



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2021 – 04:45 PM EDT

PDB ID : 7RF2
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 2.08 Angstrom
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 : 2.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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

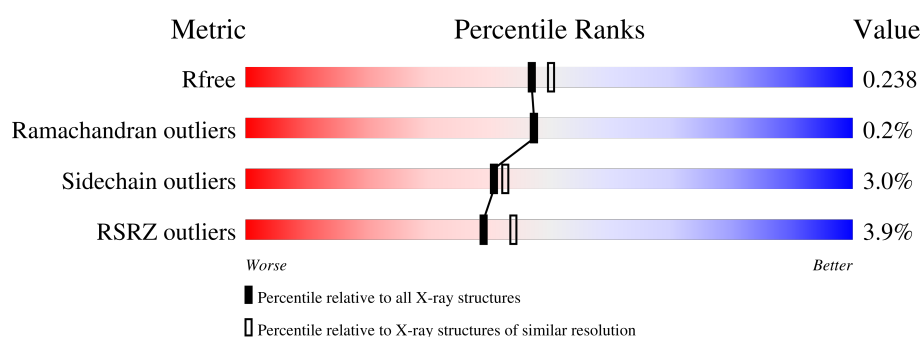
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



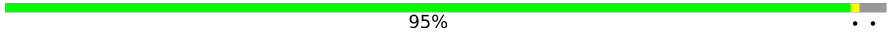
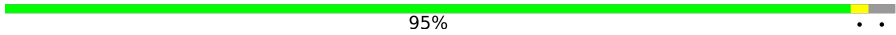
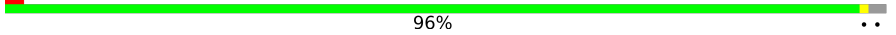
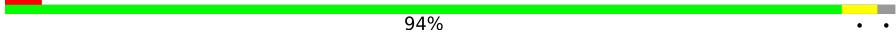


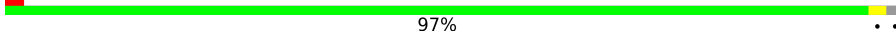







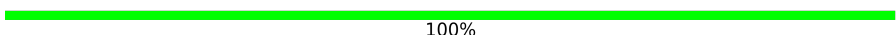

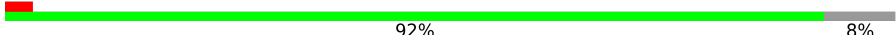








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	










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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	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	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	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	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	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	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 [i](#)

There are 36 unique types of molecules in this entry. The entry contains 103670 atoms, of which 51532 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5128	1714	2509	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			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	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	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			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			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			

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			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
			2137	675	1073	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2137	675	1073	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			

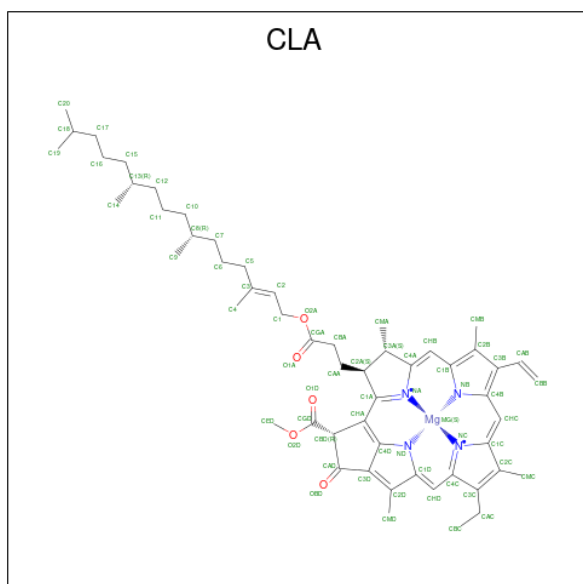
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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: C₅₅H₇₂MgN₄O₅).



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

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

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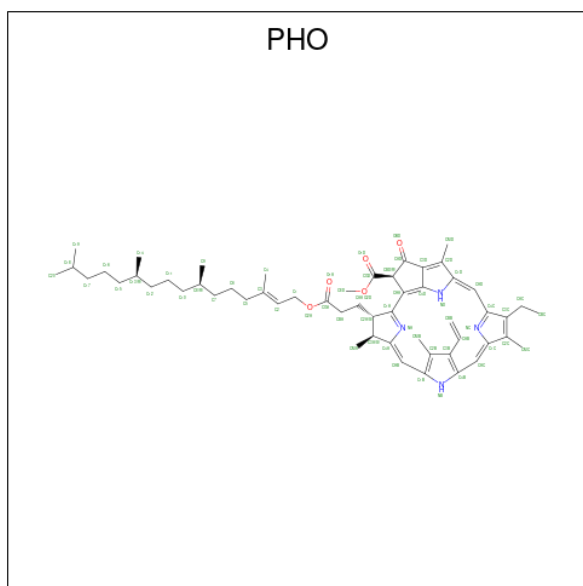
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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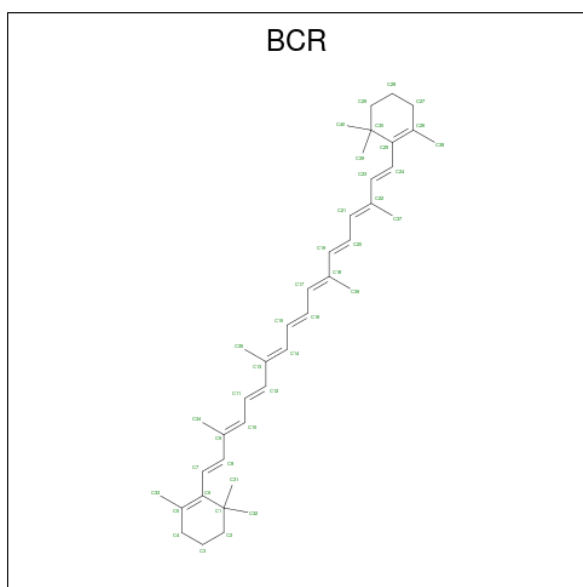
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	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	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

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



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

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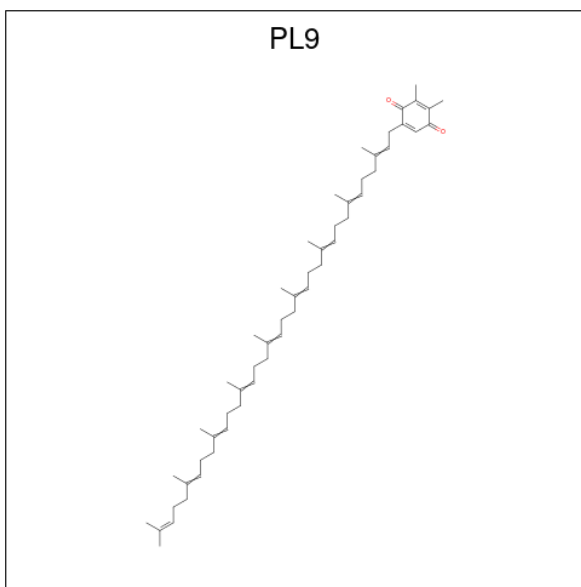
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

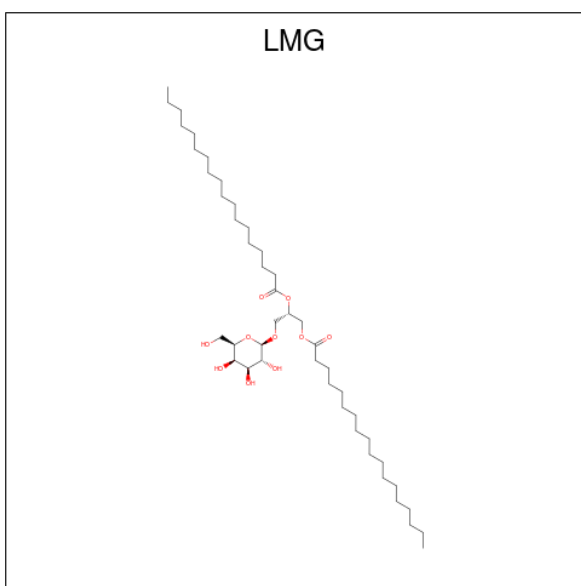
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



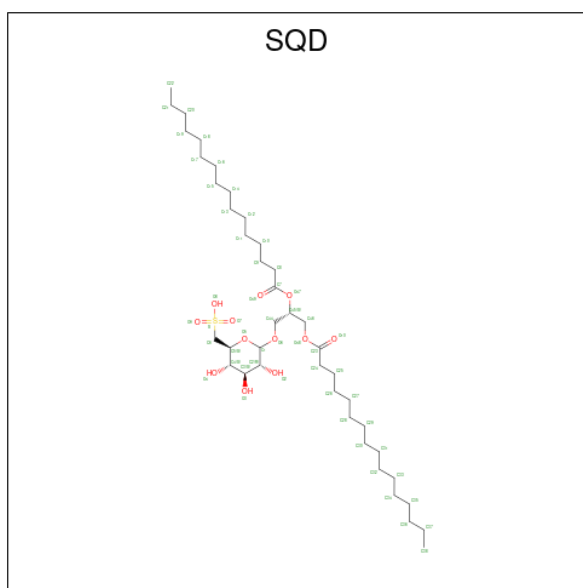
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



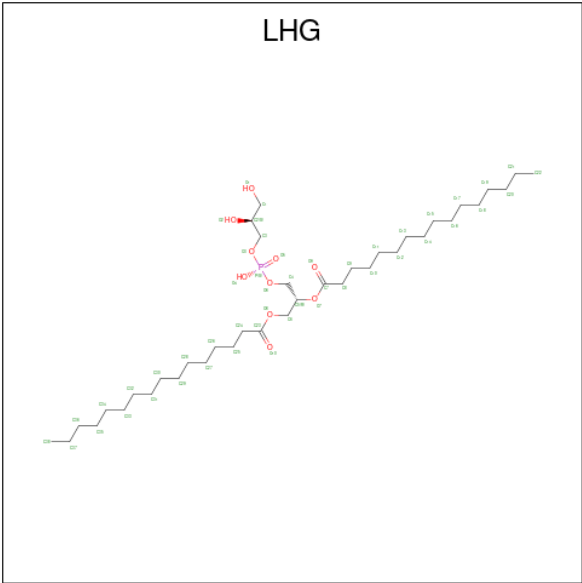
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			77	27	45	5		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	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	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	h	1	Total	C	H	O	0	0
			57	21	34	2		
27	m	1	Total	C	H	O	0	0
			123	41	72	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: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	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	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	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



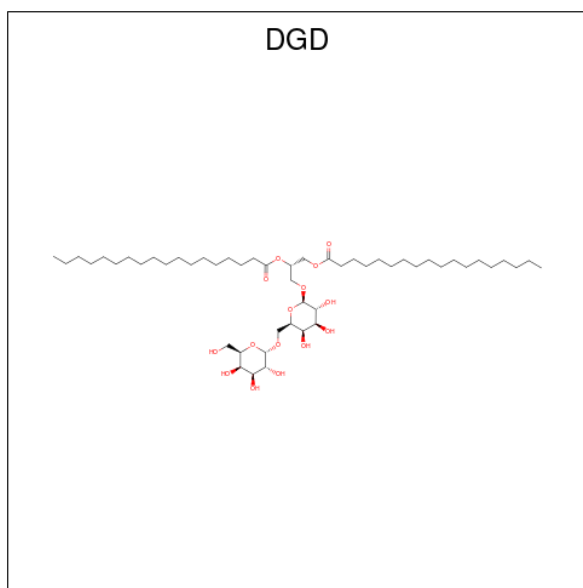
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



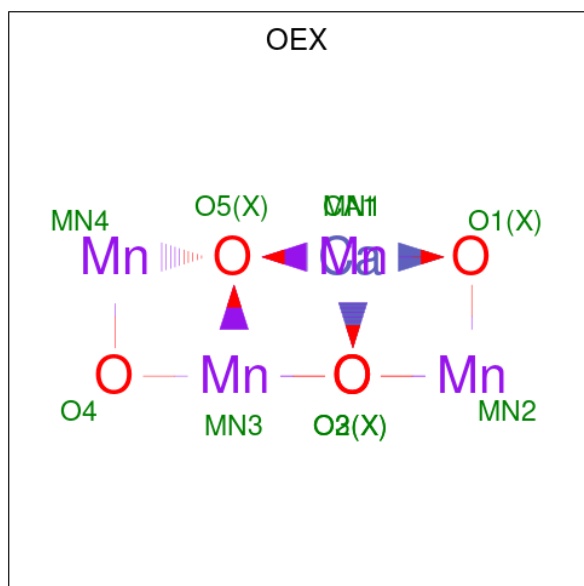
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		

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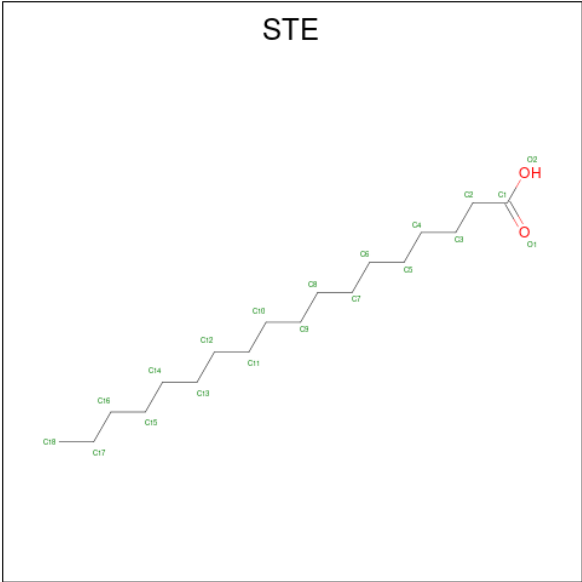
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			143	47	81	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		
30	o	1	Total	C	H	O	0	0
			119	39	75	5		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: $\text{C}_{18}\text{H}_{36}\text{O}_2$).



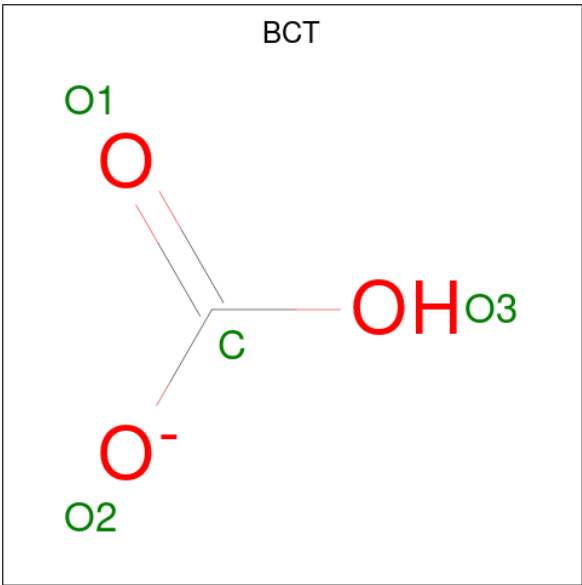
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			34	12	20	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	O		0	0
			16	14	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	D	1	Total	C	O		0	0
			15	13	2			
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			

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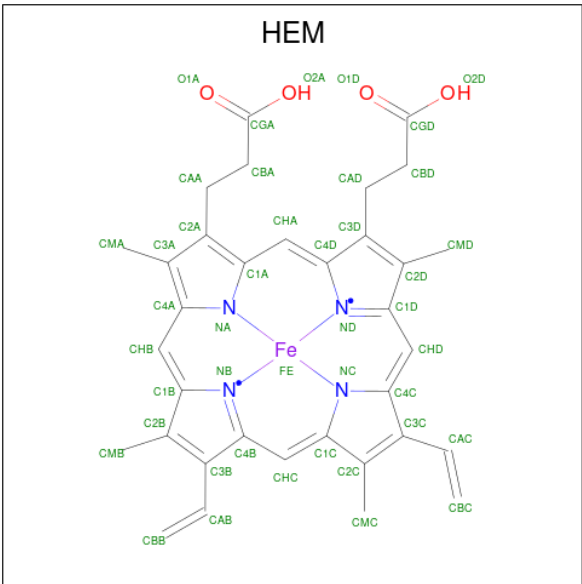
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total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

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



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

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



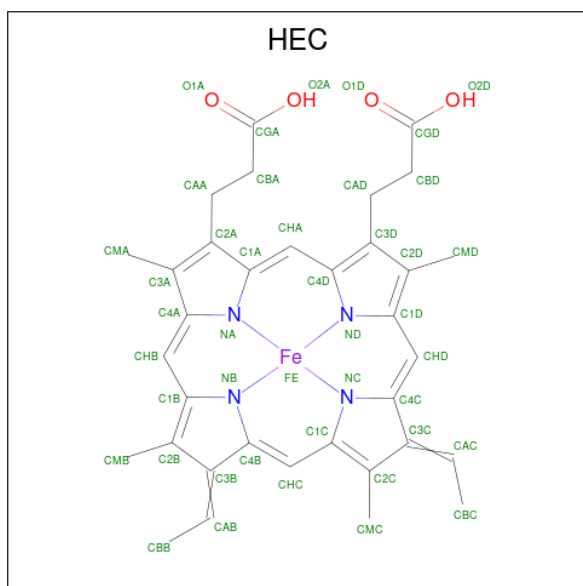
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	204	Total	O	0	0
			204	204		
36	C	182	Total	O	0	0
			182	182		
36	D	136	Total	O	0	0
			136	136		
36	E	30	Total	O	0	0
			30	30		
36	F	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	H	37	Total 37	O 37	0	0
36	I	10	Total 10	O 10	0	0
36	J	16	Total 16	O 16	0	0
36	K	8	Total 8	O 8	0	0
36	L	8	Total 8	O 8	0	0
36	M	7	Total 7	O 7	0	0
36	O	90	Total 90	O 90	0	0
36	T	10	Total 10	O 10	0	0
36	U	52	Total 52	O 52	0	0
36	V	65	Total 65	O 65	0	0
36	X	12	Total 12	O 12	0	0
36	Y	6	Total 6	O 6	0	0
36	Z	2	Total 2	O 2	0	0
36	a	126	Total 126	O 126	0	0
36	b	206	Total 206	O 206	0	0
36	c	181	Total 181	O 181	0	0
36	d	111	Total 111	O 111	0	0
36	e	21	Total 21	O 21	0	0
36	f	8	Total 8	O 8	0	0
36	h	36	Total 36	O 36	0	0
36	i	13	Total 13	O 13	0	0

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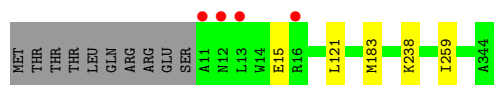
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	8	Total 8	O 8	0	0
36	k	6	Total 6	O 6	0	0
36	l	7	Total 7	O 7	0	0
36	m	6	Total 6	O 6	0	0
36	o	102	Total 102	O 102	0	0
36	r	3	Total 3	O 3	0	0
36	t	8	Total 8	O 8	0	0
36	u	58	Total 58	O 58	0	0
36	v	56	Total 56	O 56	0	0
36	x	8	Total 8	O 8	0	0
36	y	3	Total 3	O 3	0	0
36	z	9	Total 9	O 9	0	0

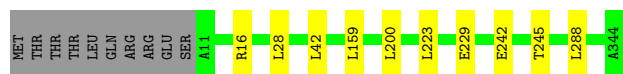
3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



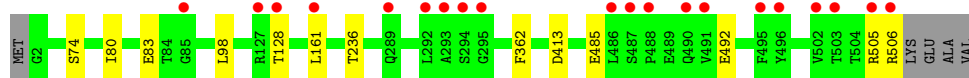
- Molecule 1: Photosystem II protein D1 1



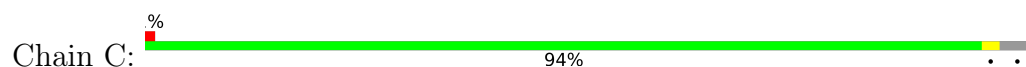
- Molecule 2: Photosystem II CP47 reaction center protein



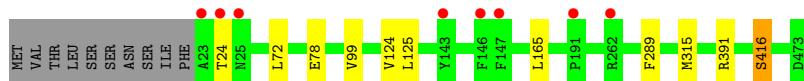
- Molecule 2: Photosystem II CP47 reaction center protein



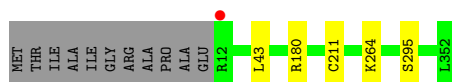
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



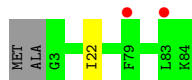
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



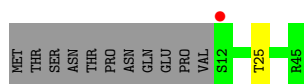
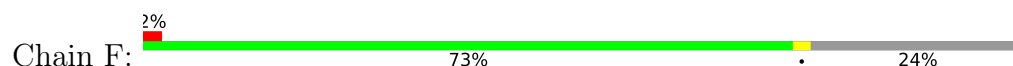
- Molecule 5: Cytochrome b559 subunit alpha



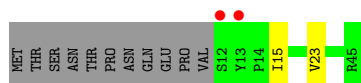
- Molecule 5: Cytochrome b559 subunit alpha



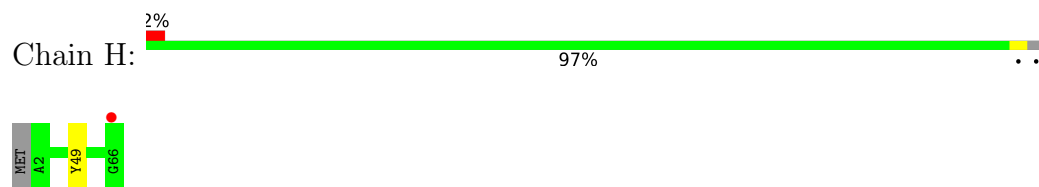
- Molecule 6: Cytochrome b559 subunit beta



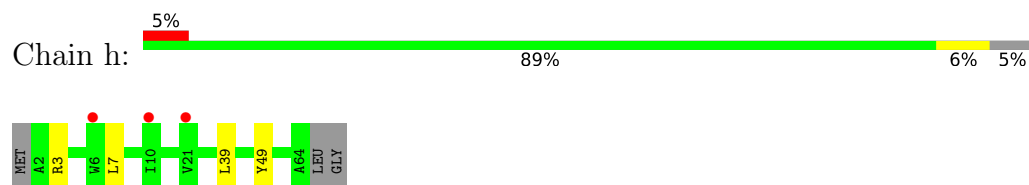
- Molecule 6: Cytochrome b559 subunit beta



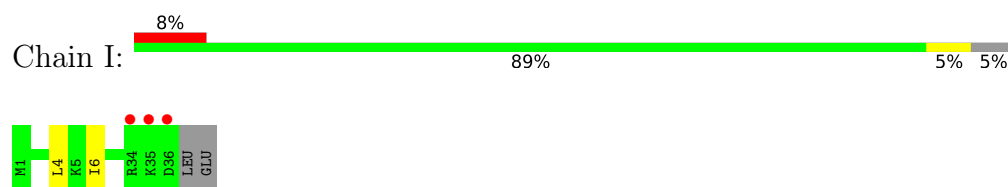
- Molecule 7: Photosystem II reaction center protein H



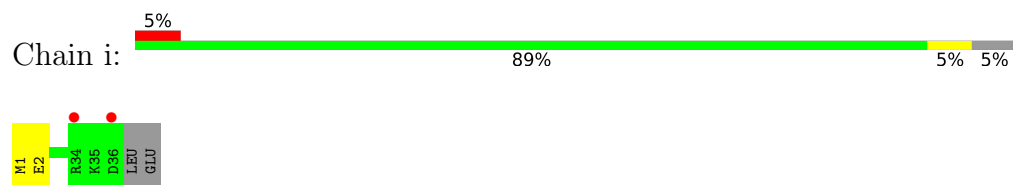
- Molecule 7: Photosystem II reaction center protein H



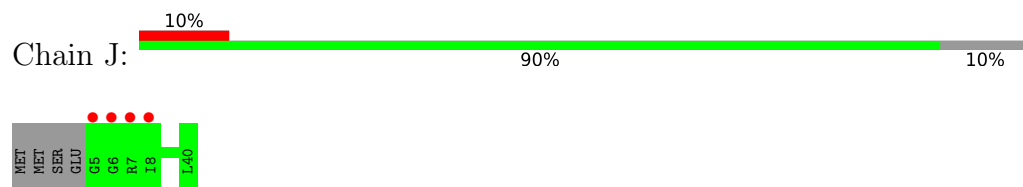
- Molecule 8: Photosystem II reaction center protein I



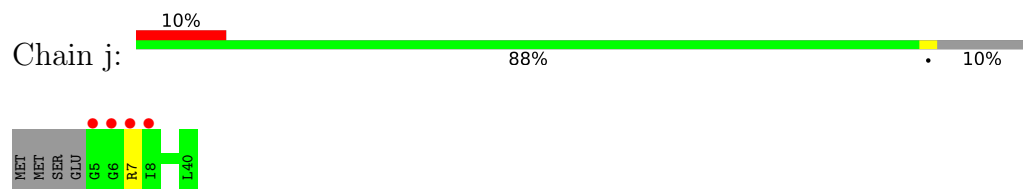
- Molecule 8: Photosystem II reaction center protein I



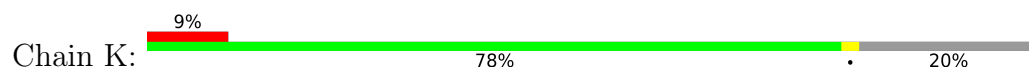
- Molecule 9: Photosystem II reaction center protein J

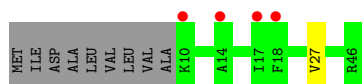


- Molecule 9: Photosystem II reaction center protein J

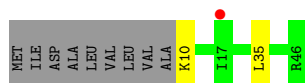
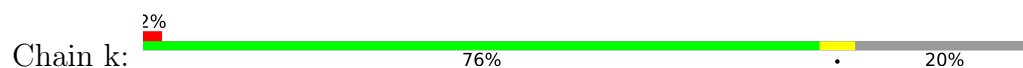


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

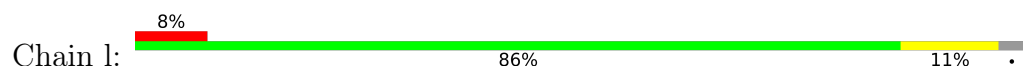


- Molecule 11: Photosystem II reaction center protein L

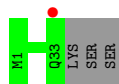


There are no outlier residues recorded for this chain.

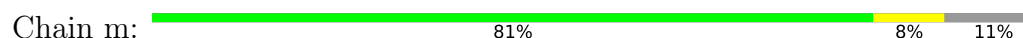
- Molecule 11: Photosystem II reaction center protein L



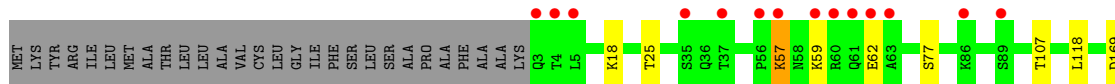
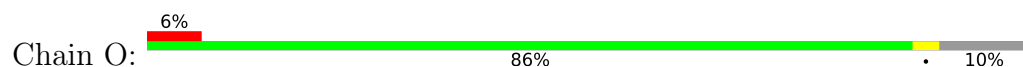
- Molecule 12: Photosystem II reaction center protein M



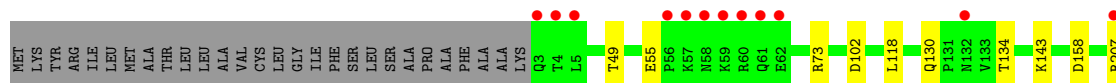
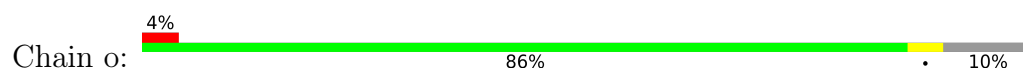
- Molecule 12: Photosystem II reaction center protein M



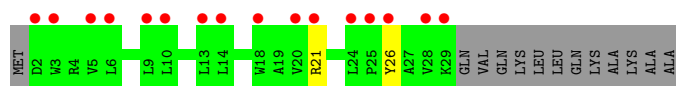
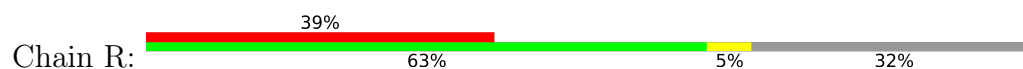
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



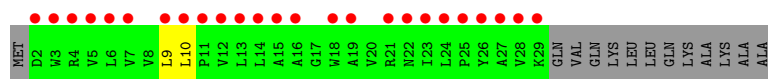
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



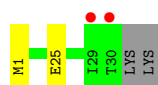
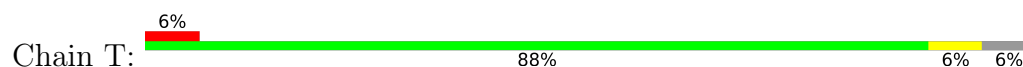
- Molecule 14: Photosystem II protein Y



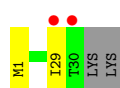
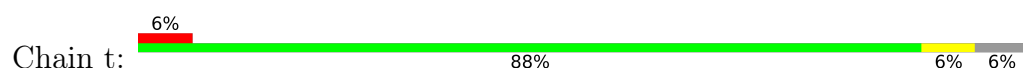
- Molecule 14: Photosystem II protein Y



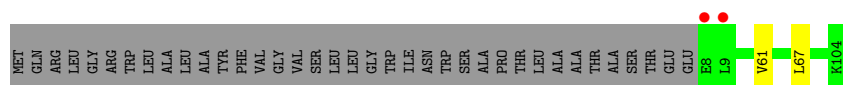
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

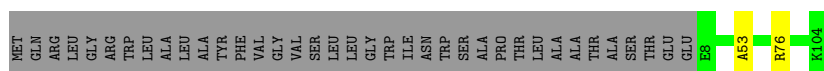


- Molecule 16: Photosystem II 12 kDa extrinsic protein

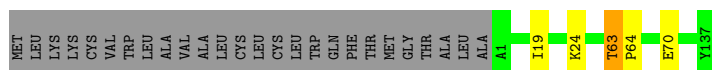
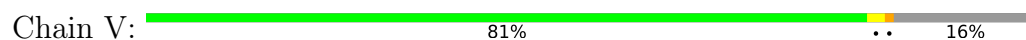


- Molecule 16: Photosystem II 12 kDa extrinsic protein

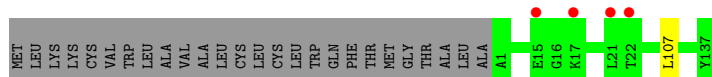
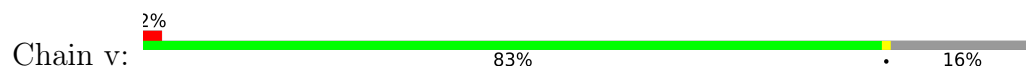




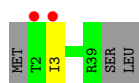
- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550



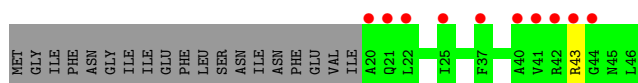
- Molecule 18: Photosystem II reaction center X protein



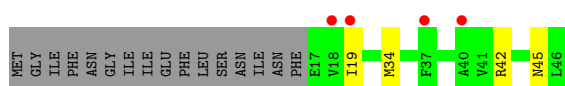
- Molecule 18: Photosystem II reaction center X protein



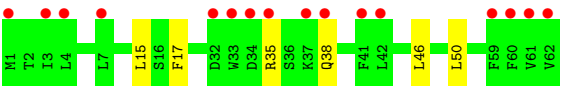
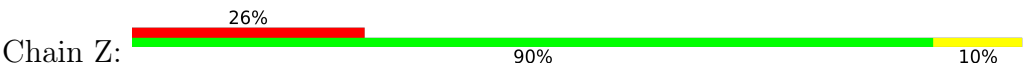
- Molecule 19: Photosystem II reaction center protein Ycf12



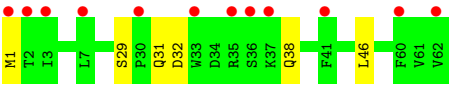
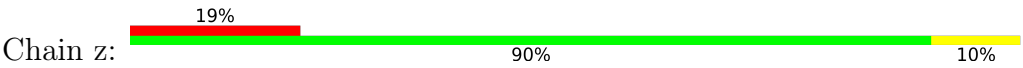
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.1 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.238 0.185 , 0.238	Depositor DCC
R_{free} test set	4226 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103670	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2707	0.66	1/3692 (0.0%)
1	a	0.62	0/2704	0.66	0/3688
2	B	0.61	0/4161	0.66	0/5669
2	b	0.60	0/4118	0.66	0/5611
3	C	0.59	0/3547	0.65	0/4830
3	c	0.57	0/3619	0.64	0/4926
4	D	0.63	1/2812 (0.0%)	0.67	0/3832
4	d	0.59	0/2821	0.65	0/3844
5	E	0.59	0/688	0.67	0/940
5	e	0.54	0/683	0.63	0/932
6	F	0.65	0/284	0.62	0/387
6	f	0.47	0/284	0.66	0/387
7	H	0.72	0/523	0.70	0/713
7	h	0.69	0/511	0.72	0/697
8	I	0.67	0/293	0.70	0/396
8	i	0.75	0/293	0.75	0/396
9	J	0.59	0/263	0.65	0/356
9	j	0.59	0/263	0.70	0/356
10	K	0.53	0/303	0.64	0/416
10	k	0.55	0/303	0.67	0/416
11	L	0.71	0/311	0.72	0/422
11	l	0.76	0/303	0.75	0/412
12	M	0.76	0/249	0.79	0/341
12	m	0.72	0/244	0.72	0/334
13	O	0.69	1/1904 (0.1%)	0.78	1/2585 (0.0%)
13	o	0.65	0/1905	0.79	2/2583 (0.1%)
14	R	0.48	0/227	0.60	0/313
14	r	0.44	0/227	0.59	0/313
15	T	0.78	0/257	0.74	0/349
15	t	0.77	0/255	0.69	0/346
16	U	0.61	0/785	0.70	0/1064
16	u	0.71	0/785	0.76	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.65	0/1085	0.76	1/1473 (0.1%)
17	v	0.62	0/1085	0.66	0/1473
18	X	0.56	0/284	0.65	0/384
18	x	0.46	0/289	0.59	0/391
19	Y	0.50	0/197	0.67	0/264
19	y	0.45	0/219	0.58	0/294
20	Z	0.51	0/490	0.57	0/669
20	z	0.48	0/488	0.56	0/666
All	All	0.61	2/42769 (0.0%)	0.68	5/58224 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	211	CYS	CB-SG	-5.97	1.72	1.81
13	O	77	SER	CB-OG	-5.16	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-7.21	104.74	120.60
13	O	169	ASP	CB-CG-OD1	6.47	124.12	118.30
13	o	158	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	183	MET	CA-CB-CG	5.56	122.75	113.30
13	o	102	ASP	CB-CG-OD1	5.01	122.81	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	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	41	39
1	a	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	47	47
3	c	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	47	47
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	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%)	226 (93%)	14 (6%)	3 (1%)	13	7
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	31
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	17
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	3	1
19	y	28/46 (61%)	24 (86%)	3 (11%)	1 (4%)	3	1
20	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5231/5700 (92%)	5092 (97%)	128 (2%)	11 (0%)	47	47

5 of 11 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	267 (99%)	3 (1%)	73	78
1	a	269/280 (96%)	259 (96%)	10 (4%)	34	34
2	B	408/407 (100%)	401 (98%)	7 (2%)	60	65
2	b	402/407 (99%)	389 (97%)	13 (3%)	39	40
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	53
3	c	354/362 (98%)	342 (97%)	12 (3%)	37	37
4	D	276/283 (98%)	272 (99%)	4 (1%)	67	72
4	d	277/283 (98%)	269 (97%)	8 (3%)	42	44
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	46
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	29
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	35
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	11
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	41
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	29
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	39
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	12
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	200 (97%)	6 (3%)	42	44
13	o	207/228 (91%)	200 (97%)	7 (3%)	37	37
14	R	22/33 (67%)	20 (91%)	2 (9%)	9	6
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	33
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	52
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	65
17	v	117/138 (85%)	116 (99%)	1 (1%)	78	83
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	40
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	13
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
All	All	4321/4654 (93%)	4188 (97%)	133 (3%)	41	41

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	134	THR
14	r	10	LEU
20	z	32	ASP
20	Z	50	LEU
20	Z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
16	u	37	GLN
5	e	60	GLN
1	a	181	ASN
4	d	338	ASN
20	Z	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.13	1 (12%)	7,9,11	0.53	0
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.97	0
8	FME	i	1	8	8,9,10	1.27	1 (12%)	7,9,11	1.04	0
15	FME	T	1	15	8,9,10	1.13	1 (12%)	7,9,11	0.77	0
12	FME	M	1	12	8,9,10	1.00	0	7,9,11	0.67	0
15	FME	t	1	15	8,9,10	1.26	2 (25%)	7,9,11	0.99	0

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.98	1.42	1.46
12	m	1	FME	CA-N	-2.43	1.42	1.46
15	t	1	FME	CA-N	-2.23	1.43	1.46
15	t	1	FME	CB-CA	2.19	1.57	1.53
15	T	1	FME	CN-N	2.08	1.40	1.33

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 6 are monoatomic - leaving 181 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	510	-	56,73,73	1.52	9 (16%)	55,113,113	1.46	8 (14%)
22	CLA	b	605	-	56,73,73	1.54	7 (12%)	55,113,113	1.76	15 (27%)
22	CLA	A	406	-	45,62,73	1.94	10 (22%)	41,99,113	2.06	11 (26%)
29	LHG	d	409	-	38,38,48	1.00	2 (5%)	41,44,54	1.05	4 (9%)
22	CLA	B	615	-	56,73,73	1.61	10 (17%)	55,113,113	1.47	9 (16%)
32	STE	D	412	-	16,19,19	0.31	0	15,19,19	0.88	0
34	HEM	F	101	5,6	27,50,50	1.96	4 (14%)	17,82,82	2.07	7 (41%)
28	SQD	A	412	-	51,52,54	1.08	5 (9%)	60,63,65	1.68	8 (13%)
29	LHG	d	408	-	48,48,48	0.90	1 (2%)	51,54,54	1.13	2 (3%)
32	STE	b	626	-	9,9,19	0.48	0	8,8,19	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
32	STE	B	623	-	8,11,19	0.40	0	7,11,19	0.89	0
22	CLA	b	612	-	56,73,73	1.40	4 (7%)	55,113,113	1.72	12 (21%)
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.11	4 (7%)
22	CLA	b	616	-	51,68,73	1.58	9 (17%)	49,107,113	2.03	11 (22%)
32	STE	B	626	-	8,11,19	0.34	0	7,11,19	0.69	0
22	CLA	b	608	-	56,73,73	1.65	8 (14%)	55,113,113	1.85	13 (23%)
32	STE	b	622	-	16,19,19	0.38	0	15,19,19	0.81	0
22	CLA	b	611	-	56,73,73	1.48	7 (12%)	55,113,113	1.85	7 (12%)
32	STE	T	102	-	14,14,19	0.41	0	13,13,19	0.82	0
24	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.55	11 (19%)
32	STE	M	102	-	11,14,19	0.60	0	10,14,19	0.46	0
32	STE	C	520	-	8,11,19	0.37	0	7,11,19	0.89	0
32	STE	E	101	-	8,11,19	0.57	0	7,11,19	0.32	0
22	CLA	b	615	-	56,73,73	2.01	8 (14%)	55,113,113	1.70	8 (14%)
29	LHG	A	413	-	48,48,48	0.98	3 (6%)	51,54,54	1.18	2 (3%)
28	SQD	f	102	-	40,41,54	1.15	4 (10%)	49,52,65	1.99	11 (22%)
22	CLA	B	601	36	56,73,73	1.93	9 (16%)	55,113,113	1.67	7 (12%)
30	DGD	o	301	-	43,43,67	1.11	2 (4%)	45,45,81	1.48	5 (11%)
22	CLA	c	505	-	56,73,73	1.46	5 (8%)	55,113,113	1.68	10 (18%)
24	BCR	C	514	-	41,41,41	1.21	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	B	606	-	56,73,73	1.59	8 (14%)	55,113,113	1.75	12 (21%)
32	STE	c	520	-	16,19,19	0.37	0	15,19,19	0.69	0
22	CLA	c	502	-	56,73,73	1.64	10 (17%)	55,113,113	1.64	11 (20%)
24	BCR	b	617	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	8 (14%)
26	PL9	D	406	-	55,55,55	1.46	6 (10%)	68,69,69	1.71	16 (23%)
22	CLA	C	504	36	50,67,73	1.65	8 (16%)	47,105,113	1.68	13 (27%)
30	DGD	C	515	-	63,63,67	1.64	14 (22%)	77,77,81	1.47	12 (15%)
22	CLA	c	509	-	56,73,73	1.47	5 (8%)	55,113,113	1.93	11 (20%)
32	STE	j	101	-	8,11,19	0.56	0	7,11,19	0.55	0
22	CLA	D	403	36	56,73,73	1.59	5 (8%)	55,113,113	1.65	9 (16%)
22	CLA	B	611	-	56,73,73	1.61	10 (17%)	55,113,113	1.68	13 (23%)
22	CLA	A	402	-	56,73,73	1.50	8 (14%)	55,113,113	1.64	10 (18%)
27	LMG	a	414	-	49,49,55	1.00	5 (10%)	57,57,63	1.33	7 (12%)
28	SQD	F	102	-	35,36,54	0.99	3 (8%)	42,45,65	1.96	10 (23%)
24	BCR	K	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	M	101	-	51,51,55	1.10	2 (3%)	59,59,63	1.43	7 (11%)
22	CLA	D	404	-	56,73,73	1.54	8 (14%)	55,113,113	1.35	6 (10%)
22	CLA	D	402	-	56,73,73	1.42	5 (8%)	55,113,113	1.67	11 (20%)
32	STE	c	522	-	8,11,19	0.40	0	7,11,19	0.84	0
24	BCR	B	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	7 (12%)
27	LMG	c	521	-	48,48,55	1.24	6 (12%)	56,56,63	1.19	4 (7%)
22	CLA	c	508	-	55,72,73	1.60	7 (12%)	53,111,113	1.61	11 (20%)
27	LMG	m	101	-	51,51,55	1.12	6 (11%)	59,59,63	1.48	11 (18%)
22	CLA	c	507	36	56,73,73	1.57	10 (17%)	55,113,113	1.58	10 (18%)
24	BCR	K	102	-	41,41,41	1.02	2 (4%)	56,56,56	1.16	3 (5%)
33	BCT	D	401	21	0,3,3	-	-	0,3,3	-	-
24	BCR	c	515	-	41,41,41	1.26	4 (9%)	56,56,56	1.28	5 (8%)
22	CLA	B	612	-	56,73,73	1.54	6 (10%)	55,113,113	1.81	11 (20%)
26	PL9	d	407	-	55,55,55	1.54	8 (14%)	68,69,69	1.83	15 (22%)
28	SQD	b	620	-	48,49,54	0.94	2 (4%)	57,60,65	2.39	14 (24%)
22	CLA	C	503	-	56,73,73	1.85	10 (17%)	55,113,113	1.70	11 (20%)
22	CLA	c	506	-	56,73,73	1.63	7 (12%)	55,113,113	1.46	7 (12%)
27	LMG	b	623	-	55,55,55	1.02	4 (7%)	63,63,63	1.74	11 (17%)
22	CLA	a	403	36	56,73,73	1.55	6 (10%)	55,113,113	1.65	11 (20%)
22	CLA	C	502	-	56,73,73	1.73	6 (10%)	55,113,113	1.48	9 (16%)
30	DGD	A	415	-	67,67,67	1.41	10 (14%)	81,81,81	1.50	16 (19%)
26	PL9	a	409	-	55,55,55	1.30	3 (5%)	68,69,69	1.84	16 (23%)
22	CLA	b	601	36	56,73,73	1.79	9 (16%)	55,113,113	1.66	9 (16%)
24	BCR	d	406	-	41,41,41	1.25	2 (4%)	56,56,56	1.22	5 (8%)
23	PHO	a	404	-	67,69,69	1.07	8 (11%)	85,99,99	1.17	8 (9%)
24	BCR	T	101	-	41,41,41	1.22	4 (9%)	56,56,56	1.14	3 (5%)
27	LMG	D	410	-	31,31,55	1.17	3 (9%)	33,33,63	1.13	1 (3%)
22	CLA	C	509	-	56,73,73	1.54	8 (14%)	55,113,113	1.63	7 (12%)
22	CLA	B	603	-	56,73,73	1.49	9 (16%)	55,113,113	1.53	10 (18%)
22	CLA	B	613	-	56,73,73	1.67	8 (14%)	55,113,113	1.78	10 (18%)
22	CLA	a	402	-	56,73,73	1.71	6 (10%)	55,113,113	1.65	10 (18%)
22	CLA	b	613	-	56,73,73	1.71	7 (12%)	55,113,113	1.85	12 (21%)
24	BCR	B	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
22	CLA	b	609	-	56,73,73	1.66	10 (17%)	55,113,113	1.55	10 (18%)
24	BCR	k	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	B	624	-	14,17,19	0.43	0	13,17,19	0.82	0
22	CLA	B	608	-	56,73,73	1.78	9 (16%)	55,113,113	1.61	9 (16%)
32	STE	C	519	-	15,15,19	0.67	0	14,14,19	0.27	0
30	DGD	H	102	-	63,63,67	1.32	8 (12%)	77,77,81	1.57	13 (16%)
24	BCR	k	101	-	41,41,41	1.01	3 (7%)	56,56,56	1.07	3 (5%)
32	STE	a	413	-	9,9,19	0.60	0	8,8,19	0.38	0
35	HEC	v	201	17	26,50,50	2.46	7 (26%)	18,82,82	2.14	6 (33%)
30	DGD	c	517	-	63,63,67	1.17	8 (12%)	77,77,81	1.39	10 (12%)
29	LHG	a	410	-	48,48,48	1.01	4 (8%)	51,54,54	1.42	6 (11%)
22	CLA	C	507	36	56,73,73	1.62	7 (12%)	55,113,113	1.92	13 (23%)
32	STE	C	518	-	8,11,19	0.44	0	7,11,19	0.73	0
23	PHO	A	405	-	67,69,69	1.22	8 (11%)	85,99,99	1.14	6 (7%)
22	CLA	C	513	-	56,73,73	1.62	9 (16%)	55,113,113	1.65	9 (16%)
22	CLA	b	606	-	56,73,73	1.83	8 (14%)	55,113,113	1.73	12 (21%)
22	CLA	b	603	-	56,73,73	1.60	7 (12%)	55,113,113	1.72	12 (21%)
30	DGD	C	517	-	63,63,67	1.27	7 (11%)	77,77,81	1.40	10 (12%)
28	SQD	a	411	-	53,54,54	0.99	5 (9%)	62,65,65	2.21	15 (24%)
32	STE	m	102	-	8,11,19	0.48	0	7,11,19	0.80	0
29	LHG	L	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	3 (5%)
27	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.38	7 (15%)
24	BCR	b	618	-	41,41,41	1.20	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	b	610	36	56,73,73	1.45	8 (14%)	55,113,113	1.59	12 (21%)
32	STE	d	411	-	13,16,19	0.38	0	12,16,19	0.72	0
32	STE	B	627	-	12,15,19	0.40	0	11,15,19	0.88	0
22	CLA	d	405	-	56,73,73	1.57	8 (14%)	55,113,113	1.48	12 (21%)
22	CLA	c	503	-	56,73,73	1.55	8 (14%)	55,113,113	1.75	15 (27%)
32	STE	a	415	-	8,11,19	0.38	0	7,11,19	0.86	0
22	CLA	b	614	-	56,73,73	1.58	9 (16%)	55,113,113	1.38	9 (16%)
27	LMG	Y	101	-	48,48,55	0.95	2 (4%)	56,56,63	1.47	10 (17%)
26	PL9	A	410	-	55,55,55	0.87	2 (3%)	68,69,69	1.53	15 (22%)
22	CLA	B	604	-	56,73,73	1.42	6 (10%)	55,113,113	1.97	14 (25%)
24	BCR	A	407	-	41,41,41	1.18	3 (7%)	56,56,56	1.40	8 (14%)
24	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	6 (10%)
28	SQD	a	412	-	35,35,54	1.23	2 (5%)	37,37,65	1.66	6 (16%)
32	STE	b	621	-	15,15,19	0.47	0	14,14,19	0.69	0
22	CLA	B	605	-	56,73,73	1.46	9 (16%)	55,113,113	1.87	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	A	404	-	67,69,69	1.24	11 (16%)	85,99,99	1.07	5 (5%)
32	STE	J	101	-	8,11,19	0.31	0	7,11,19	0.88	0
23	PHO	d	401	-	67,69,69	1.26	9 (13%)	85,99,99	1.28	9 (10%)
22	CLA	B	607	36	56,73,73	1.29	9 (16%)	55,113,113	1.63	9 (16%)
32	STE	B	622	-	10,13,19	0.42	0	9,13,19	0.80	0
22	CLA	c	511	3	56,73,73	1.87	7 (12%)	55,113,113	1.71	8 (14%)
24	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.24	7 (12%)
28	SQD	B	621	-	53,54,54	1.00	3 (5%)	62,65,65	1.80	12 (19%)
22	CLA	B	616	-	51,68,73	1.92	9 (17%)	49,107,113	1.93	12 (24%)
34	HEM	f	101	5,6	27,50,50	1.98	4 (14%)	17,82,82	2.34	5 (29%)
22	CLA	C	506	-	56,73,73	1.84	10 (17%)	55,113,113	1.52	9 (16%)
22	CLA	a	405	-	56,73,73	1.68	7 (12%)	55,113,113	1.67	12 (21%)
32	STE	H	103	-	17,17,19	0.39	0	16,16,19	0.84	0
22	CLA	C	511	3	56,73,73	1.60	7 (12%)	55,113,113	1.59	6 (10%)
33	BCT	d	402	21	0,3,3	-	-	0,3,3	-	-
27	LMG	A	411	-	48,48,55	1.02	1 (2%)	56,56,63	1.44	7 (12%)
22	CLA	B	614	-	56,73,73	1.67	7 (12%)	55,113,113	1.56	12 (21%)
24	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	9 (16%)
22	CLA	B	610	36	56,73,73	1.69	9 (16%)	55,113,113	1.72	12 (21%)
22	CLA	d	404	36	56,73,73	1.70	6 (10%)	55,113,113	1.85	10 (18%)
22	CLA	c	513	-	56,73,73	1.67	9 (16%)	55,113,113	1.38	8 (14%)
29	LHG	D	411	-	48,48,48	0.85	3 (6%)	51,54,54	1.36	8 (15%)
32	STE	B	620	-	13,16,19	0.52	0	12,16,19	0.61	0
29	LHG	D	409	-	46,46,48	0.95	3 (6%)	49,52,54	1.23	5 (10%)
31	OEX	a	416	36,3,1	0,15,15	-	-	-	-	-
30	DGD	c	516	-	63,63,67	1.38	6 (9%)	77,77,81	1.29	6 (7%)
22	CLA	c	501	-	56,73,73	1.55	6 (10%)	55,113,113	1.90	13 (23%)
27	LMG	d	410	-	44,44,55	1.23	5 (11%)	52,52,63	1.41	5 (9%)
27	LMG	h	102	-	18,21,55	0.70	0	16,20,63	0.92	0
31	OEX	A	416	36,3,1	0,15,15	-	-	-	-	-
30	DGD	C	516	-	63,63,67	1.28	7 (11%)	77,77,81	1.44	9 (11%)
30	DGD	h	103	-	63,63,67	1.23	8 (12%)	77,77,81	1.38	10 (12%)
22	CLA	c	512	-	56,73,73	1.54	7 (12%)	55,113,113	1.52	11 (20%)
32	STE	b	624	-	12,15,19	0.52	0	11,15,19	0.57	0
35	HEC	V	201	17	26,50,50	2.32	3 (11%)	18,82,82	2.04	5 (27%)
22	CLA	A	403	36	56,73,73	1.61	8 (14%)	55,113,113	1.54	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	602	-	56,73,73	1.67	9 (16%)	55,113,113	1.61	8 (14%)
22	CLA	c	510	-	56,73,73	1.57	8 (14%)	55,113,113	1.80	9 (16%)
29	LHG	D	408	-	48,48,48	0.96	2 (4%)	51,54,54	1.26	7 (13%)
32	STE	D	413	-	11,14,19	0.40	0	10,14,19	0.95	0
24	BCR	K	103	-	41,41,41	1.10	3 (7%)	56,56,56	1.31	10 (17%)
28	SQD	A	414	-	38,38,54	1.07	3 (7%)	40,40,65	1.34	3 (7%)
32	STE	M	104	-	17,17,19	0.36	0	16,16,19	0.86	0
22	CLA	B	609	-	56,73,73	1.44	9 (16%)	55,113,113	1.64	9 (16%)
24	BCR	a	406	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	5 (8%)
24	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	8 (14%)
22	CLA	b	607	36	56,73,73	1.59	9 (16%)	55,113,113	1.43	9 (16%)
22	CLA	d	403	-	56,73,73	1.50	7 (12%)	55,113,113	1.37	10 (18%)
22	CLA	b	604	-	56,73,73	1.77	6 (10%)	55,113,113	1.96	12 (21%)
30	DGD	c	518	-	63,63,67	1.21	6 (9%)	77,77,81	1.47	12 (15%)
32	STE	B	625	-	15,15,19	0.47	0	14,14,19	0.70	0
32	STE	d	412	-	16,19,19	0.51	0	15,19,19	0.52	0
32	STE	b	625	-	16,19,19	0.51	0	15,19,19	0.58	0
22	CLA	C	508	-	56,73,73	1.75	6 (10%)	55,113,113	1.69	10 (18%)
32	STE	I	101	-	14,14,19	0.58	0	13,13,19	0.35	0
29	LHG	e	101	-	41,41,48	0.98	3 (7%)	44,47,54	1.22	4 (9%)
22	CLA	C	501	-	56,73,73	1.85	10 (17%)	55,113,113	1.59	8 (14%)
24	BCR	D	405	-	41,41,41	1.22	2 (4%)	56,56,56	1.18	6 (10%)
32	STE	M	103	-	9,9,19	0.52	0	8,8,19	0.64	0
22	CLA	C	505	-	56,73,73	1.51	6 (10%)	55,113,113	1.83	11 (20%)
22	CLA	C	512	-	56,73,73	1.53	6 (10%)	55,113,113	1.50	11 (20%)
27	LMG	D	407	-	51,51,55	1.00	1 (1%)	59,59,63	1.33	8 (13%)
22	CLA	c	504	36	51,68,73	1.66	7 (13%)	49,107,113	1.72	11 (22%)
22	CLA	B	602	-	56,73,73	1.63	8 (14%)	55,113,113	1.70	9 (16%)

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	510	-	1/1/20/20	9/37/115/115	-
22	CLA	b	605	-	1/1/20/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	406	-	1/1/17/20	3/24/102/115	-
29	LHG	d	409	-	-	13/43/43/53	-
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
32	STE	D	412	-	-	7/15/17/17	-
34	HEM	F	101	5,6	-	0/6/54/54	-
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
29	LHG	d	408	-	-	21/53/53/53	-
32	STE	b	626	-	-	4/7/7/17	-
29	LHG	l	101	-	-	21/53/53/53	-
32	STE	B	623	-	-	3/7/9/17	-
22	CLA	b	612	-	1/1/20/20	7/37/115/115	-
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	b	616	-	1/1/19/20	13/31/109/115	-
32	STE	B	626	-	-	3/7/9/17	-
22	CLA	b	608	-	-	6/37/115/115	-
32	STE	b	622	-	-	10/15/17/17	-
22	CLA	b	611	-	1/1/20/20	7/37/115/115	-
32	STE	T	102	-	-	7/12/12/17	-
24	BCR	t	101	-	-	2/29/63/63	0/2/2/2
32	STE	M	102	-	-	5/10/12/17	-
32	STE	C	520	-	-	3/7/9/17	-
32	STE	E	101	-	-	4/7/9/17	-
22	CLA	b	615	-	1/1/20/20	9/37/115/115	-
29	LHG	A	413	-	-	29/53/53/53	-
28	SQD	f	102	-	-	18/36/56/69	0/1/1/1
22	CLA	B	601	36	1/1/20/20	20/37/115/115	-
30	DGD	o	301	-	-	20/45/45/95	-
22	CLA	c	505	-	1/1/20/20	8/37/115/115	-
24	BCR	C	514	-	-	11/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/20/20	15/37/115/115	-
32	STE	c	520	-	-	11/15/17/17	-
22	CLA	c	502	-	-	8/37/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	504	36	1/1/18/20	5/30/108/115	-
30	DGD	C	515	-	-	19/51/91/95	0/2/2/2
22	CLA	c	509	-	1/1/20/20	15/37/115/115	-
32	STE	j	101	-	-	3/7/9/17	-
22	CLA	D	403	36	-	9/37/115/115	-
22	CLA	B	611	-	1/1/20/20	6/37/115/115	-
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-
27	LMG	a	414	-	-	23/44/64/70	0/1/1/1
28	SQD	F	102	-	-	12/28/48/69	0/1/1/1
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
27	LMG	M	101	-	-	24/46/66/70	0/1/1/1
22	CLA	D	404	-	1/1/20/20	14/37/115/115	-
22	CLA	D	402	-	-	6/37/115/115	-
32	STE	c	522	-	-	4/7/9/17	-
24	BCR	B	619	-	-	3/29/63/63	0/2/2/2
27	LMG	c	521	-	-	25/43/63/70	0/1/1/1
22	CLA	c	508	-	-	9/36/114/115	-
27	LMG	m	101	-	-	16/46/66/70	0/1/1/1
22	CLA	c	507	36	1/1/20/20	11/37/115/115	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
24	BCR	c	515	-	-	2/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/20/20	11/37/115/115	-
26	PL9	d	407	-	-	13/53/73/73	0/1/1/1
28	SQD	b	620	-	-	23/44/64/69	0/1/1/1
22	CLA	C	503	-	1/1/20/20	5/37/115/115	-
22	CLA	c	506	-	1/1/20/20	15/37/115/115	-
27	LMG	b	623	-	-	24/50/70/70	0/1/1/1
22	CLA	a	403	36	1/1/20/20	15/37/115/115	-
22	CLA	C	502	-	1/1/20/20	10/37/115/115	-
30	DGD	A	415	-	-	34/55/95/95	0/2/2/2
26	PL9	a	409	-	-	20/53/73/73	0/1/1/1
22	CLA	b	601	36	1/1/20/20	20/37/115/115	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
23	PHO	a	404	-	-	7/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
27	LMG	D	410	-	-	13/33/33/70	-
22	CLA	C	509	-	1/1/20/20	14/37/115/115	-
22	CLA	B	603	-	1/1/20/20	13/37/115/115	-
22	CLA	B	613	-	1/1/20/20	13/37/115/115	-
22	CLA	a	402	-	1/1/20/20	5/37/115/115	-
22	CLA	b	613	-	1/1/20/20	7/37/115/115	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
22	CLA	b	609	-	-	9/37/115/115	-
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2
32	STE	B	624	-	-	11/13/15/17	-
22	CLA	B	608	-	-	3/37/115/115	-
32	STE	C	519	-	-	5/13/13/17	-
30	DGD	H	102	-	-	19/51/91/95	0/2/2/2
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2
32	STE	a	413	-	-	5/7/7/17	-
35	HEC	v	201	17	-	0/6/54/54	-
30	DGD	c	517	-	-	21/51/91/95	0/2/2/2
29	LHG	a	410	-	-	18/53/53/53	-
22	CLA	C	507	36	1/1/20/20	5/37/115/115	-
32	STE	C	518	-	-	4/7/9/17	-
23	PHO	A	405	-	-	1/53/103/103	0/5/6/6
22	CLA	C	513	-	1/1/20/20	15/37/115/115	-
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-
22	CLA	b	603	-	1/1/20/20	10/37/115/115	-
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
28	SQD	a	411	-	-	21/49/69/69	0/1/1/1
32	STE	m	102	-	-	1/7/9/17	-
29	LHG	L	101	-	-	20/53/53/53	-
27	LMG	c	519	-	-	11/31/51/70	0/1/1/1
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	b	610	36	1/1/20/20	4/37/115/115	-
32	STE	d	411	-	-	6/12/14/17	-
32	STE	B	627	-	-	6/11/13/17	-
22	CLA	d	405	-	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
32	STE	a	415	-	-	4/7/9/17	-
22	CLA	b	614	-	1/1/20/20	18/37/115/115	-
27	LMG	Y	101	-	-	23/43/63/70	0/1/1/1
26	PL9	A	410	-	-	23/53/73/73	0/1/1/1
22	CLA	B	604	-	1/1/20/20	12/37/115/115	-
24	BCR	A	407	-	-	8/29/63/63	0/2/2/2
24	BCR	B	618	-	-	10/29/63/63	0/2/2/2
28	SQD	a	412	-	-	16/37/37/69	-
32	STE	b	621	-	-	8/13/13/17	-
22	CLA	B	605	-	1/1/20/20	9/37/115/115	-
23	PHO	A	404	-	-	5/53/103/103	0/5/6/6
32	STE	J	101	-	-	3/7/9/17	-
23	PHO	d	401	-	-	6/53/103/103	0/5/6/6
22	CLA	B	607	36	1/1/20/20	7/37/115/115	-
32	STE	B	622	-	-	2/9/11/17	-
22	CLA	c	511	3	1/1/20/20	11/37/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	SQD	B	621	-	-	19/49/69/69	0/1/1/1
22	CLA	B	616	-	1/1/19/20	8/31/109/115	-
34	HEM	f	101	5,6	-	1/6/54/54	-
22	CLA	a	405	-	1/1/20/20	7/37/115/115	-
22	CLA	C	506	-	-	10/37/115/115	-
32	STE	H	103	-	-	9/15/15/17	-
22	CLA	C	511	3	1/1/20/20	9/37/115/115	-
27	LMG	A	411	-	-	16/43/63/70	0/1/1/1
22	CLA	B	614	-	1/1/20/20	11/37/115/115	-
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
22	CLA	B	610	36	1/1/20/20	4/37/115/115	-
22	CLA	d	404	36	1/1/20/20	6/37/115/115	-
22	CLA	c	513	-	1/1/20/20	12/37/115/115	-
29	LHG	D	411	-	-	19/53/53/53	-
32	STE	B	620	-	-	7/12/14/17	-
29	LHG	D	409	-	-	21/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
22	CLA	c	501	-	1/1/20/20	2/37/115/115	-
27	LMG	d	410	-	-	12/39/59/70	0/1/1/1
27	LMG	h	102	-	-	11/15/17/70	-
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2
30	DGD	h	103	-	-	19/51/91/95	0/2/2/2
22	CLA	c	512	-	1/1/20/20	16/37/115/115	-
32	STE	b	624	-	-	5/11/13/17	-
35	HEC	V	201	17	-	0/6/54/54	-
22	CLA	A	403	36	-	12/37/115/115	-
22	CLA	c	510	-	1/1/20/20	7/37/115/115	-
22	CLA	b	602	-	-	11/37/115/115	-
29	LHG	D	408	-	-	24/53/53/53	-
32	STE	D	413	-	-	5/10/12/17	-
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
28	SQD	A	414	-	-	17/39/39/69	-
32	STE	M	104	-	-	7/15/15/17	-
22	CLA	B	609	-	-	4/37/115/115	-
24	BCR	a	406	-	-	0/29/63/63	0/2/2/2
24	BCR	h	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	607	36	1/1/20/20	13/37/115/115	-
22	CLA	d	403	-	-	9/37/115/115	-
22	CLA	b	604	-	1/1/20/20	10/37/115/115	-
30	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	STE	B	625	-	-	7/13/13/17	-
32	STE	d	412	-	-	11/15/17/17	-
32	STE	b	625	-	-	8/15/17/17	-
22	CLA	C	508	-	-	8/37/115/115	-
32	STE	I	101	-	-	5/12/12/17	-
29	LHG	e	101	-	-	22/46/46/53	-
22	CLA	C	501	-	1/1/20/20	3/37/115/115	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
32	STE	M	103	-	-	4/7/7/17	-
22	CLA	C	505	-	1/1/20/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
22	CLA	c	504	36	1/1/19/20	10/31/109/115	-
22	CLA	B	602	-	1/1/20/20	8/37/115/115	-

The worst 5 of 836 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	C4B-NB	8.77	1.43	1.35
22	b	604	CLA	C4B-NB	8.75	1.43	1.35
22	b	615	CLA	C4B-NB	8.17	1.42	1.35
22	c	504	CLA	C4B-NB	8.11	1.42	1.35
22	B	601	CLA	C4B-NB	8.04	1.42	1.35

The worst 5 of 1280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O6-C1-C2	9.98	123.88	108.30
28	a	411	SQD	O6-C1-C2	9.65	123.37	108.30
22	c	509	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	C	507	CLA	C4A-NA-C1A	8.54	110.55	106.71
22	b	611	CLA	C4A-NA-C1A	8.32	110.45	106.71

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND

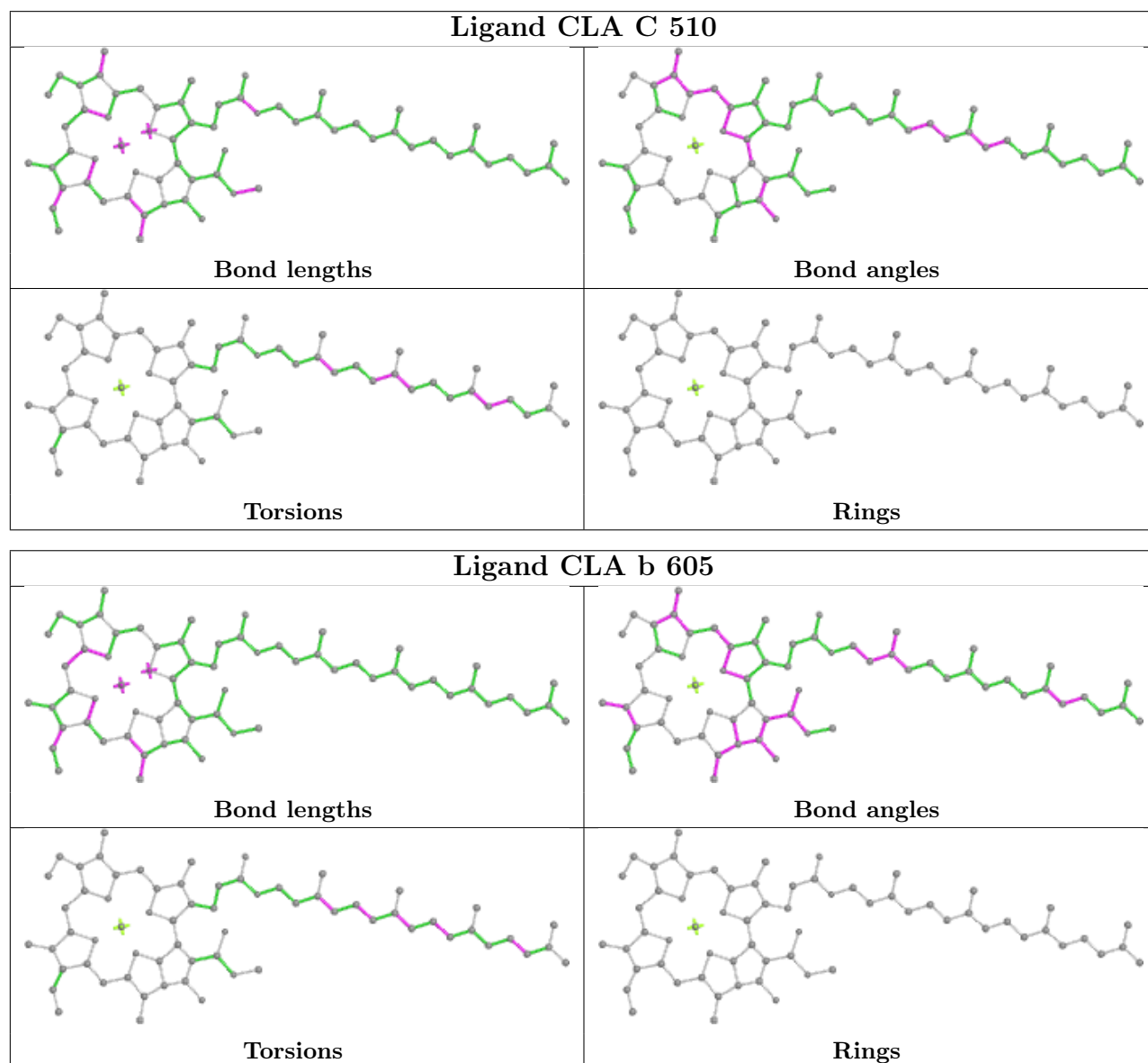
5 of 1838 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	CHA-CBD-CGD-O1D

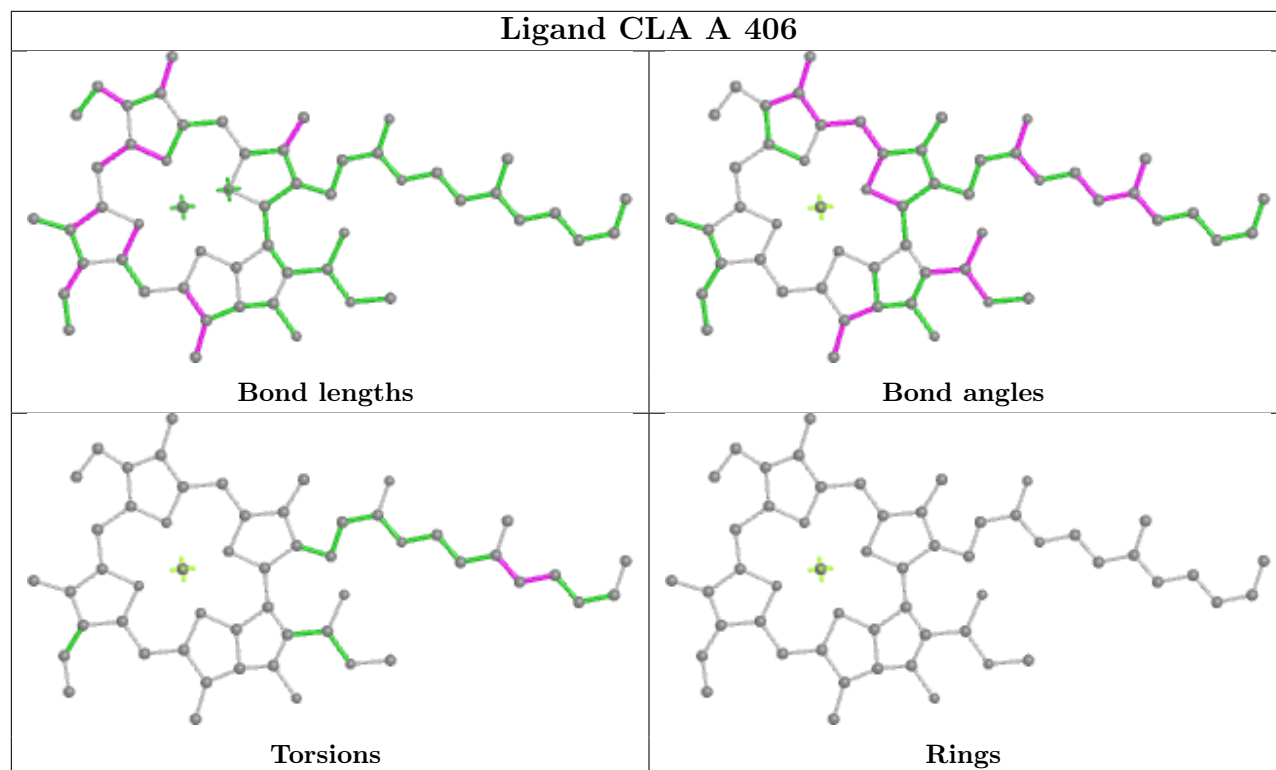
There are no ring outliers.

No monomer is involved in short contacts.

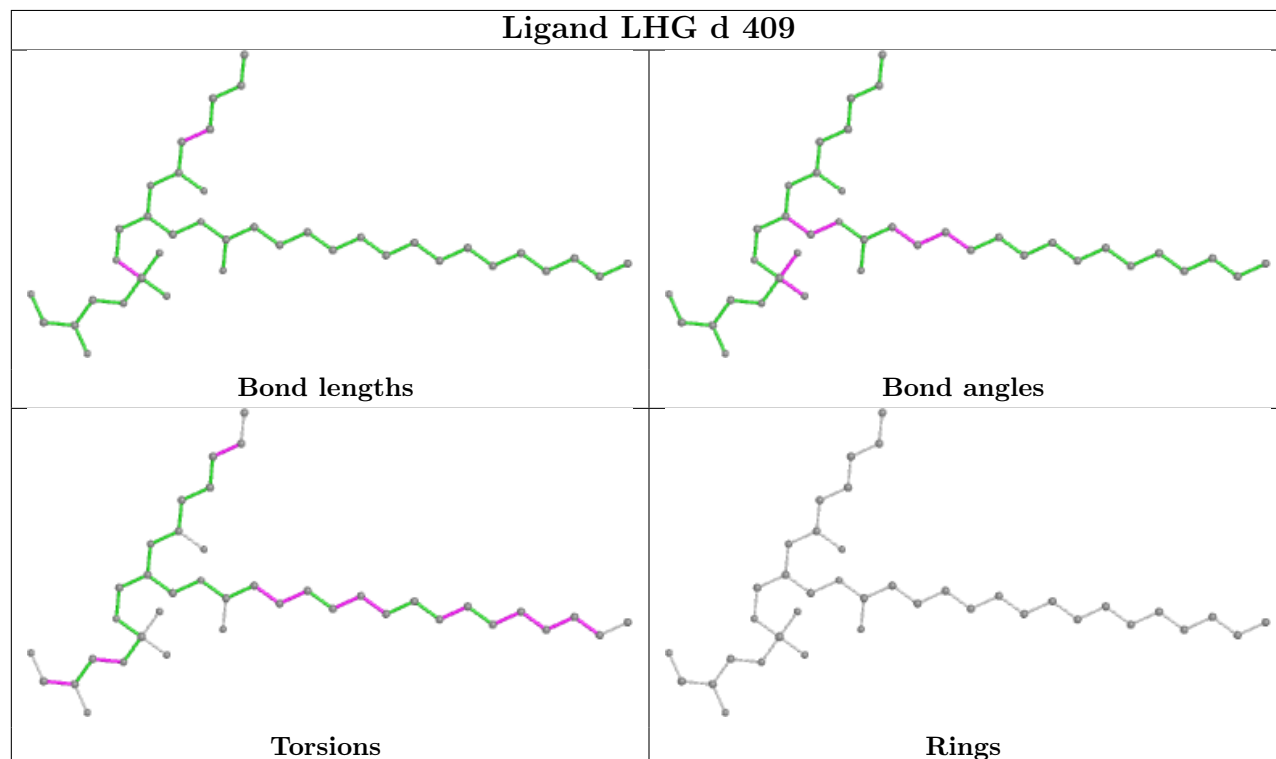
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

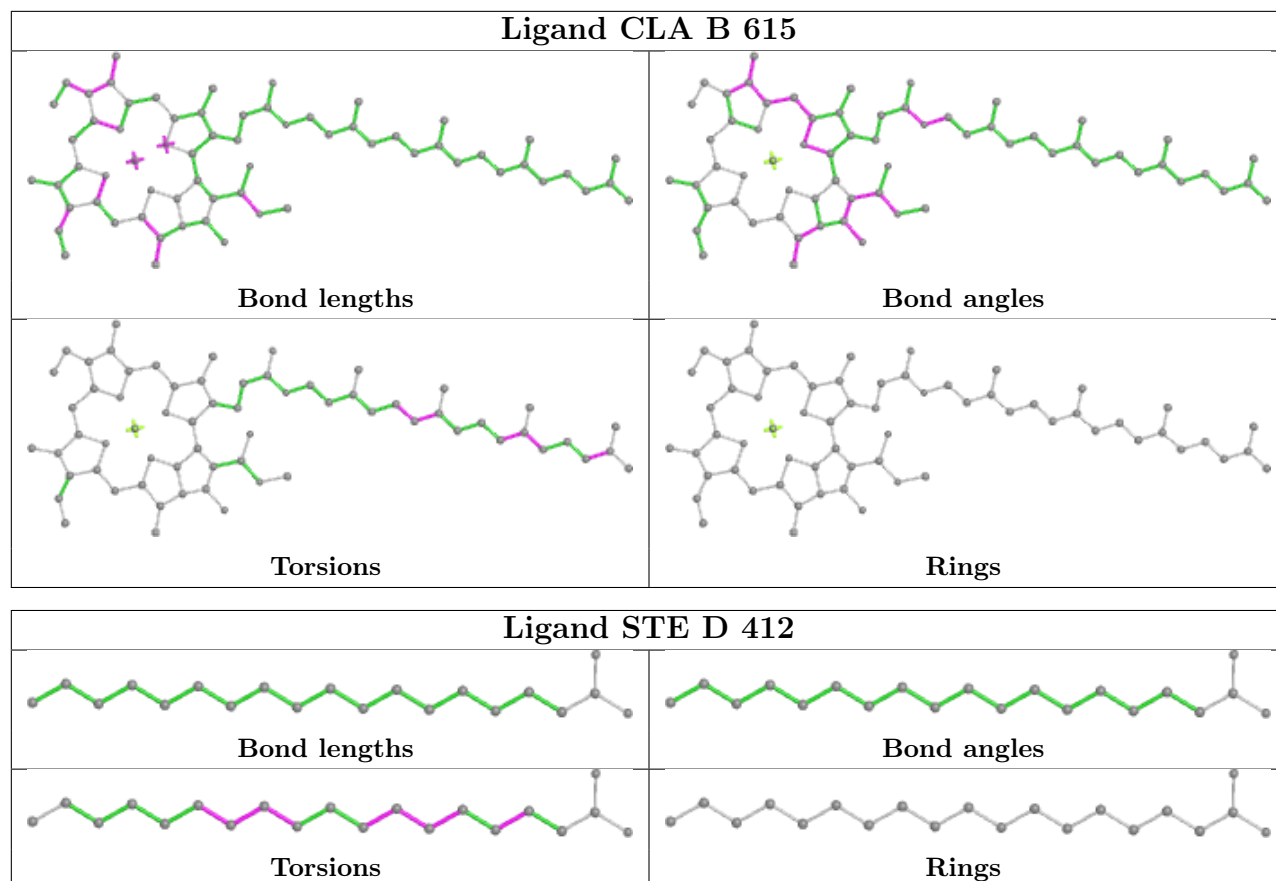


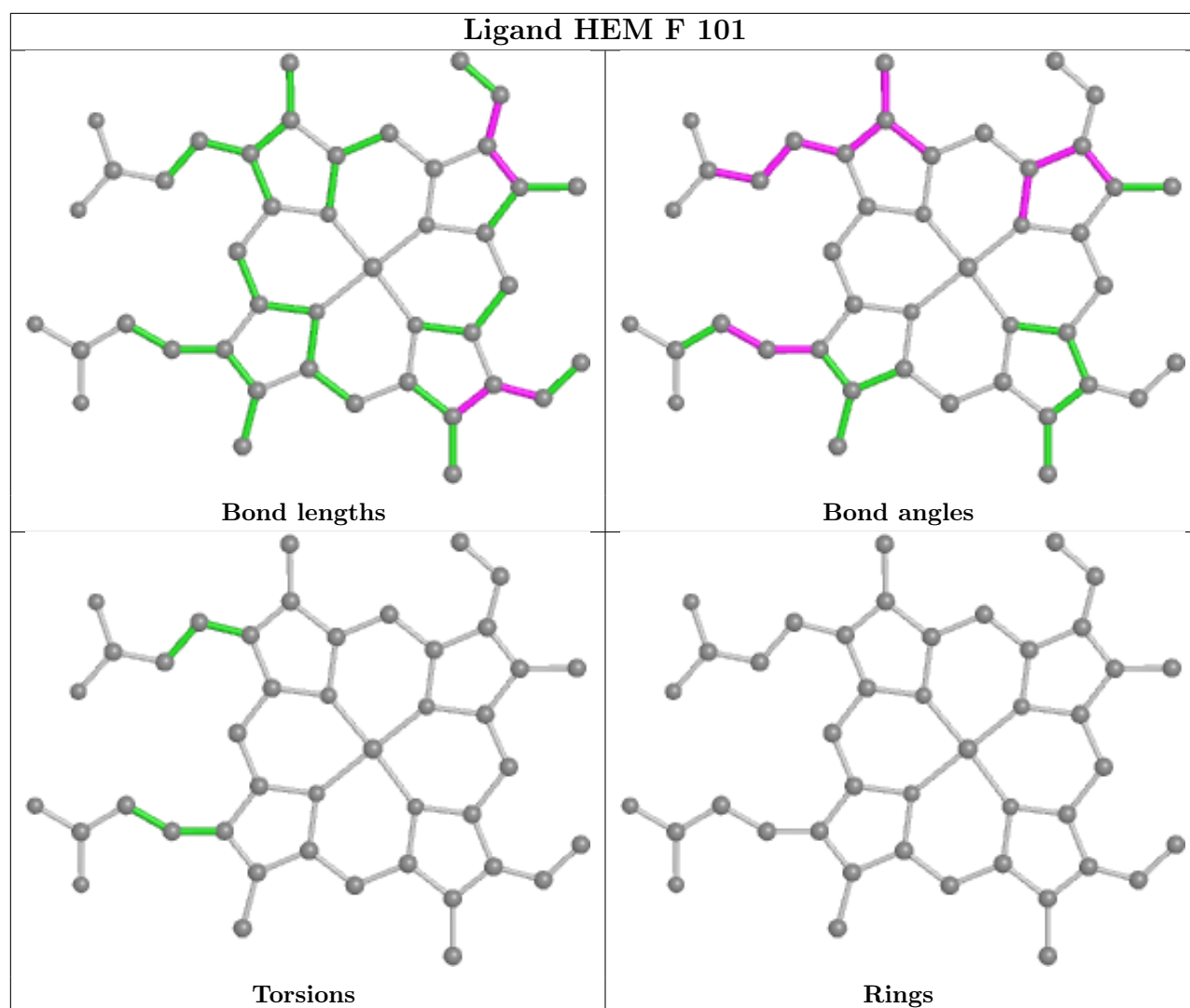
Ligand CLA A 406

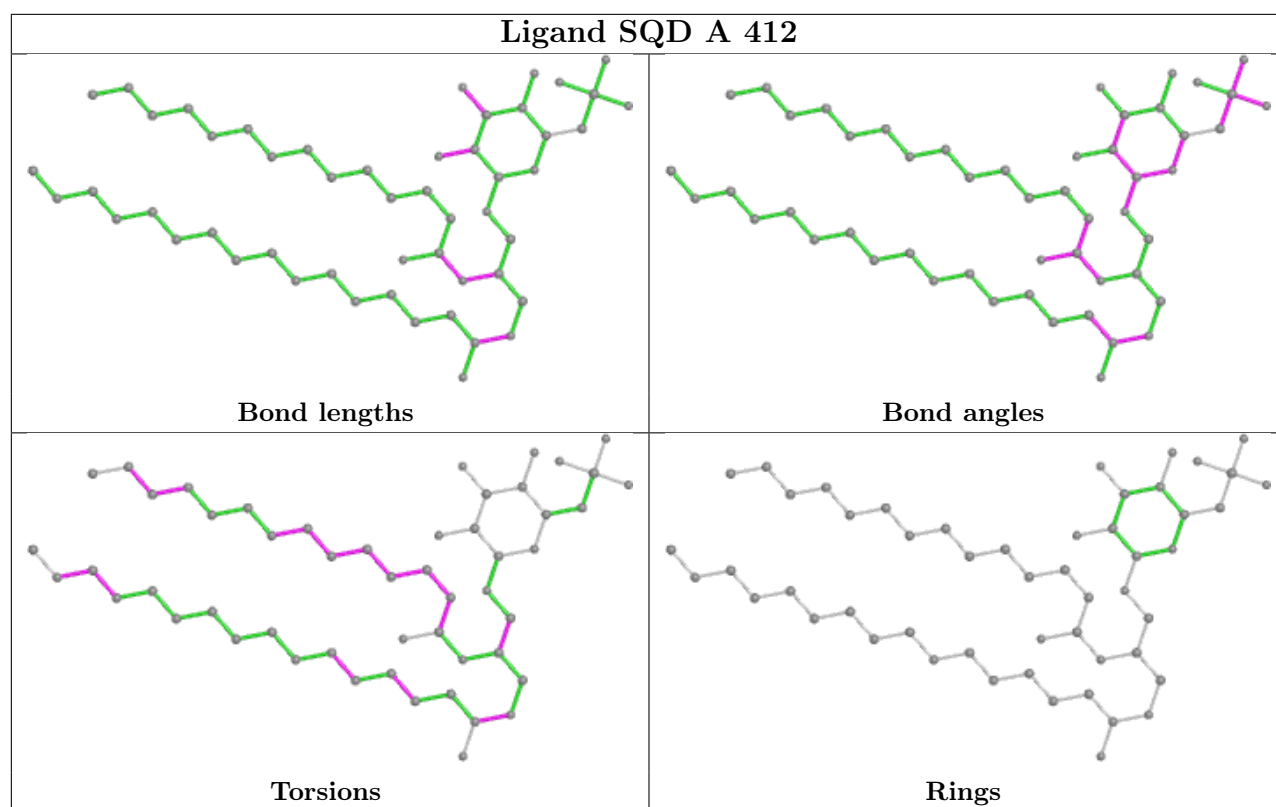


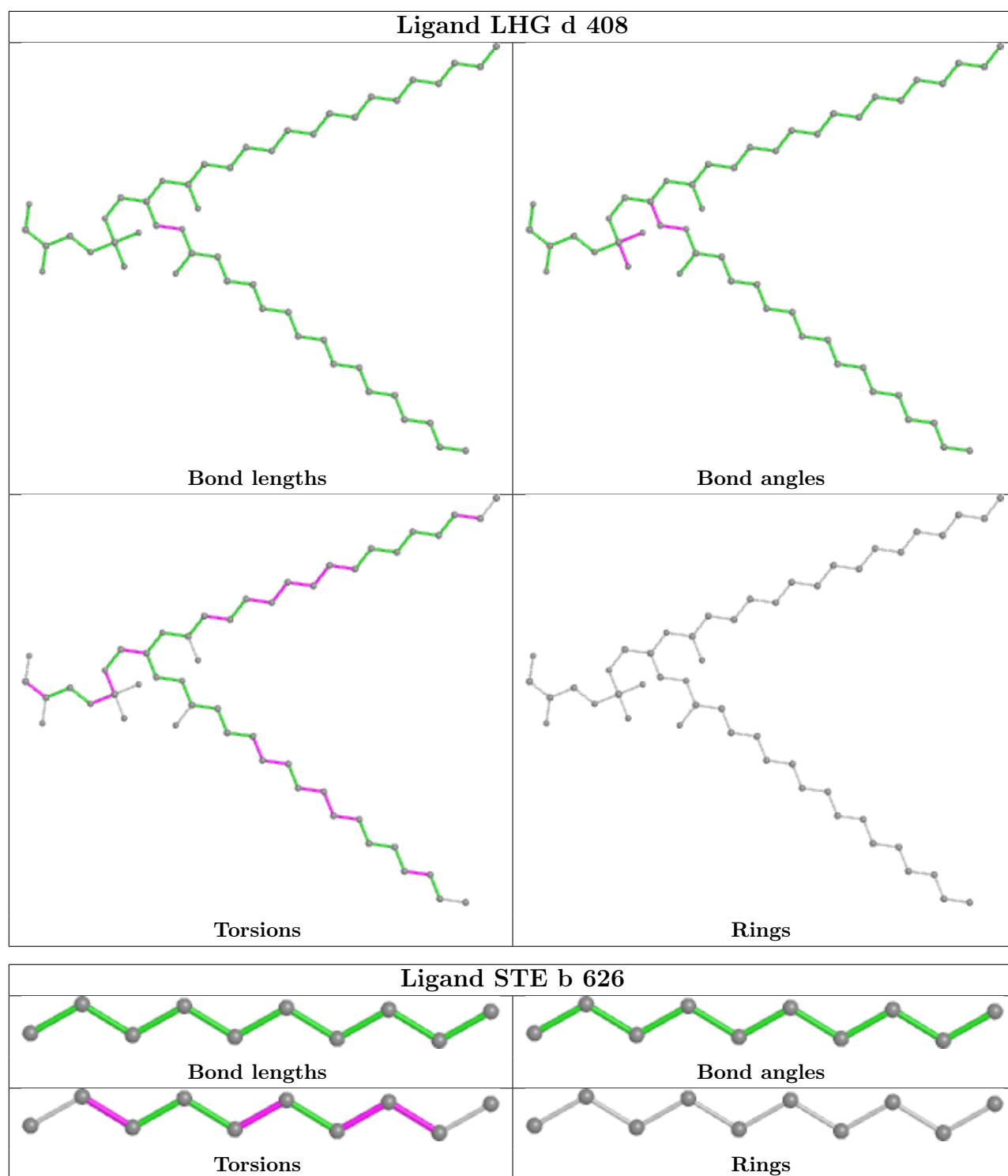
Ligand LHG d 409

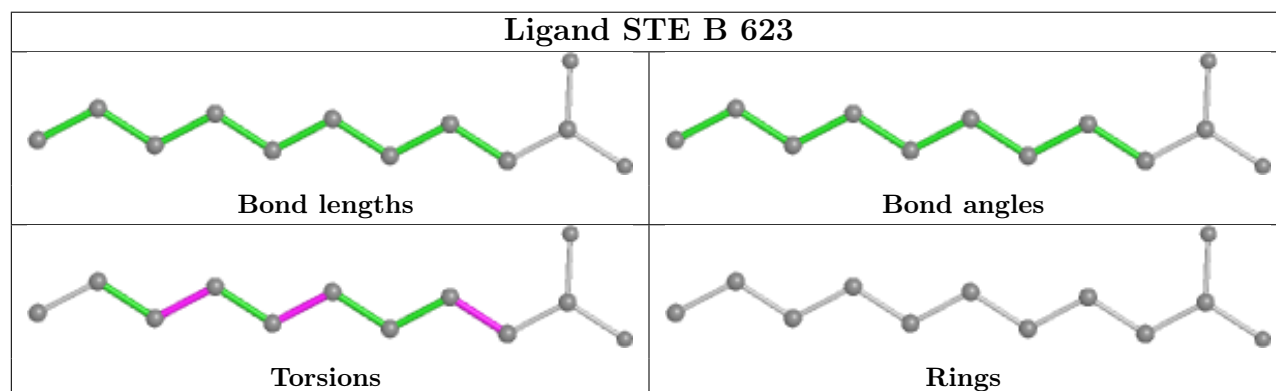
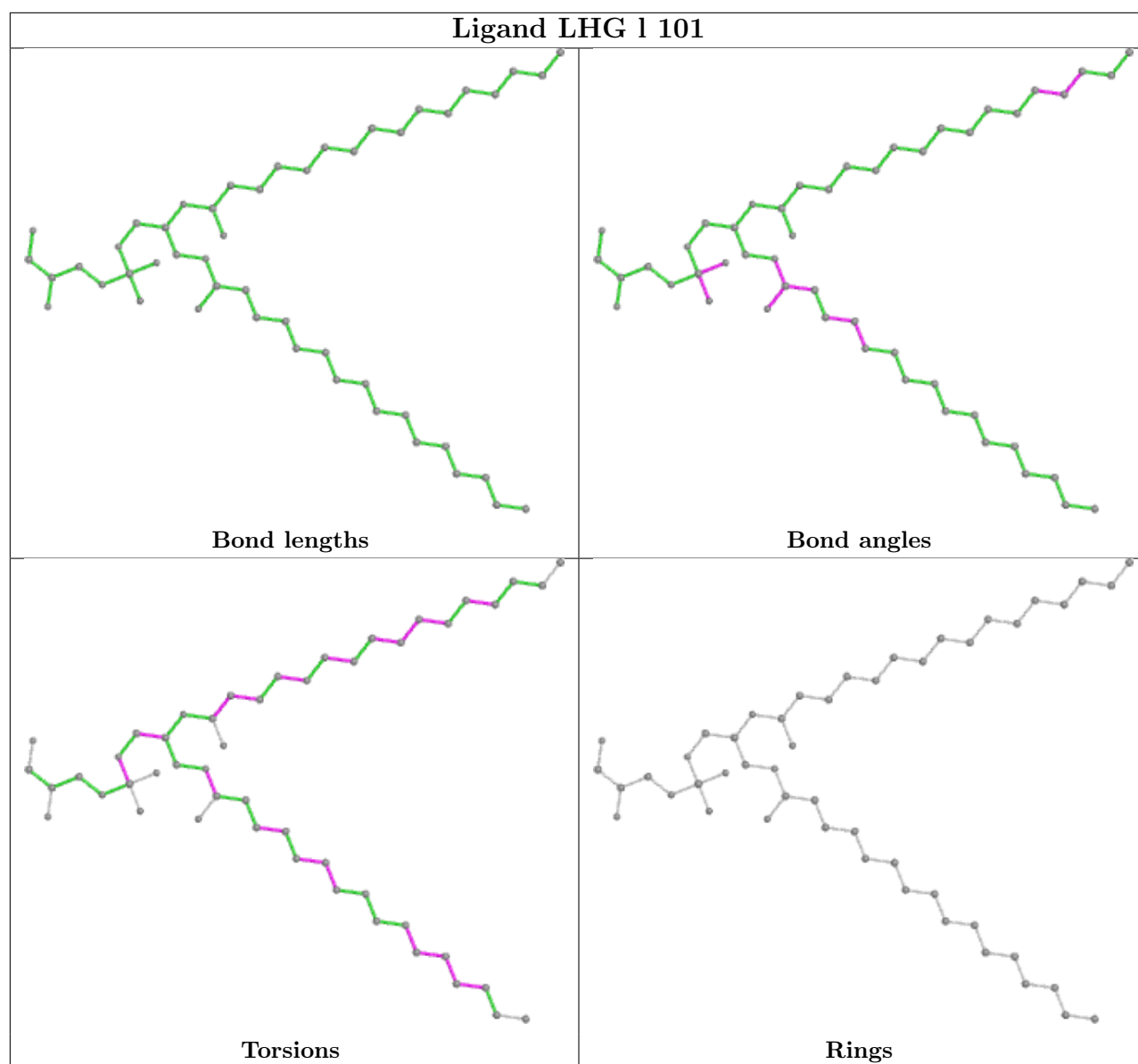




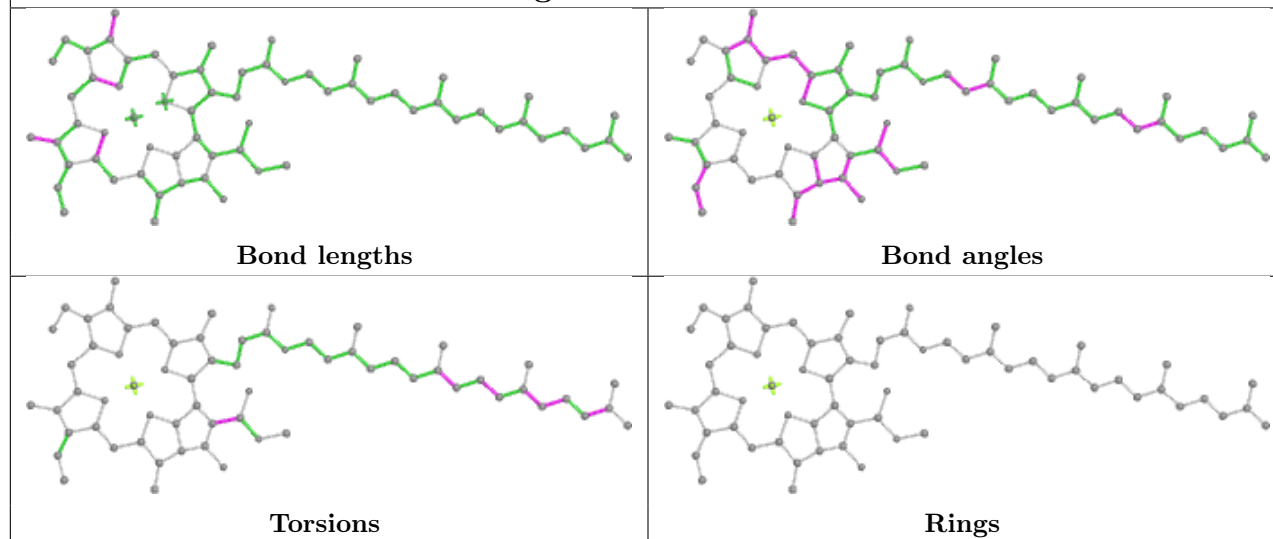




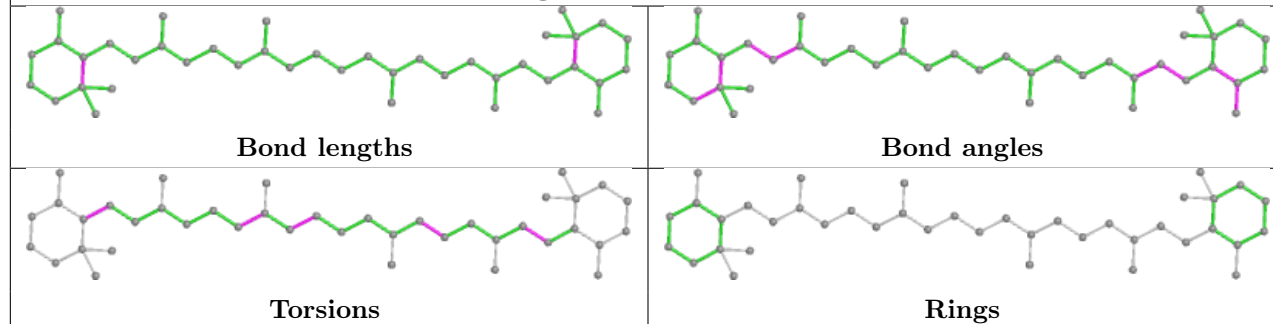




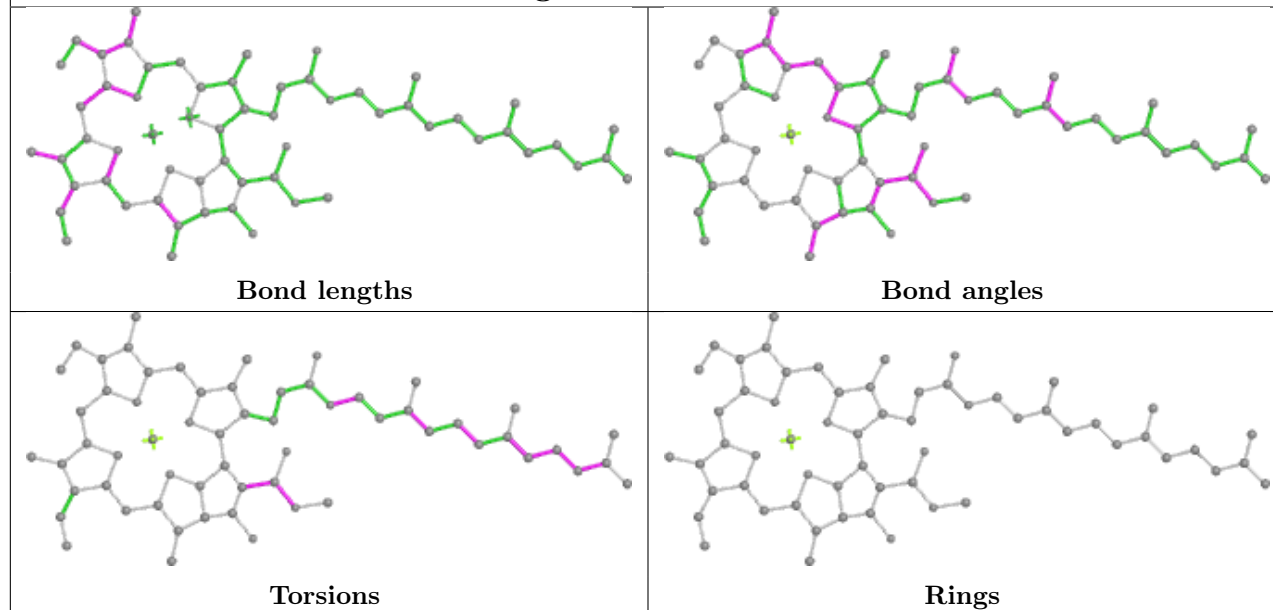
Ligand CLA b 612

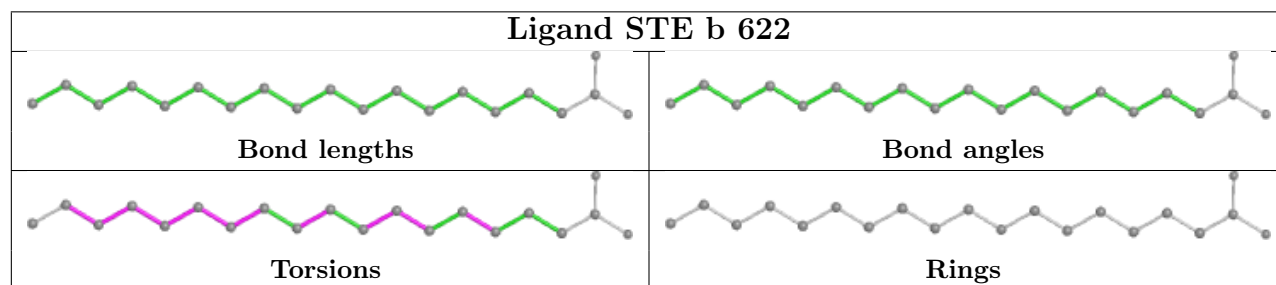
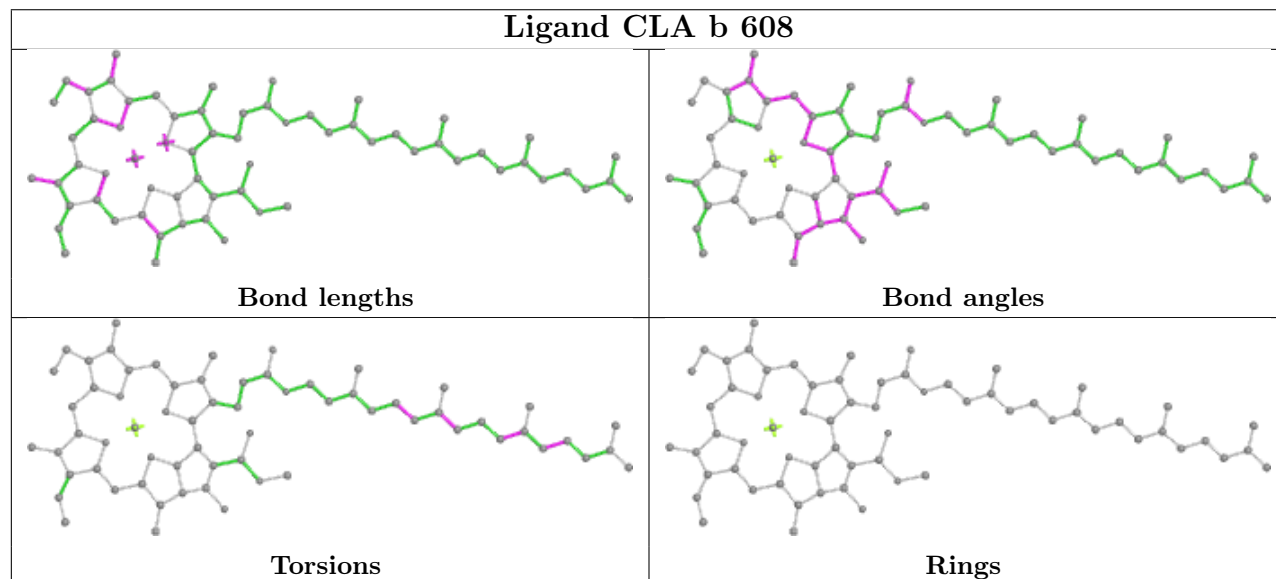
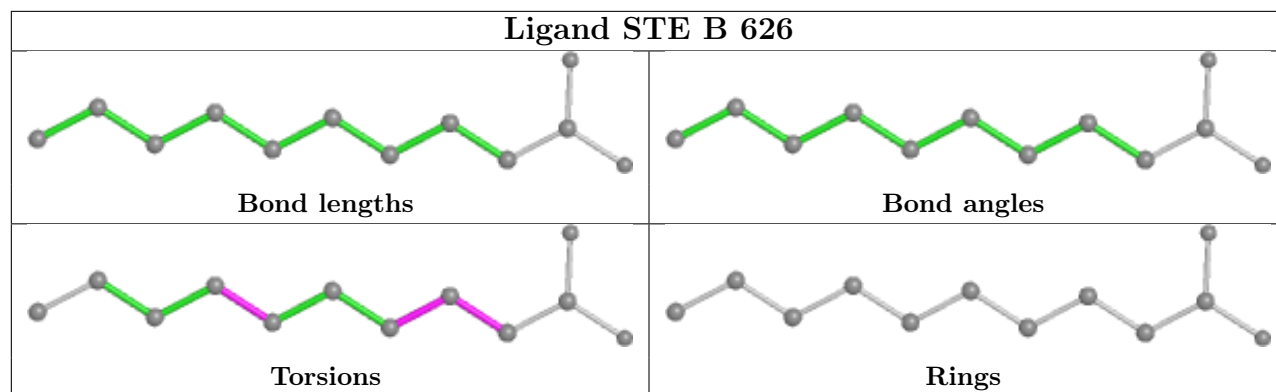


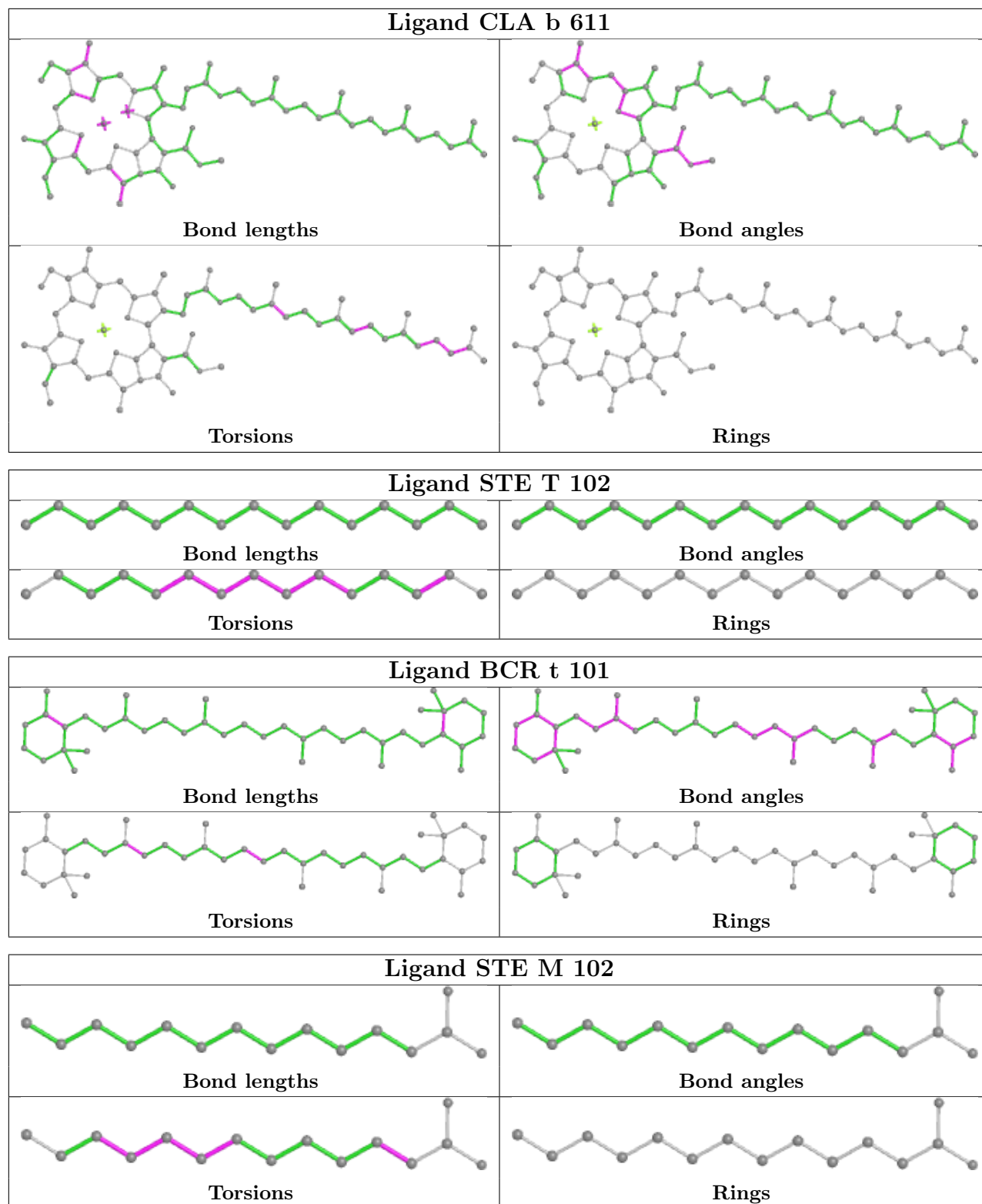
Ligand BCR c 514

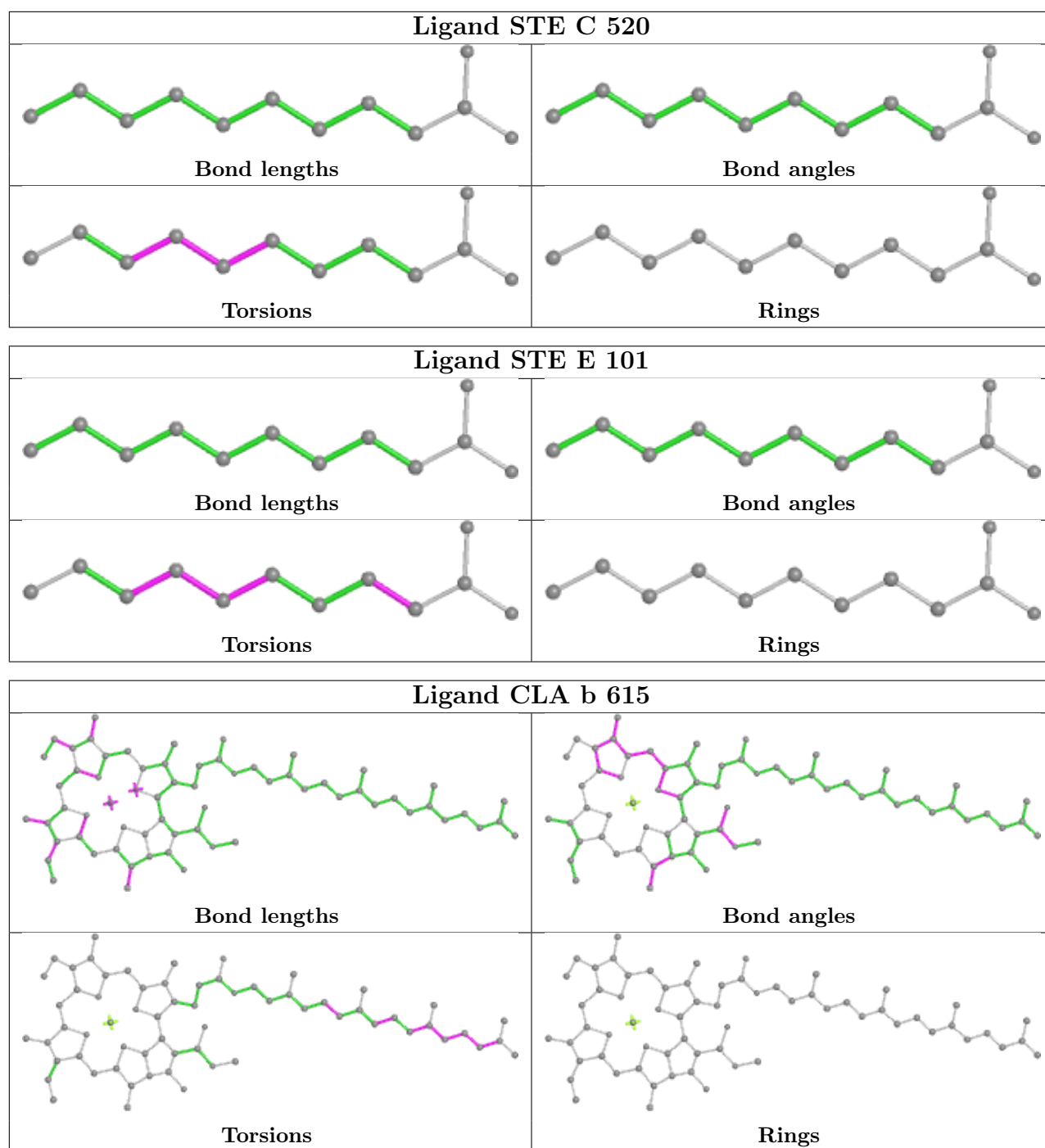


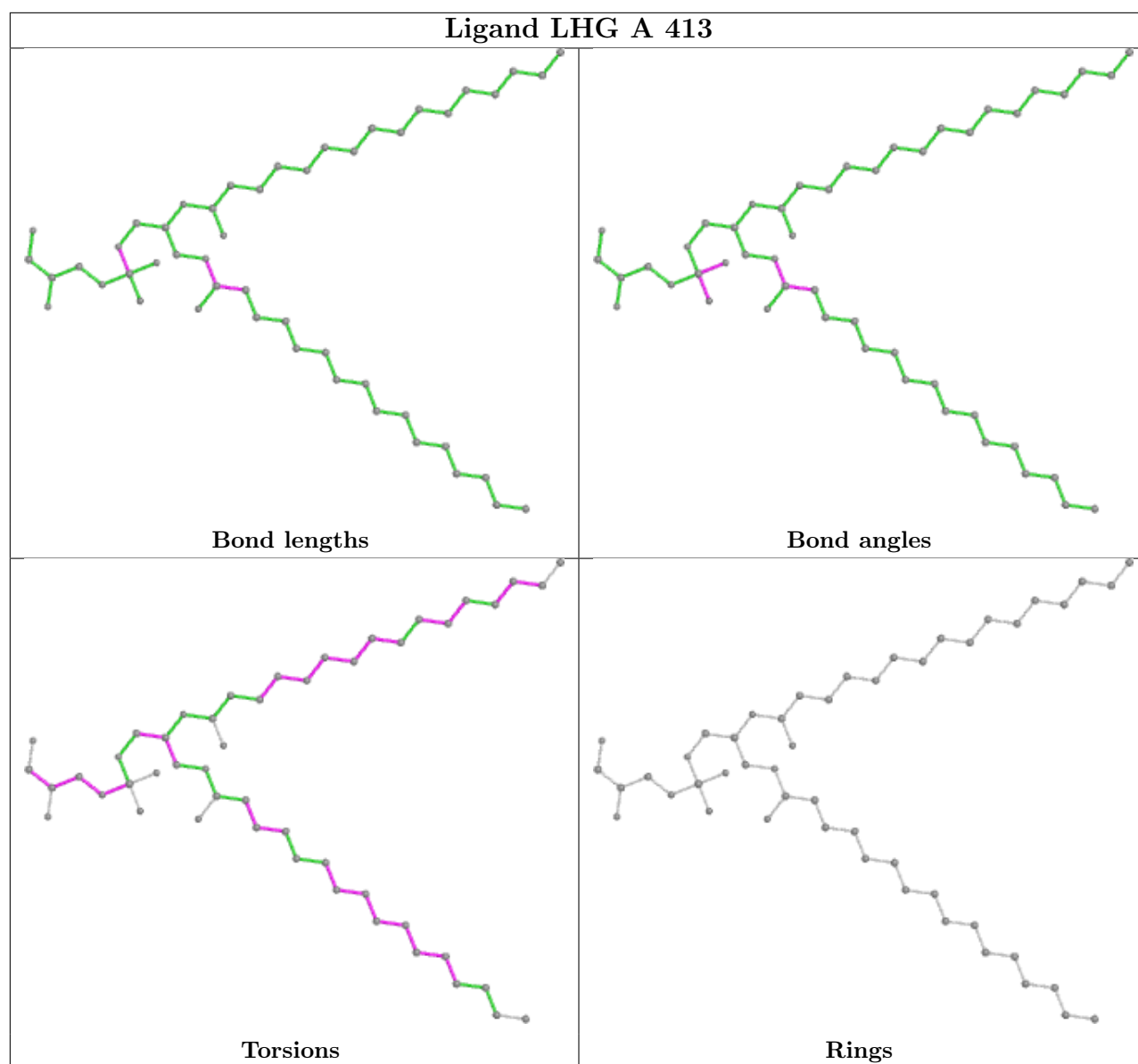
Ligand CLA b 616

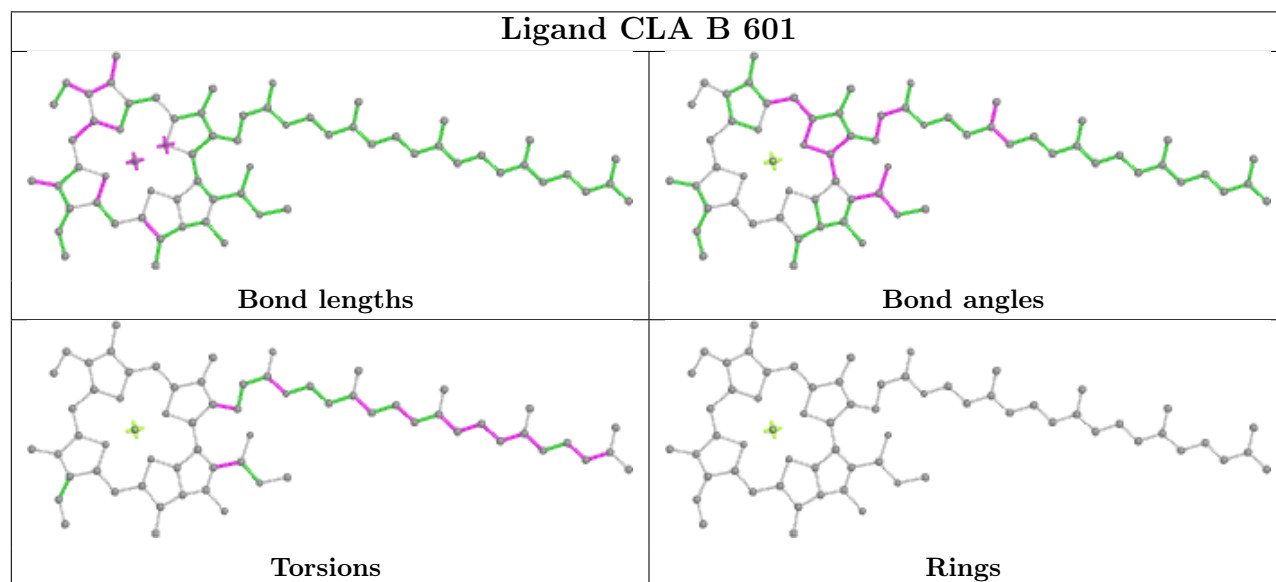
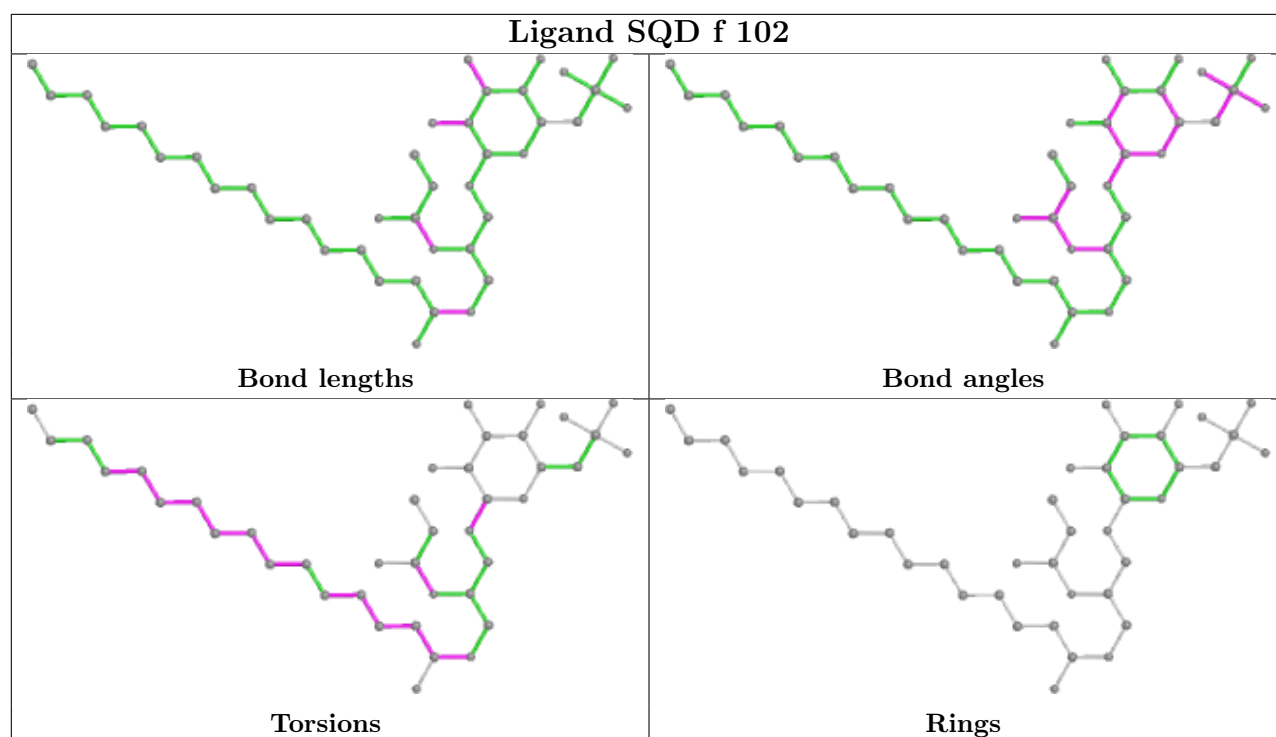


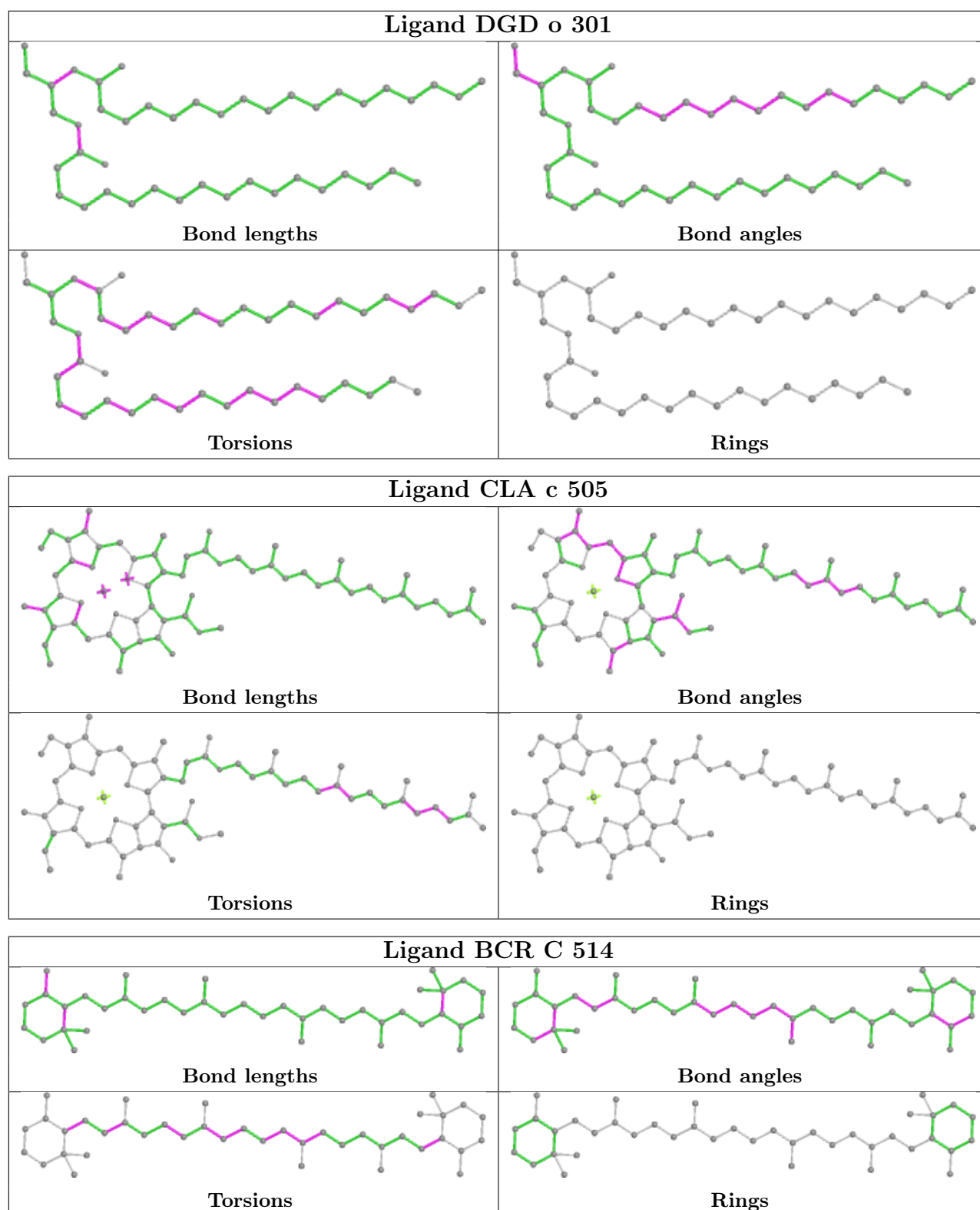


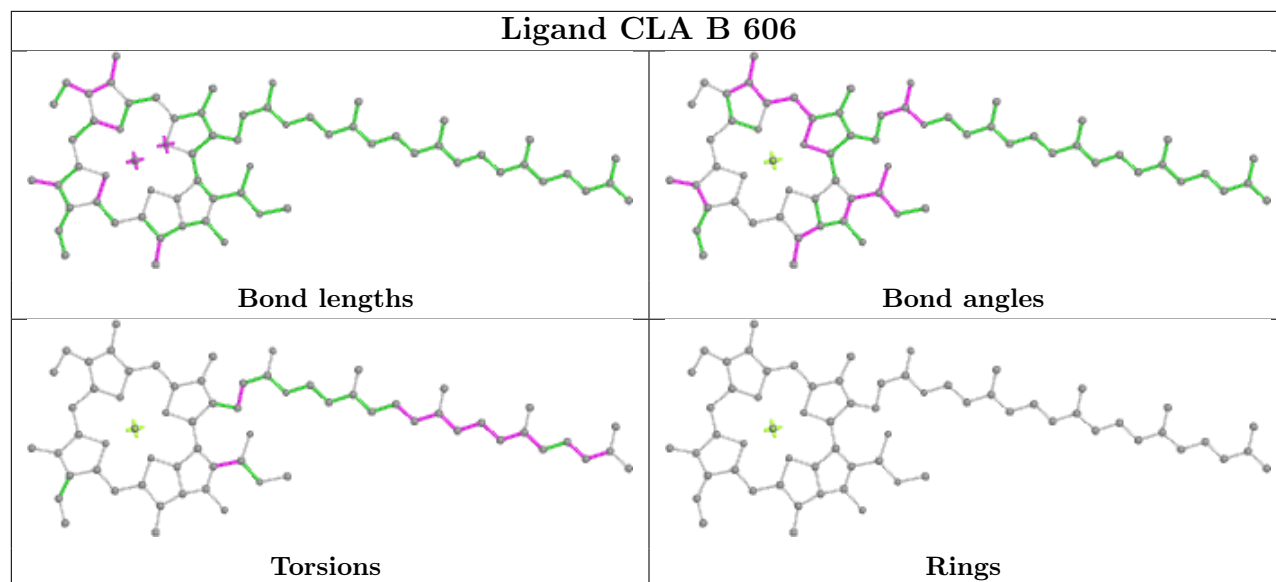
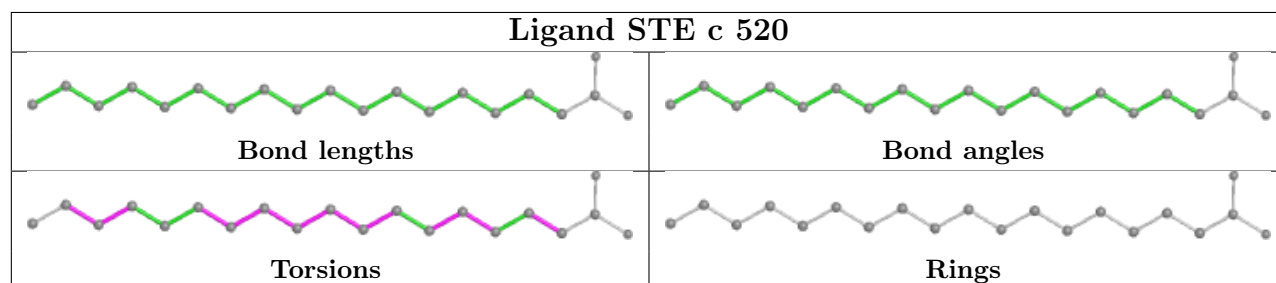
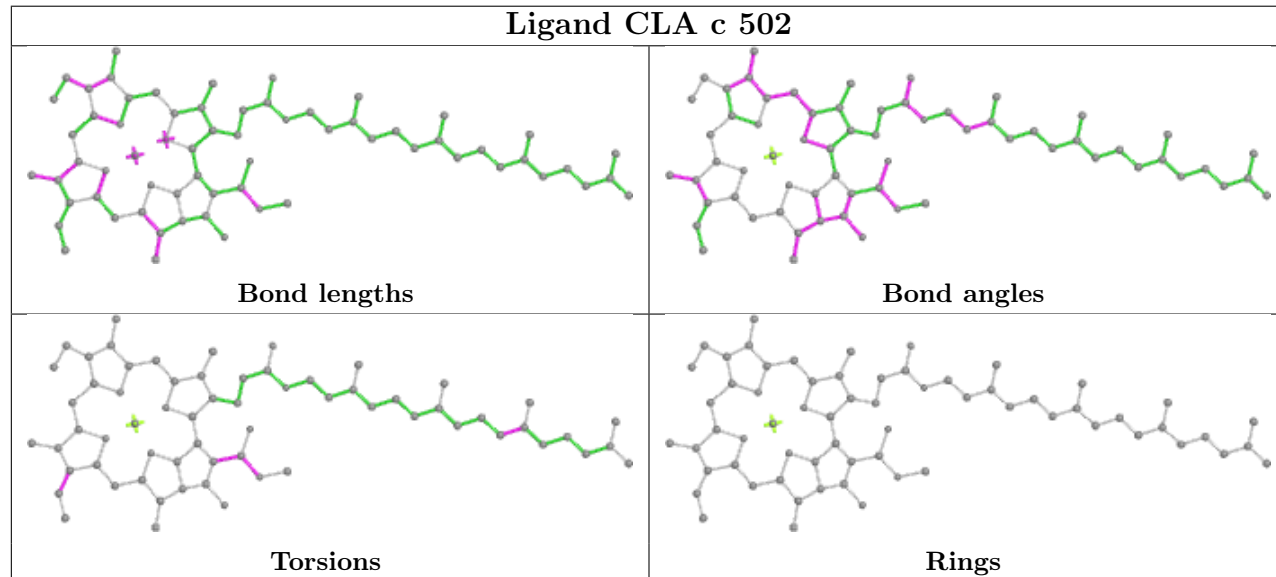


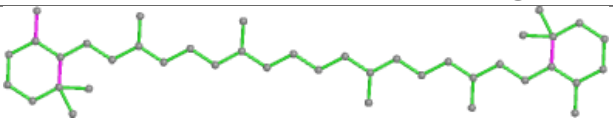
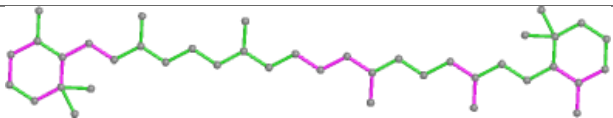
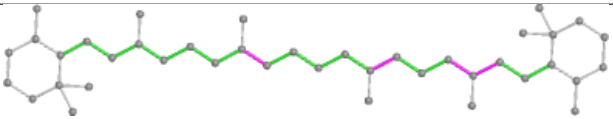
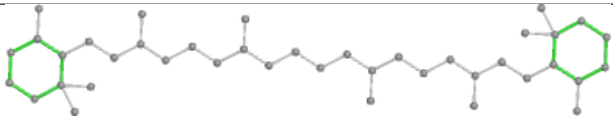


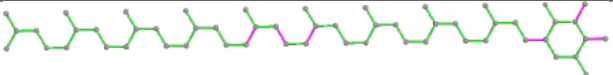
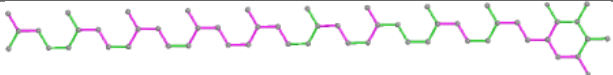
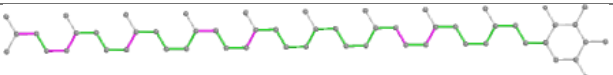
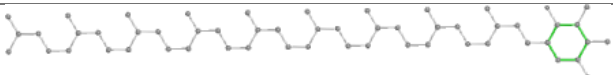


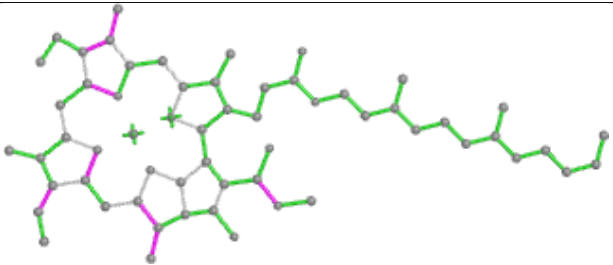
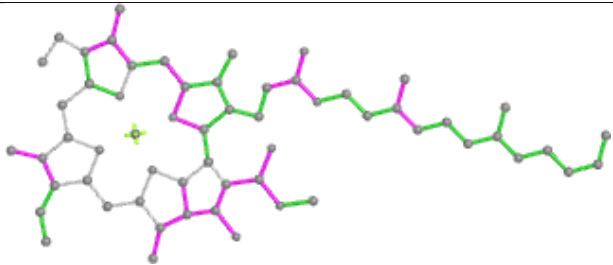
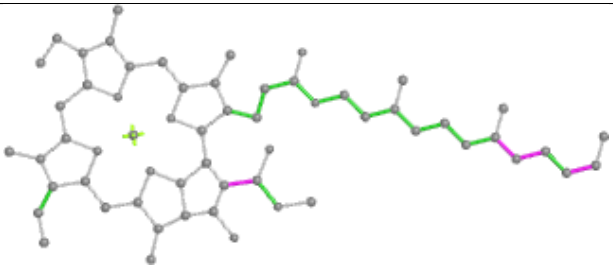
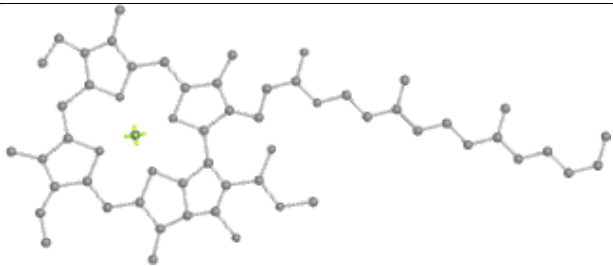


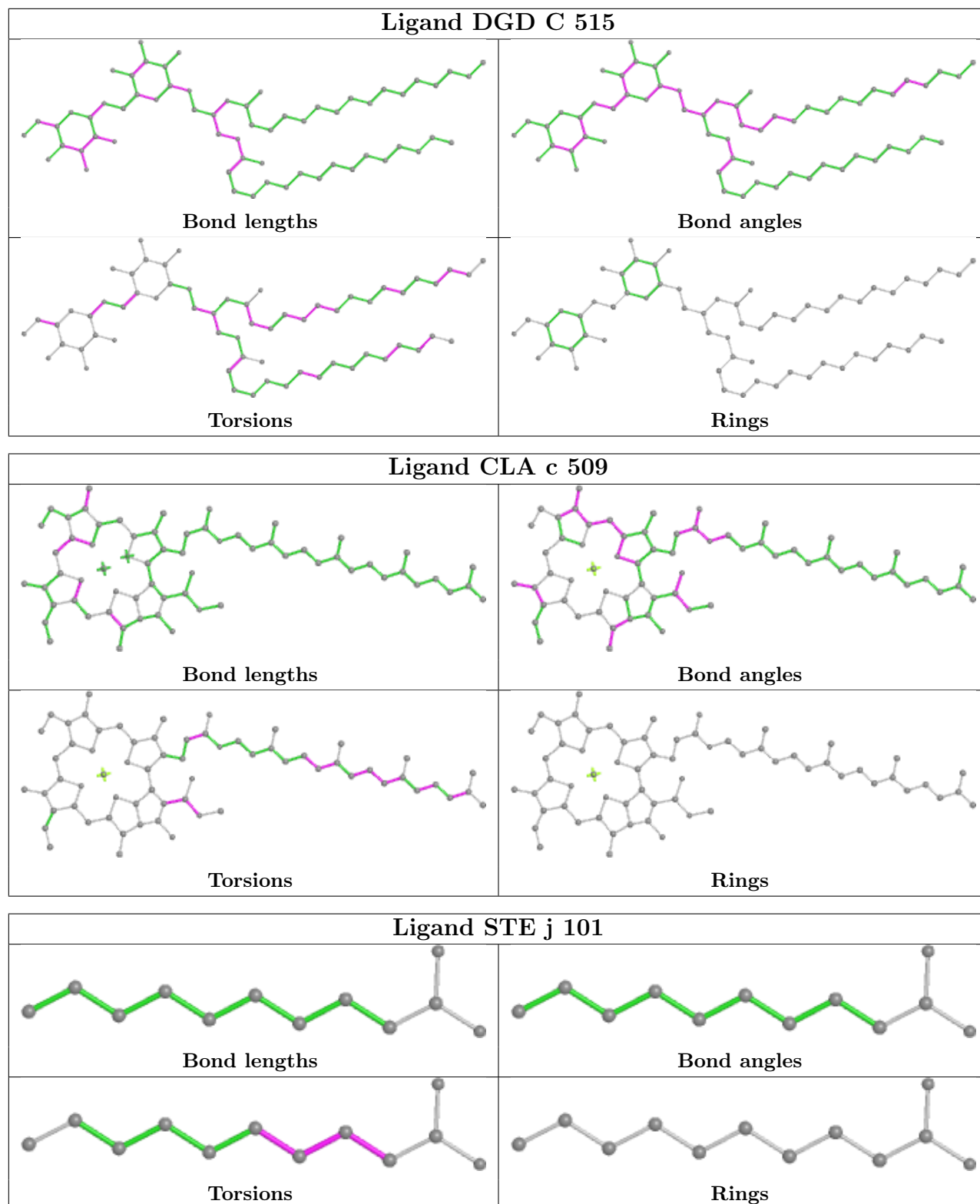


Ligand CLA B 606**Ligand STE c 520****Ligand CLA c 502**

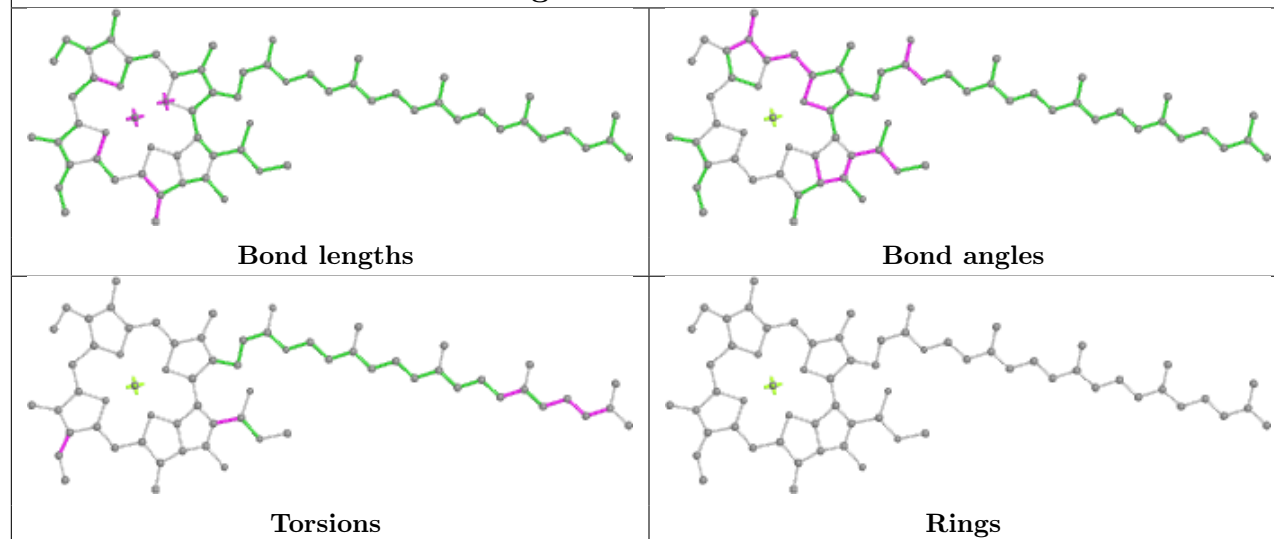
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

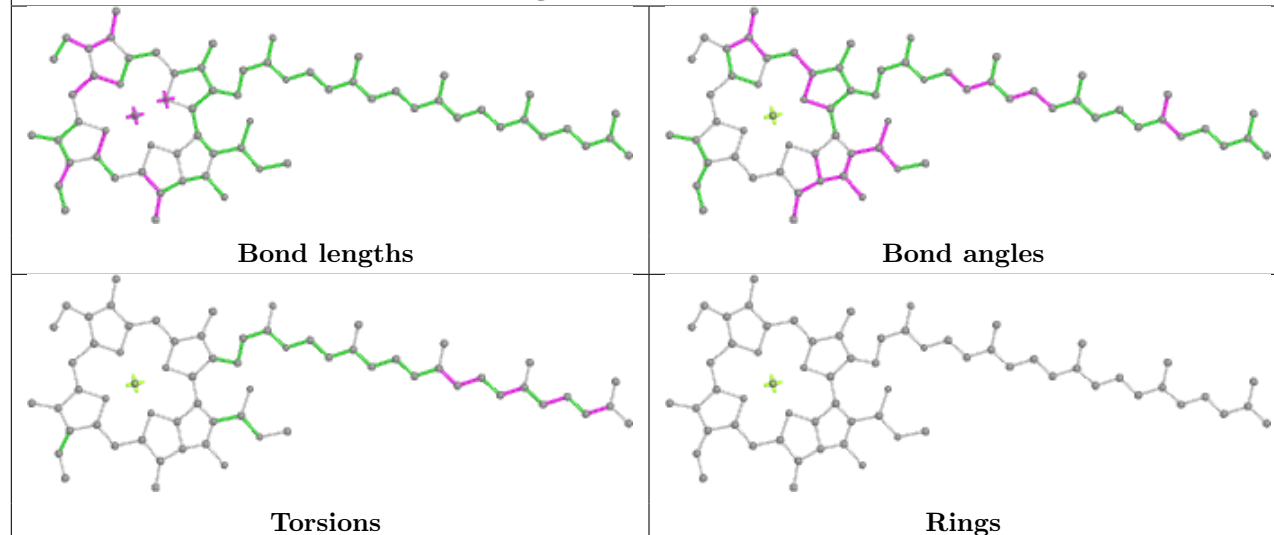
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings



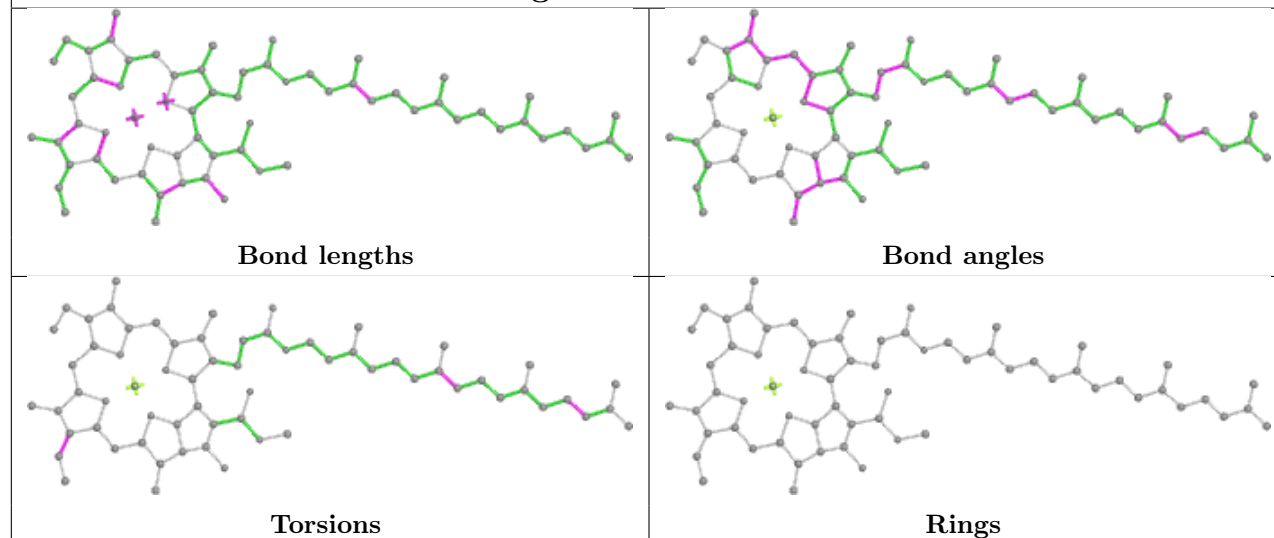
Ligand CLA D 403

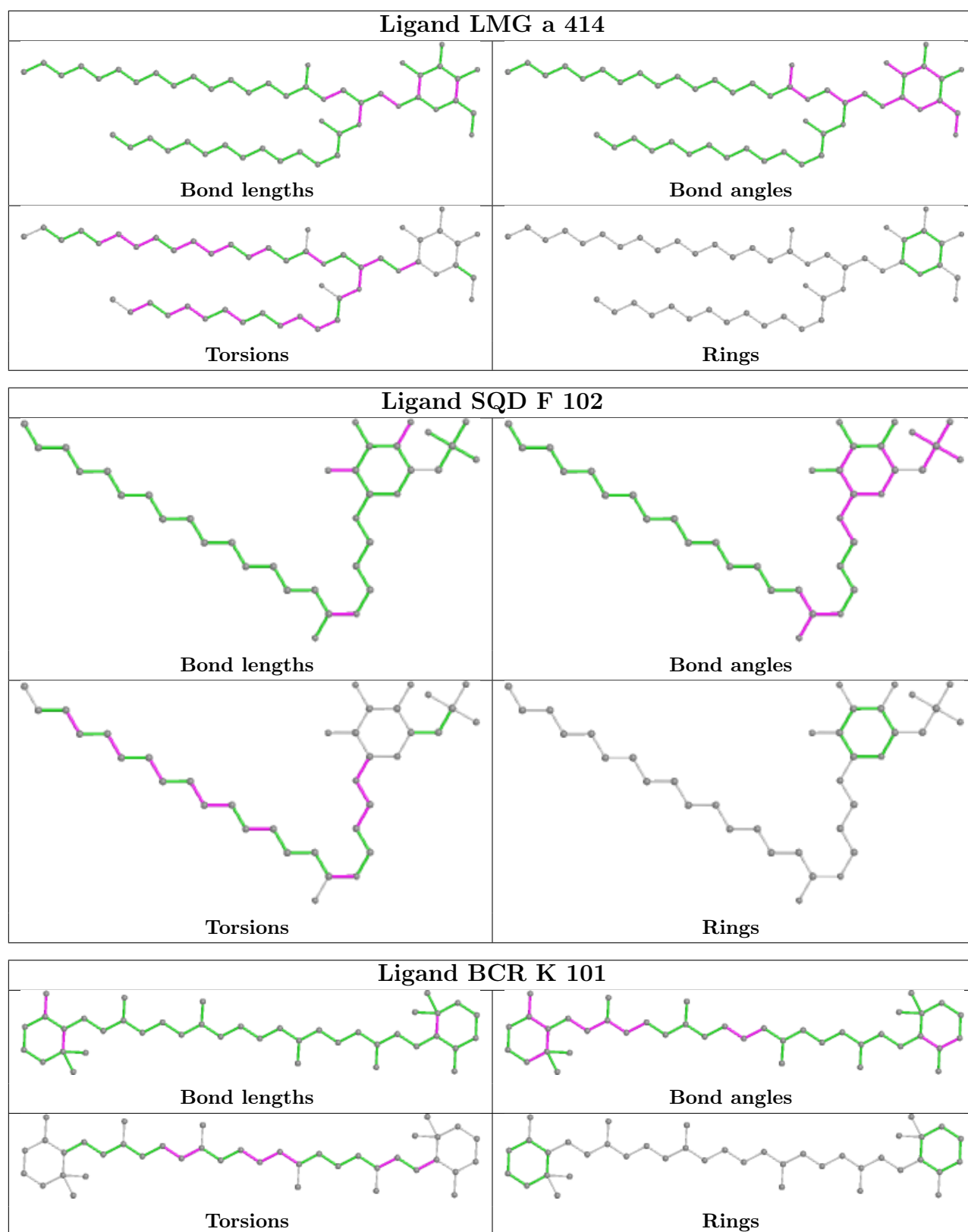


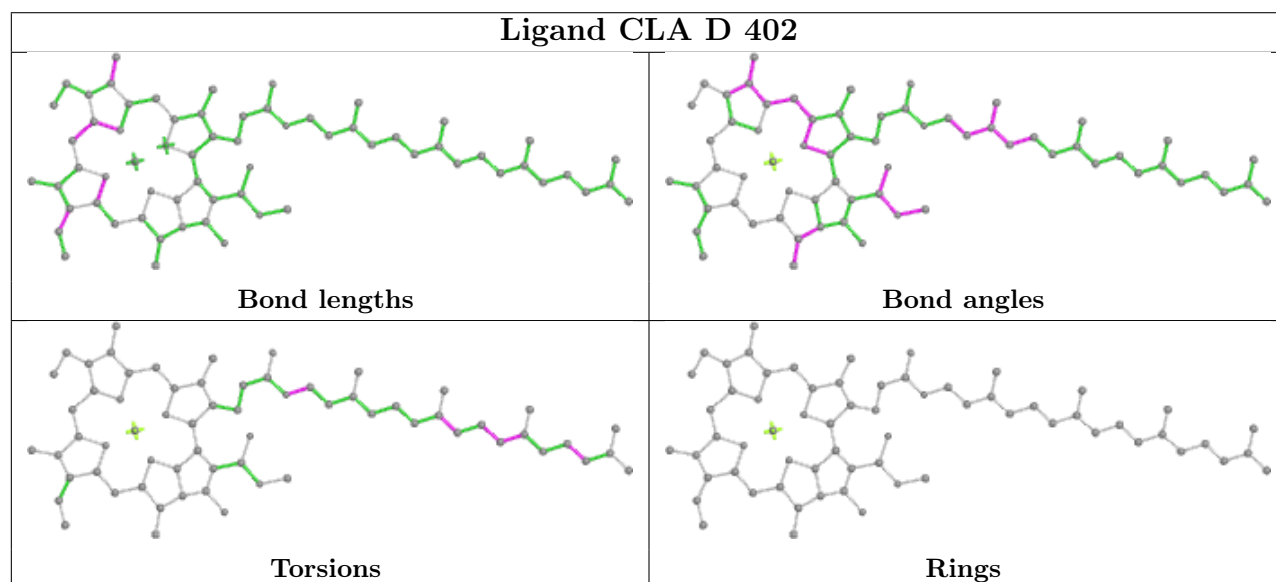
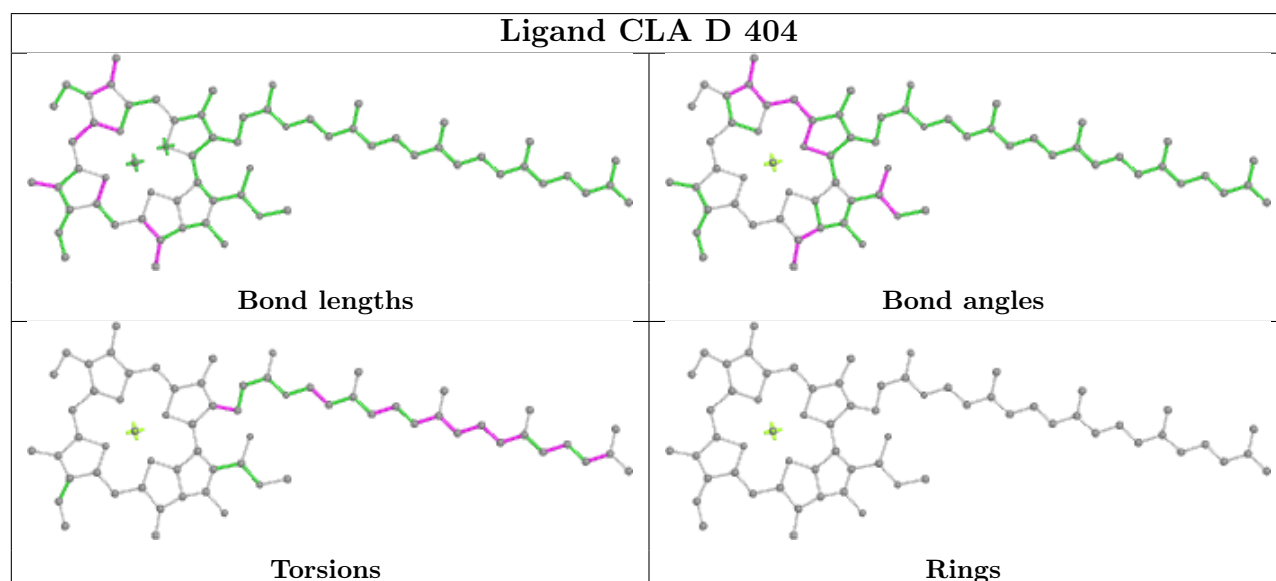
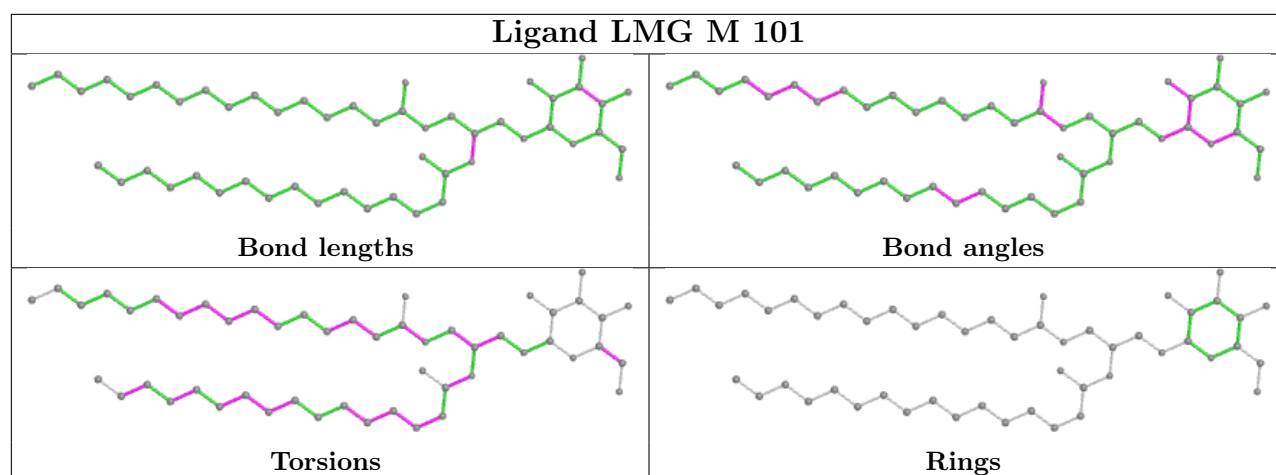
Ligand CLA B 611

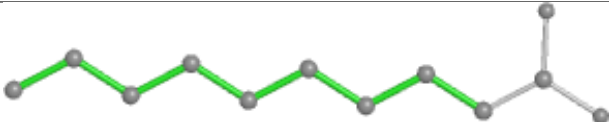
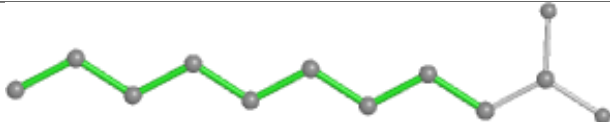
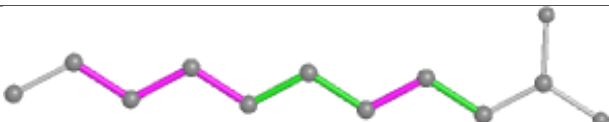
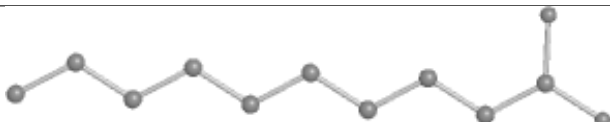


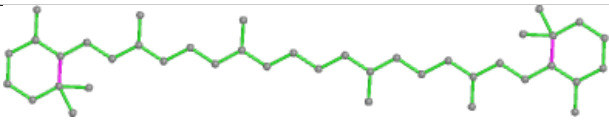
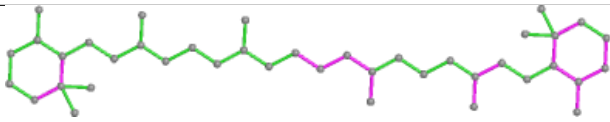
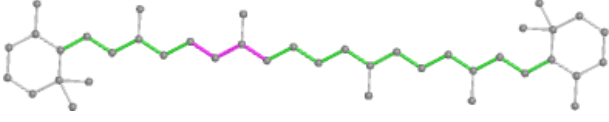
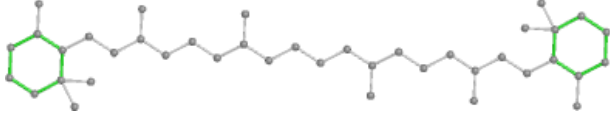
Ligand CLA A 402

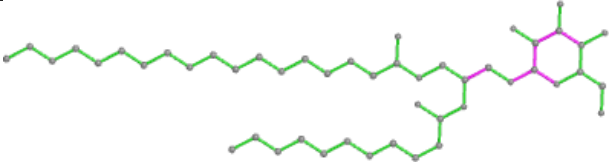
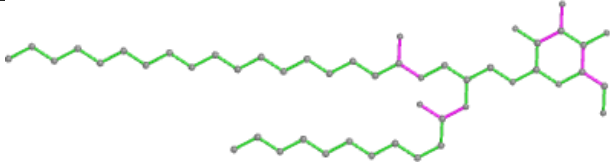
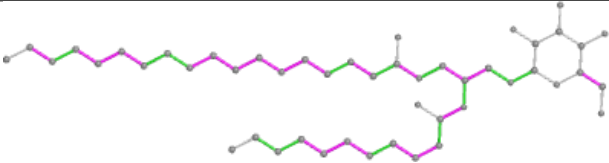
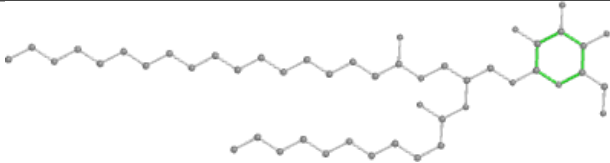




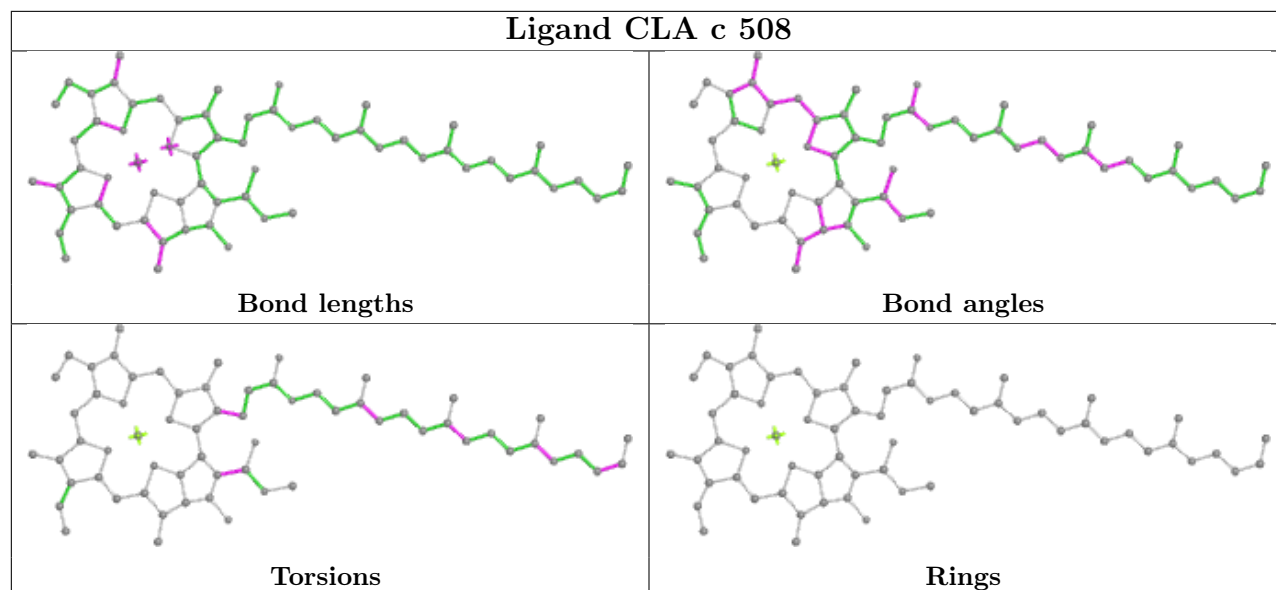


Ligand STE c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

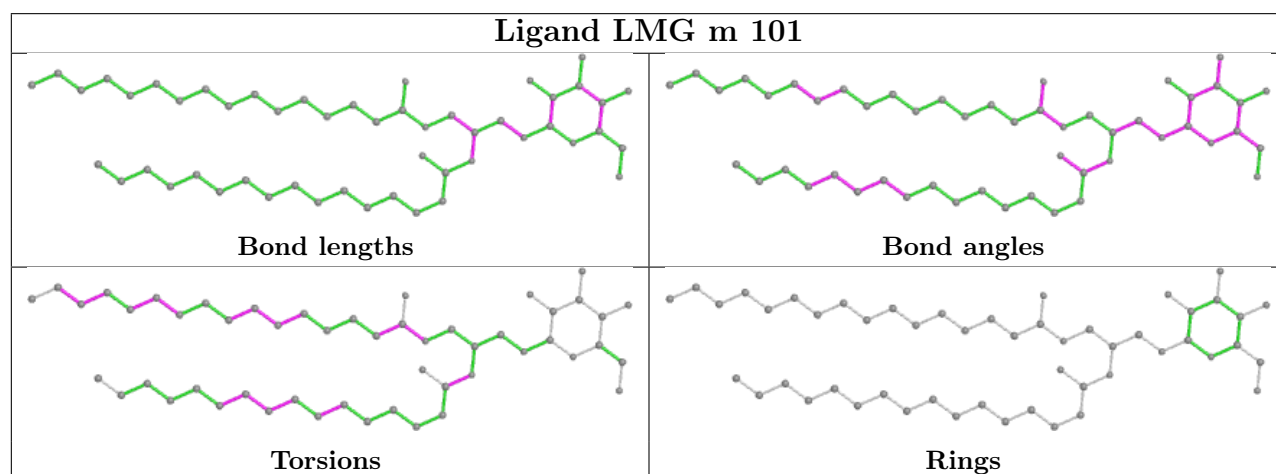
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

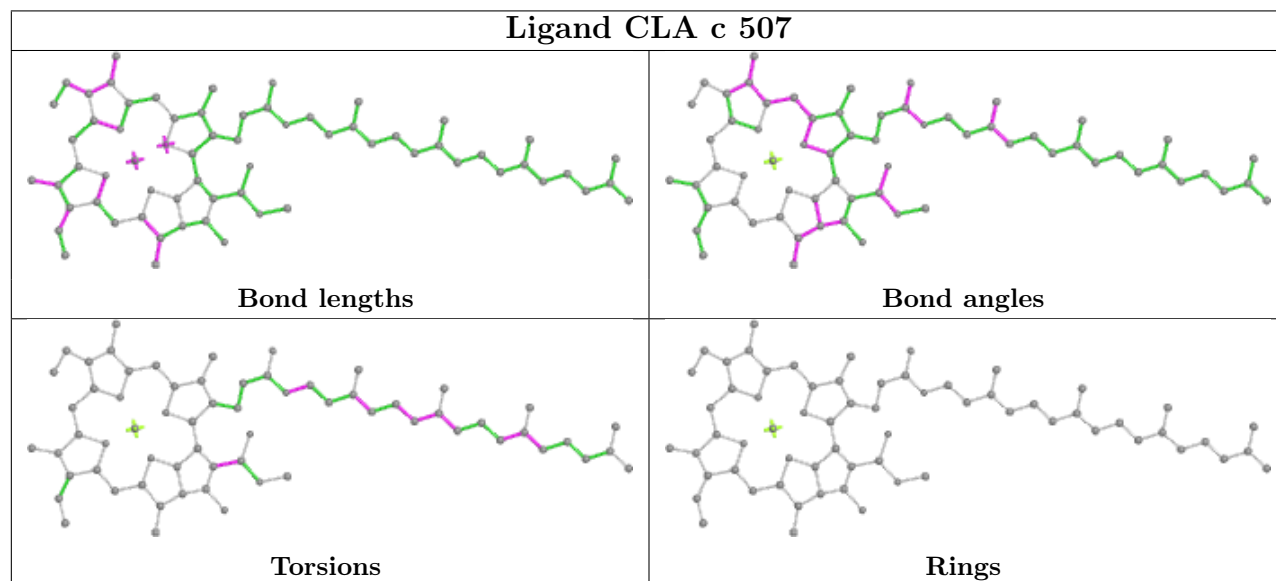
Ligand CLA c 508

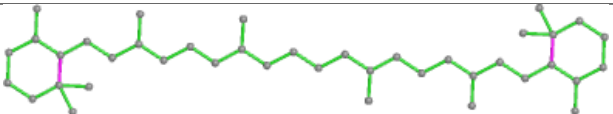
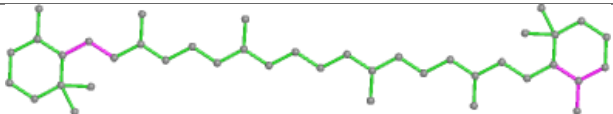
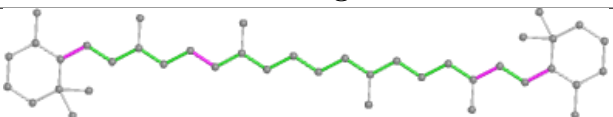
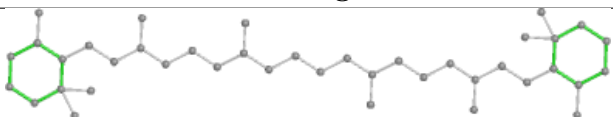


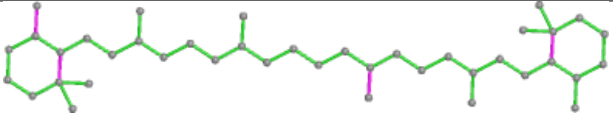
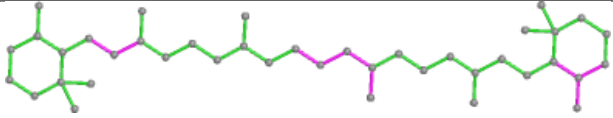
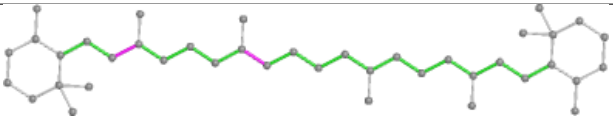
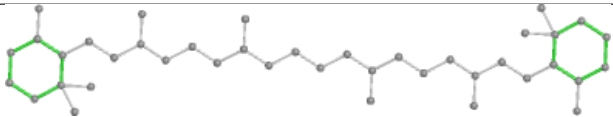
Ligand LMG m 101

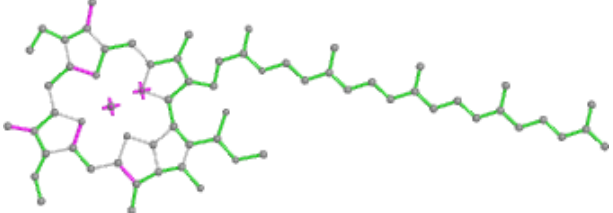
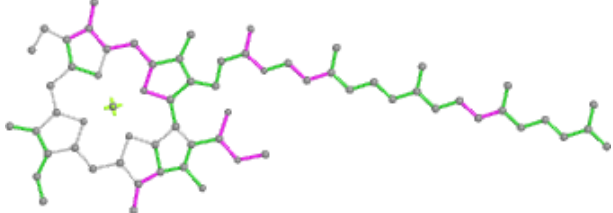
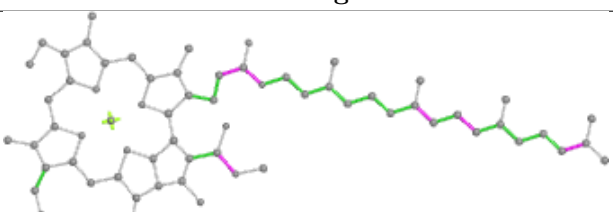
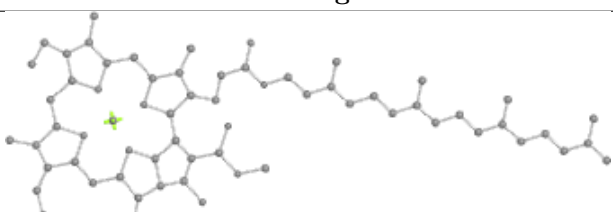


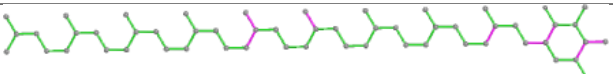
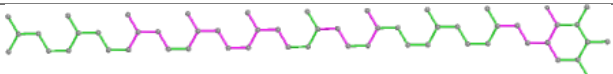
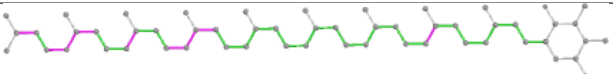
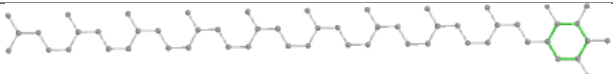
Ligand CLA c 507

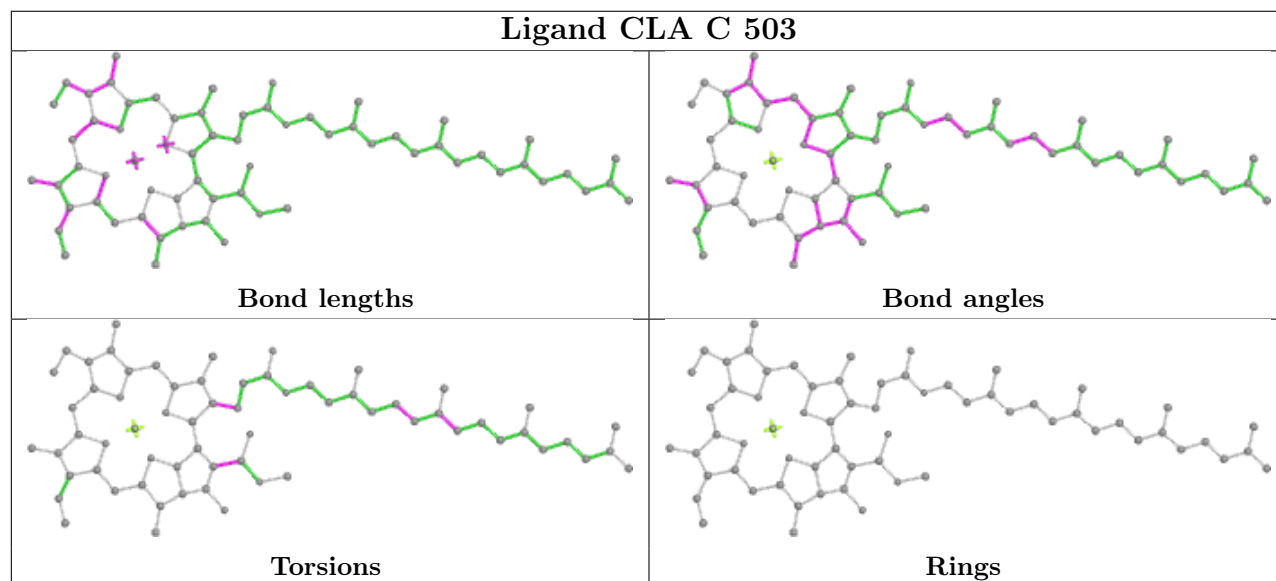
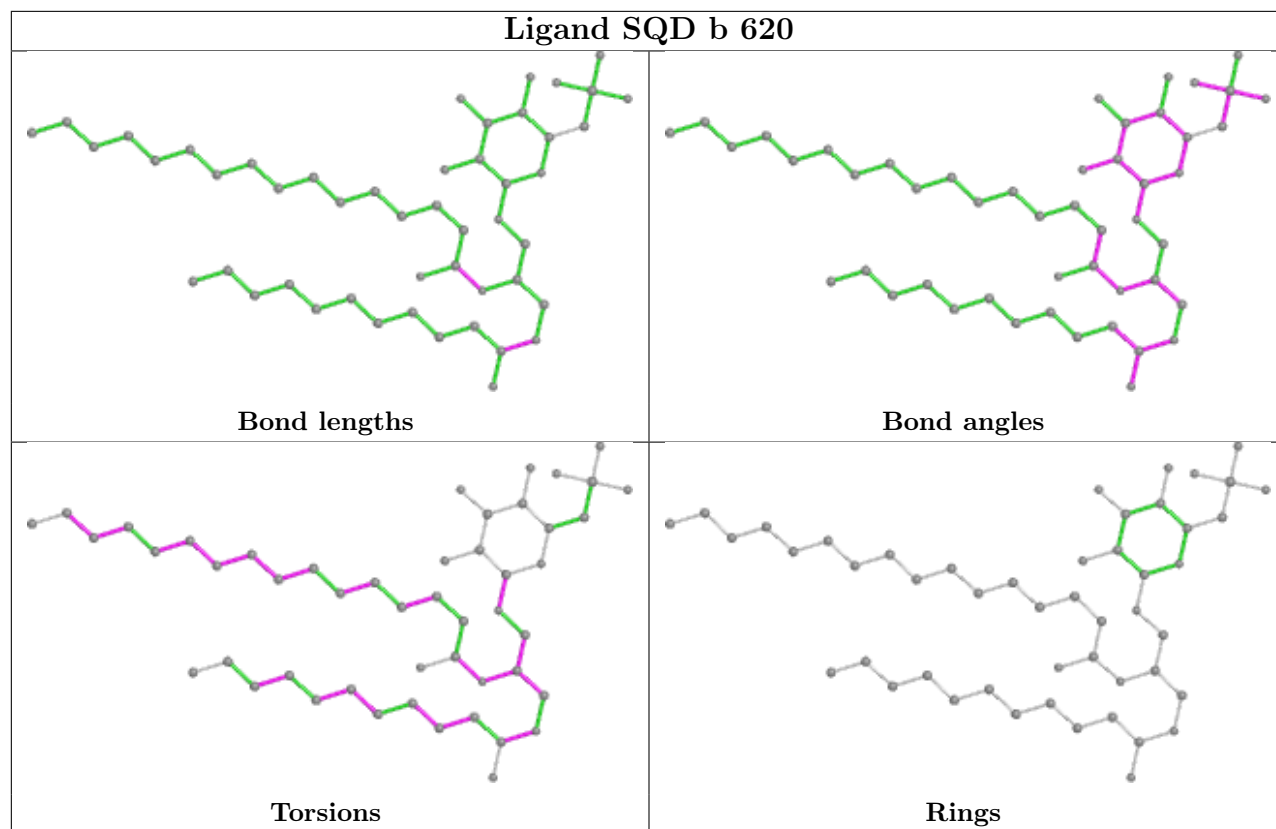


Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

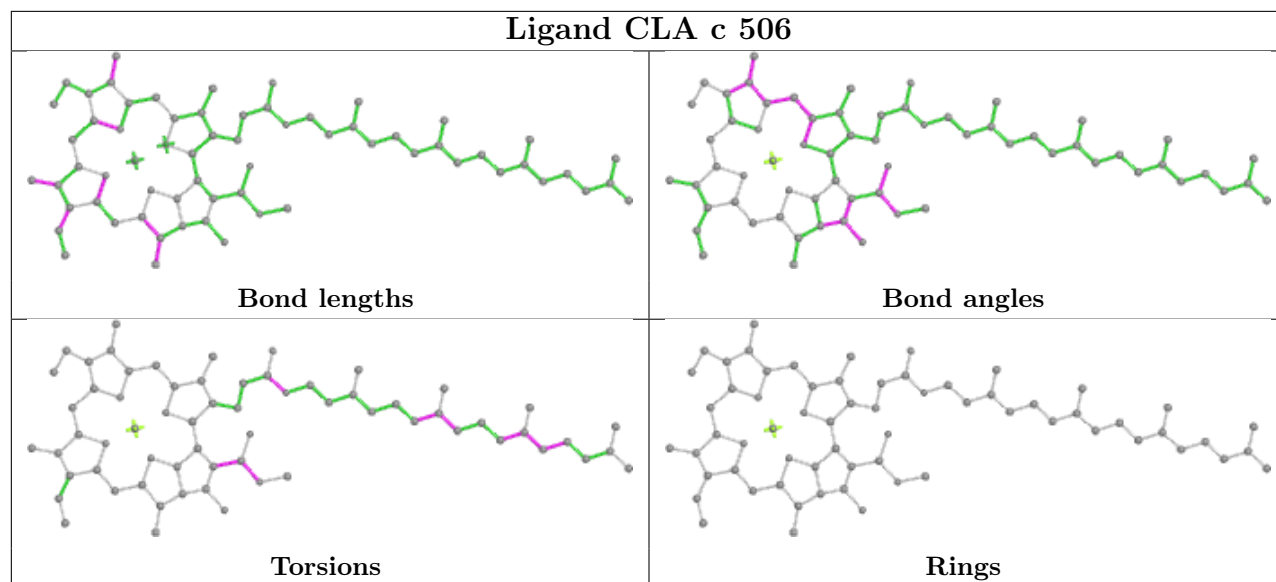
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

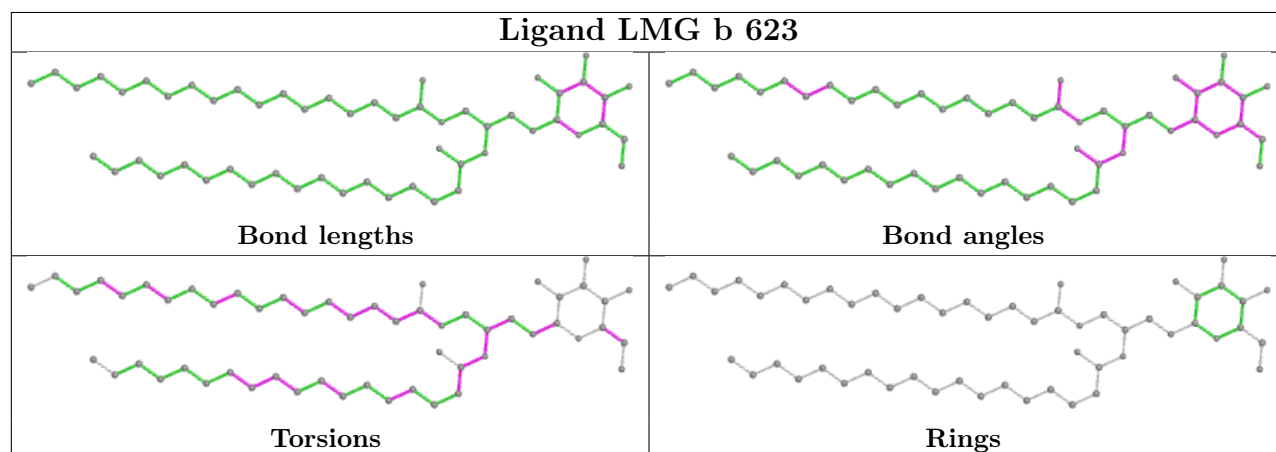
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



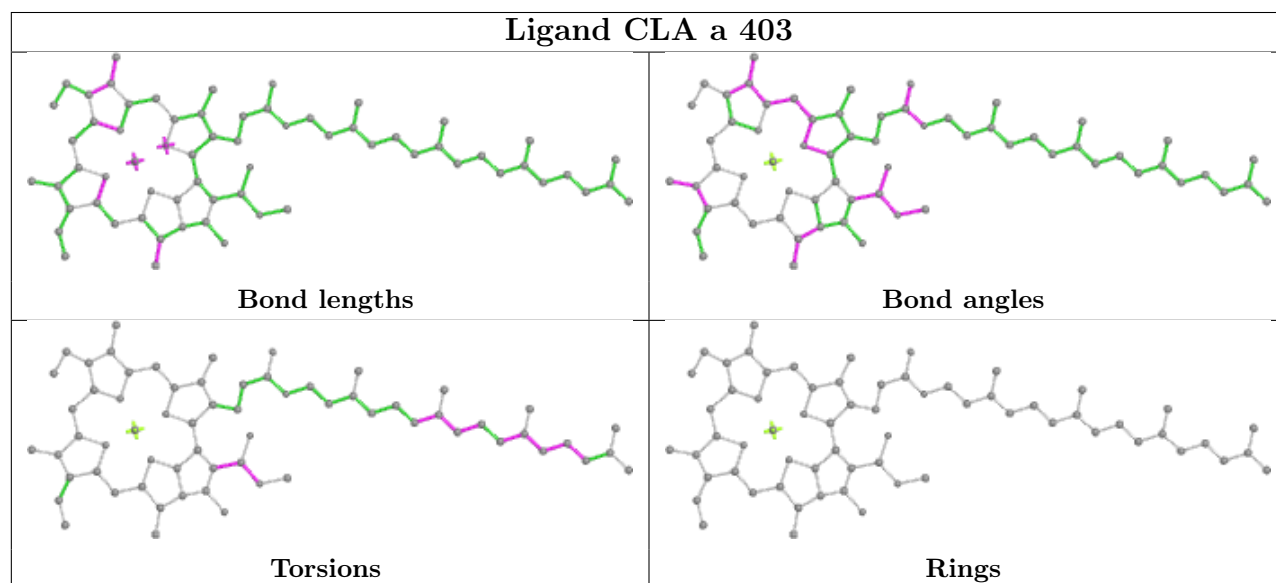
Ligand CLA c 506

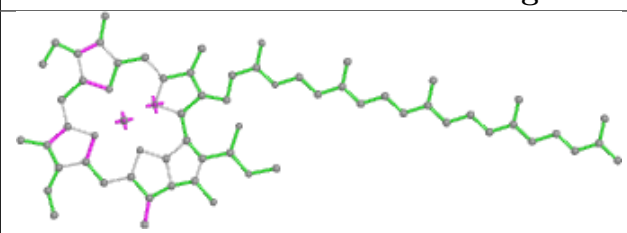
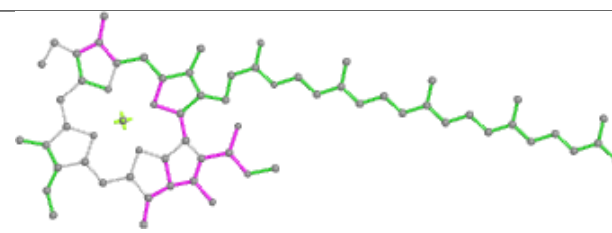
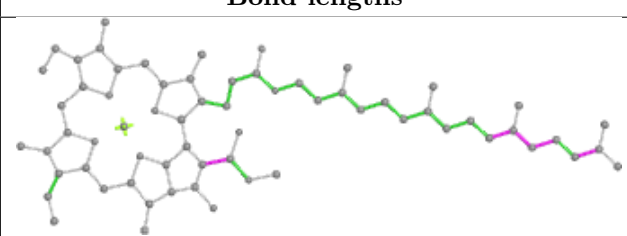
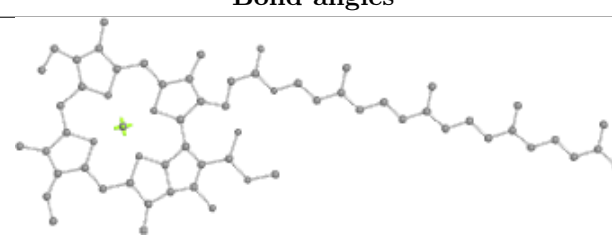


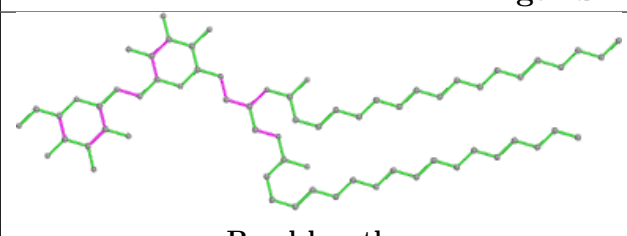
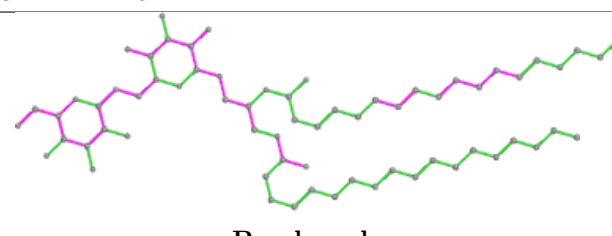
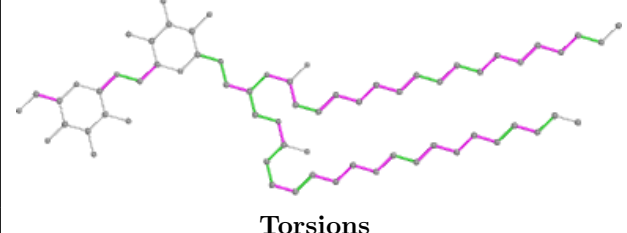
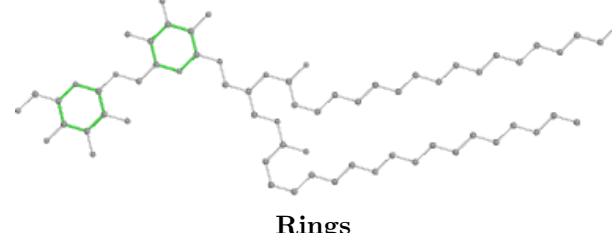
Ligand LMG b 623

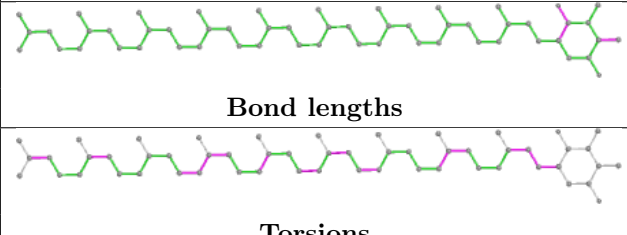
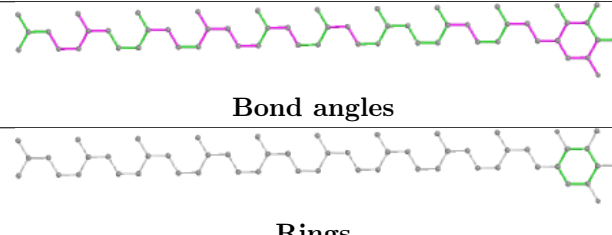
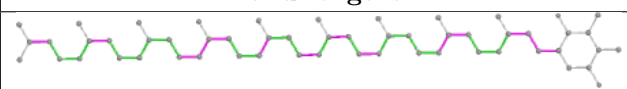
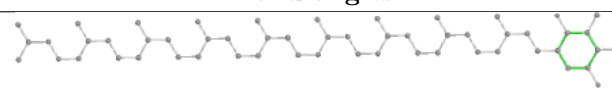


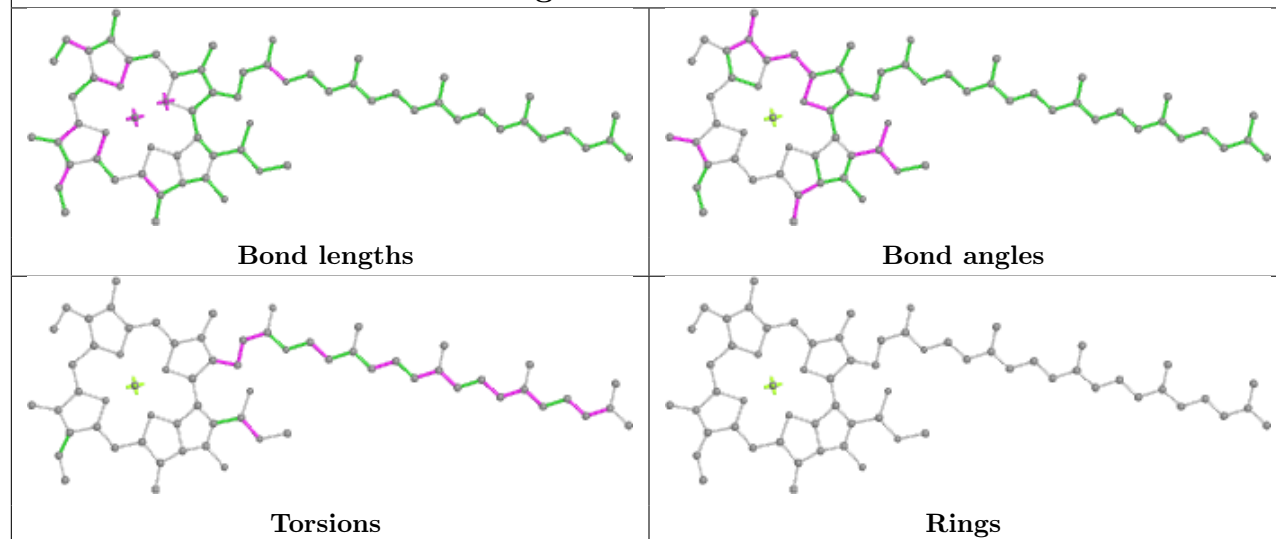
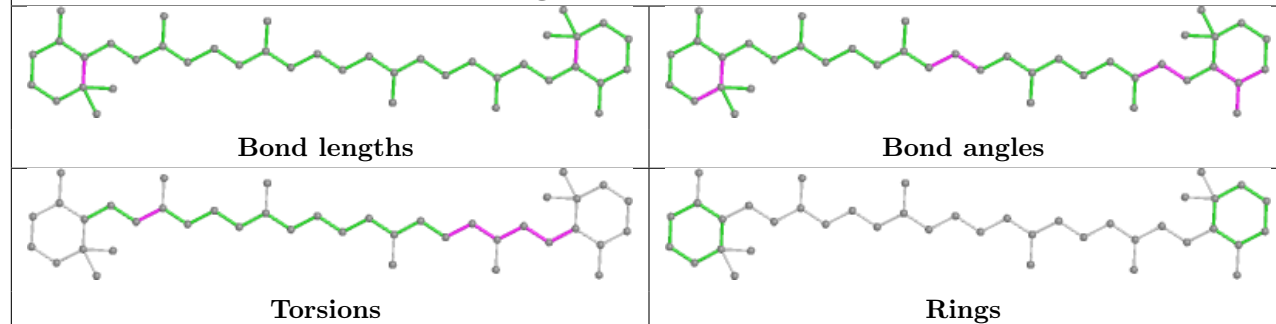
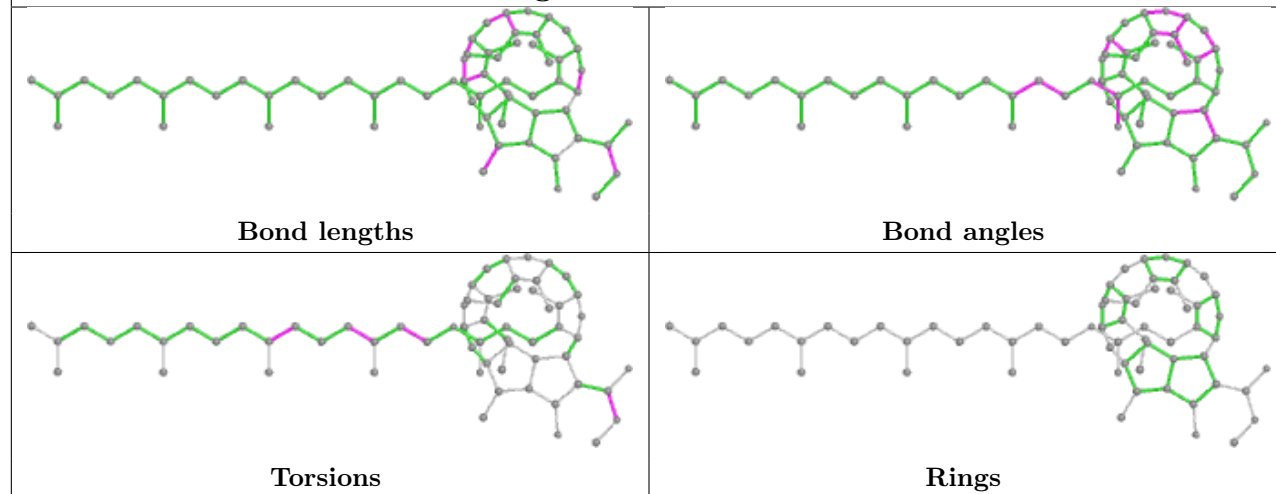
Ligand CLA a 403

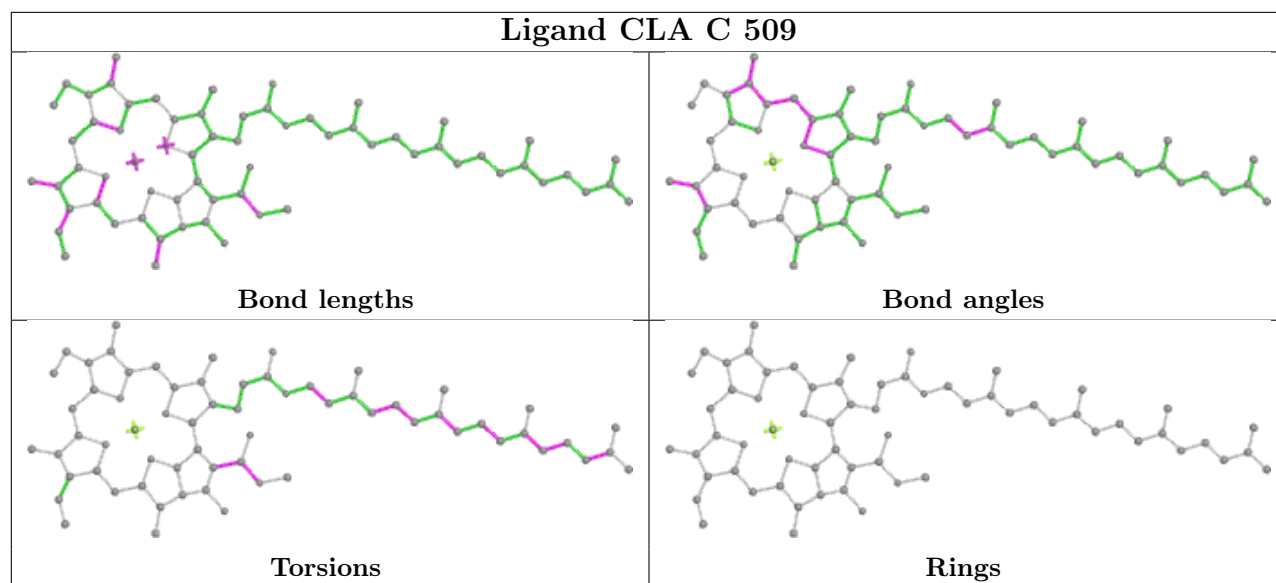
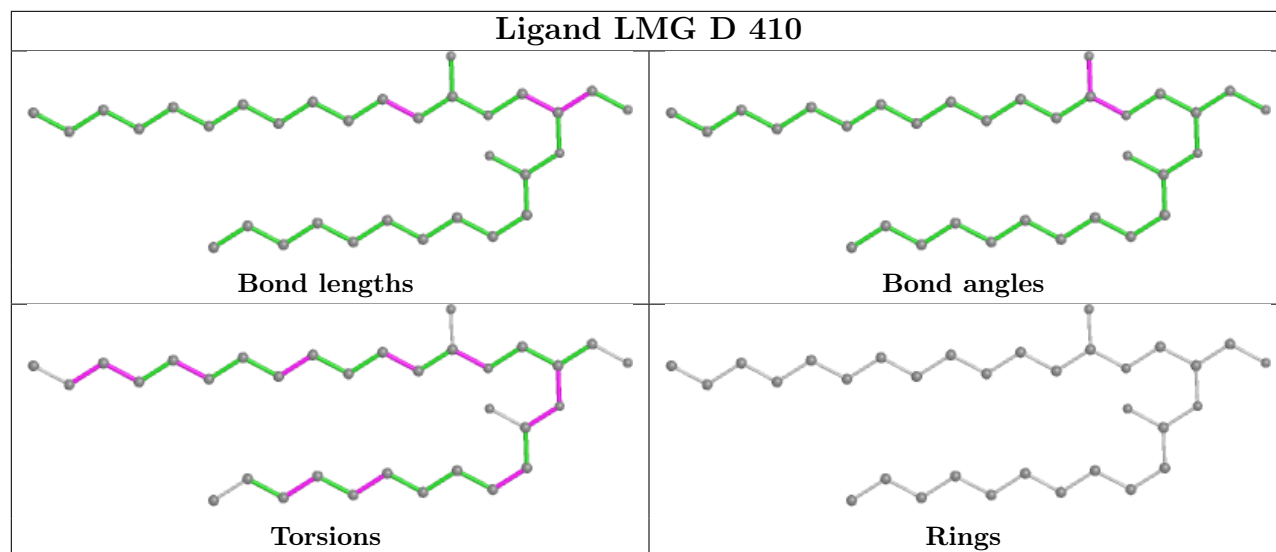
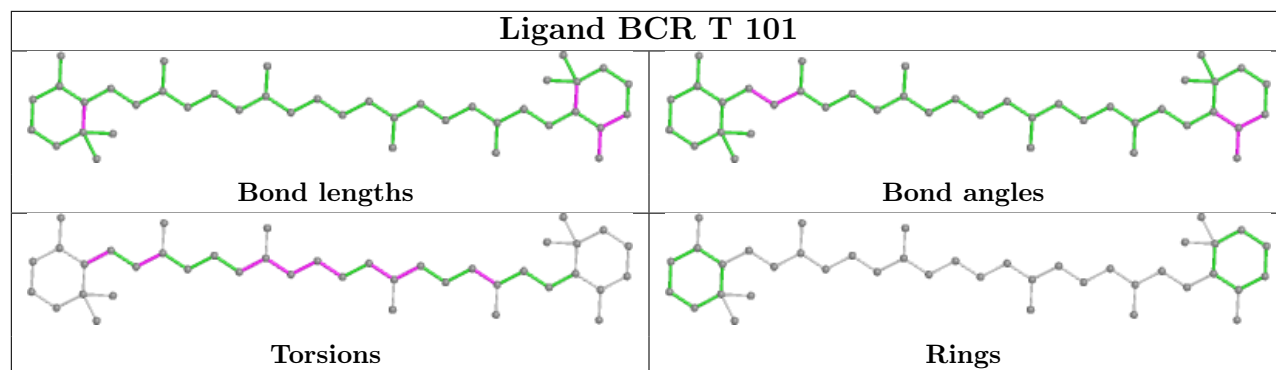


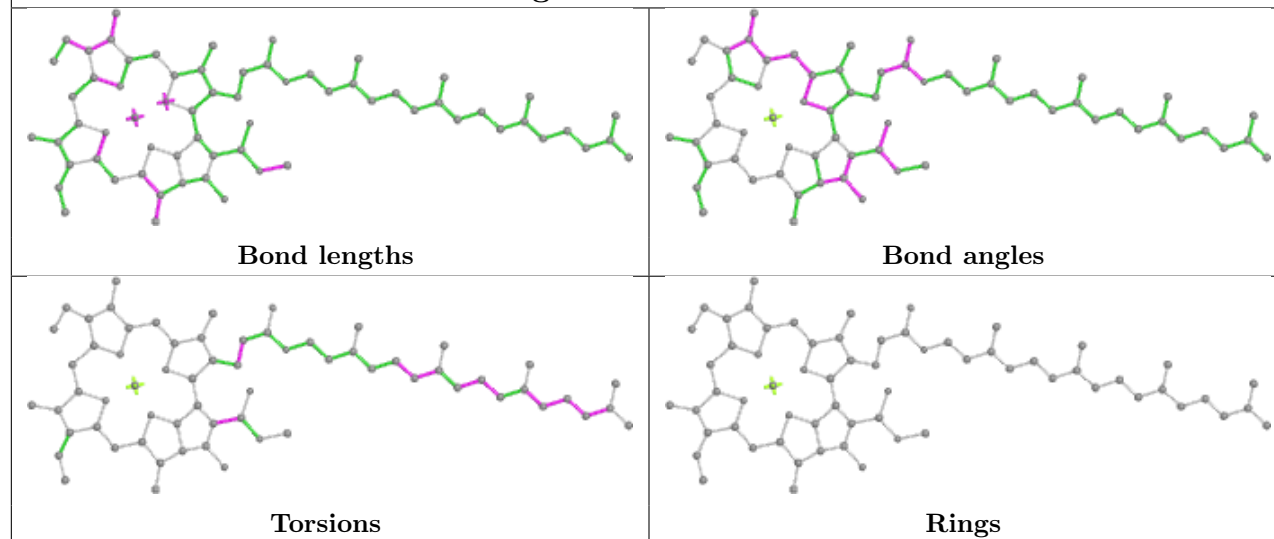
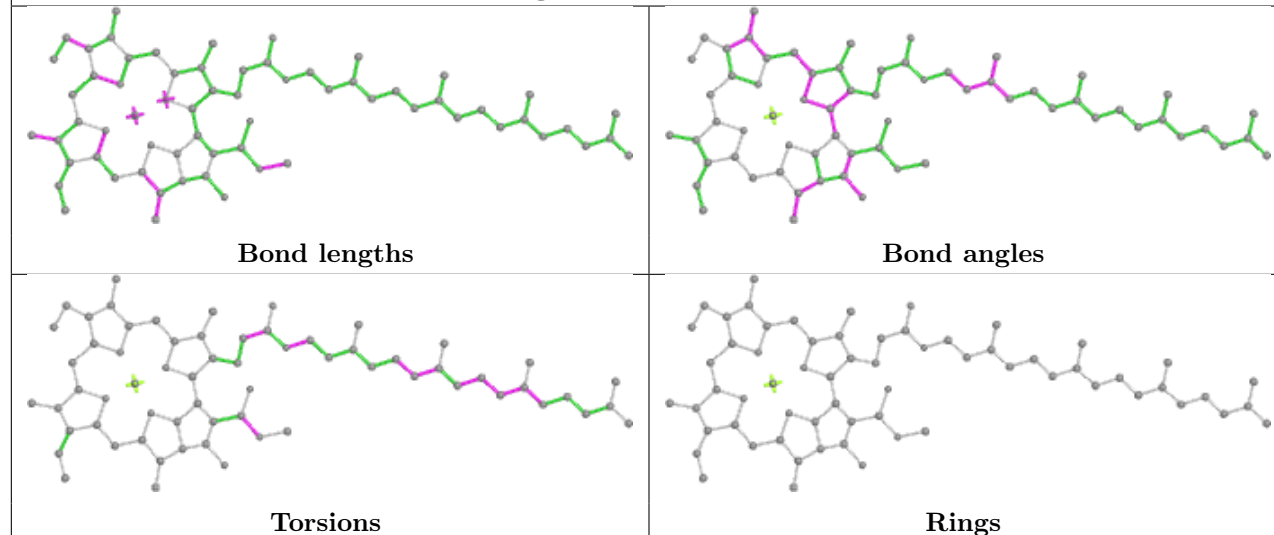
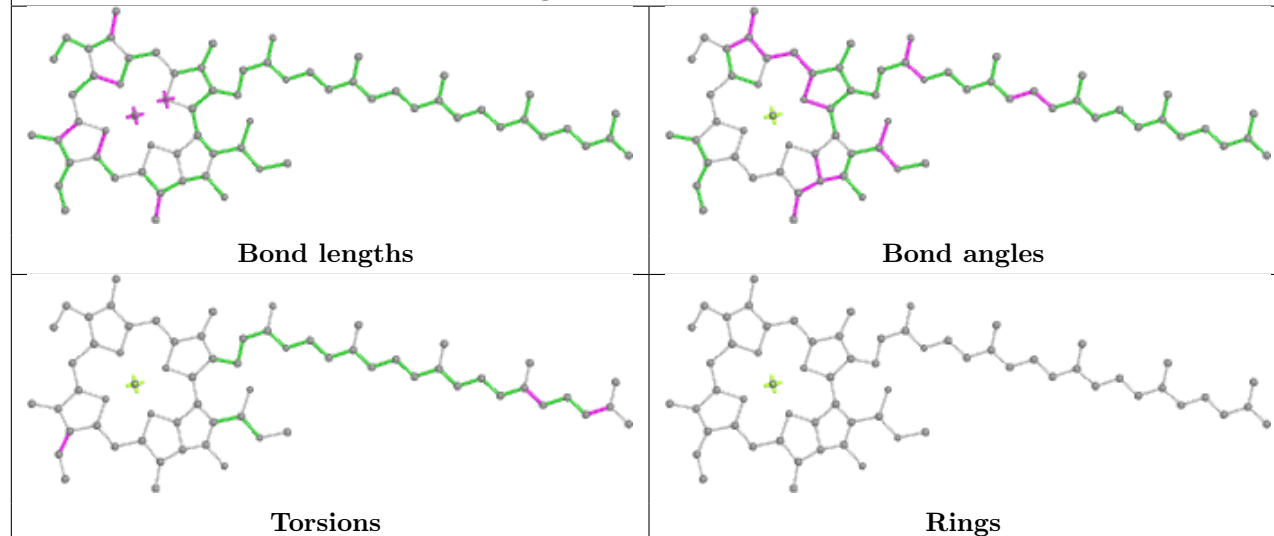
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

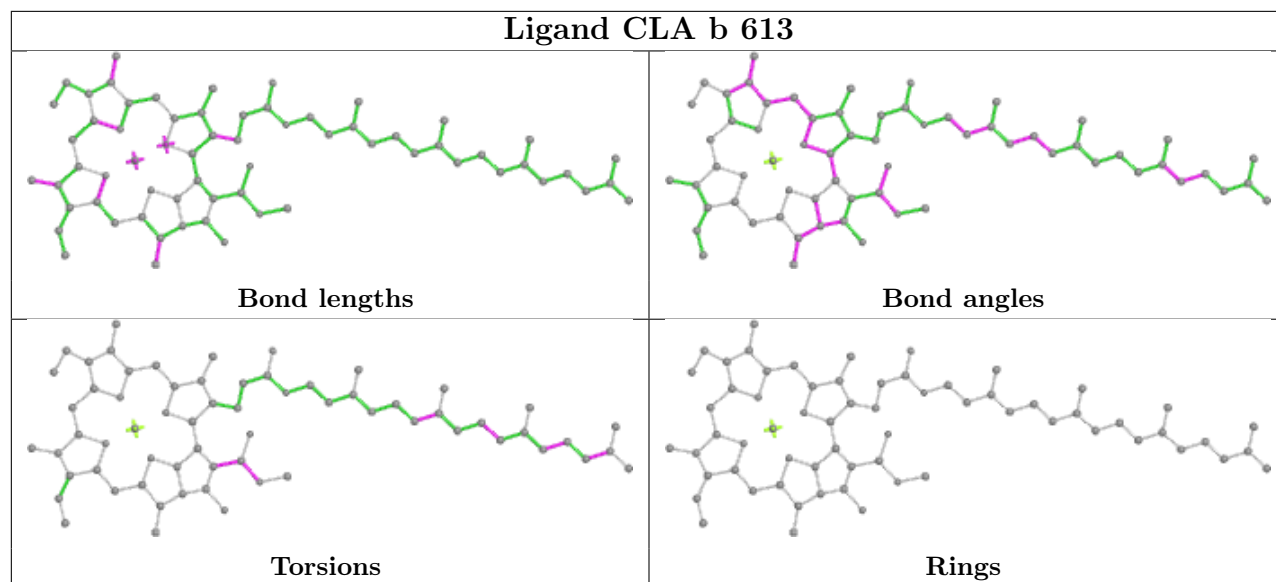
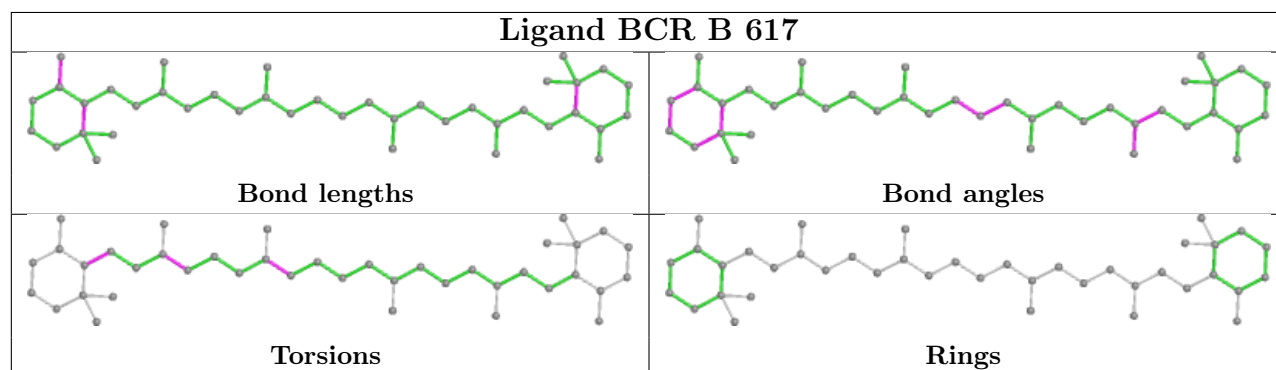
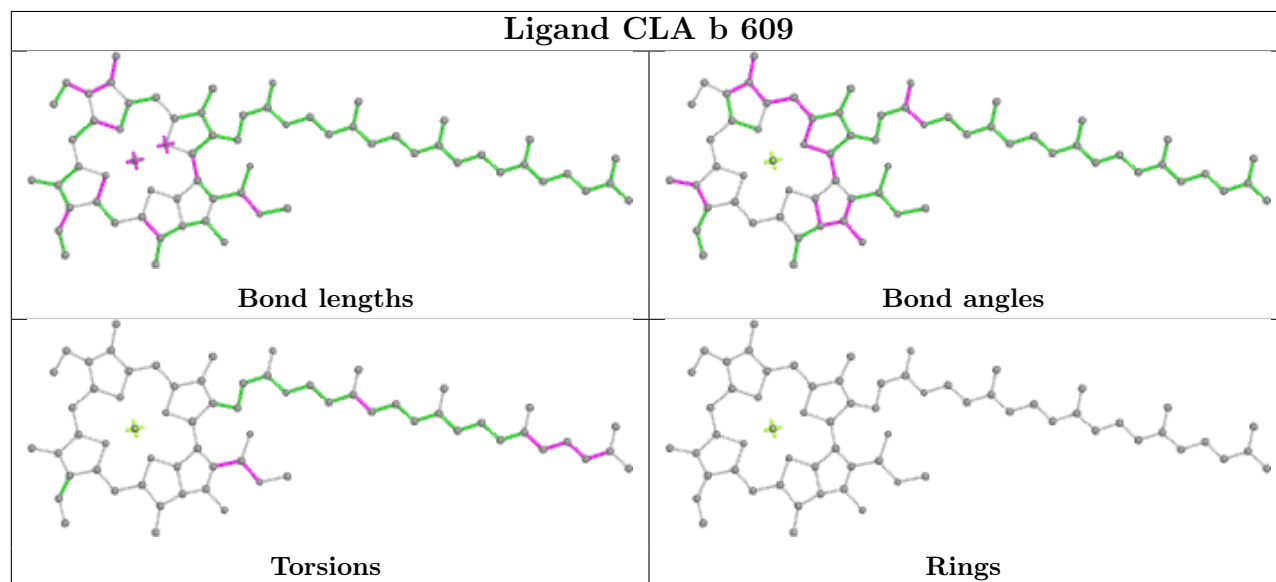
Ligand DGD A 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

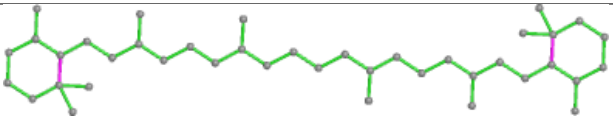
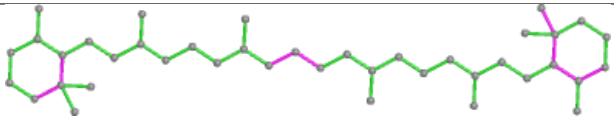
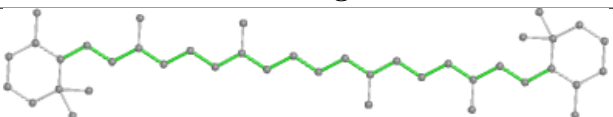
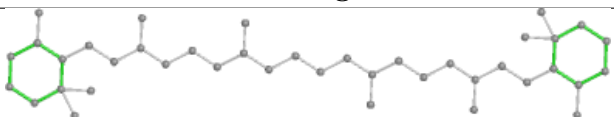
Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

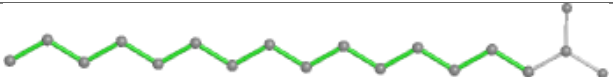
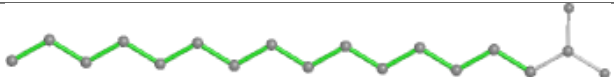
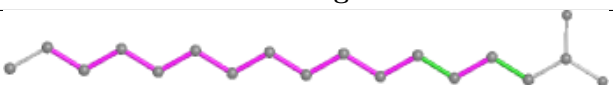

Ligand CLA b 601**Ligand BCR d 406****Ligand PHO a 404**

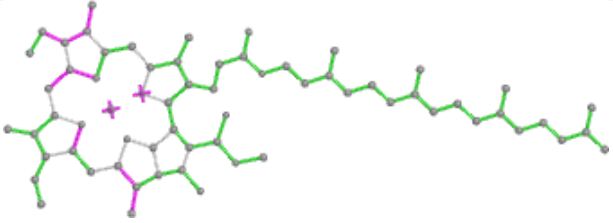
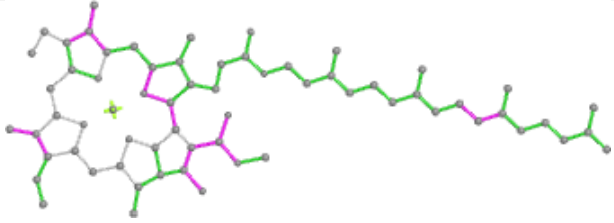
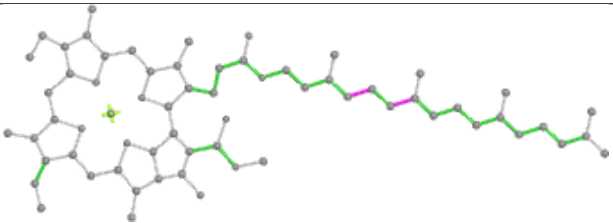
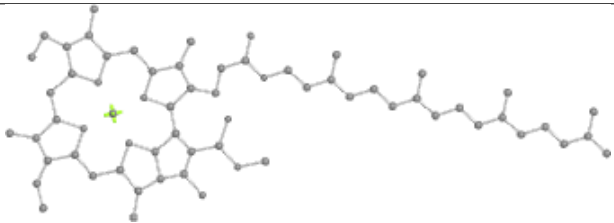


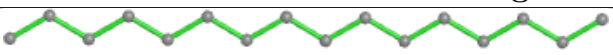
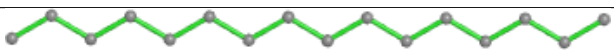
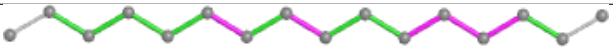

Ligand CLA B 603**Ligand CLA B 613****Ligand CLA a 402**

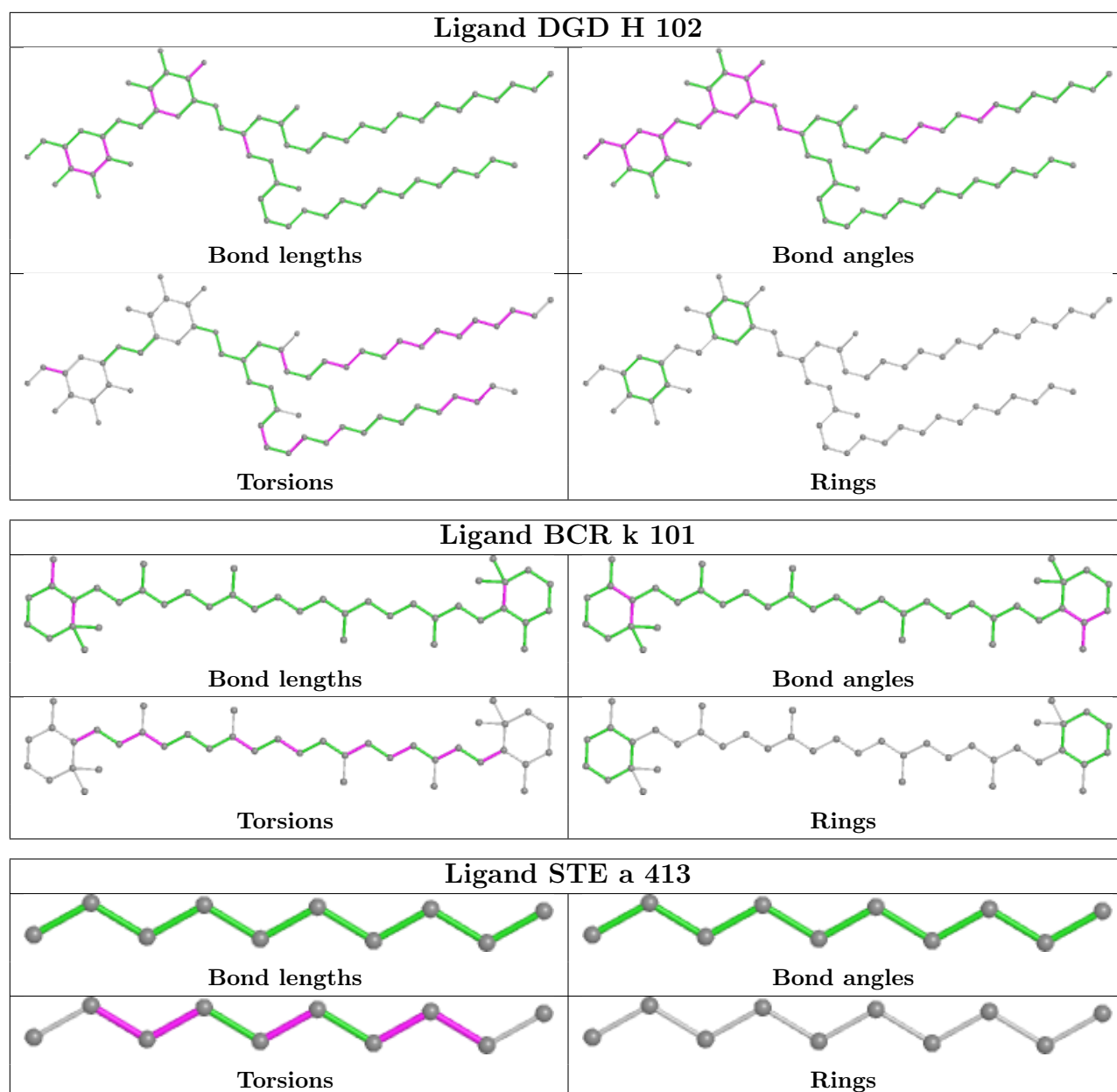
Ligand CLA b 613**Ligand BCR B 617****Ligand CLA b 609**

Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

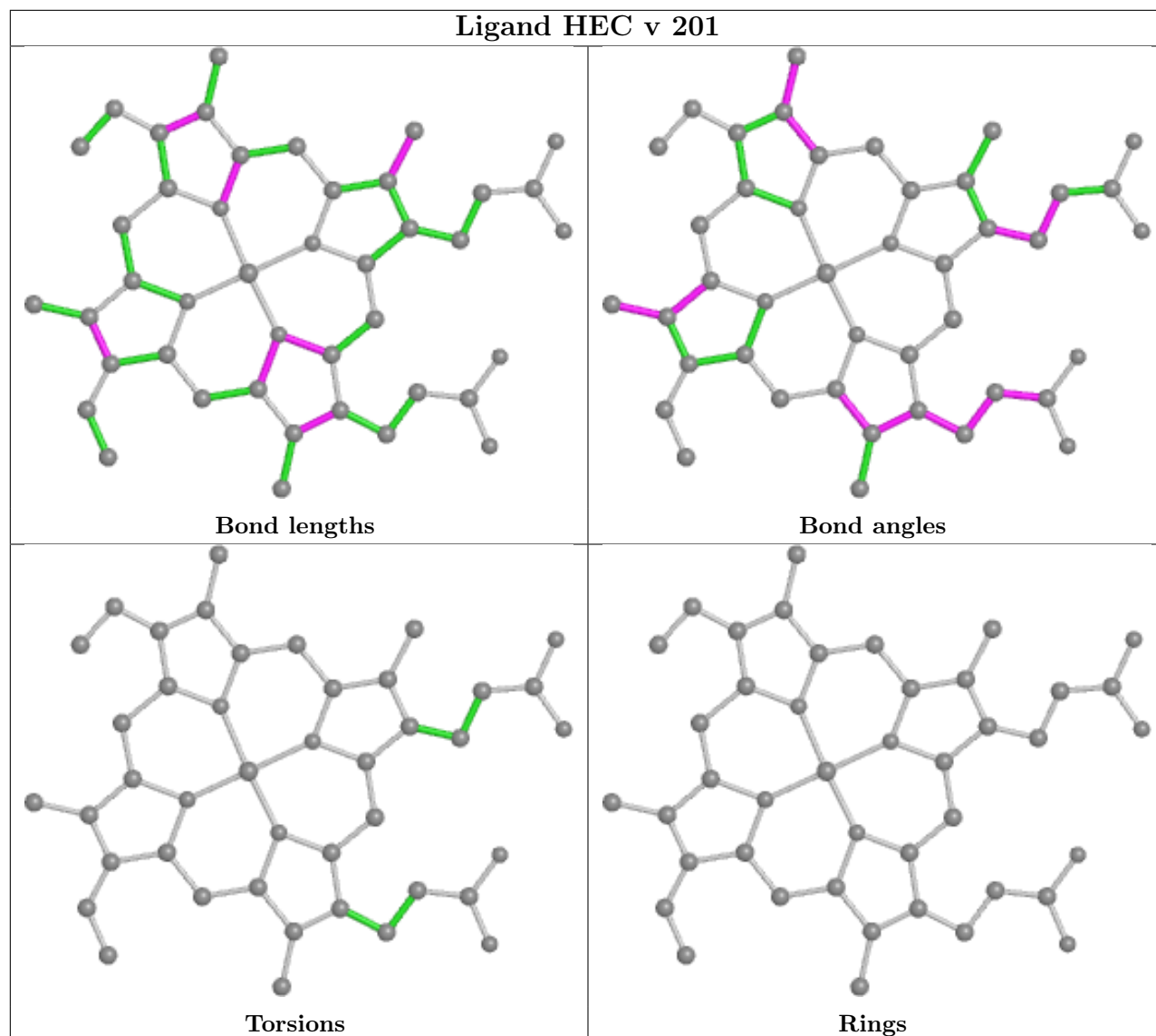
Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

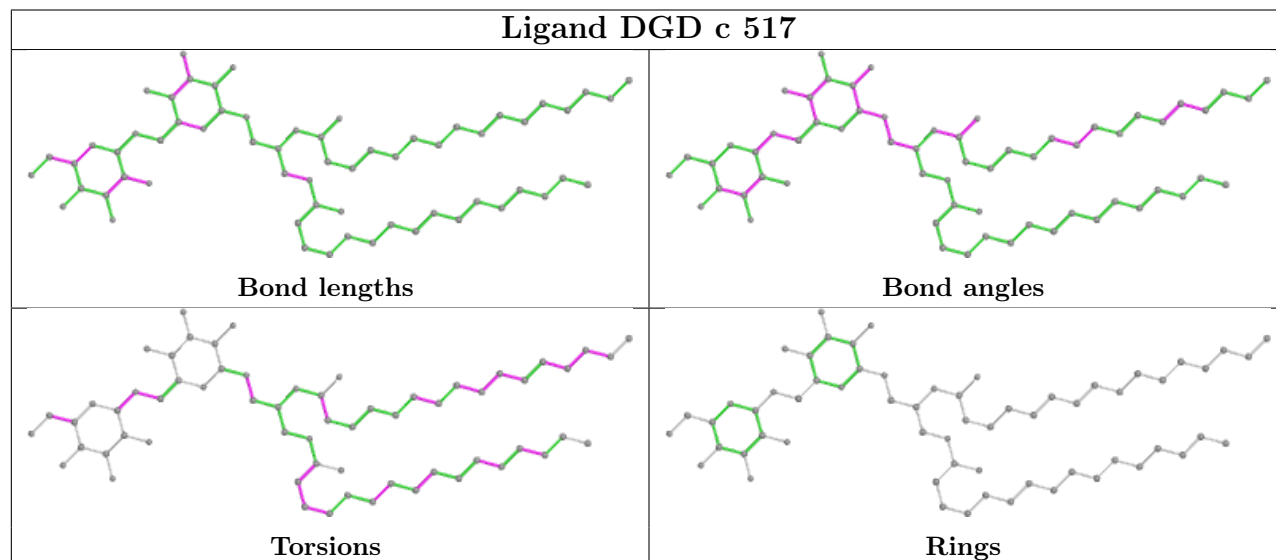
Ligand STE C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings



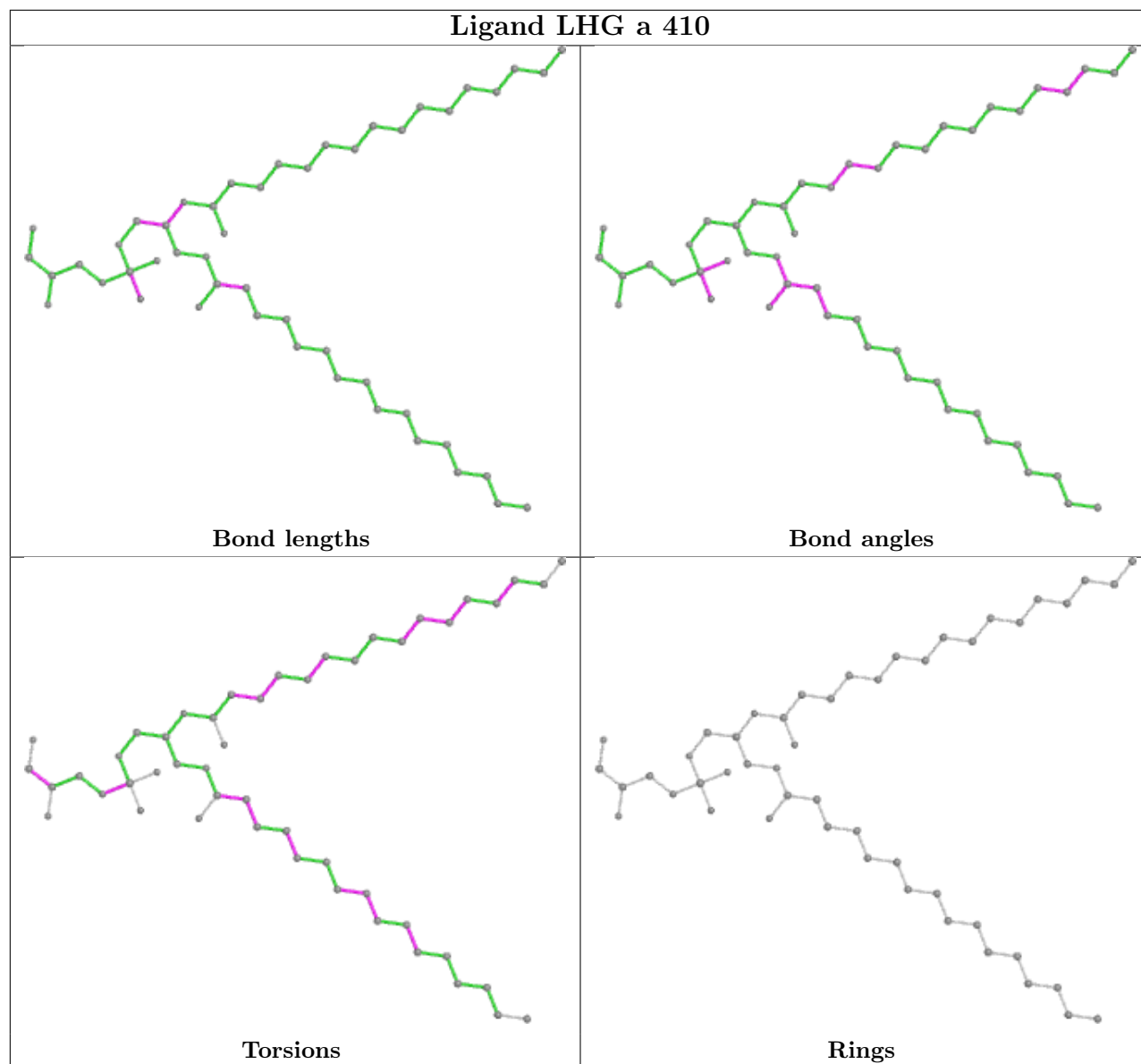
Ligand HEC v 201



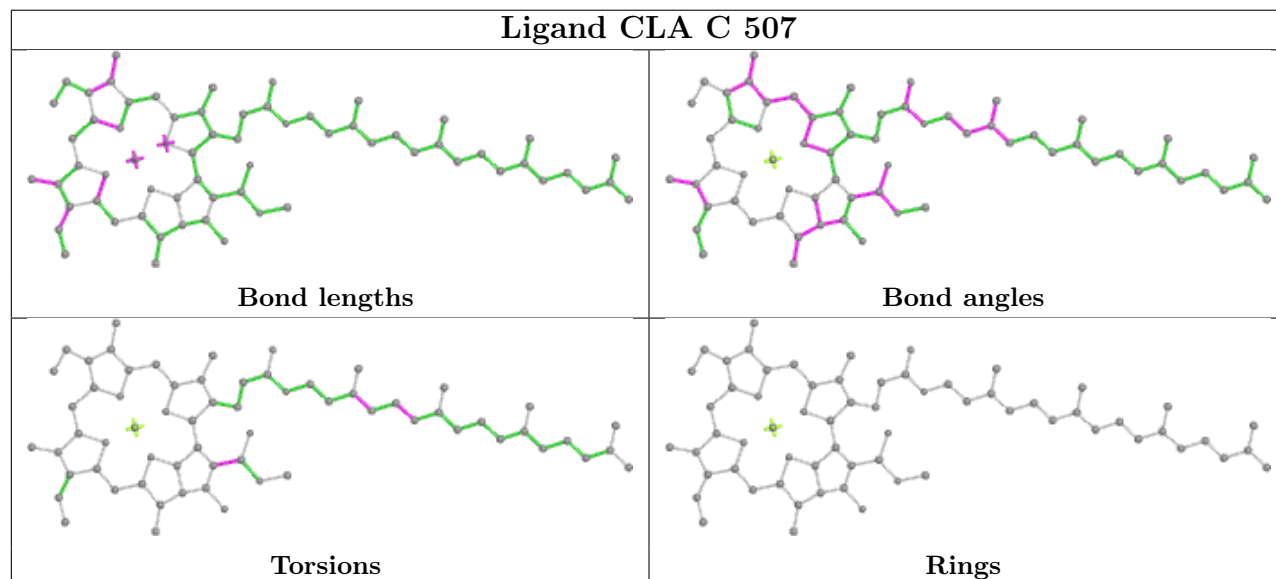
Ligand DGD c 517

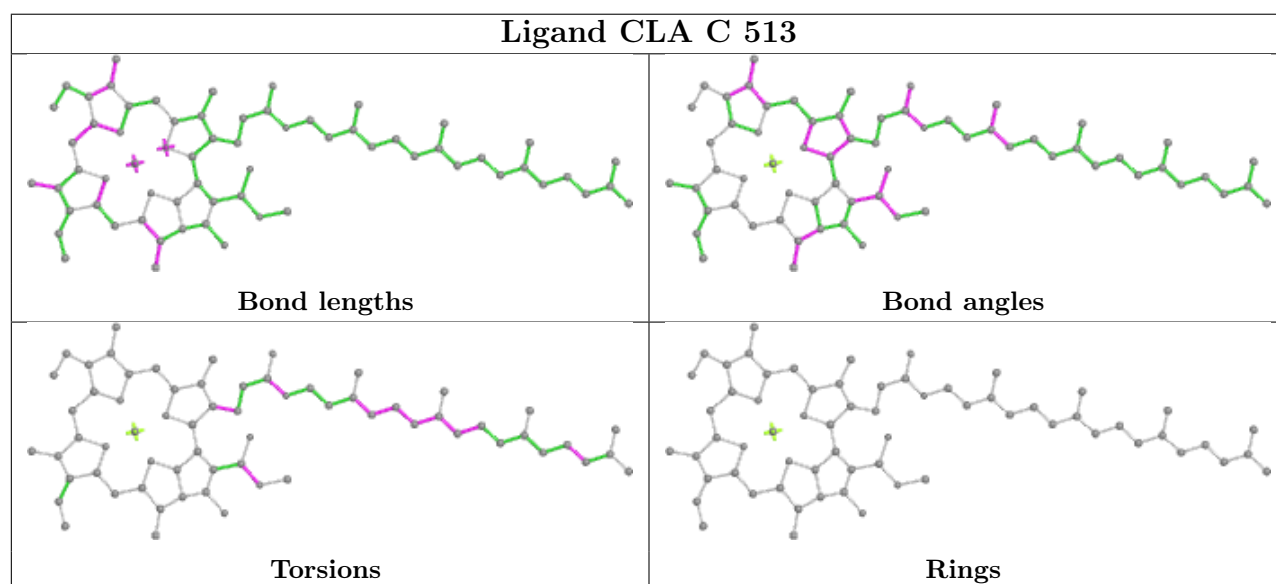
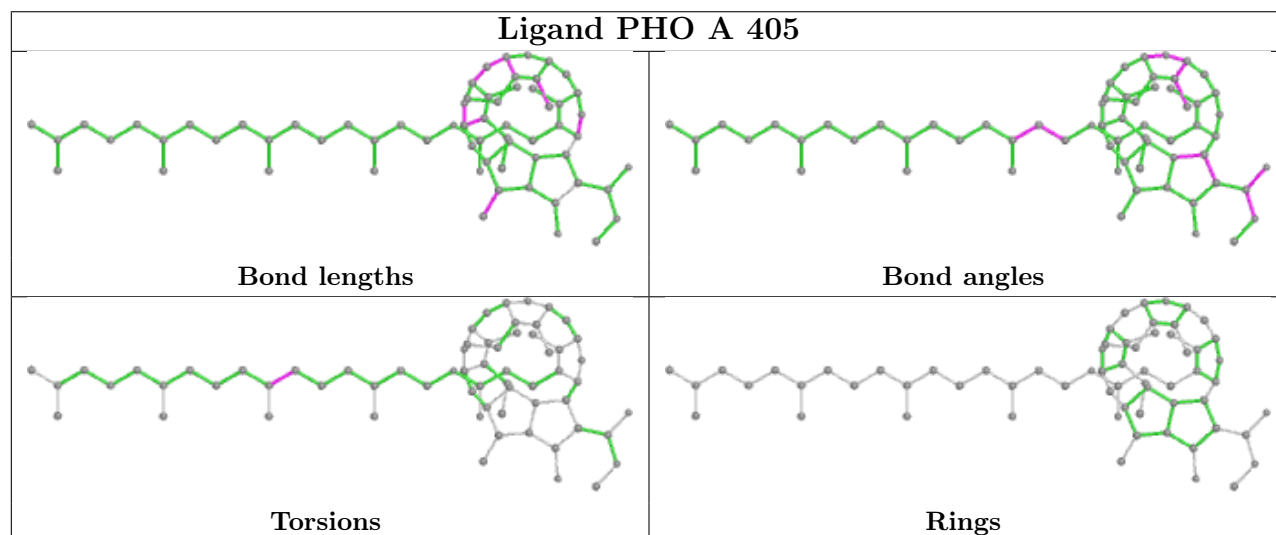
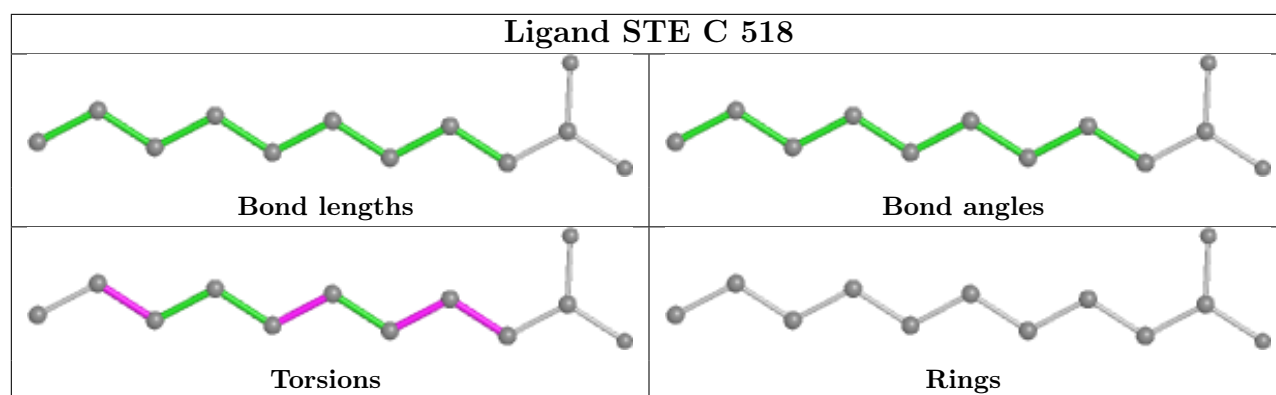


Ligand LHG a 410

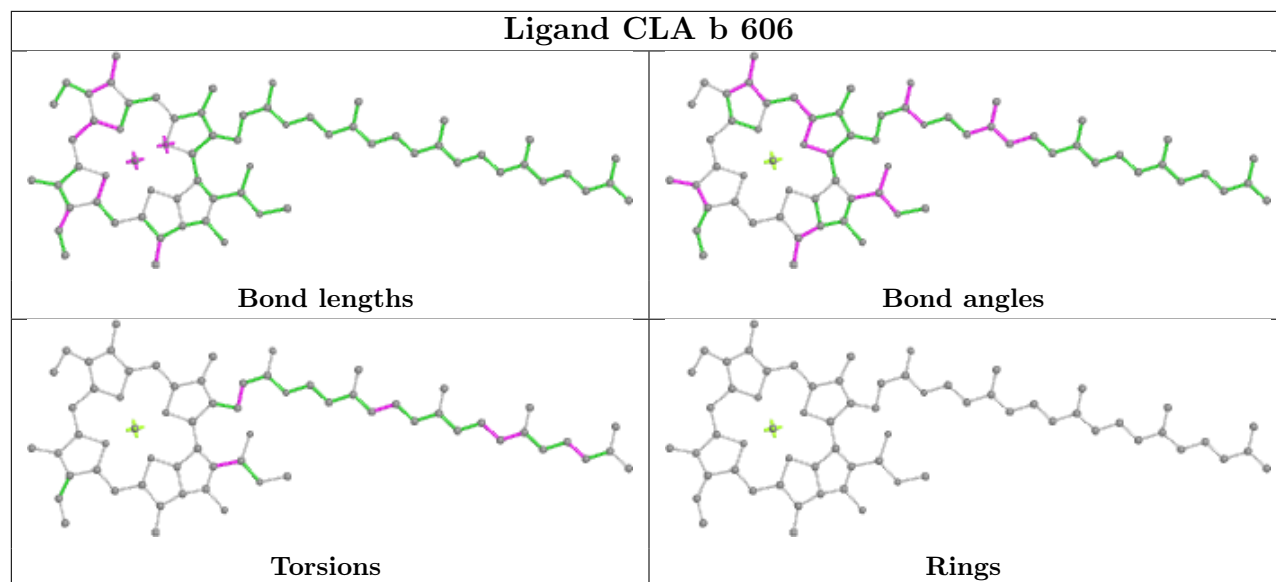


Ligand CLA C 507

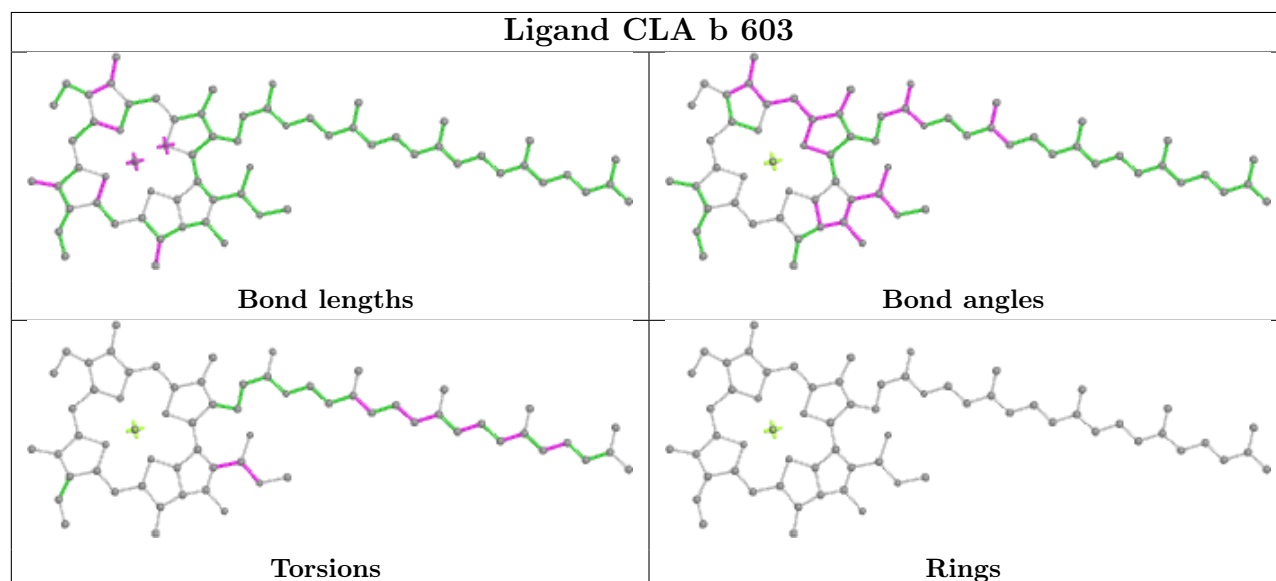




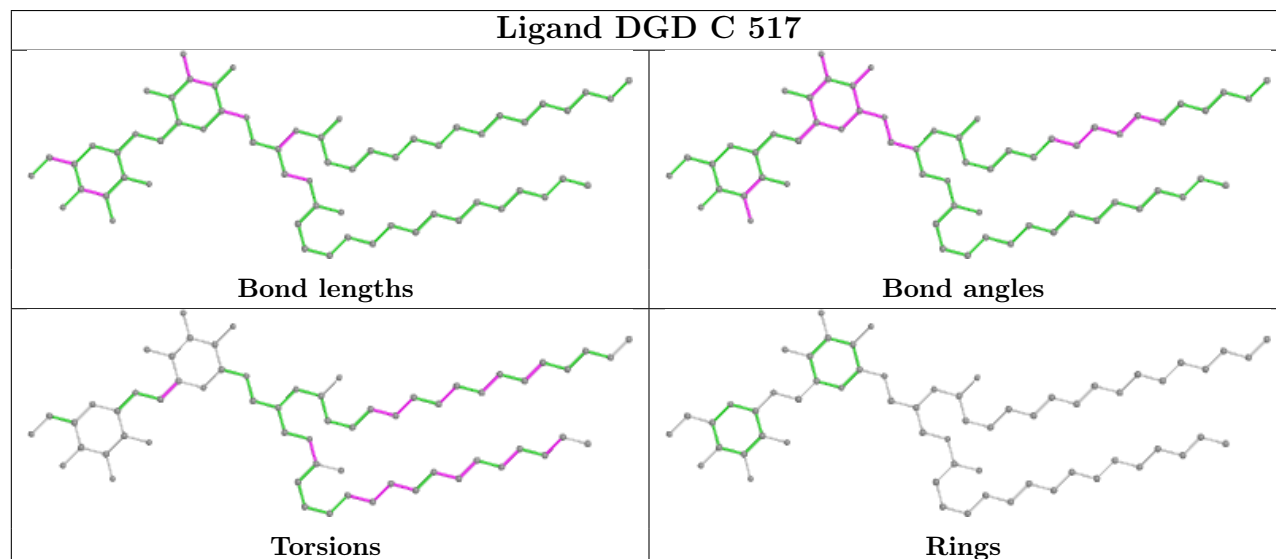
Ligand CLA b 606

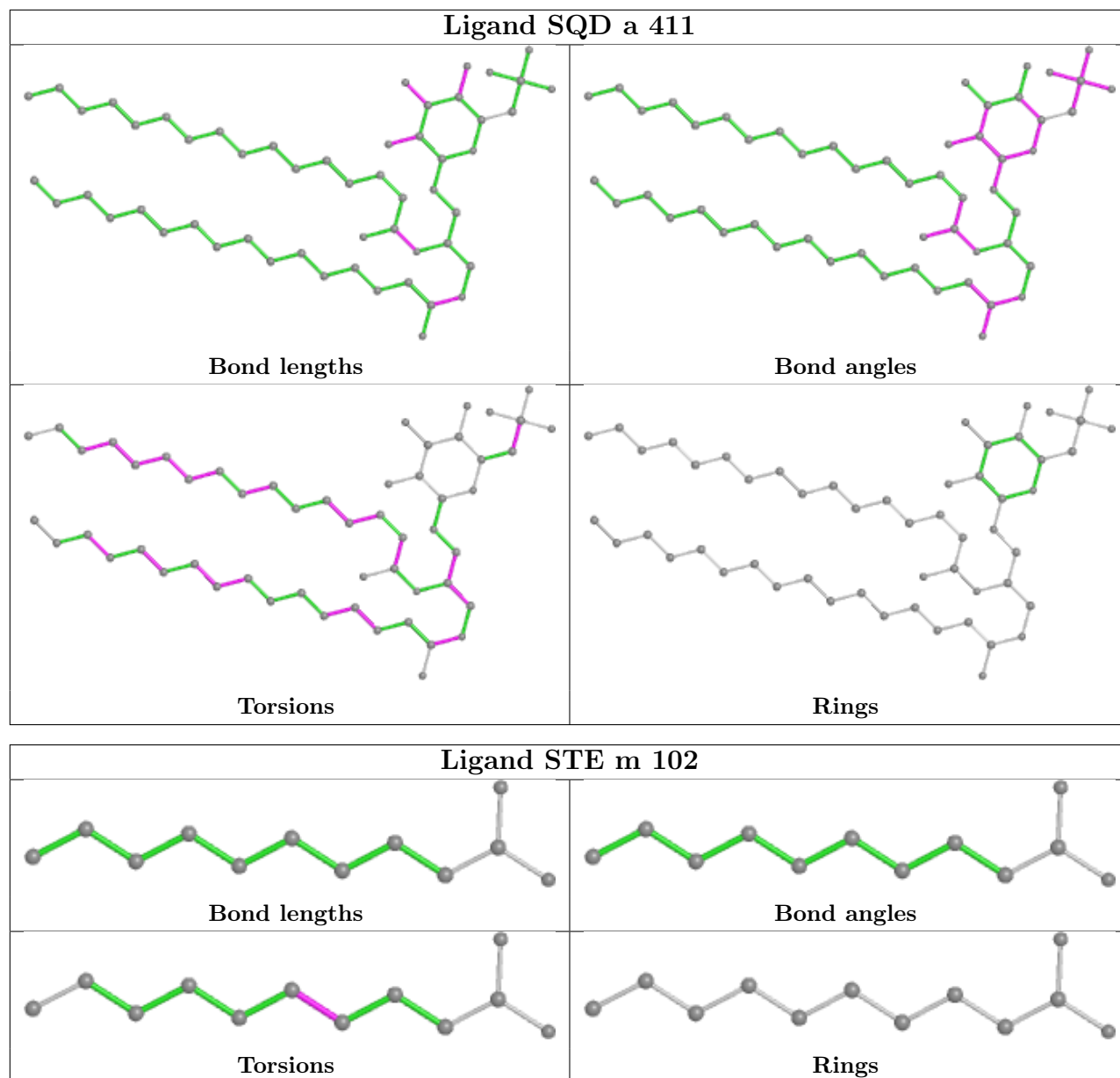


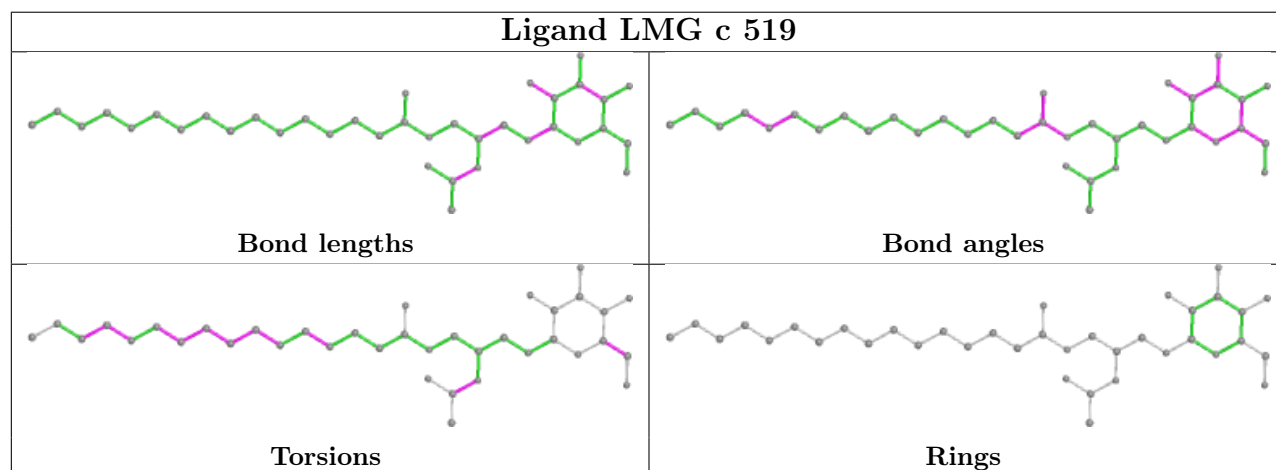
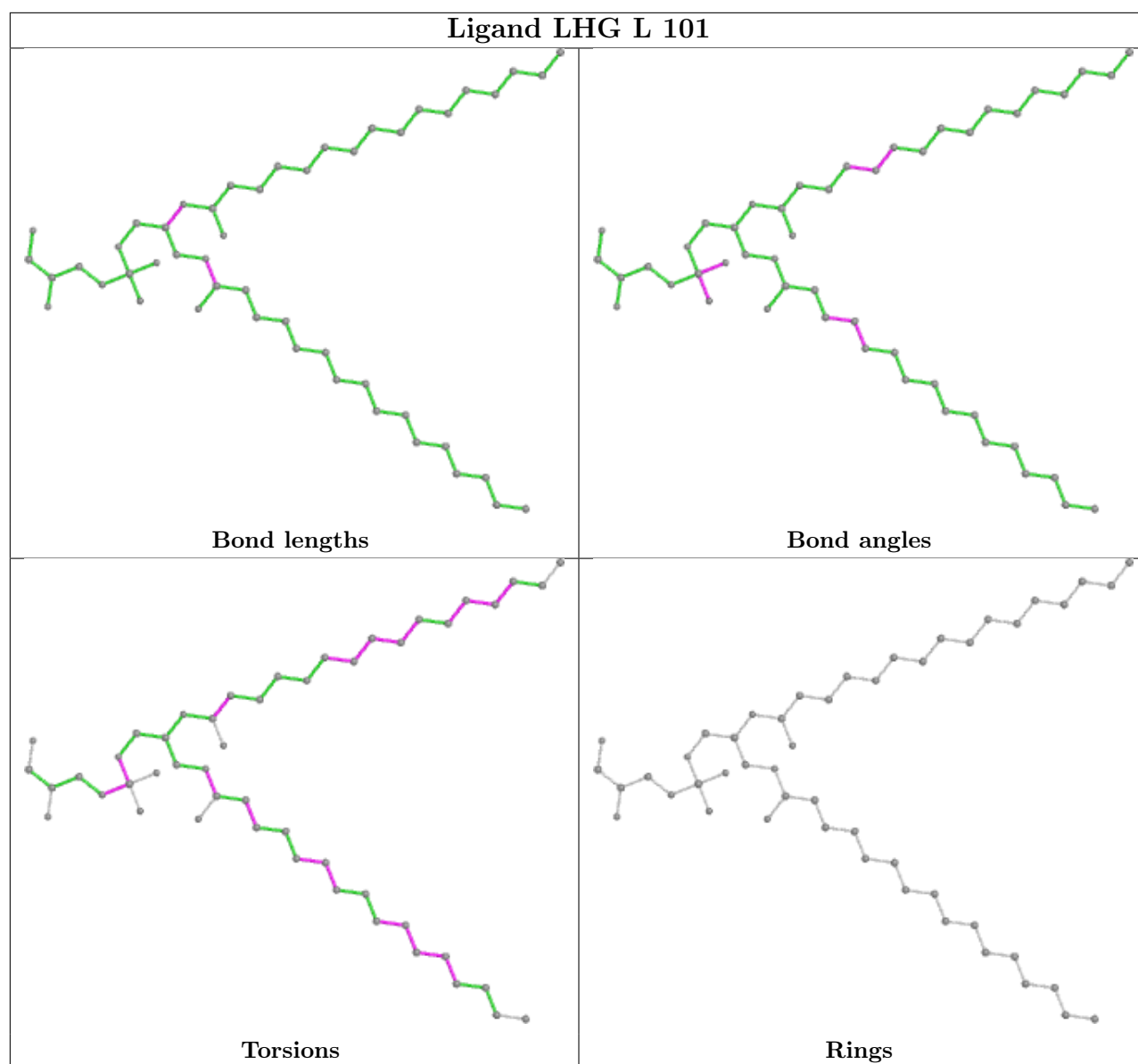
Ligand CLA b 603

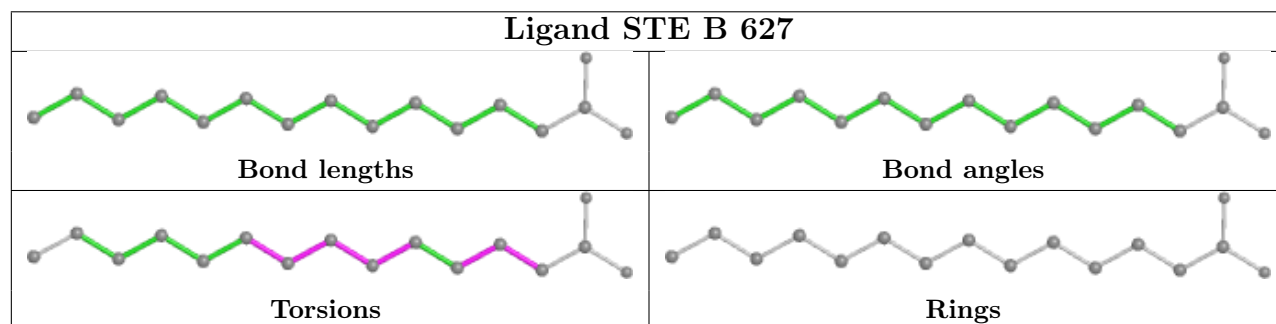
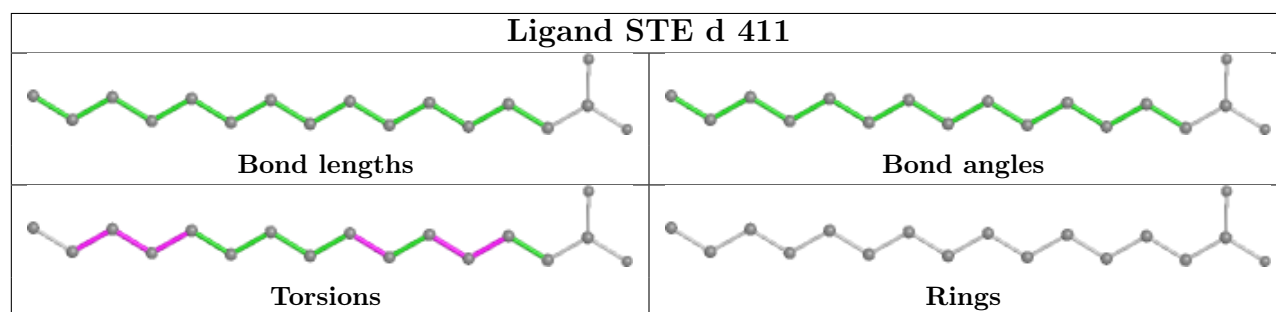
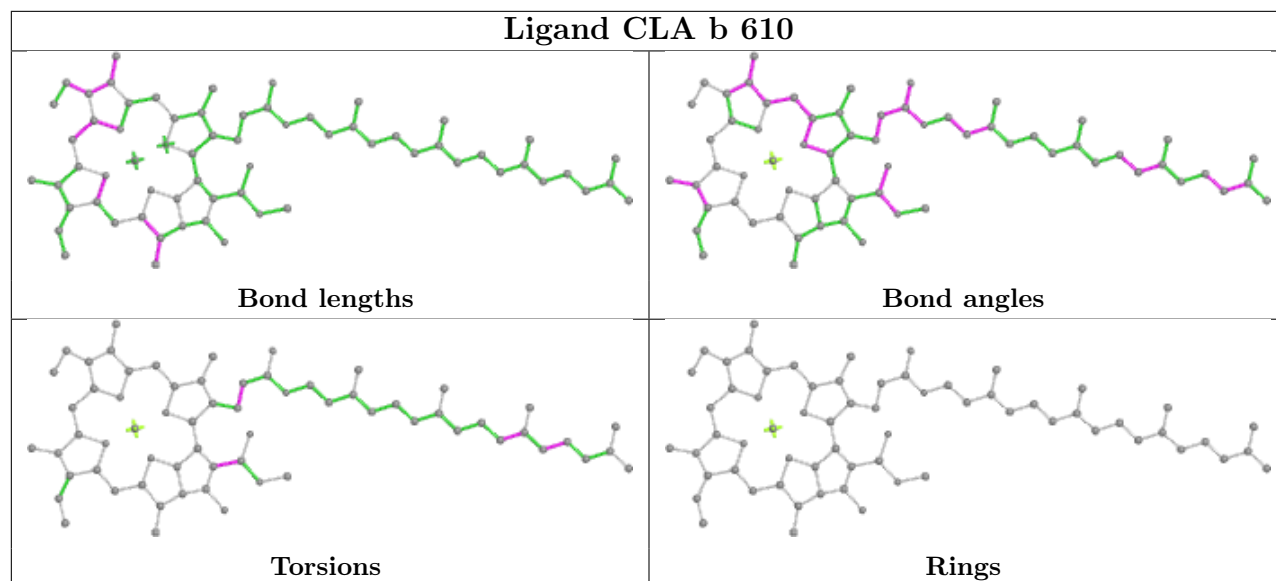
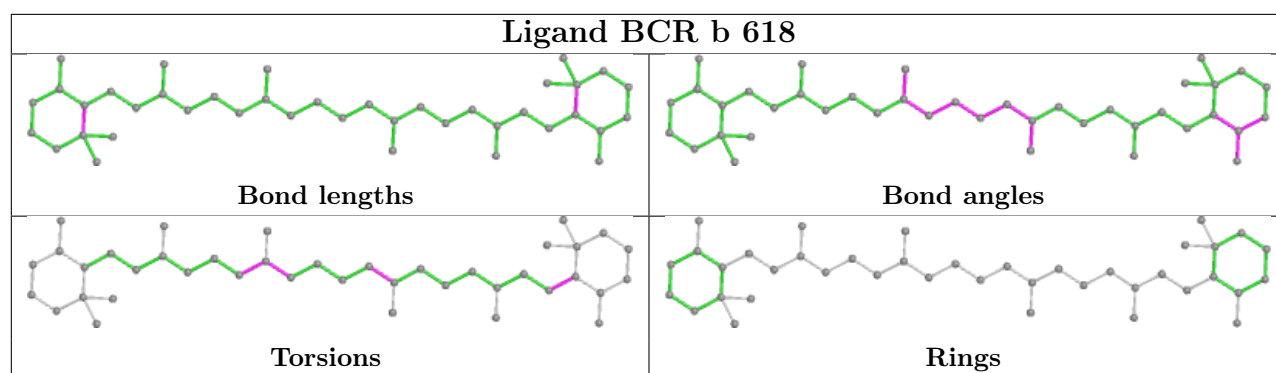


Ligand DGD C 517

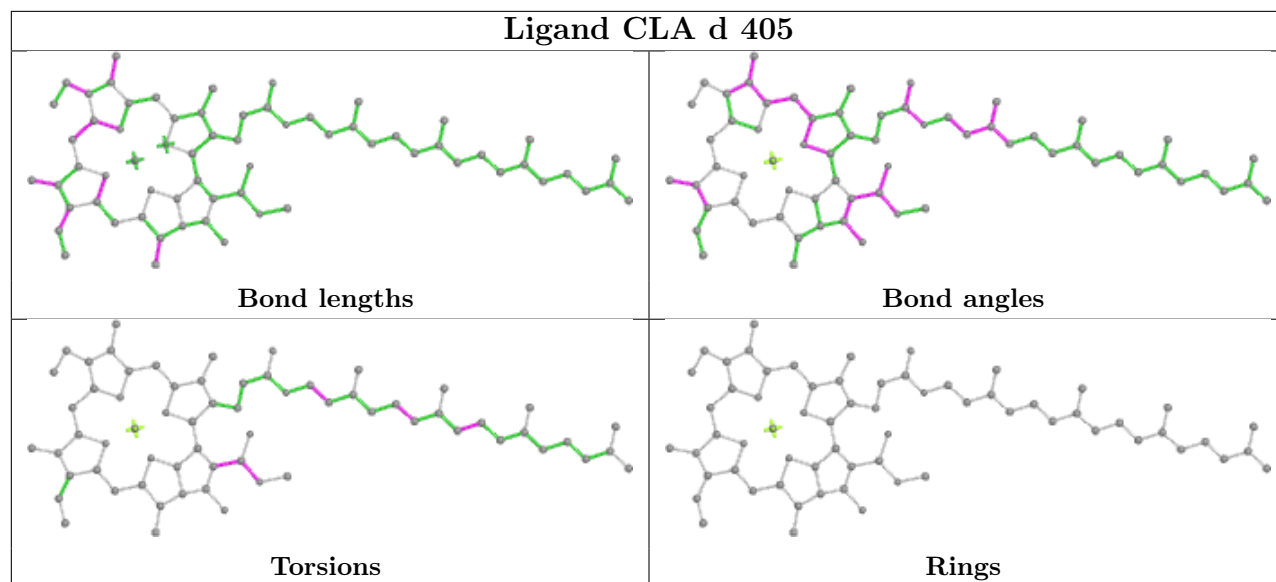




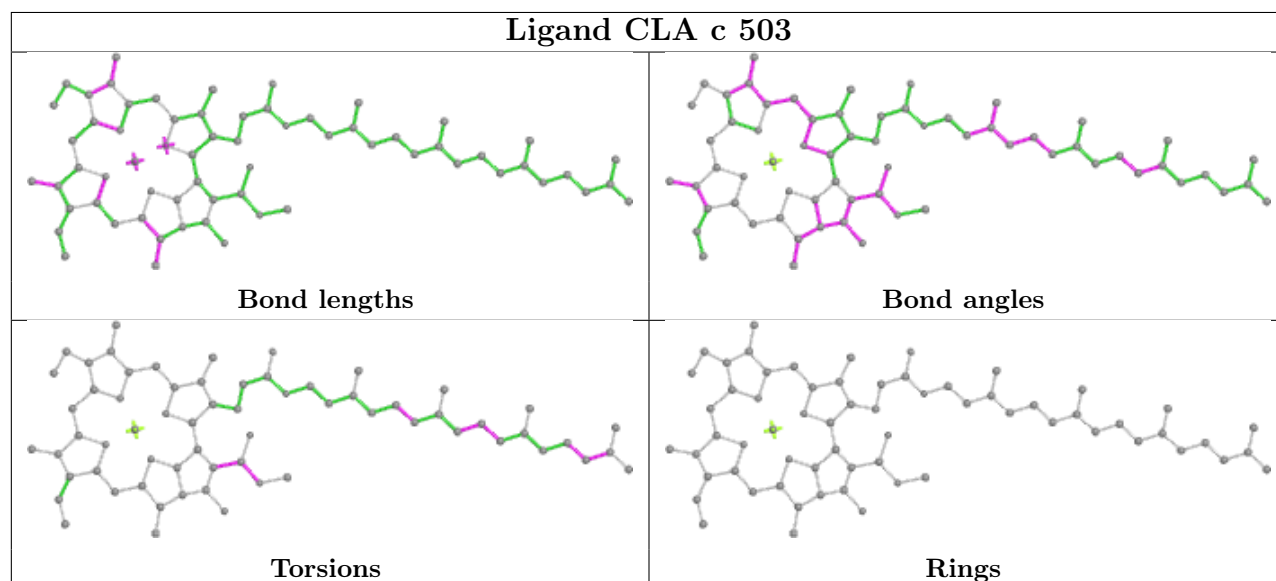




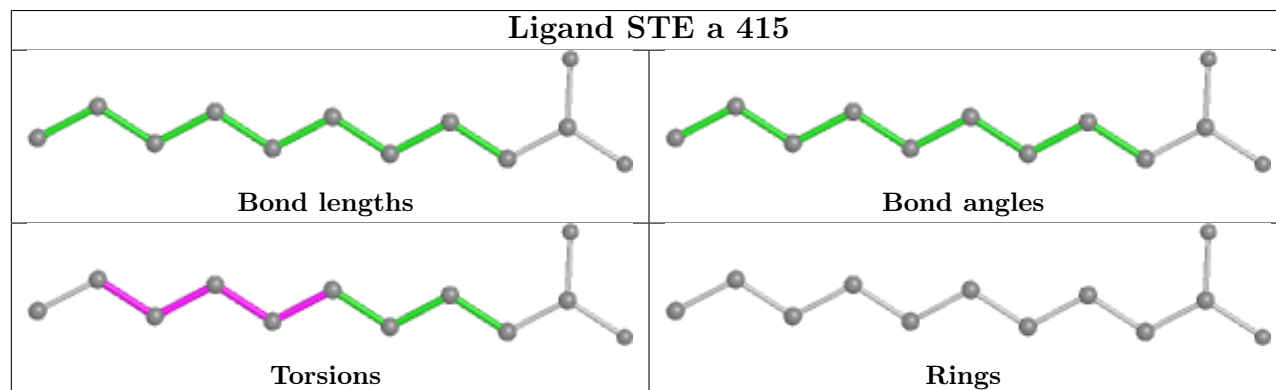
Ligand CLA d 405

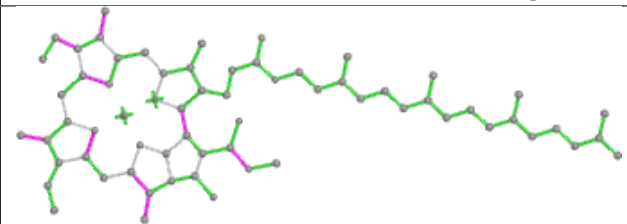
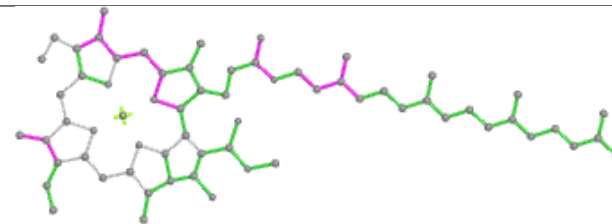
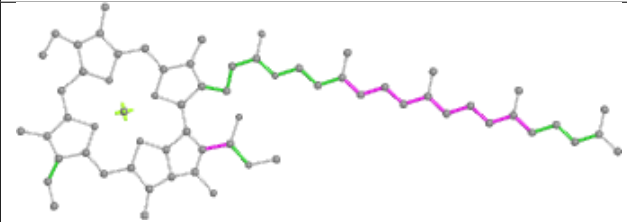
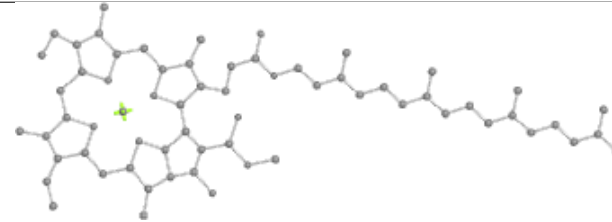


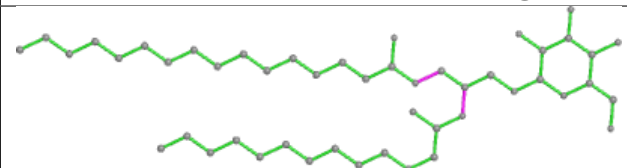
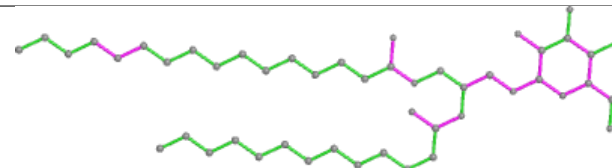
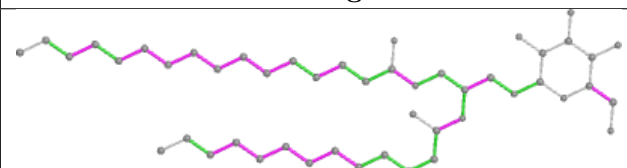
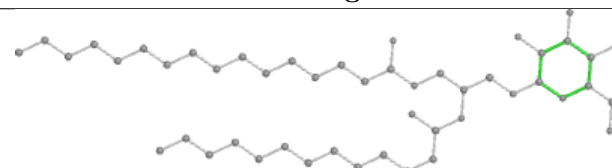
Ligand CLA c 503

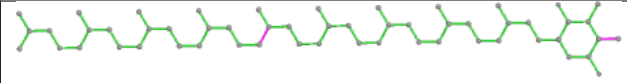
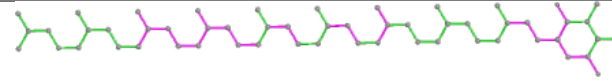
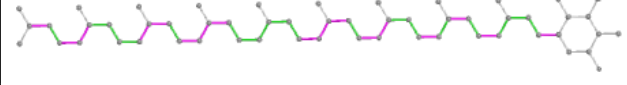
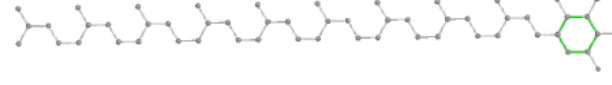


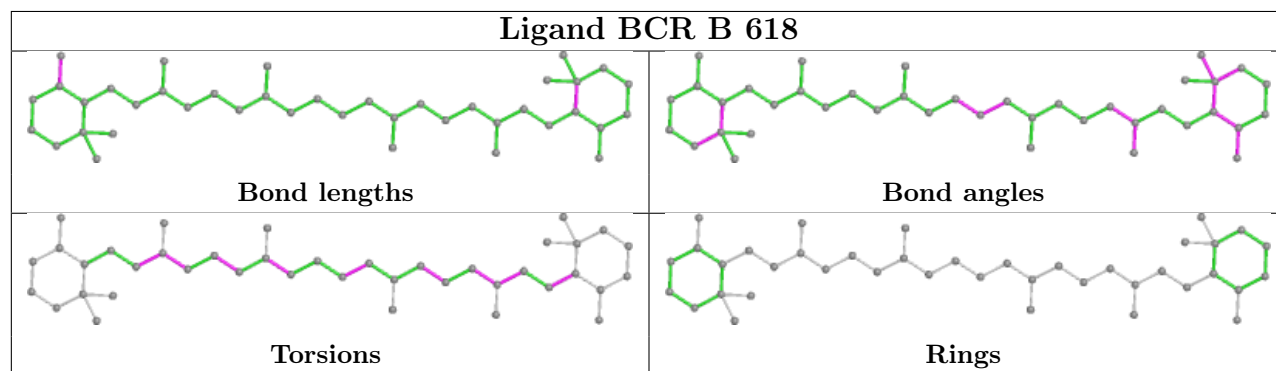
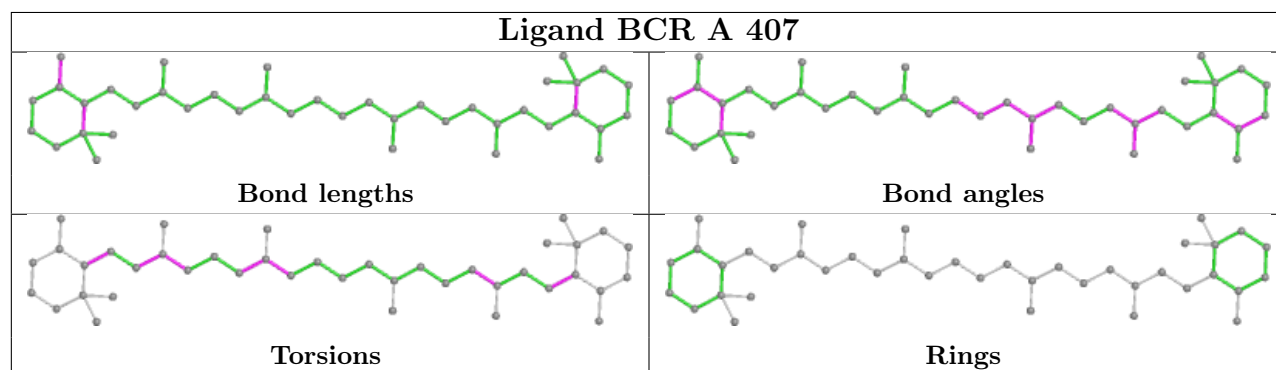
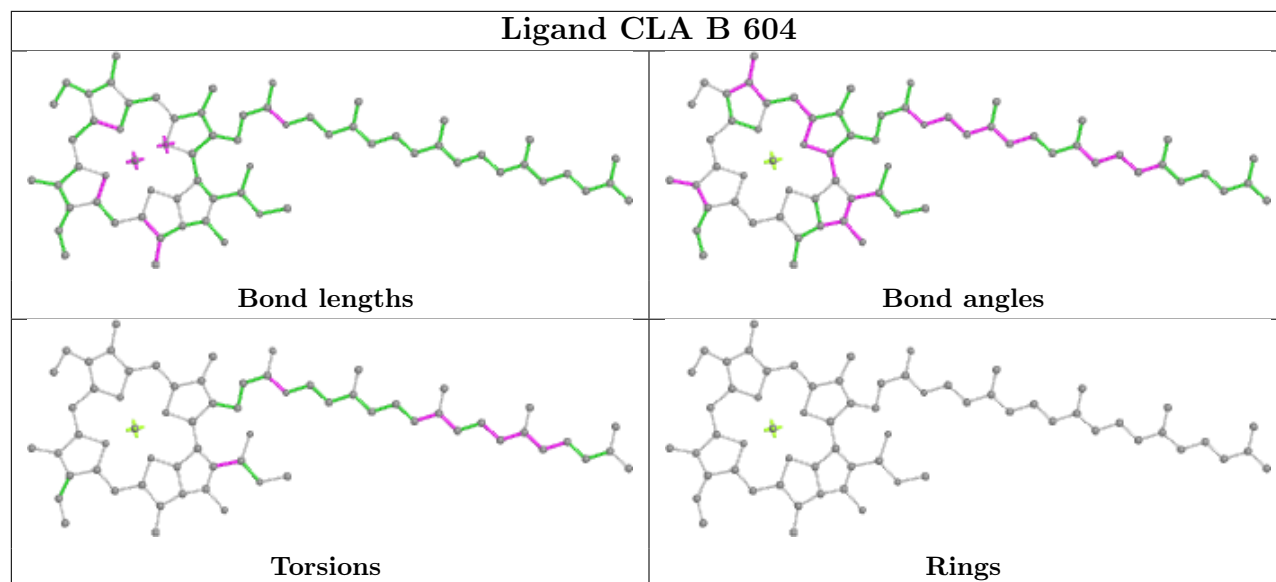
Ligand STE a 415

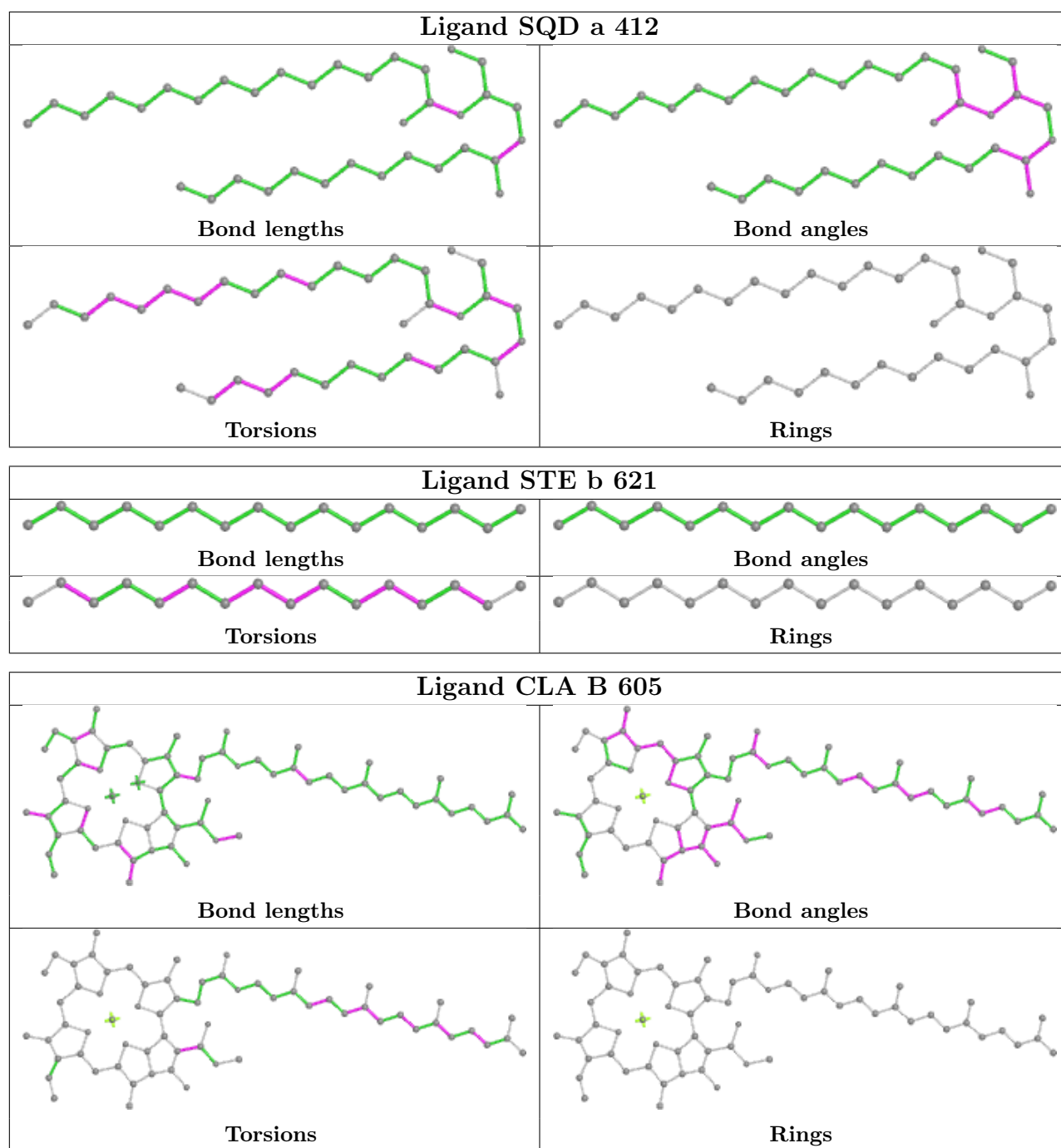


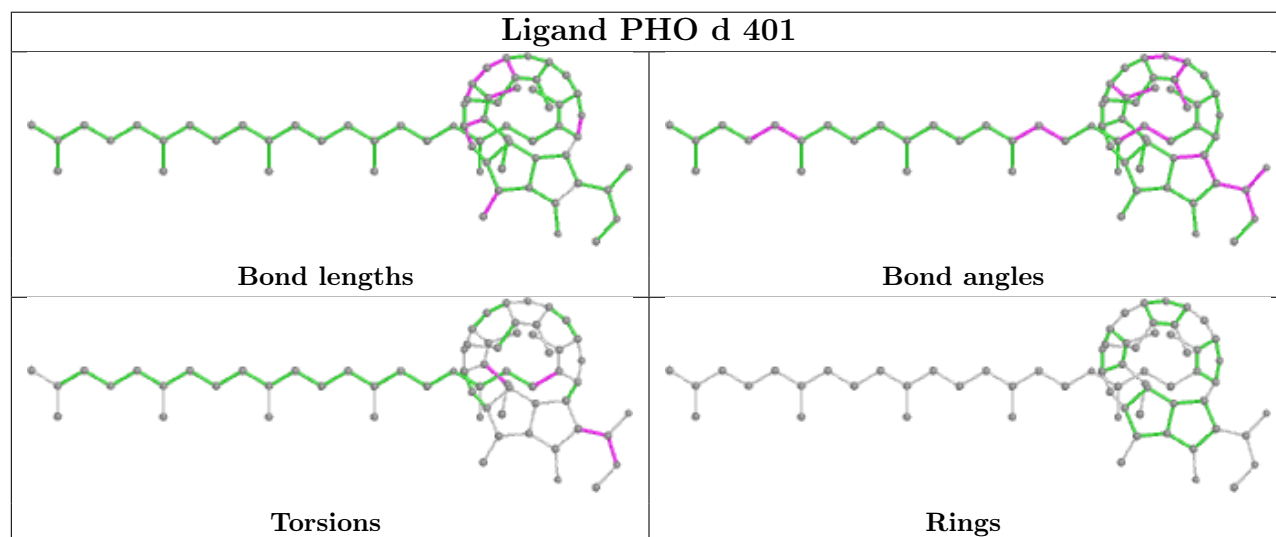
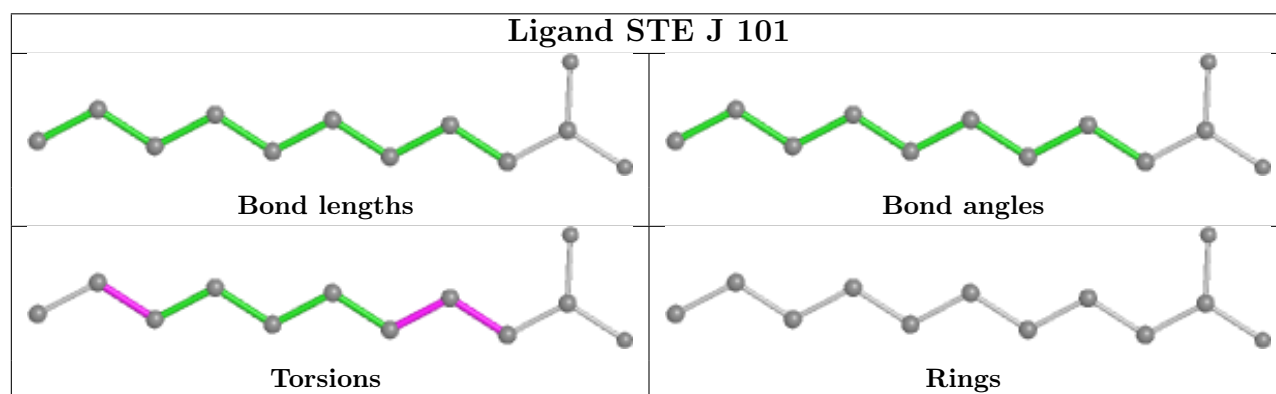
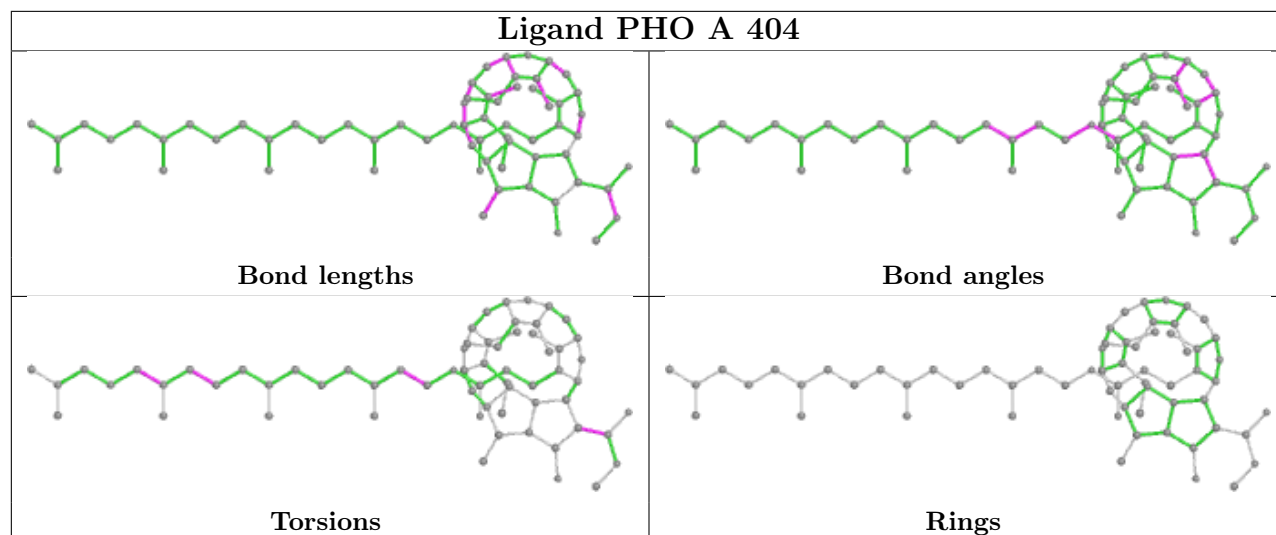
Ligand CLA b 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand LMG Y 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

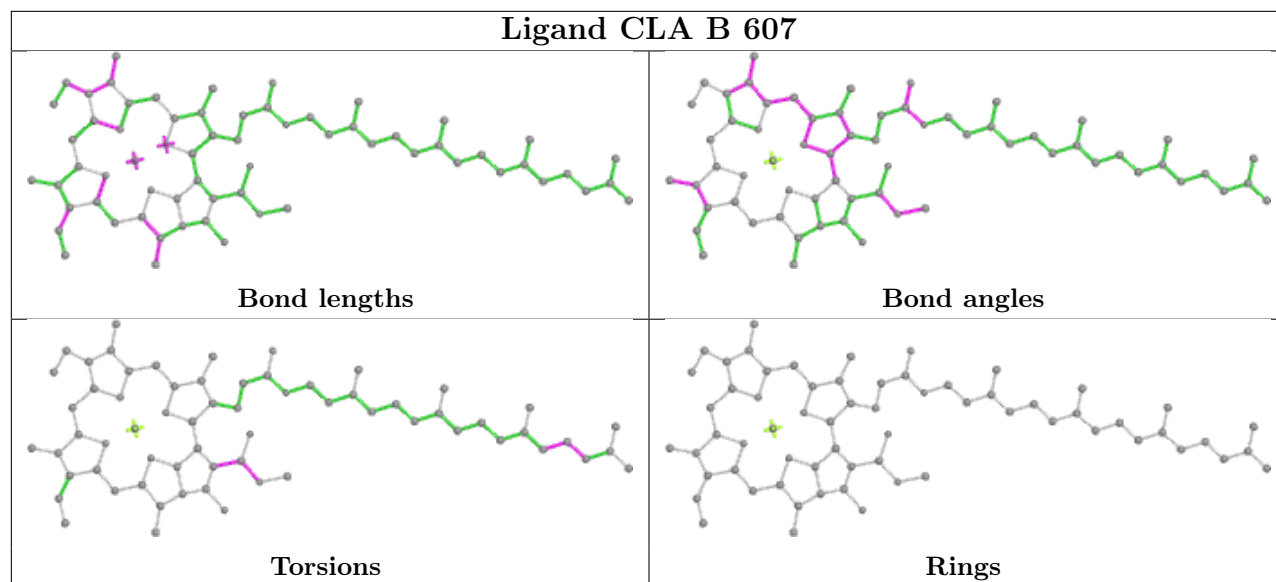
Ligand PL9 A 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



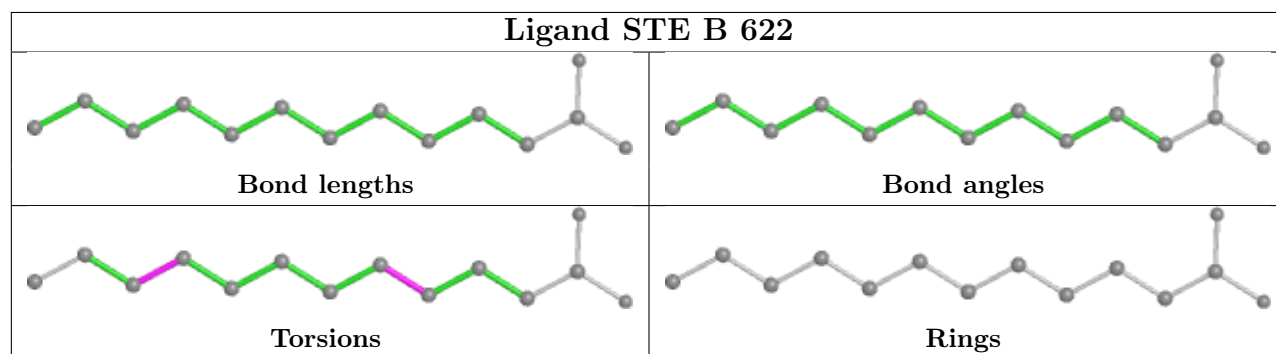




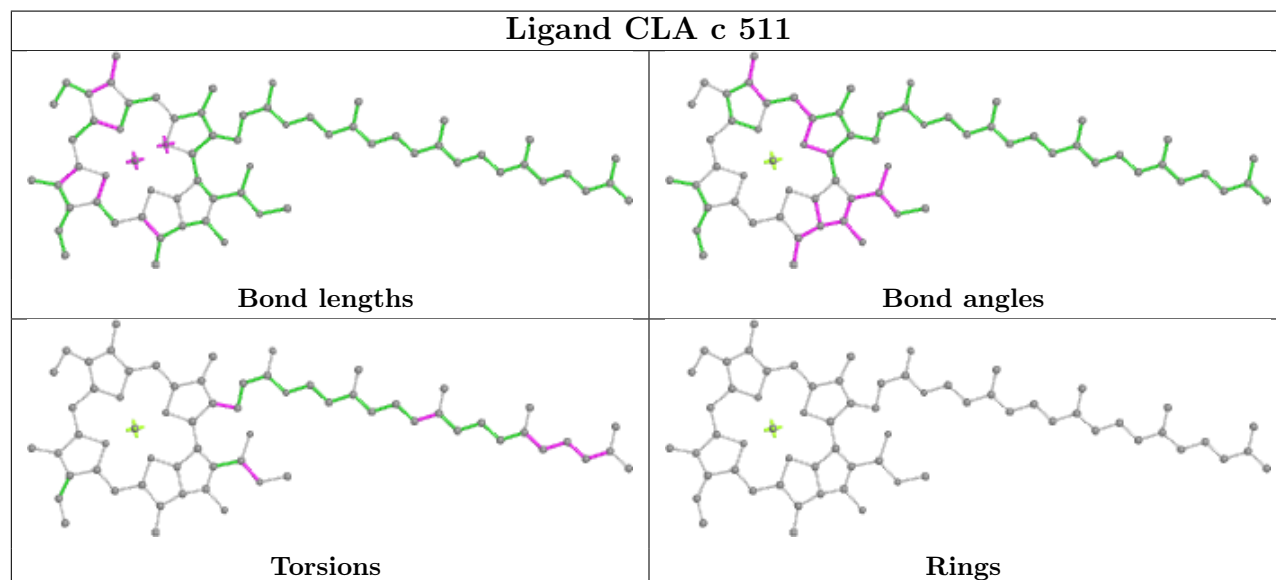
Ligand CLA B 607

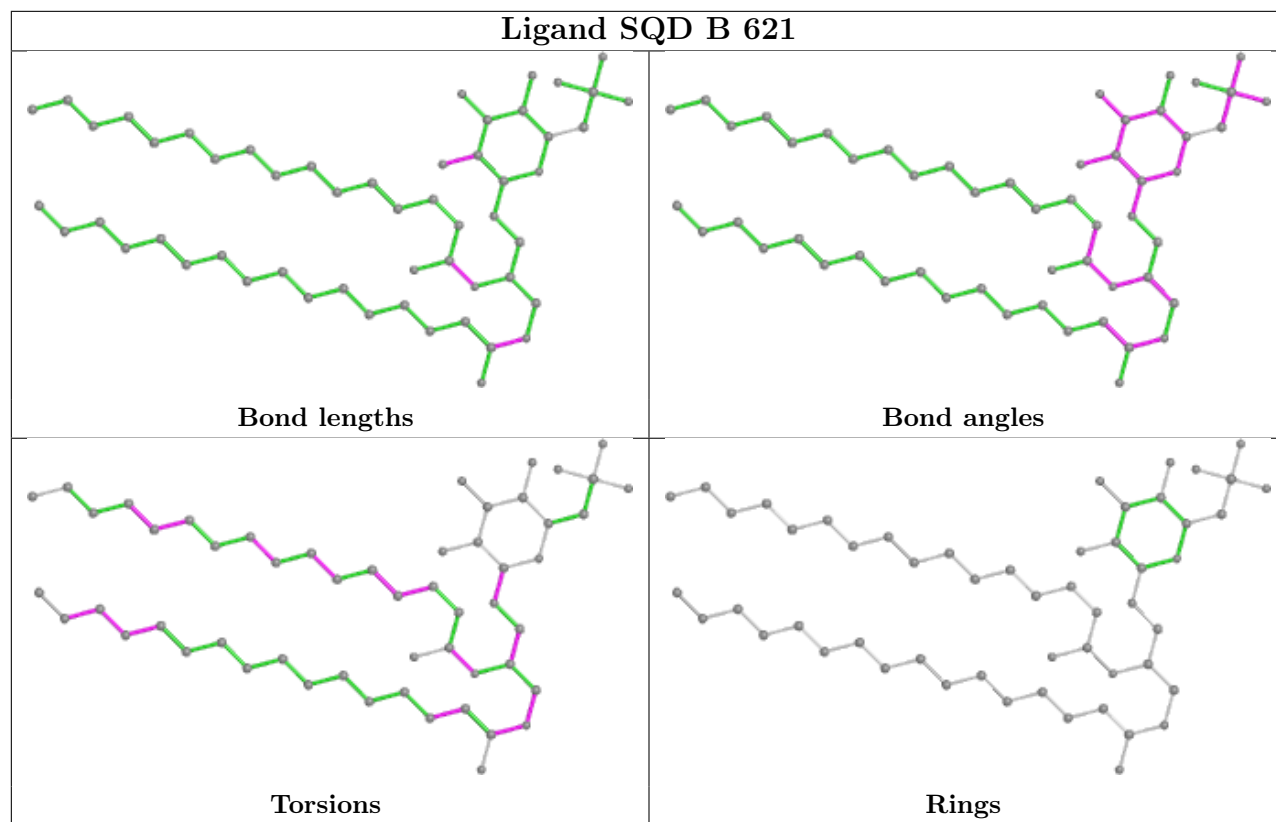
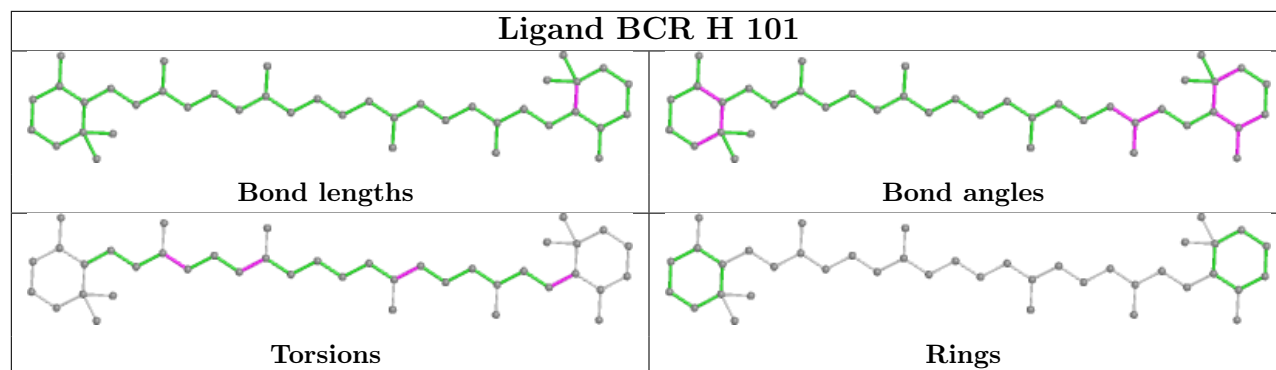


Ligand STE B 622

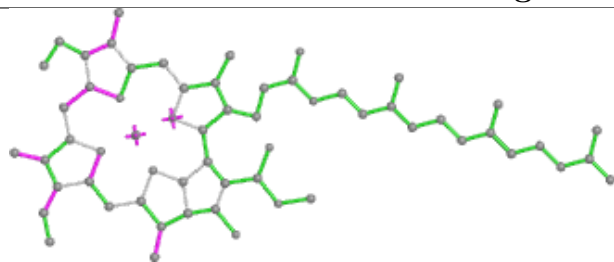


Ligand CLA c 511

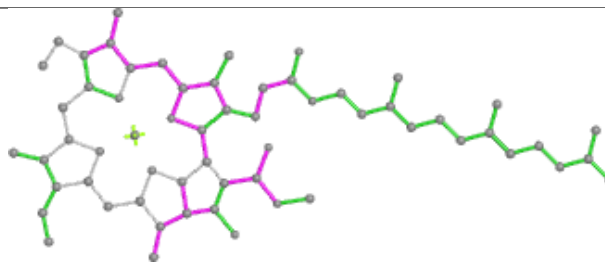




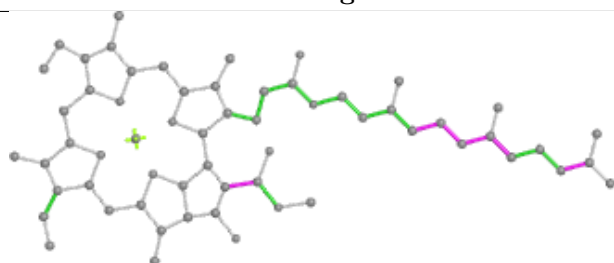
Ligand CLA B 616



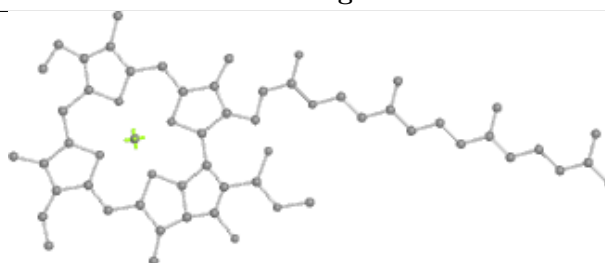
Bond lengths



Bond angles

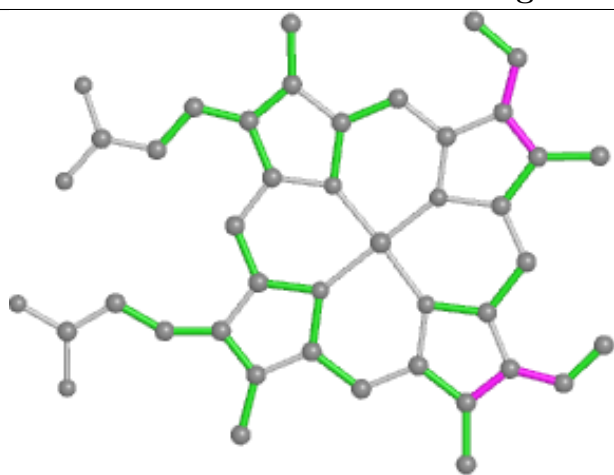


Torsions

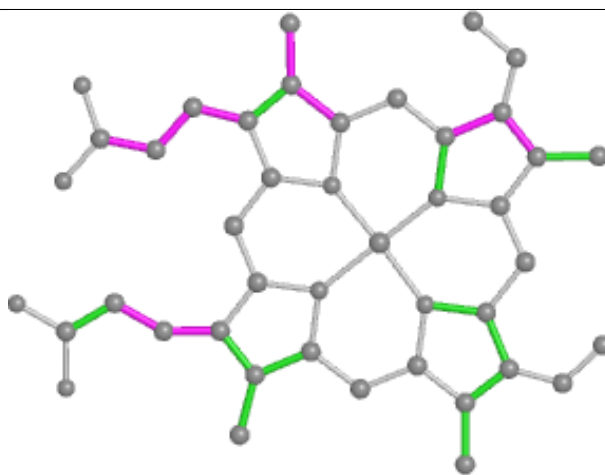


Rings

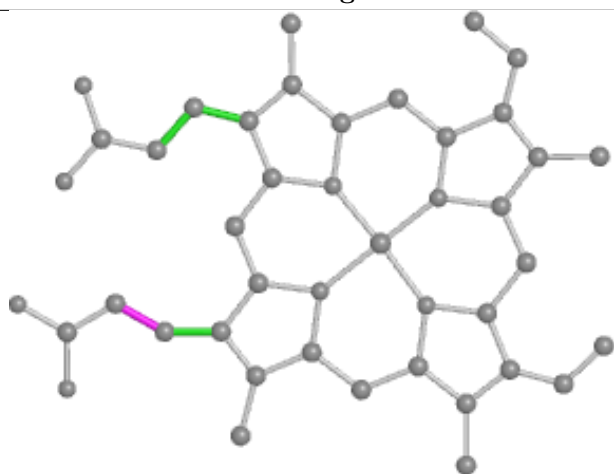
Ligand HEM f 101



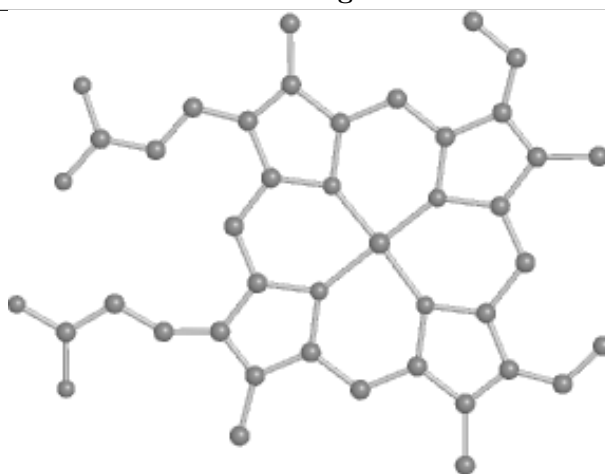
Bond lengths



Bond angles

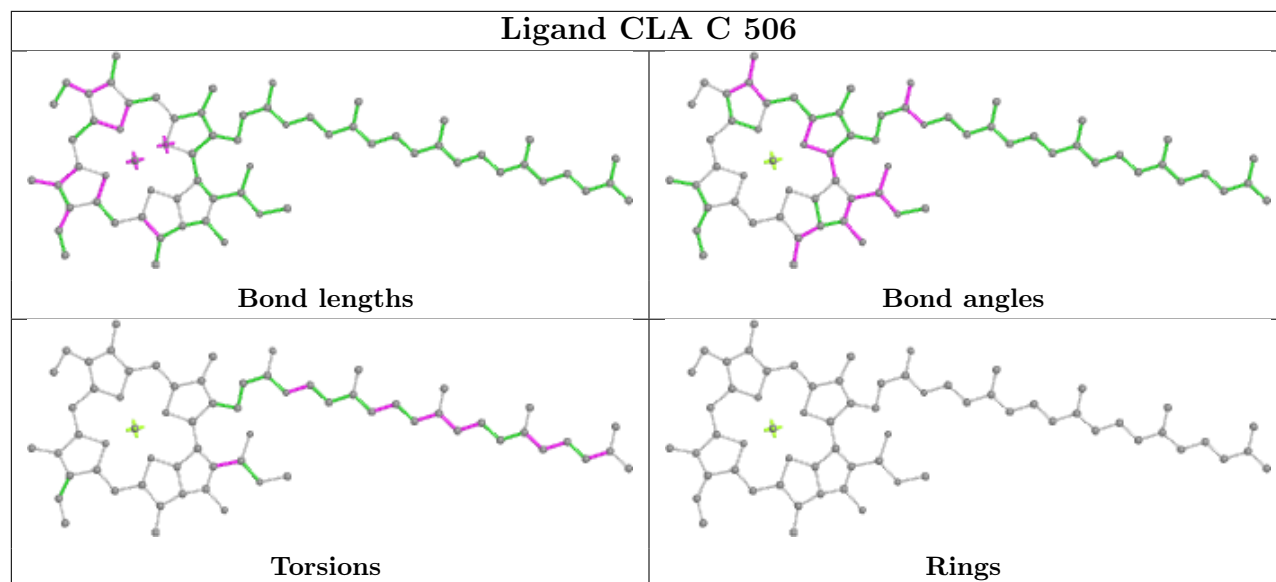


Torsions

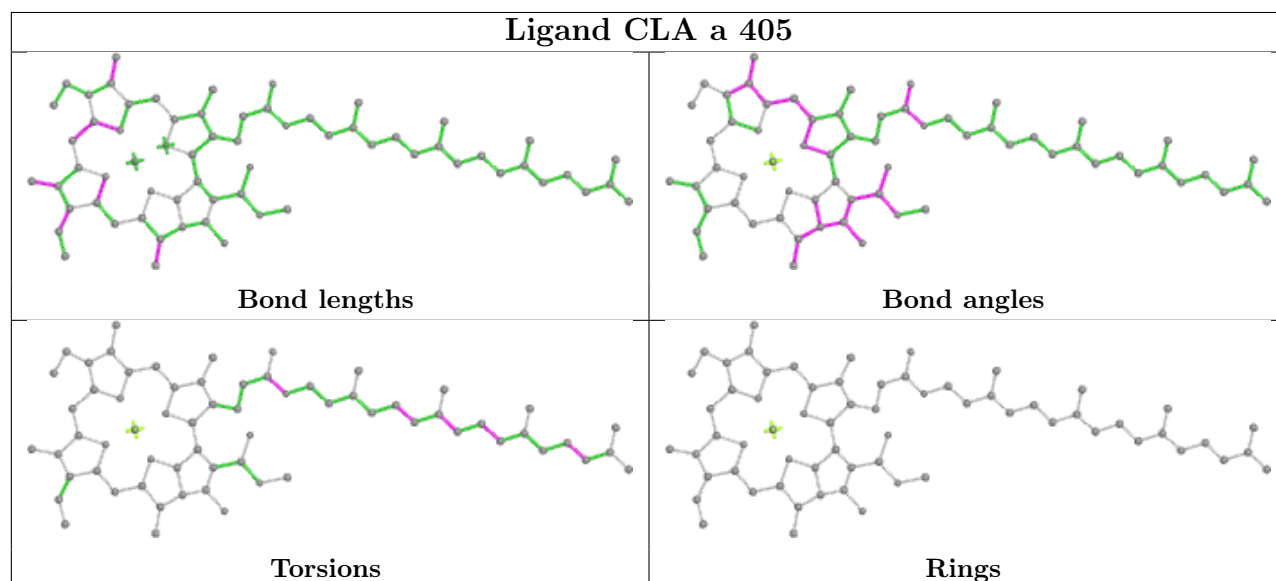


Rings

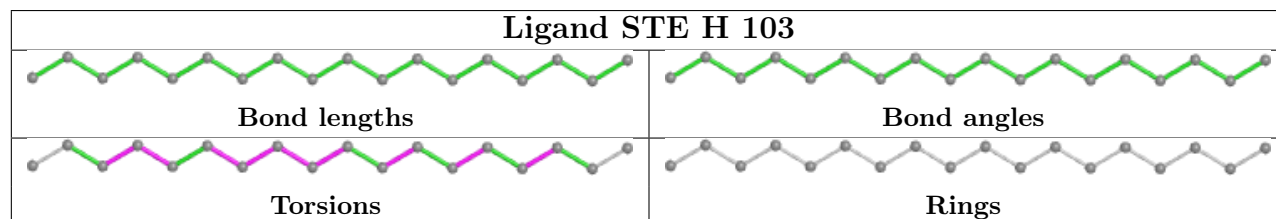
Ligand CLA C 506



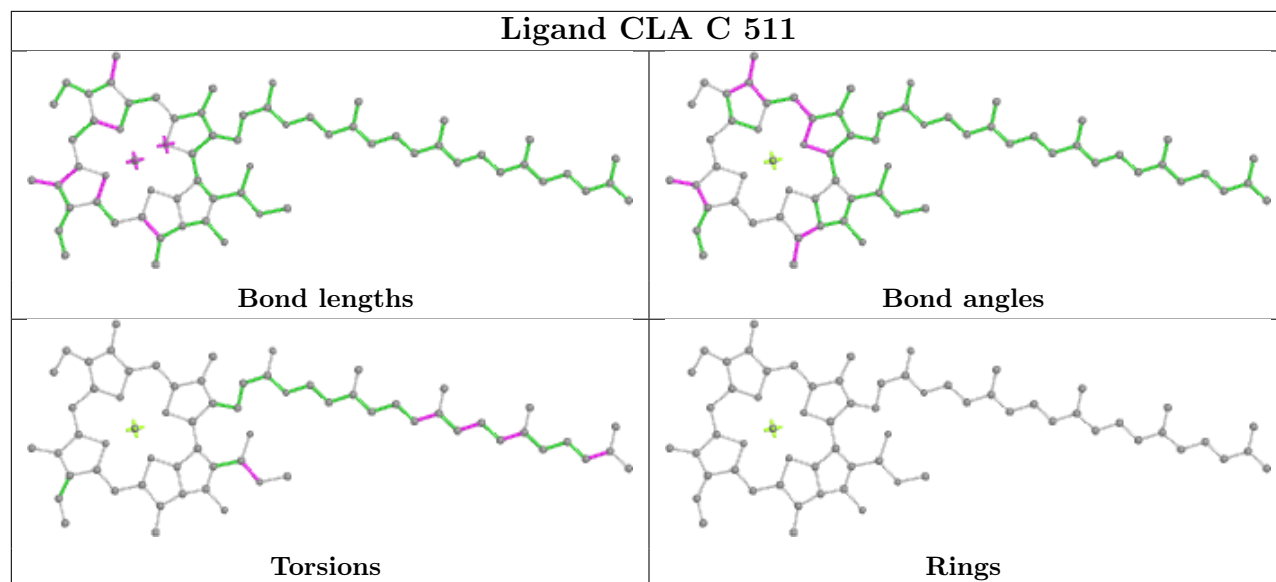
Ligand CLA a 405



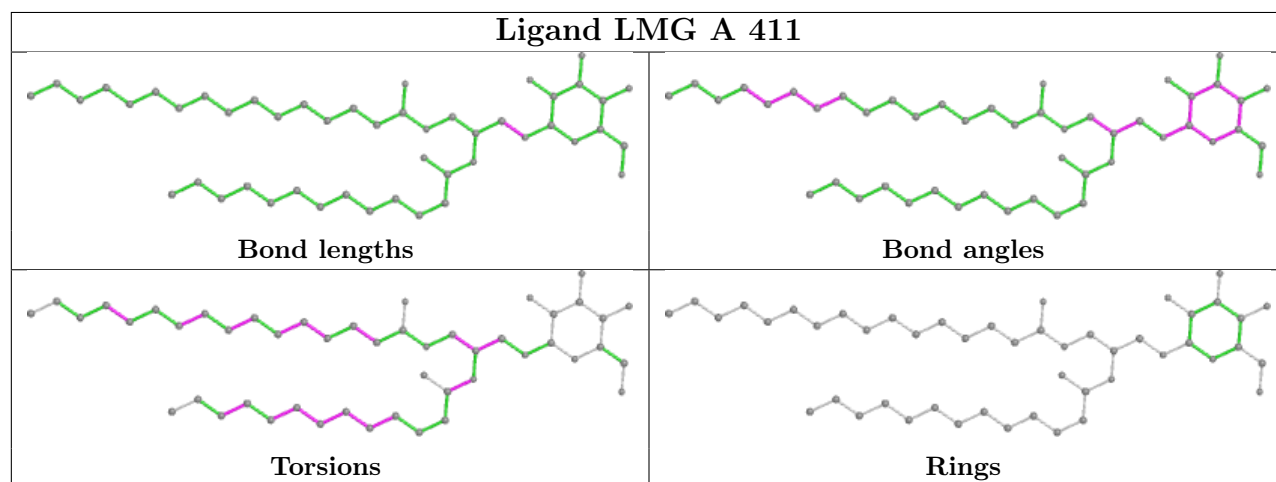
Ligand STE H 103



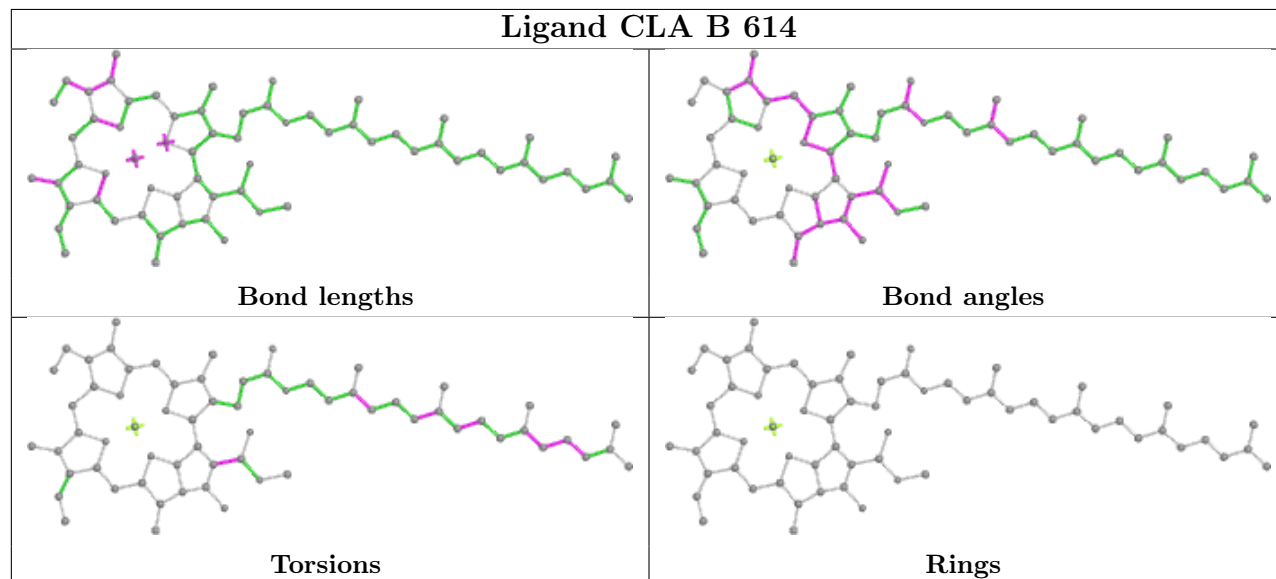
Ligand CLA C 511

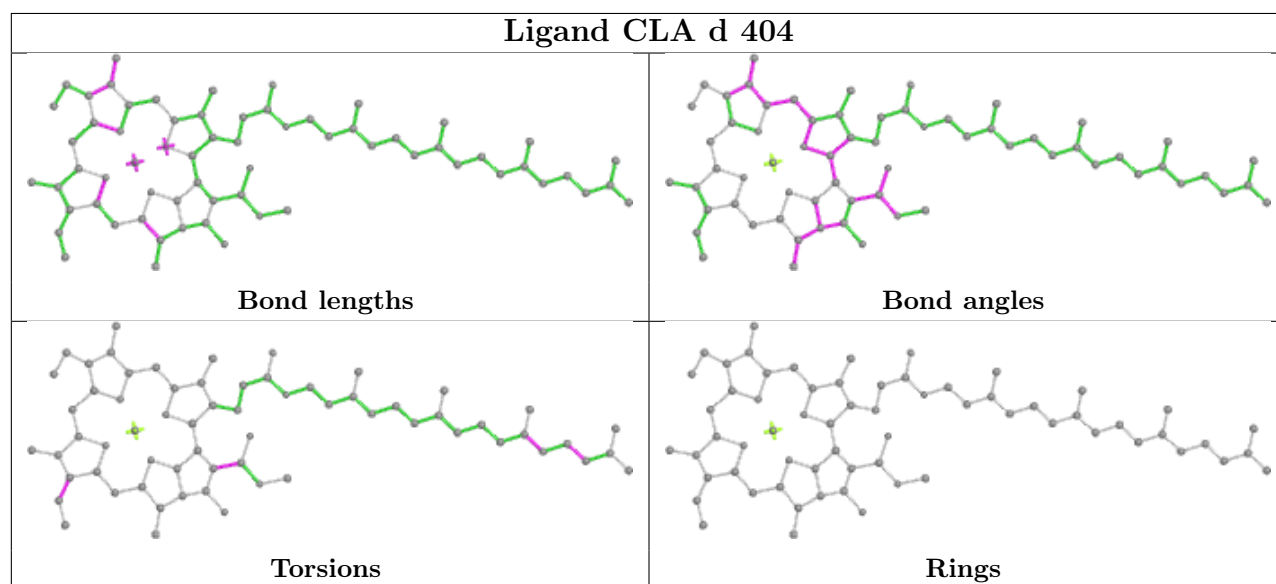
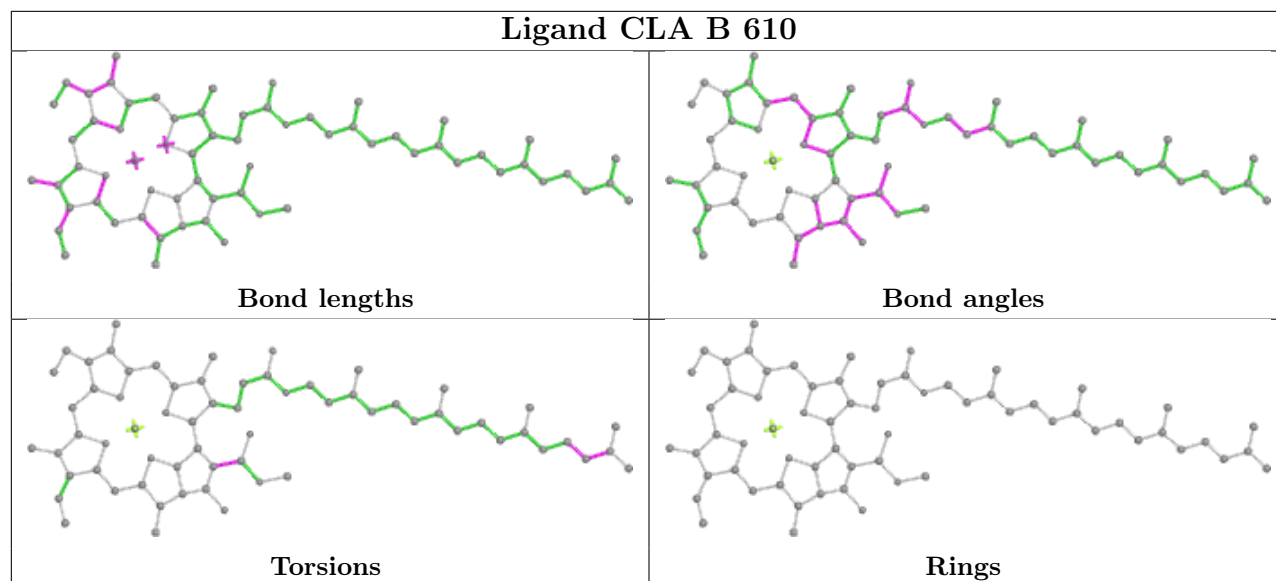
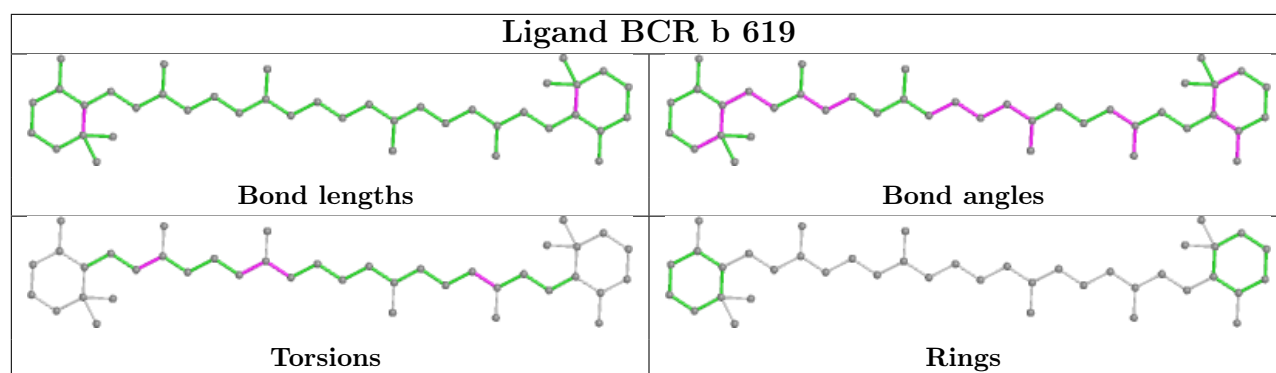


Ligand LMG A 411

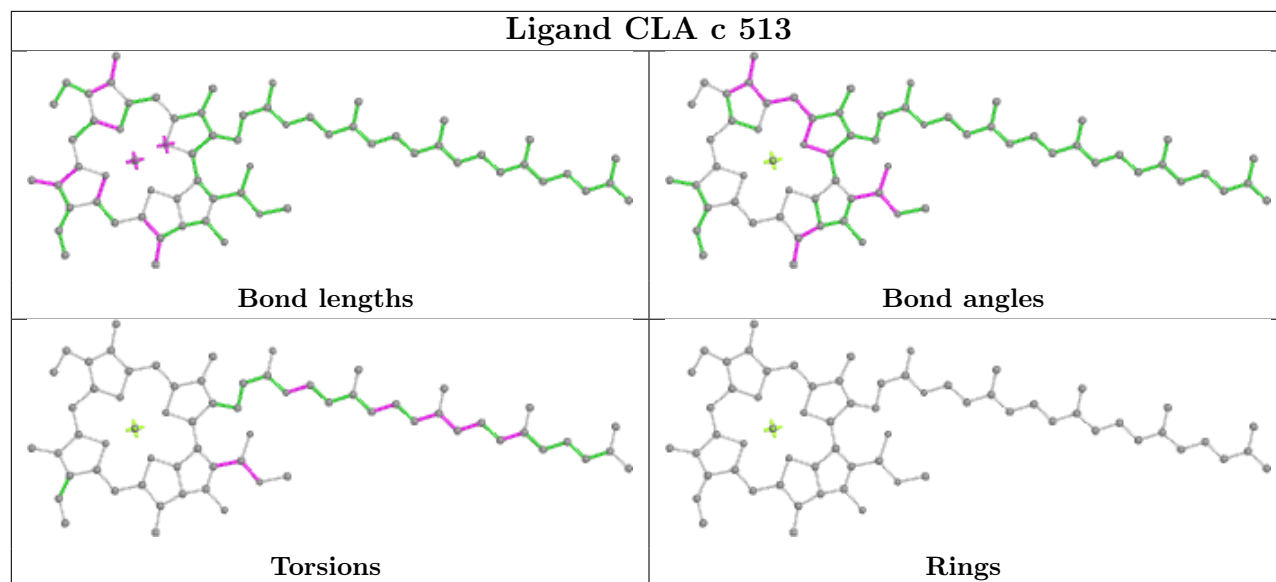


Ligand CLA B 614

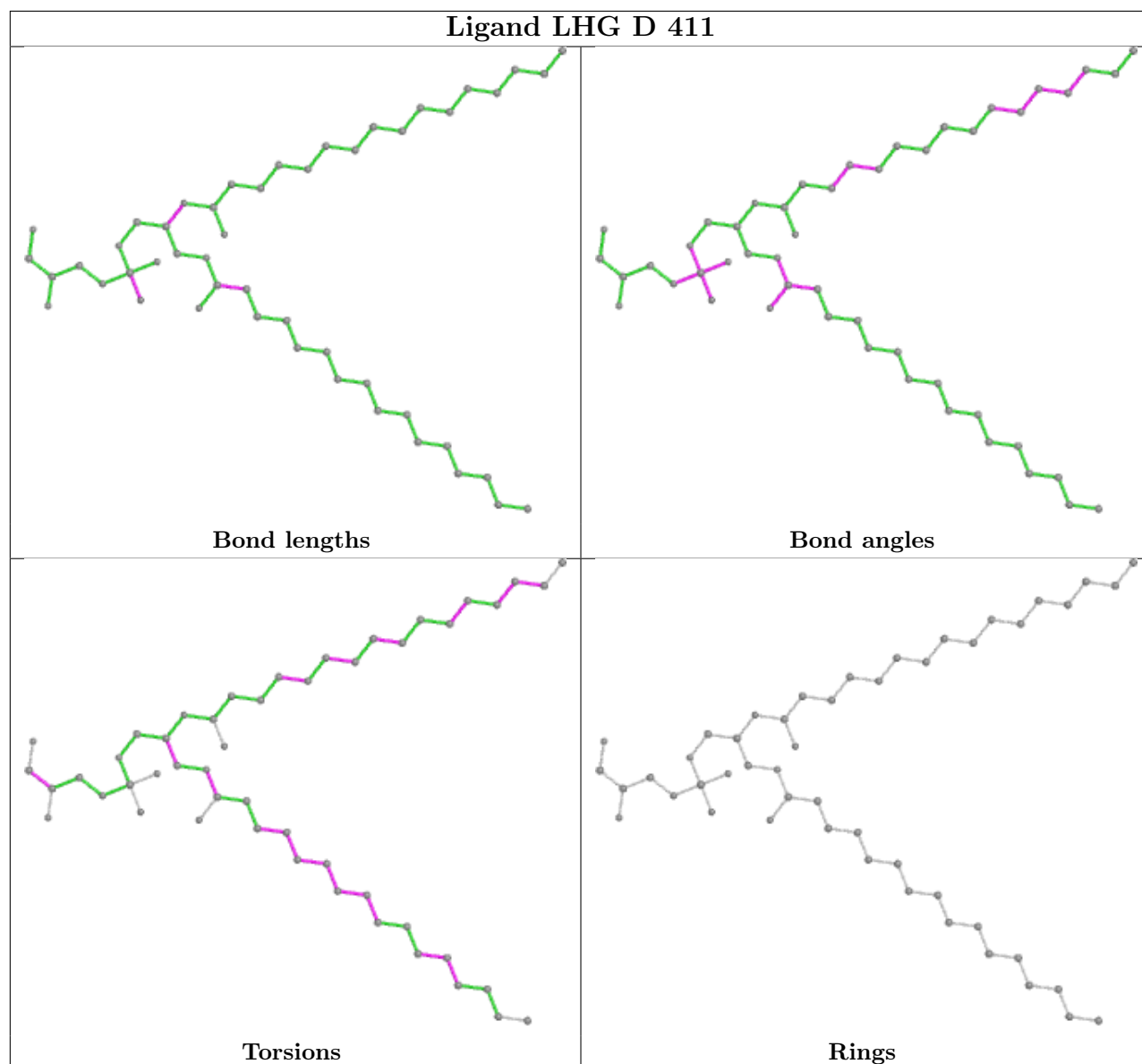


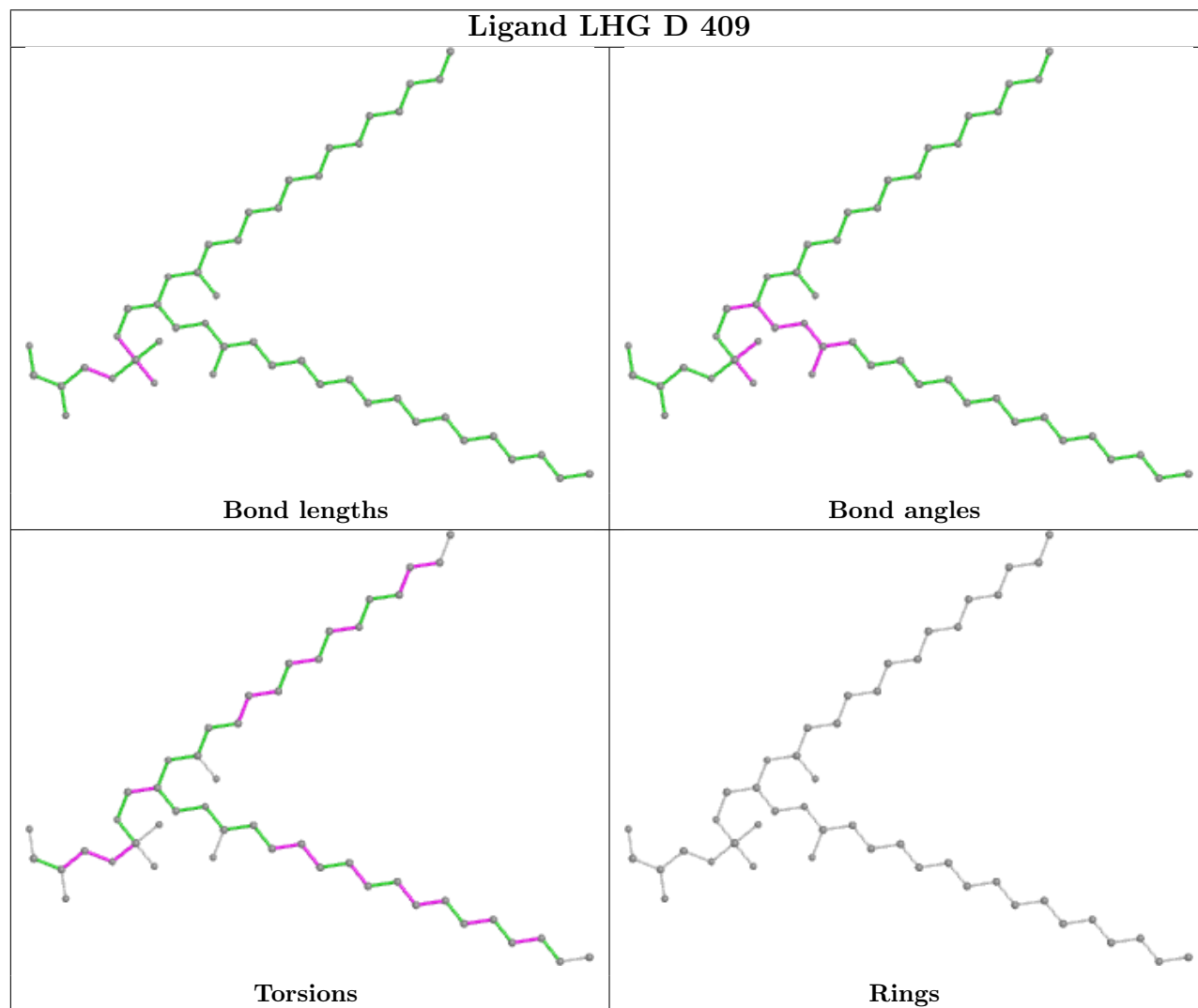
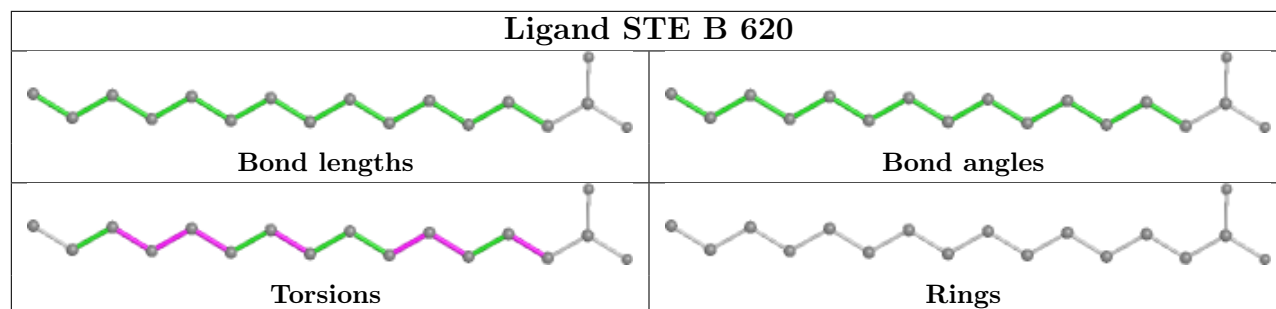


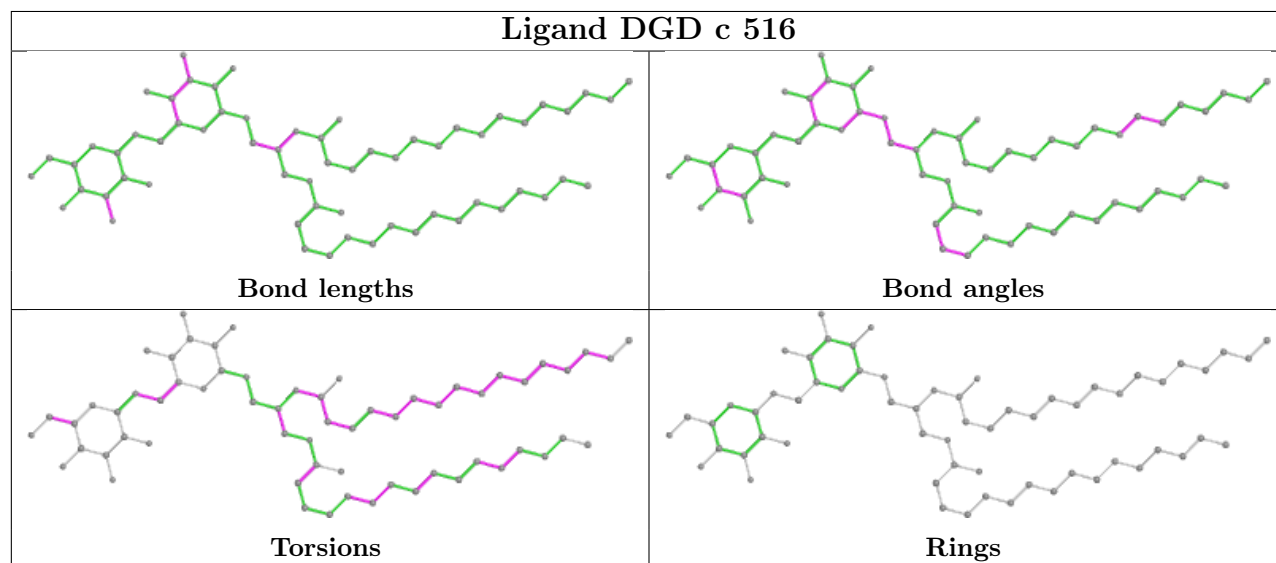
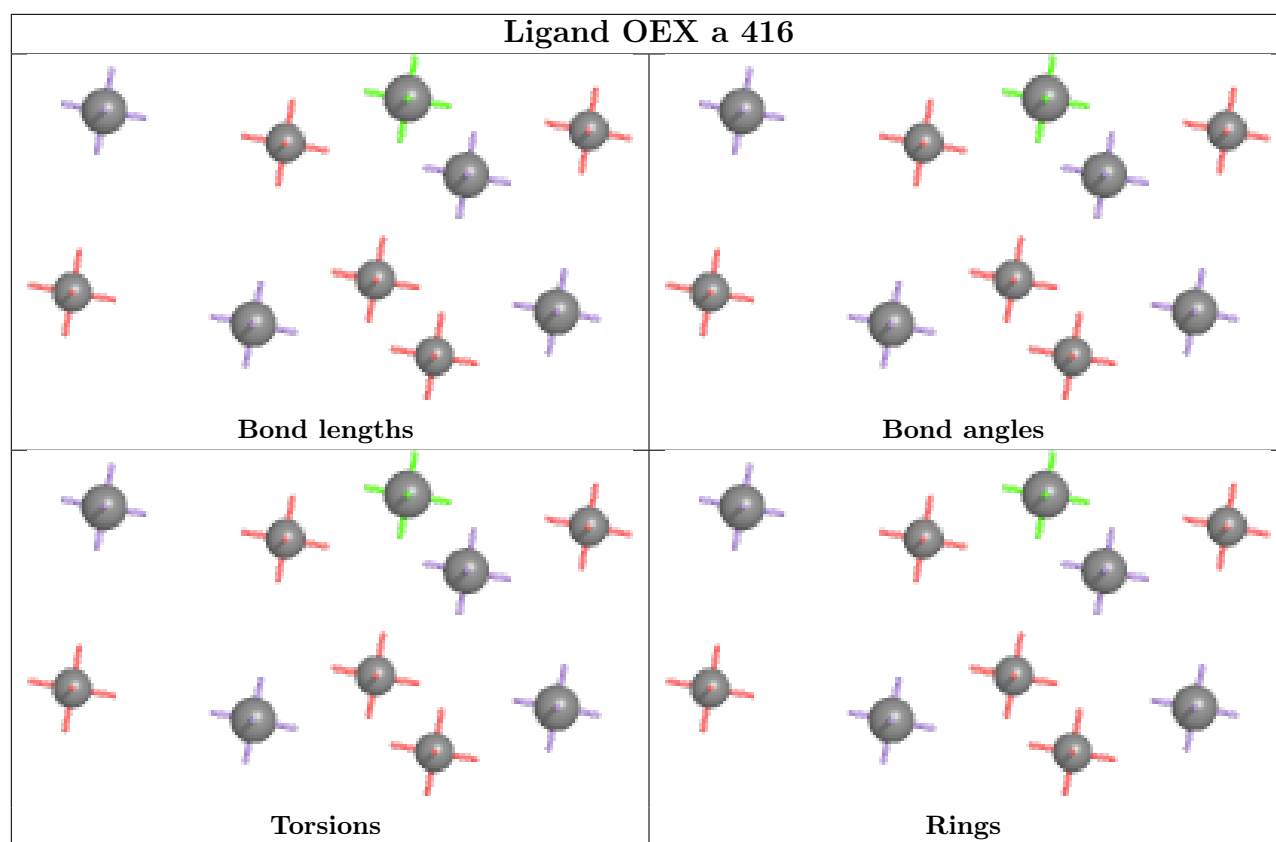
Ligand CLA c 513



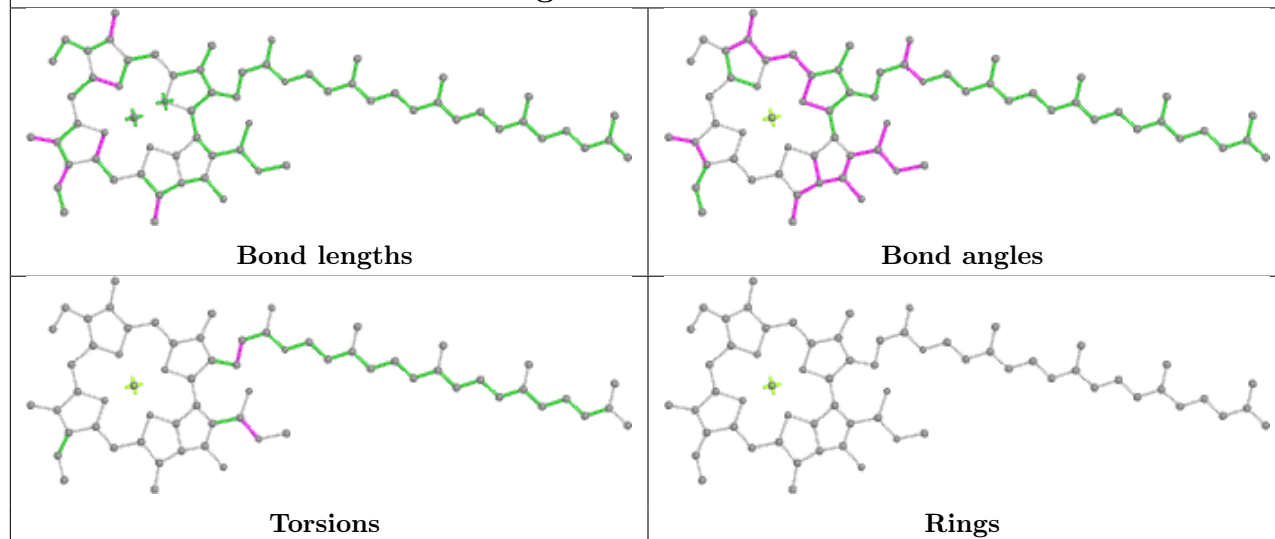
Ligand LHG D 411



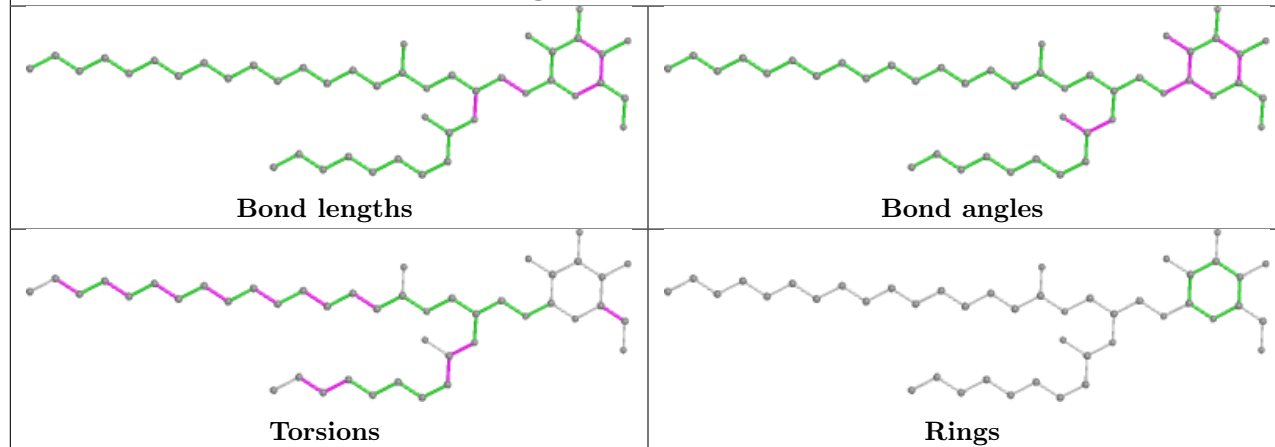




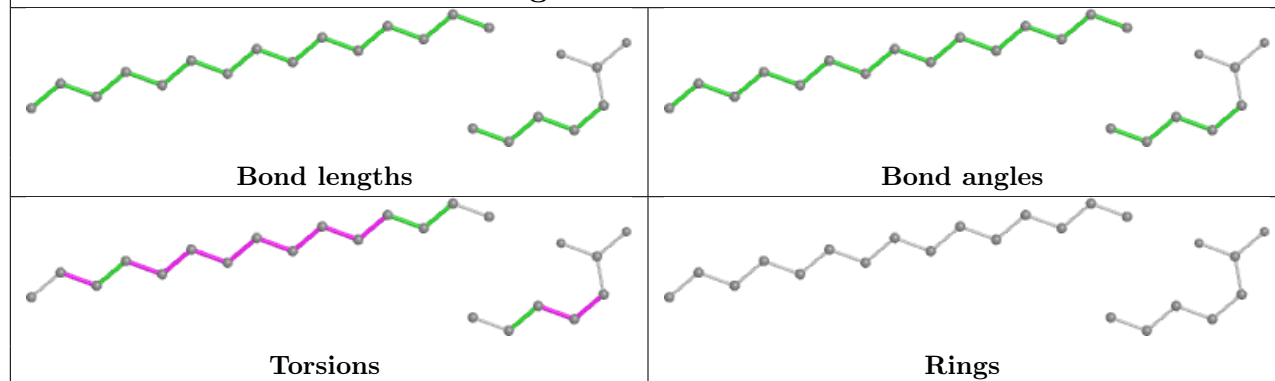
Ligand CLA c 501

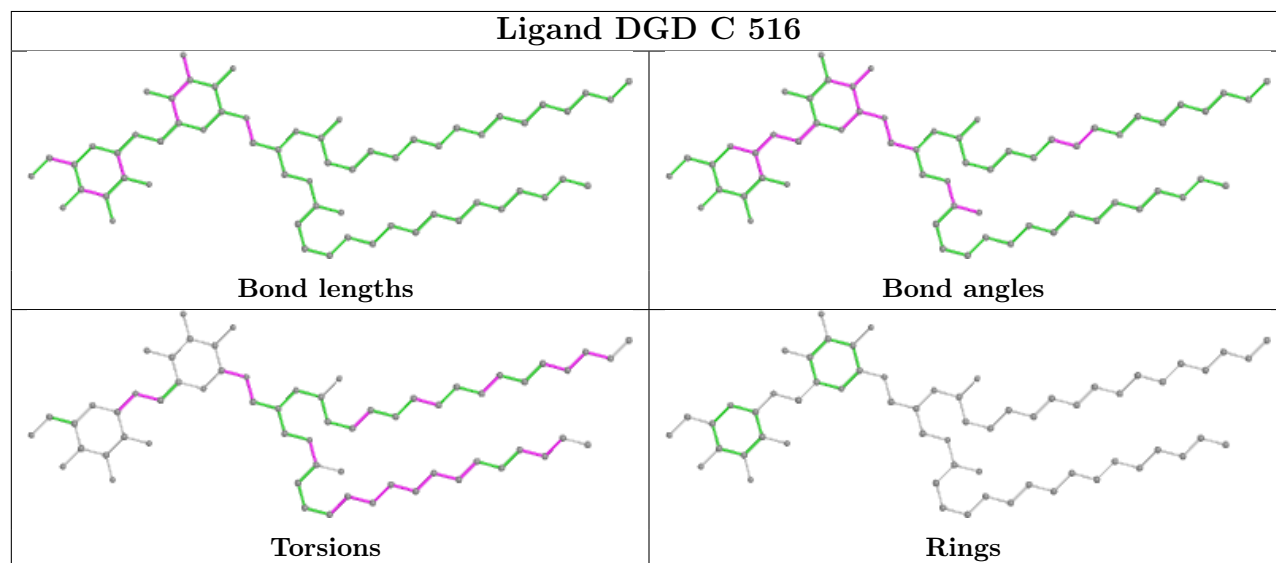
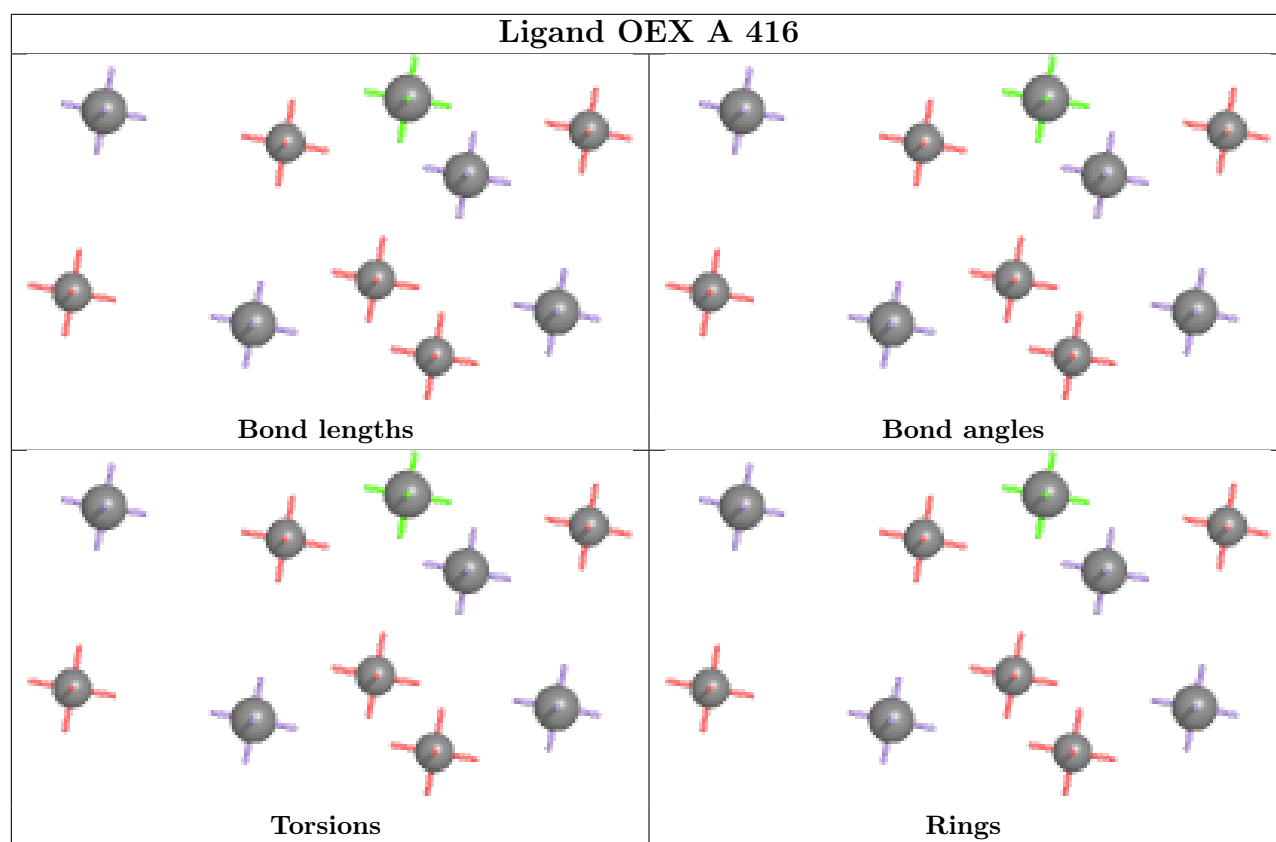


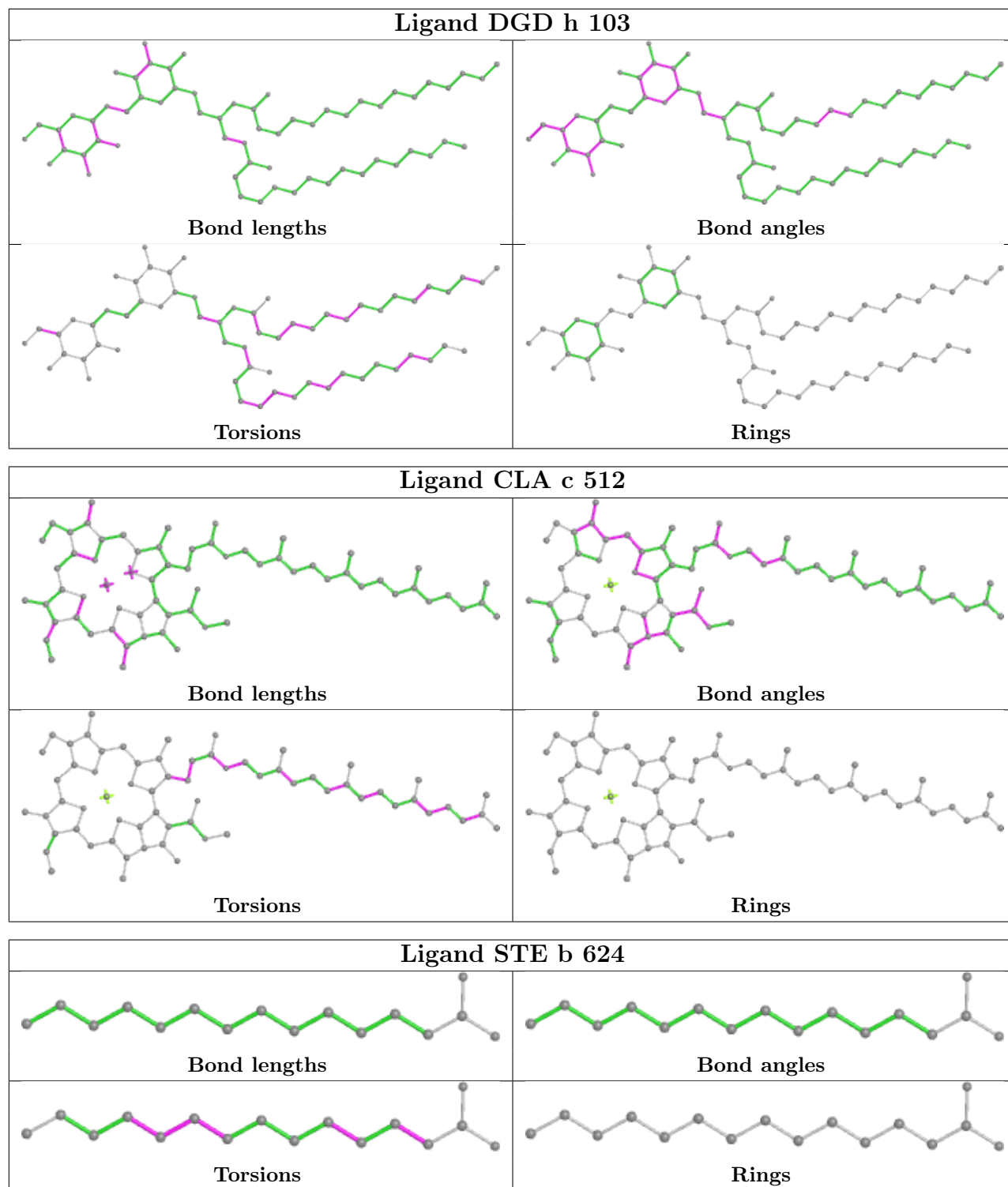
Ligand LMG d 410



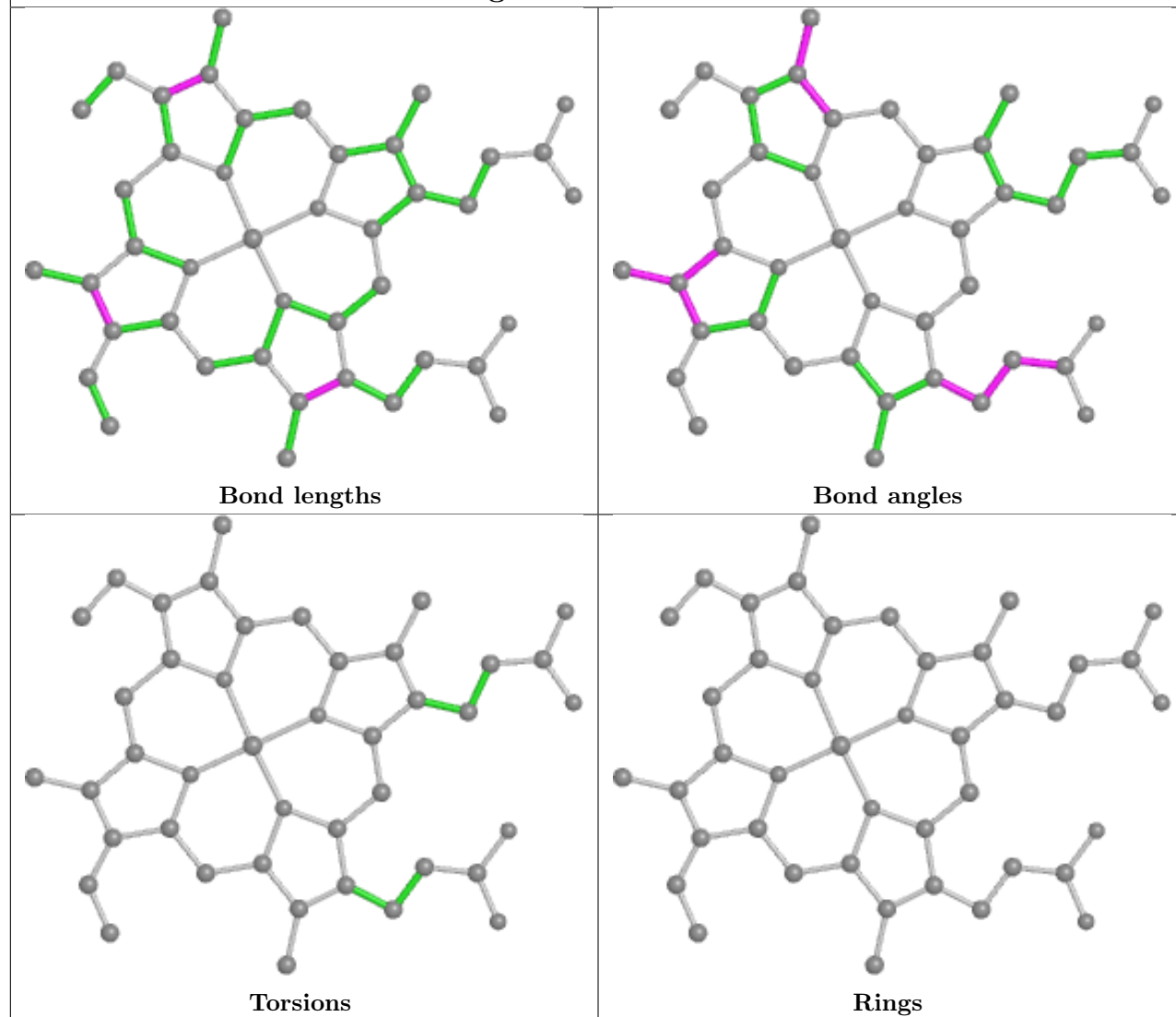
Ligand LMG h 102



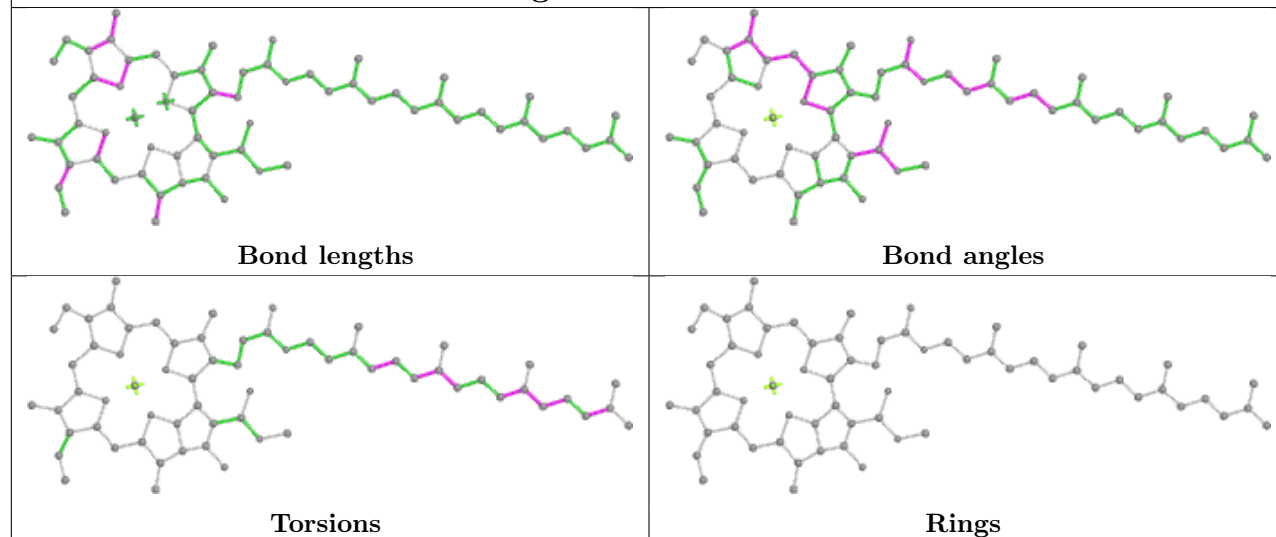


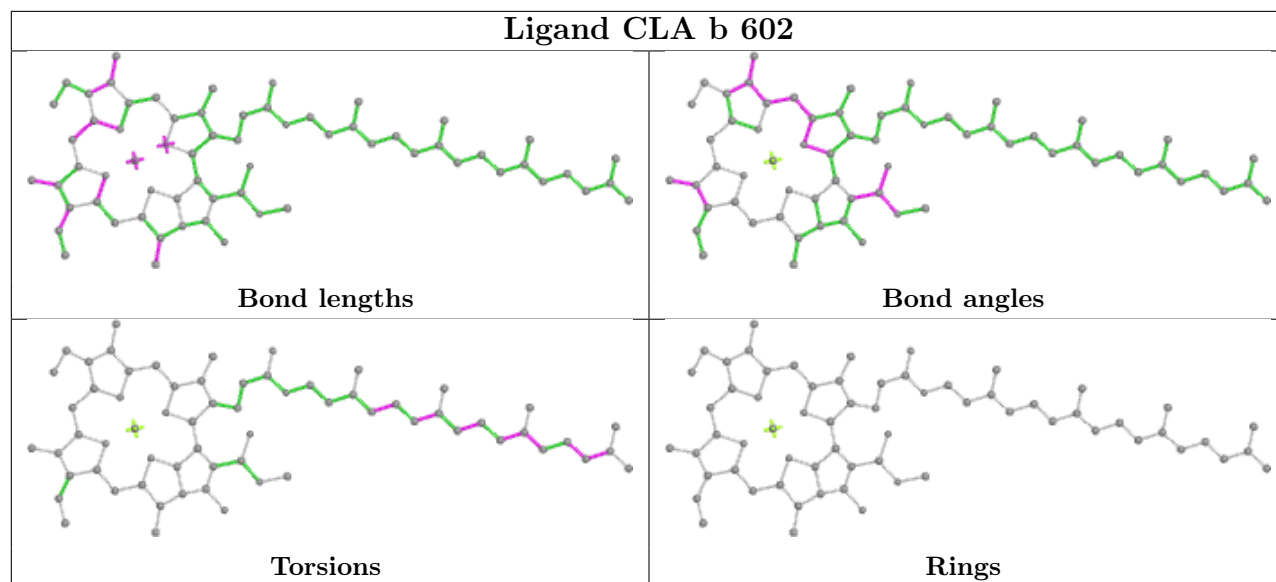
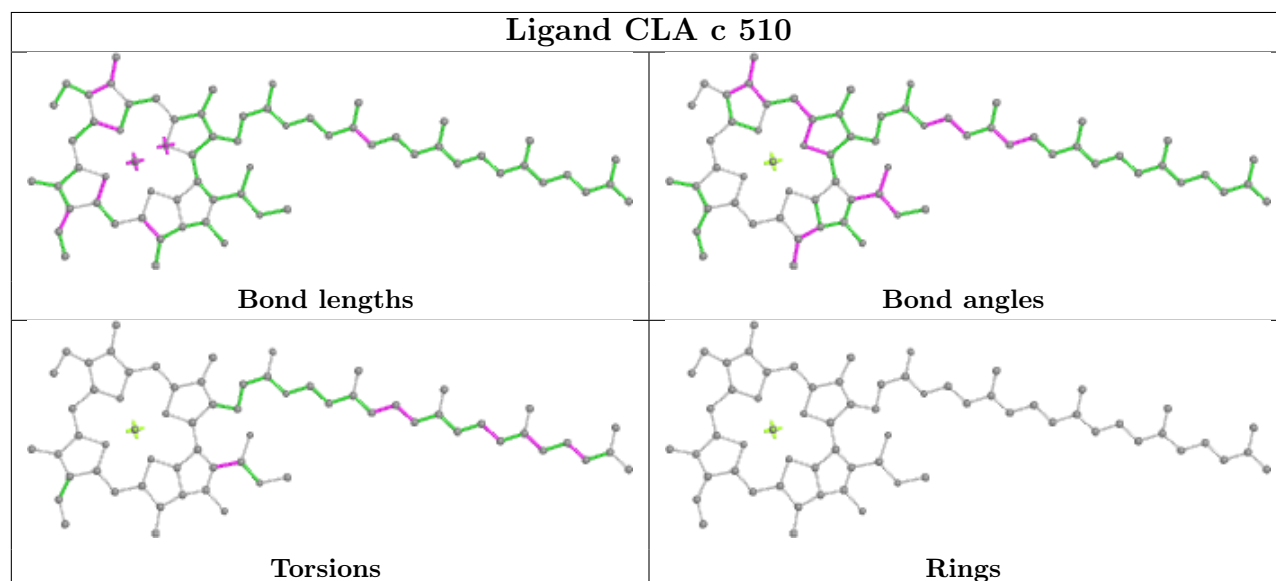


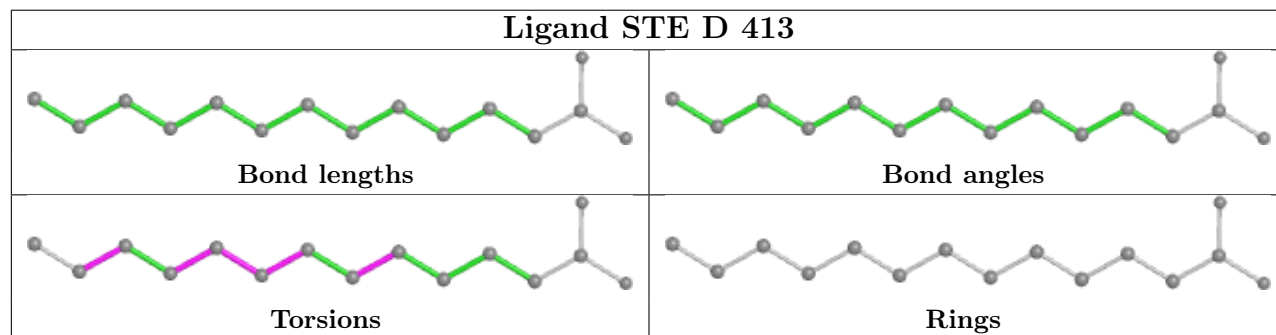
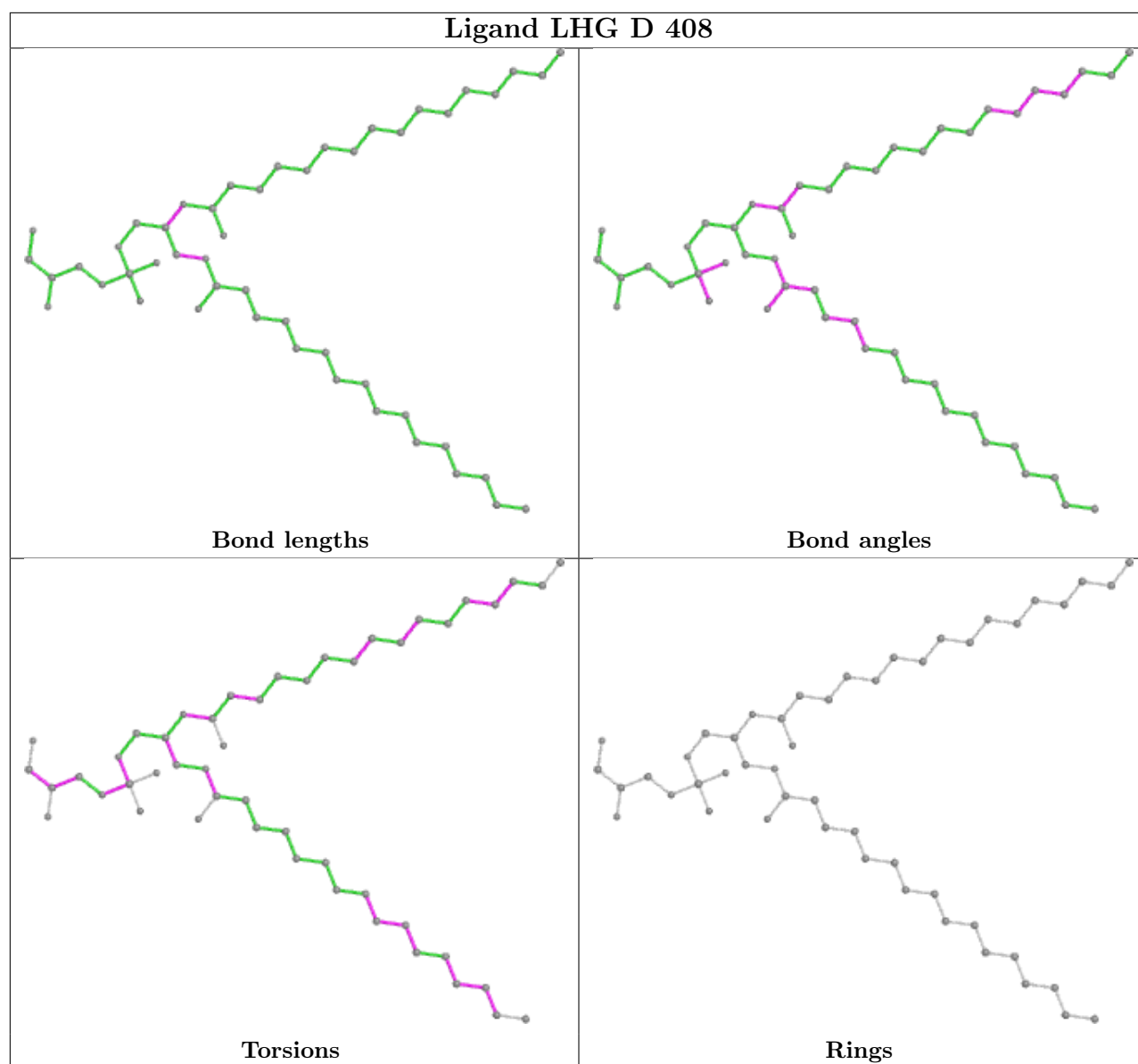
Ligand HEC V 201

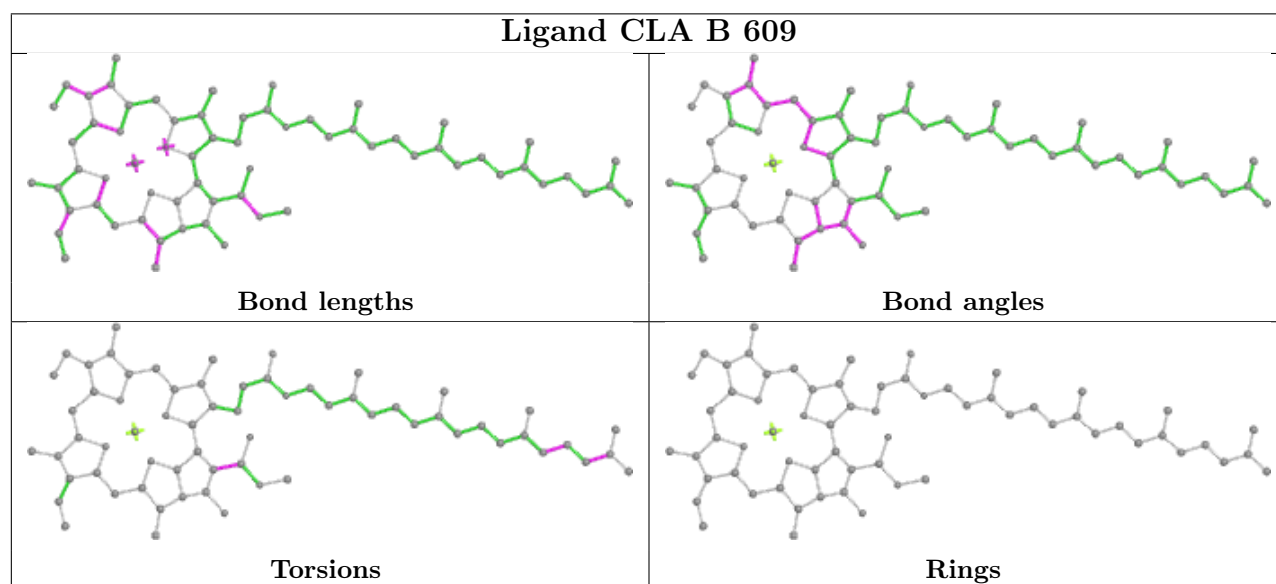
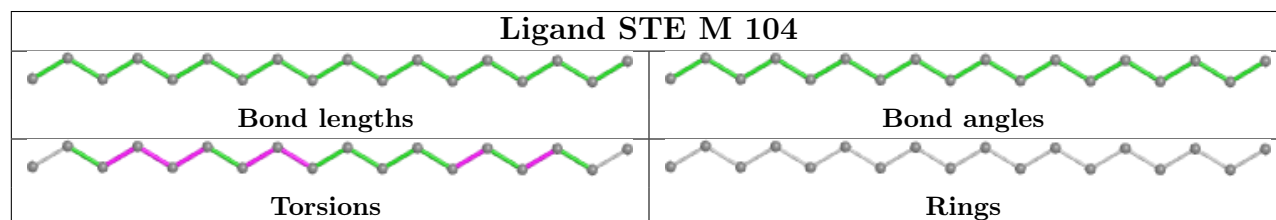
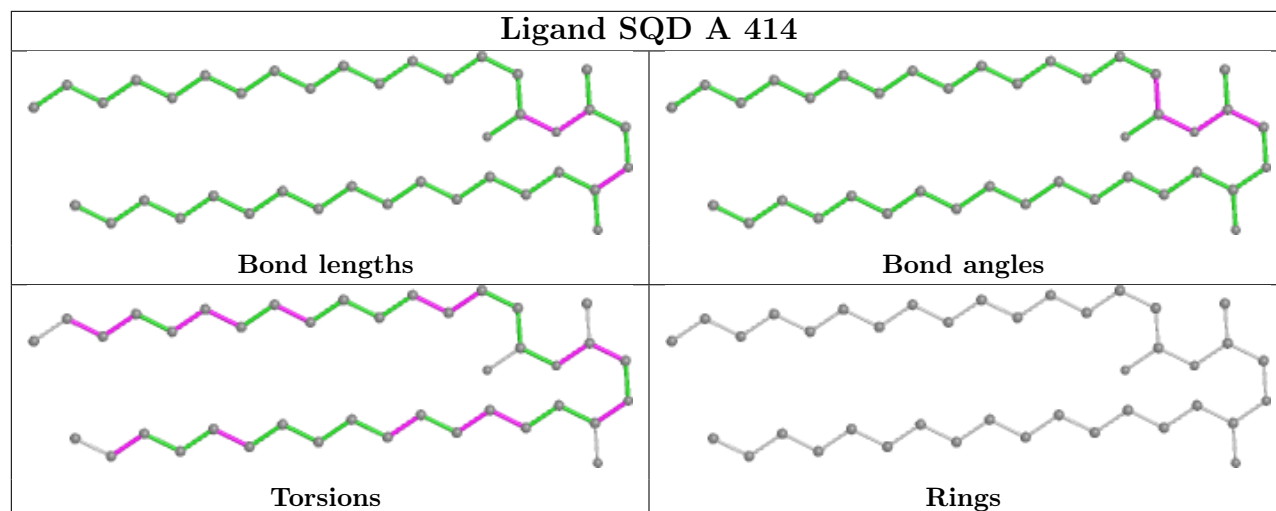
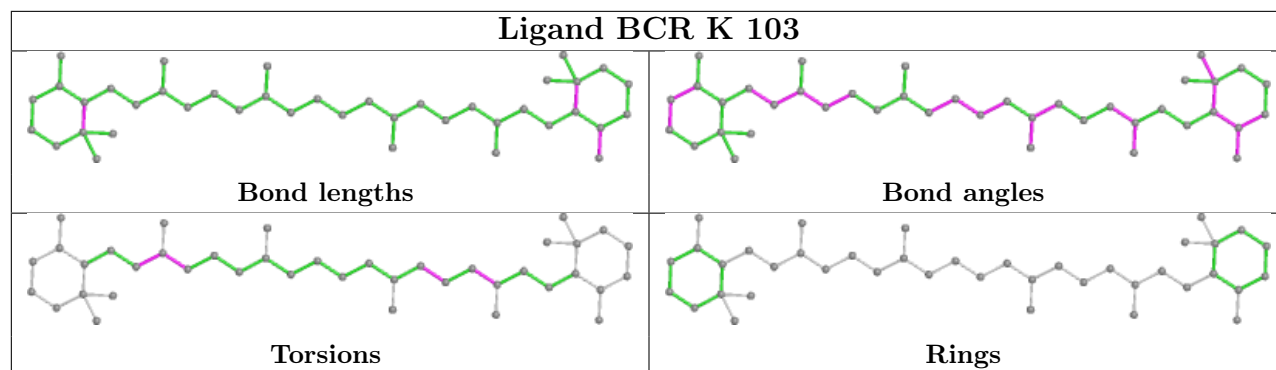


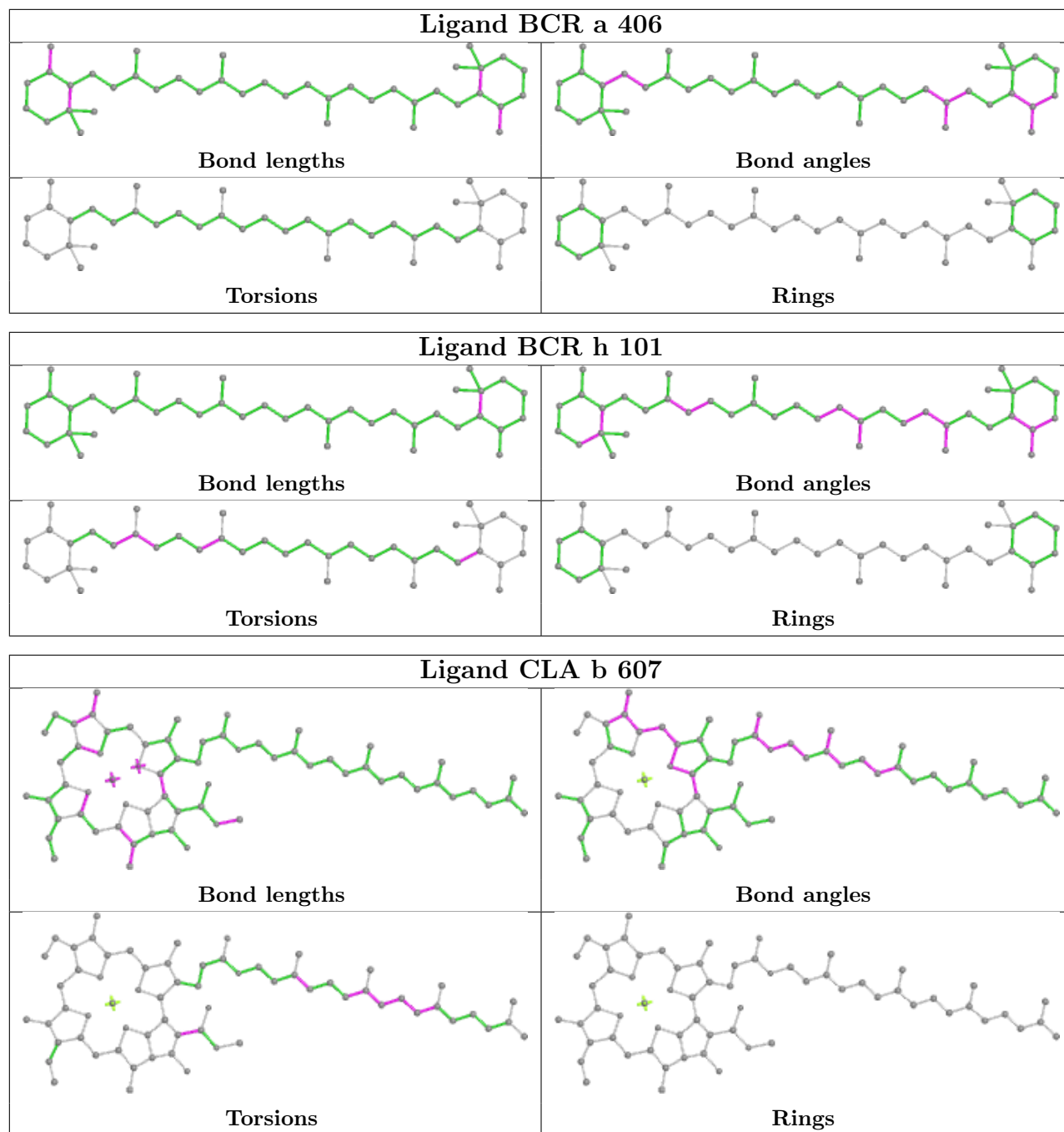
Ligand CLA A 403



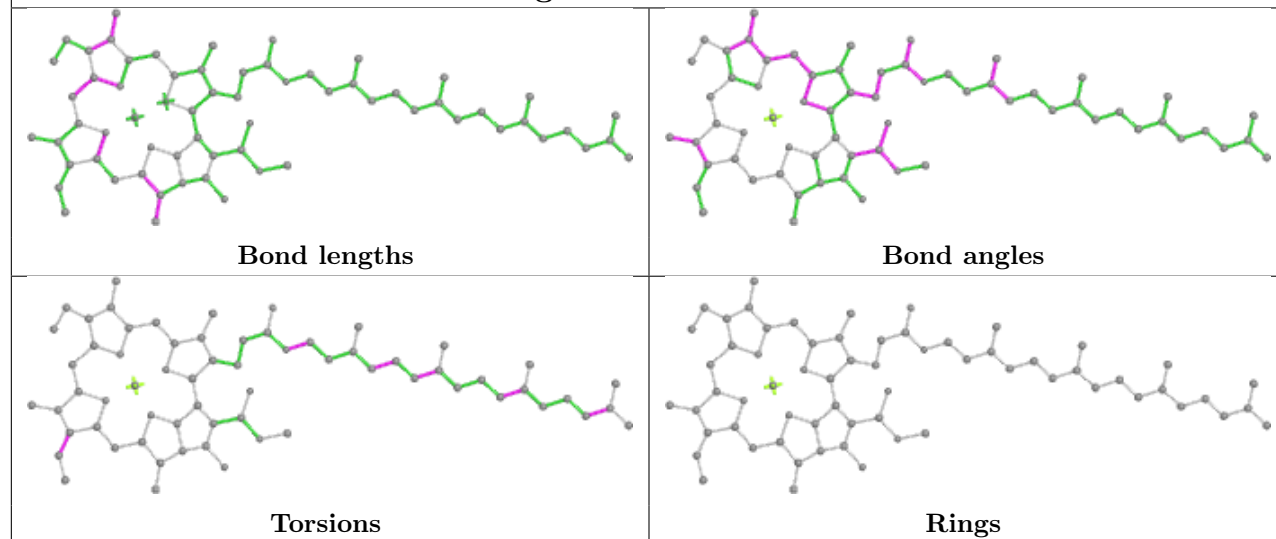
Ligand CLA b 602**Ligand CLA c 510**



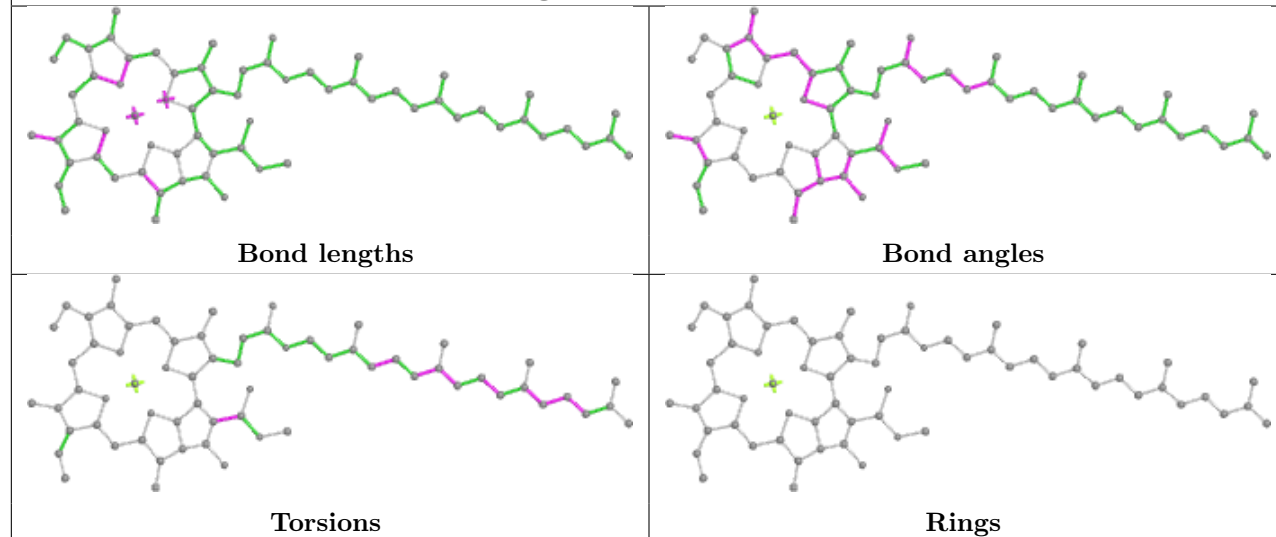




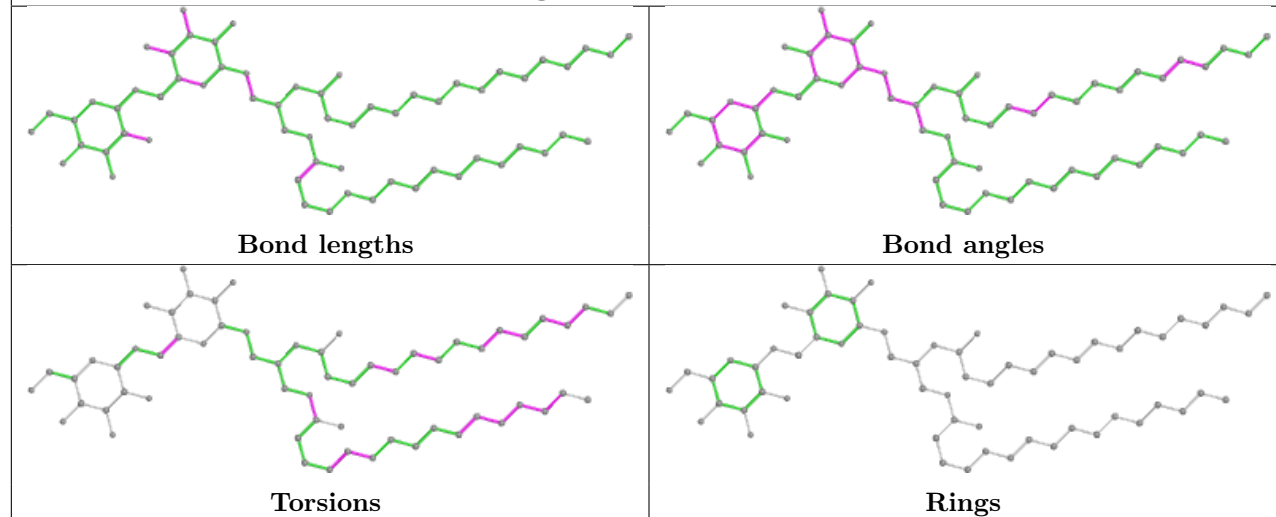
Ligand CLA d 403

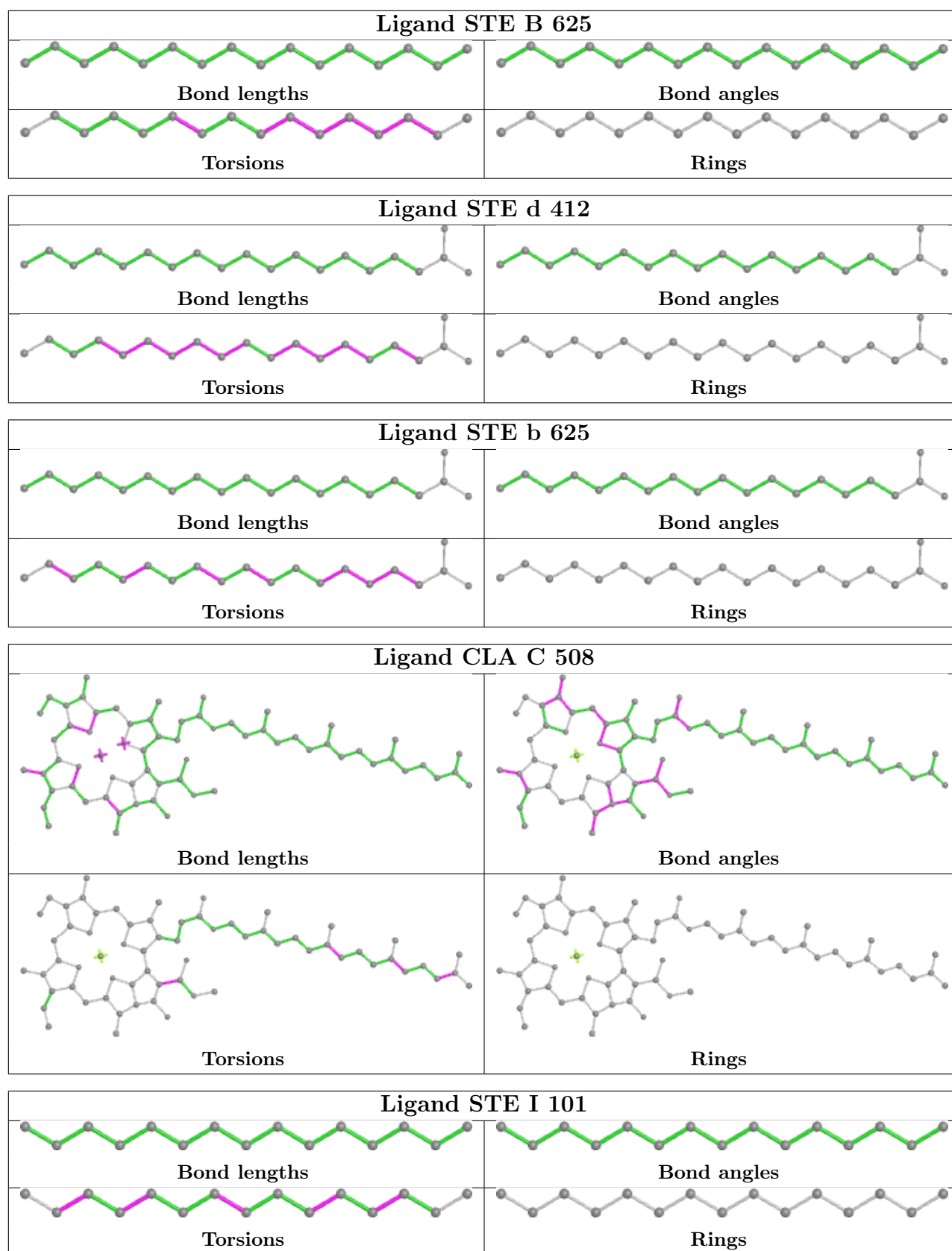


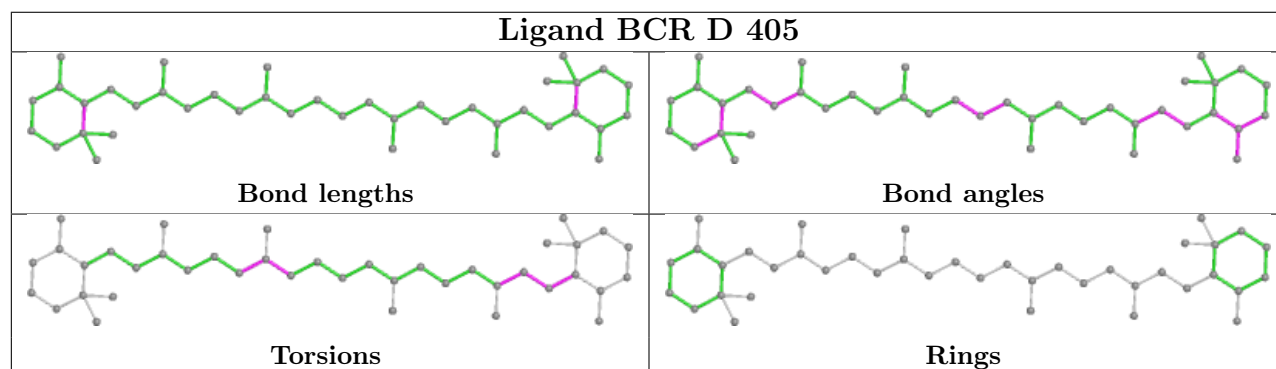
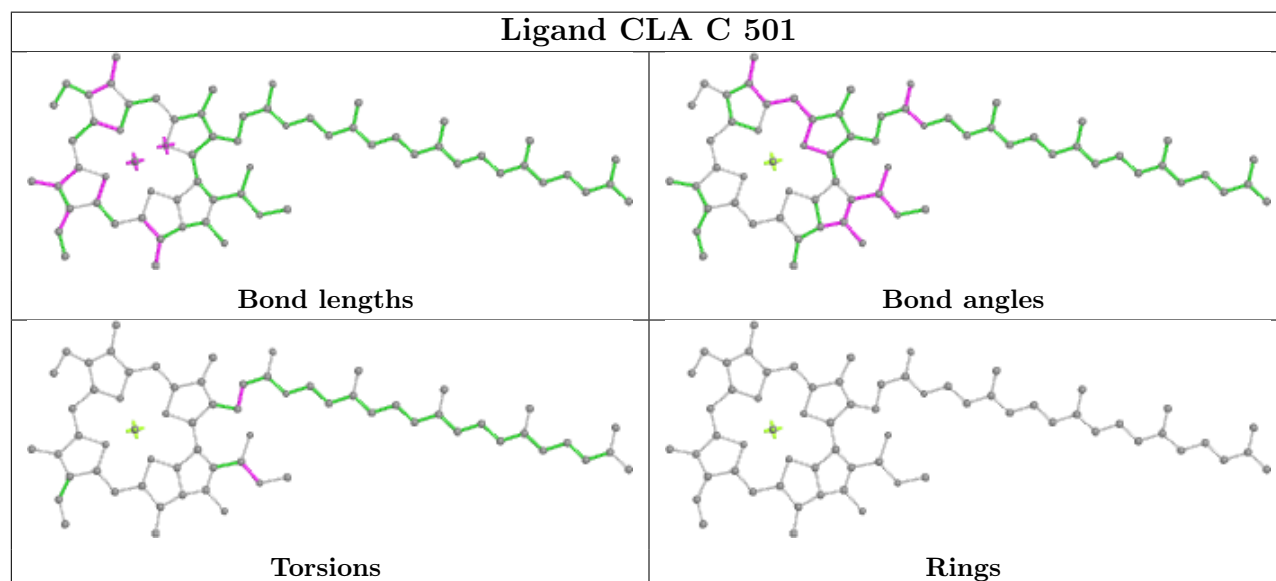
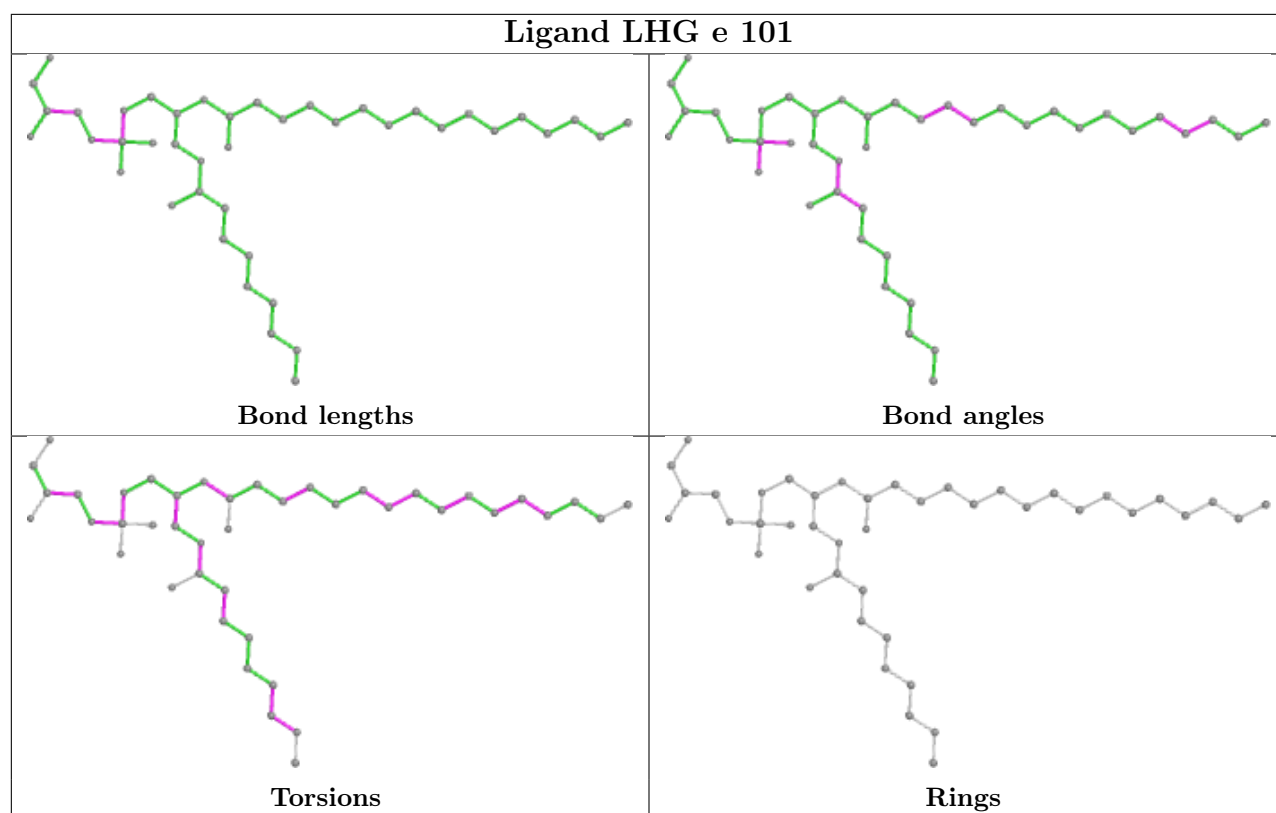
Ligand CLA b 604

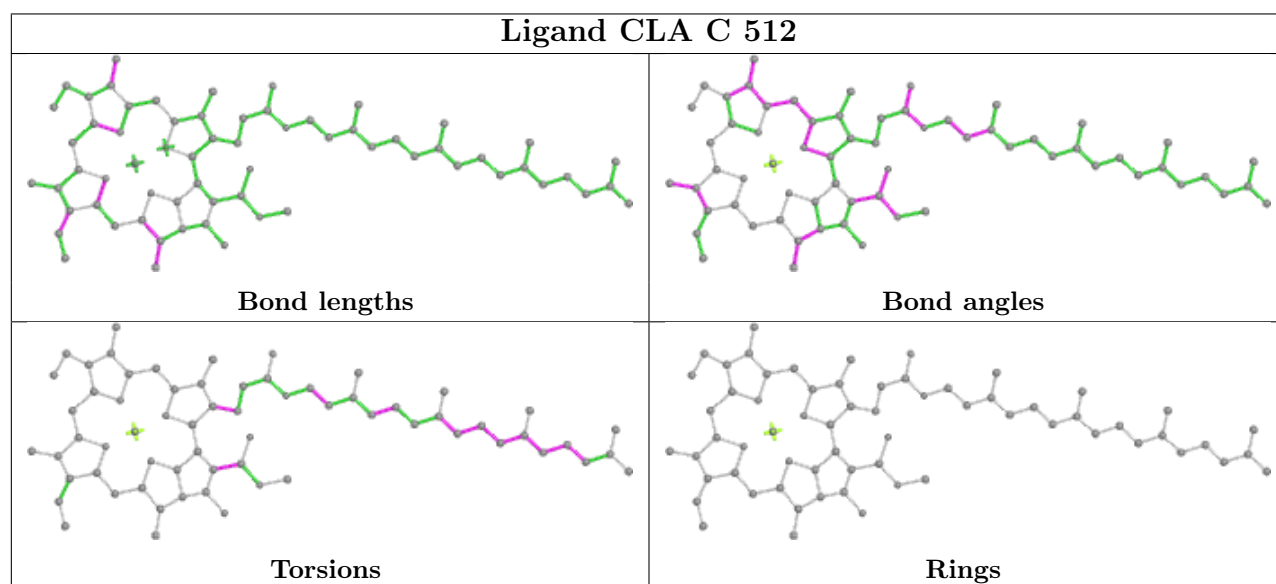
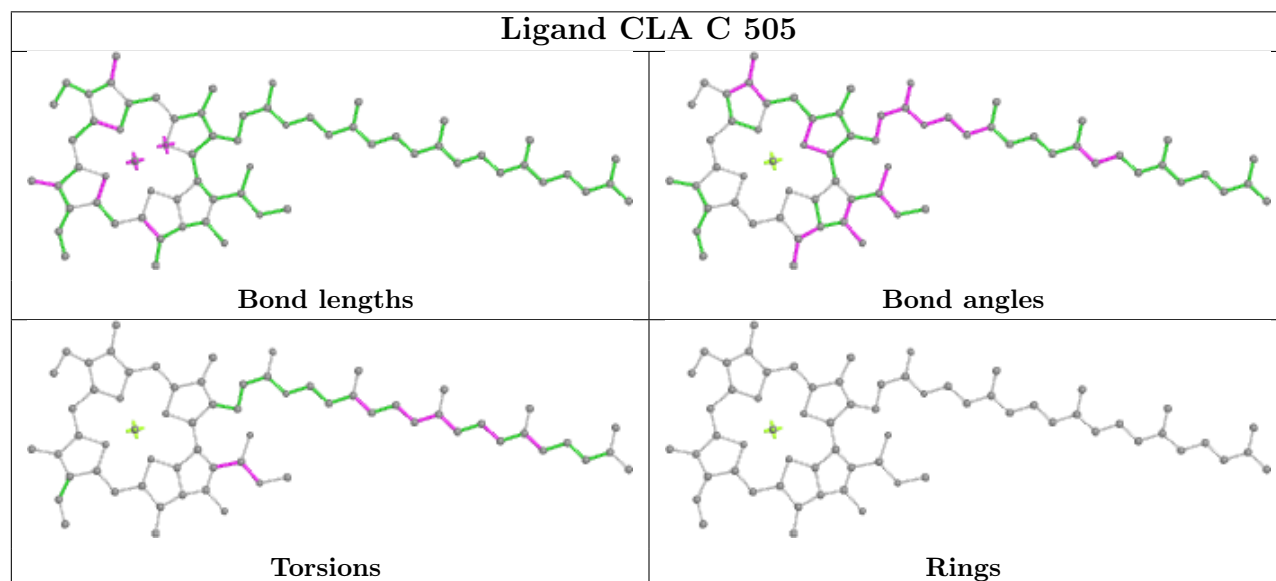
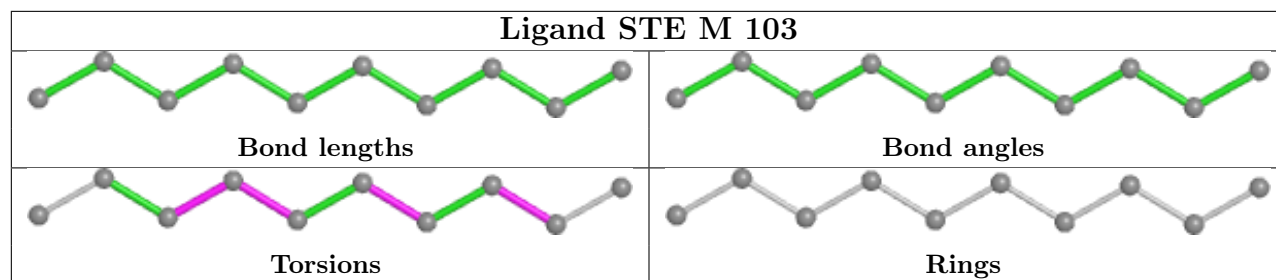


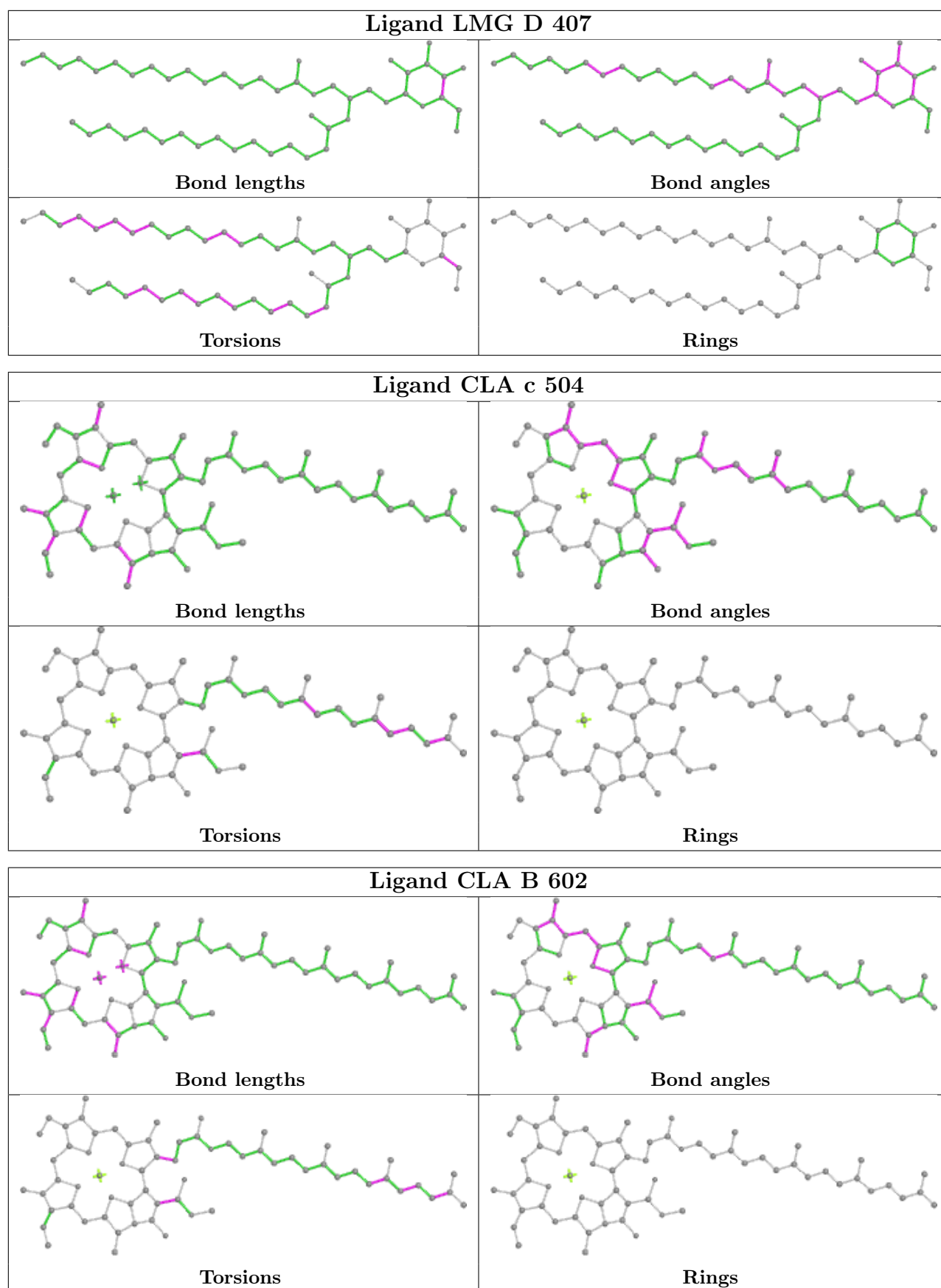
Ligand DGD c 518











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.29	4 (1%) 79 81	21, 28, 47, 72	0
1	a	334/344 (97%)	-0.34	0 100 100	21, 30, 54, 71	0
2	B	505/510 (99%)	-0.26	8 (1%) 72 75	23, 32, 59, 82	0
2	b	505/510 (99%)	-0.09	20 (3%) 38 43	21, 35, 66, 97	0
3	C	442/461 (95%)	-0.20	6 (1%) 75 78	24, 35, 49, 72	0
3	c	451/461 (97%)	-0.10	8 (1%) 68 71	26, 38, 56, 85	0
4	D	341/352 (96%)	-0.24	1 (0%) 94 94	20, 29, 46, 74	0
4	d	341/352 (96%)	-0.19	0 100 100	21, 33, 55, 78	0
5	E	82/84 (97%)	0.08	2 (2%) 59 63	32, 49, 66, 74	0
5	e	82/84 (97%)	0.27	3 (3%) 41 46	38, 55, 73, 82	0
6	F	34/45 (75%)	-0.14	1 (2%) 51 56	34, 41, 62, 85	0
6	f	34/45 (75%)	-0.17	2 (5%) 22 26	41, 48, 75, 88	0
7	H	65/66 (98%)	-0.08	1 (1%) 73 76	29, 39, 55, 66	0
7	h	63/66 (95%)	0.26	3 (4%) 30 35	39, 48, 57, 66	0
8	I	35/38 (92%)	-0.06	3 (8%) 10 12	29, 36, 64, 77	0
8	i	35/38 (92%)	-0.17	2 (5%) 23 28	30, 38, 71, 78	0
9	J	36/40 (90%)	0.21	4 (11%) 5 6	32, 47, 75, 86	0
9	j	36/40 (90%)	0.21	4 (11%) 5 6	38, 49, 83, 90	0
10	K	37/46 (80%)	0.26	4 (10%) 5 7	40, 50, 65, 73	0
10	k	37/46 (80%)	0.14	1 (2%) 54 59	45, 53, 64, 70	0
11	L	37/37 (100%)	-0.45	0 100 100	22, 29, 58, 66	0
11	l	36/37 (97%)	-0.26	3 (8%) 11 14	24, 29, 64, 79	0
12	M	32/36 (88%)	-0.06	1 (3%) 49 54	25, 31, 53, 63	0
12	m	31/36 (86%)	-0.20	0 100 100	25, 32, 47, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.01	15 (6%) 21 25	24, 38, 75, 127	0
13	o	244/272 (89%)	-0.12	12 (4%) 29 34	22, 37, 74, 103	0
14	R	28/41 (68%)	2.52	16 (57%) 0 0	58, 67, 78, 90	0
14	r	28/41 (68%)	4.52	25 (89%) 0 0	65, 90, 109, 119	0
15	T	29/32 (90%)	-0.39	2 (6%) 16 20	24, 29, 53, 70	0
15	t	29/32 (90%)	-0.17	2 (6%) 16 20	25, 30, 68, 88	0
16	U	97/134 (72%)	-0.22	2 (2%) 63 67	30, 41, 64, 83	0
16	u	97/134 (72%)	-0.36	0 100 100	28, 38, 53, 77	0
17	V	137/163 (84%)	-0.44	0 100 100	29, 38, 54, 70	0
17	v	137/163 (84%)	-0.12	4 (2%) 51 56	30, 44, 62, 83	0
18	X	38/41 (92%)	0.05	2 (5%) 26 31	38, 48, 65, 75	0
18	x	39/41 (95%)	0.54	5 (12%) 3 4	44, 56, 84, 98	0
19	Y	27/46 (58%)	1.48	10 (37%) 0 0	50, 67, 83, 89	0
19	y	30/46 (65%)	0.59	4 (13%) 3 4	57, 70, 79, 89	0
20	Z	62/62 (100%)	1.04	16 (25%) 0 0	51, 66, 106, 117	0
20	z	62/62 (100%)	0.97	12 (19%) 1 1	57, 67, 99, 111	0
All	All	5293/5700 (92%)	-0.08	208 (3%) 39 44	20, 36, 69, 127	0

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	8.5
14	r	14	LEU	8.3
13	o	58	ASN	8.3
15	t	30	THR	8.0
2	b	495	PHE	7.1

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	T	1	10/11	0.94	0.09	27,46,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	FME	t	1	10/11	0.94	0.09	29,43,65,65	0
12	FME	m	1	10/11	0.95	0.11	35,43,58,66	0
8	FME	I	1	10/11	0.96	0.13	40,48,60,60	0
8	FME	i	1	10/11	0.96	0.18	39,48,60,60	0
12	FME	M	1	10/11	0.96	0.11	39,53,66,71	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	E	101	12/20	0.68	0.35	52,76,90,92	0
32	STE	B	627	16/20	0.72	0.21	39,47,69,72	0
32	STE	b	625	20/20	0.72	0.22	45,67,80,91	0
32	STE	j	101	12/20	0.74	0.16	42,57,69,72	0
32	STE	H	103	18/20	0.75	0.29	54,82,92,98	0
32	STE	C	519	16/20	0.75	0.17	45,58,76,76	0
32	STE	B	625	16/20	0.75	0.29	37,64,85,88	0
26	PL9	a	409	55/55	0.76	0.29	44,72,88,94	0
27	LMG	h	102	23/55	0.77	0.25	47,65,83,88	0
32	STE	a	415	12/20	0.77	0.23	45,68,76,82	0
32	STE	m	102	12/20	0.77	0.23	49,64,81,90	0
32	STE	b	626	10/20	0.78	0.24	45,57,66,79	0
29	LHG	A	413	49/49	0.78	0.24	48,83,110,124	0
28	SQD	a	412	36/54	0.78	0.18	32,66,92,99	0
32	STE	I	101	15/20	0.79	0.18	43,60,76,80	0
26	PL9	A	410	55/55	0.79	0.30	46,66,88,93	0
32	STE	c	522	12/20	0.80	0.21	58,71,85,89	0
30	DGD	o	301	44/66	0.81	0.16	38,58,81,95	0
32	STE	B	620	17/20	0.81	0.15	35,52,71,82	0
27	LMG	D	410	32/55	0.81	0.18	36,58,75,85	0
27	LMG	c	521	48/55	0.81	0.23	50,77,103,106	0
24	BCR	h	101	40/40	0.81	0.15	34,52,73,80	0
32	STE	d	412	20/20	0.81	0.20	47,65,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	601	65/65	0.81	0.18	46,66,84,89	0
24	BCR	H	101	40/40	0.81	0.15	33,48,66,72	0
30	DGD	A	415	66/66	0.82	0.17	47,63,79,89	0
29	LHG	e	101	42/49	0.82	0.23	64,84,110,118	0
32	STE	a	413	10/20	0.83	0.24	40,65,68,69	0
28	SQD	A	414	39/54	0.83	0.18	44,62,91,95	0
22	CLA	C	512	65/65	0.83	0.17	35,53,82,90	0
32	STE	D	413	15/20	0.83	0.22	33,40,65,65	0
32	STE	c	520	20/20	0.84	0.17	43,58,91,99	0
22	CLA	c	513	65/65	0.84	0.20	39,65,104,105	0
32	STE	B	623	12/20	0.84	0.12	37,49,69,82	0
22	CLA	c	512	65/65	0.84	0.17	38,54,82,93	0
32	STE	T	102	15/20	0.84	0.18	52,65,79,81	0
32	STE	M	104	18/20	0.85	0.14	35,52,79,82	0
32	STE	b	624	16/20	0.86	0.16	44,61,82,89	0
24	BCR	K	102	40/40	0.86	0.12	36,54,68,73	0
32	STE	M	103	10/20	0.86	0.16	36,47,60,69	0
27	LMG	b	623	55/55	0.86	0.24	46,71,92,102	0
22	CLA	B	601	65/65	0.87	0.15	32,62,87,99	0
28	SQD	b	620	49/54	0.87	0.14	43,59,84,98	0
22	CLA	C	513	65/65	0.87	0.18	39,61,91,95	0
32	STE	d	411	17/20	0.87	0.14	44,57,65,77	0
32	STE	B	624	18/20	0.87	0.12	38,60,76,78	0
24	BCR	K	101	40/40	0.87	0.16	44,58,74,78	0
28	SQD	B	621	54/54	0.87	0.15	42,65,90,100	0
32	STE	J	101	12/20	0.88	0.11	46,58,69,77	0
32	STE	B	622	14/20	0.88	0.12	39,49,62,66	0
27	LMG	Y	101	48/55	0.88	0.15	32,67,84,92	0
24	BCR	k	101	40/40	0.89	0.13	43,60,72,77	0
22	CLA	c	502	65/65	0.89	0.16	30,42,59,62	0
24	BCR	d	406	40/40	0.89	0.13	30,52,86,93	0
32	STE	C	520	12/20	0.89	0.09	35,49,59,59	0
28	SQD	f	102	41/54	0.89	0.20	57,92,112,114	0
27	LMG	A	411	48/55	0.89	0.14	43,58,72,79	0
22	CLA	d	405	65/65	0.89	0.17	29,48,81,89	0
32	STE	b	621	16/20	0.89	0.14	41,52,70,71	0
32	STE	b	622	20/20	0.89	0.22	37,59,81,84	0
32	STE	C	518	12/20	0.90	0.12	45,56,65,67	0
22	CLA	c	508	64/65	0.90	0.15	29,44,87,101	0
22	CLA	D	404	65/65	0.90	0.14	24,41,96,106	0
32	STE	D	412	20/20	0.90	0.14	36,52,75,78	0
27	LMG	m	101	51/55	0.90	0.13	35,54,76,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	615	65/65	0.90	0.14	25,39,59,59	0
22	CLA	b	616	60/65	0.90	0.13	26,43,84,91	0
27	LMG	M	101	51/55	0.90	0.12	32,49,73,81	0
22	CLA	a	405	65/65	0.90	0.14	18,37,74,82	0
32	STE	M	102	15/20	0.90	0.15	33,50,71,73	0
24	BCR	k	102	40/40	0.90	0.17	42,53,69,69	0
32	STE	B	626	12/20	0.90	0.44	57,69,80,85	0
27	LMG	c	519	37/55	0.90	0.16	40,63,78,78	0
24	BCR	c	514	40/40	0.91	0.15	41,60,71,72	0
24	BCR	C	514	40/40	0.91	0.11	25,39,50,58	0
24	BCR	D	405	40/40	0.91	0.12	23,46,83,85	0
22	CLA	B	616	60/65	0.91	0.15	25,38,88,95	0
22	CLA	C	502	65/65	0.91	0.13	27,40,52,54	0
30	DGD	C	516	62/66	0.91	0.13	31,52,95,110	0
27	LMG	a	414	49/55	0.91	0.13	30,59,83,100	0
22	CLA	C	507	65/65	0.91	0.15	21,39,57,60	0
22	CLA	B	604	65/65	0.92	0.13	19,32,70,84	0
27	LMG	D	407	51/55	0.92	0.16	23,55,83,89	0
22	CLA	c	510	65/65	0.92	0.15	30,47,62,65	0
22	CLA	c	511	65/65	0.92	0.12	37,52,68,71	0
24	BCR	K	103	40/40	0.92	0.16	37,51,65,66	0
24	BCR	b	619	40/40	0.92	0.11	31,46,61,65	0
22	CLA	C	506	65/65	0.92	0.12	28,45,78,89	0
30	DGD	H	102	62/66	0.92	0.11	30,47,59,66	0
22	CLA	b	609	65/65	0.92	0.13	29,44,61,69	0
22	CLA	c	503	65/65	0.92	0.14	32,42,53,59	0
24	BCR	B	618	40/40	0.92	0.10	23,39,49,53	0
24	BCR	B	619	40/40	0.92	0.10	27,43,59,67	0
22	CLA	c	505	65/65	0.92	0.17	24,40,64,67	0
22	CLA	c	507	65/65	0.92	0.15	29,44,58,67	0
22	CLA	c	506	65/65	0.93	0.14	31,49,95,99	0
22	CLA	C	510	65/65	0.93	0.13	25,43,59,61	0
30	DGD	c	517	62/66	0.93	0.12	30,50,87,88	0
30	DGD	h	103	62/66	0.93	0.11	27,47,63,72	0
22	CLA	b	602	65/65	0.93	0.15	26,43,62,65	0
24	BCR	T	101	40/40	0.93	0.10	25,37,49,51	0
22	CLA	c	509	65/65	0.93	0.18	31,47,67,72	0
22	CLA	b	606	65/65	0.93	0.12	23,39,67,75	0
24	BCR	c	515	40/40	0.93	0.11	25,44,55,64	0
22	CLA	C	511	65/65	0.93	0.10	28,48,63,72	0
22	CLA	b	610	65/65	0.93	0.18	24,37,50,55	0
22	CLA	b	614	65/65	0.93	0.13	23,39,71,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	SQD	a	411	54/54	0.93	0.15	40,62,96,97	0
22	CLA	B	614	65/65	0.93	0.16	20,37,67,77	0
22	CLA	C	505	65/65	0.93	0.16	20,40,69,72	0
22	CLA	B	615	65/65	0.93	0.12	20,37,57,63	0
22	CLA	a	403	65/65	0.93	0.14	24,41,88,95	0
22	CLA	c	504	60/65	0.93	0.12	29,44,74,85	0
22	CLA	B	606	65/65	0.93	0.10	23,36,64,71	0
22	CLA	d	404	65/65	0.94	0.13	18,30,45,53	0
22	CLA	C	503	65/65	0.94	0.13	31,41,50,62	0
24	BCR	A	407	40/40	0.94	0.09	25,35,44,44	0
22	CLA	C	504	59/65	0.94	0.12	30,42,77,79	0
26	PL9	D	406	55/55	0.94	0.10	21,33,47,53	0
29	LHG	D	409	47/49	0.94	0.12	24,51,77,89	0
22	CLA	B	610	65/65	0.94	0.14	19,33,44,50	0
22	CLA	B	613	65/65	0.94	0.14	18,31,66,75	0
30	DGD	C	515	62/66	0.94	0.13	18,39,69,77	0
22	CLA	B	602	65/65	0.94	0.15	23,35,53,66	0
22	CLA	C	508	65/65	0.94	0.10	26,42,91,97	0
22	CLA	b	604	65/65	0.94	0.14	21,34,68,80	0
30	DGD	c	518	62/66	0.94	0.14	26,52,78,83	0
22	CLA	C	509	65/65	0.94	0.17	25,46,61,69	0
22	CLA	b	608	65/65	0.94	0.15	23,42,61,66	0
22	CLA	A	406	54/65	0.94	0.12	19,31,64,72	0
24	BCR	b	617	40/40	0.94	0.12	24,41,52,54	0
24	BCR	b	618	40/40	0.94	0.11	23,39,52,56	0
27	LMG	d	410	44/55	0.94	0.12	32,54,88,100	0
22	CLA	A	403	65/65	0.94	0.14	22,34,95,103	0
22	CLA	b	612	65/65	0.94	0.17	17,34,48,58	0
22	CLA	b	613	65/65	0.94	0.13	19,35,66,78	0
22	CLA	B	609	65/65	0.94	0.12	26,38,59,66	0
28	SQD	F	102	36/54	0.94	0.19	45,74,95,99	0
22	CLA	B	603	65/65	0.95	0.15	17,32,65,67	0
22	CLA	B	608	65/65	0.95	0.12	20,34,55,59	0
29	LHG	a	410	49/49	0.95	0.13	32,52,70,77	0
29	LHG	d	409	39/49	0.95	0.10	28,41,68,74	0
22	CLA	b	605	65/65	0.95	0.11	21,34,48,52	0
22	CLA	c	501	65/65	0.95	0.13	28,40,52,55	0
24	BCR	a	406	40/40	0.95	0.08	19,33,49,50	0
22	CLA	d	403	65/65	0.95	0.12	18,35,54,59	0
30	DGD	C	517	62/66	0.95	0.10	26,47,73,79	0
22	CLA	A	402	65/65	0.95	0.10	17,27,45,49	0
30	DGD	c	516	62/66	0.95	0.12	22,43,76,81	0

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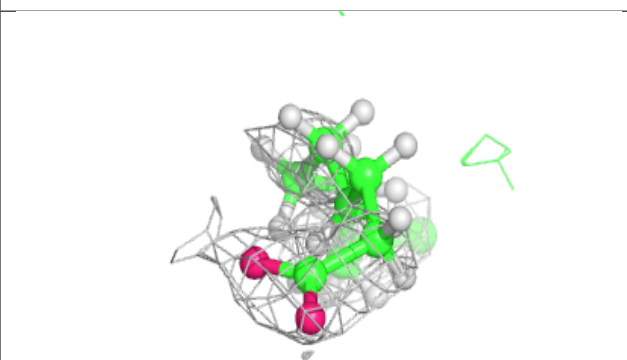
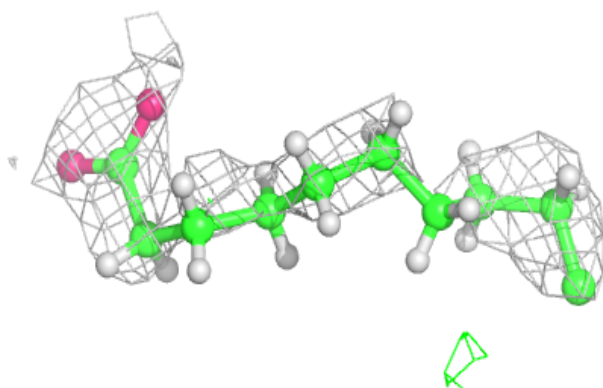
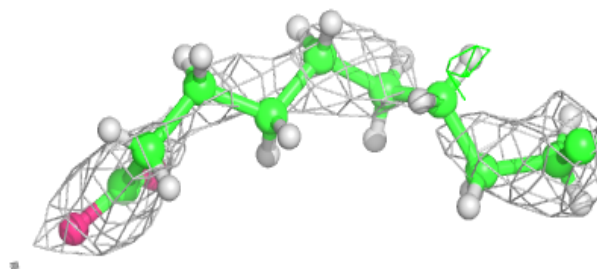
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	607	65/65	0.95	0.12	17,36,64,75	0
23	PHO	A	404	64/64	0.95	0.10	17,28,42,48	0
23	PHO	a	404	64/64	0.95	0.13	20,31,38,44	0
22	CLA	D	402	65/65	0.95	0.12	17,27,53,64	0
24	BCR	B	617	40/40	0.95	0.11	26,38,56,56	0
28	SQD	A	412	52/54	0.95	0.13	35,58,85,88	0
22	CLA	B	605	65/65	0.95	0.14	18,31,47,49	0
22	CLA	C	501	65/65	0.95	0.13	19,35,46,56	0
24	BCR	t	101	40/40	0.95	0.08	26,37,50,54	0
22	CLA	b	611	65/65	0.95	0.14	19,35,52,60	0
22	CLA	B	611	65/65	0.95	0.14	20,31,51,54	0
22	CLA	B	612	65/65	0.95	0.14	21,32,45,58	0
26	PL9	d	407	55/55	0.95	0.10	22,34,41,47	0
34	HEM	F	101	43/43	0.95	0.12	37,48,61,62	0
29	LHG	l	101	49/49	0.96	0.10	25,46,58,60	0
23	PHO	A	405	64/64	0.96	0.13	22,32,42,46	0
22	CLA	D	403	65/65	0.96	0.10	19,28,49,59	0
23	PHO	d	401	64/64	0.96	0.10	23,38,47,59	0
29	LHG	D	411	49/49	0.96	0.11	30,45,61,73	0
29	LHG	L	101	49/49	0.96	0.11	26,43,57,64	0
22	CLA	b	603	65/65	0.96	0.12	19,36,61,68	0
22	CLA	B	607	65/65	0.96	0.10	15,35,60,62	0
22	CLA	a	402	65/65	0.96	0.10	20,30,42,55	0
34	HEM	f	101	43/43	0.96	0.13	45,58,77,83	0
29	LHG	D	408	49/49	0.97	0.09	23,42,56,61	0
29	LHG	d	408	49/49	0.97	0.09	22,42,57,67	0
35	HEC	V	201	43/43	0.97	0.13	20,34,42,43	0
35	HEC	v	201	43/43	0.97	0.12	28,36,49,53	0
33	BCT	d	402	4/4	0.98	0.17	32,38,45,52	0
25	CL	a	408	1/1	0.98	0.06	28,28,28,28	0
21	FE2	a	401	1/1	0.98	0.11	35,35,35,35	0
25	CL	A	408	1/1	0.98	0.07	28,28,28,28	0
33	BCT	D	401	4/4	0.98	0.17	22,26,32,35	0
31	OEX	a	416	10/10	0.99	0.13	25,26,31,31	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.10	26,26,26,26	0
31	OEX	A	416	10/10	0.99	0.12	22,26,29,31	0
25	CL	A	409	1/1	1.00	0.04	31,31,31,31	0

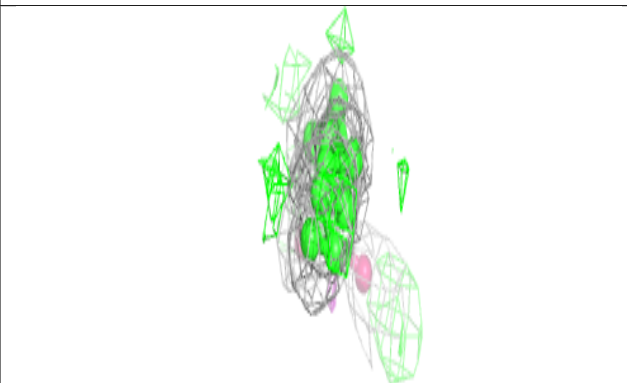
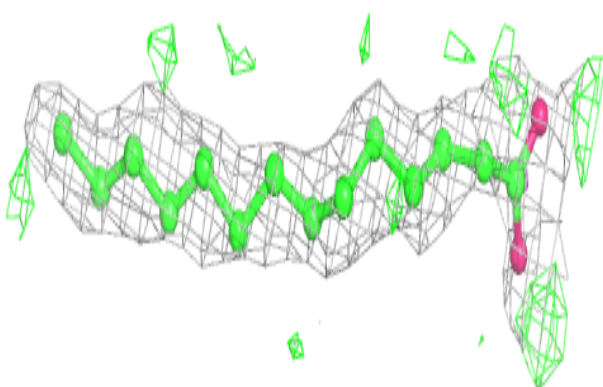
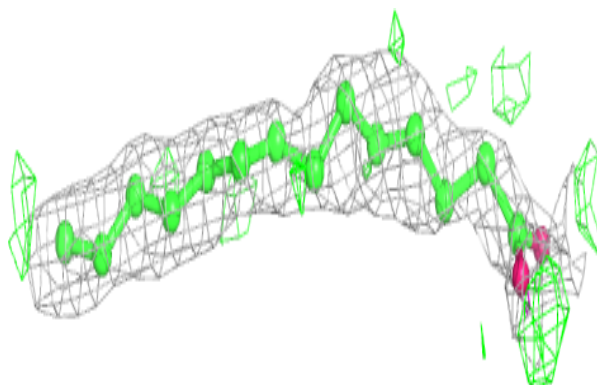
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE E 101:

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

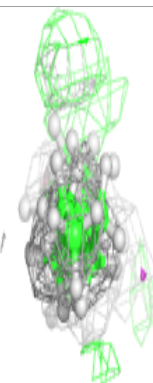
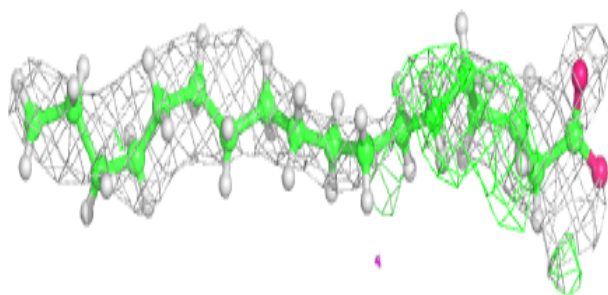
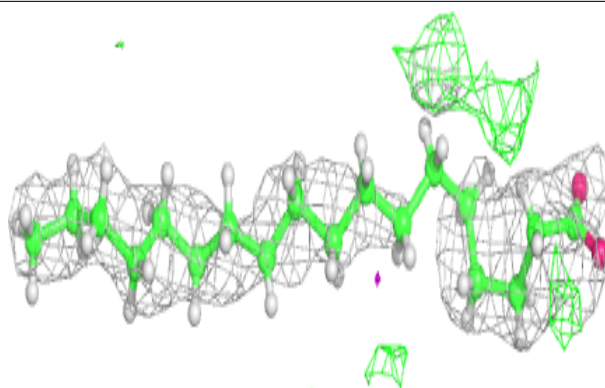
**Electron density around STE B 627:**

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

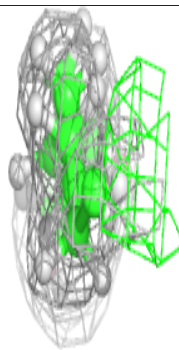
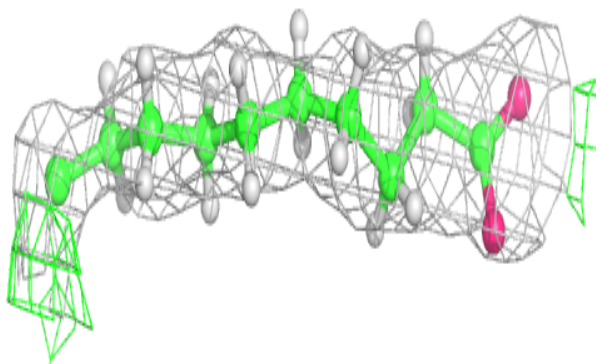
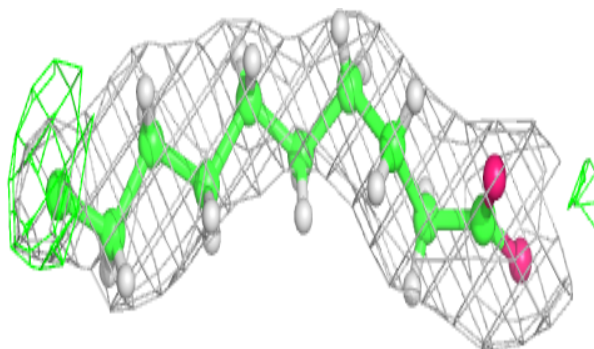


Electron density around STE b 625:

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

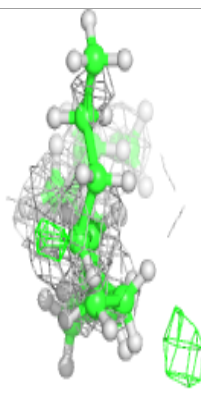
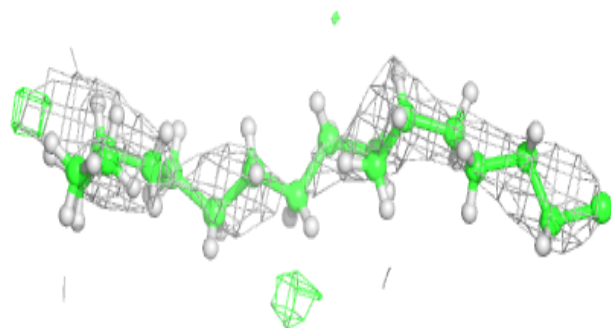
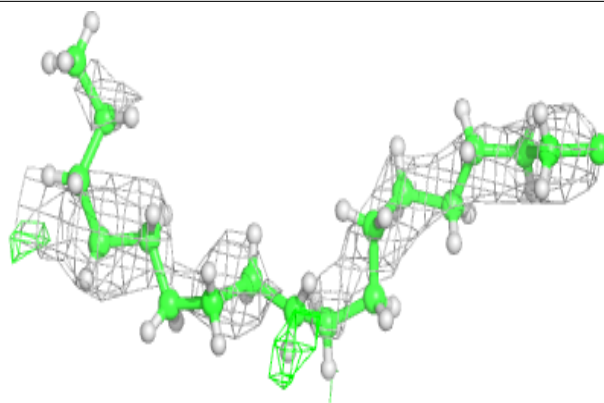
**Electron density around STE j 101:**

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

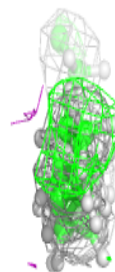
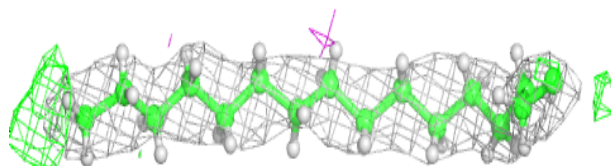
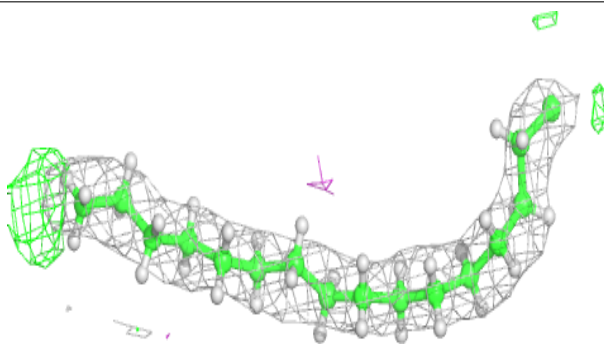


Electron density around STE H 103:

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

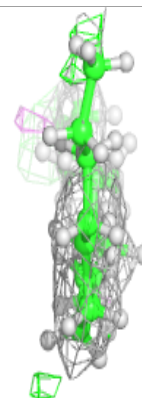
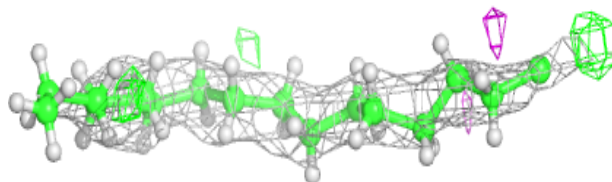
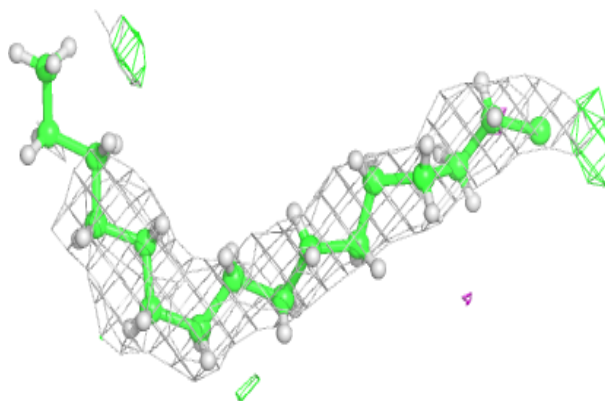
**Electron density around STE C 519:**

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

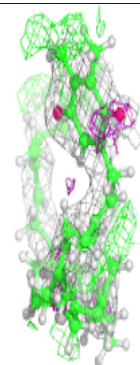
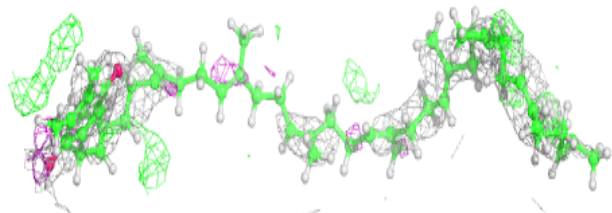
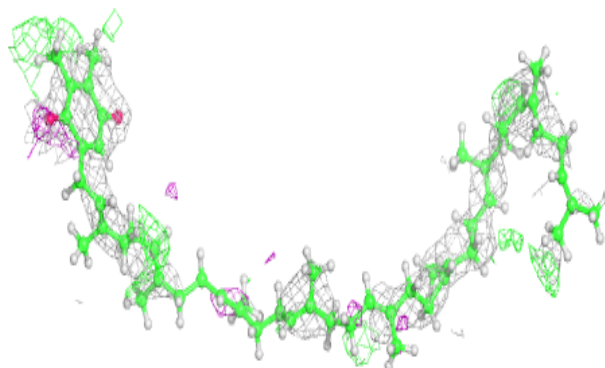


Electron density around STE B 625:

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

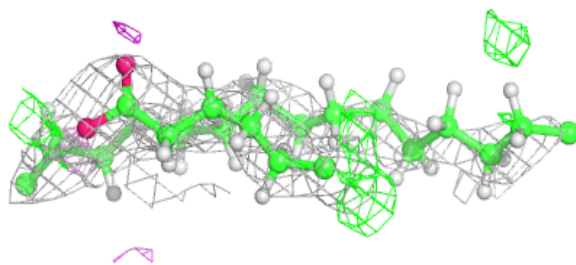
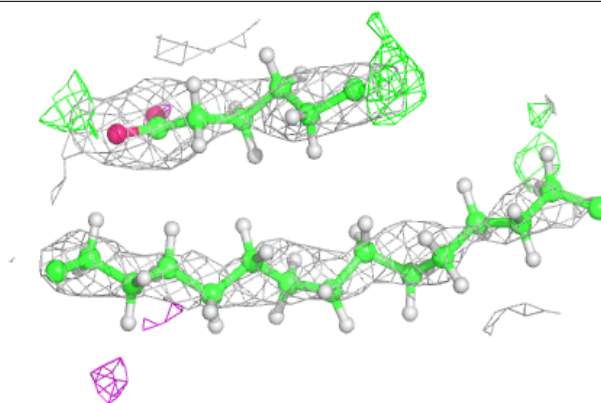
**Electron density around PL9 a 409:**

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

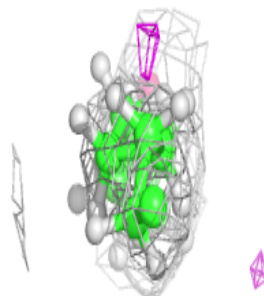
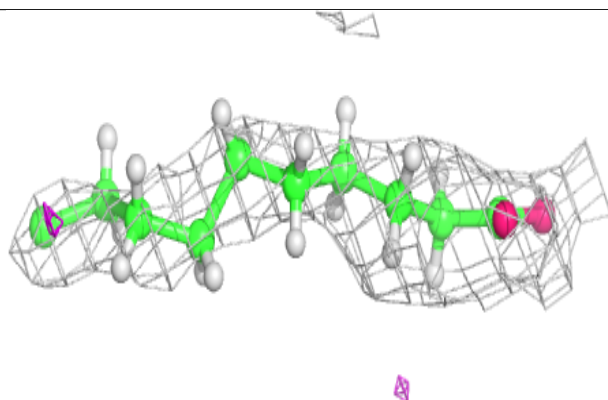
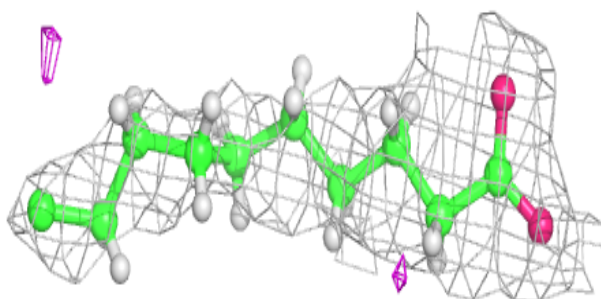


Electron density around LMG h 102:

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

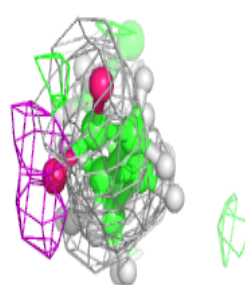
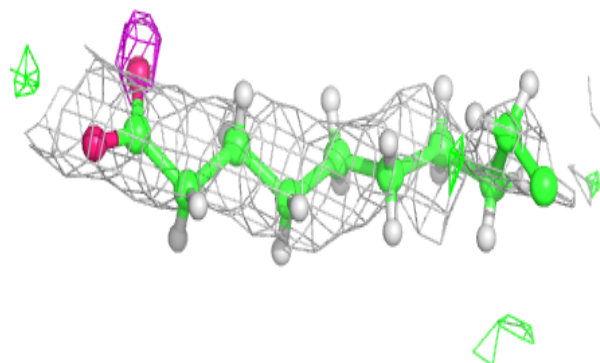
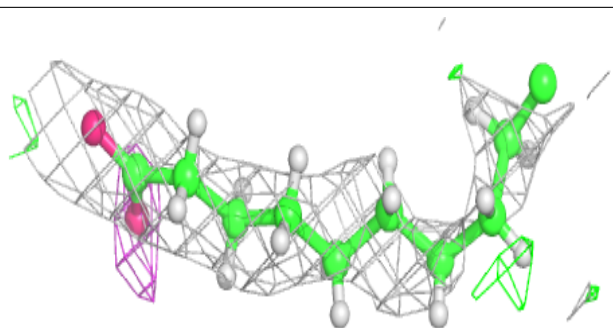
**Electron density around STE a 415:**

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

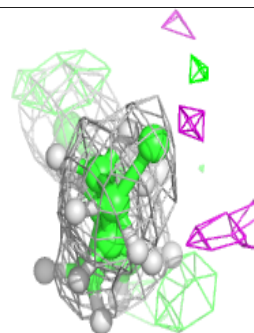
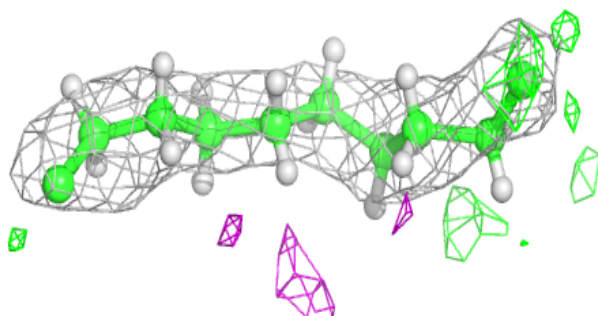
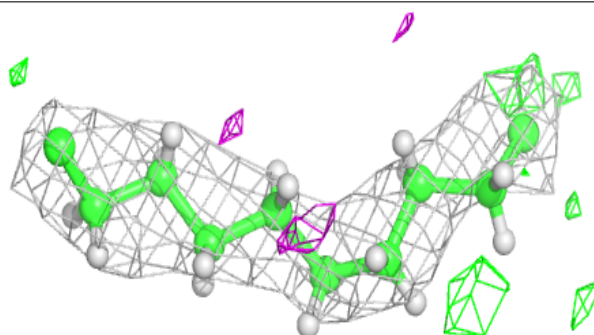


Electron density around STE m 102:

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

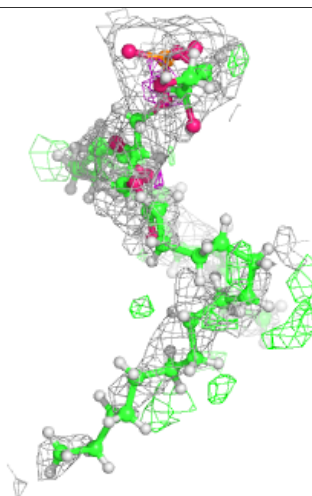
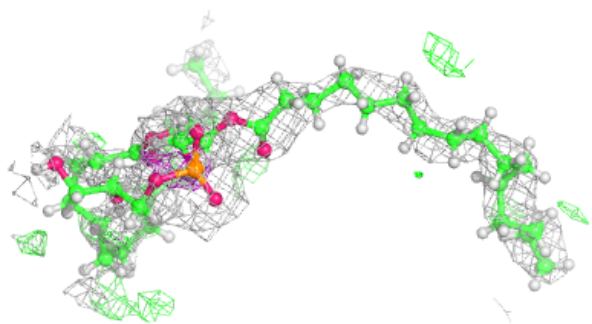
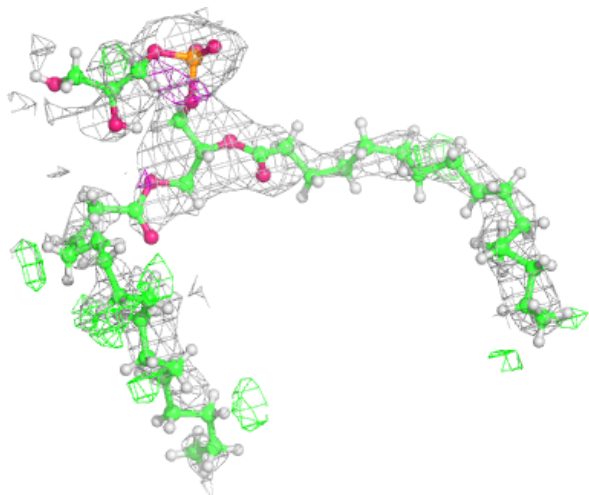
**Electron density around STE b 626:**

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



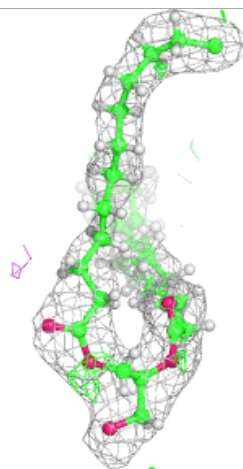
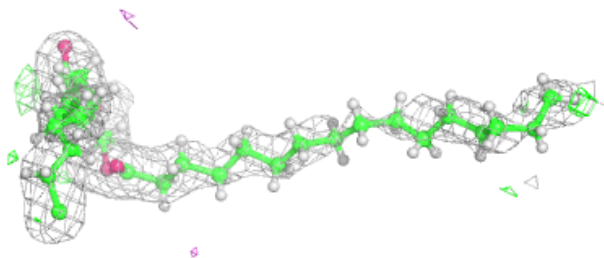
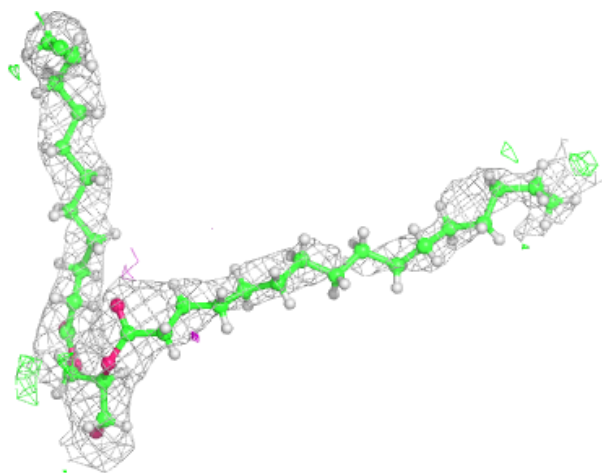
Electron density around LHG A 413:

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



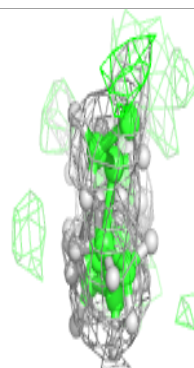
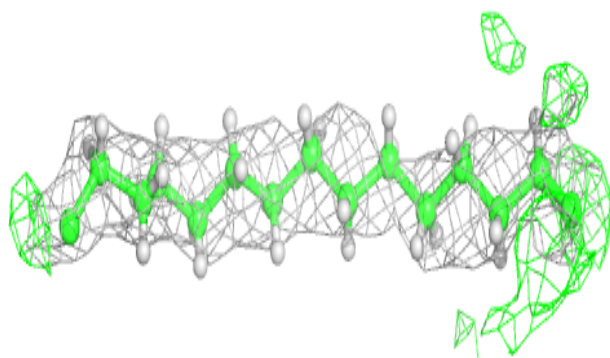
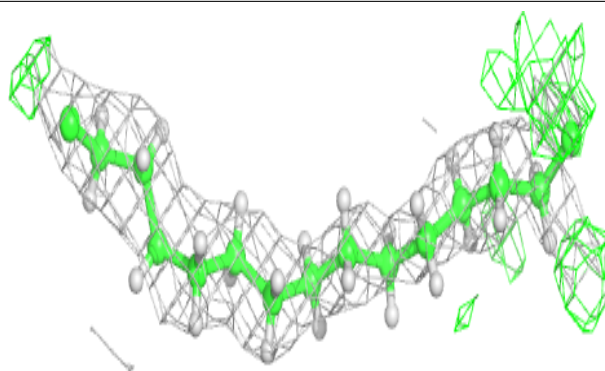
Electron density around SQD a 412:

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

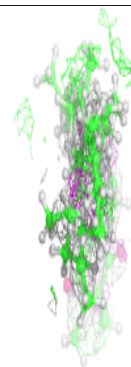
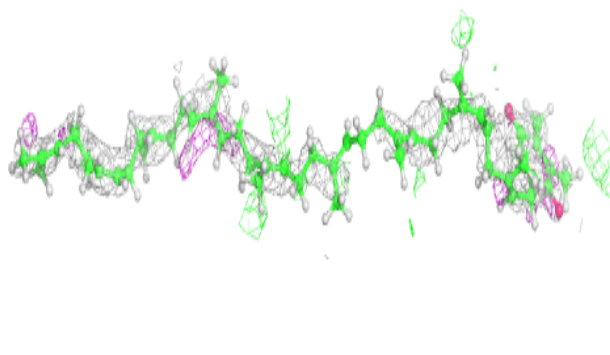
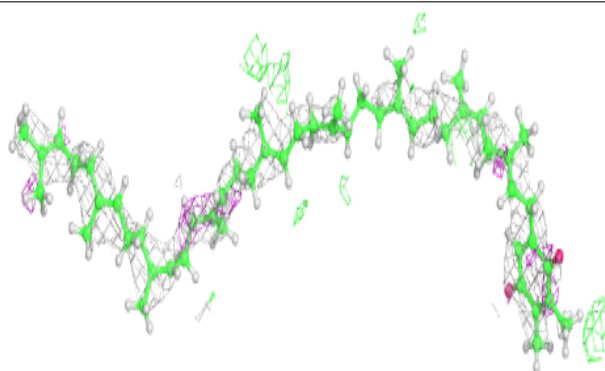


Electron density around STE I 101:

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

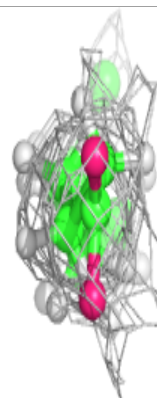
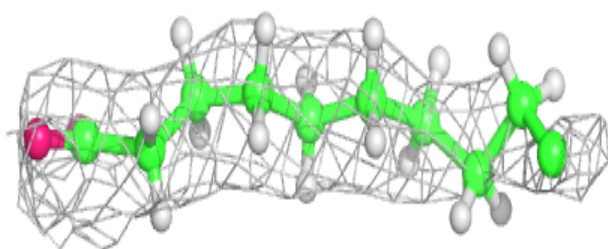
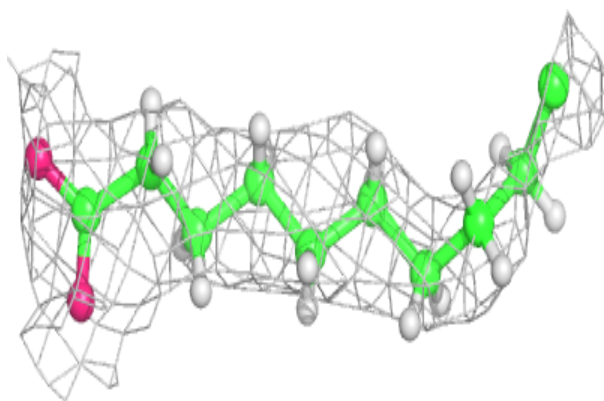
**Electron density around PL9 A 410:**

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

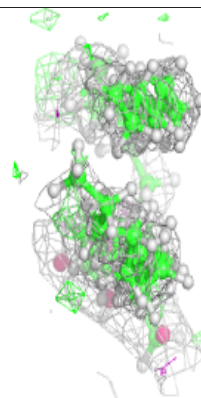
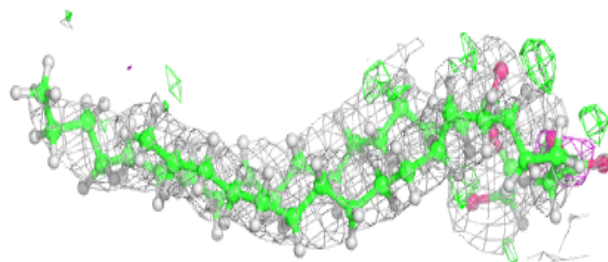
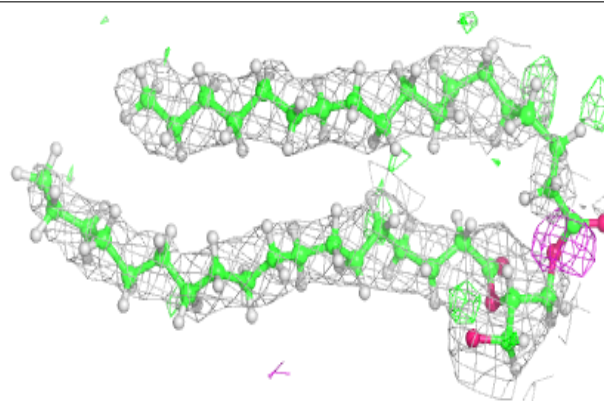


Electron density around STE c 522:

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

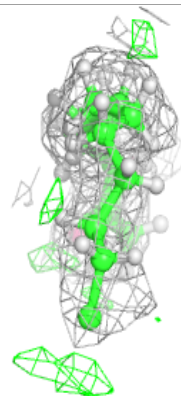
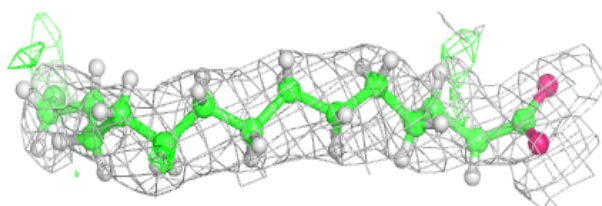
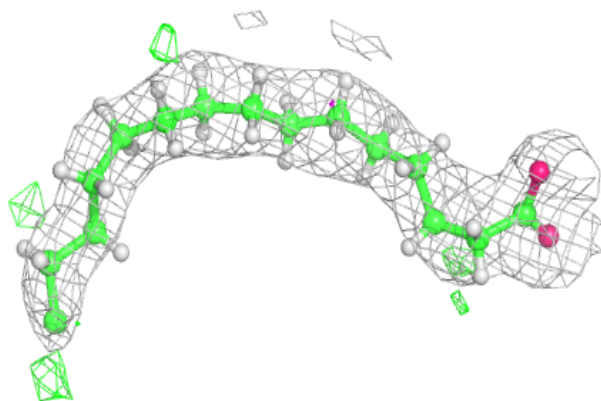
**Electron density around DGD o 301:**

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

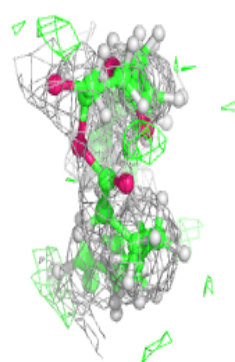
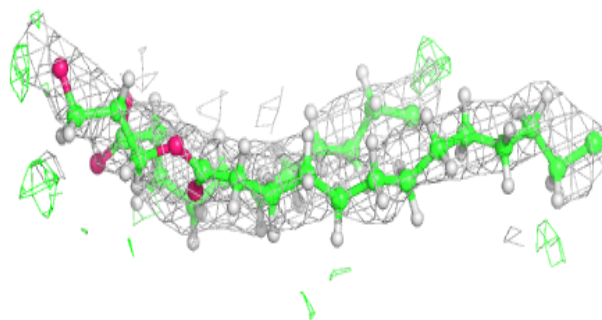
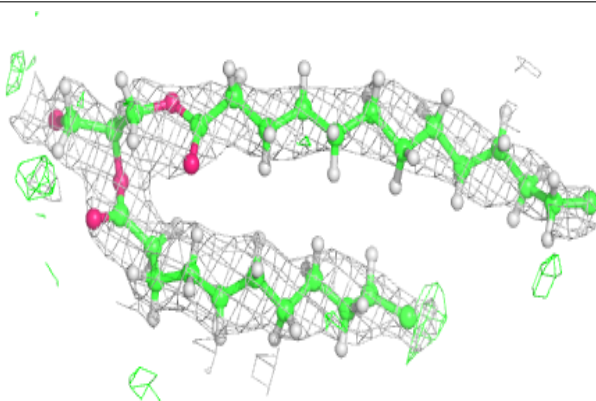


Electron density around STE B 620:

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

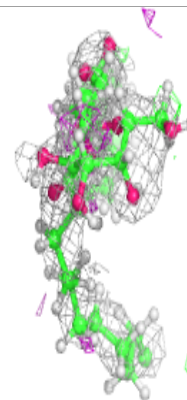
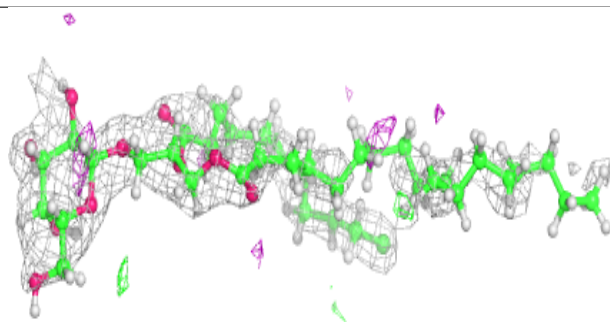
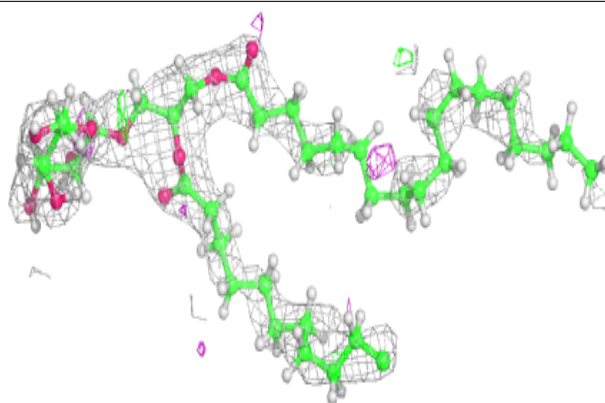
**Electron density around LMG D 410:**

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

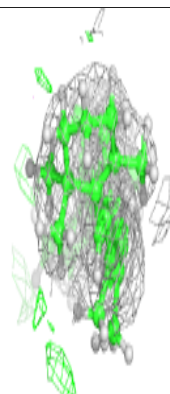
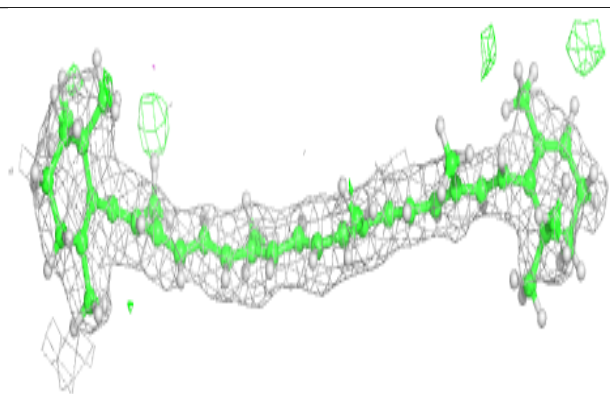
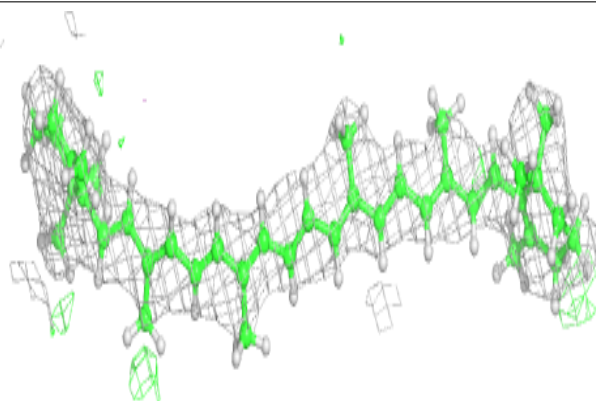


Electron density around LMG c 521:

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

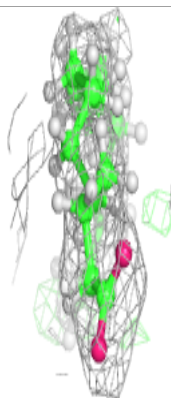
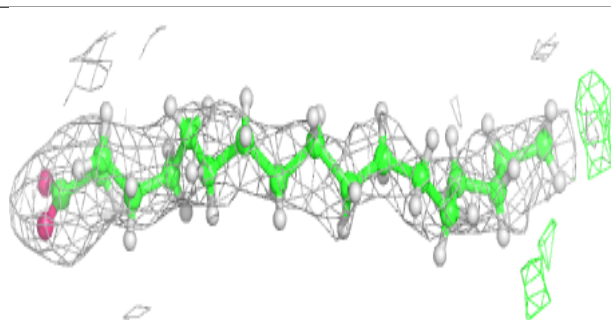
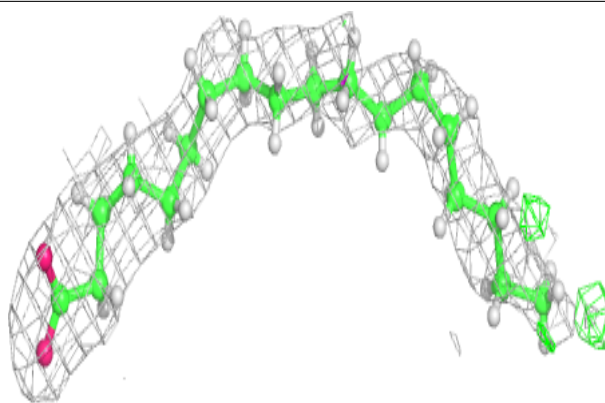
**Electron density around BCR h 101:**

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

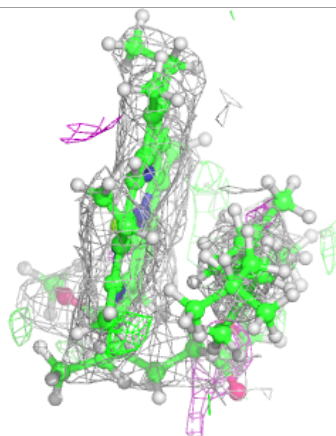
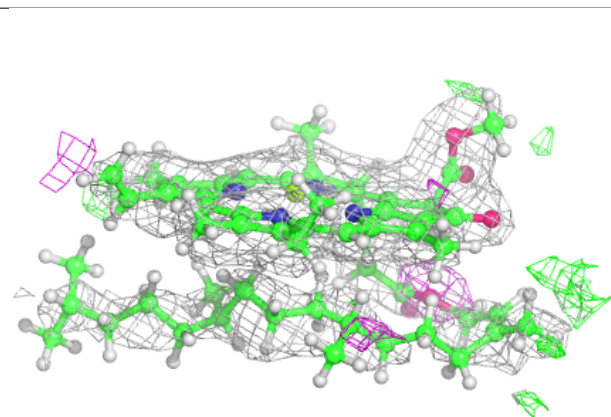
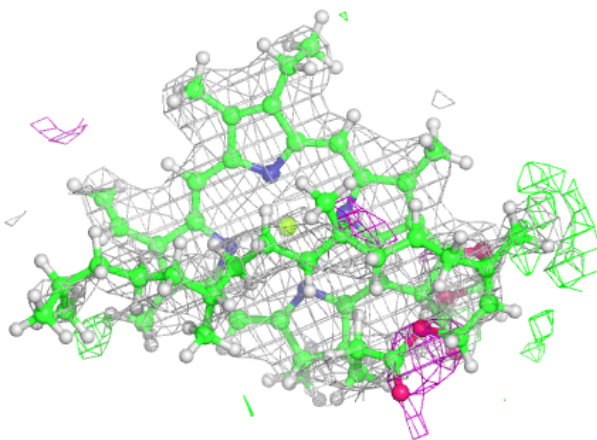


Electron density around STE d 412:

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

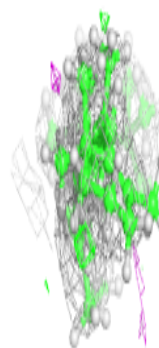
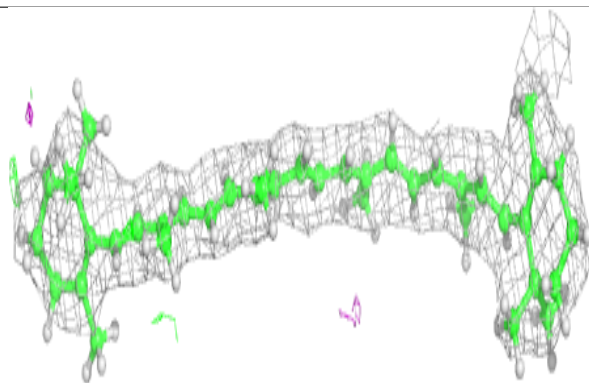
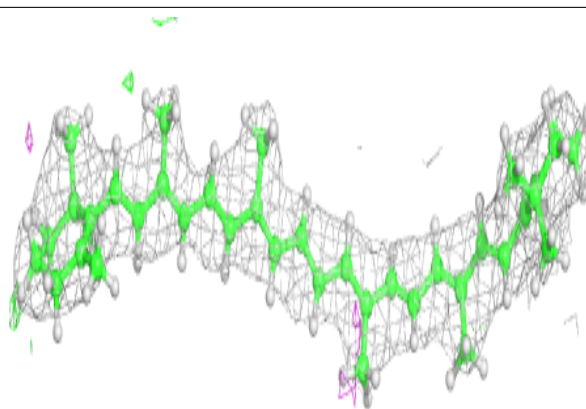
**Electron density around CLA b 601:**

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

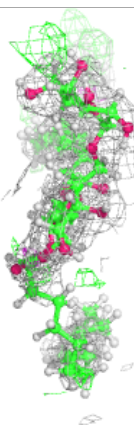
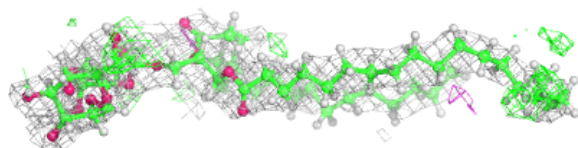
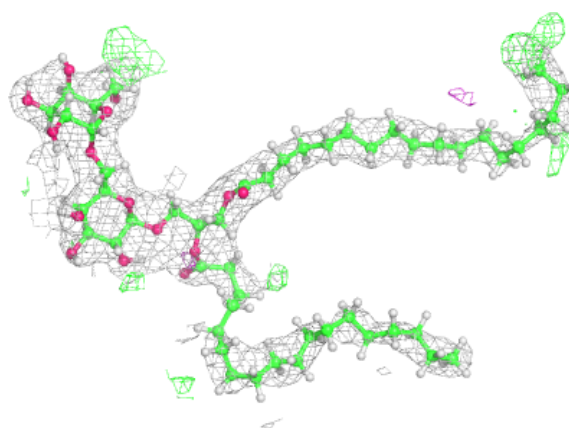


Electron density around BCR H 101:

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

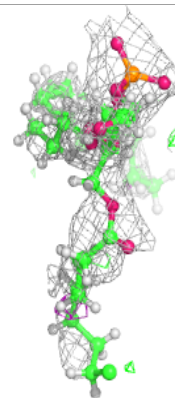
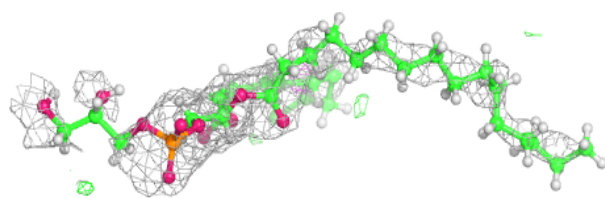
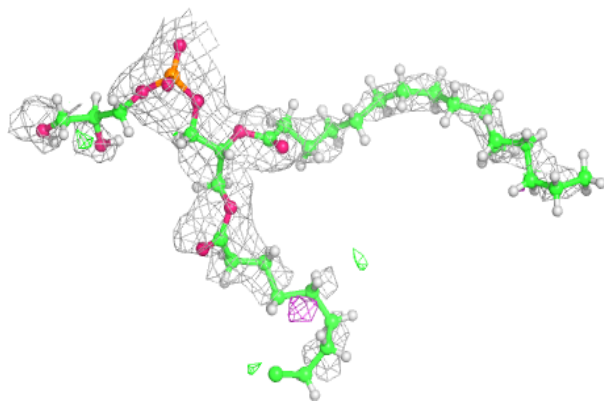
**Electron density around DGD A 415:**

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

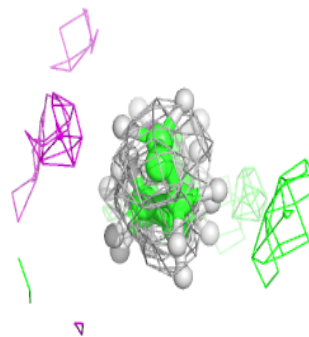
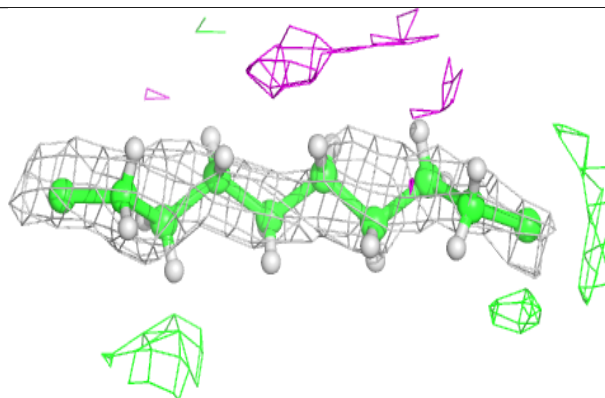
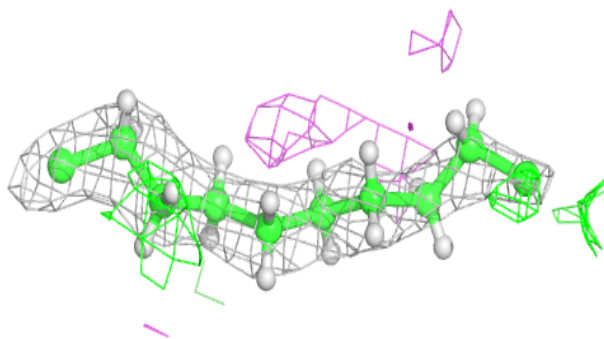


Electron density around LHG e 101:

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

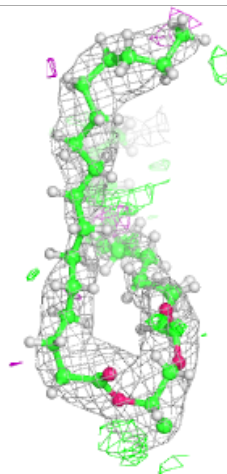
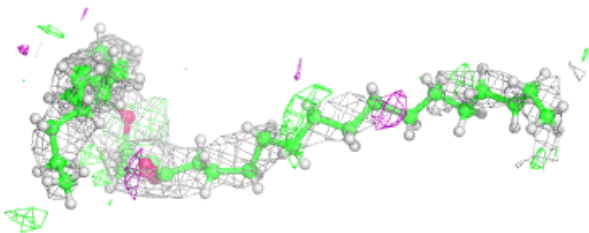
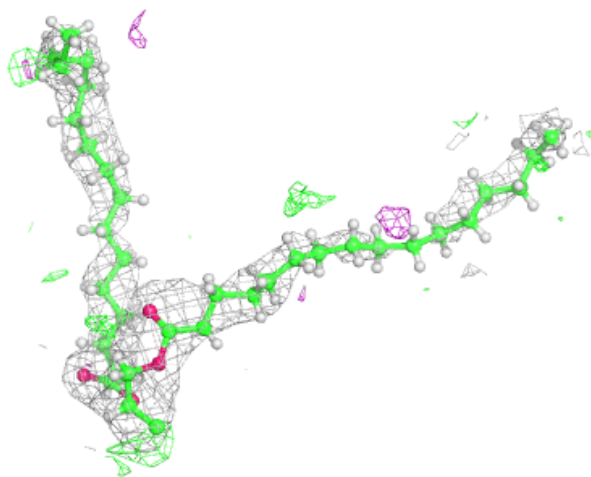
**Electron density around STE a 413:**

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



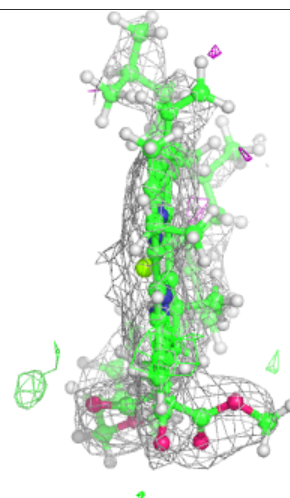
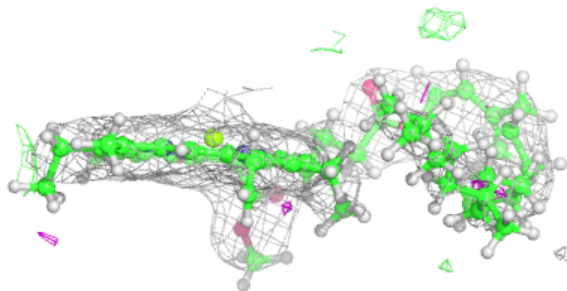
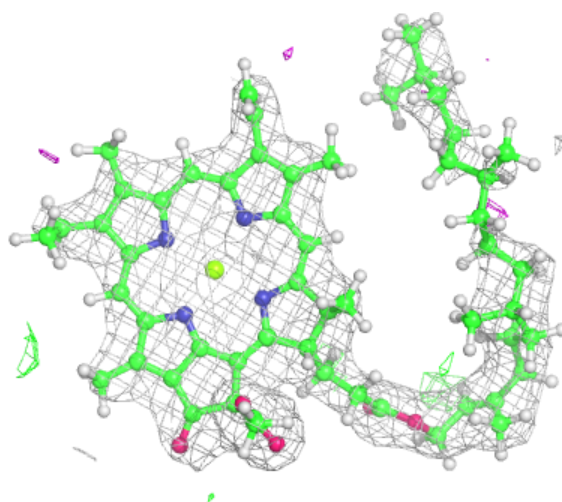
Electron density around SQD A 414:

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



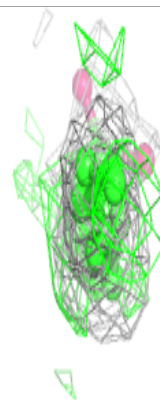
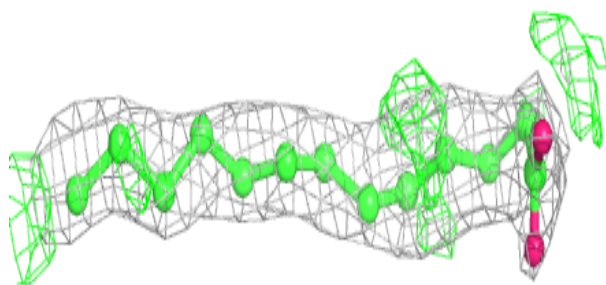
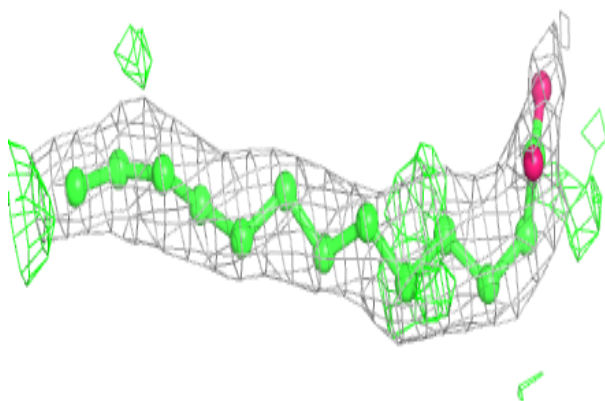
Electron density around CLA C 512:

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

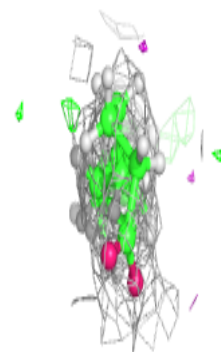
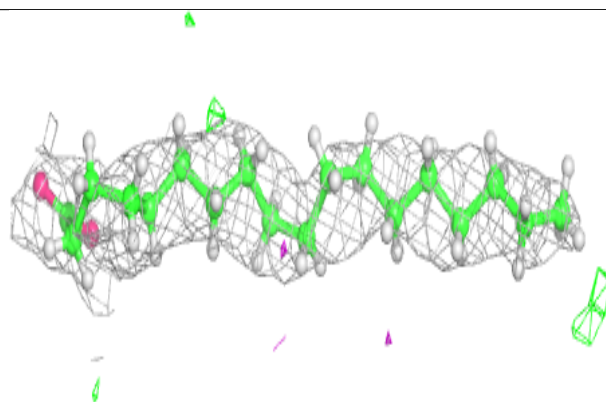
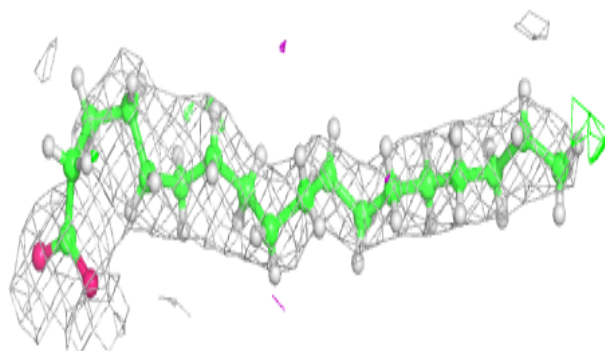


Electron density around STE D 413:

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

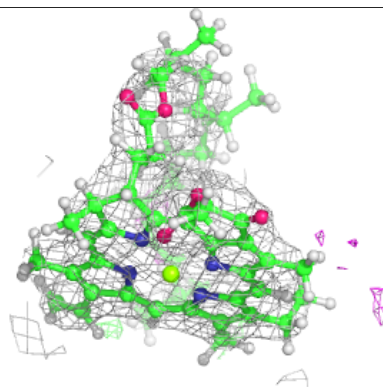
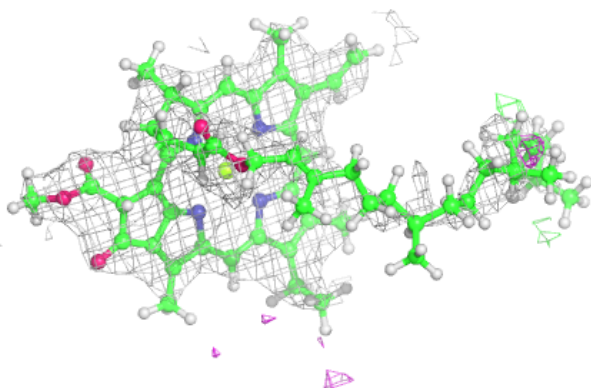
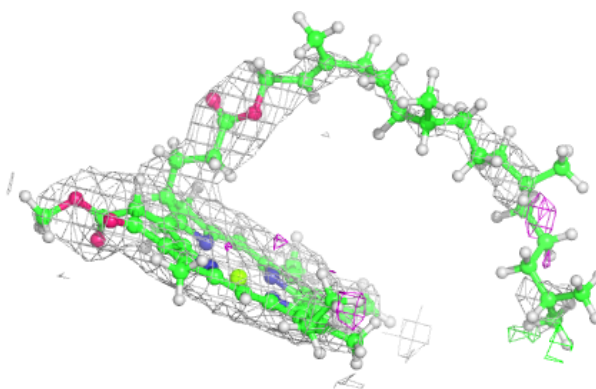
**Electron density around STE c 520:**

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

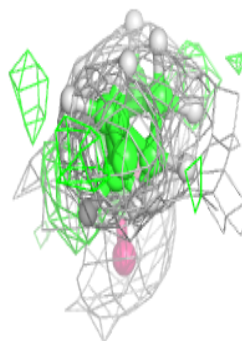
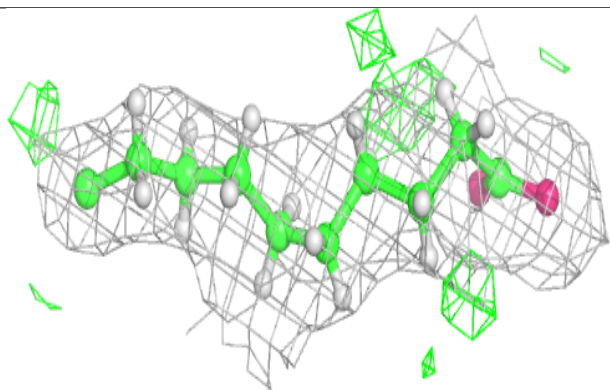
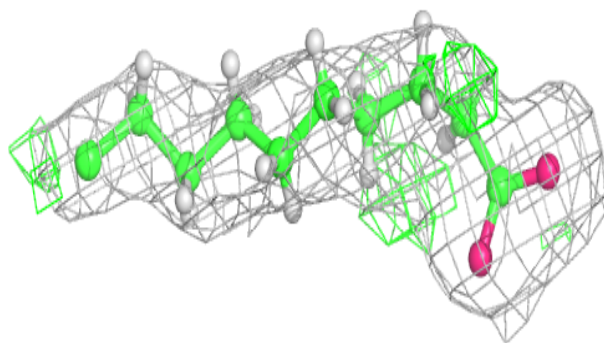


Electron density around CLA c 513:

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

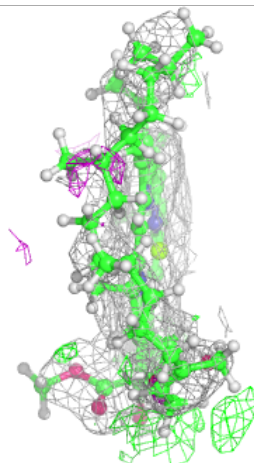
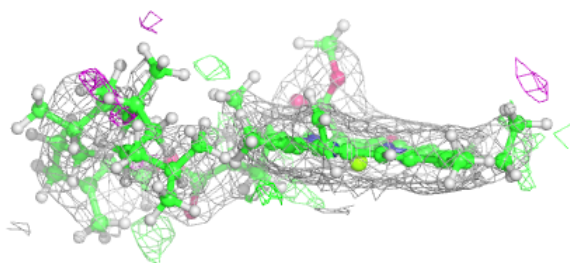
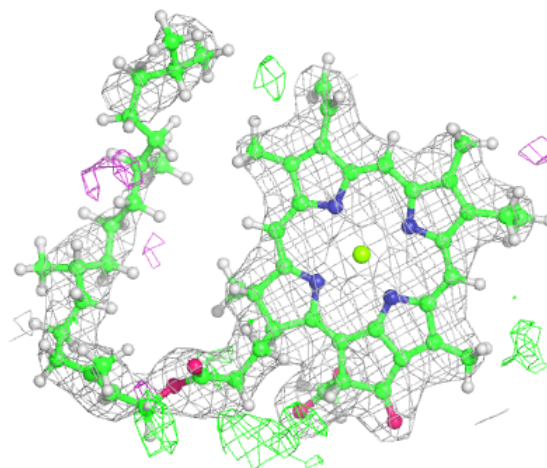
**Electron density around STE B 623:**

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



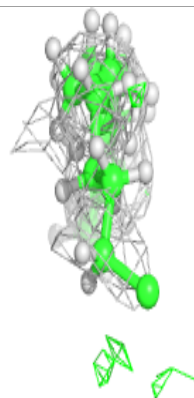
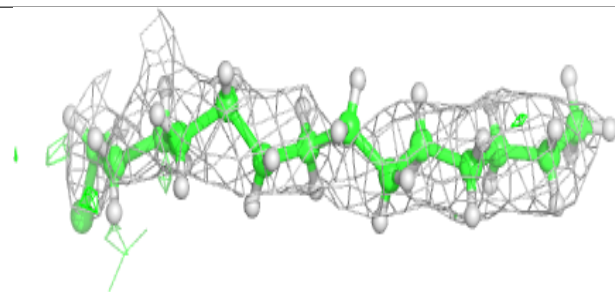
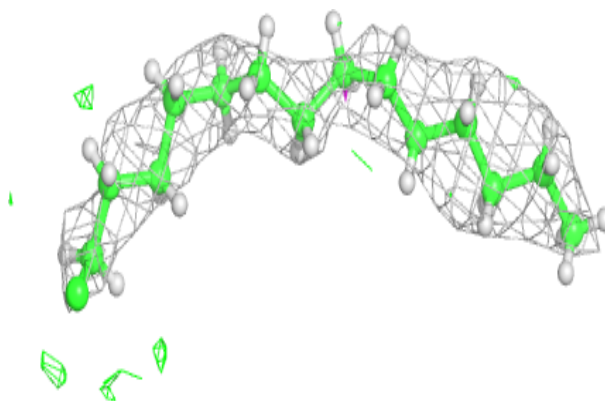
Electron density around CLA c 512:

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

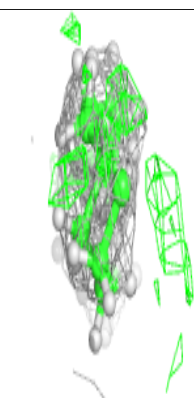
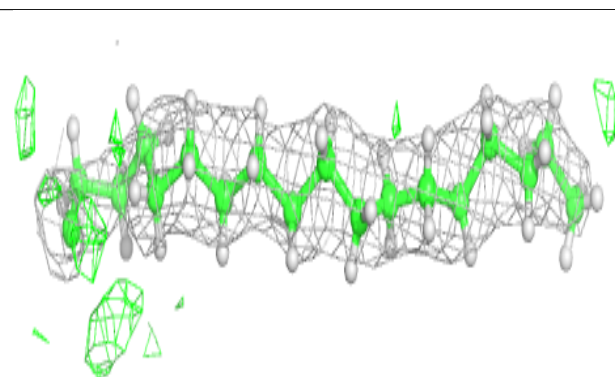
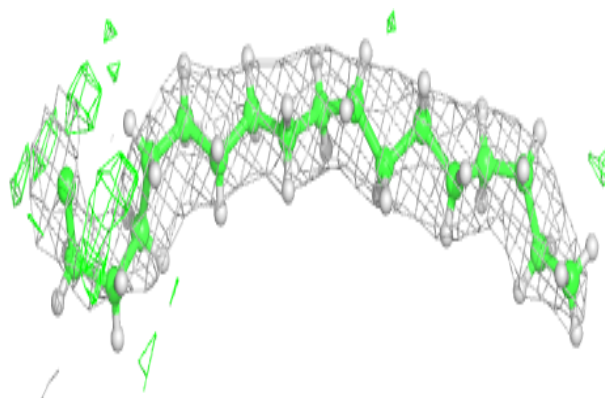


Electron density around STE T 102:

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

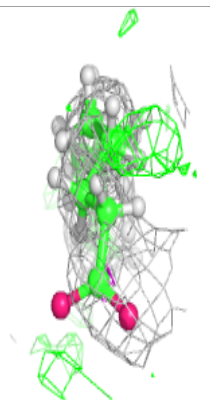
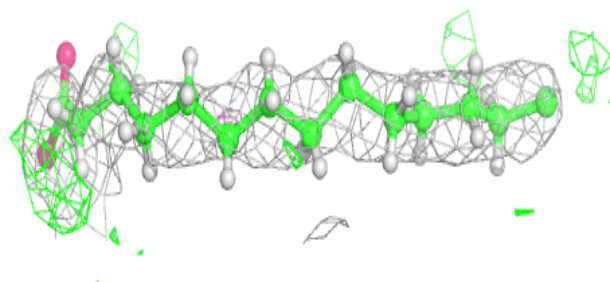
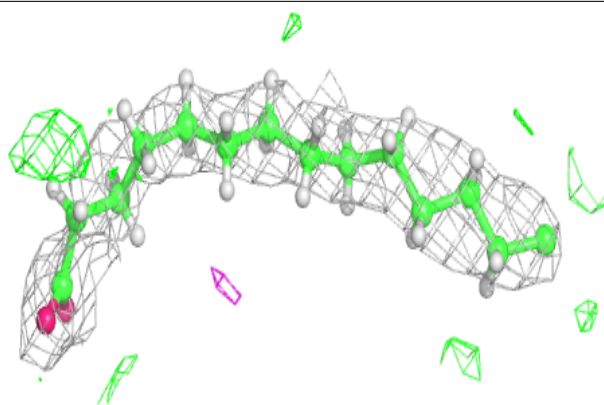
**Electron density around STE M 104:**

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

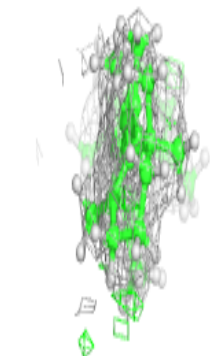
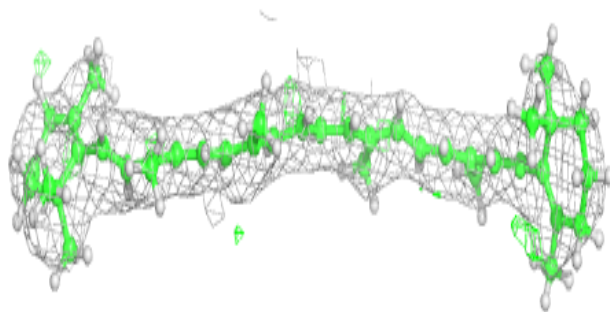
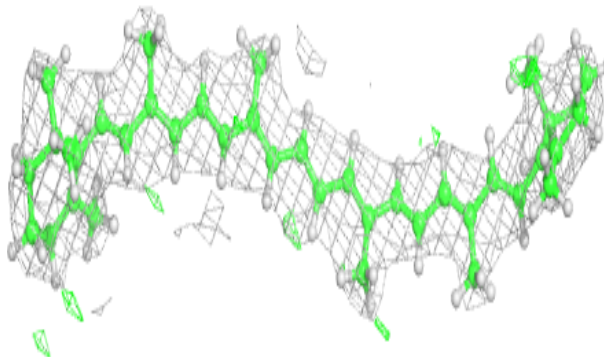


Electron density around STE b 624:

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

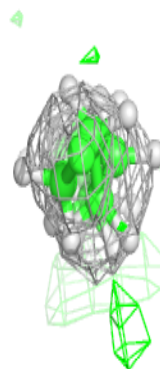
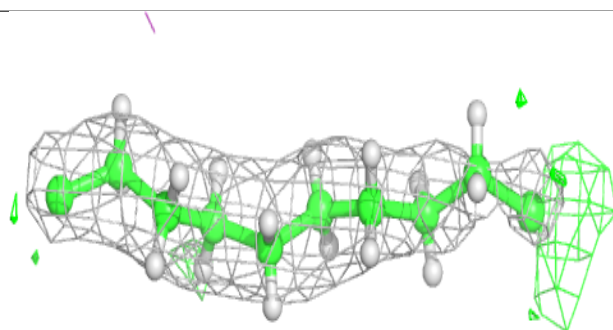
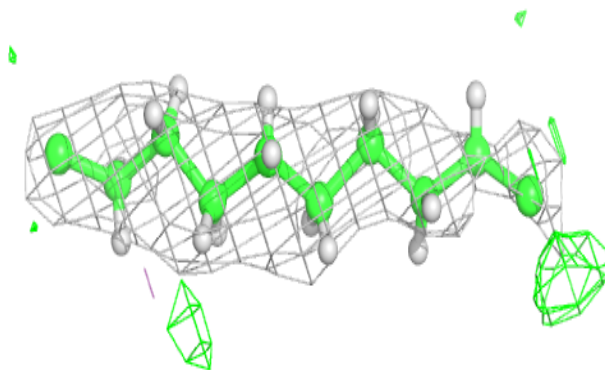
**Electron density around BCR K 102:**

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

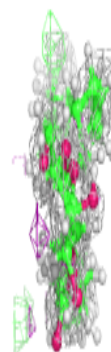
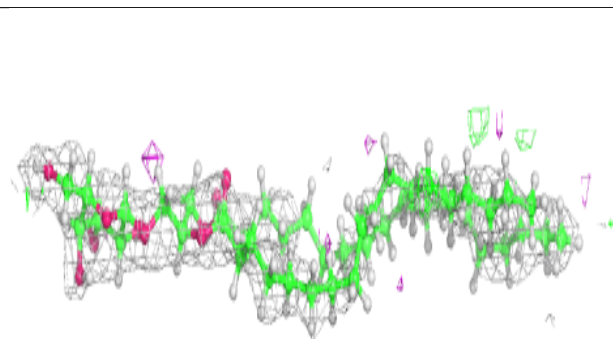
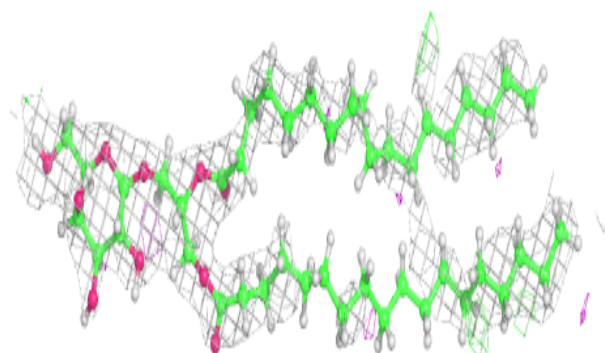


Electron density around STE M 103:

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

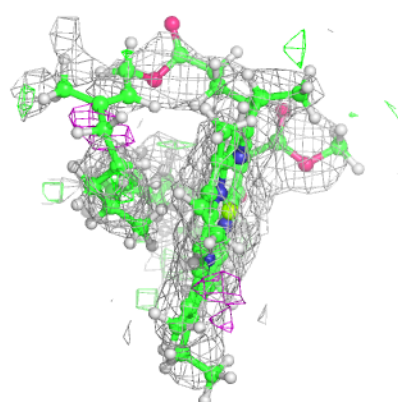
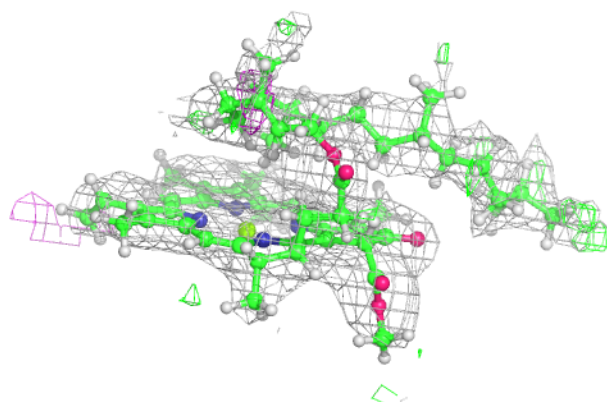
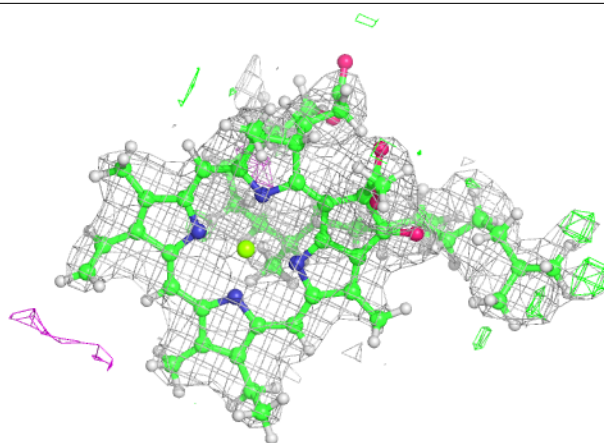
**Electron density around LMG b 623:**

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

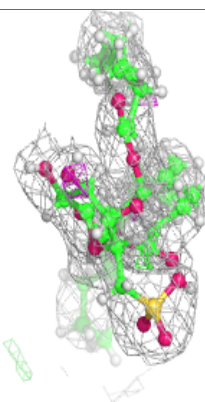
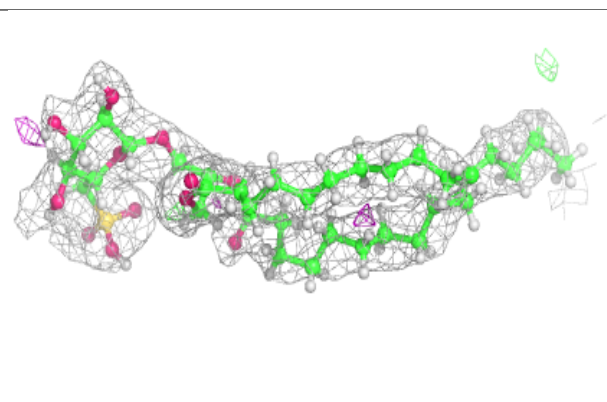
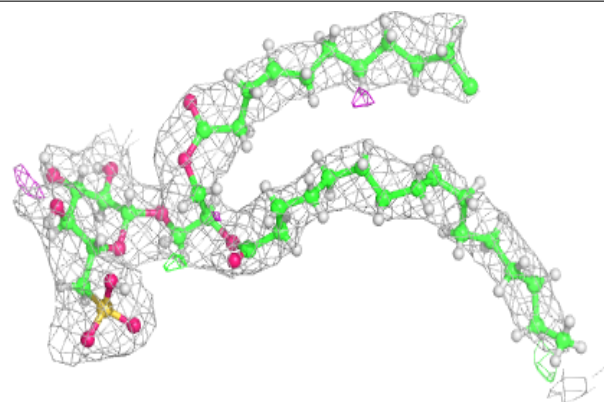


Electron density around CLA B 601:

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

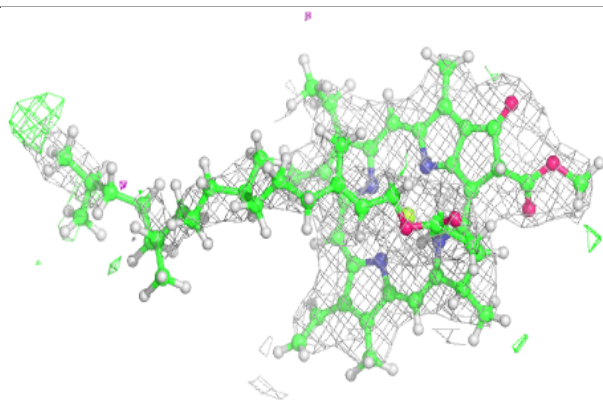
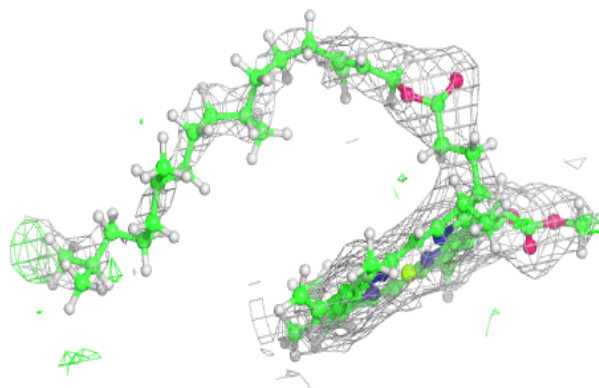
**Electron density around SQD b 620:**

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

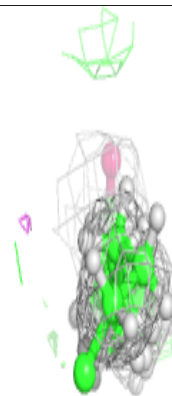
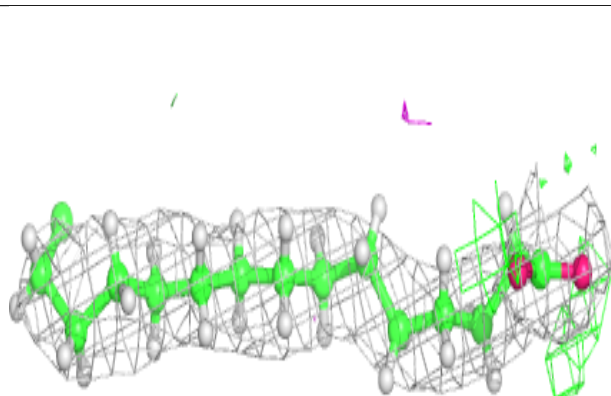
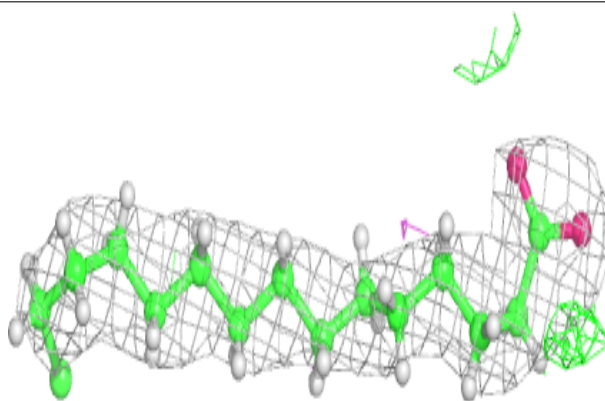


Electron density around CLA C 513:

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

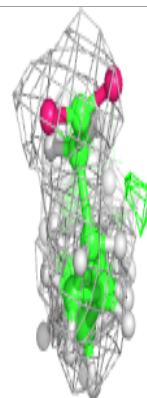
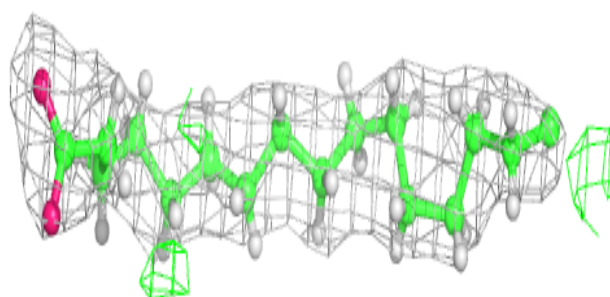
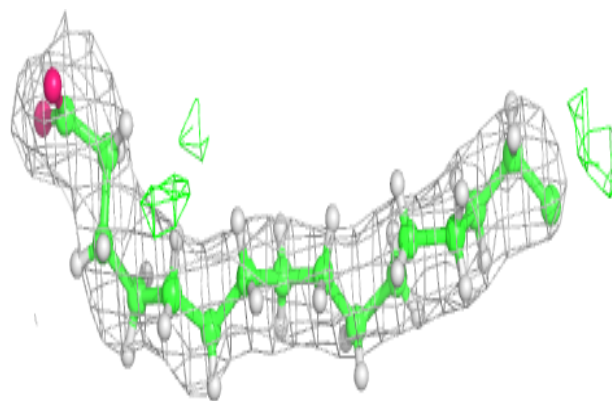
**Electron density around STE d 411:**

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

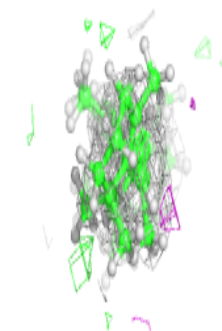
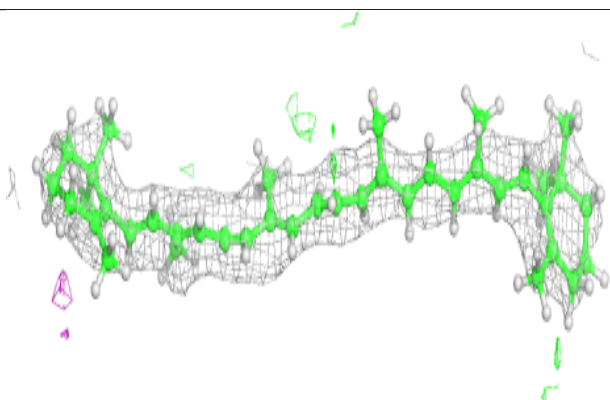
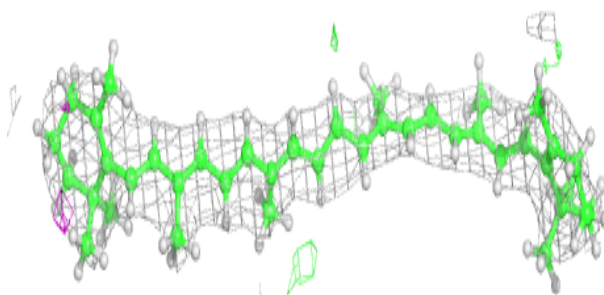


Electron density around STE B 624:

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

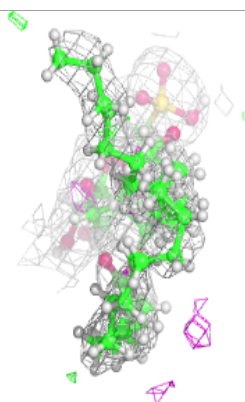
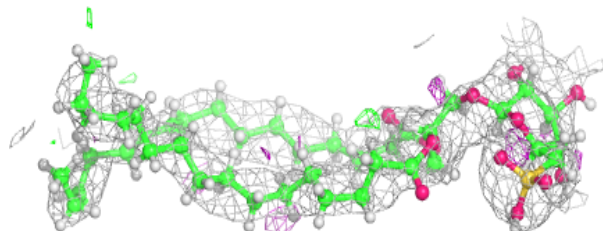
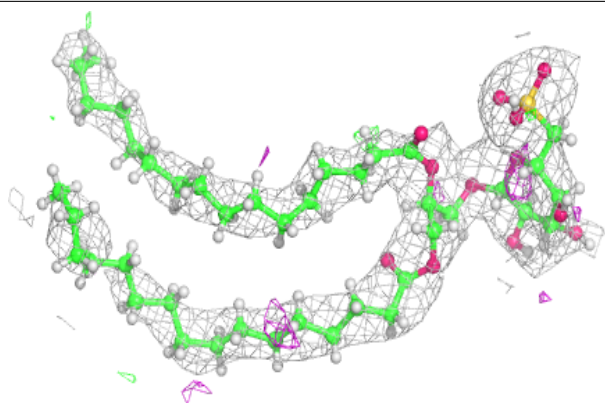
**Electron density around BCR K 101:**

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

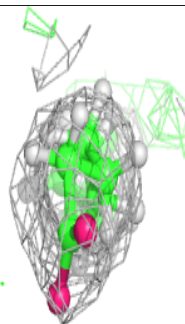
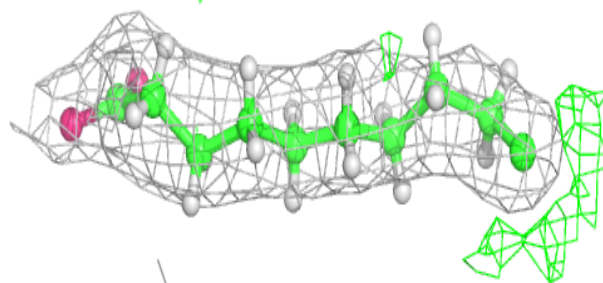
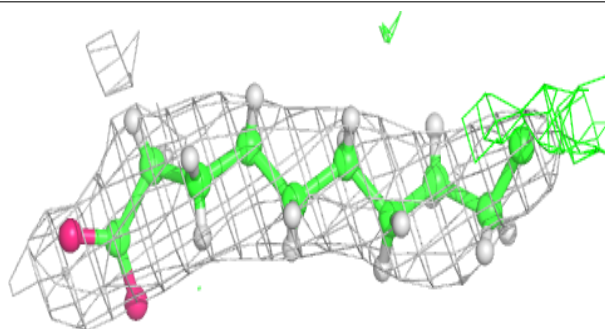


Electron density around SQD B 621:

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

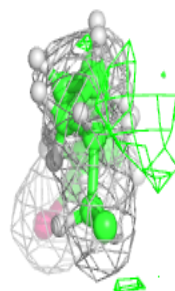
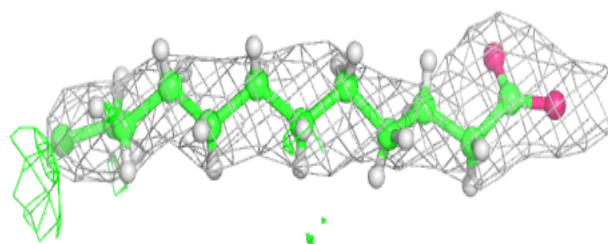
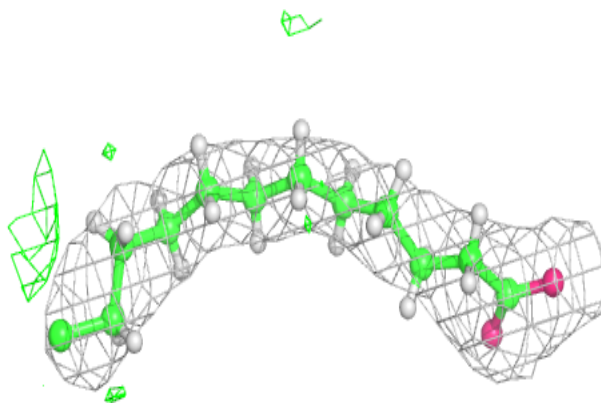
**Electron density around STE J 101:**

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



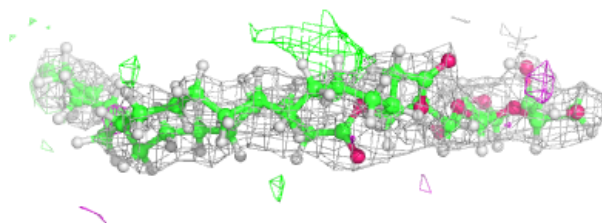
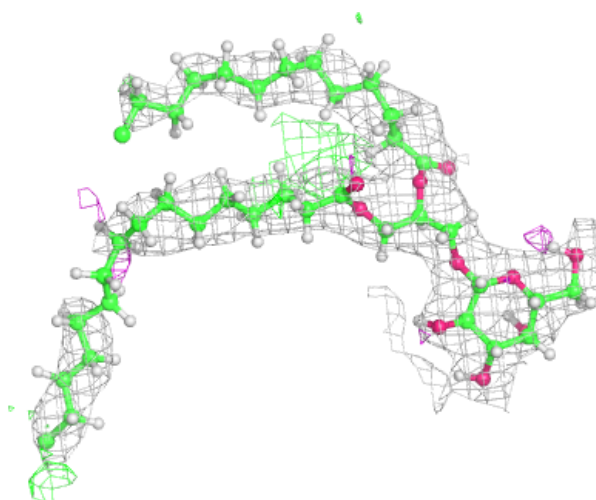
Electron density around STE B 622:

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



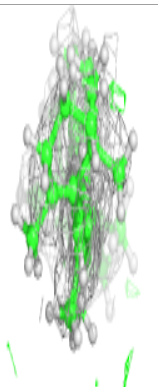
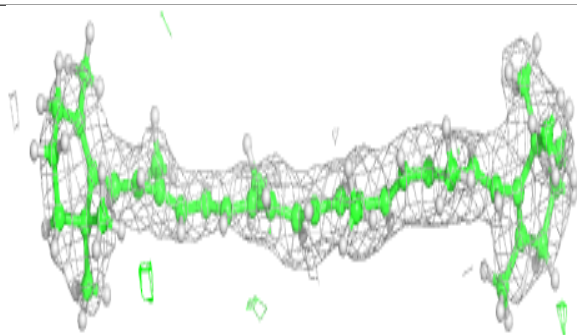
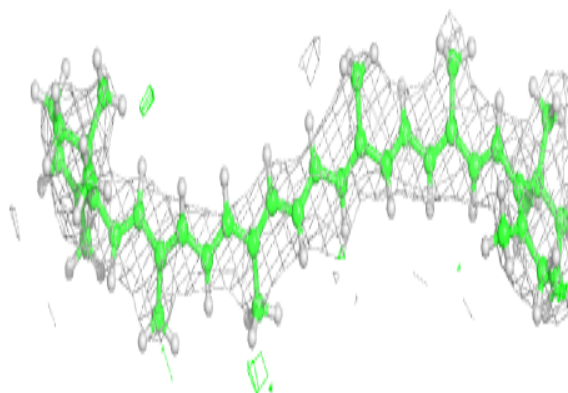
Electron density around LMG Y 101:

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

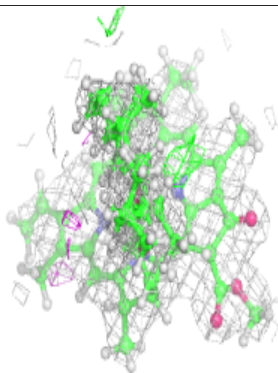
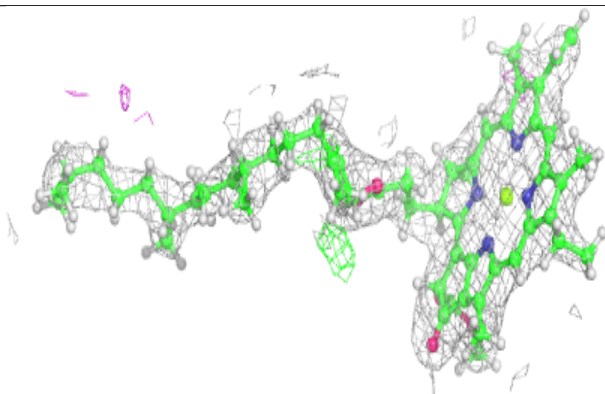
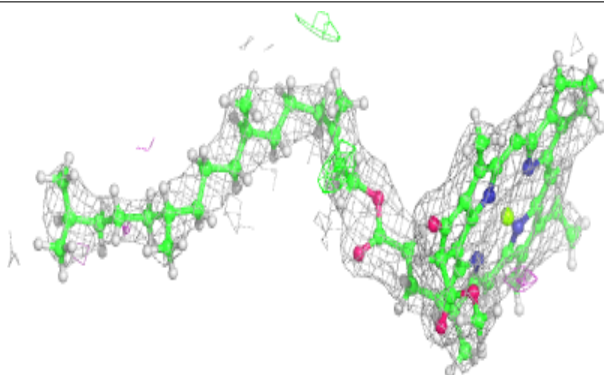


Electron density around BCR k 101:

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

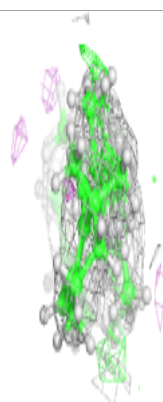
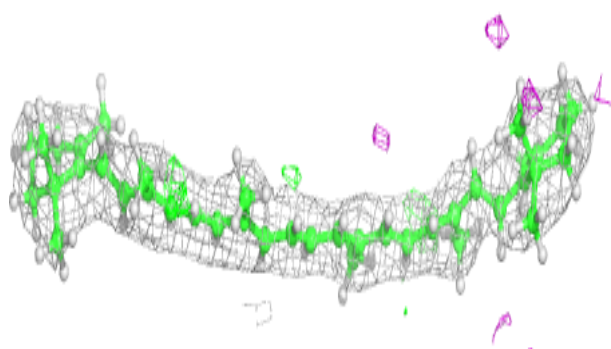
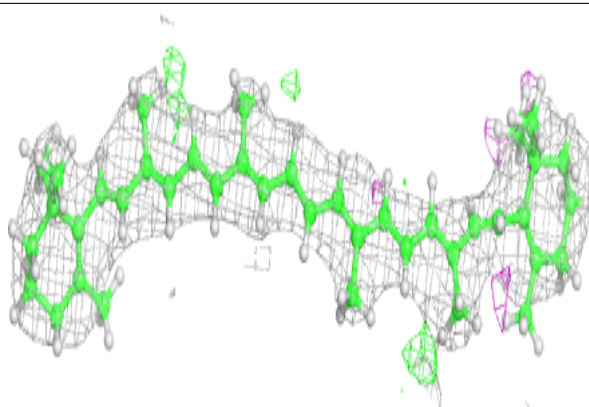
**Electron density around CLA c 502:**

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

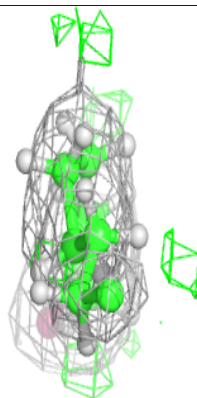
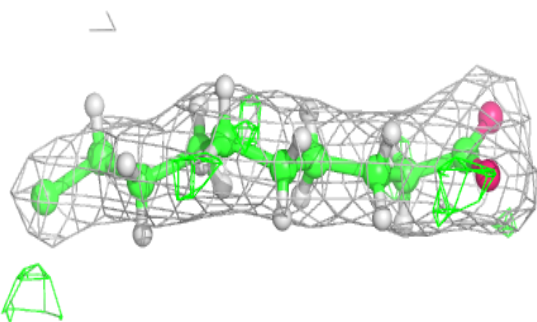
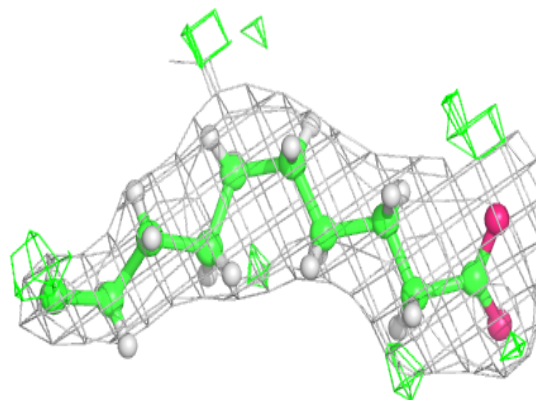


Electron density around BCR d 406:

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

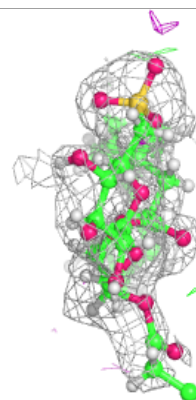
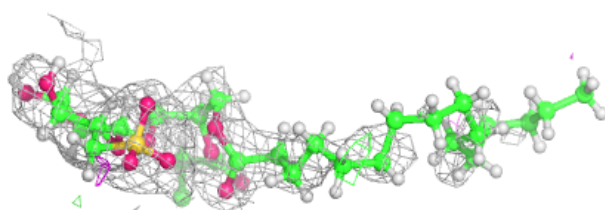
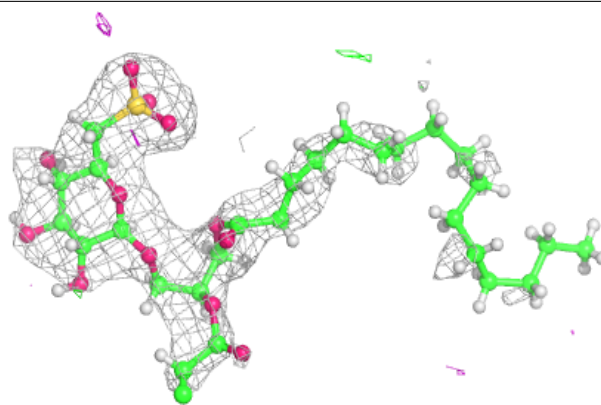
**Electron density around STE C 520:**

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

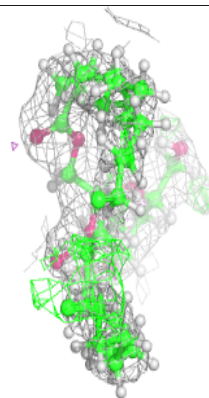
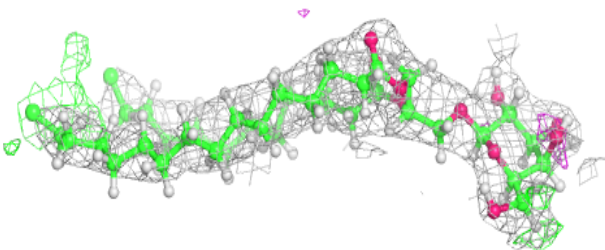
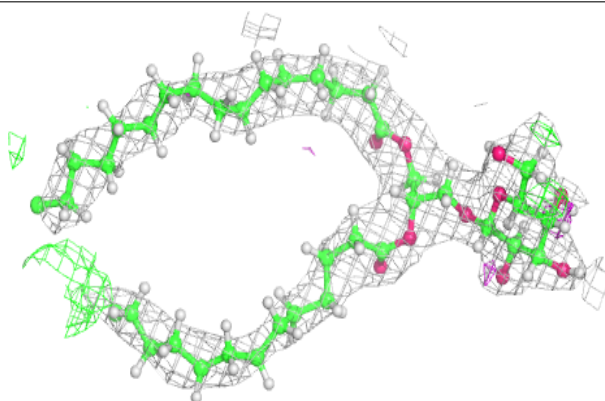


Electron density around SQD f 102:

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

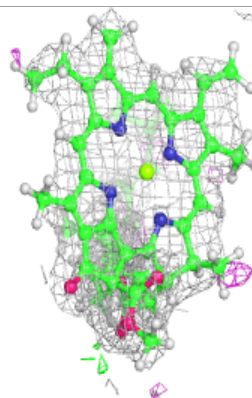
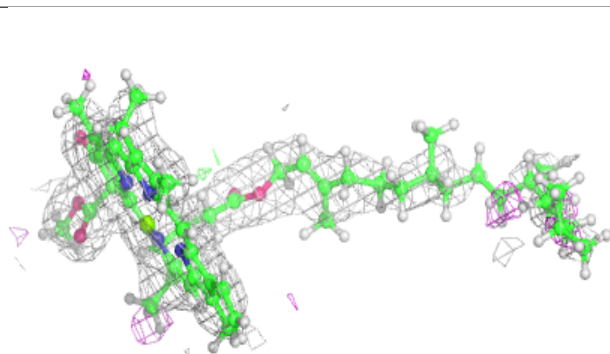
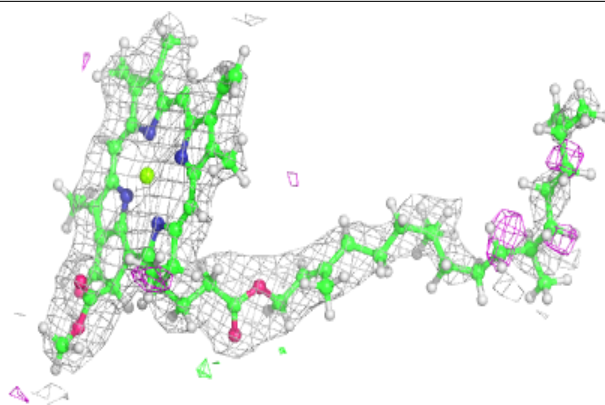
**Electron density around LMG A 411:**

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

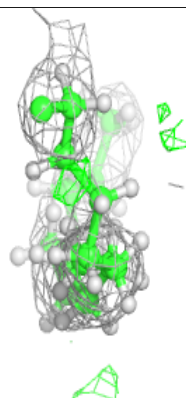
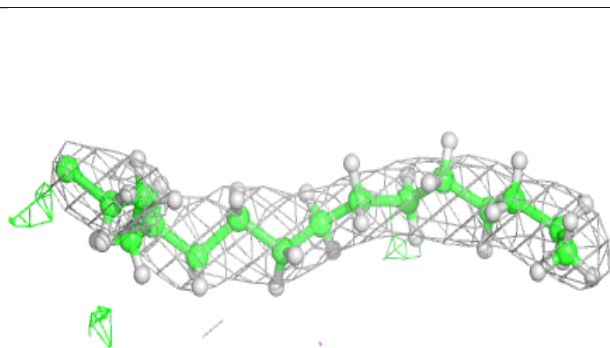
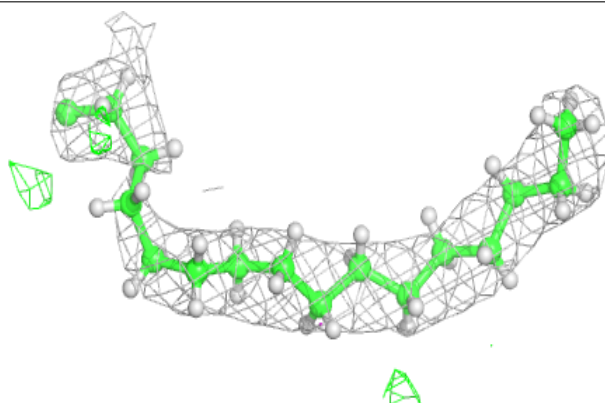


Electron density around CLA d 405:

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

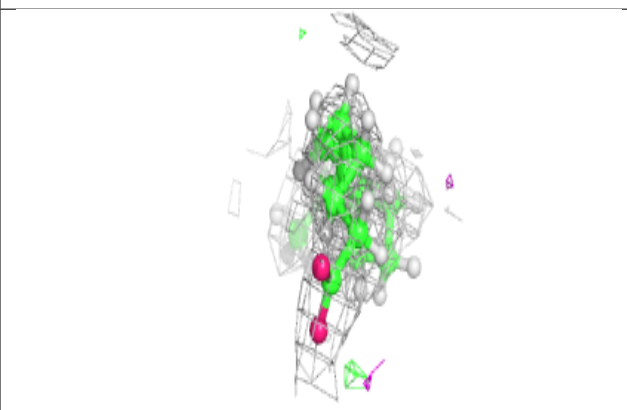
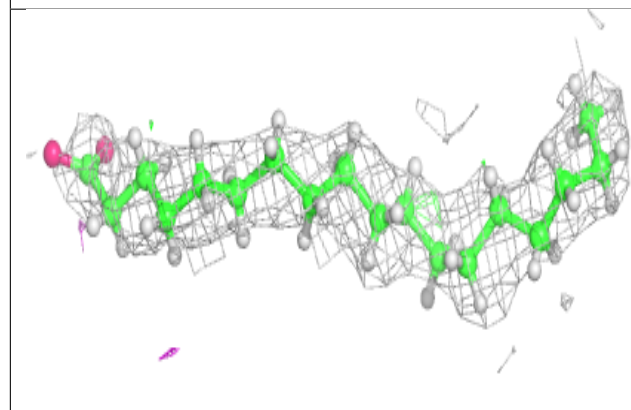
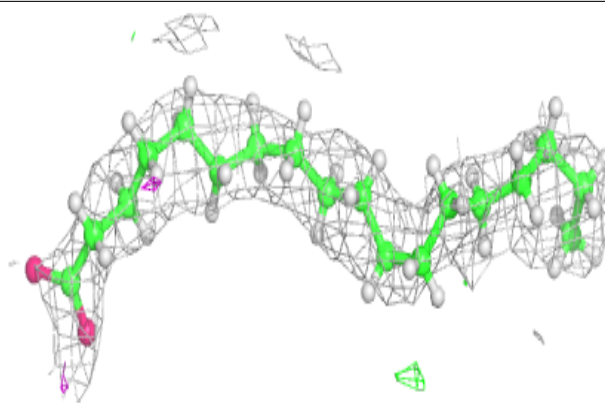
**Electron density around STE b 621:**

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

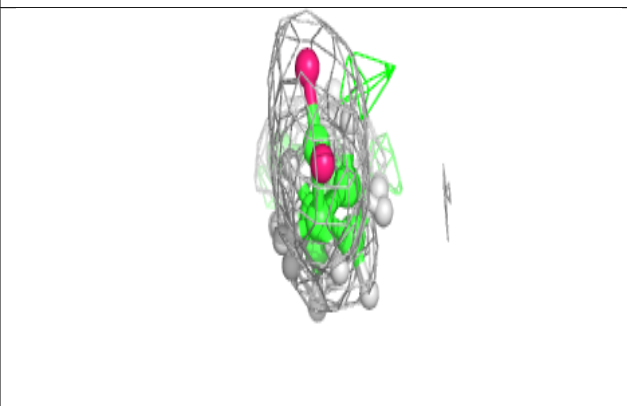
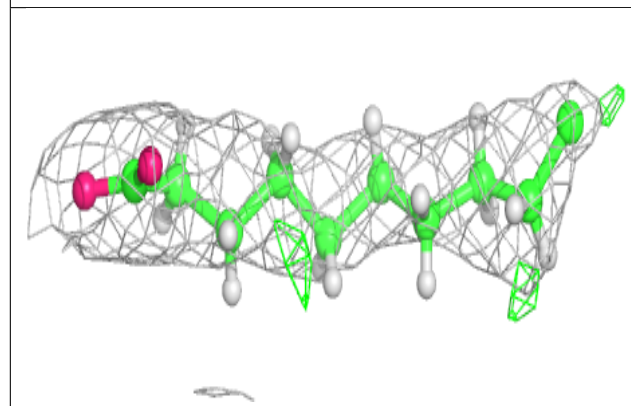
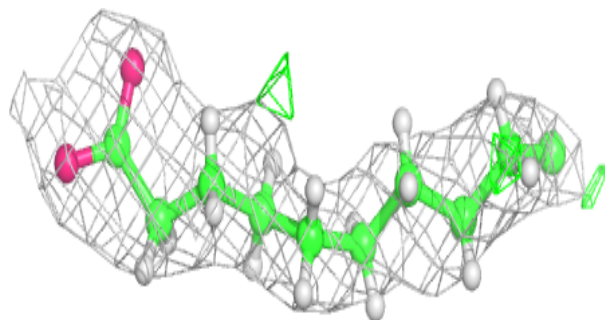


Electron density around STE b 622:

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

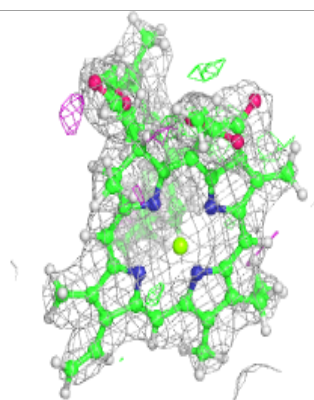
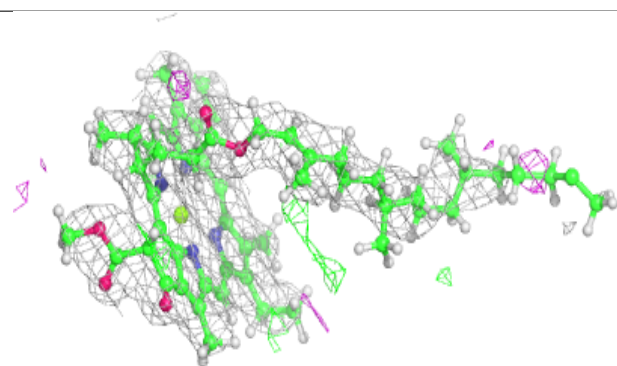
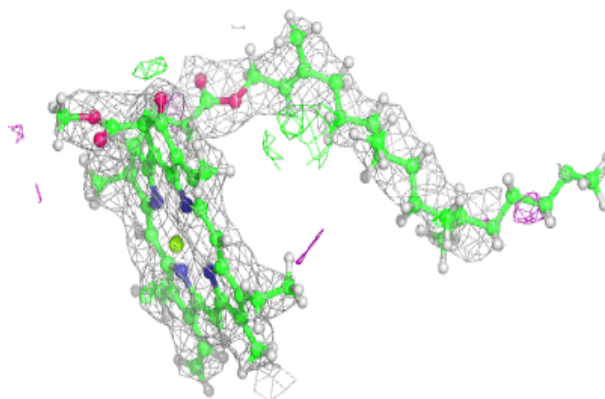
**Electron density around STE C 518:**

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

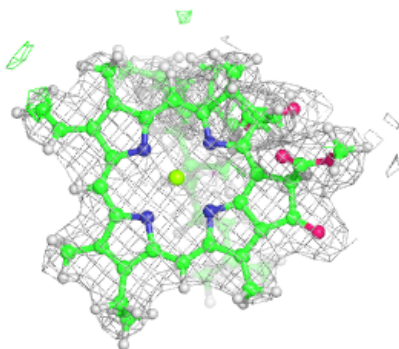
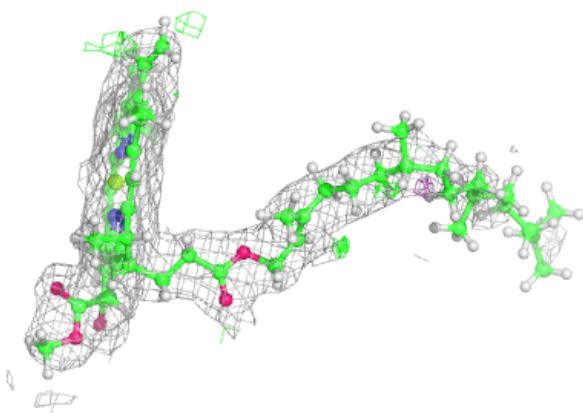
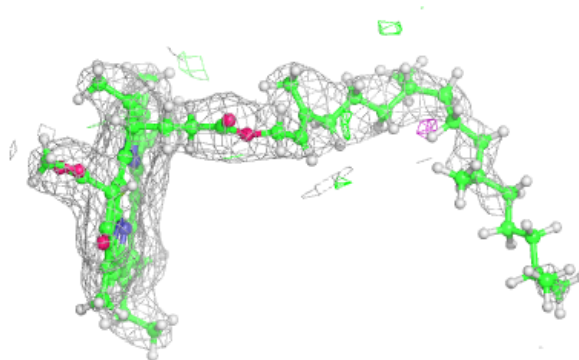


Electron density around CLA c 508:

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

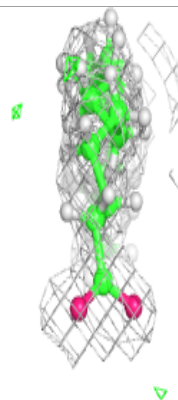
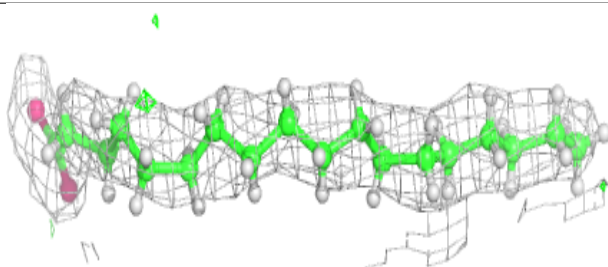
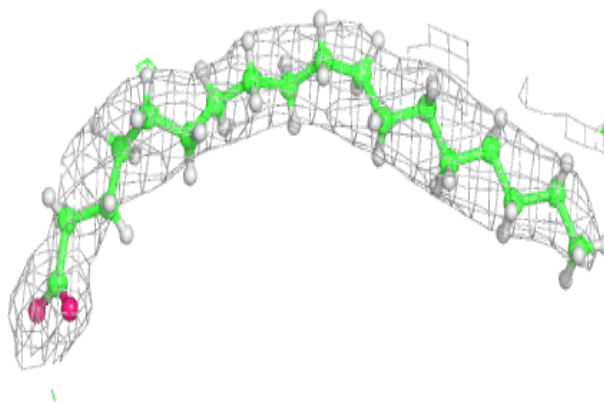
**Electron density around CLA D 404:**

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

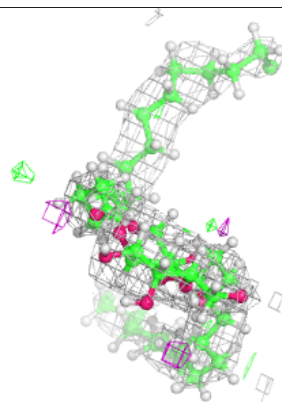
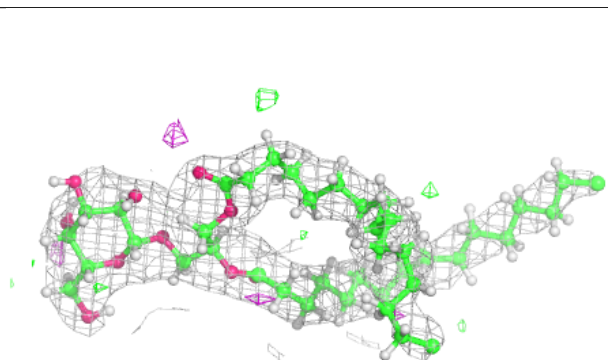
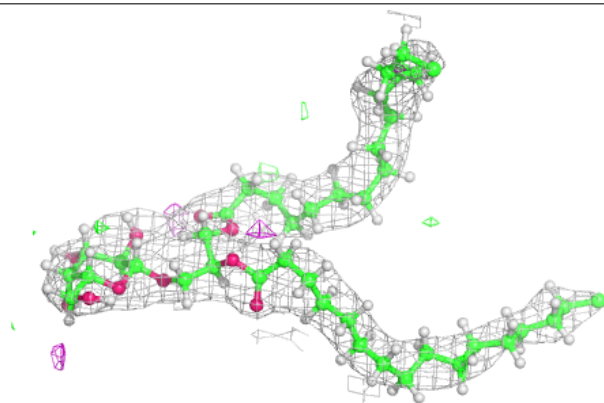


Electron density around STE D 412:

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

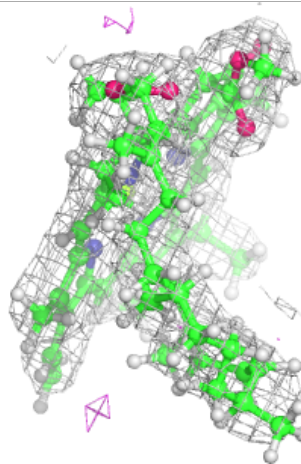
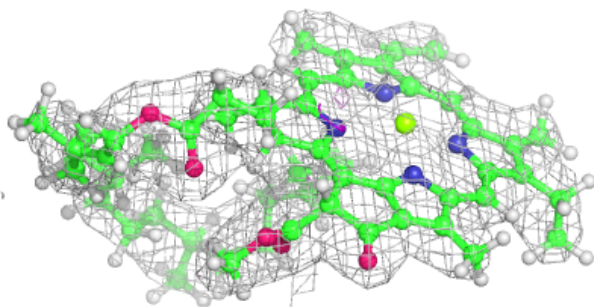
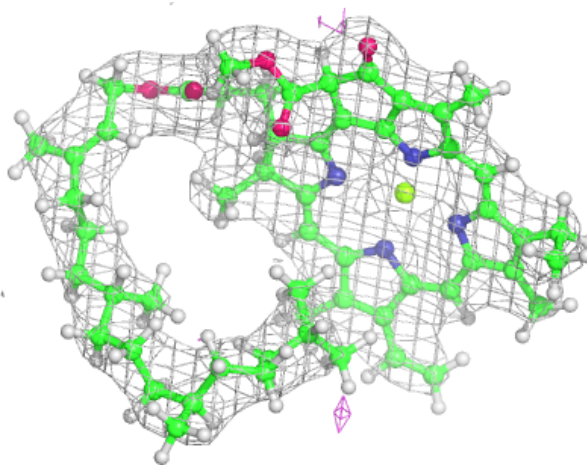
**Electron density around LMG m 101:**

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



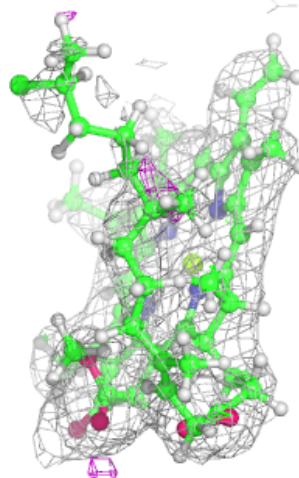
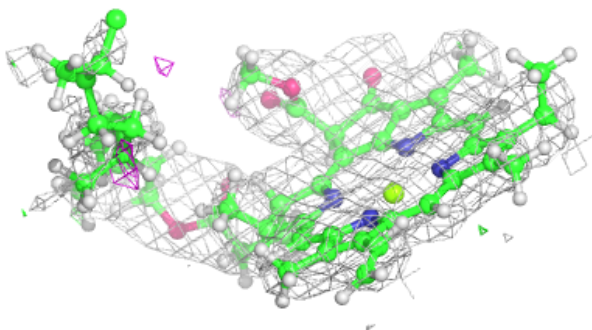
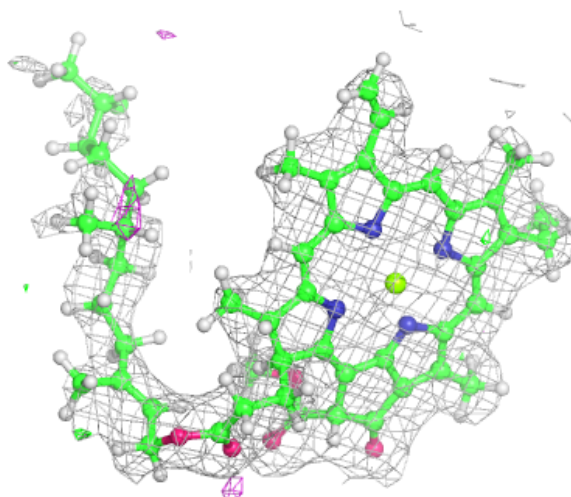
Electron density around CLA b 615:

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



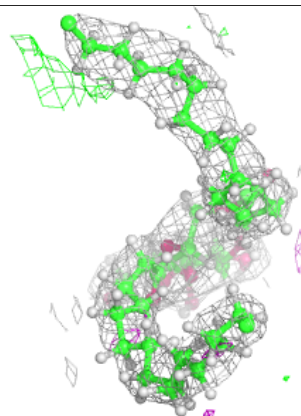
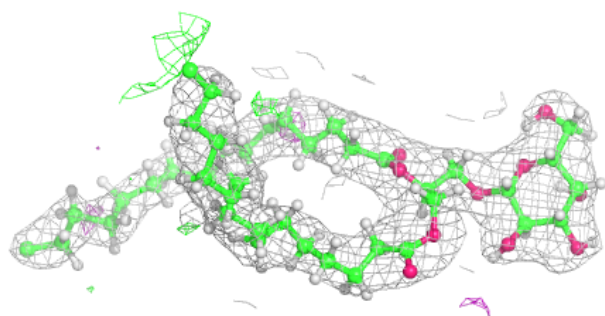
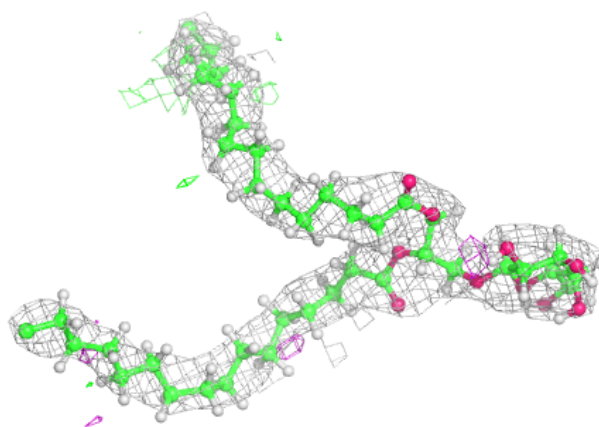
Electron density around CLA b 616:

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



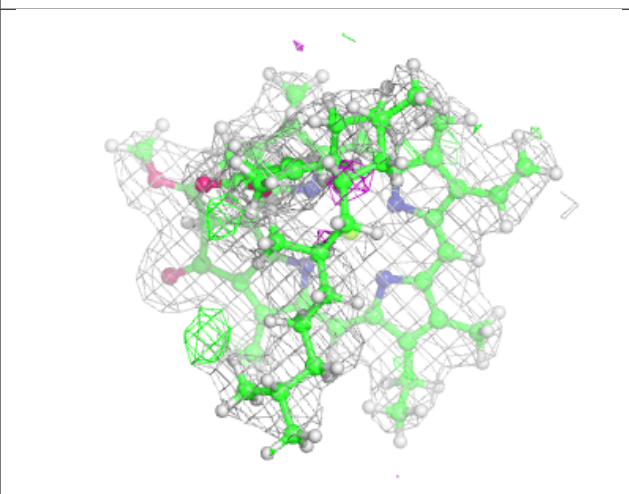
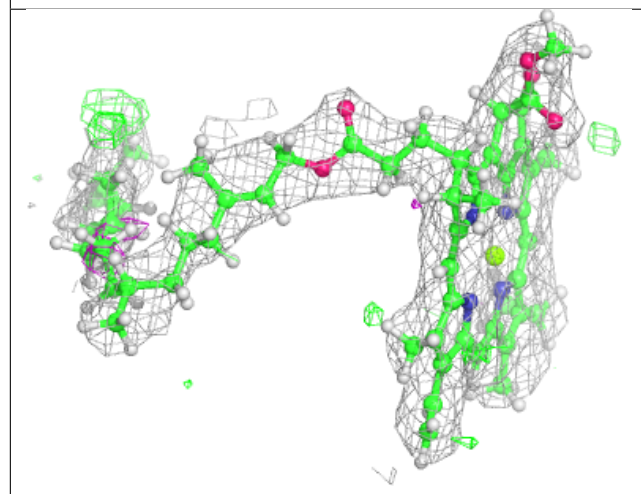
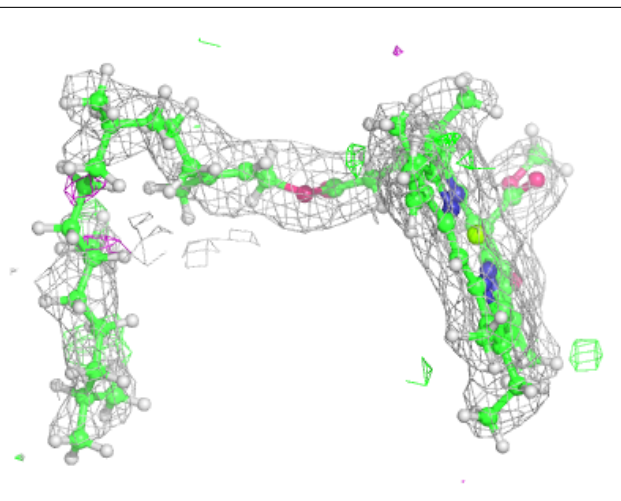
Electron density around LMG M 101:

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



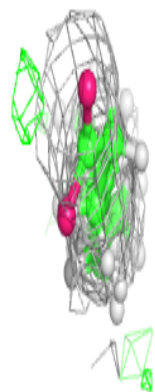
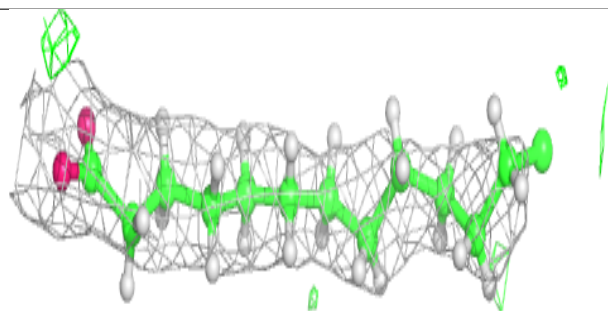
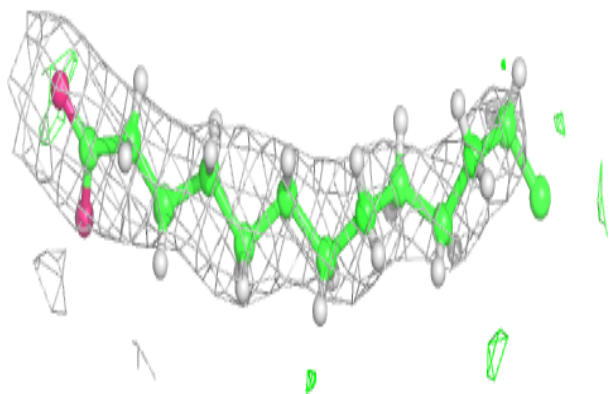
Electron density around CLA a 405:

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

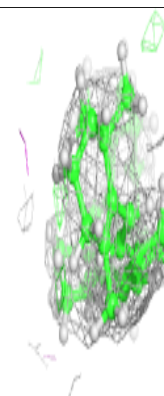
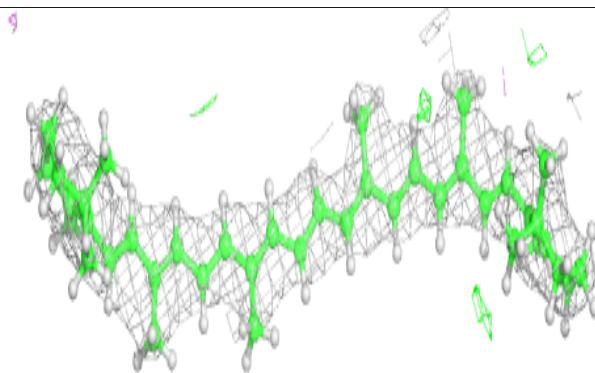
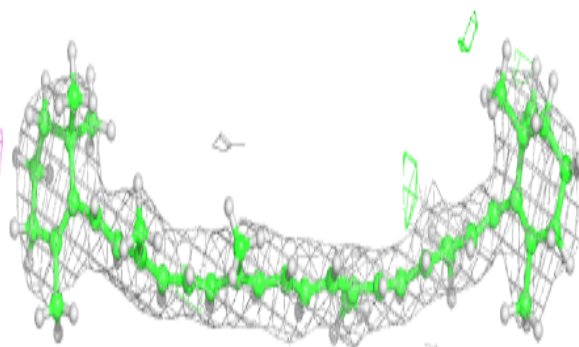


Electron density around STE M 102:

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

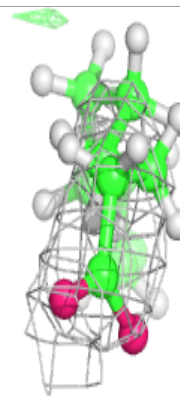
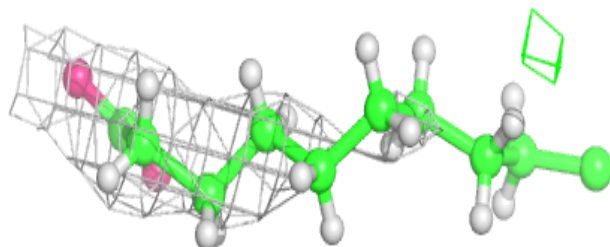
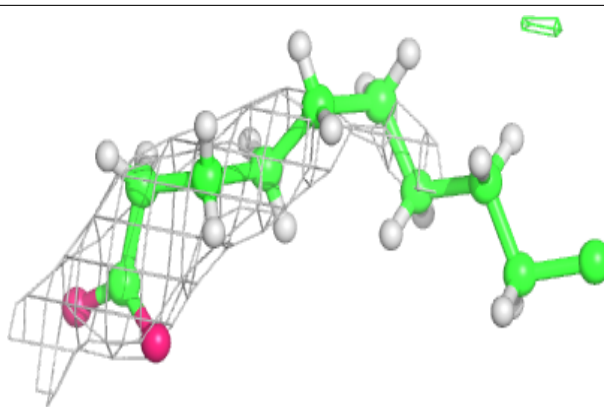
**Electron density around BCR k 102:**

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

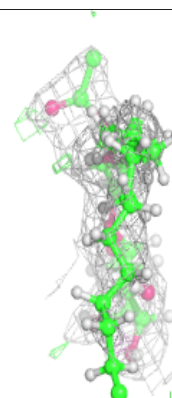
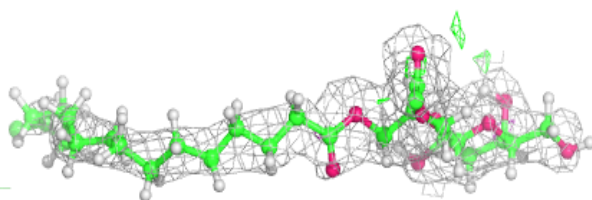
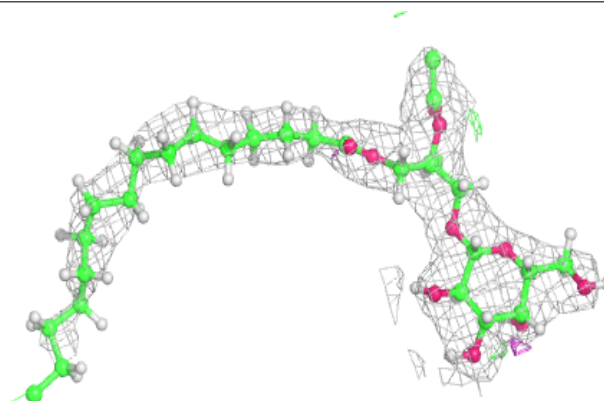


Electron density around STE B 626:

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

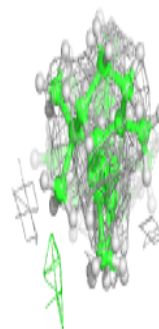
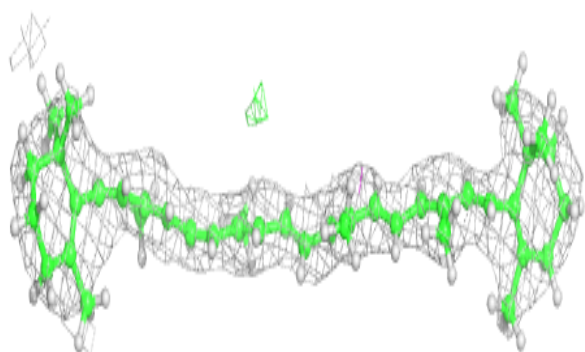
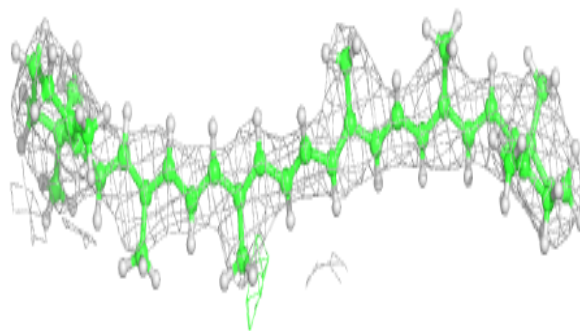
**Electron density around LMG c 519:**

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

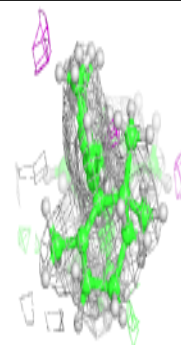
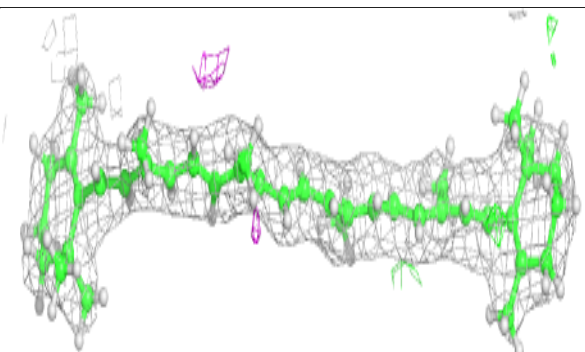
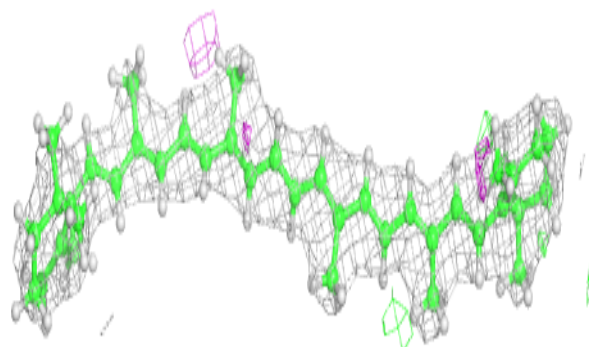


Electron density around BCR c 514:

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

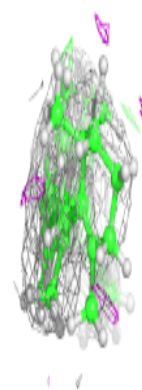
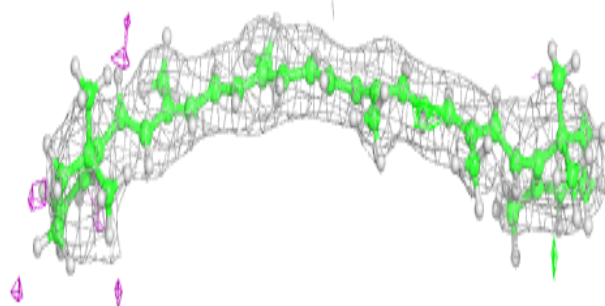
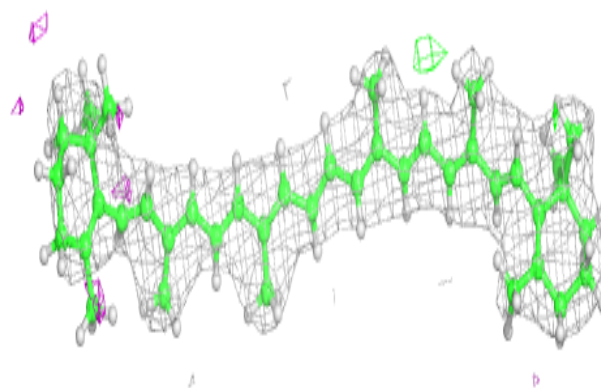
**Electron density around BCR C 514:**

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



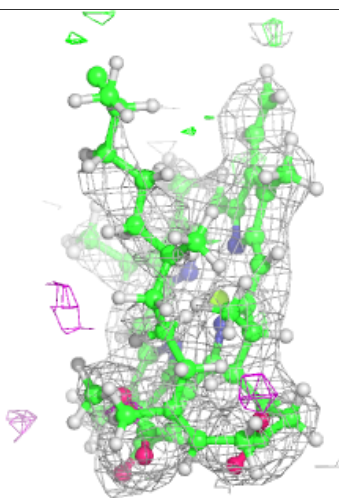
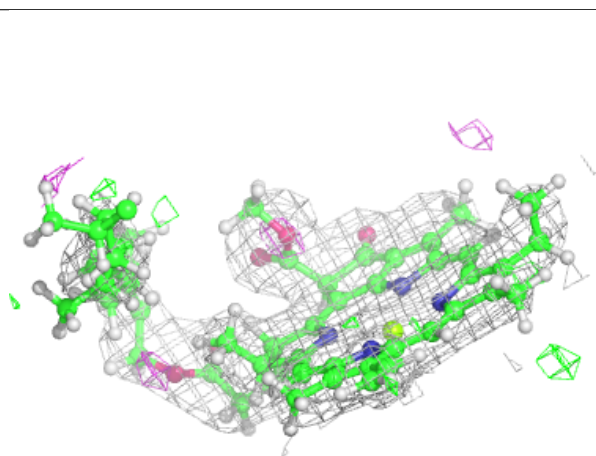
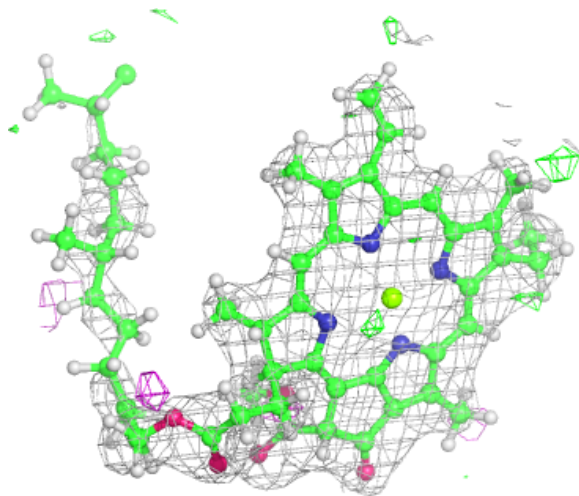
Electron density around BCR D 405:

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



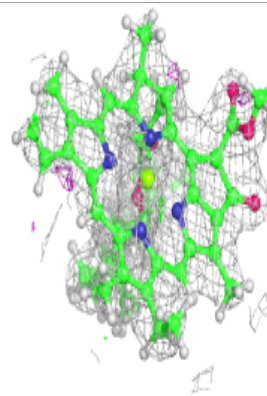
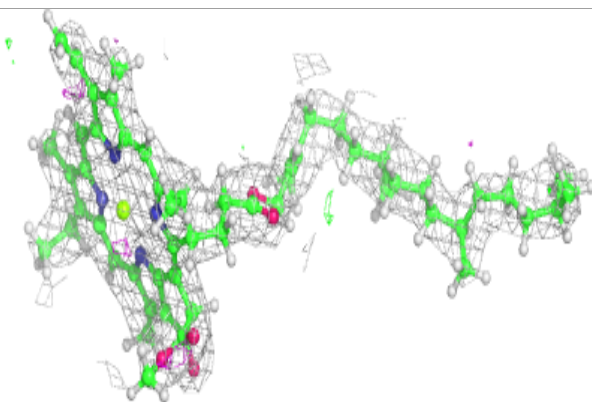
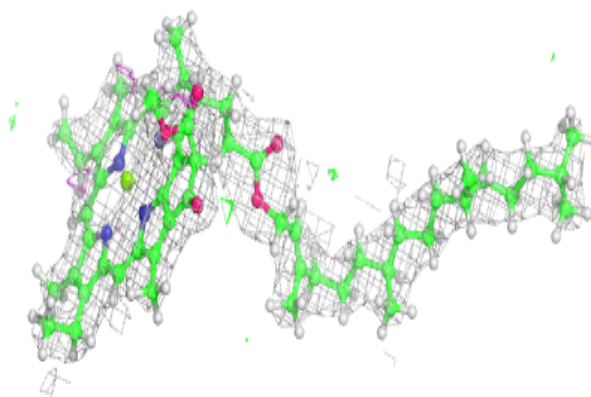
Electron density around CLA B 616:

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



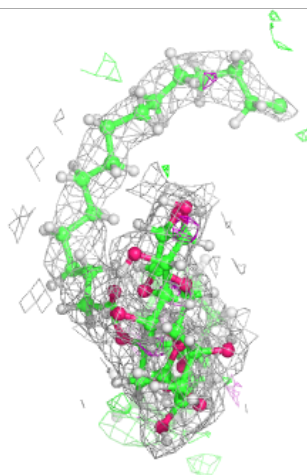
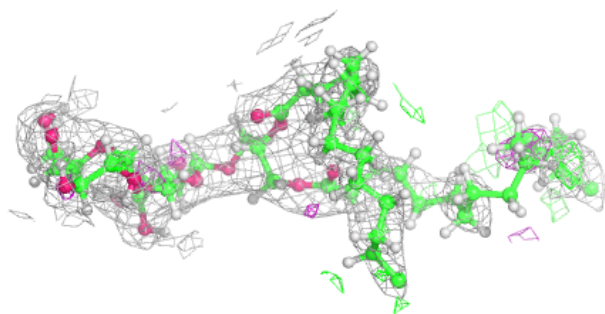
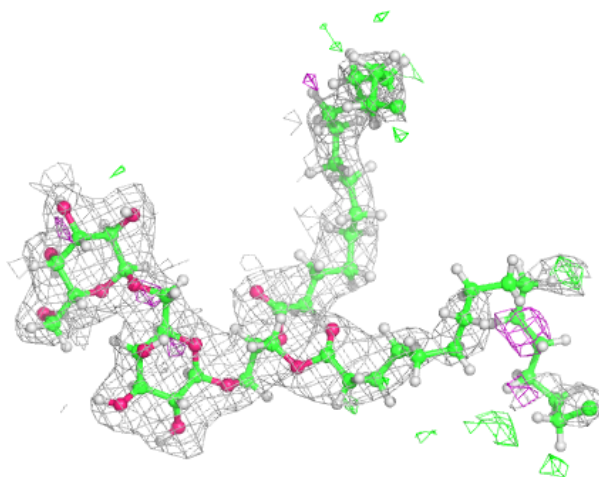
Electron density around CLA C 502:

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



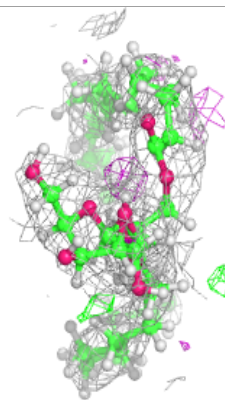
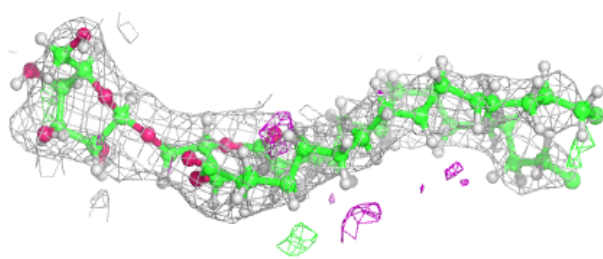
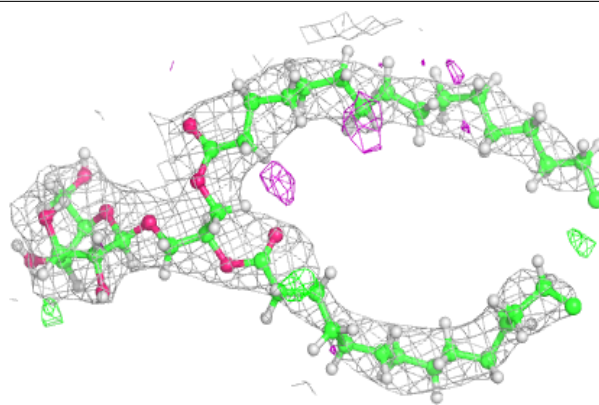
Electron density around DGD C 516:

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



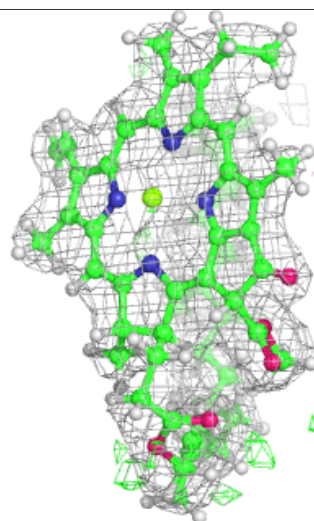
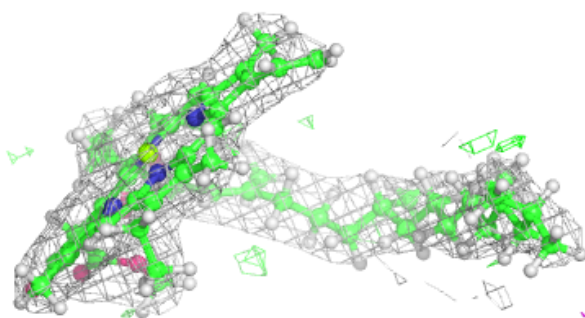
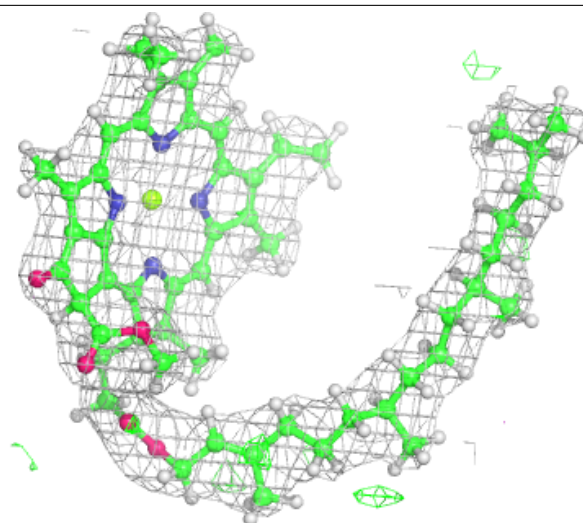
Electron density around LMG a 414:

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



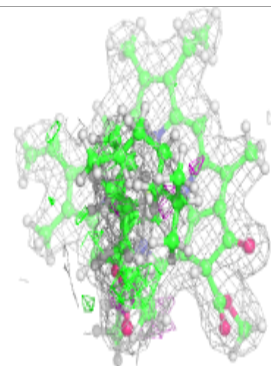
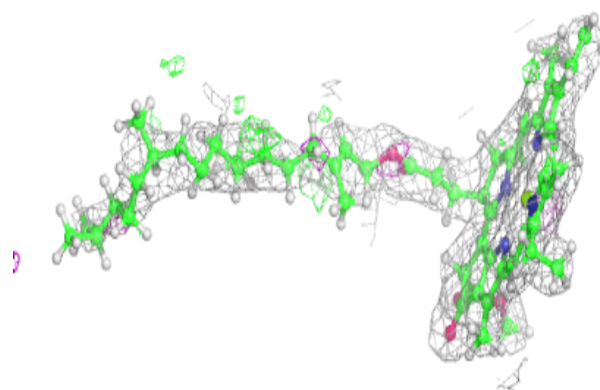
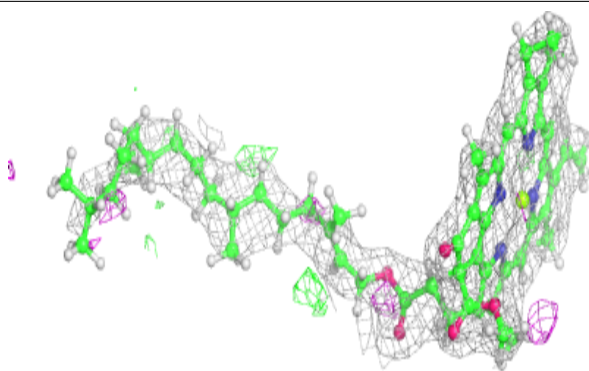
Electron density around CLA C 507:

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

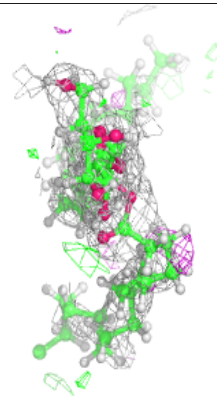
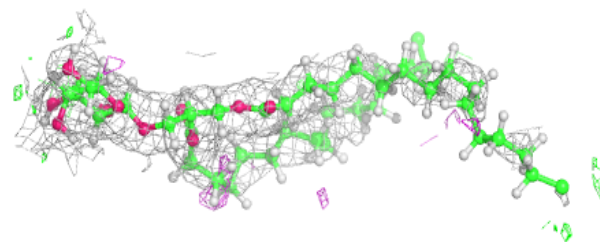
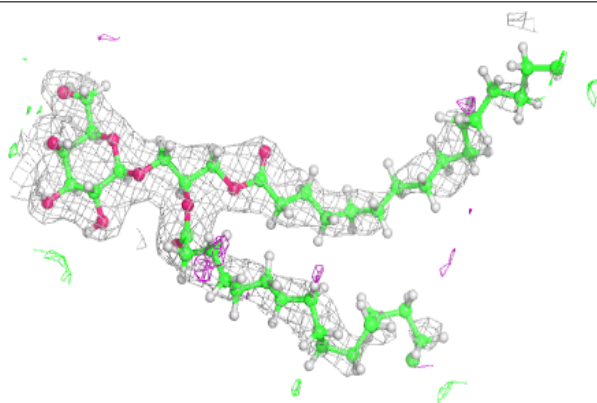


Electron density around CLA B 604:

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

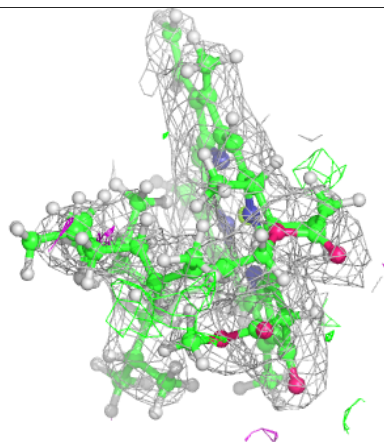
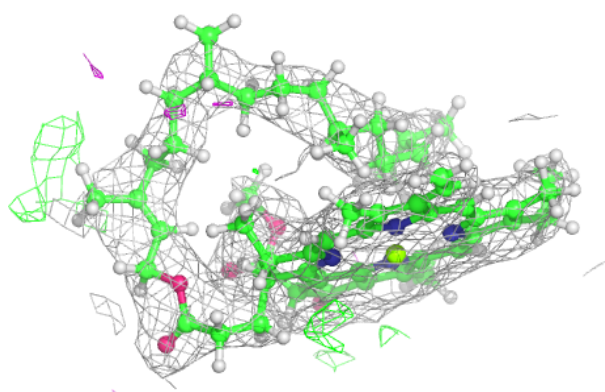
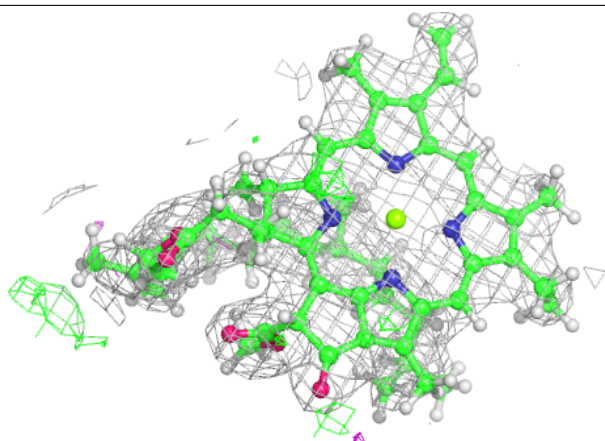
**Electron density around LMG D 407:**

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



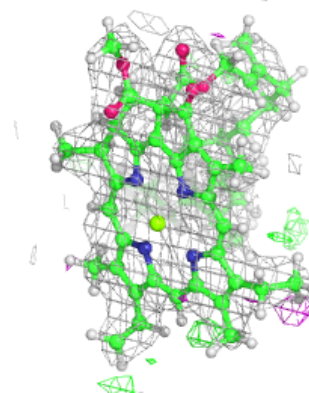
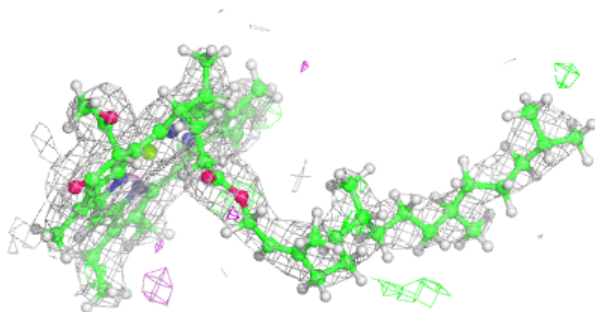
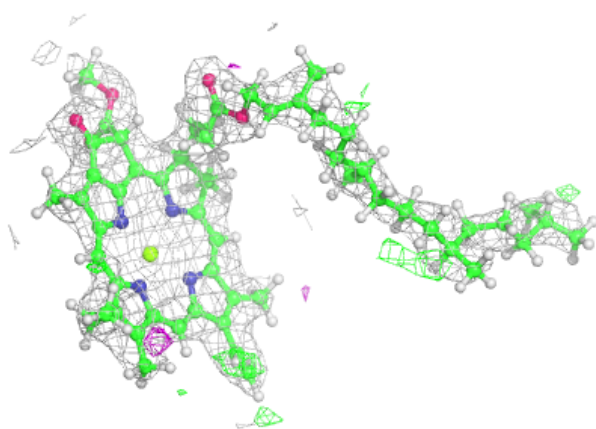
Electron density around CLA c 510:

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

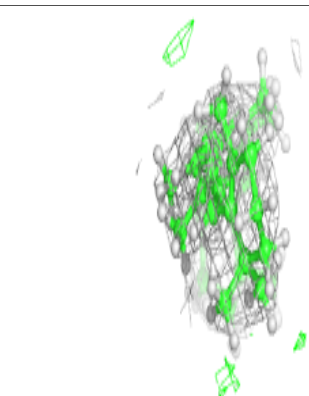
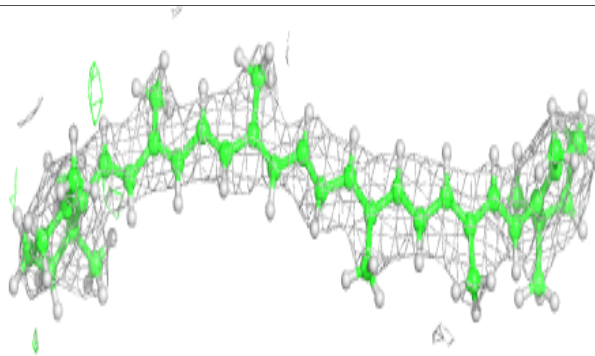
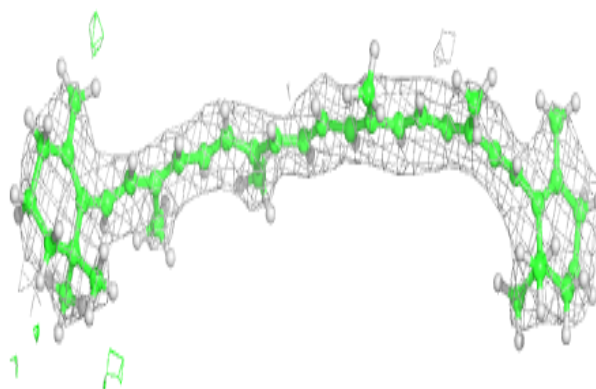


Electron density around CLA c 511:

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

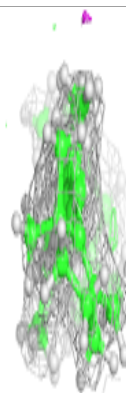
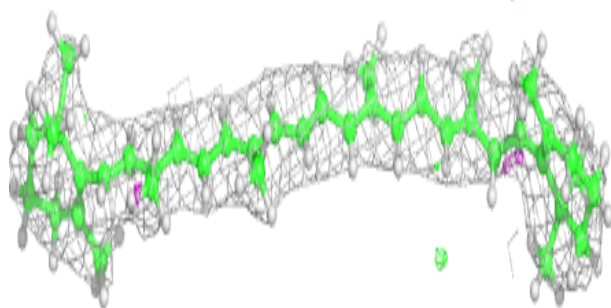
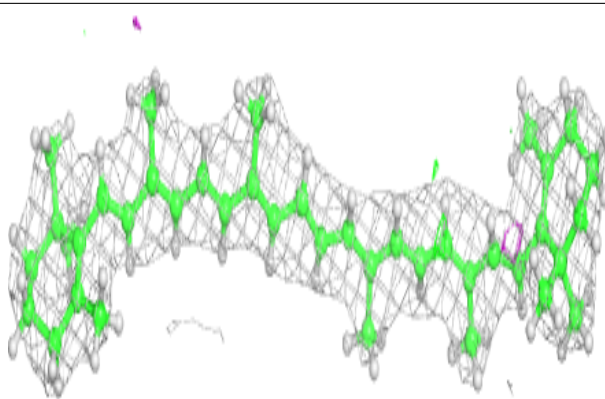
**Electron density around BCR K 103:**

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

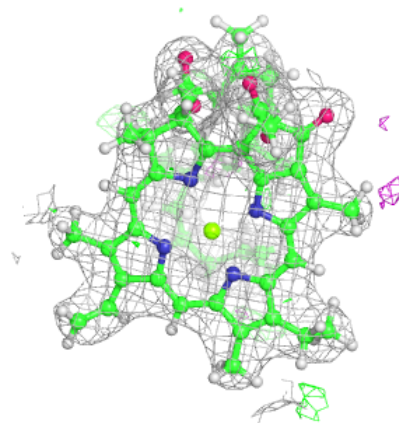
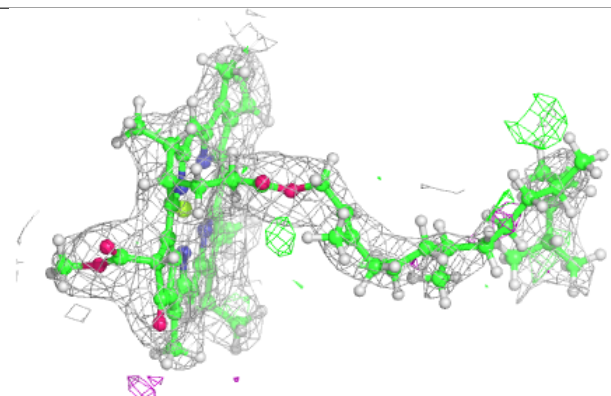
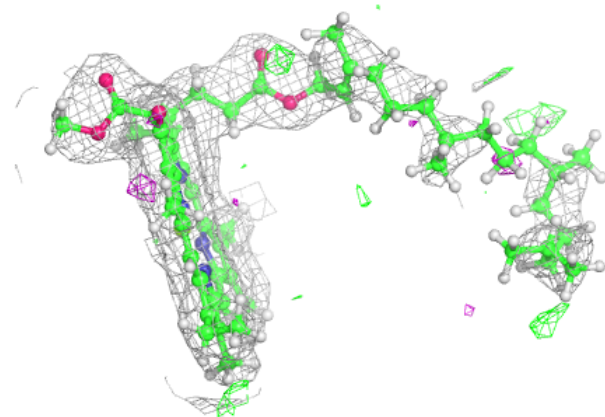


Electron density around BCR b 619:

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

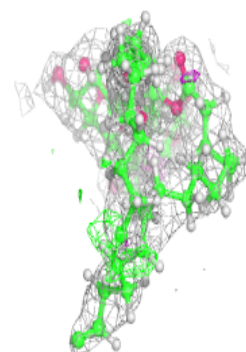
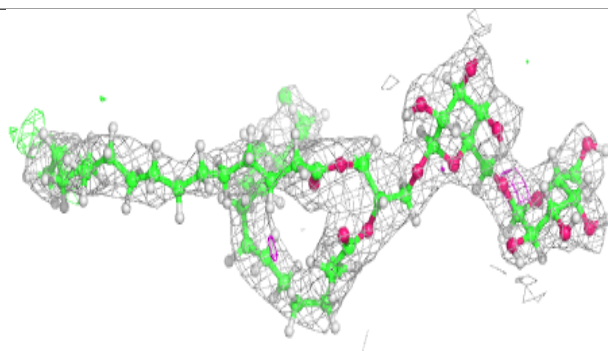
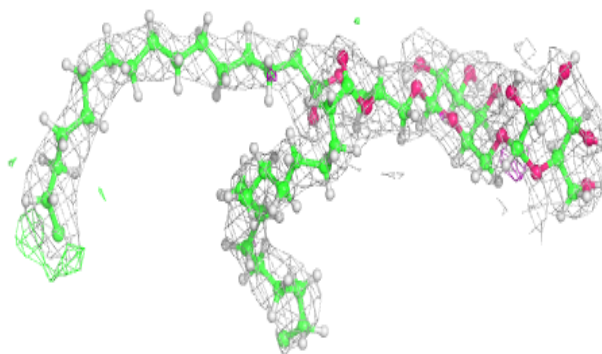
**Electron density around CLA C 506:**

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

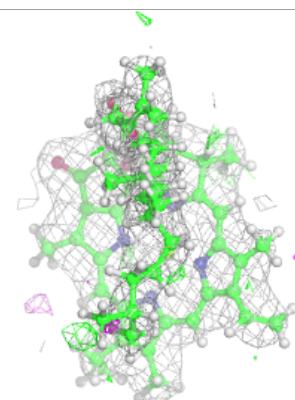
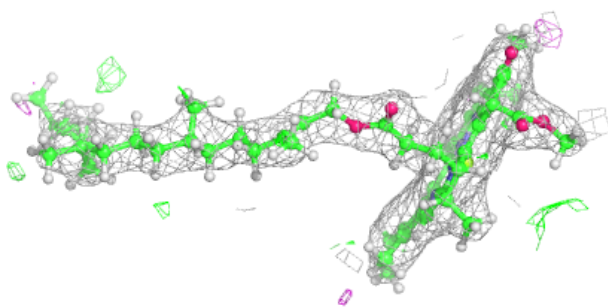
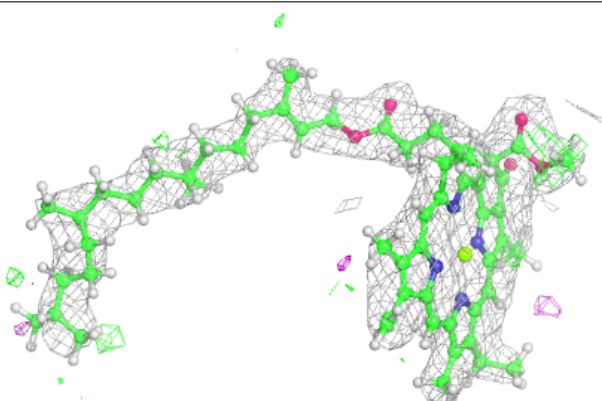


Electron density around DGD H 102:

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

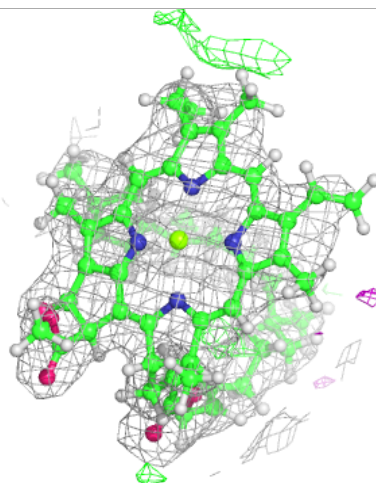
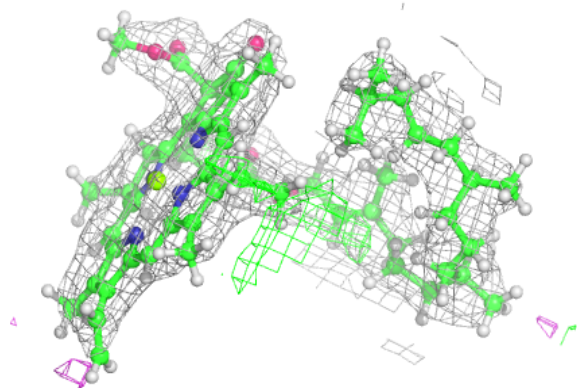
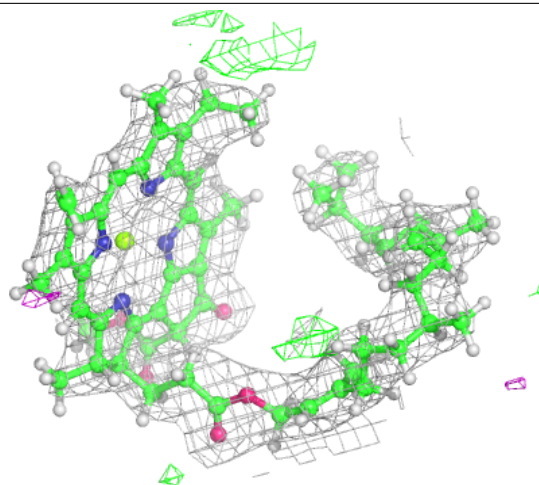
**Electron density around CLA b 609:**

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



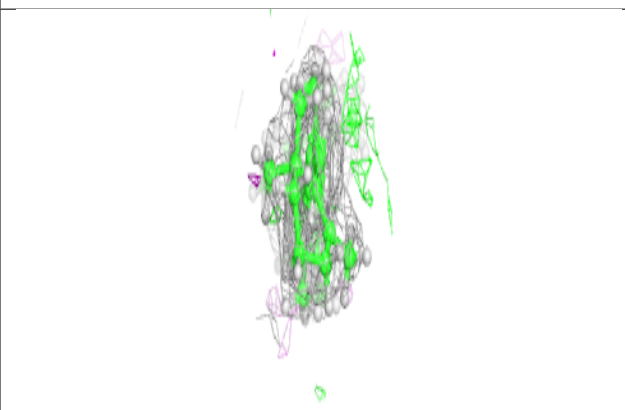
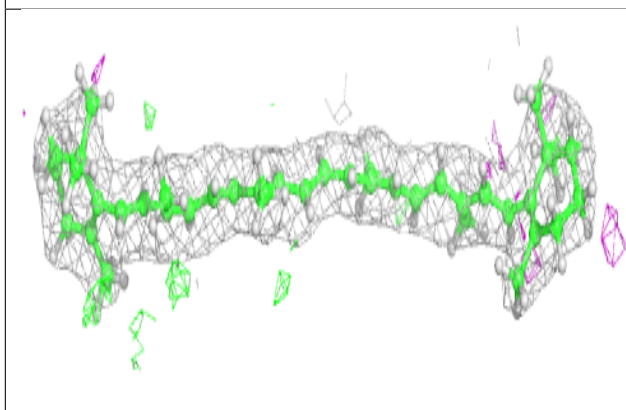
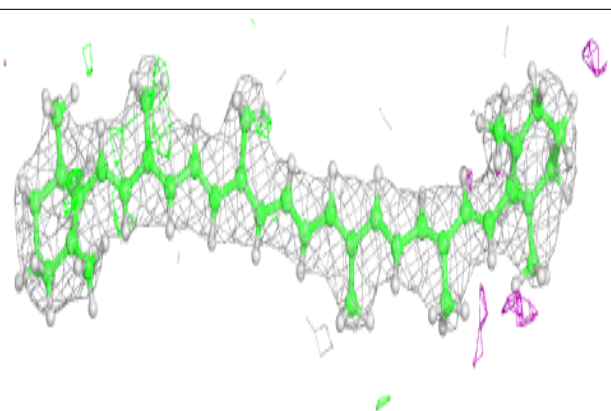
Electron density around CLA c 503:

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

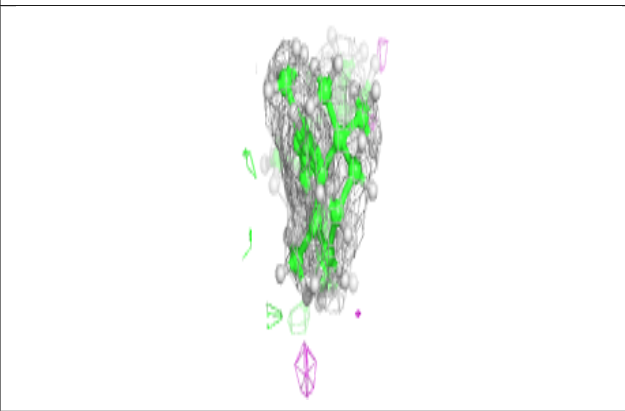
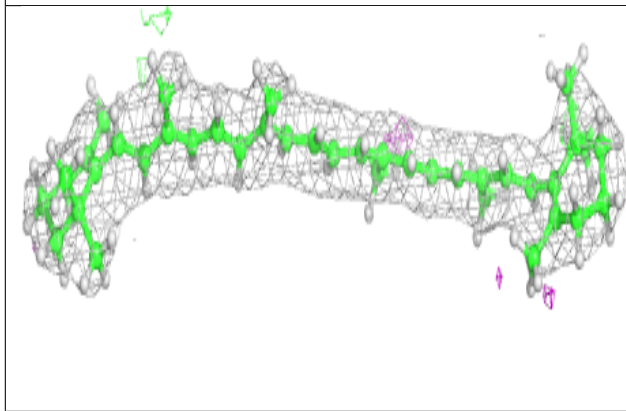
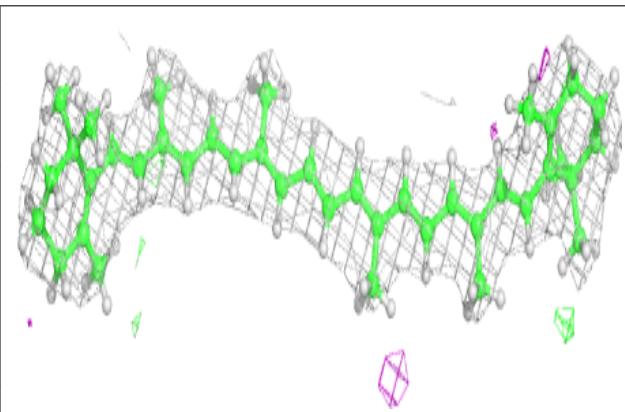


Electron density around BCR B 618:

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

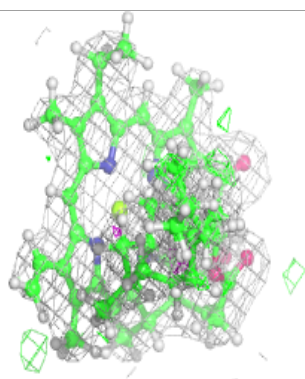
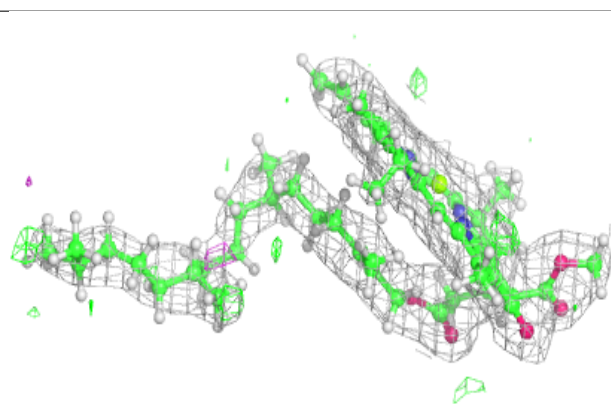
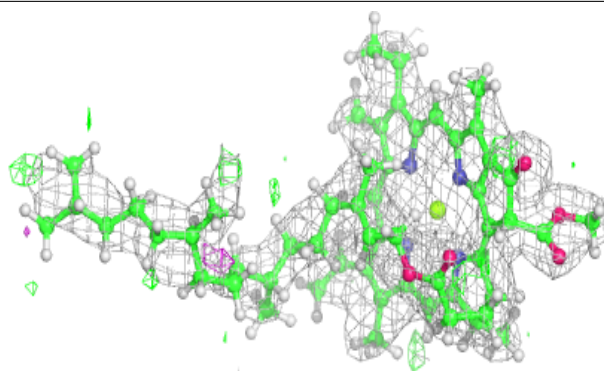
**Electron density around BCR B 619:**

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



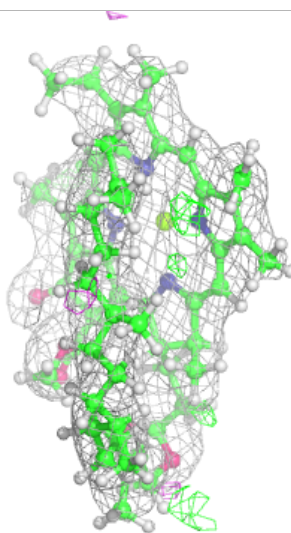
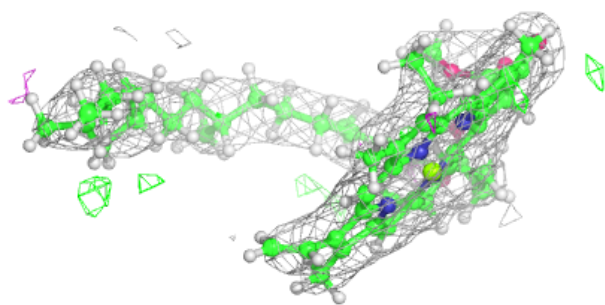
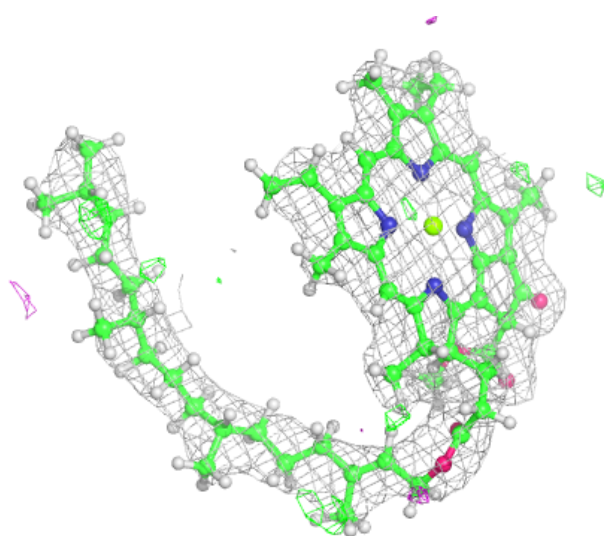
Electron density around CLA c 505:

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



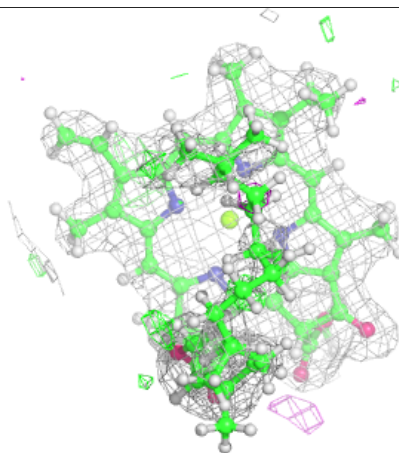
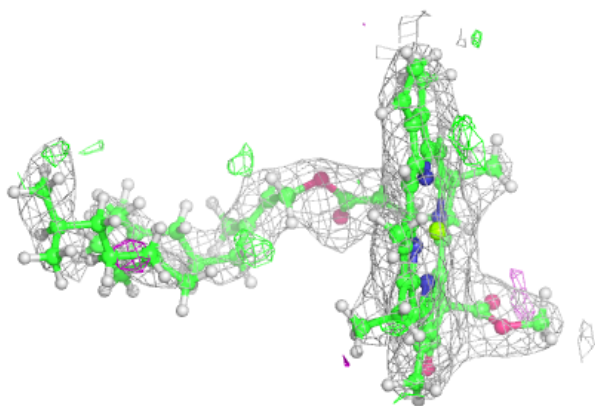
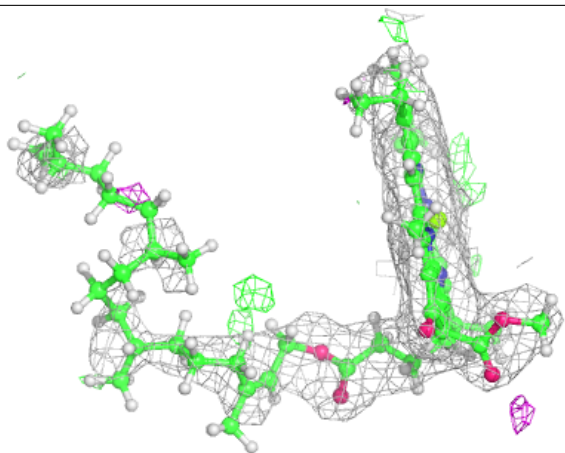
Electron density around CLA c 507:

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



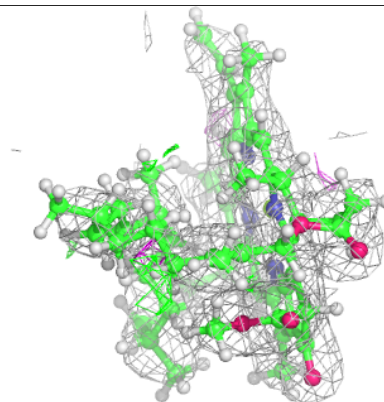
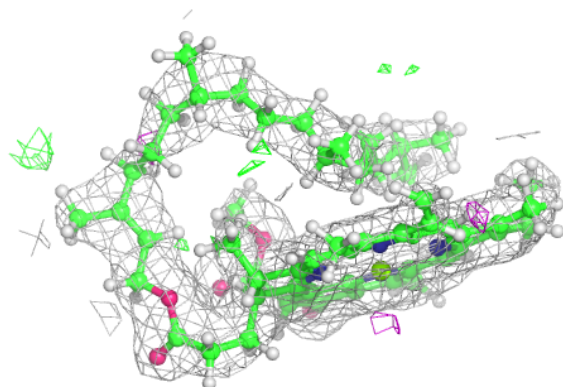
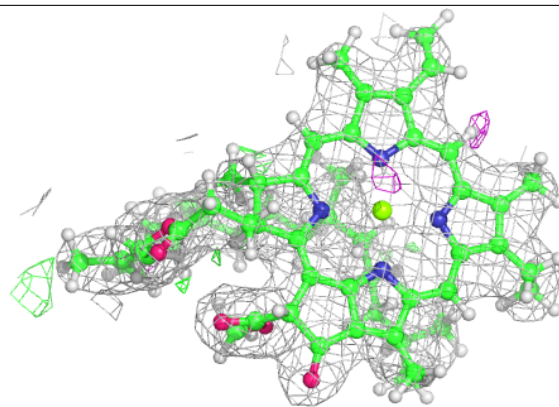
Electron density around CLA c 506:

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

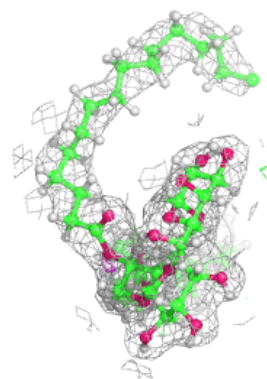
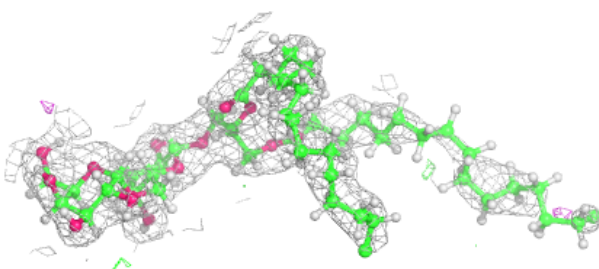
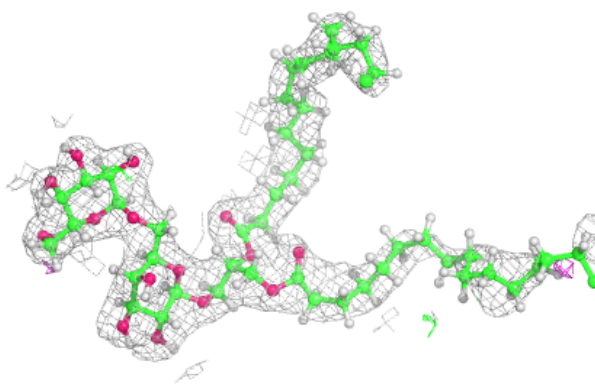


Electron density around CLA C 510:

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

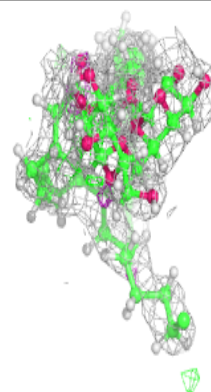
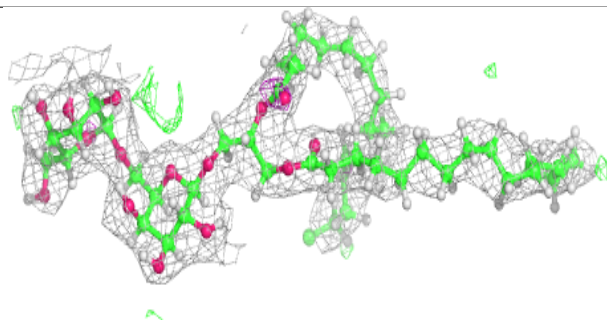
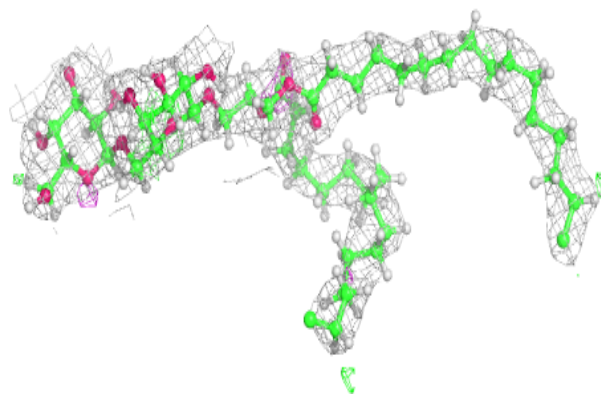
**Electron density around DGD c 517:**

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

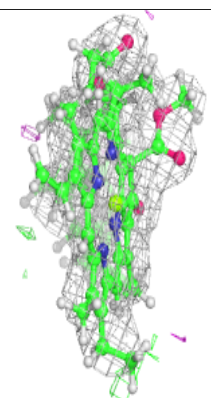
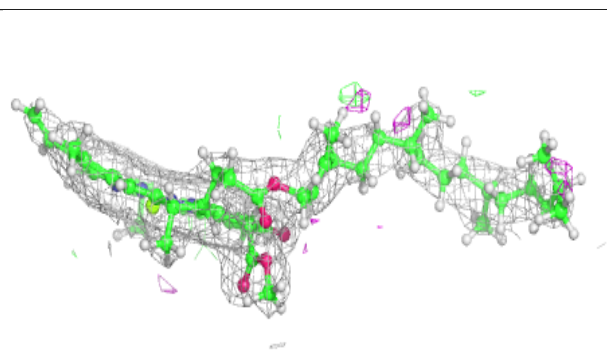
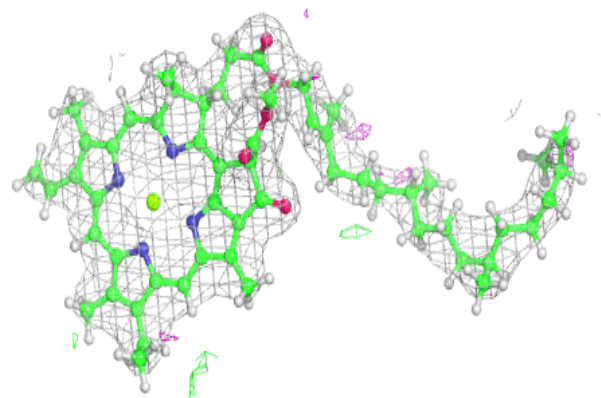


Electron density around DGD h 103:

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

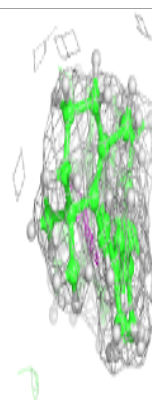
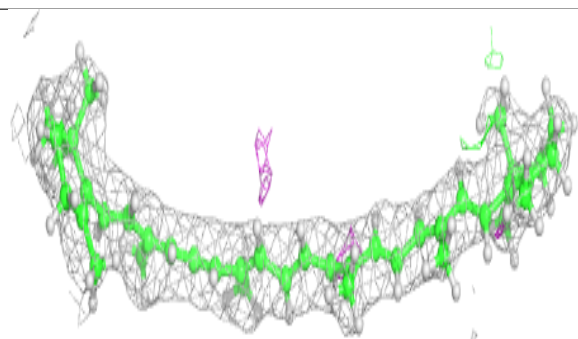
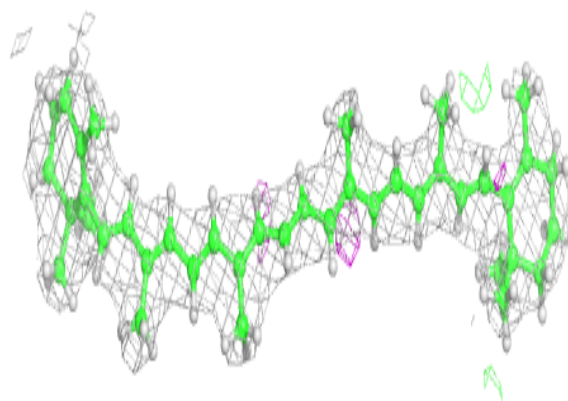
**Electron density around CLA b 602:**

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



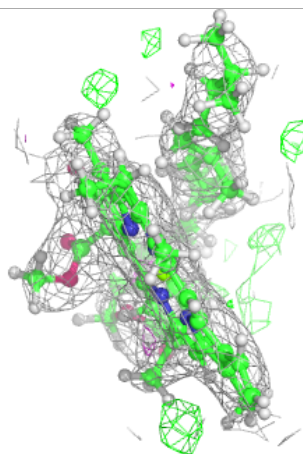
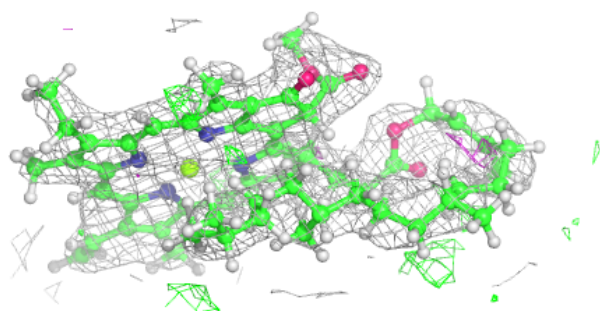
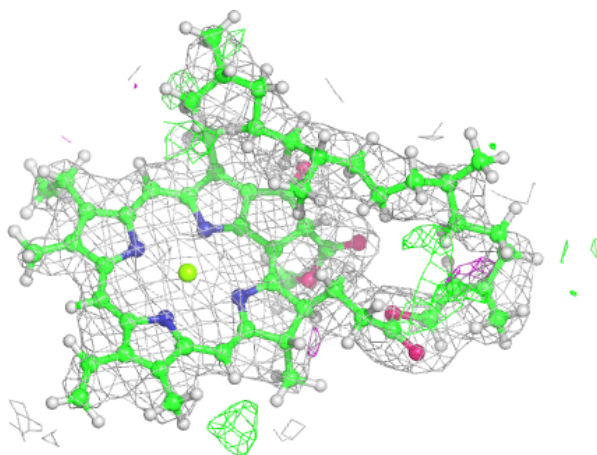
Electron density around BCR T 101:

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



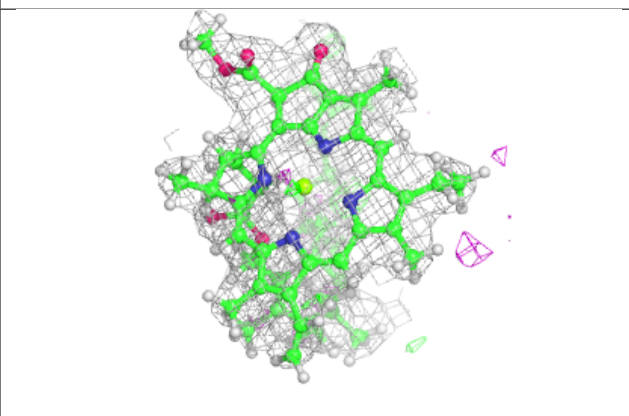
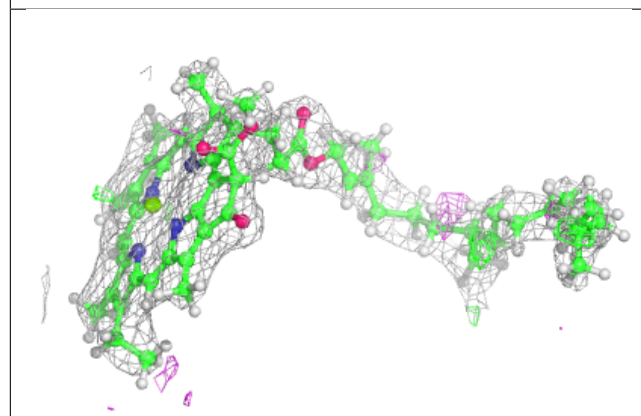
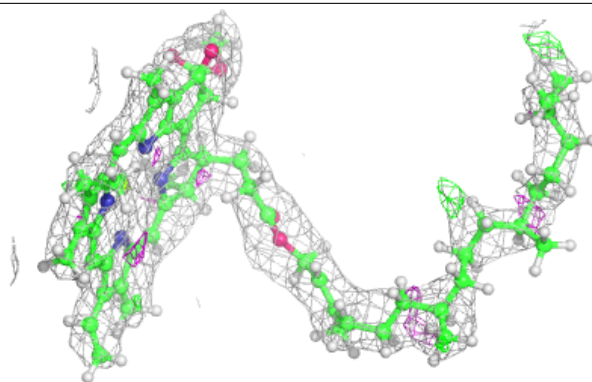
Electron density around CLA c 509:

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

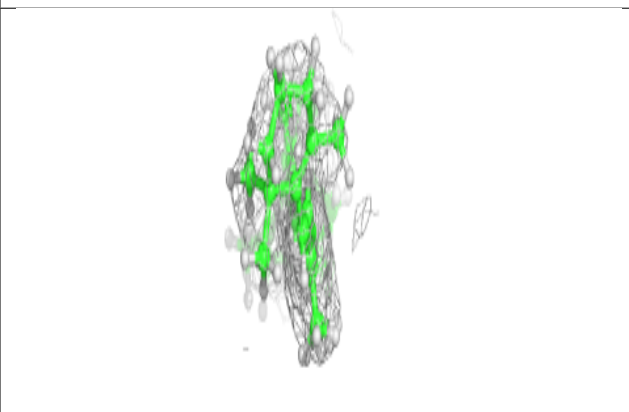
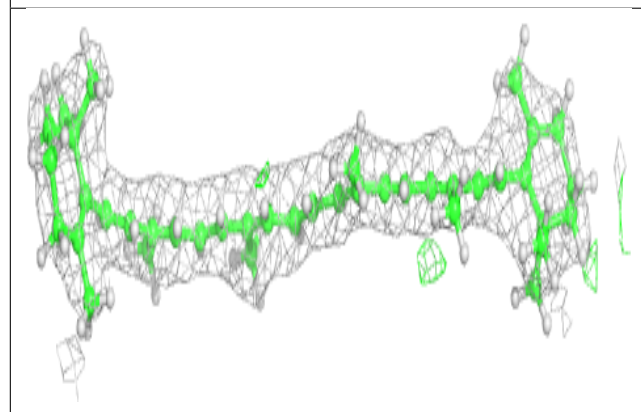
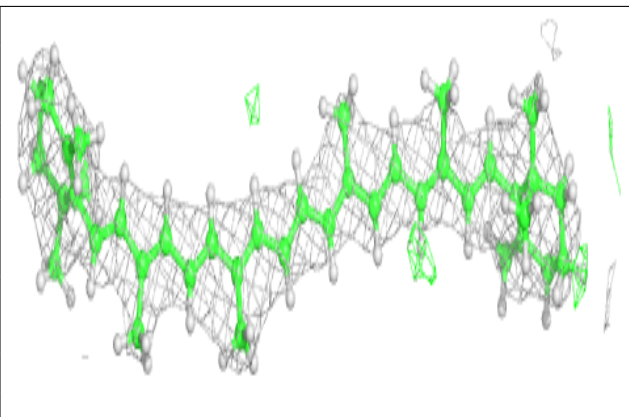


Electron density around CLA b 606:

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

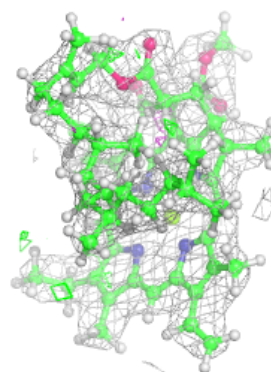
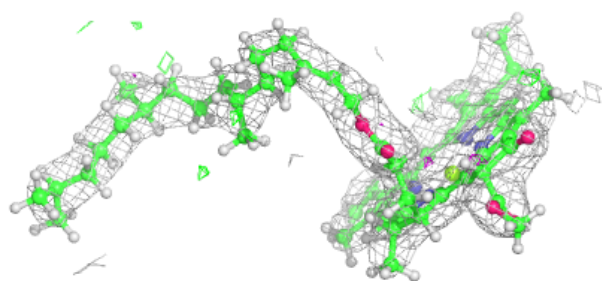
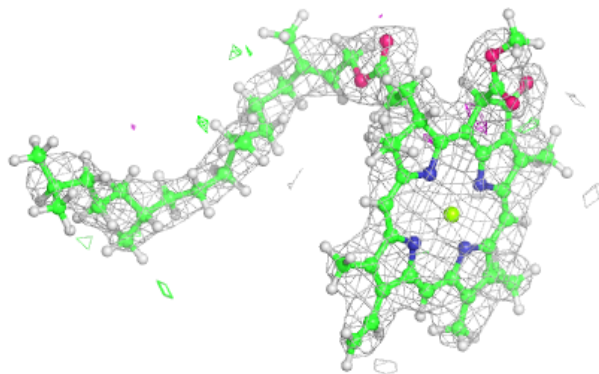
**Electron density around BCR c 515:**

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



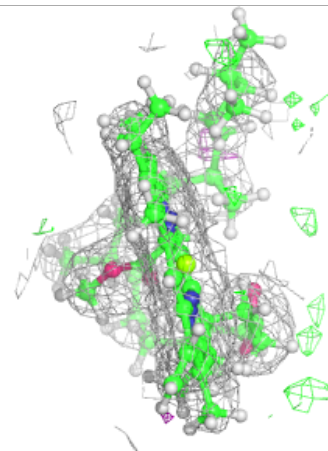
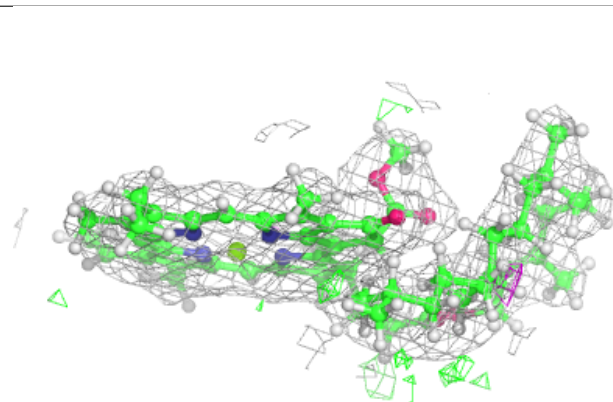
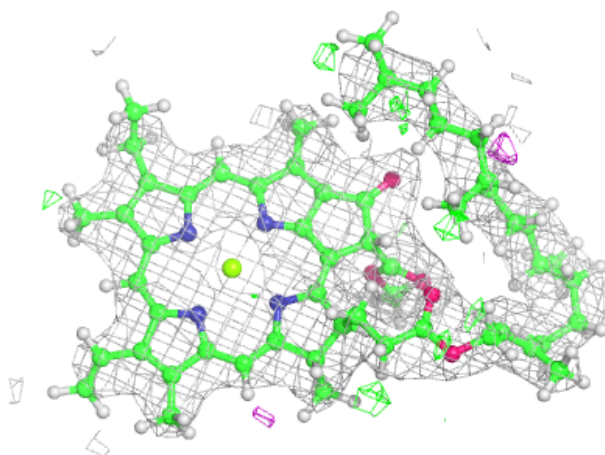
Electron density around CLA C 511:

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



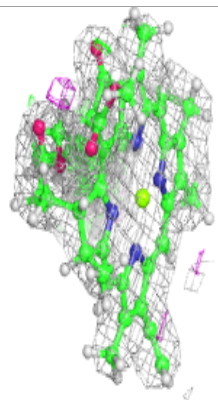
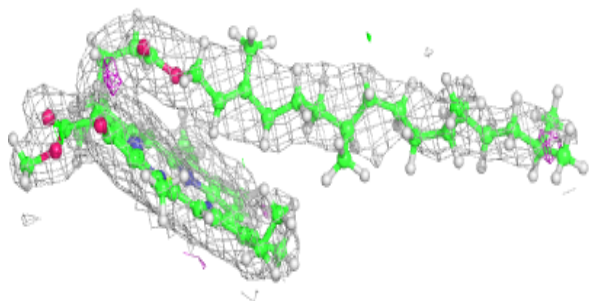
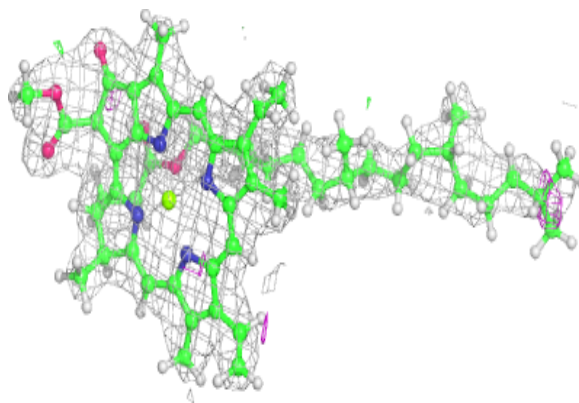
Electron density around CLA b 610:

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



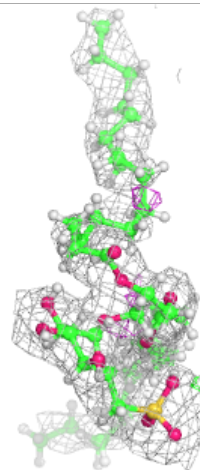
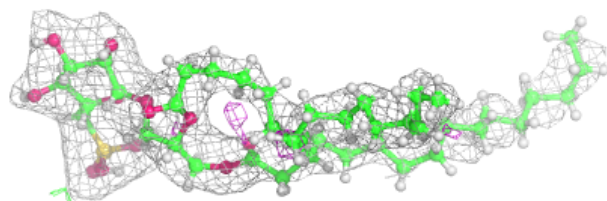
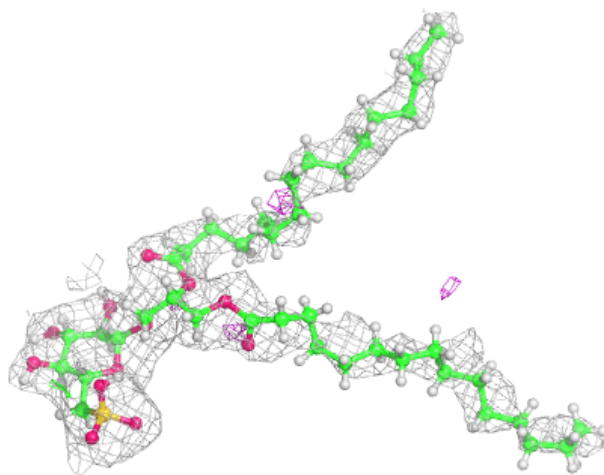
Electron density around CLA b 614:

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



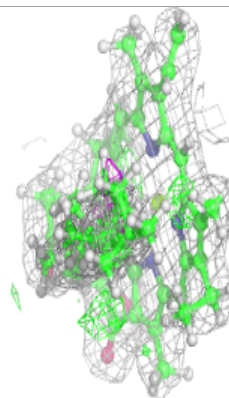
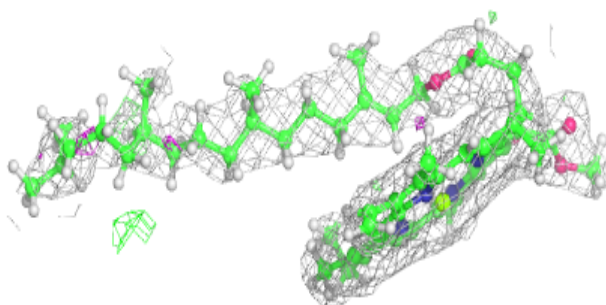
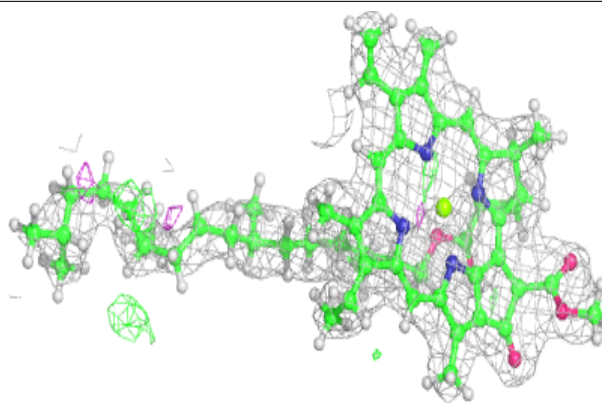
Electron density around SQD a 411:

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

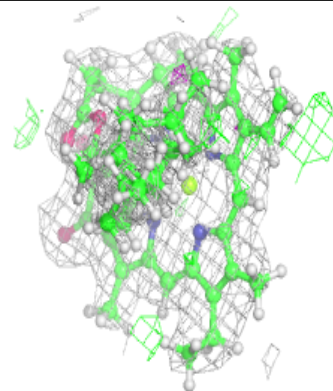
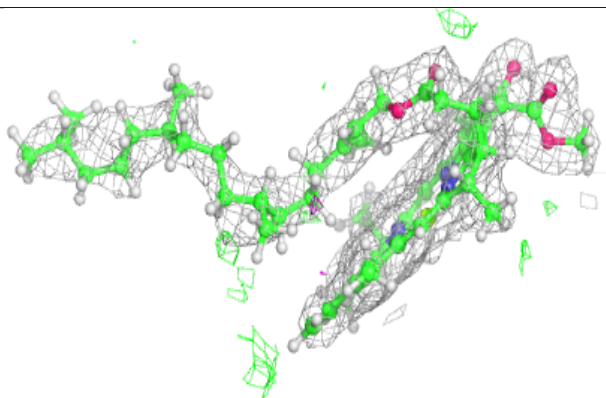
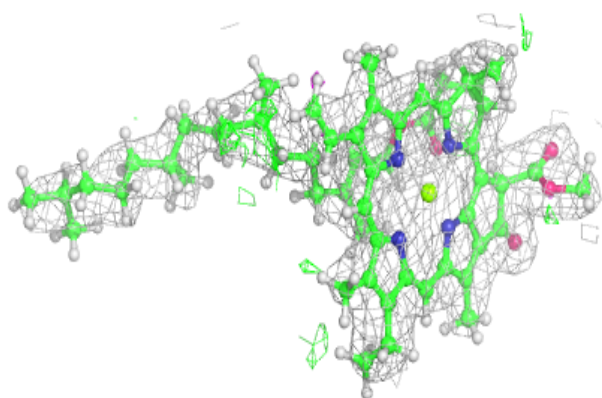


Electron density around CLA B 614:

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

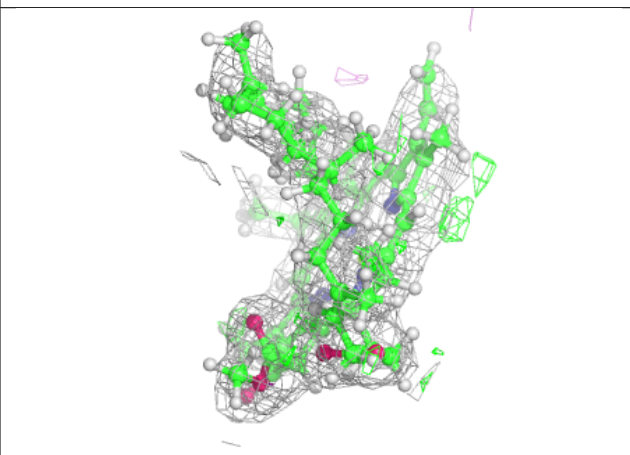
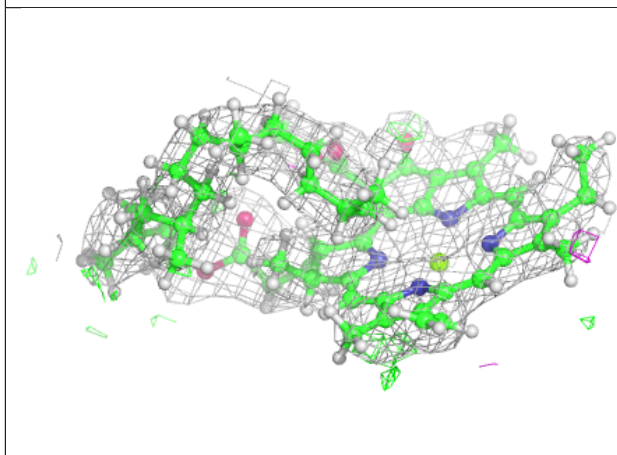
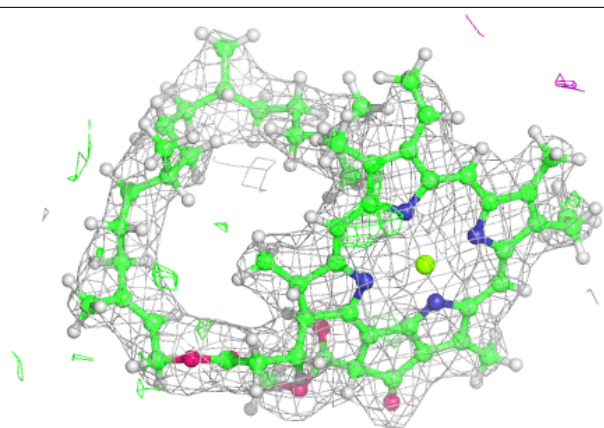
**Electron density around CLA C 505:**

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

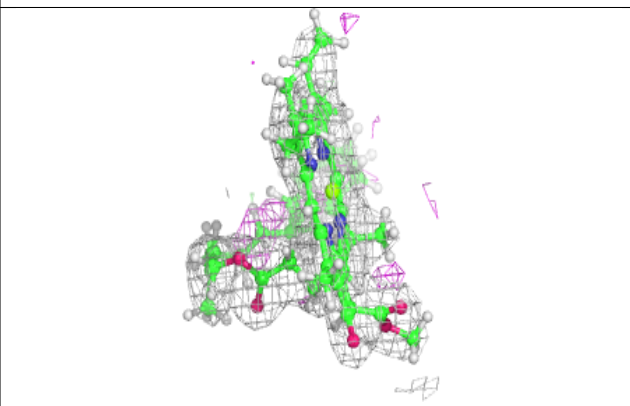
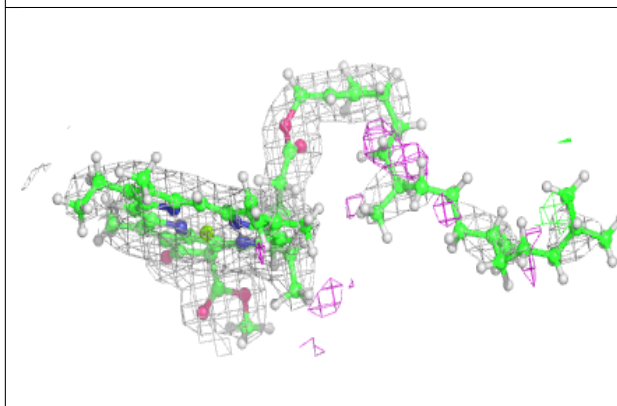
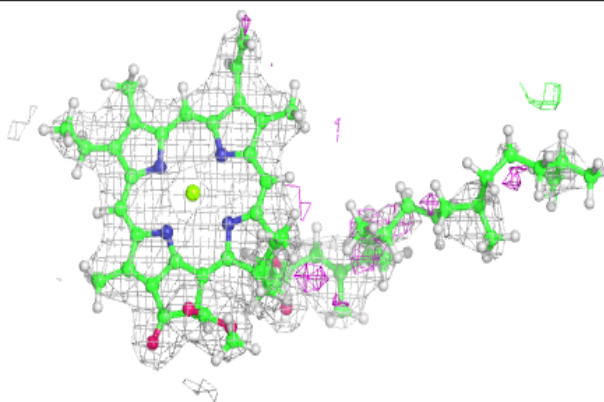


Electron density around CLA B 615:

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

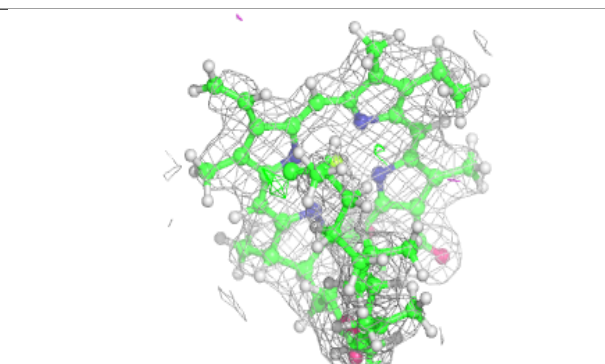
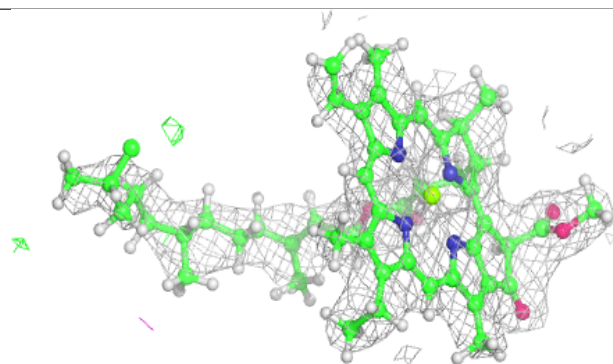
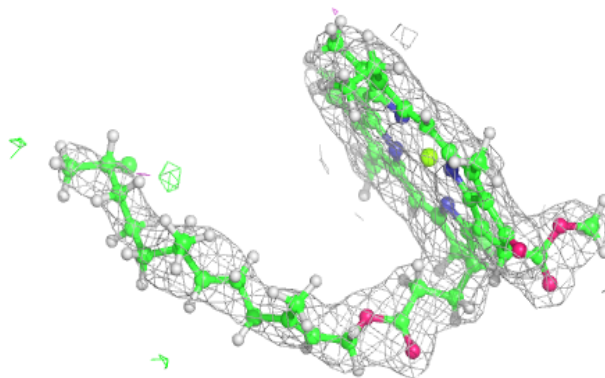
**Electron density around CLA a 403:**

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

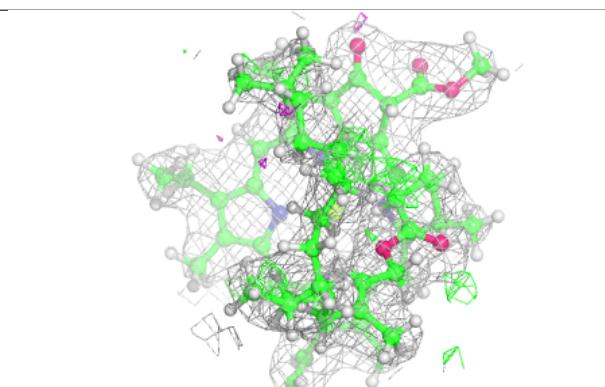
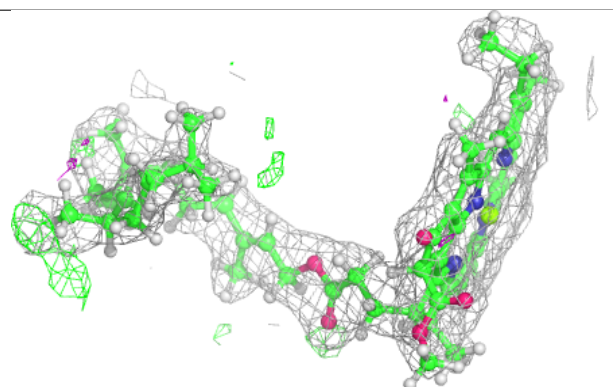
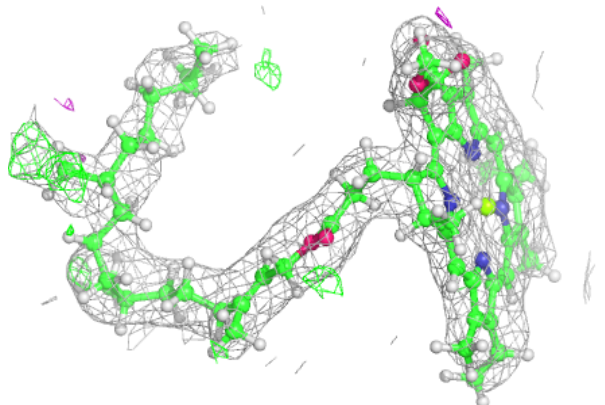


Electron density around CLA c 504:

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

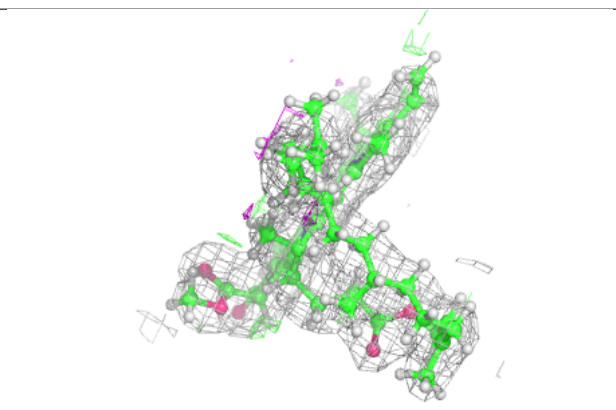
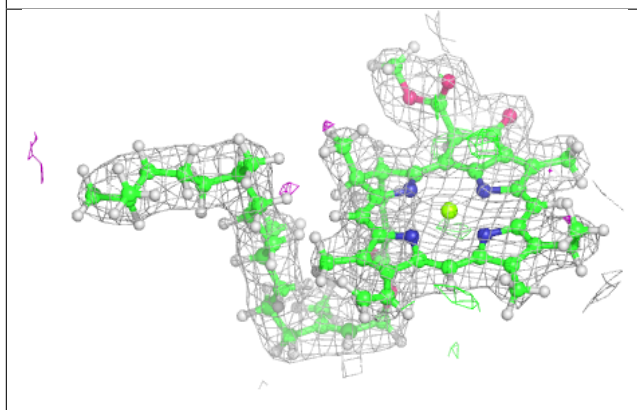
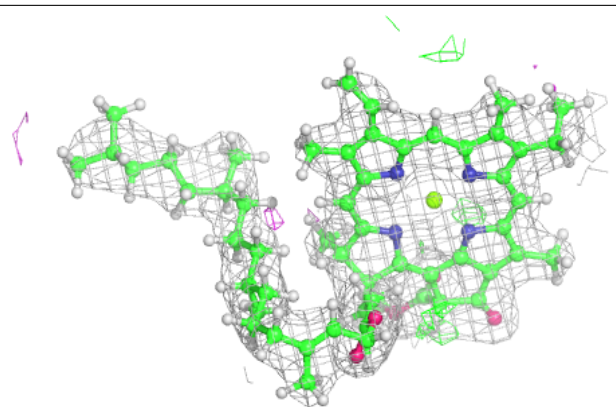
**Electron density around CLA B 606:**

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



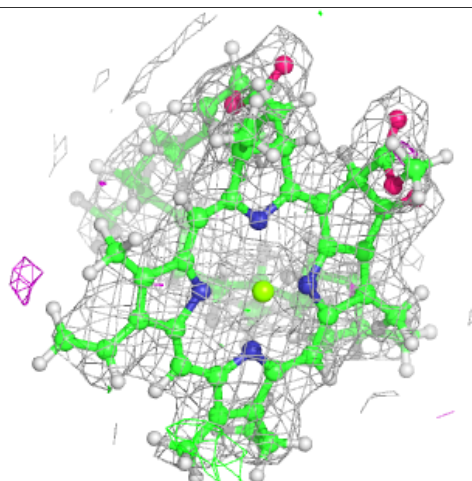
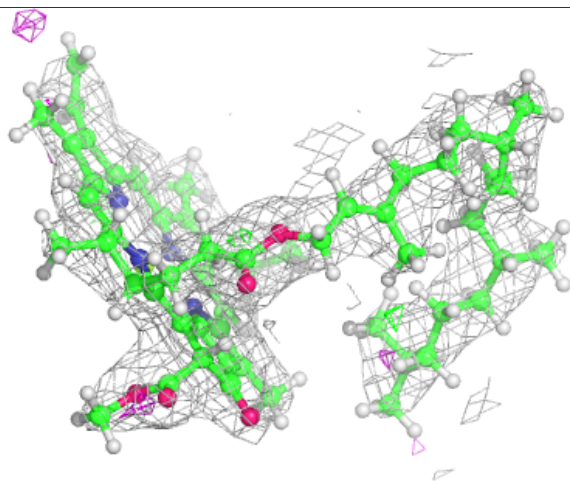
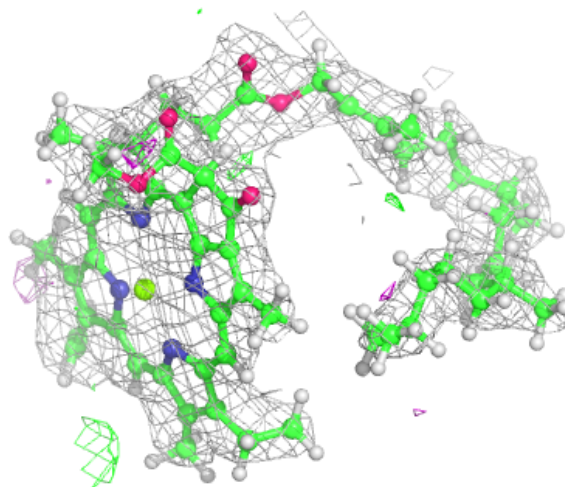
Electron density around CLA d 404:

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



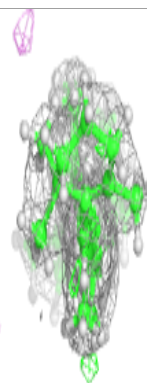
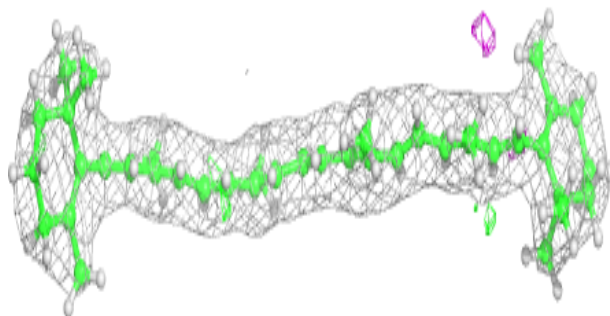
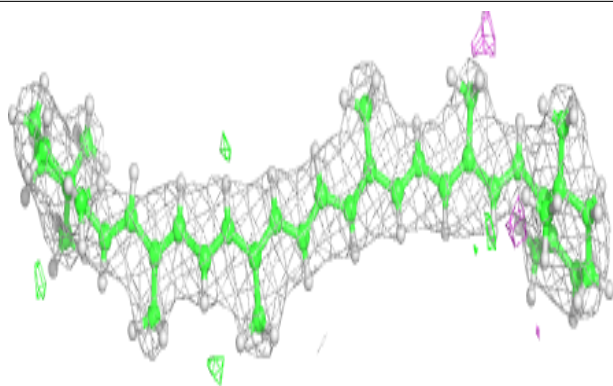
Electron density around CLA C 503:

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

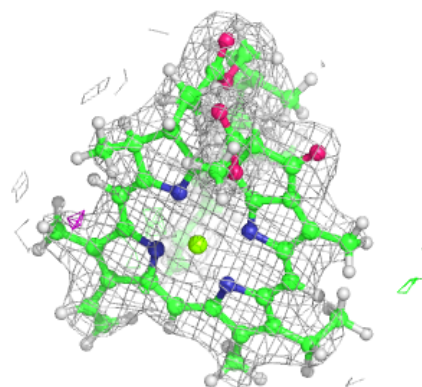
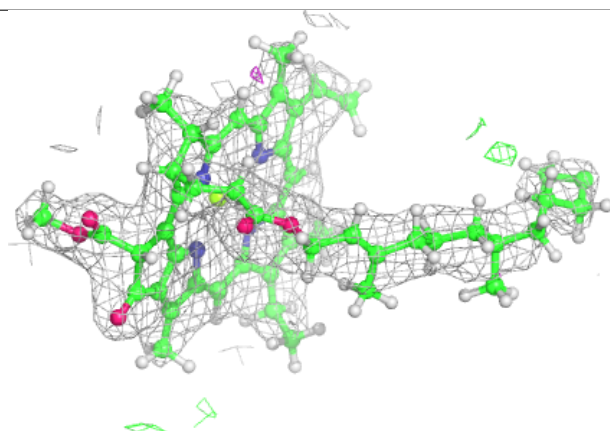
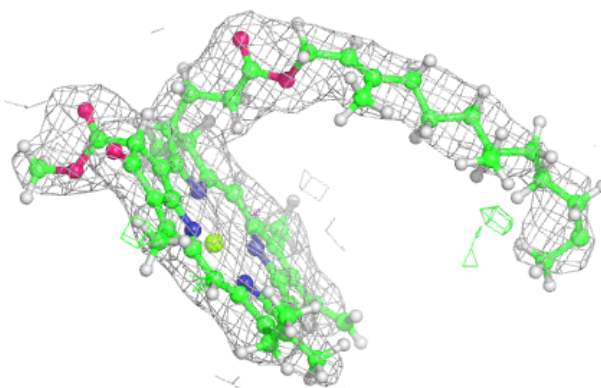


Electron density around BCR A 407:

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

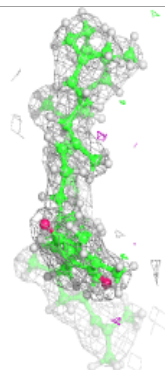
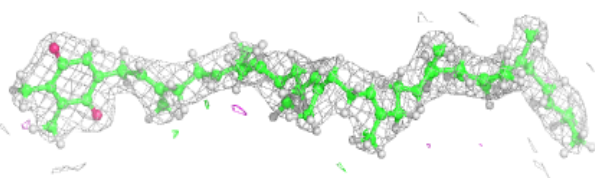
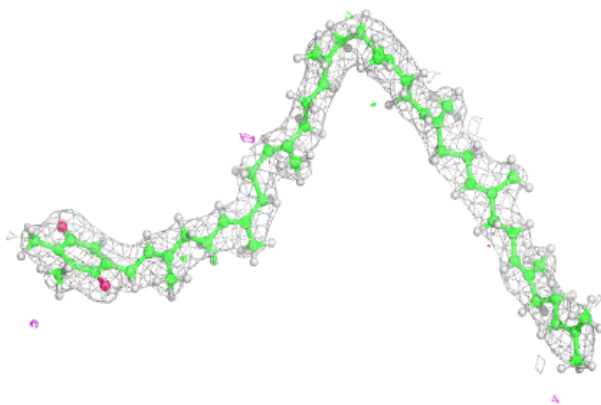
**Electron density around CLA C 504:**

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

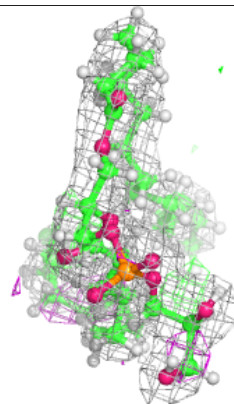
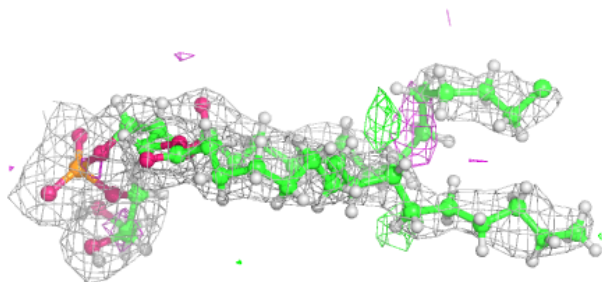
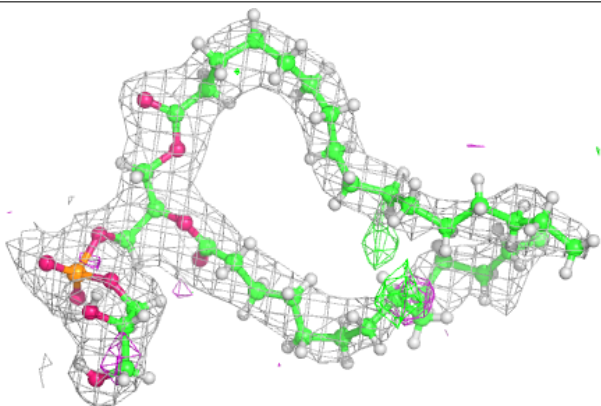


Electron density around PL9 D 406:

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

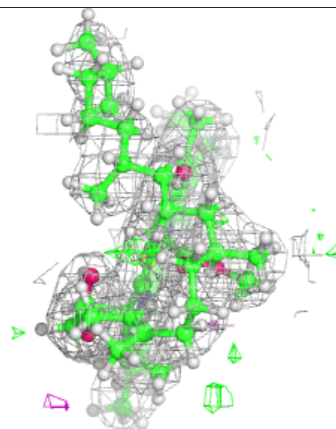
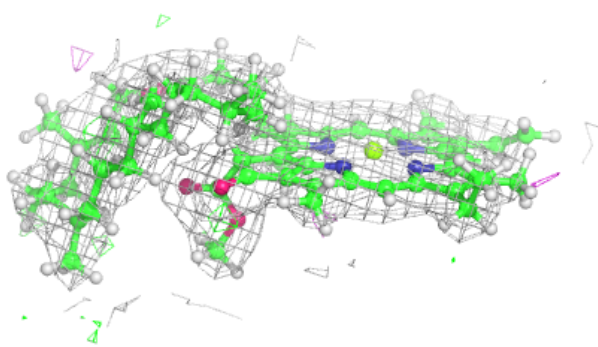
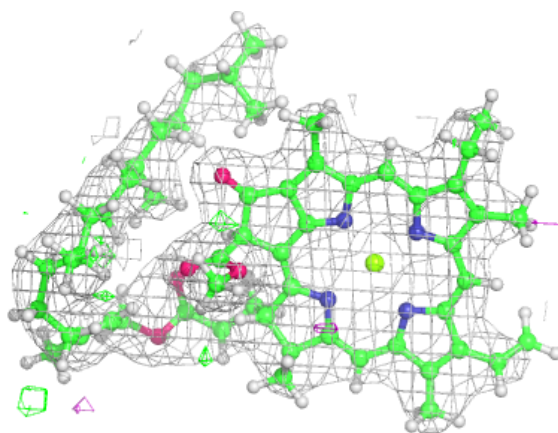
**Electron density around LHG D 409:**

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



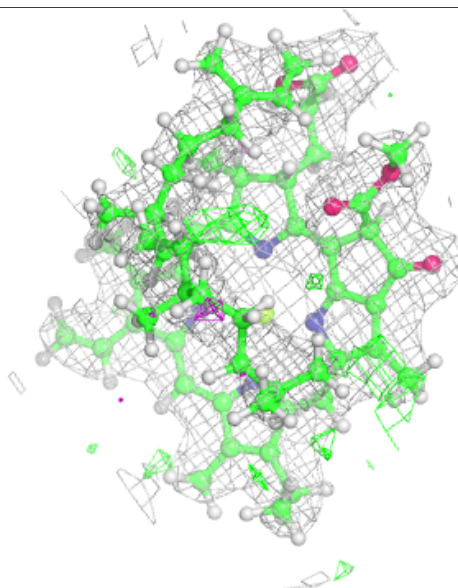
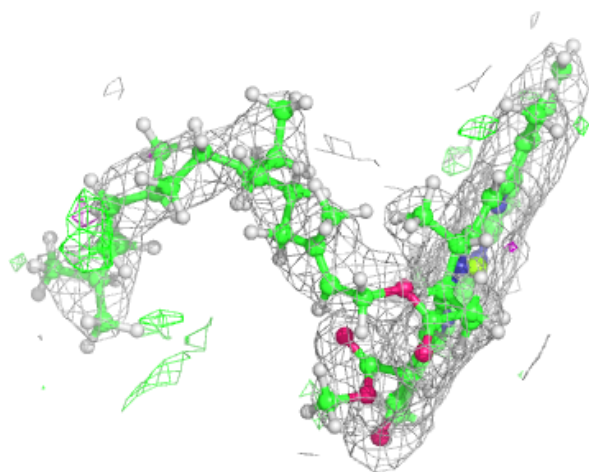
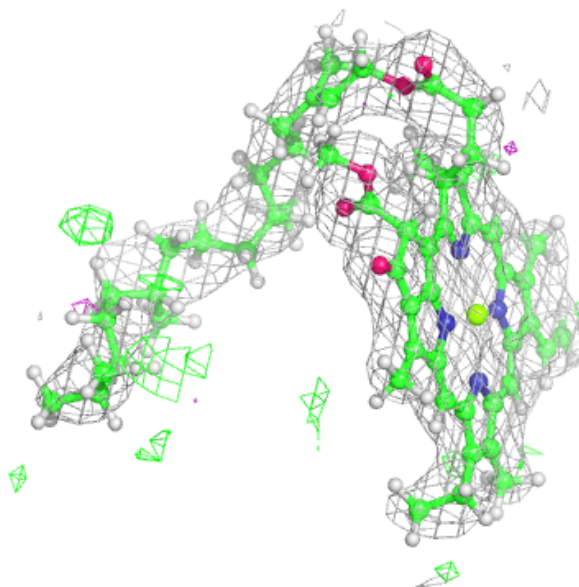
Electron density around CLA B 610:

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



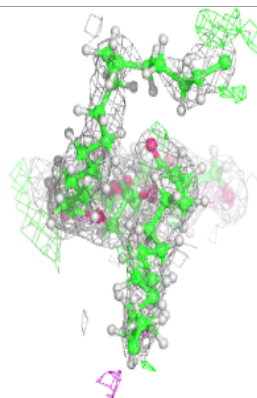
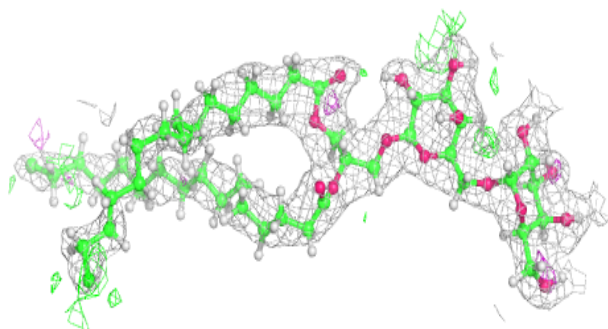
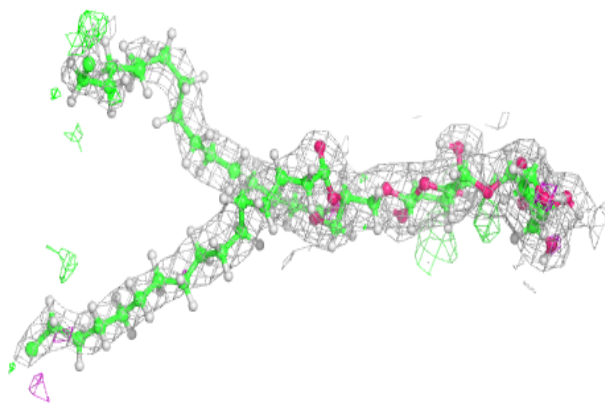
Electron density around CLA B 613:

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

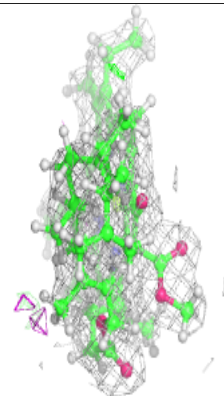
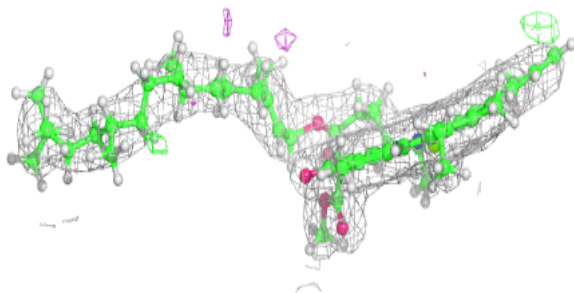
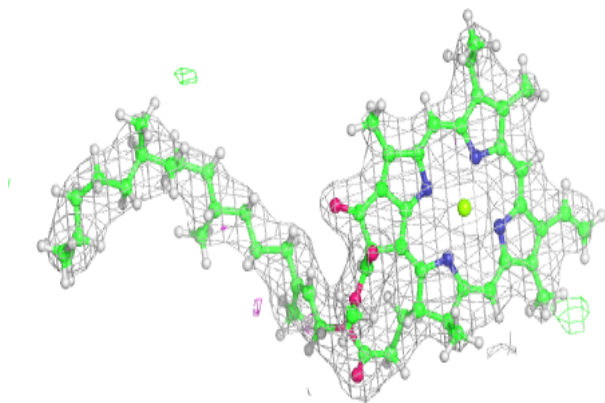


Electron density around DGD C 515:

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

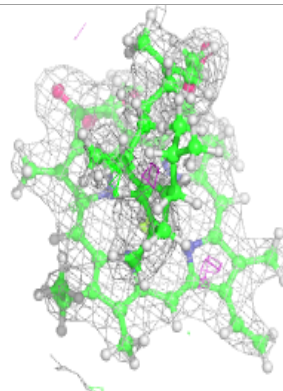
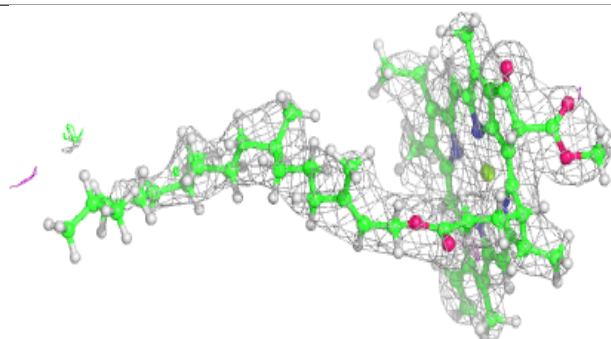
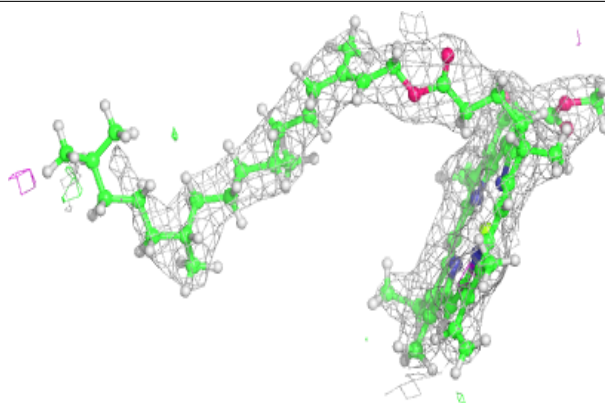
**Electron density around CLA B 602:**

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

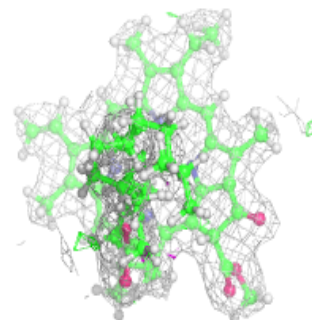
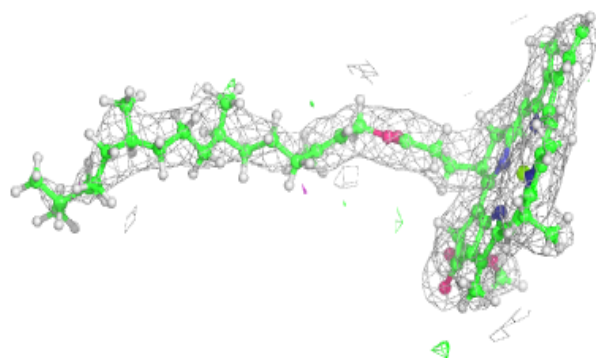
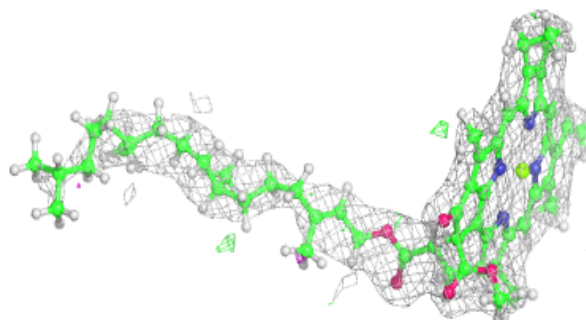


Electron density around CLA C 508:

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

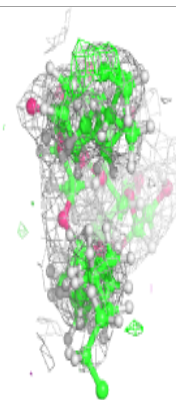
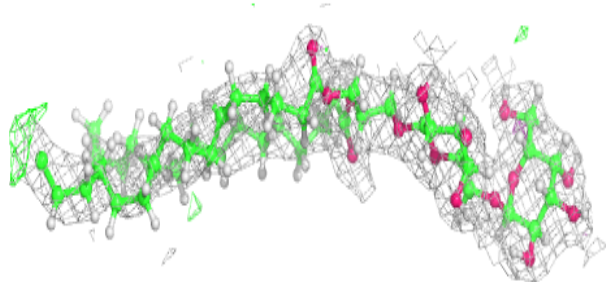
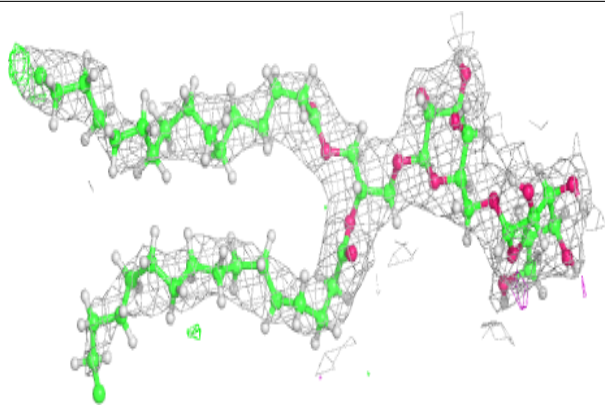
**Electron density around CLA b 604:**

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



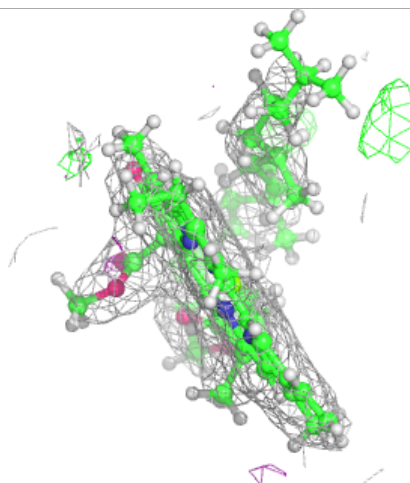
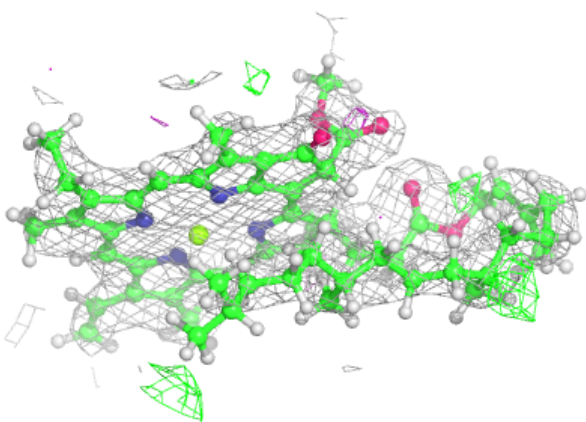
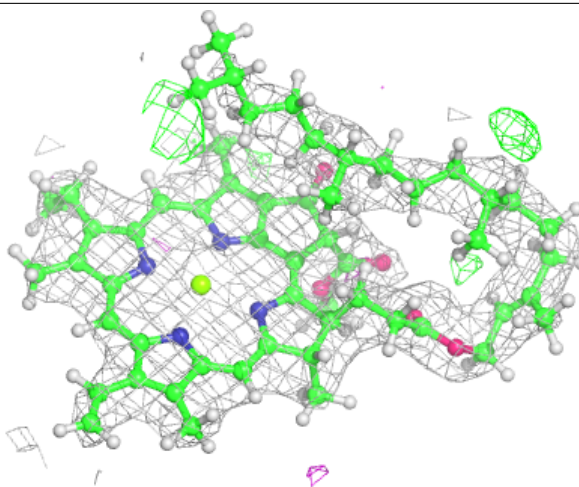
Electron density around DGD c 518:

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



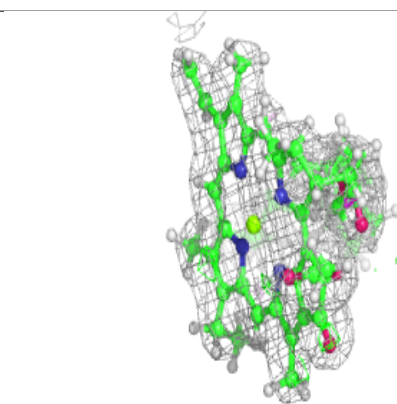
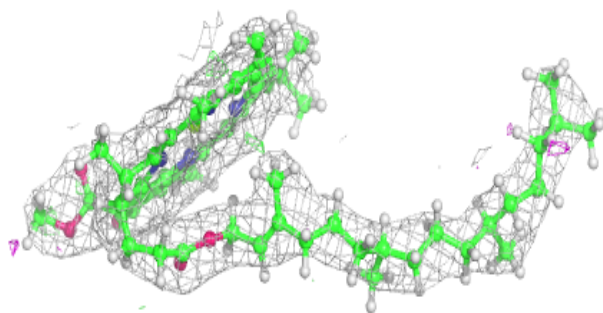
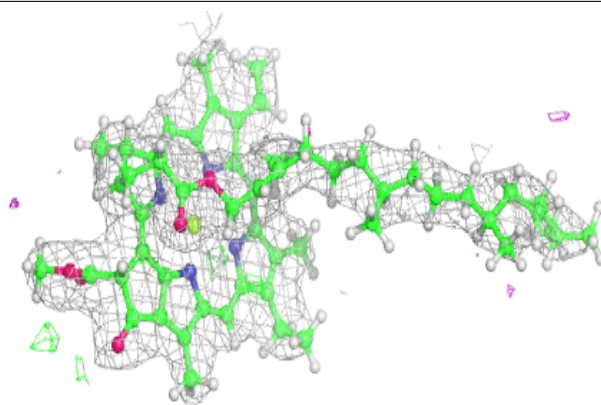
Electron density around CLA C 509:

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

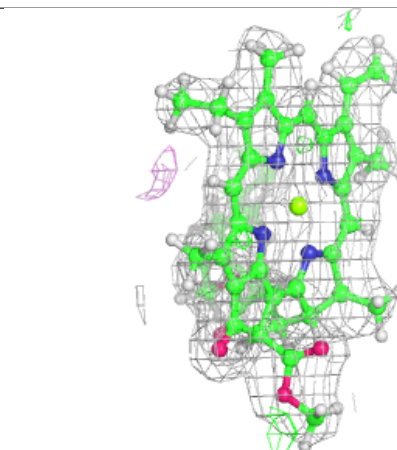
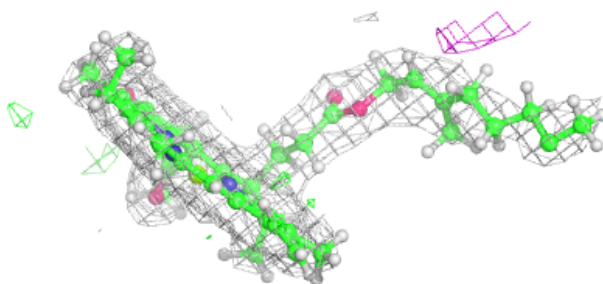
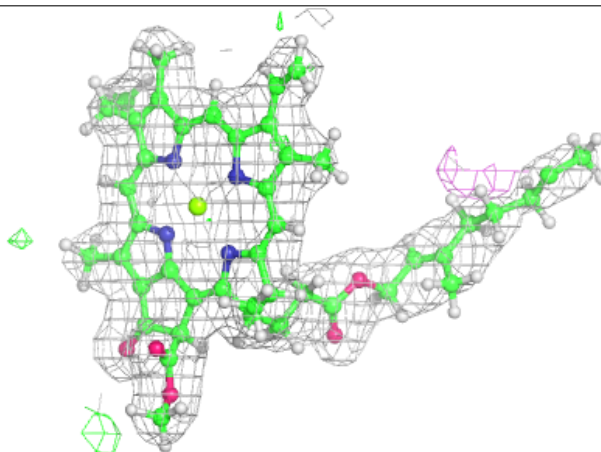


Electron density around CLA b 608:

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

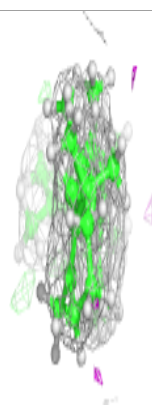
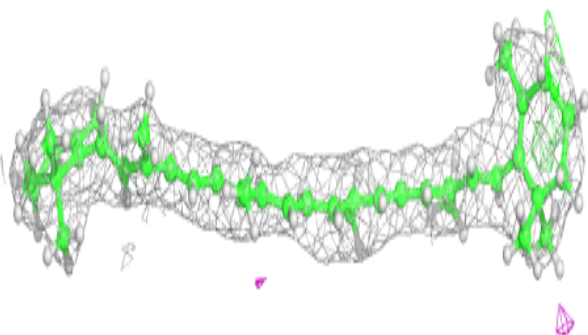
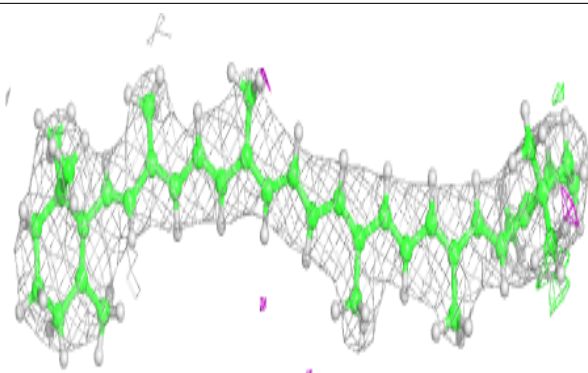
**Electron density around CLA A 406:**

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

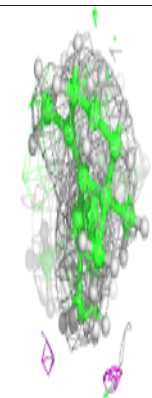
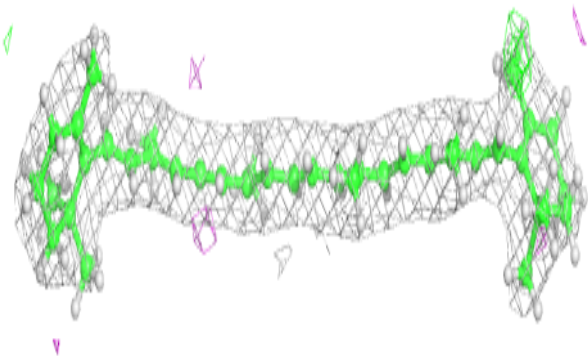
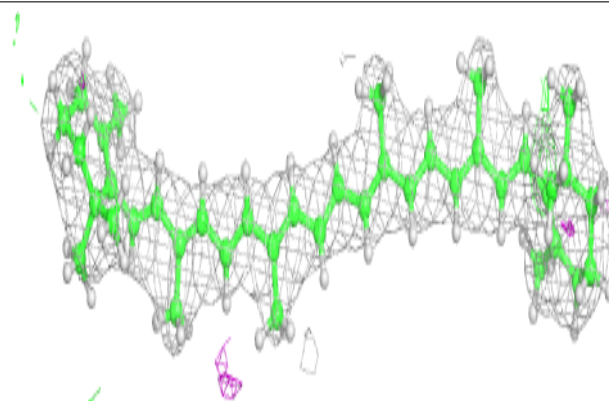


Electron density around BCR b 617:

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

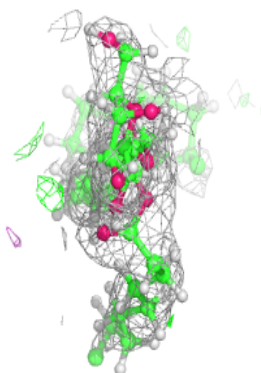
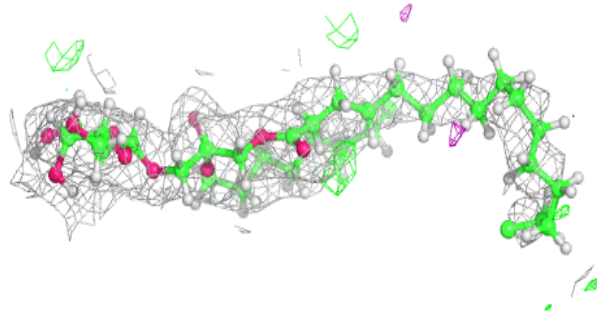
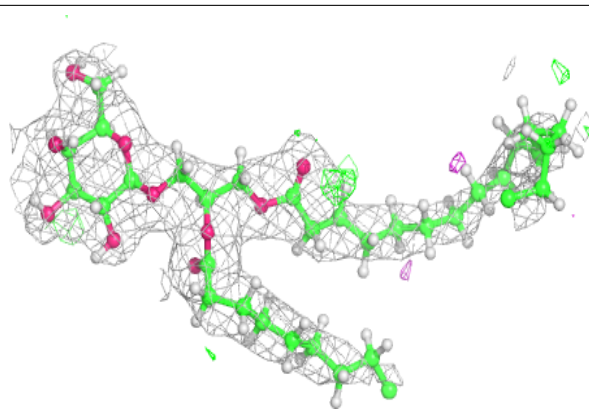
**Electron density around BCR b 618:**

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

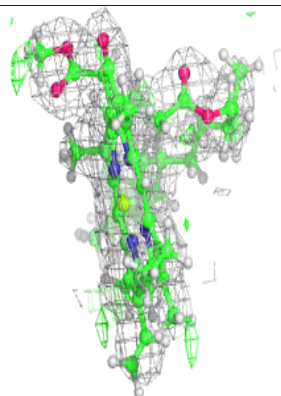
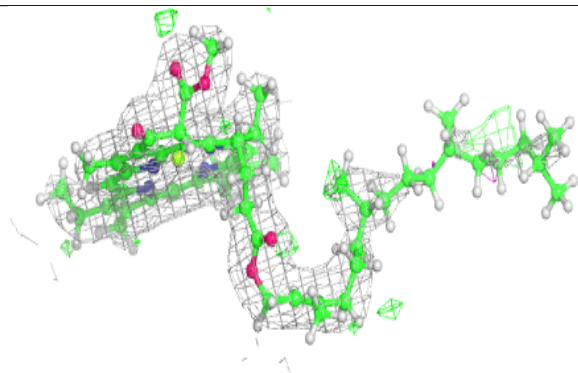
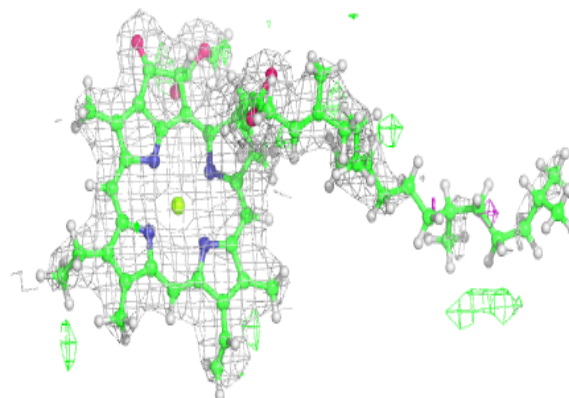


Electron density around LMG d 410:

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

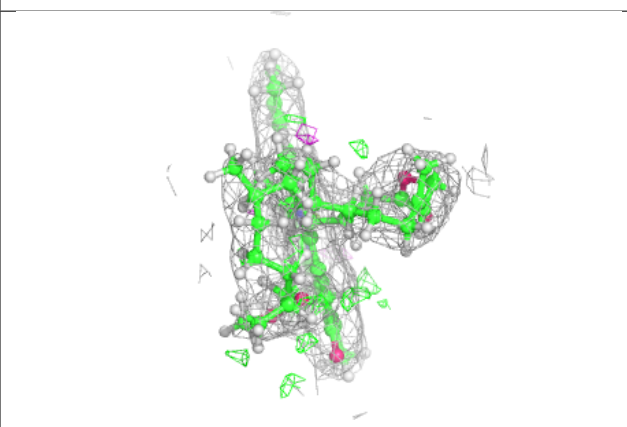
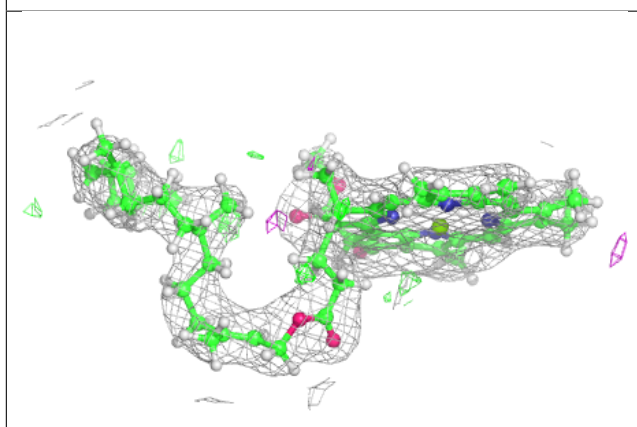
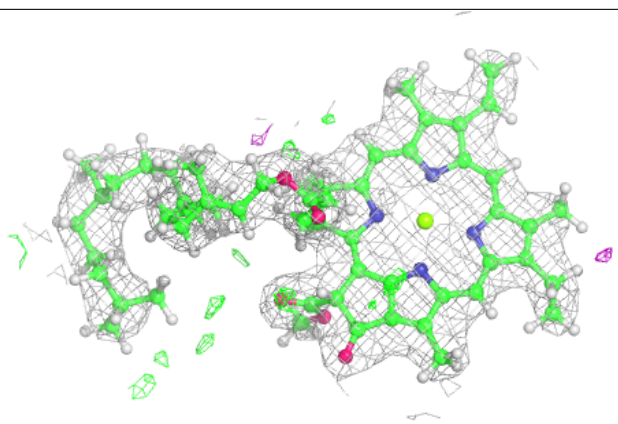
**Electron density around CLA A 403:**

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



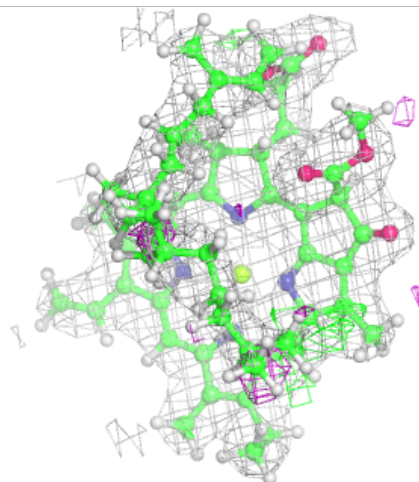
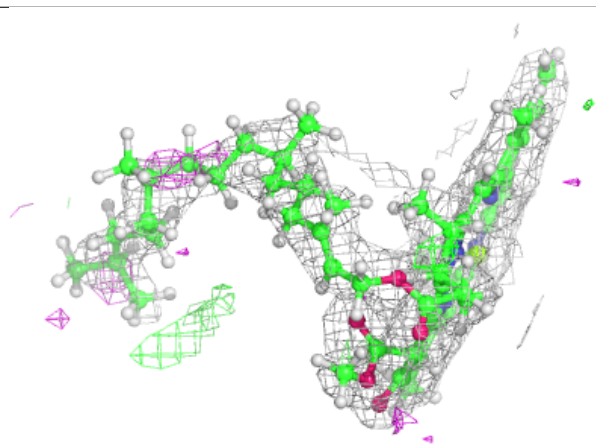
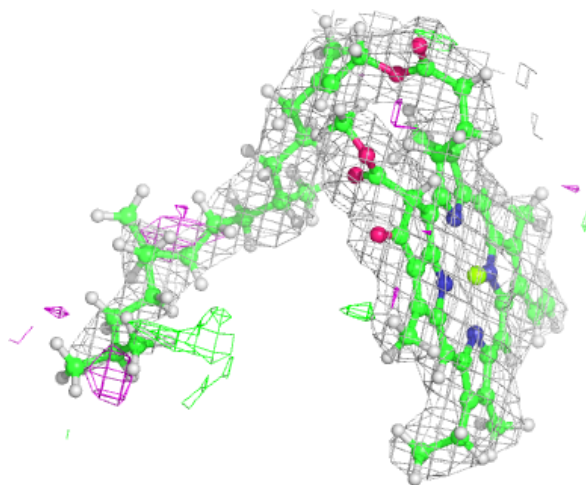
Electron density around CLA b 612:

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



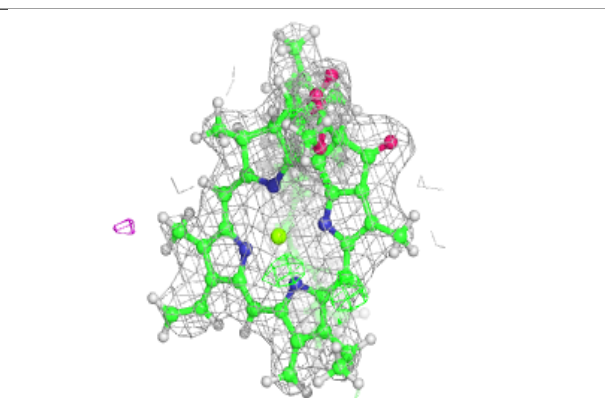
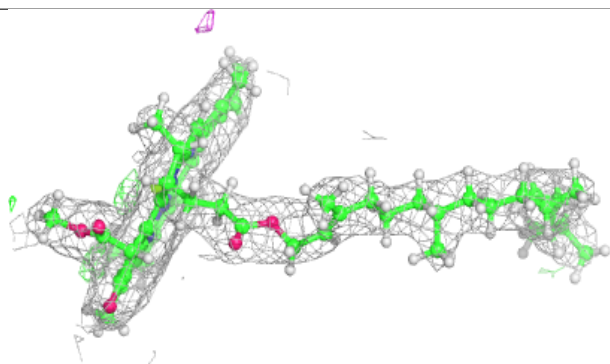
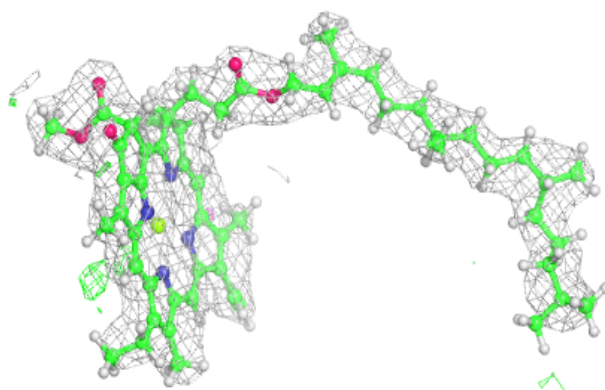
Electron density around CLA b 613:

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

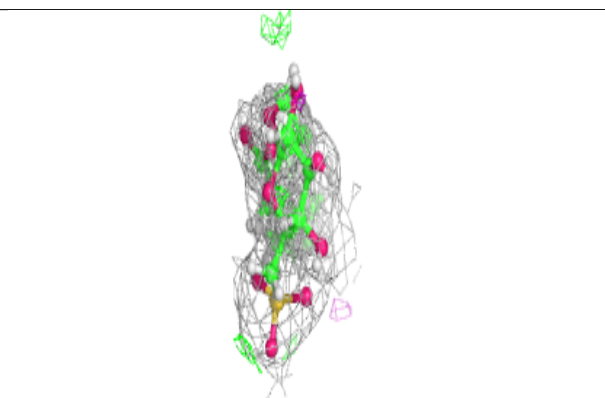
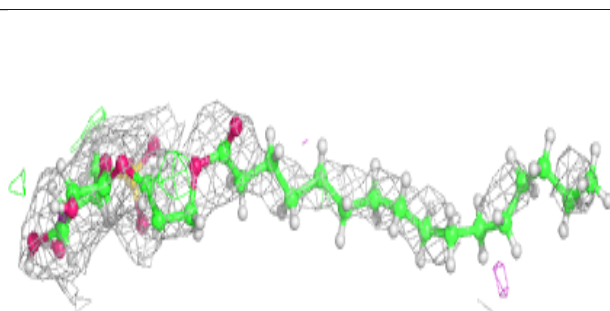
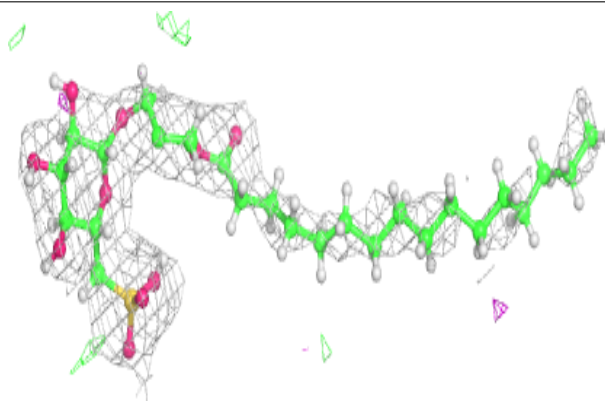


Electron density around CLA B 609:

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

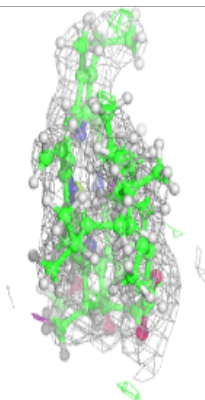
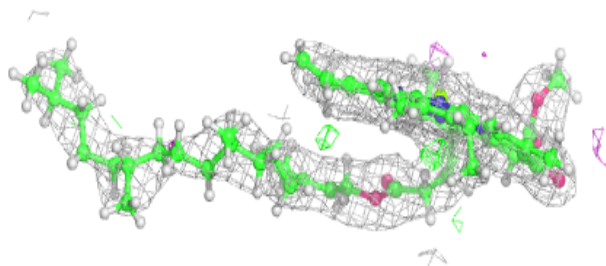
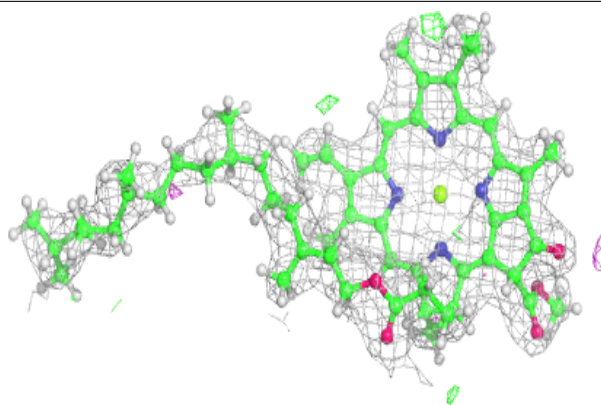
**Electron density around SQD F 102:**

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

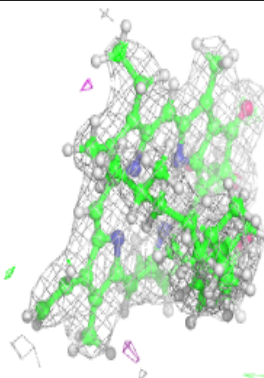
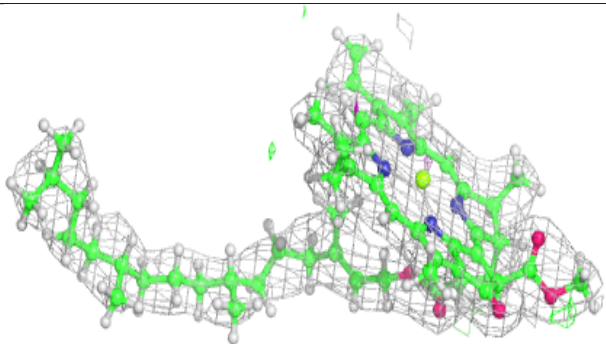
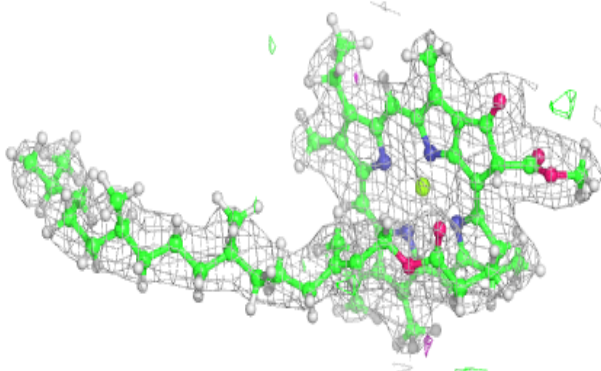


Electron density around CLA B 603:

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

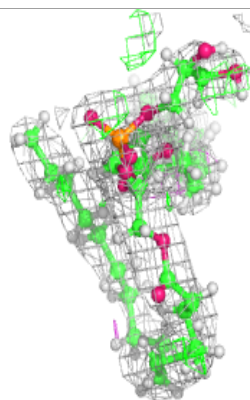
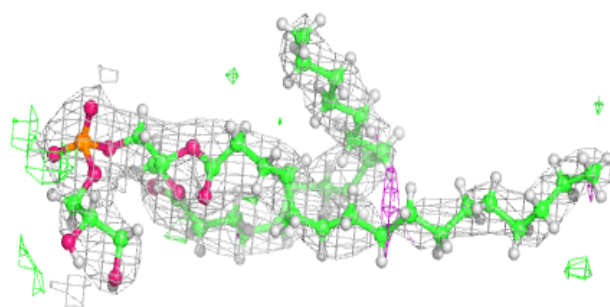
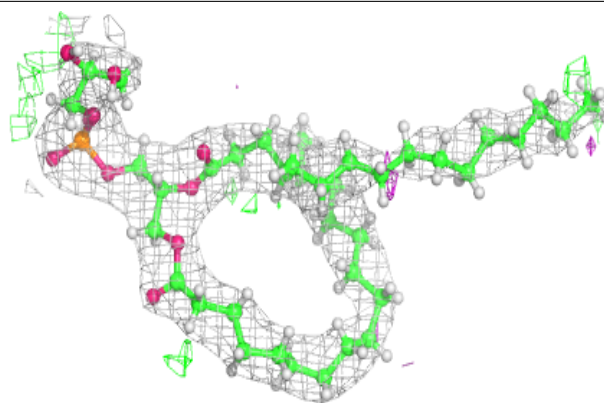
**Electron density around CLA B 608:**

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

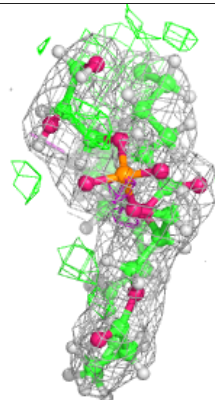
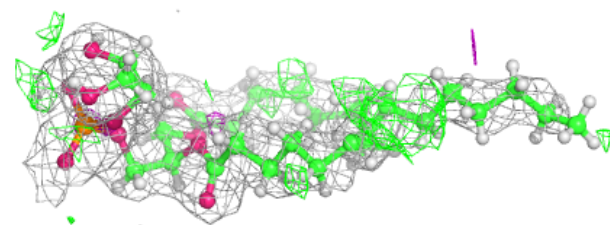
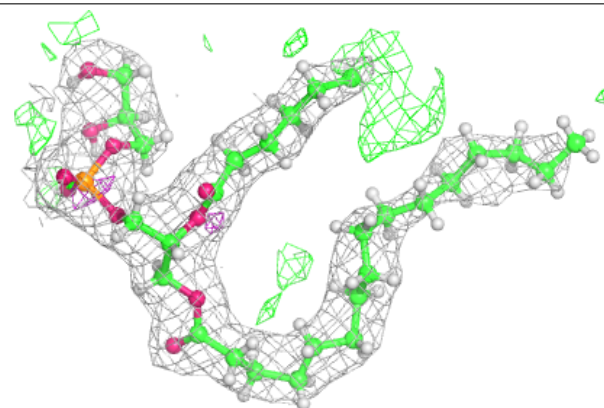


Electron density around LHG a 410:

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

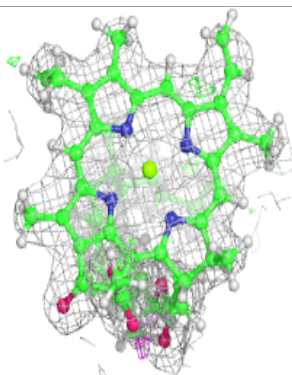
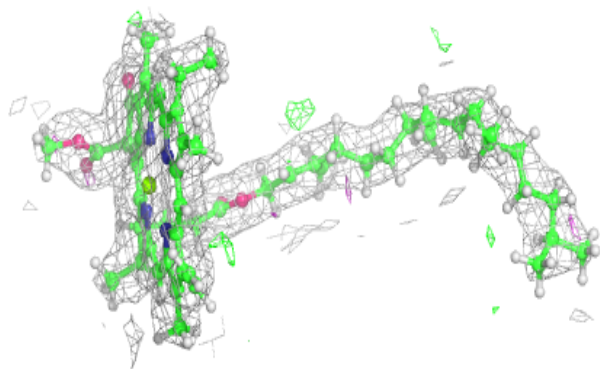
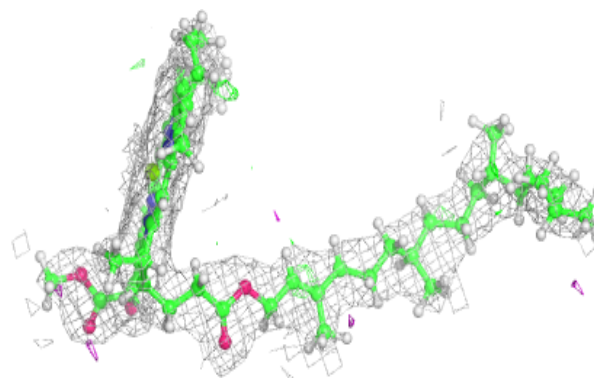
**Electron density around LHG d 409:**

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

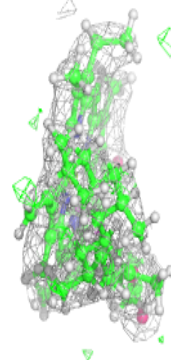
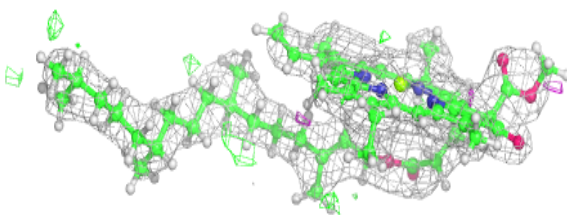
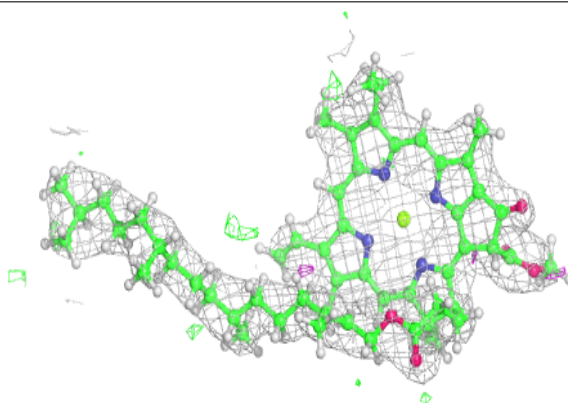


Electron density around CLA b 605:

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

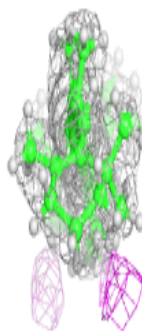
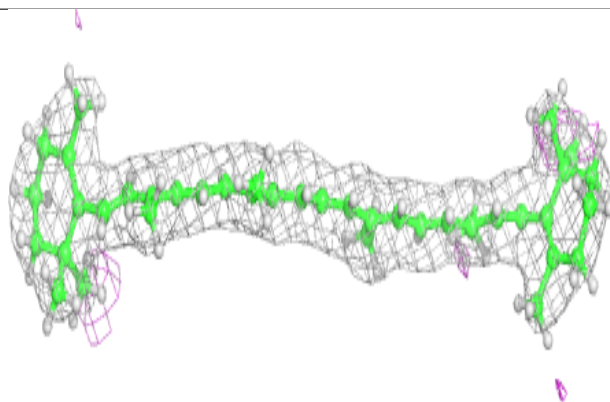
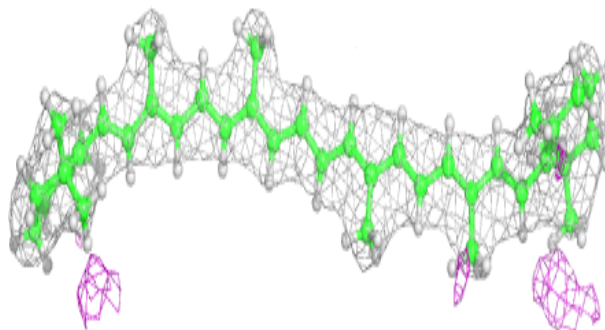
**Electron density around CLA c 501:**

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

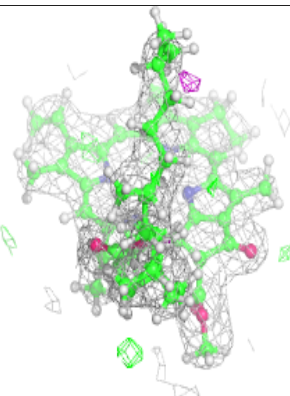
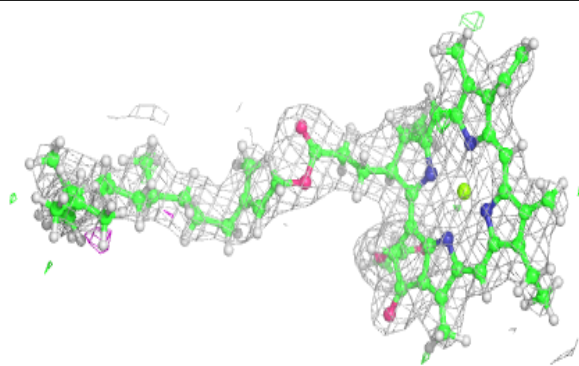
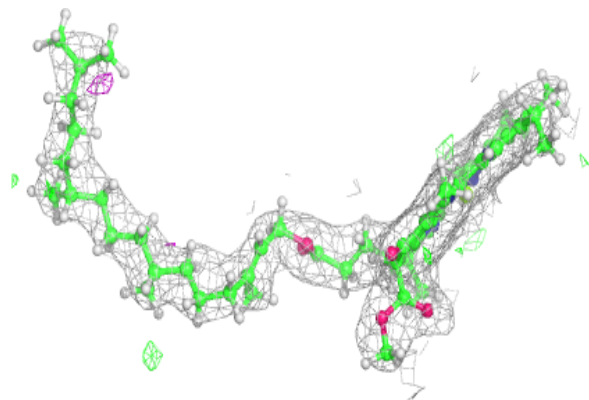


Electron density around BCR a 406:

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

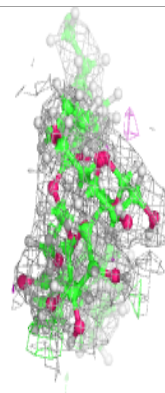
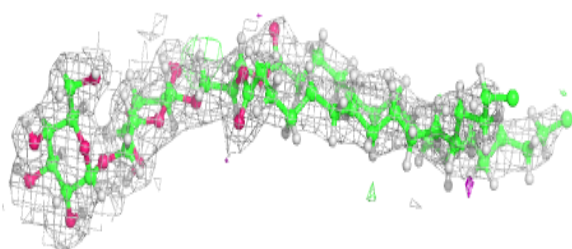
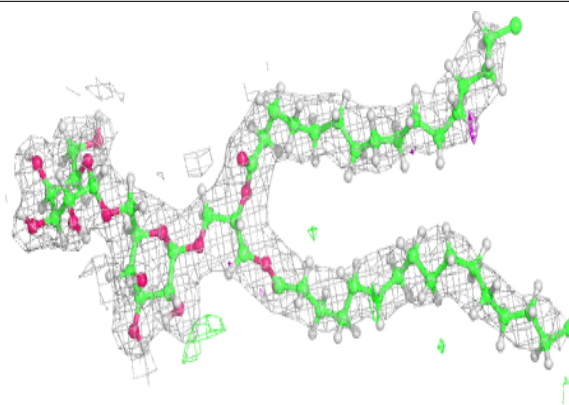
**Electron density around CLA d 403:**

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

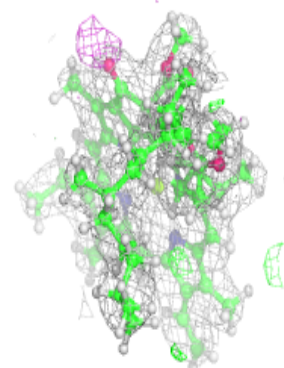
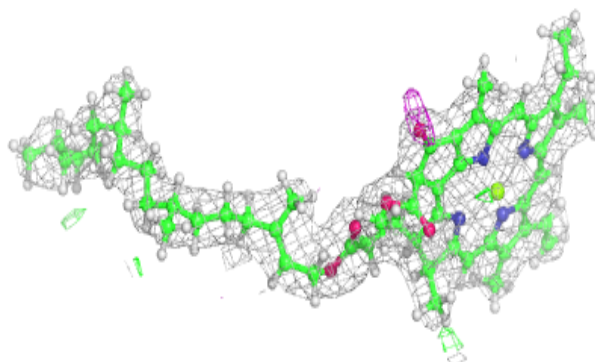
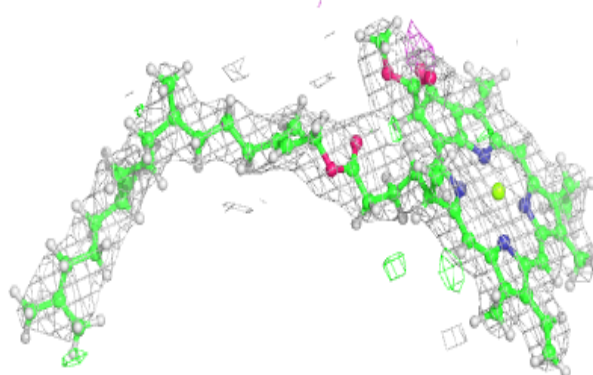


Electron density around DGD C 517:

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

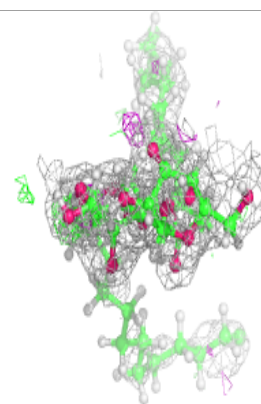
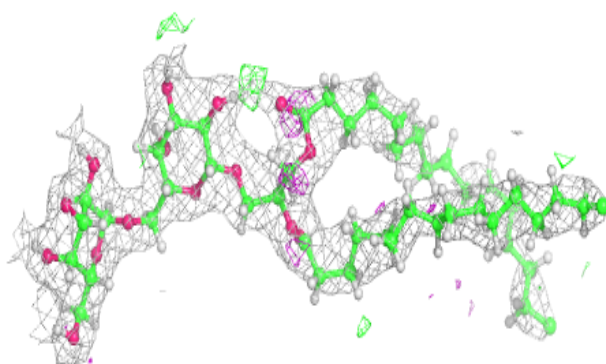
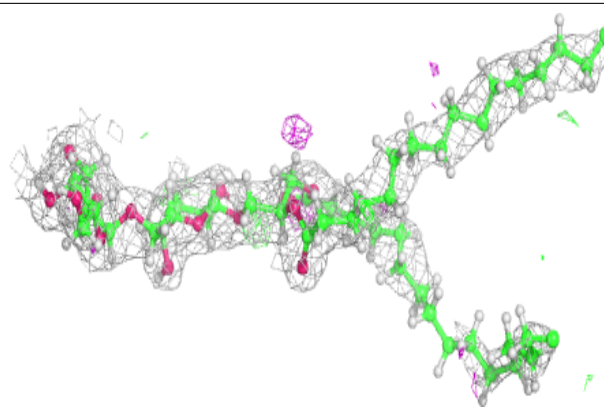
**Electron density around CLA A 402:**

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

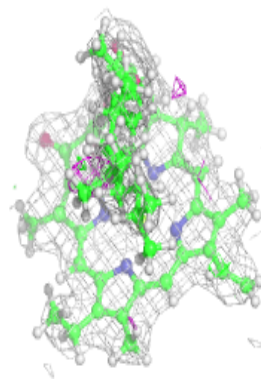
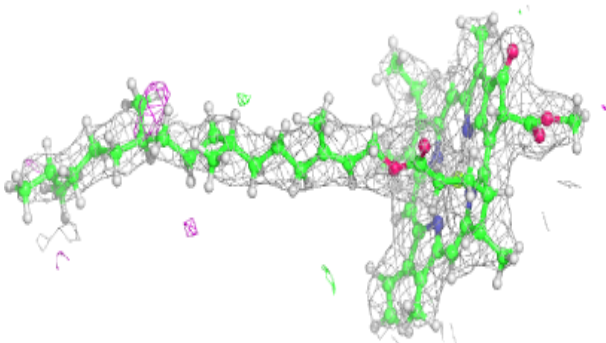
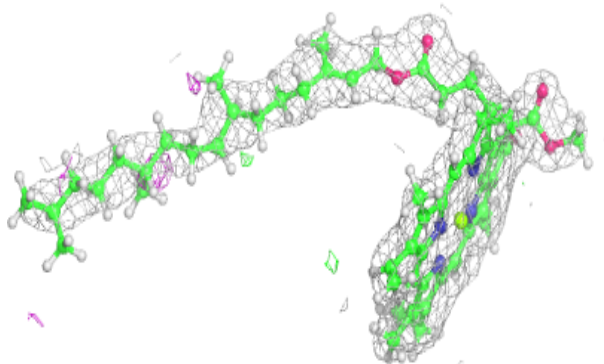


Electron density around DGD c 516:

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

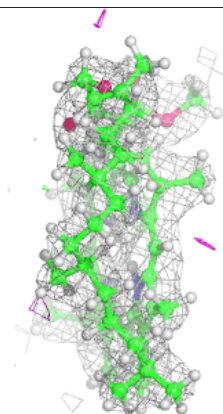
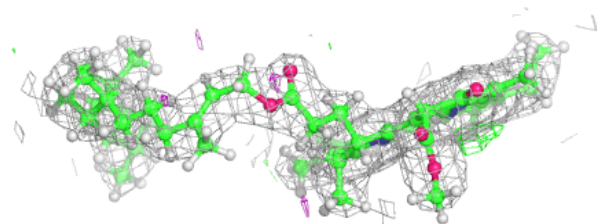
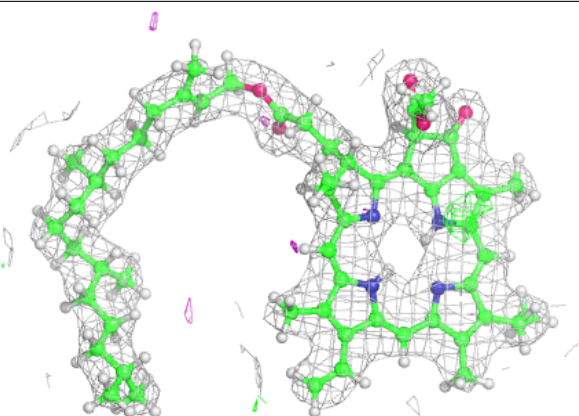
**Electron density around CLA b 607:**

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



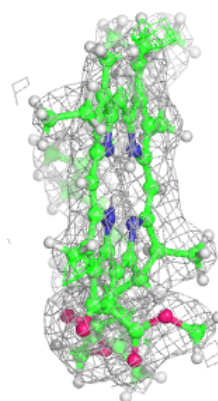
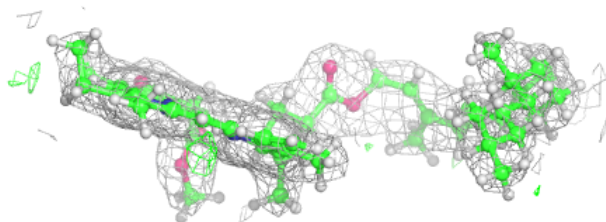
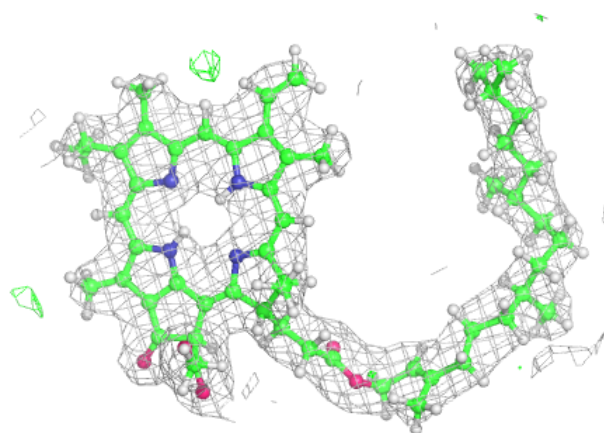
Electron density around PHO A 404:

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



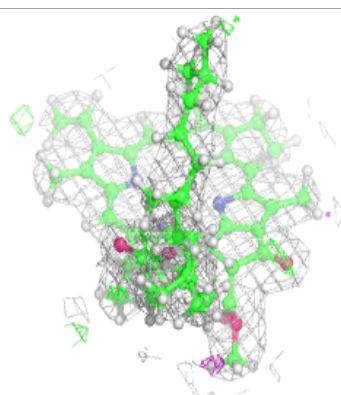
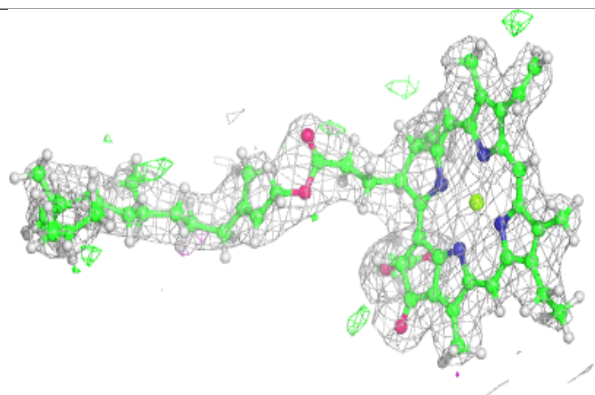
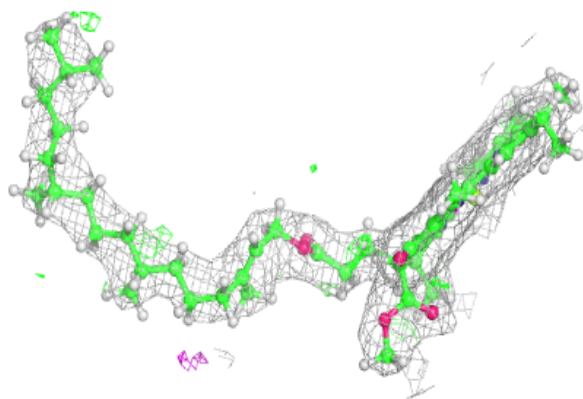
Electron density around PHO a 404:

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

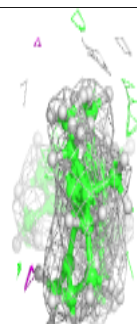
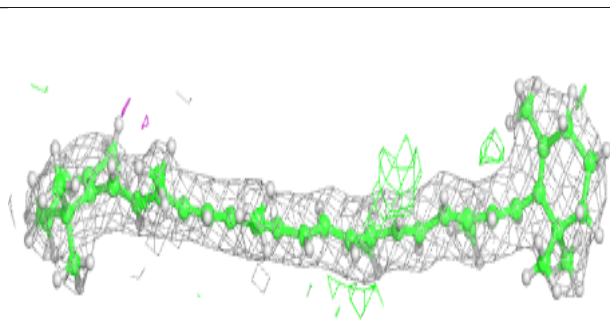
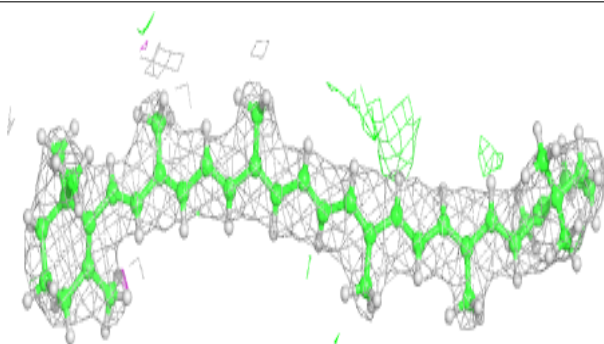


Electron density around CLA D 402:

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

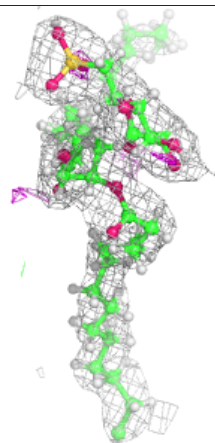
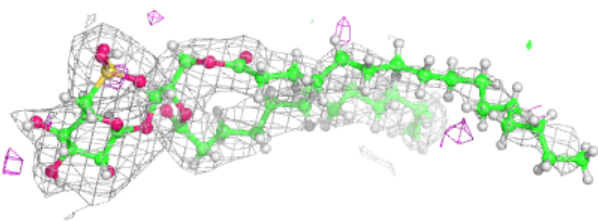
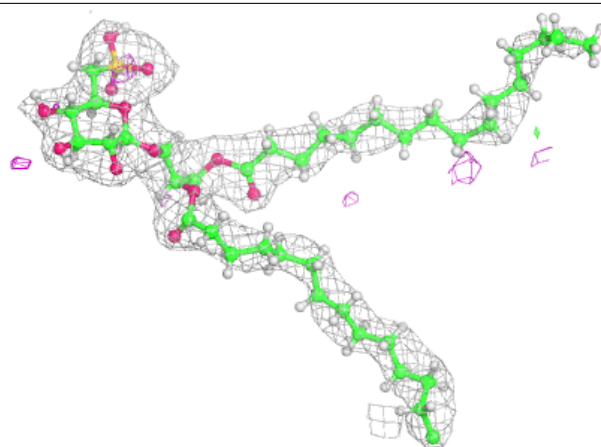
**Electron density around BCR B 617:**

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

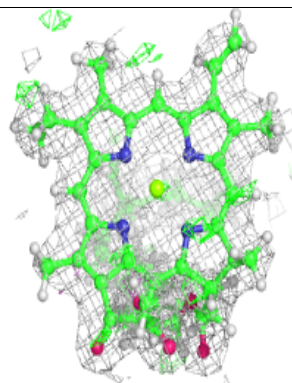
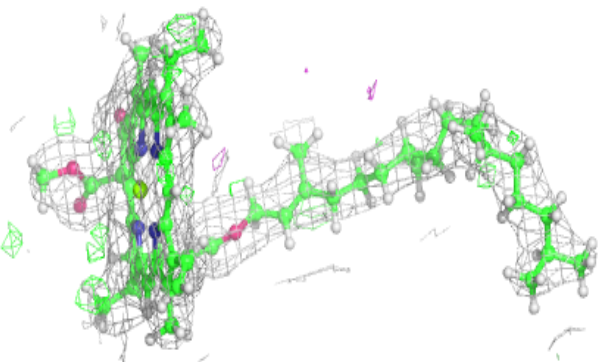
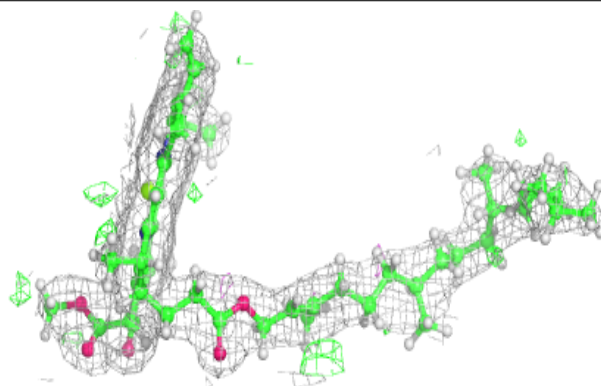


Electron density around SQD A 412:

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

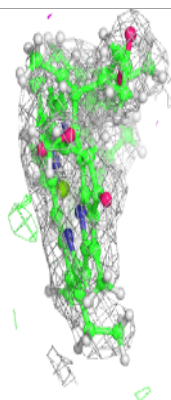
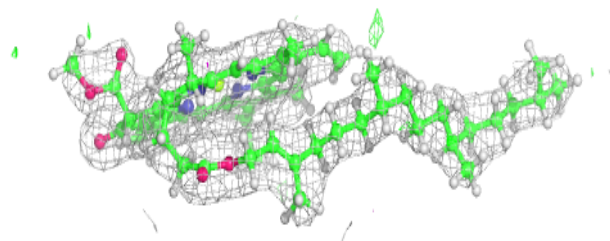
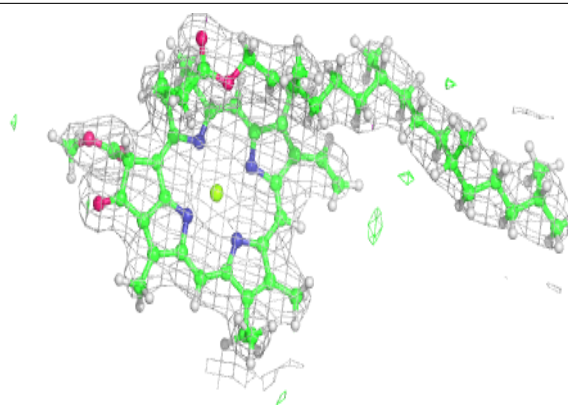
**Electron density around CLA B 605:**

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

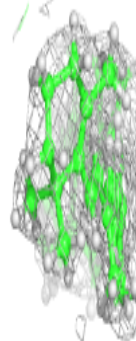
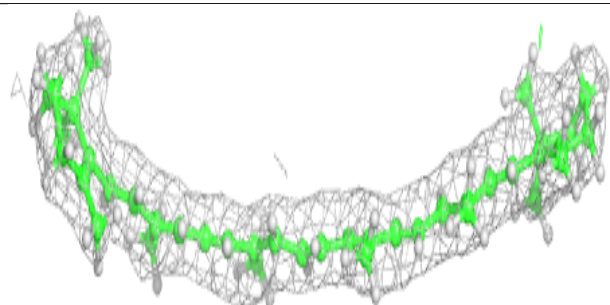
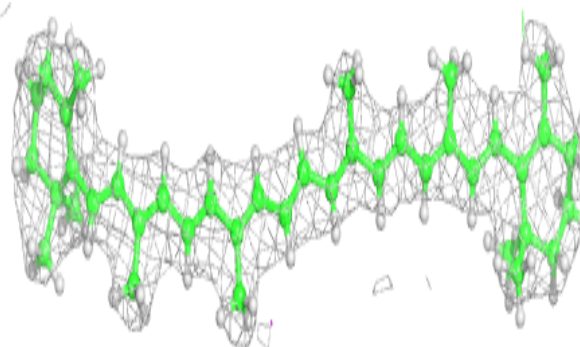


Electron density around CLA C 501:

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

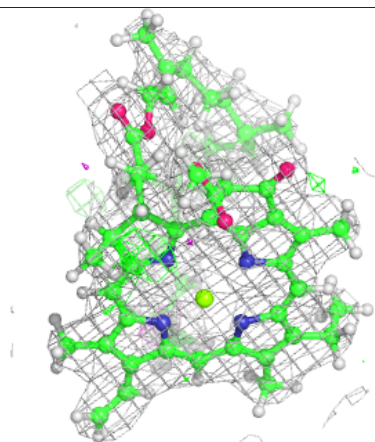
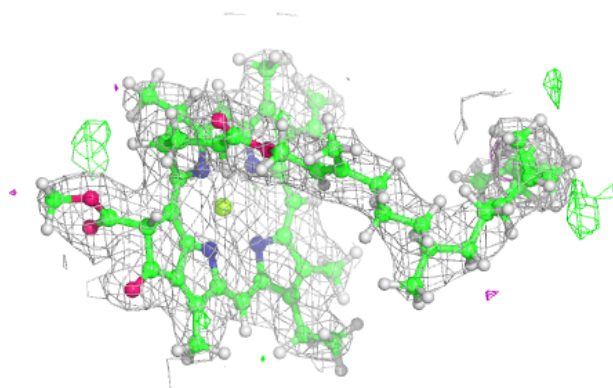
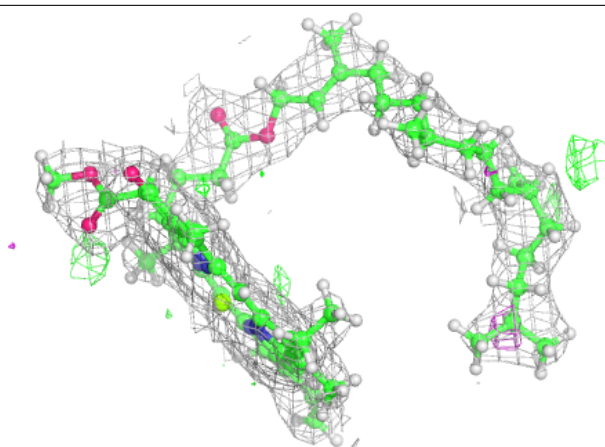
**Electron density around BCR t 101:**

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



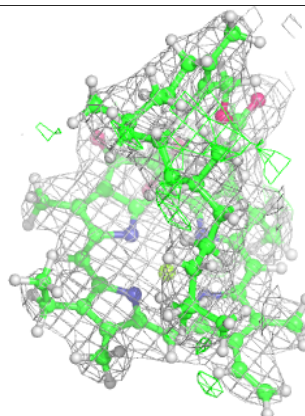
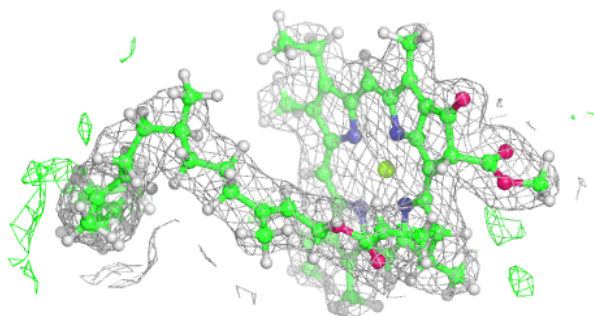
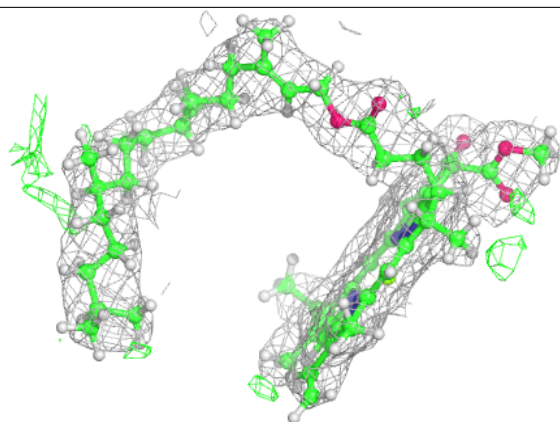
Electron density around CLA b 611:

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



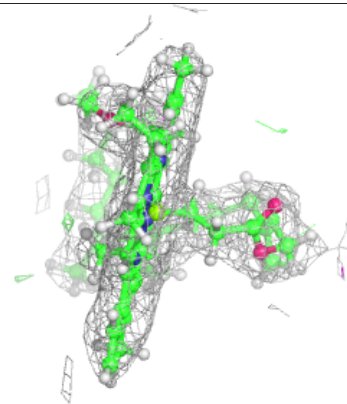
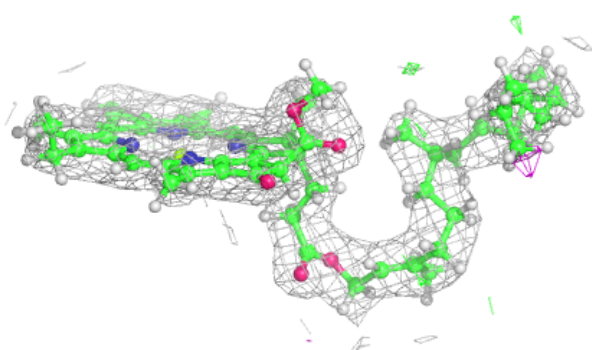
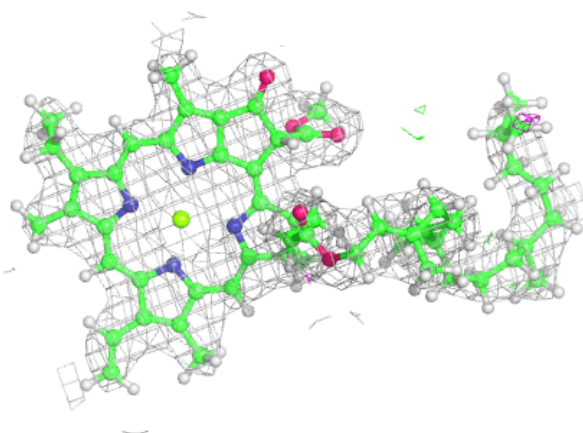
Electron density around CLA B 611:

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

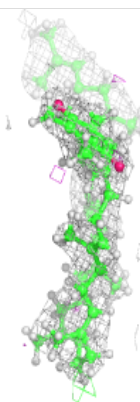
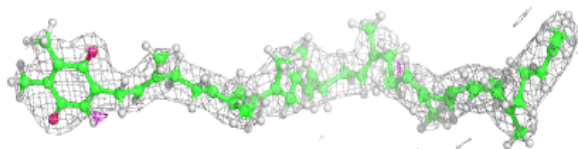
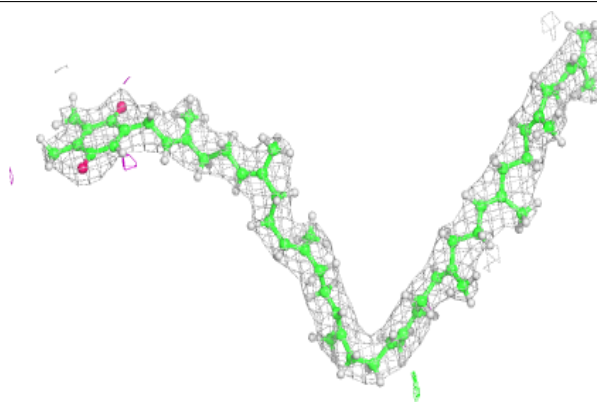


Electron density around CLA B 612:

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

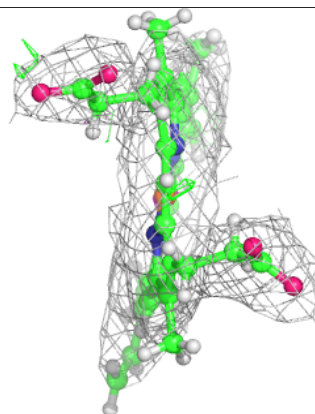
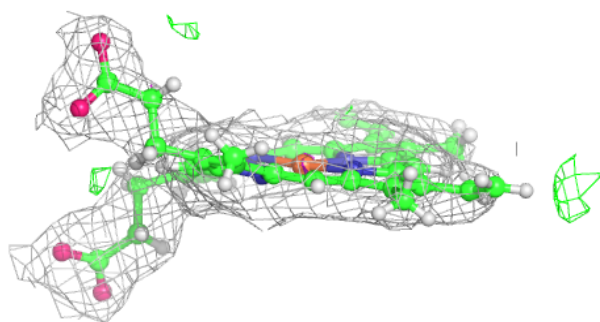
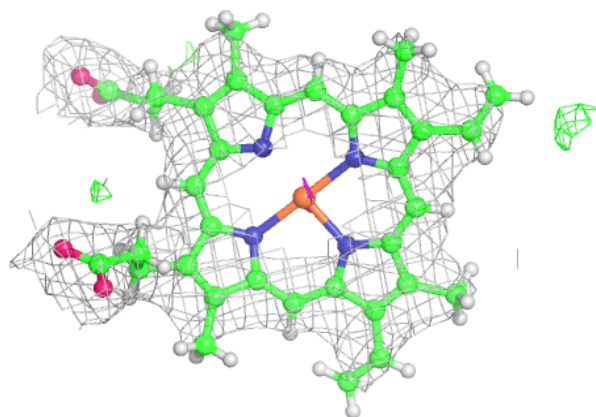
**Electron density around PL9 d 407:**

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



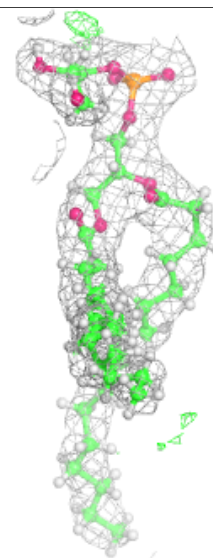
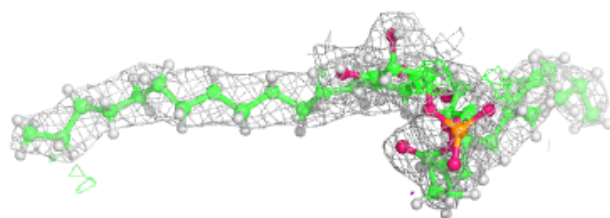
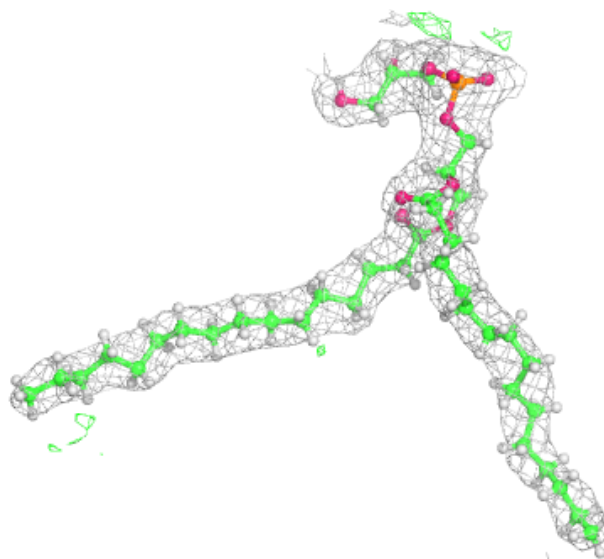
Electron density around HEM F 101:

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



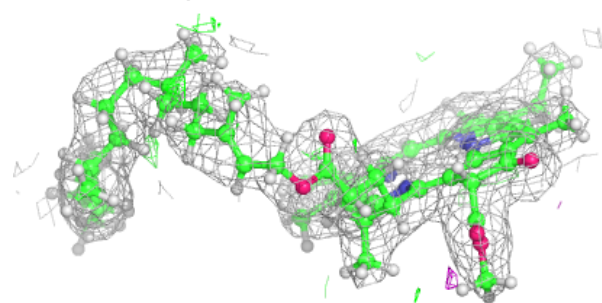
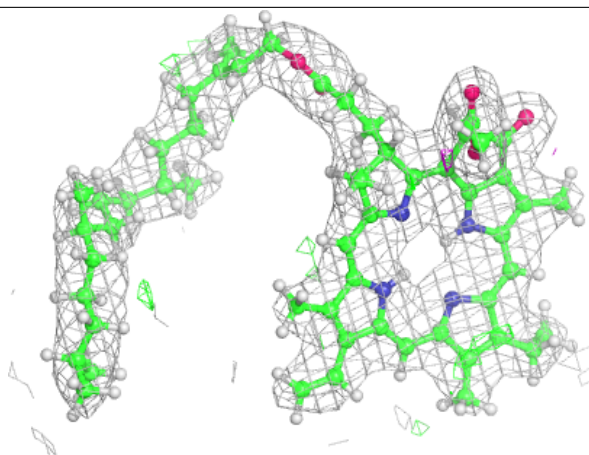
Electron density around LHG 1 101:

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



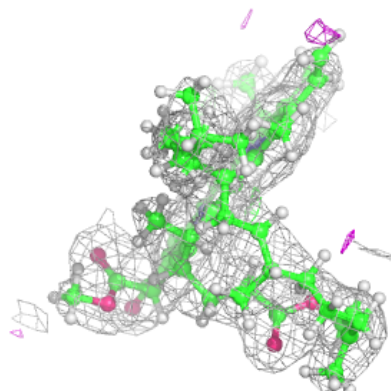
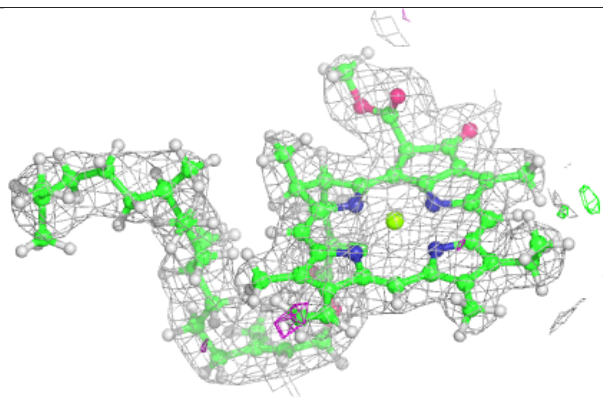
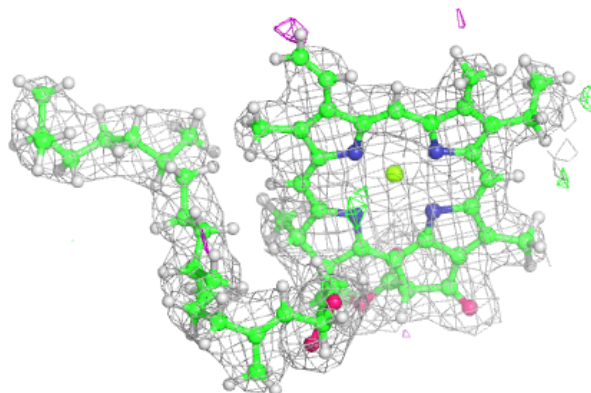
Electron density around PHO A 405:

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

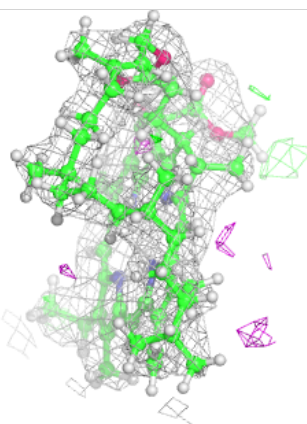
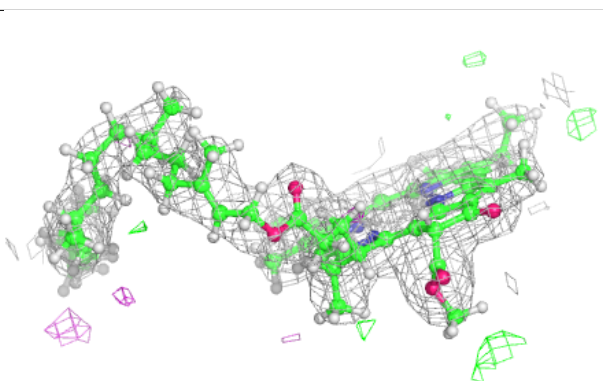
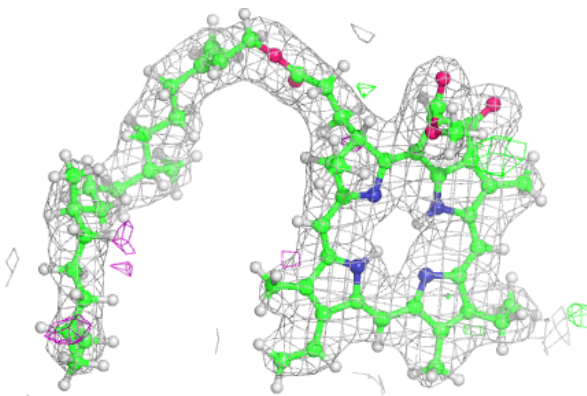


Electron density around CLA D 403:

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

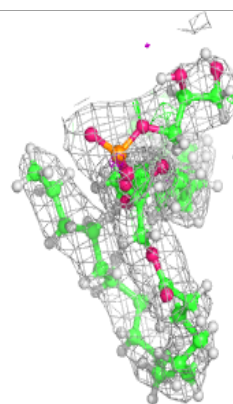
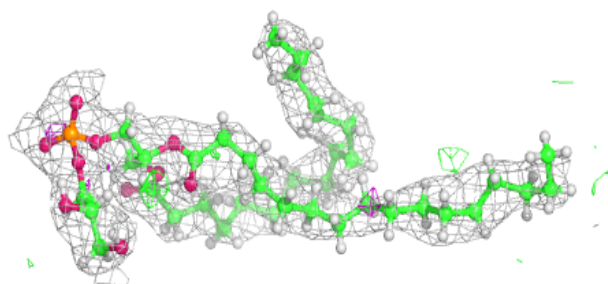
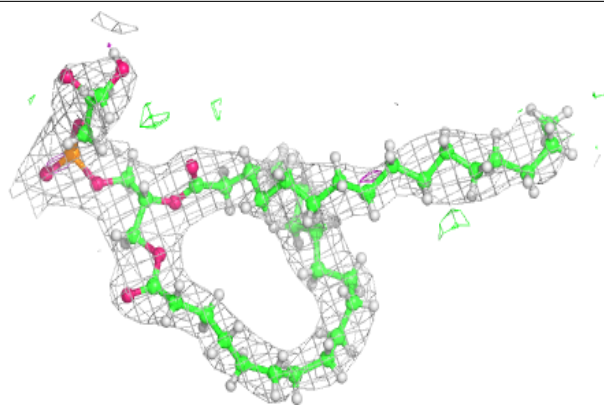
**Electron density around PHO d 401:**

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



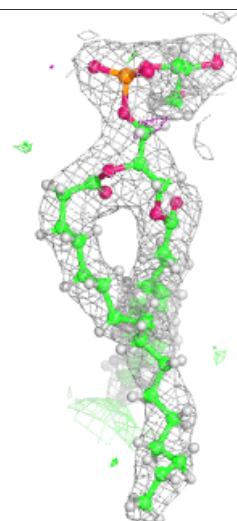
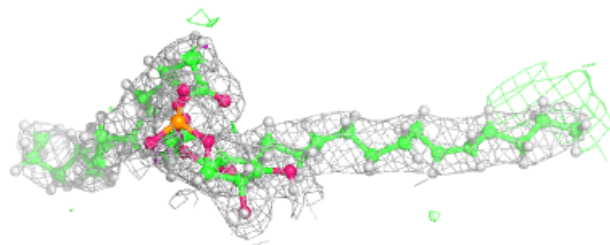
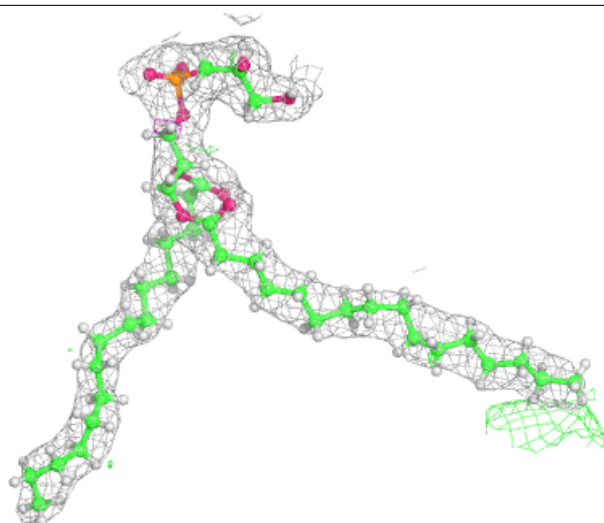
Electron density around LHG D 411:

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



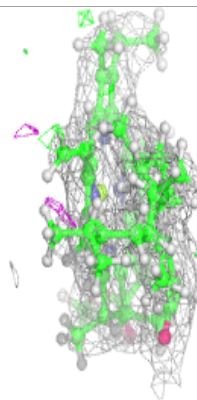
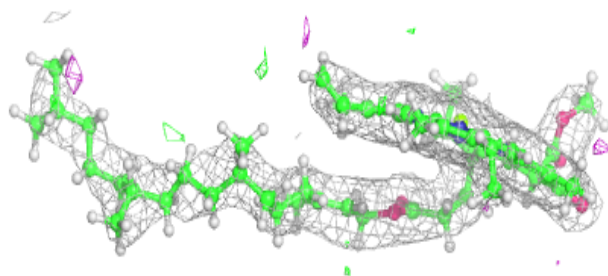
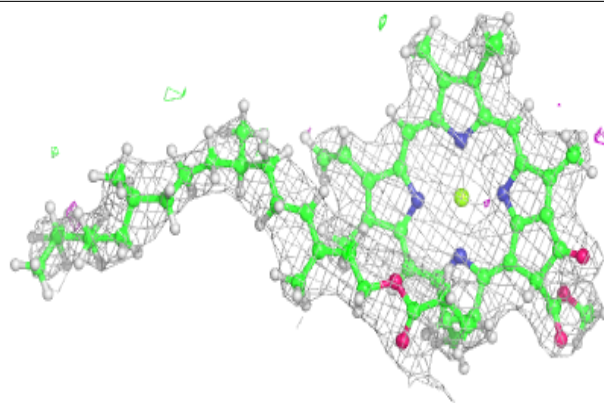
Electron density around LHG L 101:

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

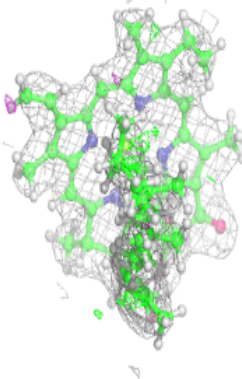
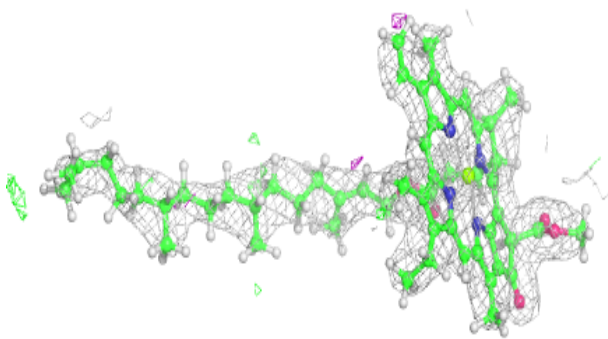
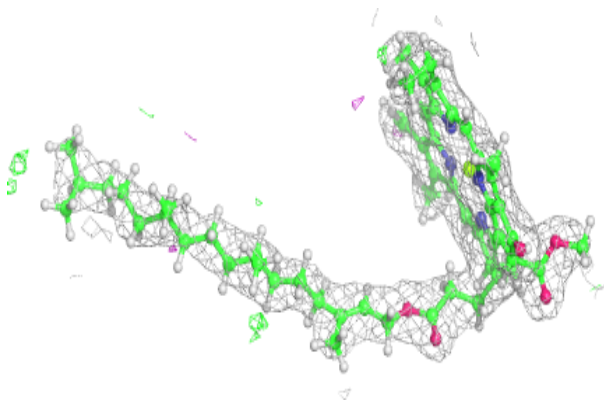


Electron density around CLA b 603:

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

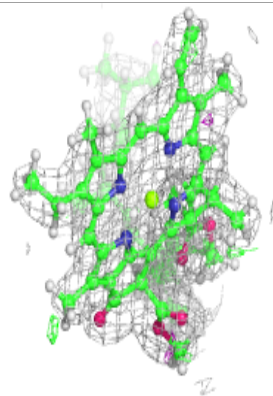
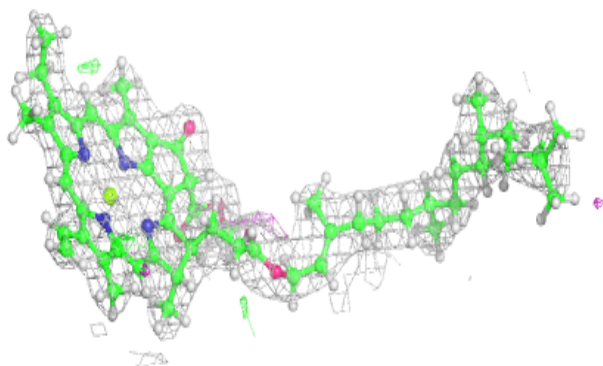
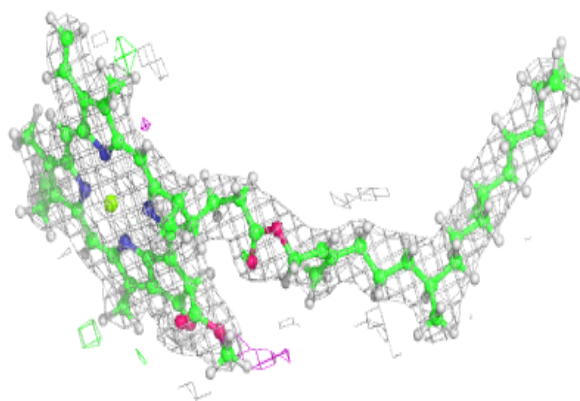
**Electron density around CLA B 607:**

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



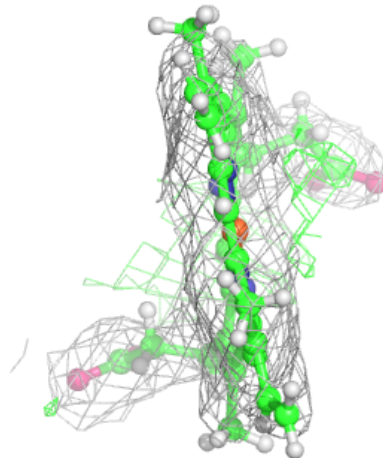
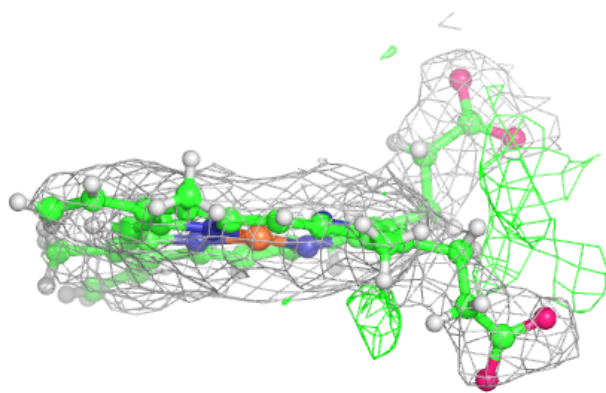
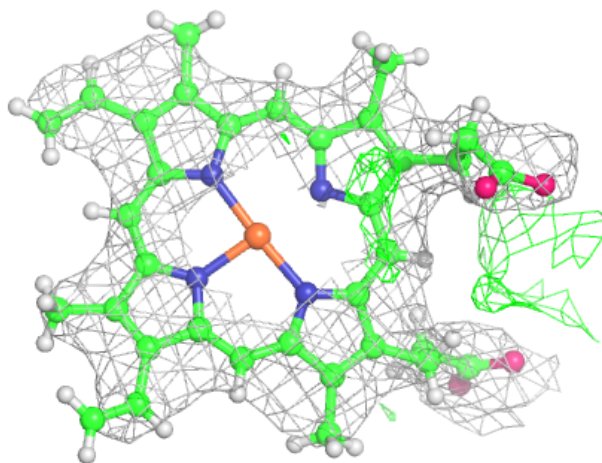
Electron density around CLA a 402:

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



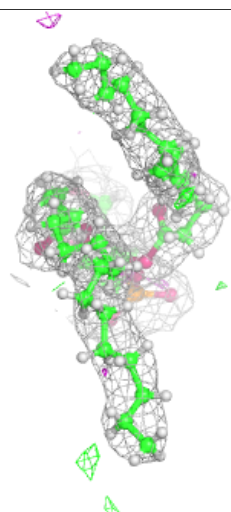
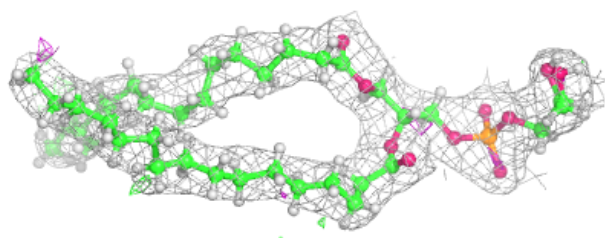
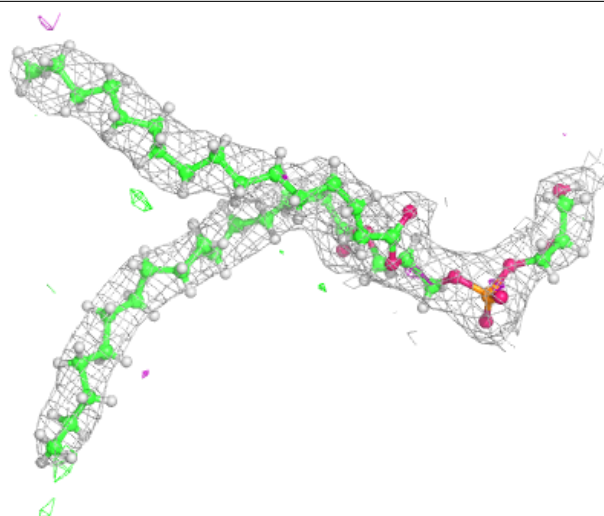
Electron density around HEM f 101:

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



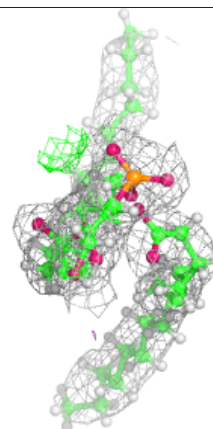
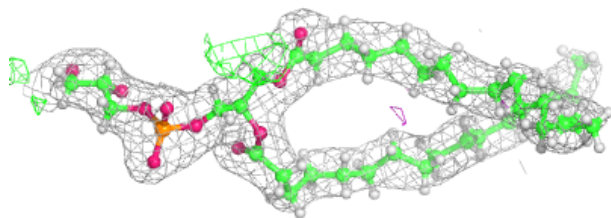
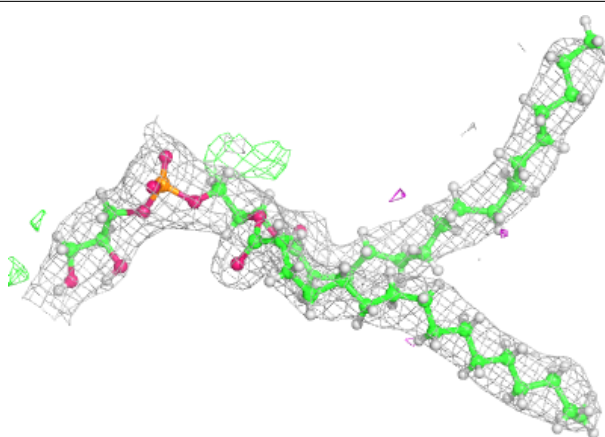
Electron density around LHG D 408:

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



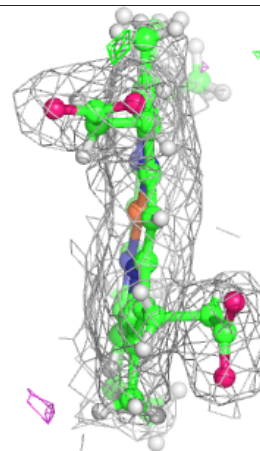
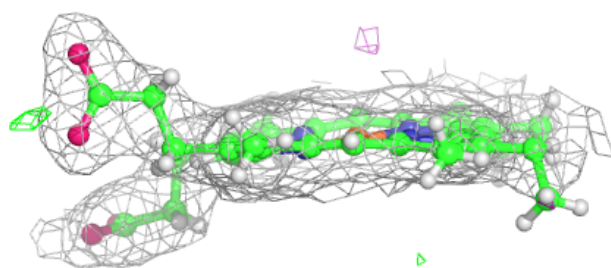
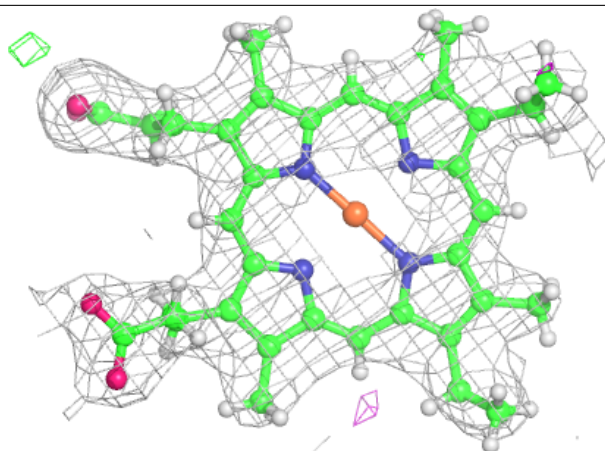
Electron density around LHG d 408:

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



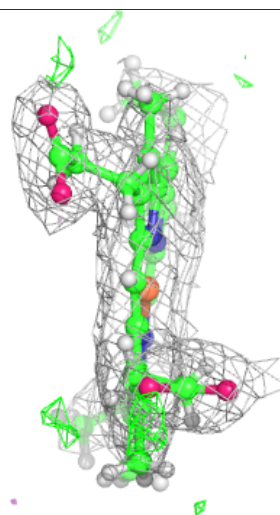
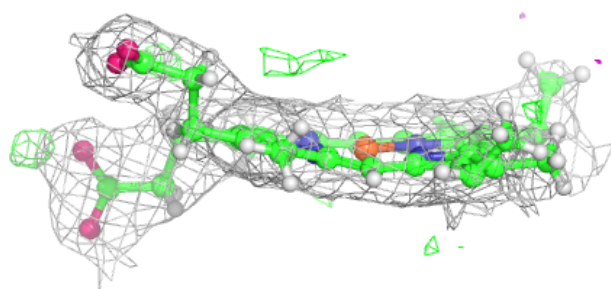
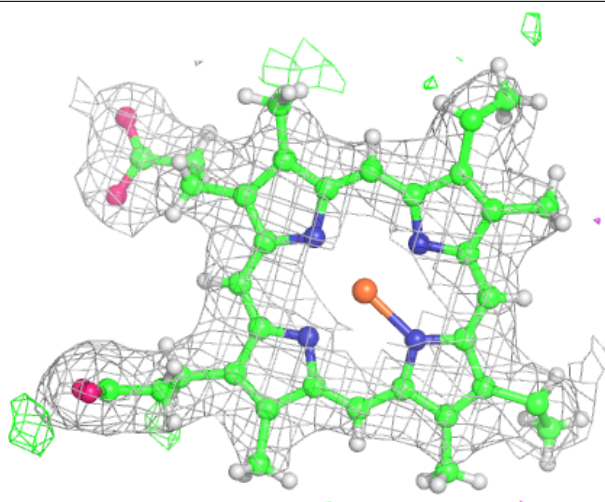
Electron density around HEC V 201:

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



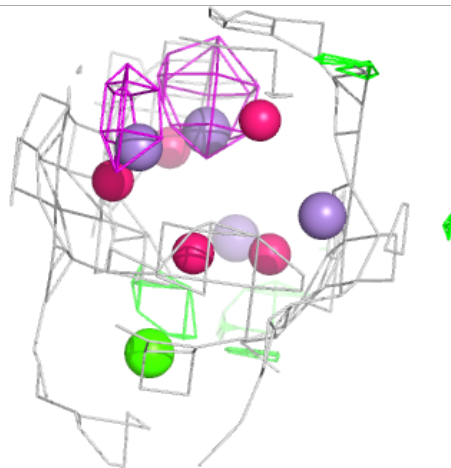
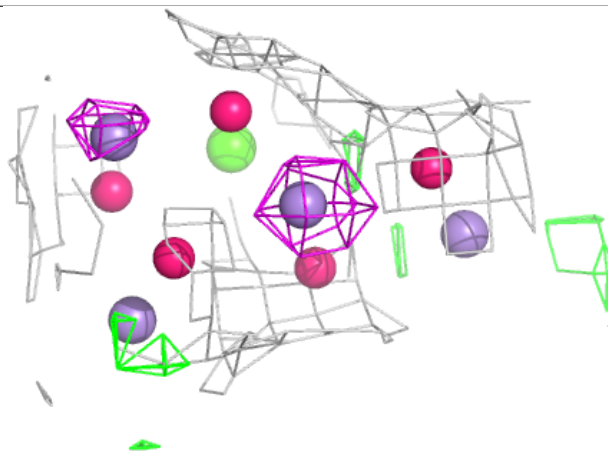
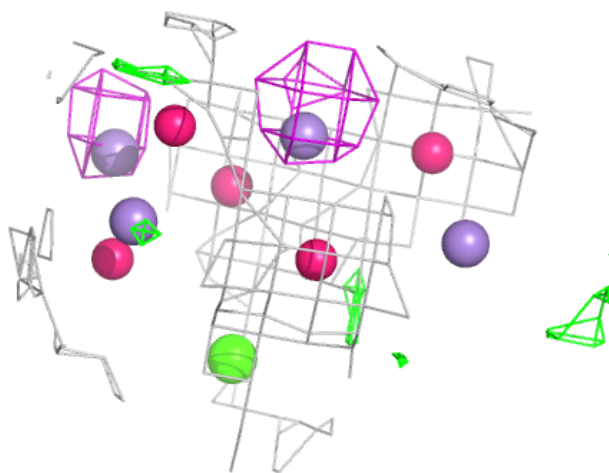
Electron density around HEC v 201:

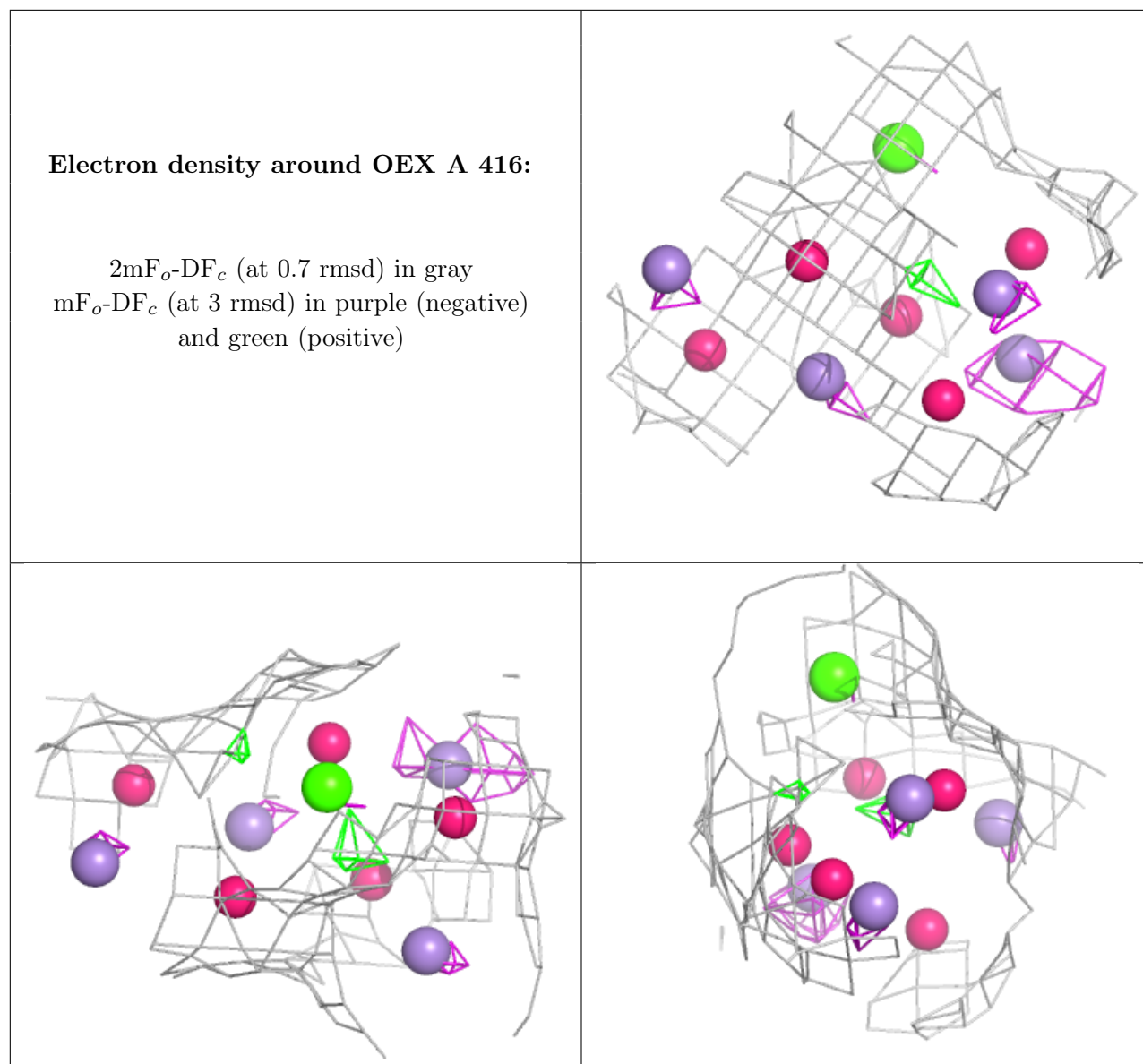
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 416:

$2mF_o-DF_c$ (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.