



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2021 – 04:44 PM EDT

PDB ID : 7RF5
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.23 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

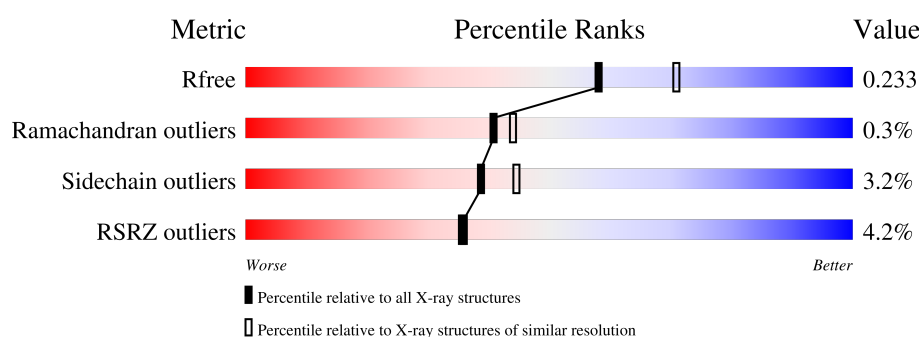
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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.



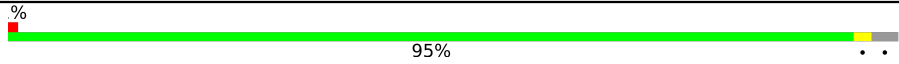
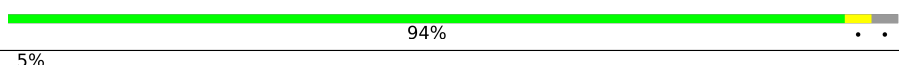
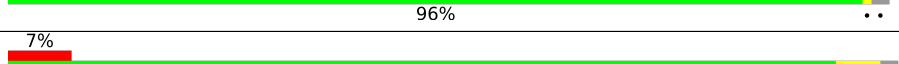
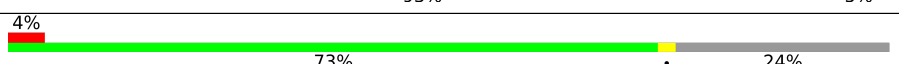

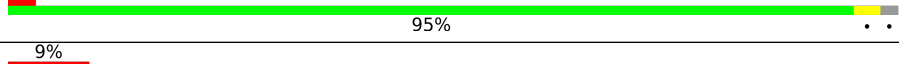
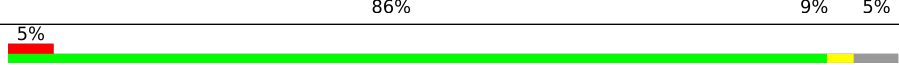
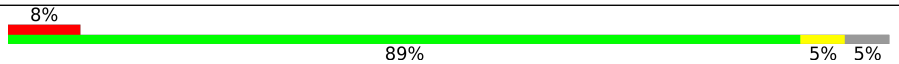


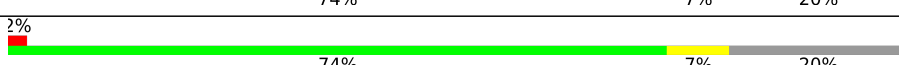
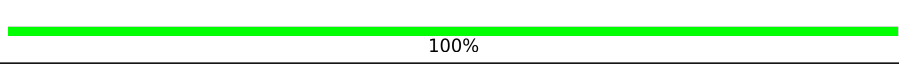
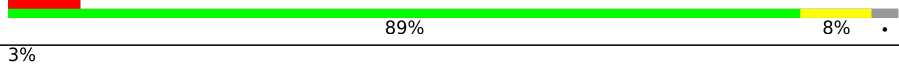


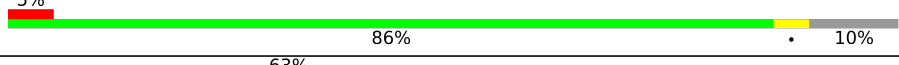

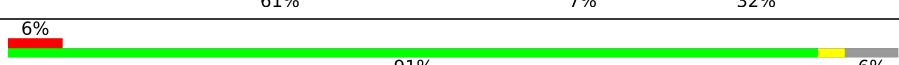
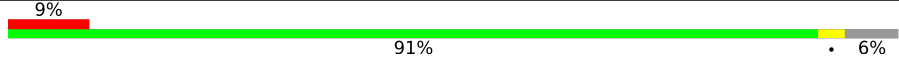
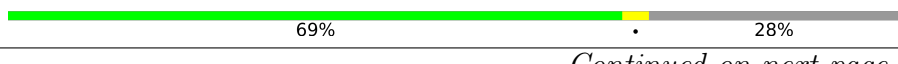



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	612	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	H	101	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	613	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
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24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105562 atoms, of which 52760 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

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

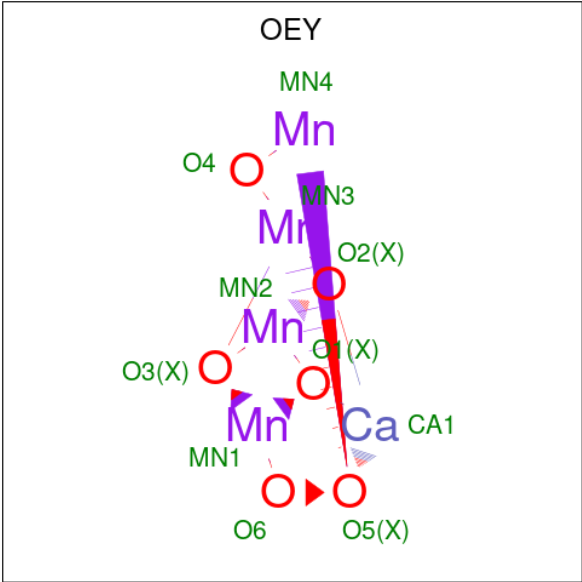
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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

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

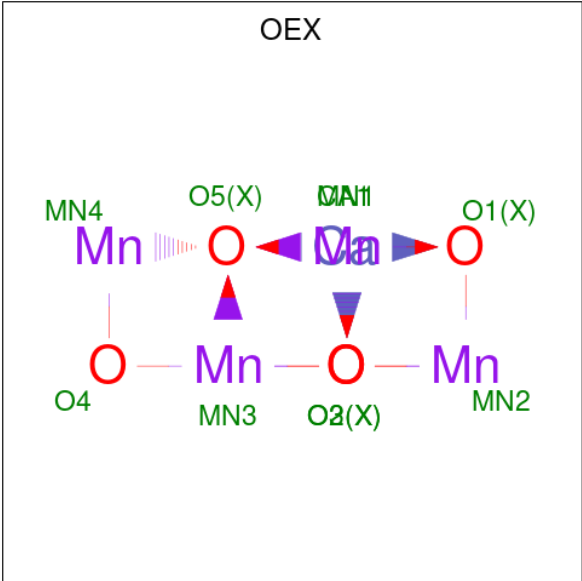
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 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
			Total	Ca	Mn	O		
22	A	1	10	1	4	5	0	1

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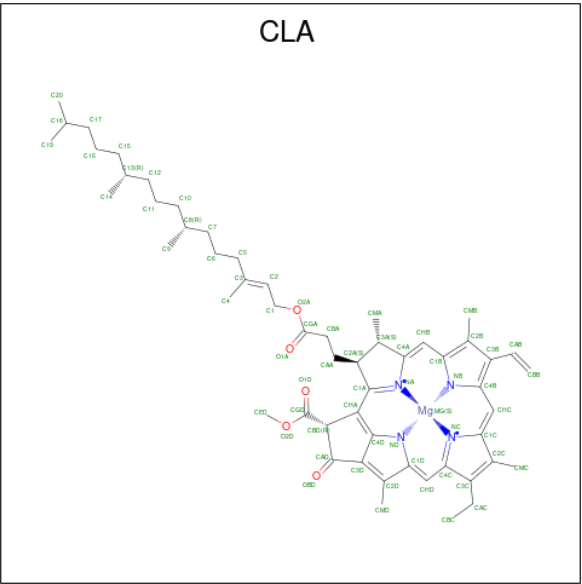
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	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
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	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
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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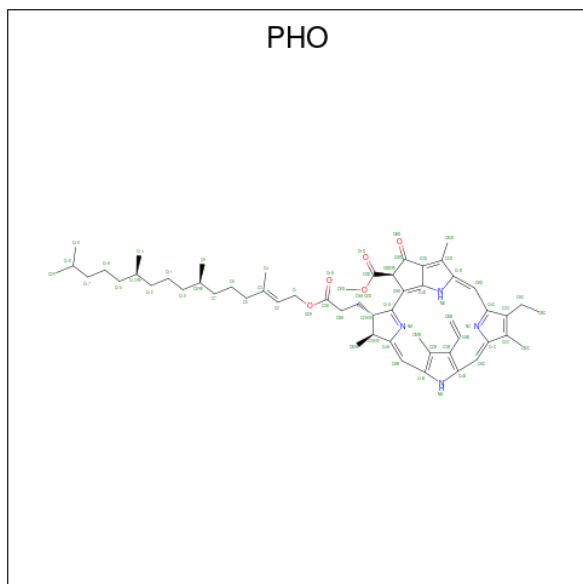
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72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

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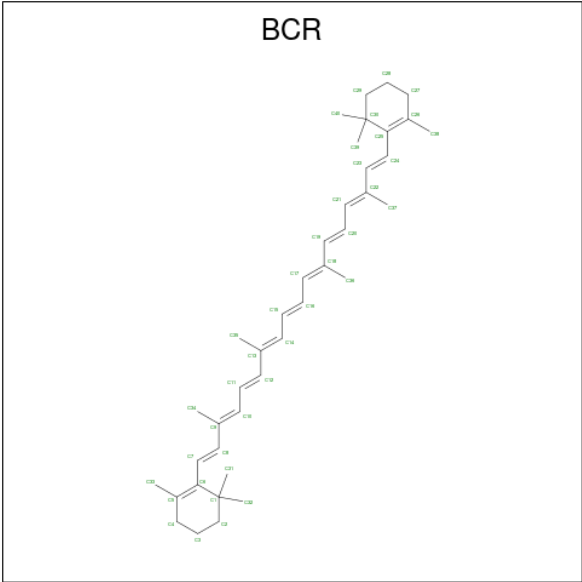
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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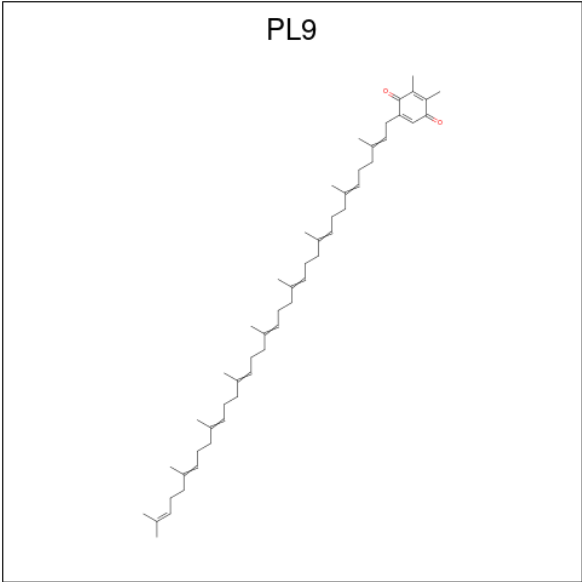
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40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

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

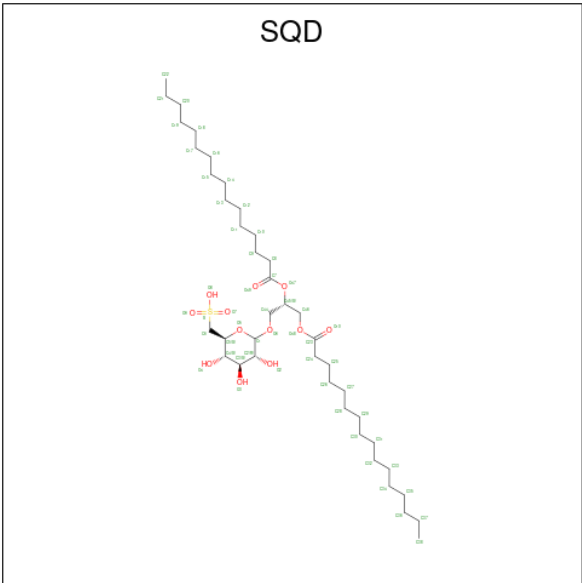
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- Molecule 28 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).



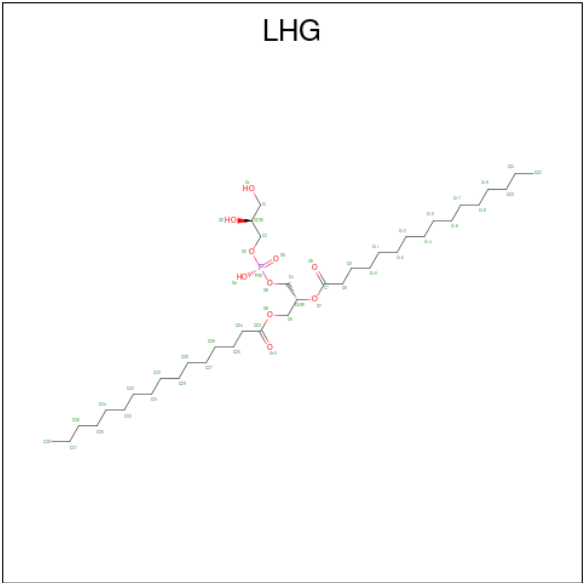
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



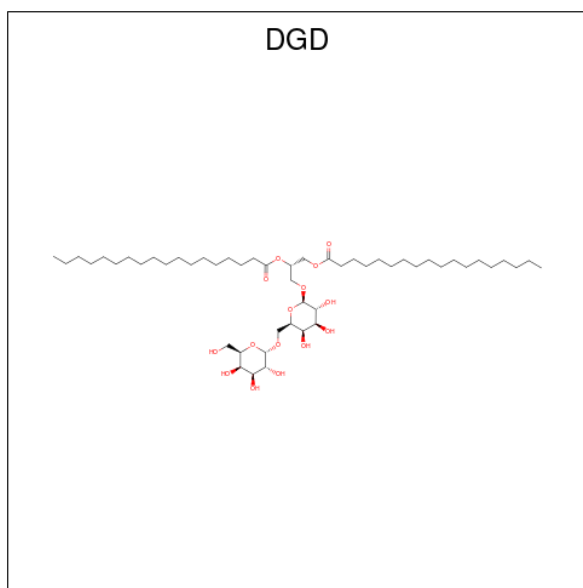
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



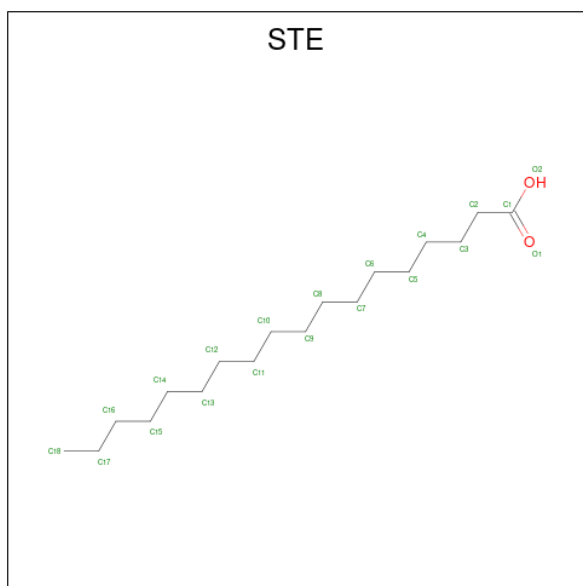
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	h	1	Total	C	H	O	0	0
			144	47	82	15		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			53	18	35			
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H		0	0
			41	15	26			

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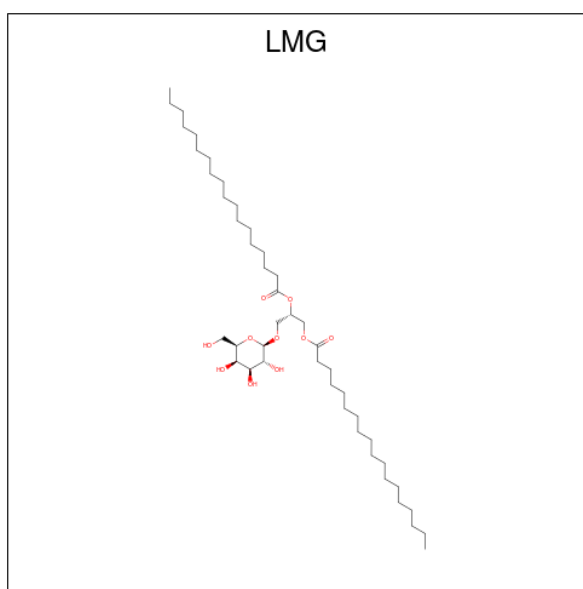
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	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	R	1	Total C H O 28 10 16 2	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	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 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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			55	18	35	2		
32	c	1	Total	C	H	O	0	0
			28	10	16	2		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	h	1	Total	C	H		0	0
			41	14	27			
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



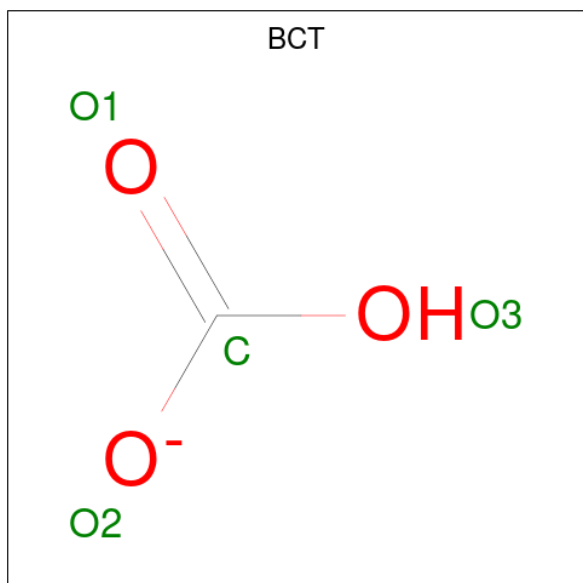
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			122	41	71	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		

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

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



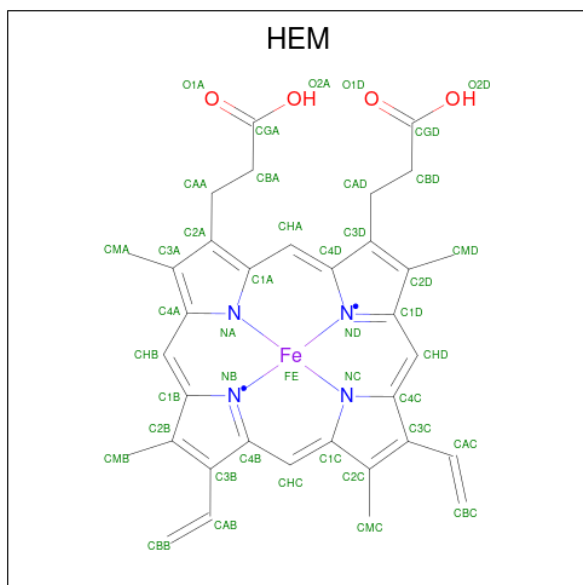
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		

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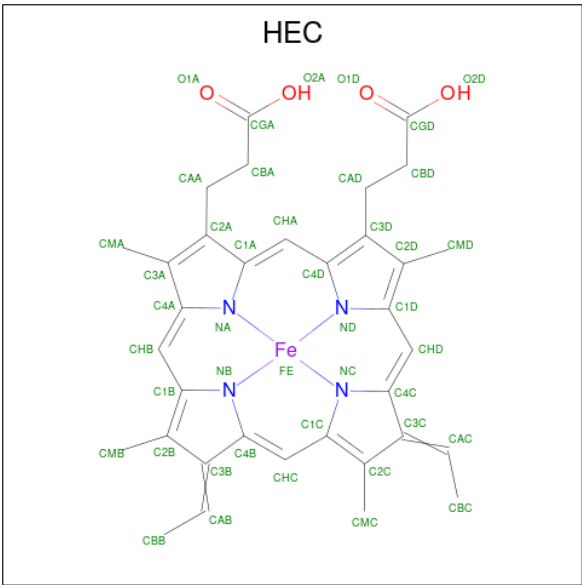
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 36 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	118	Total	O	0	0
			118	118		
37	B	141	Total	O	0	0
			141	141		
37	C	114	Total	O	0	0
			114	114		
37	D	100	Total	O	0	0
			100	100		
37	E	20	Total	O	0	0
			20	20		
37	F	3	Total	O	0	0
			3	3		
37	H	29	Total	O	0	0
			29	29		
37	I	7	Total	O	0	0
			7	7		
37	J	6	Total	O	0	0
			6	6		
37	K	6	Total	O	0	0
			6	6		

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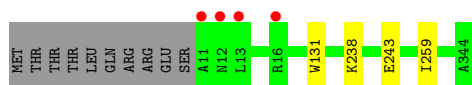
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	10	Total 10	O 10	0	0
37	M	5	Total 5	O 5	0	0
37	O	71	Total 71	O 71	0	0
37	R	1	Total 1	O 1	0	0
37	T	5	Total 5	O 5	0	0
37	U	33	Total 33	O 33	0	0
37	V	49	Total 49	O 49	0	0
37	X	7	Total 7	O 7	0	0
37	Y	4	Total 4	O 4	0	0
37	Z	2	Total 2	O 2	0	0
37	a	117	Total 117	O 117	0	0
37	b	131	Total 131	O 131	0	0
37	c	118	Total 118	O 118	0	0
37	d	100	Total 100	O 100	0	0
37	e	10	Total 10	O 10	0	0
37	f	2	Total 2	O 2	0	0
37	h	19	Total 19	O 19	0	0
37	i	8	Total 8	O 8	0	0
37	j	11	Total 11	O 11	0	0
37	k	4	Total 4	O 4	0	0
37	l	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	5	Total 5	O 5	0	0
37	o	65	Total 65	O 65	0	0
37	r	1	Total 1	O 1	0	0
37	t	5	Total 5	O 5	0	0
37	u	41	Total 41	O 41	0	0
37	v	36	Total 36	O 36	0	0
37	x	8	Total 8	O 8	0	0
37	y	1	Total 1	O 1	0	0
37	z	2	Total 2	O 2	0	0

- Molecule 1: Photosystem II protein D1 1



- Chain a: 94% . .



- Chain B:  97%



- Chain b:  3% 97%



- Chain C:  94% 2% . .



- 



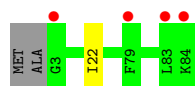
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



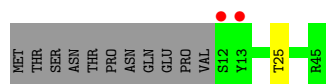
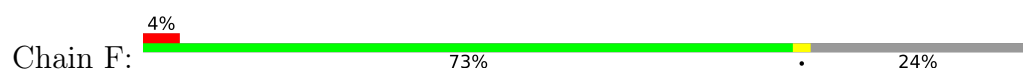
- Molecule 5: Cytochrome b559 subunit alpha



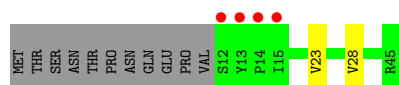
- Molecule 5: Cytochrome b559 subunit alpha



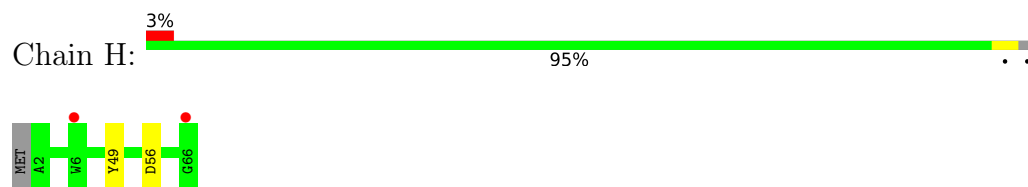
- Molecule 6: Cytochrome b559 subunit beta



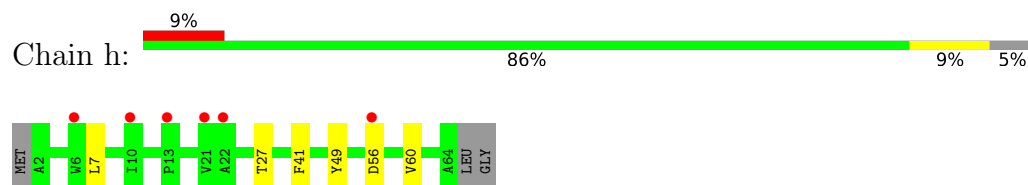
- Molecule 6: Cytochrome b559 subunit beta



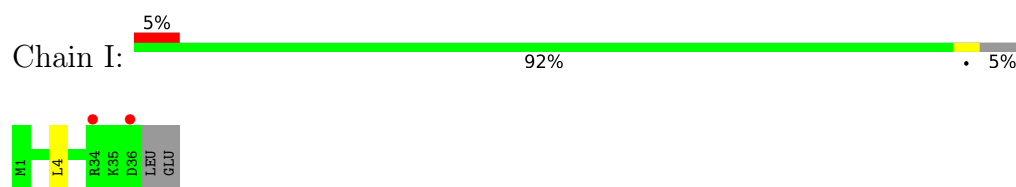
- Molecule 7: Photosystem II reaction center protein H



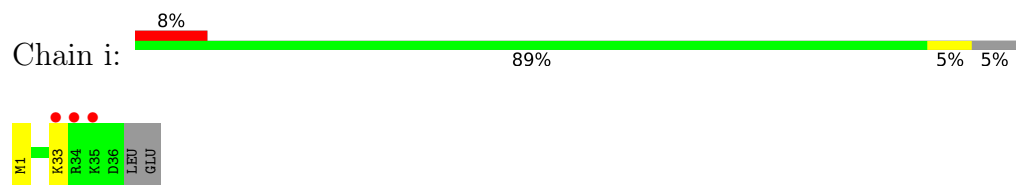
- Molecule 7: Photosystem II reaction center protein H



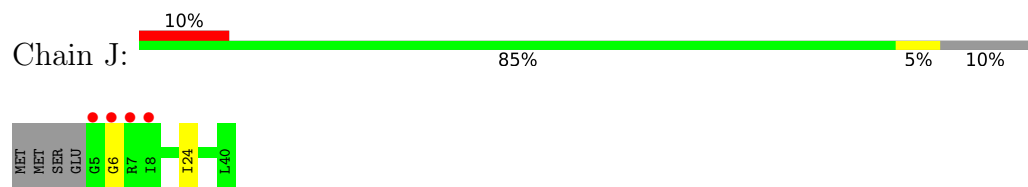
- Molecule 8: Photosystem II reaction center protein I



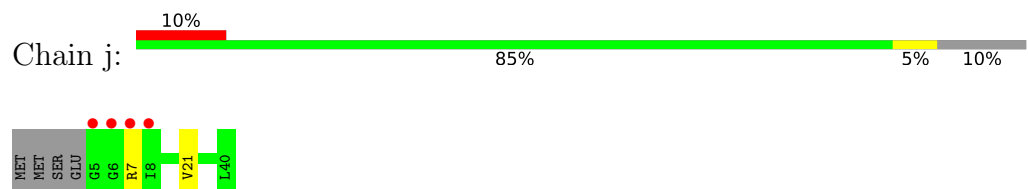
- Molecule 8: Photosystem II reaction center protein I



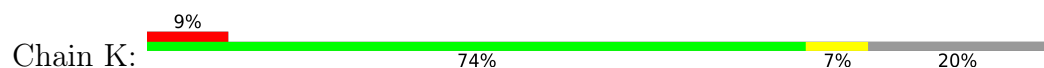
- Molecule 9: Photosystem II reaction center protein J

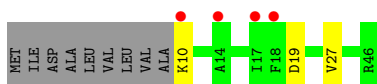


- Molecule 9: Photosystem II reaction center protein J

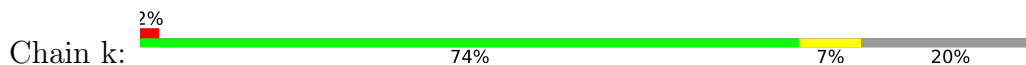


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

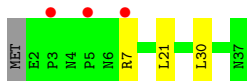
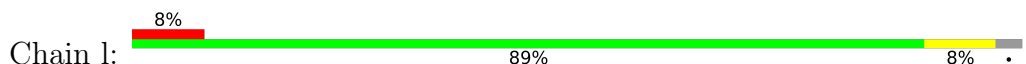


- Molecule 11: Photosystem II reaction center protein L

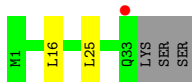
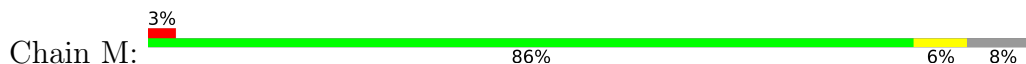


There are no outlier residues recorded for this chain.

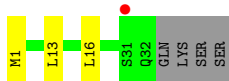
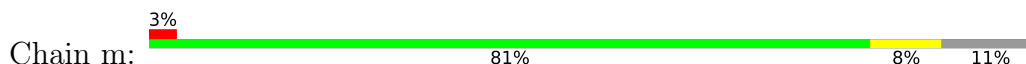
- Molecule 11: Photosystem II reaction center protein L



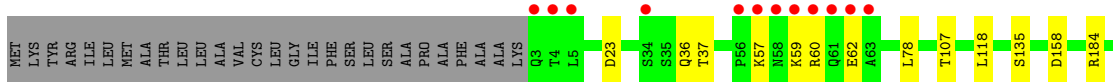
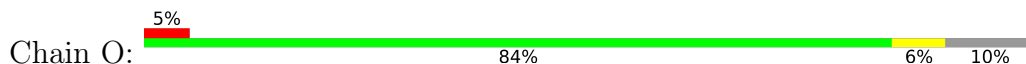
- Molecule 12: Photosystem II reaction center protein M



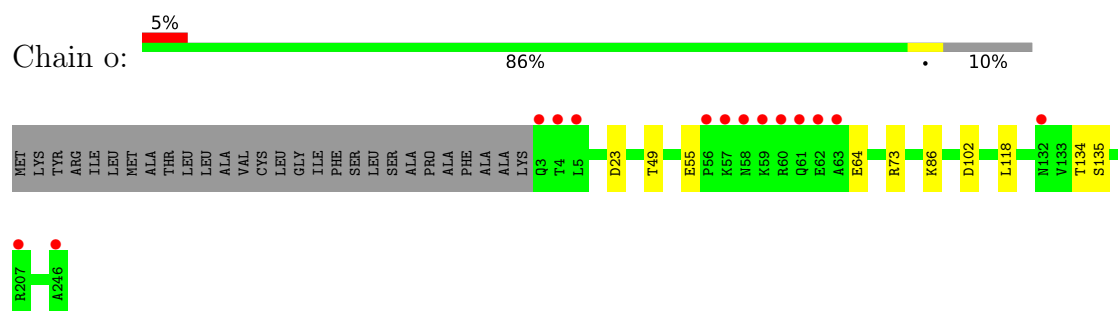
- Molecule 12: Photosystem II reaction center protein M



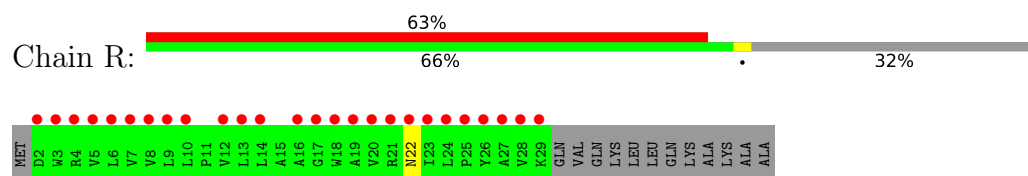
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



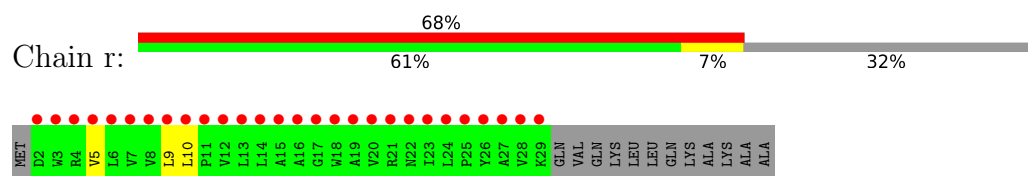
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



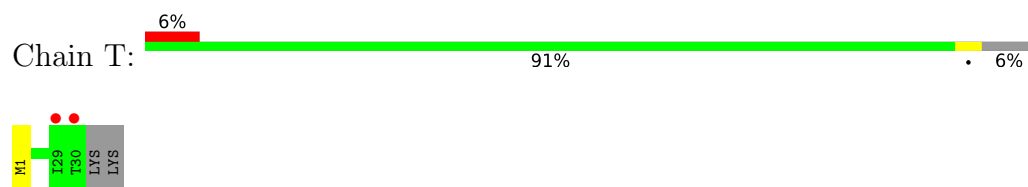
- Molecule 14: Photosystem II protein Y



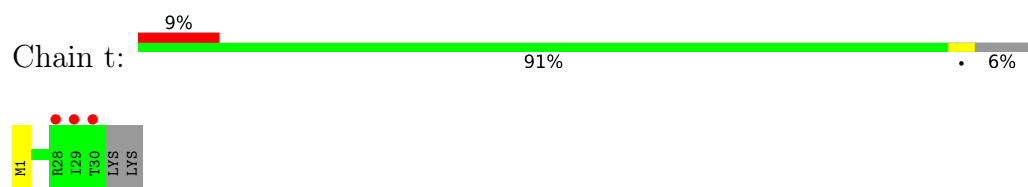
- Molecule 14: Photosystem II protein Y



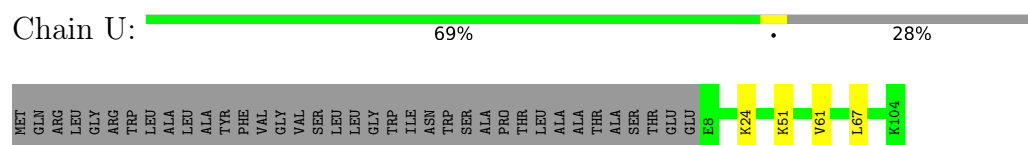
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

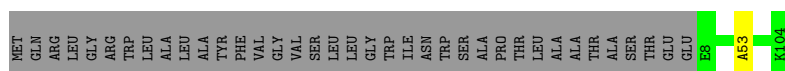


- Molecule 16: Photosystem II 12 kDa extrinsic protein



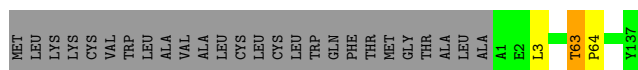
- Molecule 16: Photosystem II 12 kDa extrinsic protein





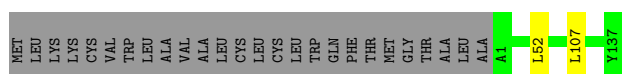
- Molecule 17: Cytochrome c-550

Chain V: 82% 16%



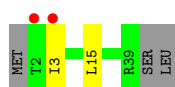
- Molecule 17: Cytochrome c-550

Chain v: 83% 16%



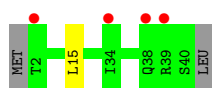
- Molecule 18: Photosystem II reaction center X protein

Chain X: 5% 88% 5% 7%



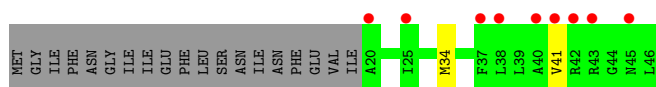
- Molecule 18: Photosystem II reaction center X protein

Chain x: 10% 93% 5%



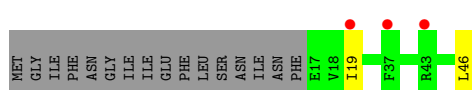
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 20% 54% 41%



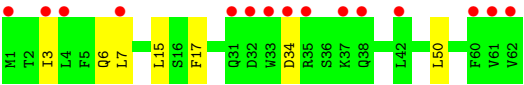
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 7% 61% 35%

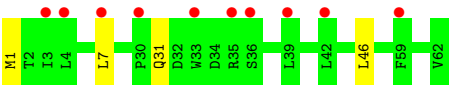
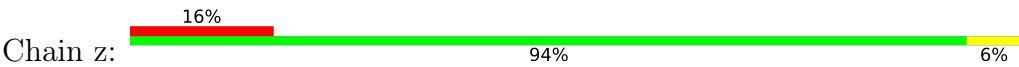


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 24% 89% 11%



● 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	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.1 (33.70-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.233 0.176 , 0.233	Depositor DCC
R_{free} test set	3445 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105562	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.58	0/3227	0.67	1/4397 (0.0%)
1	a	0.59	0/3224	0.65	0/4393
2	B	0.63	0/4161	0.68	1/5669 (0.0%)
2	b	0.59	0/4118	0.68	1/5611 (0.0%)
3	C	0.61	0/3647	0.67	2/4965 (0.0%)
3	c	0.58	0/3719	0.65	0/5061
4	D	0.66	0/2825	0.69	0/3847
4	d	0.61	0/2834	0.69	1/3859 (0.0%)
5	E	0.54	0/688	0.60	0/940
5	e	0.50	0/683	0.62	0/932
6	F	0.45	0/284	0.59	0/387
6	f	0.50	0/284	0.63	0/387
7	H	0.61	0/523	0.65	0/713
7	h	0.56	0/511	0.68	0/697
8	I	0.61	0/293	0.67	0/396
8	i	0.65	0/293	0.63	0/396
9	J	0.47	0/263	0.61	0/356
9	j	0.50	0/263	0.65	0/356
10	K	0.47	0/303	0.59	0/416
10	k	0.55	0/303	0.64	0/416
11	L	0.72	0/311	0.71	0/422
11	l	0.64	0/303	0.65	0/412
12	M	0.66	0/249	0.67	0/341
12	m	0.68	0/244	0.72	0/334
13	O	0.59	0/1904	0.74	1/2585 (0.0%)
13	o	0.61	0/1905	0.73	2/2583 (0.1%)
14	R	0.40	0/227	0.53	0/313
14	r	0.37	0/227	0.53	0/313
15	T	0.76	0/257	0.69	0/349
15	t	0.75	0/255	0.61	0/346
16	U	0.53	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.60	0/785	0.68	0/1064
17	V	0.59	0/1085	0.70	1/1473 (0.1%)
17	v	0.53	0/1085	0.65	0/1473
18	X	0.48	0/284	0.59	0/384
18	x	0.41	0/289	0.54	0/391
19	Y	0.45	0/197	0.61	0/264
19	y	0.38	0/219	0.59	0/294
20	Z	0.43	0/490	0.52	0/669
20	z	0.42	0/488	0.52	0/666
All	All	0.59	0/44035	0.67	10/59934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	102	ASP	CB-CG-OD1	7.12	124.71	118.30
2	B	380	ASP	CB-CG-OD1	6.06	123.76	118.30
2	b	98	LEU	CA-CB-CG	5.77	128.58	115.30
3	C	396	MET	CG-SD-CE	-5.73	91.04	100.20
17	V	63	THR	C-N-CD	-5.34	108.85	120.60

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	384 (97%)	12 (3%)	1 (0%)	41	44
1	a	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	488 (97%)	13 (3%)	2 (0%)	34	35
3	C	454/461 (98%)	441 (97%)	12 (3%)	1 (0%)	47	53
3	c	463/461 (100%)	453 (98%)	9 (2%)	1 (0%)	47	53
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	7
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	9	5
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	1 (3%)	1 (3%)	4	1
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	4	1
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
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%)	12 (5%)	5 (2%)	7	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	34	35
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	9
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	20
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5387/5700 (94%)	5206 (97%)	164 (3%)	17 (0%)	41	44

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	V	64	PRO
3	c	416	SER
3	C	416	SER
13	O	36	GLN
13	O	59	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	322 (99%)	2 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	46
2	B	408/407 (100%)	398 (98%)	10 (2%)	47	54
2	b	402/407 (99%)	395 (98%)	7 (2%)	60	68
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	62
3	c	364/362 (101%)	352 (97%)	12 (3%)	38	43
4	D	277/283 (98%)	271 (98%)	6 (2%)	52	59
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	44
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	49
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	32
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	11
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	38
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	5
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	46
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	32
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	7
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	26 (93%)	2 (7%)	14	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	30
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	35
14	R	22/33 (67%)	21 (96%)	1 (4%)	27	29
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	1
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	25
16	u	84/112 (75%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	116 (99%)	1 (1%)	78	84
17	v	117/138 (85%)	115 (98%)	2 (2%)	60	68
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	14
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	44
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	3
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
20	z	51/52 (98%)	47 (92%)	4 (8%)	12	9
All	All	4451/4654 (96%)	4310 (97%)	141 (3%)	39	44

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	30	VAL
12	m	13	LEU
14	r	9	LEU
16	U	51	LYS
16	U	24	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
20	Z	38	GLN
1	a	19	ASN
13	o	61	GLN
2	b	409	GLN
2	b	490	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.89	0
15	FME	T	1	15	8,9,10	1.13	0	7,9,11	1.42	1 (14%)
12	FME	M	1	12	8,9,10	0.84	0	7,9,11	0.88	0
15	FME	t	1	15	8,9,10	1.25	1 (12%)	7,9,11	0.80	0
12	FME	m	1	12	8,9,10	0.90	0	7,9,11	1.04	1 (14%)
8	FME	i	1	8	8,9,10	1.12	1 (12%)	7,9,11	0.85	0

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.87	1.42	1.46
8	i	1	FME	CA-N	-2.31	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	3.03	127.49	122.82
12	m	1	FME	CA-N-CN	-2.06	119.65	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	CLA	B	605	-	56,73,73	1.72	5 (8%)	55,113,113	1.52	12 (21%)
24	CLA	b	615	-	56,73,73	1.65	8 (14%)	55,113,113	1.50	10 (18%)
33	LMG	D	407	-	51,51,55	1.00	3 (5%)	59,59,63	1.35	5 (8%)
31	DGD	C	516	-	63,63,67	1.38	11 (17%)	77,77,81	1.35	11 (14%)
26	BCR	b	617	-	41,41,41	1.04	4 (9%)	56,56,56	1.26	6 (10%)
24	CLA	B	610	-	56,73,73	1.53	9 (16%)	55,113,113	1.50	8 (14%)
24	CLA	C	506	-	56,73,73	1.65	8 (14%)	55,113,113	1.77	9 (16%)
26	BCR	T	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	4 (7%)
32	STE	b	621	-	16,19,19	0.38	0	15,19,19	0.94	0
31	DGD	C	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.40	9 (11%)
26	BCR	K	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.21	6 (10%)
26	BCR	b	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.31	9 (16%)
24	CLA	B	608	-	56,73,73	1.54	7 (12%)	55,113,113	1.86	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	606	-	56,73,73	1.62	6 (10%)	55,113,113	2.03	11 (20%)
26	BCR	c	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	5 (8%)
24	CLA	c	509	-	56,73,73	1.55	4 (7%)	55,113,113	1.86	10 (18%)
24	CLA	B	604	-	56,73,73	1.37	7 (12%)	55,113,113	1.46	10 (18%)
26	BCR	D	405	-	41,41,41	1.20	2 (4%)	56,56,56	1.13	5 (8%)
22	OEX	A	602[A]	1,3,37	0,15,15	-	-	-	-	-
26	BCR	X	101	-	41,41,41	1.13	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	B	609	37	56,73,73	1.73	10 (17%)	55,113,113	1.62	10 (18%)
32	STE	B	626	-	8,11,19	0.39	0	7,11,19	0.67	0
30	LHG	D	409	-	48,48,48	1.16	5 (10%)	51,54,54	1.22	5 (9%)
32	STE	b	623	-	12,15,19	0.53	0	11,15,19	0.54	0
31	DGD	c	516	-	63,63,67	1.27	8 (12%)	77,77,81	1.44	15 (19%)
32	STE	B	623	-	17,17,19	0.43	0	16,16,19	0.77	0
32	STE	a	617	-	9,9,19	0.51	0	8,8,19	0.56	0
32	STE	B	619	-	13,16,19	0.41	0	12,16,19	0.87	0
24	CLA	b	612	-	56,73,73	1.41	7 (12%)	55,113,113	2.01	13 (23%)
31	DGD	c	517	-	63,63,67	1.12	6 (9%)	77,77,81	1.32	8 (10%)
24	CLA	b	613	-	56,73,73	1.72	8 (14%)	55,113,113	1.70	12 (21%)
29	SQD	D	408	-	35,36,54	0.96	3 (8%)	42,45,65	1.86	8 (19%)
31	DGD	C	518	-	63,63,67	1.17	9 (14%)	77,77,81	1.39	7 (9%)
33	LMG	c	521	-	48,48,55	1.20	5 (10%)	56,56,63	1.30	5 (8%)
24	CLA	c	513	-	56,73,73	1.61	6 (10%)	55,113,113	1.66	11 (20%)
31	DGD	c	518	-	63,63,67	1.08	8 (12%)	77,77,81	1.40	12 (15%)
24	CLA	d	403	-	56,73,73	1.70	10 (17%)	55,113,113	1.21	5 (9%)
24	CLA	c	511	3	56,73,73	1.83	7 (12%)	55,113,113	1.69	8 (14%)
29	SQD	B	620	-	53,54,54	0.96	2 (3%)	62,65,65	2.18	13 (20%)
33	LMG	D	411	-	31,31,55	1.00	3 (9%)	33,33,63	1.18	3 (9%)
29	SQD	a	616	-	35,35,54	1.05	2 (5%)	37,37,65	1.16	3 (8%)
32	STE	t	102	-	10,13,19	0.48	0	9,13,19	0.72	0
30	LHG	d	406	-	48,48,48	0.80	0	51,54,54	1.18	3 (5%)
24	CLA	C	502	-	56,73,73	1.47	8 (14%)	55,113,113	1.44	8 (14%)
24	CLA	c	510	-	56,73,73	1.74	10 (17%)	55,113,113	1.91	12 (21%)
24	CLA	A	605	37	56,73,73	1.63	7 (12%)	55,113,113	1.60	11 (20%)
34	BCT	D	402	23	0,3,3	-	-	0,3,3	-	-
32	STE	C	521	-	8,11,19	0.47	0	7,11,19	0.73	0
24	CLA	a	607	-	56,73,73	1.55	6 (10%)	55,113,113	1.49	9 (16%)
32	STE	T	103	-	14,14,19	0.40	0	13,13,19	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	513	-	56,73,73	1.62	8 (14%)	55,113,113	1.85	10 (18%)
32	STE	j	101	-	8,11,19	0.42	0	7,11,19	0.76	0
33	LMG	C	515	-	48,48,55	1.20	5 (10%)	56,56,63	1.56	12 (21%)
32	STE	d	411	-	16,19,19	0.35	0	15,19,19	0.80	0
22	OEX	a	602[A]	1,3,37	0,15,15	-	-	-		
24	CLA	b	611	-	56,73,73	1.46	9 (16%)	55,113,113	1.67	11 (20%)
26	BCR	B	616	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
24	CLA	B	601	-	56,73,73	1.65	8 (14%)	55,113,113	1.75	12 (21%)
24	CLA	C	507	37	56,73,73	1.72	10 (17%)	55,113,113	1.81	11 (20%)
24	CLA	B	612	-	56,73,73	1.71	6 (10%)	55,113,113	1.92	12 (21%)
24	CLA	C	503	-	56,73,73	1.82	10 (17%)	55,113,113	1.73	12 (21%)
26	BCR	b	618	-	41,41,41	1.35	3 (7%)	56,56,56	1.39	9 (16%)
24	CLA	c	502	-	56,73,73	1.59	7 (12%)	55,113,113	1.73	10 (18%)
26	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.37	8 (14%)
24	CLA	b	610	37	56,73,73	1.45	8 (14%)	55,113,113	1.67	10 (18%)
24	CLA	c	512	-	56,73,73	1.47	6 (10%)	55,113,113	1.74	13 (23%)
30	LHG	D	410	-	46,46,48	1.14	4 (8%)	49,52,54	1.16	2 (4%)
24	CLA	C	504	37	50,67,73	1.82	8 (16%)	47,105,113	1.44	9 (19%)
24	CLA	b	605	-	56,73,73	1.53	7 (12%)	55,113,113	1.70	9 (16%)
28	PL9	d	405	-	55,55,55	1.48	5 (9%)	68,69,69	1.59	12 (17%)
32	STE	Z	101	-	7,7,19	0.46	0	6,6,19	0.38	0
24	CLA	C	510	-	56,73,73	1.47	8 (14%)	55,113,113	1.60	7 (12%)
26	BCR	B	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.40	7 (12%)
26	BCR	c	515	-	41,41,41	1.26	4 (9%)	56,56,56	1.49	11 (19%)
25	PHO	a	606	-	67,69,69	1.11	7 (10%)	85,99,99	1.12	4 (4%)
26	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	4 (7%)
24	CLA	H	101	37	56,73,73	1.76	8 (14%)	55,113,113	1.55	9 (16%)
33	LMG	M	101	-	51,51,55	1.02	4 (7%)	59,59,63	1.40	9 (15%)
24	CLA	B	614	-	56,73,73	1.78	8 (14%)	55,113,113	1.69	7 (12%)
28	PL9	D	406	-	55,55,55	1.24	6 (10%)	68,69,69	1.88	18 (26%)
30	LHG	A	614	-	48,48,48	0.82	2 (4%)	51,54,54	1.22	6 (11%)
24	CLA	B	613	-	56,73,73	1.62	9 (16%)	55,113,113	1.50	12 (21%)
24	CLA	b	603	-	56,73,73	1.64	11 (19%)	55,113,113	1.65	9 (16%)
29	SQD	A	615	-	38,38,54	1.05	3 (7%)	40,40,65	1.45	4 (10%)
32	STE	M	104	-	17,17,19	0.35	0	16,16,19	0.86	0
30	LHG	d	407	-	38,38,48	0.95	2 (5%)	41,44,54	1.16	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	608	-	56,73,73	1.95	9 (16%)	55,113,113	1.55	10 (18%)
32	STE	a	618	-	8,11,19	0.46	0	7,11,19	0.67	0
24	CLA	d	402	-	56,73,73	1.32	8 (14%)	55,113,113	1.47	8 (14%)
24	CLA	B	607	-	56,73,73	1.69	11 (19%)	55,113,113	1.87	11 (20%)
24	CLA	C	508	-	56,73,73	1.80	9 (16%)	55,113,113	1.51	7 (12%)
32	STE	d	409	-	13,16,19	0.31	0	12,16,19	0.92	0
24	CLA	C	501	-	56,73,73	1.74	9 (16%)	55,113,113	1.50	9 (16%)
33	LMG	c	519	-	37,37,55	1.24	5 (13%)	45,45,63	1.32	6 (13%)
24	CLA	a	613	37	56,73,73	1.76	7 (12%)	55,113,113	1.40	8 (14%)
32	STE	C	519	-	8,11,19	0.51	0	7,11,19	0.55	0
26	BCR	t	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	9 (16%)
32	STE	C	520	-	15,15,19	0.44	0	14,14,19	0.63	0
33	LMG	b	622	-	55,55,55	0.91	3 (5%)	63,63,63	1.51	10 (15%)
33	LMG	a	619	-	55,55,55	1.40	7 (12%)	63,63,63	1.48	10 (15%)
24	CLA	A	604	-	56,73,73	1.61	6 (10%)	55,113,113	1.74	13 (23%)
33	LMG	d	408	-	44,44,55	1.00	4 (9%)	52,52,63	1.25	4 (7%)
24	CLA	D	404	-	56,73,73	1.39	8 (14%)	55,113,113	1.64	9 (16%)
29	SQD	b	620	-	48,49,54	0.98	3 (6%)	57,60,65	2.55	15 (26%)
31	DGD	h	102	-	63,63,67	1.19	8 (12%)	77,77,81	1.36	9 (11%)
24	CLA	C	511	3	56,73,73	1.77	8 (14%)	55,113,113	1.53	7 (12%)
32	STE	R	101	-	8,11,19	0.42	0	7,11,19	0.74	0
25	PHO	D	401	-	67,69,69	1.22	9 (13%)	85,99,99	1.12	5 (5%)
32	STE	X	102	-	16,19,19	0.34	0	15,19,19	0.95	0
24	CLA	C	512	-	56,73,73	1.71	6 (10%)	55,113,113	1.63	12 (21%)
32	STE	c	523	-	8,11,19	0.38	0	7,11,19	0.64	0
26	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	3 (5%)
26	BCR	a	608	-	41,41,41	1.13	3 (7%)	56,56,56	1.35	10 (17%)
21	OXY	a	601[B]	1,3,37	0,16,16	-	-	-	-	-
32	STE	b	624	-	16,19,19	0.47	0	15,19,19	0.79	0
36	HEC	V	201	17	26,50,50	2.27	4 (15%)	18,82,82	1.88	6 (33%)
32	STE	d	410	-	16,19,19	0.41	0	15,19,19	0.67	0
24	CLA	b	616	-	51,68,73	1.70	10 (19%)	49,107,113	1.74	12 (24%)
24	CLA	A	612	37	56,73,73	1.32	5 (8%)	55,113,113	1.62	10 (18%)
24	CLA	c	508	-	55,72,73	1.73	6 (10%)	53,111,113	1.69	11 (20%)
32	STE	B	621	-	8,11,19	0.45	0	7,11,19	0.92	0
24	CLA	B	611	-	56,73,73	1.55	6 (10%)	55,113,113	1.89	8 (14%)
24	CLA	b	614	-	56,73,73	1.55	8 (14%)	55,113,113	1.52	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	507	37	56,73,73	1.58	7 (12%)	55,113,113	1.76	11 (20%)
24	CLA	c	501	-	56,73,73	1.44	8 (14%)	55,113,113	1.57	9 (16%)
26	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.12	5 (8%)
32	STE	B	622	-	14,17,19	0.45	0	13,17,19	0.75	0
32	STE	h	103	-	13,13,19	0.42	0	12,12,19	0.64	0
33	LMG	m	101	-	51,51,55	1.21	4 (7%)	59,59,63	1.56	8 (13%)
30	LHG	e	101	-	41,41,48	0.99	2 (4%)	44,47,54	1.29	6 (13%)
24	CLA	a	604	-	56,73,73	1.71	10 (17%)	55,113,113	1.56	8 (14%)
36	HEC	v	201	17	26,50,50	2.33	3 (11%)	18,82,82	2.26	6 (33%)
24	CLA	C	505	-	56,73,73	1.67	7 (12%)	55,113,113	1.70	10 (18%)
25	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.27	7 (8%)
24	CLA	c	505	-	56,73,73	1.57	8 (14%)	55,113,113	2.01	15 (27%)
35	HEM	F	101	6,5	27,50,50	1.96	4 (14%)	17,82,82	1.93	4 (23%)
33	LMG	Y	101	-	48,48,55	1.27	7 (14%)	56,56,63	1.29	5 (8%)
24	CLA	a	605	37	56,73,73	1.56	10 (17%)	55,113,113	1.61	10 (18%)
30	LHG	l	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.24	5 (9%)
32	STE	b	625	-	9,9,19	0.40	0	8,8,19	0.51	0
26	BCR	A	608	-	41,41,41	1.22	4 (9%)	56,56,56	1.37	8 (14%)
34	BCT	a	611	23	0,3,3	-	-	0,3,3	-	-
21	OEY	A	601[B]	1,3,37	0,16,16	-	-	-	-	-
24	CLA	B	603	-	56,73,73	1.68	9 (16%)	55,113,113	2.32	13 (23%)
32	STE	B	625	-	14,14,19	0.43	0	13,13,19	0.83	0
33	LMG	D	412	-	20,26,55	0.60	0	18,26,63	1.16	0
32	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.71	0
24	CLA	c	504	37	51,68,73	1.63	7 (13%)	49,107,113	1.61	9 (18%)
29	SQD	A	613	-	51,52,54	1.10	6 (11%)	60,63,65	2.08	13 (21%)
24	CLA	b	604	-	56,73,73	1.58	5 (8%)	55,113,113	2.32	14 (25%)
30	LHG	D	413	-	48,48,48	1.01	3 (6%)	51,54,54	1.32	7 (13%)
24	CLA	c	503	-	56,73,73	1.56	10 (17%)	55,113,113	1.26	4 (7%)
28	PL9	A	611	-	55,55,55	1.27	5 (9%)	68,69,69	1.74	17 (25%)
32	STE	c	520	-	16,19,19	0.38	0	15,19,19	0.84	0
32	STE	I	101	-	14,14,19	0.50	0	13,13,19	0.61	0
32	STE	J	101	-	8,11,19	0.36	0	7,11,19	0.65	0
24	CLA	b	602	-	56,73,73	1.58	9 (16%)	55,113,113	1.78	13 (23%)
24	CLA	B	606	37	56,73,73	1.62	9 (16%)	55,113,113	1.70	7 (12%)
30	LHG	L	101	-	48,48,48	0.74	2 (4%)	51,54,54	1.16	3 (5%)
24	CLA	b	607	37	56,73,73	1.50	7 (12%)	55,113,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	f	102	-	40,41,54	1.09	4 (10%)	49,52,65	1.85	10 (20%)
32	STE	M	103	-	9,9,19	0.48	0	8,8,19	0.57	0
24	CLA	B	602	-	56,73,73	1.35	8 (14%)	55,113,113	1.47	12 (21%)
24	CLA	B	615	-	51,68,73	1.81	11 (21%)	49,107,113	1.94	10 (20%)
24	CLA	b	601	37	56,73,73	1.61	7 (12%)	55,113,113	1.80	11 (20%)
28	PL9	a	612	-	55,55,55	0.90	1 (1%)	68,69,69	1.54	11 (16%)
26	BCR	k	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.08	4 (7%)
24	CLA	D	403	-	56,73,73	1.49	8 (14%)	55,113,113	1.64	10 (18%)
32	STE	B	624	-	15,15,19	0.50	0	14,14,19	0.57	0
32	STE	L	102	-	8,11,19	0.49	0	7,11,19	0.77	0
33	LMG	c	522	-	49,49,55	0.98	4 (8%)	57,57,63	1.26	3 (5%)
24	CLA	b	609	-	56,73,73	1.66	8 (14%)	55,113,113	1.74	12 (21%)
26	BCR	h	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
24	CLA	c	506	-	56,73,73	1.51	8 (14%)	55,113,113	1.68	10 (18%)
25	PHO	A	606	-	67,69,69	1.27	9 (13%)	85,99,99	1.19	9 (10%)
24	CLA	A	607	-	45,62,73	1.51	10 (22%)	41,99,113	1.92	8 (19%)
26	BCR	C	514	-	41,41,41	1.28	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	C	509	-	56,73,73	1.60	8 (14%)	55,113,113	1.75	9 (16%)
31	DGD	A	616	-	67,67,67	1.26	9 (13%)	81,81,81	1.46	13 (16%)
35	HEM	f	101	6,5	27,50,50	1.89	4 (14%)	17,82,82	2.01	3 (17%)
26	BCR	K	103	-	41,41,41	1.24	4 (9%)	56,56,56	1.30	7 (12%)
30	LHG	a	614	-	48,48,48	1.06	4 (8%)	51,54,54	1.34	7 (13%)
31	DGD	H	102	-	63,63,67	1.32	9 (14%)	77,77,81	1.40	8 (10%)
29	SQD	a	615	-	53,54,54	0.97	6 (11%)	62,65,65	2.05	11 (17%)
32	STE	T	102	-	15,15,19	0.37	0	14,14,19	0.82	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
24	CLA	B	605	-	1/1/20/20	13/37/115/115	-
24	CLA	b	615	-	1/1/20/20	4/37/115/115	-
33	LMG	D	407	-	-	14/46/66/70	0/1/1/1
31	DGD	C	516	-	-	22/51/91/95	0/2/2/2
26	BCR	b	617	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	610	-	1/1/20/20	6/37/115/115	-
24	CLA	C	506	-	1/1/20/20	14/37/115/115	-
26	BCR	T	101	-	-	11/29/63/63	0/2/2/2
32	STE	b	621	-	-	9/15/17/17	-
31	DGD	C	517	-	-	18/51/91/95	0/2/2/2
26	BCR	K	101	-	-	9/29/63/63	0/2/2/2
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/20/20	7/37/115/115	-
24	CLA	B	608	-	-	4/37/115/115	-
26	BCR	c	514	-	-	8/29/63/63	0/2/2/2
24	CLA	c	509	-	1/1/20/20	13/37/115/115	-
24	CLA	B	604	-	1/1/20/20	14/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
26	BCR	X	101	-	-	6/29/63/63	0/2/2/2
24	CLA	B	609	37	1/1/20/20	7/37/115/115	-
32	STE	B	626	-	-	4/7/9/17	-
30	LHG	D	409	-	-	21/53/53/53	-
32	STE	b	623	-	-	6/11/13/17	-
31	DGD	c	516	-	-	20/51/91/95	0/2/2/2
32	STE	B	623	-	-	9/15/15/17	-
32	STE	a	617	-	-	4/7/7/17	-
32	STE	B	619	-	-	9/12/14/17	-
24	CLA	b	612	-	1/1/20/20	6/37/115/115	-
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	CLA	b	613	-	1/1/20/20	4/37/115/115	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
31	DGD	C	518	-	-	18/51/91/95	0/2/2/2
33	LMG	c	521	-	-	27/43/63/70	0/1/1/1
24	CLA	c	513	-	1/1/20/20	8/37/115/115	-
31	DGD	c	518	-	-	15/51/91/95	0/2/2/2
24	CLA	d	403	-	1/1/20/20	8/37/115/115	-
24	CLA	c	511	3	1/1/20/20	6/37/115/115	-
29	SQD	B	620	-	-	23/49/69/69	0/1/1/1
33	LMG	D	411	-	-	14/33/33/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	616	-	-	18/37/37/69	-
32	STE	t	102	-	-	2/9/11/17	-
30	LHG	d	406	-	-	26/53/53/53	-
24	CLA	C	502	-	1/1/20/20	6/37/115/115	-
24	CLA	c	510	-	1/1/20/20	13/37/115/115	-
24	CLA	A	605	37	1/1/20/20	14/37/115/115	-
32	STE	C	521	-	-	2/7/9/17	-
24	CLA	a	607	-	1/1/20/20	11/37/115/115	-
32	STE	T	103	-	-	8/12/12/17	-
24	CLA	C	513	-	1/1/20/20	9/37/115/115	-
32	STE	j	101	-	-	3/7/9/17	-
33	LMG	C	515	-	-	17/43/63/70	0/1/1/1
32	STE	d	411	-	-	11/15/17/17	-
24	CLA	b	611	-	1/1/20/20	4/37/115/115	-
26	BCR	B	616	-	-	7/29/63/63	0/2/2/2
24	CLA	B	601	-	1/1/20/20	8/37/115/115	-
24	CLA	C	507	37	1/1/20/20	7/37/115/115	-
24	CLA	B	612	-	1/1/20/20	12/37/115/115	-
24	CLA	C	503	-	1/1/20/20	5/37/115/115	-
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	502	-	1/1/20/20	8/37/115/115	-
26	BCR	B	618	-	-	6/29/63/63	0/2/2/2
24	CLA	b	610	37	1/1/20/20	7/37/115/115	-
24	CLA	c	512	-	1/1/20/20	16/37/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
24	CLA	C	504	37	1/1/18/20	8/30/108/115	-
24	CLA	b	605	-	1/1/20/20	6/37/115/115	-
28	PL9	d	405	-	-	12/53/73/73	0/1/1/1
32	STE	Z	101	-	-	2/5/5/17	-
24	CLA	C	510	-	1/1/20/20	8/37/115/115	-
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
26	BCR	c	515	-	-	5/29/63/63	0/2/2/2
25	PHO	a	606	-	-	2/53/103/103	0/5/6/6
26	BCR	d	404	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	H	101	37	1/1/20/20	18/37/115/115	-
33	LMG	M	101	-	-	23/46/66/70	0/1/1/1
24	CLA	B	614	-	1/1/20/20	6/37/115/115	-
28	PL9	D	406	-	-	11/53/73/73	0/1/1/1
30	LHG	A	614	-	-	30/53/53/53	-
24	CLA	B	613	-	1/1/20/20	16/37/115/115	-
24	CLA	b	603	-	1/1/20/20	4/37/115/115	-
29	SQD	A	615	-	-	17/39/39/69	-
32	STE	M	104	-	-	10/15/15/17	-
30	LHG	d	407	-	-	15/43/43/53	-
24	CLA	b	608	-	1/1/20/20	6/37/115/115	-
32	STE	a	618	-	-	4/7/9/17	-
24	CLA	d	402	-	-	6/37/115/115	-
24	CLA	B	607	-	1/1/20/20	4/37/115/115	-
24	CLA	C	508	-	-	7/37/115/115	-
32	STE	d	409	-	-	10/12/14/17	-
24	CLA	C	501	-	1/1/20/20	4/37/115/115	-
33	LMG	c	519	-	-	9/31/51/70	0/1/1/1
24	CLA	a	613	37	1/1/20/20	4/37/115/115	-
32	STE	C	519	-	-	3/7/9/17	-
26	BCR	t	101	-	-	7/29/63/63	0/2/2/2
32	STE	C	520	-	-	7/13/13/17	-
33	LMG	b	622	-	-	25/50/70/70	0/1/1/1
33	LMG	a	619	-	-	36/50/70/70	0/1/1/1
24	CLA	A	604	-	1/1/20/20	9/37/115/115	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
24	CLA	D	404	-	1/1/20/20	13/37/115/115	-
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	C	511	3	1/1/20/20	9/37/115/115	-
32	STE	R	101	-	-	4/7/9/17	-
25	PHO	D	401	-	-	3/53/103/103	0/5/6/6
32	STE	X	102	-	-	12/15/17/17	-
24	CLA	C	512	-	1/1/20/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	c	523	-	-	7/7/9/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
26	BCR	a	608	-	-	6/29/63/63	0/2/2/2
32	STE	b	624	-	-	9/15/17/17	-
36	HEC	V	201	17	-	0/6/54/54	-
32	STE	d	410	-	-	11/15/17/17	-
24	CLA	b	616	-	1/1/19/20	8/31/109/115	-
24	CLA	A	612	37	1/1/20/20	7/37/115/115	-
24	CLA	c	508	-	1/1/19/20	8/36/114/115	-
32	STE	B	621	-	-	6/7/9/17	-
24	CLA	B	611	-	1/1/20/20	13/37/115/115	-
24	CLA	b	614	-	1/1/20/20	14/37/115/115	-
24	CLA	c	507	37	1/1/20/20	11/37/115/115	-
24	CLA	c	501	-	1/1/20/20	4/37/115/115	-
26	BCR	k	102	-	-	8/29/63/63	0/2/2/2
32	STE	B	622	-	-	8/13/15/17	-
32	STE	h	103	-	-	6/11/11/17	-
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
30	LHG	e	101	-	-	21/46/46/53	-
24	CLA	a	604	-	1/1/20/20	4/37/115/115	-
36	HEC	v	201	17	-	0/6/54/54	-
24	CLA	C	505	-	1/1/20/20	11/37/115/115	-
25	PHO	d	401	-	-	9/53/103/103	0/5/6/6
24	CLA	c	505	-	1/1/20/20	9/37/115/115	-
35	HEM	F	101	6,5	-	1/6/54/54	-
33	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
24	CLA	a	605	37	-	12/37/115/115	-
30	LHG	l	101	-	-	16/53/53/53	-
32	STE	b	625	-	-	5/7/7/17	-
26	BCR	A	608	-	-	6/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/20/20	13/37/115/115	-
32	STE	B	625	-	-	8/12/12/17	-
33	LMG	D	412	-	-	9/18/22/70	-
32	STE	M	102	-	-	5/10/12/17	-
24	CLA	c	504	37	1/1/19/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	613	-	-	22/47/67/69	0/1/1/1
24	CLA	b	604	-	1/1/20/20	13/37/115/115	-
30	LHG	D	413	-	-	15/53/53/53	-
24	CLA	c	503	-	1/1/20/20	7/37/115/115	-
28	PL9	A	611	-	-	21/53/73/73	0/1/1/1
32	STE	c	520	-	-	7/15/17/17	-
32	STE	I	101	-	-	7/12/12/17	-
32	STE	J	101	-	-	2/7/9/17	-
24	CLA	b	602	-	-	8/37/115/115	-
24	CLA	B	606	37	1/1/20/20	14/37/115/115	-
30	LHG	L	101	-	-	19/53/53/53	-
24	CLA	b	607	37	1/1/20/20	13/37/115/115	-
29	SQD	f	102	-	-	17/36/56/69	0/1/1/1
32	STE	M	103	-	-	2/7/7/17	-
24	CLA	B	602	-	1/1/20/20	11/37/115/115	-
24	CLA	B	615	-	1/1/19/20	7/31/109/115	-
24	CLA	b	601	37	1/1/20/20	18/37/115/115	-
28	PL9	a	612	-	-	19/53/73/73	0/1/1/1
26	BCR	k	101	-	-	11/29/63/63	0/2/2/2
24	CLA	D	403	-	-	10/37/115/115	-
32	STE	B	624	-	-	11/13/13/17	-
32	STE	L	102	-	-	3/7/9/17	-
33	LMG	c	522	-	-	26/44/64/70	0/1/1/1
24	CLA	b	609	-	-	8/37/115/115	-
26	BCR	h	101	-	-	6/29/63/63	0/2/2/2
24	CLA	c	506	-	1/1/20/20	15/37/115/115	-
25	PHO	A	606	-	-	3/53/103/103	0/5/6/6
24	CLA	A	607	-	1/1/17/20	2/24/102/115	-
26	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/20/20	12/37/115/115	-
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
35	HEM	f	101	6,5	-	0/6/54/54	-
26	BCR	K	103	-	-	6/29/63/63	0/2/2/2
30	LHG	a	614	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
29	SQD	a	615	-	-	25/49/69/69	0/1/1/1
32	STE	T	102	-	-	9/13/13/17	-

The worst 5 of 859 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C4B-NB	8.42	1.42	1.35
24	B	605	CLA	MG-NA	8.14	2.25	2.06
24	B	613	CLA	C4B-NB	8.10	1.42	1.35
24	H	101	CLA	C4B-NB	8.08	1.42	1.35
24	A	605	CLA	C4B-NB	8.07	1.42	1.35

The worst 5 of 1244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4A-NA-C1A	11.93	112.07	106.71
29	b	620	SQD	O6-C1-C2	11.85	126.80	108.30
24	b	604	CLA	C4A-NA-C1A	11.25	111.76	106.71
24	b	606	CLA	C4A-NA-C1A	9.39	110.93	106.71
29	B	620	SQD	O6-C1-C2	9.11	122.52	108.30

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	607	CLA	ND
24	A	612	CLA	ND
24	B	601	CLA	ND

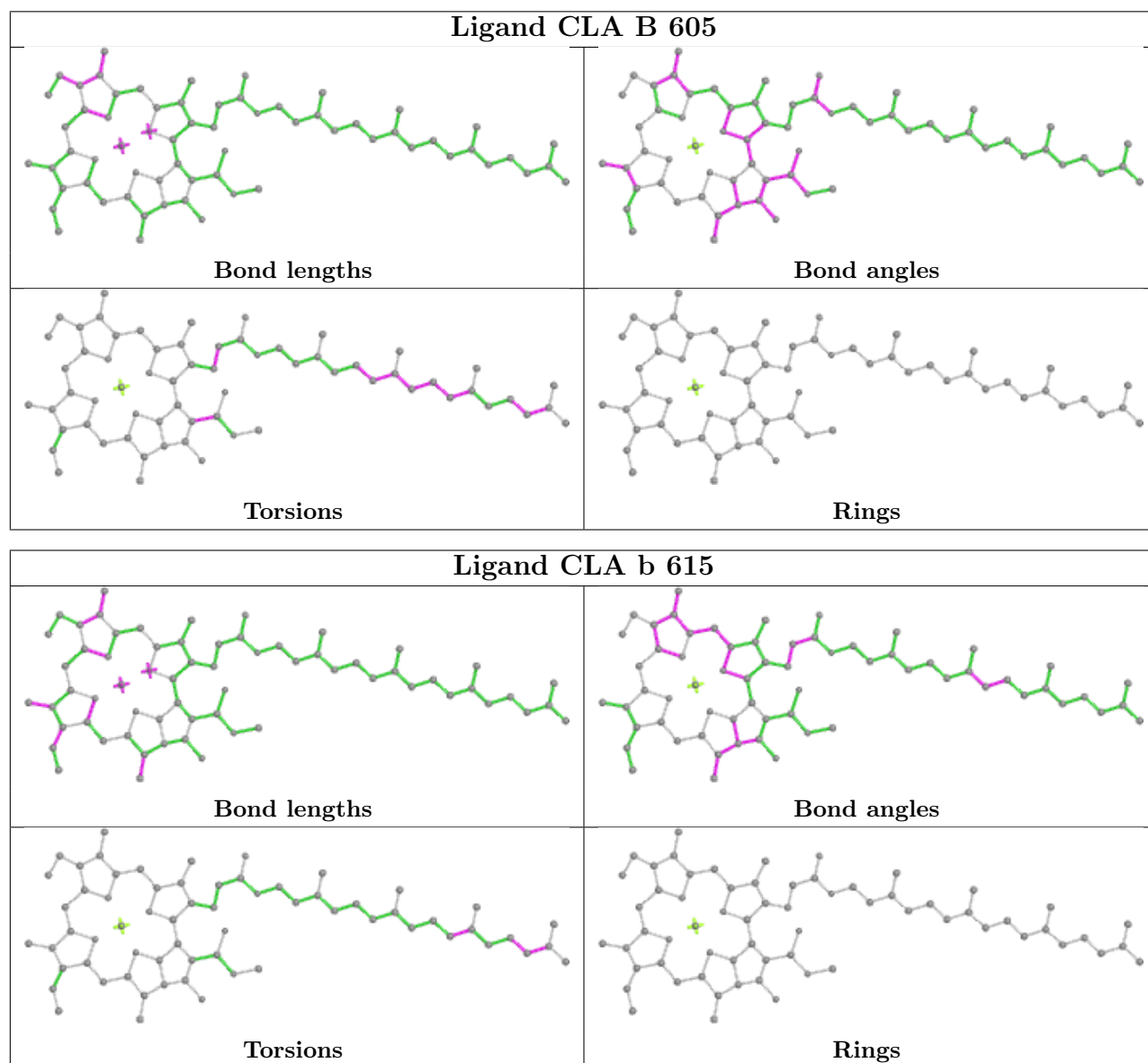
5 of 1880 torsion outliers are listed below:

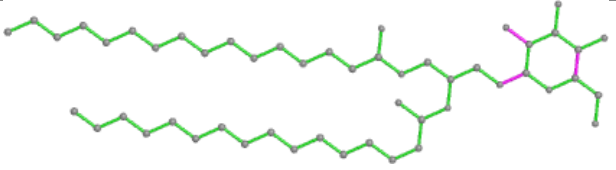
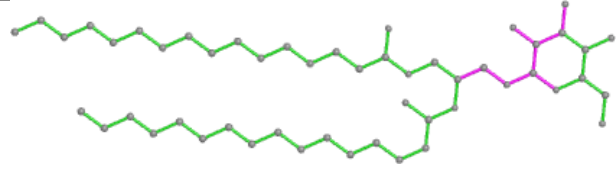
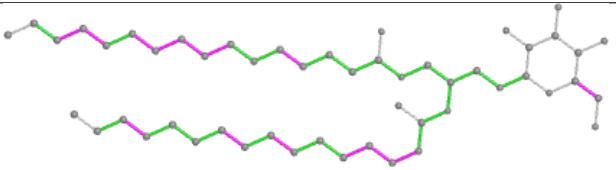
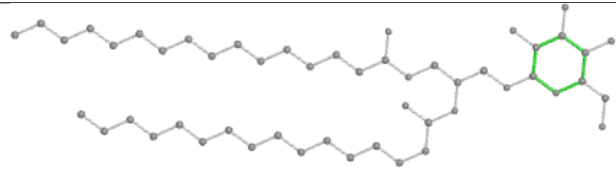
Mol	Chain	Res	Type	Atoms
24	A	604	CLA	C2C-C3C-CAC-CBC
24	A	612	CLA	CHA-CBD-CGD-O1D
24	A	612	CLA	CHA-CBD-CGD-O2D
24	B	613	CLA	CHA-CBD-CGD-O1D
24	B	613	CLA	CHA-CBD-CGD-O2D

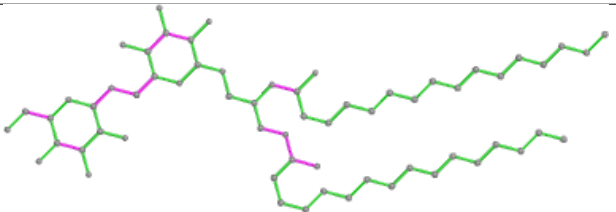
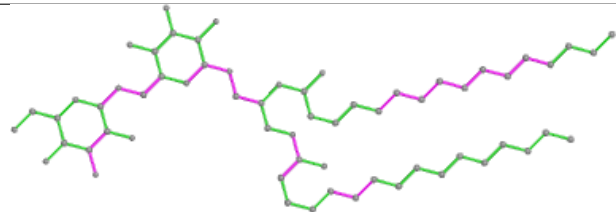
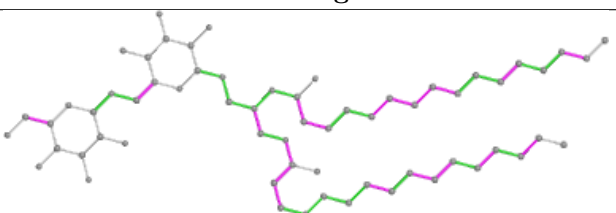
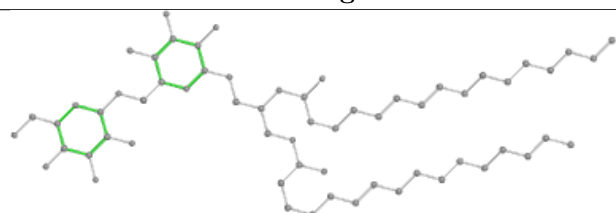
There are no ring outliers.

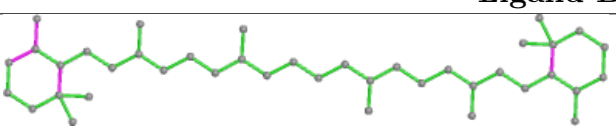
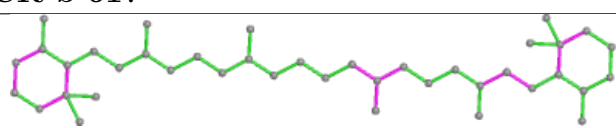
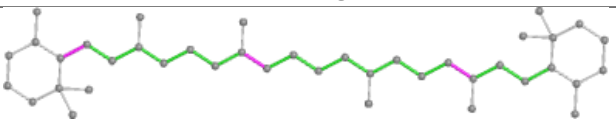
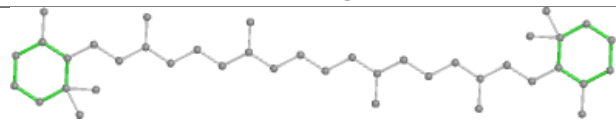
No monomer is involved in short contacts.

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

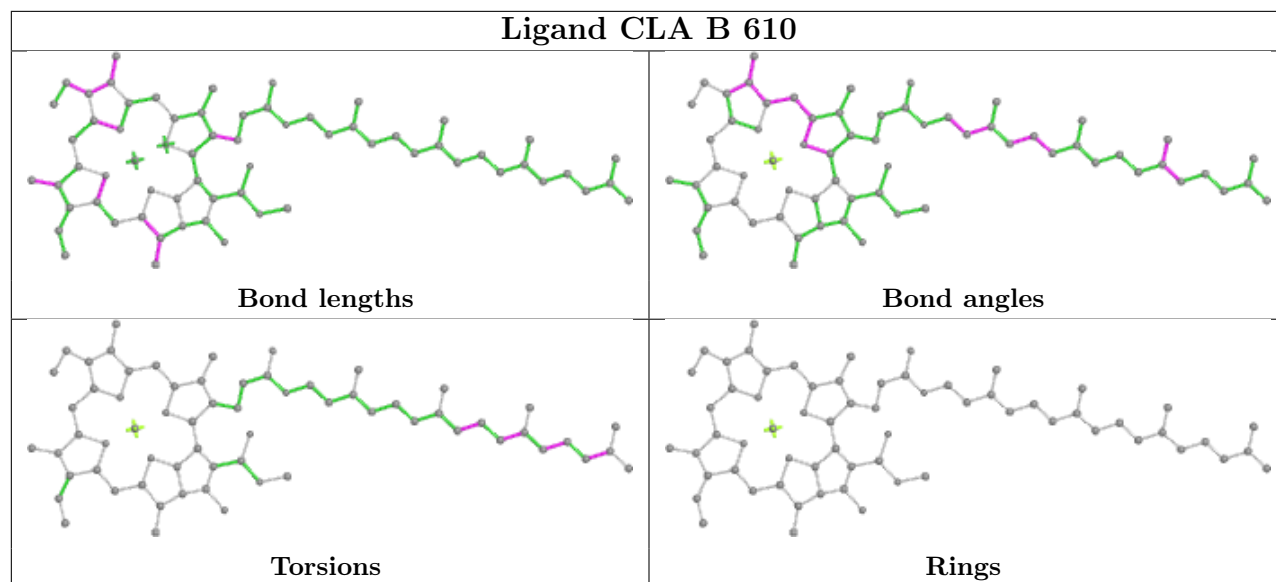


Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

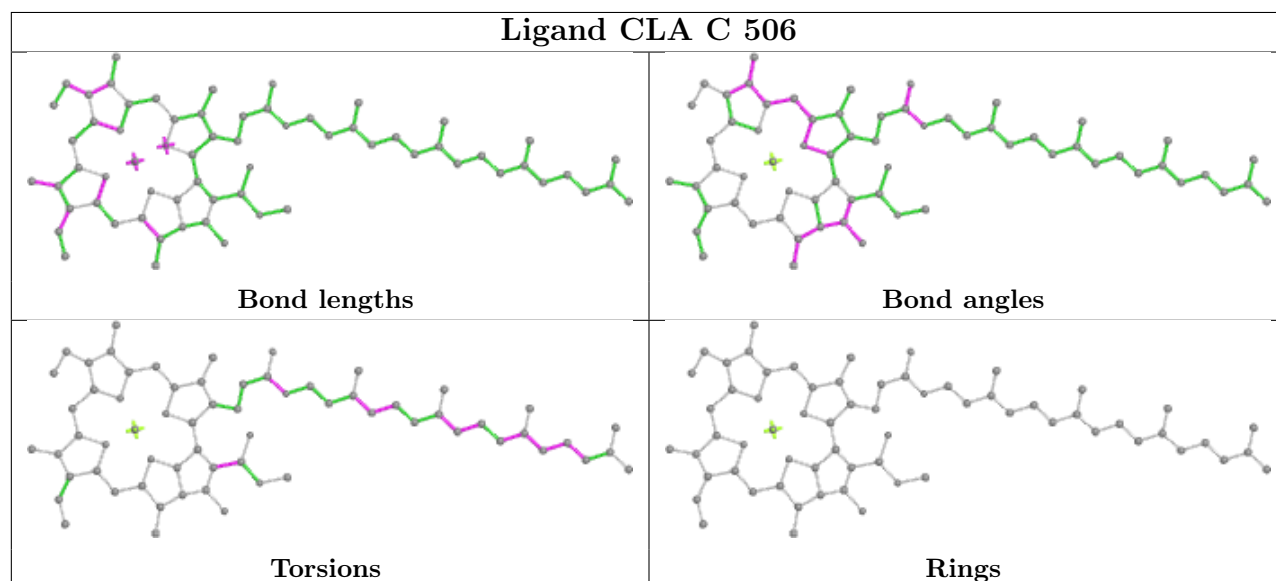
Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

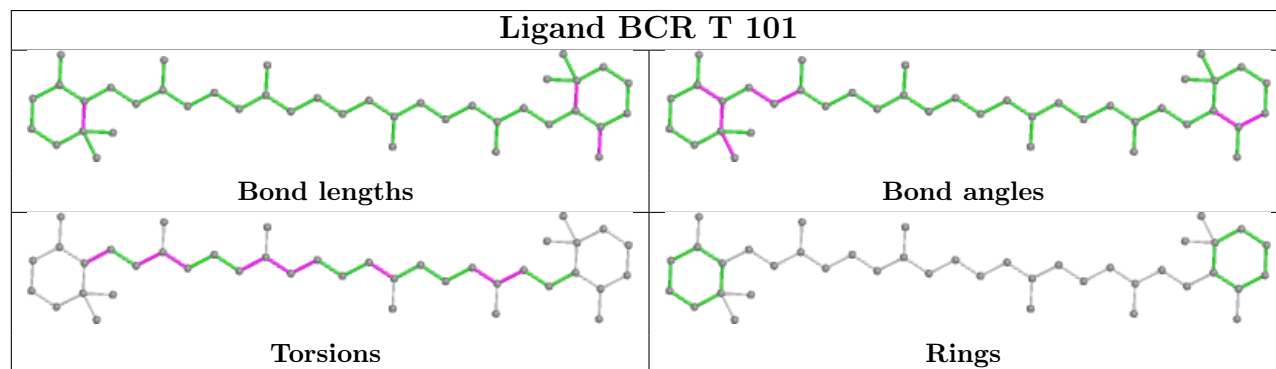
Ligand CLA B 610

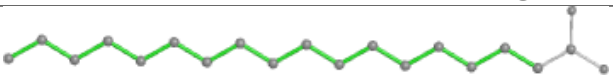
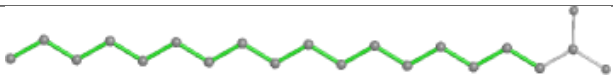
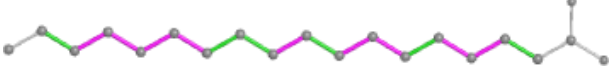
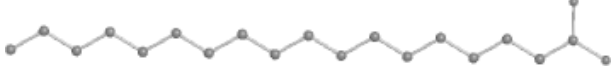


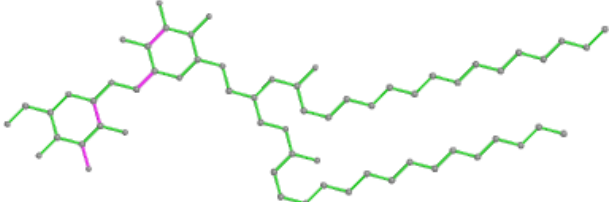
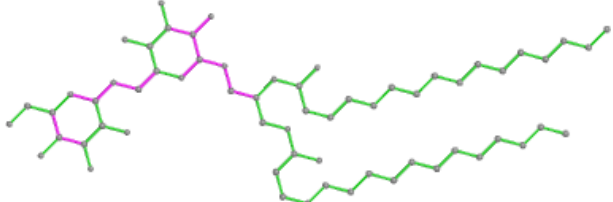
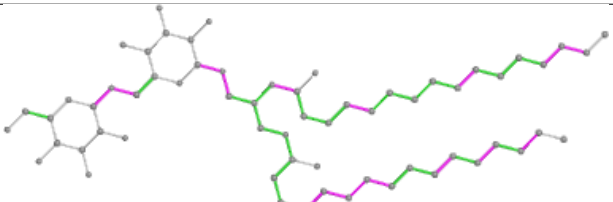
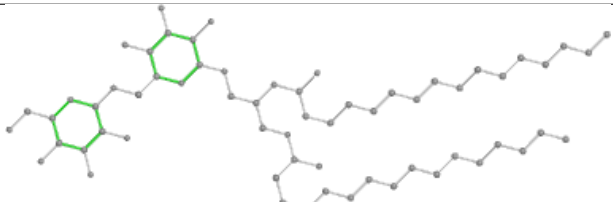
Ligand CLA C 506

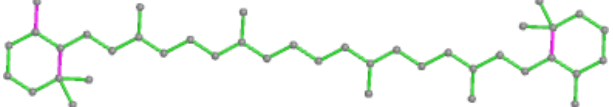
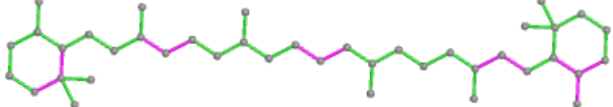
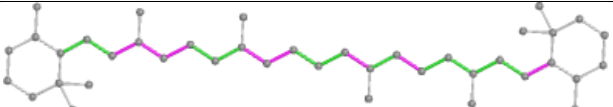
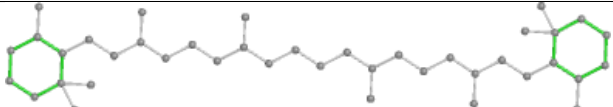


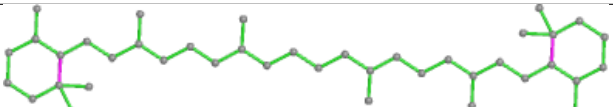
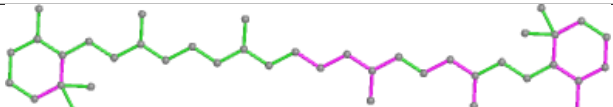
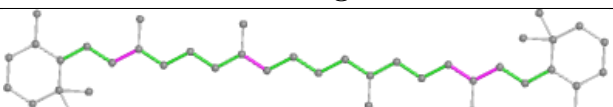
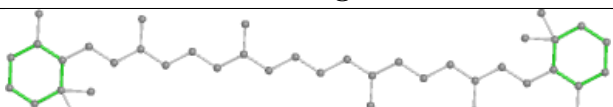
Ligand BCR T 101

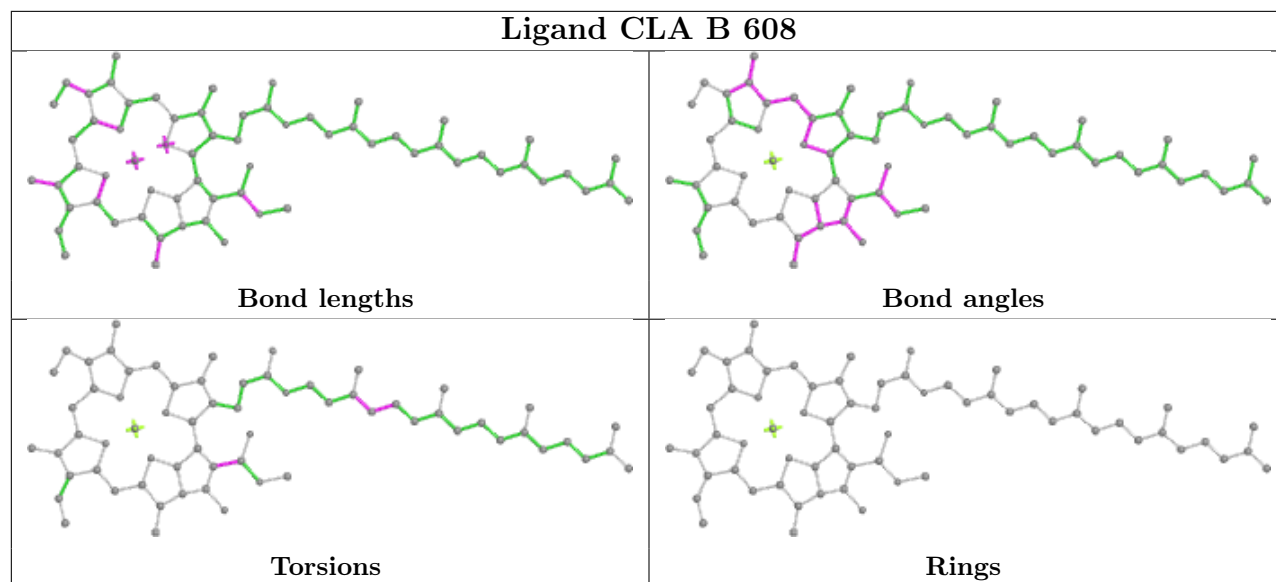
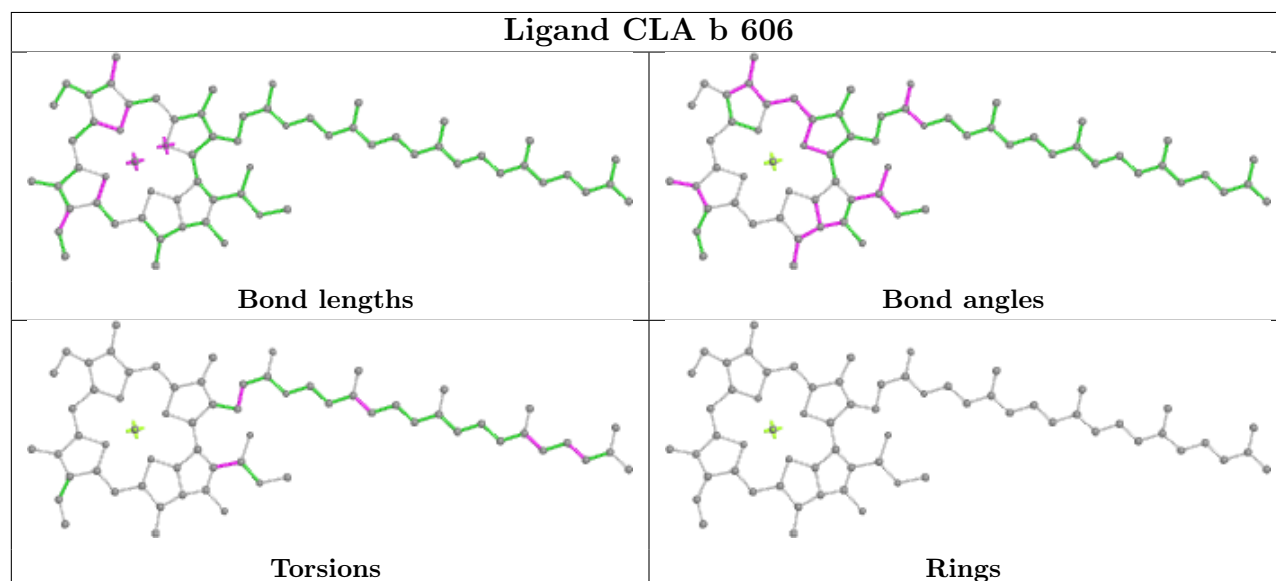
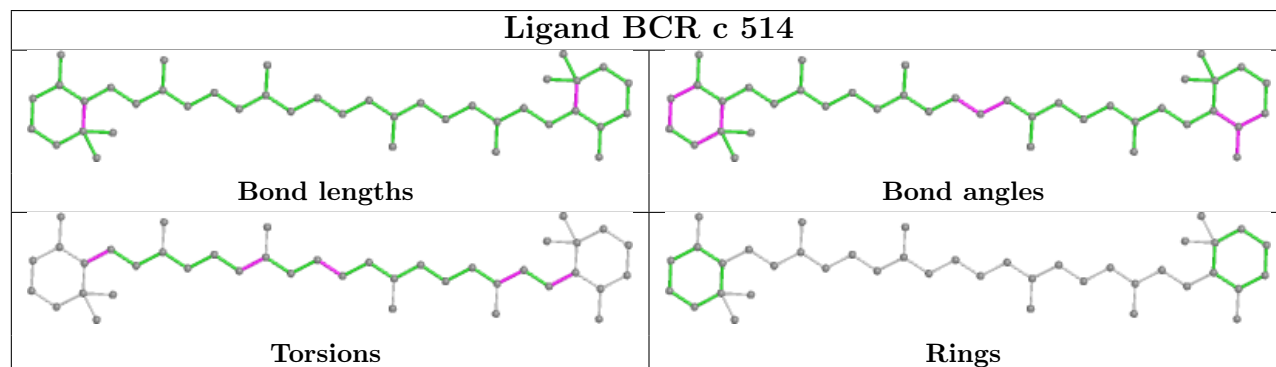


Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

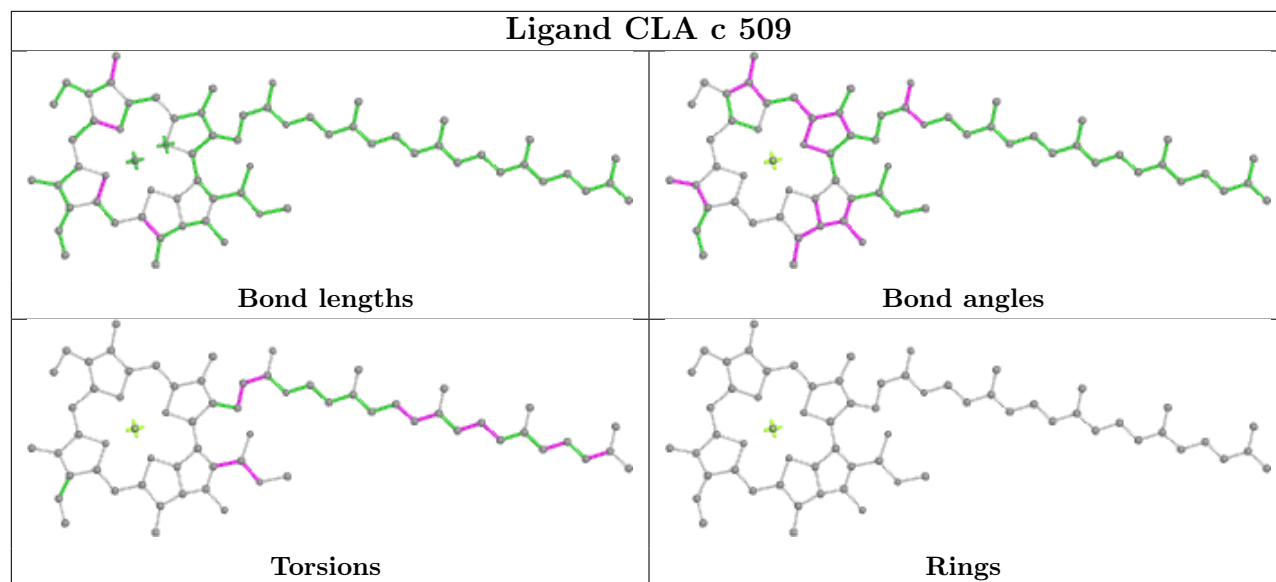
Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

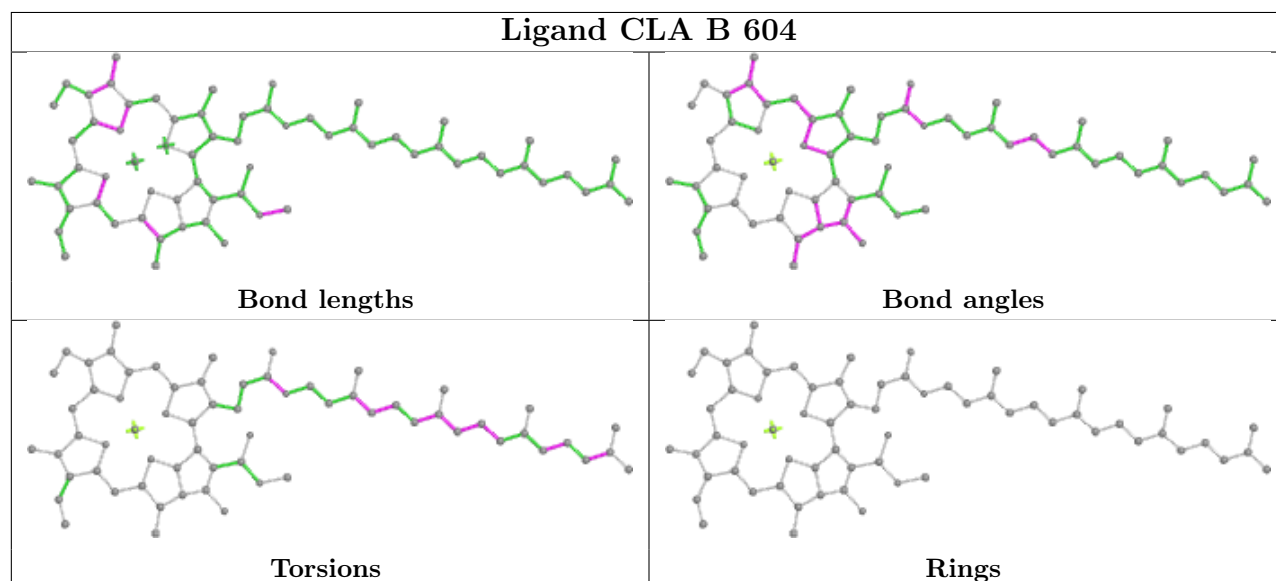
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608**Ligand CLA b 606****Ligand BCR c 514**

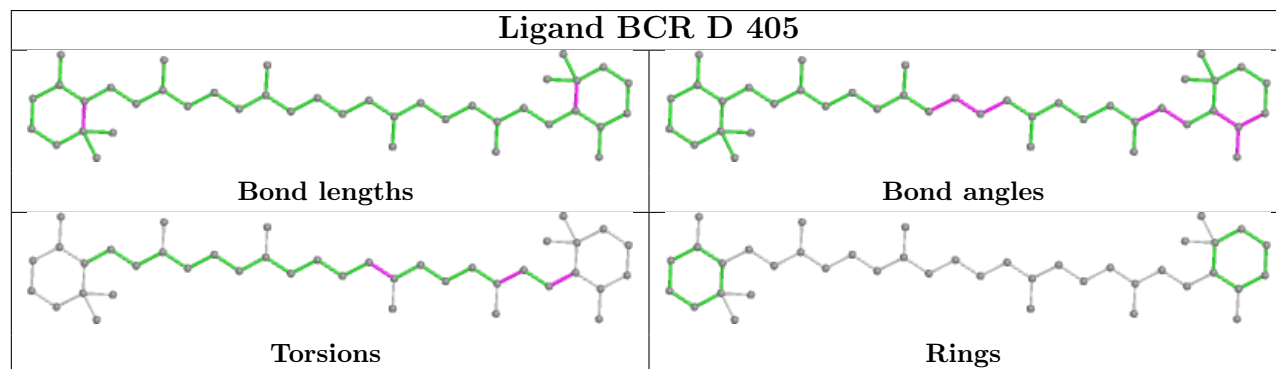
Ligand CLA c 509

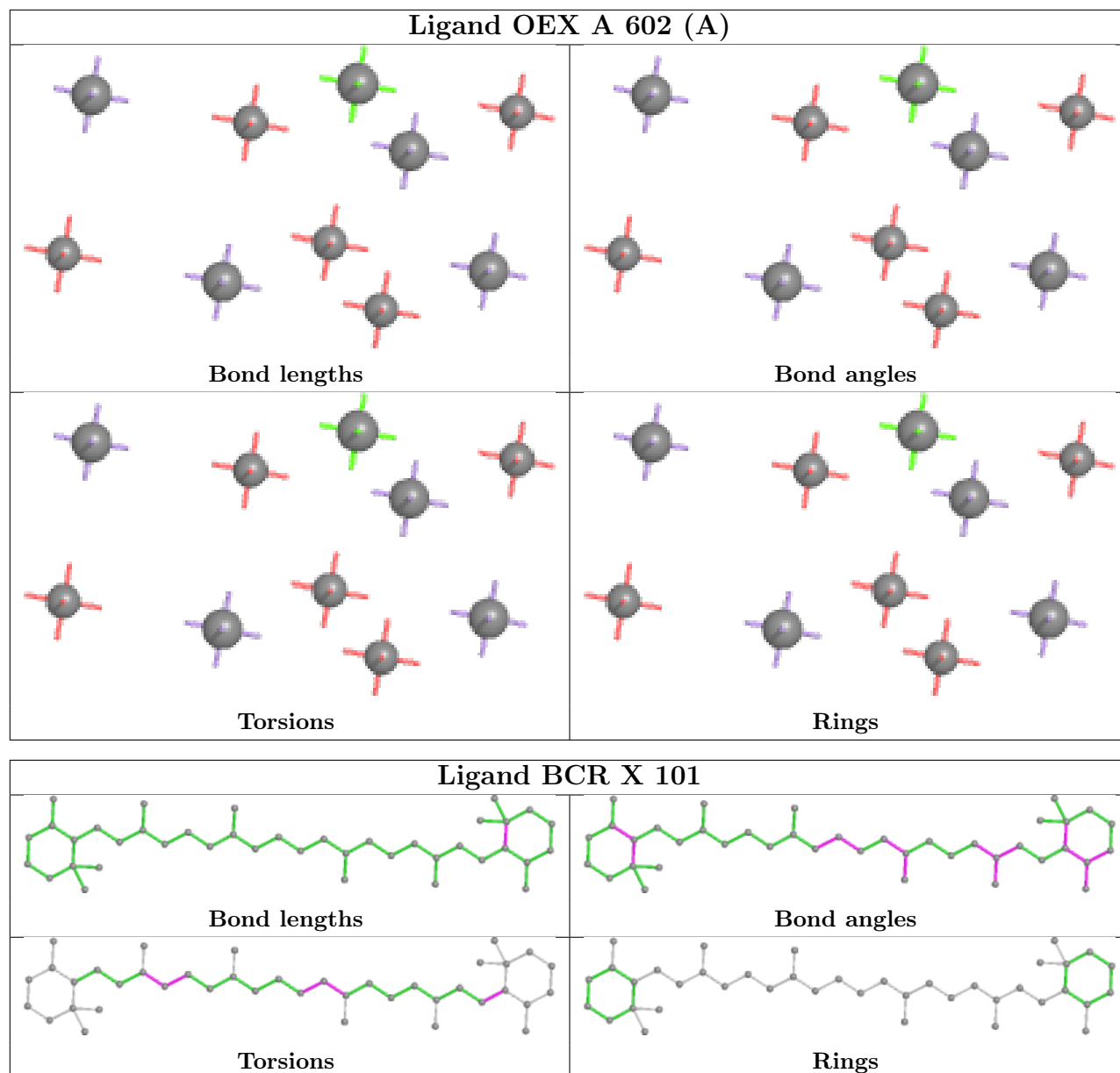


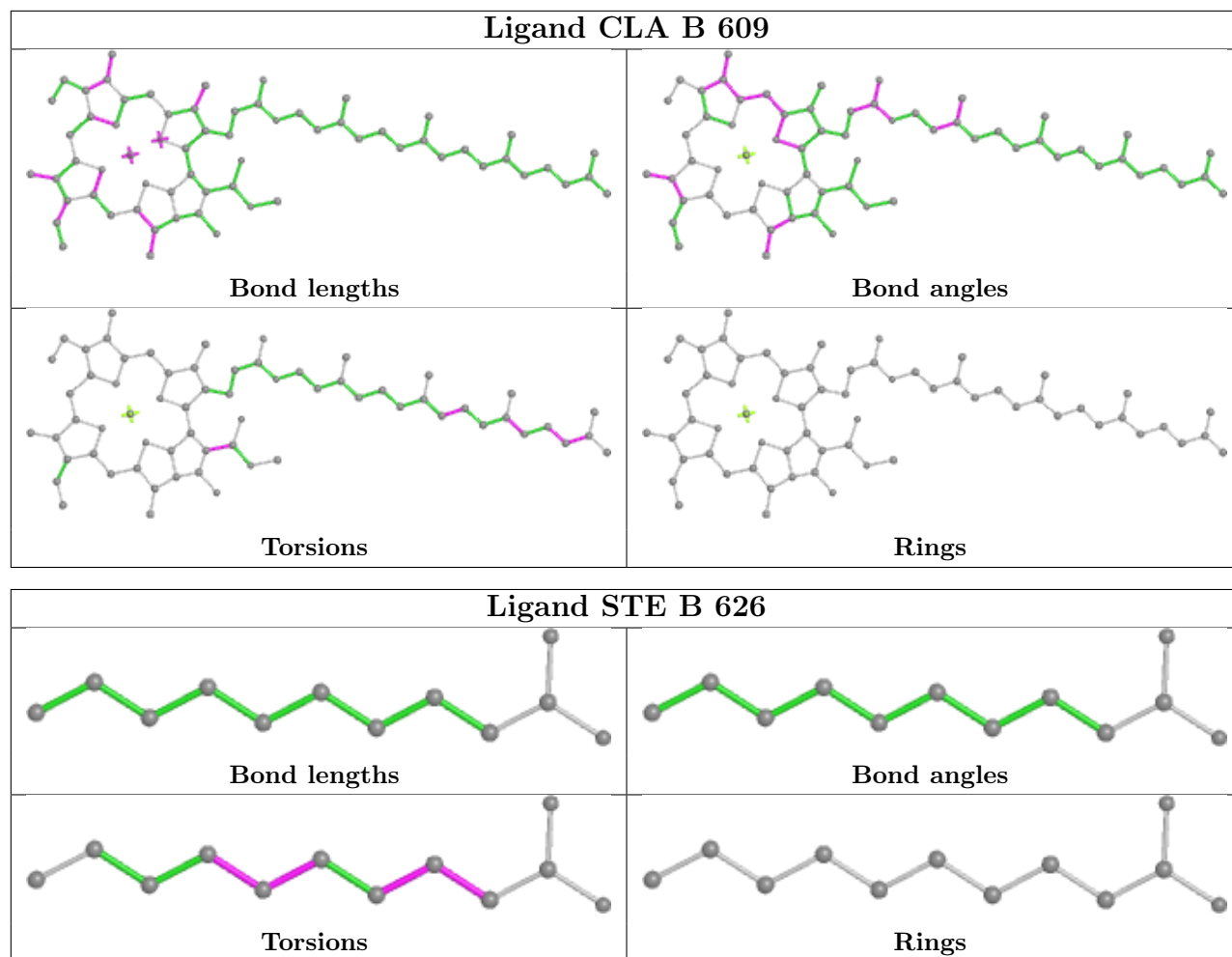
Ligand CLA B 604

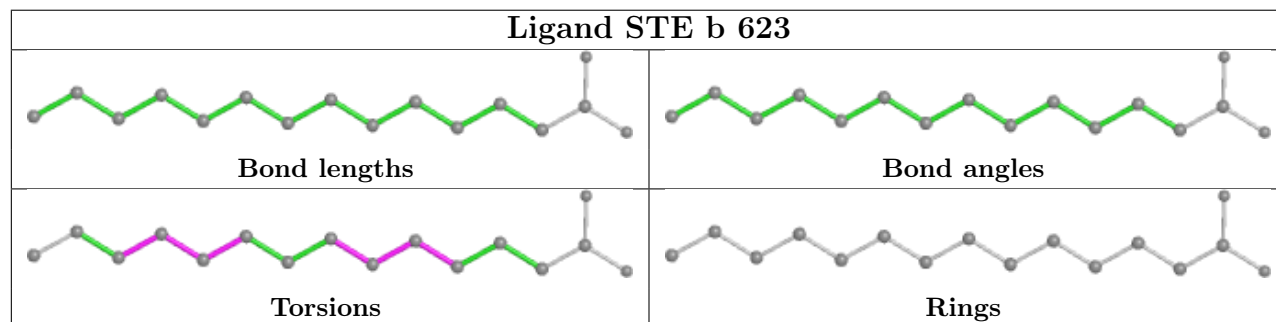
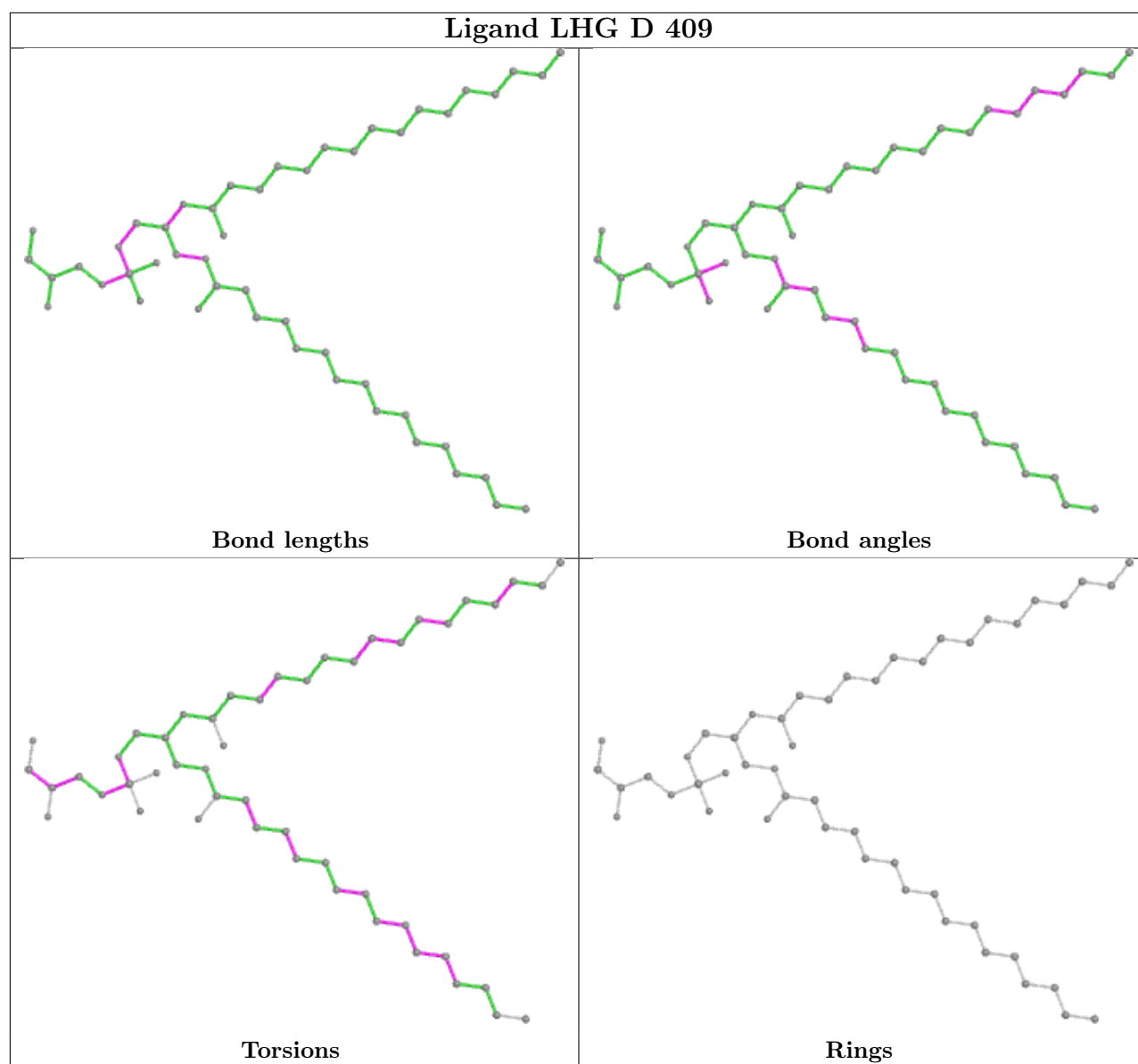


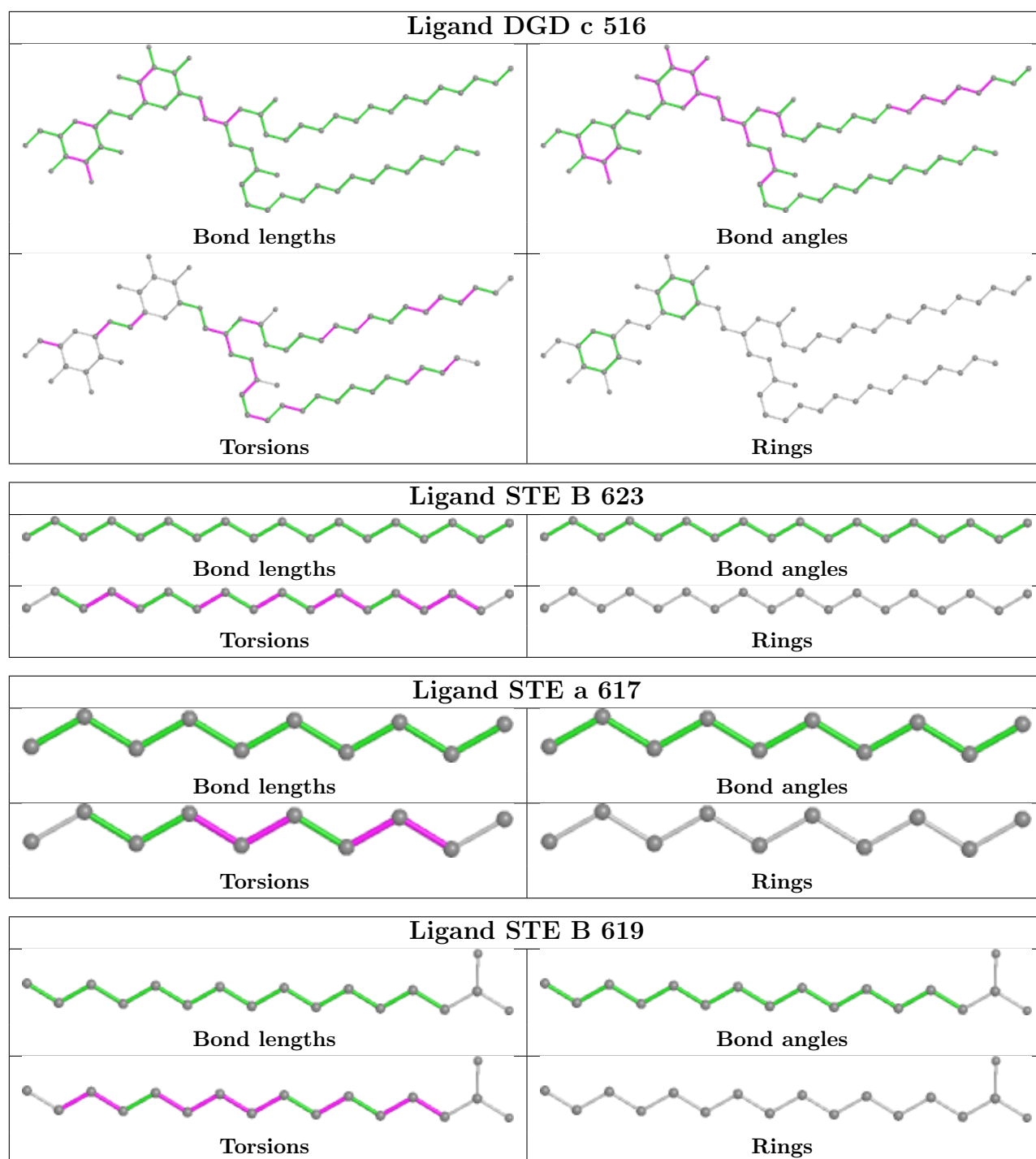
Ligand BCR D 405



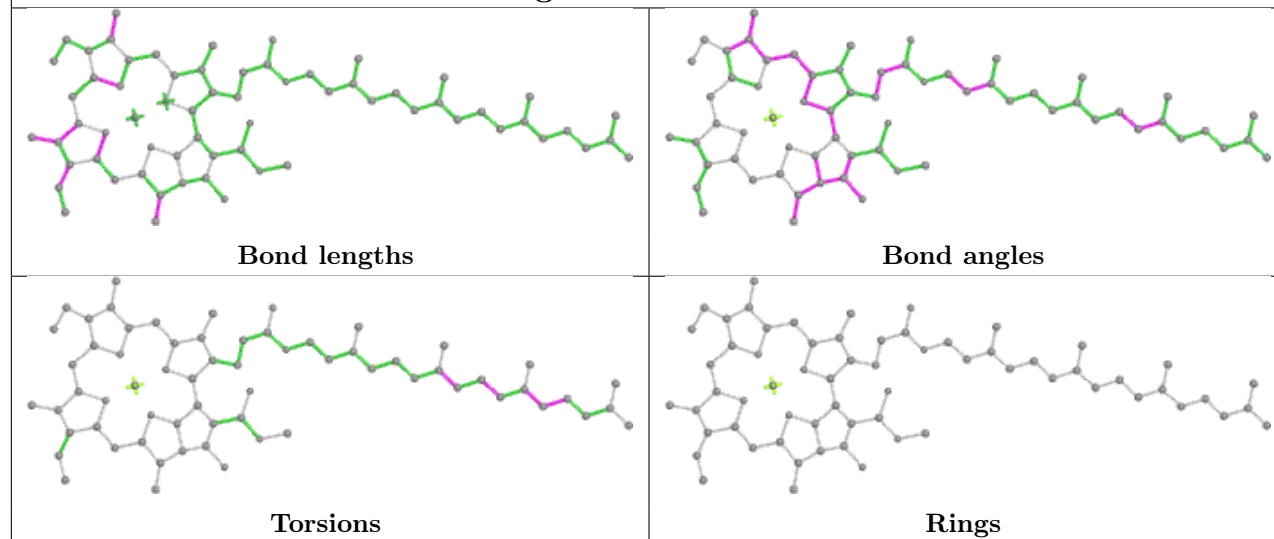




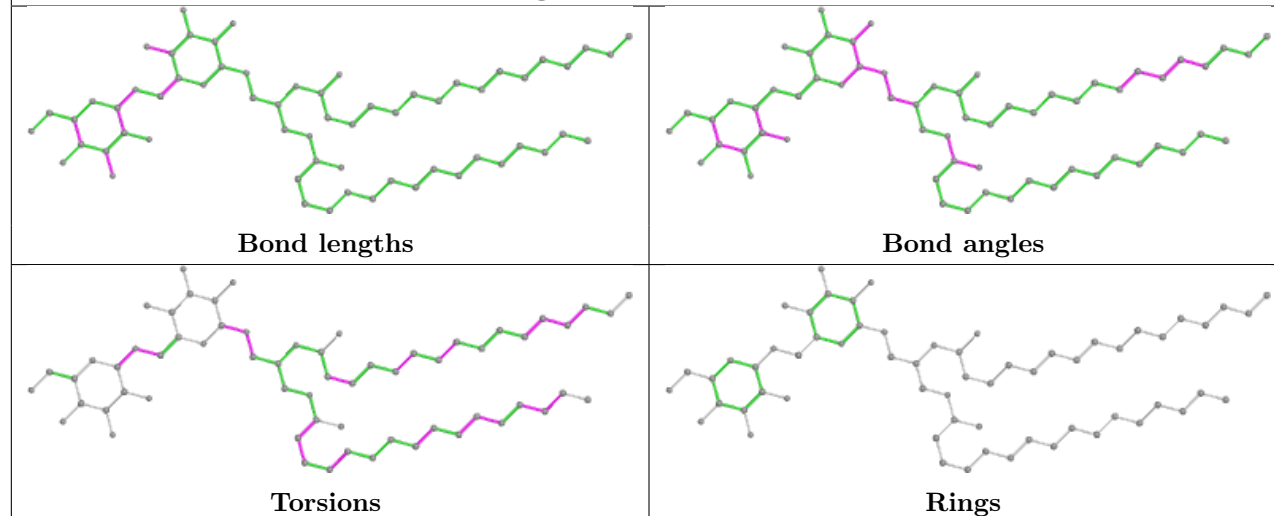




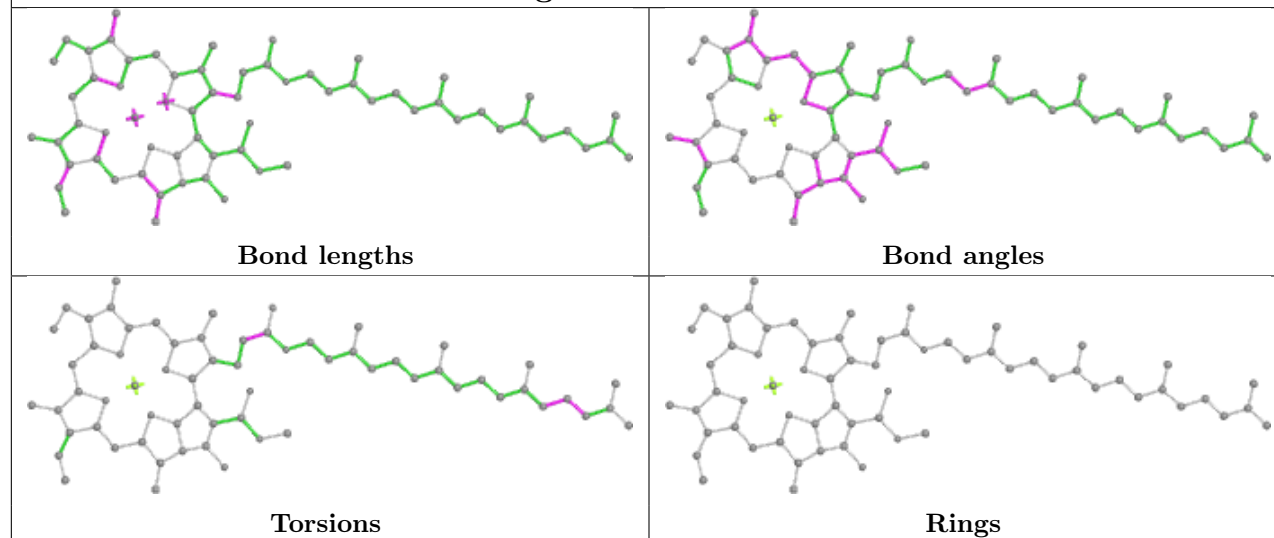
Ligand CLA b 612

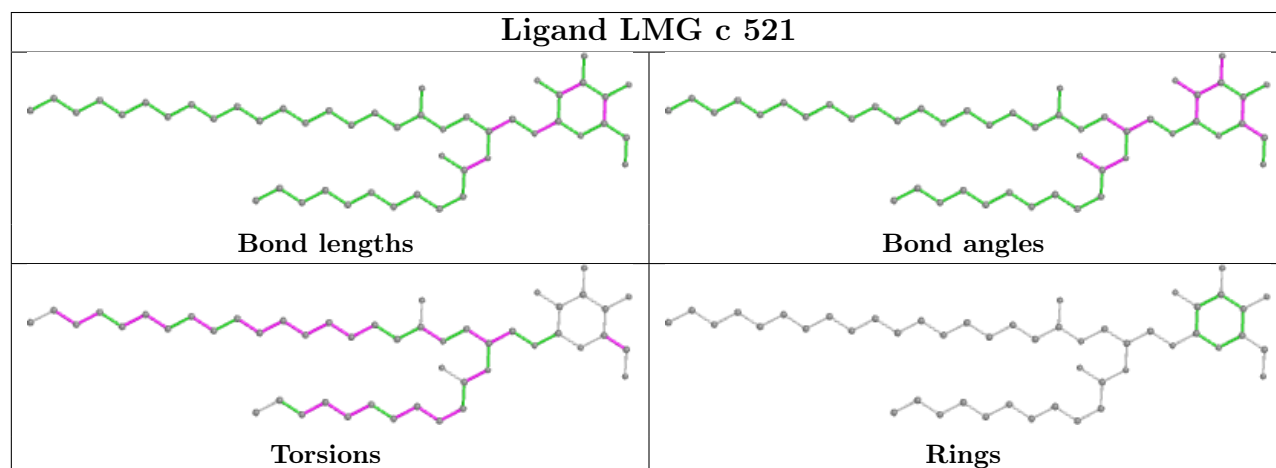
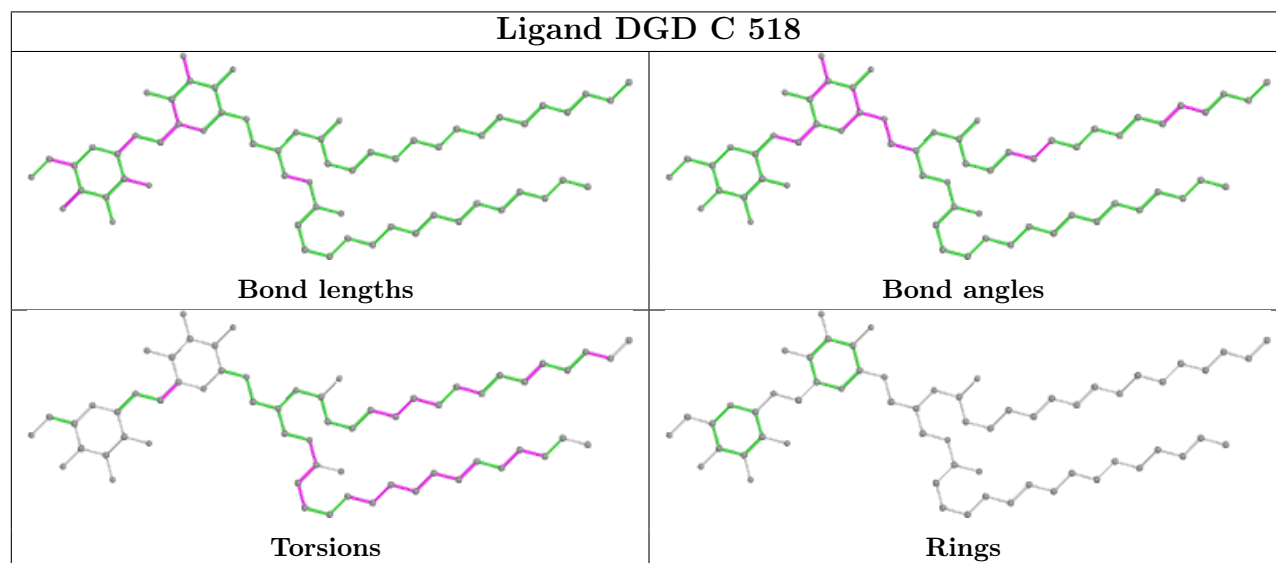
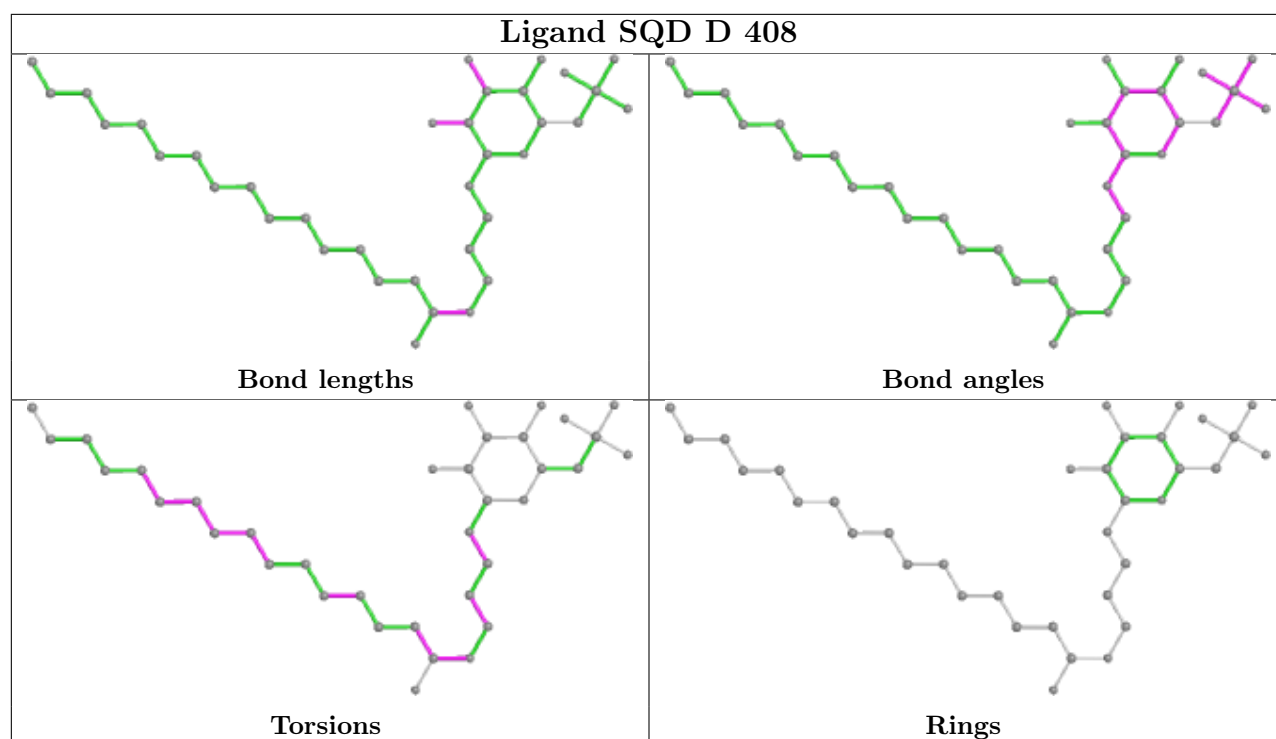


Ligand DGD c 517

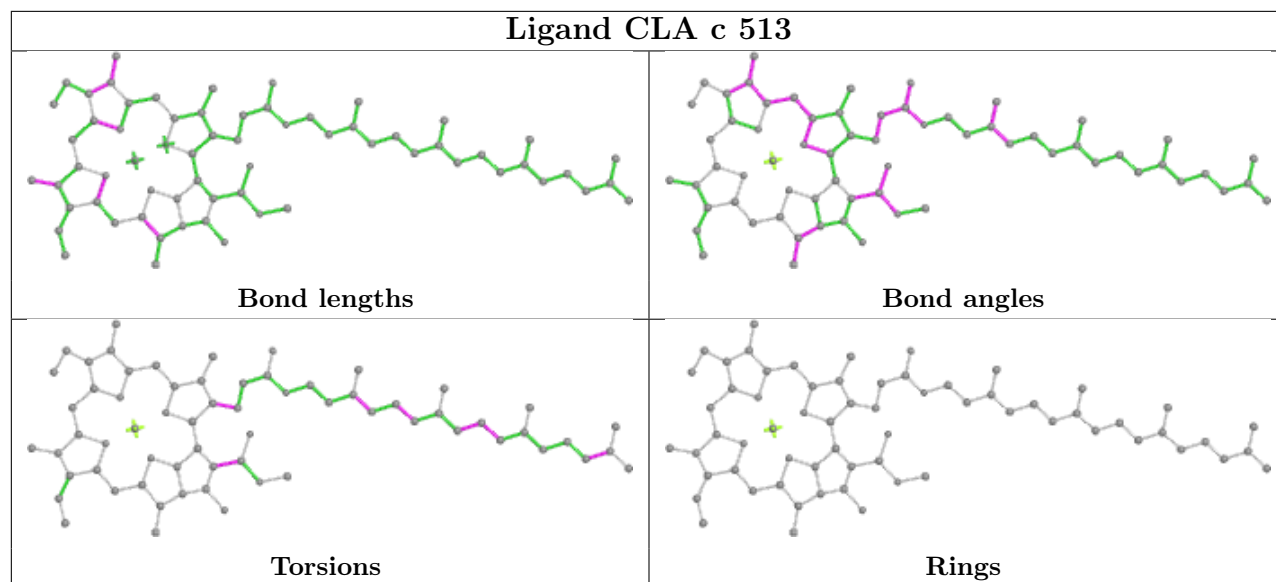


Ligand CLA b 613

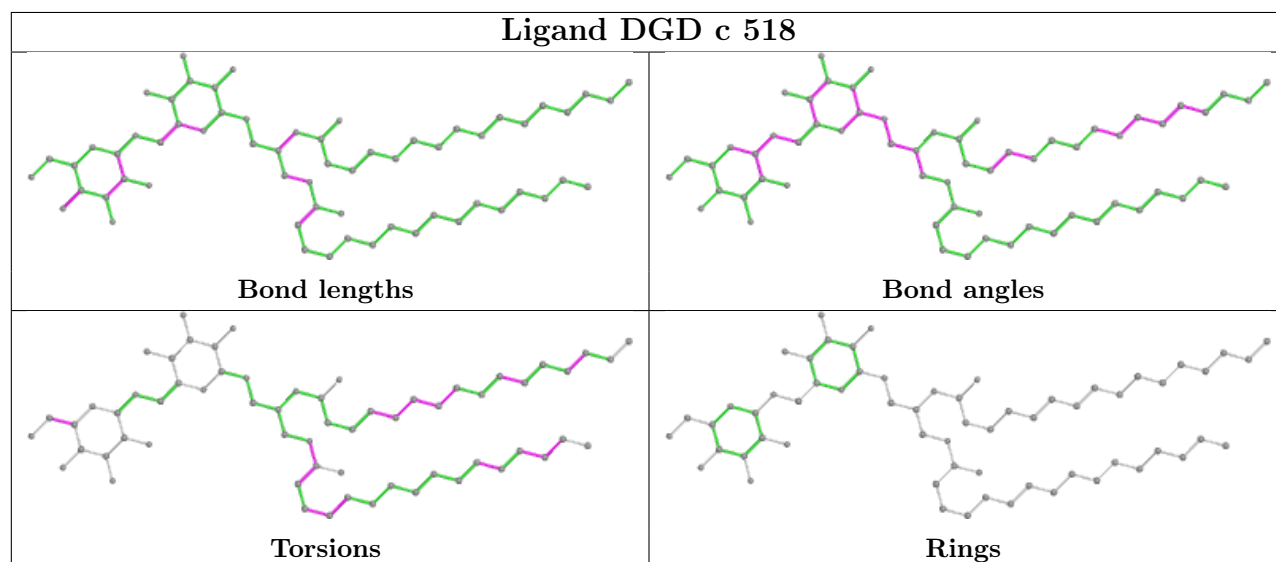




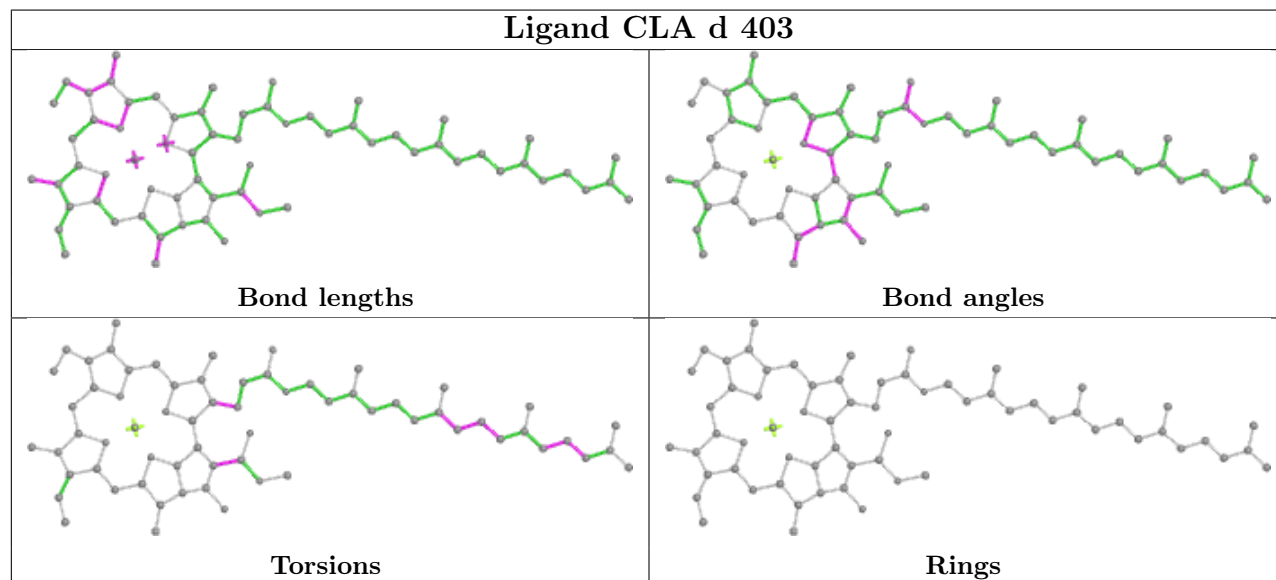
Ligand CLA c 513



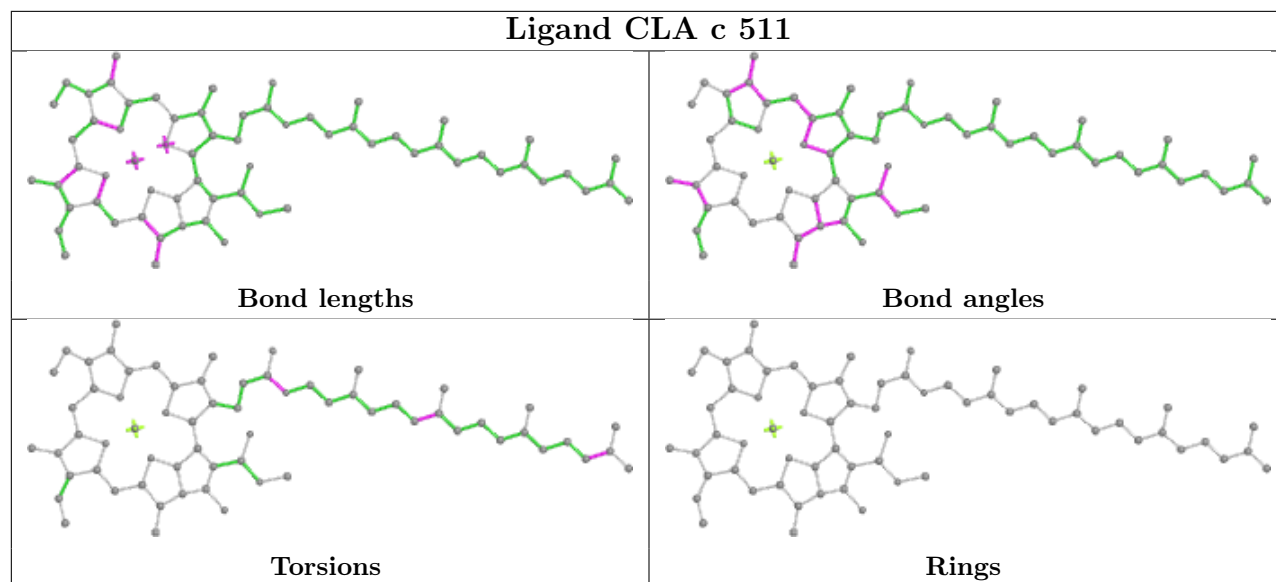
Ligand DGD c 518



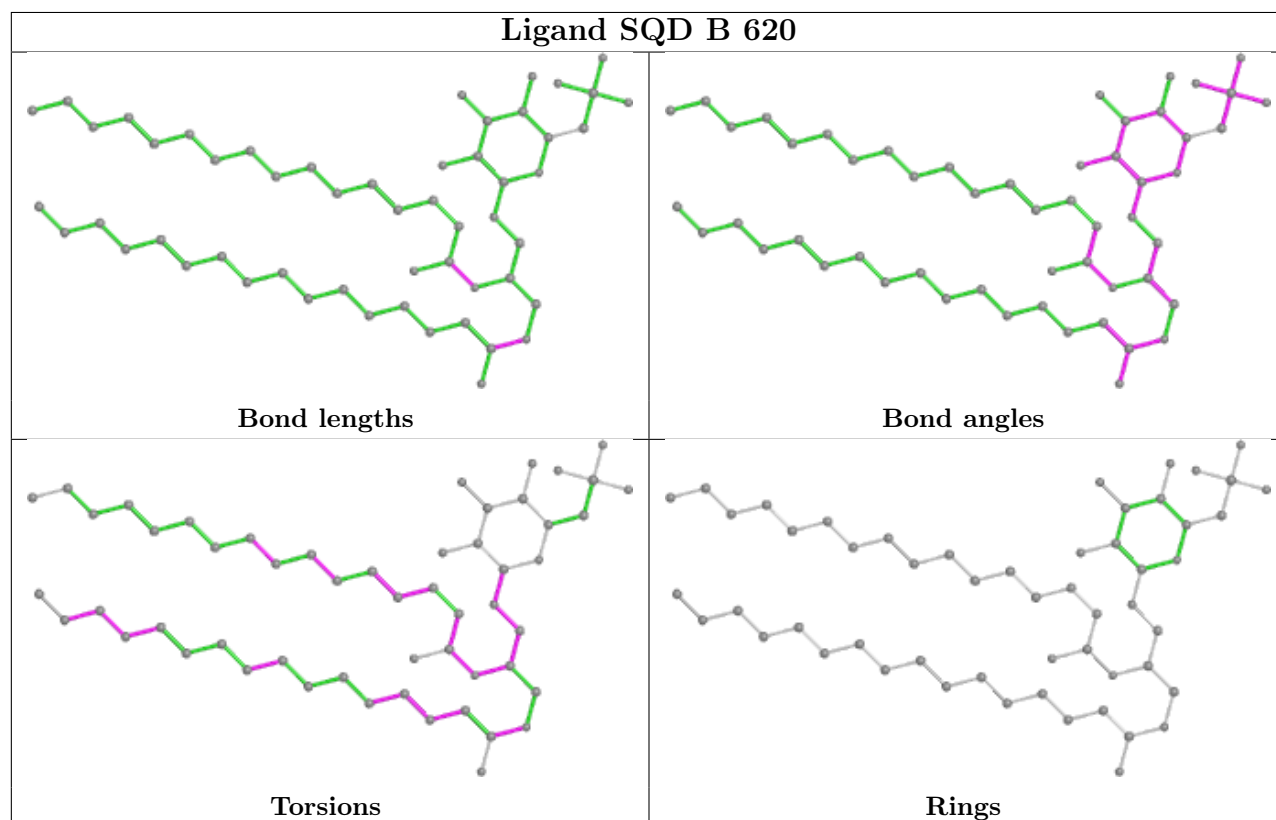
Ligand CLA d 403

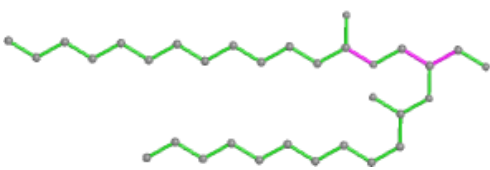
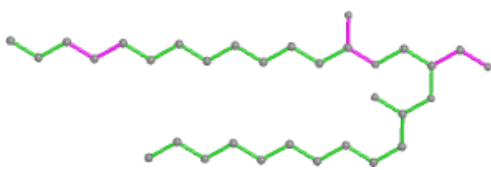
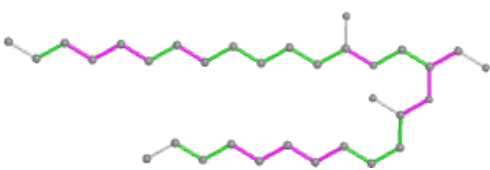



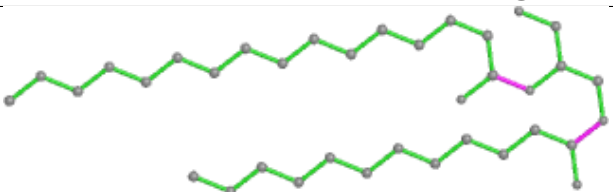
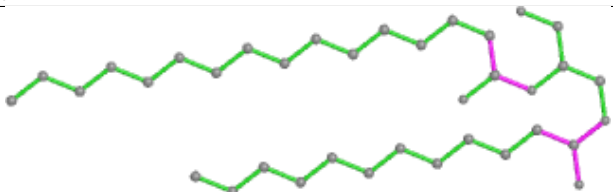
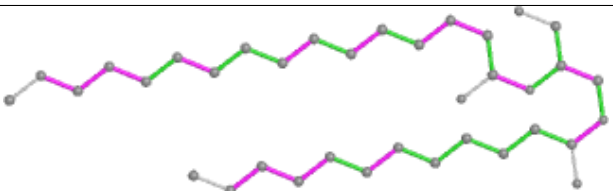
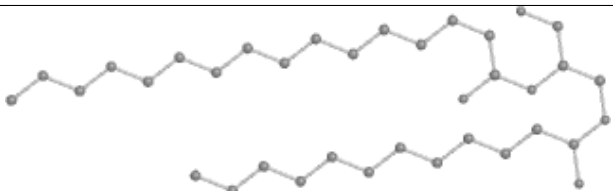
Ligand CLA c 511

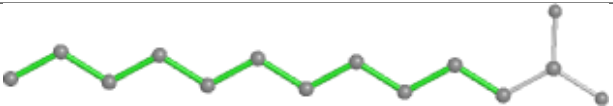
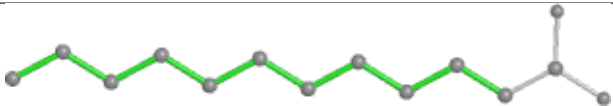
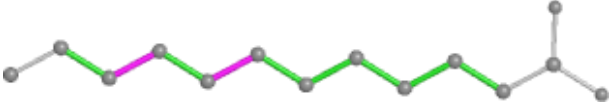
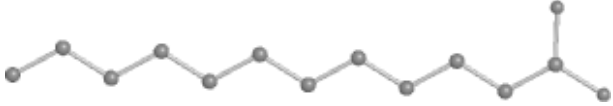


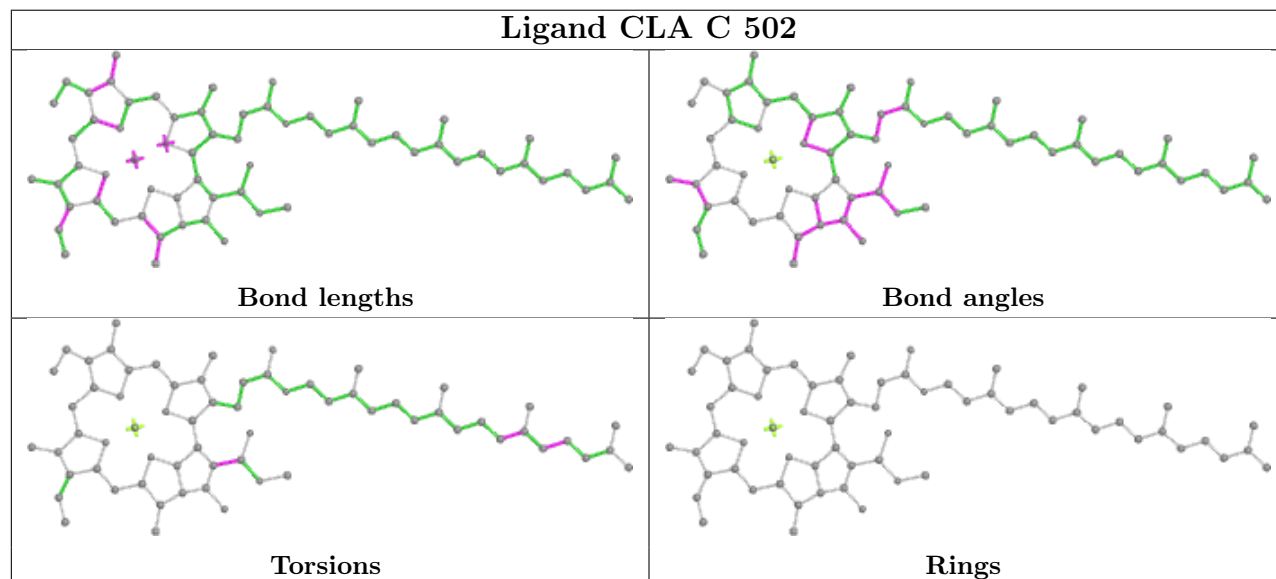
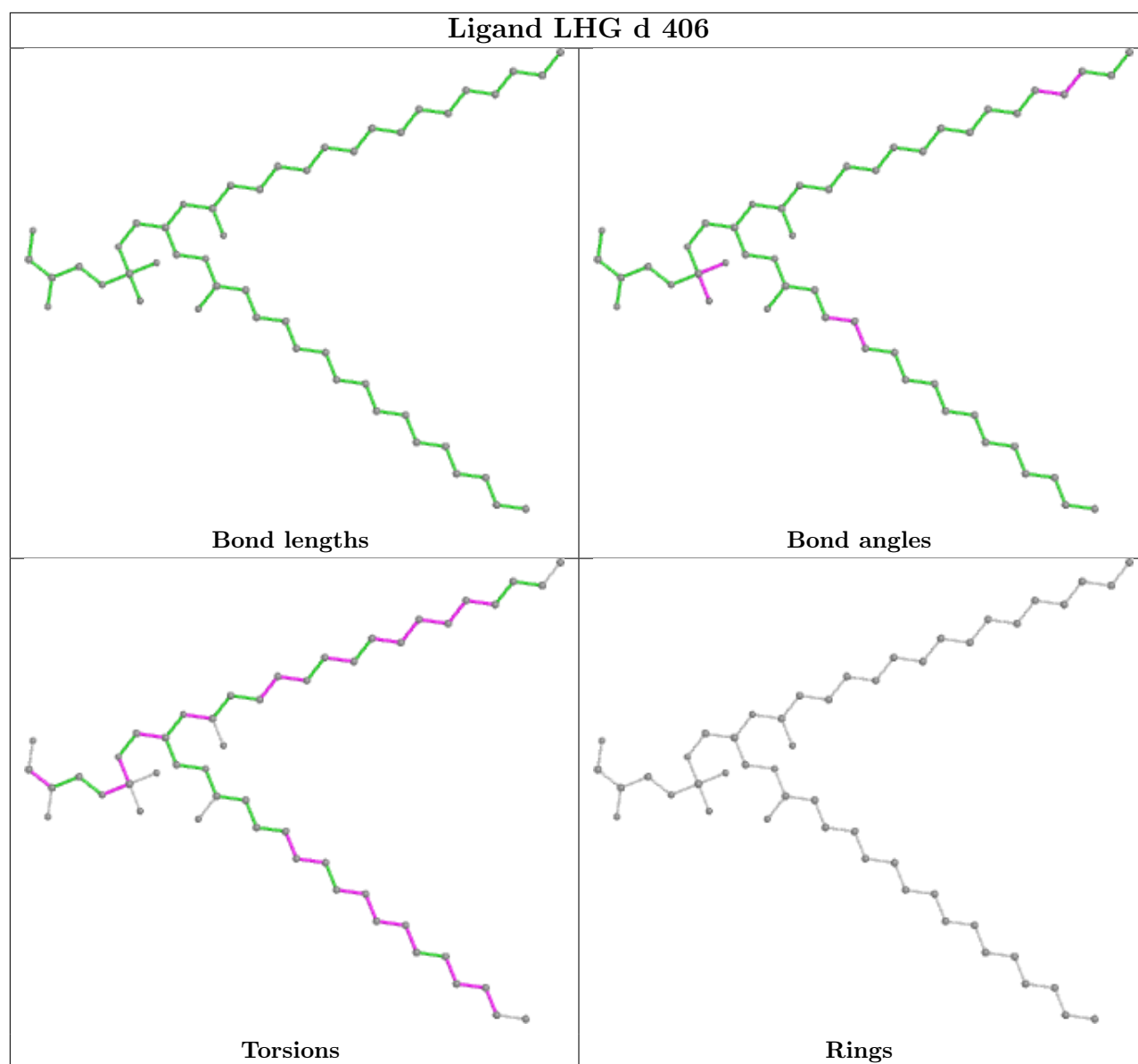
Ligand SQD B 620



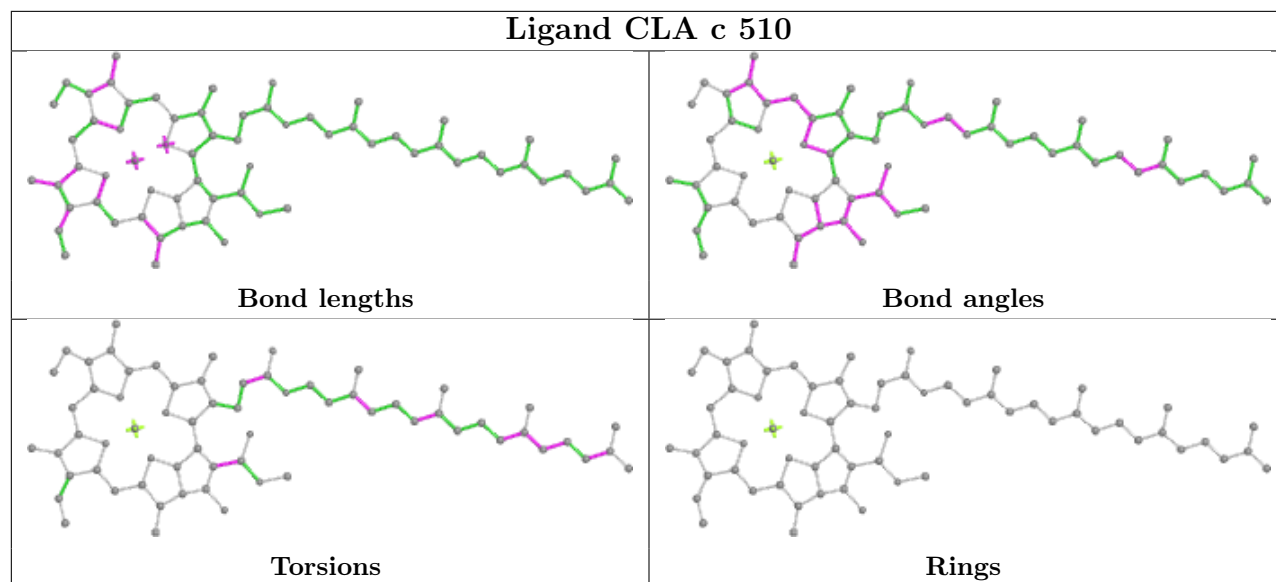
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SQD a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

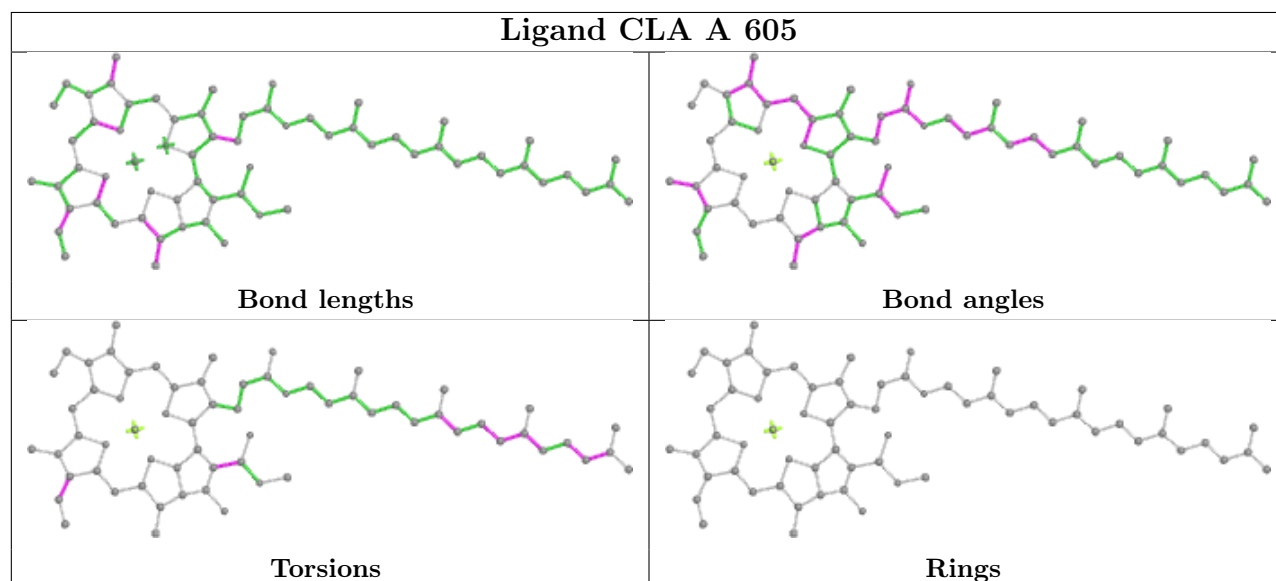
Ligand STE t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



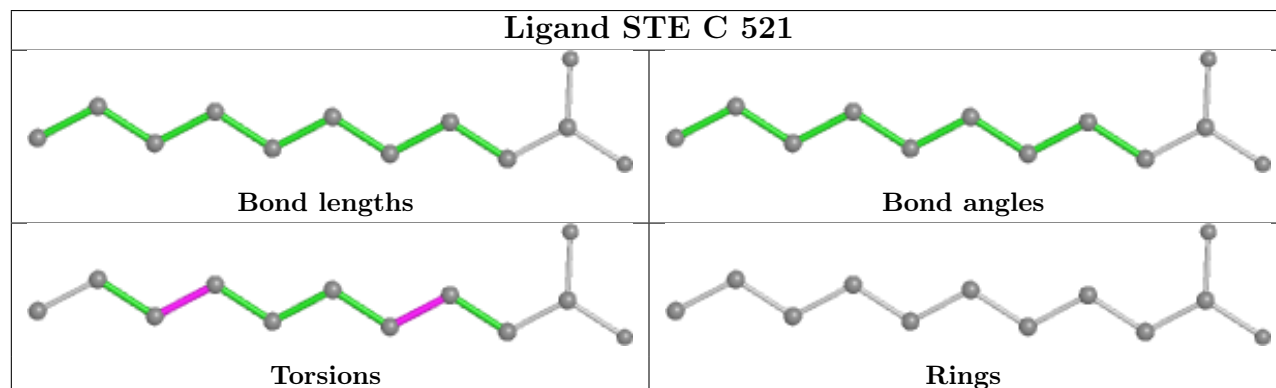
Ligand CLA c 510

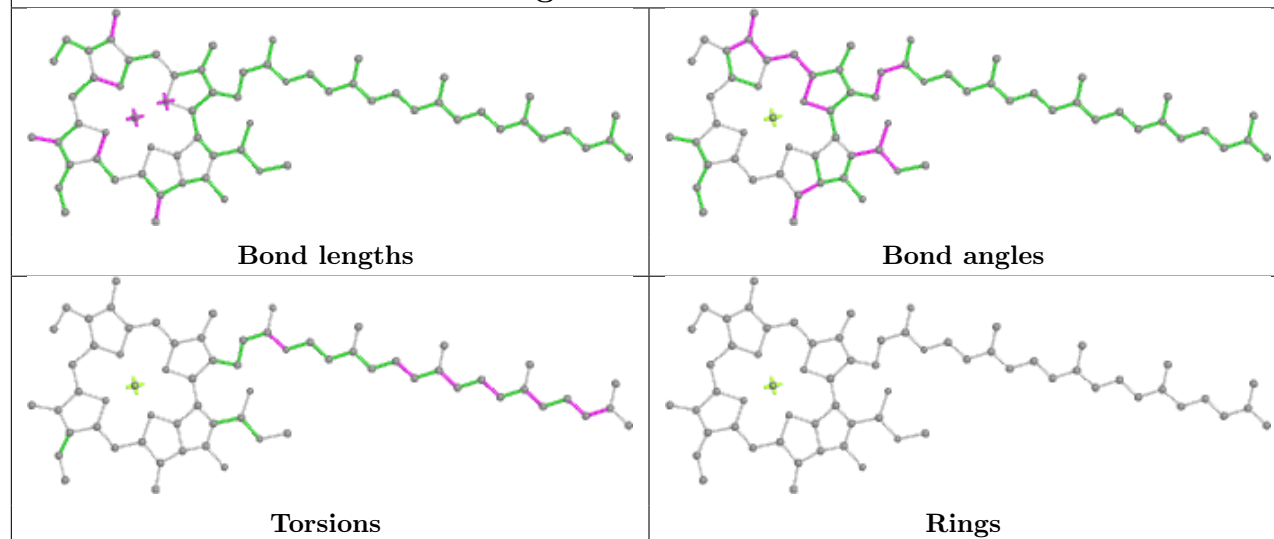
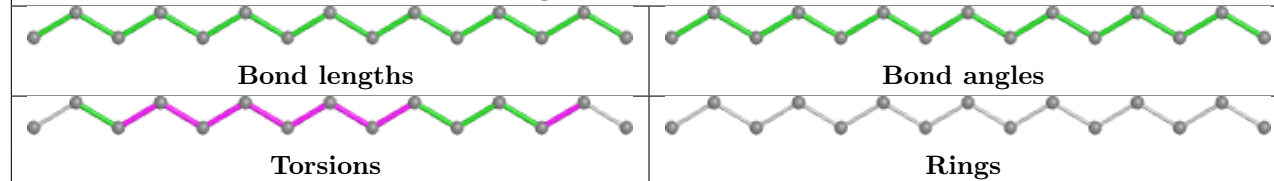
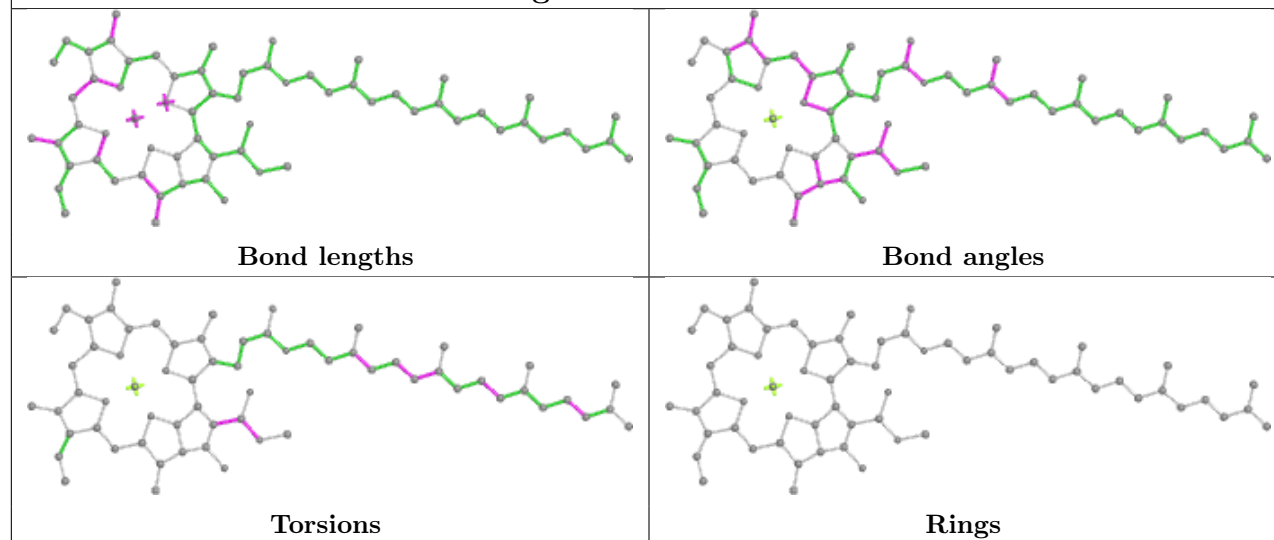


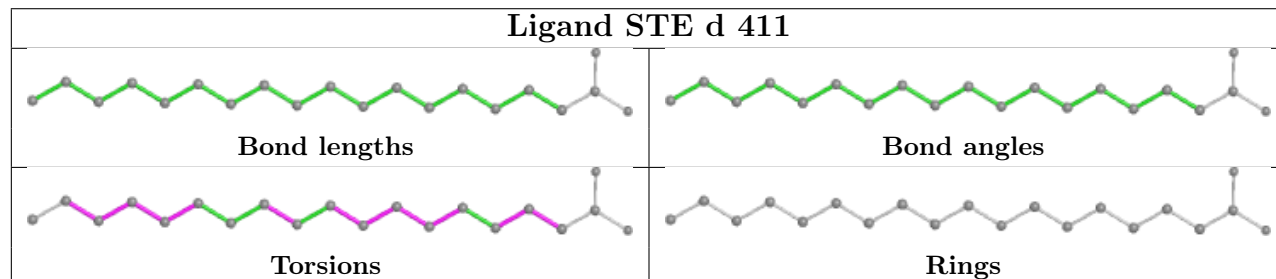
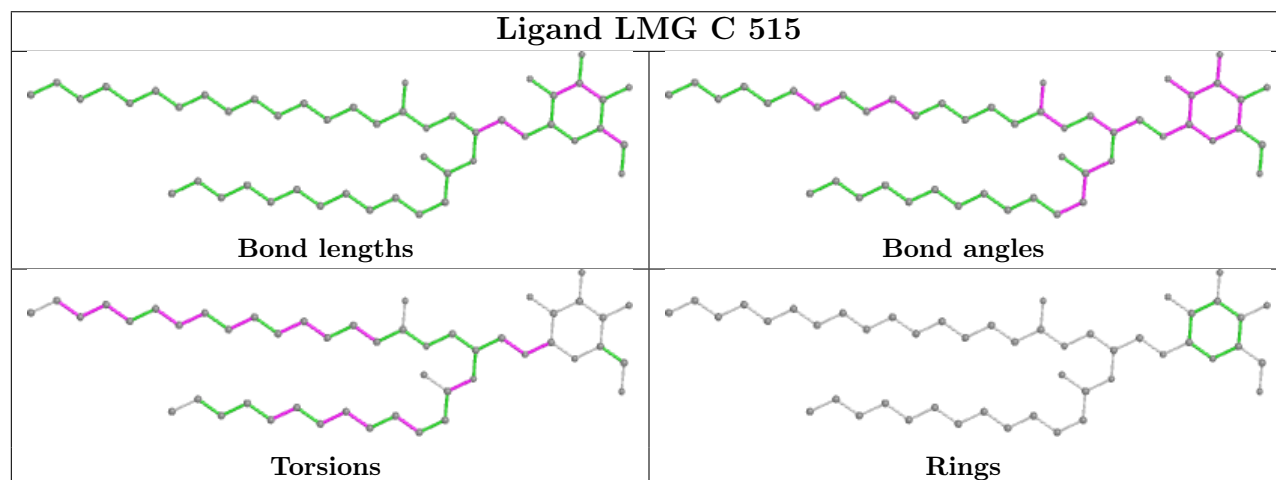
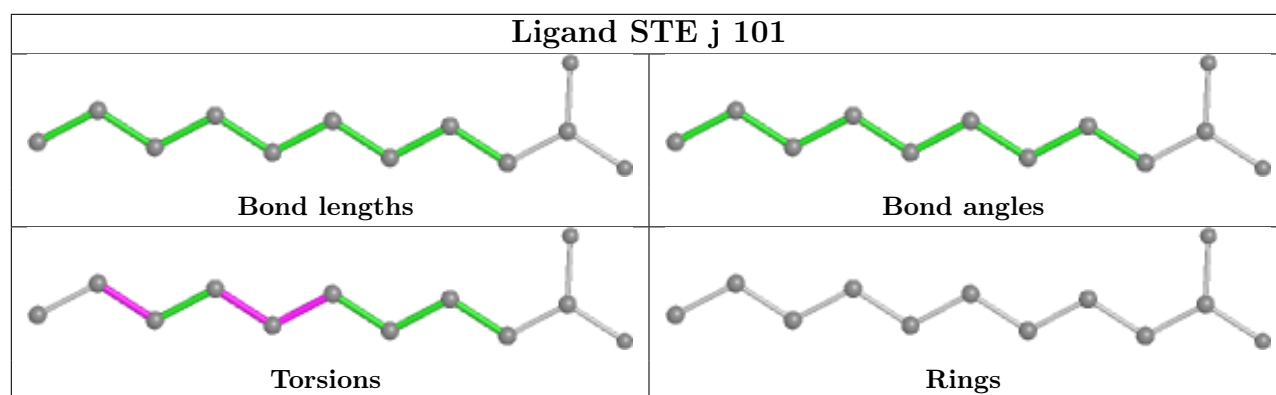
Ligand CLA A 605

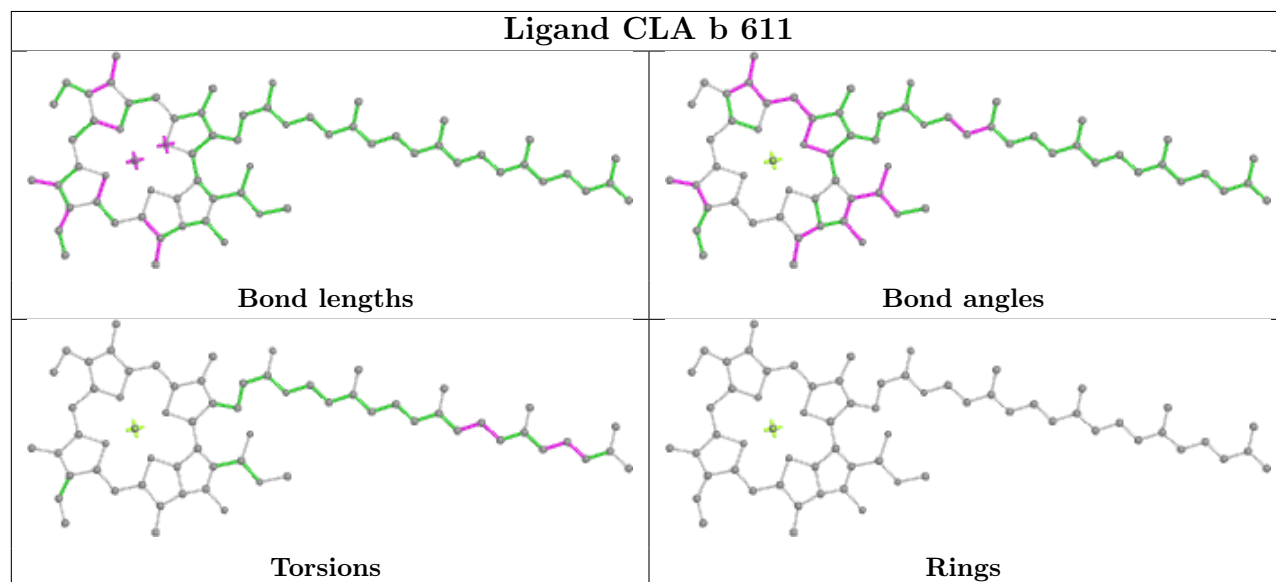
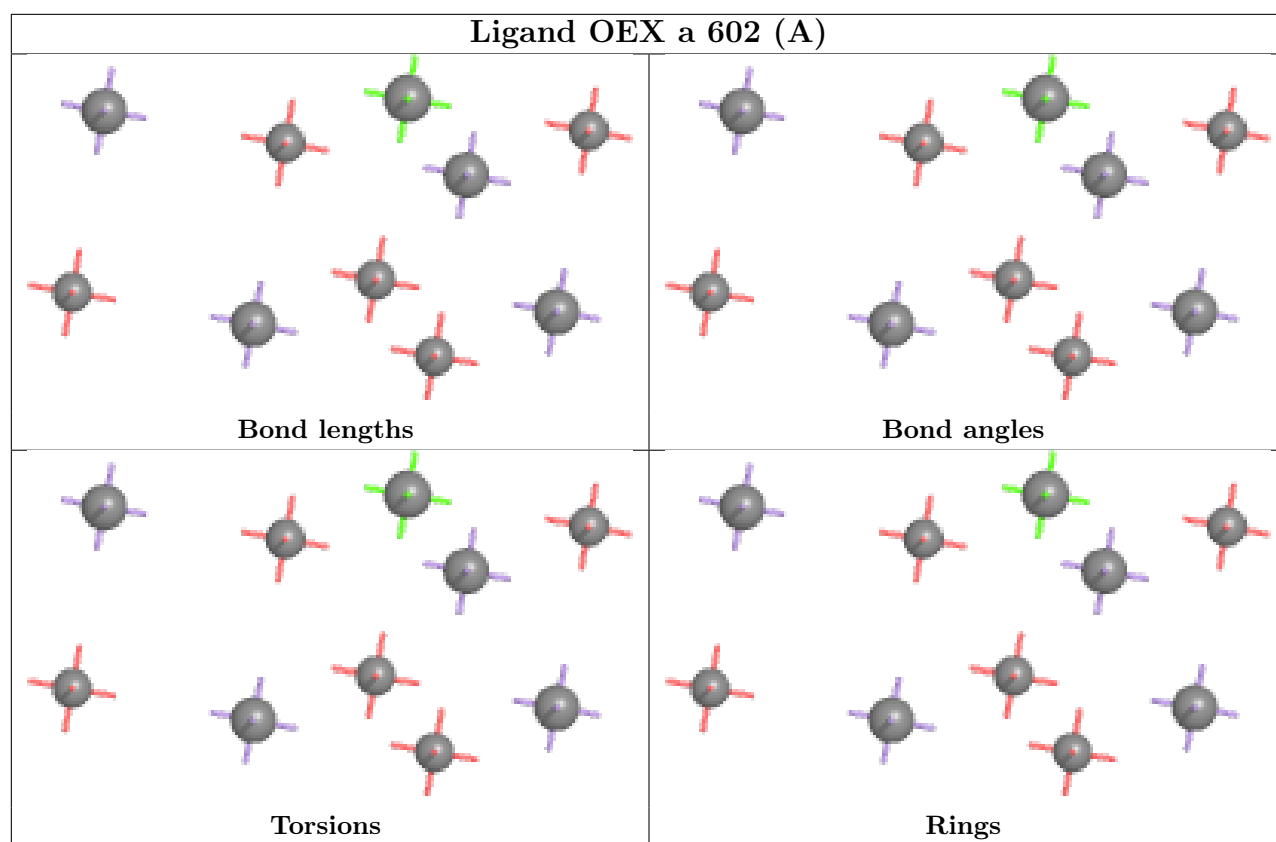


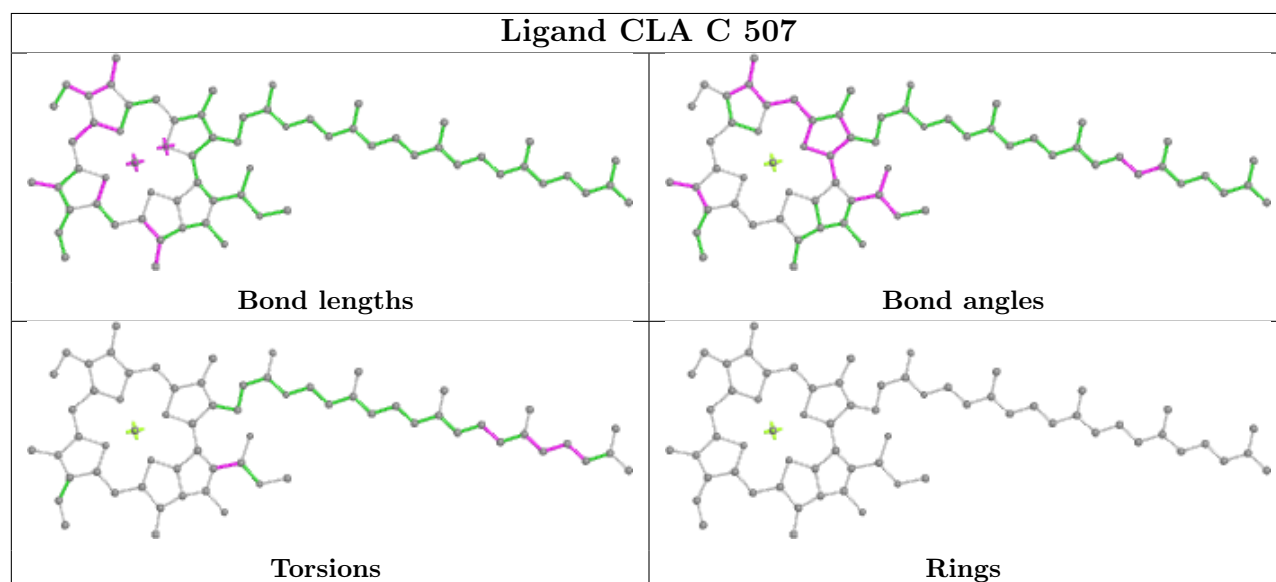
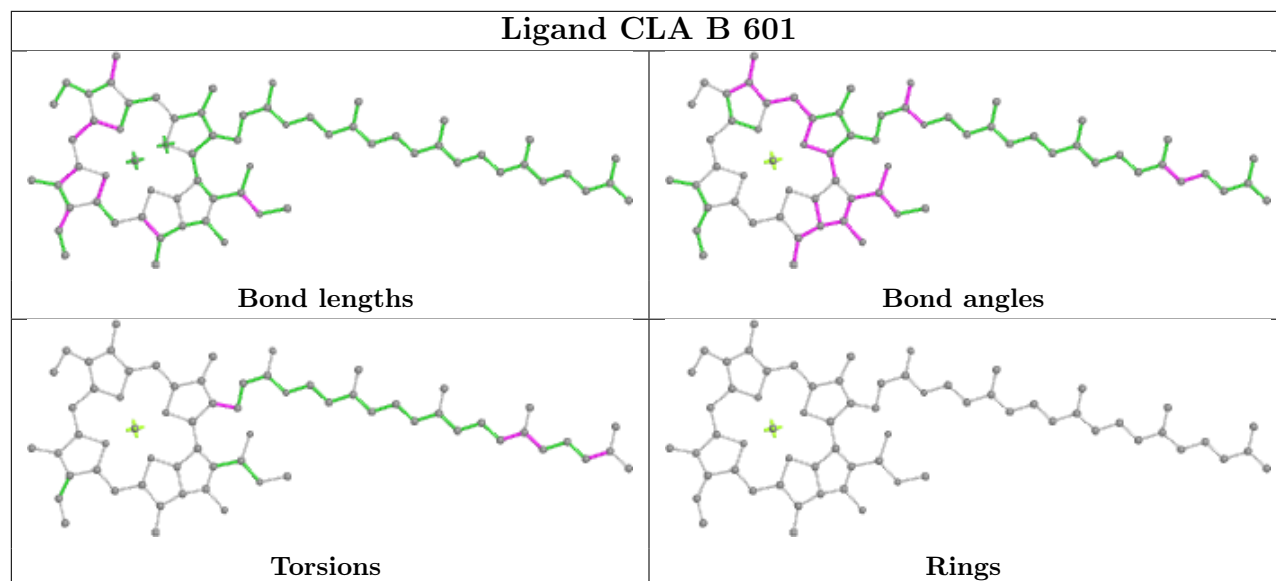
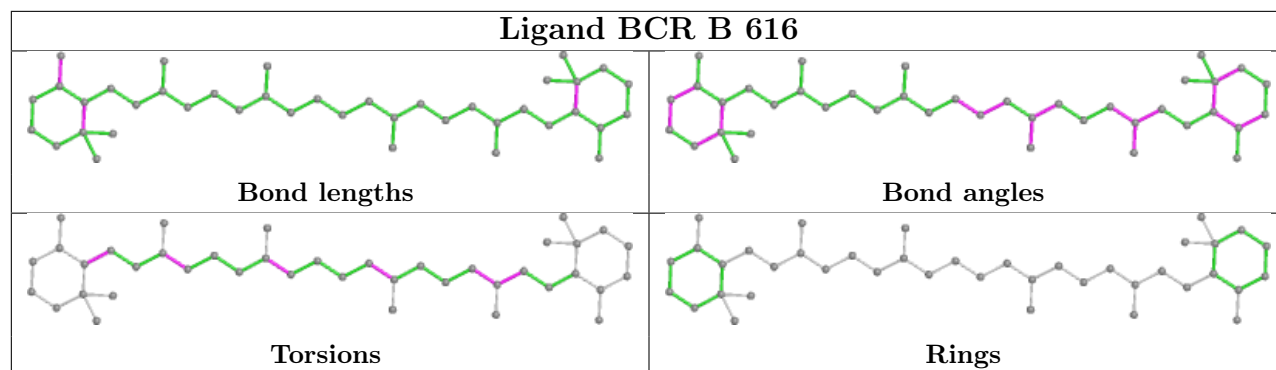
Ligand STE C 521

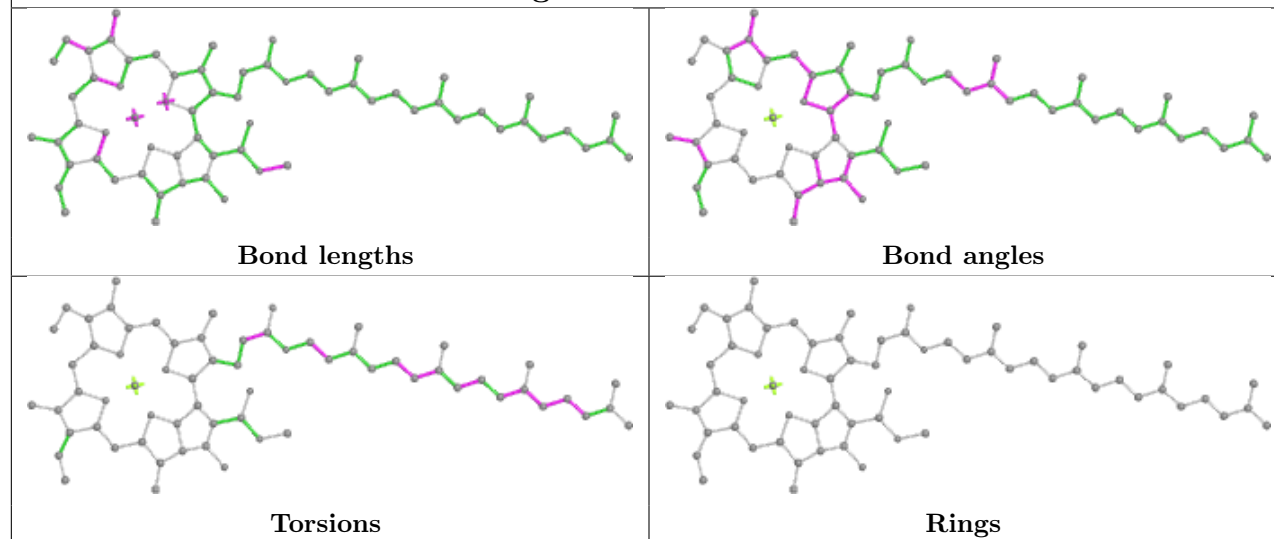
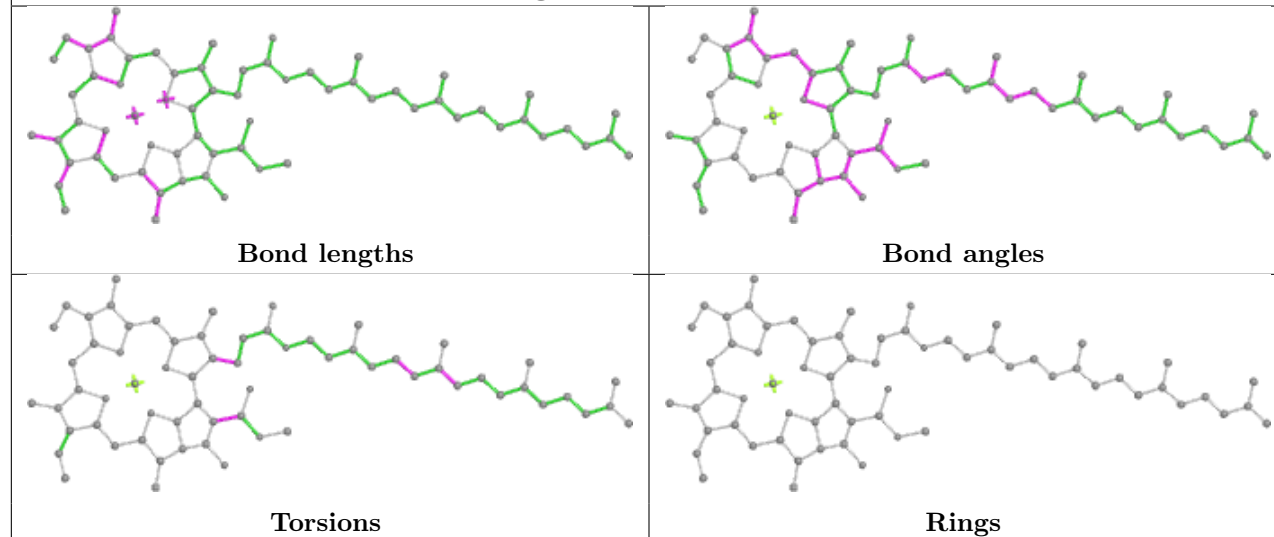
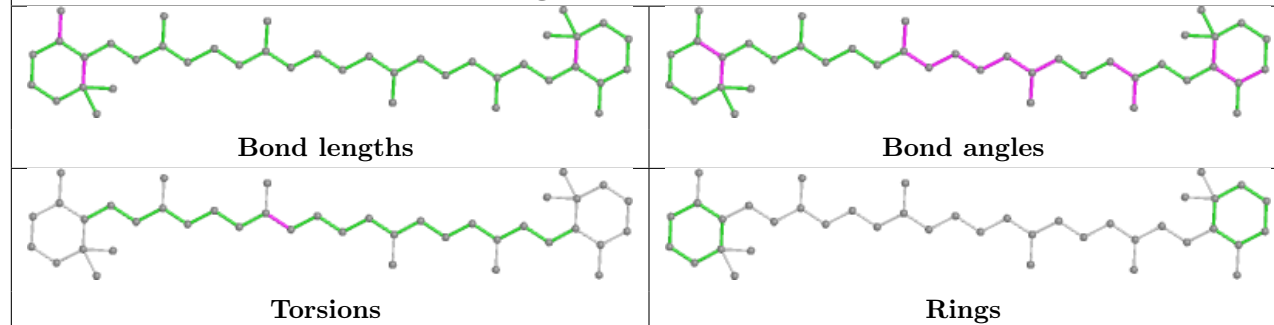


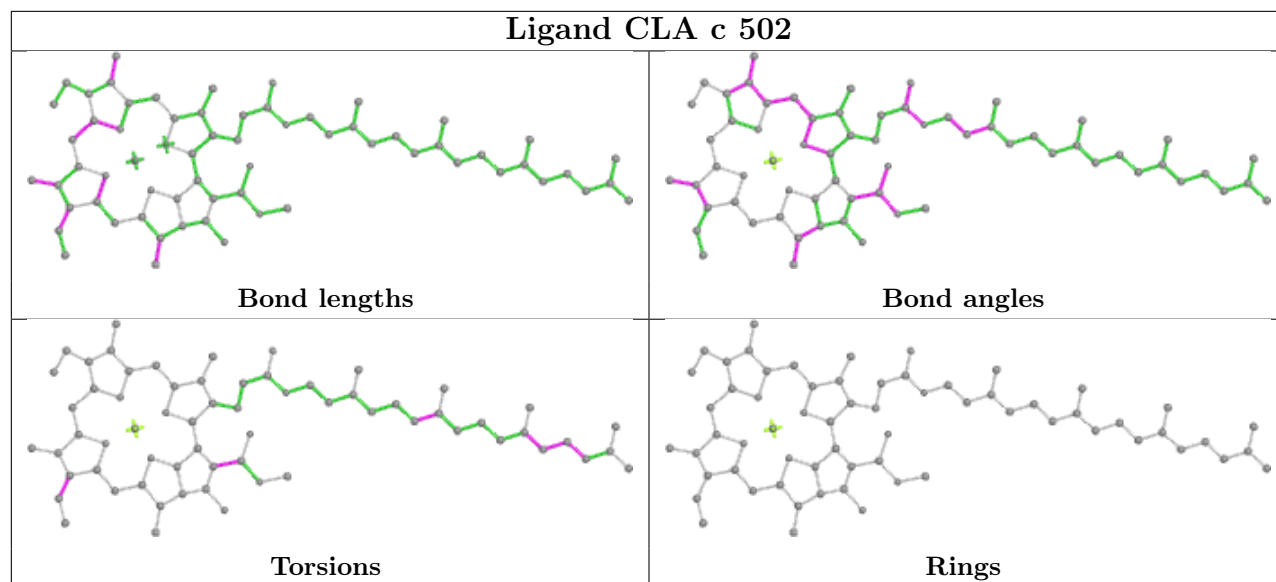
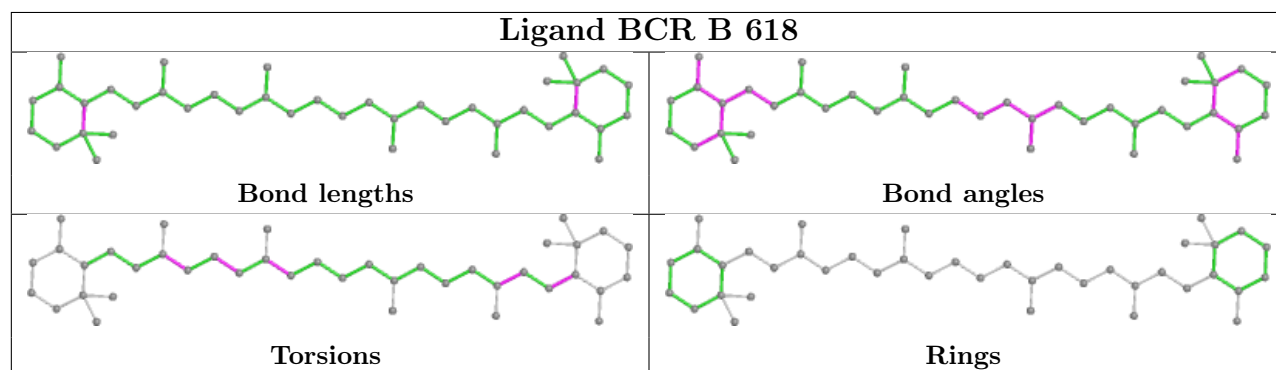
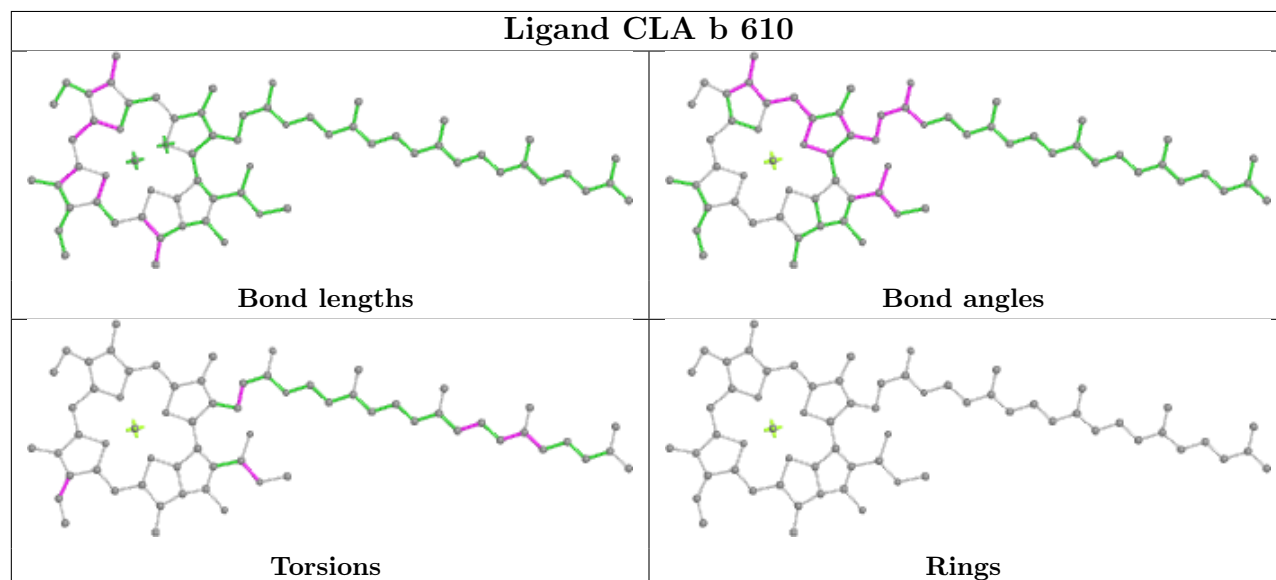
Ligand CLA a 607**Ligand STE T 103****Ligand CLA C 513**



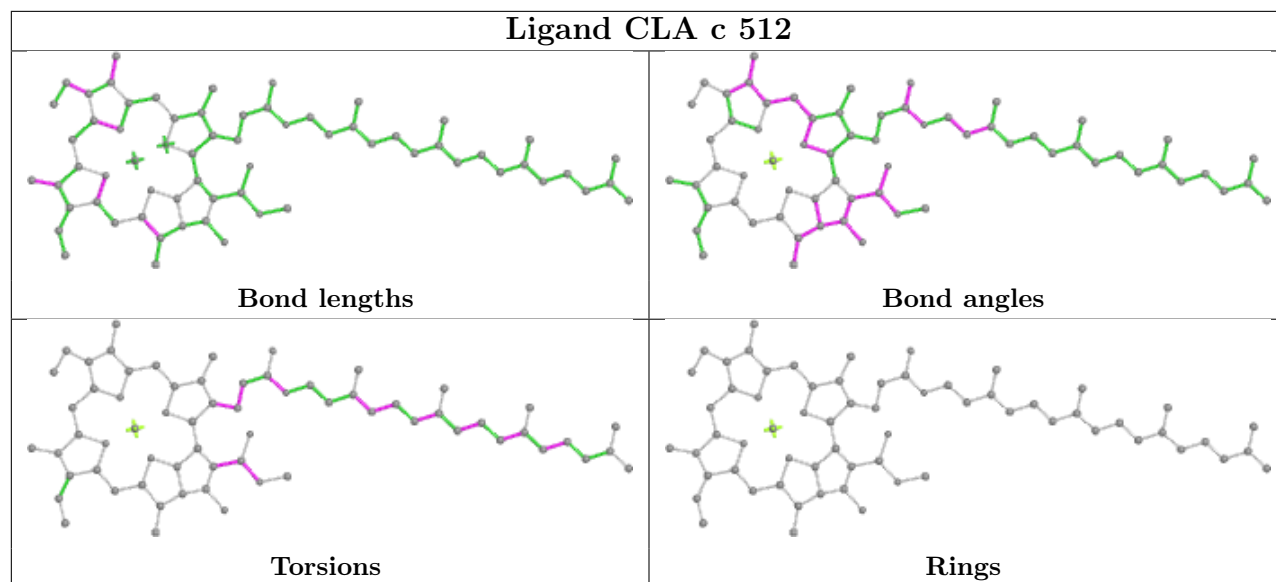




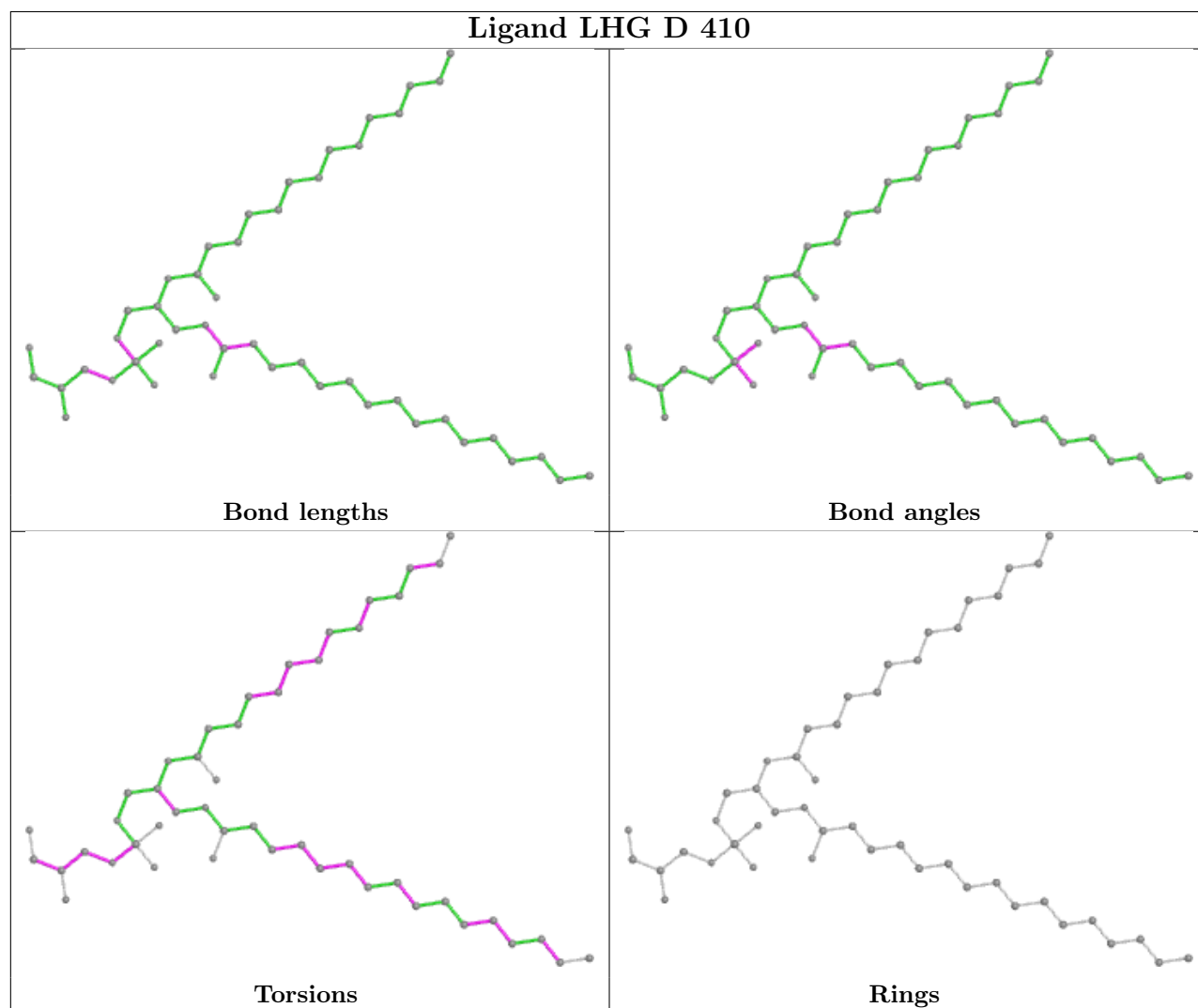
Ligand CLA B 612**Ligand CLA C 503****Ligand BCR b 618**

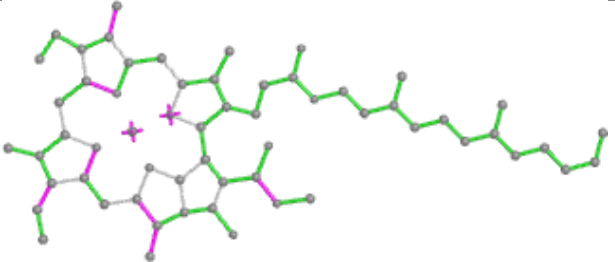
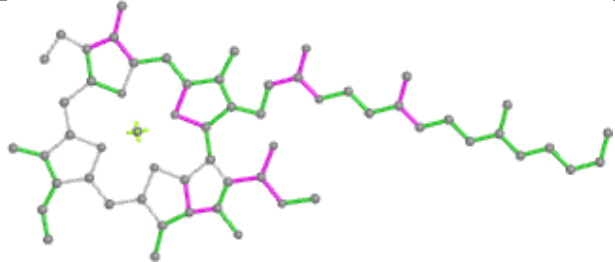
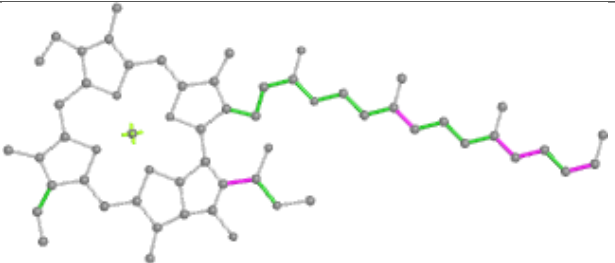
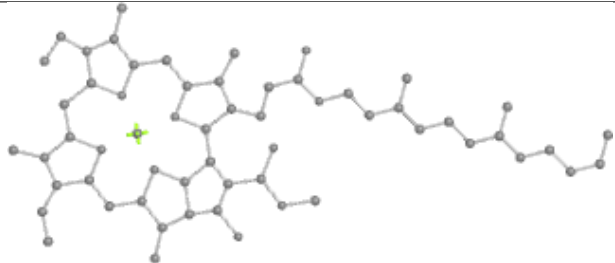
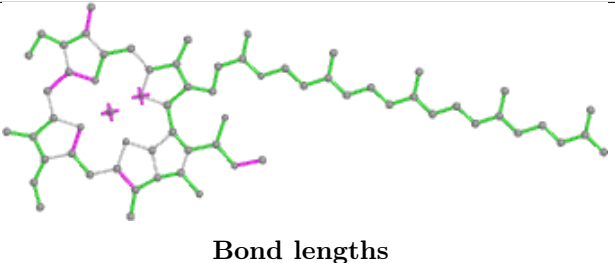
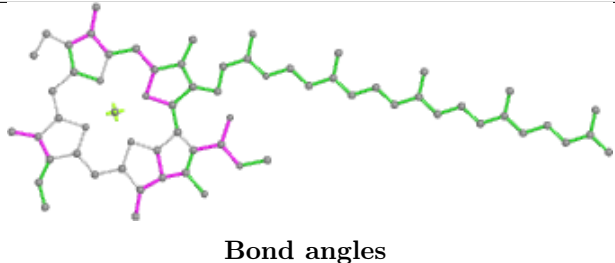
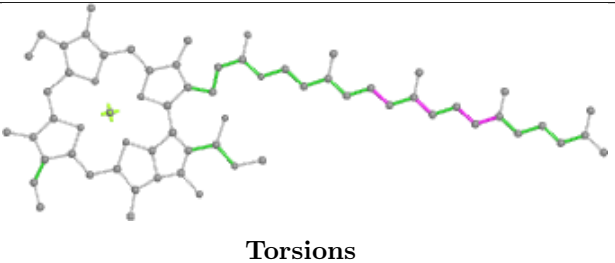
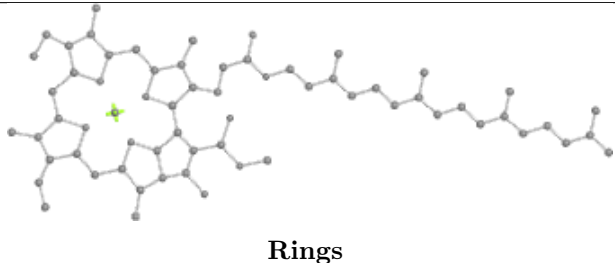
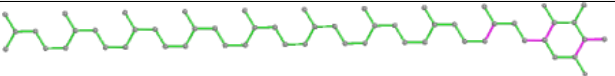
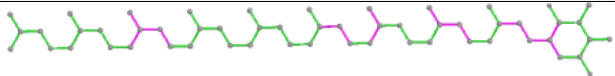
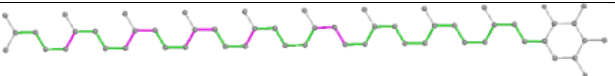
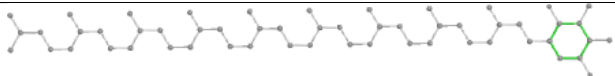
Ligand CLA c 502**Ligand BCR B 618****Ligand CLA b 610**

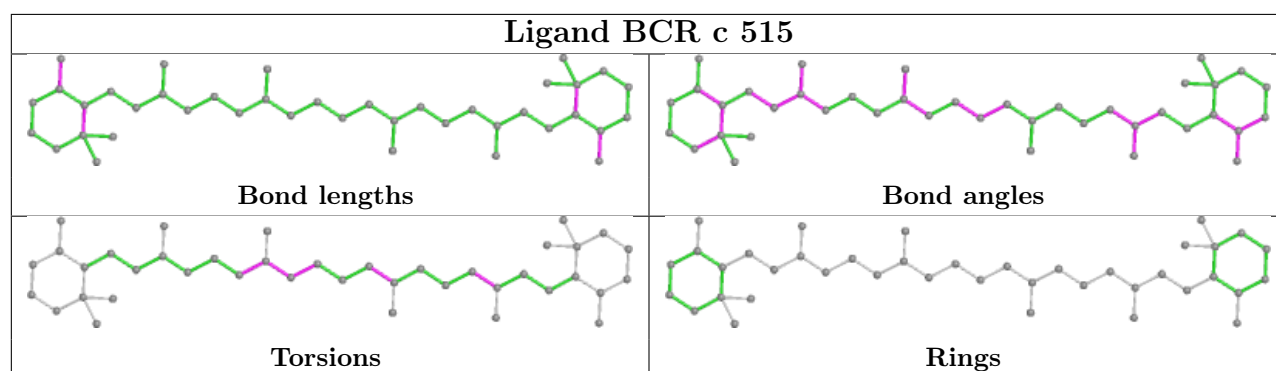
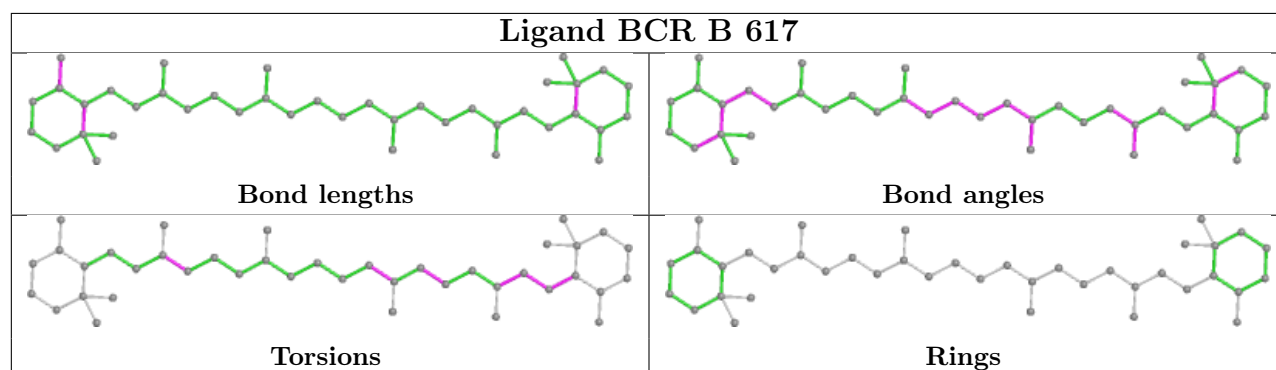
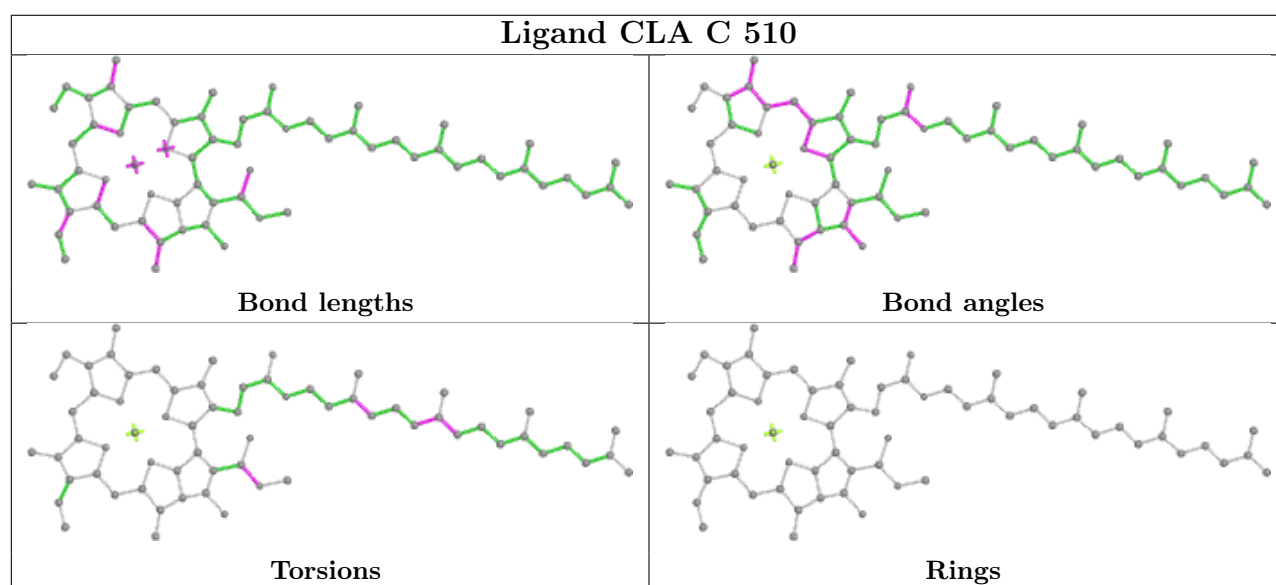
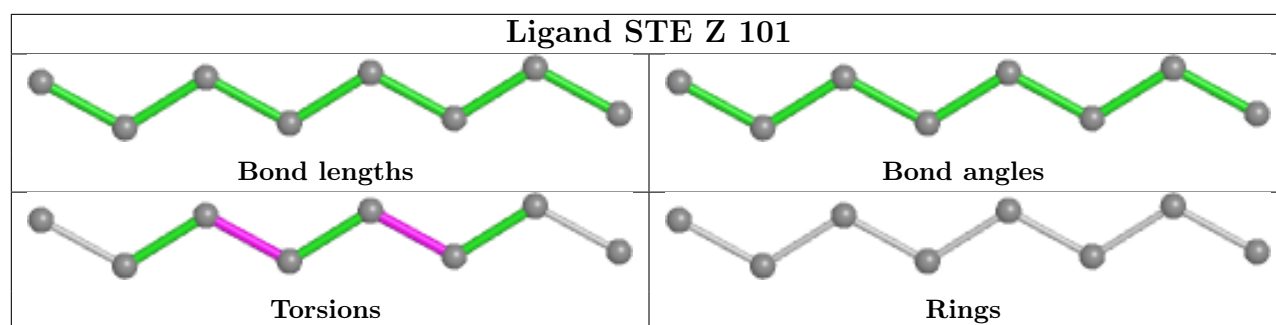
Ligand CLA c 512

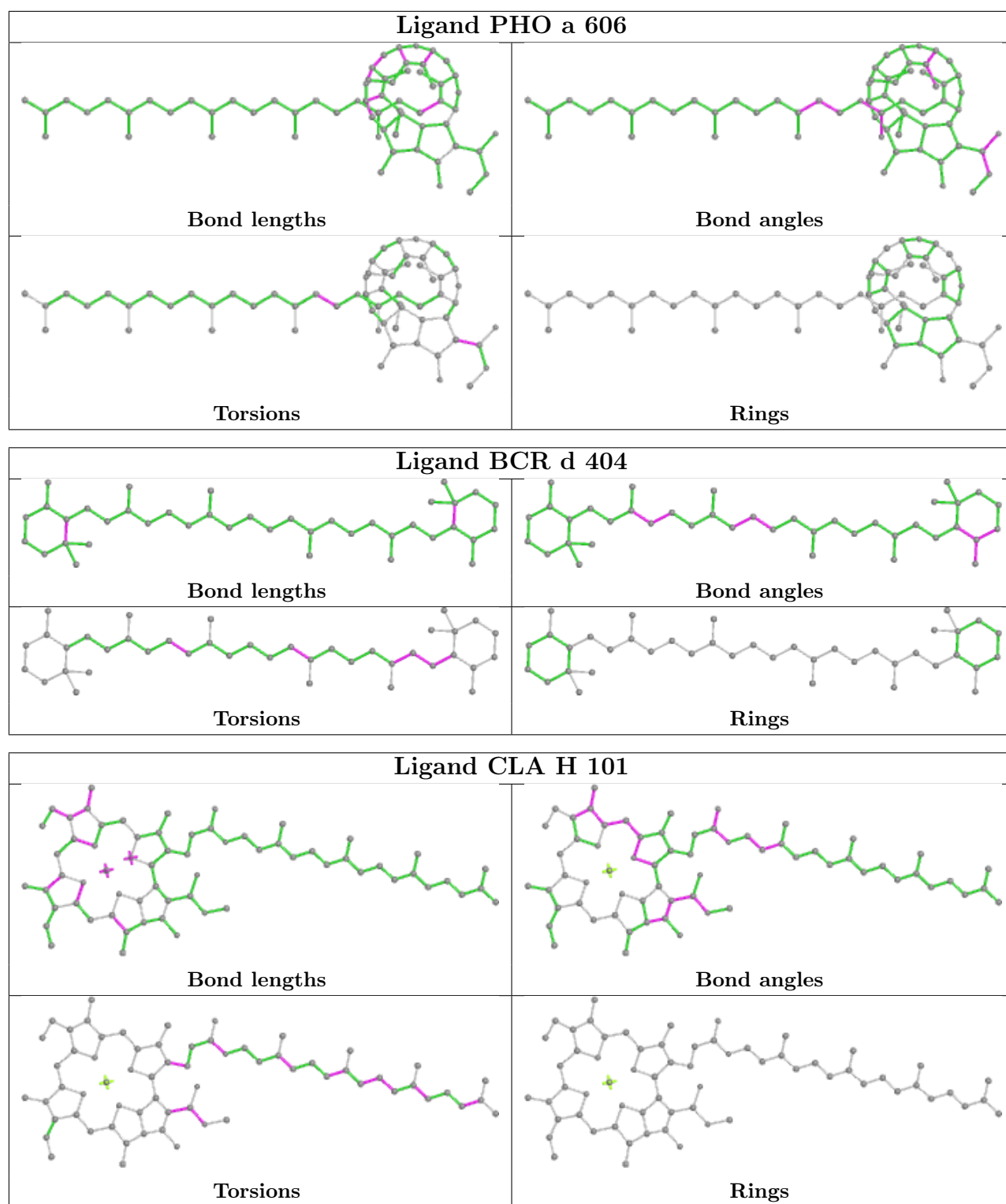


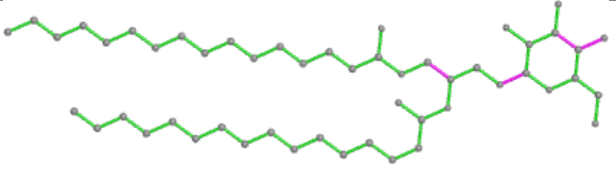
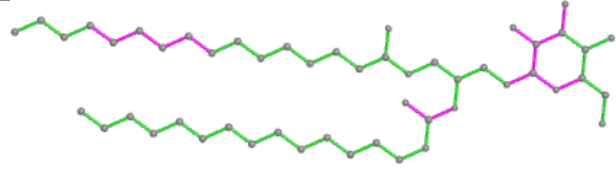
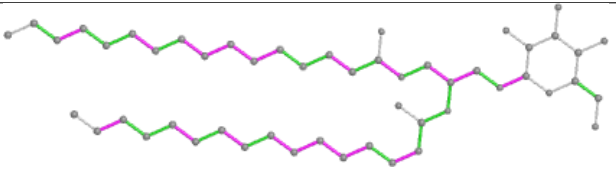
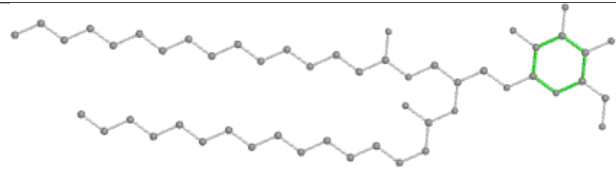
Ligand LHG D 410

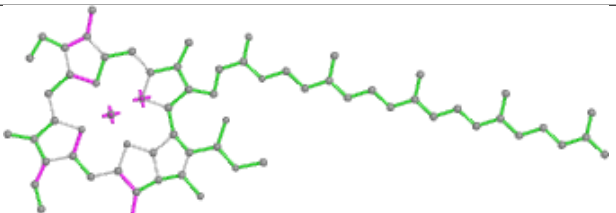
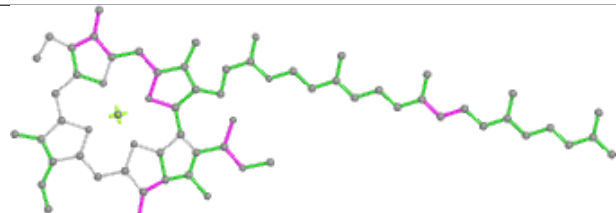
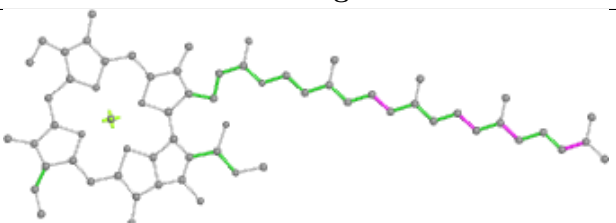
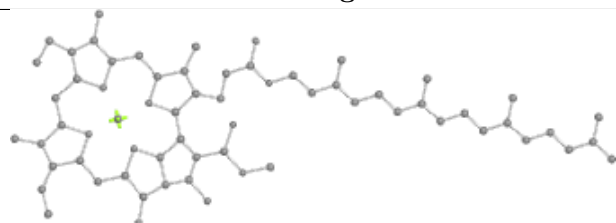


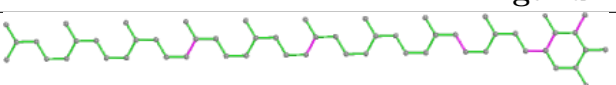
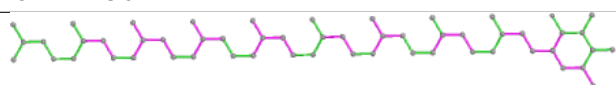
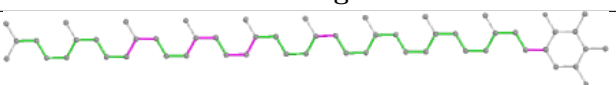
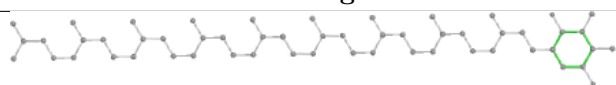
Ligand CLA C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 605	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 405	
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 <p>Torsions</p>	 <p>Rings</p>

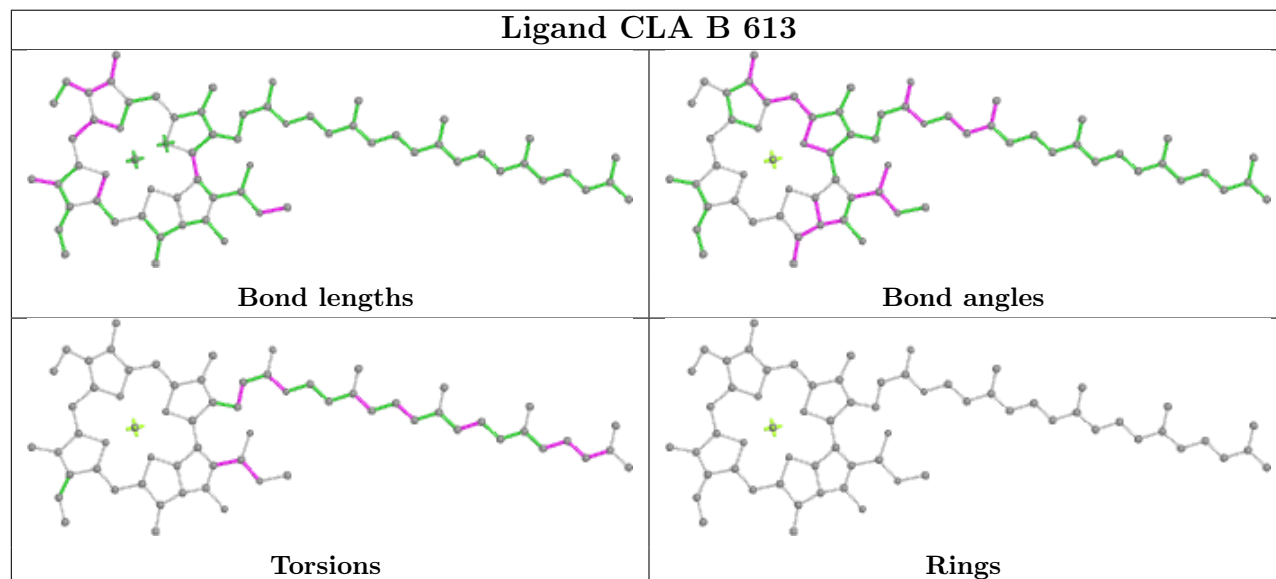
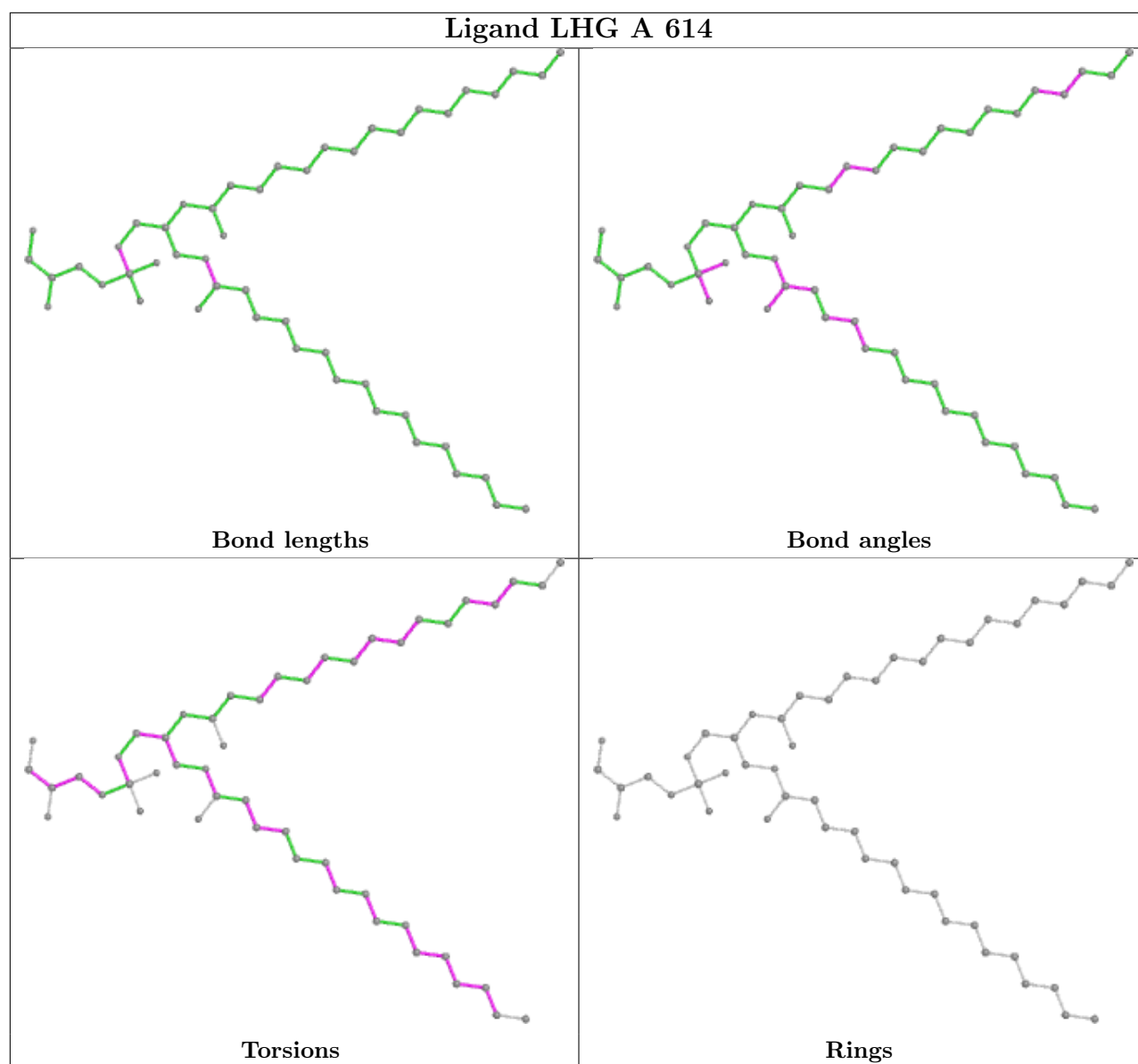


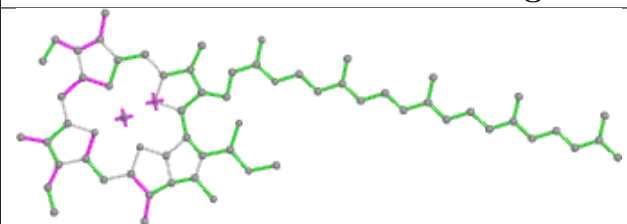
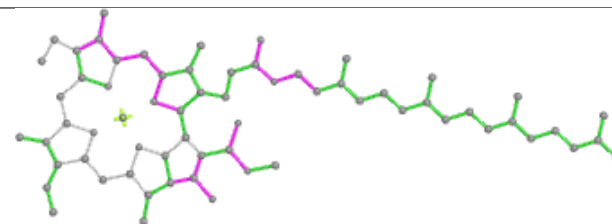
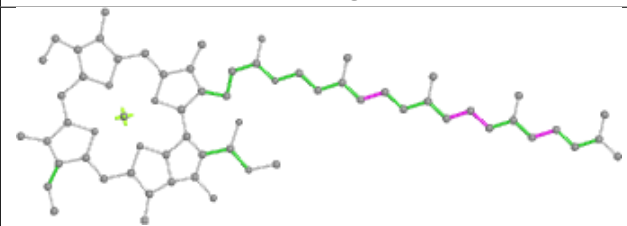
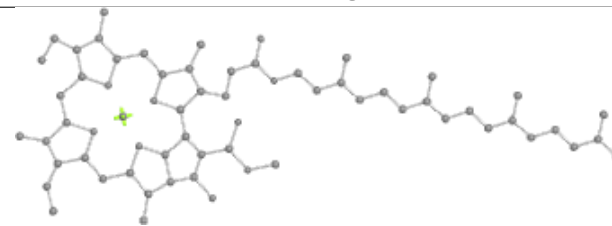


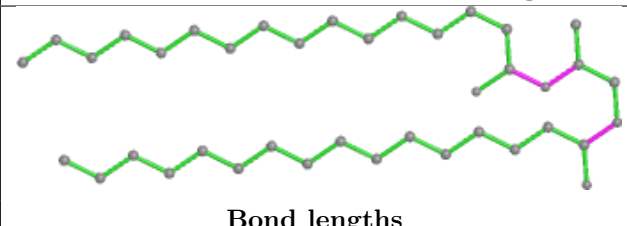
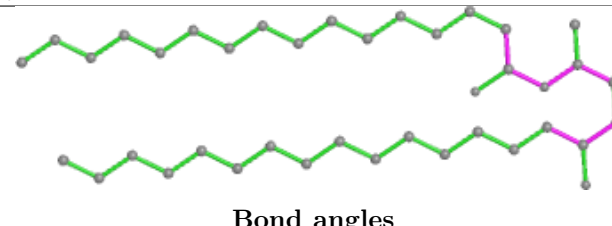
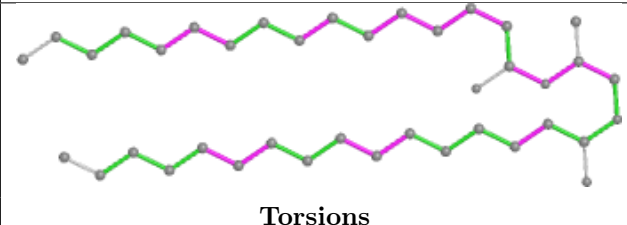
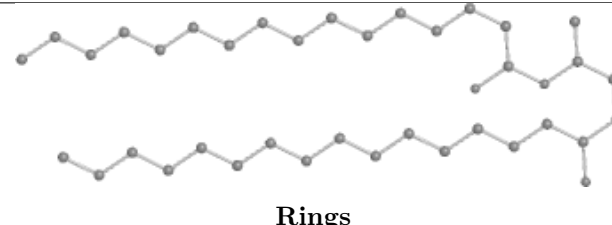
Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

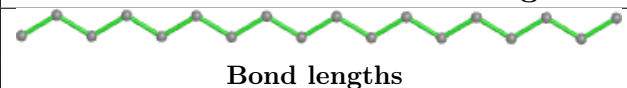
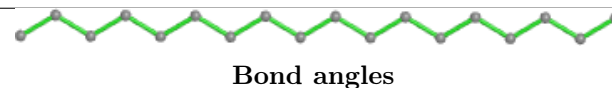
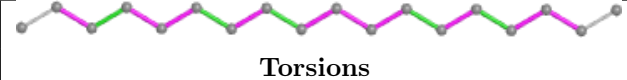

Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

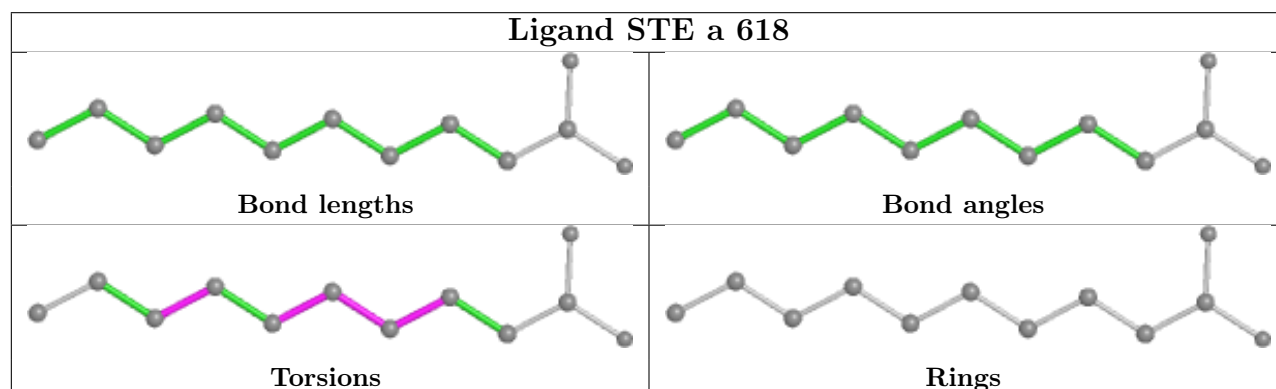
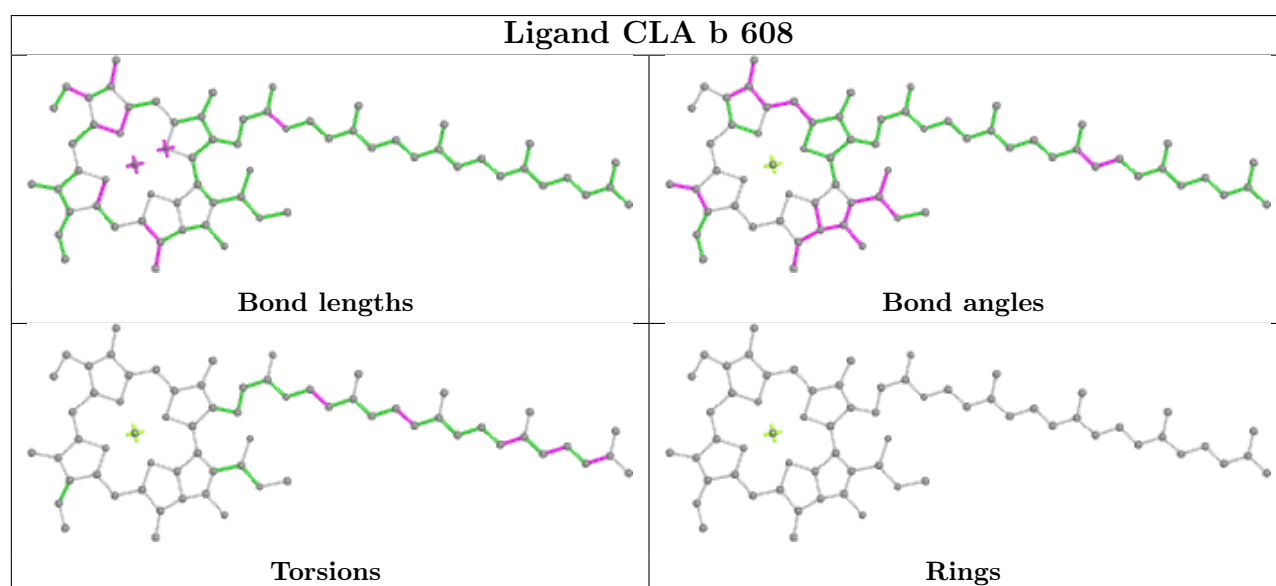
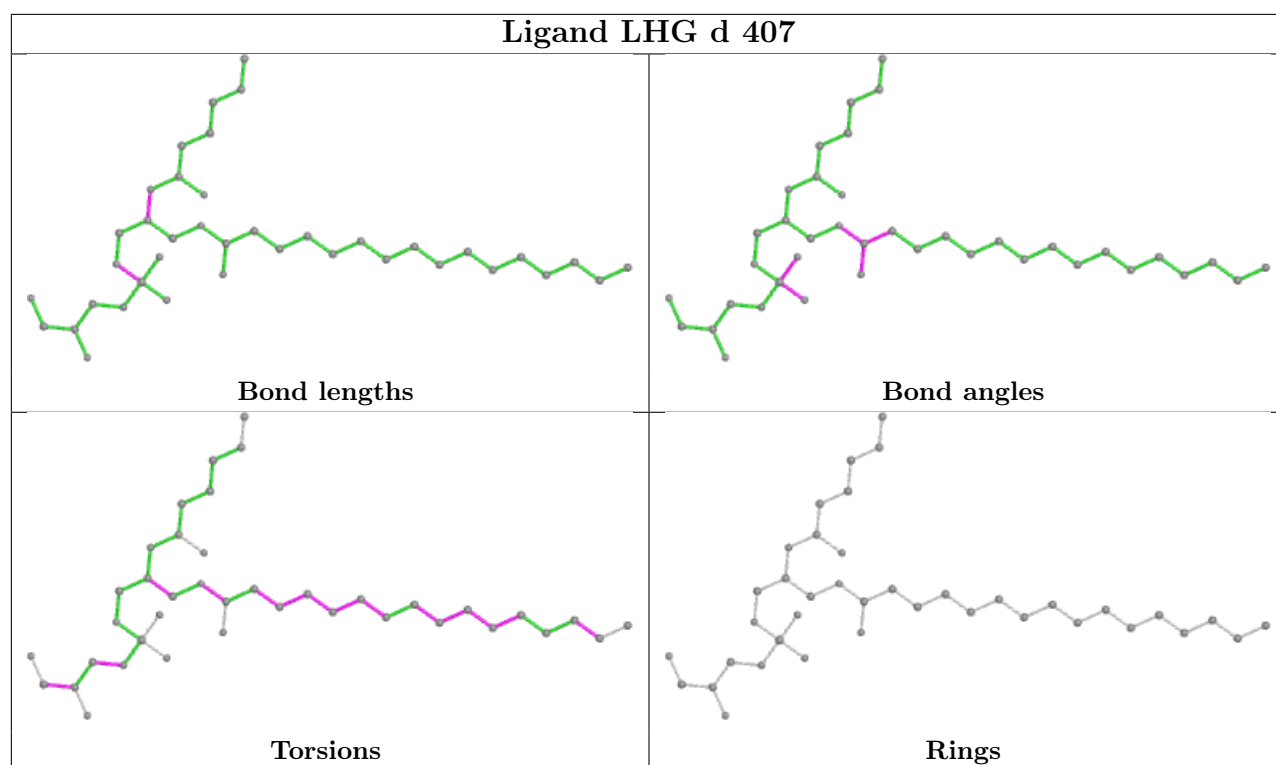
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

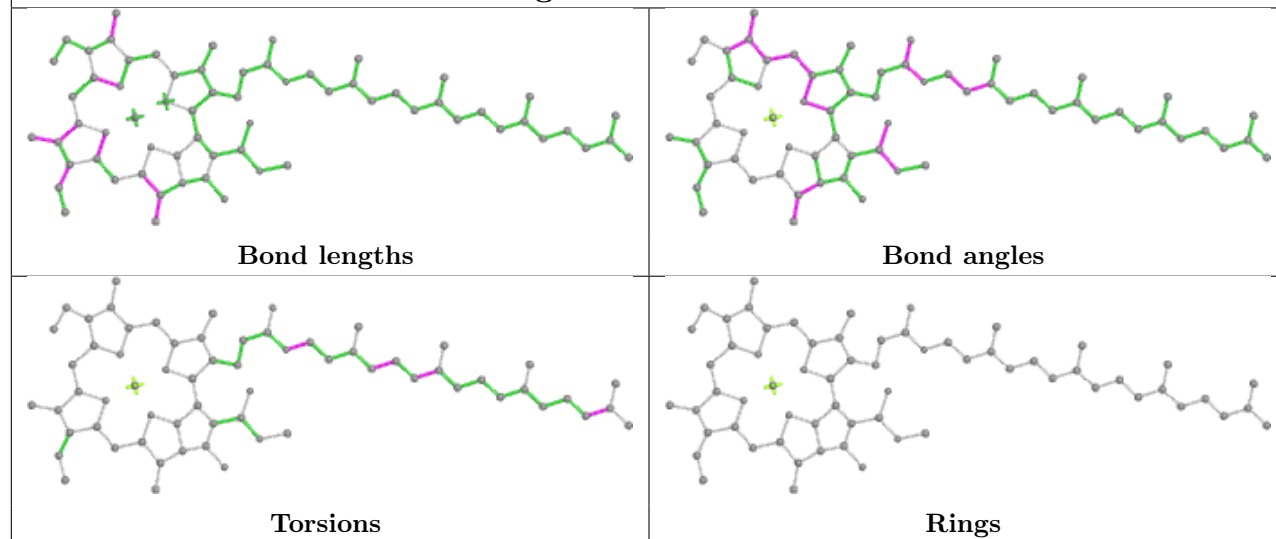
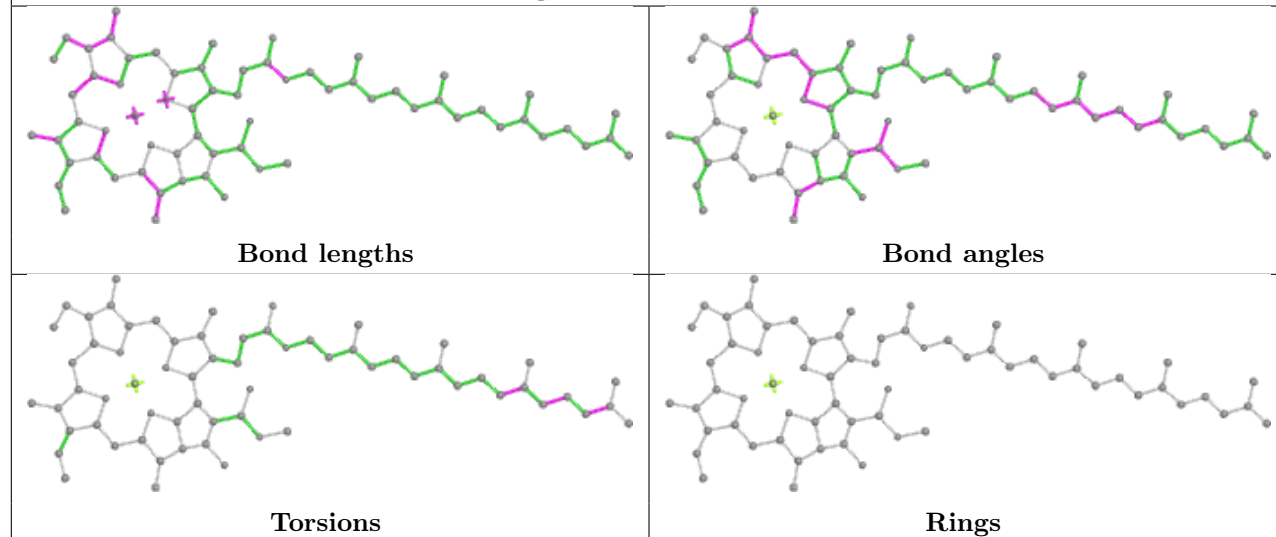
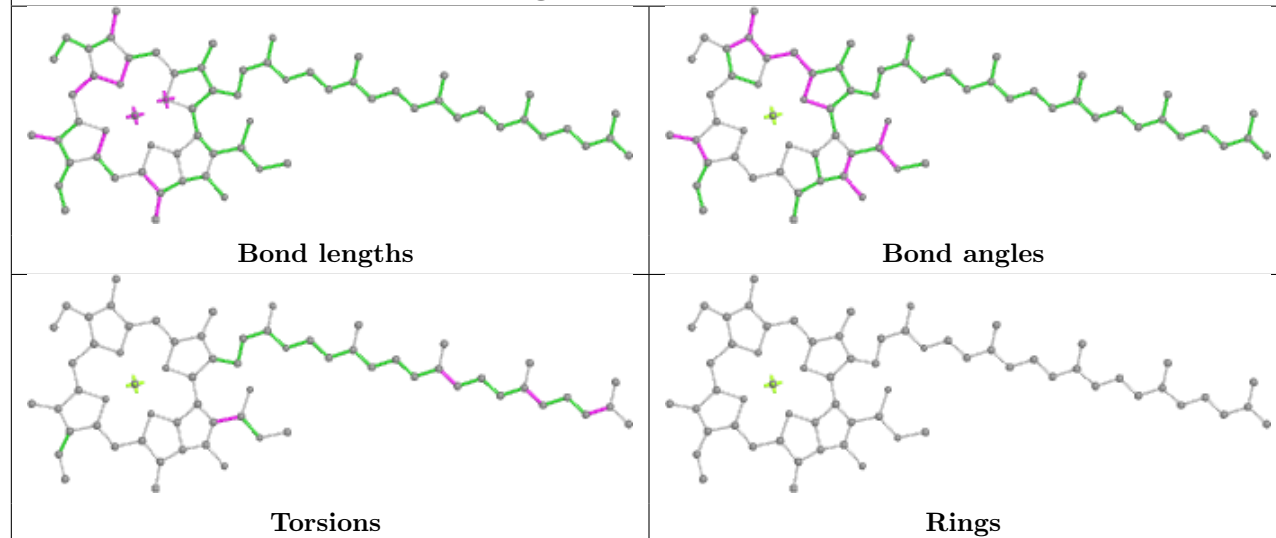


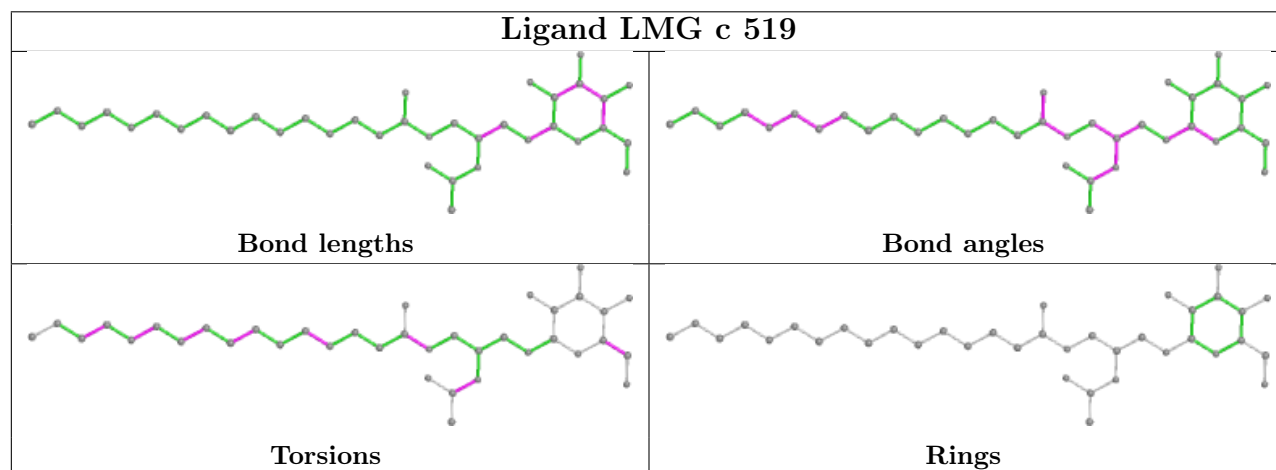
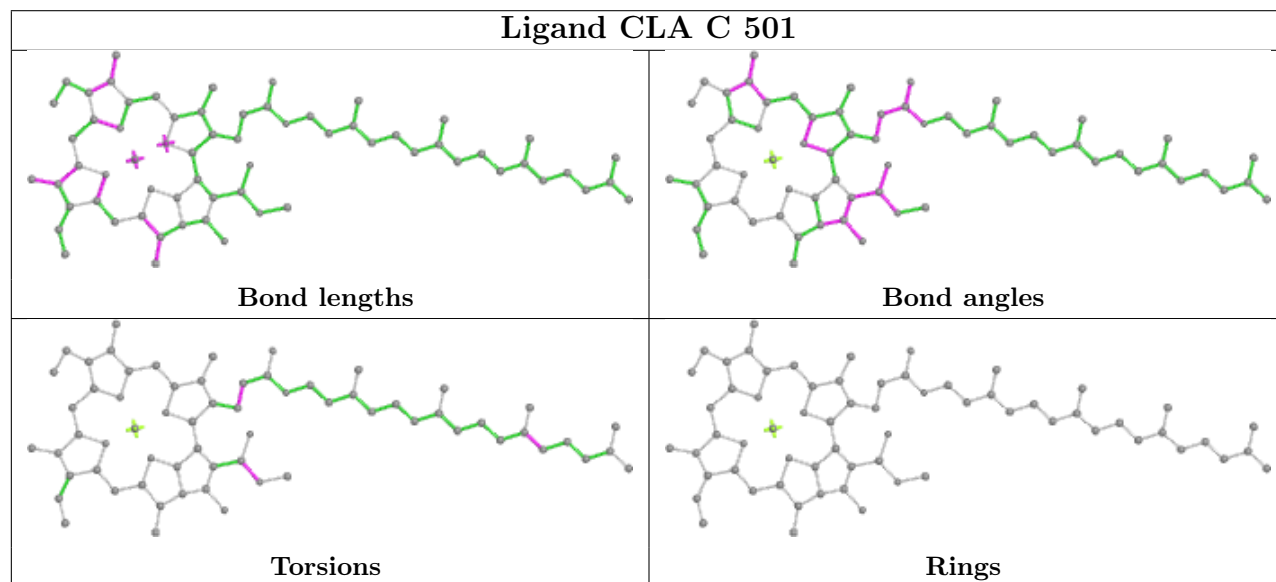
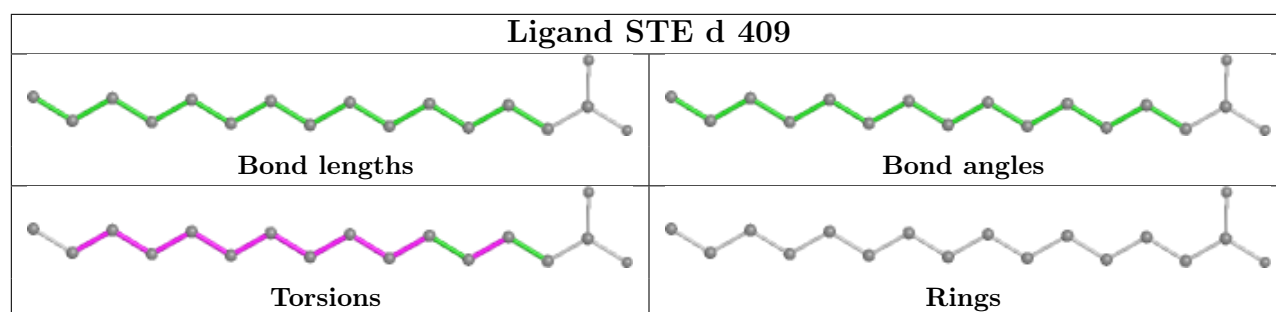
Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

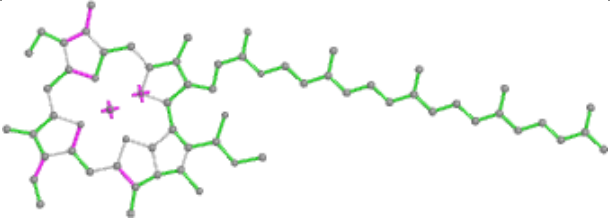
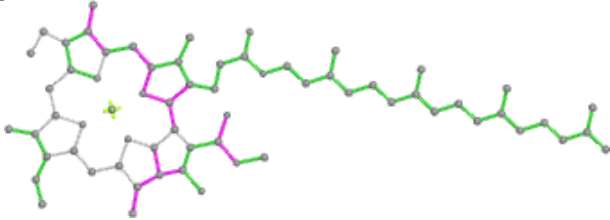
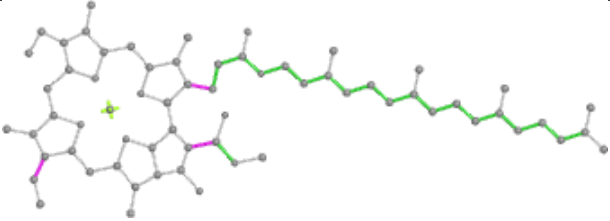
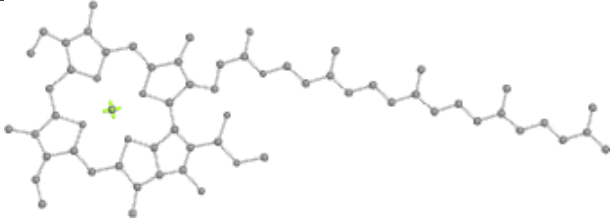
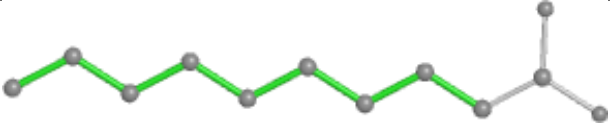
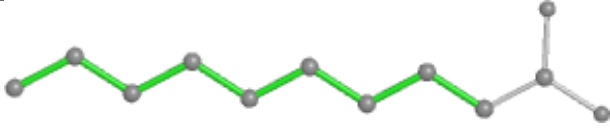
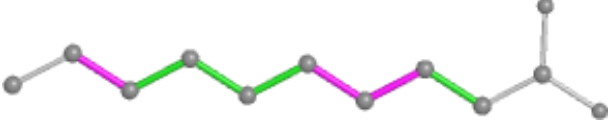
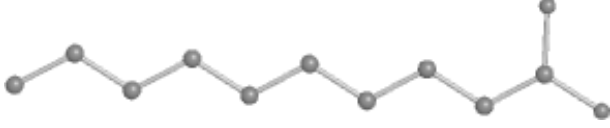
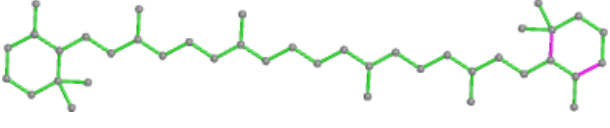
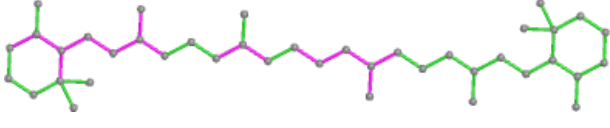


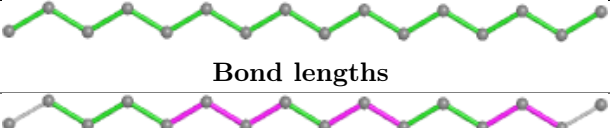
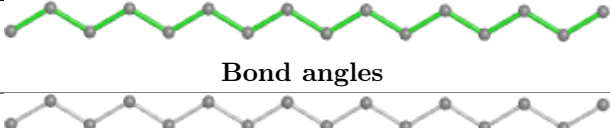

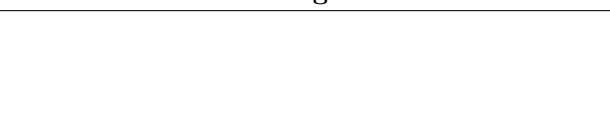
Ligand SQD A 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

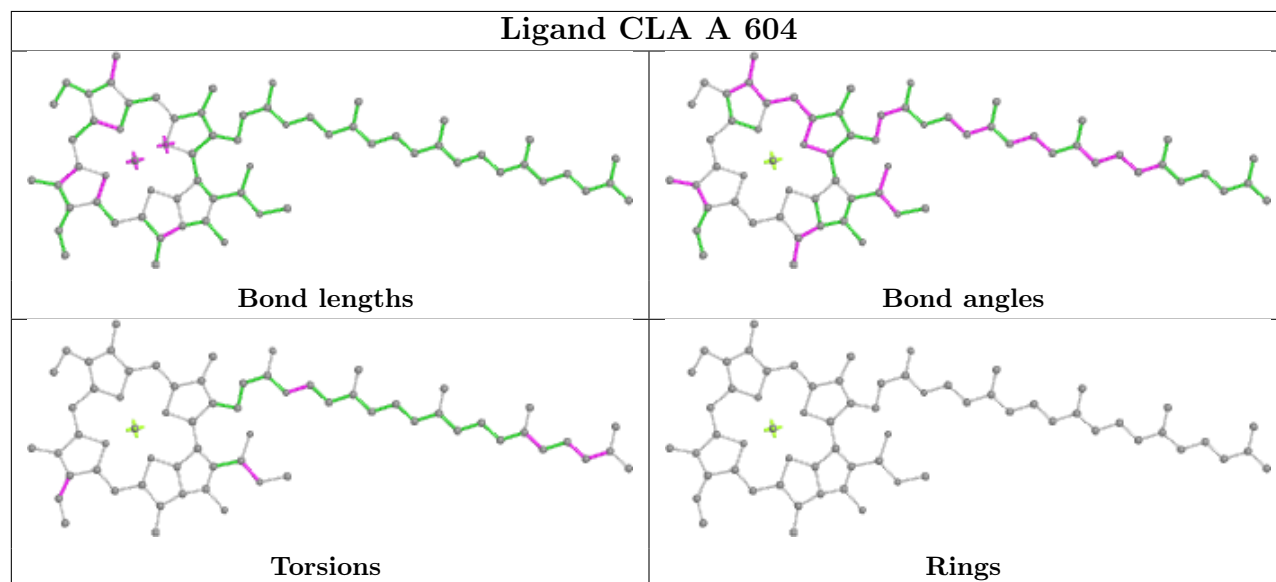
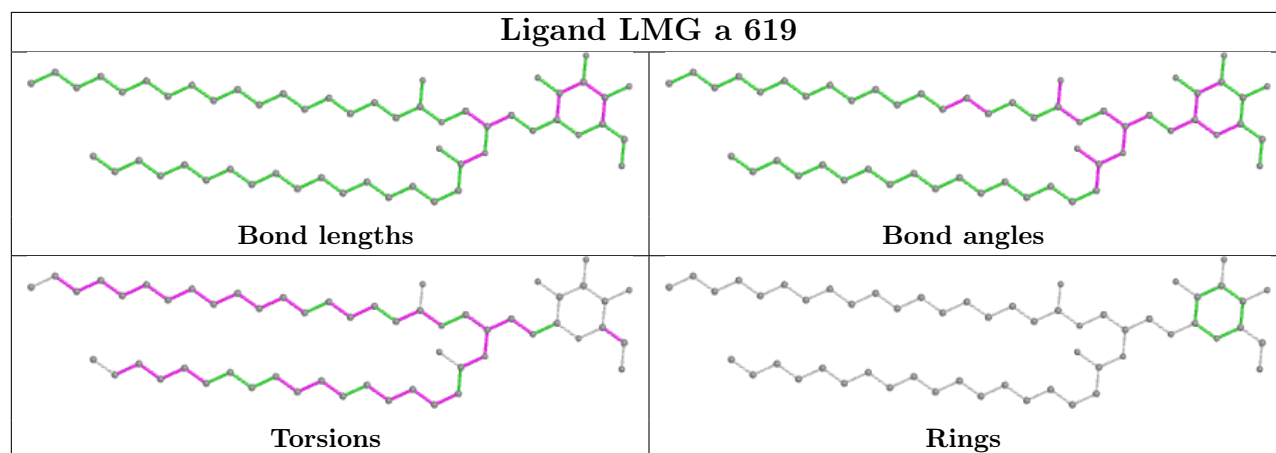
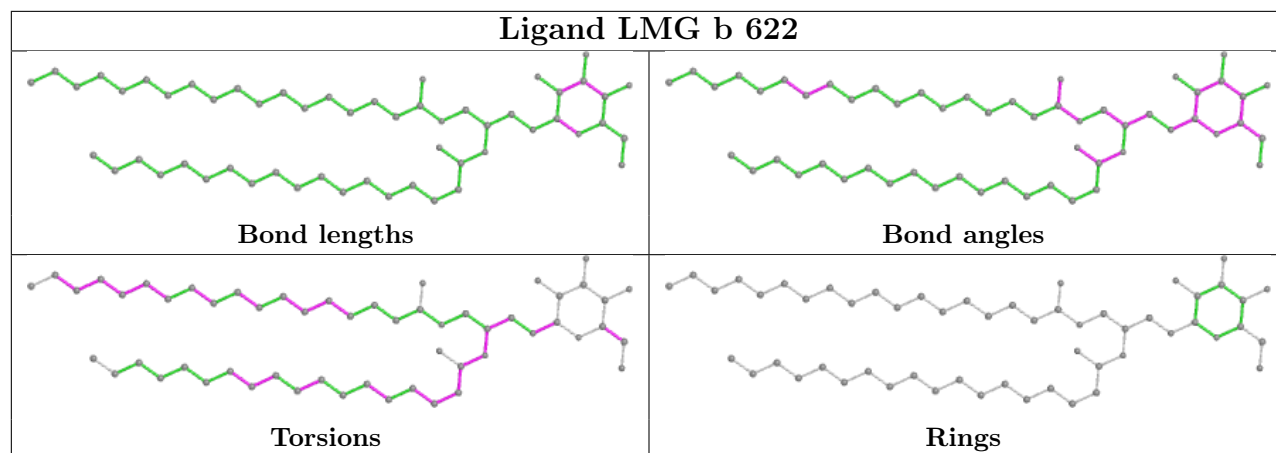
Ligand STE M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

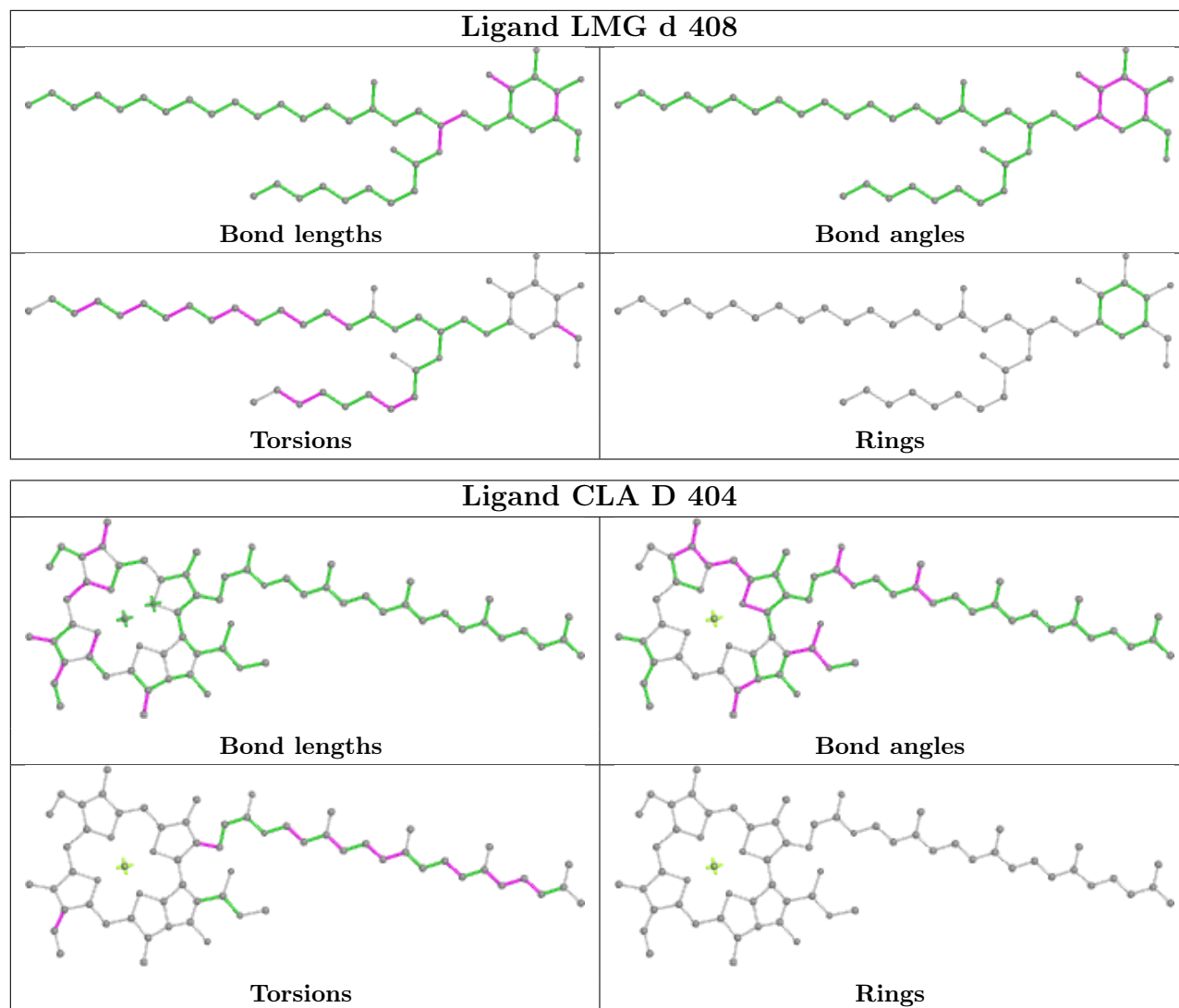


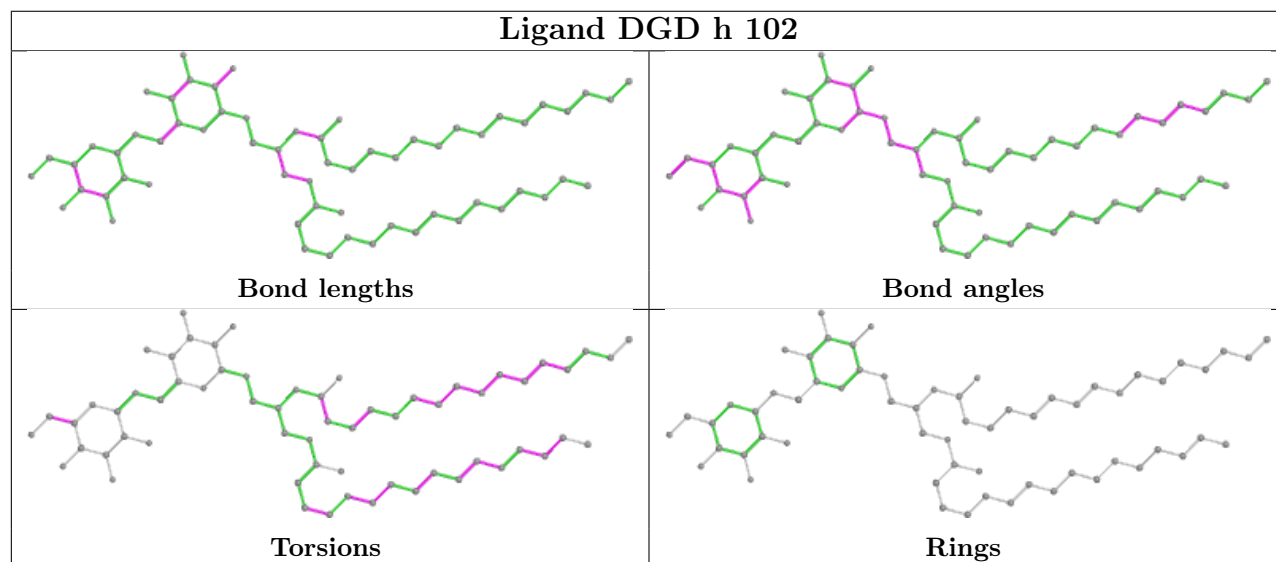
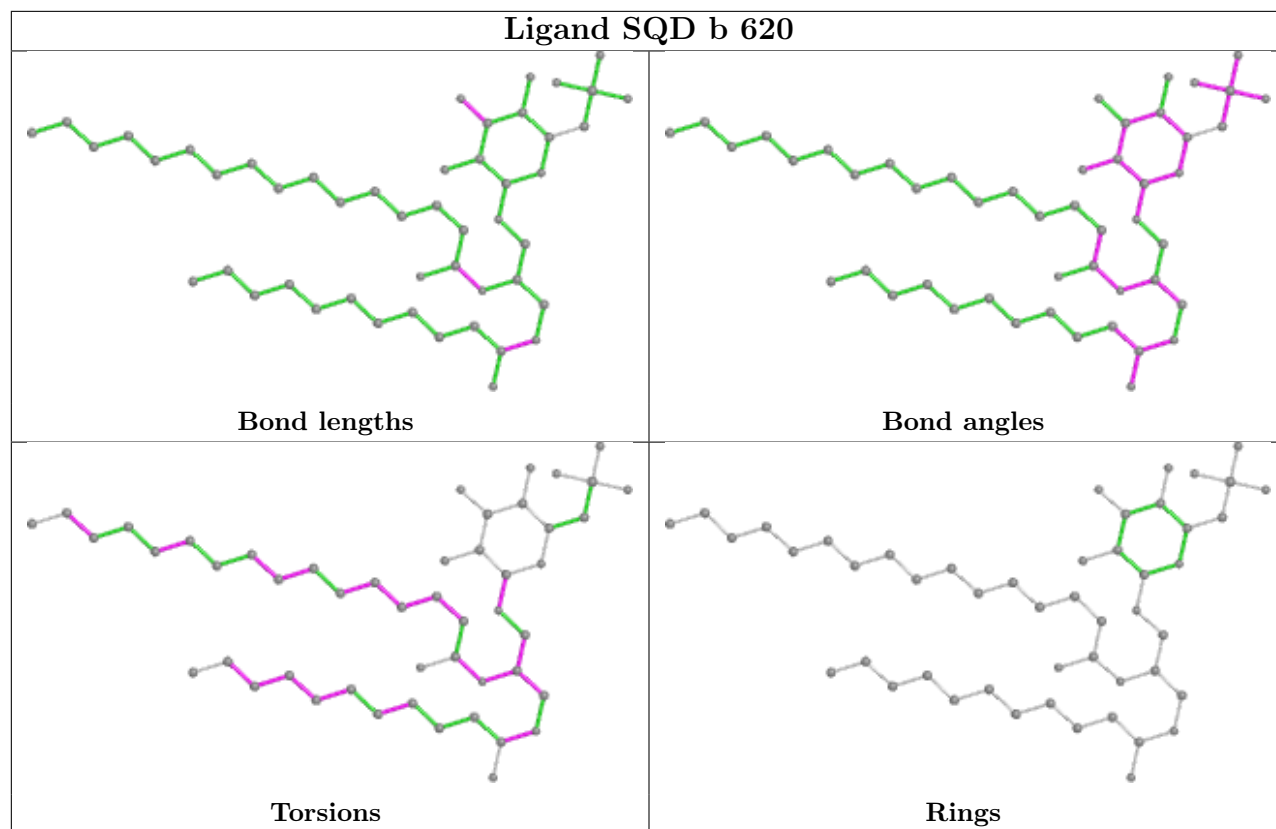
Ligand CLA d 402**Ligand CLA B 607****Ligand CLA C 508**

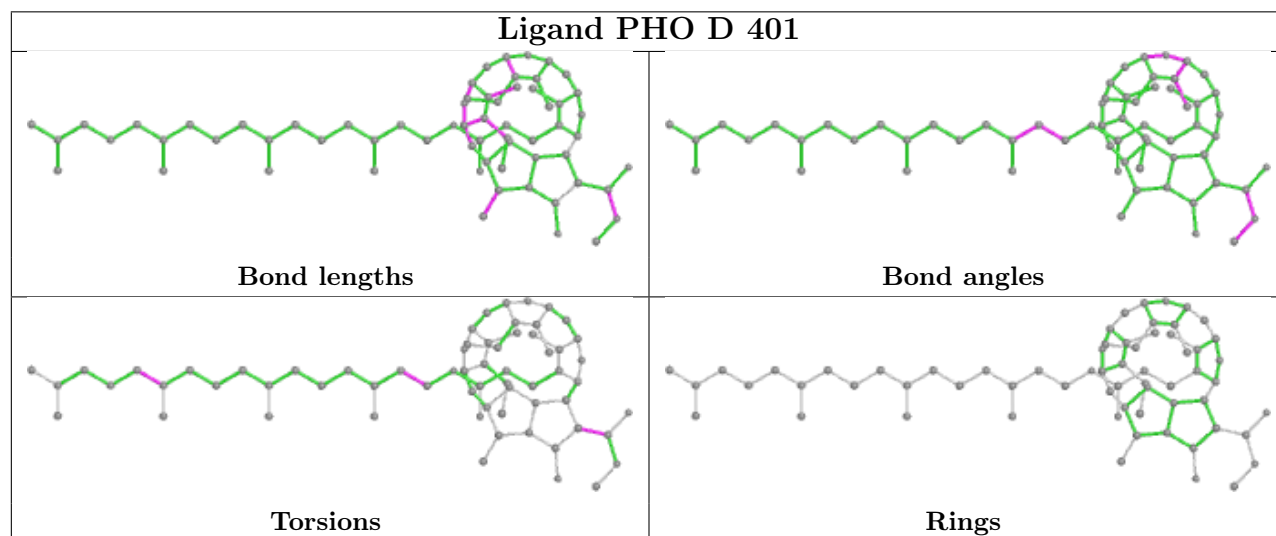
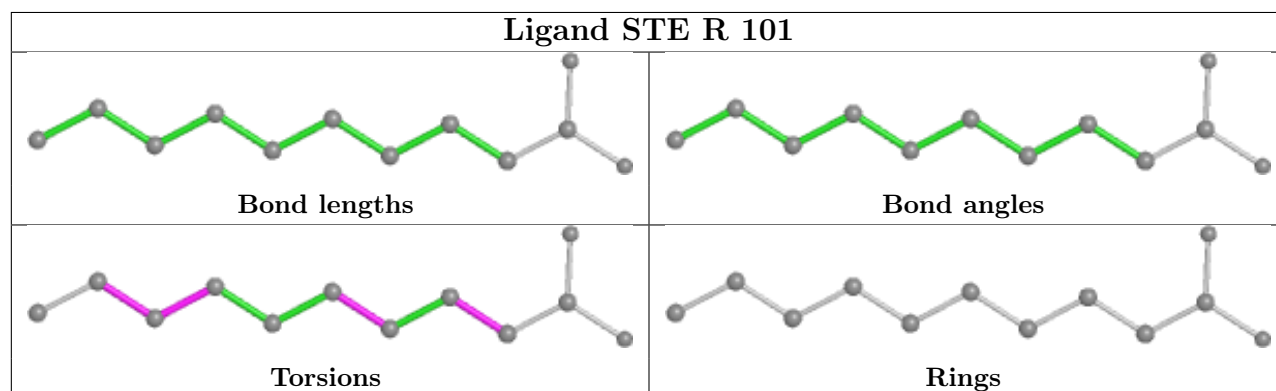
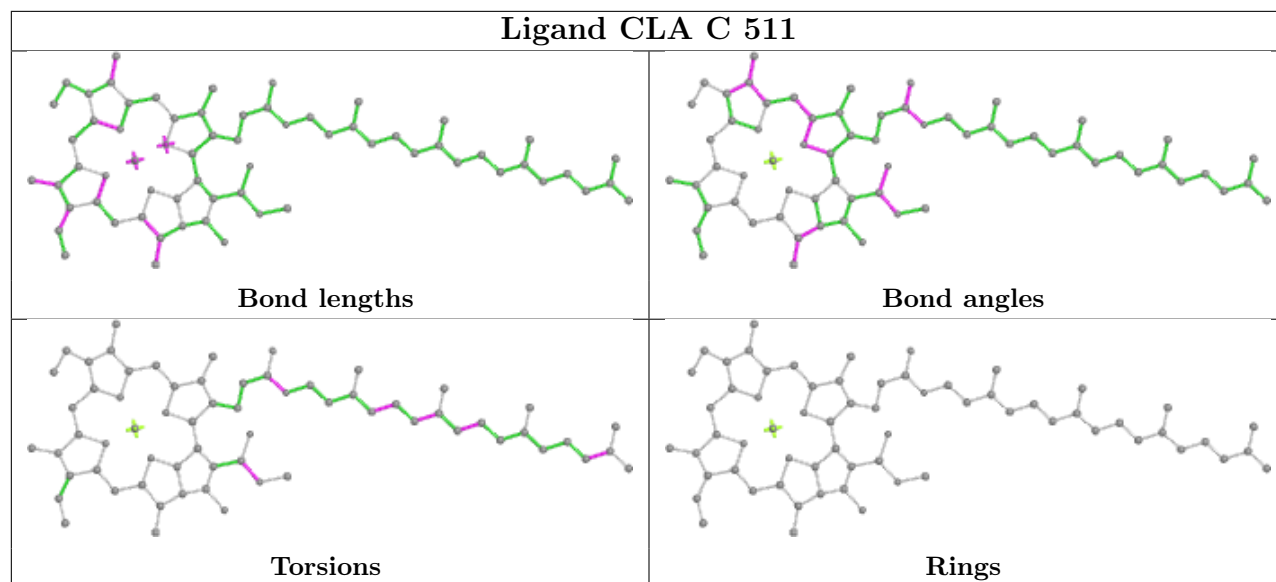


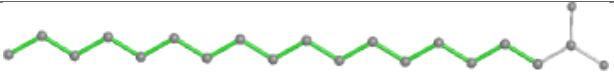
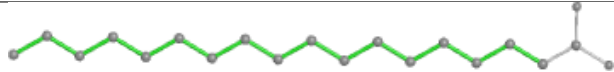
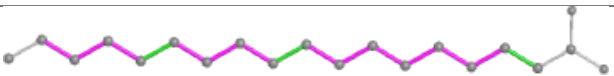
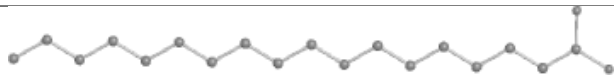
Ligand CLA a 613	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE C 519	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR t 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE C 520	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

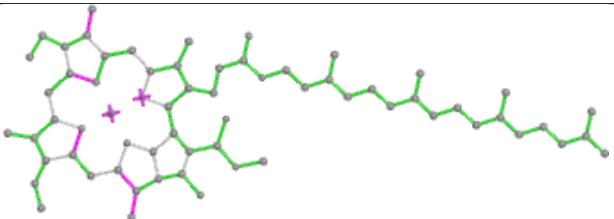
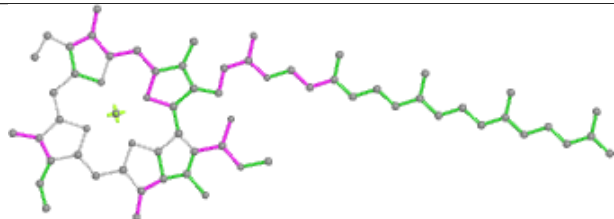
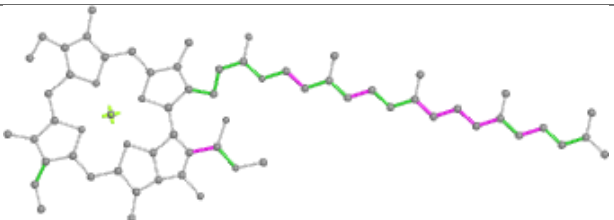
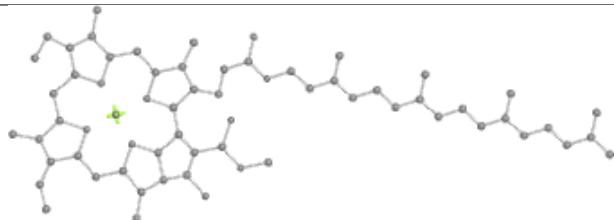


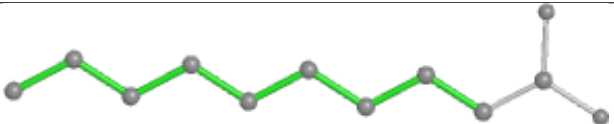
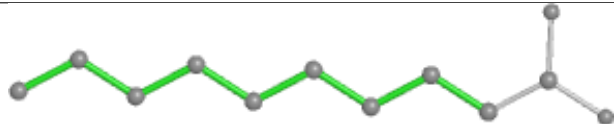
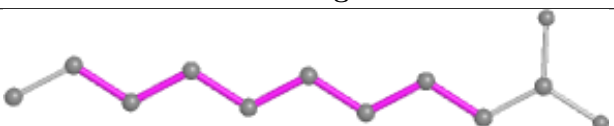
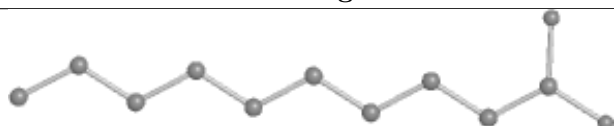


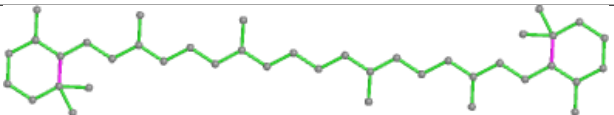
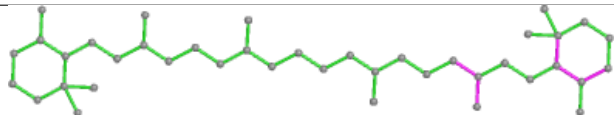
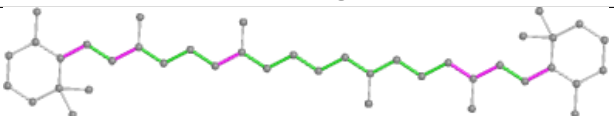
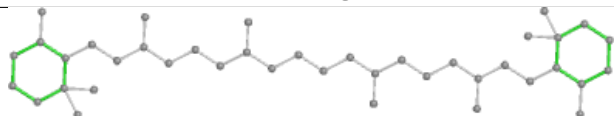


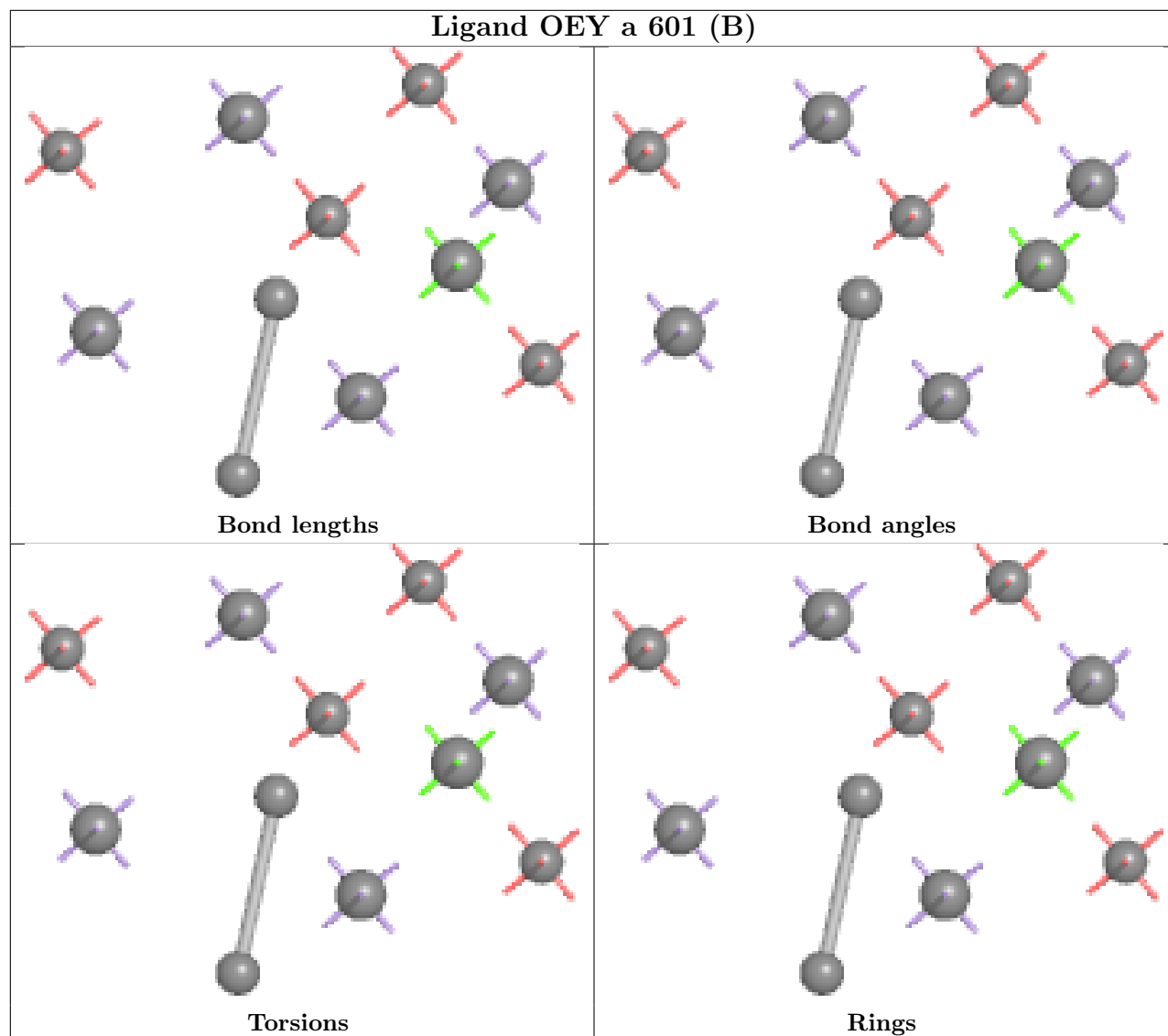
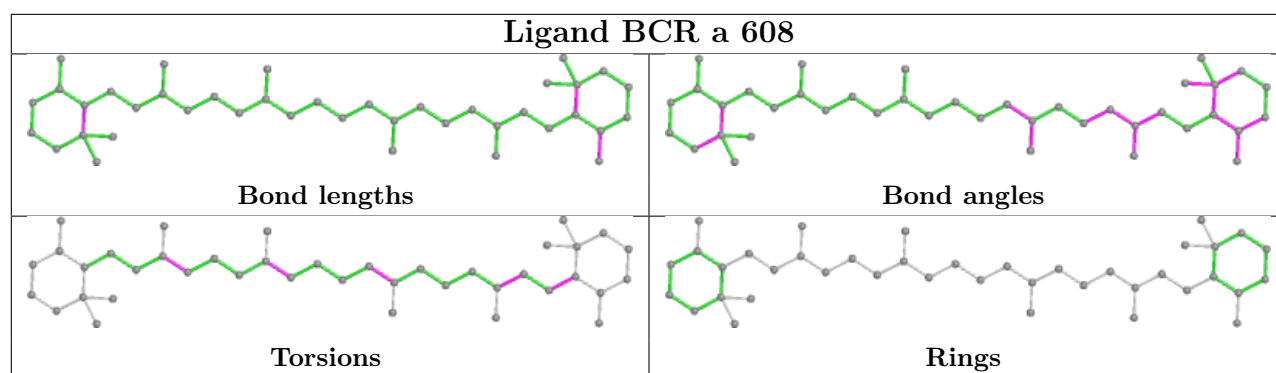


Ligand STE X 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

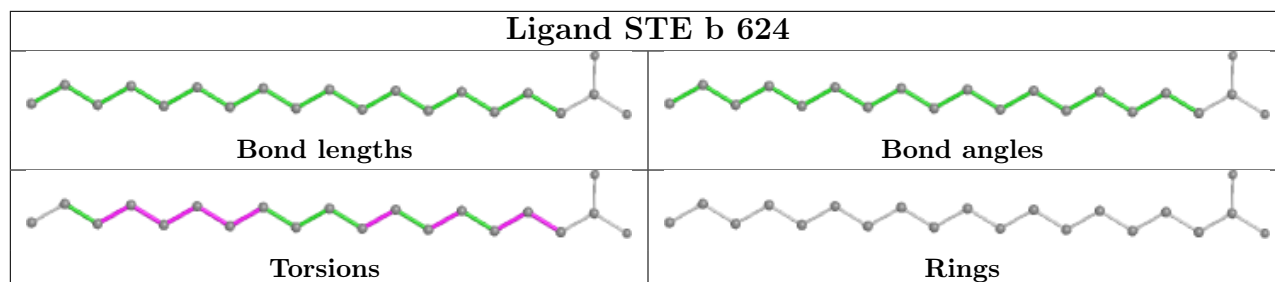
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE c 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

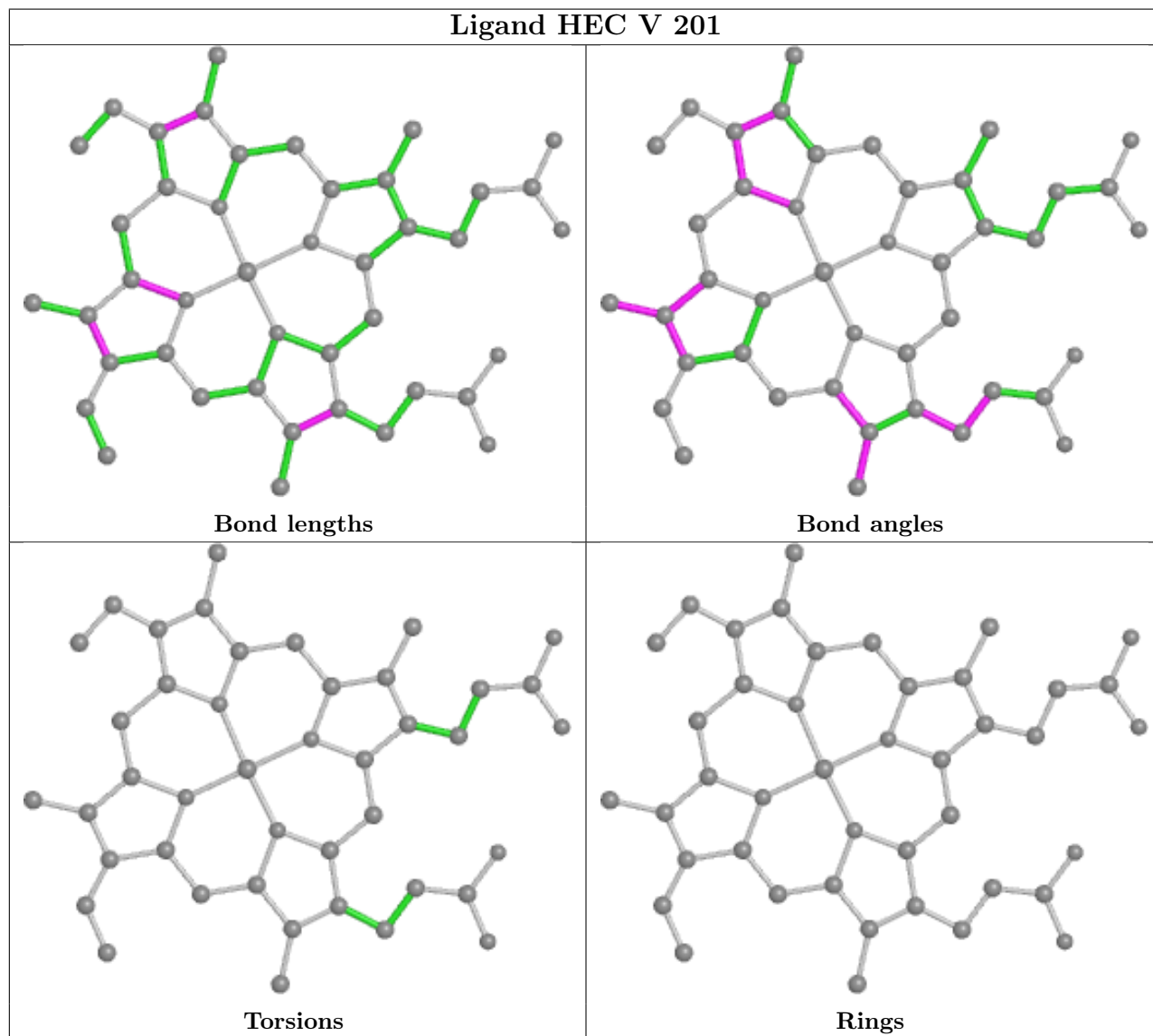
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



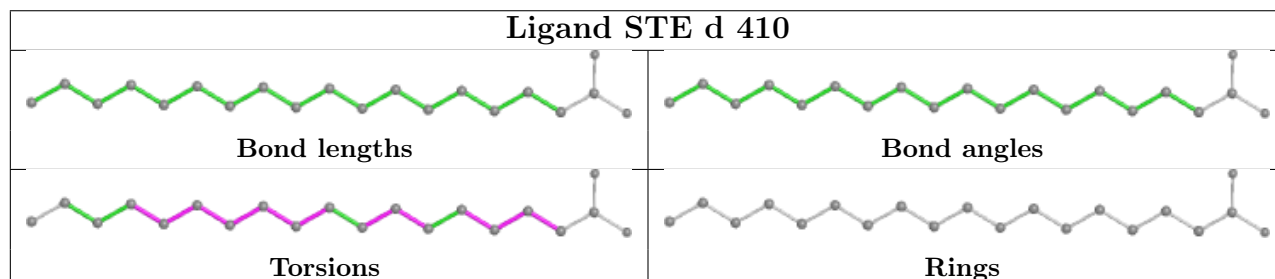
Ligand STE b 624

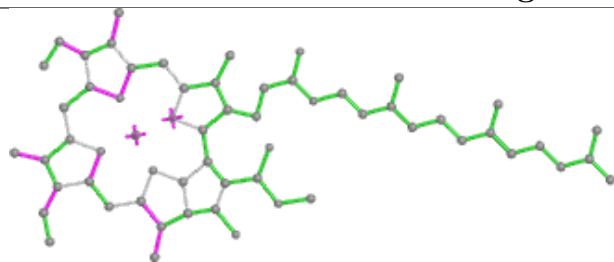


Ligand HEC V 201

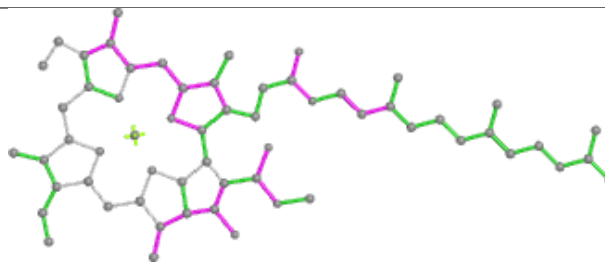


Ligand STE d 410

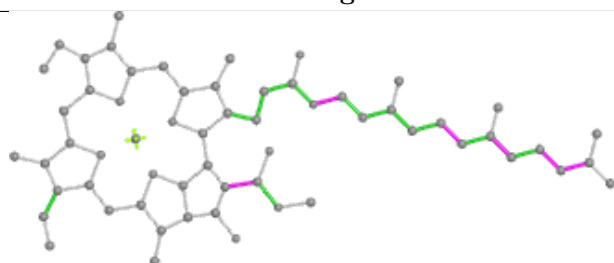


Ligand CLA b 616

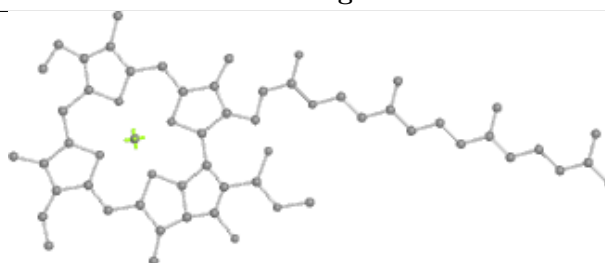
Bond lengths



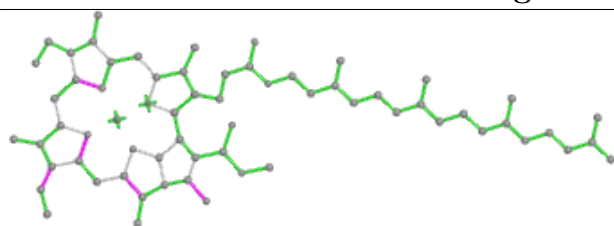
Bond angles



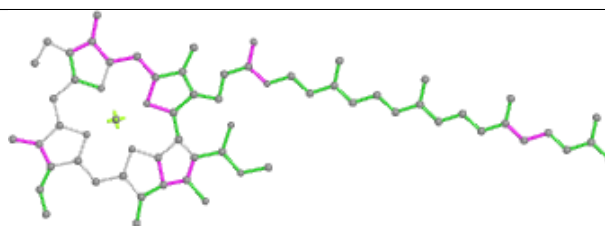
Torsions



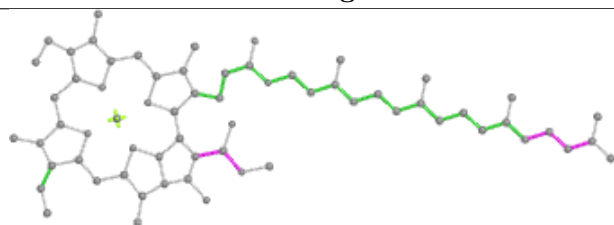
Rings

Ligand CLA A 612

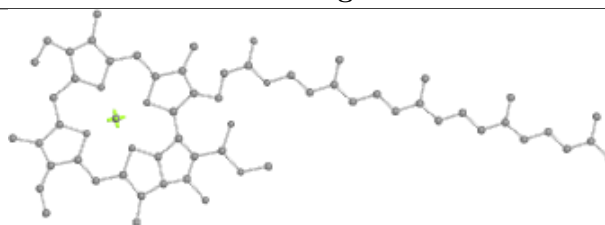
Bond lengths



Bond angles

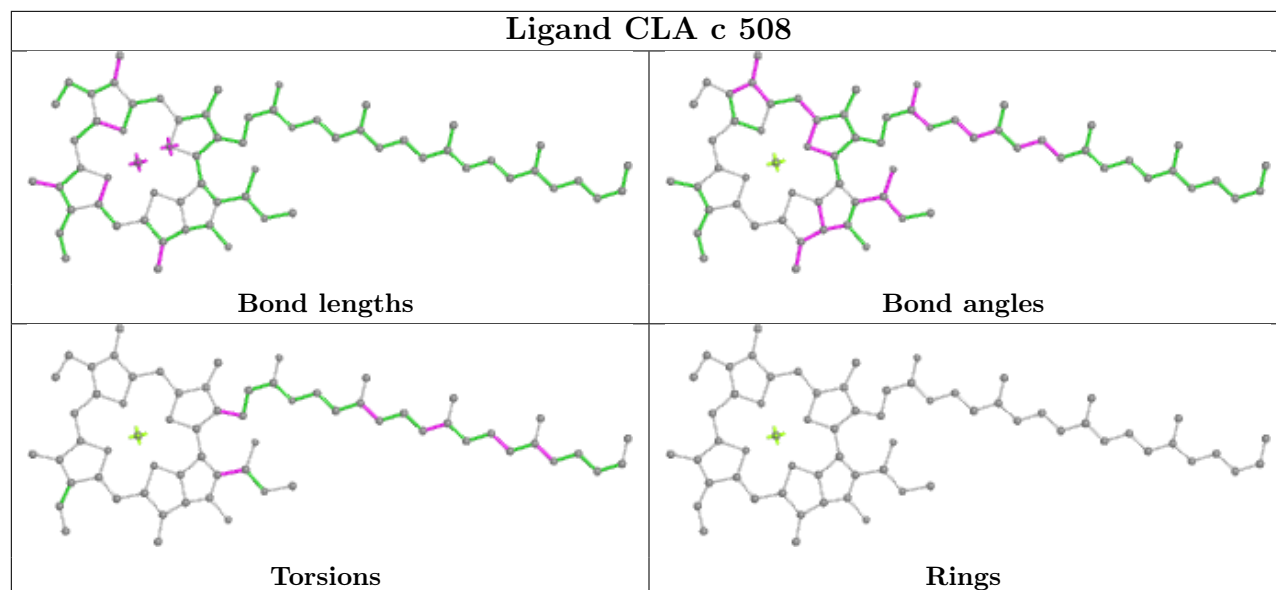


Torsions

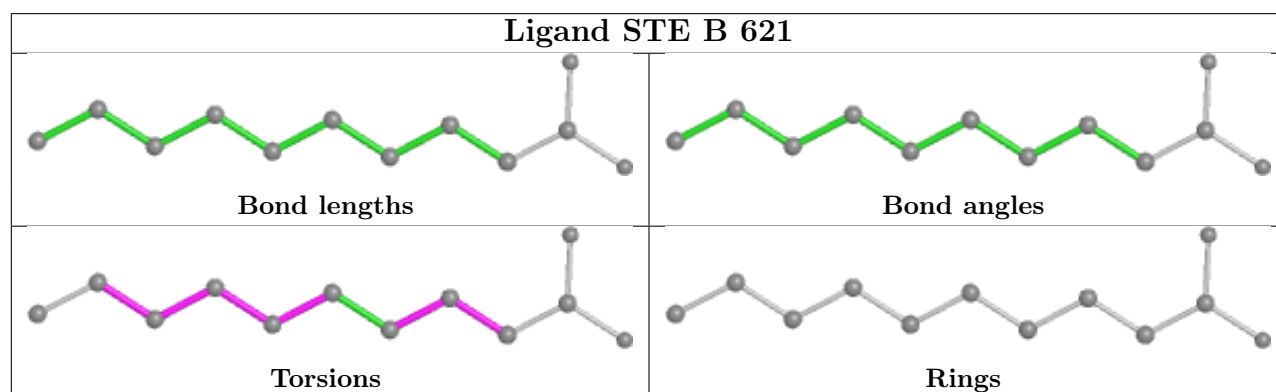


Rings

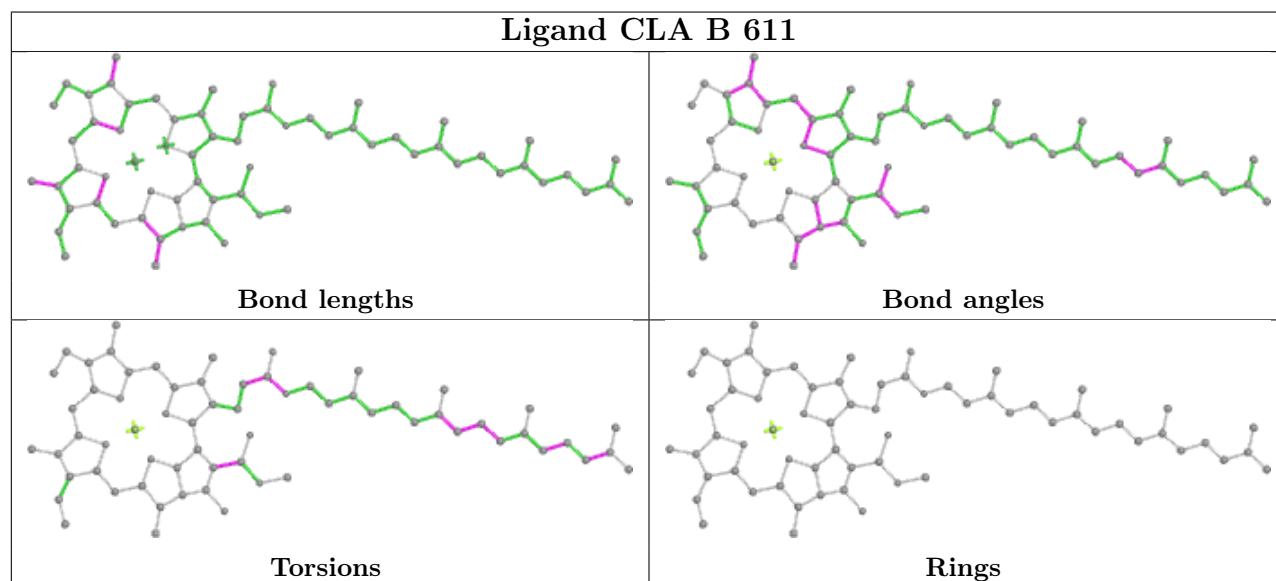
Ligand CLA c 508



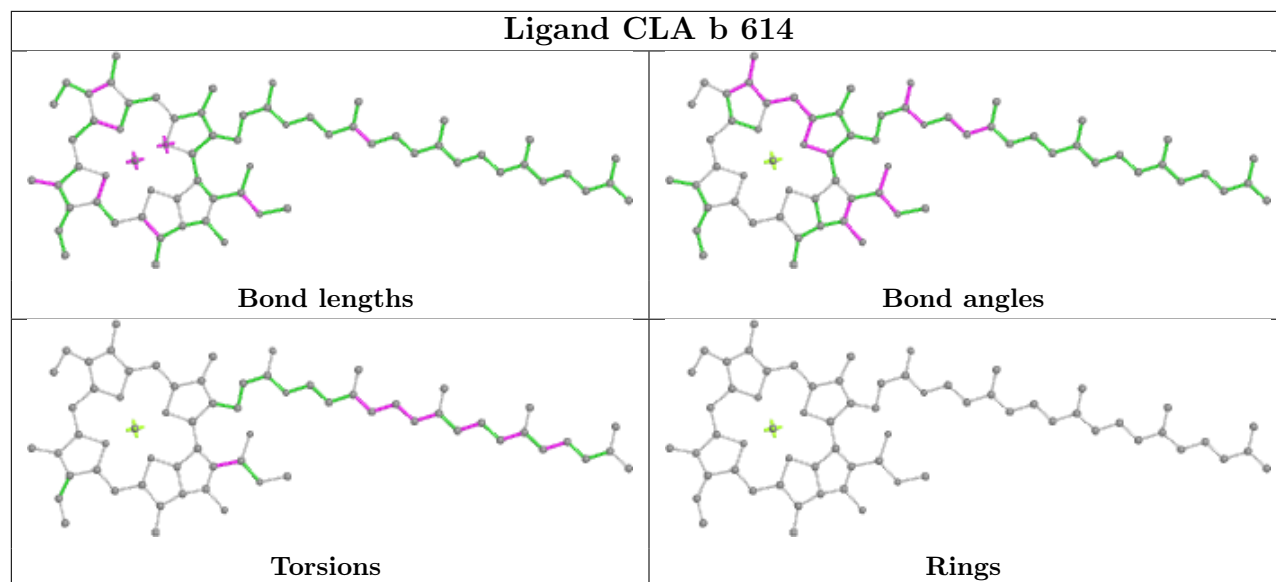
Ligand STE B 621



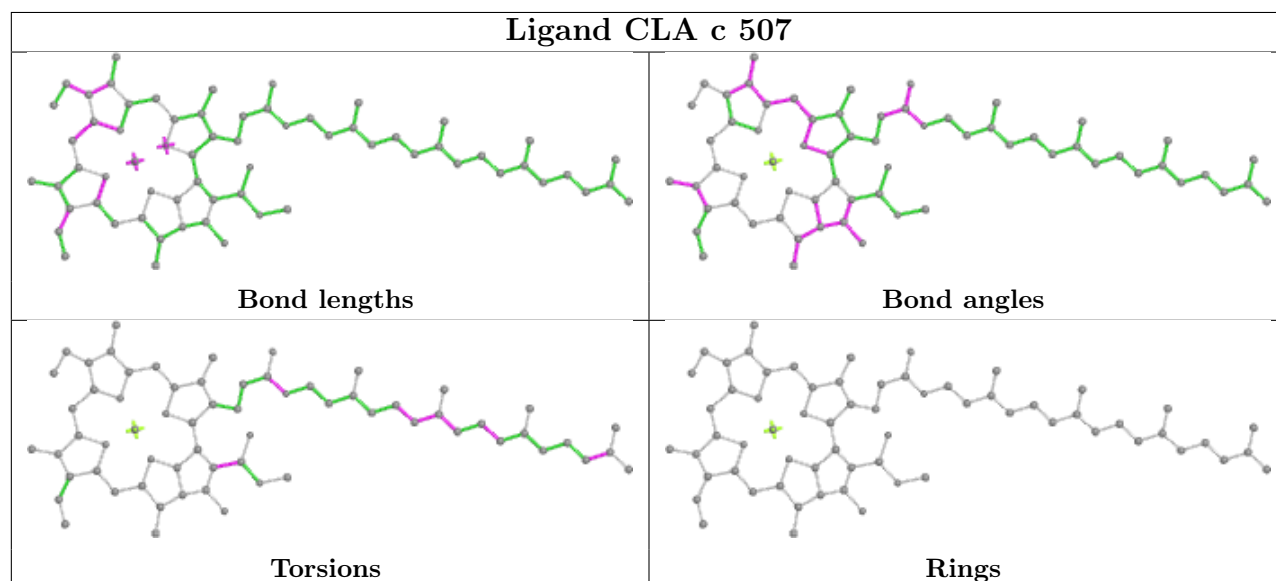
Ligand CLA B 611



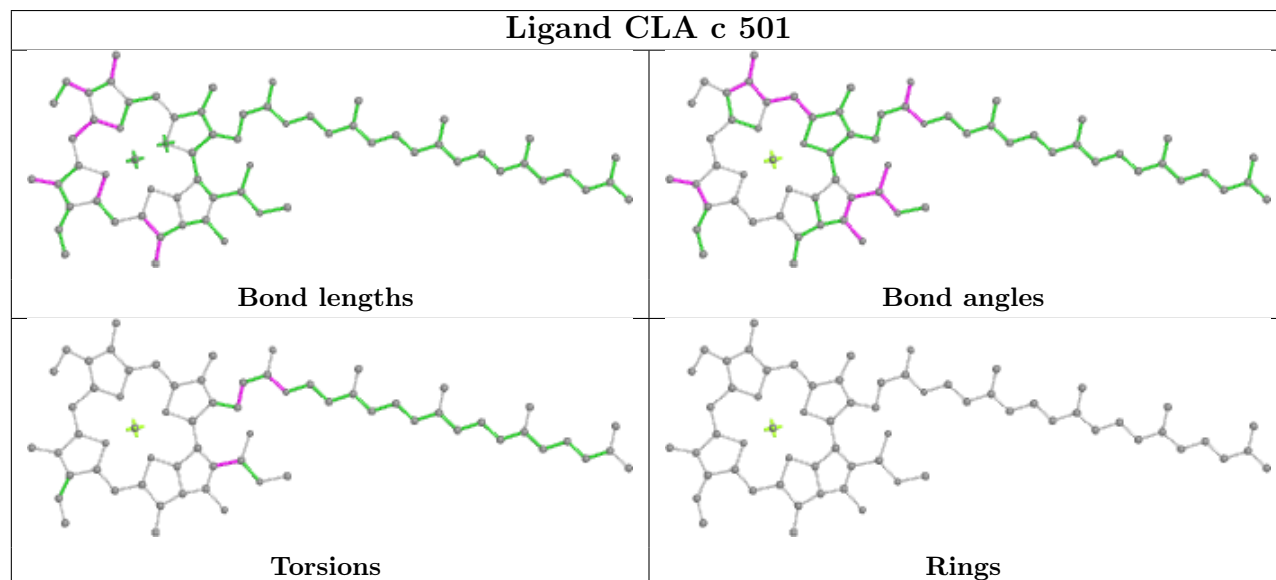
Ligand CLA b 614

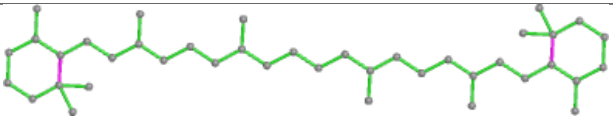
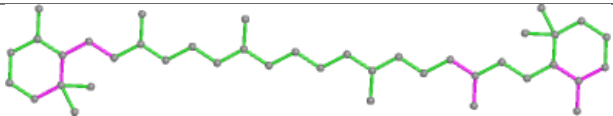
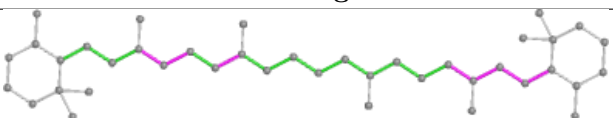
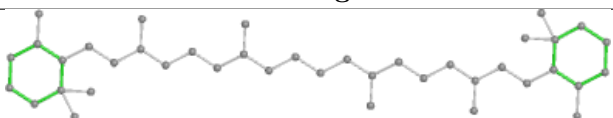


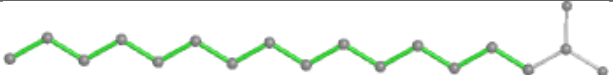
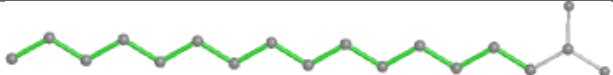

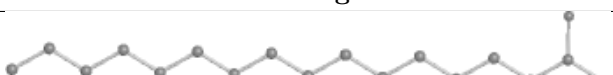
Ligand CLA c 507



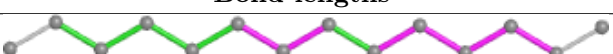



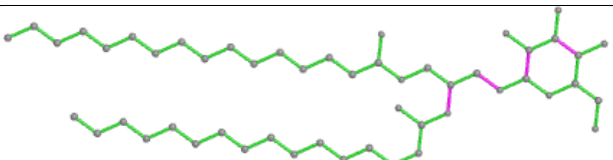
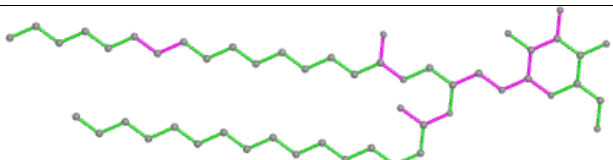
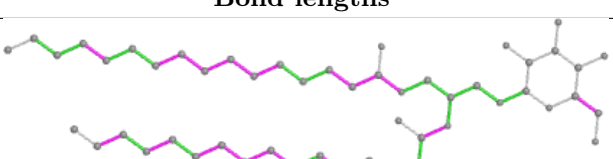
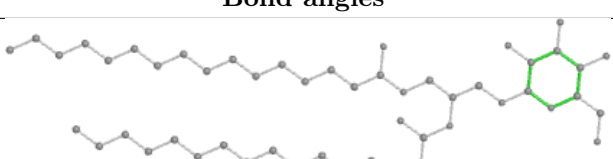
Ligand CLA c 501

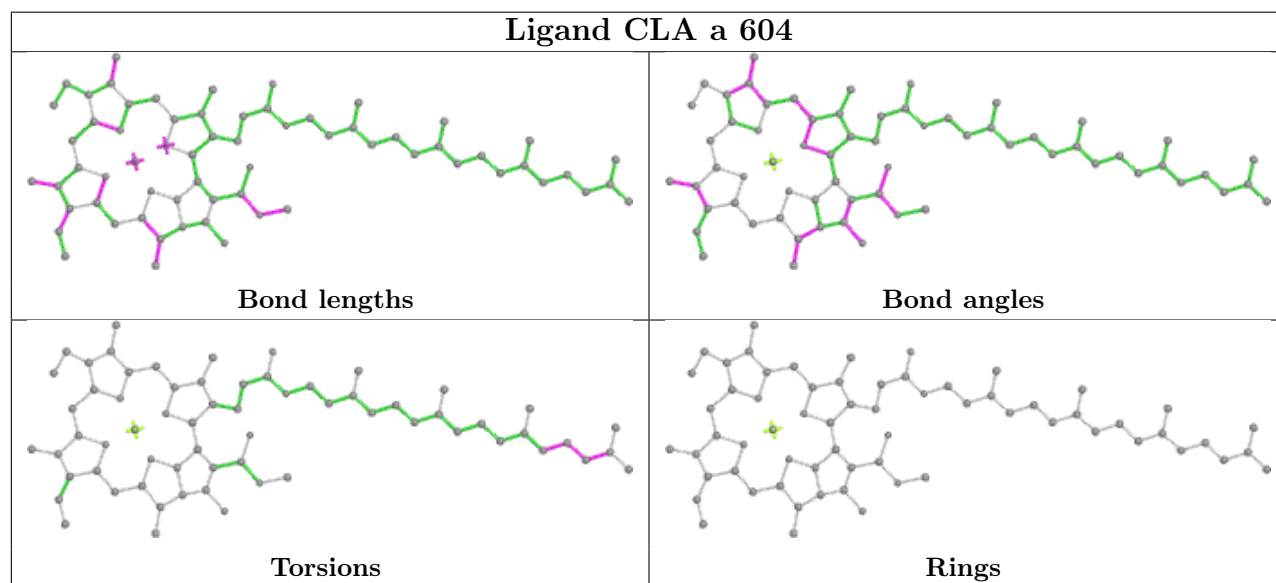
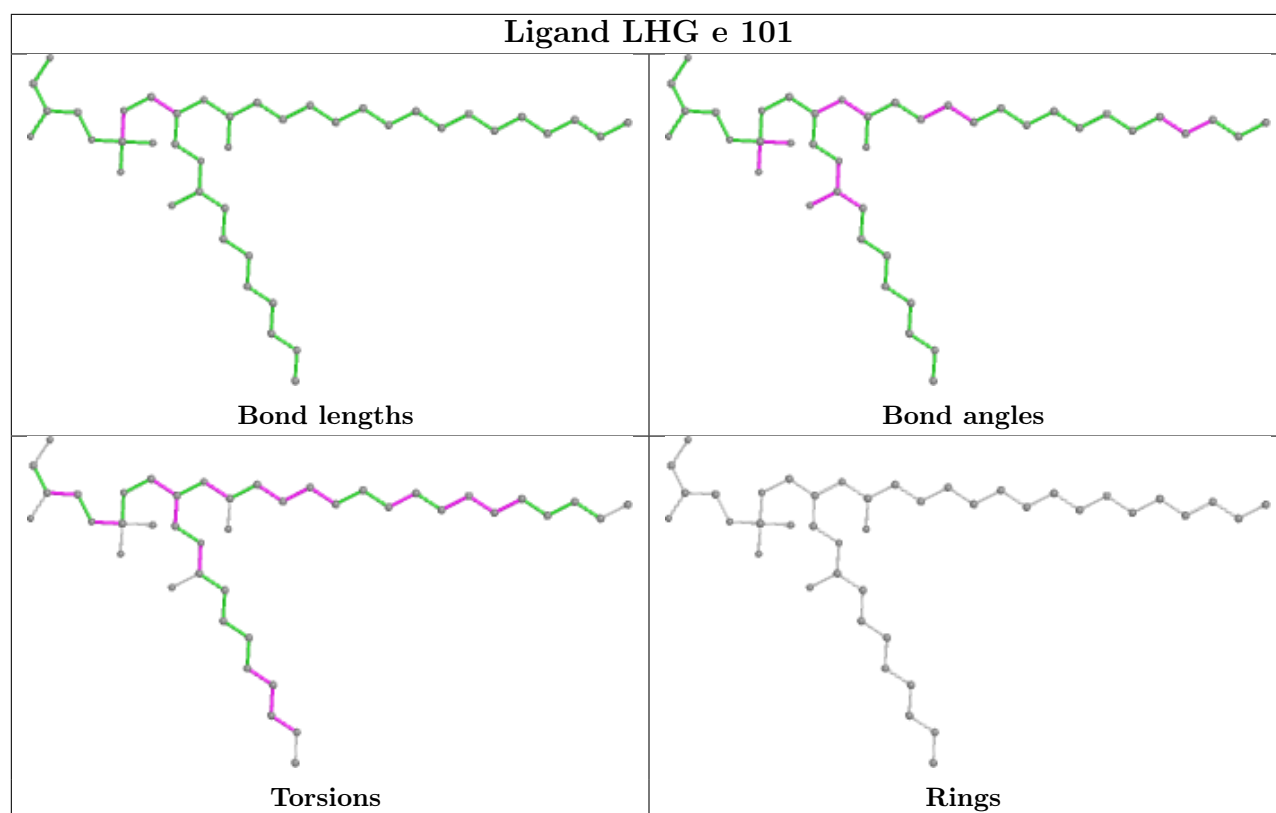


Ligand BCR k 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

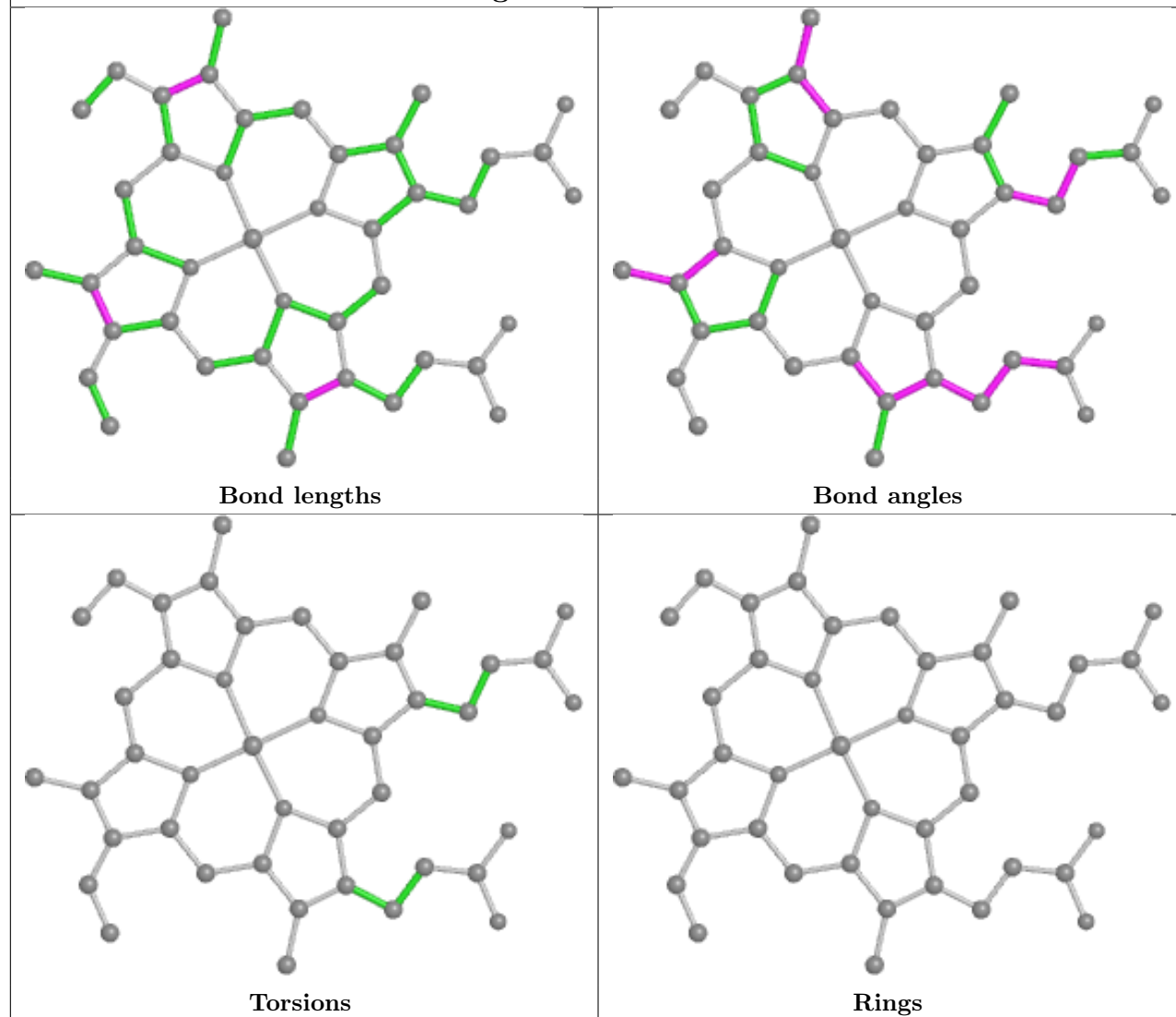
Ligand STE B 622	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand STE h 103	
	Bond lengths
	Bond angles
	Torsions
	Rings

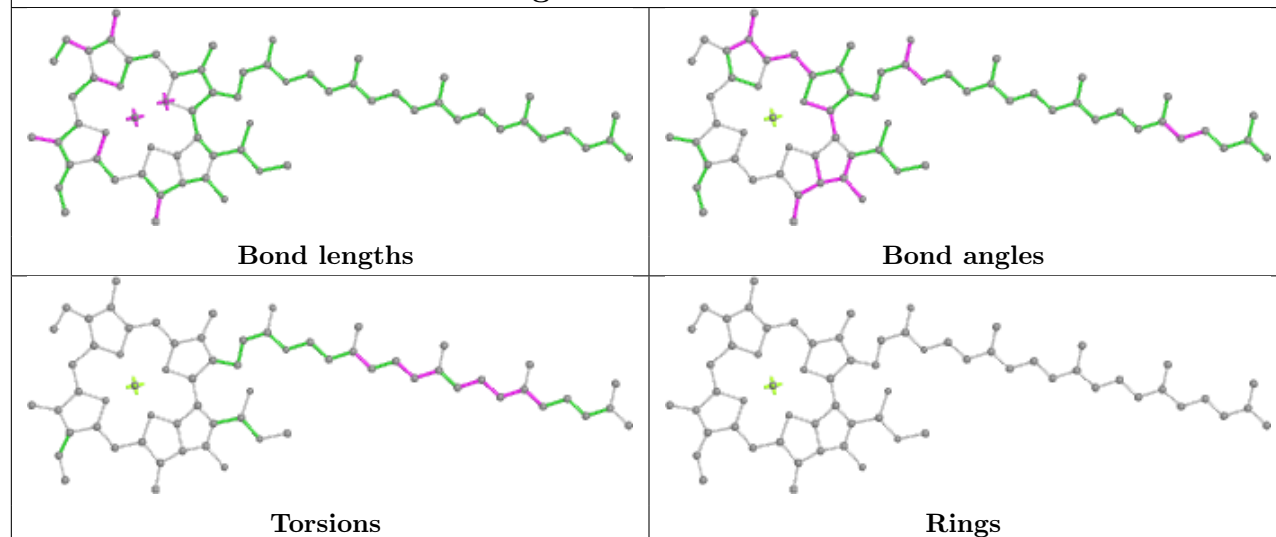
Ligand LMG m 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

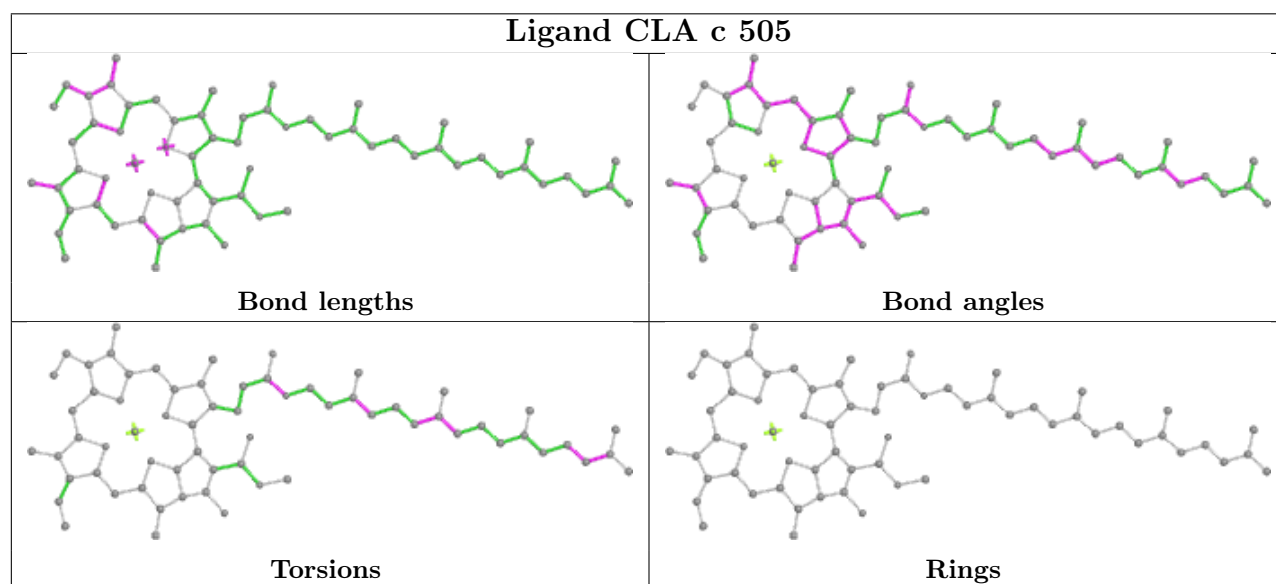
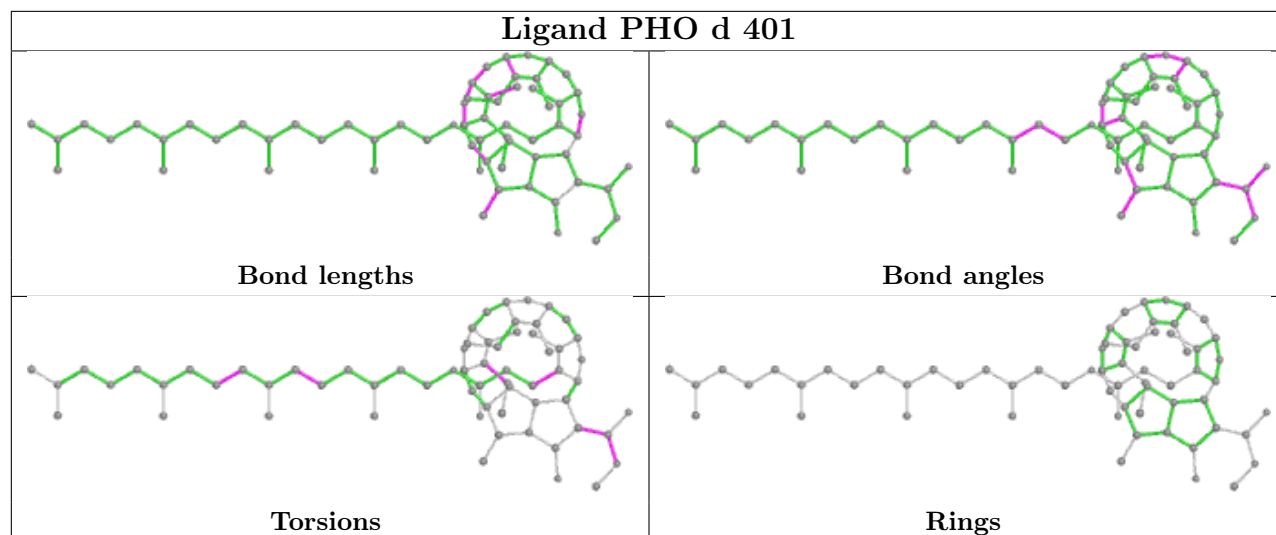


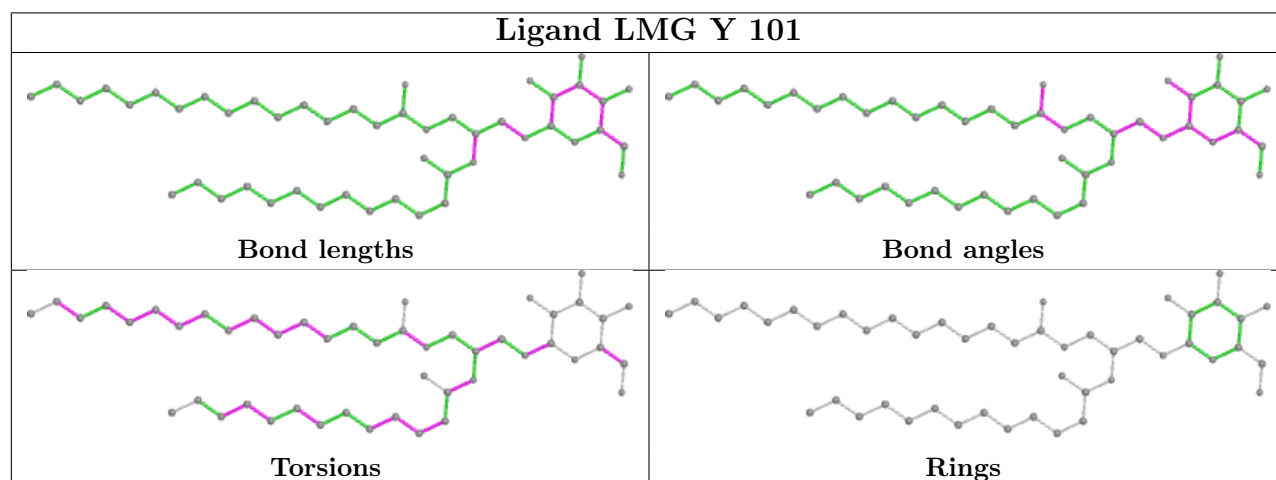
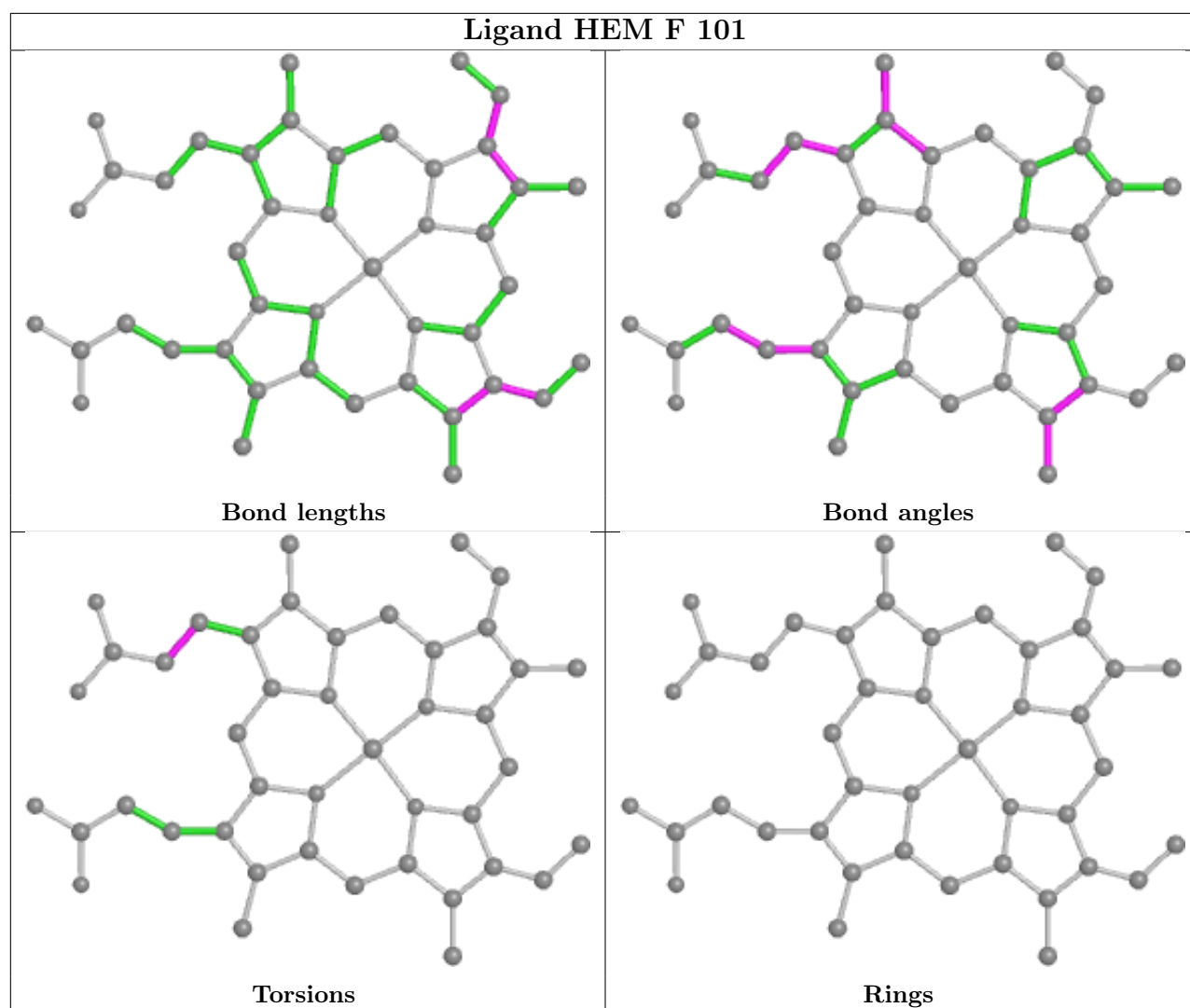
Ligand HEC v 201



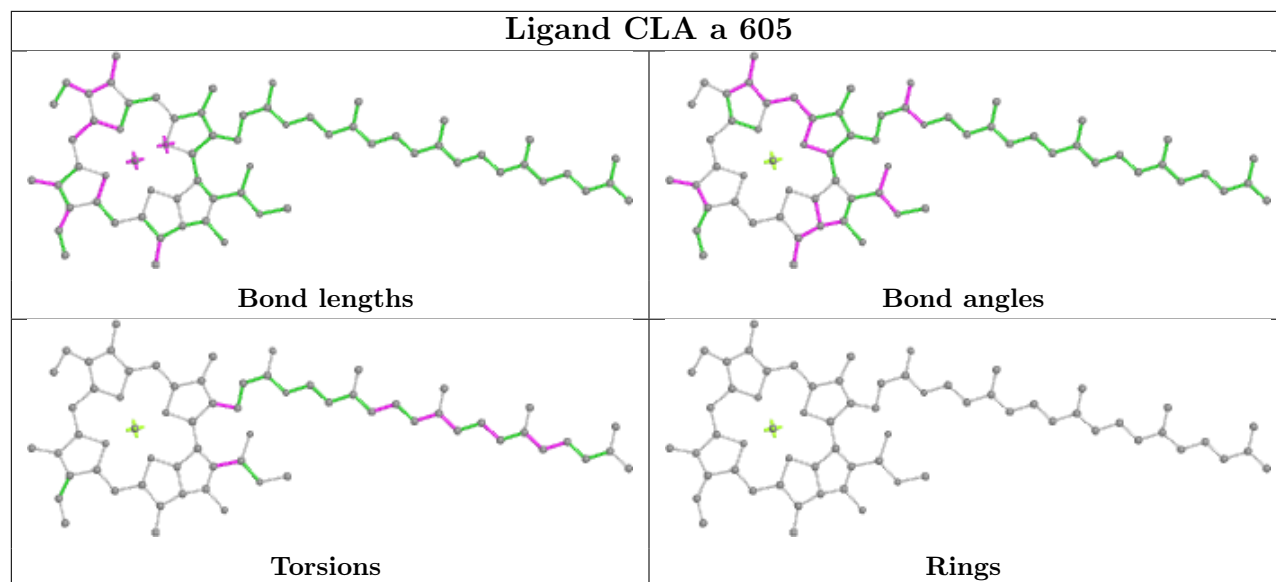
Ligand CLA C 505



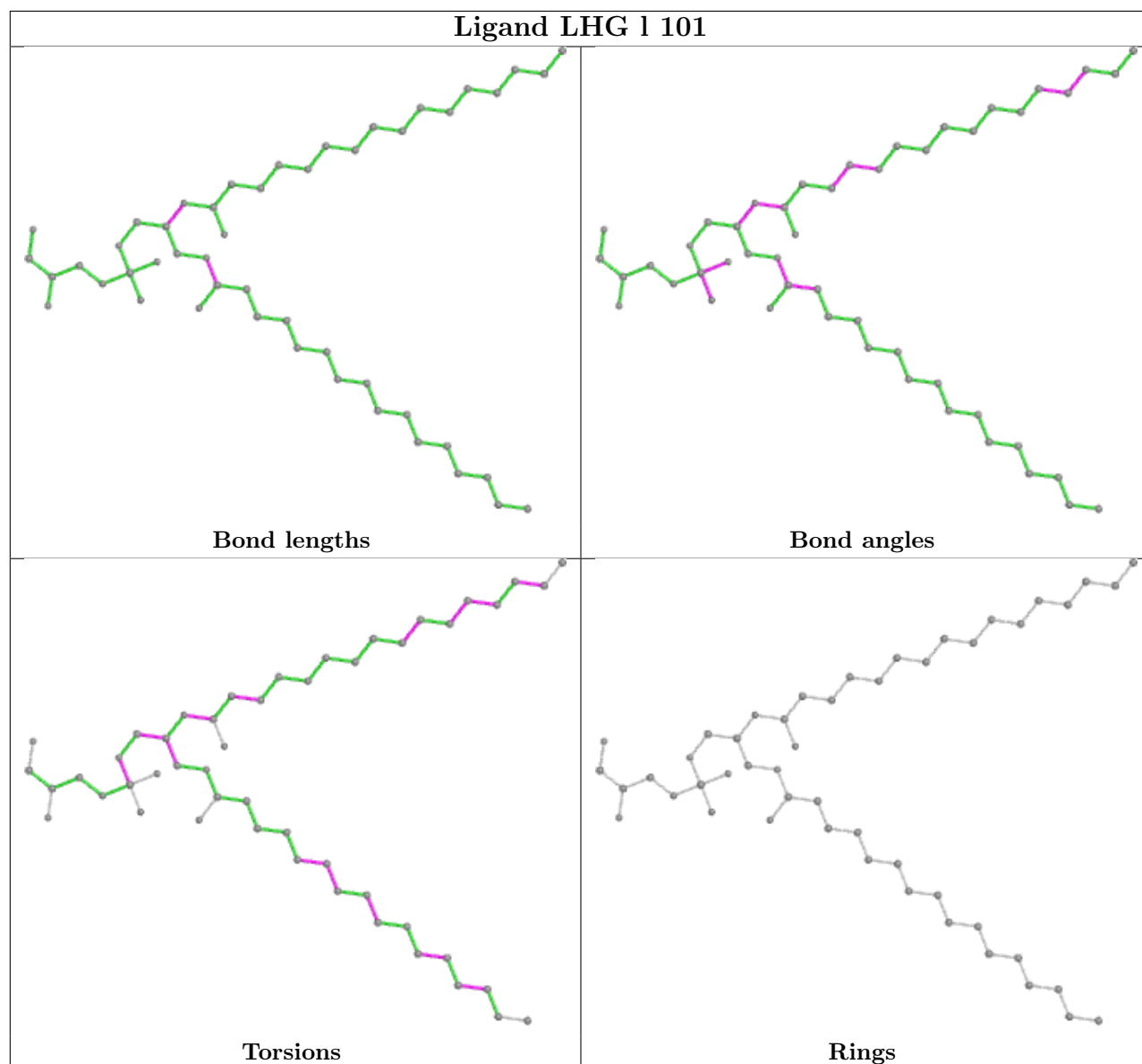


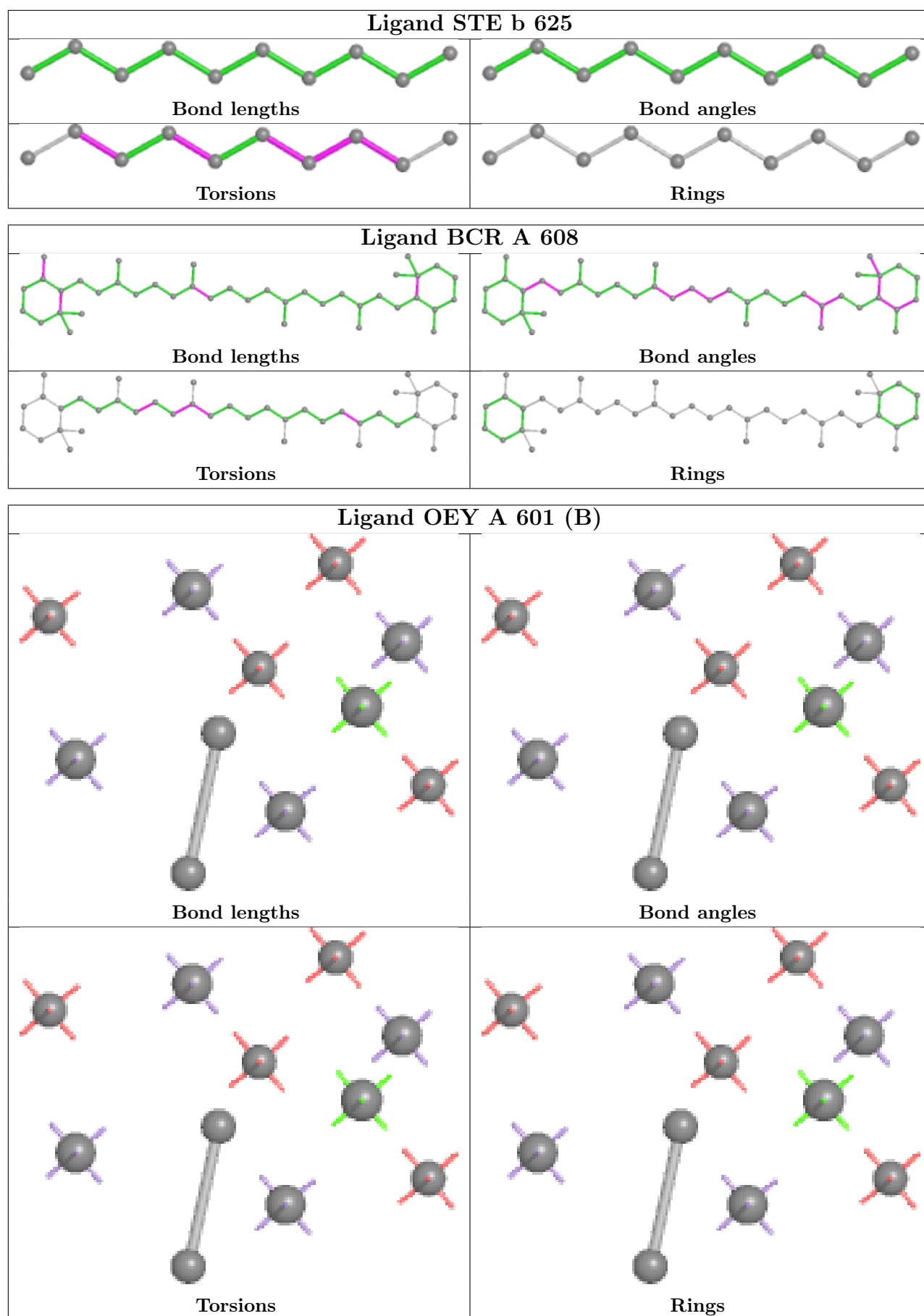


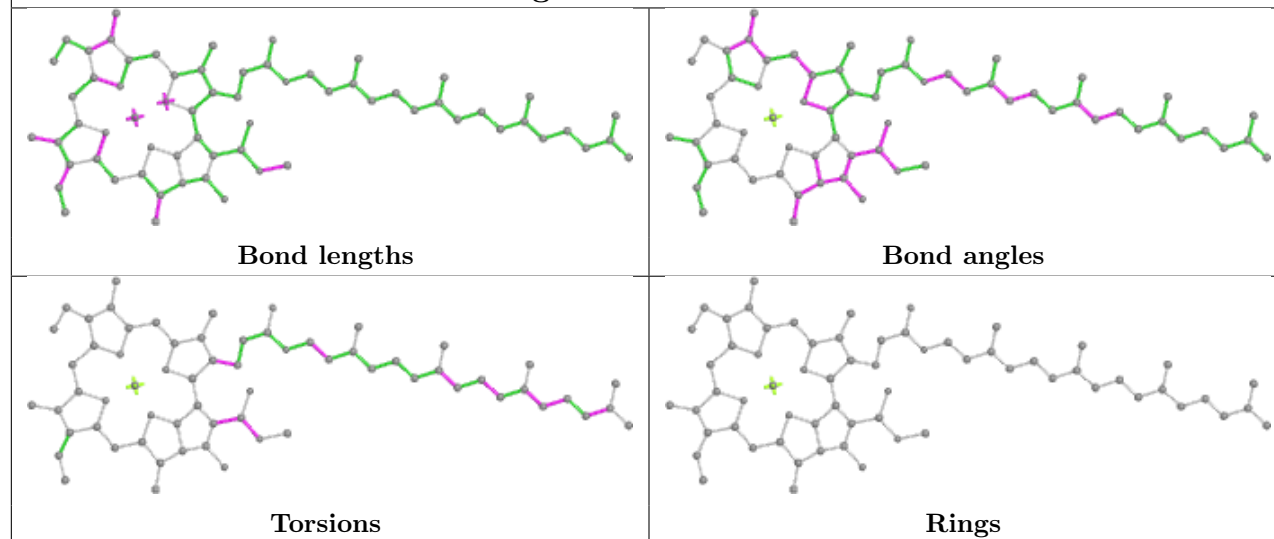
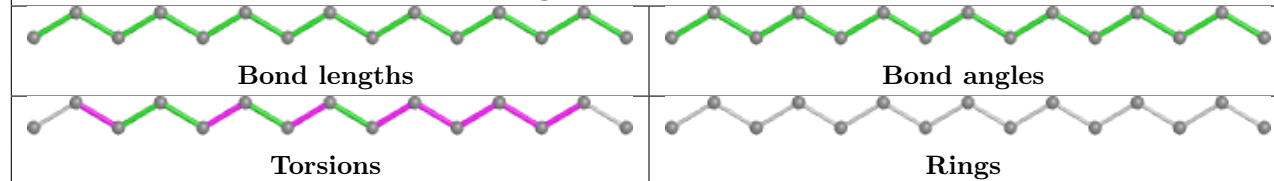
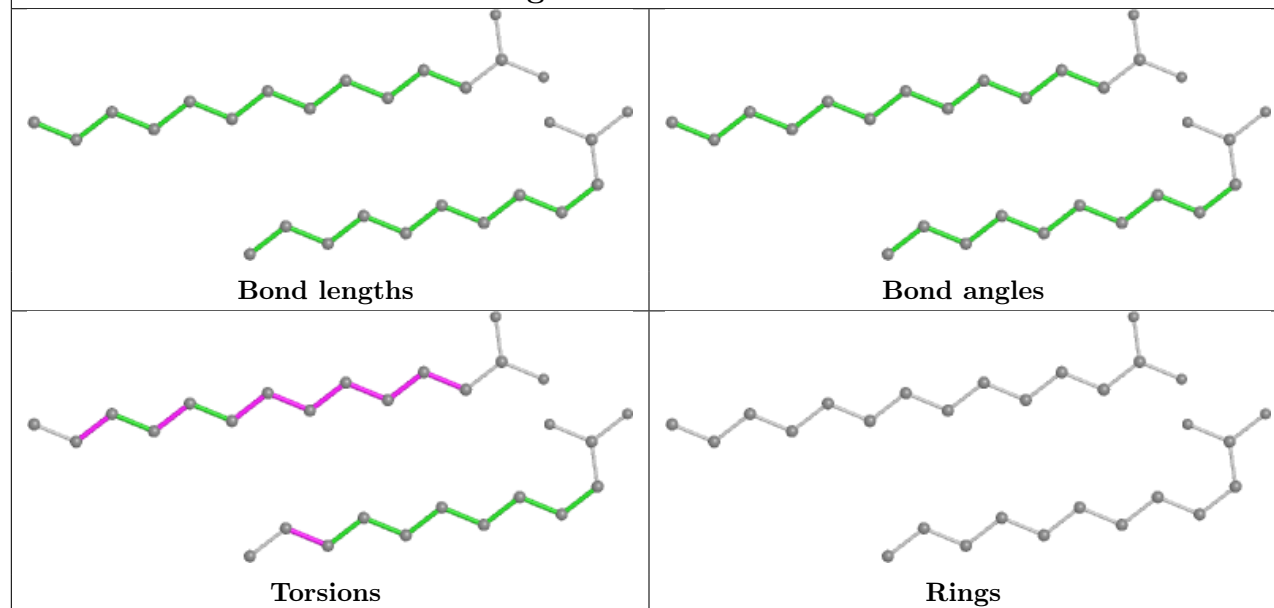
Ligand CLA a 605

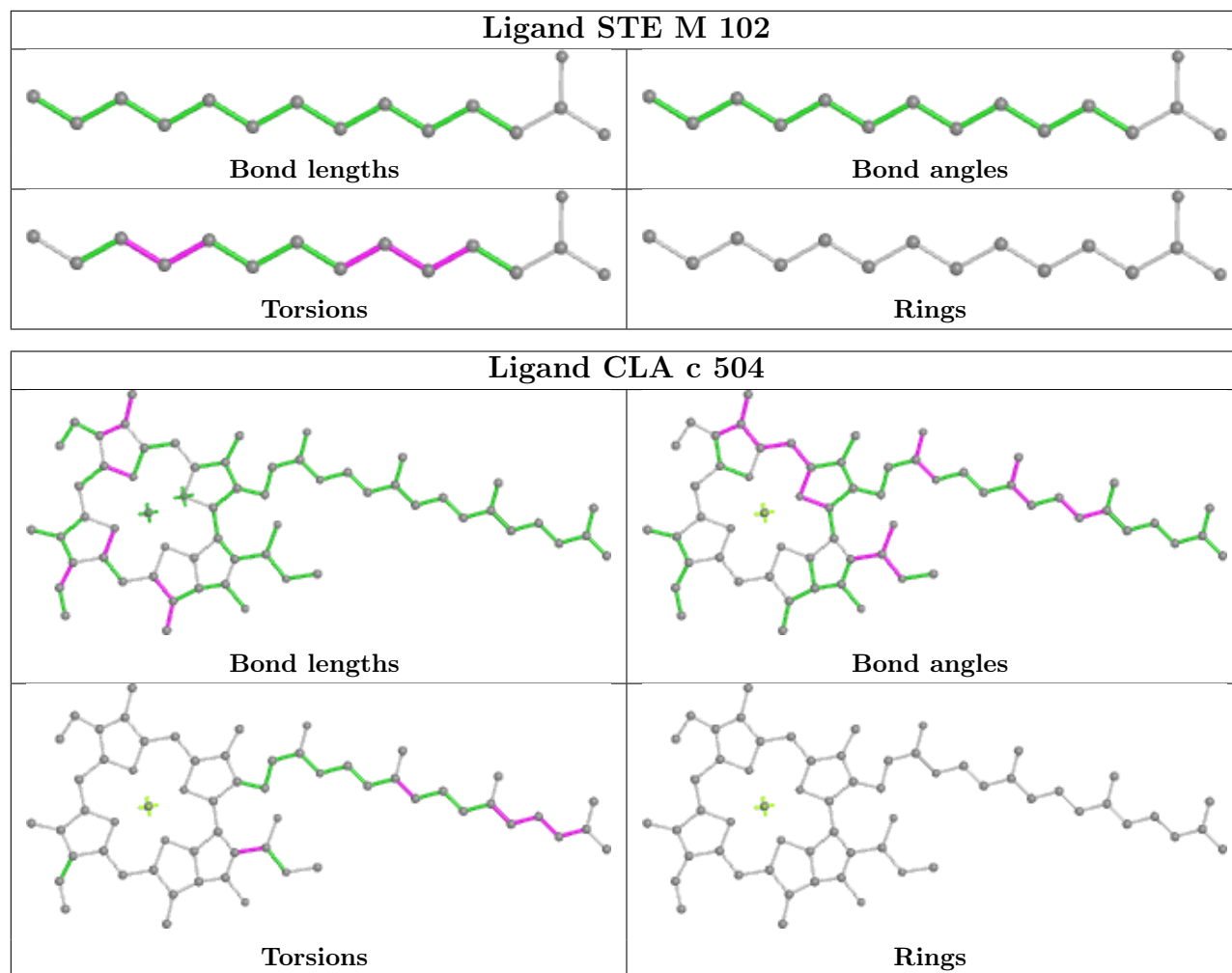


Ligand LHG 1 101

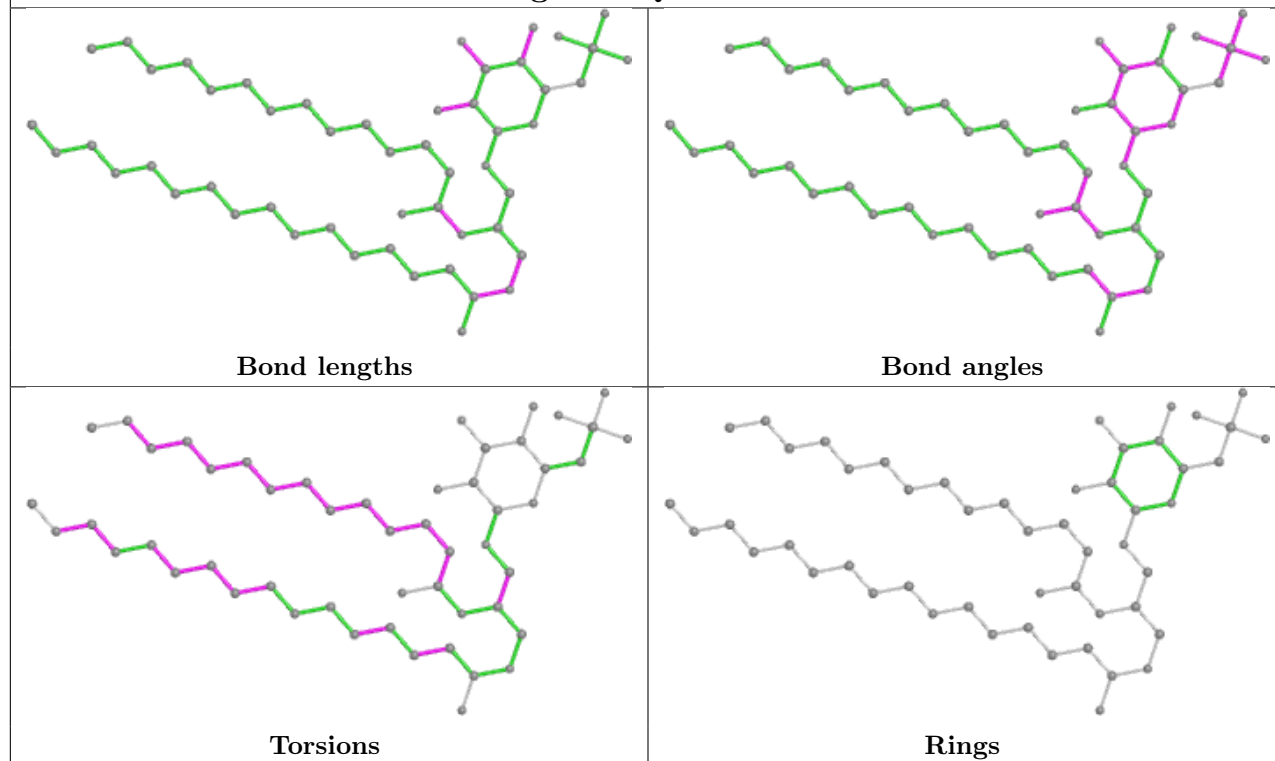




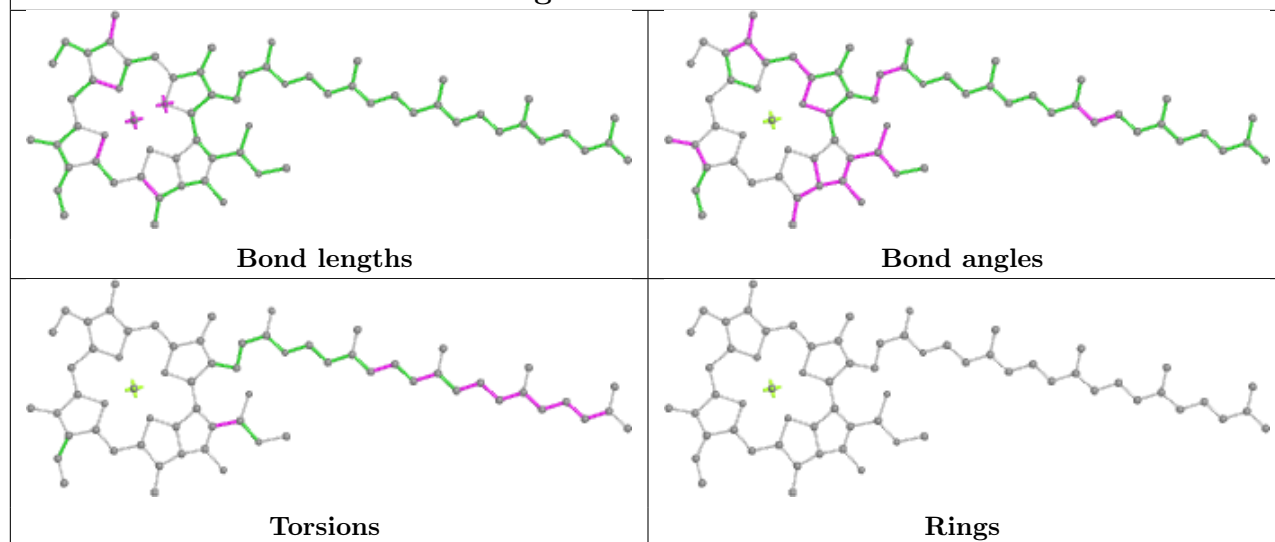
Ligand CLA B 603**Ligand STE B 625****Ligand LMG D 412**

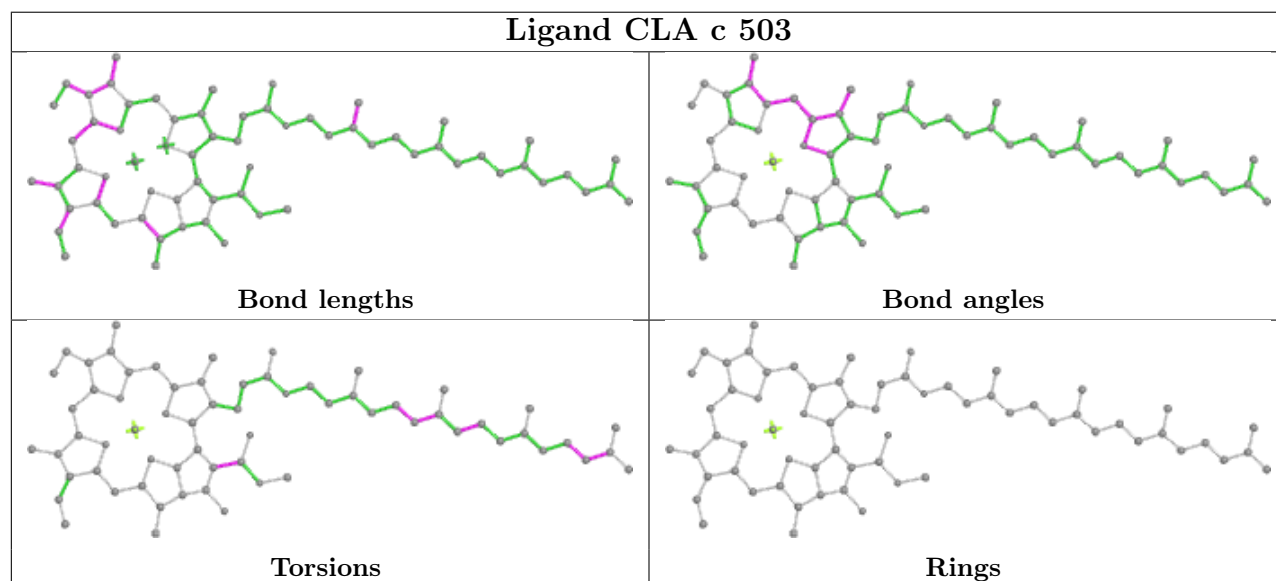
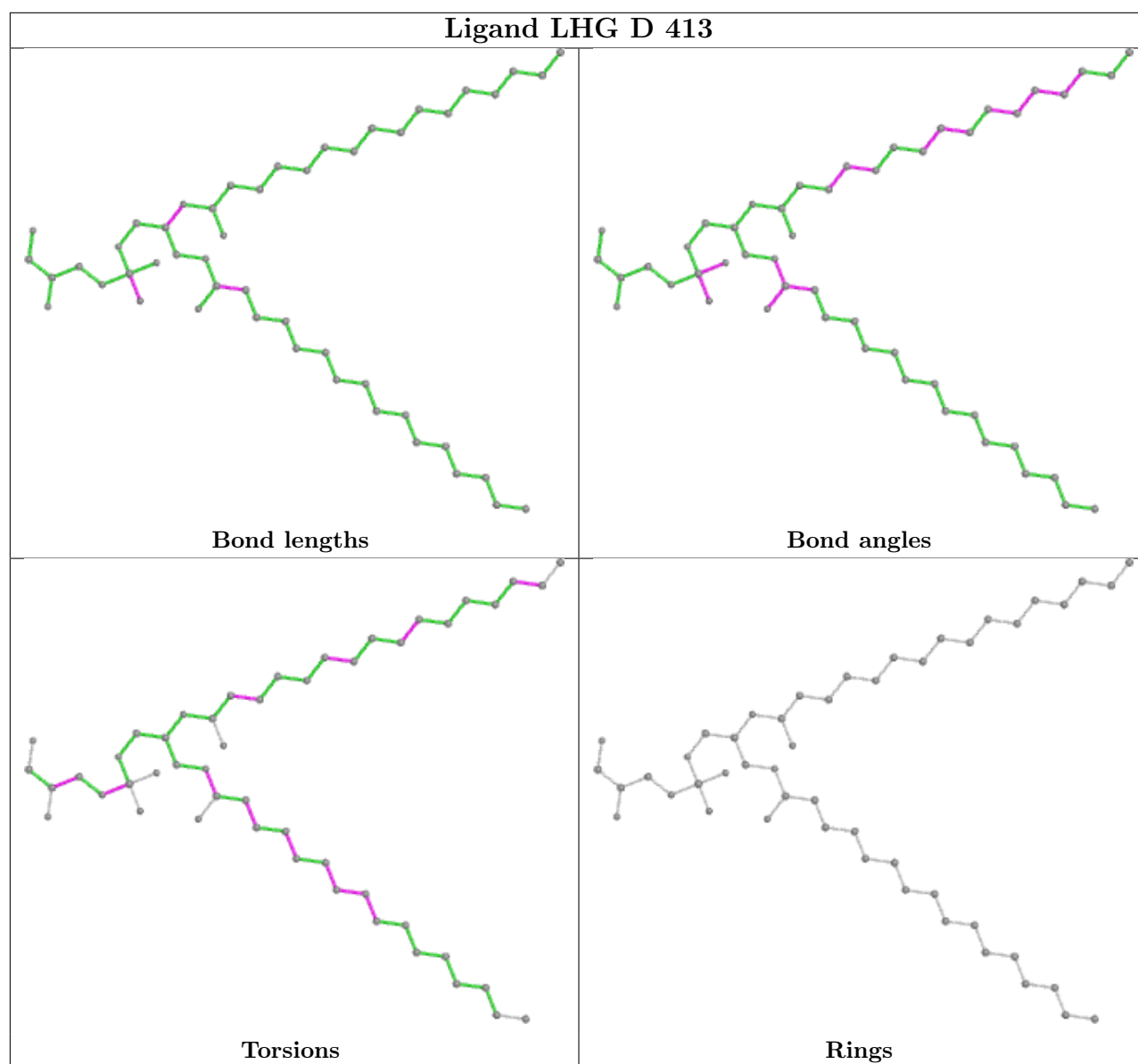


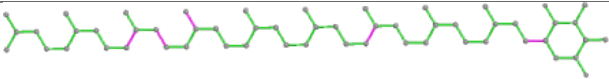
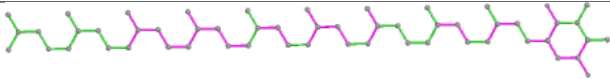
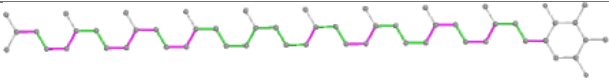
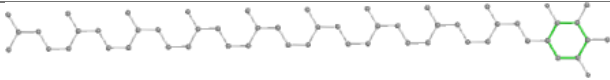
Ligand SQD A 613

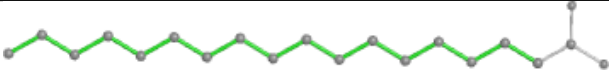
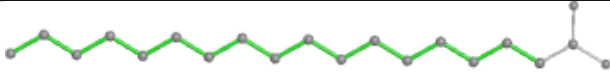
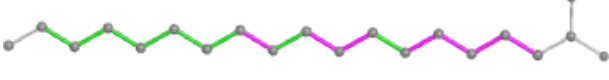
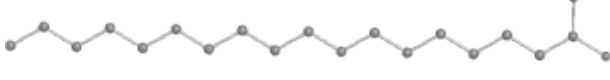



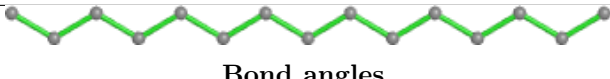


Ligand CLA b 604

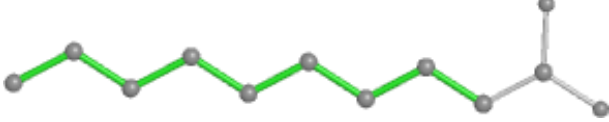
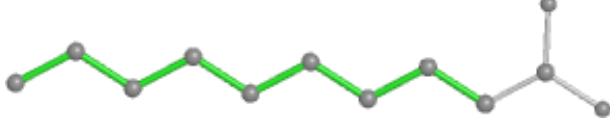
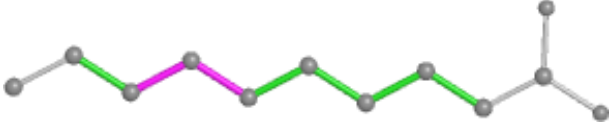
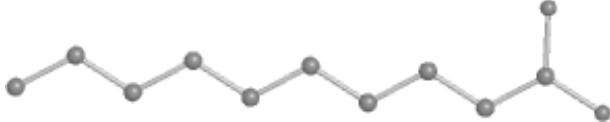


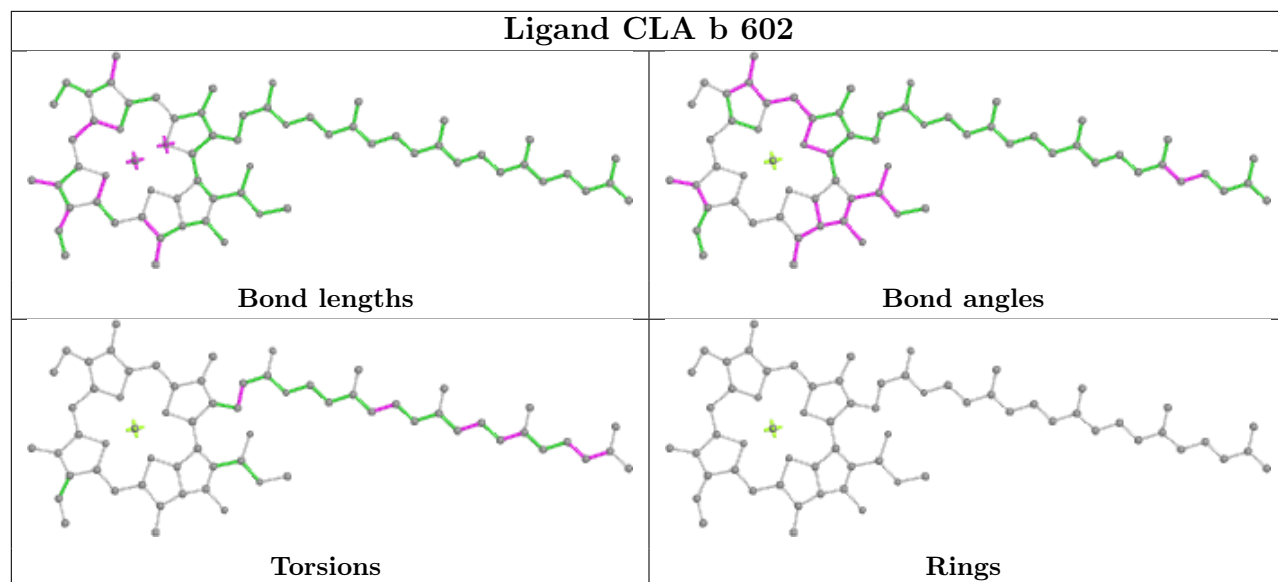
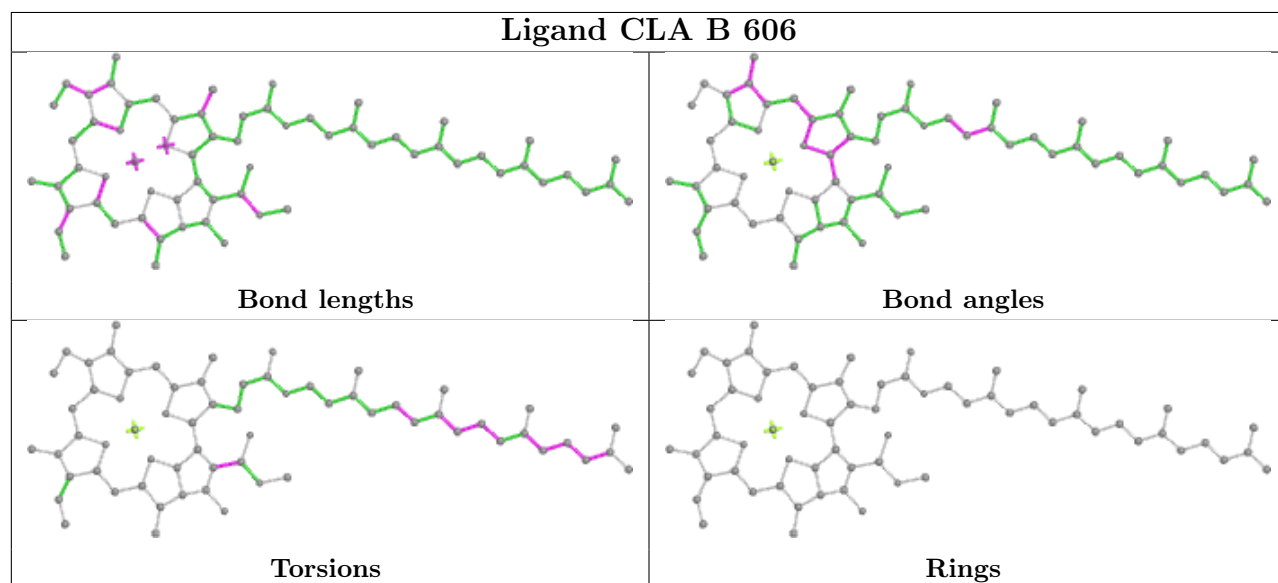


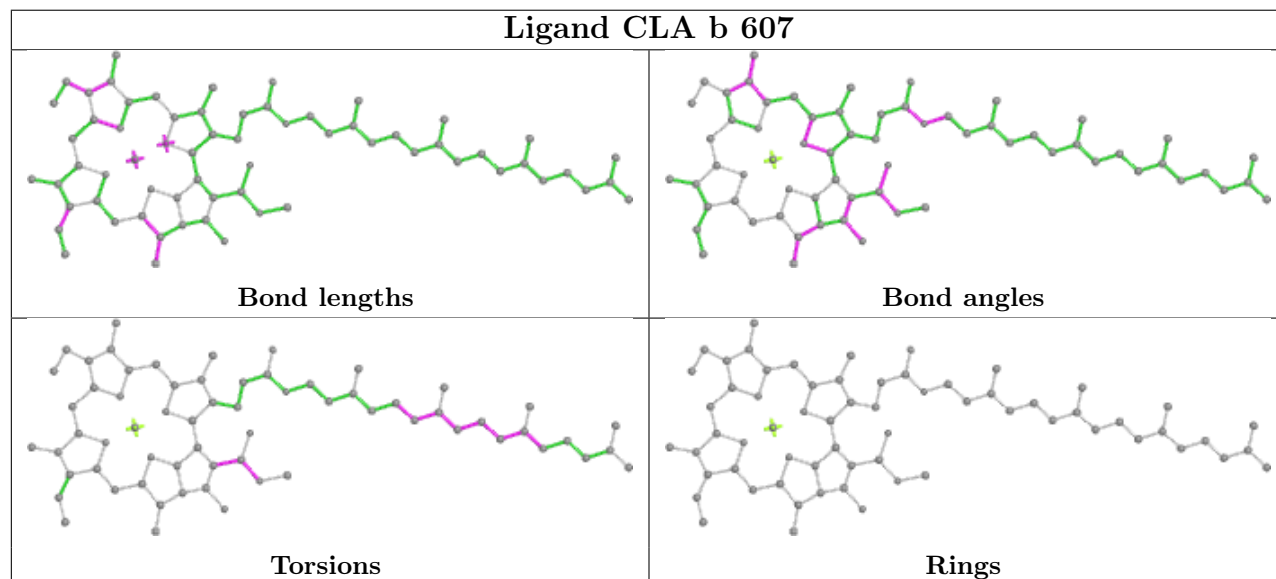
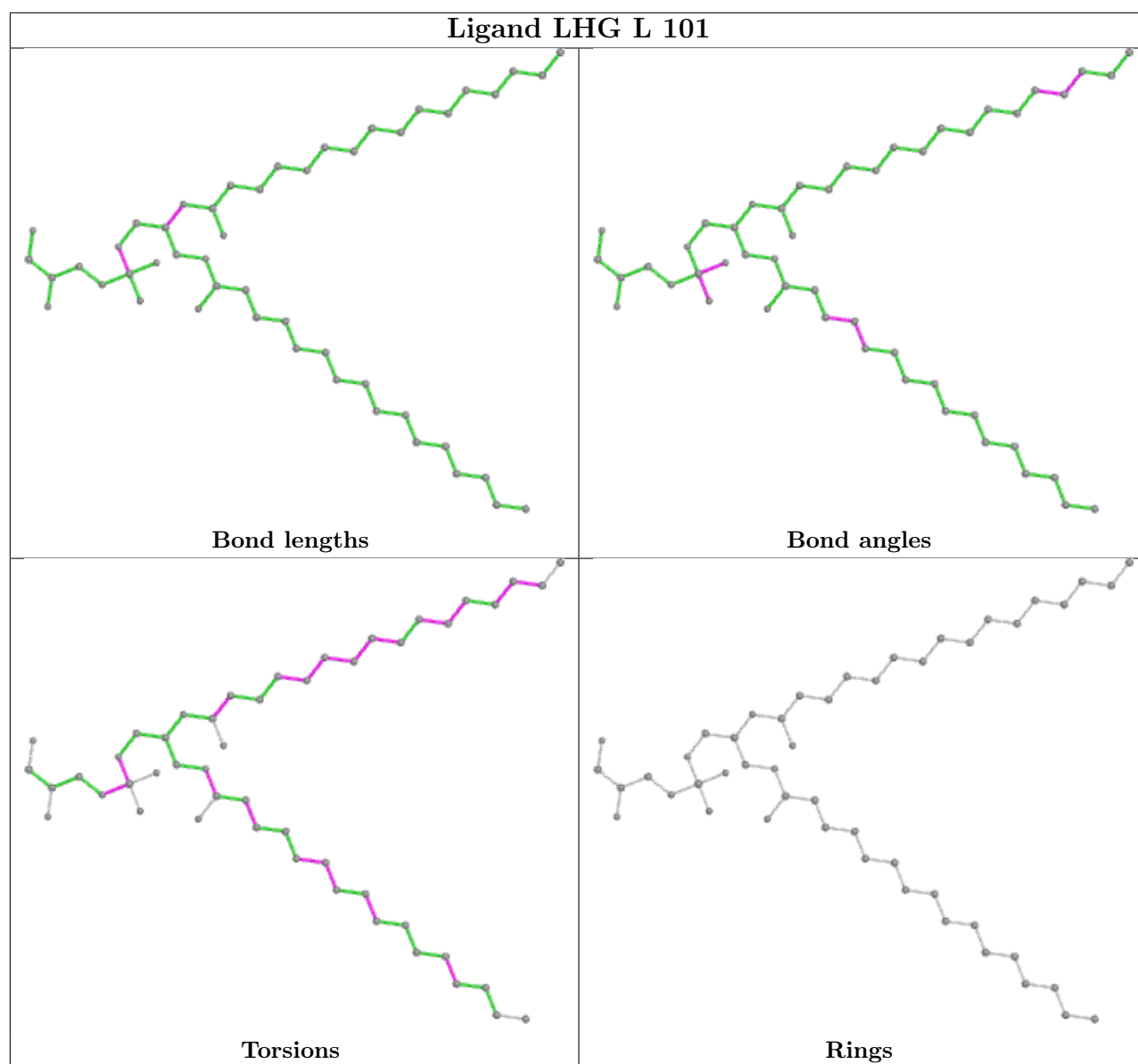
Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

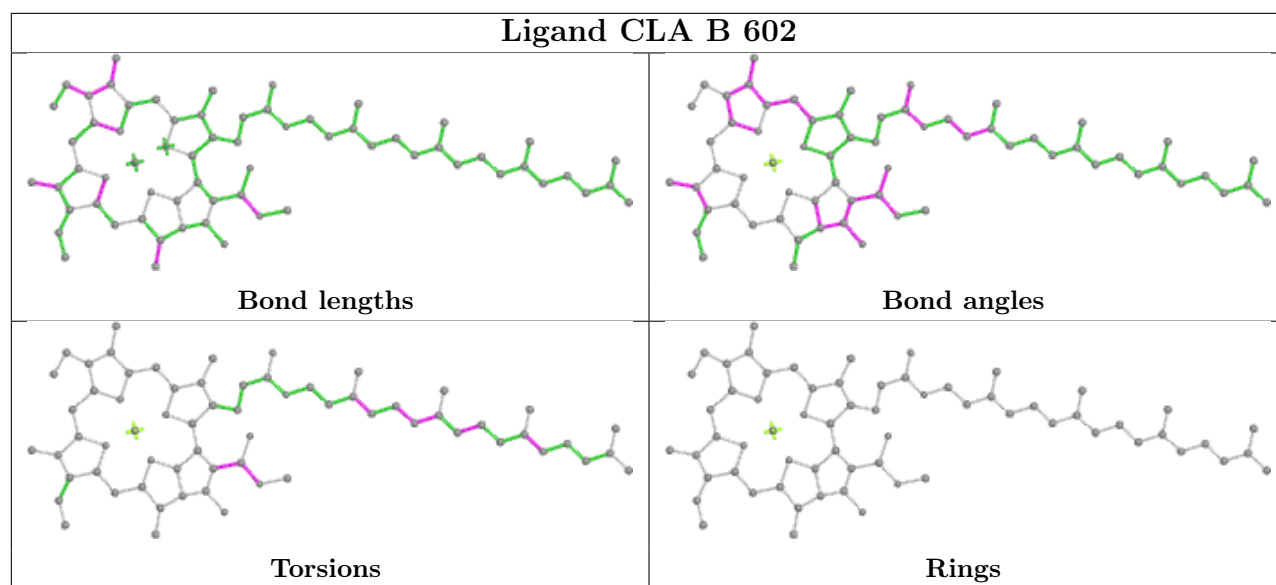
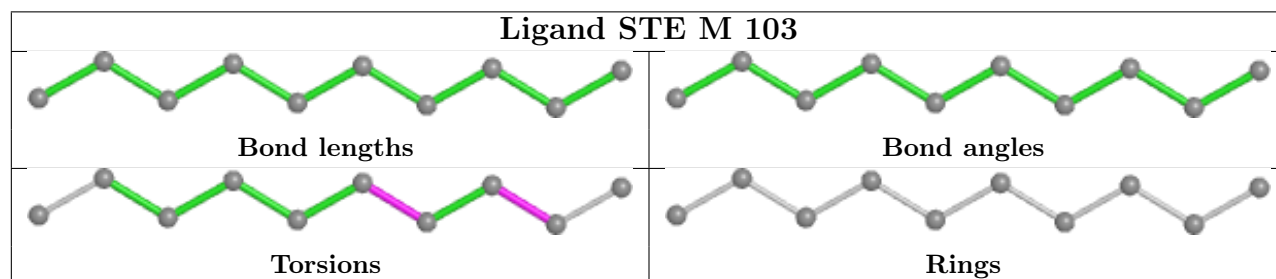
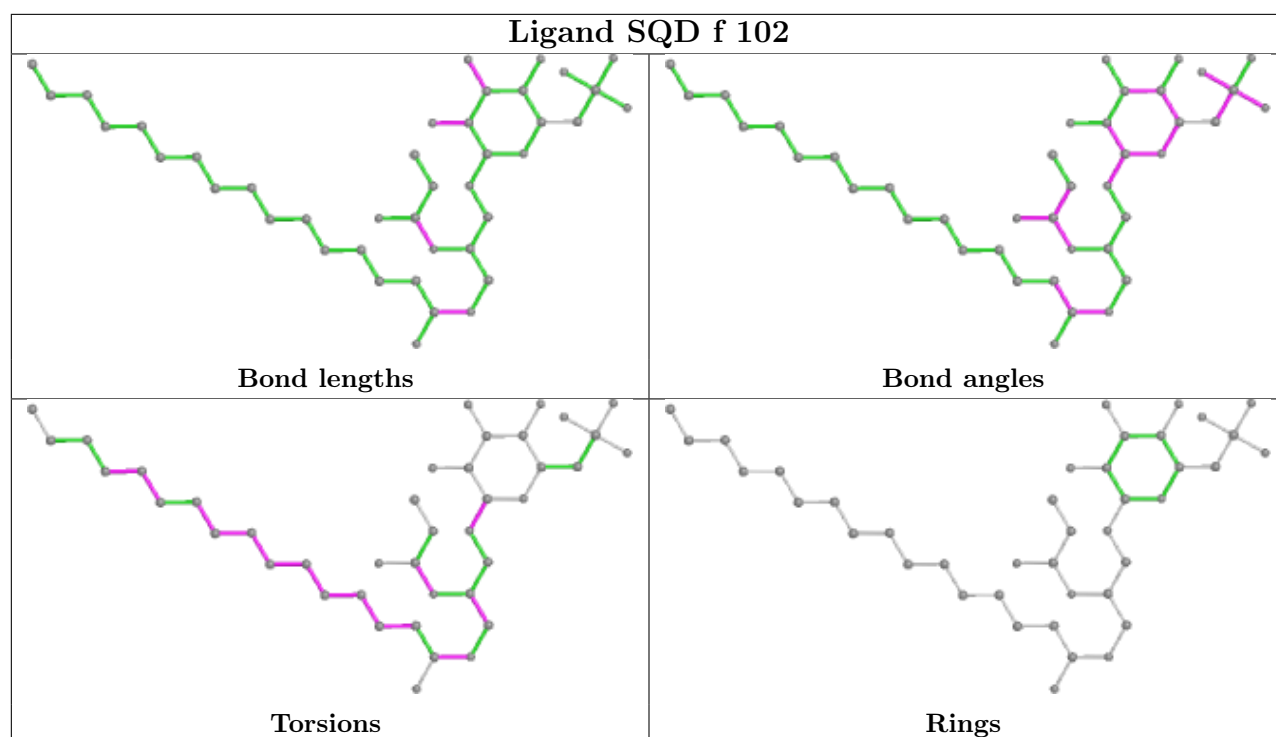
Ligand STE c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

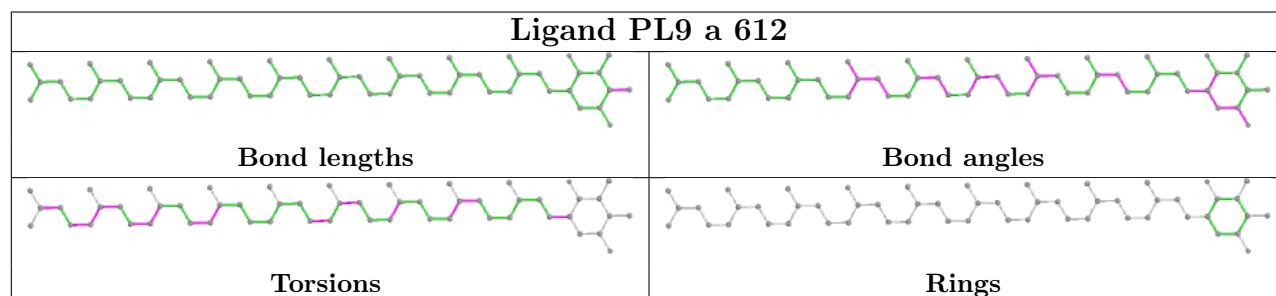
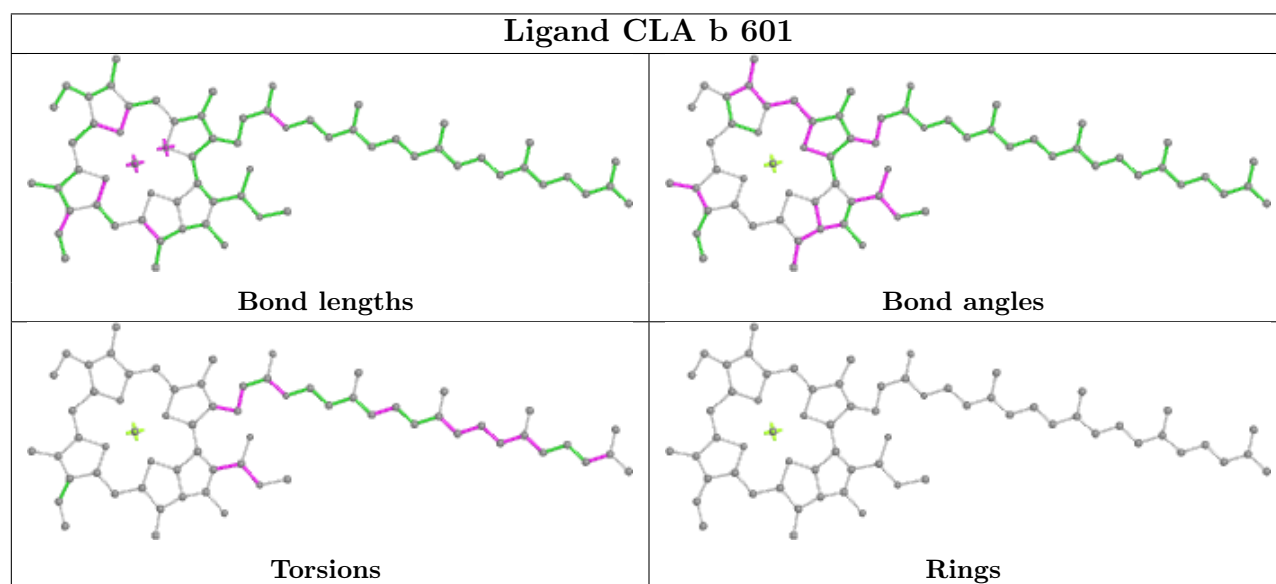
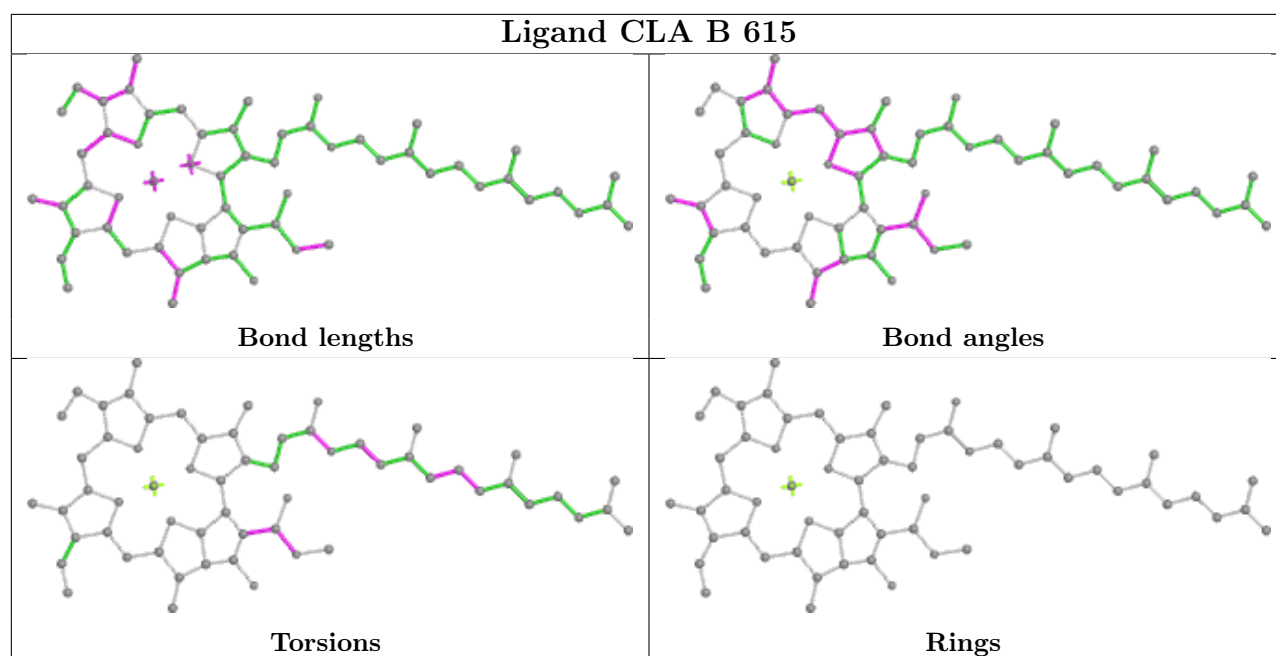
Ligand STE I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

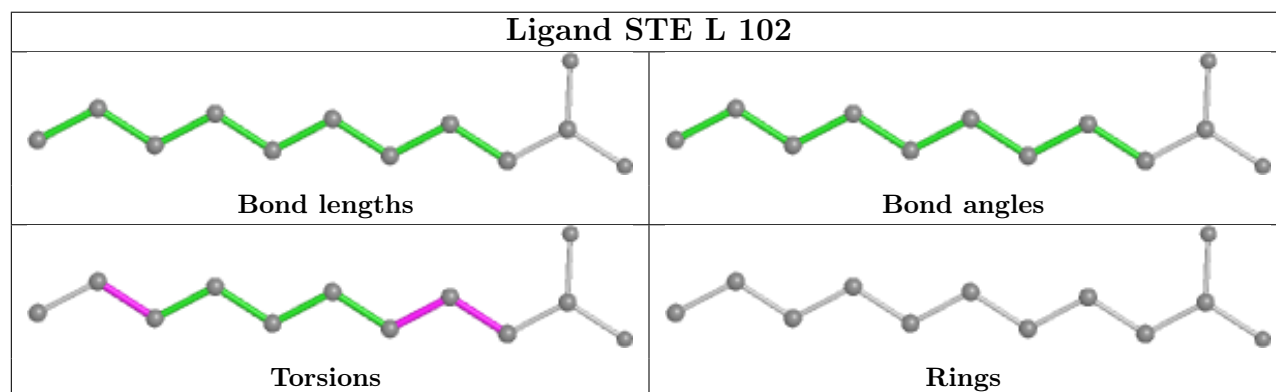
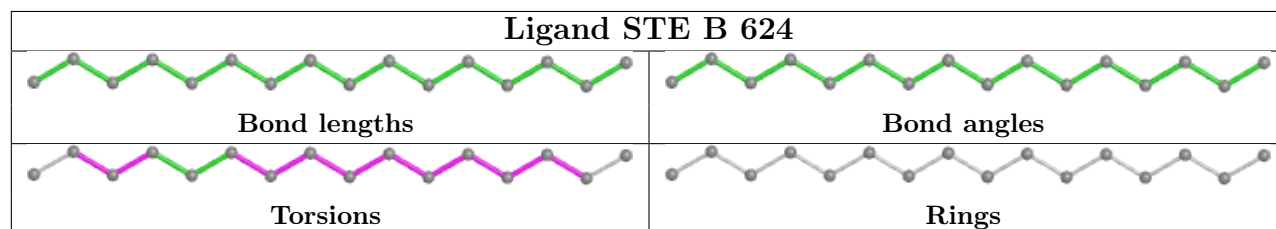
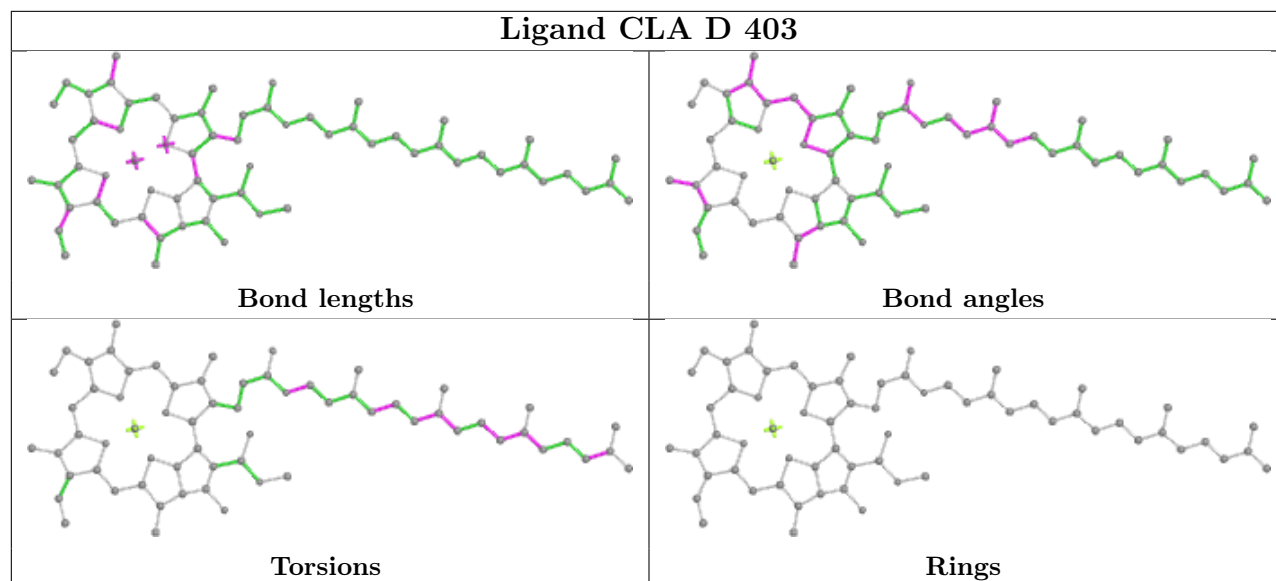
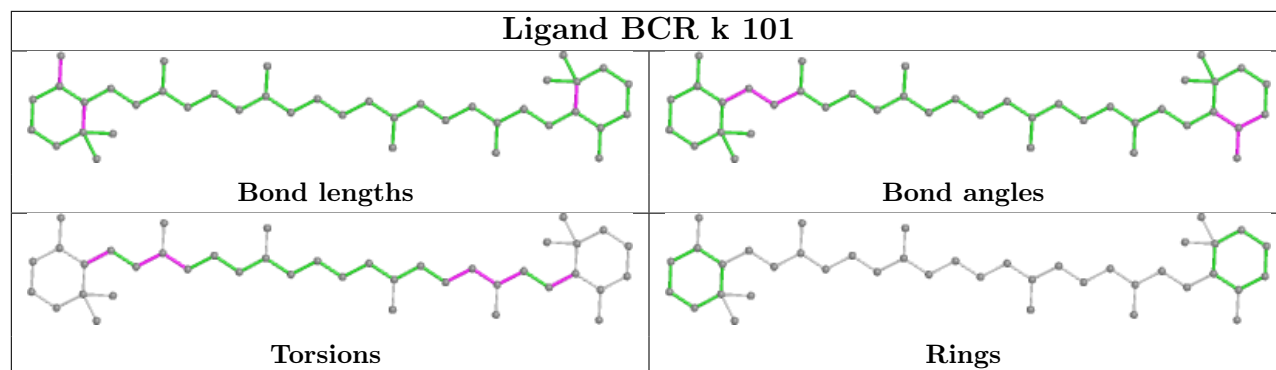
Ligand STE J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

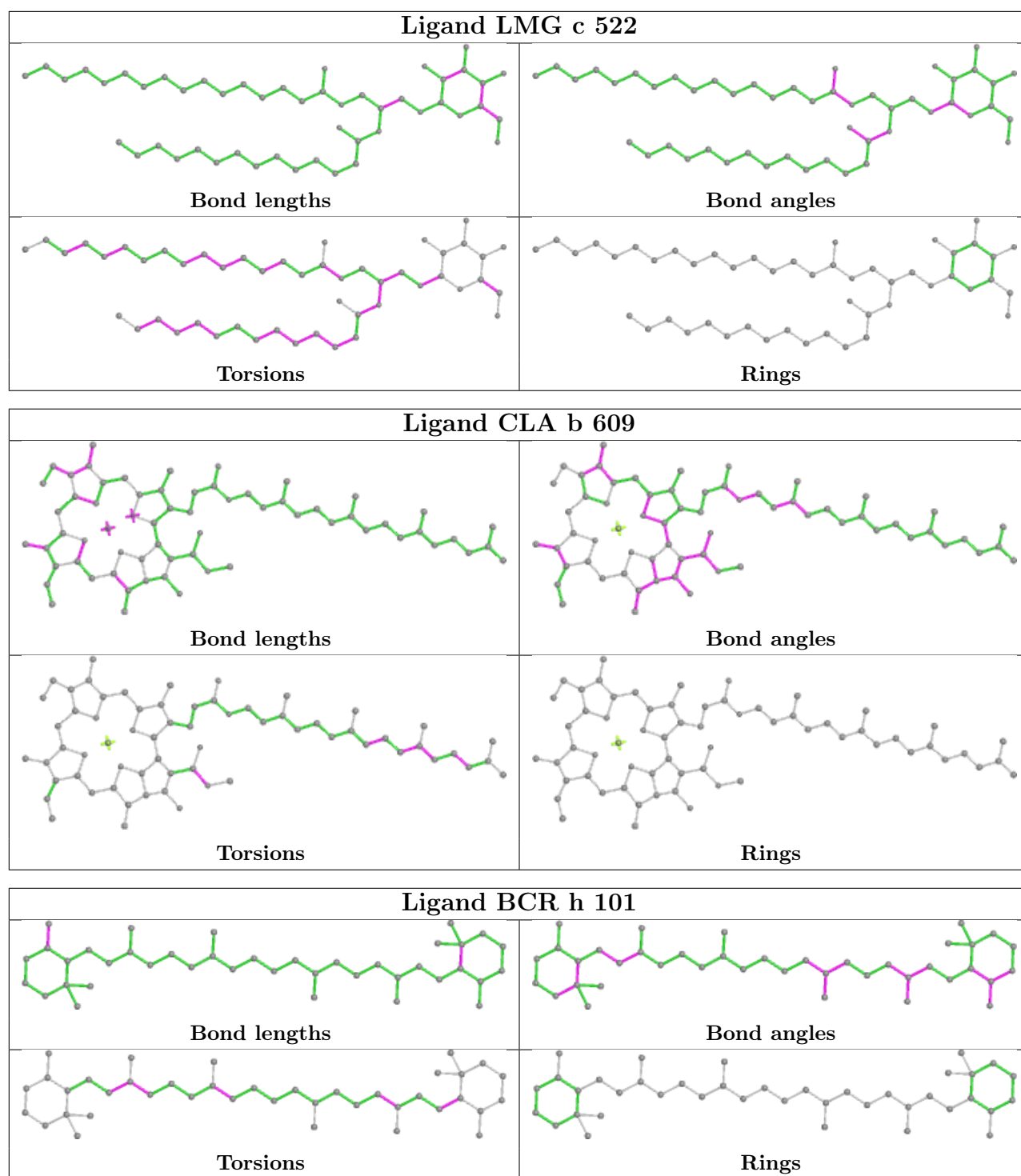
Ligand CLA b 602**Ligand CLA B 606**

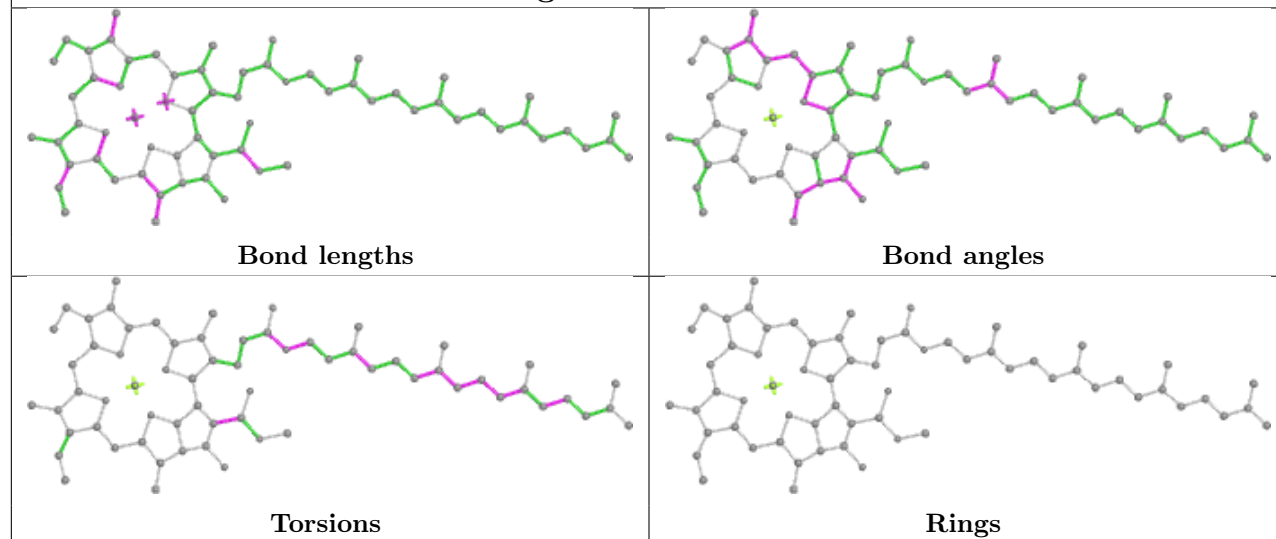
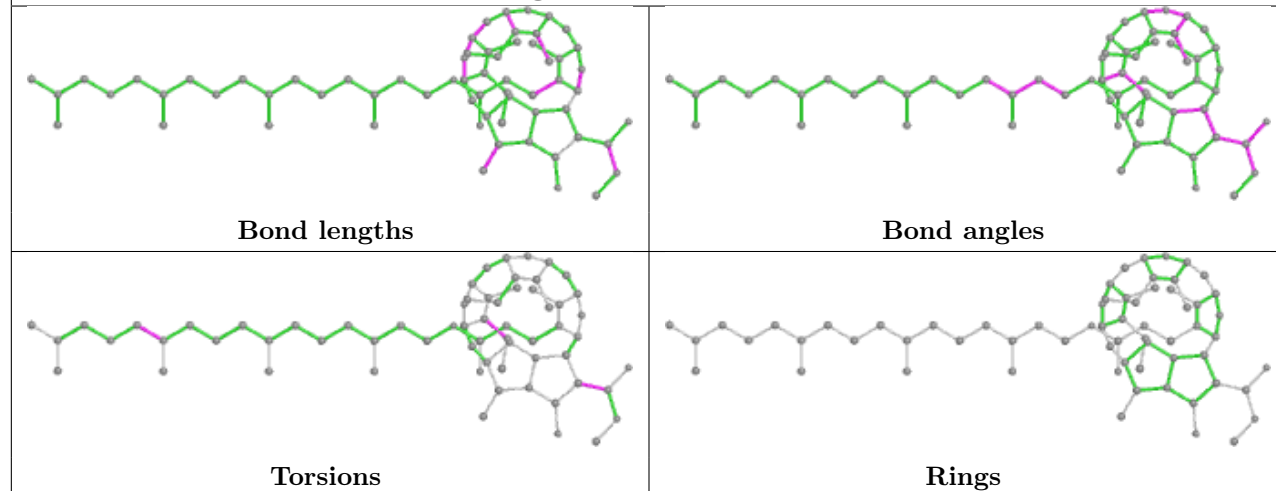




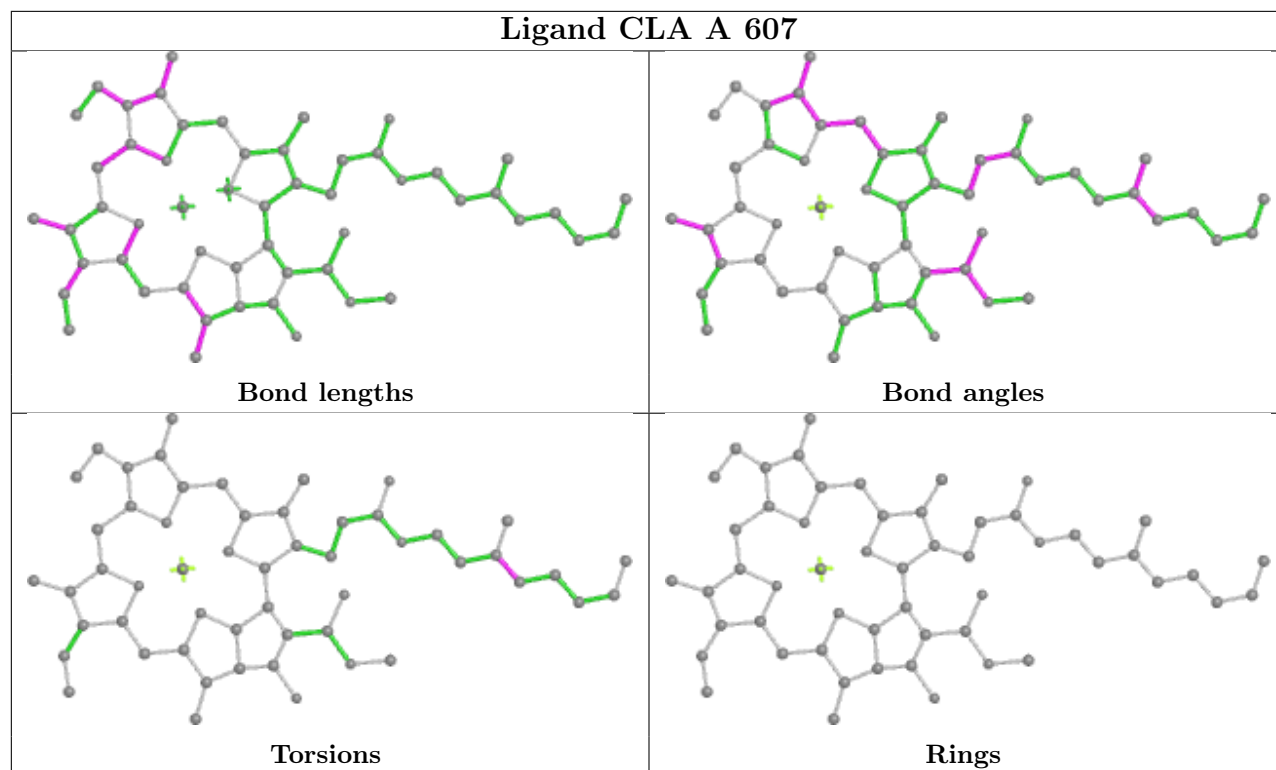




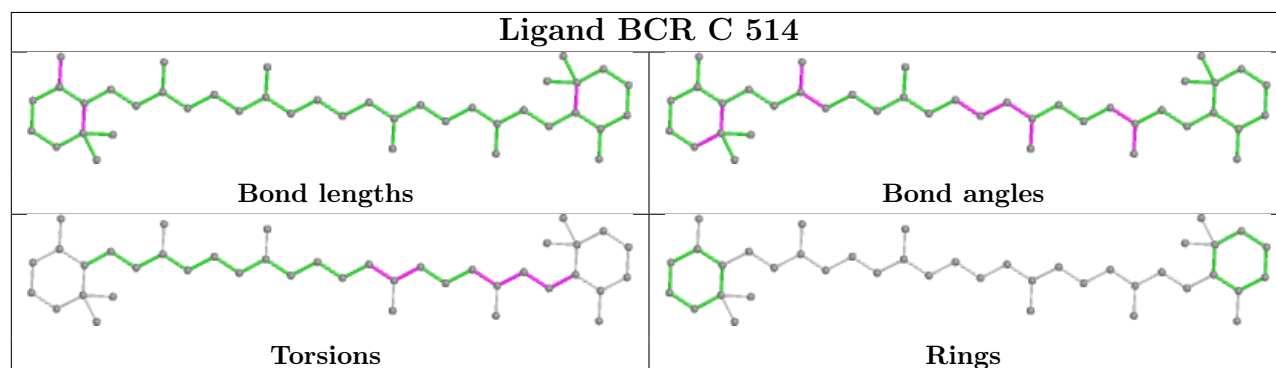


Ligand CLA c 506**Ligand PHO A 606**

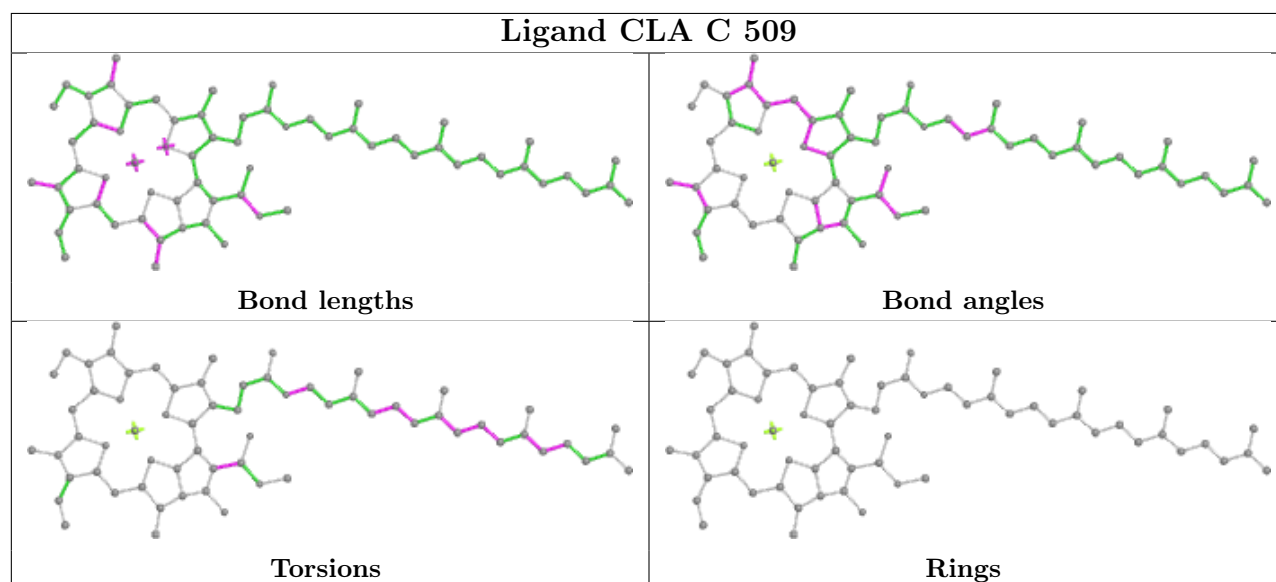
Ligand CLA A 607

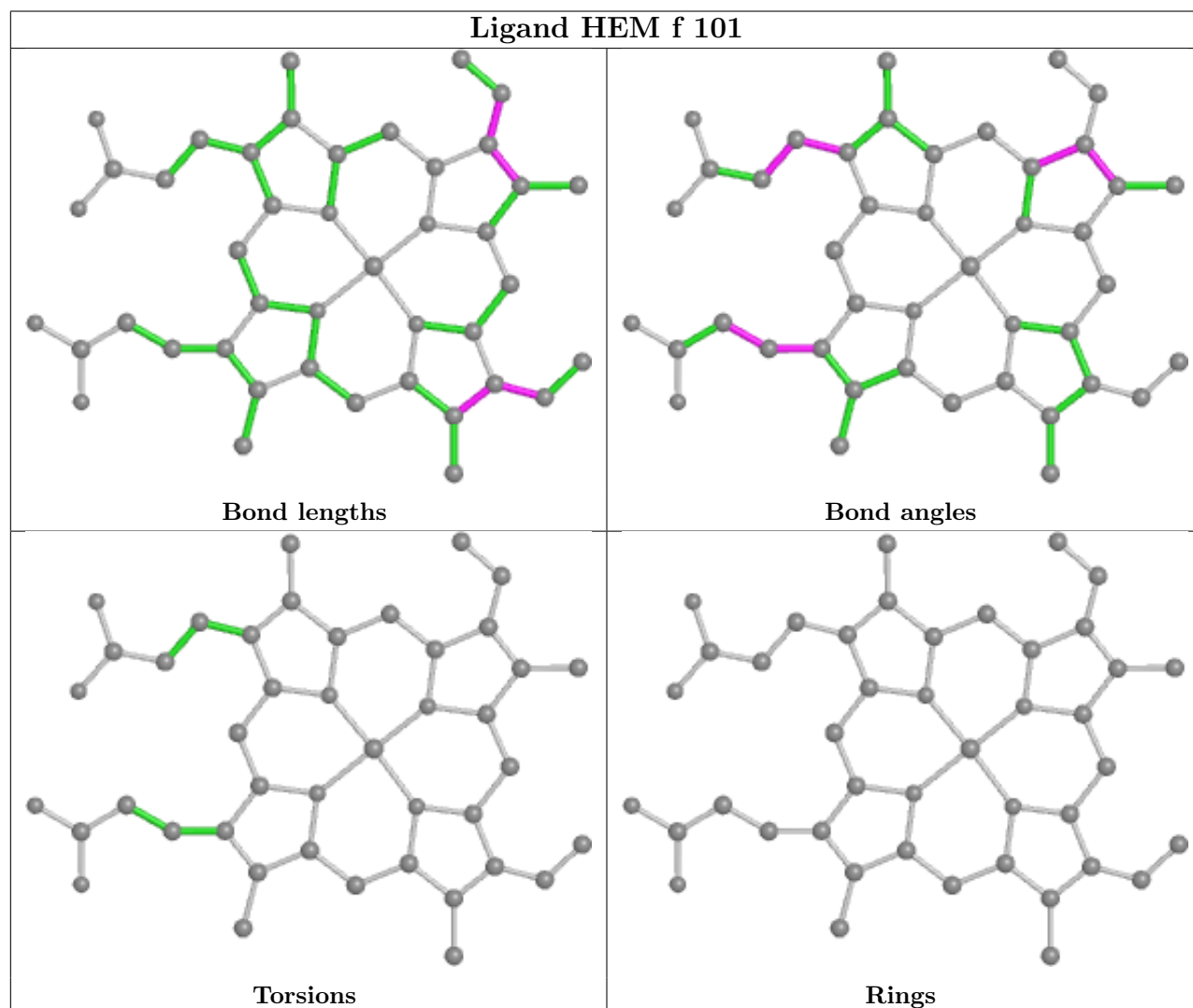
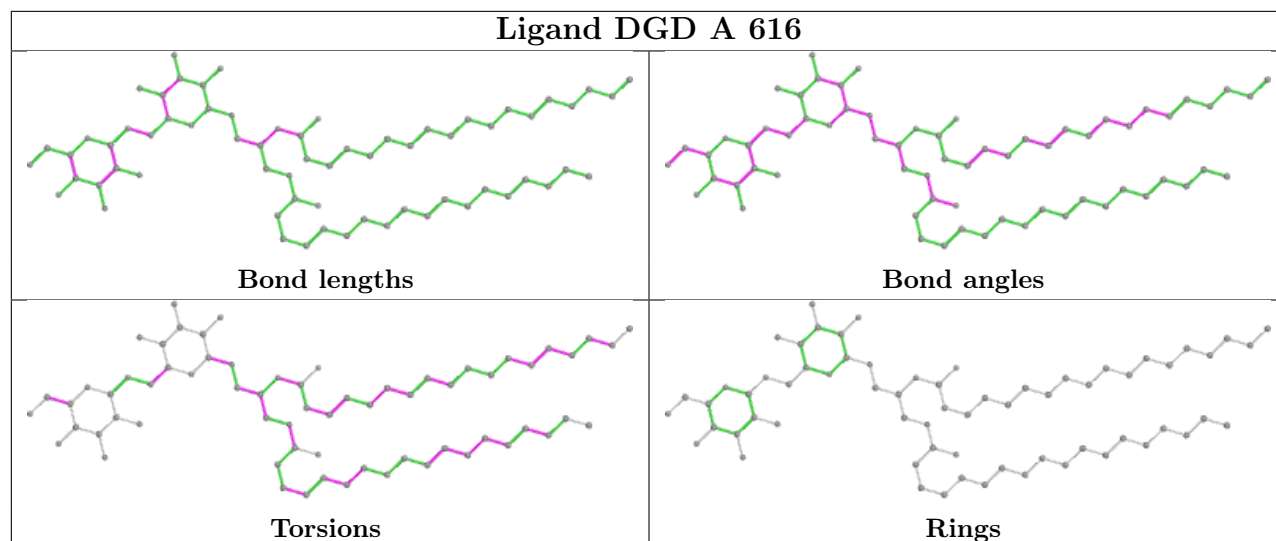


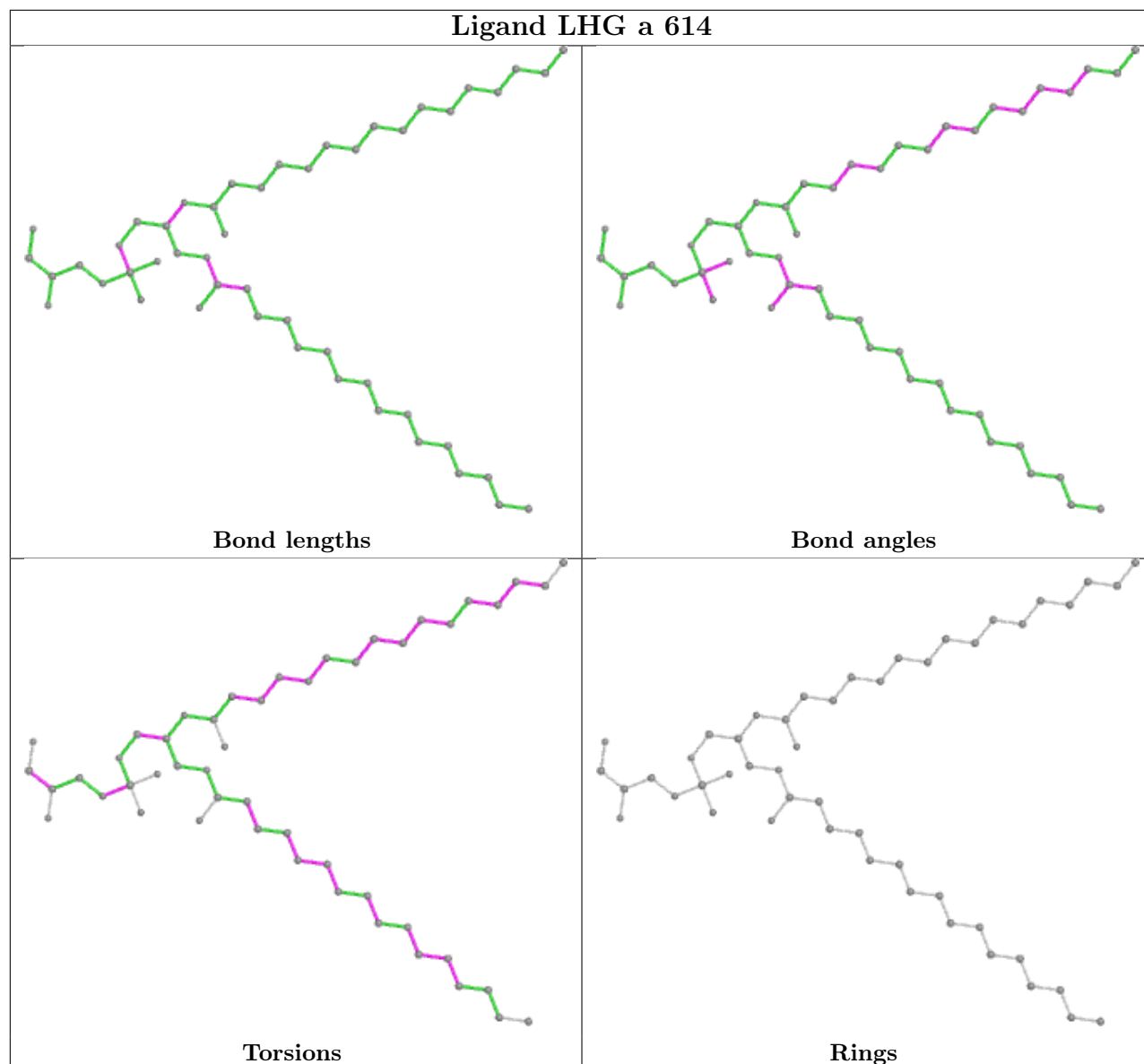
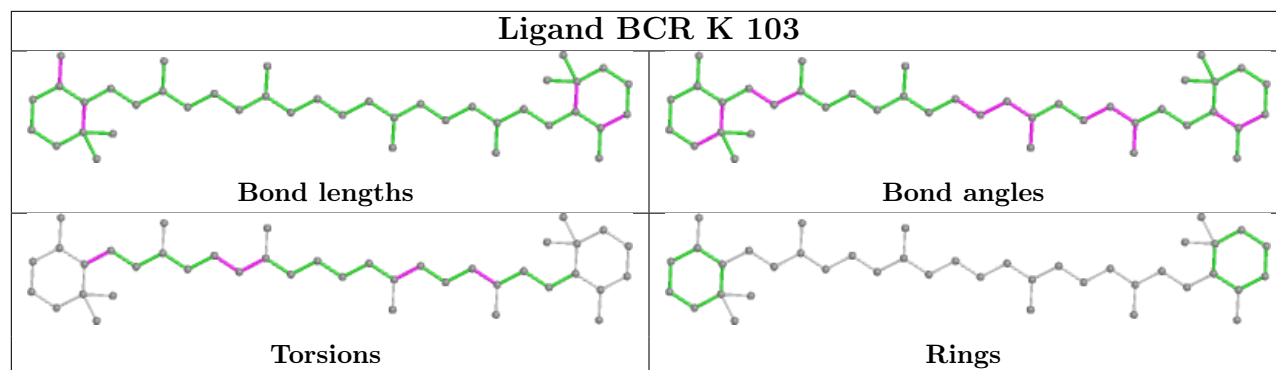
Ligand BCR C 514

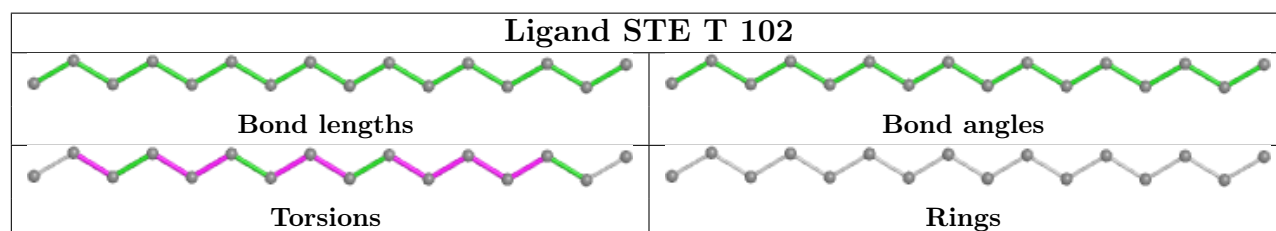
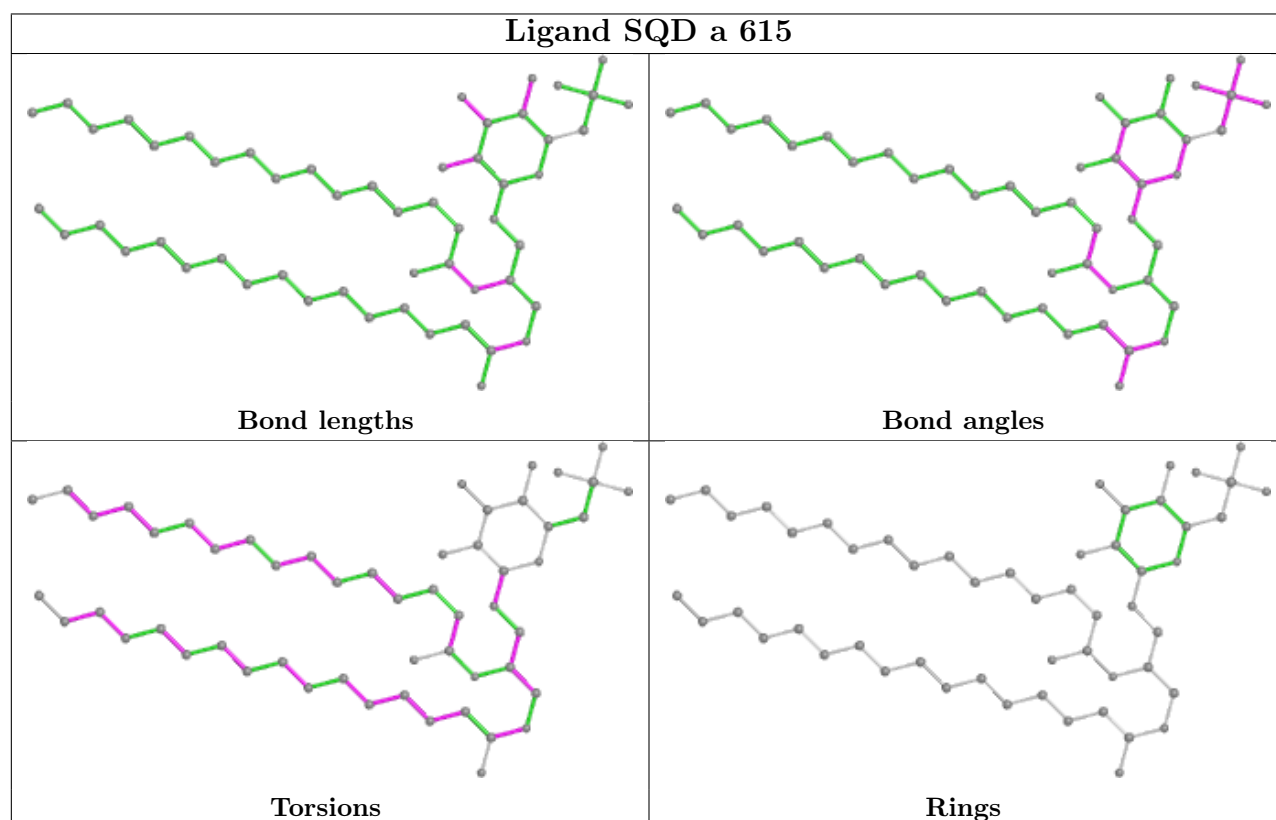
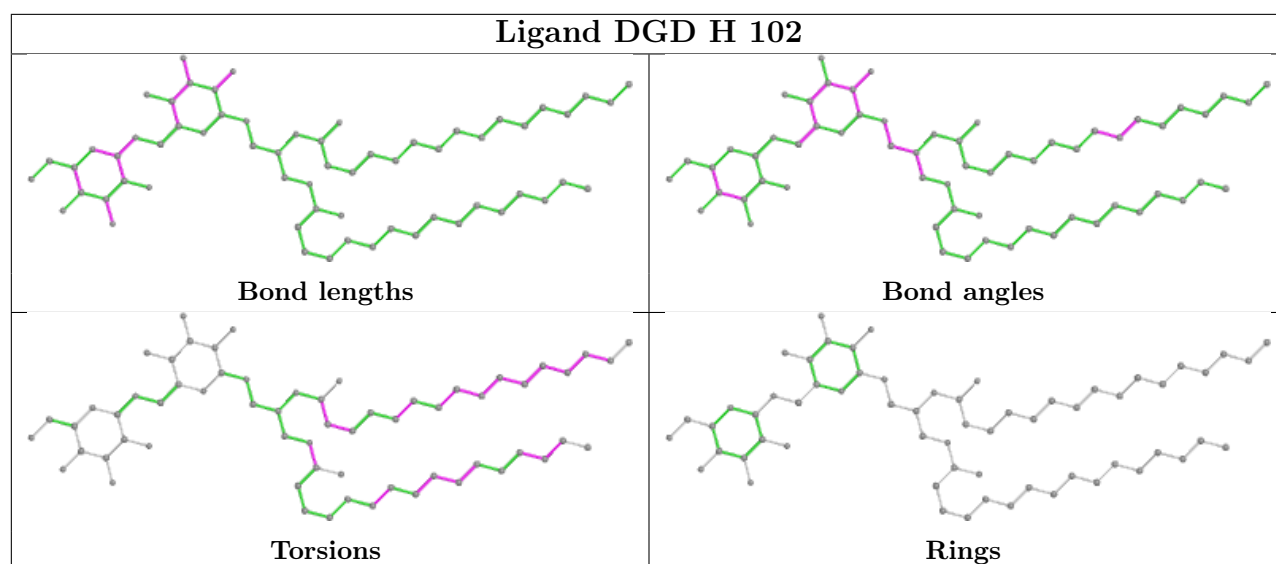


Ligand CLA C 509









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%)	-0.39	4 (1%) 79 80	25, 33, 53, 84	0
1	a	334/344 (97%)	-0.36	1 (0%) 94 94	24, 35, 61, 85	0
2	B	505/510 (99%)	-0.40	6 (1%) 79 80	27, 37, 64, 93	0
2	b	505/510 (99%)	-0.23	16 (3%) 47 47	28, 39, 74, 106	0
3	C	442/461 (95%)	-0.31	8 (1%) 68 69	29, 40, 56, 78	0
3	c	451/461 (97%)	-0.25	8 (1%) 68 69	29, 43, 63, 97	0
4	D	341/352 (96%)	-0.41	3 (0%) 84 84	26, 34, 54, 82	0
4	d	341/352 (96%)	-0.34	0 100 100	27, 38, 63, 84	0
5	E	82/84 (97%)	-0.02	4 (4%) 29 29	37, 55, 74, 87	0
5	e	82/84 (97%)	0.19	6 (7%) 15 14	40, 64, 84, 93	0
6	F	34/45 (75%)	-0.30	2 (5%) 22 21	41, 48, 71, 97	0
6	f	34/45 (75%)	-0.17	4 (11%) 4 3	45, 54, 92, 109	0
7	H	65/66 (98%)	-0.12	2 (3%) 49 49	37, 45, 62, 77	0
7	h	63/66 (95%)	0.25	6 (9%) 8 7	44, 55, 66, 69	0
8	I	35/38 (92%)	-0.33	2 (5%) 23 23	35, 42, 70, 89	0
8	i	35/38 (92%)	-0.18	3 (8%) 10 10	36, 43, 72, 80	0
9	J	36/40 (90%)	0.02	4 (11%) 5 4	39, 54, 84, 92	0
9	j	36/40 (90%)	0.07	4 (11%) 5 4	42, 57, 94, 101	0
10	K	37/46 (80%)	0.16	4 (10%) 5 5	48, 56, 76, 86	0
10	k	37/46 (80%)	-0.10	1 (2%) 54 55	51, 59, 76, 84	0
11	L	37/37 (100%)	-0.56	0 100 100	28, 33, 62, 71	0
11	l	36/37 (97%)	-0.27	3 (8%) 11 11	28, 34, 65, 88	0
12	M	32/36 (88%)	-0.18	1 (3%) 49 49	29, 36, 63, 74	0
12	m	31/36 (86%)	-0.31	1 (3%) 47 47	30, 37, 58, 71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.12	13 (5%) 26 26	29, 45, 82, 128	0
13	o	244/272 (89%)	-0.19	14 (5%) 23 23	29, 44, 80, 121	0
14	R	28/41 (68%)	3.55	26 (92%) 0 0	77, 89, 101, 107	0
14	r	28/41 (68%)	5.75	28 (100%) 0 0	86, 118, 129, 134	0
15	T	29/32 (90%)	-0.40	2 (6%) 16 16	30, 35, 60, 81	0
15	t	29/32 (90%)	-0.24	3 (10%) 6 5	31, 36, 71, 78	0
16	U	97/134 (72%)	-0.39	0 100 100	36, 46, 69, 89	0
16	u	97/134 (72%)	-0.47	0 100 100	34, 44, 60, 85	0
17	V	137/163 (84%)	-0.64	0 100 100	31, 44, 59, 76	0
17	v	137/163 (84%)	-0.28	0 100 100	37, 51, 69, 81	0
18	X	38/41 (92%)	0.22	2 (5%) 26 26	45, 55, 75, 79	0
18	x	39/41 (95%)	0.47	4 (10%) 6 5	49, 65, 92, 106	0
19	Y	27/46 (58%)	1.35	9 (33%) 0 0	58, 76, 89, 93	0
19	y	30/46 (65%)	0.60	3 (10%) 7 6	63, 76, 92, 97	0
20	Z	62/62 (100%)	0.78	15 (24%) 0 0	59, 74, 112, 126	0
20	z	62/62 (100%)	0.73	10 (16%) 1 1	61, 73, 108, 120	0
All	All	5293/5700 (92%)	-0.19	222 (4%) 36 35	24, 41, 77, 134	0

The worst 5 of 222 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	10.8
14	r	9	LEU	10.2
13	o	58	ASN	8.8
14	r	10	LEU	8.7
14	r	3	TRP	8.1

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	0.10	37,46,65,67	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	0.95	0.10	34,48,77,77	0
12	FME	M	1	10/11	0.96	0.10	45,54,73,74	0
8	FME	i	1	10/11	0.97	0.17	46,57,67,70	0
12	FME	m	1	10/11	0.97	0.14	39,54,76,81	0
8	FME	I	1	10/11	0.97	0.16	45,56,68,71	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	R	101	12/20	0.66	0.29	66,87,95,107	0
32	STE	a	618	12/20	0.77	0.29	40,72,79,81	0
32	STE	B	623	18/20	0.78	0.33	54,80,90,94	0
32	STE	h	103	14/20	0.78	0.28	60,77,87,92	0
33	LMG	c	521	48/55	0.79	0.24	43,78,104,111	0
32	STE	b	623	16/20	0.80	0.20	50,67,85,92	0
32	STE	d	411	20/20	0.80	0.21	54,78,96,100	0
30	LHG	e	101	42/49	0.80	0.29	59,92,114,126	0
26	BCR	X	101	40/40	0.80	0.17	34,52,70,73	0
26	BCR	h	101	40/40	0.81	0.18	42,63,87,92	0
30	LHG	A	614	49/49	0.81	0.25	51,87,115,118	0
32	STE	B	625	15/20	0.81	0.19	46,67,82,96	0
24	CLA	b	601	65/65	0.82	0.21	54,74,95,108	0
32	STE	b	621	20/20	0.82	0.22	45,62,80,86	0
32	STE	B	624	16/20	0.82	0.24	38,69,90,91	0
32	STE	B	626	12/20	0.83	0.43	57,71,88,88	0
32	STE	b	624	20/20	0.83	0.20	42,67,87,89	0
32	STE	c	520	20/20	0.83	0.24	43,68,86,100	0
28	PL9	A	611	55/55	0.83	0.27	38,69,87,92	0
29	SQD	a	616	36/54	0.83	0.19	31,69,93,98	0
33	LMG	D	411	33/55	0.83	0.19	44,61,84,94	0
33	LMG	b	622	55/55	0.83	0.29	54,76,98,109	0
32	STE	B	622	18/20	0.83	0.17	45,66,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	PL9	a	612	55/55	0.84	0.21	43,77,95,103	0
32	STE	L	102	12/20	0.84	0.20	54,70,85,93	0
24	CLA	c	512	65/65	0.84	0.17	47,65,93,98	0
32	STE	T	103	15/20	0.84	0.19	46,65,87,88	0
32	STE	a	617	10/20	0.84	0.23	37,70,76,81	0
24	CLA	C	512	65/65	0.85	0.19	41,62,97,102	0
32	STE	B	619	17/20	0.85	0.17	35,53,73,77	0
32	STE	B	621	12/20	0.85	0.12	38,62,74,78	0
32	STE	I	101	15/20	0.85	0.17	45,62,89,90	0
24	CLA	c	513	65/65	0.85	0.21	47,75,105,109	0
26	BCR	K	102	40/40	0.85	0.15	44,62,77,85	0
33	LMG	c	522	49/55	0.85	0.17	36,61,90,107	0
32	STE	d	410	20/20	0.86	0.24	50,65,79,81	0
24	CLA	C	513	65/65	0.86	0.21	50,69,101,107	0
31	DGD	A	616	66/66	0.86	0.17	46,68,85,98	0
24	CLA	H	101	65/65	0.86	0.16	44,68,98,103	0
32	STE	C	521	12/20	0.86	0.14	36,54,66,68	0
32	STE	X	102	20/20	0.86	0.18	38,57,80,83	0
32	STE	Z	101	8/20	0.86	0.18	50,64,77,77	0
29	SQD	f	102	41/54	0.87	0.23	64,94,114,118	0
33	LMG	Y	101	48/55	0.87	0.19	47,75,101,104	0
32	STE	M	104	18/20	0.87	0.16	39,52,86,91	0
32	STE	c	523	12/20	0.87	0.19	58,75,87,90	0
33	LMG	C	515	48/55	0.87	0.16	31,61,83,93	0
29	SQD	B	620	54/54	0.88	0.15	41,62,87,95	0
33	LMG	a	619	55/55	0.88	0.16	39,61,83,85	0
32	STE	C	519	12/20	0.88	0.14	43,63,75,76	0
32	STE	M	103	10/20	0.88	0.17	44,55,60,69	0
29	SQD	A	615	39/54	0.88	0.18	45,65,95,96	0
26	BCR	D	405	40/40	0.89	0.14	35,51,89,97	0
33	LMG	D	412	28/55	0.89	0.14	39,56,67,75	0
29	SQD	b	620	49/54	0.89	0.14	40,62,90,107	0
32	STE	C	520	16/20	0.89	0.12	47,59,68,73	0
32	STE	b	625	10/20	0.89	0.28	47,58,68,69	0
32	STE	t	102	14/20	0.89	0.14	42,54,65,66	0
32	STE	M	102	15/20	0.89	0.15	42,58,67,69	0
26	BCR	k	102	40/40	0.90	0.19	45,61,74,77	0
24	CLA	a	607	65/65	0.90	0.14	23,41,90,102	0
26	BCR	c	514	40/40	0.90	0.18	45,65,82,84	0
24	CLA	C	502	65/65	0.90	0.16	32,47,64,67	0
26	BCR	k	101	40/40	0.90	0.13	40,67,79,81	0
33	LMG	M	101	51/55	0.91	0.13	34,53,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	j	101	12/20	0.91	0.16	49,65,78,78	0
26	BCR	d	404	40/40	0.91	0.13	40,59,99,107	0
24	CLA	c	502	65/65	0.91	0.16	33,48,67,71	0
24	CLA	D	404	65/65	0.91	0.14	24,47,107,122	0
26	BCR	K	101	40/40	0.91	0.15	45,64,76,82	0
33	LMG	m	101	51/55	0.91	0.14	37,55,75,85	0
24	CLA	d	403	65/65	0.92	0.15	31,55,98,106	0
24	CLA	c	508	64/65	0.92	0.15	36,53,99,120	0
33	LMG	D	407	51/55	0.92	0.18	31,64,87,89	0
33	LMG	c	519	37/55	0.92	0.15	48,69,83,87	0
24	CLA	b	616	60/65	0.92	0.15	33,50,93,101	0
24	CLA	b	615	65/65	0.92	0.15	30,46,69,80	0
32	STE	T	102	16/20	0.92	0.14	43,58,78,83	0
24	CLA	c	506	65/65	0.93	0.13	35,55,90,101	0
26	BCR	K	103	40/40	0.93	0.16	42,59,74,83	0
24	CLA	C	508	65/65	0.93	0.14	31,49,105,118	0
29	SQD	D	408	36/54	0.93	0.19	57,78,93,96	0
26	BCR	b	617	40/40	0.93	0.12	33,49,64,65	0
26	BCR	b	619	40/40	0.93	0.10	33,54,68,72	0
24	CLA	B	615	60/65	0.93	0.14	27,46,103,111	0
24	CLA	B	614	65/65	0.93	0.14	28,43,63,67	0
24	CLA	C	505	65/65	0.93	0.16	25,48,71,77	0
26	BCR	C	514	40/40	0.93	0.11	27,47,60,72	0
31	DGD	C	517	62/66	0.93	0.13	38,58,106,117	0
31	DGD	c	518	62/66	0.93	0.14	32,59,84,90	0
32	STE	d	409	17/20	0.93	0.12	43,58,66,77	0
24	CLA	C	507	65/65	0.93	0.15	31,47,67,70	0
33	LMG	d	408	44/55	0.93	0.15	37,61,93,102	0
24	CLA	c	503	65/65	0.93	0.15	36,50,65,65	0
24	CLA	b	602	65/65	0.94	0.15	29,48,67,71	0
24	CLA	b	604	65/65	0.94	0.15	26,41,79,98	0
24	CLA	b	606	65/65	0.94	0.12	29,46,76,85	0
24	CLA	b	609	65/65	0.94	0.14	34,51,74,79	0
24	CLA	b	614	65/65	0.94	0.12	29,44,78,91	0
31	DGD	C	518	62/66	0.94	0.12	28,53,75,87	0
31	DGD	H	102	62/66	0.94	0.11	32,49,62,71	0
31	DGD	c	517	62/66	0.94	0.12	36,56,97,103	0
26	BCR	T	101	40/40	0.94	0.10	26,47,62,63	0
31	DGD	h	102	62/66	0.94	0.12	35,53,66,79	0
24	CLA	C	510	65/65	0.94	0.15	33,51,68,70	0
24	CLA	C	511	65/65	0.94	0.12	38,55,72,78	0
24	CLA	B	605	65/65	0.94	0.11	22,41,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	503	65/65	0.94	0.15	36,49,61,63	0
24	CLA	c	505	65/65	0.94	0.18	30,48,69,76	0
24	CLA	B	608	65/65	0.94	0.13	27,45,63,72	0
24	CLA	c	507	65/65	0.94	0.14	32,49,62,74	0
24	CLA	C	506	65/65	0.94	0.12	28,47,91,95	0
24	CLA	c	509	65/65	0.94	0.19	34,55,70,75	0
28	PL9	D	406	55/55	0.94	0.12	25,39,50,65	0
24	CLA	c	511	65/65	0.94	0.12	41,60,78,81	0
32	STE	J	101	12/20	0.94	0.13	50,62,78,78	0
29	SQD	A	613	52/54	0.94	0.16	36,63,92,97	0
24	CLA	a	605	65/65	0.94	0.14	30,45,99,110	0
24	CLA	B	601	65/65	0.94	0.16	27,41,63,71	0
24	CLA	B	603	65/65	0.94	0.14	23,38,77,86	0
29	SQD	a	615	54/54	0.94	0.15	45,70,92,96	0
26	BCR	B	616	40/40	0.94	0.13	31,44,61,67	0
26	BCR	B	618	40/40	0.94	0.11	29,46,61,71	0
26	BCR	c	515	40/40	0.95	0.12	32,50,72,73	0
24	CLA	b	612	65/65	0.95	0.17	23,39,55,56	0
31	DGD	c	516	62/66	0.95	0.12	28,45,75,84	0
24	CLA	b	613	65/65	0.95	0.15	23,41,81,88	0
24	CLA	C	509	65/65	0.95	0.18	30,50,66,77	0
26	BCR	A	608	40/40	0.95	0.09	29,40,48,49	0
26	BCR	t	101	40/40	0.95	0.10	29,44,55,58	0
24	CLA	B	613	65/65	0.95	0.16	25,42,82,92	0
26	BCR	B	617	40/40	0.95	0.10	29,44,58,59	0
24	CLA	C	504	59/65	0.95	0.12	34,47,85,97	0
28	PL9	d	405	55/55	0.95	0.12	27,41,52,54	0
24	CLA	A	607	54/65	0.95	0.11	20,36,69,78	0
24	CLA	A	605	65/65	0.95	0.14	24,39,100,106	0
24	CLA	c	504	60/65	0.95	0.11	36,52,83,88	0
24	CLA	b	605	65/65	0.95	0.15	28,42,56,59	0
24	CLA	C	501	65/65	0.95	0.12	29,41,55,61	0
24	CLA	b	608	65/65	0.95	0.15	30,48,71,80	0
24	CLA	B	602	65/65	0.95	0.17	22,38,61,72	0
26	BCR	a	608	40/40	0.95	0.09	26,39,47,55	0
24	CLA	b	610	65/65	0.95	0.17	27,43,54,62	0
30	LHG	D	410	47/49	0.95	0.14	33,53,93,98	0
30	LHG	a	614	49/49	0.95	0.12	33,54,72,75	0
26	BCR	b	618	40/40	0.95	0.11	28,46,61,65	0
30	LHG	l	101	49/49	0.95	0.12	34,51,61,71	0
24	CLA	c	510	65/65	0.95	0.15	38,54,70,72	0
31	DGD	C	516	62/66	0.95	0.13	27,43,82,94	0

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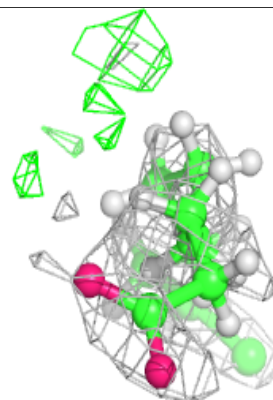
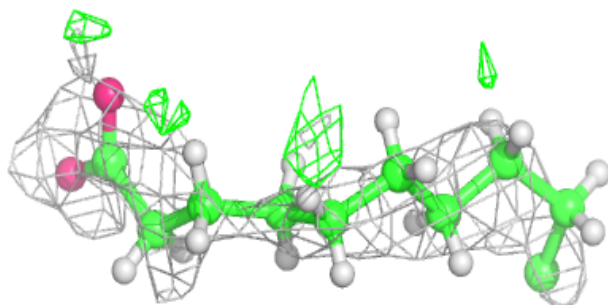
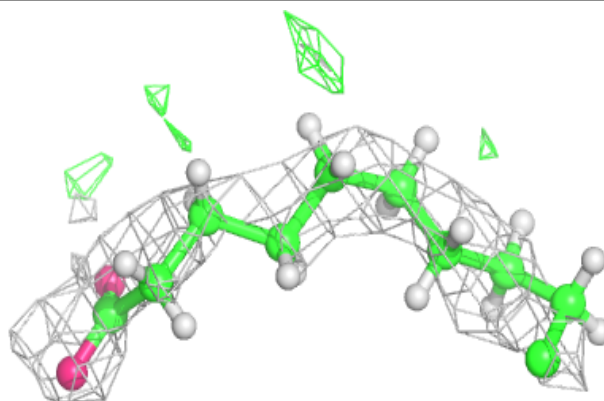
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	611	65/65	0.95	0.14	25,38,62,75	0
30	LHG	D	413	49/49	0.96	0.12	34,47,70,76	0
30	LHG	L	101	49/49	0.96	0.13	32,46,60,67	0
24	CLA	D	403	65/65	0.96	0.12	19,33,57,66	0
30	LHG	d	407	39/49	0.96	0.11	38,54,74,77	0
24	CLA	B	607	65/65	0.96	0.12	24,40,63,68	0
24	CLA	b	607	65/65	0.96	0.11	22,43,71,75	0
24	CLA	B	604	65/65	0.96	0.15	25,38,51,54	0
24	CLA	a	604	65/65	0.96	0.11	24,35,49,57	0
24	CLA	B	609	65/65	0.96	0.14	22,36,48,51	0
24	CLA	B	611	65/65	0.96	0.14	23,37,51,60	0
24	CLA	a	613	65/65	0.96	0.13	23,37,48,53	0
24	CLA	B	612	65/65	0.96	0.14	22,39,78,86	0
24	CLA	A	612	65/65	0.96	0.11	22,34,54,58	0
24	CLA	b	603	65/65	0.96	0.15	26,42,74,82	0
24	CLA	B	606	65/65	0.96	0.11	22,37,71,79	0
24	CLA	d	402	65/65	0.96	0.12	25,40,67,76	0
24	CLA	c	501	65/65	0.96	0.13	31,45,60,63	0
25	PHO	A	606	64/64	0.96	0.14	25,37,46,48	0
25	PHO	D	401	64/64	0.96	0.10	21,34,45,47	0
25	PHO	a	606	64/64	0.96	0.13	23,35,43,45	0
25	PHO	d	401	64/64	0.96	0.10	27,43,53,64	0
35	HEM	f	101	43/43	0.96	0.14	49,67,93,97	0
30	LHG	D	409	49/49	0.97	0.10	29,42,55,71	0
24	CLA	B	610	65/65	0.97	0.15	21,35,51,55	0
30	LHG	d	406	49/49	0.97	0.10	28,45,61,66	0
34	BCT	a	611	4/4	0.97	0.23	35,36,48,53	0
35	HEM	F	101	43/43	0.97	0.11	42,58,73,76	0
24	CLA	A	604	65/65	0.97	0.10	19,33,50,61	0
36	HEC	V	201	43/43	0.97	0.12	28,38,45,53	0
36	HEC	v	201	43/43	0.97	0.13	32,41,54,58	0
27	CL	A	609	1/1	0.99	0.12	34,34,34,34	0
27	CL	A	610	1/1	0.99	0.03	37,37,37,37	0
27	CL	a	609	1/1	0.99	0.04	32,32,32,32	0
34	BCT	D	402	4/4	0.99	0.14	34,36,43,47	0
27	CL	a	610	1/1	0.99	0.03	35,35,35,35	0
21	OEY	A	601[B]	11/11	0.99	0.14	21,25,29,31	11
21	OEY	a	601[B]	11/11	0.99	0.12	21,26,32,32	11
22	OEX	A	602[A]	10/10	0.99	0.14	33,36,40,40	10
22	OEX	a	602[A]	10/10	0.99	0.12	31,36,39,40	10
23	FE2	a	603	1/1	1.00	0.05	32,32,32,32	0
23	FE2	A	603	1/1	1.00	0.08	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.

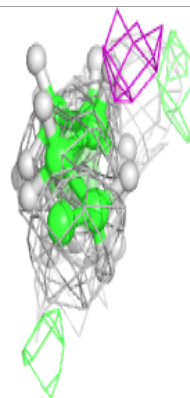
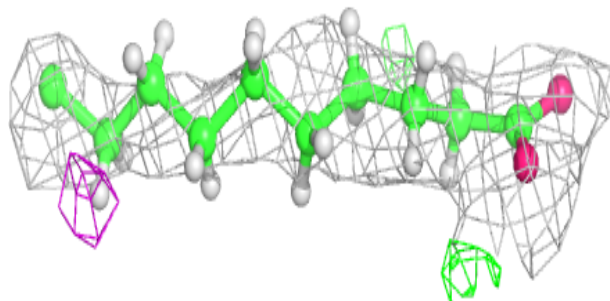
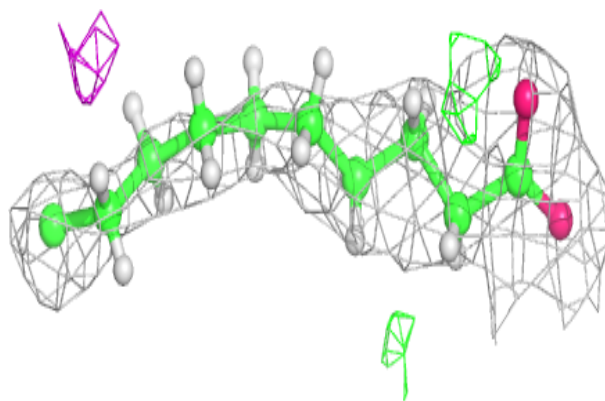
Electron density around STE R 101:

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

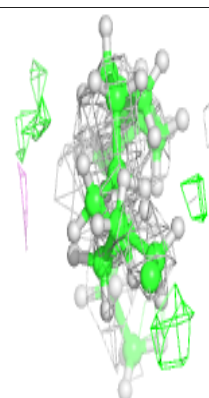
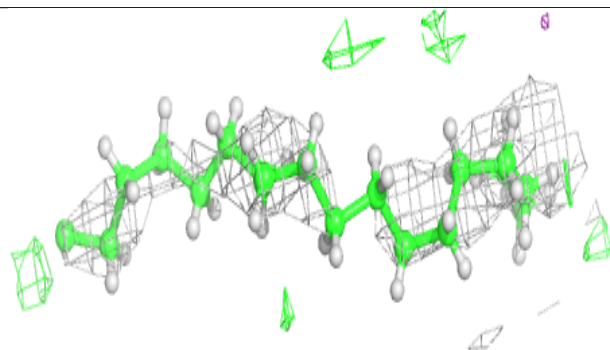
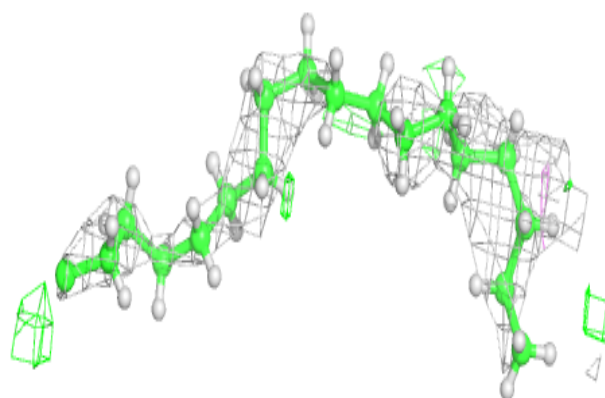


Electron density around STE a 618:

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

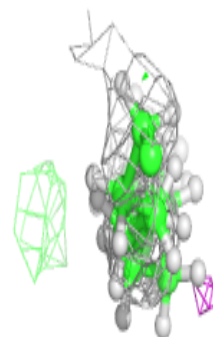
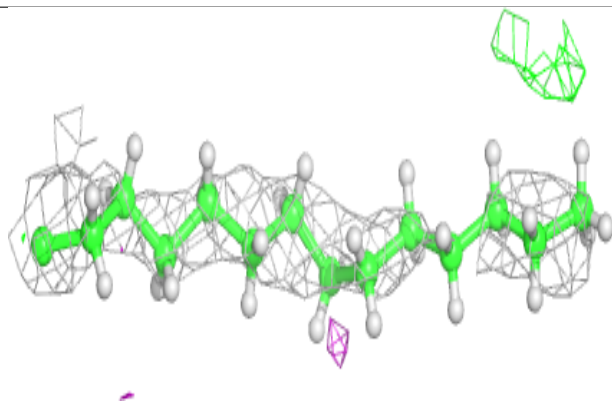
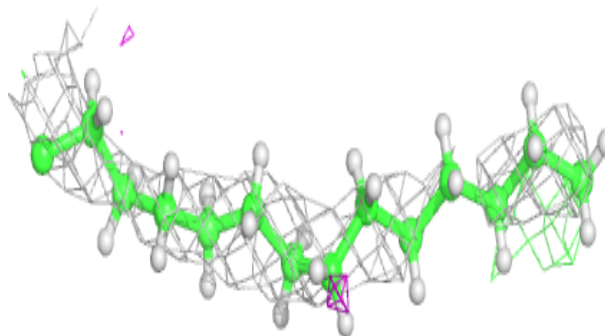
**Electron density around STE B 623:**

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

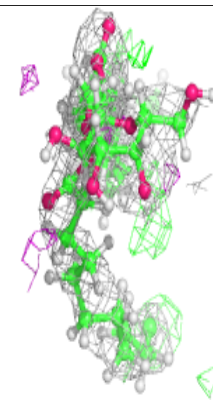
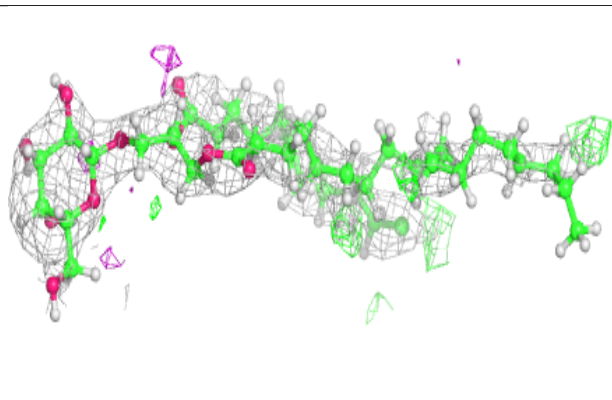
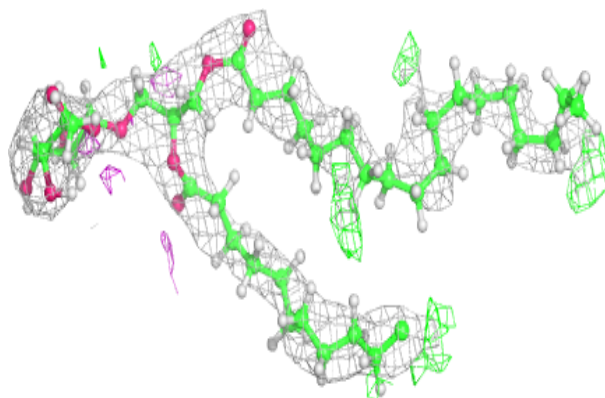


Electron density around STE h 103:

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

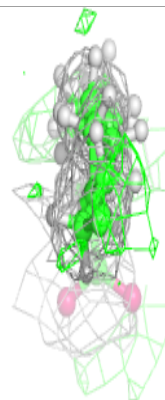
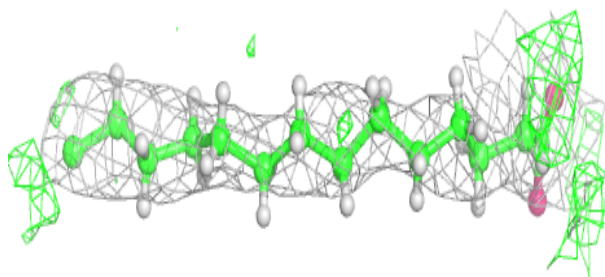
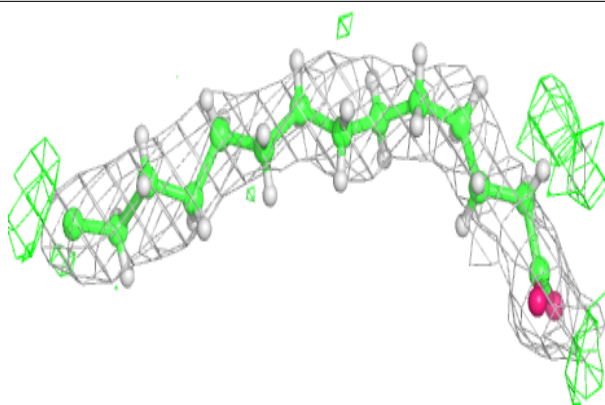
**Electron density around LMG c 521:**

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

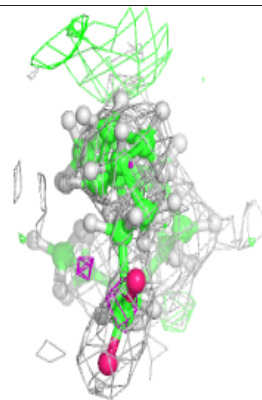
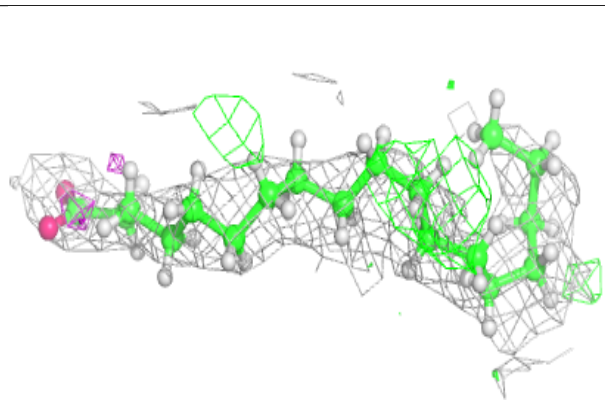
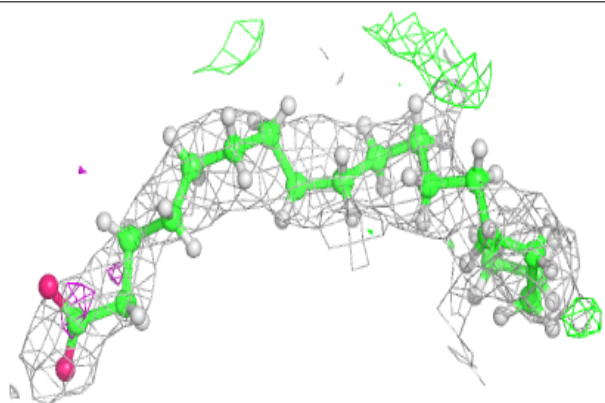


Electron density around STE b 623:

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

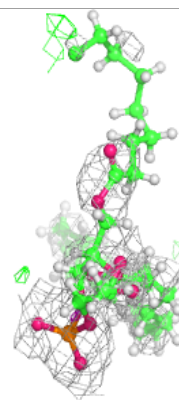
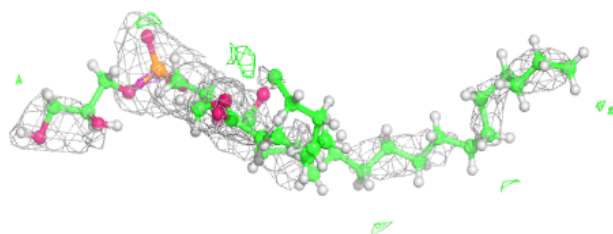
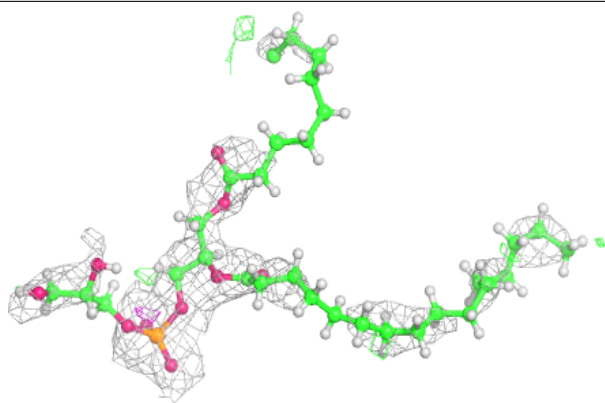
**Electron density around STE d 411:**

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

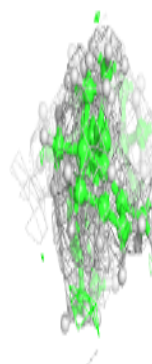
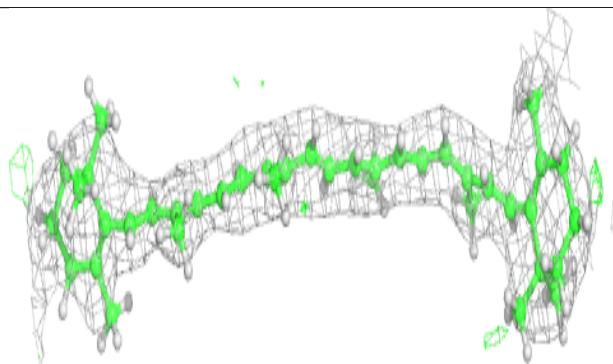
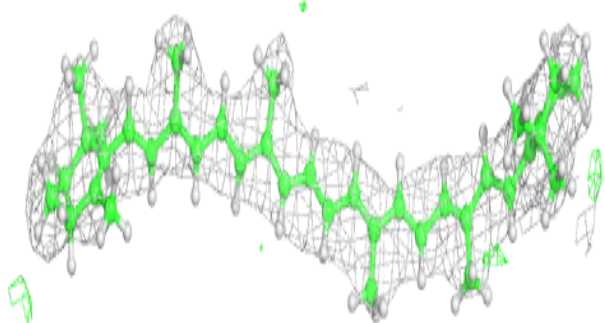


Electron density around LHG e 101:

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

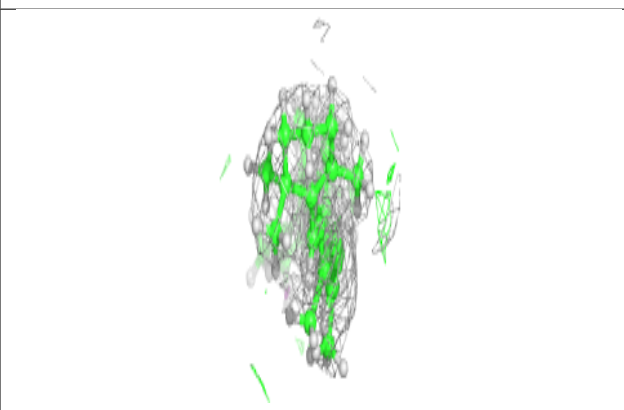
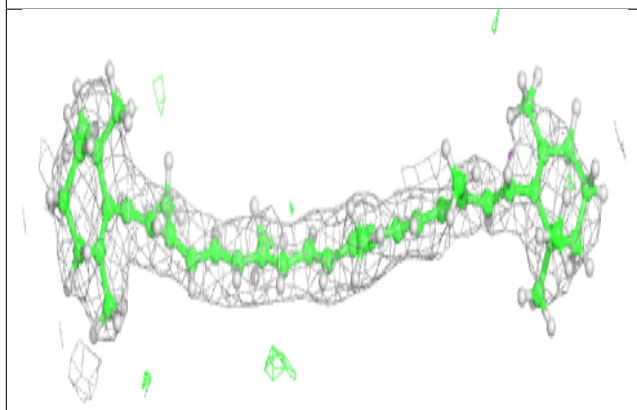
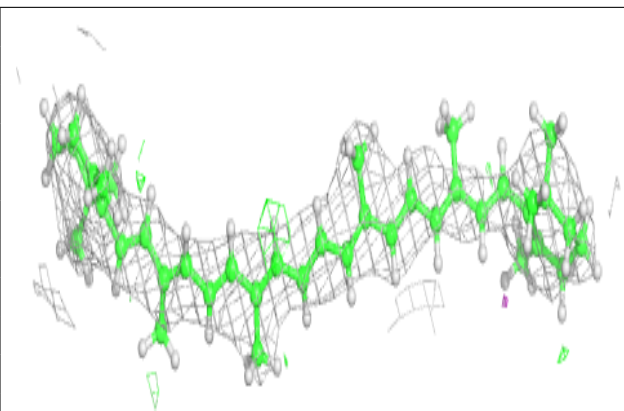
**Electron density around BCR X 101:**

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



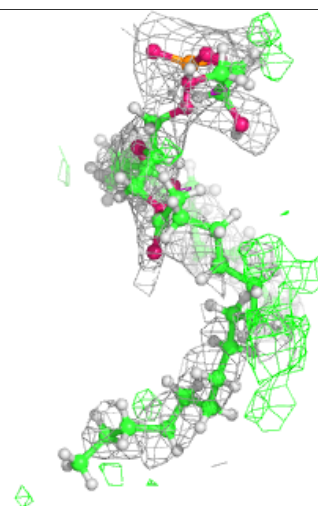
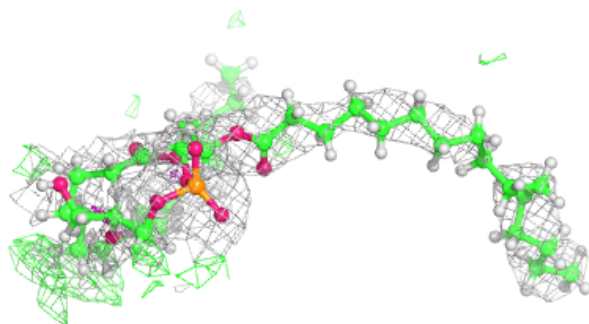
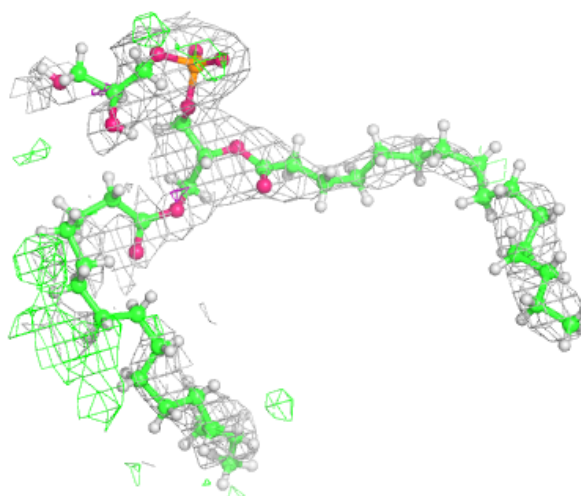
Electron density around BCR h 101:

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



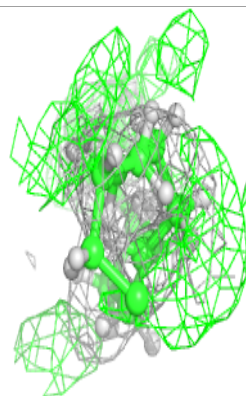
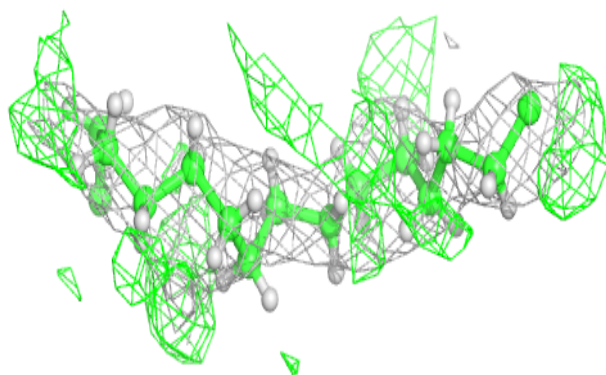
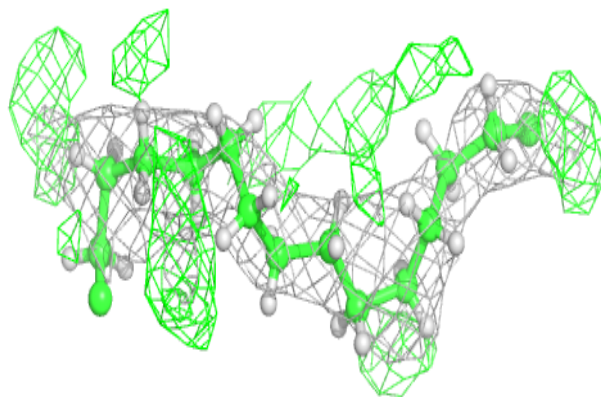
Electron density around LHG A 614:

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

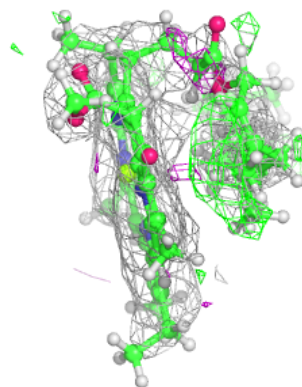
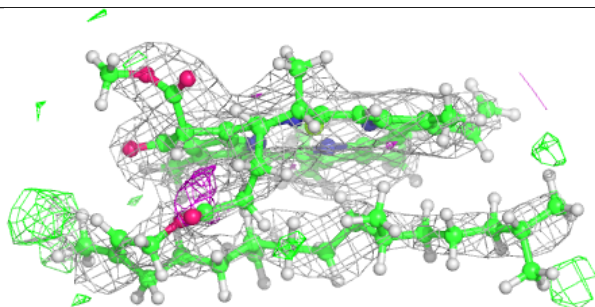
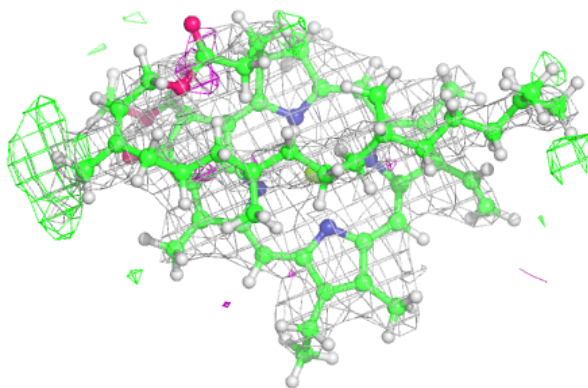


Electron density around STE B 625:

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

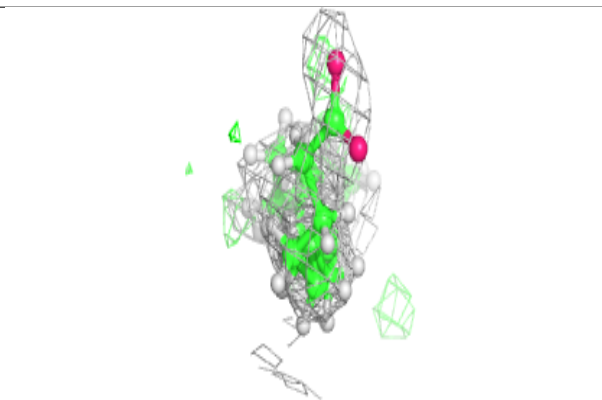
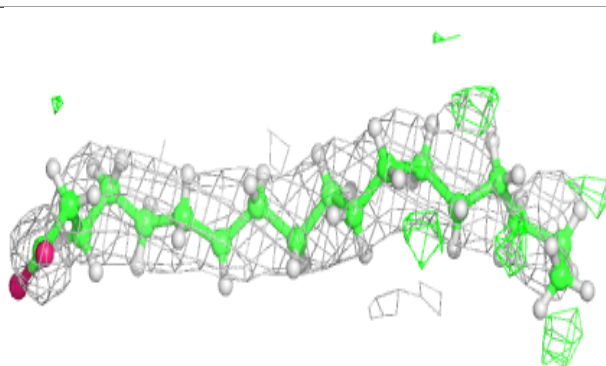
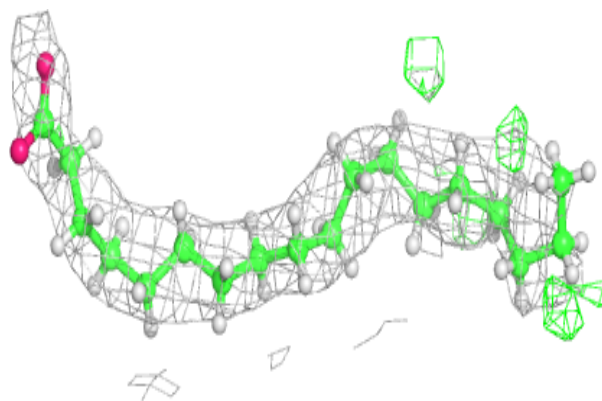
**Electron density around CLA b 601:**

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

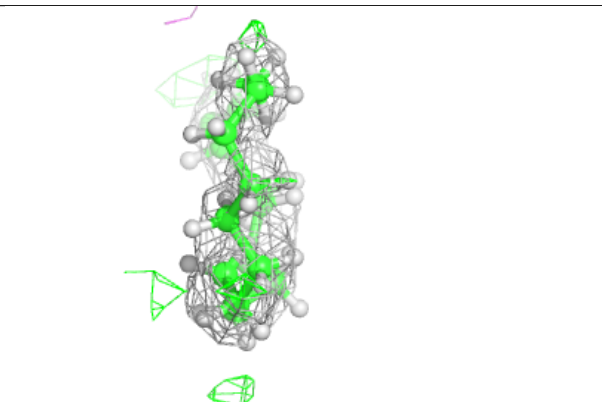
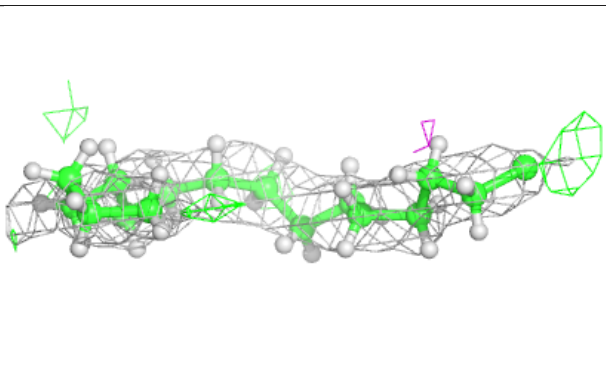
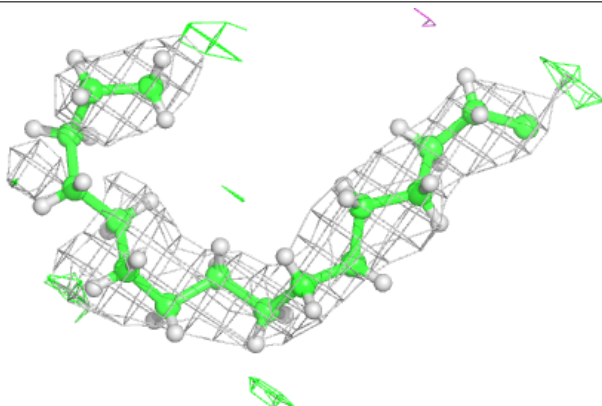


Electron density around STE b 621:

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

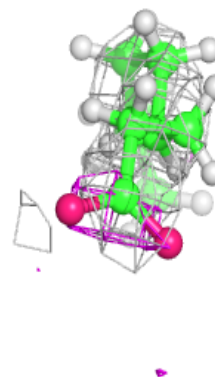
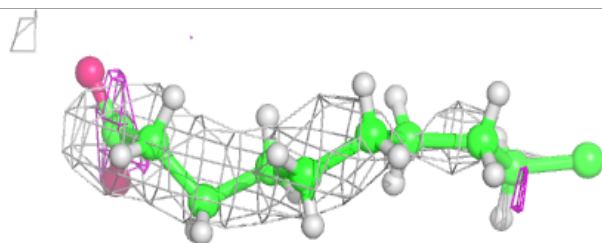
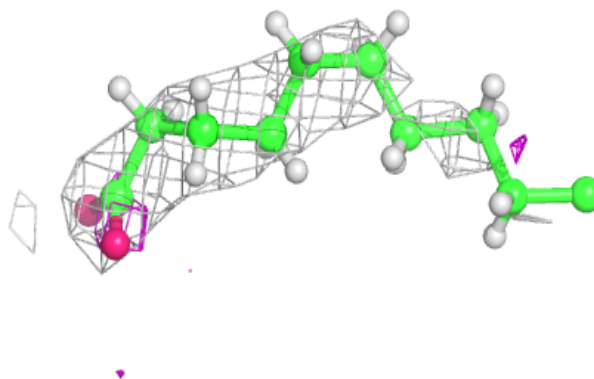
**Electron density around STE B 624:**

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

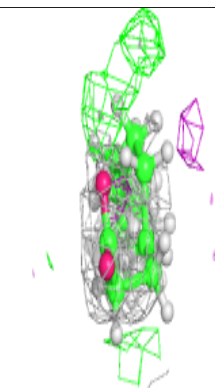
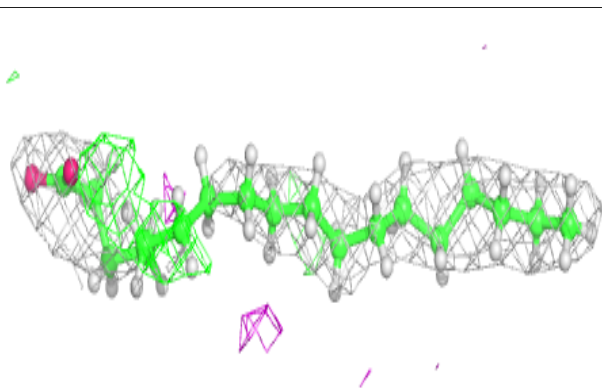
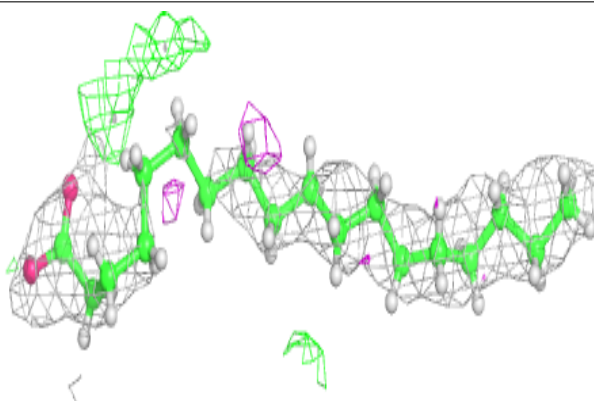


Electron density around STE B 626:

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

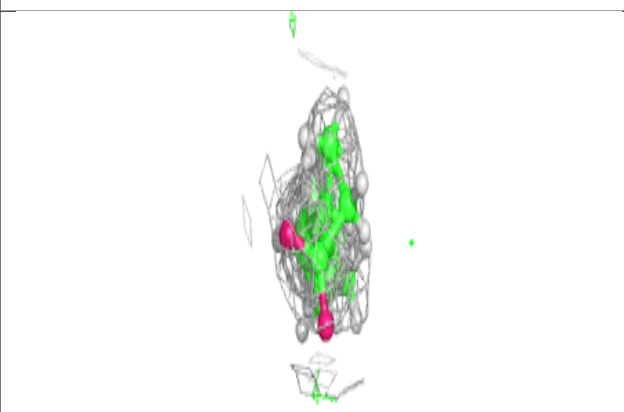
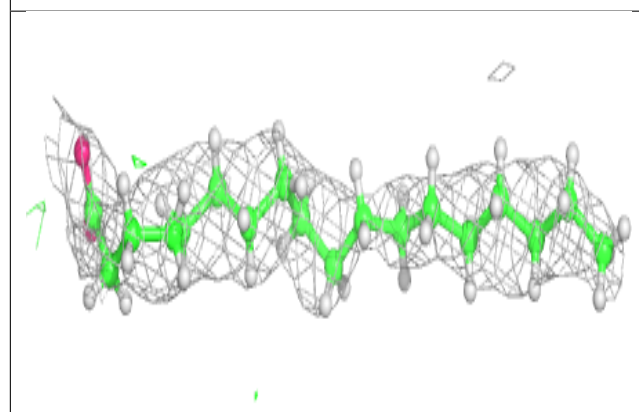
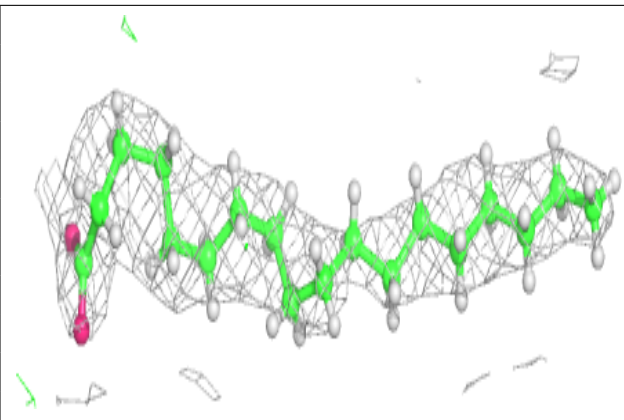
**Electron density around STE b 624:**

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

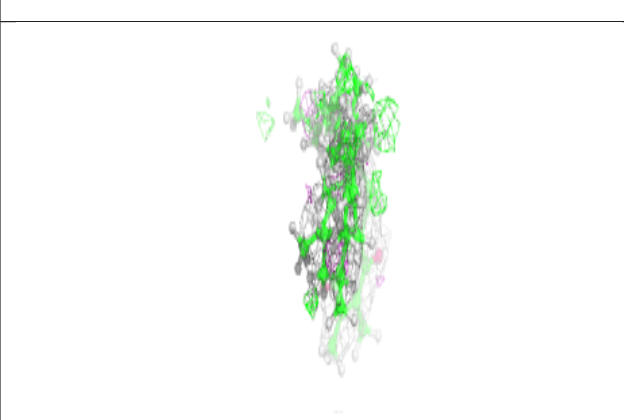
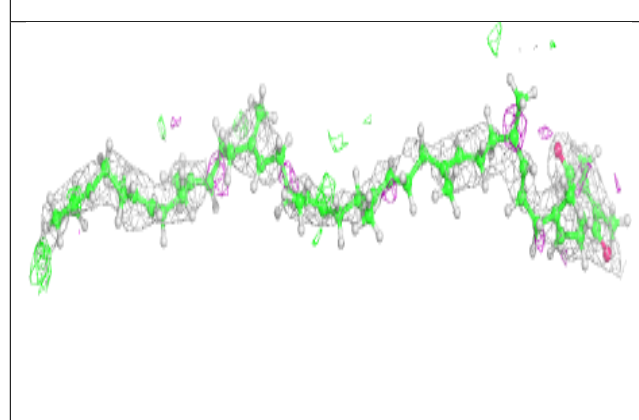
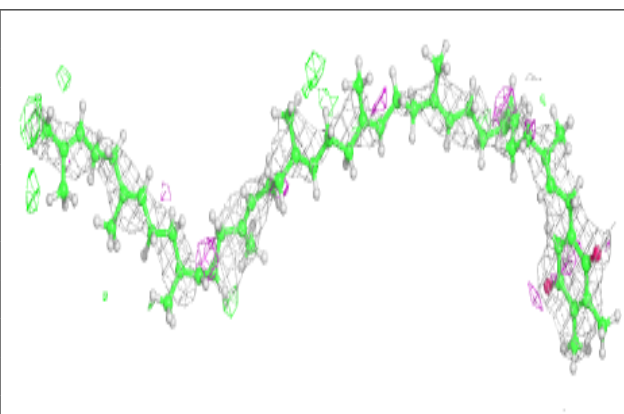


Electron density around STE c 520:

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

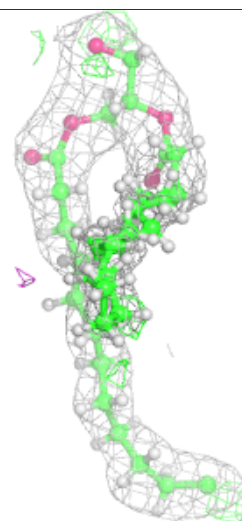
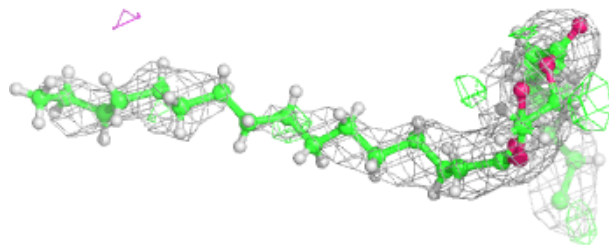
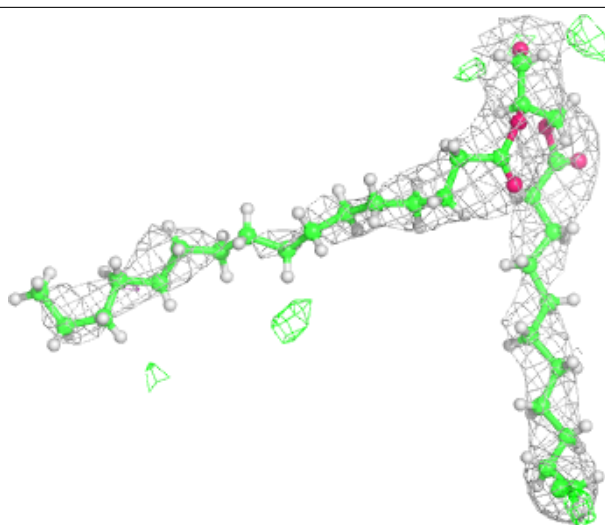
**Electron density around PL9 A 611:**

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



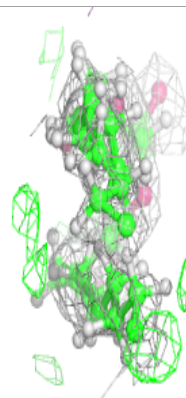
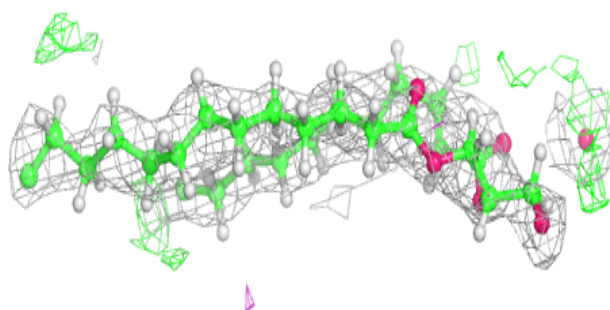
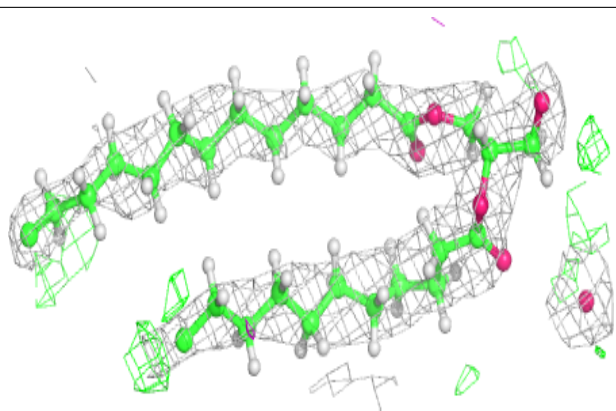
Electron density around SQD a 616:

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

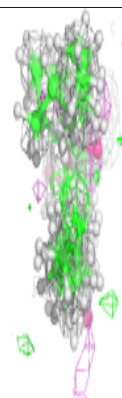
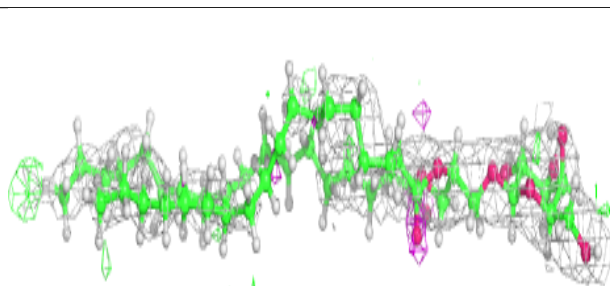
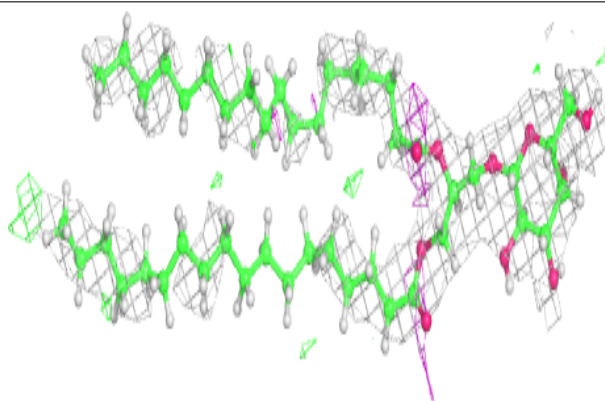


Electron density around LMG D 411:

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

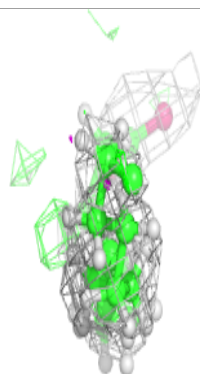
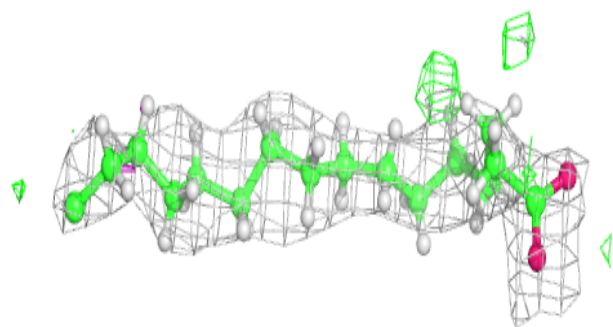
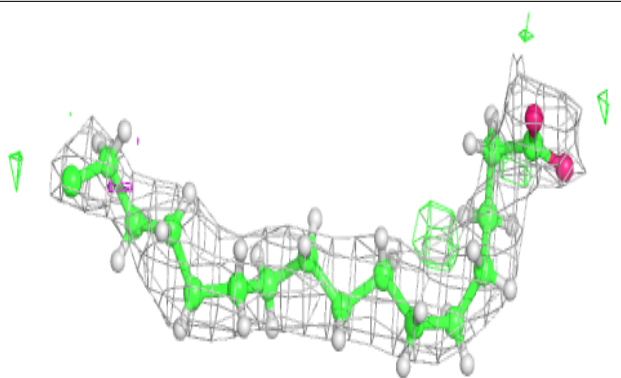
**Electron density around LMG b 622:**

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

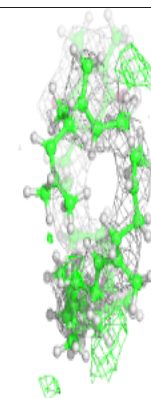
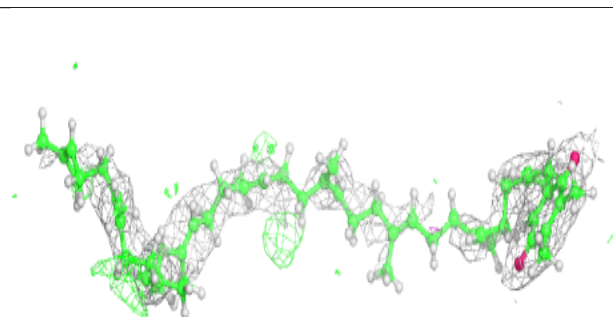
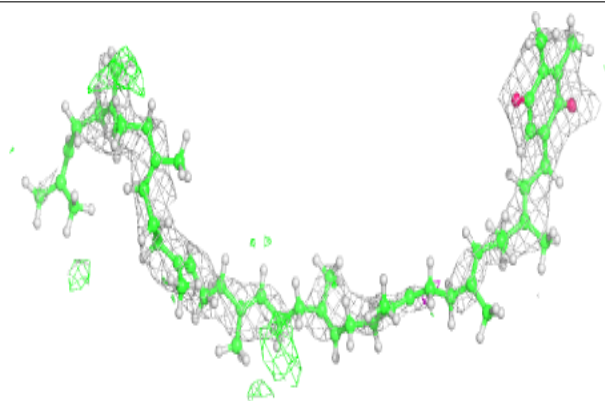


Electron density around STE B 622:

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

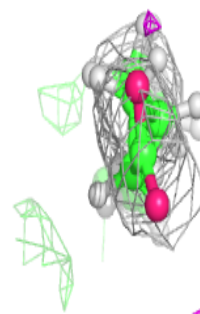
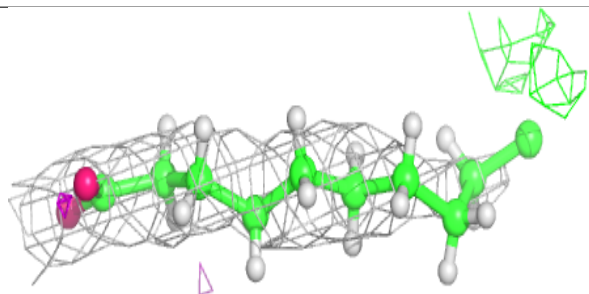
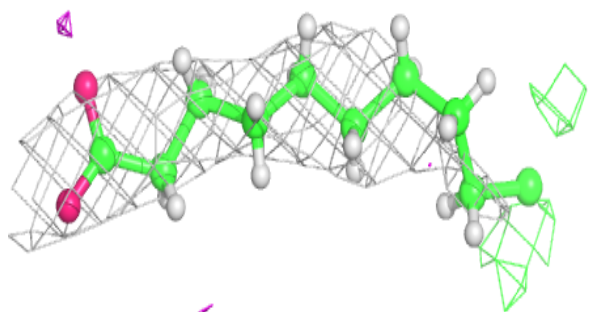
**Electron density around PL9 a 612:**

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



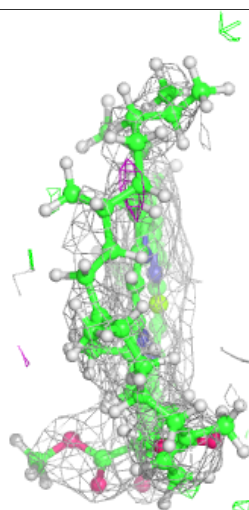
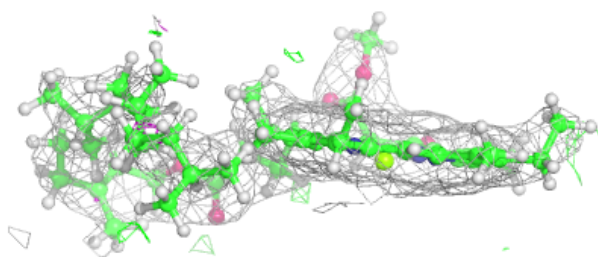
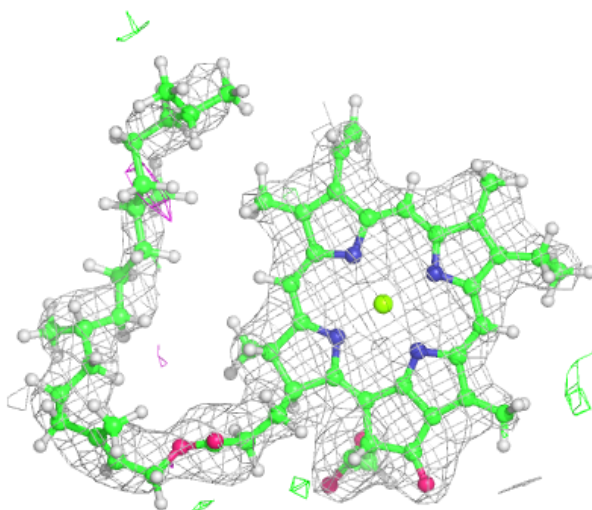
Electron density around STE L 102:

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



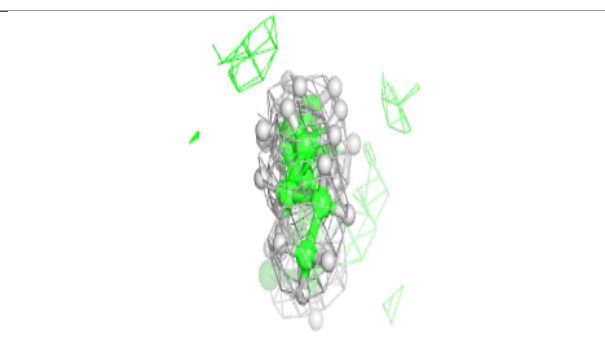
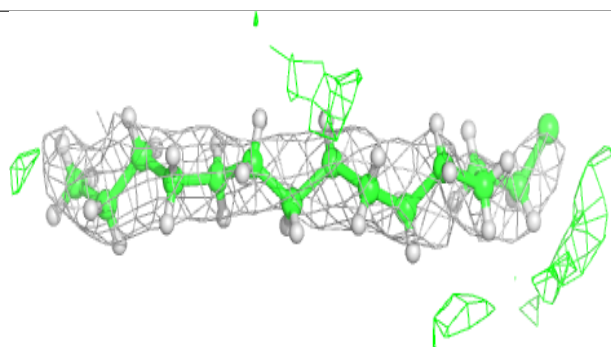
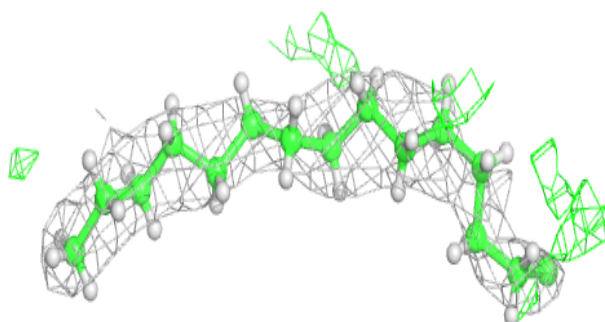
Electron density around CLA c 512:

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

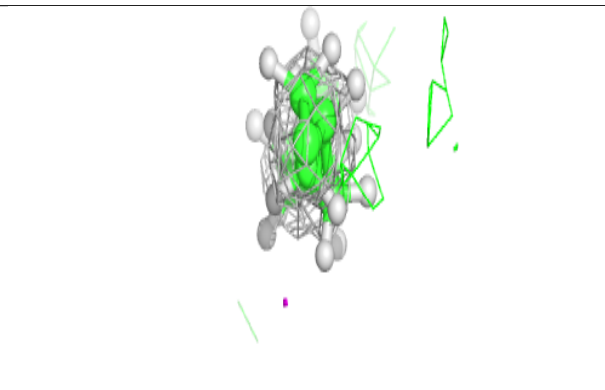
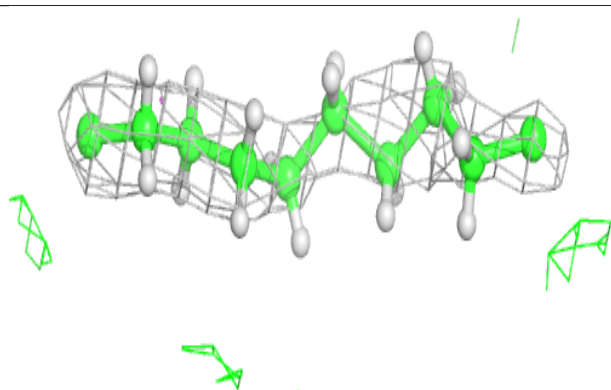
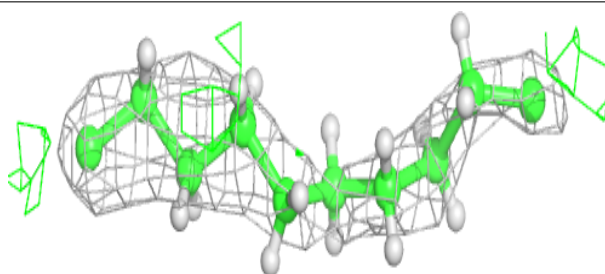


Electron density around STE T 103:

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

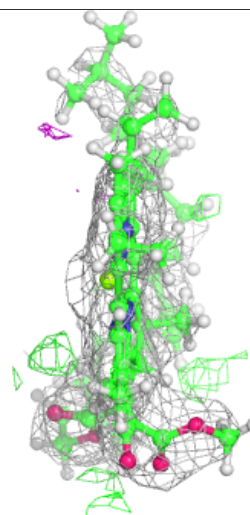
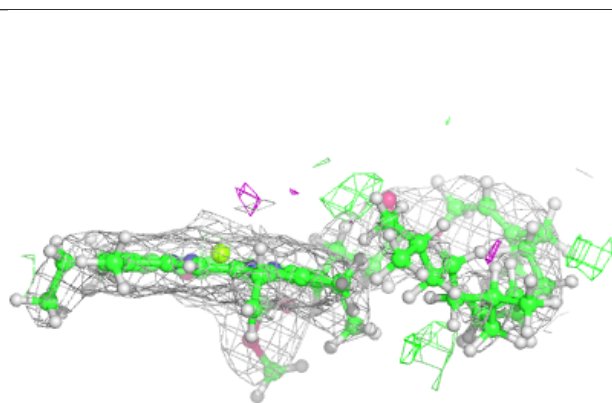
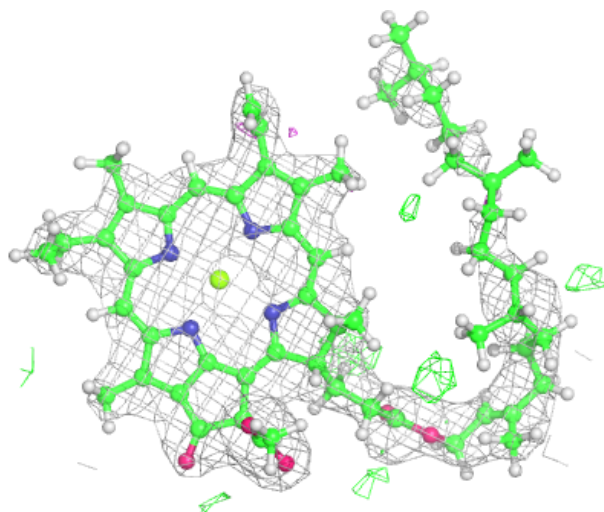
**Electron density around STE a 617:**

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



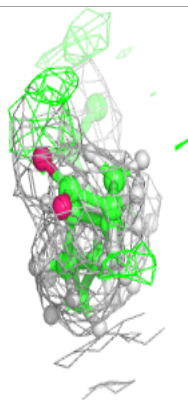
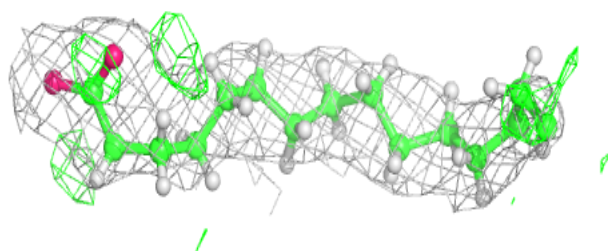
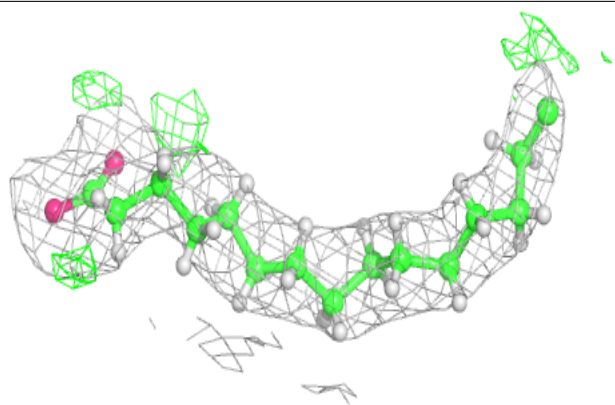
Electron density around CLA C 512:

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

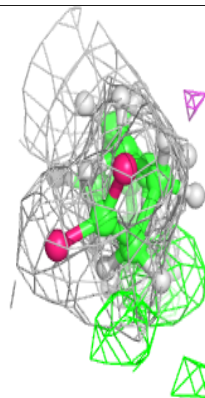
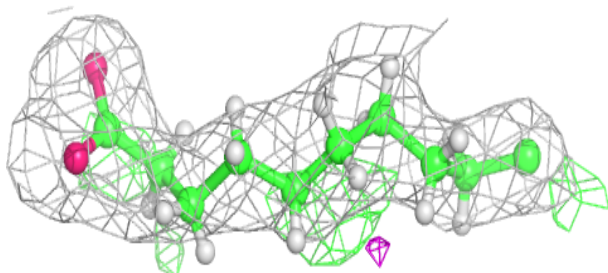
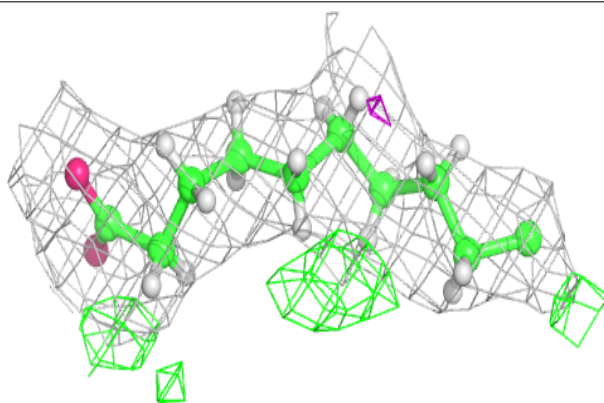


Electron density around STE B 619:

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

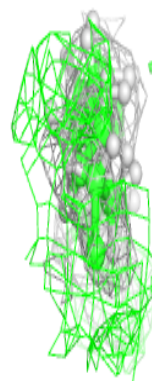
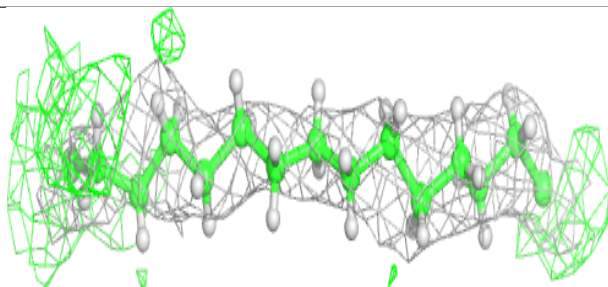
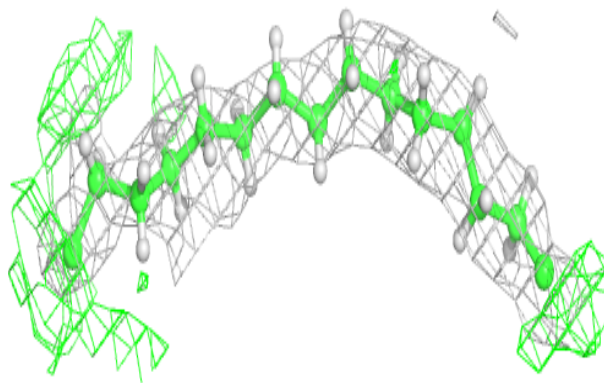
**Electron density around STE B 621:**

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

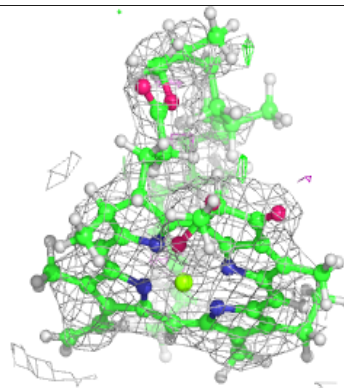
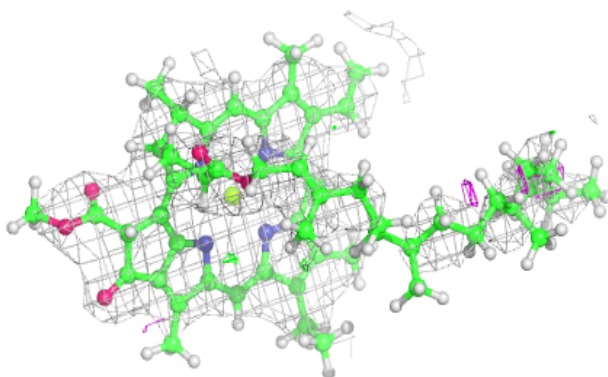
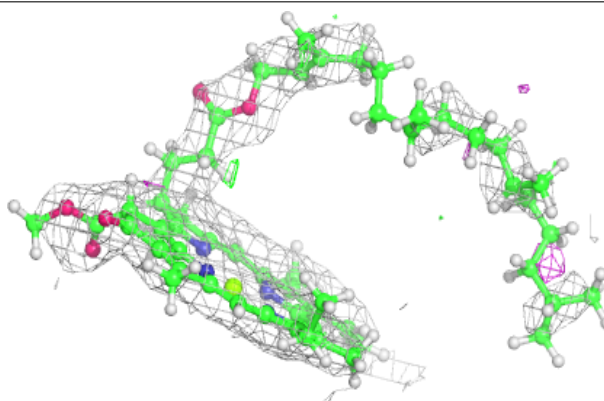


Electron density around STE I 101:

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

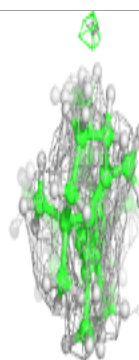
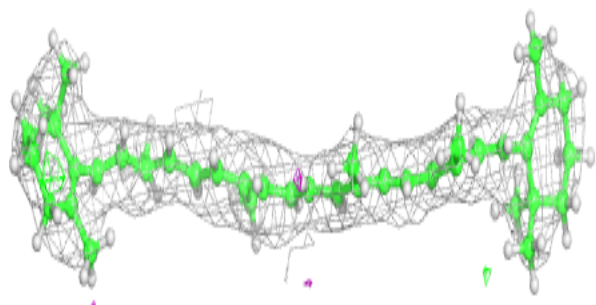
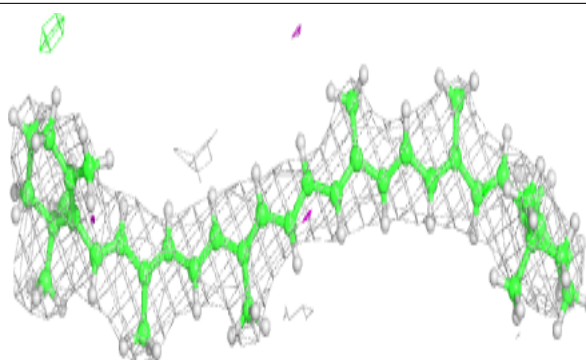
**Electron density around CLA c 513:**

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

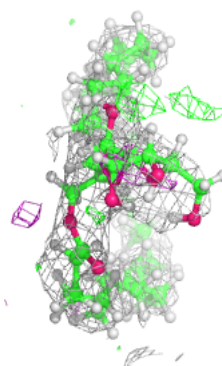
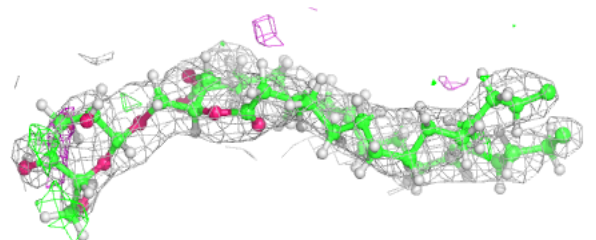
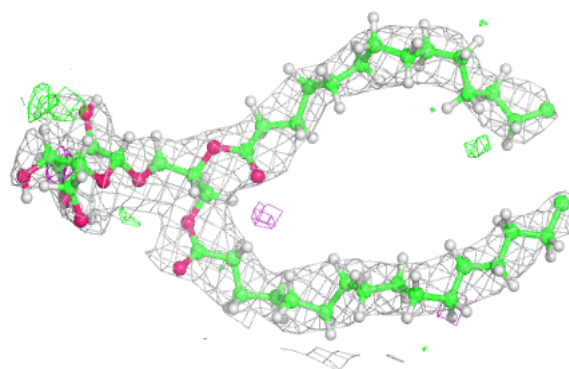


Electron density around BCR K 102:

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

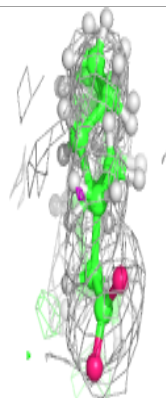
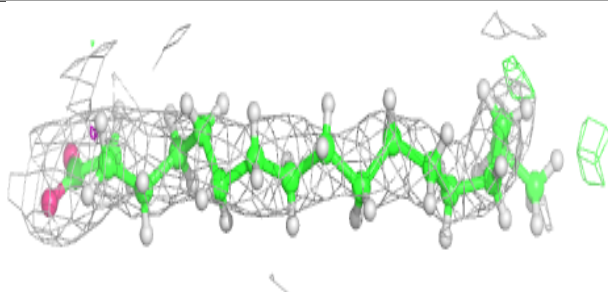
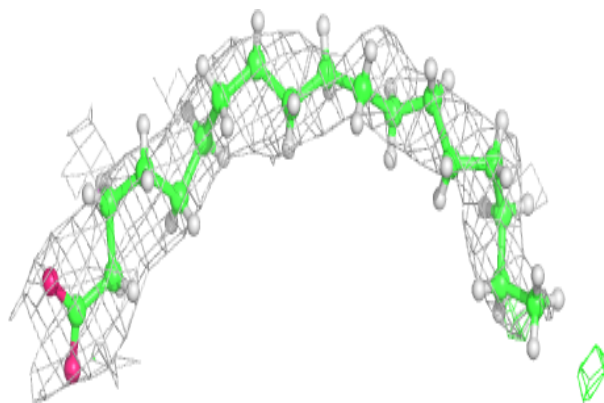
**Electron density around LMG c 522:**

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

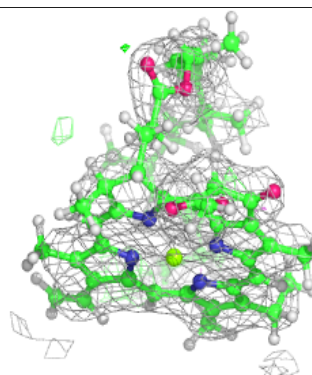
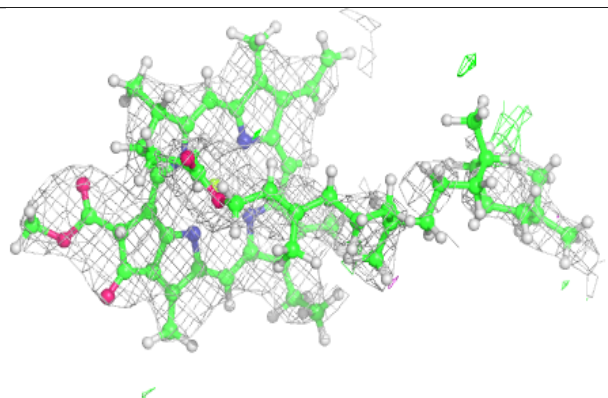
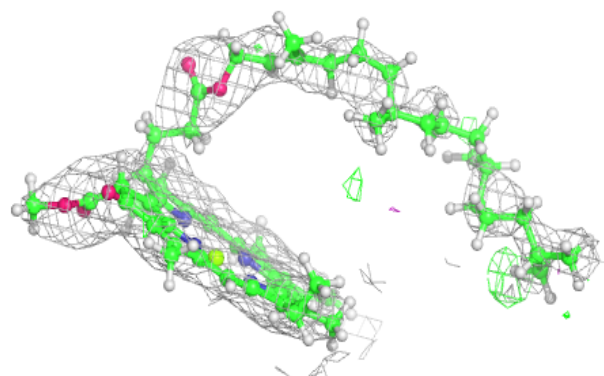


Electron density around STE d 410:

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

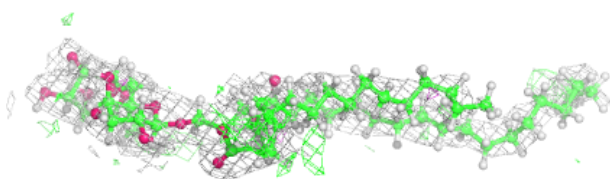
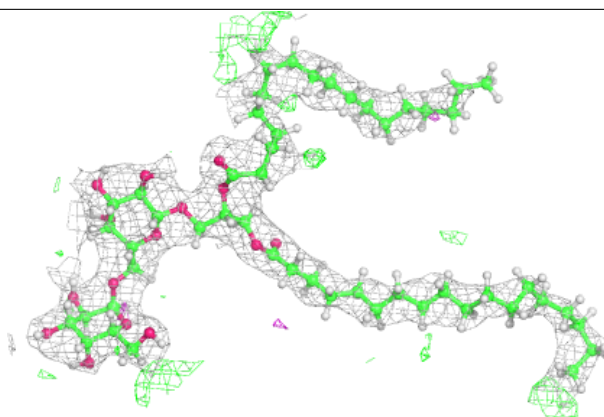
**Electron density around CLA C 513:**

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

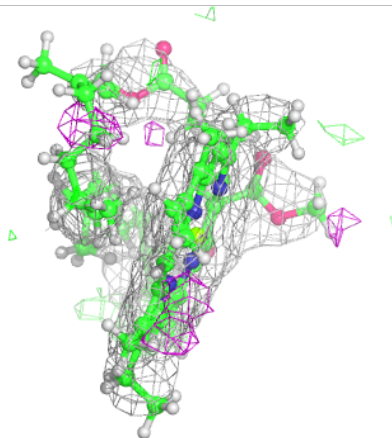
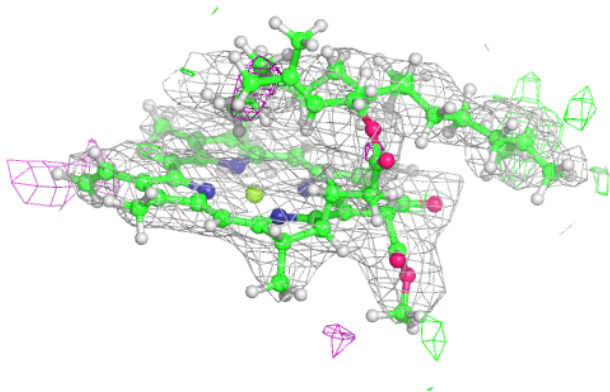
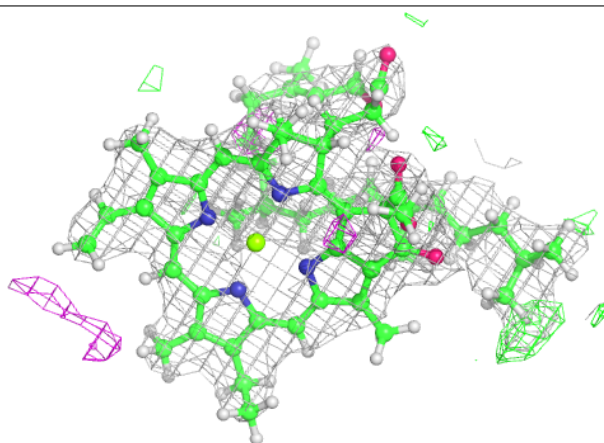


Electron density around DGD A 616:

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

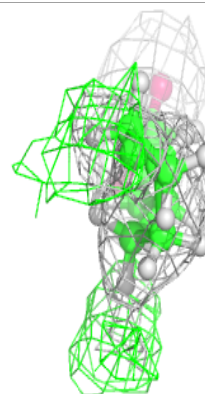
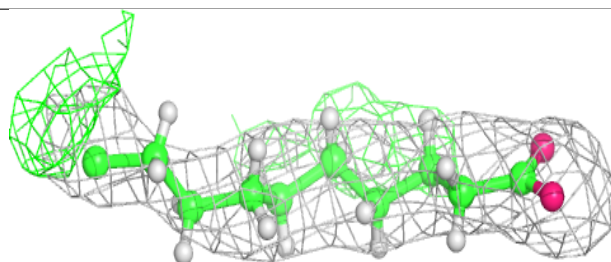
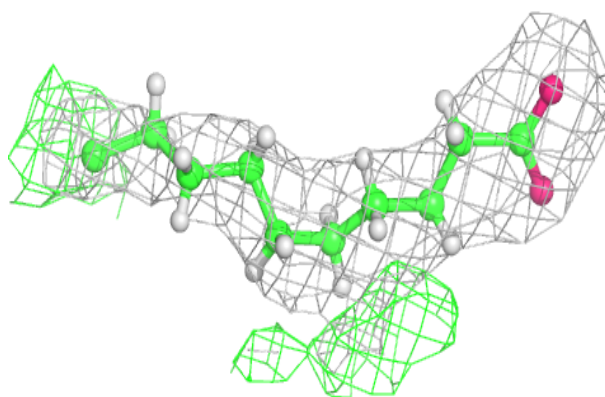
**Electron density around CLA H 101:**

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

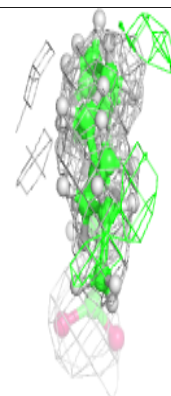
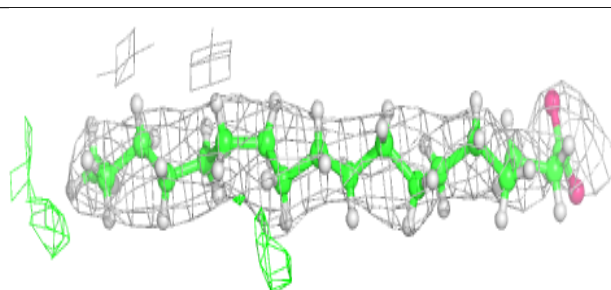
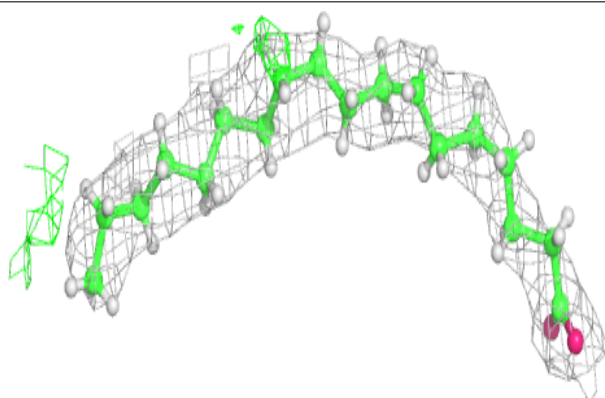


Electron density around STE C 521:

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

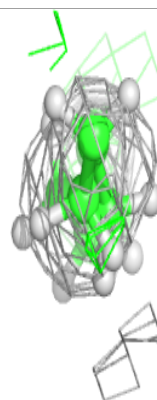
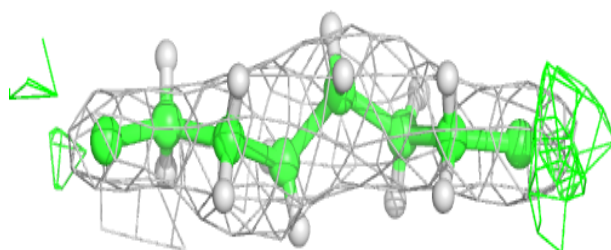
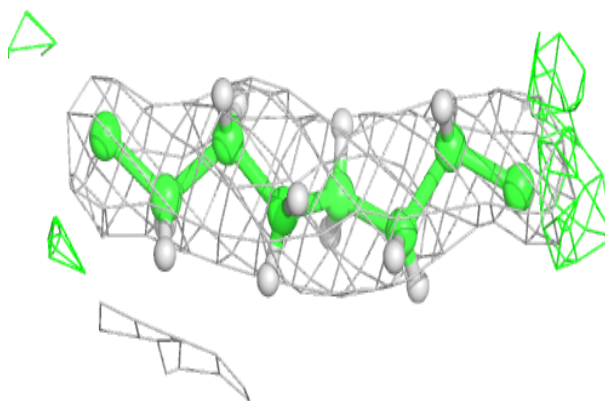
**Electron density around STE X 102:**

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

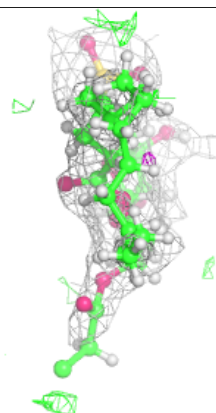
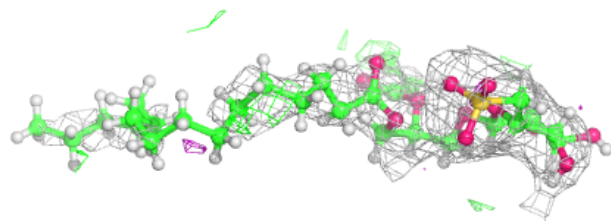
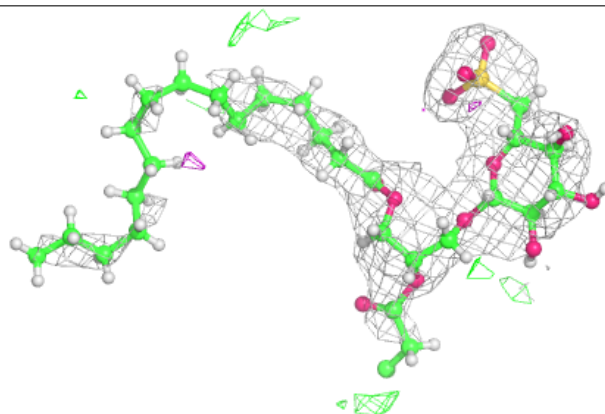


Electron density around STE Z 101:

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

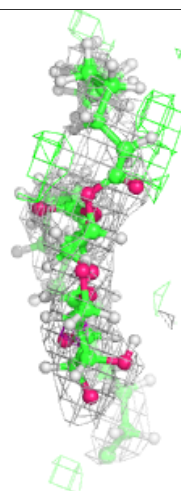
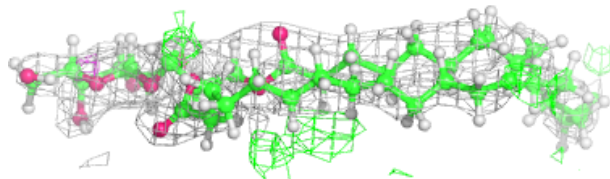
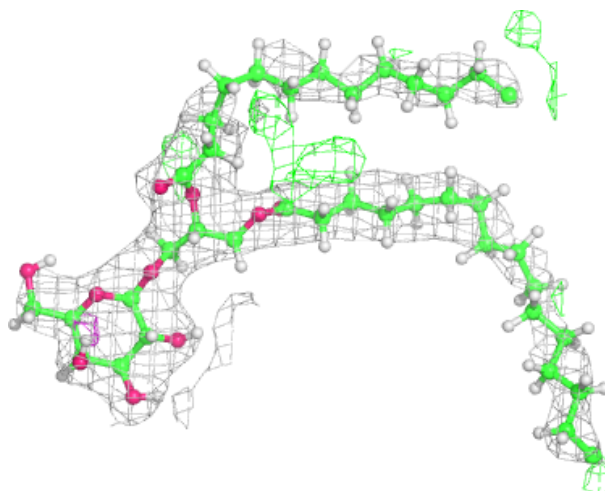
**Electron density around SQD f 102:**

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



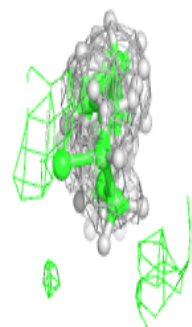
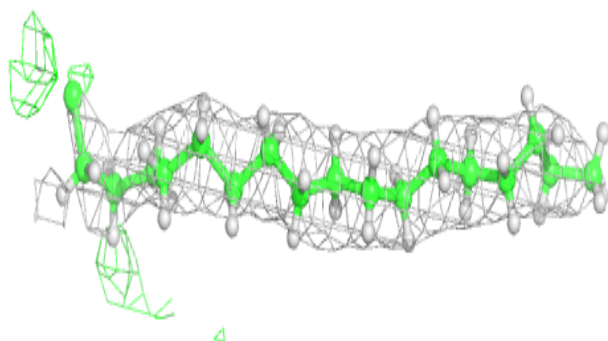
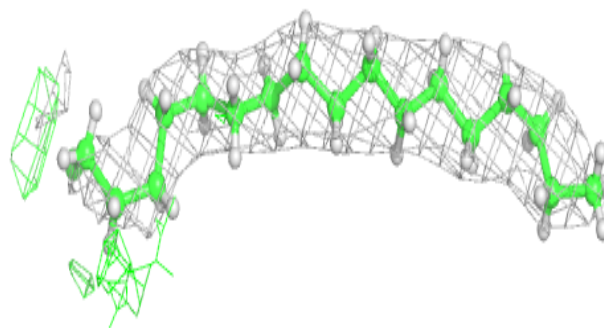
Electron density around LMG Y 101:

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

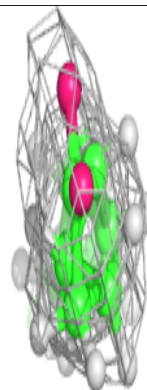
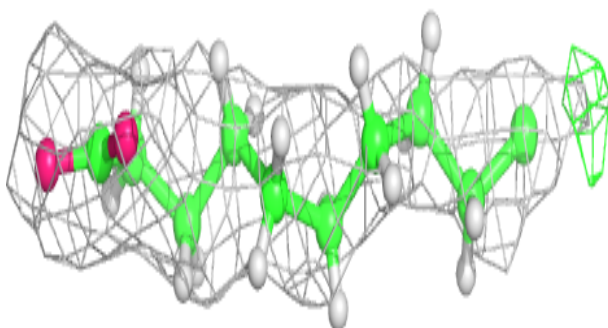
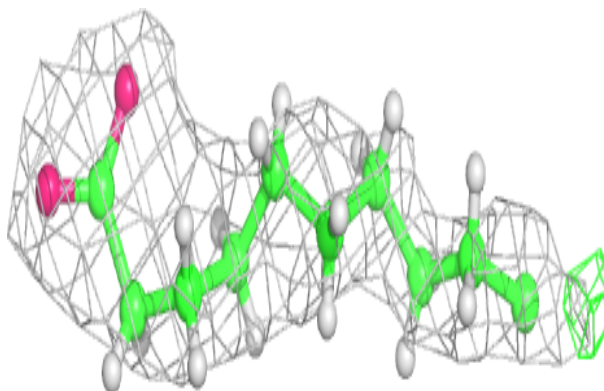


Electron density around STE M 104:

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

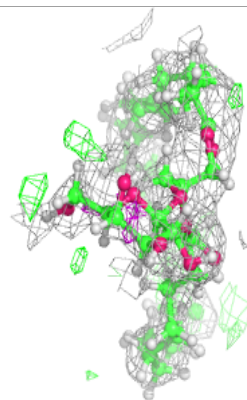
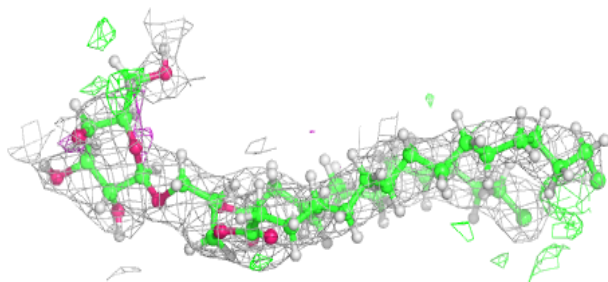
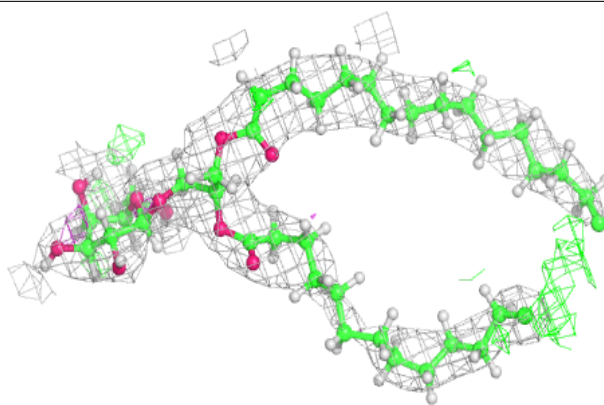
**Electron density around STE c 523:**

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

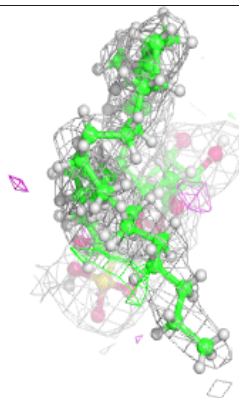
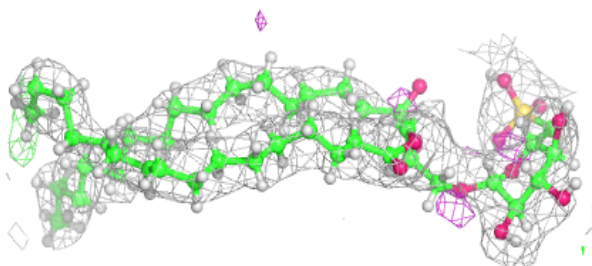
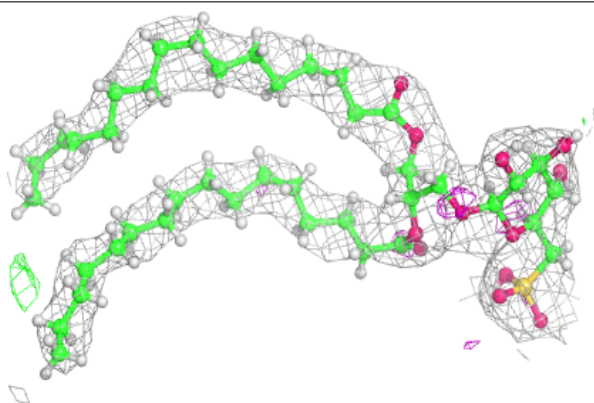


Electron density around LMG C 515:

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

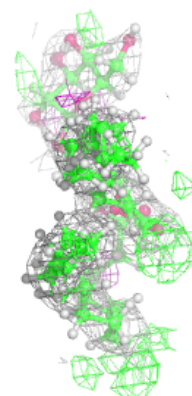
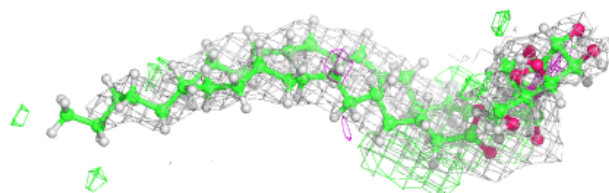
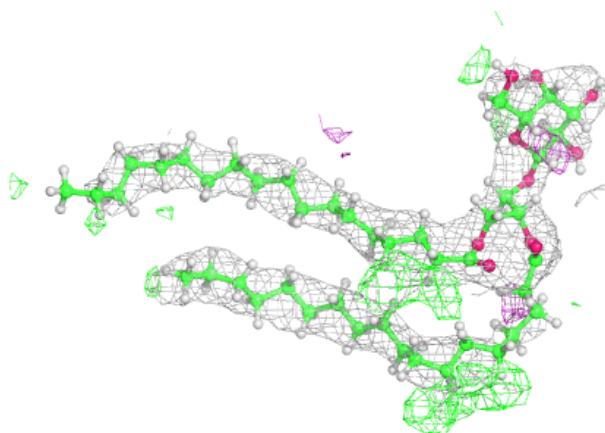
**Electron density around SQD B 620:**

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

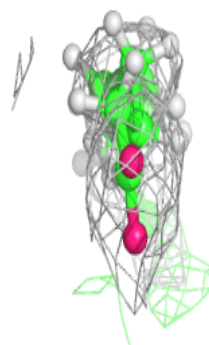
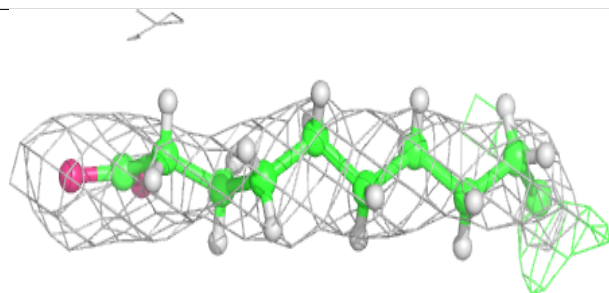
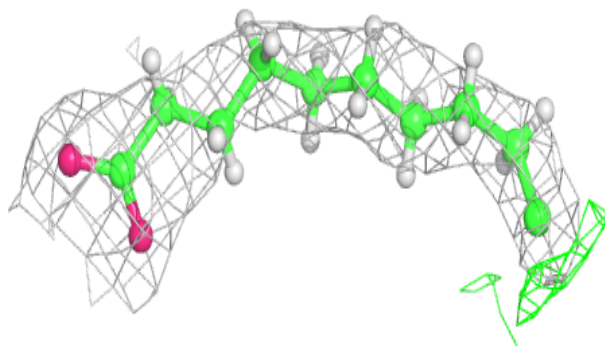


Electron density around LMG a 619:

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

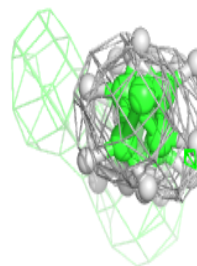
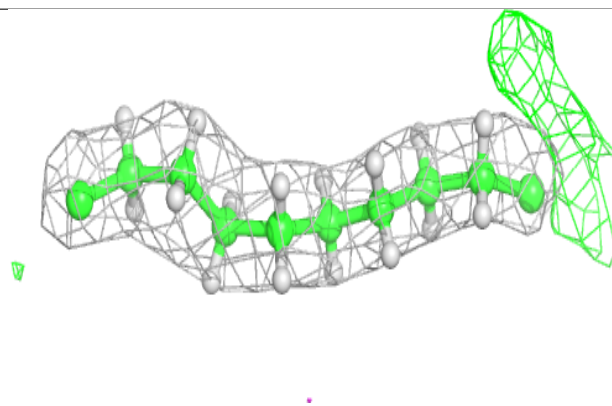
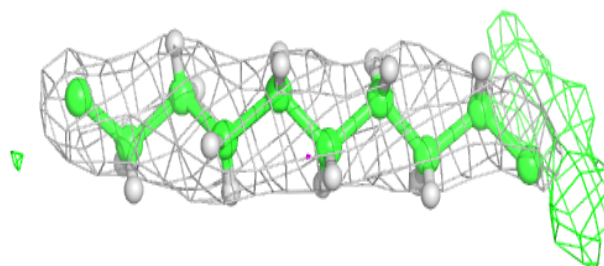
**Electron density around STE C 519:**

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



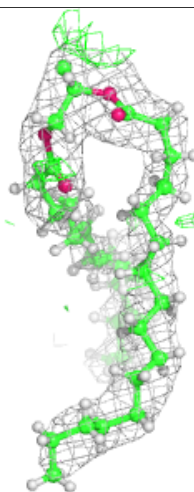
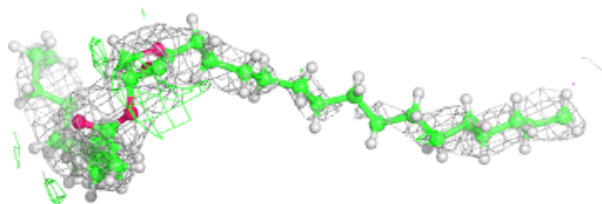
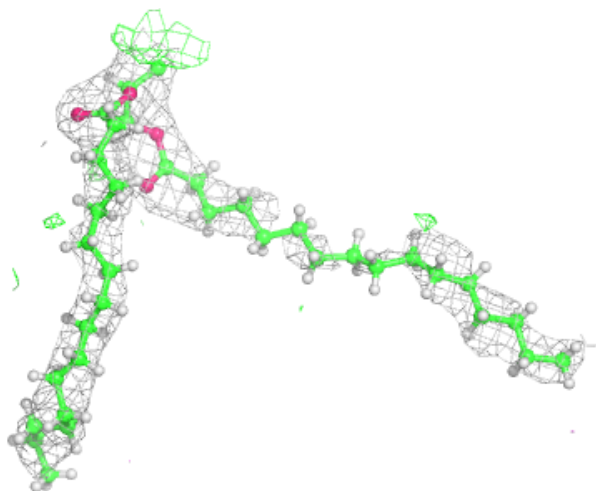
Electron density around STE M 103:

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



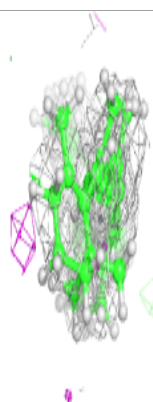
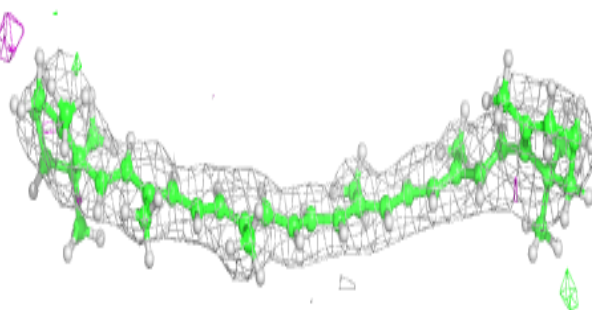
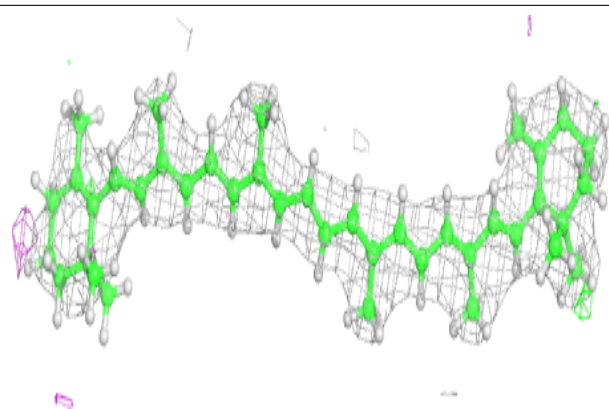
Electron density around SQD A 615:

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

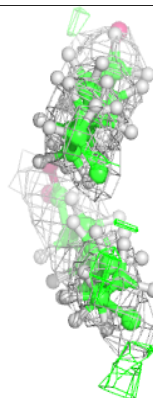
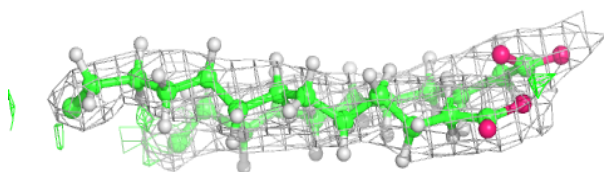
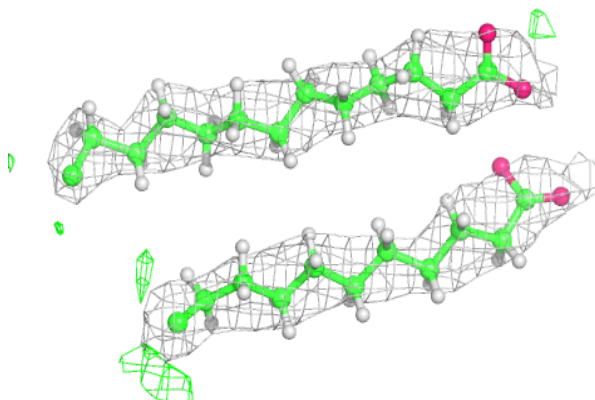


Electron density around BCR D 405:

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

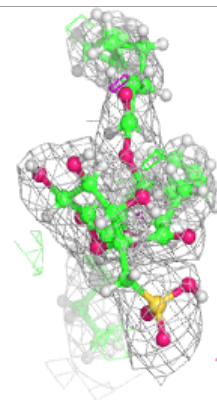
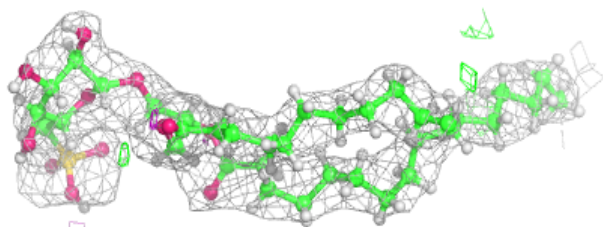
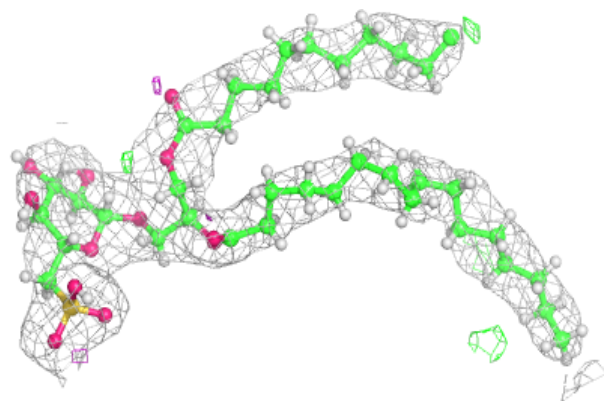
**Electron density around LMG D 412:**

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

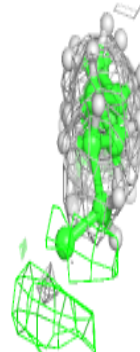
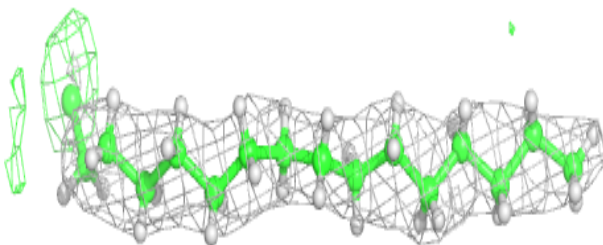
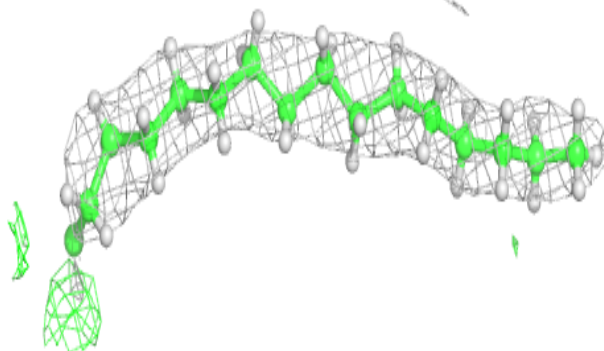


Electron density around SQD b 620:

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

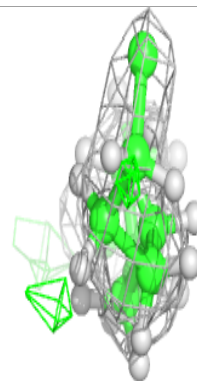
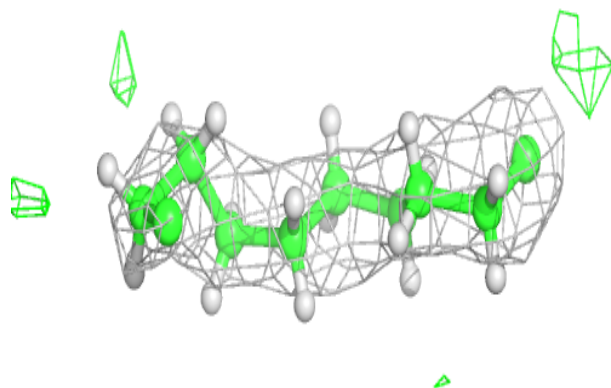
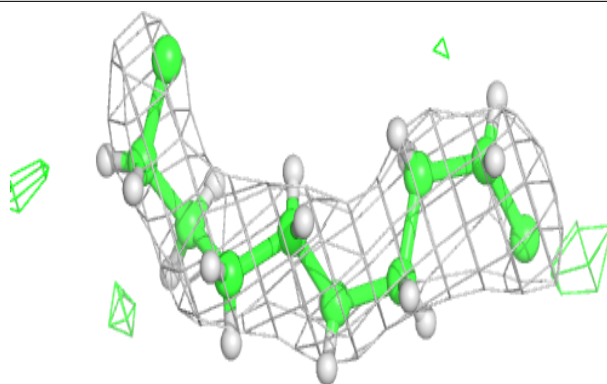
**Electron density around STE C 520:**

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

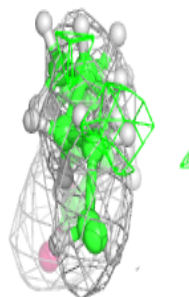
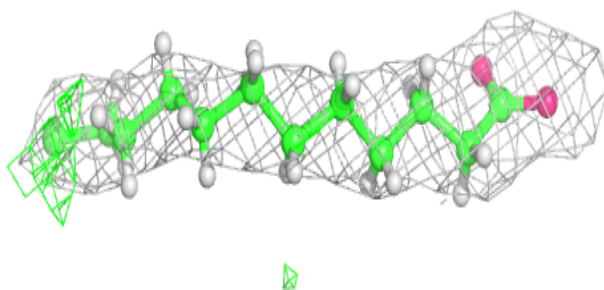
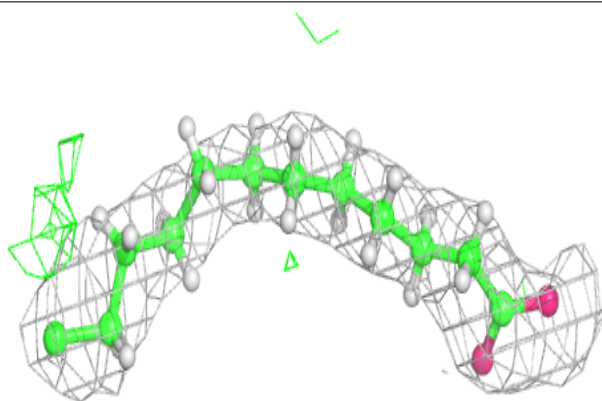


Electron density around STE b 625:

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

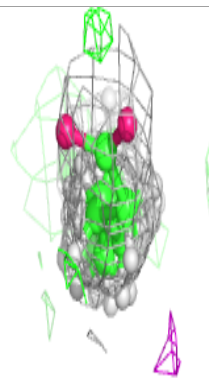
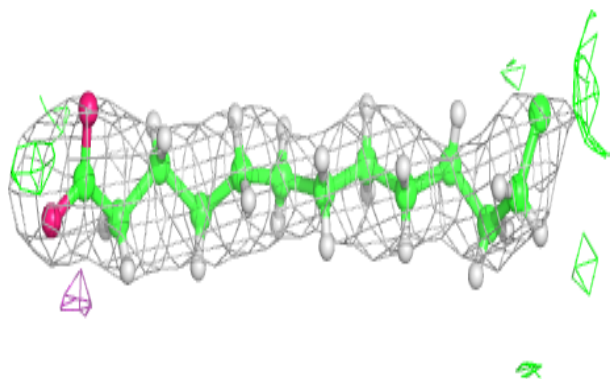
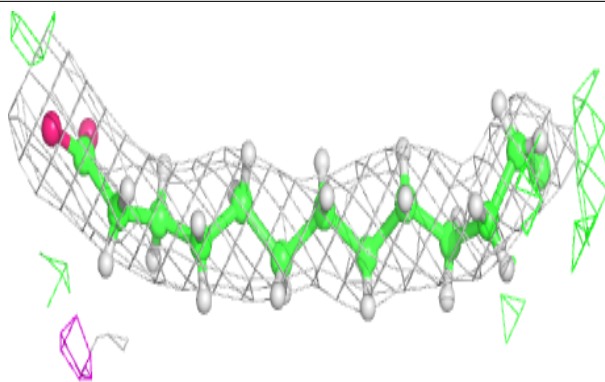
**Electron density around STE t 102:**

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

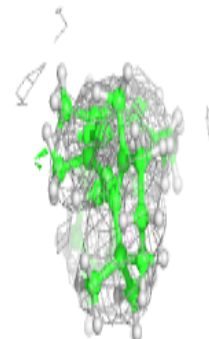
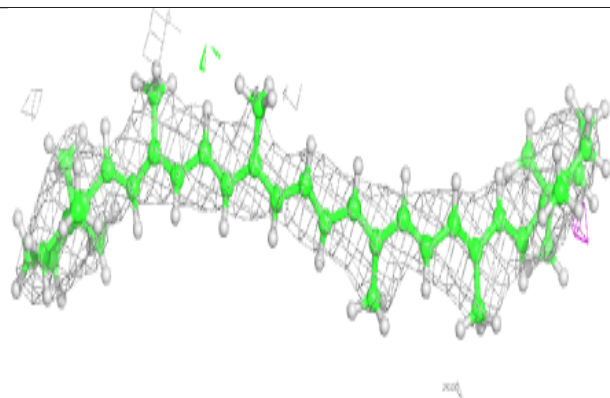
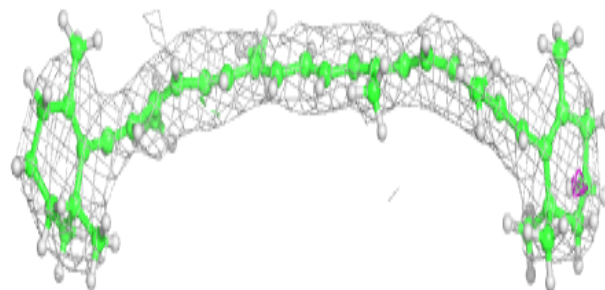


Electron density around STE M 102:

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

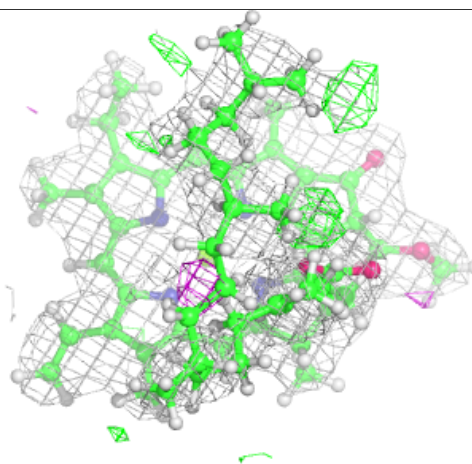
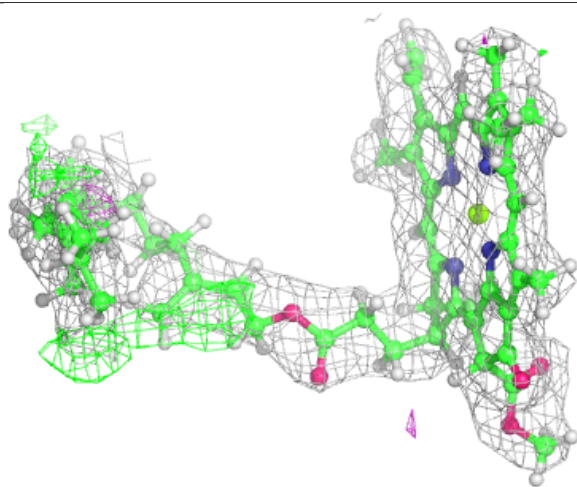
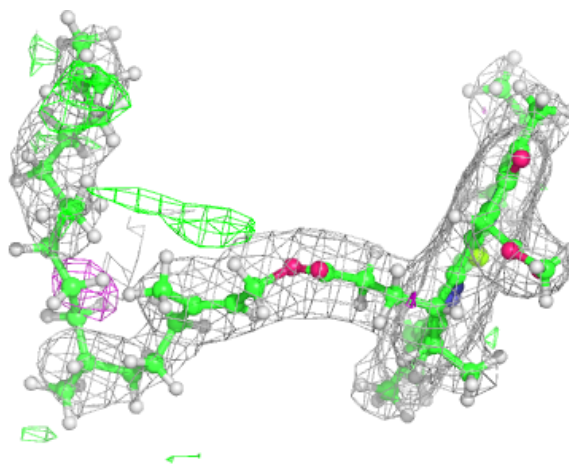
**Electron density around BCR k 102:**

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



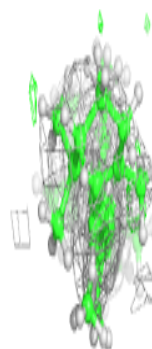
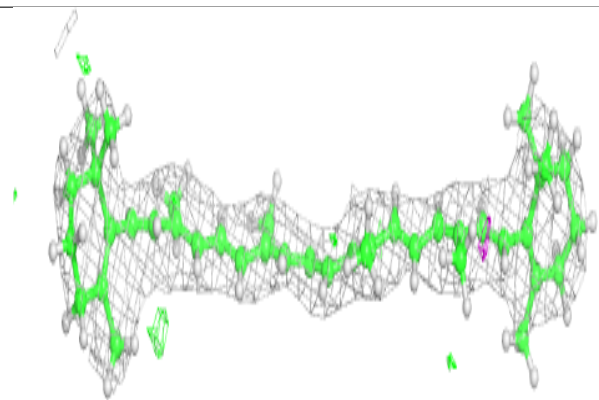
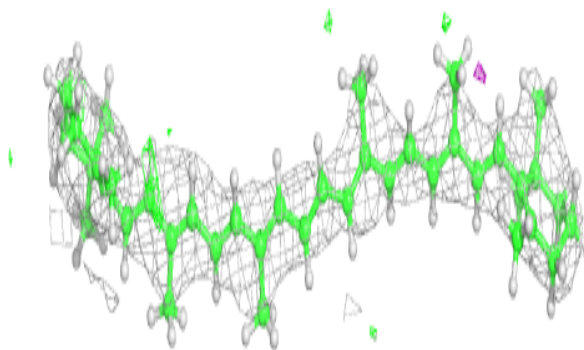
Electron density around CLA a 607:

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

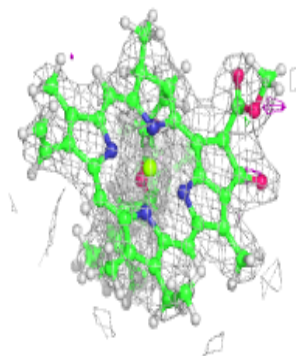
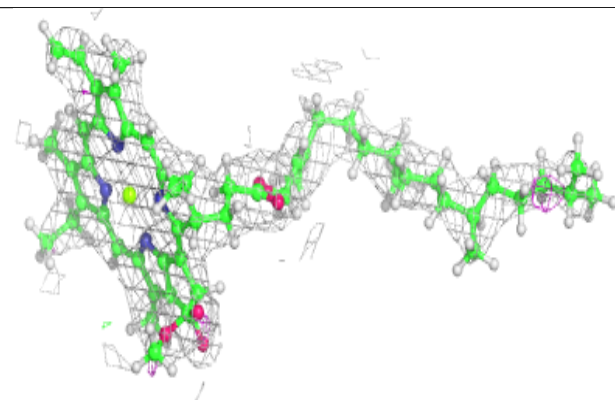
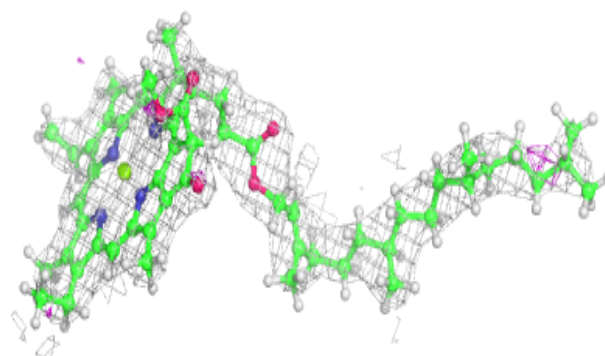


Electron density around BCR c 514:

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

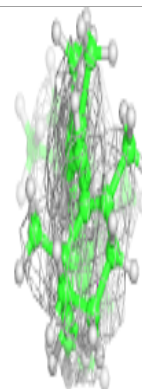
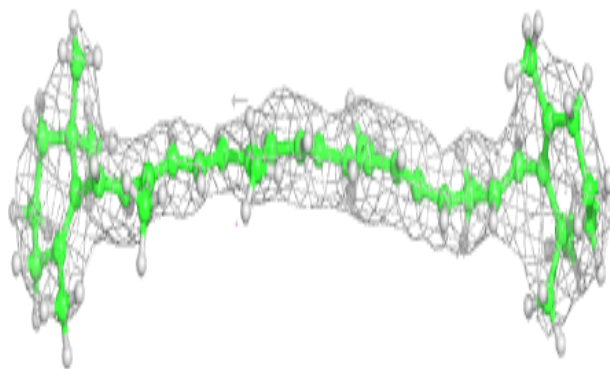
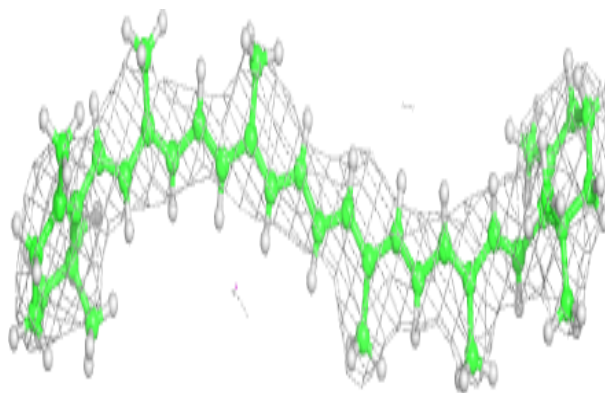
**Electron density around CLA C 502:**

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

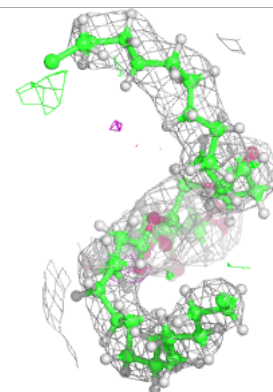
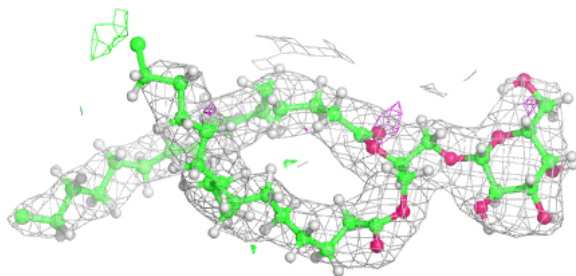
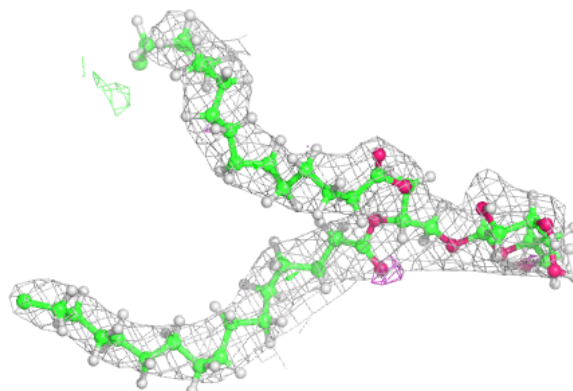


Electron density around BCR k 101:

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

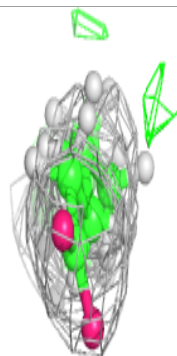
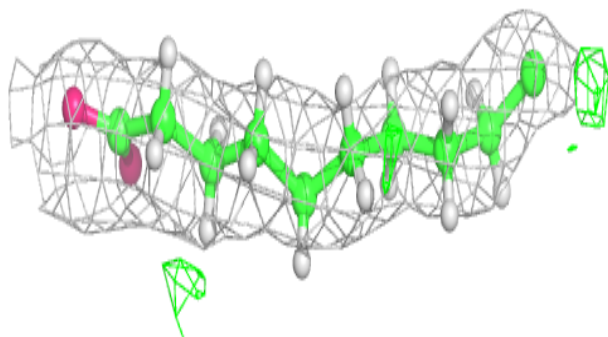
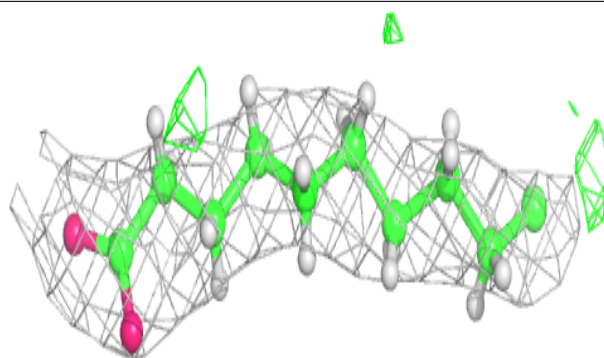
**Electron density around LMG M 101:**

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

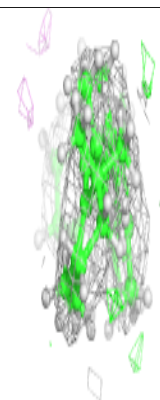
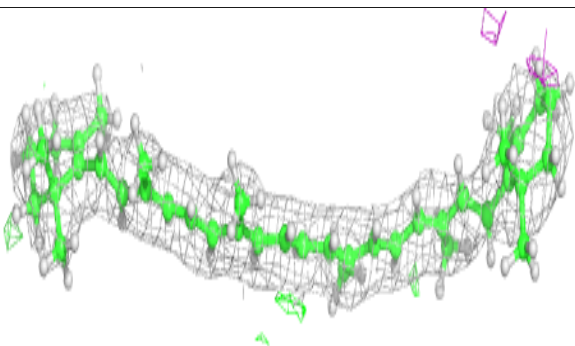
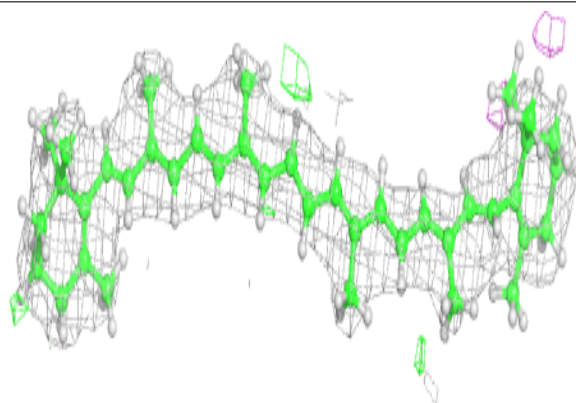


Electron density around STE j 101:

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

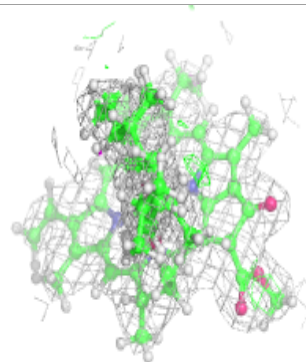
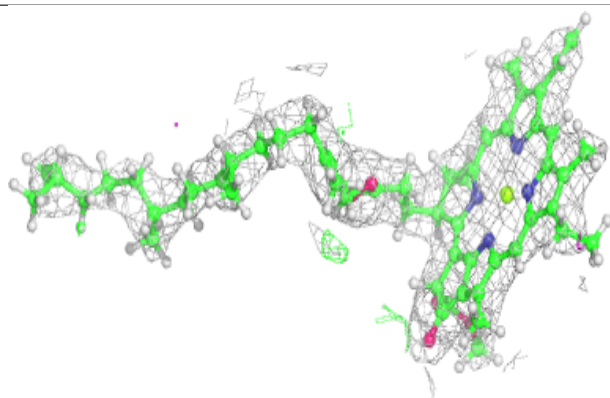
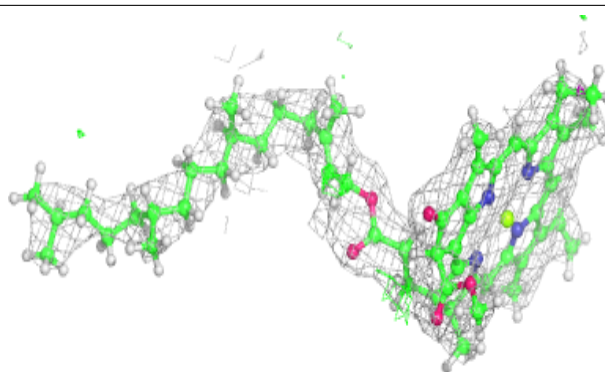
**Electron density around BCR d 404:**

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

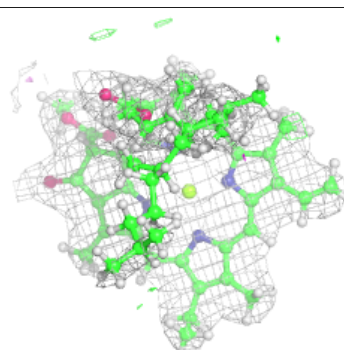
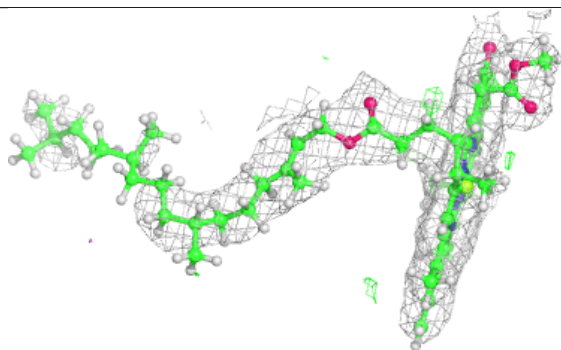
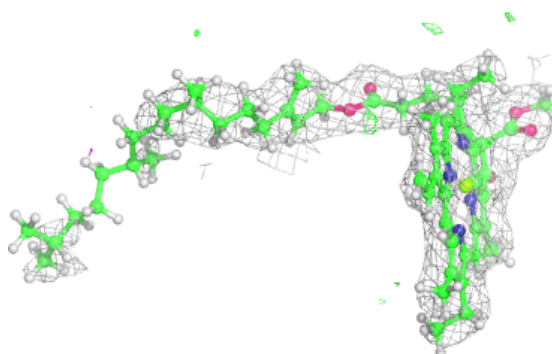


Electron density around CLA c 502:

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

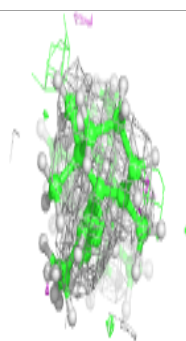
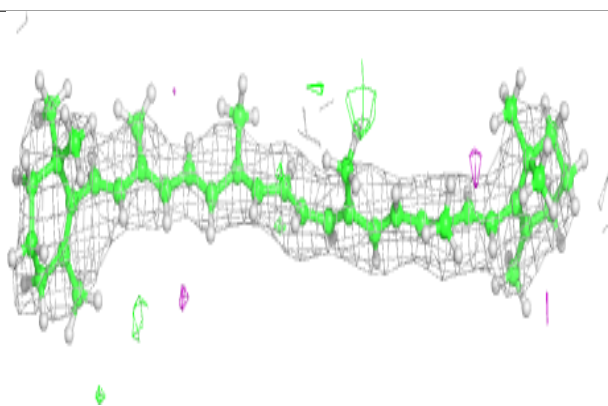
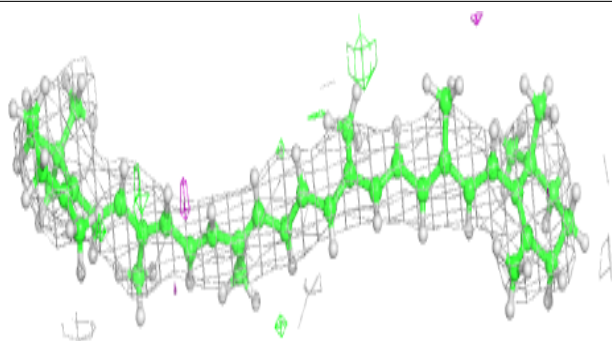
**Electron density around CLA D 404:**

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

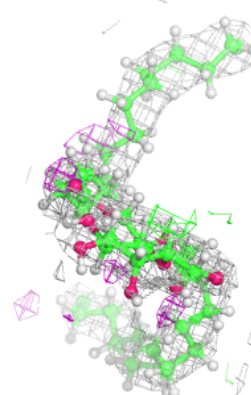
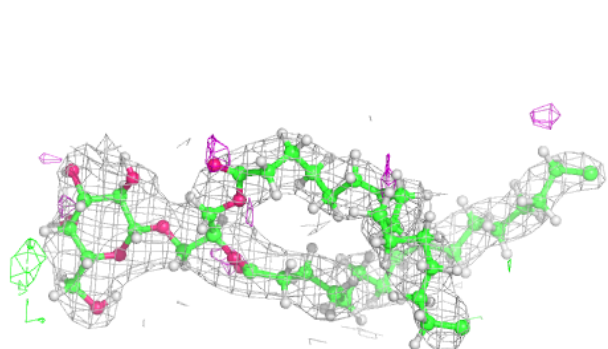
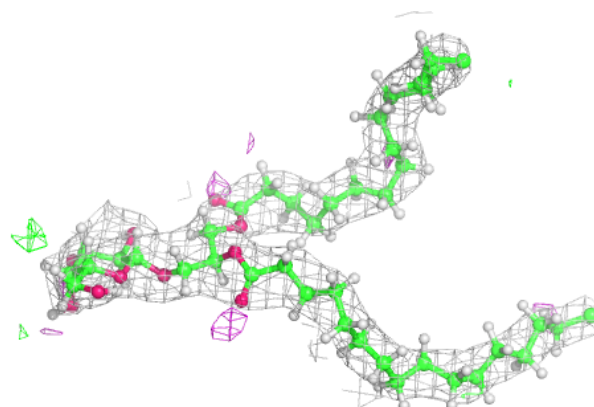


Electron density around BCR K 101:

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

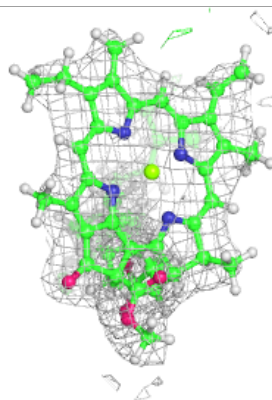
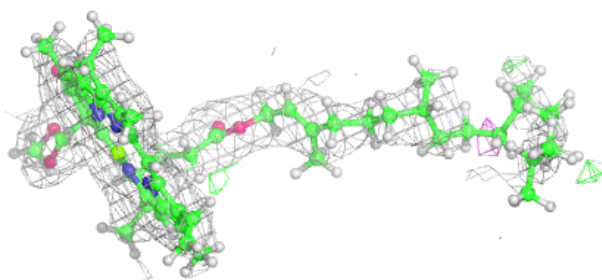
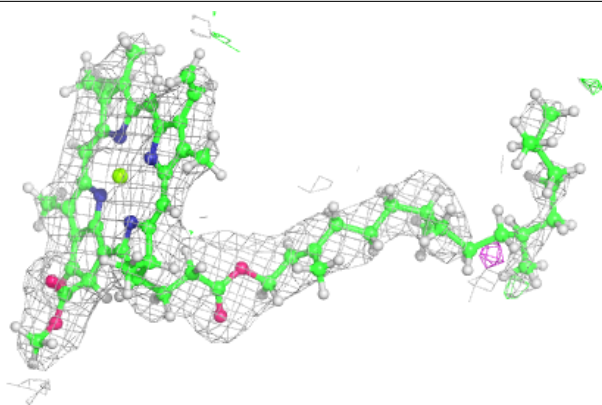
**Electron density around LMG m 101:**

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

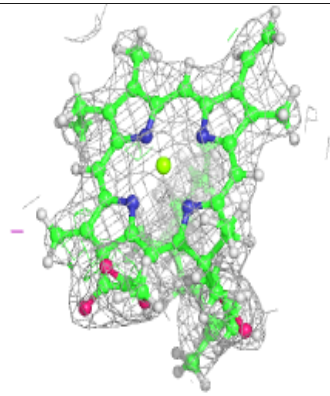
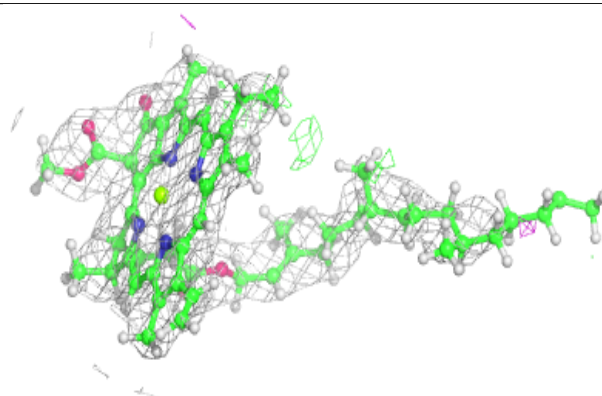
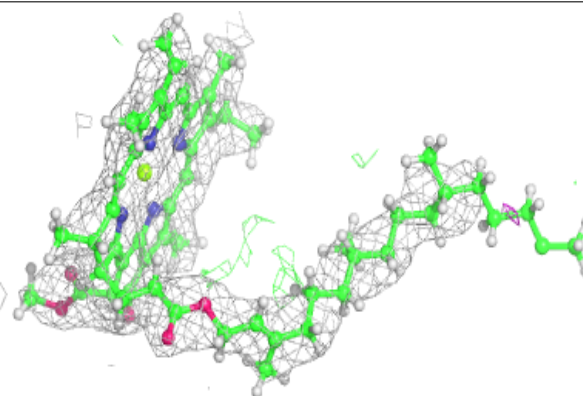


Electron density around CLA d 403:

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

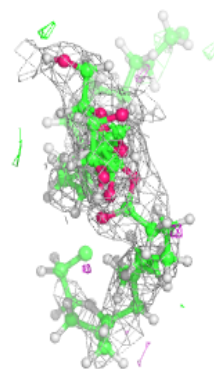
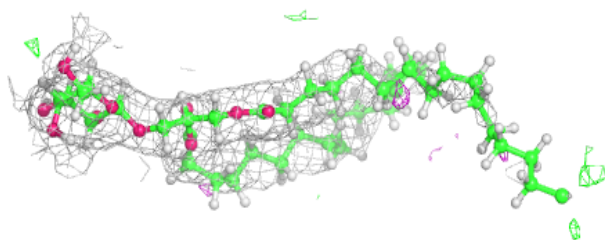
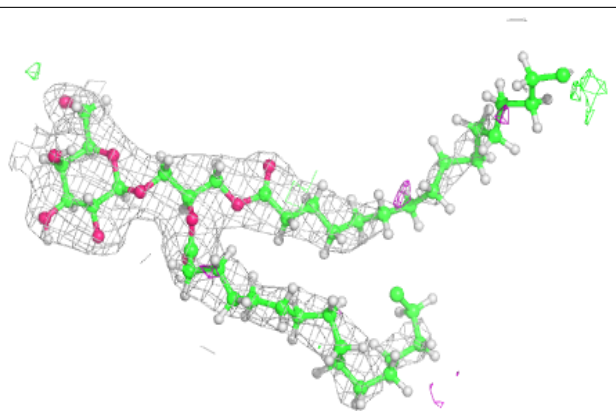
**Electron density around CLA c 508:**

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

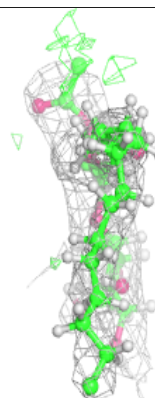
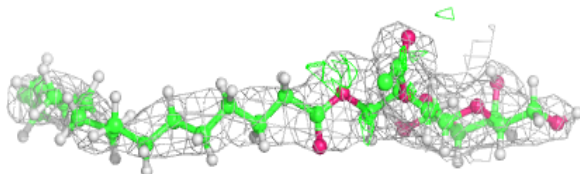
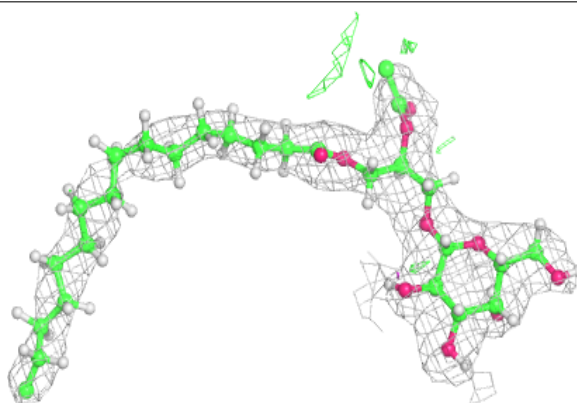


Electron density around LMG D 407:

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

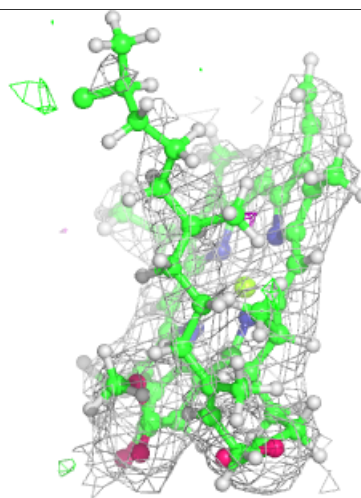
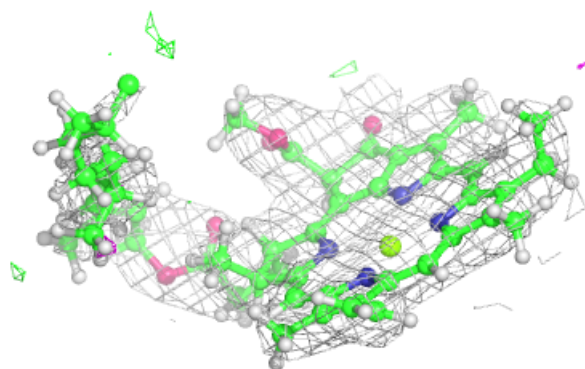
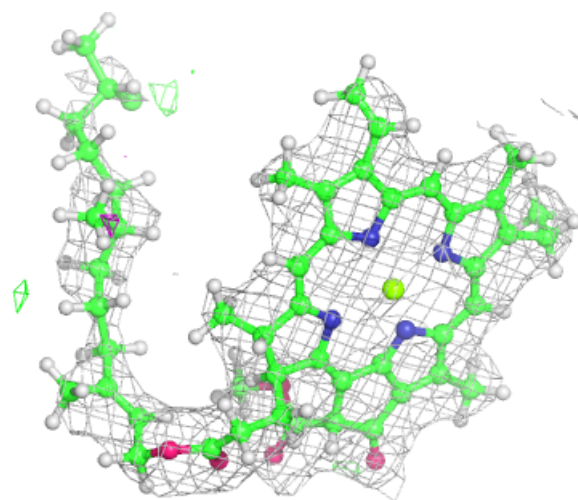
**Electron density around LMG c 519:**

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



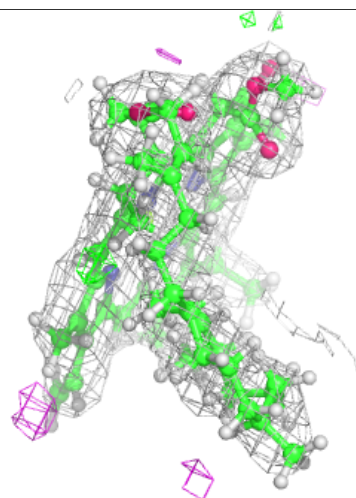
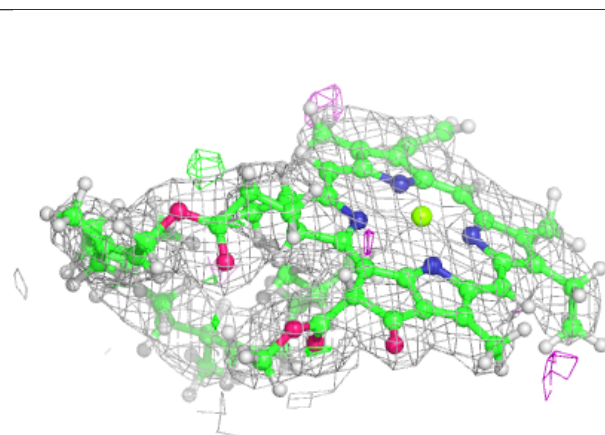
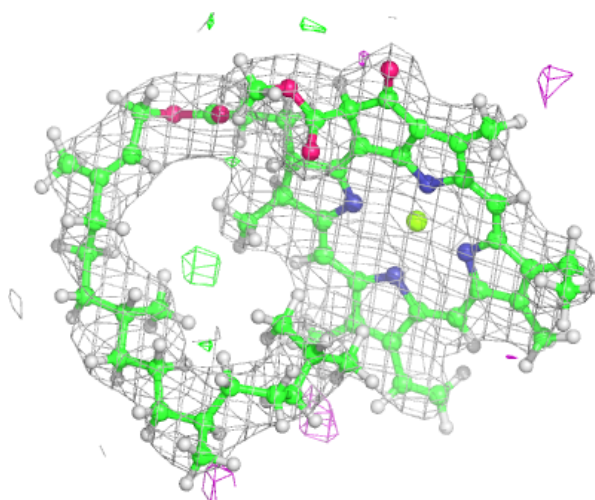
Electron density around CLA b 616:

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



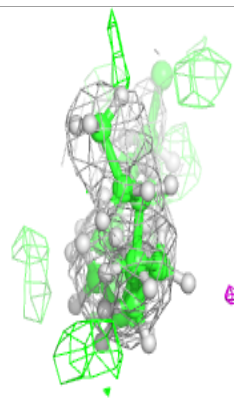
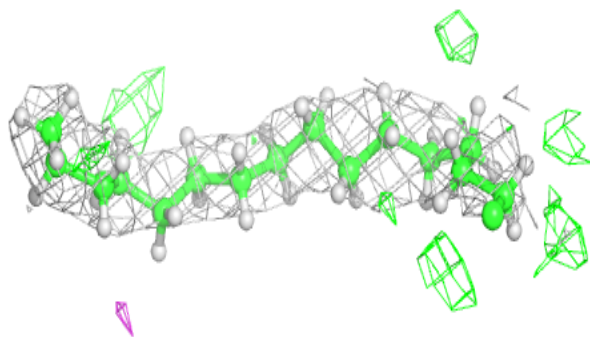
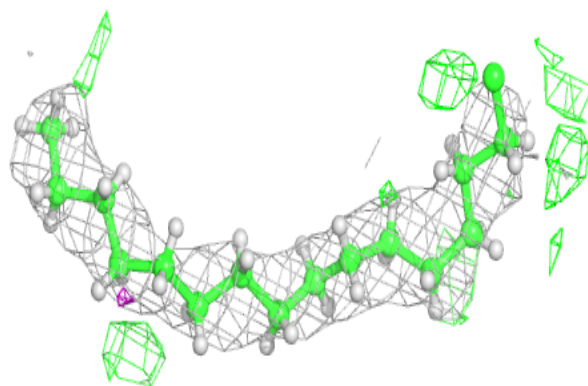
Electron density around CLA b 615:

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



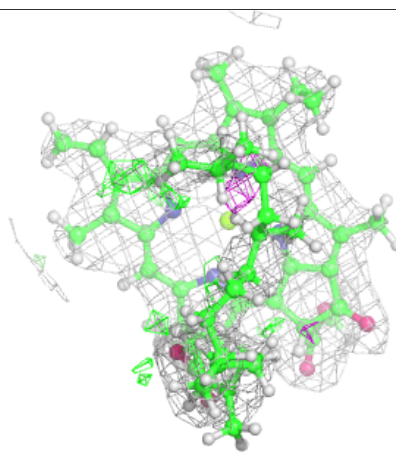
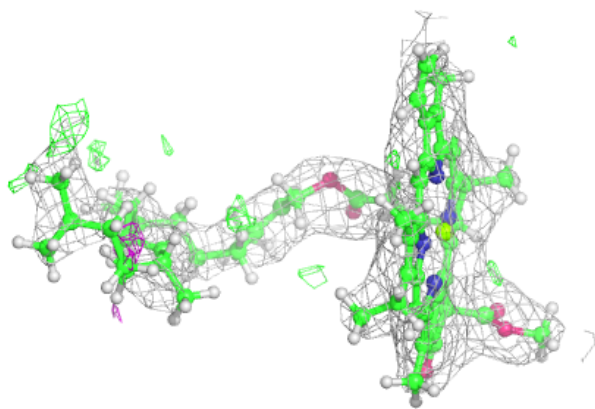
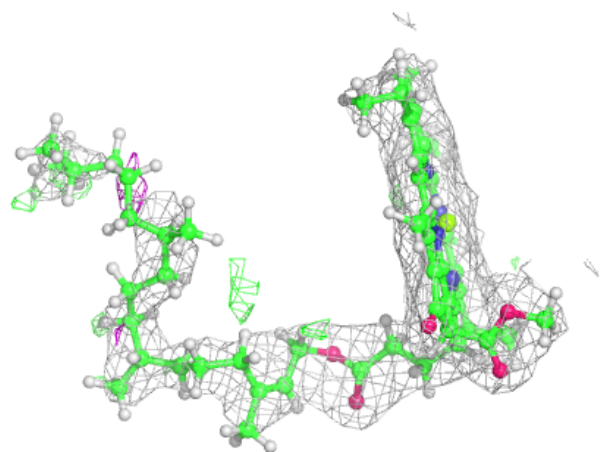
Electron density around STE T 102:

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



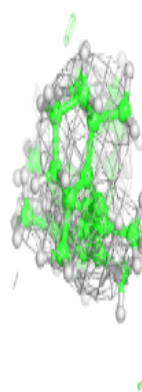
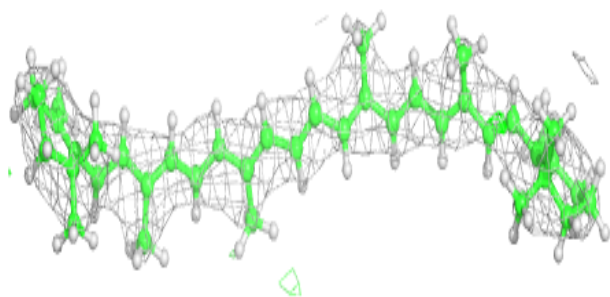
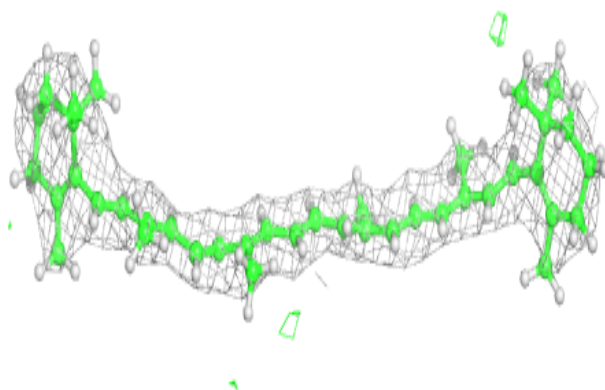
Electron density around CLA c 506:

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

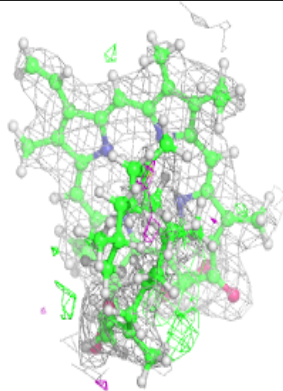
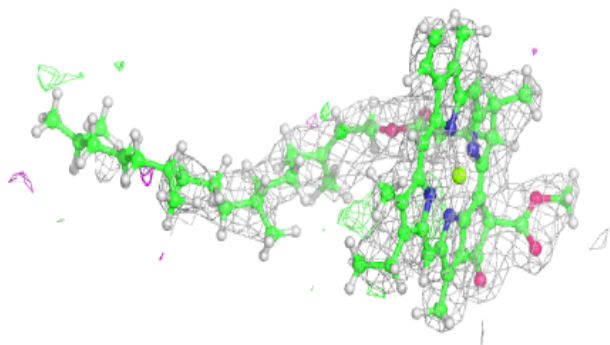
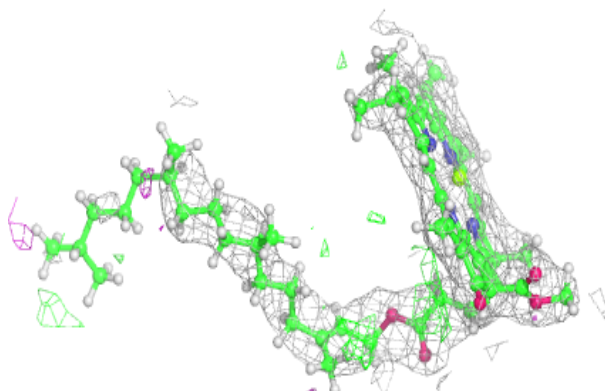


Electron density around BCR K 103:

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

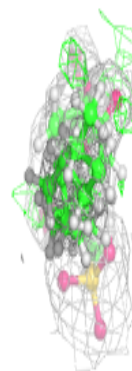
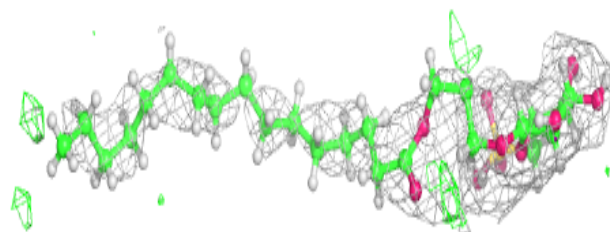
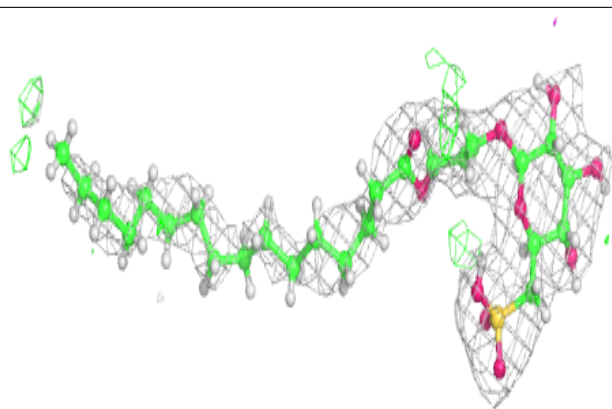
**Electron density around CLA C 508:**

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

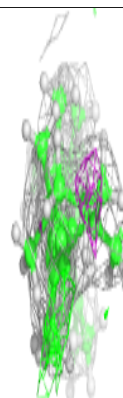
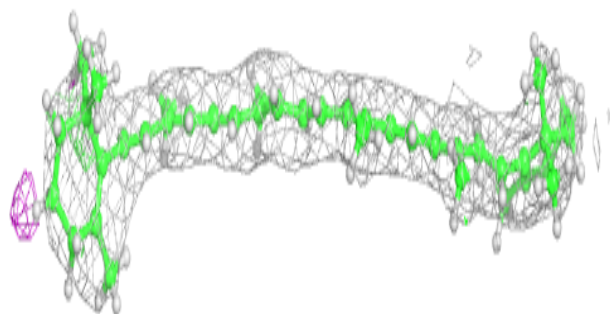
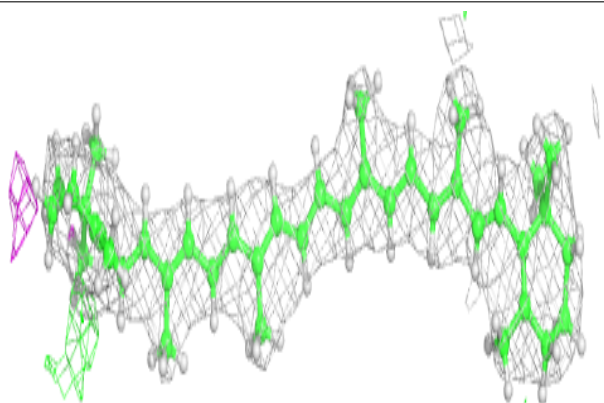


Electron density around SQD D 408:

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

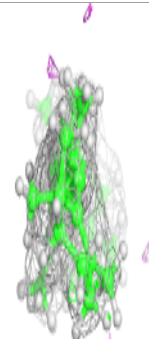
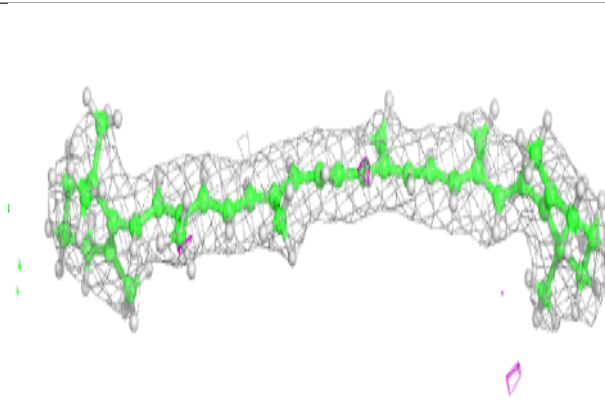
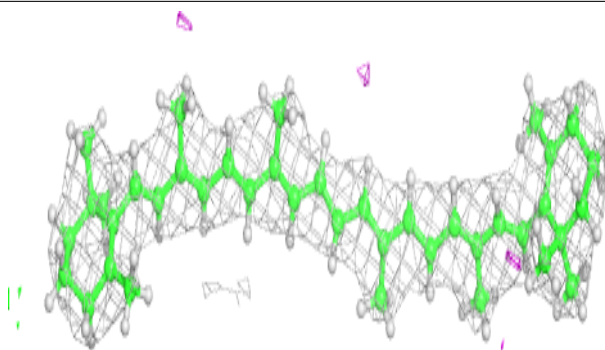
**Electron density around BCR b 617:**

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



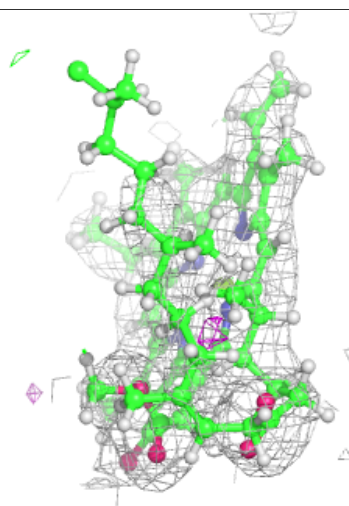
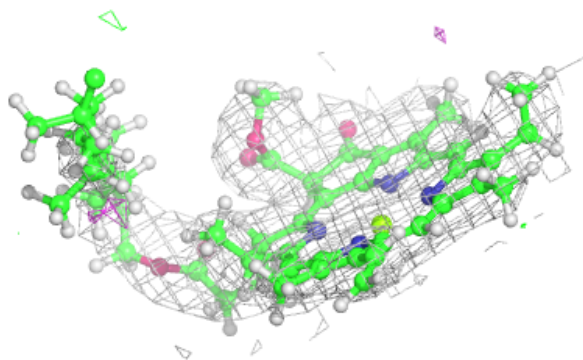
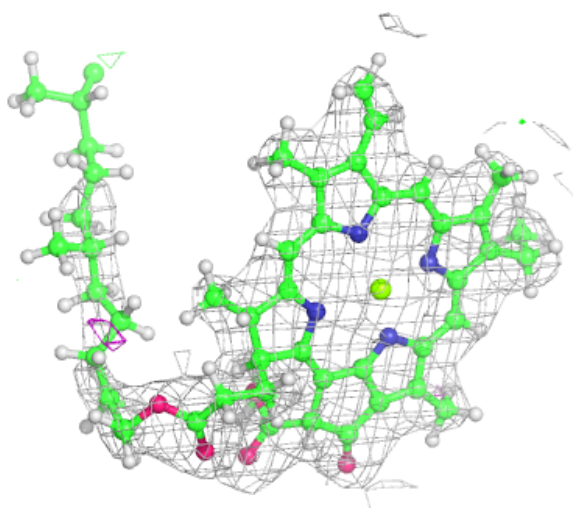
Electron density around BCR b 619:

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



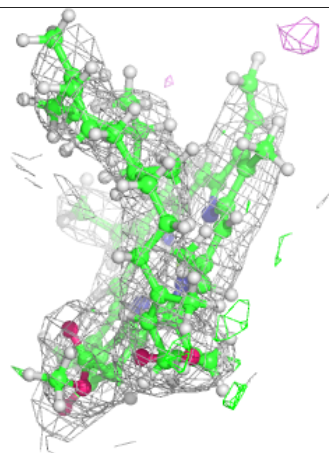
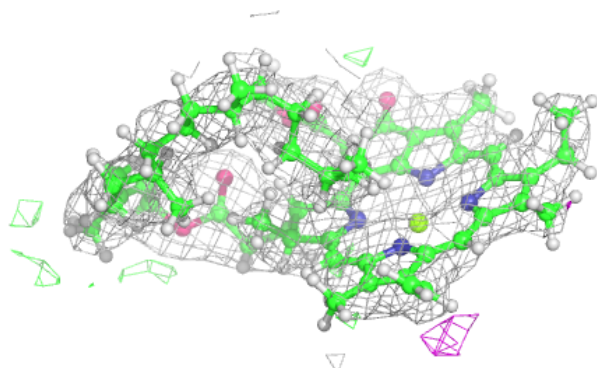
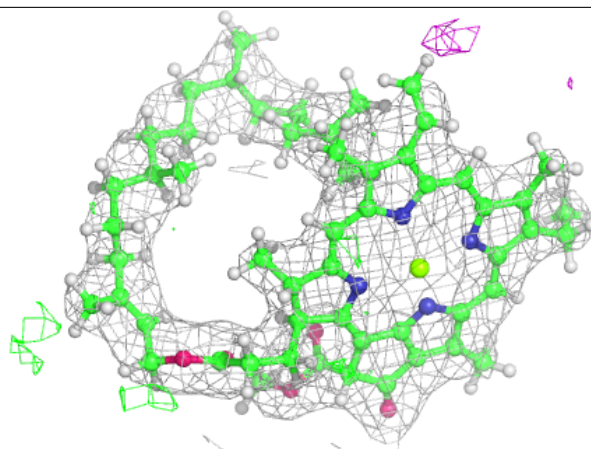
Electron density around CLA B 615:

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

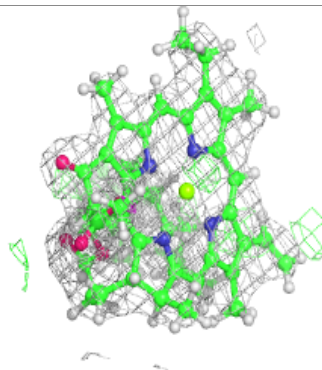
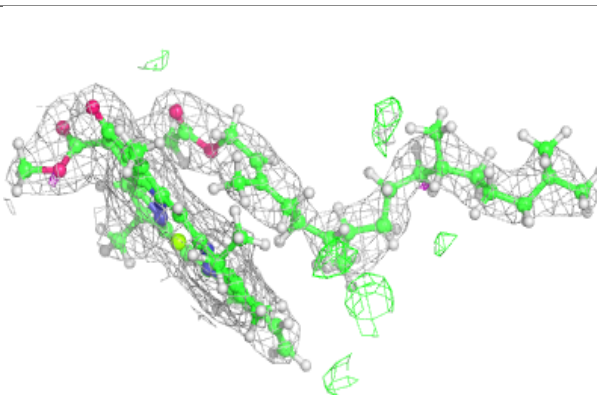
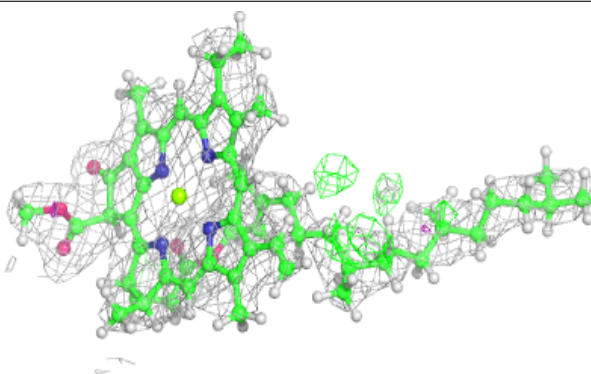


Electron density around CLA B 614:

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

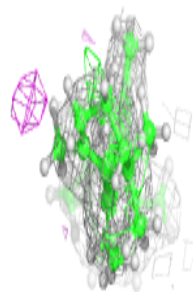
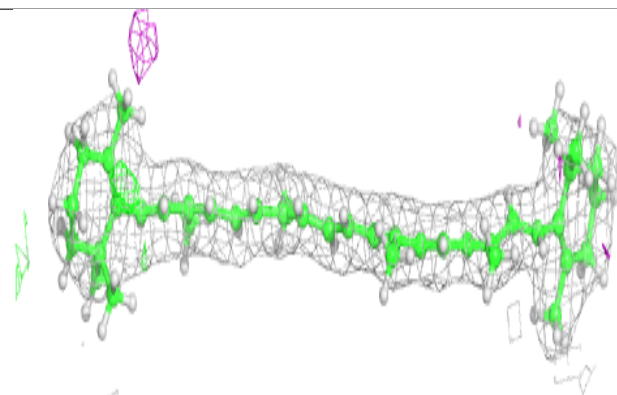
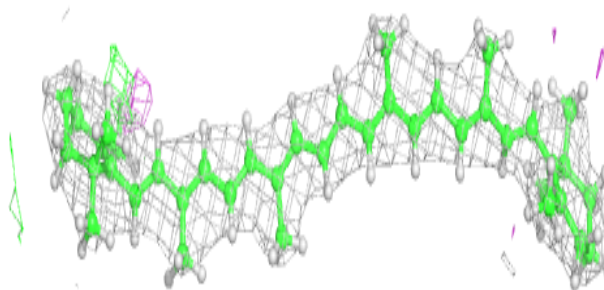
**Electron density around CLA C 505:**

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



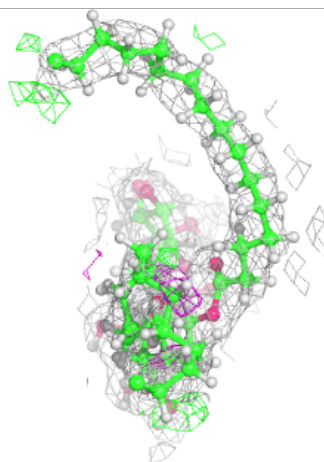
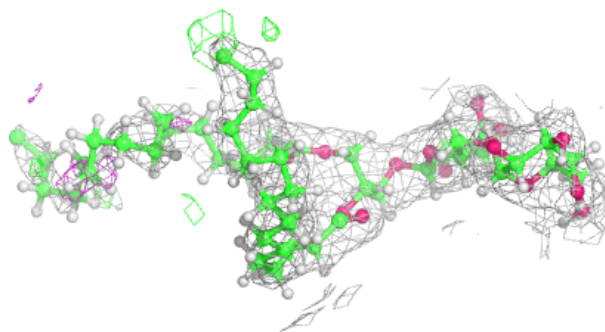
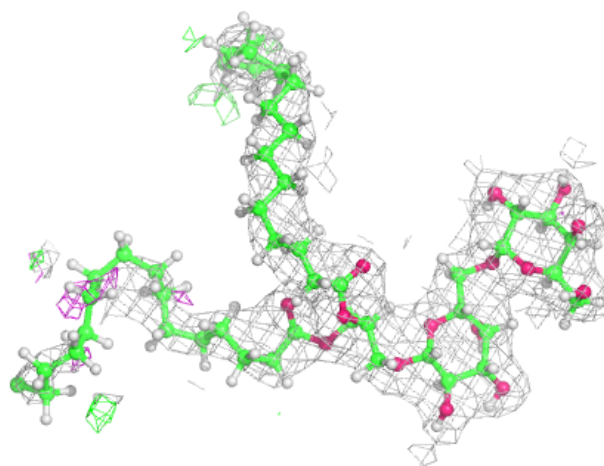
Electron density around BCR C 514:

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



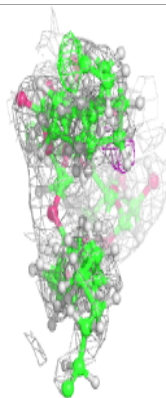
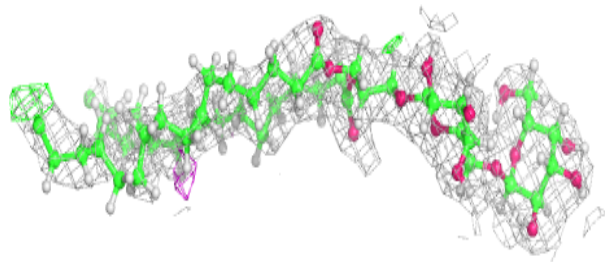
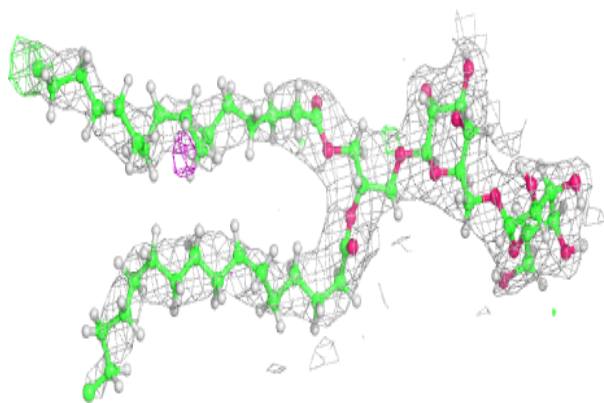
Electron density around DGD C 517:

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

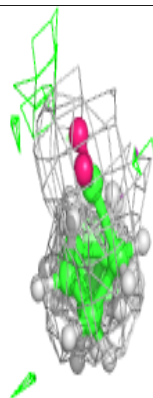
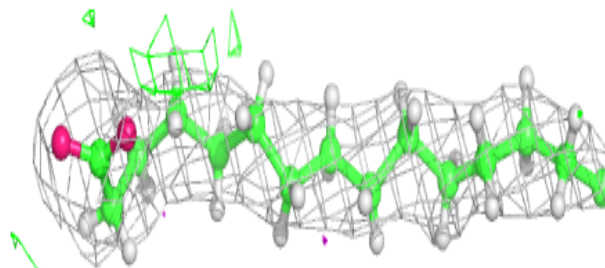
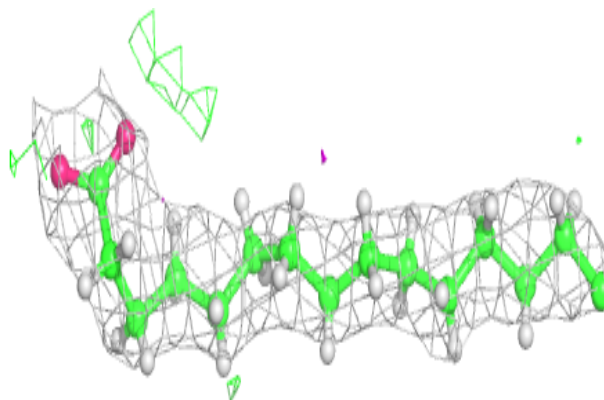


Electron density around DGD c 518:

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

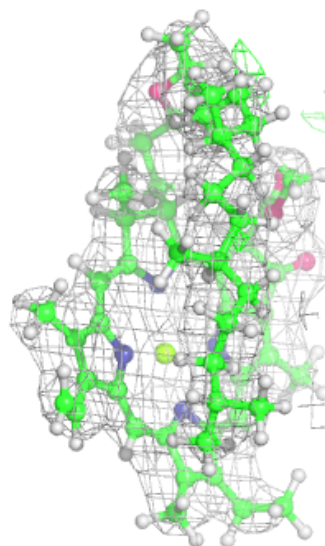
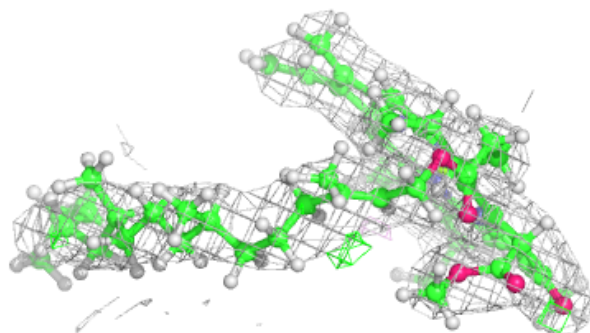
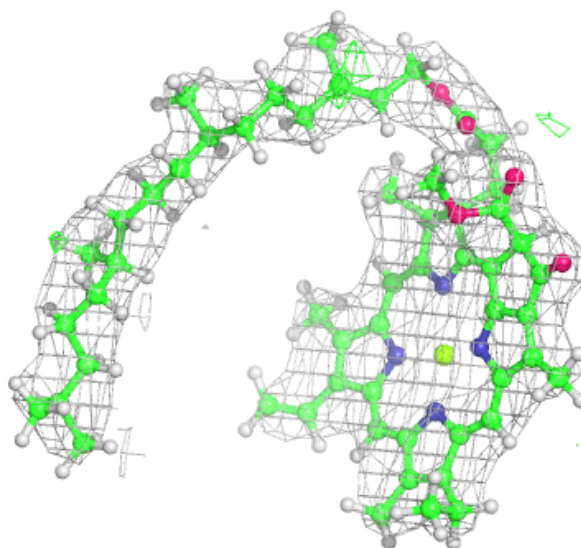
**Electron density around STE d 409:**

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



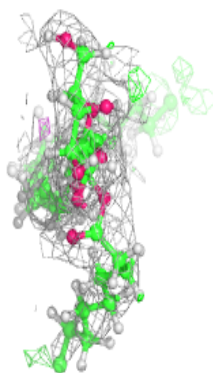
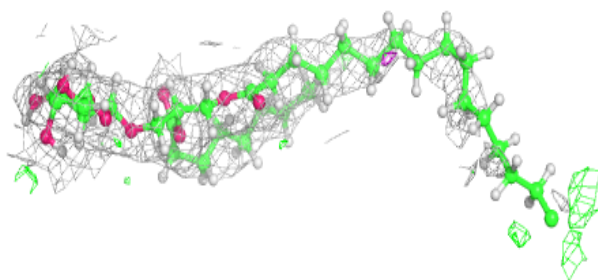
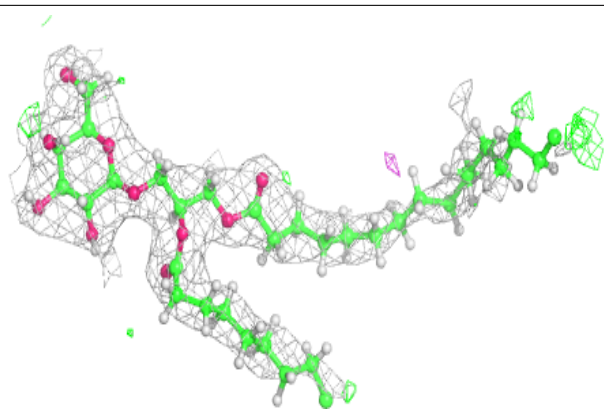
Electron density around CLA C 507:

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



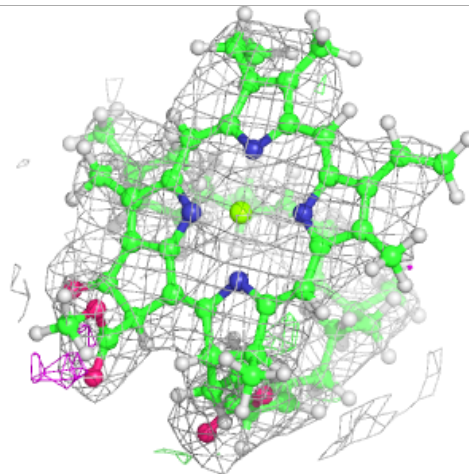
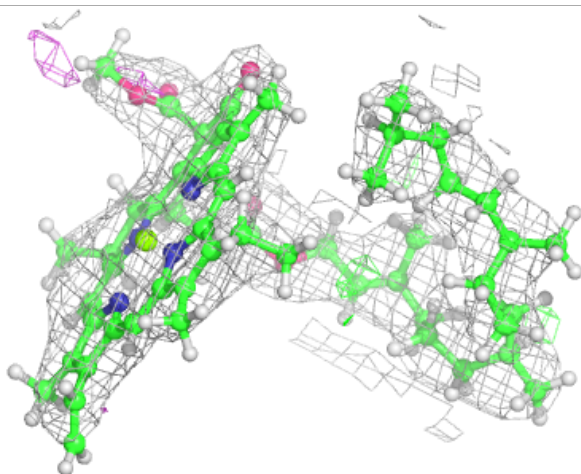
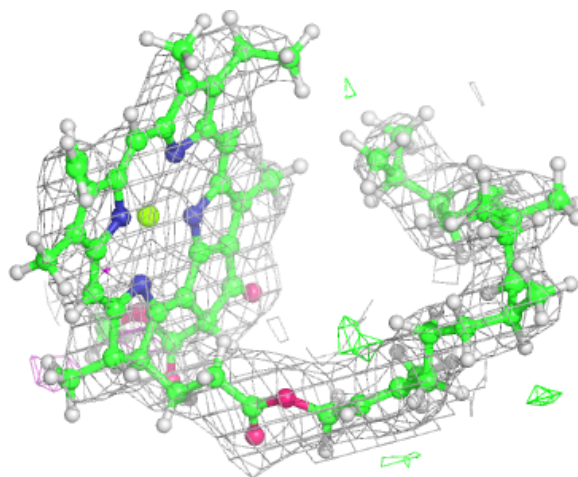
Electron density around LMG d 408:

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



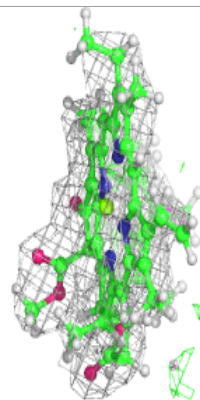
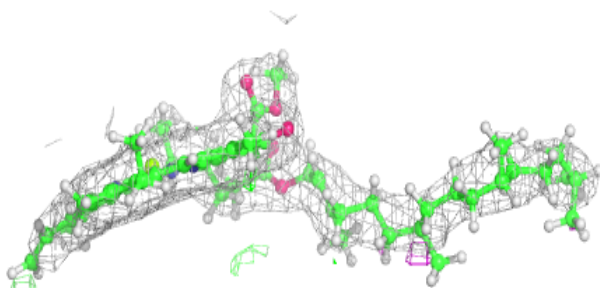
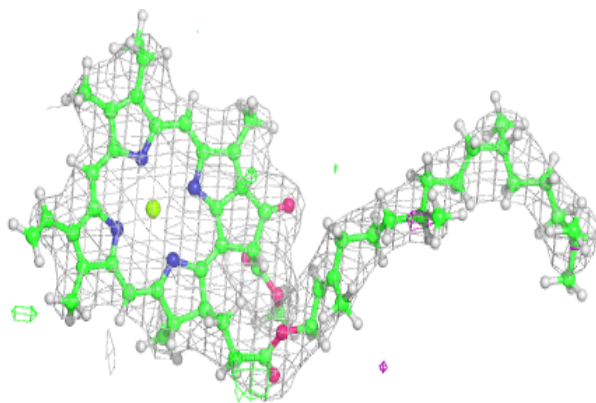
Electron density around CLA c 503:

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

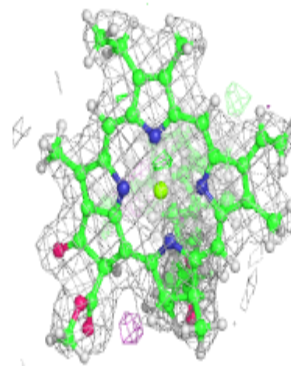
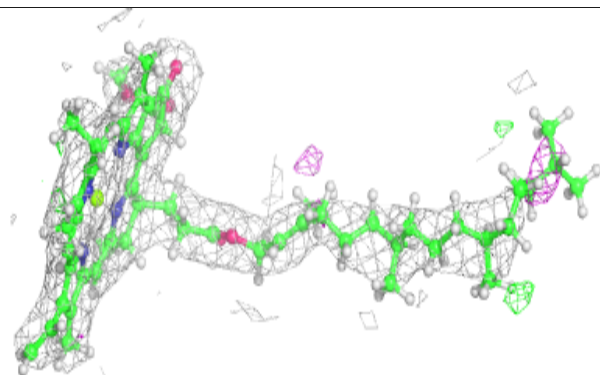
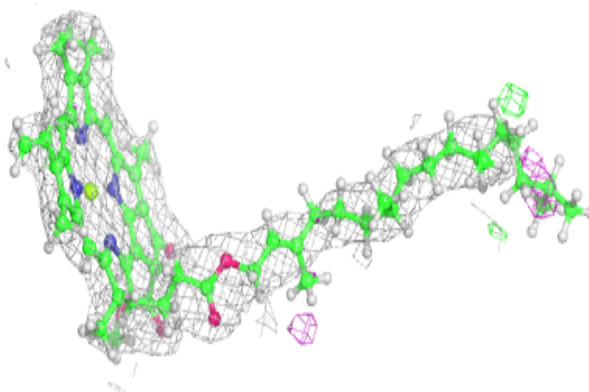


Electron density around CLA b 602:

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

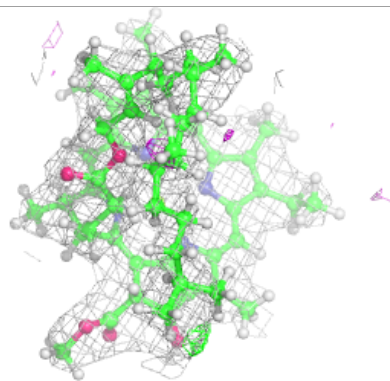
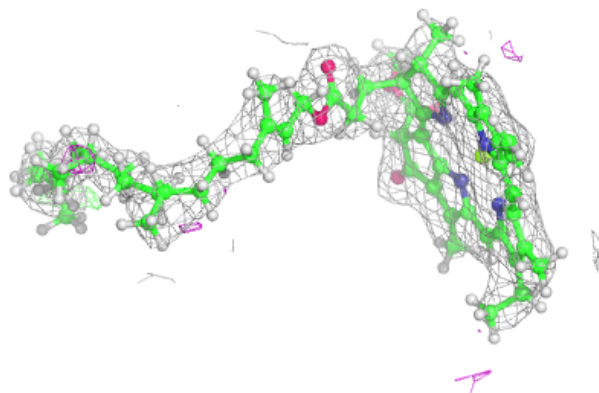
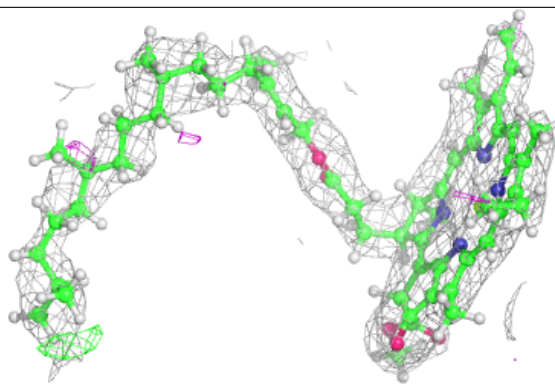
**Electron density around CLA b 604:**

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

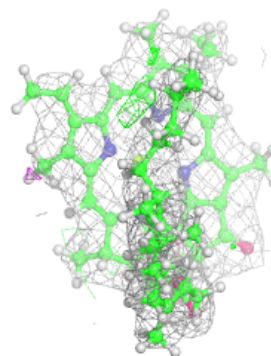
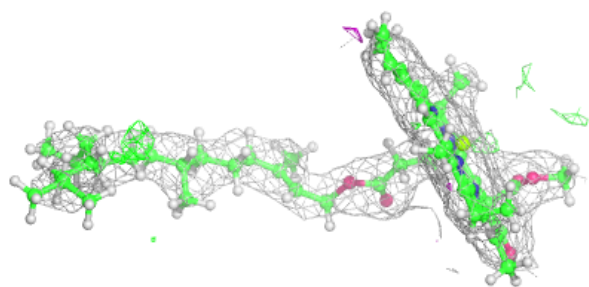
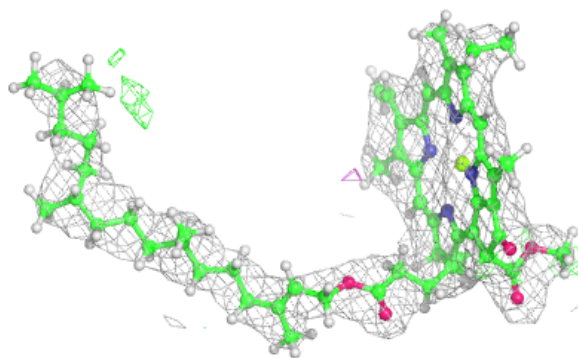


Electron density around CLA b 606:

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

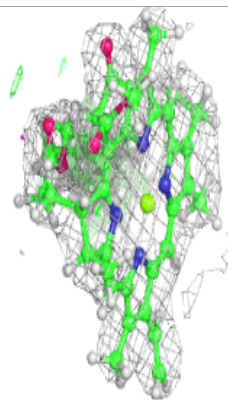
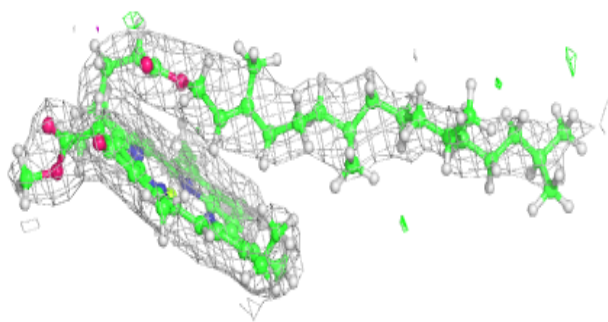
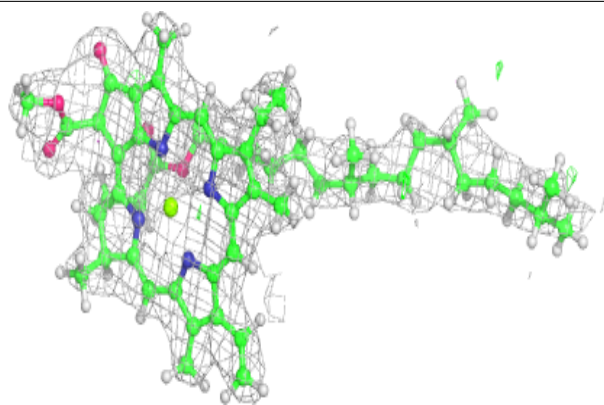
**Electron density around CLA b 609:**

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

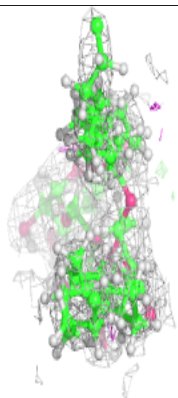
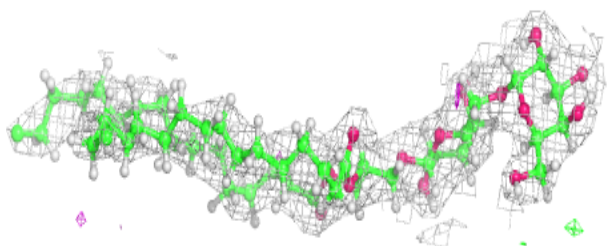
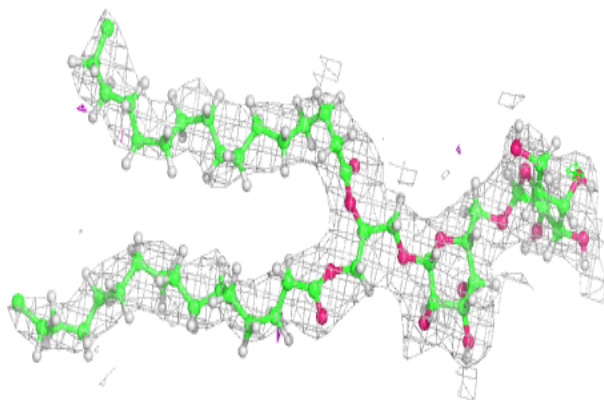


Electron density around CLA b 614:

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

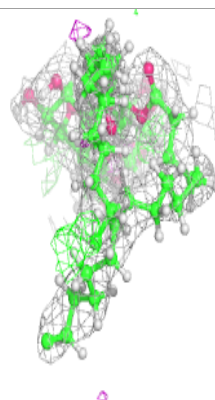
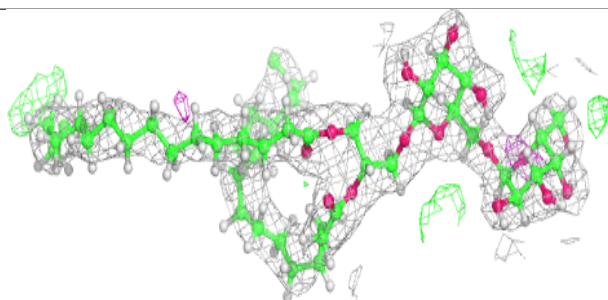
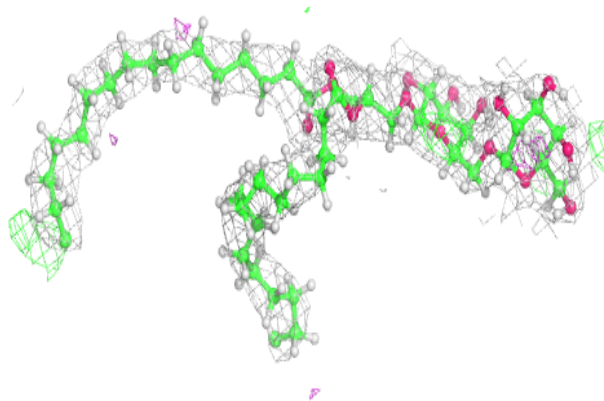
**Electron density around DGD C 518:**

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

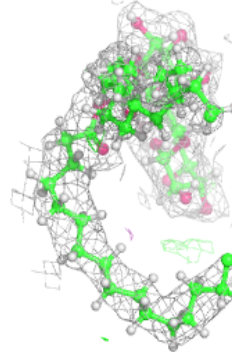
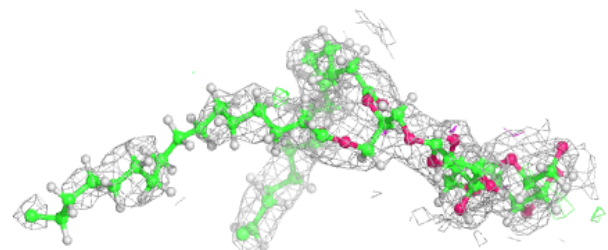
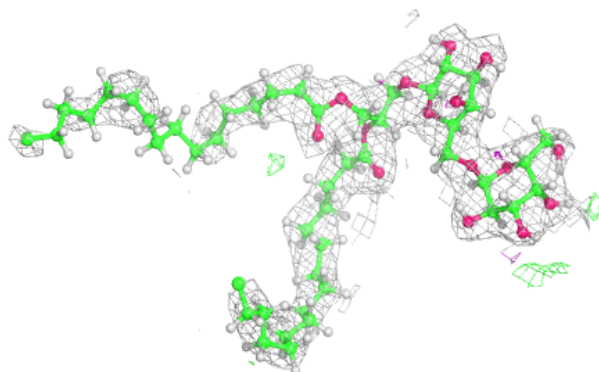


Electron density around DGD H 102:

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

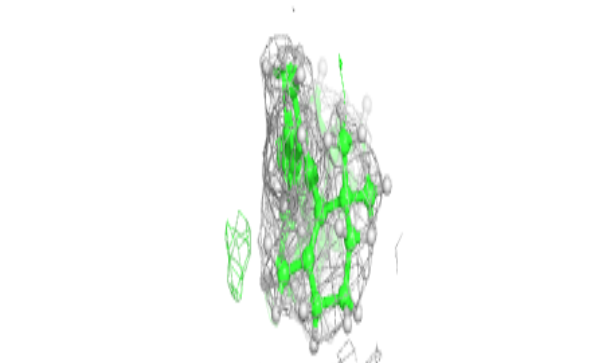
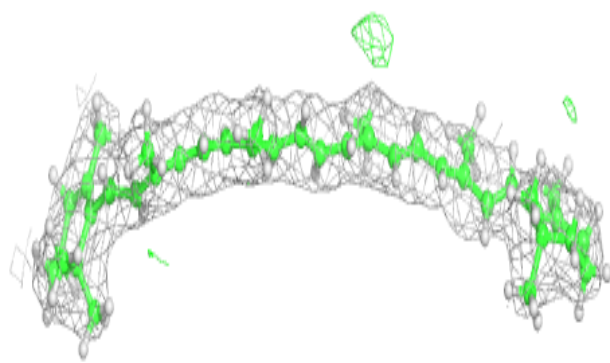
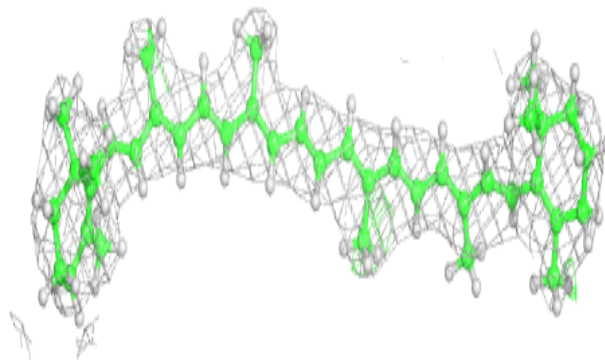
**Electron density around DGD c 517:**

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

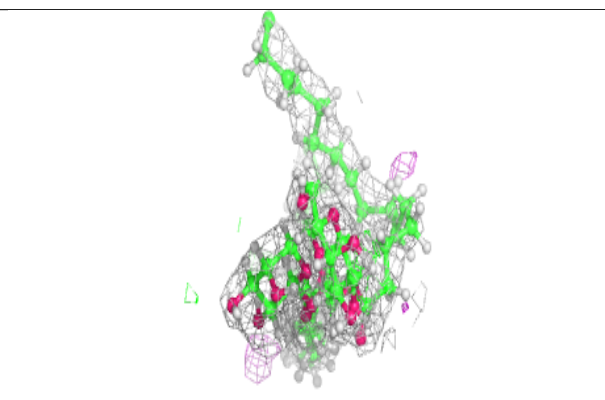
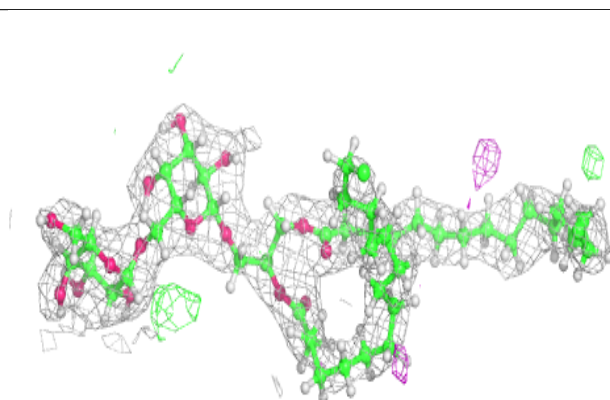
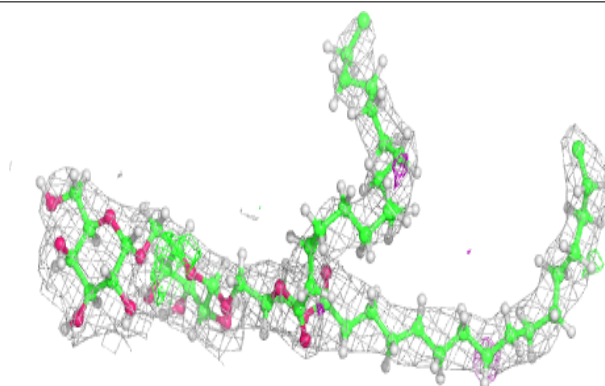


Electron density around BCR T 101:

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

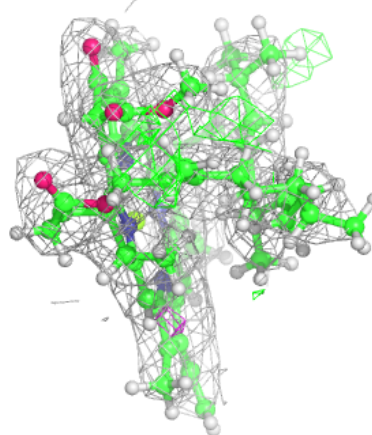
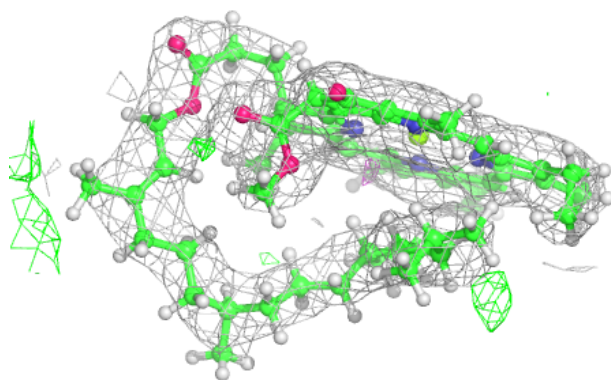
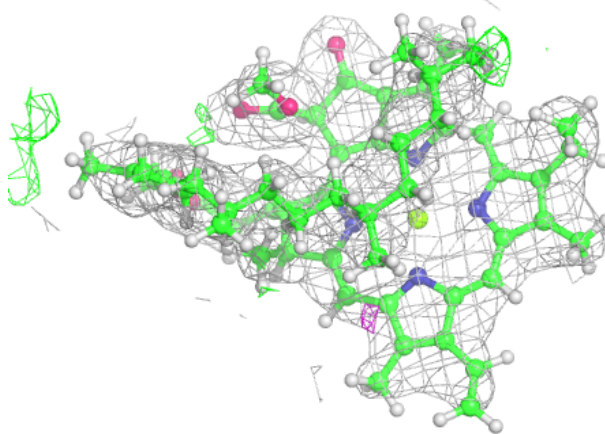
**Electron density around DGD h 102:**

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



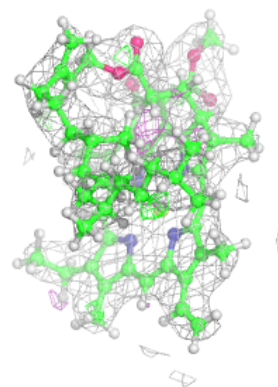
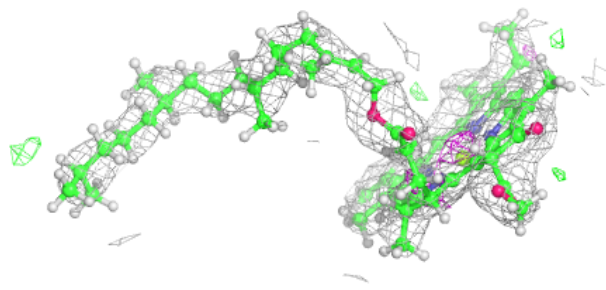
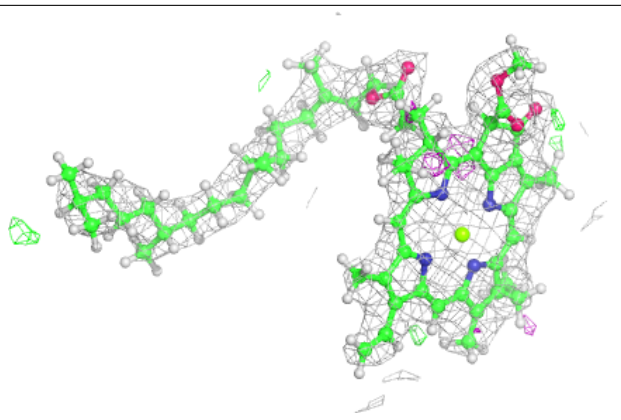
Electron density around CLA C 510:

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

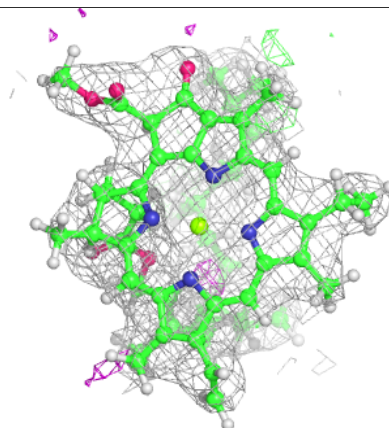
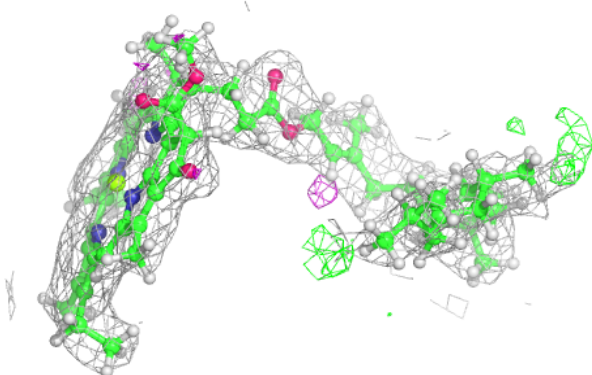
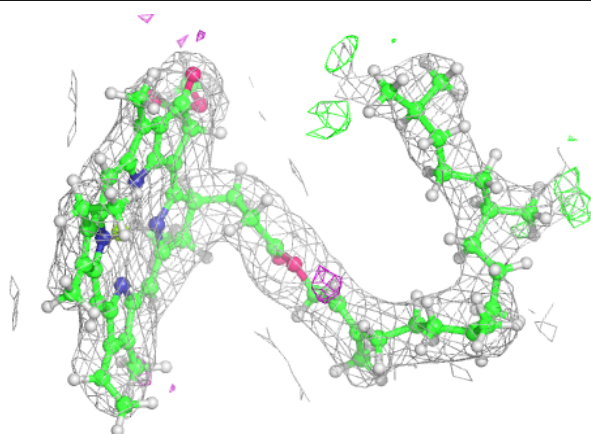


Electron density around CLA C 511:

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

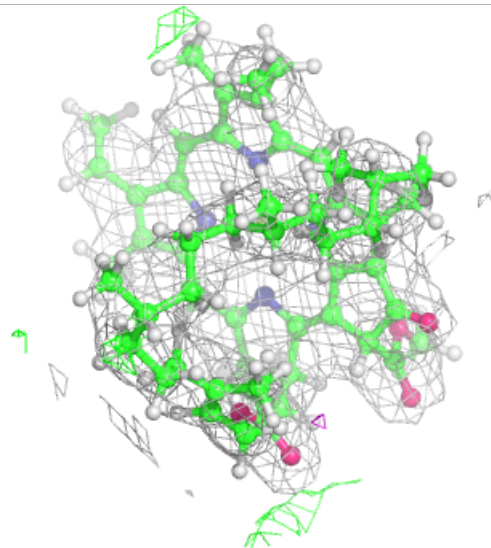
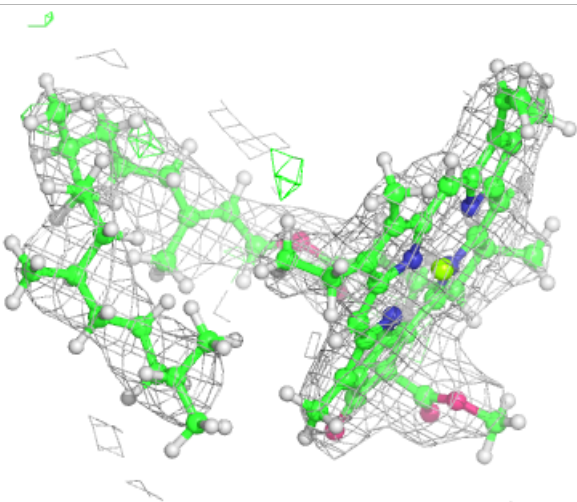
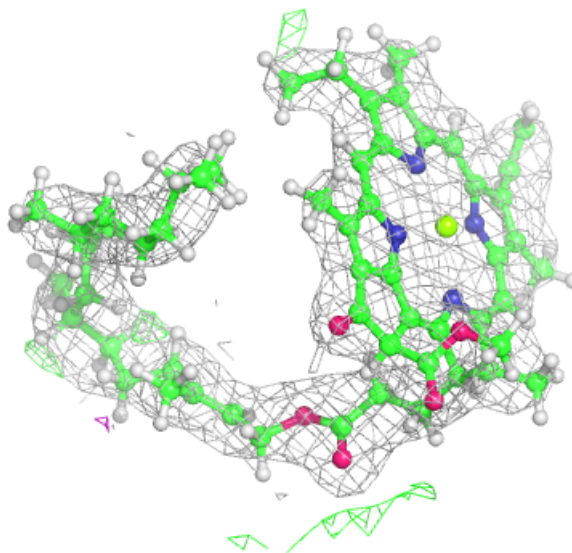
**Electron density around CLA B 605:**

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



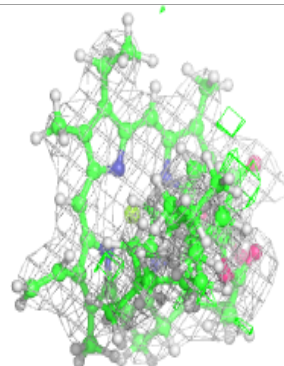
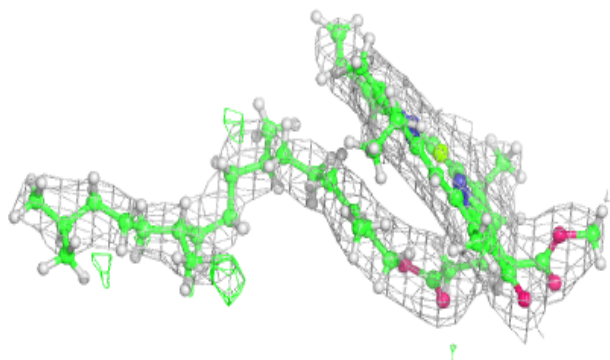
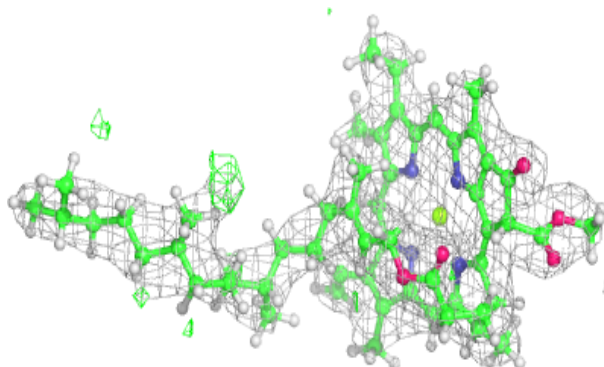
Electron density around CLA C 503:

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

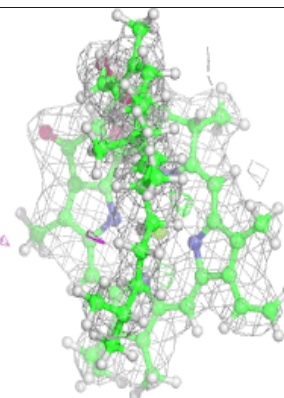
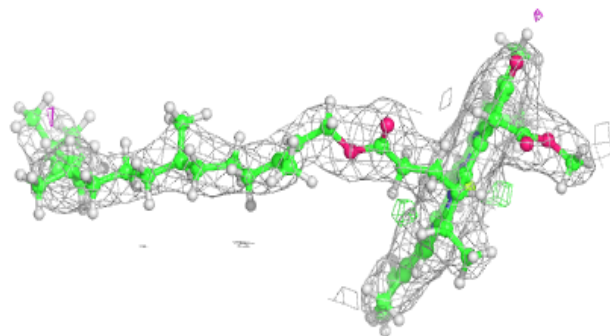
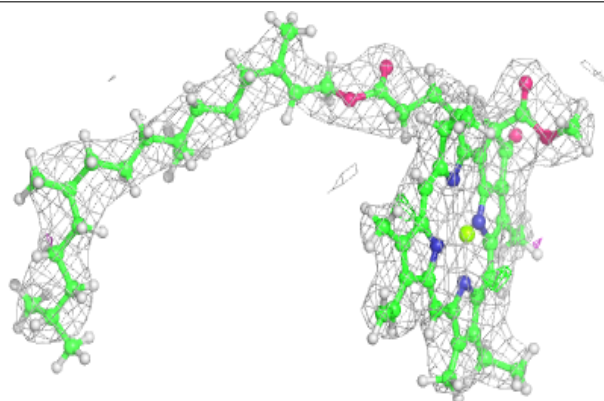


Electron density around CLA c 505:

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

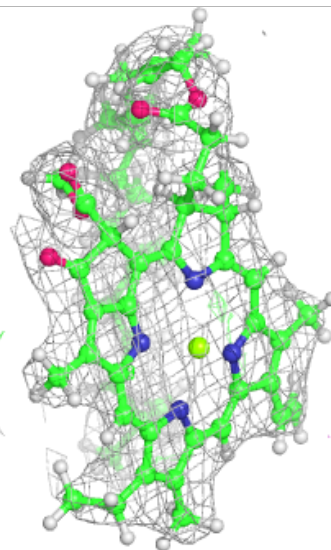
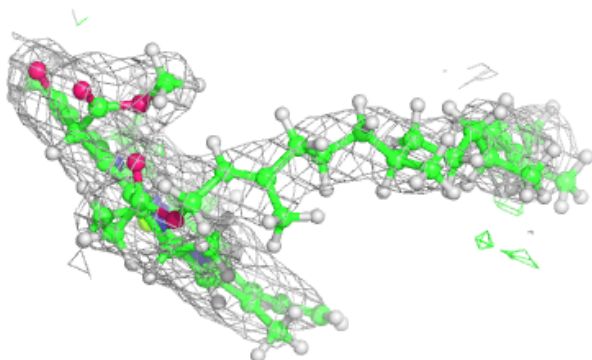
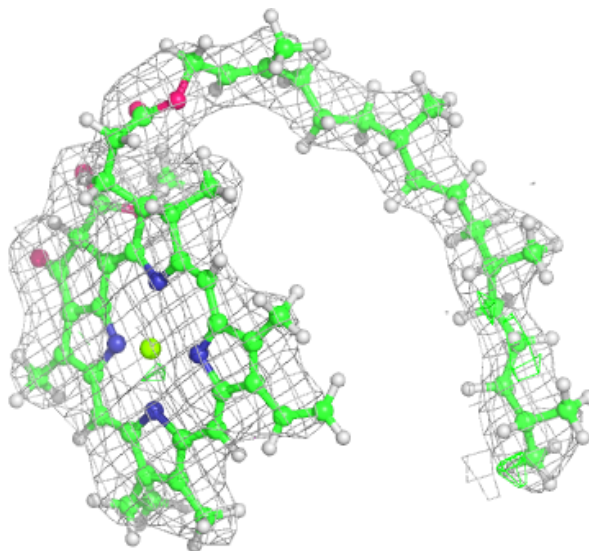
**Electron density around CLA B 608:**

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



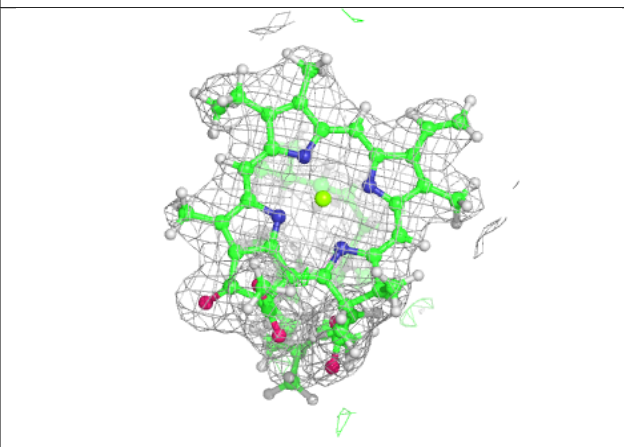
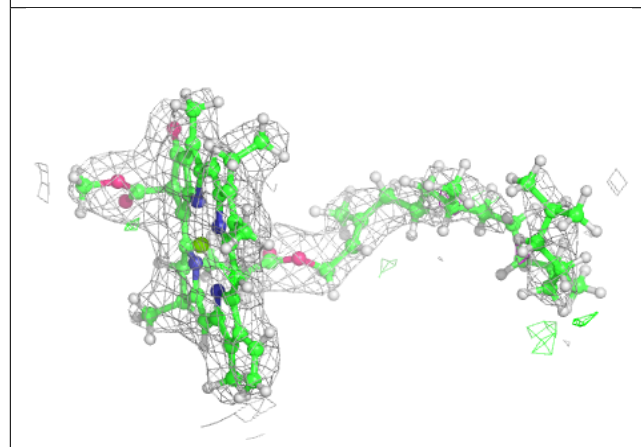
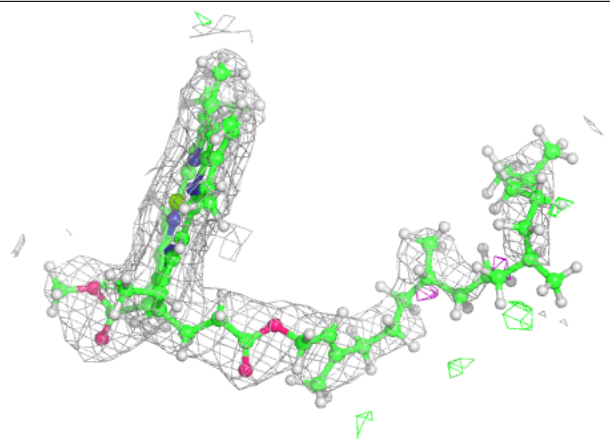
Electron density around CLA c 507:

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



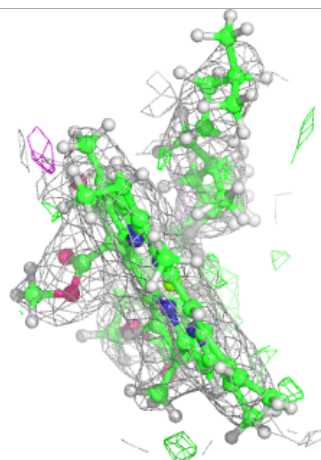
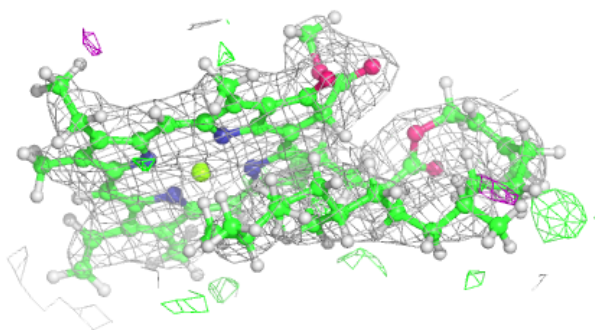
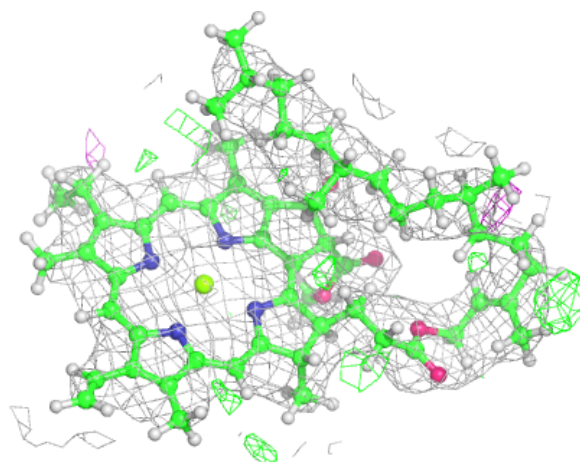
Electron density around CLA C 506:

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



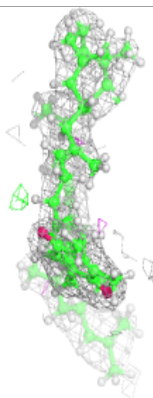
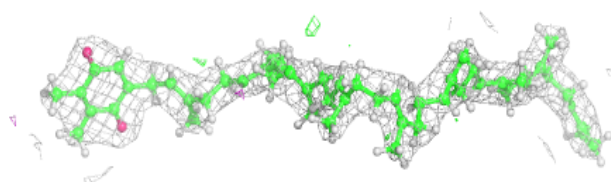
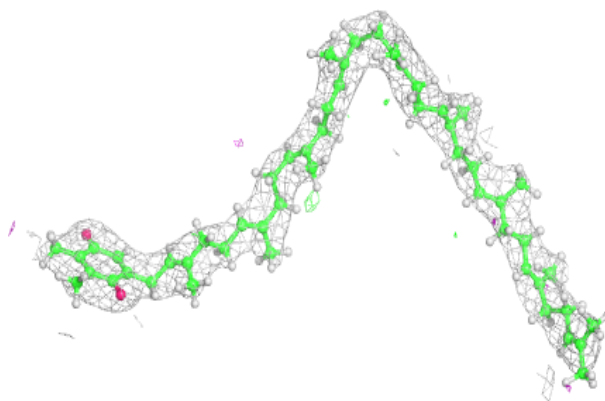
Electron density around CLA c 509:

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

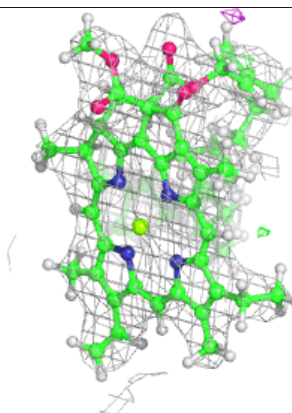
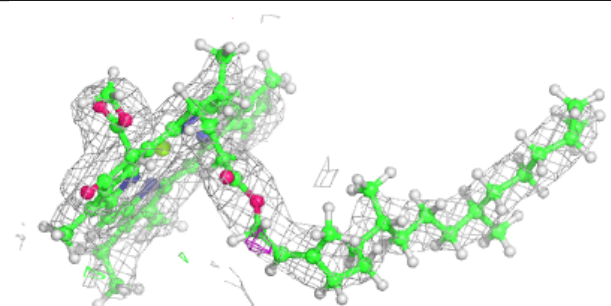
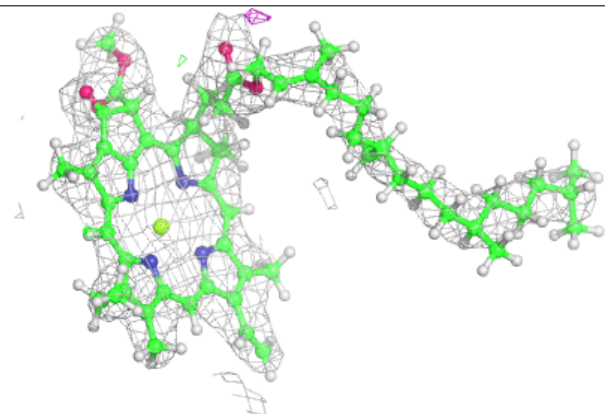


Electron density around PL9 D 406:

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

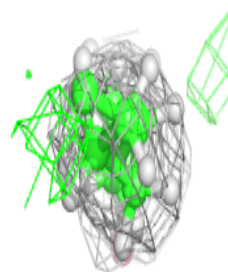
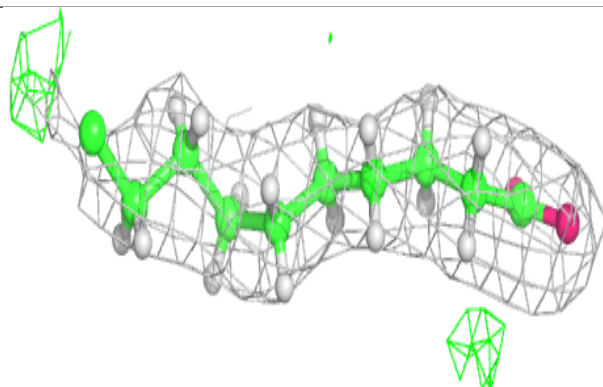
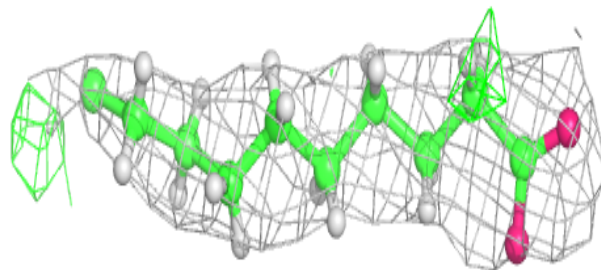
**Electron density around CLA c 511:**

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

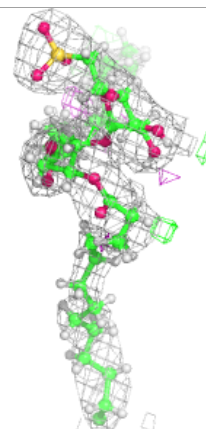
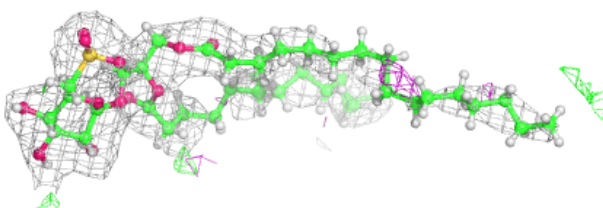
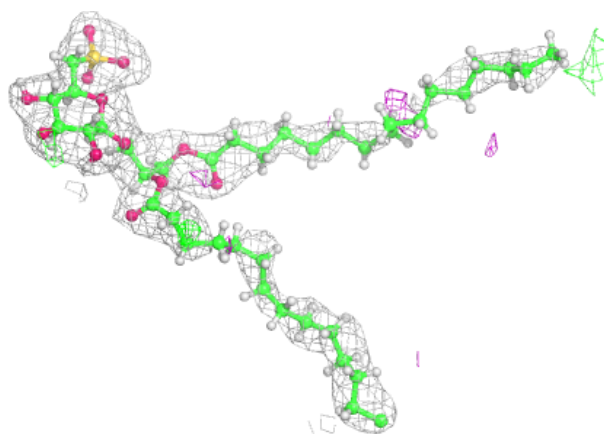


Electron density around STE J 101:

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

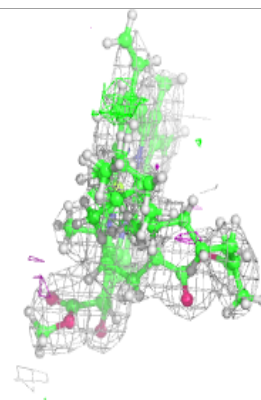
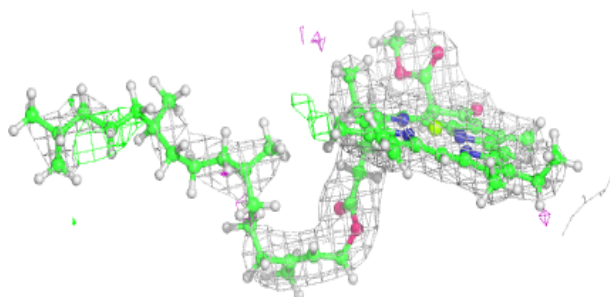
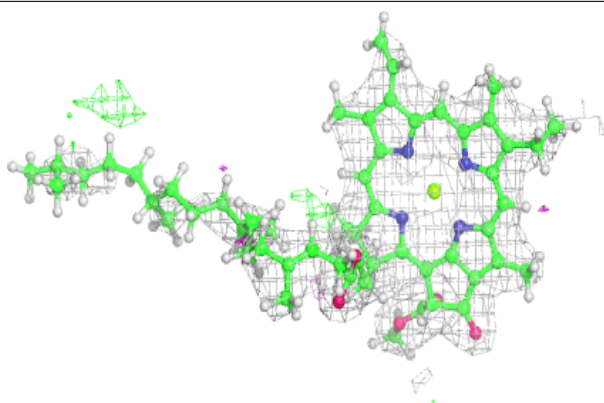
**Electron density around SQD A 613:**

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

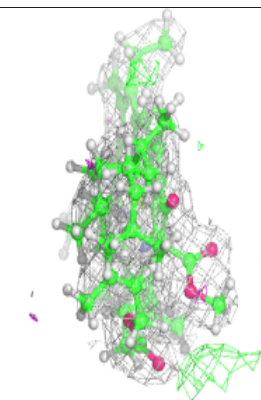
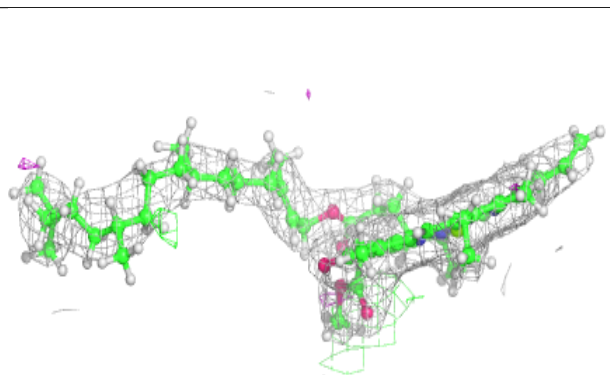
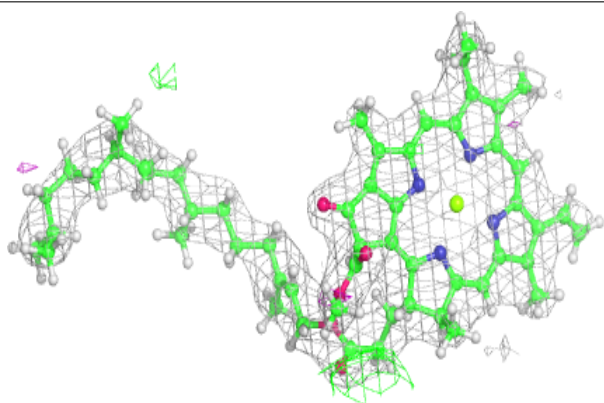


Electron density around CLA a 605:

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

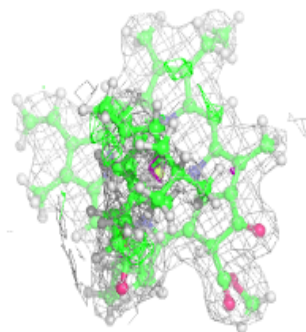
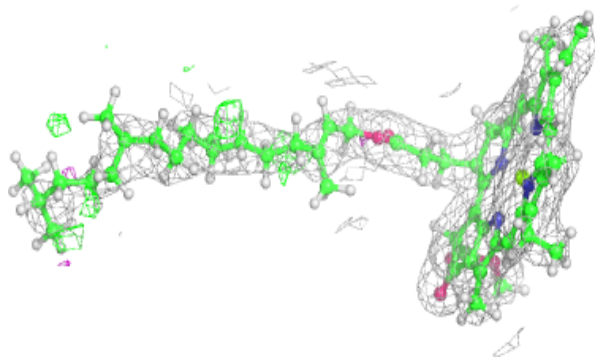
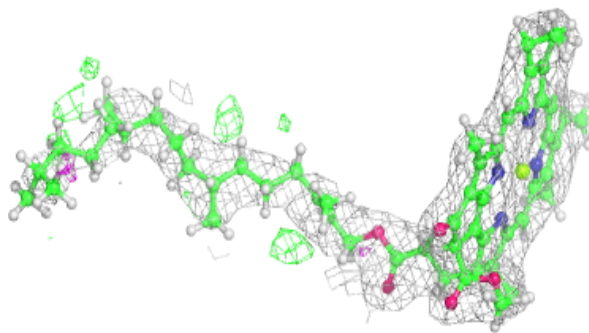
**Electron density around CLA B 601:**

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



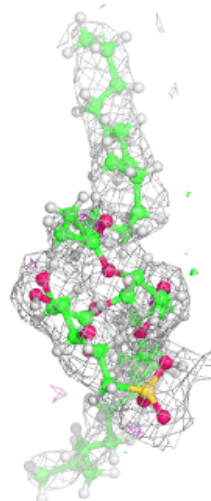
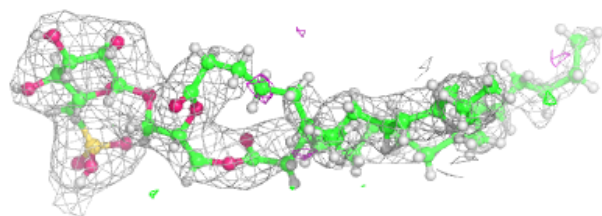
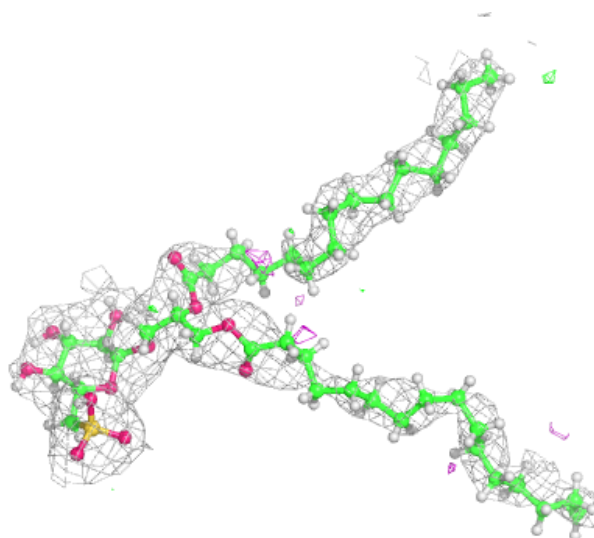
Electron density around CLA B 603:

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



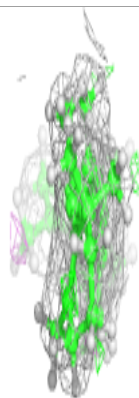
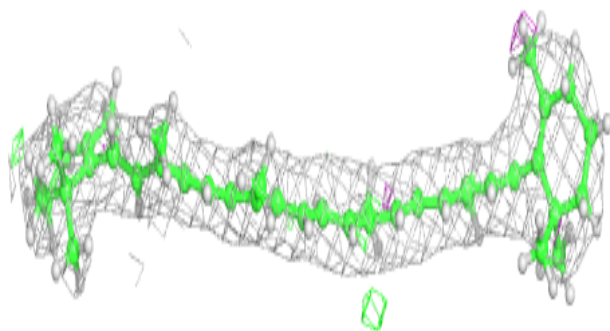
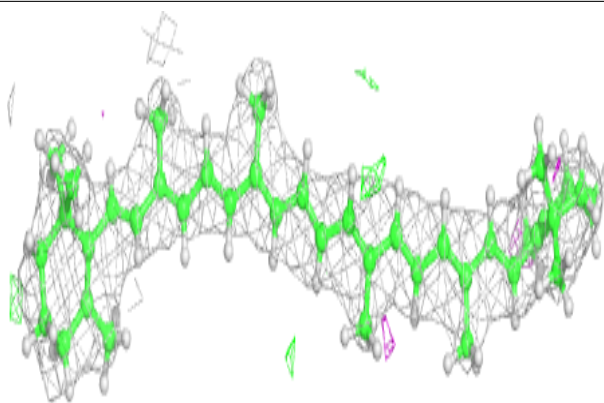
Electron density around SQD a 615:

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

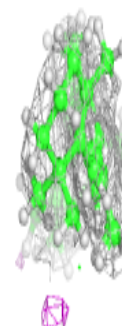
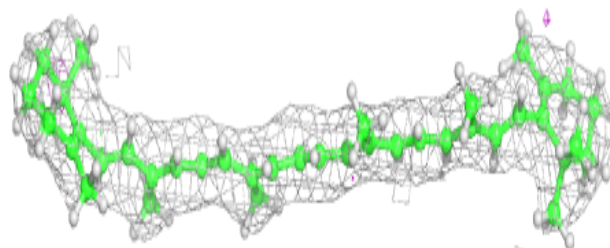
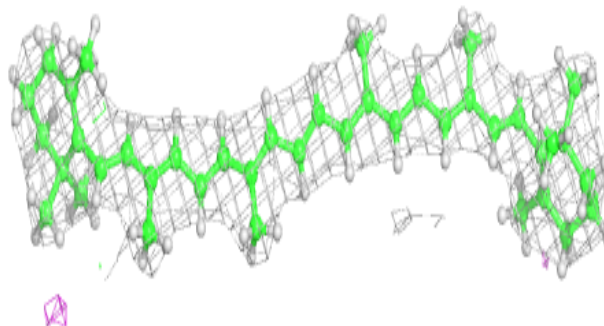


Electron density around BCR B 616:

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

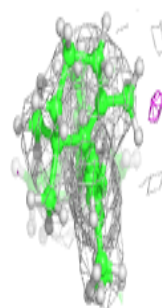
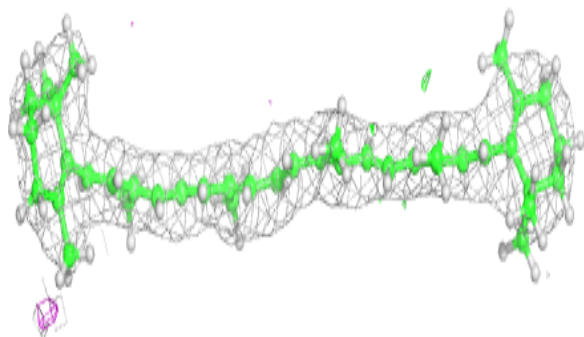
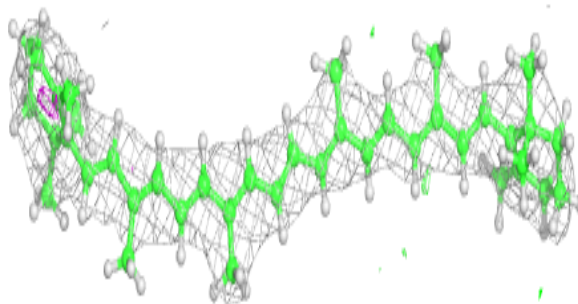
**Electron density around BCR B 618:**

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

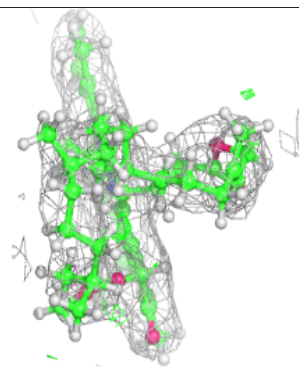
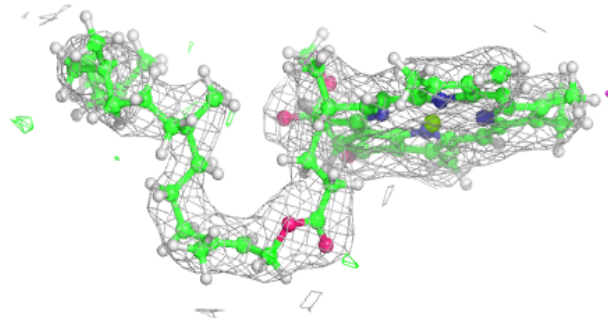
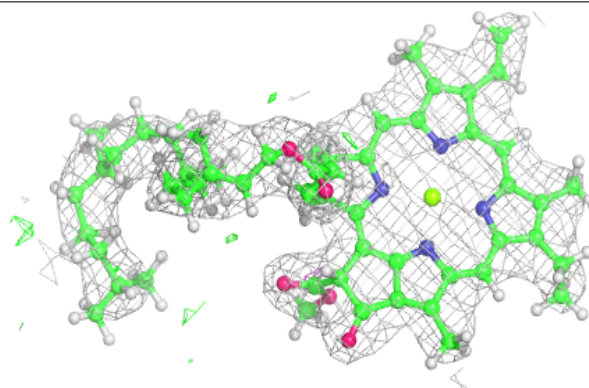


Electron density around BCR c 515:

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

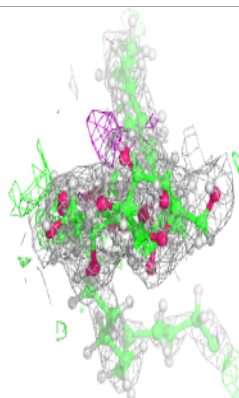
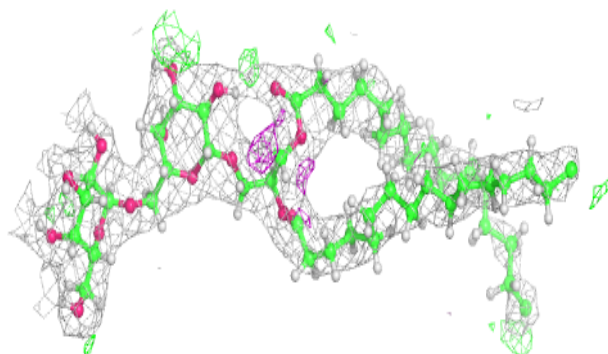
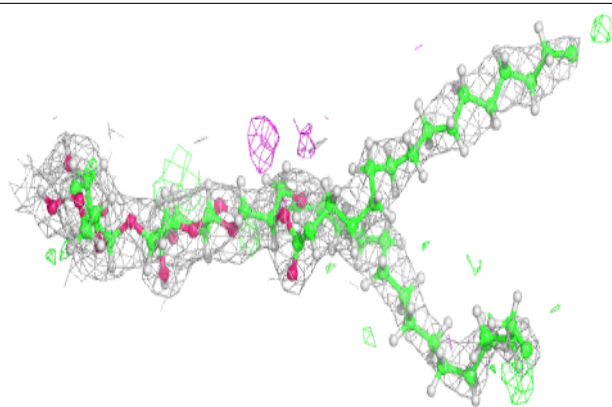
**Electron density around CLA b 612:**

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



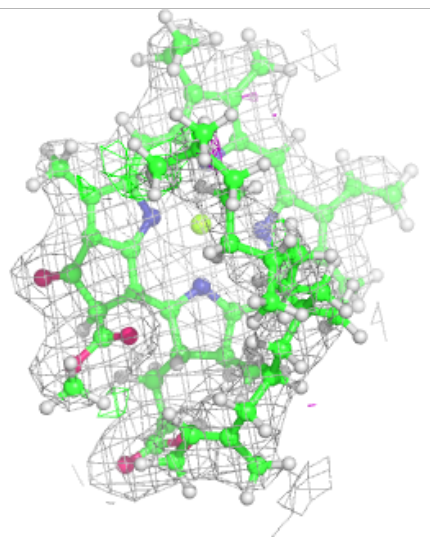
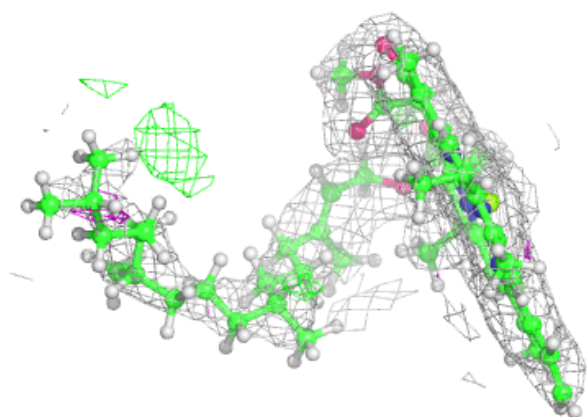
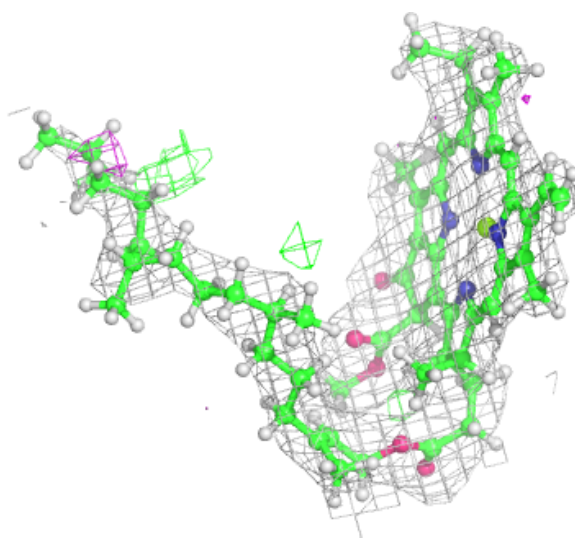
Electron density around DGD c 516:

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



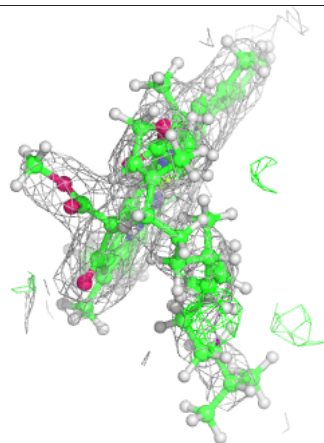
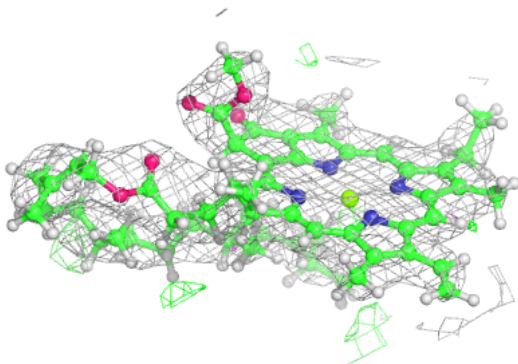
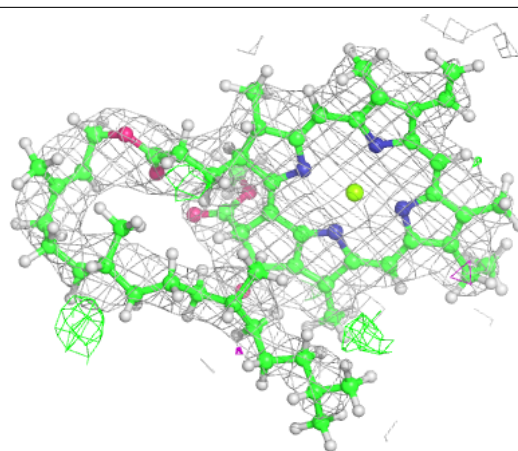
Electron density around CLA b 613:

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

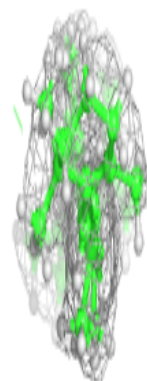
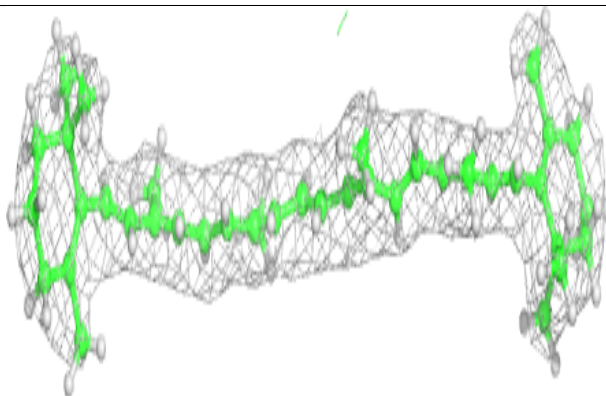
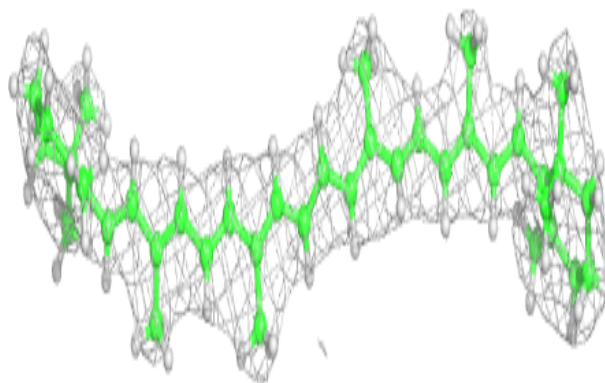


Electron density around CLA C 509:

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

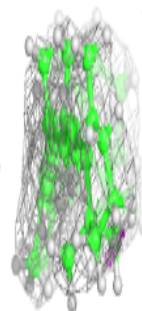
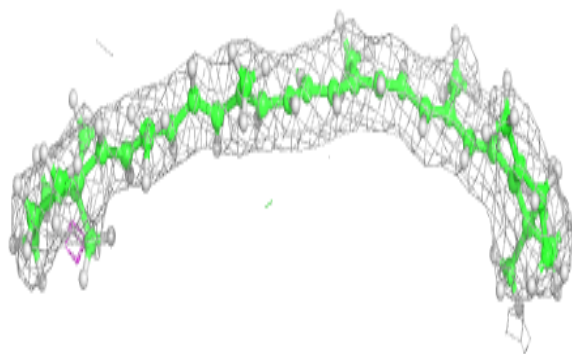
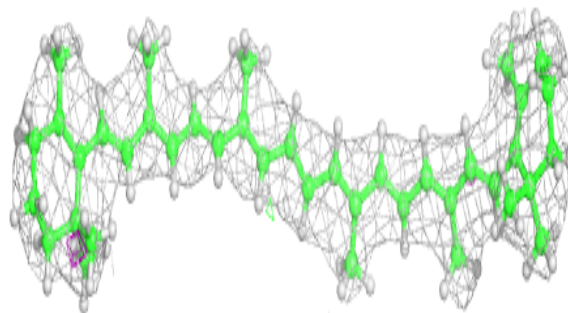
**Electron density around BCR A 608:**

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

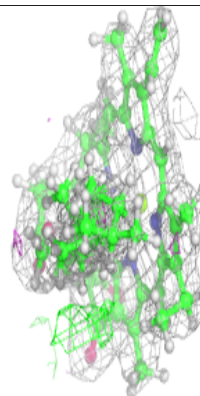
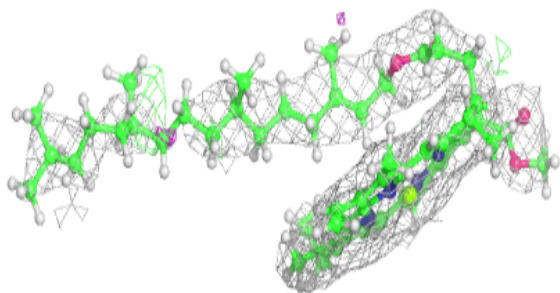
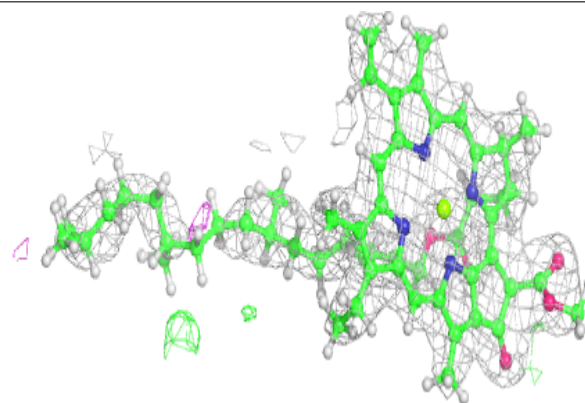


Electron density around BCR t 101:

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

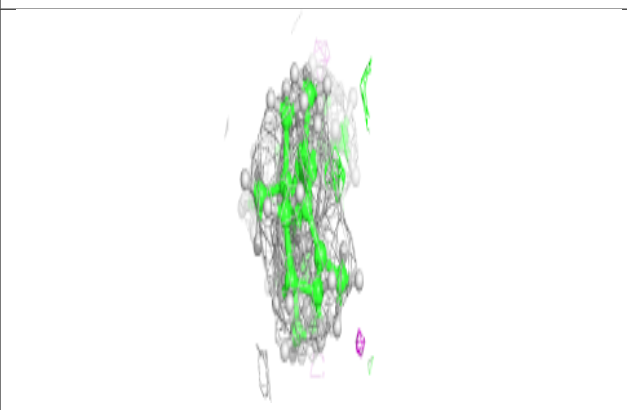
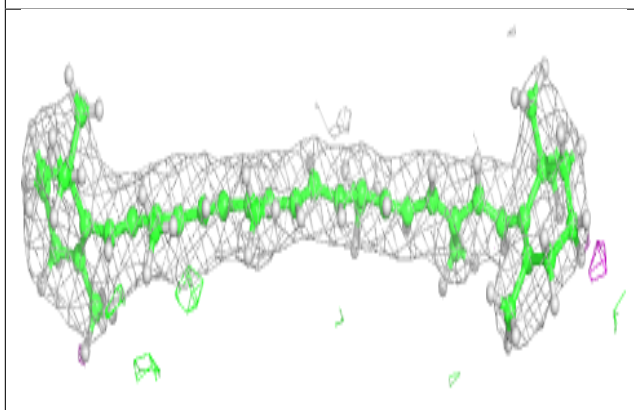
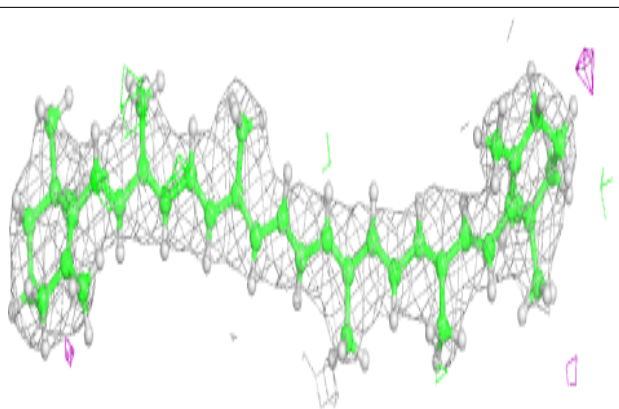
**Electron density around CLA B 613:**

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

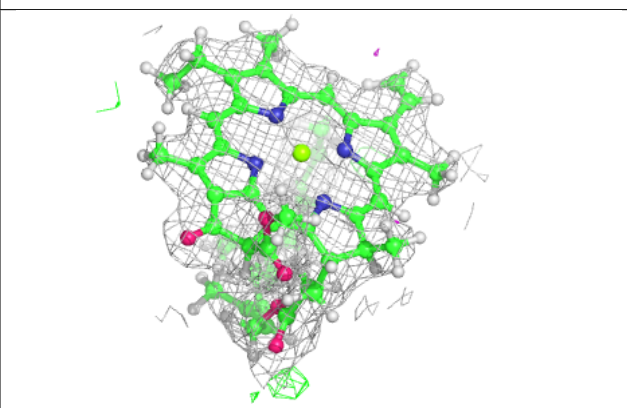
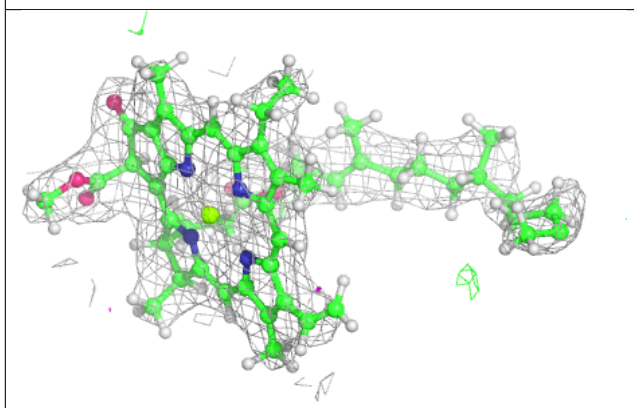
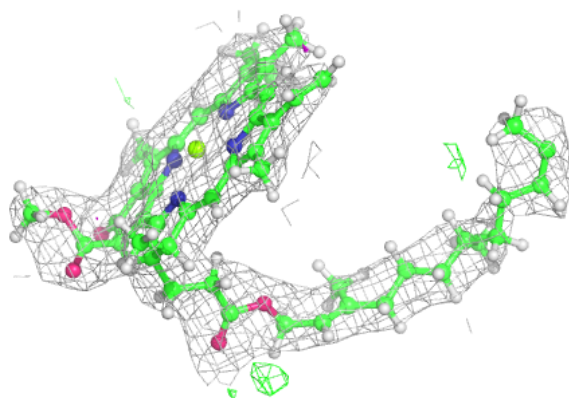


Electron density around BCR B 617:

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

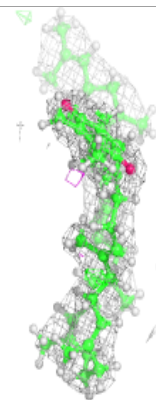
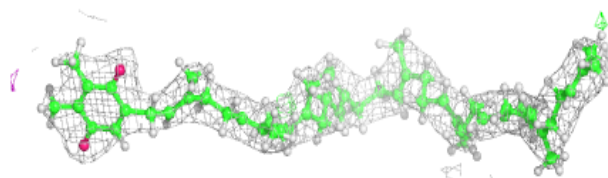
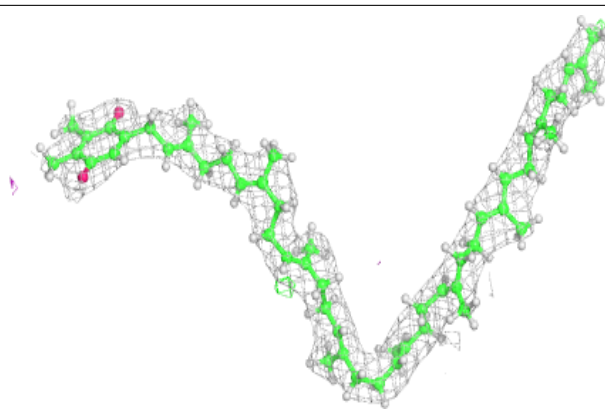
**Electron density around CLA C 504:**

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



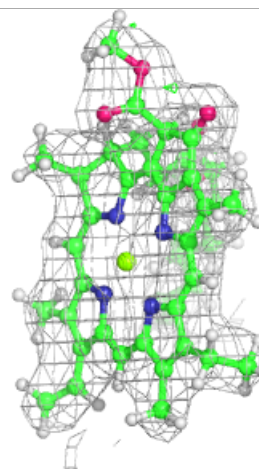
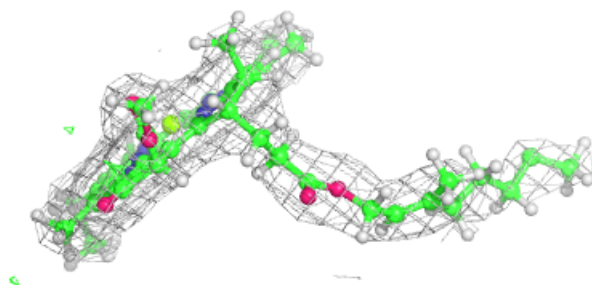
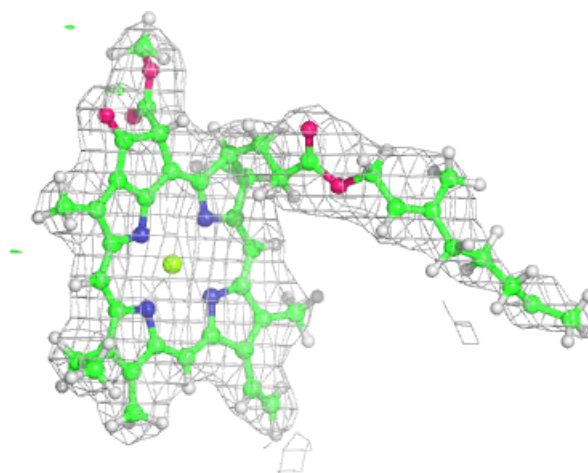
Electron density around PL9 d 405:

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



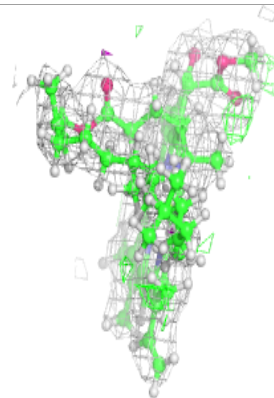
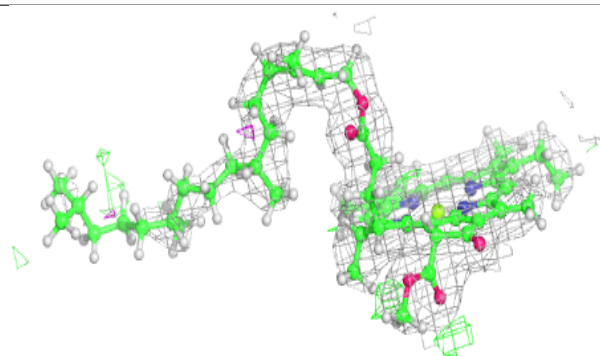
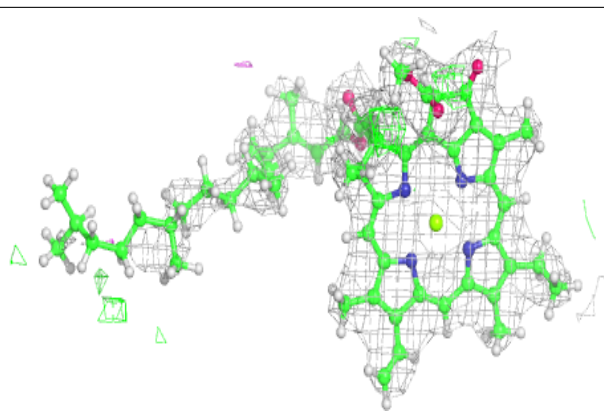
Electron density around CLA A 607:

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

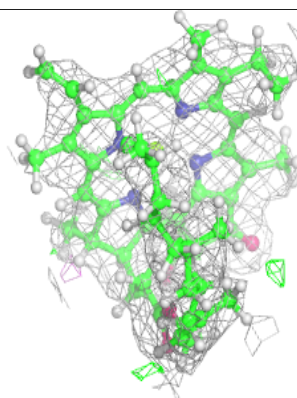
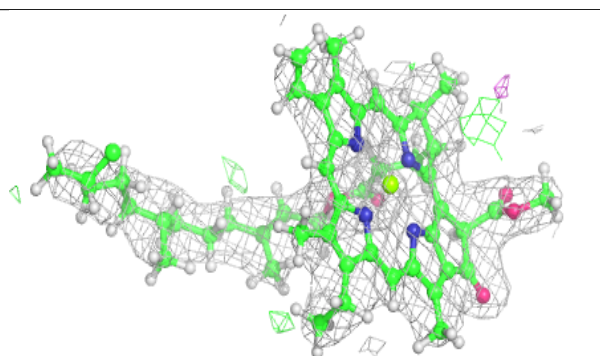
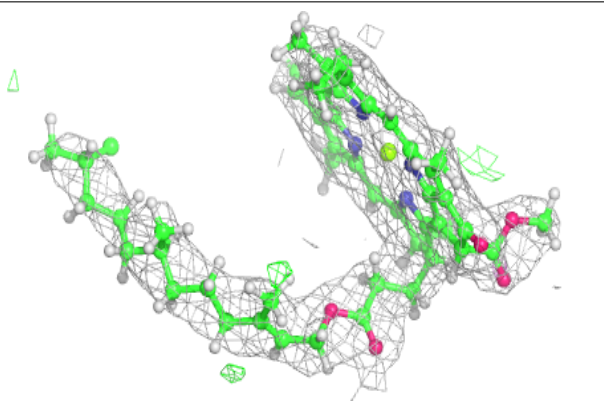


Electron density around CLA A 605:

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

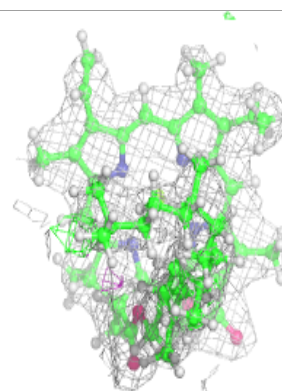
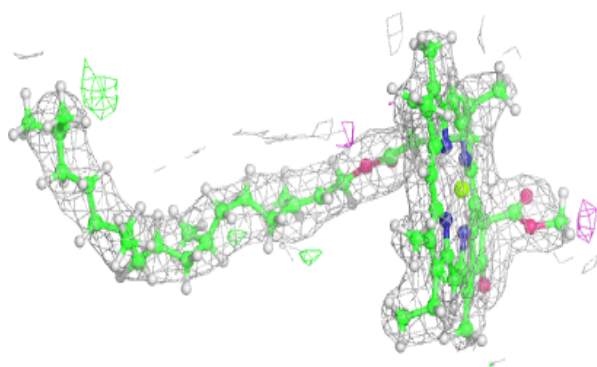
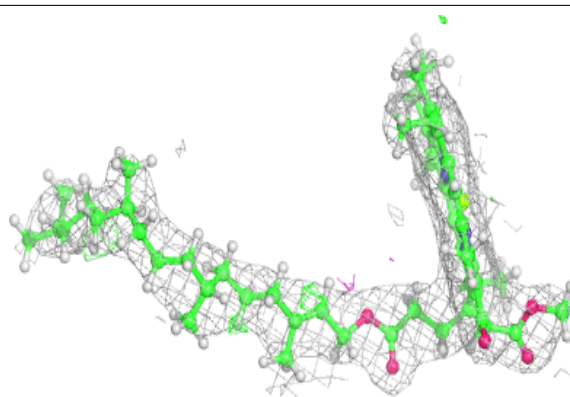
**Electron density around CLA c 504:**

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

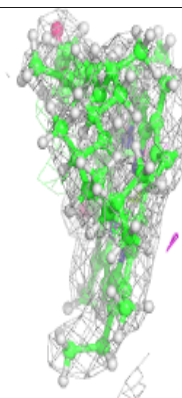
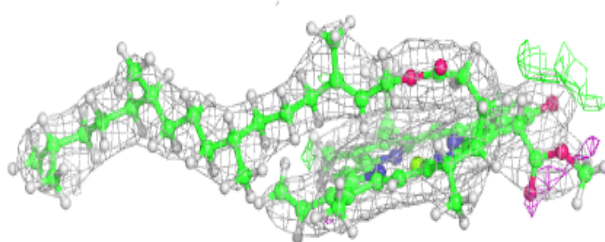
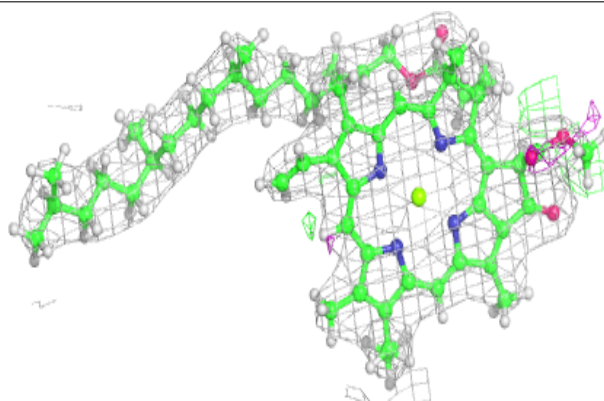


Electron density around CLA b 605:

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

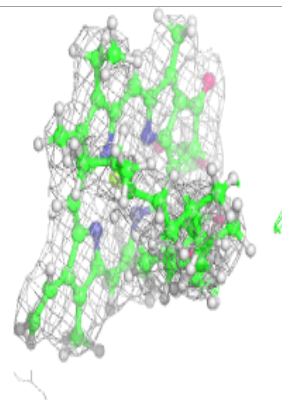
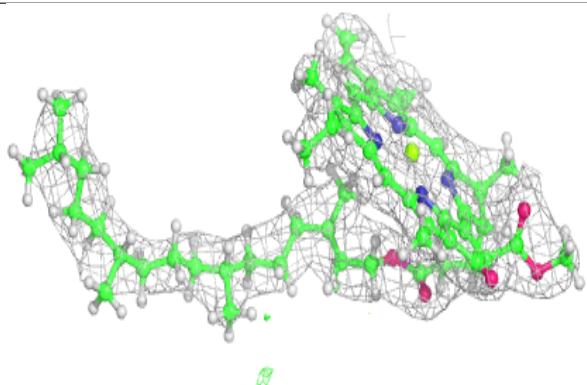
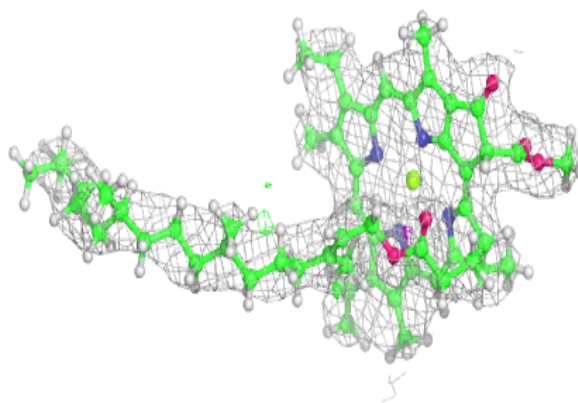
**Electron density around CLA C 501:**

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

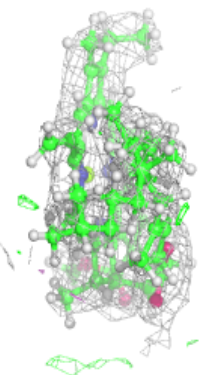
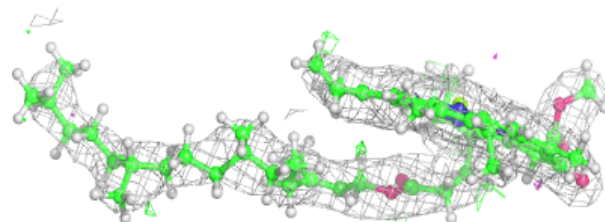
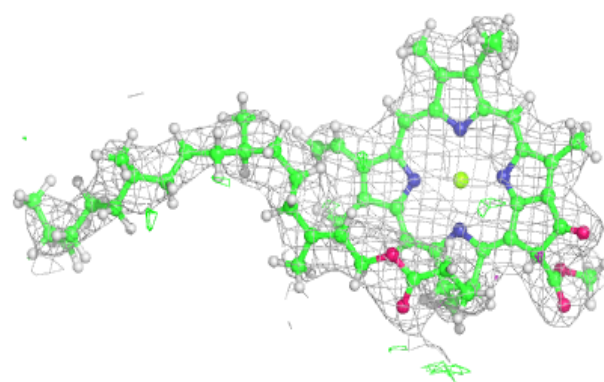


Electron density around CLA b 608:

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

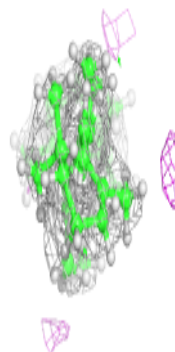
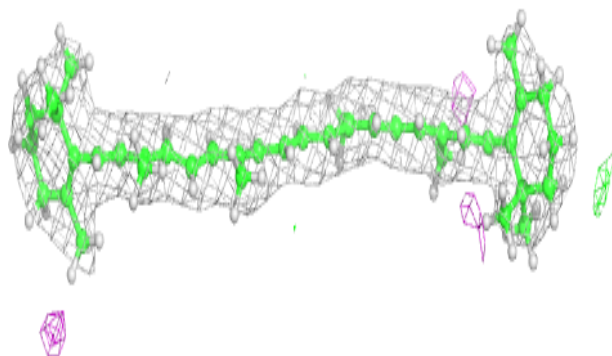
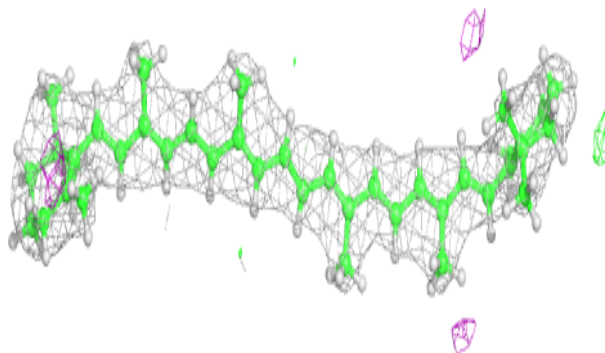
**Electron density around CLA B 602:**

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



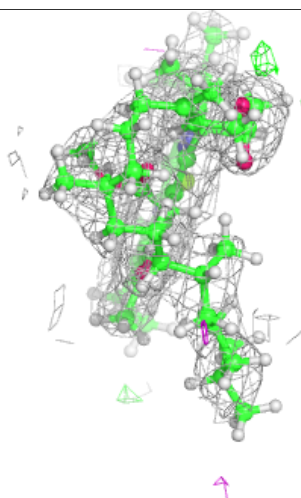
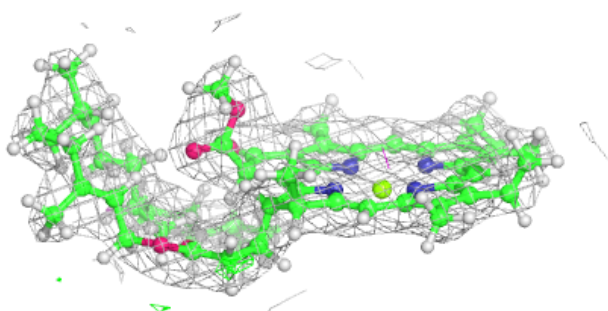
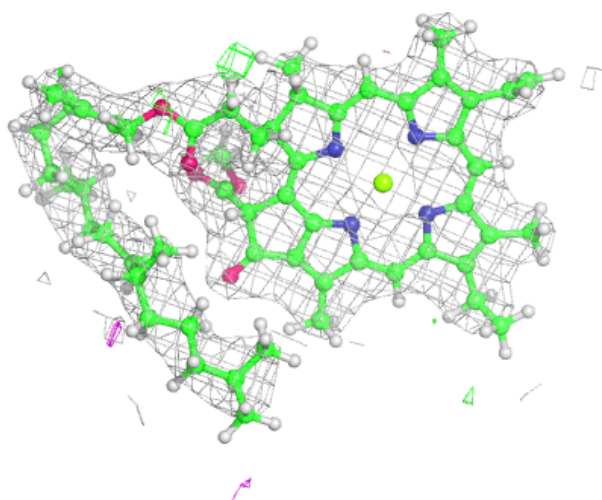
Electron density around BCR a 608:

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



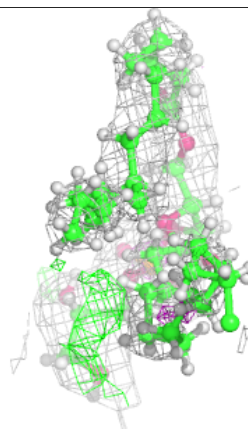
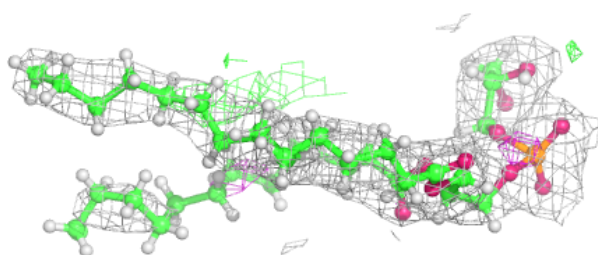
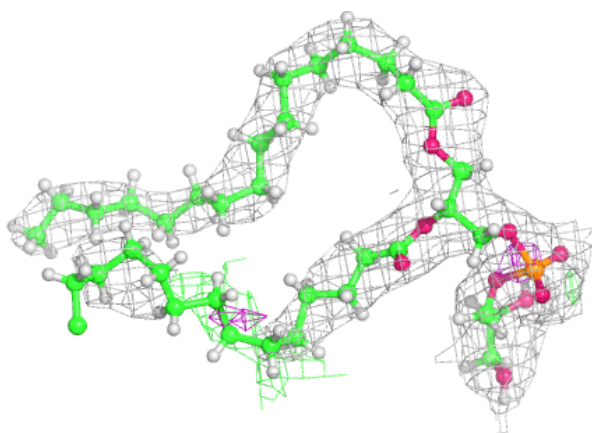
Electron density around CLA b 610:

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

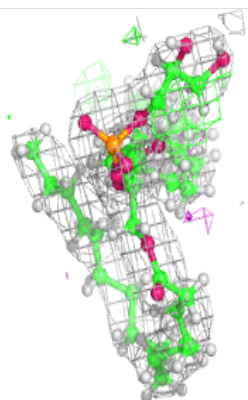
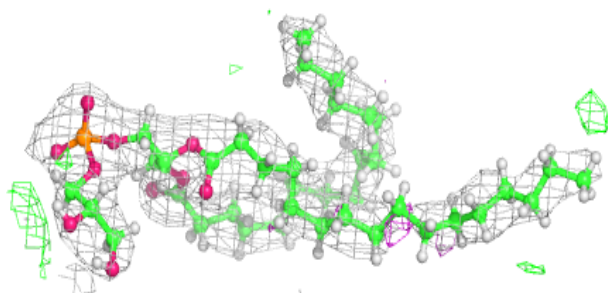
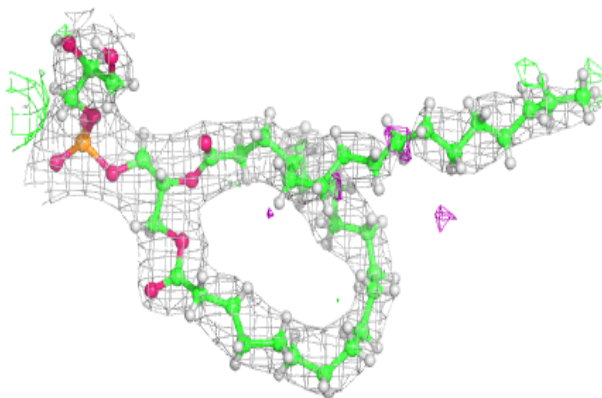


Electron density around LHG D 410:

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

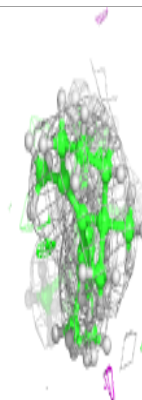
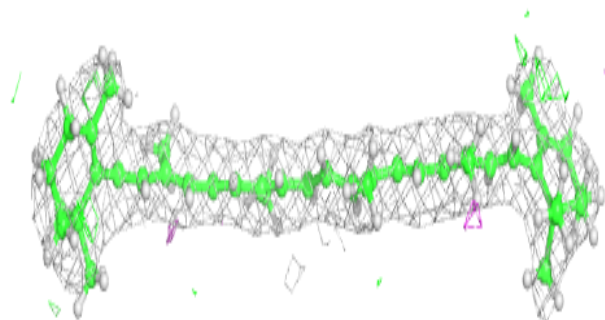
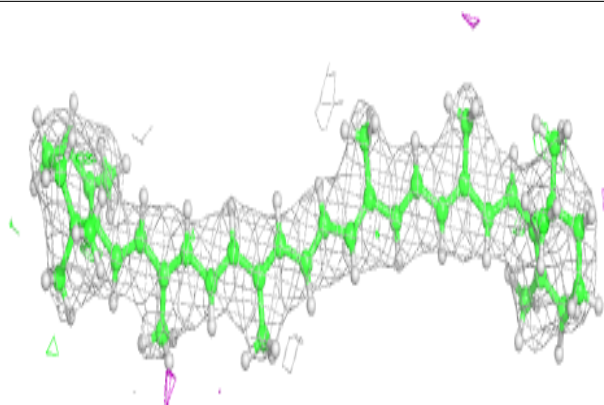
**Electron density around LHG a 614:**

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



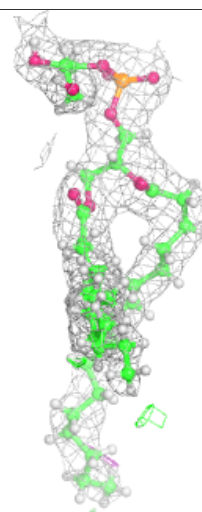
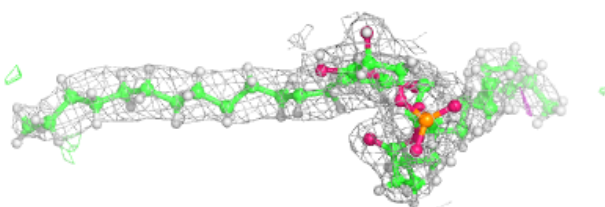
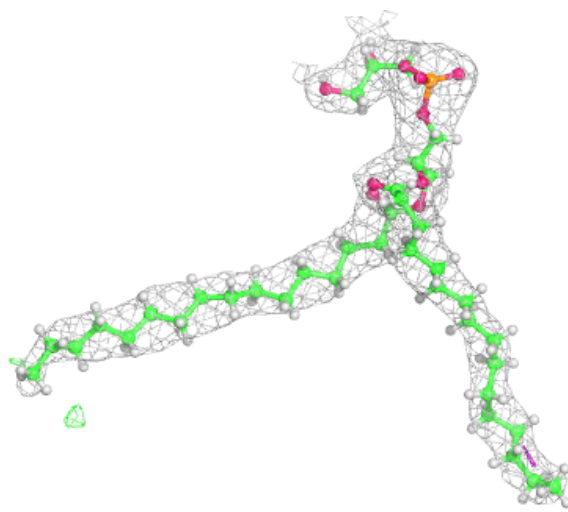
Electron density around BCR b 618:

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



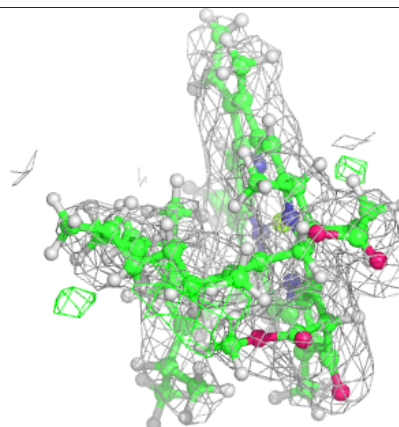
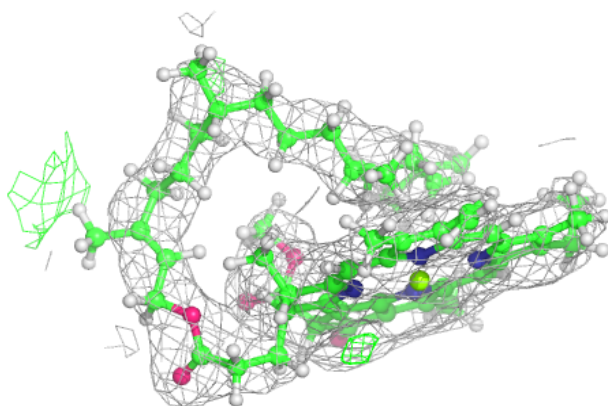
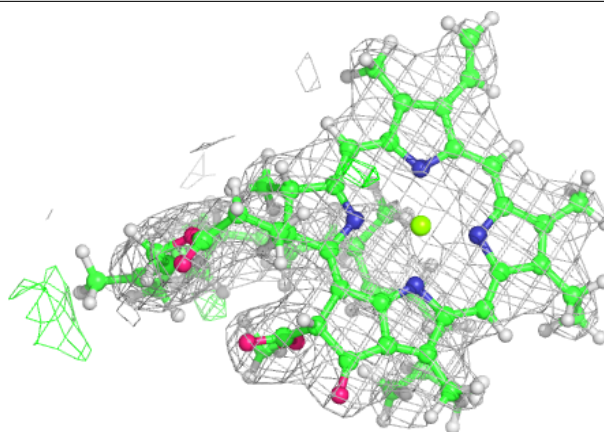
Electron density around LHG 1 101:

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

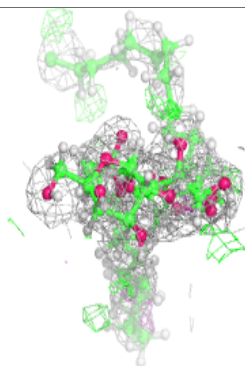
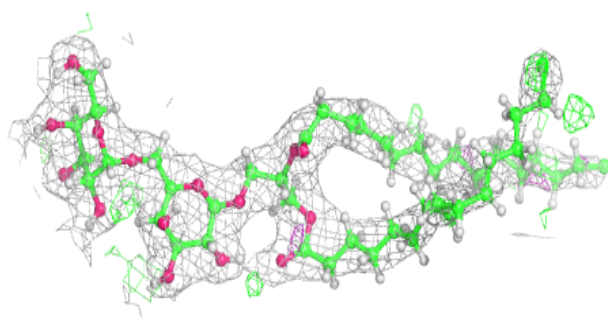
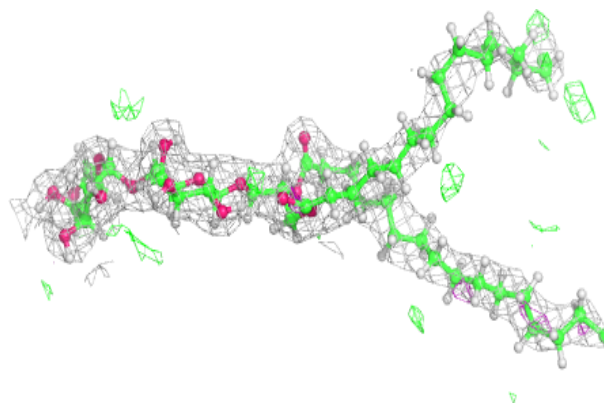


Electron density around CLA c 510:

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

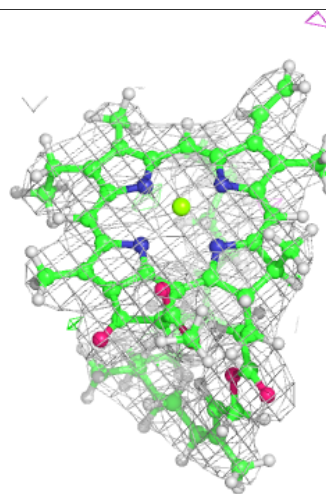
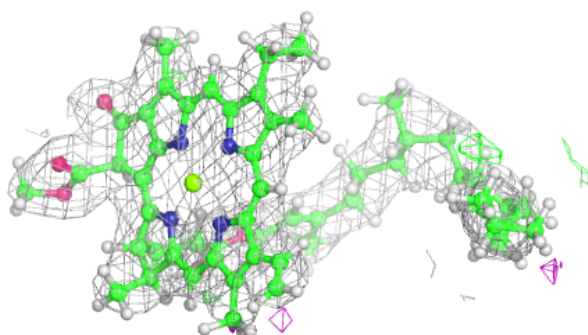
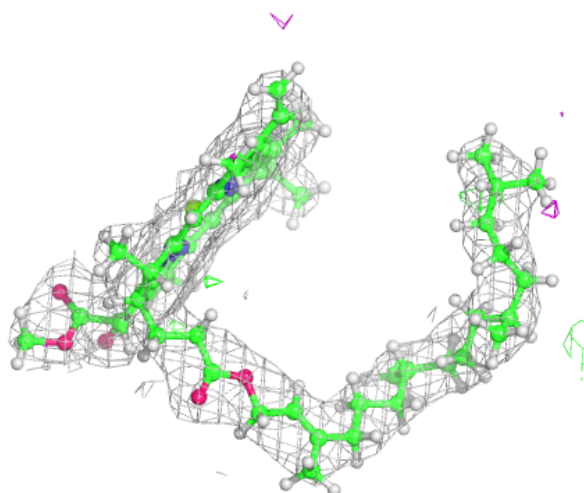
**Electron density around DGD C 516:**

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



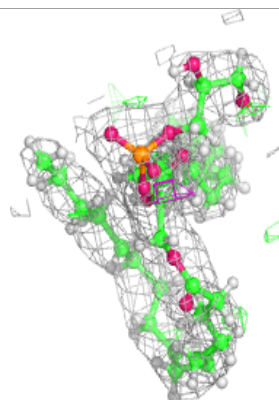
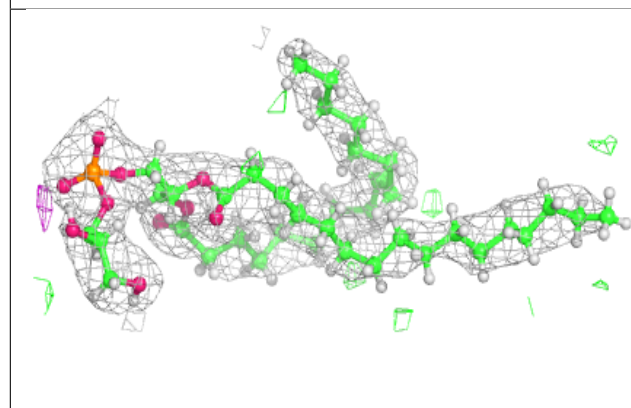
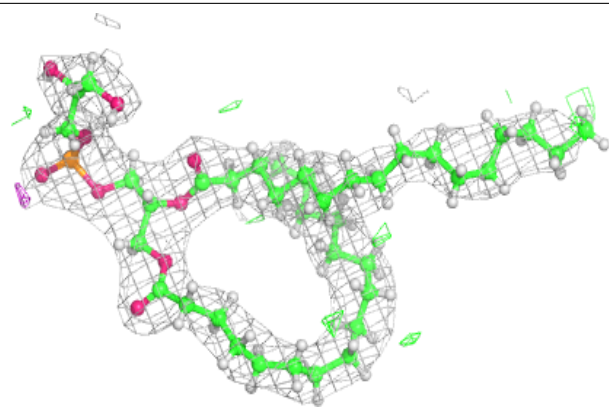
Electron density around CLA b 611:

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



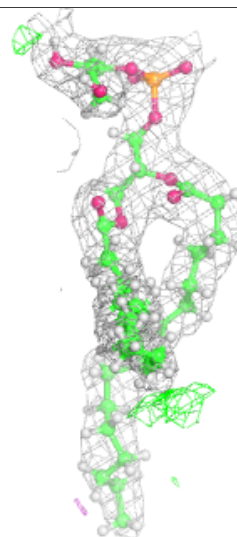
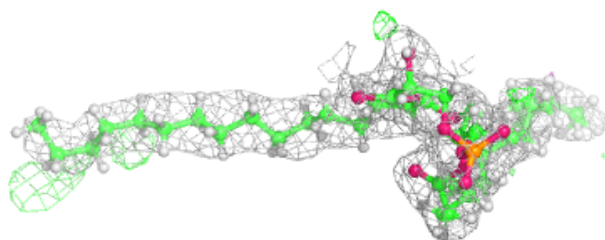
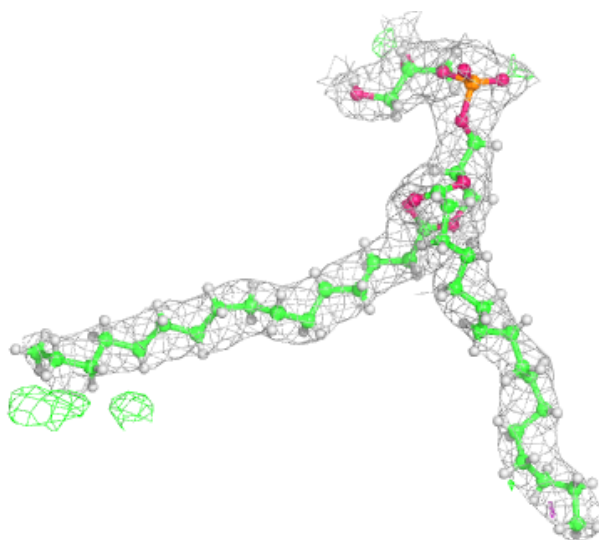
Electron density around LHG D 413:

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



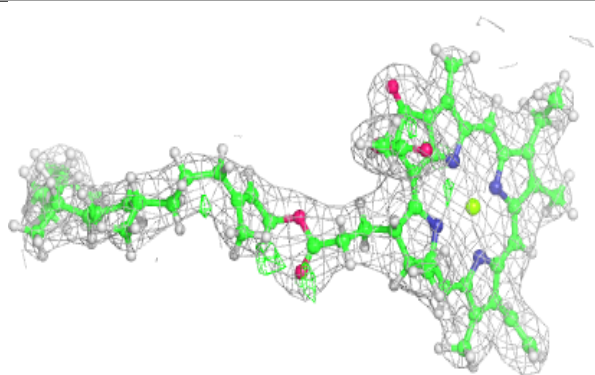
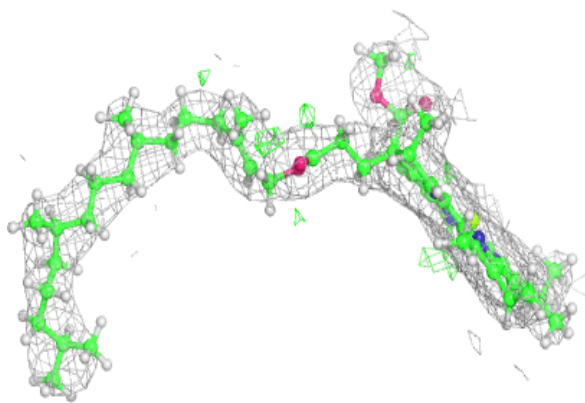
Electron density around LHG L 101:

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

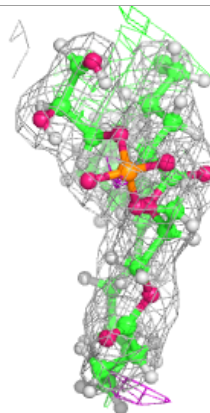
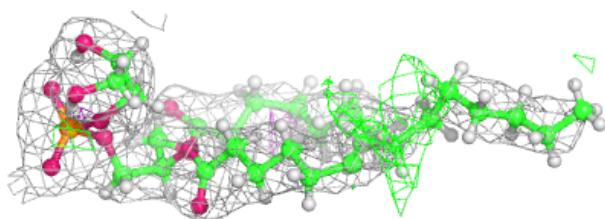
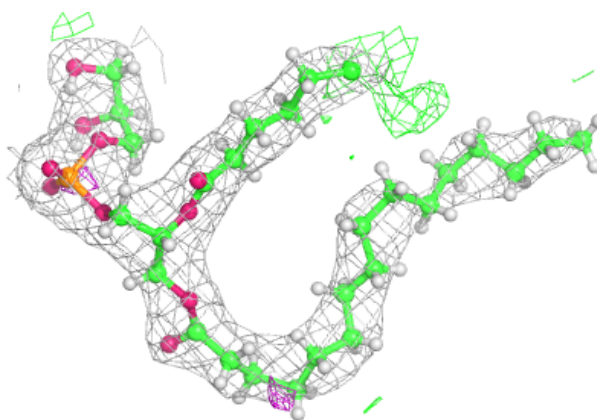


Electron density around CLA D 403:

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

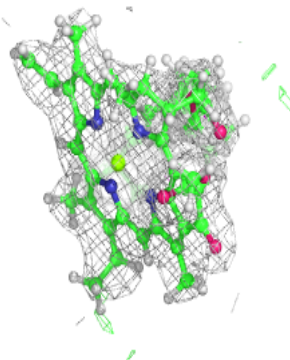
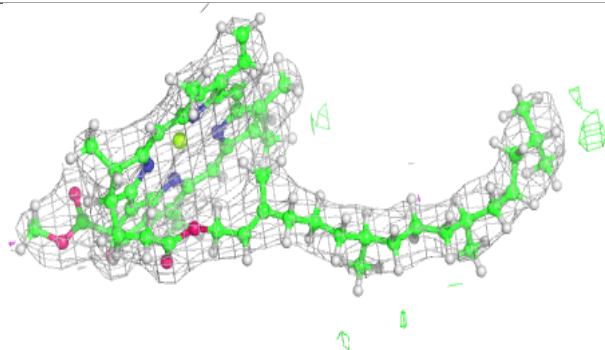
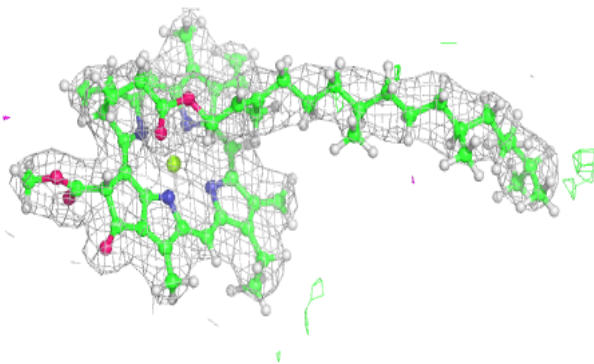
**Electron density around LHG d 407:**

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

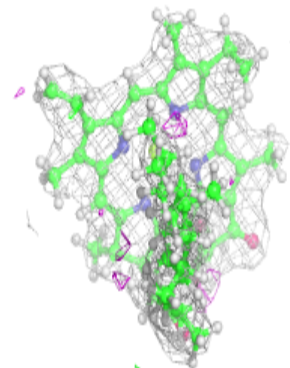
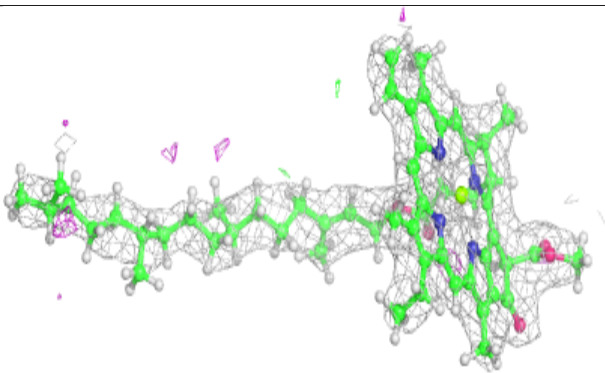
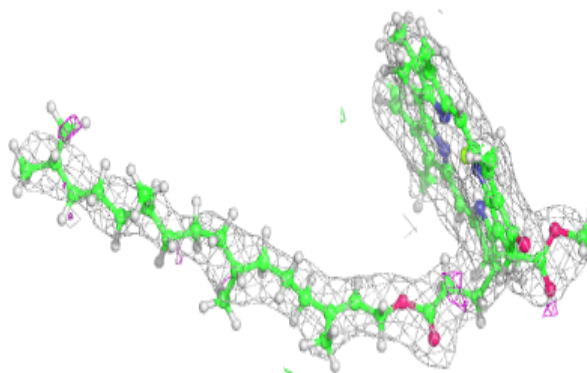


Electron density around CLA B 607:

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

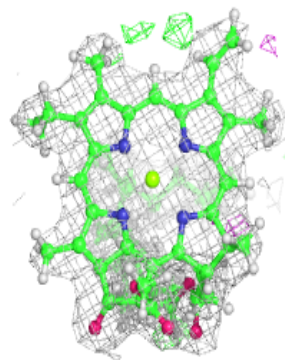
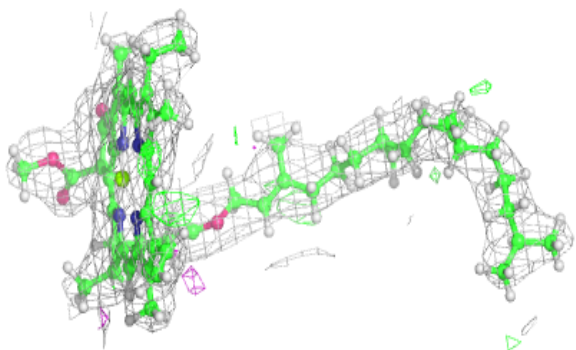
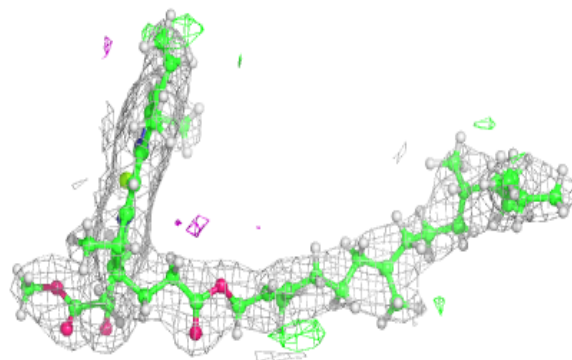
**Electron density around CLA b 607:**

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

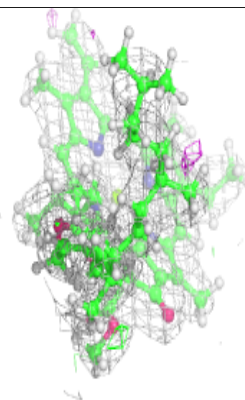
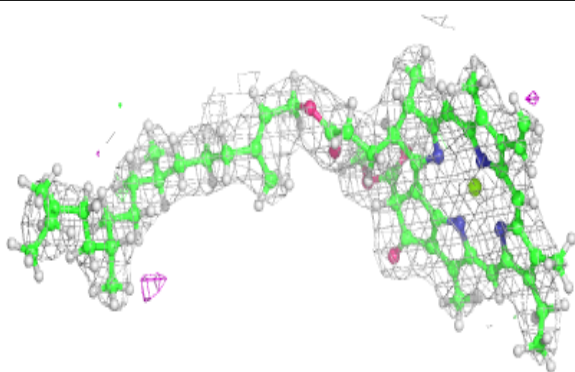
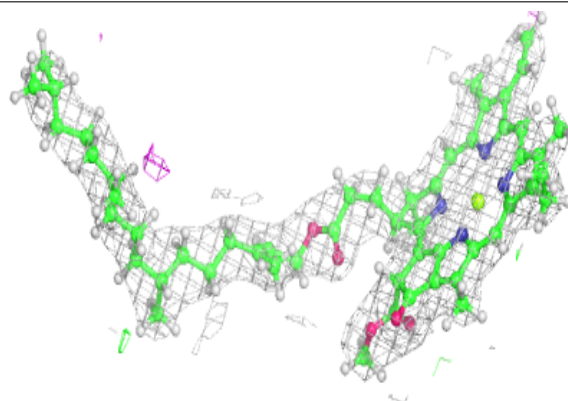


Electron density around CLA B 604:

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

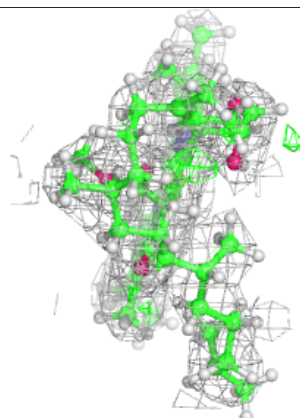
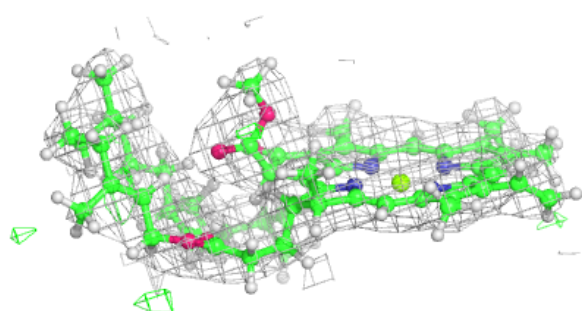
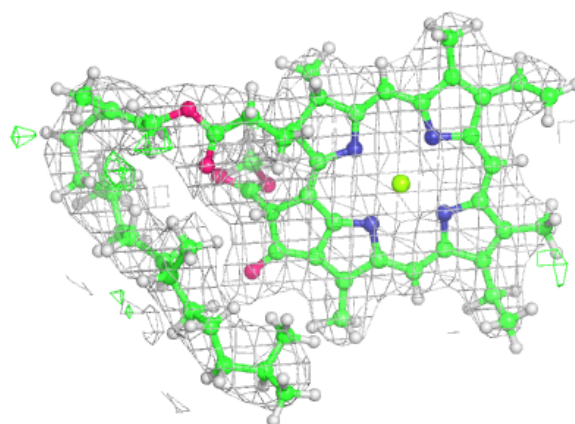
**Electron density around CLA a 604:**

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



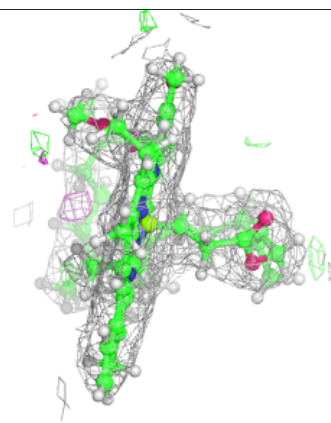
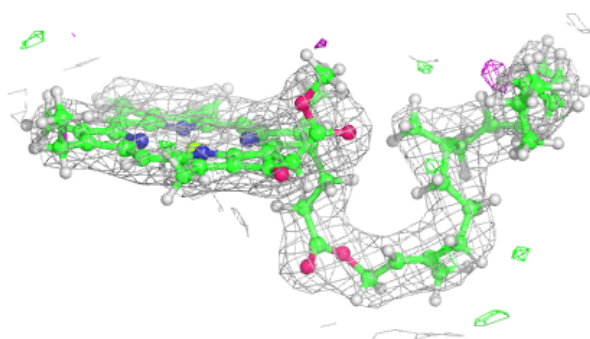
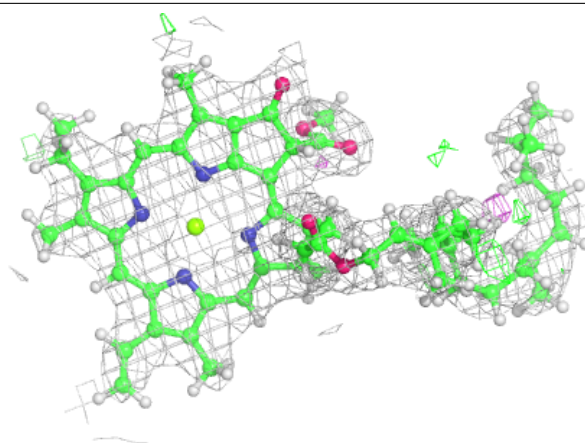
Electron density around CLA B 609:

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

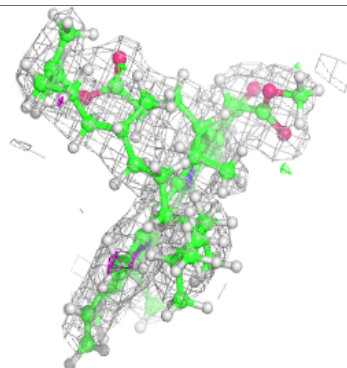
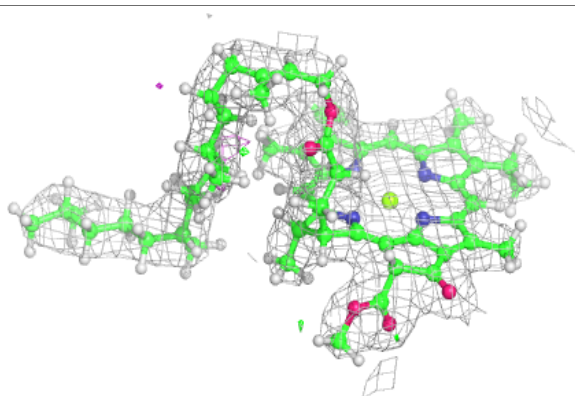
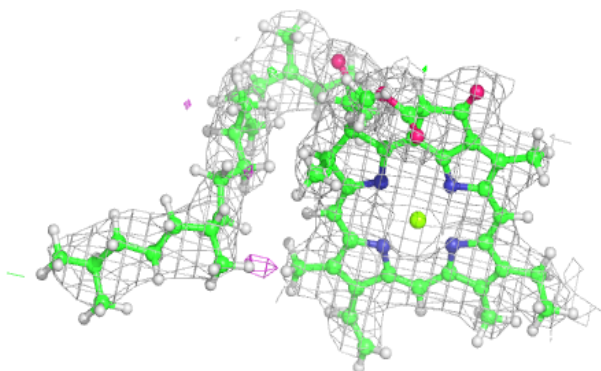


Electron density around CLA B 611:

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

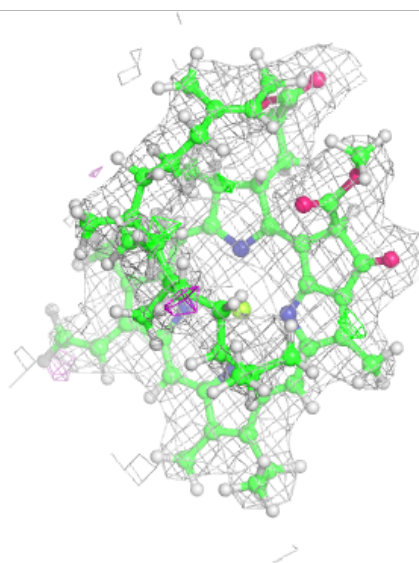
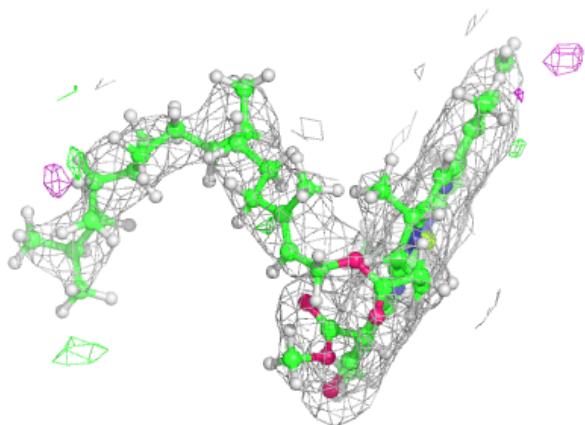
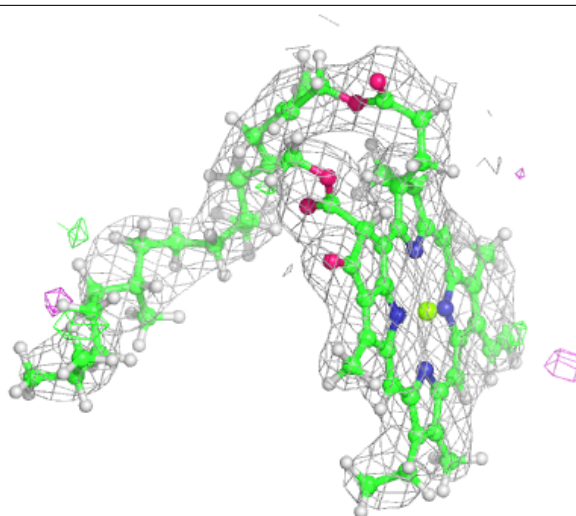
**Electron density around CLA a 613:**

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



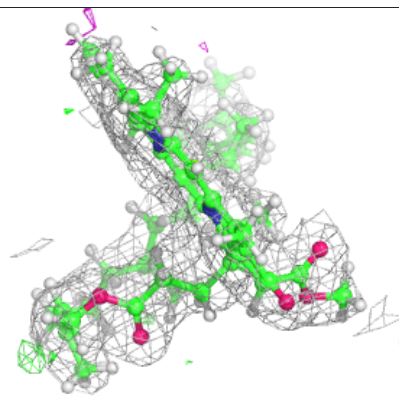
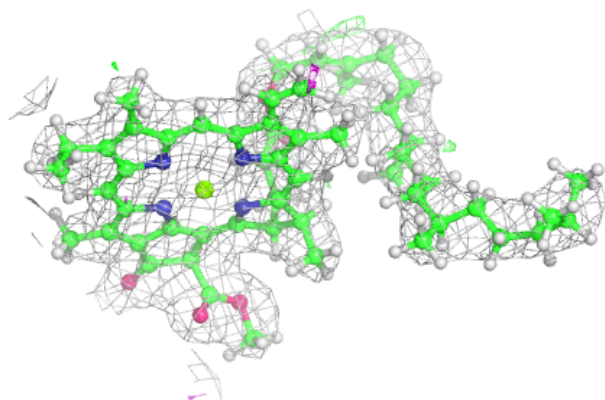
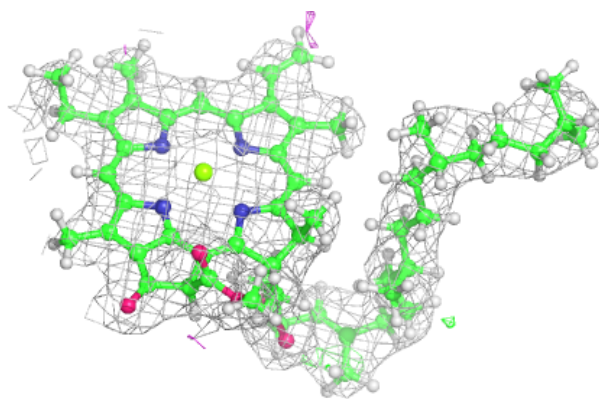
Electron density around CLA B 612:

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

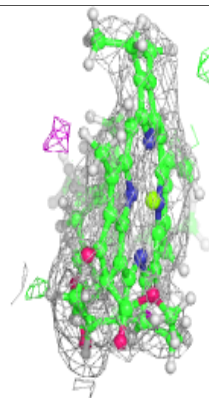
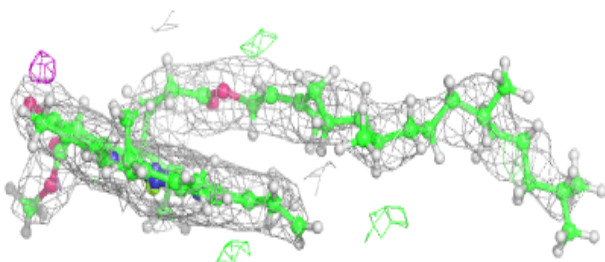
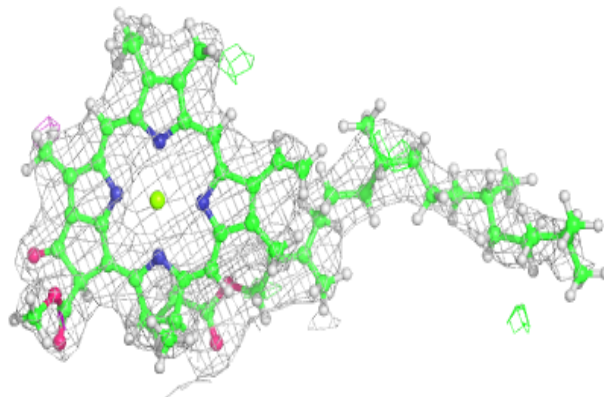


Electron density around CLA A 612:

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

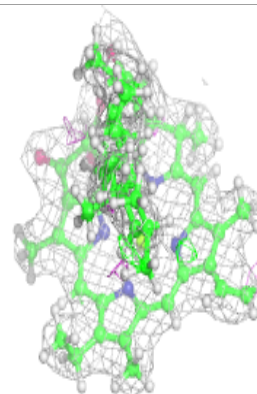
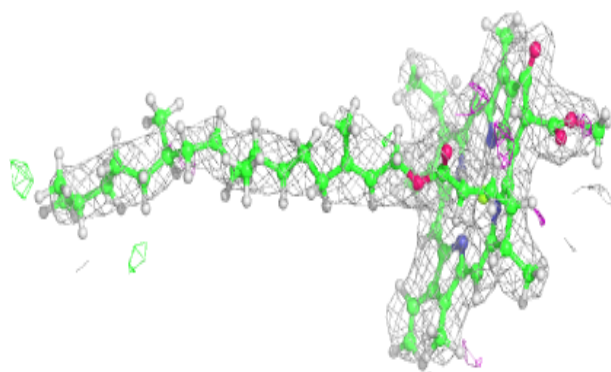
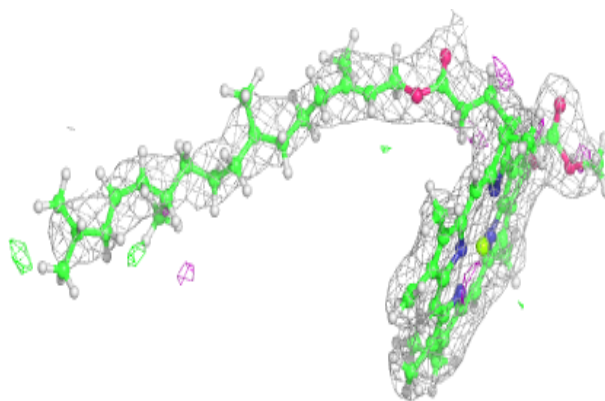
**Electron density around CLA b 603:**

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

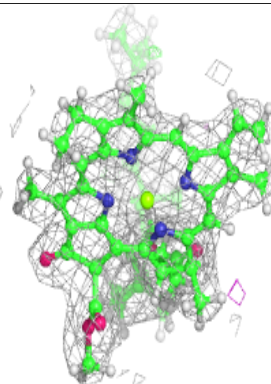
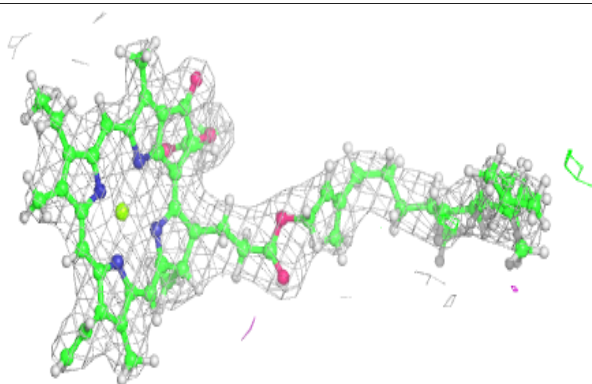
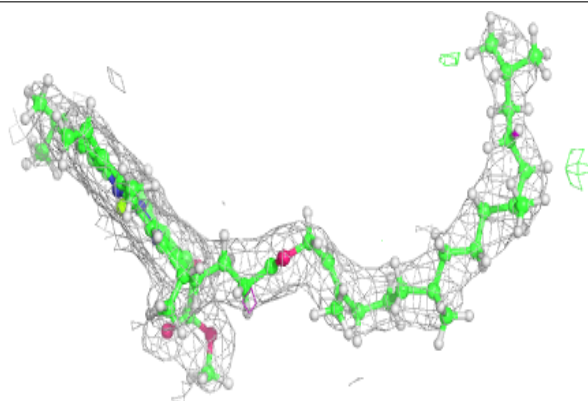


Electron density around CLA B 606:

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

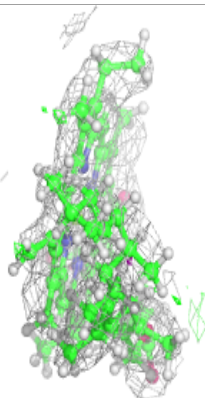
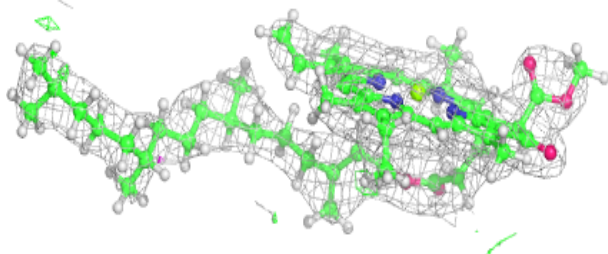
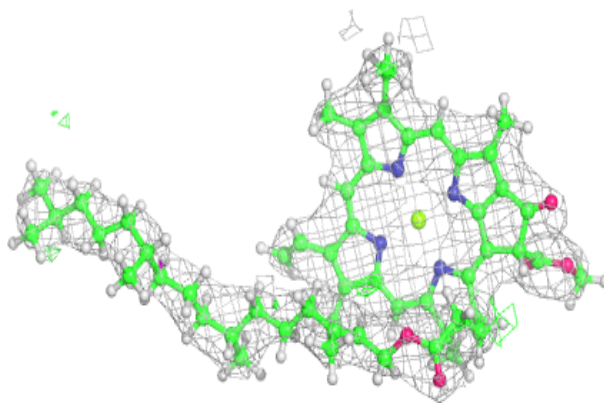
**Electron density around CLA d 402:**

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

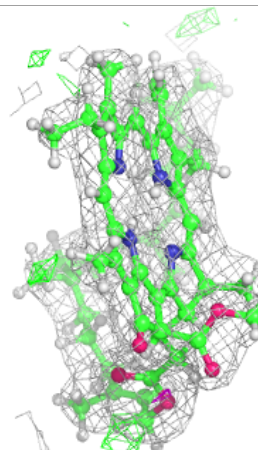
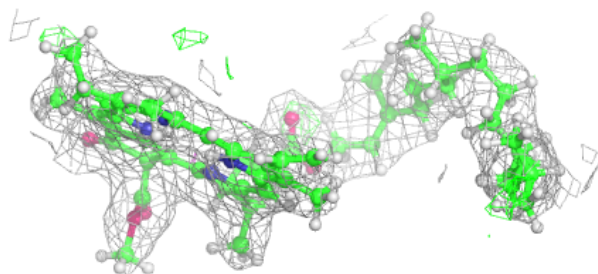
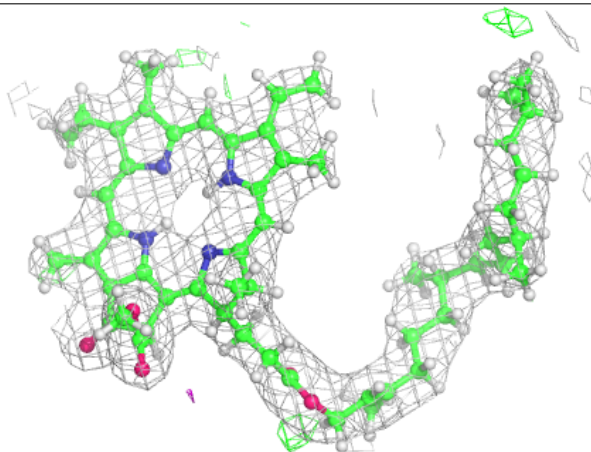


Electron density around CLA c 501:

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

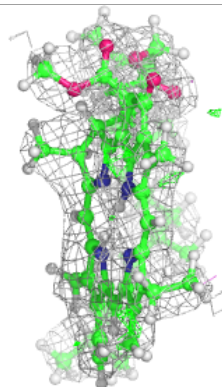
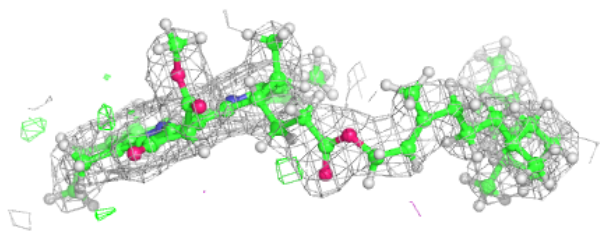
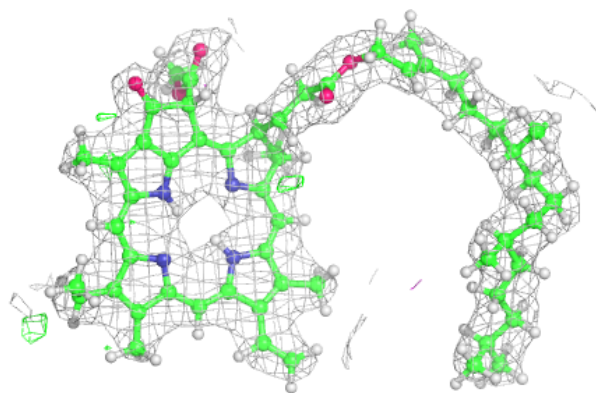
**Electron density around PHO A 606:**

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

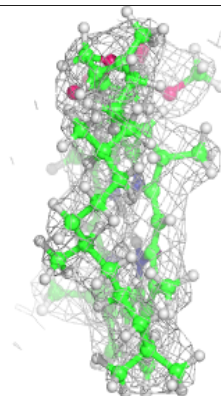
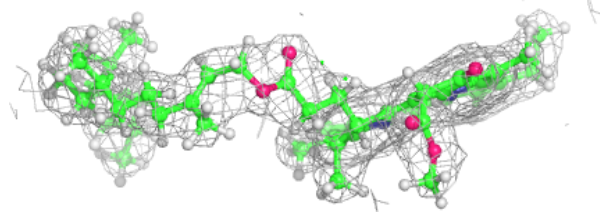
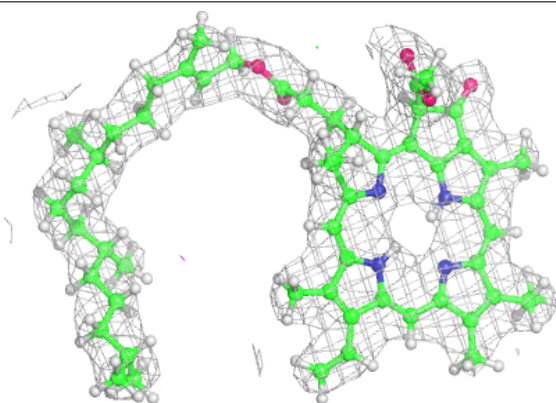


Electron density around PHO D 401:

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

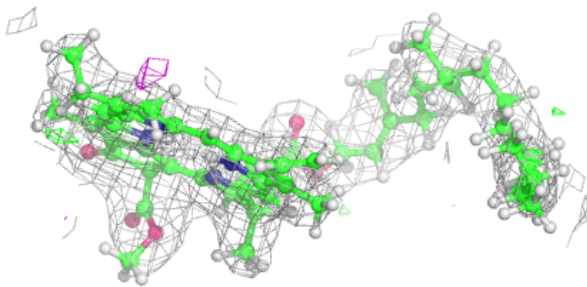
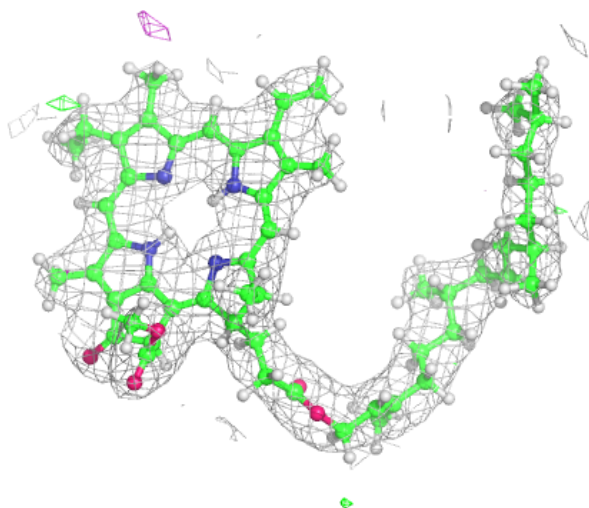
**Electron density around PHO a 606:**

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



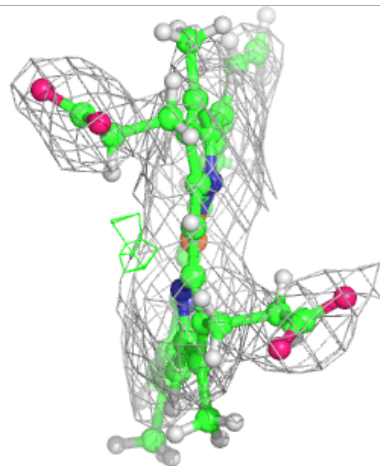
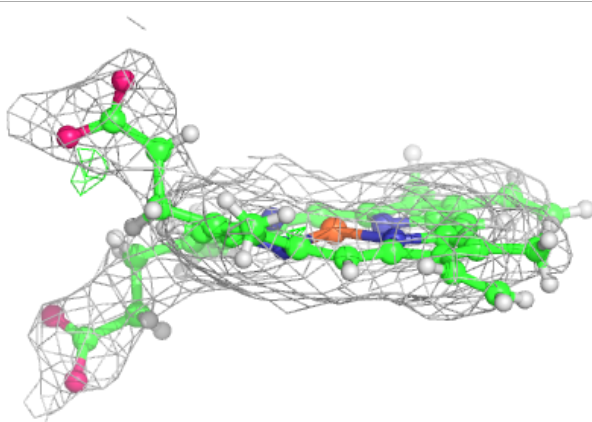
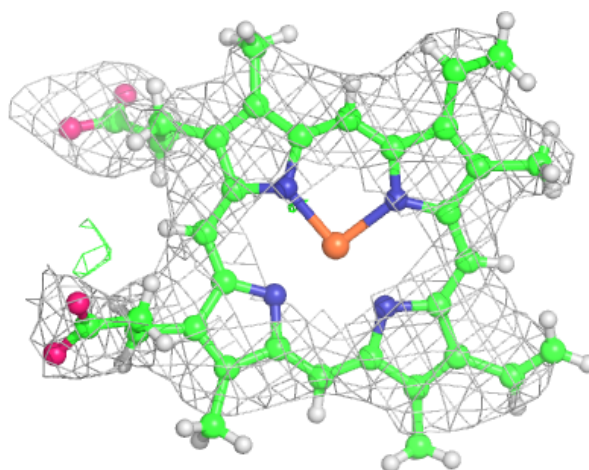
Electron density around PHO d 401:

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



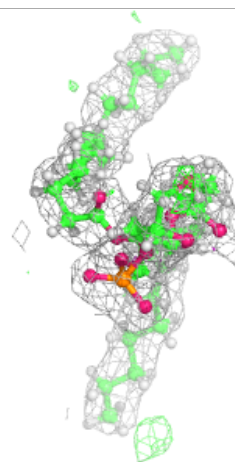
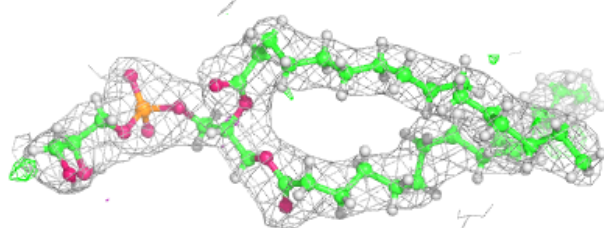
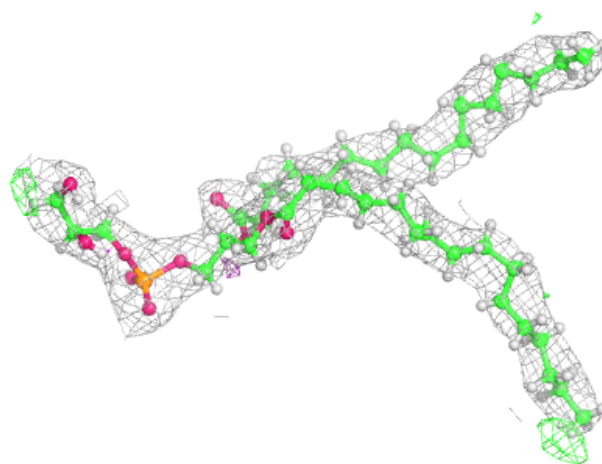
Electron density around HEM f 101:

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



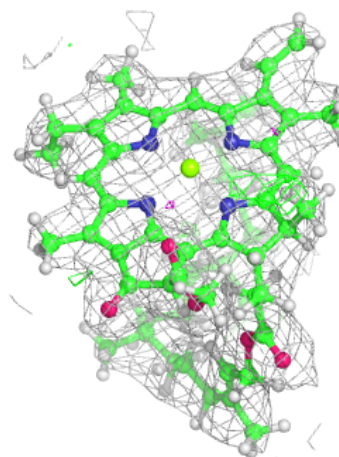
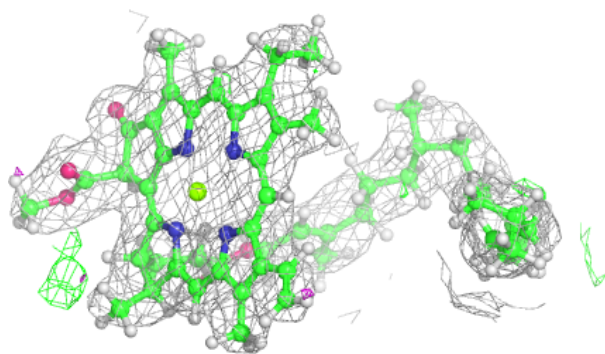
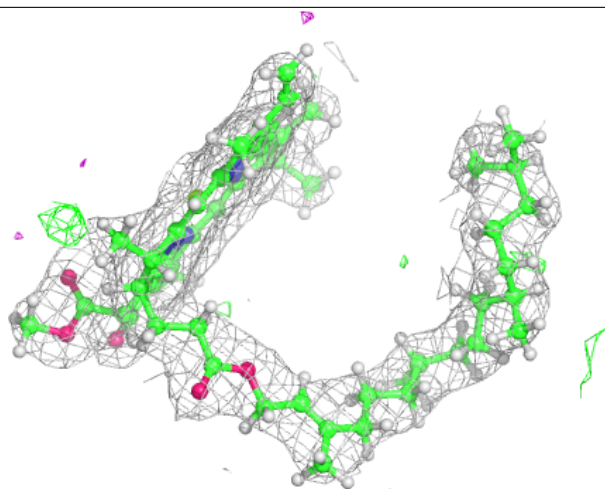
Electron density around LHG D 409:

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



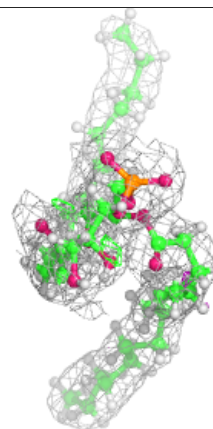
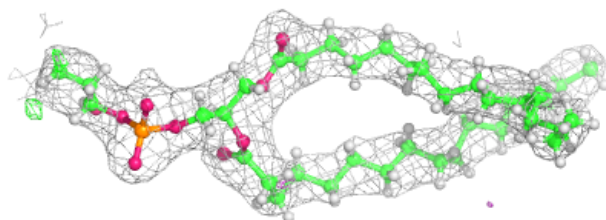
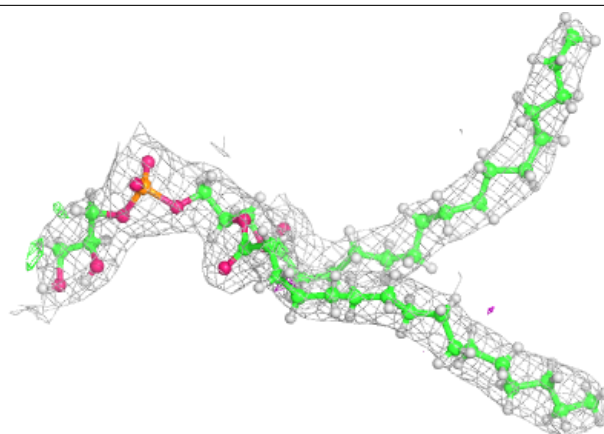
Electron density around CLA B 610:

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



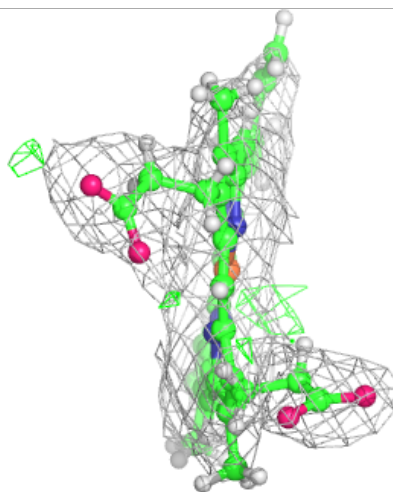
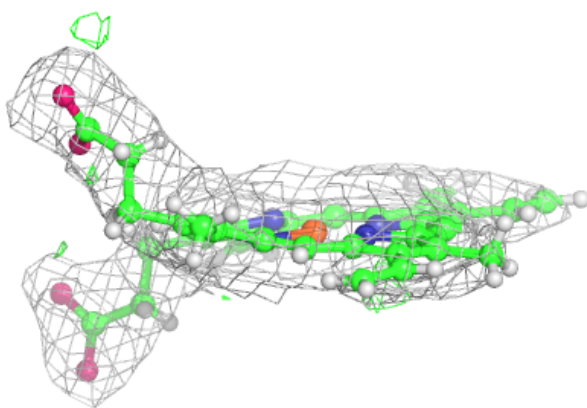
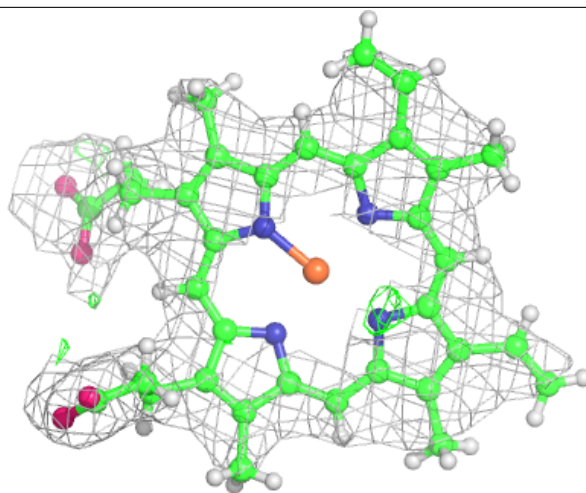
Electron density around LHG d 406:

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



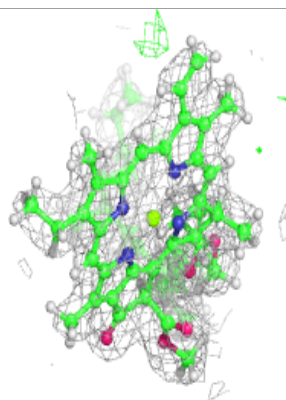
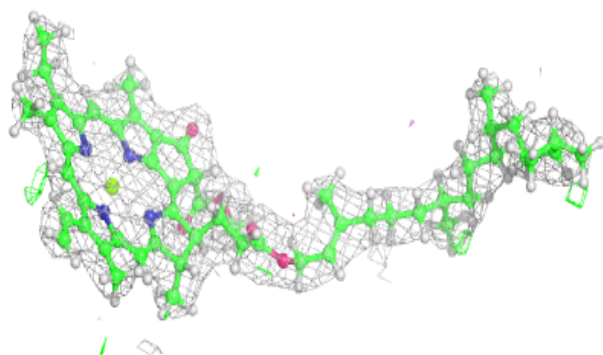
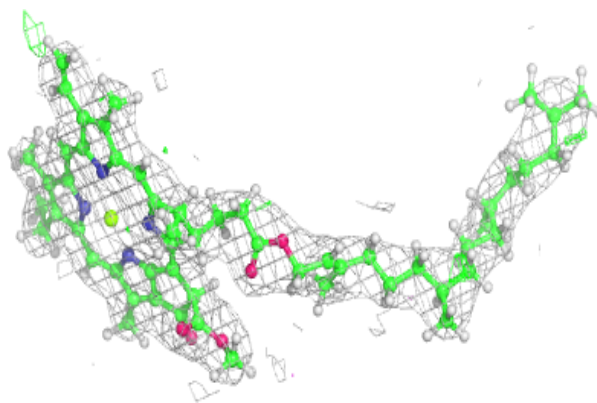
Electron density around HEM F 101:

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



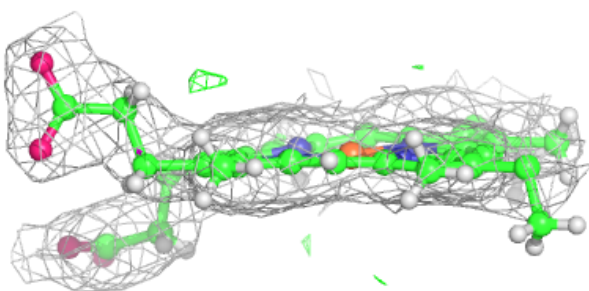
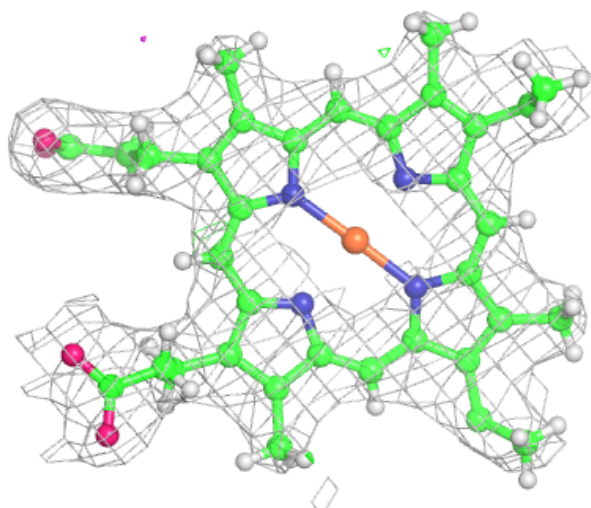
Electron density around CLA A 604:

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



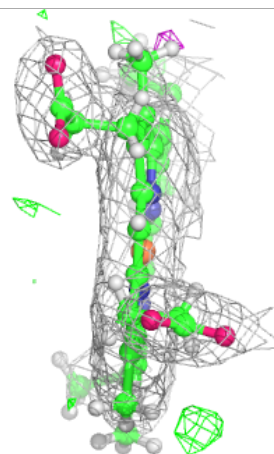
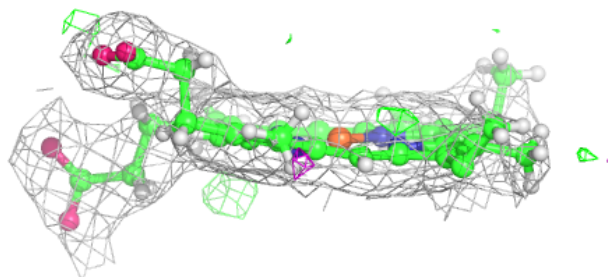
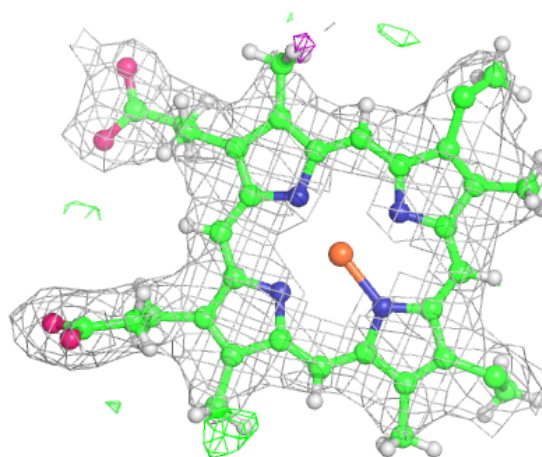
Electron density around HEC V 201:

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



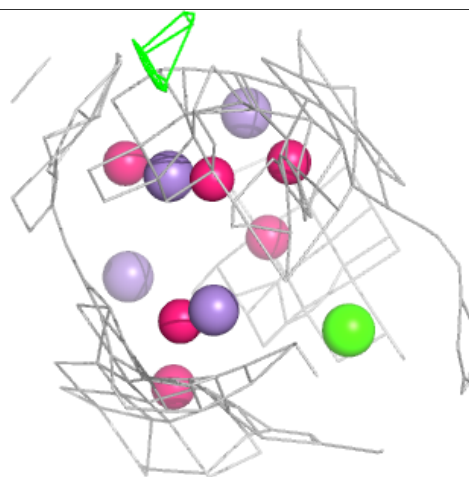
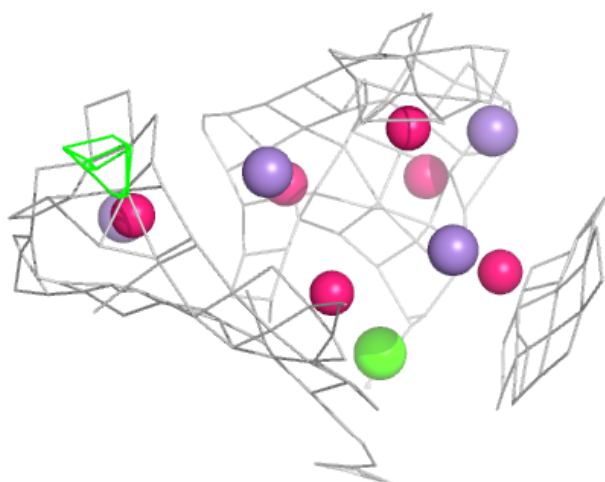
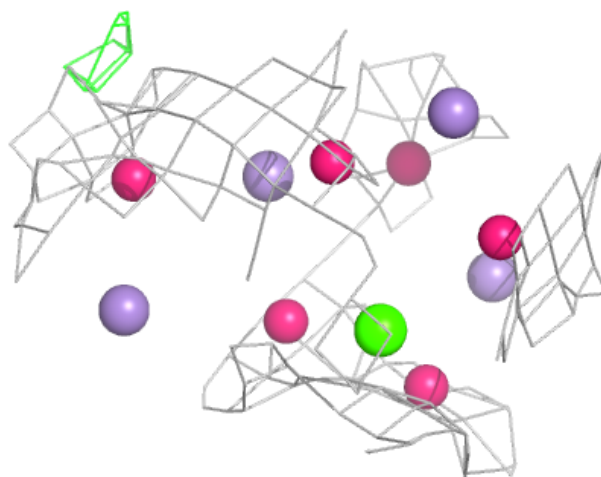
Electron density around HEC v 201:

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



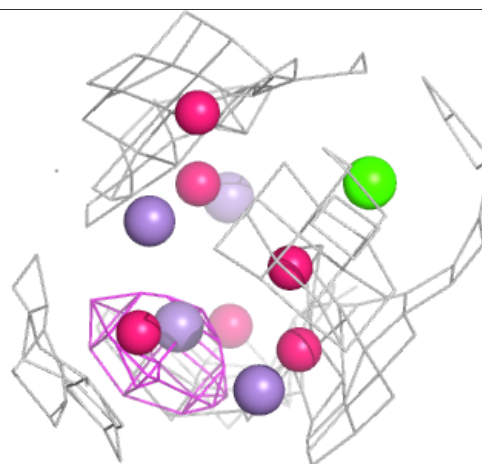
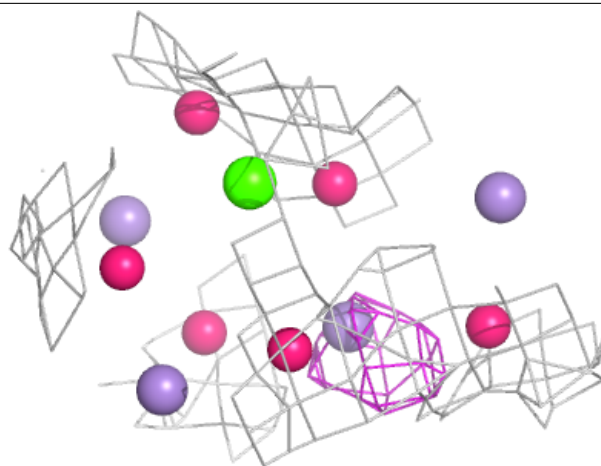
Electron density around OEY A 601 (B):

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



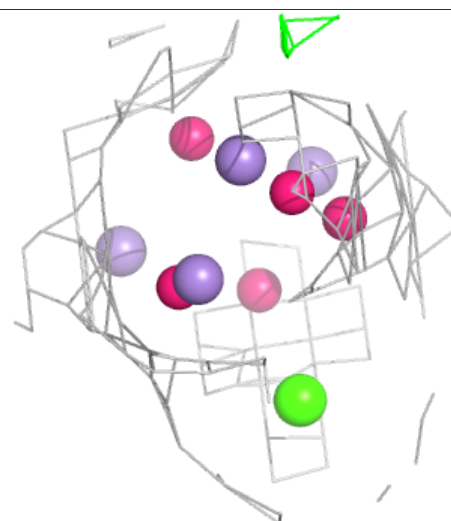
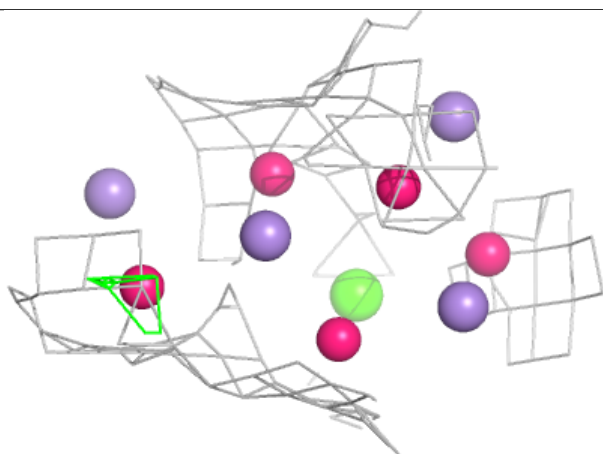
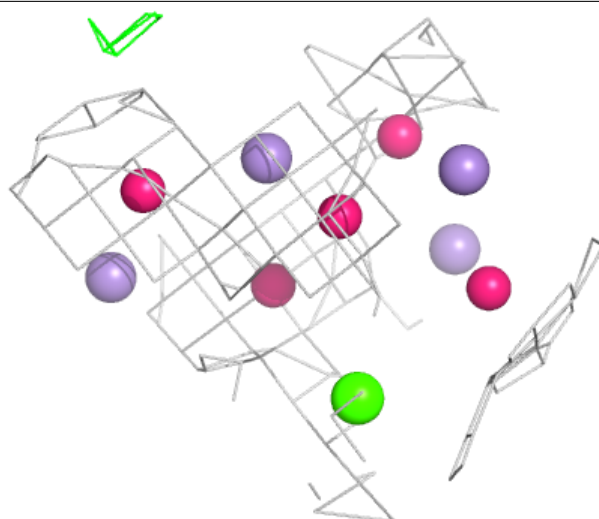
Electron density around OEY a 601 (B):

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



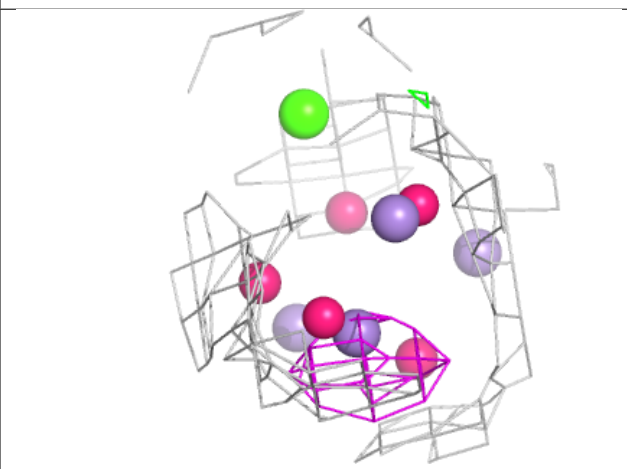
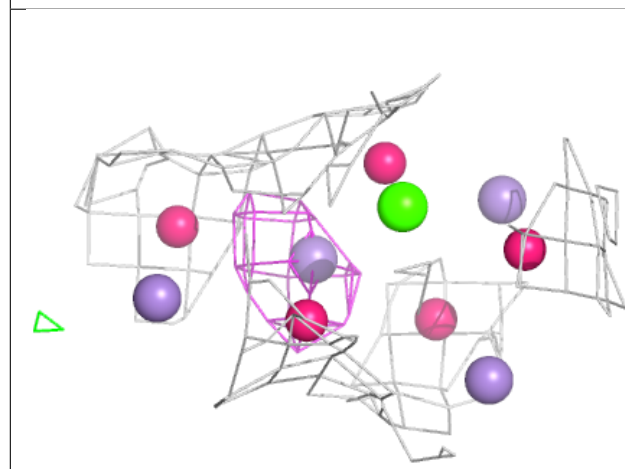
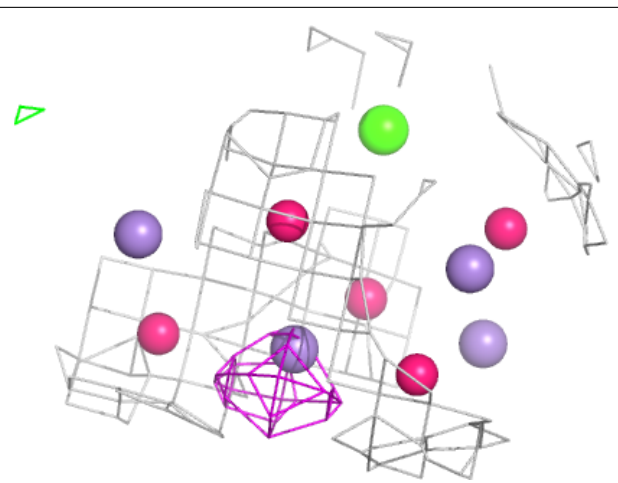
Electron density around OEX A 602 (A):

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



Electron density around OEX a 602 (A):

$2mF_o-DF_c$ (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.