



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2021 – 10:51 AM EDT

PDB ID : 7RF7
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.09 Å(reported)

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

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

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

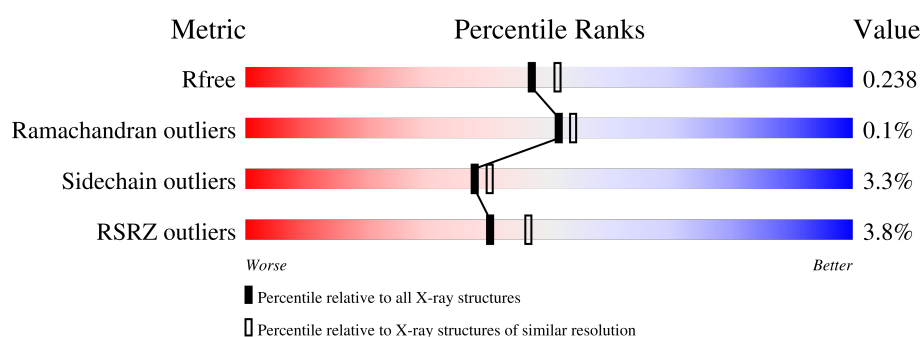
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



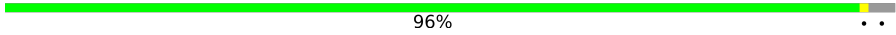
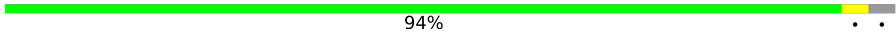
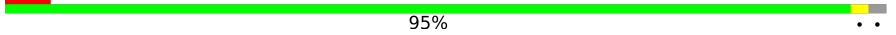
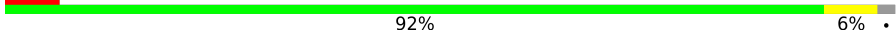


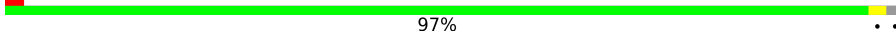







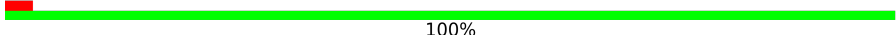







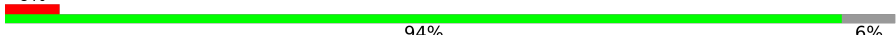


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>0%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>94%</div> <div>..</div> </div>
2	B	510	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
2	b	510	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
3	C	461	<div> <div>0%</div> <div>94%</div> <div>..</div> </div>
3	c	461	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>










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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106082 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	0	0	0
			598	204	305	43			

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- | 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 |

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

- # CLA

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



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



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

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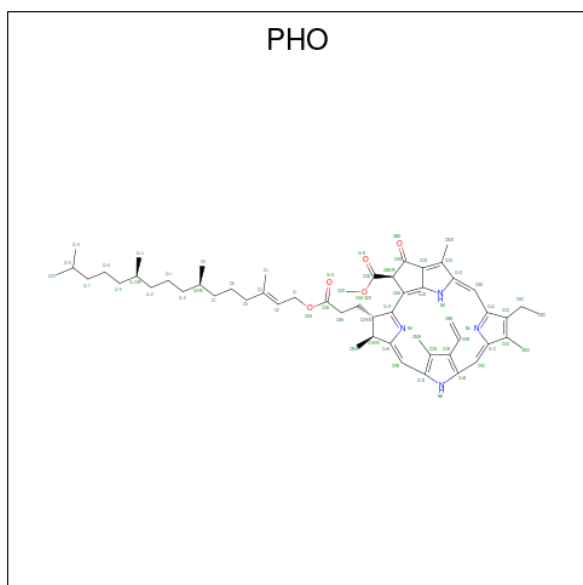
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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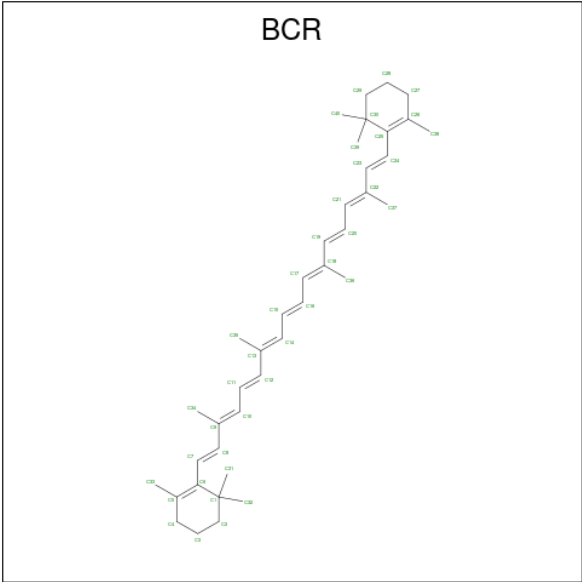
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

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



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

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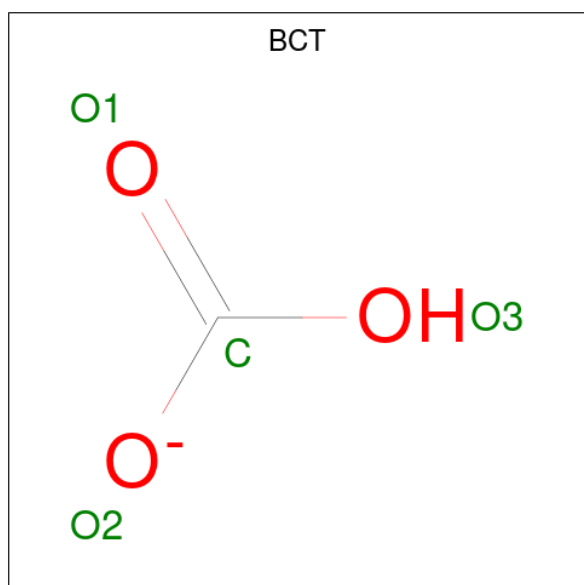
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

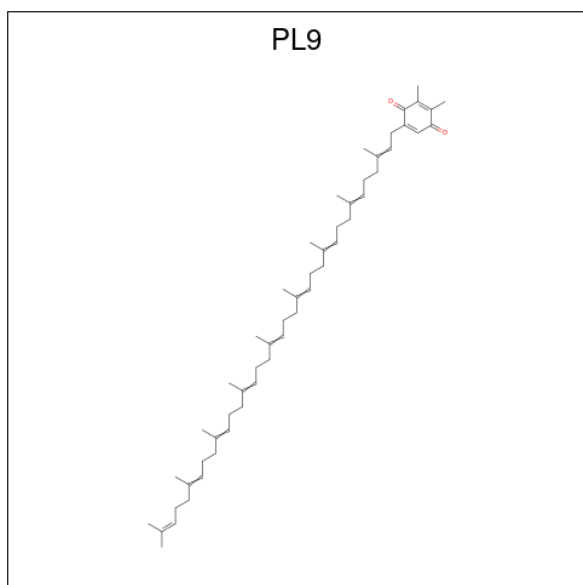
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



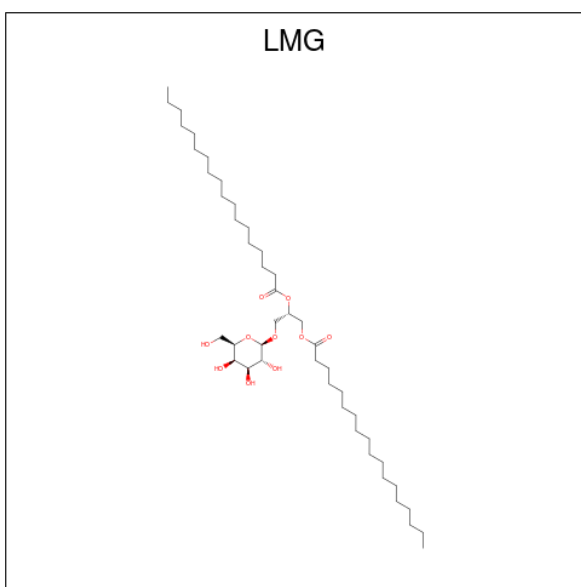
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

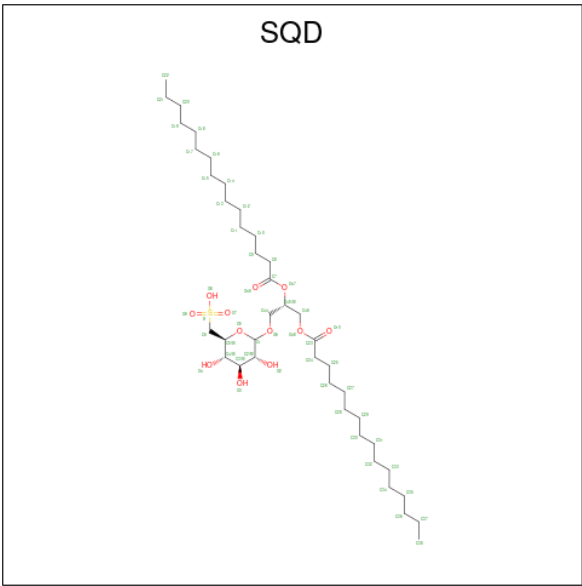
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

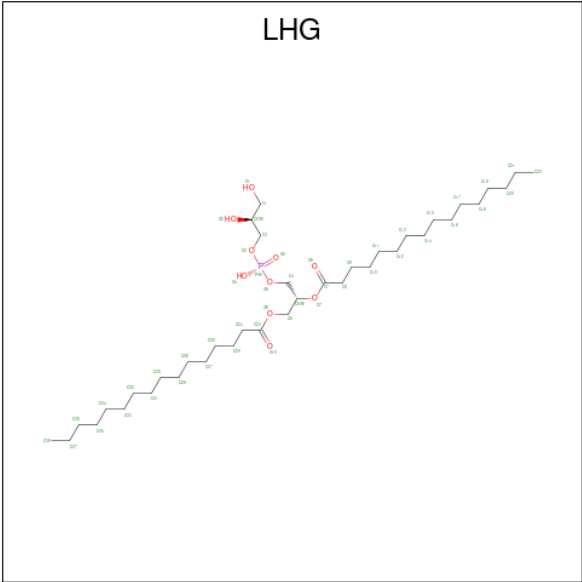
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



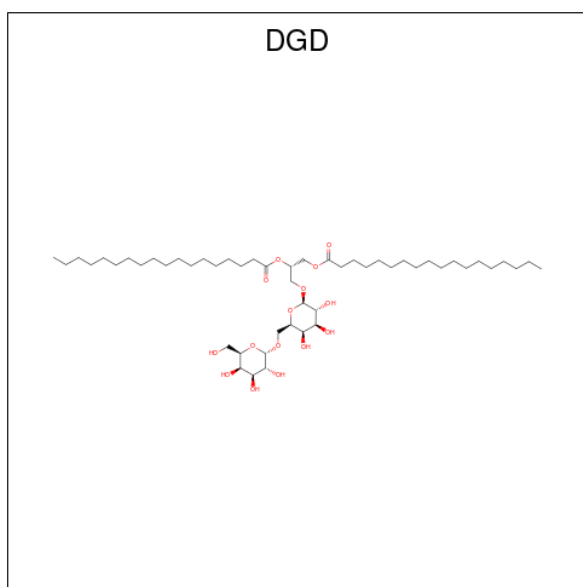
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	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).



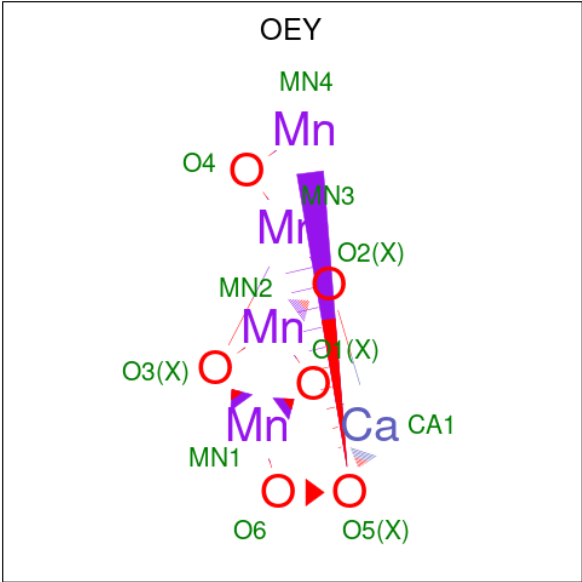
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			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: C₅₁H₉₆O₁₅).



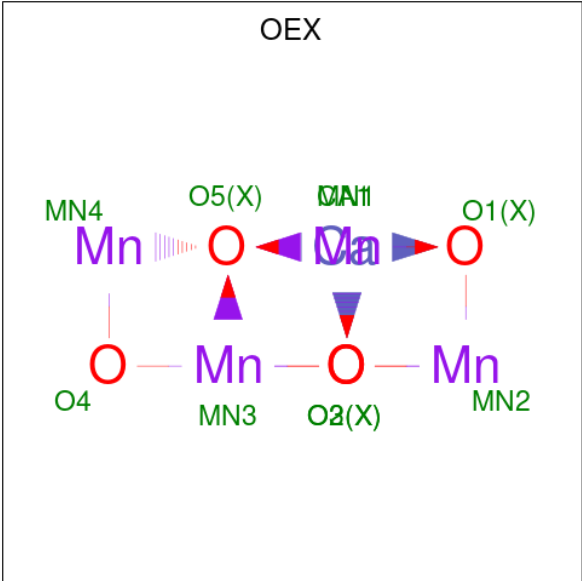
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	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 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
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 33 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



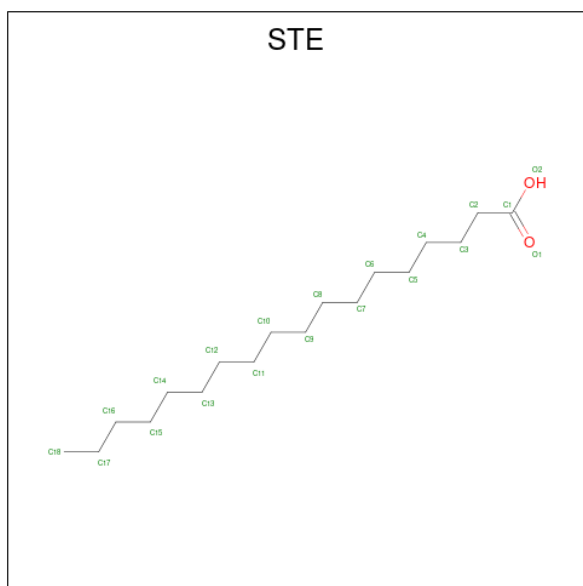
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 34 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



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

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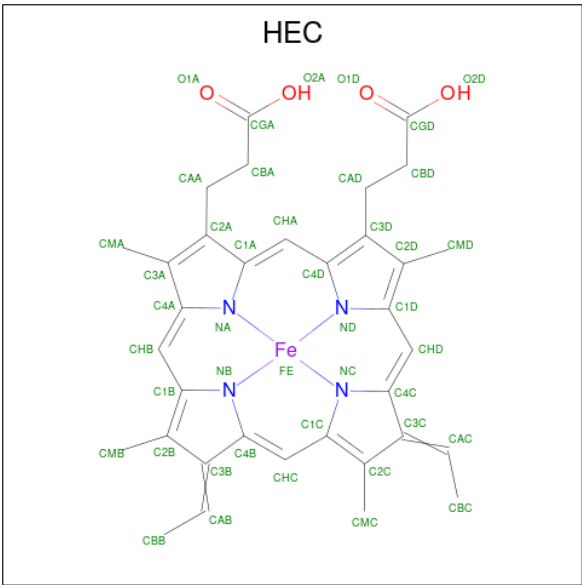
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	1	Total C H O 28 10 16 2	0	0
34	L	1	Total C H O 28 10 16 2	0	0
34	M	1	Total C H O 37 13 22 2	0	0
34	M	1	Total C H 26 10 16	0	0
34	R	1	Total C H O 28 10 16 2	0	0
34	T	1	Total C H 44 15 29	0	0
34	X	1	Total C H O 55 18 35 2	0	0
34	Z	1	Total C H 20 8 12	0	0
34	a	1	Total C H 26 10 16	0	0
34	a	1	Total C H O 28 10 16 2	0	0
34	a	1	Total C H 41 15 26	0	0
34	b	1	Total C H 47 16 31	0	0
34	b	1	Total C H O 55 18 35 2	0	0
34	b	1	Total C H O 40 14 24 2	0	0
34	b	1	Total C H O 55 18 35 2	0	0
34	b	1	Total C H 26 10 16	0	0
34	c	1	Total C H O 55 18 35 2	0	0
34	c	1	Total C H O 28 10 16 2	0	0
34	d	1	Total C H O 43 15 26 2	0	0
34	d	1	Total C H O 55 18 35 2	0	0
34	d	1	Total C H O 55 18 35 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	h	1	Total C H 41 14 27	0	0
34	j	1	Total C H O 28 10 16 2	0	0
34	l	1	Total C H 53 18 35	0	0
34	t	1	Total C H O 34 12 20 2	0	0

- # HEM

- 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	151	Total	O	0	8
			151	151		
37	B	204	Total	O	0	0
			204	204		
37	C	173	Total	O	0	0
			173	173		
37	D	131	Total	O	0	0
			131	131		
37	E	33	Total	O	0	0
			33	33		
37	F	8	Total	O	0	0
			8	8		
37	H	34	Total	O	0	0
			34	34		
37	I	17	Total	O	0	0
			17	17		
37	J	24	Total	O	0	0
			24	24		
37	K	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	10	Total 10	O 10	0	0
37	M	8	Total 8	O 8	0	0
37	O	86	Total 86	O 86	0	0
37	R	4	Total 4	O 4	0	0
37	T	8	Total 8	O 8	0	0
37	U	34	Total 34	O 34	0	0
37	V	64	Total 64	O 64	0	0
37	X	15	Total 15	O 15	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	10	Total 10	O 10	0	0
37	a	132	Total 132	O 132	0	8
37	b	172	Total 172	O 172	0	0
37	c	157	Total 157	O 157	0	0
37	d	110	Total 110	O 110	0	0
37	e	28	Total 28	O 28	0	0
37	f	6	Total 6	O 6	0	0
37	h	20	Total 20	O 20	0	0
37	i	11	Total 11	O 11	0	0
37	j	8	Total 8	O 8	0	0
37	k	5	Total 5	O 5	0	0
37	l	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	7	Total 7	O 7	0	0
37	o	100	Total 100	O 100	0	0
37	r	7	Total 7	O 7	0	0
37	t	8	Total 8	O 8	0	0
37	u	48	Total 48	O 48	0	0
37	v	59	Total 59	O 59	0	0
37	x	11	Total 11	O 11	0	0
37	y	4	Total 4	O 4	0	0
37	z	12	Total 12	O 12	0	0

3 Residue-property plots [i](#)

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

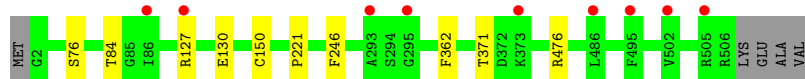
- Molecule 1: Photosystem II protein D1 1



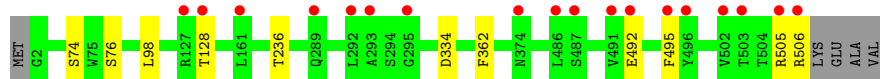
- Molecule 1: Photosystem II protein D1 1



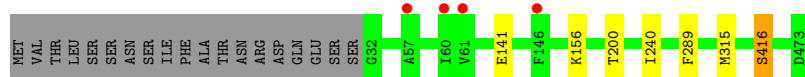
- Molecule 2: Photosystem II CP47 reaction center protein



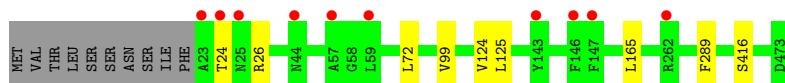
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



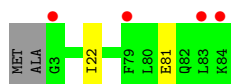
- Molecule 4: Photosystem II D2 protein



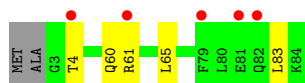
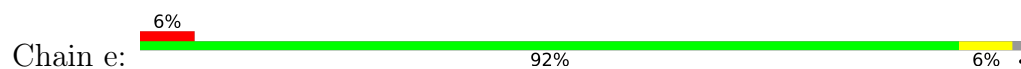
- Molecule 4: Photosystem II D2 protein



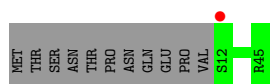
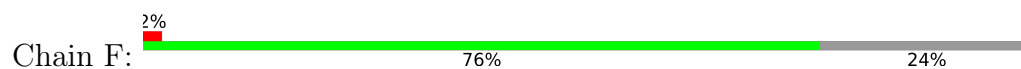
- Molecule 5: Cytochrome b559 subunit alpha



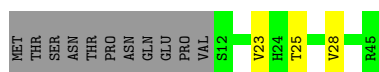
- Molecule 5: Cytochrome b559 subunit alpha



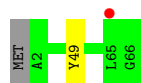
- Molecule 6: Cytochrome b559 subunit beta



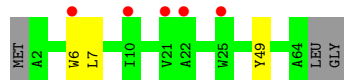
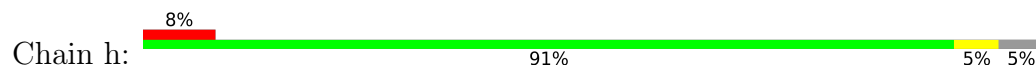
- Molecule 6: Cytochrome b559 subunit beta



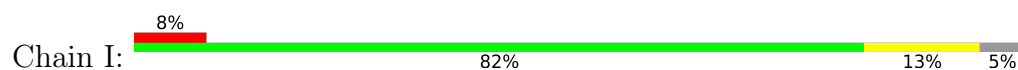
- Molecule 7: Photosystem II reaction center protein H



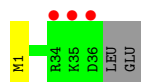
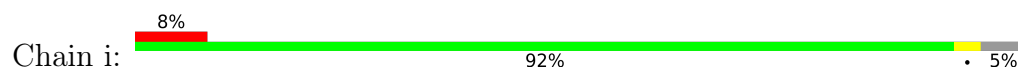
- Molecule 7: Photosystem II reaction center protein H



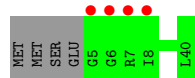
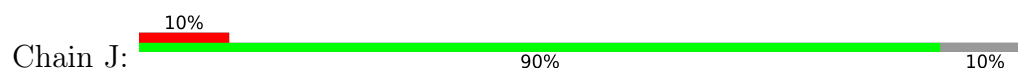
- Molecule 8: Photosystem II reaction center protein I



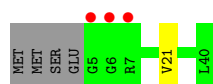
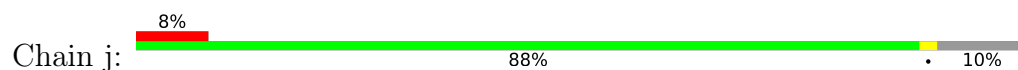
- Molecule 8: Photosystem II reaction center protein I



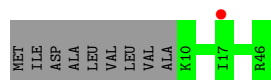
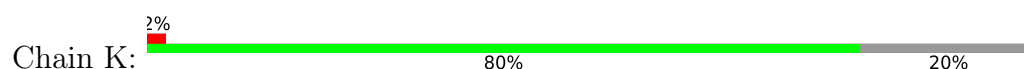
- Molecule 9: Photosystem II reaction center protein J



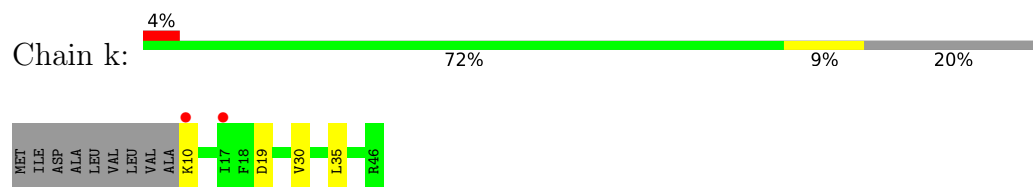
- Molecule 9: Photosystem II reaction center protein J



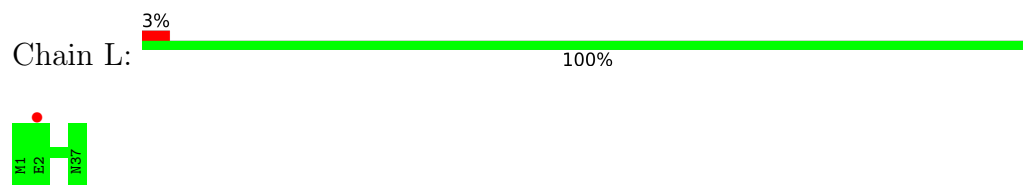
- Molecule 10: Photosystem II reaction center protein K



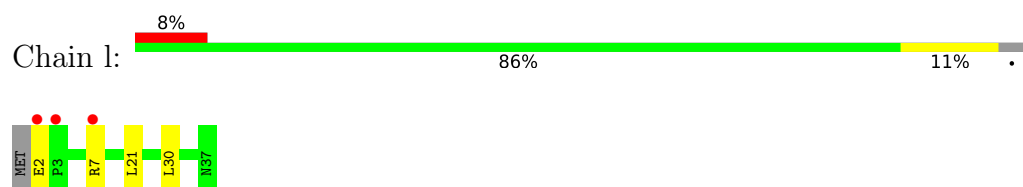
- Molecule 10: Photosystem II reaction center protein K



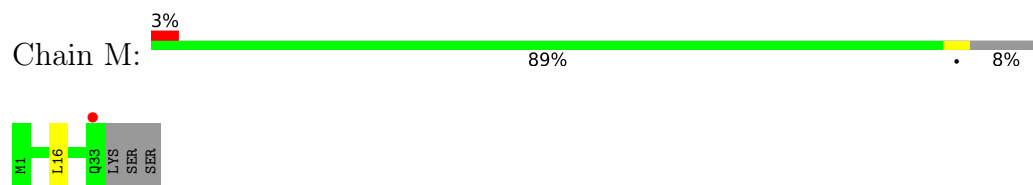
- Molecule 11: Photosystem II reaction center protein L



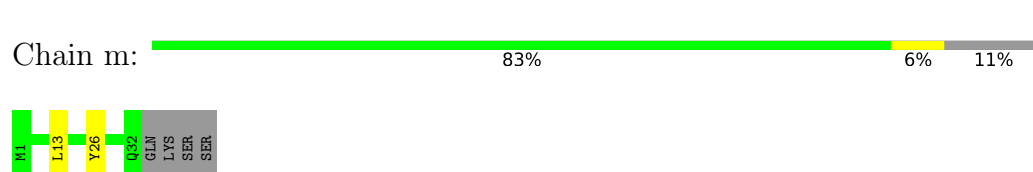
- Molecule 11: Photosystem II reaction center protein L



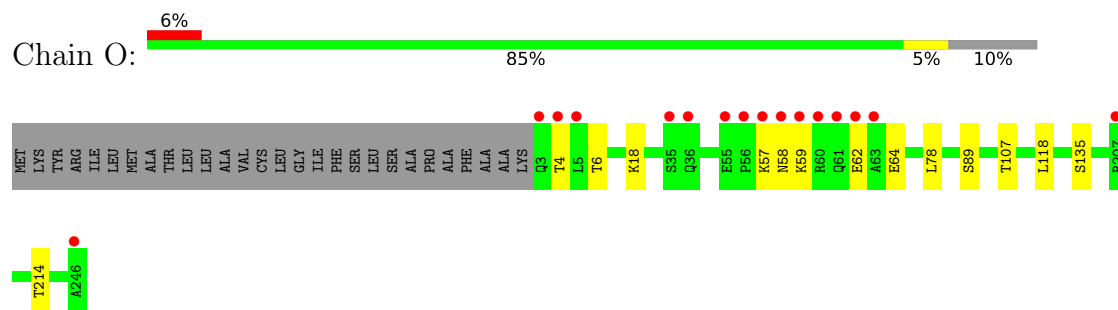
- Molecule 12: Photosystem II reaction center protein M



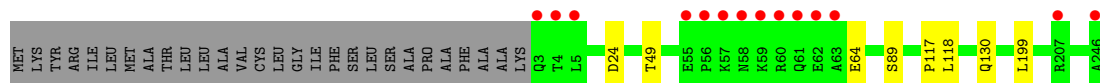
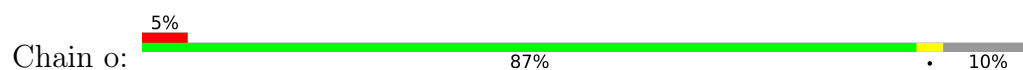
- Molecule 12: Photosystem II reaction center protein M



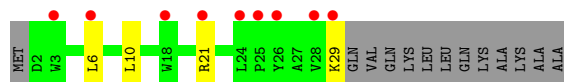
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



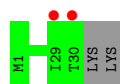
- Molecule 14: Photosystem II protein Y



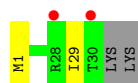
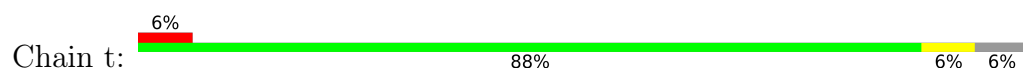
- Molecule 14: Photosystem II protein Y



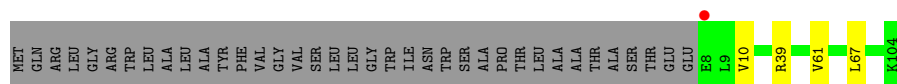
- Molecule 15: Photosystem II reaction center protein T



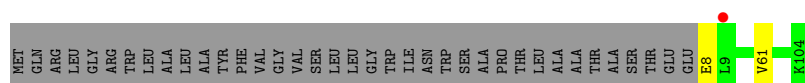
- Molecule 15: Photosystem II reaction center protein T




- Molecule 16: Photosystem II 12 kDa extrinsic protein

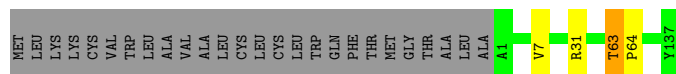


- Molecule 16: Photosystem II 12 kDa extrinsic protein




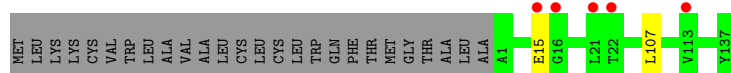
- Molecule 17: Cytochrome c-550

Chain V:  82% 16%




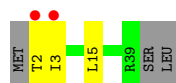
- Molecule 17: Cytochrome c-550

Chain v:  83% 16%




- Molecule 18: Photosystem II reaction center X protein

Chain X:  85% 7% 7%



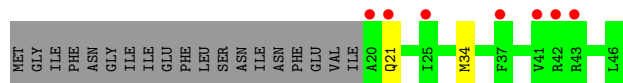
- Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5%



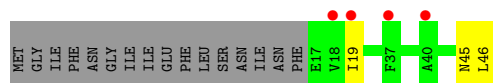
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  54% 41%




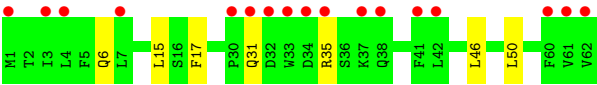
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  59% 7% 35%

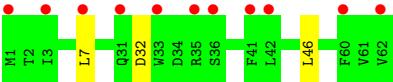
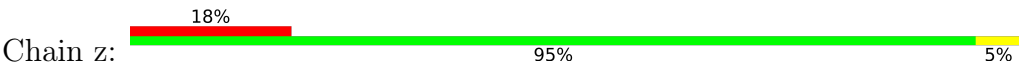


- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  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	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 86.0 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 0.238	Depositor DCC
R_{free} test set	4171 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	106082	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: SQD, PHO, HEC, BCR, BCT, STE, FME, LHG, HEM, OEY, FE2, CL, LMG, OEX, DGD, CLA, PL9

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	0.57	0/3227	0.64	1/4397 (0.0%)
1	a	0.57	0/3224	0.64	0/4393
2	B	0.61	2/4161 (0.0%)	0.66	0/5669
2	b	0.60	0/4118	0.66	1/5611 (0.0%)
3	C	0.57	0/3647	0.65	0/4965
3	c	0.54	0/3719	0.64	0/5061
4	D	0.62	0/2825	0.67	0/3847
4	d	0.59	0/2834	0.68	0/3859
5	E	0.56	0/688	0.61	0/940
5	e	0.50	0/683	0.63	0/932
6	F	0.52	0/284	0.55	0/387
6	f	0.45	0/284	0.56	0/387
7	H	0.60	0/523	0.71	0/713
7	h	0.53	0/511	0.69	0/697
8	I	0.57	0/293	0.64	0/396
8	i	0.60	0/293	0.64	0/396
9	J	0.55	0/263	0.63	0/356
9	j	0.47	0/263	0.66	0/356
10	K	0.51	0/303	0.60	0/416
10	k	0.49	0/303	0.62	0/416
11	L	0.58	0/311	0.68	0/422
11	l	0.64	0/303	0.66	0/412
12	M	0.57	0/249	0.62	0/341
12	m	0.78	1/244 (0.4%)	0.64	0/334
13	O	0.57	0/1904	0.72	0/2585
13	o	0.58	0/1905	0.71	0/2583
14	R	0.39	0/227	0.55	0/313
14	r	0.35	0/227	0.54	0/313
15	T	0.67	0/257	0.70	0/349
15	t	0.66	0/255	0.61	0/346
16	U	0.54	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.61	0/785	0.68	0/1064
17	V	0.59	0/1085	0.66	1/1473 (0.1%)
17	v	0.55	0/1085	0.65	0/1473
18	X	0.52	0/284	0.66	0/384
18	x	0.44	0/289	0.58	0/391
19	Y	0.45	0/197	0.58	0/264
19	y	0.36	0/219	0.57	0/294
20	Z	0.45	0/490	0.54	0/669
20	z	0.40	0/488	0.51	0/666
All	All	0.57	3/44035 (0.0%)	0.65	3/59934 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	26	TYR	CD1-CE1	-6.25	1.29	1.39
2	B	150	CYS	CB-SG	-5.75	1.72	1.81
2	B	221	PRO	CA-C	-5.37	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-5.33	108.87	120.60
2	b	334	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	131	TRP	CA-CB-CG	-5.05	104.10	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	41	41
1	a	397/344 (115%)	388 (98%)	9 (2%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	454/461 (98%)	444 (98%)	9 (2%)	1 (0%)	47	49
3	c	463/461 (100%)	452 (98%)	10 (2%)	1 (0%)	47	49
4	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	13	8
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	22	18
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
All	All	5387/5700 (94%)	5241 (97%)	139 (3%)	7 (0%)	51	54

5 of 7 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	322 (99%)	2 (1%)	86	90
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	43
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	60
2	b	402/407 (99%)	392 (98%)	10 (2%)	47	52
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	60
3	c	364/362 (101%)	356 (98%)	8 (2%)	52	57
4	D	277/283 (98%)	274 (99%)	3 (1%)	73	79
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	41
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	30
5	e	71/73 (97%)	66 (93%)	5 (7%)	15	12
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	63
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	18
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	2
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	30
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	36
12	m	28/32 (88%)	27 (96%)	1 (4%)	35	36
13	O	206/228 (90%)	195 (95%)	11 (5%)	22	20
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	33
14	R	22/33 (67%)	18 (82%)	4 (18%)	1	1
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	24
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	53
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	67
17	v	117/138 (85%)	115 (98%)	2 (2%)	60	67
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	14
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	48 (94%)	3 (6%)	19	17
All	All	4451/4654 (96%)	4308 (97%)	143 (3%)	38	41

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	l	2	GLU
12	m	13	LEU
15	t	29	ILE
17	V	7	VAL
16	U	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	378	ASN
13	o	36	GLN
7	h	59	ASN
13	o	132	ASN
14	R	22	ASN

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	$\# Z > 2$
15	FME	T	1	15	8,9,10	1.04	0	7,9,11	1.23	0
8	FME	i	1	8	8,9,10	0.89	0	7,9,11	1.41	1 (14%)
12	FME	M	1	12	8,9,10	0.83	0	7,9,11	0.82	0
12	FME	m	1	12	8,9,10	0.98	0	7,9,11	1.13	0
15	FME	t	1	15	8,9,10	1.10	1 (12%)	7,9,11	1.13	0
8	FME	I	1	8	8,9,10	1.08	1 (12%)	7,9,11	1.26	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	T	1	15	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.69	1.42	1.46
15	t	1	FME	CA-N	-2.35	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.15	117.98	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.05	119.67	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
22	CLA	D	402	-	56,73,73	1.37	5 (8%)	55,113,113	1.65	9 (16%)
22	CLA	a	402	-	56,73,73	1.62	7 (12%)	55,113,113	1.70	9 (16%)
26	BCT	A	409	21	0,3,3	-	-	0,3,3	-	-
22	CLA	A	405	-	45,62,73	1.65	5 (11%)	41,99,113	1.74	12 (29%)
24	BCR	t	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	8 (14%)
22	CLA	B	611	-	56,73,73	1.60	7 (12%)	55,113,113	1.81	14 (25%)
31	DGD	h	101	-	63,63,67	1.04	5 (7%)	77,77,81	1.48	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	512	-	56,73,73	1.63	6 (10%)	55,113,113	1.78	10 (18%)
24	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	3 (5%)
22	CLA	C	503	-	56,73,73	1.84	7 (12%)	55,113,113	1.92	9 (16%)
24	BCR	c	515	-	41,41,41	1.13	3 (7%)	56,56,56	1.23	7 (12%)
22	CLA	c	502	-	56,73,73	1.83	9 (16%)	55,113,113	1.69	8 (14%)
29	SQD	A	413	-	51,52,54	0.96	5 (9%)	60,63,65	1.83	12 (20%)
22	CLA	a	410	37	56,73,73	1.90	6 (10%)	55,113,113	1.66	9 (16%)
24	BCR	a	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.38	8 (14%)
22	CLA	b	606	-	56,73,73	1.85	12 (21%)	55,113,113	2.20	13 (23%)
29	SQD	a	411	-	53,54,54	1.02	5 (9%)	62,65,65	1.79	12 (19%)
22	CLA	c	506	-	56,73,73	1.47	7 (12%)	55,113,113	1.66	11 (20%)
28	LMG	a	416	-	55,55,55	1.21	4 (7%)	63,63,63	1.49	7 (11%)
35	HEM	e	101	5,6	27,50,50	2.04	5 (18%)	17,82,82	2.13	4 (23%)
22	CLA	B	609	-	56,73,73	1.73	8 (14%)	55,113,113	1.62	10 (18%)
22	CLA	C	513	-	56,73,73	1.68	7 (12%)	55,113,113	1.52	10 (18%)
22	CLA	C	508	-	56,73,73	1.65	6 (10%)	55,113,113	1.89	10 (18%)
22	CLA	A	402	-	56,73,73	1.57	9 (16%)	55,113,113	1.60	8 (14%)
22	CLA	d	403	-	56,73,73	1.58	8 (14%)	55,113,113	1.59	10 (18%)
24	BCR	d	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
22	CLA	b	608	-	56,73,73	1.70	8 (14%)	55,113,113	1.49	11 (20%)
24	BCR	A	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	7 (12%)
26	BCT	a	408	21	0,3,3	-	-	0,3,3	-	-
22	CLA	C	504	37	50,67,73	1.68	7 (14%)	47,105,113	1.67	13 (27%)
22	CLA	b	615	-	56,73,73	1.68	9 (16%)	55,113,113	1.69	8 (14%)
34	STE	d	411	-	13,16,19	0.32	0	12,16,19	1.16	1 (8%)
22	CLA	B	616	-	51,68,73	1.81	10 (19%)	49,107,113	2.15	16 (32%)
34	STE	B	626	-	15,15,19	0.44	0	14,14,19	0.62	0
22	CLA	c	503	-	56,73,73	1.54	9 (16%)	55,113,113	1.69	9 (16%)
22	CLA	C	505	-	56,73,73	1.68	5 (8%)	55,113,113	1.57	11 (20%)
22	CLA	a	403	37	56,73,73	1.56	6 (10%)	55,113,113	1.56	9 (16%)
27	PL9	a	409	-	55,55,55	1.18	5 (9%)	68,69,69	1.58	14 (20%)
28	LMG	D	411	-	20,26,55	0.42	0	18,26,63	1.19	0
29	SQD	a	412	-	35,35,54	1.10	2 (5%)	37,37,65	1.44	4 (10%)
36	HEC	v	201	17	26,50,50	2.37	4 (15%)	18,82,82	2.14	5 (27%)
23	PHO	d	401	-	67,69,69	1.13	6 (8%)	85,99,99	1.03	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	K	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.18	5 (8%)
29	SQD	f	101	-	40,41,54	1.12	5 (12%)	49,52,65	2.05	11 (22%)
28	LMG	D	406	-	51,51,55	0.87	3 (5%)	59,59,63	1.43	9 (15%)
34	STE	B	625	-	14,17,19	0.37	0	13,17,19	1.03	0
22	CLA	b	604	-	56,73,73	1.45	7 (12%)	55,113,113	1.84	12 (21%)
23	PHO	D	401	-	67,69,69	1.15	5 (7%)	85,99,99	1.25	10 (11%)
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.21	6 (10%)
34	STE	H	103	-	17,17,19	0.43	0	16,16,19	0.68	0
34	STE	l	102	-	17,17,19	0.31	0	16,16,19	1.00	0
31	DGD	c	516	-	63,63,67	1.26	11 (17%)	77,77,81	1.43	13 (16%)
30	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.17	4 (7%)
29	SQD	b	620	-	48,49,54	0.95	4 (8%)	57,60,65	2.15	17 (29%)
22	CLA	B	612	-	56,73,73	1.63	5 (8%)	55,113,113	1.86	12 (21%)
34	STE	B	620	-	13,16,19	0.32	0	12,16,19	1.10	0
30	LHG	D	409	-	46,46,48	0.98	3 (6%)	49,52,54	1.32	4 (8%)
34	STE	C	519	-	8,11,19	0.39	0	7,11,19	0.81	0
30	LHG	A	414	-	48,48,48	0.85	3 (6%)	51,54,54	1.18	4 (7%)
34	STE	J	101	-	8,11,19	0.33	0	7,11,19	0.99	0
34	STE	L	101	-	8,11,19	0.44	0	7,11,19	0.70	0
28	LMG	C	518	-	48,48,55	1.15	5 (10%)	56,56,63	1.34	6 (10%)
30	LHG	D	408	-	48,48,48	1.05	3 (6%)	51,54,54	1.27	7 (13%)
22	CLA	B	601	37	56,73,73	1.62	9 (16%)	55,113,113	1.99	13 (23%)
34	STE	c	523	-	8,11,19	0.38	0	7,11,19	0.77	0
27	PL9	D	405	-	55,55,55	1.71	9 (16%)	68,69,69	1.72	14 (20%)
32	OXY	a	418[B]	37,1,3	0,16,16	-	-	-	-	-
22	CLA	b	607	37	56,73,73	1.39	6 (10%)	55,113,113	1.89	11 (20%)
24	BCR	C	514	-	41,41,41	1.27	3 (7%)	56,56,56	1.37	5 (8%)
28	LMG	D	410	-	31,31,55	0.89	2 (6%)	33,33,63	1.16	2 (6%)
22	CLA	c	508	-	55,72,73	1.66	8 (14%)	53,111,113	1.67	11 (20%)
30	LHG	d	409	-	38,38,48	0.71	1 (2%)	41,44,54	1.13	3 (7%)
34	STE	d	413	-	16,19,19	0.39	0	15,19,19	0.76	0
28	LMG	c	522	-	49,49,55	0.92	3 (6%)	57,57,63	1.32	4 (7%)
34	STE	C	521	-	8,11,19	0.29	0	7,11,19	1.29	1 (14%)
24	BCR	B	618	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	7 (12%)
22	CLA	c	504	37	51,68,73	1.58	6 (11%)	49,107,113	1.51	8 (16%)
22	CLA	b	605	-	56,73,73	1.50	8 (14%)	55,113,113	1.70	12 (21%)
22	CLA	b	611	-	56,73,73	1.52	5 (8%)	55,113,113	1.62	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	c	518	-	63,63,67	1.01	4 (6%)	77,77,81	1.38	12 (15%)
33	OEX	A	418[A]	37,1,3	0,15,15	-	-	-		
36	HEC	V	201	17	26,50,50	2.07	3 (11%)	18,82,82	2.17	6 (33%)
34	STE	b	627	-	9,9,19	0.48	0	8,8,19	0.55	0
34	STE	B	624	-	8,11,19	0.32	0	7,11,19	0.93	0
22	CLA	B	614	-	56,73,73	1.63	8 (14%)	55,113,113	1.77	13 (23%)
34	STE	t	102	-	10,13,19	0.41	0	9,13,19	0.92	0
22	CLA	b	602	-	56,73,73	1.51	7 (12%)	55,113,113	1.88	10 (18%)
34	STE	T	102	-	14,14,19	0.39	0	13,13,19	0.83	0
35	HEM	F	101	5,6	27,50,50	1.95	5 (18%)	17,82,82	2.37	8 (47%)
22	CLA	c	501	-	56,73,73	1.56	5 (8%)	55,113,113	1.75	11 (20%)
22	CLA	b	613	-	56,73,73	1.57	7 (12%)	55,113,113	1.98	14 (25%)
24	BCR	D	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.11	3 (5%)
24	BCR	T	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.25	5 (8%)
32	OEY	A	417[B]	37,1,3	0,16,16	-	-	-		
28	LMG	A	412	-	48,48,55	1.04	3 (6%)	56,56,63	1.35	7 (12%)
22	CLA	A	403	37	56,73,73	1.56	8 (14%)	55,113,113	1.52	9 (16%)
22	CLA	B	605	-	56,73,73	1.43	6 (10%)	55,113,113	1.42	9 (16%)
22	CLA	C	501	-	56,73,73	1.69	8 (14%)	55,113,113	1.72	6 (10%)
22	CLA	B	608	-	56,73,73	1.40	8 (14%)	55,113,113	1.70	9 (16%)
34	STE	b	623	-	16,19,19	0.36	0	15,19,19	0.82	0
28	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.31	6 (10%)
22	CLA	B	610	37	56,73,73	1.72	7 (12%)	55,113,113	1.85	14 (25%)
23	PHO	A	404	-	67,69,69	1.22	9 (13%)	85,99,99	1.24	8 (9%)
34	STE	a	414	-	8,11,19	0.47	0	7,11,19	0.79	0
24	BCR	k	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	5 (8%)
28	LMG	M	101	-	51,51,55	1.05	6 (11%)	59,59,63	1.43	9 (15%)
34	STE	b	621	-	15,15,19	0.40	0	14,14,19	0.78	0
24	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.33	8 (14%)
28	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.33	7 (15%)
22	CLA	C	509	-	56,73,73	1.38	7 (12%)	55,113,113	1.97	9 (16%)
34	STE	b	625	-	12,15,19	0.40	0	11,15,19	0.71	0
22	CLA	b	614	-	56,73,73	1.71	8 (14%)	55,113,113	1.49	9 (16%)
28	LMG	b	622	-	51,51,55	1.01	5 (9%)	59,59,63	1.47	7 (11%)
31	DGD	C	515	-	63,63,67	1.11	3 (4%)	77,77,81	1.39	13 (16%)
30	LHG	e	102	-	41,41,48	1.04	4 (9%)	44,47,54	1.36	5 (11%)
27	PL9	A	410	-	55,55,55	1.25	4 (7%)	68,69,69	1.83	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	601	37	56,73,73	1.63	4 (7%)	55,113,113	1.92	8 (14%)
34	STE	Z	101	-	7,7,19	0.33	0	6,6,19	0.67	0
34	STE	h	102	-	13,13,19	0.42	0	12,12,19	0.63	0
22	CLA	C	510	-	56,73,73	1.55	6 (10%)	55,113,113	1.58	6 (10%)
24	BCR	b	617	-	41,41,41	1.16	4 (9%)	56,56,56	1.40	8 (14%)
27	PL9	d	406	-	55,55,55	1.64	7 (12%)	68,69,69	1.69	15 (22%)
31	DGD	c	517	-	63,63,67	0.97	4 (6%)	77,77,81	1.42	10 (12%)
28	LMG	d	410	-	44,44,55	1.01	2 (4%)	52,52,63	1.36	8 (15%)
30	LHG	B	621	-	48,48,48	0.99	2 (4%)	51,54,54	1.09	3 (5%)
34	STE	a	413	-	9,9,19	0.49	0	8,8,19	0.52	0
22	CLA	b	616	-	51,68,73	1.44	10 (19%)	49,107,113	1.80	9 (18%)
24	BCR	b	618	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	8 (14%)
34	STE	b	626	-	16,19,19	0.45	0	15,19,19	0.72	0
34	STE	c	520	-	16,19,19	0.37	0	15,19,19	0.80	0
22	CLA	c	505	-	56,73,73	1.36	6 (10%)	55,113,113	1.58	9 (16%)
24	BCR	B	619	-	41,41,41	1.15	3 (7%)	56,56,56	1.29	7 (12%)
29	SQD	D	407	-	35,36,54	0.97	2 (5%)	42,45,65	2.28	12 (28%)
22	CLA	A	411	37	56,73,73	1.56	8 (14%)	55,113,113	1.59	9 (16%)
31	DGD	A	416	-	67,67,67	1.27	10 (14%)	81,81,81	1.44	11 (13%)
31	DGD	C	517	-	63,63,67	0.90	5 (7%)	77,77,81	1.32	6 (7%)
22	CLA	c	509	-	56,73,73	1.46	4 (7%)	55,113,113	1.86	12 (21%)
30	LHG	B	622	-	48,48,48	0.87	3 (6%)	51,54,54	1.40	8 (15%)
22	CLA	B	602	-	56,73,73	1.63	6 (10%)	55,113,113	1.75	10 (18%)
24	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
34	STE	C	520	-	15,15,19	0.39	0	14,14,19	0.80	0
22	CLA	C	507	37	56,73,73	1.60	5 (8%)	55,113,113	1.88	12 (21%)
34	STE	X	101	-	16,19,19	0.29	0	15,19,19	1.10	1 (6%)
34	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.68	0
22	CLA	C	506	-	56,73,73	1.66	9 (16%)	55,113,113	1.55	10 (18%)
30	LHG	d	408	-	48,48,48	0.92	3 (6%)	51,54,54	1.19	4 (7%)
28	LMG	b	624	-	55,55,55	0.87	3 (5%)	63,63,63	1.49	10 (15%)
22	CLA	c	513	-	56,73,73	1.54	5 (8%)	55,113,113	1.49	9 (16%)
22	CLA	C	511	3	56,73,73	1.92	6 (10%)	55,113,113	1.56	4 (7%)
22	CLA	D	403	-	56,73,73	1.57	11 (19%)	55,113,113	1.65	12 (21%)
34	STE	M	102	-	11,14,19	0.43	0	10,14,19	0.71	0
22	CLA	c	510	-	56,73,73	1.65	8 (14%)	55,113,113	1.69	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	607	37	56,73,73	1.61	10 (17%)	55,113,113	1.69	7 (12%)
22	CLA	d	404	-	56,73,73	1.65	8 (14%)	55,113,113	1.56	10 (18%)
22	CLA	c	511	3	56,73,73	1.53	6 (10%)	55,113,113	1.75	8 (14%)
22	CLA	b	610	37	56,73,73	1.48	8 (14%)	55,113,113	1.67	12 (21%)
23	PHO	d	402	-	67,69,69	1.24	7 (10%)	85,99,99	1.16	6 (7%)
22	CLA	b	603	-	56,73,73	1.56	8 (14%)	55,113,113	1.74	12 (21%)
22	CLA	B	615	-	56,73,73	1.64	7 (12%)	55,113,113	1.52	11 (20%)
34	STE	B	627	-	8,11,19	0.35	0	7,11,19	0.58	0
22	CLA	C	512	-	56,73,73	1.59	10 (17%)	55,113,113	1.57	12 (21%)
31	DGD	C	516	-	63,63,67	1.25	8 (12%)	77,77,81	1.34	9 (11%)
34	STE	j	101	-	8,11,19	0.54	0	7,11,19	0.39	0
34	STE	a	415	-	14,14,19	0.41	0	13,13,19	0.86	0
34	STE	I	101	-	14,14,19	0.45	0	13,13,19	0.59	0
22	CLA	b	612	-	56,73,73	1.38	6 (10%)	55,113,113	1.76	13 (23%)
34	STE	d	412	-	16,19,19	0.41	0	15,19,19	0.63	0
24	BCR	x	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
22	CLA	a	404	-	56,73,73	1.70	10 (17%)	55,113,113	1.76	11 (20%)
31	DGD	H	102	-	63,63,67	1.23	8 (12%)	77,77,81	1.47	12 (15%)
24	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	7 (12%)
30	LHG	d	407	-	48,48,48	0.95	2 (4%)	51,54,54	1.35	7 (13%)
33	OEX	a	417[A]	37,1,3	0,15,15	-	-	-	-	-
34	STE	R	101	-	8,11,19	0.42	0	7,11,19	0.64	0
22	CLA	C	502	-	56,73,73	1.54	6 (10%)	55,113,113	1.79	9 (16%)
29	SQD	A	415	-	38,38,54	1.00	3 (7%)	40,40,65	1.29	4 (10%)
24	BCR	k	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.05	3 (5%)
22	CLA	B	613	-	56,73,73	1.64	9 (16%)	55,113,113	1.84	9 (16%)
22	CLA	B	604	-	56,73,73	1.51	6 (10%)	55,113,113	2.02	14 (25%)
24	BCR	B	617	-	41,41,41	1.17	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	B	606	-	56,73,73	1.75	8 (14%)	55,113,113	1.47	9 (16%)
22	CLA	c	507	37	56,73,73	1.29	7 (12%)	55,113,113	1.73	14 (25%)
29	SQD	B	623	-	53,54,54	0.97	3 (5%)	62,65,65	1.76	11 (17%)
22	CLA	b	609	-	56,73,73	1.67	9 (16%)	55,113,113	1.59	10 (18%)
22	CLA	B	603	-	56,73,73	1.62	8 (14%)	55,113,113	1.52	11 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	402	-	1/1/20/20	9/37/115/115	-
22	CLA	a	402	-	1/1/20/20	6/37/115/115	-
22	CLA	A	405	-	1/1/17/20	6/24/102/115	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/20/20	7/37/115/115	-
31	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	c	512	-	1/1/20/20	21/37/115/115	-
24	BCR	Y	101	-	-	9/29/63/63	0/2/2/2
22	CLA	C	503	-	-	4/37/115/115	-
24	BCR	c	515	-	-	8/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/20/20	8/37/115/115	-
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
22	CLA	a	410	37	-	6/37/115/115	-
24	BCR	a	405	-	-	2/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/20/20	14/37/115/115	-
29	SQD	a	411	-	-	25/49/69/69	0/1/1/1
22	CLA	c	506	-	1/1/20/20	16/37/115/115	-
28	LMG	a	416	-	-	25/50/70/70	0/1/1/1
35	HEM	e	101	5,6	-	0/6/54/54	-
22	CLA	B	609	-	-	7/37/115/115	-
22	CLA	C	513	-	1/1/20/20	11/37/115/115	-
22	CLA	C	508	-	-	6/37/115/115	-
22	CLA	A	402	-	1/1/20/20	4/37/115/115	-
22	CLA	d	403	-	1/1/20/20	9/37/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/20/20	8/37/115/115	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
22	CLA	C	504	37	1/1/18/20	9/30/108/115	-
22	CLA	b	615	-	1/1/20/20	12/37/115/115	-
34	STE	d	411	-	-	9/12/14/17	-
22	CLA	B	616	-	1/1/19/20	9/31/109/115	-
34	STE	B	626	-	-	10/13/13/17	-
22	CLA	c	503	-	-	4/37/115/115	-
22	CLA	C	505	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	37	-	13/37/115/115	-
27	PL9	a	409	-	-	23/53/73/73	0/1/1/1
28	LMG	D	411	-	-	9/18/22/70	-
29	SQD	a	412	-	-	14/37/37/69	-
36	HEC	v	201	17	-	0/6/54/54	-
23	PHO	d	401	-	-	6/53/103/103	0/5/6/6
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
29	SQD	f	101	-	-	15/36/56/69	0/1/1/1
28	LMG	D	406	-	-	16/46/66/70	0/1/1/1
34	STE	B	625	-	-	7/13/15/17	-
22	CLA	b	604	-	1/1/20/20	5/37/115/115	-
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
34	STE	H	103	-	-	11/15/15/17	-
34	STE	l	102	-	-	9/15/15/17	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	LHG	l	101	-	-	18/53/53/53	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
22	CLA	B	612	-	1/1/20/20	11/37/115/115	-
34	STE	B	620	-	-	6/12/14/17	-
30	LHG	D	409	-	-	26/51/51/53	-
34	STE	C	519	-	-	5/7/9/17	-
30	LHG	A	414	-	-	31/53/53/53	-
34	STE	J	101	-	-	2/7/9/17	-
34	STE	L	101	-	-	4/7/9/17	-
28	LMG	C	518	-	-	20/43/63/70	0/1/1/1
30	LHG	D	408	-	-	24/53/53/53	-
22	CLA	B	601	37	1/1/20/20	20/37/115/115	-
34	STE	c	523	-	-	3/7/9/17	-
27	PL9	D	405	-	-	10/53/73/73	0/1/1/1
22	CLA	b	607	37	1/1/20/20	17/37/115/115	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
28	LMG	D	410	-	-	14/33/33/70	-
22	CLA	c	508	-	-	16/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	d	409	-	-	19/43/43/53	-
34	STE	d	413	-	-	9/15/17/17	-
28	LMG	c	522	-	-	19/44/64/70	0/1/1/1
34	STE	C	521	-	-	4/7/9/17	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	c	504	37	1/1/19/20	9/31/109/115	-
22	CLA	b	605	-	1/1/20/20	11/37/115/115	-
22	CLA	b	611	-	1/1/20/20	9/37/115/115	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
36	HEC	V	201	17	-	0/6/54/54	-
34	STE	b	627	-	-	5/7/7/17	-
34	STE	B	624	-	-	3/7/9/17	-
22	CLA	B	614	-	1/1/20/20	14/37/115/115	-
34	STE	t	102	-	-	3/9/11/17	-
22	CLA	b	602	-	1/1/20/20	12/37/115/115	-
34	STE	T	102	-	-	7/12/12/17	-
35	HEM	F	101	5,6	-	0/6/54/54	-
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
22	CLA	b	613	-	1/1/20/20	4/37/115/115	-
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
28	LMG	A	412	-	-	17/43/63/70	0/1/1/1
22	CLA	A	403	37	1/1/20/20	14/37/115/115	-
22	CLA	B	605	-	1/1/20/20	11/37/115/115	-
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
22	CLA	B	608	-	-	1/37/115/115	-
34	STE	b	623	-	-	9/15/17/17	-
28	LMG	c	521	-	-	24/43/63/70	0/1/1/1
22	CLA	B	610	37	1/1/20/20	7/37/115/115	-
23	PHO	A	404	-	-	4/53/103/103	0/5/6/6
34	STE	a	414	-	-	4/7/9/17	-
24	BCR	k	102	-	-	7/29/63/63	0/2/2/2
28	LMG	M	101	-	-	17/46/66/70	0/1/1/1
34	STE	b	621	-	-	5/13/13/17	-
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
22	CLA	C	509	-	1/1/20/20	9/37/115/115	-
34	STE	b	625	-	-	4/11/13/17	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-
28	LMG	b	622	-	-	24/46/66/70	0/1/1/1
31	DGD	C	515	-	-	22/51/91/95	0/2/2/2
30	LHG	e	102	-	-	25/46/46/53	-
27	PL9	A	410	-	-	22/53/73/73	0/1/1/1
22	CLA	b	601	37	1/1/20/20	17/37/115/115	-
34	STE	Z	101	-	-	3/5/5/17	-
34	STE	h	102	-	-	5/11/11/17	-
22	CLA	C	510	-	1/1/20/20	9/37/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
27	PL9	d	406	-	-	14/53/73/73	0/1/1/1
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
28	LMG	d	410	-	-	12/39/59/70	0/1/1/1
30	LHG	B	621	-	-	26/53/53/53	-
34	STE	a	413	-	-	3/7/7/17	-
22	CLA	b	616	-	1/1/19/20	13/31/109/115	-
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	STE	b	626	-	-	4/15/17/17	-
34	STE	c	520	-	-	9/15/17/17	-
22	CLA	c	505	-	1/1/20/20	7/37/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
22	CLA	A	411	37	-	11/37/115/115	-
31	DGD	A	416	-	-	24/55/95/95	0/2/2/2
31	DGD	C	517	-	-	15/51/91/95	0/2/2/2
22	CLA	c	509	-	1/1/20/20	10/37/115/115	-
30	LHG	B	622	-	-	22/53/53/53	-
22	CLA	B	602	-	-	6/37/115/115	-
24	BCR	K	101	-	-	14/29/63/63	0/2/2/2
34	STE	C	520	-	-	5/13/13/17	-
22	CLA	C	507	37	1/1/20/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	STE	X	101	-	-	9/15/17/17	-
34	STE	M	103	-	-	1/7/7/17	-
22	CLA	C	506	-	1/1/20/20	12/37/115/115	-
30	LHG	d	408	-	-	22/53/53/53	-
28	LMG	b	624	-	-	29/50/70/70	0/1/1/1
22	CLA	c	513	-	1/1/20/20	9/37/115/115	-
22	CLA	C	511	3	1/1/20/20	12/37/115/115	-
22	CLA	D	403	-	-	10/37/115/115	-
34	STE	M	102	-	-	4/10/12/17	-
22	CLA	c	510	-	1/1/20/20	12/37/115/115	-
22	CLA	B	607	37	1/1/20/20	10/37/115/115	-
22	CLA	d	404	-	1/1/20/20	9/37/115/115	-
22	CLA	c	511	3	1/1/20/20	13/37/115/115	-
22	CLA	b	610	37	1/1/20/20	7/37/115/115	-
23	PHO	d	402	-	-	9/53/103/103	0/5/6/6
22	CLA	b	603	-	1/1/20/20	7/37/115/115	-
22	CLA	B	615	-	1/1/20/20	8/37/115/115	-
34	STE	B	627	-	-	5/7/9/17	-
22	CLA	C	512	-	1/1/20/20	15/37/115/115	-
31	DGD	C	516	-	-	20/51/91/95	0/2/2/2
34	STE	j	101	-	-	4/7/9/17	-
34	STE	a	415	-	-	7/12/12/17	-
34	STE	I	101	-	-	6/12/12/17	-
22	CLA	b	612	-	1/1/20/20	6/37/115/115	-
34	STE	d	412	-	-	10/15/17/17	-
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2
22	CLA	a	404	-	1/1/20/20	8/37/115/115	-
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	BCR	b	619	-	-	3/29/63/63	0/2/2/2
30	LHG	d	407	-	-	22/53/53/53	-
34	STE	R	101	-	-	4/7/9/17	-
22	CLA	C	502	-	1/1/20/20	6/37/115/115	-
29	SQD	A	415	-	-	11/39/39/69	-
24	BCR	k	101	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	613	-	1/1/20/20	12/37/115/115	-
22	CLA	B	604	-	1/1/20/20	10/37/115/115	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/20/20	12/37/115/115	-
22	CLA	c	507	37	1/1/20/20	8/37/115/115	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
22	CLA	b	609	-	-	4/37/115/115	-
22	CLA	B	603	-	1/1/20/20	12/37/115/115	-

The worst 5 of 792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	MG-NA	8.45	2.26	2.06
22	C	511	CLA	MG-NA	8.43	2.26	2.06
22	B	613	CLA	C4B-NB	8.39	1.42	1.35
22	B	614	CLA	C4B-NB	8.14	1.42	1.35
22	a	410	CLA	MG-NA	7.99	2.25	2.06

The worst 5 of 1282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	10.68	111.51	106.71
22	B	601	CLA	C4A-NA-C1A	10.55	111.45	106.71
22	b	601	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	B	604	CLA	C4A-NA-C1A	9.36	110.91	106.71
29	b	620	SQD	O6-C1-C2	9.26	122.76	108.30

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND
22	B	603	CLA	ND

5 of 1883 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC

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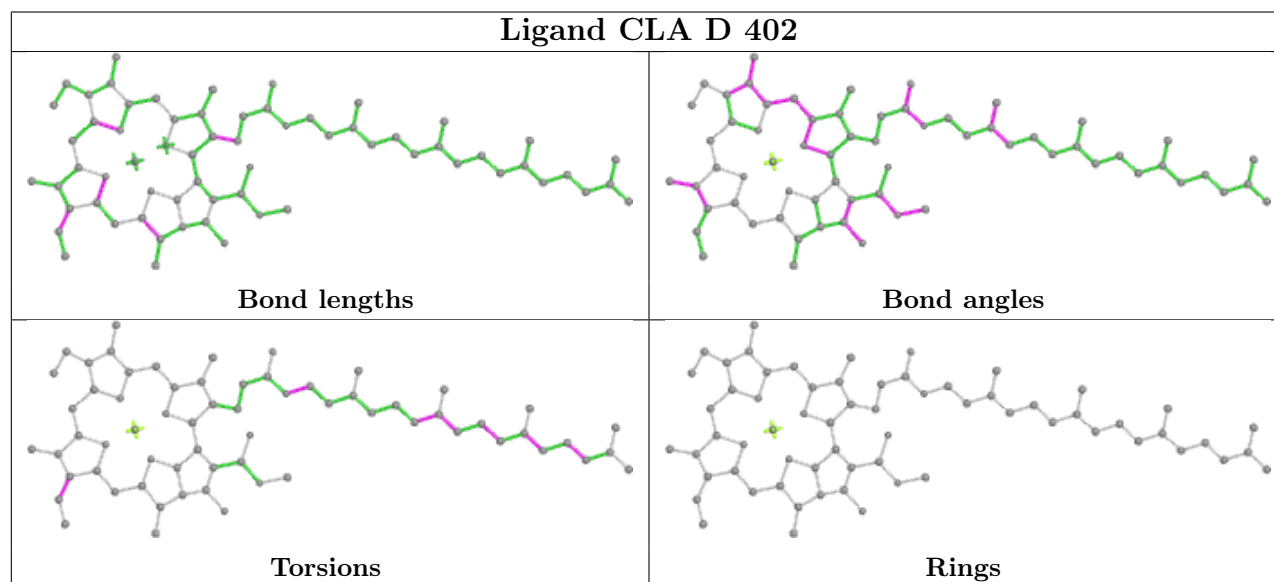
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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C2-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
22	A	411	CLA	CHA-CBD-CGD-O1D
22	A	411	CLA	CHA-CBD-CGD-O2D

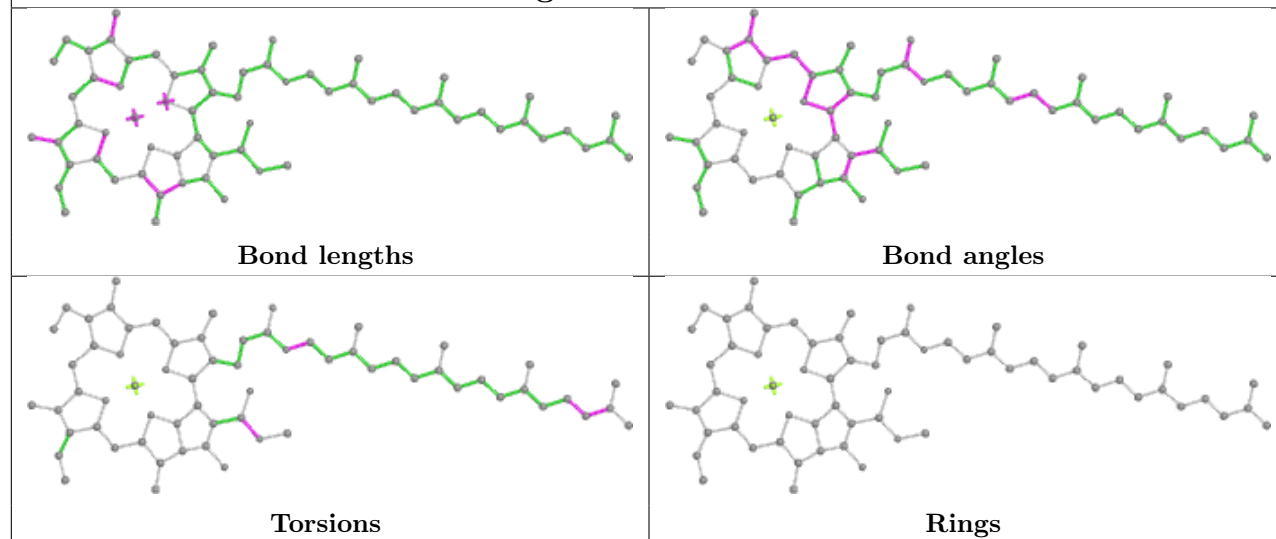
There are no ring outliers.

No monomer is involved in short contacts.

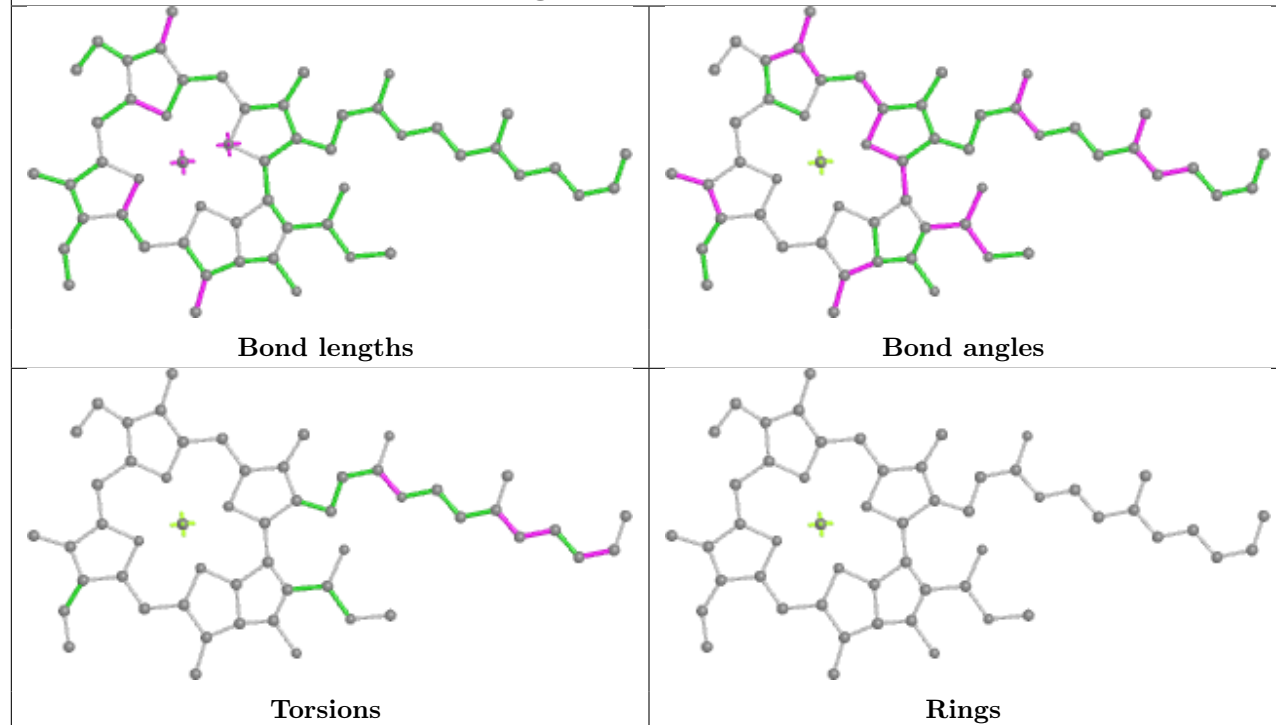
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



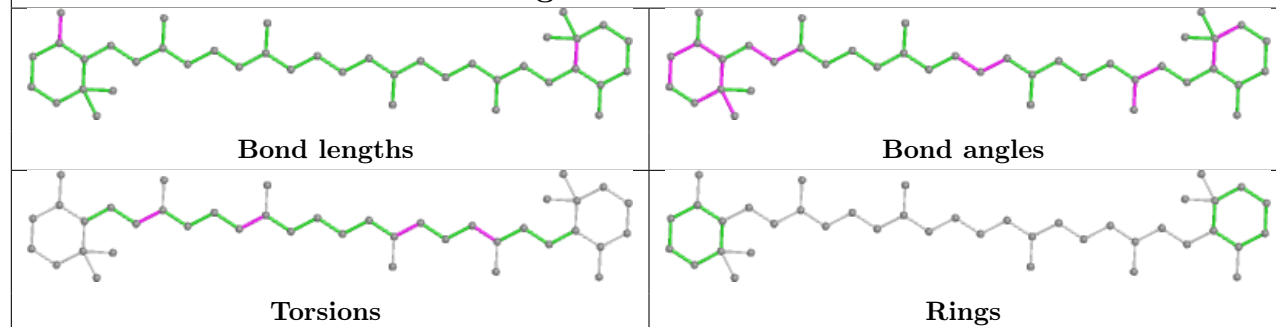
Ligand CLA a 402



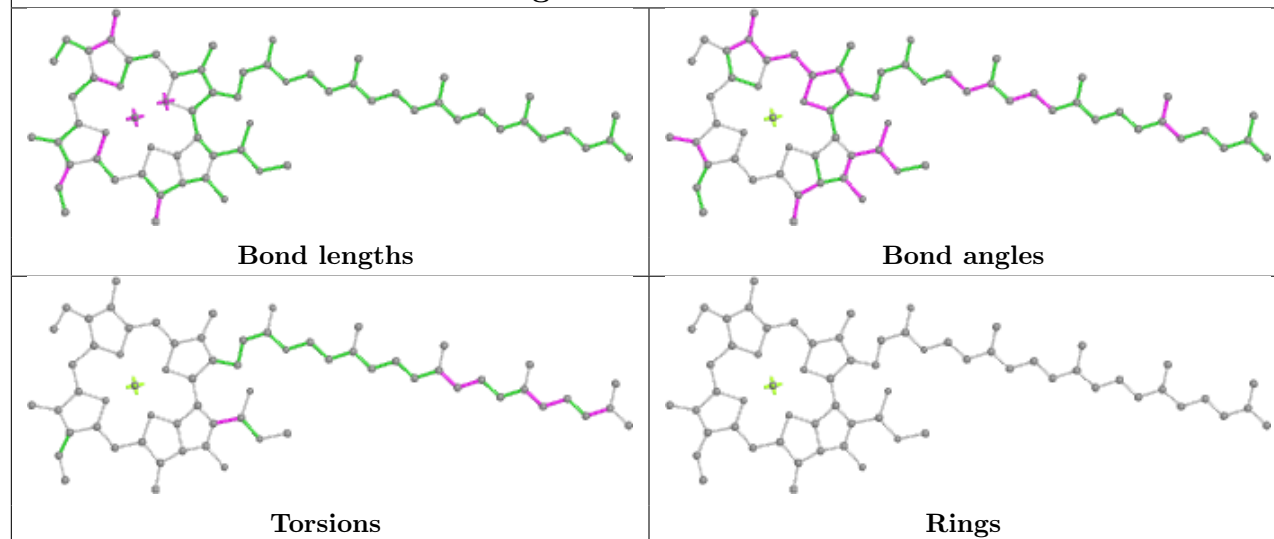
Ligand CLA A 405



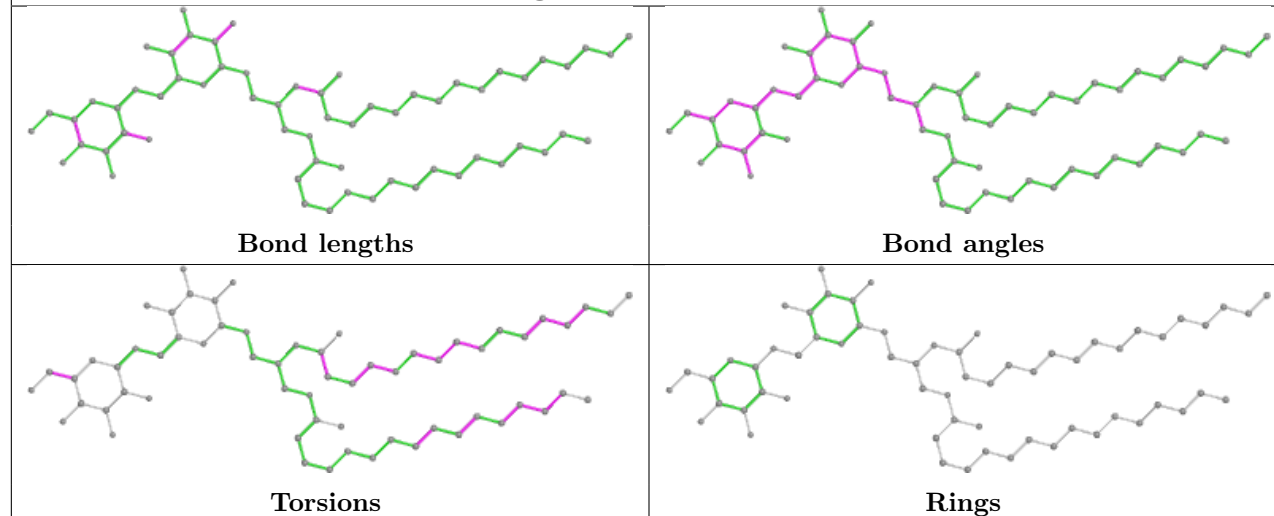
Ligand BCR t 101



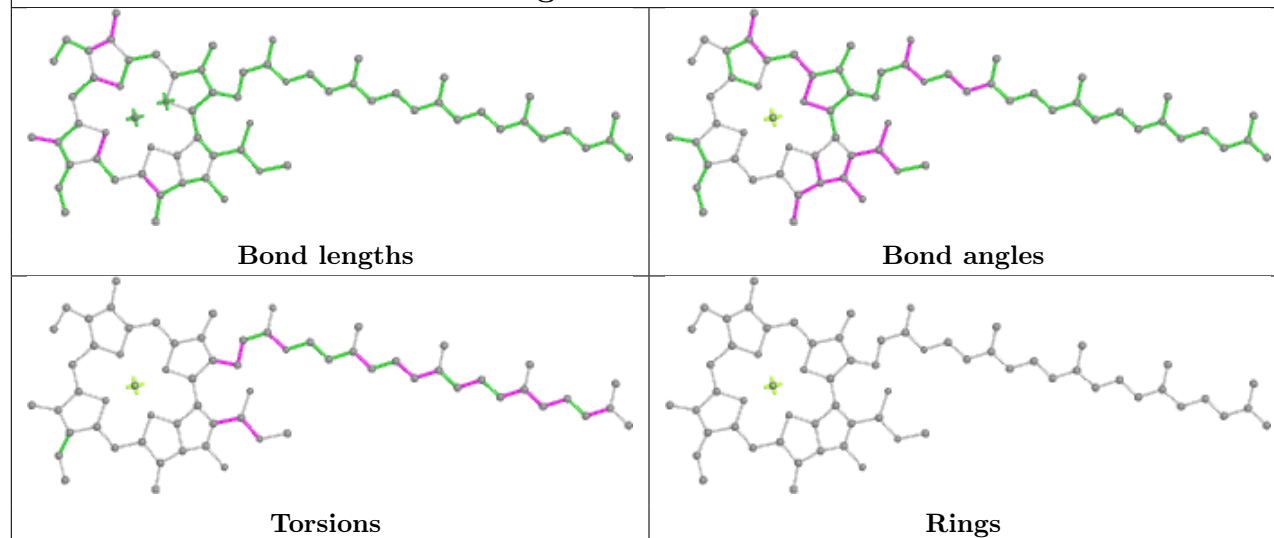
Ligand CLA B 611

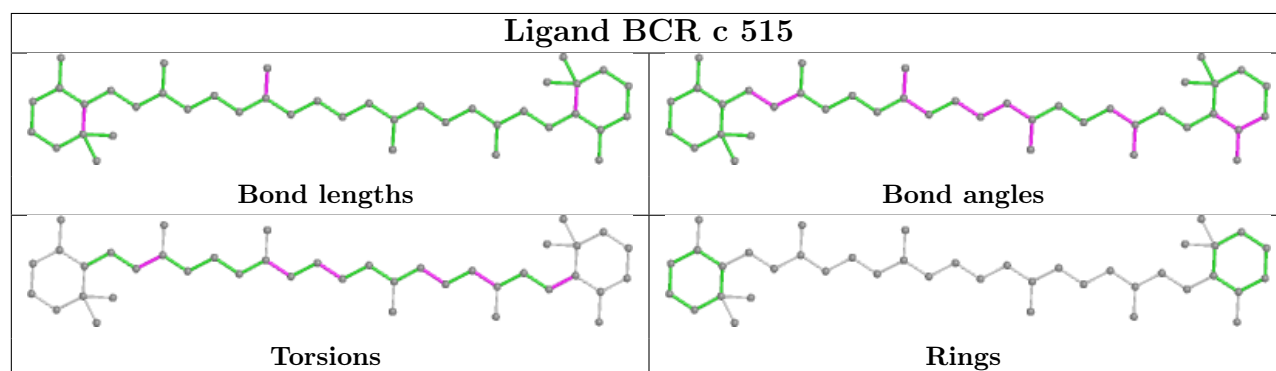
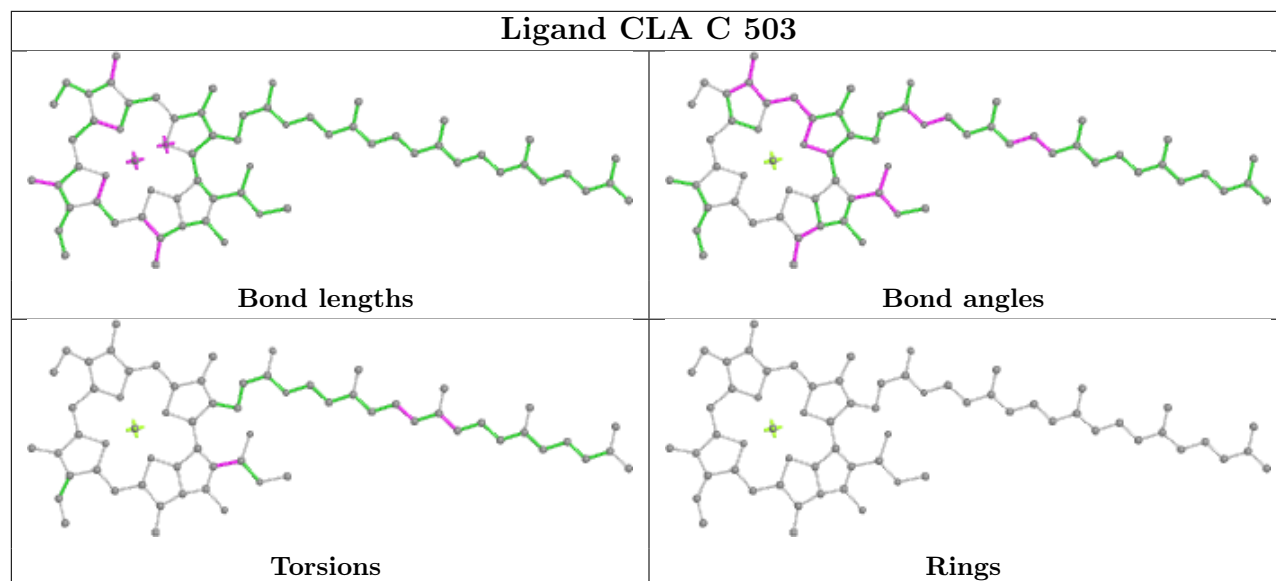
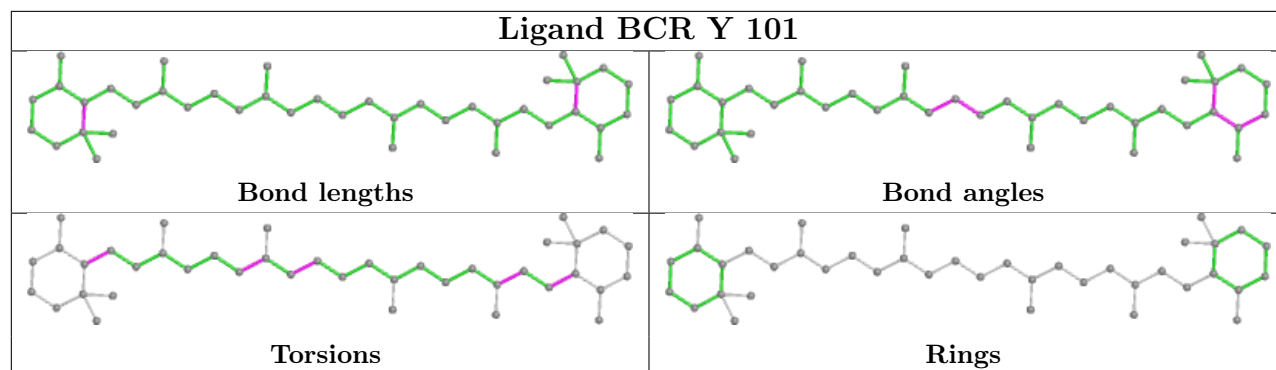


Ligand DGD h 101

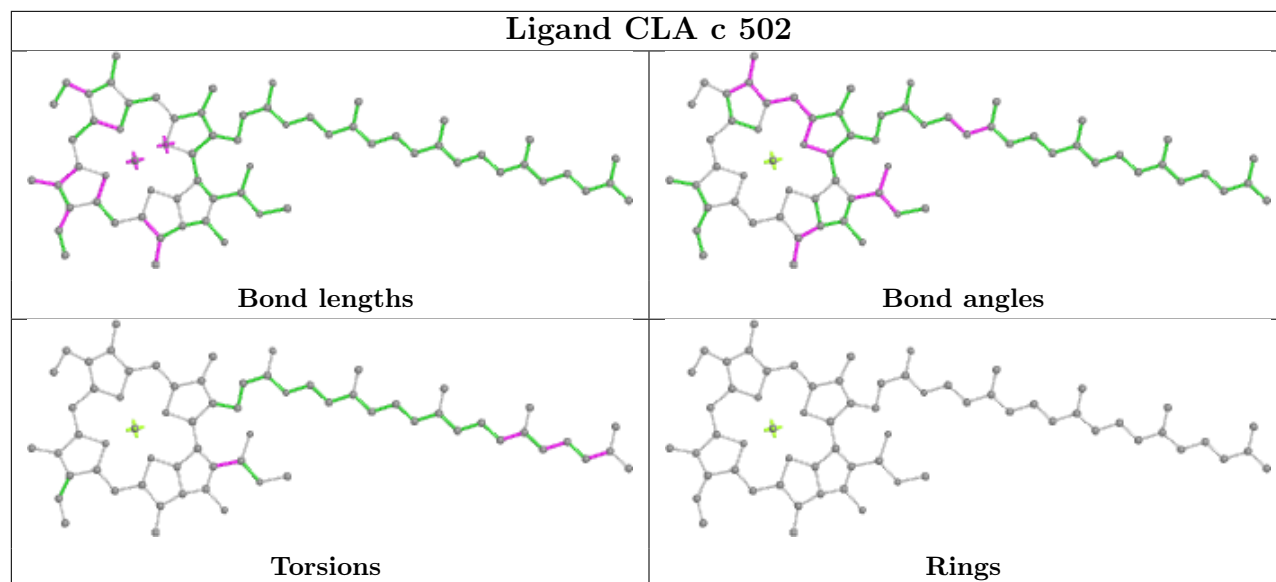


Ligand CLA c 512

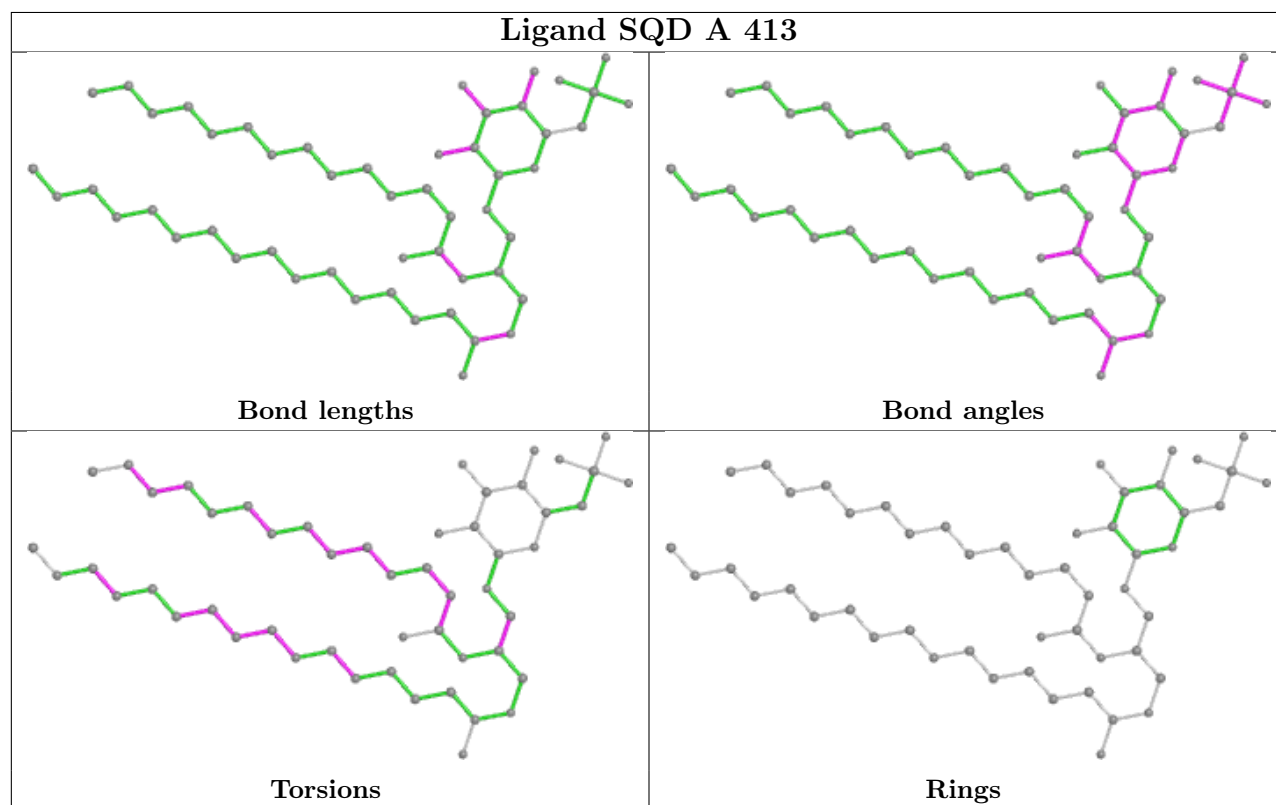


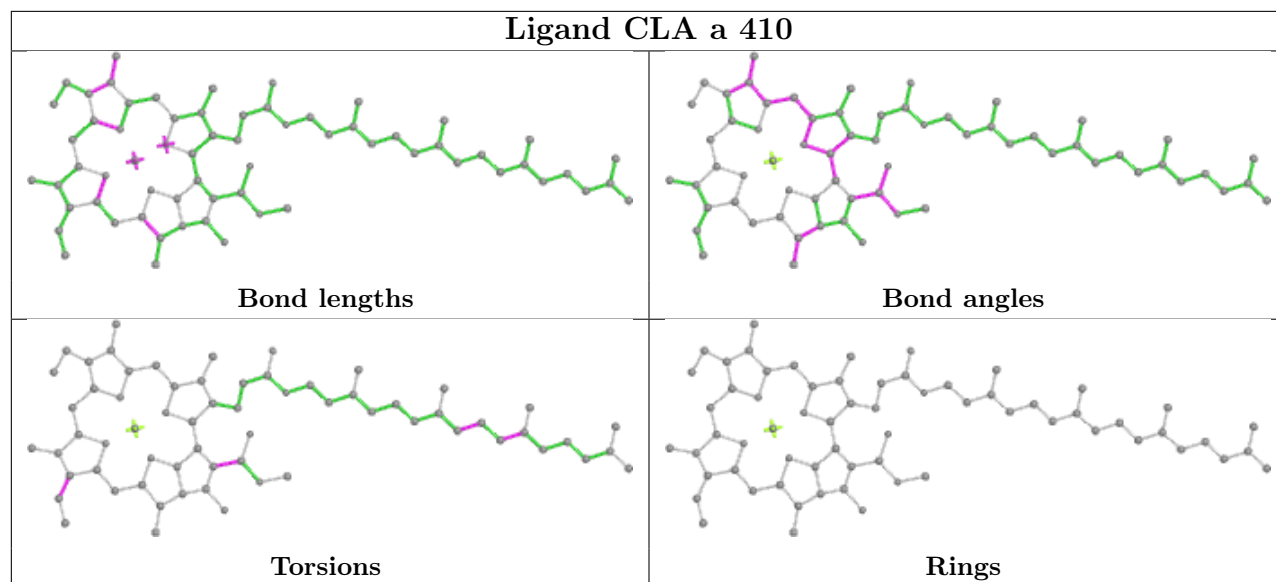
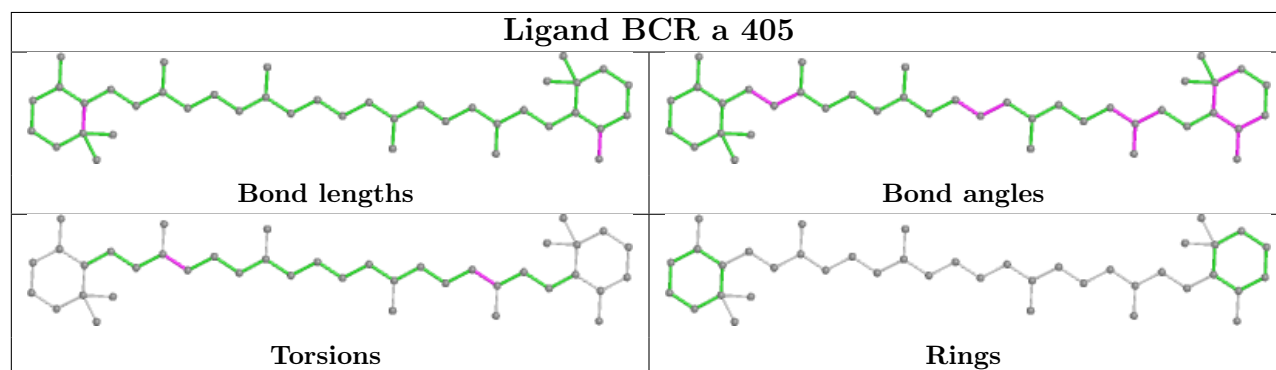
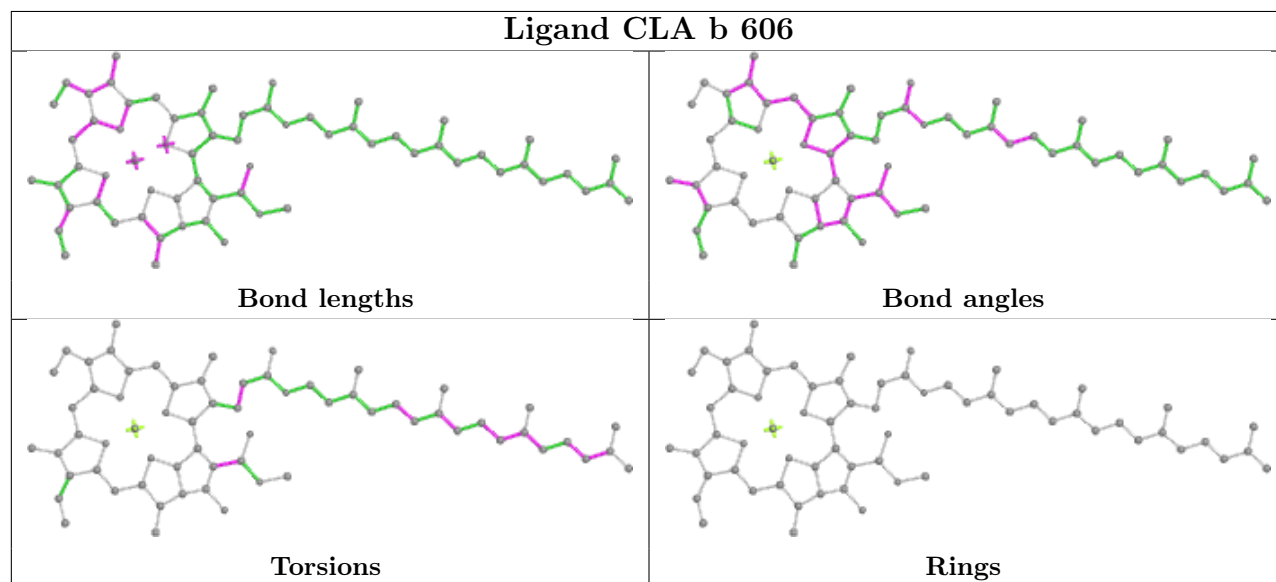


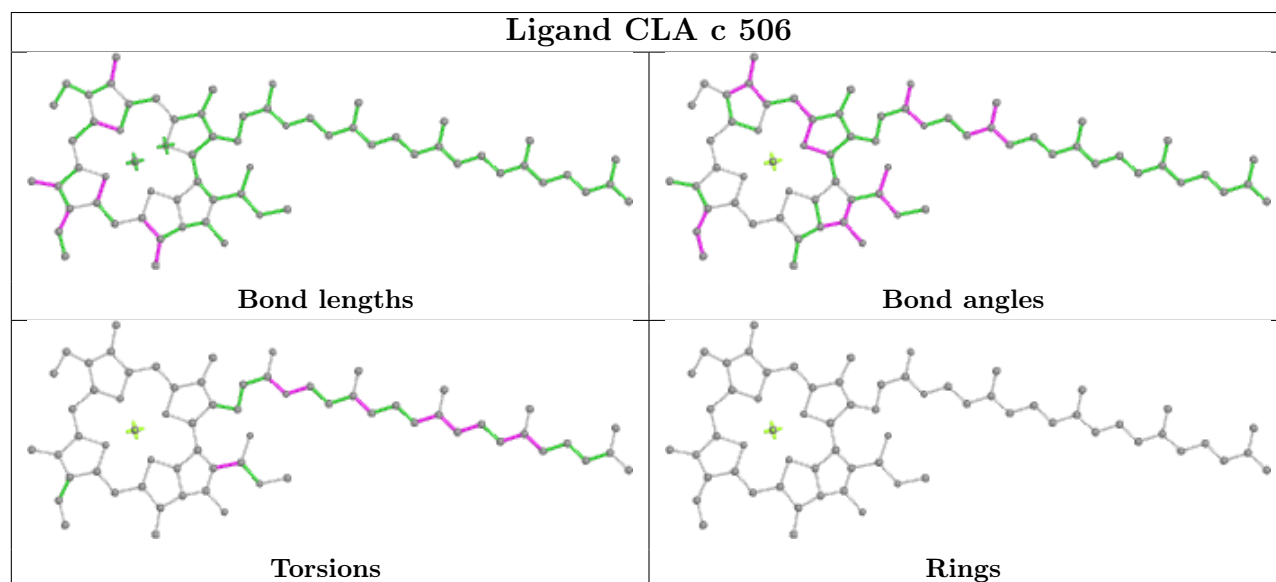
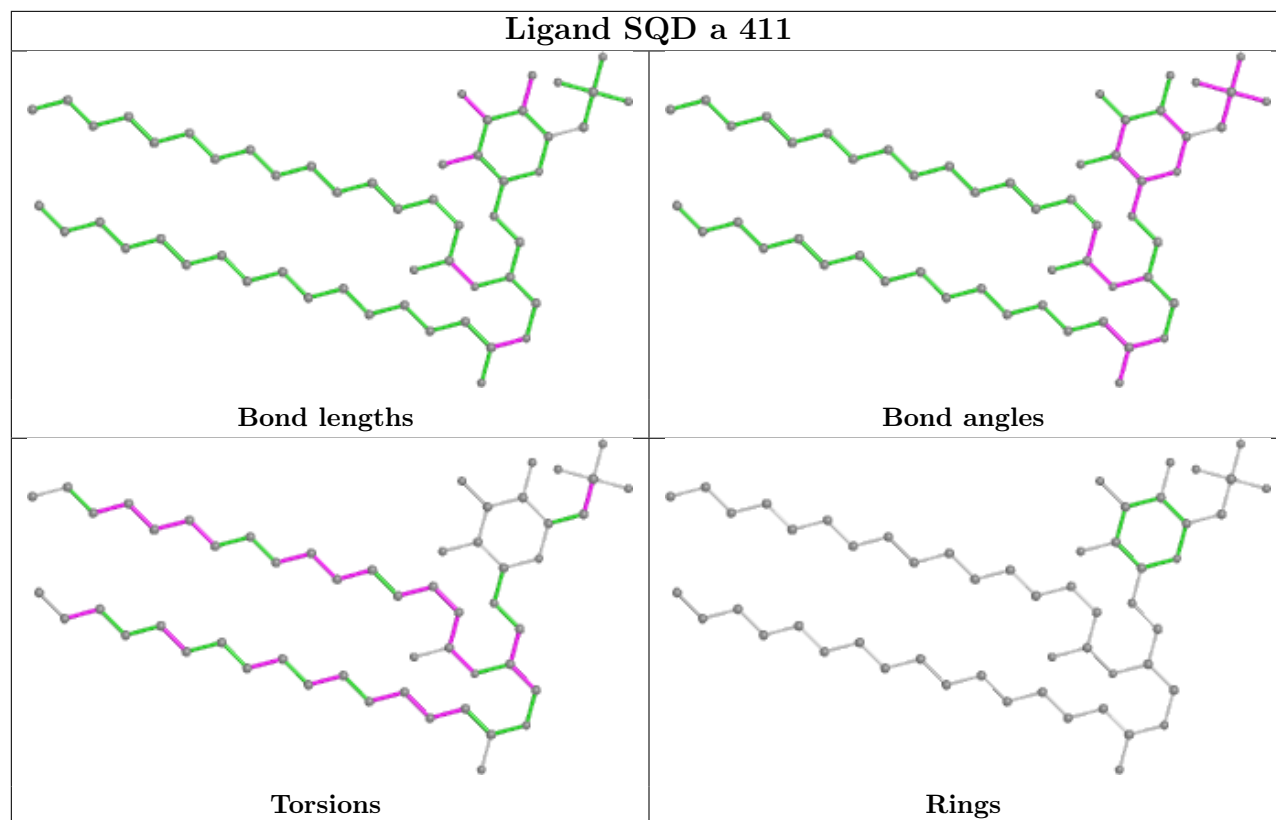
Ligand CLA c 502

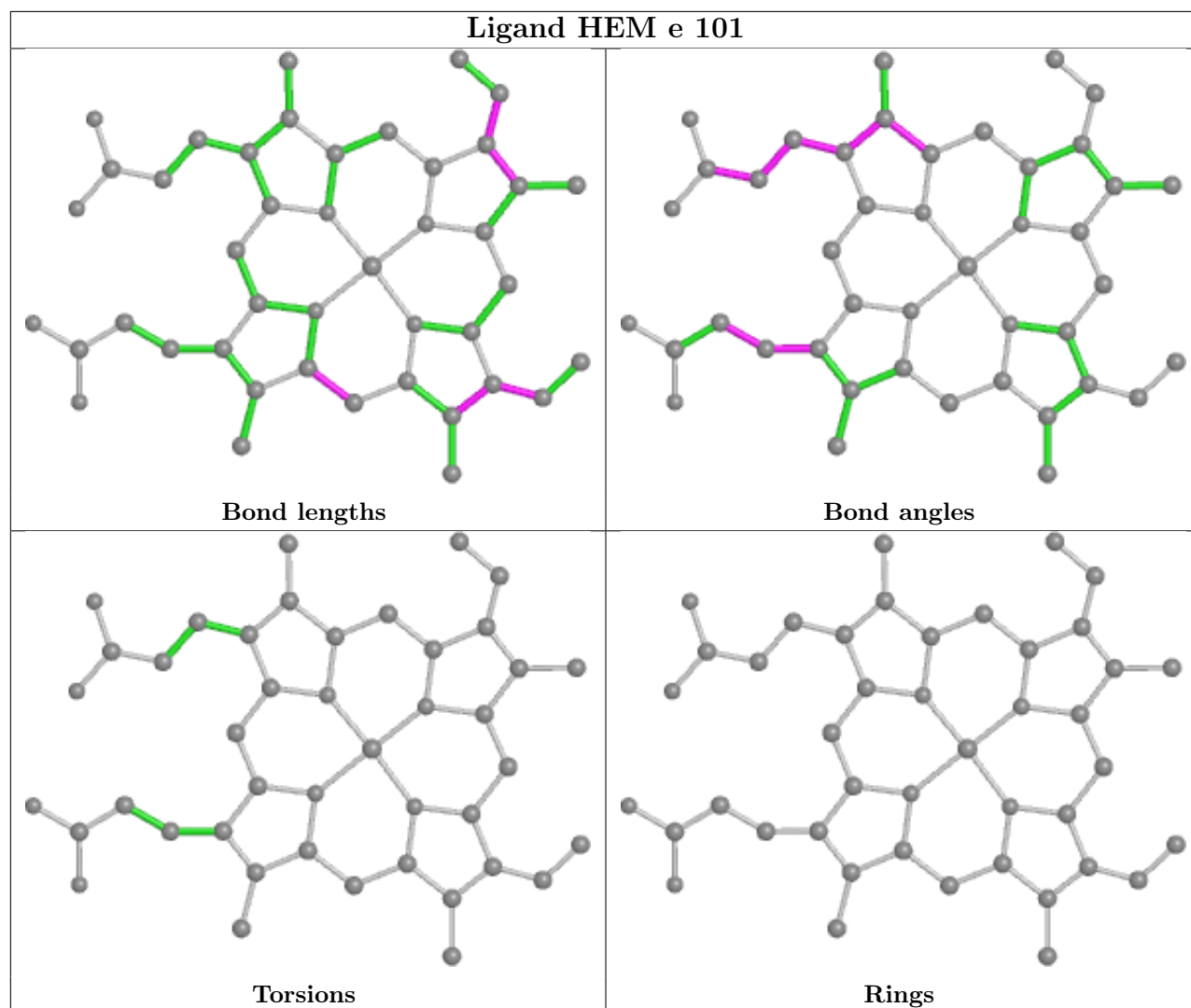
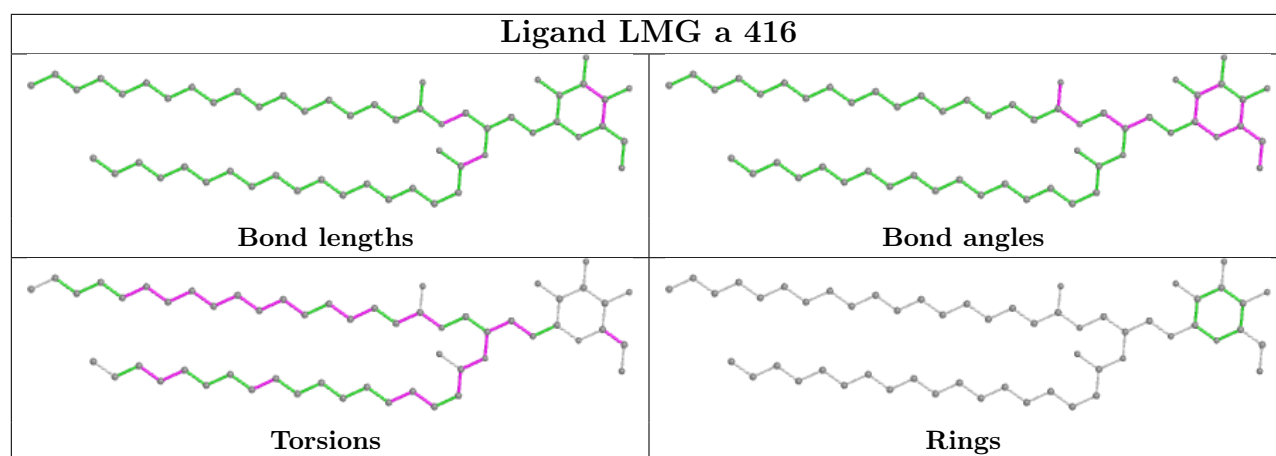


Ligand SQD A 413

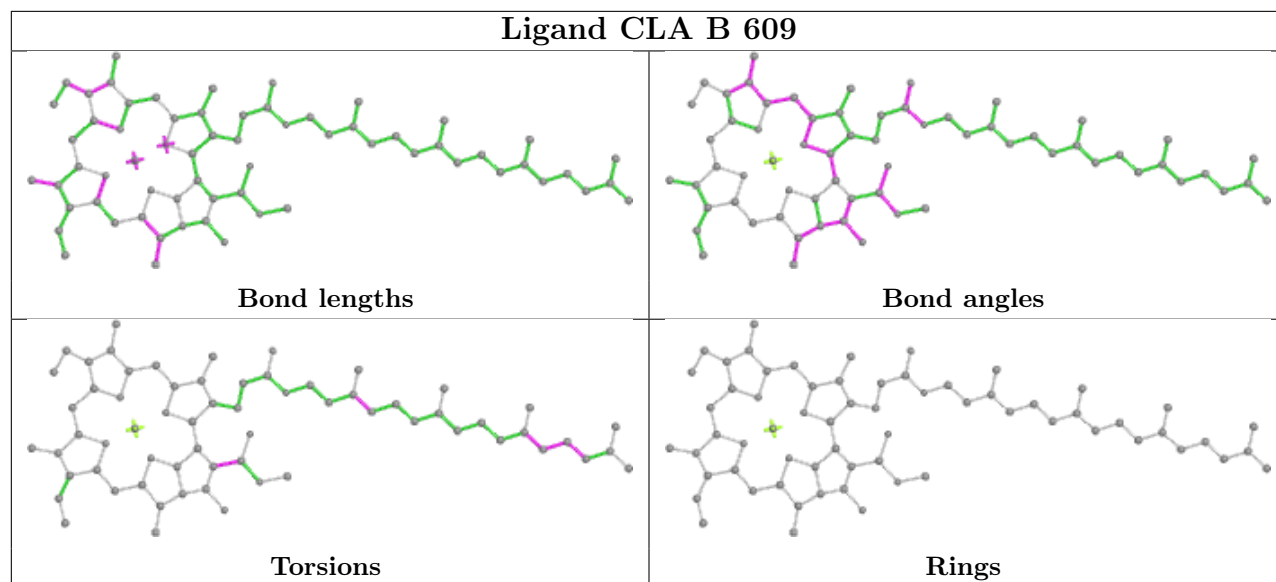


Ligand CLA a 410**Ligand BCR a 405****Ligand CLA b 606**

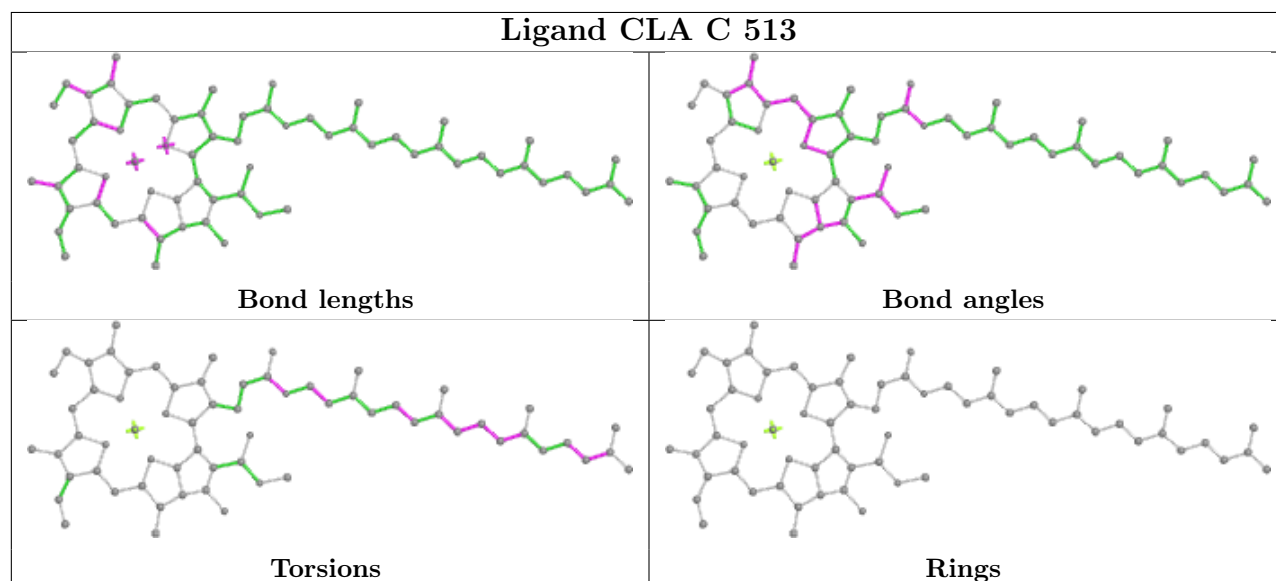




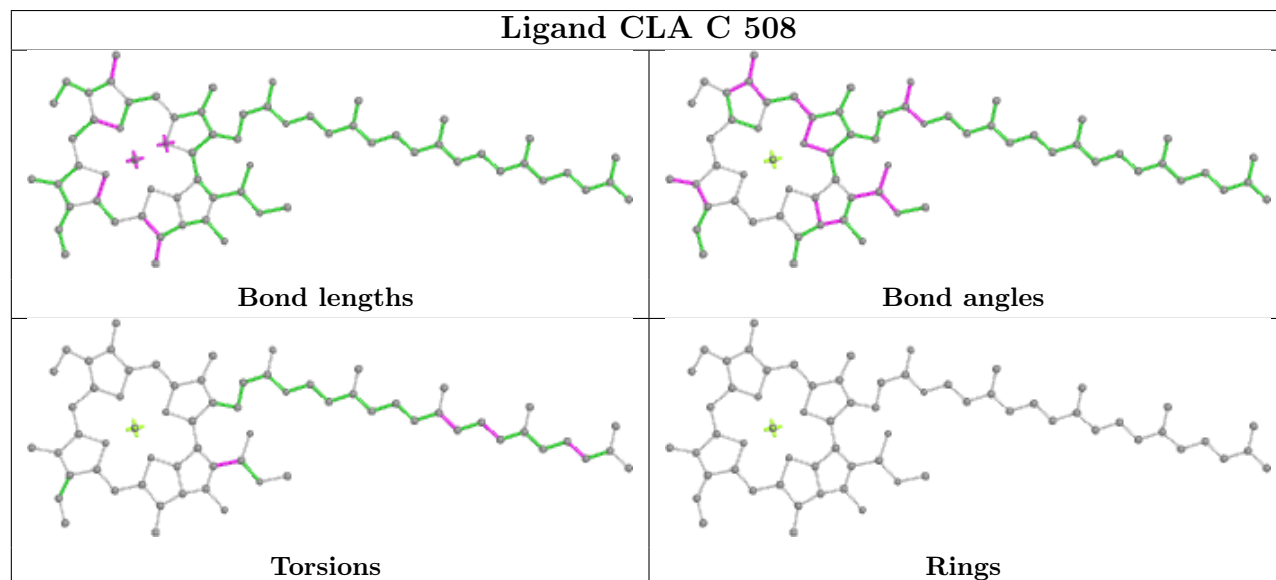
Ligand CLA B 609



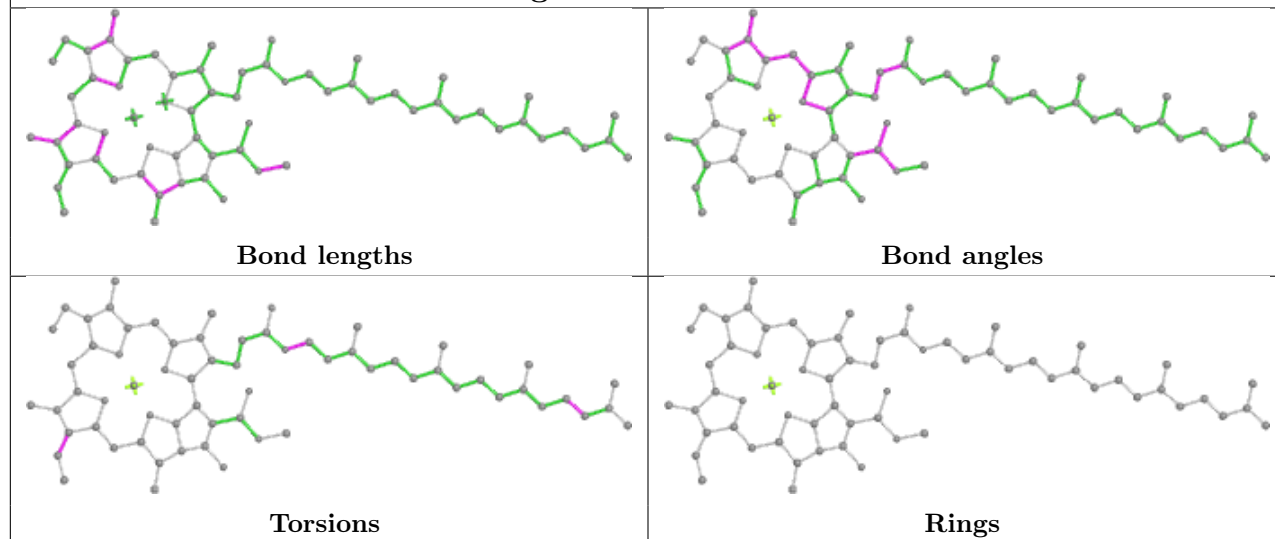
Ligand CLA C 513



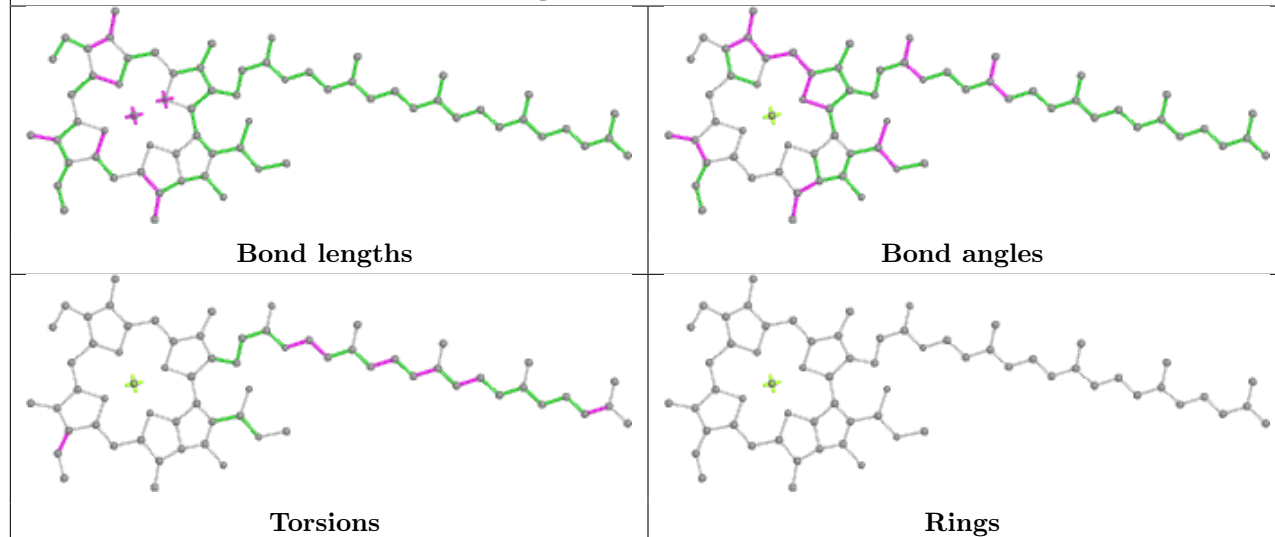
Ligand CLA C 508



Ligand CLA A 402

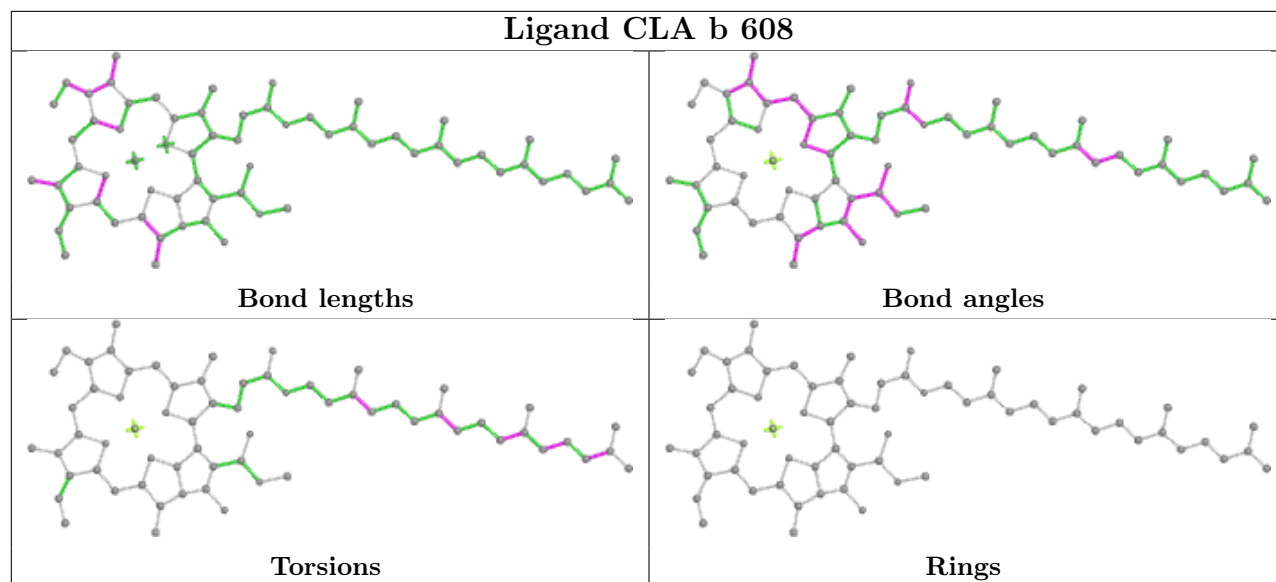
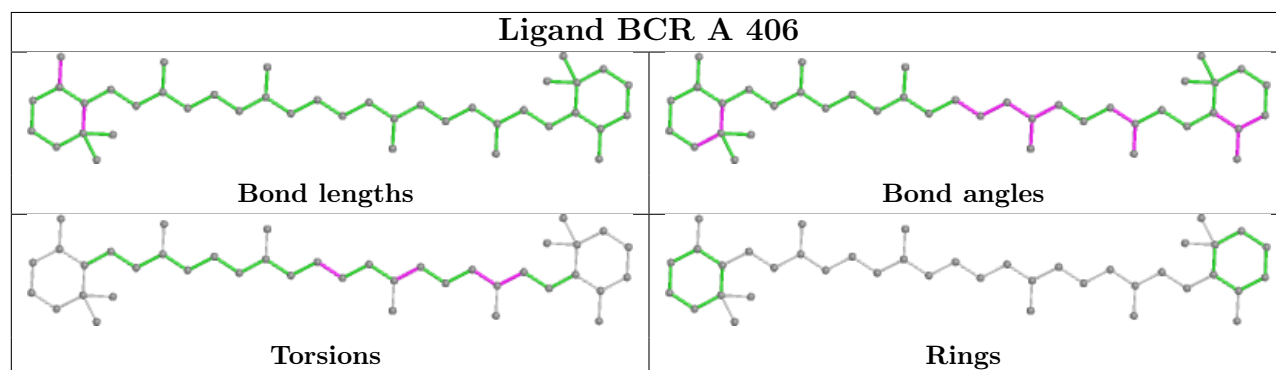
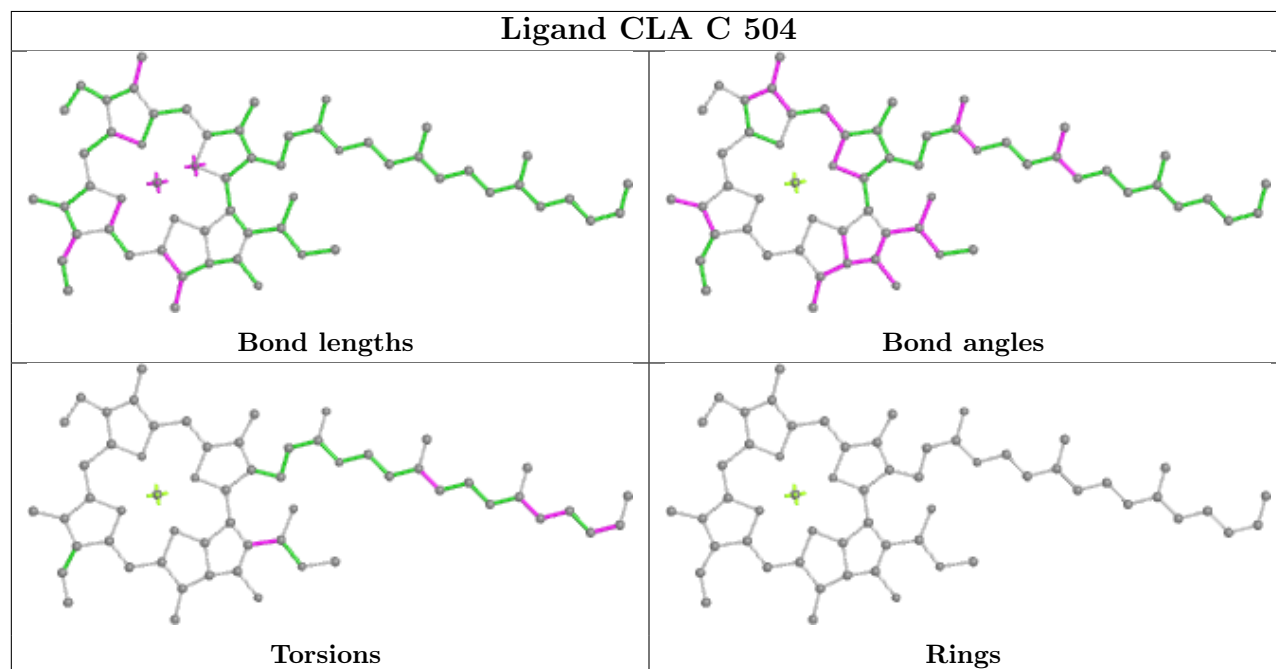


Ligand CLA d 403

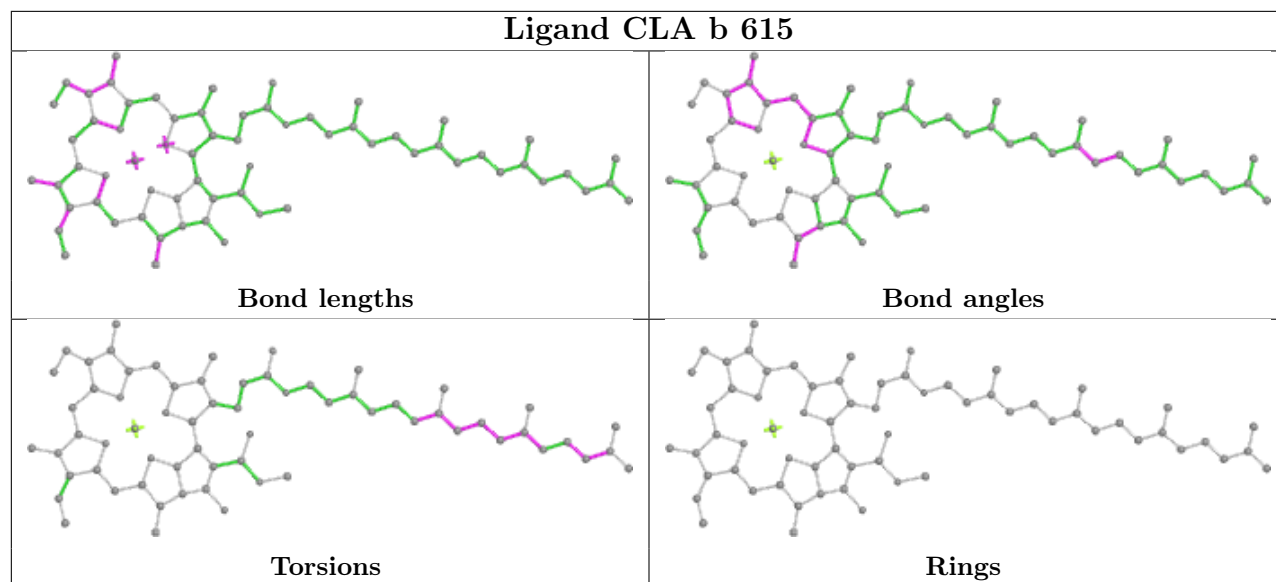


Ligand BCR d 405

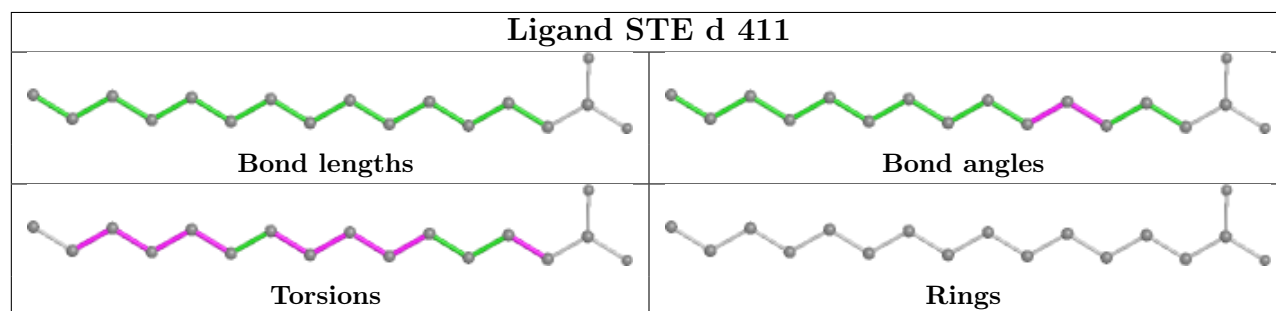


Ligand CLA b 608**Ligand BCR A 406****Ligand CLA C 504**

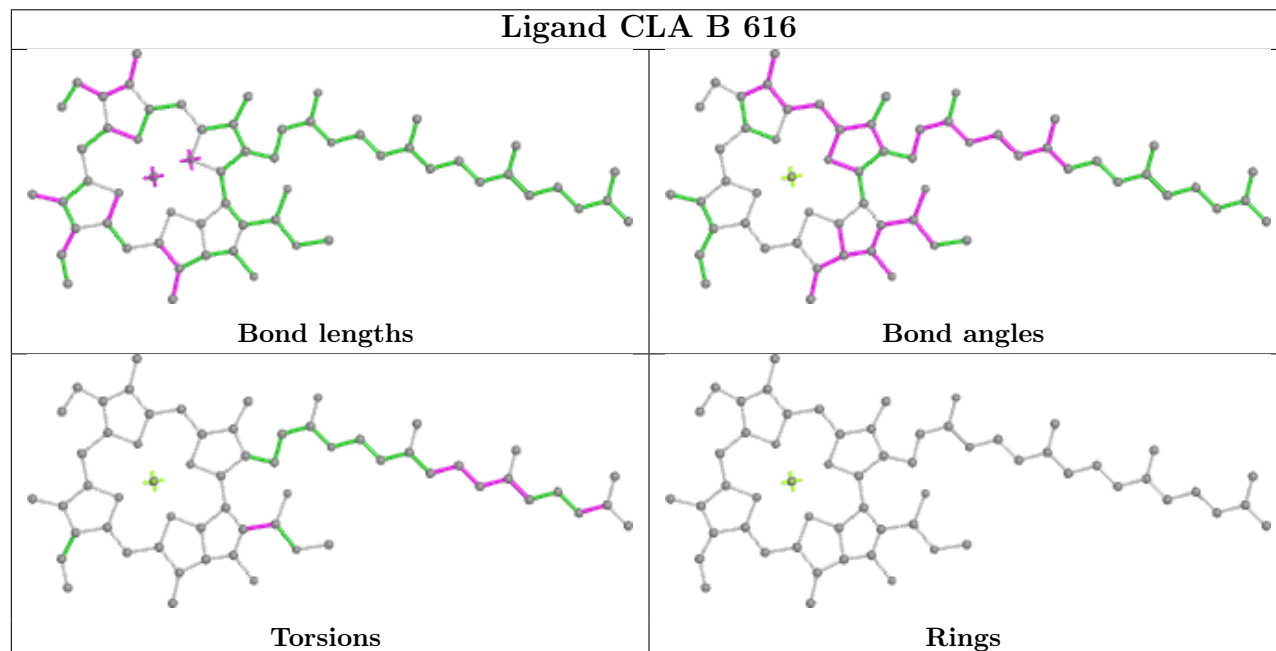
Ligand CLA b 615

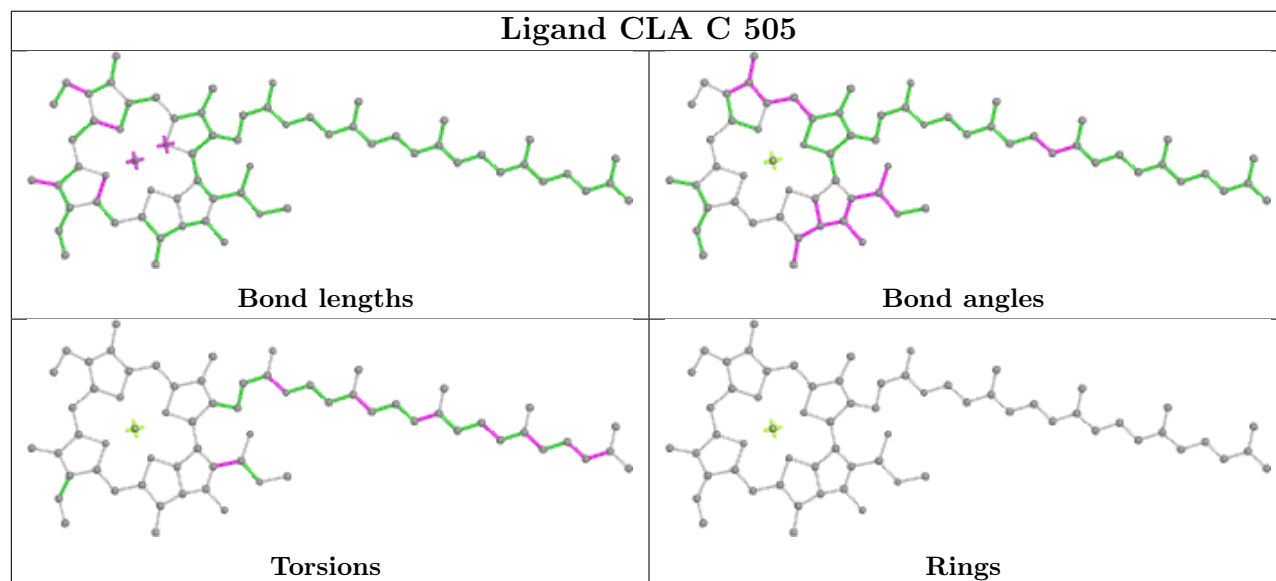
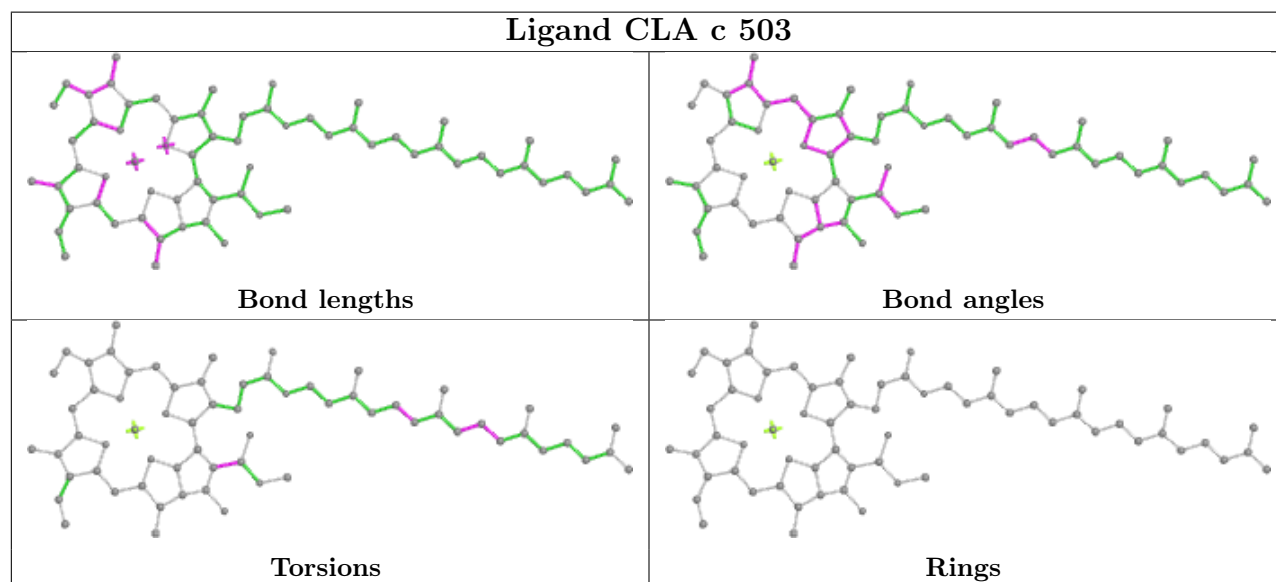
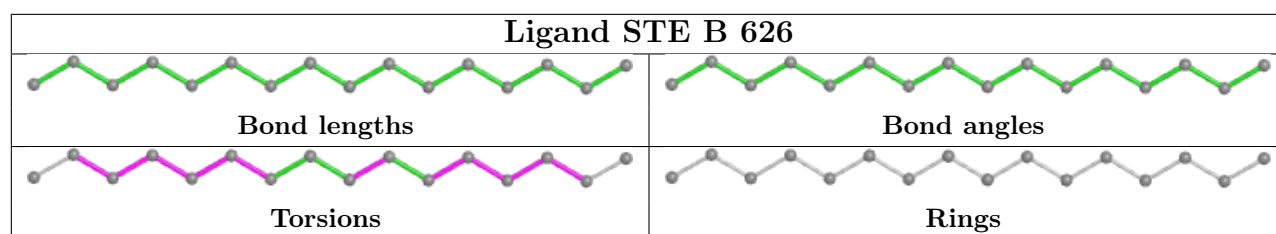


Ligand STE d 411

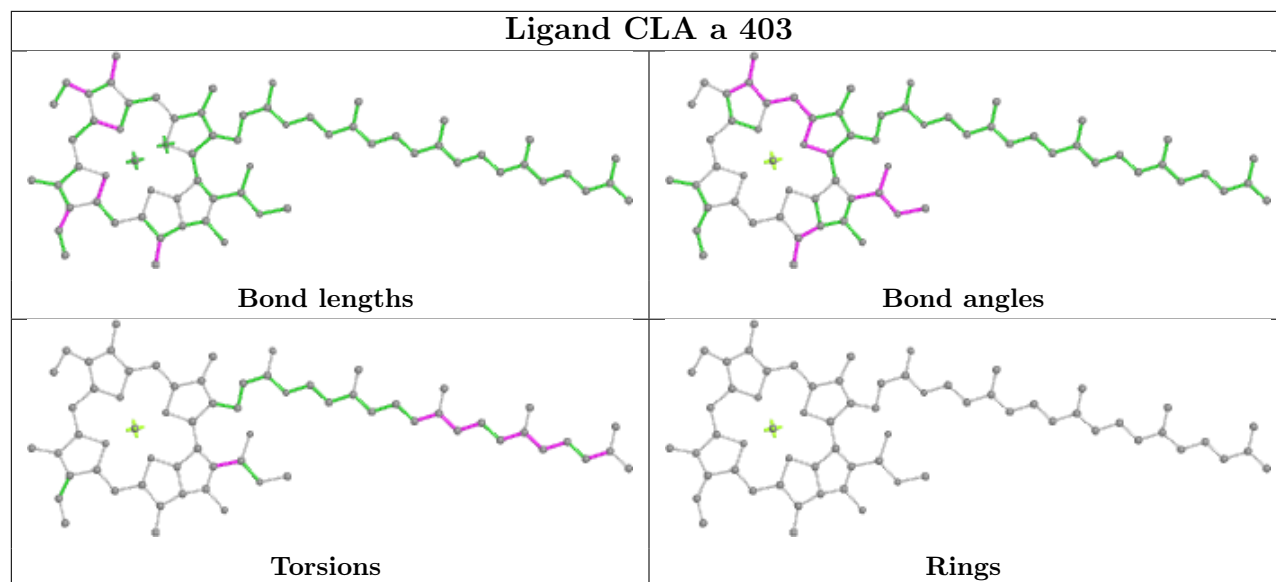


Ligand CLA B 616

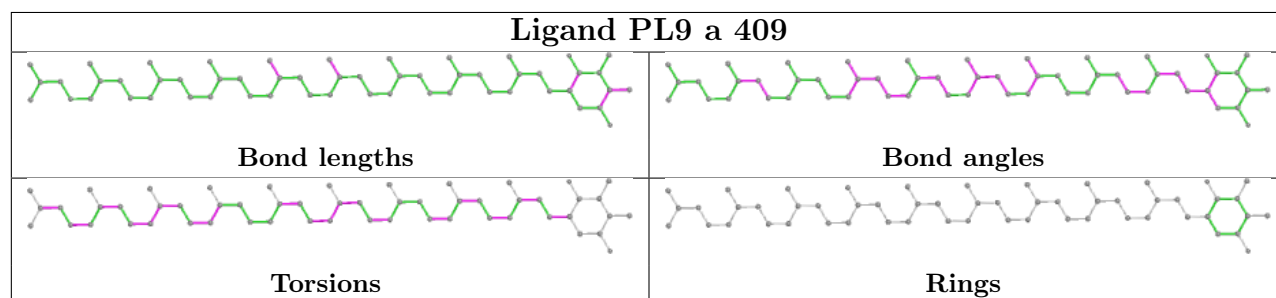




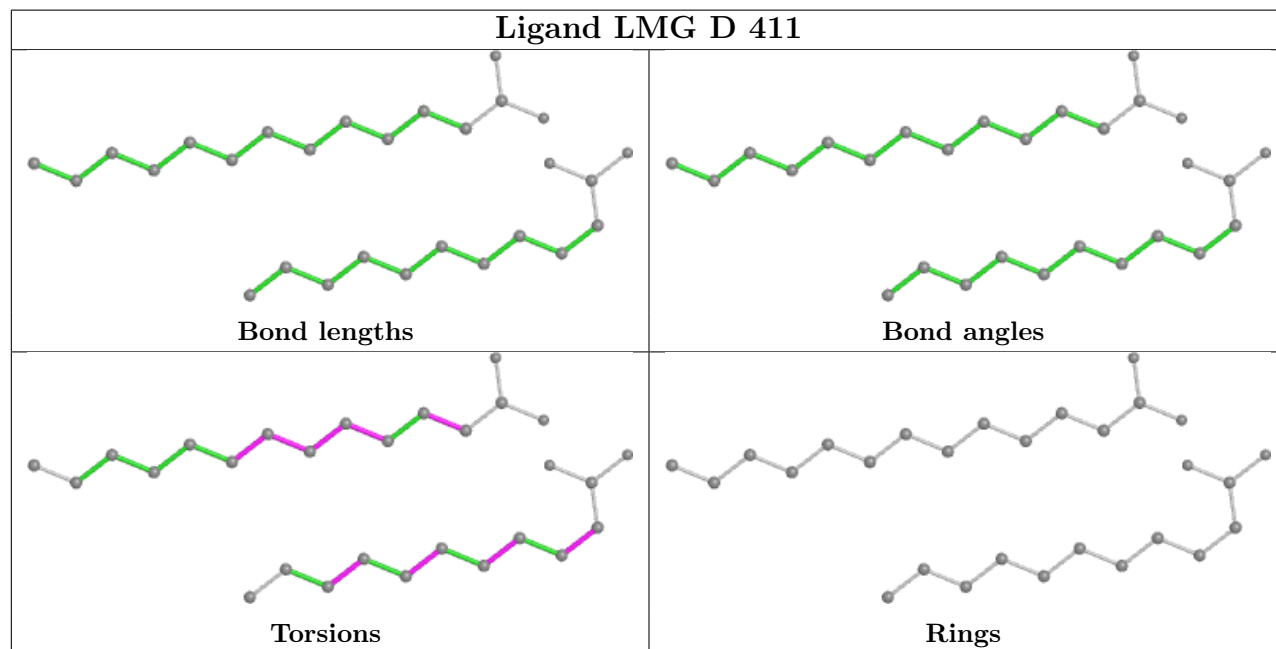
Ligand CLA a 403



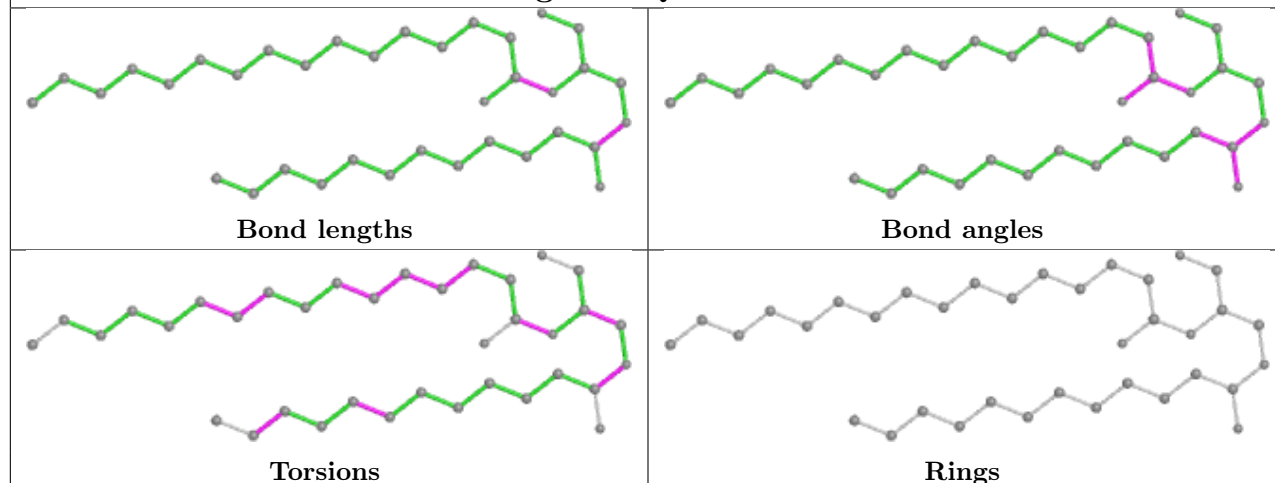
Ligand PL9 a 409



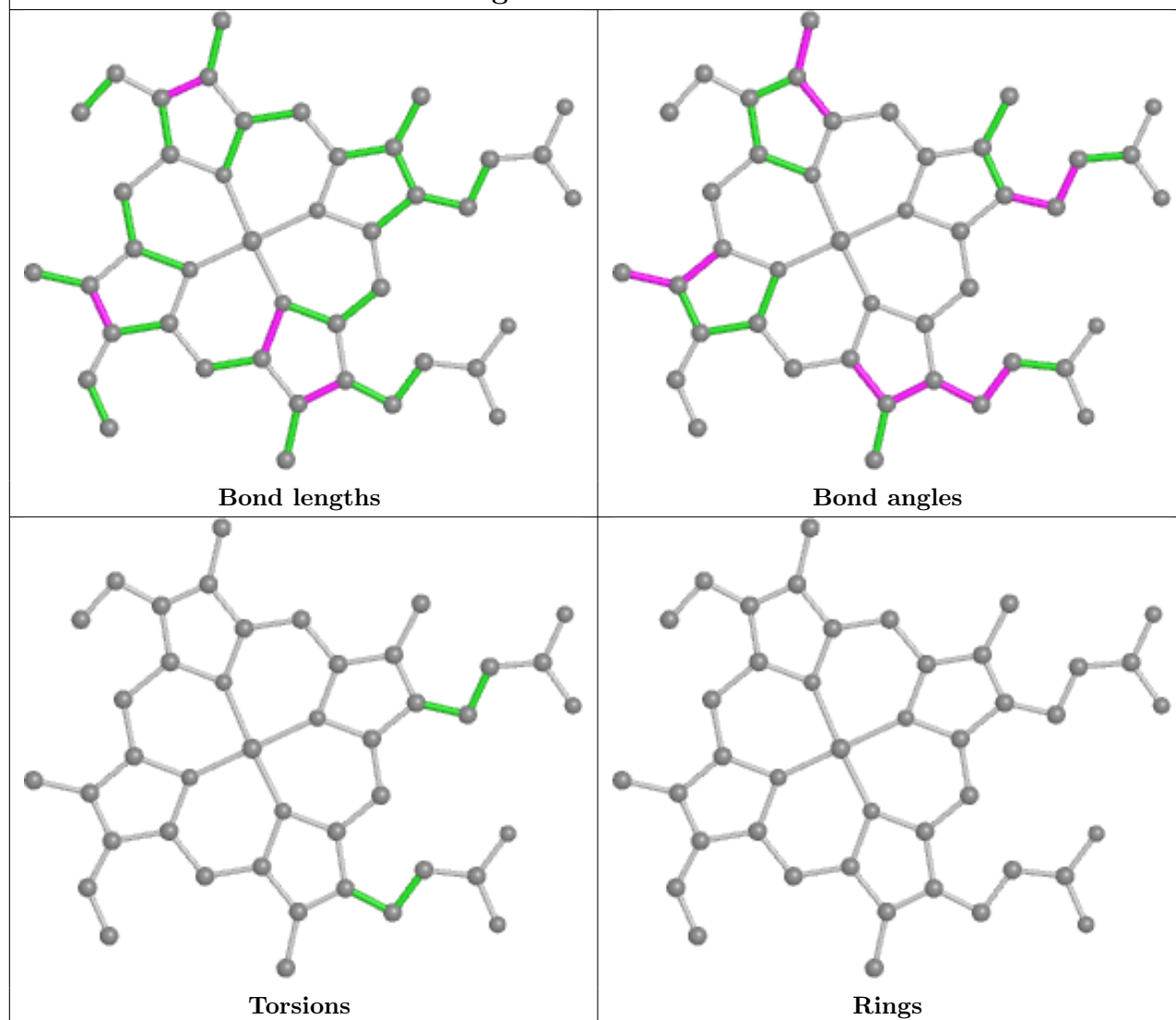
Ligand LMG D 411



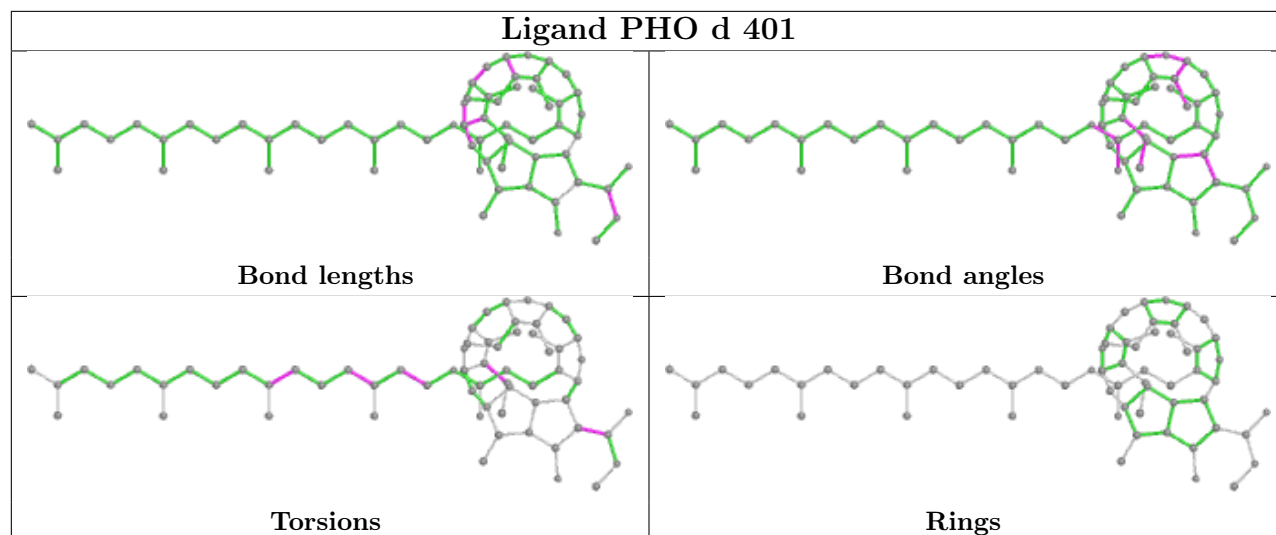
Ligand SQD a 412



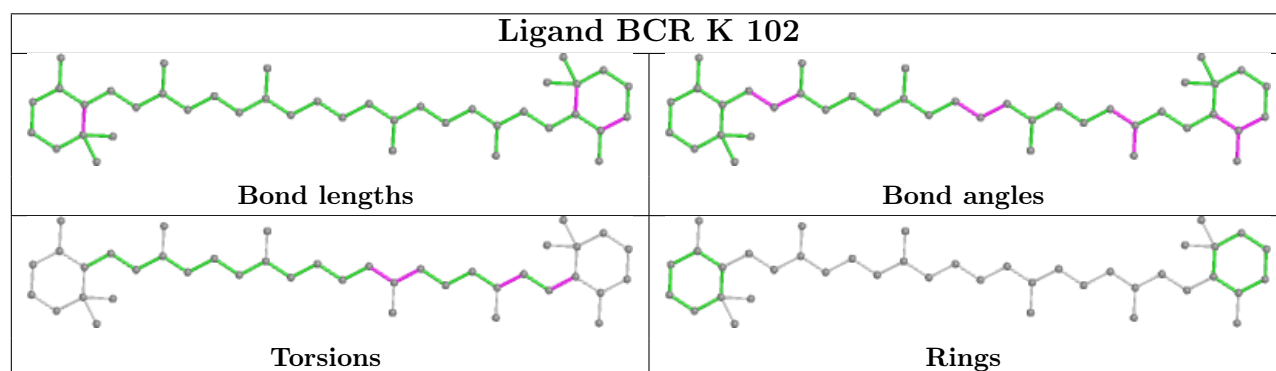
Ligand HEC v 201



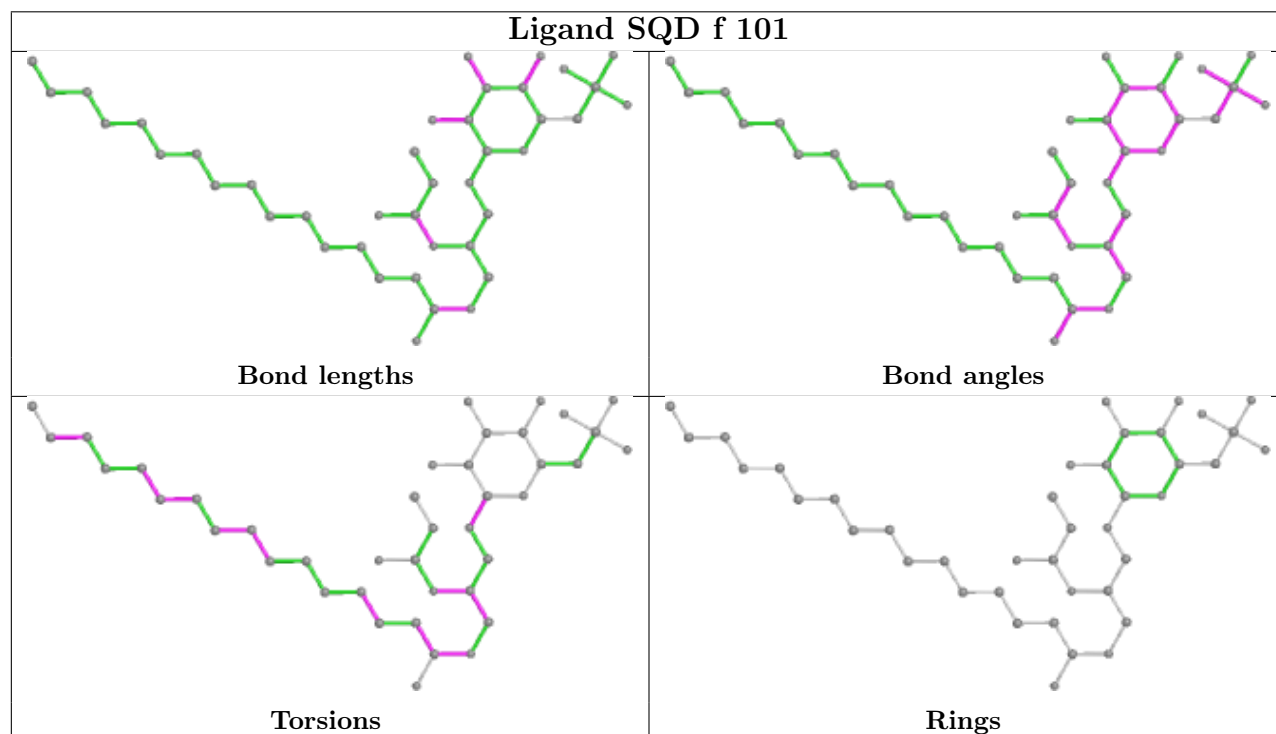
Ligand PHO d 401

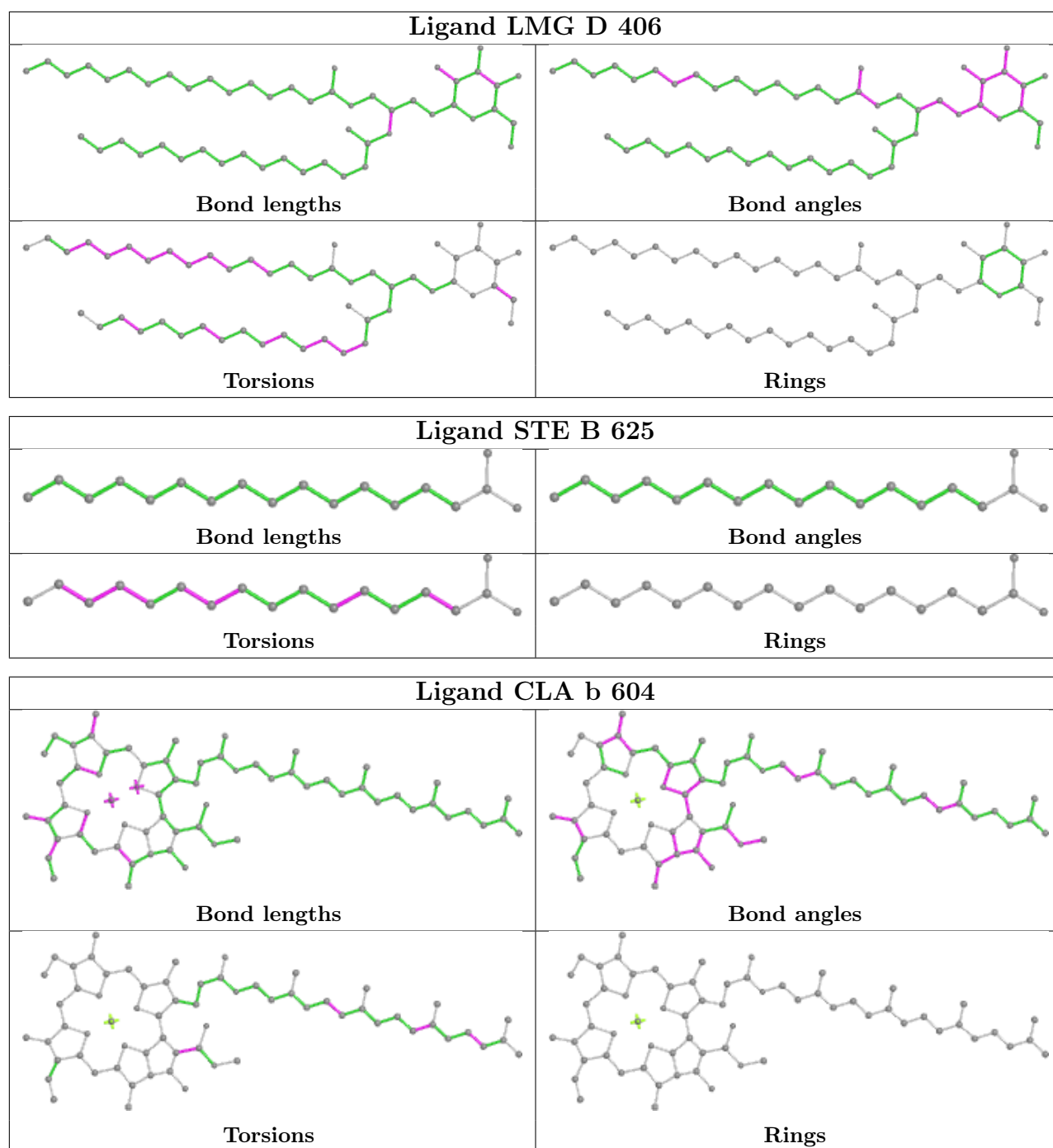


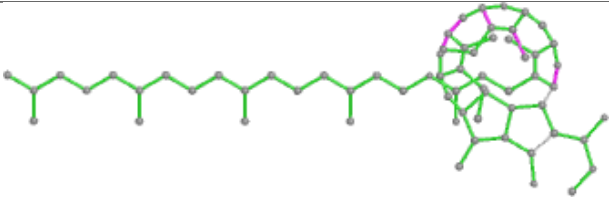
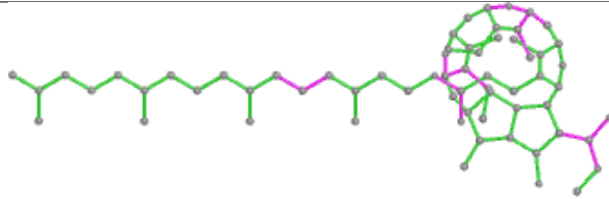
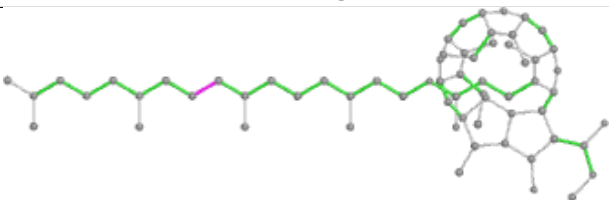
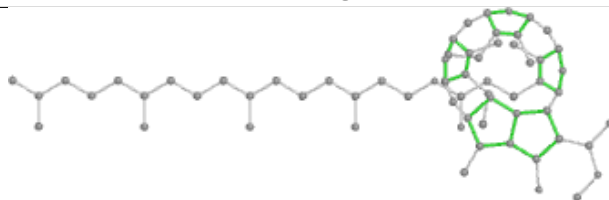

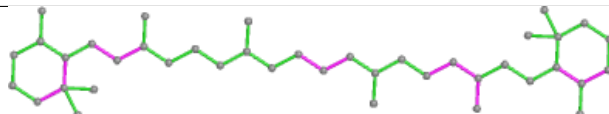
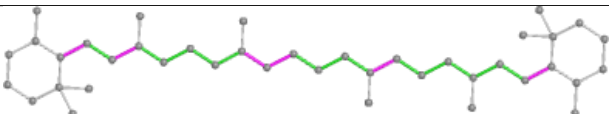
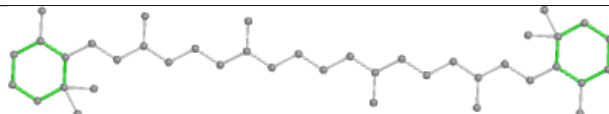








Ligand BCR K 102

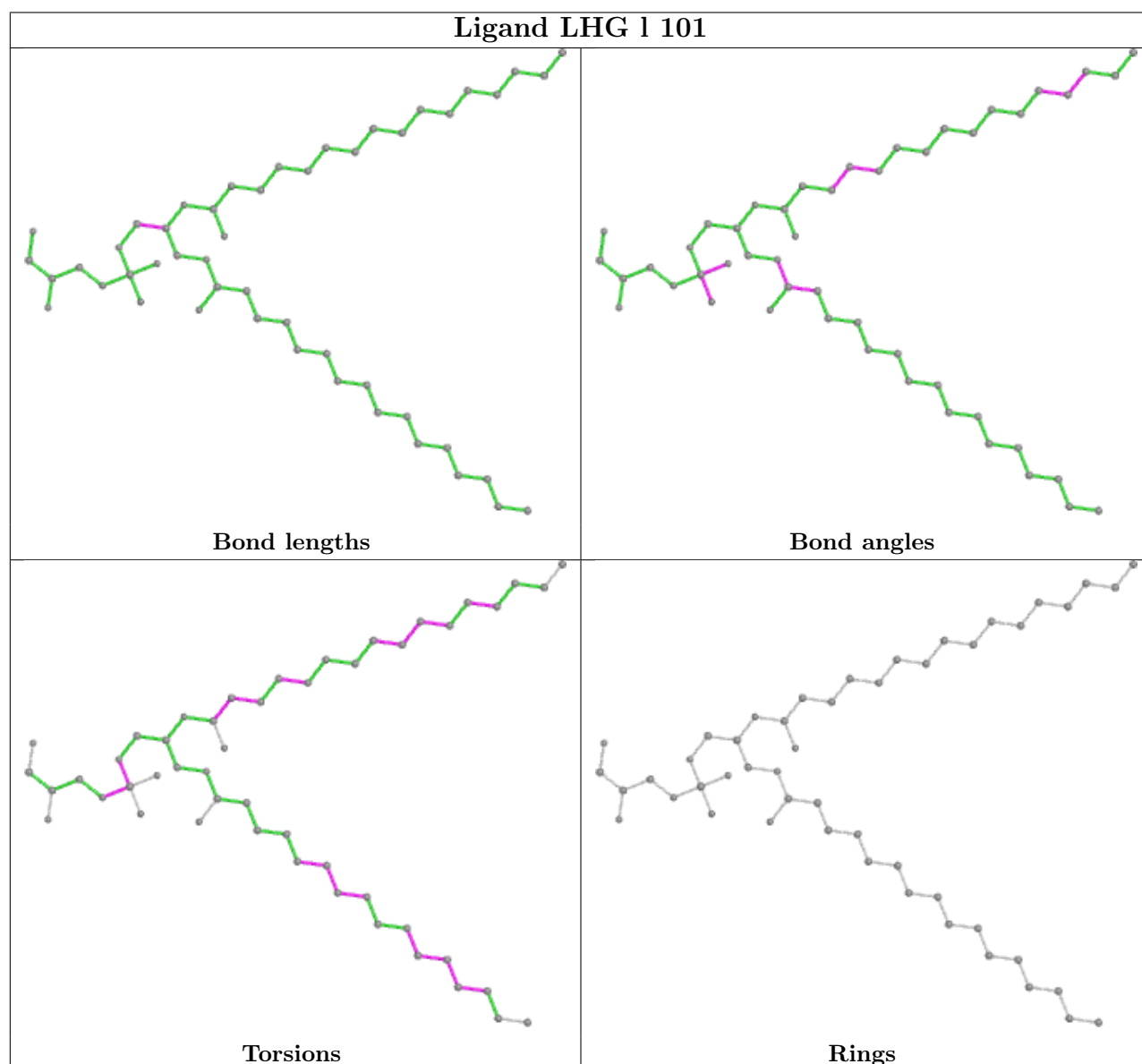
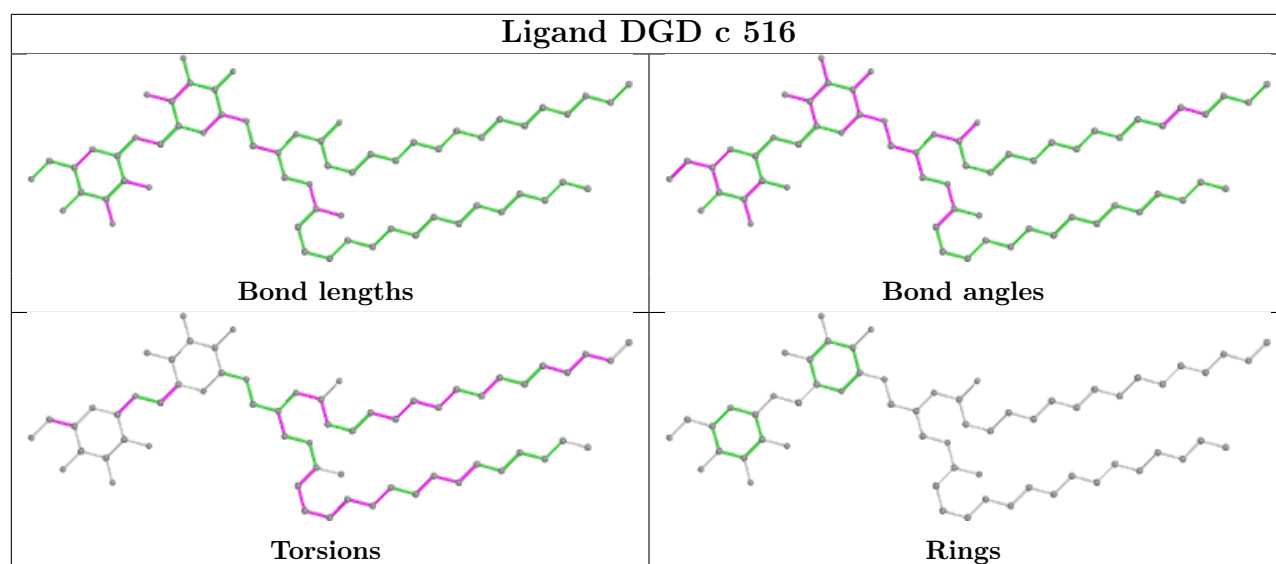


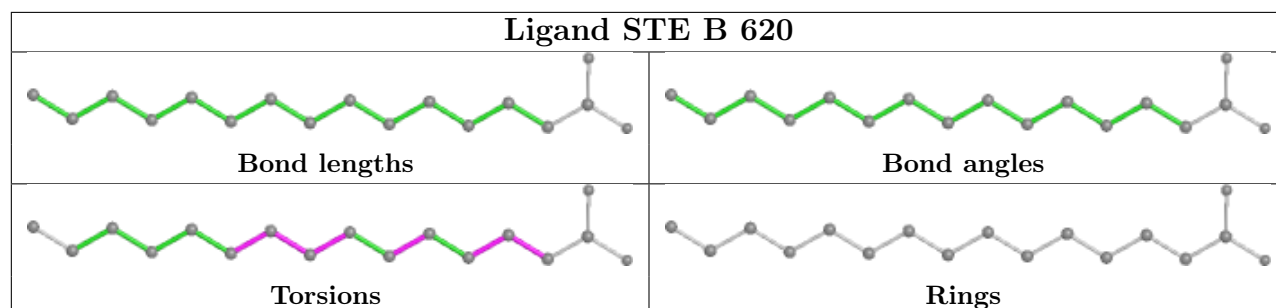
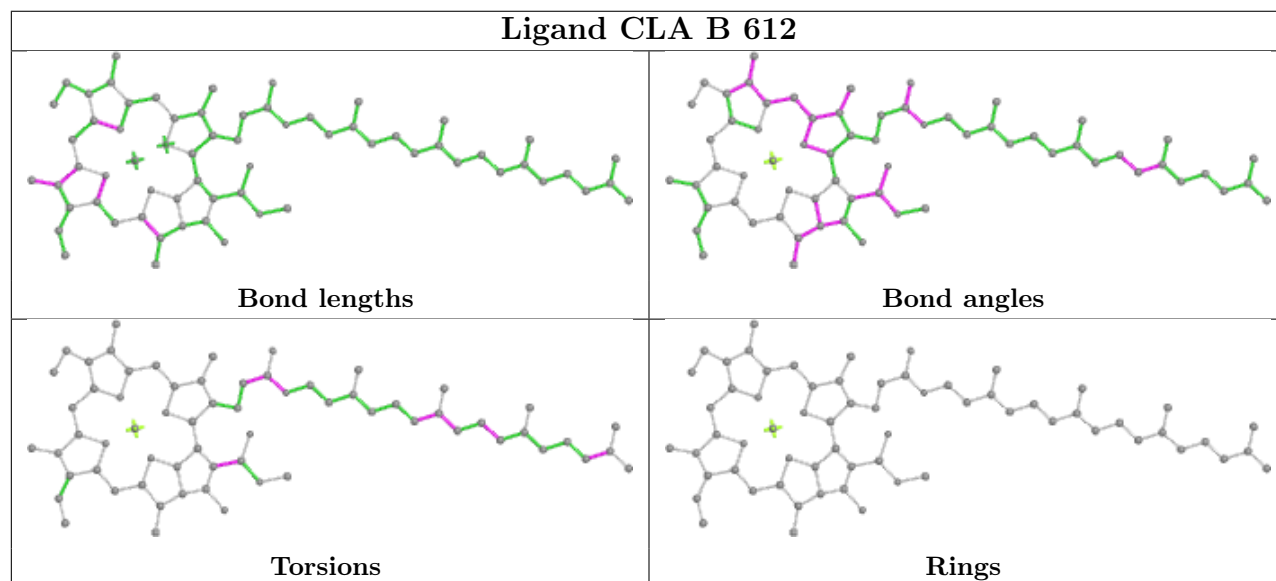
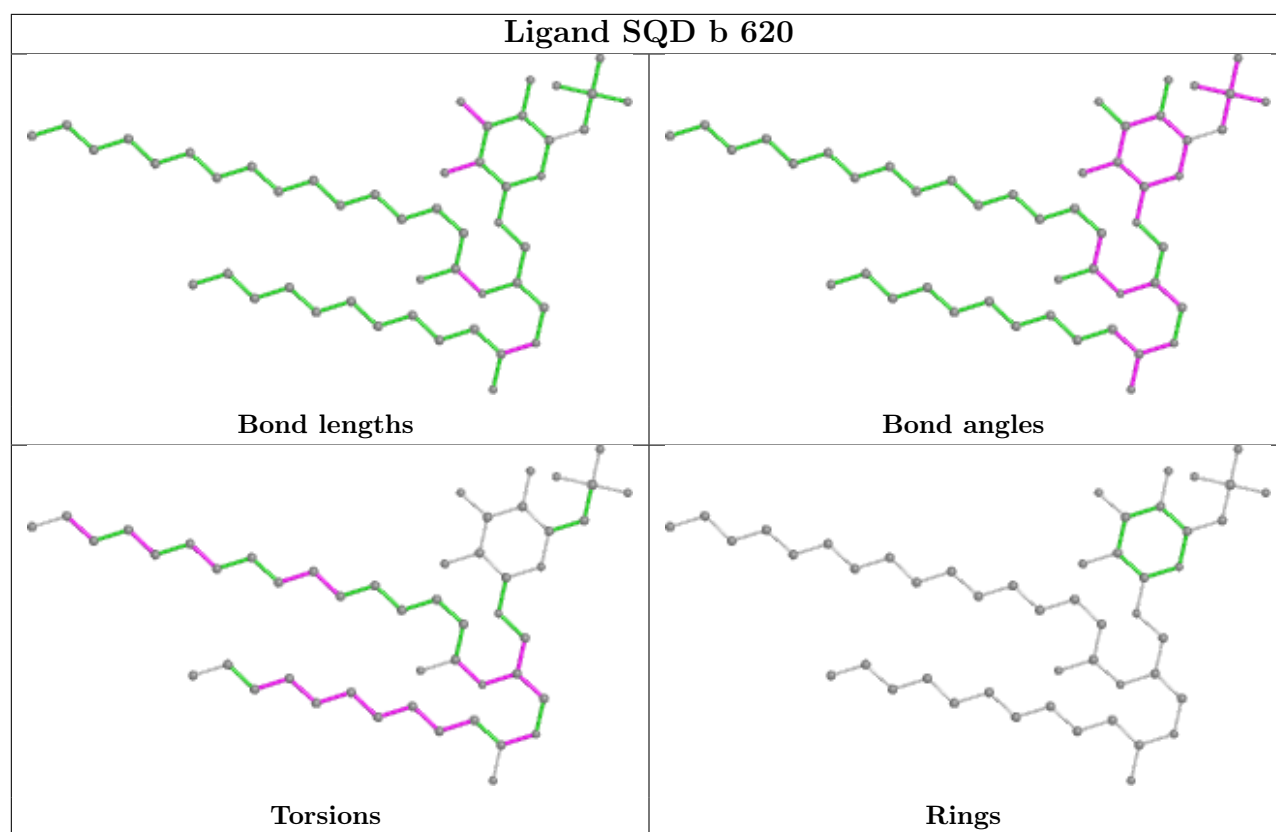
Ligand SQD f 101

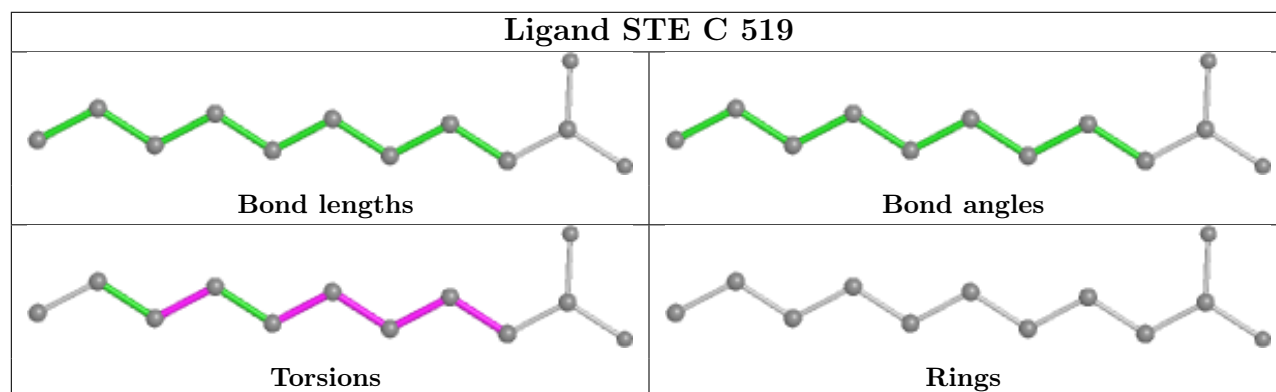
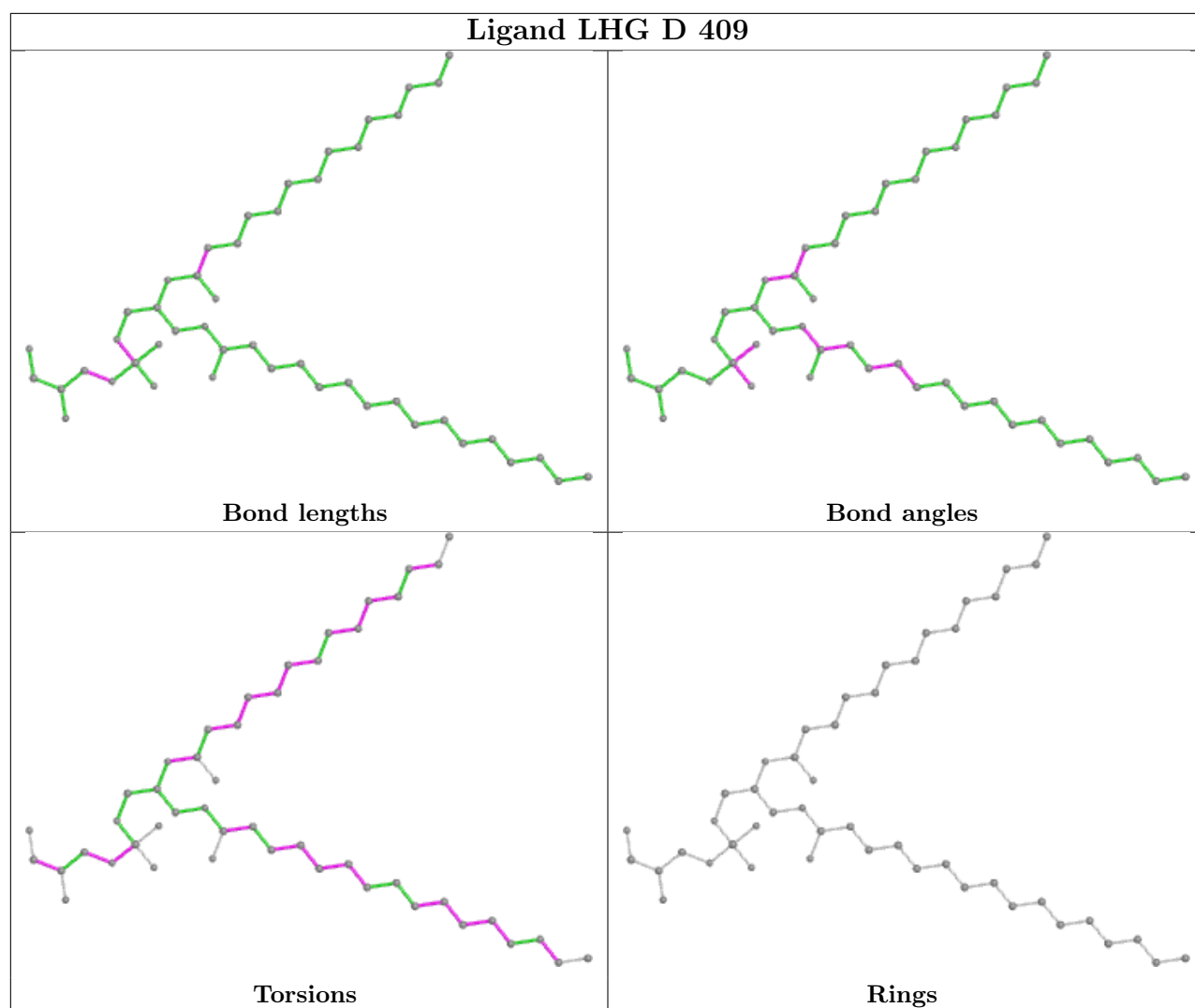


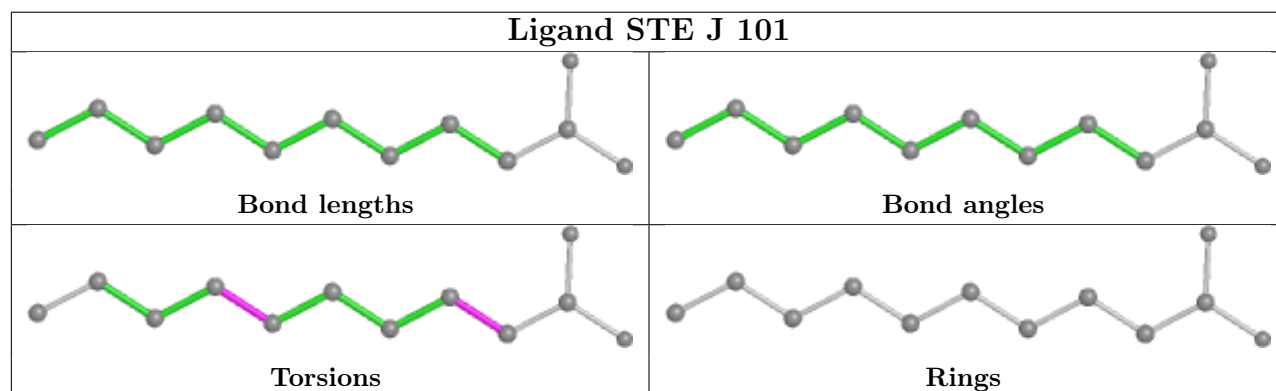
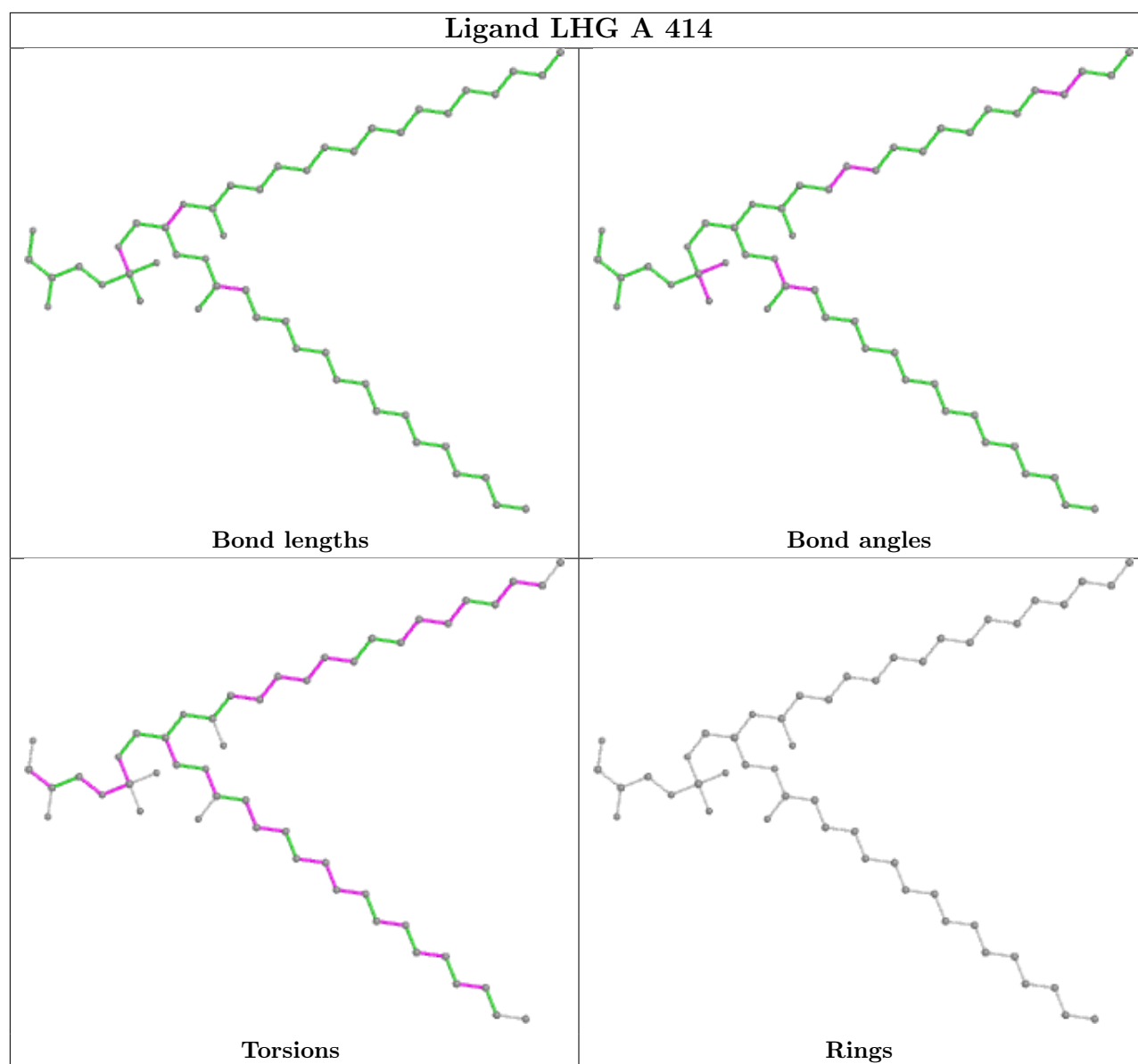


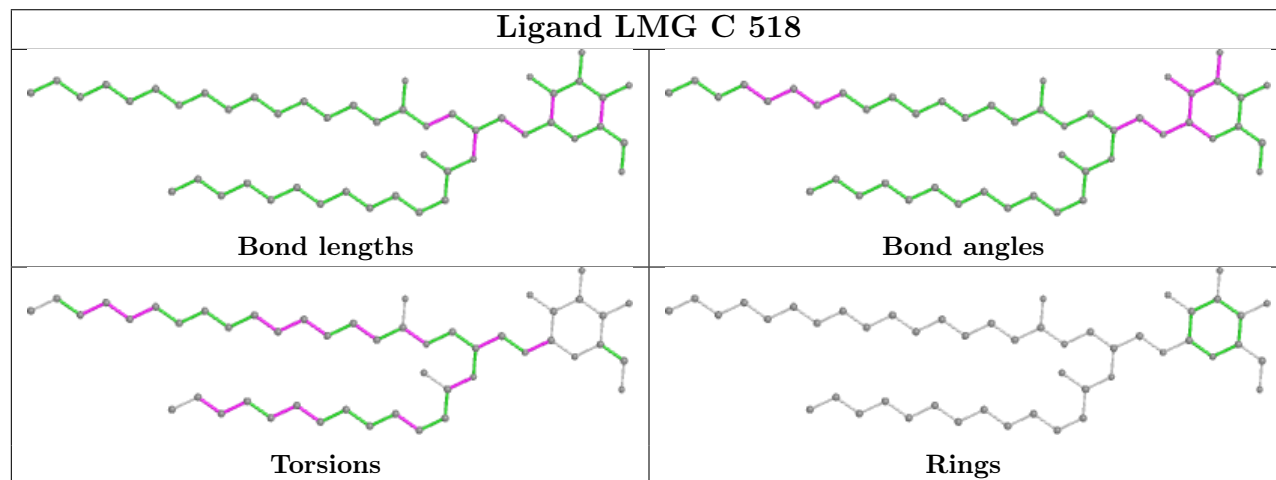
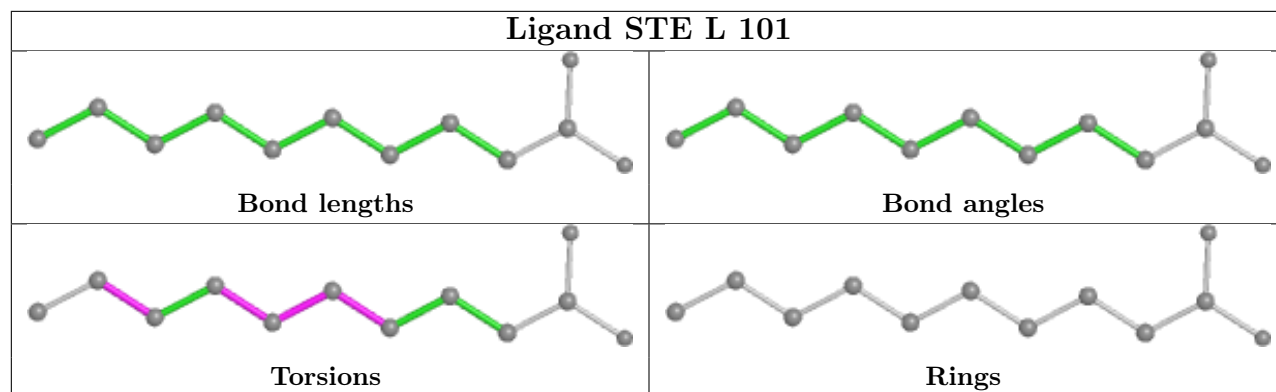
Ligand PHO D 401	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE H 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE l 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

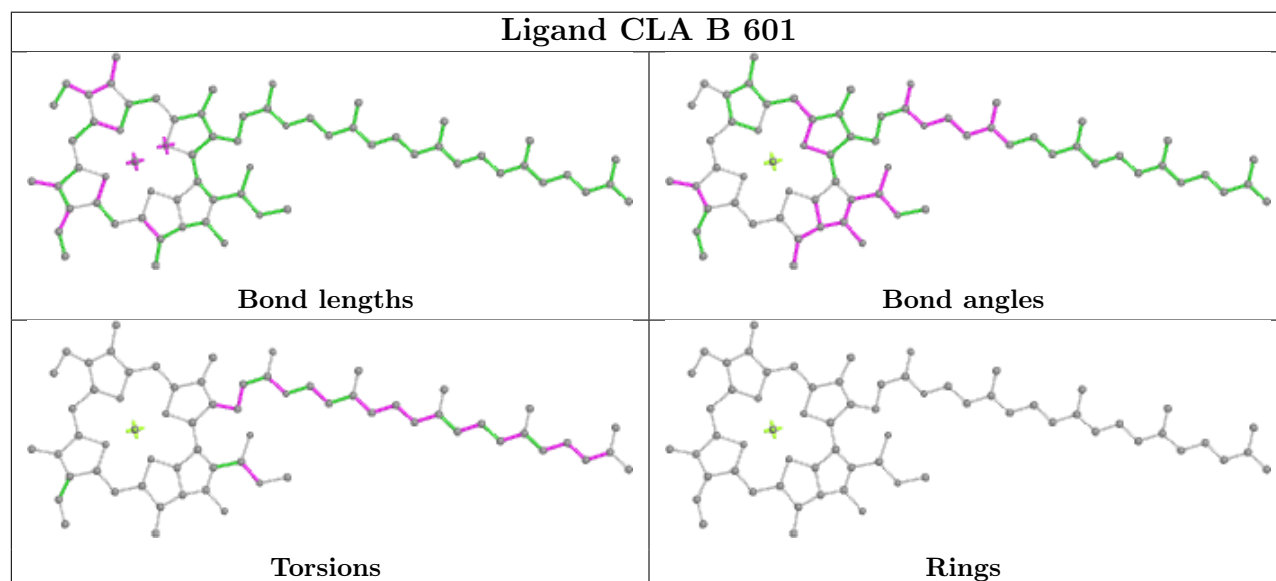
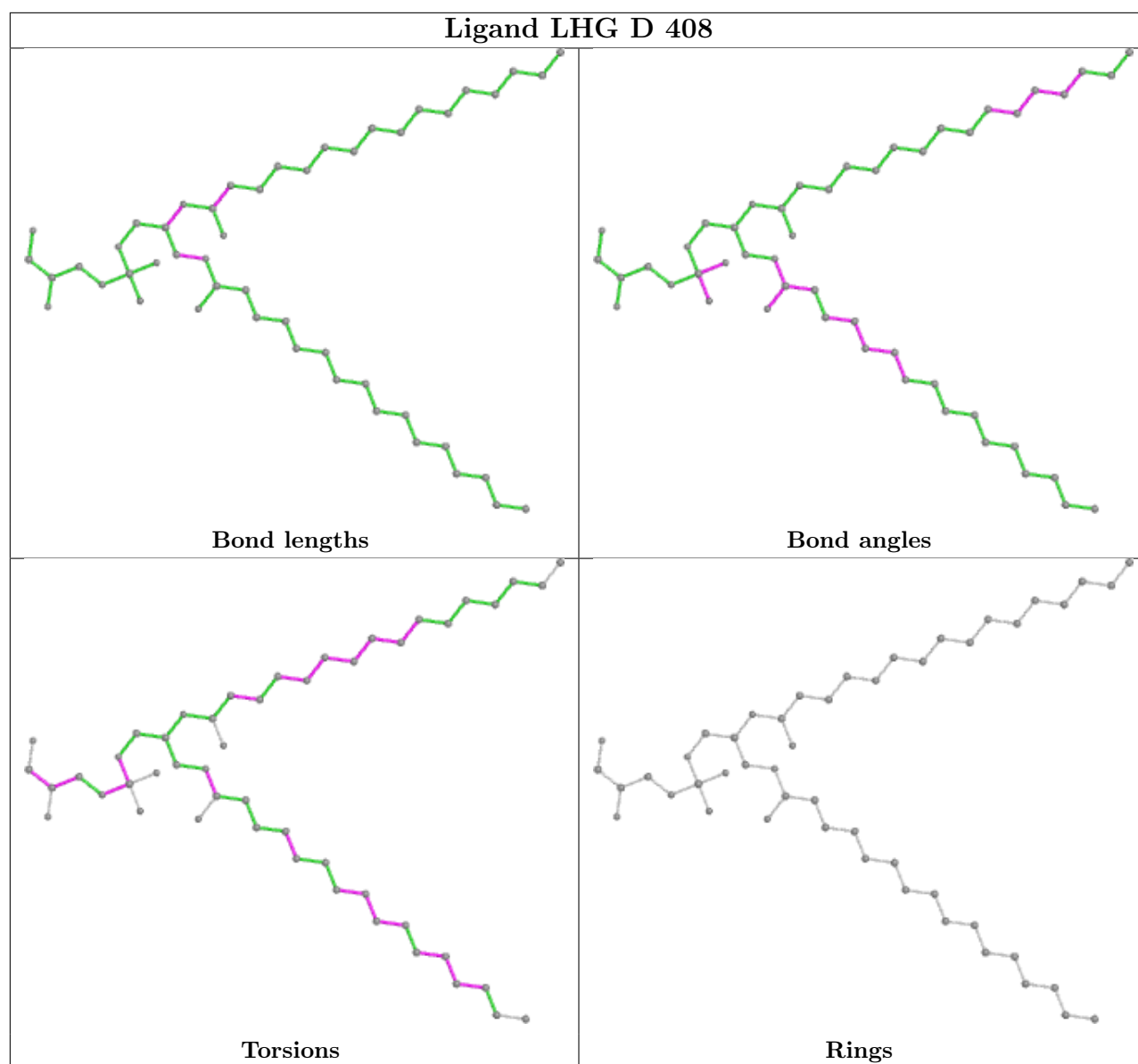


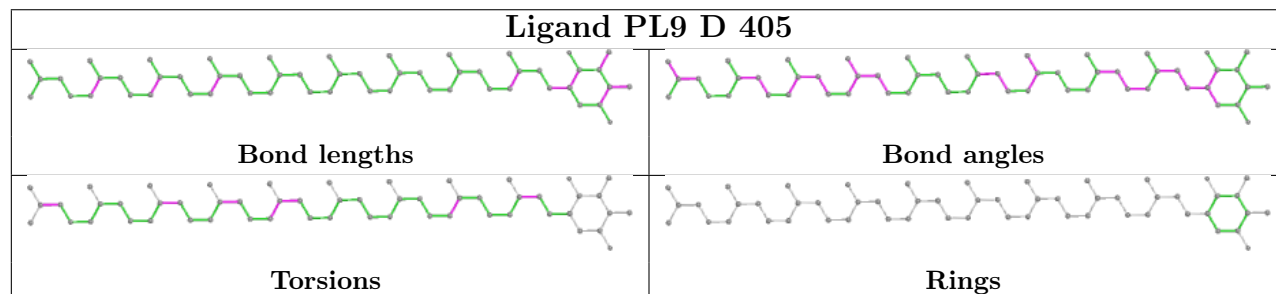
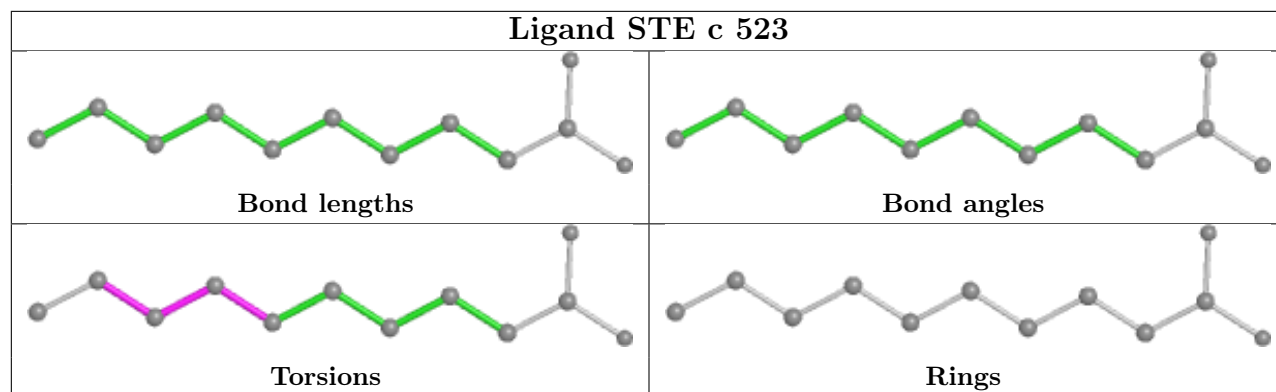




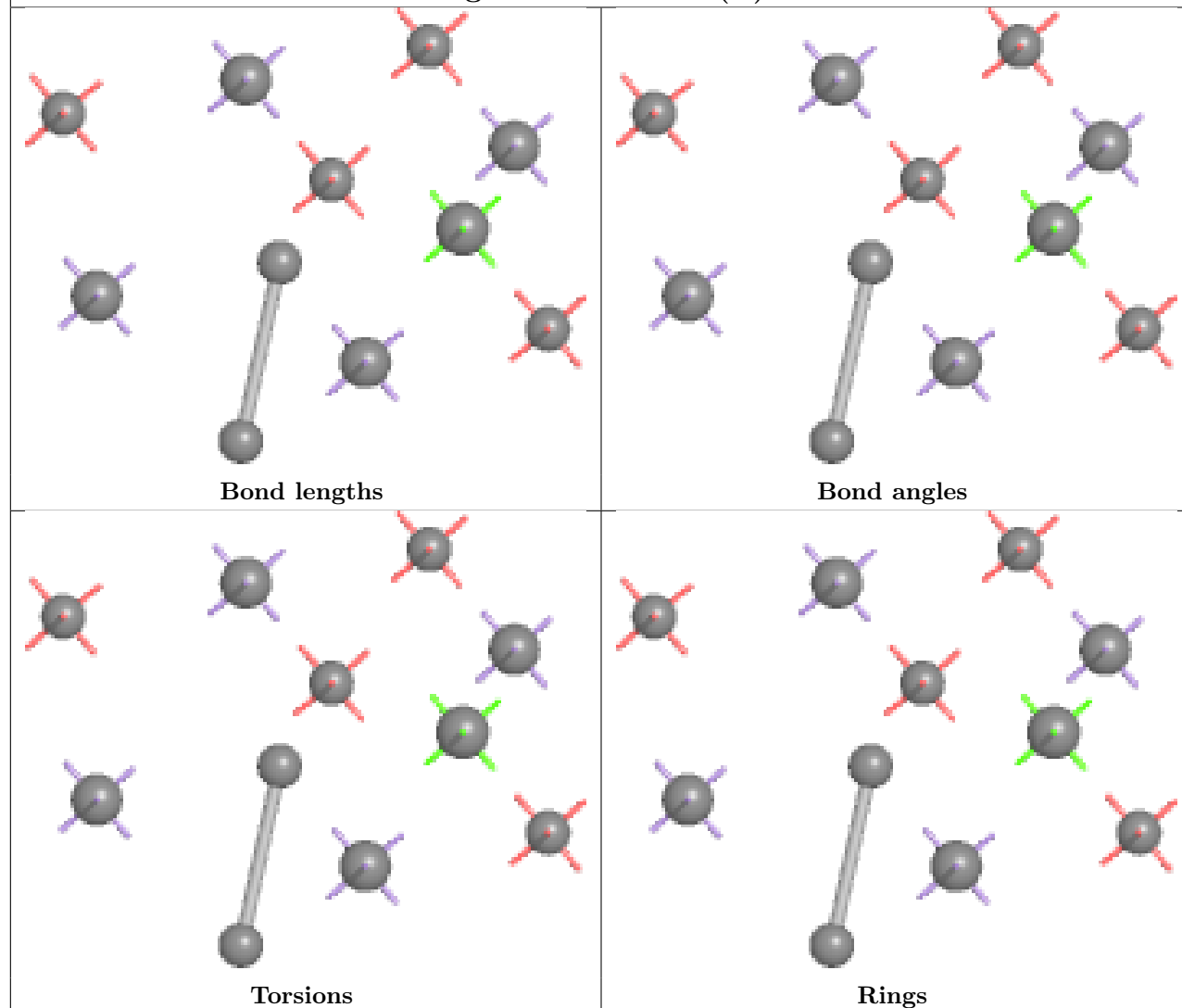




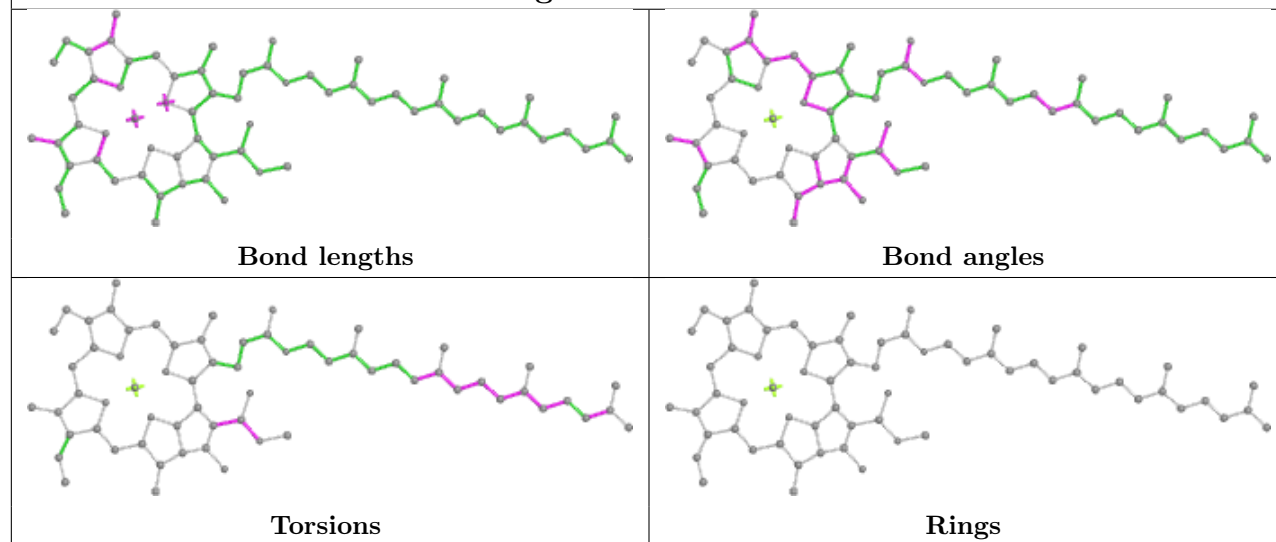


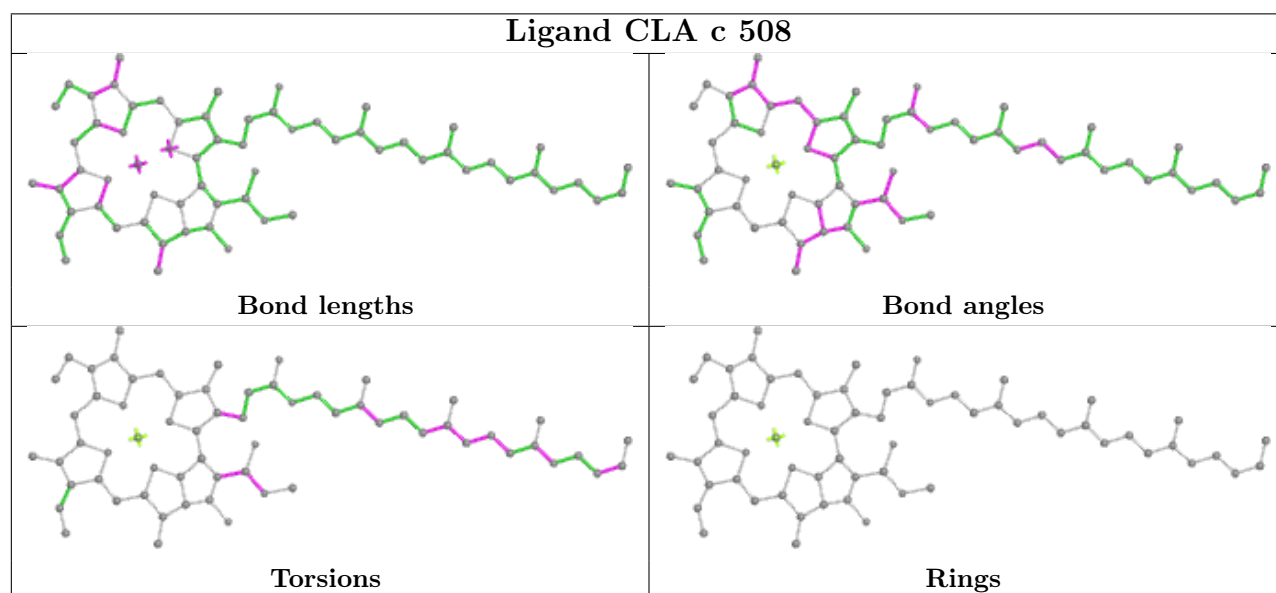
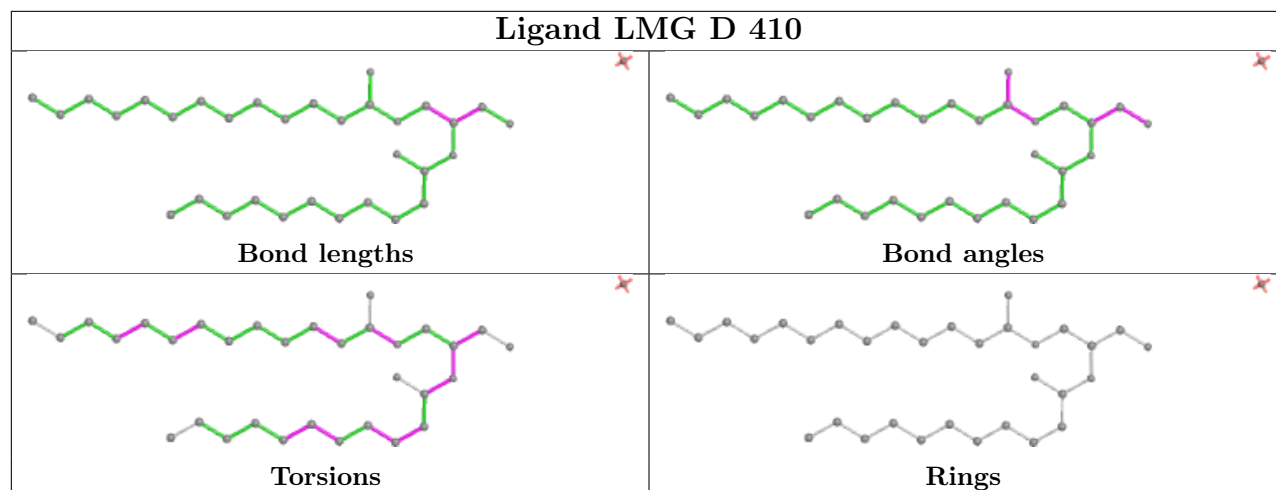
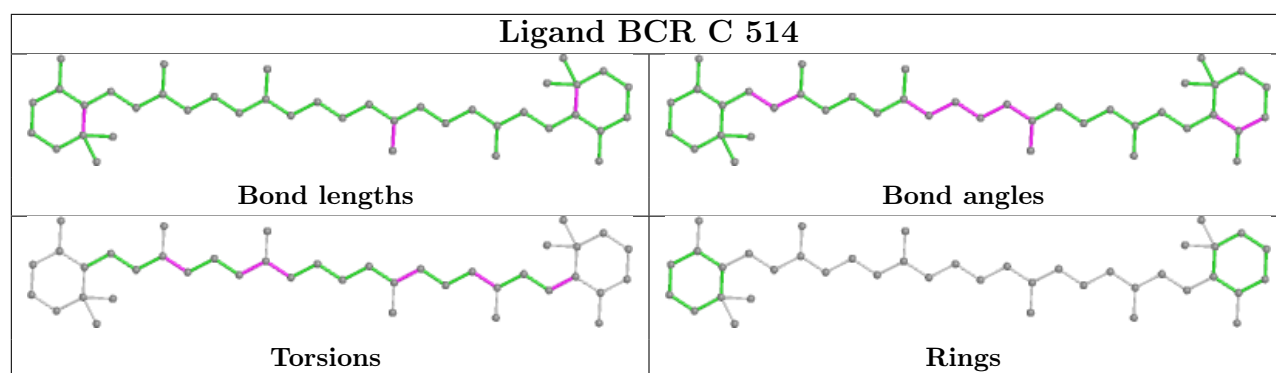


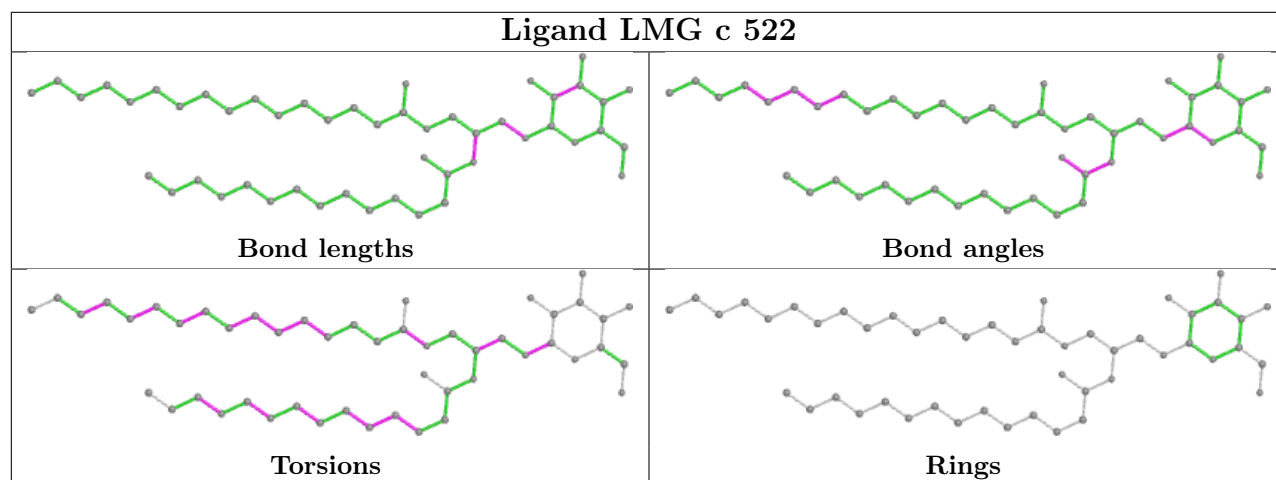
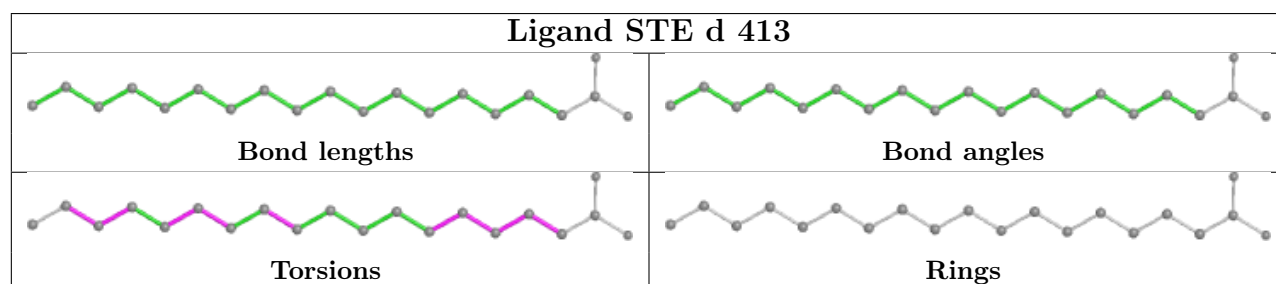
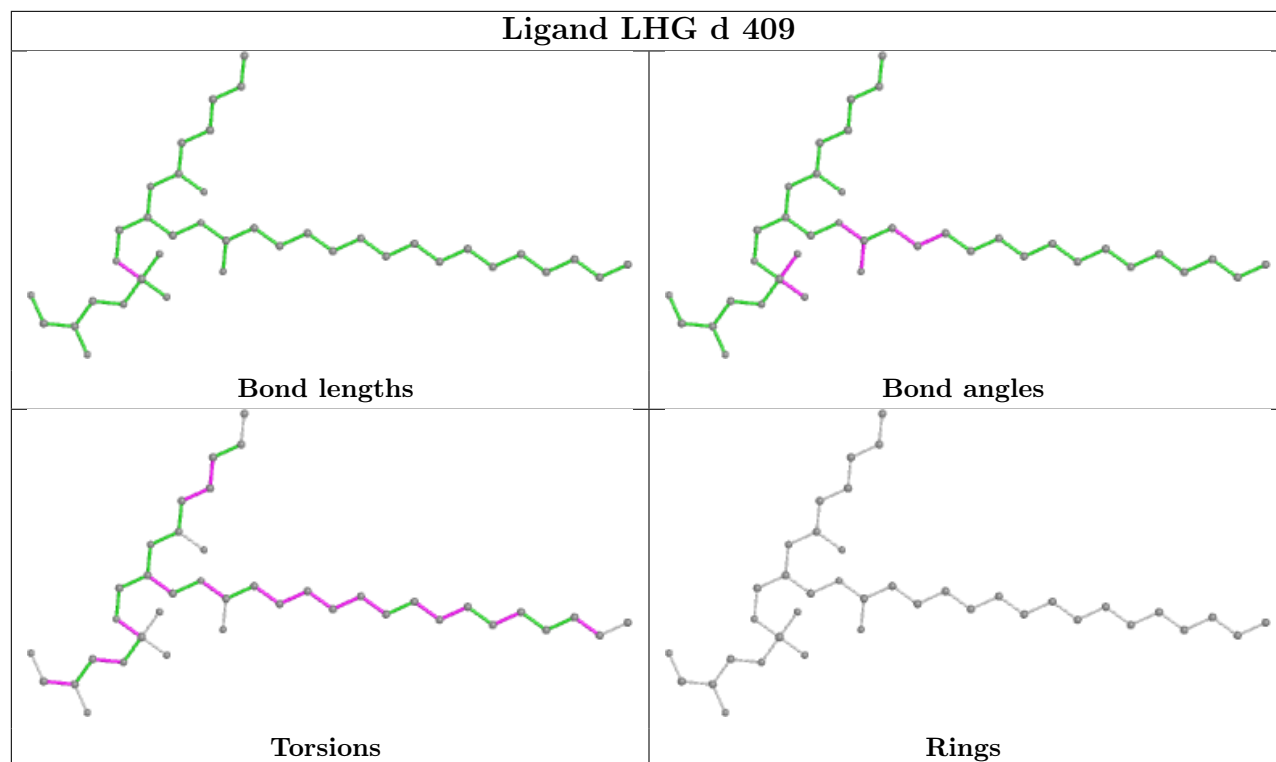
Ligand OEY a 418 (B)

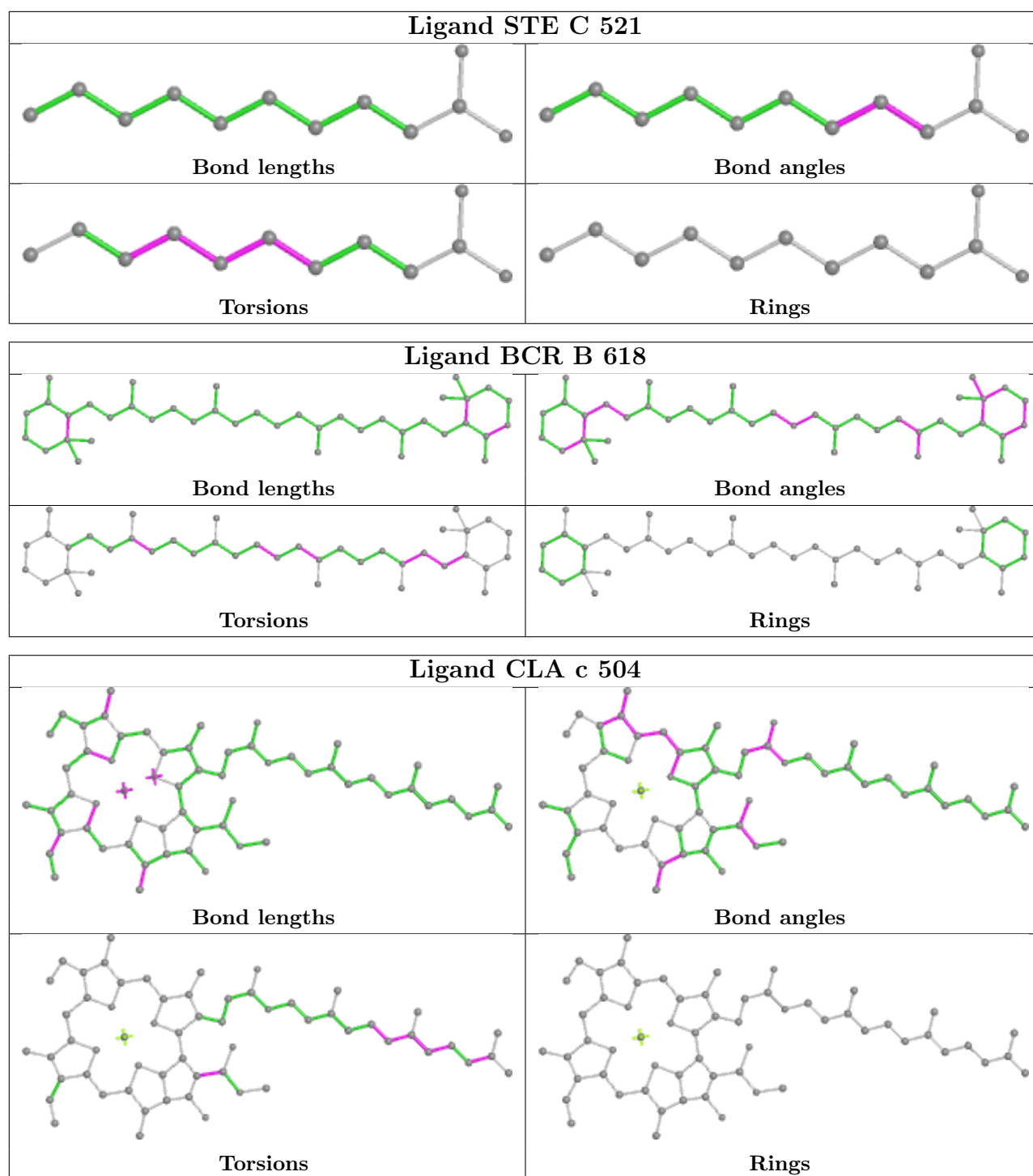


Ligand CLA b 607

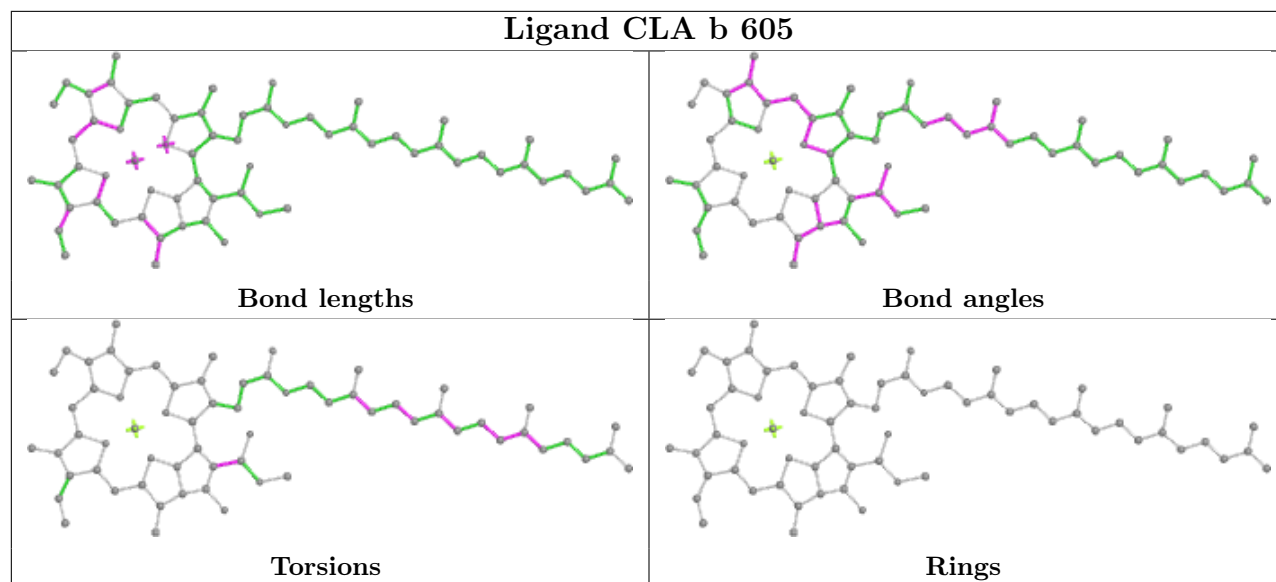




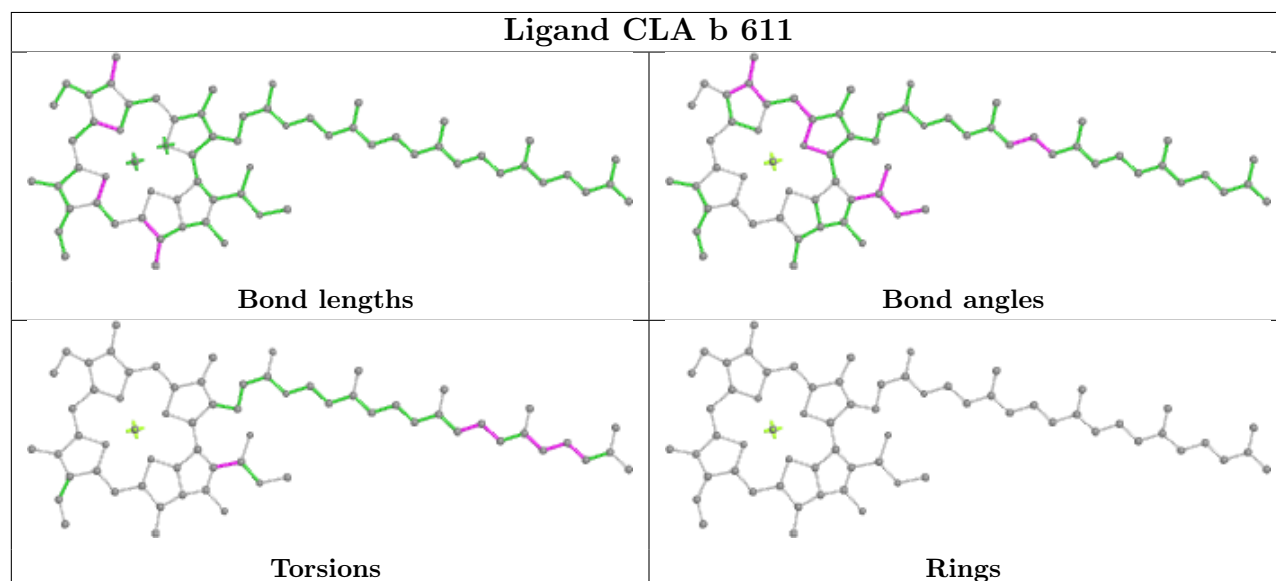




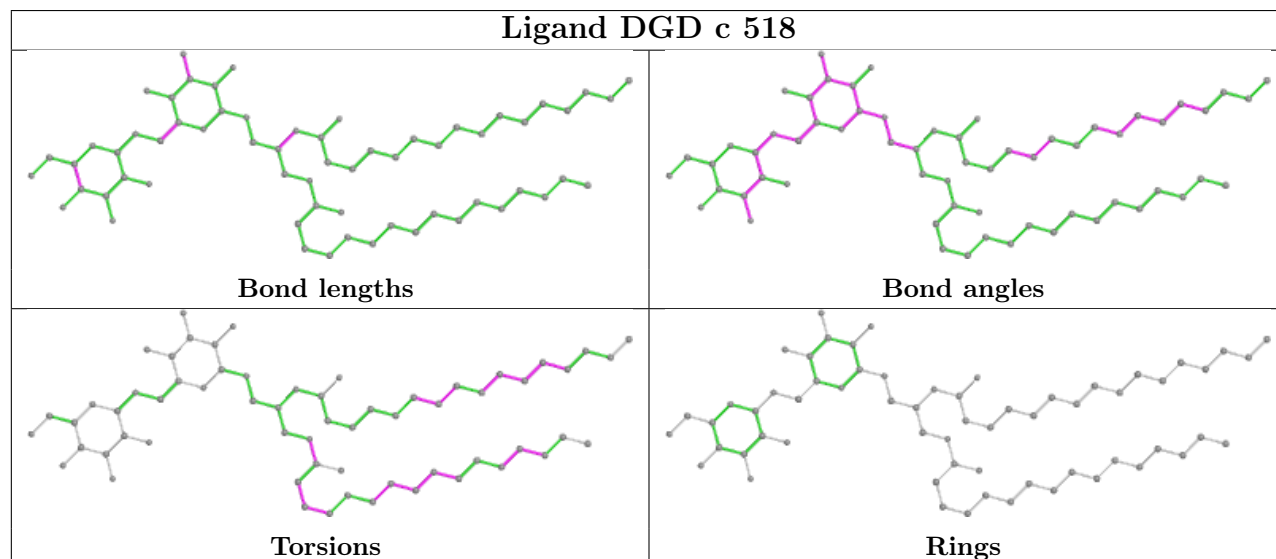
Ligand CLA b 605

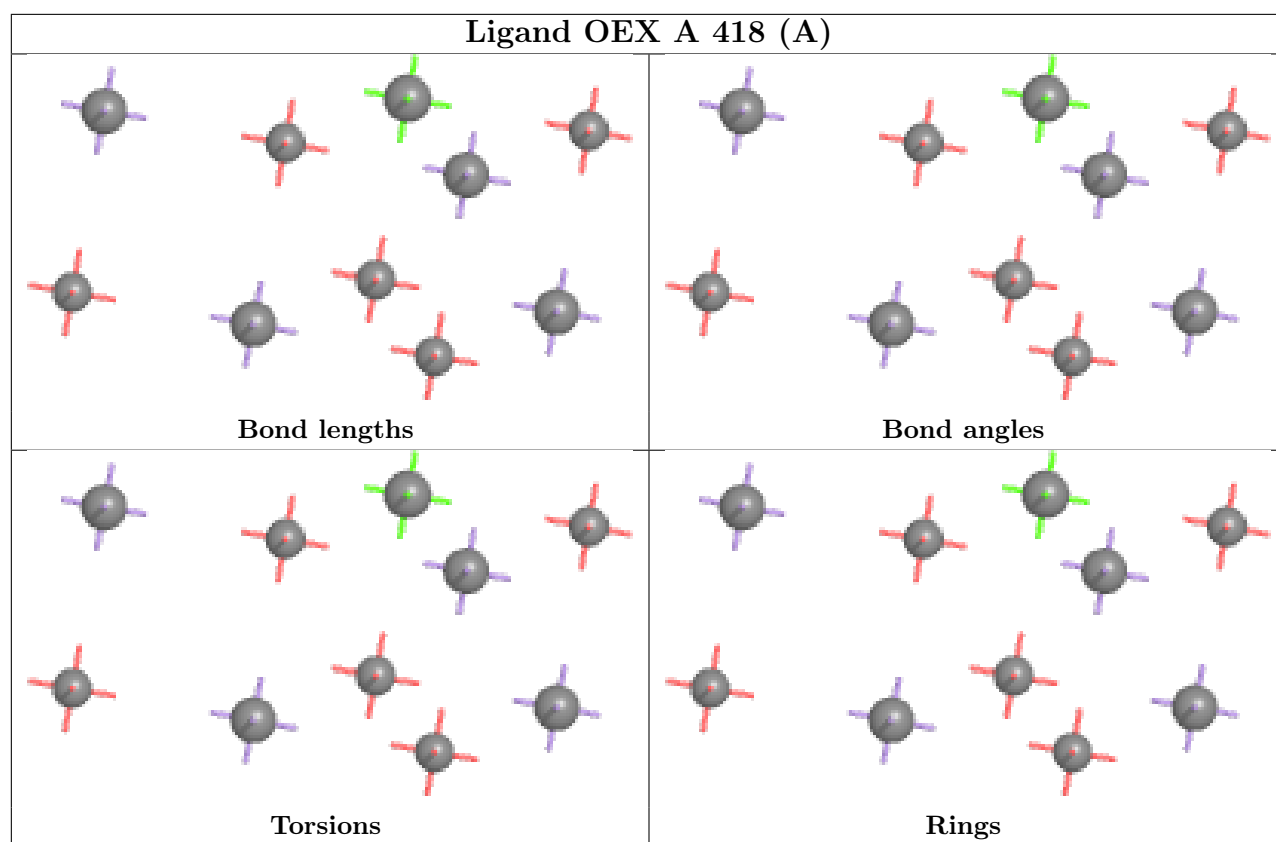


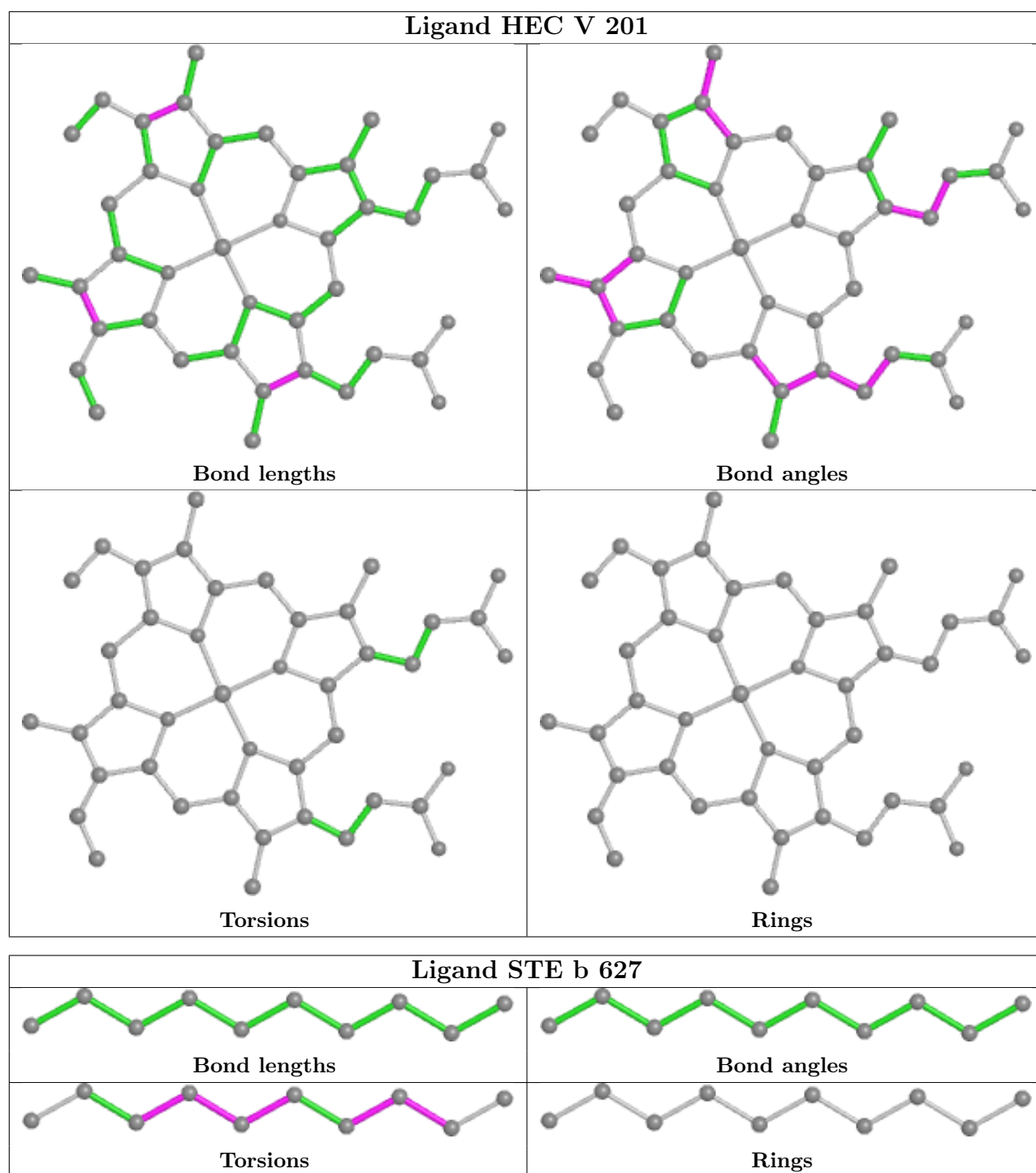
Ligand CLA b 611

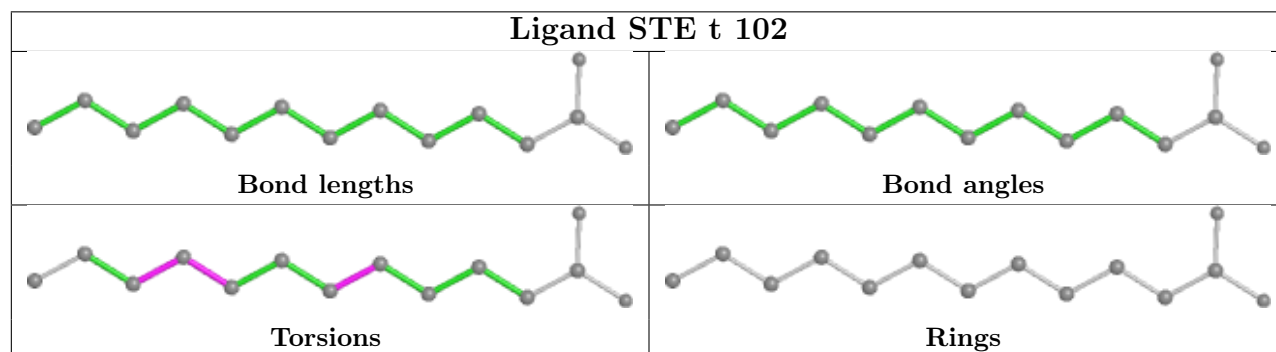
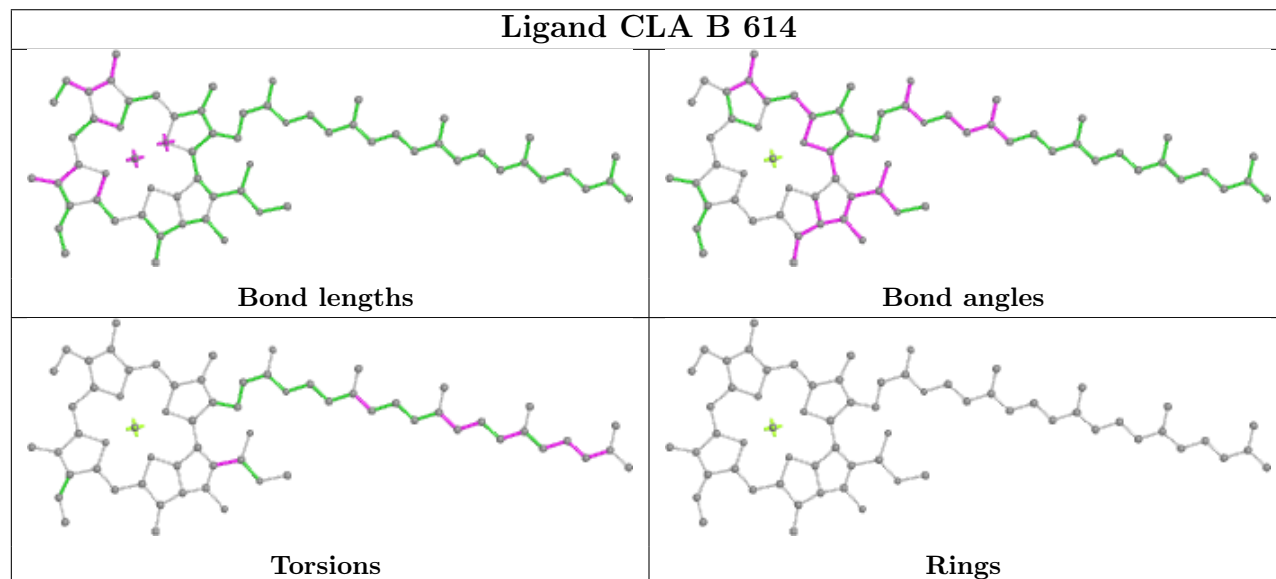
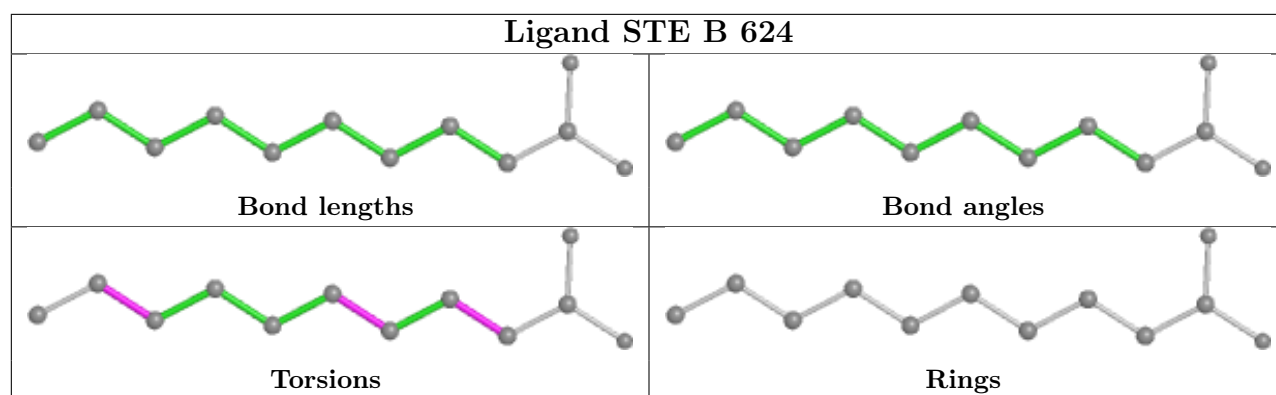


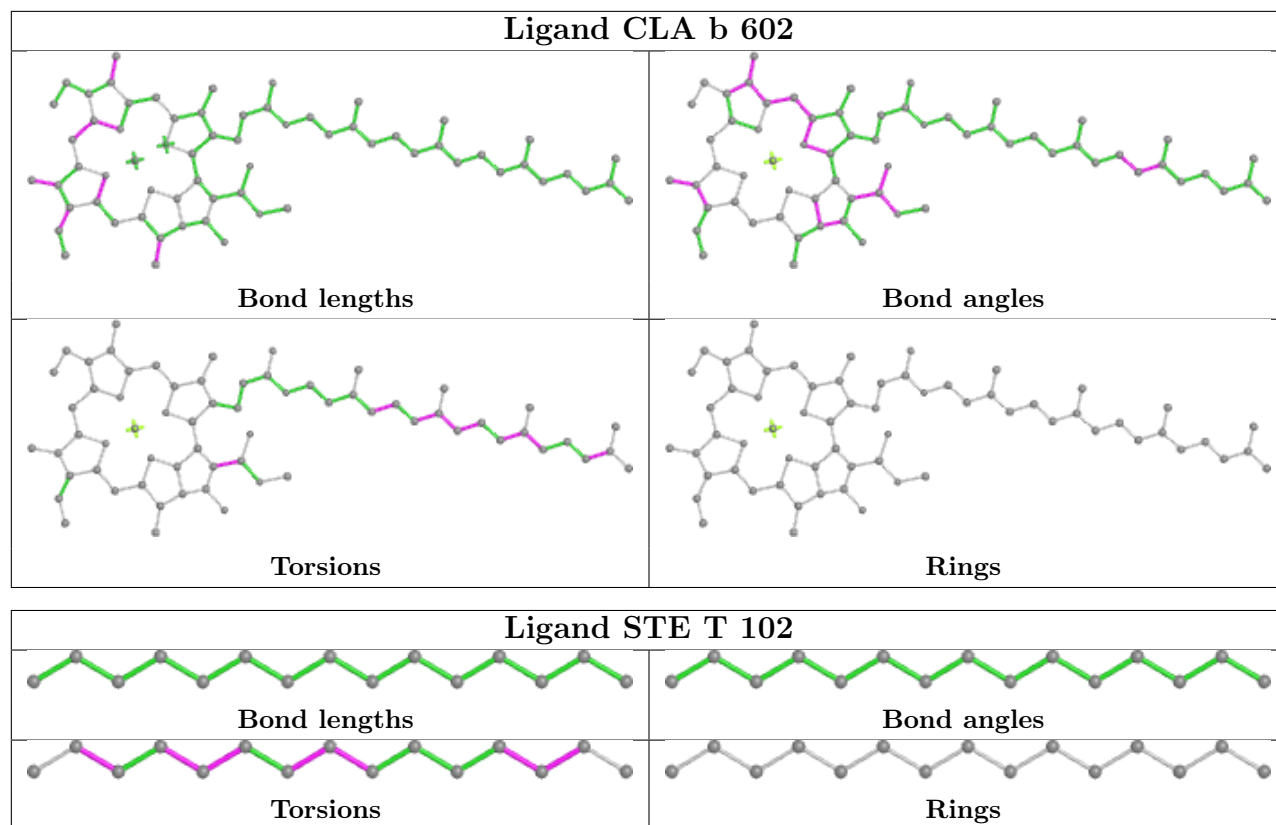
Ligand DGD c 518

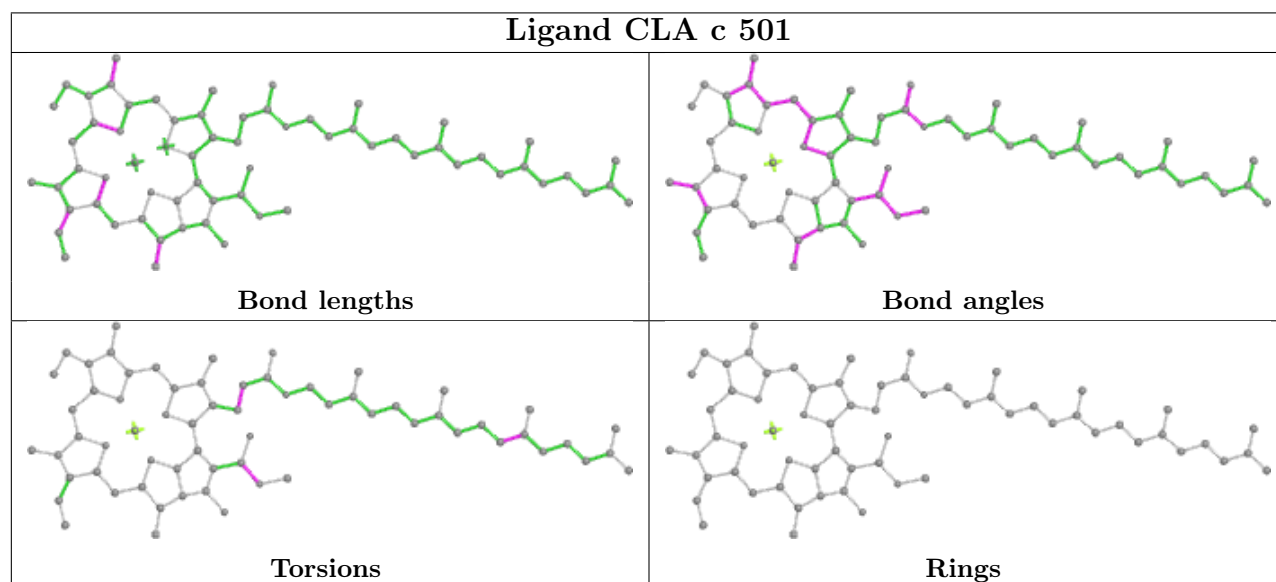
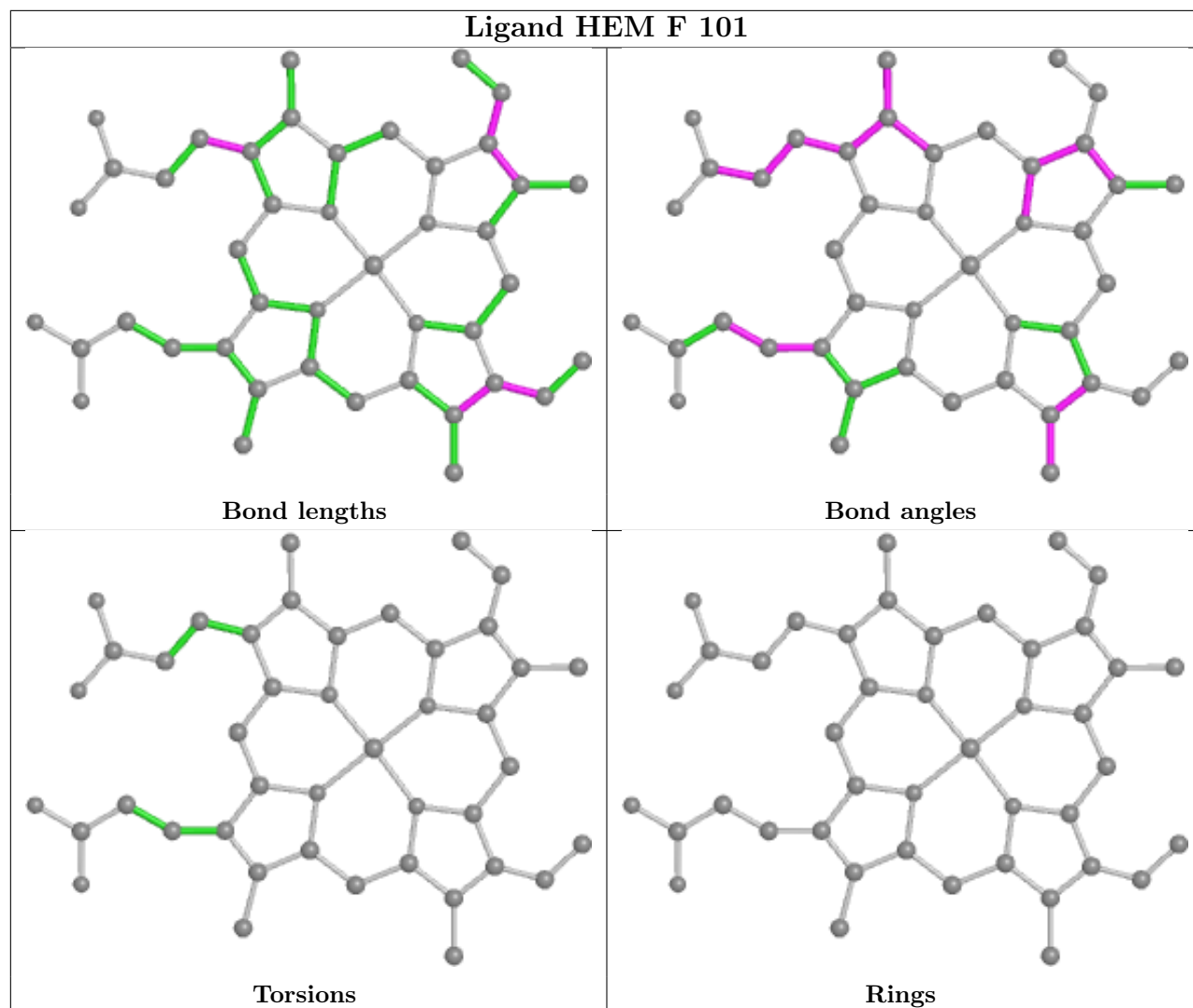


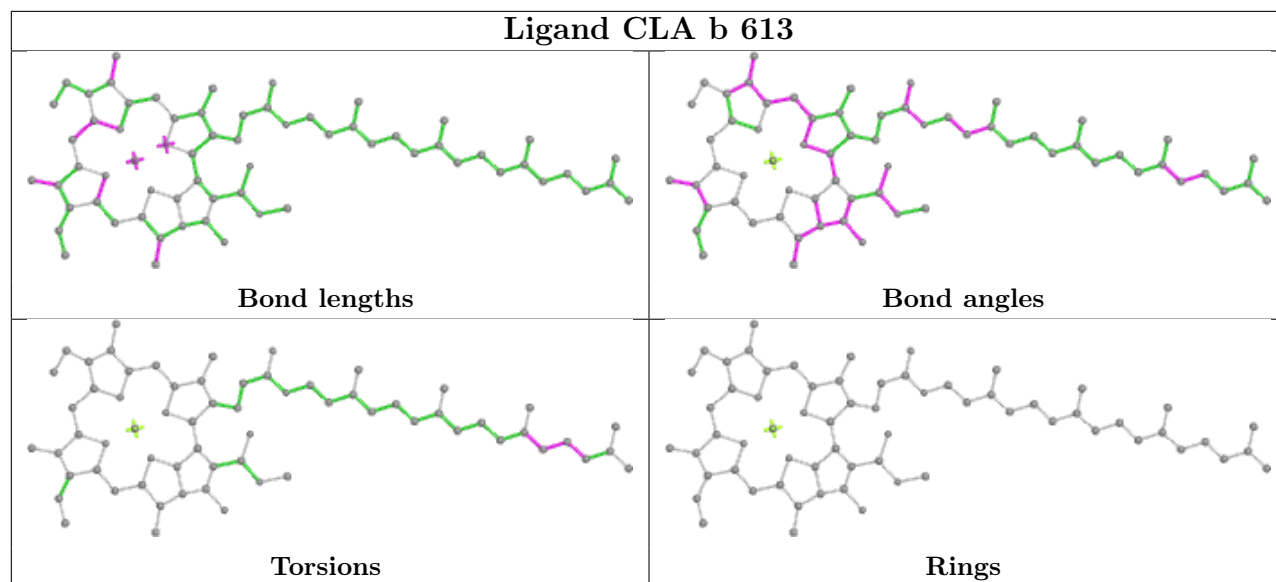
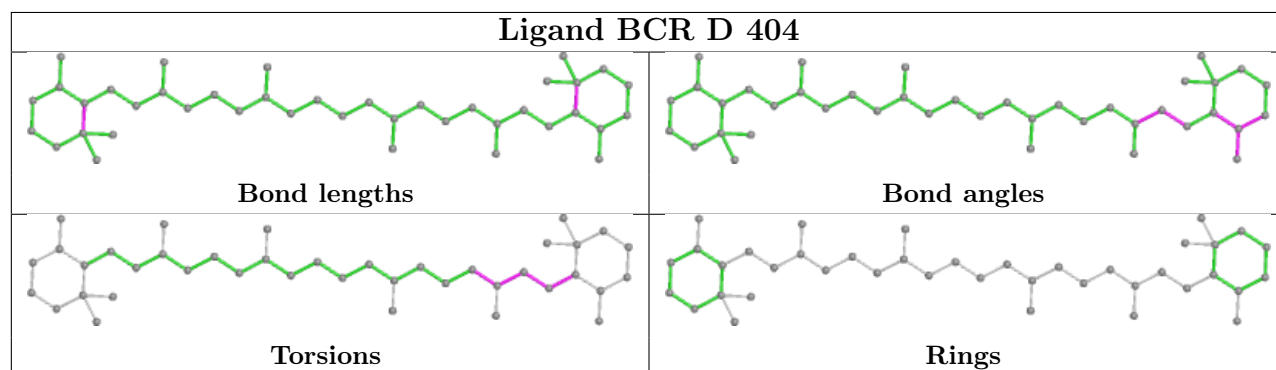
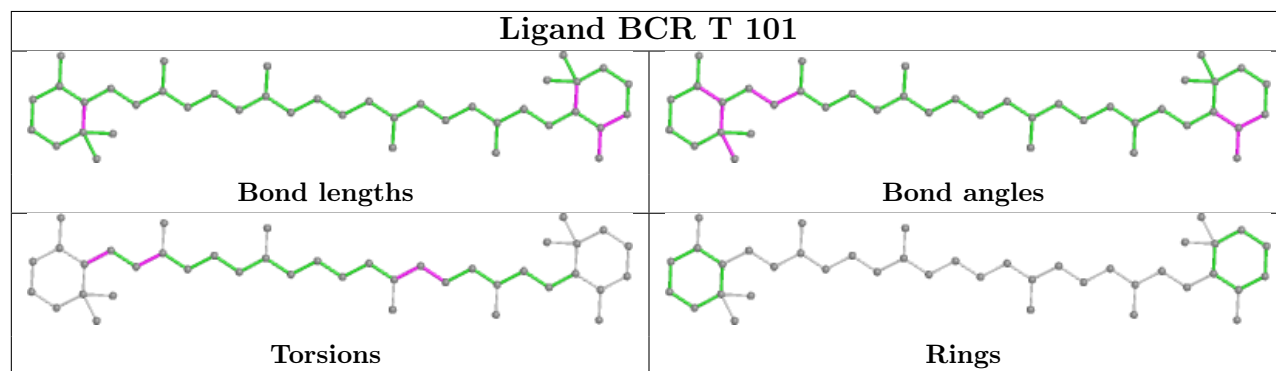


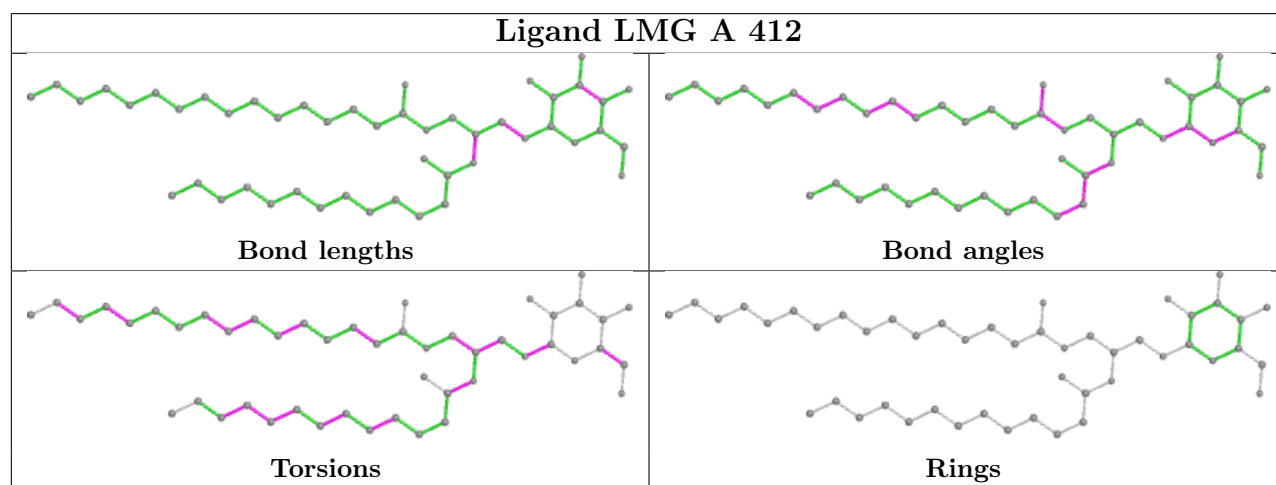
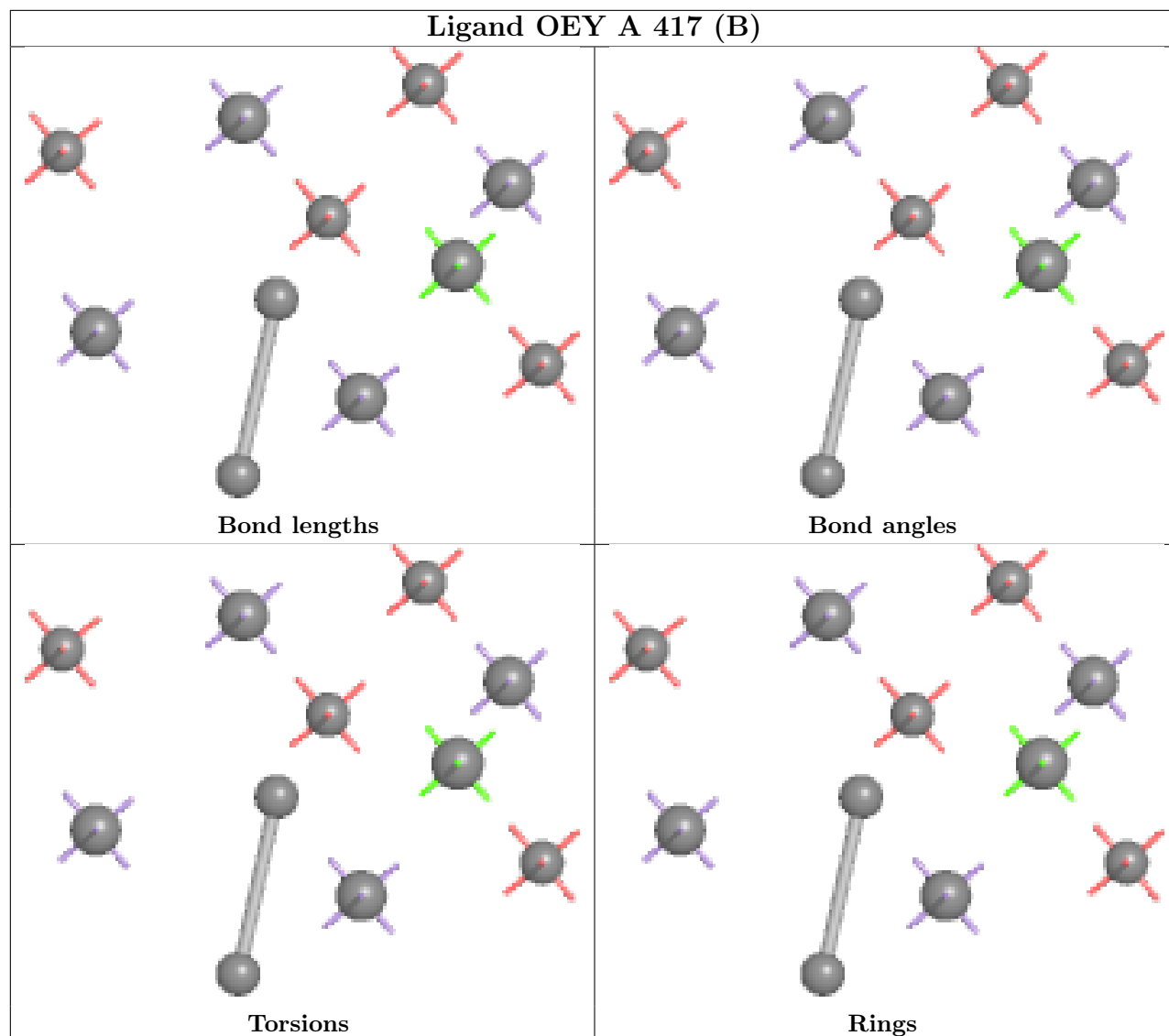


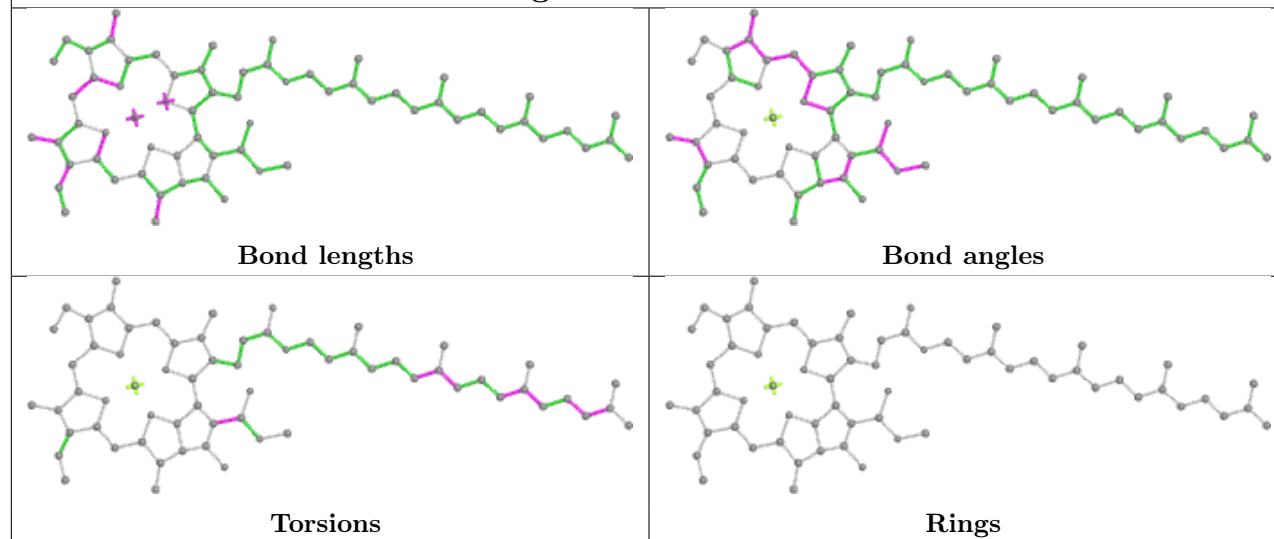
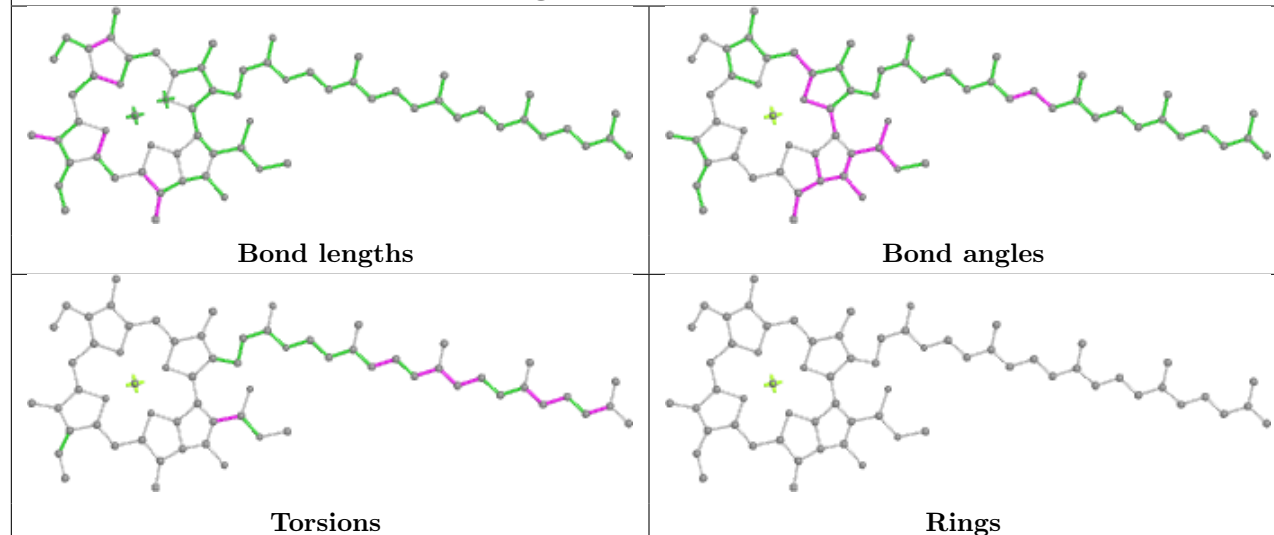
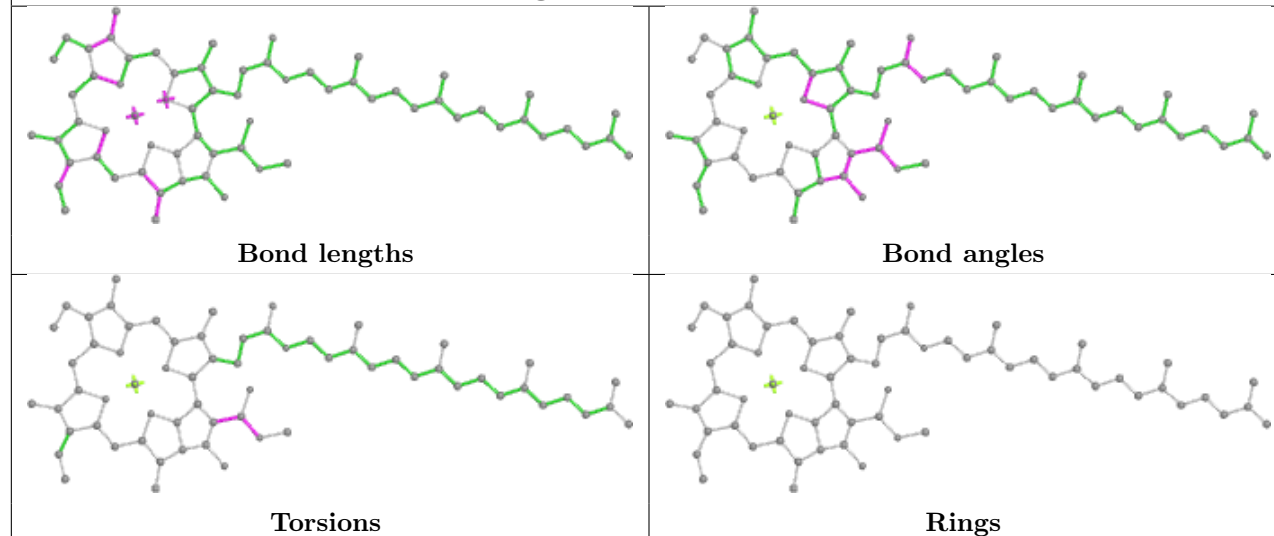


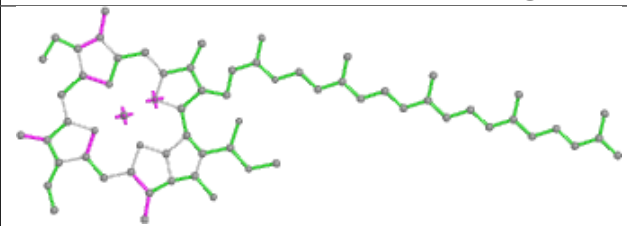
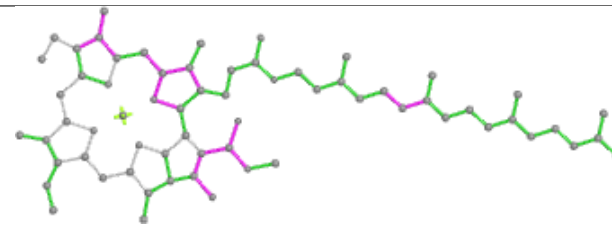
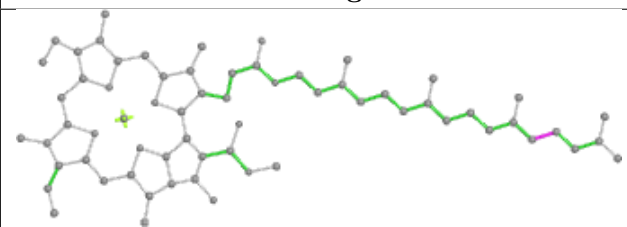
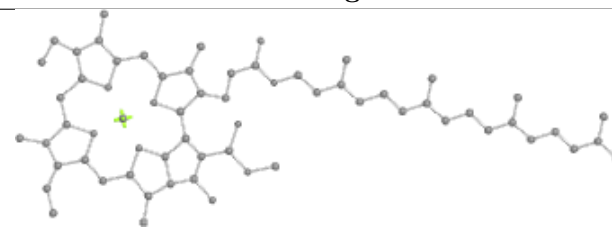
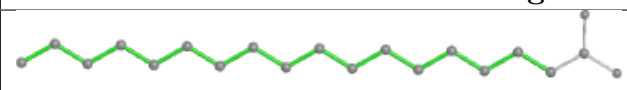
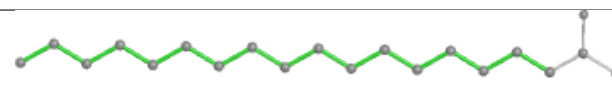
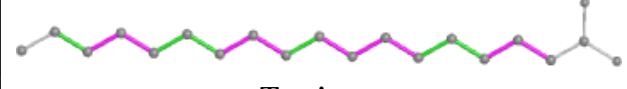
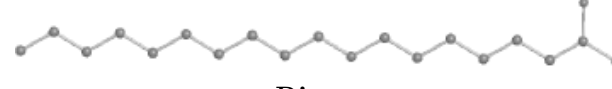
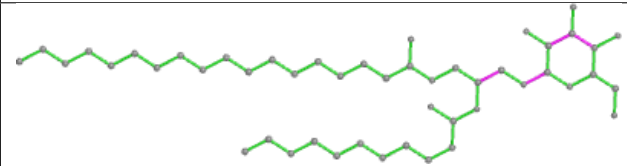
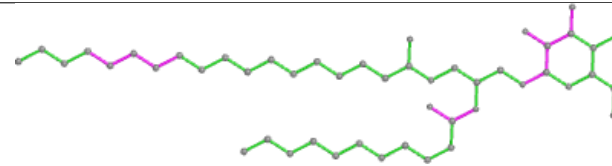
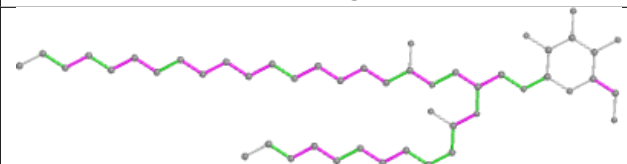
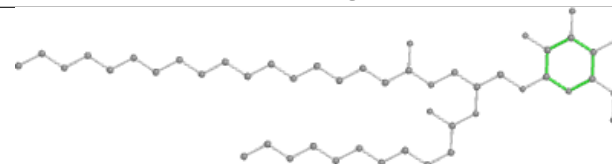




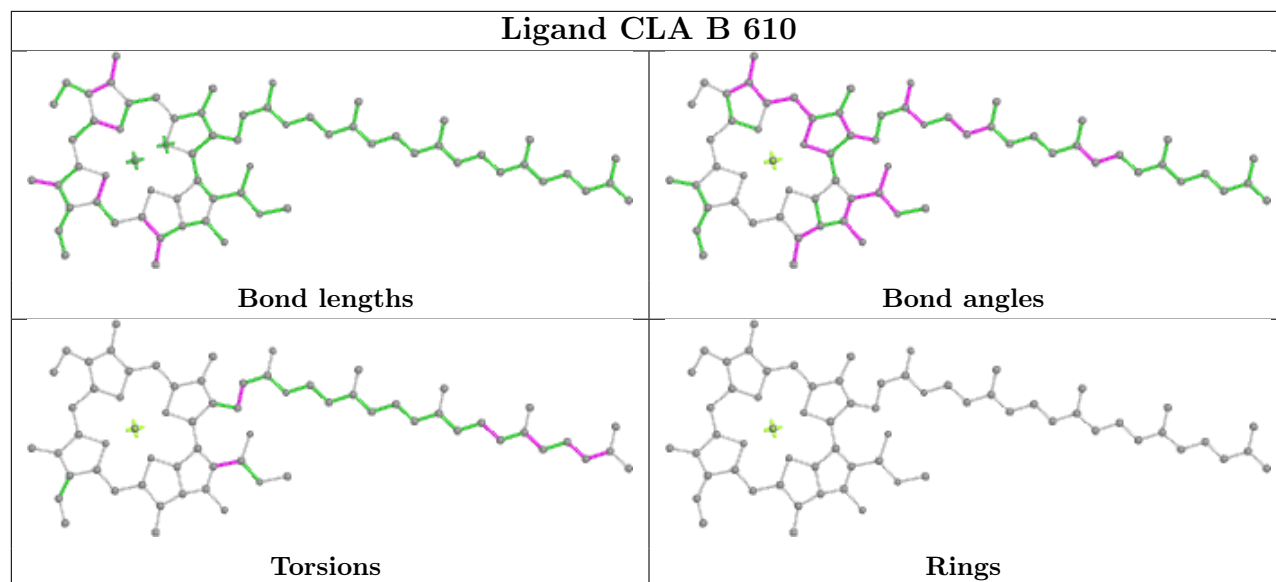
Ligand CLA b 613**Ligand BCR D 404****Ligand BCR T 101**



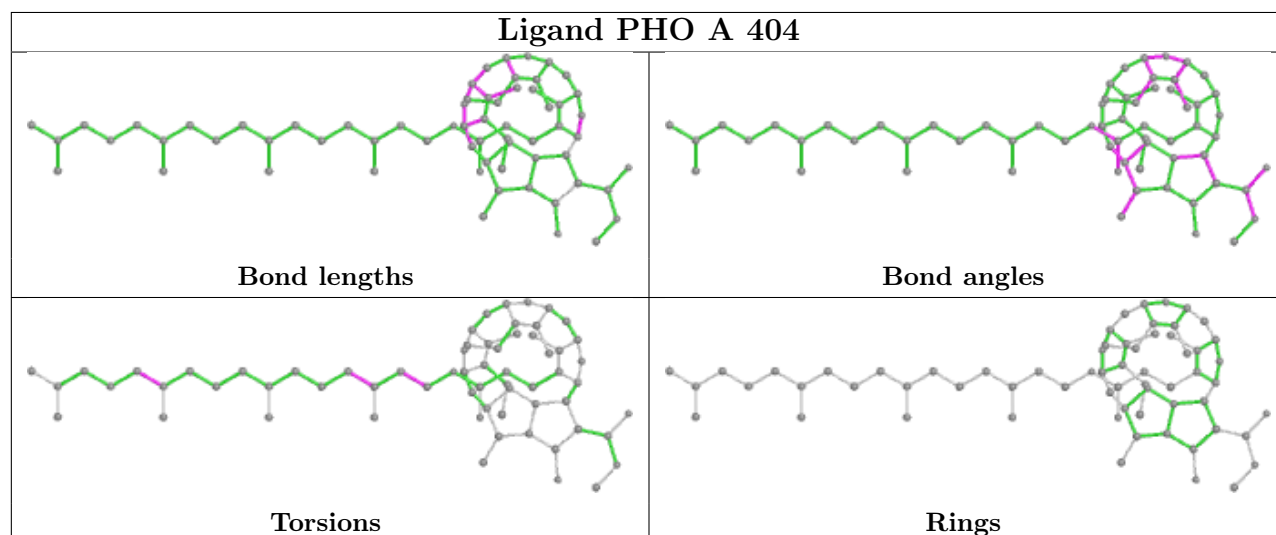
Ligand CLA A 403**Ligand CLA B 605****Ligand CLA C 501**

Ligand CLA B 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE b 623	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG c 521	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

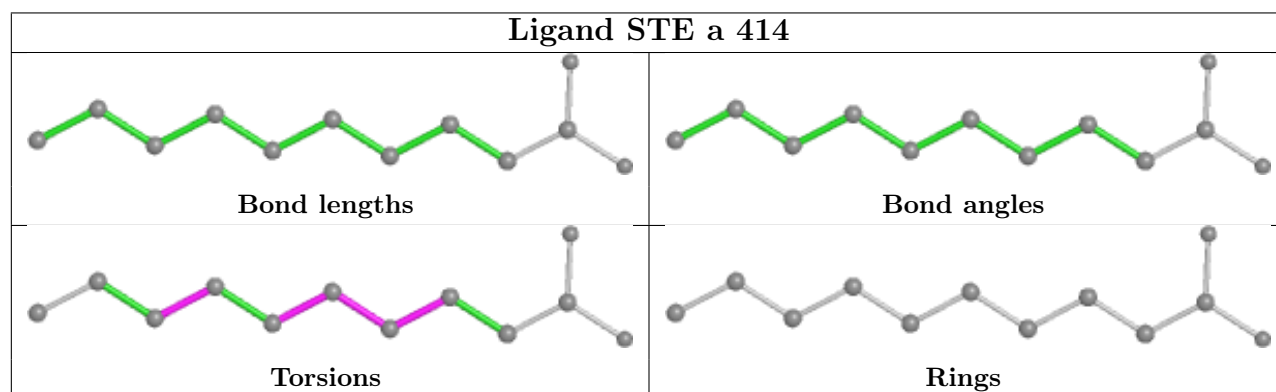
Ligand CLA B 610



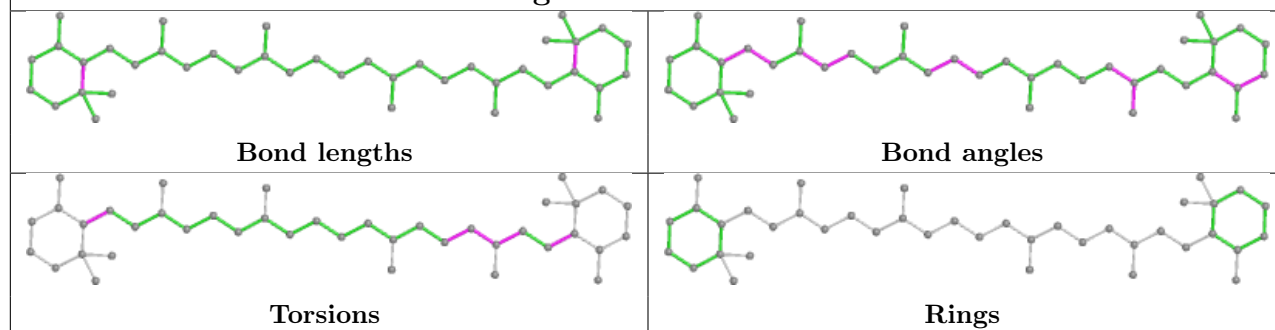
Ligand PHO A 404



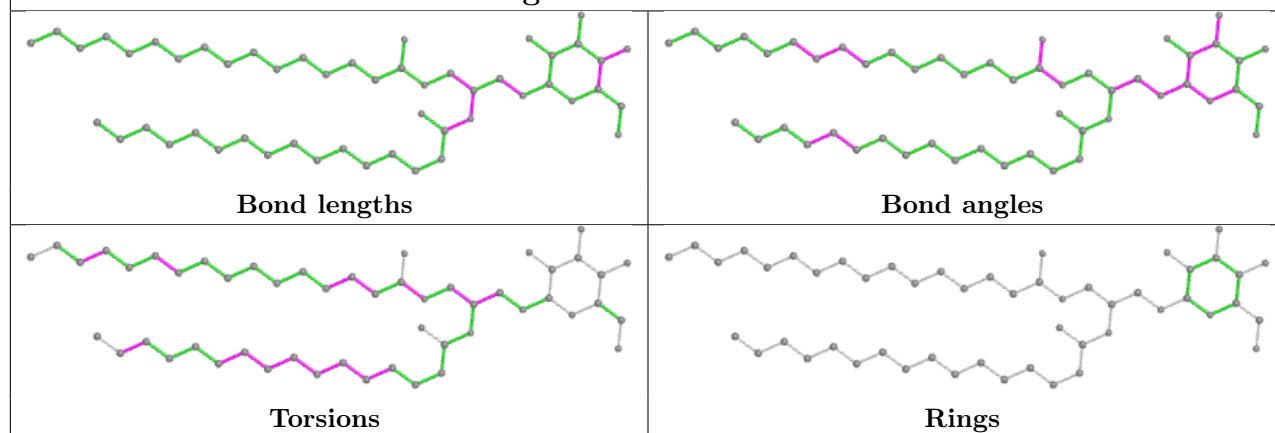
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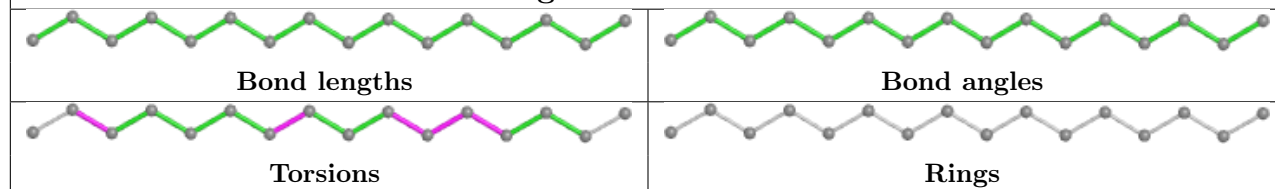
Ligand BCR k 102



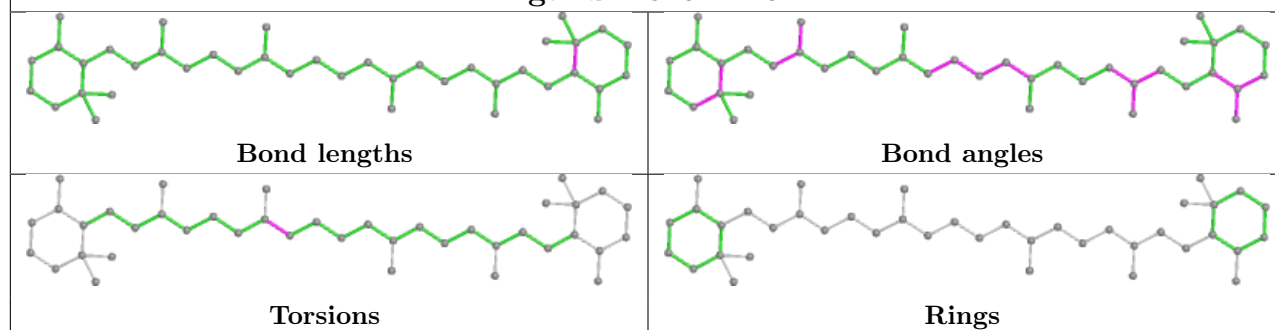
Ligand LMG M 101

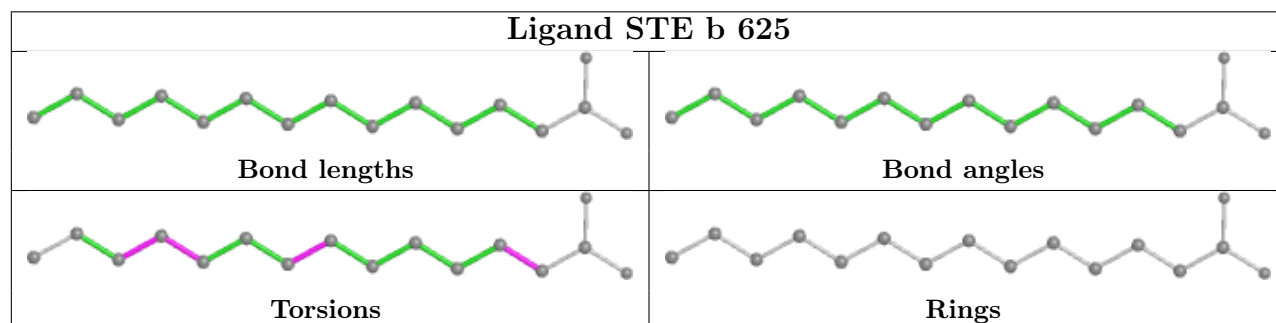
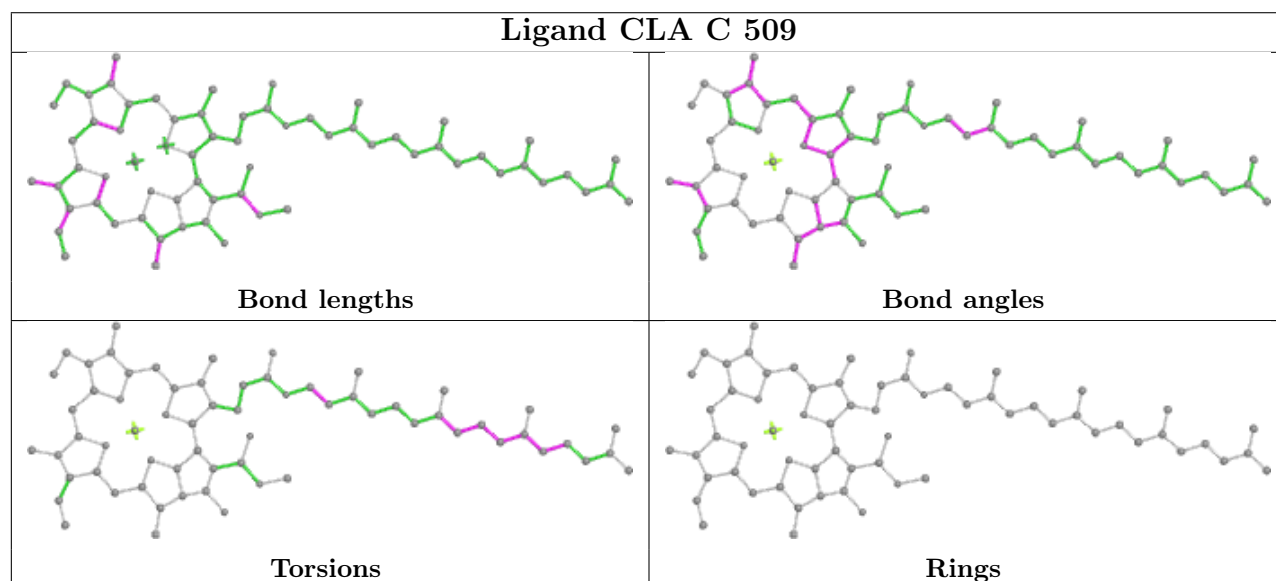
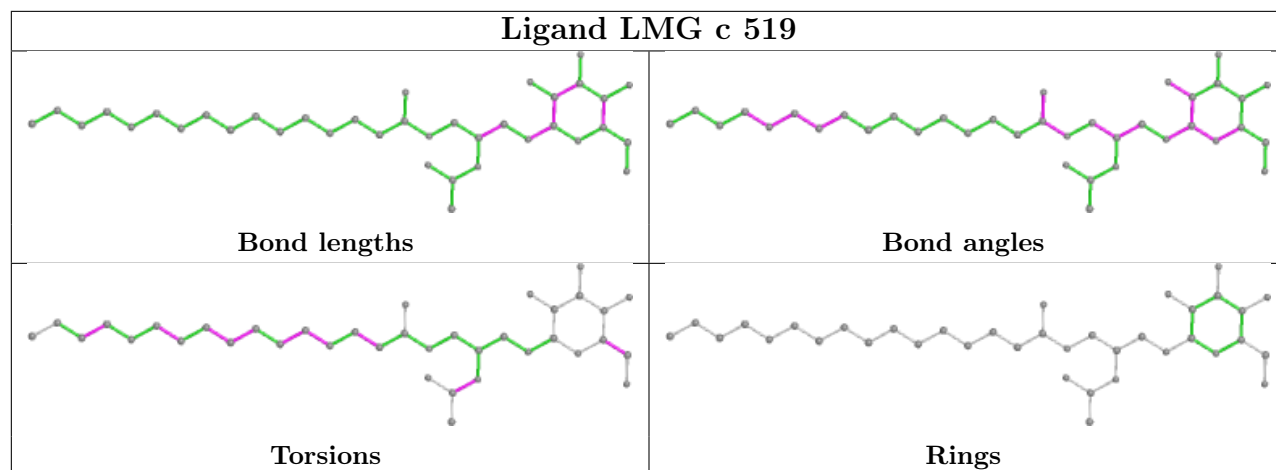


Ligand STE b 621

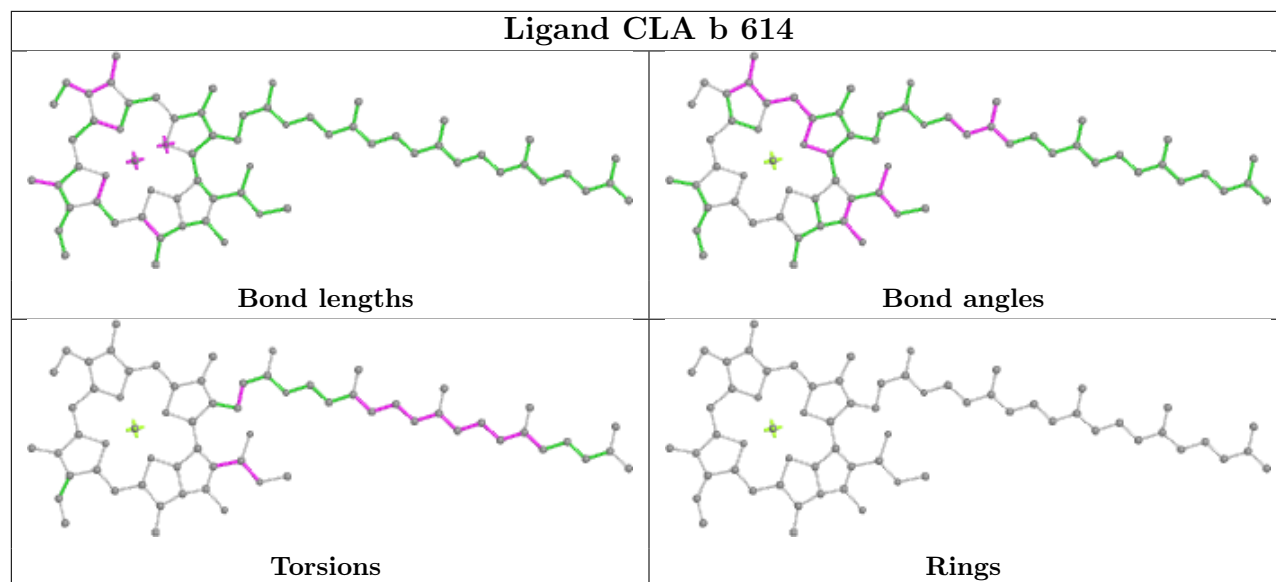


Ligand BCR H 101

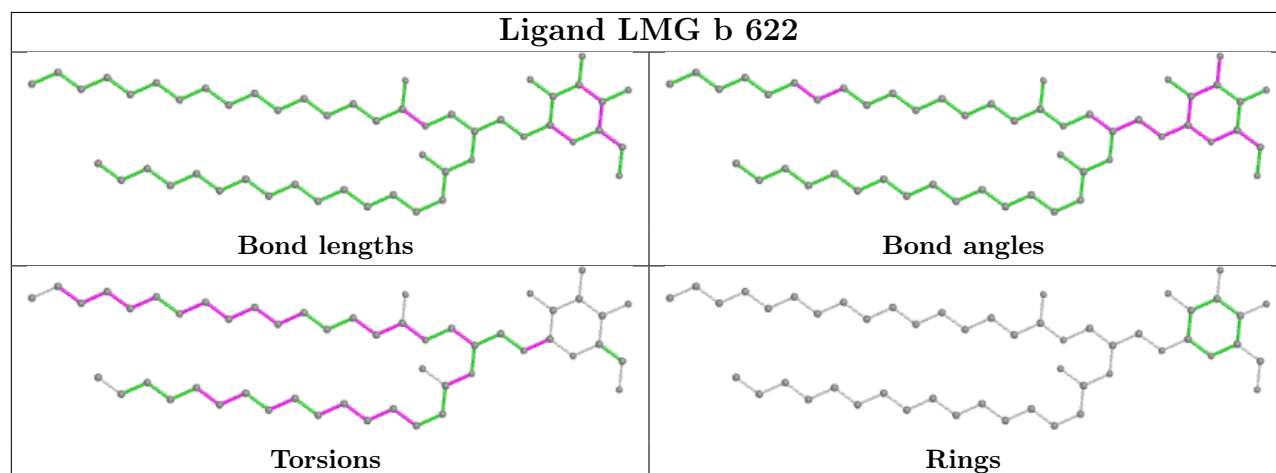




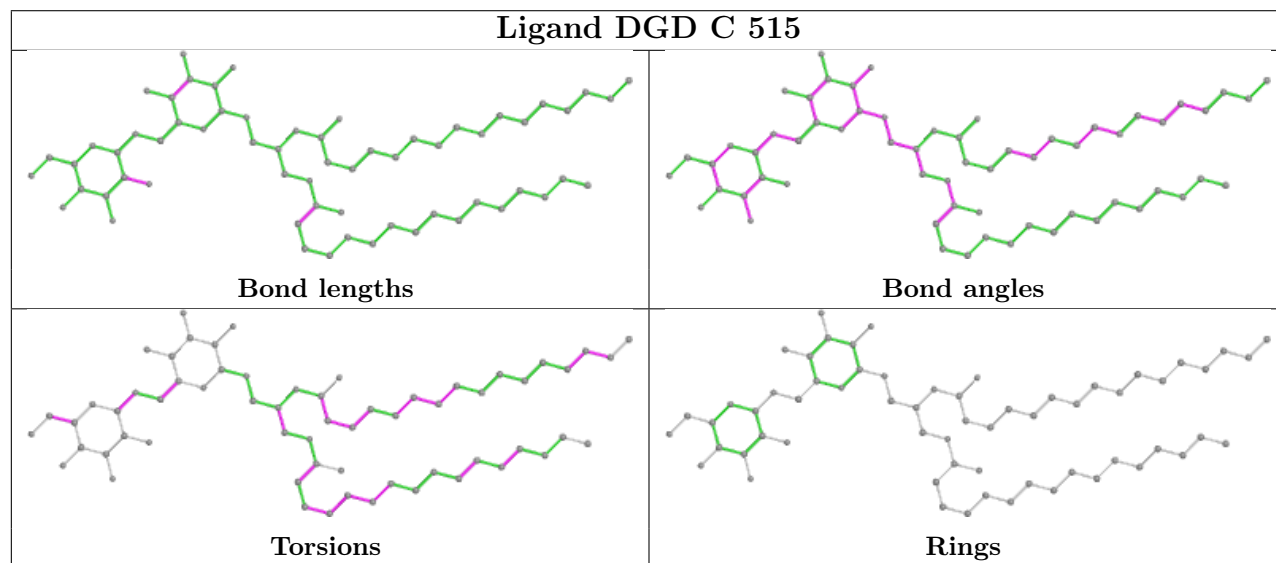
Ligand CLA b 614

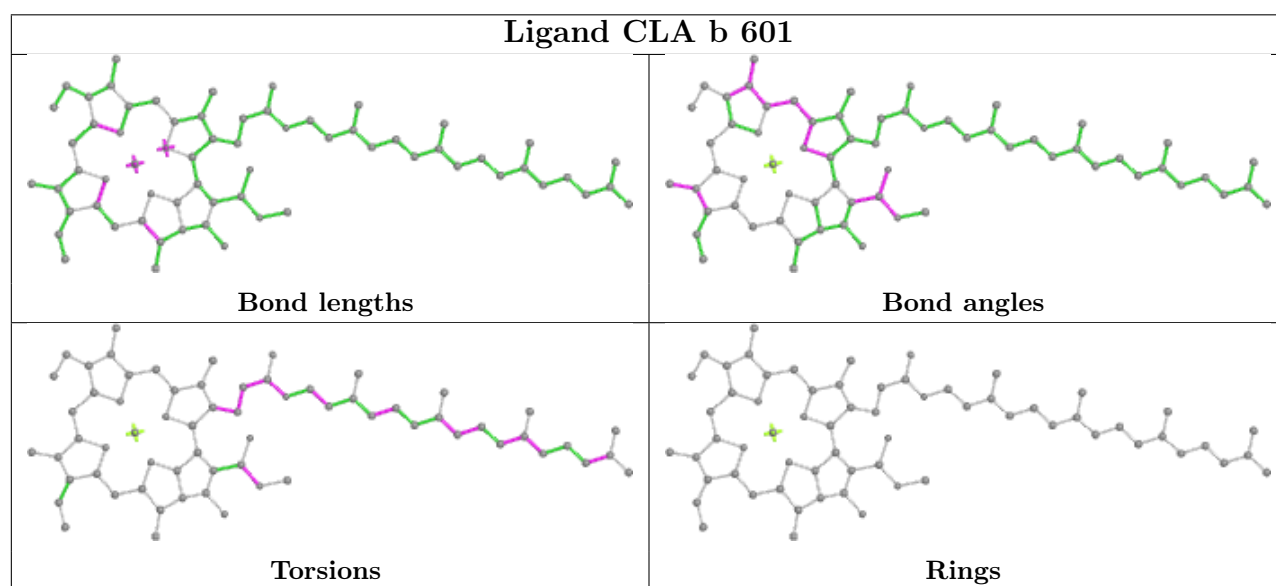
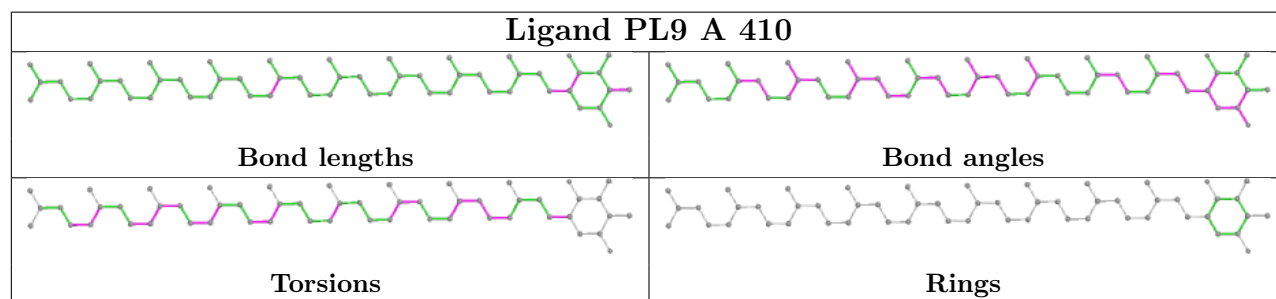
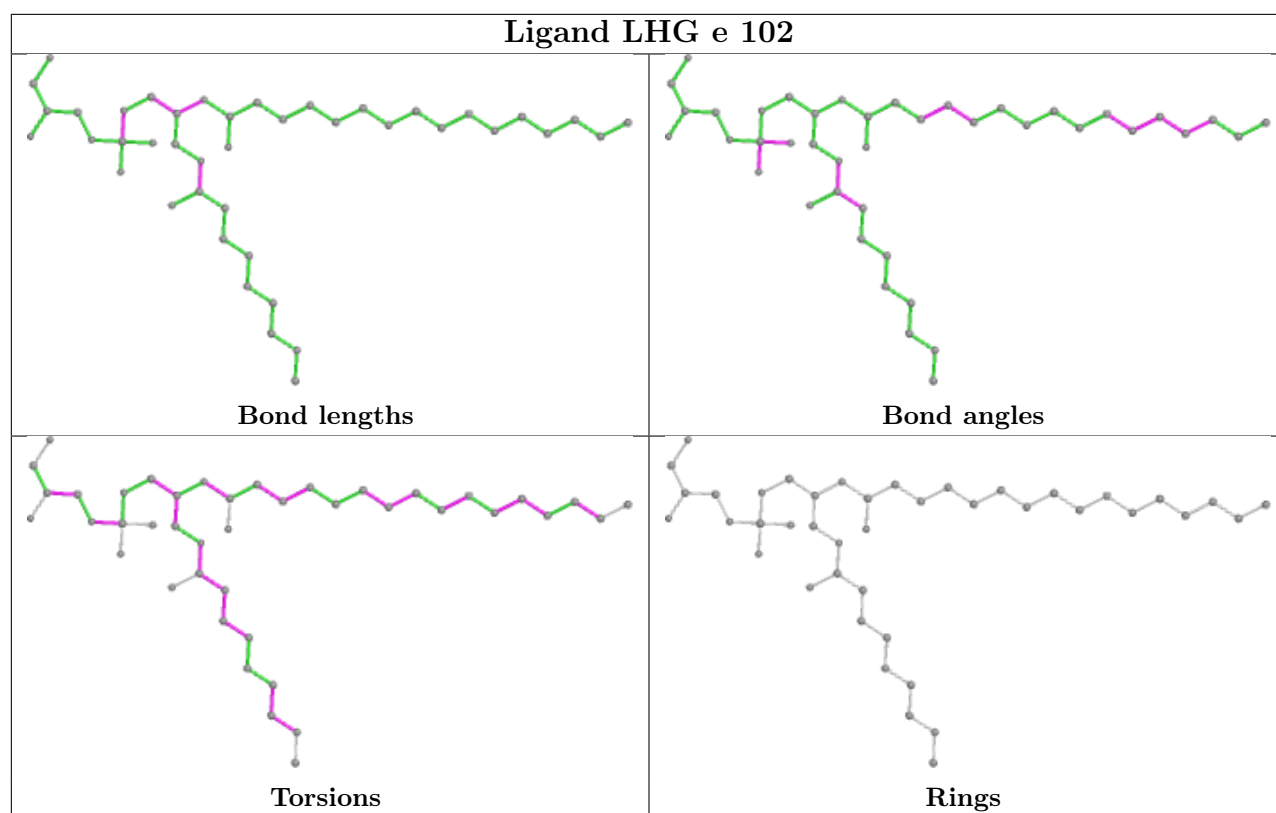


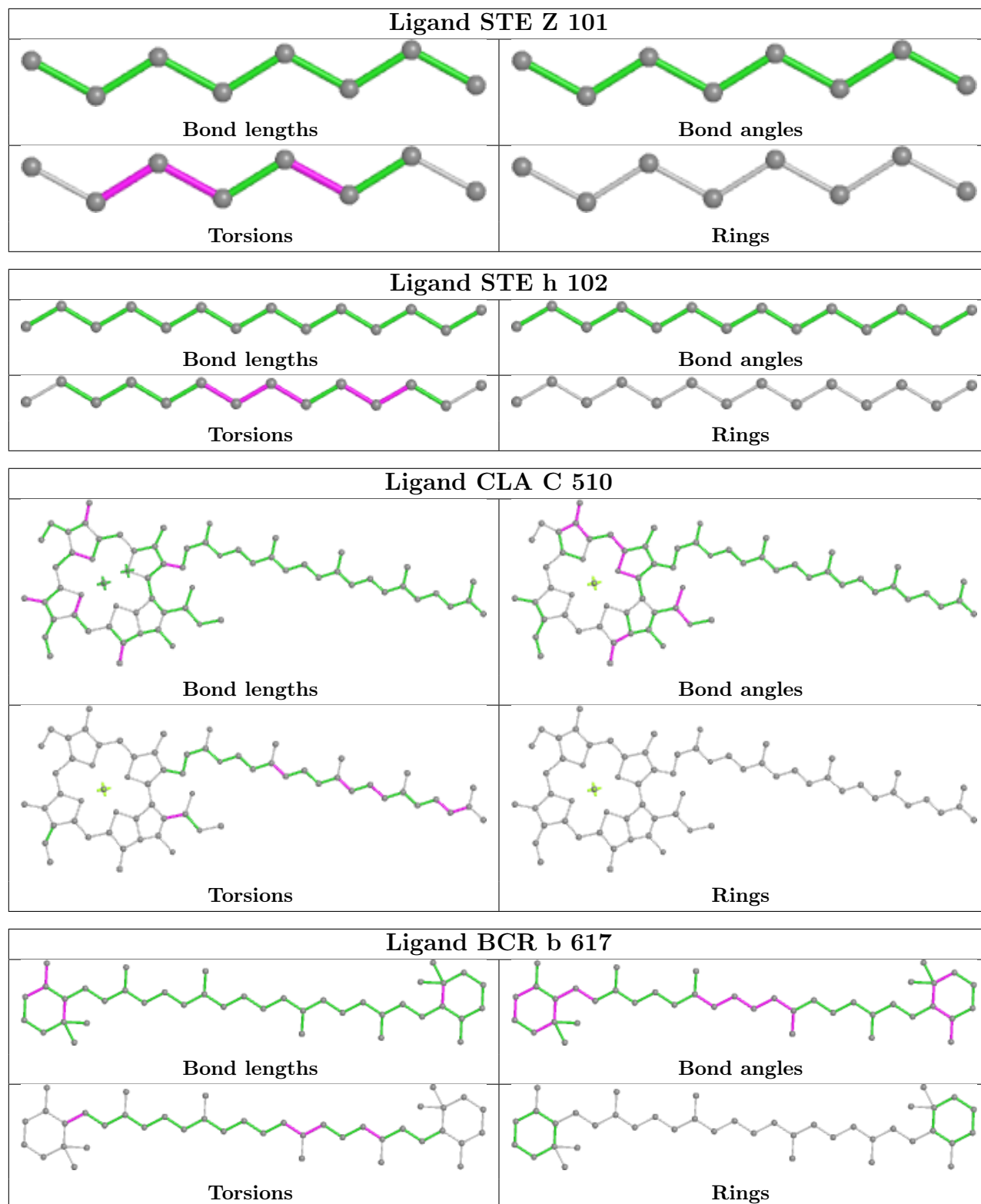
Ligand LMG b 622

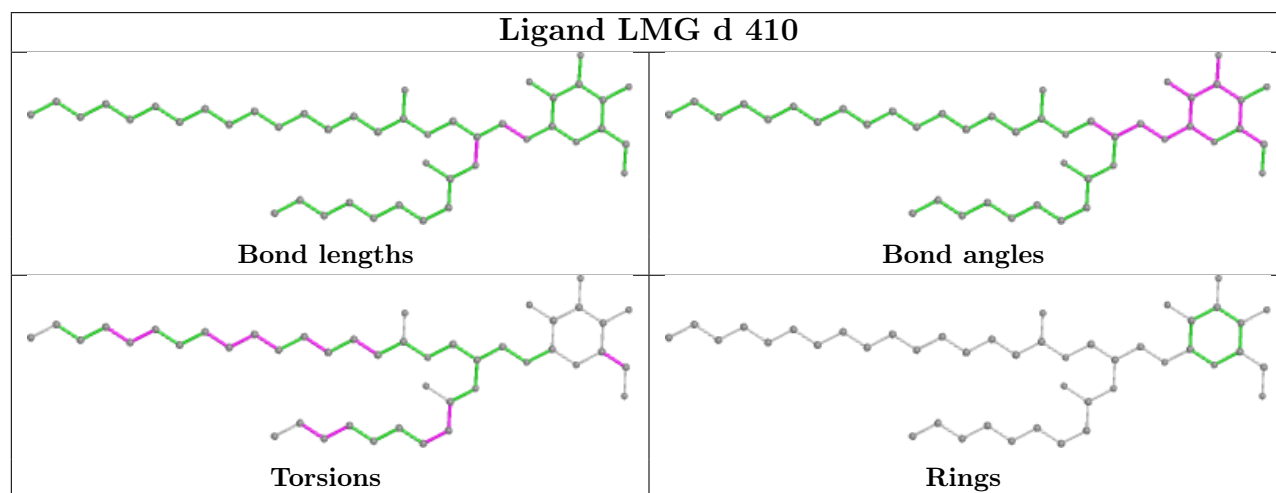
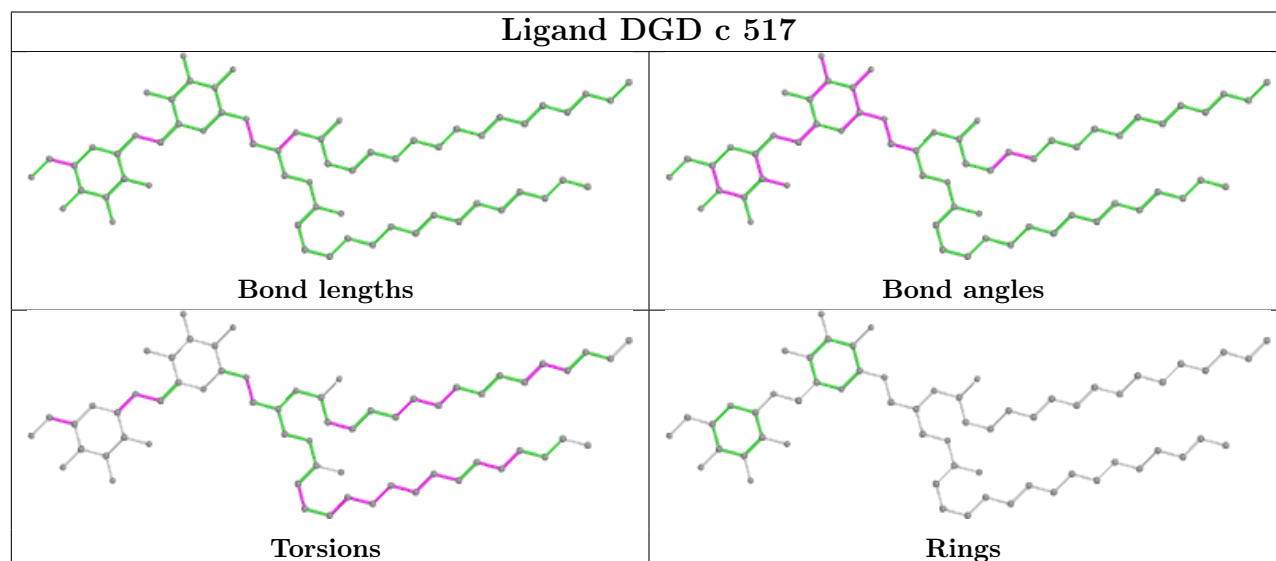
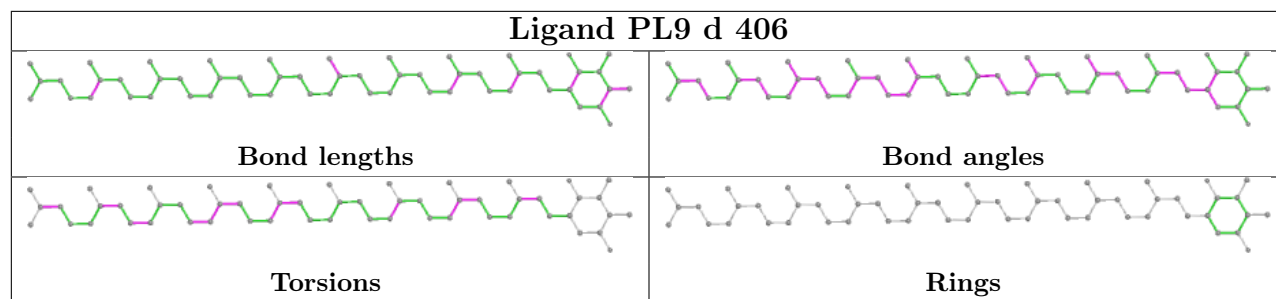


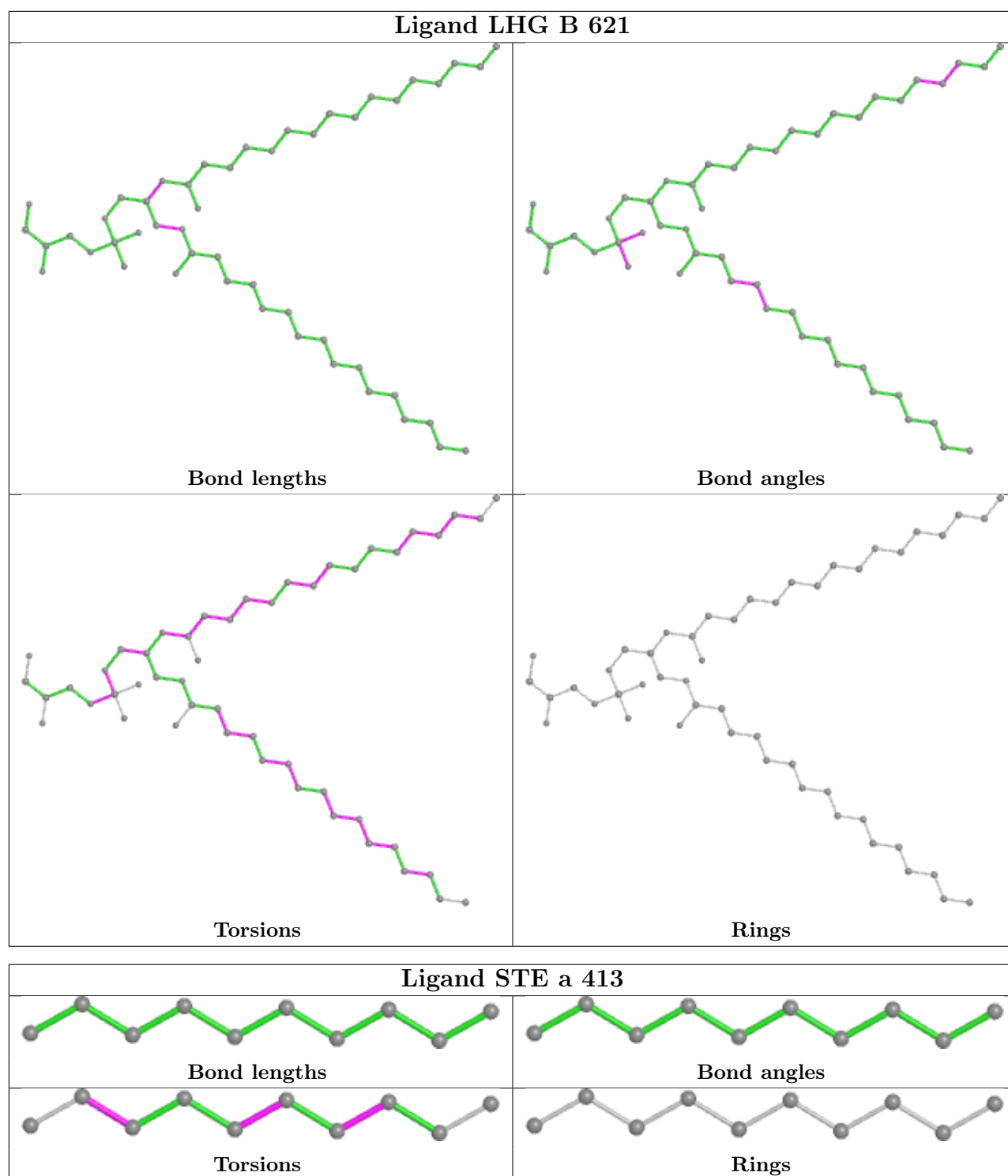
Ligand DGD C 515

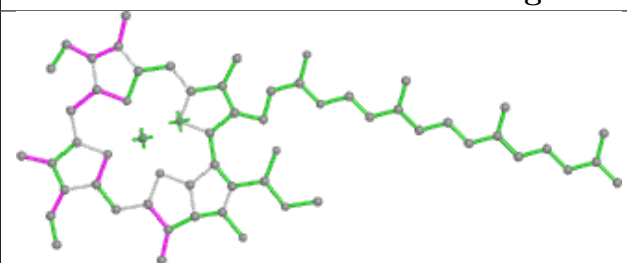
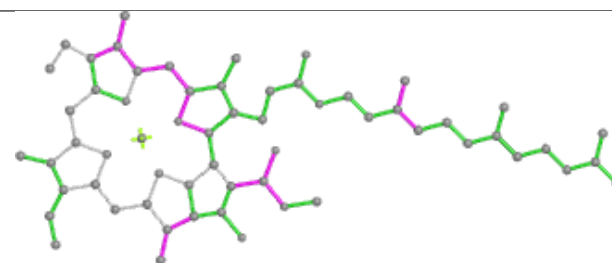
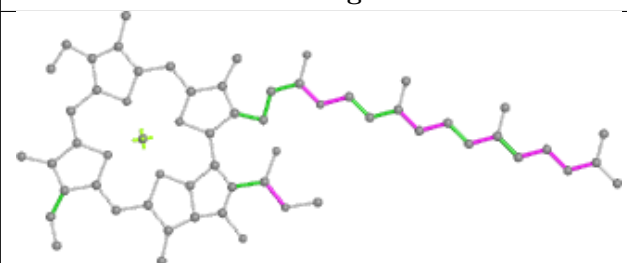
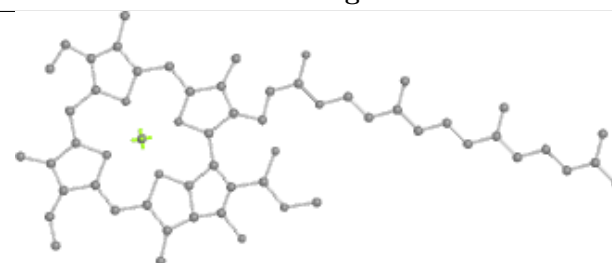


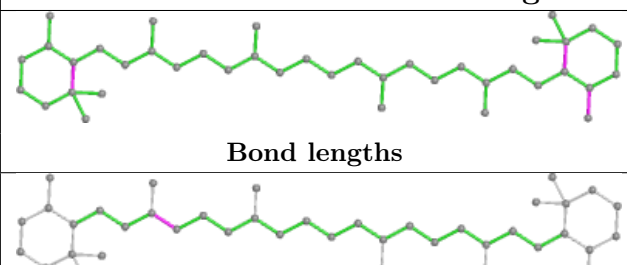
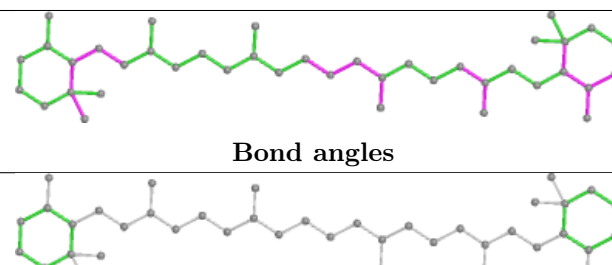
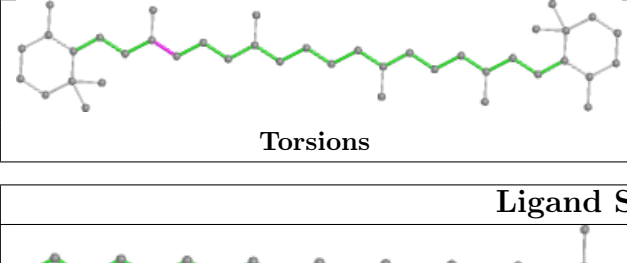
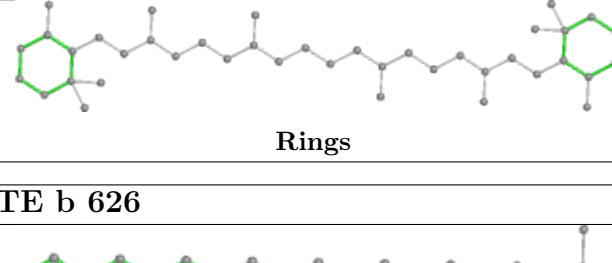


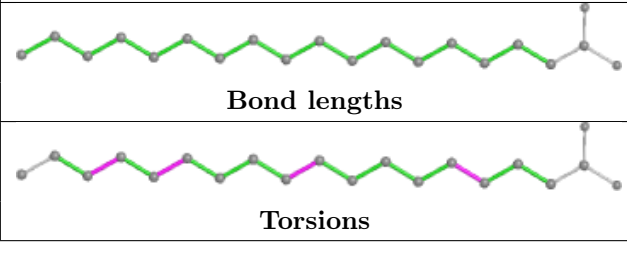
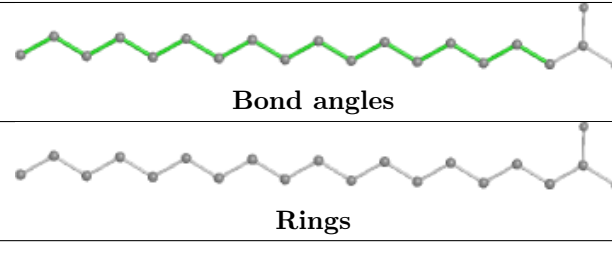
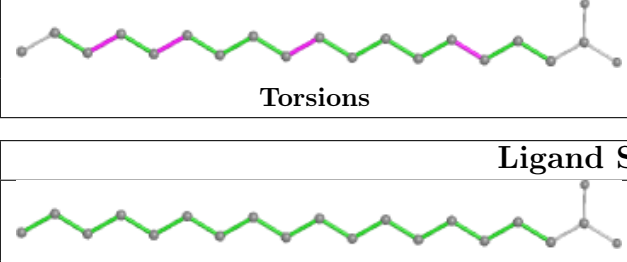
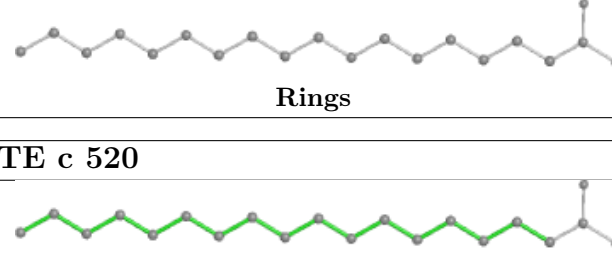


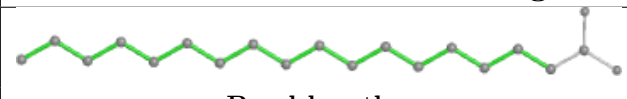
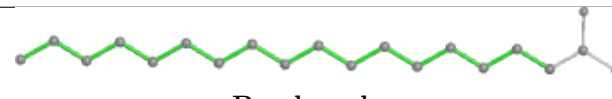
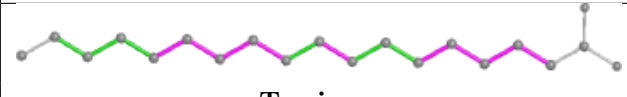
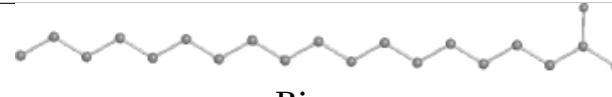




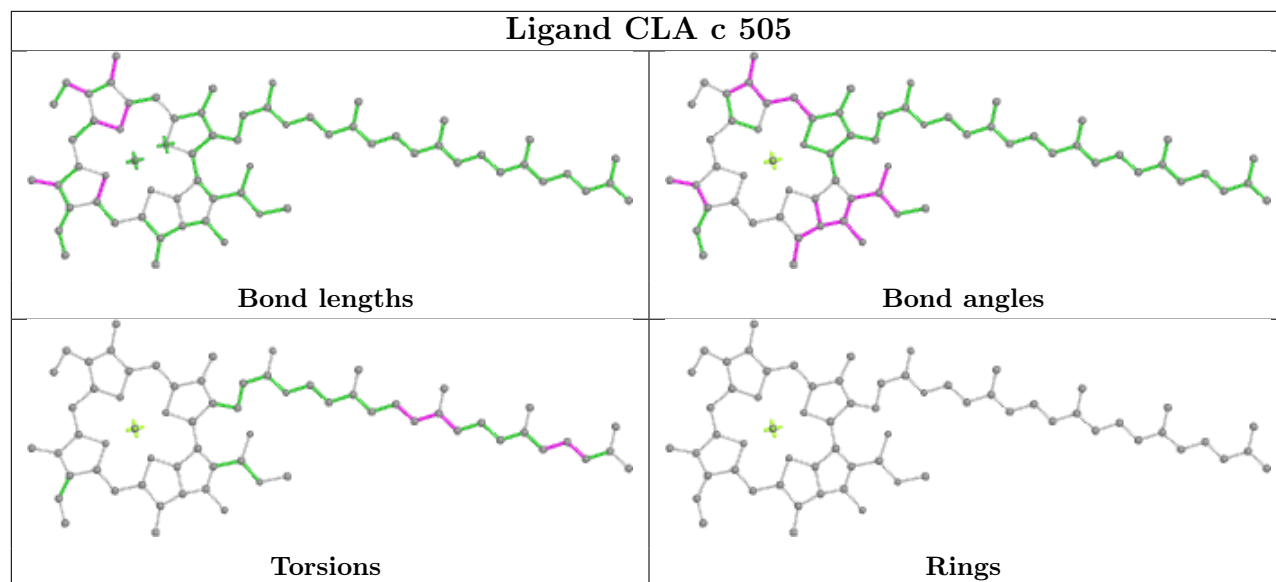
Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

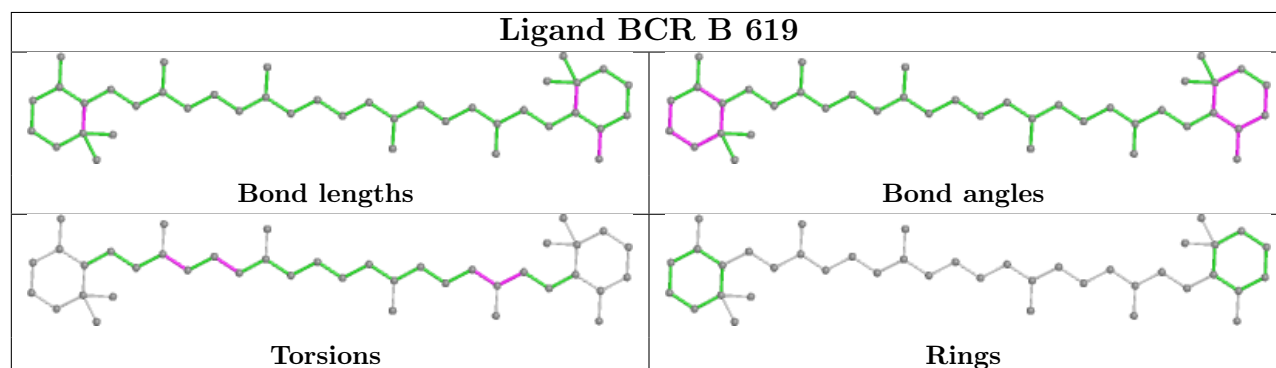
Ligand STE b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

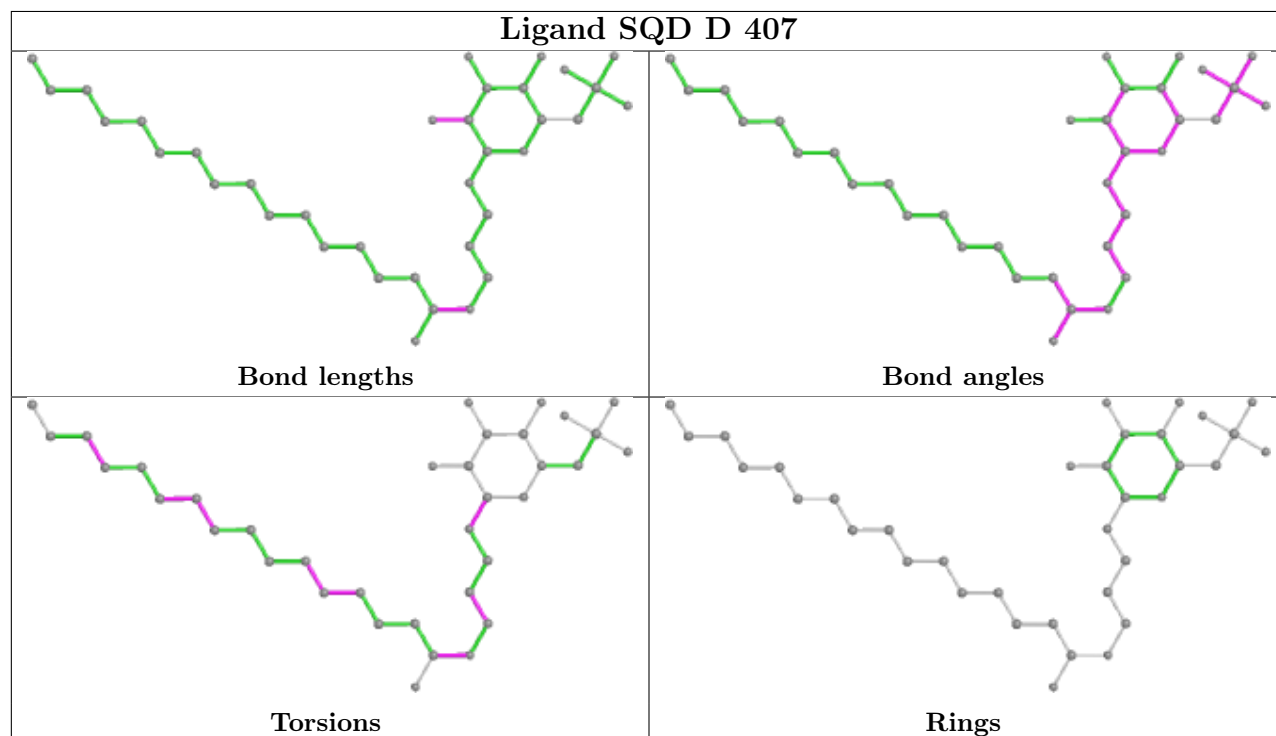
Ligand CLA c 505



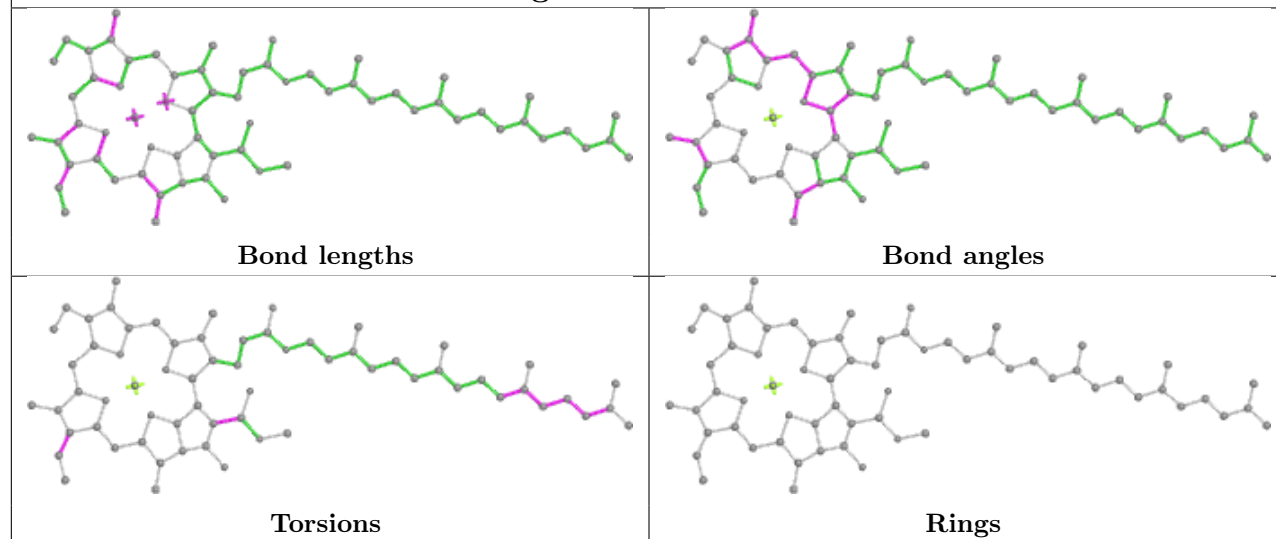
Ligand BCR B 619



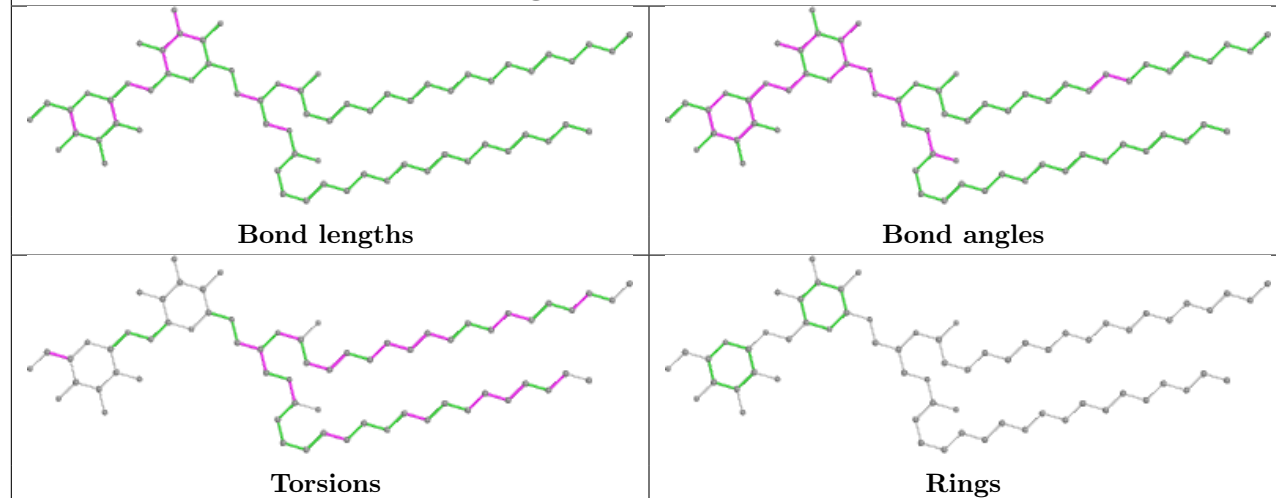
Ligand SQD D 407



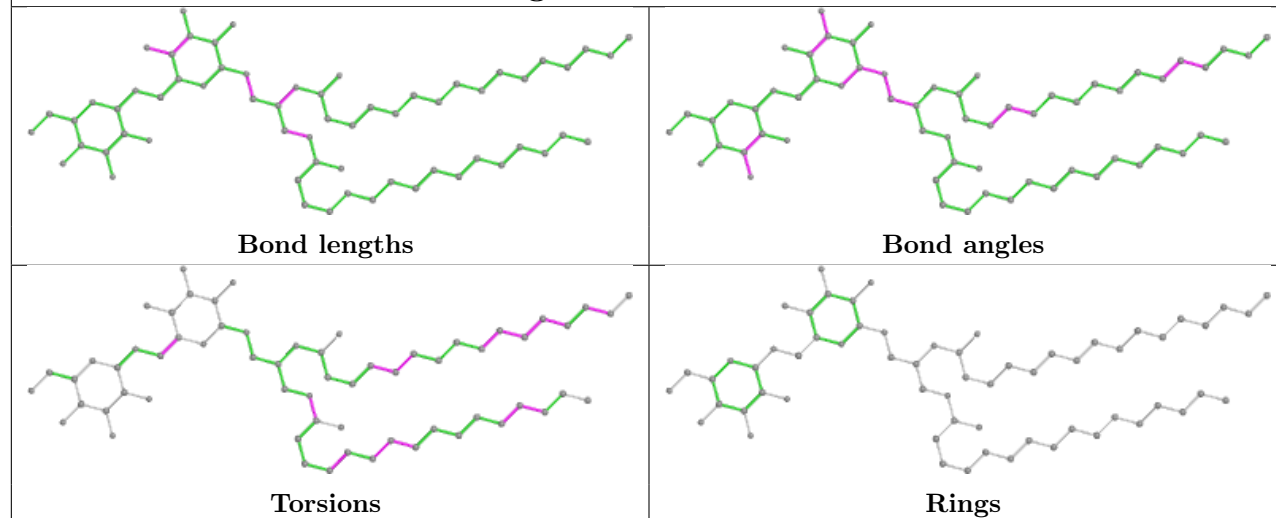
Ligand CLA A 411



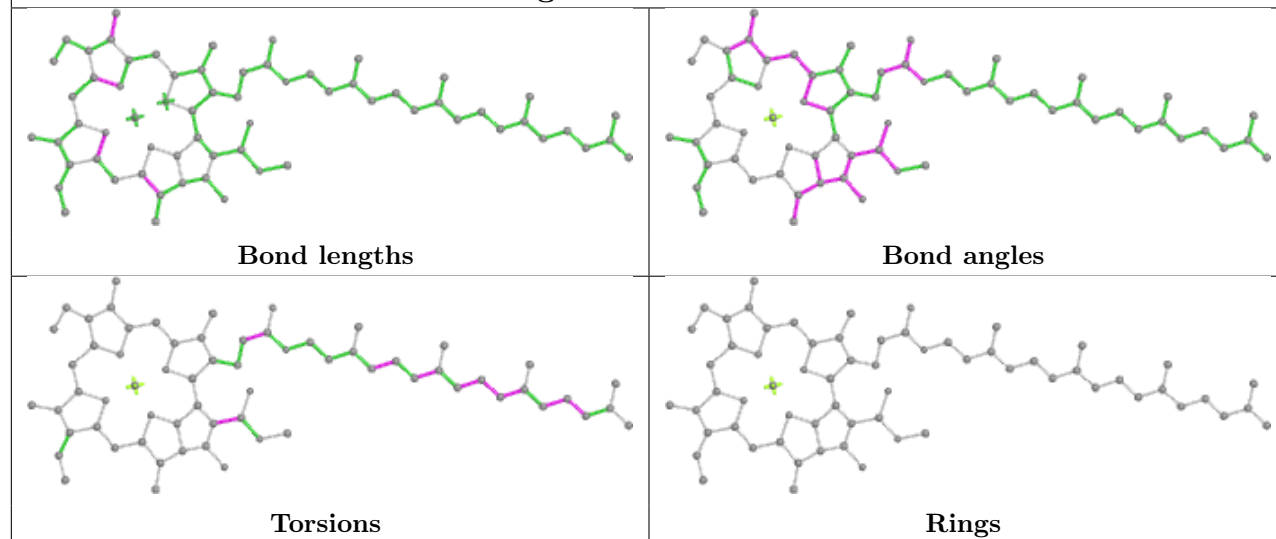
Ligand DGD A 416



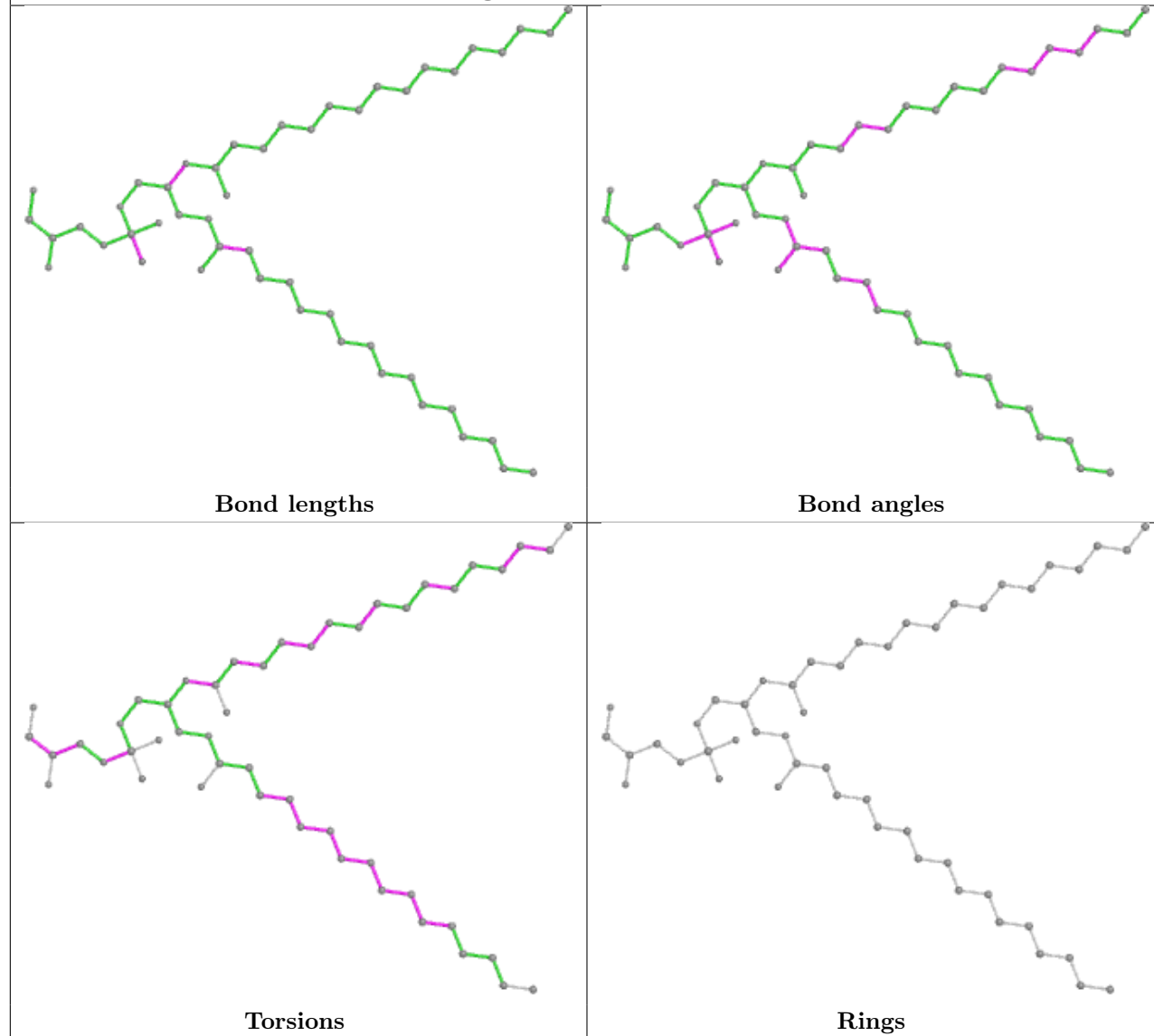
Ligand DGD C 517

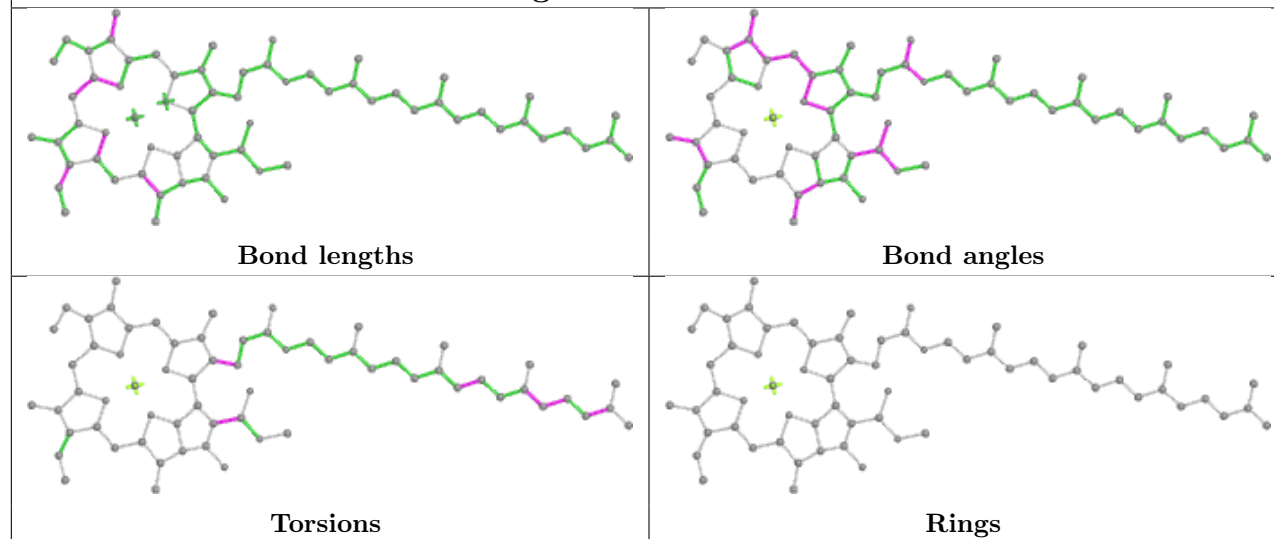
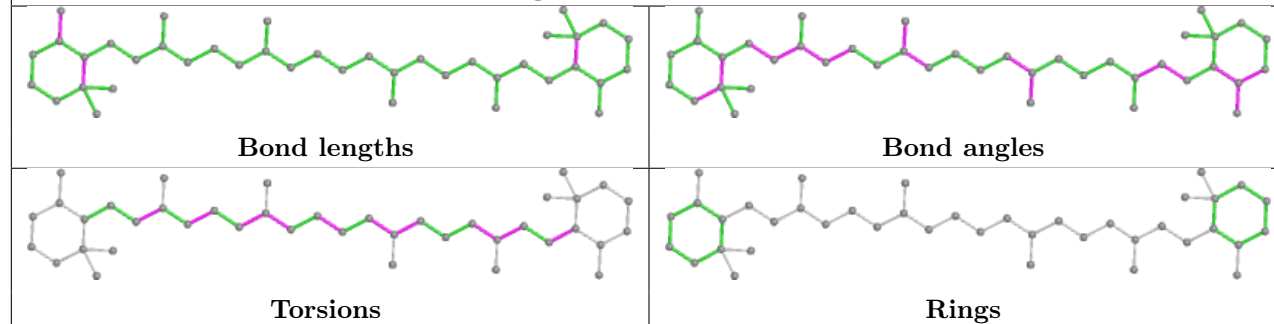
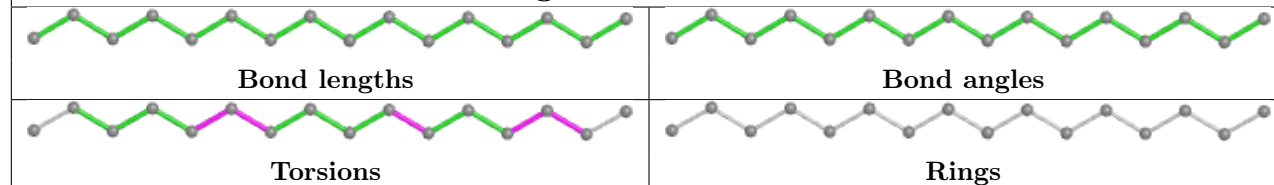
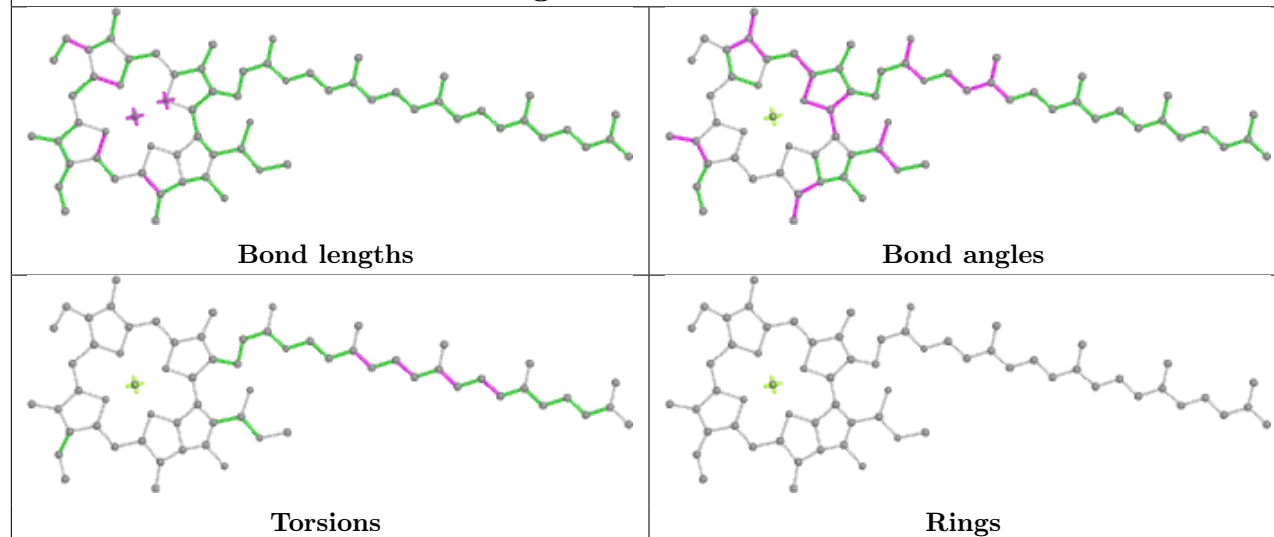


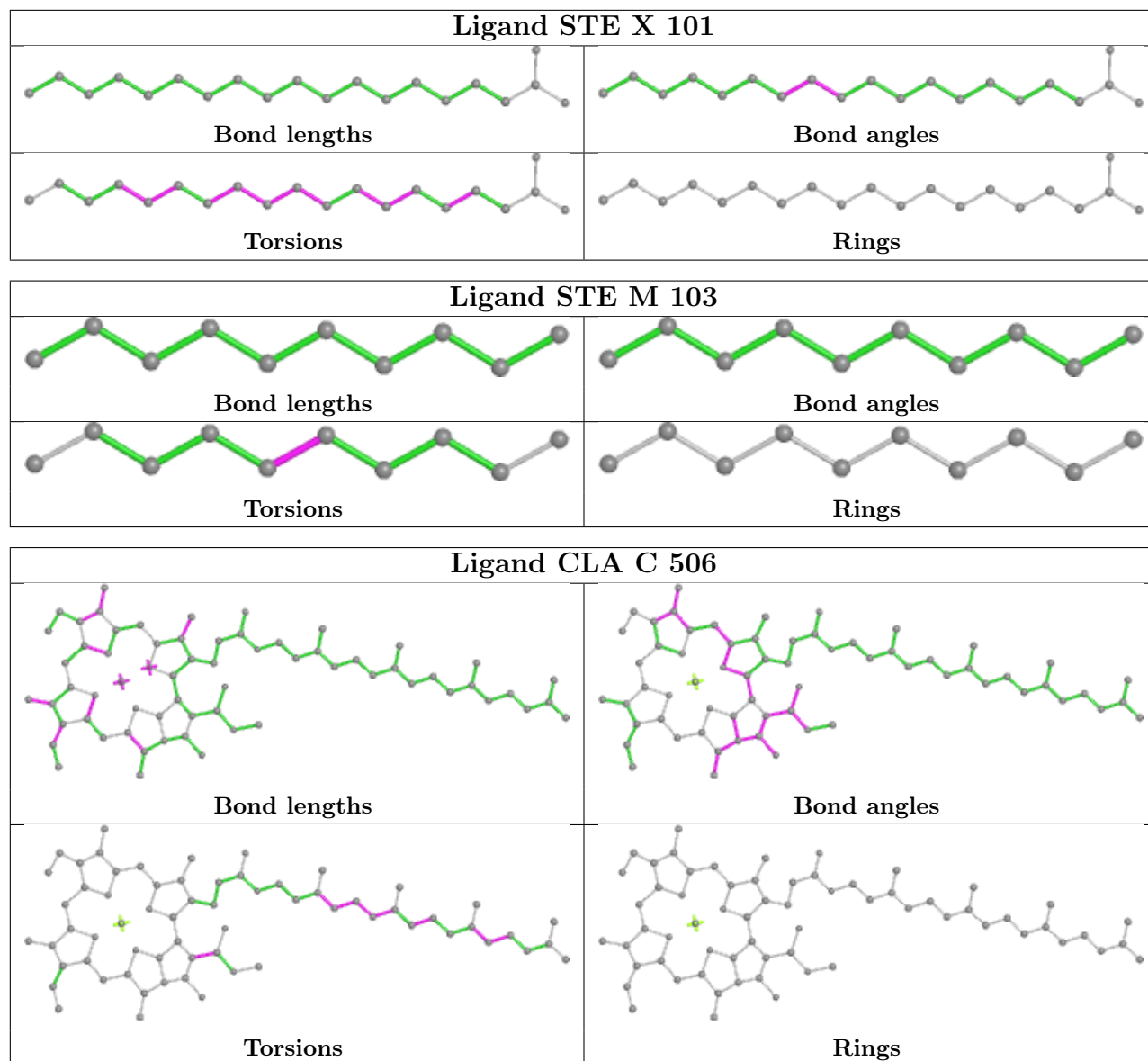
Ligand CLA c 509

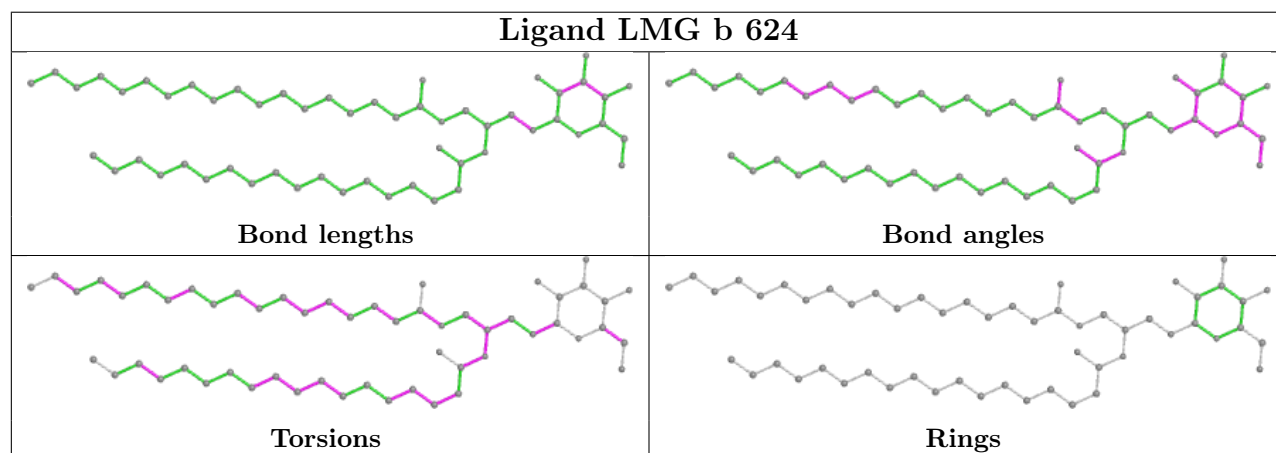
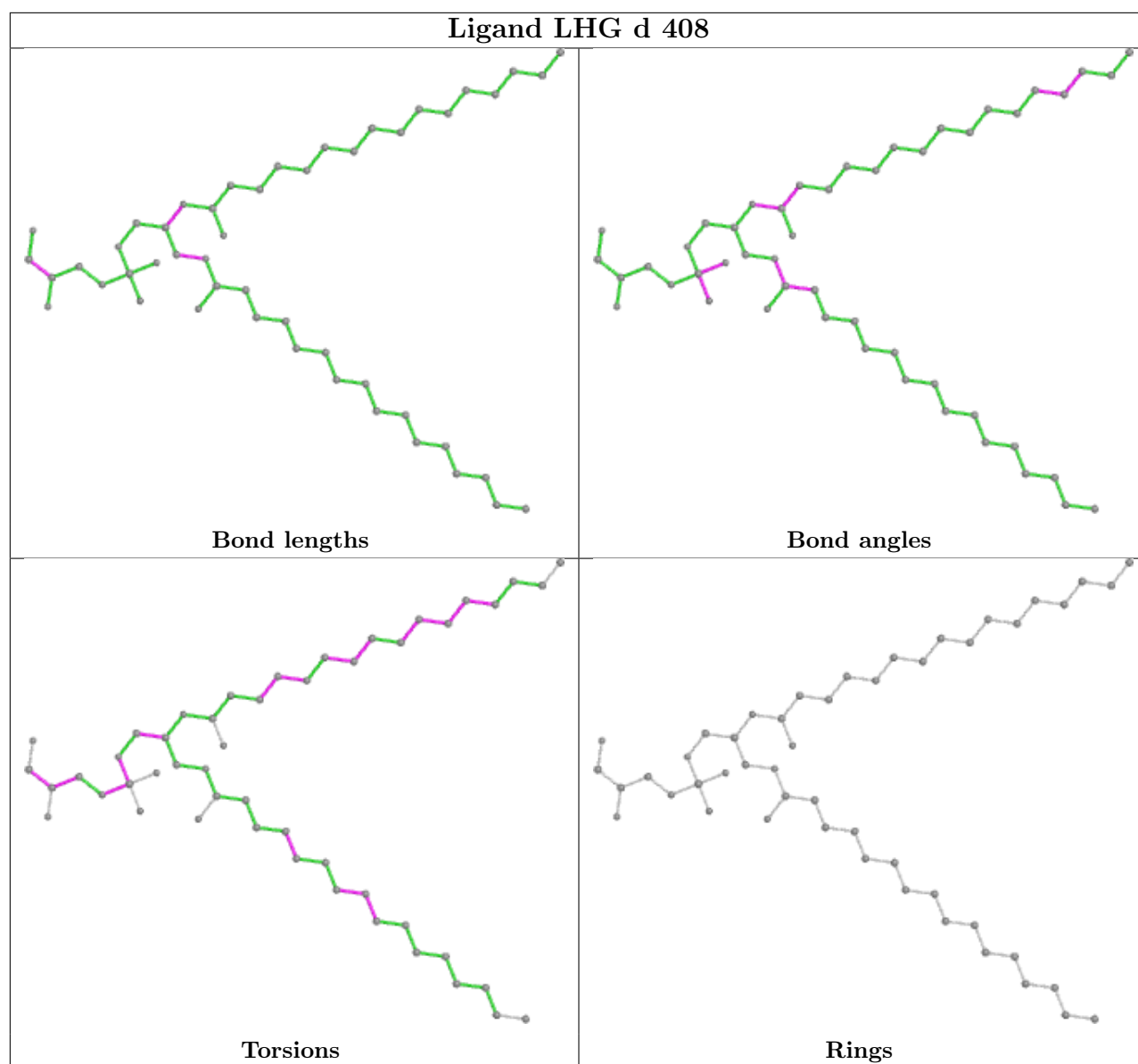


Ligand LHG B 622

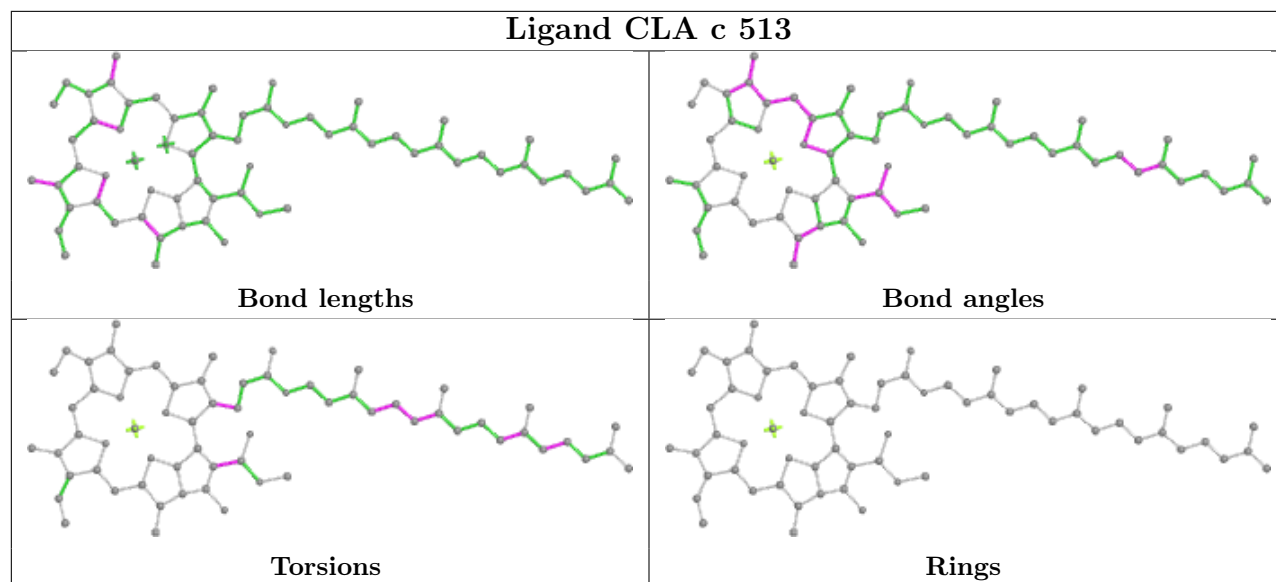


Ligand CLA B 602**Ligand BCR K 101****Ligand STE C 520****Ligand CLA C 507**

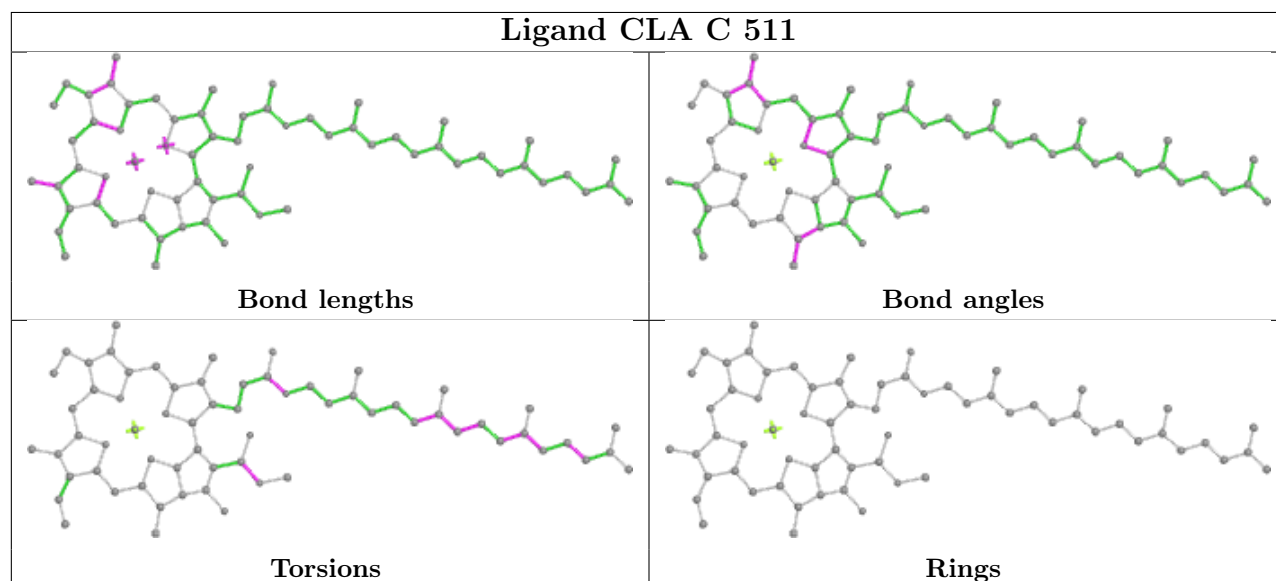




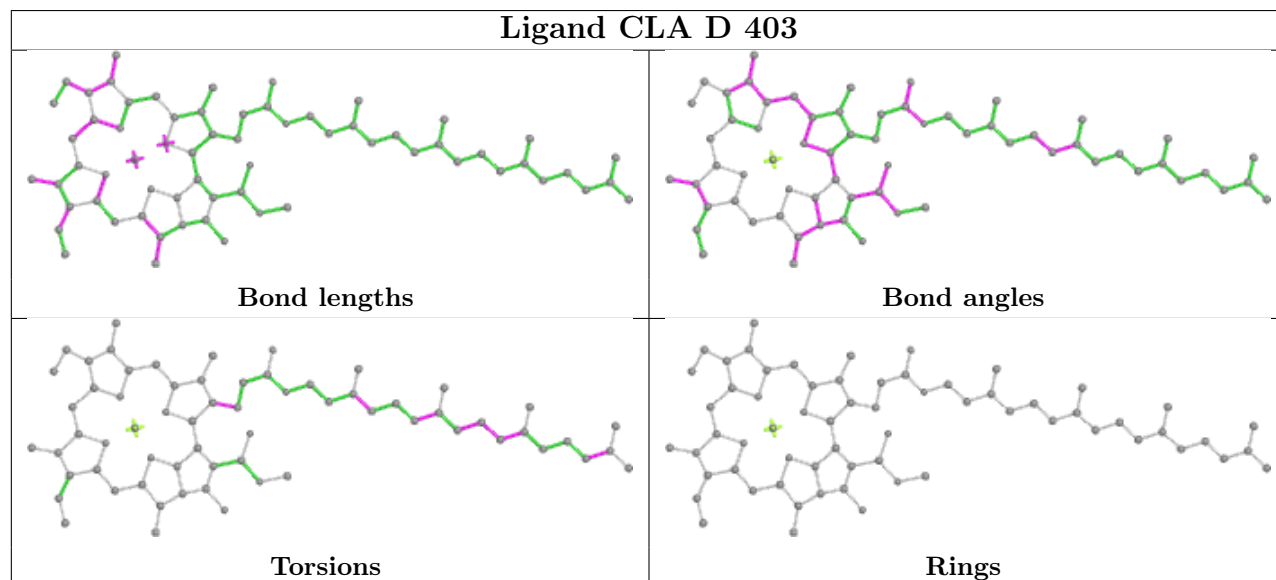
Ligand CLA c 513

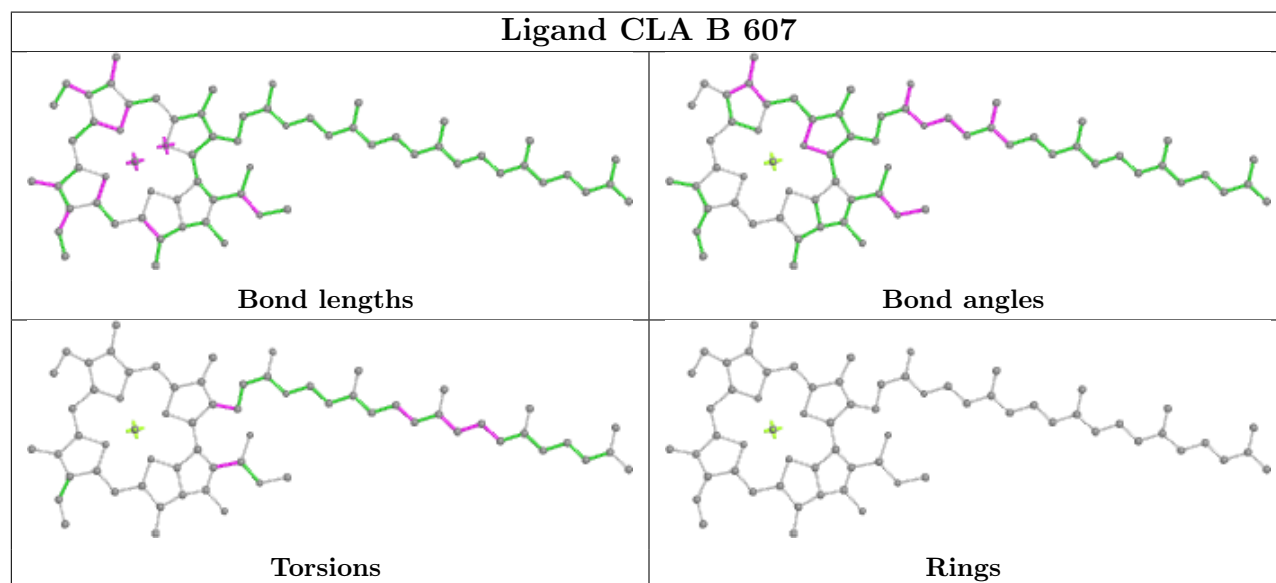
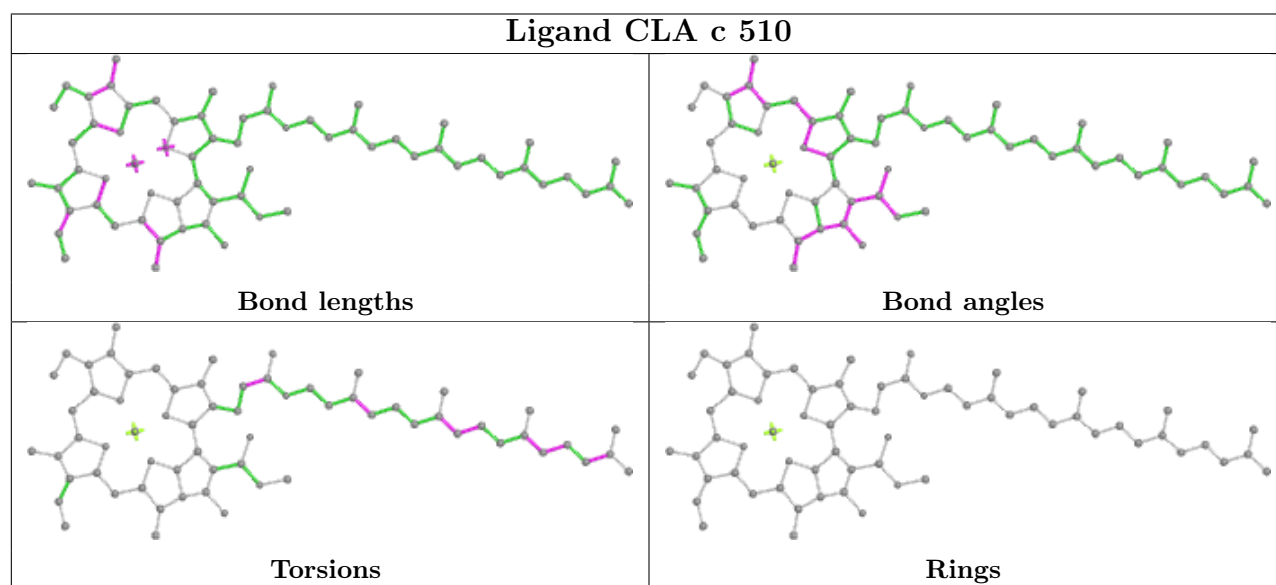
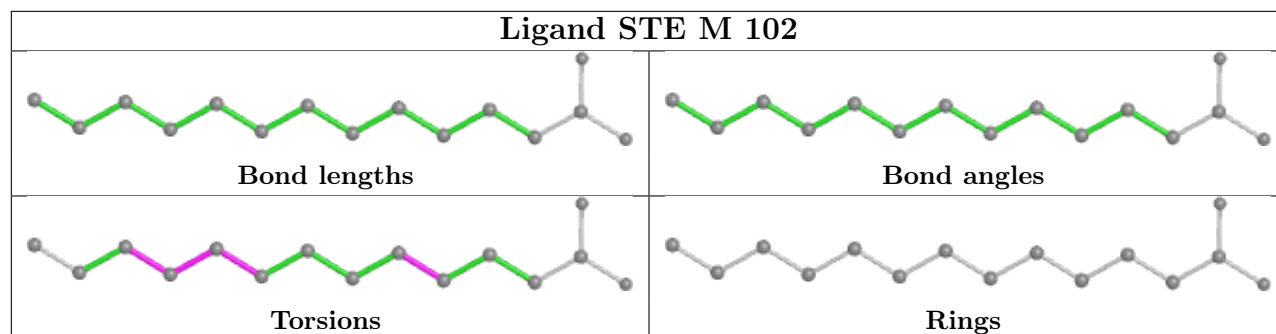


Ligand CLA C 511

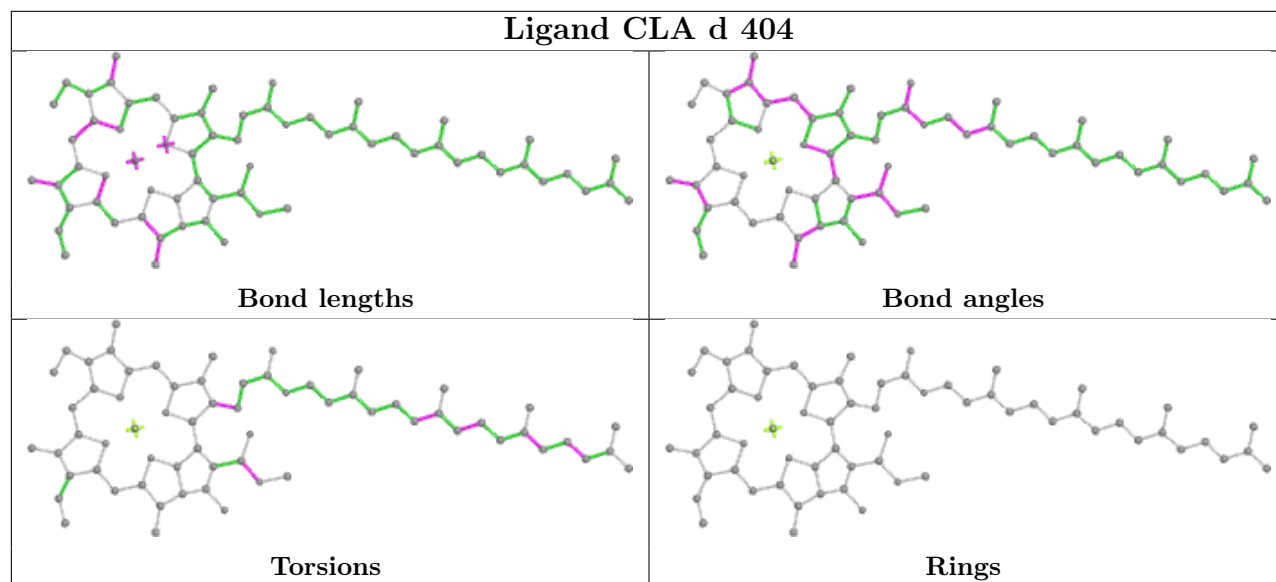


Ligand CLA D 403

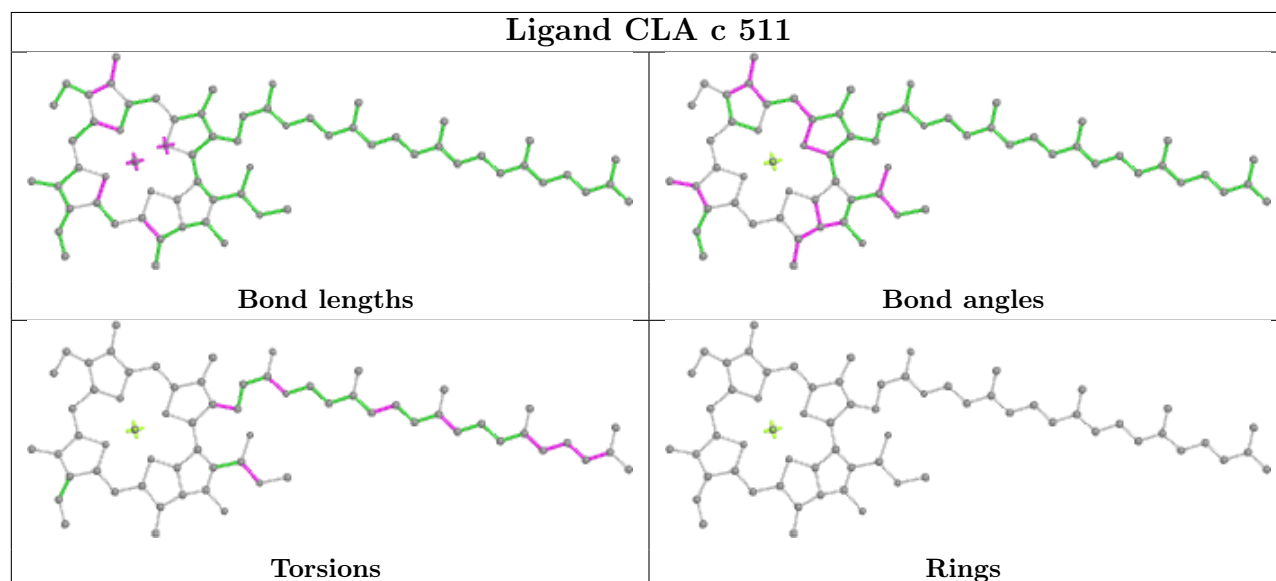




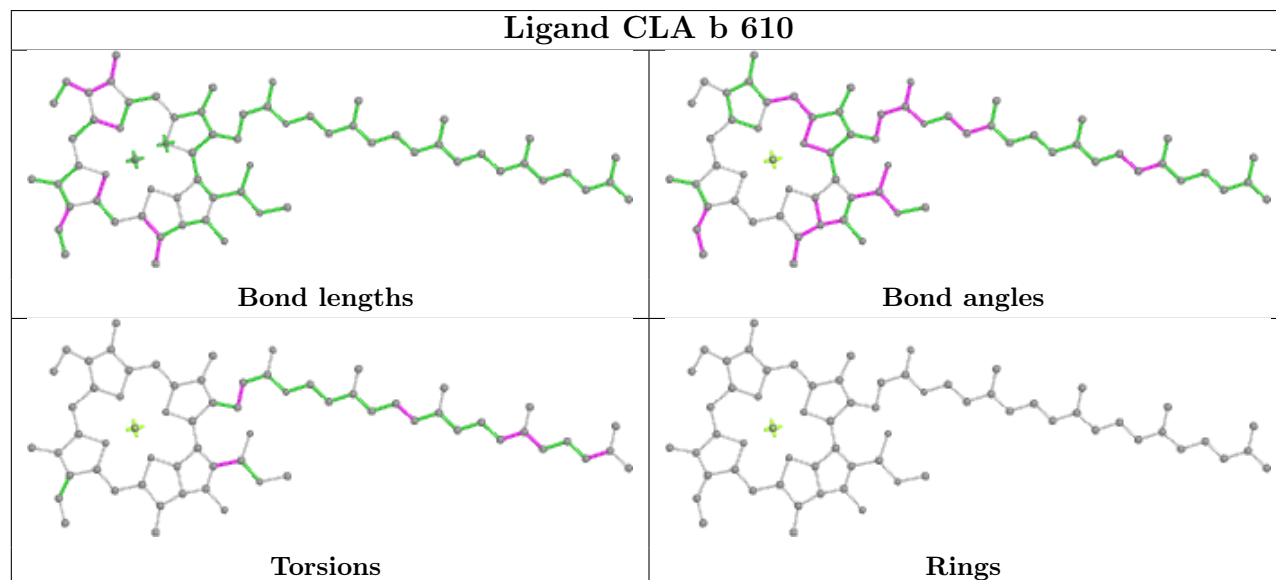
Ligand CLA d 404

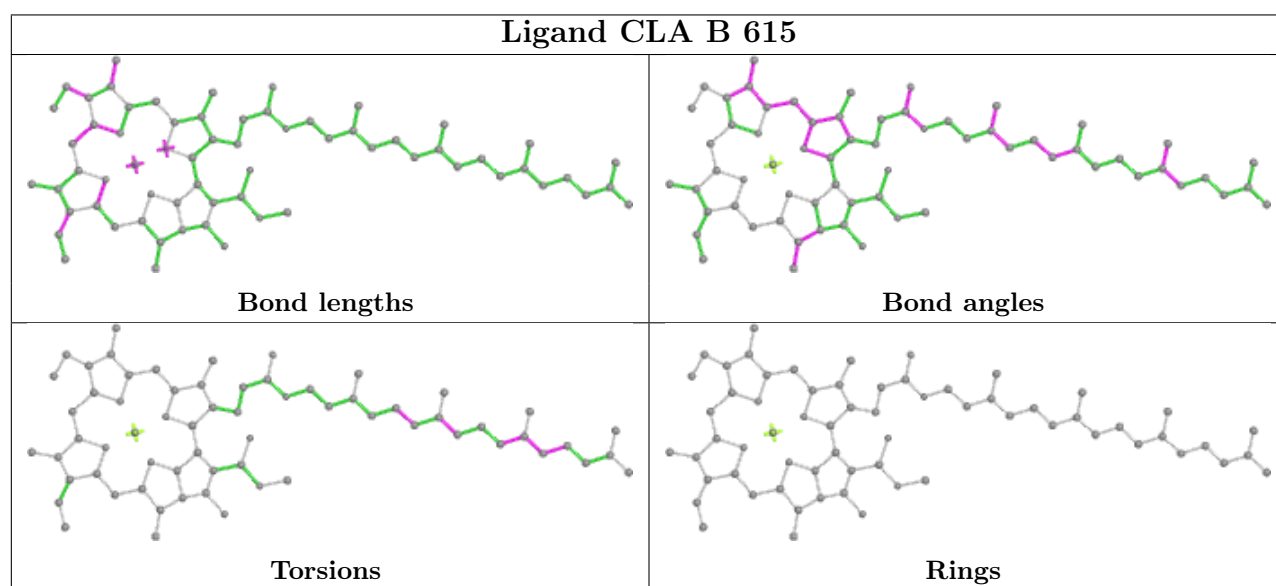
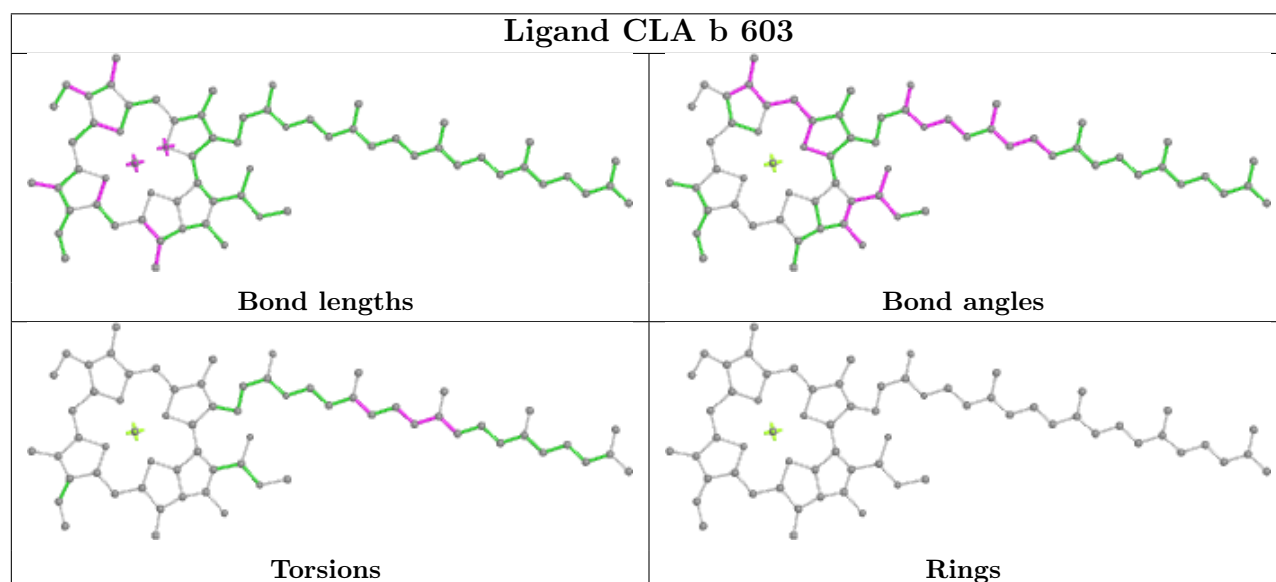
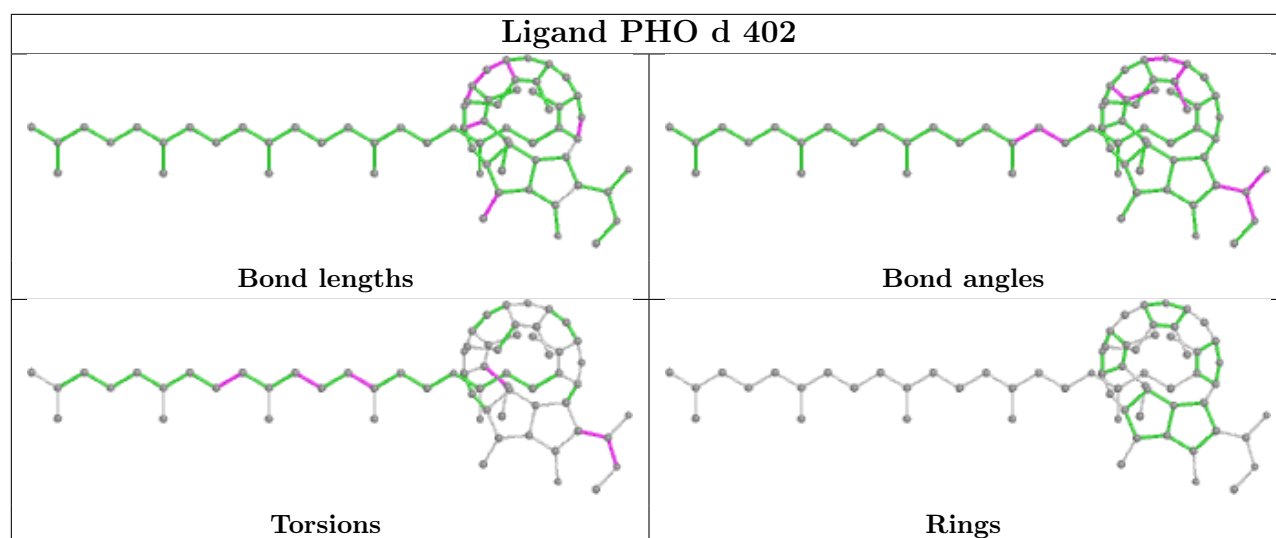


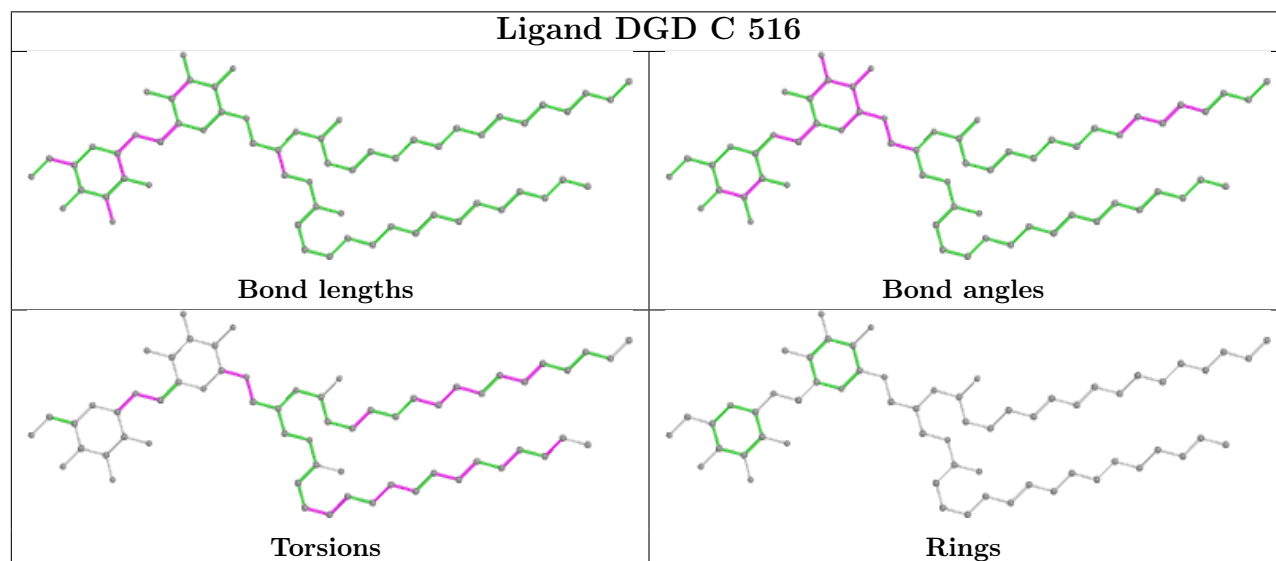
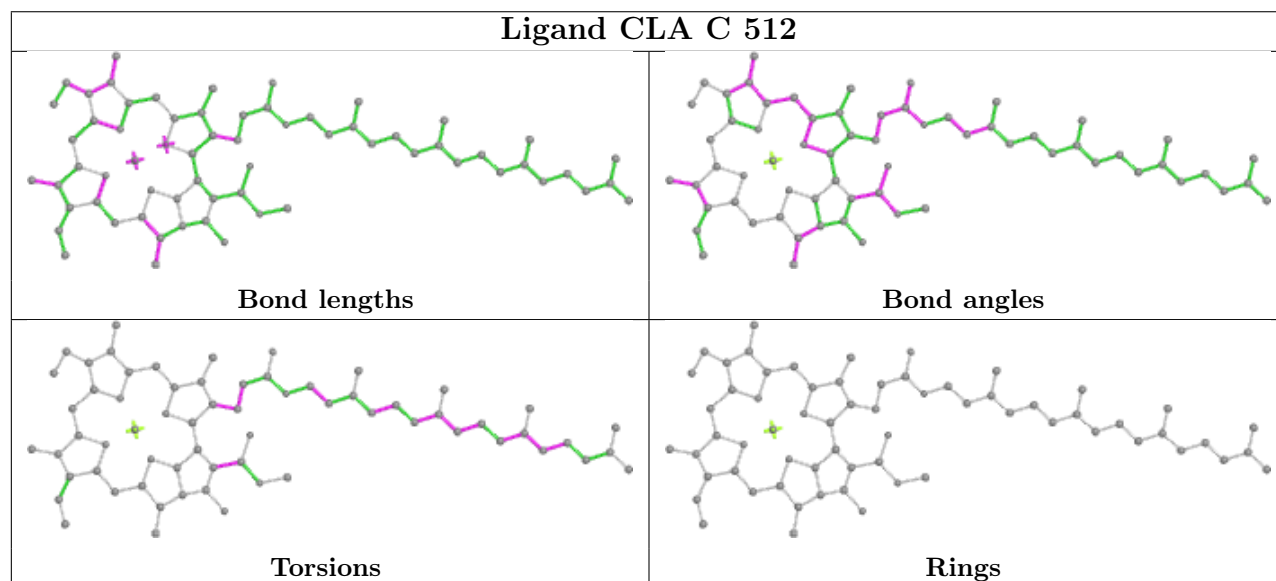
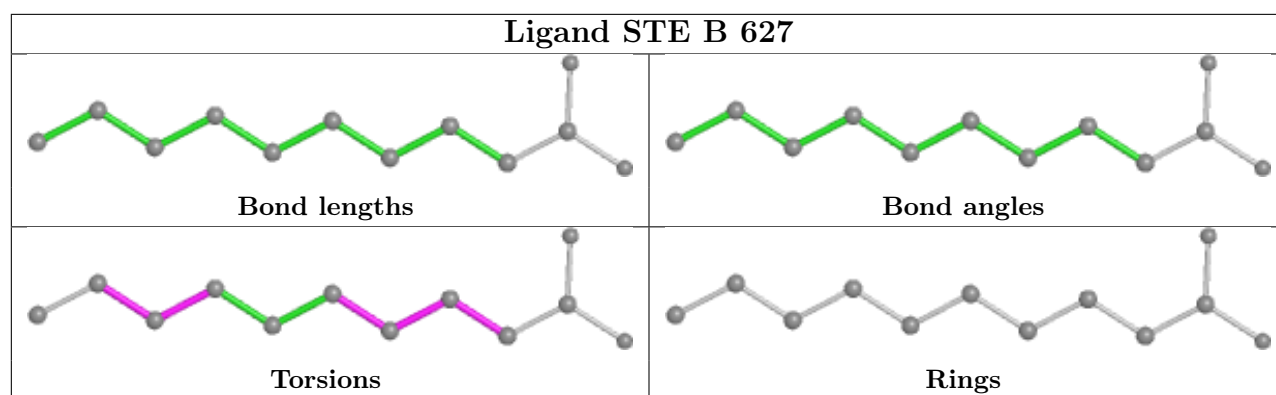
Ligand CLA c 511

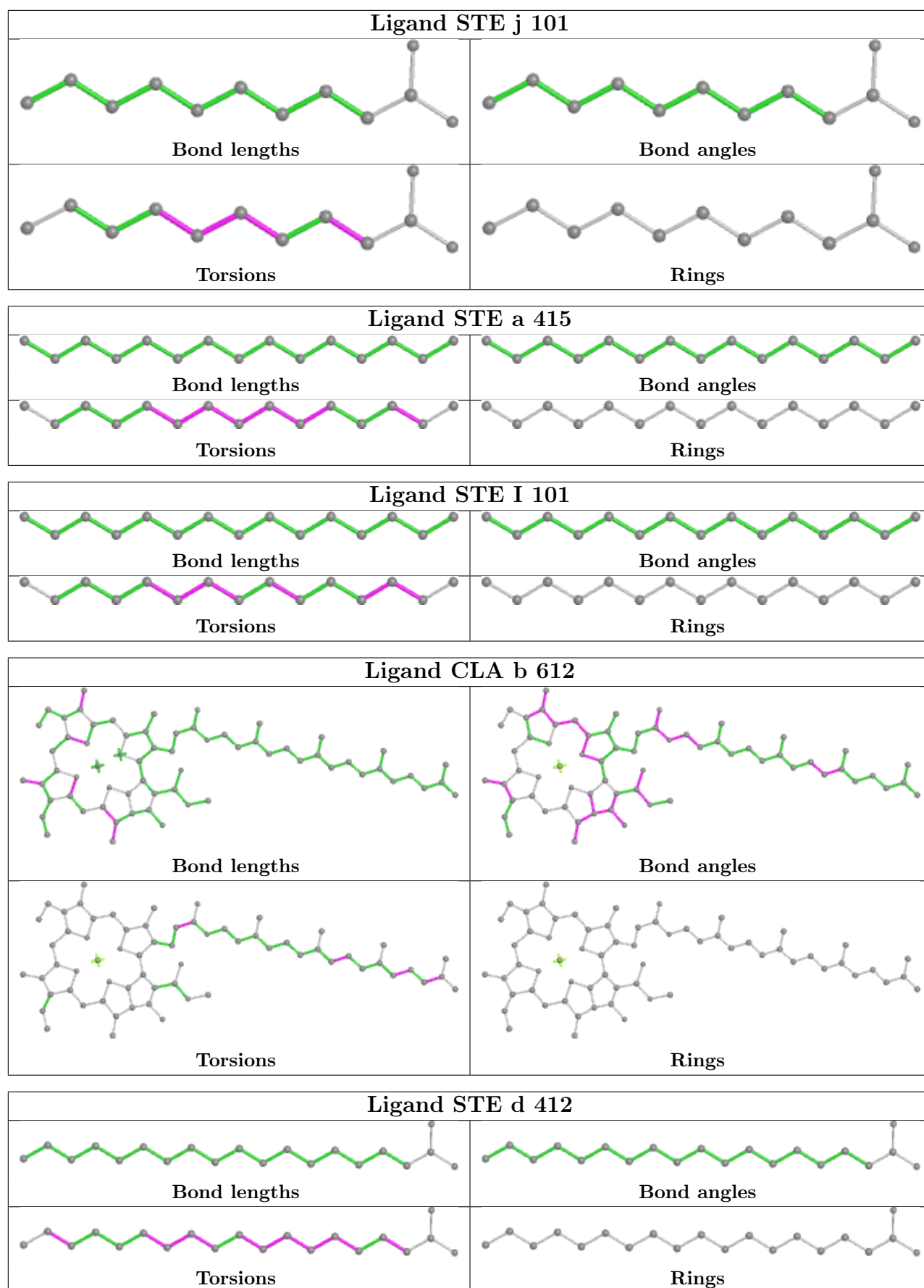


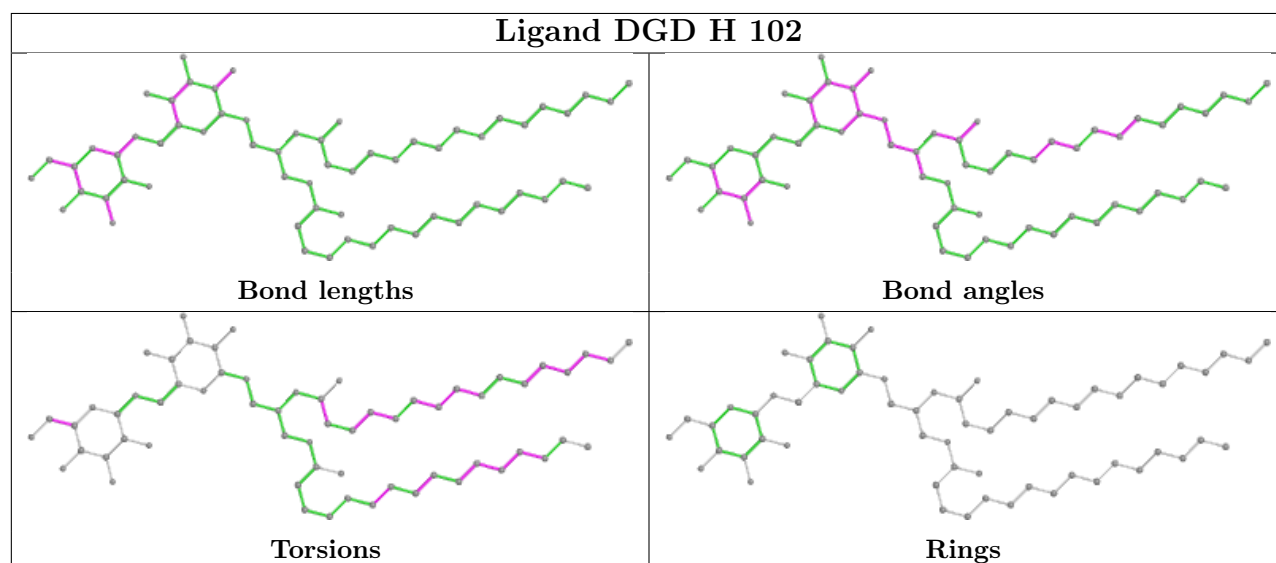
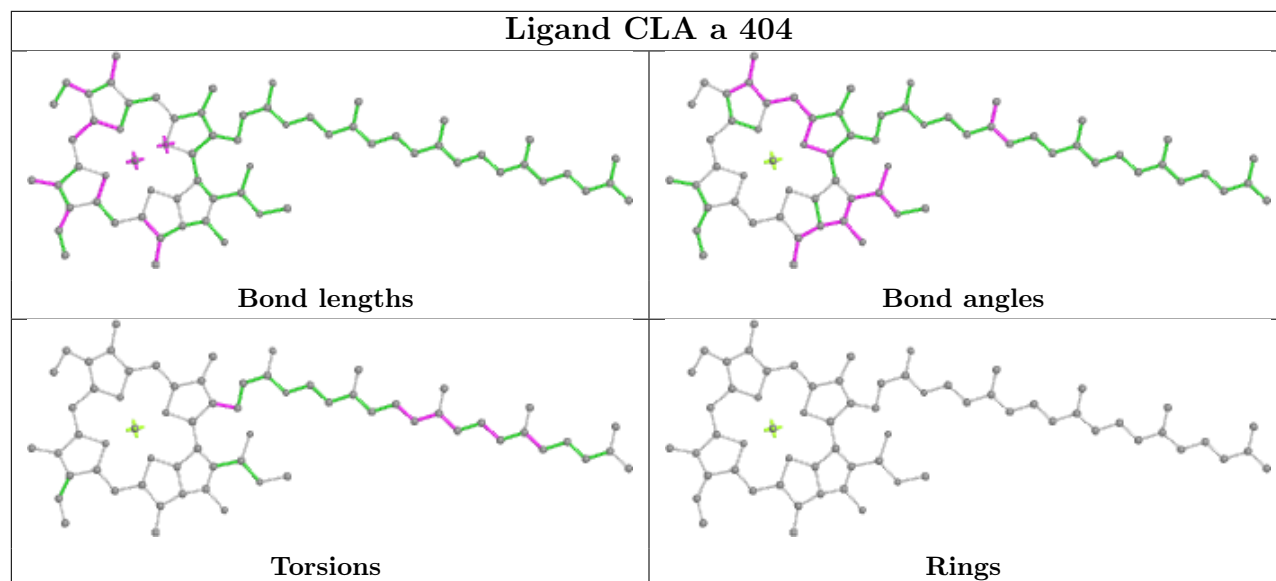
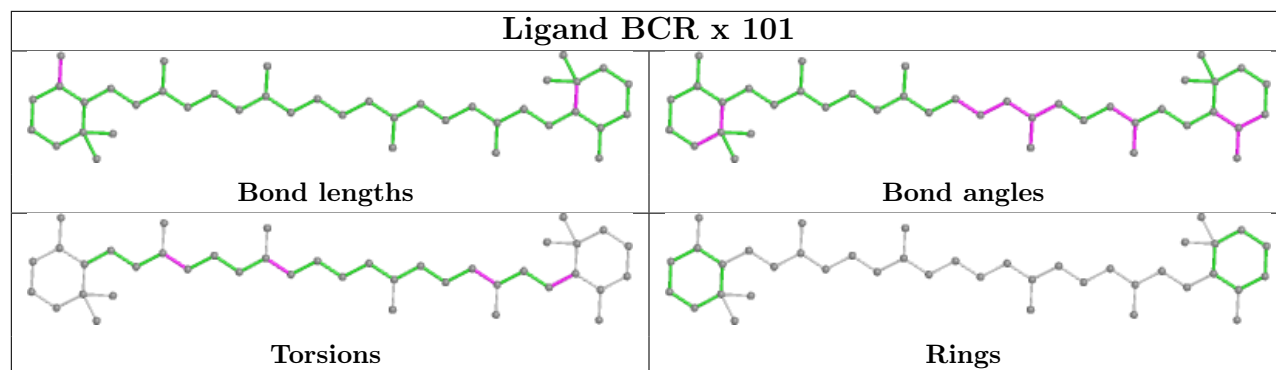
Ligand CLA b 610

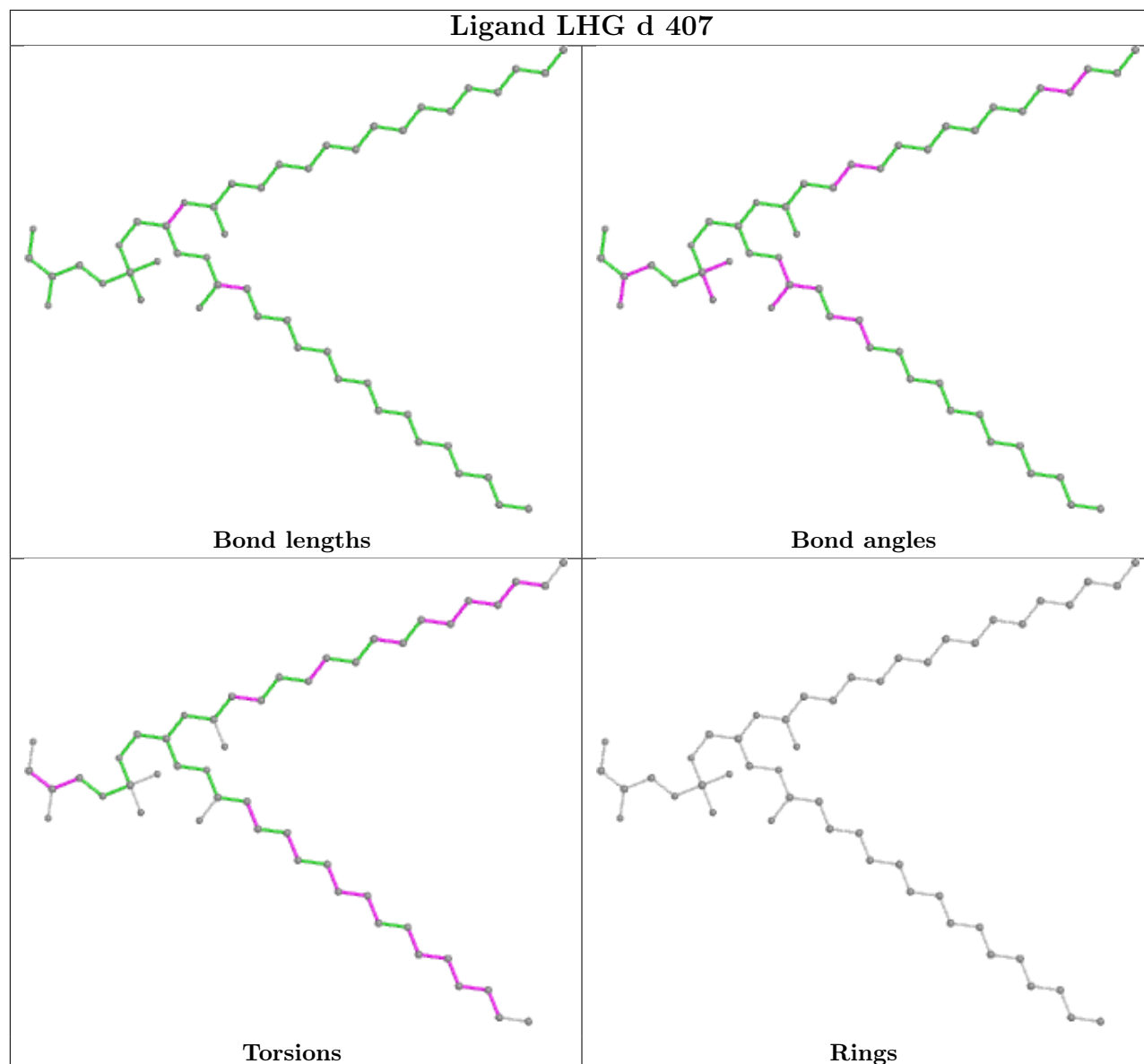
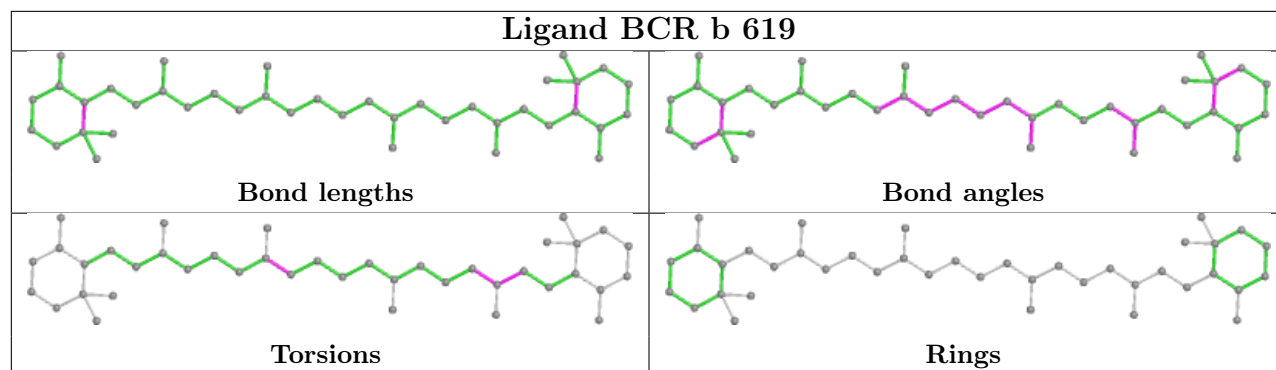


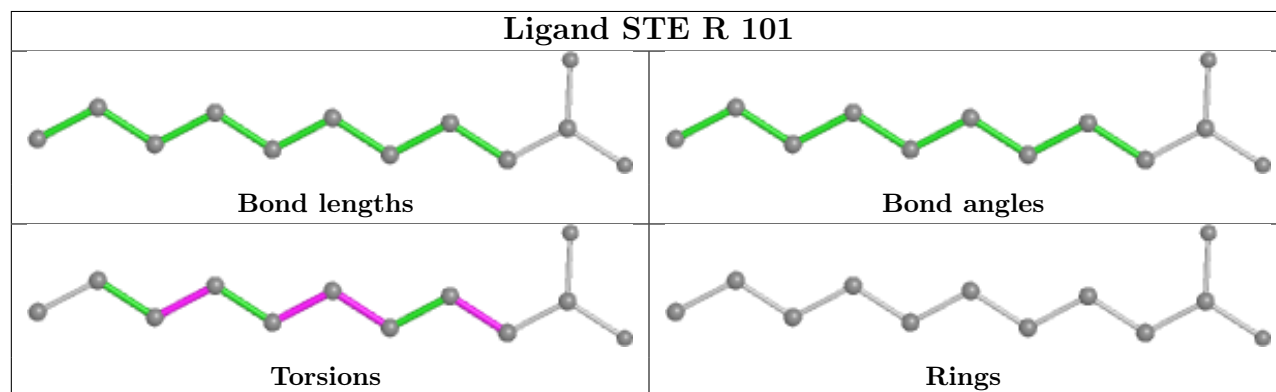
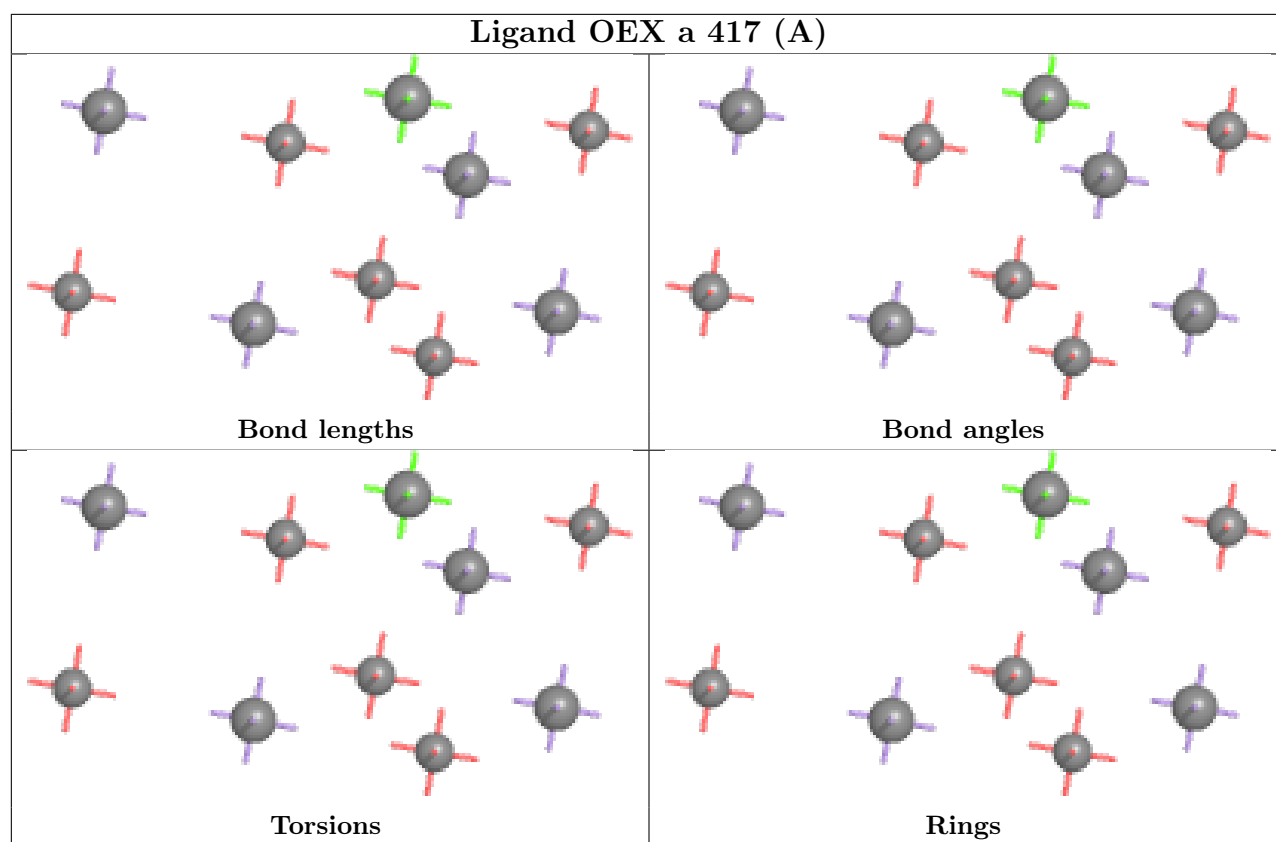


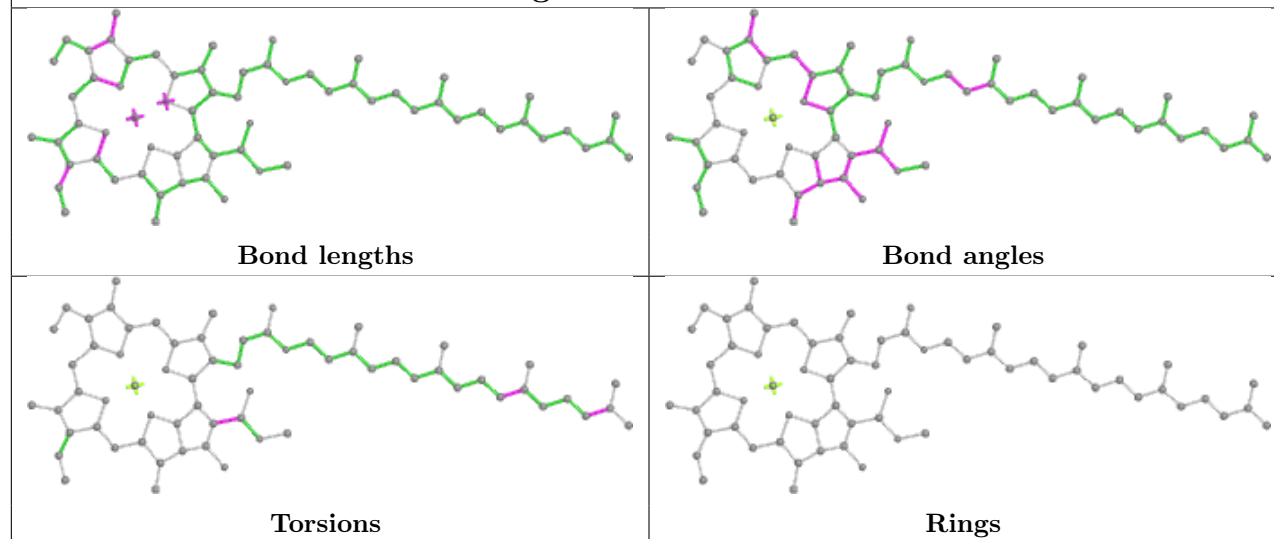
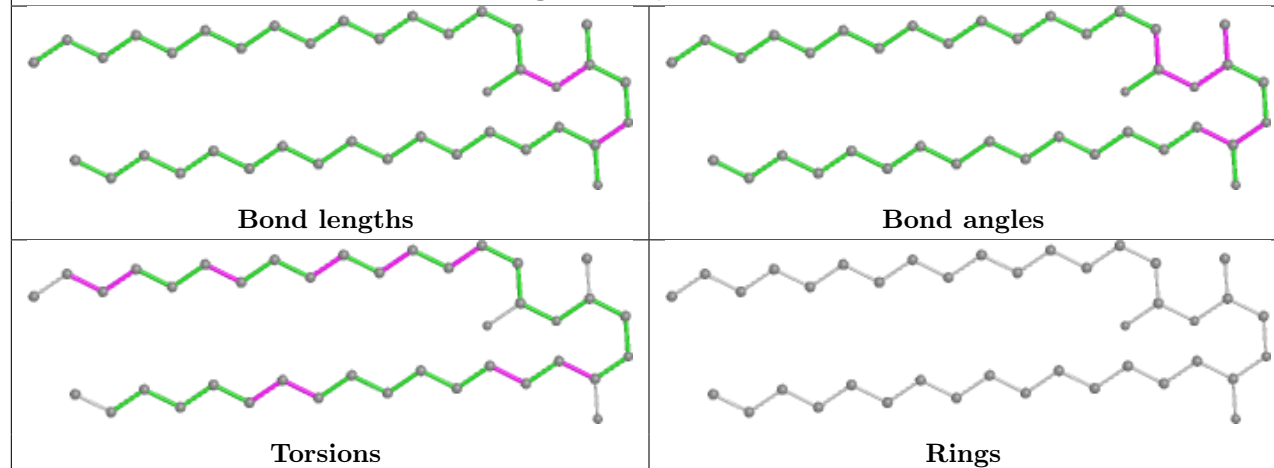
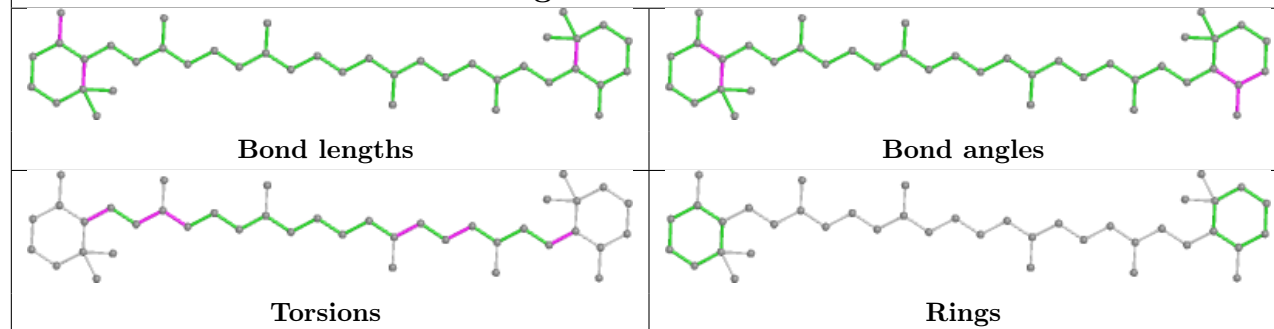


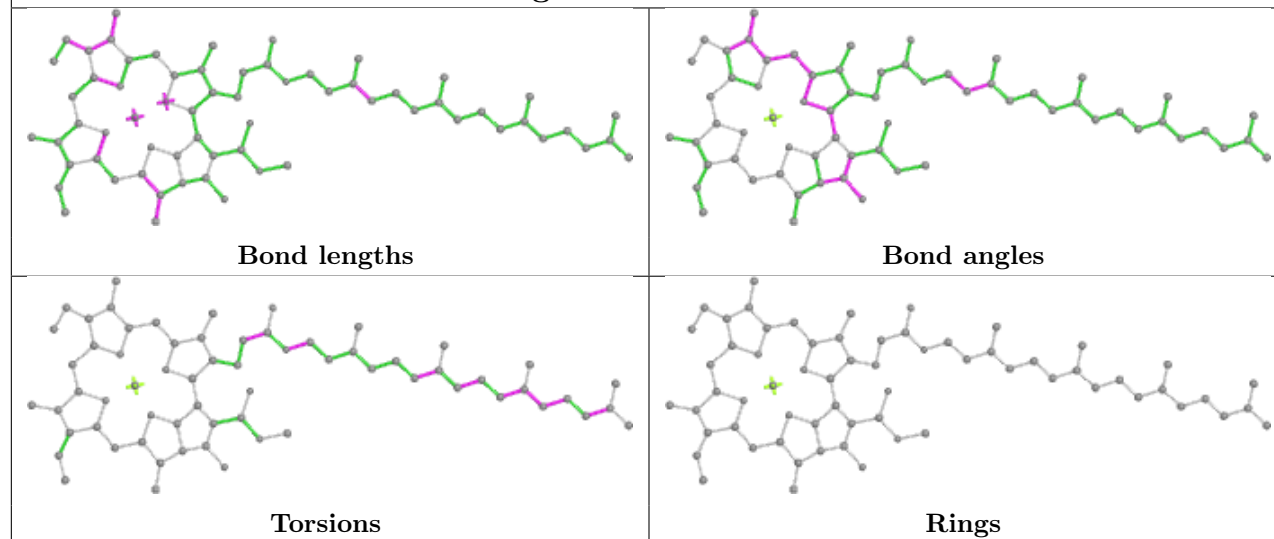
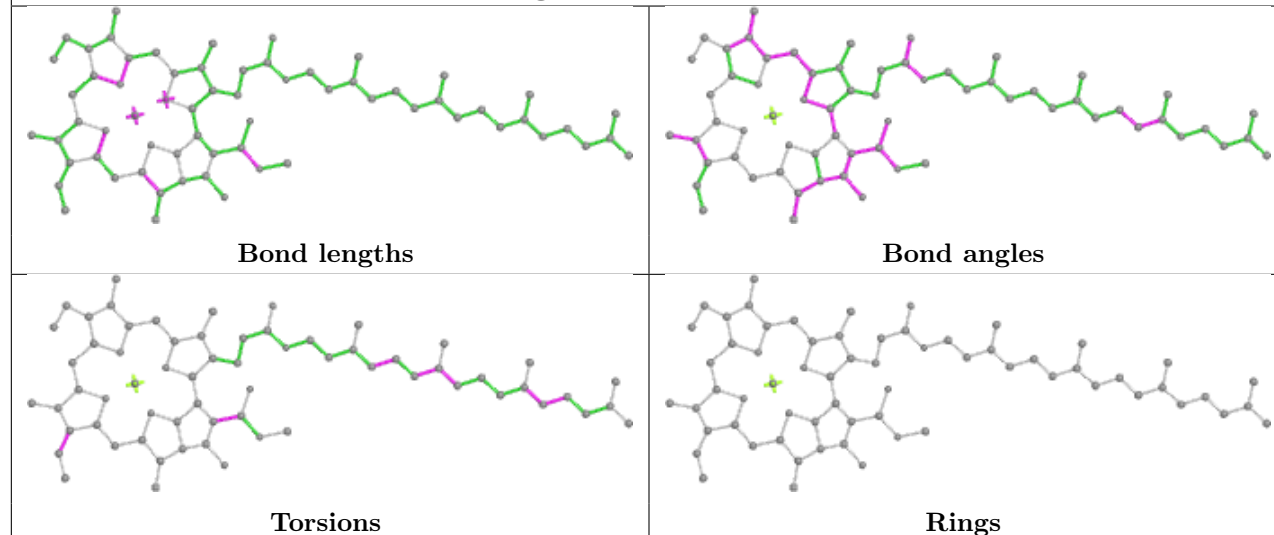
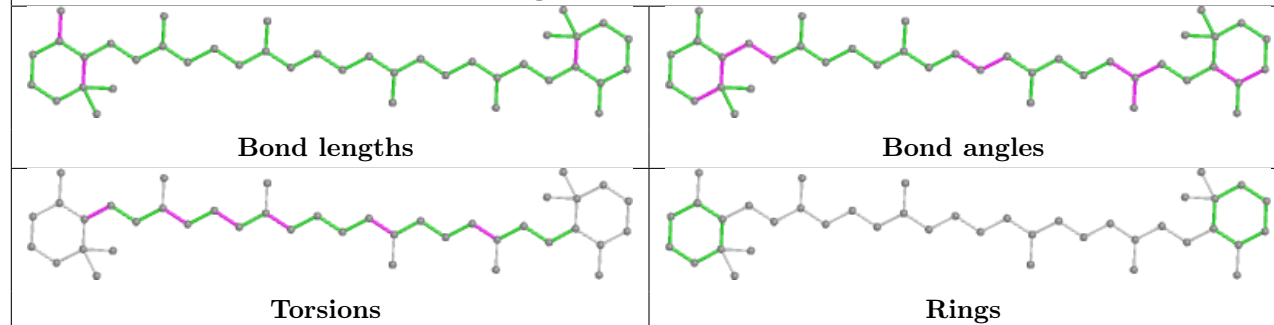


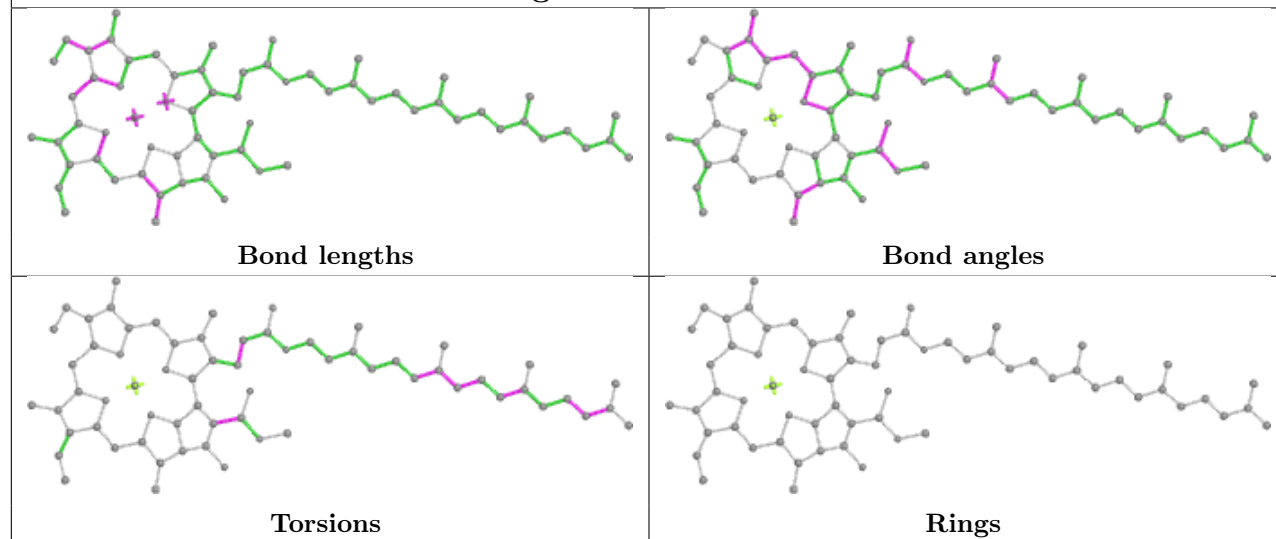
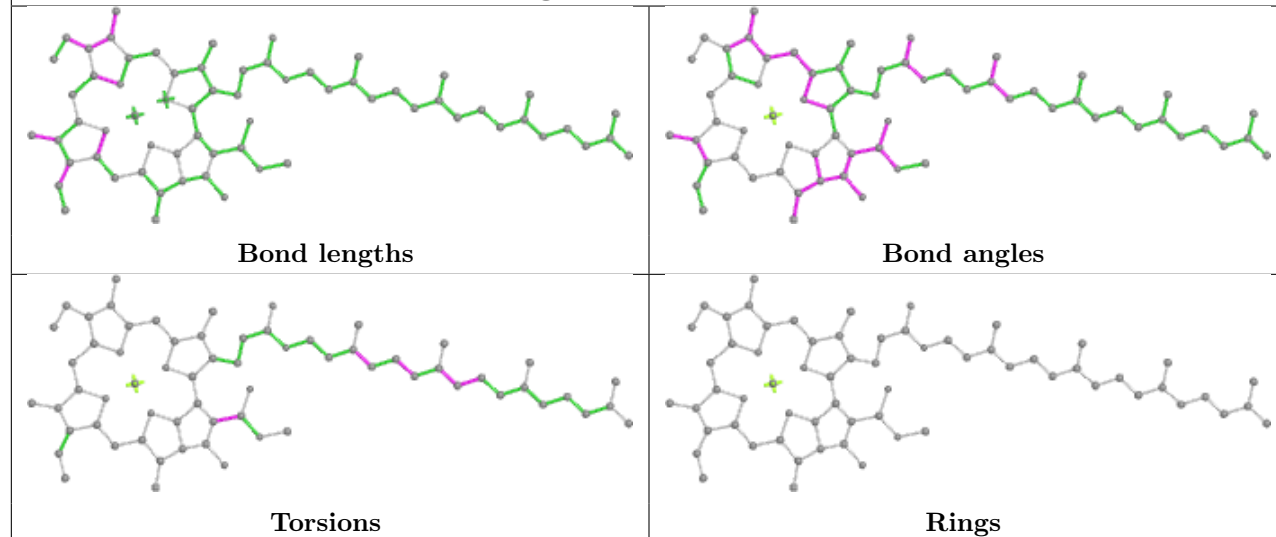


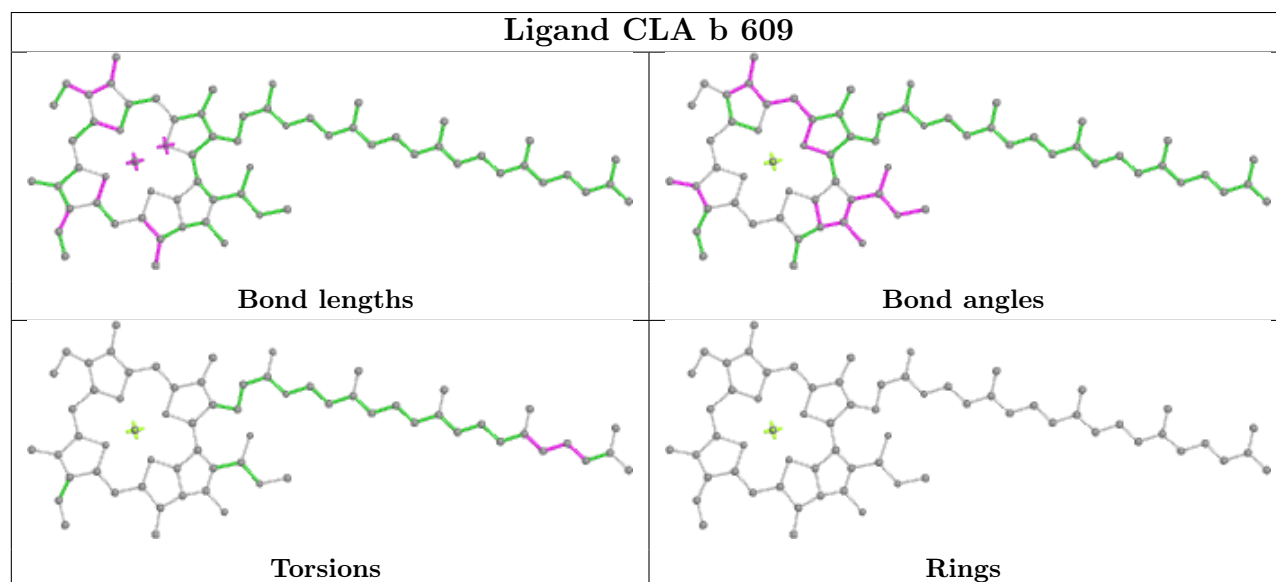
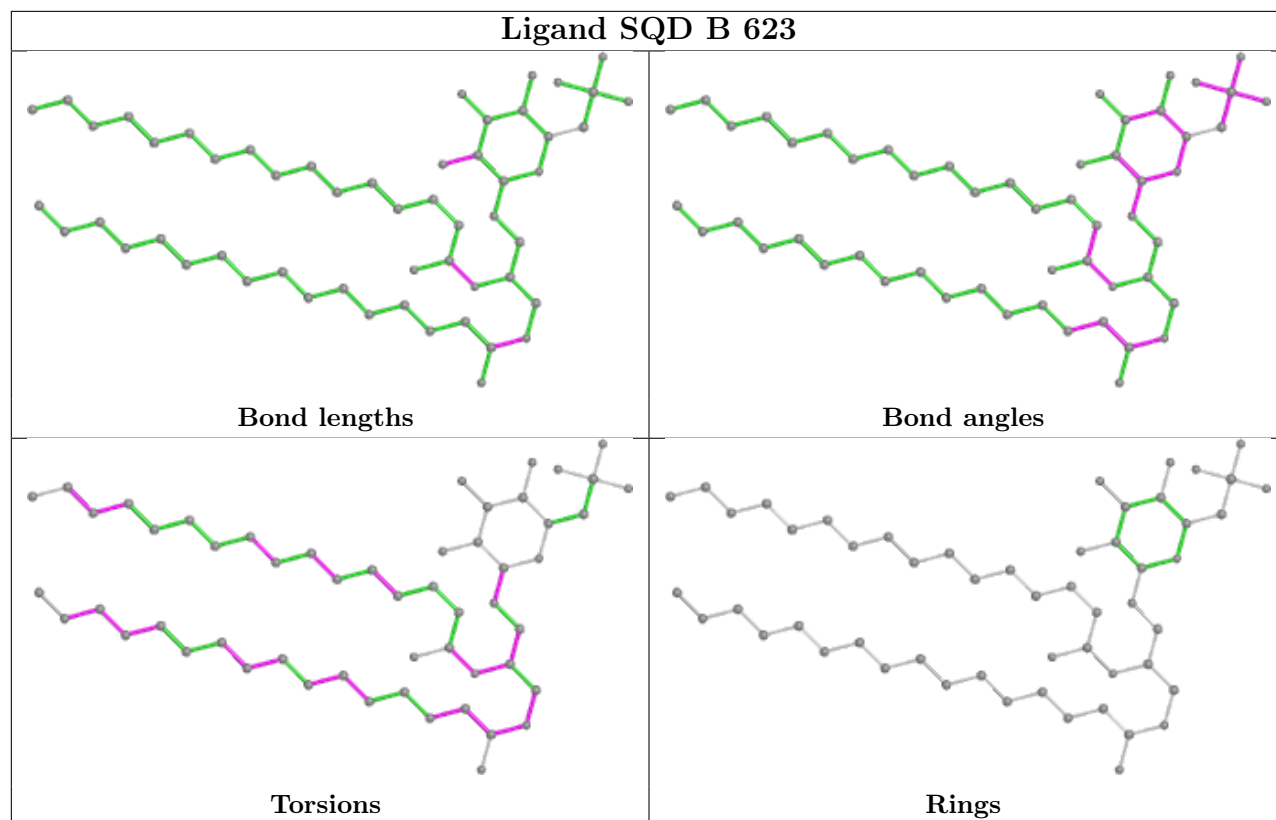


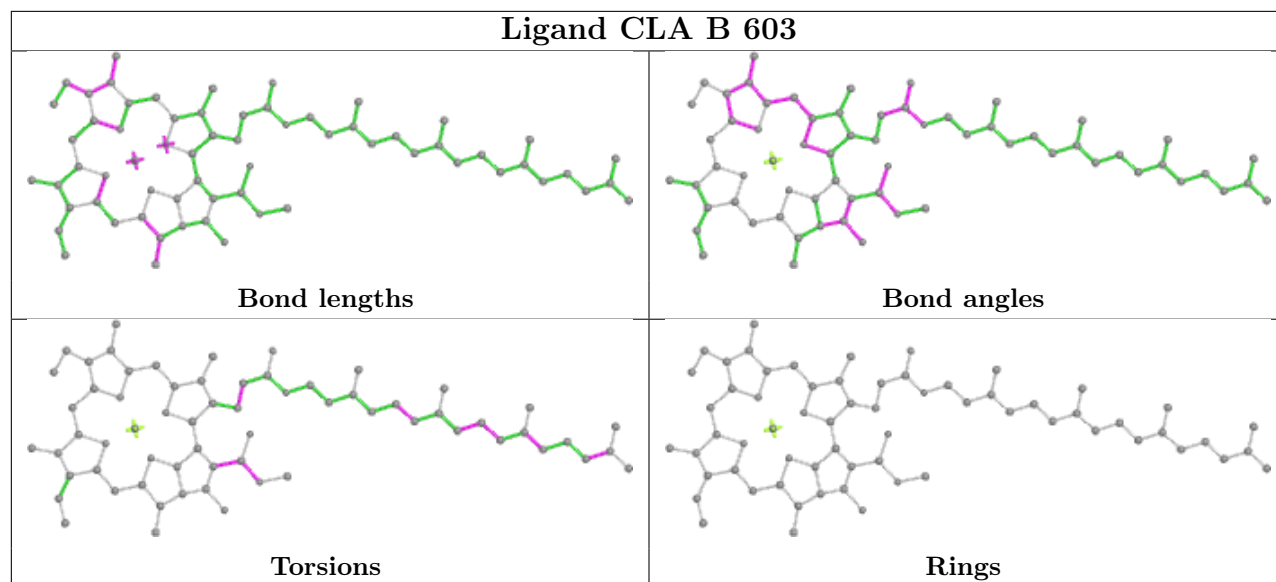


Ligand CLA C 502**Ligand SQD A 415****Ligand BCR k 101**

Ligand CLA B 613**Ligand CLA B 604****Ligand BCR B 617**

Ligand CLA B 606**Ligand CLA c 507**





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%)	-0.36	4 (1%) 79 82	21, 28, 43, 73	0
1	a	334/344 (97%)	-0.39	1 (0%) 94 94	22, 30, 52, 73	0
2	B	505/510 (99%)	-0.36	9 (1%) 68 72	24, 32, 57, 80	0
2	b	505/510 (99%)	-0.15	18 (3%) 42 49	23, 35, 65, 90	0
3	C	442/461 (95%)	-0.26	4 (0%) 84 86	25, 34, 49, 67	0
3	c	451/461 (97%)	-0.18	10 (2%) 62 66	26, 38, 57, 86	0
4	D	341/352 (96%)	-0.32	1 (0%) 94 94	23, 29, 43, 69	0
4	d	341/352 (96%)	-0.29	0 100 100	24, 33, 52, 74	0
5	E	82/84 (97%)	-0.00	4 (4%) 29 35	33, 48, 62, 78	0
5	e	82/84 (97%)	0.27	5 (6%) 21 26	37, 54, 70, 79	0
6	F	34/45 (75%)	-0.36	1 (2%) 51 57	34, 40, 54, 74	0
6	f	34/45 (75%)	-0.22	0 100 100	38, 47, 65, 82	0
7	H	65/66 (98%)	-0.05	1 (1%) 73 77	30, 38, 53, 65	0
7	h	63/66 (95%)	0.27	5 (7%) 12 16	36, 45, 57, 60	0
8	I	35/38 (92%)	-0.23	3 (8%) 10 13	33, 37, 62, 76	0
8	i	35/38 (92%)	-0.12	3 (8%) 10 13	30, 39, 70, 82	0
9	J	36/40 (90%)	-0.04	4 (11%) 5 7	33, 46, 67, 85	0
9	j	36/40 (90%)	0.00	3 (8%) 11 14	34, 48, 78, 86	0
10	K	37/46 (80%)	0.14	1 (2%) 54 60	37, 48, 62, 70	0
10	k	37/46 (80%)	0.03	2 (5%) 25 31	43, 51, 65, 73	0
11	L	37/37 (100%)	-0.44	1 (2%) 54 60	24, 29, 58, 66	0
11	l	36/37 (97%)	-0.19	3 (8%) 11 14	25, 30, 65, 81	0
12	M	32/36 (88%)	-0.04	1 (3%) 49 55	28, 33, 56, 67	0
12	m	31/36 (86%)	-0.11	0 100 100	27, 33, 51, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.03	16 (6%) 18 23	24, 41, 77, 133	0
13	o	244/272 (89%)	-0.03	14 (5%) 23 29	25, 40, 77, 114	0
14	R	28/41 (68%)	1.65	9 (32%) 0 0	54, 62, 75, 82	0
14	r	28/41 (68%)	3.12	20 (71%) 0 0	62, 76, 92, 100	0
15	T	29/32 (90%)	-0.32	2 (6%) 16 21	26, 30, 54, 74	0
15	t	29/32 (90%)	-0.20	2 (6%) 16 21	28, 32, 74, 91	0
16	U	97/134 (72%)	-0.23	1 (1%) 82 85	31, 41, 64, 79	0
16	u	97/134 (72%)	-0.39	1 (1%) 82 85	30, 38, 56, 74	0
17	V	137/163 (84%)	-0.45	0 100 100	30, 39, 52, 73	0
17	v	137/163 (84%)	-0.18	5 (3%) 42 49	31, 44, 62, 75	0
18	X	38/41 (92%)	-0.06	2 (5%) 26 32	36, 47, 64, 69	0
18	x	39/41 (95%)	0.37	4 (10%) 6 8	44, 51, 77, 88	0
19	Y	27/46 (58%)	1.15	7 (25%) 0 0	48, 66, 85, 89	0
19	y	30/46 (65%)	0.45	4 (13%) 3 4	56, 67, 78, 86	0
20	Z	62/62 (100%)	0.87	17 (27%) 0 0	49, 62, 97, 104	0
20	z	62/62 (100%)	0.76	11 (17%) 1 1	53, 66, 99, 111	0
All	All	5293/5700 (92%)	-0.15	199 (3%) 40 46	21, 36, 66, 133	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	10.5
13	O	56	PRO	6.7
2	b	495	PHE	6.5
14	r	3	TRP	6.0
1	A	13	LEU	6.0

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	0.93	0.10	29,41,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	FME	t	1	10/11	0.94	0.09	29,43,62,63	0
8	FME	i	1	10/11	0.96	0.16	35,44,57,58	0
12	FME	m	1	10/11	0.97	0.13	33,47,63,74	0
8	FME	I	1	10/11	0.97	0.17	34,41,49,59	0
12	FME	M	1	10/11	0.97	0.13	40,49,68,70	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
34	STE	a	414	12/20	0.68	0.25	50,64,74,78	0
34	STE	b	627	10/20	0.69	0.22	44,59,69,70	0
34	STE	L	101	12/20	0.75	0.16	46,59,75,80	0
34	STE	R	101	12/20	0.76	0.28	51,75,78,85	0
34	STE	H	103	18/20	0.77	0.25	48,66,76,79	0
29	SQD	a	412	36/54	0.79	0.18	33,59,78,86	0
29	SQD	A	415	39/54	0.79	0.18	37,59,88,94	0
30	LHG	A	414	49/49	0.80	0.20	47,70,98,111	0
34	STE	b	625	16/20	0.80	0.17	45,62,72,74	0
28	LMG	c	521	48/55	0.80	0.22	47,69,94,103	0
34	STE	d	412	20/20	0.80	0.23	36,55,71,73	0
34	STE	c	523	12/20	0.81	0.26	49,64,81,82	0
34	STE	b	626	20/20	0.81	0.18	44,62,74,79	0
34	STE	h	102	14/20	0.81	0.26	47,62,75,78	0
34	STE	j	101	12/20	0.81	0.13	42,56,70,73	0
31	DGD	A	416	66/66	0.82	0.17	41,61,75,79	0
22	CLA	C	512	65/65	0.82	0.17	33,53,82,92	0
34	STE	B	626	16/20	0.83	0.24	45,63,72,75	0
28	LMG	D	410	33/55	0.83	0.17	36,55,74,80	0
34	STE	d	413	20/20	0.83	0.16	42,62,76,76	0
30	LHG	e	102	42/49	0.83	0.24	57,79,100,109	0
24	BCR	H	101	40/40	0.83	0.15	26,44,57,61	0
22	CLA	b	601	65/65	0.84	0.17	42,65,85,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	STE	B	625	18/20	0.84	0.13	38,57,69,74	0
24	BCR	x	101	40/40	0.84	0.14	31,51,66,74	0
22	CLA	c	512	65/65	0.85	0.16	39,57,86,92	0
28	LMG	a	416	55/55	0.85	0.15	38,56,75,80	0
28	LMG	b	624	55/55	0.85	0.28	50,72,91,96	0
34	STE	c	520	20/20	0.85	0.20	43,57,79,88	0
28	LMG	A	412	48/55	0.85	0.16	36,55,74,89	0
28	LMG	c	522	49/55	0.85	0.15	37,55,79,96	0
34	STE	a	413	10/20	0.85	0.17	37,60,68,72	0
34	STE	B	624	12/20	0.85	0.11	44,55,64,66	0
34	STE	a	415	15/20	0.85	0.13	42,58,69,74	0
34	STE	b	621	16/20	0.86	0.18	35,49,65,75	0
24	BCR	Y	101	40/40	0.86	0.13	35,50,68,71	0
34	STE	I	101	15/20	0.86	0.15	39,56,70,70	0
34	STE	B	627	12/20	0.86	0.38	44,59,76,79	0
34	STE	M	102	15/20	0.86	0.14	34,48,63,63	0
34	STE	b	623	20/20	0.87	0.21	39,55,69,79	0
22	CLA	B	601	65/65	0.87	0.16	30,59,82,94	0
22	CLA	C	513	65/65	0.87	0.17	40,60,87,89	0
34	STE	C	520	16/20	0.87	0.12	36,52,62,69	0
29	SQD	B	623	54/54	0.87	0.15	40,57,86,96	0
34	STE	B	620	17/20	0.88	0.18	36,50,62,62	0
29	SQD	b	620	49/54	0.88	0.14	38,57,85,89	0
22	CLA	c	513	65/65	0.88	0.19	39,68,104,108	0
27	PL9	A	410	55/55	0.88	0.23	34,63,84,90	0
27	PL9	a	409	55/55	0.88	0.19	37,66,80,89	0
34	STE	C	519	12/20	0.88	0.11	46,56,66,67	0
34	STE	X	101	20/20	0.88	0.15	31,48,62,64	0
34	STE	C	521	12/20	0.89	0.09	34,47,54,58	0
24	BCR	k	101	40/40	0.89	0.11	42,61,73,75	0
22	CLA	a	404	65/65	0.89	0.13	20,37,74,79	0
24	BCR	K	101	40/40	0.89	0.15	41,55,70,71	0
22	CLA	d	404	65/65	0.89	0.16	27,46,81,87	0
24	BCR	c	514	40/40	0.89	0.15	43,59,70,72	0
24	BCR	d	405	40/40	0.89	0.13	32,51,85,98	0
34	STE	l	102	18/20	0.89	0.14	34,47,72,80	0
22	CLA	C	502	65/65	0.90	0.14	28,39,61,73	0
28	LMG	c	519	37/55	0.90	0.17	39,61,75,81	0
28	LMG	C	518	48/55	0.90	0.14	36,65,86,89	0
22	CLA	c	502	65/65	0.90	0.15	29,41,61,65	0
22	CLA	c	508	64/65	0.90	0.15	30,45,85,96	0
22	CLA	b	615	65/65	0.91	0.14	26,40,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	616	60/65	0.91	0.13	26,42,85,88	0
34	STE	J	101	12/20	0.91	0.10	45,59,70,72	0
22	CLA	D	403	65/65	0.91	0.13	24,43,100,108	0
24	BCR	B	619	40/40	0.91	0.10	29,41,54,60	0
24	BCR	D	404	40/40	0.91	0.13	25,43,76,85	0
34	STE	T	102	15/20	0.91	0.17	41,56,70,76	0
28	LMG	M	101	51/55	0.91	0.11	29,47,70,84	0
34	STE	Z	101	8/20	0.91	0.15	46,57,66,66	0
24	BCR	k	102	40/40	0.91	0.16	39,54,66,67	0
28	LMG	b	622	51/55	0.91	0.11	29,50,68,80	0
22	CLA	b	602	65/65	0.91	0.15	28,42,60,61	0
34	STE	t	102	14/20	0.91	0.10	33,52,62,65	0
28	LMG	D	411	28/55	0.92	0.13	28,48,59,61	0
29	SQD	f	101	41/54	0.92	0.17	49,76,94,100	0
22	CLA	B	606	65/65	0.92	0.11	24,36,74,79	0
22	CLA	c	503	65/65	0.92	0.16	30,43,53,62	0
24	BCR	C	514	40/40	0.92	0.11	25,41,53,63	0
31	DGD	C	516	62/66	0.92	0.12	30,48,91,108	0
22	CLA	c	506	65/65	0.92	0.12	30,48,87,97	0
34	STE	d	411	17/20	0.92	0.10	40,54,61,61	0
22	CLA	C	505	65/65	0.92	0.17	24,39,69,74	0
22	CLA	c	511	65/65	0.92	0.13	39,52,71,74	0
22	CLA	C	506	65/65	0.92	0.12	23,42,82,89	0
24	BCR	b	619	40/40	0.92	0.11	28,45,65,68	0
28	LMG	D	406	51/55	0.92	0.16	28,50,76,88	0
22	CLA	C	507	65/65	0.92	0.14	22,40,52,57	0
22	CLA	B	615	65/65	0.93	0.13	23,36,61,64	0
22	CLA	c	510	65/65	0.93	0.15	32,47,64,67	0
22	CLA	B	616	60/65	0.93	0.14	22,38,79,86	0
22	CLA	B	614	65/65	0.93	0.17	21,37,73,79	0
22	CLA	b	606	65/65	0.93	0.11	27,39,69,74	0
31	DGD	H	102	62/66	0.93	0.10	26,41,58,63	0
31	DGD	c	517	62/66	0.93	0.12	33,51,82,89	0
31	DGD	c	518	62/66	0.93	0.14	30,49,77,88	0
34	STE	M	103	10/20	0.93	0.12	35,48,55,58	0
31	DGD	h	101	62/66	0.93	0.12	24,47,62,66	0
22	CLA	c	504	60/65	0.93	0.12	29,42,80,83	0
22	CLA	c	505	65/65	0.93	0.16	26,39,64,73	0
29	SQD	a	411	54/54	0.93	0.15	41,61,84,85	0
22	CLA	b	609	65/65	0.93	0.14	29,45,60,68	0
22	CLA	c	507	65/65	0.93	0.14	27,44,59,61	0
27	PL9	D	405	55/55	0.94	0.10	21,33,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	B	618	40/40	0.94	0.09	24,37,49,55	0
30	LHG	d	407	49/49	0.94	0.14	32,50,70,76	0
22	CLA	C	508	65/65	0.94	0.12	27,43,95,106	0
22	CLA	C	509	65/65	0.94	0.17	26,43,64,72	0
22	CLA	C	510	65/65	0.94	0.13	25,42,58,62	0
31	DGD	C	517	62/66	0.94	0.12	25,45,68,74	0
22	CLA	b	604	65/65	0.94	0.14	18,35,71,83	0
22	CLA	C	511	65/65	0.94	0.12	28,49,64,66	0
24	BCR	K	102	40/40	0.94	0.14	32,48,61,64	0
22	CLA	B	604	65/65	0.94	0.12	20,34,66,70	0
24	BCR	b	618	40/40	0.94	0.11	25,39,57,61	0
22	CLA	c	509	65/65	0.94	0.17	32,46,62,68	0
22	CLA	b	611	65/65	0.94	0.14	22,34,54,60	0
24	BCR	c	515	40/40	0.94	0.12	27,43,56,61	0
22	CLA	b	614	65/65	0.94	0.13	24,41,73,77	0
28	LMG	d	410	44/55	0.94	0.12	31,50,73,88	0
22	CLA	C	503	65/65	0.94	0.14	26,41,51,57	0
22	CLA	C	504	59/65	0.94	0.13	28,40,76,84	0
29	SQD	D	407	36/54	0.94	0.14	44,68,83,94	0
24	BCR	t	101	40/40	0.94	0.10	24,39,52,55	0
22	CLA	a	403	65/65	0.94	0.14	23,41,91,95	0
24	BCR	B	617	40/40	0.94	0.11	28,39,55,60	0
22	CLA	b	607	65/65	0.95	0.13	20,36,67,71	0
29	SQD	A	413	52/54	0.95	0.14	29,55,82,90	0
22	CLA	b	608	65/65	0.95	0.14	25,41,58,61	0
22	CLA	C	501	65/65	0.95	0.13	22,36,50,53	0
22	CLA	b	610	65/65	0.95	0.17	24,39,48,56	0
22	CLA	B	603	65/65	0.95	0.14	16,34,59,61	0
22	CLA	b	612	65/65	0.95	0.16	20,34,51,54	0
22	CLA	d	403	65/65	0.95	0.11	20,35,57,67	0
22	CLA	b	613	65/65	0.95	0.14	18,34,72,79	0
23	PHO	A	404	64/64	0.95	0.10	18,28,36,40	0
30	LHG	B	622	49/49	0.95	0.12	27,45,65,70	0
30	LHG	D	409	47/49	0.95	0.12	27,48,73,88	0
23	PHO	d	402	64/64	0.95	0.10	27,38,48,50	0
30	LHG	d	409	39/49	0.95	0.10	28,46,69,71	0
22	CLA	A	403	65/65	0.95	0.13	21,35,85,91	0
30	LHG	l	101	49/49	0.95	0.11	31,43,57,64	0
22	CLA	A	405	54/65	0.95	0.10	18,33,58,67	0
31	DGD	C	515	62/66	0.95	0.12	22,40,74,80	0
22	CLA	B	609	65/65	0.95	0.12	23,37,61,73	0
22	CLA	c	501	65/65	0.95	0.12	23,41,52,56	0

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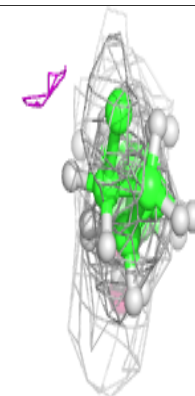
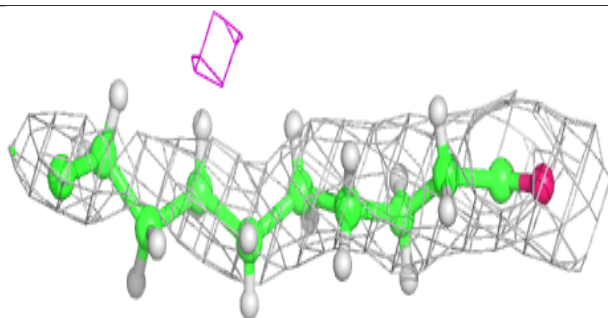
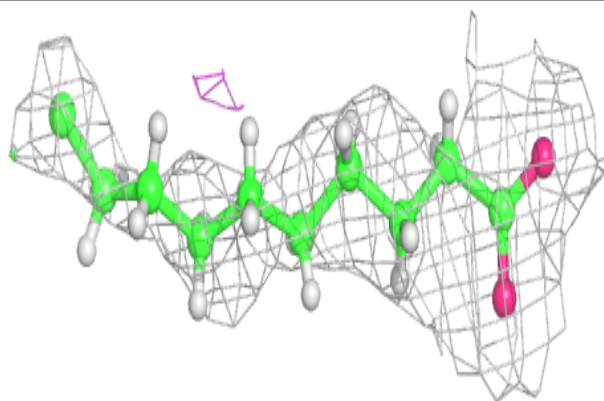
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	610	65/65	0.95	0.14	20,34,46,47	0
31	DGD	c	516	62/66	0.95	0.10	22,41,70,78	0
22	CLA	a	410	65/65	0.95	0.11	20,29,47,54	0
22	CLA	B	613	65/65	0.95	0.14	19,32,63,67	0
22	CLA	A	411	65/65	0.95	0.10	18,27,56,59	0
24	BCR	T	101	40/40	0.95	0.09	22,39,54,62	0
22	CLA	A	402	65/65	0.95	0.10	16,27,41,55	0
24	BCR	a	405	40/40	0.95	0.09	22,33,46,49	0
24	BCR	b	617	40/40	0.95	0.10	23,41,53,57	0
22	CLA	B	602	65/65	0.95	0.14	23,36,55,60	0
35	HEM	F	101	43/43	0.95	0.11	32,45,60,66	0
22	CLA	a	402	65/65	0.96	0.09	18,30,47,60	0
24	BCR	A	406	40/40	0.96	0.08	23,35,45,47	0
27	PL9	d	406	55/55	0.96	0.10	22,34,42,44	0
22	CLA	B	611	65/65	0.96	0.15	22,32,51,54	0
22	CLA	B	612	65/65	0.96	0.15	19,34,46,50	0
22	CLA	B	608	65/65	0.96	0.12	22,35,54,62	0
22	CLA	B	605	65/65	0.96	0.13	21,32,46,53	0
22	CLA	D	402	65/65	0.96	0.10	13,30,54,60	0
22	CLA	b	603	65/65	0.96	0.13	23,36,68,70	0
22	CLA	B	607	65/65	0.96	0.10	18,34,60,69	0
22	CLA	b	605	65/65	0.96	0.12	21,35,49,52	0
30	LHG	B	621	49/49	0.96	0.11	27,42,59,64	0
23	PHO	D	401	64/64	0.96	0.13	22,34,43,48	0
26	BCT	a	408	4/4	0.96	0.18	26,32,39,46	0
23	PHO	d	401	64/64	0.96	0.12	18,32,39,48	0
30	LHG	d	408	49/49	0.96	0.10	26,42,52,57	0
35	HEM	e	101	43/43	0.96	0.12	40,51,71,74	0
36	HEC	v	201	43/43	0.96	0.14	25,37,47,49	0
30	LHG	D	408	49/49	0.97	0.10	21,40,51,57	0
36	HEC	V	201	43/43	0.98	0.11	23,33,44,47	0
33	OEX	a	417[A]	10/10	0.99	0.11	26,32,35,35	10
25	CL	a	406	1/1	0.99	0.07	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.02	28,28,28,28	0
26	BCT	A	409	4/4	0.99	0.16	31,32,33,40	0
21	FE2	a	401	1/1	0.99	0.06	32,32,32,32	0
25	CL	A	407	1/1	0.99	0.06	28,28,28,28	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
32	OEY	A	417[B]	11/11	0.99	0.13	20,26,30,32	11
32	OEY	a	418[B]	11/11	0.99	0.11	22,25,29,31	11
33	OEX	A	418[A]	10/10	0.99	0.13	29,31,35,35	10
21	FE2	A	401	1/1	1.00	0.08	27,27,27,27	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.

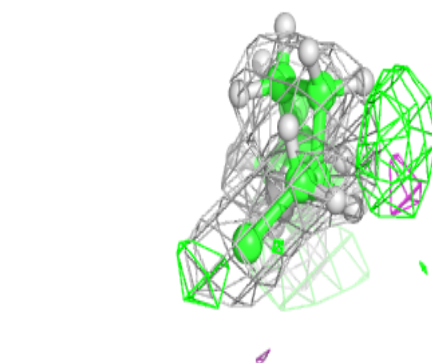
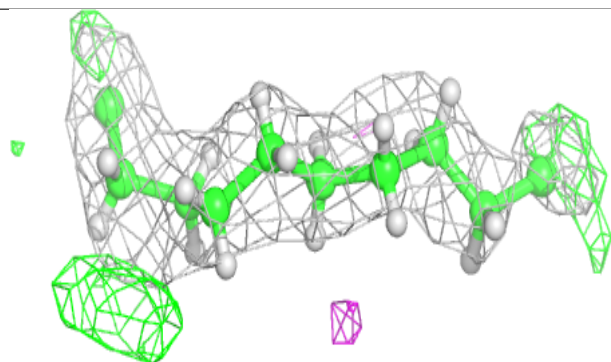
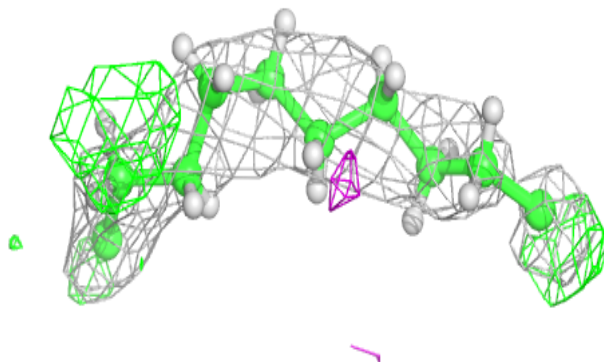
Electron density around STE a 414:

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

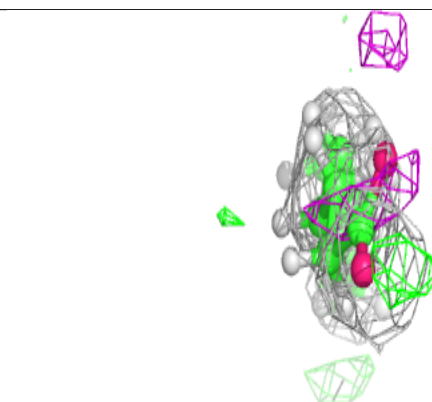
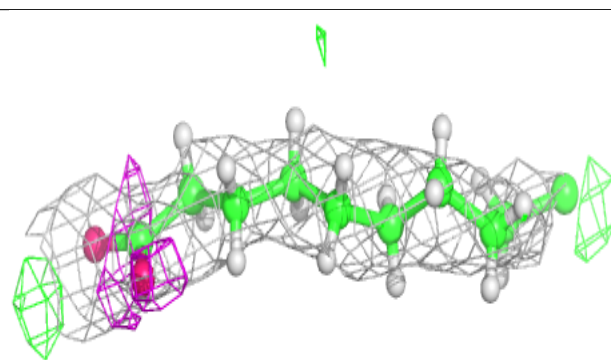
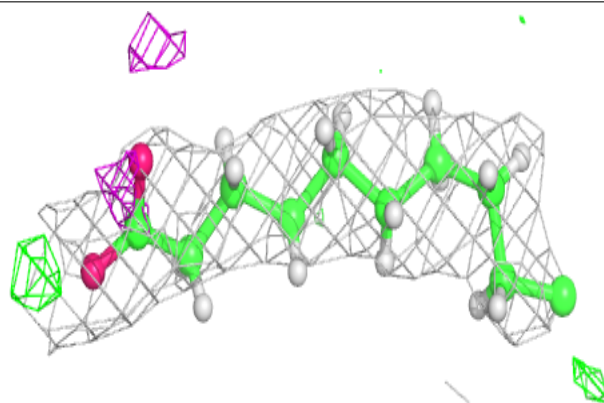


Electron density around STE b 627:

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

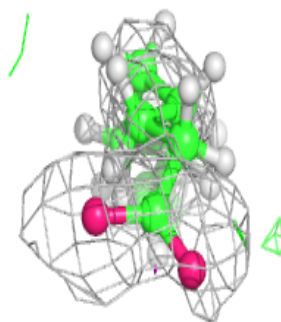
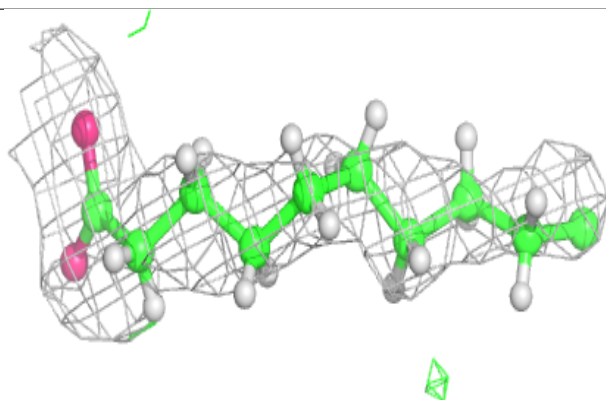
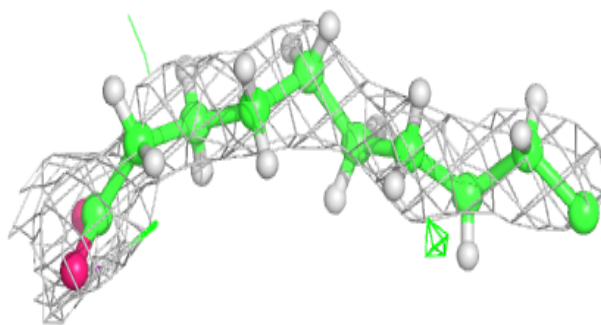
**Electron density around STE L 101:**

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

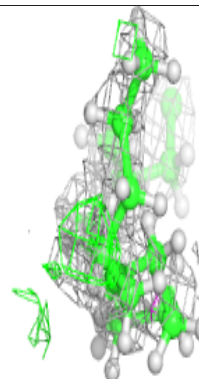
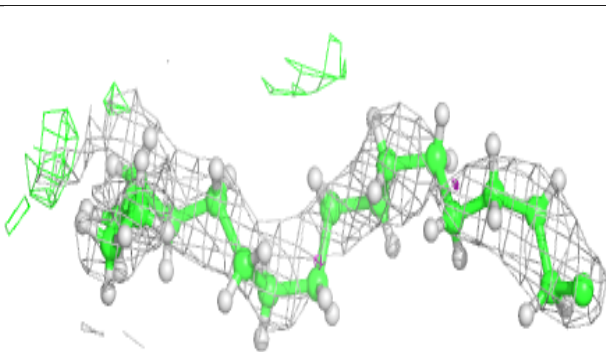
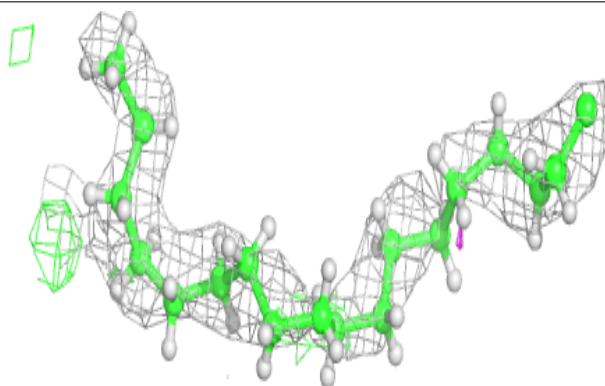


Electron density around STE R 101:

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

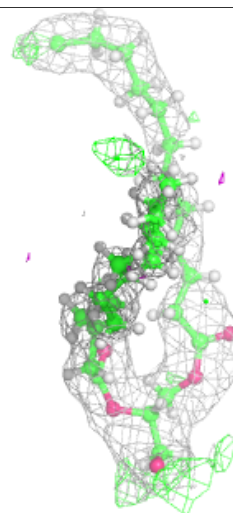
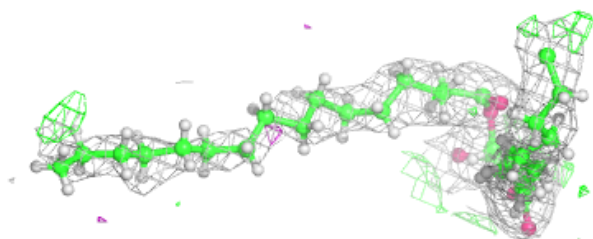
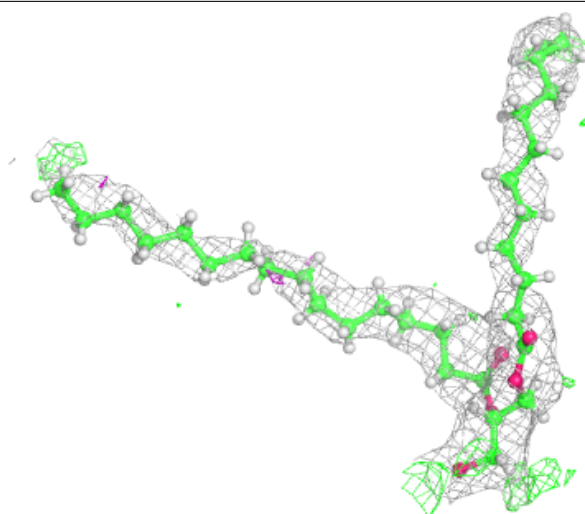
**Electron density around STE H 103:**

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



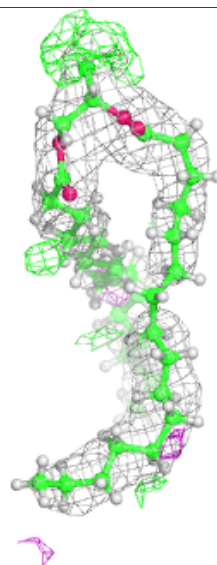
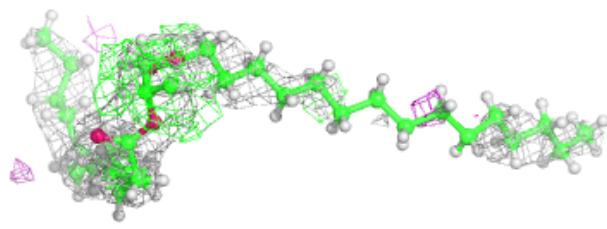
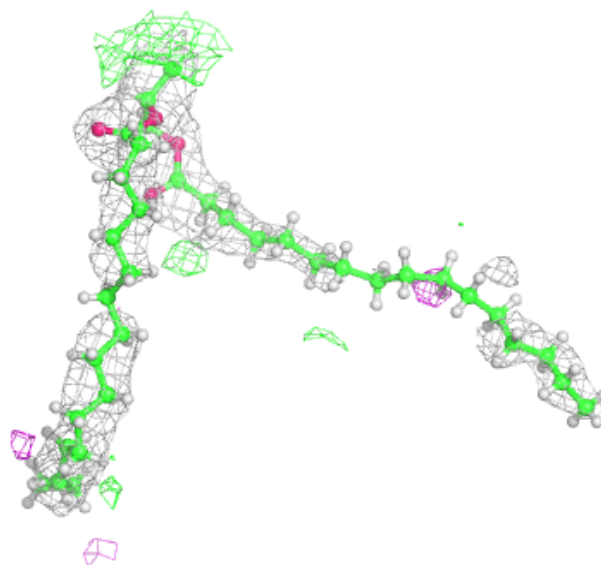
Electron density around SQD a 412:

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



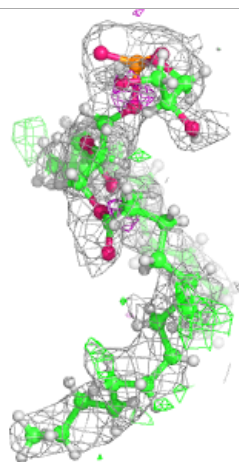
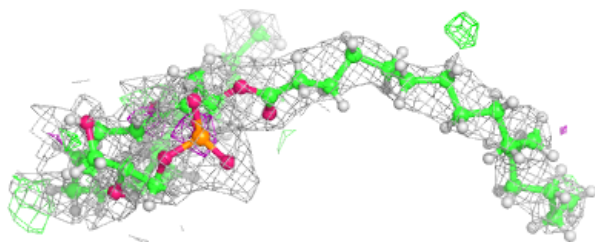
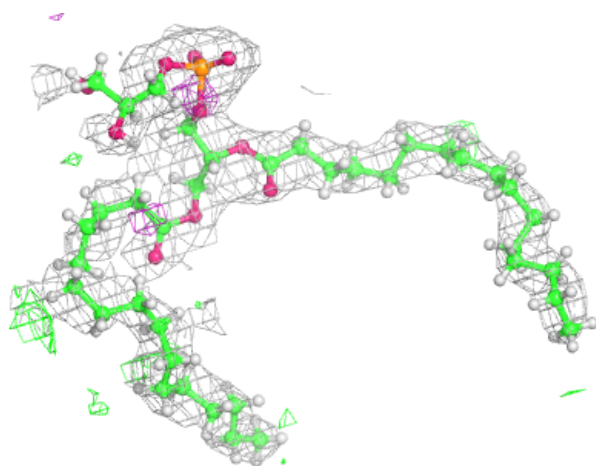
Electron density around SQD A 415:

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



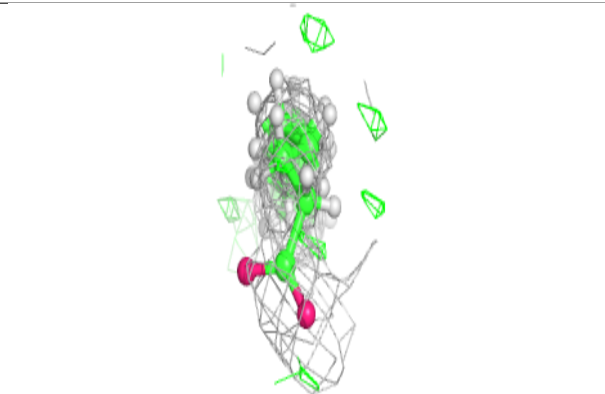
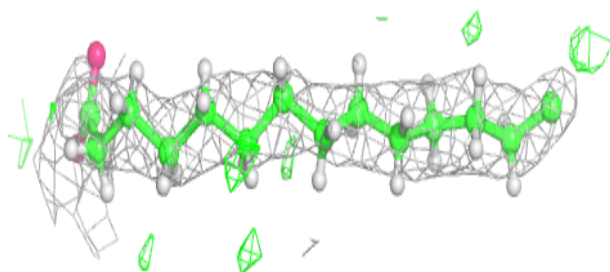
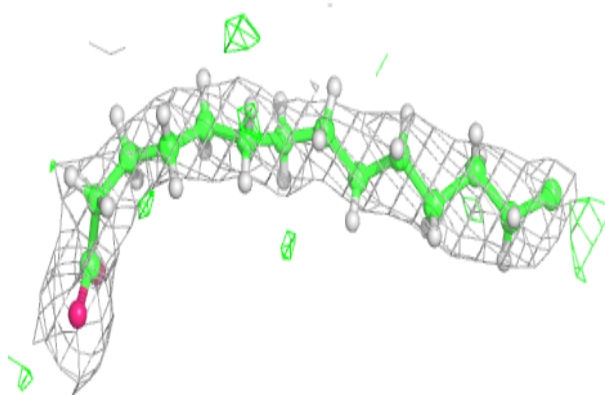
Electron density around LHG A 414:

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

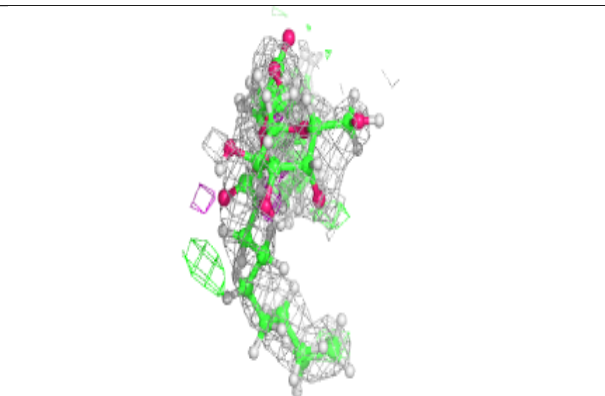
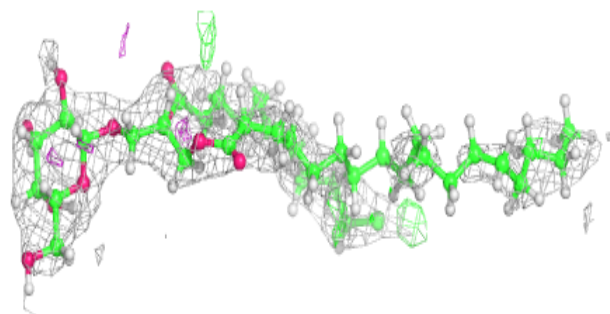
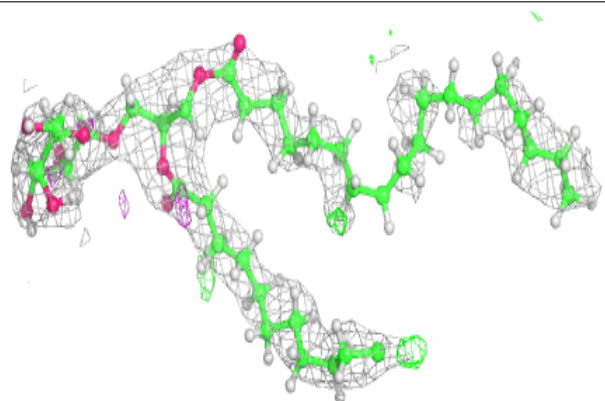


Electron density around STE b 625:

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

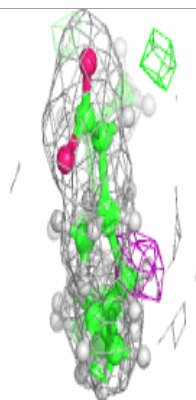
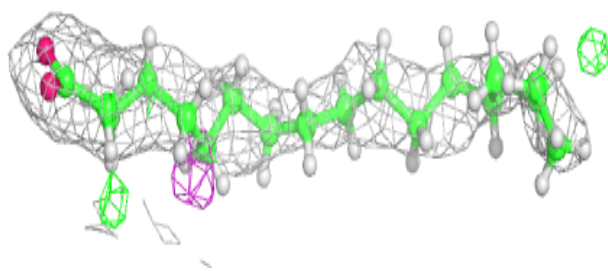
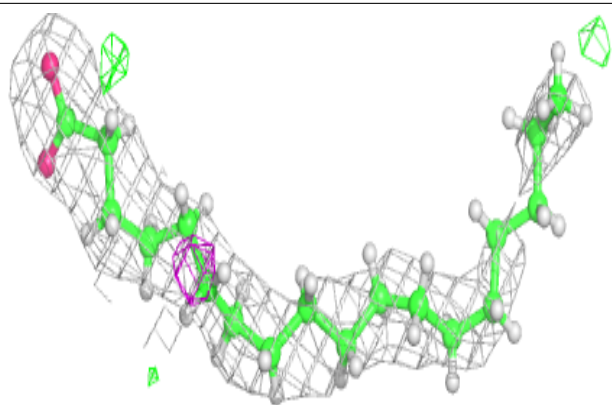
**Electron density around LMG c 521:**

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

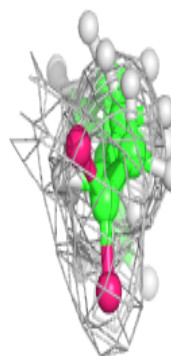
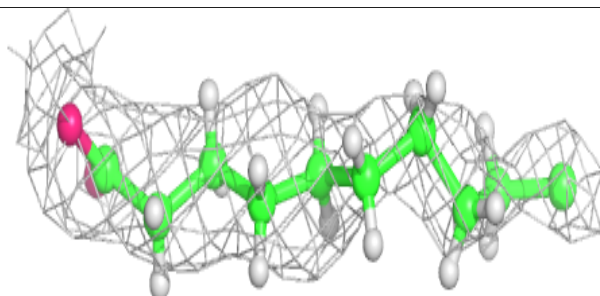
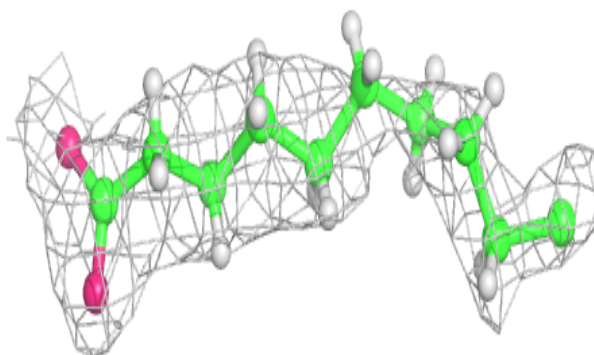


Electron density around STE d 412:

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

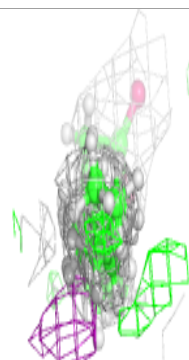
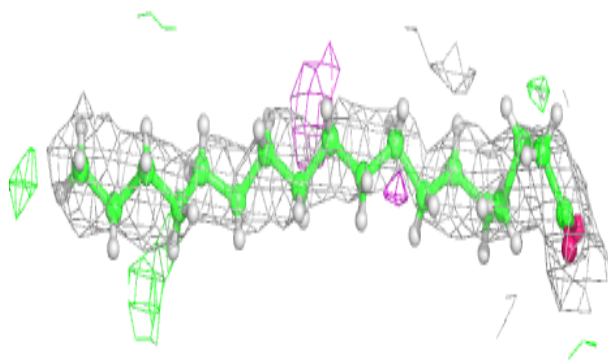
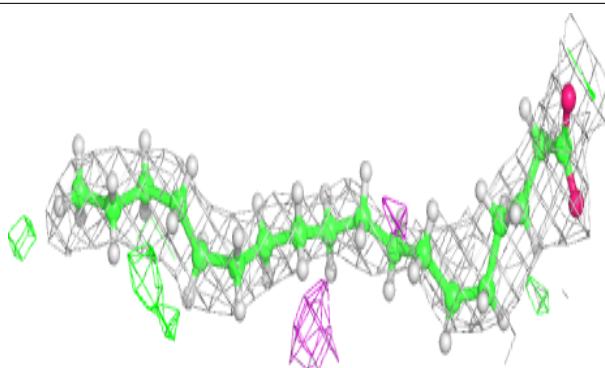
**Electron density around STE c 523:**

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

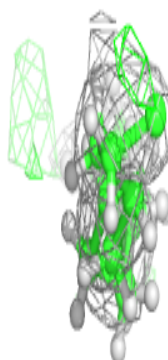
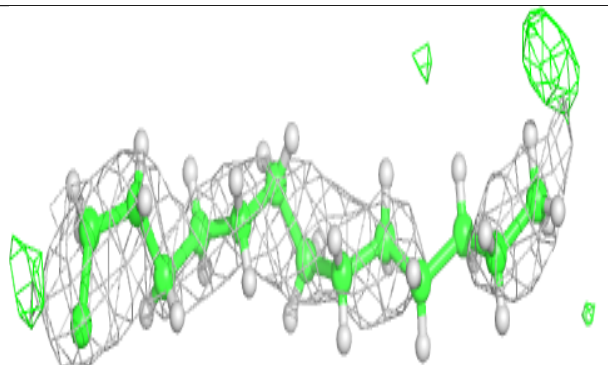
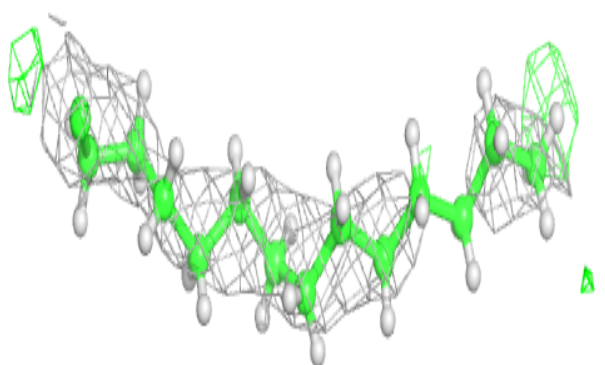


Electron density around STE b 626:

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

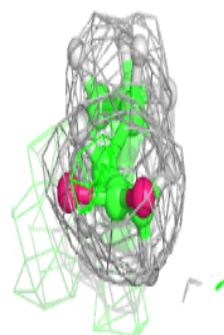
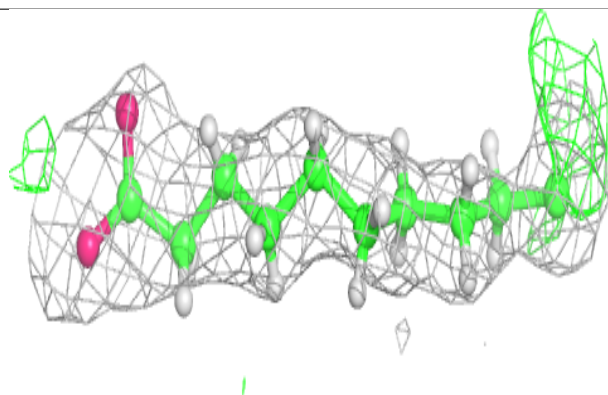
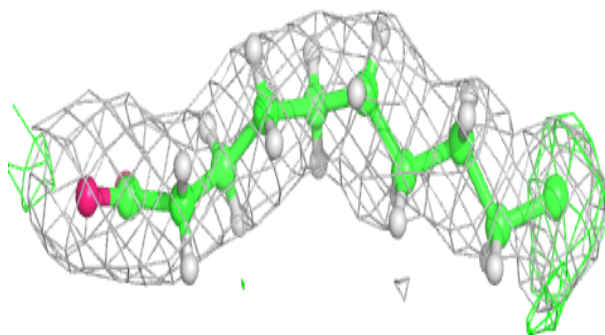
**Electron density around STE h 102:**

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

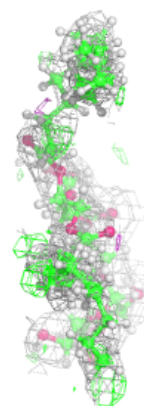
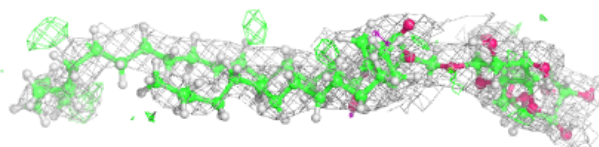
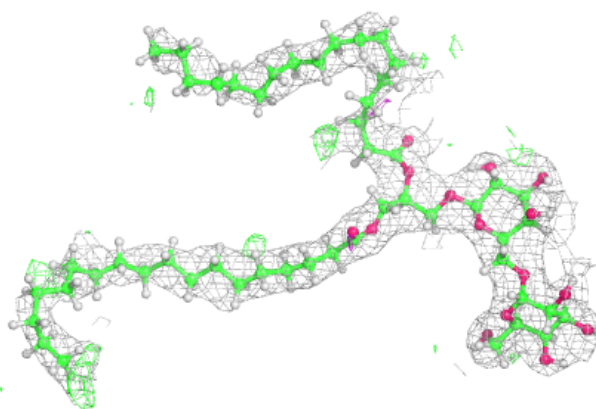


Electron density around STE j 101:

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

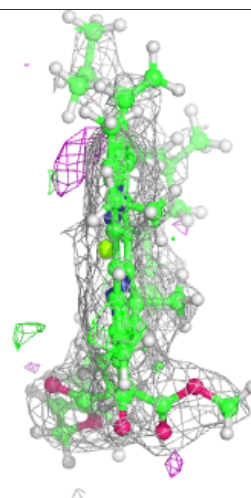
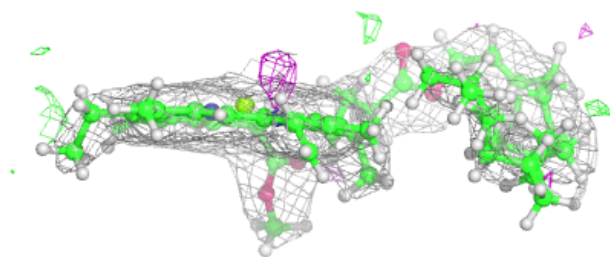
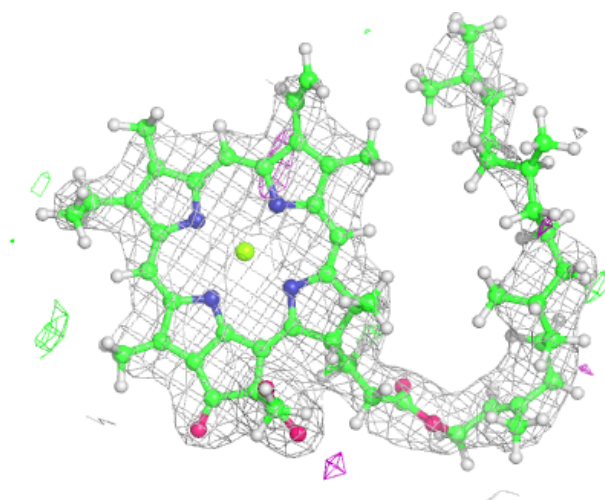
**Electron density around DGD A 416:**

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



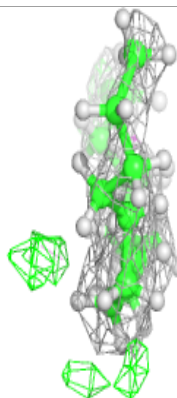
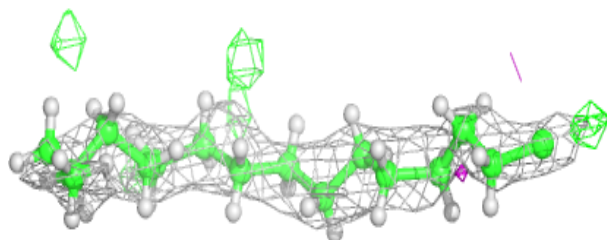
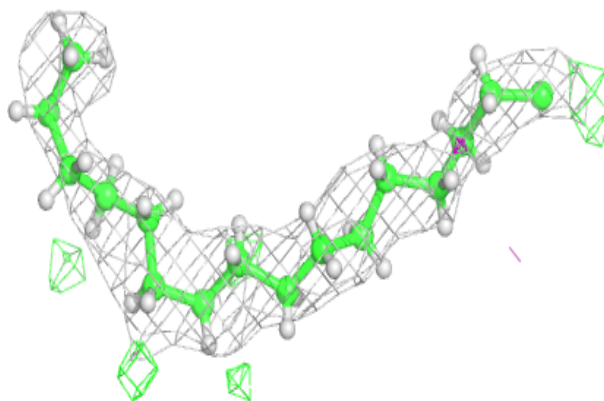
Electron density around CLA C 512:

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

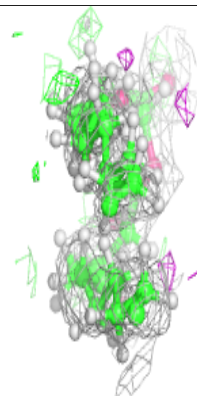
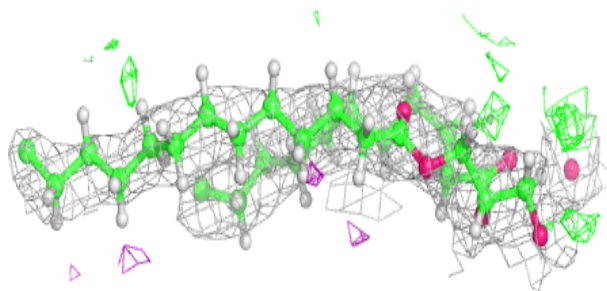
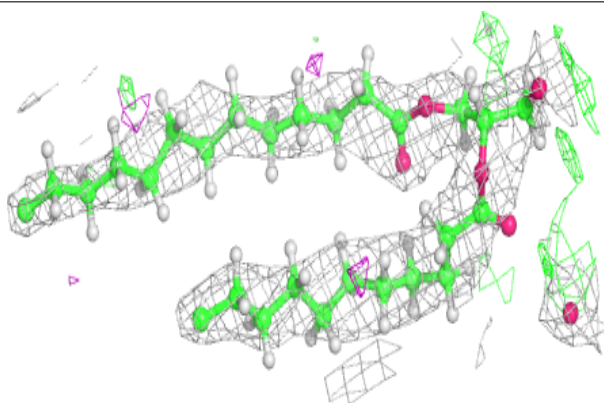


Electron density around STE B 626:

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

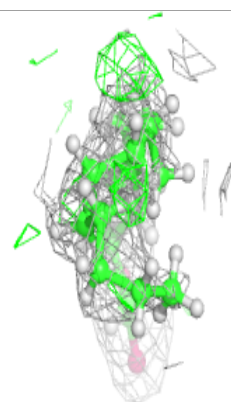
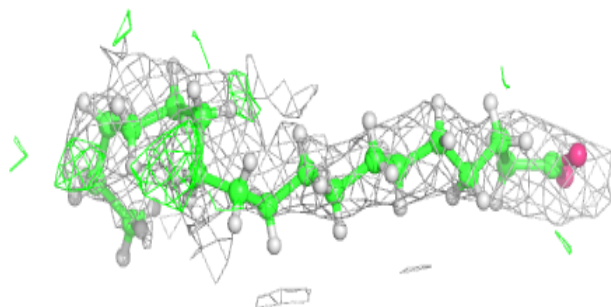
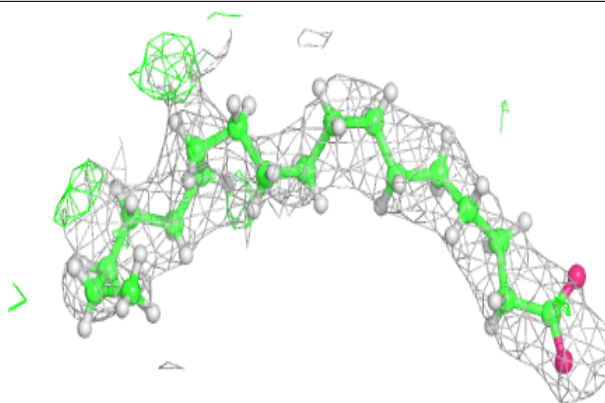
**Electron density around LMG D 410:**

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

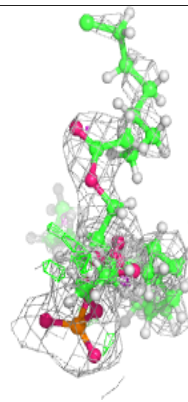
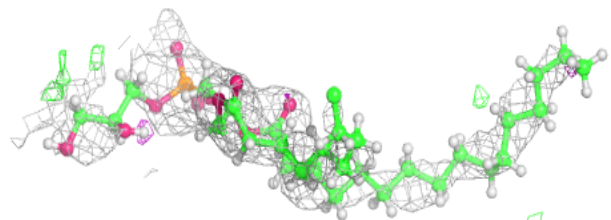
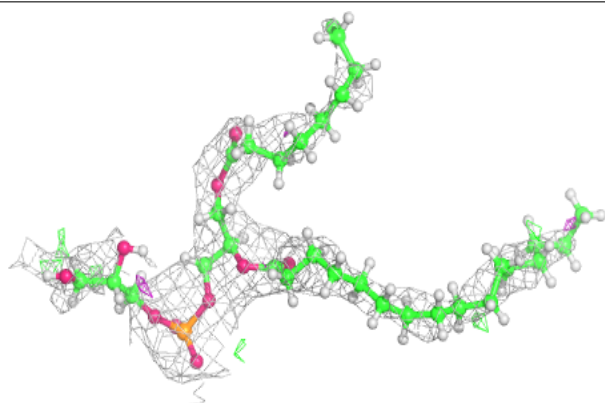


Electron density around STE d 413:

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

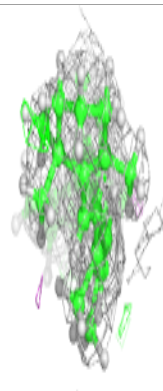
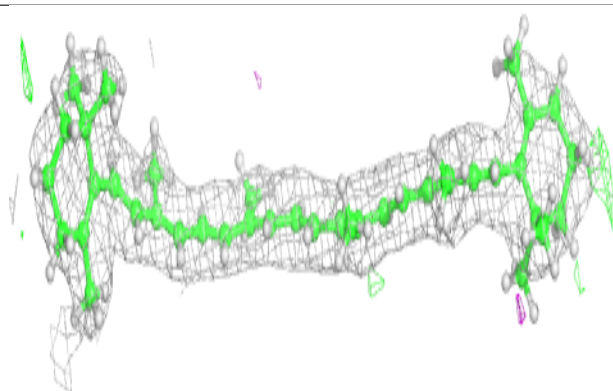
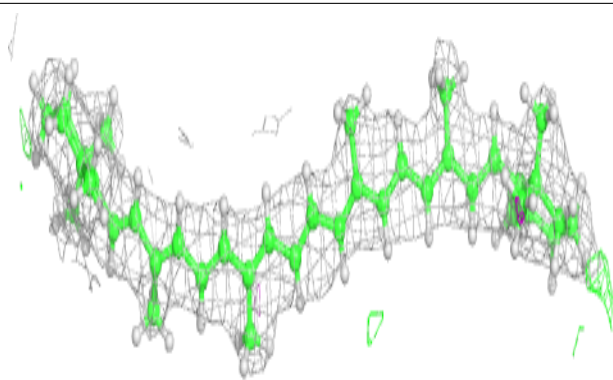
**Electron density around LHG e 102:**

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



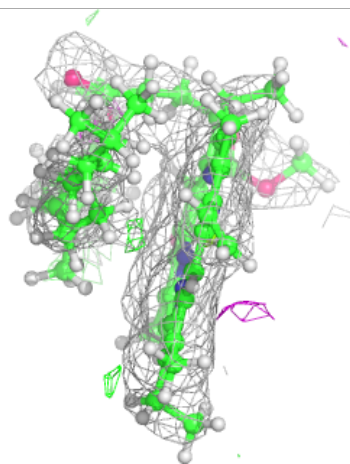
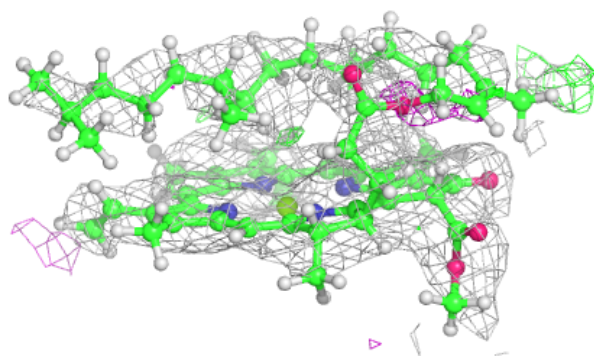
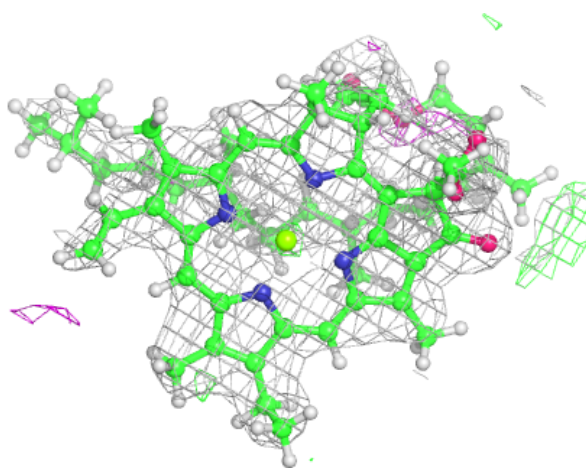
Electron density around BCR H 101:

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



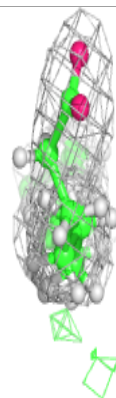
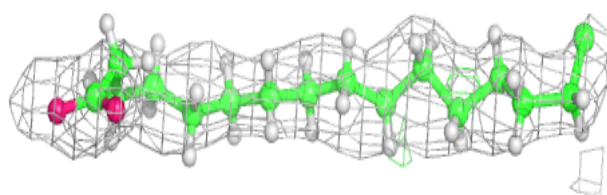
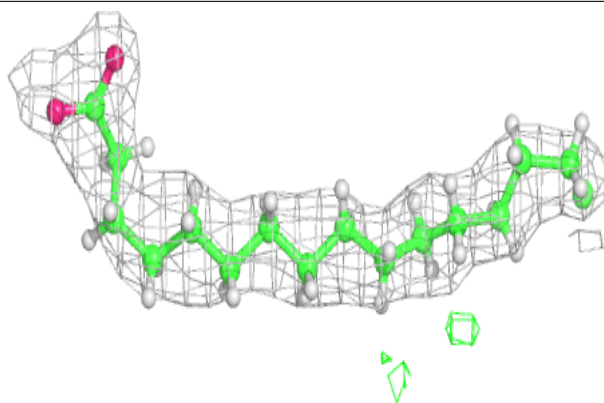
Electron density around CLA b 601:

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

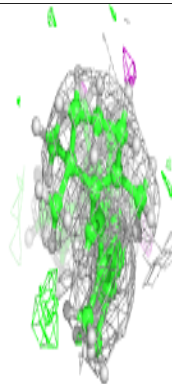
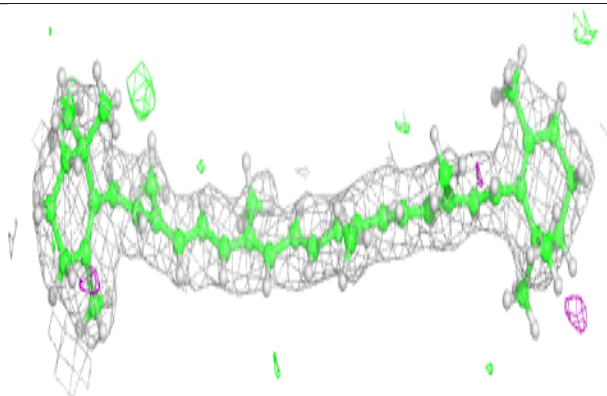
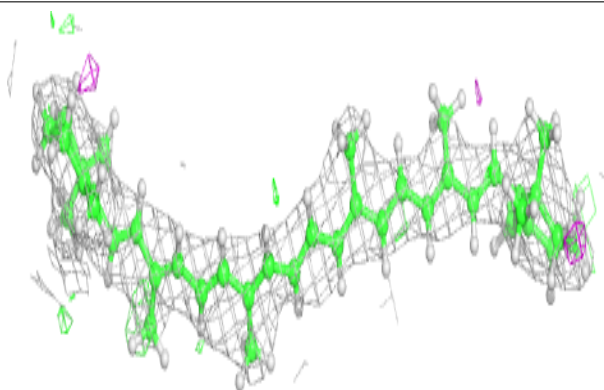


Electron density around STE B 625:

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

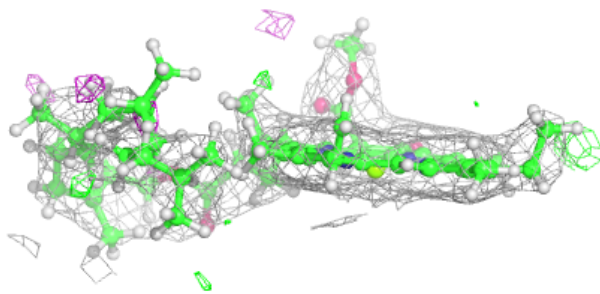
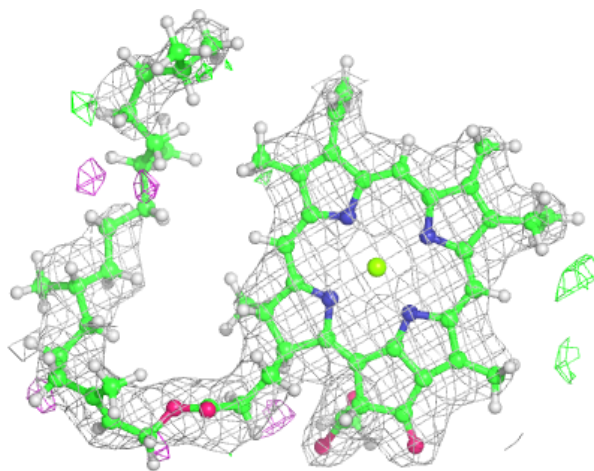
**Electron density around BCR x 101:**

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



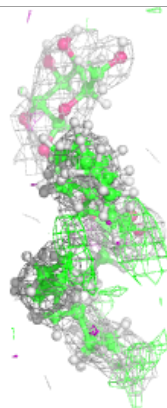
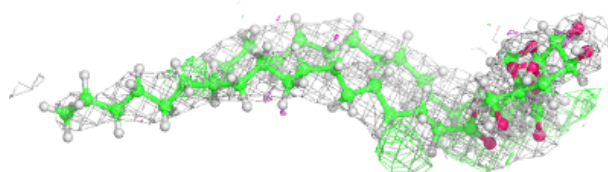
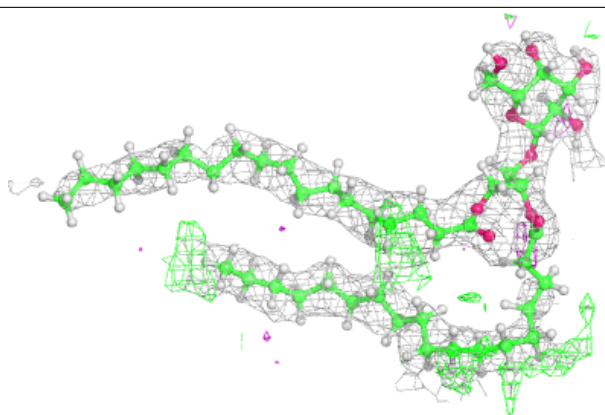
Electron density around CLA c 512:

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

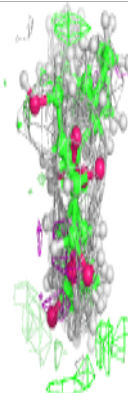
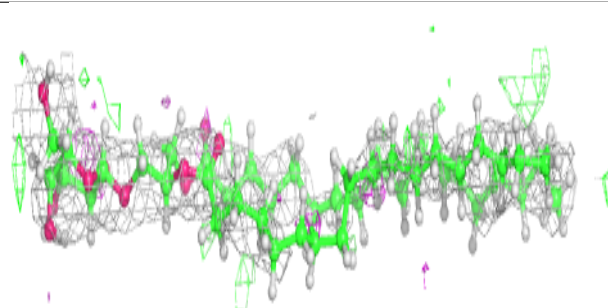
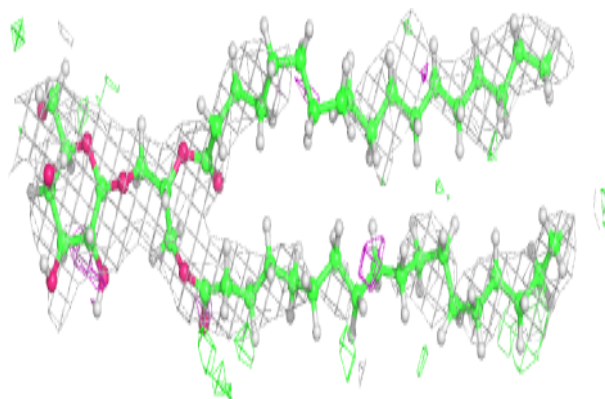


Electron density around LMG a 416:

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

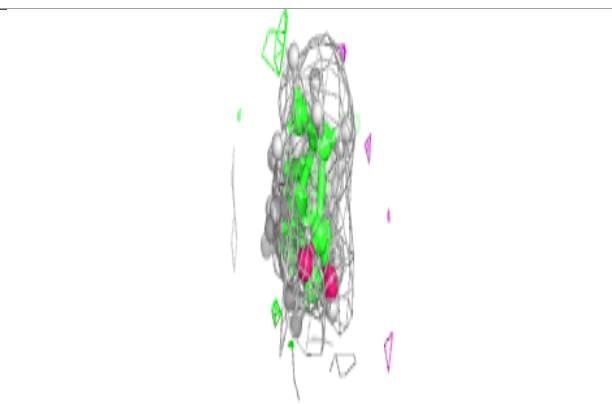
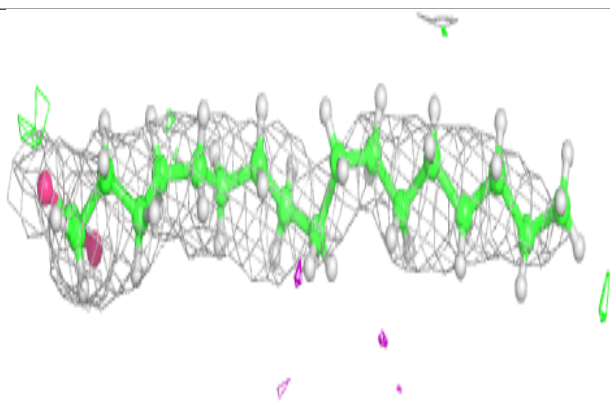
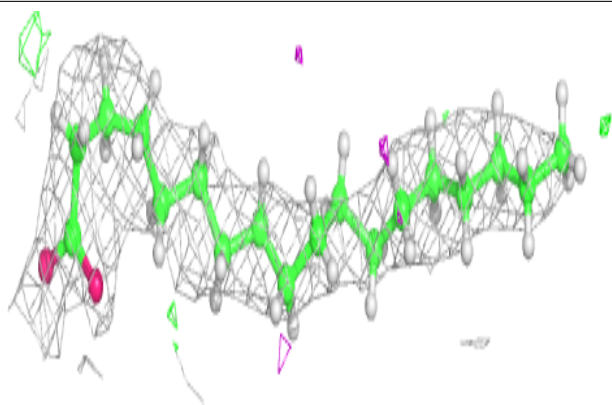
**Electron density around LMG b 624:**

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

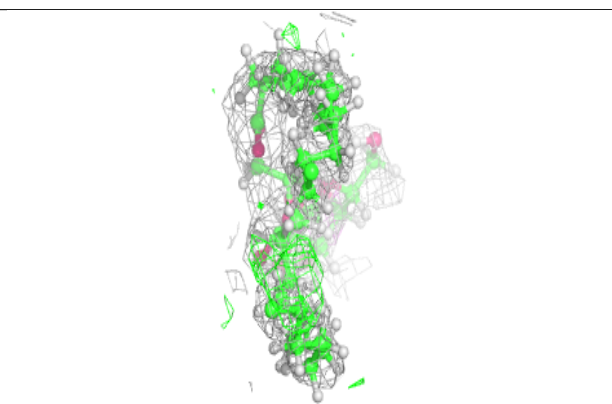
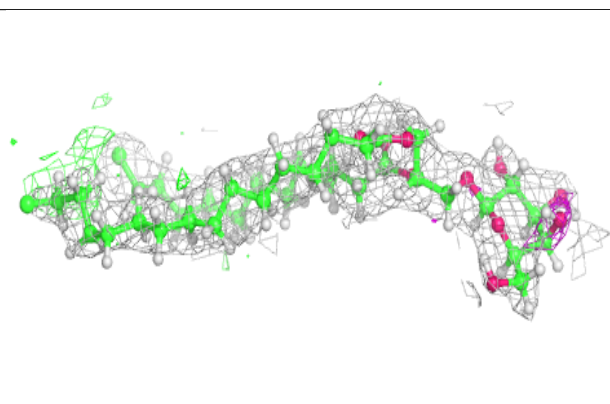
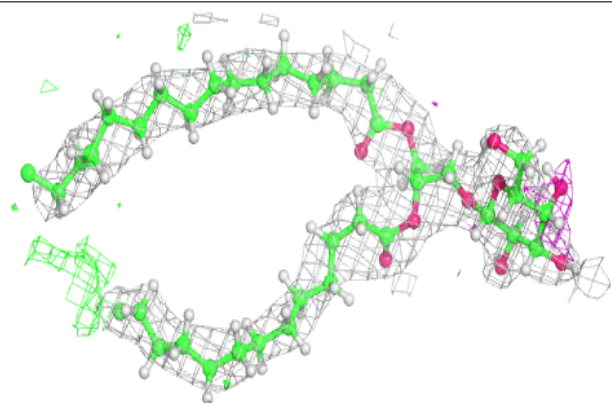


Electron density around STE c 520:

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

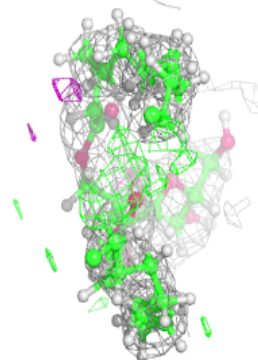
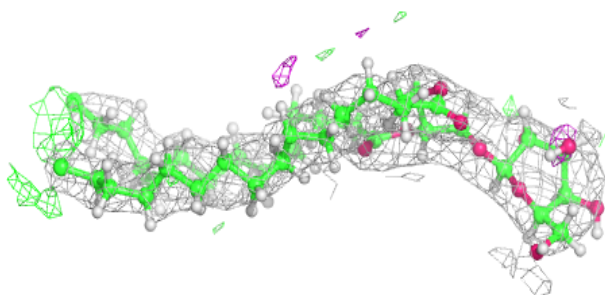
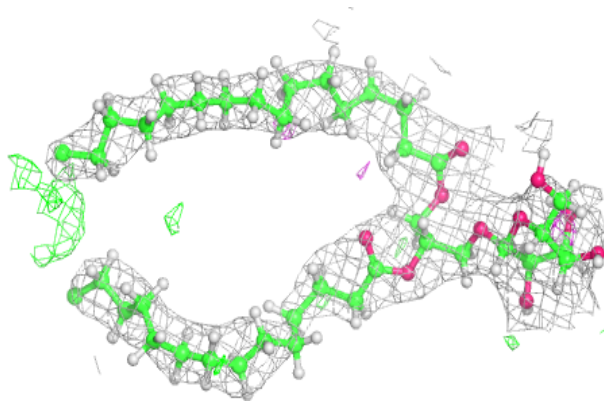
**Electron density around LMG A 412:**

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

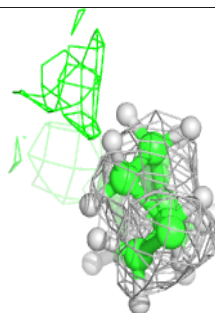
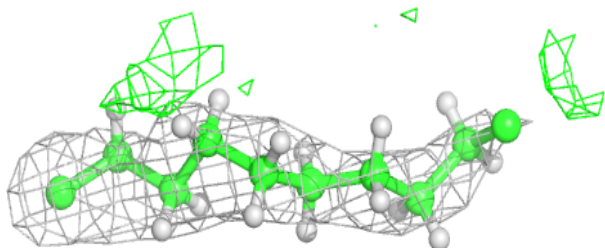
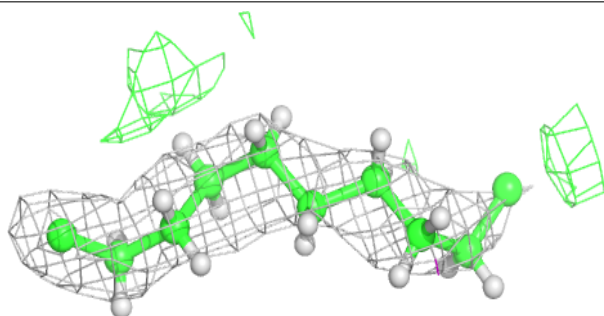


Electron density around LMG c 522:

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

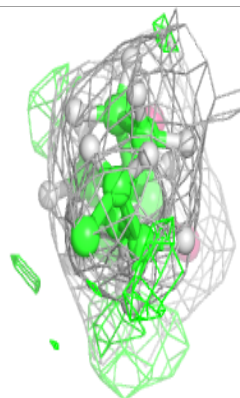
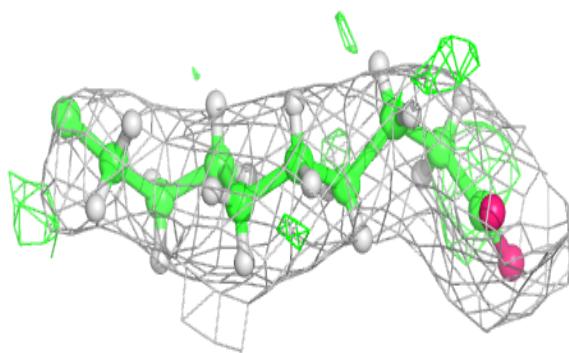
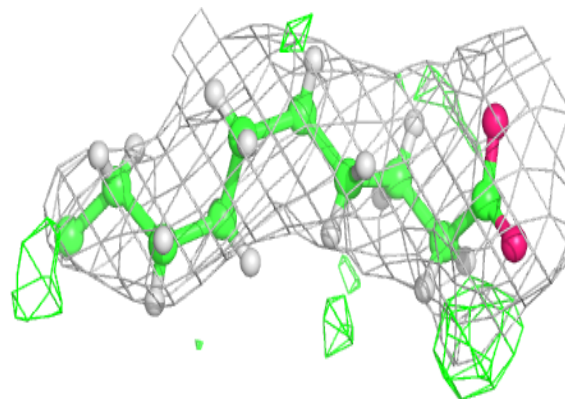
**Electron density around STE a 413:**

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

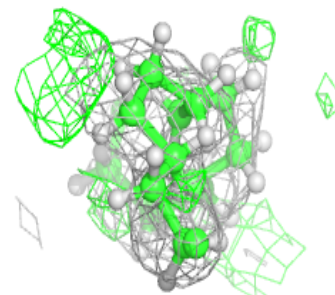
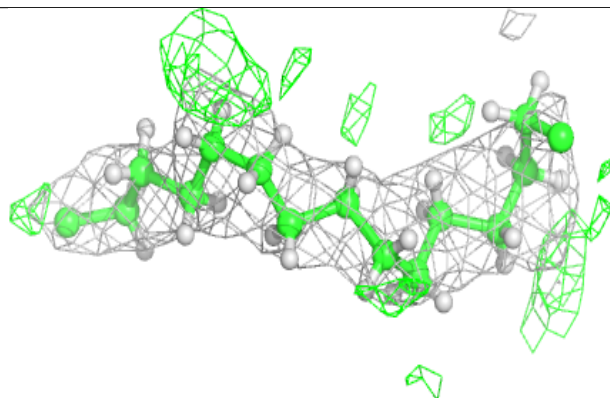
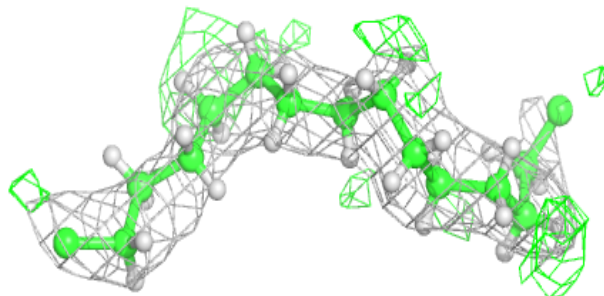


Electron density around STE B 624:

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

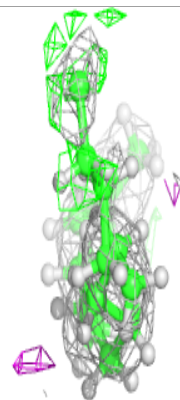
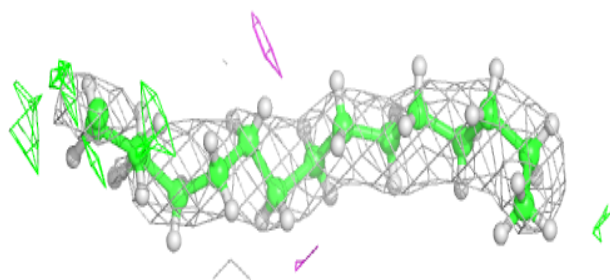
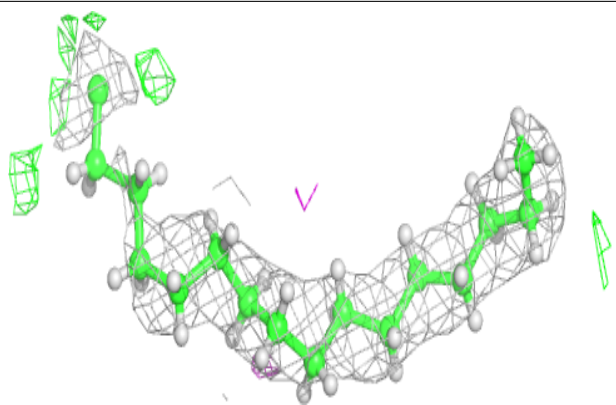
**Electron density around STE a 415:**

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

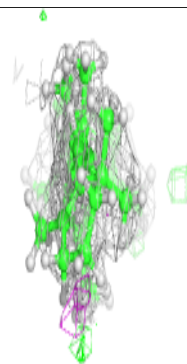
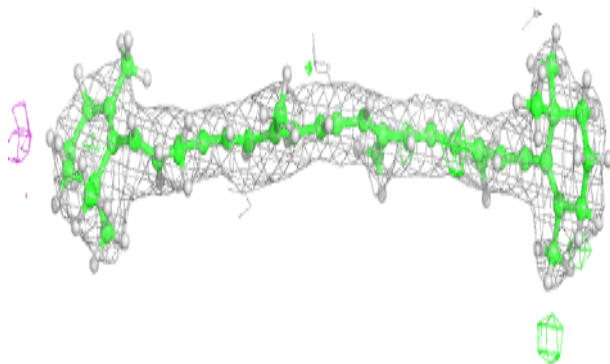
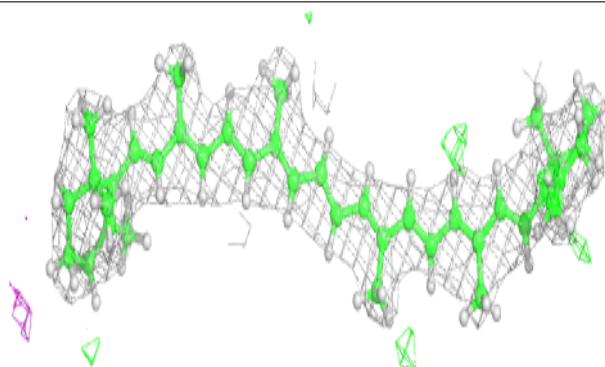


Electron density around STE b 621:

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

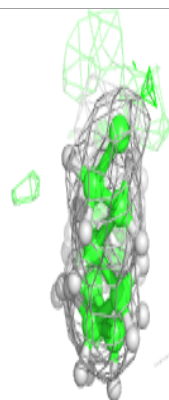
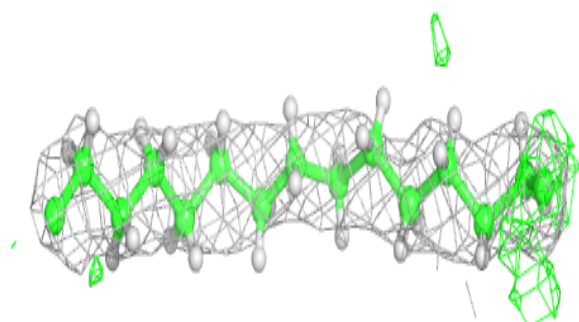
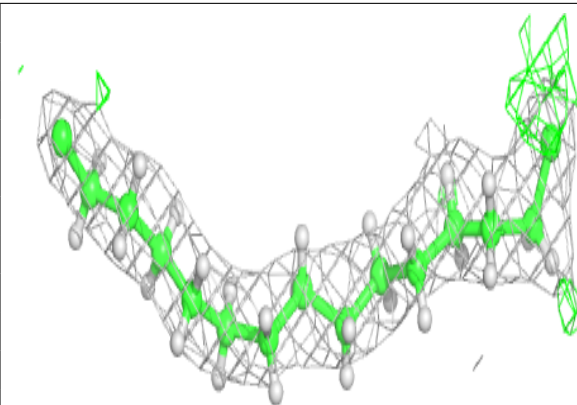
**Electron density around BCR Y 101:**

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

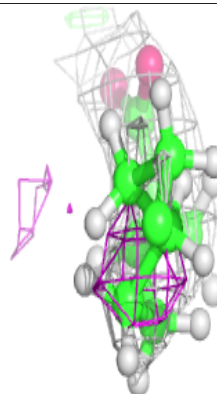
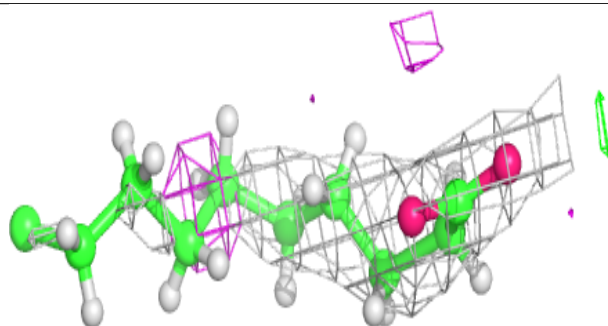
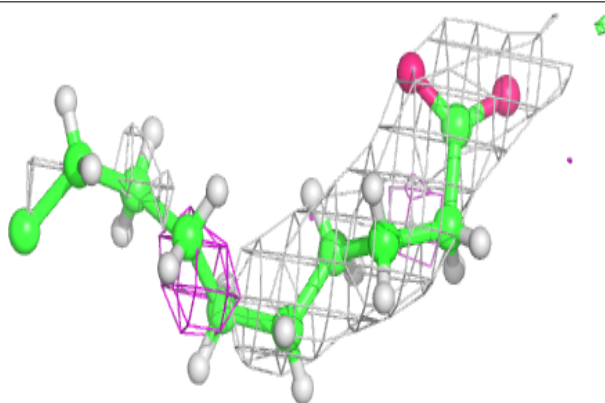


Electron density around STE I 101:

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

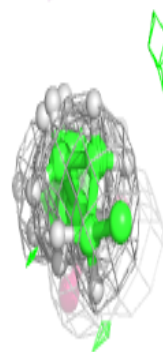
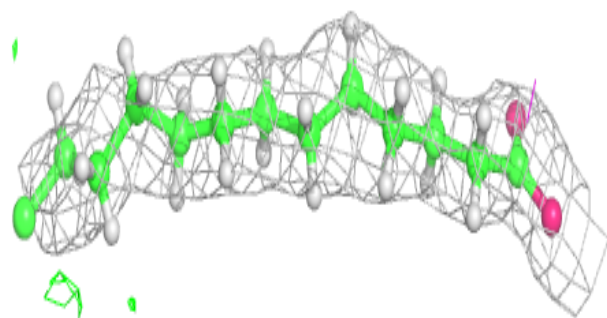
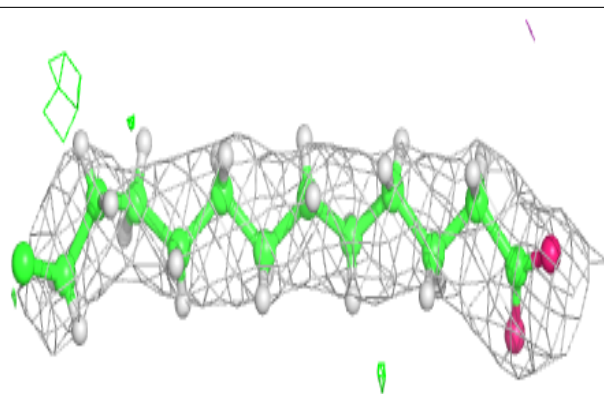
**Electron density around STE B 627:**

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

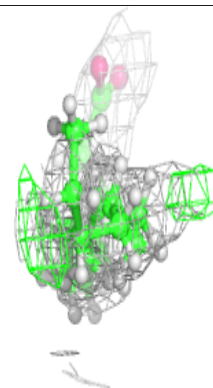
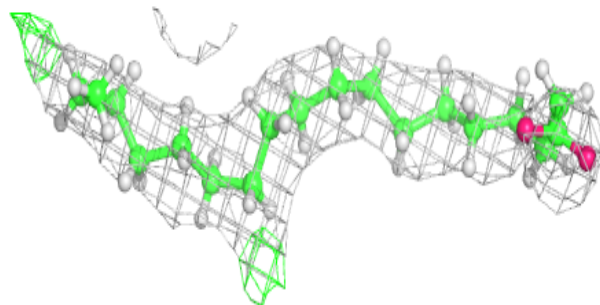
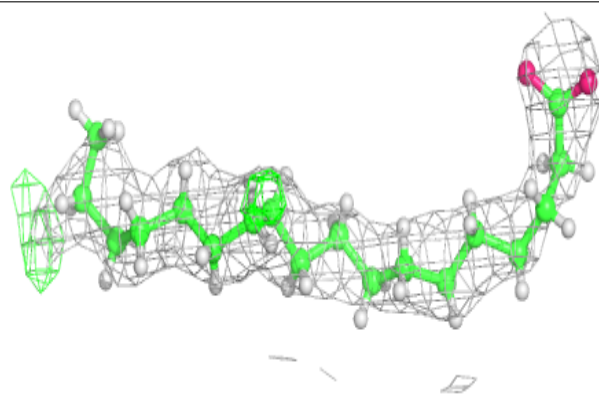


Electron density around STE M 102:

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

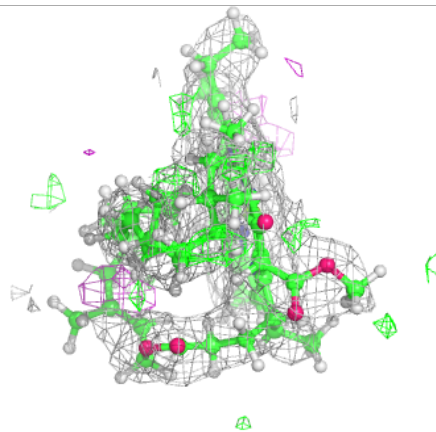
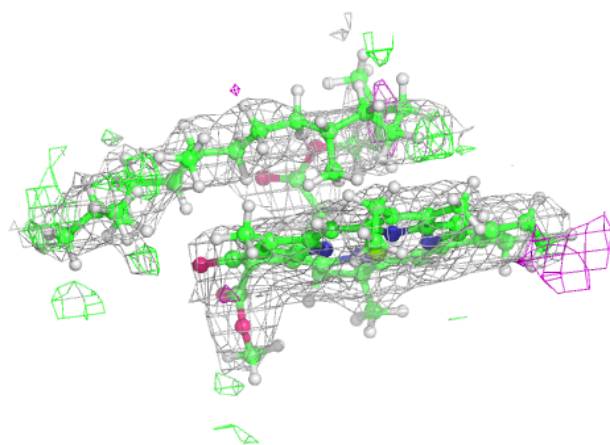
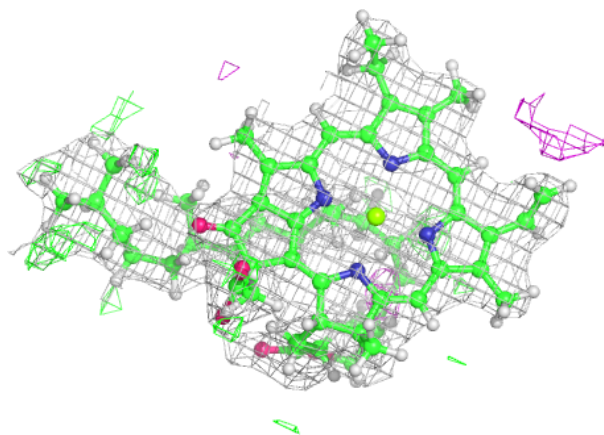
**Electron density around STE b 623:**

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



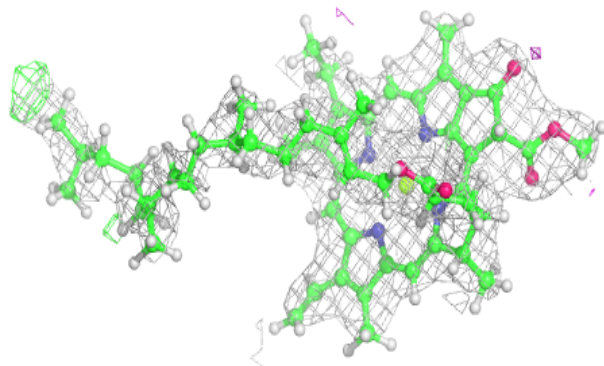
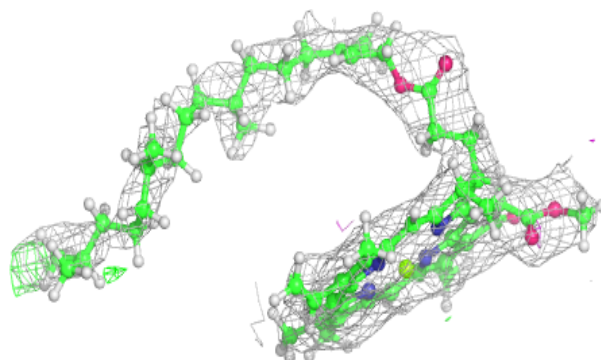
Electron density around CLA B 601:

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

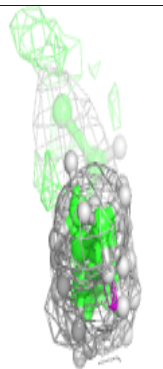
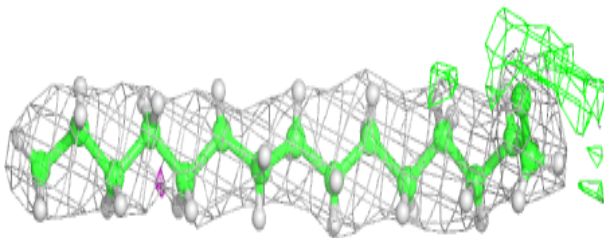
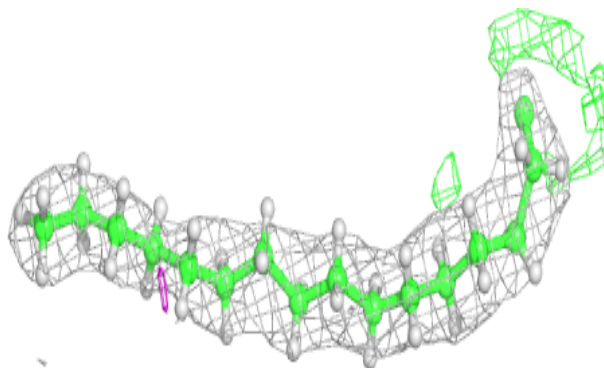


Electron density around CLA C 513:

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

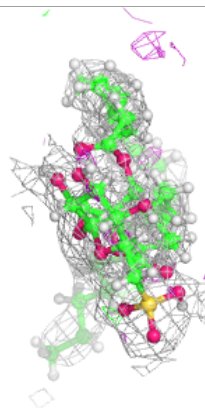
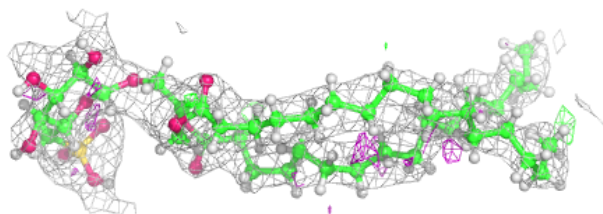
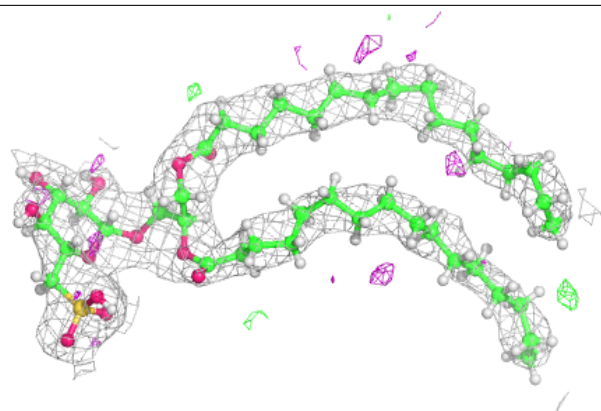
**Electron density around STE C 520:**

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

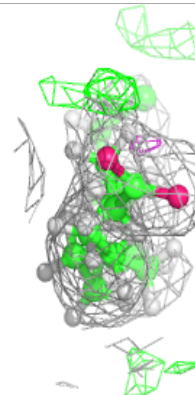
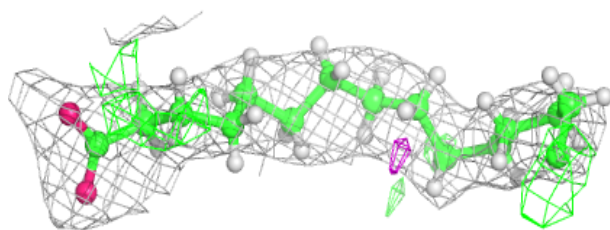
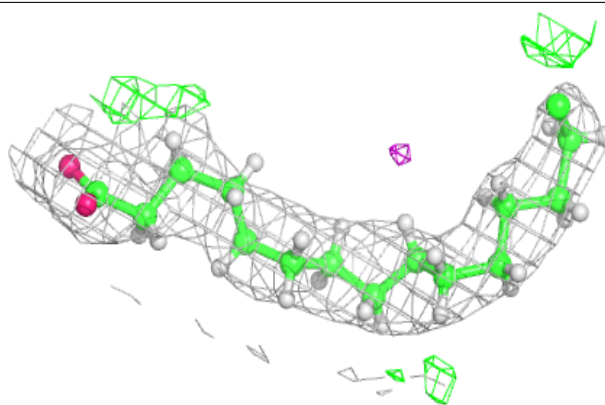


Electron density around SQD B 623:

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

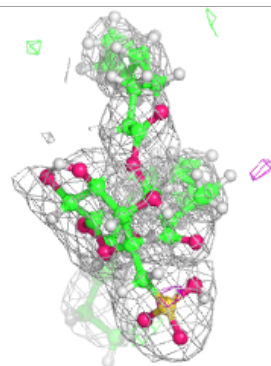
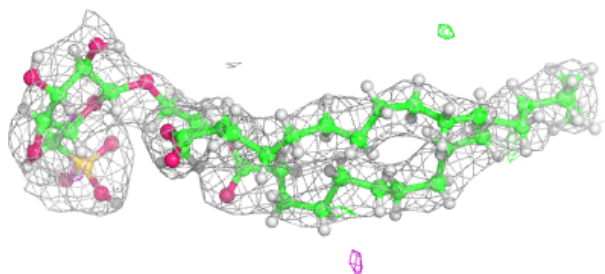
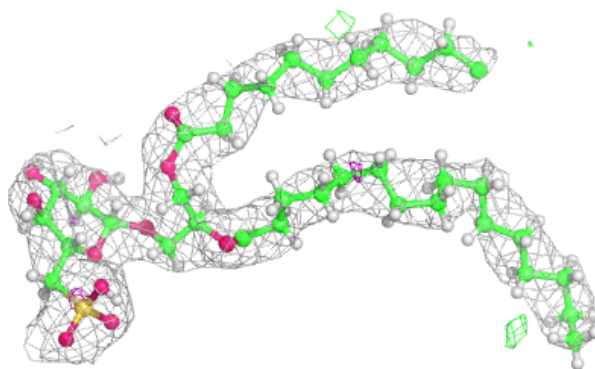
**Electron density around STE B 620:**

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

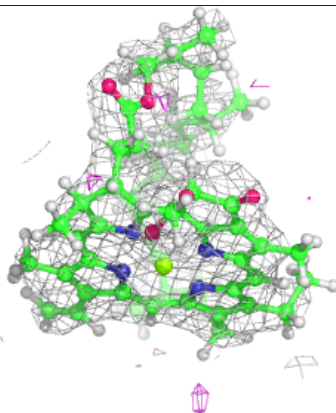
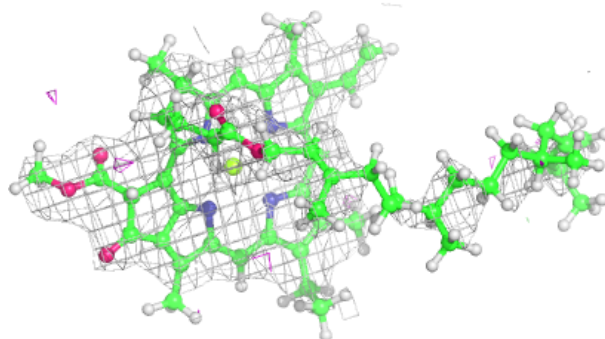
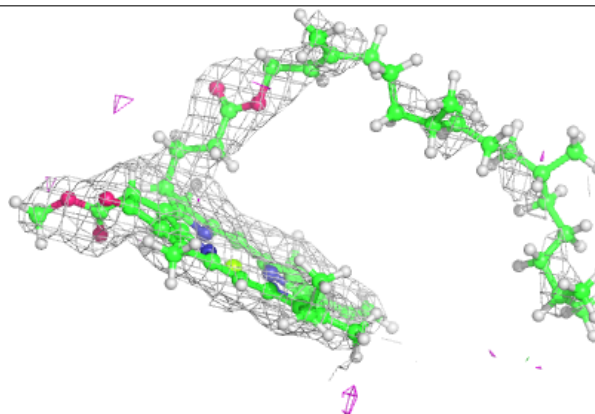


Electron density around SQD b 620:

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

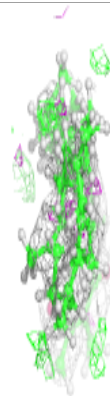
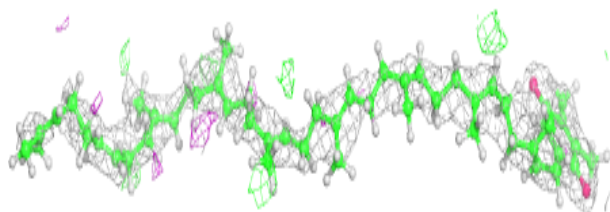
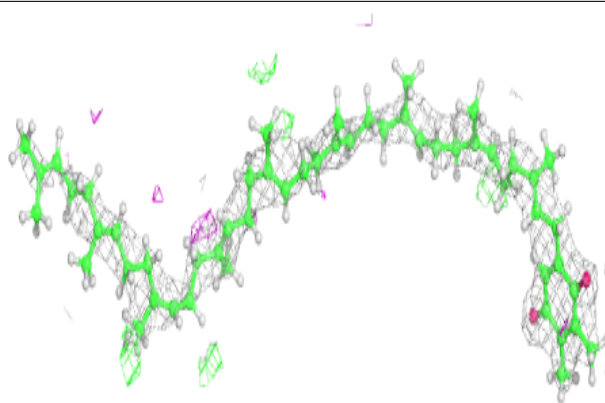
**Electron density around CLA c 513:**

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

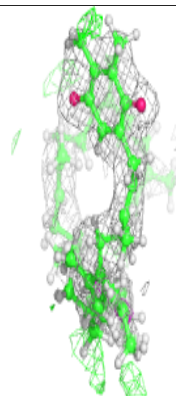
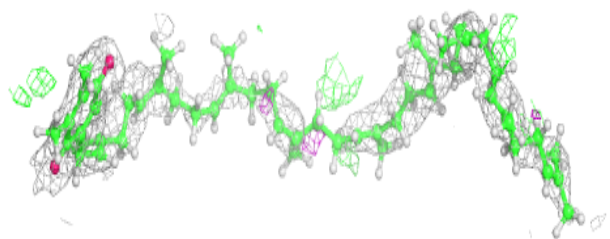
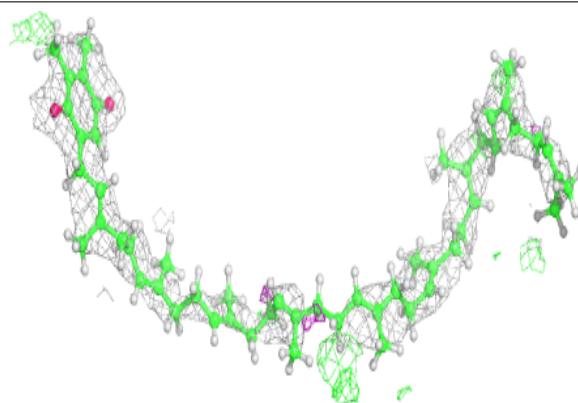


Electron density around PL9 A 410:

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

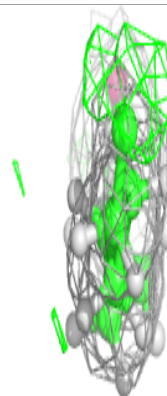
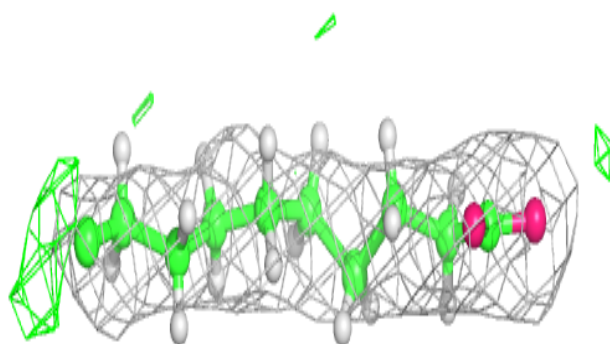
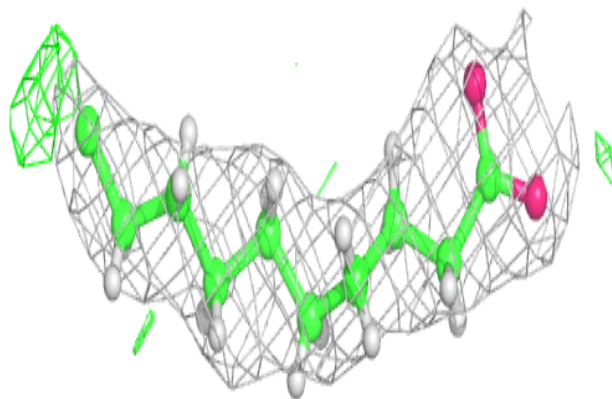
**Electron density around PL9 a 409:**

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

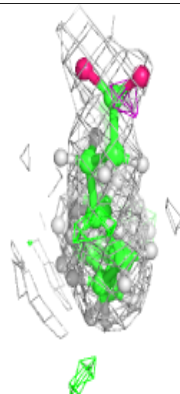
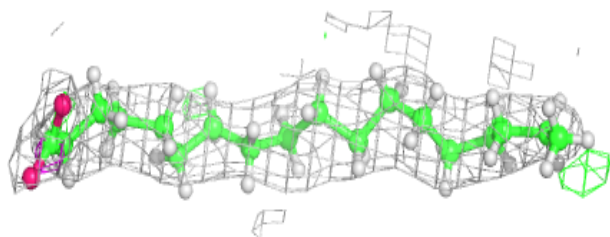
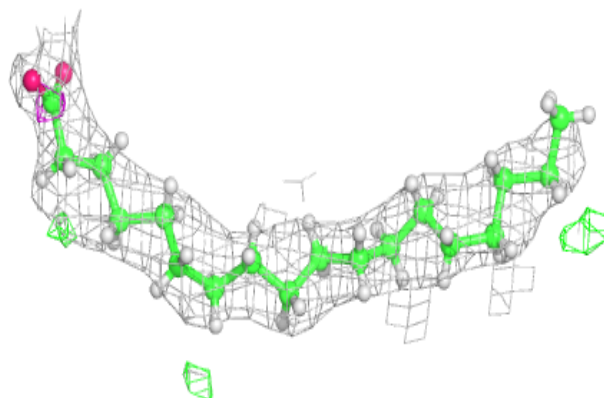


Electron density around STE C 519:

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

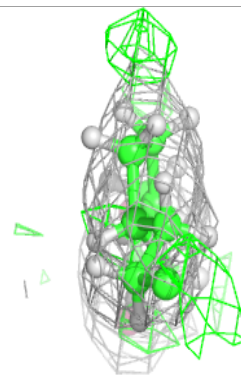
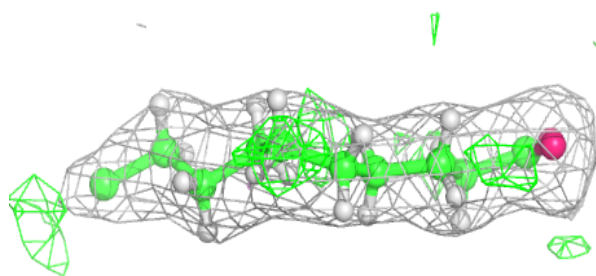
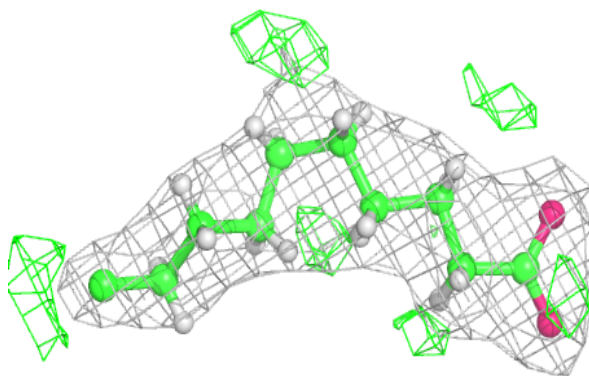
**Electron density around STE X 101:**

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

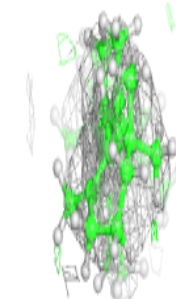
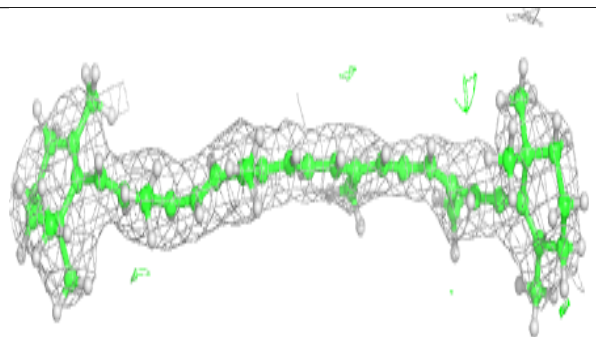
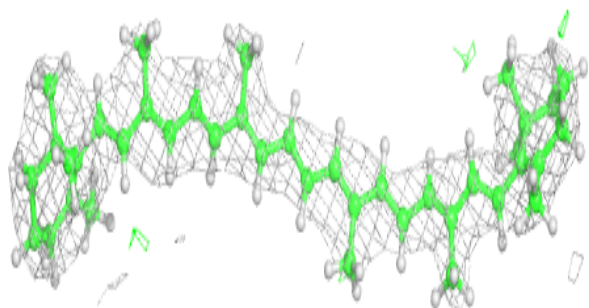


Electron density around STE C 521:

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

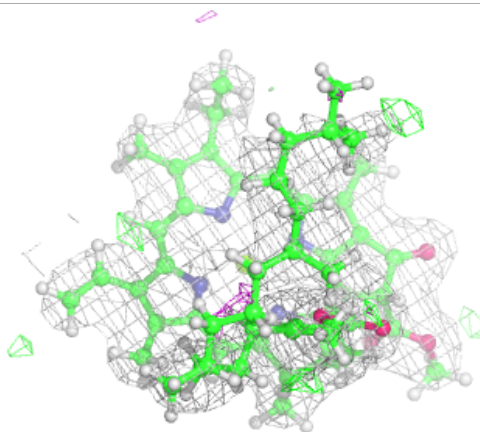
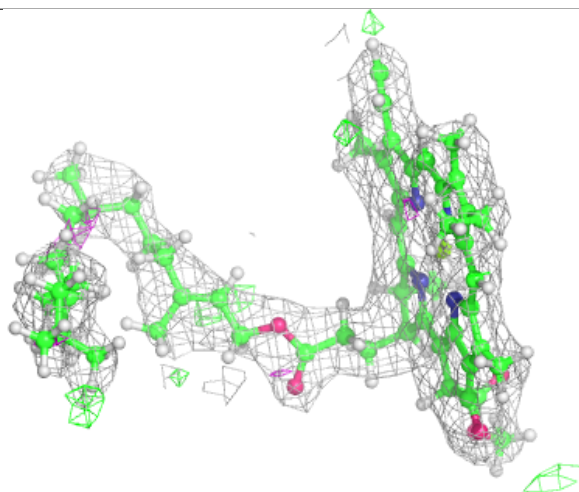
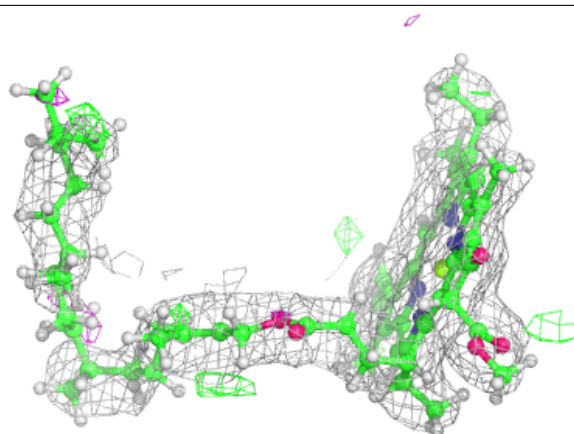
**Electron density around BCR k 101:**

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



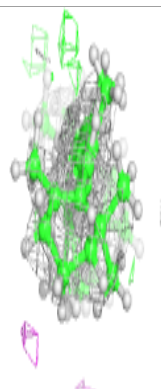
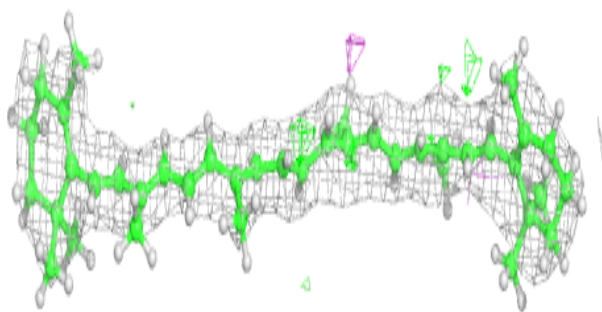
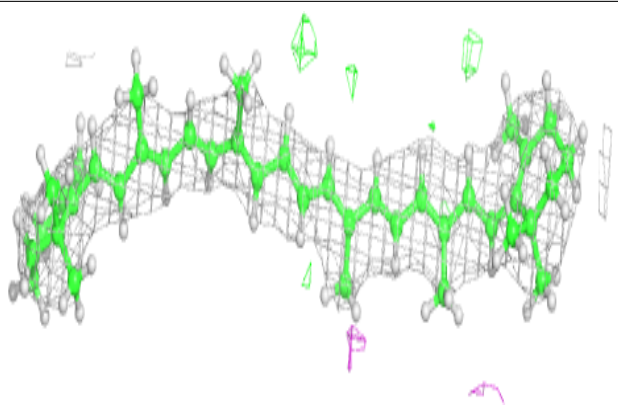
Electron density around CLA a 404:

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

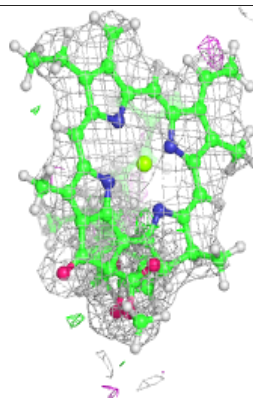
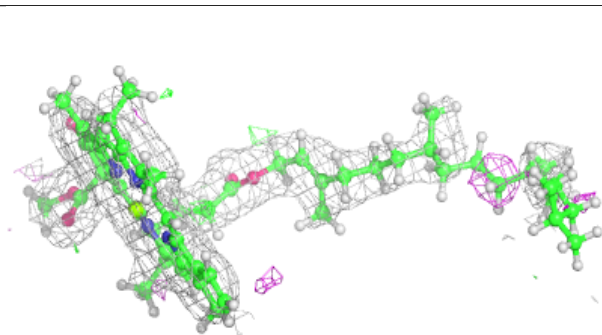
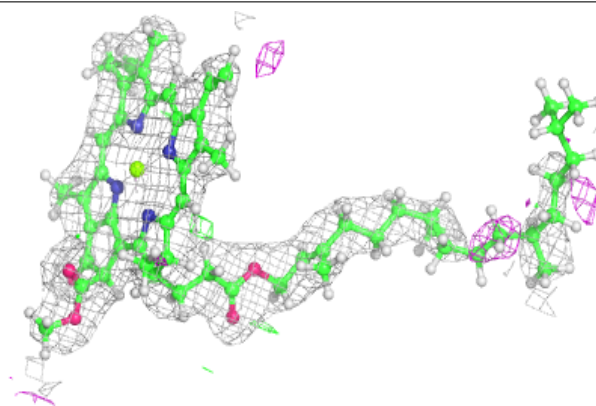


Electron density around BCR K 101:

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

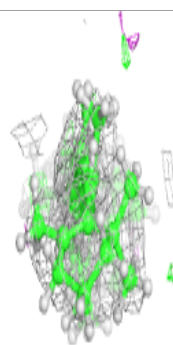
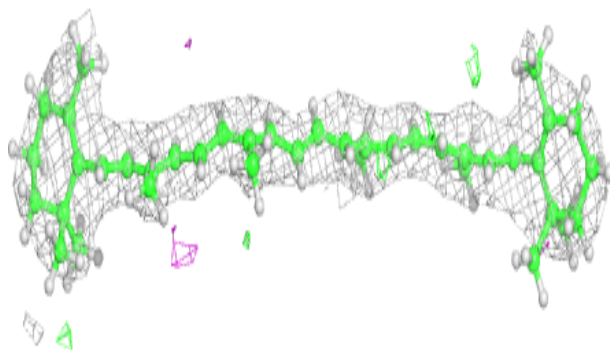
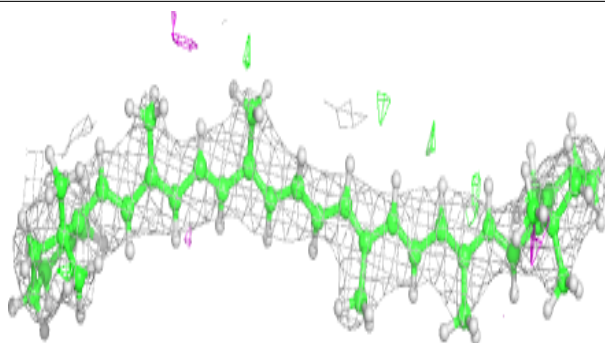
**Electron density around CLA d 404:**

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

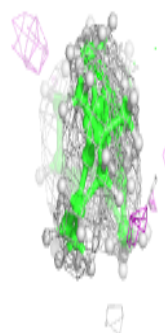
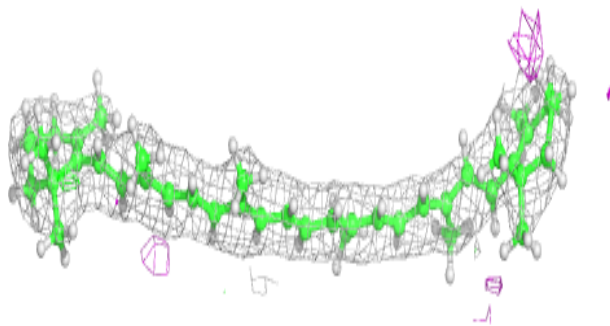
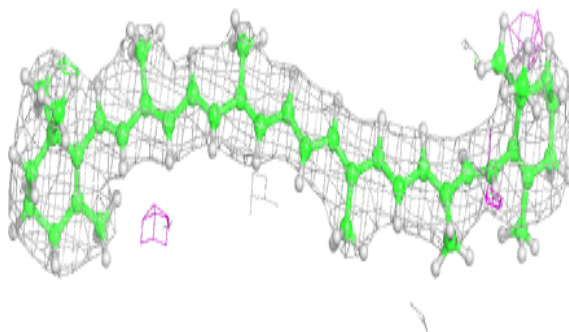


Electron density around BCR c 514:

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

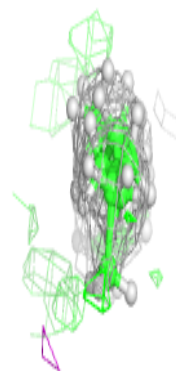
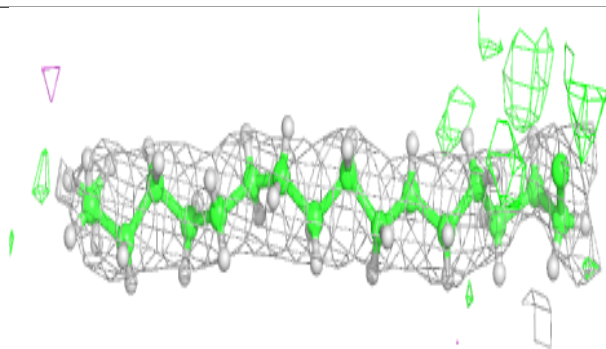
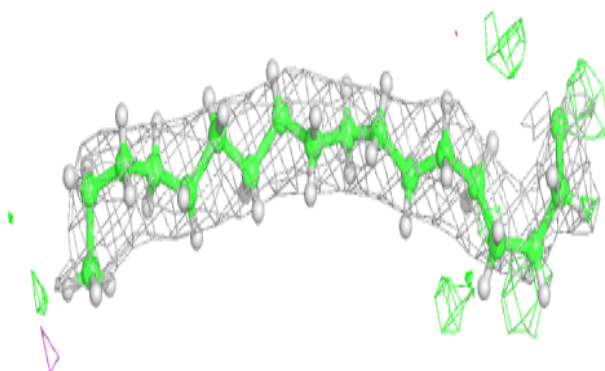
**Electron density around BCR d 405:**

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

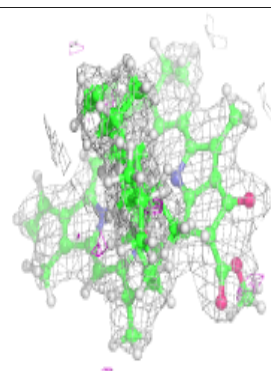
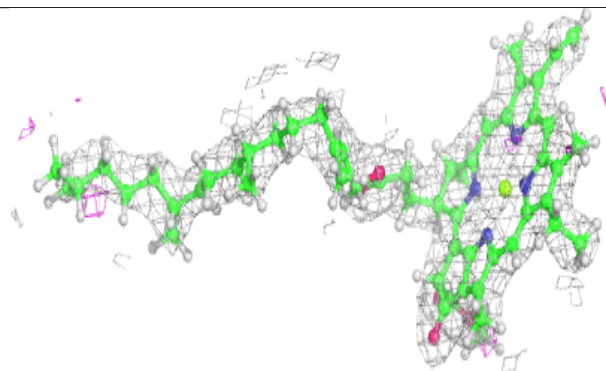
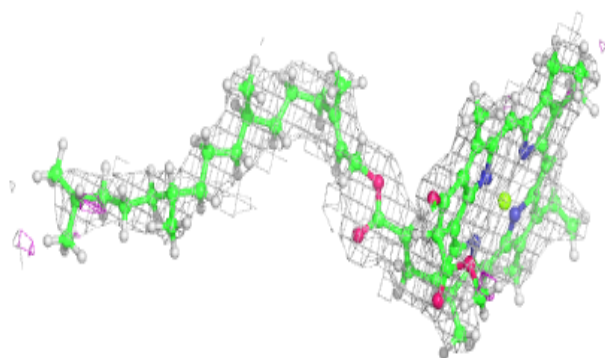


Electron density around STE I 102:

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

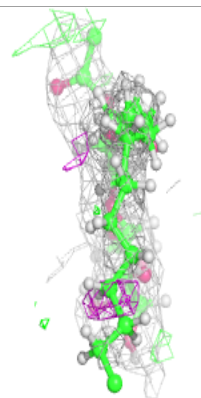
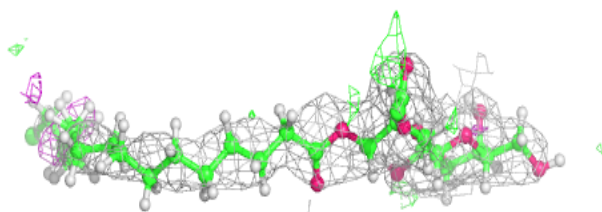
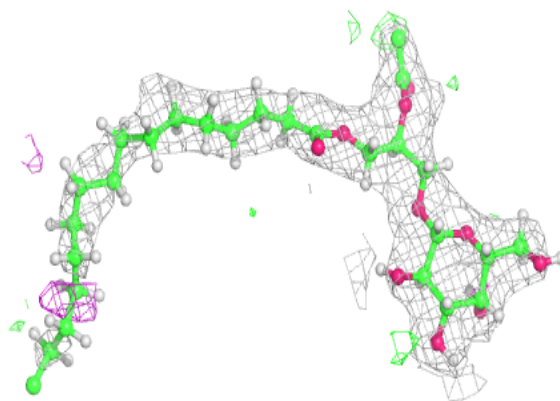
**Electron density around CLA C 502:**

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



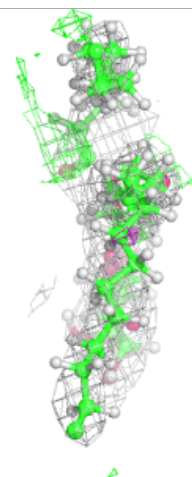
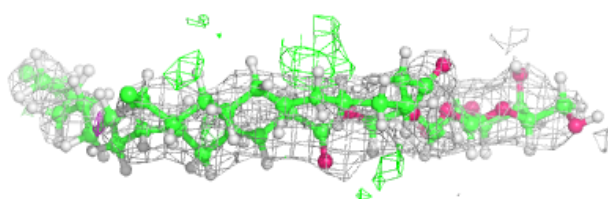
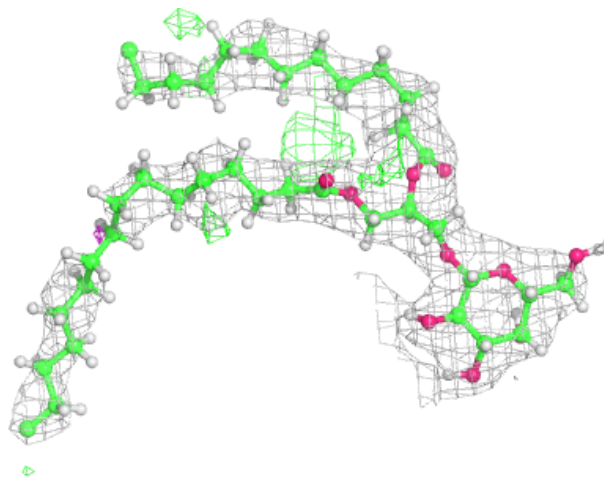
Electron density around LMG c 519:

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



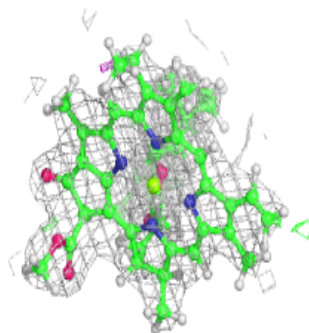
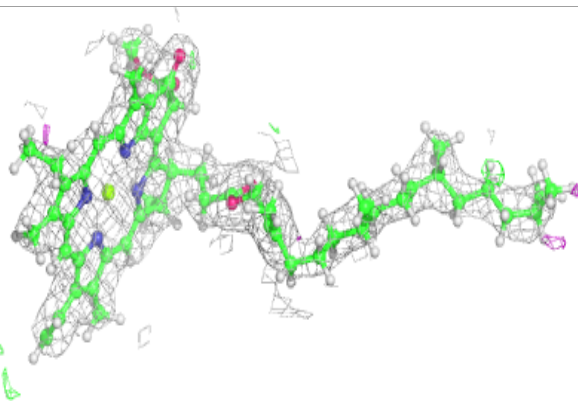
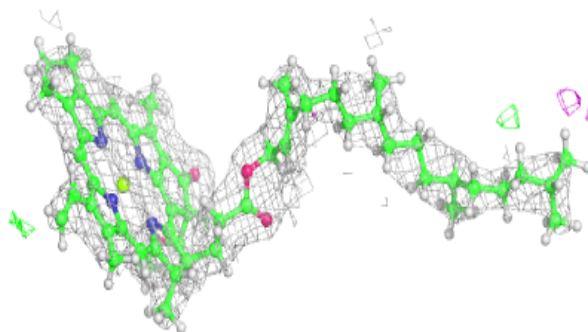
Electron density around LMG C 518:

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

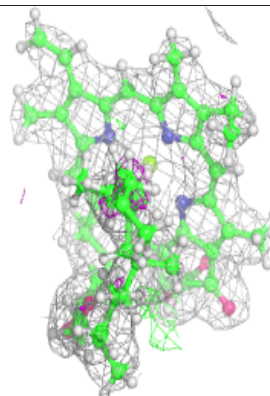
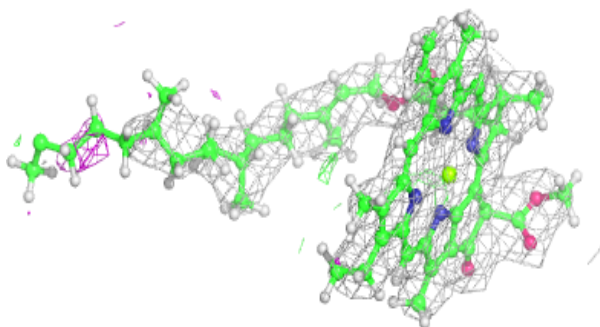
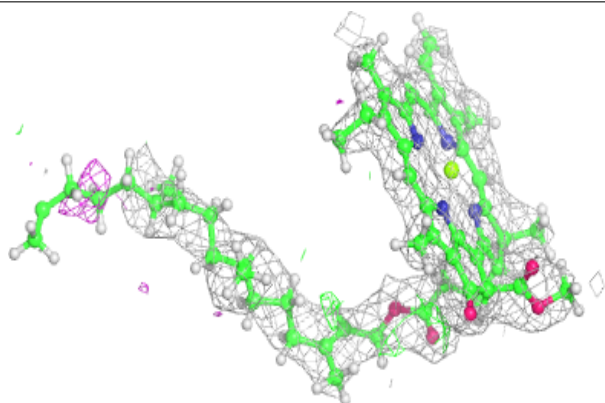


Electron density around CLA c 502:

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

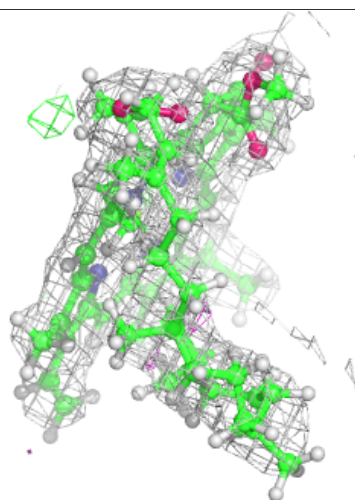
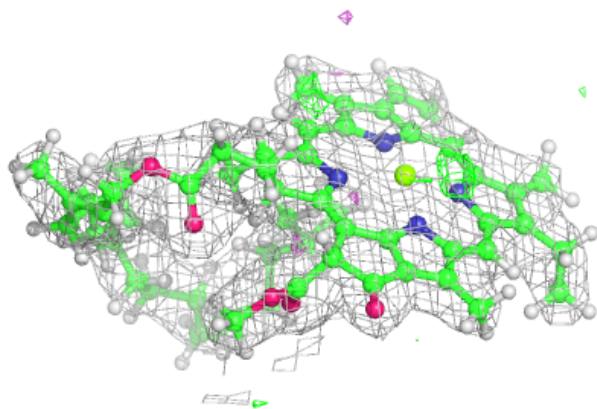
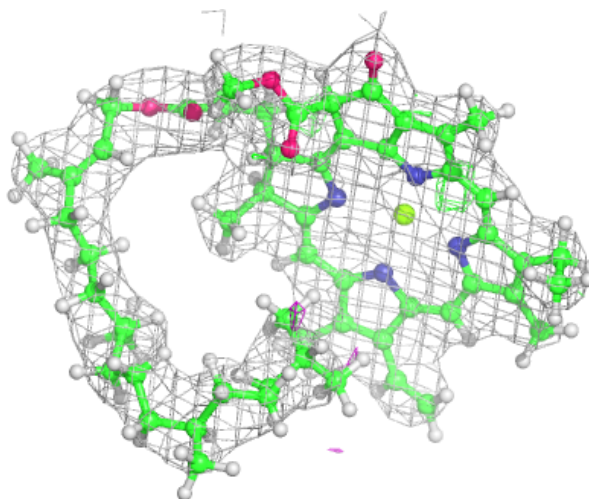
**Electron density around CLA c 508:**

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



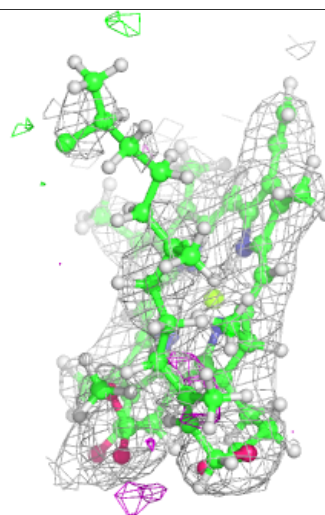
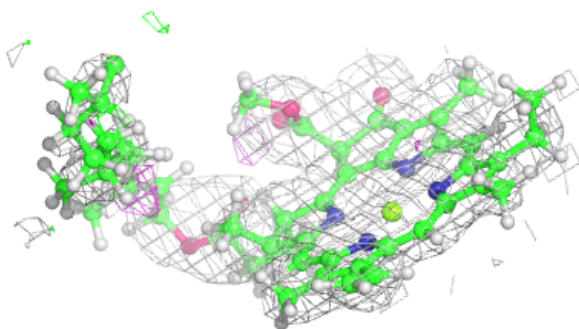
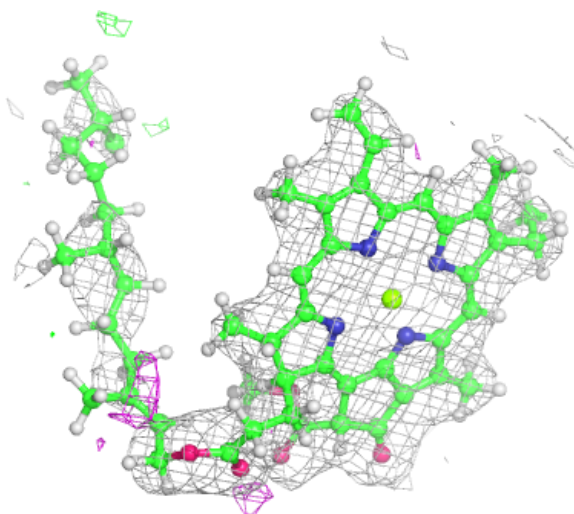
Electron density around CLA b 615:

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



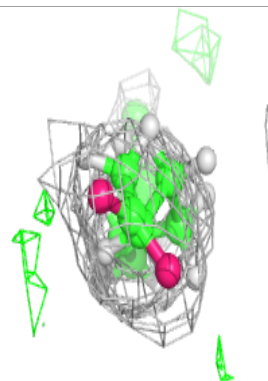
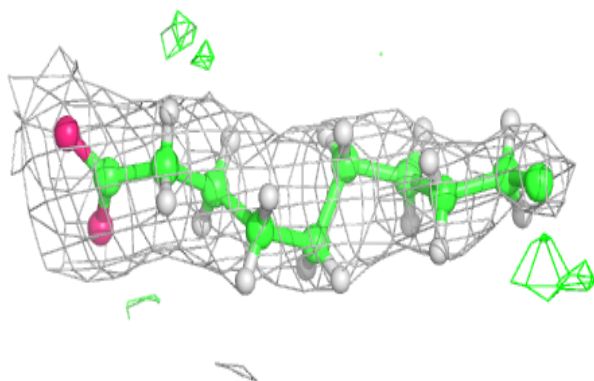
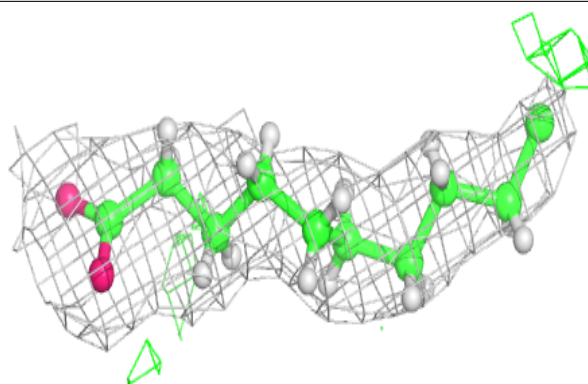
Electron density around CLA b 616:

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

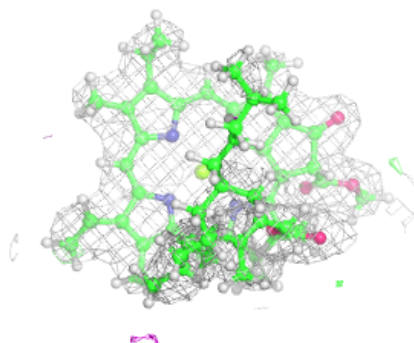
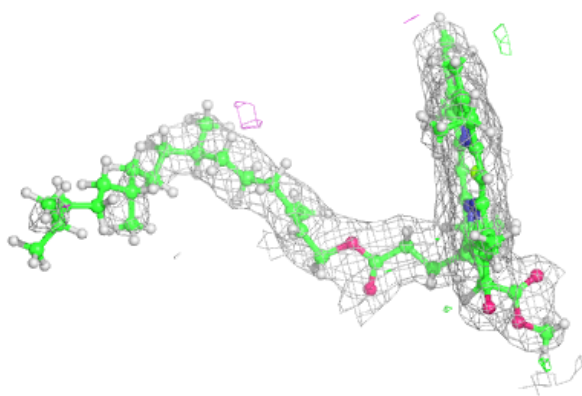
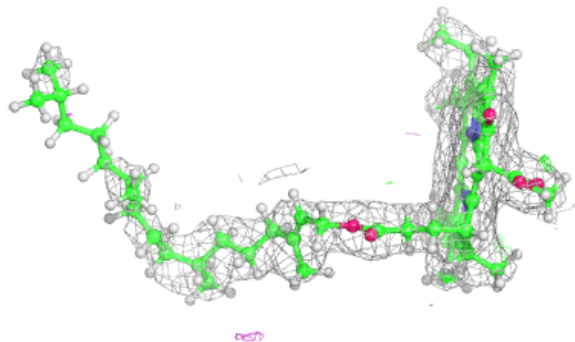


Electron density around STE J 101:

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

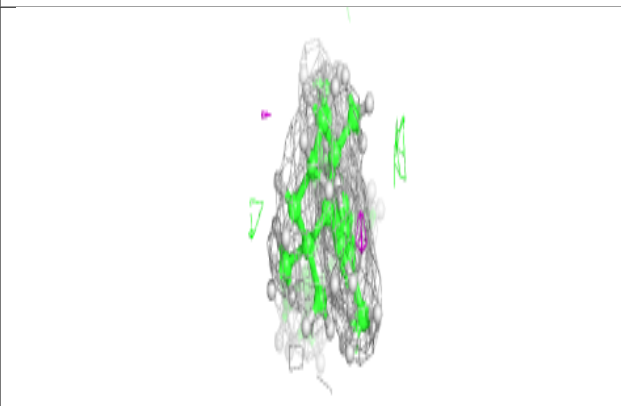
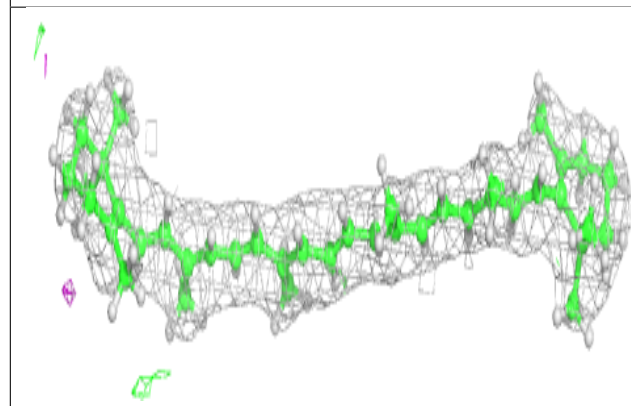
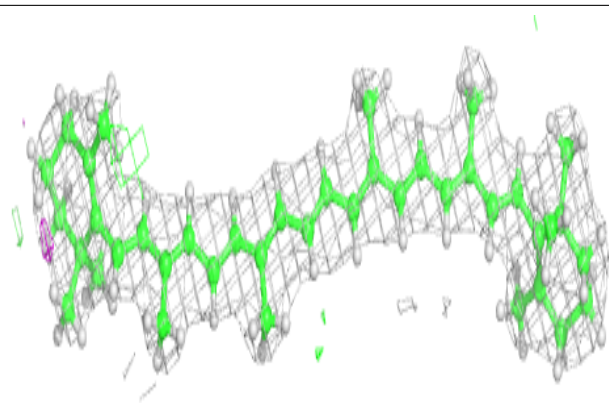
**Electron density around CLA D 403:**

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

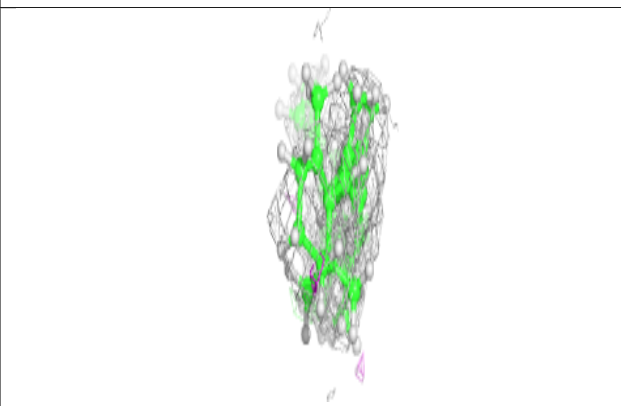
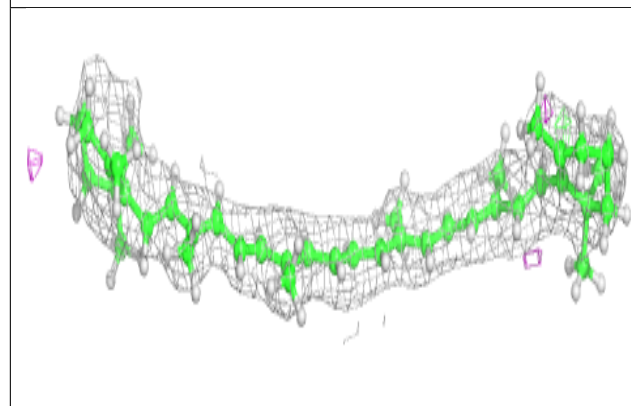
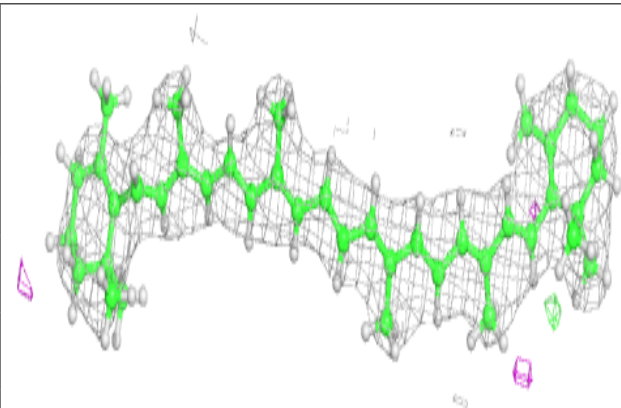


Electron density around BCR B 619:

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

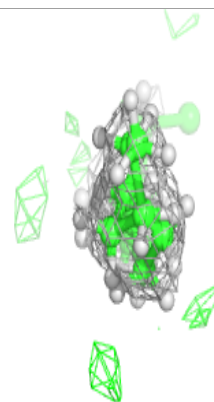
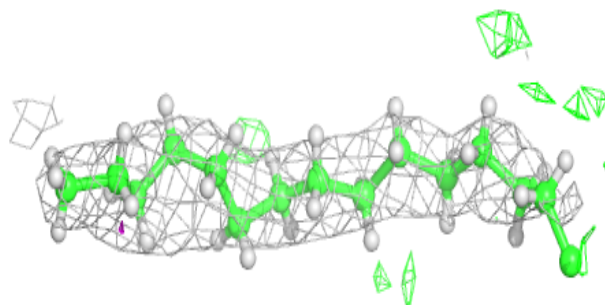
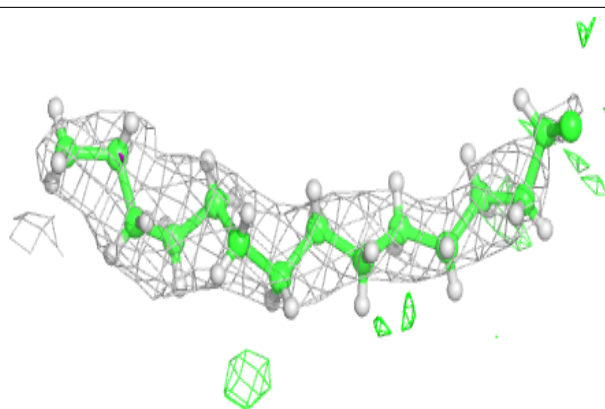
**Electron density around BCR D 404:**

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

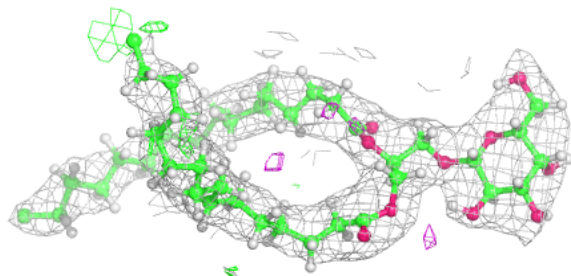
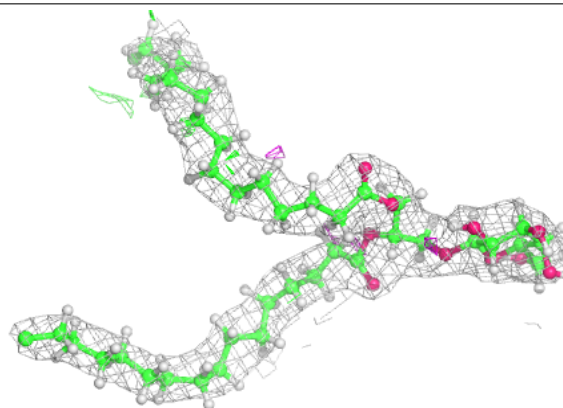


Electron density around STE T 102:

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

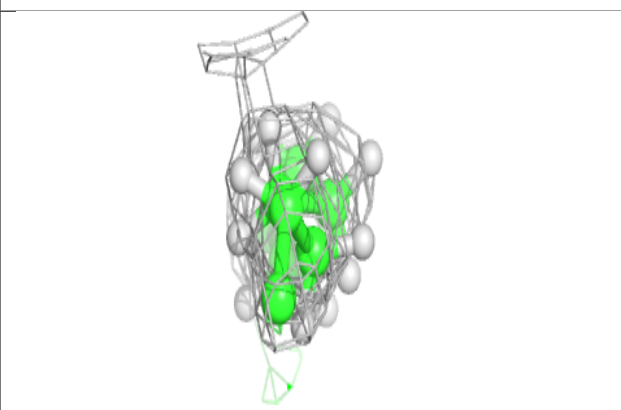
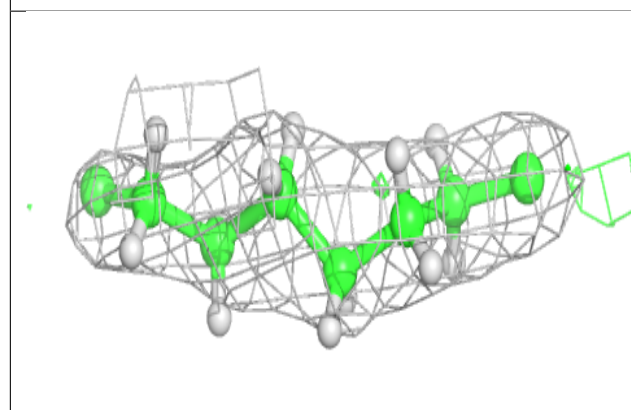
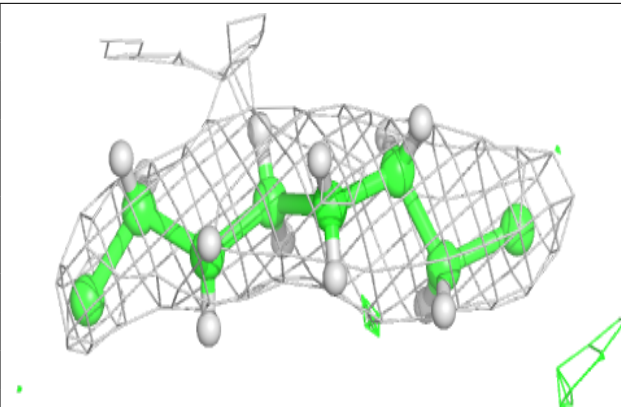
**Electron density around LMG M 101:**

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

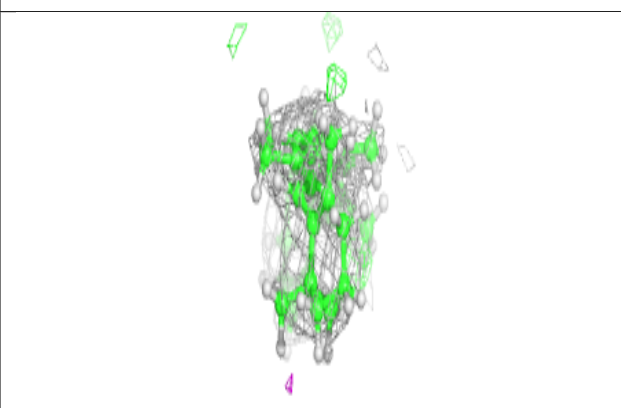
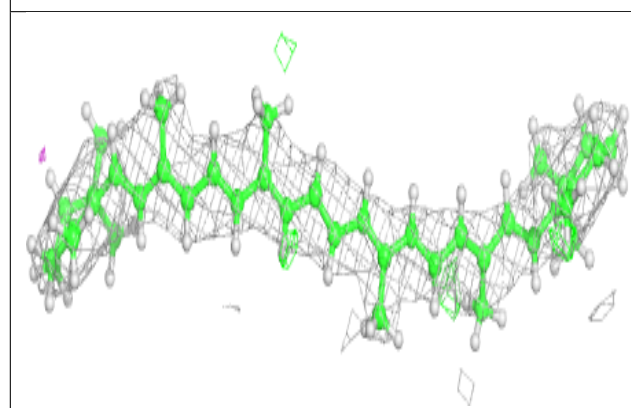
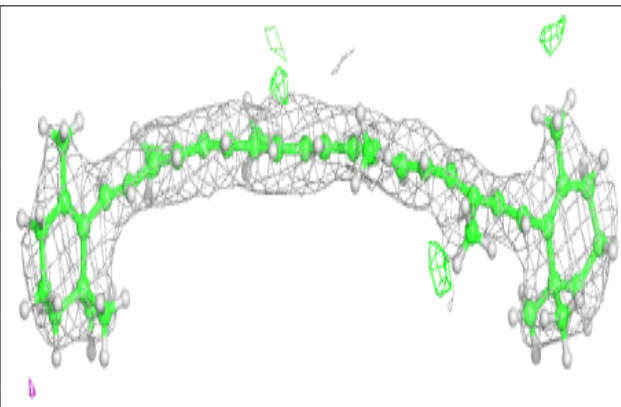


Electron density around STE Z 101:

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

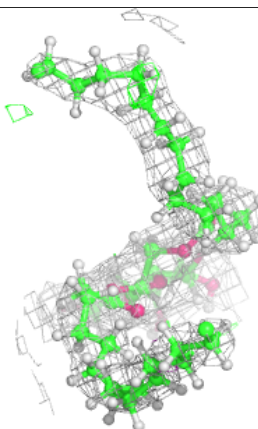
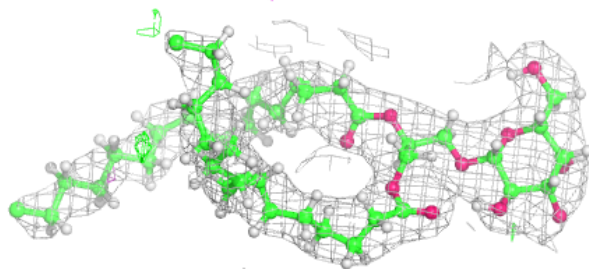
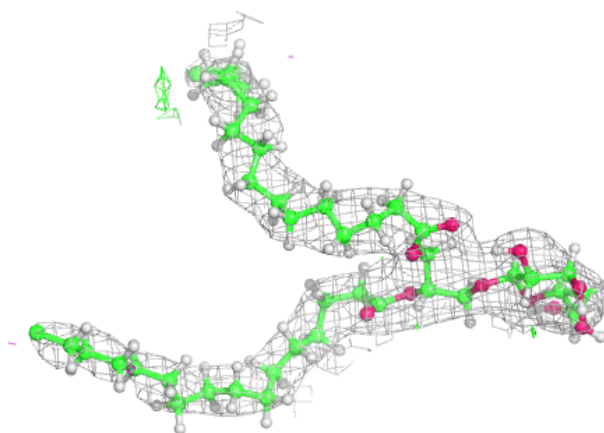
**Electron density around BCR k 102:**

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

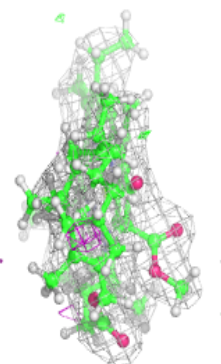
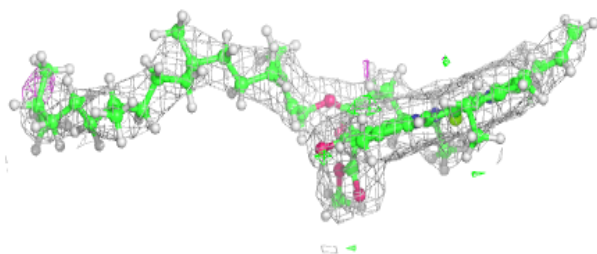
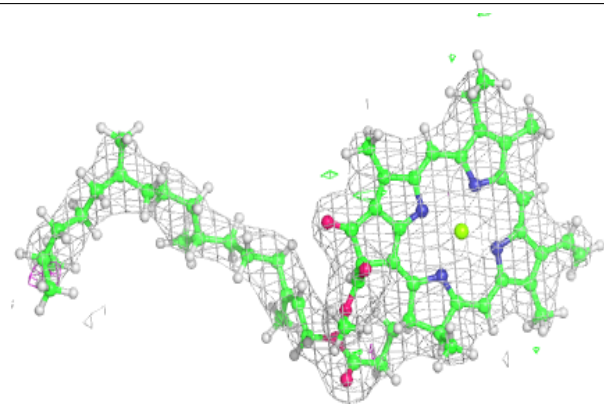


Electron density around LMG b 622:

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

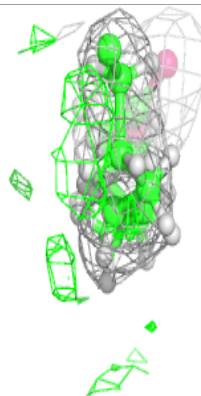
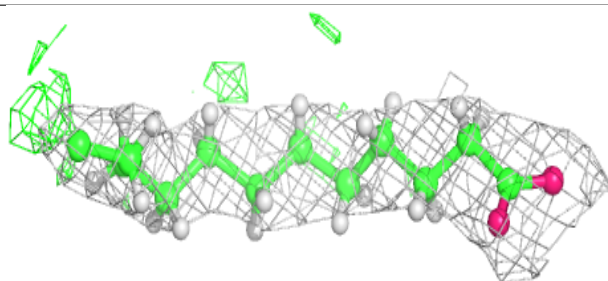
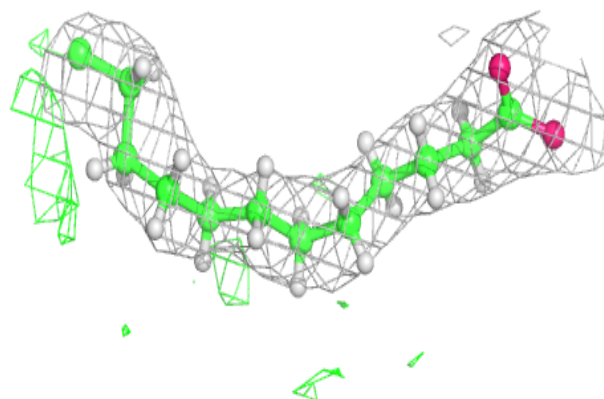
**Electron density around CLA b 602:**

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

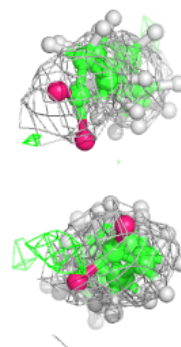
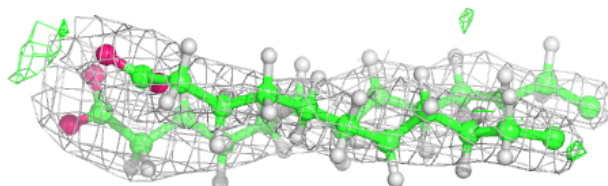
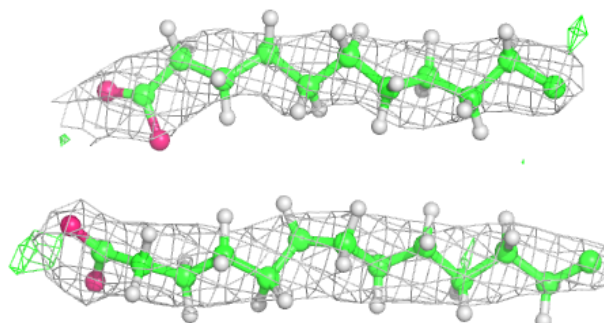


Electron density around STE t 102:

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

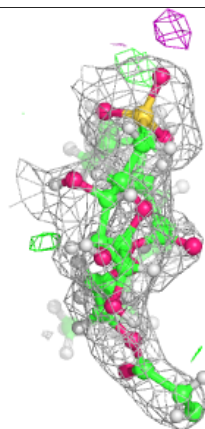
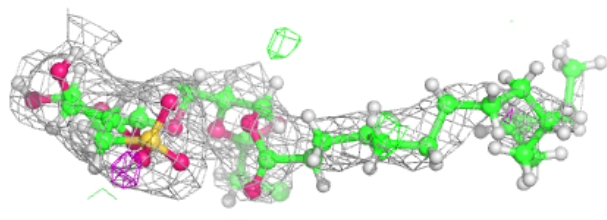
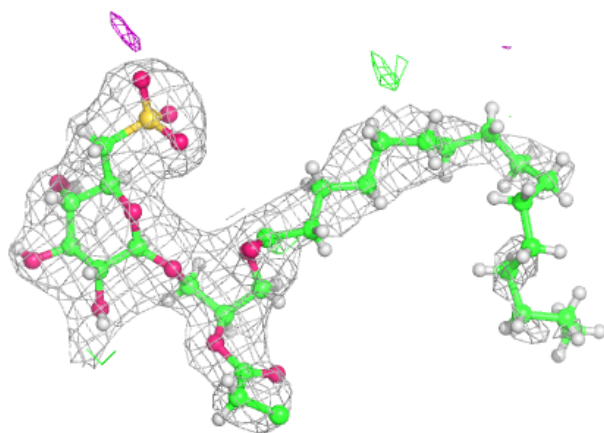
**Electron density around LMG D 411:**

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



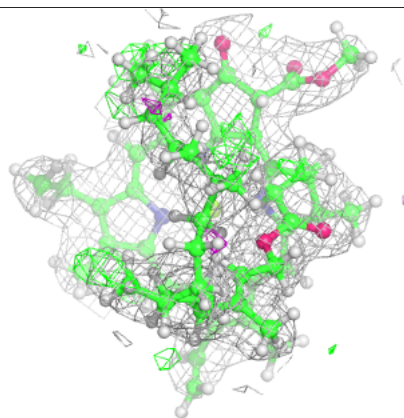
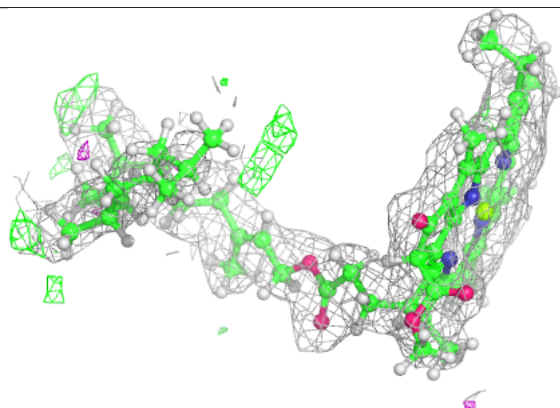
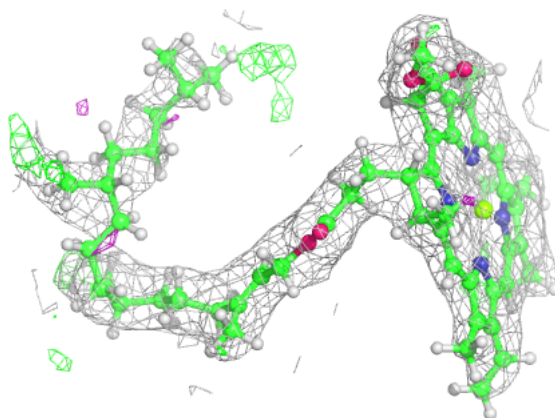
Electron density around SQD f 101:

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



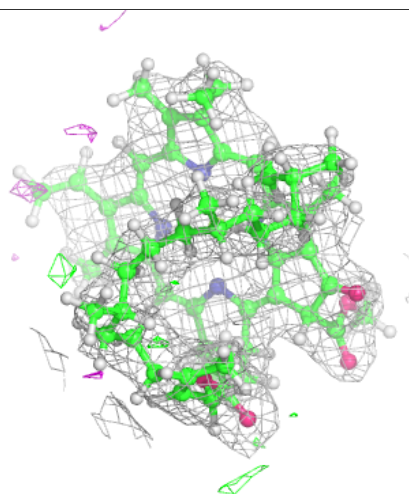
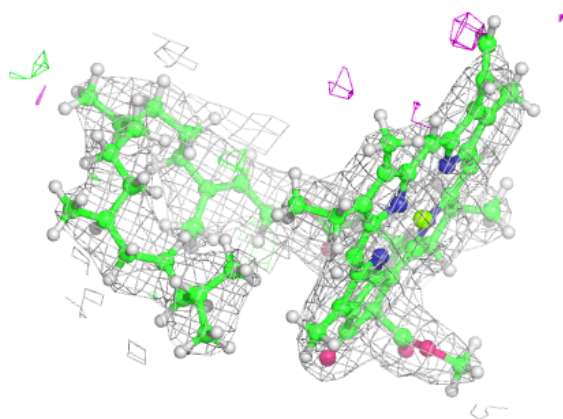
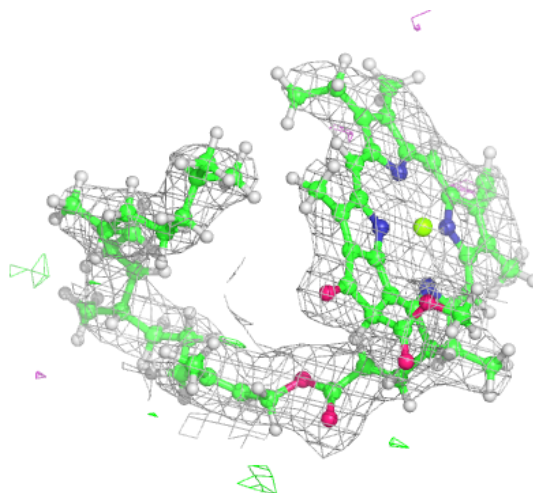
Electron density around CLA B 606:

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



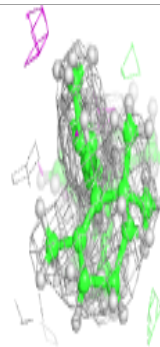
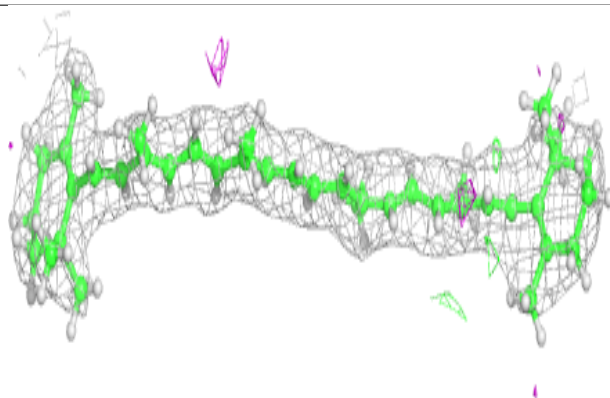
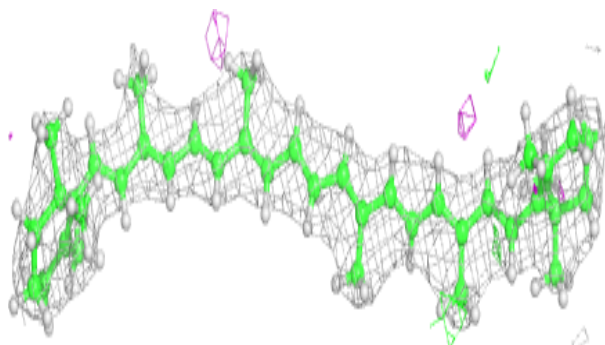
Electron density around CLA c 503:

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

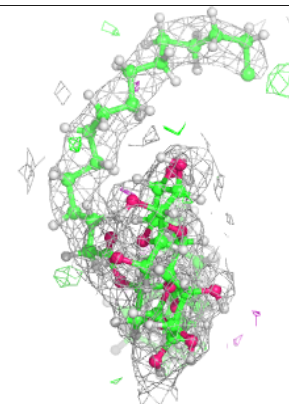
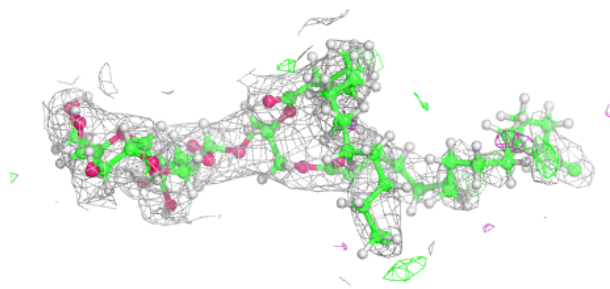
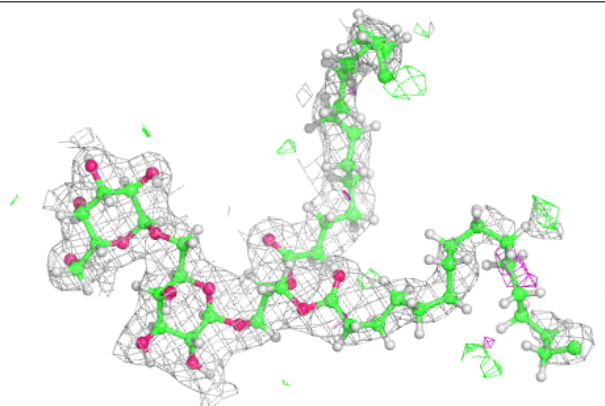


Electron density around BCR C 514:

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

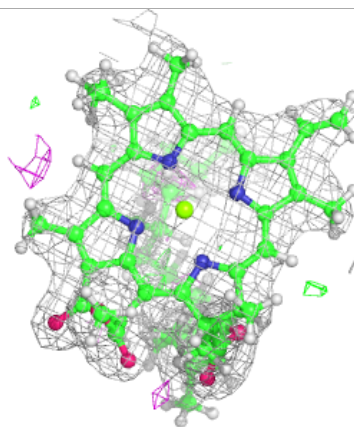
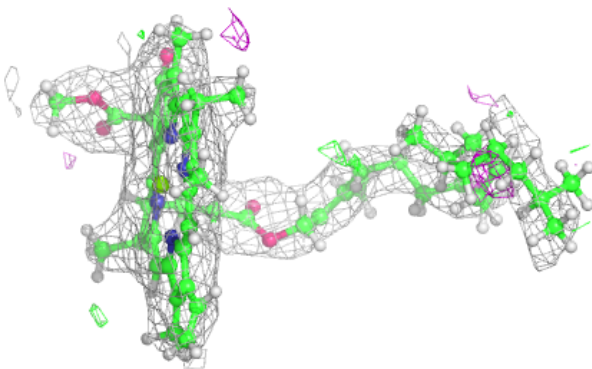
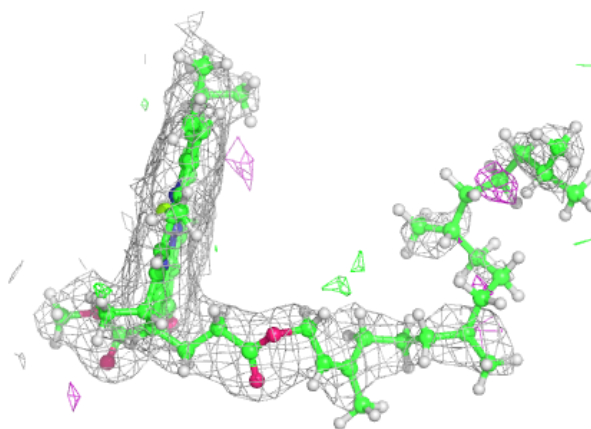
**Electron density around DGD C 516:**

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



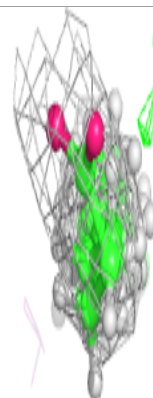
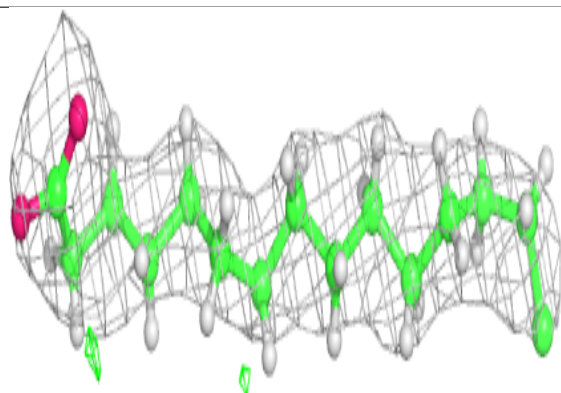
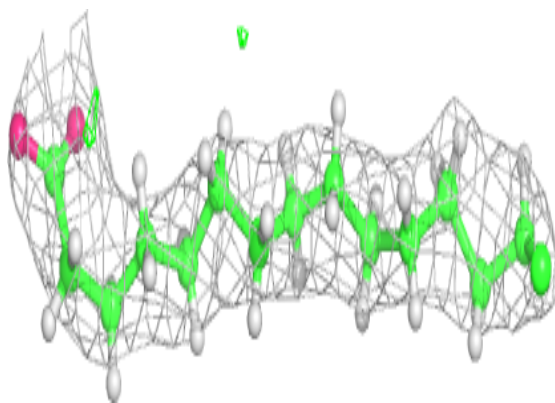
Electron density around CLA c 506:

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

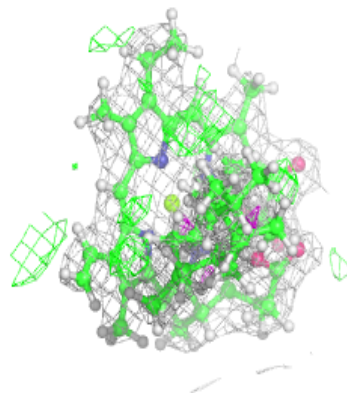
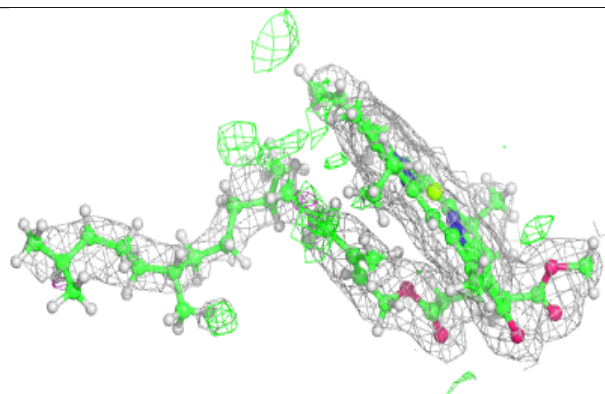
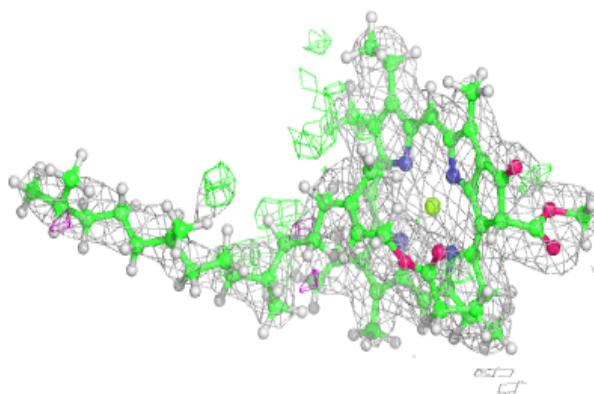


Electron density around STE d 411:

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

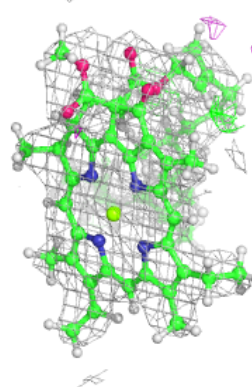
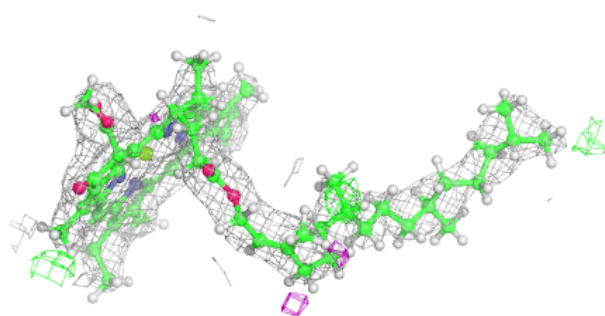
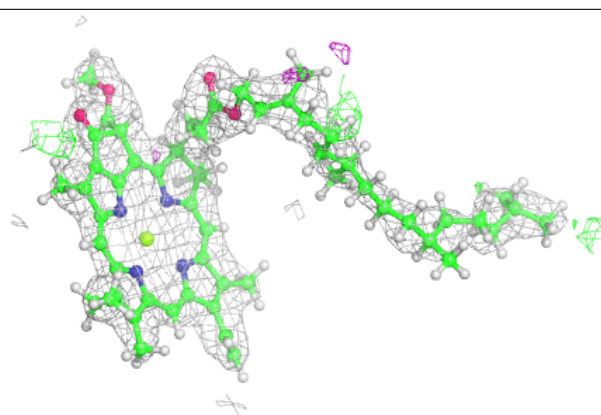
**Electron density around CLA C 505:**

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

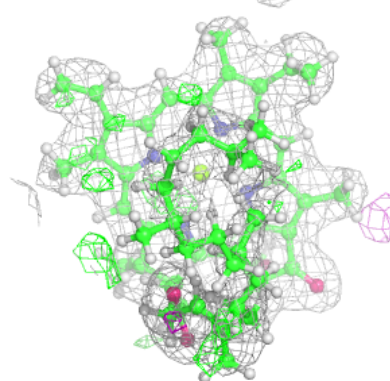
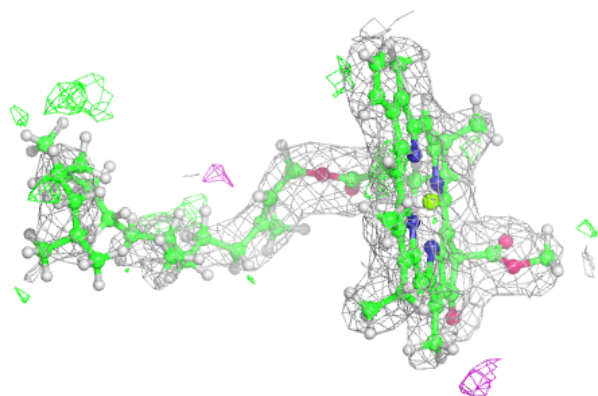
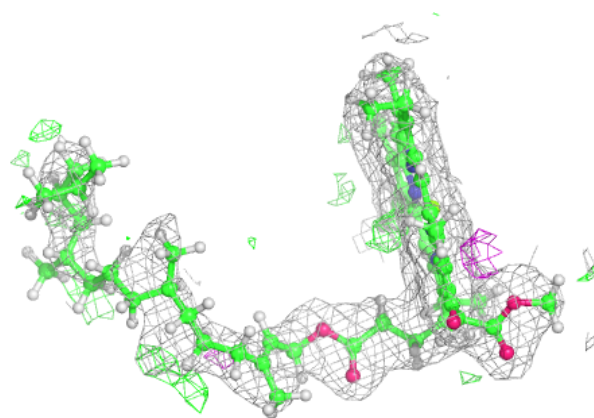


Electron density around CLA c 511:

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

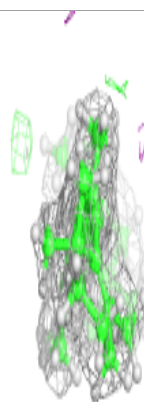
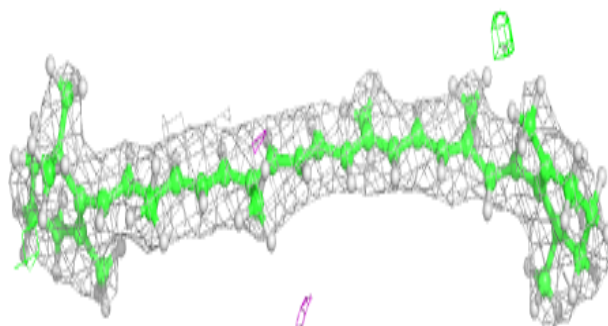
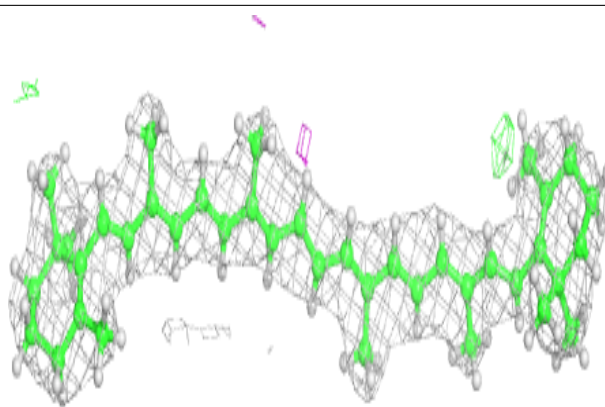
**Electron density around CLA C 506:**

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

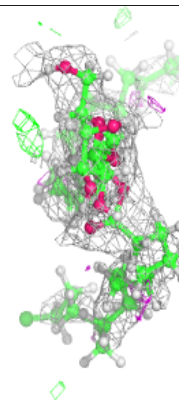
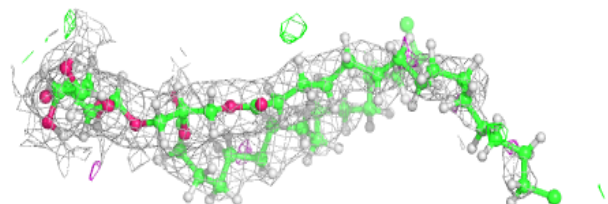
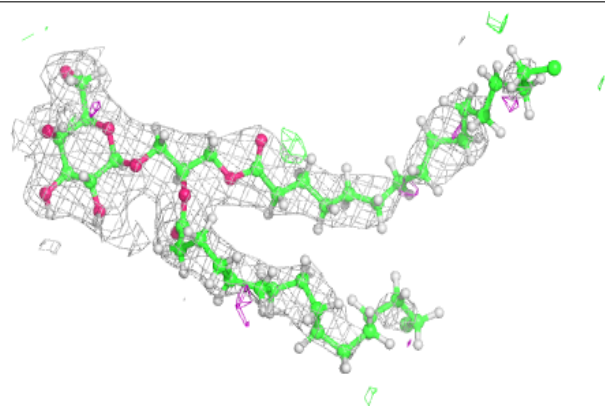


Electron density around BCR b 619:

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

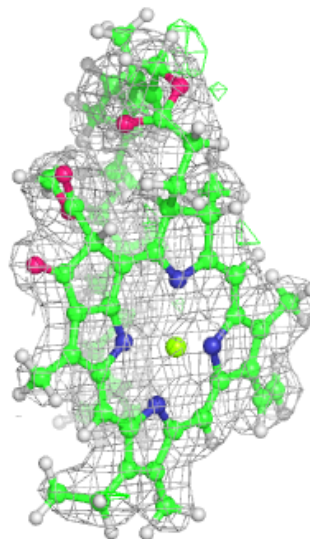
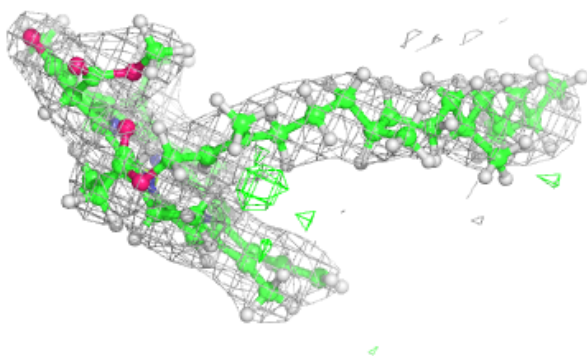
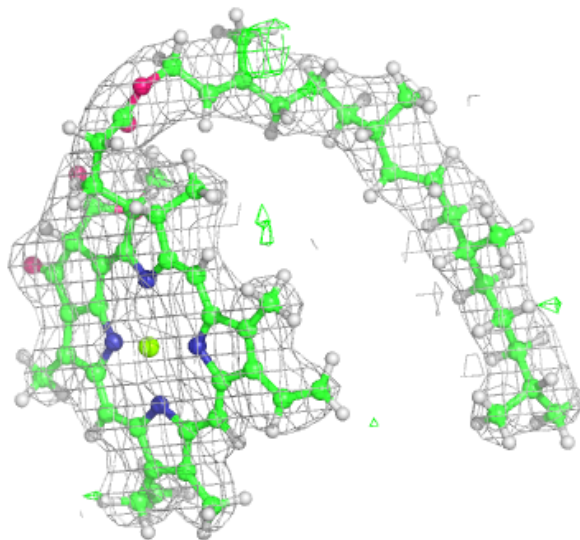
**Electron density around LMG D 406:**

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



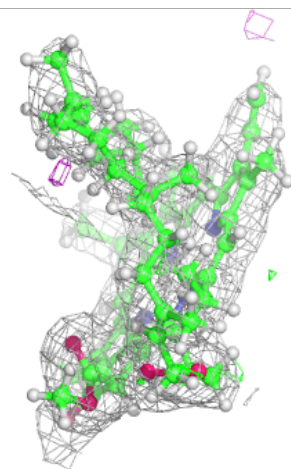
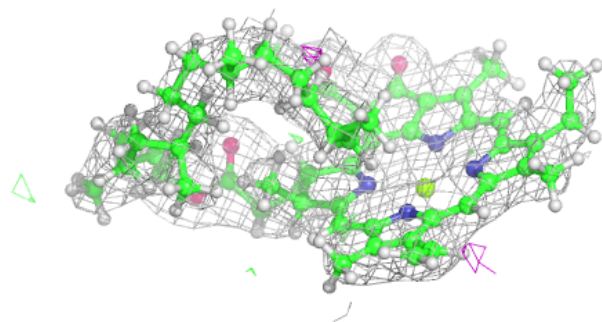
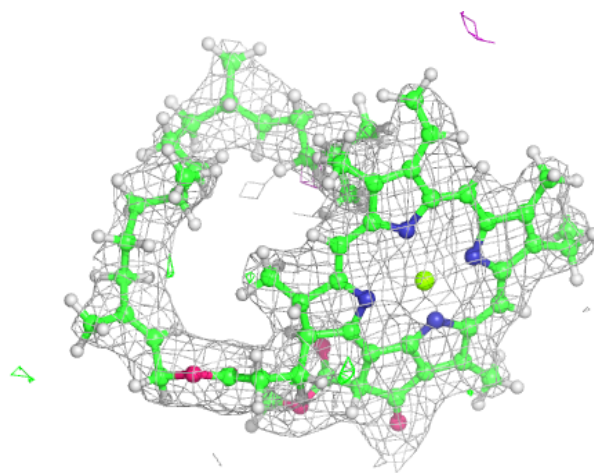
Electron density around CLA C 507:

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



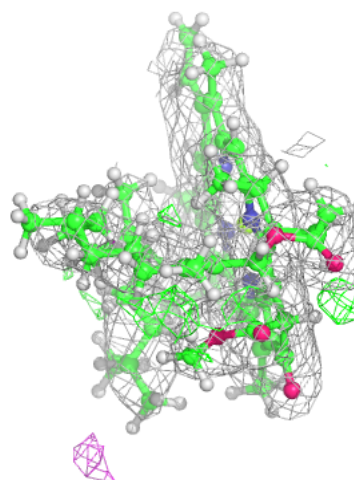
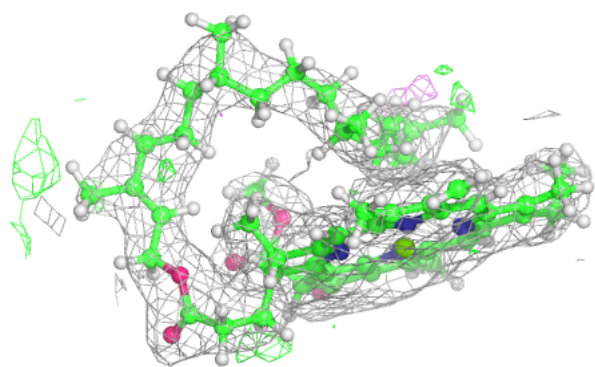
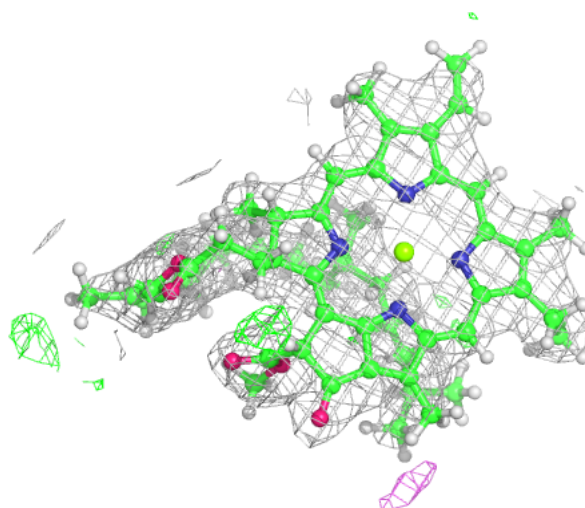
Electron density around CLA B 615:

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



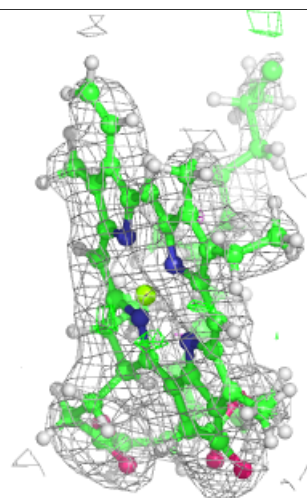
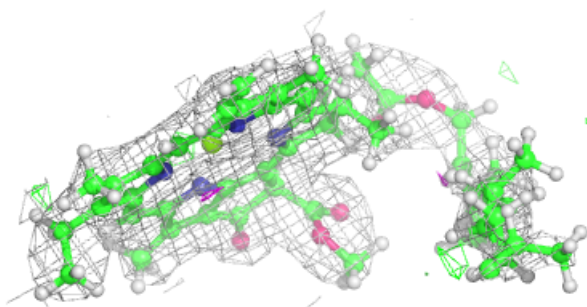
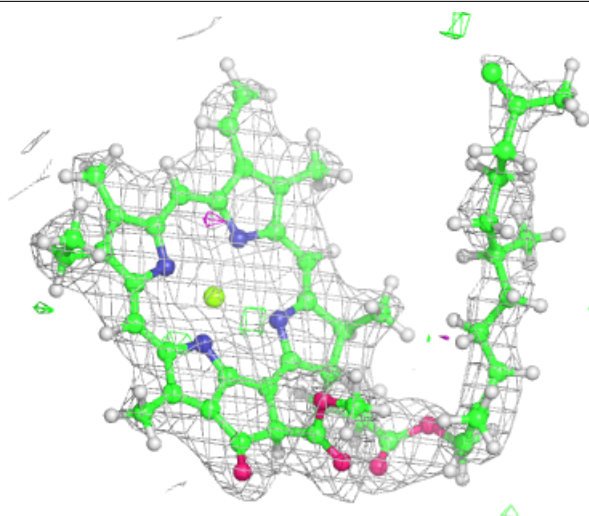
Electron density around CLA c 510:

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



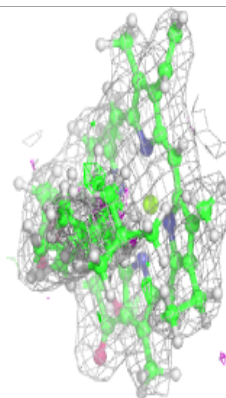
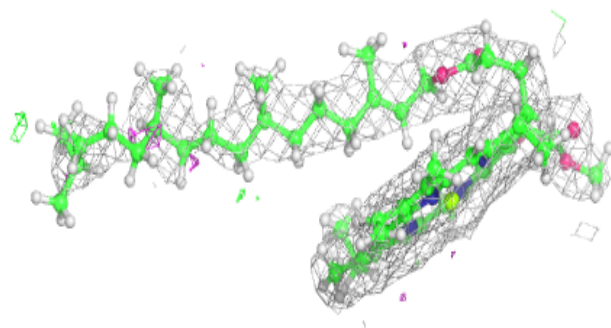
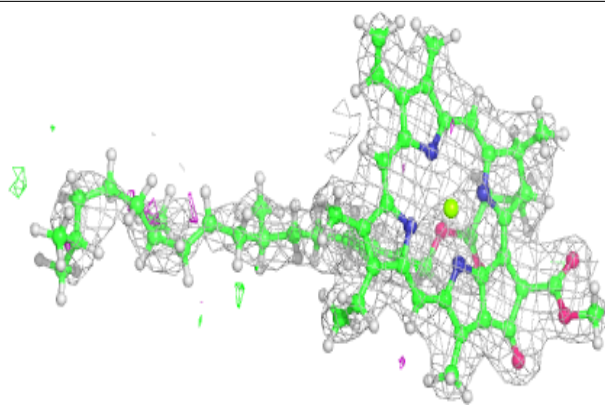
Electron density around CLA B 616:

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

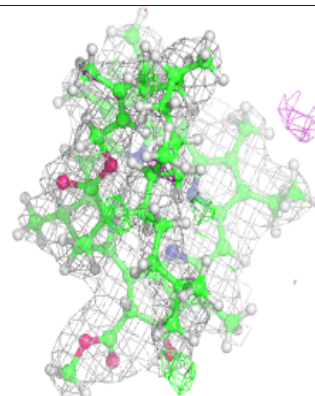
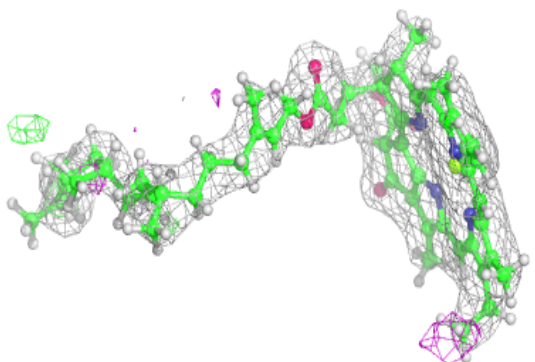
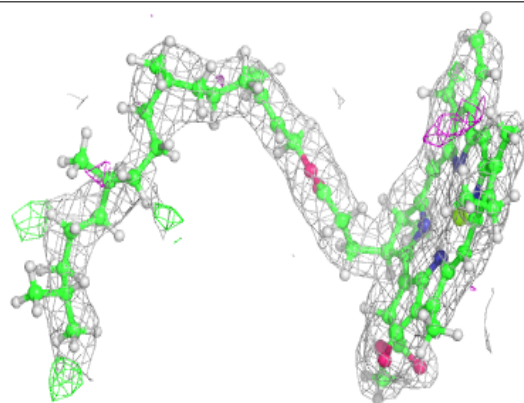


Electron density around CLA B 614:

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

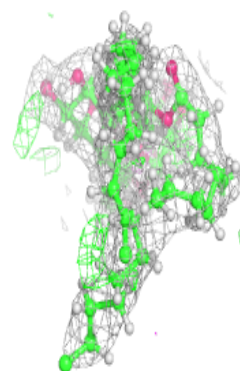
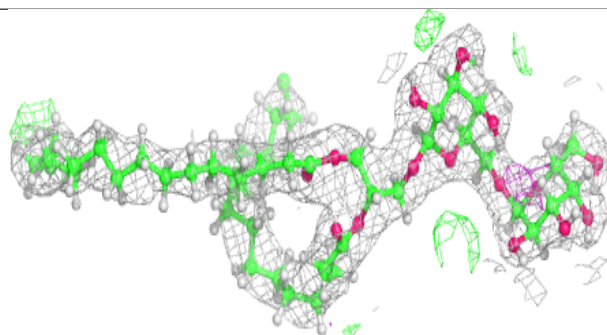
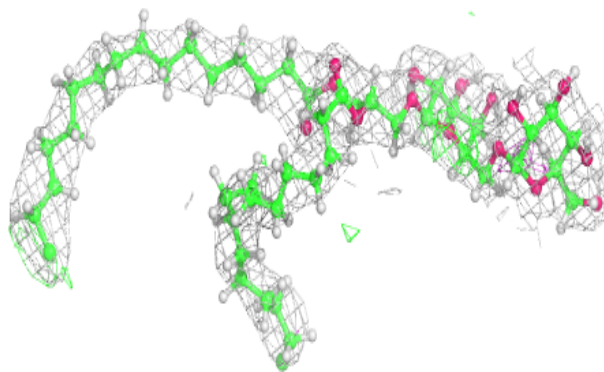
**Electron density around CLA b 606:**

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

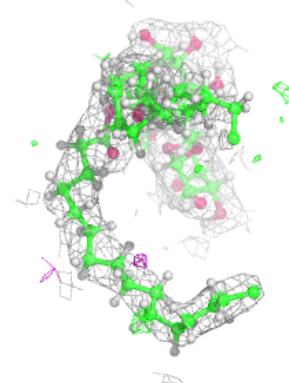
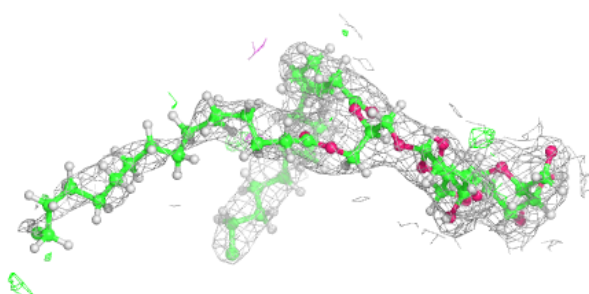
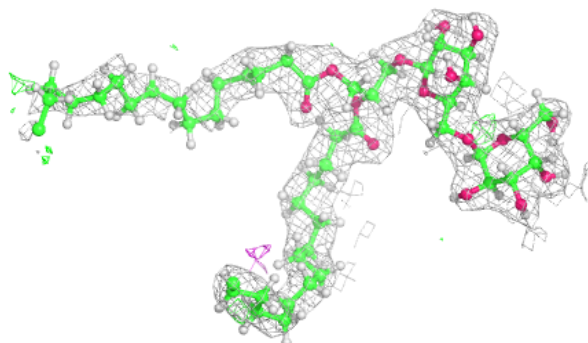


Electron density around DGD H 102:

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

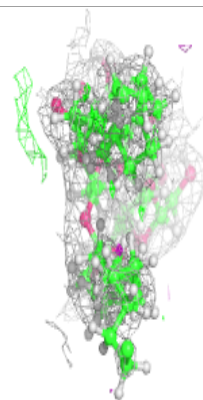
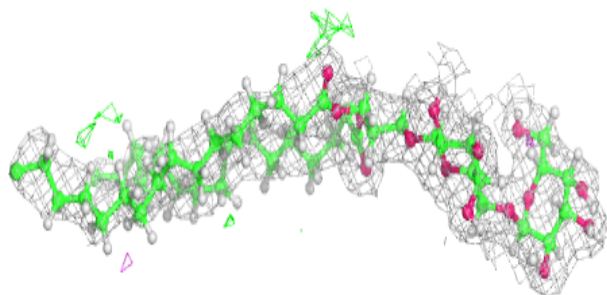
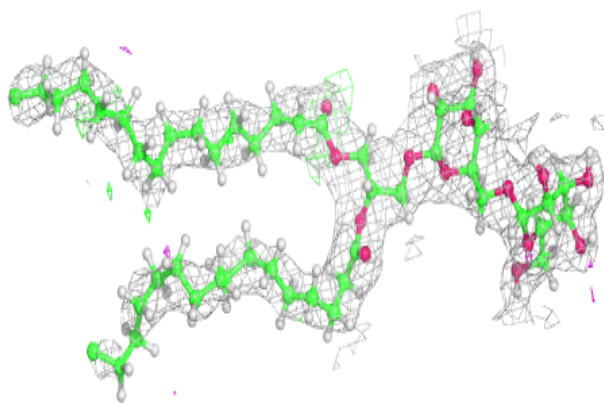
**Electron density around DGD c 517:**

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

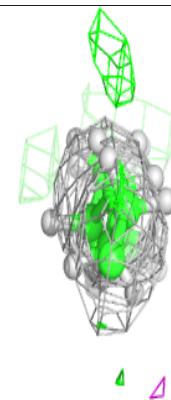
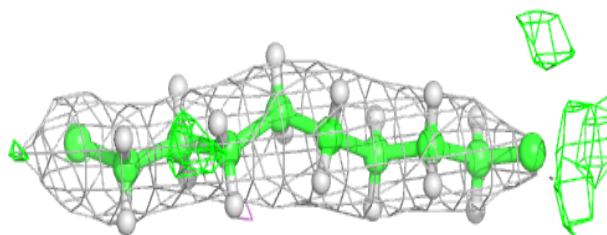
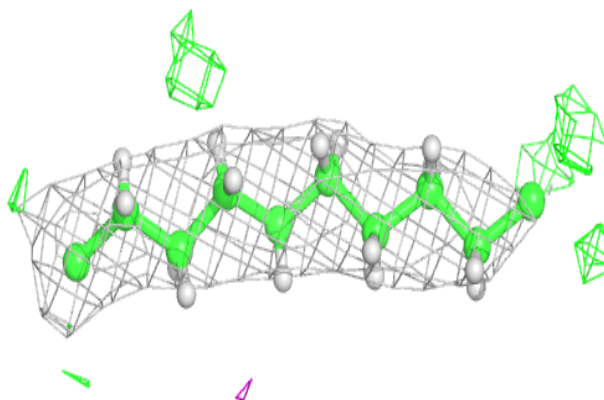


Electron density around DGD c 518:

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

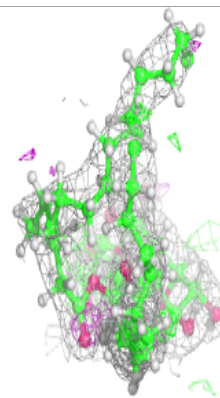
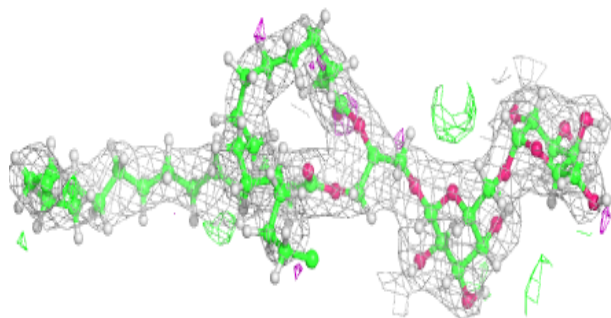
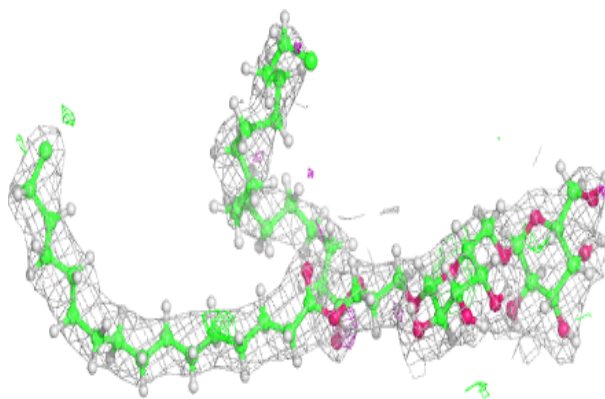
**Electron density around STE M 103:**

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

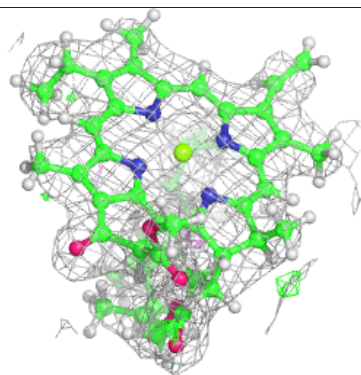
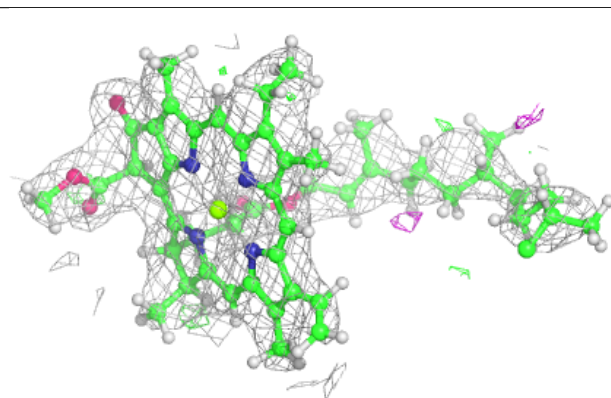
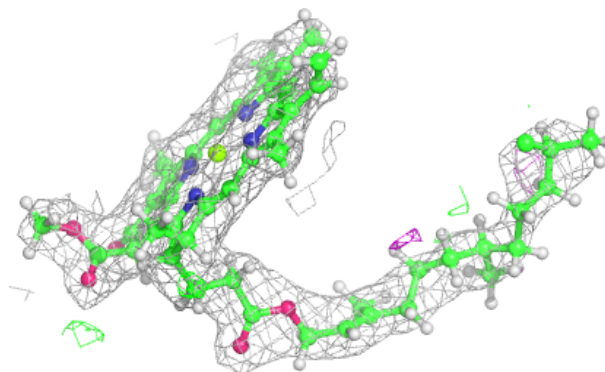


Electron density around DGD h 101:

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

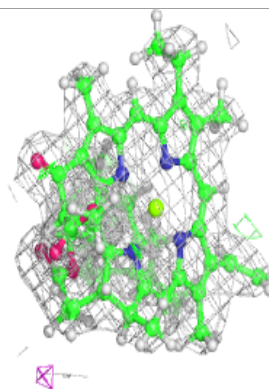
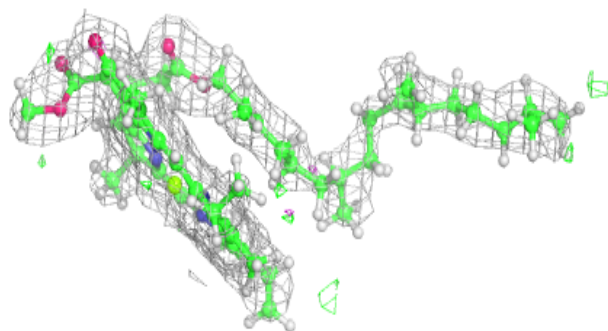
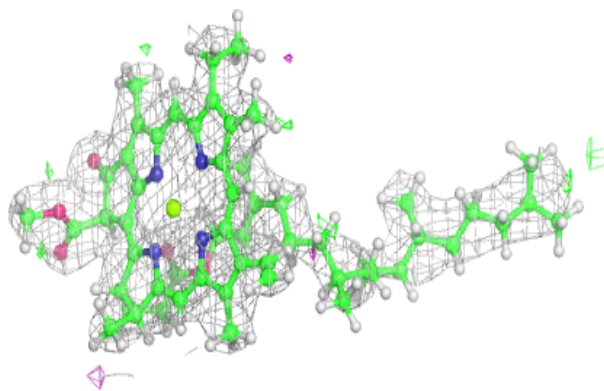
**Electron density around CLA c 504:**

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



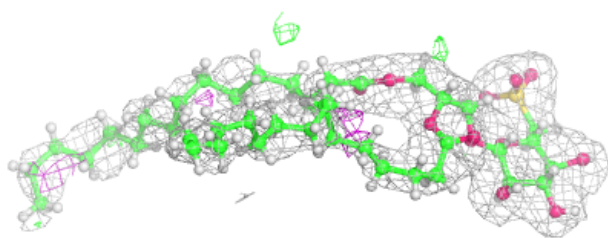
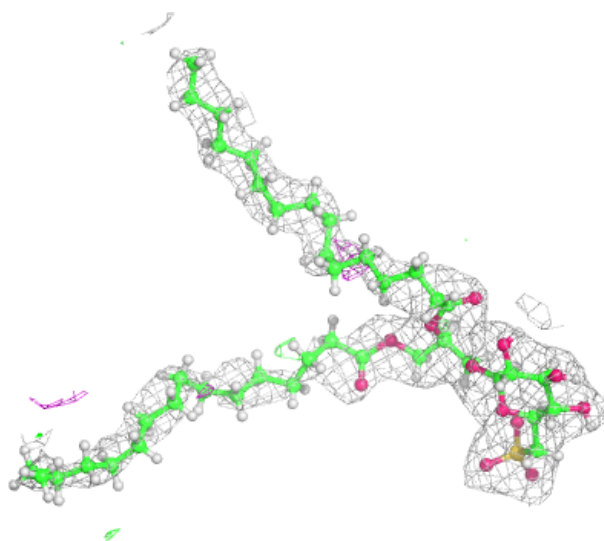
Electron density around CLA c 505:

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



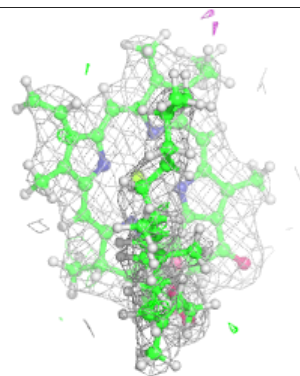
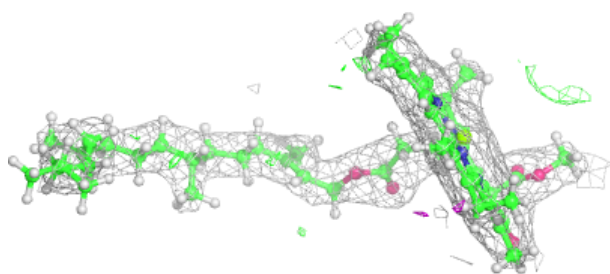
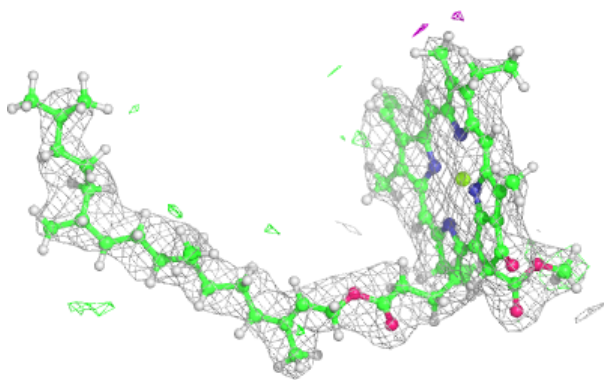
Electron density around SQD a 411:

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



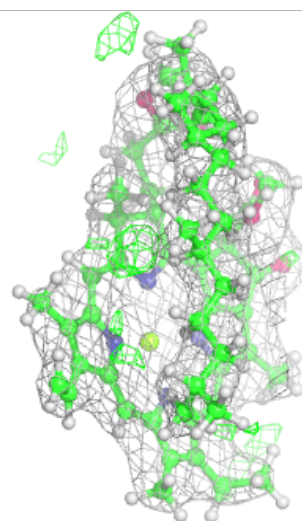
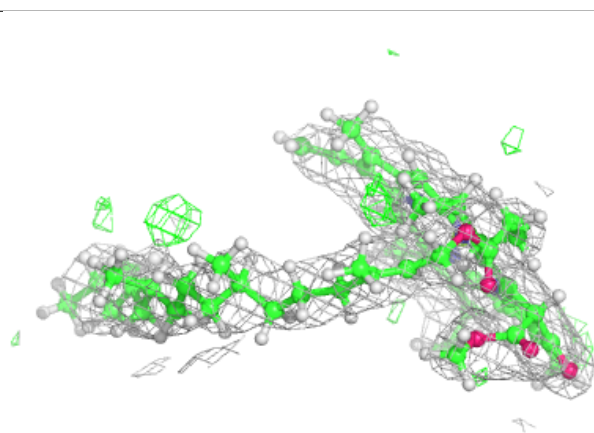
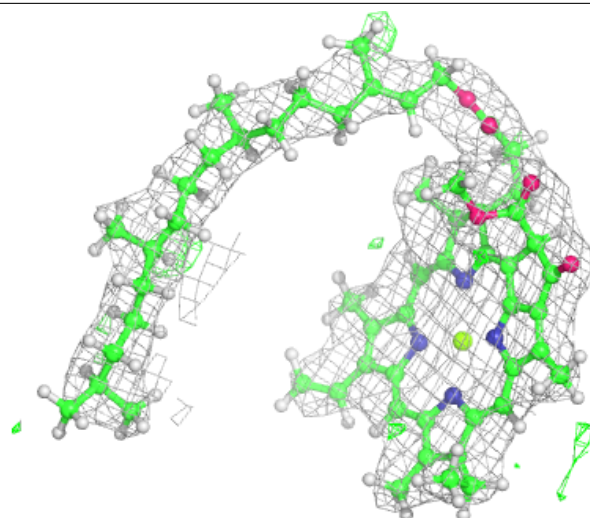
Electron density around CLA b 609:

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



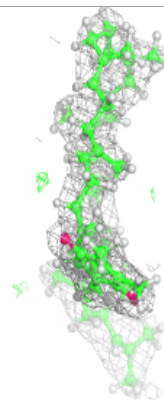
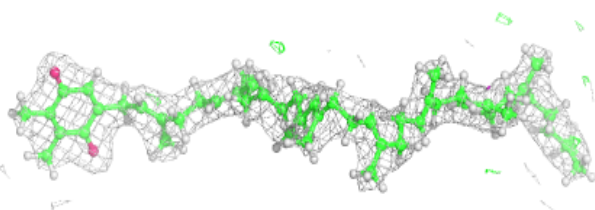
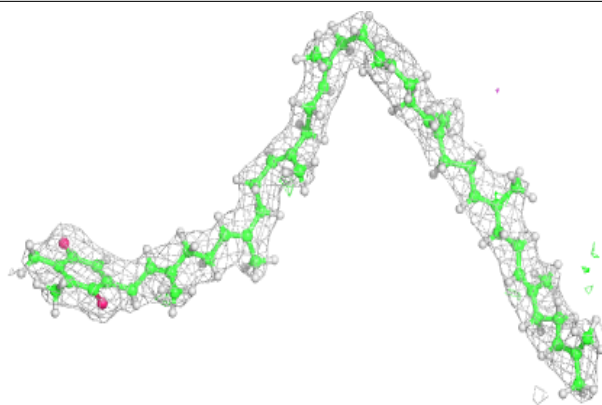
Electron density around CLA c 507:

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

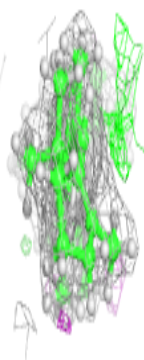
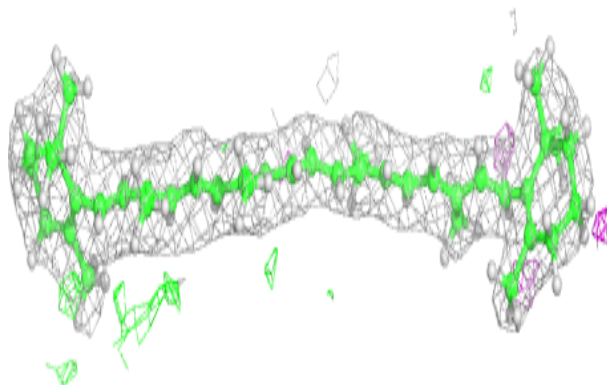
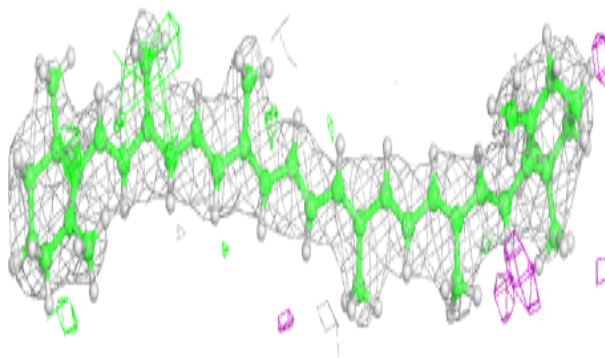


Electron density around PL9 D 405:

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

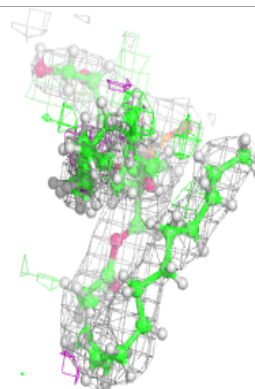
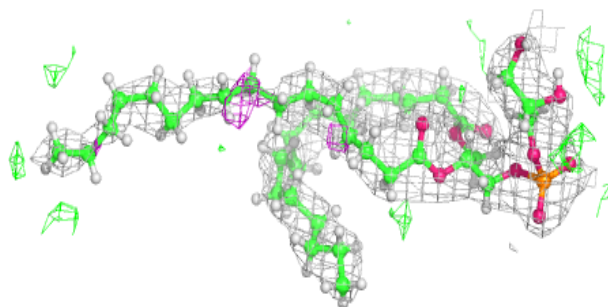
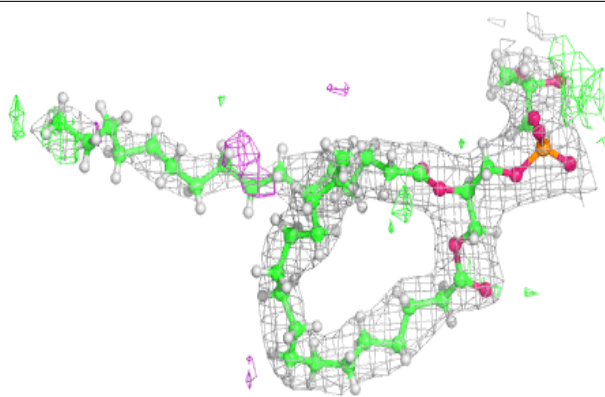
**Electron density around BCR B 618:**

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

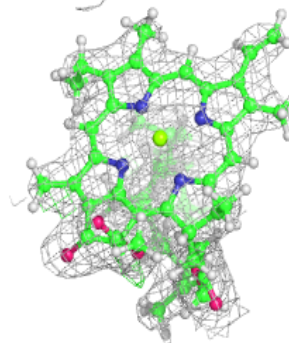
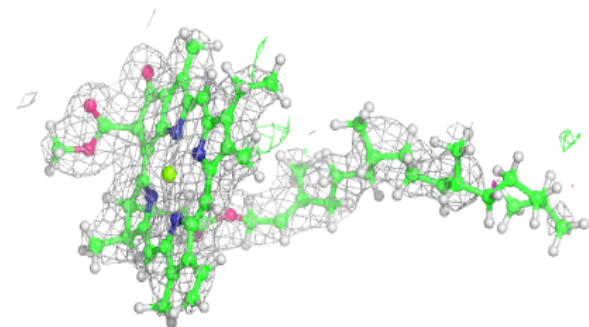
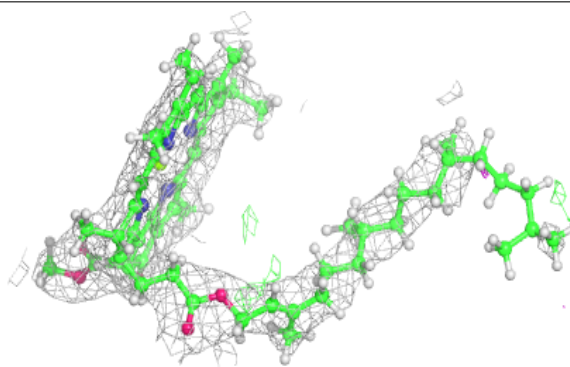


Electron density around LHG d 407:

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

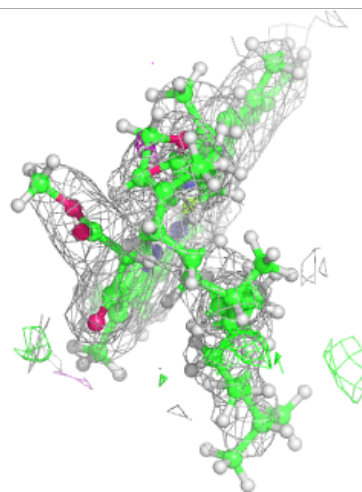
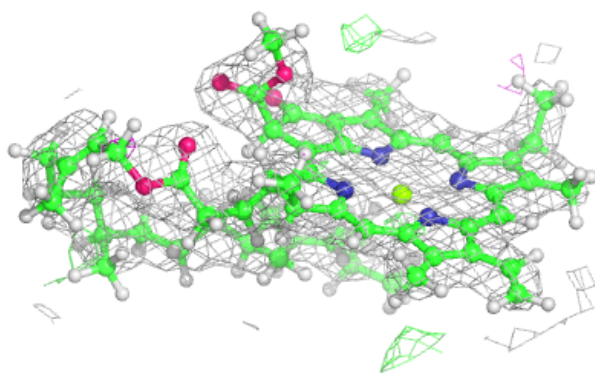
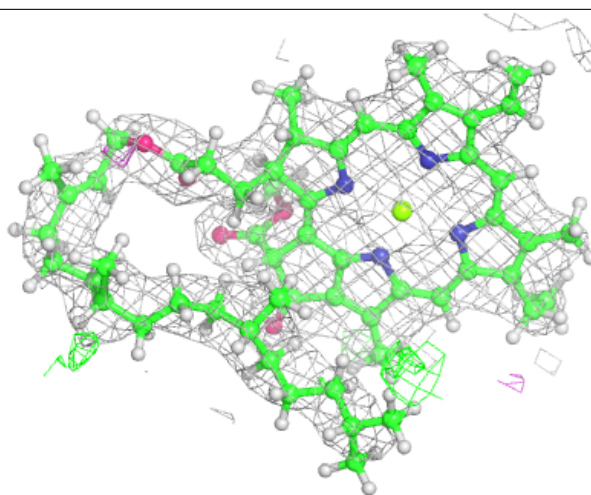
**Electron density around CLA C 508:**

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



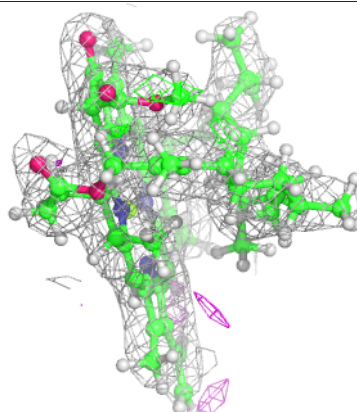
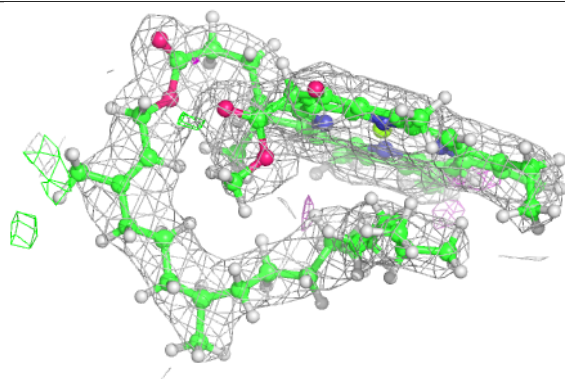
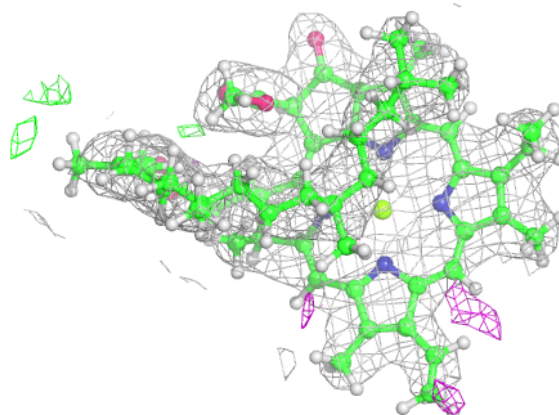
Electron density around CLA C 509:

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

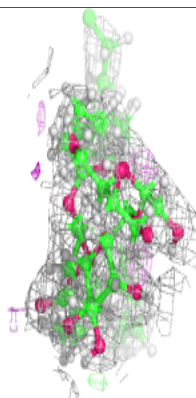
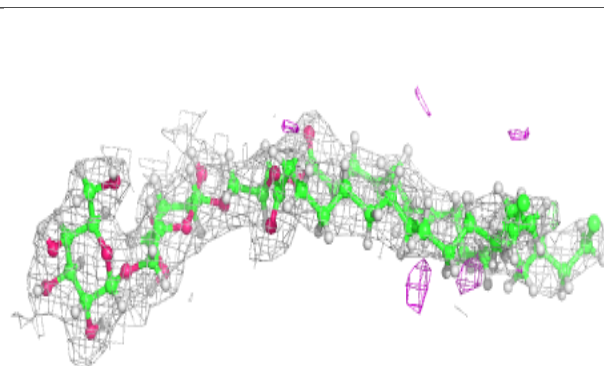
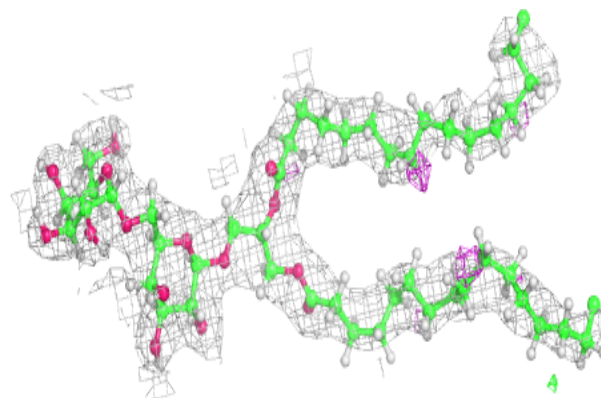


Electron density around CLA C 510:

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

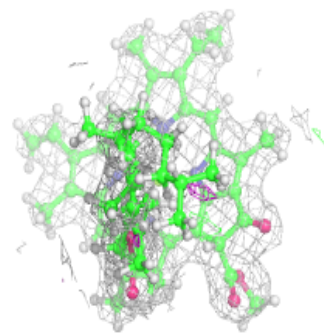
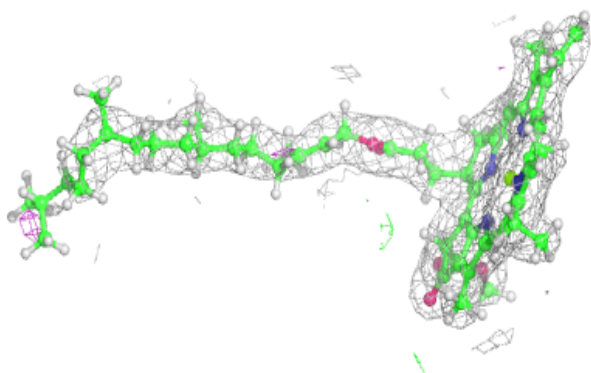
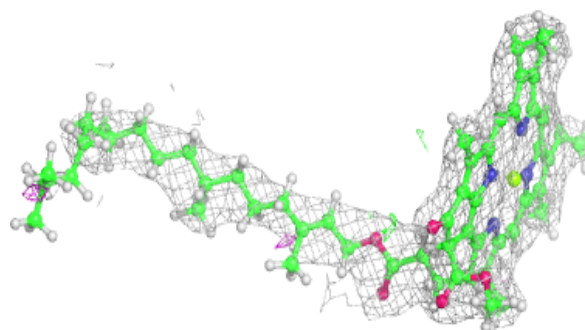
**Electron density around DGD C 517:**

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

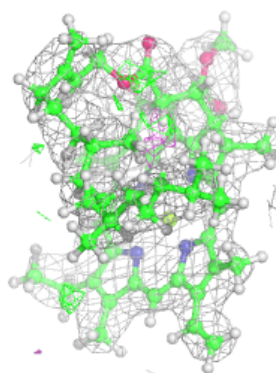
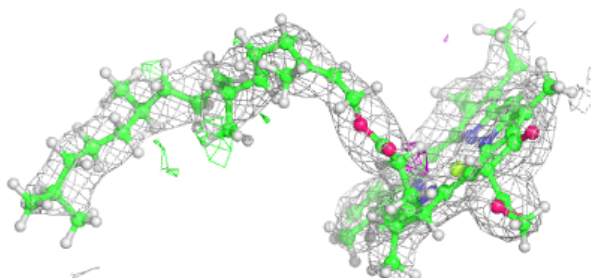
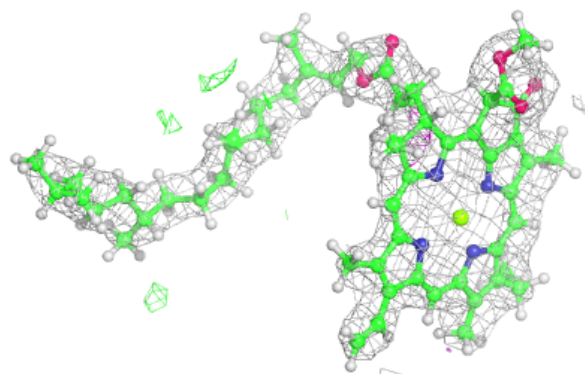


Electron density around CLA b 604:

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

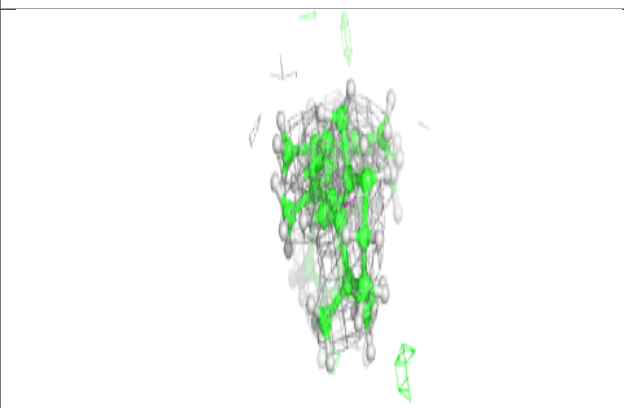
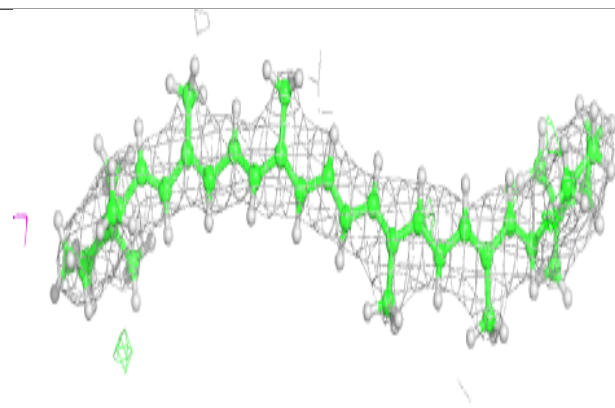
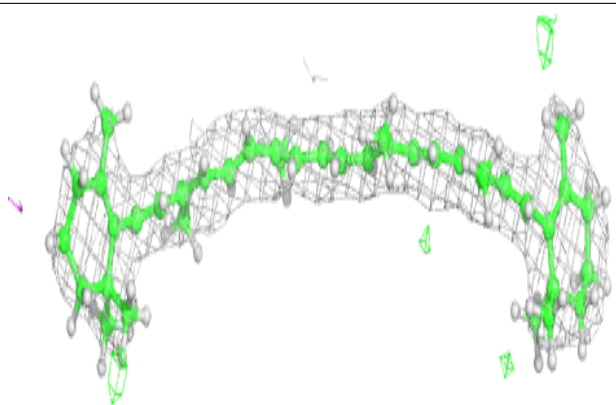
**Electron density around CLA C 511:**

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

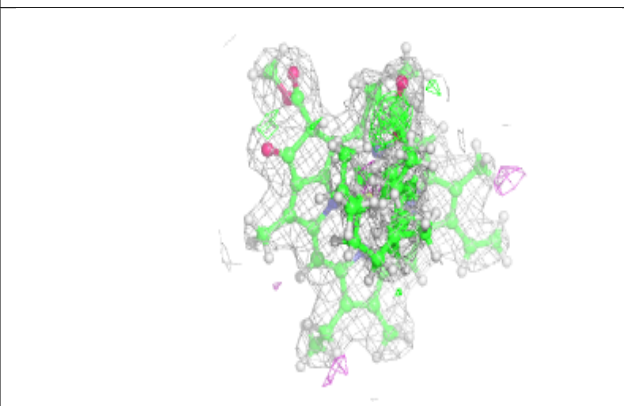
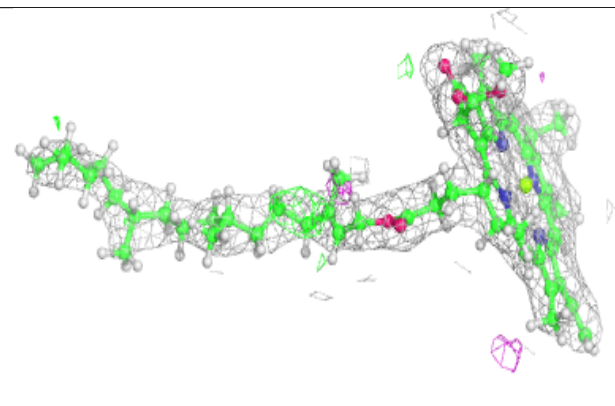
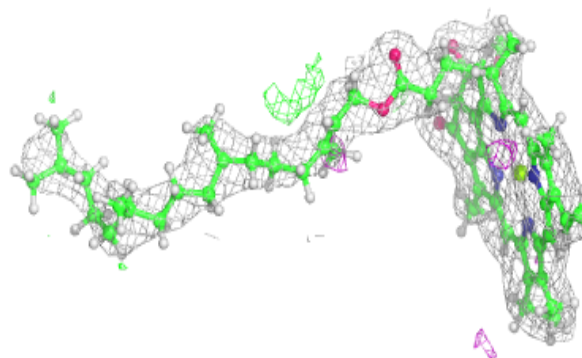


Electron density around BCR K 102:

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

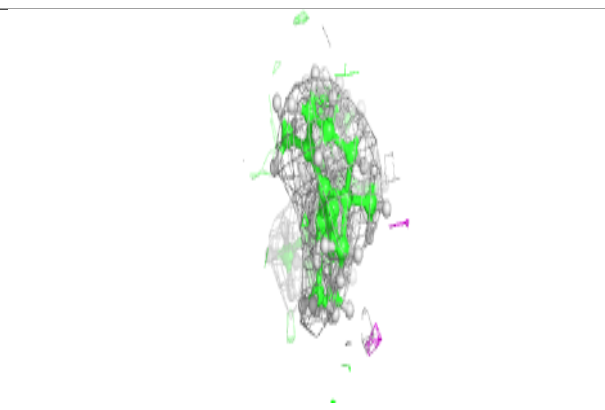
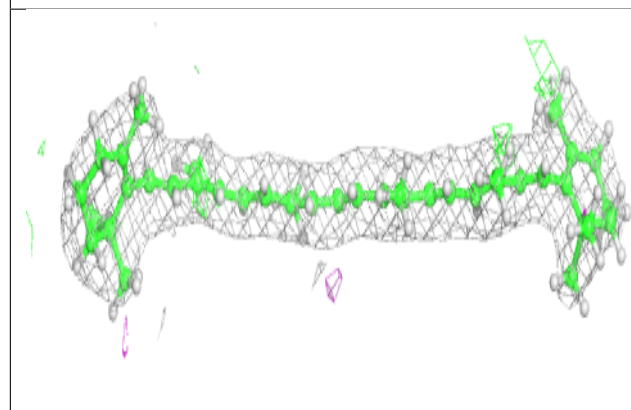
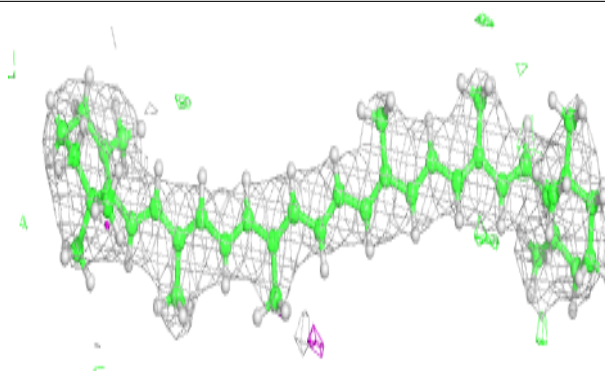
**Electron density around CLA B 604:**

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



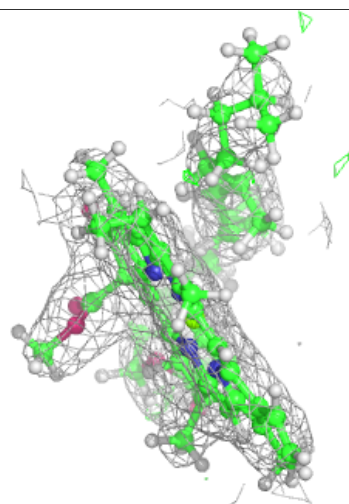
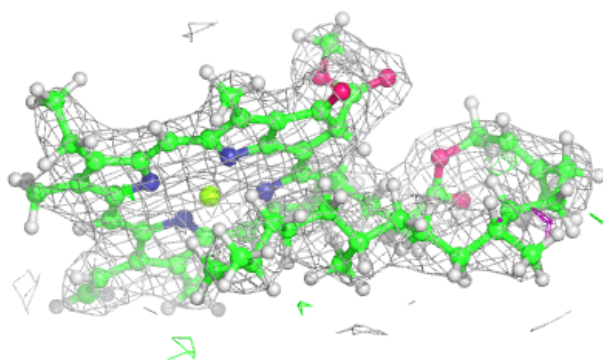
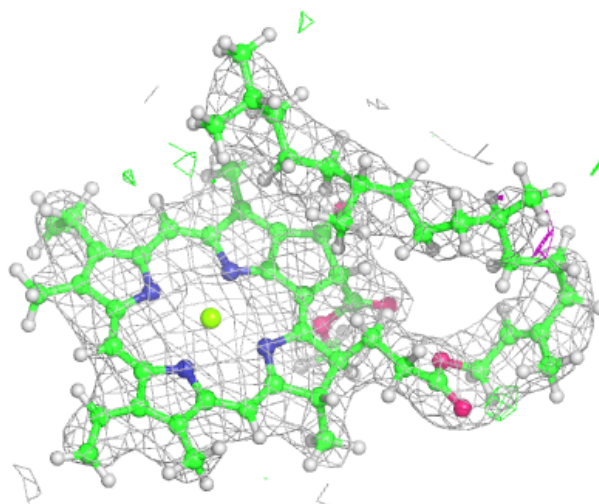
Electron density around BCR b 618:

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



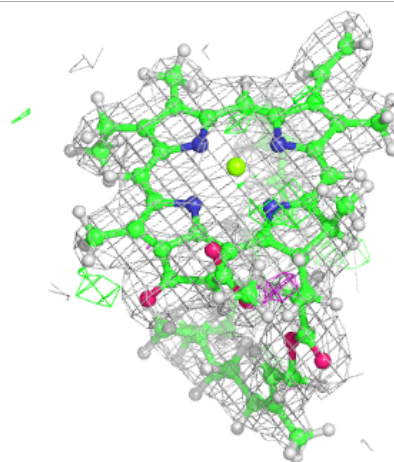
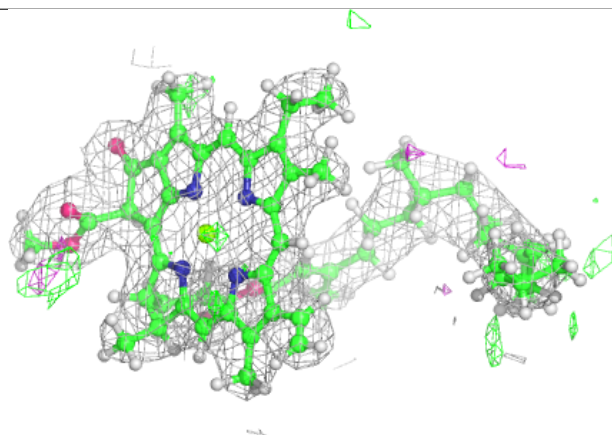
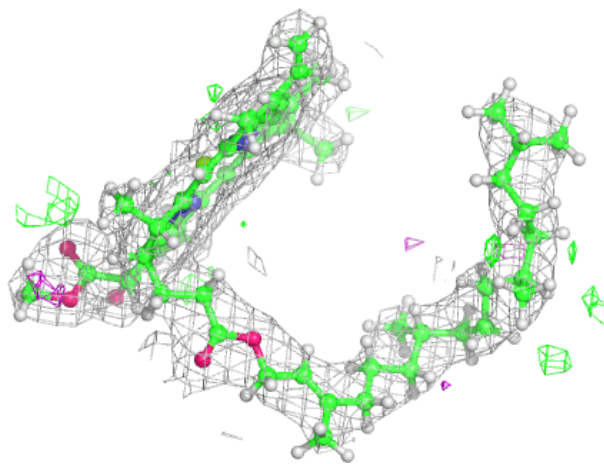
Electron density around CLA c 509:

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



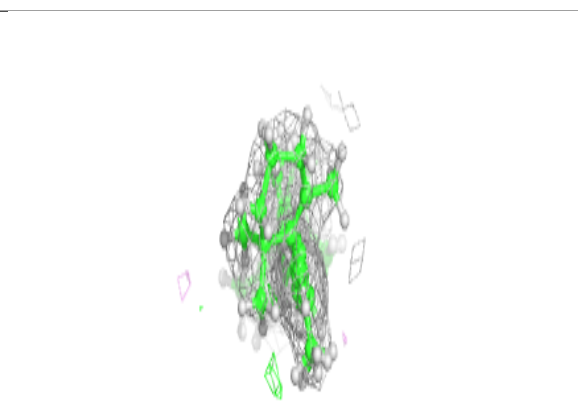
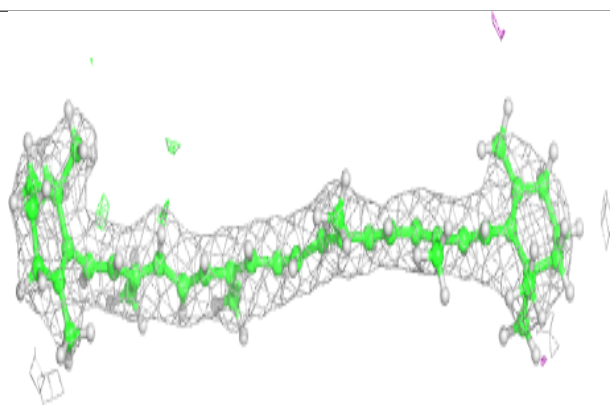
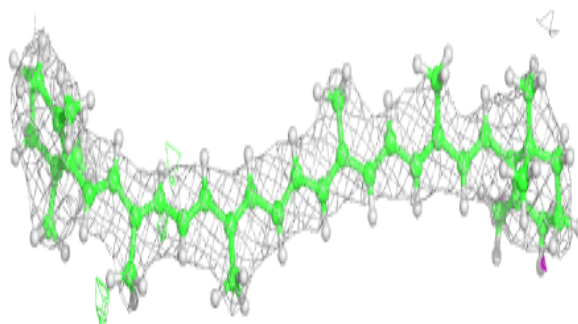
Electron density around CLA b 611:

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

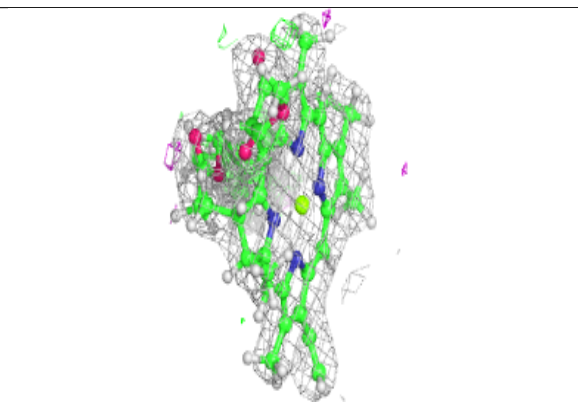
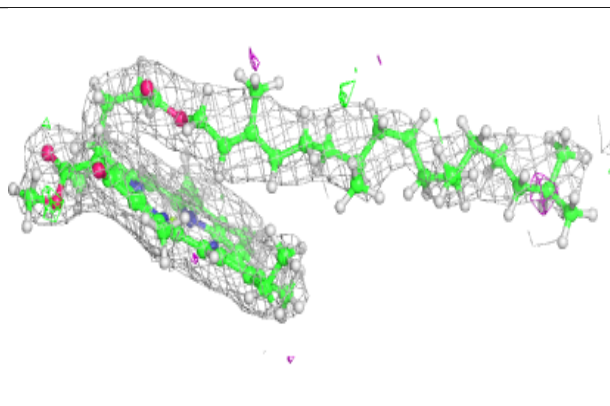
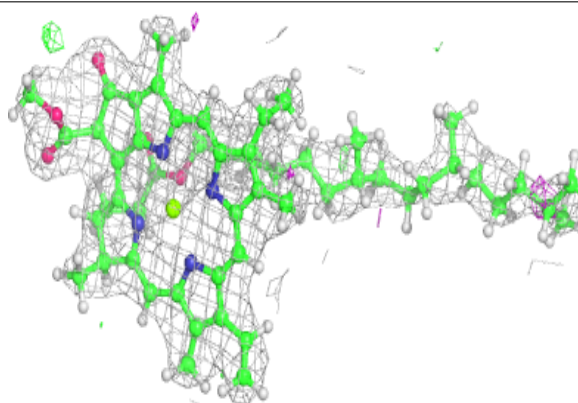


Electron density around BCR c 515:

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

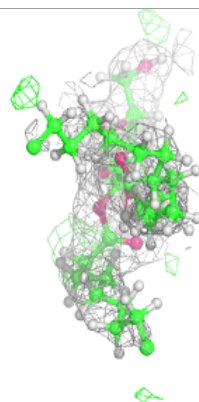
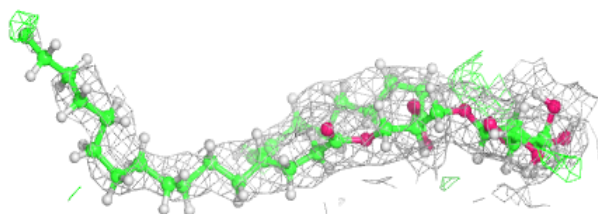
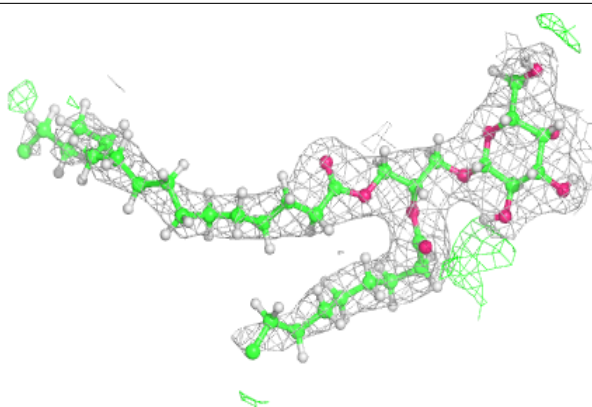
**Electron density around CLA b 614:**

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



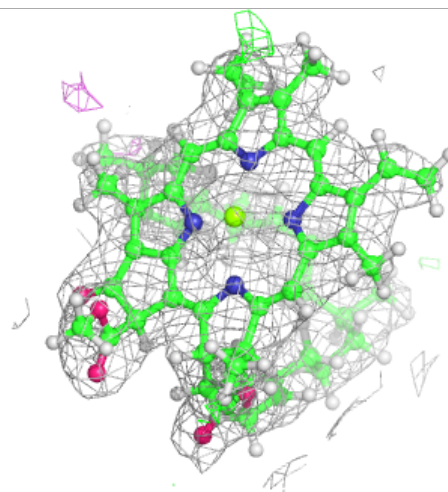
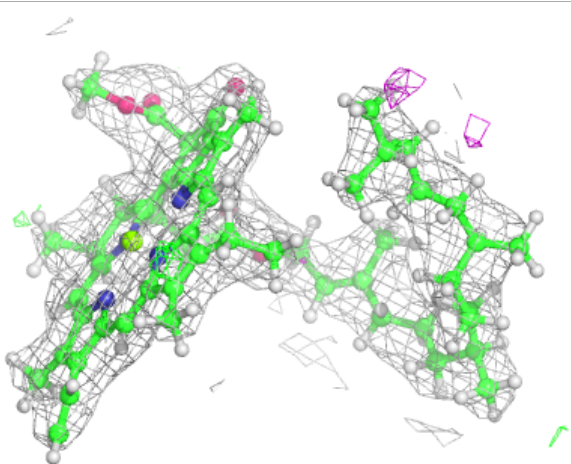
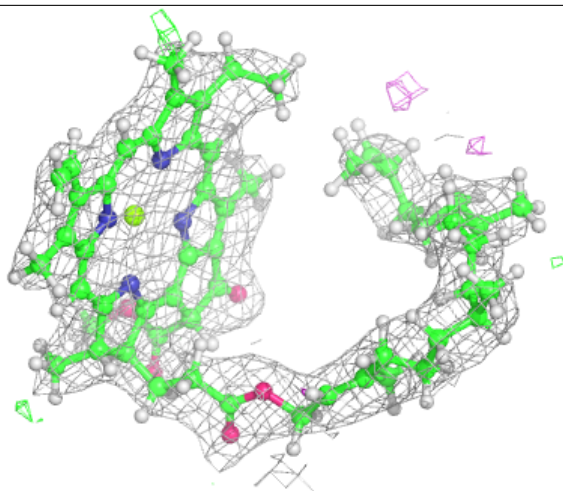
Electron density around LMG d 410:

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



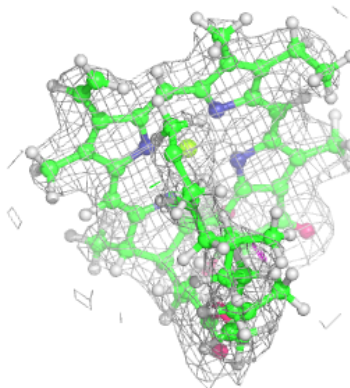
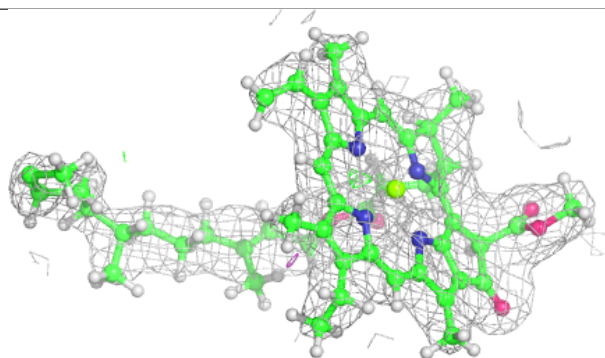
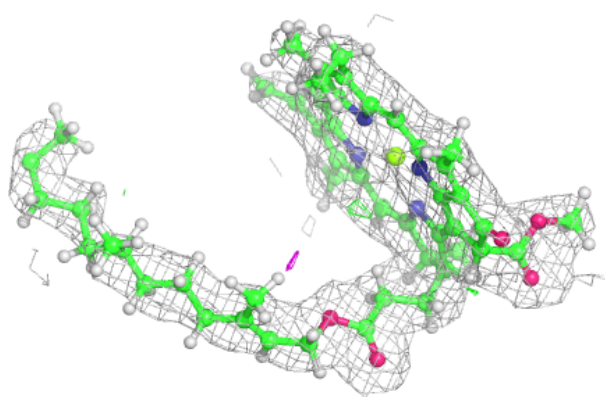
Electron density around CLA C 503:

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

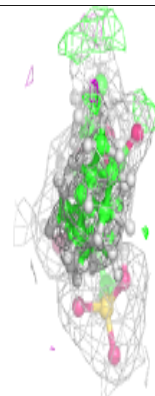
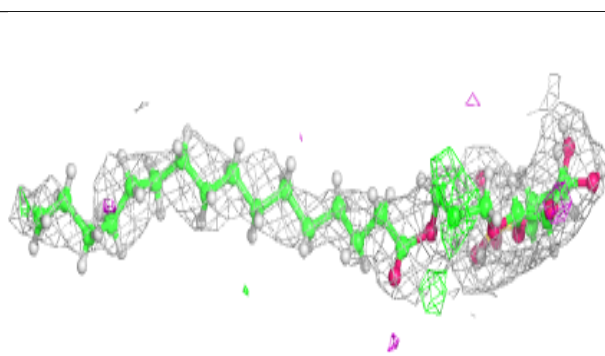
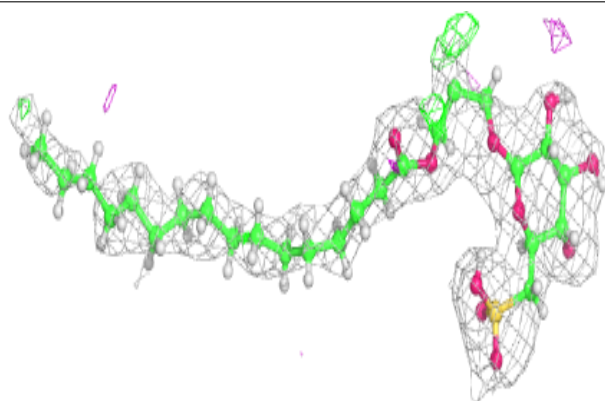


Electron density around CLA C 504:

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

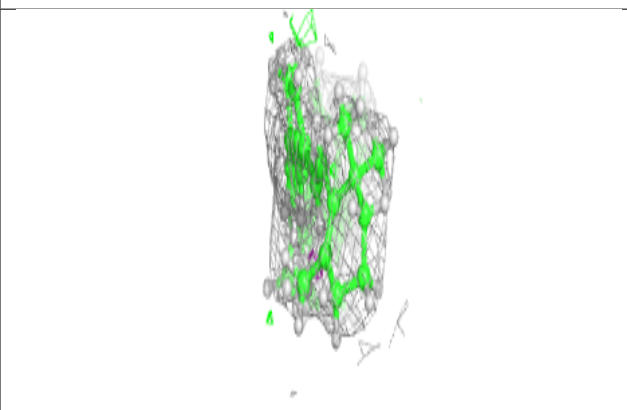
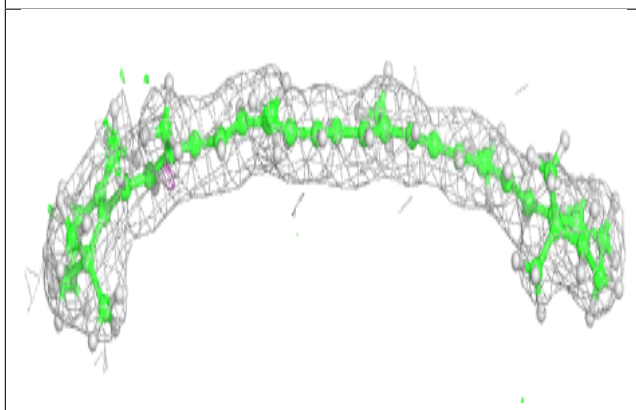
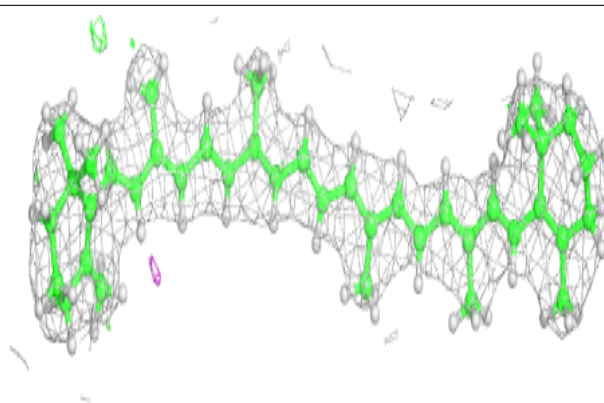
**Electron density around SQD D 407:**

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

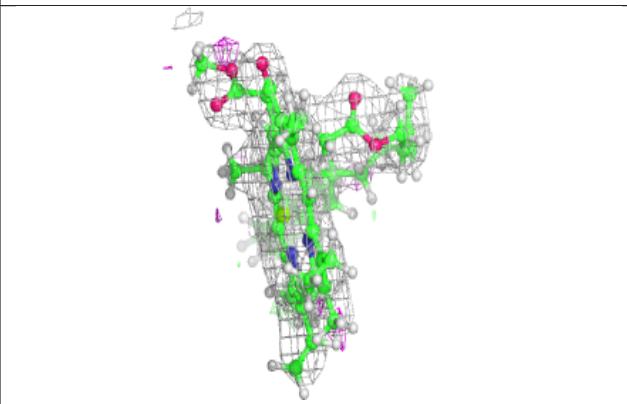
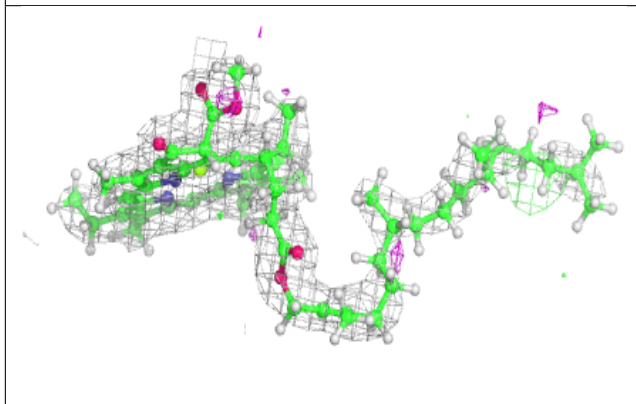
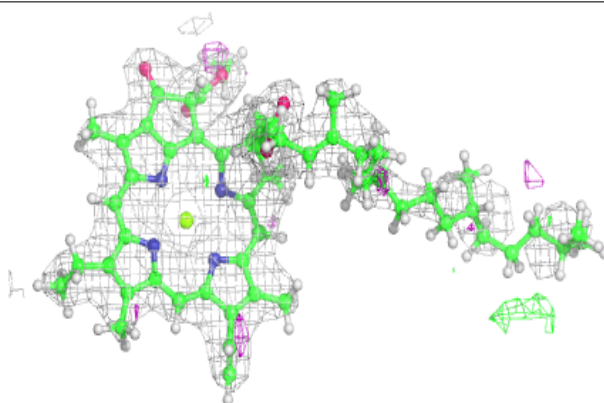


Electron density around BCR t 101:

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

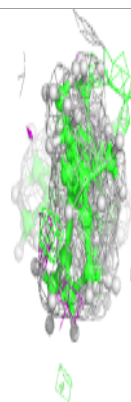
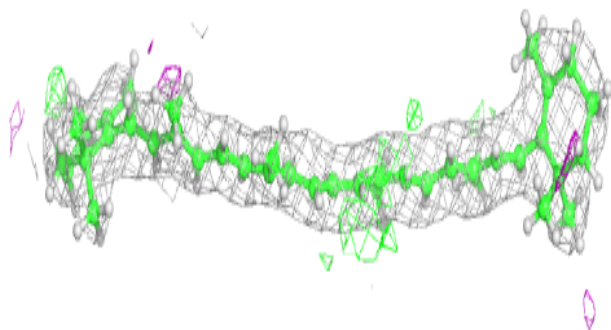
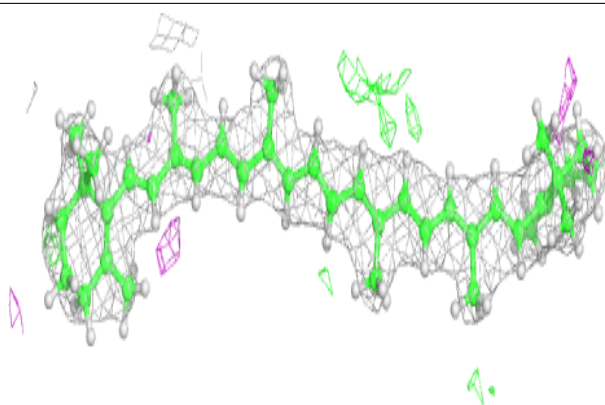
**Electron density around CLA a 403:**

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

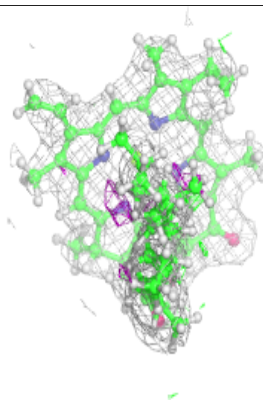
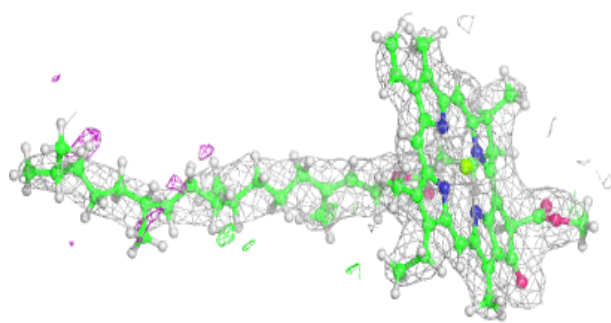
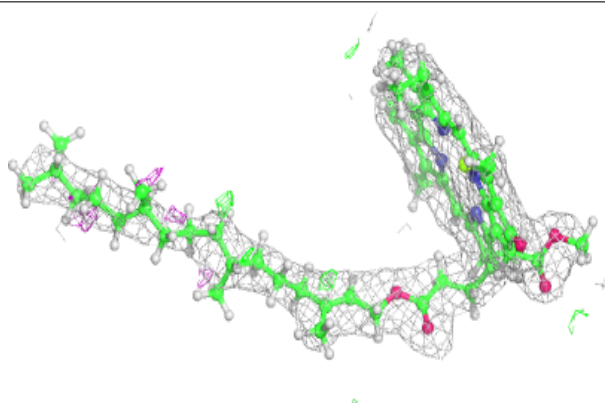


Electron density around BCR B 617:

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

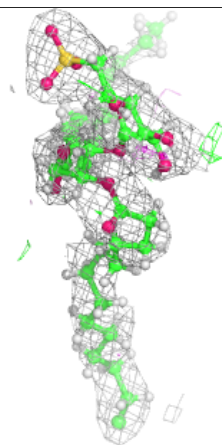
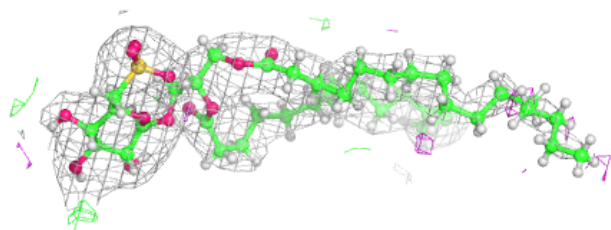
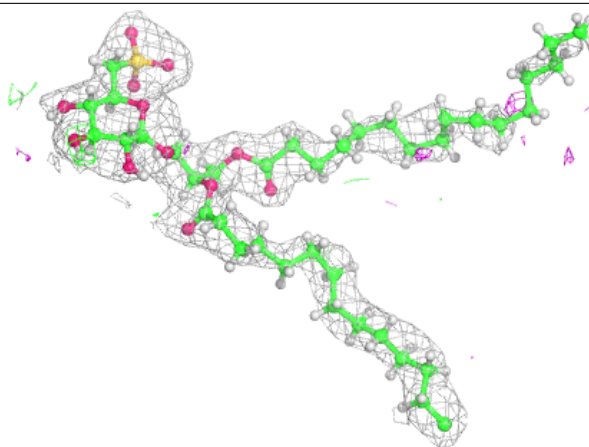
**Electron density around CLA b 607:**

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

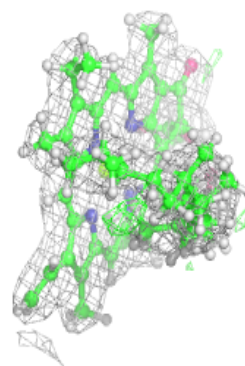
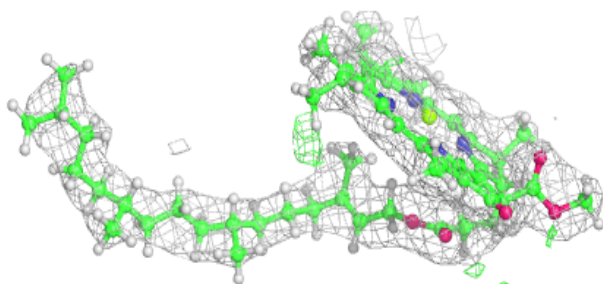
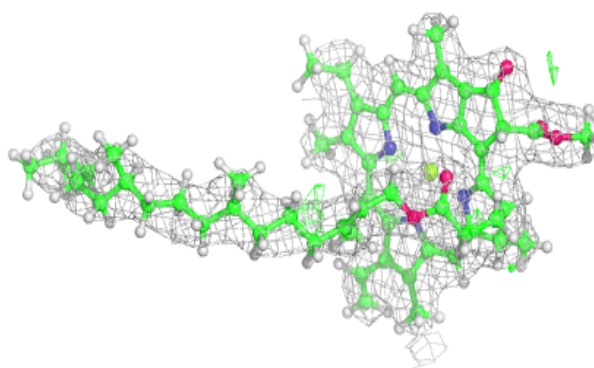


Electron density around SQD A 413:

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

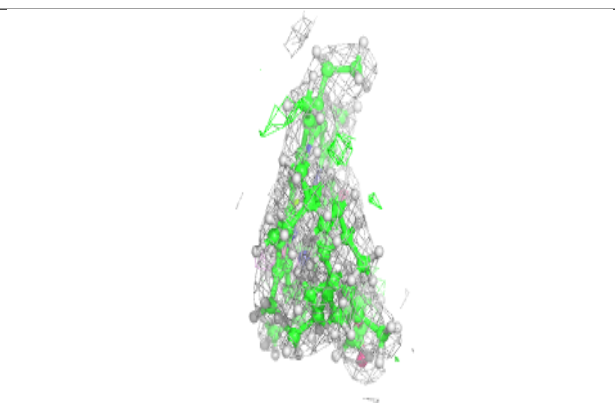
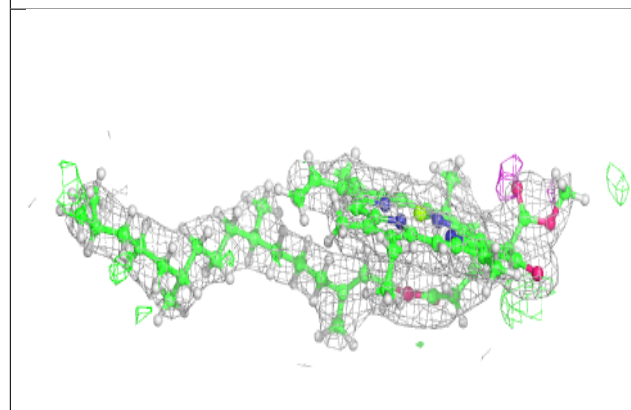
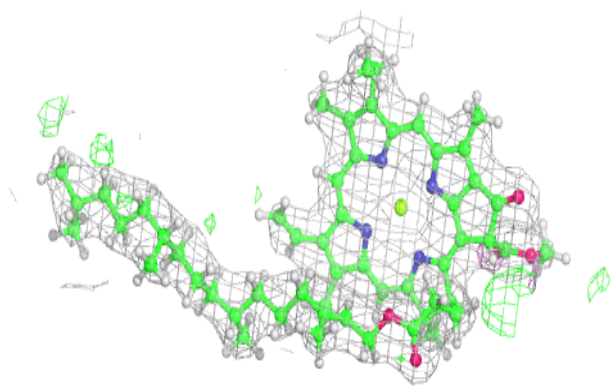
**Electron density around CLA b 608:**

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



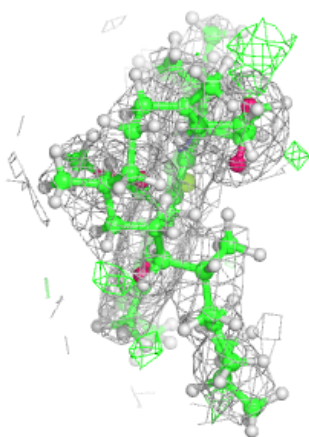
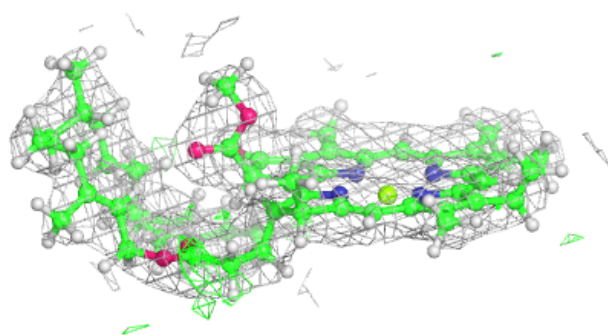
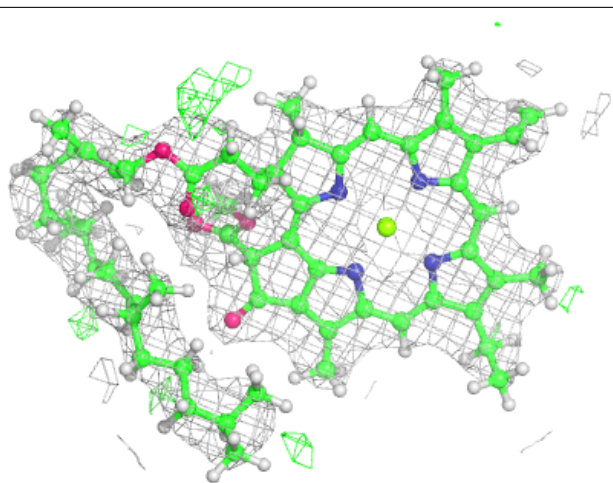
Electron density around CLA C 501:

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



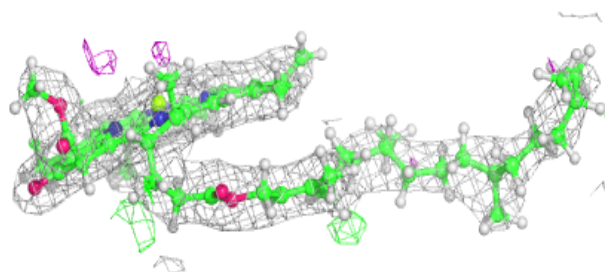
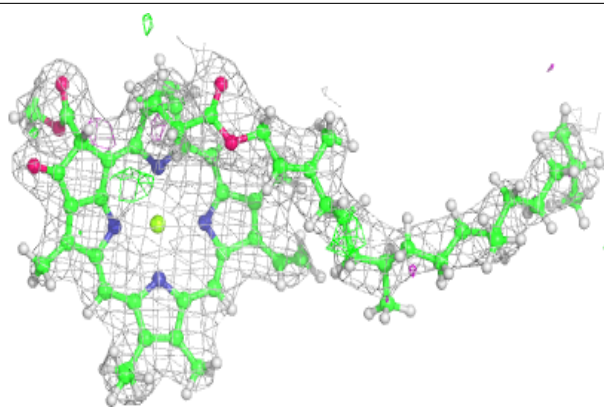
Electron density around CLA b 610:

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

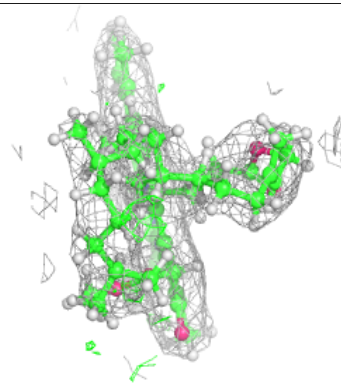
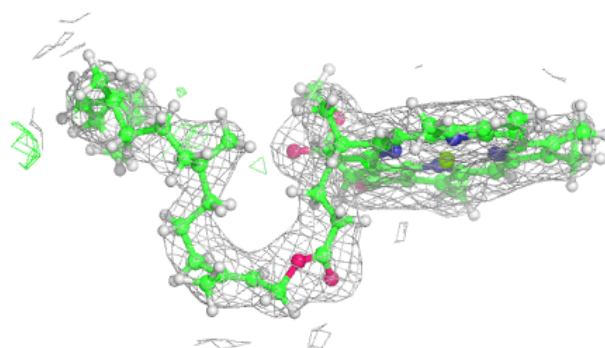
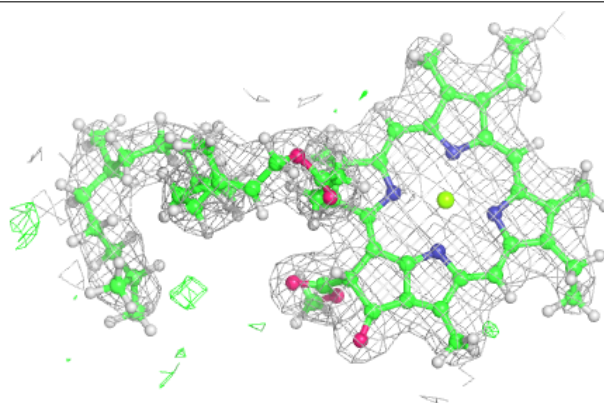


Electron density around CLA B 603:

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

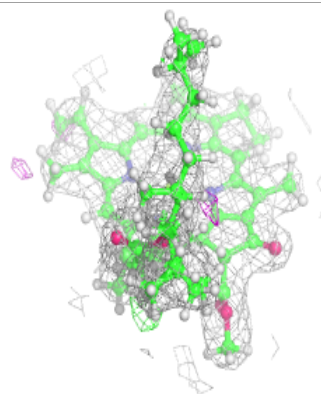
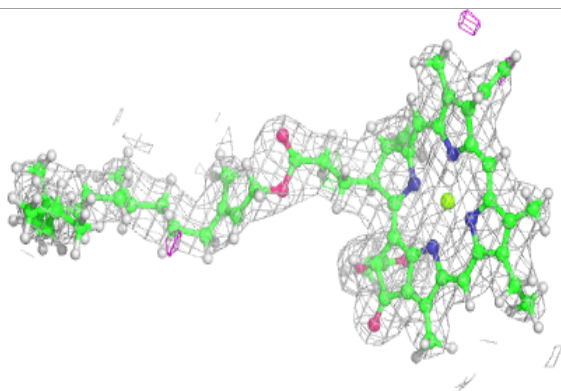
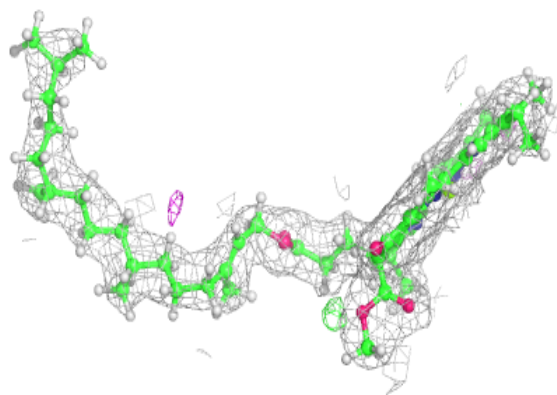
**Electron density around CLA b 612:**

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



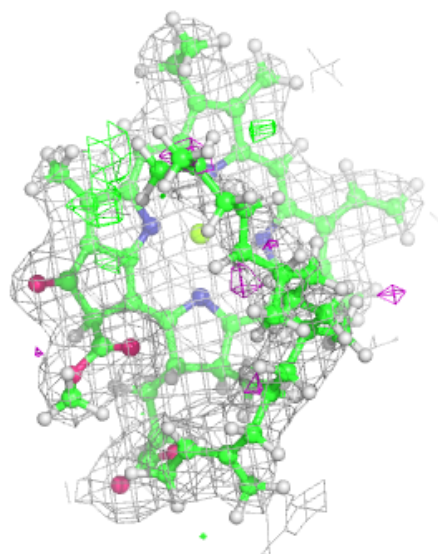
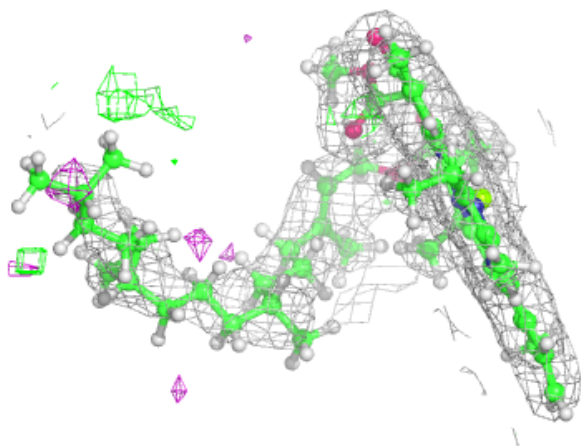
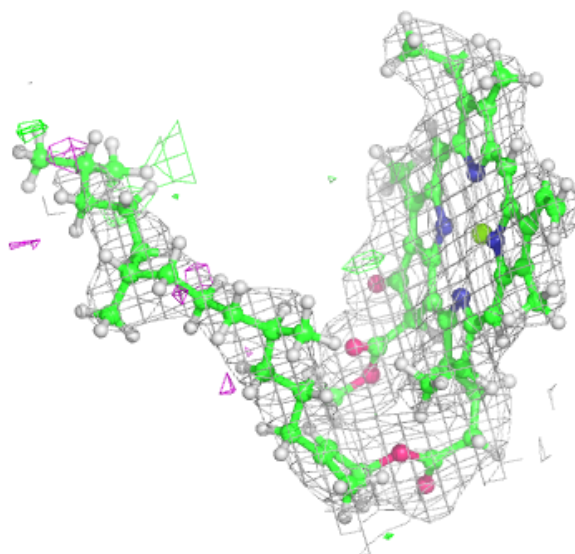
Electron density around CLA d 403:

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



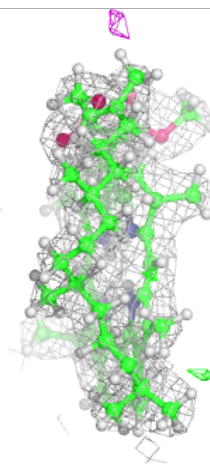
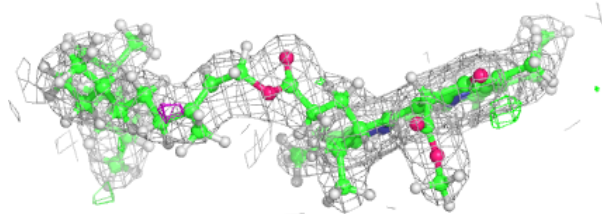
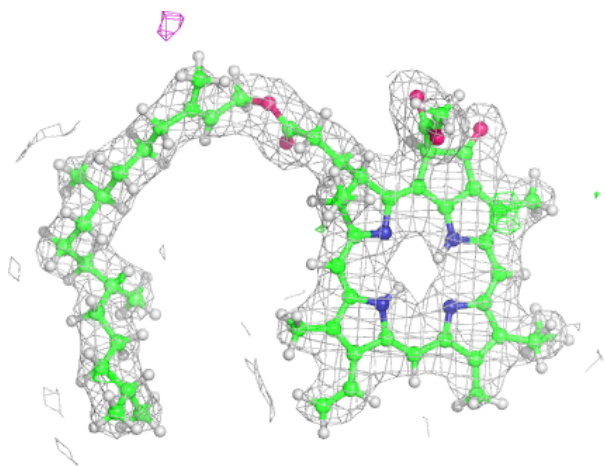
Electron density around CLA b 613:

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



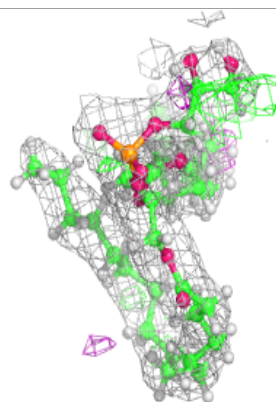
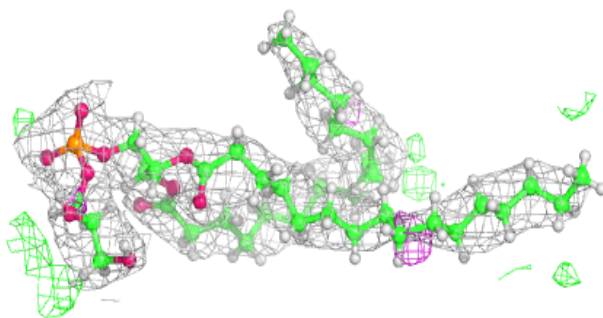
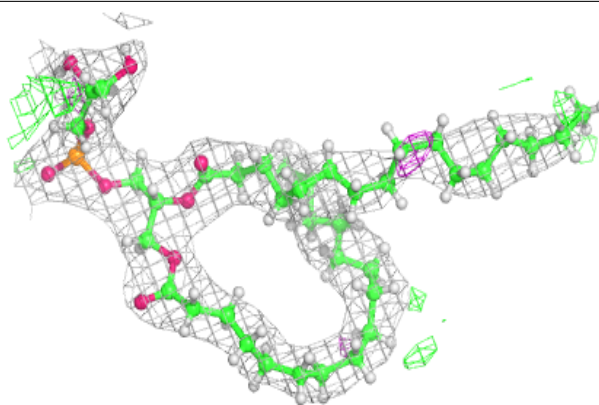
Electron density around PHO A 404:

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

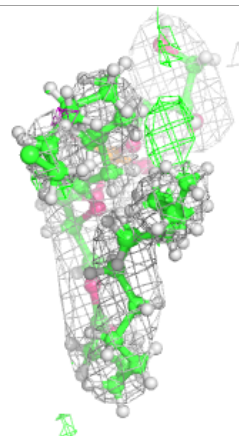
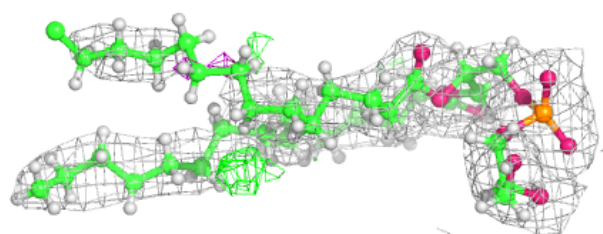
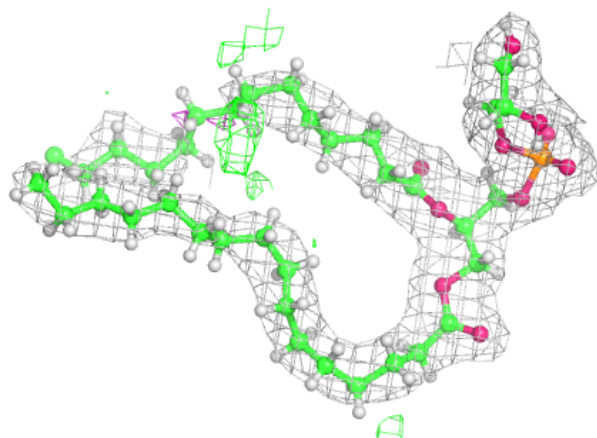


Electron density around LHG B 622:

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

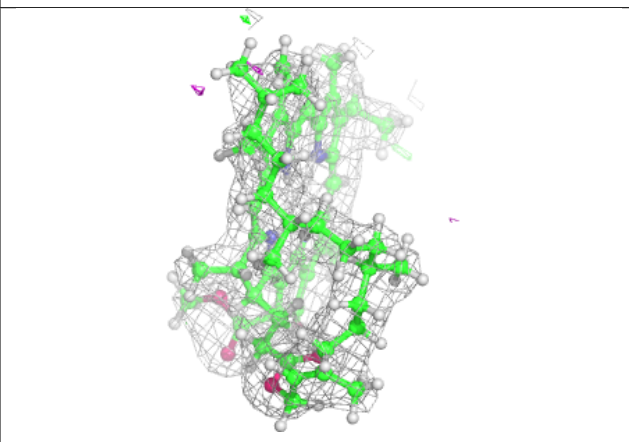
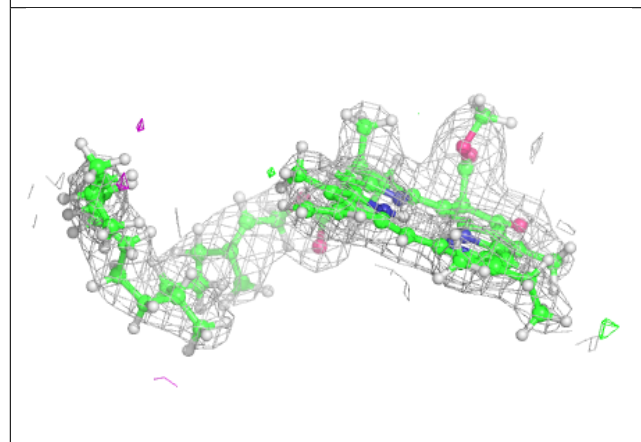
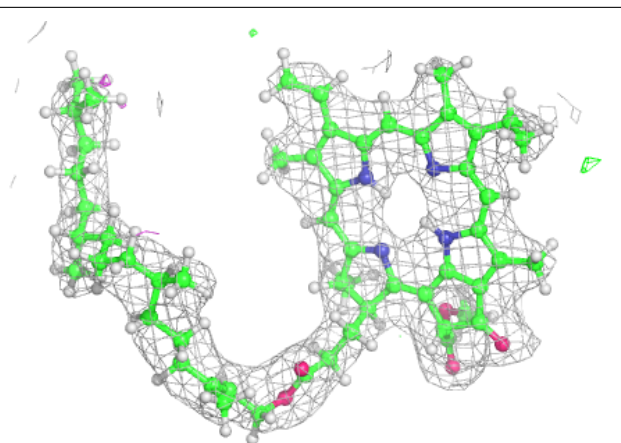
**Electron density around LHG D 409:**

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



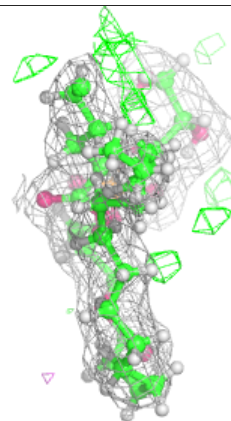
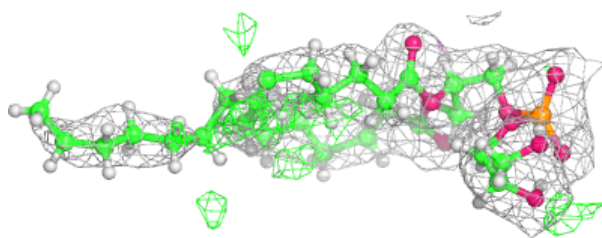
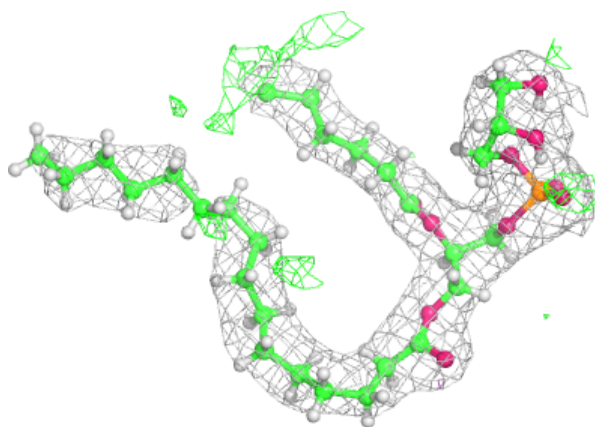
Electron density around PHO d 402:

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

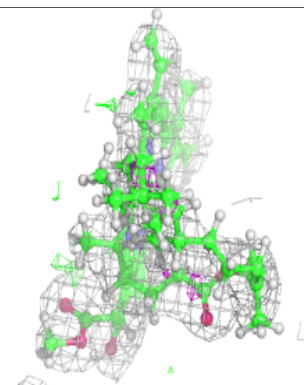
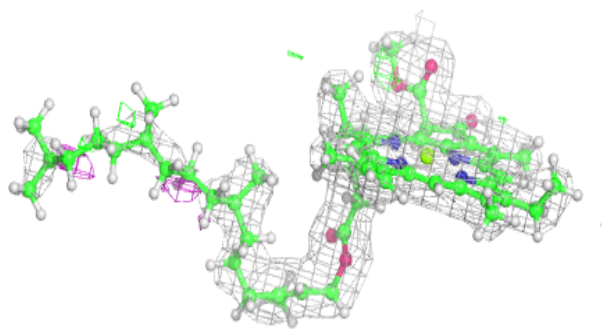
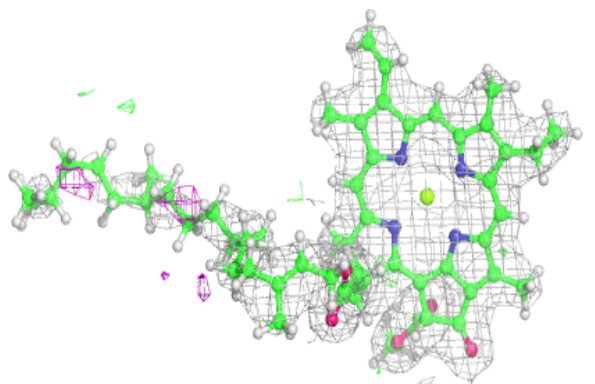


Electron density around LHG d 409:

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

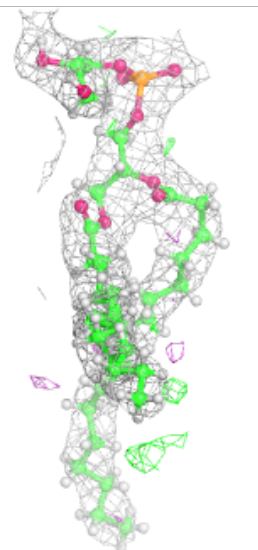
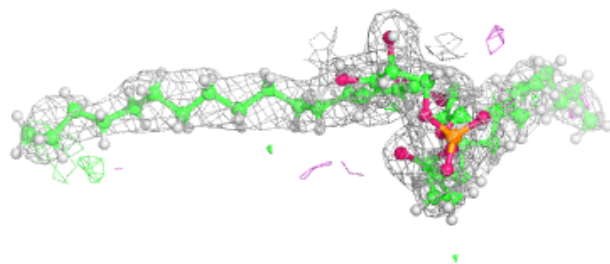
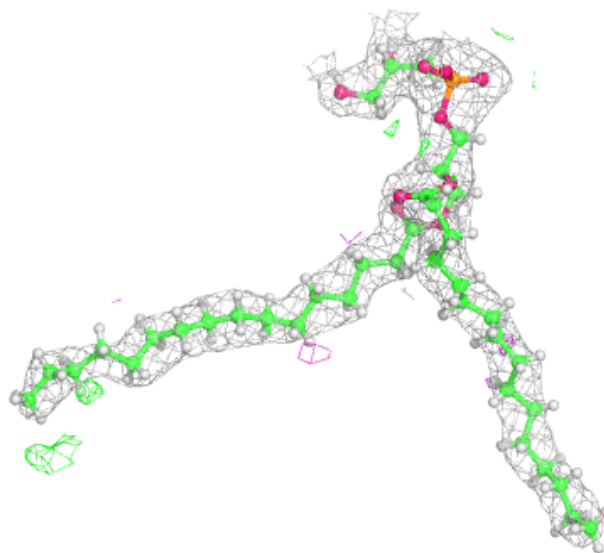
**Electron density around CLA A 403:**

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



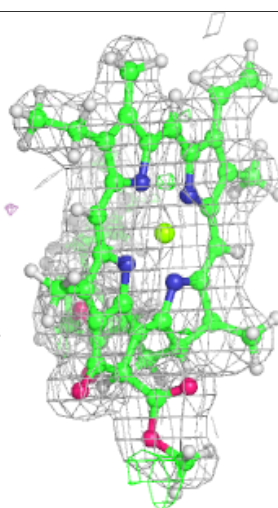
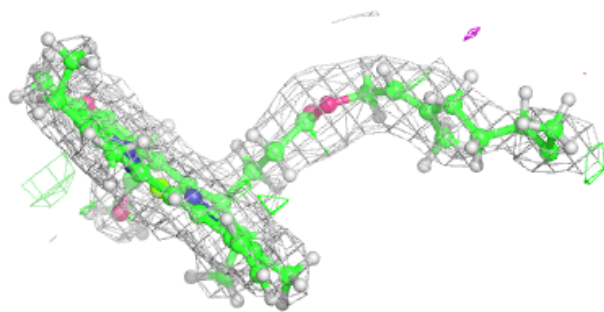
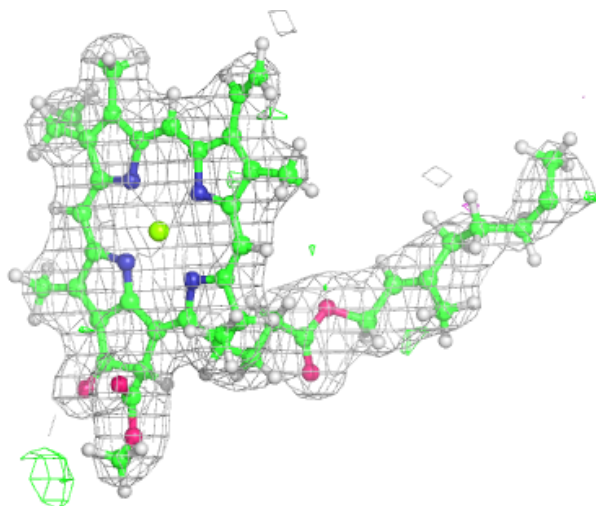
Electron density around LHG 1 101:

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



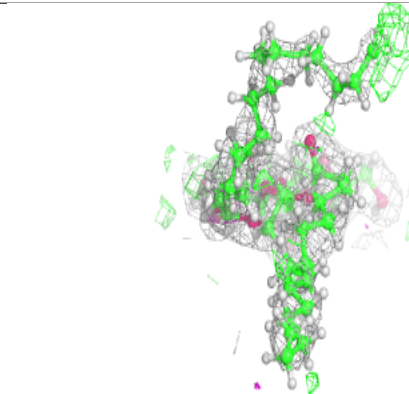
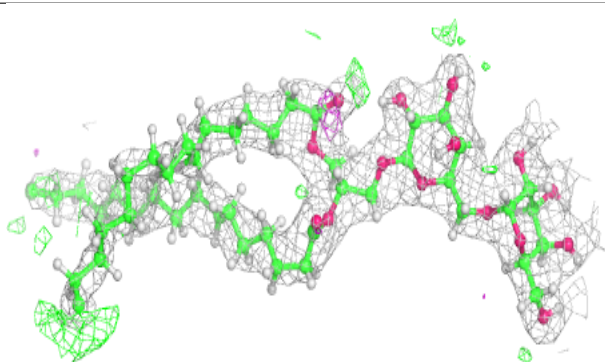
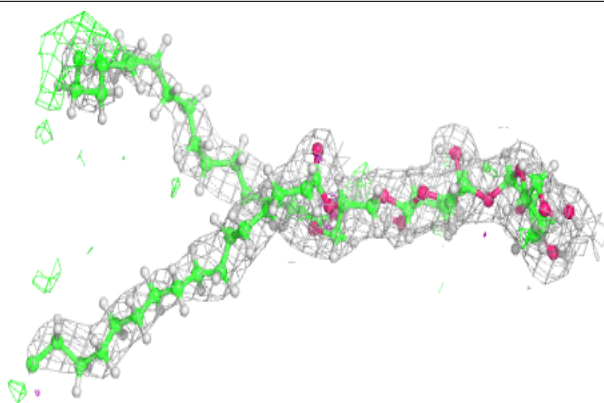
Electron density around CLA A 405:

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

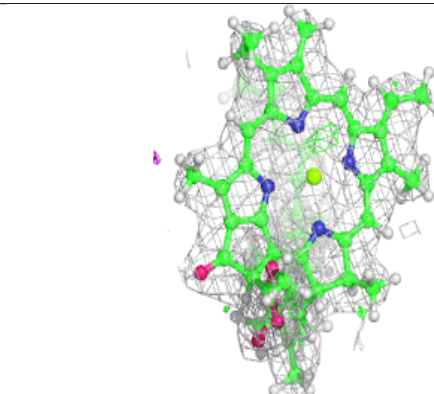
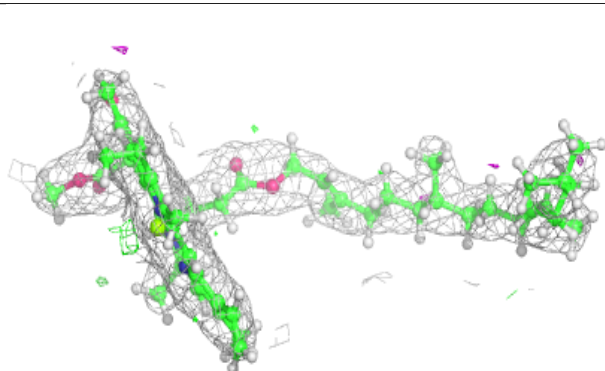
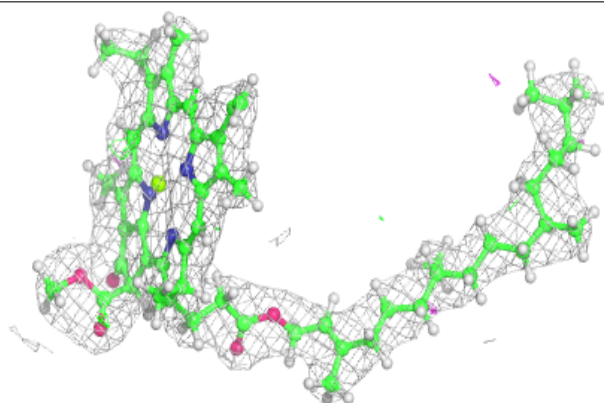


Electron density around DGD C 515:

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

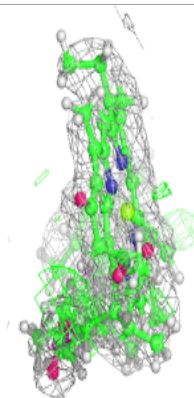
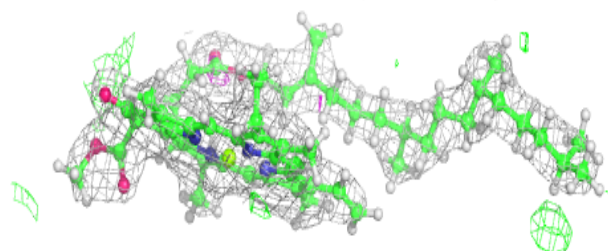
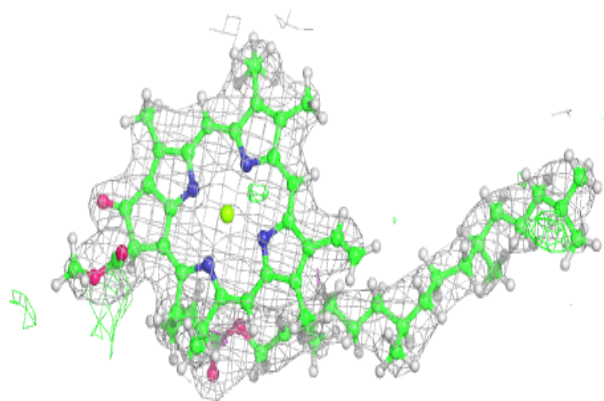
**Electron density around CLA B 609:**

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



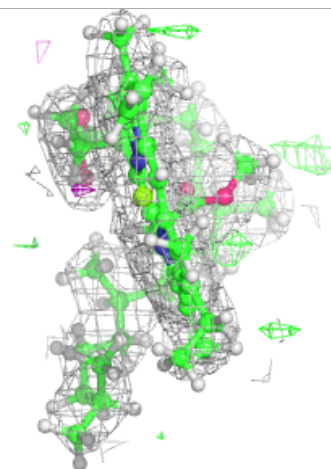
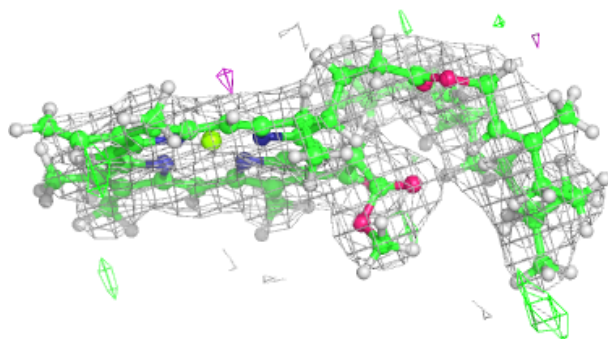
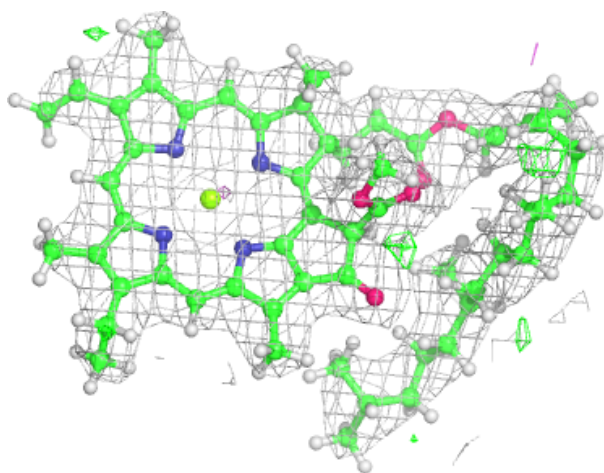
Electron density around CLA c 501:

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



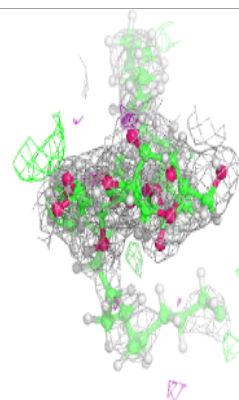
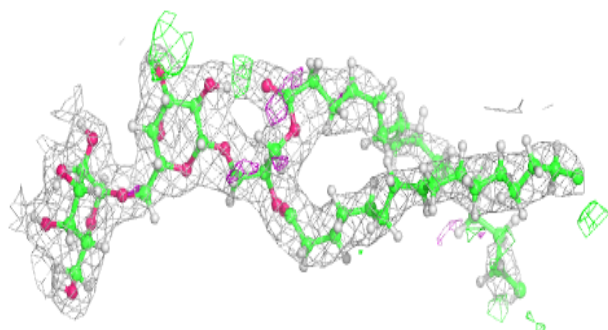
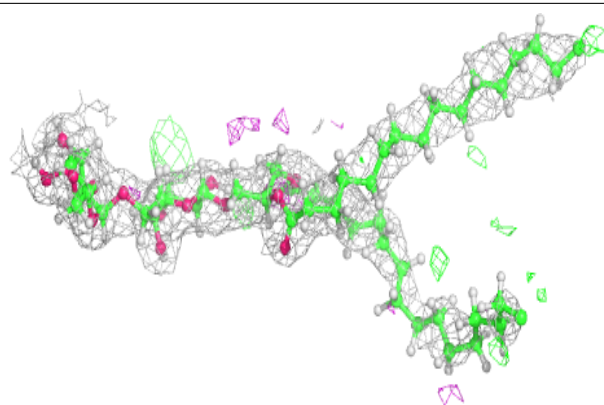
Electron density around CLA B 610:

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

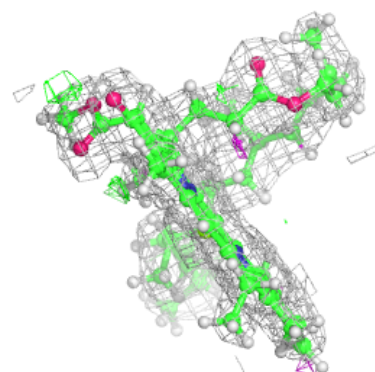
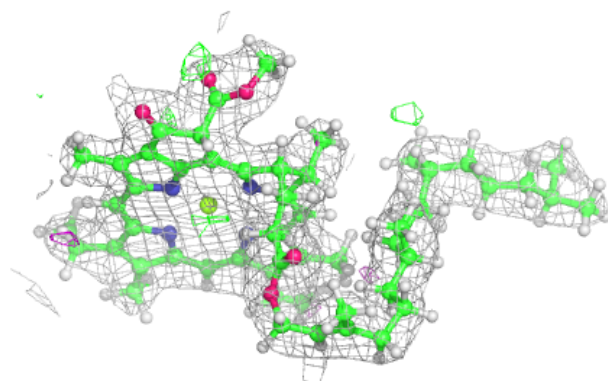
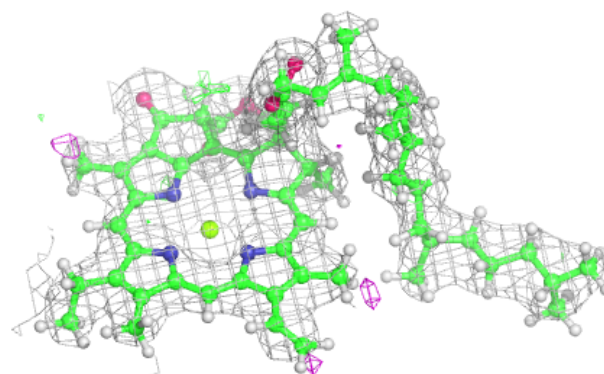


Electron density around DGD c 516:

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

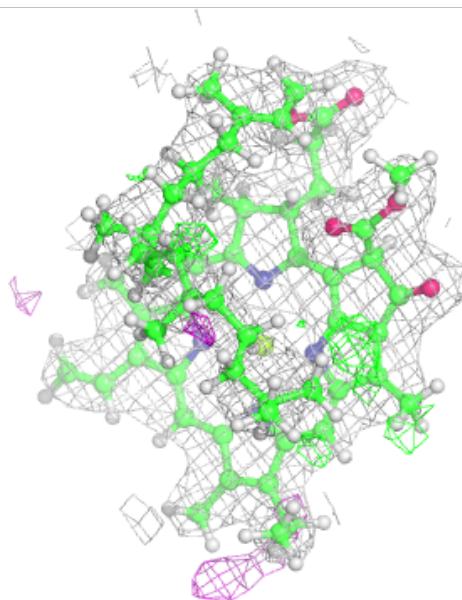
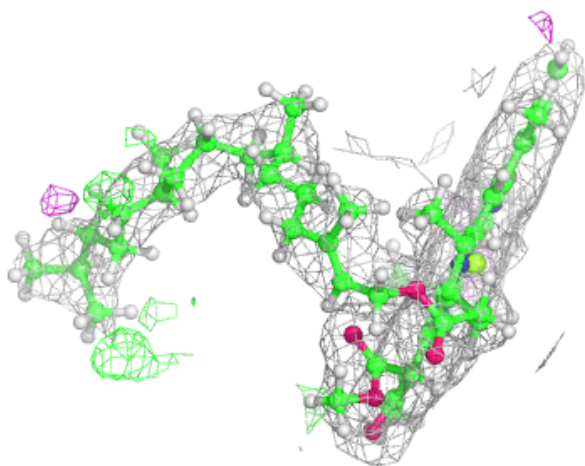
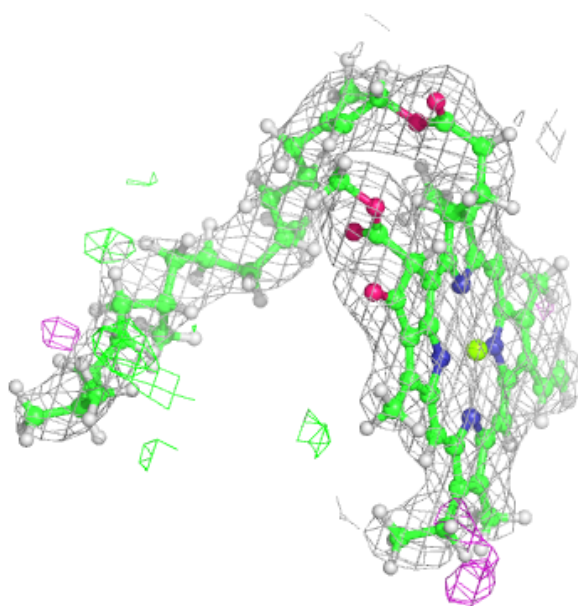
**Electron density around CLA a 410:**

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



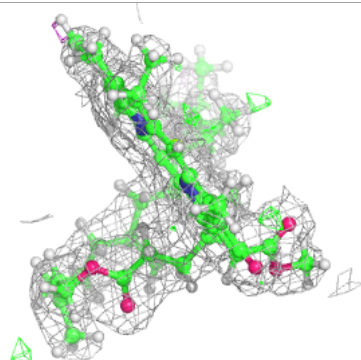
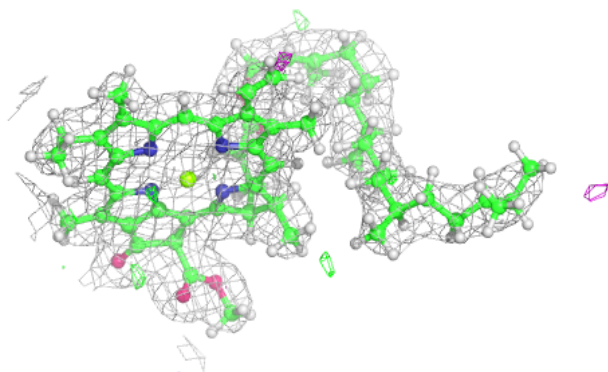
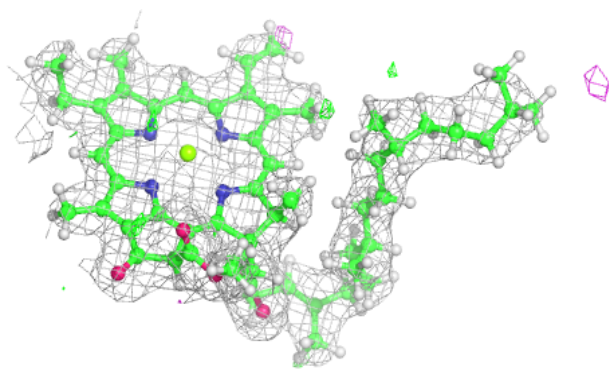
Electron density around CLA B 613:

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

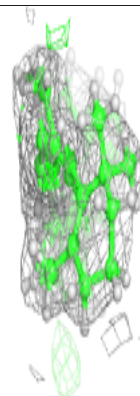
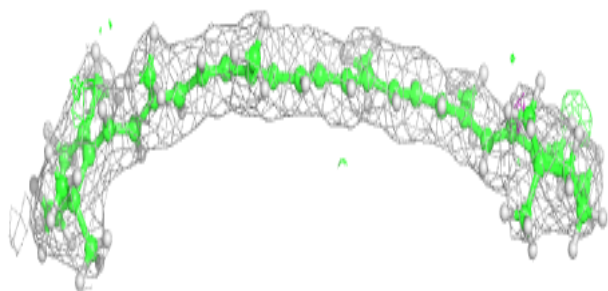
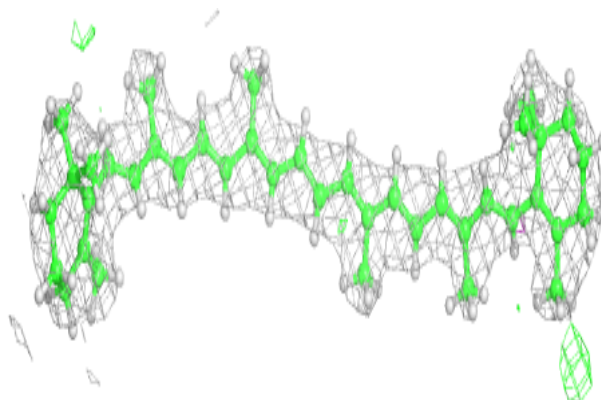


Electron density around CLA A 411:

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

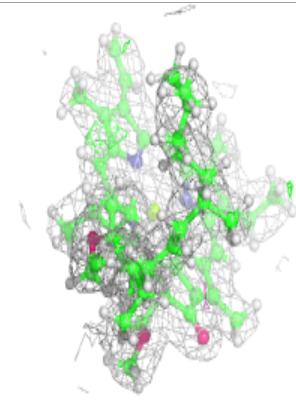
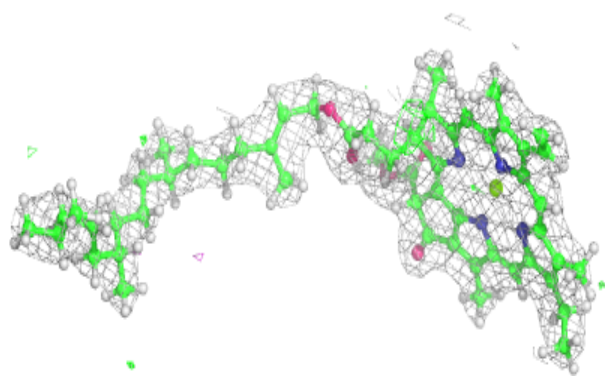
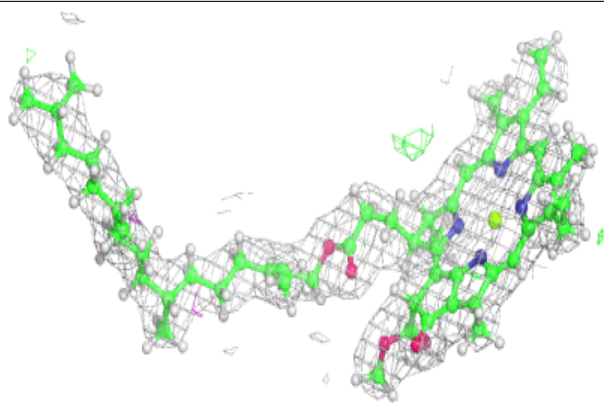
**Electron density around BCR T 101:**

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

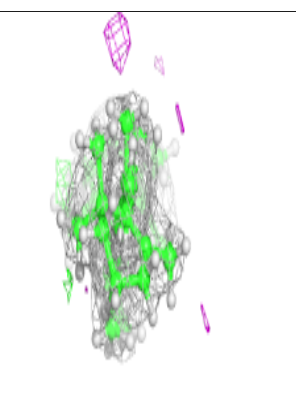
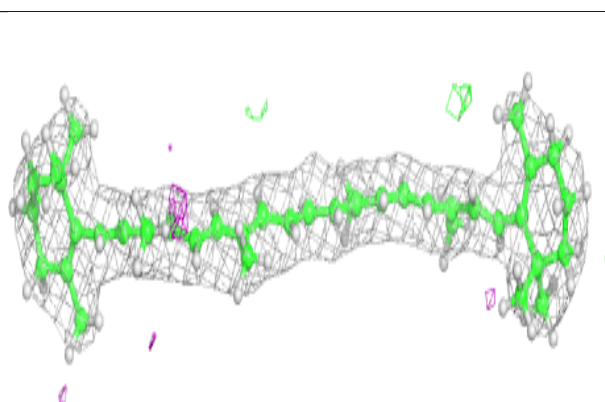
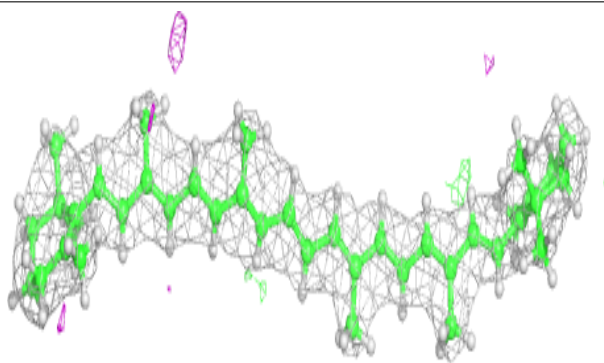


Electron density around CLA A 402:

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

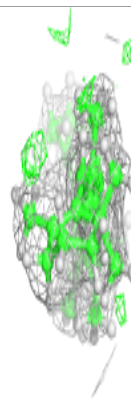
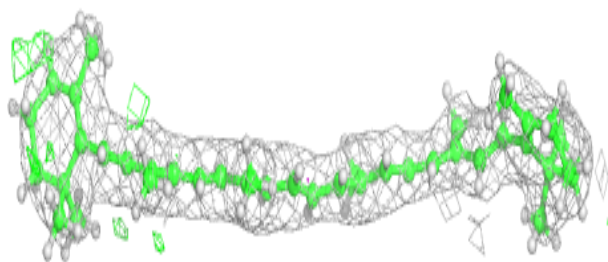
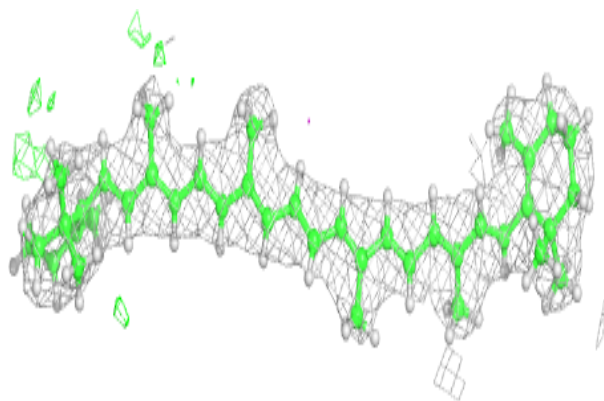
**Electron density around BCR a 405:**

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

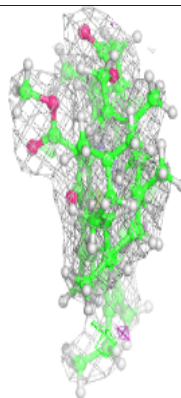
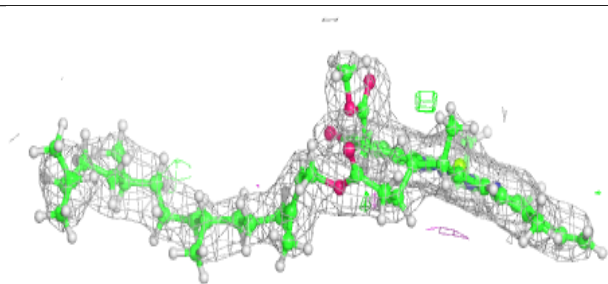
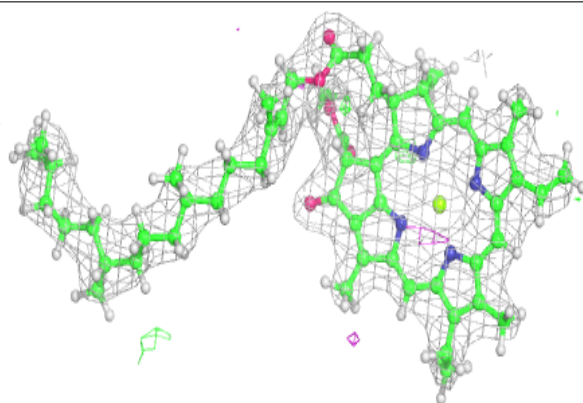


Electron density around BCR b 617:

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

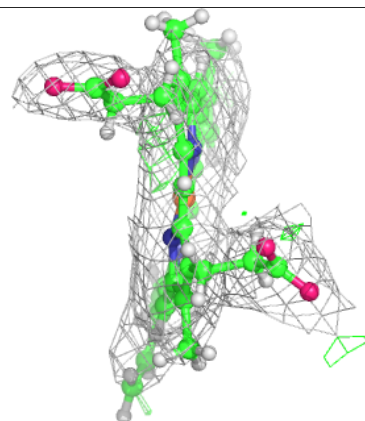
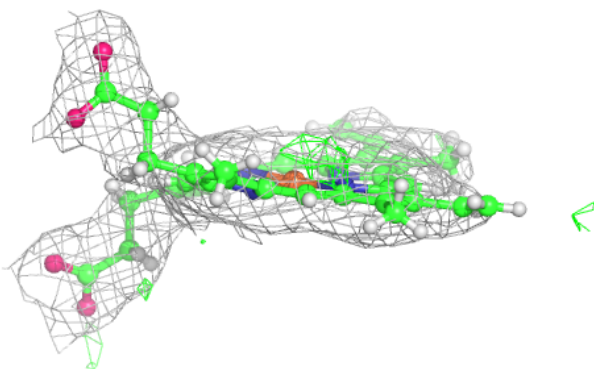
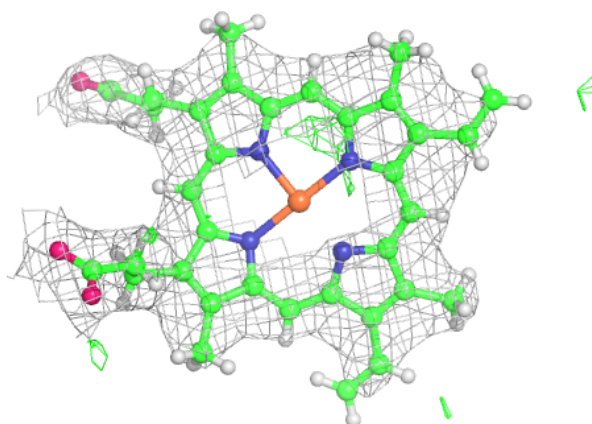
**Electron density around CLA B 602:**

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

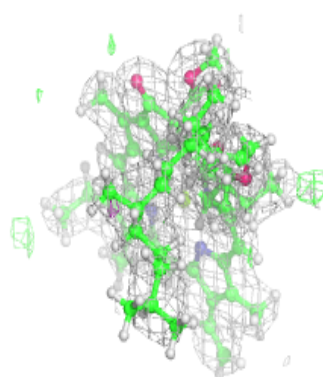
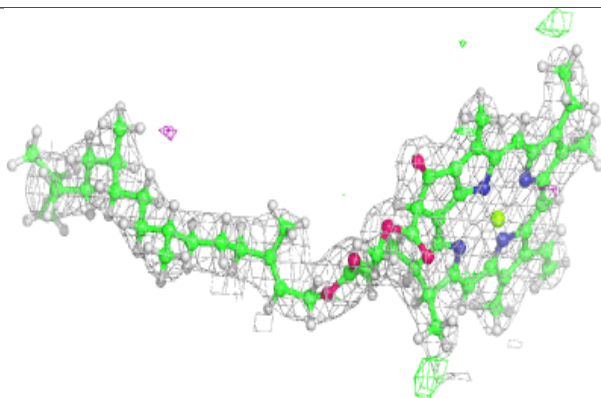
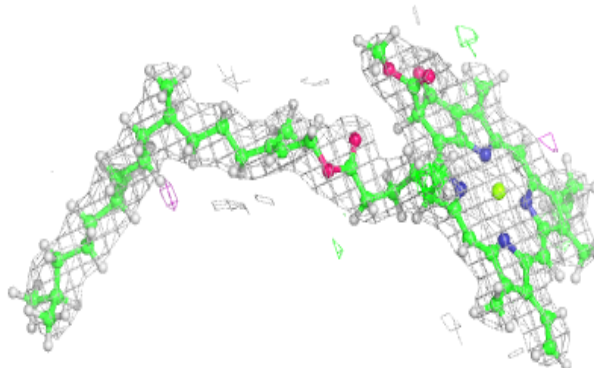


Electron density around HEM F 101:

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

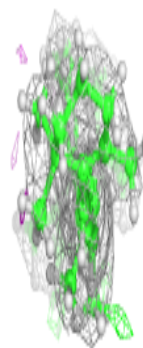
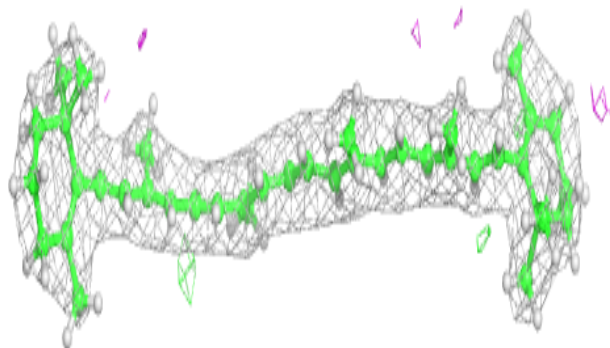
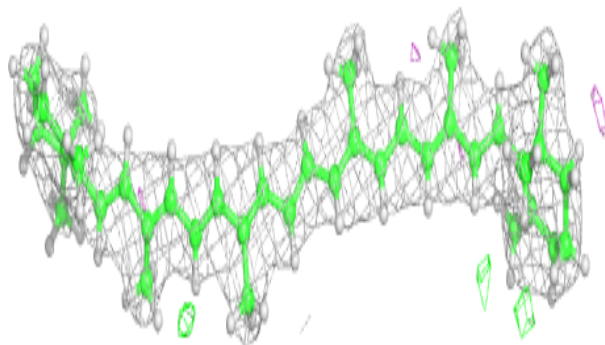
**Electron density around CLA a 402:**

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

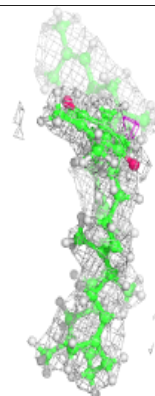
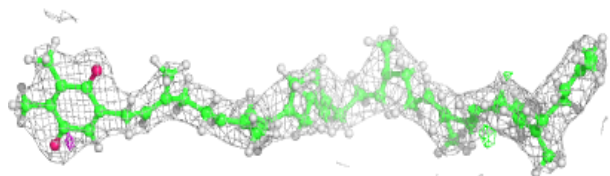
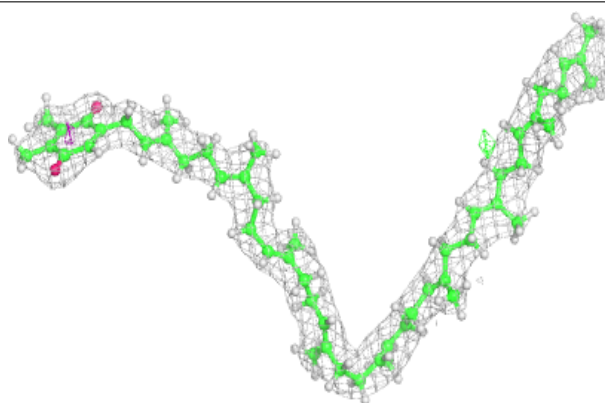


Electron density around BCR A 406:

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

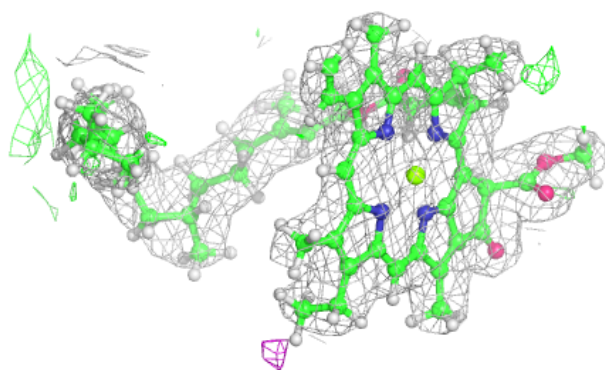
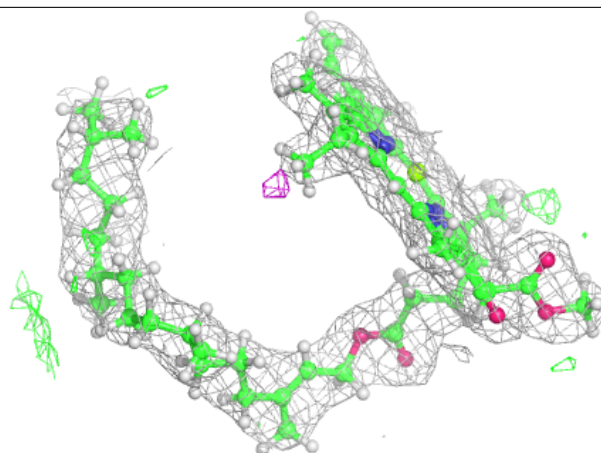
**Electron density around PL9 d 406:**

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



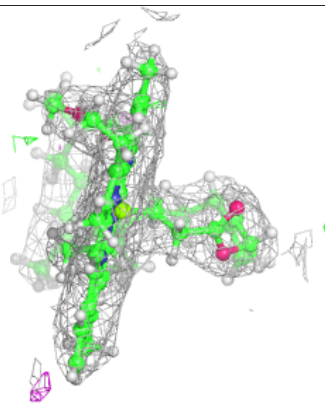
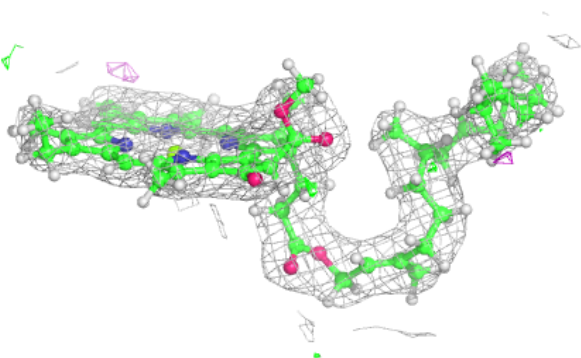
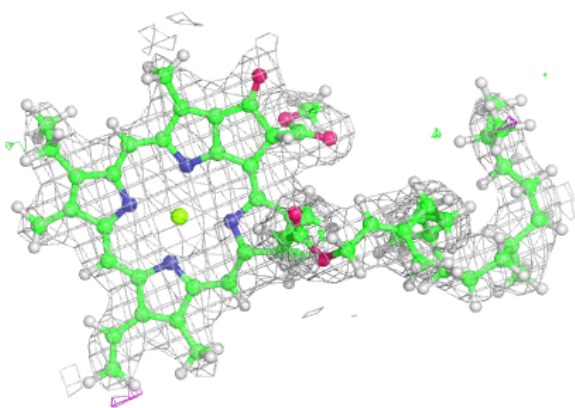
Electron density around CLA B 611:

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

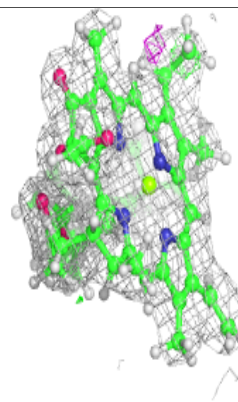
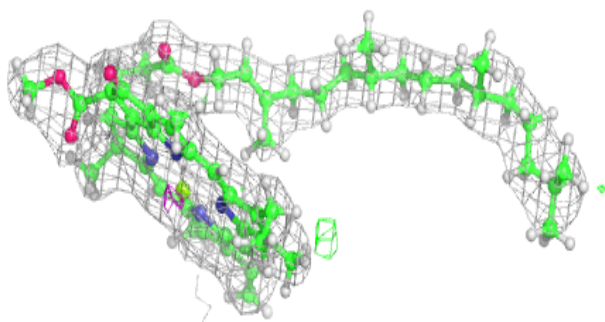
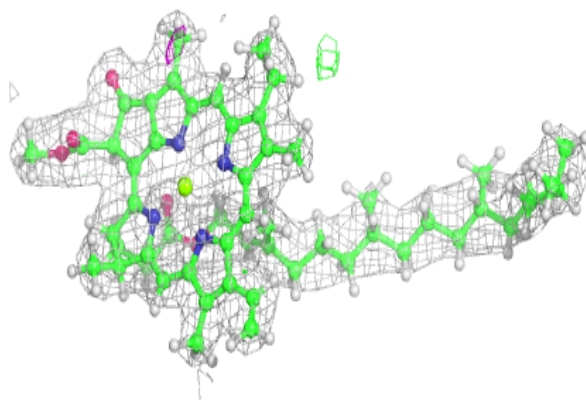


Electron density around CLA B 612:

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

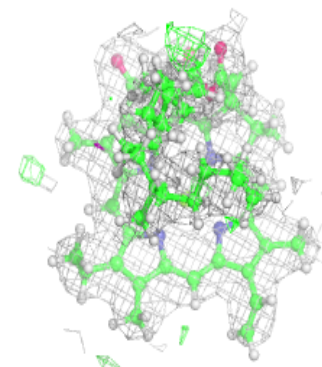
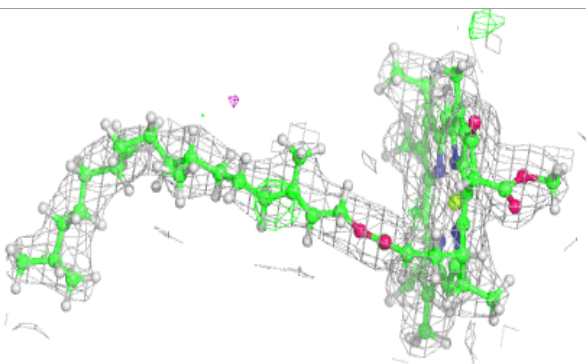
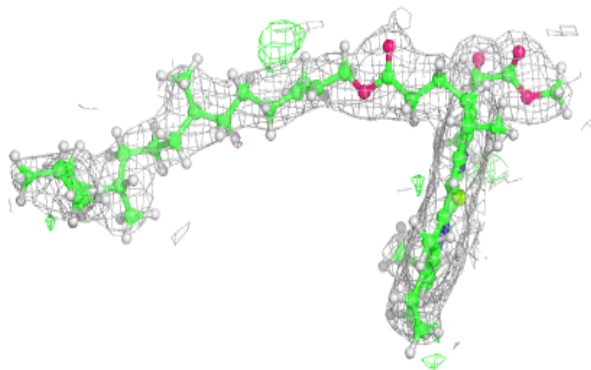
**Electron density around CLA B 608:**

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

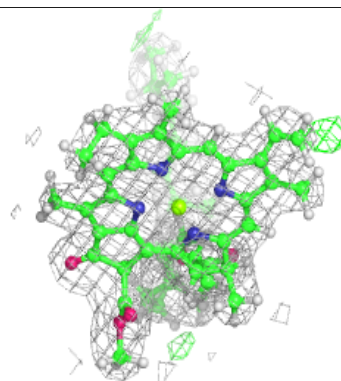
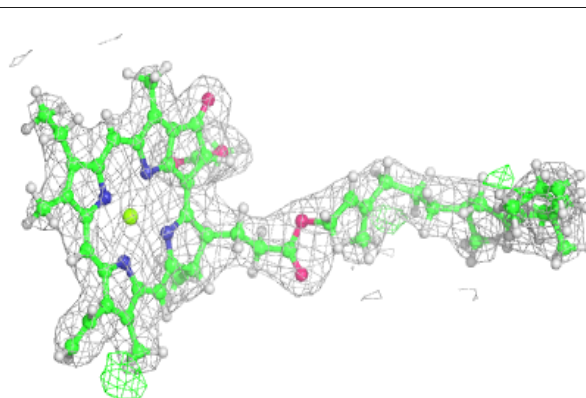
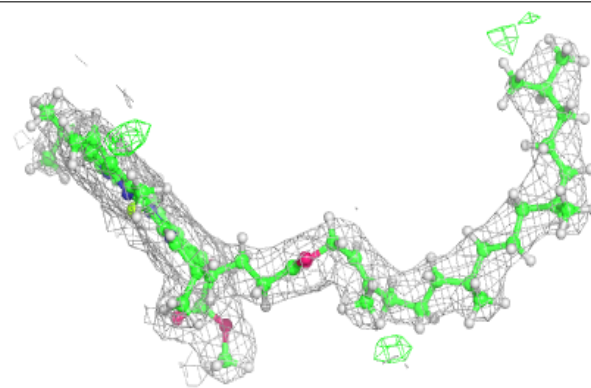


Electron density around CLA B 605:

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

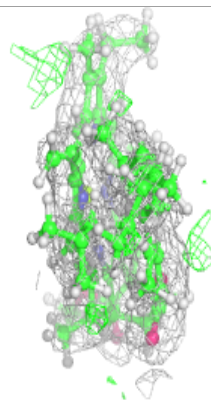
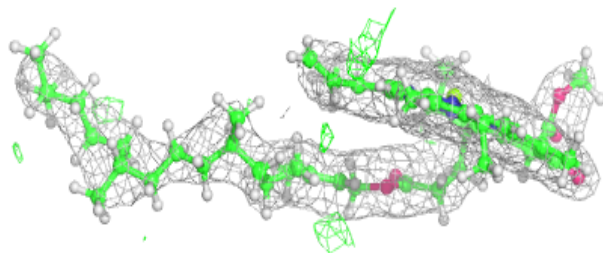
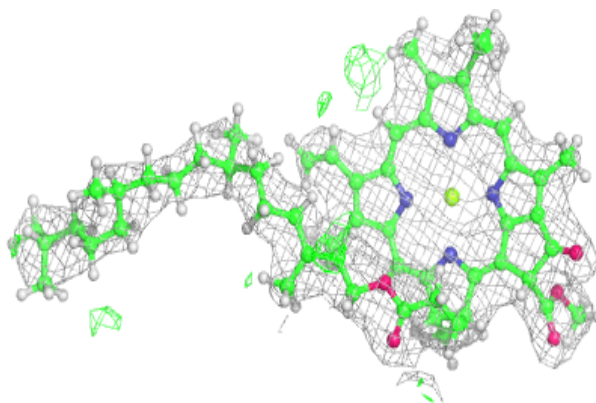
**Electron density around CLA D 402:**

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

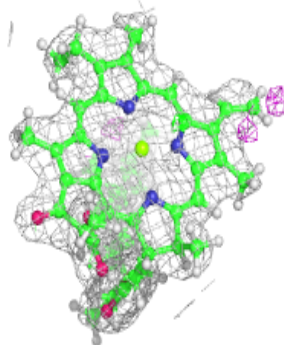
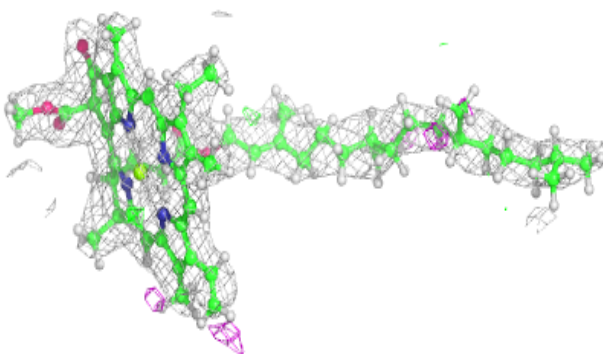
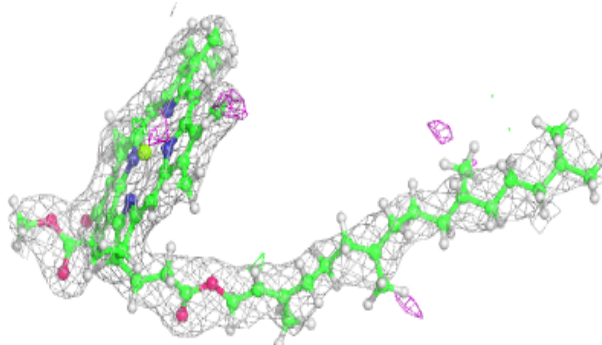


Electron density around CLA b 603:

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

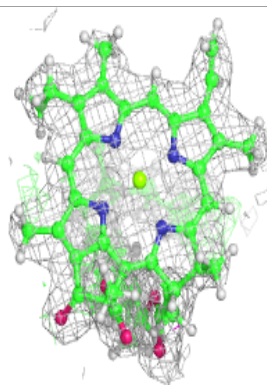
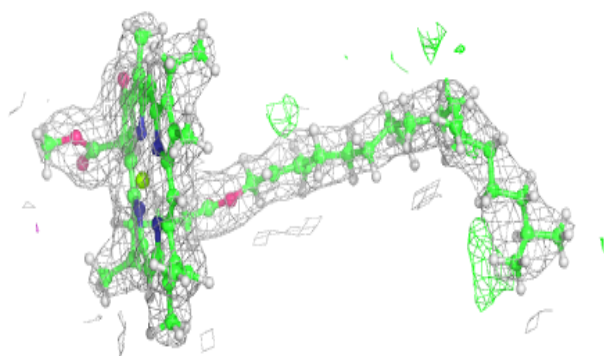
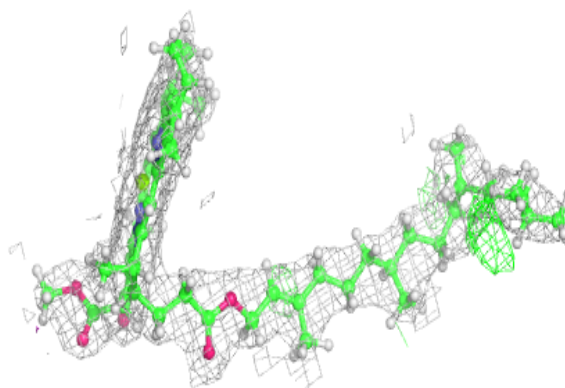
**Electron density around CLA B 607:**

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



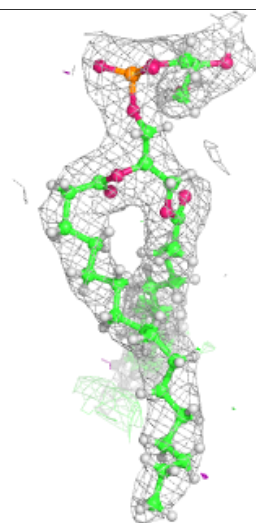
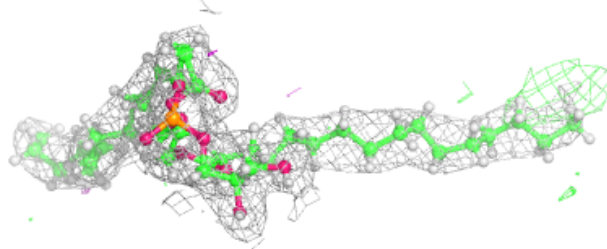
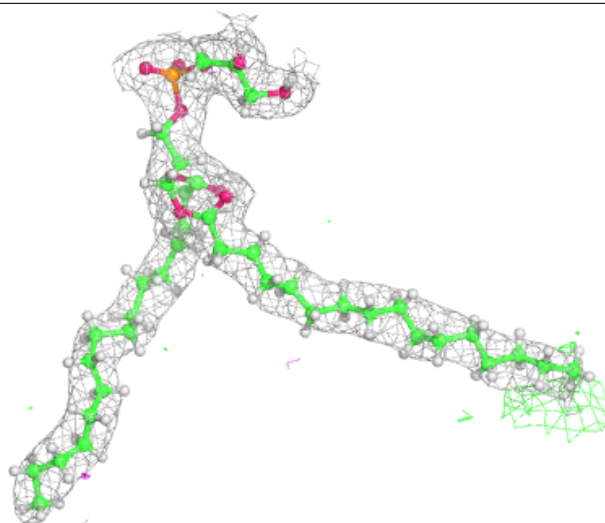
Electron density around CLA b 605:

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



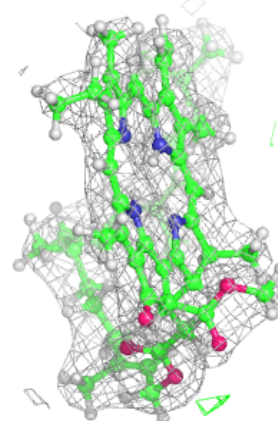
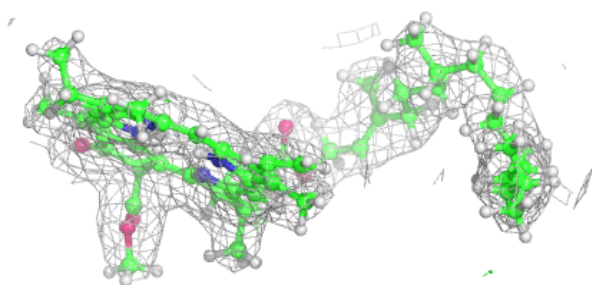
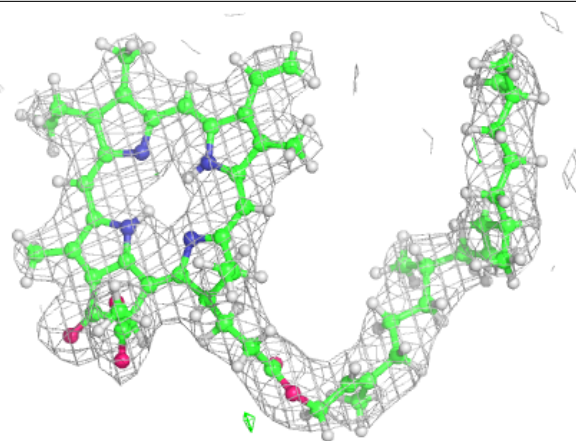
Electron density around LHG B 621:

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



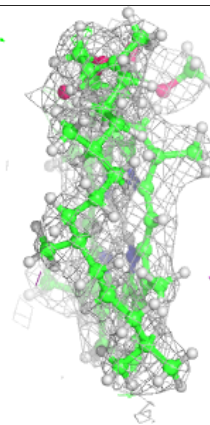
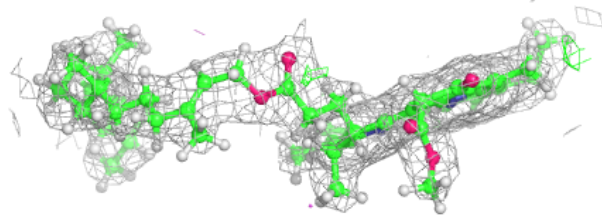
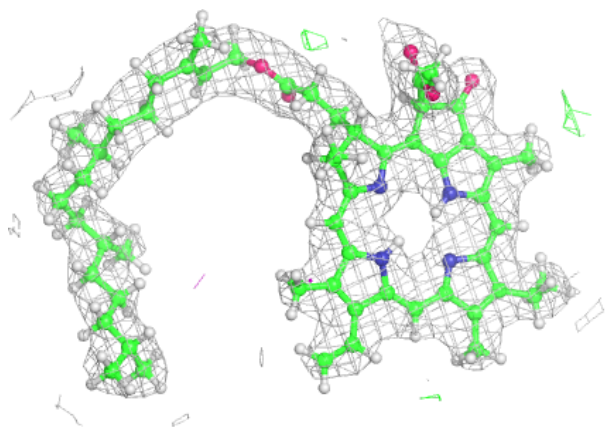
Electron density around PHO D 401:

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

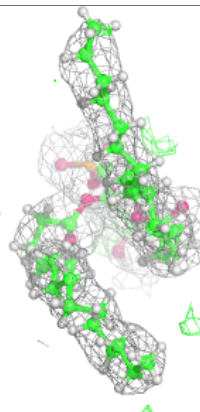
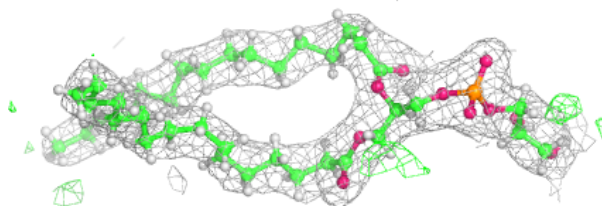
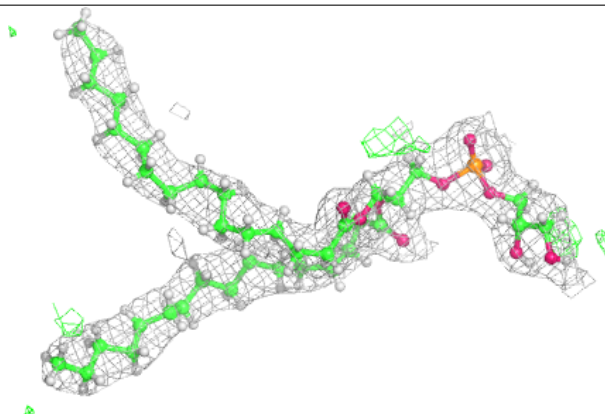


Electron density around PHO d 401:

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

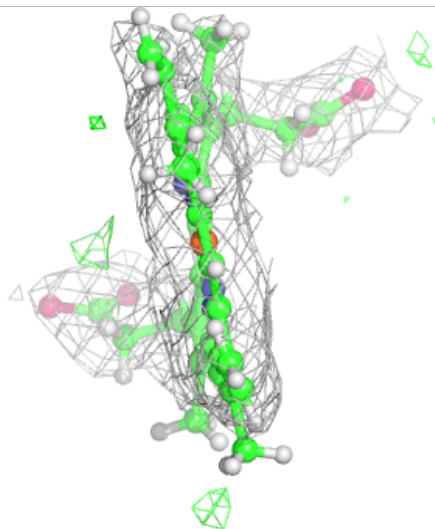
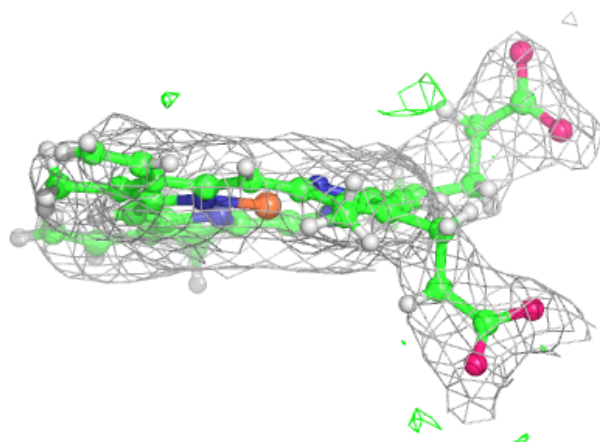
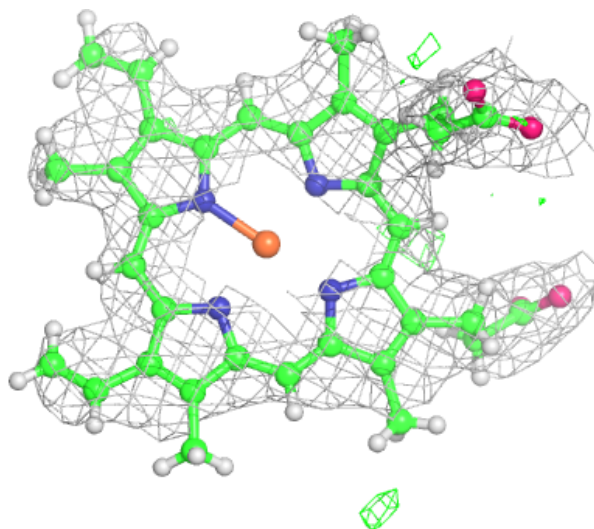
**Electron density around LHG d 408:**

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



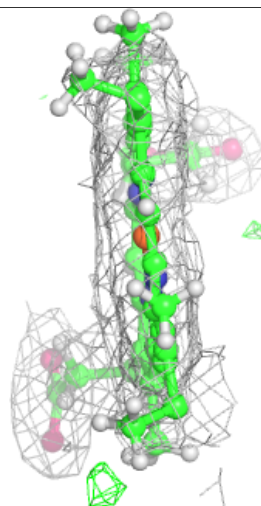
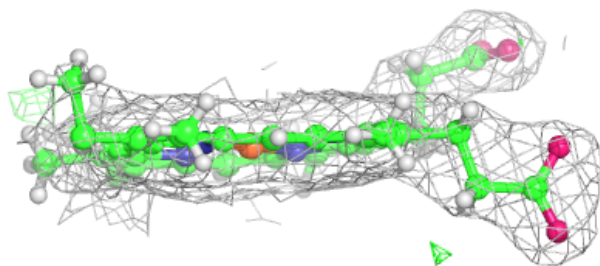
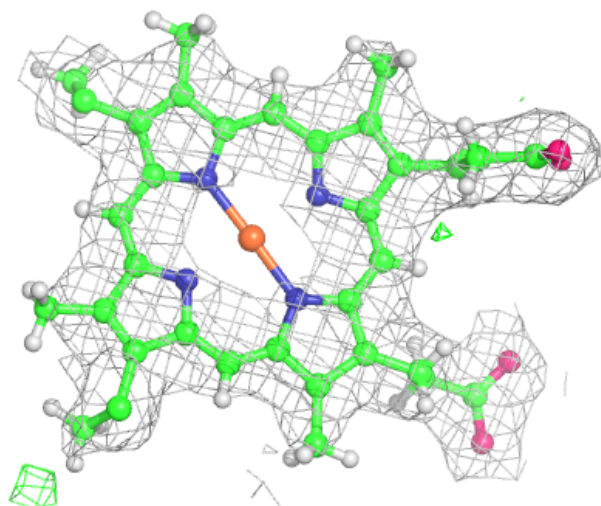
Electron density around HEM e 101:

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



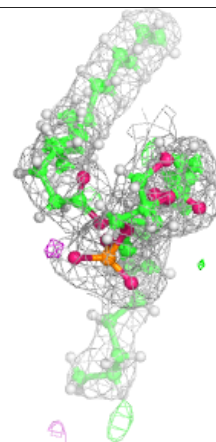
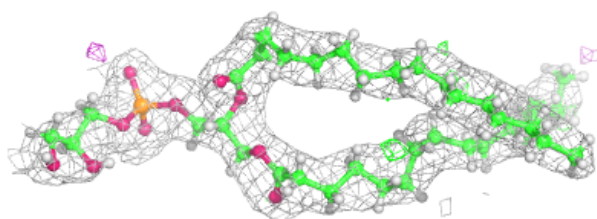
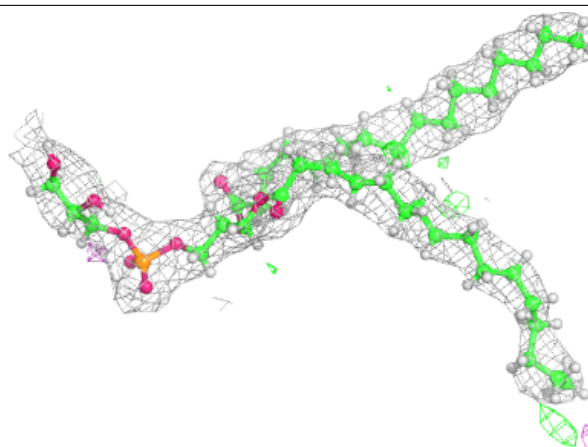
Electron density around HEC v 201:

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



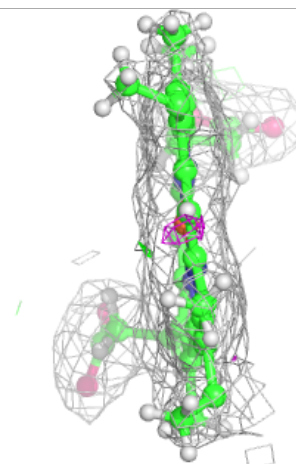
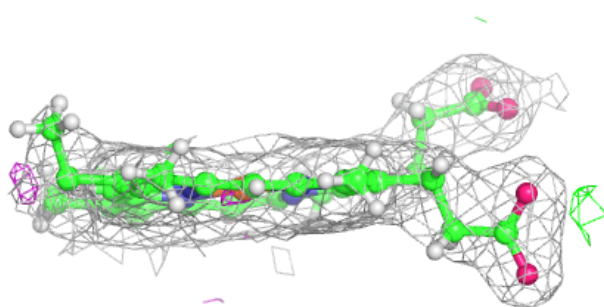
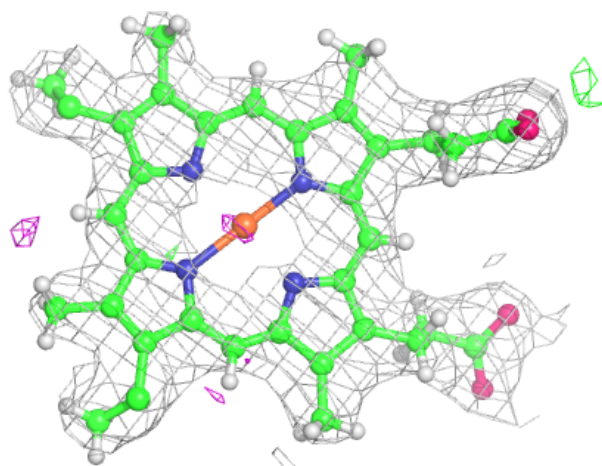
Electron density around LHG D 408:

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



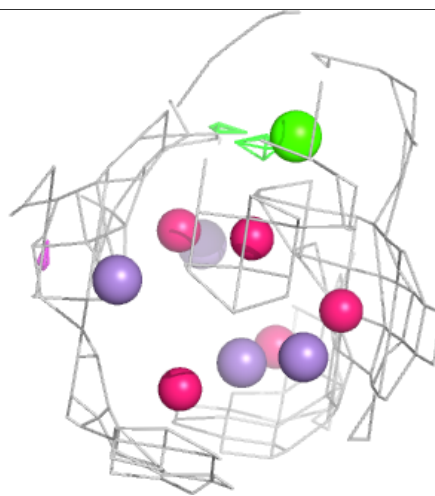
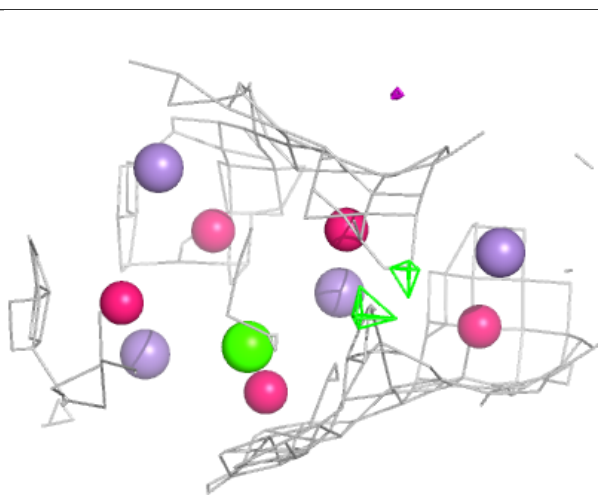
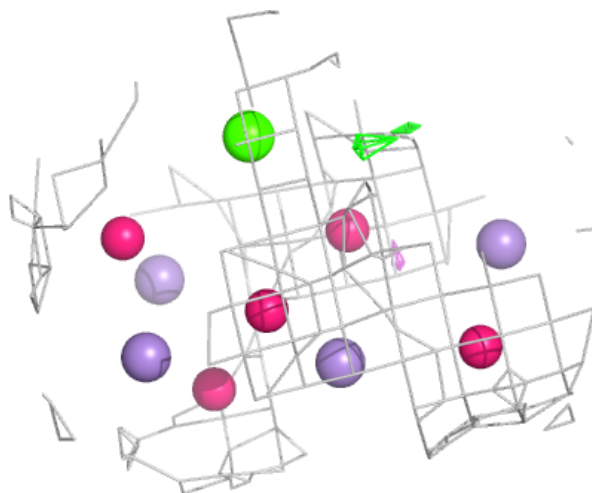
Electron density around HEC V 201:

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



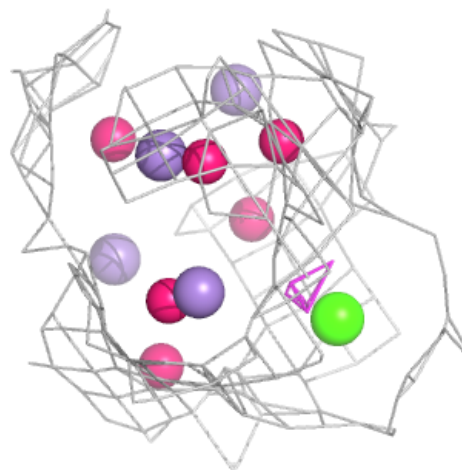
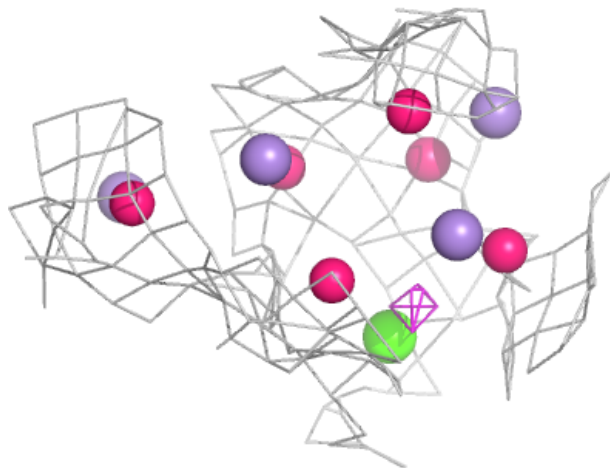
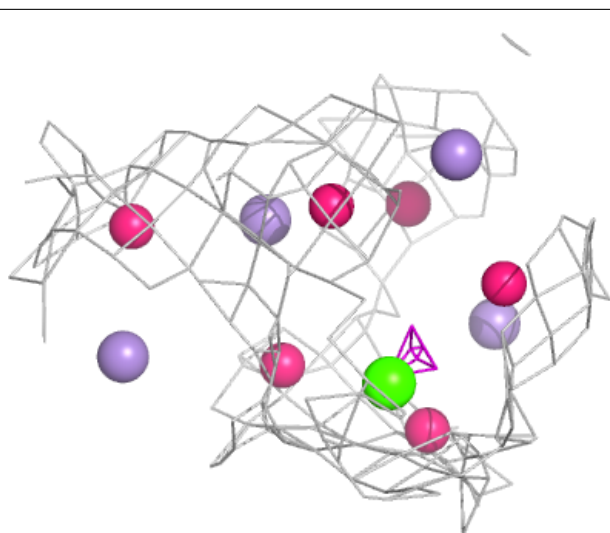
Electron density around OEX a 417 (A):

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



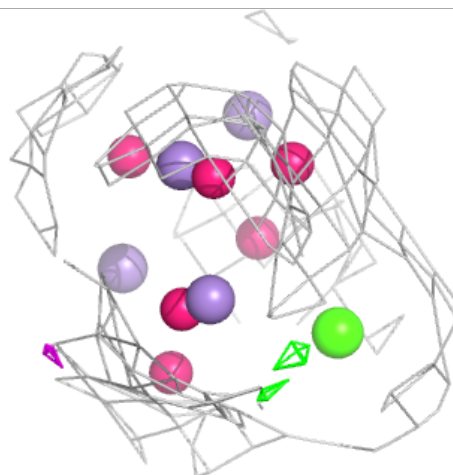
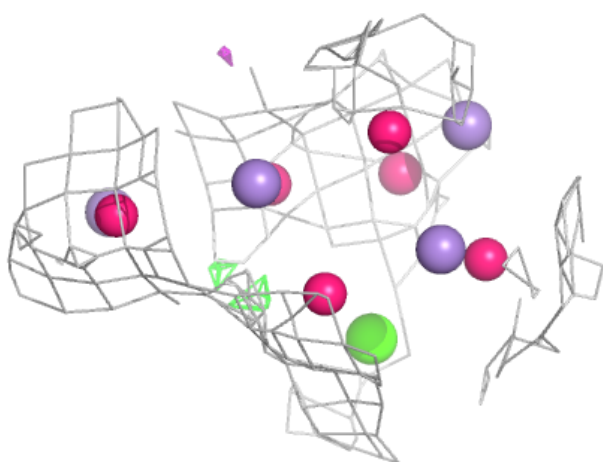
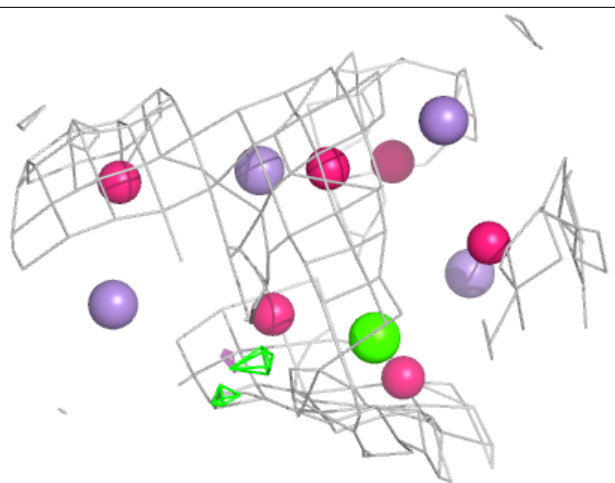
Electron density around OEY A 417 (B):

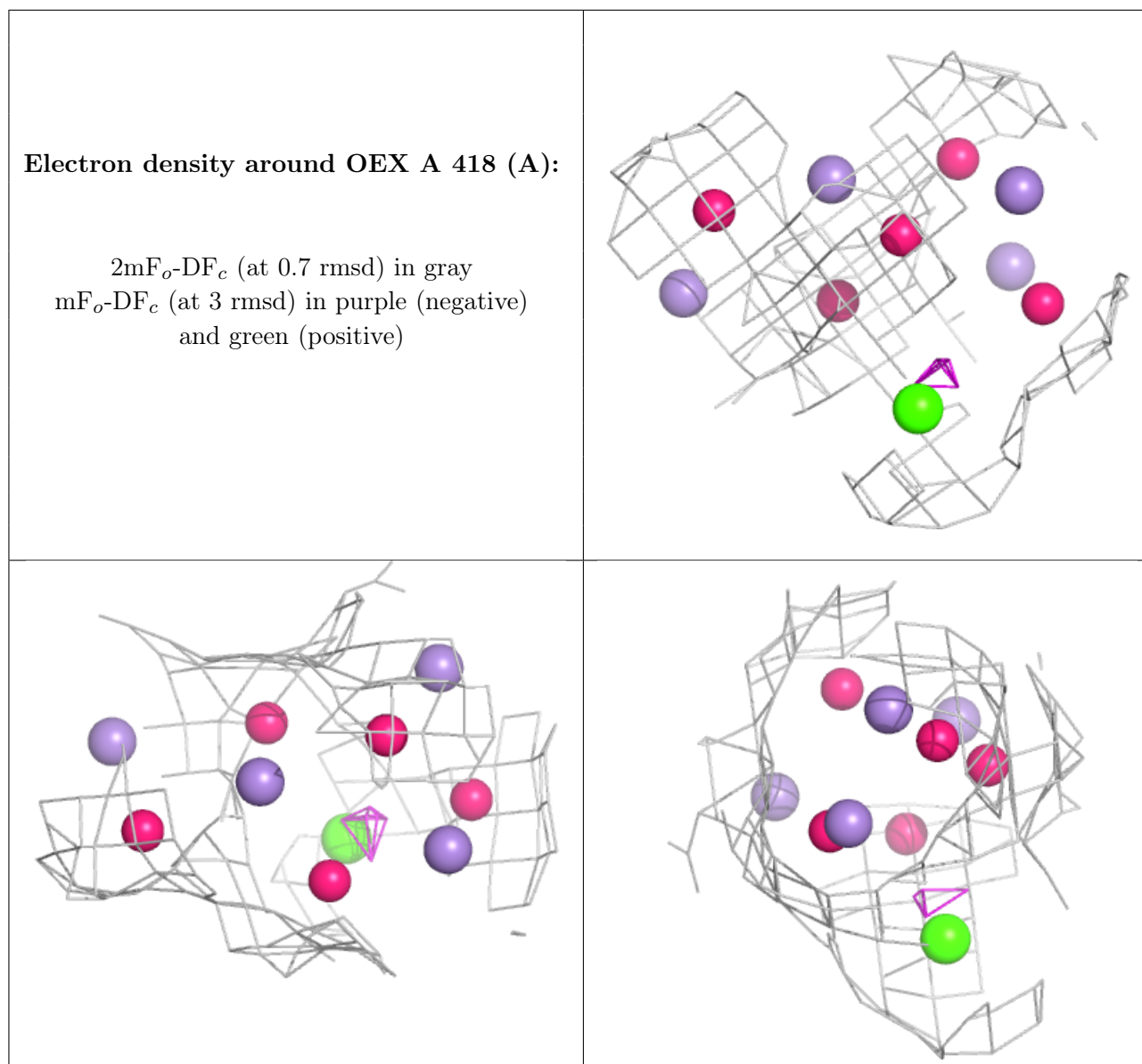
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEY a 418 (B):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.