



## wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2021 – 12:38 PM EDT

PDB ID : 7RF8  
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 2.09 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2



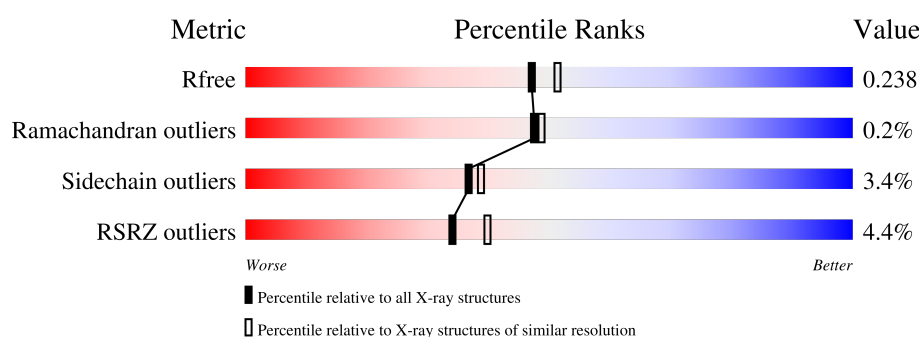
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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.



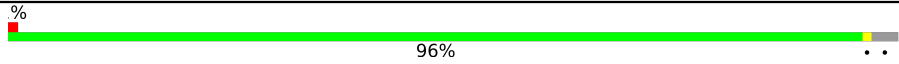
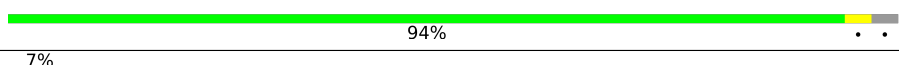
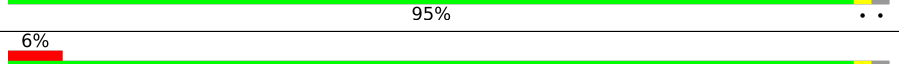
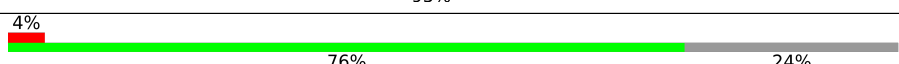

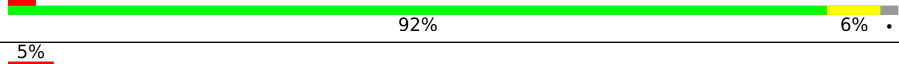
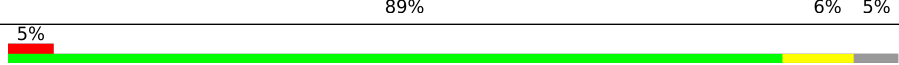
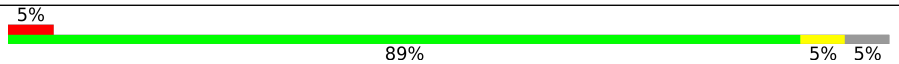
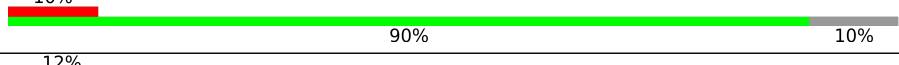

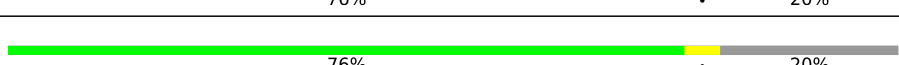
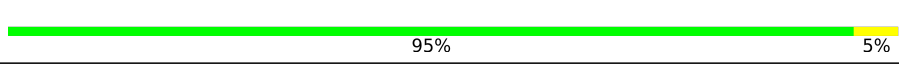
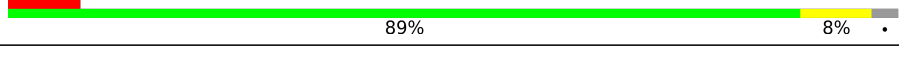


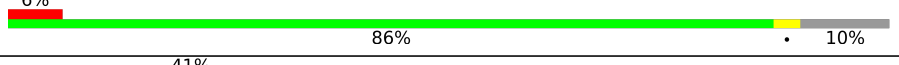


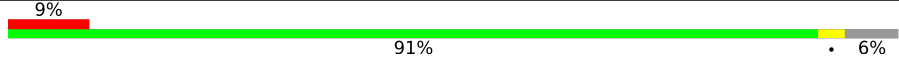
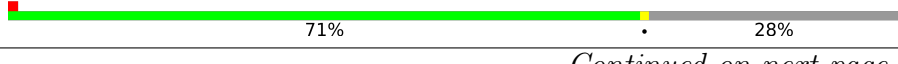

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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	344	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	a	344	<div> <div>93%</div> <div>..</div> </div>
2	B	510	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
2	b	510	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
3	C	461	<div> <div>2%</div> <div>94%</div> <div>..</div> </div>
3	c	461	<div> <div>3%</div> <div>95%</div> <div>..</div> </div>




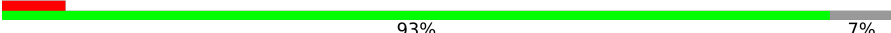





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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

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Mol	Chain	Length	Quality of chain
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	405	X	-	-	-
22	CLA	A	410	X	-	-	-
22	CLA	B	601	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	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	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	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	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	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	-	-	-
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	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	404	X	-	-	-
22	CLA	d	405	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105937 atoms, of which 52685 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	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

- 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
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	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	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

- 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	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	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	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	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
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- 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	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	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
			1547	491	773	129	154				
16	u	97	Total	C	H	N	O		0	0	0
			1547	491	773	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	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	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			



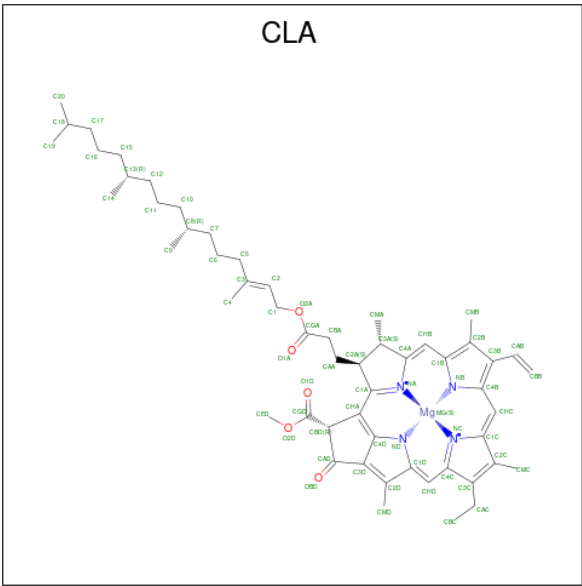
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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		
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	A	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		

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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
			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
			117	49	58	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		

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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	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	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
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
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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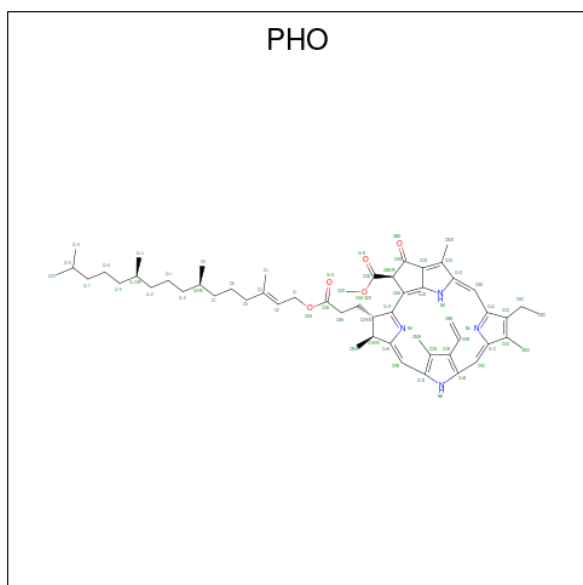
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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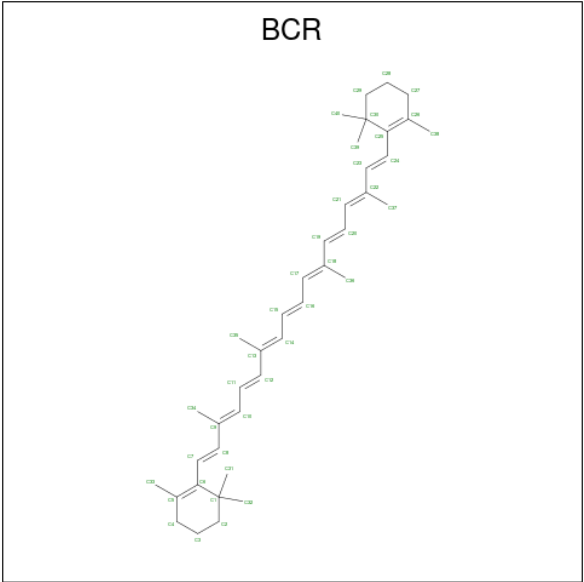
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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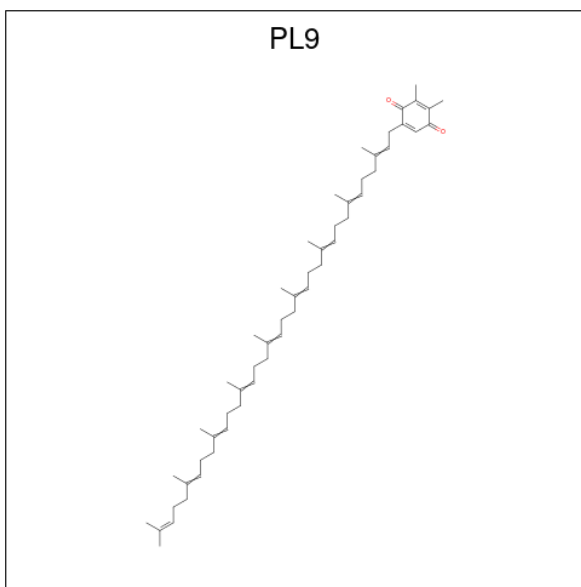
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40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

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

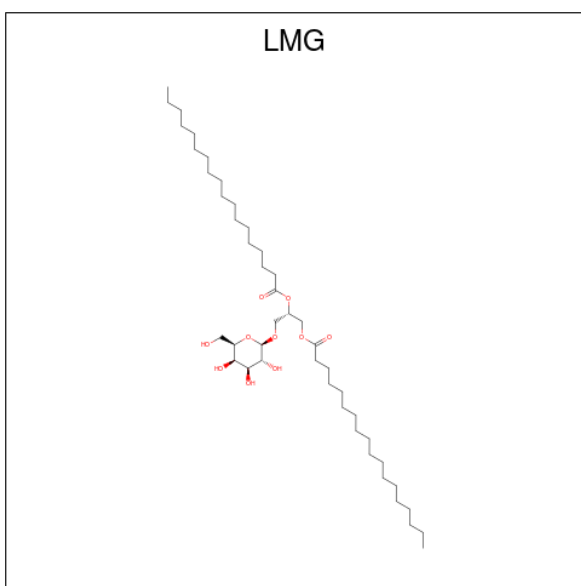
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- 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>).



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		

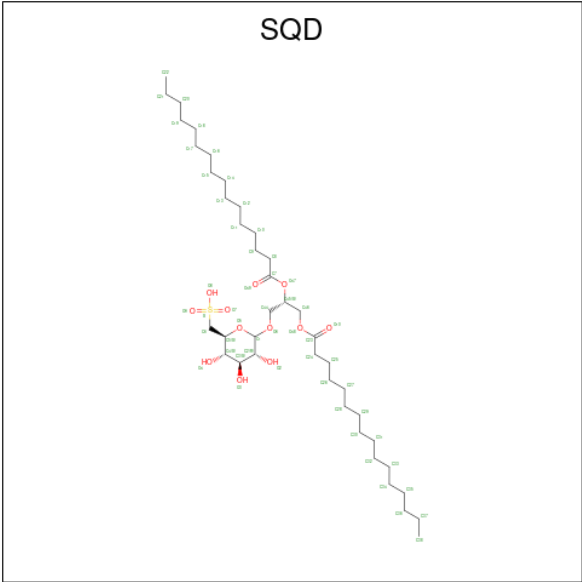
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





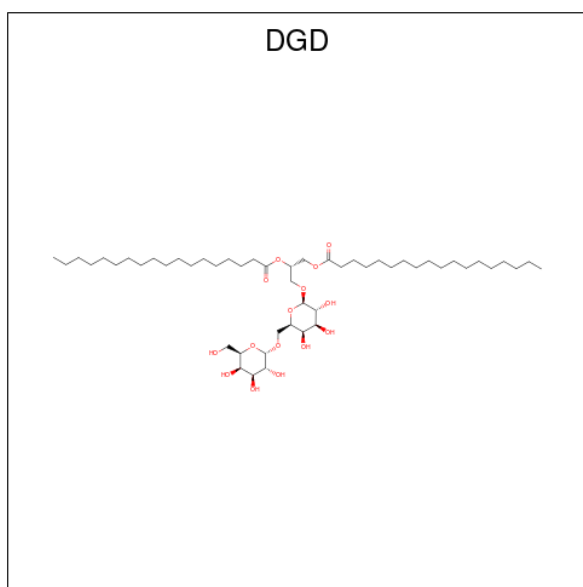
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	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
			57	21	34	2		
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).



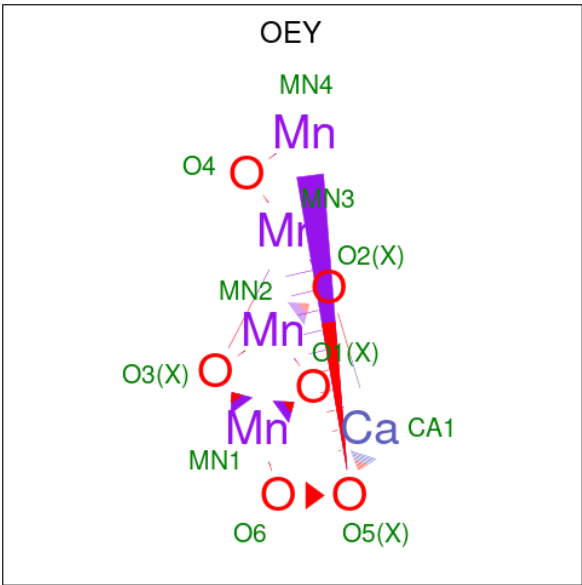
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	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>).



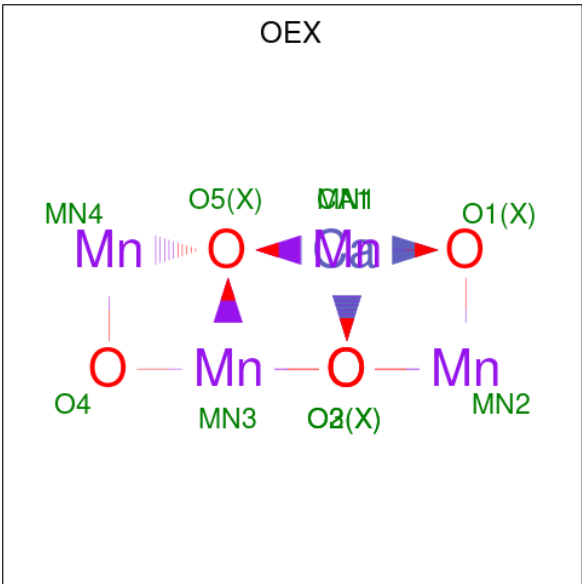
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	a	1	Total	C	H	O	0	0
			119	39	75	5		
29	c	1	Total	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		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



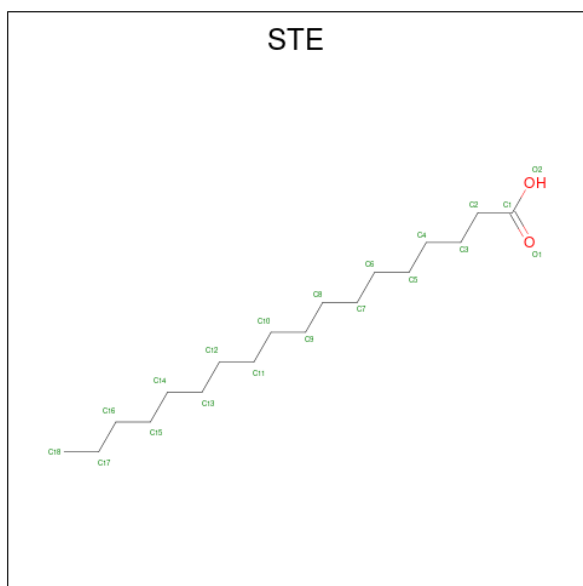
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula:  $C_{18}H_{36}O_2$ ).



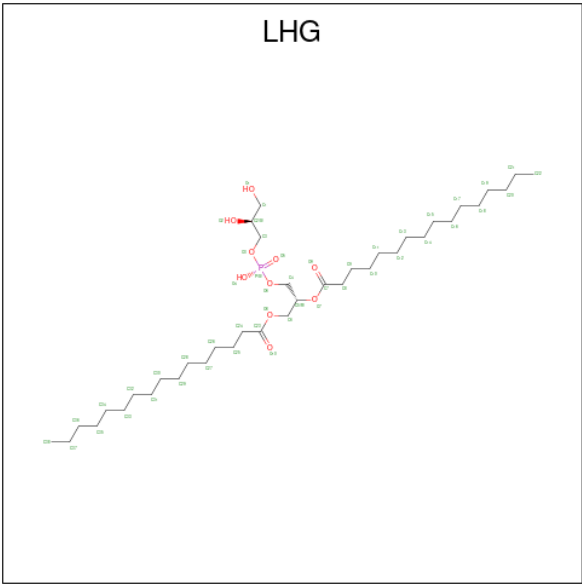
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		

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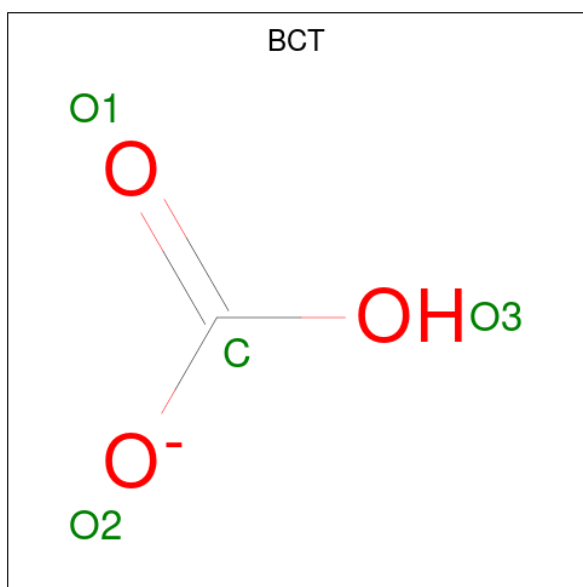
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	1	Total	C	H	O	0	0
			37	13	22	2		
32	M	1	Total	C	H		0	0
			26	10	16			
32	T	1	Total	C	H		0	0
			47	16	31			
32	T	1	Total	C	H		0	0
			44	15	29			
32	a	1	Total	C	H		0	0
			26	10	16			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	1	Total	C	H	O	0	0
			55	18	35	2		
32	b	1	Total	C	H	O	0	0
			40	14	24	2		
32	b	1	Total	C	H	O	0	0
			55	18	35	2		
32	b	1	Total	C	H		0	0
			26	10	16			
32	c	1	Total	C	H	O	0	0
			55	18	35	2		
32	c	1	Total	C	H	O	0	0
			28	10	16	2		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- 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).



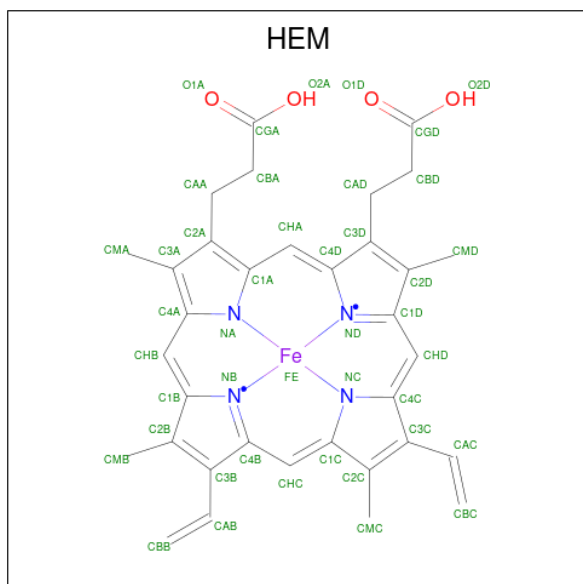
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	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		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

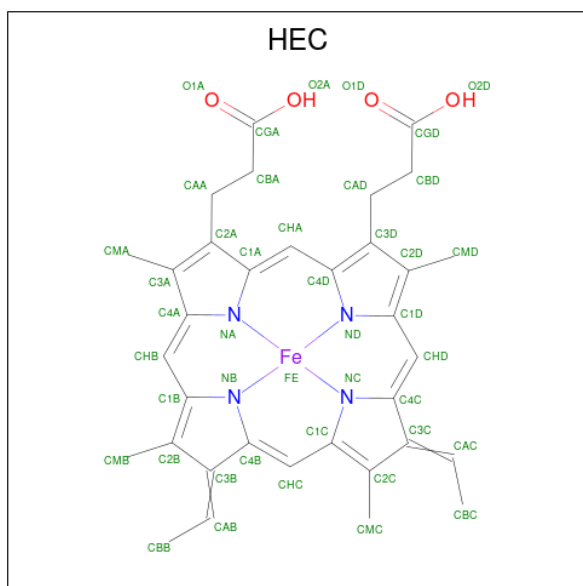
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	136	Total	O	1	12
			136	136		
37	B	213	Total	O	0	0
			213	213		
37	C	159	Total	O	0	0
			159	159		
37	D	130	Total	O	0	0
			130	130		
37	E	40	Total	O	0	0
			40	40		
37	F	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	42	Total 42	O 42	0	0
37	I	12	Total 12	O 12	0	0
37	J	13	Total 13	O 13	0	0
37	K	4	Total 4	O 4	0	0
37	L	9	Total 9	O 9	0	0
37	M	9	Total 9	O 9	0	0
37	O	99	Total 99	O 99	0	0
37	R	4	Total 4	O 4	0	0
37	T	9	Total 9	O 9	0	0
37	U	33	Total 33	O 33	0	0
37	V	64	Total 64	O 64	0	0
37	X	14	Total 14	O 14	0	0
37	Y	4	Total 4	O 4	0	0
37	Z	3	Total 3	O 3	0	0
37	a	118	Total 118	O 118	0	8
37	b	191	Total 191	O 191	0	0
37	c	157	Total 157	O 157	0	0
37	d	105	Total 105	O 105	0	0
37	e	17	Total 17	O 17	0	0
37	f	6	Total 6	O 6	0	0
37	h	30	Total 30	O 30	0	0

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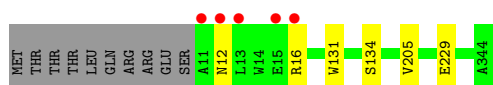
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	21	Total 21	O 21	0	0
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	12	Total 12	O 12	0	0
37	m	5	Total 5	O 5	0	0
37	o	93	Total 93	O 93	0	0
37	r	5	Total 5	O 5	0	0
37	t	8	Total 8	O 8	0	0
37	u	65	Total 65	O 65	0	0
37	v	59	Total 59	O 59	0	0
37	x	9	Total 9	O 9	0	0
37	y	4	Total 4	O 4	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



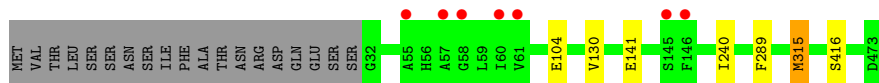
- Molecule 2: Photosystem II CP47 reaction center protein



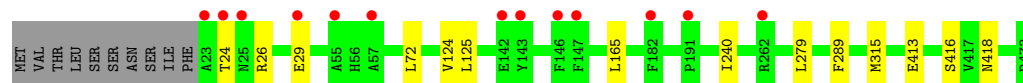
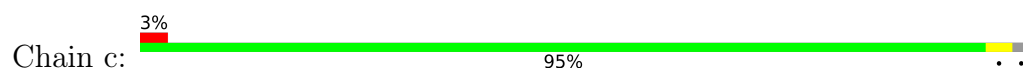
- Molecule 2: Photosystem II CP47 reaction center protein



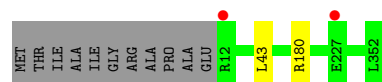
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



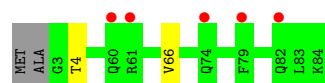
- Molecule 4: Photosystem II D2 protein



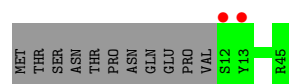
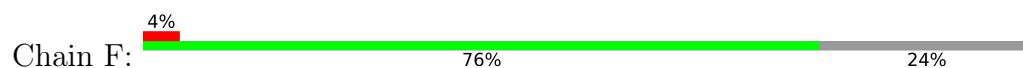
- Molecule 5: Cytochrome b559 subunit alpha



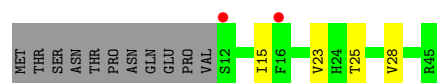
- Molecule 5: Cytochrome b559 subunit alpha



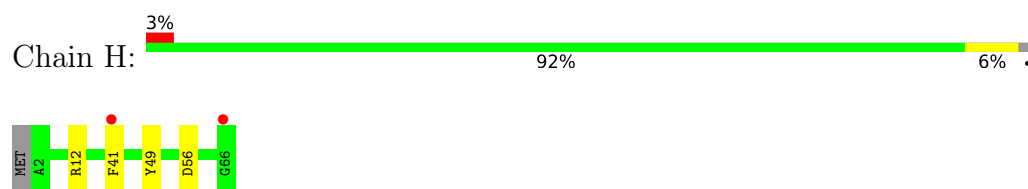
- Molecule 6: Cytochrome b559 subunit beta



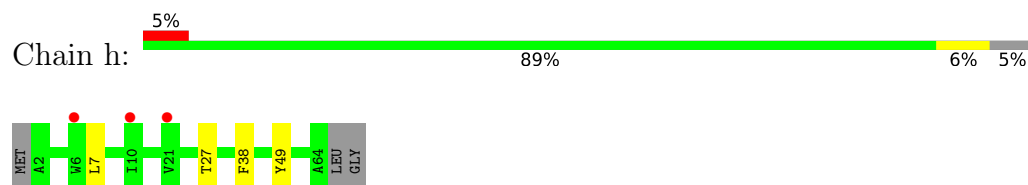
- Molecule 6: Cytochrome b559 subunit beta



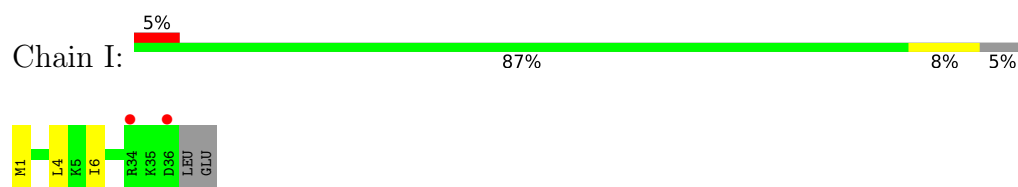
- Molecule 7: Photosystem II reaction center protein H



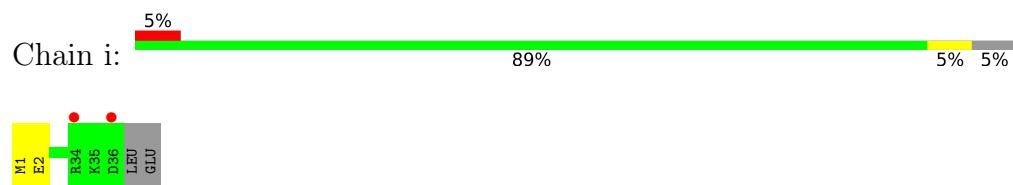
- Molecule 7: Photosystem II reaction center protein H



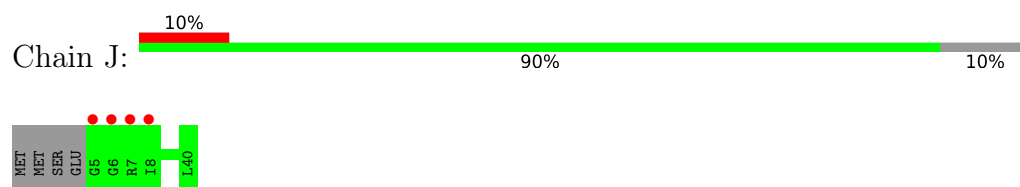
- Molecule 8: Photosystem II reaction center protein I



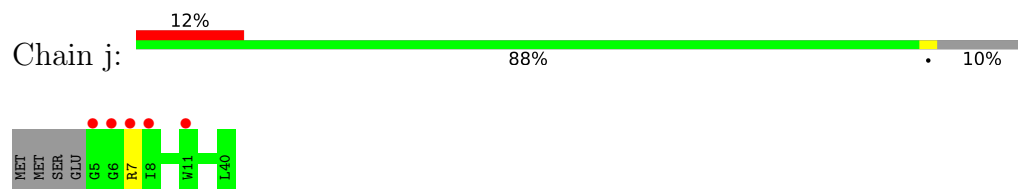
- Molecule 8: Photosystem II reaction center protein I



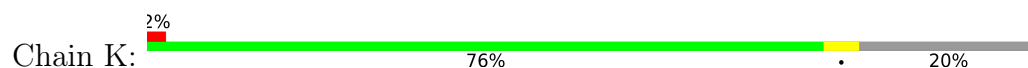
- Molecule 9: Photosystem II reaction center protein J

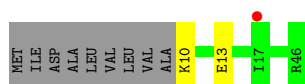


- Molecule 9: Photosystem II reaction center protein J



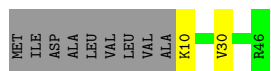
- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 76% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 95% 5%



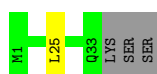
- Molecule 11: Photosystem II reaction center protein L

Chain l: 8% 89% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 89% 8%



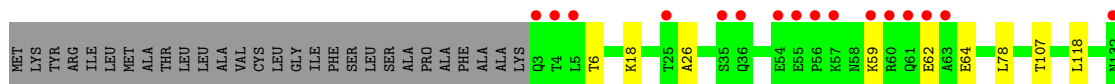
- Molecule 12: Photosystem II reaction center protein M

Chain m: 78% 11% 11%

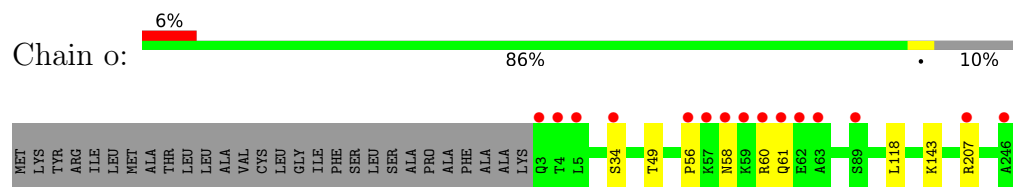


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

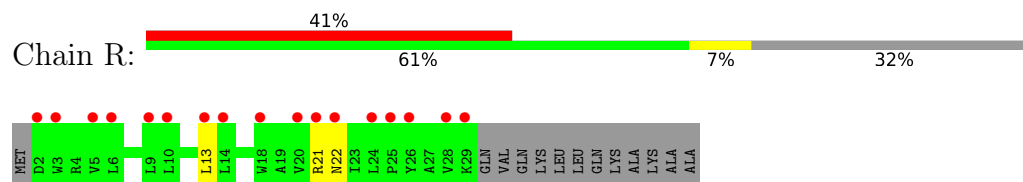
Chain O: 6% 86% 10%



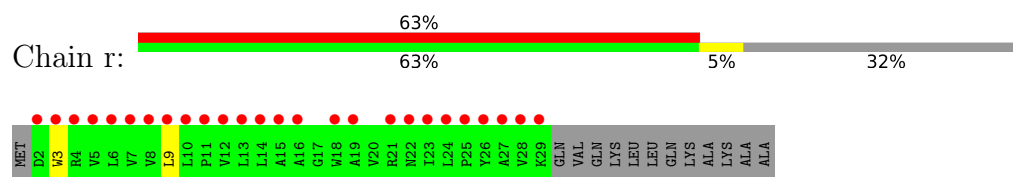
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



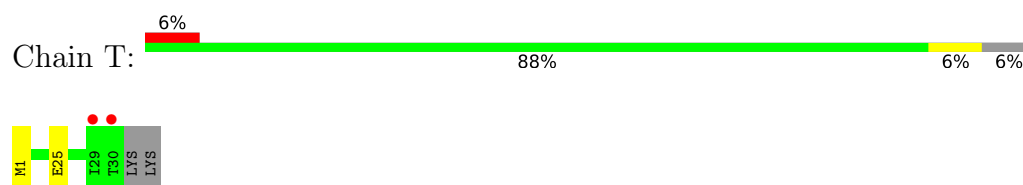
- Molecule 14: Photosystem II protein Y



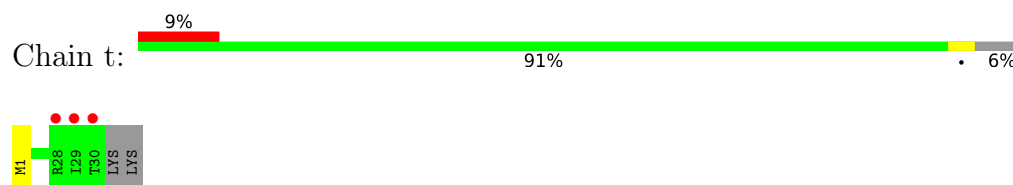
- Molecule 14: Photosystem II protein Y



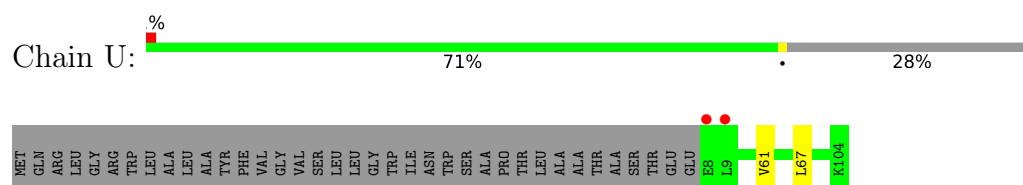
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T



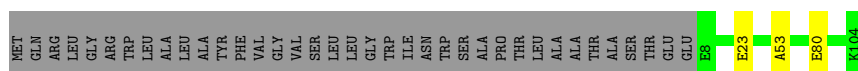
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein

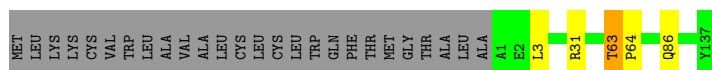






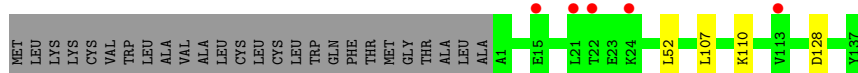
- Molecule 17: Cytochrome c-550

Chain V: 81% 16%



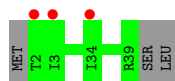
- Molecule 17: Cytochrome c-550

Chain v: 82% 16%



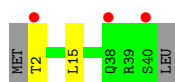
- Molecule 18: Photosystem II reaction center X protein

Chain X: 93% 7%



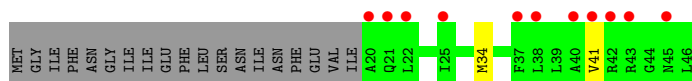
- Molecule 18: Photosystem II reaction center X protein

Chain x: 90% 5% 5%



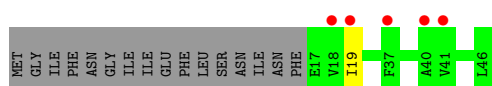
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 54% 41% 24%

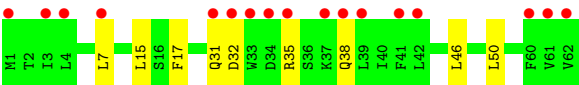
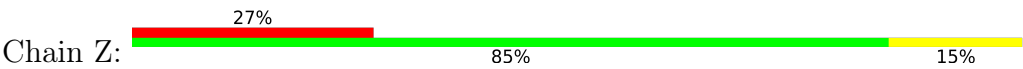


- Molecule 19: Photosystem II reaction center protein Ycf12

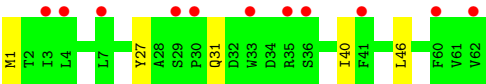
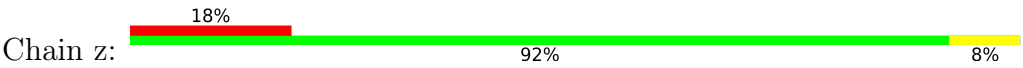
Chain y: 63% 35% 11%



- 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, $\alpha$ , $\beta$ , $\gamma$	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.181 , 0.239 0.181 , 0.238	Depositor DCC
$R_{free}$ test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	105937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: HEM, OEX, SQD, LHG, FME, CLA, LMG, HEC, STE, BCR, PL9, OEY, FE2, CL, DGD, BCT, PHO

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	0.61	0/3227	0.66	1/4397 (0.0%)
1	a	0.59	0/3224	0.65	0/4393
2	B	0.63	0/4161	0.68	1/5669 (0.0%)
2	b	0.60	0/4118	0.66	2/5611 (0.0%)
3	C	0.60	0/3647	0.65	1/4965 (0.0%)
3	c	0.56	0/3719	0.65	0/5061
4	D	0.65	0/2825	0.66	0/3847
4	d	0.60	0/2834	0.68	0/3859
5	E	0.58	0/688	0.62	0/940
5	e	0.53	0/683	0.63	0/932
6	F	0.56	0/284	0.58	0/387
6	f	0.53	0/284	0.66	0/387
7	H	0.69	1/523 (0.2%)	0.70	0/713
7	h	0.66	0/511	0.74	0/697
8	I	0.62	0/293	0.67	0/396
8	i	0.78	0/293	0.71	0/396
9	J	0.60	0/263	0.67	0/356
9	j	0.57	0/263	0.68	0/356
10	K	0.57	0/303	0.64	0/416
10	k	0.54	0/303	0.65	0/416
11	L	0.72	0/311	0.73	0/422
11	l	0.71	0/303	0.76	0/412
12	M	0.68	0/249	0.69	0/341
12	m	0.80	0/244	0.70	0/334
13	O	0.67	0/1904	0.77	0/2585
13	o	0.67	0/1905	0.75	0/2583
14	R	0.45	0/227	0.59	0/313
14	r	0.42	0/227	0.60	0/313
15	T	0.78	0/257	0.68	0/349
15	t	0.76	0/255	0.71	0/346
16	U	0.62	0/785	0.71	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.68	0/785	0.74	0/1064
17	V	0.63	0/1085	0.75	1/1473 (0.1%)
17	v	0.60	0/1085	0.68	0/1473
18	X	0.56	0/284	0.64	0/384
18	x	0.46	0/289	0.58	0/391
19	Y	0.46	0/197	0.63	0/264
19	y	0.41	0/219	0.57	0/294
20	Z	0.51	0/490	0.61	0/669
20	z	0.45	0/488	0.53	0/666
All	All	0.61	1/44035 (0.0%)	0.67	6/59934 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	41	PHE	CB-CG	-5.10	1.42	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	98	LEU	CA-CB-CG	5.97	129.04	115.30
17	V	63	THR	C-N-CD	-5.92	107.59	120.60
2	B	15	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	131	TRP	CA-CB-CG	-5.18	103.86	113.70
2	b	334	ASP	CB-CG-OD1	5.09	122.89	118.30

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	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
1	a	397/344 (115%)	388 (98%)	8 (2%)	1 (0%)	41	41
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	47	49
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	47	49
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	9	5
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	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%)	227 (93%)	13 (5%)	3 (1%)	13	8
13	o	242/272 (89%)	231 (96%)	8 (3%)	3 (1%)	13	8
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	14	9
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	18
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5387/5700 (94%)	5225 (97%)	150 (3%)	12 (0%)	47	49

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
17	V	64	PRO
3	c	416	SER
13	O	62	GLU

### 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	324/280 (116%)	319 (98%)	5 (2%)	65	71
1	a	323/280 (115%)	310 (96%)	13 (4%)	31	32
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	60
2	b	402/407 (99%)	391 (97%)	11 (3%)	44	48
3	C	356/362 (98%)	350 (98%)	6 (2%)	60	67
3	c	364/362 (101%)	350 (96%)	14 (4%)	33	34
4	D	277/283 (98%)	275 (99%)	2 (1%)	84	88
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	41
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	30
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	47
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	35
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	10
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	15
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	43
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	30
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	13
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	13
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	18
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	36
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	33
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	46
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	34
15	t	25/28 (89%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	53
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	53
17	V	117/138 (85%)	114 (97%)	3 (3%)	46	50
17	v	117/138 (85%)	113 (97%)	4 (3%)	37	39
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	14
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	4
19	y	22/37 (60%)	21 (96%)	1 (4%)	27	27
20	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
20	z	51/52 (98%)	46 (90%)	5 (10%)	8	5
All	All	4451/4654 (96%)	4301 (97%)	150 (3%)	37	39

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	27	THR
18	x	15	LEU
9	j	7	ARG
13	o	60	ARG
17	V	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	490	GLN
5	e	74	GLN
20	z	31	GLN
13	o	61	GLN
17	V	86	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
8	FME	i	1	8	8,9,10	0.98	0	7,9,11	1.53	1 (14%)
8	FME	I	1	8	8,9,10	0.95	0	7,9,11	1.30	1 (14%)
12	FME	m	1	12	8,9,10	1.05	1 (12%)	7,9,11	1.12	0
15	FME	t	1	15	8,9,10	1.68	1 (12%)	7,9,11	0.80	0
12	FME	M	1	12	8,9,10	0.87	0	7,9,11	1.03	0
15	FME	T	1	15	8,9,10	1.13	1 (12%)	7,9,11	1.09	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
8	FME	i	1	8	-	4/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.20	1.40	1.46
12	m	1	FME	CA-N	-2.22	1.43	1.46
15	T	1	FME	CA-N	-2.17	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.62	114.46	109.73
8	I	1	FME	CA-N-CN	-2.47	119.02	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
8	i	1	FME	CA-CB-CG-SD

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 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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
22	CLA	C	502	-	56,73,73	1.57	9 (16%)	55,113,113	1.57	7 (12%)
24	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	7 (12%)
29	DGD	A	414	-	67,67,67	1.38	7 (10%)	81,81,81	1.50	12 (14%)
28	SQD	a	410	-	53,54,54	0.95	4 (7%)	62,65,65	2.05	13 (20%)
24	BCR	C	515	-	41,41,41	1.16	4 (9%)	56,56,56	1.13	3 (5%)
33	LHG	D	408	-	48,48,48	0.97	5 (10%)	51,54,54	1.28	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.73	0
22	CLA	B	613	-	56,73,73	1.49	7 (12%)	55,113,113	1.79	13 (23%)
22	CLA	C	513	-	56,73,73	1.60	8 (14%)	55,113,113	1.74	8 (14%)
24	BCR	d	406	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)
22	CLA	C	509	-	56,73,73	1.64	9 (16%)	55,113,113	1.73	11 (20%)
24	BCR	D	405	-	41,41,41	1.16	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	c	506	-	56,73,73	1.45	9 (16%)	55,113,113	1.60	10 (18%)
22	CLA	B	610	37	56,73,73	1.68	7 (12%)	55,113,113	1.76	13 (23%)
24	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
22	CLA	b	612	-	56,73,73	1.24	6 (10%)	55,113,113	1.78	14 (25%)
32	STE	B	624	-	8,11,19	0.48	0	7,11,19	1.01	1 (14%)
27	LMG	D	407	-	51,51,55	1.18	4 (7%)	59,59,63	1.34	9 (15%)
32	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.83	0
29	DGD	C	518	-	63,63,67	1.15	9 (14%)	77,77,81	1.36	10 (12%)
22	CLA	b	601	37	56,73,73	1.68	10 (17%)	55,113,113	1.77	5 (9%)
29	DGD	C	516	-	63,63,67	1.36	11 (17%)	77,77,81	1.40	10 (12%)
22	CLA	c	505	-	56,73,73	1.35	6 (10%)	55,113,113	1.67	11 (20%)
35	HEM	f	101	5,6	27,50,50	2.03	5 (18%)	17,82,82	2.18	5 (29%)
22	CLA	C	511	3	56,73,73	1.72	7 (12%)	55,113,113	1.50	7 (12%)
23	PHO	D	401	-	67,69,69	1.17	6 (8%)	85,99,99	1.16	7 (8%)
28	SQD	A	412	-	51,52,54	1.02	3 (5%)	60,63,65	2.11	12 (20%)
32	STE	b	625	-	9,9,19	0.59	0	8,8,19	0.46	0
24	BCR	B	619	-	41,41,41	1.10	3 (7%)	56,56,56	1.38	5 (8%)
33	LHG	L	102	-	48,48,48	1.00	2 (4%)	51,54,54	1.23	2 (3%)
24	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.46	10 (17%)
36	HEC	V	201	17	26,50,50	2.26	3 (11%)	18,82,82	2.18	6 (33%)
22	CLA	c	503	-	56,73,73	1.55	9 (16%)	55,113,113	1.68	9 (16%)
22	CLA	B	605	-	56,73,73	1.46	9 (16%)	55,113,113	1.60	8 (14%)
22	CLA	c	508	-	55,72,73	1.70	7 (12%)	53,111,113	1.71	8 (15%)
32	STE	B	625	-	14,17,19	0.38	0	13,17,19	0.90	0
22	CLA	b	609	-	56,73,73	1.60	8 (14%)	55,113,113	1.68	11 (20%)
33	LHG	d	410	-	38,38,48	0.88	3 (7%)	41,44,54	1.12	3 (7%)
23	PHO	d	402	-	67,69,69	1.31	12 (17%)	85,99,99	1.25	8 (9%)
24	BCR	B	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.18	7 (12%)
26	PL9	D	406	-	55,55,55	1.46	6 (10%)	68,69,69	1.63	13 (19%)
32	STE	C	520	-	8,11,19	0.39	0	7,11,19	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	STE	a	414	-	8,11,19	0.44	0	7,11,19	0.73	0
22	CLA	A	405	-	45,62,73	1.83	9 (20%)	41,99,113	1.80	9 (21%)
22	CLA	c	507	37	56,73,73	1.48	9 (16%)	55,113,113	1.50	12 (21%)
22	CLA	B	607	37	56,73,73	1.52	10 (17%)	55,113,113	1.86	10 (18%)
27	LMG	c	520	-	37,37,55	1.26	6 (16%)	45,45,63	1.31	6 (13%)
27	LMG	A	411	-	48,48,55	0.99	3 (6%)	56,56,63	1.32	7 (12%)
24	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	6 (10%)
22	CLA	b	606	-	56,73,73	1.46	6 (10%)	55,113,113	1.93	10 (18%)
33	LHG	d	409	-	48,48,48	0.74	1 (2%)	51,54,54	1.13	4 (7%)
27	LMG	B	621	-	20,26,55	0.62	0	18,26,63	1.09	0
22	CLA	C	508	-	56,73,73	1.73	7 (12%)	55,113,113	1.58	6 (10%)
32	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.60	0
29	DGD	C	517	-	63,63,67	1.39	7 (11%)	77,77,81	1.58	14 (18%)
22	CLA	c	504	37	51,68,73	1.57	7 (13%)	49,107,113	1.77	8 (16%)
22	CLA	C	505	-	56,73,73	1.69	9 (16%)	55,113,113	1.64	10 (18%)
24	BCR	H	101	-	41,41,41	1.13	1 (2%)	56,56,56	1.28	8 (14%)
24	BCR	b	617	-	41,41,41	1.05	3 (7%)	56,56,56	1.45	10 (17%)
26	PL9	A	409	-	55,55,55	1.15	3 (5%)	68,69,69	1.62	14 (20%)
26	PL9	a	409	-	55,55,55	0.93	2 (3%)	68,69,69	1.69	18 (26%)
28	SQD	a	411	-	35,35,54	1.10	2 (5%)	37,37,65	1.18	5 (13%)
34	BCT	D	402	21	0,3,3	-	-	0,3,3	-	-
28	SQD	F	101	-	35,36,54	1.02	3 (8%)	42,45,65	1.95	9 (21%)
33	LHG	d	408	-	48,48,48	1.03	3 (6%)	51,54,54	1.45	8 (15%)
22	CLA	A	410	37	56,73,73	1.54	5 (8%)	55,113,113	1.48	7 (12%)
22	CLA	b	602	-	56,73,73	1.51	7 (12%)	55,113,113	1.76	11 (20%)
27	LMG	d	412	-	44,44,55	1.21	6 (13%)	52,52,63	1.39	8 (15%)
32	STE	x	101	-	16,19,19	0.56	0	15,19,19	0.49	0
35	HEM	E	101	5,6	27,50,50	1.97	5 (18%)	17,82,82	2.03	5 (29%)
24	BCR	t	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.46	10 (17%)
32	STE	C	521	-	15,15,19	0.54	0	14,14,19	0.51	0
32	STE	c	524	-	8,11,19	0.34	0	7,11,19	0.85	0
22	CLA	d	405	-	56,73,73	1.55	10 (17%)	55,113,113	1.46	5 (9%)
22	CLA	C	512	-	56,73,73	1.60	8 (14%)	55,113,113	1.58	12 (21%)
22	CLA	c	509	-	56,73,73	1.58	5 (8%)	55,113,113	2.05	11 (20%)
33	LHG	D	409	-	46,46,48	1.09	3 (6%)	49,52,54	1.12	3 (6%)
32	STE	C	522	-	8,11,19	0.34	0	7,11,19	1.62	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	501	-	56,73,73	1.62	8 (14%)	55,113,113	1.69	11 (20%)
22	CLA	a	404	-	56,73,73	1.67	10 (17%)	55,113,113	1.52	10 (18%)
22	CLA	B	612	-	56,73,73	1.52	7 (12%)	55,113,113	1.75	10 (18%)
24	BCR	c	514	-	41,41,41	1.22	2 (4%)	56,56,56	1.33	8 (14%)
22	CLA	c	510	-	56,73,73	1.52	10 (17%)	55,113,113	1.75	10 (18%)
29	DGD	a	412	-	43,43,67	1.13	3 (6%)	45,45,81	1.45	7 (15%)
32	STE	d	413	-	13,16,19	0.43	0	12,16,19	0.78	0
22	CLA	b	616	-	51,68,73	1.50	8 (15%)	49,107,113	1.93	10 (20%)
22	CLA	b	614	-	56,73,73	1.86	7 (12%)	55,113,113	1.58	12 (21%)
29	DGD	c	518	-	63,63,67	1.32	9 (14%)	77,77,81	1.53	10 (12%)
32	STE	T	103	-	14,14,19	0.42	0	13,13,19	0.89	0
26	PL9	d	407	-	55,55,55	1.39	6 (10%)	68,69,69	1.85	18 (26%)
31	OEX	A	416[A]	37,1,3	0,15,15	-	-	-	-	-
27	LMG	M	101	-	51,51,55	1.10	5 (9%)	59,59,63	1.41	7 (11%)
32	STE	j	101	-	8,11,19	0.62	0	7,11,19	0.55	0
22	CLA	d	403	-	56,73,73	1.45	7 (12%)	55,113,113	1.37	5 (9%)
29	DGD	h	102	-	63,63,67	1.29	11 (17%)	77,77,81	1.54	13 (16%)
34	BCT	a	408	21	0,3,3	-	-	0,3,3	-	-
24	BCR	c	515	-	41,41,41	1.22	3 (7%)	56,56,56	1.42	10 (17%)
22	CLA	B	609	-	56,73,73	1.43	7 (12%)	55,113,113	1.42	10 (18%)
32	STE	H	103	-	17,17,19	0.56	0	16,16,19	0.59	0
22	CLA	b	603	-	56,73,73	1.63	10 (17%)	55,113,113	1.68	10 (18%)
22	CLA	B	604	-	56,73,73	1.32	5 (8%)	55,113,113	2.06	15 (27%)
22	CLA	B	602	-	56,73,73	1.68	9 (16%)	55,113,113	1.89	11 (20%)
22	CLA	c	511	3	56,73,73	1.89	8 (14%)	55,113,113	1.83	10 (18%)
27	LMG	b	620	-	51,51,55	1.13	6 (11%)	59,59,63	1.51	11 (18%)
32	STE	t	102	-	10,13,19	0.54	0	9,13,19	0.84	0
24	BCR	B	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	6 (10%)
32	STE	m	101	-	8,11,19	0.54	0	7,11,19	0.43	0
30	OEY	A	415[B]	37,1,3	0,16,16	-	-	-	-	-
22	CLA	D	403	-	56,73,73	1.66	8 (14%)	55,113,113	1.58	12 (21%)
28	SQD	A	413	-	38,38,54	1.03	3 (7%)	40,40,65	1.46	6 (15%)
29	DGD	c	519	-	63,63,67	1.38	10 (15%)	77,77,81	1.44	12 (15%)
32	STE	B	620	-	13,16,19	0.44	0	12,16,19	0.79	0
22	CLA	B	611	-	56,73,73	1.40	5 (8%)	55,113,113	1.63	12 (21%)
28	SQD	B	623	-	53,54,54	1.00	3 (5%)	62,65,65	1.86	11 (17%)
22	CLA	C	503	-	56,73,73	1.93	8 (14%)	55,113,113	1.77	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	STE	b	621	-	16,19,19	0.41	0	15,19,19	0.77	0
31	OEX	a	416[A]	37,1,3	0,15,15	-	-	-		
22	CLA	B	606	-	56,73,73	1.59	7 (12%)	55,113,113	1.63	14 (25%)
27	LMG	c	523	-	49,49,55	1.03	4 (8%)	57,57,63	1.27	6 (10%)
22	CLA	B	601	37	56,73,73	1.86	8 (14%)	55,113,113	1.65	7 (12%)
27	LMG	c	522	-	48,48,55	1.19	5 (10%)	56,56,63	1.37	8 (14%)
22	CLA	b	607	37	56,73,73	1.62	9 (16%)	55,113,113	1.49	10 (18%)
24	BCR	T	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.25	6 (10%)
32	STE	c	521	-	16,19,19	0.41	0	15,19,19	0.81	0
23	PHO	d	401	-	67,69,69	1.20	6 (8%)	85,99,99	1.02	4 (4%)
24	BCR	b	618	-	41,41,41	1.31	4 (9%)	56,56,56	1.24	4 (7%)
32	STE	E	103	-	8,11,19	0.46	0	7,11,19	0.61	0
32	STE	B	627	-	8,11,19	0.45	0	7,11,19	0.60	0
22	CLA	B	615	-	56,73,73	1.97	8 (14%)	55,113,113	1.65	9 (16%)
32	STE	T	102	-	15,15,19	0.50	0	14,14,19	0.70	0
28	SQD	f	102	-	40,41,54	1.19	5 (12%)	49,52,65	1.83	11 (22%)
22	CLA	B	608	-	56,73,73	1.52	9 (16%)	55,113,113	1.91	12 (21%)
22	CLA	b	604	-	56,73,73	1.63	8 (14%)	55,113,113	2.04	14 (25%)
27	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.09	2 (6%)
28	SQD	L	101	-	48,49,54	1.00	3 (6%)	57,60,65	2.31	17 (29%)
29	DGD	H	102	-	63,63,67	1.39	9 (14%)	77,77,81	1.43	8 (10%)
22	CLA	B	616	-	51,68,73	1.67	8 (15%)	49,107,113	2.05	10 (20%)
22	CLA	C	506	-	56,73,73	1.53	9 (16%)	55,113,113	1.66	8 (14%)
33	LHG	B	622	-	48,48,48	1.01	4 (8%)	51,54,54	1.40	6 (11%)
29	DGD	c	517	-	63,63,67	1.09	7 (11%)	77,77,81	1.35	7 (9%)
22	CLA	b	611	-	56,73,73	1.68	9 (16%)	55,113,113	1.56	7 (12%)
32	STE	I	101	-	14,14,19	0.60	0	13,13,19	0.39	0
22	CLA	C	501	-	56,73,73	1.63	9 (16%)	55,113,113	1.91	11 (20%)
27	LMG	b	622	-	55,55,55	1.03	7 (12%)	63,63,63	1.44	7 (11%)
32	STE	b	624	-	16,19,19	0.62	0	15,19,19	0.64	0
24	BCR	a	405	-	41,41,41	1.17	5 (12%)	56,56,56	1.42	8 (14%)
22	CLA	c	502	-	56,73,73	1.67	9 (16%)	55,113,113	1.63	11 (20%)
22	CLA	c	512	-	56,73,73	1.66	9 (16%)	55,113,113	1.63	9 (16%)
22	CLA	B	614	-	56,73,73	1.76	7 (12%)	55,113,113	1.45	11 (20%)
24	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.31	9 (16%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	11 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	510	-	56,73,73	1.51	7 (12%)	55,113,113	1.59	11 (20%)
33	LHG	l	101	-	48,48,48	0.85	1 (2%)	51,54,54	1.15	5 (9%)
32	STE	b	623	-	12,15,19	0.52	0	11,15,19	0.51	0
22	CLA	c	513	-	56,73,73	1.45	6 (10%)	55,113,113	1.64	11 (20%)
24	BCR	Y	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.21	4 (7%)
30	OEY	a	415[B]	37,1,3	0,16,16	-	-	-	-	-
33	LHG	e	101	-	41,41,48	0.86	1 (2%)	44,47,54	1.26	4 (9%)
22	CLA	D	404	-	56,73,73	1.62	8 (14%)	55,113,113	1.88	8 (14%)
22	CLA	A	403	37	56,73,73	1.60	8 (14%)	55,113,113	1.37	9 (16%)
22	CLA	b	615	-	56,73,73	1.61	9 (16%)	55,113,113	1.67	12 (21%)
22	CLA	b	605	-	56,73,73	1.42	7 (12%)	55,113,113	1.60	14 (25%)
22	CLA	A	402	-	56,73,73	1.53	5 (8%)	55,113,113	1.71	11 (20%)
22	CLA	b	608	-	56,73,73	1.60	9 (16%)	55,113,113	1.77	13 (23%)
22	CLA	C	504	37	50,67,73	1.59	5 (10%)	47,105,113	1.46	6 (12%)
32	STE	a	413	-	9,9,19	0.64	0	8,8,19	0.41	0
27	LMG	C	519	-	48,48,55	1.18	7 (14%)	56,56,63	1.43	7 (12%)
22	CLA	a	403	37	56,73,73	1.49	7 (12%)	55,113,113	1.85	15 (27%)
27	LMG	d	411	-	18,21,55	0.75	0	16,20,63	0.89	0
32	STE	D	411	-	16,19,19	0.27	0	15,19,19	1.09	0
22	CLA	a	402	-	56,73,73	1.55	7 (12%)	55,113,113	1.68	11 (20%)
22	CLA	B	603	-	56,73,73	1.54	12 (21%)	55,113,113	1.63	12 (21%)
23	PHO	A	404	-	67,69,69	1.19	8 (11%)	85,99,99	1.18	9 (10%)
22	CLA	b	613	-	56,73,73	1.83	7 (12%)	55,113,113	1.85	16 (29%)
22	CLA	C	507	37	56,73,73	1.36	8 (14%)	55,113,113	2.02	13 (23%)
22	CLA	b	610	37	56,73,73	1.43	9 (16%)	55,113,113	1.49	12 (21%)
33	LHG	E	102	-	48,48,48	0.86	3 (6%)	51,54,54	1.18	3 (5%)
22	CLA	d	404	37	56,73,73	1.70	7 (12%)	55,113,113	1.71	9 (16%)
36	HEC	v	201	17	26,50,50	2.38	5 (19%)	18,82,82	1.76	5 (27%)
24	BCR	C	514	-	41,41,41	1.20	4 (9%)	56,56,56	1.33	5 (8%)
32	STE	J	101	-	8,11,19	0.29	0	7,11,19	1.02	0
32	STE	l	102	-	17,17,19	0.44	0	16,16,19	0.81	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
22	CLA	C	502	-	1/1/20/20	11/37/115/115	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
29	DGD	A	414	-	-	25/55/95/95	0/2/2/2
28	SQD	a	410	-	-	19/49/69/69	0/1/1/1
24	BCR	C	515	-	-	14/29/63/63	0/2/2/2
33	LHG	D	408	-	-	26/53/53/53	-
32	STE	B	626	-	-	6/13/13/17	-
22	CLA	B	613	-	1/1/20/20	12/37/115/115	-
22	CLA	C	513	-	1/1/20/20	17/37/115/115	-
24	BCR	d	406	-	-	7/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/20/20	14/37/115/115	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
22	CLA	c	506	-	1/1/20/20	16/37/115/115	-
22	CLA	B	610	37	1/1/20/20	7/37/115/115	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
22	CLA	b	612	-	1/1/20/20	8/37/115/115	-
32	STE	B	624	-	-	4/7/9/17	-
27	LMG	D	407	-	-	17/46/66/70	0/1/1/1
32	STE	M	102	-	-	4/10/12/17	-
29	DGD	C	518	-	-	12/51/91/95	0/2/2/2
22	CLA	b	601	37	1/1/20/20	14/37/115/115	-
29	DGD	C	516	-	-	22/51/91/95	0/2/2/2
22	CLA	c	505	-	1/1/20/20	10/37/115/115	-
35	HEM	f	101	5,6	-	0/6/54/54	-
22	CLA	C	511	3	1/1/20/20	6/37/115/115	-
23	PHO	D	401	-	-	4/53/103/103	0/5/6/6
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
32	STE	b	625	-	-	5/7/7/17	-
24	BCR	B	619	-	-	1/29/63/63	0/2/2/2
33	LHG	L	102	-	-	20/53/53/53	-
24	BCR	A	406	-	-	5/29/63/63	0/2/2/2
36	HEC	V	201	17	-	0/6/54/54	-
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
22	CLA	c	508	-	-	7/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	B	625	-	-	9/13/15/17	-
22	CLA	b	609	-	1/1/20/20	9/37/115/115	-
33	LHG	d	410	-	-	14/43/43/53	-
23	PHO	d	402	-	-	9/53/103/103	0/5/6/6
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	PL9	D	406	-	-	8/53/73/73	0/1/1/1
32	STE	C	520	-	-	4/7/9/17	-
32	STE	a	414	-	-	6/7/9/17	-
22	CLA	A	405	-	1/1/17/20	3/24/102/115	-
22	CLA	c	507	37	1/1/20/20	8/37/115/115	-
22	CLA	B	607	37	1/1/20/20	13/37/115/115	-
27	LMG	c	520	-	-	8/31/51/70	0/1/1/1
27	LMG	A	411	-	-	23/43/63/70	0/1/1/1
24	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/20/20	15/37/115/115	-
33	LHG	d	409	-	-	17/53/53/53	-
27	LMG	B	621	-	-	10/18/22/70	-
22	CLA	C	508	-	-	9/37/115/115	-
32	STE	M	103	-	-	2/7/7/17	-
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
22	CLA	c	504	37	1/1/19/20	5/31/109/115	-
22	CLA	C	505	-	1/1/20/20	19/37/115/115	-
24	BCR	H	101	-	-	7/29/63/63	0/2/2/2
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
26	PL9	a	409	-	-	18/53/73/73	0/1/1/1
28	SQD	a	411	-	-	17/37/37/69	-
28	SQD	F	101	-	-	10/28/48/69	0/1/1/1
33	LHG	d	408	-	-	25/53/53/53	-
22	CLA	A	410	37	1/1/20/20	11/37/115/115	-
22	CLA	b	602	-	-	11/37/115/115	-
27	LMG	d	412	-	-	11/39/59/70	0/1/1/1
32	STE	x	101	-	-	9/15/17/17	-
35	HEM	E	101	5,6	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	t	101	-	-	11/29/63/63	0/2/2/2
32	STE	C	521	-	-	5/13/13/17	-
32	STE	c	524	-	-	5/7/9/17	-
22	CLA	d	405	-	1/1/20/20	10/37/115/115	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
22	CLA	c	509	-	1/1/20/20	11/37/115/115	-
33	LHG	D	409	-	-	16/51/51/53	-
32	STE	C	522	-	-	4/7/9/17	-
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
22	CLA	a	404	-	1/1/20/20	9/37/115/115	-
22	CLA	B	612	-	1/1/20/20	12/37/115/115	-
24	BCR	c	514	-	-	11/29/63/63	0/2/2/2
22	CLA	c	510	-	1/1/20/20	16/37/115/115	-
29	DGD	a	412	-	-	27/45/45/95	-
32	STE	d	413	-	-	9/12/14/17	-
22	CLA	b	616	-	1/1/19/20	7/31/109/115	-
22	CLA	b	614	-	1/1/20/20	17/37/115/115	-
29	DGD	c	518	-	-	23/51/91/95	0/2/2/2
32	STE	T	103	-	-	7/12/12/17	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
27	LMG	M	101	-	-	23/46/66/70	0/1/1/1
32	STE	j	101	-	-	3/7/9/17	-
22	CLA	d	403	-	-	10/37/115/115	-
29	DGD	h	102	-	-	15/51/91/95	0/2/2/2
24	BCR	c	515	-	-	4/29/63/63	0/2/2/2
22	CLA	B	609	-	-	5/37/115/115	-
32	STE	H	103	-	-	6/15/15/17	-
22	CLA	b	603	-	1/1/20/20	4/37/115/115	-
22	CLA	B	602	-	-	9/37/115/115	-
22	CLA	B	604	-	1/1/20/20	14/37/115/115	-
22	CLA	c	511	3	1/1/20/20	11/37/115/115	-
27	LMG	b	620	-	-	14/46/66/70	0/1/1/1
32	STE	t	102	-	-	4/9/11/17	-
24	BCR	B	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	m	101	-	-	5/7/9/17	-
22	CLA	D	403	-	1/1/20/20	4/37/115/115	-
28	SQD	A	413	-	-	13/39/39/69	-
29	DGD	c	519	-	-	19/51/91/95	0/2/2/2
32	STE	B	620	-	-	8/12/14/17	-
22	CLA	B	611	-	1/1/20/20	8/37/115/115	-
28	SQD	B	623	-	-	26/49/69/69	0/1/1/1
22	CLA	C	503	-	1/1/20/20	7/37/115/115	-
32	STE	b	621	-	-	10/15/17/17	-
22	CLA	B	606	-	1/1/20/20	13/37/115/115	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
22	CLA	B	601	37	1/1/20/20	18/37/115/115	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	b	607	37	1/1/20/20	17/37/115/115	-
24	BCR	T	101	-	-	10/29/63/63	0/2/2/2
32	STE	c	521	-	-	8/15/17/17	-
23	PHO	d	401	-	-	4/53/103/103	0/5/6/6
24	BCR	b	618	-	-	7/29/63/63	0/2/2/2
32	STE	E	103	-	-	6/7/9/17	-
32	STE	B	627	-	-	4/7/9/17	-
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
32	STE	T	102	-	-	5/13/13/17	-
28	SQD	f	102	-	-	11/36/56/69	0/1/1/1
22	CLA	B	608	-	1/1/20/20	3/37/115/115	-
22	CLA	b	604	-	1/1/20/20	9/37/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
29	DGD	H	102	-	-	22/51/91/95	0/2/2/2
22	CLA	B	616	-	1/1/19/20	12/31/109/115	-
22	CLA	C	506	-	1/1/20/20	12/37/115/115	-
33	LHG	B	622	-	-	18/53/53/53	-
29	DGD	c	517	-	-	27/51/91/95	0/2/2/2
22	CLA	b	611	-	1/1/20/20	7/37/115/115	-
32	STE	I	101	-	-	8/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	501	-	1/1/20/20	4/37/115/115	-
27	LMG	b	622	-	-	29/50/70/70	0/1/1/1
32	STE	b	624	-	-	5/15/17/17	-
24	BCR	a	405	-	-	4/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/20/20	12/37/115/115	-
22	CLA	c	512	-	1/1/20/20	21/37/115/115	-
22	CLA	B	614	-	1/1/20/20	14/37/115/115	-
24	BCR	h	101	-	-	10/29/63/63	0/2/2/2
24	BCR	b	619	-	-	5/29/63/63	0/2/2/2
22	CLA	C	510	-	1/1/20/20	10/37/115/115	-
33	LHG	l	101	-	-	28/53/53/53	-
32	STE	b	623	-	-	6/11/13/17	-
22	CLA	c	513	-	1/1/20/20	6/37/115/115	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
33	LHG	e	101	-	-	22/46/46/53	-
22	CLA	D	404	-	-	9/37/115/115	-
22	CLA	A	403	37	-	11/37/115/115	-
22	CLA	b	615	-	1/1/20/20	11/37/115/115	-
22	CLA	b	605	-	1/1/20/20	10/37/115/115	-
22	CLA	A	402	-	1/1/20/20	4/37/115/115	-
22	CLA	b	608	-	1/1/20/20	8/37/115/115	-
22	CLA	C	504	37	1/1/18/20	8/30/108/115	-
32	STE	a	413	-	-	3/7/7/17	-
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
22	CLA	a	403	37	-	13/37/115/115	-
27	LMG	d	411	-	-	8/15/17/70	-
32	STE	D	411	-	-	10/15/17/17	-
22	CLA	a	402	-	1/1/20/20	7/37/115/115	-
22	CLA	B	603	-	1/1/20/20	12/37/115/115	-
23	PHO	A	404	-	-	5/53/103/103	0/5/6/6
22	CLA	b	613	-	1/1/20/20	5/37/115/115	-
22	CLA	C	507	37	1/1/20/20	5/37/115/115	-
22	CLA	b	610	37	1/1/20/20	3/37/115/115	-
33	LHG	E	102	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	404	37	1/1/20/20	7/37/115/115	-
36	HEC	v	201	17	-	0/6/54/54	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
32	STE	J	101	-	-	3/7/9/17	-
32	STE	l	102	-	-	9/15/15/17	-

The worst 5 of 870 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C4B-NB	9.27	1.43	1.35
22	B	615	CLA	C4B-NB	8.98	1.43	1.35
22	b	604	CLA	C4B-NB	8.35	1.42	1.35
22	B	602	CLA	C4B-NB	8.13	1.42	1.35
22	c	504	CLA	C4B-NB	7.81	1.42	1.35

The worst 5 of 1296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	9.93	111.17	106.71
22	c	511	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	B	616	CLA	C4A-NA-C1A	9.36	110.91	106.71
22	C	507	CLA	C4A-NA-C1A	9.33	110.90	106.71
28	L	101	SQD	O6-C1-C2	9.25	122.74	108.30

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	A	410	CLA	ND
22	B	601	CLA	ND
22	B	603	CLA	ND

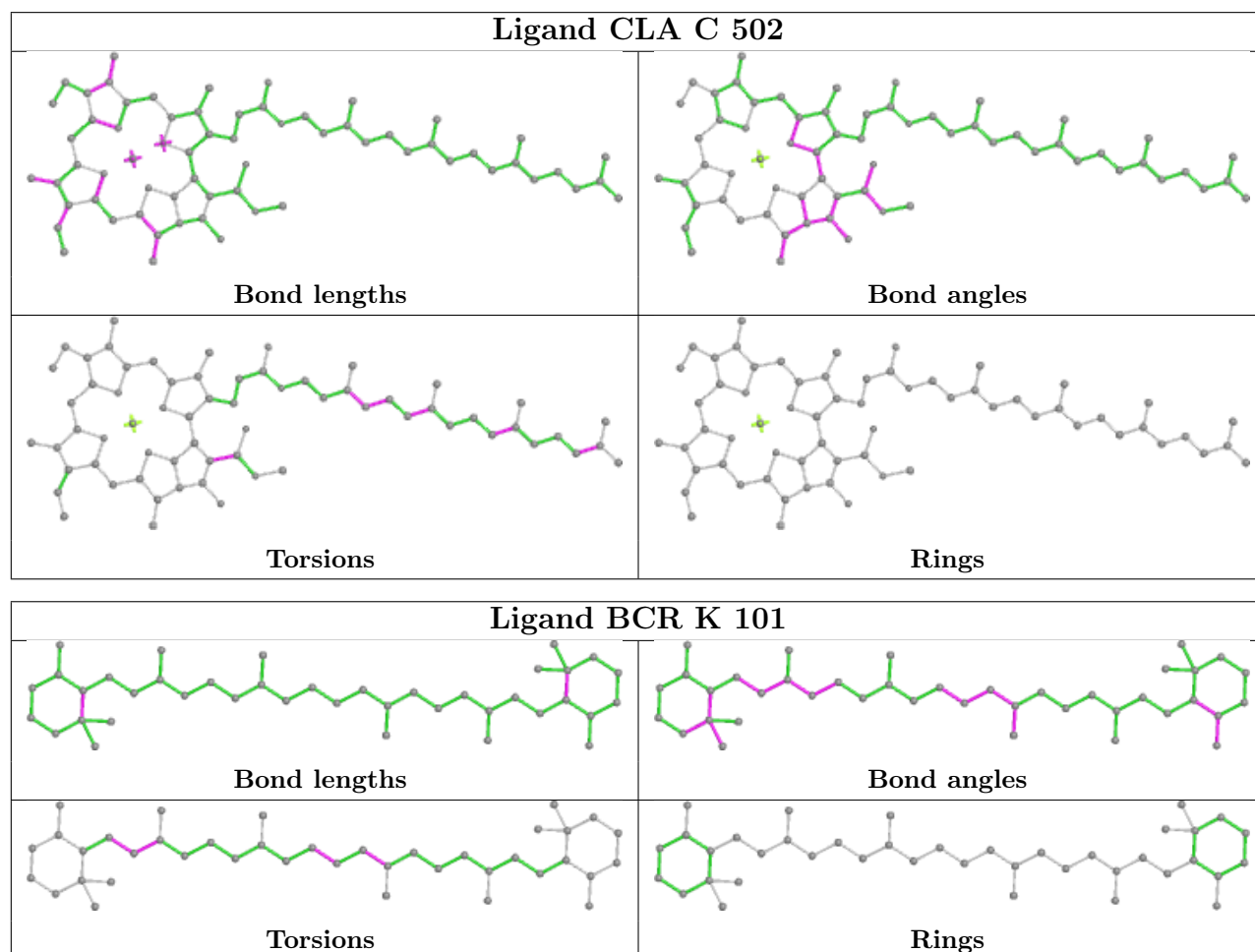
5 of 1891 torsion outliers are listed below:

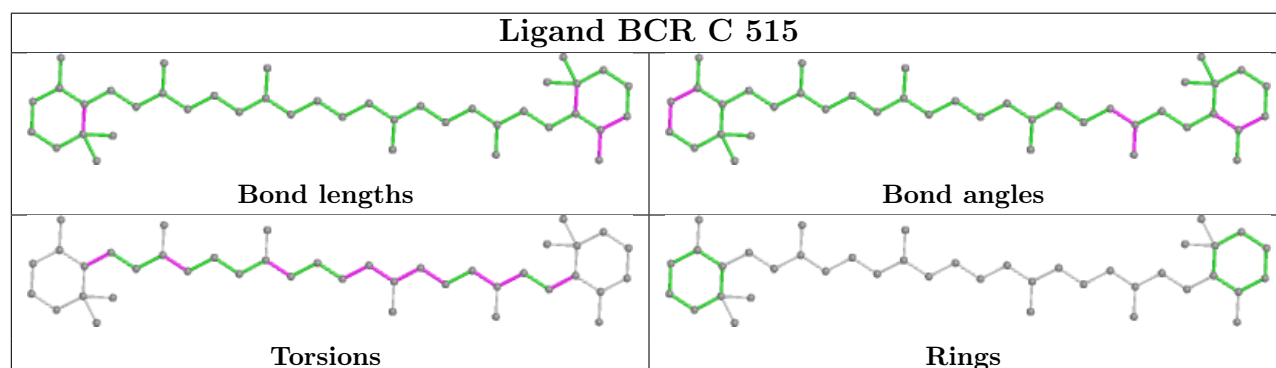
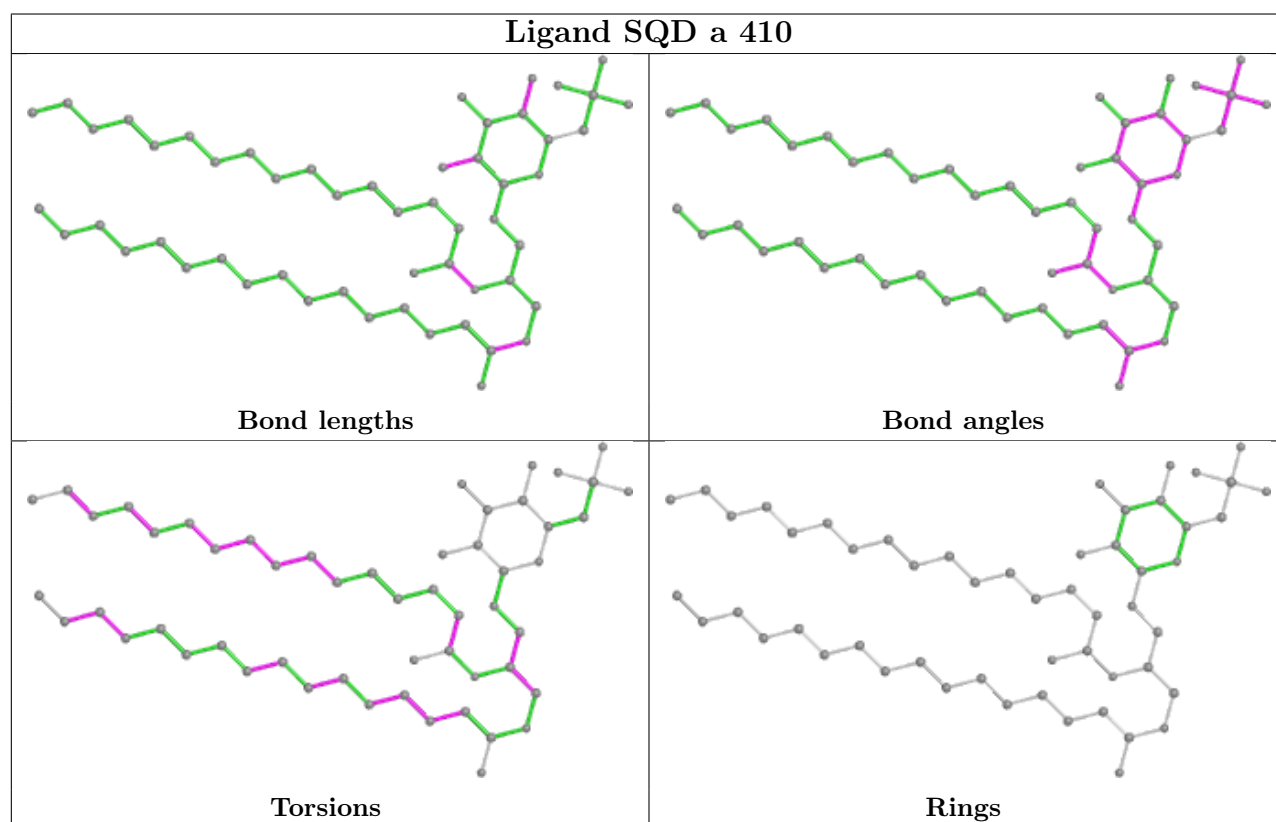
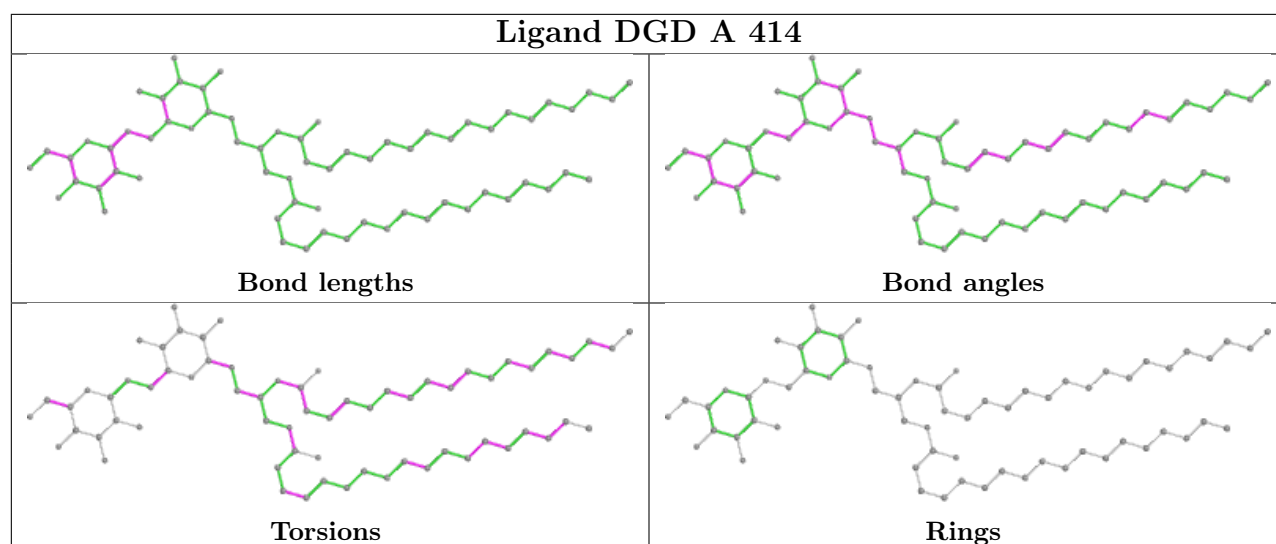
Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
22	A	410	CLA	CHA-CBD-CGD-O1D
22	A	410	CLA	CHA-CBD-CGD-O2D
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

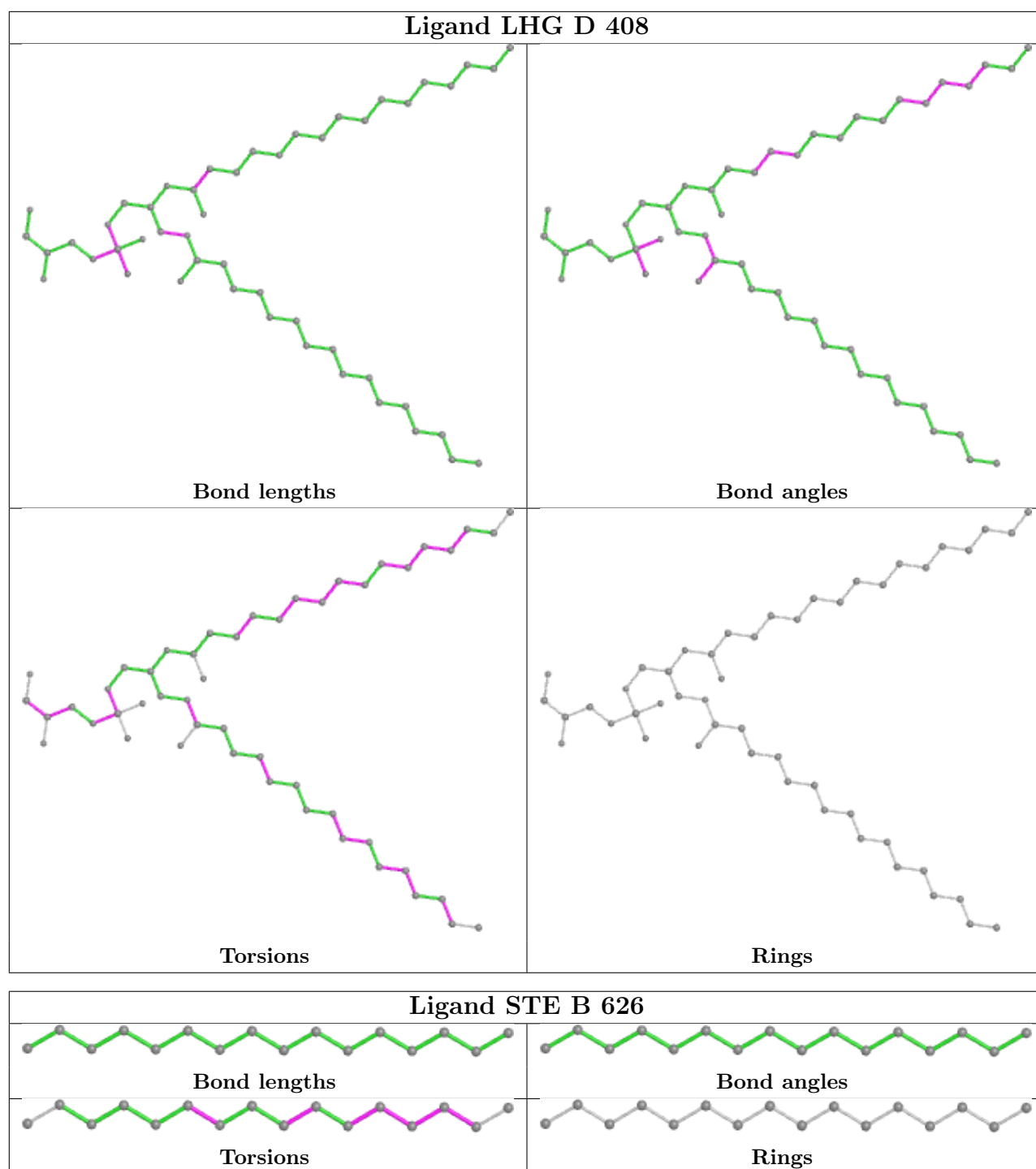
No monomer is involved in short contacts.

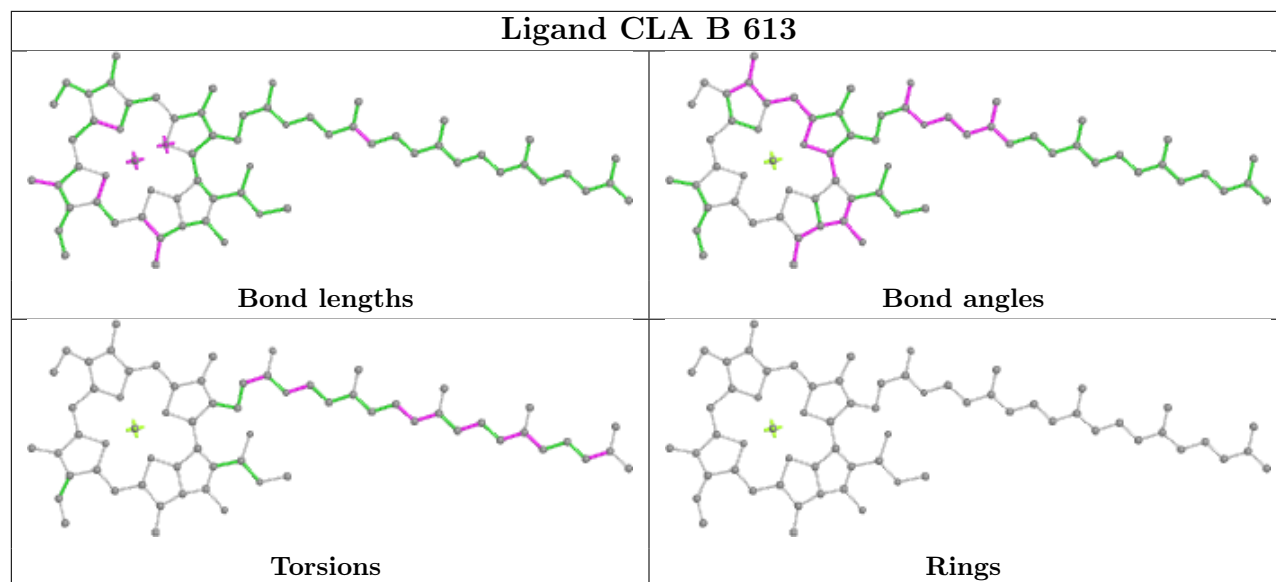
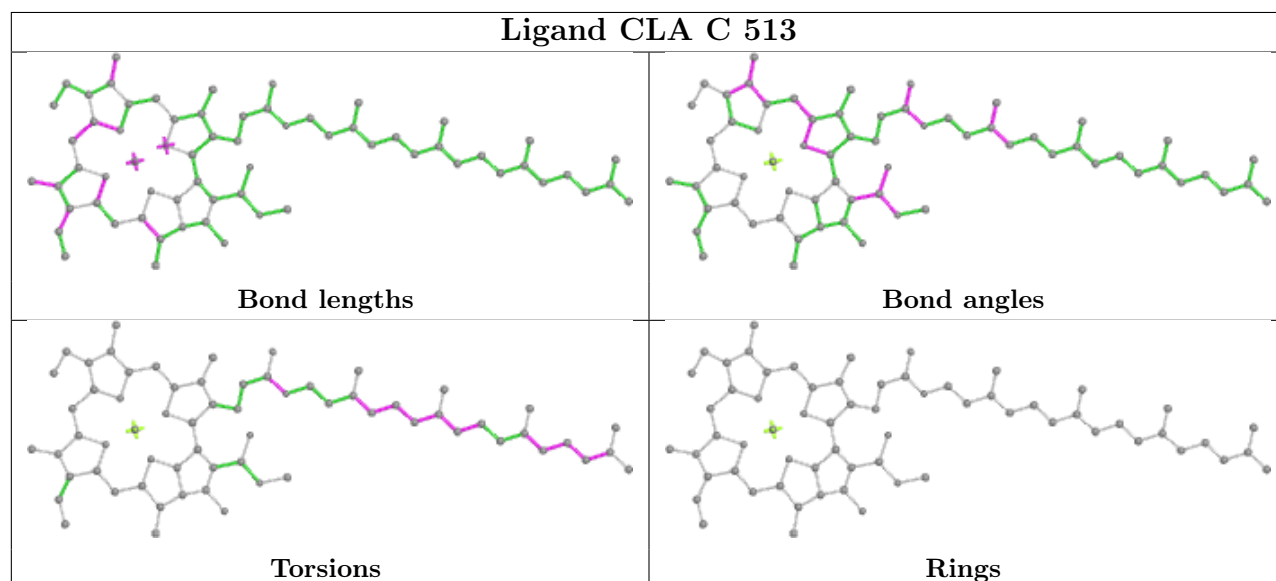
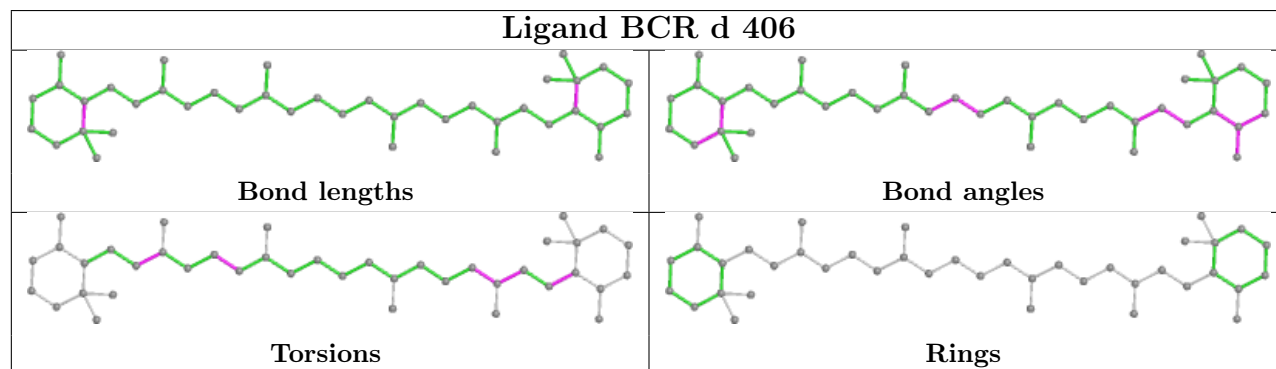
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



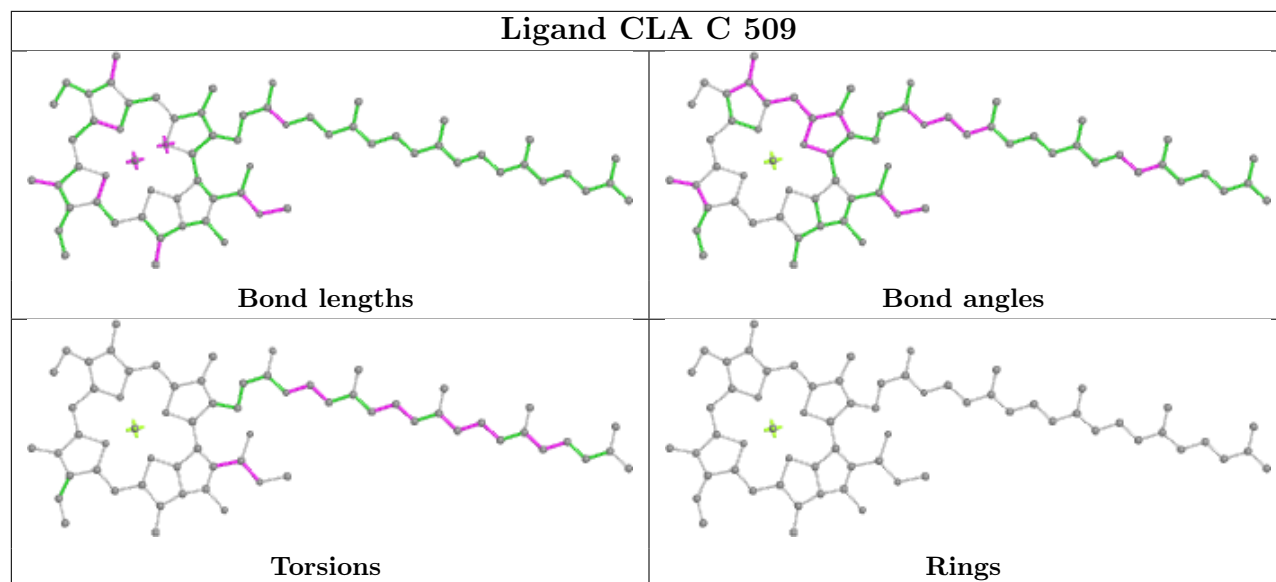




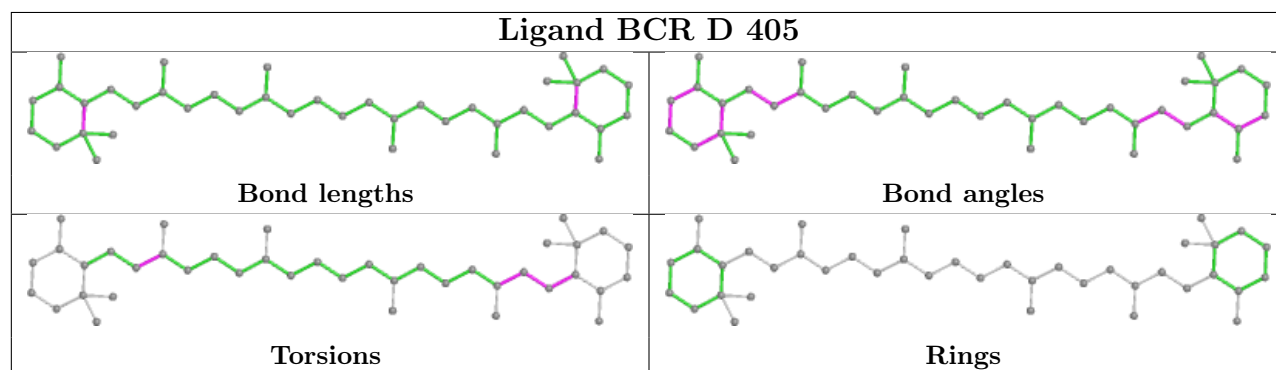


**Ligand CLA B 613****Ligand CLA C 513****Ligand BCR d 406**

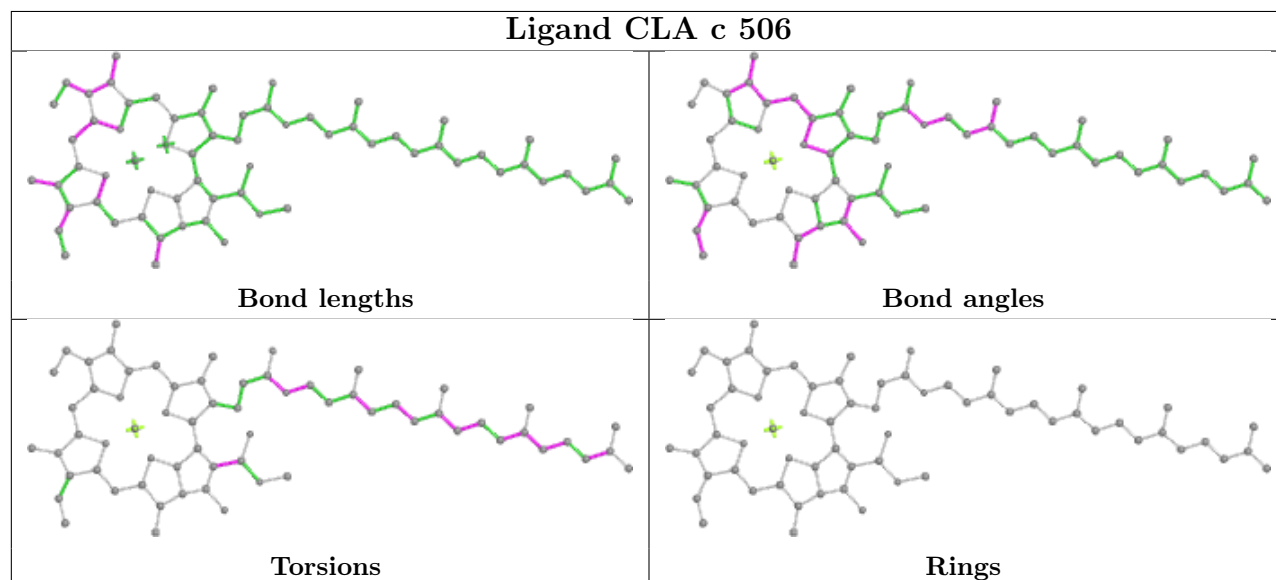
## Ligand CLA C 509

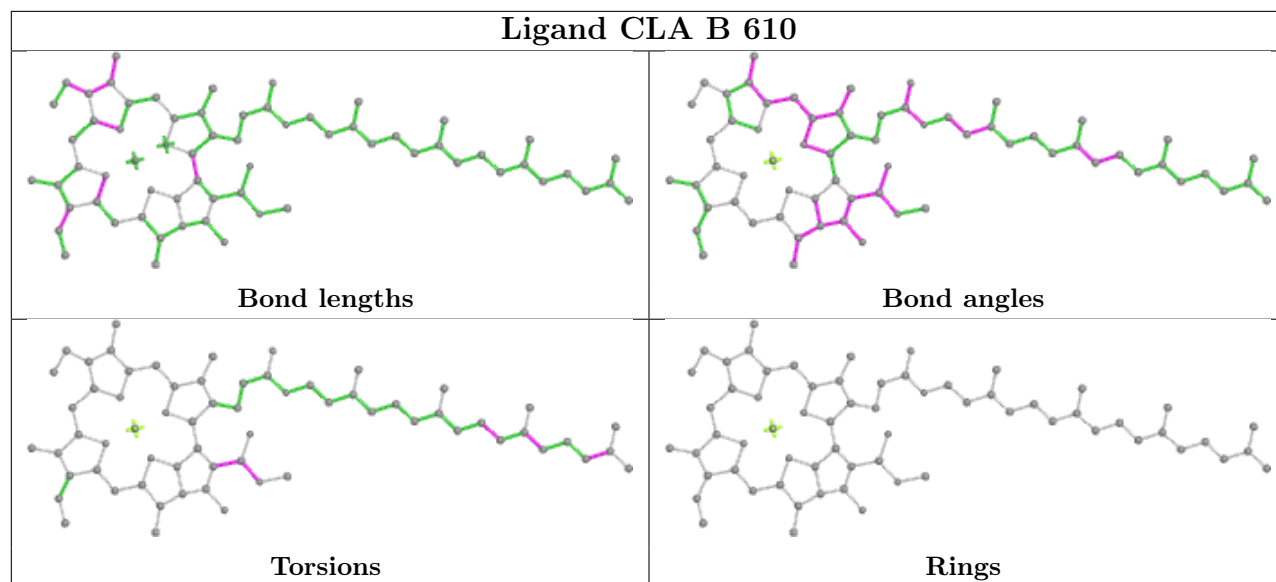
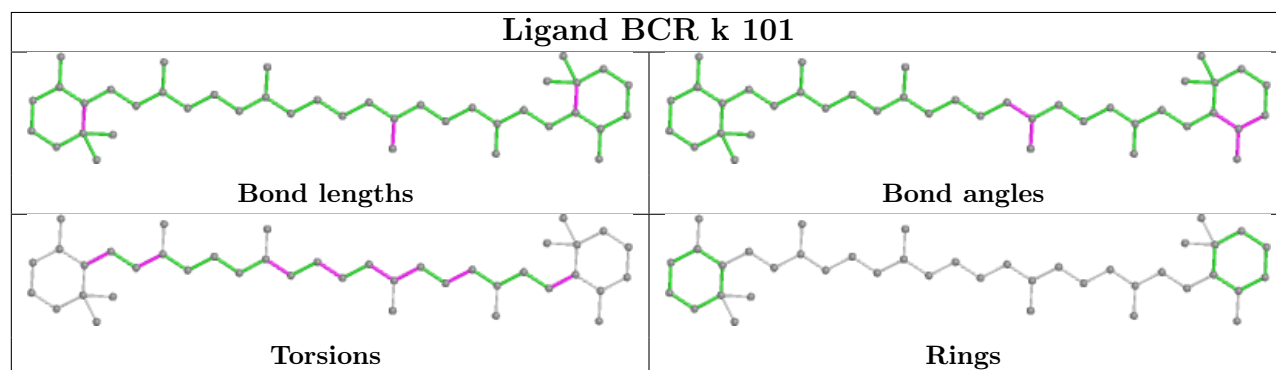
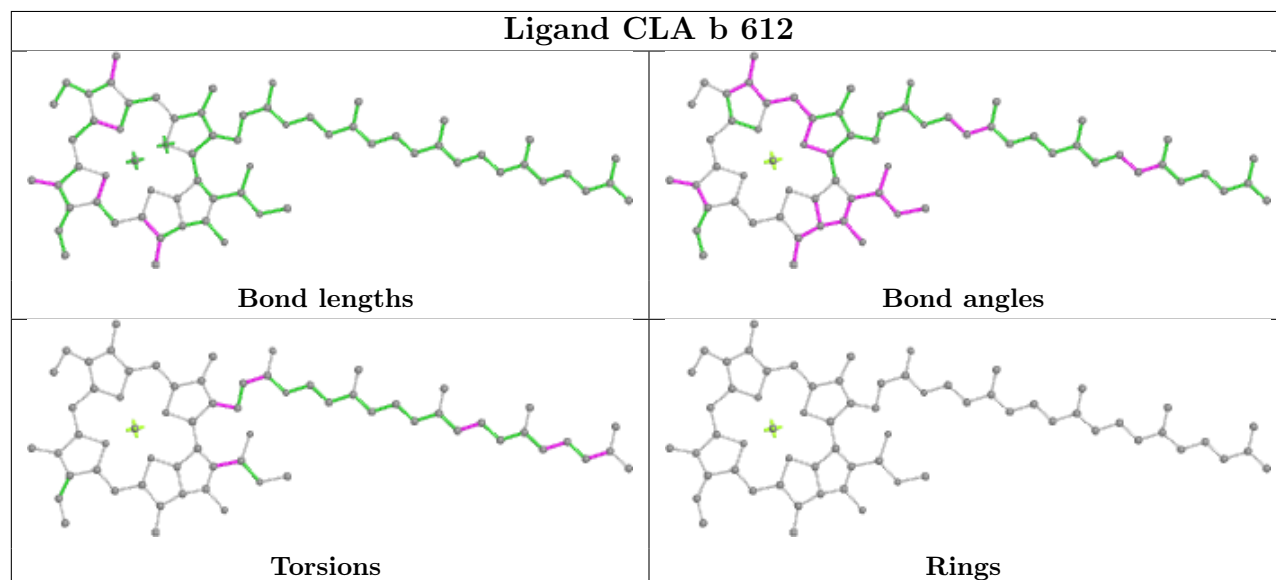


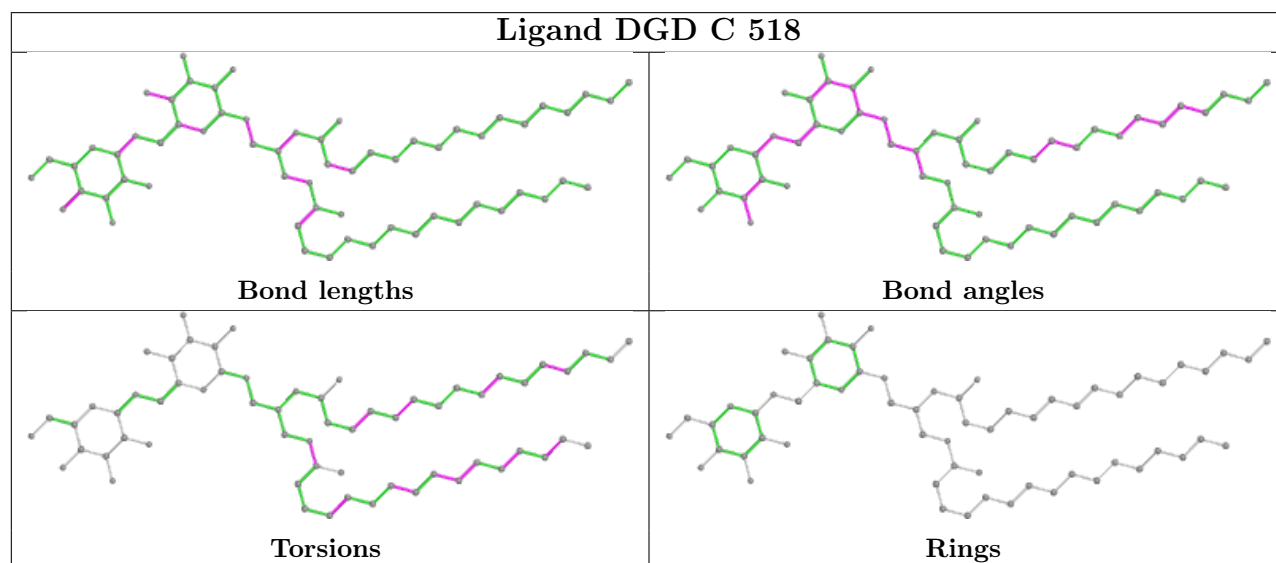
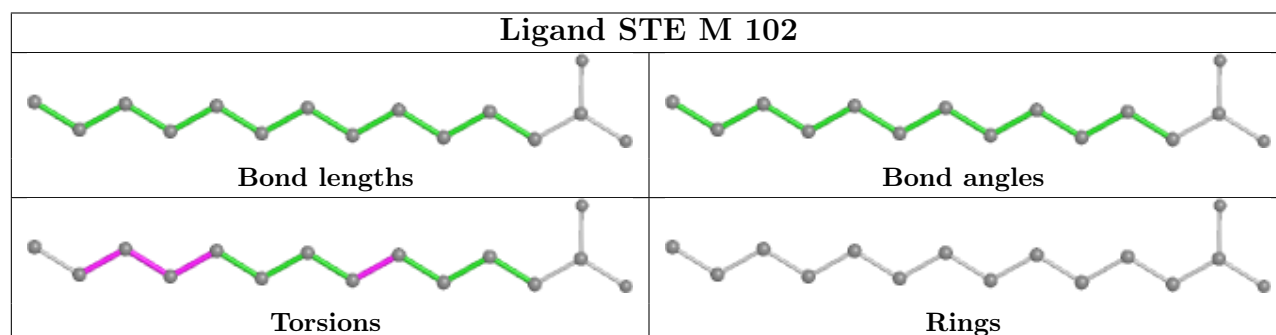
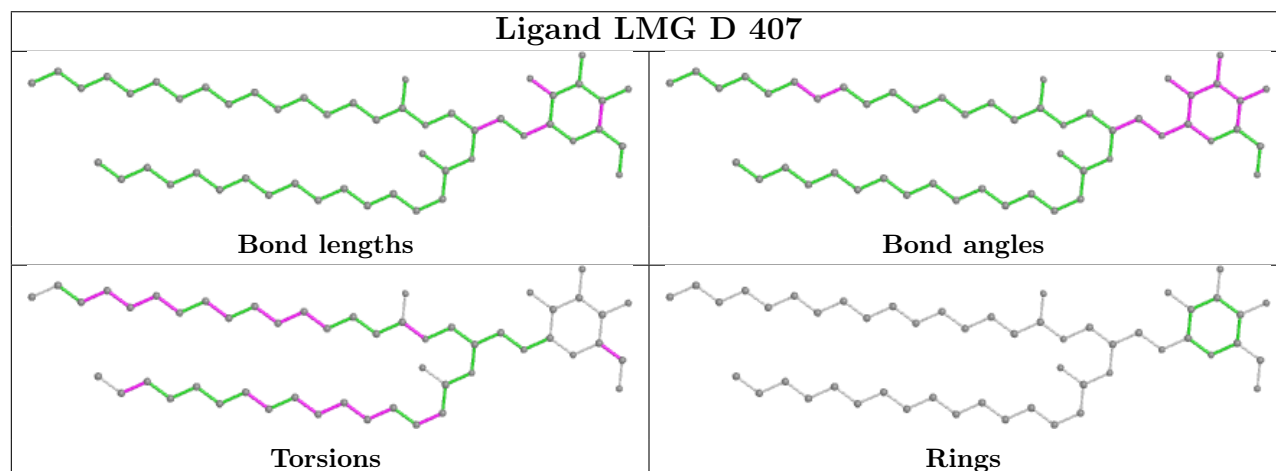
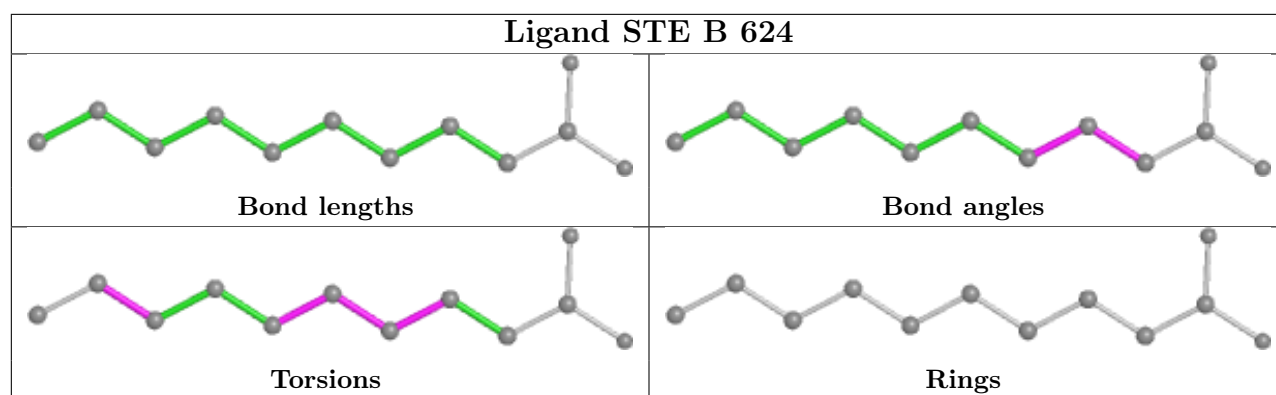
## Ligand BCR D 405



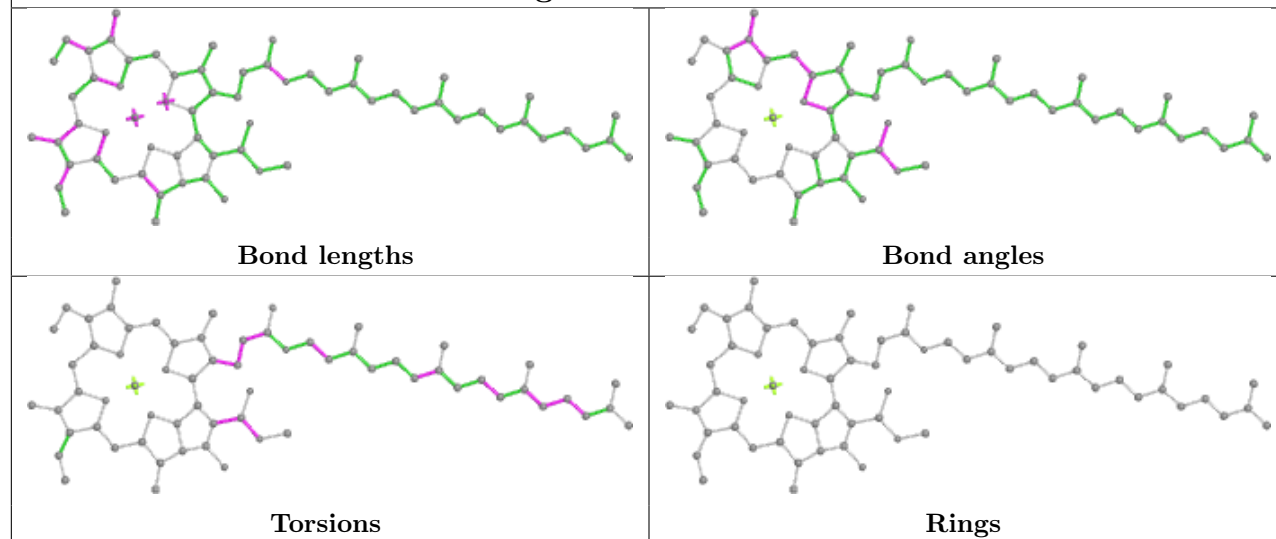
## Ligand CLA c 506



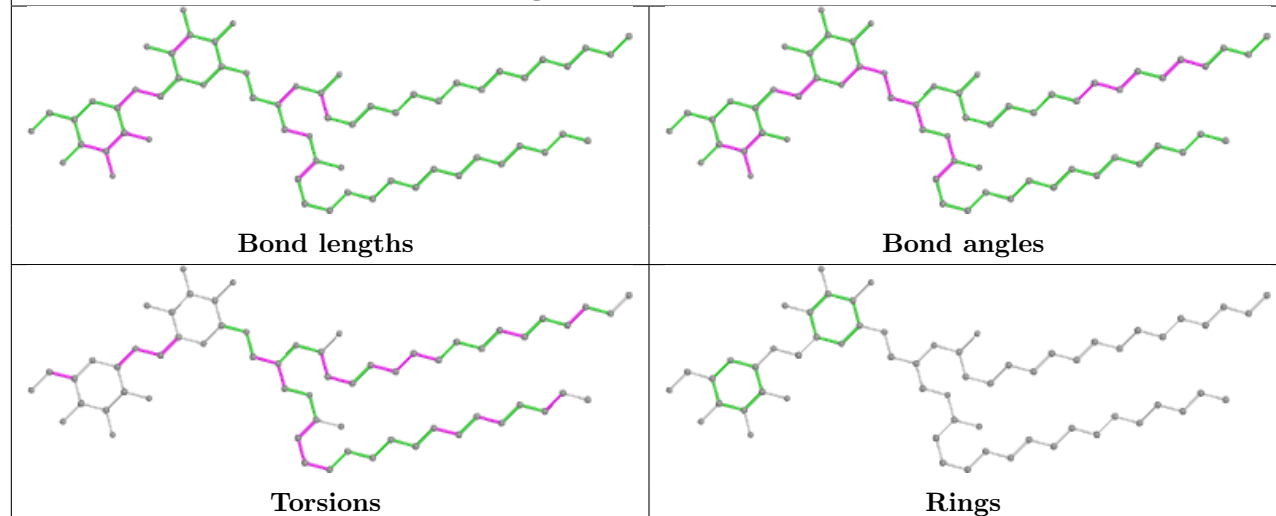
**Ligand CLA B 610****Ligand BCR k 101****Ligand CLA b 612**



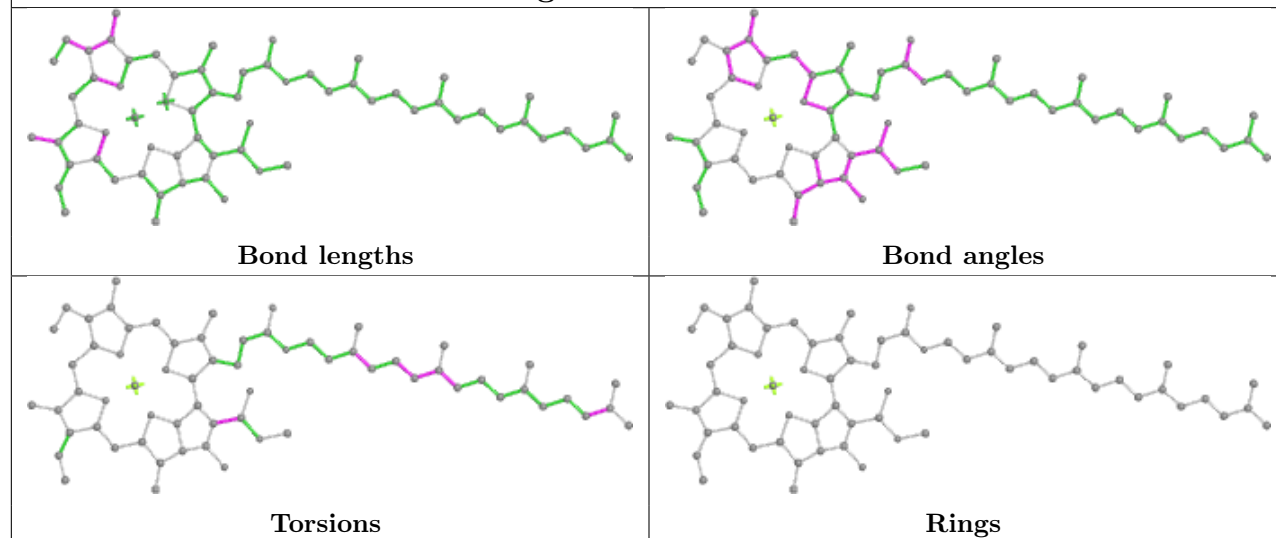
## Ligand CLA b 601



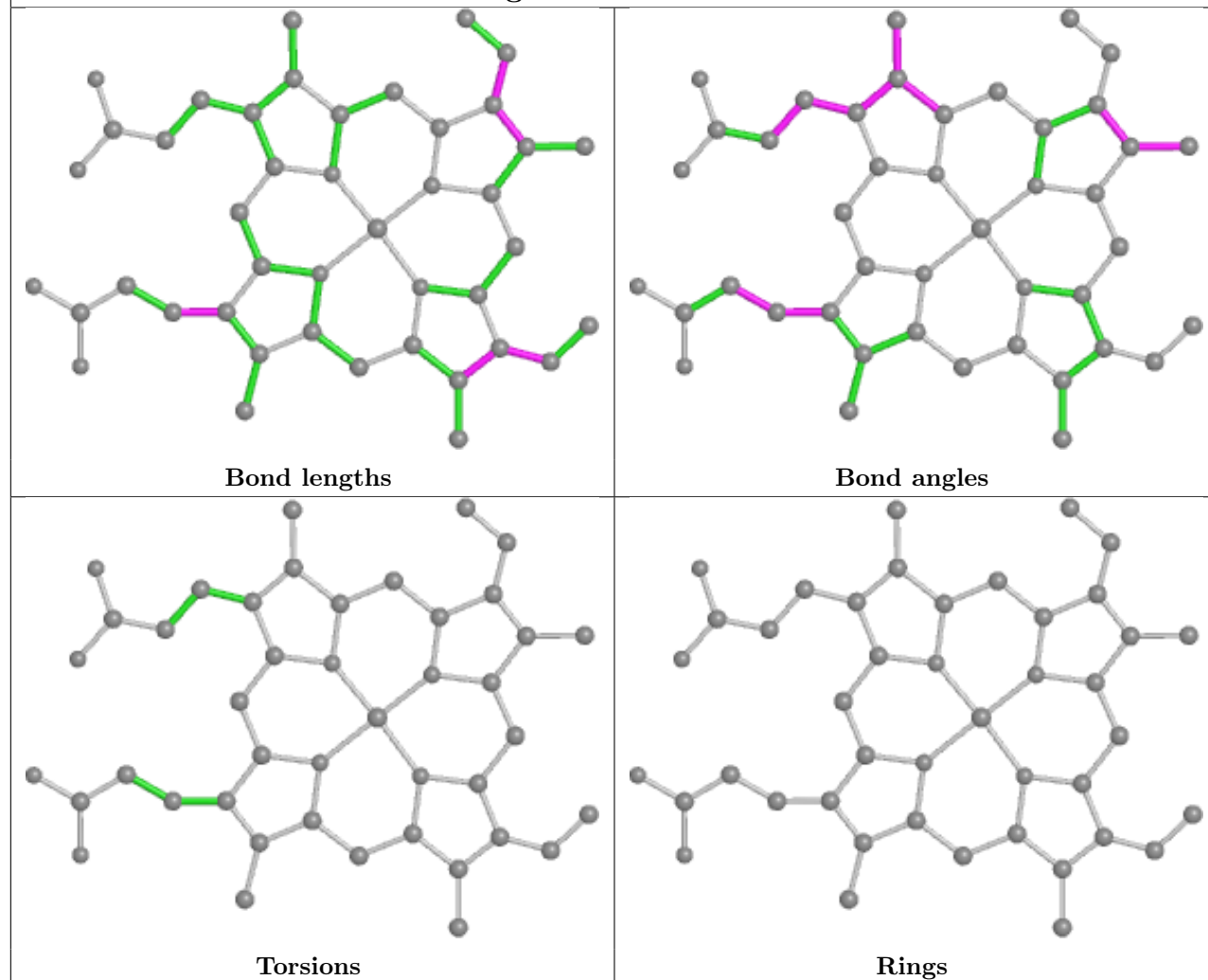
## Ligand DGD C 516



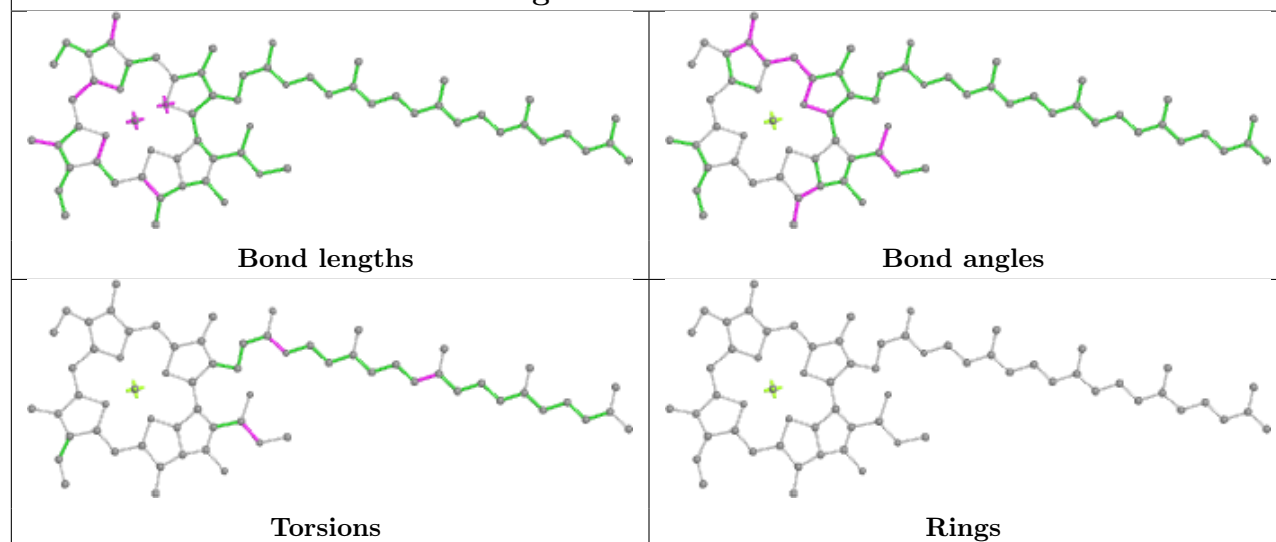
## Ligand CLA c 505

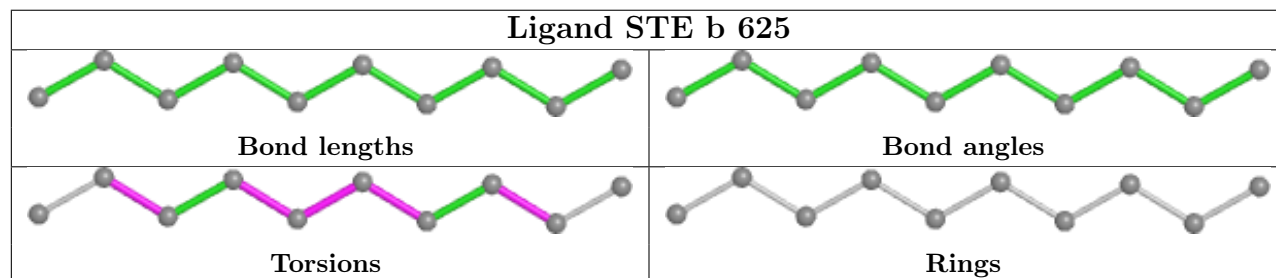
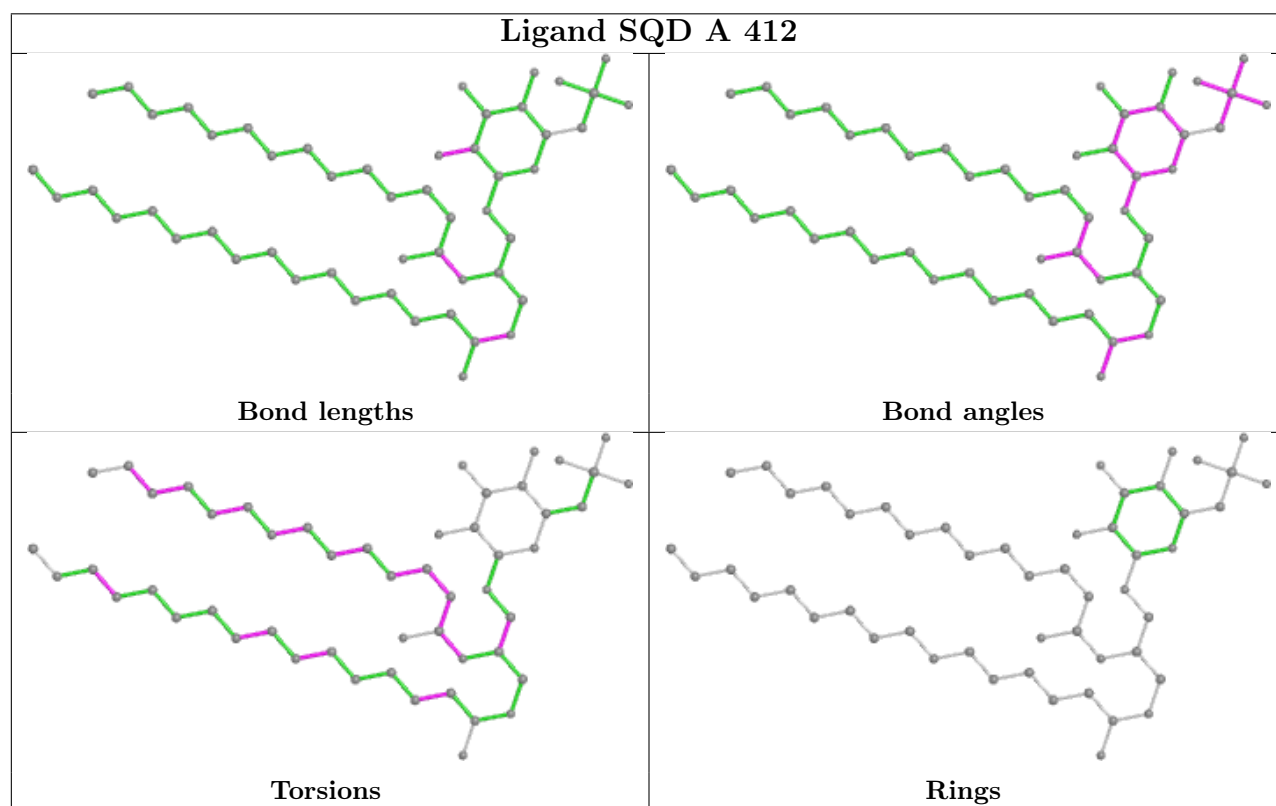
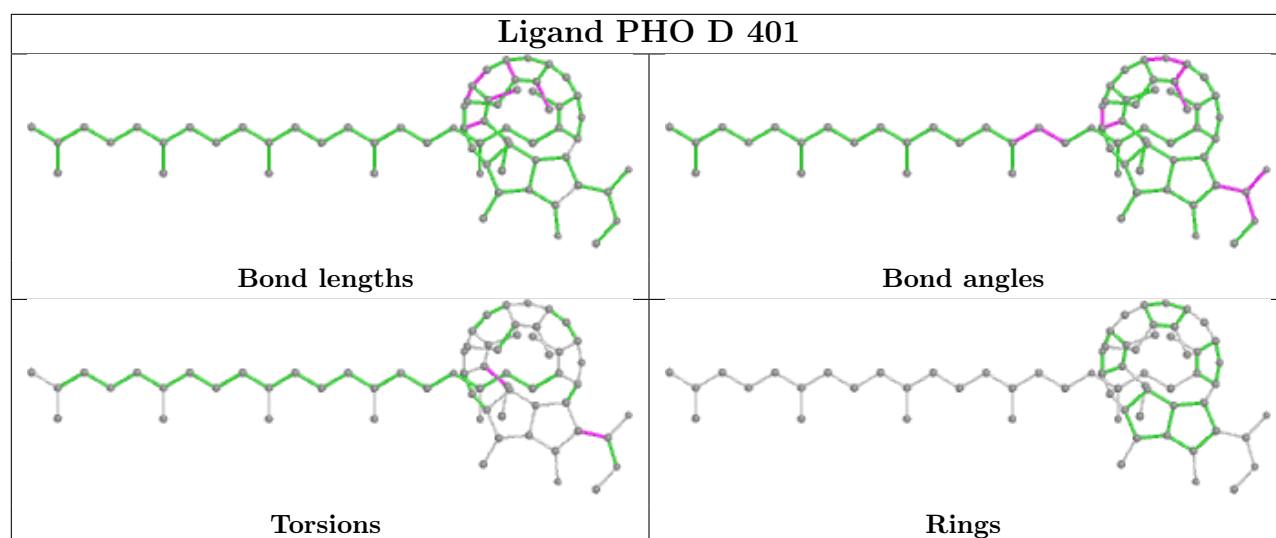


## Ligand HEM f 101

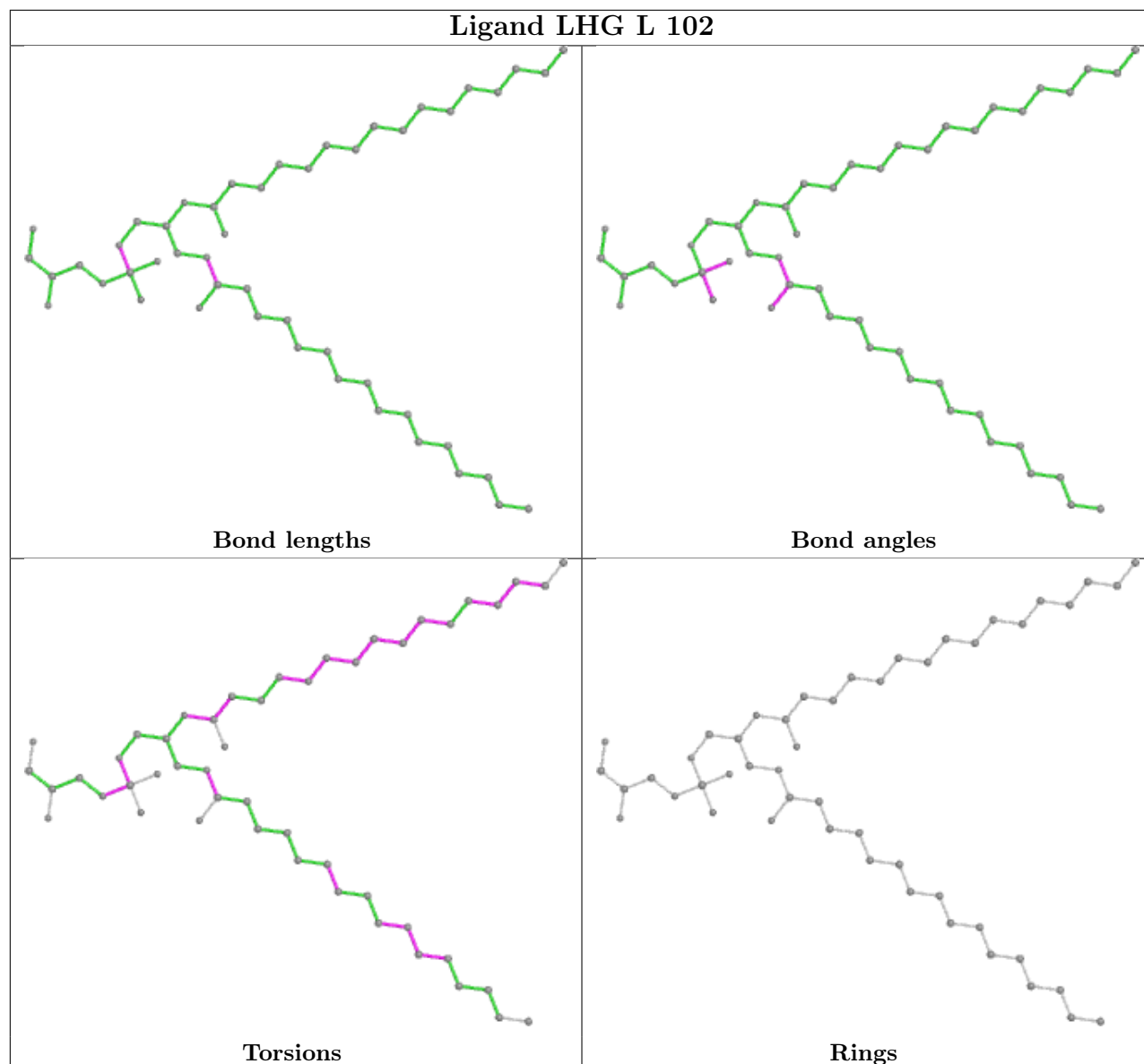
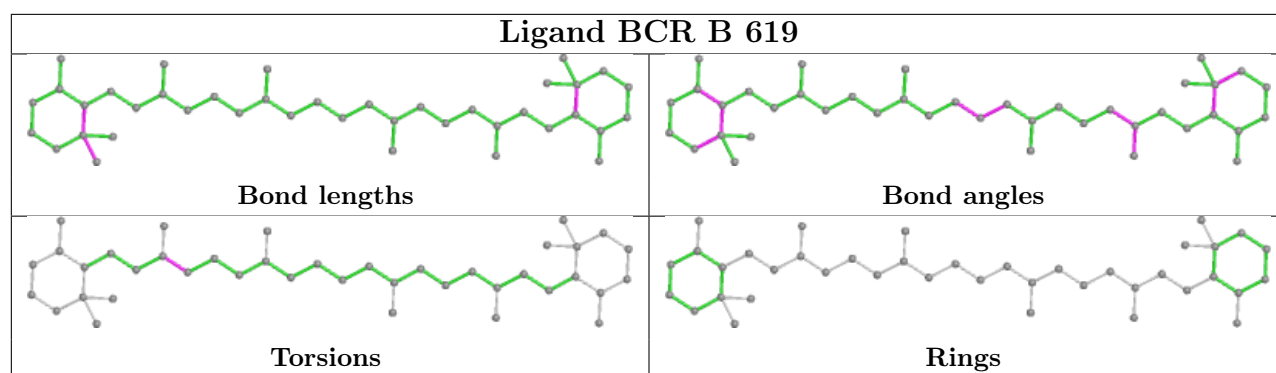


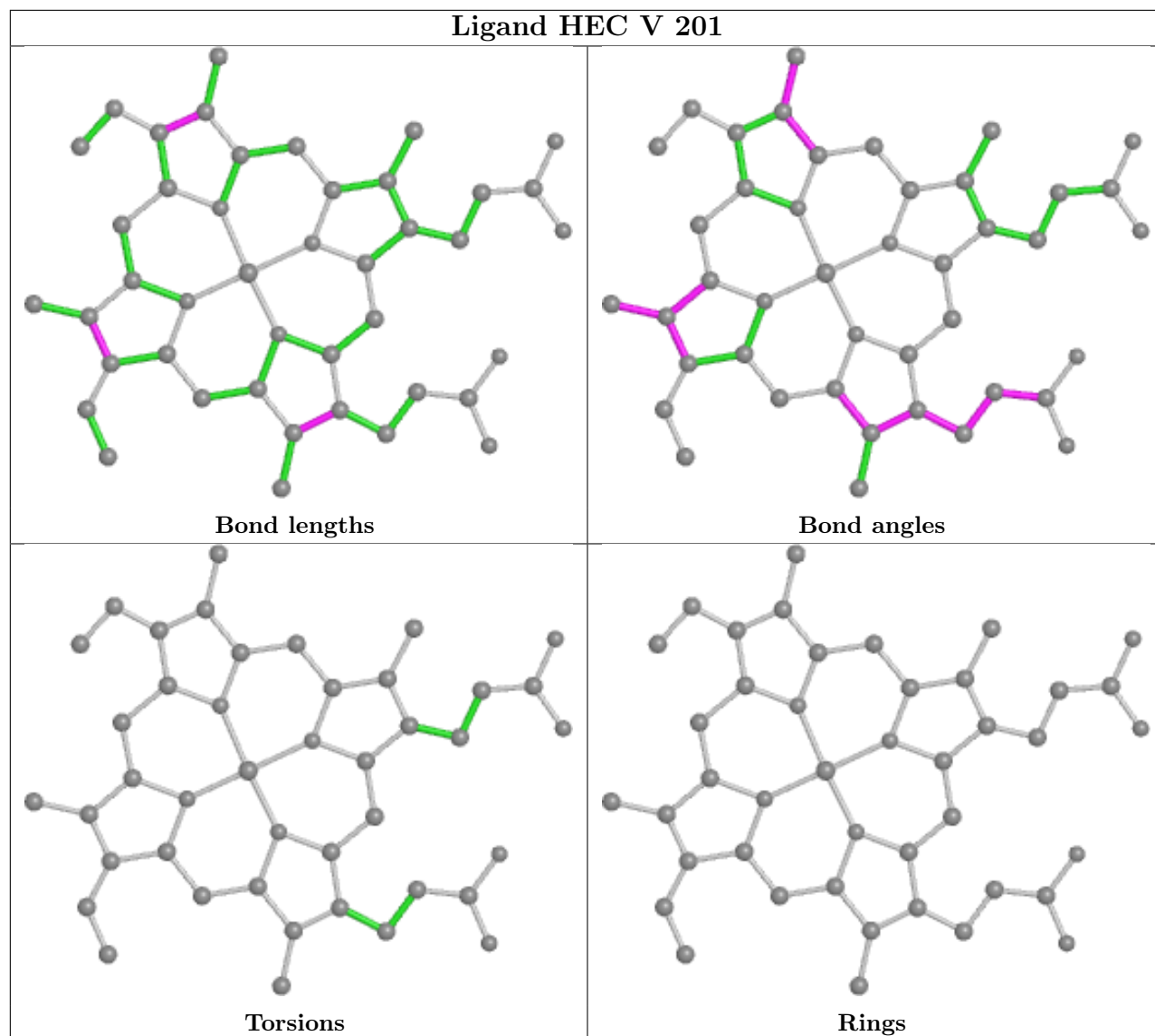
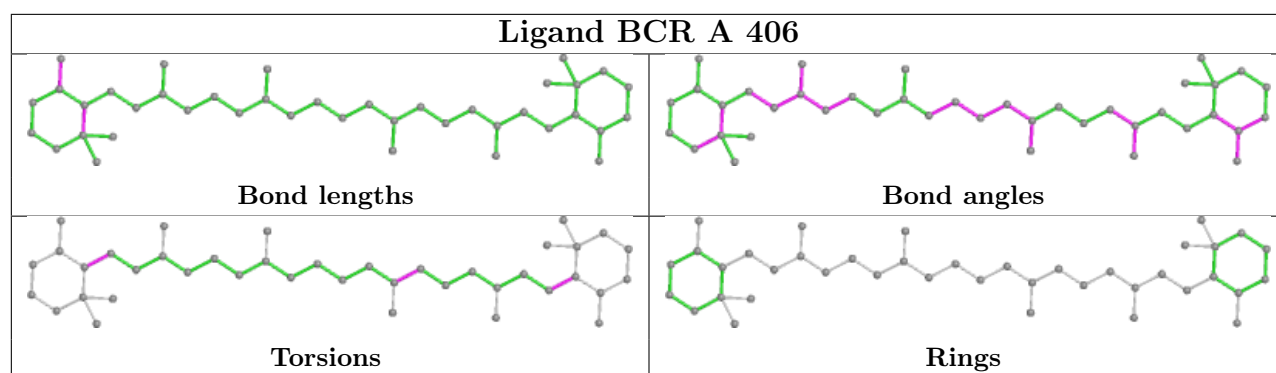
## Ligand CLA C 511



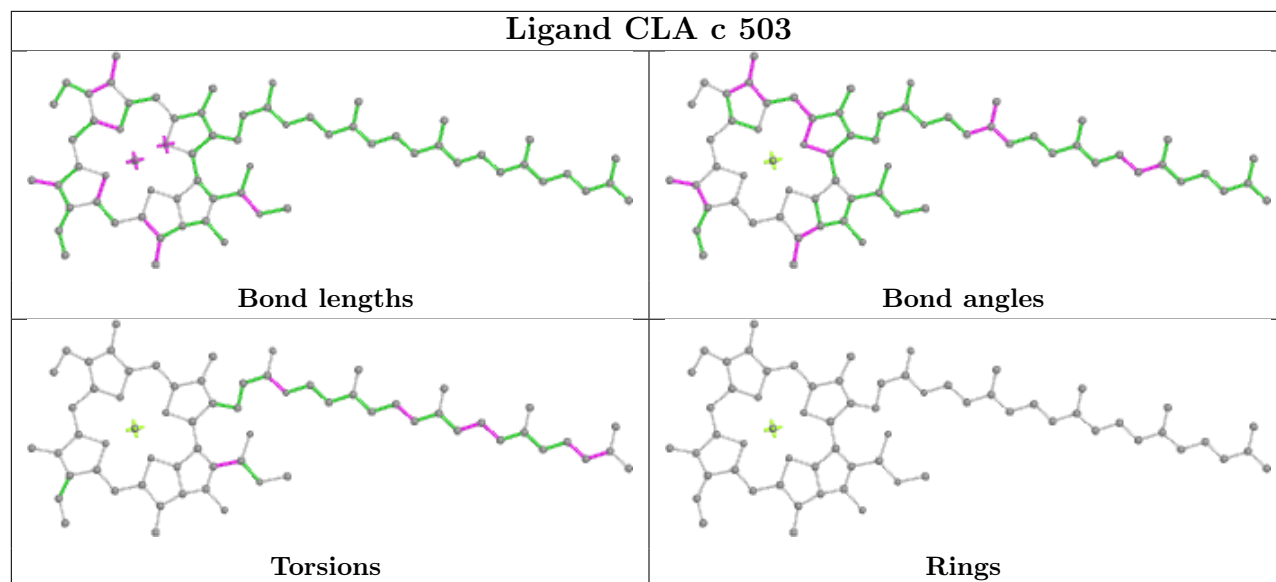




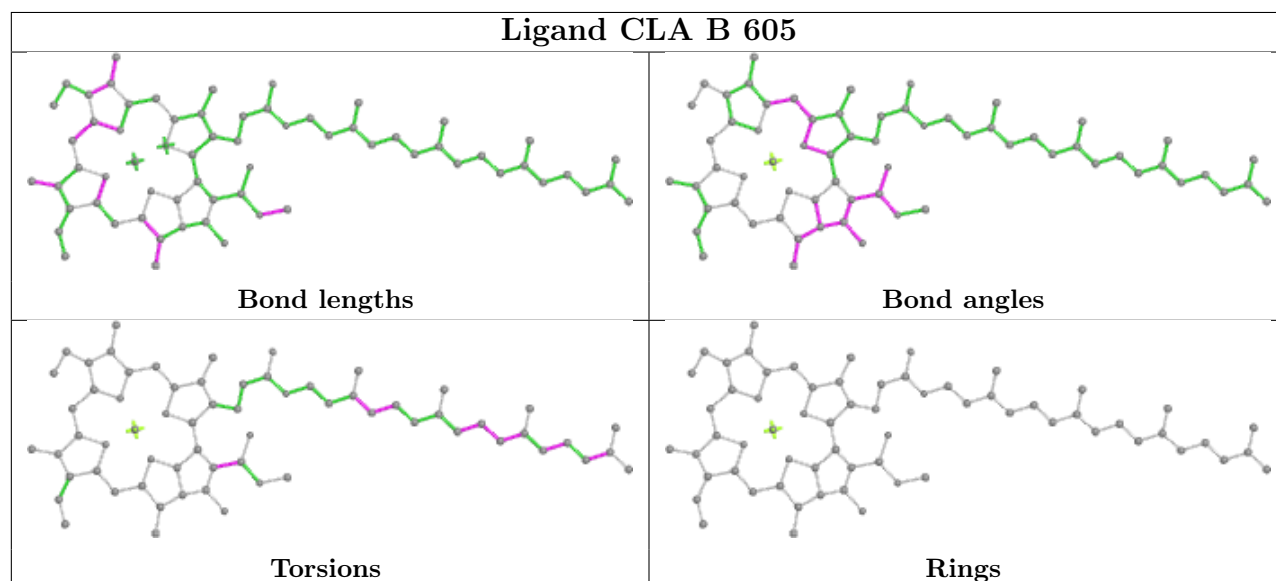




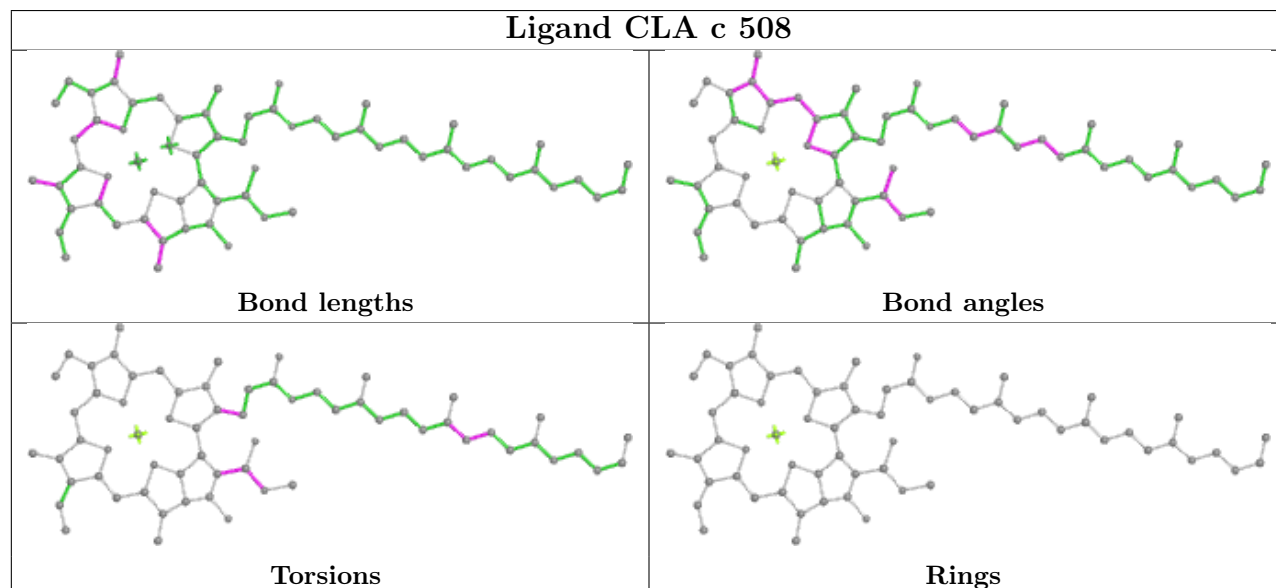
## Ligand CLA c 503

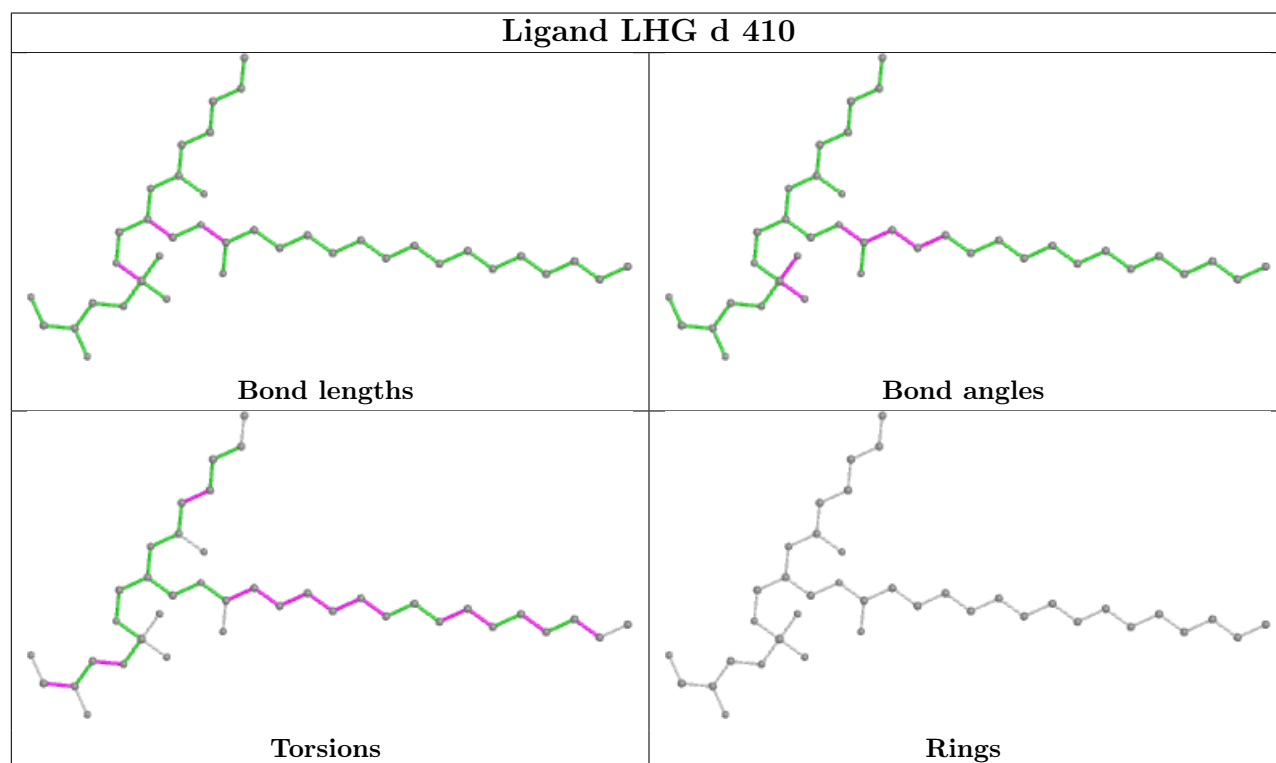
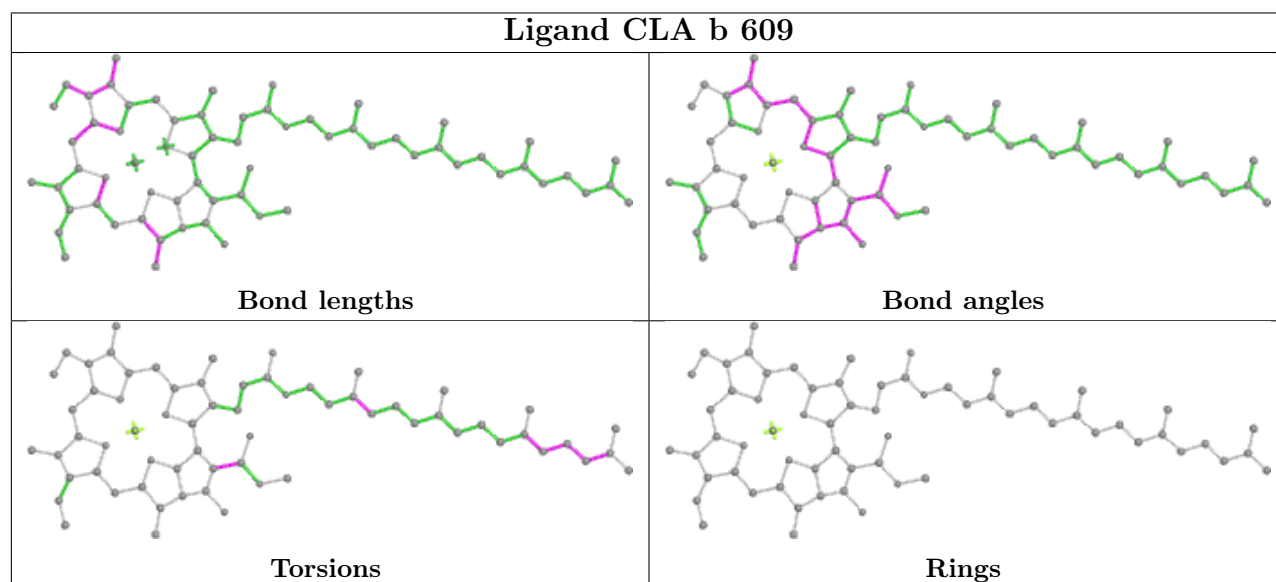
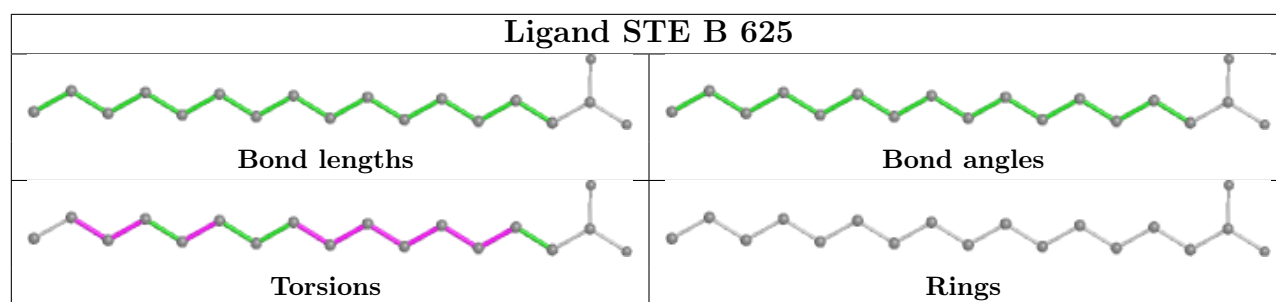


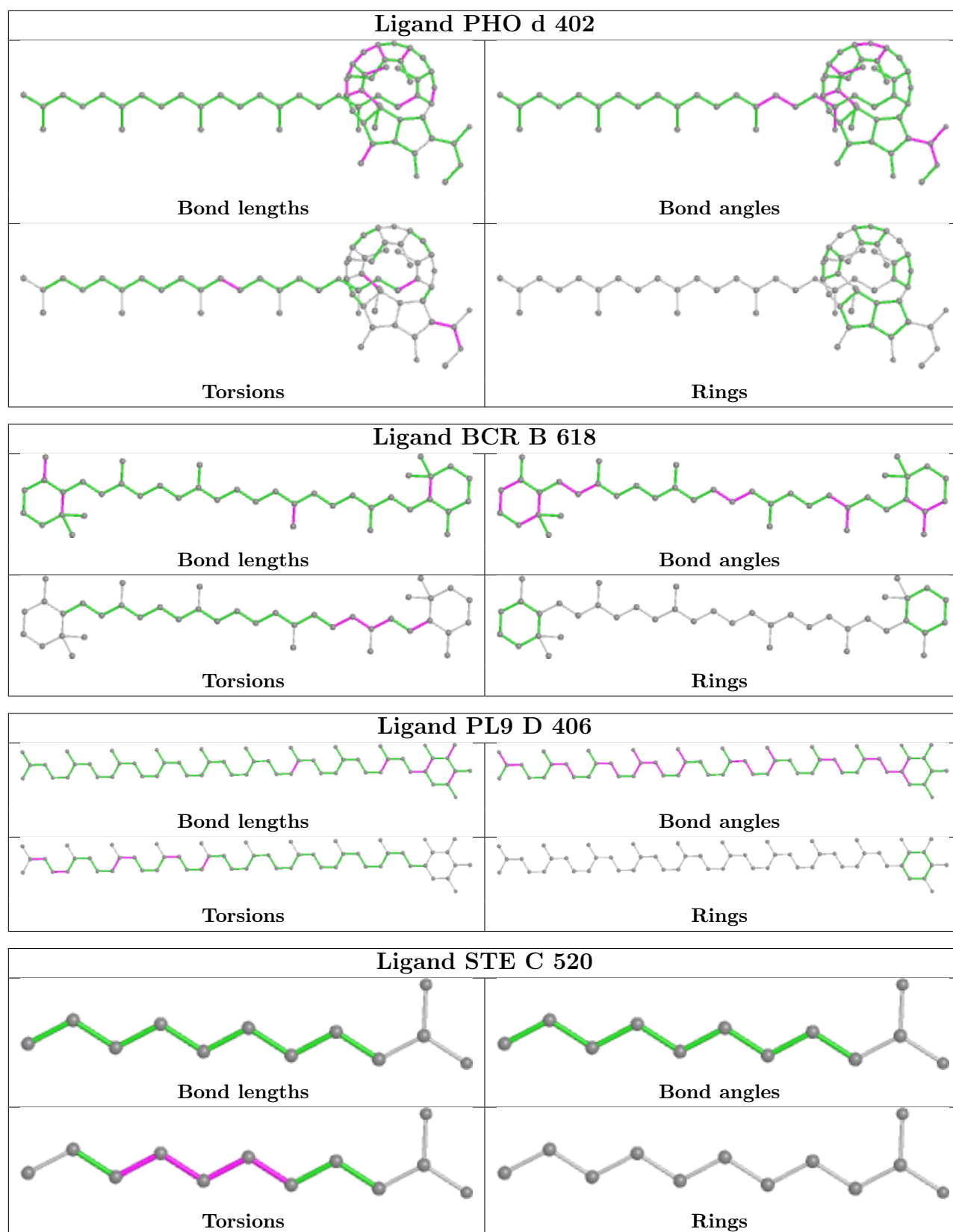
## Ligand CLA B 605

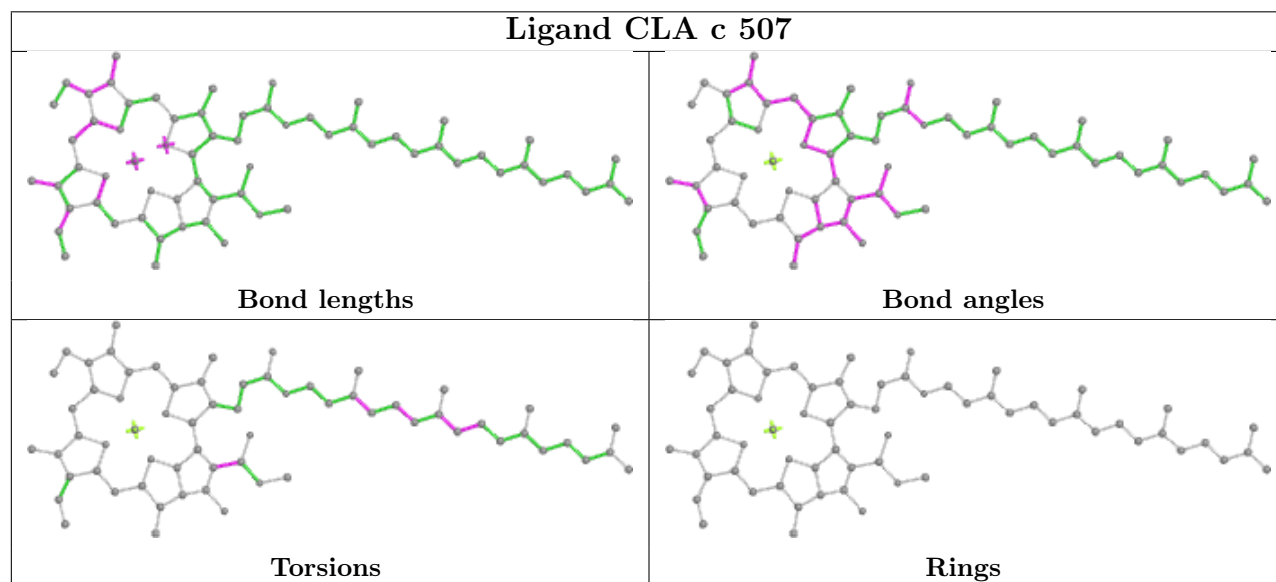
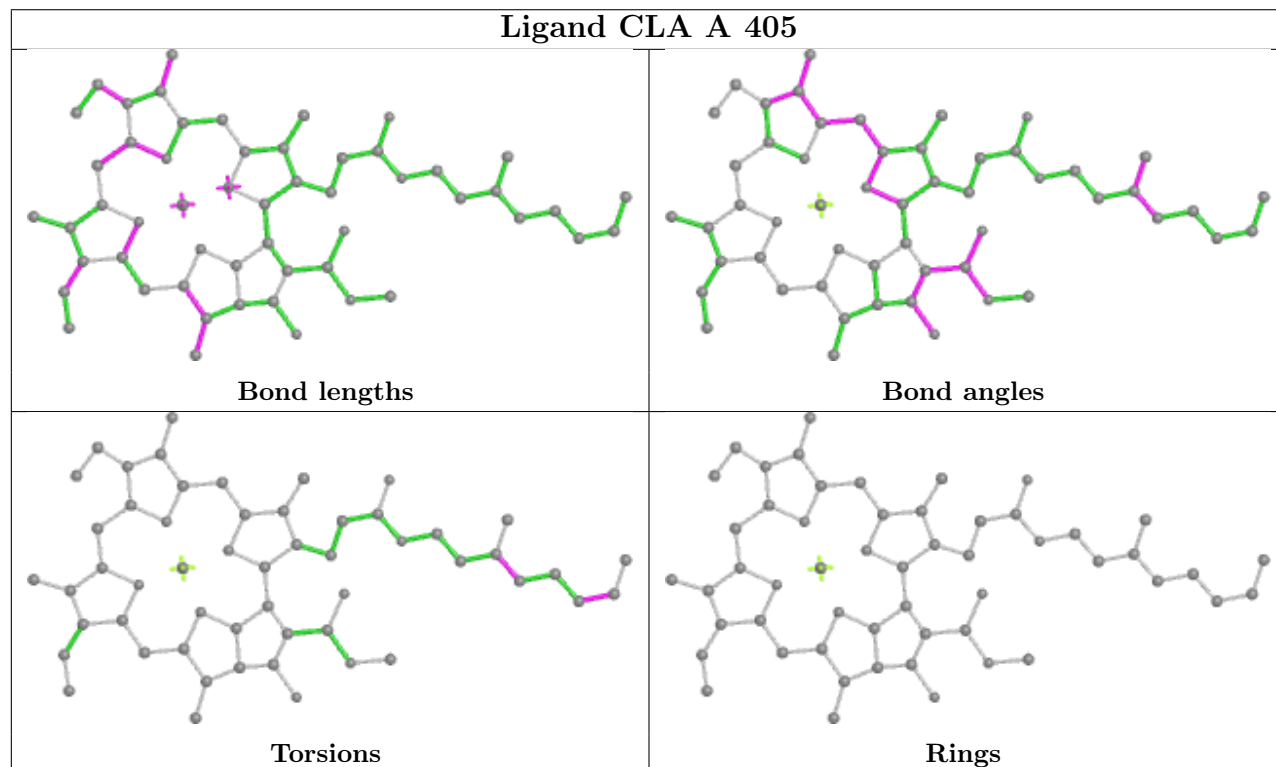
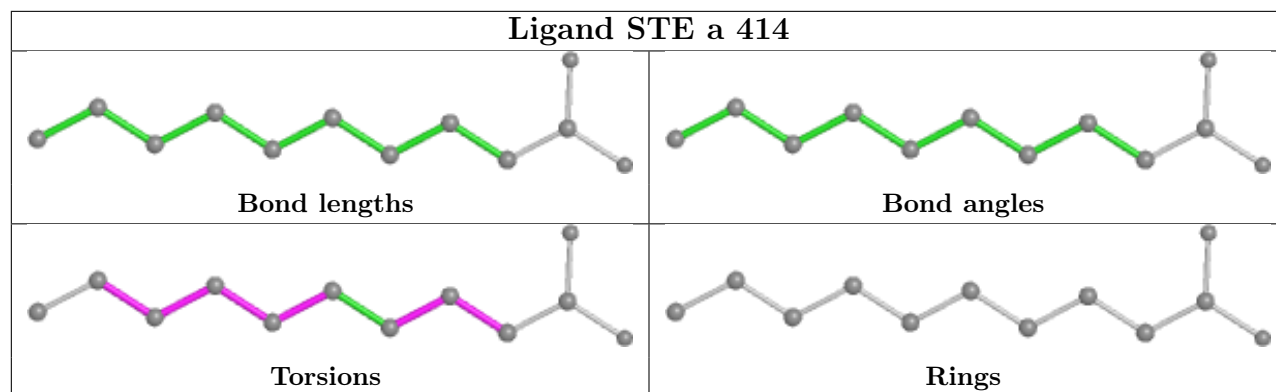


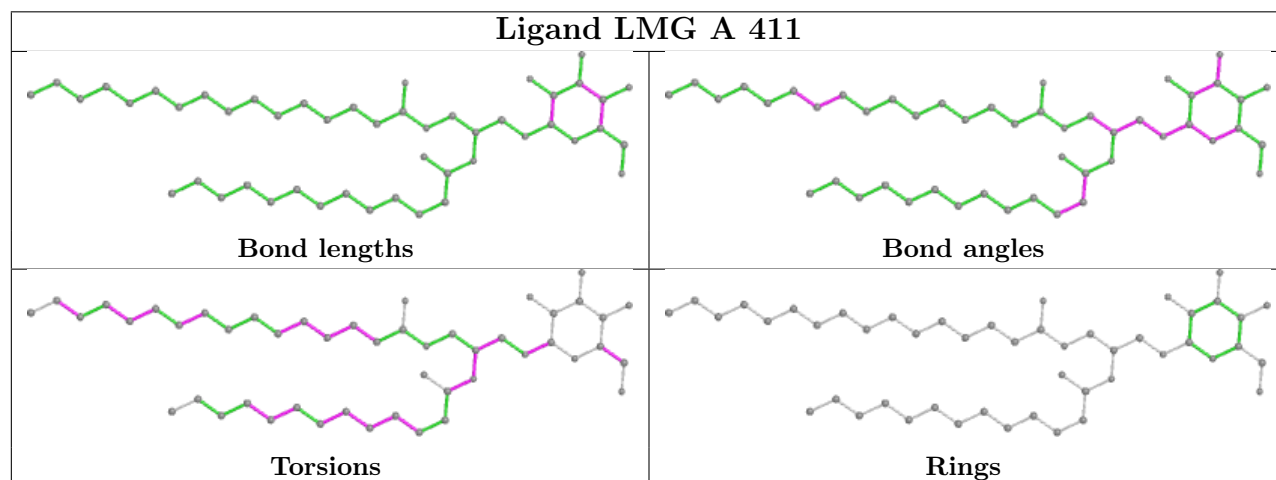
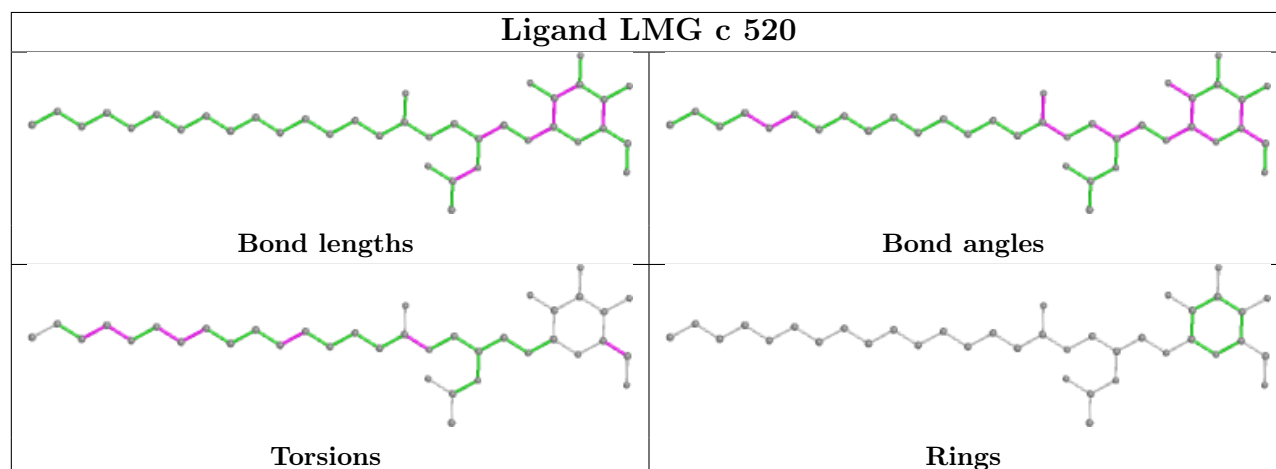
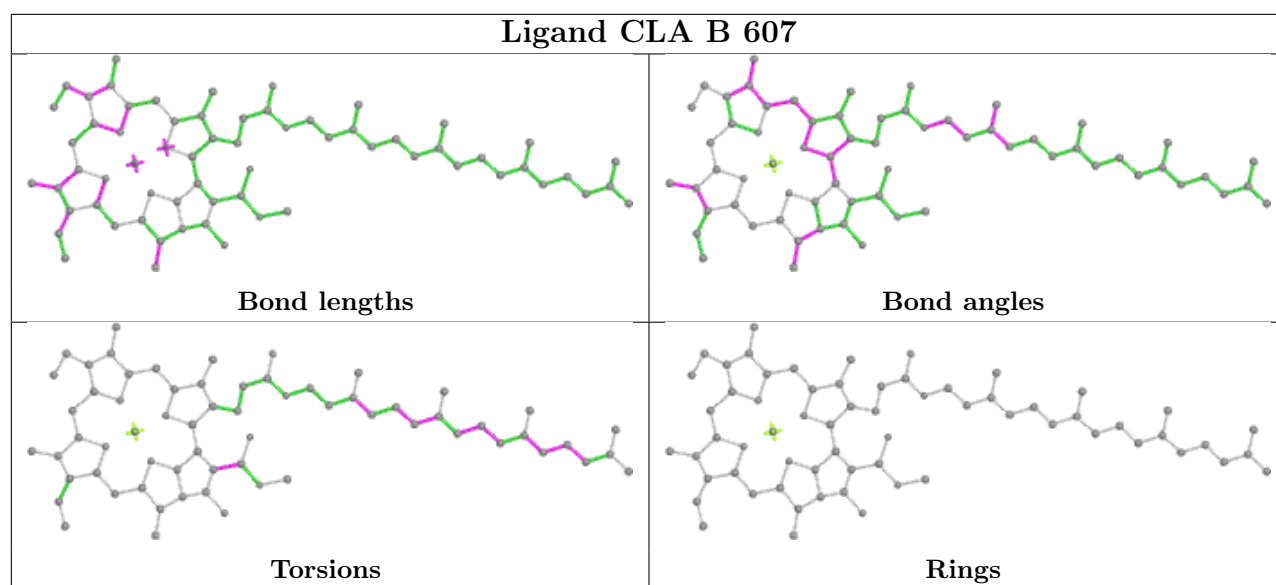
## Ligand CLA c 508

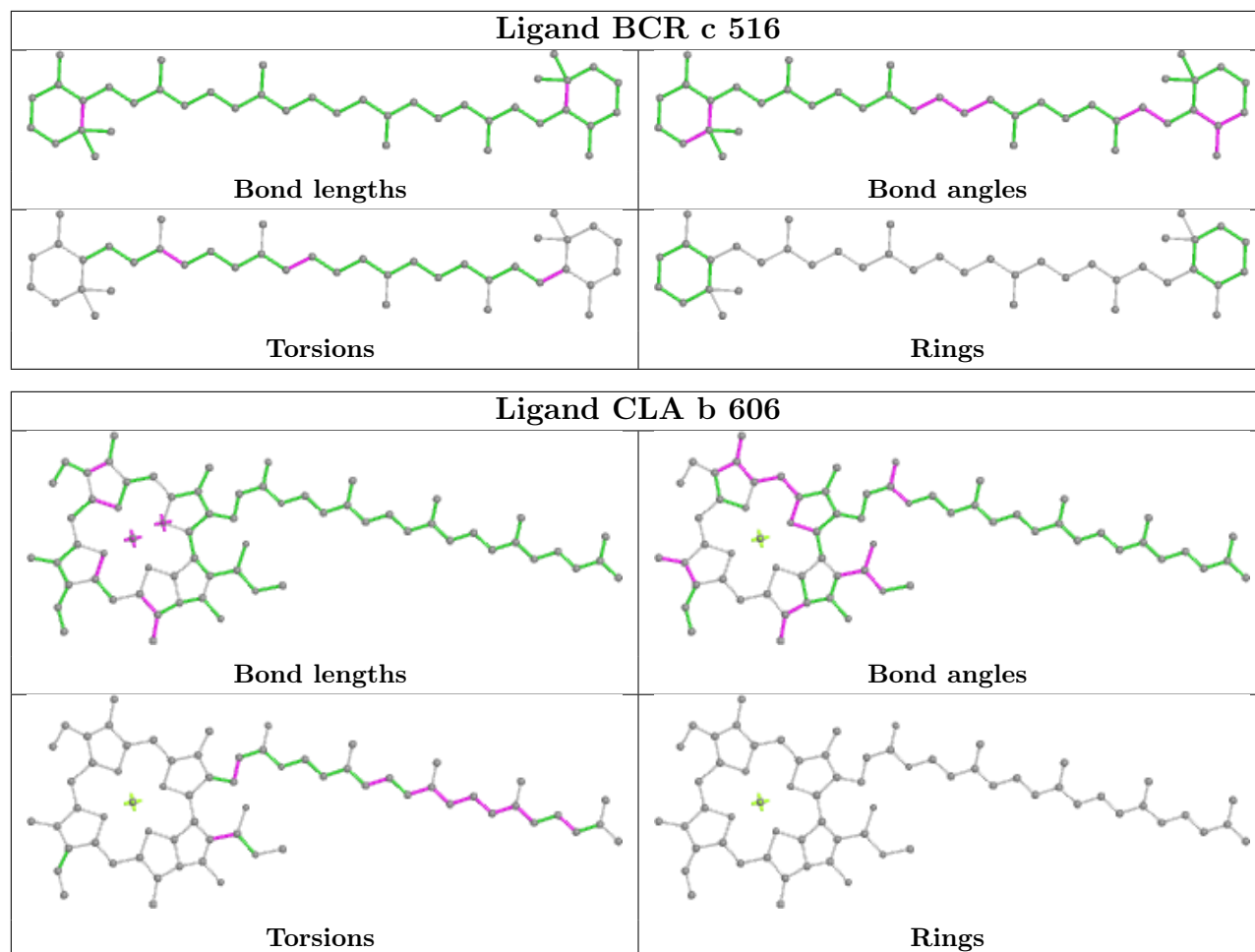




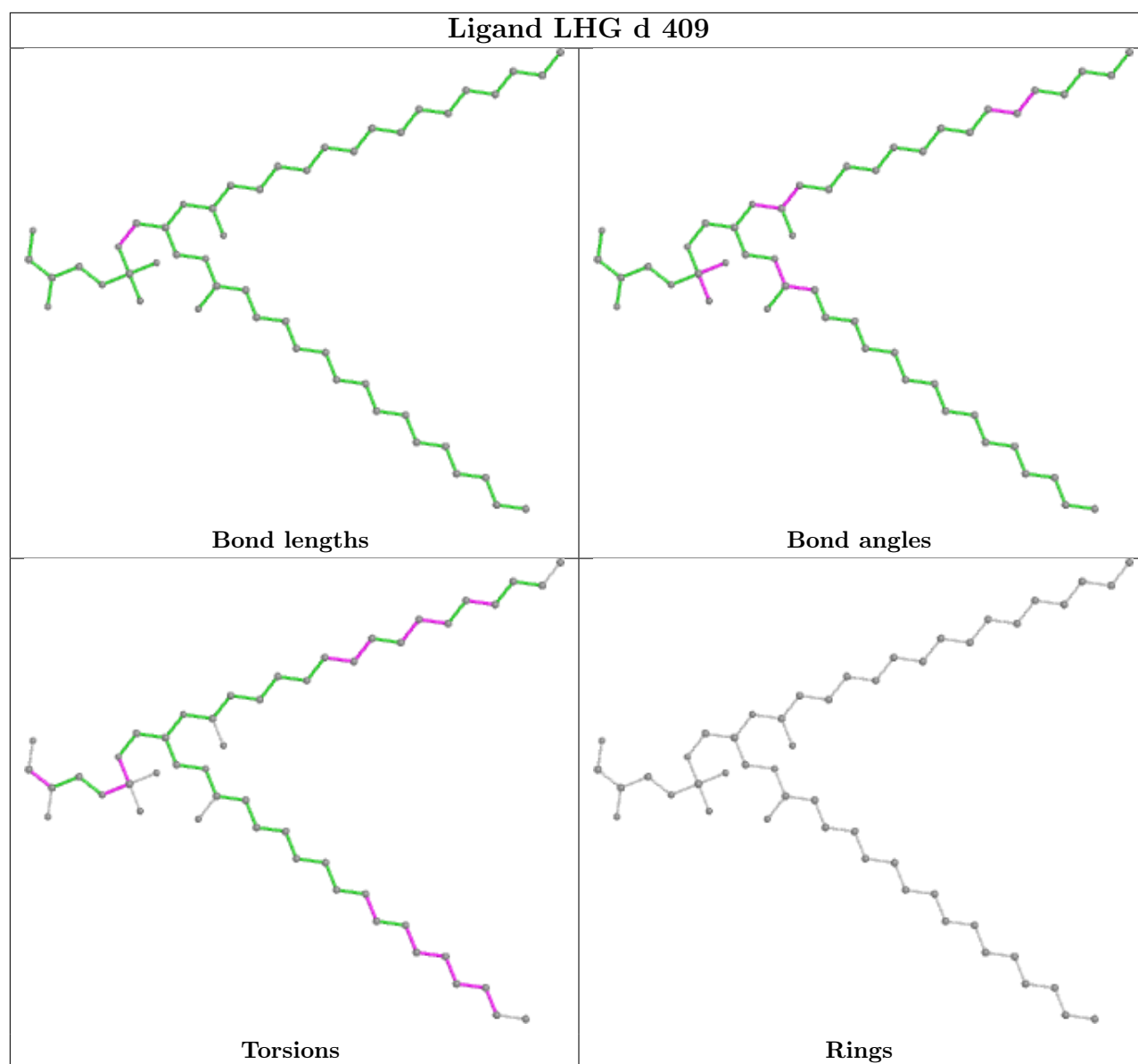


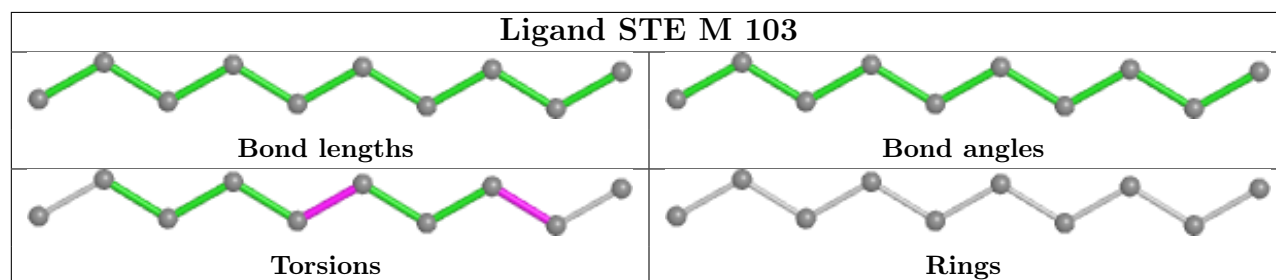
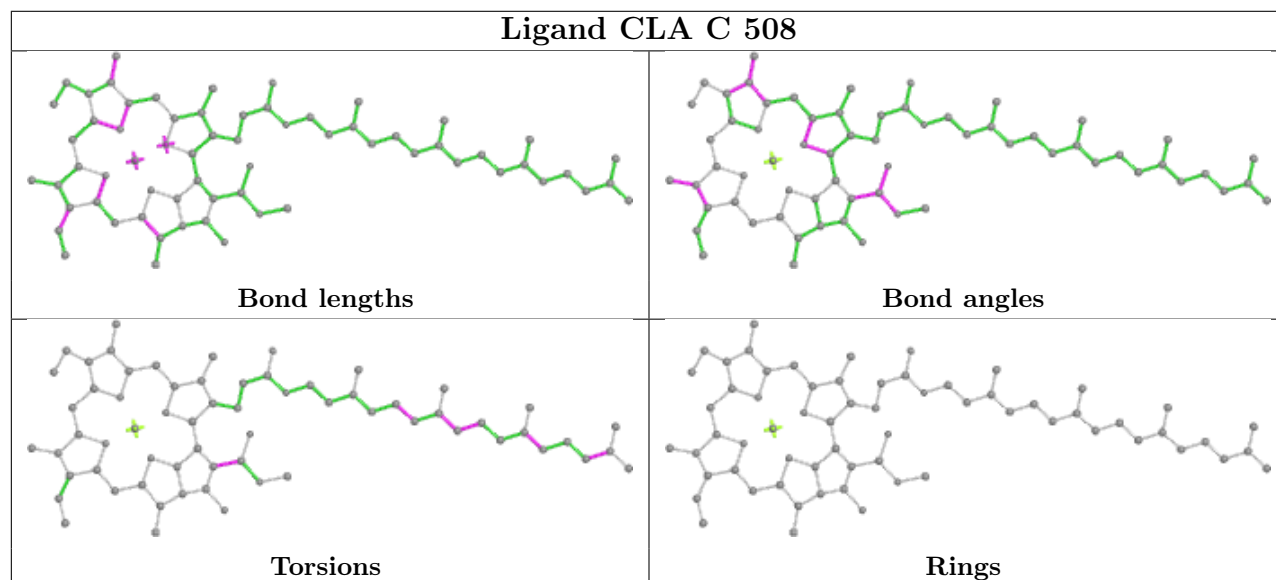
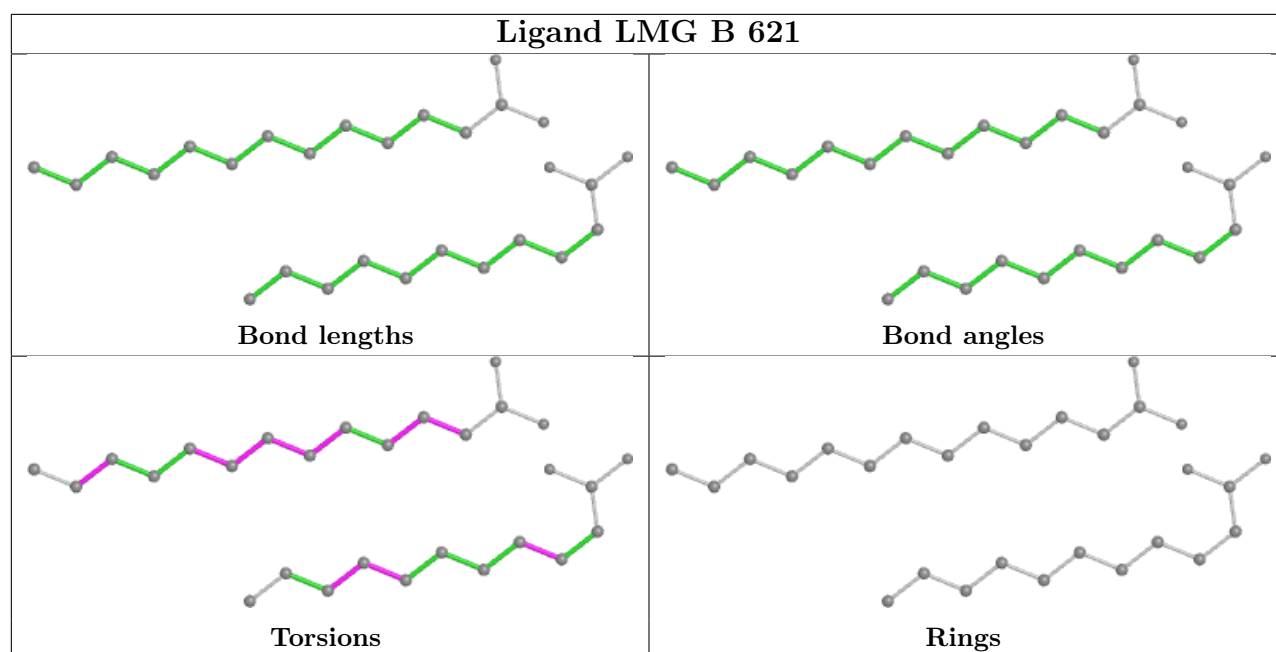


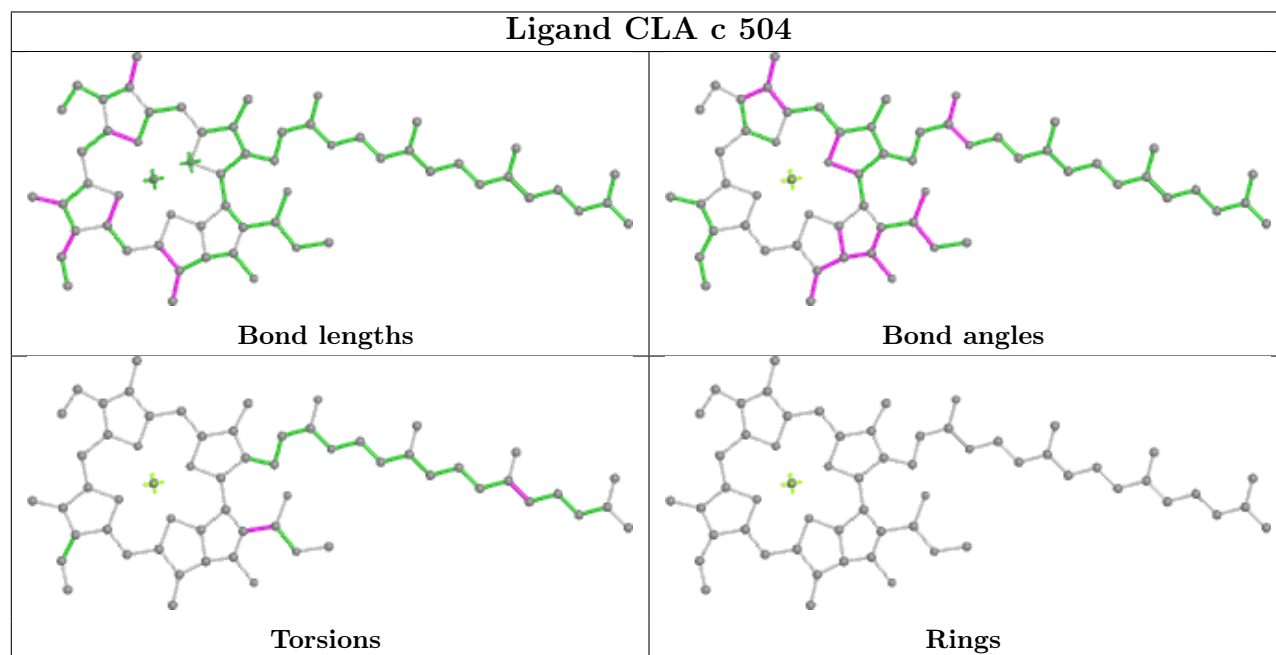
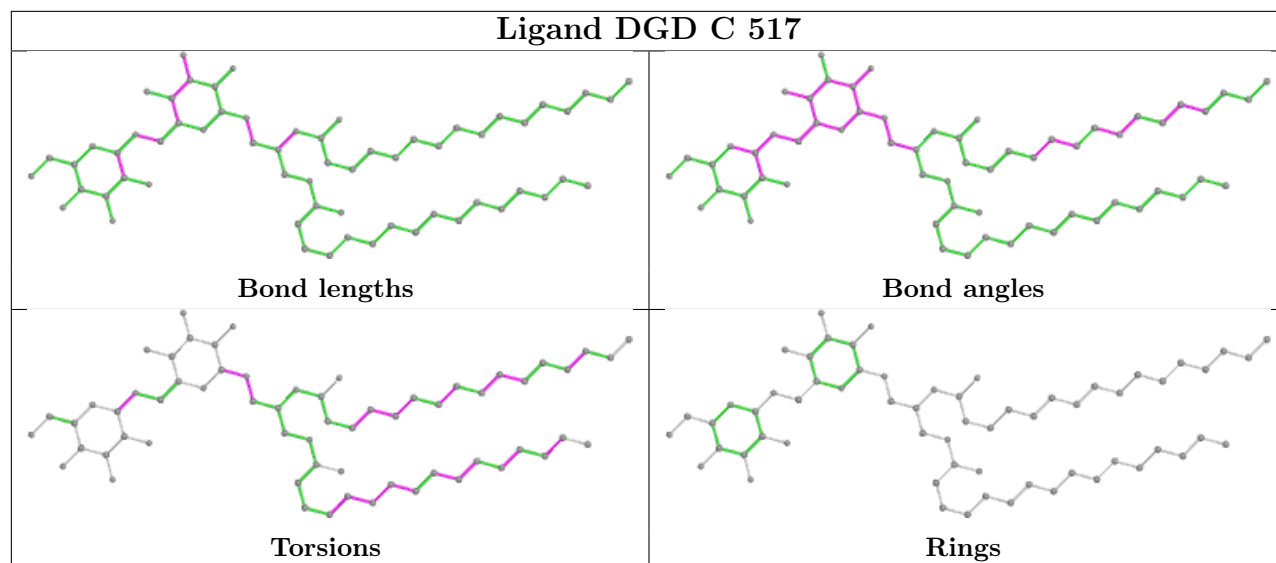


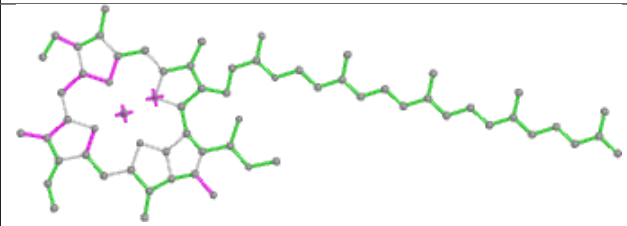
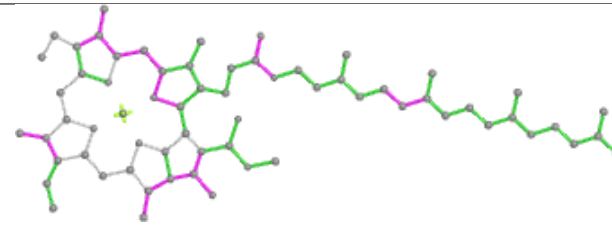
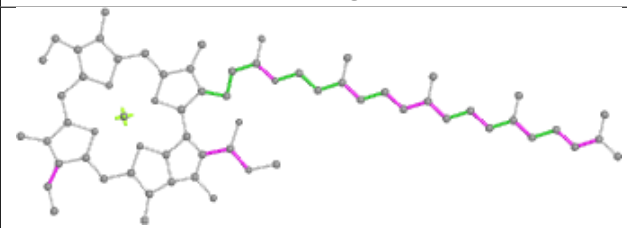
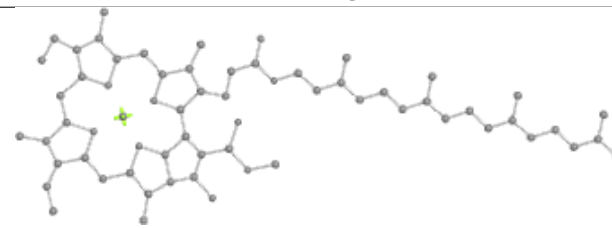


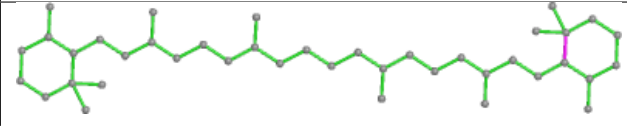
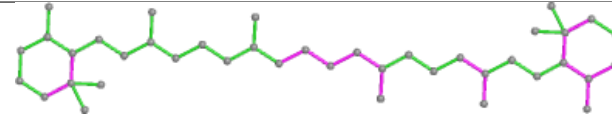
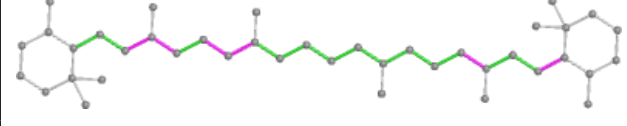
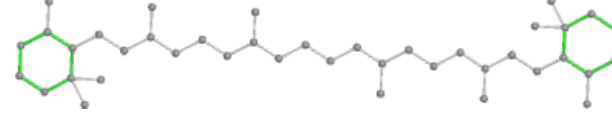


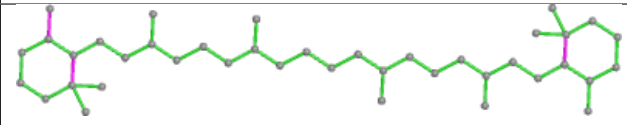
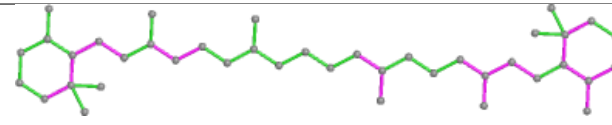
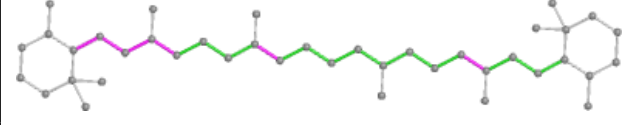
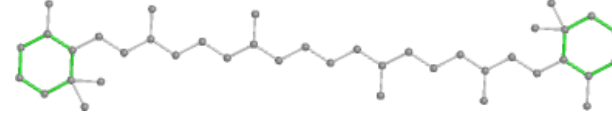


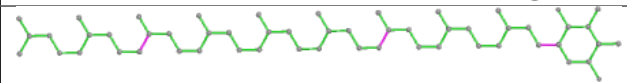
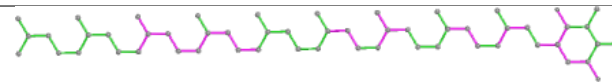
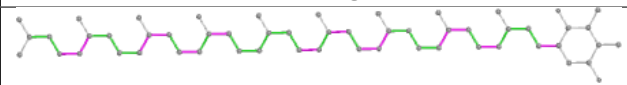
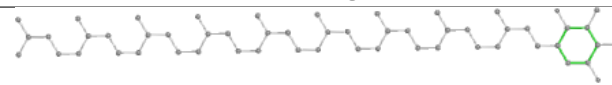


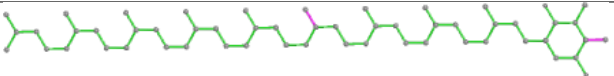
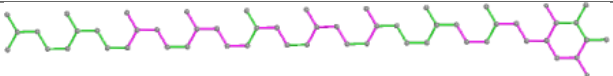
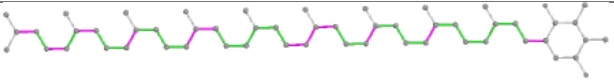
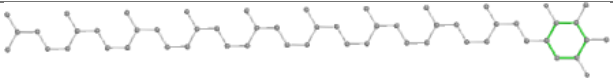


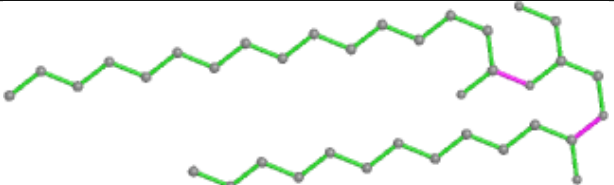
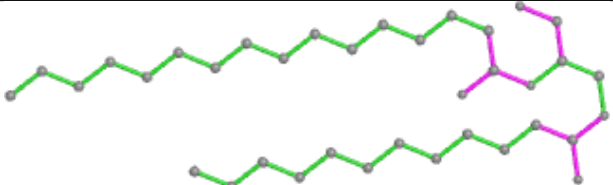
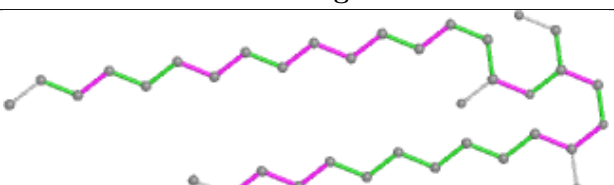
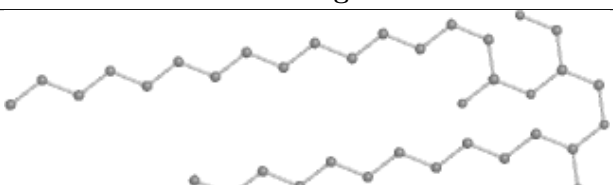
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

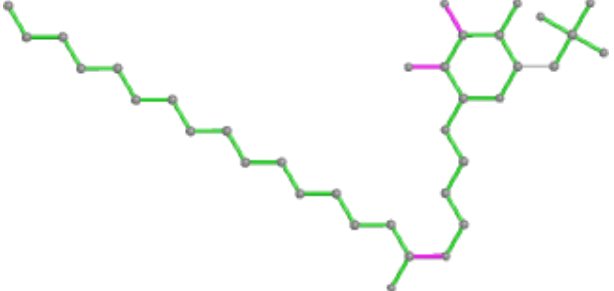
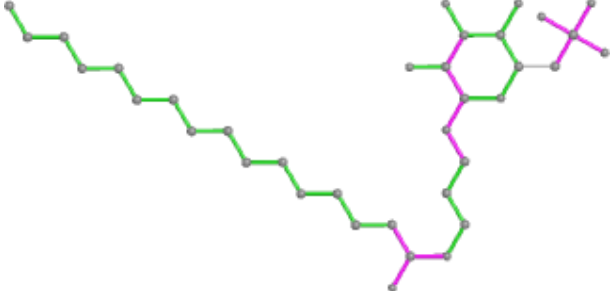
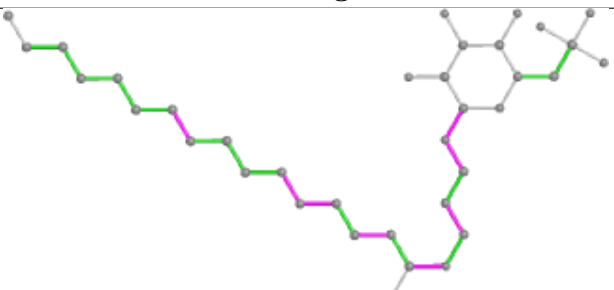
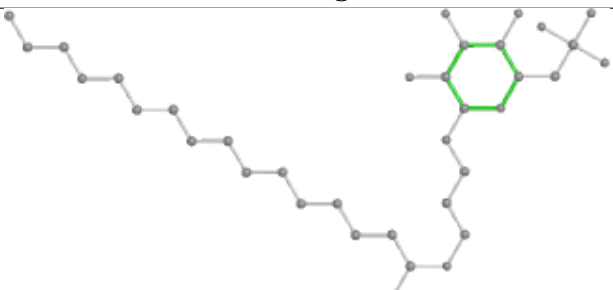
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

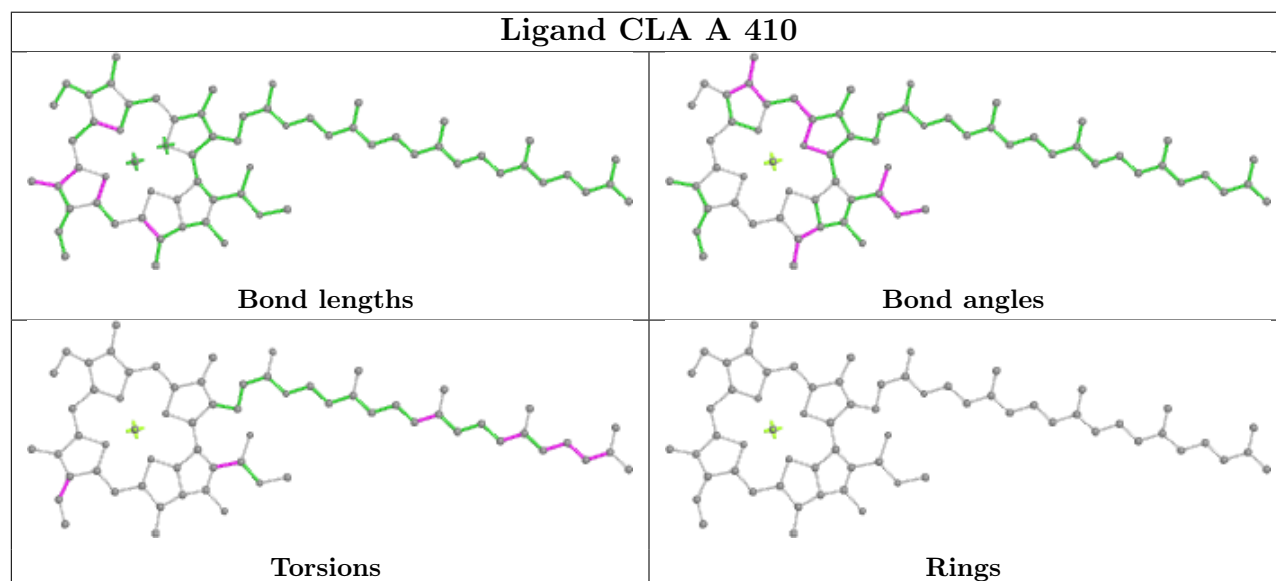
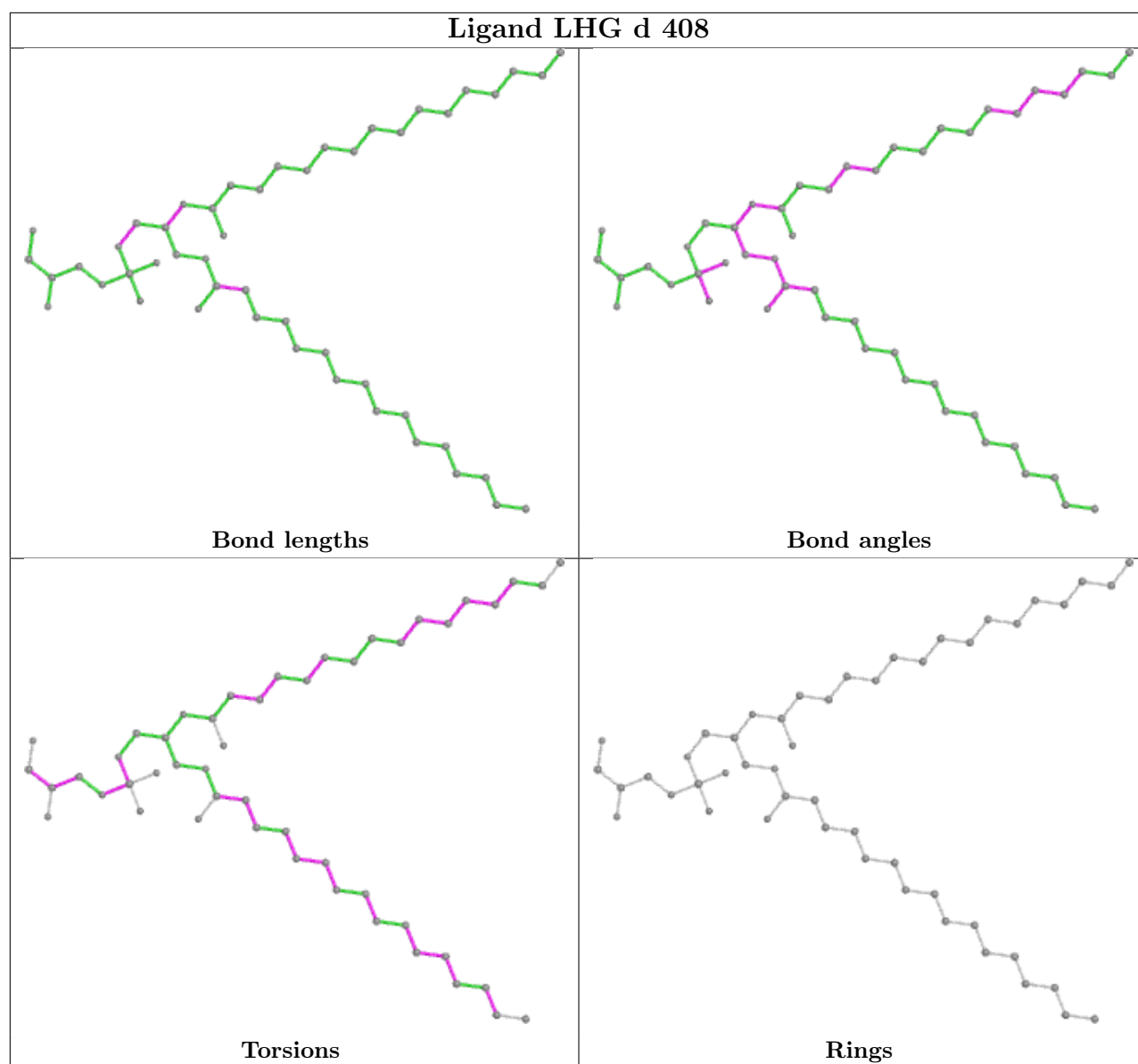
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

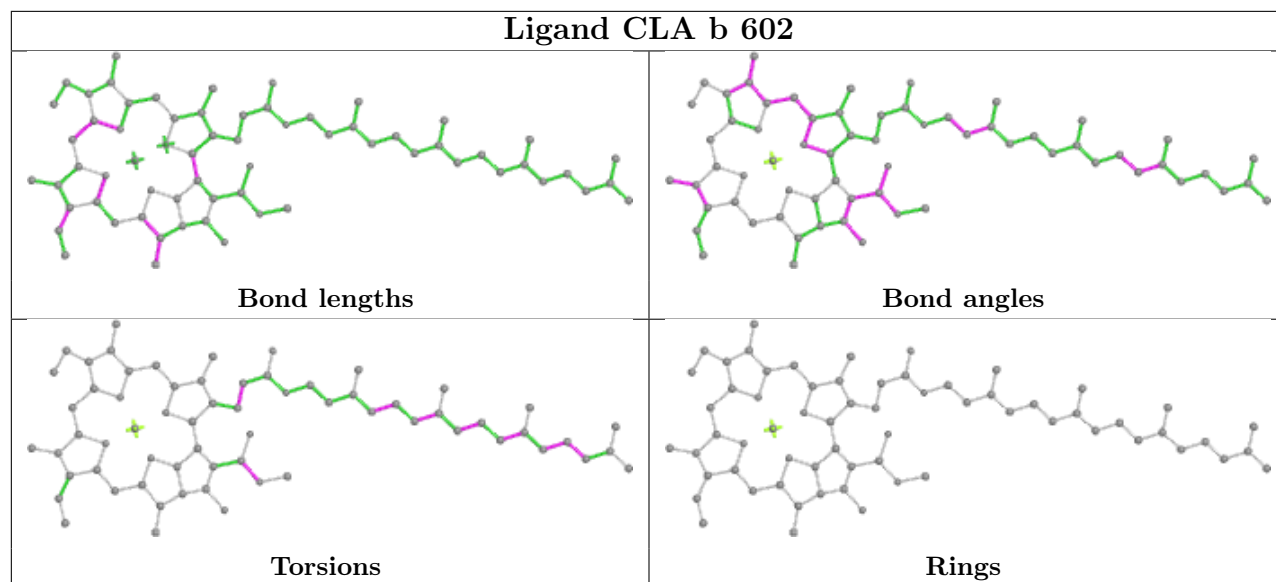
Ligand PL9 a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

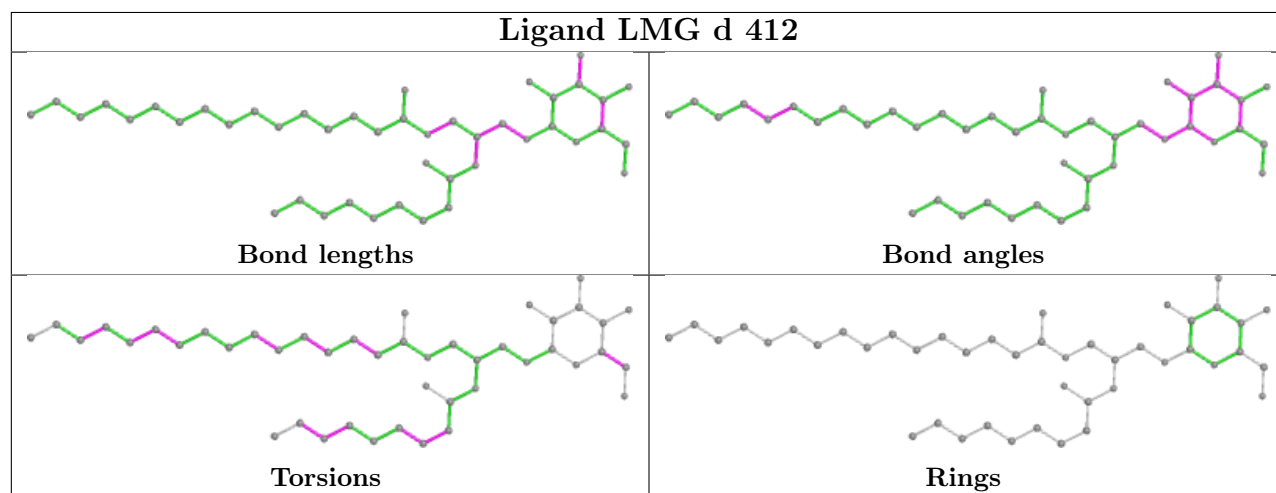
Ligand SQD F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



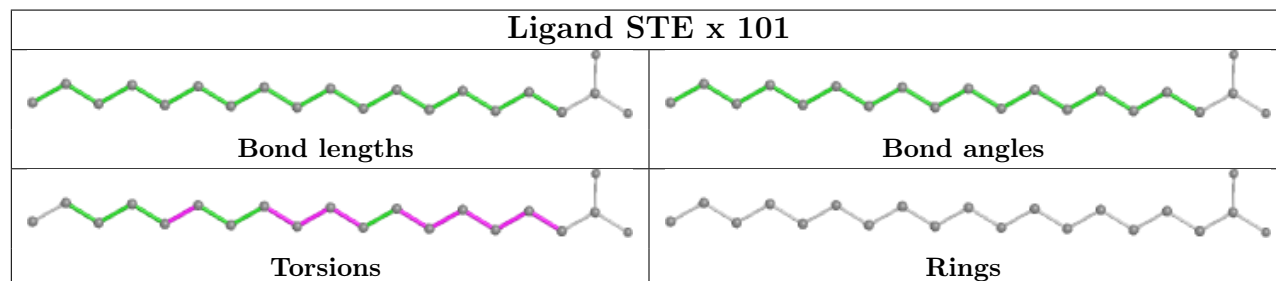
## Ligand CLA b 602

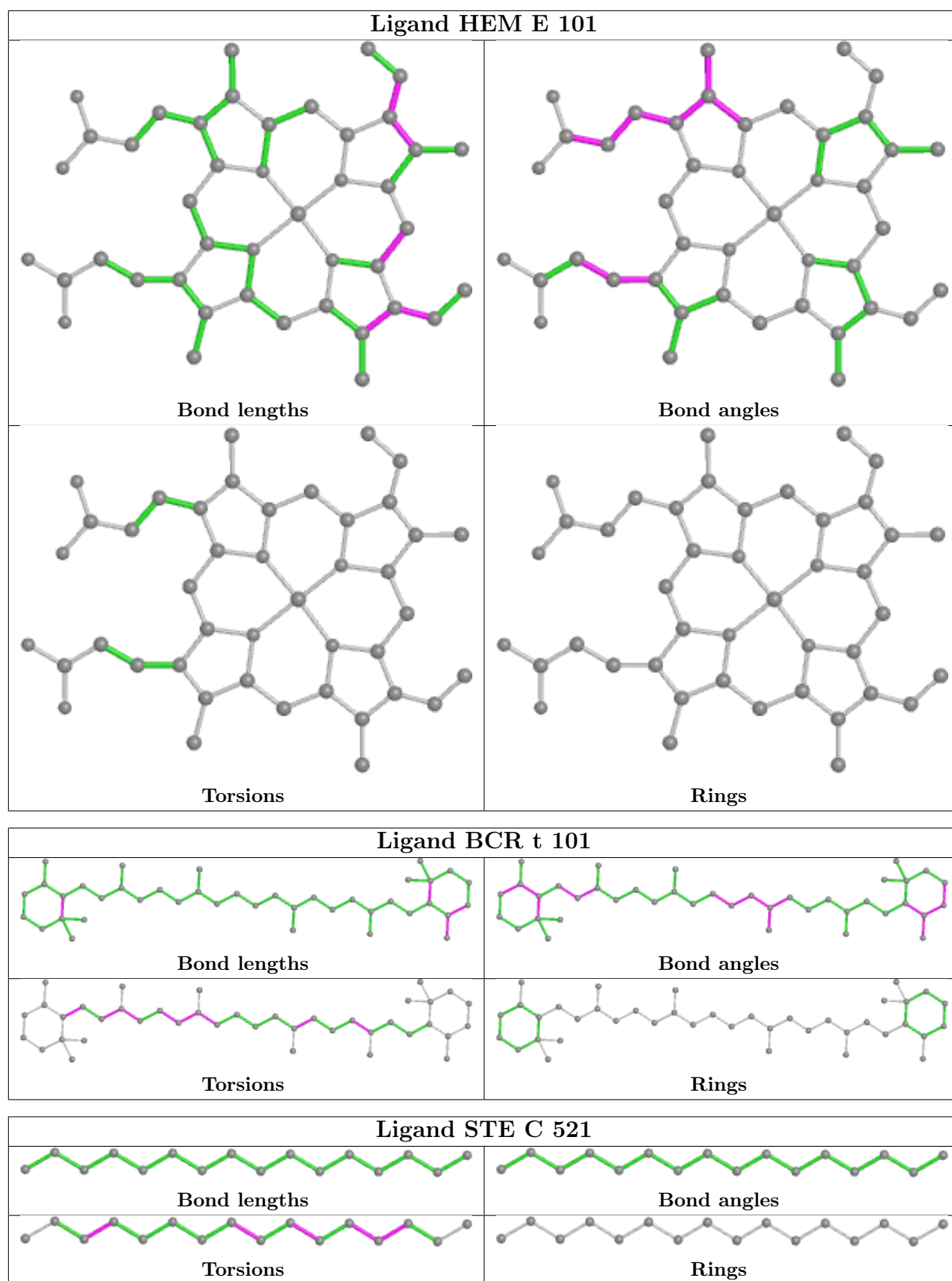


## Ligand LMG d 412

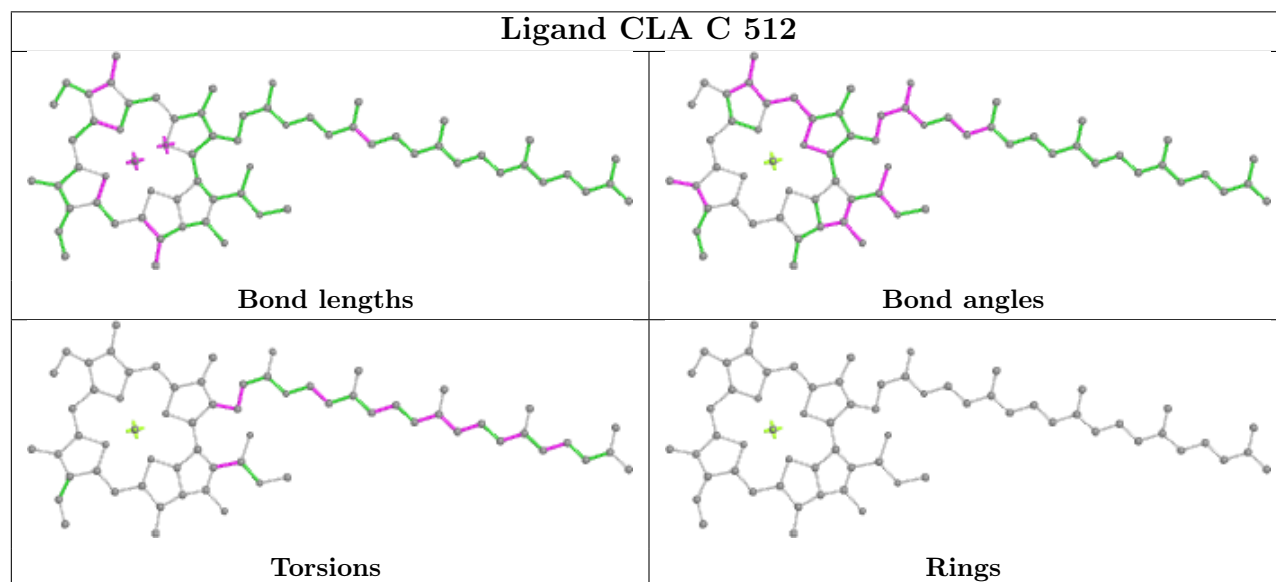
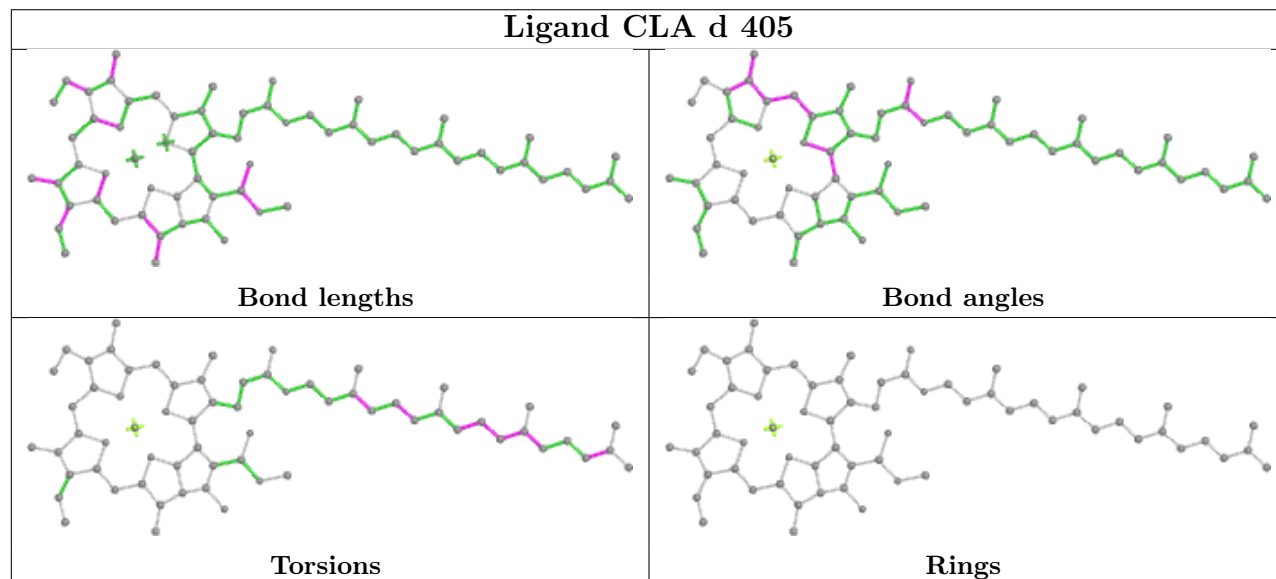
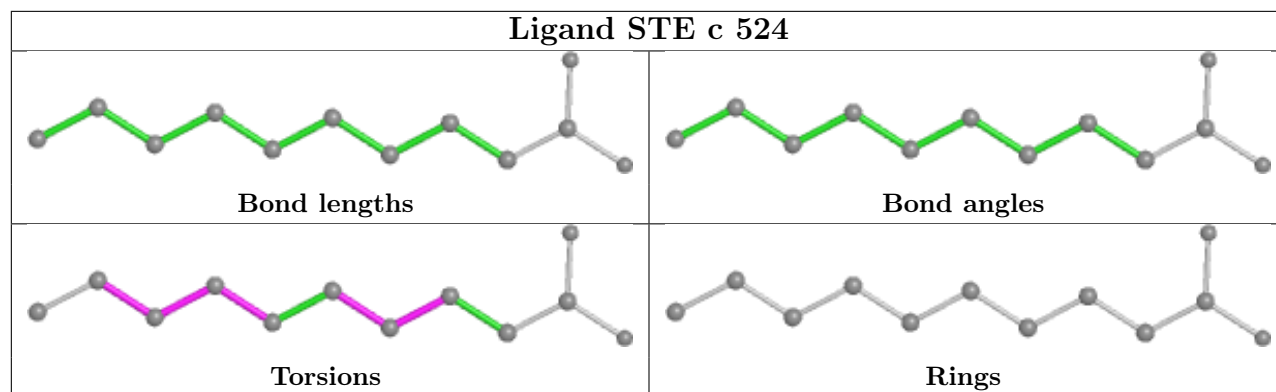


## Ligand STE x 101

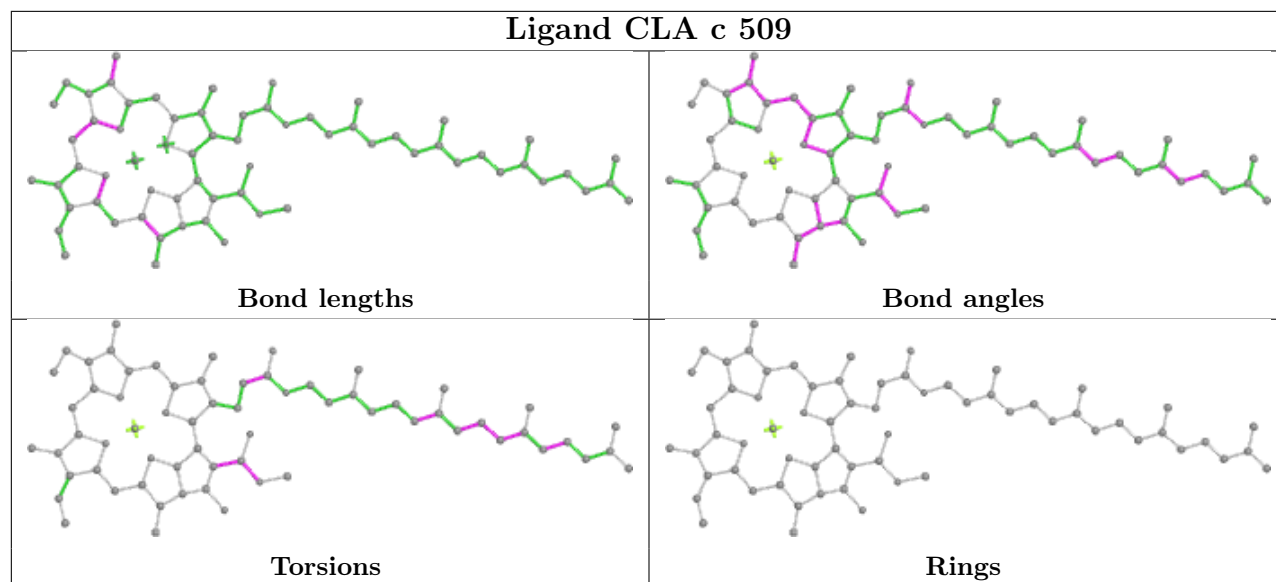




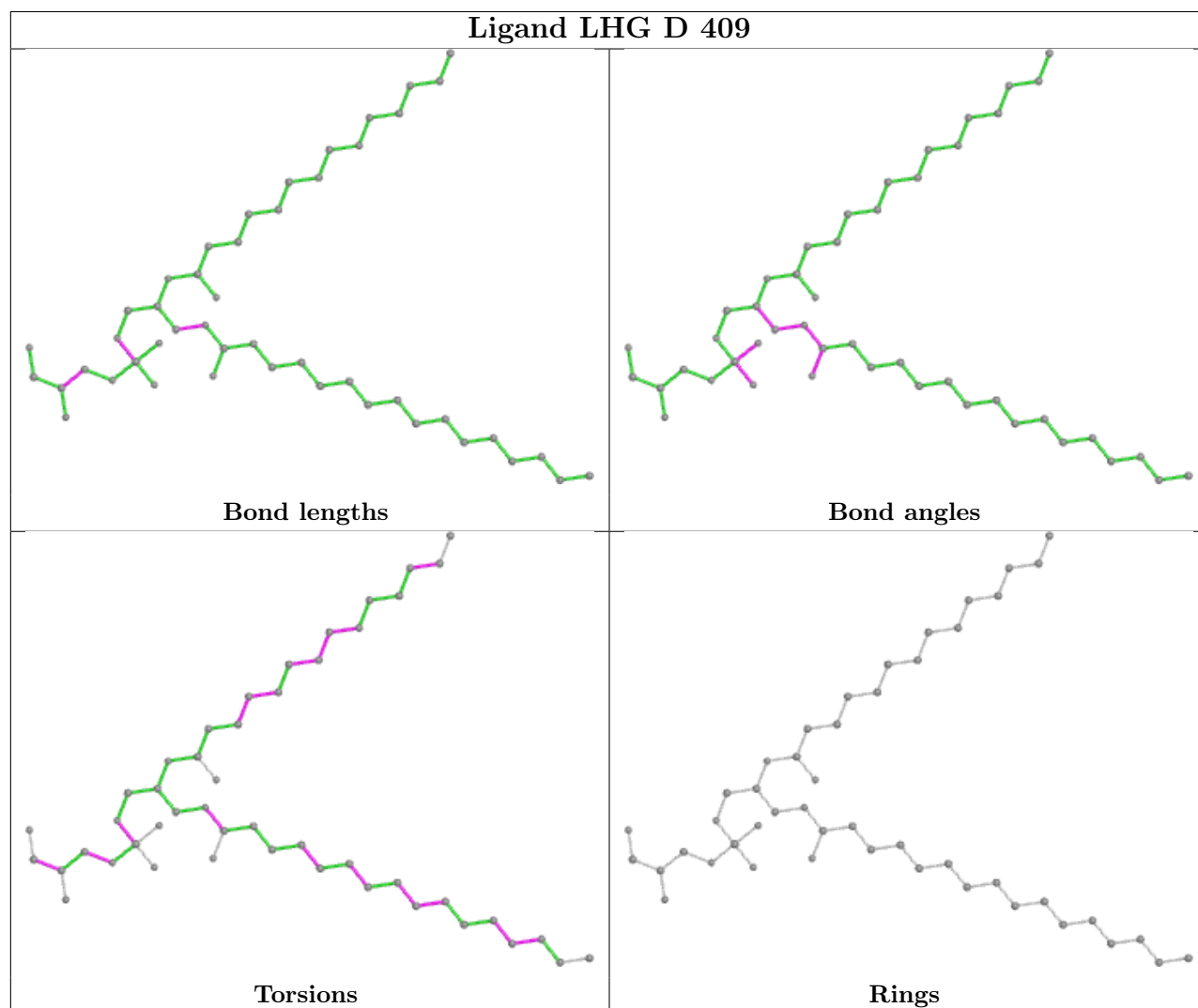


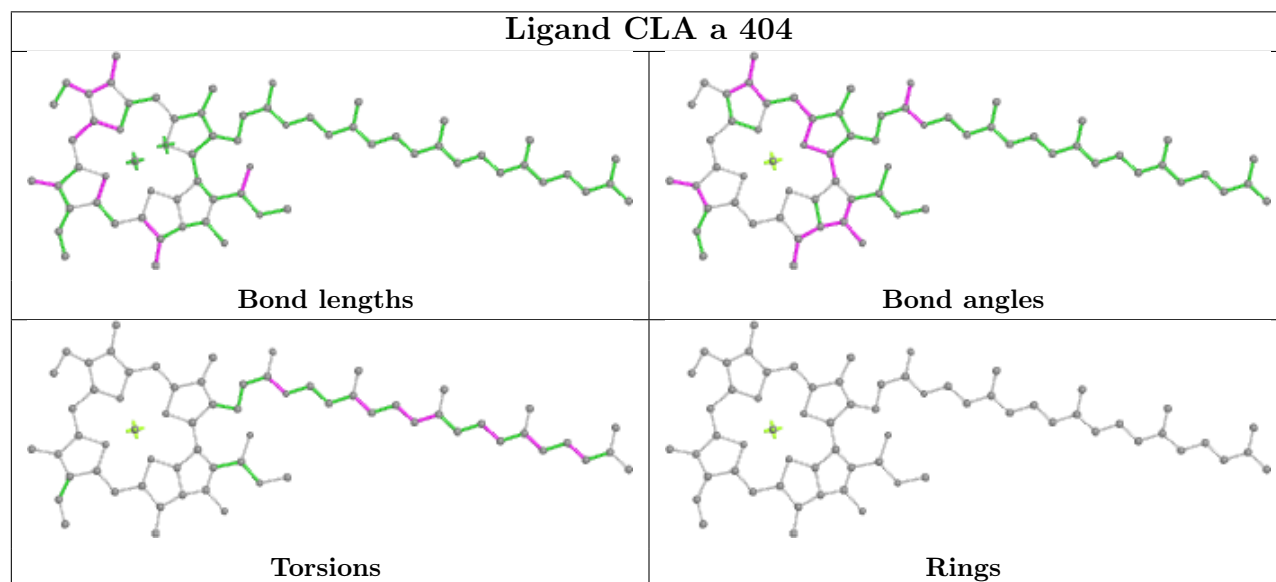
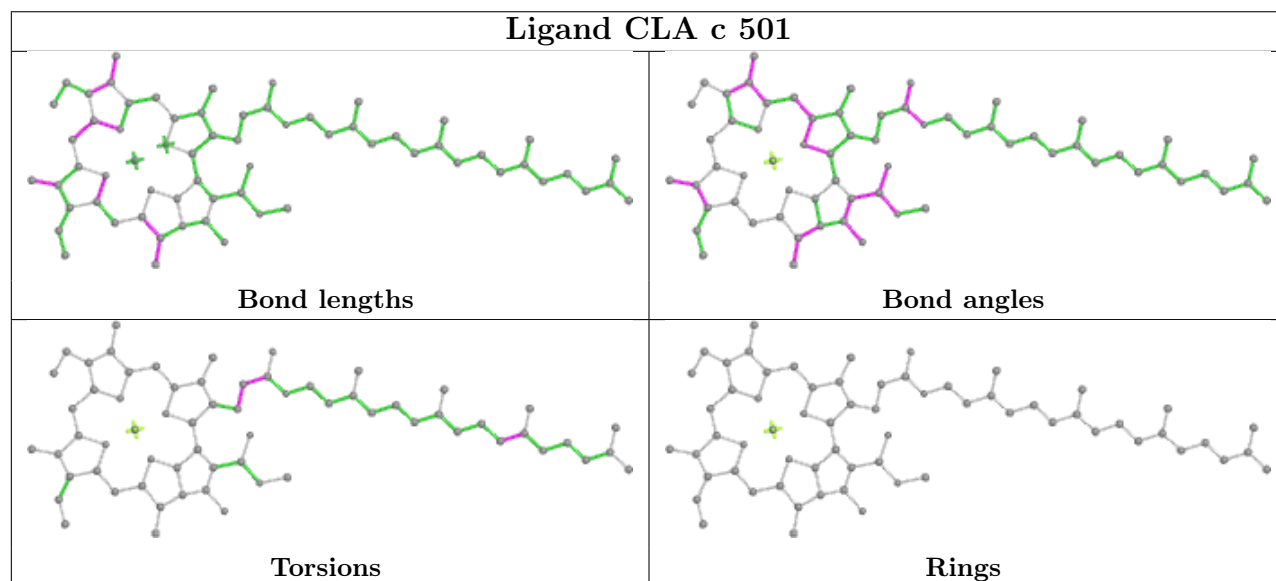
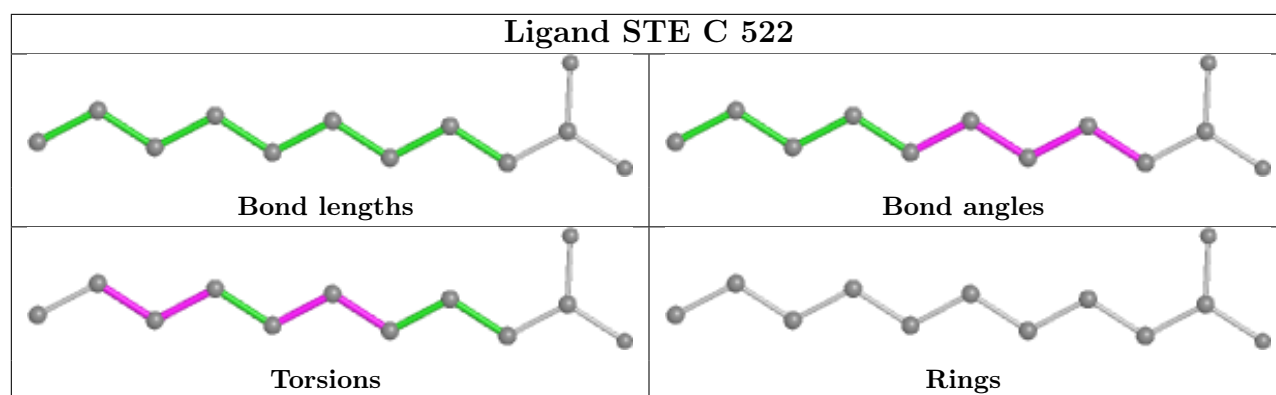


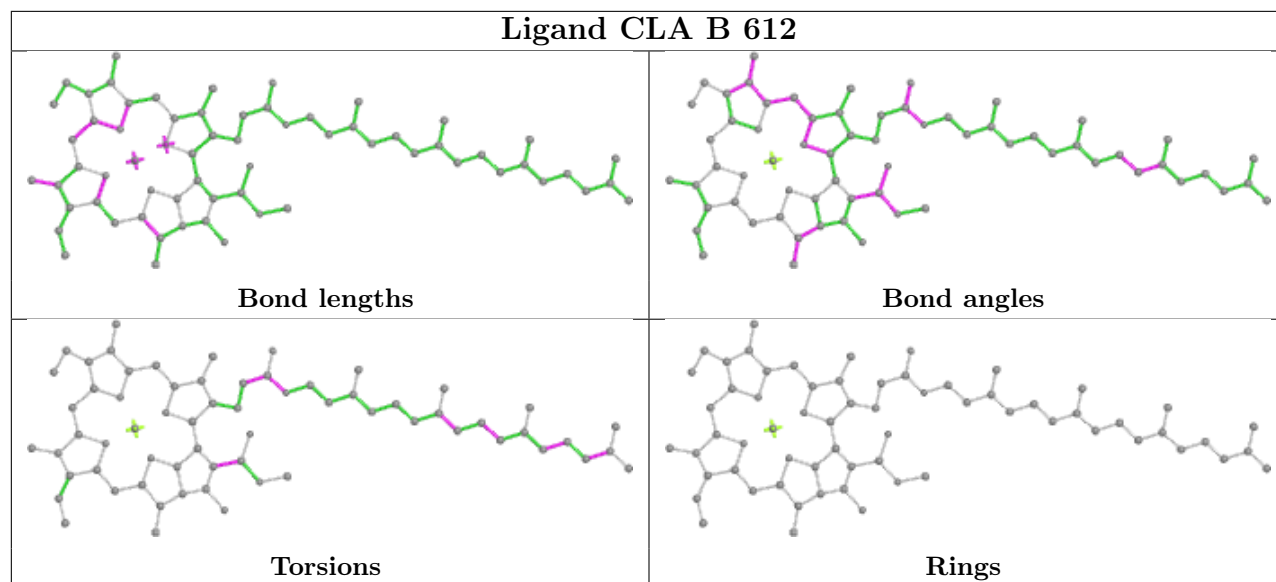
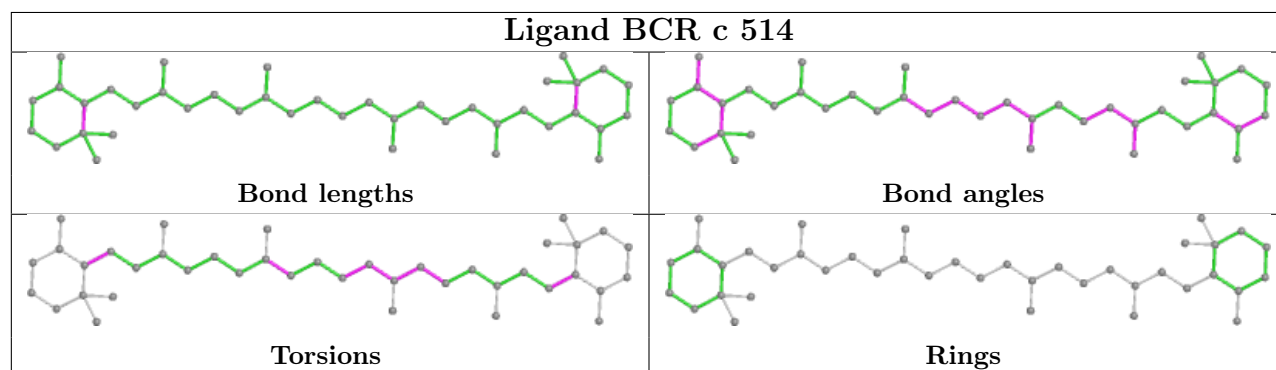
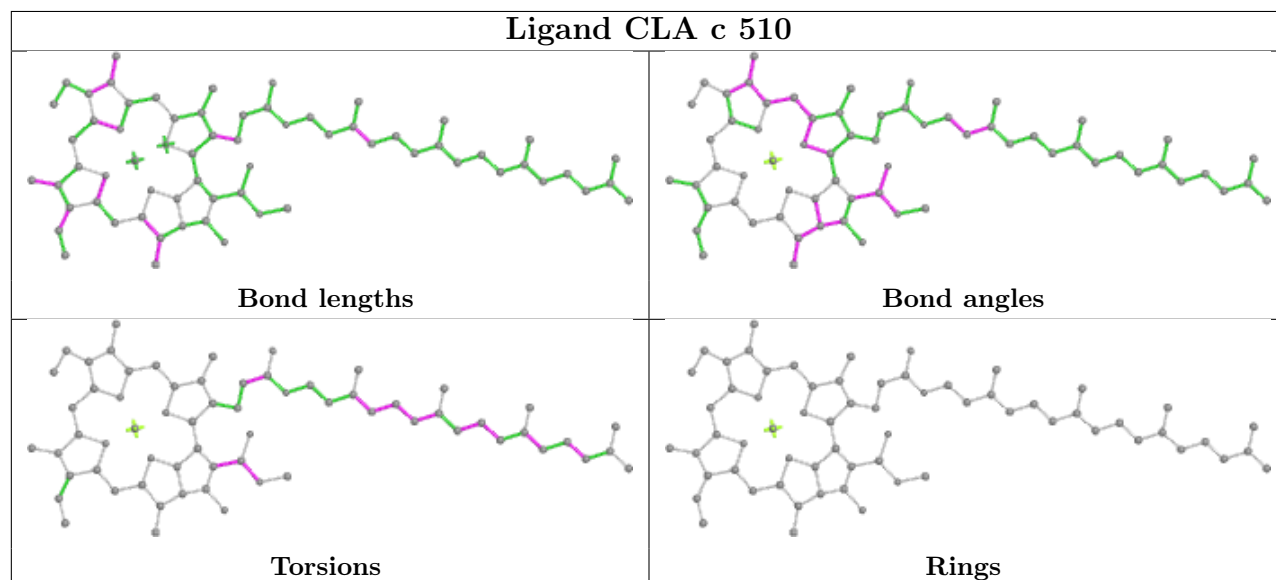
## Ligand CLA c 509

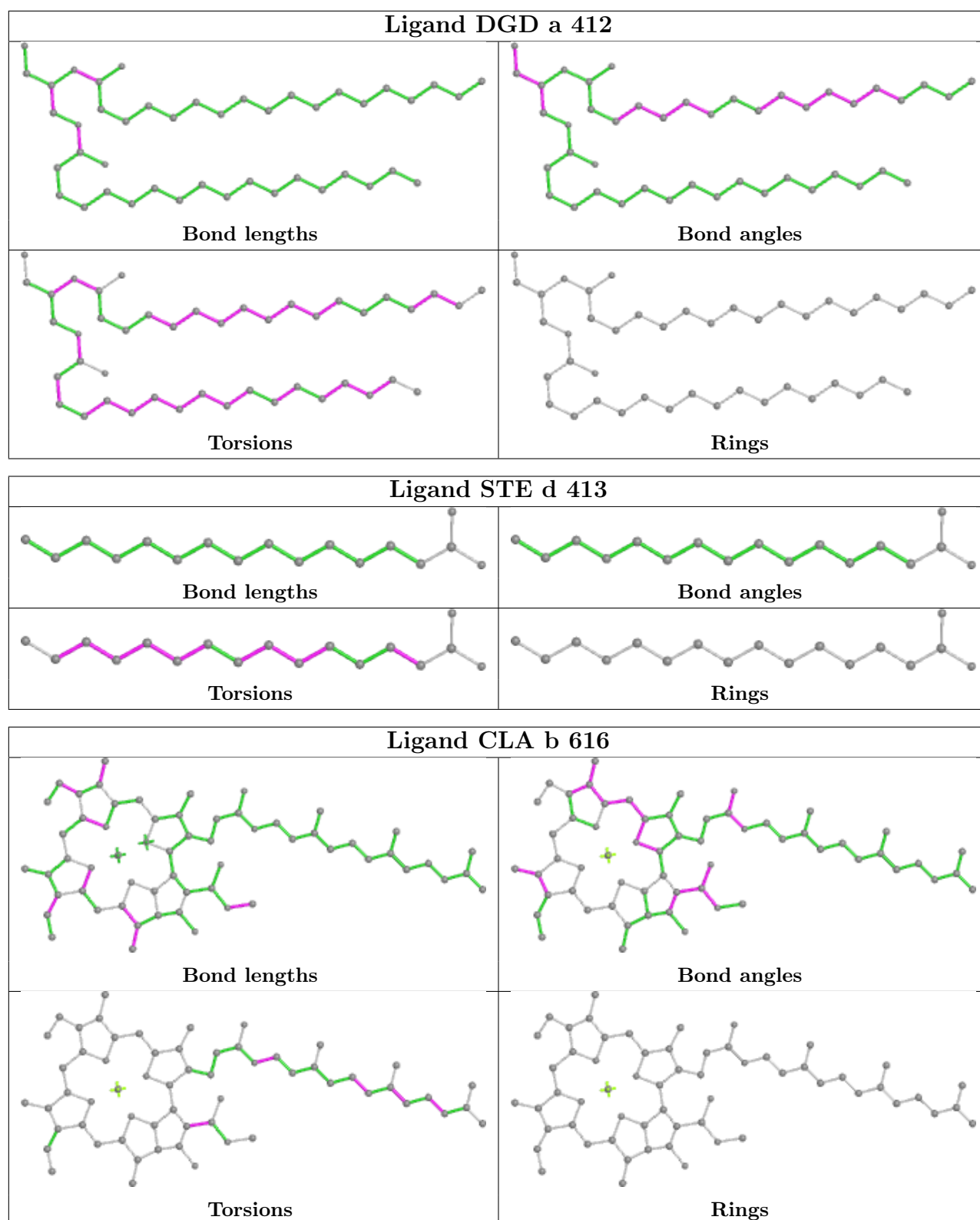


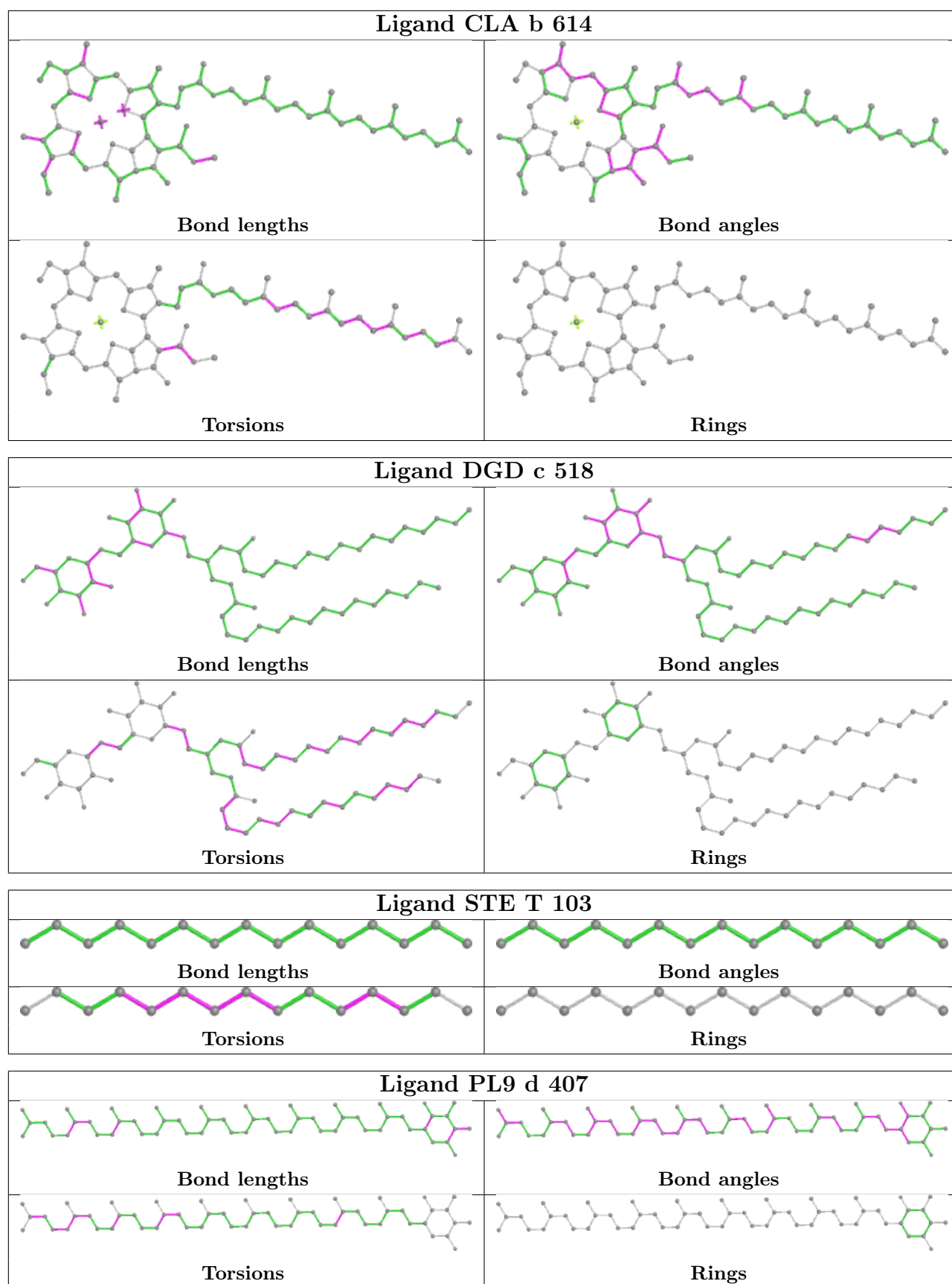
## Ligand LHG D 409

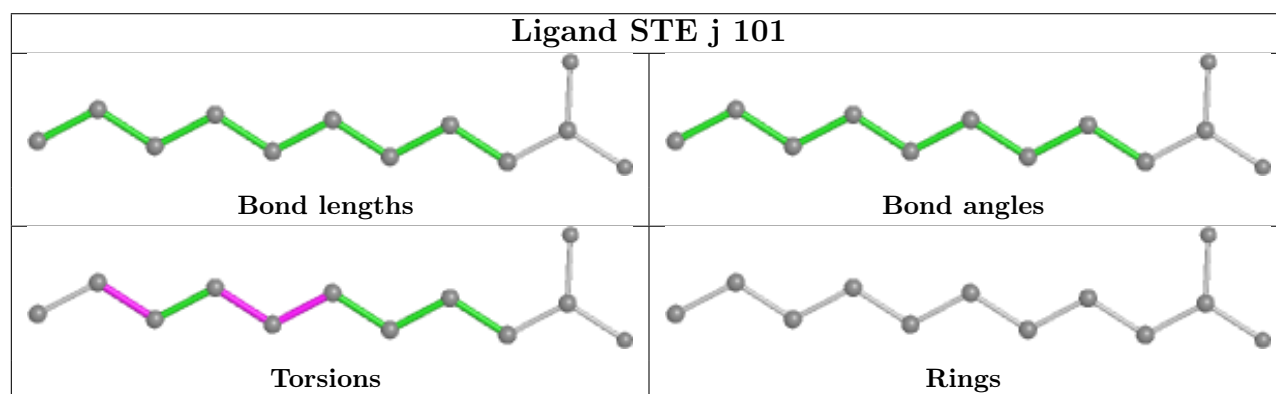
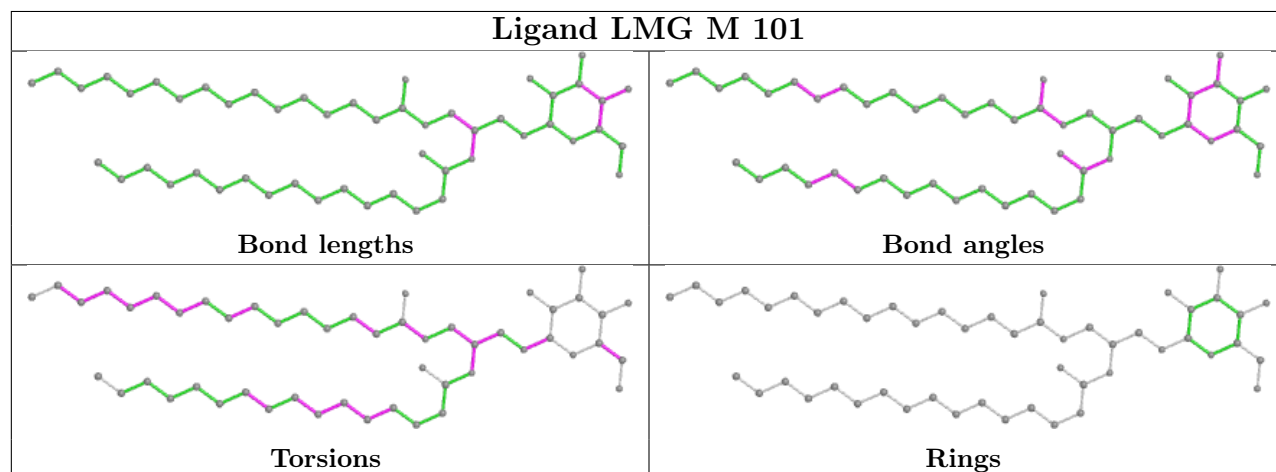
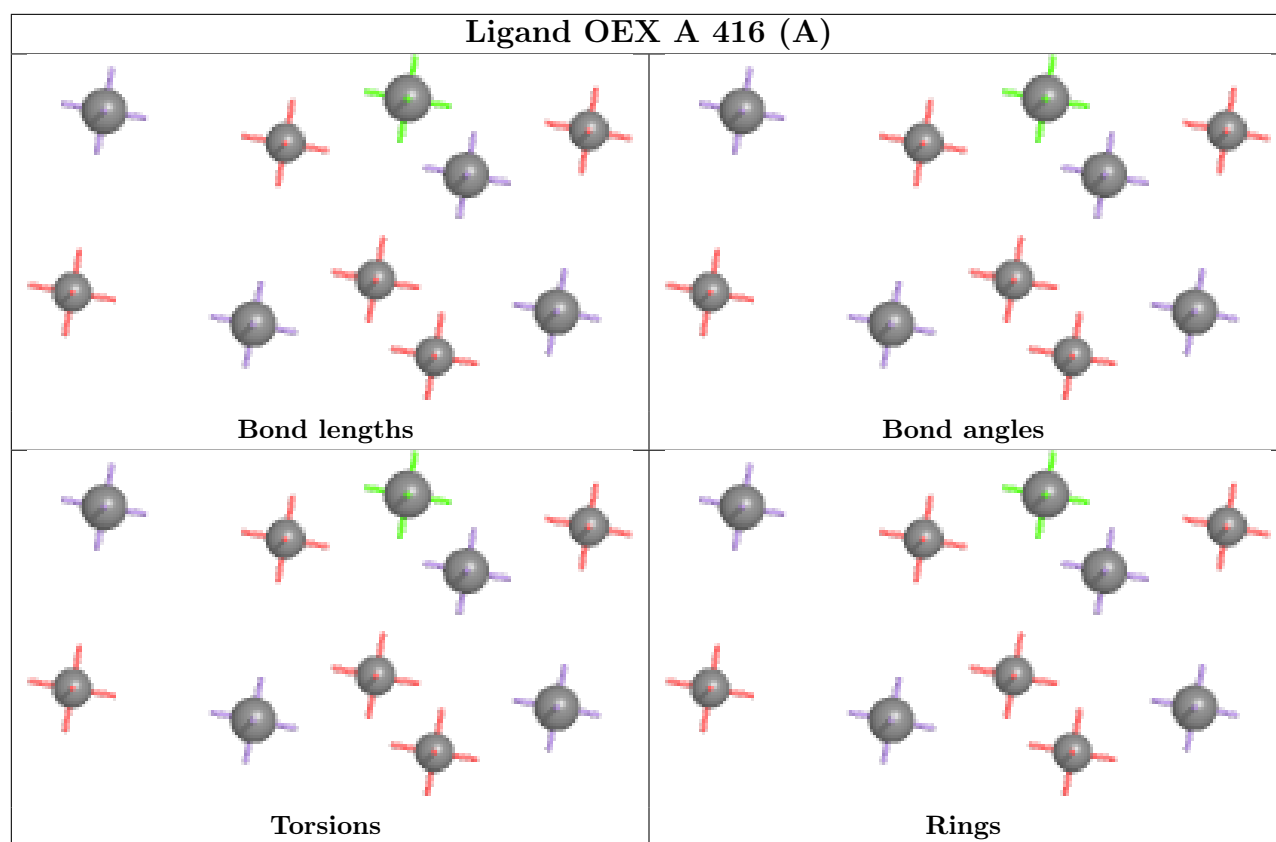




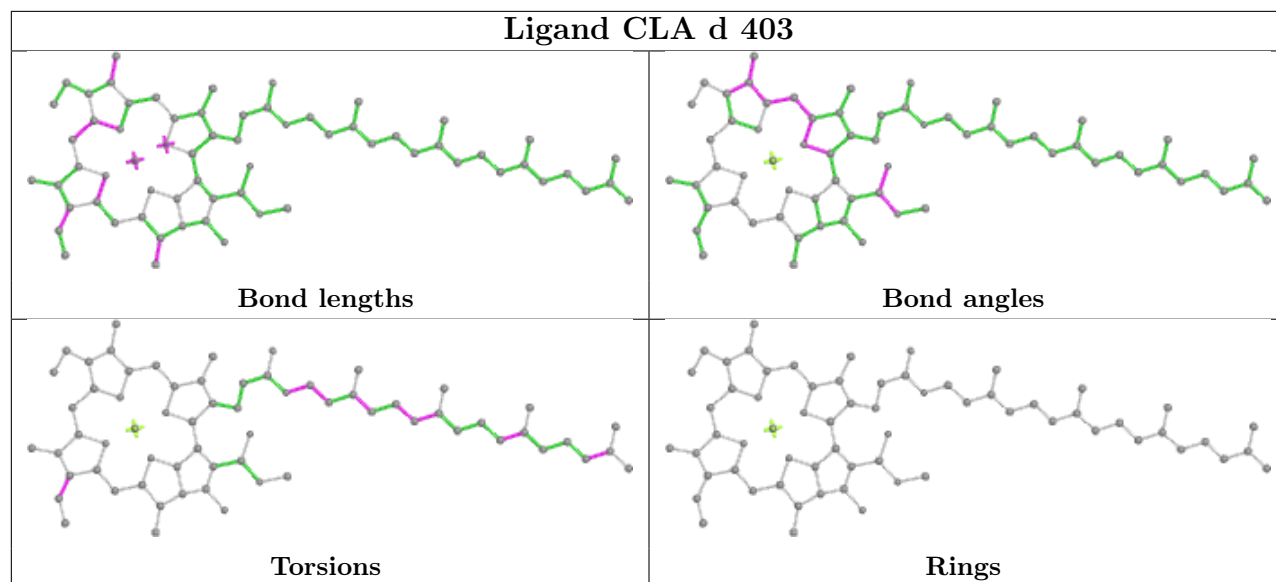
**Ligand CLA B 612****Ligand BCR c 514****Ligand CLA c 510**



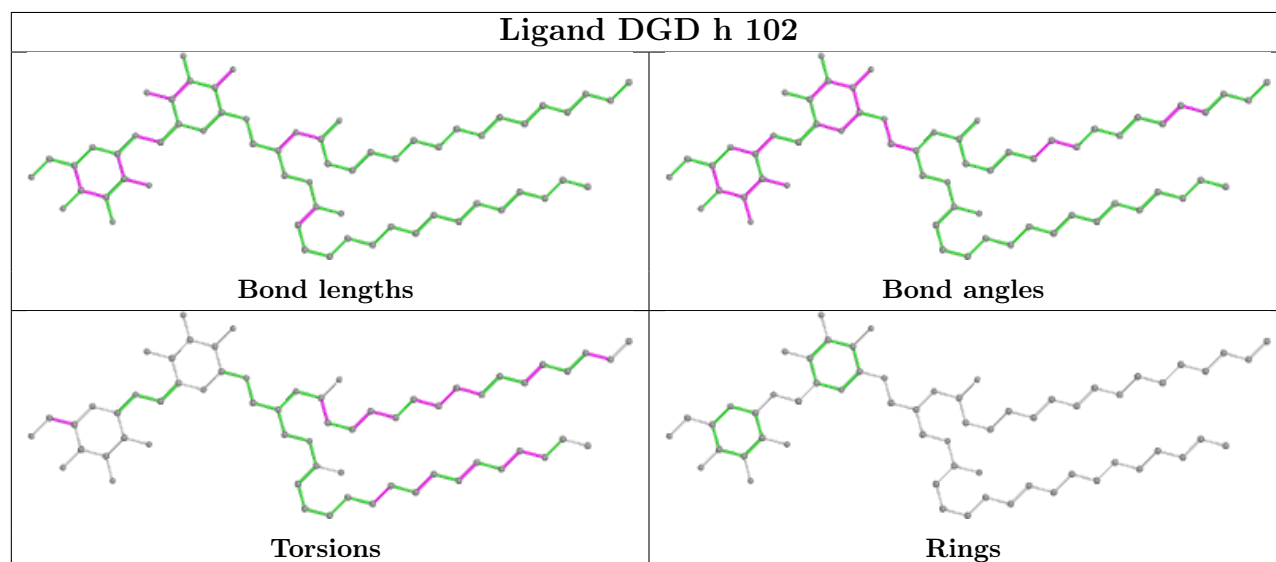




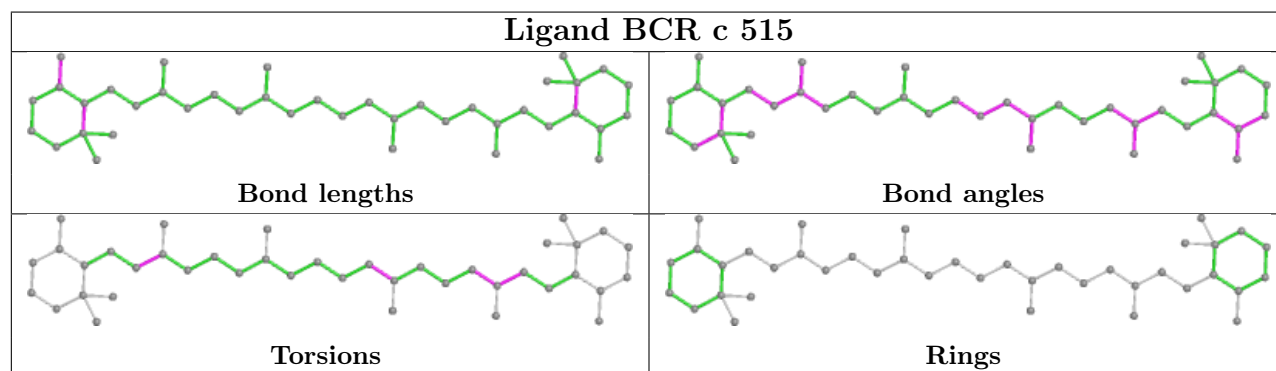
## Ligand CLA d 403



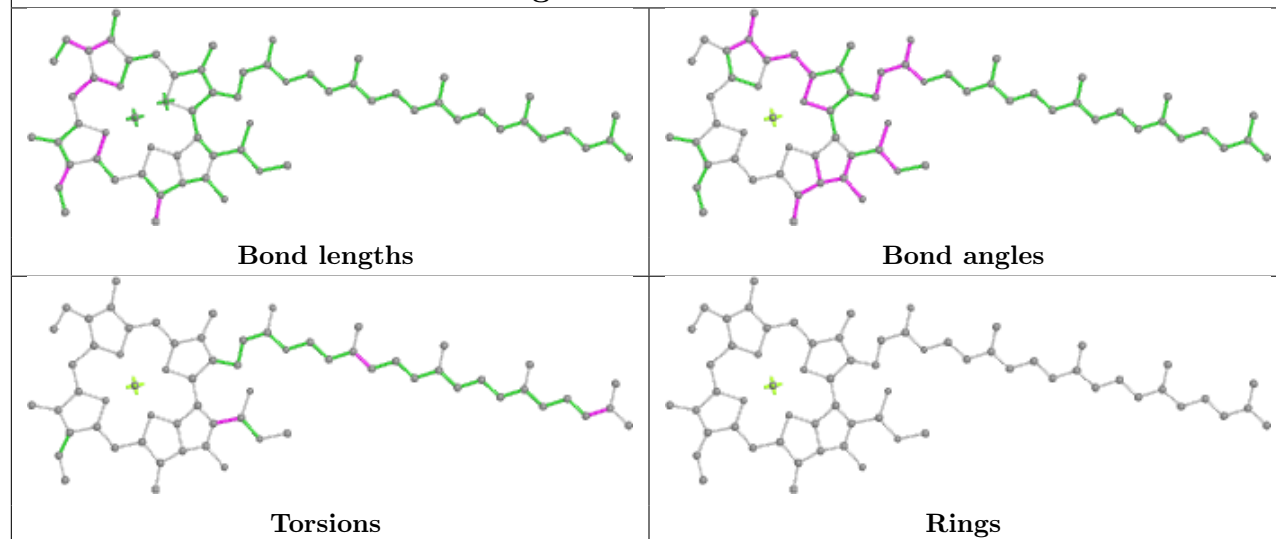
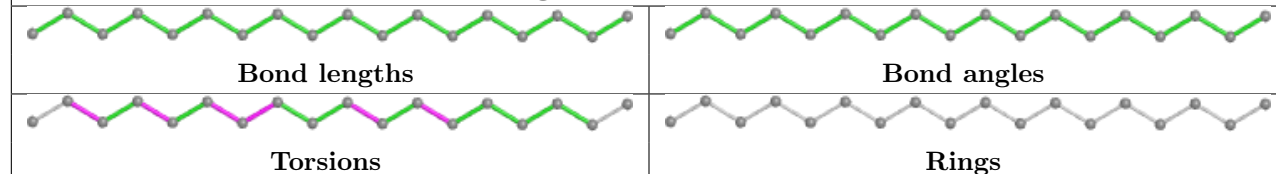
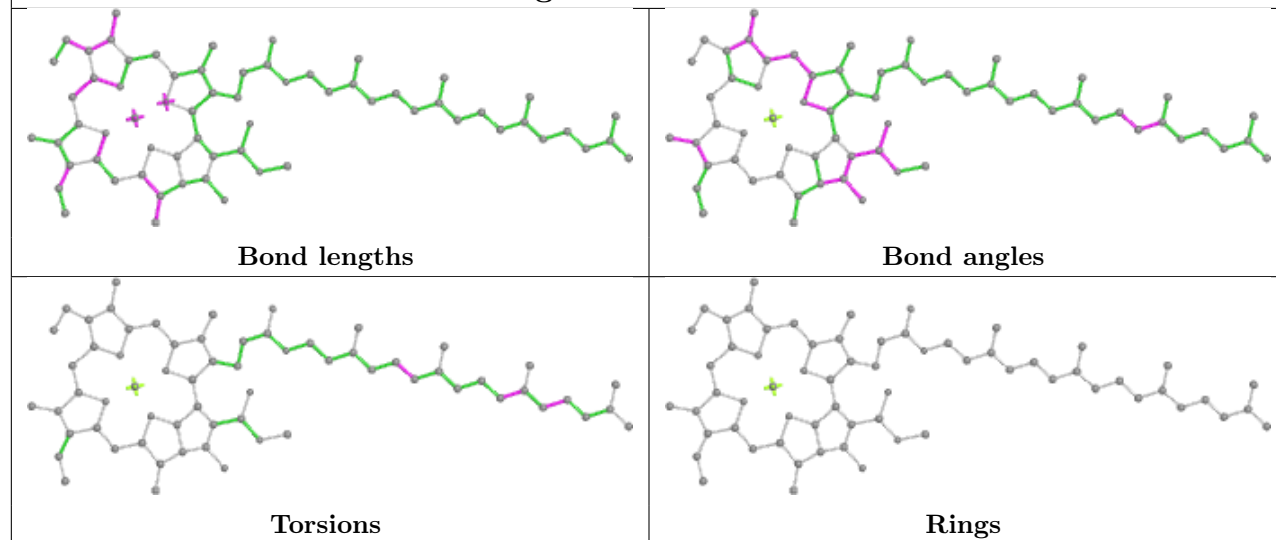
## Ligand DGD h 102



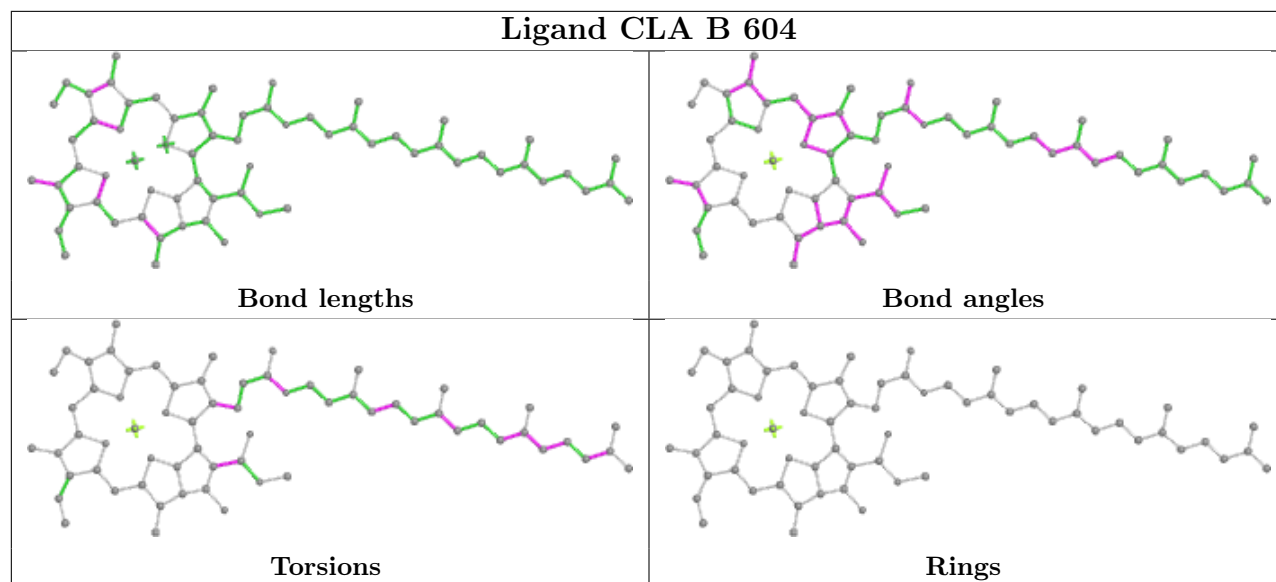
## Ligand BCR c 515



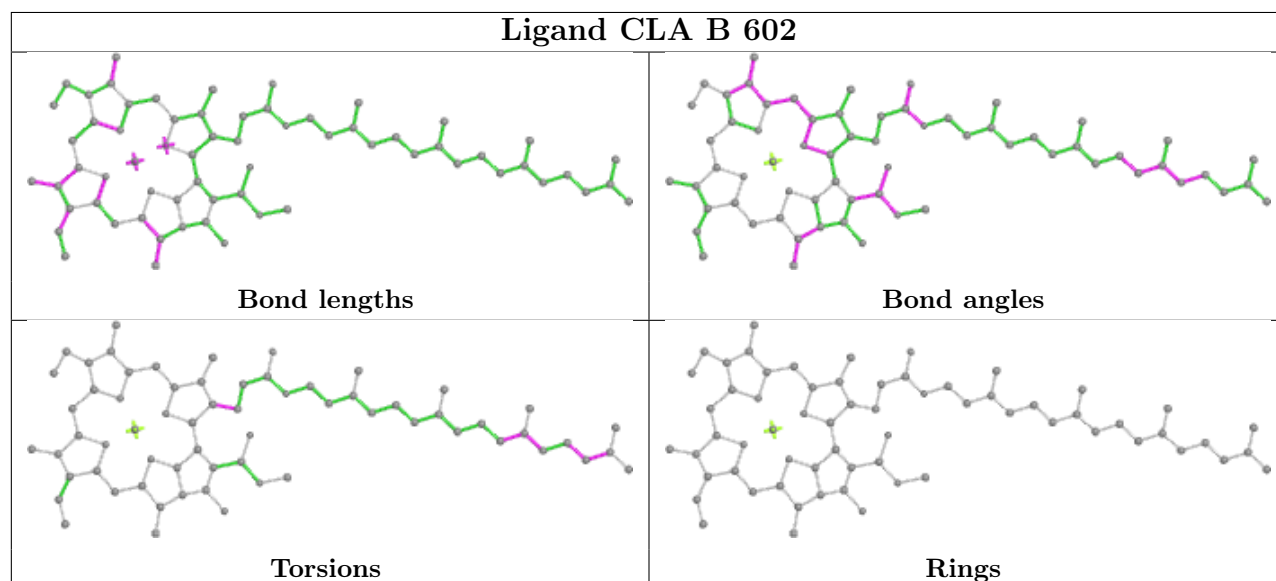


**Ligand CLA B 609****Ligand STE H 103****Ligand CLA b 603**

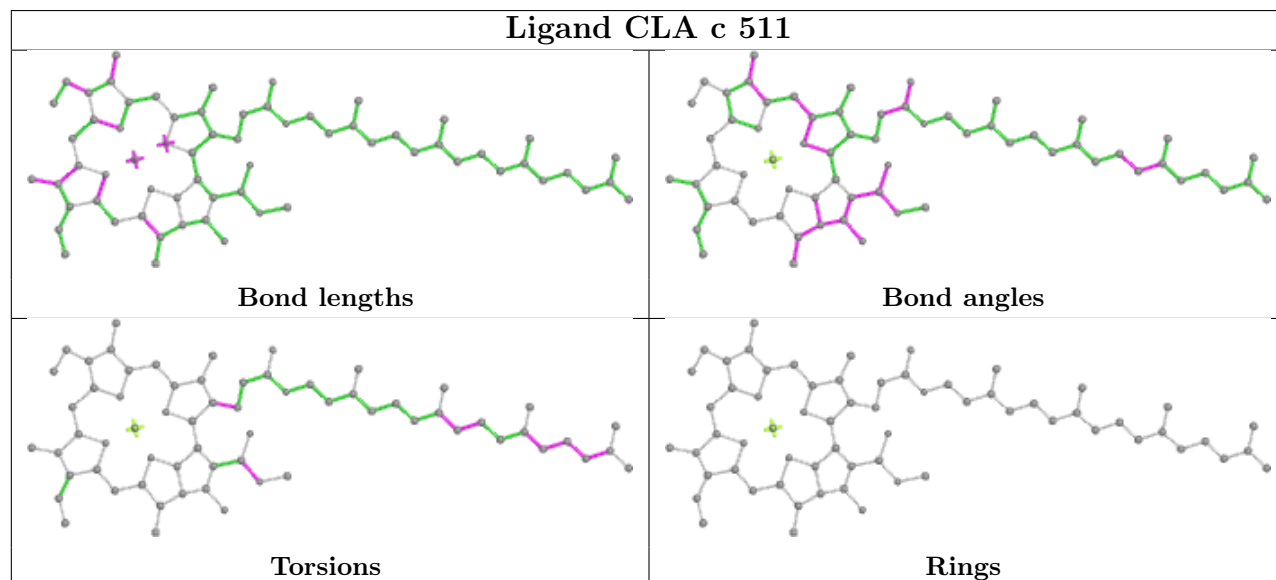
## Ligand CLA B 604

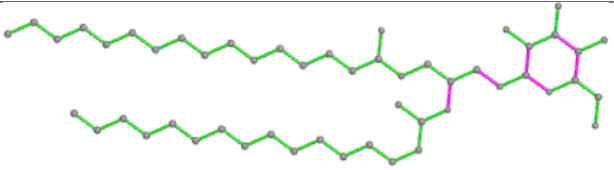
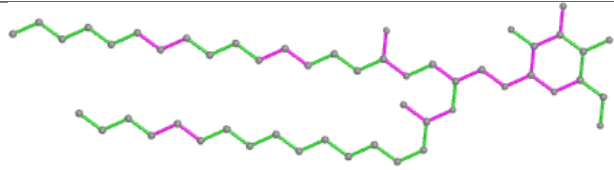
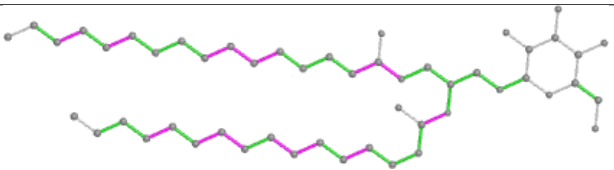
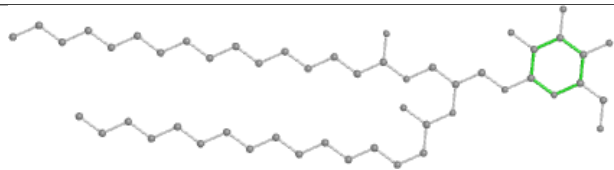


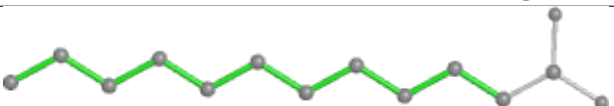
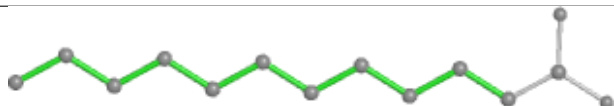
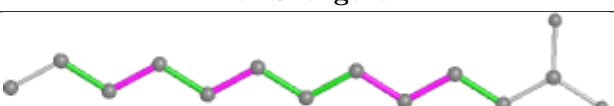
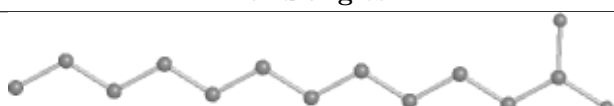
## Ligand CLA B 602

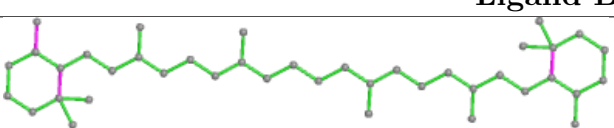
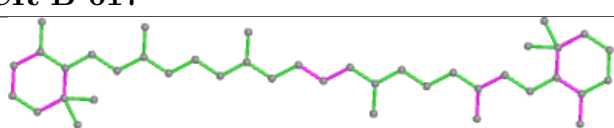
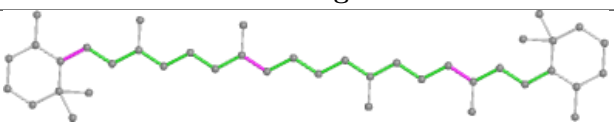
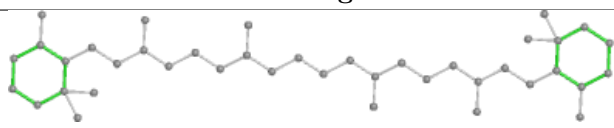


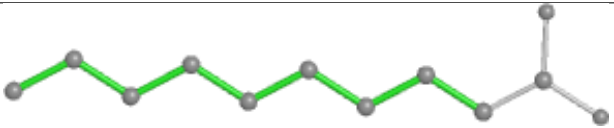
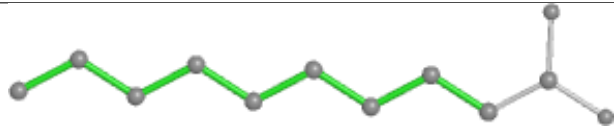
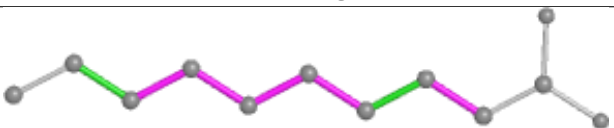
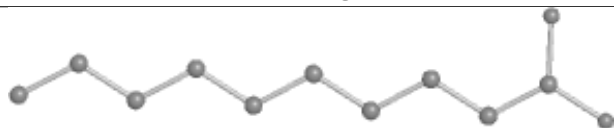
## Ligand CLA c 511



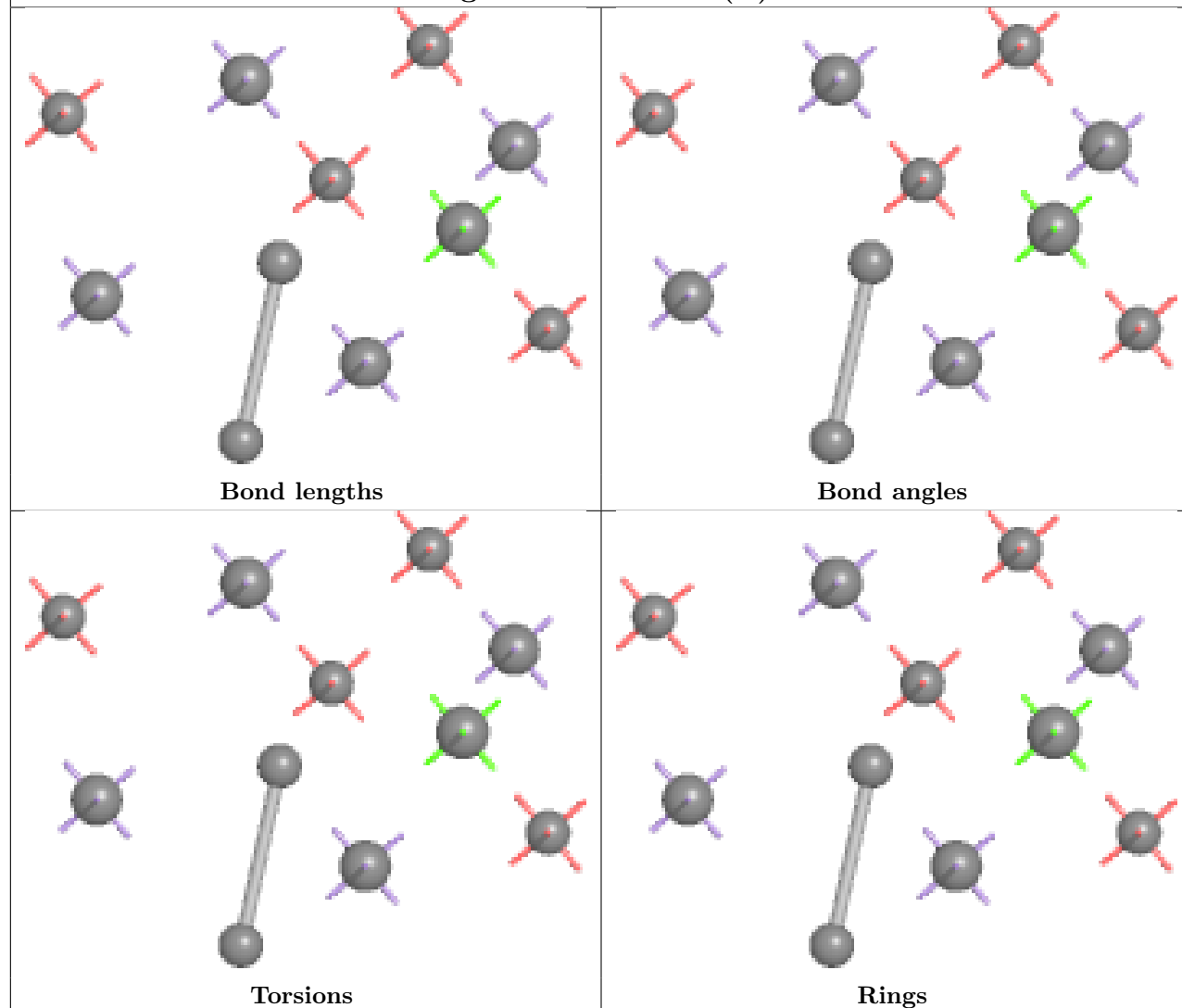
Ligand LMG b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

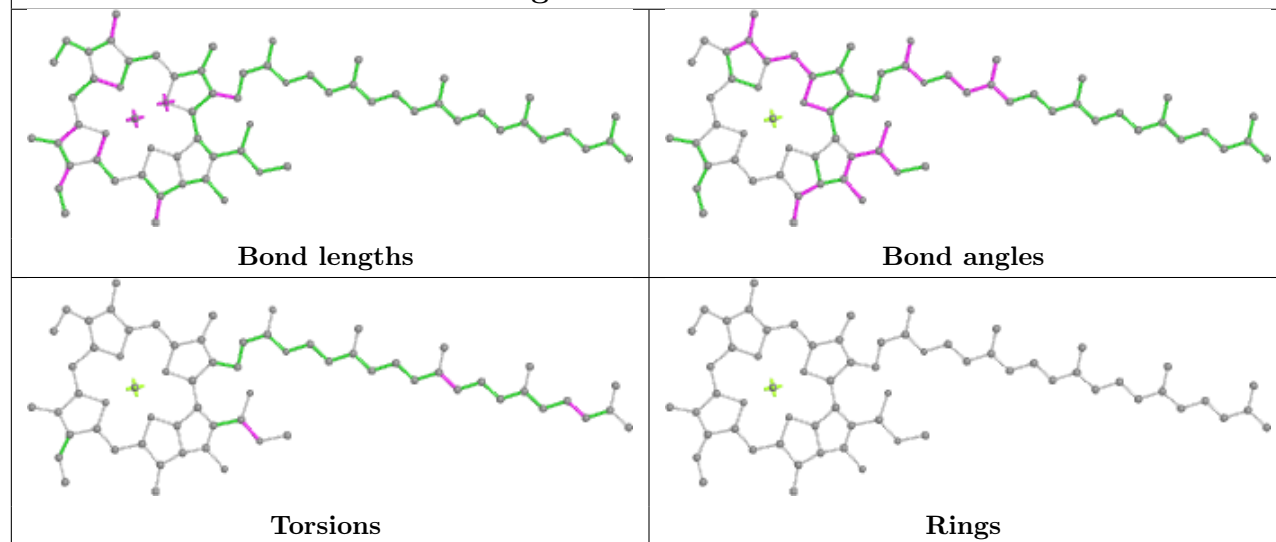
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

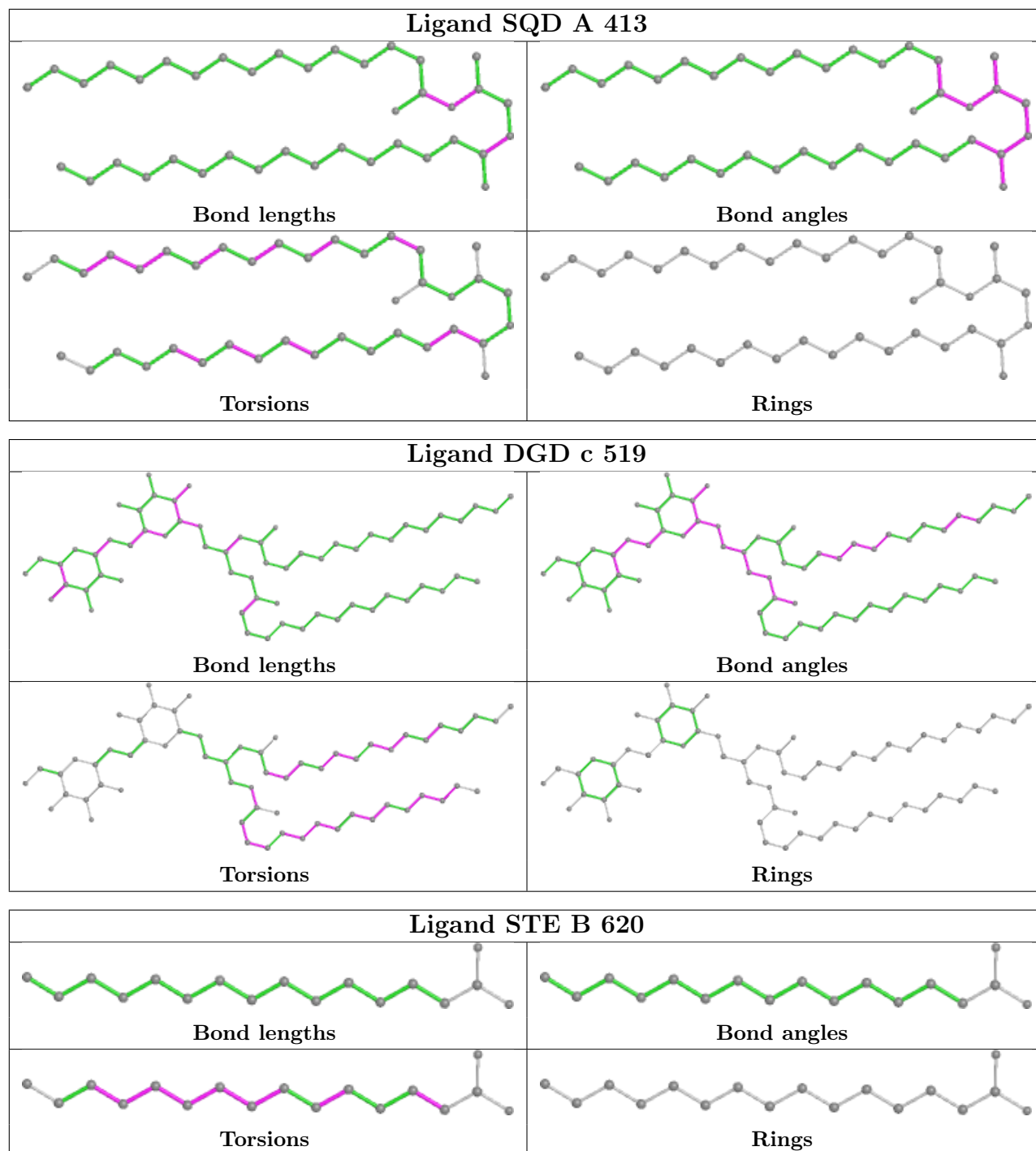
Ligand STE m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

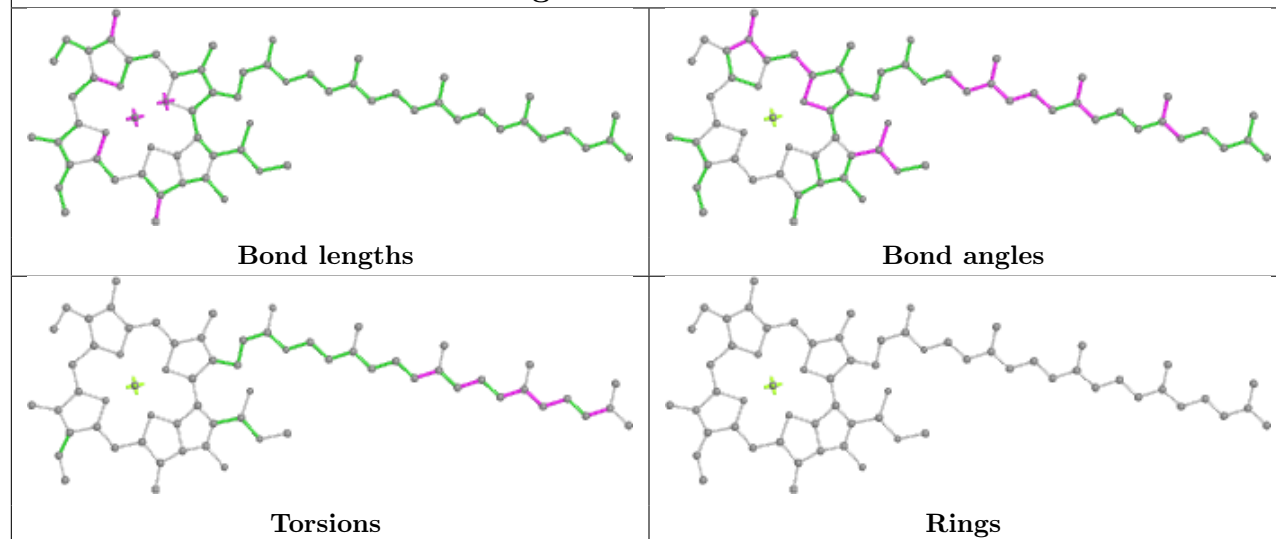
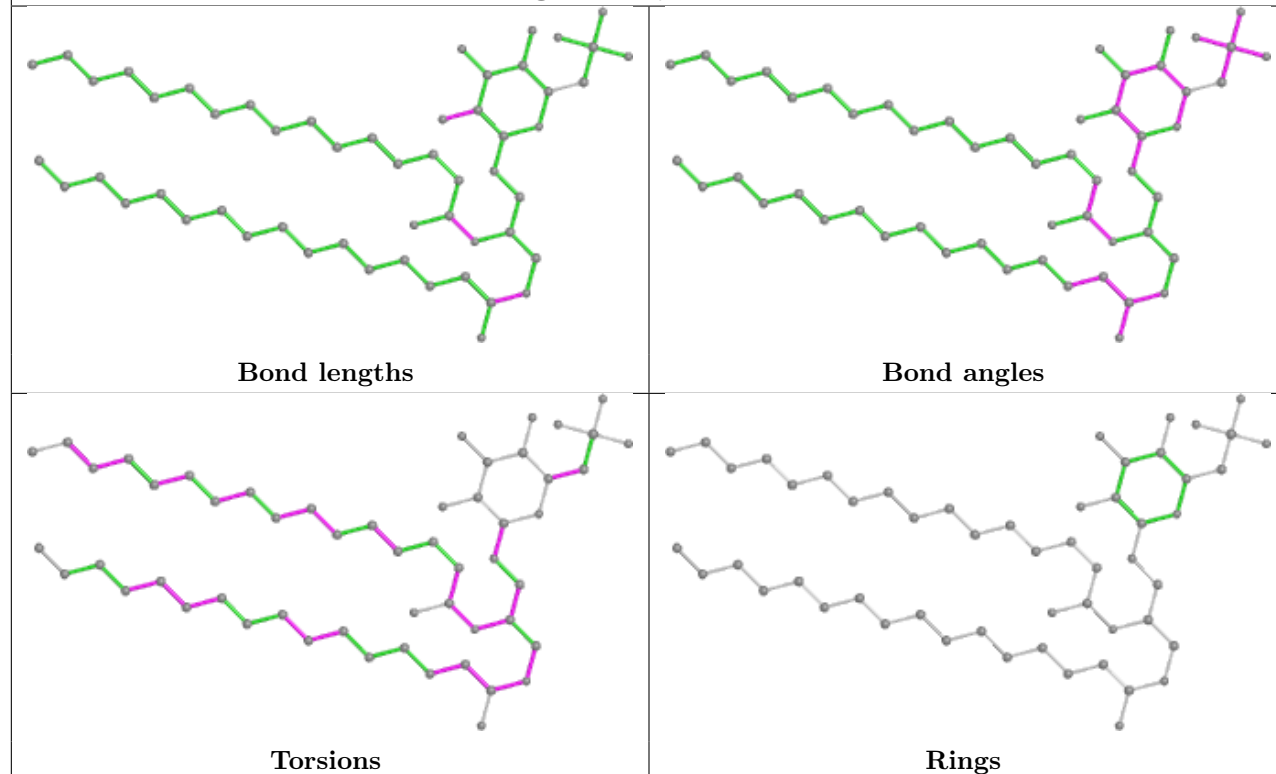
## Ligand OEY A 415 (B)

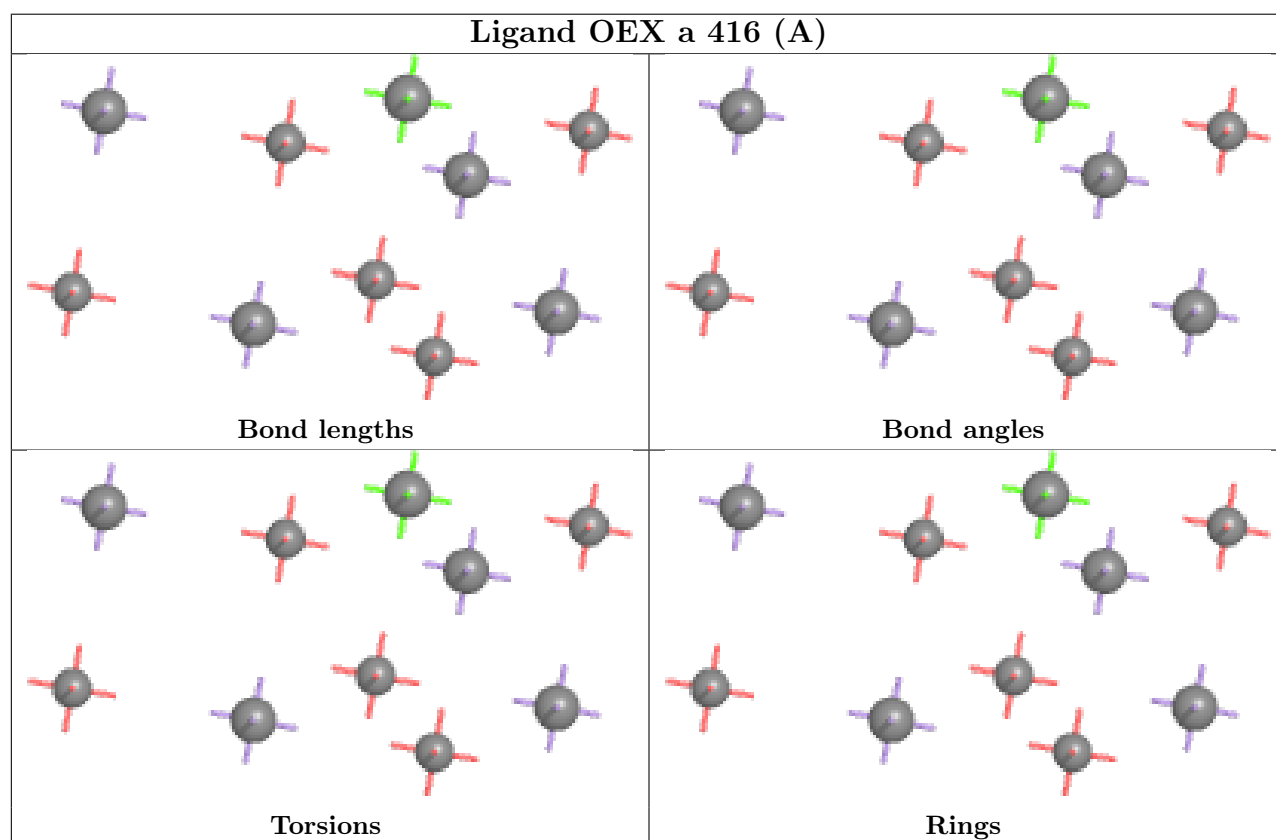
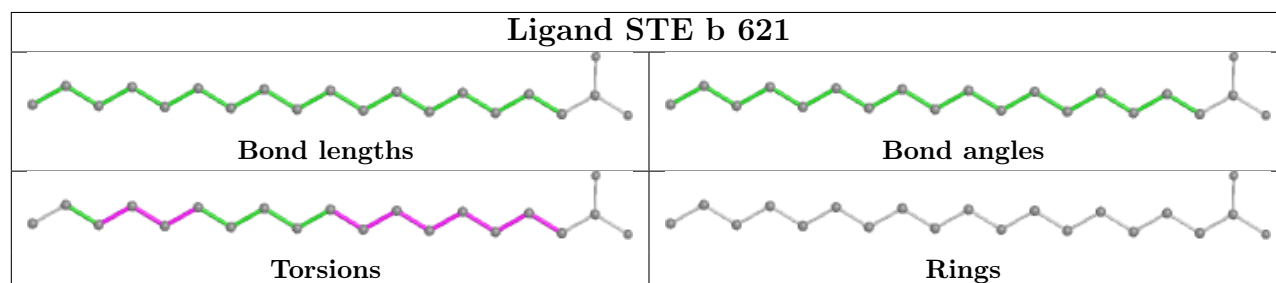
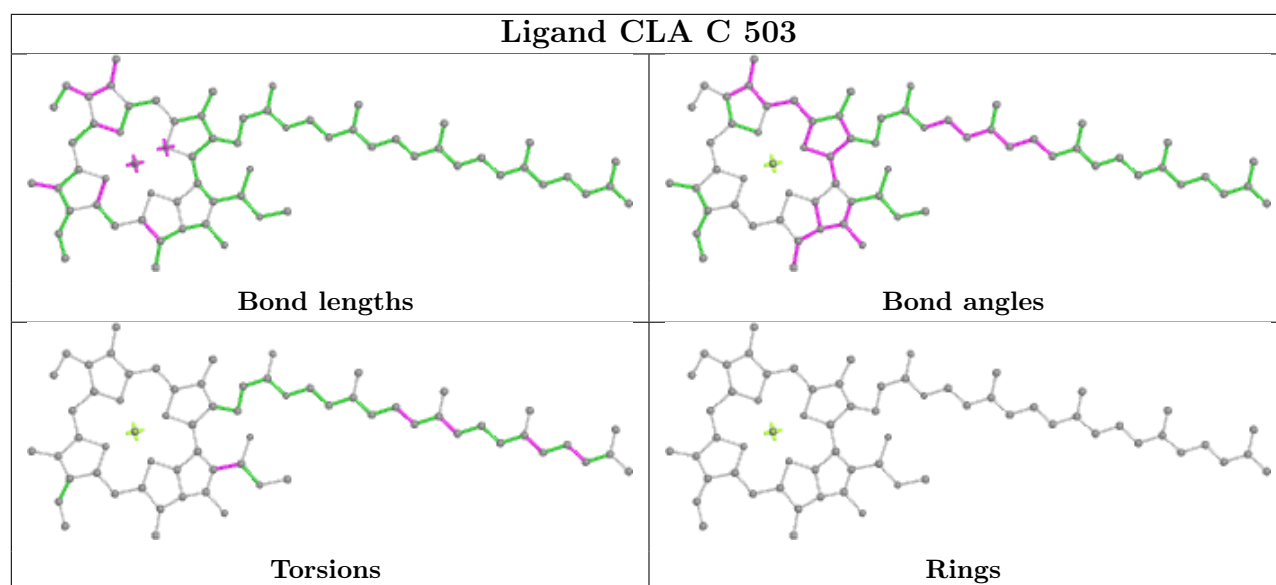


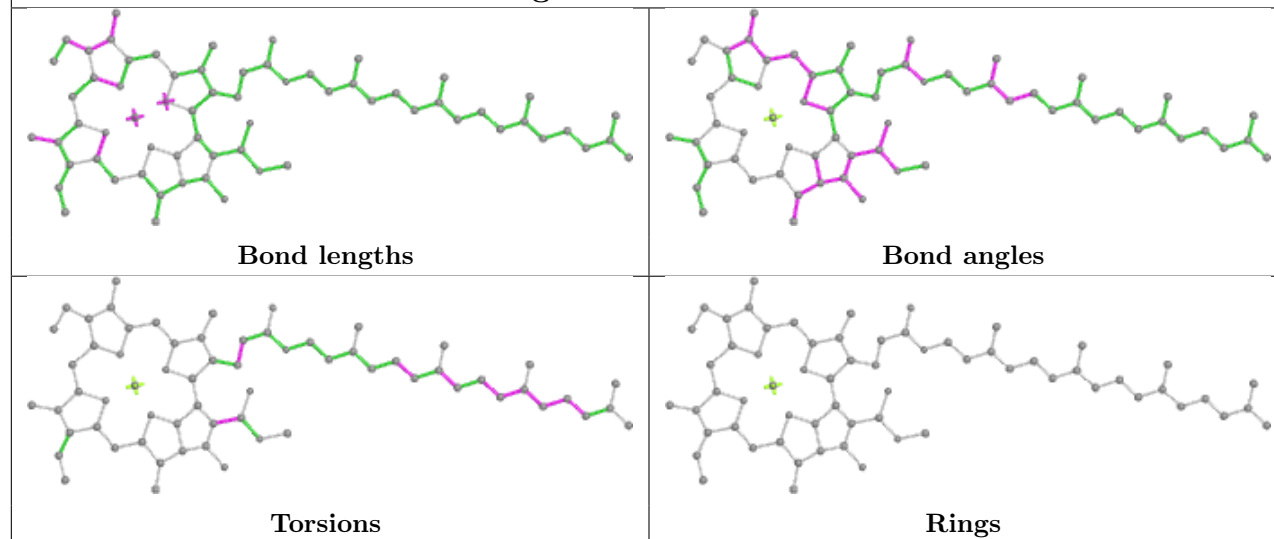
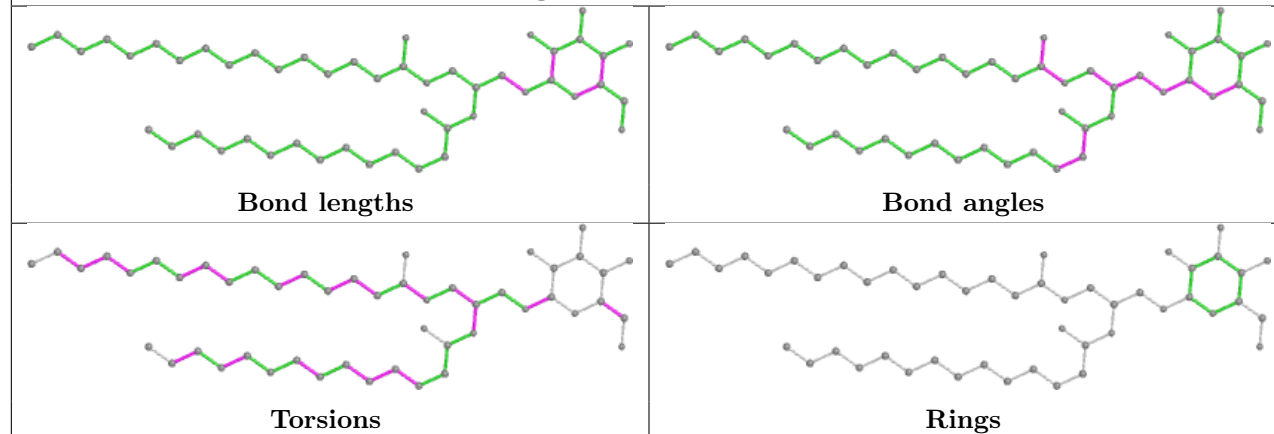
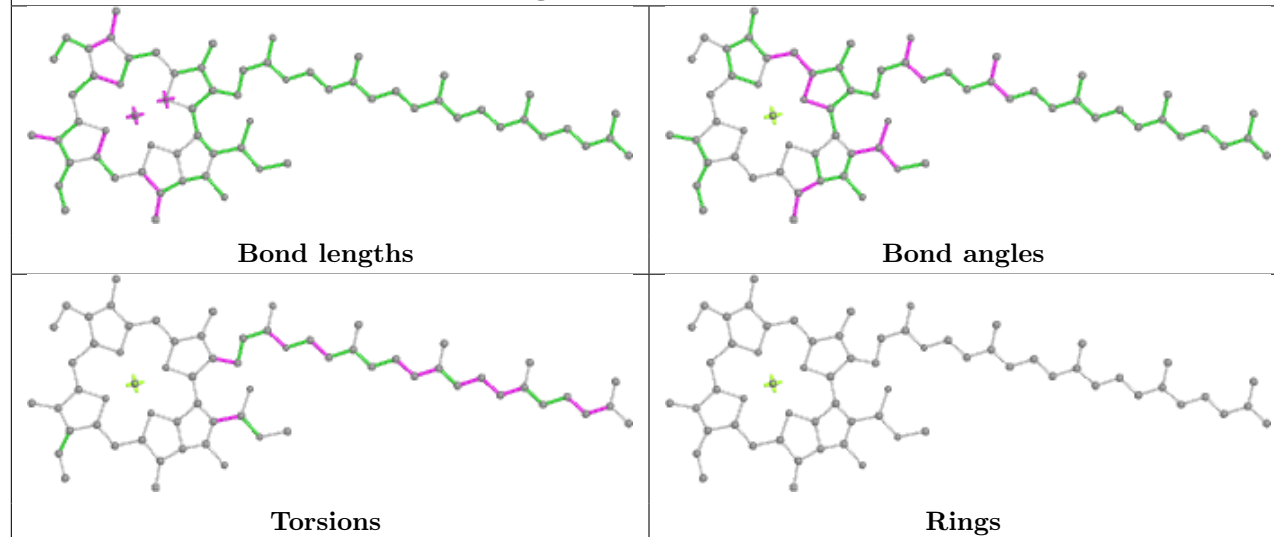
## Ligand CLA D 403



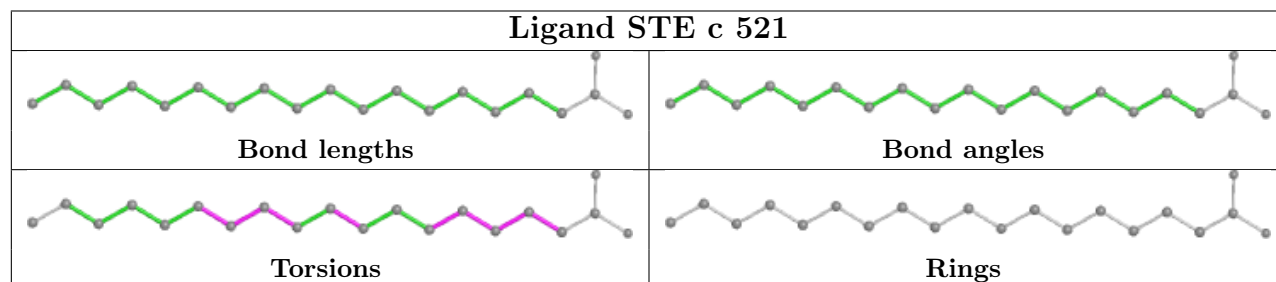
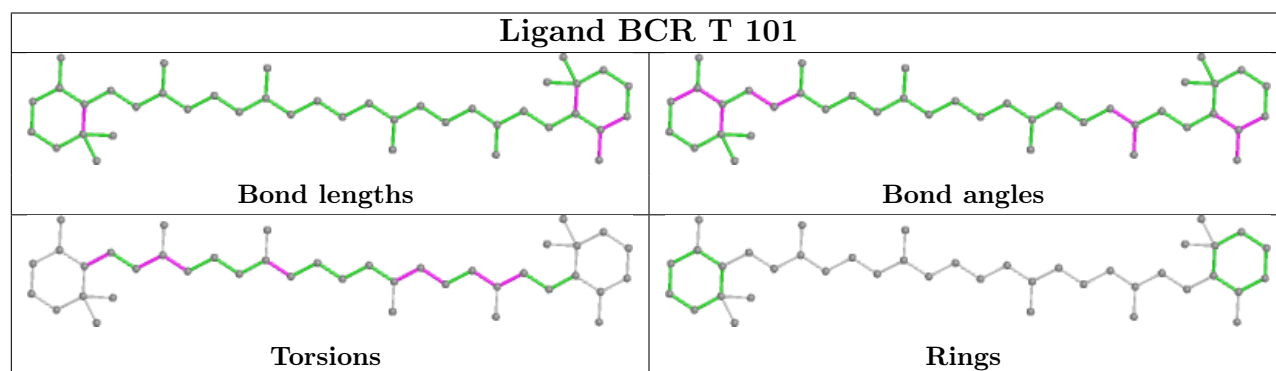
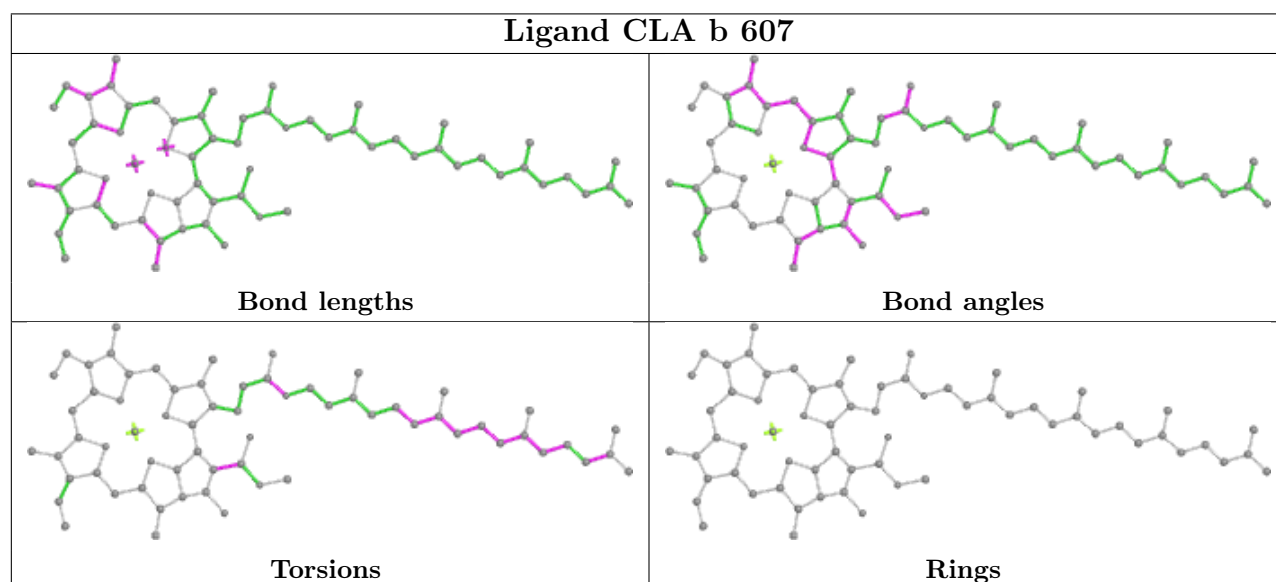
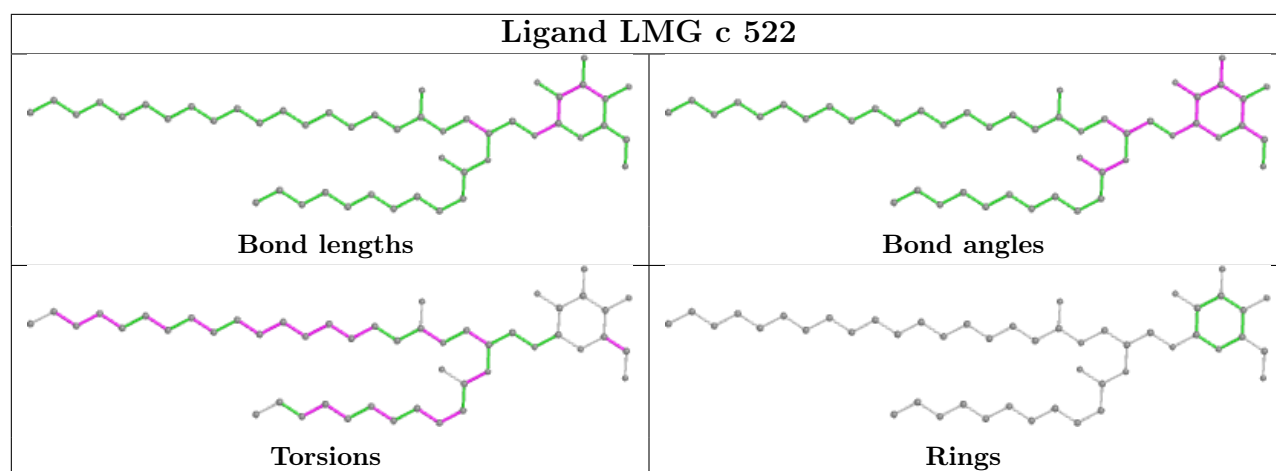


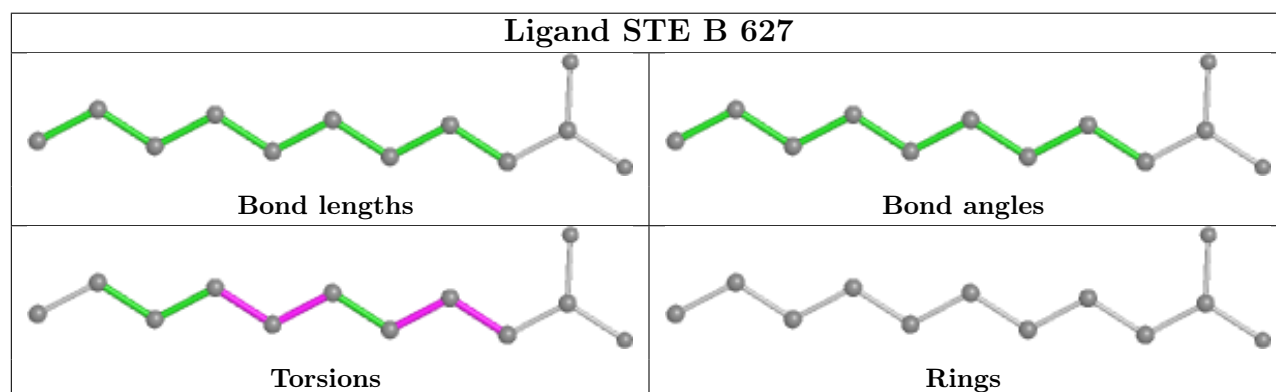
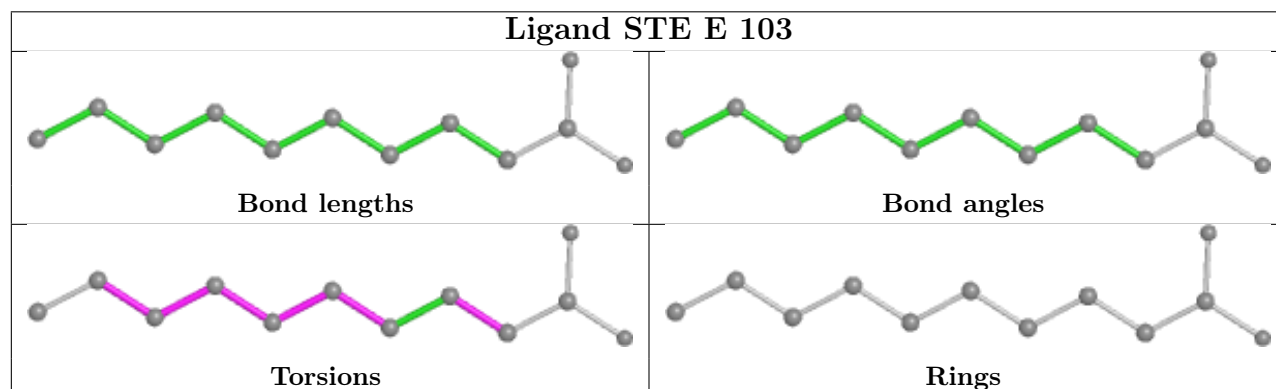
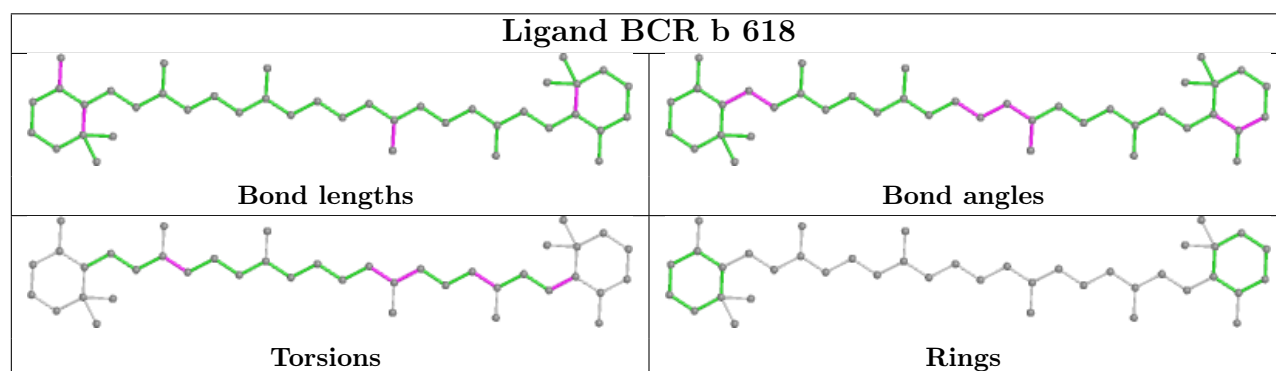
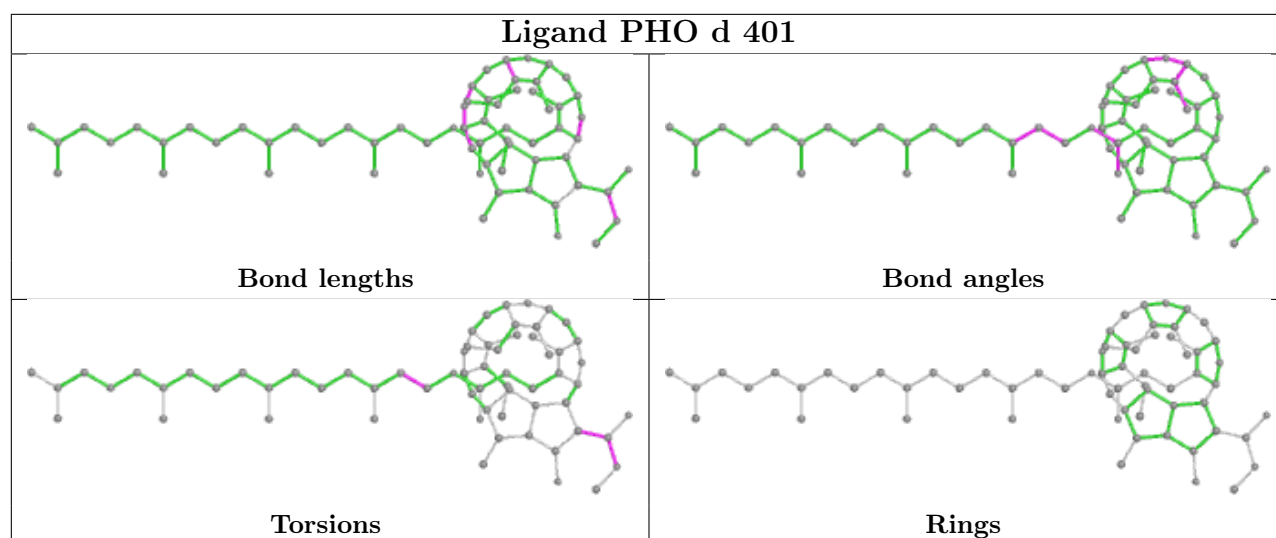
**Ligand CLA B 611****Ligand SQD B 623**



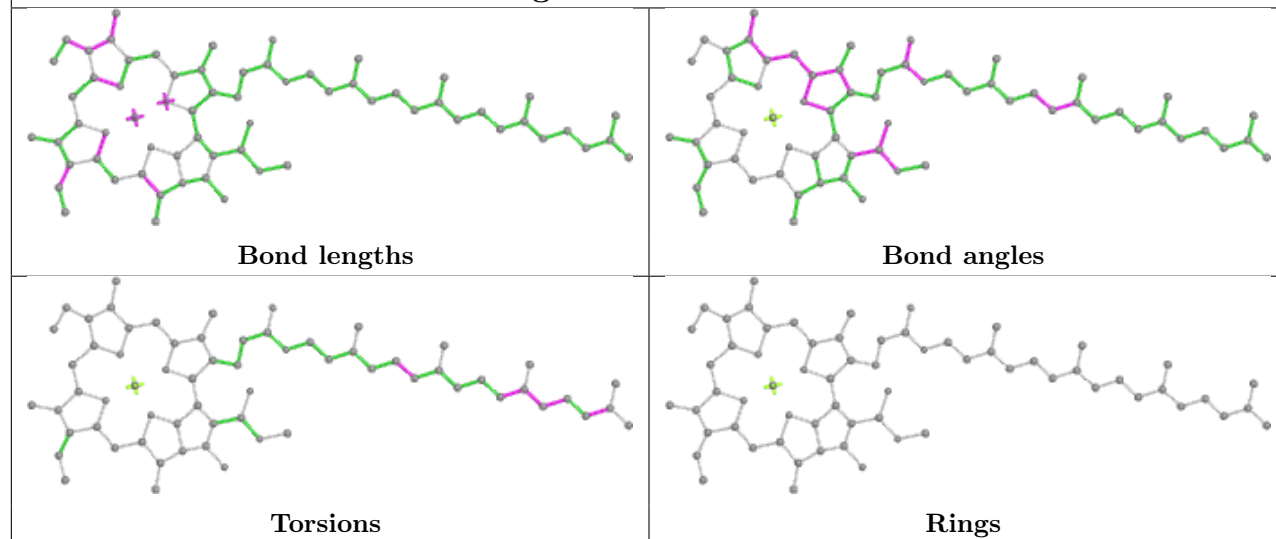
**Ligand CLA B 606****Ligand LMG c 523****Ligand CLA B 601**



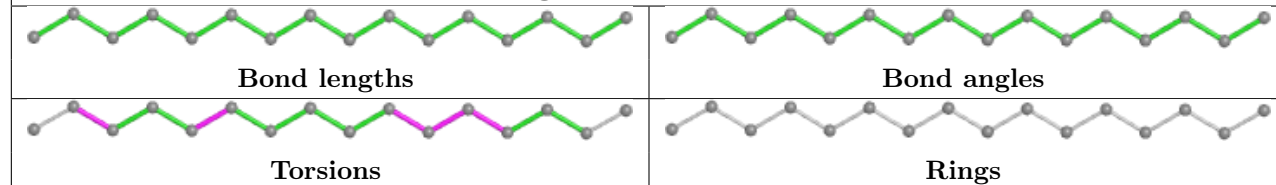




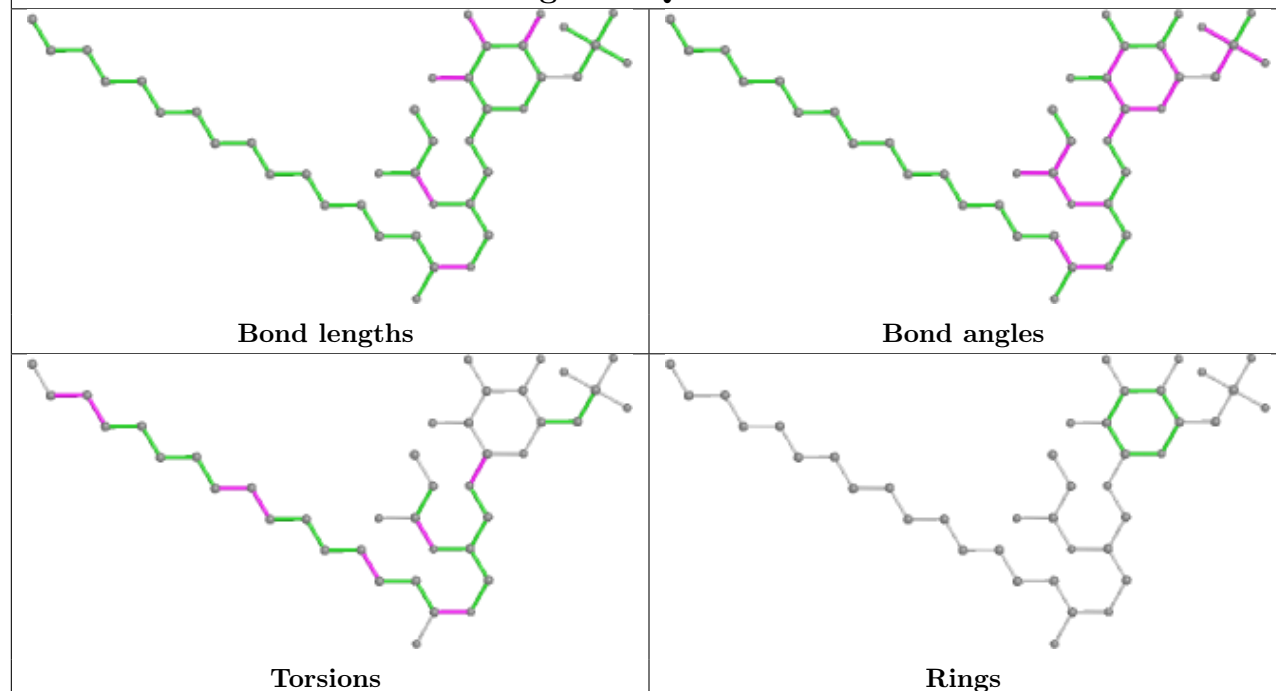
## Ligand CLA B 615



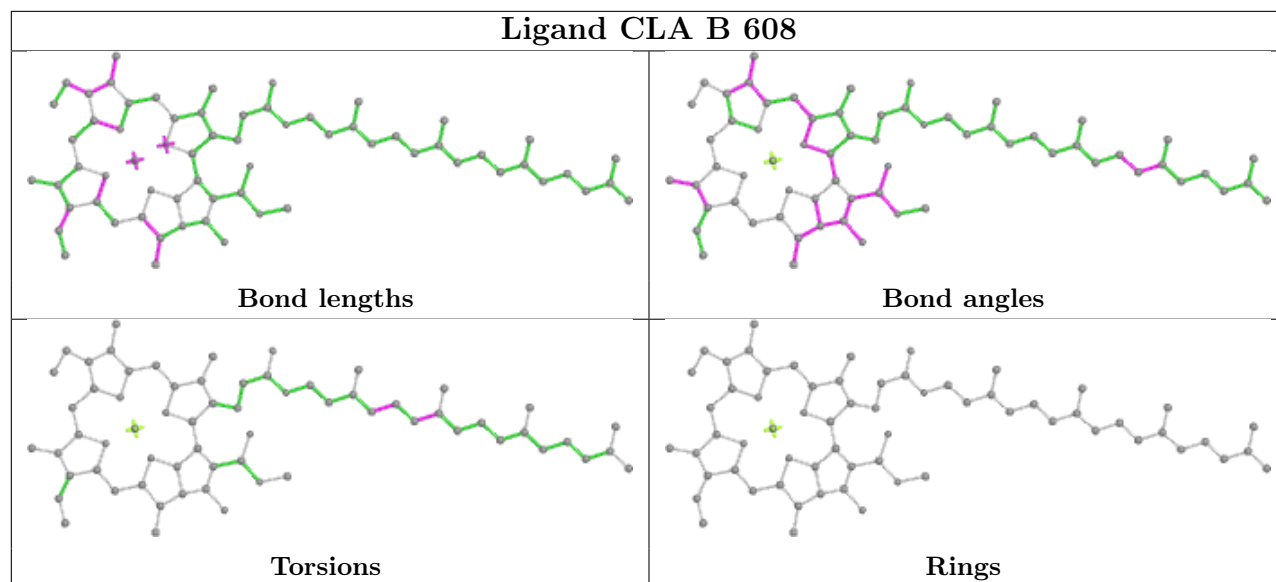
## Ligand STE T 102



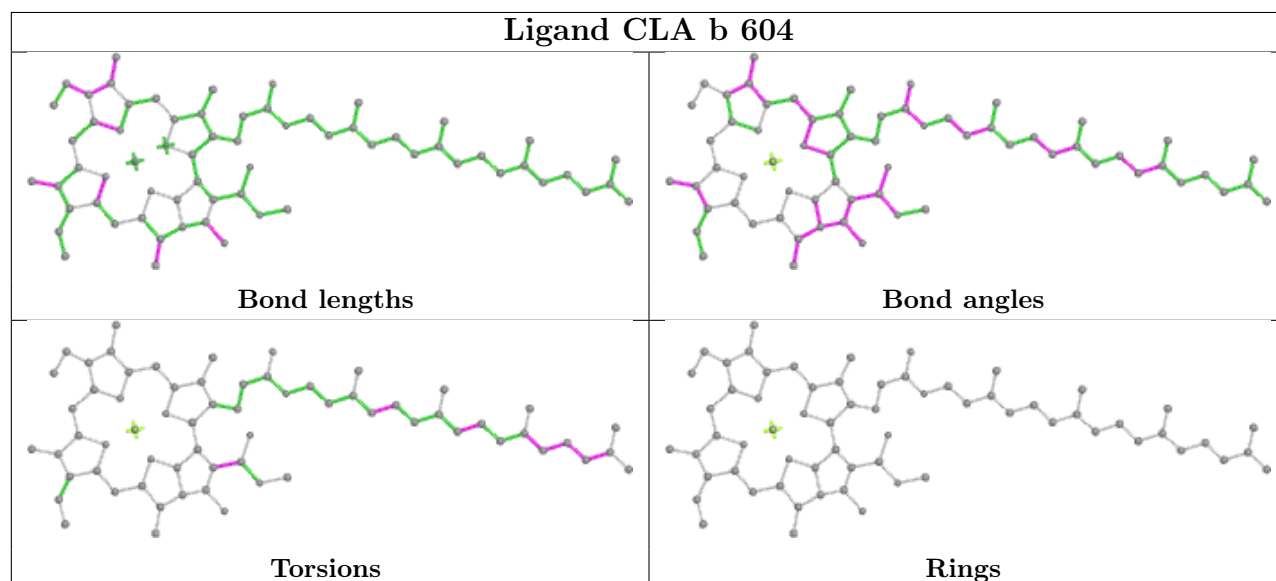
## Ligand SQD f 102



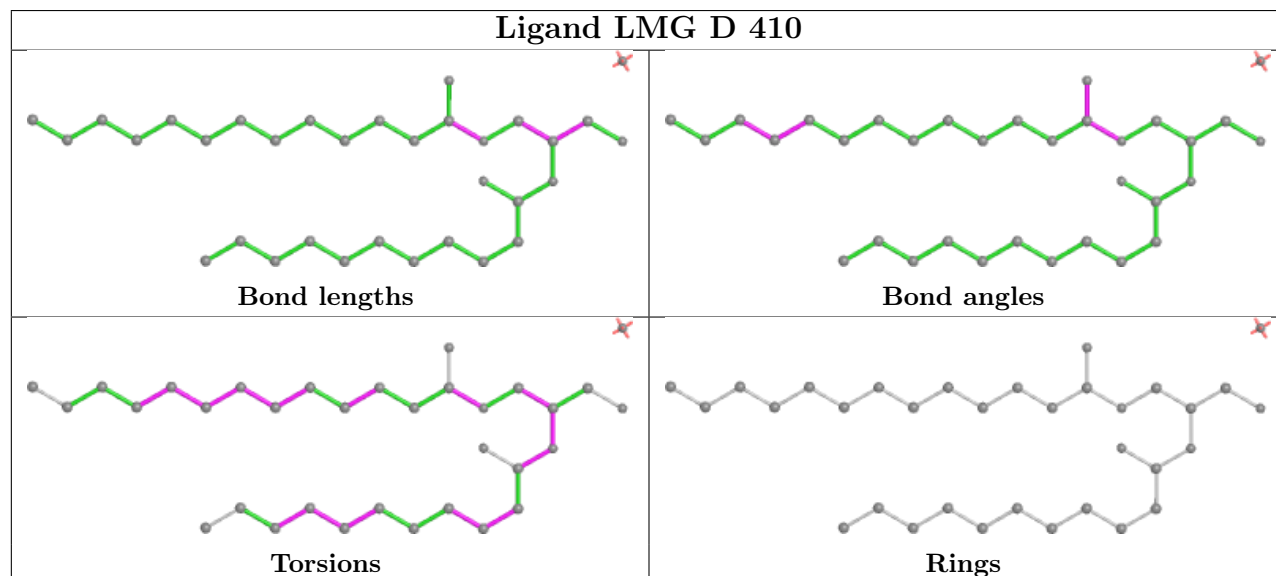
## Ligand CLA B 608

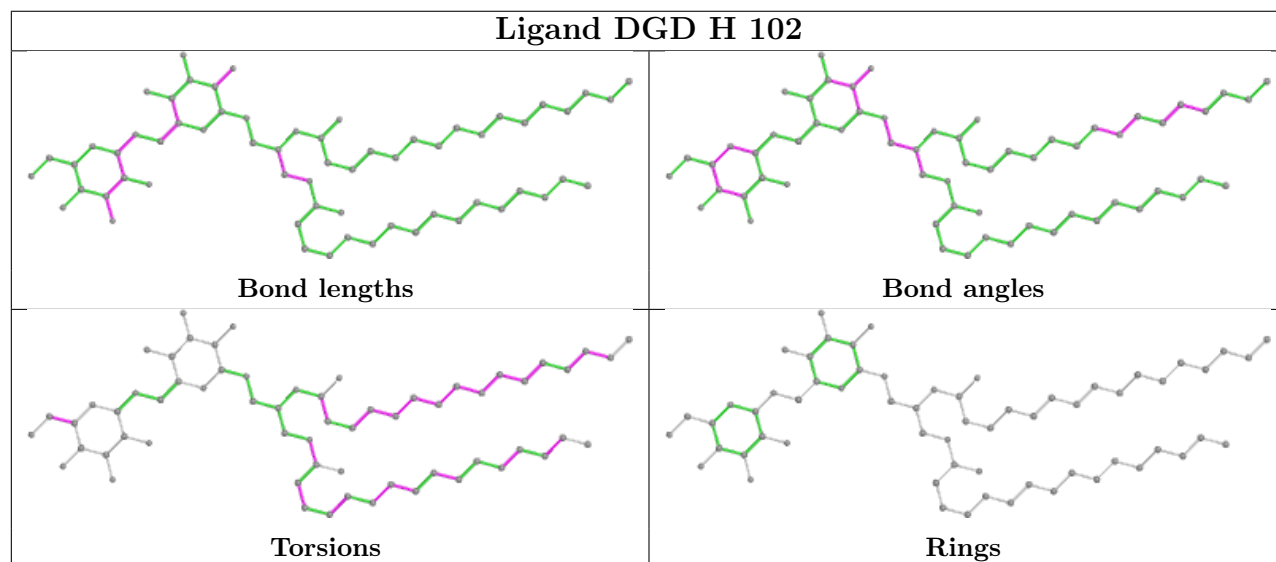
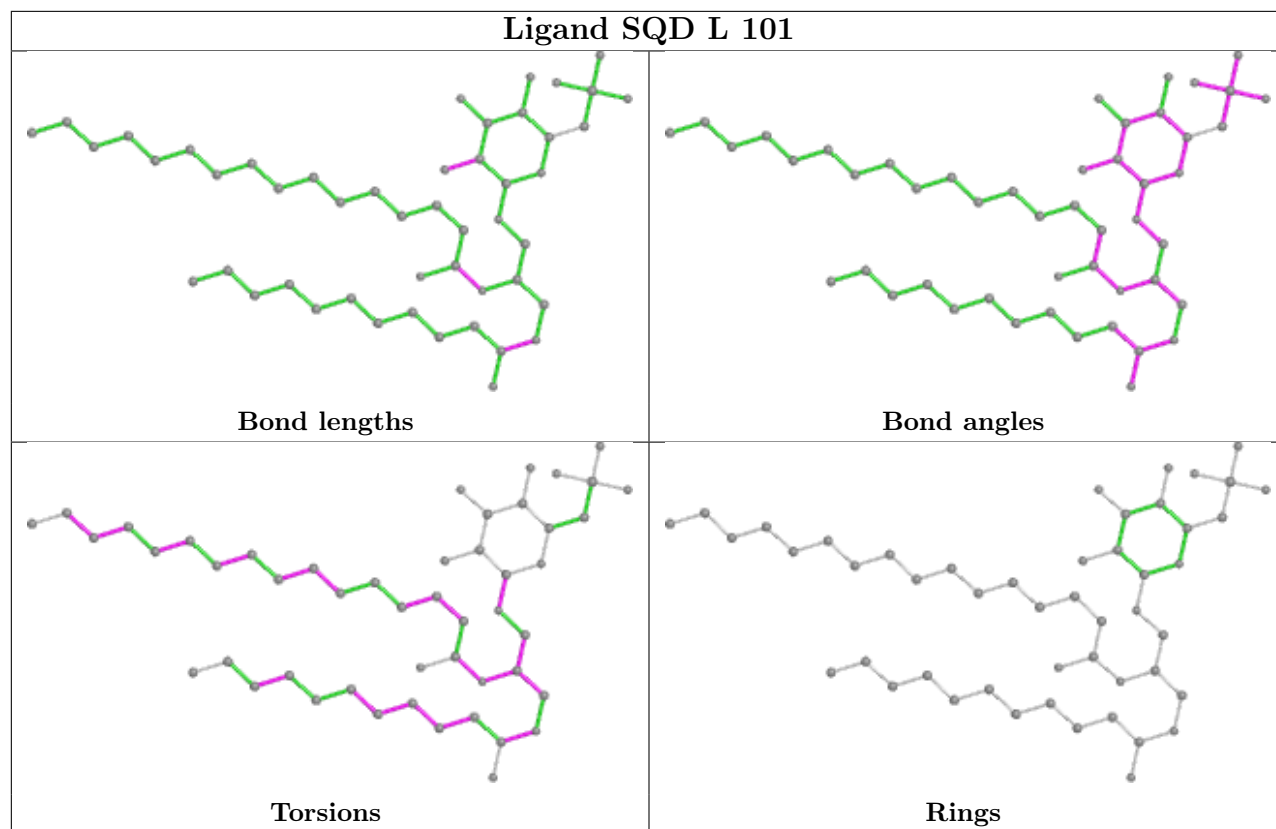


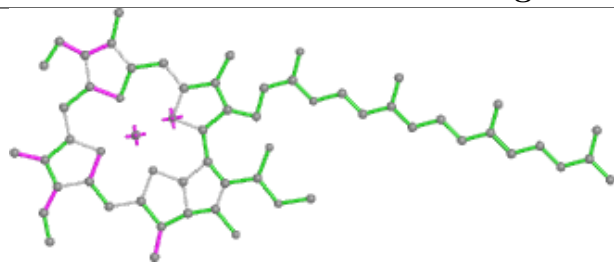
## Ligand CLA b 604



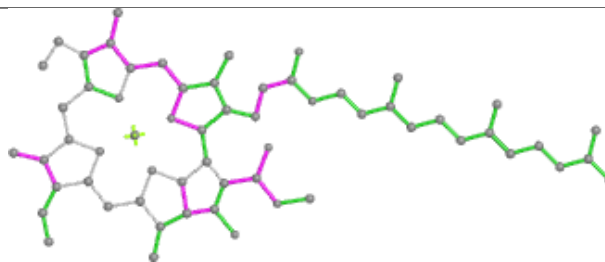
## Ligand LMG D 410



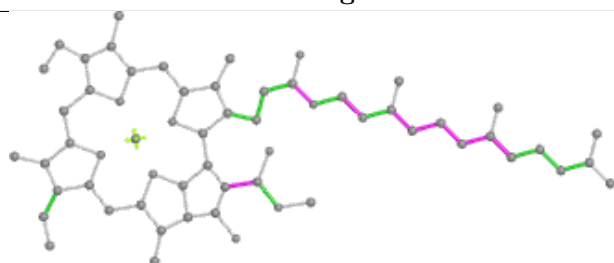


**Ligand CLA B 616**

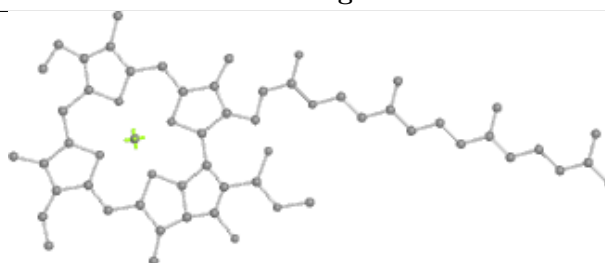
Bond lengths



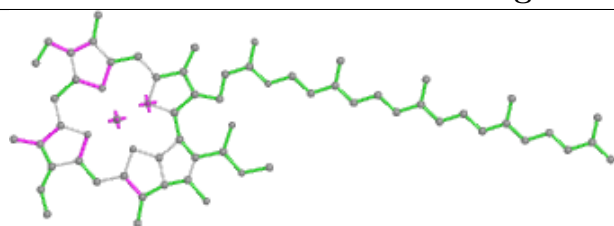
Bond angles



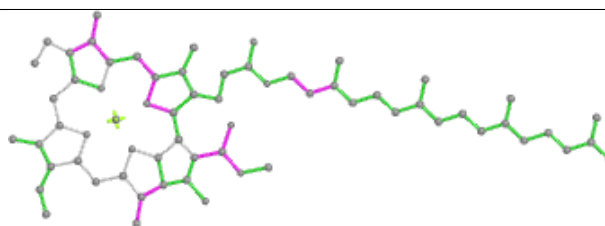
Torsions



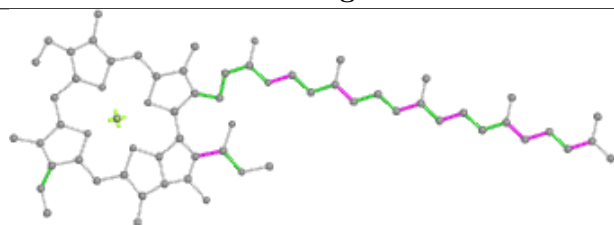
Rings

**Ligand CLA C 506**

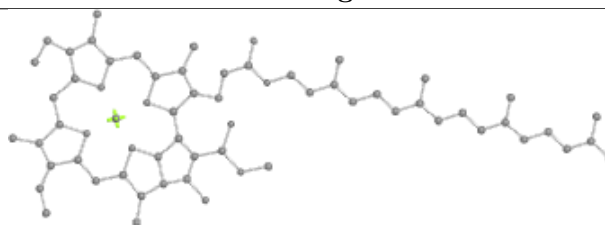
Bond lengths



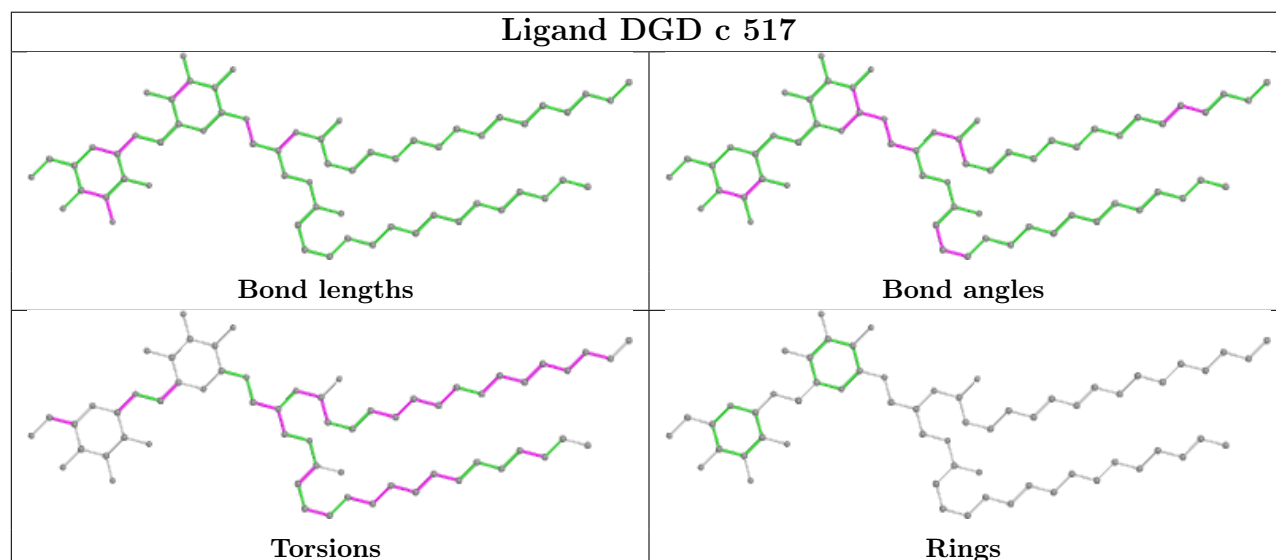
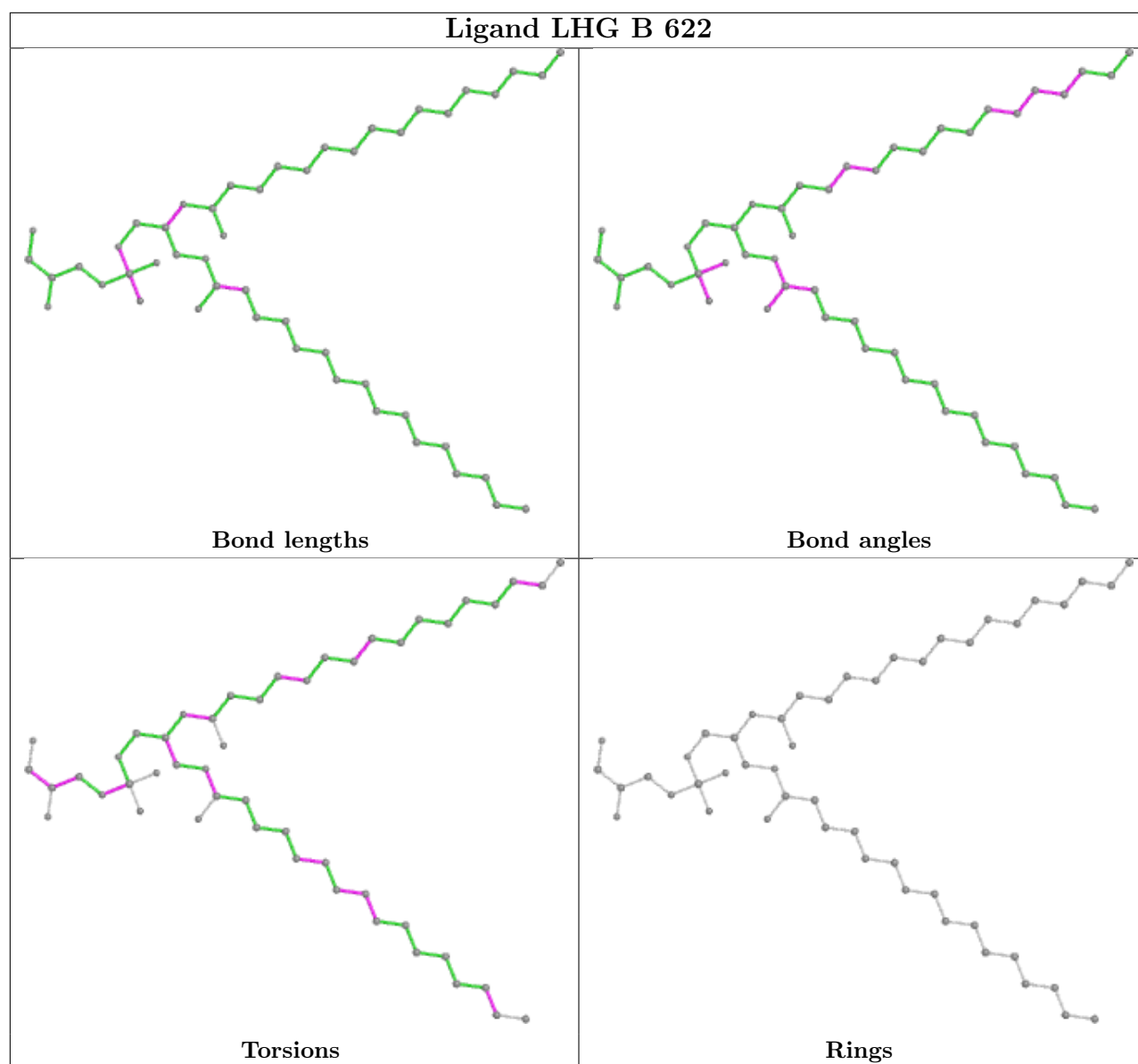
Bond angles



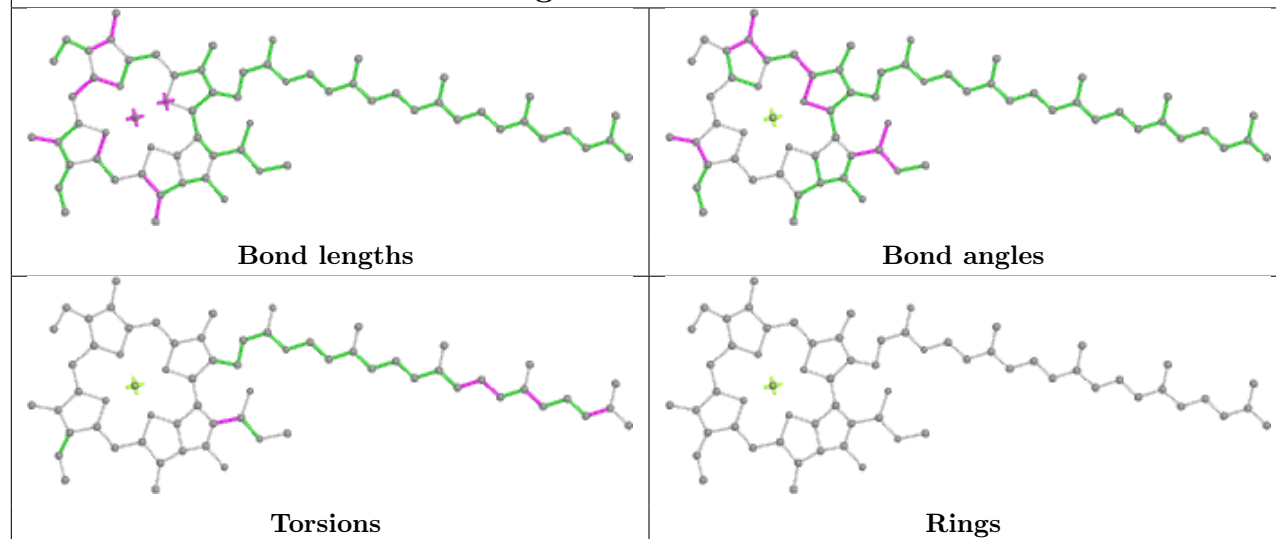
Torsions



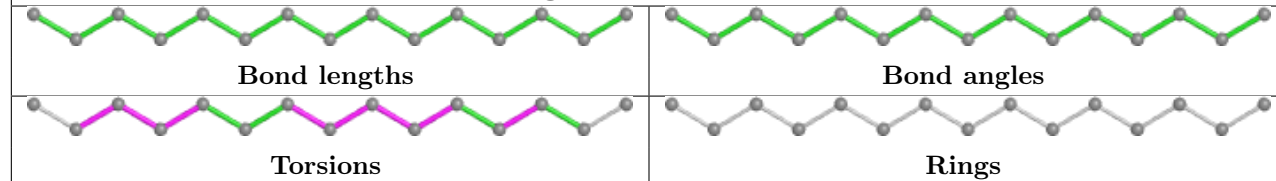
Rings



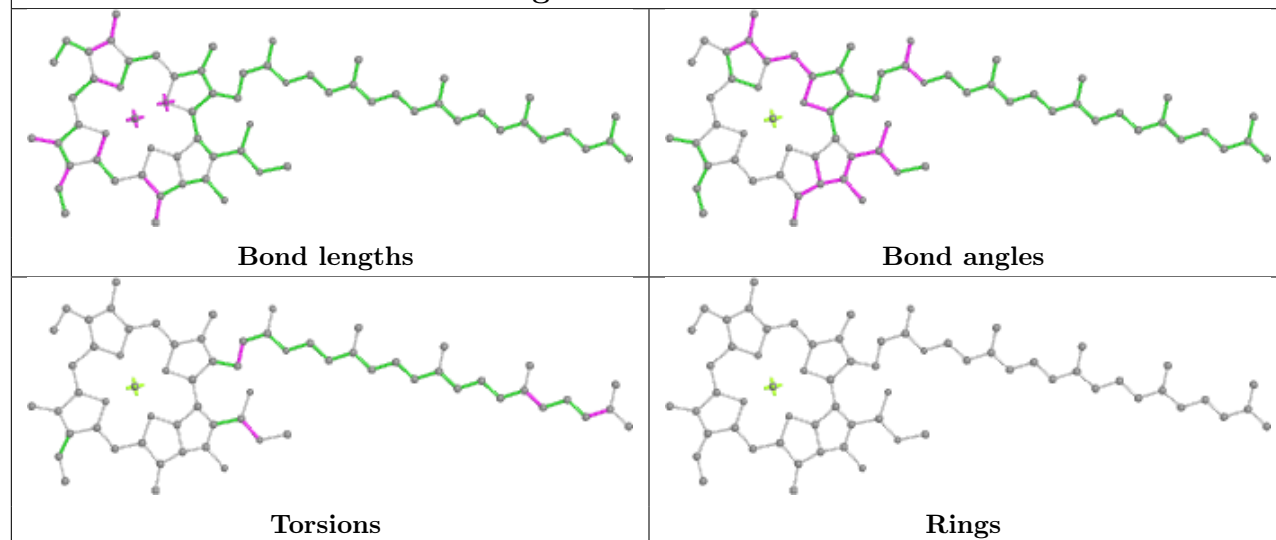
## Ligand CLA b 611



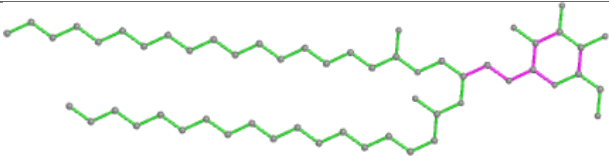
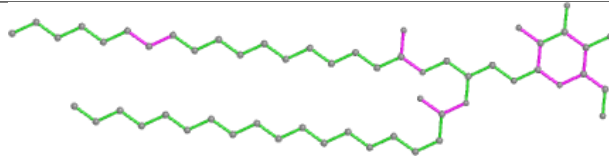
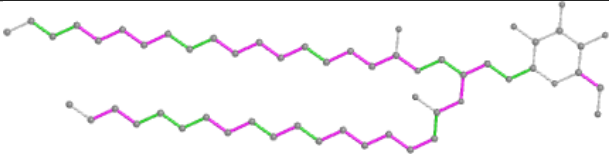

## Ligand STE I 101

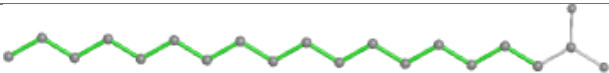
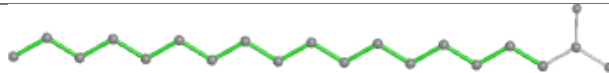
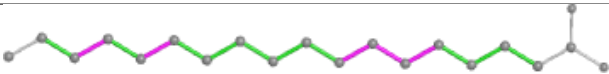
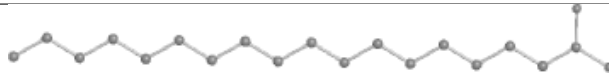


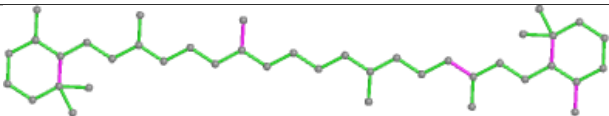
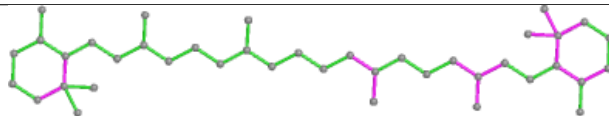
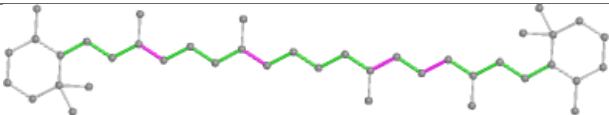
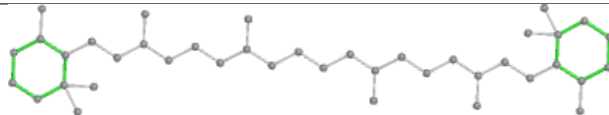
## Ligand CLA C 501

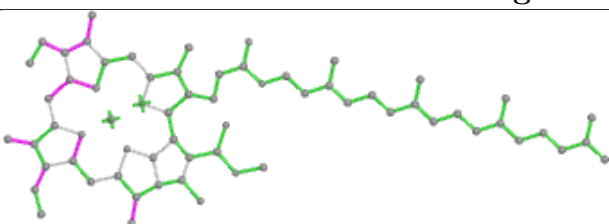
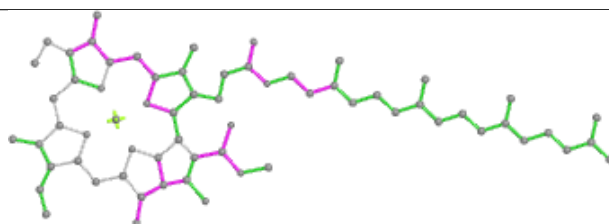
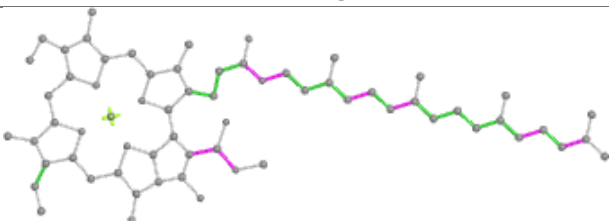
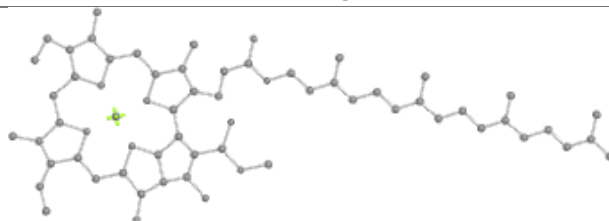




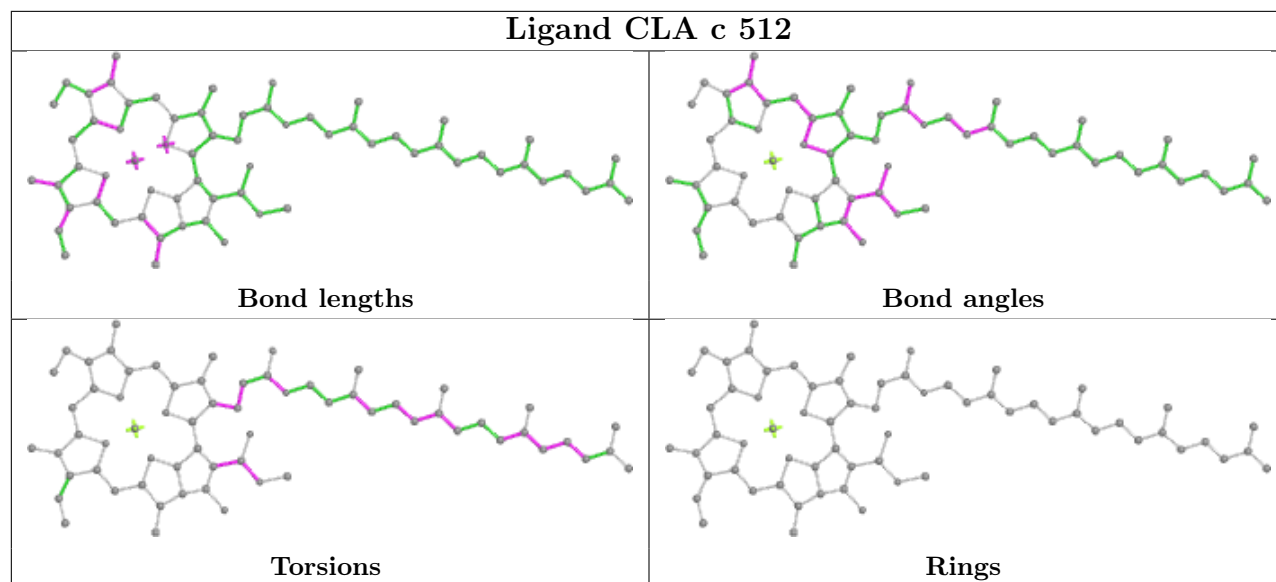
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

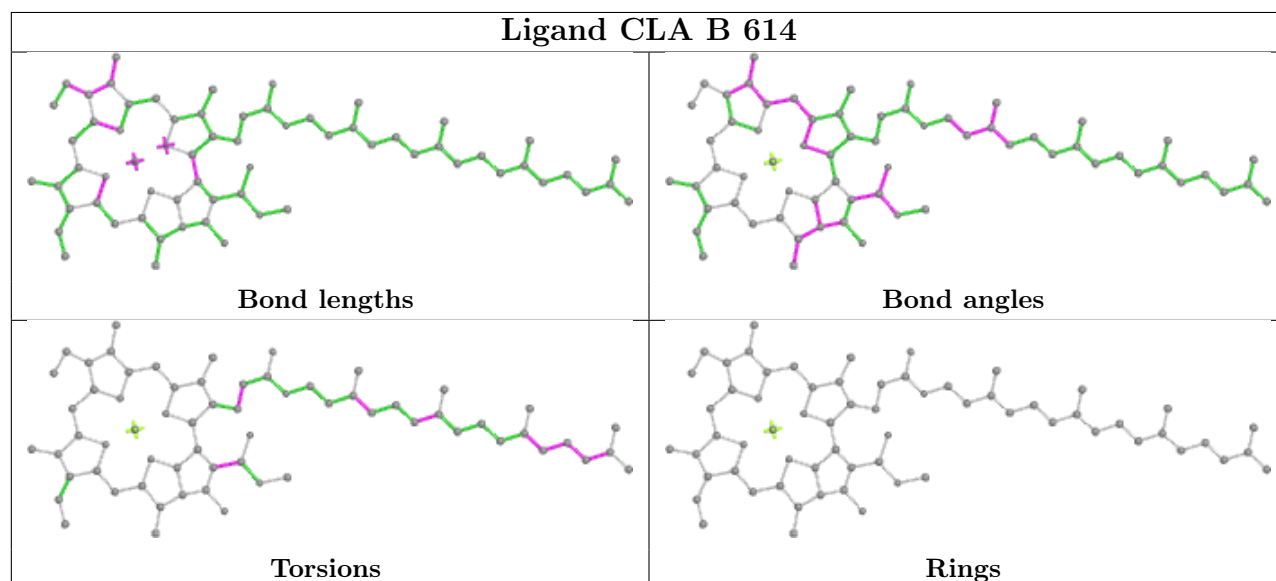
Ligand BCR a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

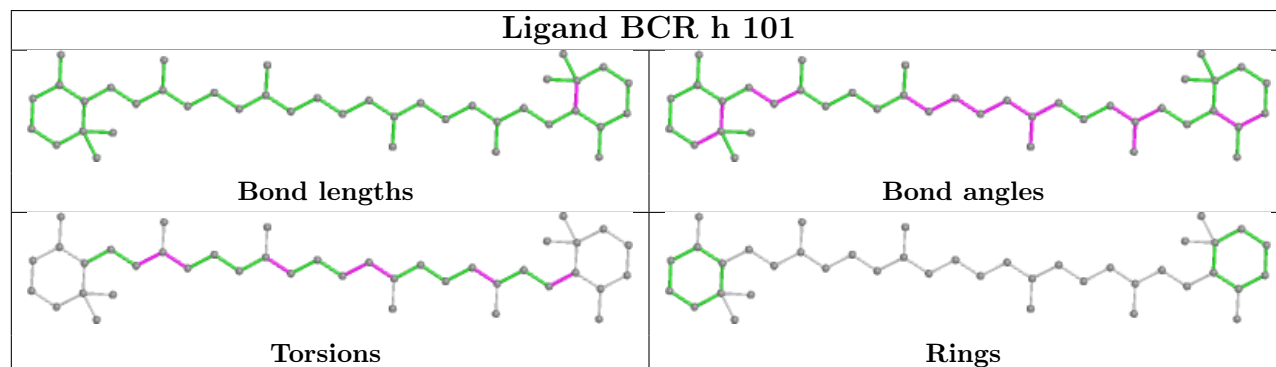
## Ligand CLA c 512

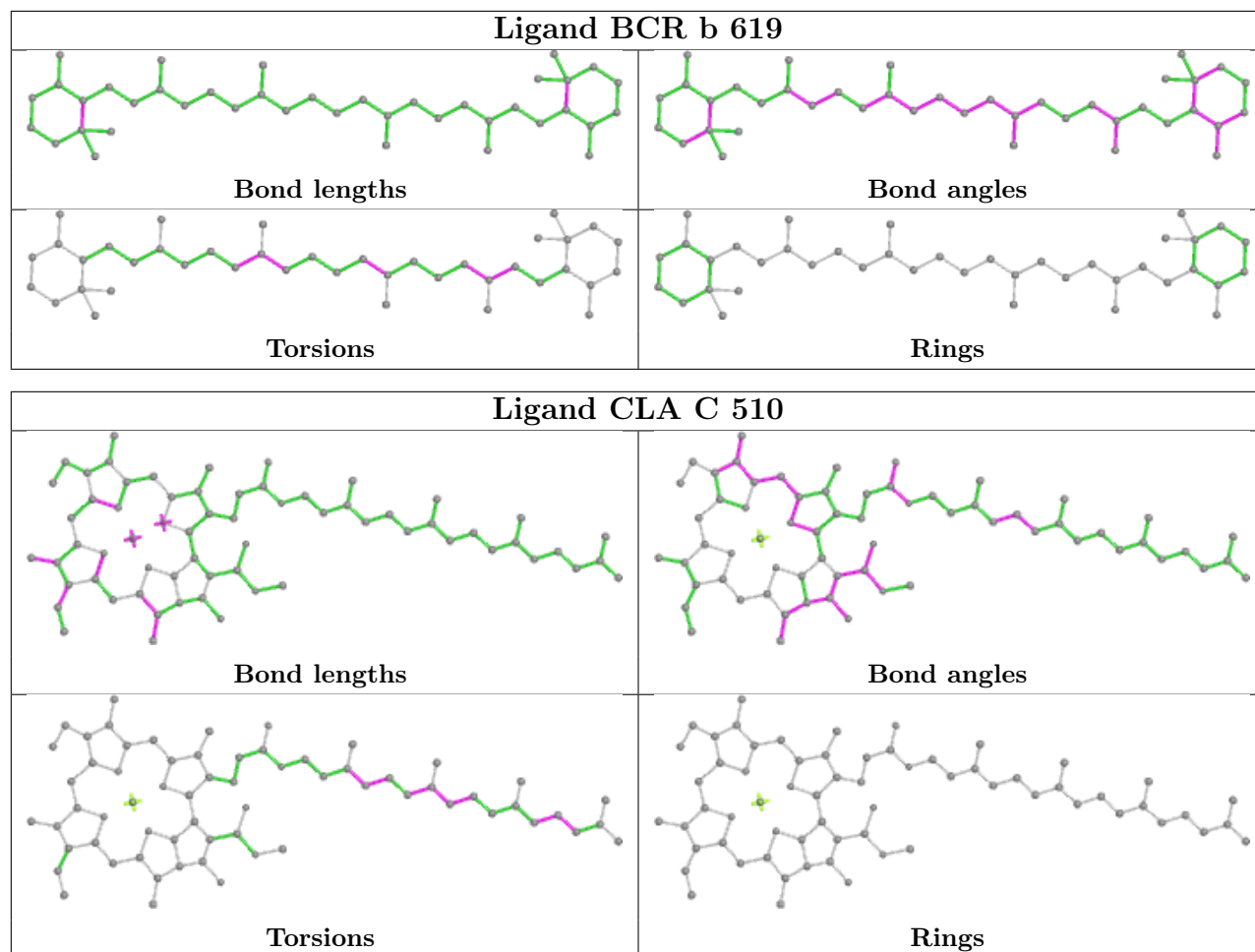


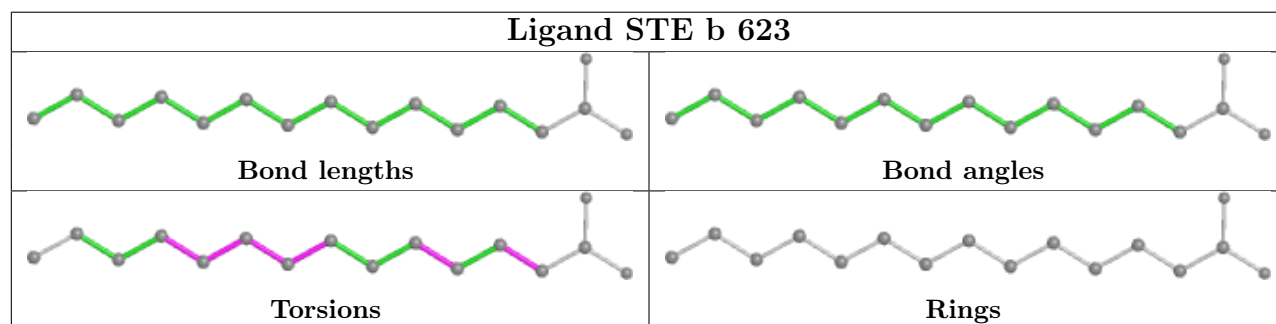
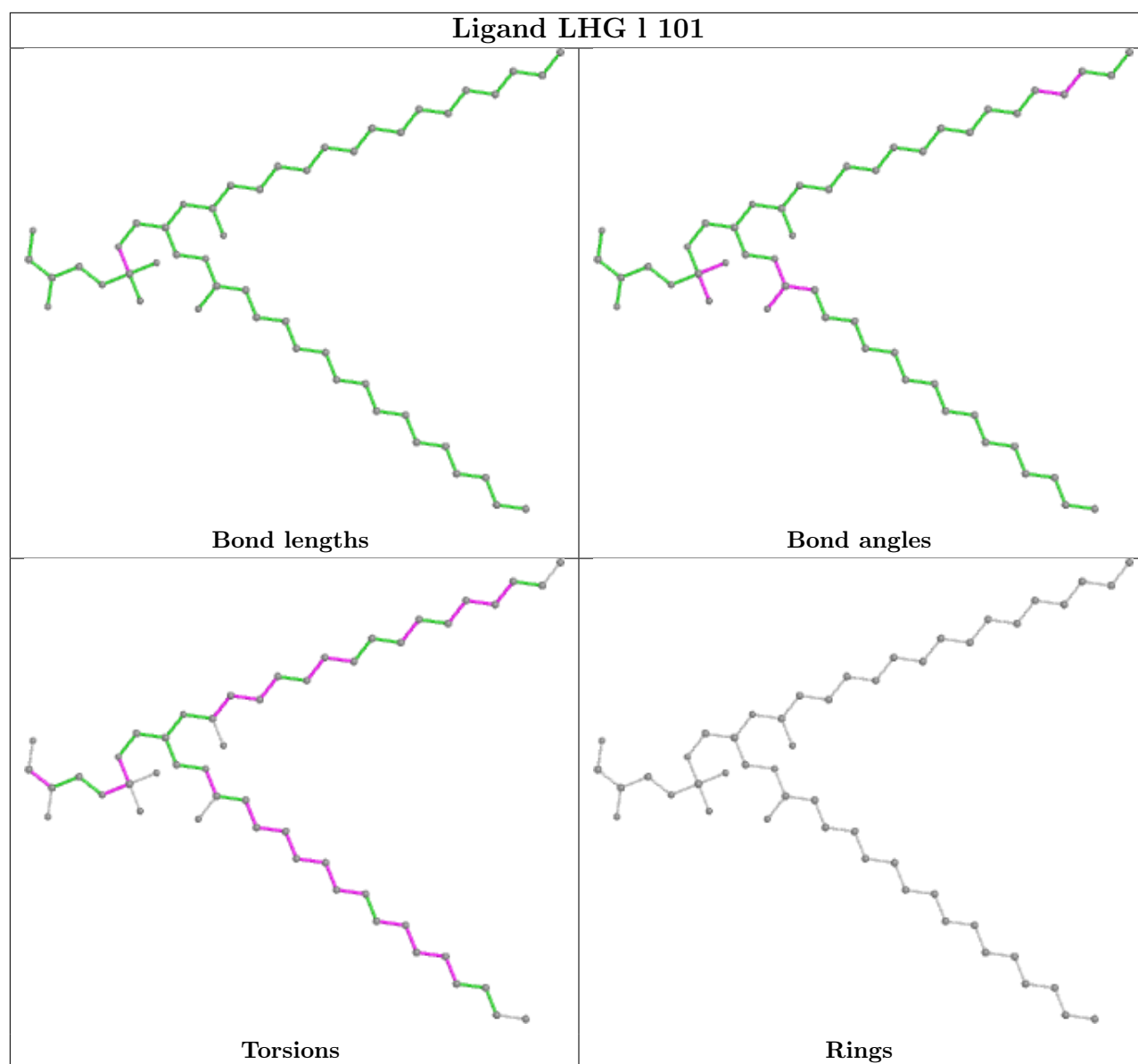
## Ligand CLA B 614

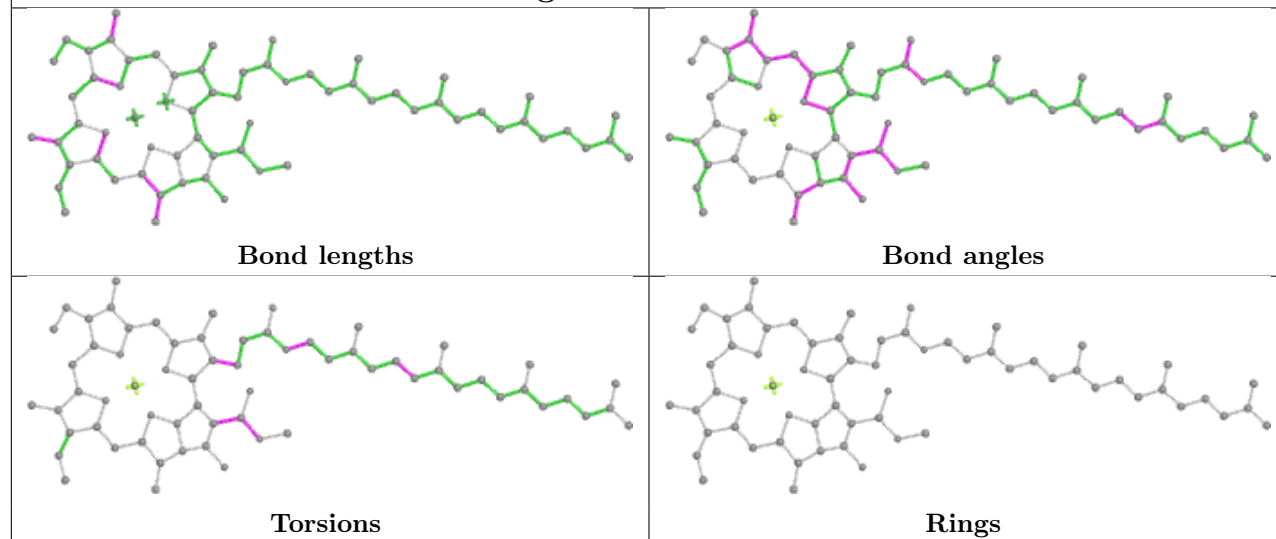
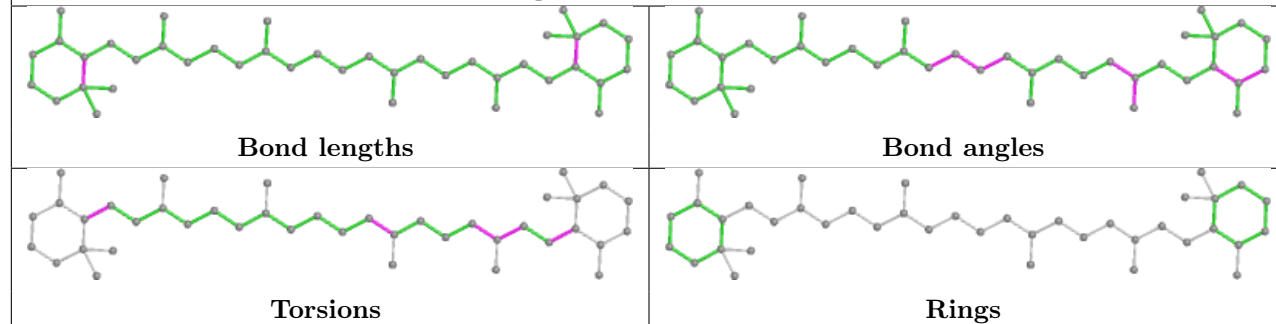


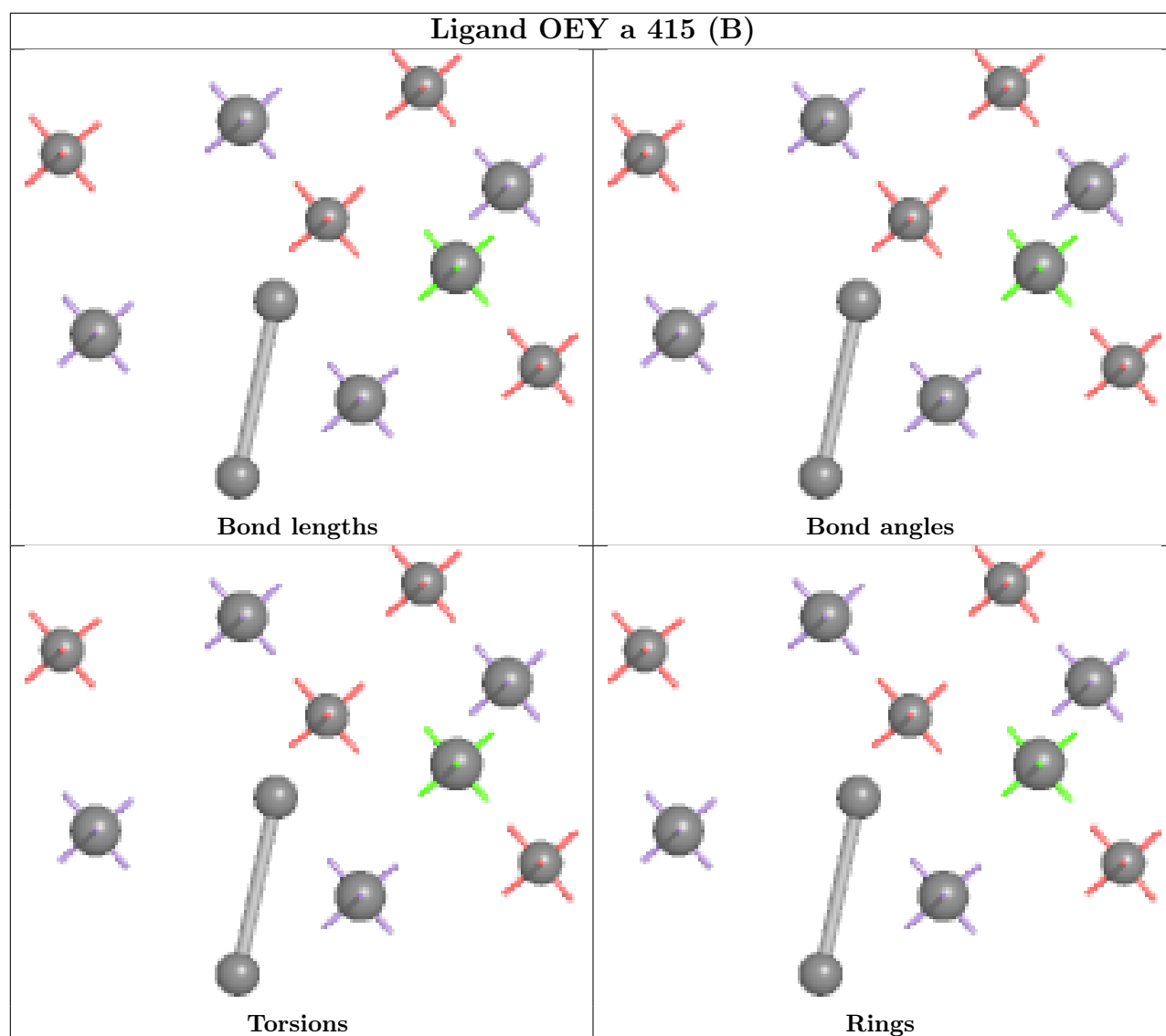
## Ligand BCR h 101

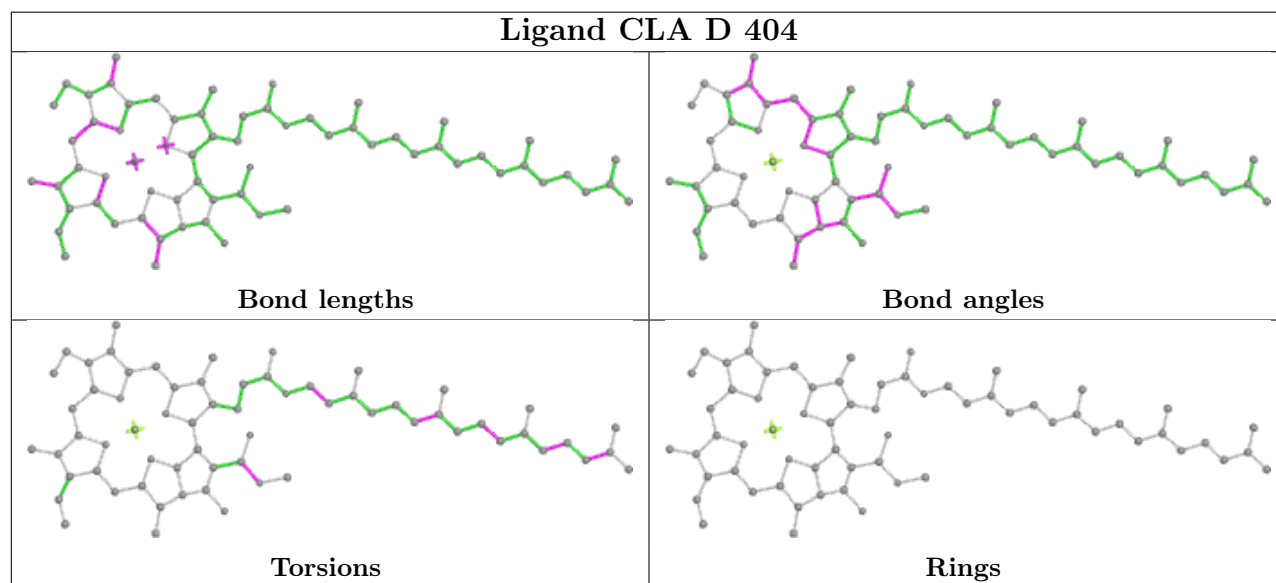
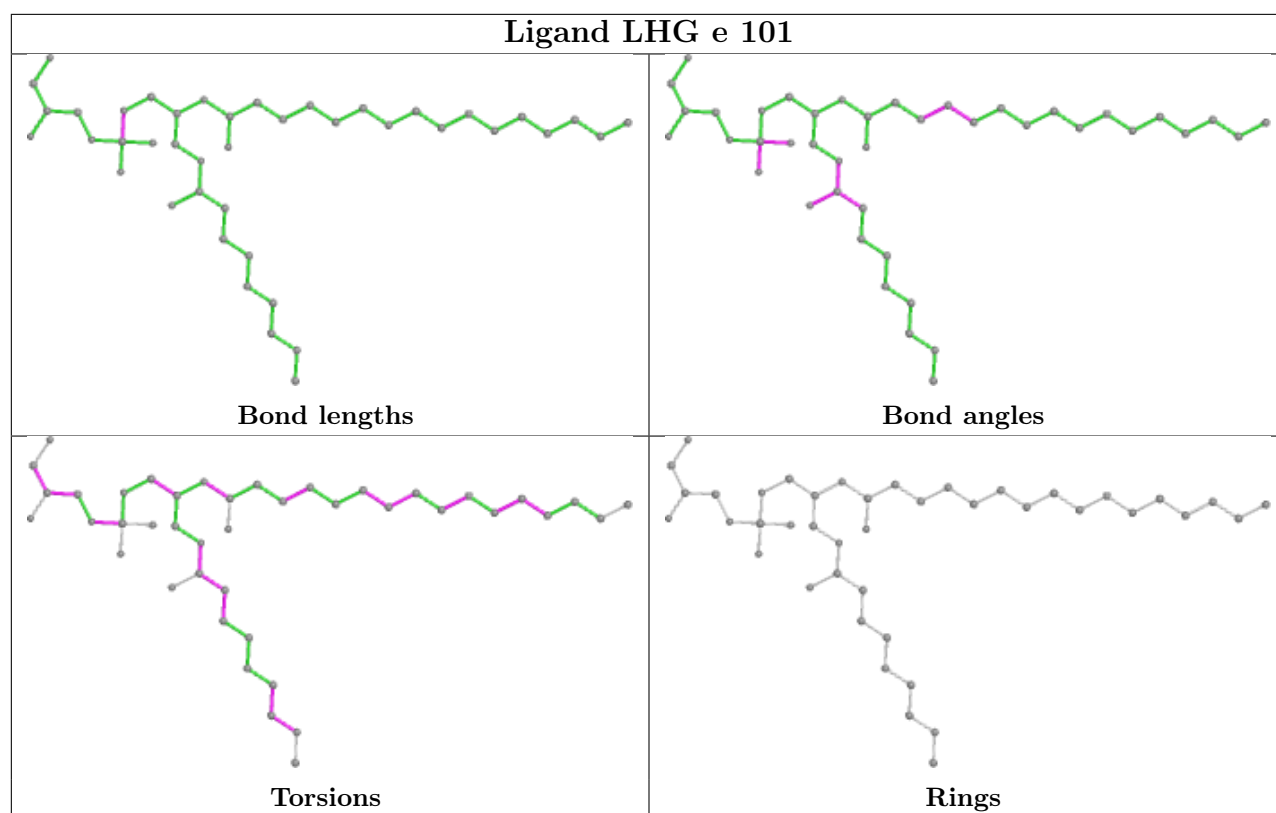




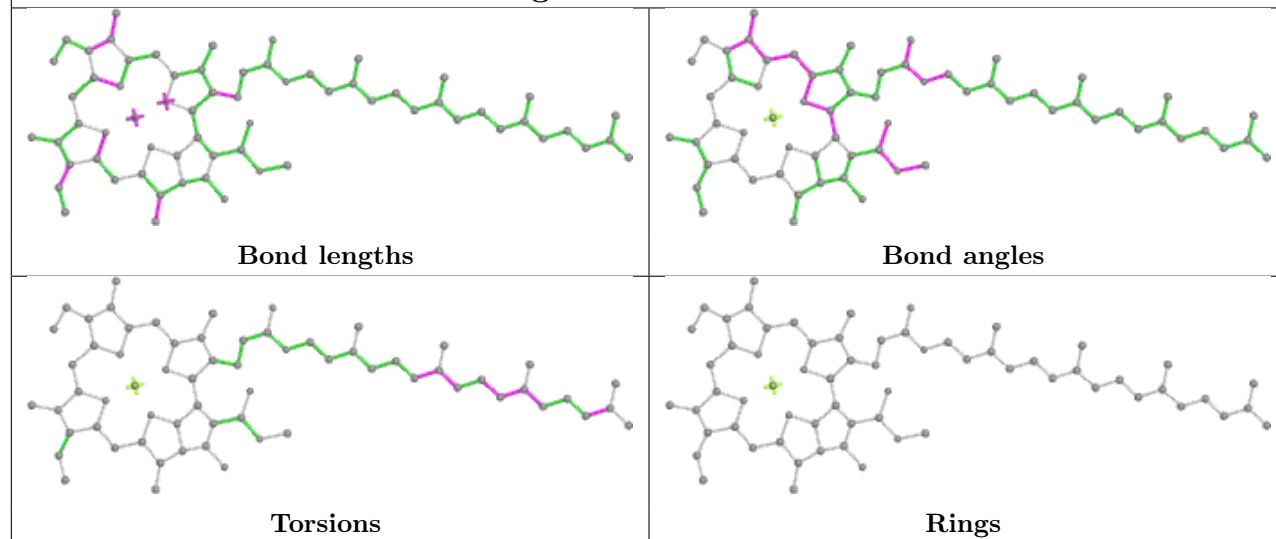


**Ligand CLA c 513****Ligand BCR Y 101**

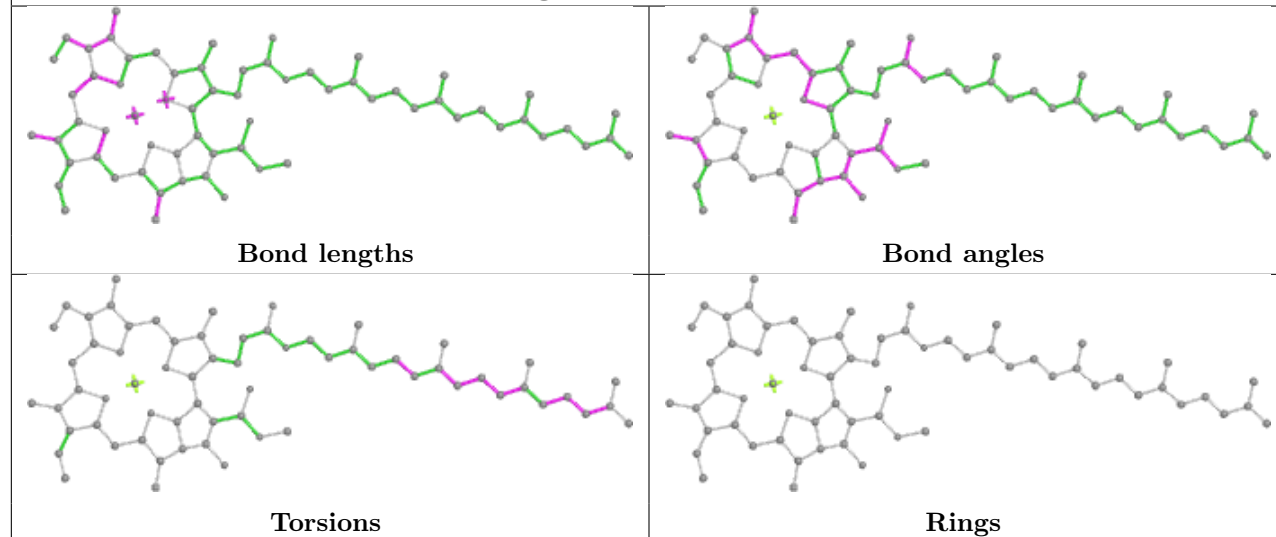




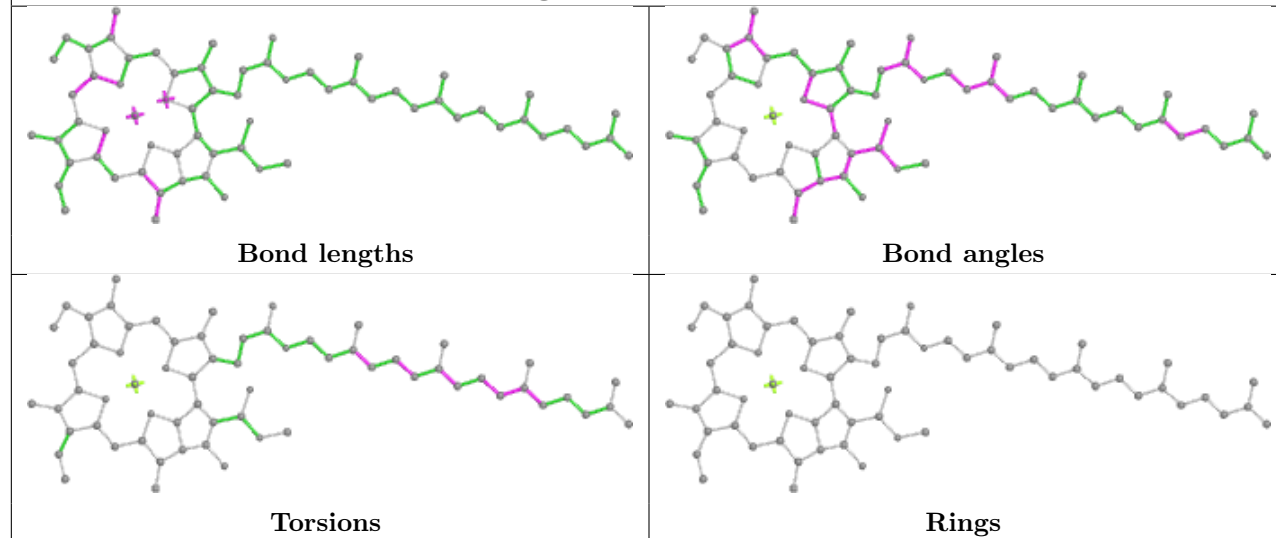
## Ligand CLA A 403



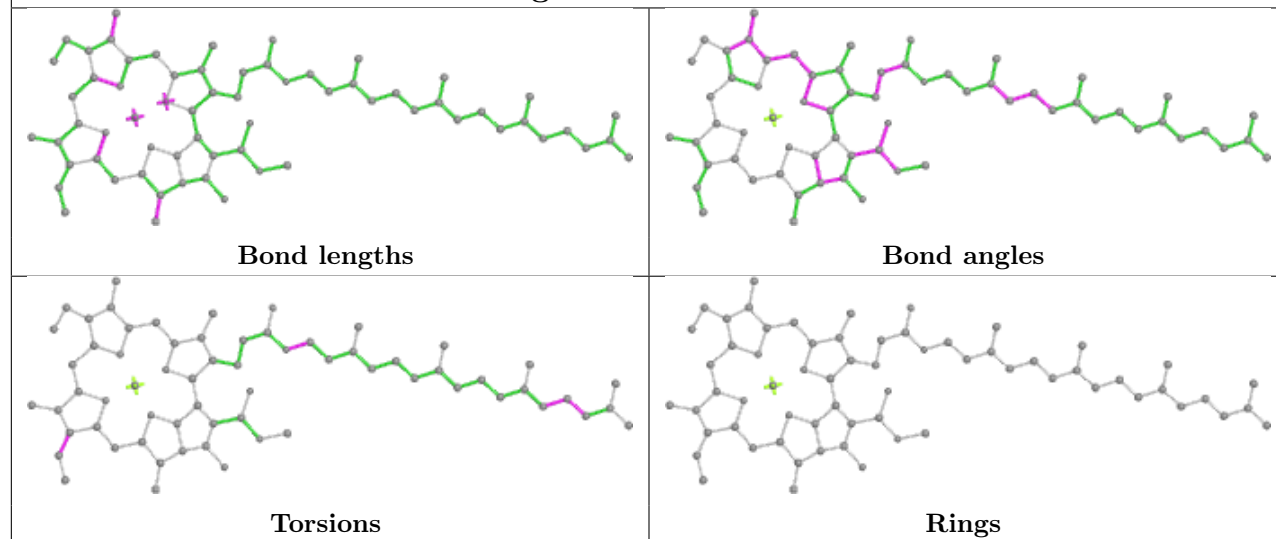
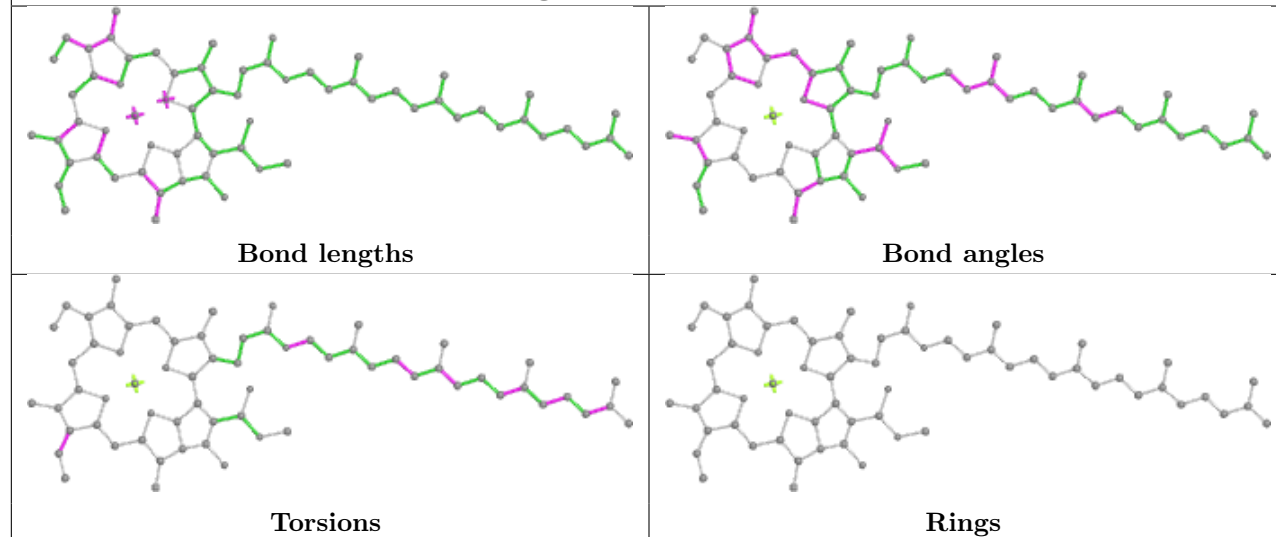
## Ligand CLA b 615



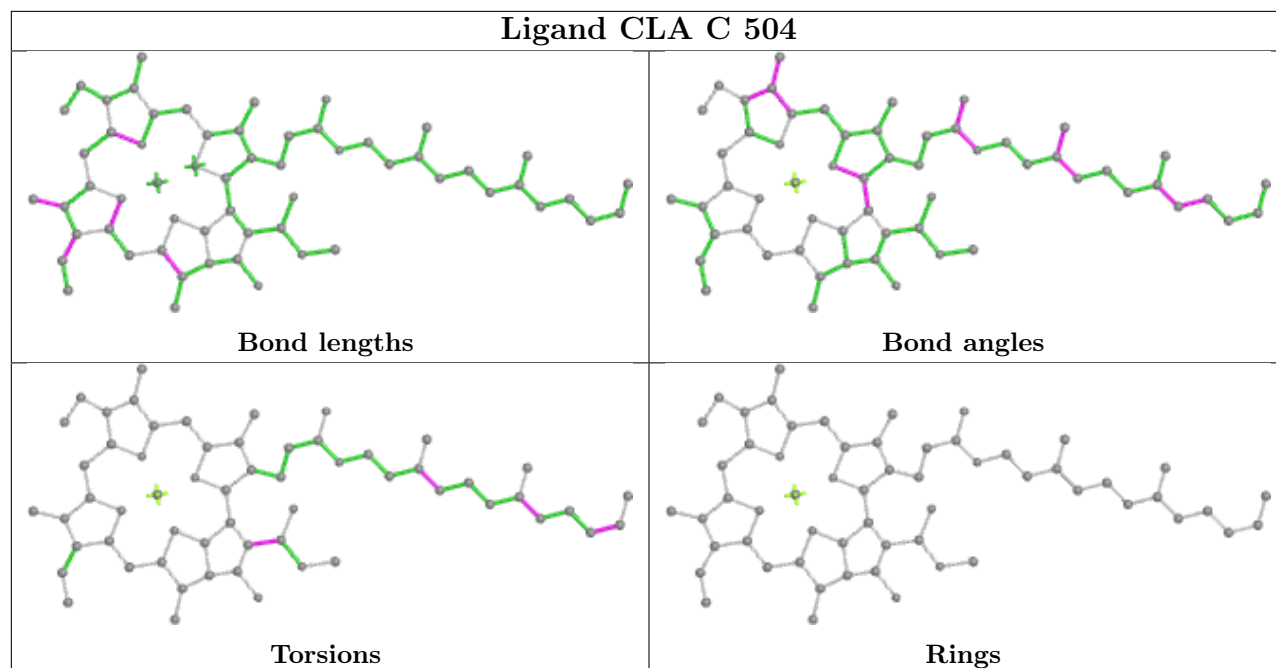
## Ligand CLA b 605



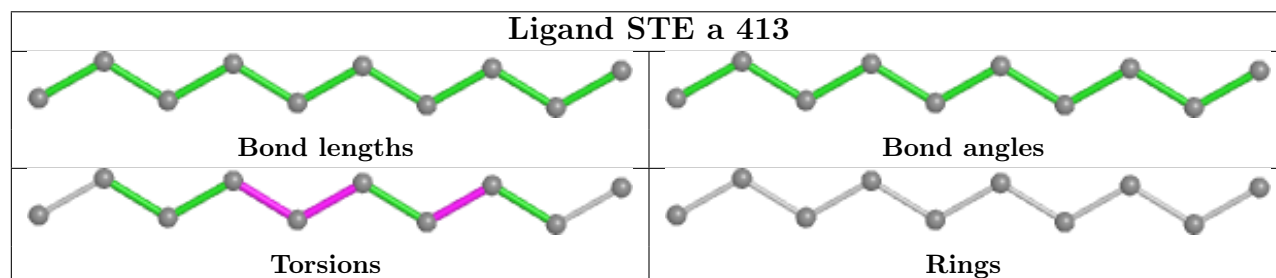


**Ligand CLA A 402****Ligand CLA b 608**

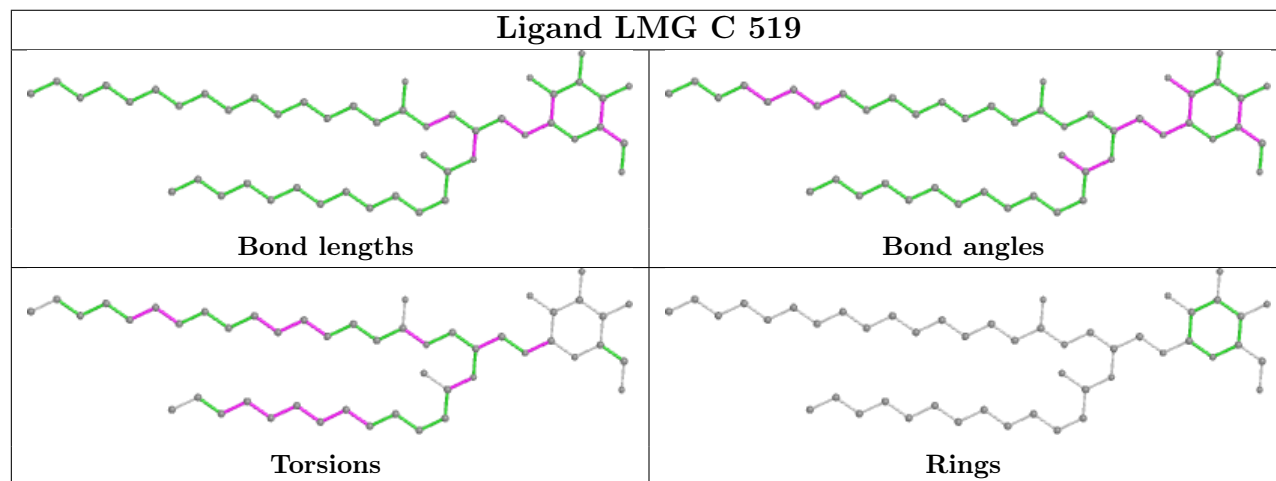
## Ligand CLA C 504



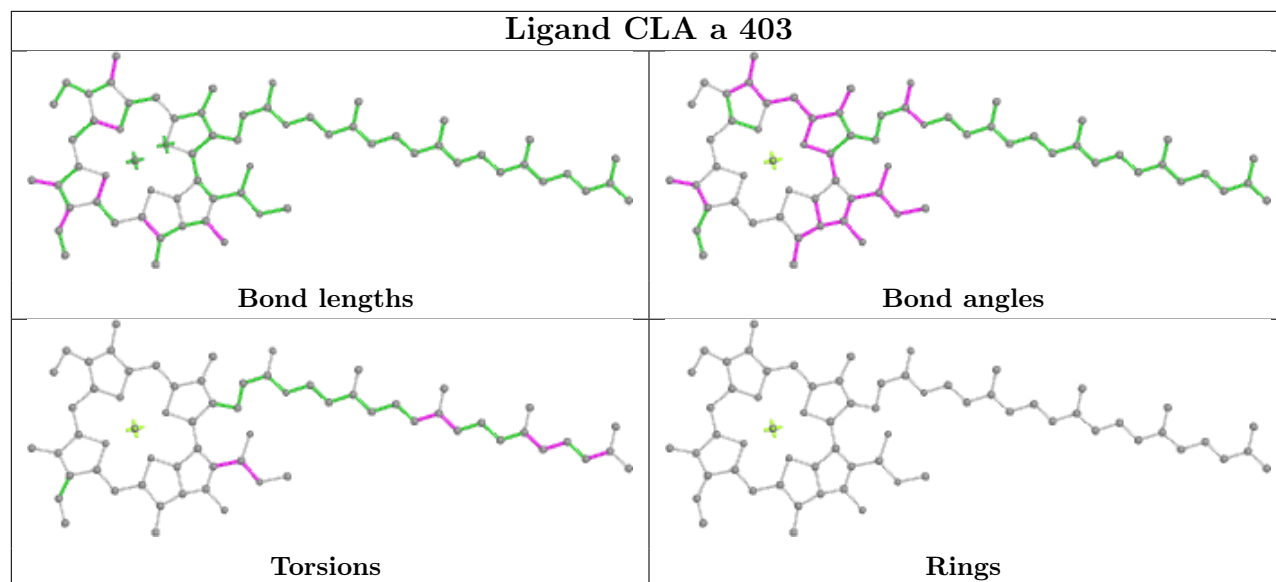
## Ligand STE a 413



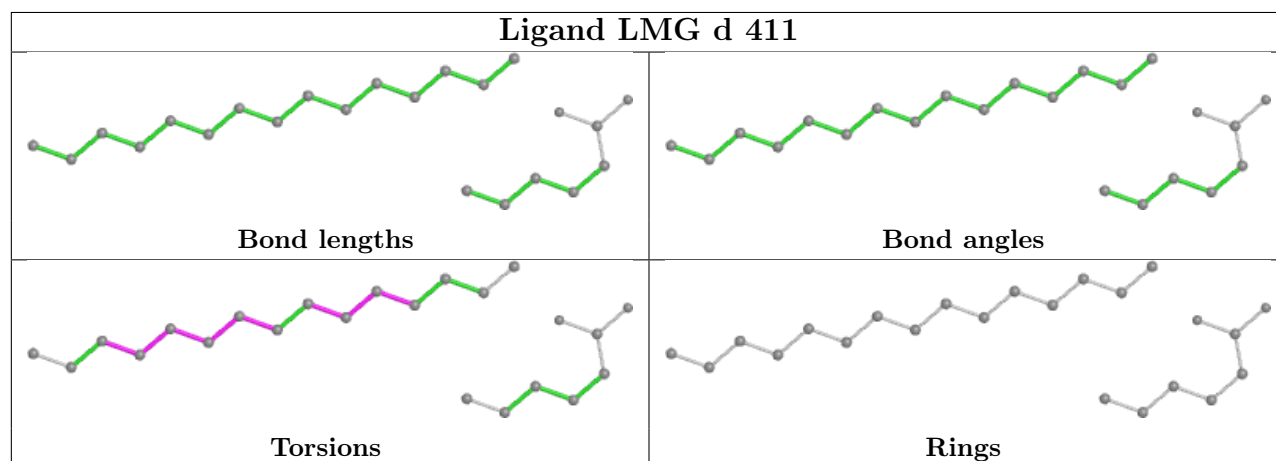
## Ligand LMG C 519



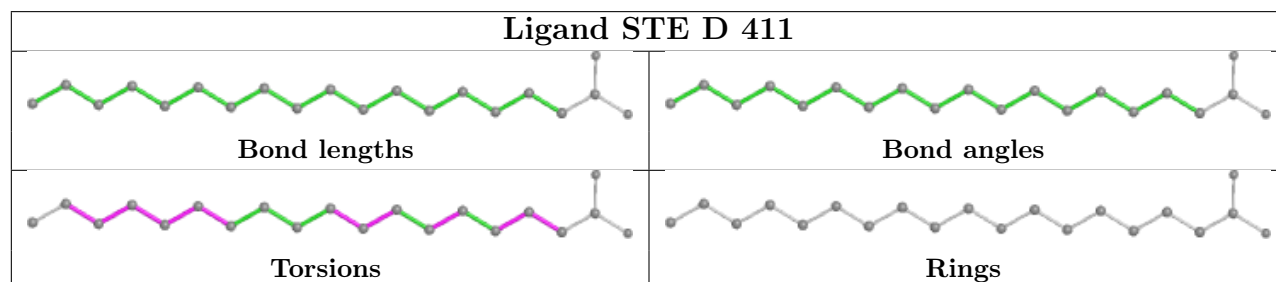
## Ligand CLA a 403



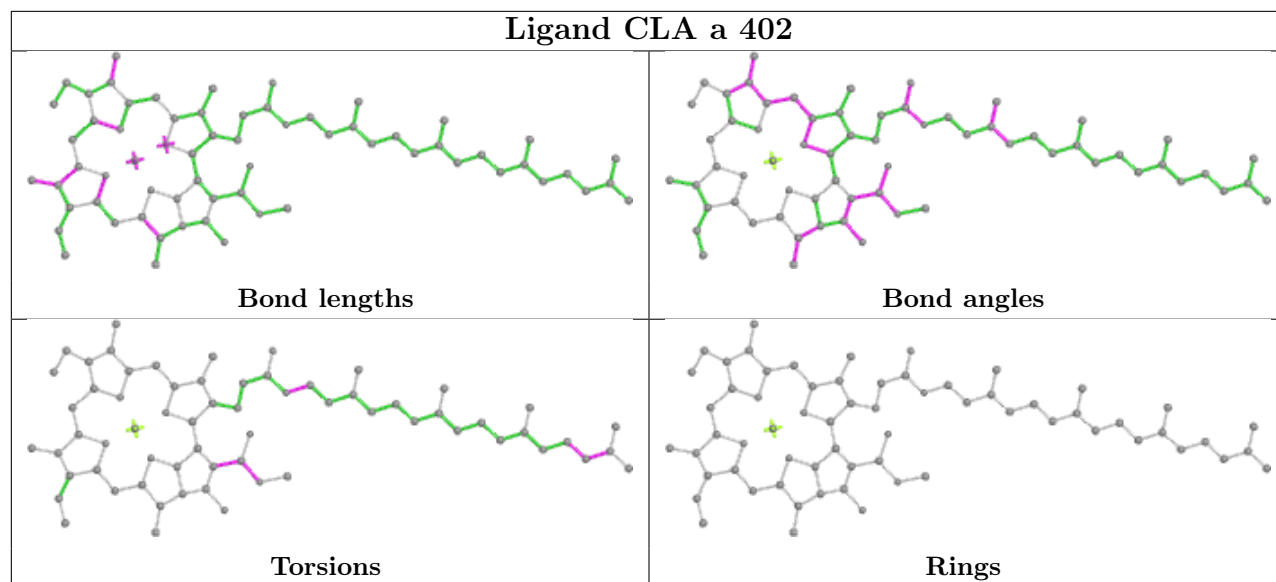
## Ligand LMG d 411



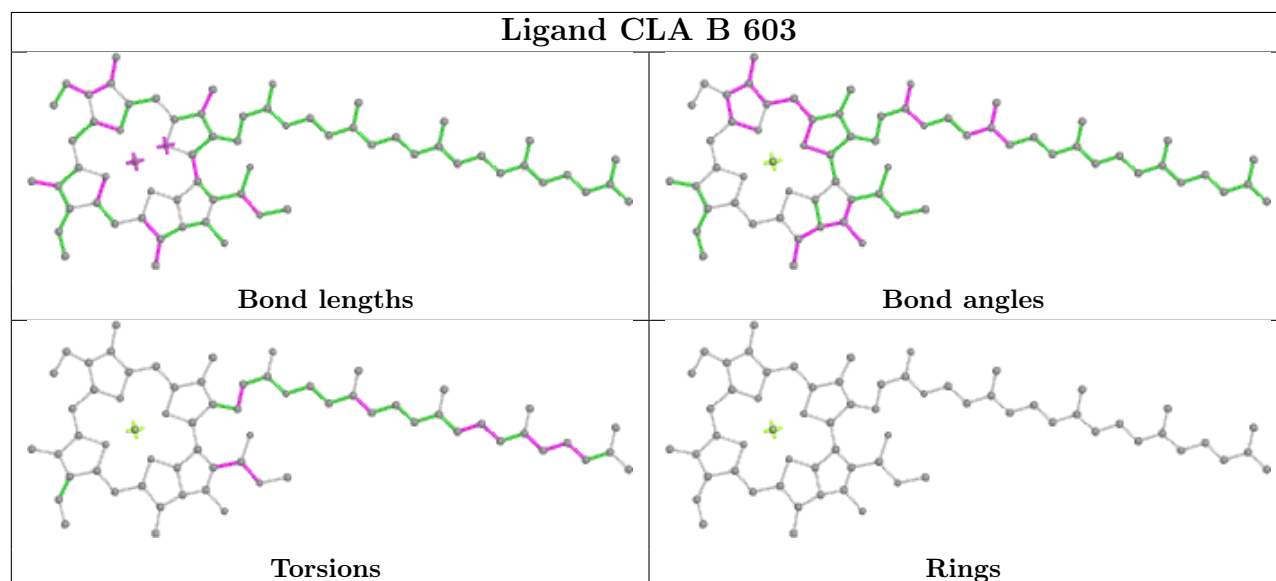
## Ligand STE D 411



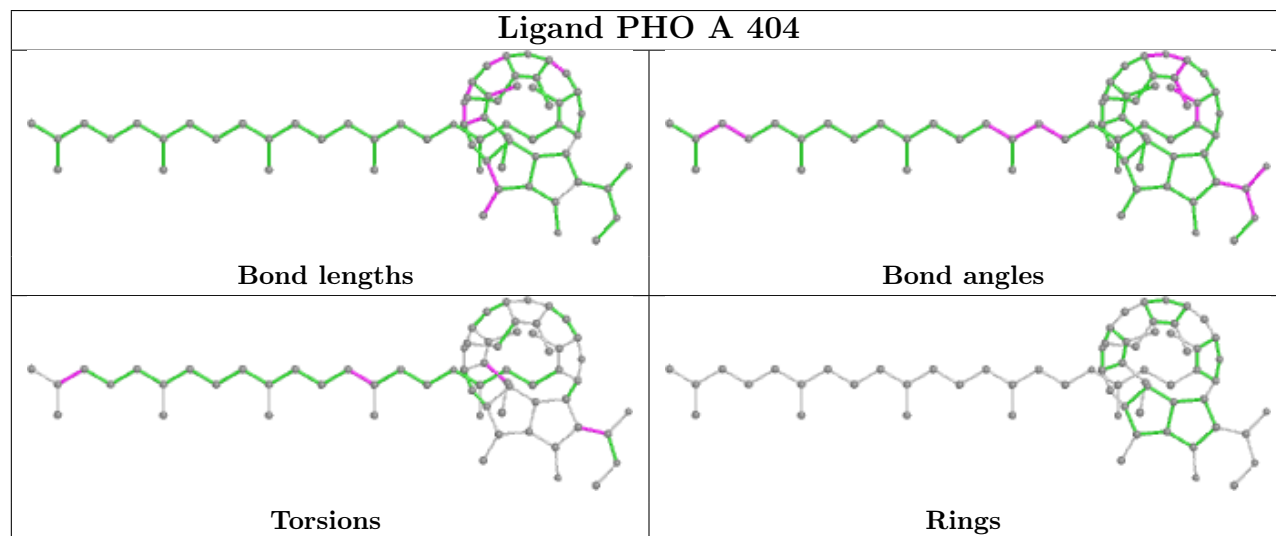
## Ligand CLA a 402



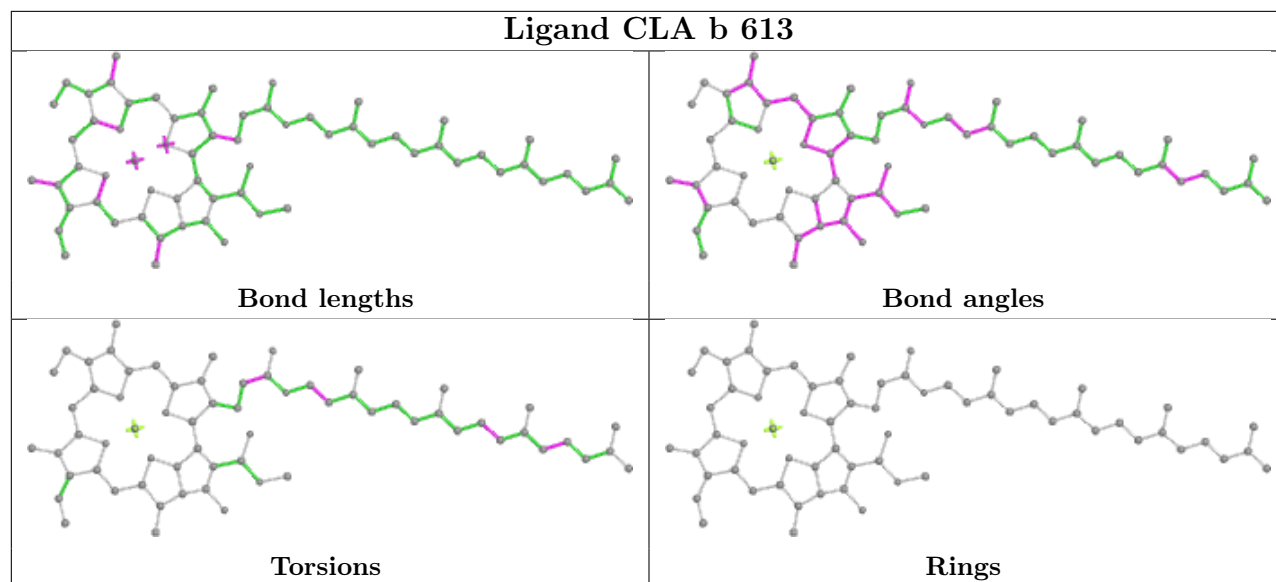
## Ligand CLA B 603



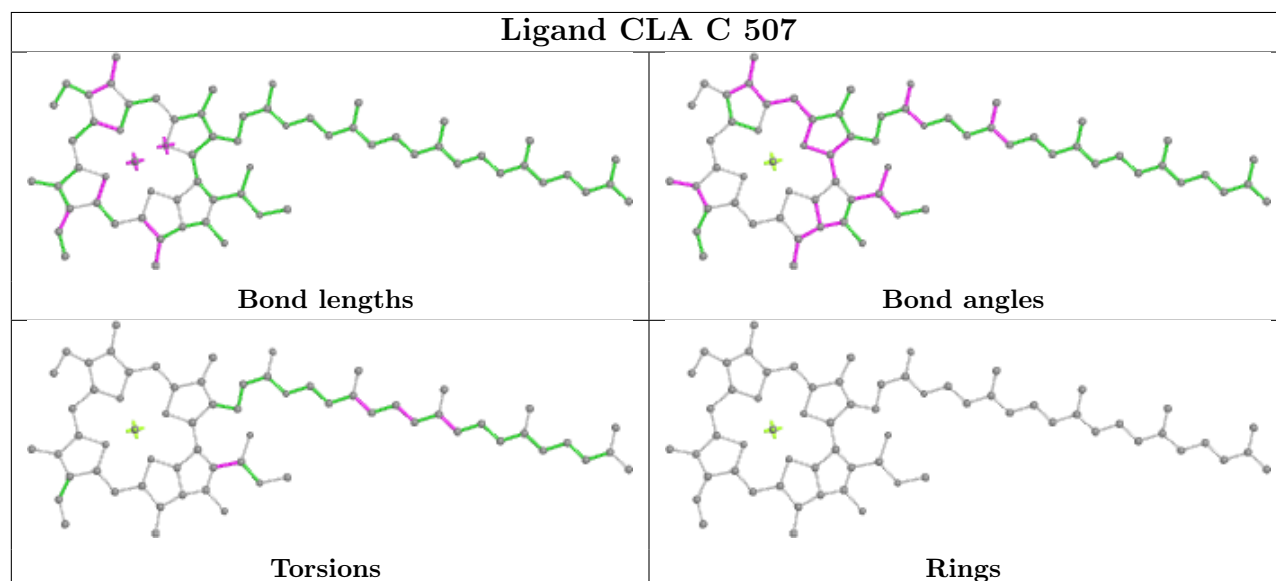
## Ligand PHO A 404



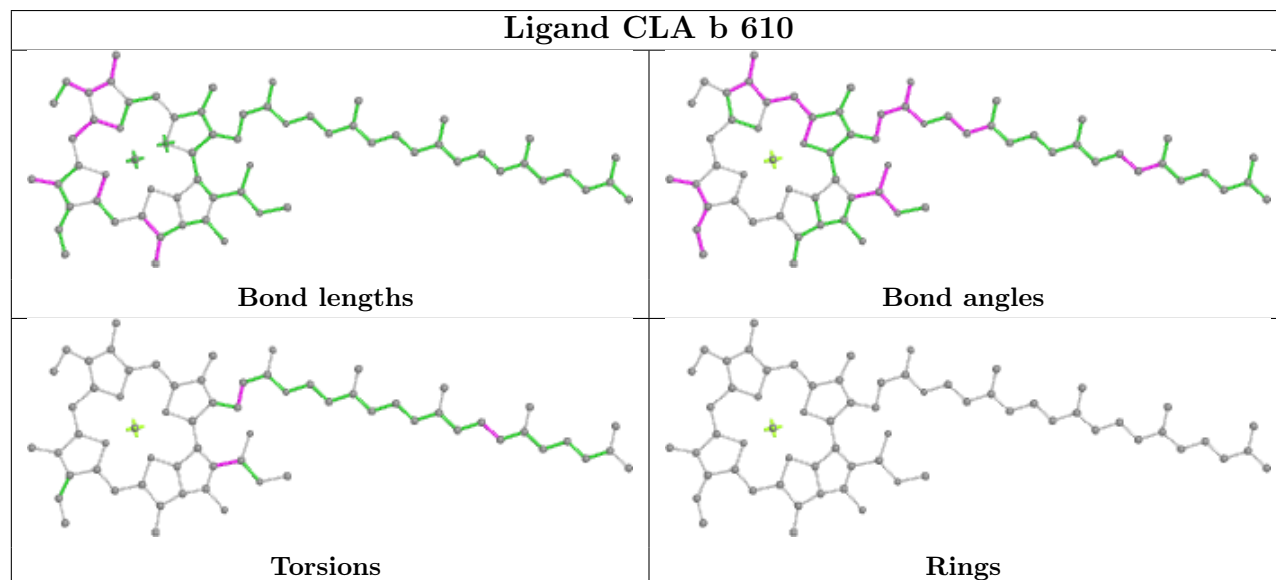
## Ligand CLA b 613

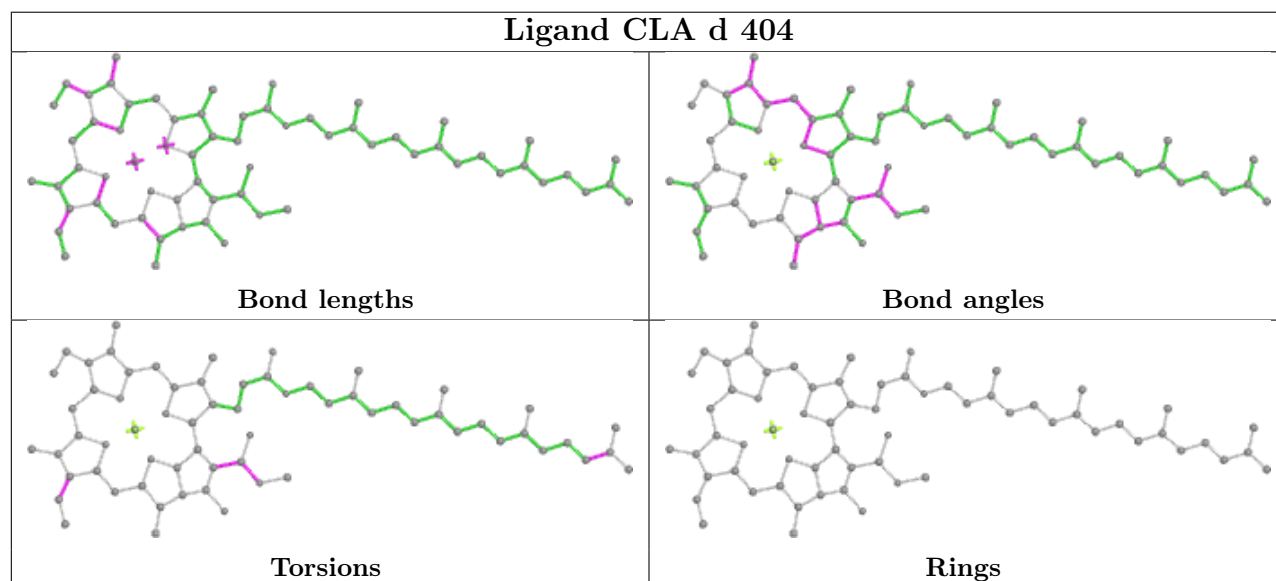
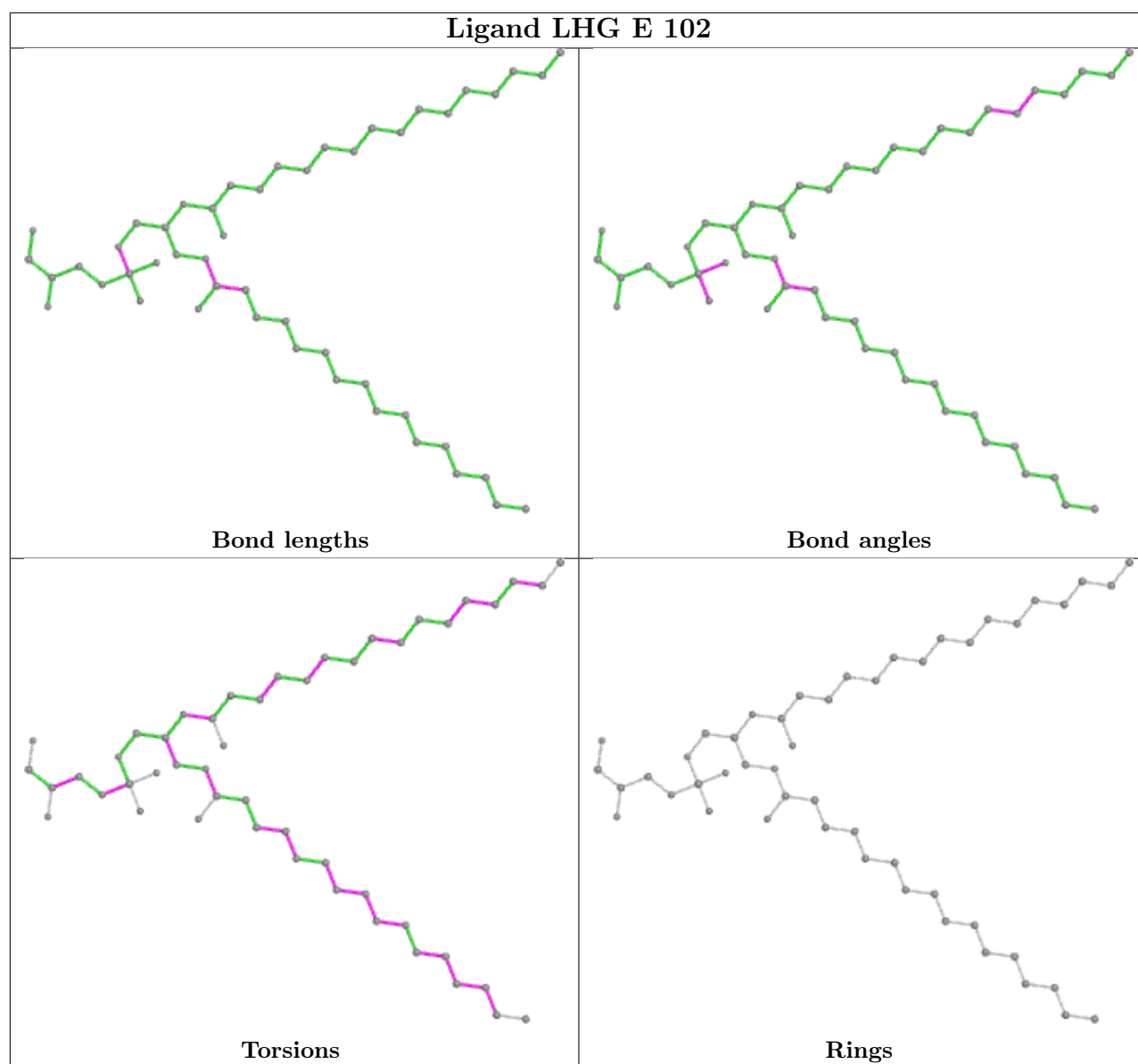


## Ligand CLA C 507

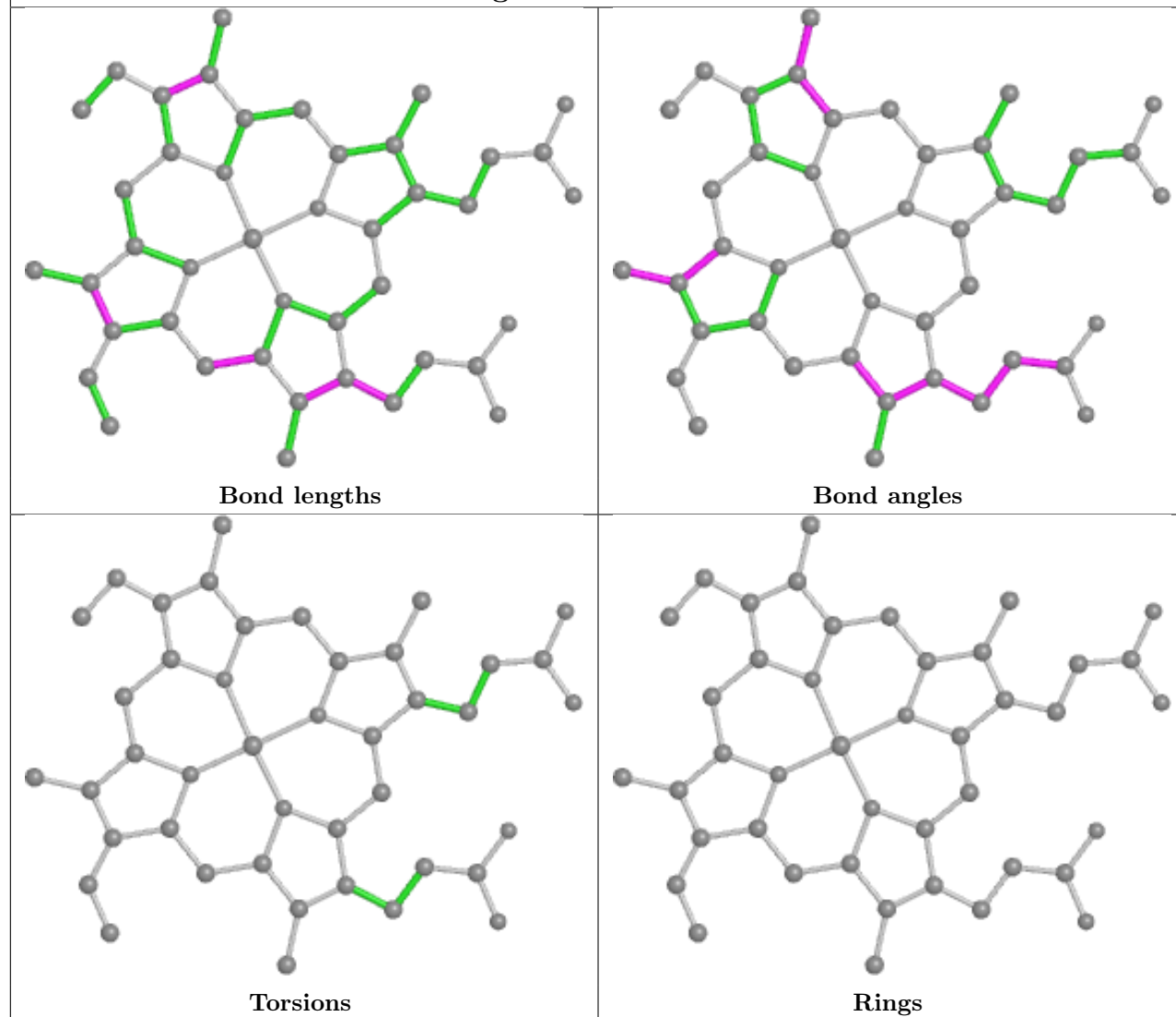


## Ligand CLA b 610

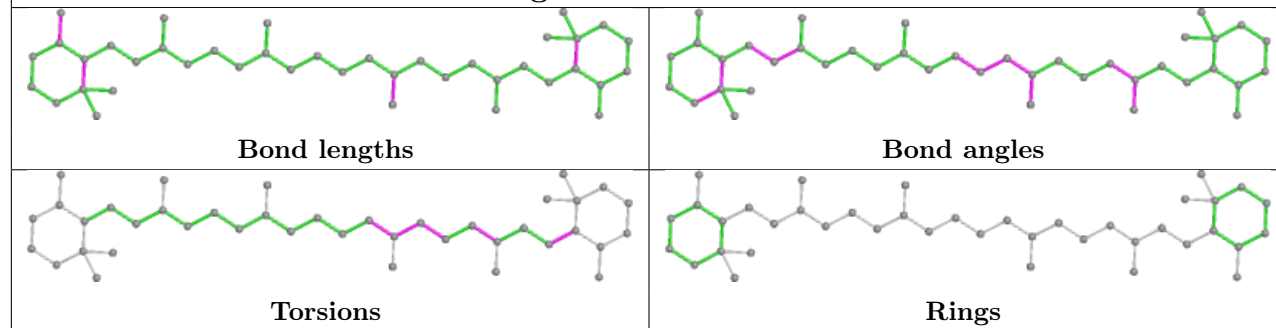


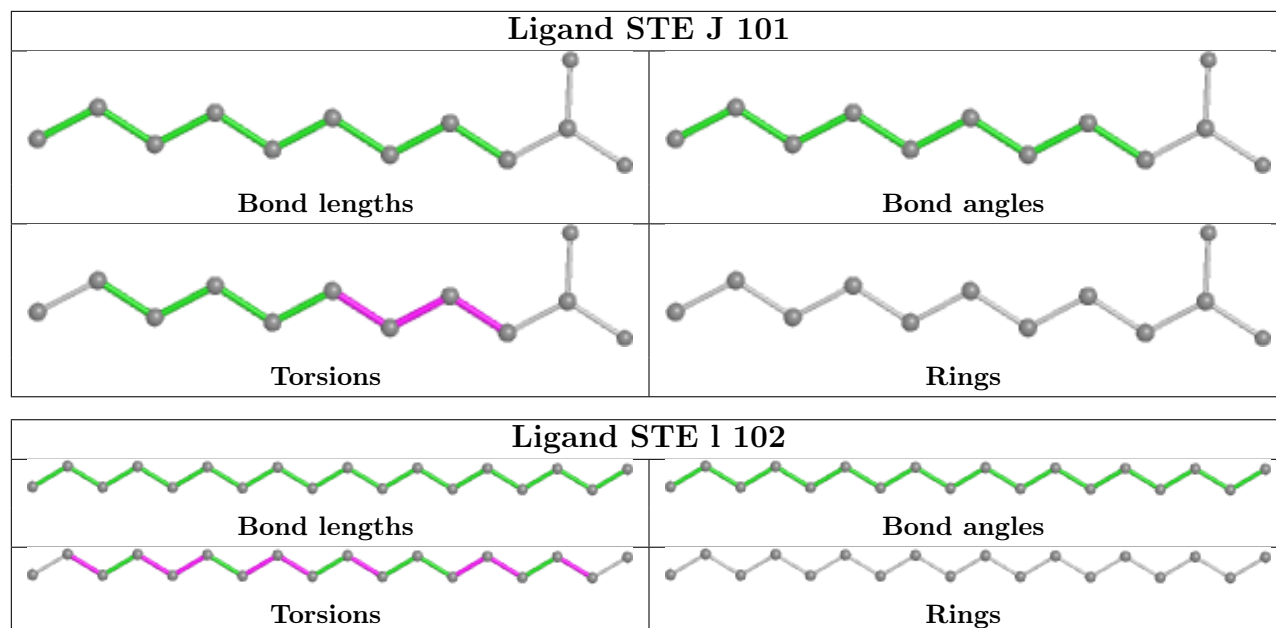


## Ligand HEC v 201



## Ligand BCR C 514





## 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	334/344 (97%)	-0.26	5 (1%) 73 77	23, 32, 53, 84	0
1	a	334/344 (97%)	-0.29	1 (0%) 94 94	26, 34, 61, 80	0
2	B	505/510 (99%)	-0.27	12 (2%) 59 64	26, 36, 65, 92	0
2	b	505/510 (99%)	-0.07	20 (3%) 38 44	28, 39, 75, 115	0
3	C	442/461 (95%)	-0.18	7 (1%) 72 75	27, 39, 56, 81	0
3	c	451/461 (97%)	-0.05	13 (2%) 51 57	28, 43, 64, 99	0
4	D	341/352 (96%)	-0.22	2 (0%) 89 91	27, 34, 51, 78	0
4	d	341/352 (96%)	-0.20	1 (0%) 94 94	27, 38, 62, 84	0
5	E	82/84 (97%)	0.16	6 (7%) 15 19	37, 55, 73, 86	0
5	e	82/84 (97%)	0.26	5 (6%) 21 26	40, 62, 82, 90	0
6	F	34/45 (75%)	-0.20	2 (5%) 22 27	41, 48, 70, 91	0
6	f	34/45 (75%)	-0.14	2 (5%) 22 27	44, 52, 80, 93	0
7	H	65/66 (98%)	-0.06	2 (3%) 49 55	36, 44, 61, 76	0
7	h	63/66 (95%)	0.30	3 (4%) 30 36	44, 52, 65, 70	0
8	I	35/38 (92%)	-0.15	2 (5%) 23 29	35, 40, 72, 82	0
8	i	35/38 (92%)	-0.12	2 (5%) 23 29	34, 43, 77, 84	0
9	J	36/40 (90%)	0.03	4 (11%) 5 7	37, 52, 78, 91	0
9	j	36/40 (90%)	0.26	5 (13%) 2 3	43, 54, 89, 102	0
10	K	37/46 (80%)	0.22	1 (2%) 54 60	48, 56, 74, 83	0
10	k	37/46 (80%)	0.12	0 100 100	48, 57, 72, 84	0
11	L	37/37 (100%)	-0.38	0 100 100	27, 33, 65, 73	0
11	l	36/37 (97%)	-0.22	3 (8%) 11 14	26, 34, 70, 89	0
12	M	32/36 (88%)	0.04	0 100 100	30, 36, 62, 71	0
12	m	31/36 (86%)	-0.21	0 100 100	27, 37, 53, 69	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	17 (6%) 16 20	29, 44, 82, 140	0
13	o	244/272 (89%)	-0.02	15 (6%) 21 26	29, 44, 85, 124	0
14	R	28/41 (68%)	2.35	17 (60%) 0 0	65, 78, 90, 100	0
14	r	28/41 (68%)	4.32	26 (92%) 0 0	79, 101, 115, 123	0
15	T	29/32 (90%)	-0.36	2 (6%) 16 21	29, 33, 65, 73	0
15	t	29/32 (90%)	-0.20	3 (10%) 6 8	29, 34, 78, 90	0
16	U	97/134 (72%)	-0.18	2 (2%) 63 68	34, 46, 71, 92	0
16	u	97/134 (72%)	-0.34	0 100 100	33, 42, 60, 84	0
17	V	137/163 (84%)	-0.45	0 100 100	32, 43, 59, 85	0
17	v	137/163 (84%)	-0.08	5 (3%) 42 49	35, 49, 69, 88	0
18	X	38/41 (92%)	0.03	3 (7%) 12 16	43, 53, 75, 84	0
18	x	39/41 (95%)	0.45	3 (7%) 13 17	52, 63, 92, 105	0
19	Y	27/46 (58%)	1.54	11 (40%) 0 0	55, 76, 92, 98	0
19	y	30/46 (65%)	0.54	5 (16%) 1 2	64, 77, 90, 97	0
20	Z	62/62 (100%)	1.01	17 (27%) 0 0	58, 71, 112, 129	0
20	z	62/62 (100%)	0.89	11 (17%) 1 1	63, 73, 116, 123	0
All	All	5293/5700 (92%)	-0.06	235 (4%) 34 40	23, 41, 76, 140	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	8.5
14	r	28	VAL	7.8
14	r	9	LEU	7.3
13	O	56	PRO	7.1
14	r	29	LYS	7.1

## 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
15	FME	t	1	10/11	0.93	0.09	33,48,71,72	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	0.94	0.10	29,52,69,69	0
12	FME	M	1	10/11	0.95	0.11	44,54,68,76	0
8	FME	I	1	10/11	0.95	0.16	40,52,64,70	0
8	FME	i	1	10/11	0.95	0.19	41,51,64,67	0
12	FME	m	1	10/11	0.96	0.14	33,50,72,82	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
32	STE	E	103	12/20	0.67	0.35	63,80,88,95	0
32	STE	H	103	18/20	0.69	0.31	43,78,89,95	0
32	STE	b	624	20/20	0.70	0.18	51,69,78,93	0
26	PL9	A	409	55/55	0.74	0.29	44,72,93,105	0
32	STE	c	521	20/20	0.76	0.23	44,63,94,107	0
27	LMG	d	411	23/55	0.77	0.23	42,72,88,92	0
32	STE	B	626	16/20	0.77	0.28	39,72,94,94	0
32	STE	a	413	10/20	0.78	0.20	37,66,75,80	0
32	STE	x	101	20/20	0.78	0.24	49,67,79,79	0
24	BCR	h	101	40/40	0.79	0.16	43,60,79,91	0
27	LMG	c	522	48/55	0.79	0.24	39,82,115,118	0
28	SQD	a	411	36/54	0.80	0.17	32,65,86,91	0
26	PL9	a	409	55/55	0.80	0.24	42,76,96,107	0
32	STE	C	521	16/20	0.80	0.16	38,58,85,88	0
33	LHG	E	102	49/49	0.80	0.23	55,87,113,120	0
29	DGD	A	414	66/66	0.81	0.16	47,67,82,90	0
29	DGD	a	412	44/66	0.81	0.16	35,58,82,91	0
32	STE	B	620	17/20	0.81	0.16	39,59,71,80	0
24	BCR	H	101	40/40	0.81	0.16	38,53,64,74	0
22	CLA	b	601	65/65	0.81	0.17	53,72,92,96	0
27	LMG	D	410	33/55	0.81	0.15	41,58,86,90	0
32	STE	a	414	12/20	0.82	0.23	54,67,77,79	0
22	CLA	C	512	65/65	0.82	0.18	35,61,88,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	STE	b	625	10/20	0.82	0.25	40,53,63,74	0
32	STE	B	627	12/20	0.82	0.38	53,66,83,86	0
32	STE	I	101	15/20	0.82	0.18	38,59,77,81	0
27	LMG	b	622	55/55	0.82	0.25	53,80,98,112	0
32	STE	b	623	16/20	0.83	0.17	50,68,83,94	0
28	SQD	A	413	39/54	0.83	0.18	43,66,94,100	0
33	LHG	e	101	42/49	0.83	0.23	56,93,112,132	0
22	CLA	c	512	65/65	0.84	0.17	47,64,99,104	0
22	CLA	c	513	65/65	0.85	0.20	49,74,106,110	0
32	STE	b	621	20/20	0.85	0.23	39,58,79,80	0
32	STE	l	102	18/20	0.85	0.17	37,54,88,89	0
32	STE	j	101	12/20	0.86	0.13	48,62,70,79	0
32	STE	T	103	15/20	0.86	0.15	44,60,81,84	0
22	CLA	B	601	65/65	0.86	0.15	35,64,90,100	0
22	CLA	C	513	65/65	0.86	0.19	45,68,103,112	0
32	STE	T	102	16/20	0.86	0.17	41,53,78,79	0
24	BCR	k	101	40/40	0.87	0.13	45,67,78,80	0
24	BCR	Y	101	40/40	0.87	0.12	43,58,76,83	0
32	STE	B	625	18/20	0.87	0.14	41,59,81,88	0
32	STE	c	524	12/20	0.87	0.21	57,73,82,84	0
32	STE	d	413	17/20	0.87	0.17	48,62,75,82	0
28	SQD	B	623	54/54	0.88	0.15	43,66,97,109	0
27	LMG	A	411	48/55	0.88	0.15	43,65,84,101	0
32	STE	m	101	12/20	0.88	0.15	48,64,76,82	0
24	BCR	c	516	40/40	0.88	0.19	45,60,71,79	0
32	STE	J	101	12/20	0.88	0.12	49,62,72,73	0
32	STE	D	411	20/20	0.88	0.18	38,55,79,84	0
32	STE	C	520	12/20	0.89	0.13	43,57,68,70	0
28	SQD	f	102	41/54	0.89	0.18	63,89,107,109	0
24	BCR	c	514	40/40	0.89	0.15	47,64,79,81	0
22	CLA	c	502	65/65	0.89	0.16	34,49,69,75	0
24	BCR	d	406	40/40	0.89	0.14	40,57,98,114	0
24	BCR	K	101	40/40	0.89	0.14	51,65,74,78	0
28	SQD	L	101	49/54	0.89	0.13	40,61,93,97	0
24	BCR	D	405	40/40	0.89	0.12	35,49,85,89	0
22	CLA	c	508	64/65	0.90	0.15	37,50,94,112	0
22	CLA	c	510	65/65	0.90	0.17	36,53,67,73	0
27	LMG	c	523	49/55	0.90	0.12	35,62,83,99	0
22	CLA	C	502	65/65	0.90	0.14	35,47,60,68	0
32	STE	M	103	10/20	0.90	0.13	36,54,57,61	0
22	CLA	b	615	65/65	0.90	0.14	31,45,61,65	0
22	CLA	d	405	65/65	0.90	0.16	32,53,93,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	B	621	28/55	0.90	0.16	37,53,66,72	0
27	LMG	C	519	48/55	0.90	0.15	49,74,93,98	0
32	STE	C	522	12/20	0.90	0.10	34,45,58,64	0
22	CLA	D	404	65/65	0.90	0.14	27,47,106,117	0
22	CLA	b	616	60/65	0.91	0.14	34,48,89,91	0
27	LMG	c	520	37/55	0.91	0.15	43,72,92,96	0
24	BCR	B	619	40/40	0.91	0.10	33,45,59,61	0
24	BCR	C	515	40/40	0.91	0.19	45,60,78,81	0
24	BCR	b	619	40/40	0.91	0.11	35,52,70,70	0
22	CLA	c	503	65/65	0.91	0.16	35,48,61,64	0
32	STE	t	102	14/20	0.91	0.11	35,55,65,68	0
27	LMG	M	101	51/55	0.91	0.11	33,53,76,92	0
27	LMG	b	620	51/55	0.91	0.11	38,57,76,91	0
32	STE	M	102	15/20	0.91	0.14	37,50,66,69	0
22	CLA	C	507	65/65	0.92	0.14	27,45,60,65	0
22	CLA	b	602	65/65	0.92	0.16	31,46,65,71	0
27	LMG	D	407	51/55	0.92	0.16	31,60,86,92	0
22	CLA	c	511	65/65	0.92	0.14	43,60,78,82	0
22	CLA	b	604	65/65	0.92	0.15	24,39,80,93	0
22	CLA	B	616	60/65	0.92	0.15	28,45,84,100	0
29	DGD	h	102	62/66	0.92	0.11	33,53,64,71	0
22	CLA	C	503	65/65	0.92	0.14	36,47,59,62	0
24	BCR	B	618	40/40	0.92	0.10	28,41,58,61	0
22	CLA	C	506	65/65	0.92	0.12	29,49,89,94	0
22	CLA	a	404	65/65	0.92	0.13	21,40,80,85	0
22	CLA	c	505	65/65	0.92	0.17	28,45,71,75	0
22	CLA	c	507	65/65	0.92	0.14	30,49,61,66	0
22	CLA	B	606	65/65	0.93	0.12	28,41,71,77	0
22	CLA	c	509	65/65	0.93	0.19	37,53,70,75	0
24	BCR	c	515	40/40	0.93	0.11	35,47,58,72	0
22	CLA	B	615	65/65	0.93	0.12	29,42,67,77	0
22	CLA	C	508	65/65	0.93	0.12	32,46,104,115	0
28	SQD	F	101	36/54	0.93	0.17	43,77,93,98	0
22	CLA	b	606	65/65	0.93	0.11	29,45,77,78	0
22	CLA	b	609	65/65	0.93	0.14	32,50,71,77	0
22	CLA	b	614	65/65	0.93	0.14	25,44,78,85	0
26	PL9	D	406	55/55	0.93	0.11	24,38,49,50	0
29	DGD	C	517	62/66	0.93	0.12	41,56,102,121	0
29	DGD	H	102	62/66	0.93	0.11	33,48,61,66	0
24	BCR	B	617	40/40	0.93	0.12	30,45,60,65	0
29	DGD	c	518	62/66	0.93	0.12	35,58,94,103	0
22	CLA	C	511	65/65	0.93	0.12	36,57,71,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	A	403	65/65	0.93	0.14	26,40,103,112	0
32	STE	B	624	12/20	0.93	0.10	37,56,70,74	0
24	BCR	C	514	40/40	0.93	0.11	32,43,56,61	0
22	CLA	B	602	65/65	0.93	0.16	27,40,62,65	0
22	CLA	B	604	65/65	0.93	0.13	26,38,75,80	0
22	CLA	a	403	65/65	0.93	0.14	30,45,99,107	0
22	CLA	c	506	65/65	0.93	0.12	36,53,94,101	0
22	CLA	C	505	65/65	0.93	0.16	22,44,72,75	0
24	BCR	b	618	40/40	0.93	0.11	30,44,56,60	0
22	CLA	C	509	65/65	0.94	0.19	32,50,65,74	0
22	CLA	b	608	65/65	0.94	0.14	34,48,64,68	0
27	LMG	d	412	44/55	0.94	0.13	37,58,89,92	0
22	CLA	C	510	65/65	0.94	0.14	34,49,66,74	0
22	CLA	b	611	65/65	0.94	0.15	27,39,57,66	0
22	CLA	b	612	65/65	0.94	0.18	26,39,54,63	0
22	CLA	b	613	65/65	0.94	0.15	26,40,76,83	0
28	SQD	a	410	54/54	0.94	0.14	44,67,96,99	0
23	PHO	d	401	64/64	0.94	0.13	23,35,43,48	0
24	BCR	A	406	40/40	0.94	0.09	28,38,49,52	0
22	CLA	A	402	65/65	0.94	0.10	21,32,46,56	0
29	DGD	C	516	62/66	0.94	0.12	25,48,84,91	0
22	CLA	A	405	54/65	0.94	0.11	20,34,68,73	0
29	DGD	C	518	62/66	0.94	0.12	33,54,82,91	0
26	PL9	d	407	55/55	0.94	0.11	27,38,45,52	0
22	CLA	B	609	65/65	0.94	0.14	29,42,56,59	0
22	CLA	B	610	65/65	0.94	0.14	23,35,47,51	0
29	DGD	c	519	62/66	0.94	0.14	31,57,86,101	0
22	CLA	C	504	59/65	0.94	0.13	32,47,85,92	0
22	CLA	c	504	60/65	0.94	0.11	35,50,87,88	0
22	CLA	B	611	65/65	0.94	0.15	23,35,50,56	0
22	CLA	B	612	65/65	0.94	0.15	25,36,50,55	0
24	BCR	T	101	40/40	0.94	0.10	29,44,58,62	0
22	CLA	B	613	65/65	0.94	0.14	21,35,71,75	0
24	BCR	a	405	40/40	0.94	0.09	25,36,52,56	0
22	CLA	B	614	65/65	0.94	0.17	26,43,77,92	0
22	CLA	b	610	65/65	0.95	0.18	28,42,53,58	0
22	CLA	C	501	65/65	0.95	0.12	26,41,54,58	0
22	CLA	A	410	65/65	0.95	0.09	20,32,52,58	0
24	BCR	t	101	40/40	0.95	0.09	27,39,55,58	0
28	SQD	A	412	52/54	0.95	0.15	33,66,94,99	0
22	CLA	B	605	65/65	0.95	0.14	24,35,49,54	0
22	CLA	b	603	65/65	0.95	0.14	24,40,71,79	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	D	403	65/65	0.95	0.12	22,32,59,60	0
22	CLA	b	605	65/65	0.95	0.12	24,39,54,60	0
22	CLA	c	501	65/65	0.95	0.13	31,44,54,62	0
22	CLA	d	403	65/65	0.95	0.12	23,40,60,68	0
22	CLA	d	404	65/65	0.95	0.12	24,35,46,50	0
24	BCR	b	617	40/40	0.95	0.10	29,43,52,56	0
22	CLA	B	603	65/65	0.95	0.14	24,38,63,64	0
23	PHO	A	404	64/64	0.95	0.09	20,31,40,48	0
22	CLA	b	607	65/65	0.95	0.14	21,40,65,77	0
33	LHG	B	622	49/49	0.95	0.12	28,48,68,77	0
22	CLA	a	402	65/65	0.95	0.10	24,35,48,62	0
22	CLA	B	607	65/65	0.95	0.11	17,37,68,76	0
33	LHG	l	101	49/49	0.95	0.10	34,48,59,67	0
22	CLA	B	608	65/65	0.96	0.11	22,39,59,65	0
33	LHG	D	409	47/49	0.96	0.11	29,53,82,99	0
29	DGD	c	517	62/66	0.96	0.10	25,46,77,83	0
33	LHG	L	102	49/49	0.96	0.11	30,44,59,74	0
33	LHG	d	408	49/49	0.96	0.12	30,55,77,83	0
33	LHG	d	409	49/49	0.96	0.10	30,49,61,71	0
33	LHG	d	410	39/49	0.96	0.10	34,50,72,74	0
23	PHO	d	402	64/64	0.96	0.10	32,43,54,63	0
23	PHO	D	401	64/64	0.96	0.14	25,37,45,53	0
34	BCT	a	408	4/4	0.96	0.18	35,40,48,58	0
35	HEM	E	101	43/43	0.96	0.12	42,57,75,75	0
35	HEM	f	101	43/43	0.96	0.12	46,64,89,90	0
36	HEC	V	201	43/43	0.96	0.13	24,37,49,51	0
36	HEC	v	201	43/43	0.96	0.13	32,41,52,55	0
34	BCT	D	402	4/4	0.97	0.20	32,33,37,44	0
33	LHG	D	408	49/49	0.97	0.09	26,44,56,63	0
31	OEX	A	416[A]	10/10	0.98	0.13	35,37,41,41	10
25	CL	a	407	1/1	0.98	0.05	33,33,33,33	0
21	FE2	a	401	1/1	0.98	0.06	37,37,37,37	0
30	OEY	A	415[B]	11/11	0.98	0.13	21,26,30,34	11
31	OEX	a	416[A]	10/10	0.99	0.11	32,38,41,41	10
25	CL	A	408	1/1	0.99	0.03	32,32,32,32	0
25	CL	a	406	1/1	0.99	0.04	30,30,30,30	0
21	FE2	A	401	1/1	0.99	0.11	33,33,33,33	0
30	OEY	a	415[B]	11/11	0.99	0.11	25,27,31,37	11
25	CL	A	407	1/1	0.99	0.06	33,33,33,33	0

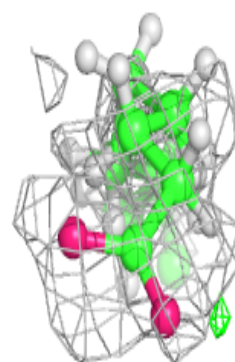
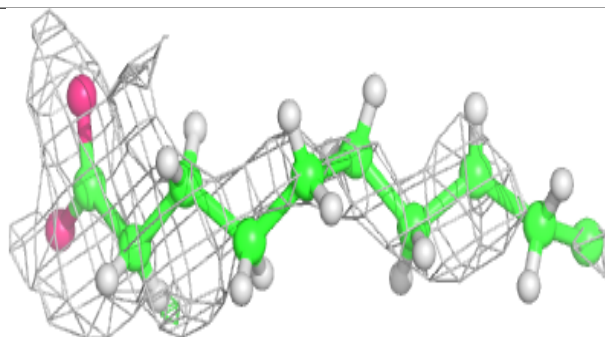
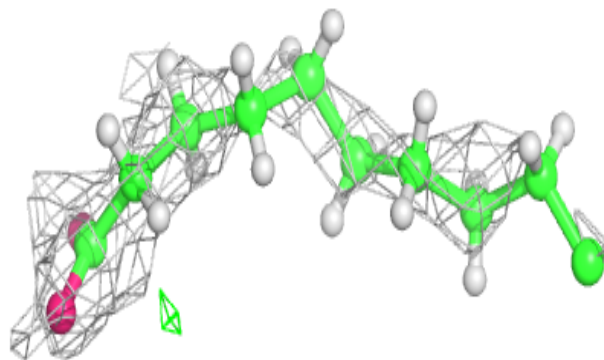
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.

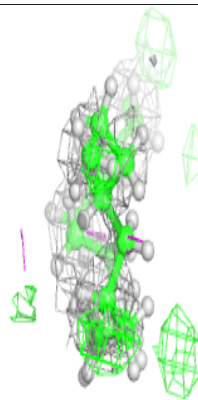
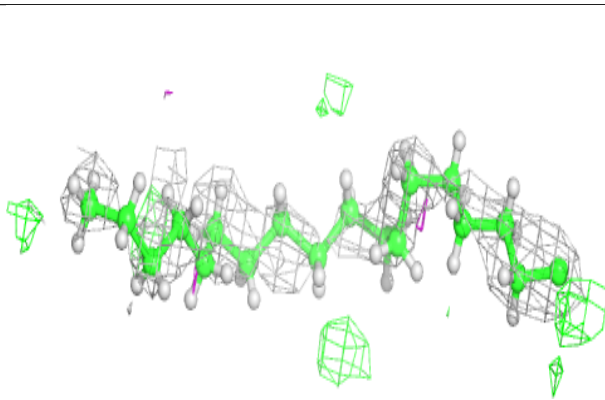
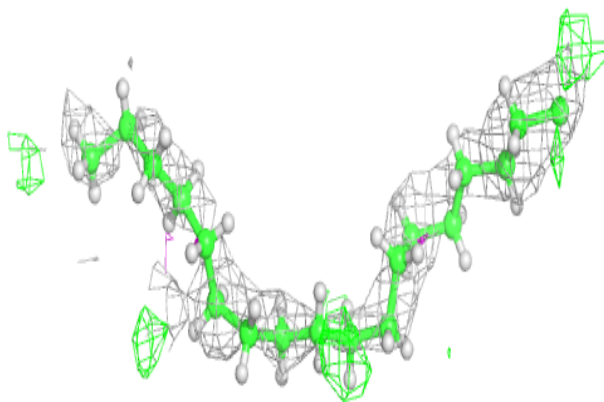
**Electron density around STE E 103:**

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



**Electron density around STE H 103:**

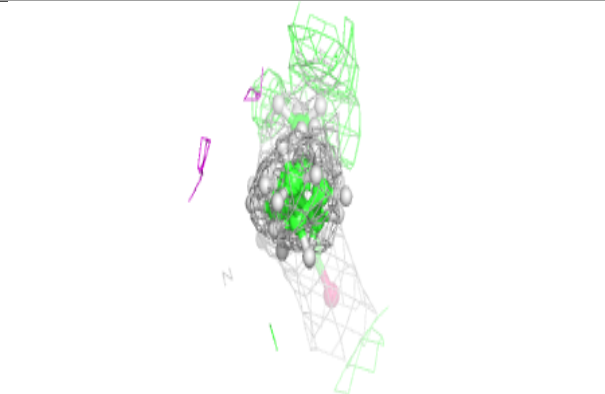
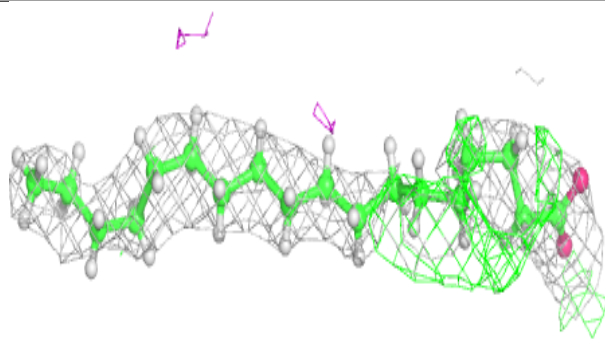
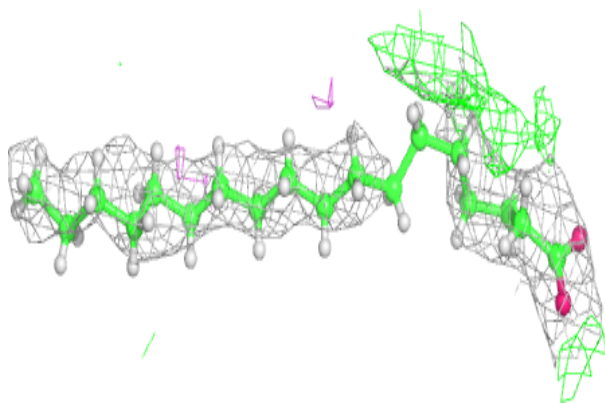
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



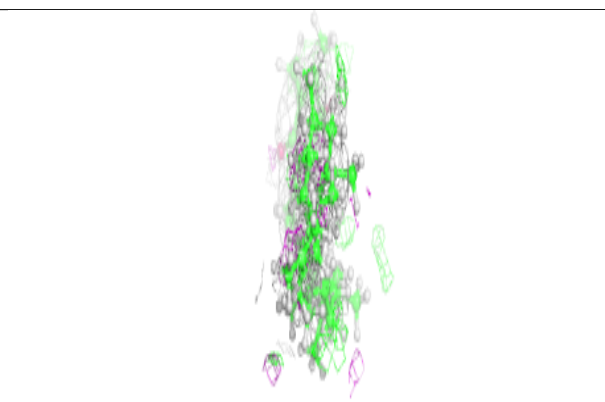
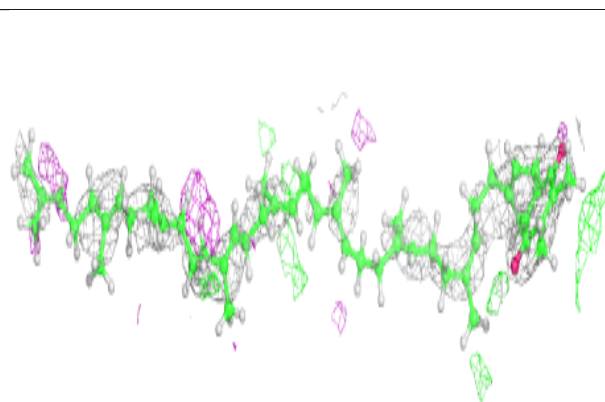
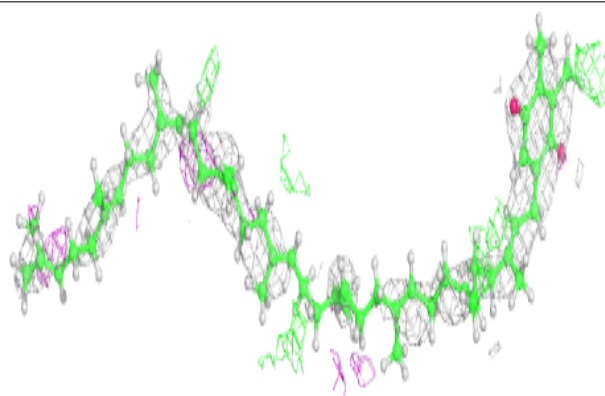


**Electron density around STE b 624:**

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

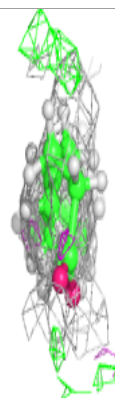
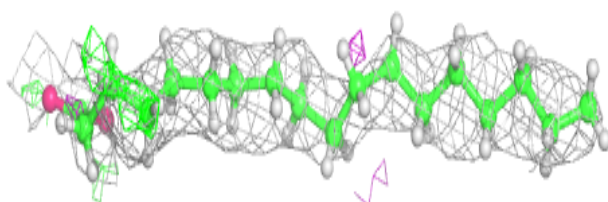
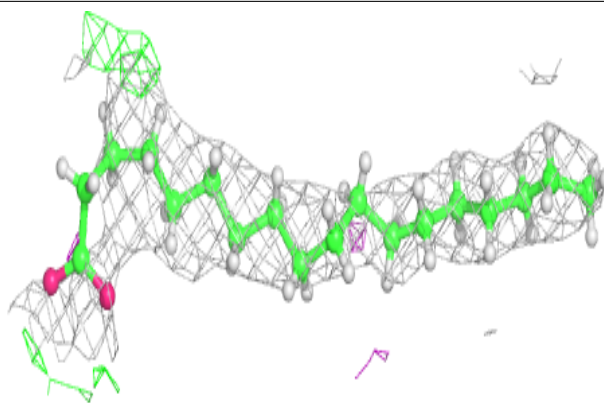
**Electron density around PL9 A 409:**

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

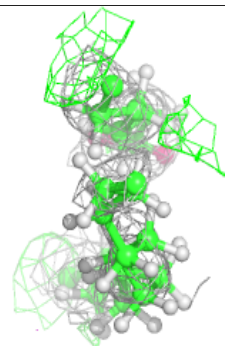
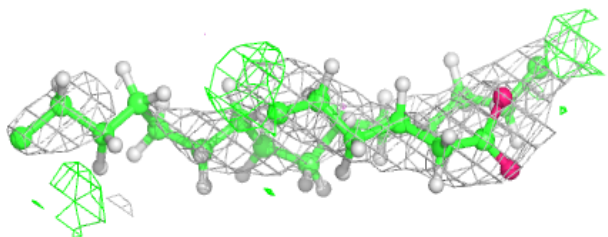
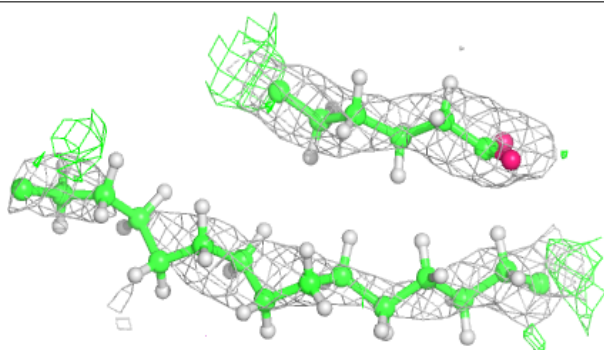


**Electron density around STE c 521:**

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

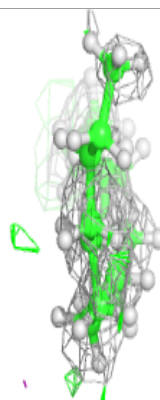
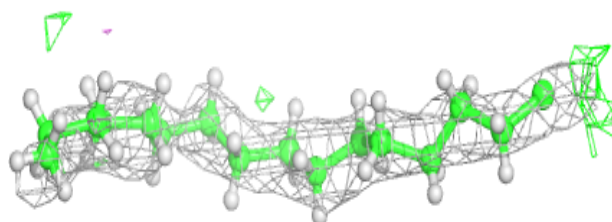
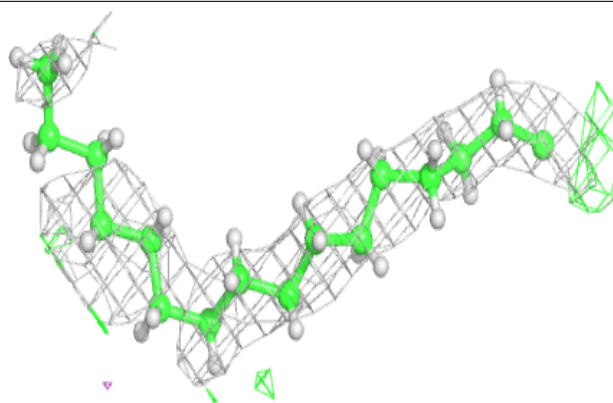
**Electron density around LMG d 411:**

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

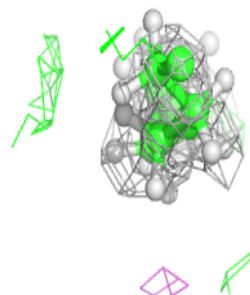
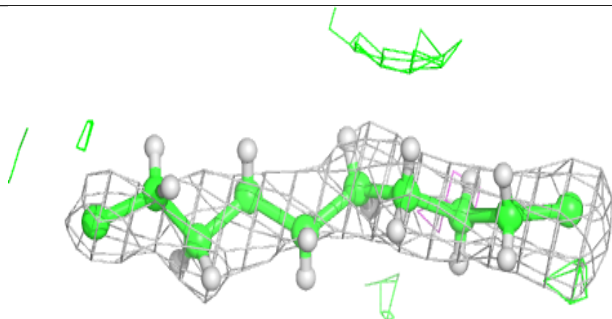
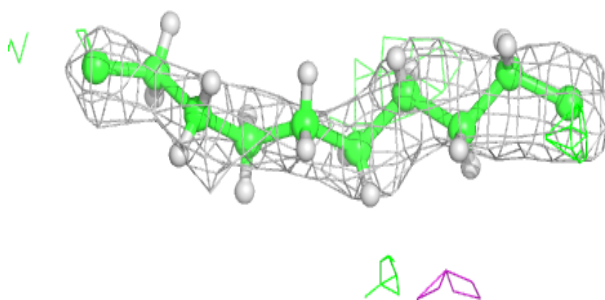


**Electron density around STE B 626:**

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

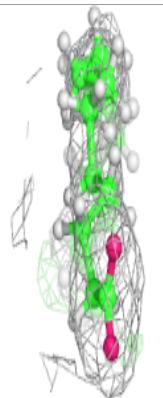
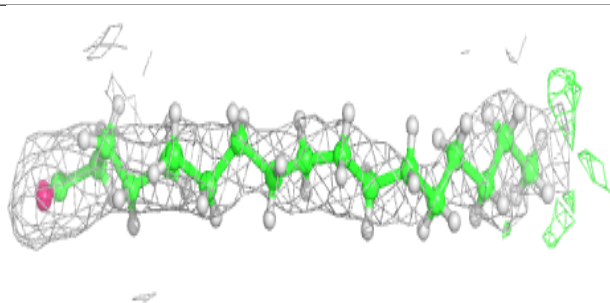
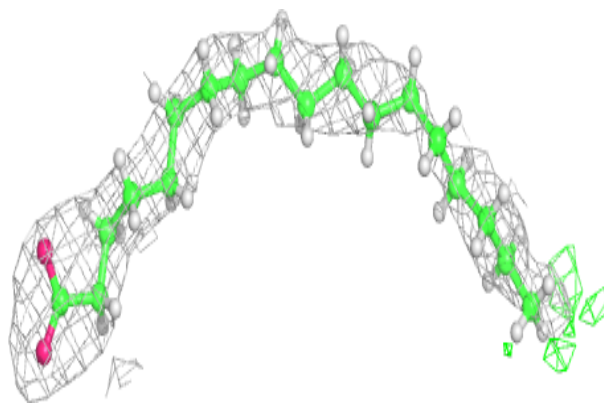
**Electron density around STE a 413:**

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

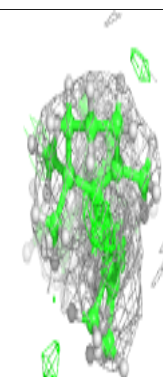
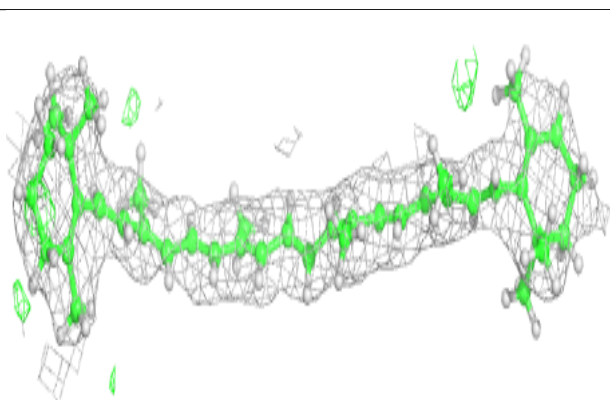
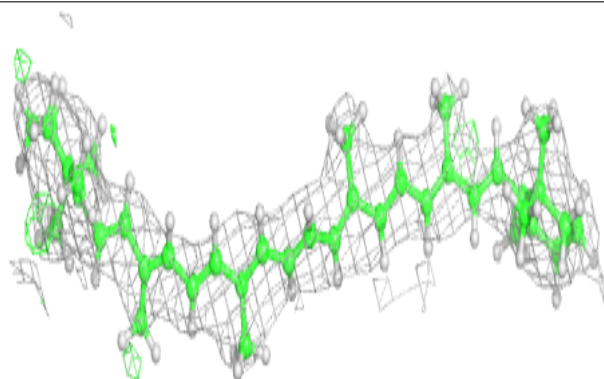


**Electron density around STE x 101:**

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

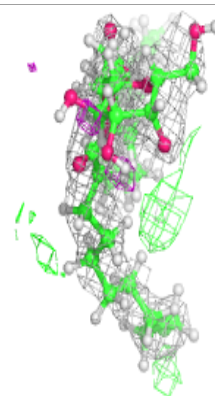
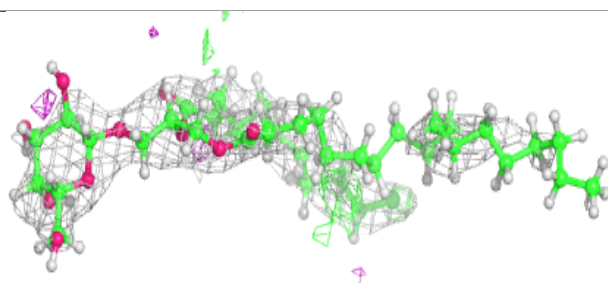
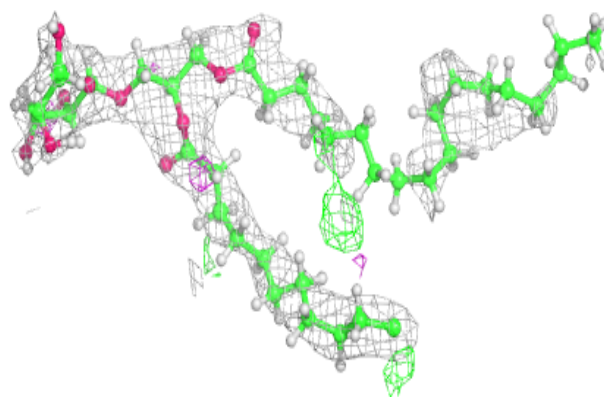
**Electron density around BCR h 101:**

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



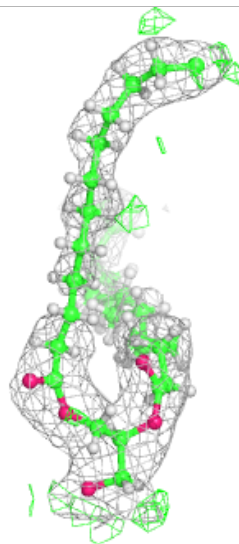
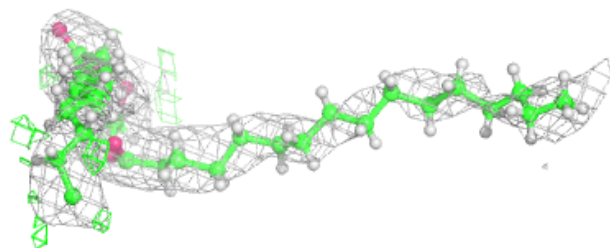
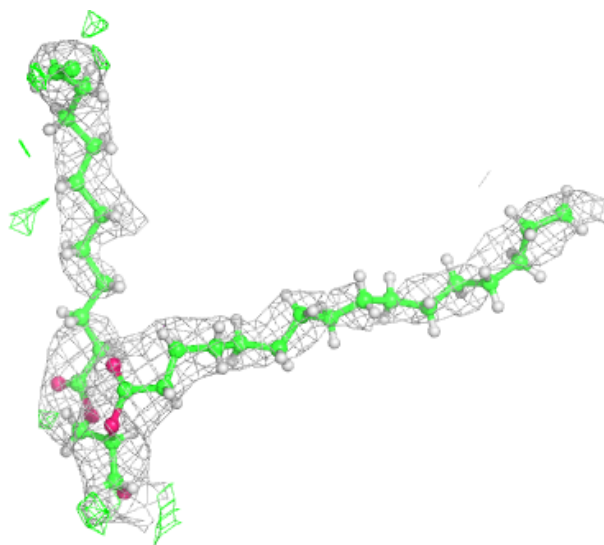
**Electron density around LMG c 522:**

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



**Electron density around SQD a 411:**

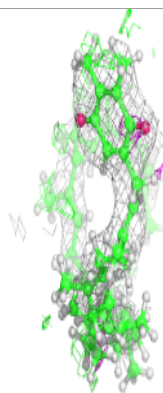
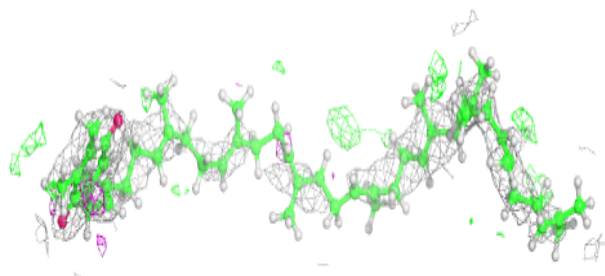
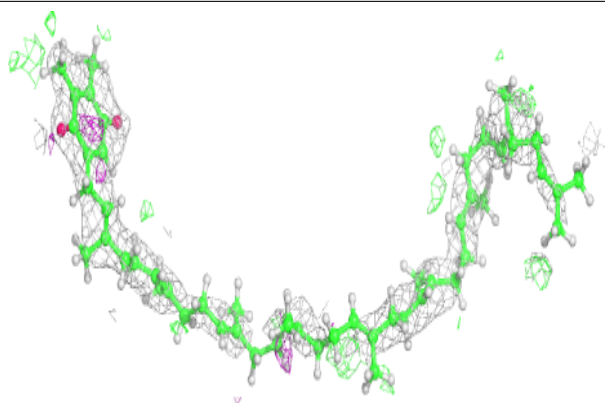
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



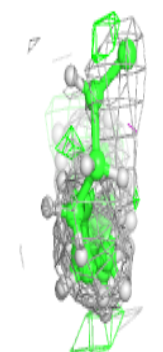
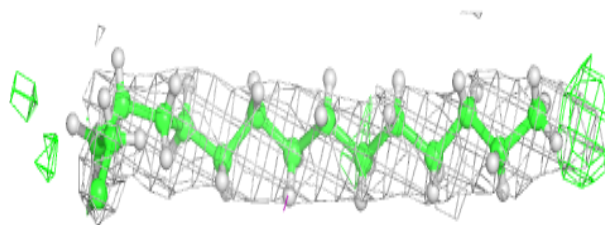
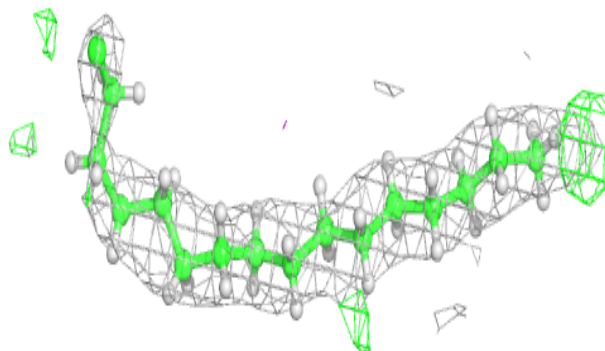


**Electron density around PL9 a 409:**

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

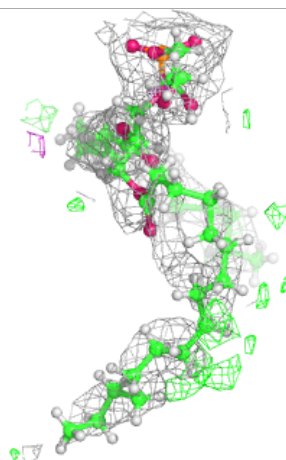
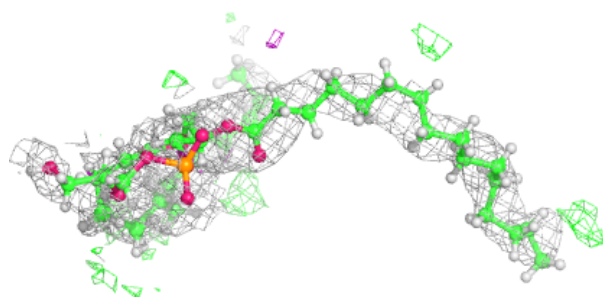
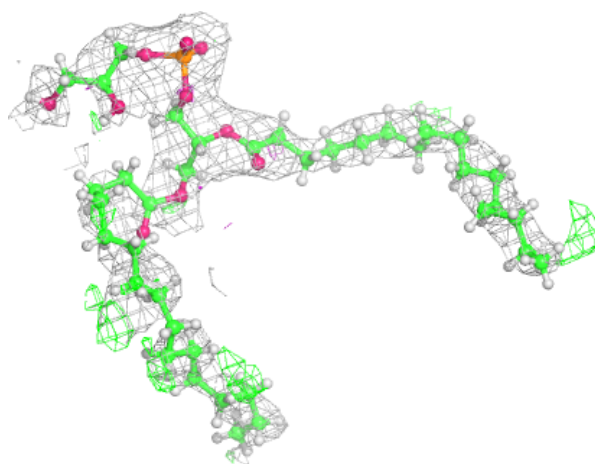
**Electron density around STE C 521:**

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



**Electron density around LHG E 102:**

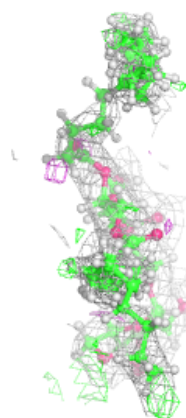
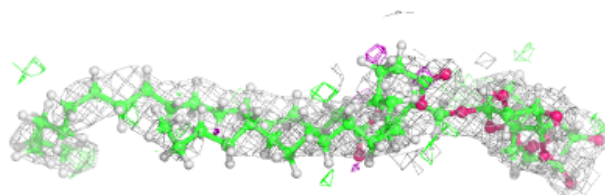
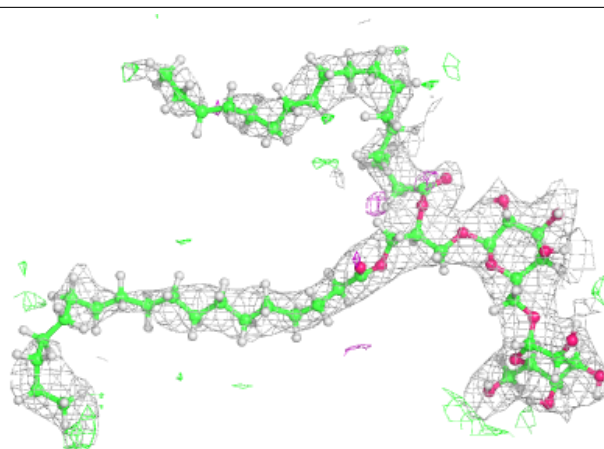
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



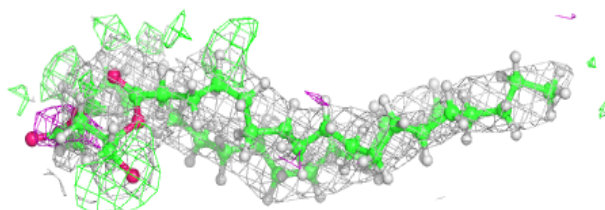
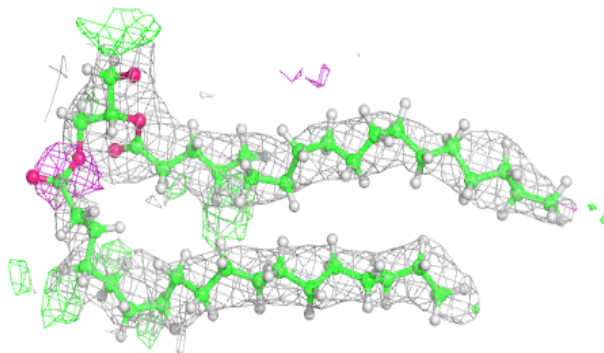


**Electron density around DGD A 414:**

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

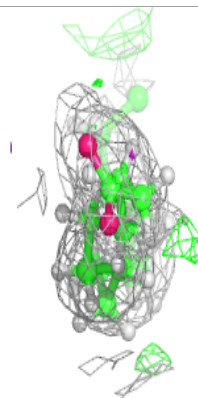
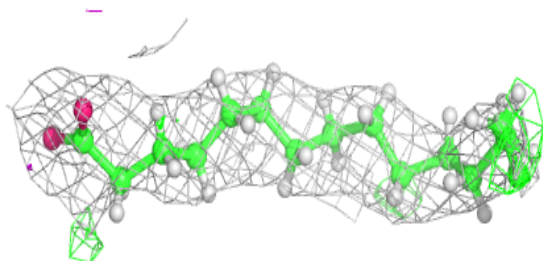
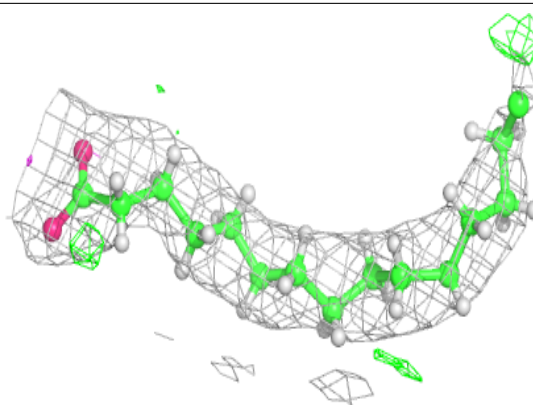
**Electron density around DGD a 412:**

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

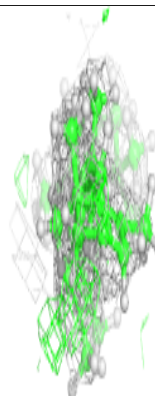
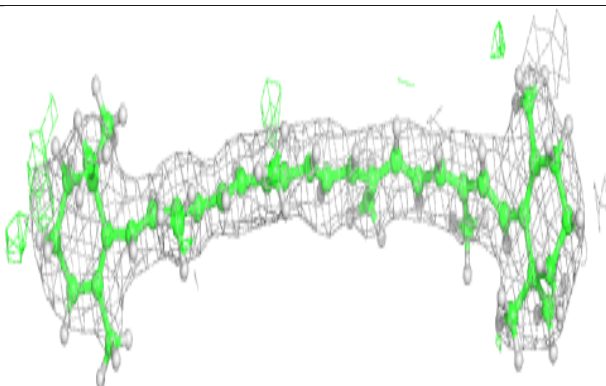
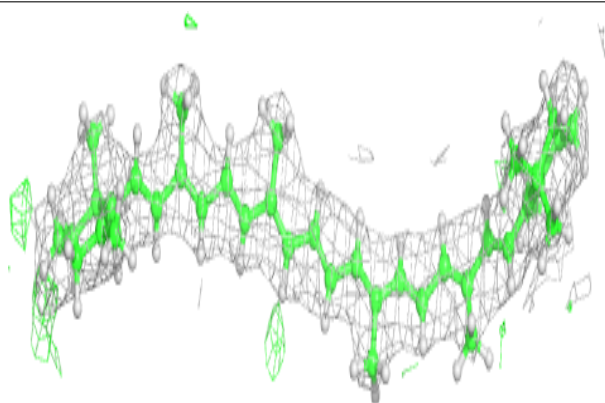


**Electron density around STE B 620:**

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

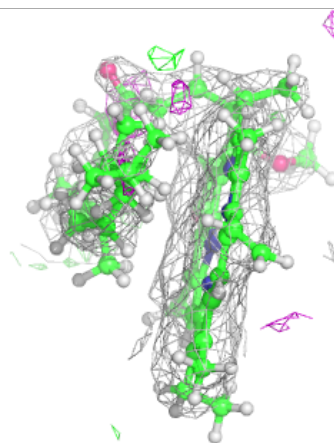
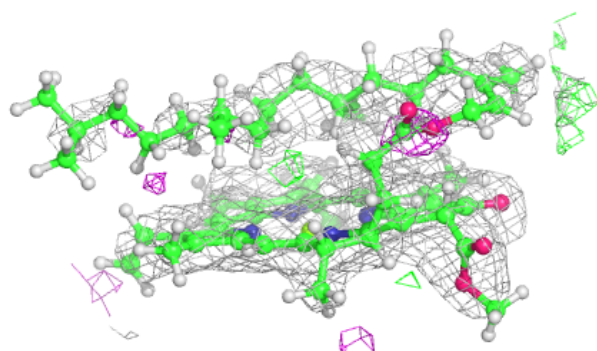
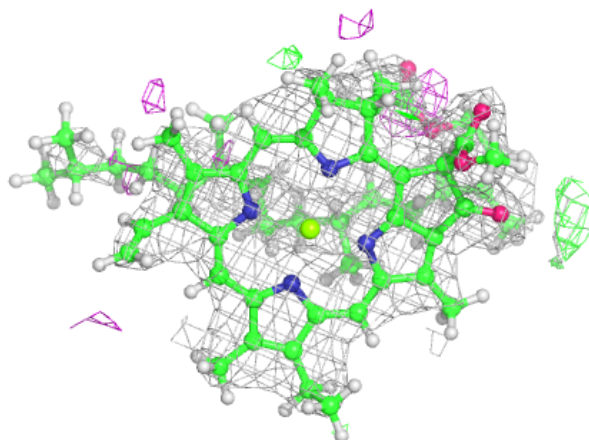
**Electron density around BCR H 101:**

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



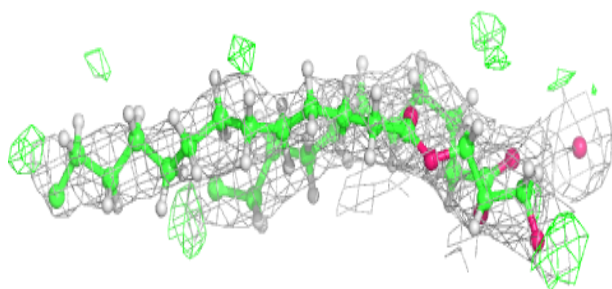
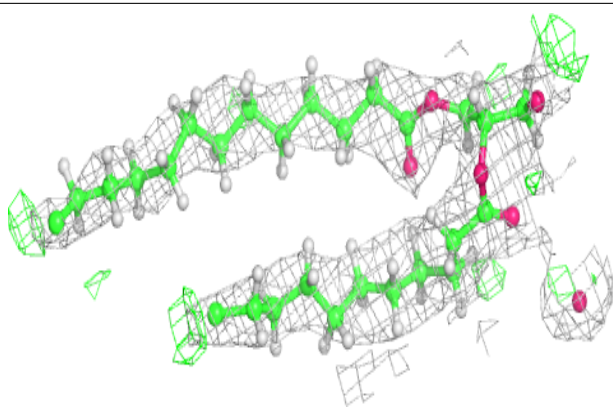
**Electron density around CLA b 601:**

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

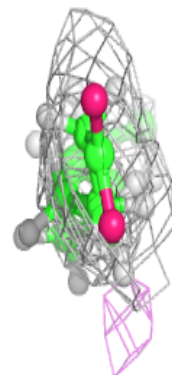
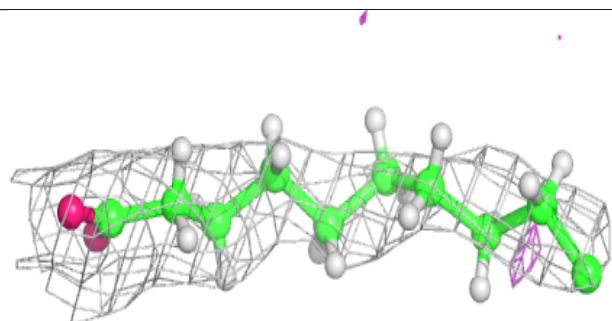
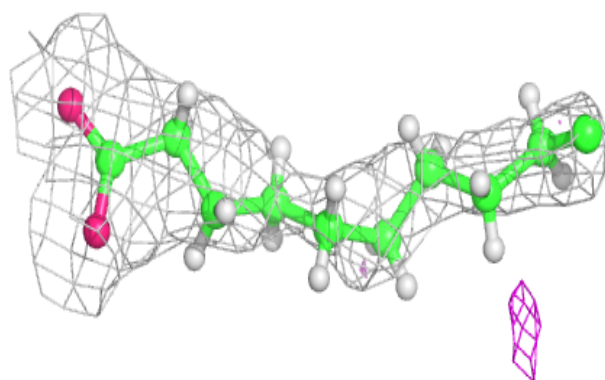


**Electron density around LMG D 410:**

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

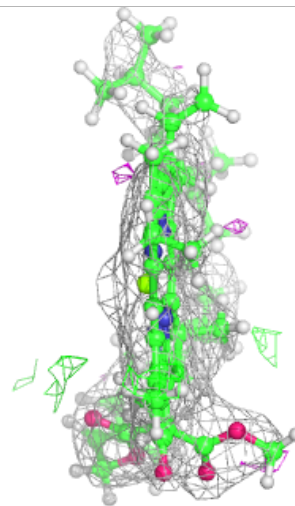
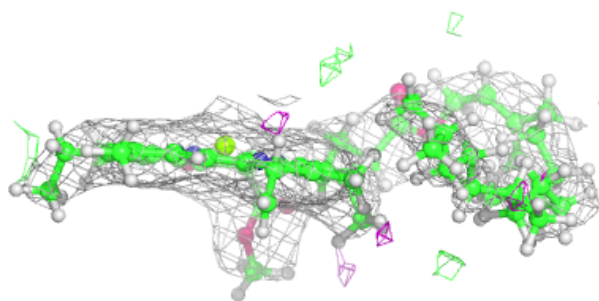
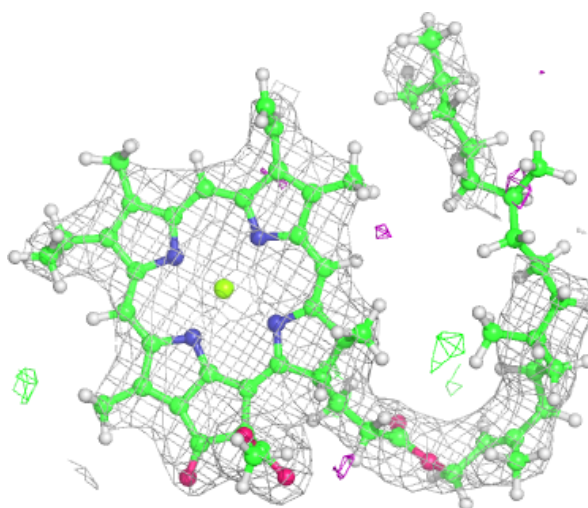
**Electron density around STE a 414:**

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



**Electron density around CLA C 512:**

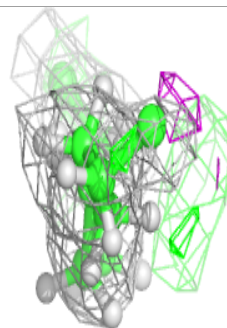
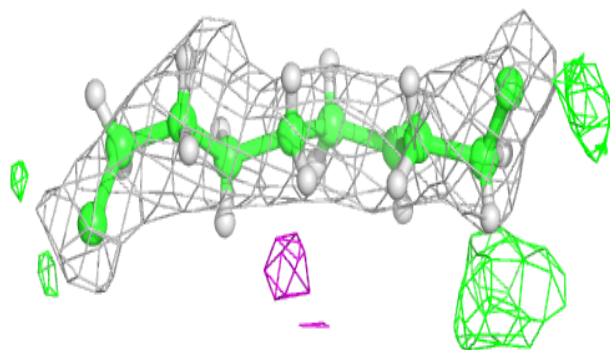
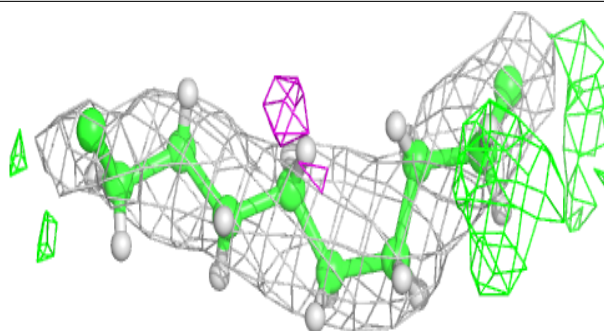
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



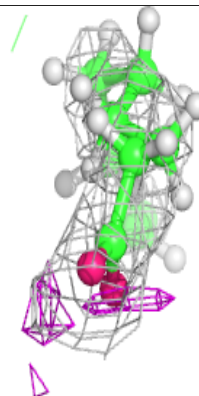
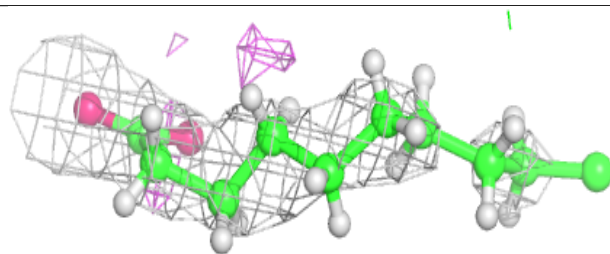
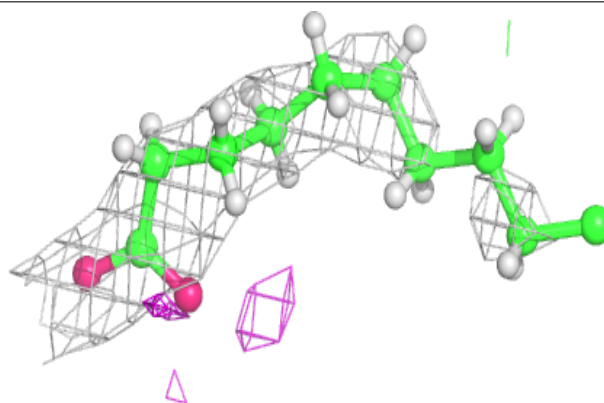


**Electron density around STE b 625:**

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

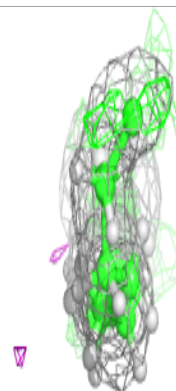
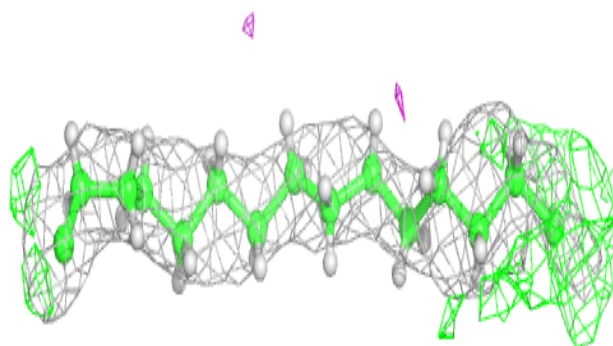
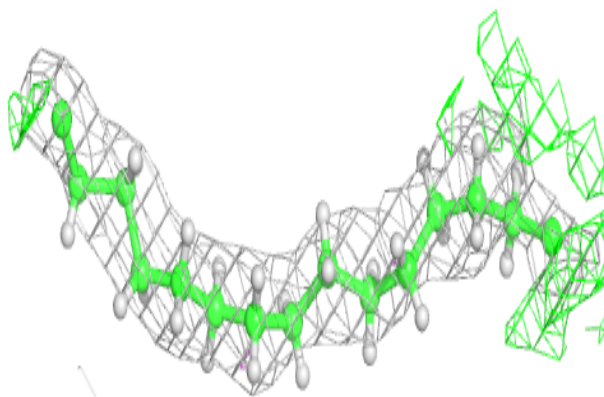
**Electron density around STE B 627:**

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

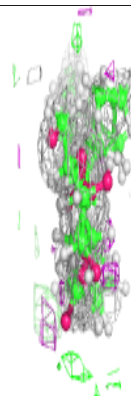
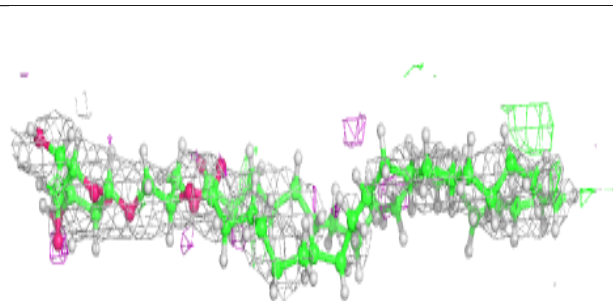
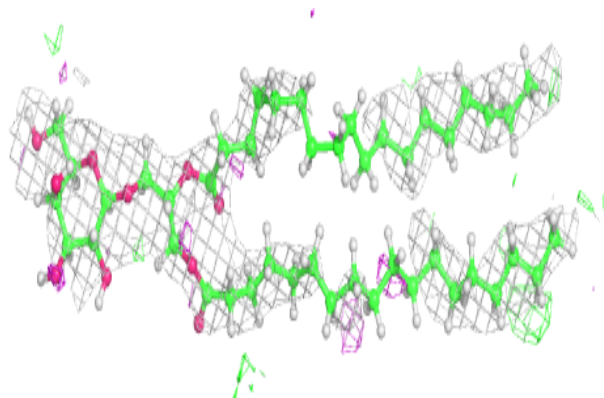


**Electron density around STE I 101:**

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

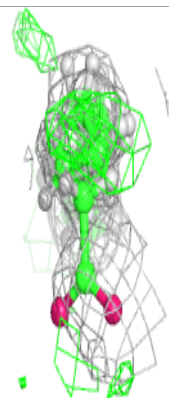
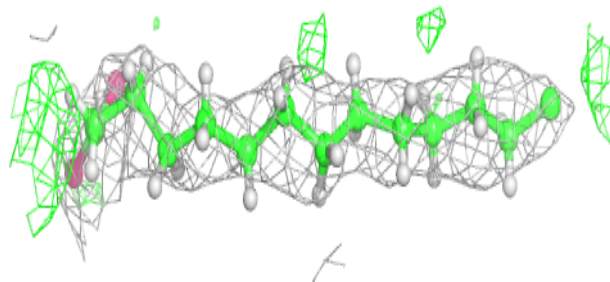
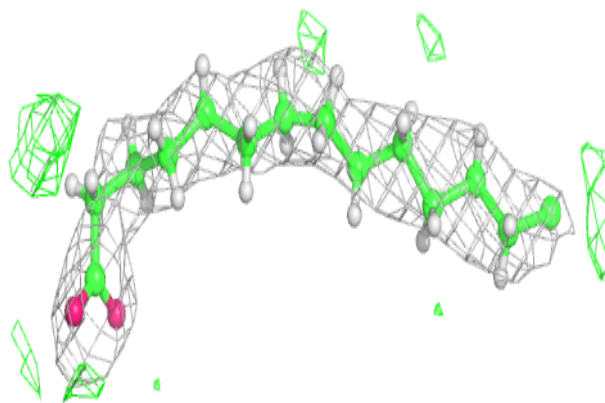
**Electron density around LMG b 622:**

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



**Electron density around STE b 623:**

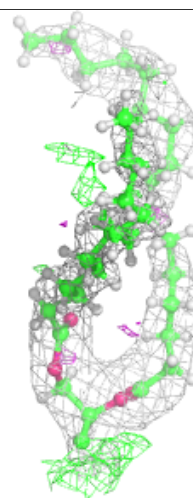
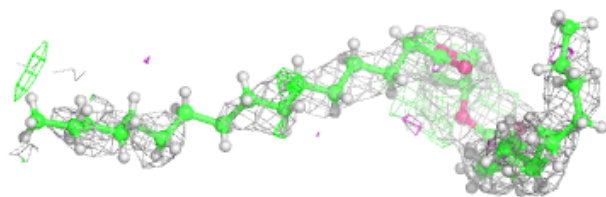
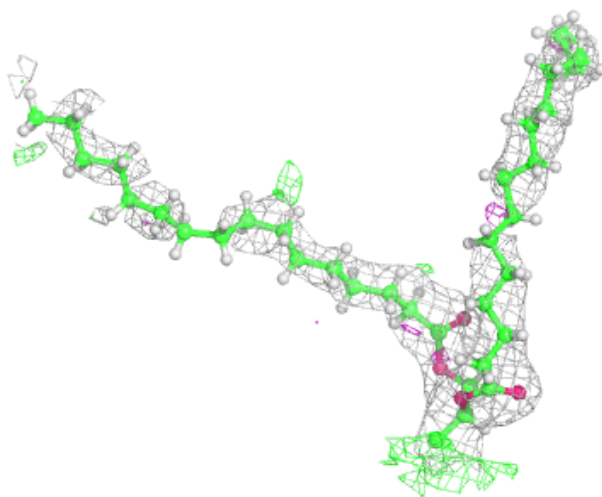
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





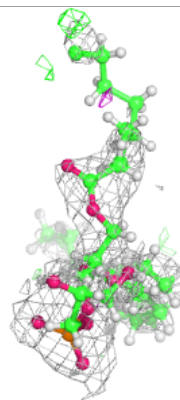
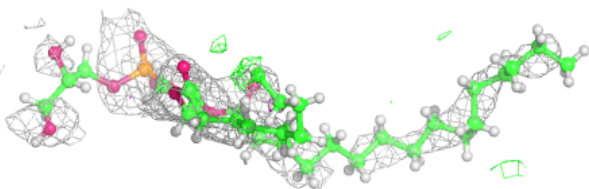
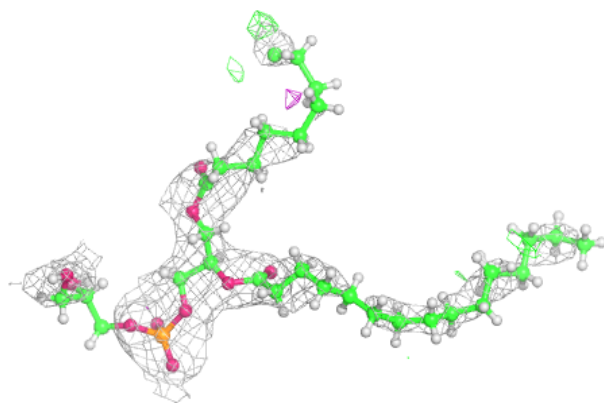
**Electron density around SQD A 413:**

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



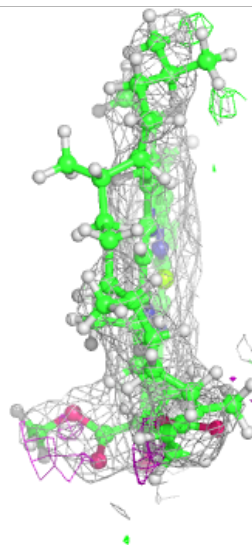
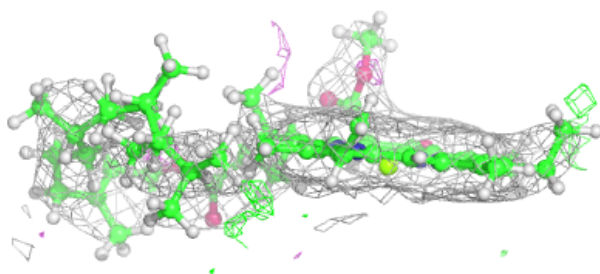
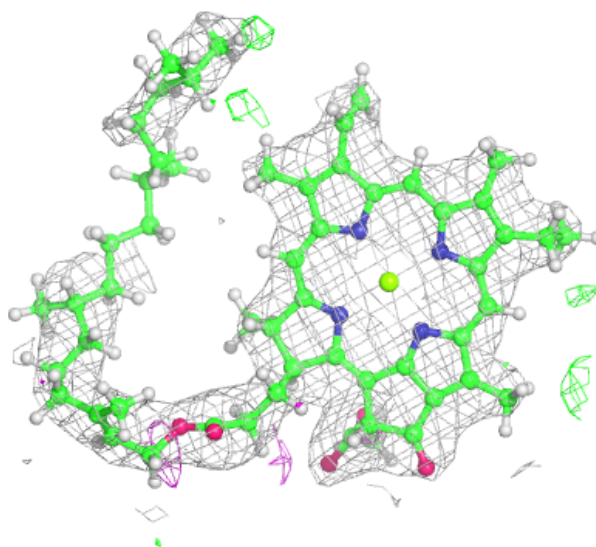
**Electron density around LHG e 101:**

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



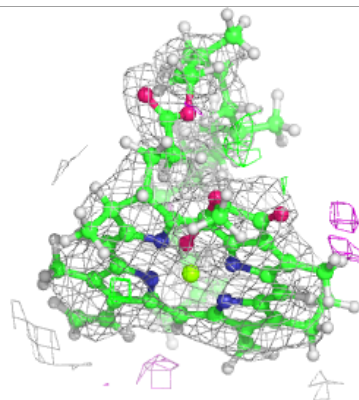
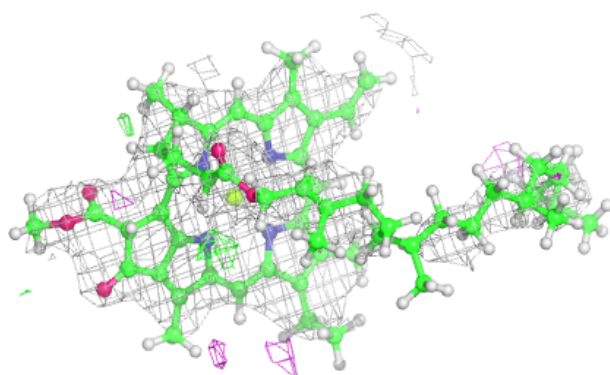
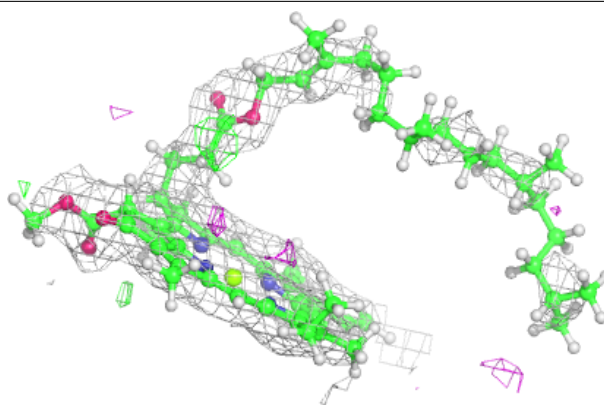
**Electron density around CLA c 512:**

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

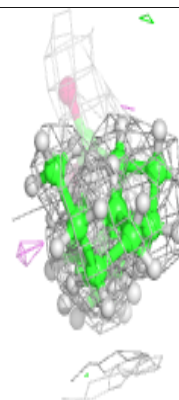
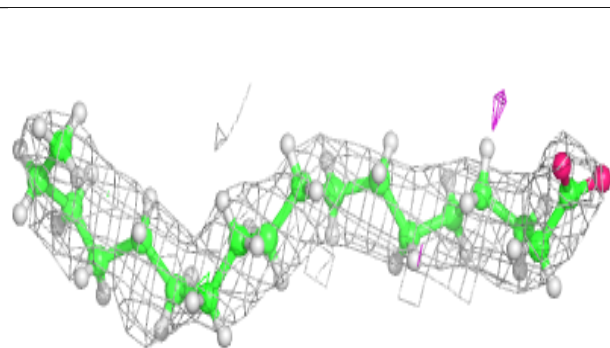
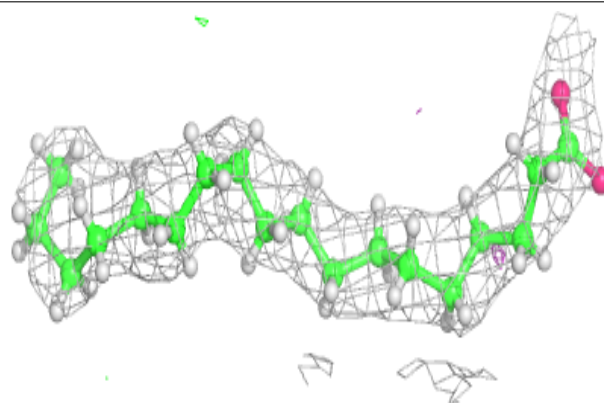


**Electron density around CLA c 513:**

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

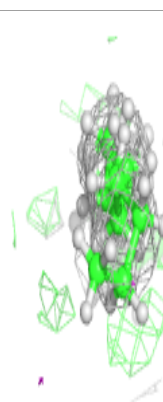
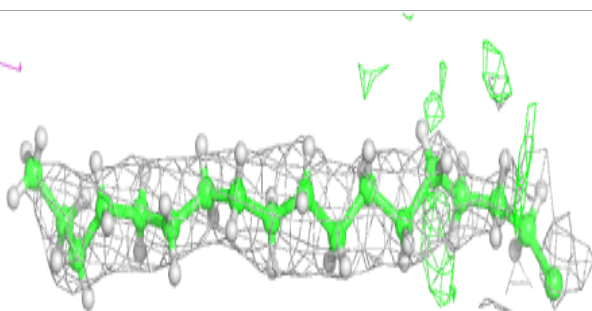
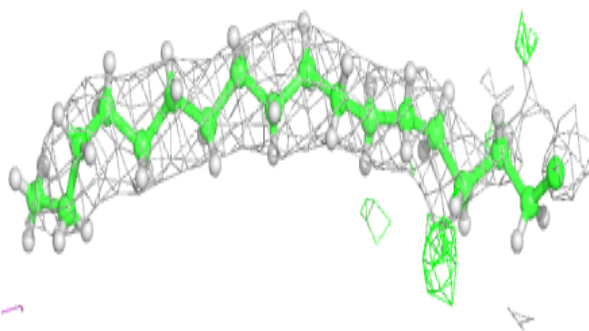
**Electron density around STE b 621:**

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

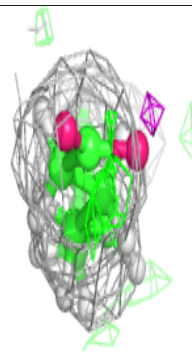
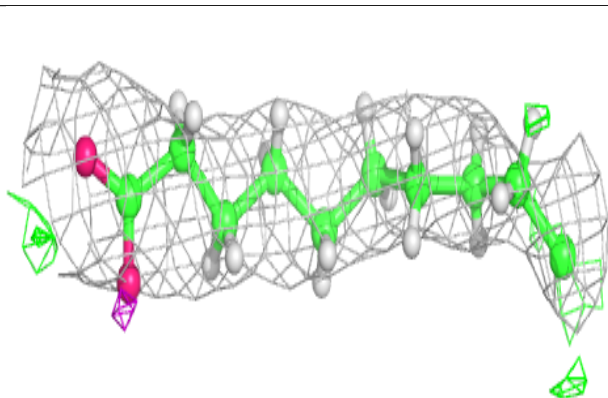
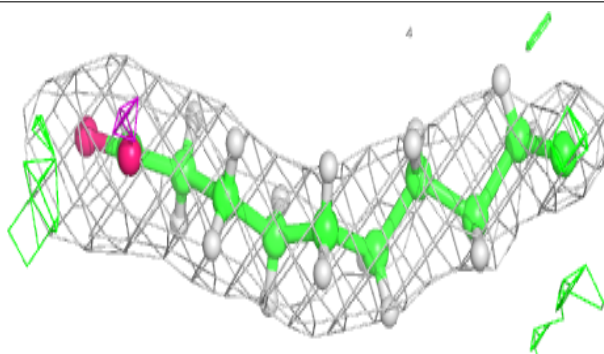


**Electron density around STE l 102:**

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

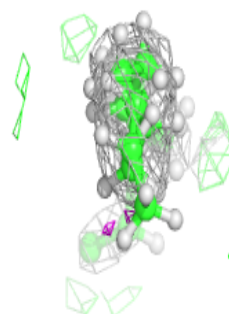
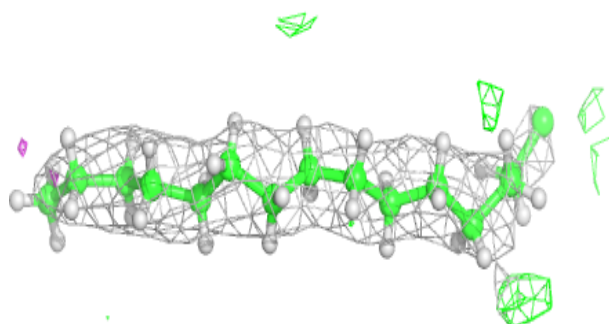
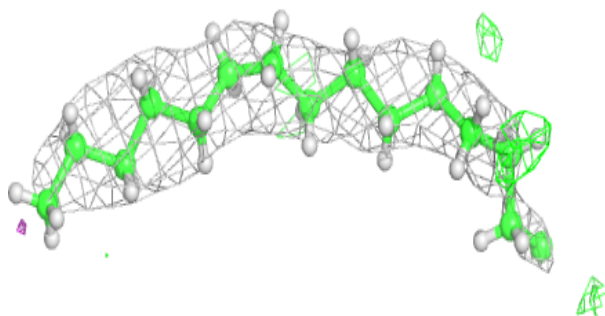
**Electron density around STE j 101:**

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

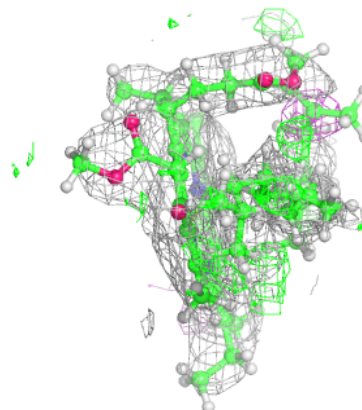
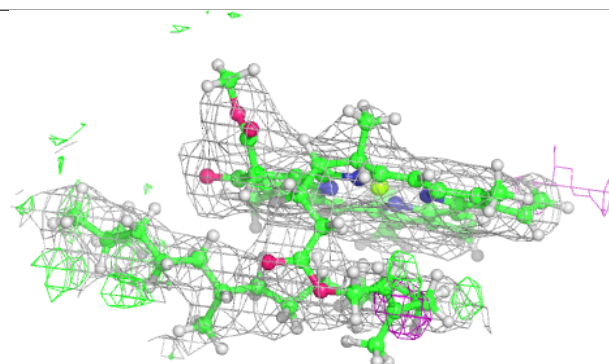
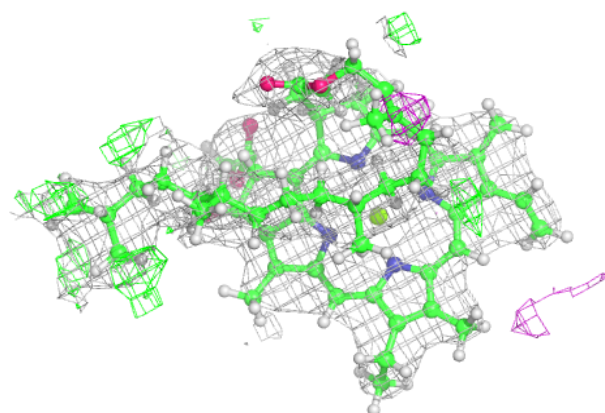


**Electron density around STE T 103:**

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

**Electron density around CLA B 601:**

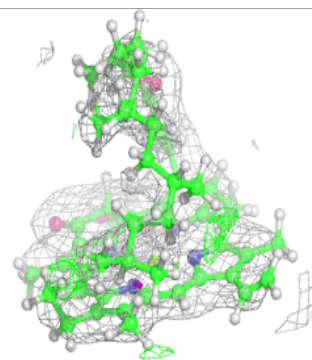
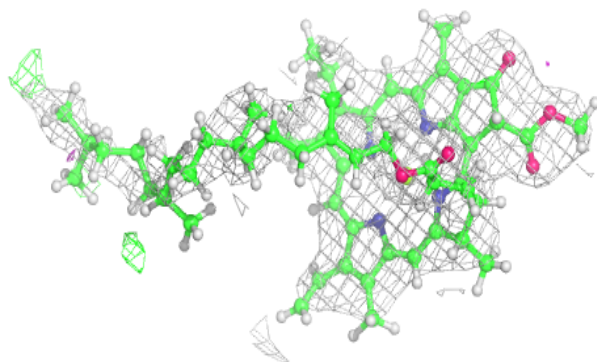
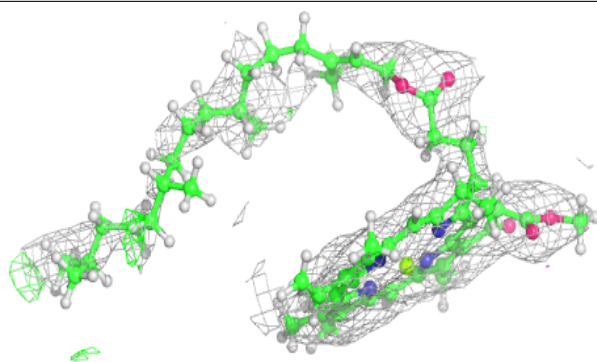
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



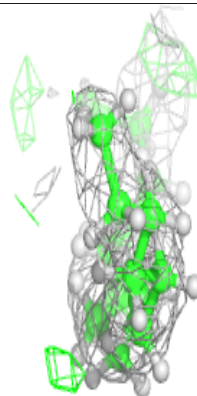
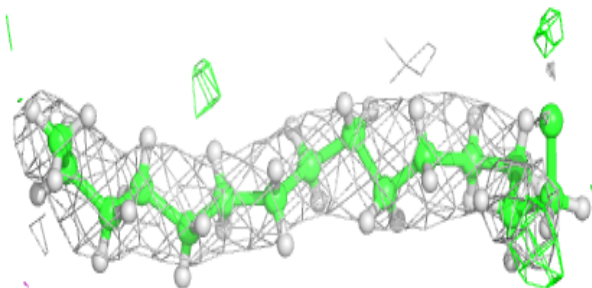
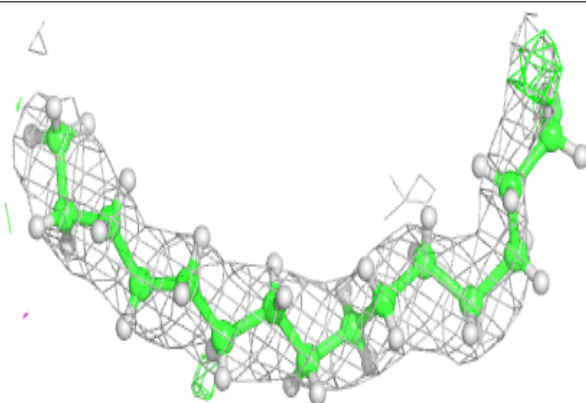


**Electron density around CLA C 513:**

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

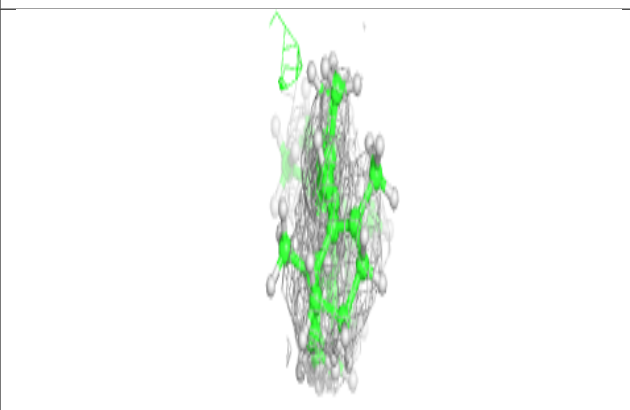
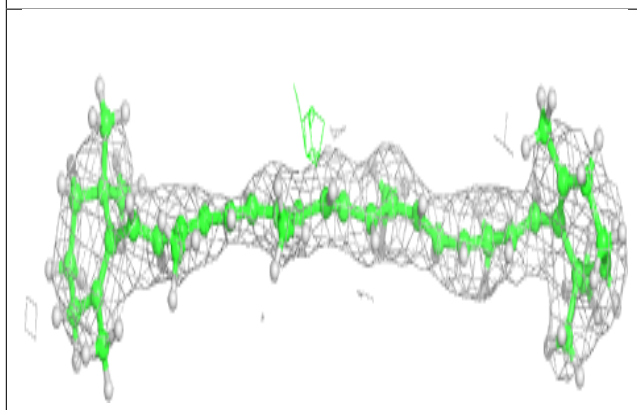
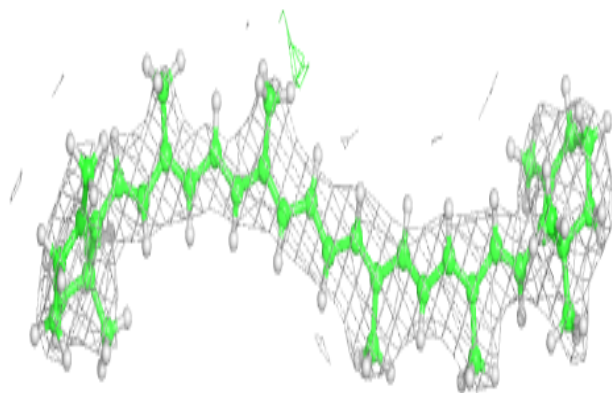
**Electron density around STE T 102:**

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

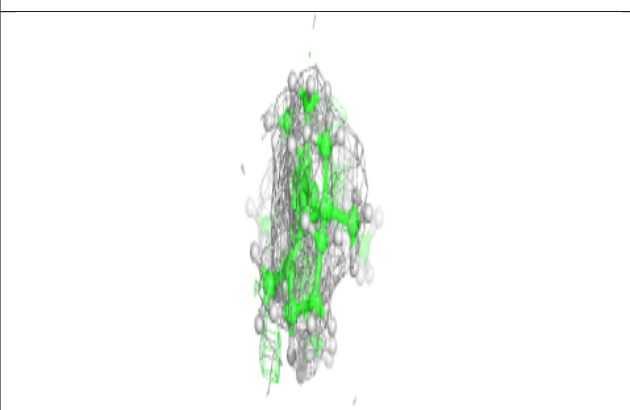
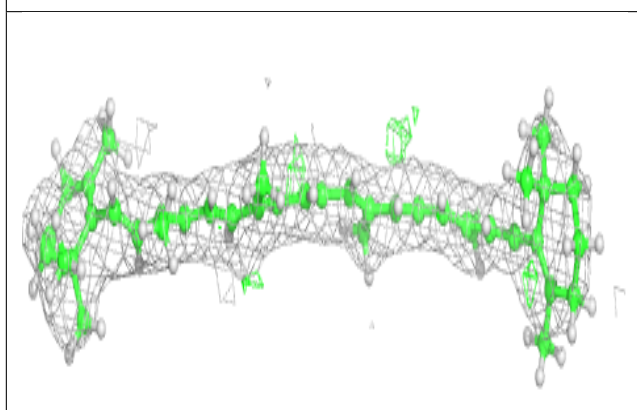
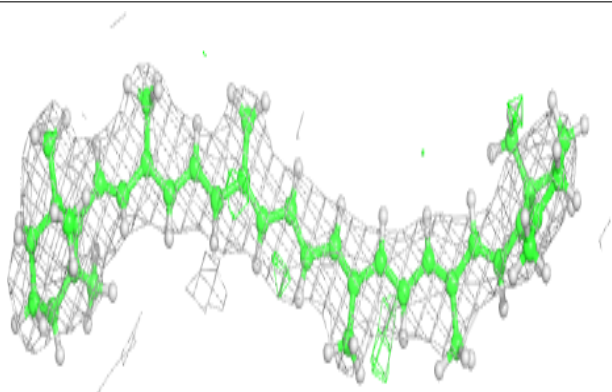


**Electron density around BCR k 101:**

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

**Electron density around BCR Y 101:**

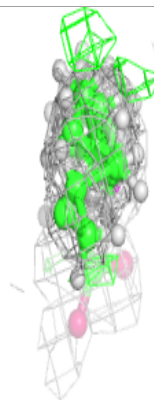
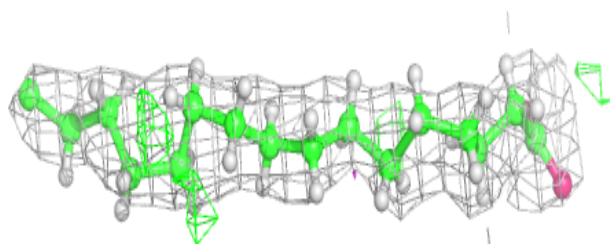
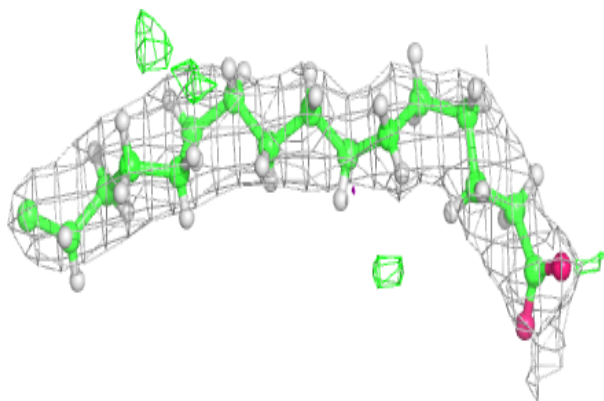
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



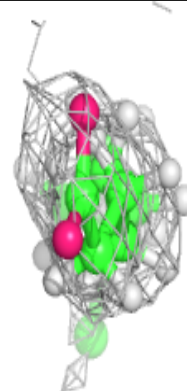
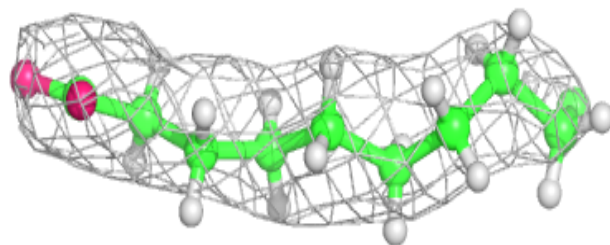
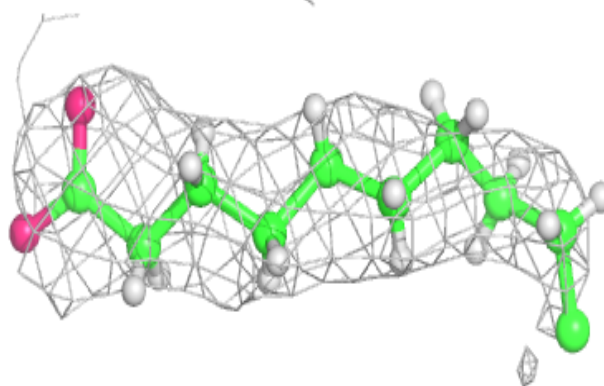


**Electron density around STE B 625:**

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

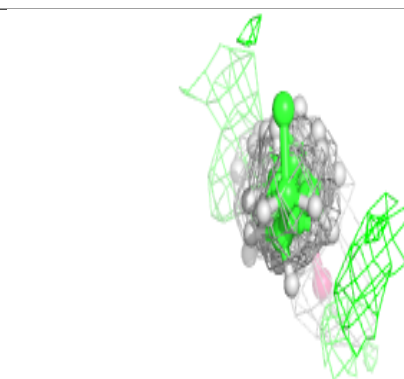
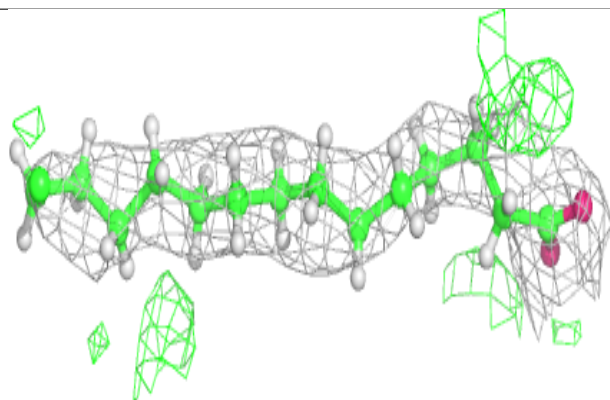
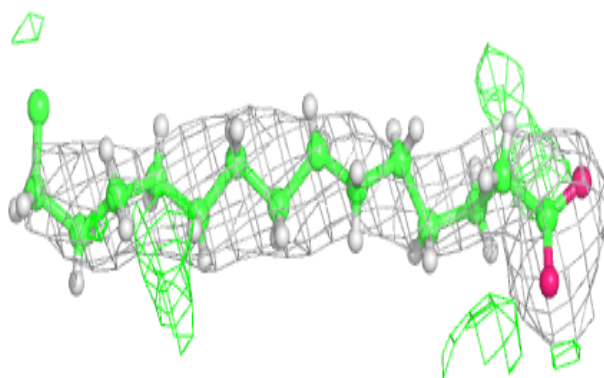
**Electron density around STE c 524:**

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

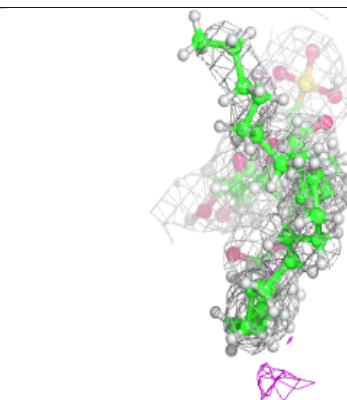
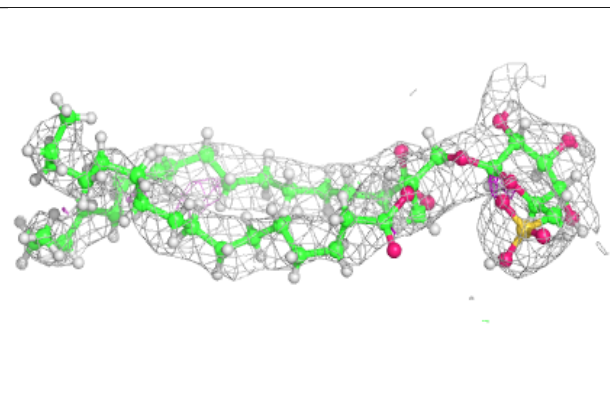
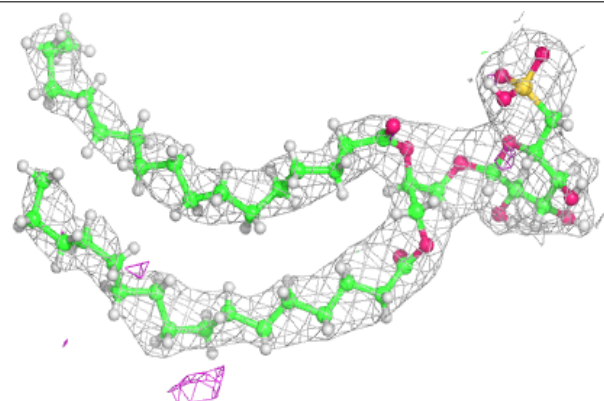


**Electron density around STE d 413:**

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

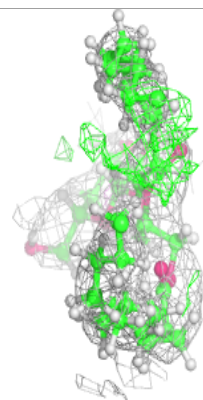
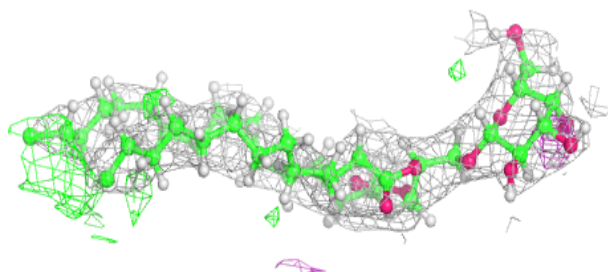
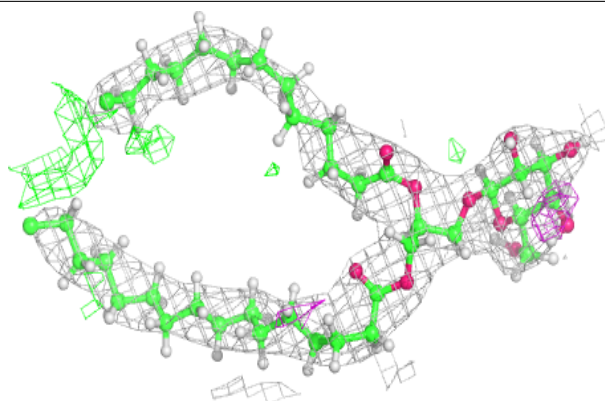
**Electron density around SQD B 623:**

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

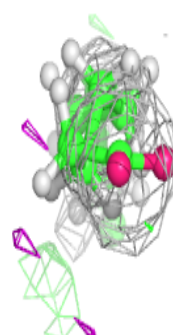
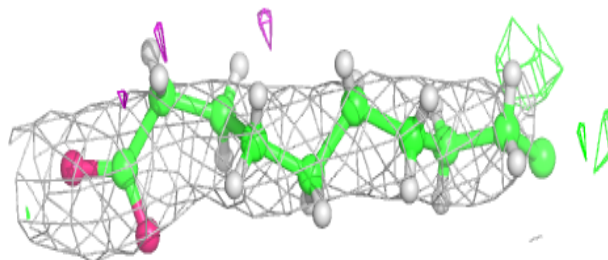
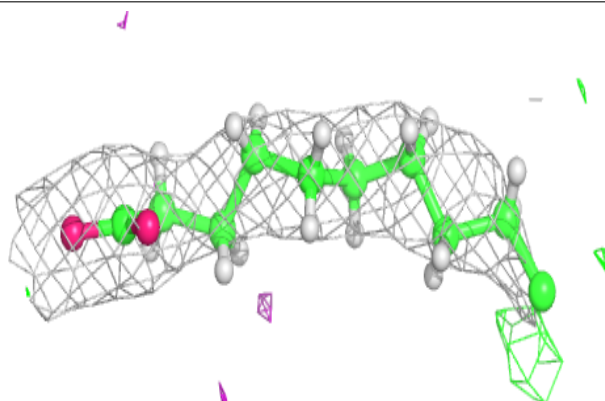


**Electron density around LMG A 411:**

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

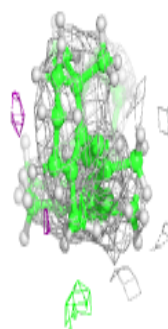
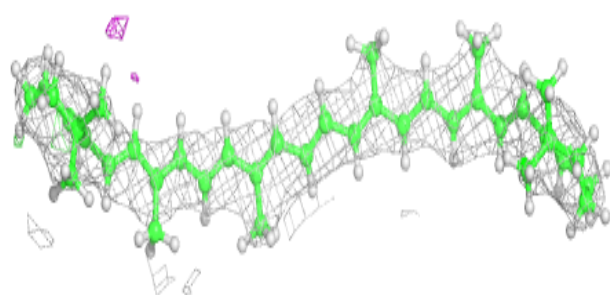
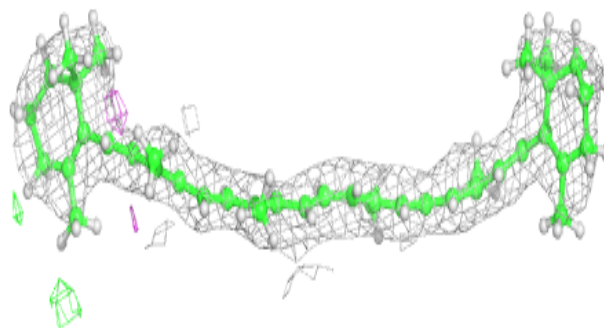
**Electron density around STE m 101:**

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

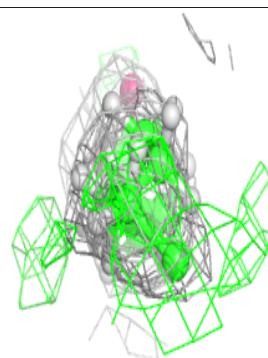
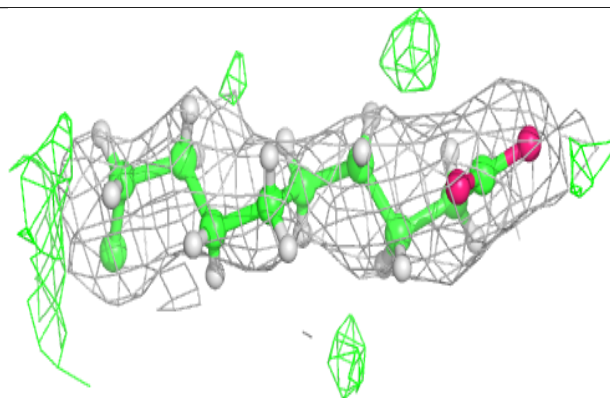
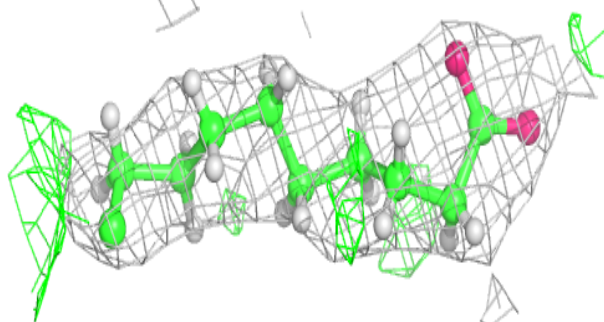


**Electron density around BCR c 516:**

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

**Electron density around STE J 101:**

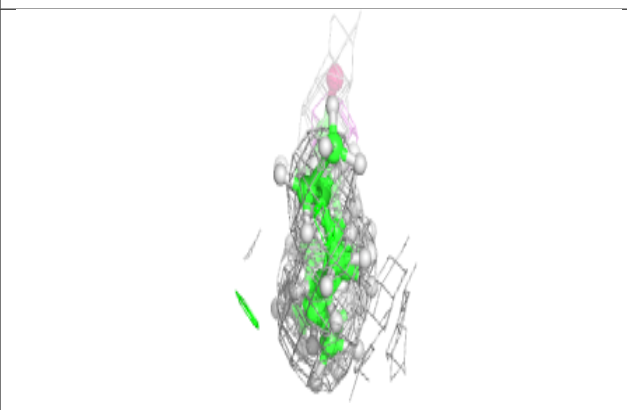
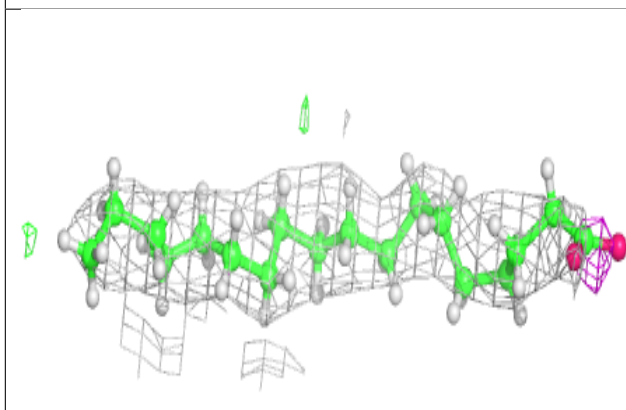
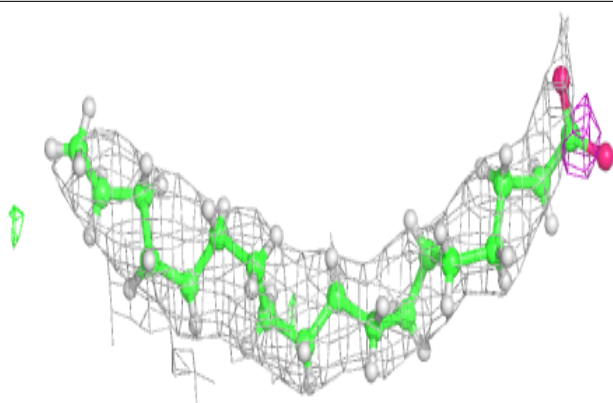
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



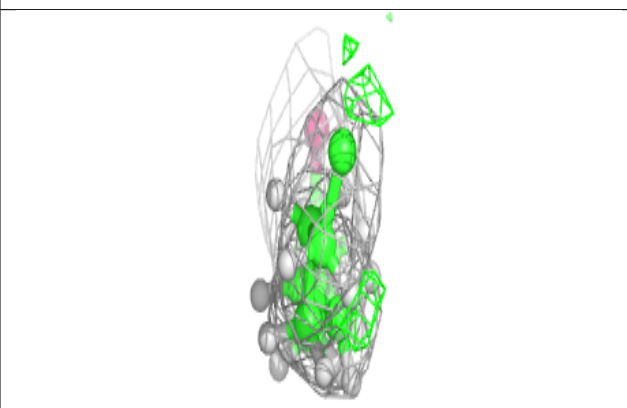
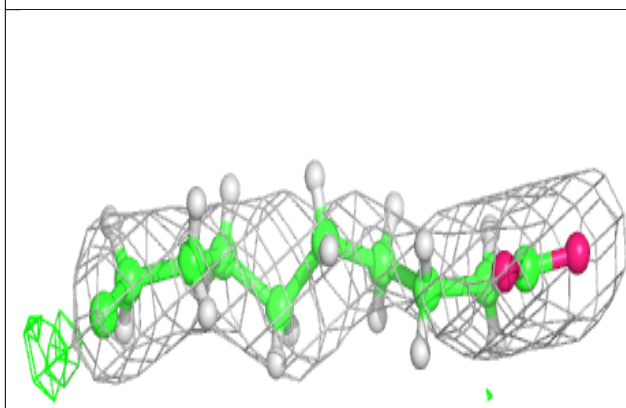
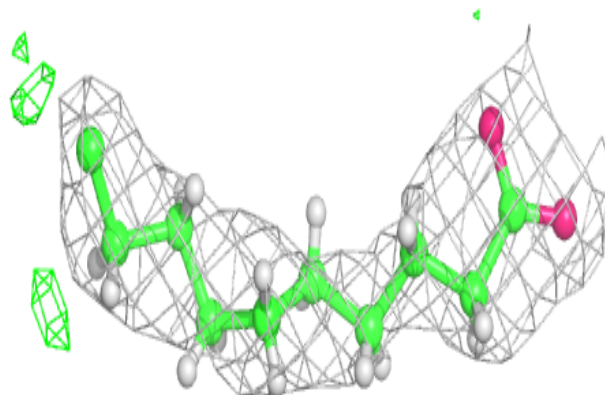


**Electron density around STE D 411:**

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

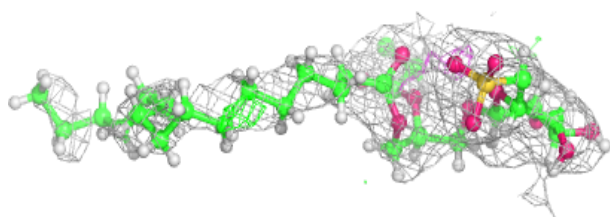
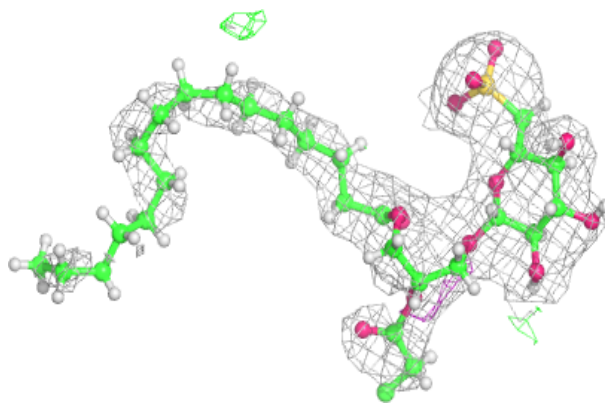
**Electron density around STE C 520:**

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

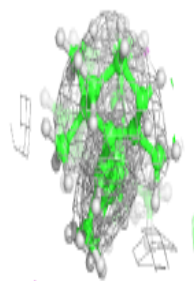
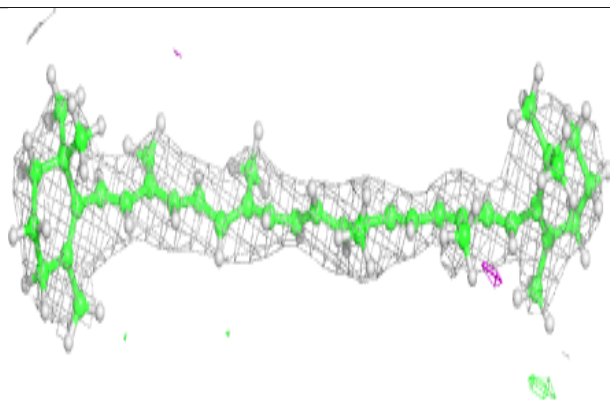
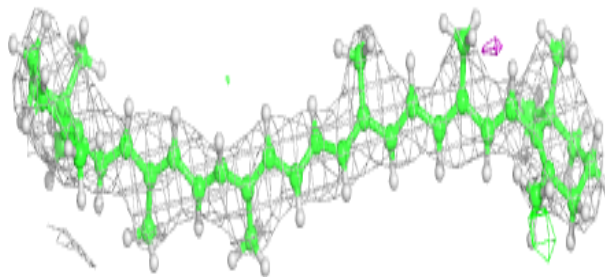


**Electron density around SQD f 102:**

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

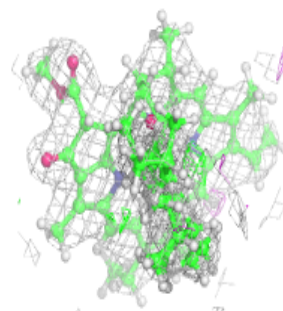
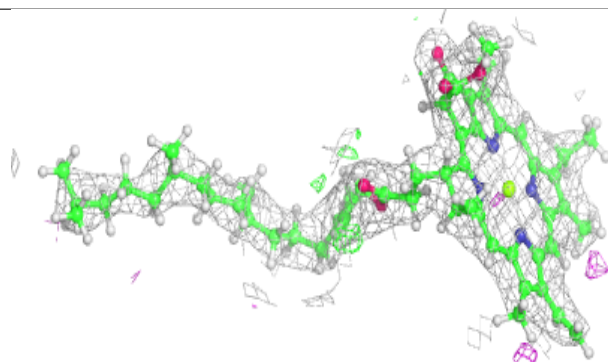
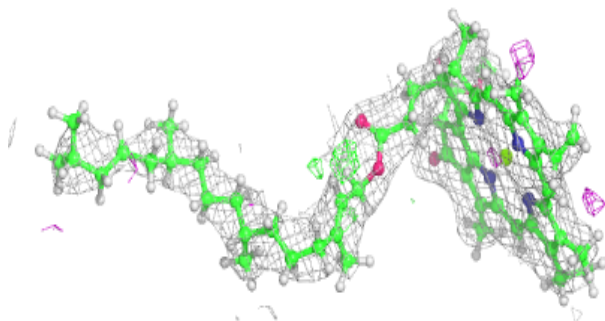
**Electron density around BCR c 514:**

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

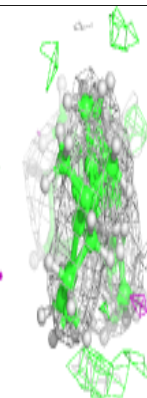
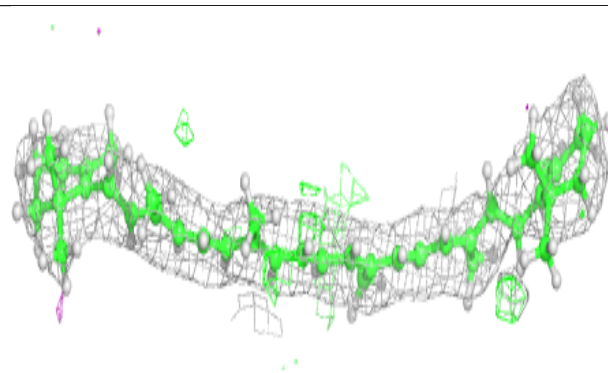
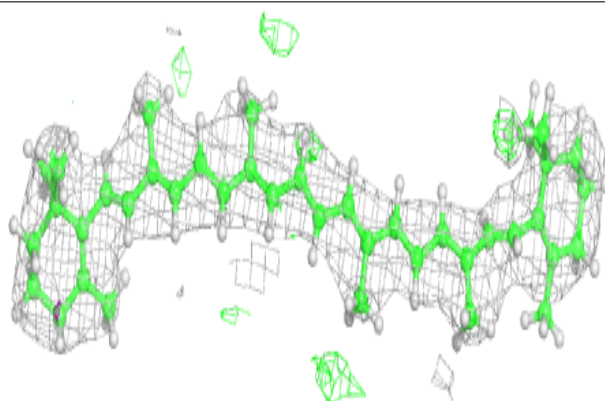


**Electron density around CLA c 502:**

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

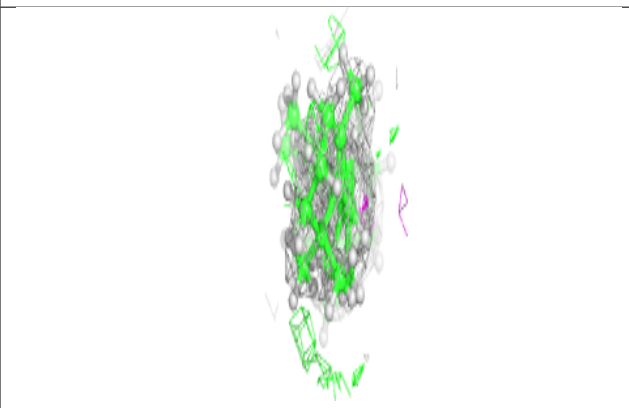
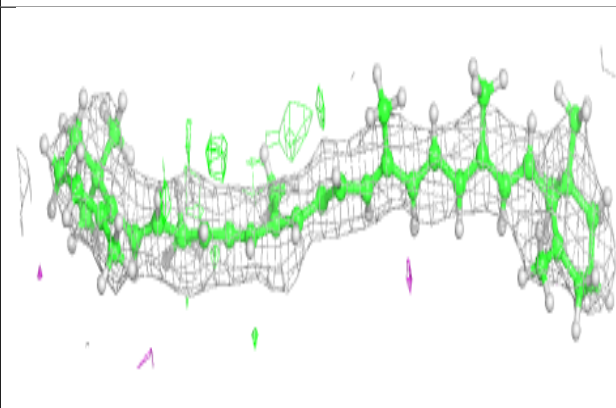
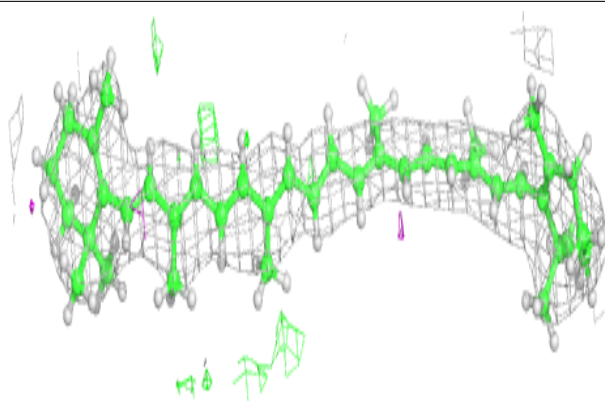
**Electron density around BCR d 406:**

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

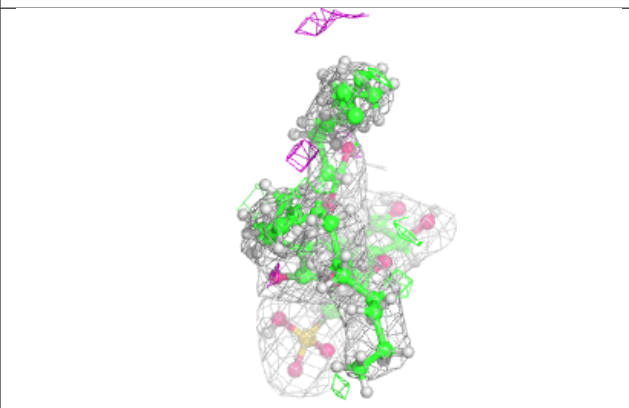
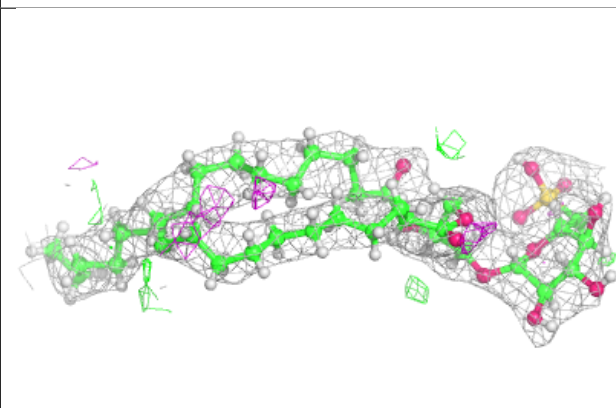
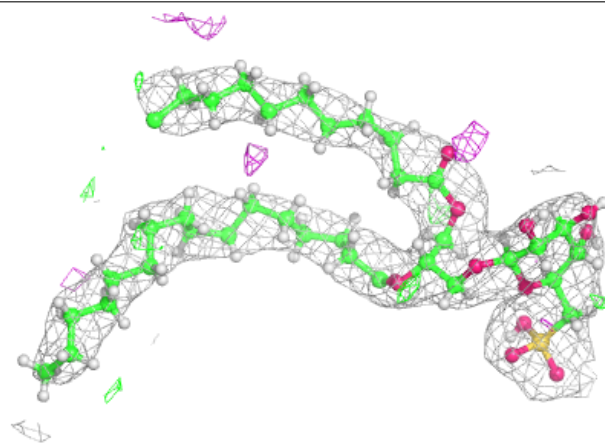


**Electron density around BCR K 101:**

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

**Electron density around SQD L 101:**

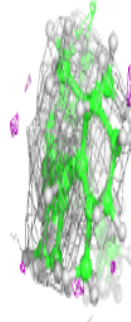
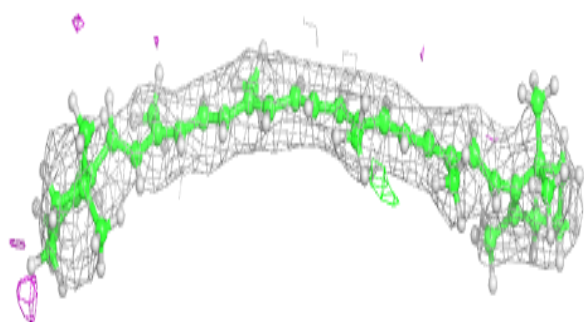
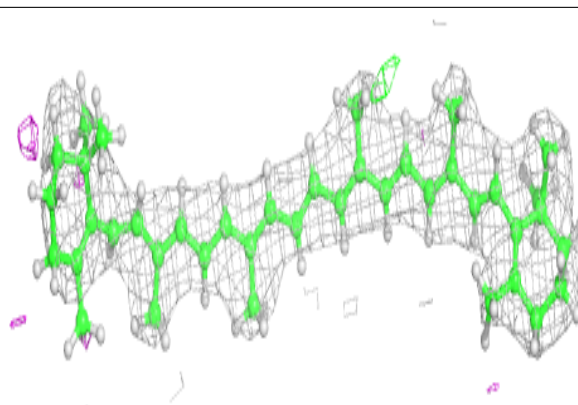
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



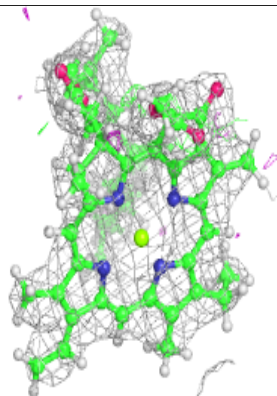
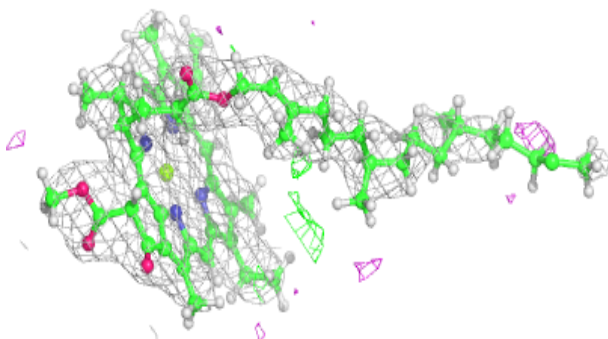
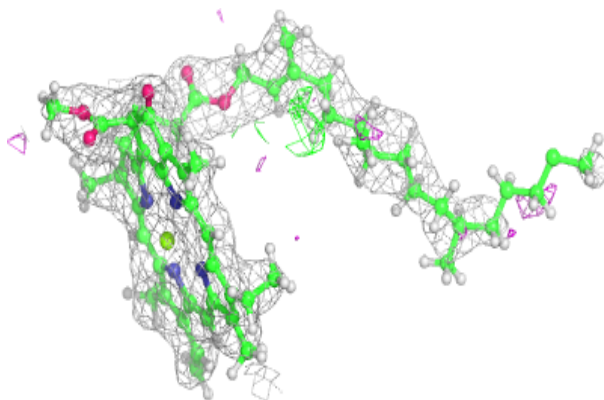


**Electron density around BCR D 405:**

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

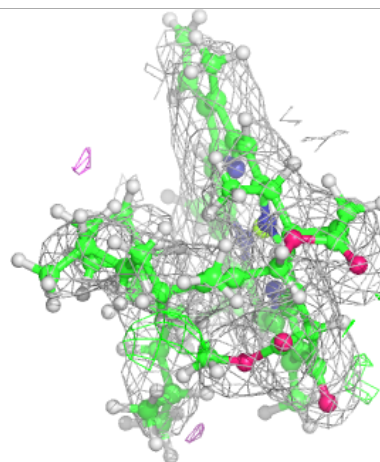
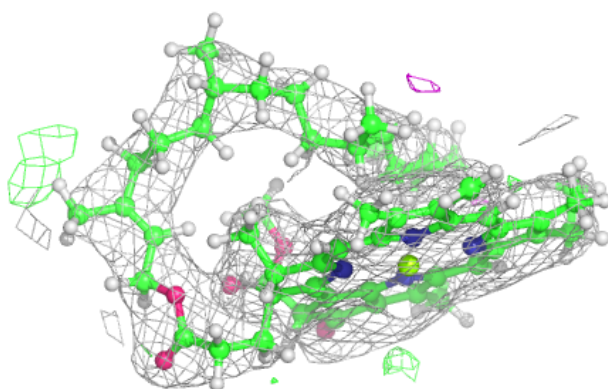
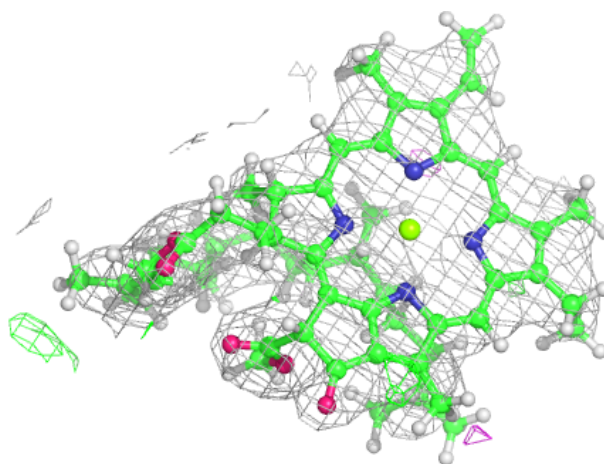
**Electron density around CLA c 508:**

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



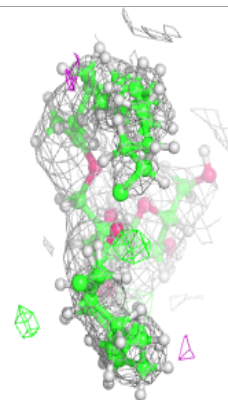
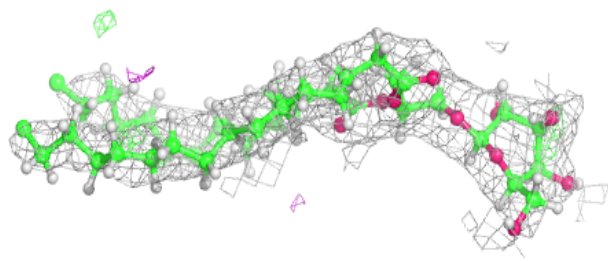
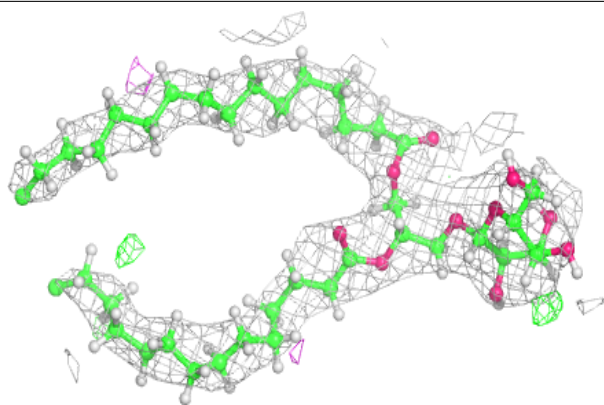
**Electron density around CLA c 510:**

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

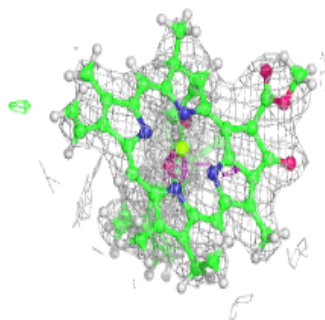
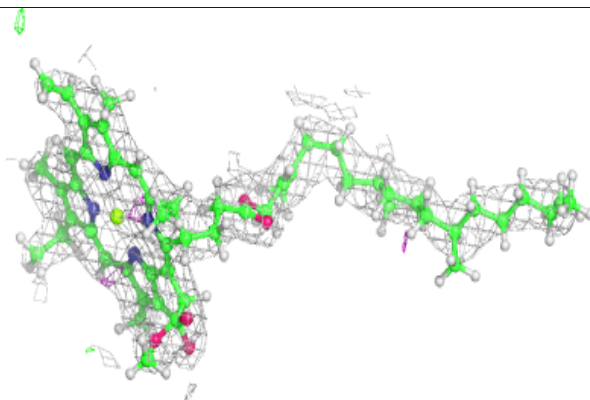
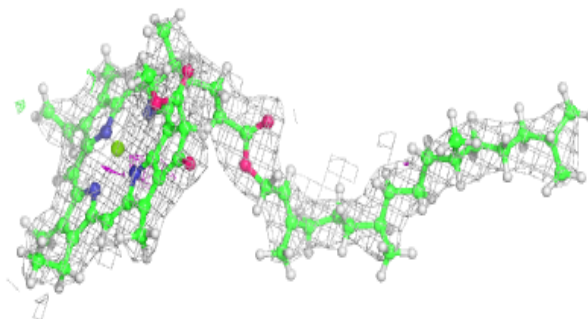


**Electron density around LMG c 523:**

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

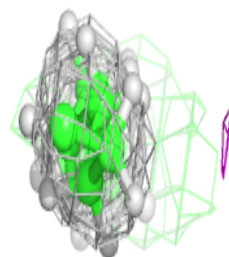
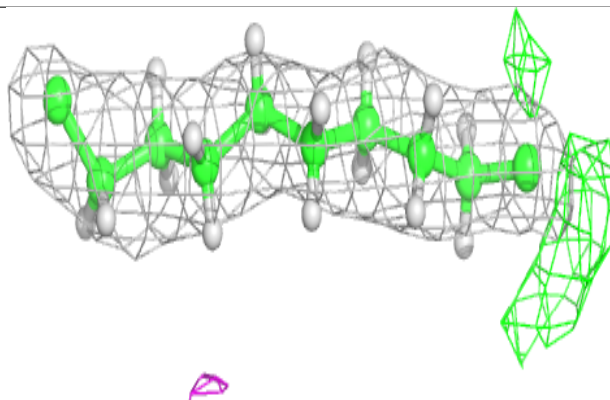
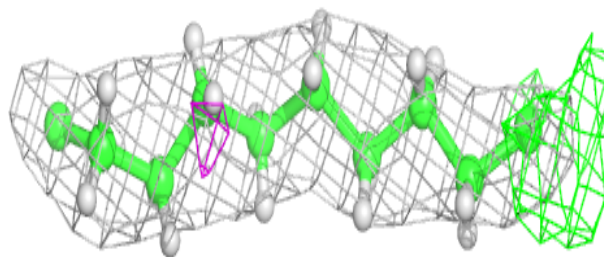
**Electron density around CLA C 502:**

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



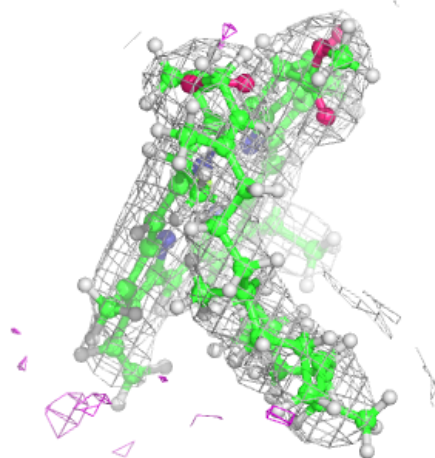
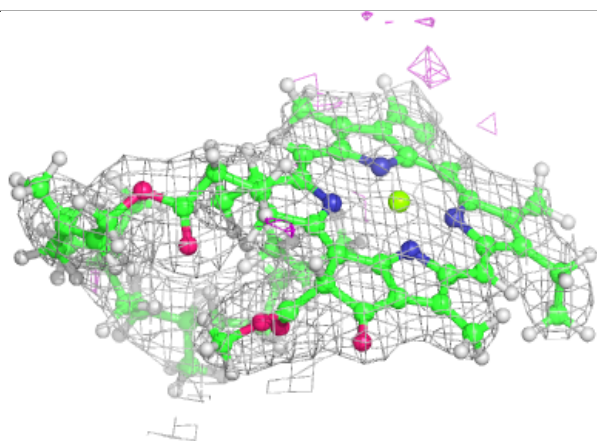
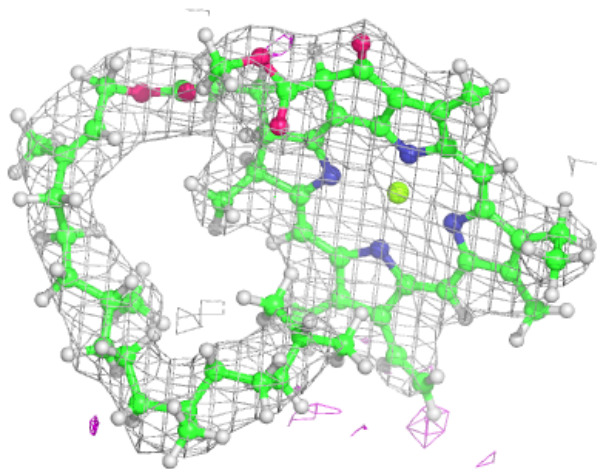
**Electron density around STE M 103:**

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



**Electron density around CLA b 615:**

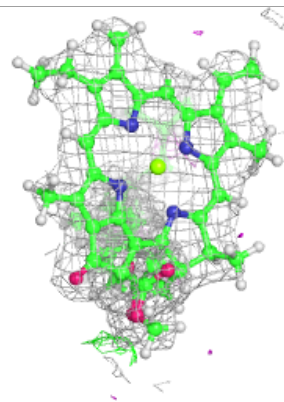
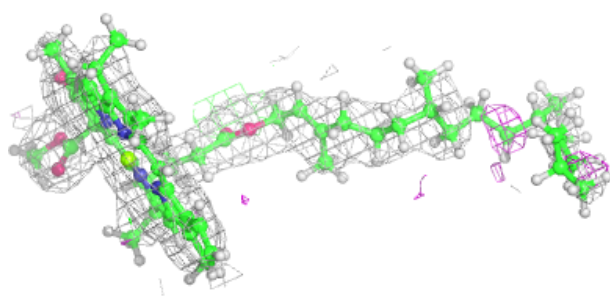
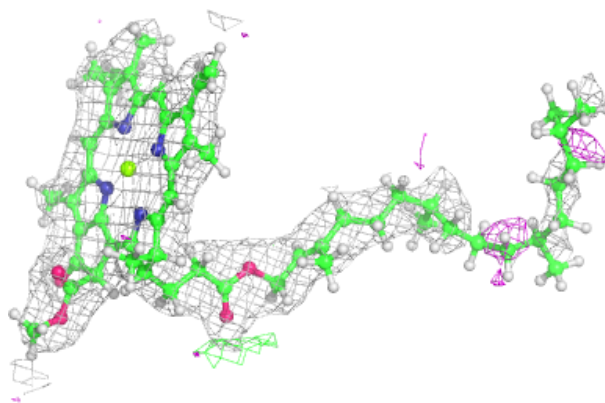
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



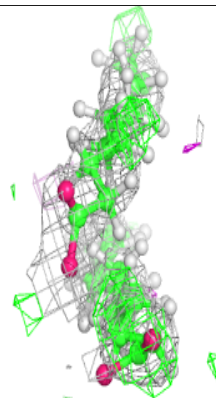
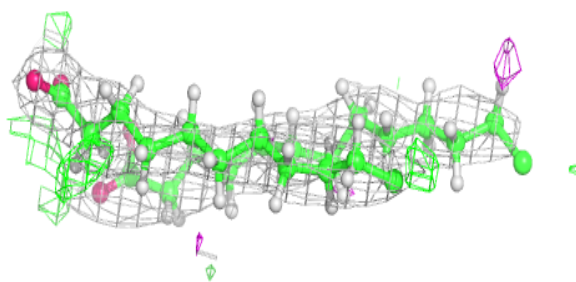
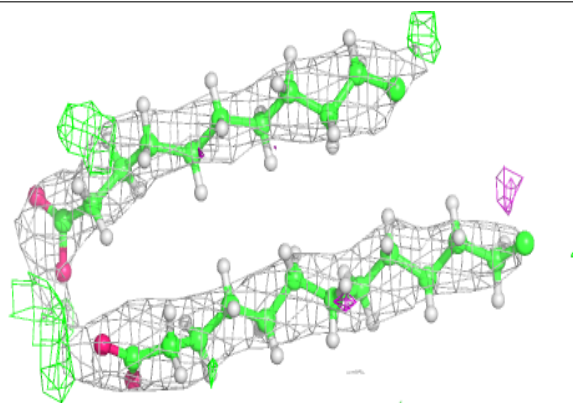


**Electron density around CLA d 405:**

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

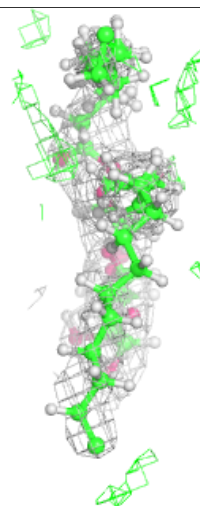
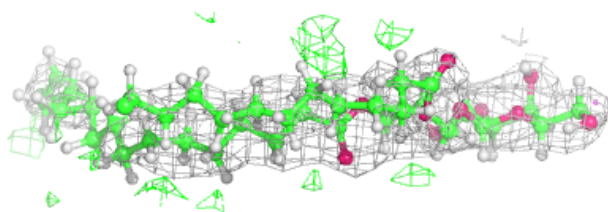
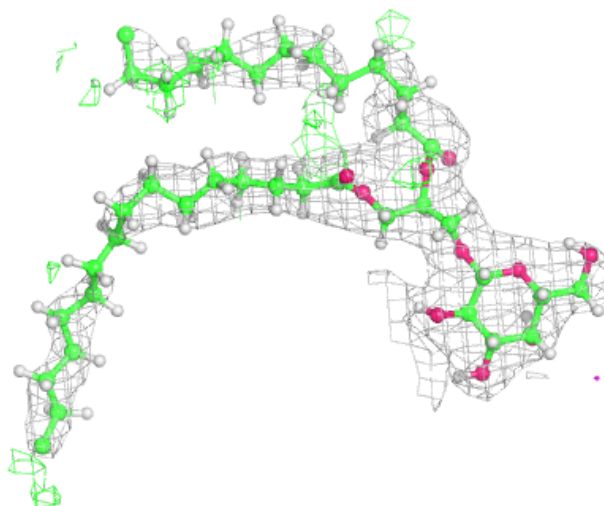
**Electron density around LMG B 621:**

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



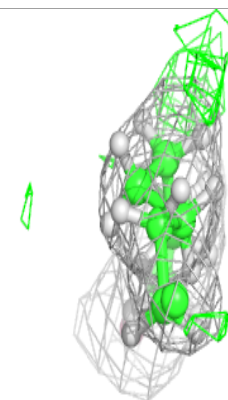
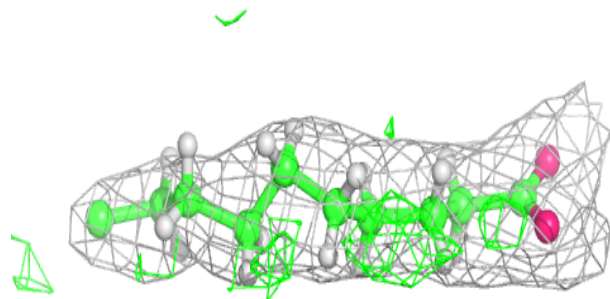
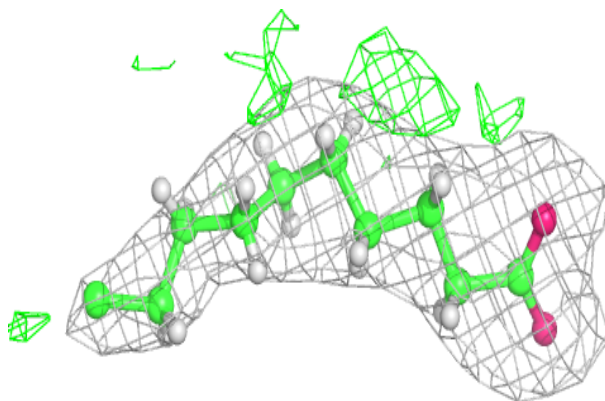
**Electron density around LMG C 519:**

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

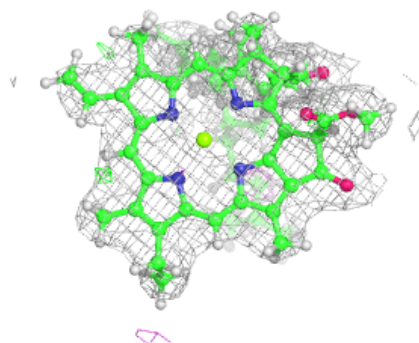
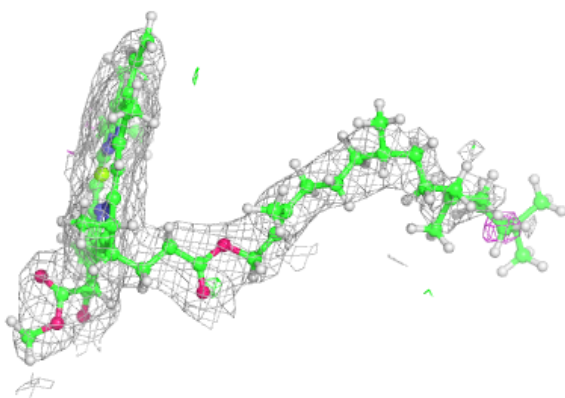
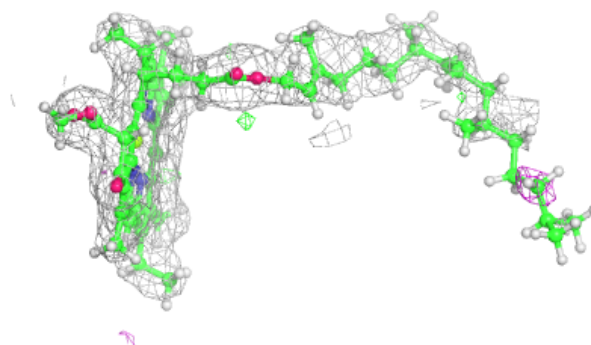


**Electron density around STE C 522:**

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

**Electron density around CLA D 404:**

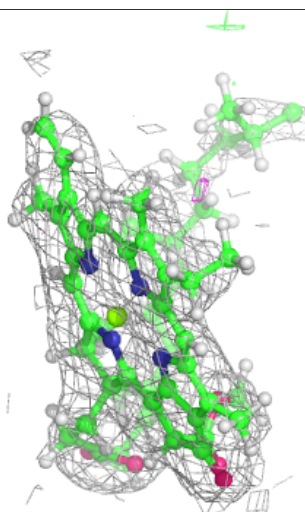
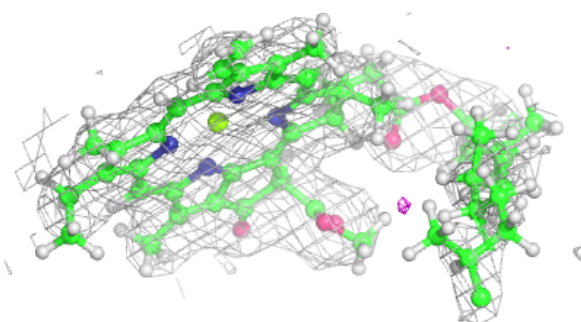
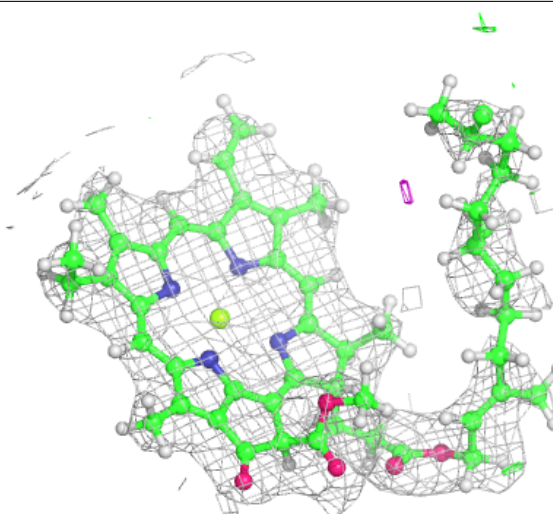
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





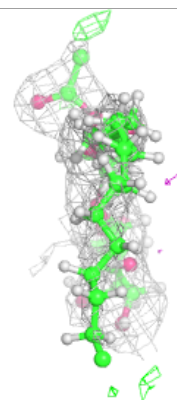
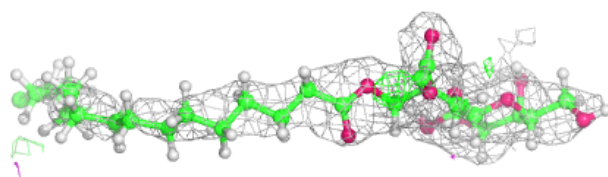
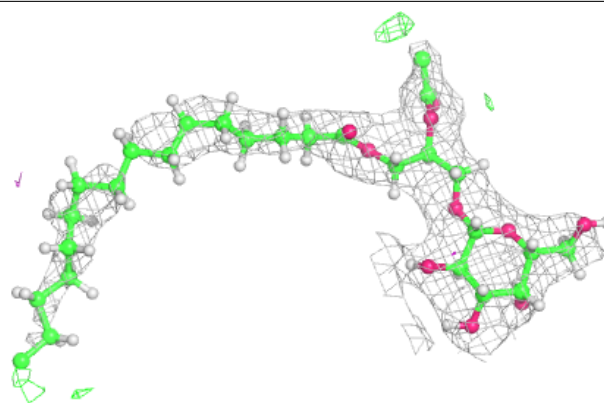
**Electron density around CLA b 616:**

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

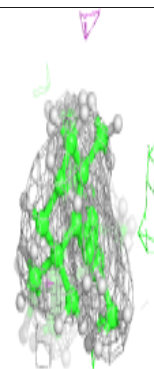
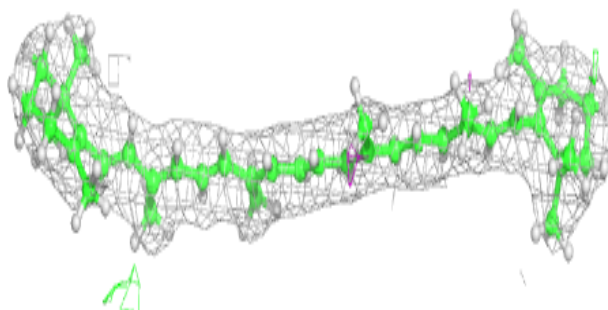
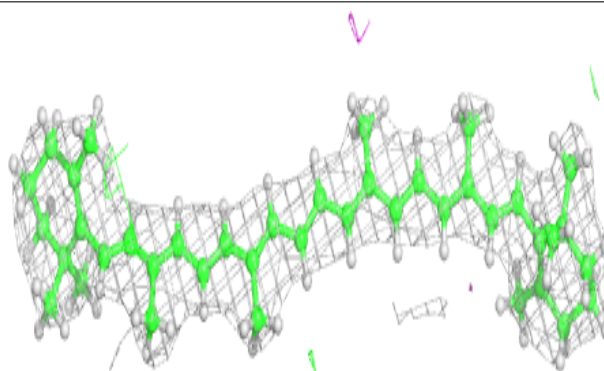


**Electron density around LMG c 520:**

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

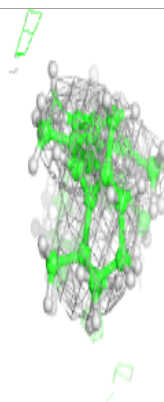
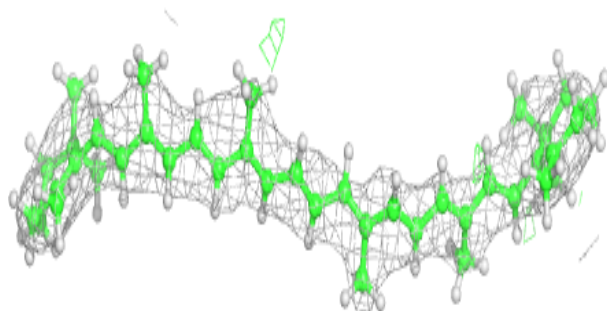
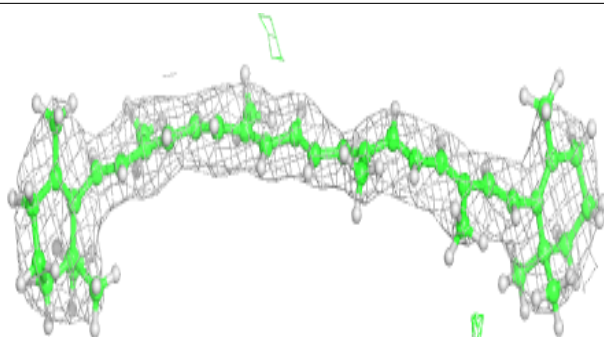
**Electron density around BCR B 619:**

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

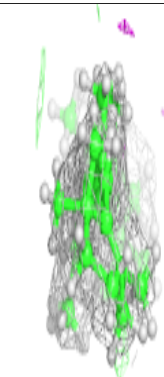
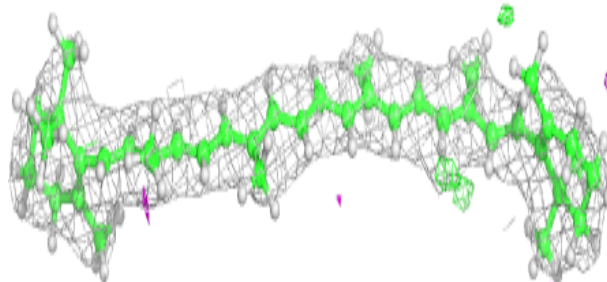
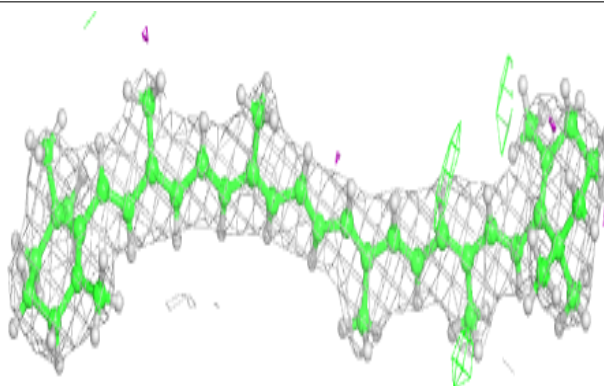


**Electron density around BCR C 515:**

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

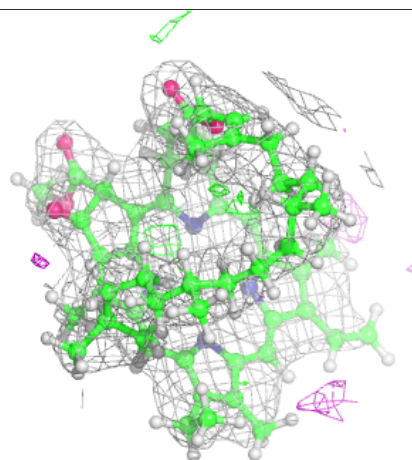
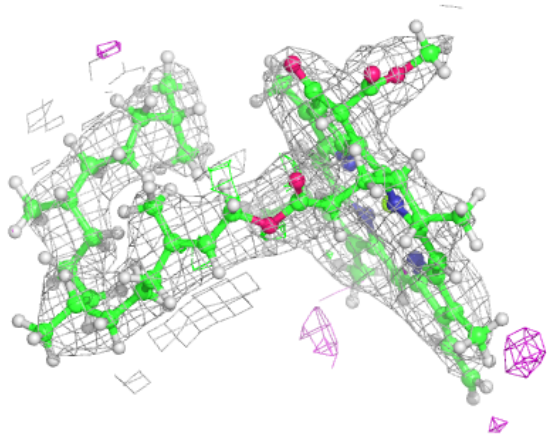
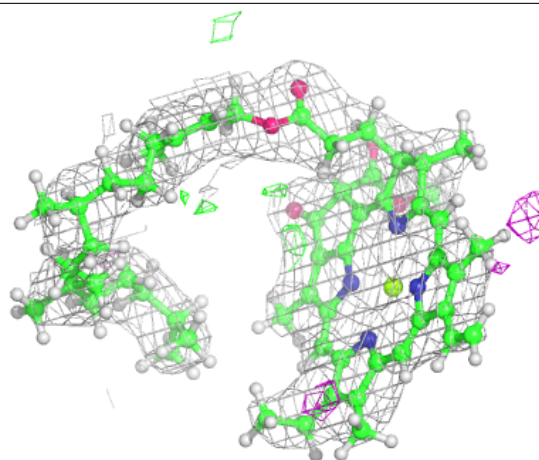
**Electron density around BCR b 619:**

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



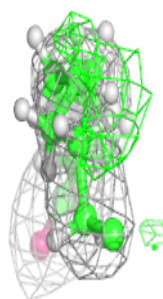
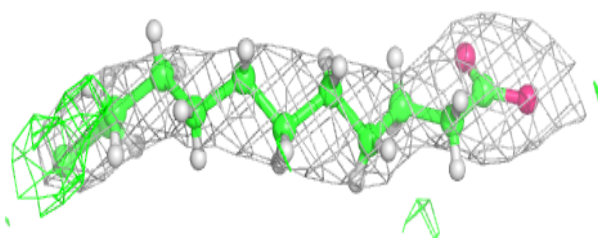
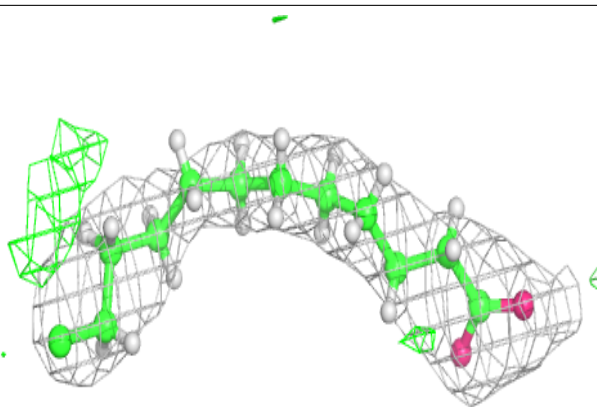
**Electron density around CLA c 503:**

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

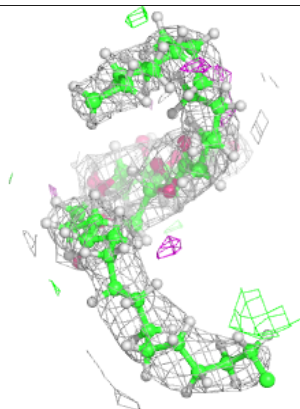
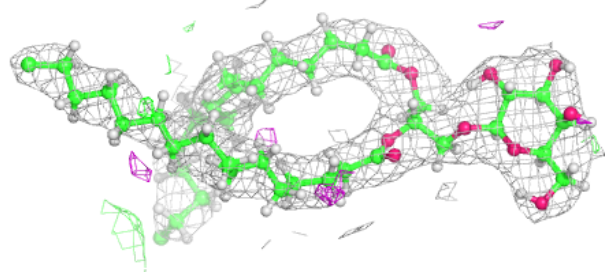
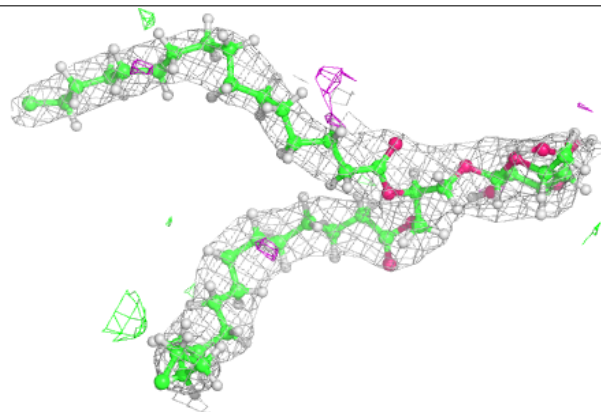


**Electron density around STE t 102:**

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

**Electron density around LMG M 101:**

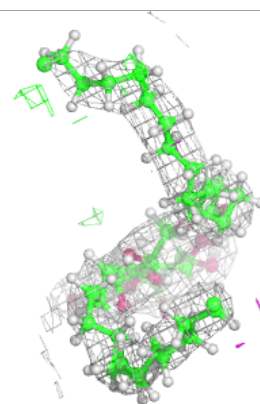
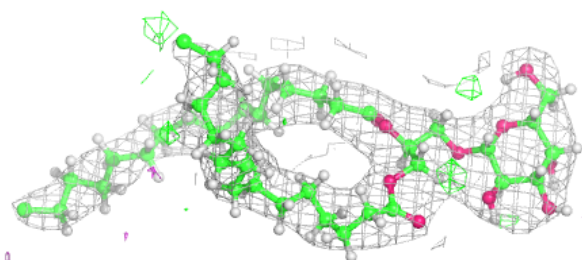
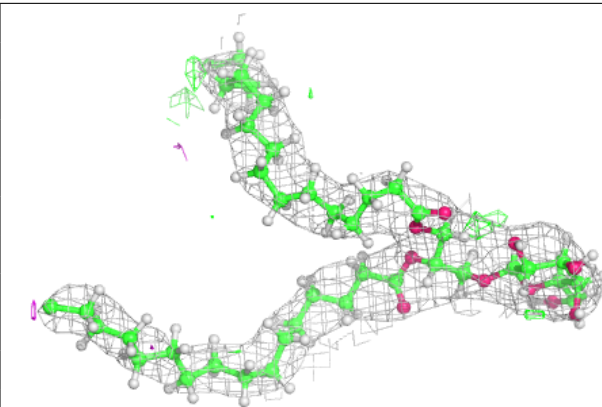
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



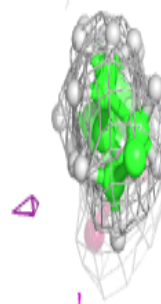
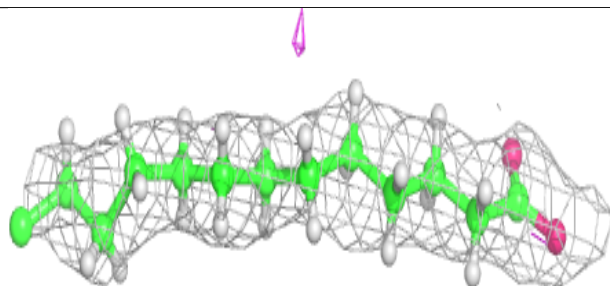
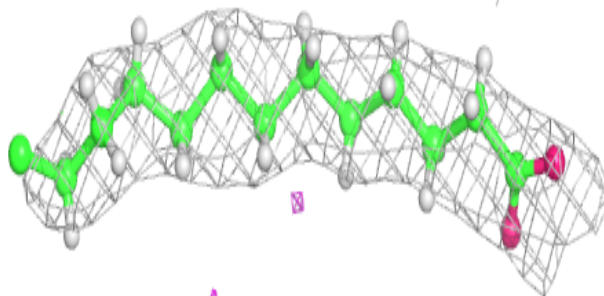


**Electron density around LMG b 620:**

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

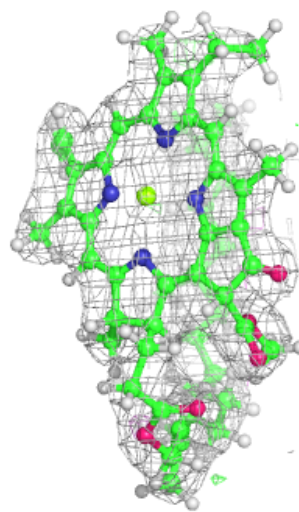
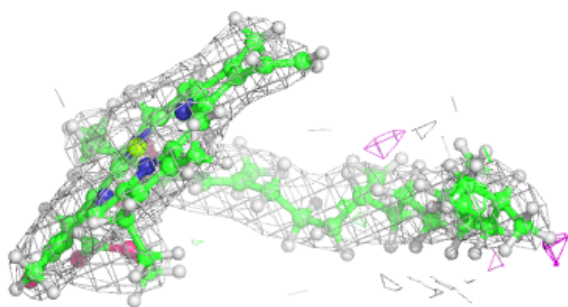
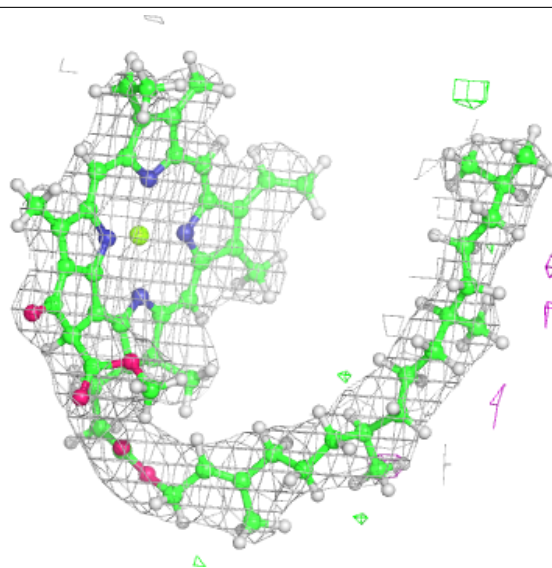
**Electron density around STE M 102:**

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



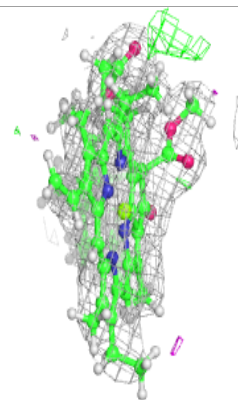
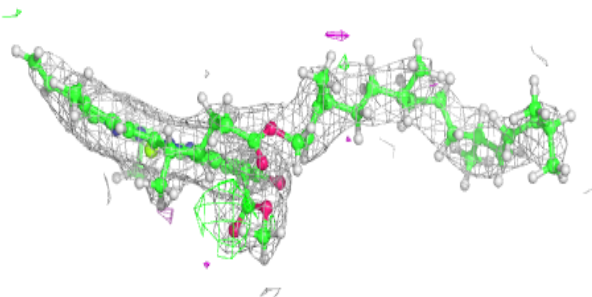
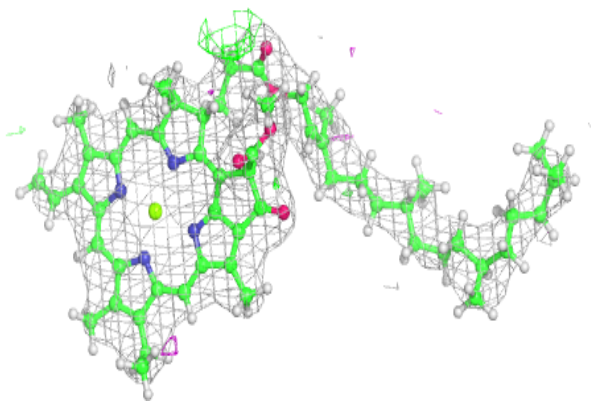
**Electron density around CLA C 507:**

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

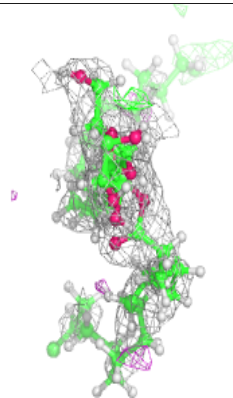
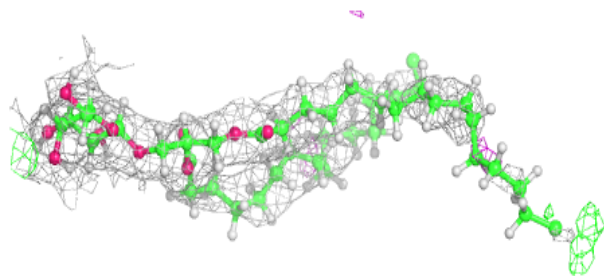
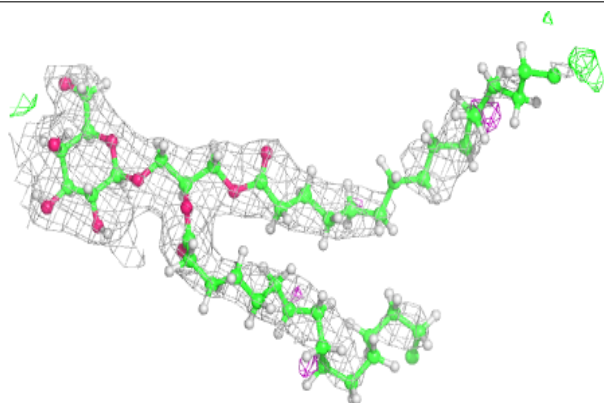


**Electron density around CLA b 602:**

$2mF_o-DF_c$  (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:**

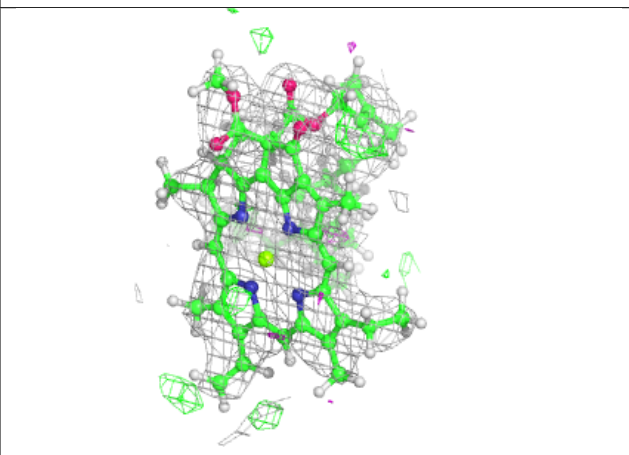
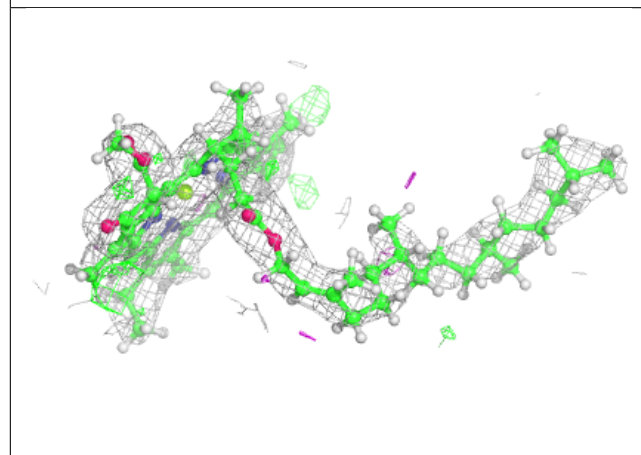
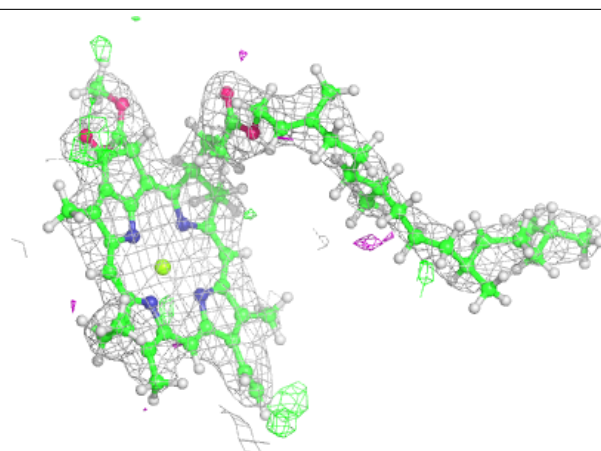
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



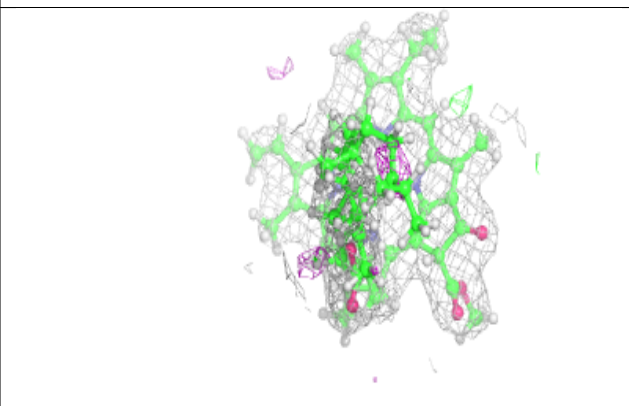
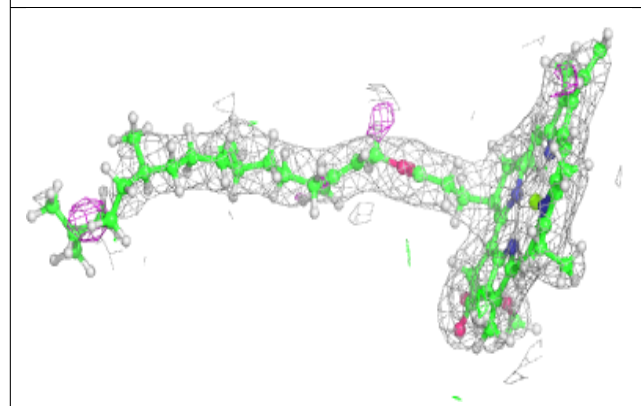
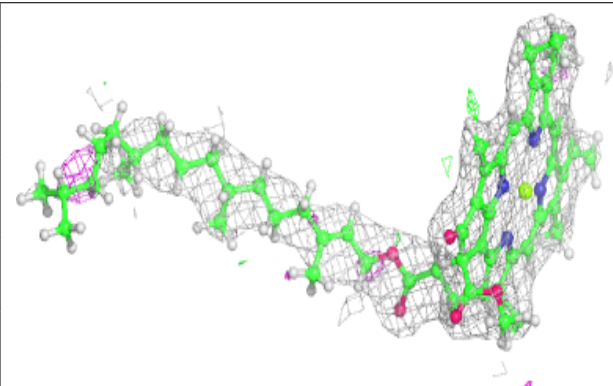


**Electron density around CLA c 511:**

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

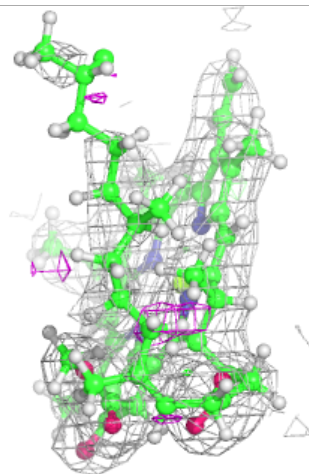
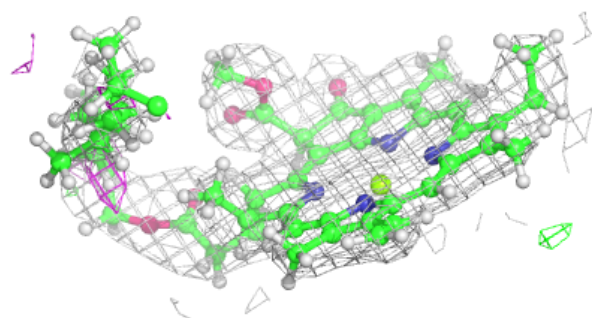
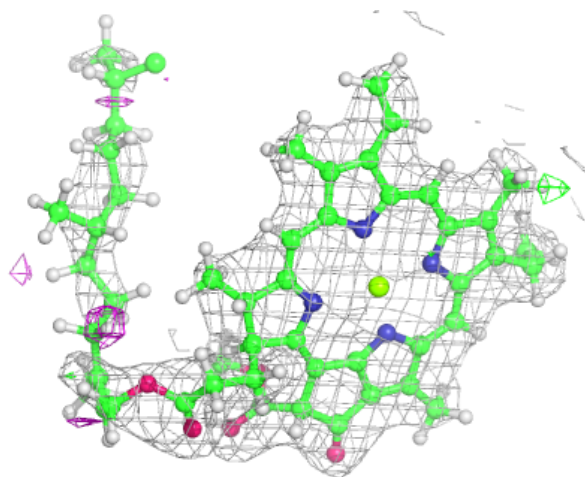
**Electron density around CLA b 604:**

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



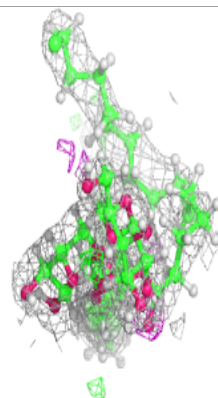
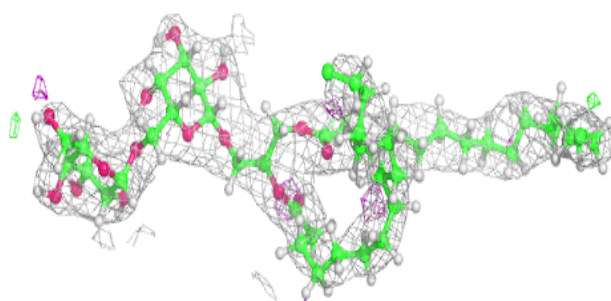
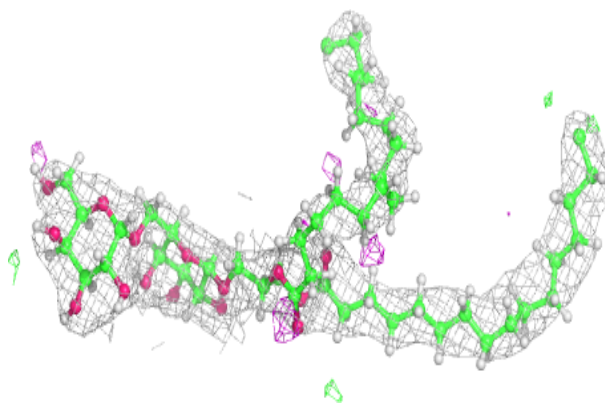
**Electron density around CLA B 616:**

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



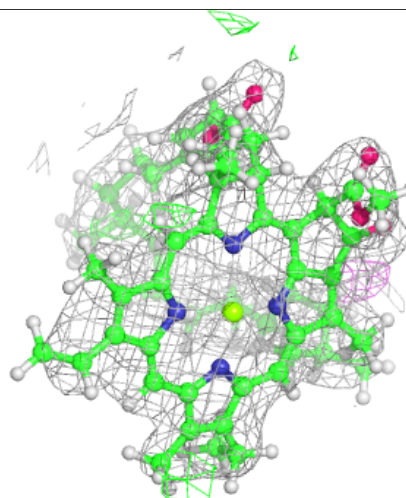
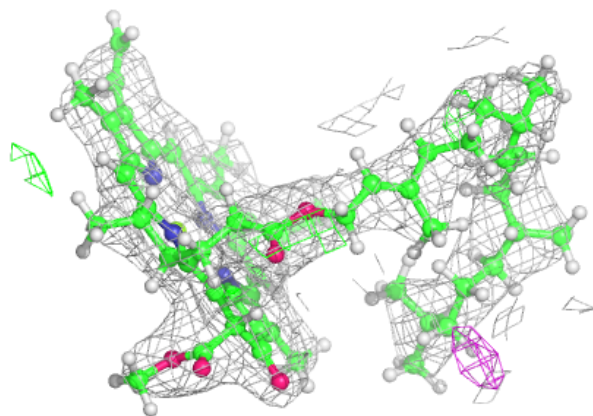
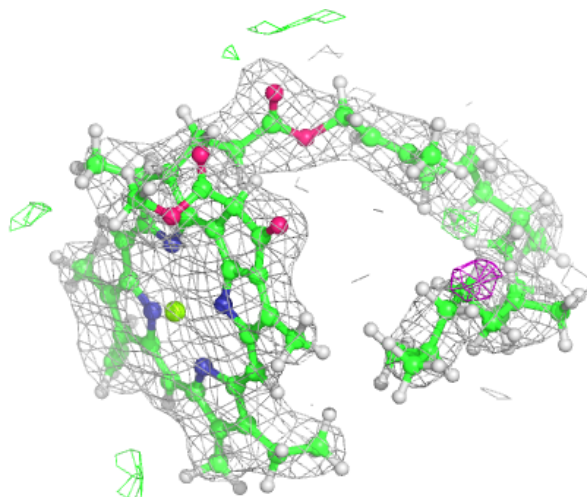
**Electron density around DGD h 102:**

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



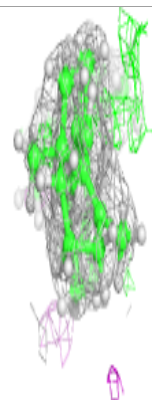
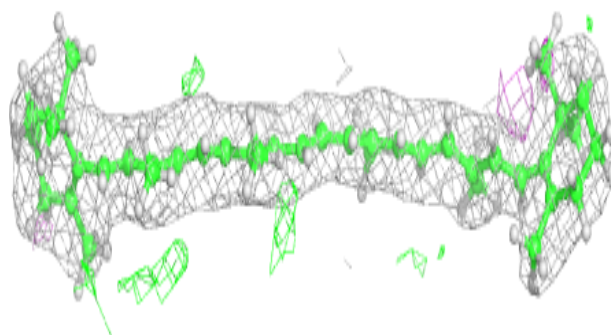
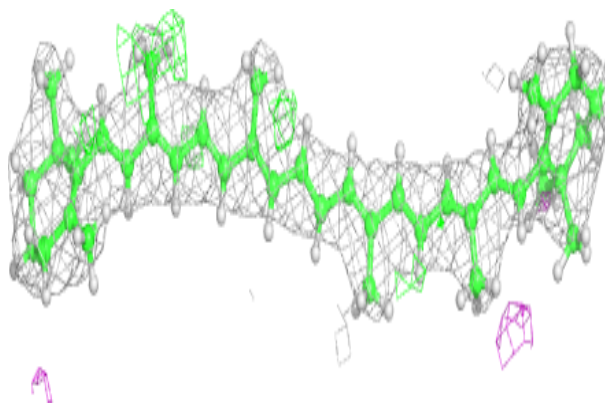
**Electron density around CLA C 503:**

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

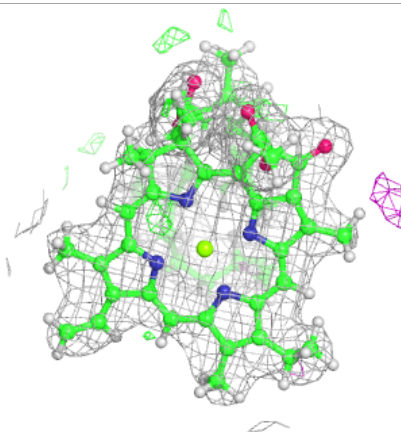
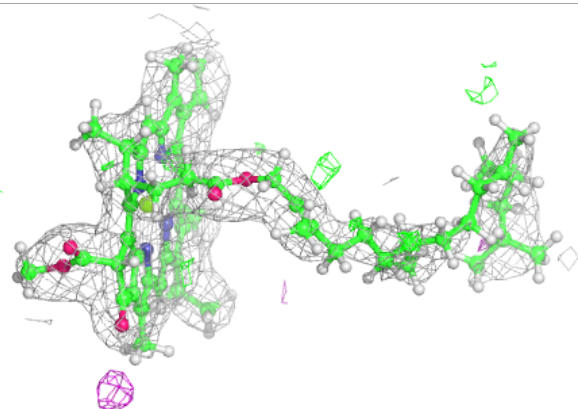
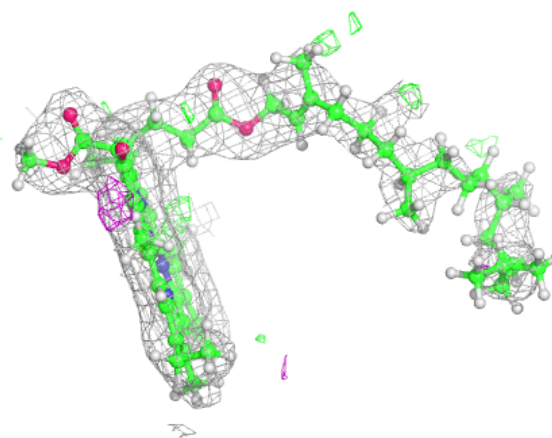


**Electron density around BCR B 618:**

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

**Electron density around CLA C 506:**

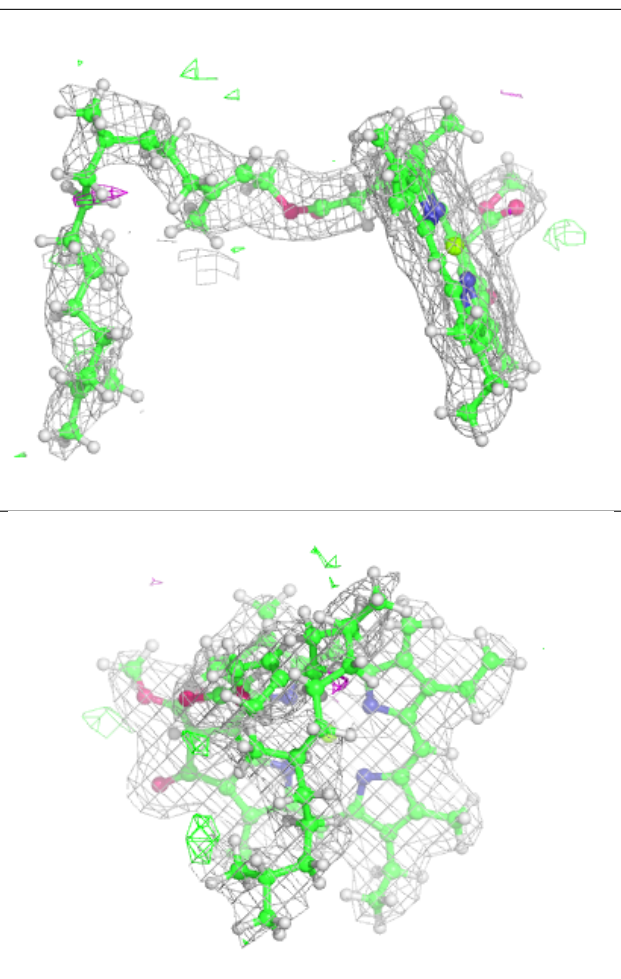
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





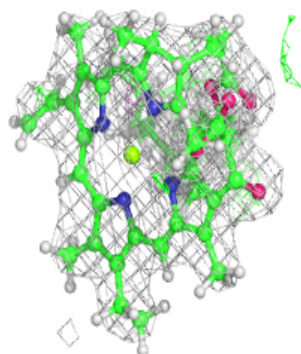
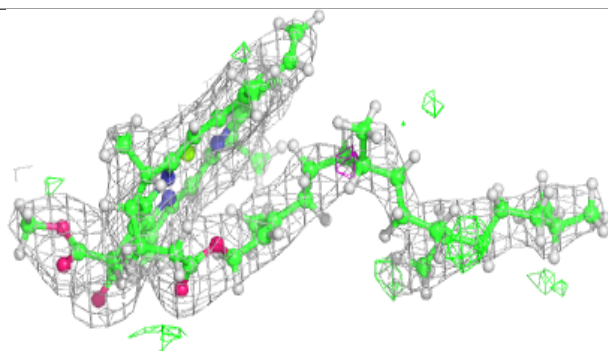
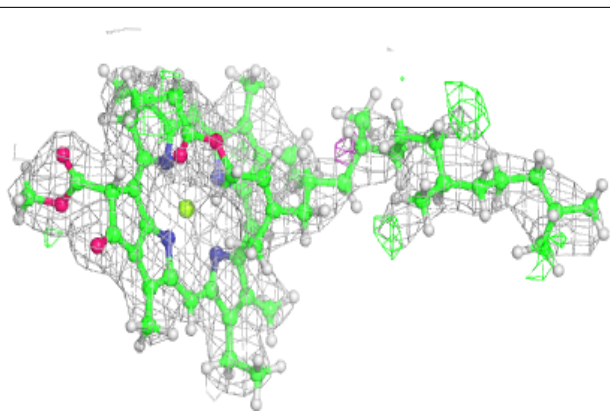
**Electron density around CLA a 404:**

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



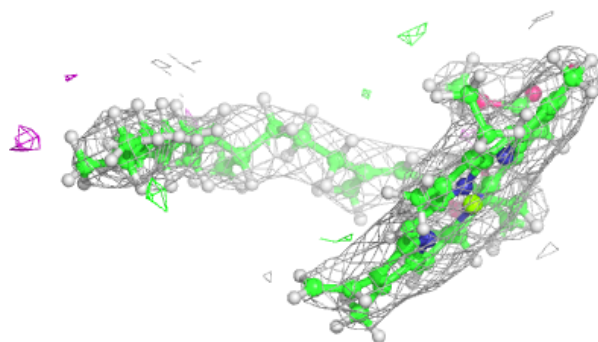
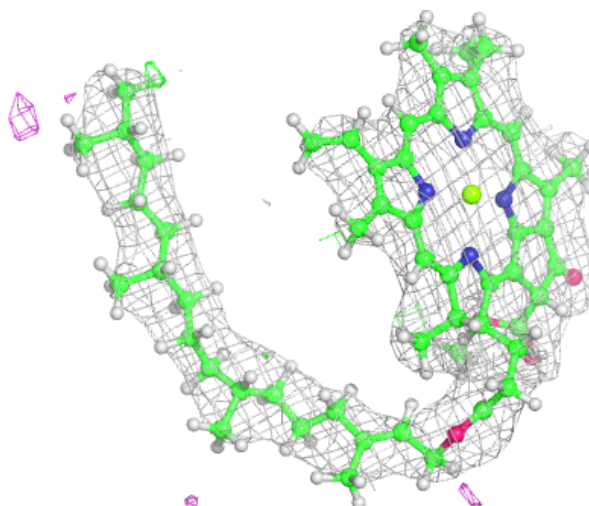
**Electron density around CLA c 505:**

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



**Electron density around CLA c 507:**

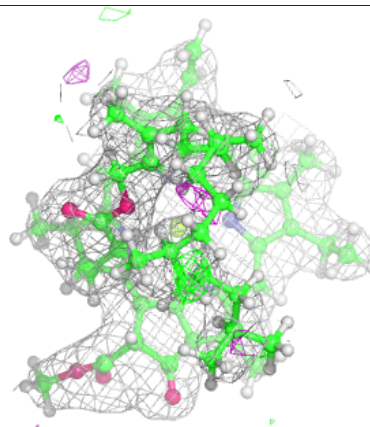
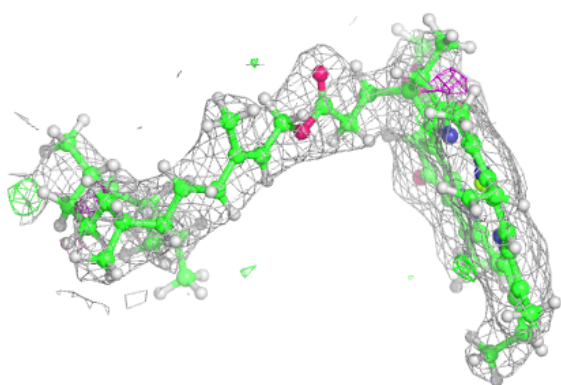
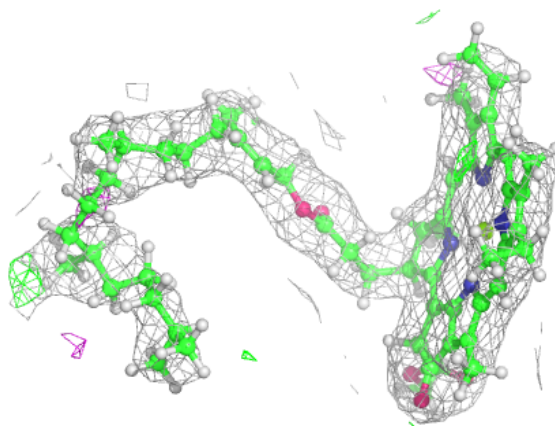
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





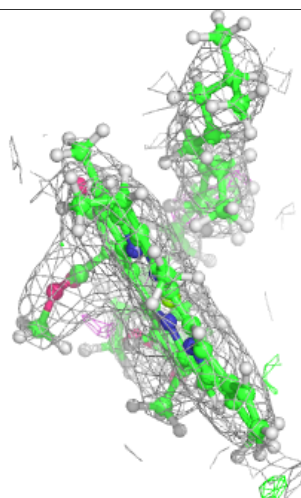
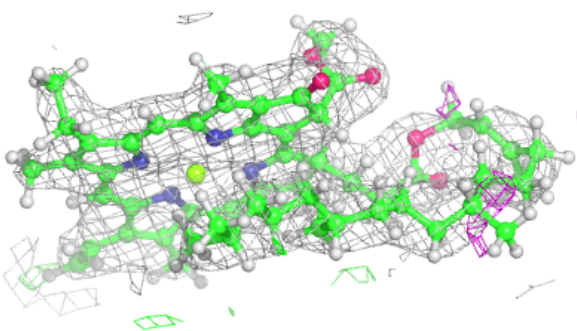
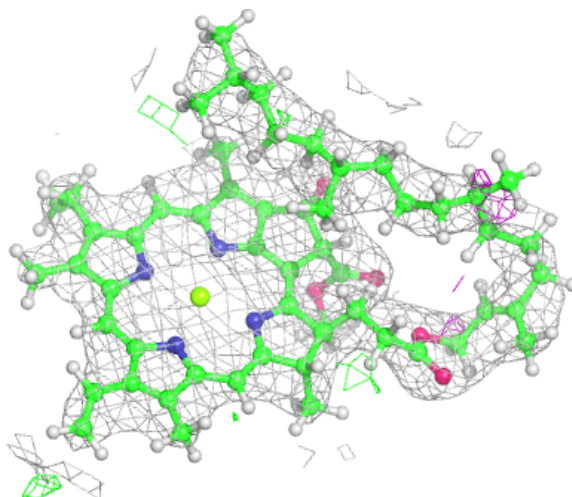
**Electron density around CLA B 606:**

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



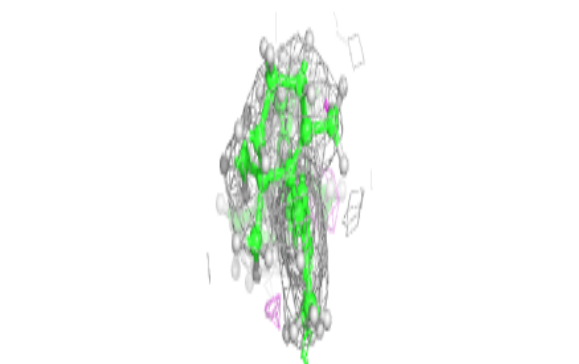
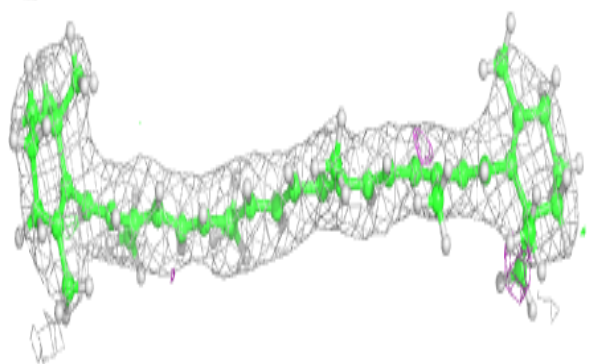
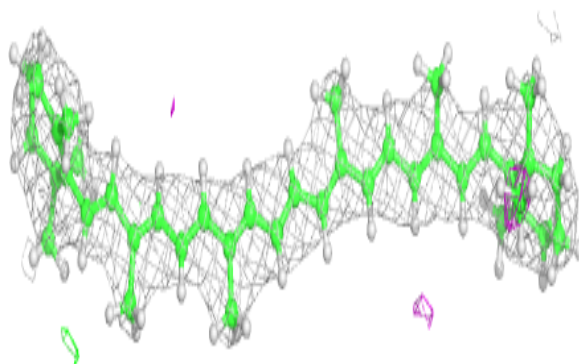
**Electron density around CLA c 509:**

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

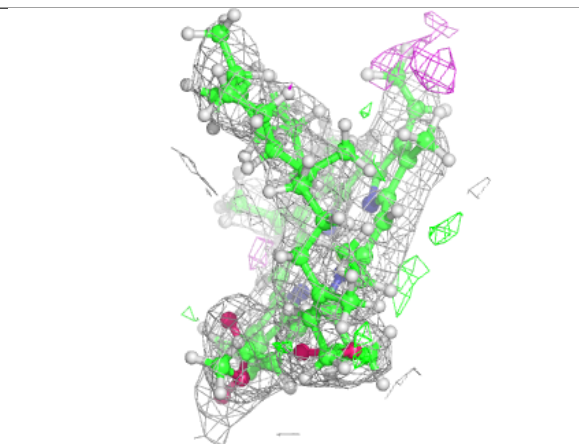
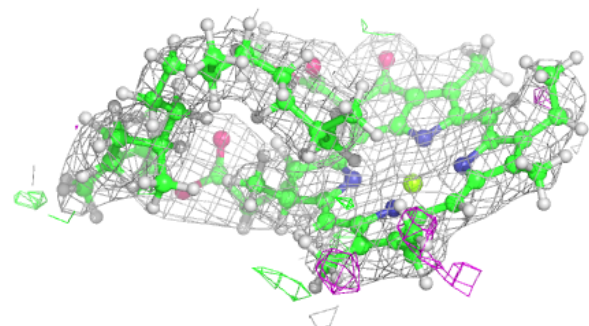
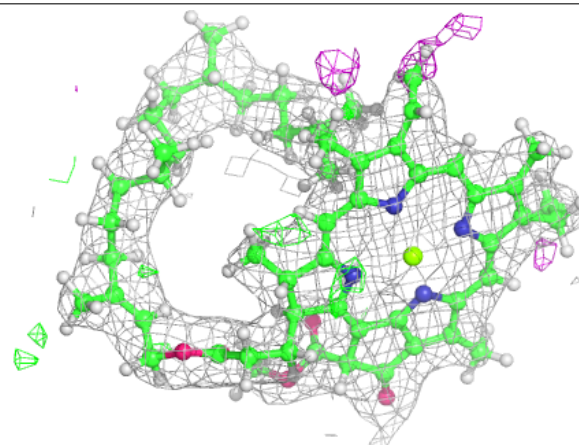


**Electron density around BCR c 515:**

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

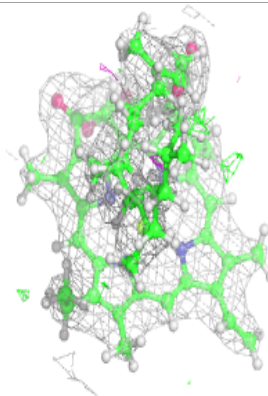
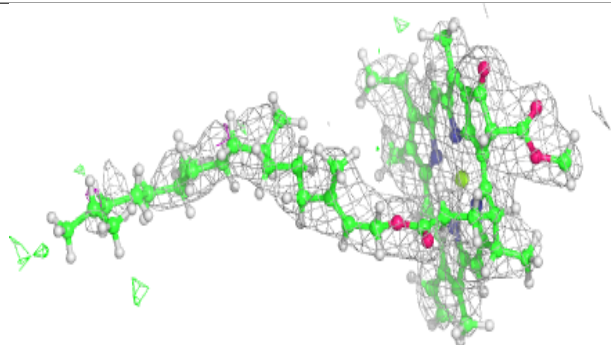
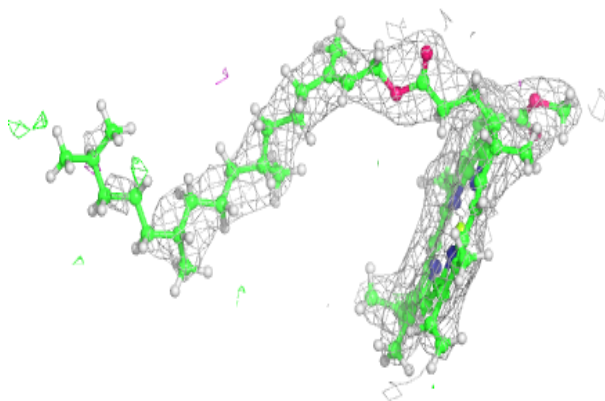
**Electron density around CLA B 615:**

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

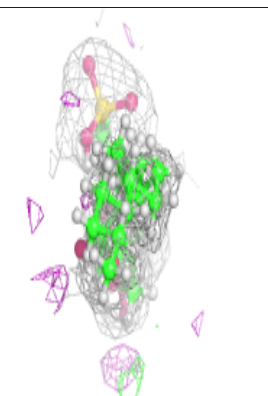
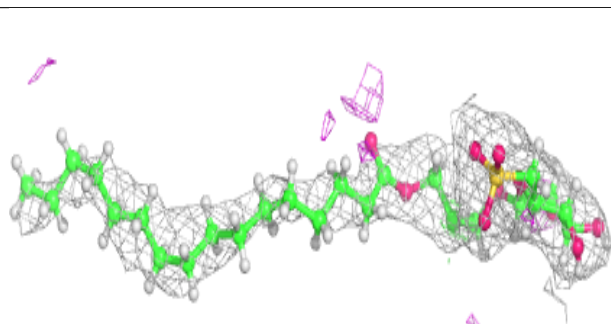
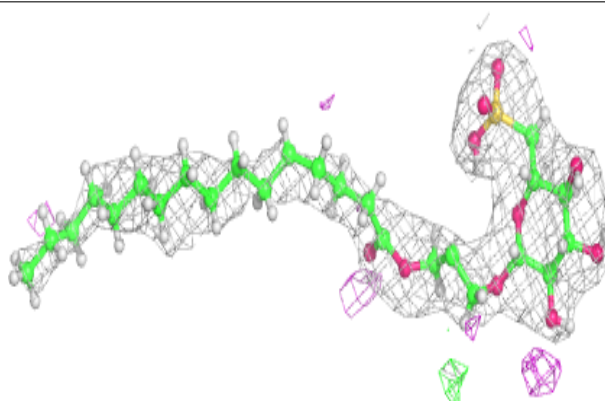


**Electron density around CLA C 508:**

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

**Electron density around SQD F 101:**

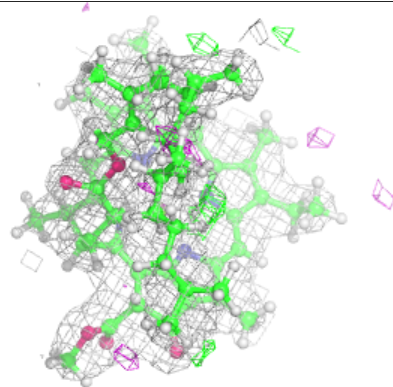
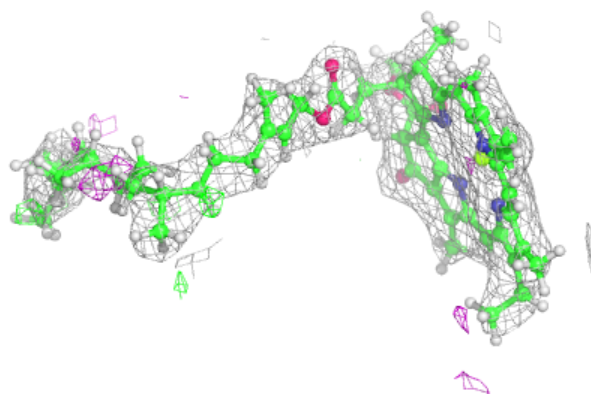
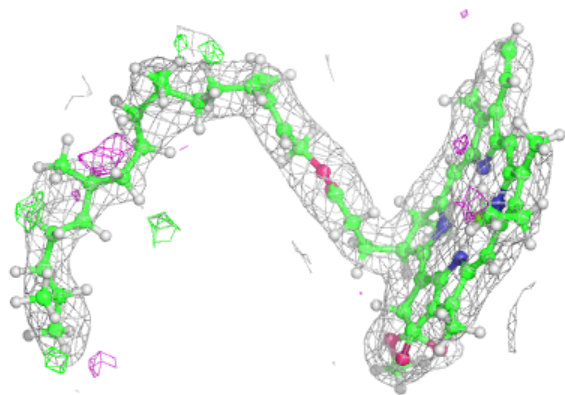
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



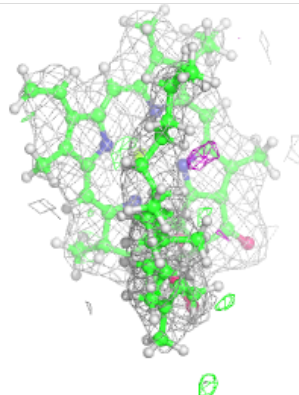
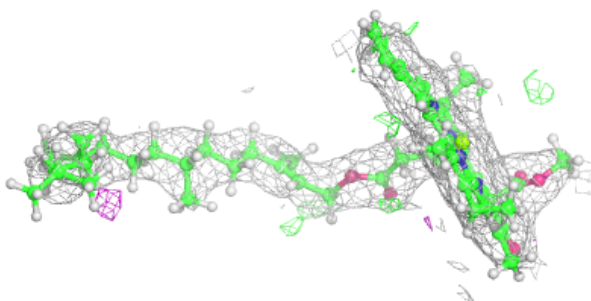
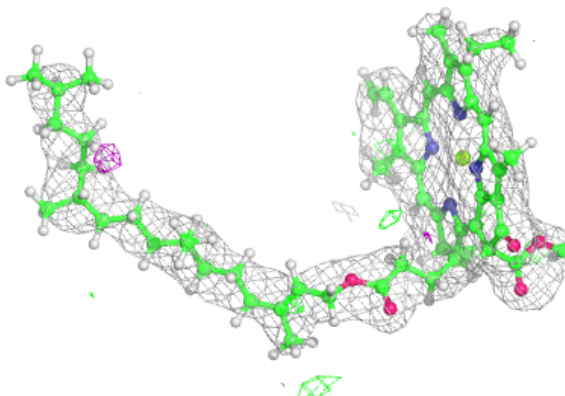


**Electron density around CLA b 606:**

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

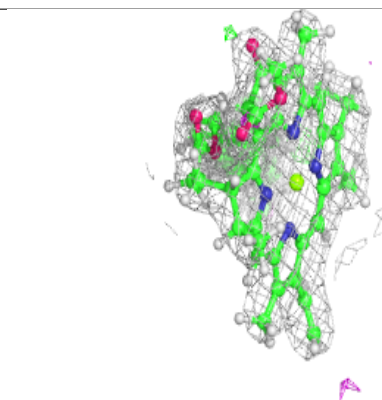
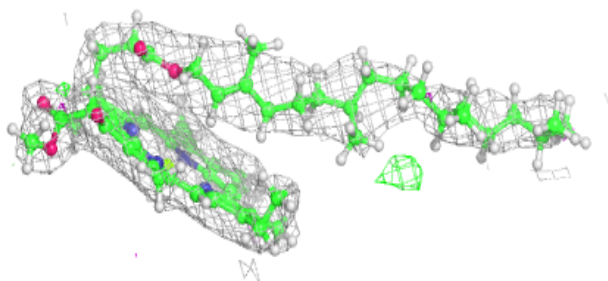
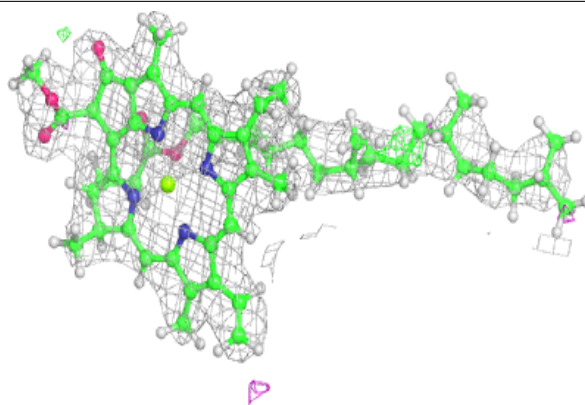
**Electron density around CLA b 609:**

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

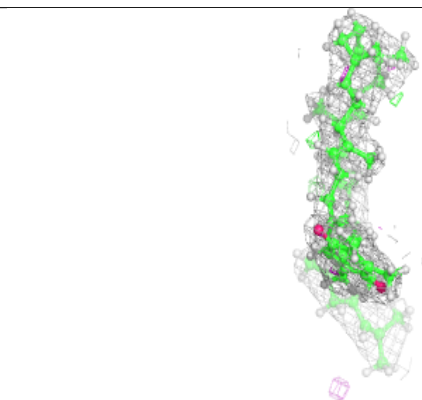
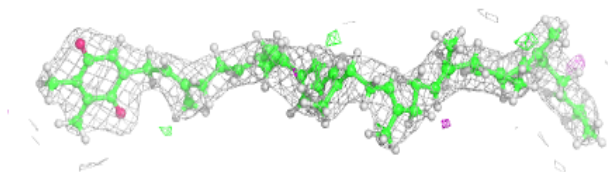
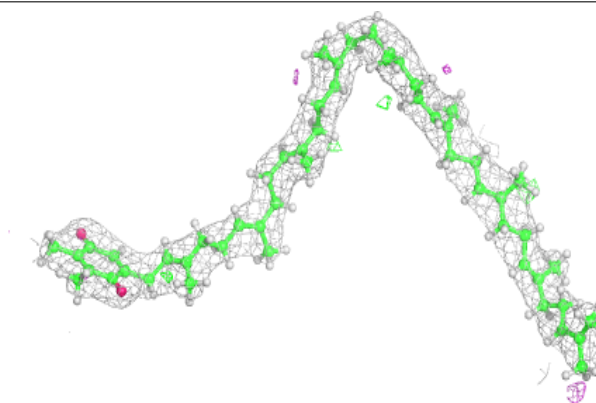


**Electron density around CLA b 614:**

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

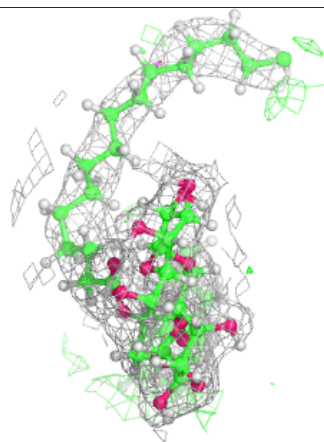
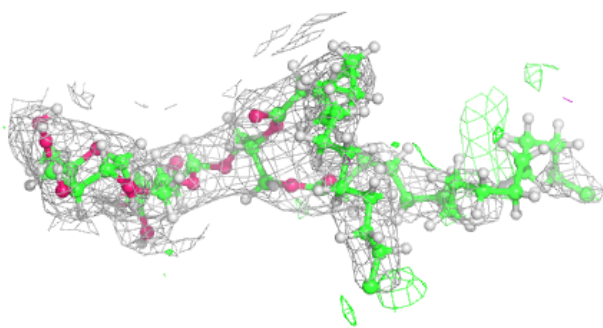
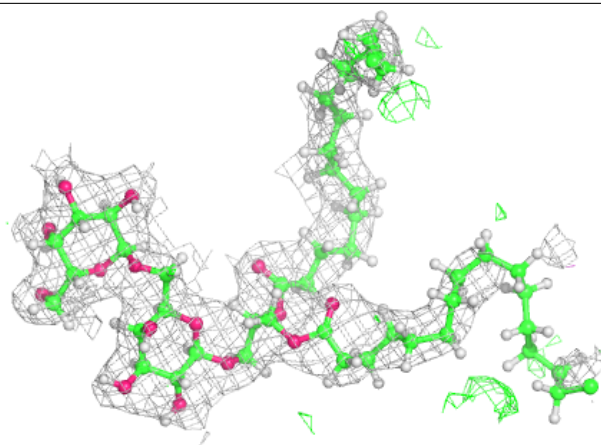
**Electron density around PL9 D 406:**

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

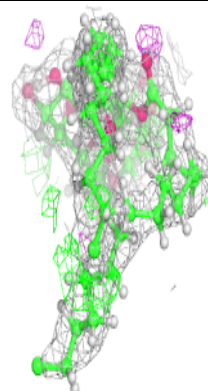
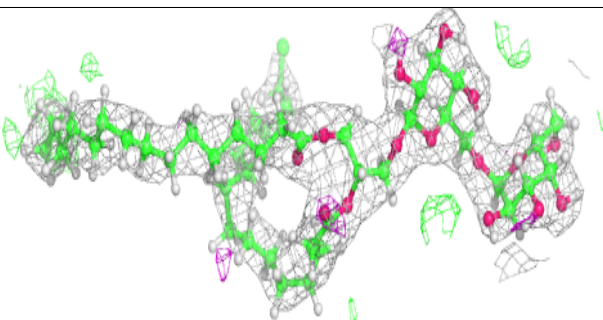
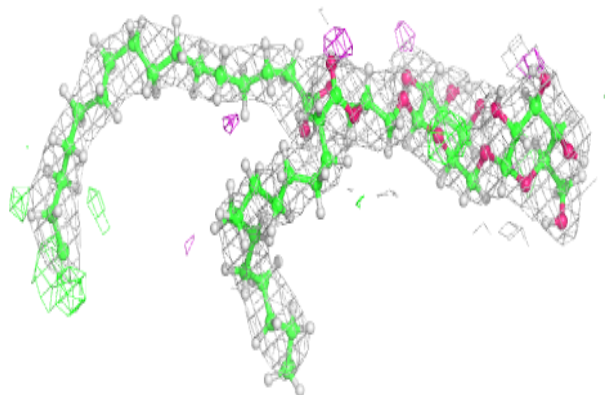


**Electron density around DGD C 517:**

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

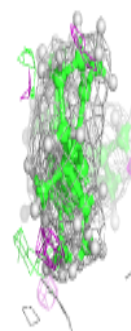
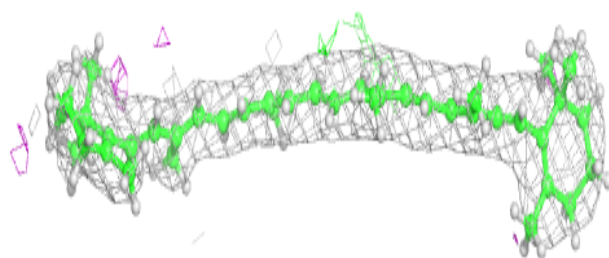
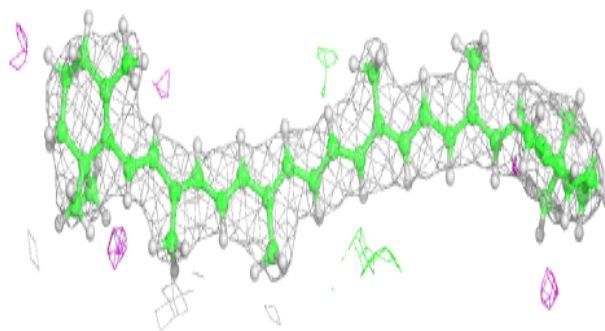
**Electron density around DGD H 102:**

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

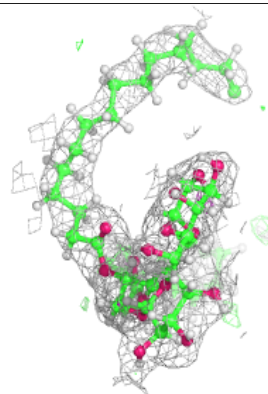
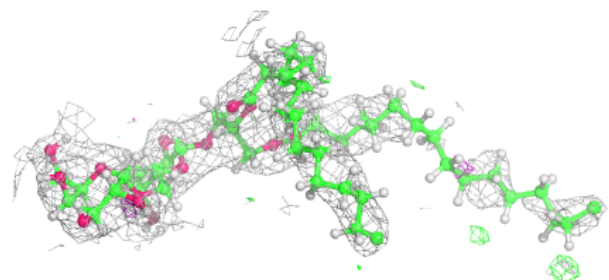
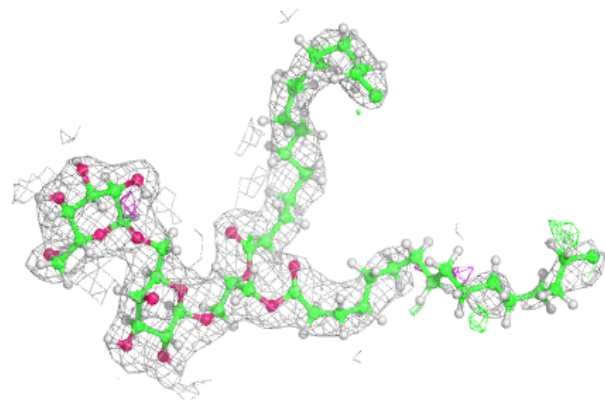


**Electron density around BCR B 617:**

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

**Electron density around DGD c 518:**

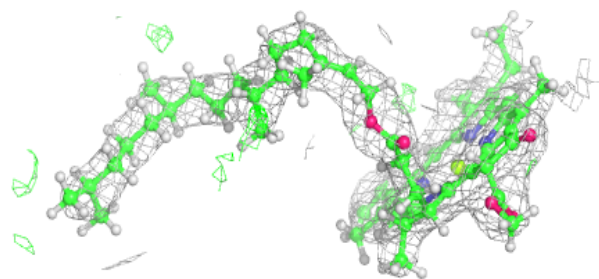
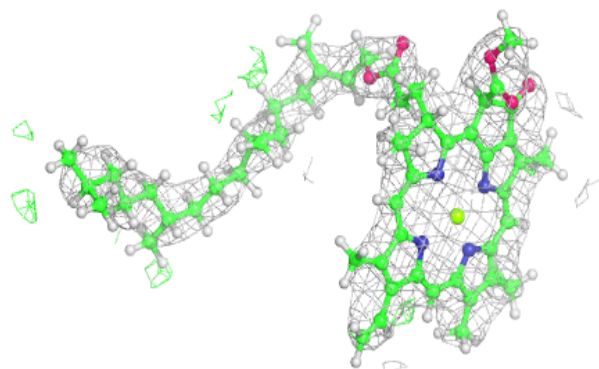
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



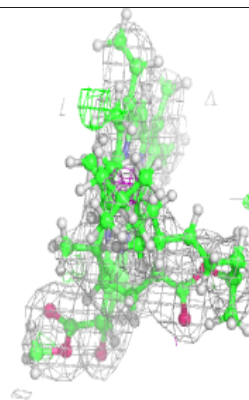
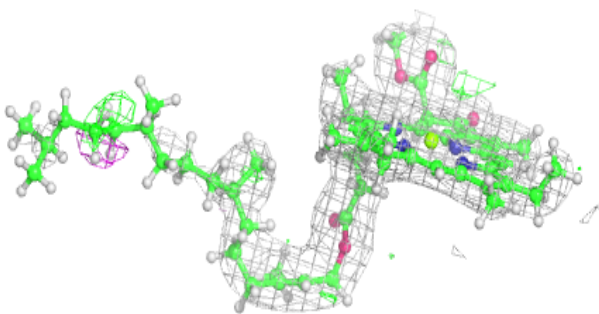
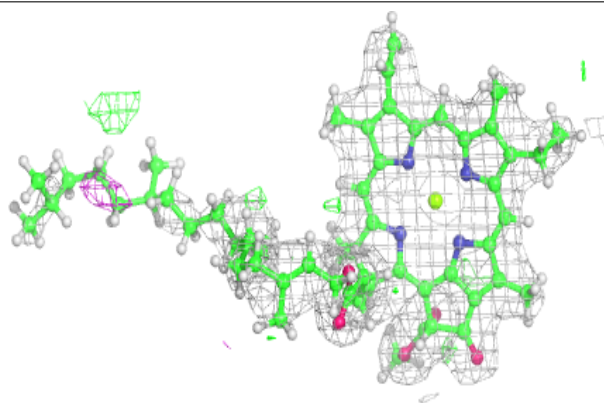


**Electron density around CLA C 511:**

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

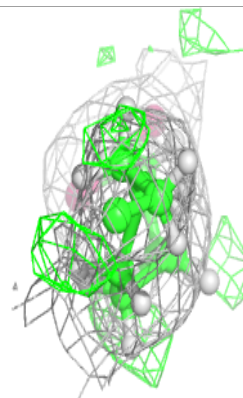
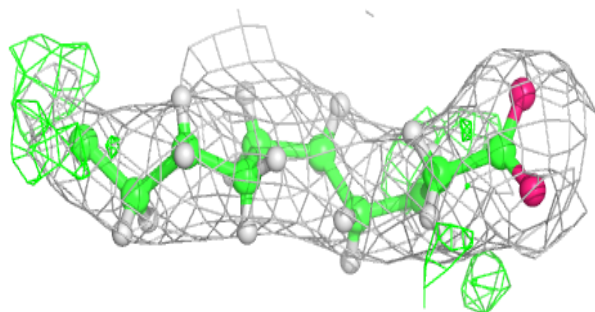
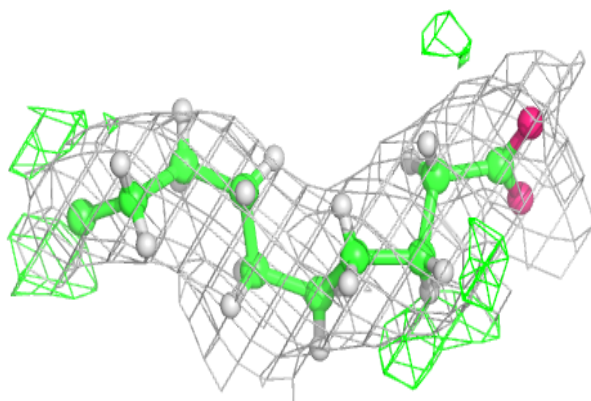
**Electron density around CLA A 403:**

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

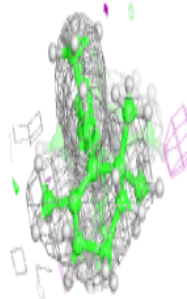
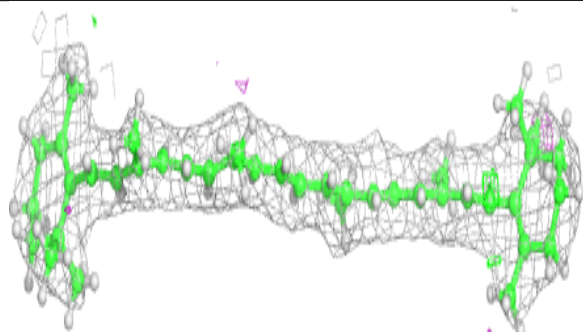
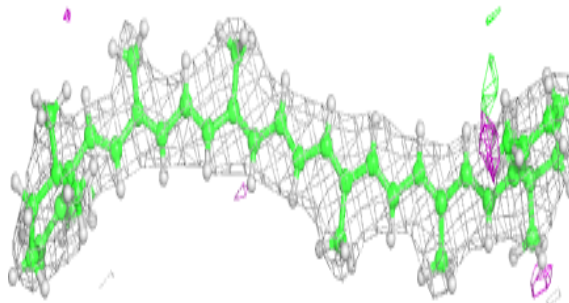


**Electron density around STE B 624:**

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

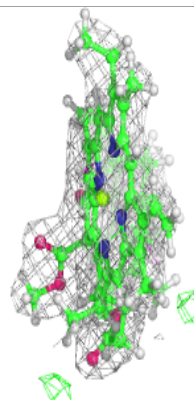
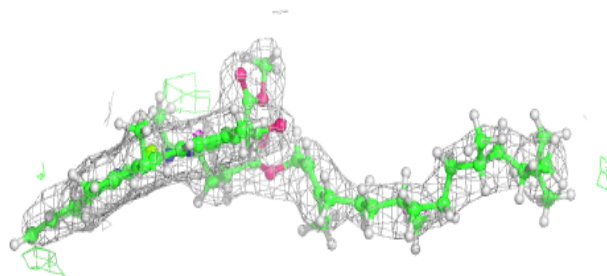
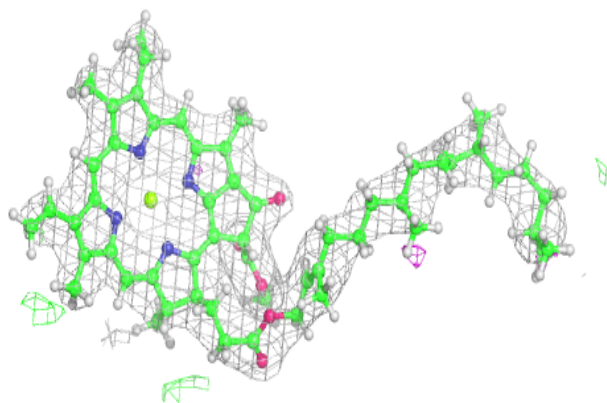
**Electron density around BCR C 514:**

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

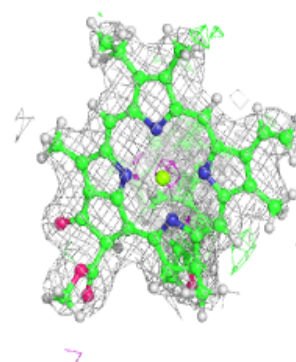
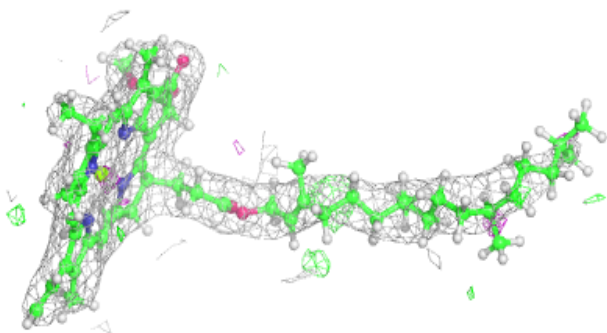
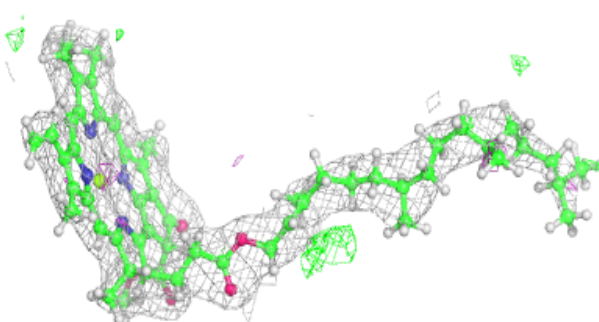


**Electron density around CLA B 602:**

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

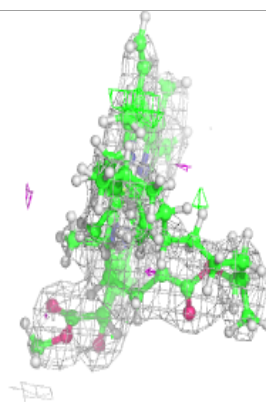
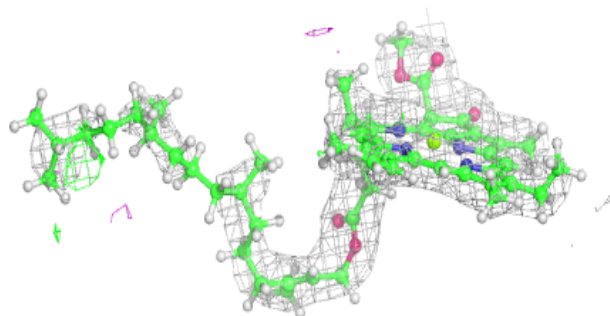
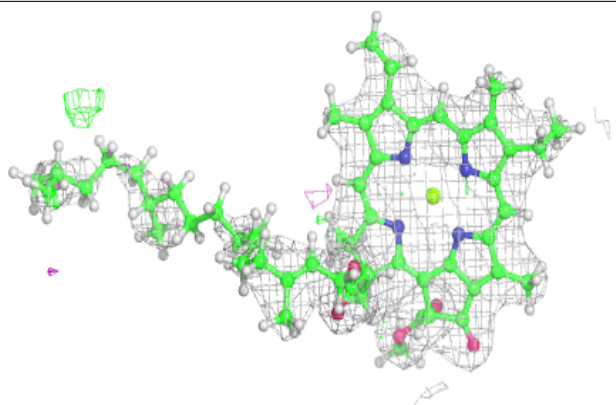
**Electron density around CLA B 604:**

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

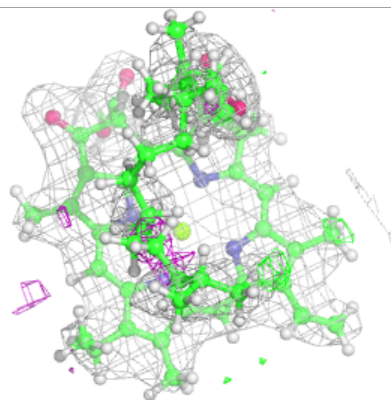
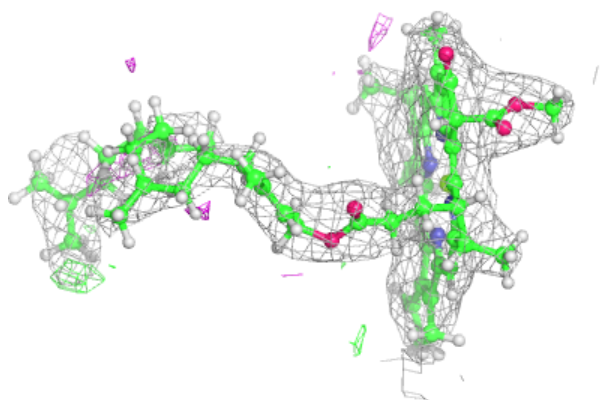
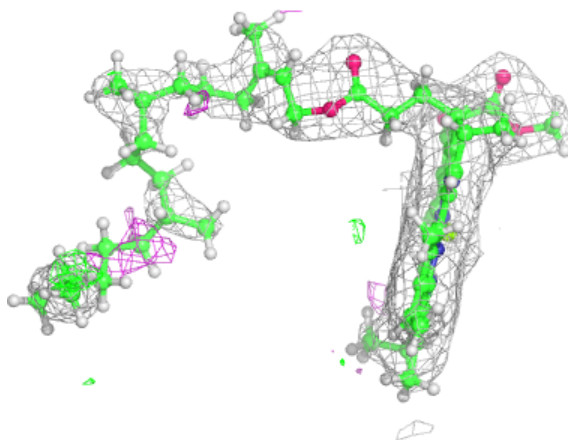


**Electron density around CLA a 403:**

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

**Electron density around CLA c 506:**

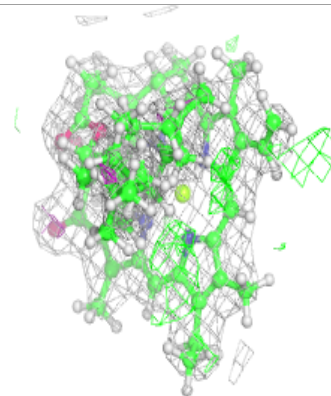
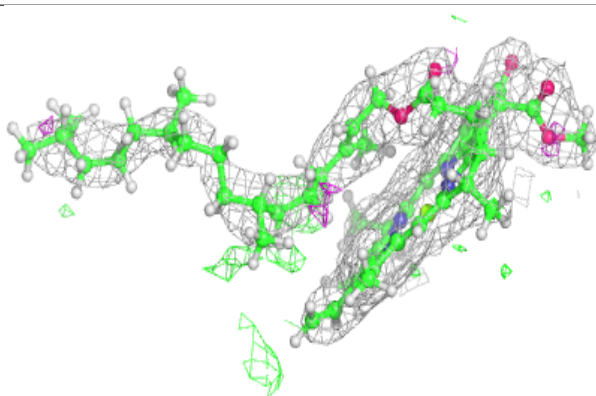
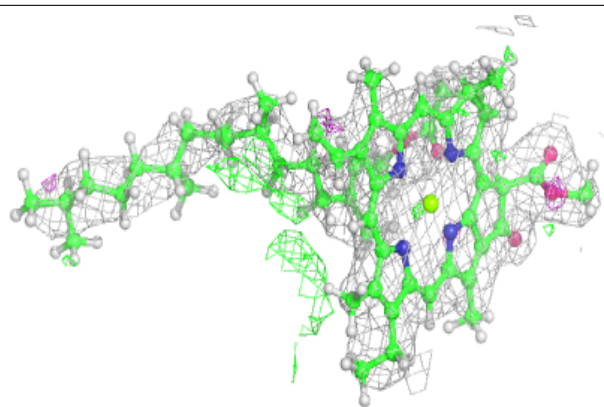
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



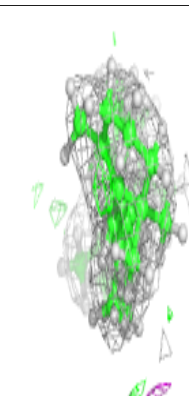
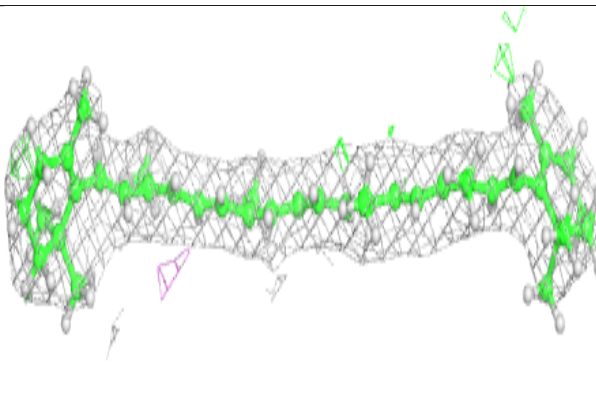
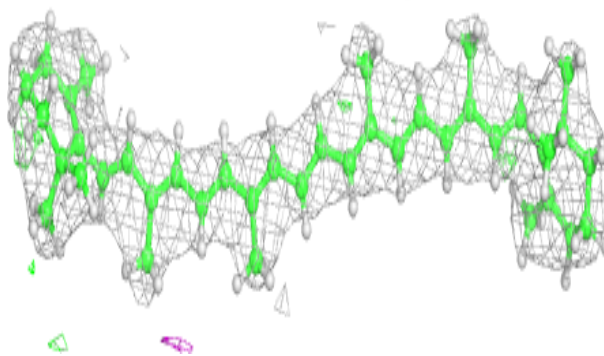


**Electron density around CLA C 505:**

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

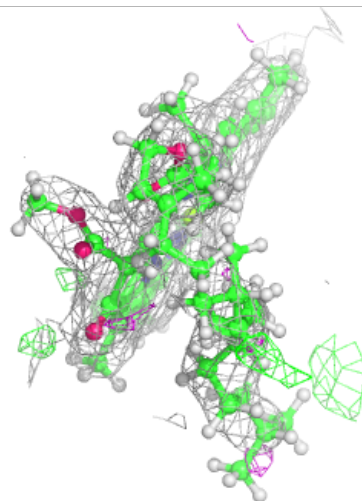
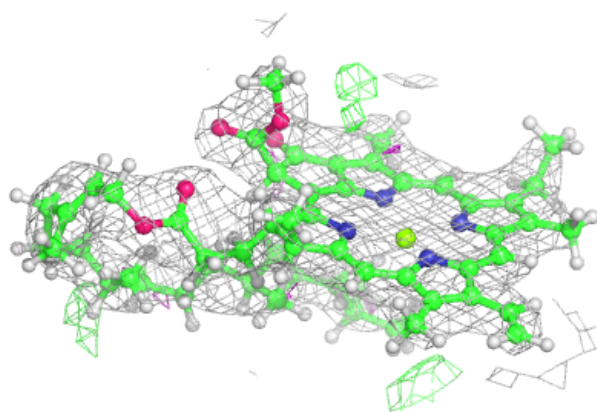
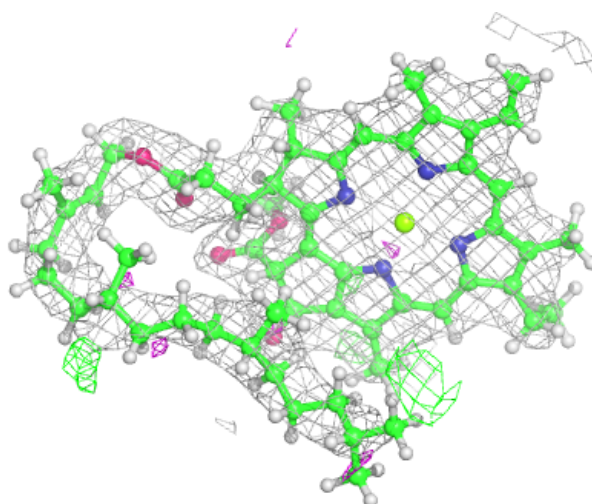
**Electron density around BCR b 618:**

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



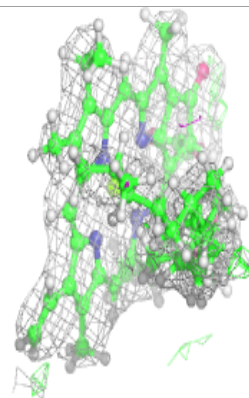
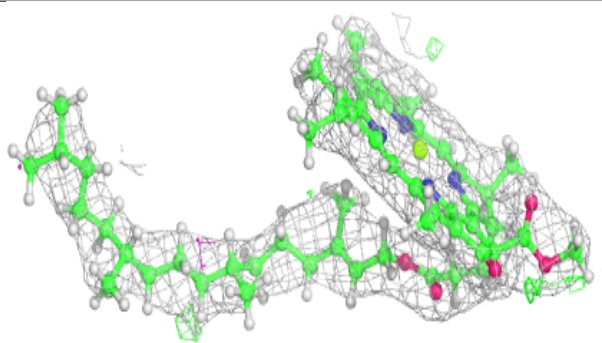
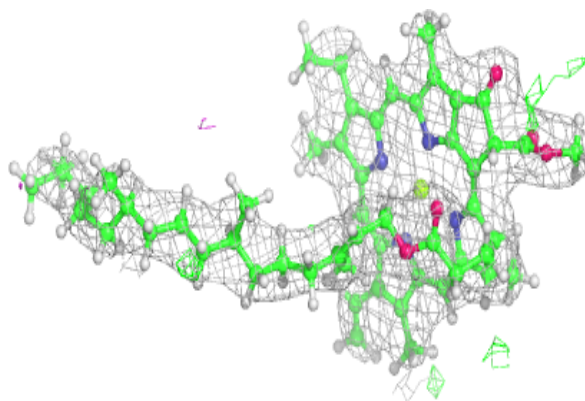
**Electron density around CLA C 509:**

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

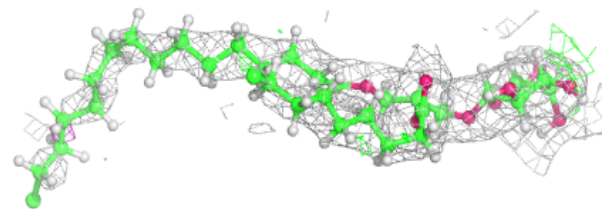
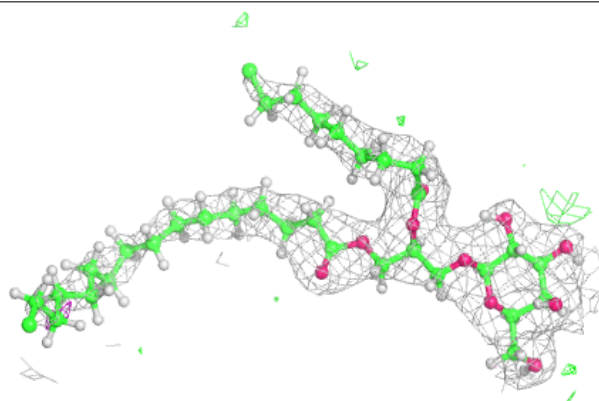


**Electron density around CLA b 608:**

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

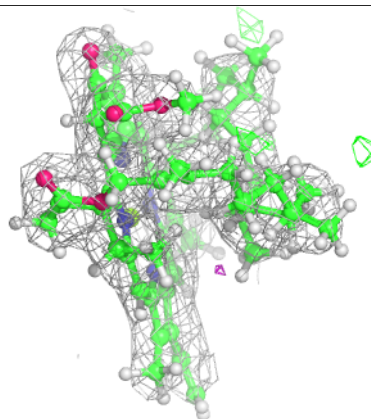
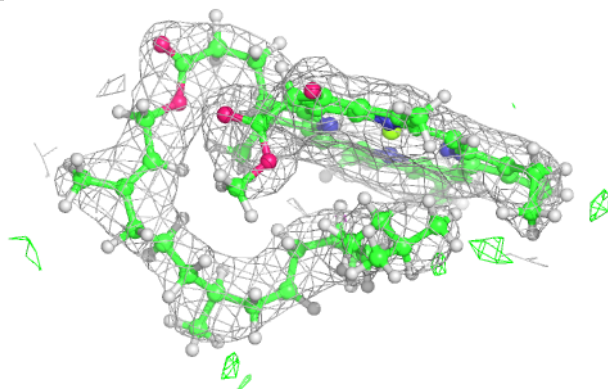
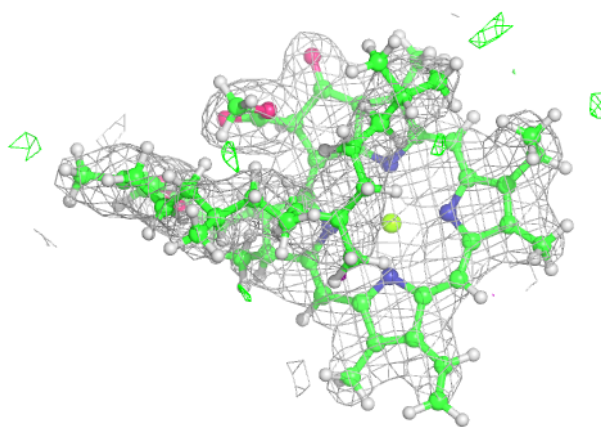
**Electron density around LMG d 412:**

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



**Electron density around CLA C 510:**

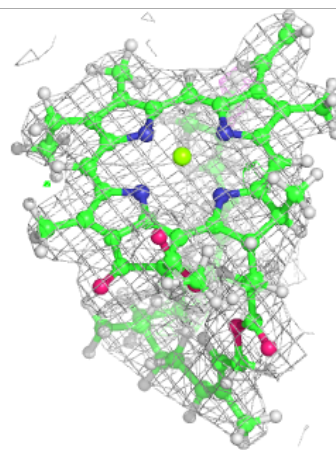
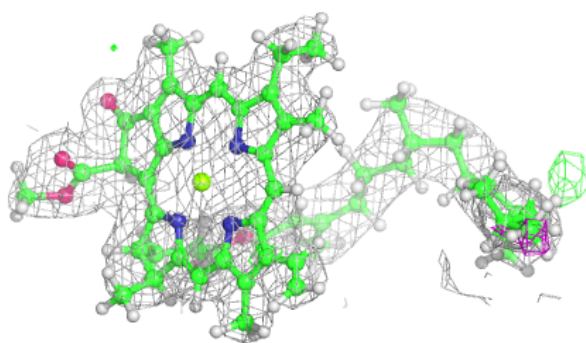
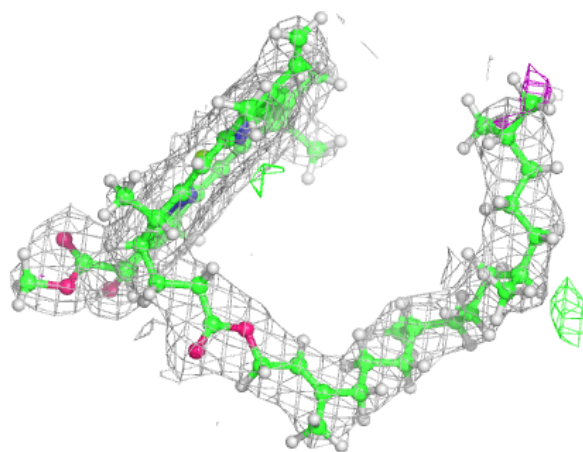
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





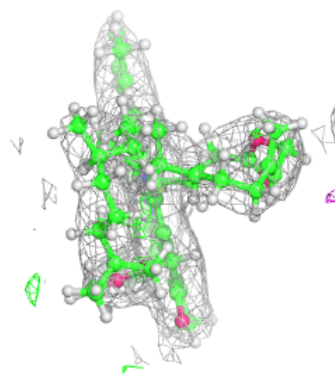
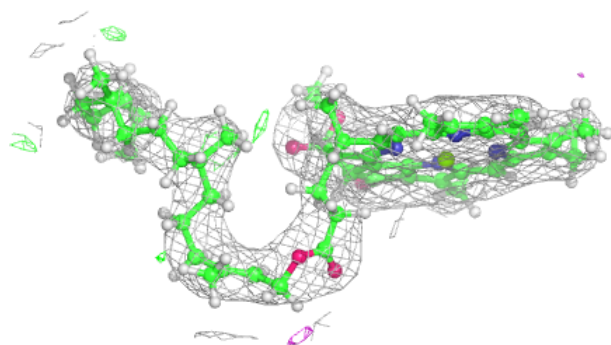
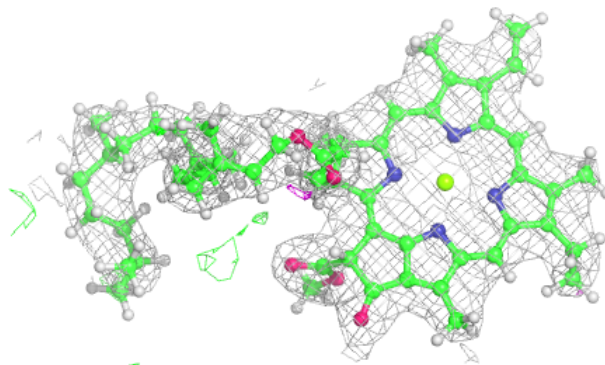
**Electron density around CLA b 611:**

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



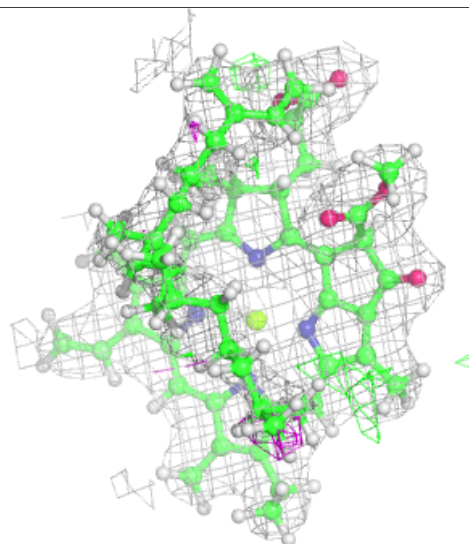
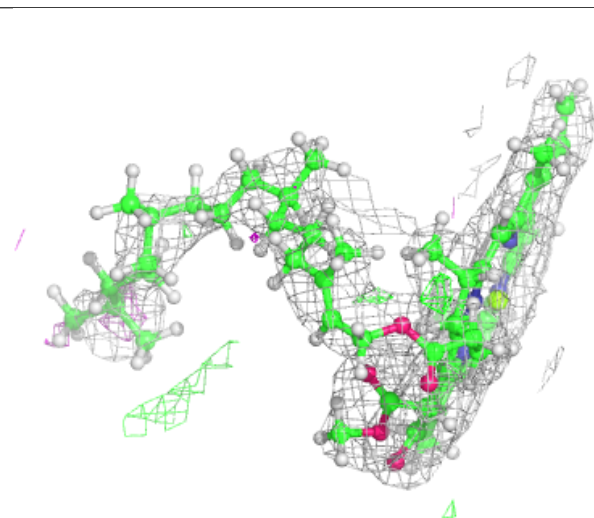
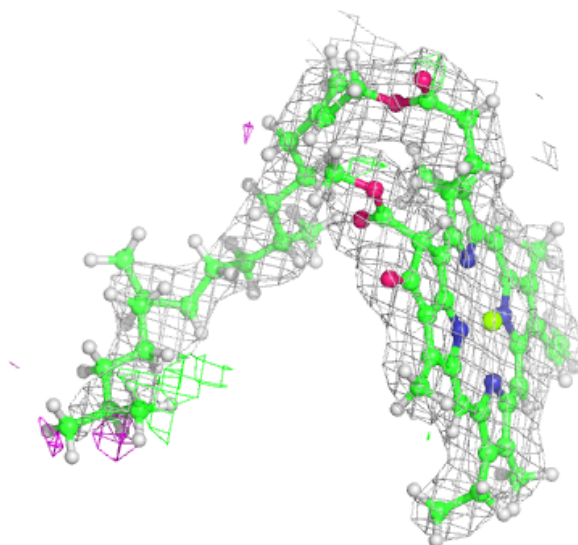
**Electron density around CLA b 612:**

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



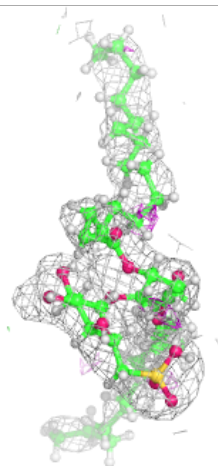
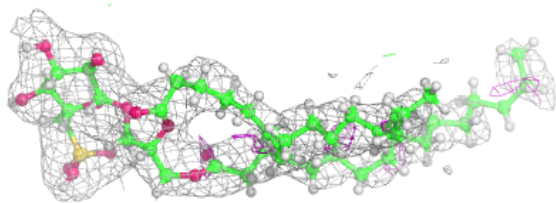
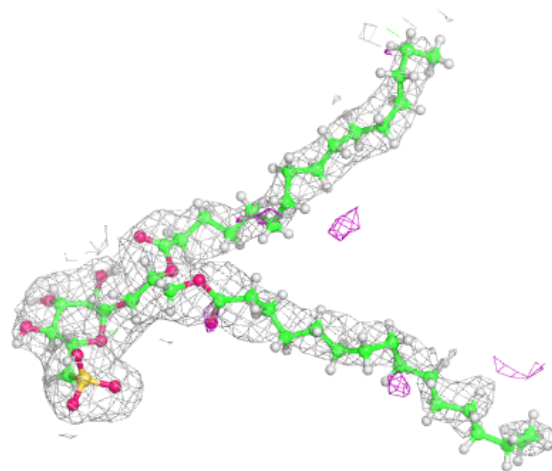
**Electron density around CLA b 613:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



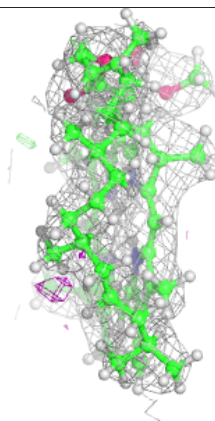
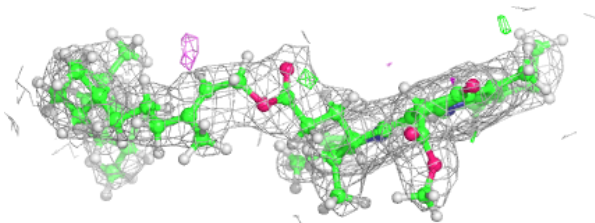
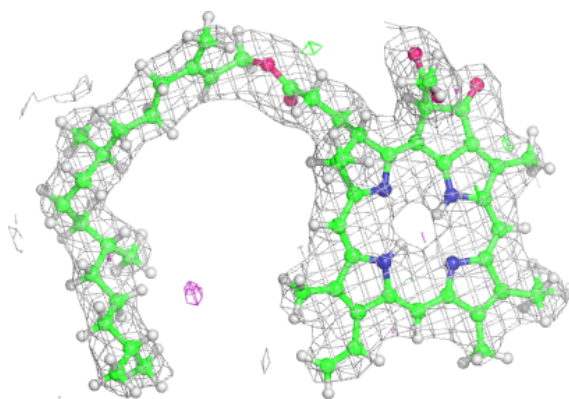
**Electron density around SQD a 410:**

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

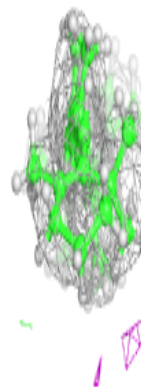
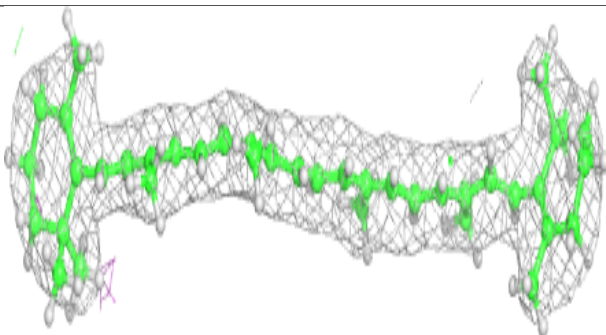
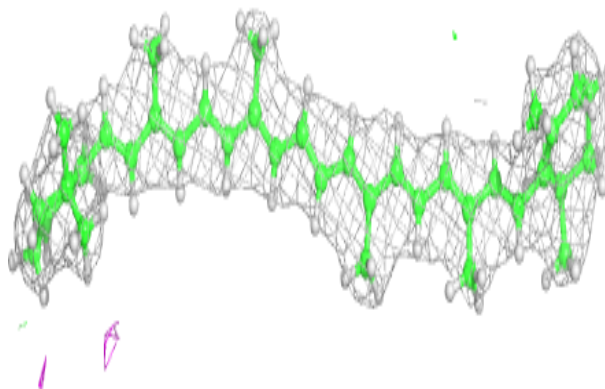


**Electron density around PHO d 401:**

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

**Electron density around BCR A 406:**

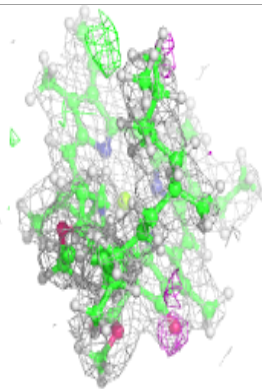
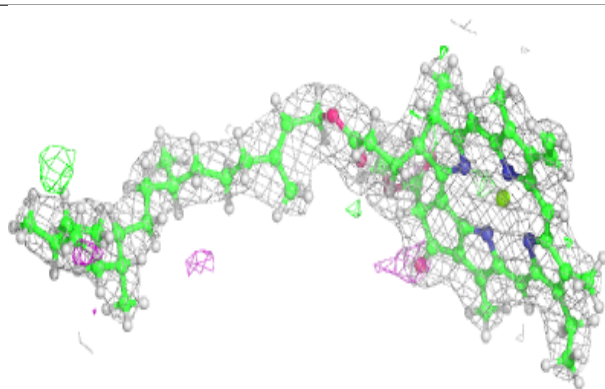
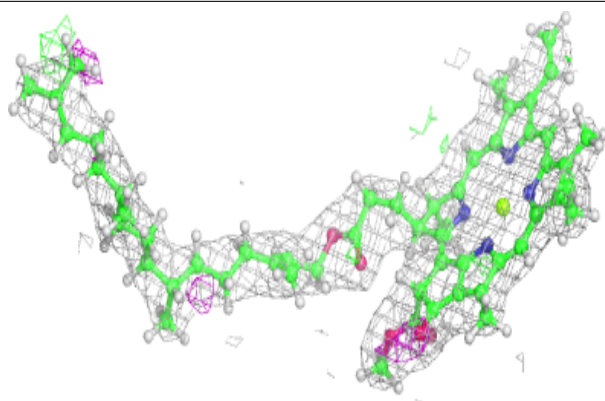
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



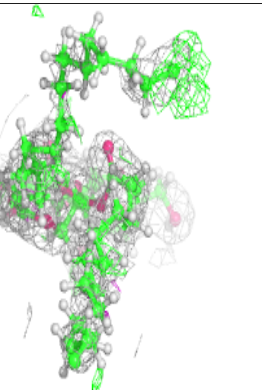
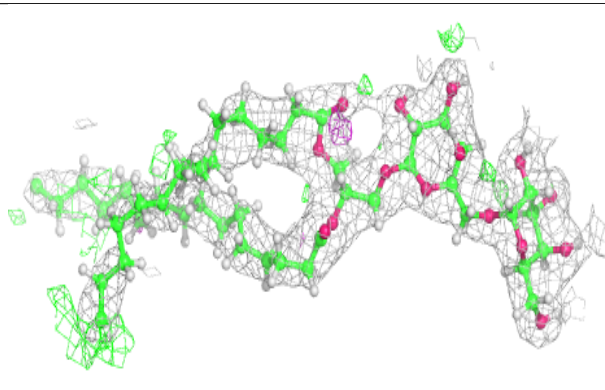
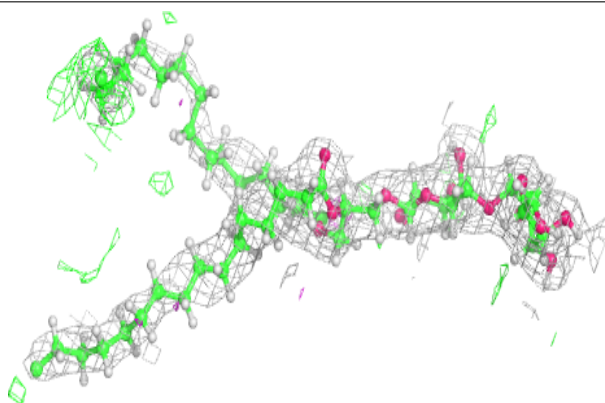


**Electron density around CLA A 402:**

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

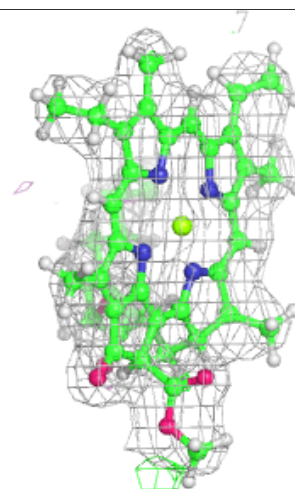
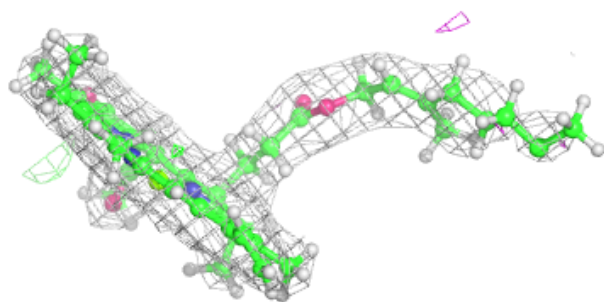
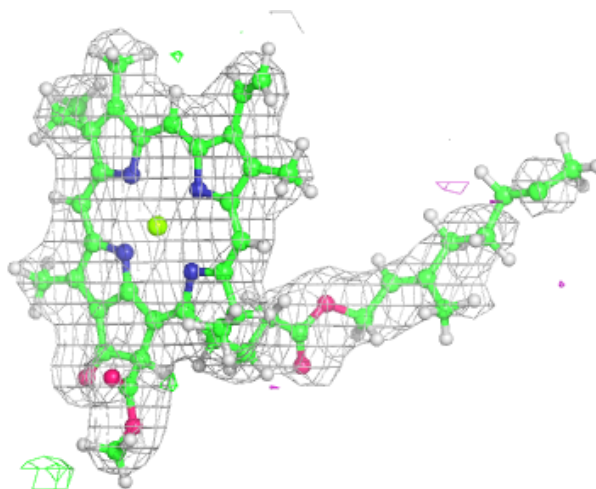
**Electron density around DGD C 516:**

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



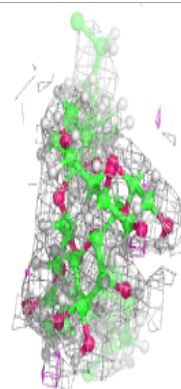
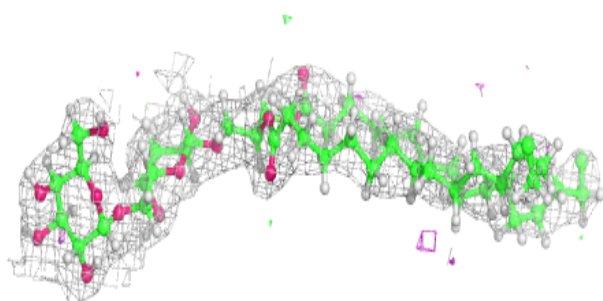
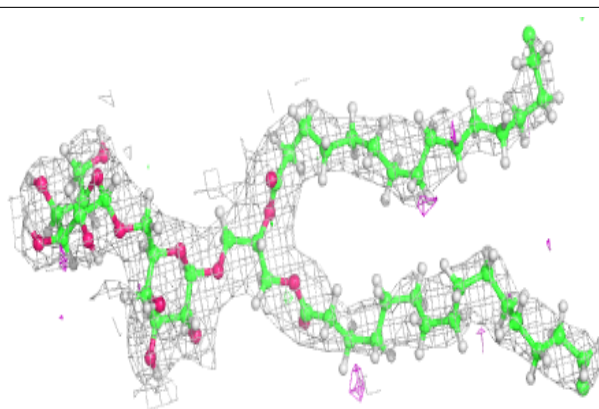
**Electron density around CLA A 405:**

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

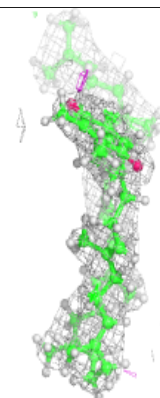
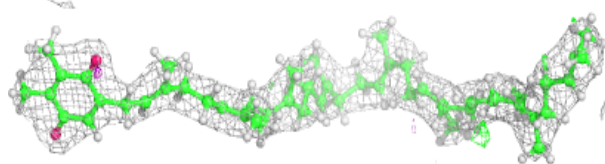
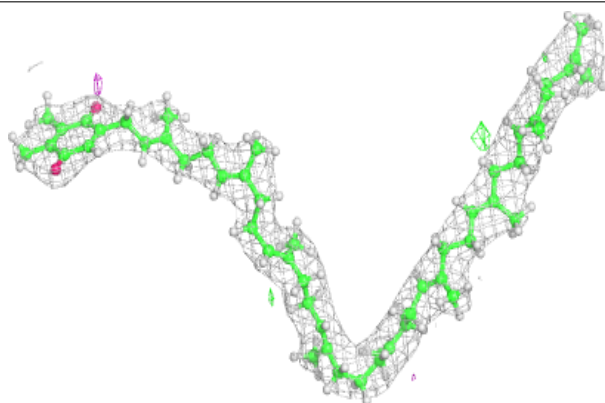


**Electron density around DGD C 518:**

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

**Electron density around PL9 d 407:**

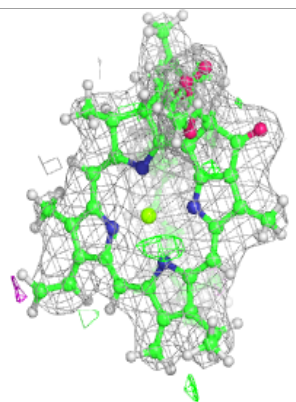
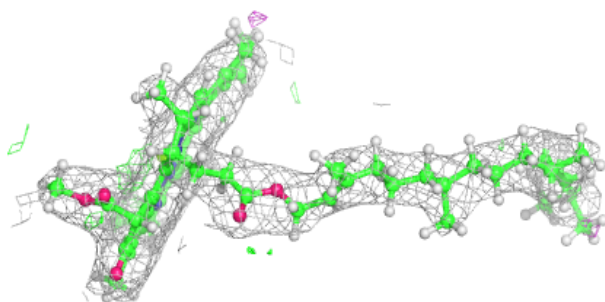
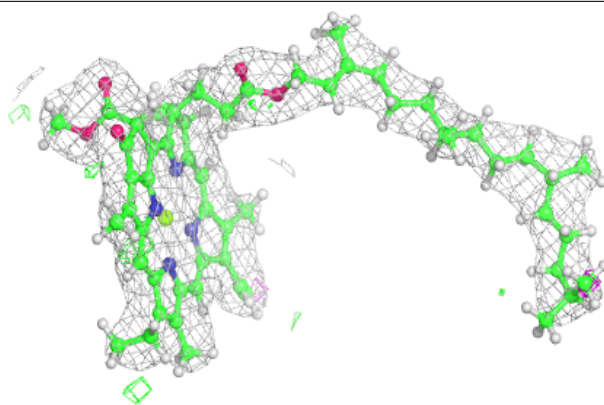
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





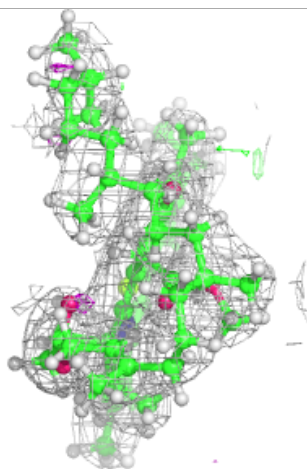
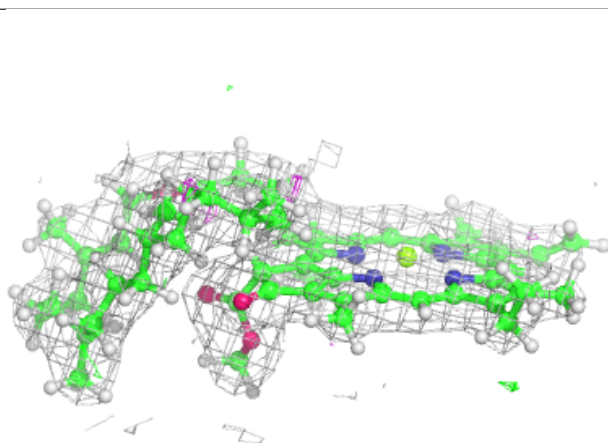
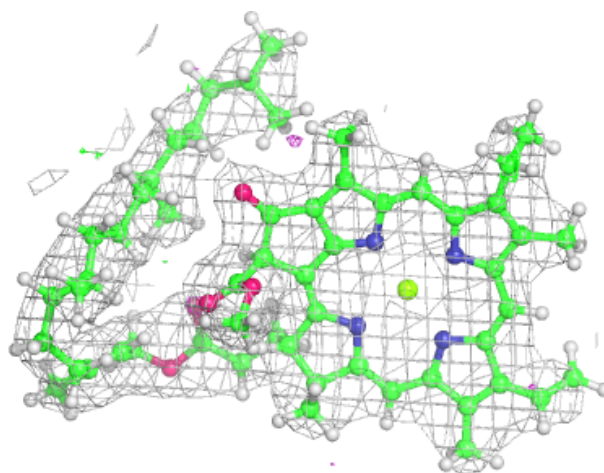
**Electron density around CLA B 609:**

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



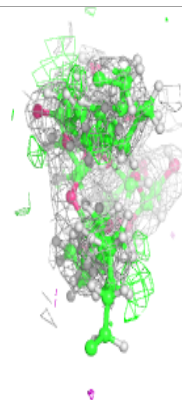
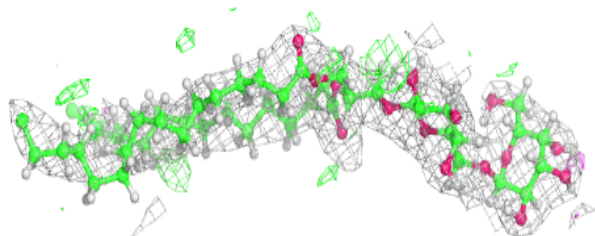
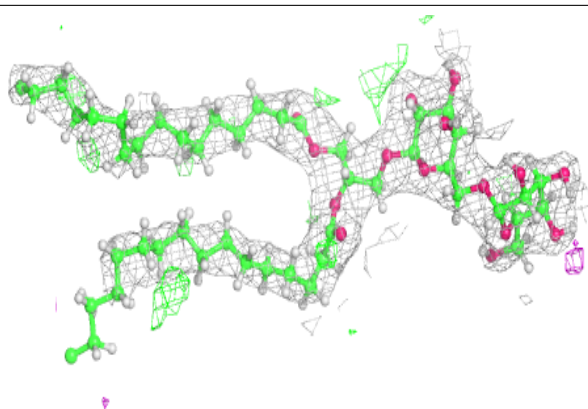
**Electron density around CLA B 610:**

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

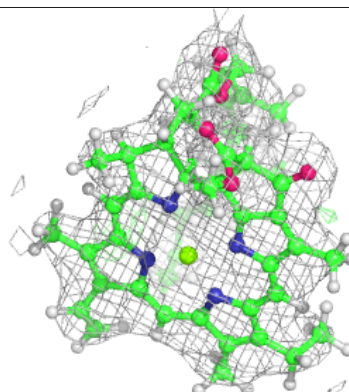
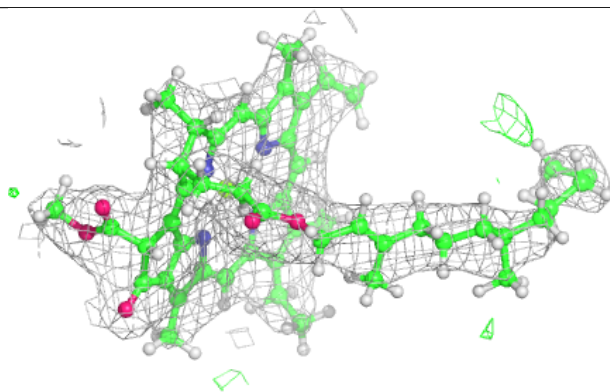
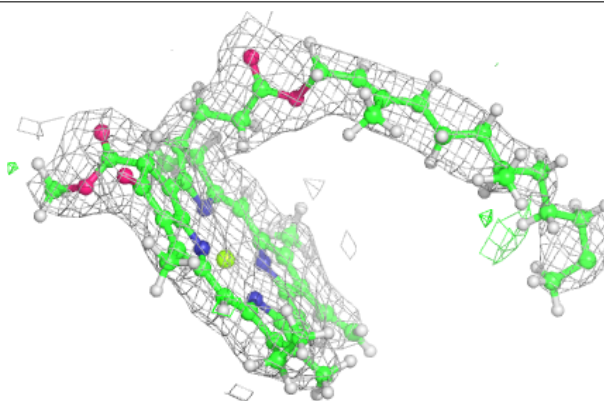


**Electron density around DGD c 519:**

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

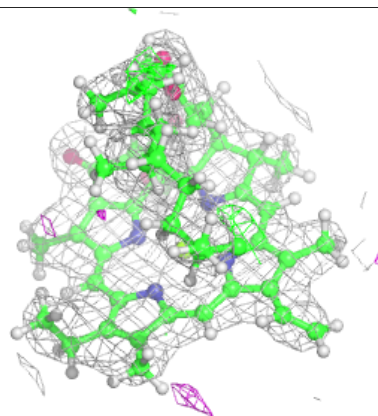
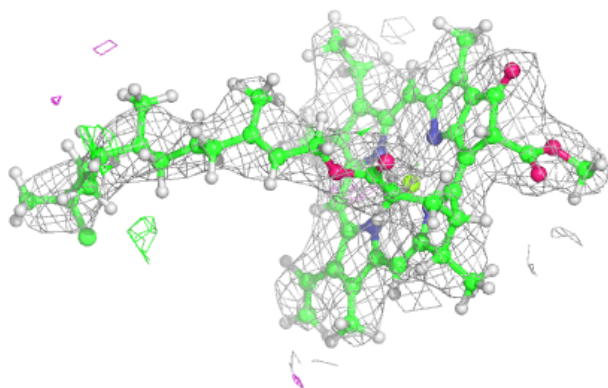
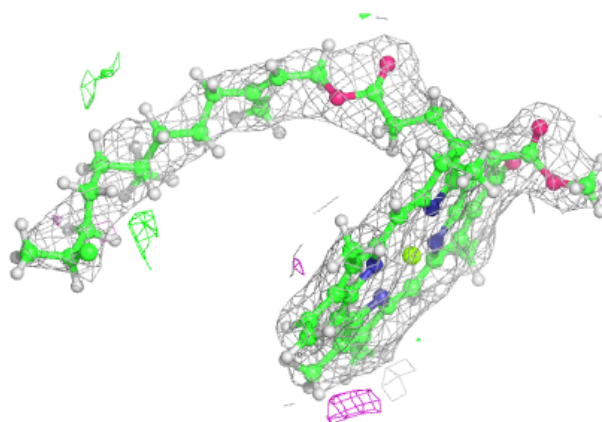
**Electron density around CLA C 504:**

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



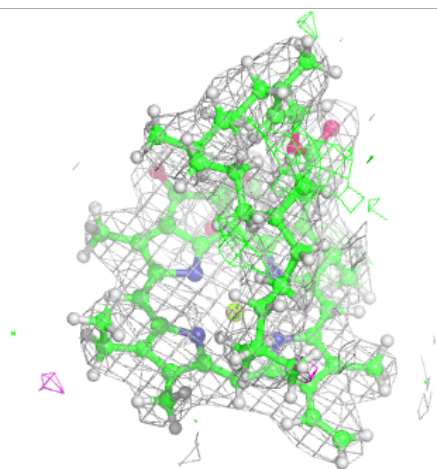
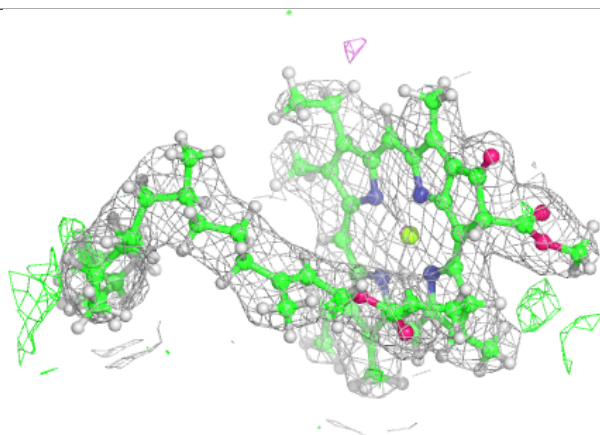
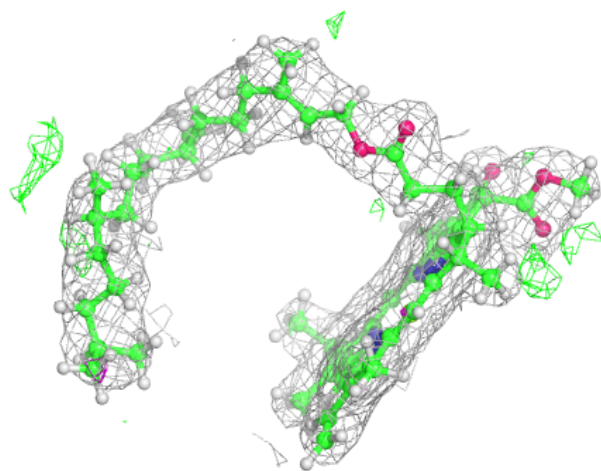
**Electron density around CLA c 504:**

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



**Electron density around CLA B 611:**

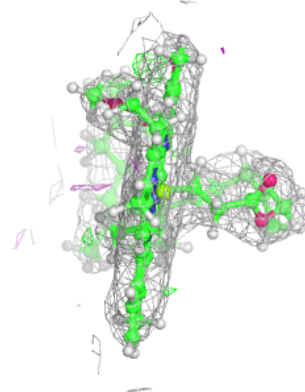
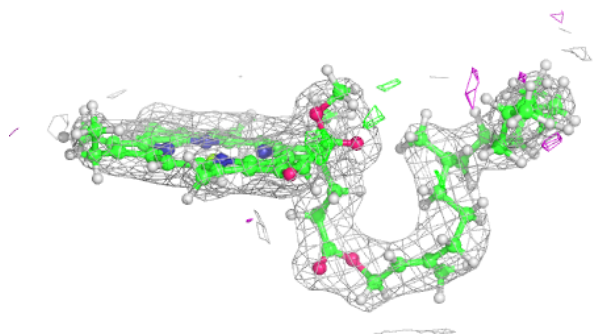
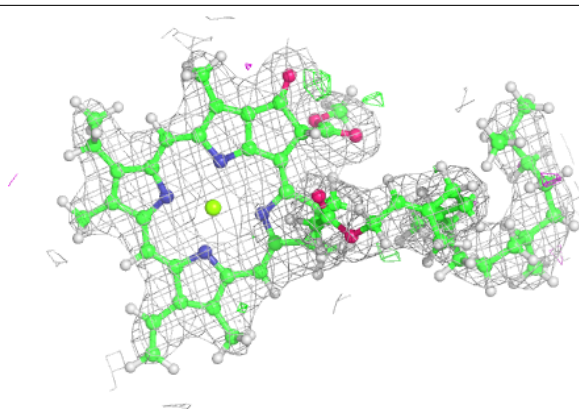
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



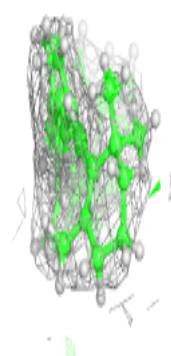
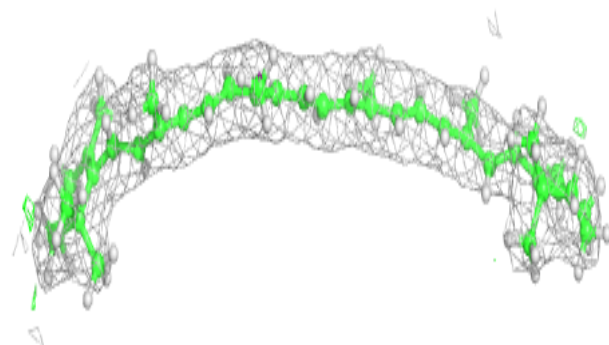
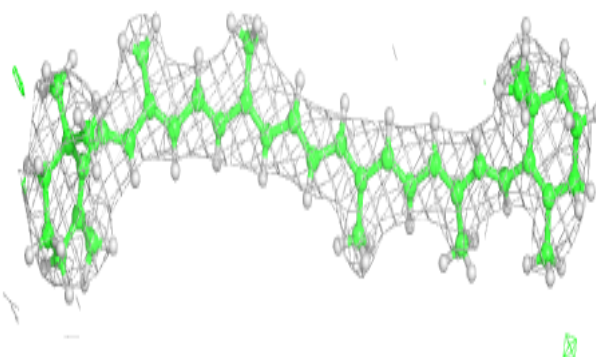


**Electron density around CLA B 612:**

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

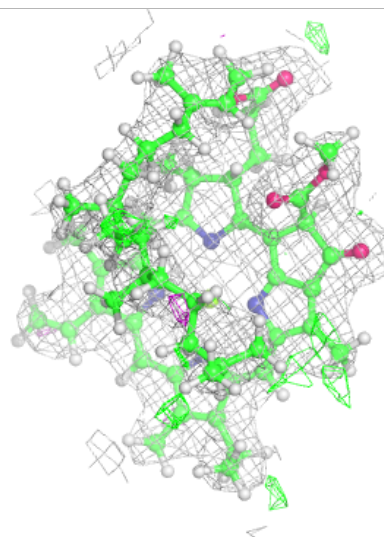
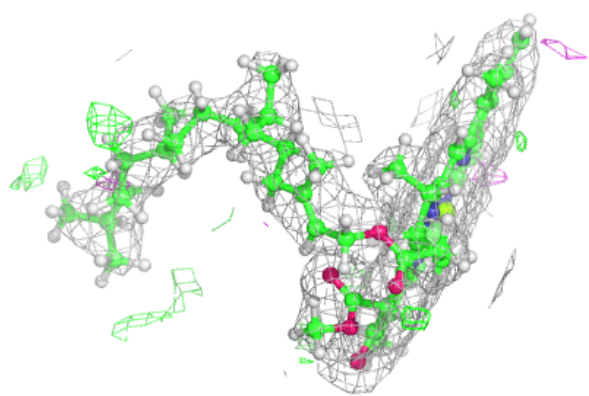
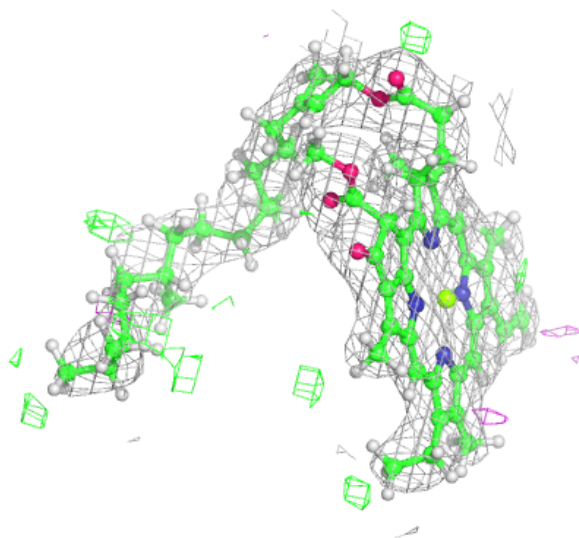
**Electron density around BCR T 101:**

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



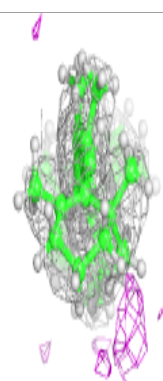
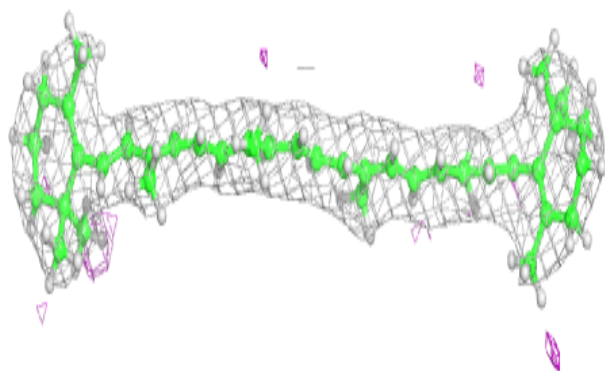
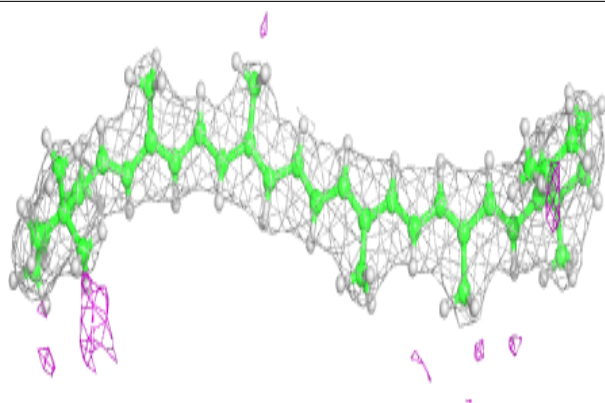
**Electron density around CLA B 613:**

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

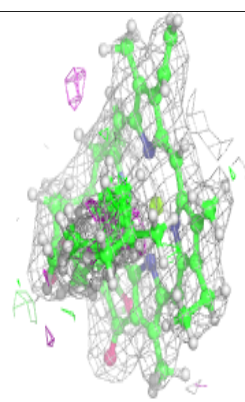
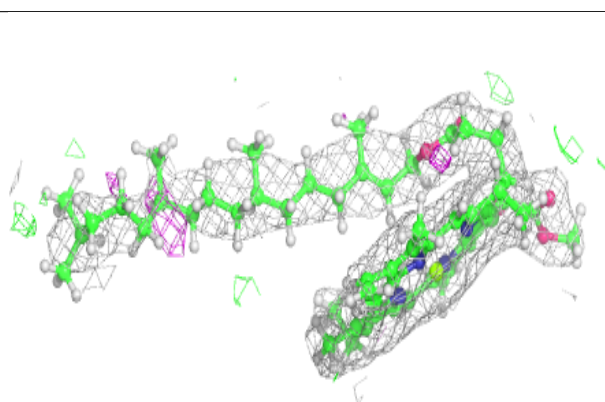
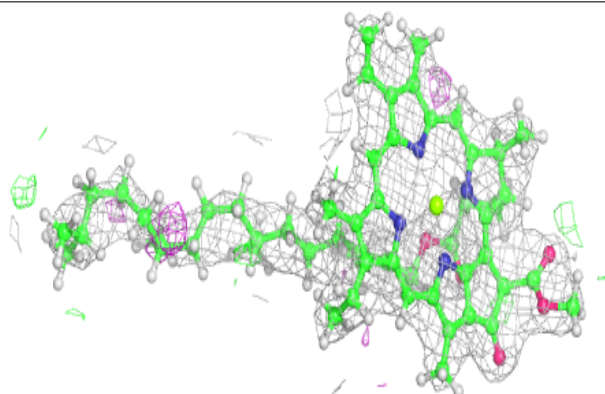


**Electron density around BCR a 405:**

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

**Electron density around CLA B 614:**

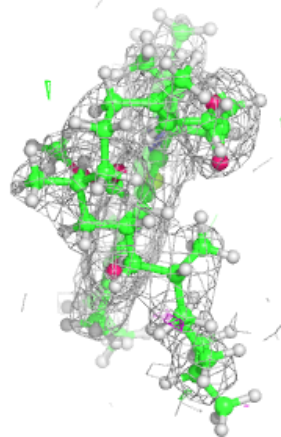
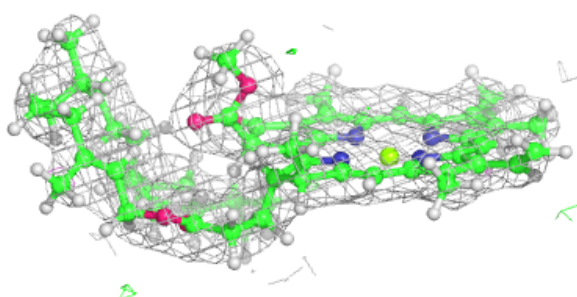
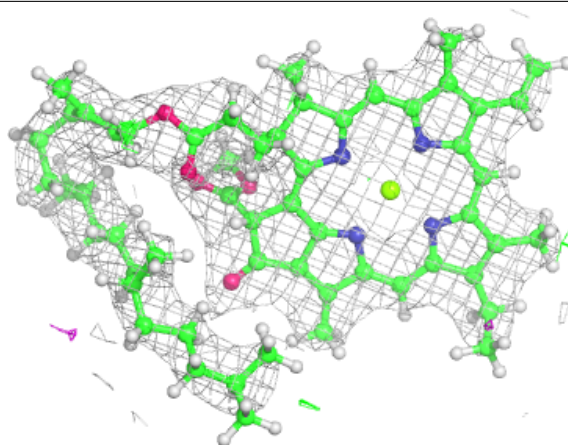
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



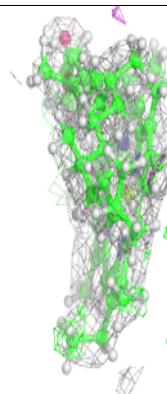
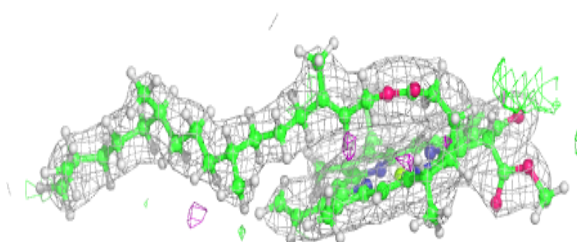
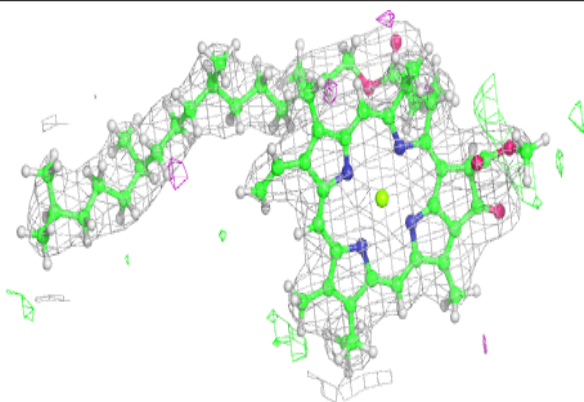


**Electron density around CLA b 610:**

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

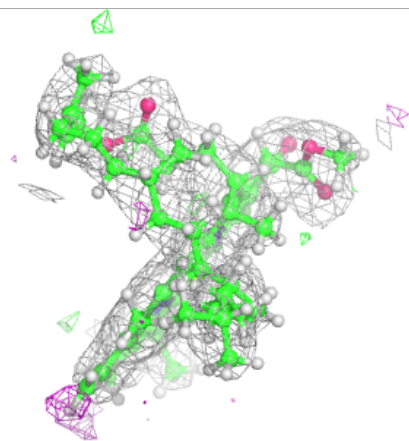
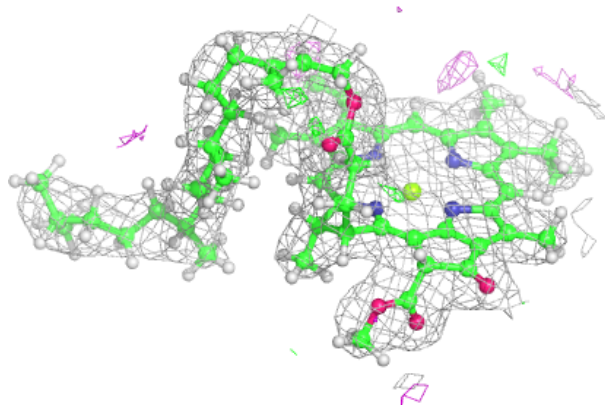
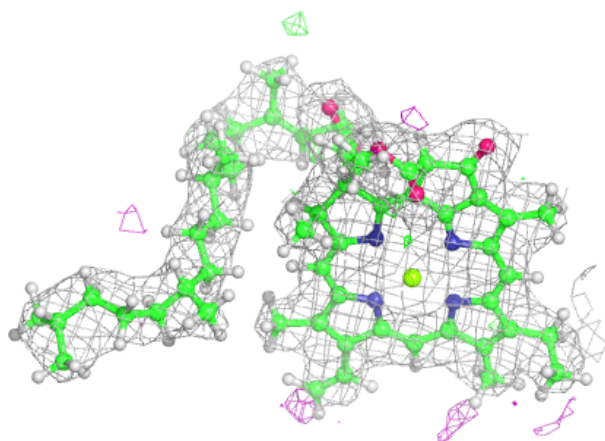
**Electron density around CLA C 501:**

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



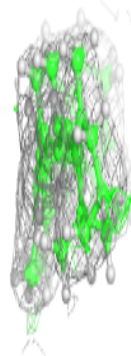
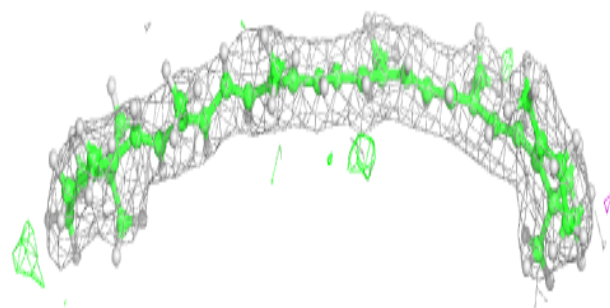
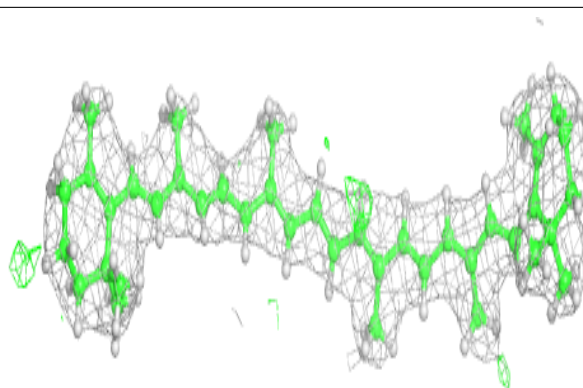
**Electron density around CLA A 410:**

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

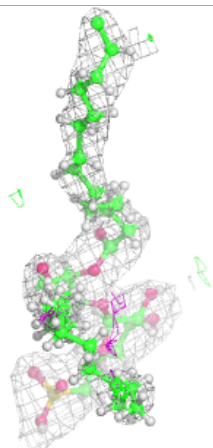
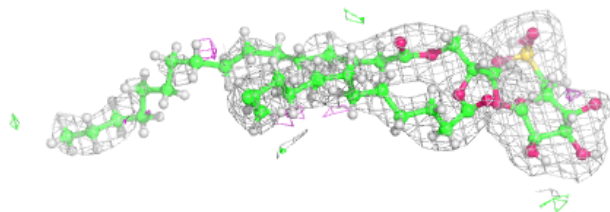
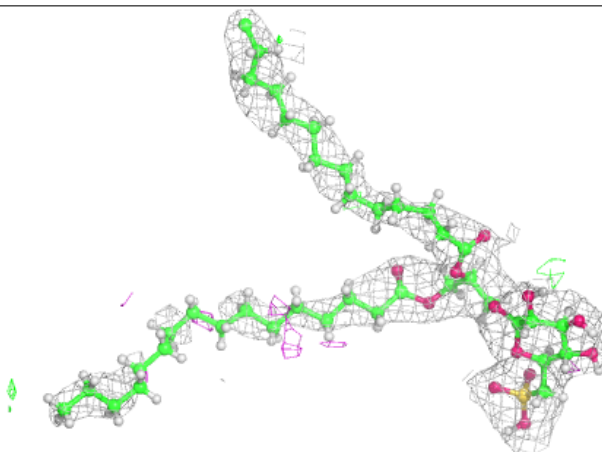


**Electron density around BCR t 101:**

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

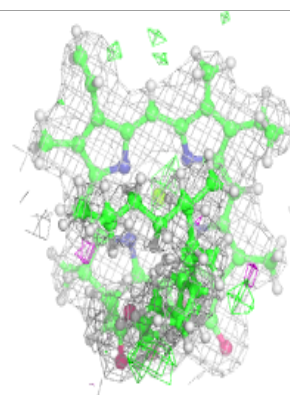
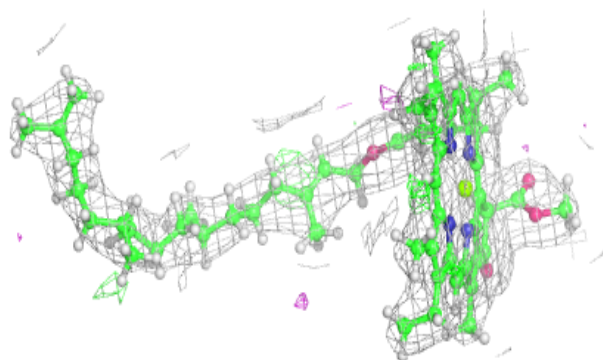
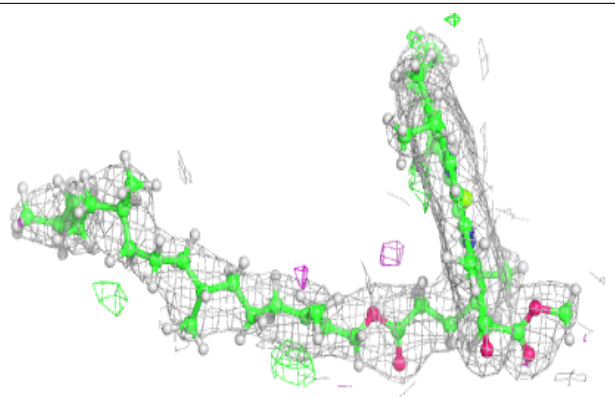
**Electron density around SQD A 412:**

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

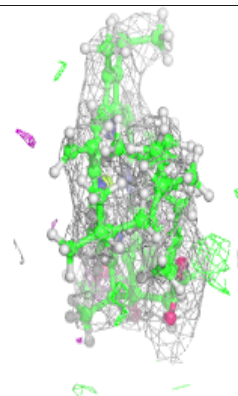
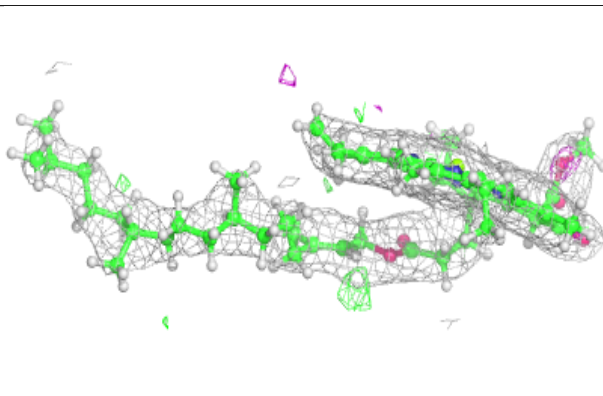
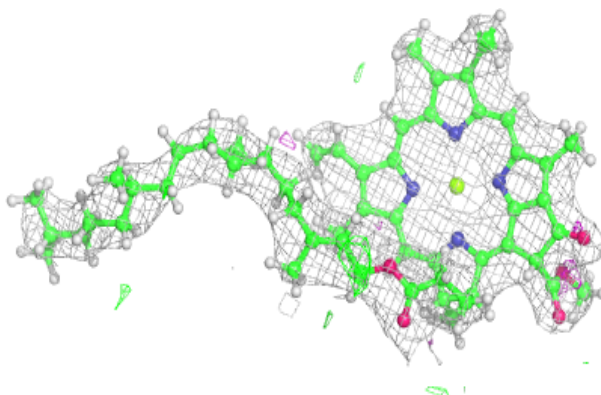


**Electron density around CLA B 605:**

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

**Electron density around CLA b 603:**

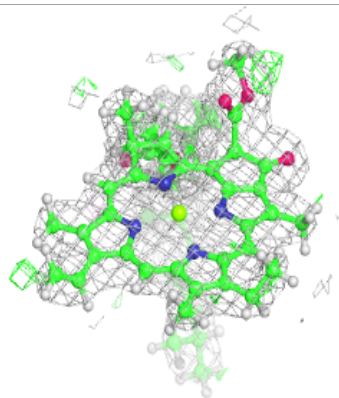
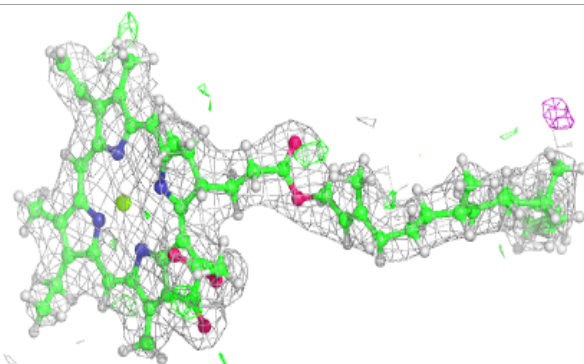
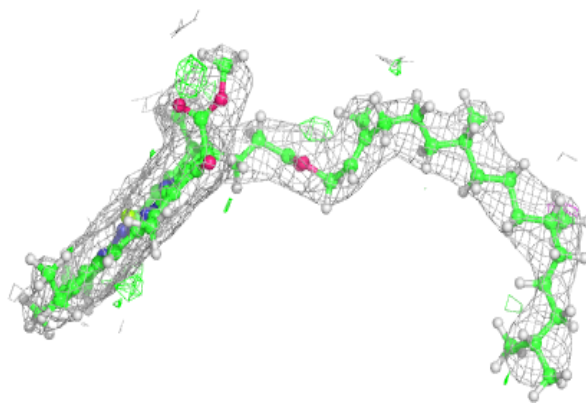
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



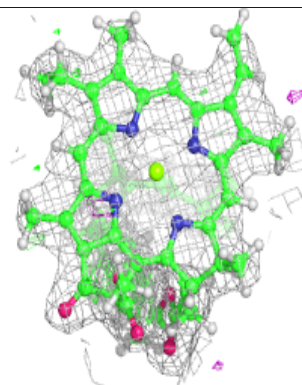
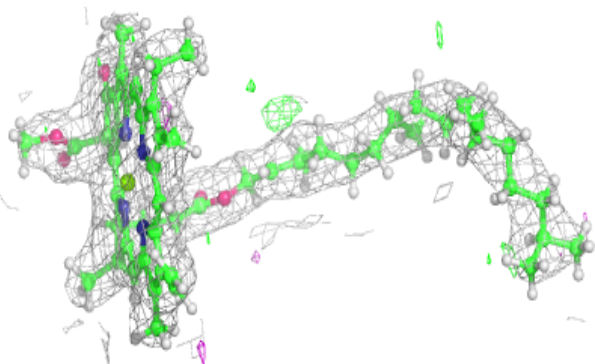
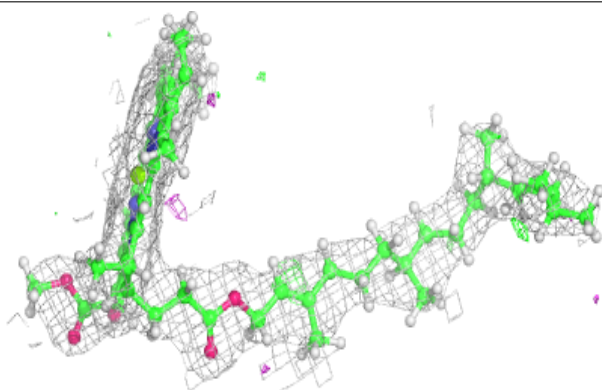


**Electron density around CLA D 403:**

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

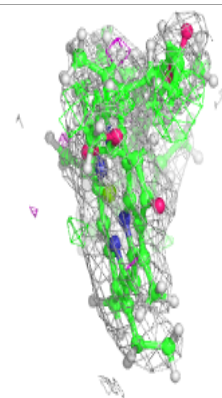
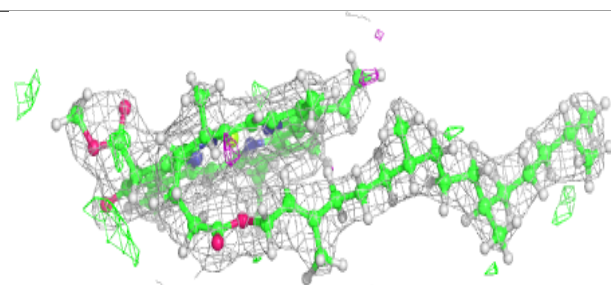
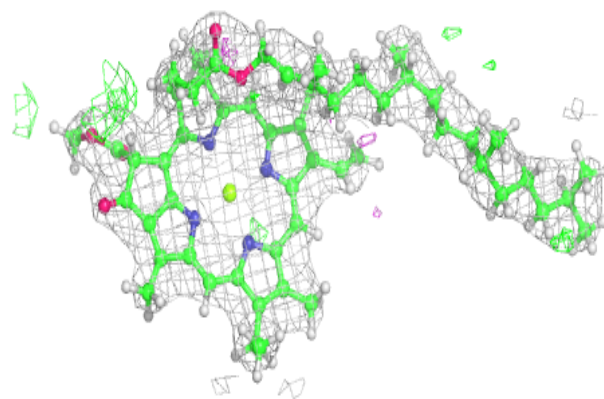
**Electron density around CLA b 605:**

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

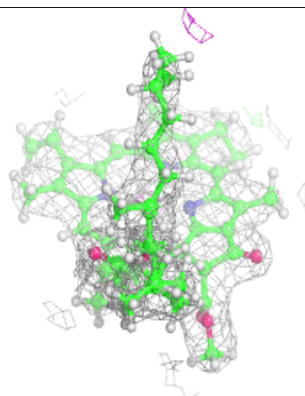
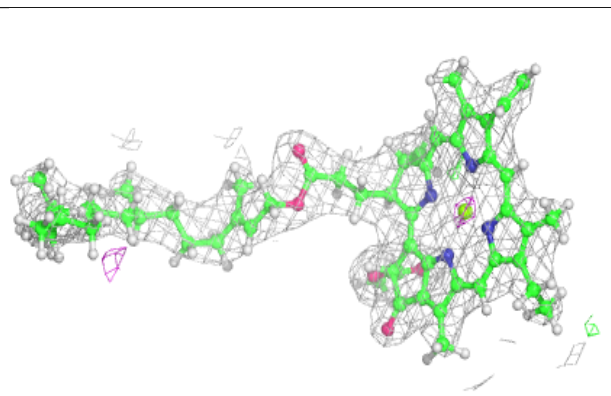
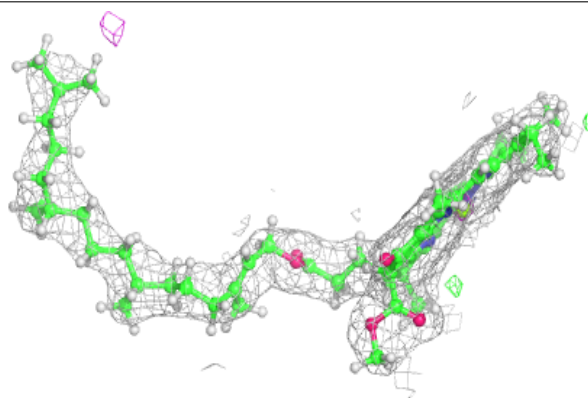


**Electron density around CLA c 501:**

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

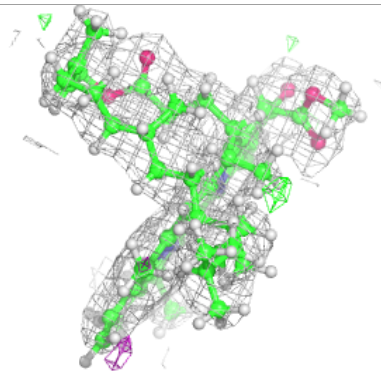
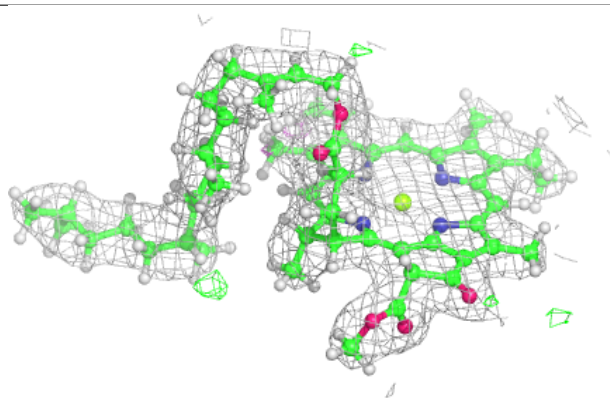
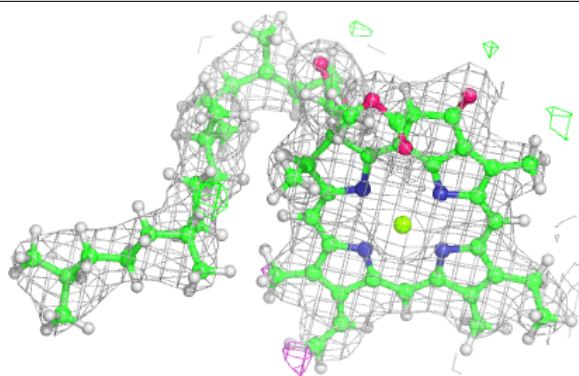
**Electron density around CLA d 403:**

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

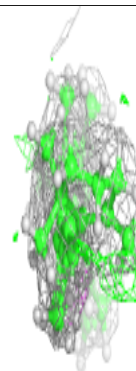
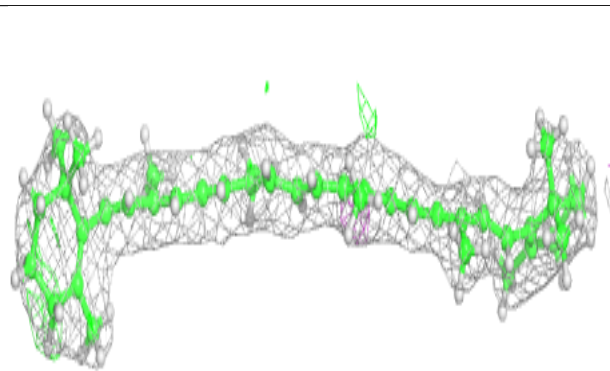
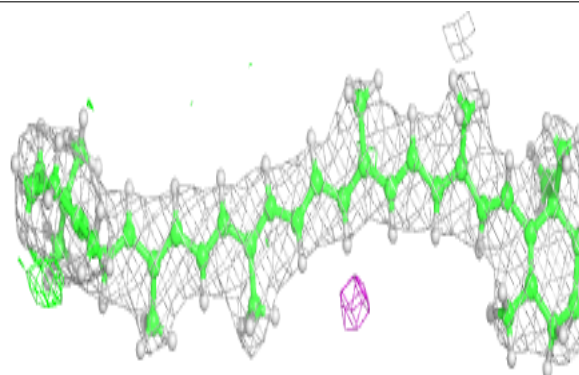


**Electron density around CLA d 404:**

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

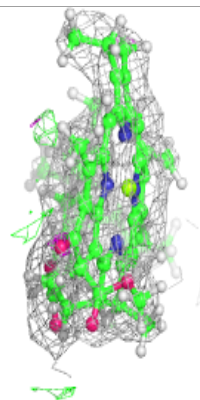
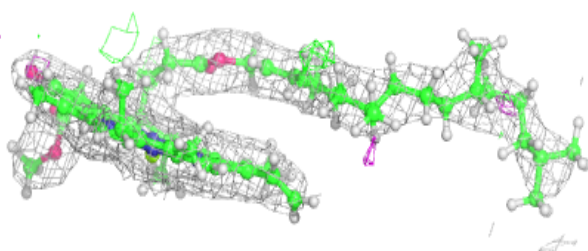
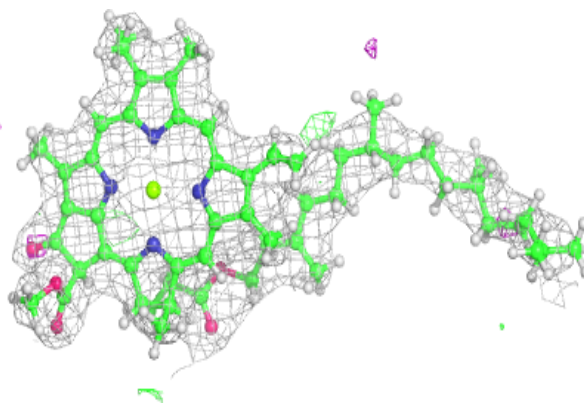
**Electron density around BCR b 617:**

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

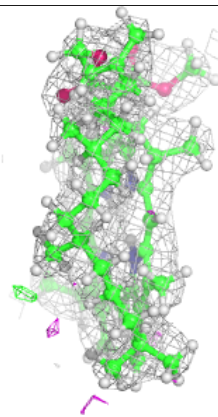
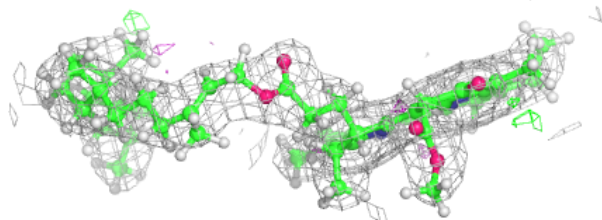
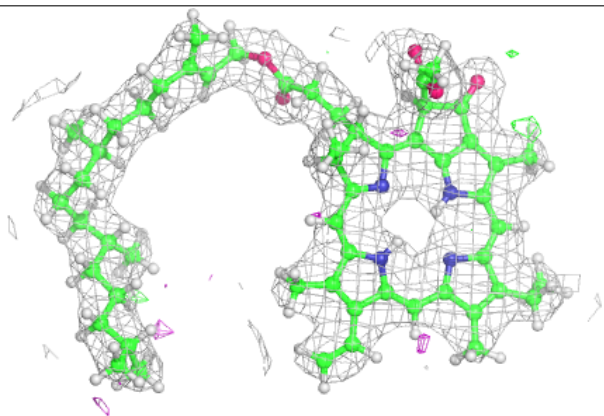


**Electron density around CLA B 603:**

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

**Electron density around PHO A 404:**

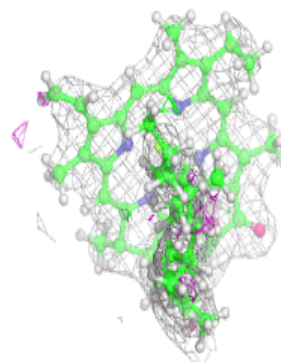
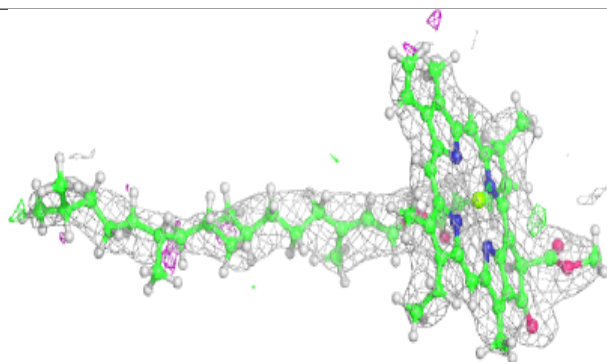
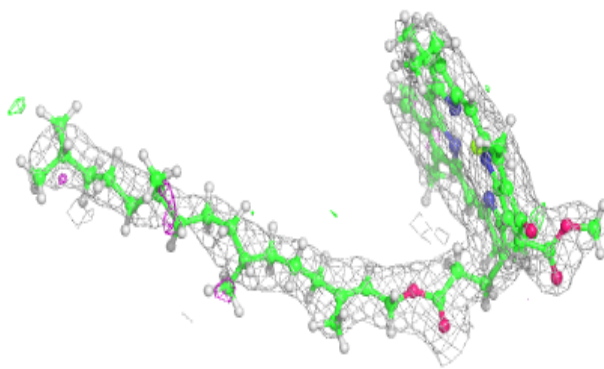
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



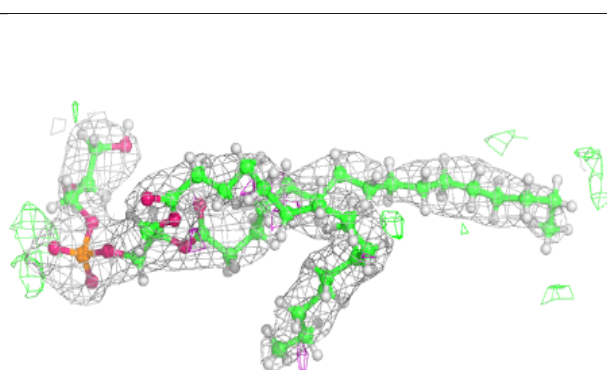
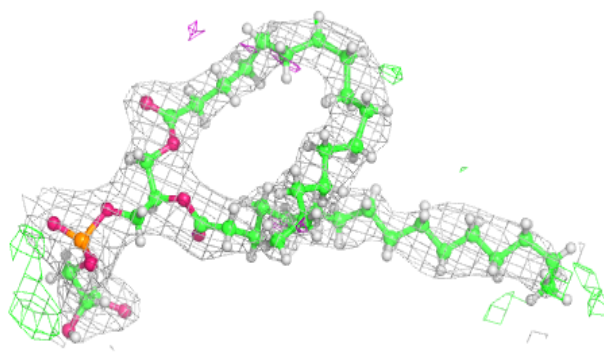


**Electron density around CLA b 607:**

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

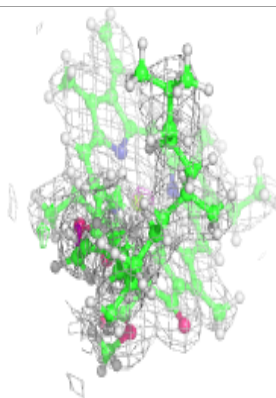
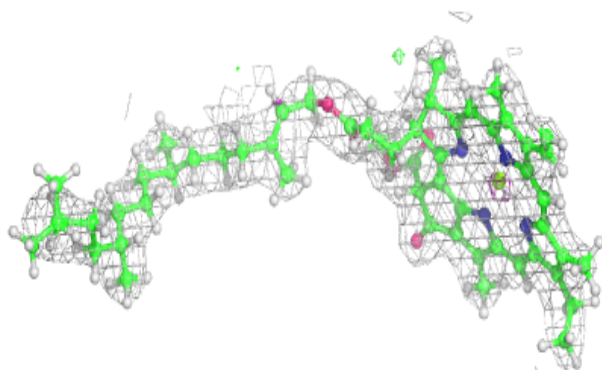
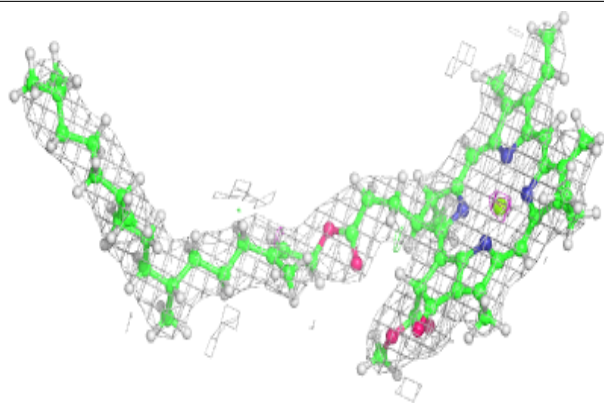
**Electron density around LHG B 622:**

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

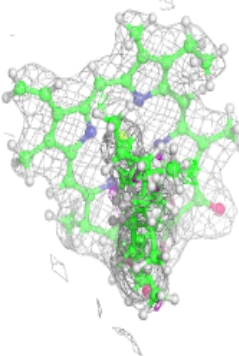
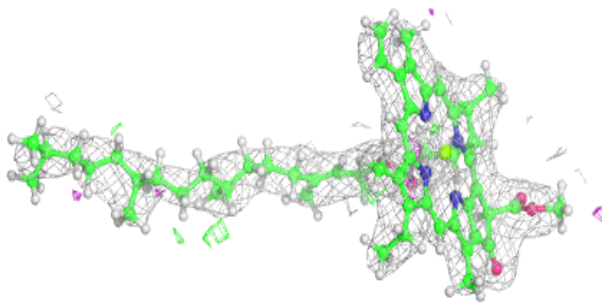
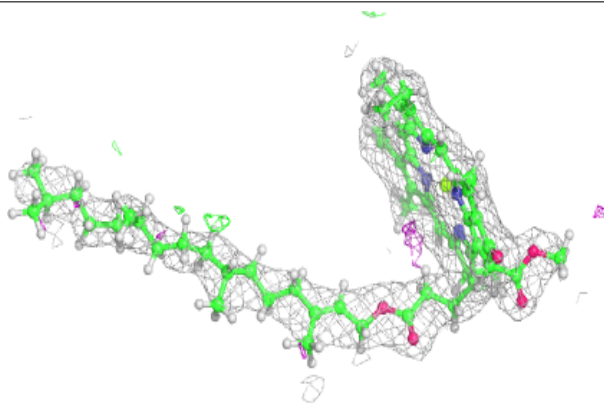


**Electron density around CLA a 402:**

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

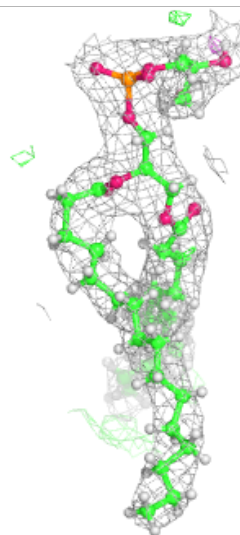
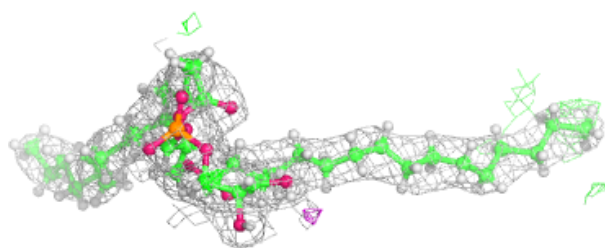
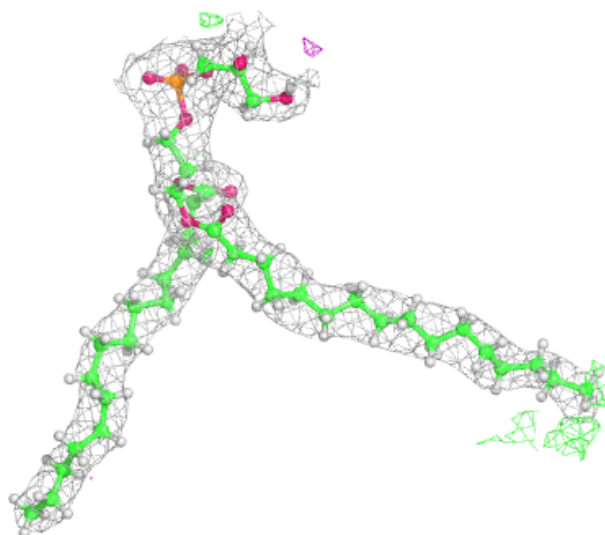
**Electron density around CLA B 607:**

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



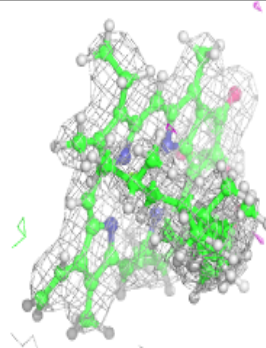
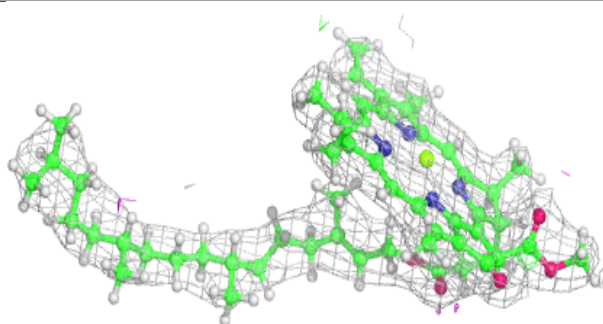
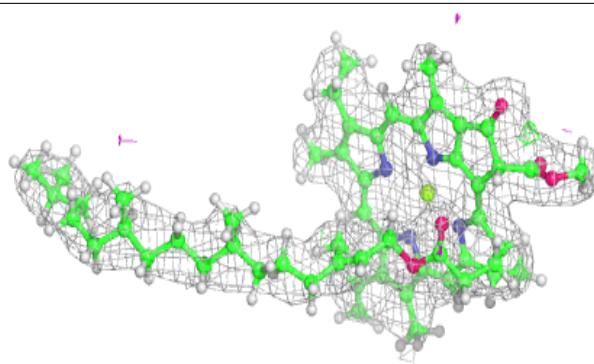
**Electron density around LHG 1 101:**

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

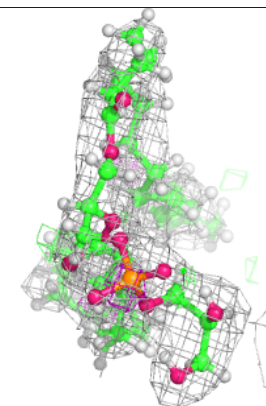
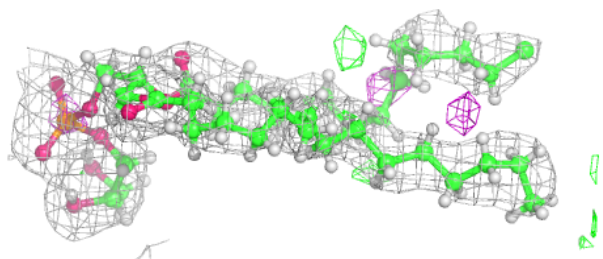
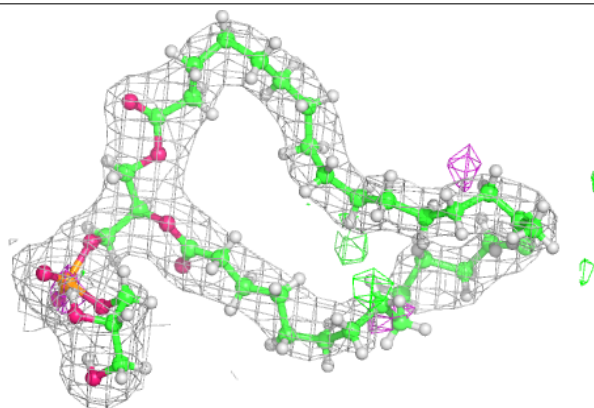


**Electron density around CLA B 608:**

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

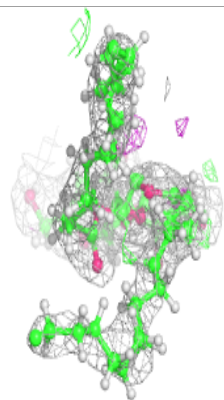
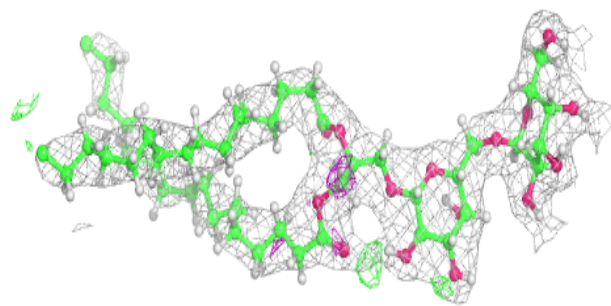
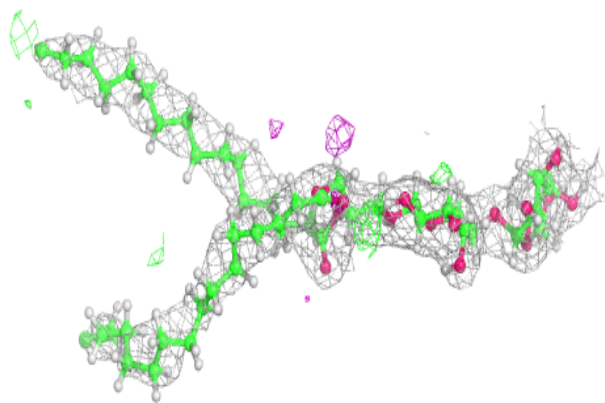
**Electron density around LHG D 409:**

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



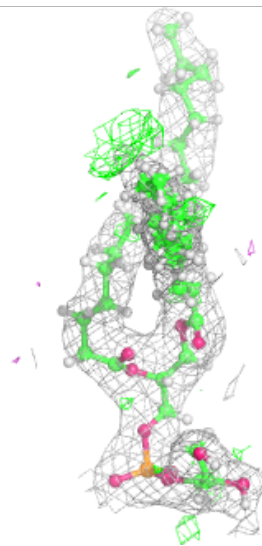
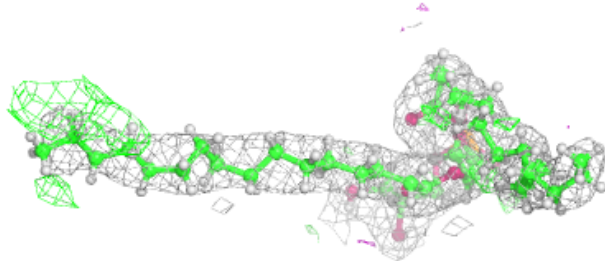
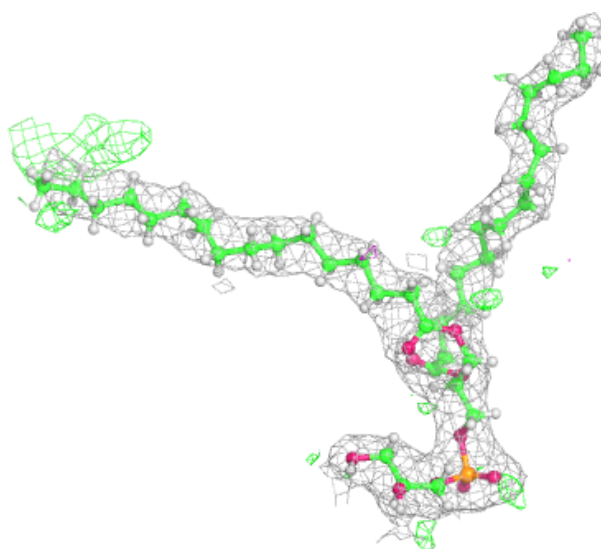
**Electron density around DGD c 517:**

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



**Electron density around LHG L 102:**

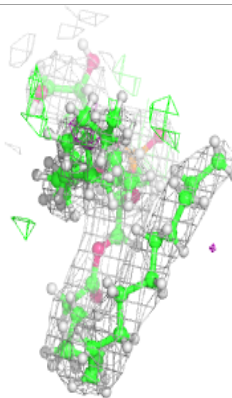
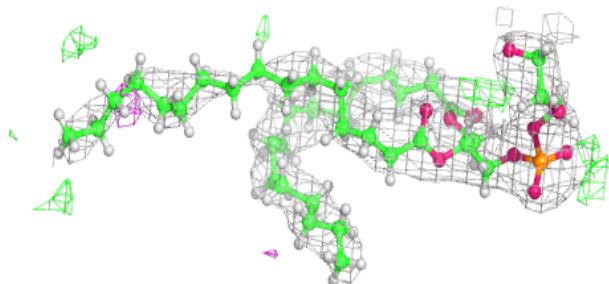
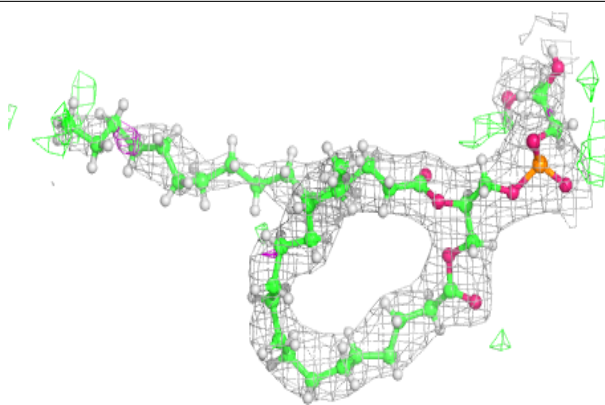
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



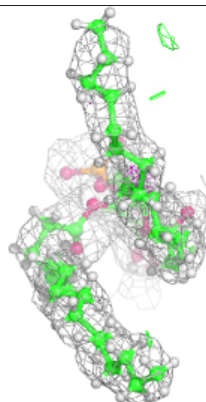
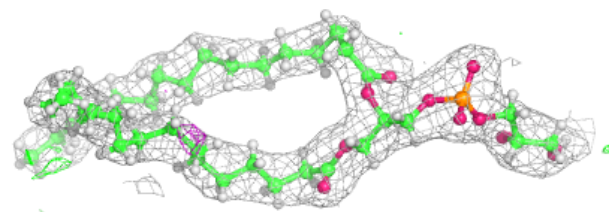
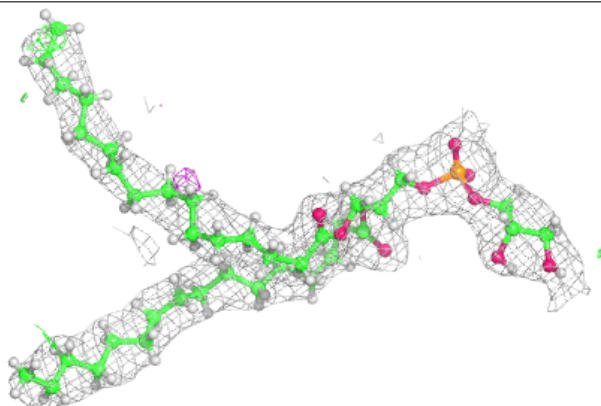


**Electron density around LHG d 408:**

$2mF_o-DF_c$  (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:**

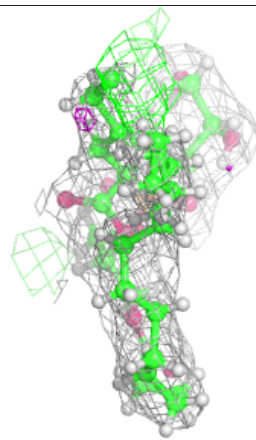
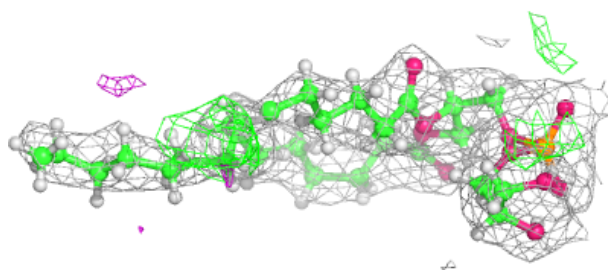
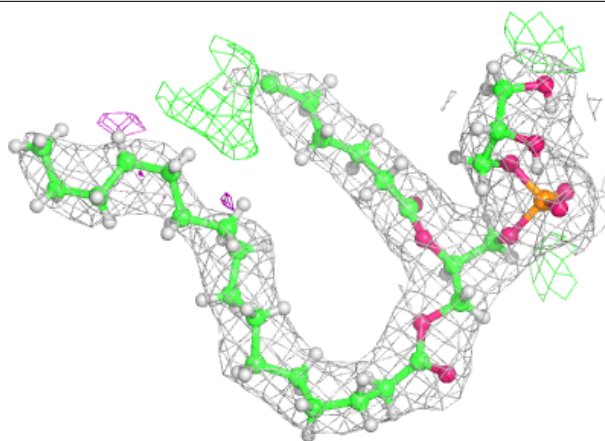
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





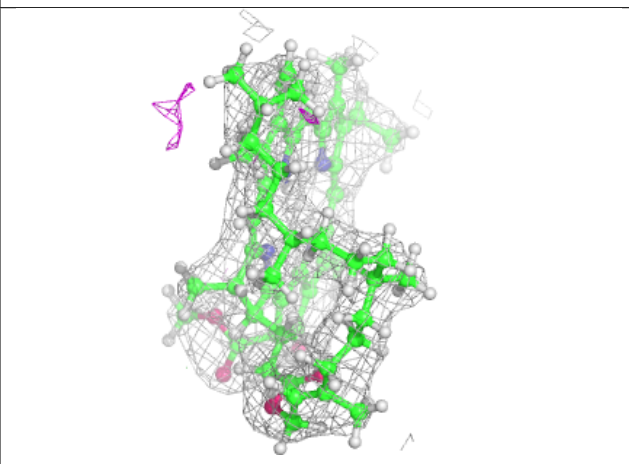
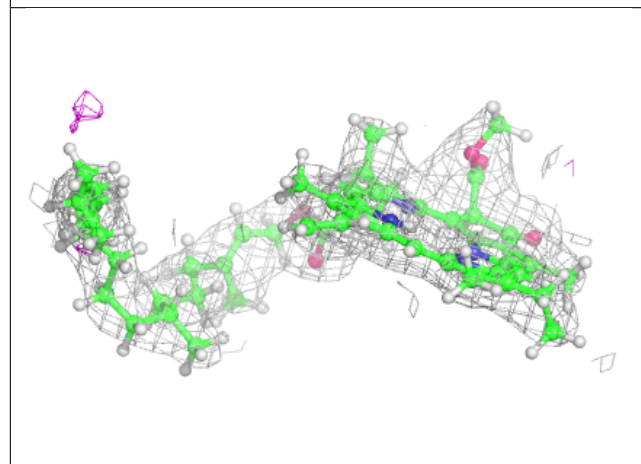
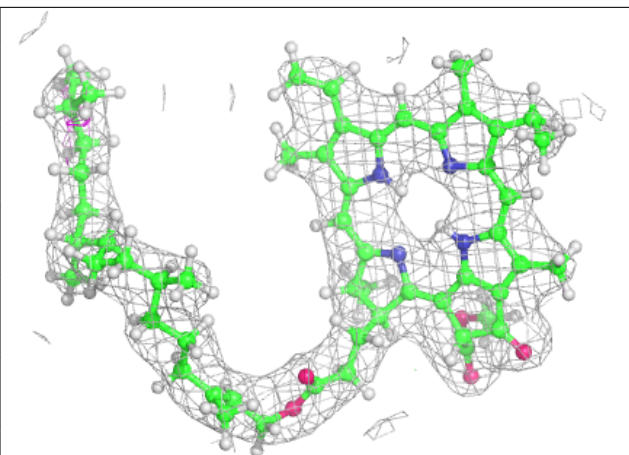
**Electron density around LHG d 410:**

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



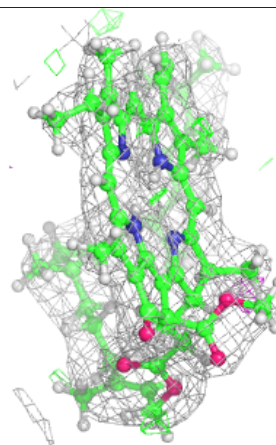
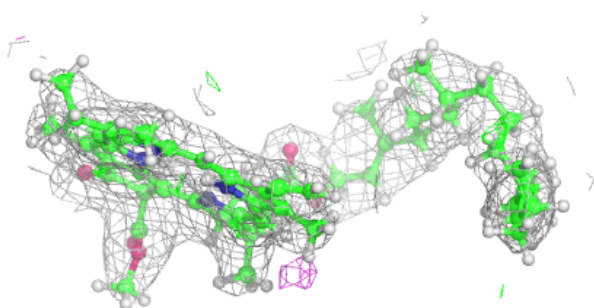
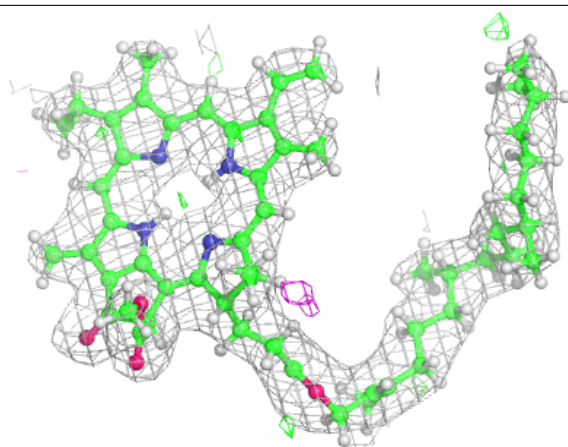
**Electron density around PHO d 402:**

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



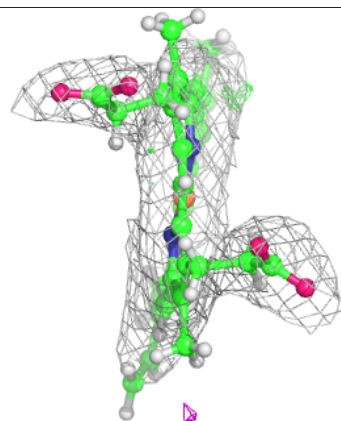
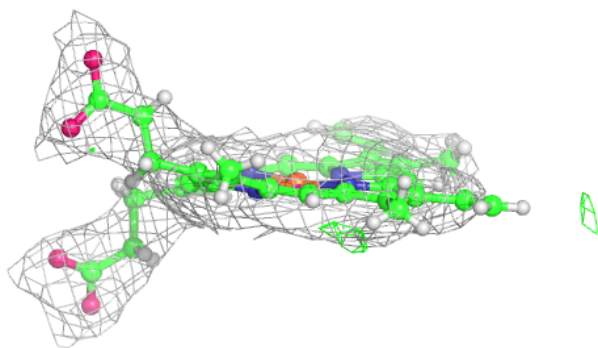
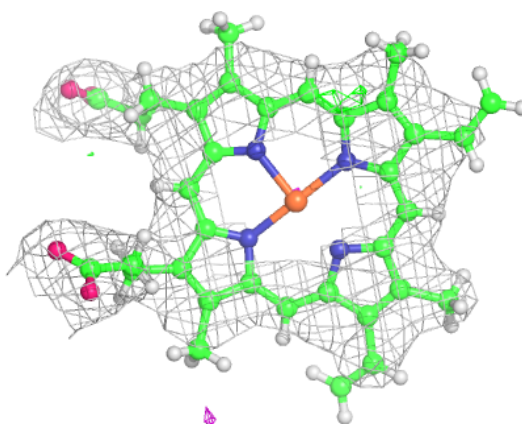
**Electron density around PHO D 401:**

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



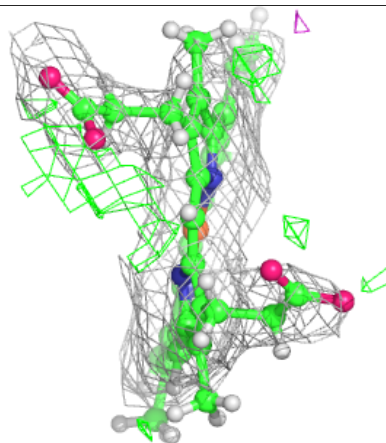
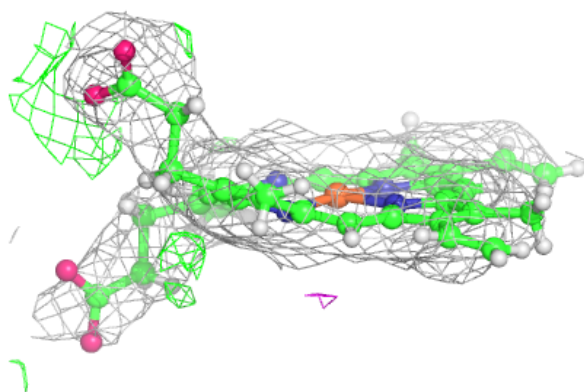
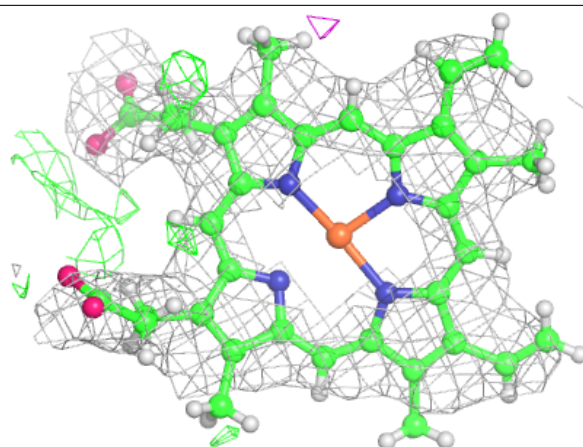
**Electron density around HEM E 101:**

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



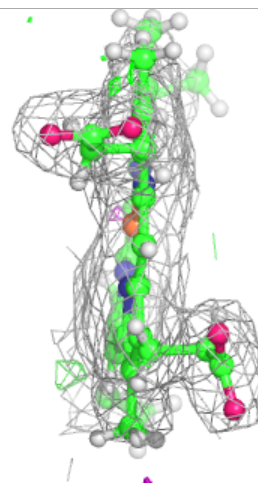
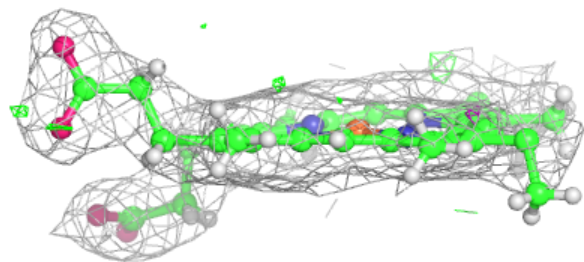
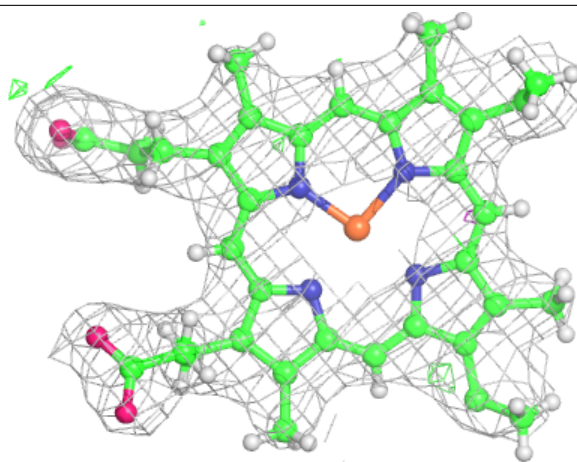
**Electron density around HEM f 101:**

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



**Electron density around HEC V 201:**

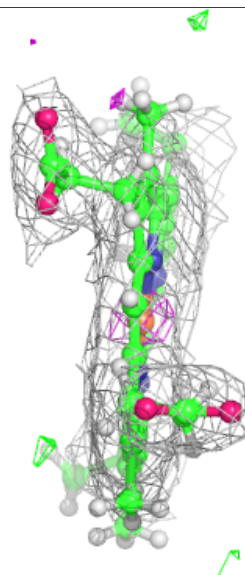
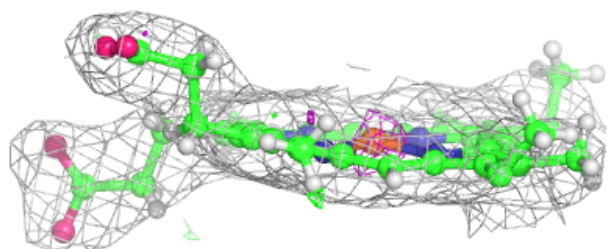
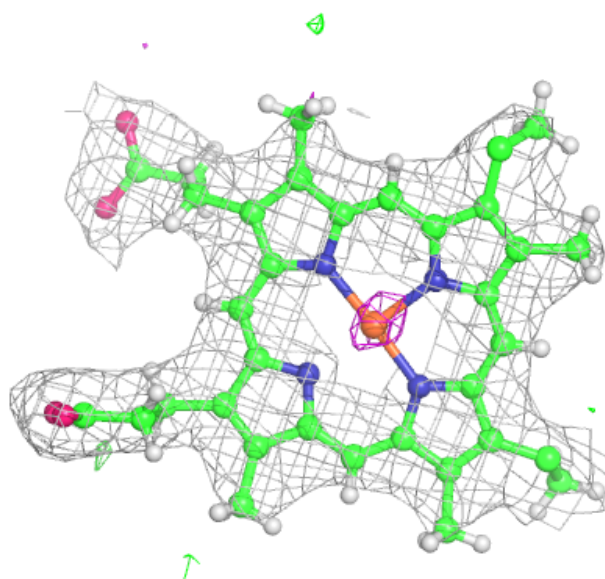
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC v 201:**

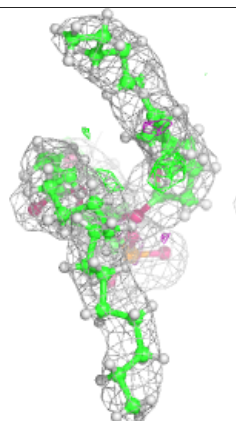
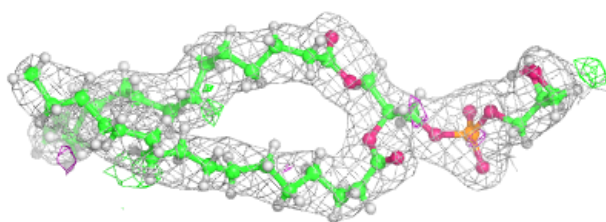
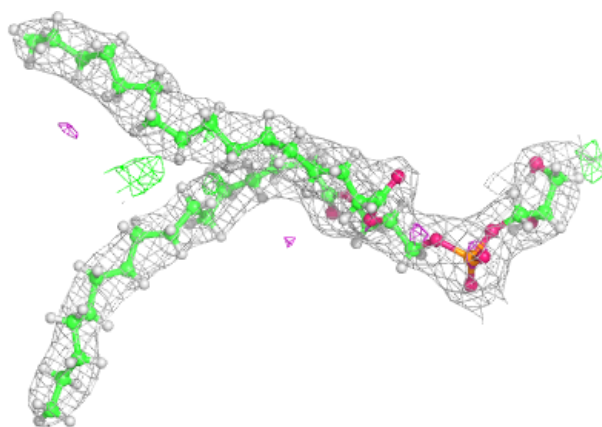
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





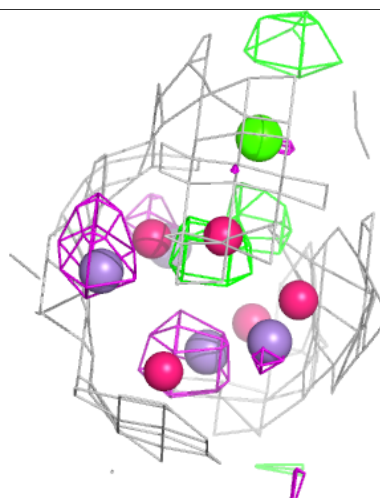
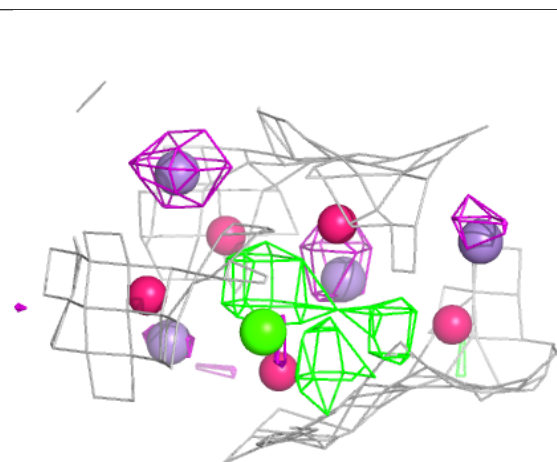
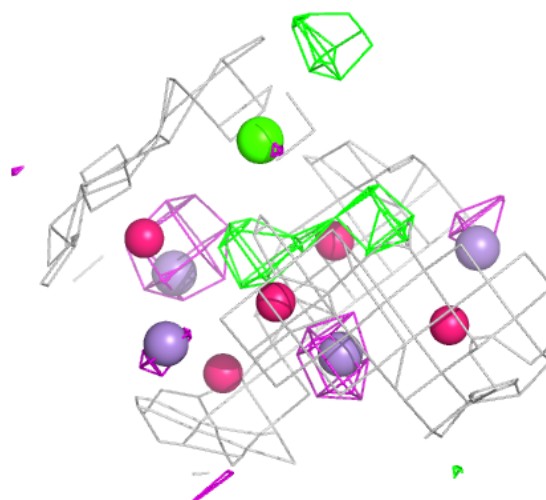
**Electron density around LHG D 408:**

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



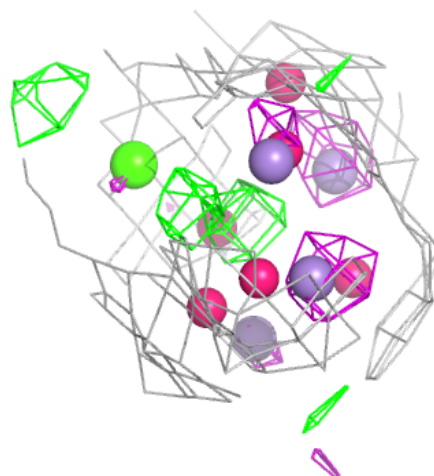
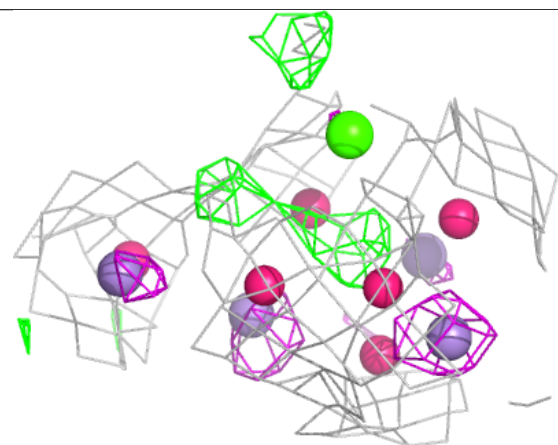
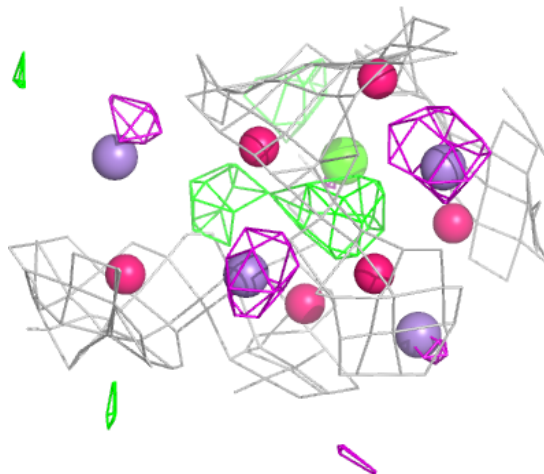
**Electron density around OEX A 416 (A):**

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



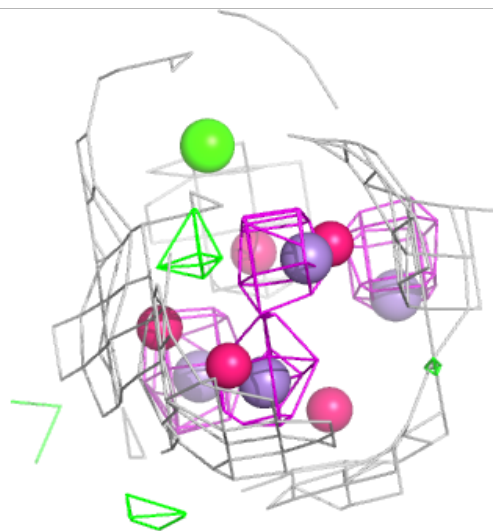
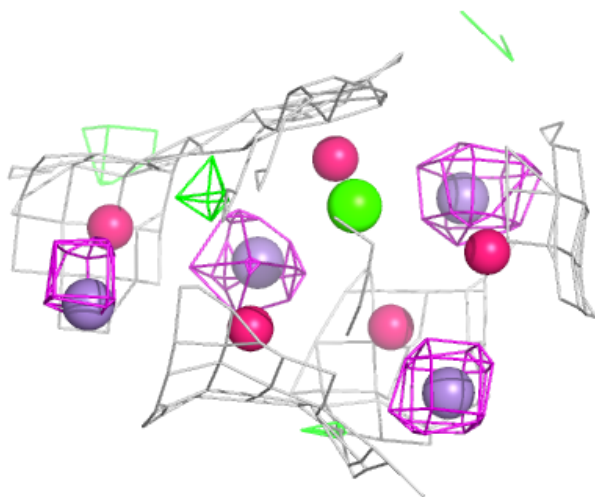
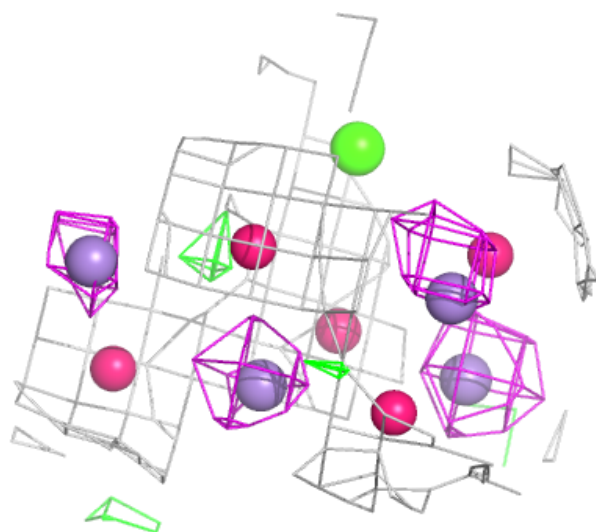
**Electron density around OEY A 415 (B):**

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



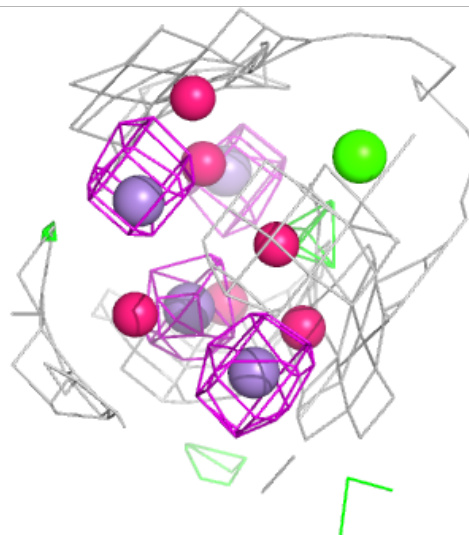
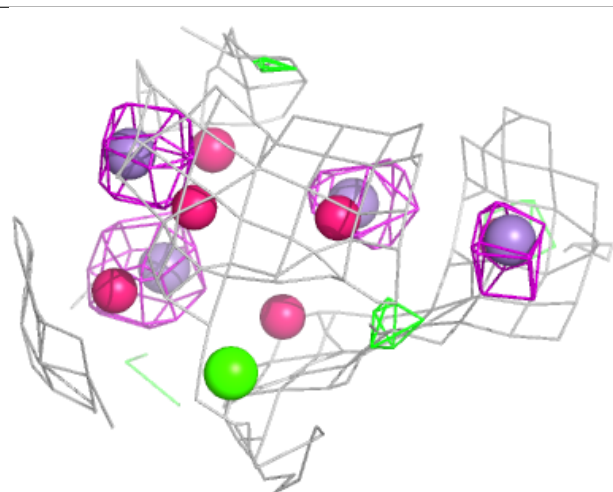
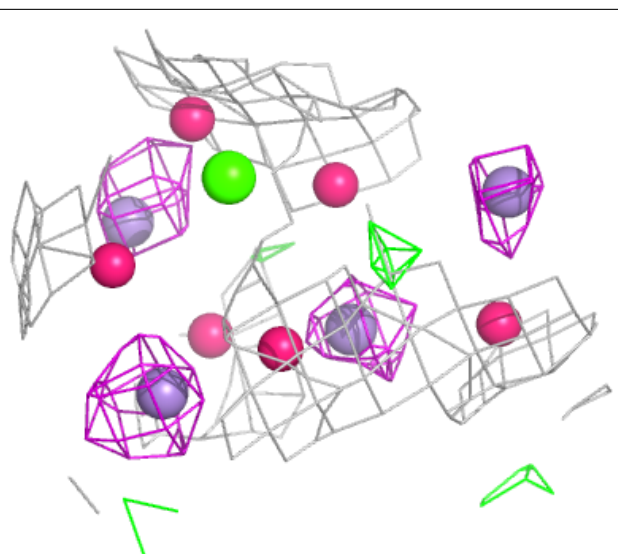
**Electron density around OEX a 416 (A):**

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



**Electron density around OEY a 415 (B):**

$2mF_o-DF_c$  (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.