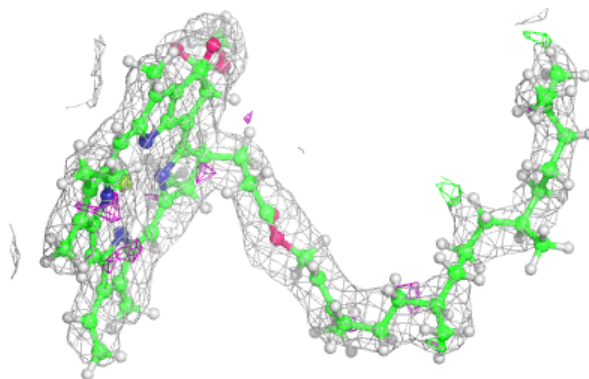
**Electron density around CLA a 403:**

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

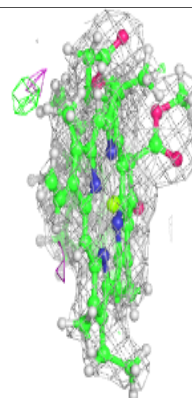
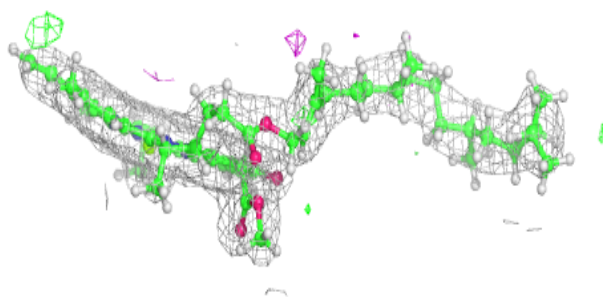
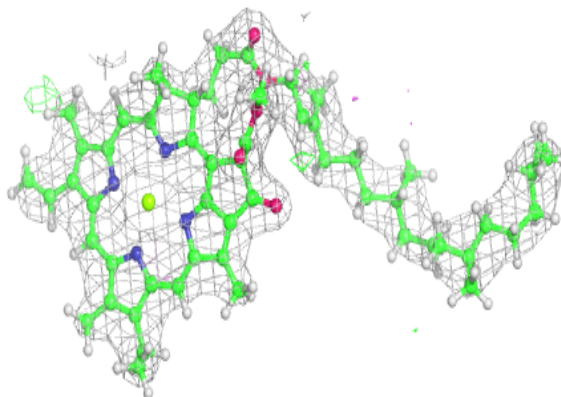


**Electron density around CLA b 606:**

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

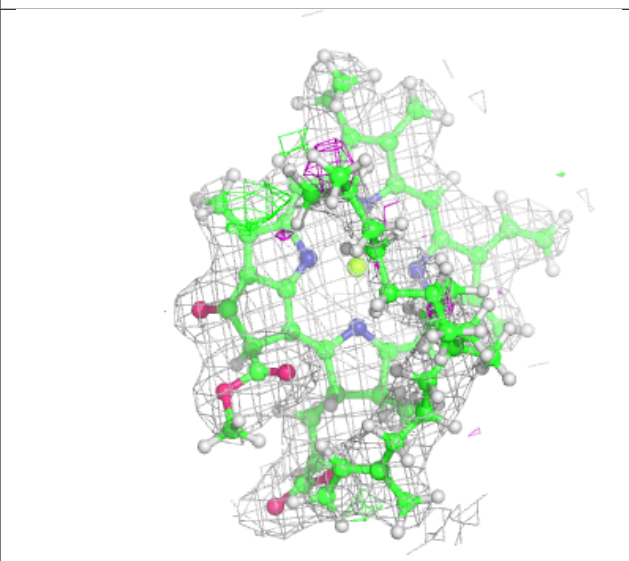
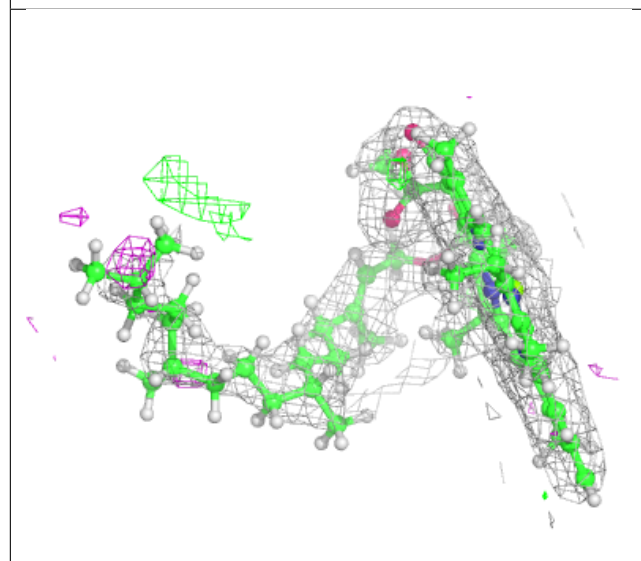
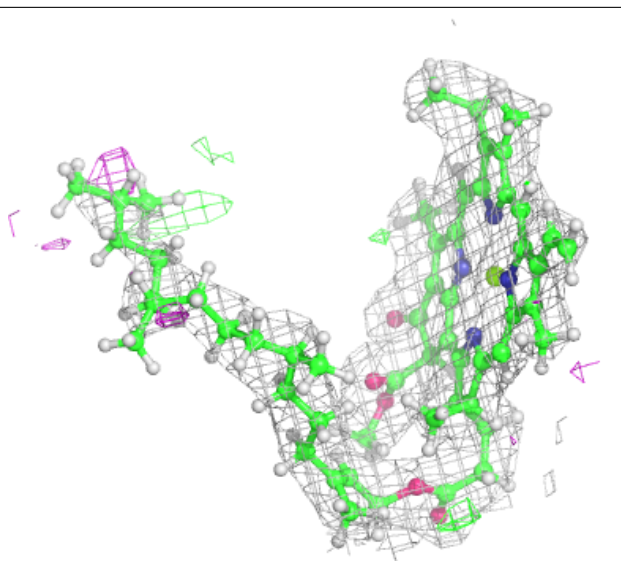
**Electron density around CLA B 602:**

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



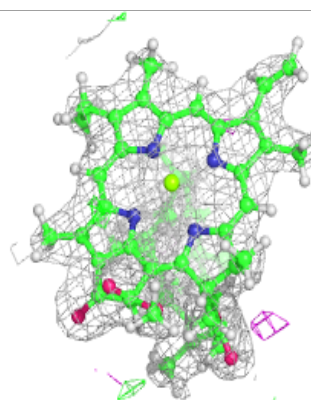
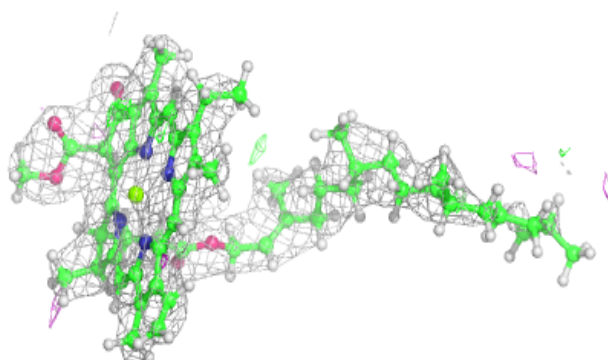
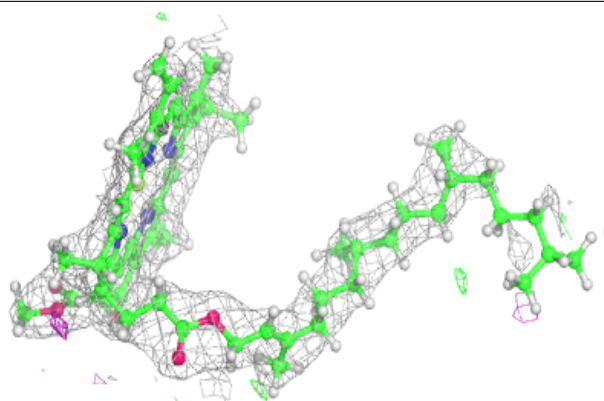
**Electron density around CLA b 613:**

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

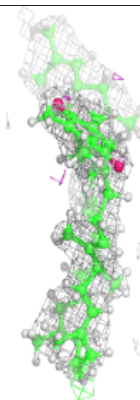
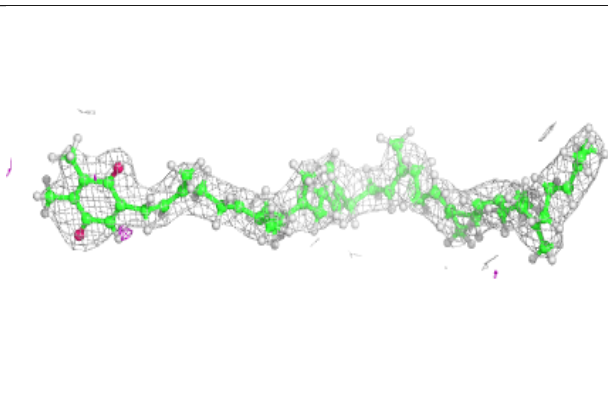
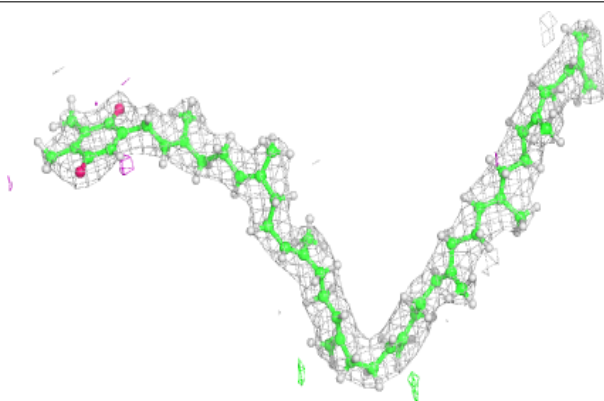


**Electron density around CLA C 508:**

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

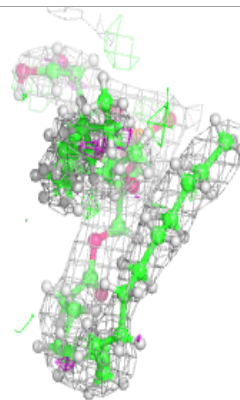
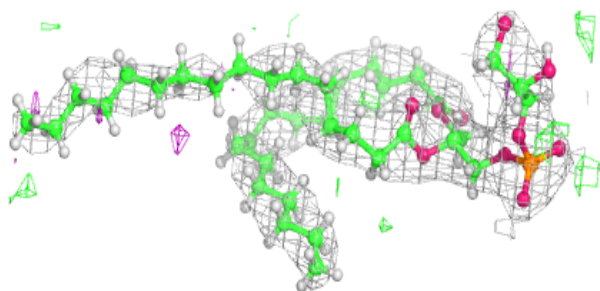
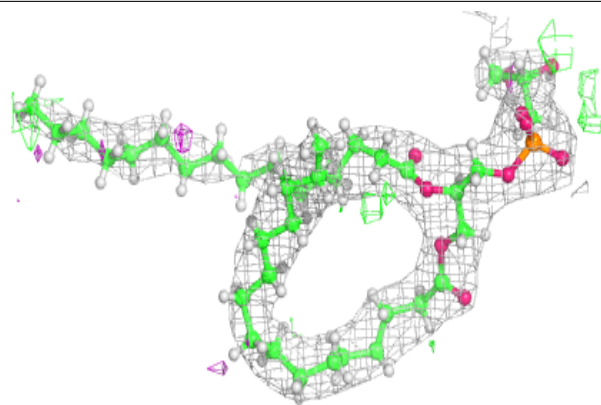
**Electron density around PL9 d 406:**

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

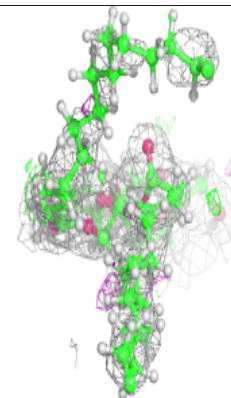
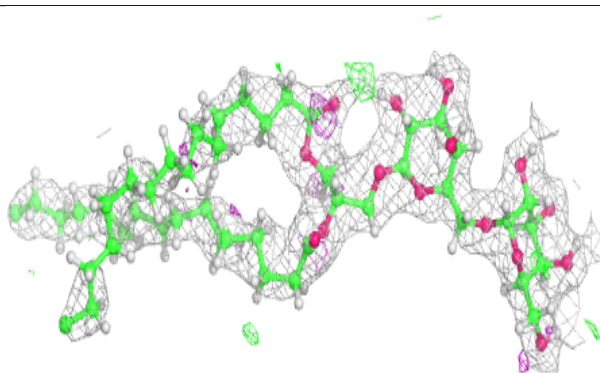
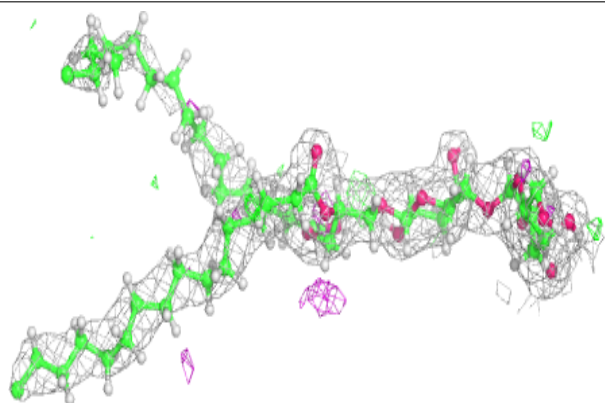


**Electron density around LHG d 407:**

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

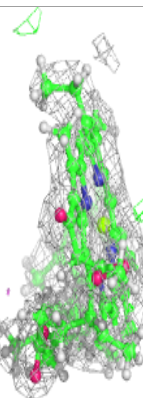
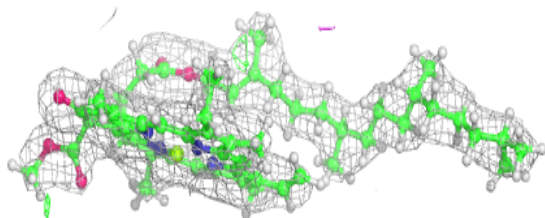
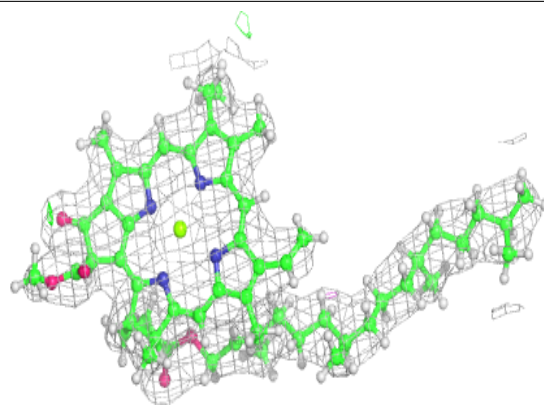
**Electron density around DGD c 517:**

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

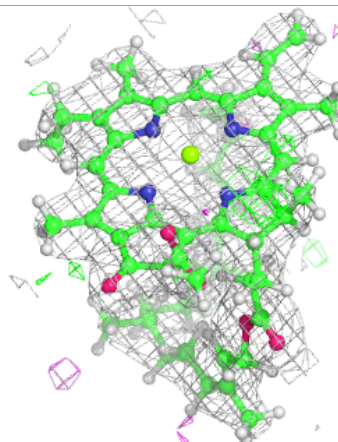
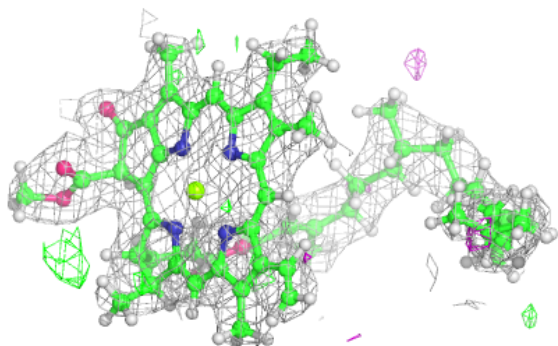
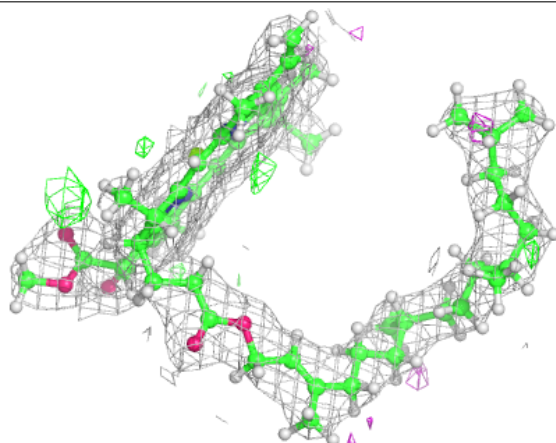


**Electron density around CLA C 501:**

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

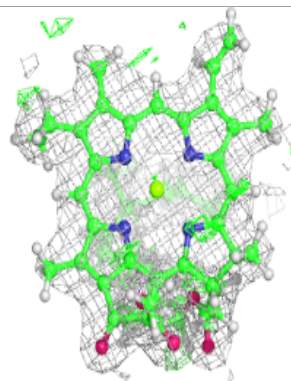
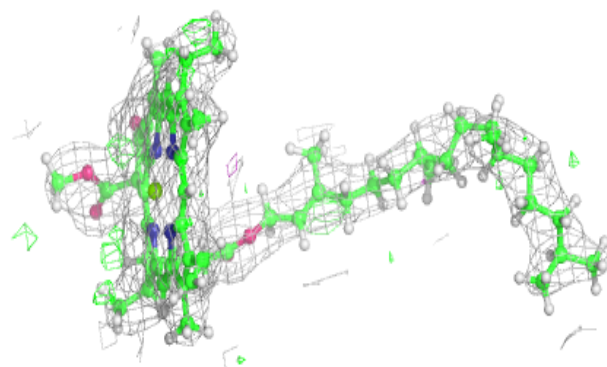
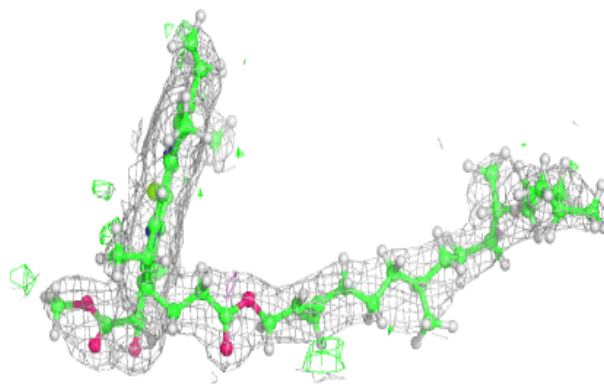
**Electron density around CLA b 611:**

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



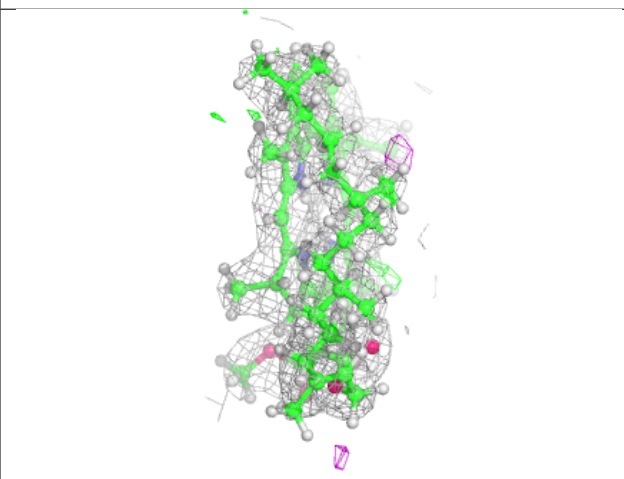
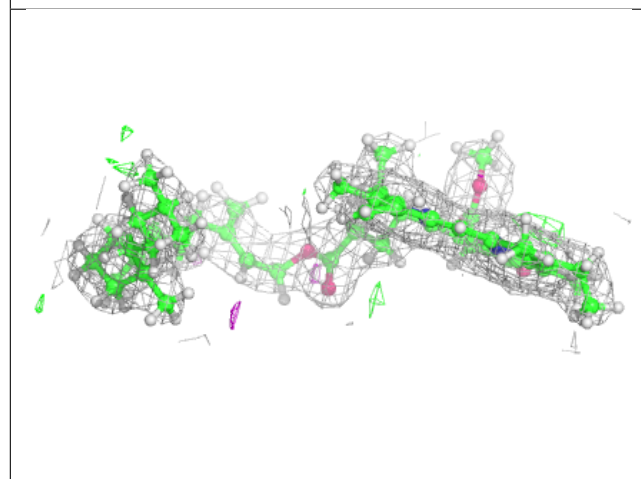
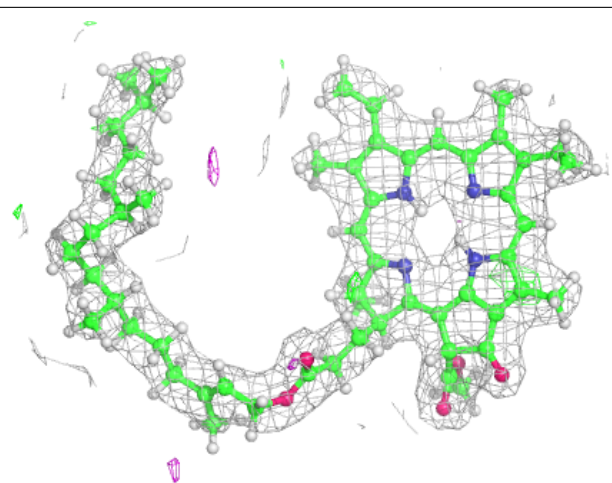
**Electron density around CLA B 605:**

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



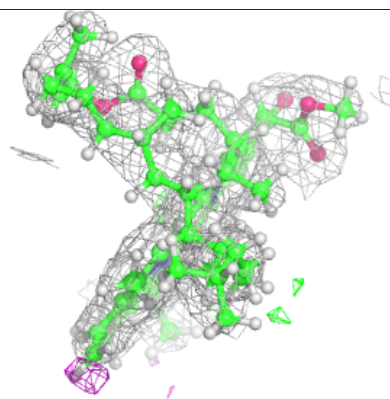
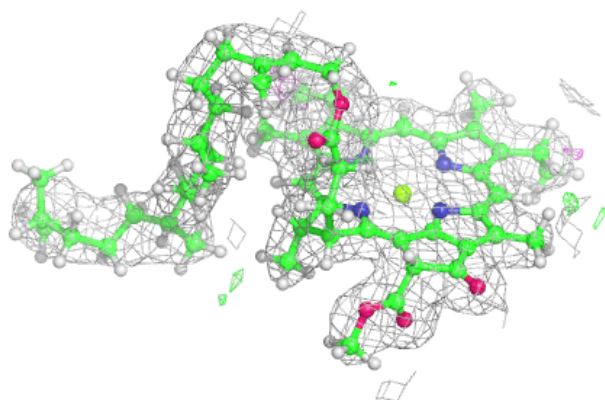
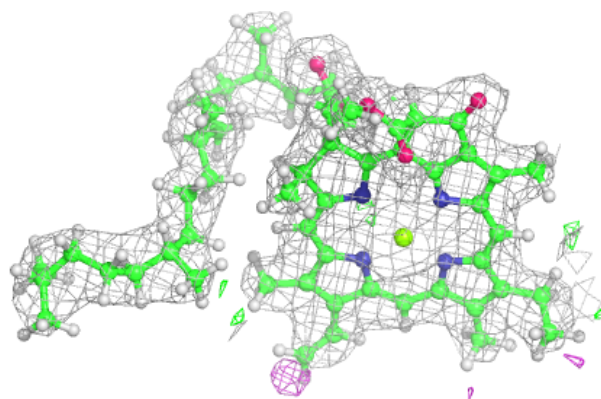
**Electron density around PHO A 404:**

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

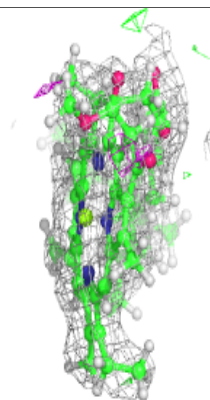
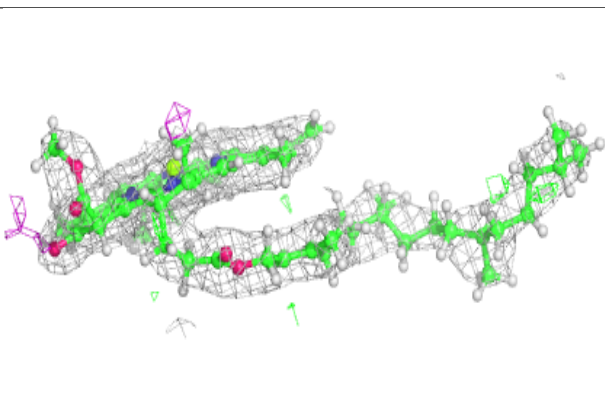
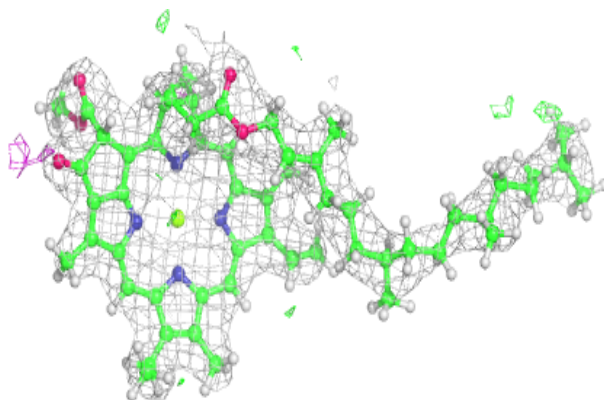


**Electron density around CLA D 404:**

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

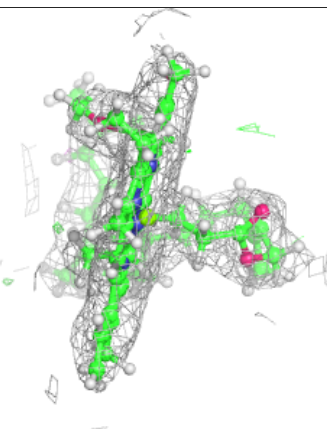
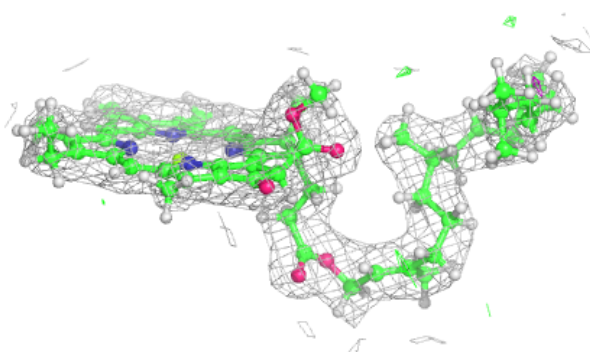
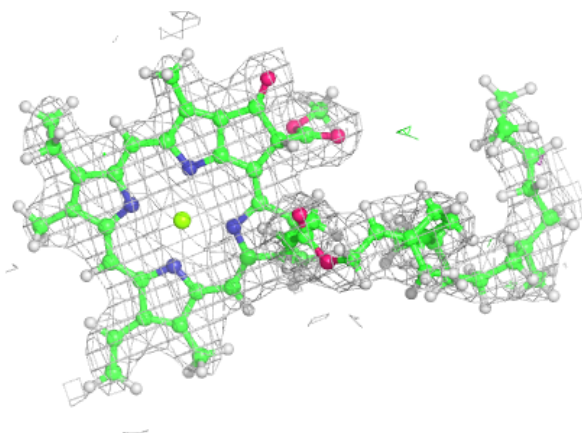
**Electron density around CLA B 603:**

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

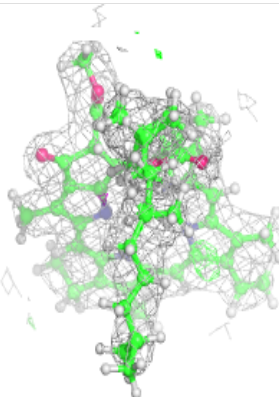
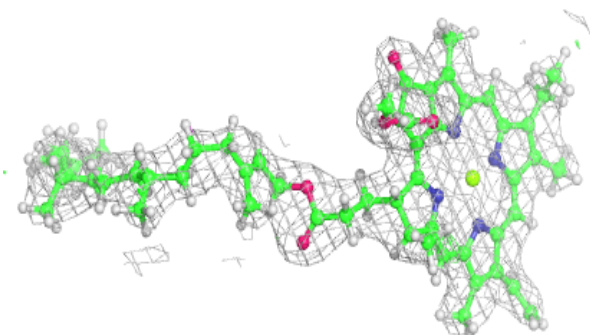
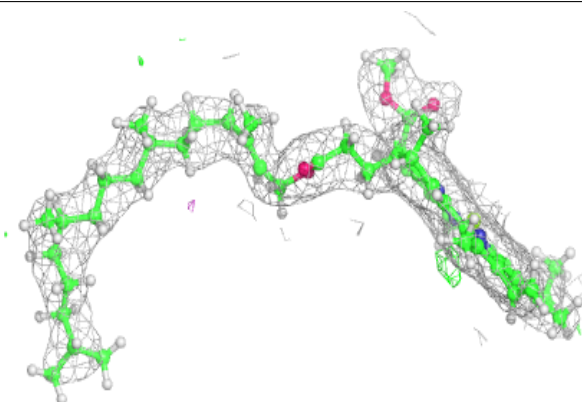


**Electron density around CLA B 612:**

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

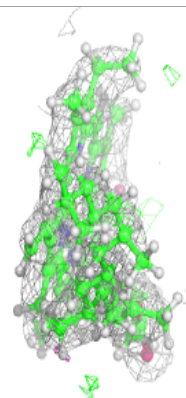
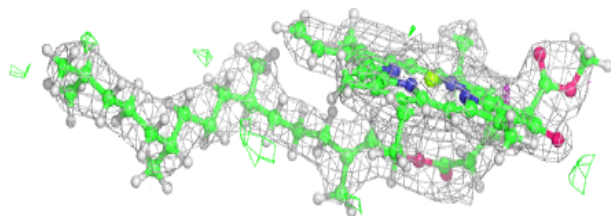
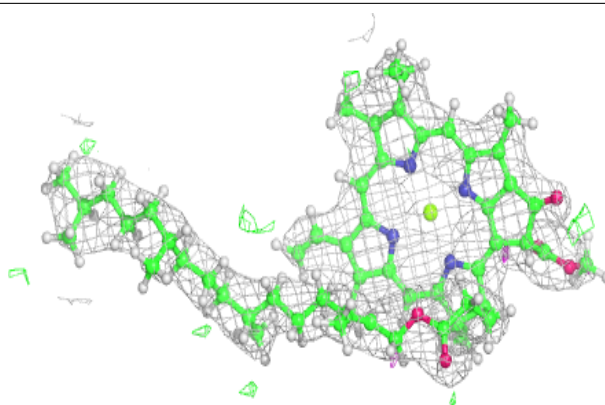
**Electron density around CLA d 403:**

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

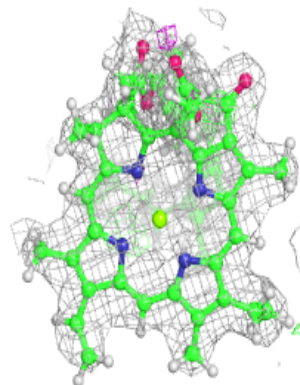
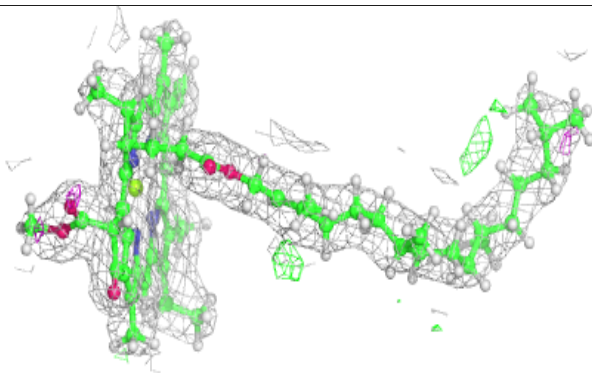
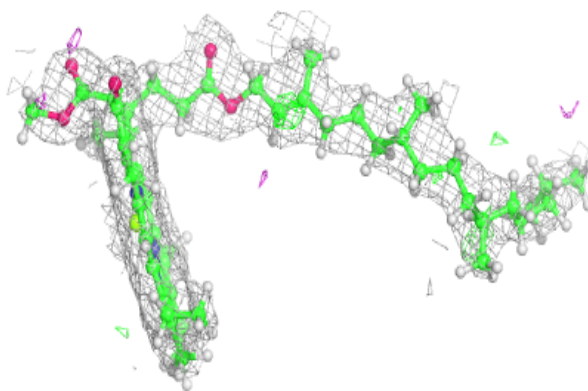


**Electron density around CLA c 502:**

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

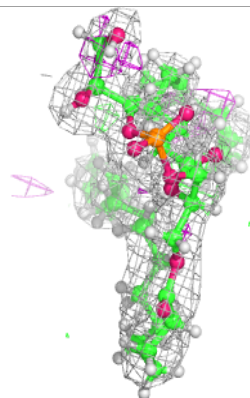
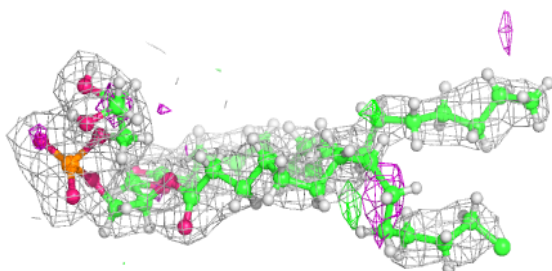
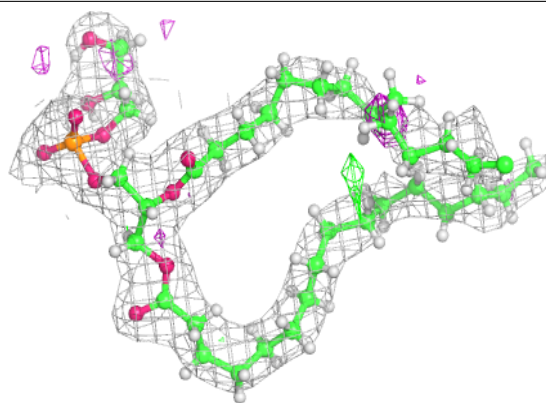
**Electron density around CLA b 605:**

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

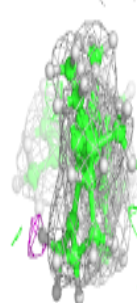
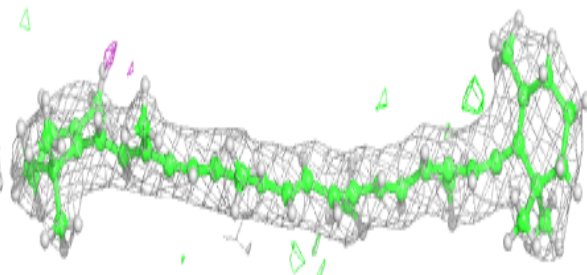
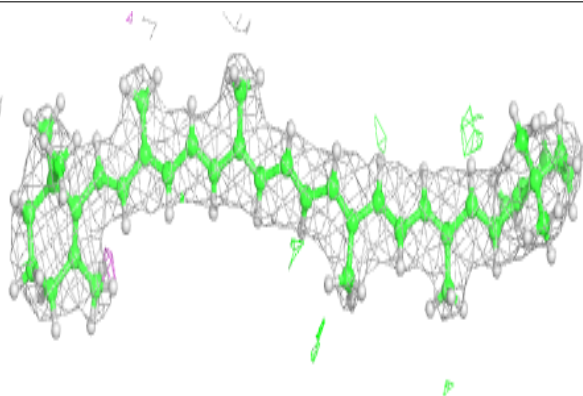


**Electron density around LHG D 410:**

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

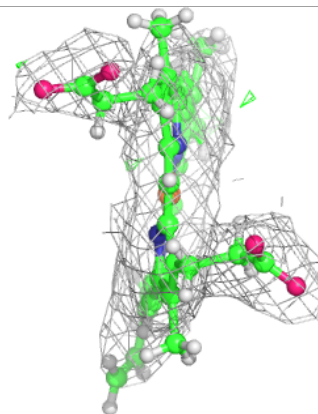
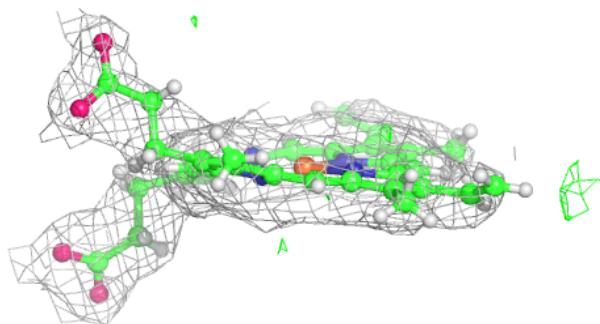
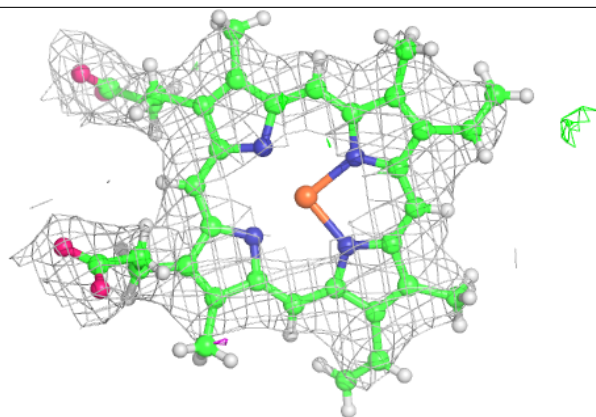
**Electron density around BCR B 617:**

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

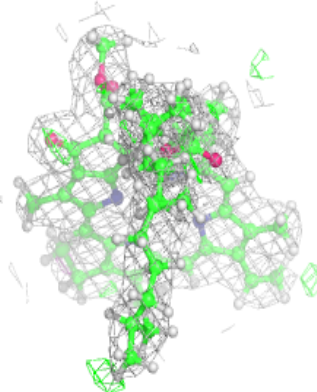
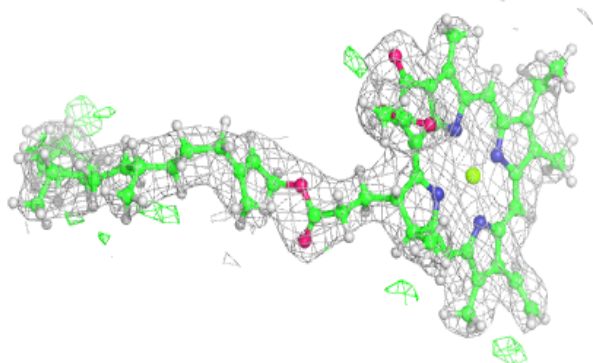
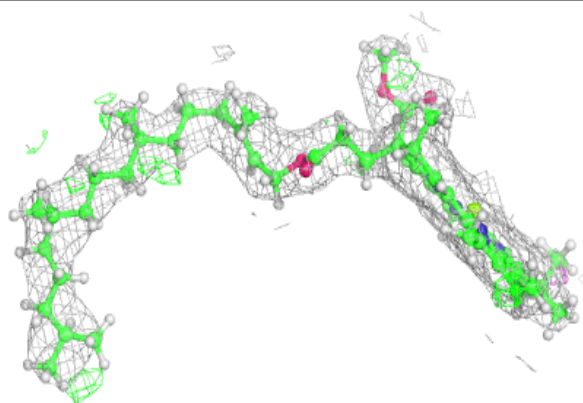


**Electron density around HEC F 102:**

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

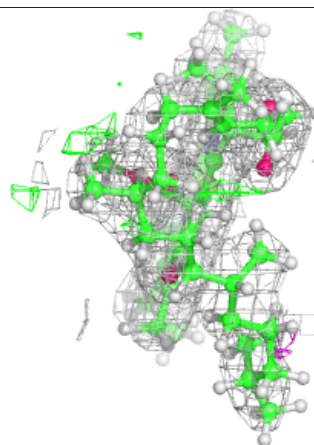
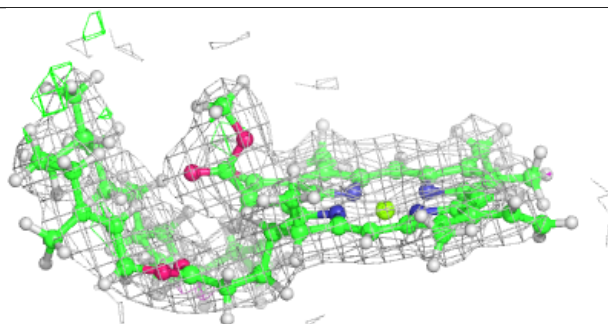
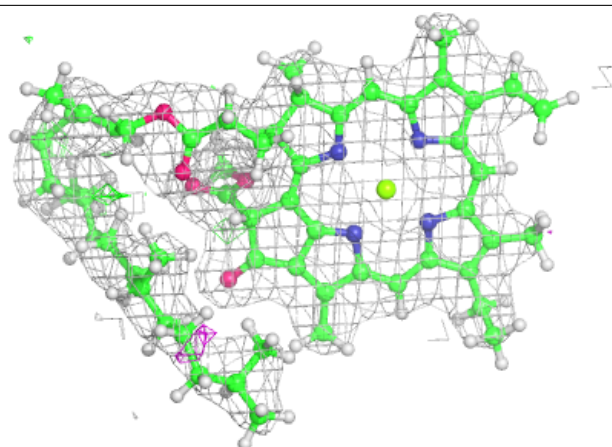
**Electron density around CLA D 403:**

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

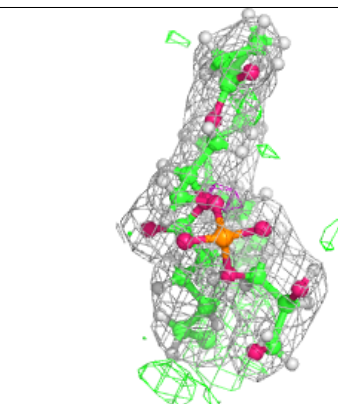
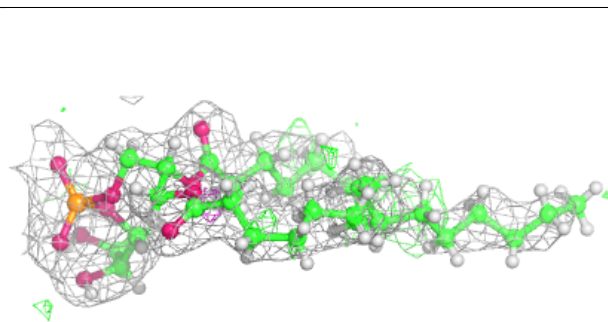
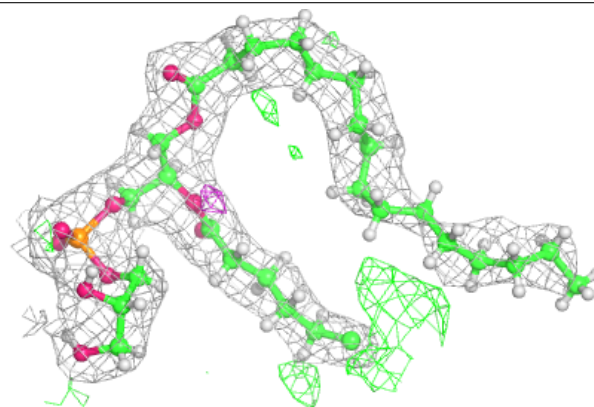


**Electron density around CLA B 610:**

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

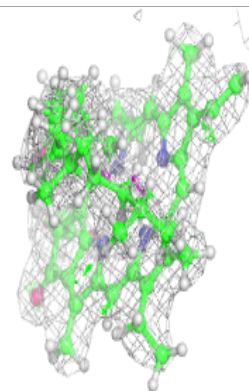
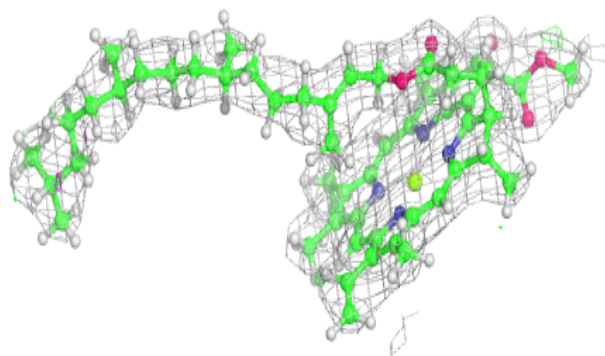
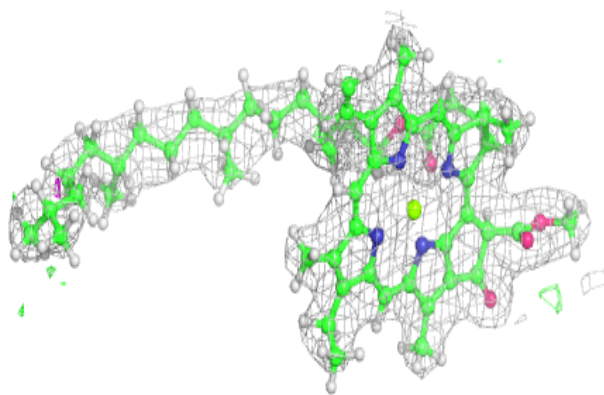
**Electron density around LHG d 409:**

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

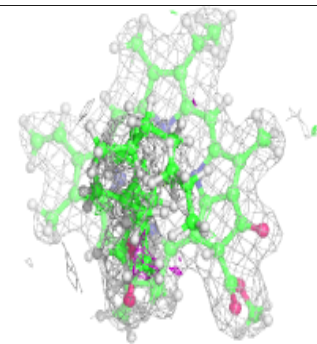
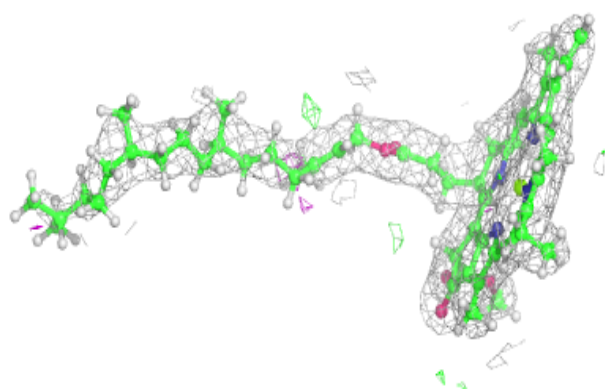
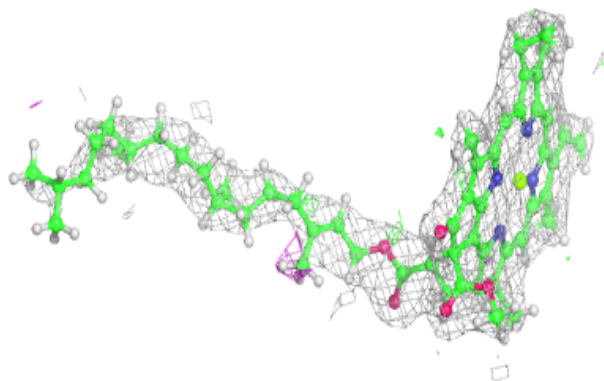


**Electron density around CLA B 608:**

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

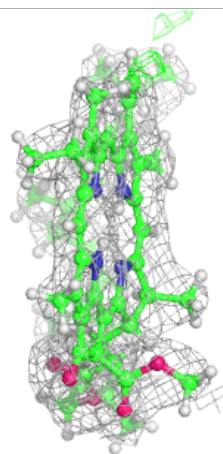
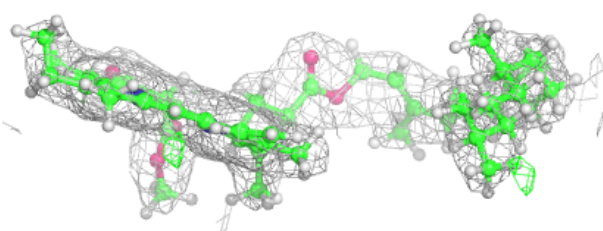
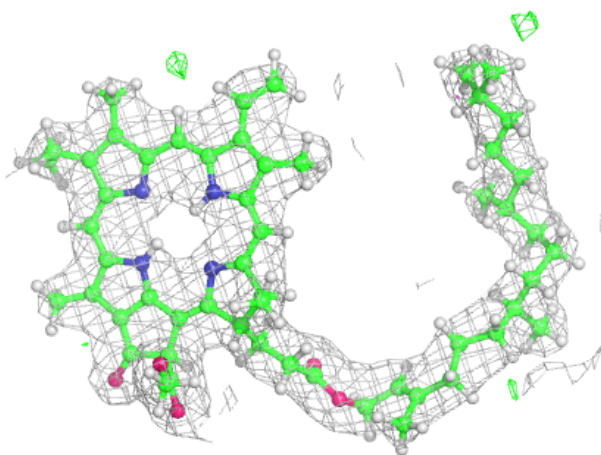
**Electron density around CLA b 604:**

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



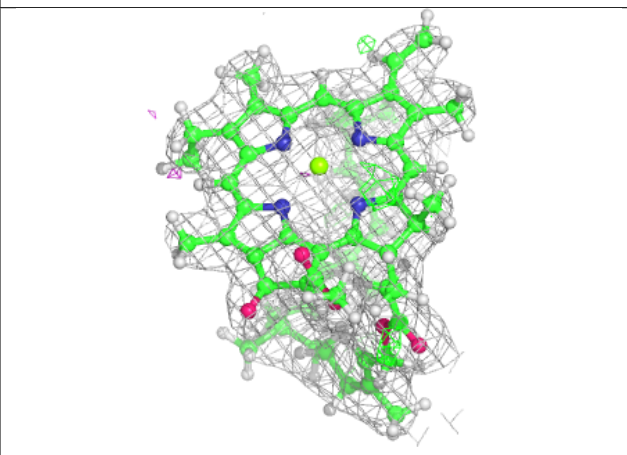
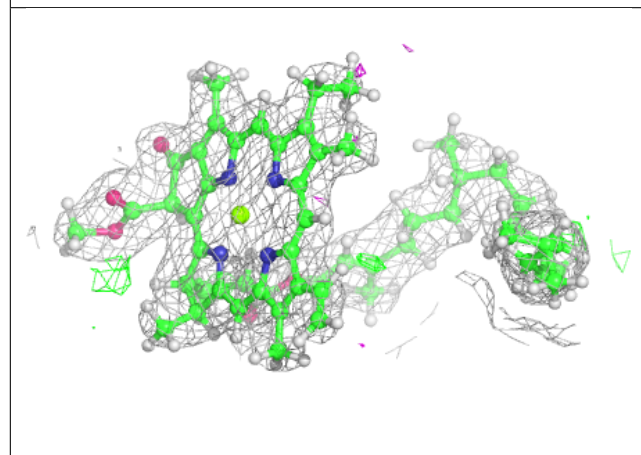
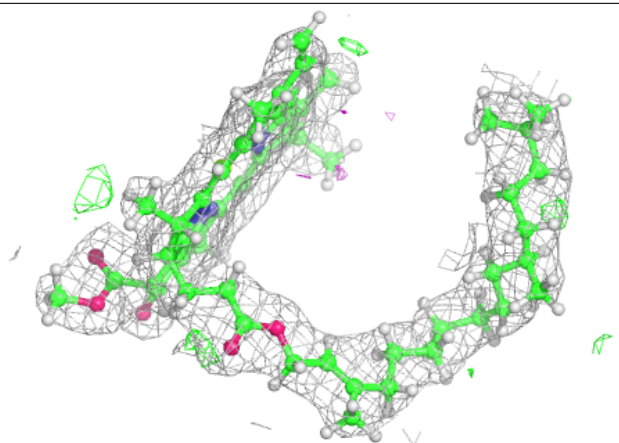
**Electron density around PHO a 404:**

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



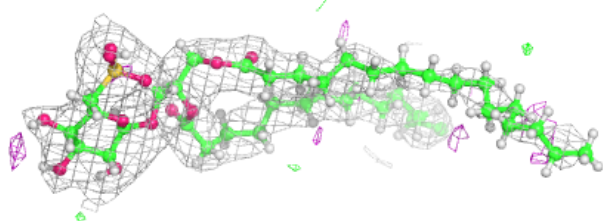
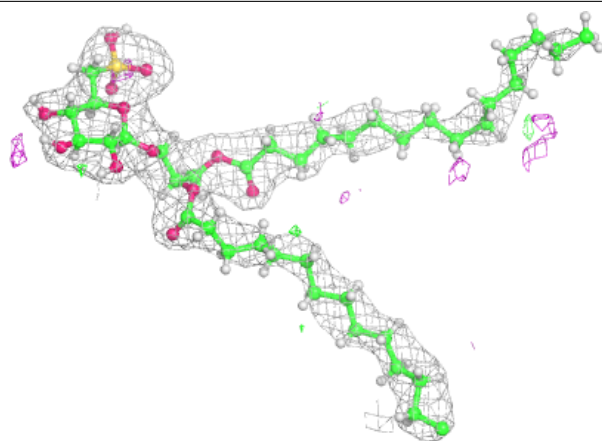
**Electron density around CLA B 611:**

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

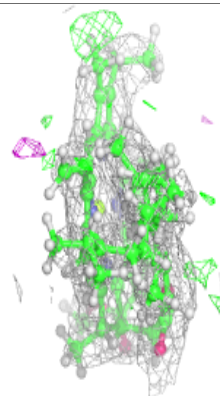
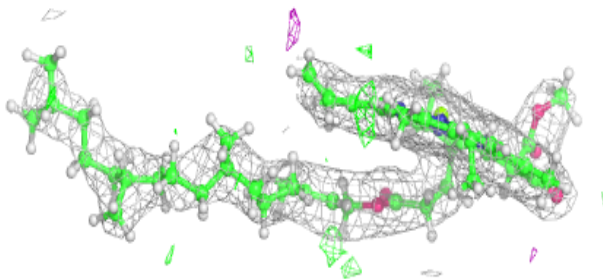
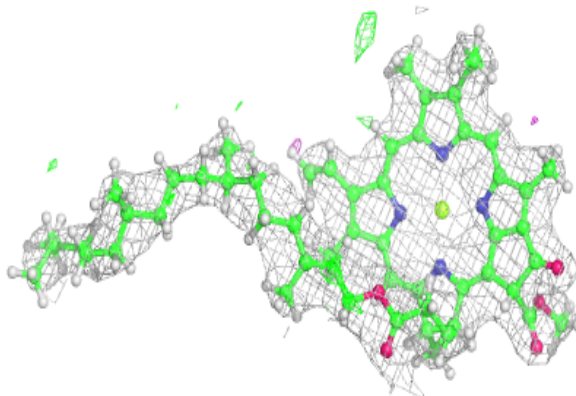


**Electron density around SQD A 411:**

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

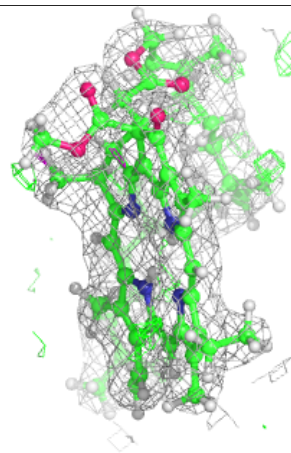
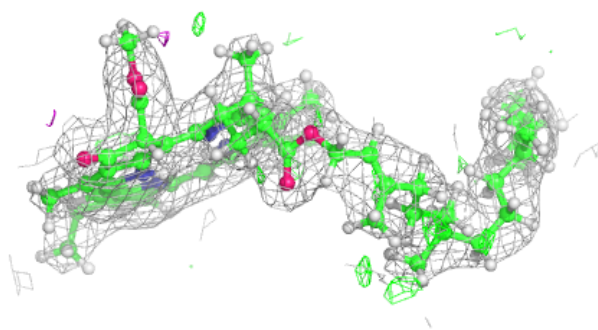
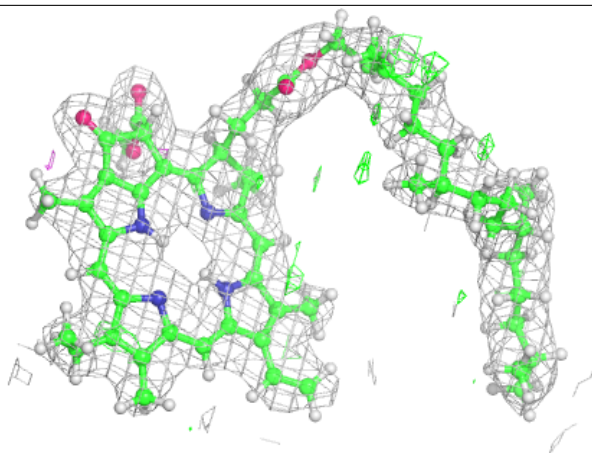
**Electron density around CLA b 603:**

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



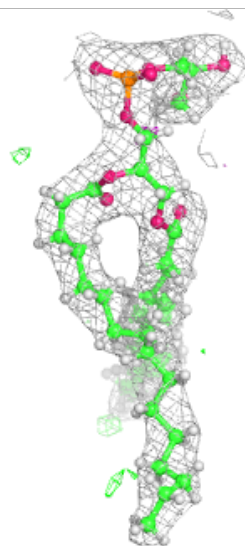
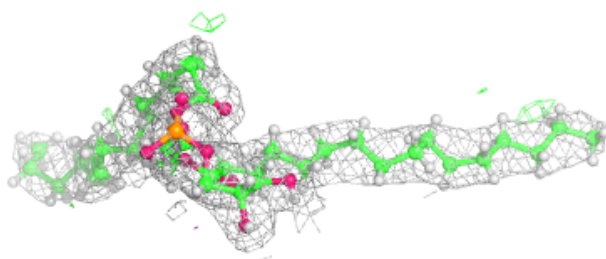
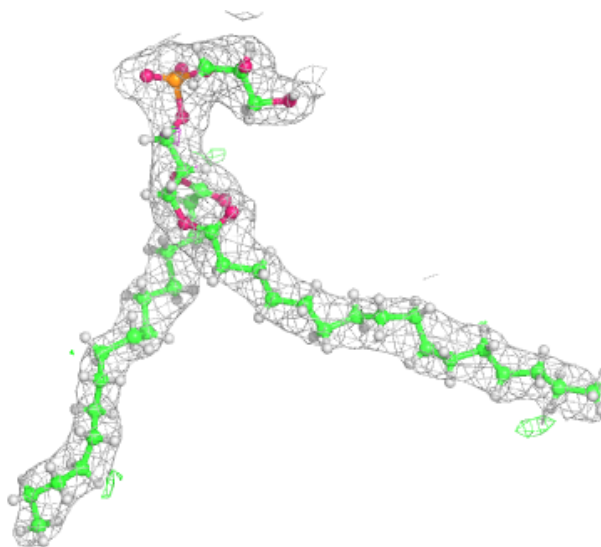
**Electron density around PHO D 401:**

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



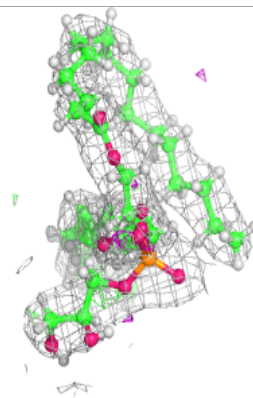
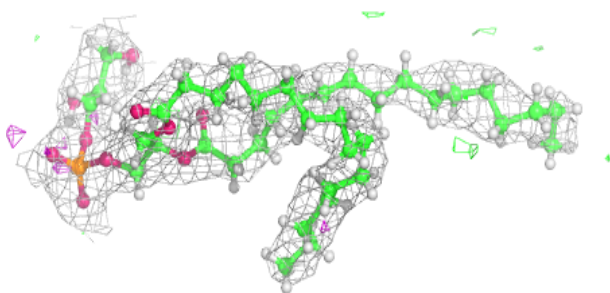
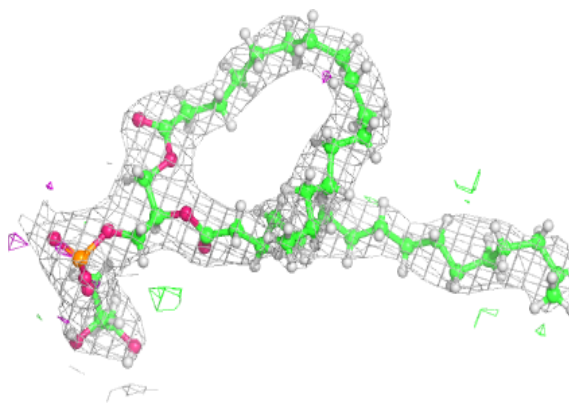
**Electron density around LHG L 102:**

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

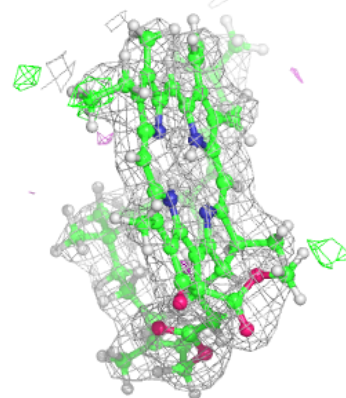
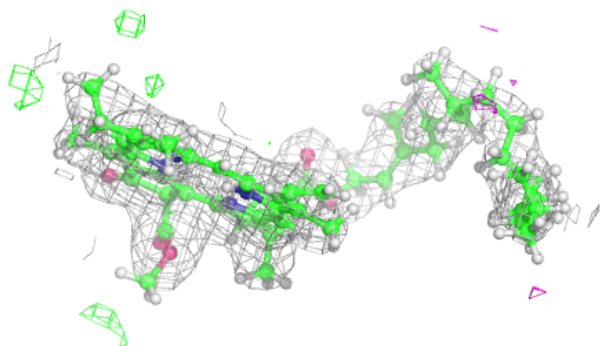
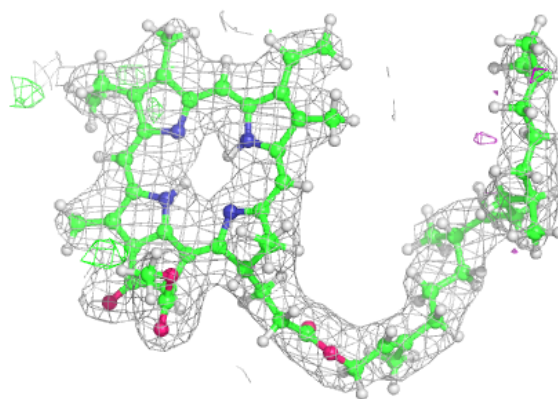


**Electron density around LHG D 412:**

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

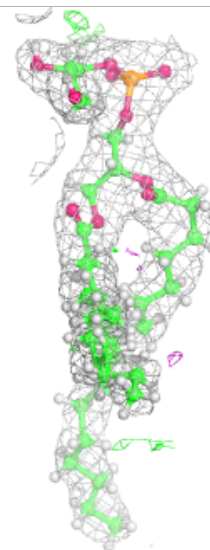
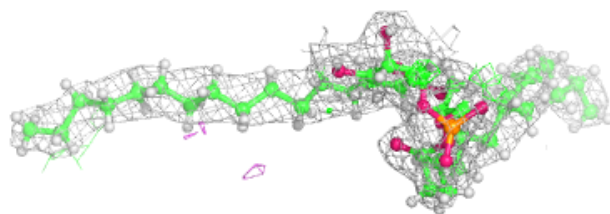
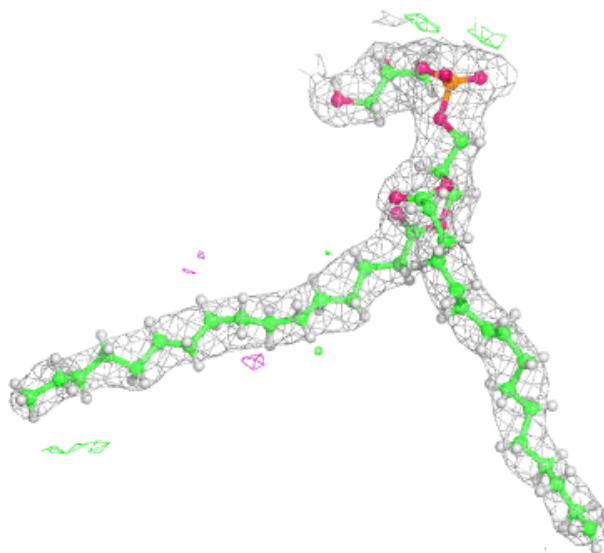
**Electron density around PHO d 401:**

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



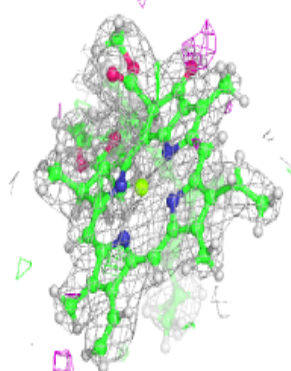
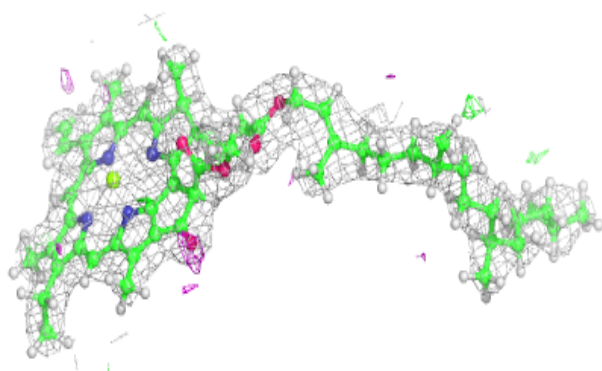
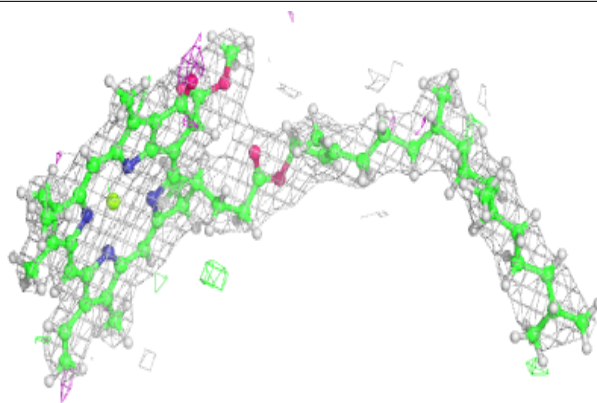
**Electron density around LHG 1 101:**

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

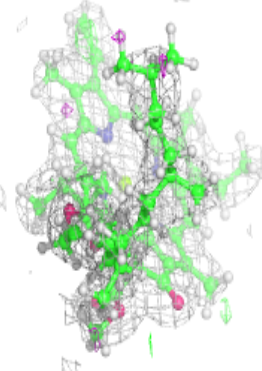
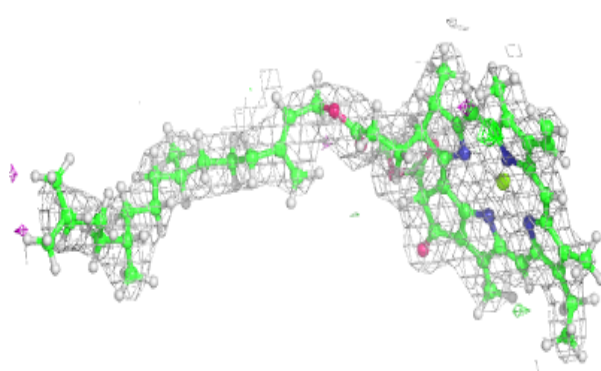
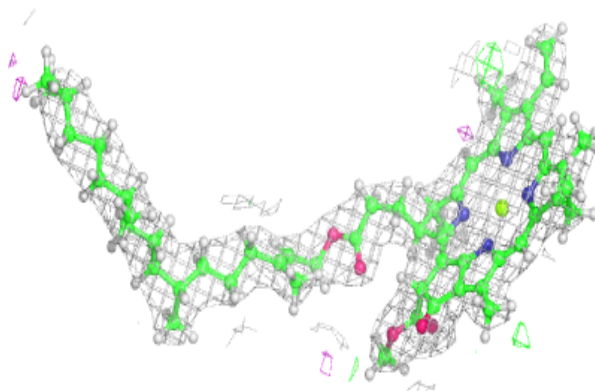


**Electron density around CLA A 402:**

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

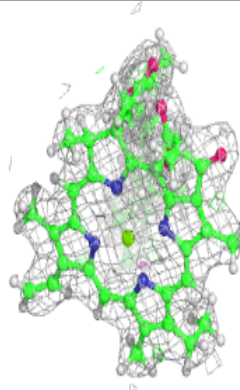
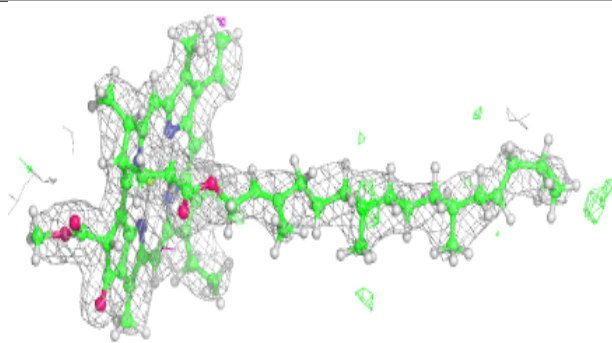
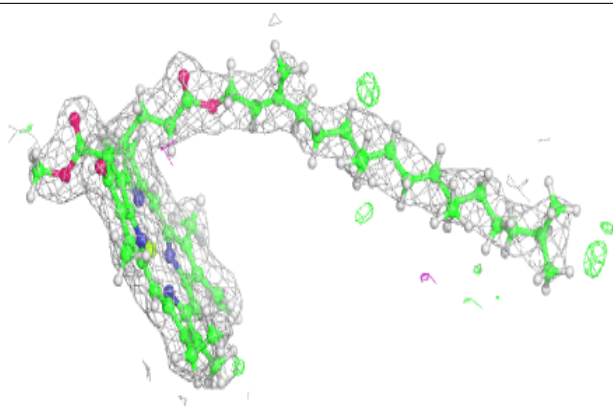
**Electron density around CLA a 402:**

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

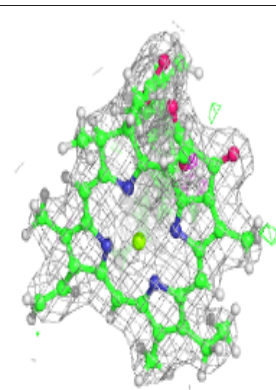
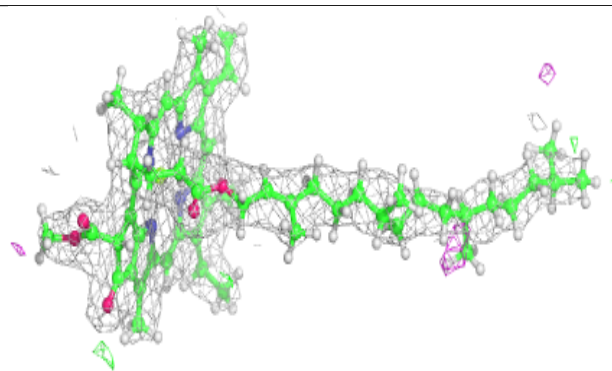
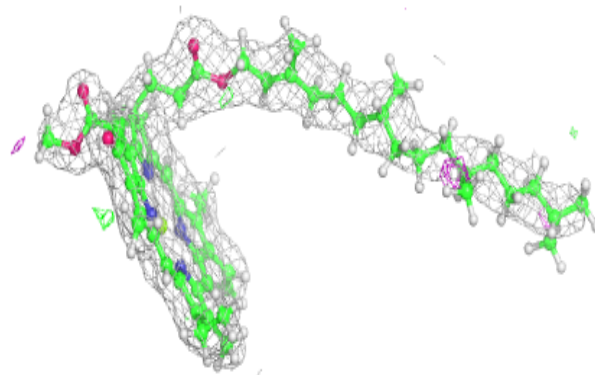


**Electron density around CLA B 607:**

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

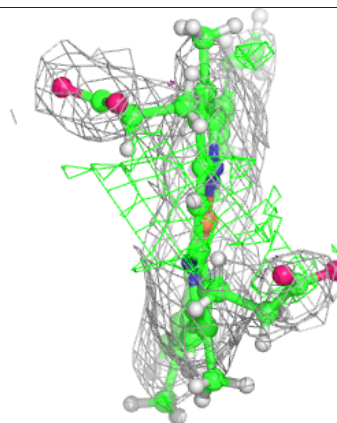
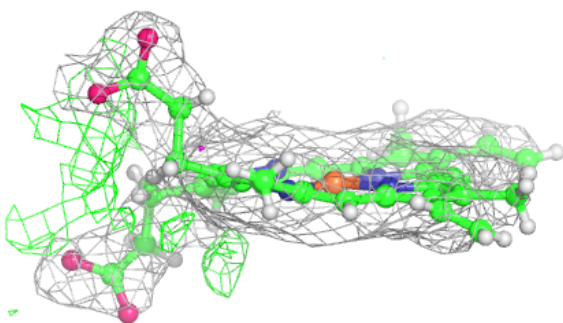
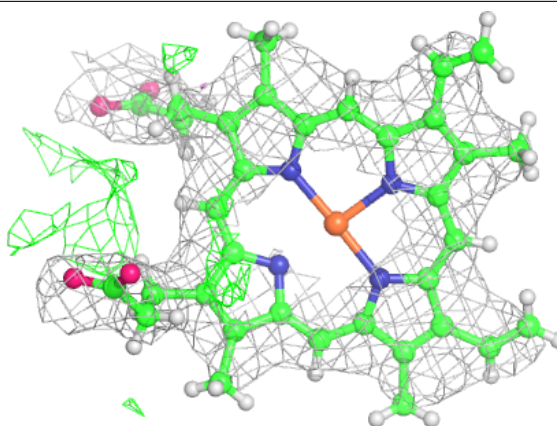
**Electron density around CLA b 607:**

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



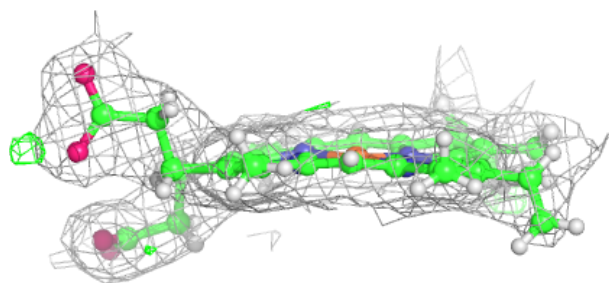
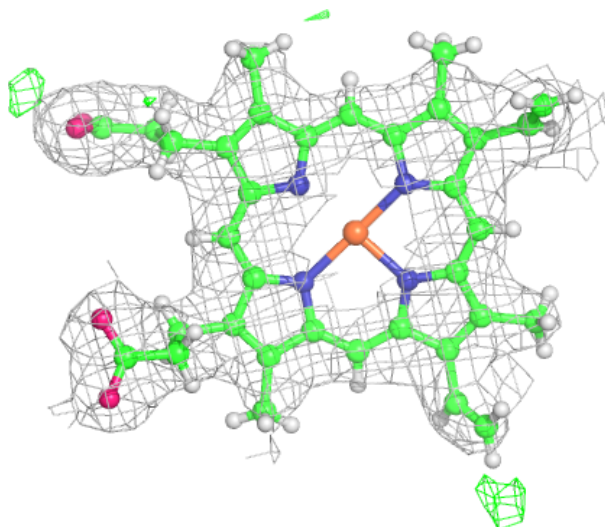
**Electron density around HEC f 101:**

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



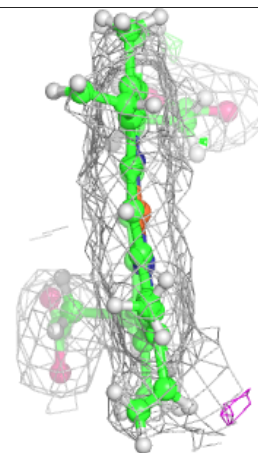
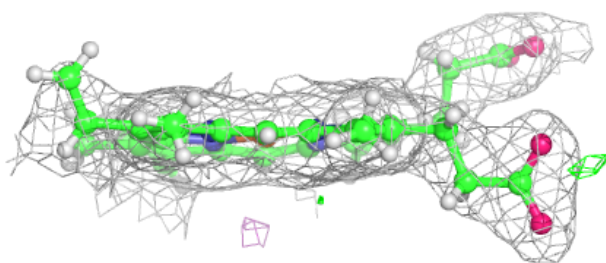
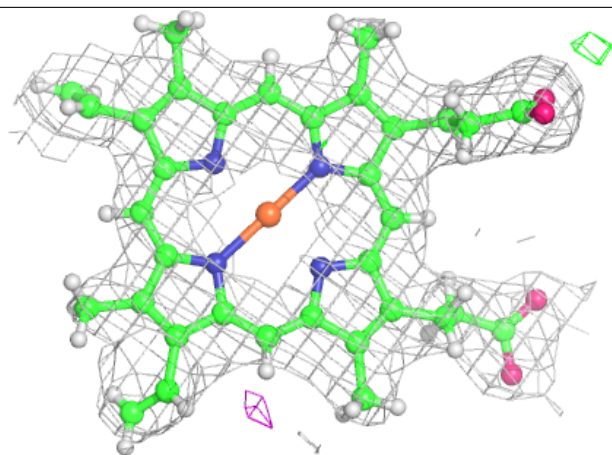
**Electron density around HEC v 201:**

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



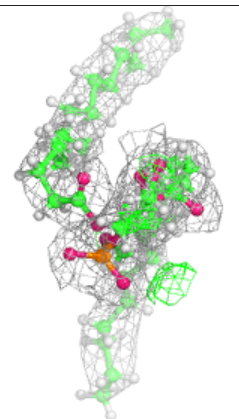
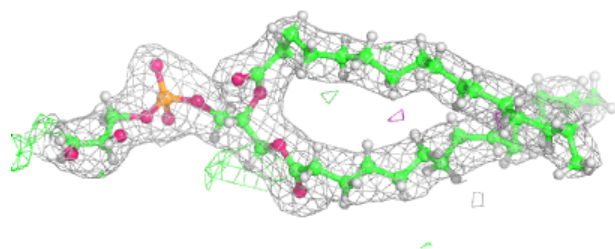
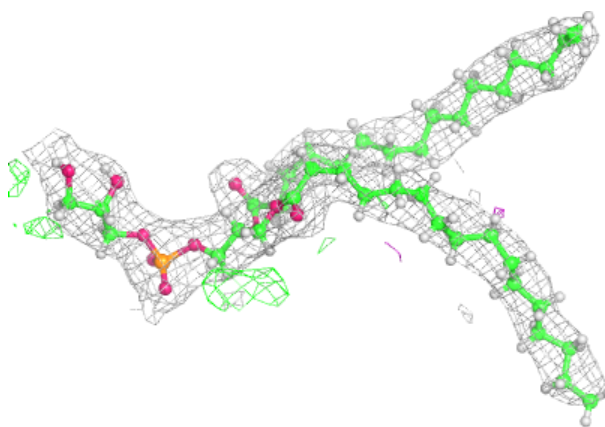
**Electron density around HEC V 201:**

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



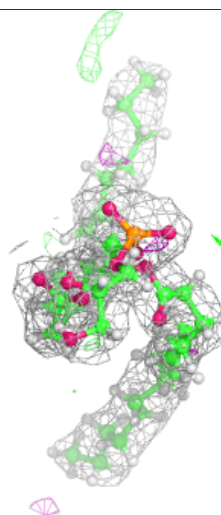
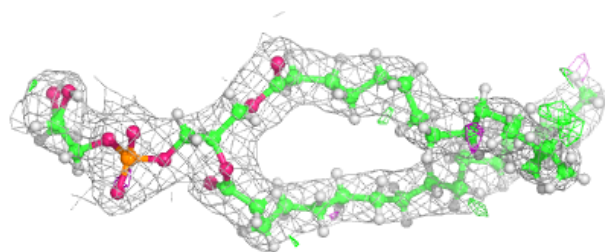
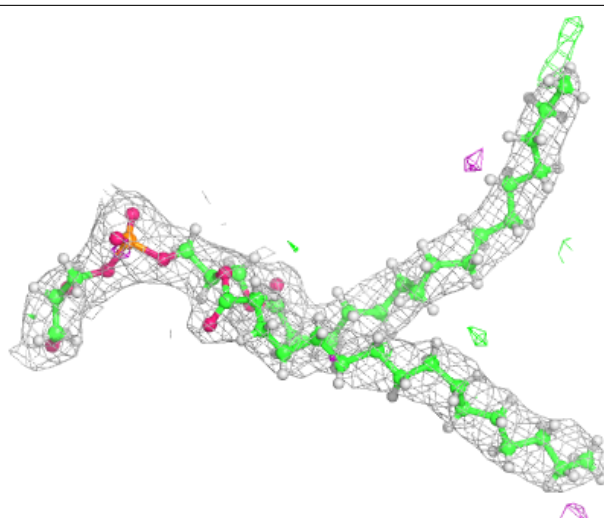
**Electron density around LHG d 408:**

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



**Electron density around LHG 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.