



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:54 AM EDT

PDB ID : 7RF3 / pdb_00007rf3
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 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 : 2.26 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.015 (Gargrove)

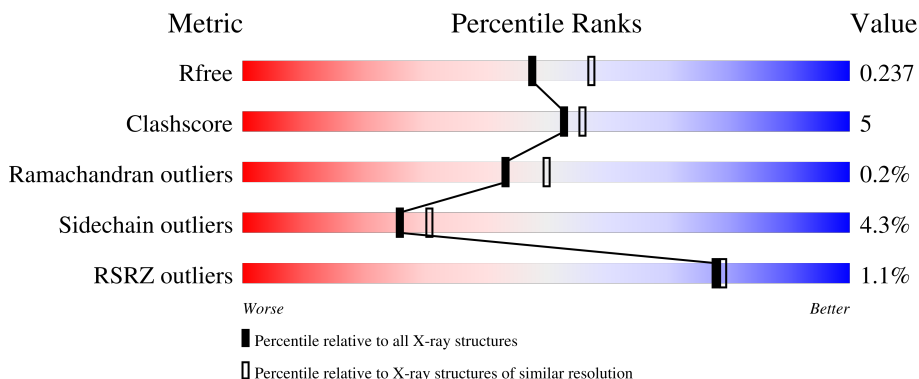
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

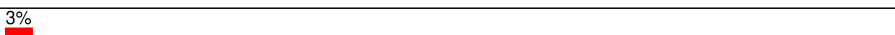
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	

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Mol	Chain	Length	Quality of chain
14	r	41	
15	T	32	
15	t	32	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103278 atoms, of which 51563 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

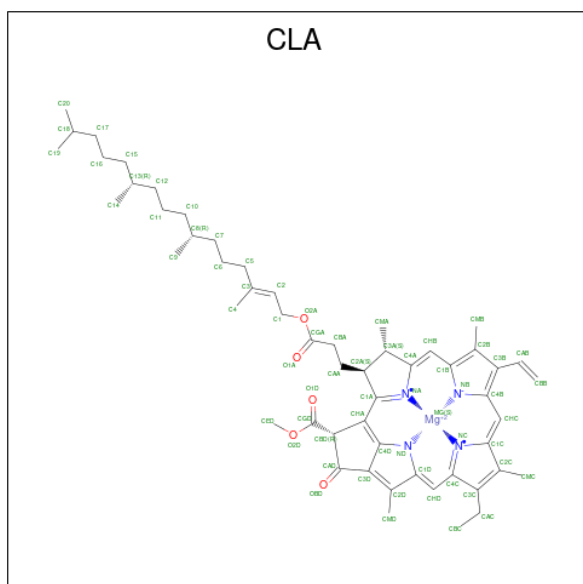
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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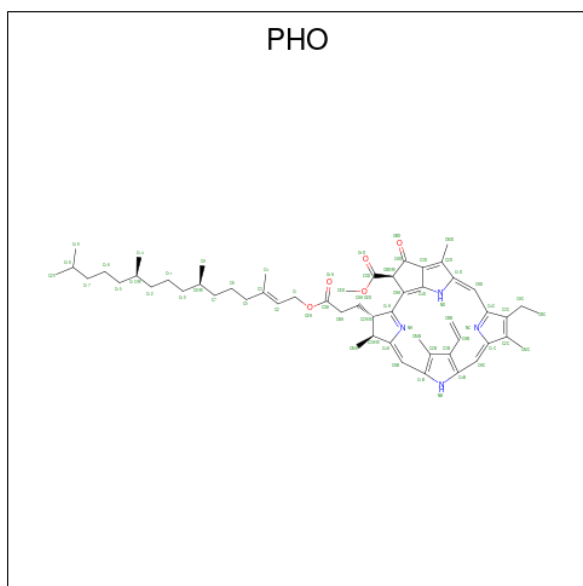
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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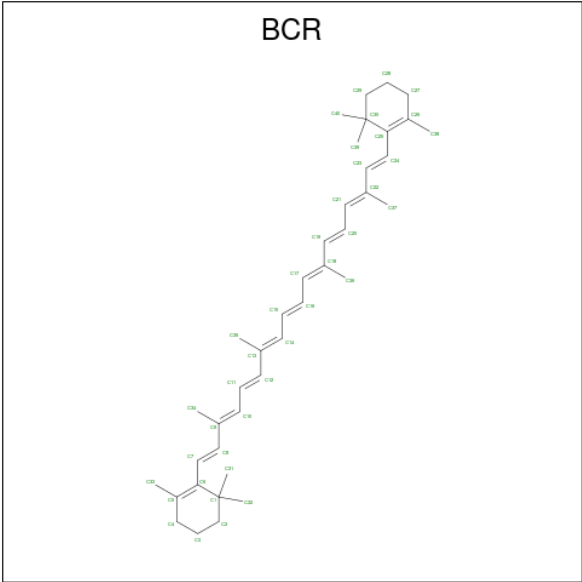
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

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



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

- Molecule 24 is BETA-CAROTENE (CCD ID: 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	Z	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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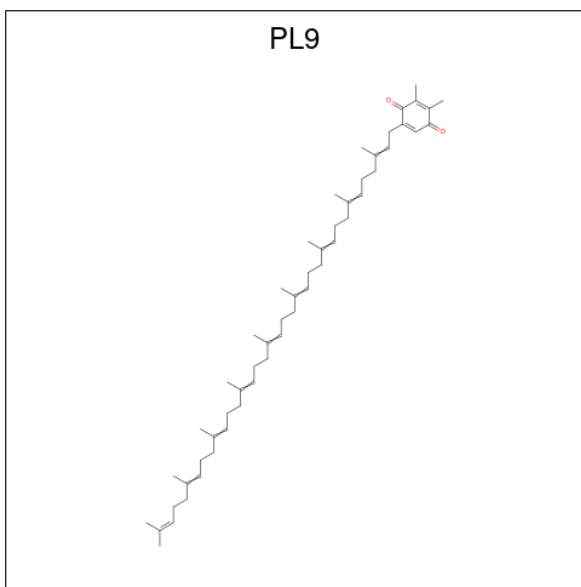
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	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 (CCD ID: CL) (formula: Cl).

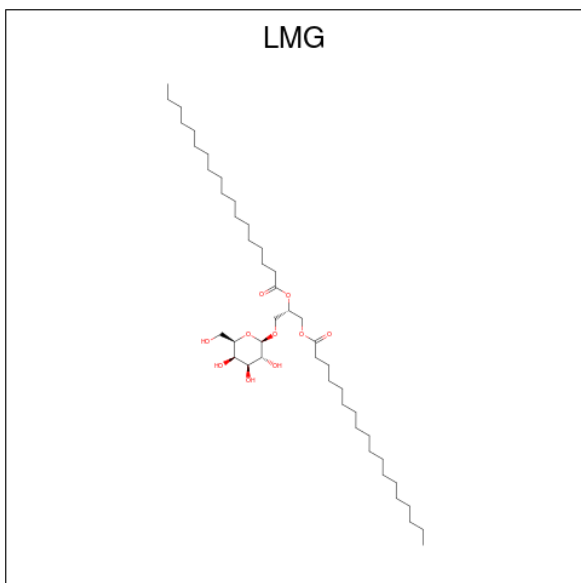
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

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



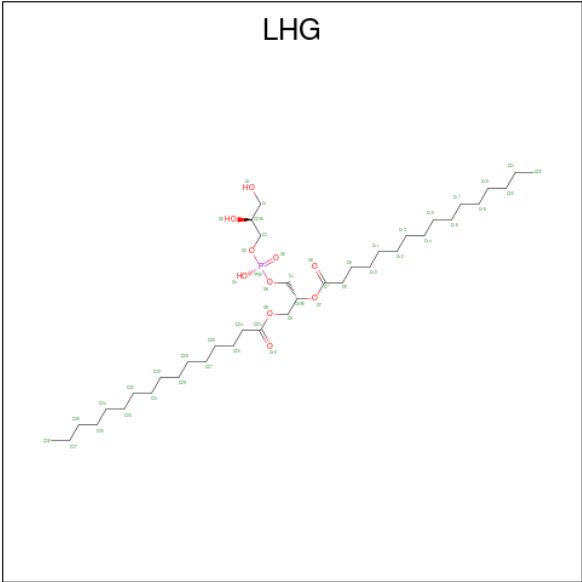
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



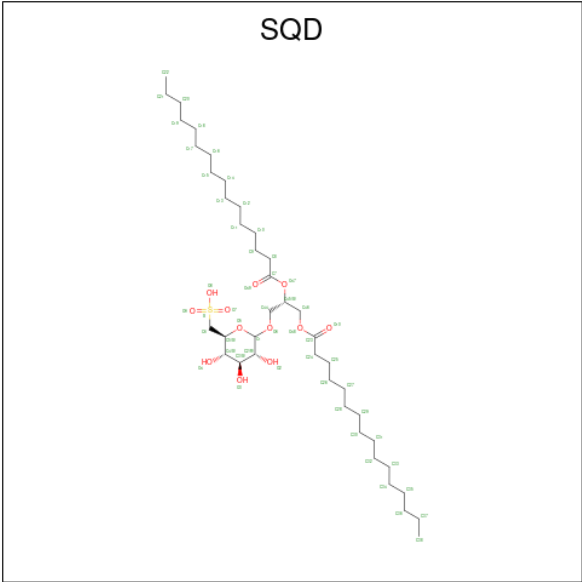
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



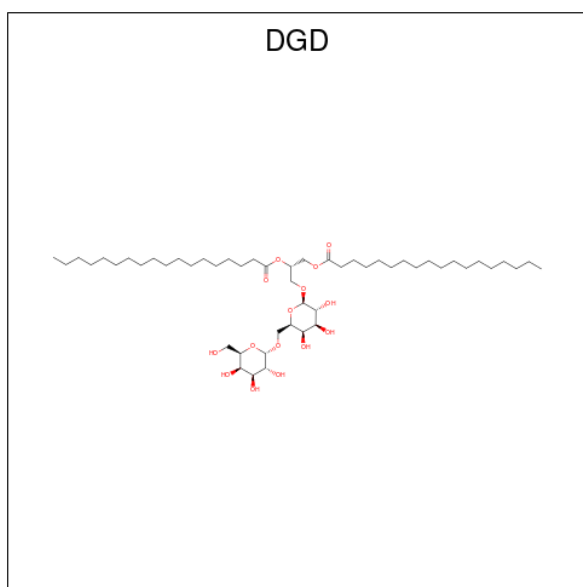
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	b	1	Total	C	H	O	P	0	0
			123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

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



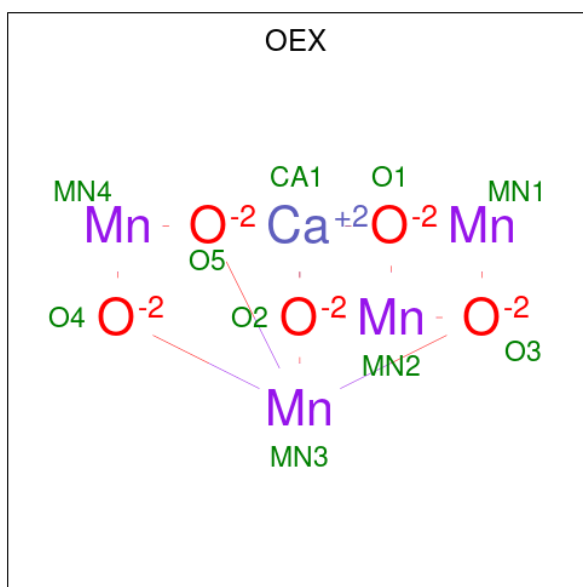
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



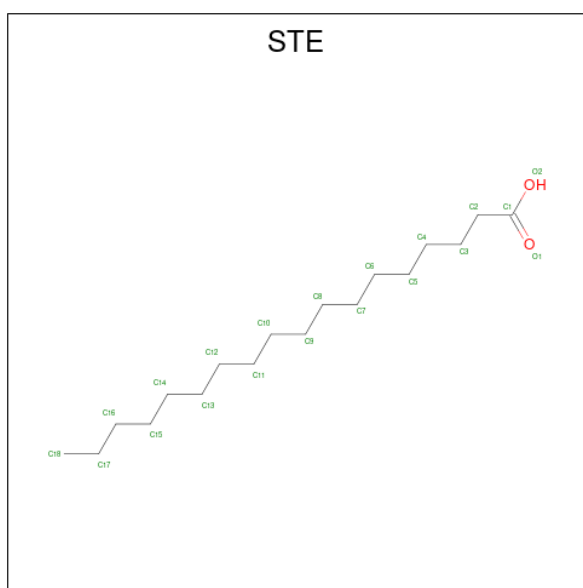
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	B	1	Total	C	H	O	0	0
			119	39	75	5		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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



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

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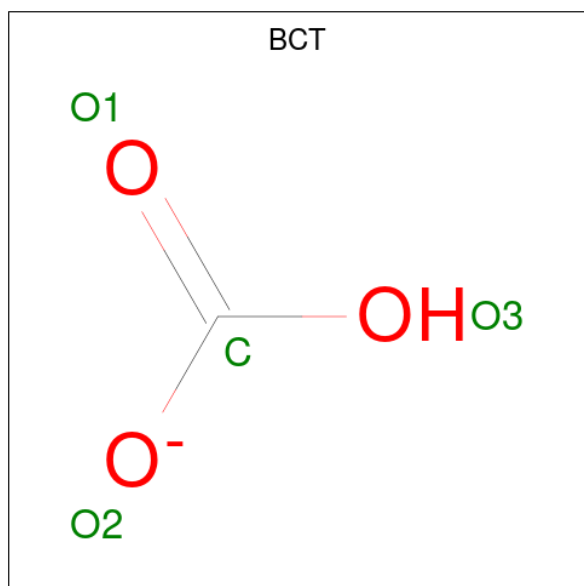
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 46 16 28 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 44 15 29	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0

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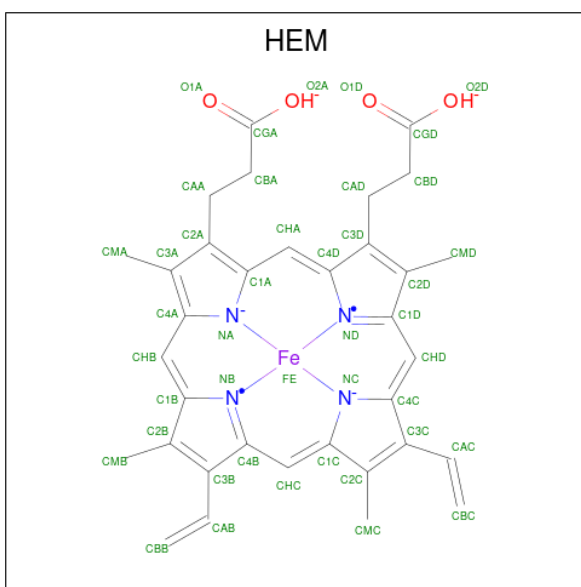
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	k	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



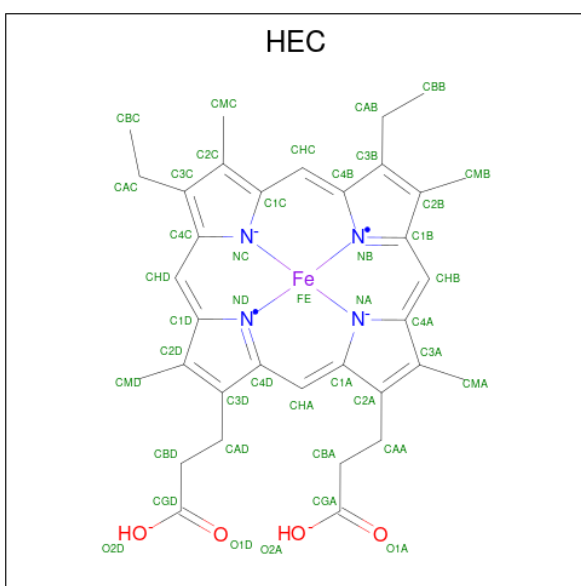
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	124	Total O 124 124	0	0
36	B	170	Total O 170 170	0	0
36	C	137	Total O 137 137	0	0
36	D	106	Total O 106 106	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	20	Total O 20 20	0	0
36	I	9	Total O 9 9	0	0
36	J	9	Total O 9 9	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	10	Total O 10 10	0	0
36	O	82	Total O 82 82	0	0
36	R	1	Total O 1 1	0	0
36	T	9	Total O 9 9	0	0
36	U	32	Total O 32 32	0	0
36	V	46	Total O 46 46	0	0
36	X	11	Total O 11 11	0	0
36	Y	3	Total O 3 3	0	0
36	Z	4	Total O 4 4	0	0
36	a	111	Total O 111 111	0	0

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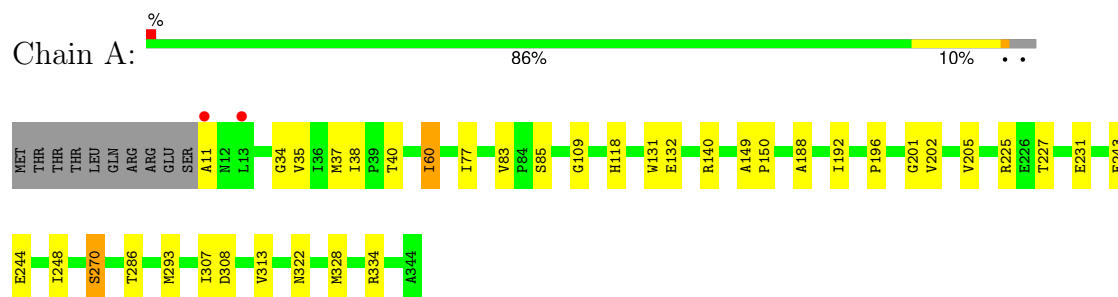
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	140	Total 140	O 140	0	0
36	c	115	Total 115	O 115	0	0
36	d	102	Total 102	O 102	0	0
36	e	19	Total 19	O 19	0	0
36	f	10	Total 10	O 10	0	0
36	h	22	Total 22	O 22	0	0
36	i	10	Total 10	O 10	0	0
36	j	10	Total 10	O 10	0	0
36	k	7	Total 7	O 7	0	0
36	l	7	Total 7	O 7	0	0
36	m	7	Total 7	O 7	0	0
36	o	79	Total 79	O 79	0	0
36	r	12	Total 12	O 12	0	0
36	t	10	Total 10	O 10	0	0
36	u	40	Total 40	O 40	0	0
36	v	39	Total 39	O 39	0	0
36	x	5	Total 5	O 5	0	0
36	y	5	Total 5	O 5	0	0
36	z	6	Total 6	O 6	0	0

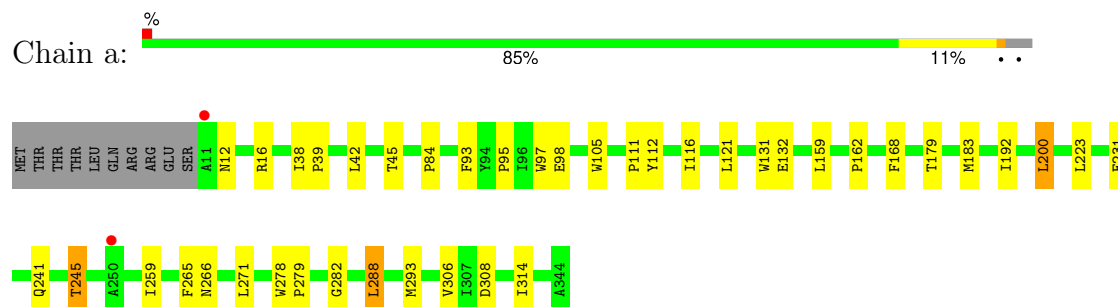
3 Residue-property plots [i](#)

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.

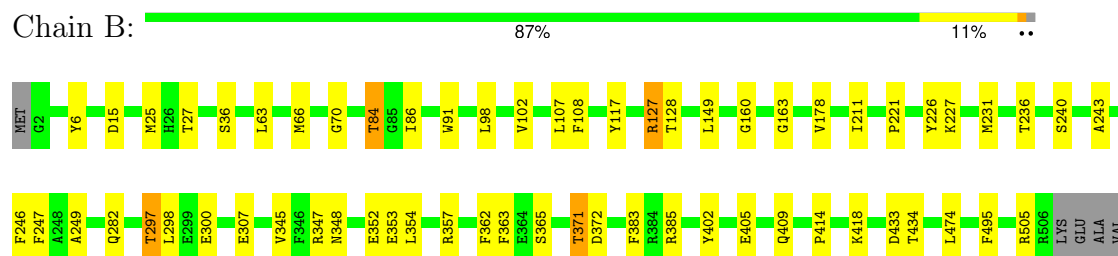
- Molecule 1: Photosystem II protein D1 1



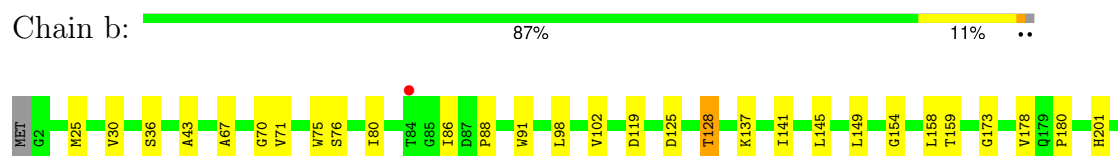
- Molecule 1: Photosystem II protein D1 1

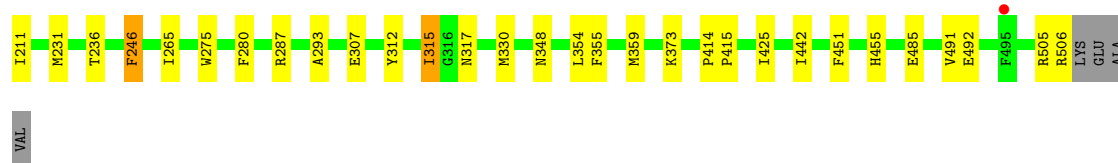


- Molecule 2: Photosystem II CP47 reaction center protein



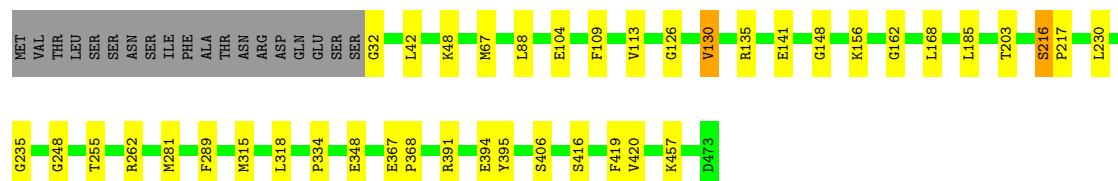
- Molecule 2: Photosystem II CP47 reaction center protein





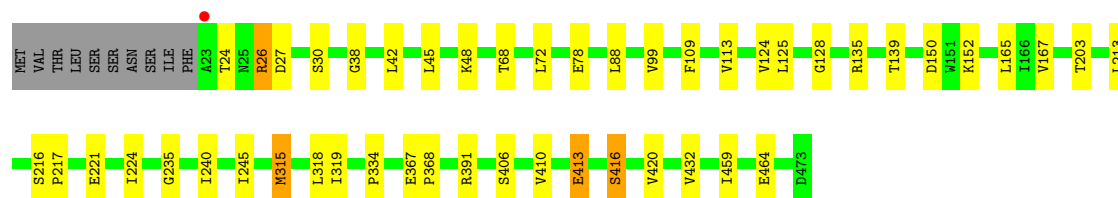
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



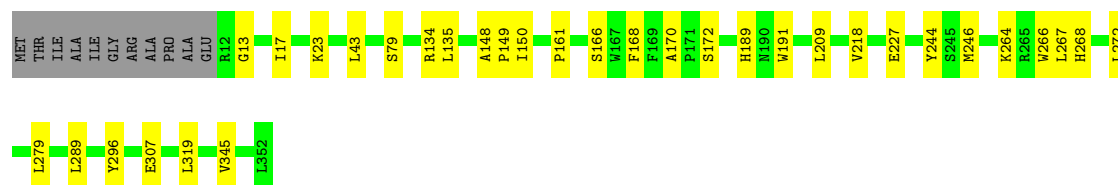
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% ..



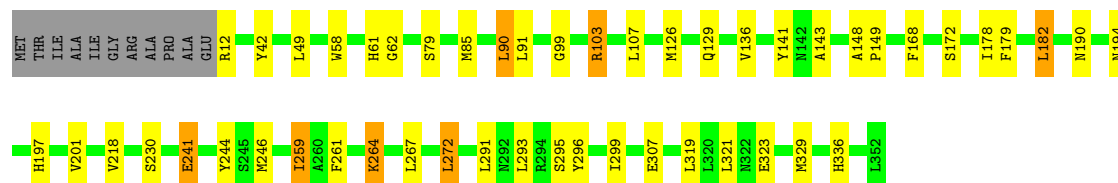
- Molecule 4: Photosystem II D2 protein

Chain D: 88% 9% .



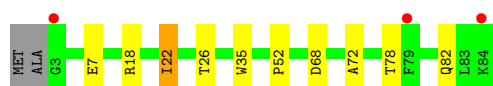
- Molecule 4: Photosystem II D2 protein

Chain d: 83% 12% ..



- Molecule 5: Cytochrome b559 subunit alpha

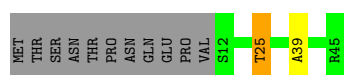
Chain E: 4% 86% 11% ..



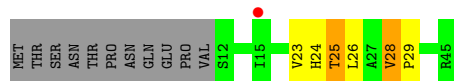
- Molecule 5: Cytochrome b559 subunit alpha



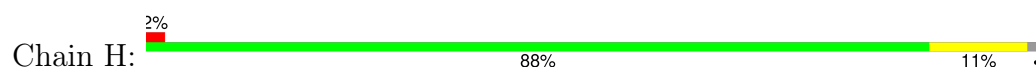
- Molecule 6: Cytochrome b559 subunit beta



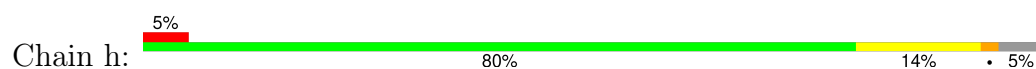
- Molecule 6: Cytochrome b559 subunit beta



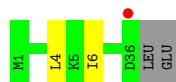
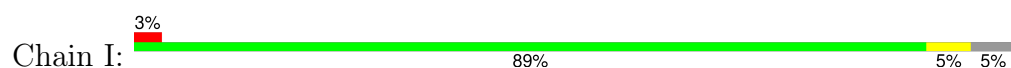
- Molecule 7: Photosystem II reaction center protein H



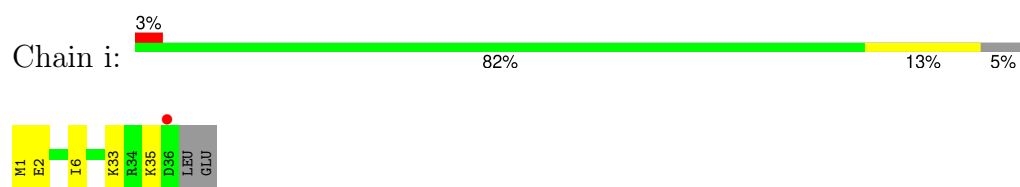
- Molecule 7: Photosystem II reaction center protein H



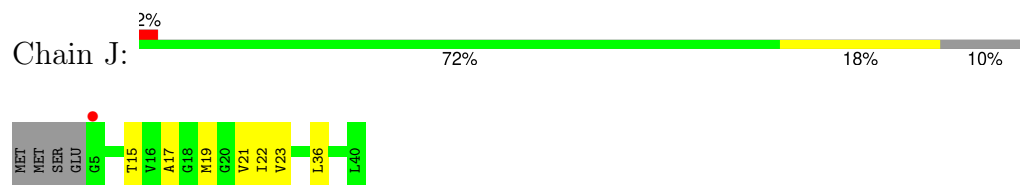
- Molecule 8: Photosystem II reaction center protein I



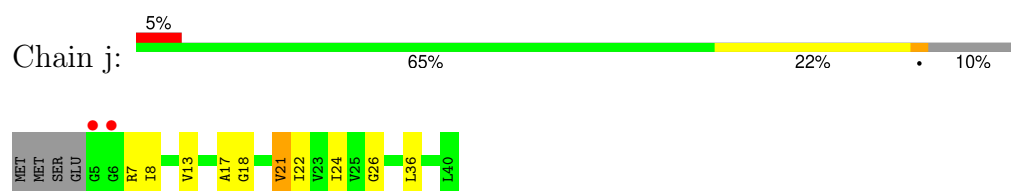
- Molecule 8: Photosystem II reaction center protein I



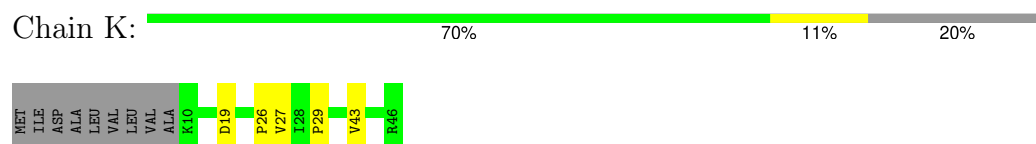
- Molecule 9: Photosystem II reaction center protein J



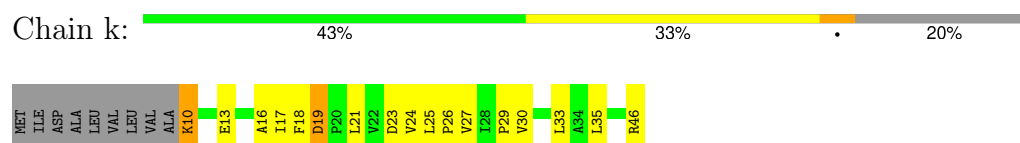
- Molecule 9: Photosystem II reaction center protein J



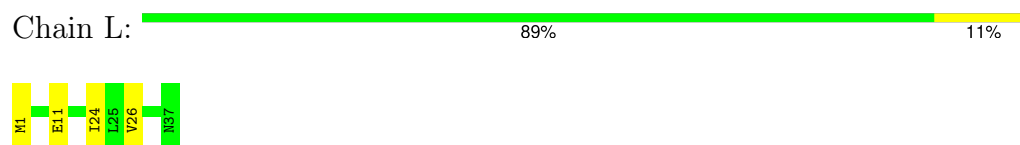
- Molecule 10: Photosystem II reaction center protein K



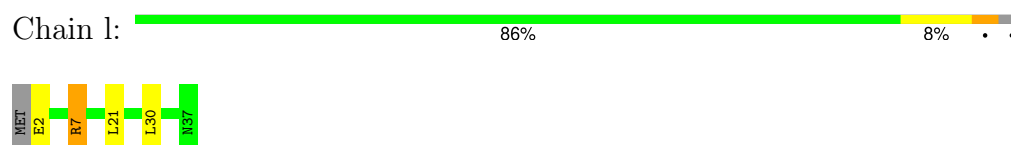
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



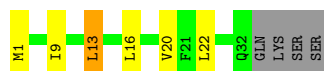
- Molecule 11: Photosystem II reaction center protein L



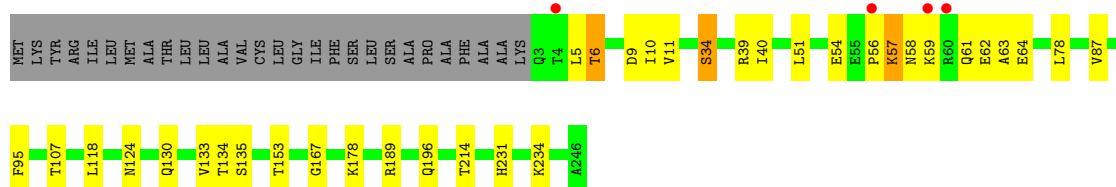
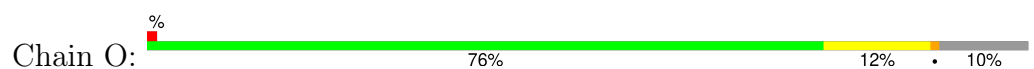
- Molecule 12: Photosystem II reaction center protein M



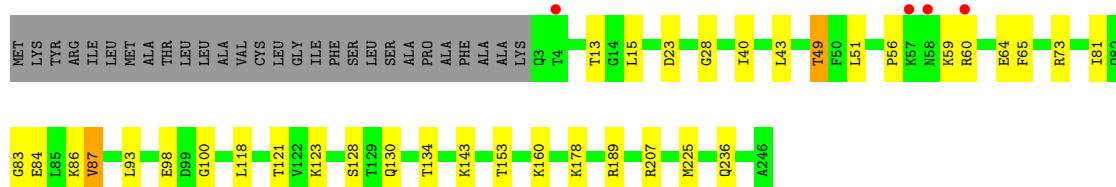
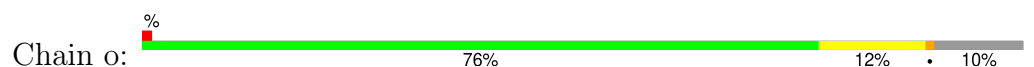
• Molecule 12: Photosystem II reaction center protein M



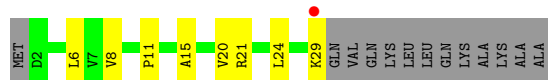
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• 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

Chain T:  81% 9% 6%



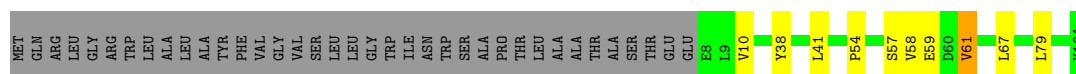
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 84% 9% 6%



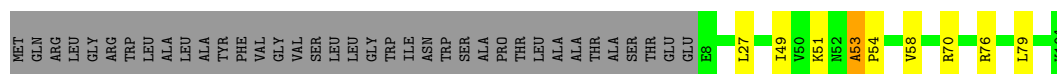
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  65% 7% 28%



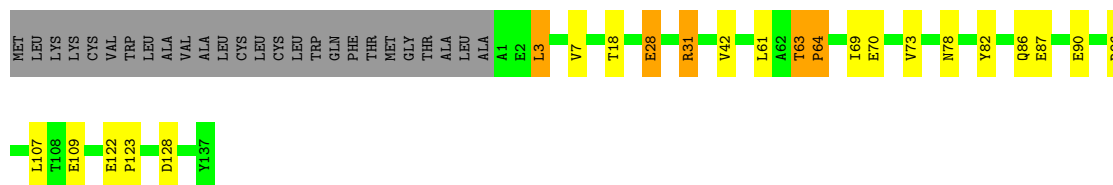
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  66% 6% 28%



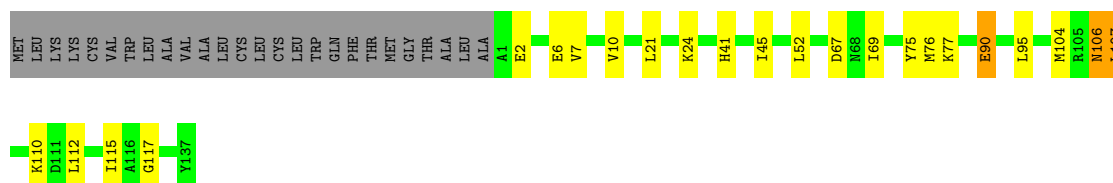
- Molecule 17: Cytochrome c-550

Chain V:  70% 11% 16%



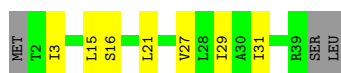
- Molecule 17: Cytochrome c-550

Chain v:  70% 12% 16%

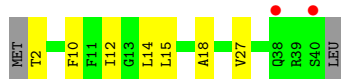
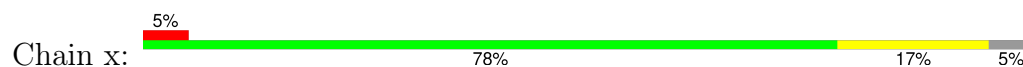


- Molecule 18: Photosystem II reaction center X protein

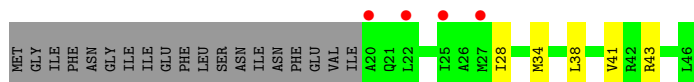
Chain X:  76% 17% 7%



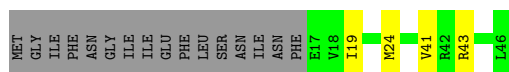
- Molecule 18: Photosystem II reaction center X protein



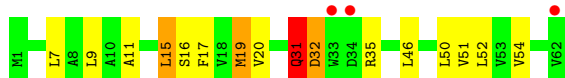
- Molecule 19: Photosystem II reaction center protein Ycf12



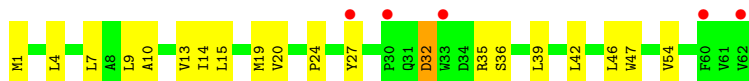
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26 33.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.54-2.26) 86.7 (33.54-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.238 0.179 , 0.237	Depositor DCC
R_{free} test set	3302 reflections (0.53%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	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	103278	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	1/2707 (0.0%)	0.67	0/3692
1	a	0.58	0/2704	0.65	0/3688
2	B	0.56	0/4161	0.63	0/5669
2	b	0.53	0/4118	0.62	0/5611
3	C	0.54	0/3547	0.62	0/4830
3	c	0.50	0/3619	0.60	0/4926
4	D	0.58	0/2812	0.64	0/3832
4	d	0.56	0/2821	0.65	0/3844
5	E	0.45	0/688	0.54	0/940
5	e	0.43	0/683	0.57	0/932
6	F	0.48	0/284	0.60	0/387
6	f	0.51	0/284	0.62	0/387
7	H	0.59	0/523	0.59	0/713
7	h	0.50	0/511	0.59	0/697
8	I	0.55	0/293	0.65	0/396
8	i	0.55	0/293	0.53	0/396
9	J	0.45	0/263	0.54	0/356
9	j	0.40	0/263	0.55	0/356
10	K	0.44	0/303	0.63	0/416
10	k	0.41	0/303	0.54	0/416
11	L	0.62	0/311	0.62	0/422
11	l	0.60	0/303	0.63	0/412
12	M	0.65	0/249	0.66	0/341
12	m	0.59	0/244	0.64	0/334
13	O	0.54	0/1904	0.65	0/2585
13	o	0.56	0/1905	0.64	0/2583
14	R	0.41	0/227	0.54	0/313
14	r	0.36	0/227	0.45	0/313
15	T	0.60	0/257	0.60	0/349
15	t	0.60	0/255	0.58	0/346
16	U	0.51	0/785	0.60	0/1064
16	u	0.54	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.54	0/1085	0.63	0/1473
17	v	0.52	0/1085	0.58	0/1473
18	X	0.45	0/284	0.58	0/384
18	x	0.39	0/289	0.49	0/391
19	Y	0.43	0/197	0.51	0/264
19	y	0.35	0/219	0.47	0/294
20	Z	0.40	0/490	0.50	0/669
20	z	0.35	0/488	0.44	0/666
All	All	0.54	1/42769 (0.0%)	0.62	0/58224

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	-7.55	1.50	1.54

There are no bond angle outliers.

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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2519	2519	23	0
1	a	2619	2510	2510	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4005	3873	3867	42	0
2	b	3978	3836	3836	37	0
3	C	3426	3355	3343	25	0
3	c	3500	3426	3426	28	0
4	D	2717	2621	2621	22	0
4	d	2723	2627	2627	31	0
5	E	666	651	651	7	0
5	e	664	648	648	18	0
6	F	275	282	282	2	0
6	f	275	282	282	5	0
7	H	510	532	532	5	0
7	h	498	518	518	5	0
8	I	296	311	311	0	0
8	i	296	311	311	2	0
9	J	257	268	268	5	0
9	j	257	268	268	7	0
10	K	293	305	305	1	0
10	k	293	305	305	12	0
11	L	304	316	316	4	0
11	l	296	304	304	1	0
12	M	256	269	269	9	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	20	0
13	o	1874	1846	1846	21	0
14	R	221	238	238	3	0
14	r	221	238	238	7	0
15	T	258	261	261	5	0
15	t	256	256	256	1	0
16	U	774	773	773	5	0
16	u	774	773	773	5	1
17	V	1064	1071	1073	11	1
17	v	1064	1071	1073	14	0
18	X	281	312	312	4	0
18	x	286	316	314	4	0
19	Y	196	217	217	2	0
19	y	218	241	241	2	0
20	Z	479	516	516	8	0
20	z	477	509	509	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	2	0
22	B	1035	1139	1139	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	839	922	922	8	0
22	D	195	216	216	3	0
22	a	260	288	288	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	15	0
22	d	130	144	144	4	0
23	A	64	74	74	0	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	40	56	56	0	0
24	B	120	168	168	4	0
24	C	40	56	56	1	0
24	D	40	56	56	1	0
24	H	40	56	56	0	0
24	K	80	112	112	2	0
24	T	40	56	56	3	0
24	Z	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	2	0
24	c	40	56	56	2	0
24	d	40	56	56	3	0
24	k	120	168	168	0	0
24	t	40	56	56	3	0
24	x	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	3	0
26	D	55	80	80	1	0
26	a	55	80	80	3	0
26	d	55	80	80	0	0
27	A	48	66	66	3	0
27	C	48	66	66	1	0
27	D	112	157	156	1	0
27	M	51	72	72	1	0
27	a	49	68	68	0	0
27	b	55	86	86	0	0
27	c	85	113	113	1	0
27	d	67	92	92	1	0
27	m	51	72	72	0	0
28	A	47	67	67	2	0
28	B	49	74	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	74	74	2	0
28	E	49	74	74	2	0
28	L	49	74	74	6	0
28	b	49	74	74	1	0
28	d	88	125	125	5	0
28	e	42	57	57	3	0
28	l	49	74	74	1	0
29	A	91	135	135	5	0
29	B	54	78	77	1	0
29	F	36	45	45	0	0
29	L	49	65	64	2	0
29	a	90	133	132	6	0
29	f	41	48	48	2	0
30	A	66	96	96	3	0
30	B	44	75	75	4	0
30	C	186	245	243	6	0
30	H	62	82	81	1	0
30	c	186	246	244	4	0
30	h	62	82	81	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	75	117	114	5	0
32	C	40	63	60	0	0
32	D	20	35	35	3	0
32	E	12	16	16	0	0
32	H	18	35	35	3	0
32	I	15	26	26	1	0
32	J	12	16	16	1	0
32	M	40	67	64	1	0
32	a	12	16	16	0	0
32	b	82	141	138	5	0
32	c	20	35	35	0	0
32	d	17	26	26	0	0
32	j	12	16	16	1	0
32	k	12	16	16	2	0
32	l	18	35	35	1	0
32	m	12	16	16	0	0
32	t	24	36	36	0	0
32	x	20	35	35	2	0
33	D	4	1	1	1	0
33	a	4	1	1	0	0
34	F	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	43	30	30	4	0
35	V	43	30	30	1	0
35	v	43	30	30	0	0
36	A	124	0	0	7	0
36	B	170	0	0	13	0
36	C	137	0	0	4	0
36	D	106	0	0	6	0
36	E	26	0	0	1	0
36	F	8	0	0	0	0
36	H	20	0	0	1	0
36	I	9	0	0	0	0
36	J	9	0	0	1	0
36	K	7	0	0	0	0
36	L	11	0	0	1	0
36	M	10	0	0	2	0
36	O	82	0	0	3	0
36	R	1	0	0	0	0
36	T	9	0	0	4	0
36	U	32	0	0	1	0
36	V	46	0	0	3	0
36	X	11	0	0	0	0
36	Y	3	0	0	0	0
36	Z	4	0	0	0	0
36	a	111	0	0	4	0
36	b	140	0	0	5	0
36	c	115	0	0	1	0
36	d	102	0	0	1	0
36	e	19	0	0	3	0
36	f	10	0	0	0	0
36	h	22	0	0	0	0
36	i	10	0	0	0	0
36	j	10	0	0	1	0
36	k	7	0	0	2	0
36	l	7	0	0	1	0
36	m	7	0	0	0	0
36	o	79	0	0	5	0
36	r	12	0	0	0	0
36	t	10	0	0	0	0
36	u	40	0	0	0	0
36	v	39	0	0	3	0
36	x	5	0	0	0	0
36	y	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	6	0	0	0	0
All	All	51715	51563	51525	508	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 508 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:OD1	36:B:704:HOH:O	1.88	0.92
2:B:354:LEU:O	36:B:702:HOH:O	1.87	0.91
2:B:84:THR:O	36:B:703:HOH:O	1.87	0.91
11:L:11:GLU:OE1	36:L:201:HOH:O	1.88	0.90
1:a:266:ASN:ND2	36:a:501:HOH:O	2.01	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:70:GLU:OE2	16:u:76:ARG:HE[3_457]	1.56	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	40
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	442/461 (96%)	431 (98%)	10 (2%)	1 (0%)	43	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	50
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	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%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
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%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	232 (96%)	8 (3%)	3 (1%)	10	7
13	o	242/272 (89%)	229 (95%)	11 (4%)	2 (1%)	16	14
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%)	27 (96%)	1 (4%)	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	17
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	1
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	3
20	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5231/5700 (92%)	5087 (97%)	132 (2%)	12 (0%)	43	50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	264 (98%)	6 (2%)	45	56
1	a	269/280 (96%)	260 (97%)	9 (3%)	33	42
2	B	408/407 (100%)	395 (97%)	13 (3%)	34	43
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	49
3	C	346/362 (96%)	339 (98%)	7 (2%)	48	59
3	c	354/362 (98%)	338 (96%)	16 (4%)	24	29
4	D	276/283 (98%)	272 (99%)	4 (1%)	59	70
4	d	277/283 (98%)	262 (95%)	15 (5%)	20	21
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	20
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	11
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	16
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	20 (83%)	4 (17%)	2	0
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
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	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	12
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	12
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	24
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	35
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	34
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	39
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	74
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	14
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	18
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	6
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	14
19	Y	19/37 (51%)	18 (95%)	1 (5%)	20	22
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	29
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4321/4654 (93%)	4134 (96%)	187 (4%)	26	31

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	416	SER
9	j	7	ARG
4	d	178	ILE
4	d	329	MET
10	k	35	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
6	f	44	GLN
13	o	61	GLN
13	O	88	ASN
13	O	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	1.35	2 (25%)
8	FME	I	1	8	8,9,10	1.05	0	8,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.86	0	8,9,11	1.28	1 (12%)
12	FME	m	1	12	8,9,10	1.12	1 (12%)	8,9,11	0.58	0
8	FME	i	1	8	8,9,10	0.88	0	8,9,11	0.92	0
15	FME	t	1	15	8,9,10	1.17	1 (12%)	8,9,11	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.51	1.42	1.46
12	m	1	FME	CA-N	-2.48	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CB-CA-N	2.38	114.85	110.52
12	M	1	FME	CA-N-CN	-2.37	119.18	122.82
15	T	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic - leaving 180 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	A	405	1	58,62,73	1.63	8 (13%)	68,99,113	1.46	8 (11%)
22	CLA	B	609	2	69,73,73	1.21	9 (13%)	82,113,113	1.30	7 (8%)
22	CLA	c	511	3	69,73,73	1.63	11 (15%)	82,113,113	1.30	4 (4%)
32	STE	a	415	-	11,11,19	0.96	1 (9%)	11,11,19	0.97	1 (9%)
22	CLA	b	614	2	69,73,73	1.49	11 (15%)	82,113,113	1.34	7 (8%)
22	CLA	c	501	3	69,73,73	1.18	9 (13%)	82,113,113	1.48	8 (9%)
24	BCR	b	617	-	41,41,41	1.24	3 (7%)	56,56,56	1.37	8 (14%)
24	BCR	k	103	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	7 (12%)
27	LMG	D	411	-	26,26,55	0.95	2 (7%)	26,26,63	1.34	3 (11%)
29	SQD	F	102	-	34,36,54	0.95	3 (8%)	42,45,65	2.00	11 (26%)
22	CLA	d	402	4	69,73,73	1.24	6 (8%)	82,113,113	1.36	6 (7%)
30	DGD	C	516	-	63,63,67	1.24	7 (11%)	77,77,81	1.48	12 (15%)
30	DGD	h	101	-	63,63,67	1.22	10 (15%)	77,77,81	1.48	14 (18%)
22	CLA	B	614	2	69,73,73	1.43	6 (8%)	82,113,113	1.46	11 (13%)
22	CLA	b	615	2	69,73,73	1.57	11 (15%)	82,113,113	1.28	8 (9%)
32	STE	B	620	-	16,16,19	0.86	1 (6%)	16,16,19	0.87	1 (6%)
23	PHO	a	404	-	58,69,69	1.97	12 (20%)	55,99,99	1.60	9 (16%)
28	LHG	d	406	-	48,48,48	0.74	1 (2%)	51,54,54	1.27	5 (9%)
28	LHG	E	101	-	48,48,48	0.97	4 (8%)	51,54,54	1.26	8 (15%)
22	CLA	c	508	3	68,72,73	1.30	12 (17%)	80,111,113	1.41	10 (12%)
29	SQD	A	412	-	50,52,54	1.06	5 (10%)	60,63,65	1.94	10 (16%)
22	CLA	C	510	3	69,73,73	1.36	12 (17%)	82,113,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	x	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	b	603	2	69,73,73	1.27	11 (15%)	82,113,113	1.52	12 (14%)
22	CLA	b	602	2	69,73,73	1.25	8 (11%)	82,113,113	1.51	11 (13%)
35	HEC	V	201	17	50,50,50	1.65	3 (6%)	68,82,82	1.44	14 (20%)
22	CLA	B	610	36	69,73,73	1.33	8 (11%)	82,113,113	1.27	8 (9%)
27	LMG	d	409	-	44,44,55	1.05	4 (9%)	52,52,63	1.36	6 (11%)
32	STE	B	627	-	11,11,19	0.78	0	11,11,19	1.09	1 (9%)
26	PL9	a	410	-	55,55,55	0.85	2 (3%)	68,69,69	1.74	14 (20%)
24	BCR	a	406	-	41,41,41	1.11	4 (9%)	56,56,56	1.17	2 (3%)
22	CLA	a	411	36	69,73,73	1.29	10 (14%)	82,113,113	1.49	11 (13%)
32	STE	M	104	-	14,14,19	0.41	0	13,13,19	0.83	0
27	LMG	m	101	-	51,51,55	1.09	4 (7%)	59,59,63	1.47	8 (13%)
32	STE	b	626	-	9,9,19	0.43	0	8,8,19	0.67	0
24	BCR	T	101	-	41,41,41	1.26	5 (12%)	56,56,56	1.34	5 (8%)
32	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.74	0
24	BCR	Z	101	-	41,41,41	1.14	4 (9%)	56,56,56	1.46	10 (17%)
26	PL9	D	407	-	55,55,55	1.47	8 (14%)	68,69,69	1.69	14 (20%)
22	CLA	c	502	3	69,73,73	1.26	11 (15%)	82,113,113	1.25	11 (13%)
22	CLA	d	403	4	69,73,73	1.26	10 (14%)	82,113,113	1.13	8 (9%)
22	CLA	b	608	2	69,73,73	1.19	7 (10%)	82,113,113	1.09	6 (7%)
24	BCR	A	406	-	41,41,41	1.07	3 (7%)	56,56,56	1.39	11 (19%)
27	LMG	C	518	-	48,48,55	1.05	6 (12%)	56,56,63	1.37	5 (8%)
32	STE	B	626	-	15,15,19	0.47	0	14,14,19	0.72	0
24	BCR	H	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.36	8 (14%)
22	CLA	C	503	3	69,73,73	1.50	8 (11%)	82,113,113	1.73	8 (9%)
22	CLA	b	606	2	69,73,73	1.42	6 (8%)	82,113,113	1.52	5 (6%)
24	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.20	6 (10%)
32	STE	B	625	-	17,17,19	0.76	0	17,17,19	0.95	0
28	LHG	d	407	-	38,38,48	0.84	2 (5%)	41,44,54	1.21	2 (4%)
22	CLA	b	604	2	69,73,73	1.12	8 (11%)	82,113,113	1.55	9 (10%)
30	DGD	A	414	-	67,67,67	1.23	8 (11%)	81,81,81	1.32	9 (11%)
22	CLA	c	505	3	69,73,73	1.08	7 (10%)	82,113,113	1.29	6 (7%)
28	LHG	A	411	-	46,46,48	1.02	3 (6%)	49,52,54	1.25	3 (6%)
22	CLA	b	611	2	69,73,73	1.25	8 (11%)	82,113,113	1.43	8 (9%)
22	CLA	B	615	2	69,73,73	1.30	8 (11%)	82,113,113	1.34	10 (12%)
32	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	510	3	69,73,73	1.43	8 (11%)	82,113,113	1.39	10 (12%)
22	CLA	c	512	3	69,73,73	1.29	9 (13%)	82,113,113	1.48	13 (15%)
32	STE	l	102	-	17,17,19	0.43	0	16,16,19	0.79	0
27	LMG	b	622	-	55,55,55	1.13	6 (10%)	63,63,63	1.46	8 (12%)
22	CLA	D	403	4	69,73,73	1.23	7 (10%)	82,113,113	1.44	9 (10%)
30	DGD	c	515	-	63,63,67	1.14	7 (11%)	77,77,81	1.37	10 (12%)
22	CLA	B	606	2	69,73,73	1.40	5 (7%)	82,113,113	1.58	7 (8%)
23	PHO	A	404	-	58,69,69	1.79	12 (20%)	55,99,99	1.73	13 (23%)
24	BCR	b	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	8 (14%)
22	CLA	B	602	2	69,73,73	1.40	9 (13%)	82,113,113	1.31	12 (14%)
27	LMG	c	518	-	37,37,55	0.98	1 (2%)	45,45,63	1.34	7 (15%)
32	STE	D	412	-	19,19,19	0.65	0	19,19,19	1.21	0
32	STE	b	625	-	19,19,19	0.80	1 (5%)	19,19,19	0.87	0
32	STE	M	102	-	14,14,19	0.75	0	14,14,19	1.16	2 (14%)
22	CLA	C	501	3	69,73,73	1.46	10 (14%)	82,113,113	1.28	9 (10%)
24	BCR	K	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.28	6 (10%)
30	DGD	C	517	-	63,63,67	1.16	6 (9%)	77,77,81	1.34	11 (14%)
22	CLA	B	613	2	69,73,73	1.32	10 (14%)	82,113,113	1.34	9 (10%)
32	STE	d	410	-	16,16,19	0.65	0	16,16,19	1.04	0
35	HEC	v	201	17	50,50,50	1.62	5 (10%)	68,82,82	1.41	7 (10%)
24	BCR	B	619	-	41,41,41	1.32	3 (7%)	56,56,56	1.44	8 (14%)
22	CLA	C	505	3	69,73,73	1.39	10 (14%)	82,113,113	1.33	10 (12%)
22	CLA	B	604	2	69,73,73	1.33	9 (13%)	82,113,113	1.66	16 (19%)
24	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.12	2 (3%)
22	CLA	b	609	2	69,73,73	1.50	10 (14%)	82,113,113	1.48	9 (10%)
32	STE	t	103	-	9,9,19	0.41	0	8,8,19	0.64	0
27	LMG	A	410	-	48,48,55	0.94	3 (6%)	56,56,63	1.29	5 (8%)
22	CLA	c	504	36	64,68,73	1.24	9 (14%)	76,107,113	1.25	7 (9%)
22	CLA	c	506	3	69,73,73	1.25	9 (13%)	82,113,113	1.19	6 (7%)
23	PHO	D	401	-	58,69,69	2.07	12 (20%)	55,99,99	1.41	8 (14%)
24	BCR	b	618	-	41,41,41	1.34	5 (12%)	56,56,56	1.32	10 (17%)
24	BCR	D	406	-	41,41,41	1.23	2 (4%)	56,56,56	1.16	5 (8%)
28	LHG	L	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.18	4 (7%)
22	CLA	B	608	2	69,73,73	1.46	8 (11%)	82,113,113	1.33	13 (15%)
28	LHG	b	623	-	48,48,48	1.02	4 (8%)	51,54,54	1.26	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	610	36	69,73,73	1.26	9 (13%)	82,113,113	1.29	10 (12%)
29	SQD	L	101	-	47,49,54	0.95	2 (4%)	57,60,65	2.19	16 (28%)
32	STE	m	102	-	11,11,19	0.65	0	11,11,19	1.28	1 (9%)
22	CLA	C	504	36	63,67,73	1.24	9 (14%)	74,105,113	1.24	7 (9%)
22	CLA	C	506	3	69,73,73	1.21	7 (10%)	82,113,113	1.15	8 (9%)
29	SQD	a	413	-	35,35,54	1.11	2 (5%)	37,37,65	1.34	4 (10%)
29	SQD	A	413	-	38,38,54	1.06	3 (7%)	40,40,65	1.54	6 (15%)
32	STE	c	519	-	19,19,19	0.61	0	19,19,19	1.21	1 (5%)
32	STE	j	101	-	11,11,19	0.99	0	11,11,19	0.86	0
27	LMG	a	414	-	49,49,55	0.92	2 (4%)	57,57,63	1.36	5 (8%)
28	LHG	e	102	-	41,41,48	0.94	3 (7%)	44,47,54	1.32	4 (9%)
22	CLA	D	404	36	69,73,73	1.14	4 (5%)	82,113,113	1.30	7 (8%)
22	CLA	A	402	1	69,73,73	1.41	7 (10%)	82,113,113	1.27	8 (9%)
32	STE	x	102	-	19,19,19	0.66	0	19,19,19	1.13	1 (5%)
31	OEX	a	416	3,1,36	0,14,14	-	-	-	-	-
24	BCR	B	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.31	8 (14%)
22	CLA	B	611	2	69,73,73	1.19	9 (13%)	82,113,113	1.37	11 (13%)
24	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
29	SQD	B	622	-	52,54,54	0.98	3 (5%)	62,65,65	1.89	13 (20%)
22	CLA	a	403	36	69,73,73	1.26	8 (11%)	82,113,113	1.48	14 (17%)
32	STE	C	519	-	11,11,19	0.81	0	11,11,19	1.42	2 (18%)
32	STE	b	621	-	19,19,19	0.68	0	19,19,19	0.90	0
22	CLA	C	507	36	69,73,73	1.12	7 (10%)	82,113,113	1.29	7 (8%)
24	BCR	C	514	-	41,41,41	1.27	5 (12%)	56,56,56	1.27	4 (7%)
26	PL9	A	409	-	55,55,55	1.12	2 (3%)	68,69,69	1.66	13 (19%)
33	BCT	a	409	21	3,3,3	1.35	0	2,3,3	3.77	2 (100%)
22	CLA	b	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.27	9 (10%)
32	STE	b	624	-	15,15,19	0.93	1 (6%)	15,15,19	0.73	0
30	DGD	H	102	-	63,63,67	1.43	14 (22%)	77,77,81	1.38	10 (12%)
32	STE	E	102	-	11,11,19	0.86	0	11,11,19	0.97	1 (9%)
22	CLA	C	511	3	69,73,73	1.27	9 (13%)	82,113,113	1.34	9 (10%)
32	STE	J	101	-	11,11,19	0.59	0	11,11,19	1.48	2 (18%)
22	CLA	B	612	2	69,73,73	1.09	4 (5%)	82,113,113	1.37	10 (12%)
30	DGD	B	623	-	43,43,67	1.24	6 (13%)	45,45,81	1.27	5 (11%)
27	LMG	D	410	-	31,31,55	0.88	1 (3%)	33,33,63	1.20	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCT	D	402	21	3,3,3	1.16	0	2,3,3	2.80	1 (50%)
32	STE	C	521	-	11,11,19	0.62	0	11,11,19	1.40	3 (27%)
22	CLA	B	607	36	69,73,73	1.26	9 (13%)	82,113,113	1.46	10 (12%)
32	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.55	0
22	CLA	C	509	3	69,73,73	1.14	7 (10%)	82,113,113	1.42	10 (12%)
22	CLA	b	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.47	10 (12%)
22	CLA	c	509	3	69,73,73	1.64	9 (13%)	82,113,113	1.28	6 (7%)
30	DGD	c	516	-	63,63,67	1.08	5 (7%)	77,77,81	1.39	11 (14%)
22	CLA	C	502	3	69,73,73	1.21	10 (14%)	82,113,113	1.31	11 (13%)
23	PHO	d	401	-	58,69,69	2.03	11 (18%)	55,99,99	1.52	9 (16%)
28	LHG	D	409	-	48,48,48	0.81	3 (6%)	51,54,54	1.34	7 (13%)
24	BCR	c	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	6 (10%)
24	BCR	t	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.32	8 (14%)
22	CLA	b	613	2	69,73,73	1.17	10 (14%)	82,113,113	1.42	12 (14%)
22	CLA	b	616	2	64,68,73	1.22	8 (12%)	76,107,113	1.50	9 (11%)
22	CLA	B	605	2	69,73,73	1.25	9 (13%)	82,113,113	1.36	8 (9%)
32	STE	C	520	-	15,15,19	0.56	0	14,14,19	0.59	0
29	SQD	f	101	-	39,41,54	1.13	4 (10%)	49,52,65	1.77	9 (18%)
27	LMG	D	408	-	51,51,55	0.99	4 (7%)	59,59,63	1.27	6 (10%)
22	CLA	B	616	2	64,68,73	1.31	8 (12%)	76,107,113	1.65	9 (11%)
22	CLA	a	405	1	69,73,73	1.42	10 (14%)	82,113,113	1.24	8 (9%)
22	CLA	D	405	4	69,73,73	1.67	8 (11%)	82,113,113	1.45	14 (17%)
22	CLA	b	607	36	69,73,73	1.22	10 (14%)	82,113,113	1.32	6 (7%)
27	LMG	c	520	-	48,48,55	1.10	5 (10%)	56,56,63	1.25	6 (10%)
29	SQD	a	412	-	52,54,54	0.99	3 (5%)	62,65,65	1.85	13 (20%)
24	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
26	PL9	d	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.70	13 (19%)
34	HEM	F	101	6,5	50,50,50	1.43	7 (14%)	67,82,82	1.09	5 (7%)
24	BCR	k	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	5 (8%)
22	CLA	c	513	3	69,73,73	1.23	10 (14%)	82,113,113	1.23	6 (7%)
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.14	1 (7%)
22	CLA	C	512	3	69,73,73	1.27	5 (7%)	82,113,113	1.50	11 (13%)
32	STE	B	624	-	11,11,19	0.86	0	11,11,19	0.98	0
30	DGD	c	517	-	63,63,67	1.14	6 (9%)	77,77,81	1.50	14 (18%)
30	DGD	C	515	-	63,63,67	1.26	8 (12%)	77,77,81	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	OEX	A	415	3,1,36	0,14,14	-	-	-		
22	CLA	b	601	36	69,73,73	1.42	6 (8%)	82,113,113	1.47	6 (7%)
28	LHG	l	101	-	48,48,48	0.69	0	51,54,54	1.28	5 (9%)
22	CLA	C	508	3	69,73,73	1.45	9 (13%)	82,113,113	1.24	9 (10%)
22	CLA	B	603	2	69,73,73	1.53	7 (10%)	82,113,113	1.40	17 (20%)
27	LMG	d	408	-	21,21,55	0.69	1 (4%)	20,20,63	1.05	0
32	STE	k	104	-	11,11,19	0.96	1 (9%)	11,11,19	1.15	1 (9%)
22	CLA	C	513	3	69,73,73	1.28	12 (17%)	82,113,113	1.28	10 (12%)
34	HEM	e	101	6,5	50,50,50	1.43	7 (14%)	67,82,82	1.21	6 (8%)
22	CLA	a	402	1	69,73,73	1.35	11 (15%)	82,113,113	1.24	7 (8%)
22	CLA	B	601	36	69,73,73	1.62	9 (13%)	82,113,113	1.27	5 (6%)
27	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.36	6 (10%)
22	CLA	A	403	36	69,73,73	1.27	10 (14%)	82,113,113	1.19	10 (12%)
28	LHG	B	621	-	48,48,48	1.03	3 (6%)	51,54,54	1.35	7 (13%)
32	STE	b	620	-	15,15,19	0.56	0	14,14,19	0.70	0
22	CLA	c	503	3	69,73,73	1.28	7 (10%)	82,113,113	1.47	7 (8%)
22	CLA	c	507	36	69,73,73	1.40	9 (13%)	82,113,113	1.28	6 (7%)

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	A	405	1	-	6/26/102/115	-
22	CLA	B	609	2	-	4/39/115/115	-
22	CLA	c	511	3	-	12/39/115/115	-
32	STE	a	415	-	-	3/9/9/17	-
22	CLA	b	614	2	-	21/39/115/115	-
22	CLA	c	501	3	-	3/39/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
24	BCR	k	103	-	-	8/29/63/63	0/2/2/2
27	LMG	D	411	-	-	15/22/22/70	-
29	SQD	F	102	-	-	11/28/48/69	0/1/1/1
22	CLA	d	402	4	-	7/39/115/115	-
30	DGD	C	516	-	-	25/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	B	614	2	-	12/39/115/115	-
22	CLA	b	615	2	-	9/39/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
28	LHG	d	406	-	-	20/53/53/53	-
28	LHG	E	101	-	-	24/53/53/53	-
22	CLA	c	508	3	-	13/38/114/115	-
29	SQD	A	412	-	-	17/47/67/69	0/1/1/1
22	CLA	C	510	3	-	8/39/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	603	2	-	13/39/115/115	-
35	HEC	V	201	17	1/1/7/7	5/14/54/54	-
22	CLA	b	602	2	-	11/39/115/115	-
22	CLA	B	610	36	-	4/39/115/115	-
27	LMG	d	409	-	-	12/39/59/70	0/1/1/1
32	STE	B	627	-	-	7/9/9/17	-
26	PL9	a	410	-	-	26/53/73/73	0/1/1/1
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	a	411	36	-	12/39/115/115	-
32	STE	M	104	-	-	8/12/12/17	-
27	LMG	m	101	-	-	23/46/66/70	0/1/1/1
32	STE	b	626	-	-	5/7/7/17	-
24	BCR	T	101	-	-	11/29/63/63	0/2/2/2
32	STE	M	103	-	-	3/7/7/17	-
24	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
22	CLA	c	502	3	-	15/39/115/115	-
22	CLA	d	403	4	-	5/39/115/115	-
22	CLA	b	608	2	-	7/39/115/115	-
24	BCR	A	406	-	-	3/29/63/63	0/2/2/2
27	LMG	C	518	-	-	20/43/63/70	0/1/1/1
32	STE	B	626	-	-	6/13/13/17	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	503	3	-	4/39/115/115	-
22	CLA	b	606	2	-	9/39/115/115	-
24	BCR	d	404	-	-	5/29/63/63	0/2/2/2
32	STE	B	625	-	-	10/15/15/17	-
28	LHG	d	407	-	-	14/43/43/53	-
22	CLA	b	604	2	-	8/39/115/115	-
30	DGD	A	414	-	-	27/55/95/95	0/2/2/2
22	CLA	c	505	3	-	9/39/115/115	-
28	LHG	A	411	-	-	22/51/51/53	-
22	CLA	b	611	2	-	10/39/115/115	-
22	CLA	B	615	2	-	7/39/115/115	-
32	STE	I	101	-	-	7/12/12/17	-
22	CLA	c	510	3	-	9/39/115/115	-
22	CLA	c	512	3	-	20/39/115/115	-
32	STE	l	102	-	-	13/15/15/17	-
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
22	CLA	D	403	4	-	7/39/115/115	-
30	DGD	c	515	-	-	25/51/91/95	0/2/2/2
22	CLA	B	606	2	-	10/39/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
24	BCR	b	619	-	-	14/29/63/63	0/2/2/2
22	CLA	B	602	2	-	9/39/115/115	-
27	LMG	c	518	-	-	8/31/51/70	0/1/1/1
32	STE	D	412	-	-	10/17/17/17	-
32	STE	b	625	-	-	5/17/17/17	-
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	C	501	3	-	3/39/115/115	-
24	BCR	K	102	-	-	4/29/63/63	0/2/2/2
30	DGD	C	517	-	-	12/51/91/95	0/2/2/2
22	CLA	B	613	2	-	14/39/115/115	-
35	HEC	v	201	17	1/1/7/7	4/14/54/54	-
32	STE	d	410	-	-	7/14/14/17	-
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	C	505	3	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	604	2	-	11/39/115/115	-
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
22	CLA	b	609	2	-	6/39/115/115	-
32	STE	t	103	-	-	4/7/7/17	-
27	LMG	A	410	-	-	24/43/63/70	0/1/1/1
22	CLA	c	504	36	-	11/33/109/115	-
22	CLA	c	506	3	-	13/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
24	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	LHG	L	102	-	-	20/53/53/53	-
22	CLA	B	608	2	-	2/39/115/115	-
28	LHG	b	623	-	-	24/53/53/53	-
22	CLA	b	610	36	-	7/39/115/115	-
29	SQD	L	101	-	-	26/44/64/69	0/1/1/1
32	STE	m	102	-	-	4/9/9/17	-
22	CLA	C	504	36	-	10/32/108/115	-
22	CLA	C	506	3	-	12/39/115/115	-
29	SQD	a	413	-	-	16/37/37/69	-
29	SQD	A	413	-	-	13/39/39/69	-
32	STE	c	519	-	-	12/17/17/17	-
32	STE	j	101	-	-	2/9/9/17	-
27	LMG	a	414	-	-	21/44/64/70	0/1/1/1
28	LHG	e	102	-	-	25/46/46/53	-
22	CLA	D	404	36	-	5/39/115/115	-
22	CLA	A	402	1	-	2/39/115/115	-
32	STE	x	102	-	-	13/17/17/17	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	B	611	2	-	6/39/115/115	-
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2
29	SQD	B	622	-	-	16/49/69/69	0/1/1/1
22	CLA	a	403	36	-	14/39/115/115	-
32	STE	C	519	-	-	6/9/9/17	-
32	STE	b	621	-	-	9/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	36	-	9/39/115/115	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
26	PL9	A	409	-	-	25/53/73/73	0/1/1/1
22	CLA	b	612	2	-	15/39/115/115	-
32	STE	b	624	-	-	8/13/13/17	-
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
32	STE	E	102	-	-	7/9/9/17	-
22	CLA	C	511	3	-	11/39/115/115	-
32	STE	J	101	-	-	5/9/9/17	-
22	CLA	B	612	2	-	9/39/115/115	-
30	DGD	B	623	-	-	24/45/45/95	-
27	LMG	D	410	-	-	17/33/33/70	-
32	STE	C	521	-	-	1/9/9/17	-
22	CLA	B	607	36	-	10/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
22	CLA	C	509	3	-	7/39/115/115	-
22	CLA	b	605	2	-	9/39/115/115	-
22	CLA	c	509	3	-	16/39/115/115	-
30	DGD	c	516	-	-	21/51/91/95	0/2/2/2
22	CLA	C	502	3	-	6/39/115/115	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
28	LHG	D	409	-	-	19/53/53/53	-
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	613	2	-	8/39/115/115	-
22	CLA	b	616	2	-	8/33/109/115	-
22	CLA	B	605	2	-	10/39/115/115	-
32	STE	C	520	-	-	4/13/13/17	-
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
27	LMG	D	408	-	-	17/46/66/70	0/1/1/1
22	CLA	B	616	2	-	8/33/109/115	-
22	CLA	a	405	1	-	10/39/115/115	-
22	CLA	D	405	4	-	9/39/115/115	-
22	CLA	b	607	36	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	520	-	-	26/43/63/70	0/1/1/1
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
24	BCR	K	101	-	-	11/29/63/63	0/2/2/2
26	PL9	d	405	-	-	18/53/73/73	0/1/1/1
34	HEM	F	101	6,5	-	3/14/54/54	-
24	BCR	k	102	-	-	12/29/63/63	0/2/2/2
22	CLA	c	513	3	-	9/39/115/115	-
32	STE	t	102	-	-	3/11/11/17	-
22	CLA	C	512	3	-	21/39/115/115	-
32	STE	B	624	-	-	6/9/9/17	-
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
30	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	b	601	36	-	17/39/115/115	-
28	LHG	l	101	-	-	18/53/53/53	-
22	CLA	C	508	3	-	5/39/115/115	-
22	CLA	B	603	2	-	10/39/115/115	-
27	LMG	d	408	-	-	9/17/17/70	-
32	STE	k	104	-	-	2/9/9/17	-
22	CLA	C	513	3	-	16/39/115/115	-
34	HEM	e	101	6,5	-	1/14/54/54	-
22	CLA	a	402	1	-	1/39/115/115	-
22	CLA	B	601	36	-	19/39/115/115	-
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
22	CLA	A	403	36	-	5/39/115/115	-
28	LHG	B	621	-	-	16/53/53/53	-
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	c	503	3	-	11/39/115/115	-
22	CLA	c	507	36	-	12/39/115/115	-

The worst 5 of 927 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	8.96	1.49	1.39
22	D	405	CLA	MG-NB	-8.64	1.88	2.05
23	D	401	PHO	C3B-C4B	8.45	1.50	1.41
23	D	401	PHO	C1B-C2B	8.45	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	C1B-C2B	8.38	1.48	1.39

The worst 5 of 1223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	10.19	111.33	106.68
22	B	616	CLA	C4A-NA-C1A	9.47	111.00	106.68
29	a	412	SQD	O6-C1-C2	8.95	121.87	108.27
29	A	412	SQD	O6-C1-C2	8.85	121.72	108.27
22	B	606	CLA	C4A-NA-C1A	8.78	110.69	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA
35	v	201	HEC	NA

5 of 1923 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

116 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	609	CLA	1	0
22	c	511	CLA	5	0
22	b	614	CLA	2	0
22	c	501	CLA	2	0
24	b	617	BCR	1	0
22	d	402	CLA	1	0
30	C	516	DGD	4	0
22	B	614	CLA	2	0
22	b	615	CLA	3	0
32	B	620	STE	1	0
23	a	404	PHO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	406	LHG	3	0
28	E	101	LHG	2	0
22	c	508	CLA	1	0
29	A	412	SQD	4	0
22	C	510	CLA	1	0
24	x	101	BCR	1	0
22	b	602	CLA	1	0
35	V	201	HEC	1	0
32	B	627	STE	2	0
26	a	410	PL9	3	0
24	a	406	BCR	1	0
22	a	411	CLA	1	0
32	M	104	STE	1	0
32	b	626	STE	1	0
24	T	101	BCR	3	0
24	Z	101	BCR	2	0
26	D	407	PL9	1	0
22	c	502	CLA	1	0
22	d	403	CLA	3	0
27	C	518	LMG	1	0
22	b	606	CLA	2	0
24	d	404	BCR	3	0
28	d	407	LHG	2	0
22	b	604	CLA	1	0
30	A	414	DGD	3	0
28	A	411	LHG	2	0
22	B	615	CLA	1	0
32	I	101	STE	1	0
22	c	510	CLA	2	0
22	c	512	CLA	1	0
32	l	102	STE	1	0
30	c	515	DGD	1	0
22	B	606	CLA	3	0
22	B	602	CLA	2	0
32	D	412	STE	3	0
32	b	625	STE	1	0
30	C	517	DGD	2	0
22	B	613	CLA	3	0
24	B	619	BCR	1	0
22	B	604	CLA	2	0
24	B	618	BCR	2	0
27	A	410	LMG	3	0

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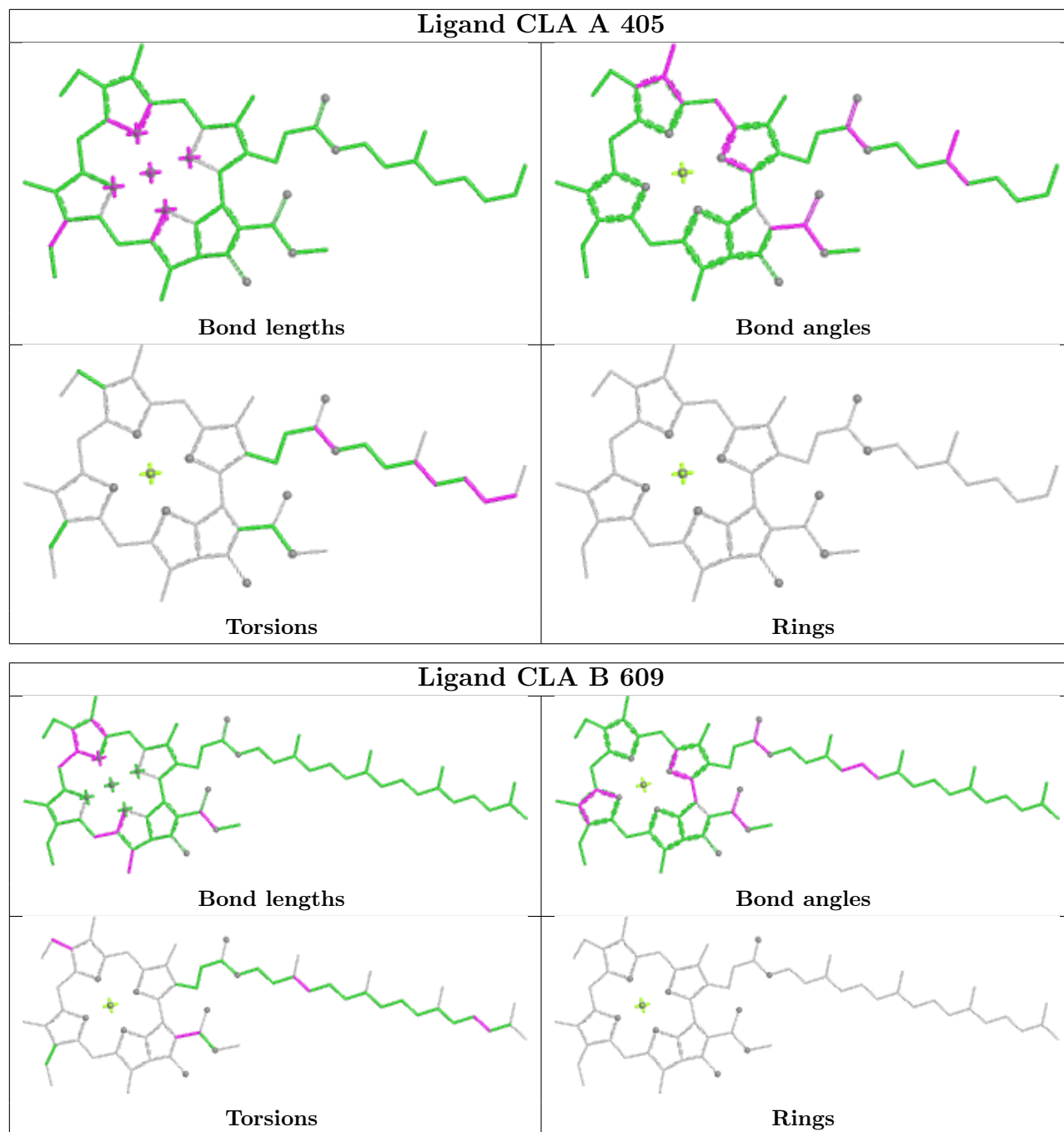
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	401	PHO	1	0
24	b	618	BCR	1	0
24	D	406	BCR	1	0
28	L	102	LHG	6	0
28	b	623	LHG	1	0
22	b	610	CLA	2	0
29	L	101	SQD	2	0
22	C	504	CLA	1	0
29	a	413	SQD	2	0
29	A	413	SQD	1	0
32	j	101	STE	1	0
28	e	102	LHG	3	0
22	D	404	CLA	3	0
22	A	402	CLA	1	0
32	x	102	STE	2	0
24	B	617	BCR	1	0
22	B	611	CLA	3	0
29	B	622	SQD	1	0
32	b	621	STE	1	0
22	C	507	CLA	1	0
24	C	514	BCR	1	0
26	A	409	PL9	3	0
32	b	624	STE	1	0
30	H	102	DGD	1	0
22	C	511	CLA	2	0
32	J	101	STE	1	0
30	B	623	DGD	4	0
33	D	402	BCT	1	0
32	H	103	STE	3	0
22	C	509	CLA	2	0
22	b	605	CLA	2	0
30	c	516	DGD	2	0
22	C	502	CLA	1	0
23	d	401	PHO	1	0
28	D	409	LHG	2	0
24	c	514	BCR	2	0
24	t	101	BCR	3	0
22	b	616	CLA	2	0
22	B	605	CLA	4	0
29	f	101	SQD	2	0
27	D	408	LMG	1	0
22	a	405	CLA	1	0

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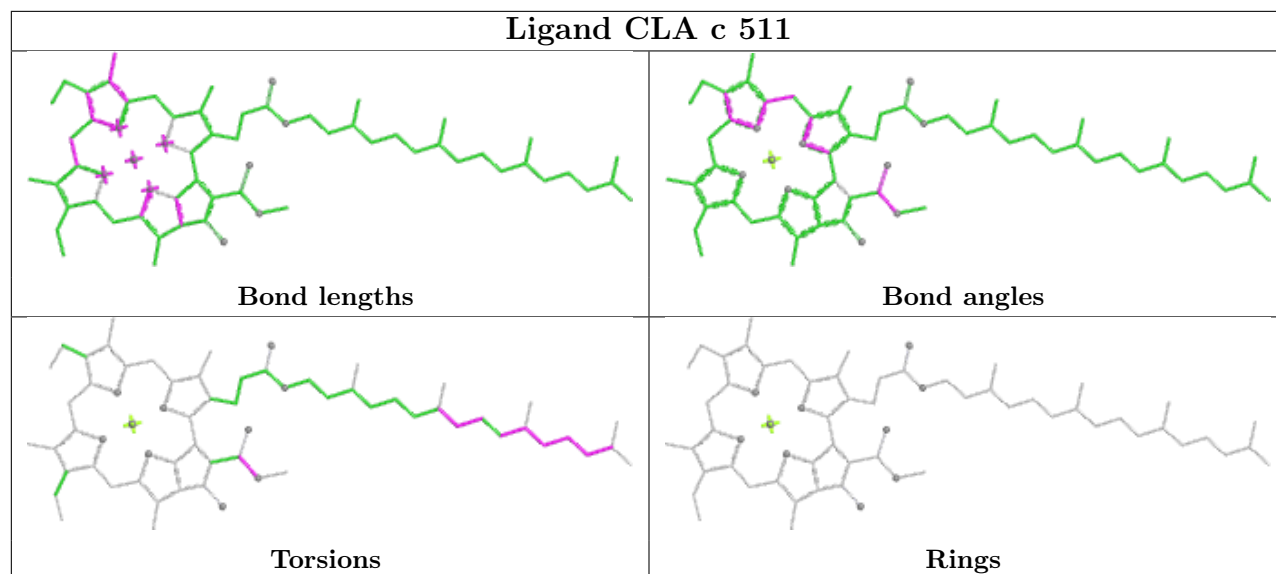
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	607	CLA	1	0
27	c	520	LMG	1	0
29	a	412	SQD	4	0
24	K	101	BCR	2	0
34	F	101	HEM	2	0
22	c	513	CLA	1	0
32	B	624	STE	2	0
30	c	517	DGD	2	0
22	b	601	CLA	2	0
28	l	101	LHG	1	0
22	B	603	CLA	2	0
27	d	408	LMG	1	0
32	k	104	STE	2	0
34	e	101	HEM	4	0
22	B	601	CLA	3	0
27	M	101	LMG	1	0
22	A	403	CLA	1	0
28	B	621	LHG	4	0
32	b	620	STE	1	0
22	c	503	CLA	3	0
22	c	507	CLA	1	0

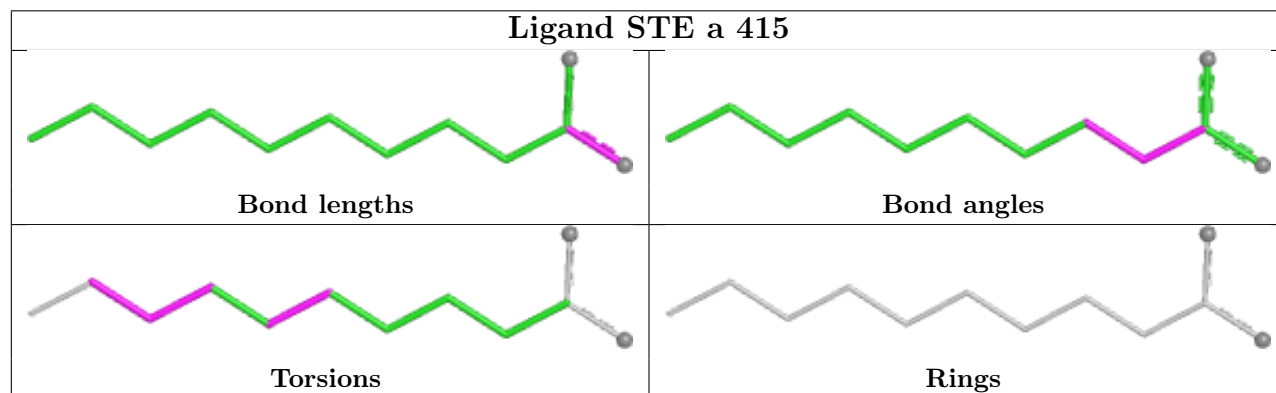
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



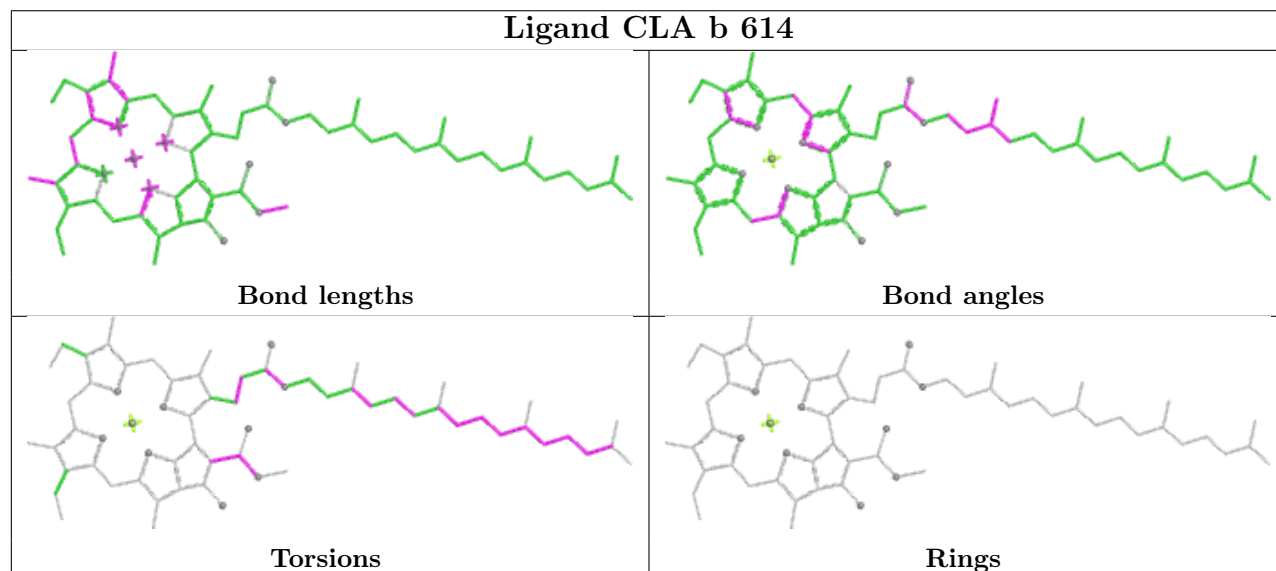
Ligand CLA c 511

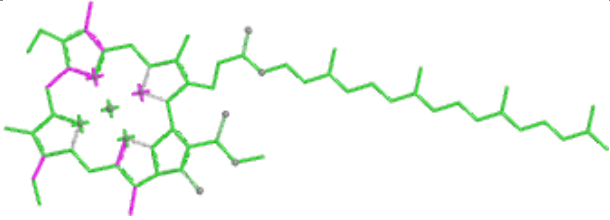
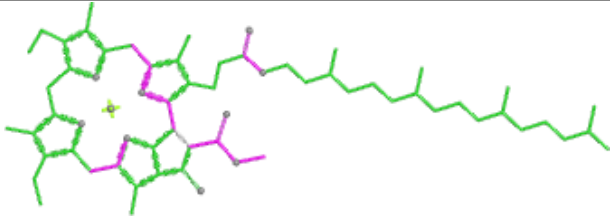
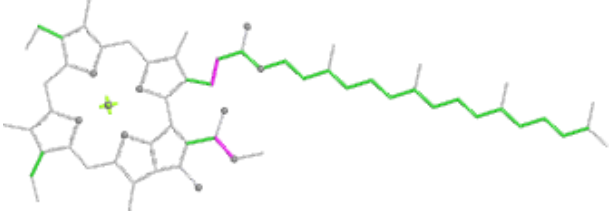
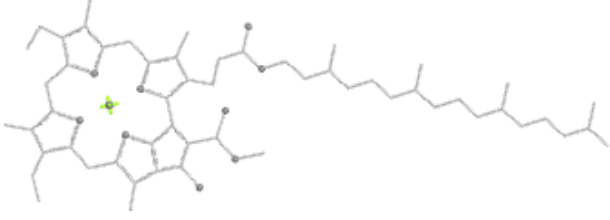
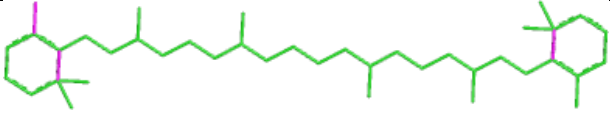
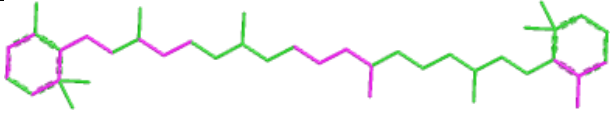
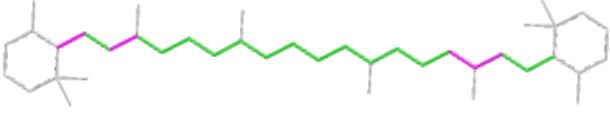
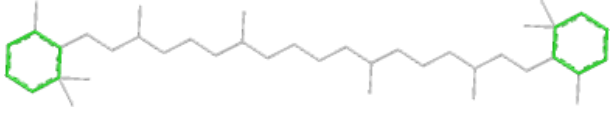
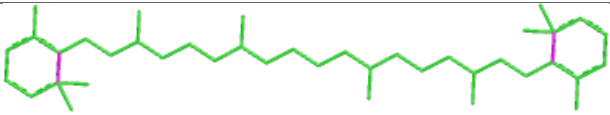
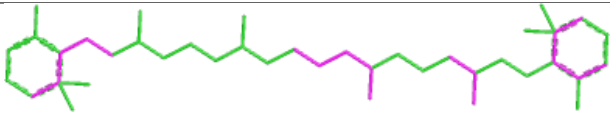
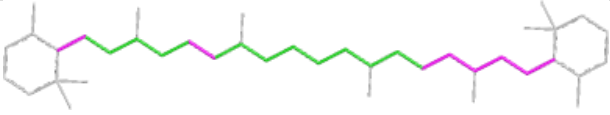
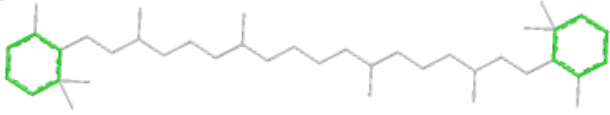


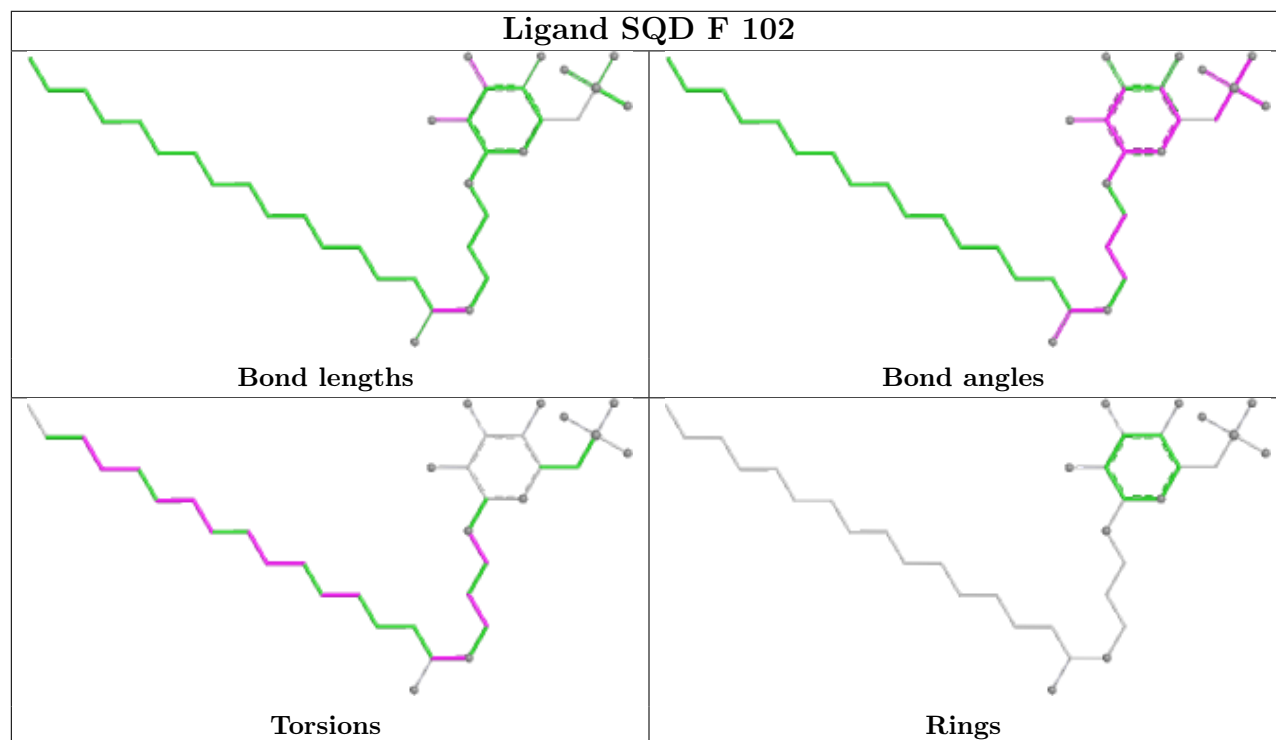
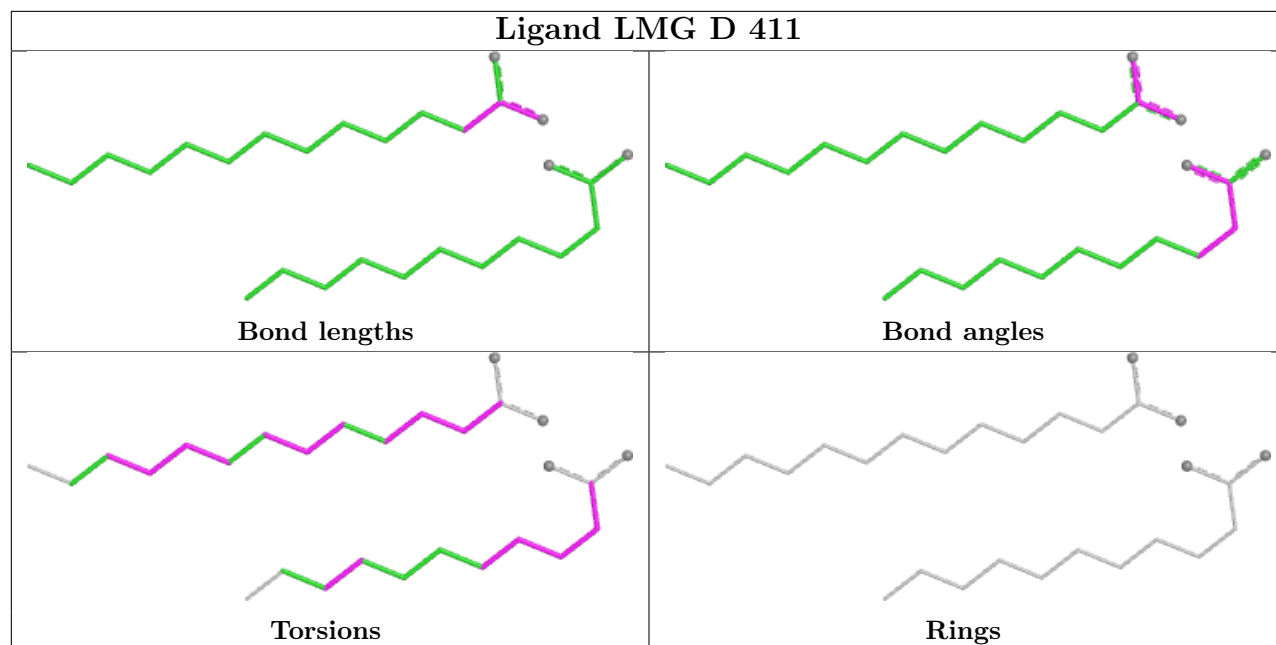
Ligand STE a 415



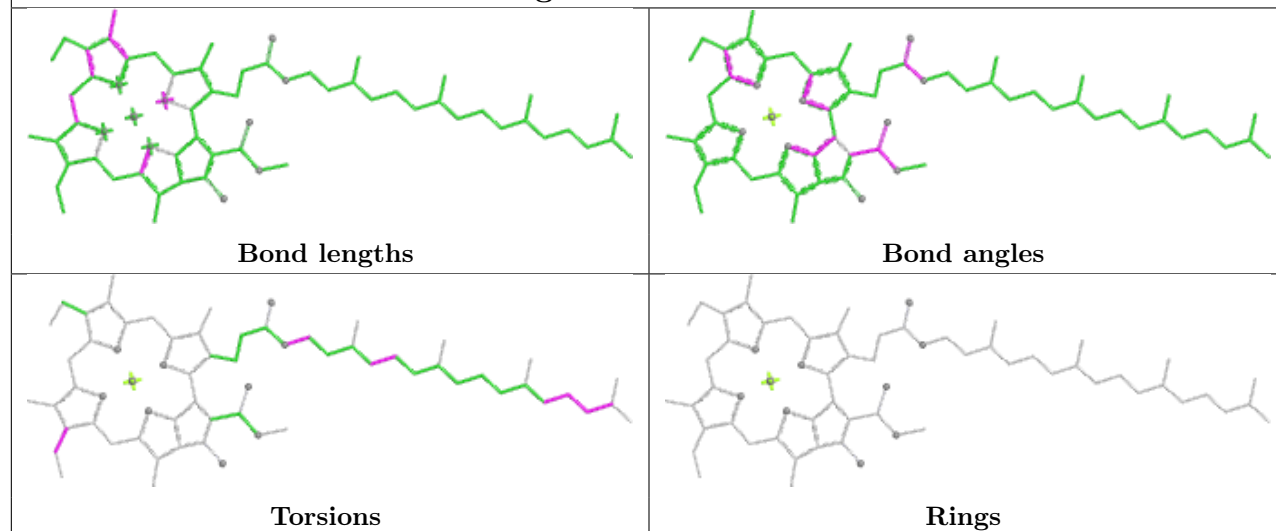
Ligand CLA b 614



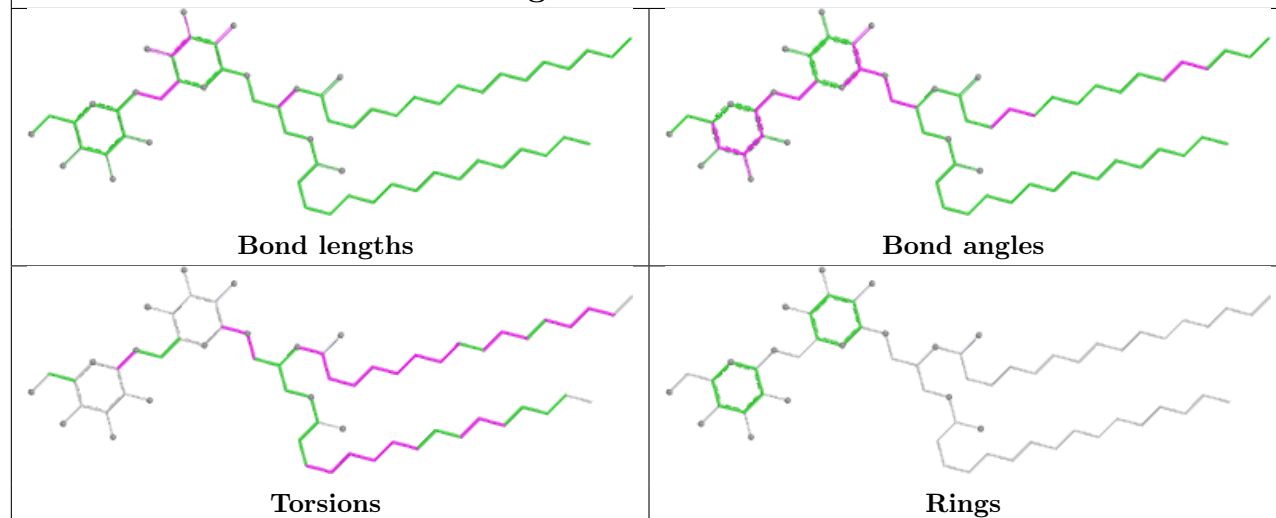
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Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand BCR b 617			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand BCR k 103			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	



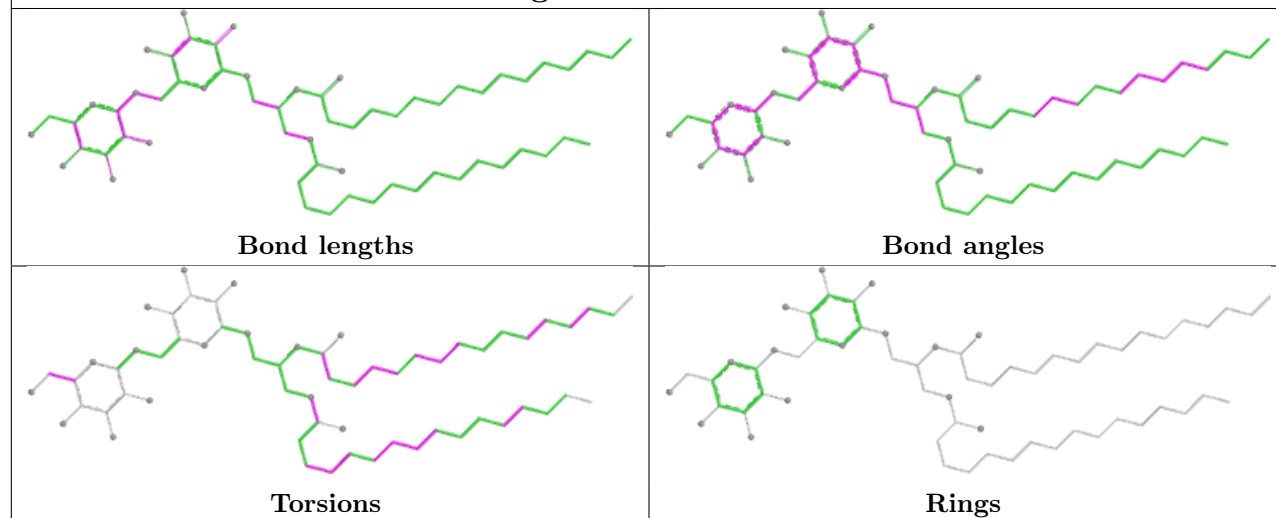
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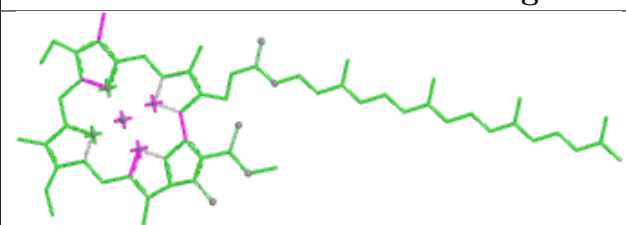
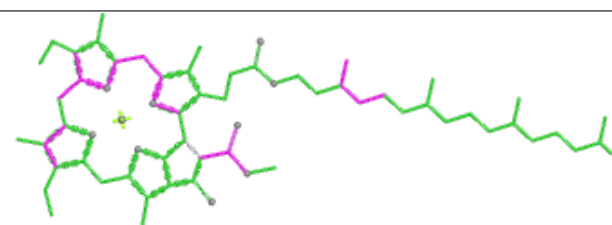
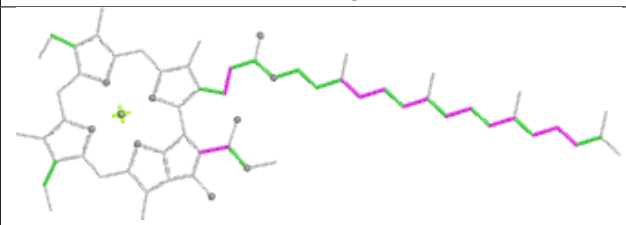
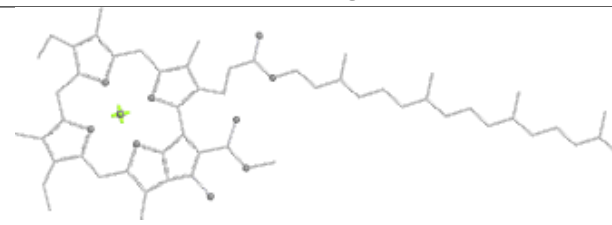


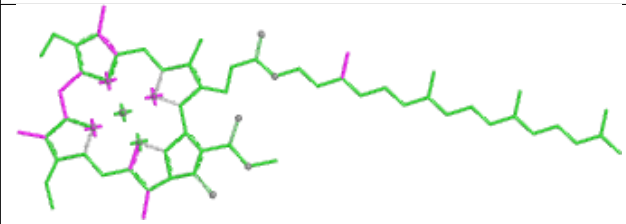
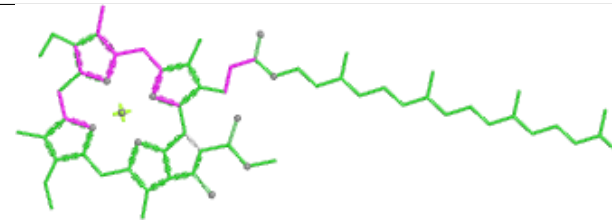
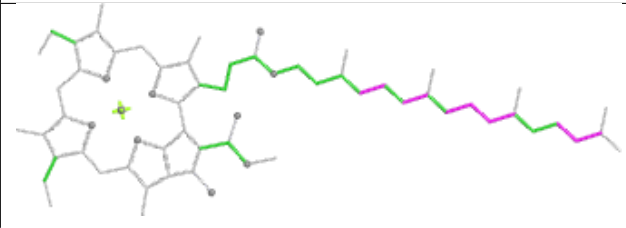
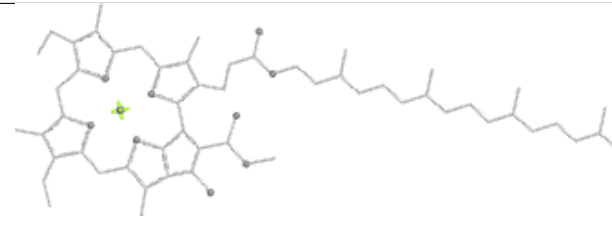
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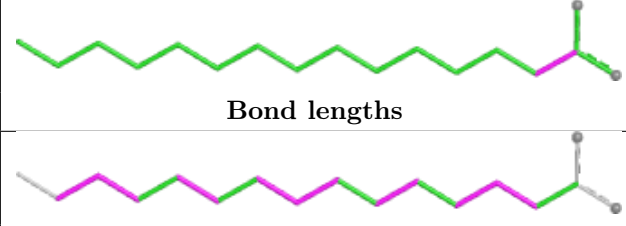
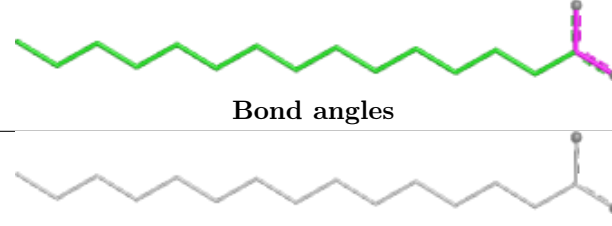
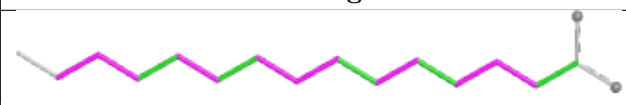
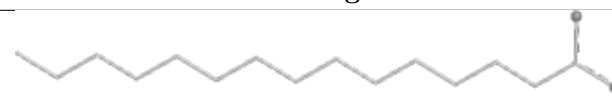


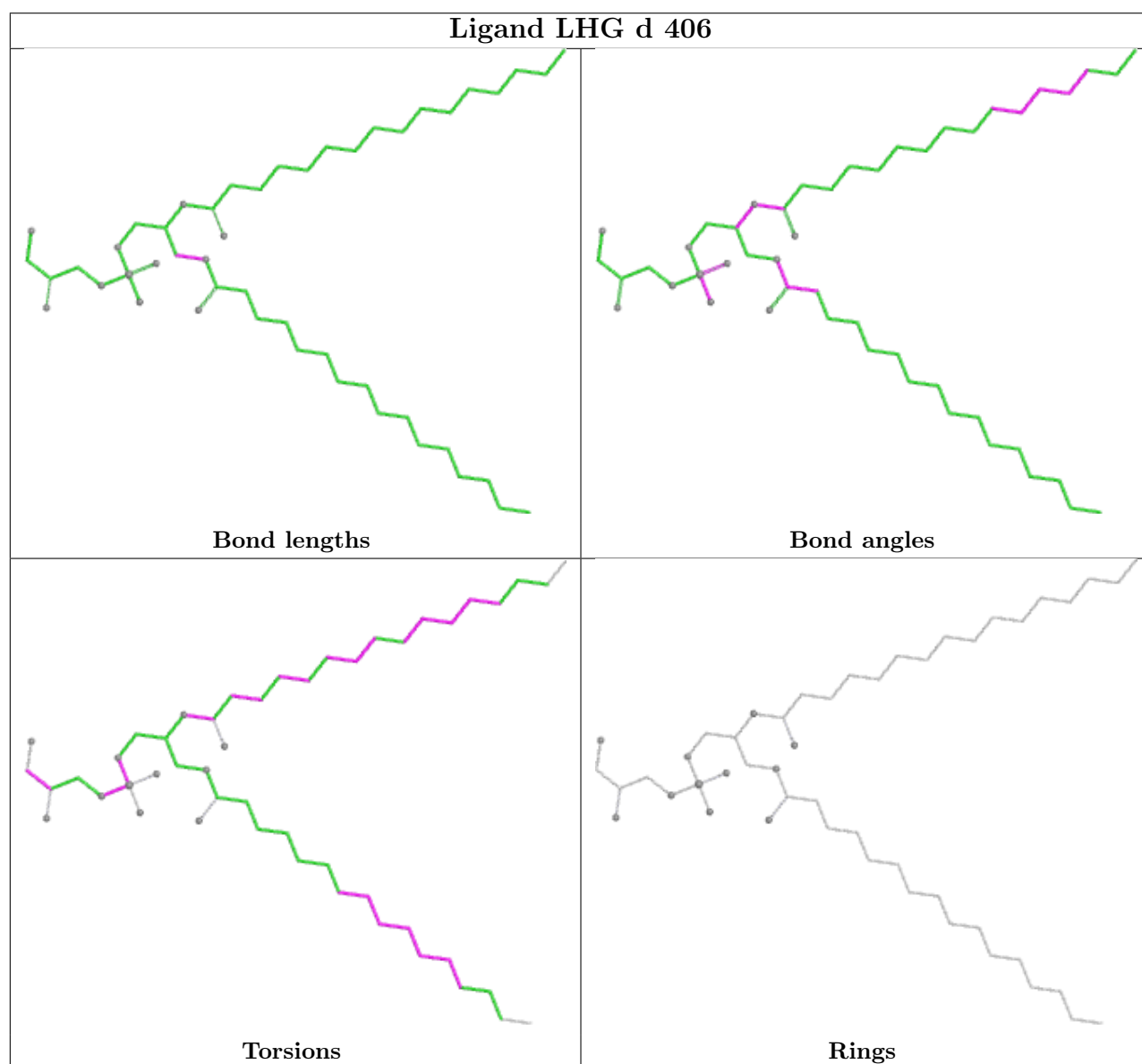
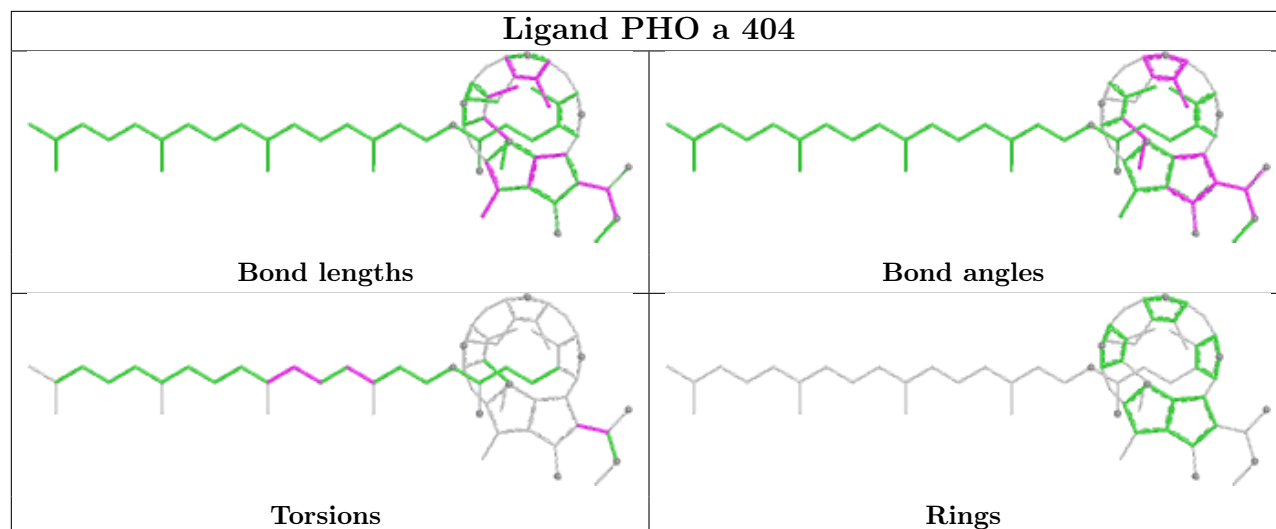
Ligand DGD h 101

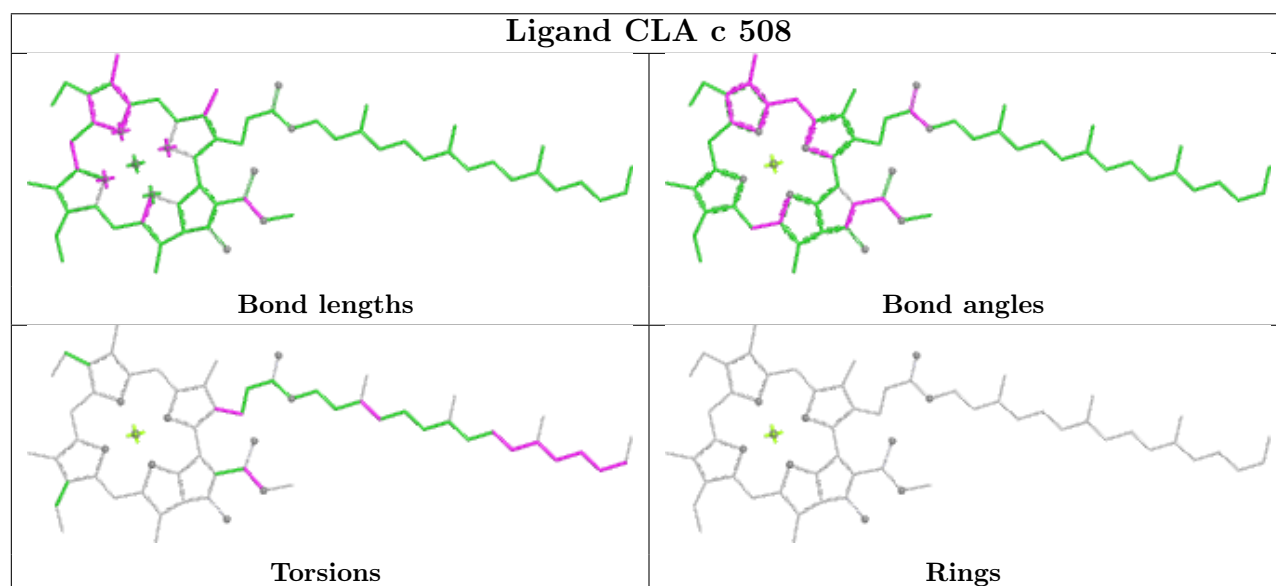
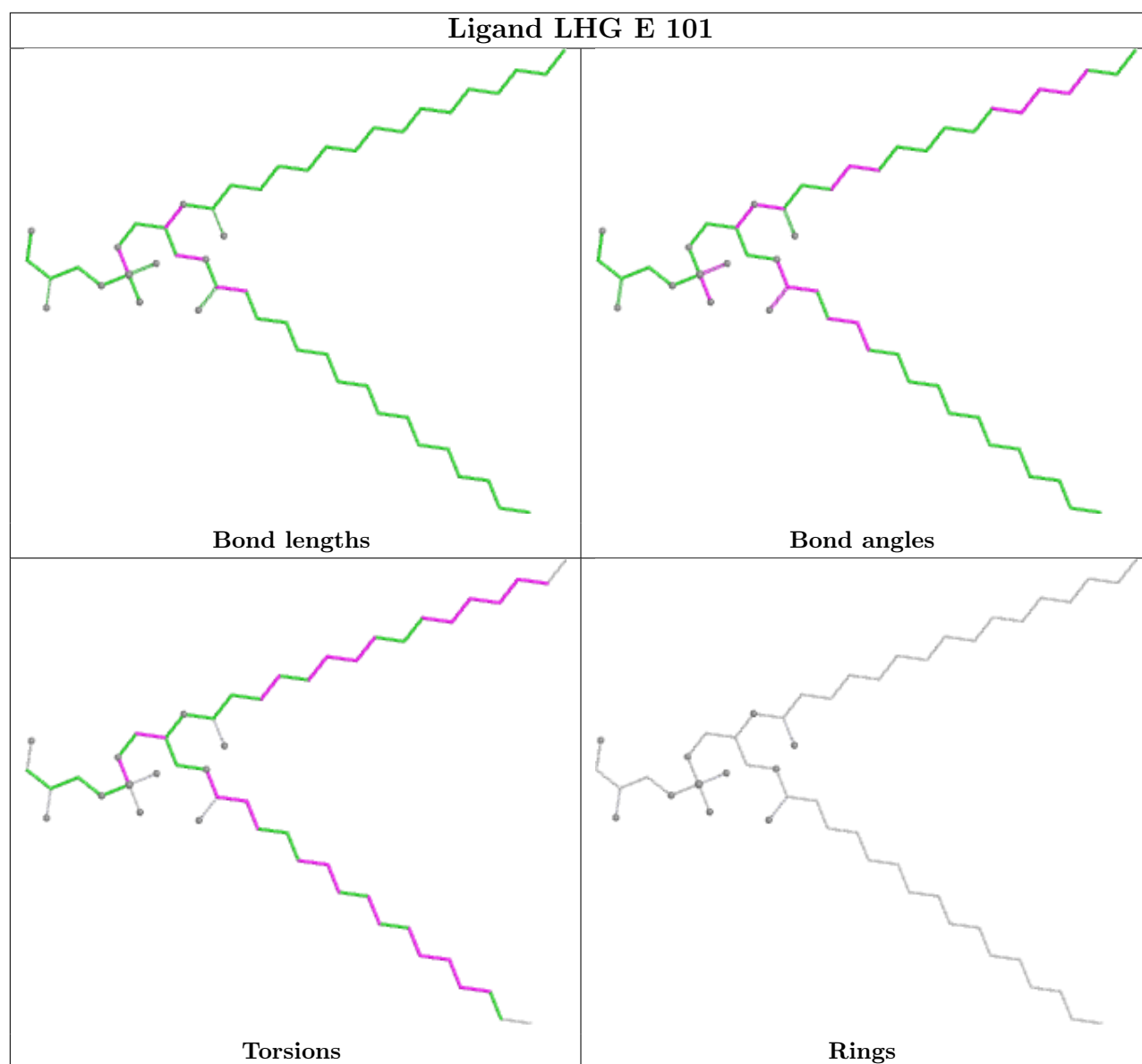


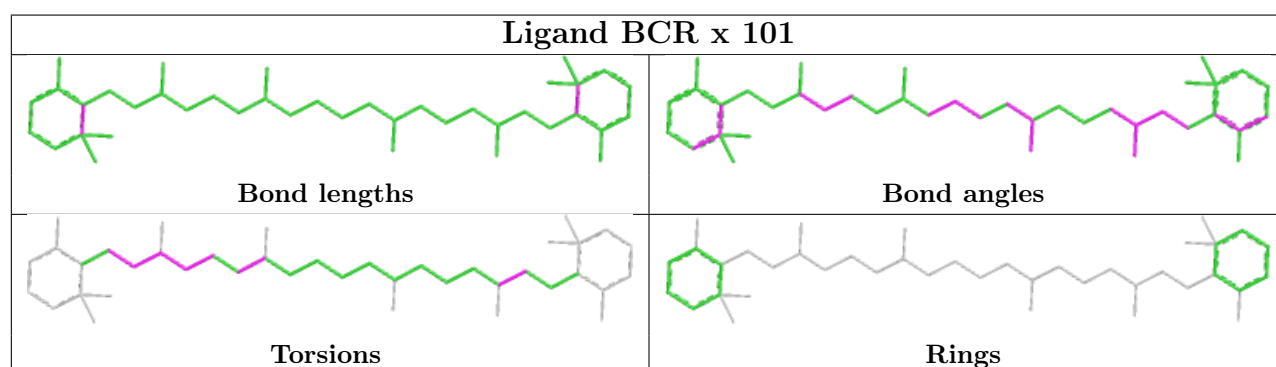
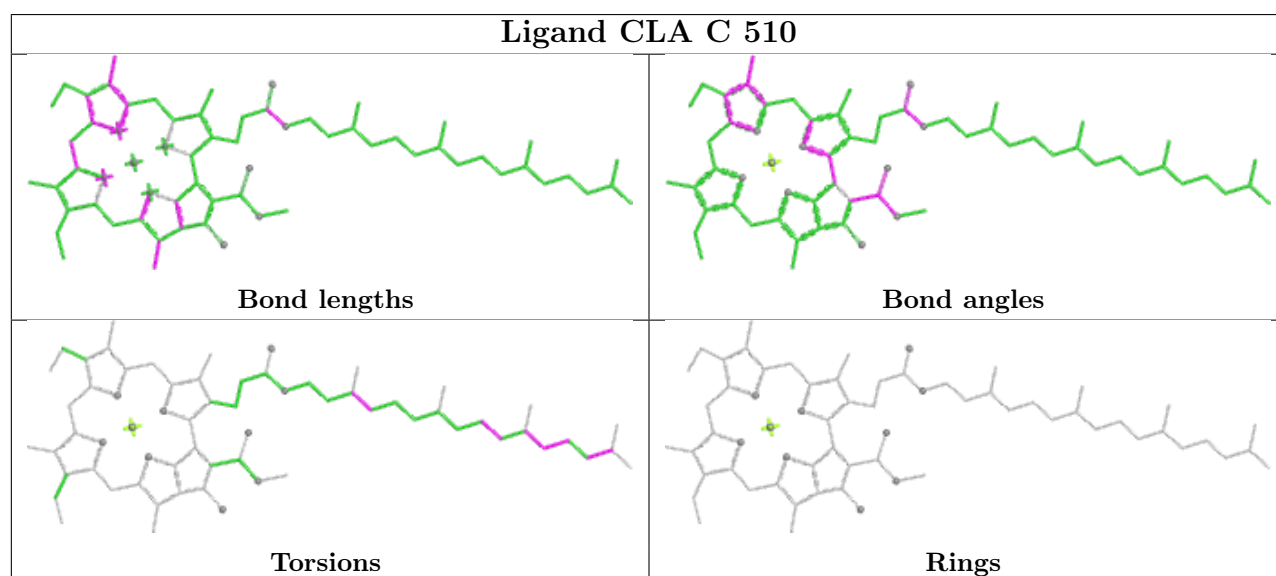
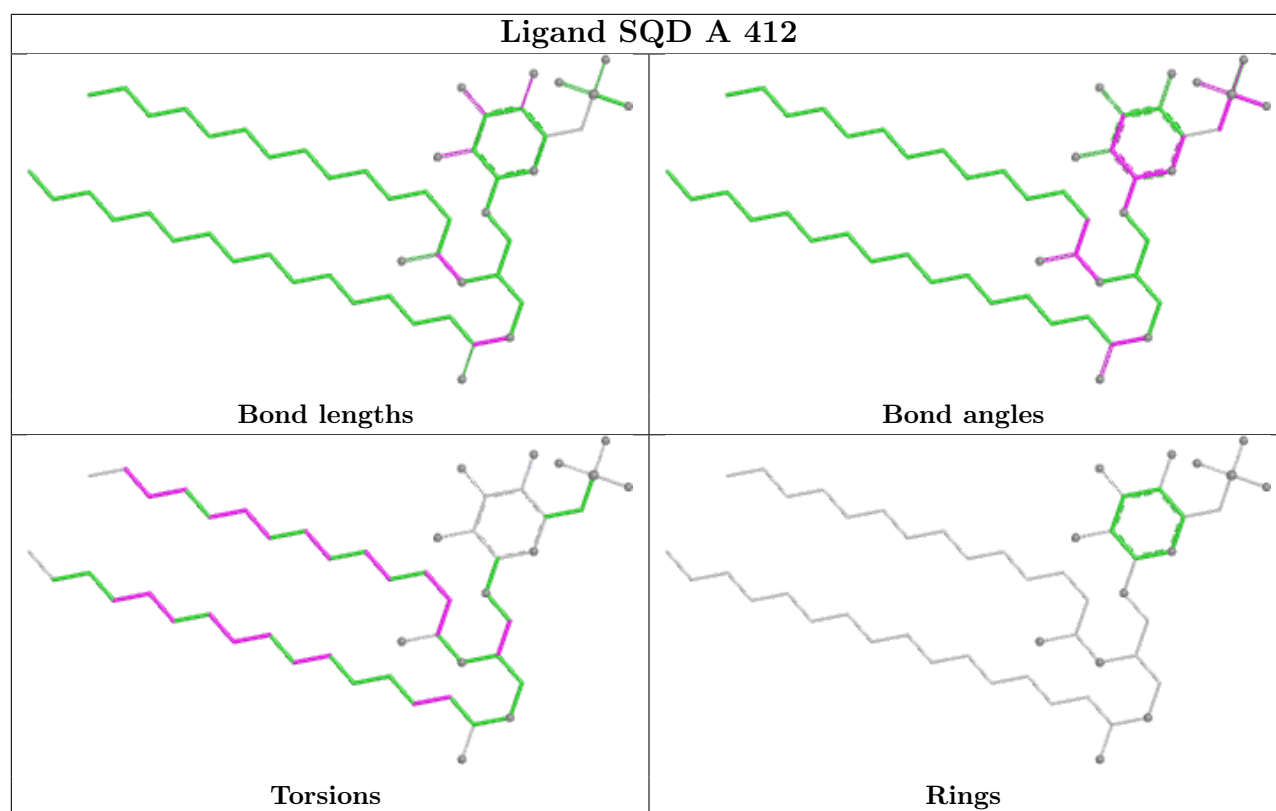
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

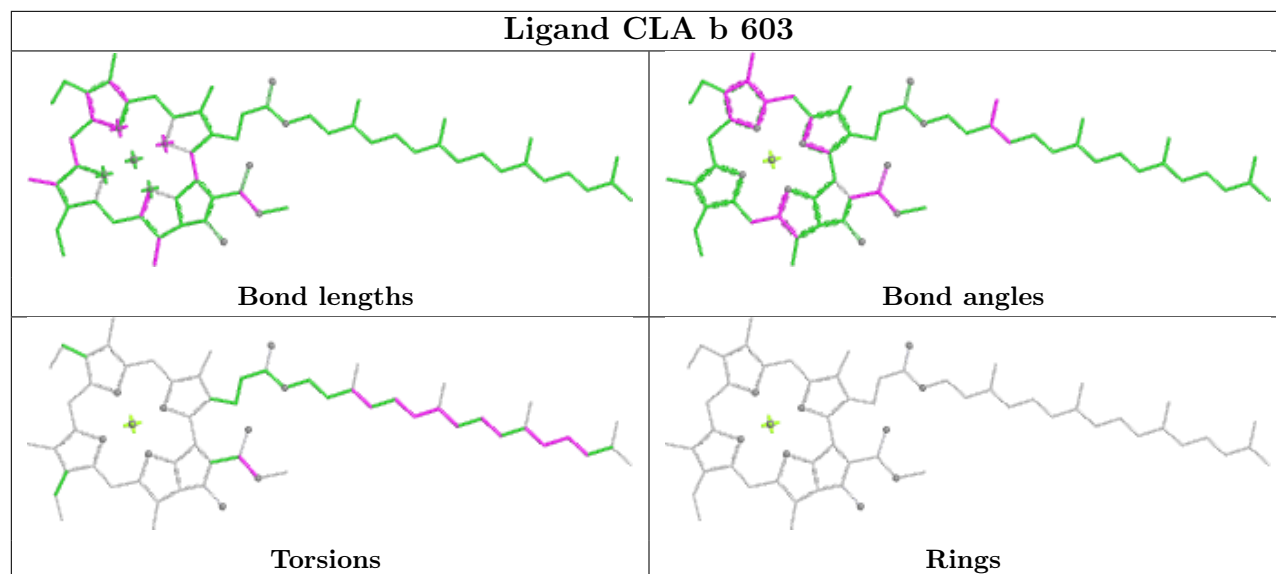
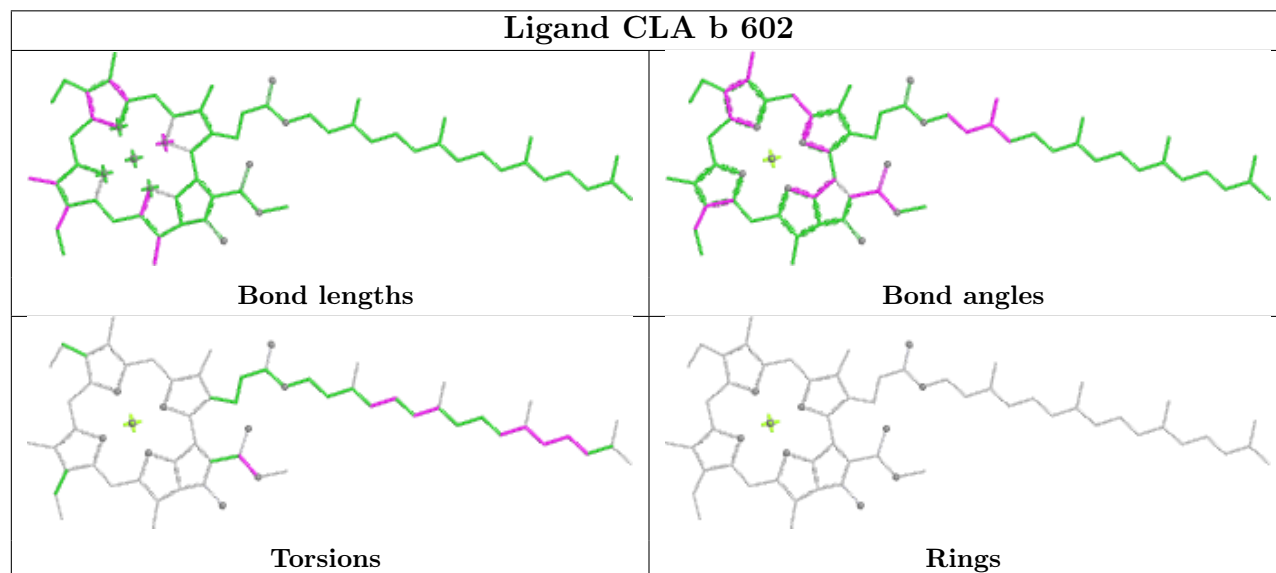
Ligand CLA b 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

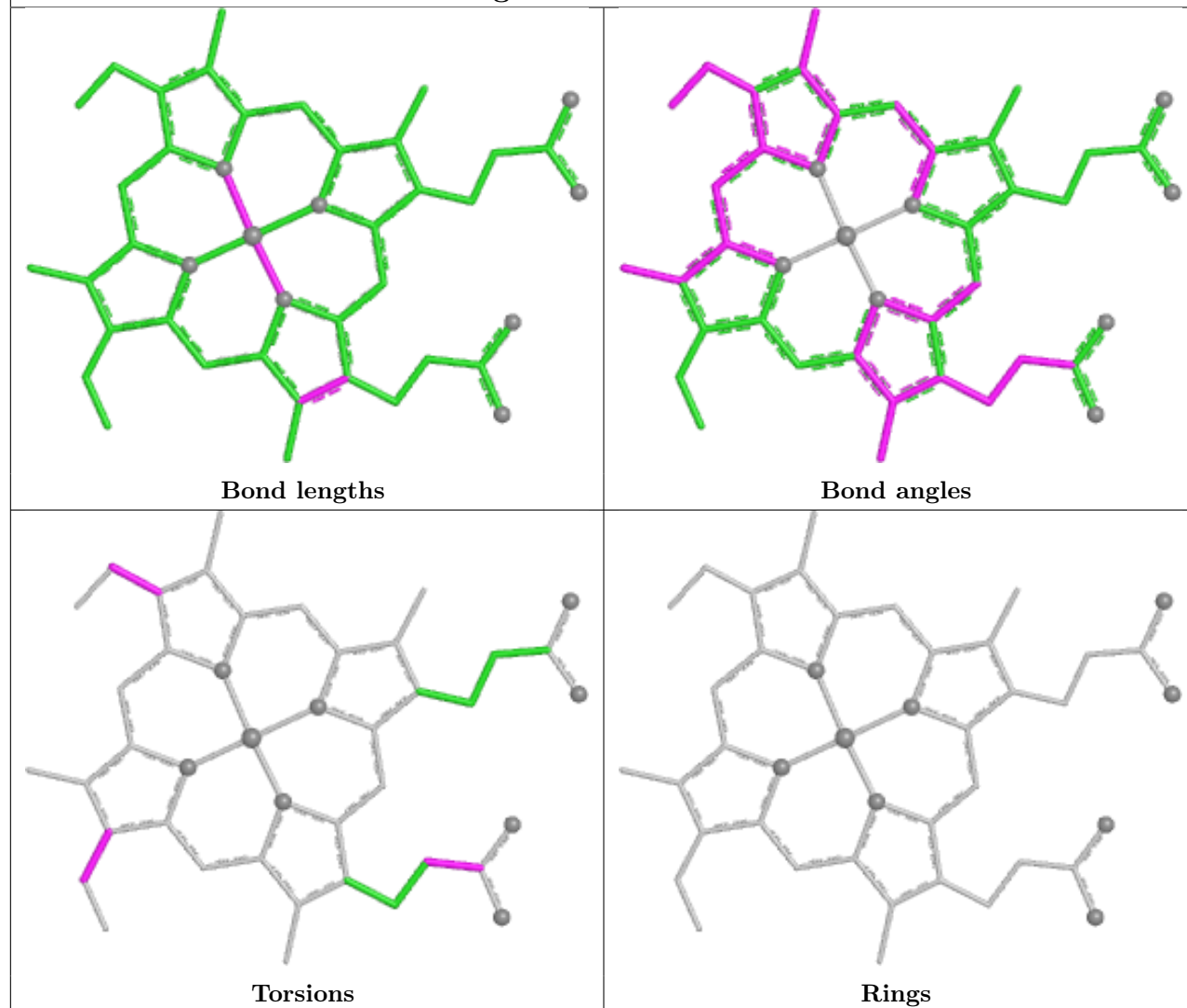




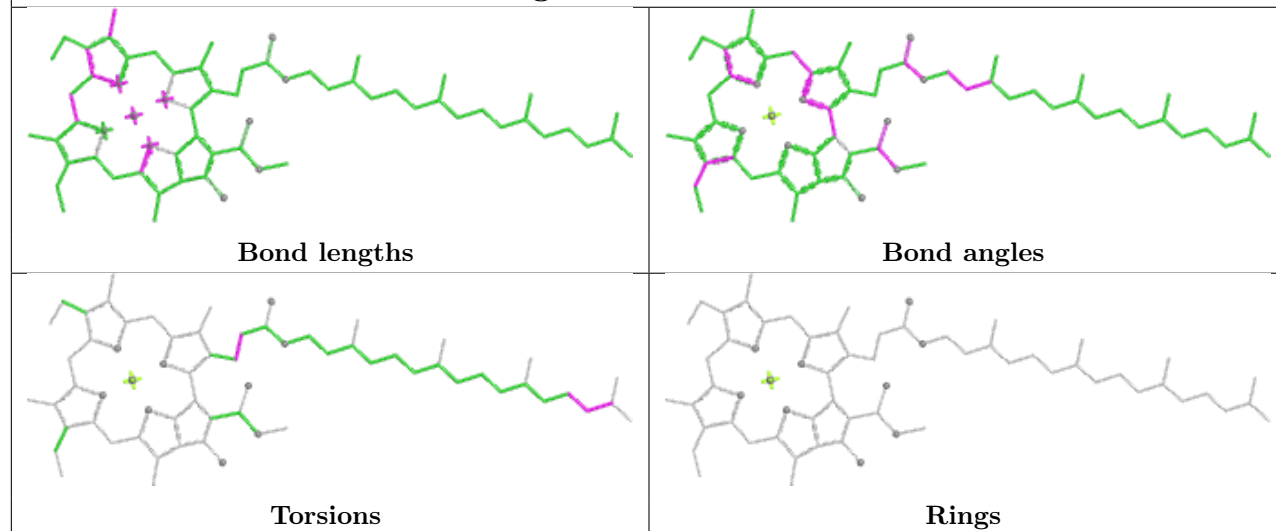


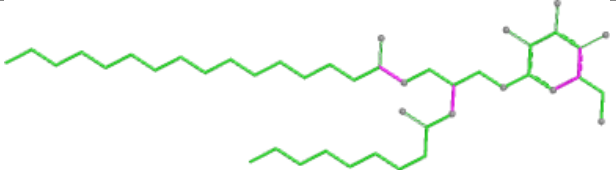
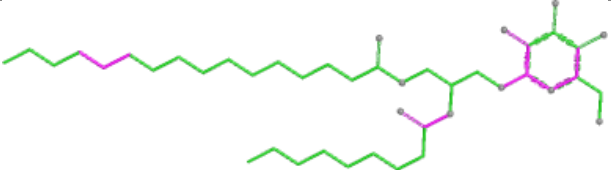
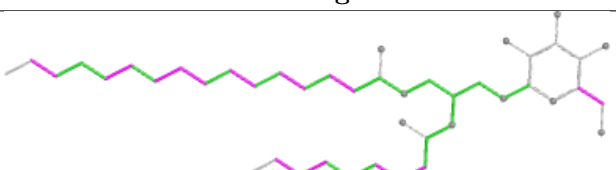
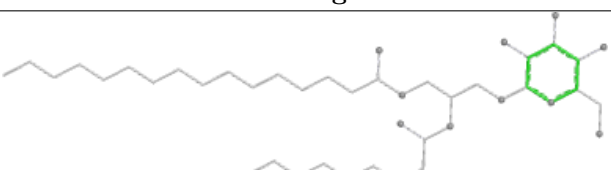
Ligand CLA b 603**Ligand CLA b 602**

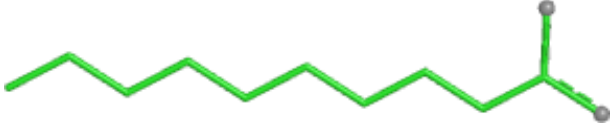
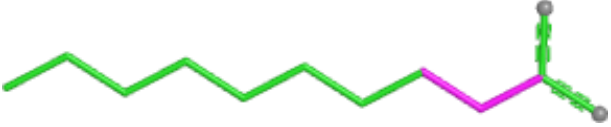
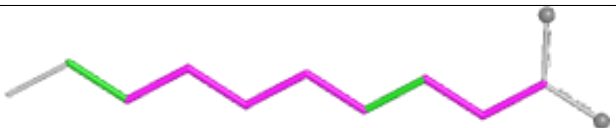
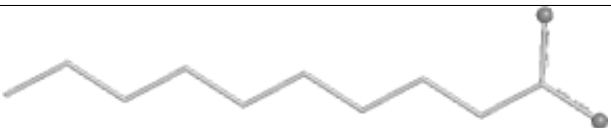
Ligand HEC V 201

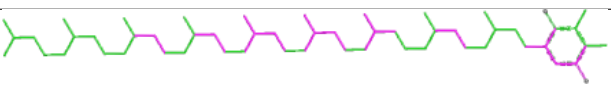
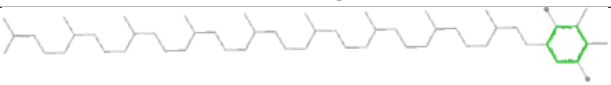


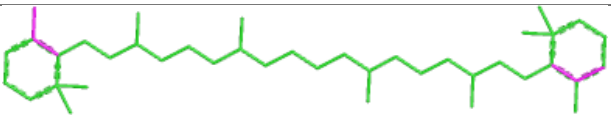
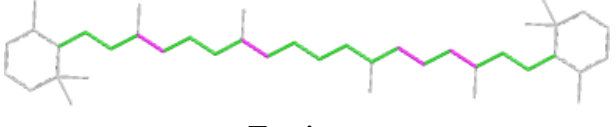
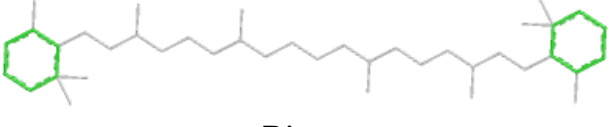
Ligand CLA B 610

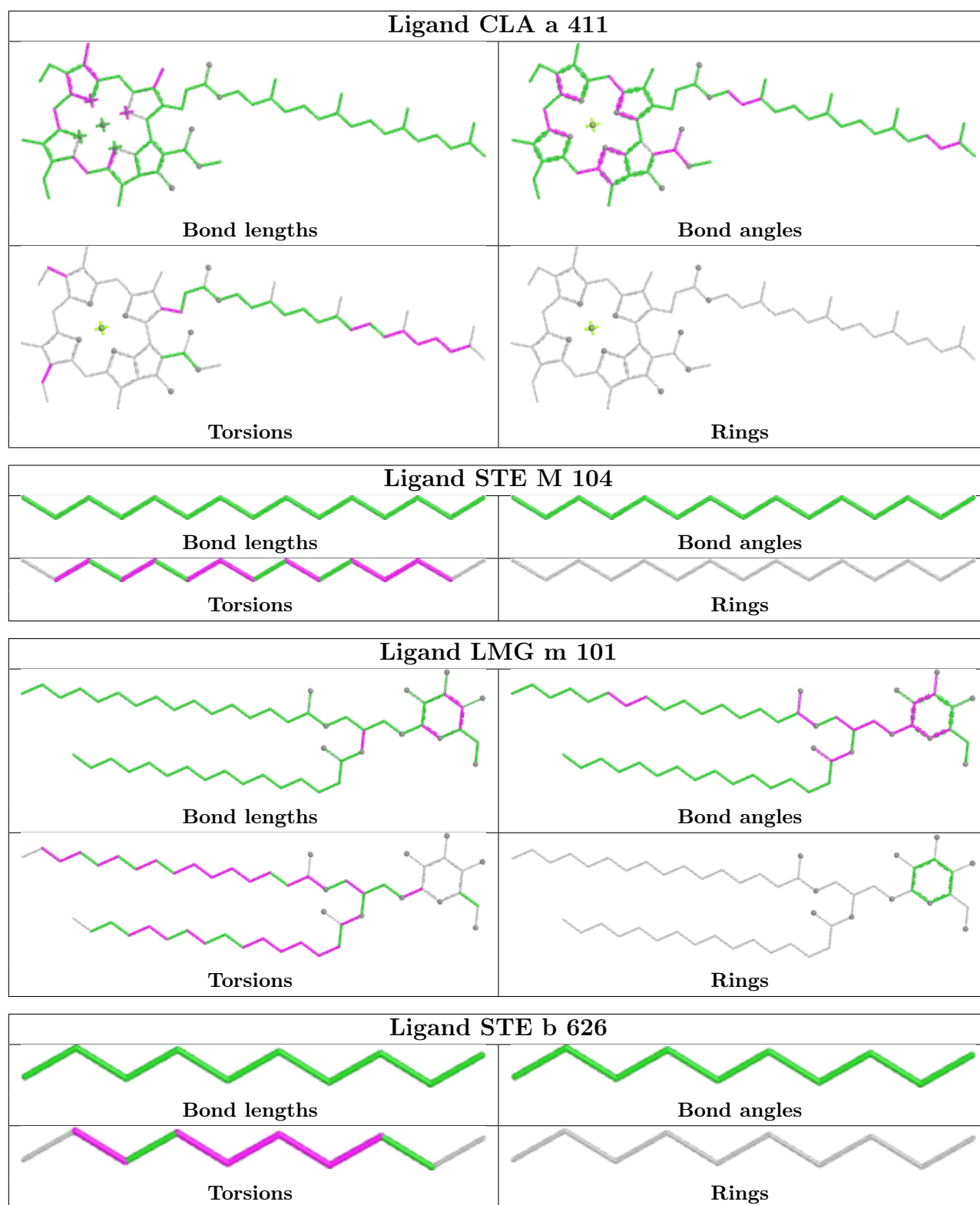


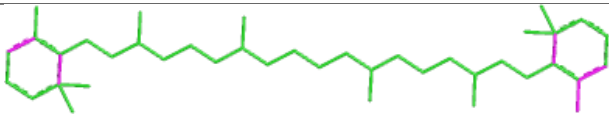
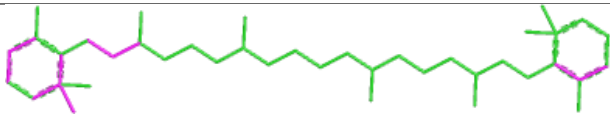
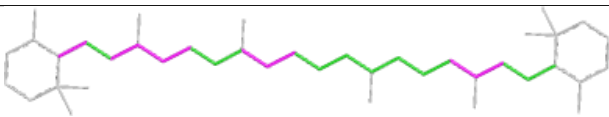
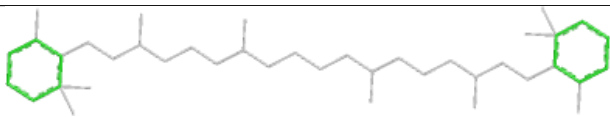
Ligand LMG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

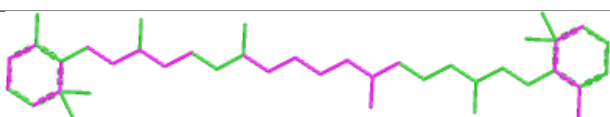
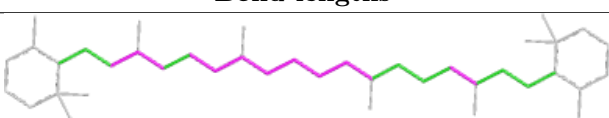
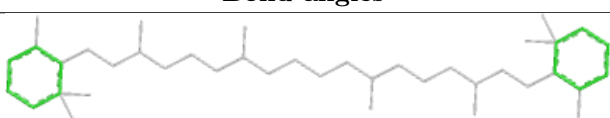
Ligand PL9 a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

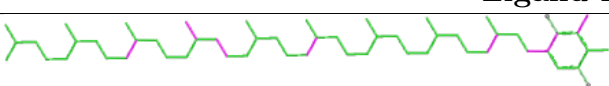
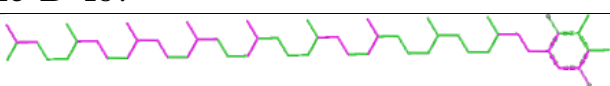
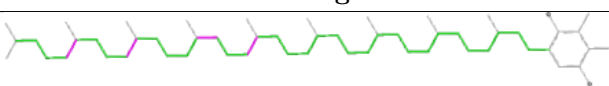
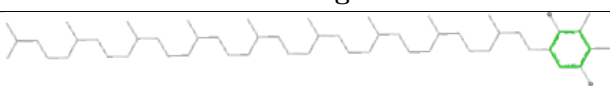
Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

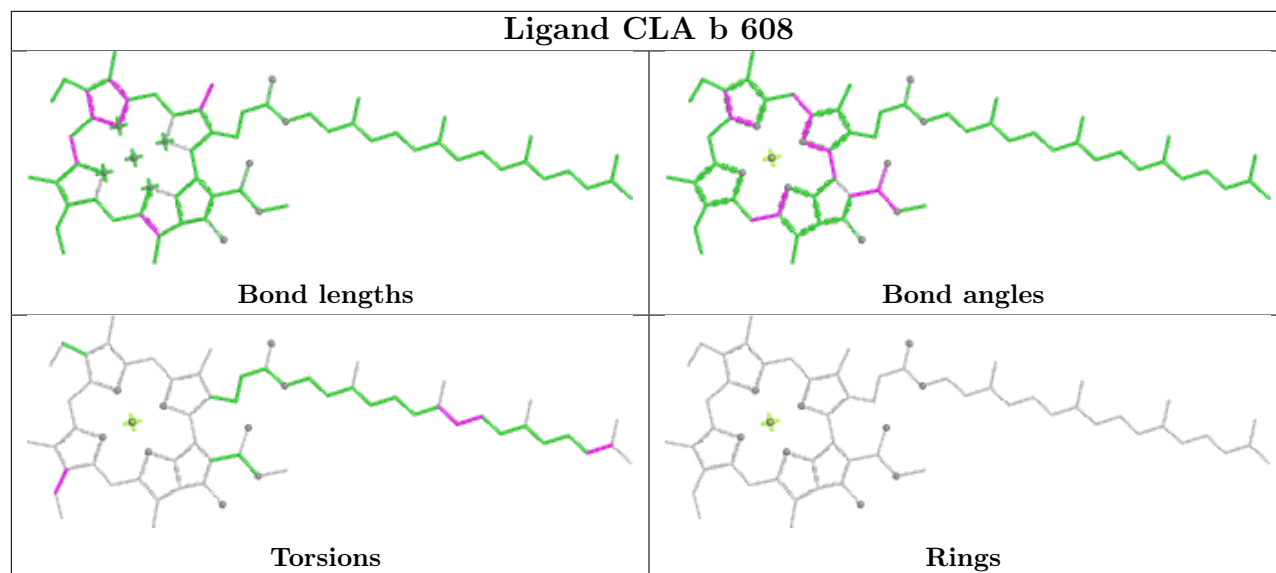
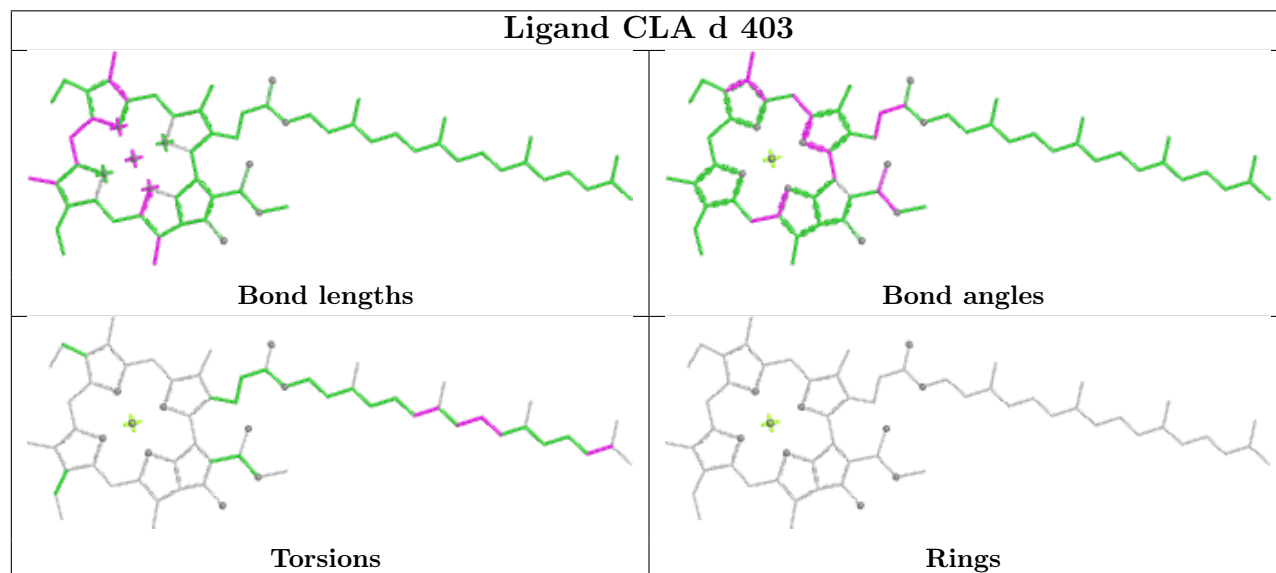
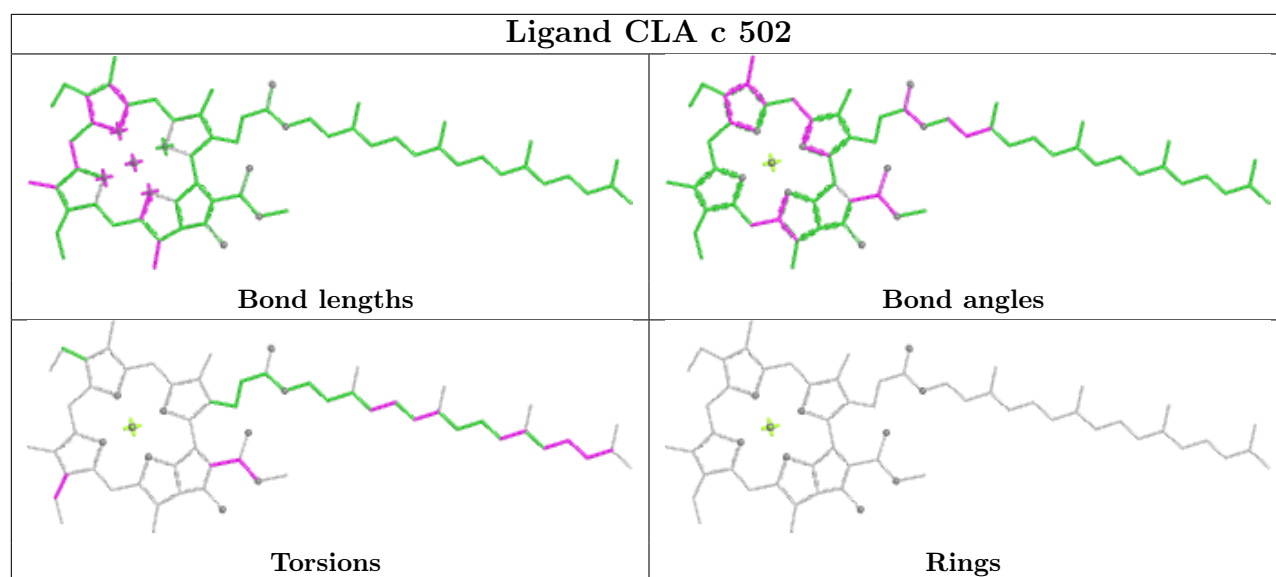


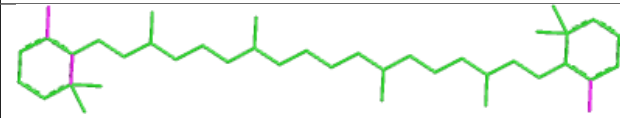
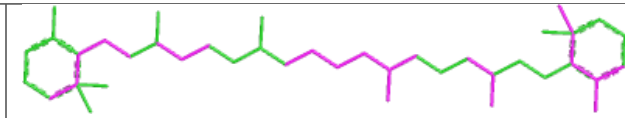
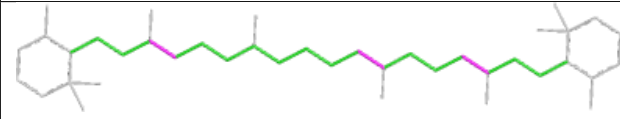
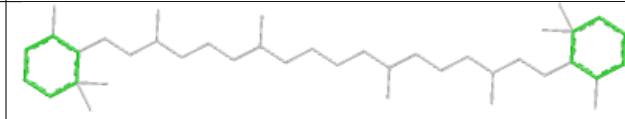
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

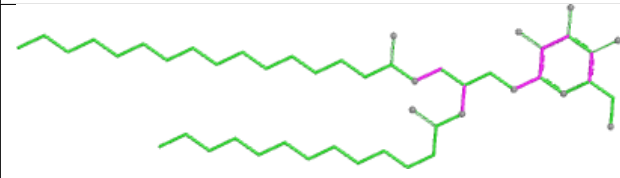
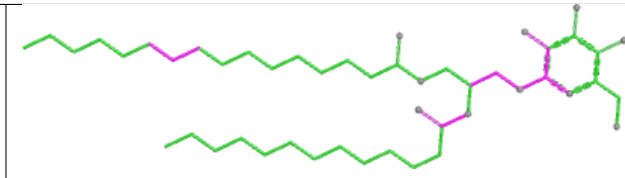
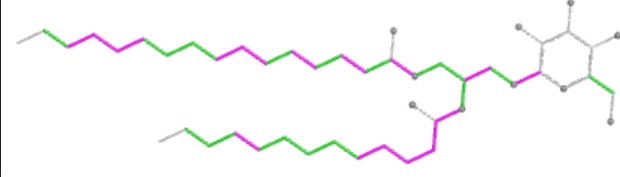
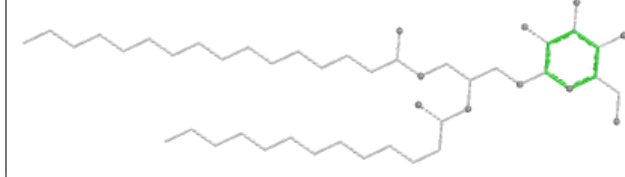
Ligand STE M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

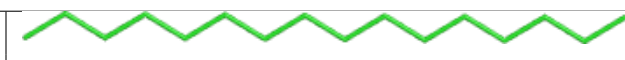
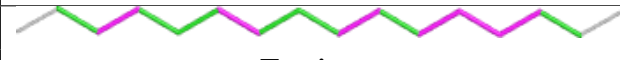
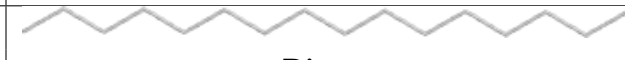
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

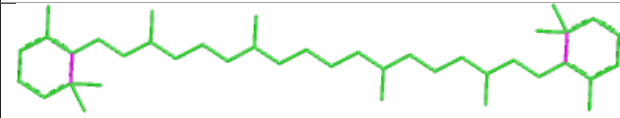
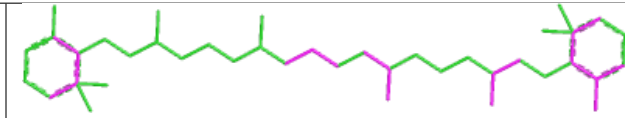
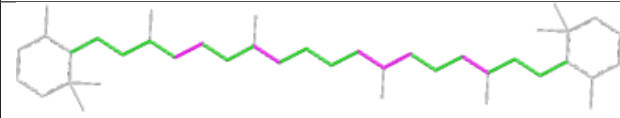
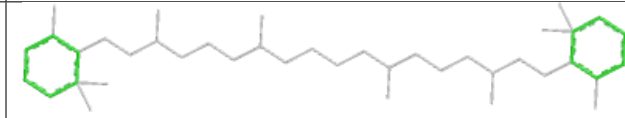
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

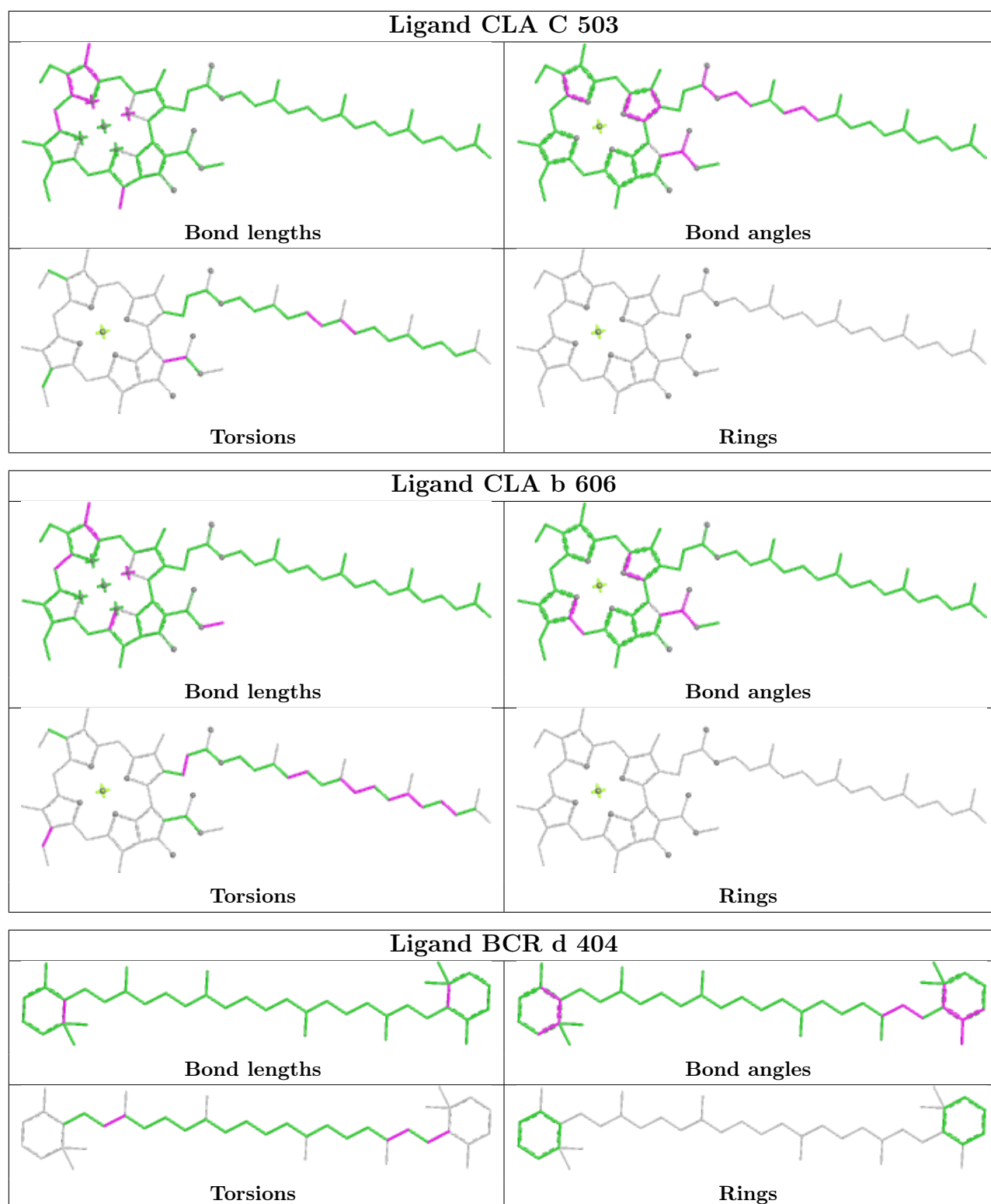


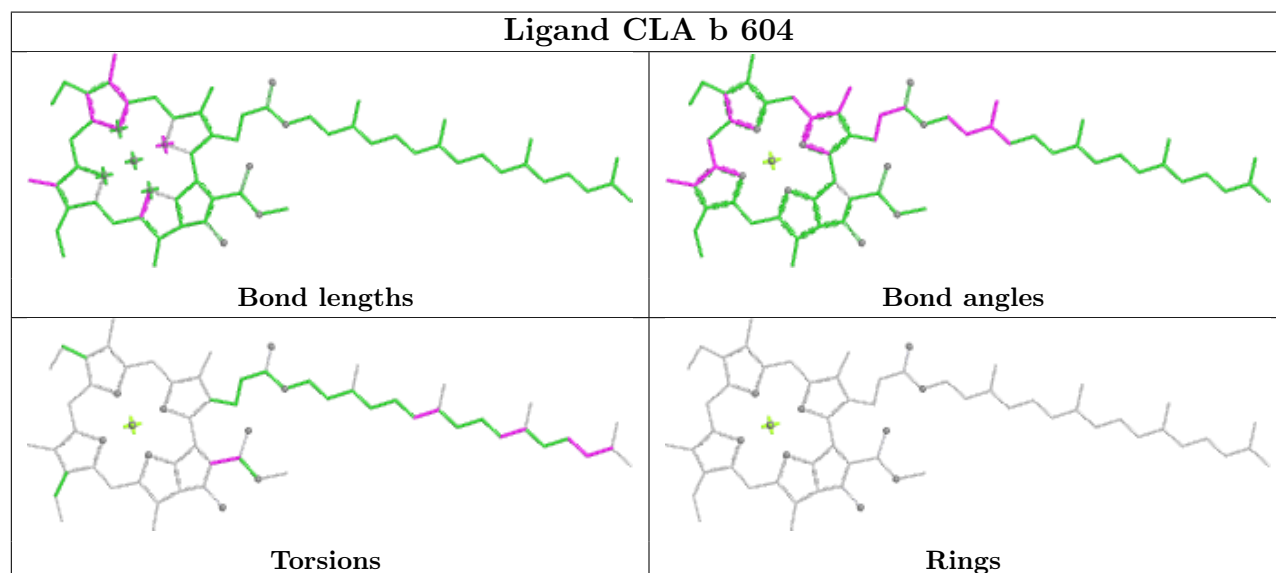
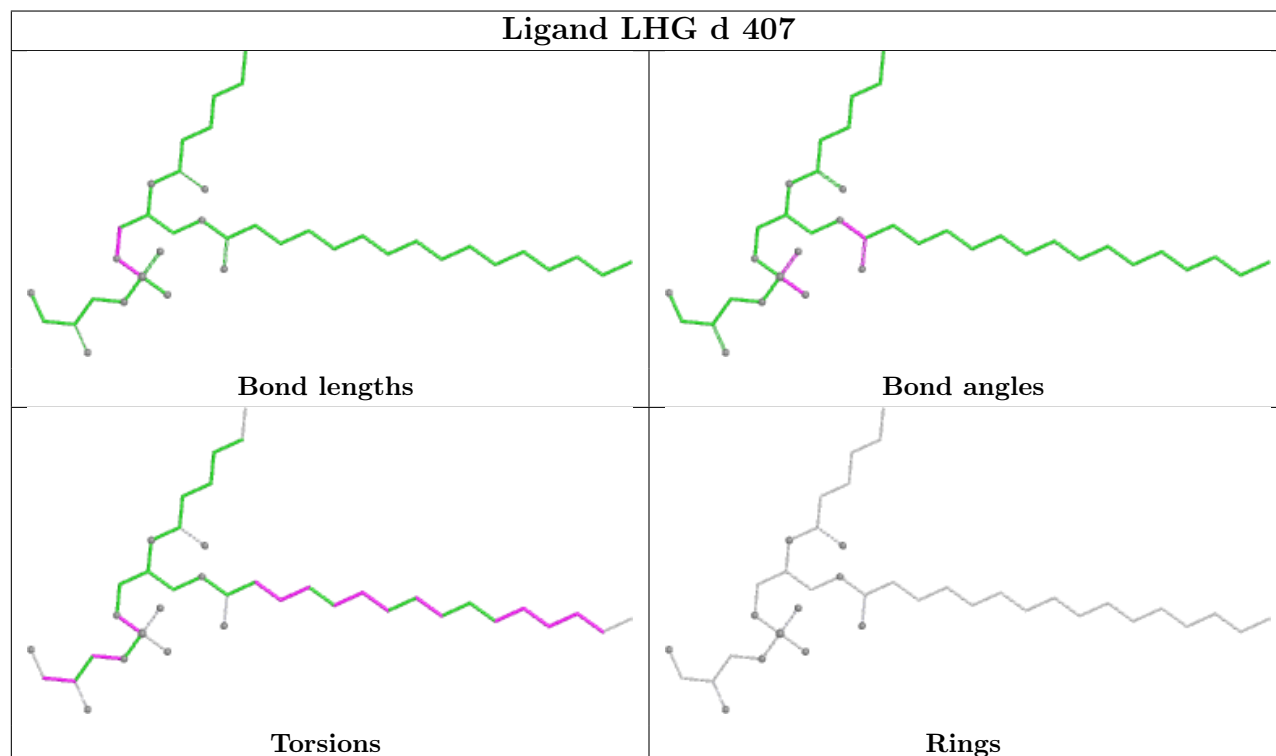
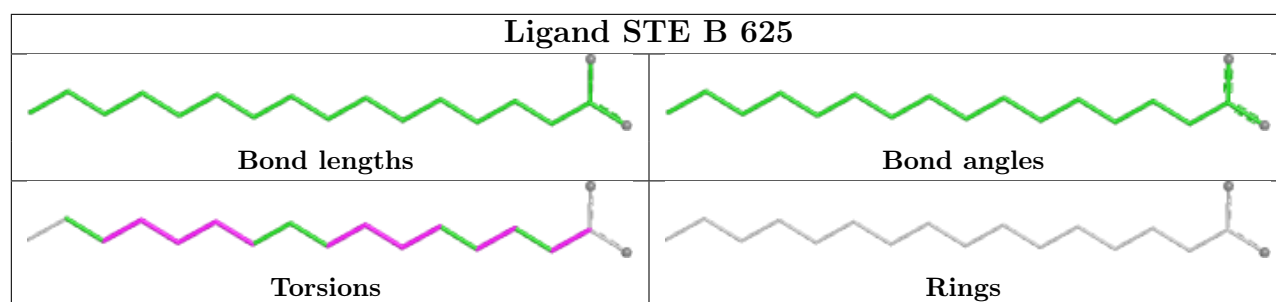
Ligand BCR A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

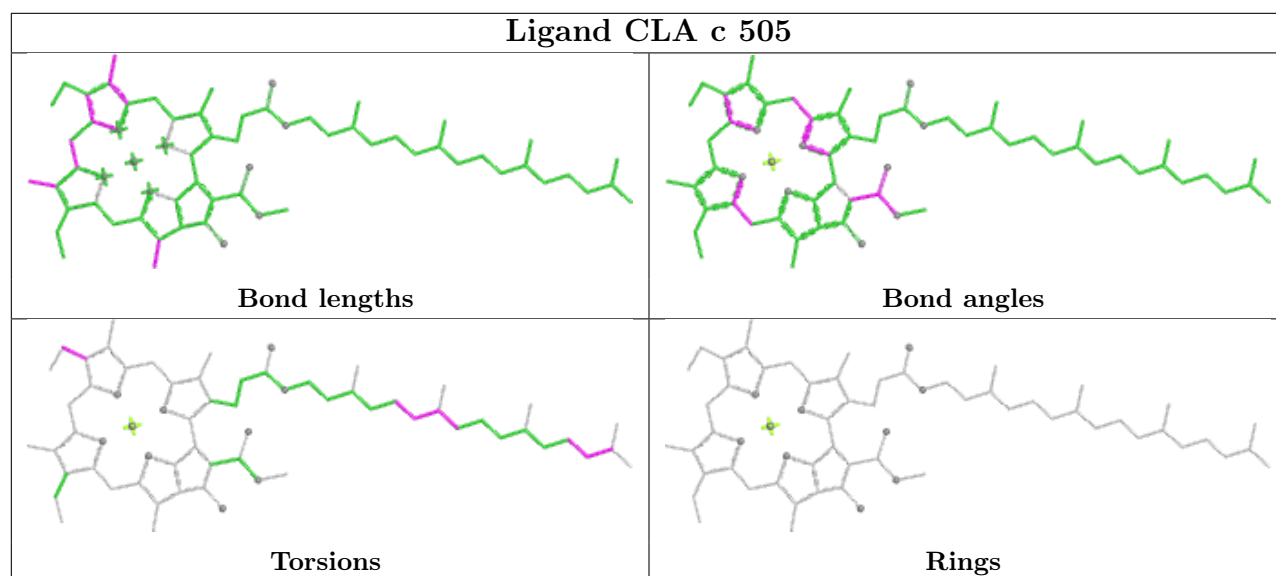
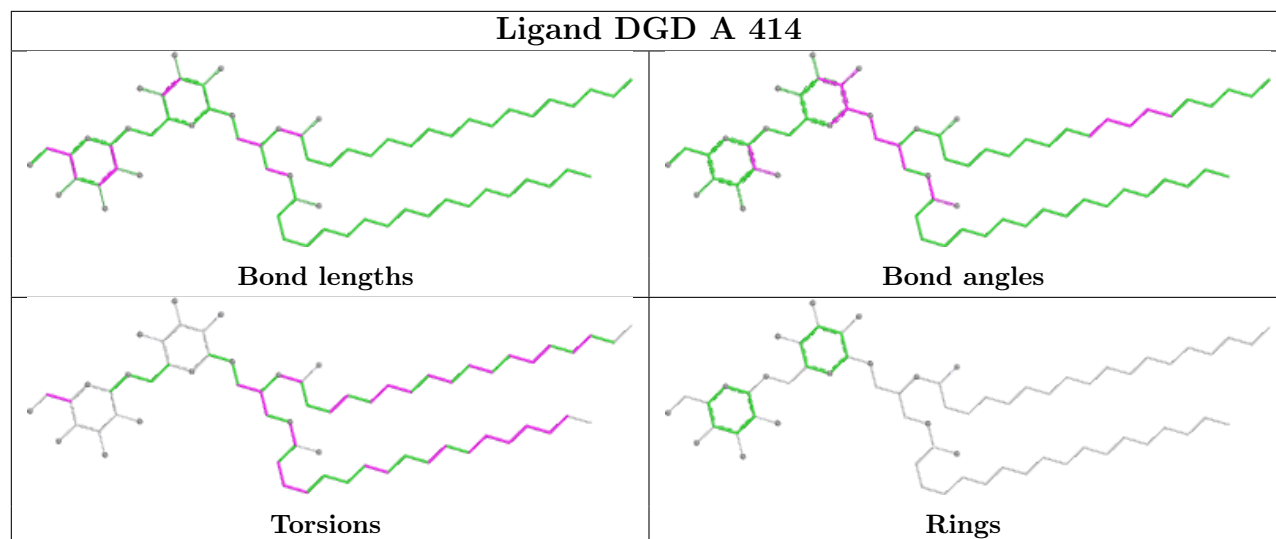
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Bond lengths	Bond angles
	
Torsions	Rings

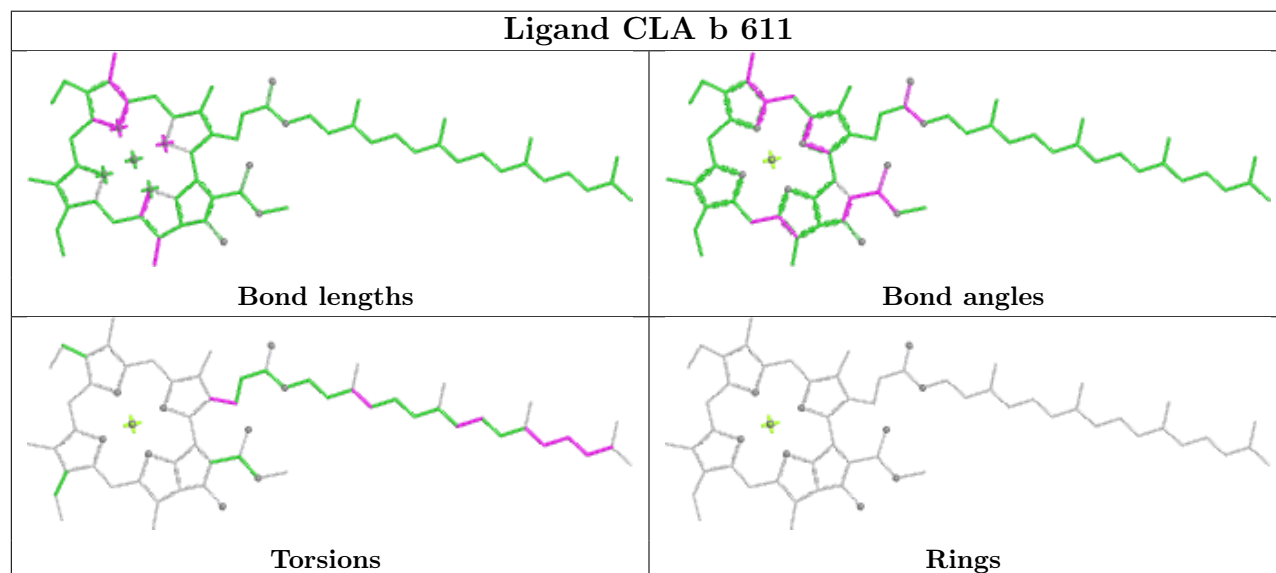
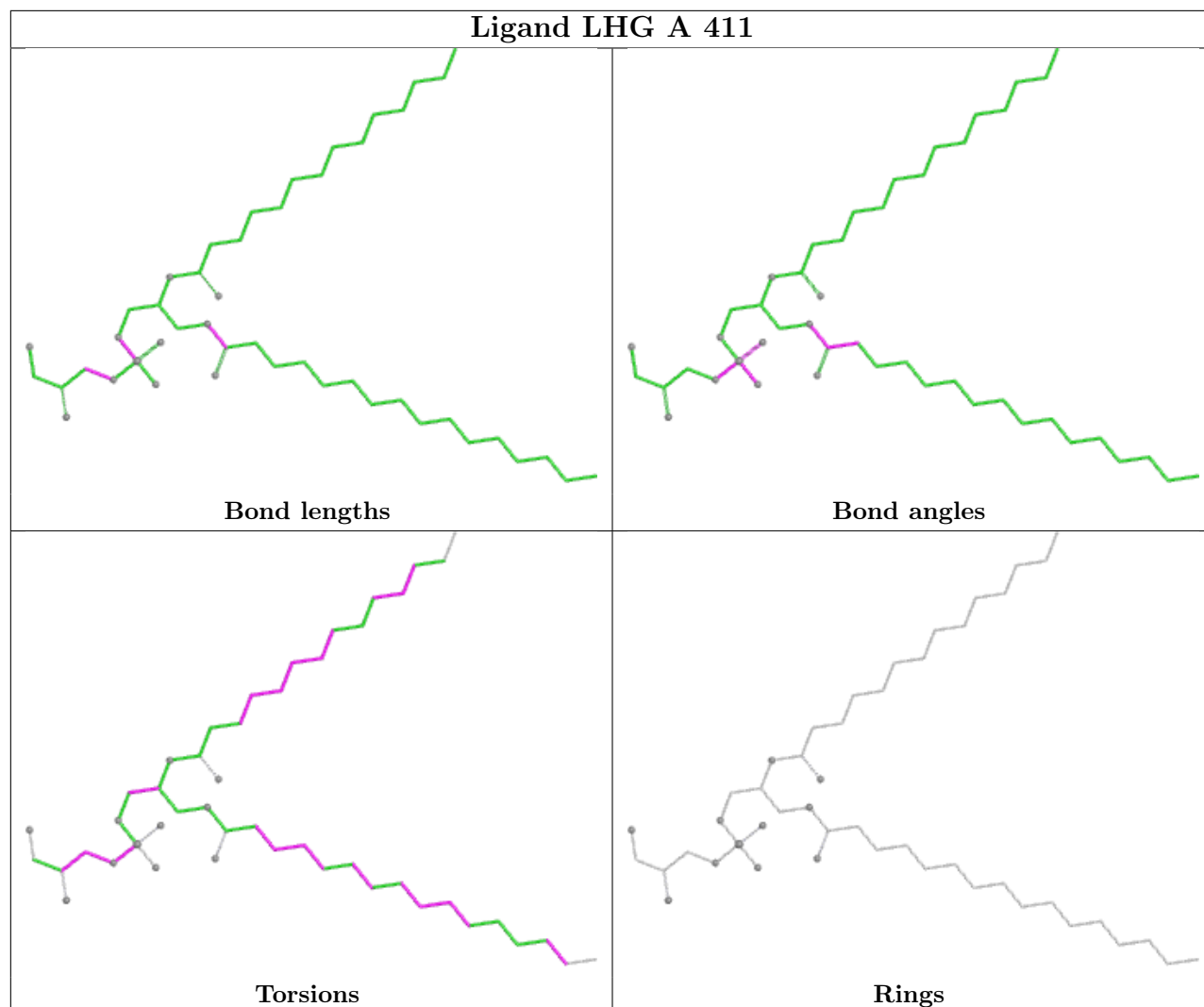
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Bond lengths	Bond angles
	
Torsions	Rings

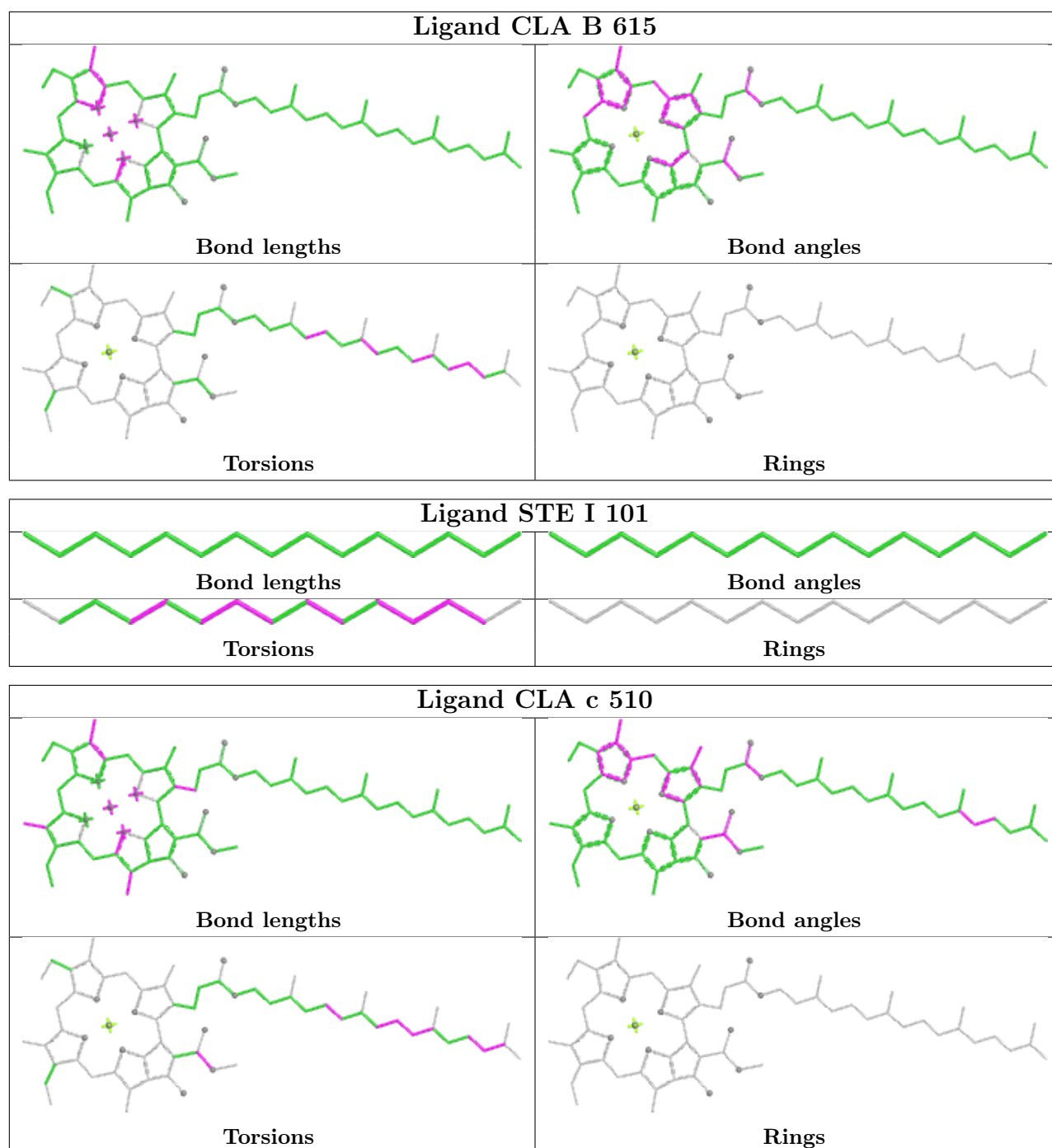
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Bond lengths	Bond angles
	
Torsions	Rings

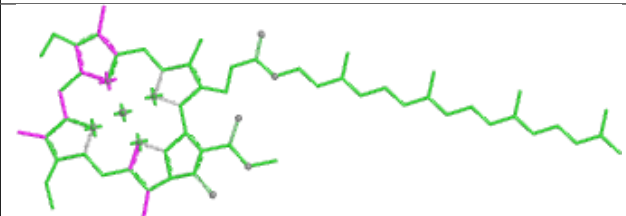
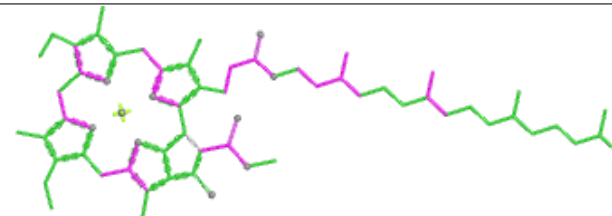
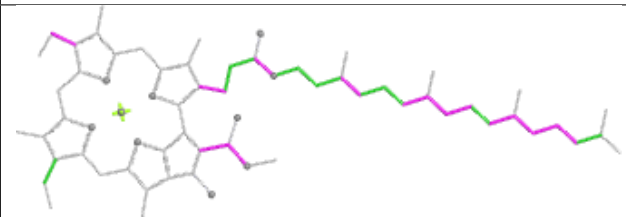
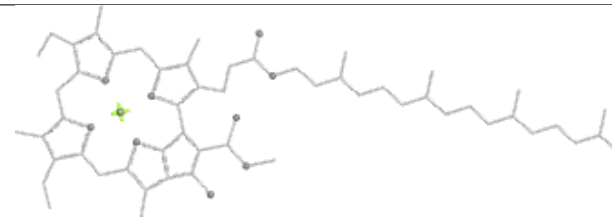




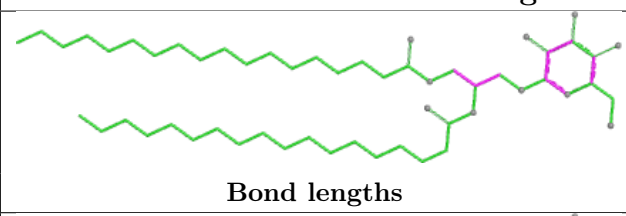
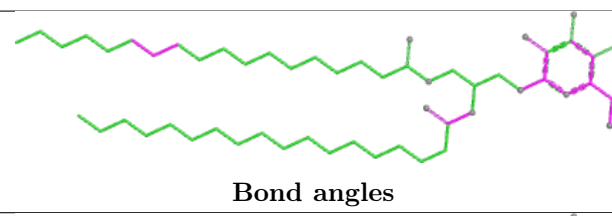
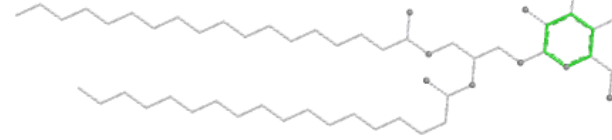


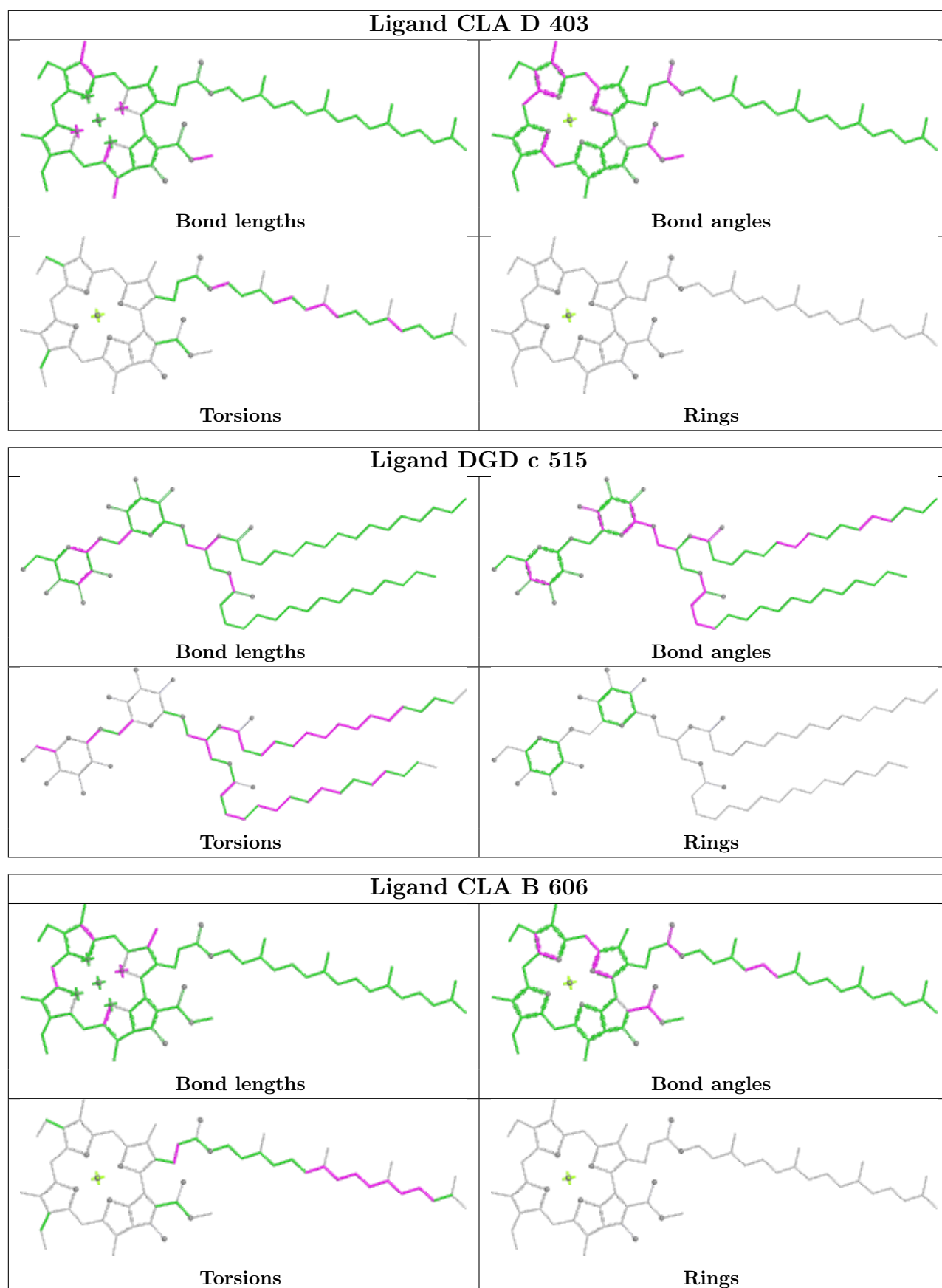


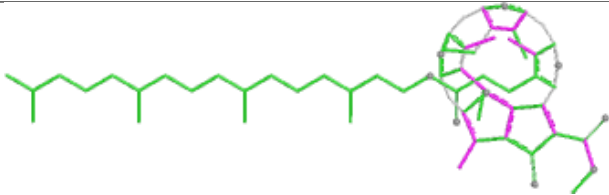
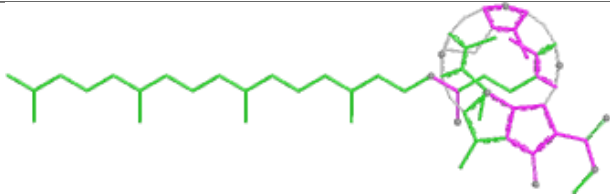
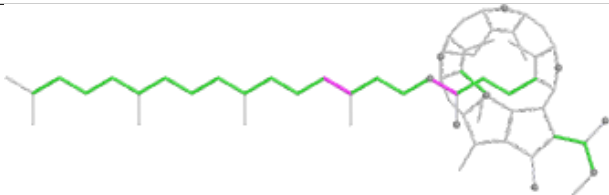
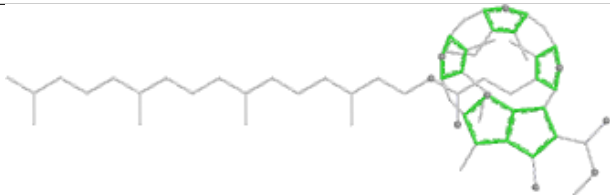


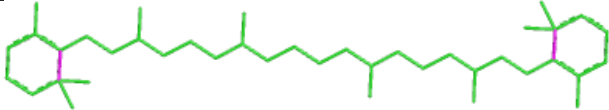
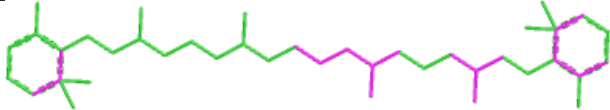
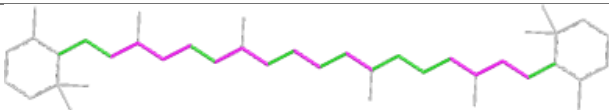
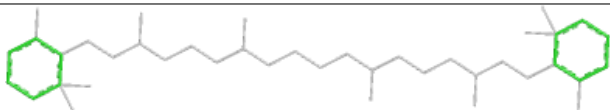
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

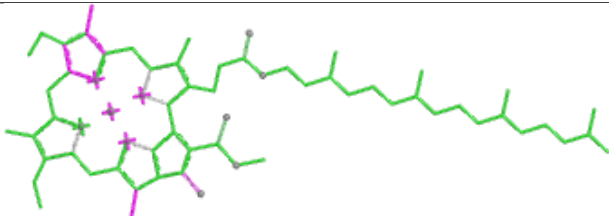
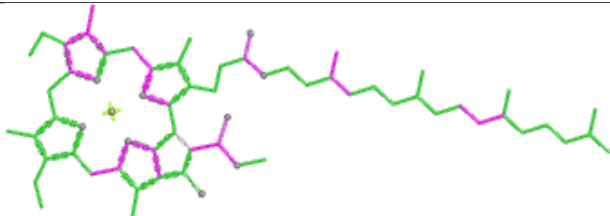
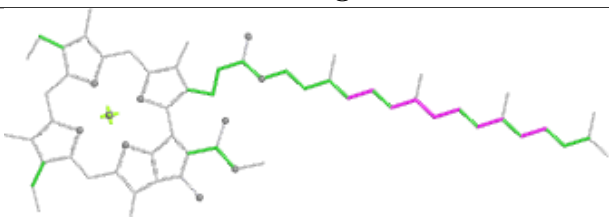
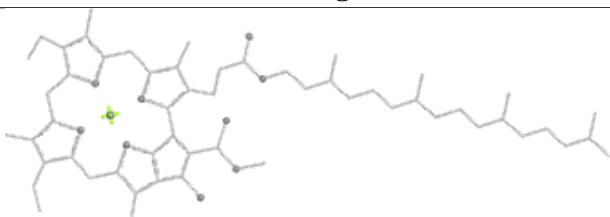
Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

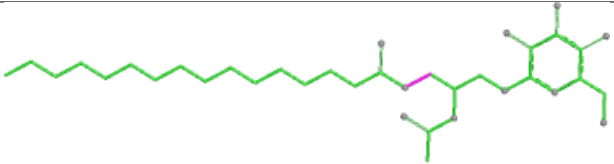
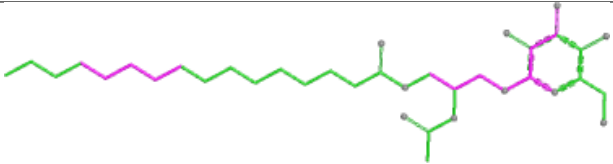
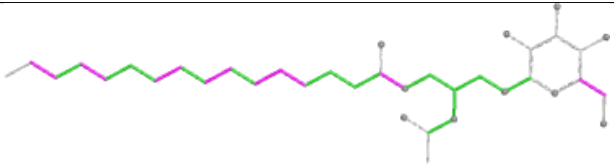
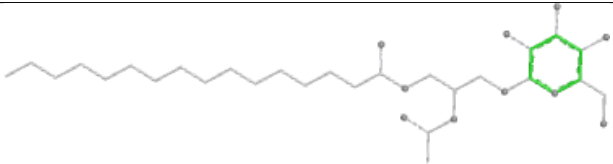
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

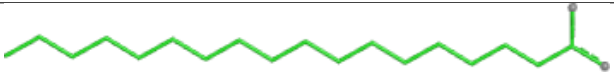
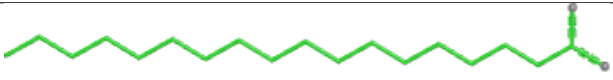
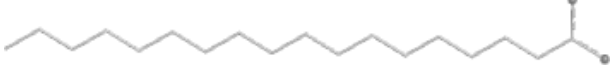


Ligand PHO A 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

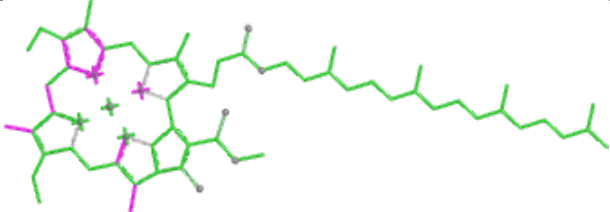
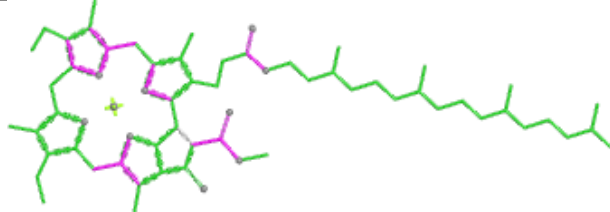
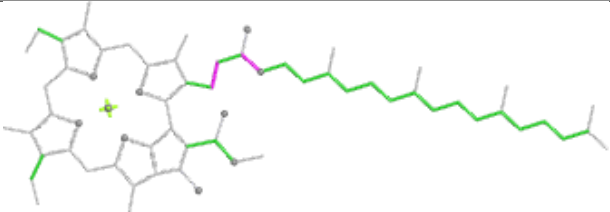
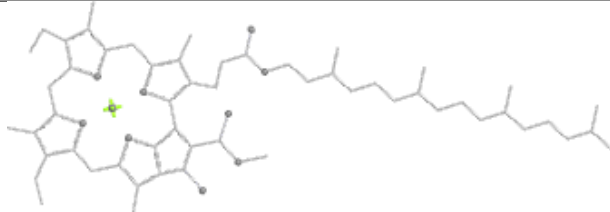
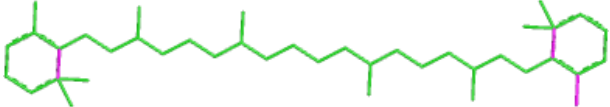
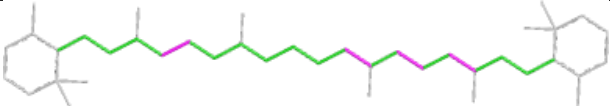
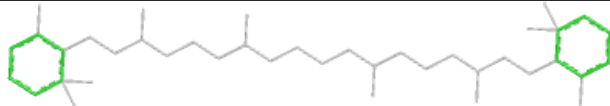
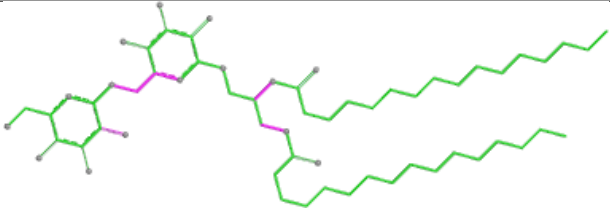
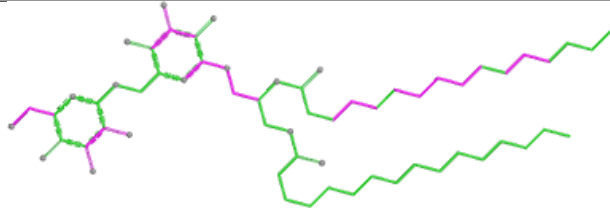
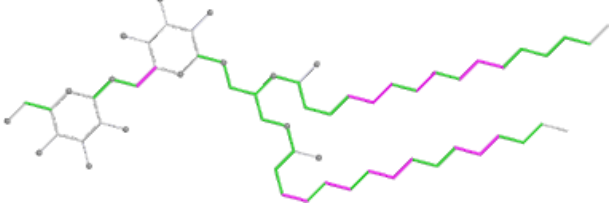
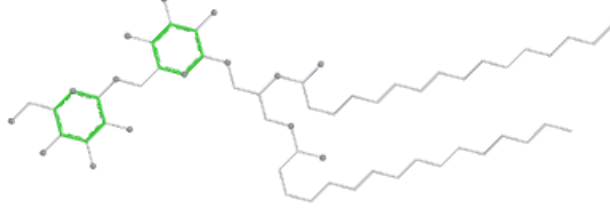
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

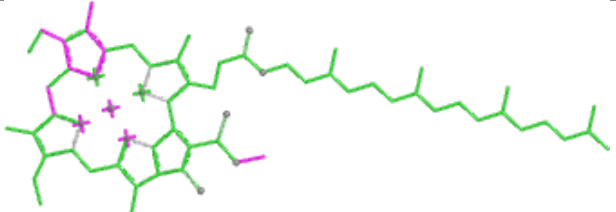
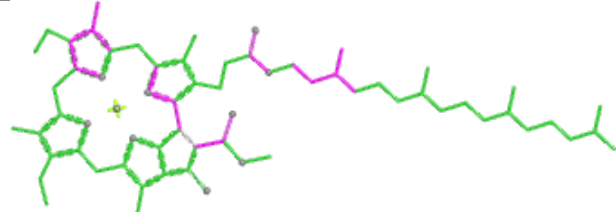
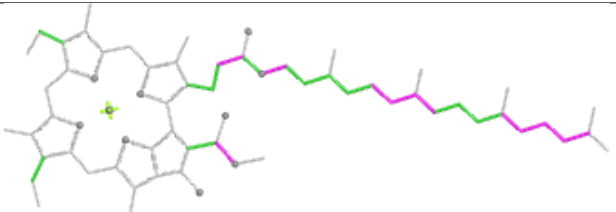
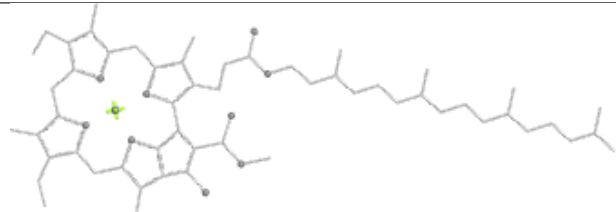
Ligand LMG c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

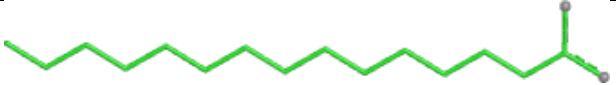
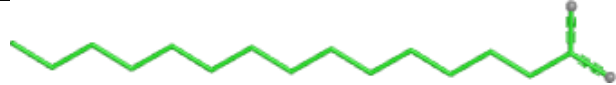
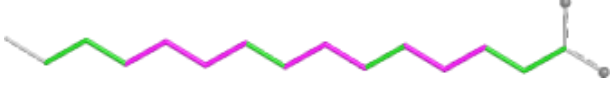
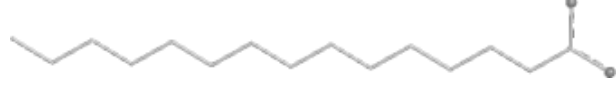
Ligand STE D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

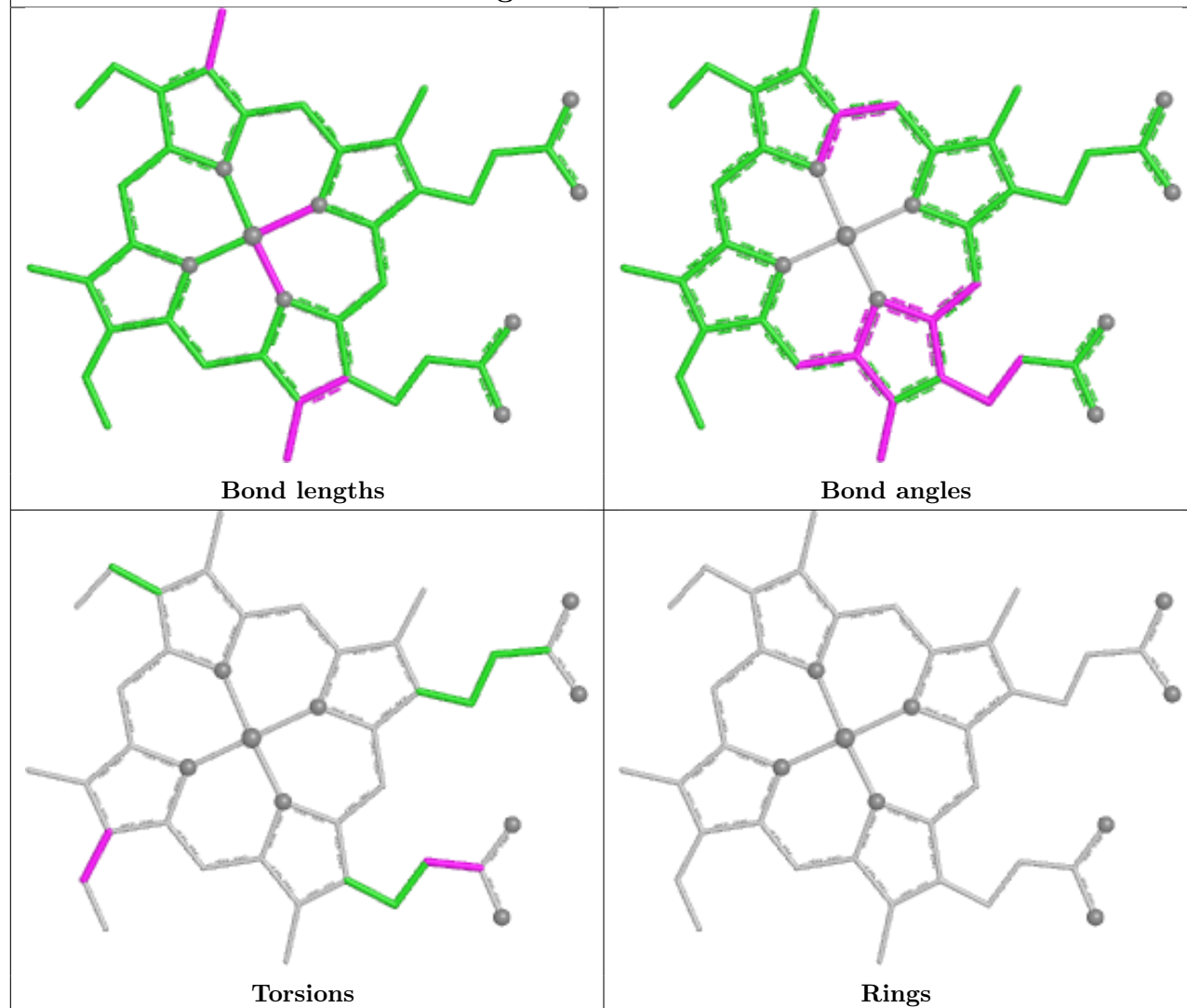
Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

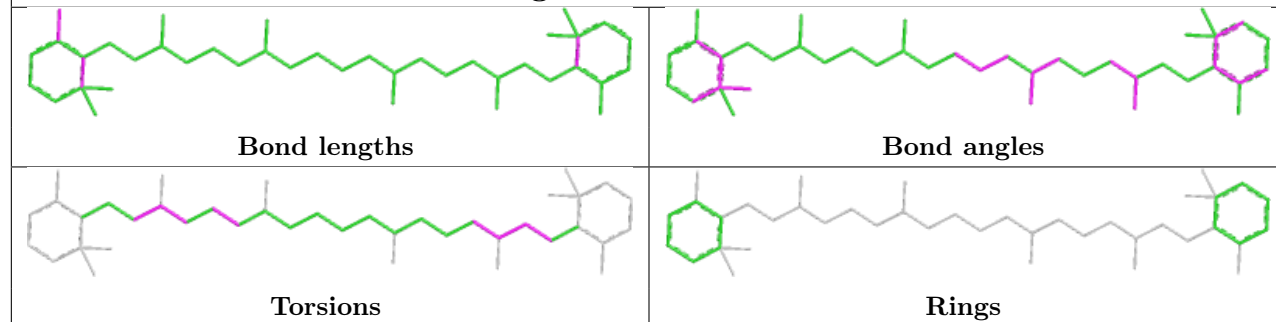
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

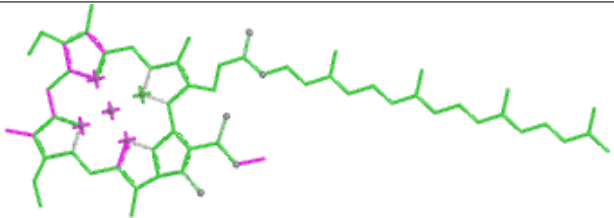
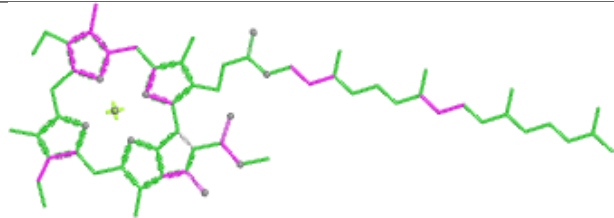
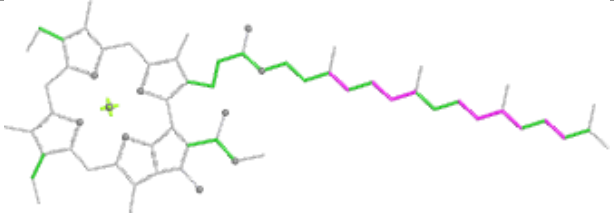
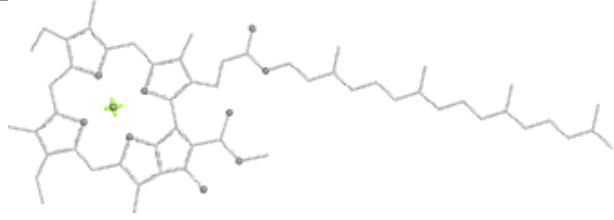
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Bond lengths	Bond angles
	
Torsions	Rings

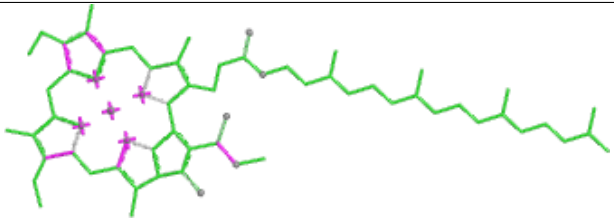
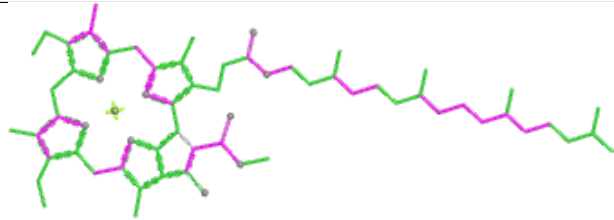
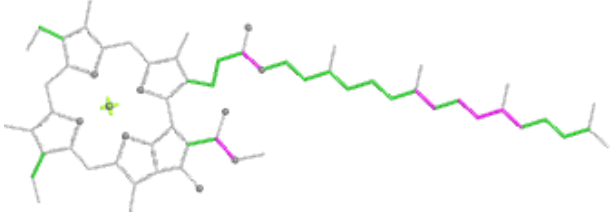
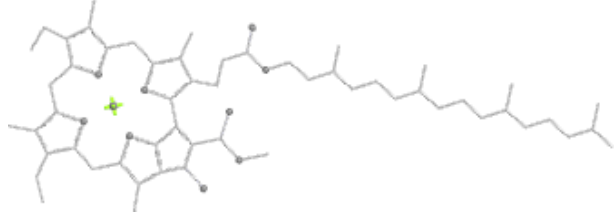
Ligand HEC v 201

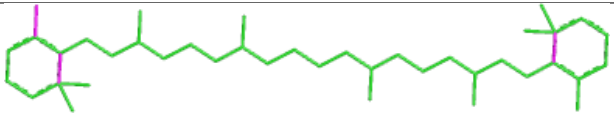
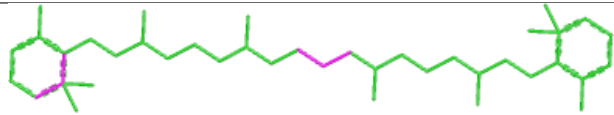
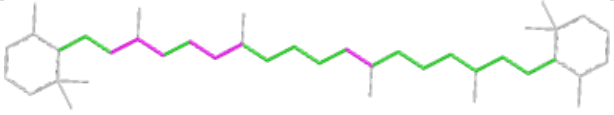
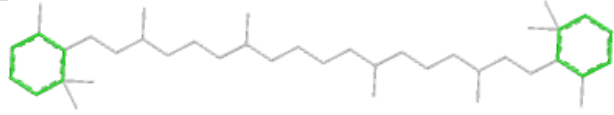


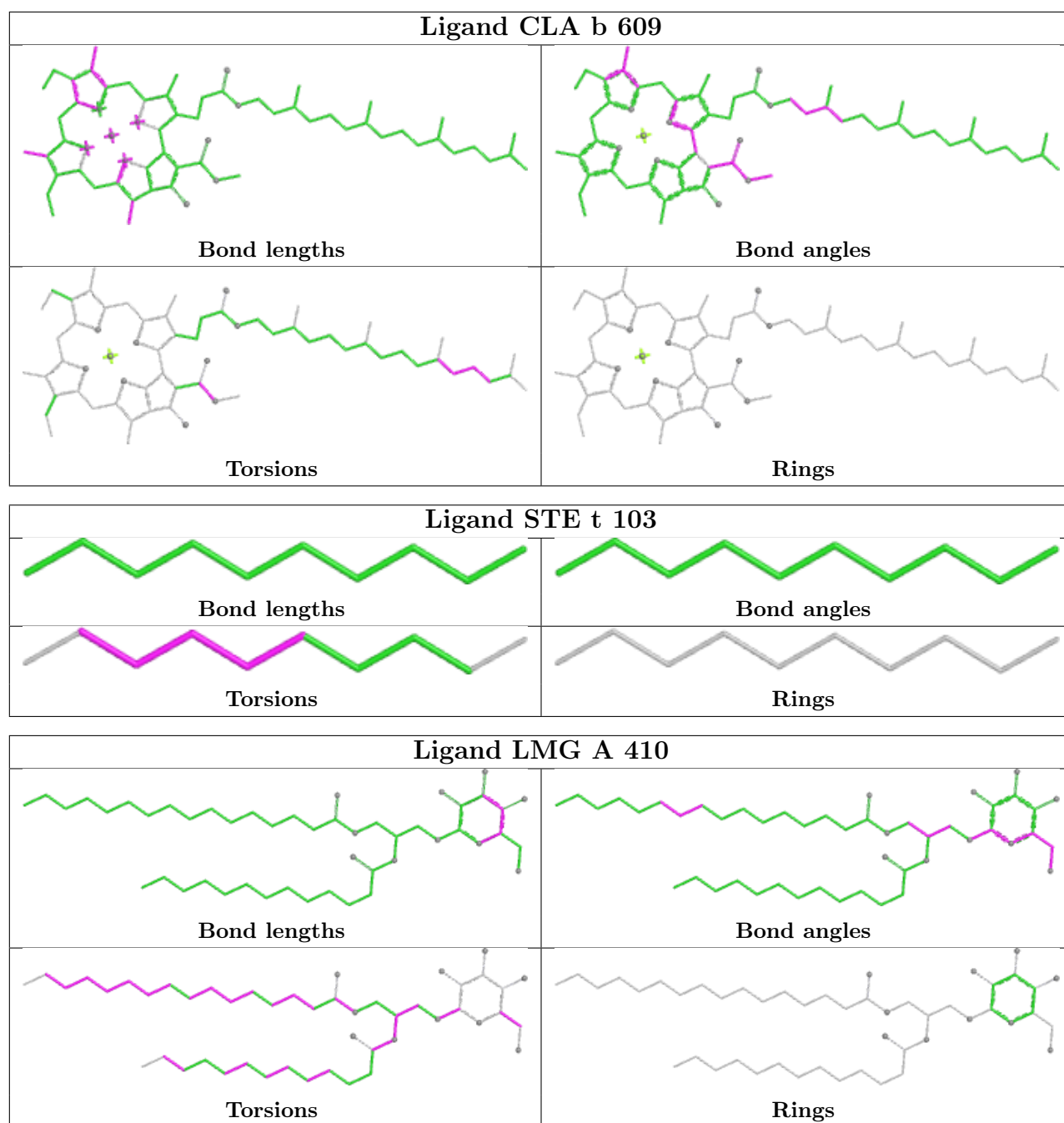
Ligand BCR B 619



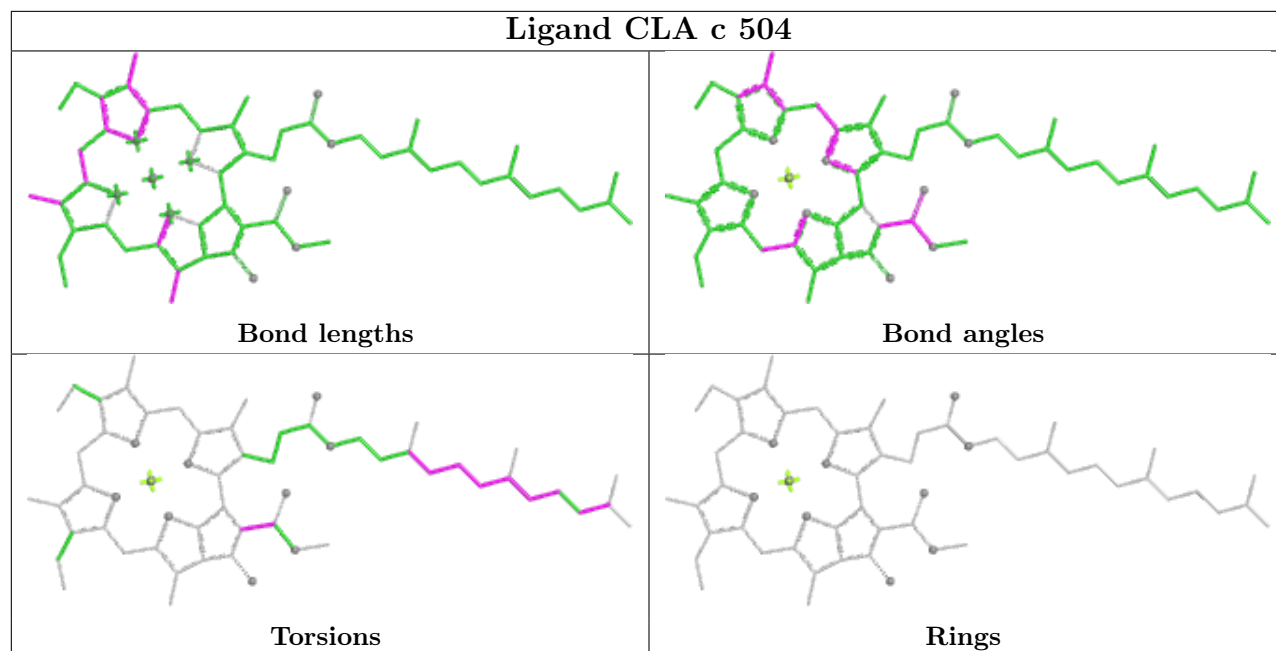
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

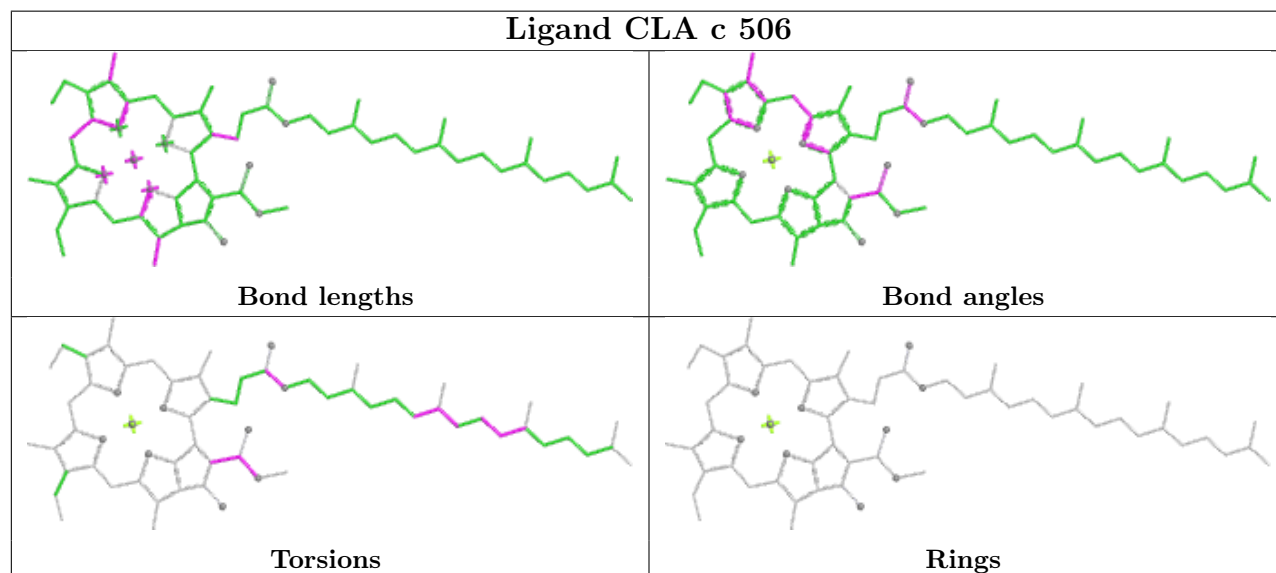
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



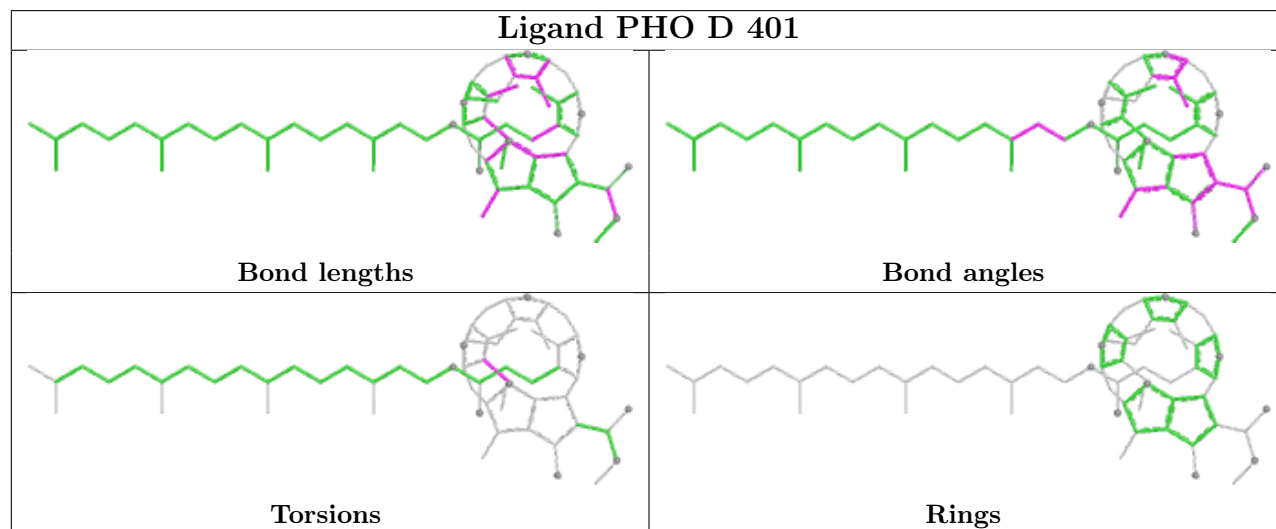
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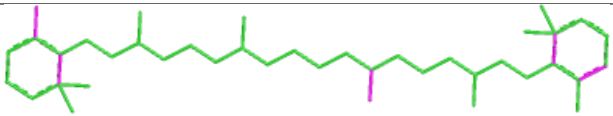
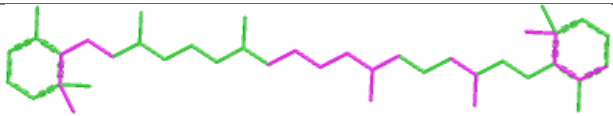
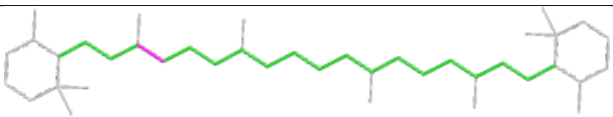
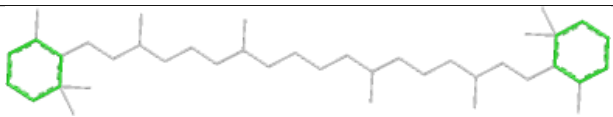


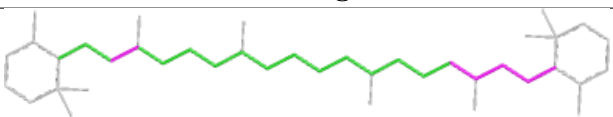
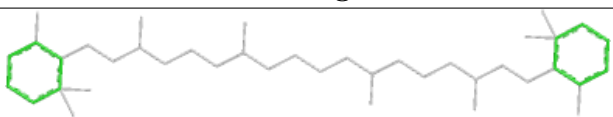
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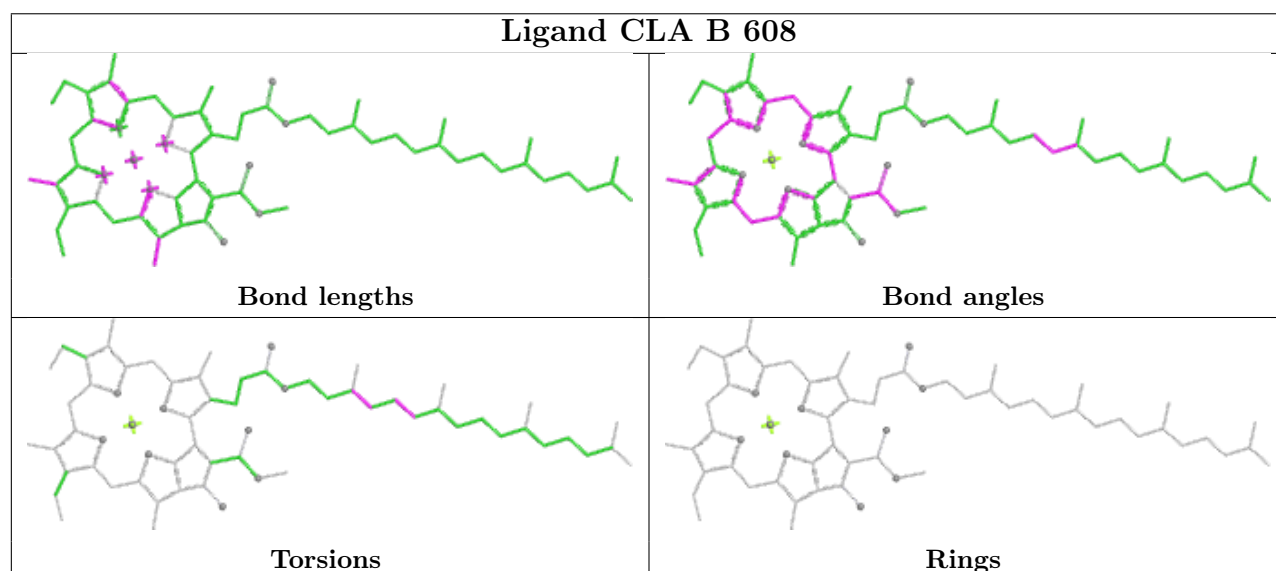
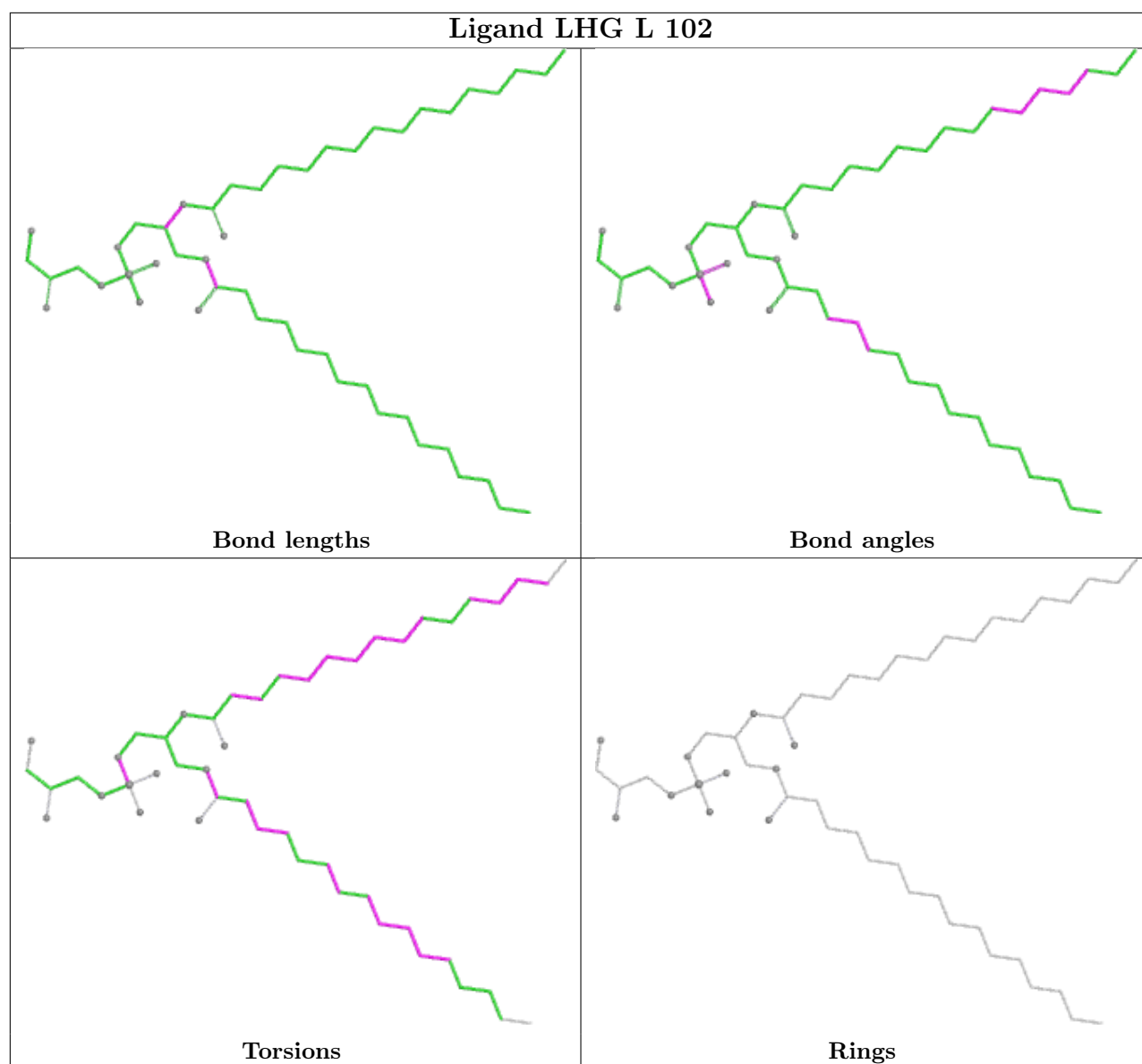


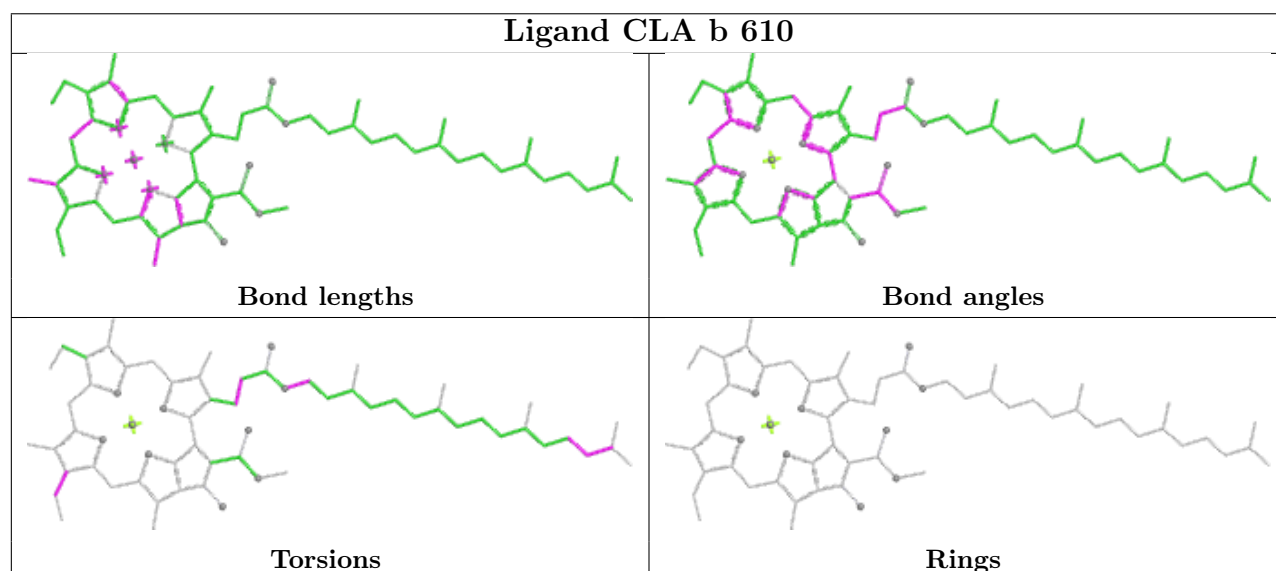
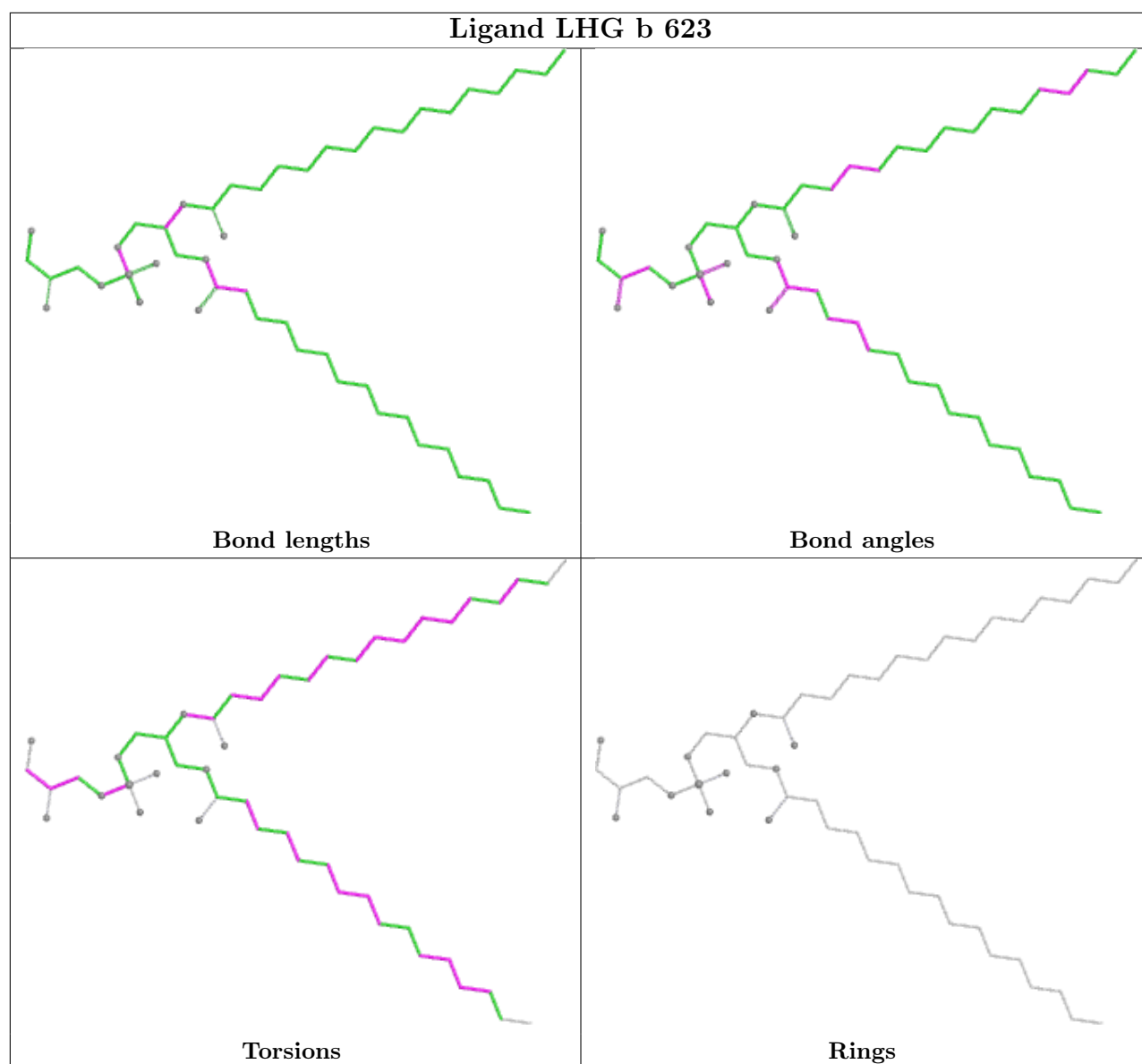
Ligand PHO D 401

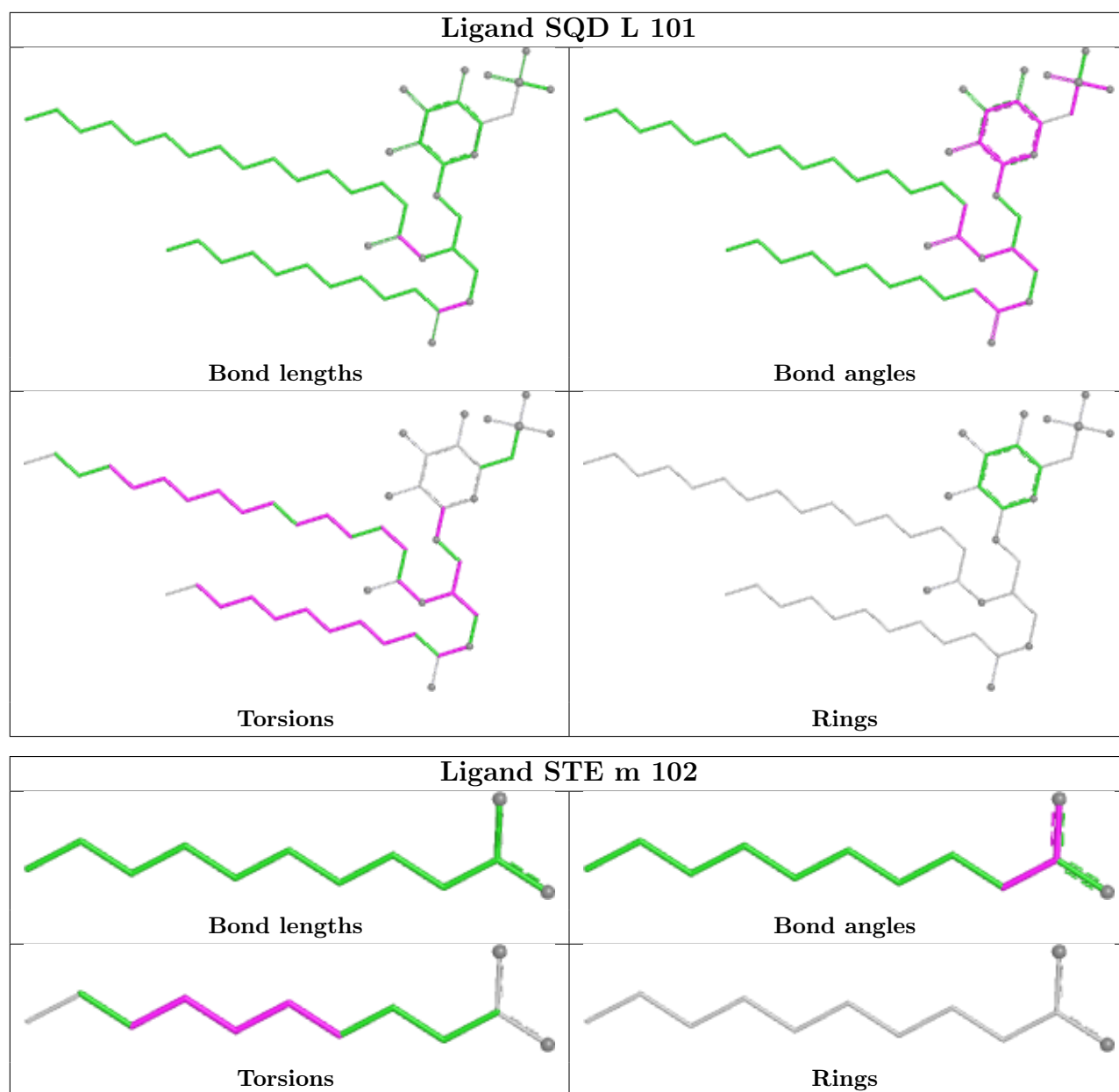


Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

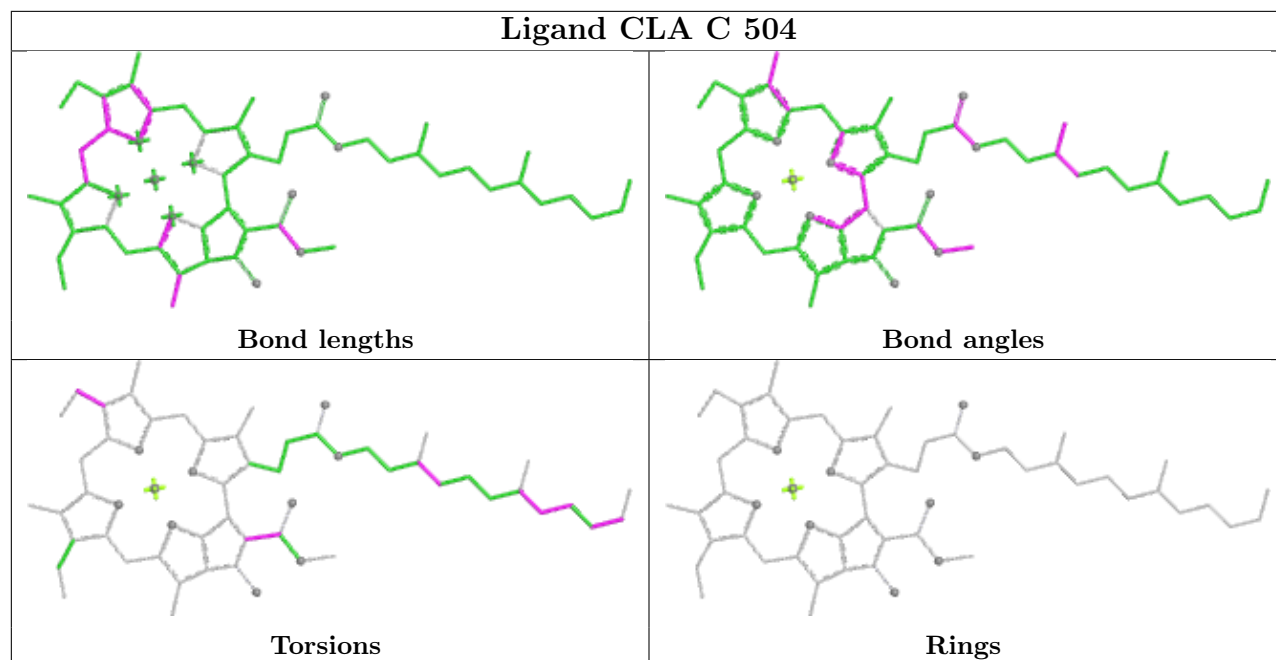
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



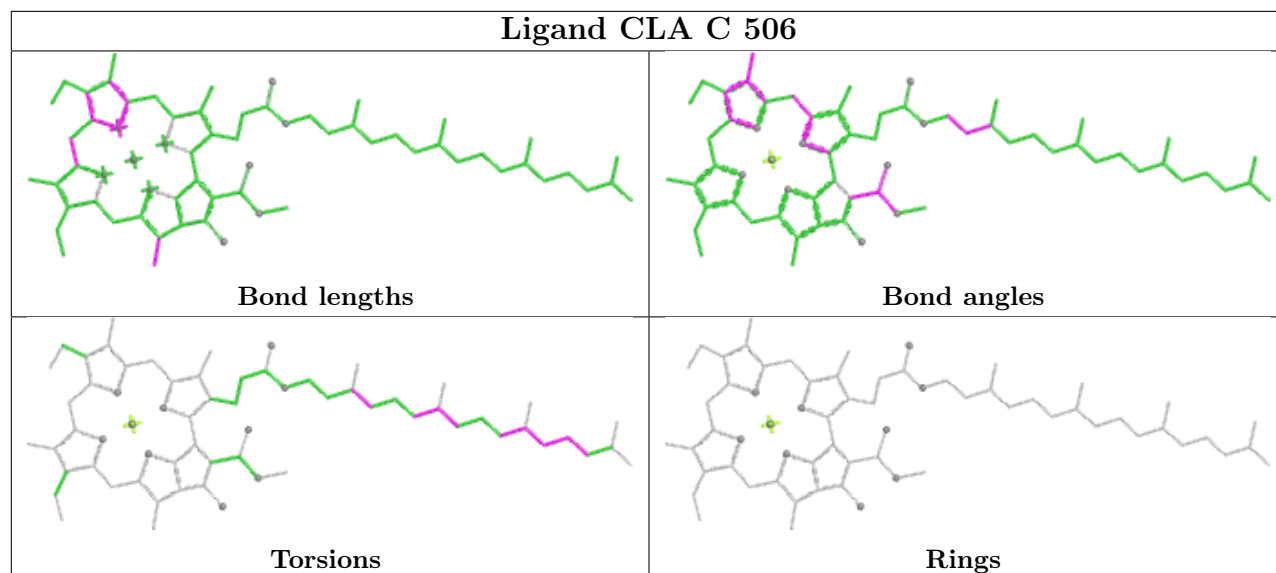




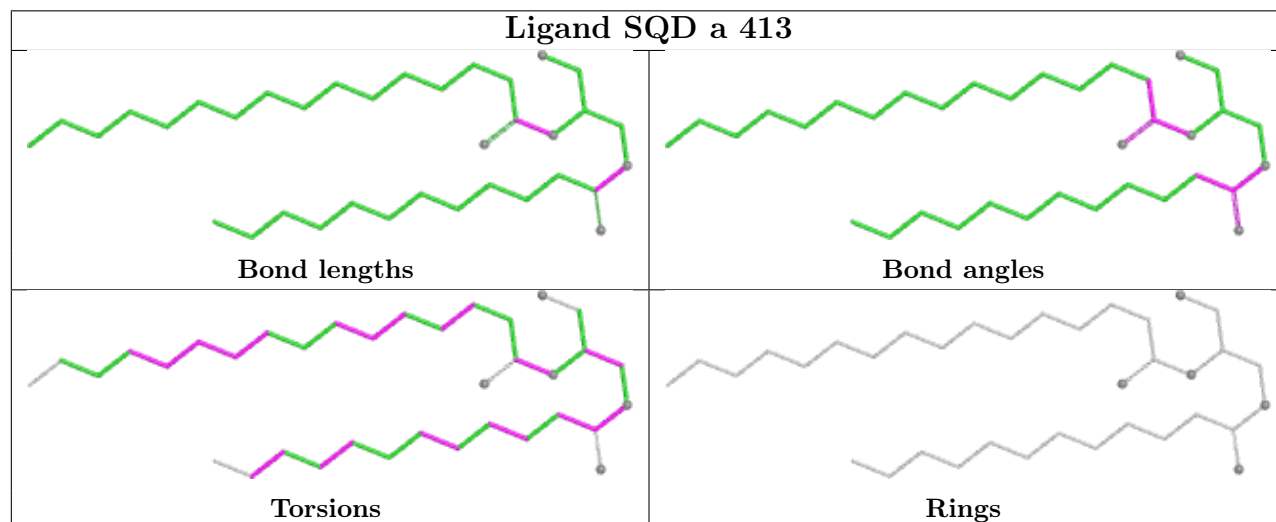
Ligand CLA C 504

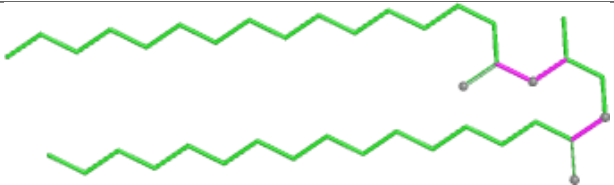
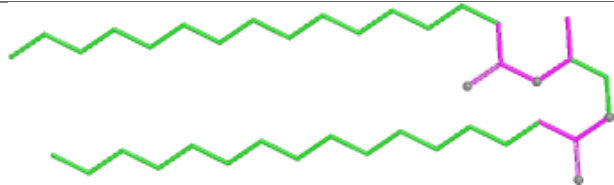
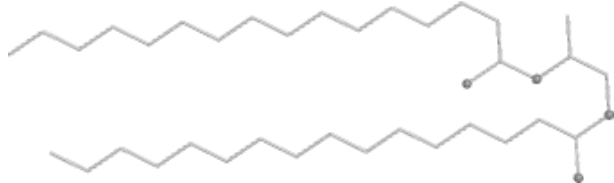


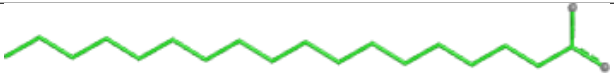
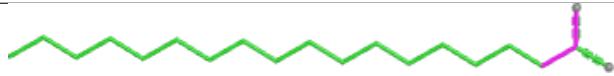
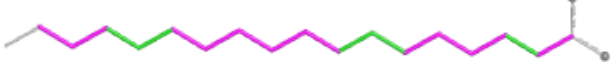
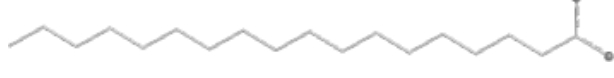
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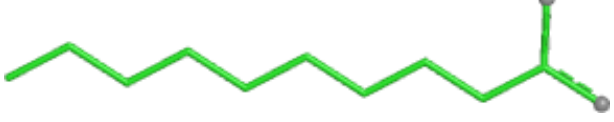
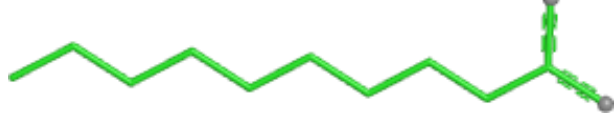
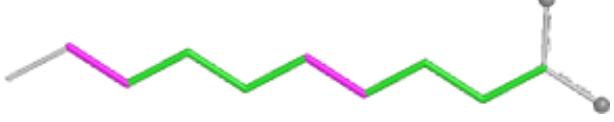
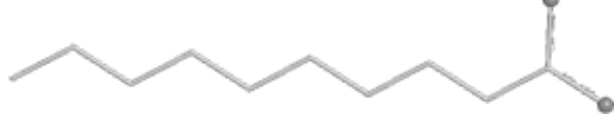


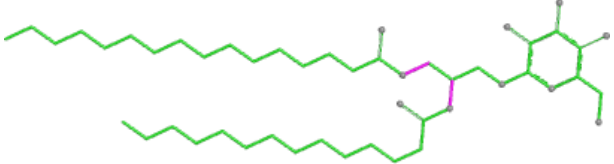
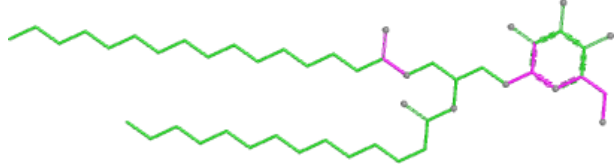
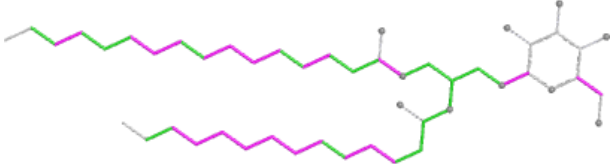
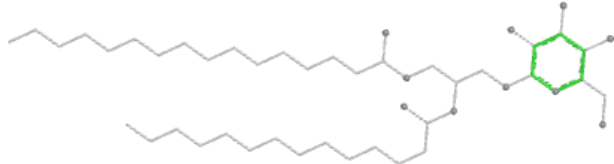
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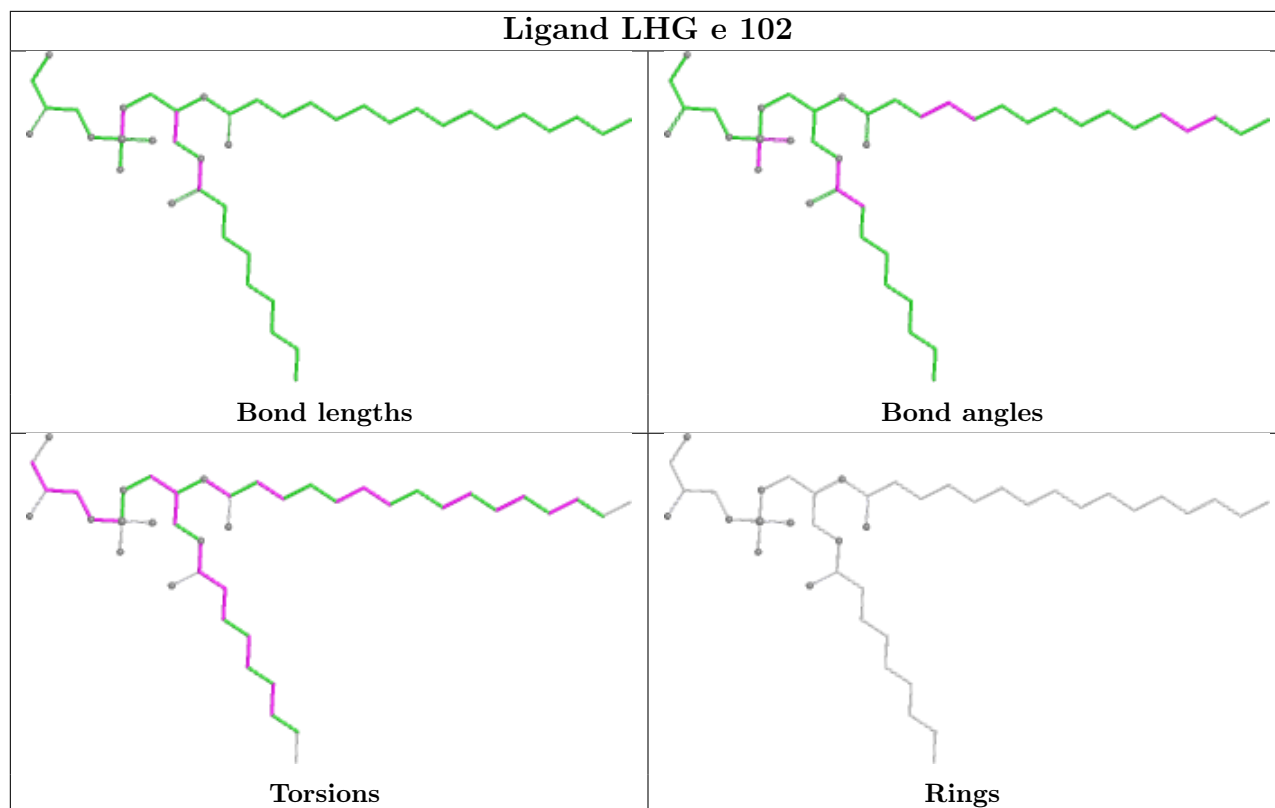
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

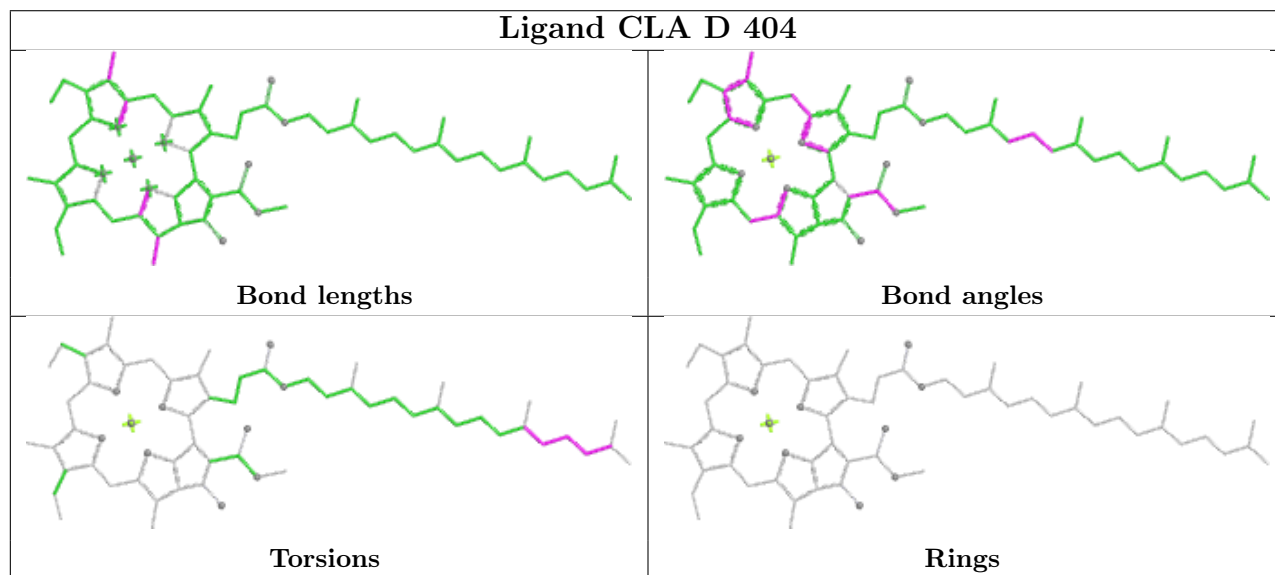
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

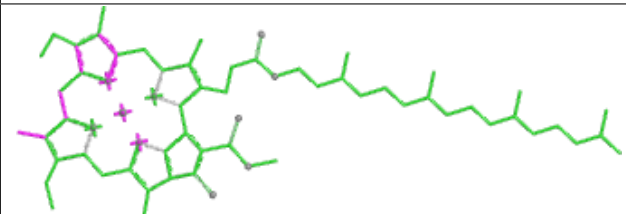
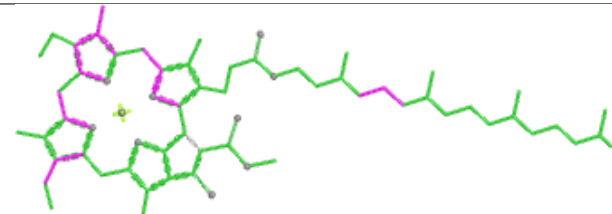
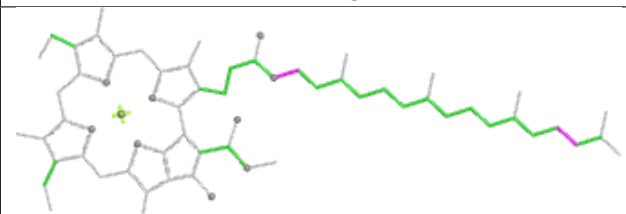
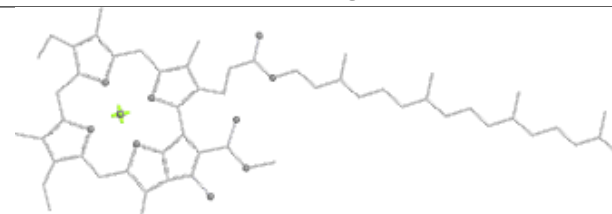
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Bond lengths	Bond angles
	
Torsions	Rings

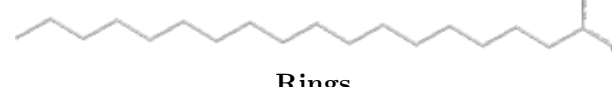
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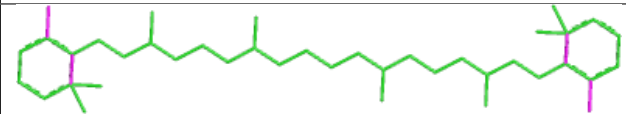
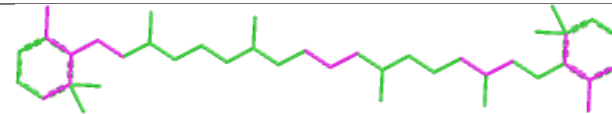
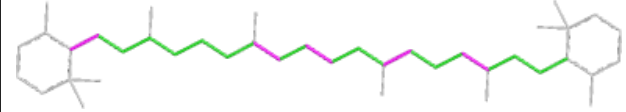
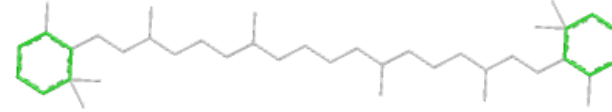


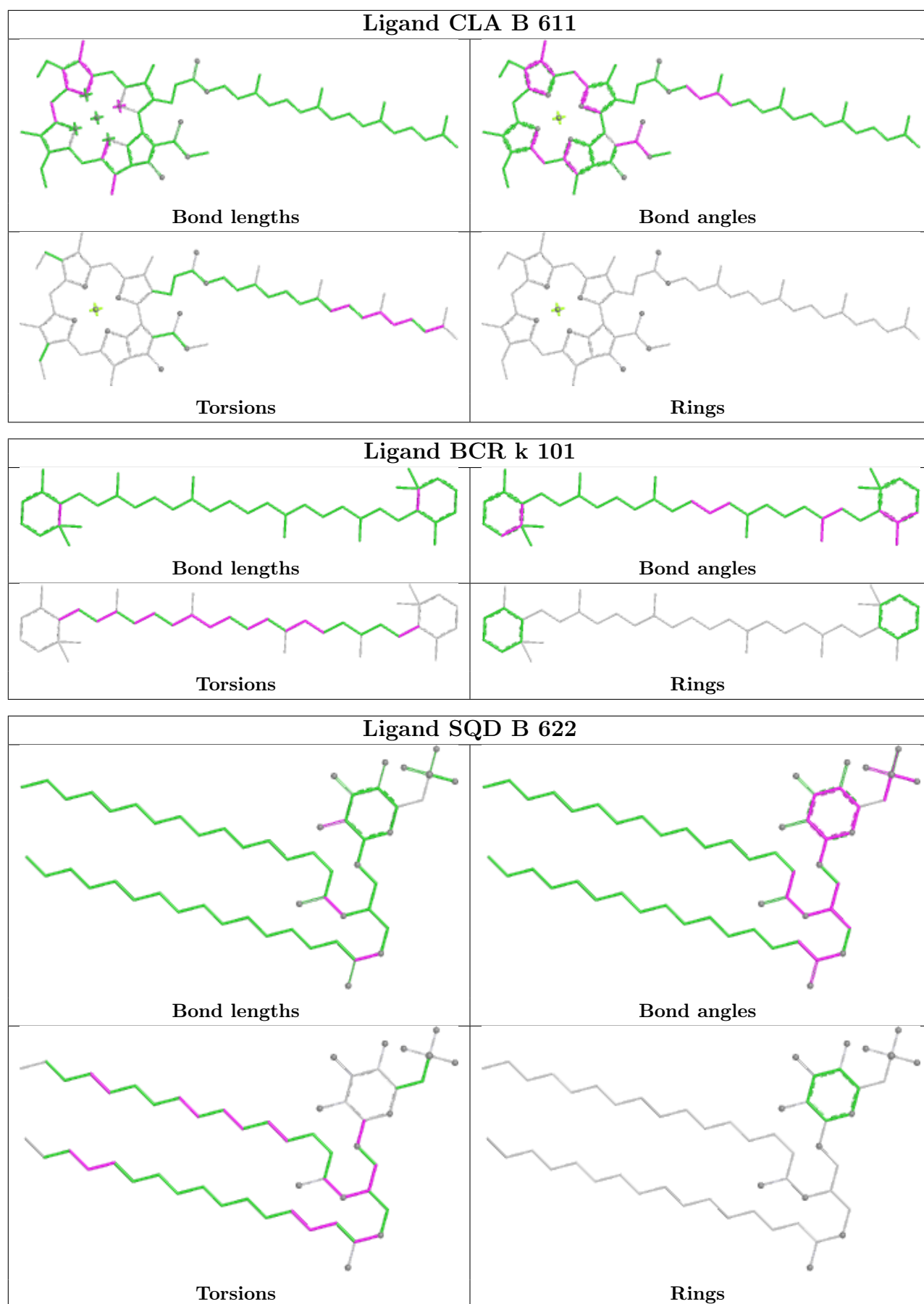
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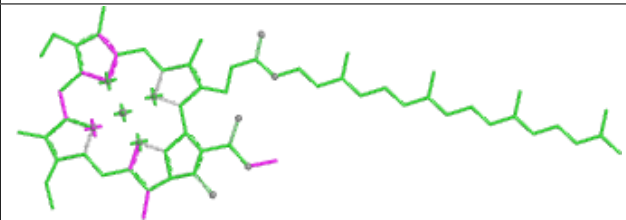
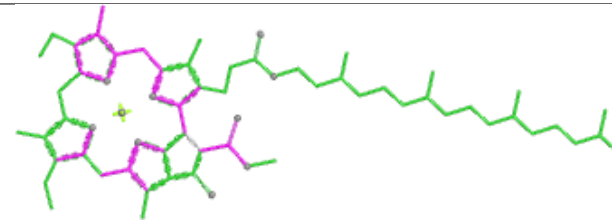
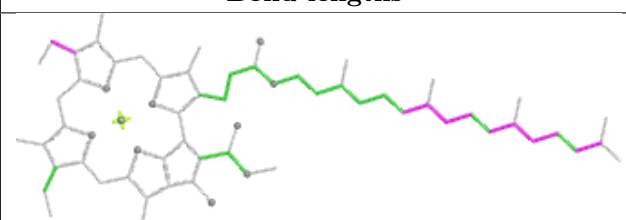
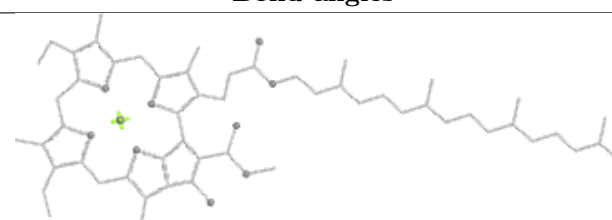


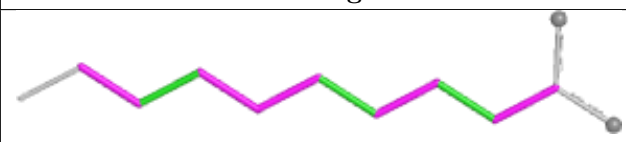
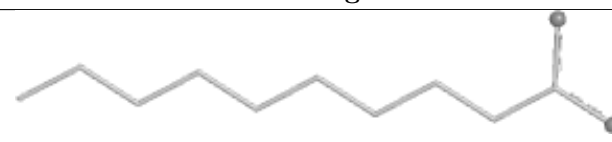
Ligand CLA A 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

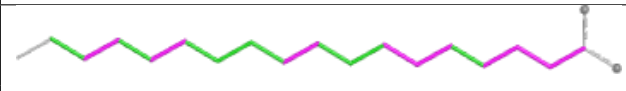
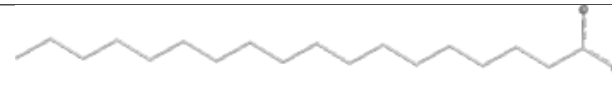
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Bond lengths	Bond angles
	
Torsions	Rings

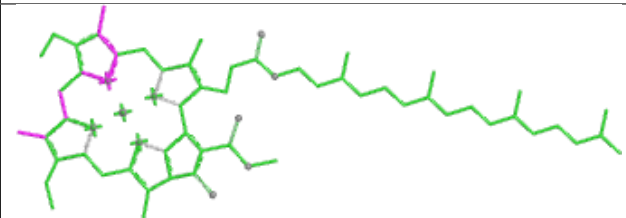
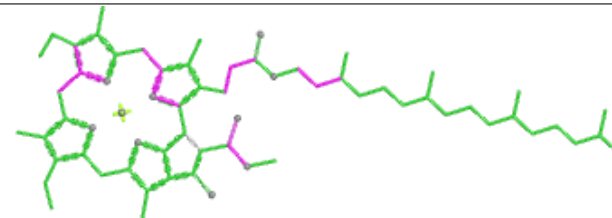
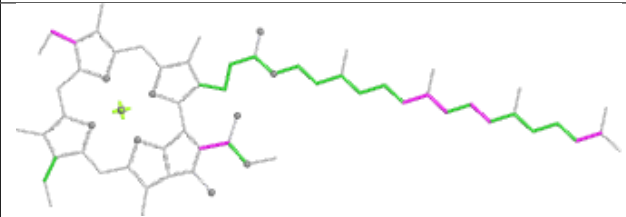
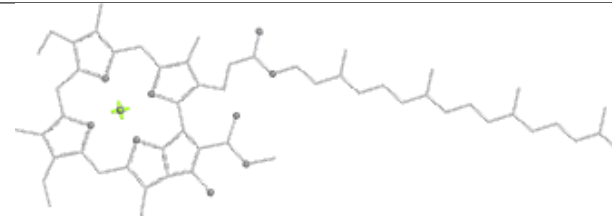
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Bond lengths	Bond angles
	
Torsions	Rings

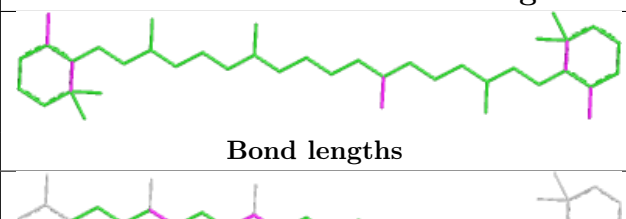
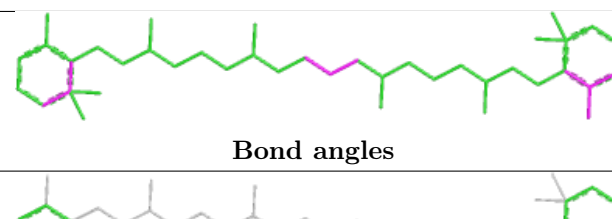
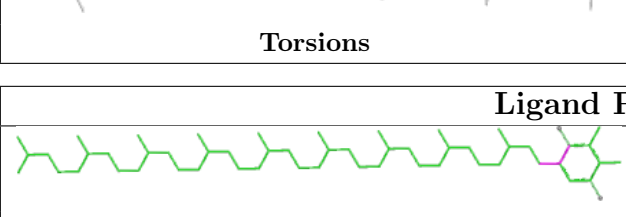
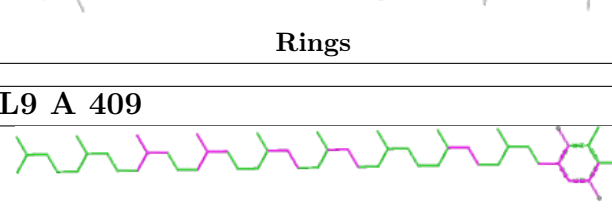


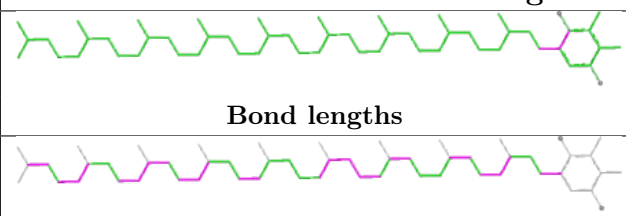
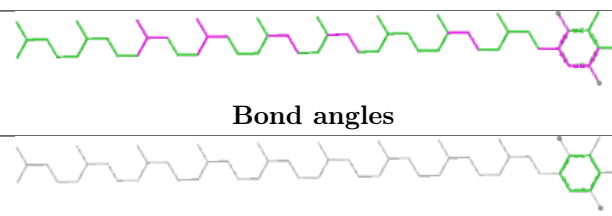
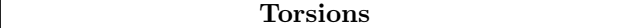
Ligand CLA a 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

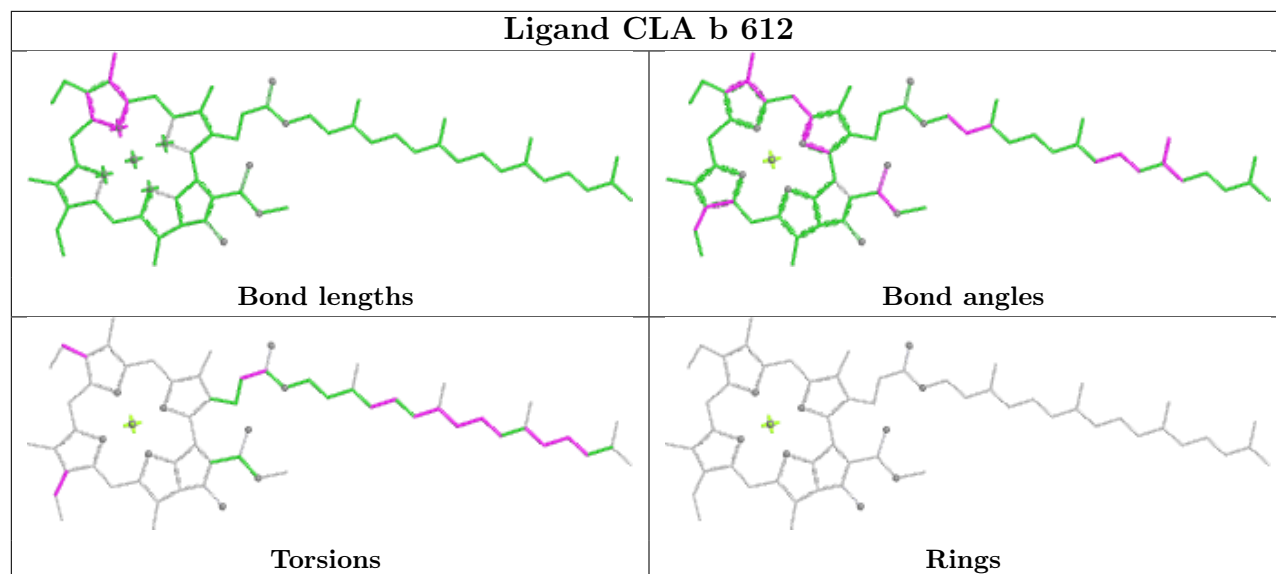
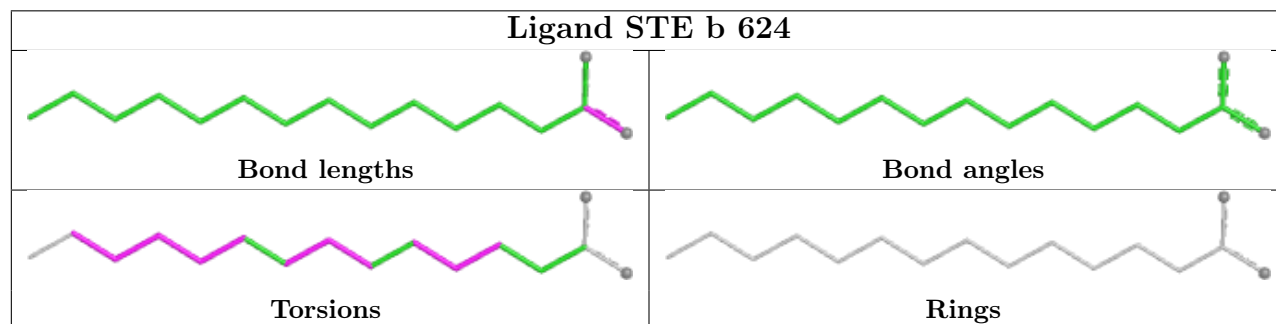
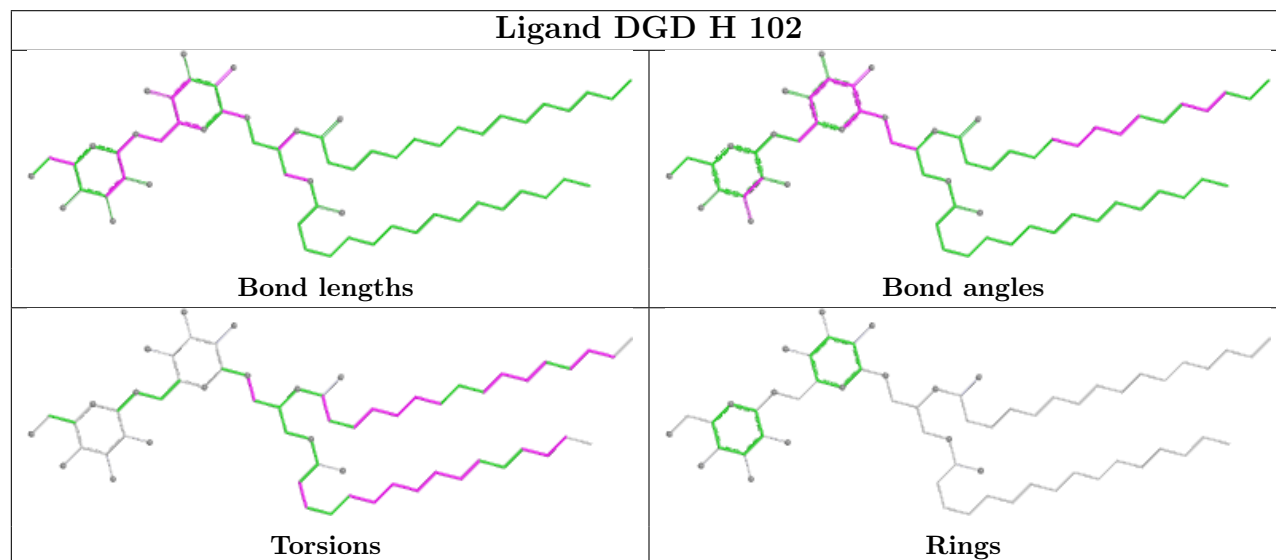
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Bond lengths	Bond angles
	
Torsions	Rings

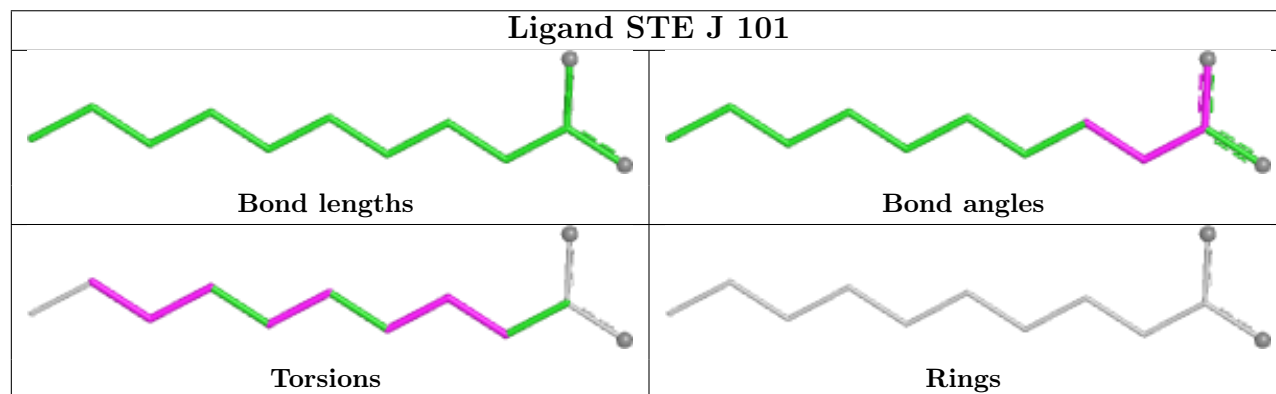
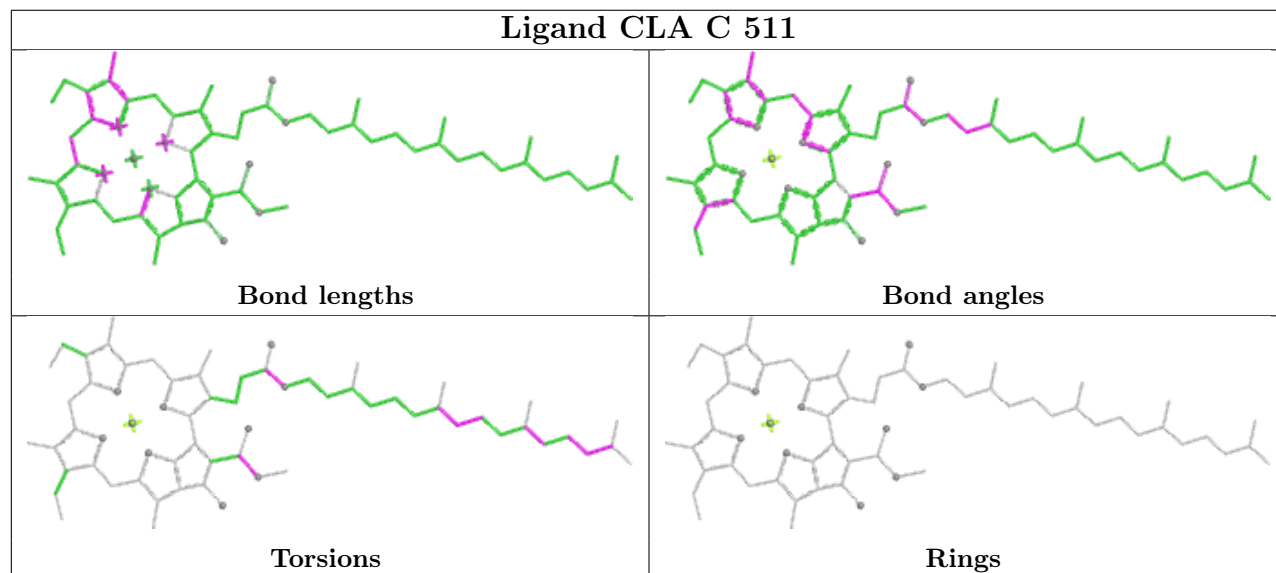
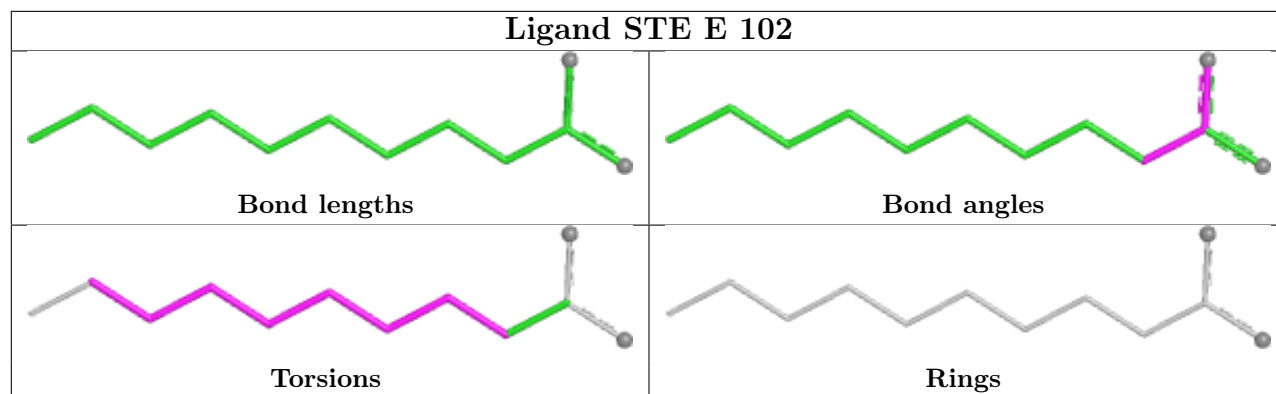
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Bond lengths	Bond angles
	
Torsions	Rings

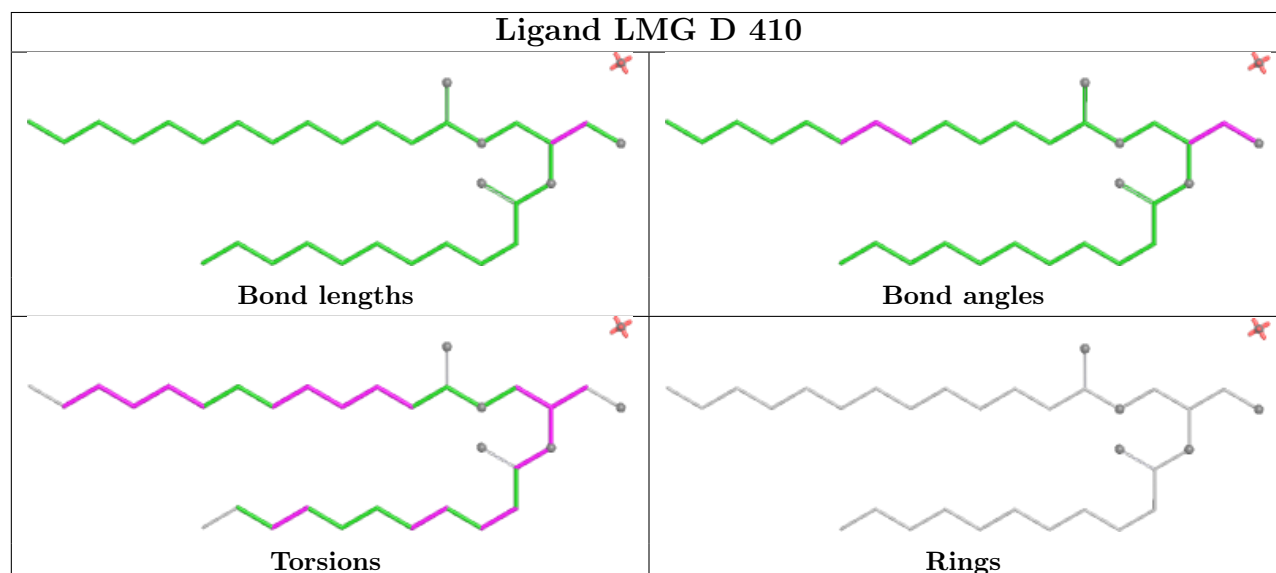
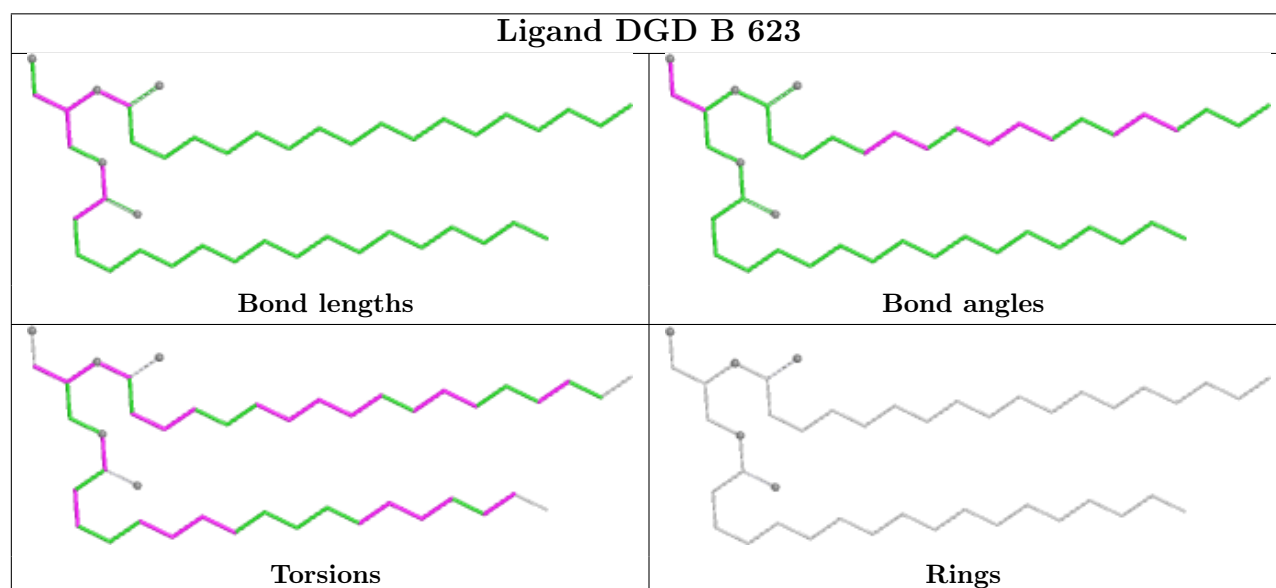
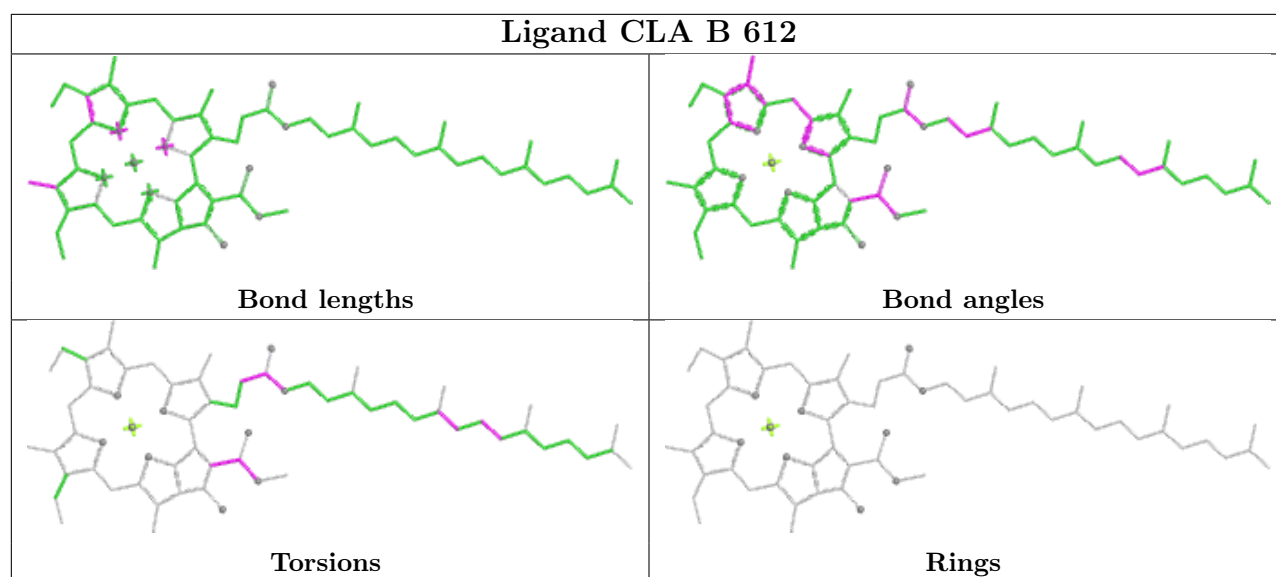
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Bond lengths	Bond angles
	
Torsions	Rings

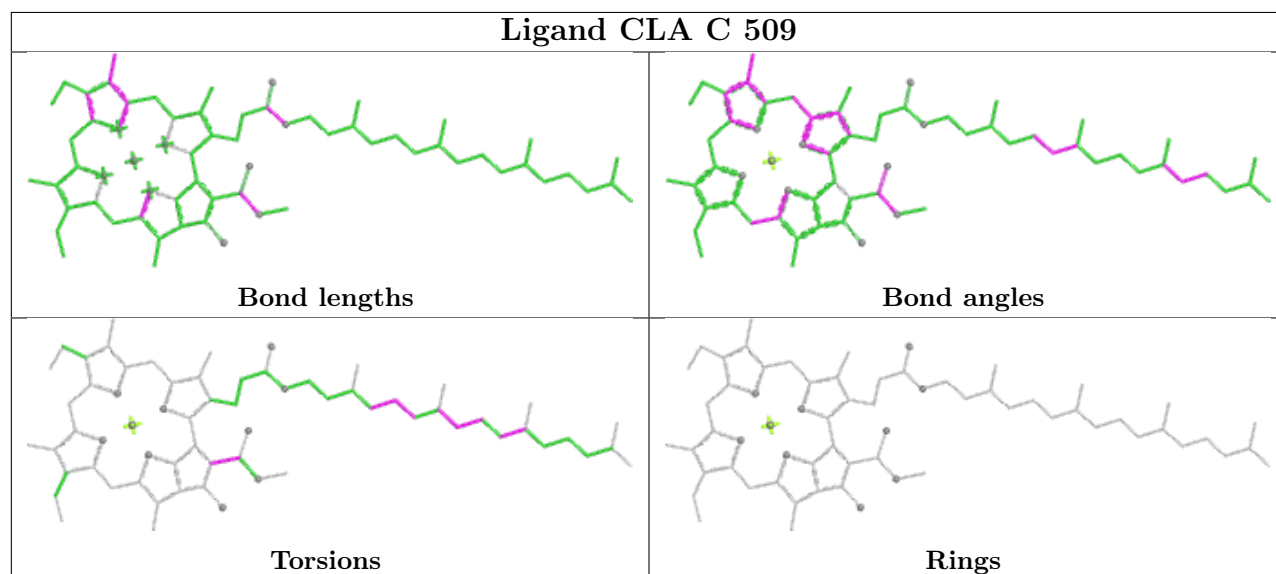
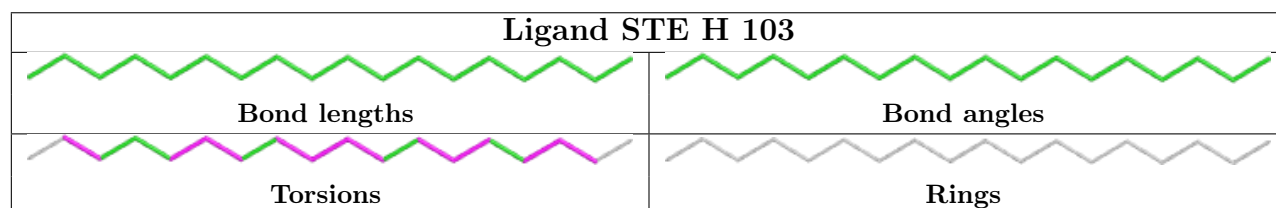
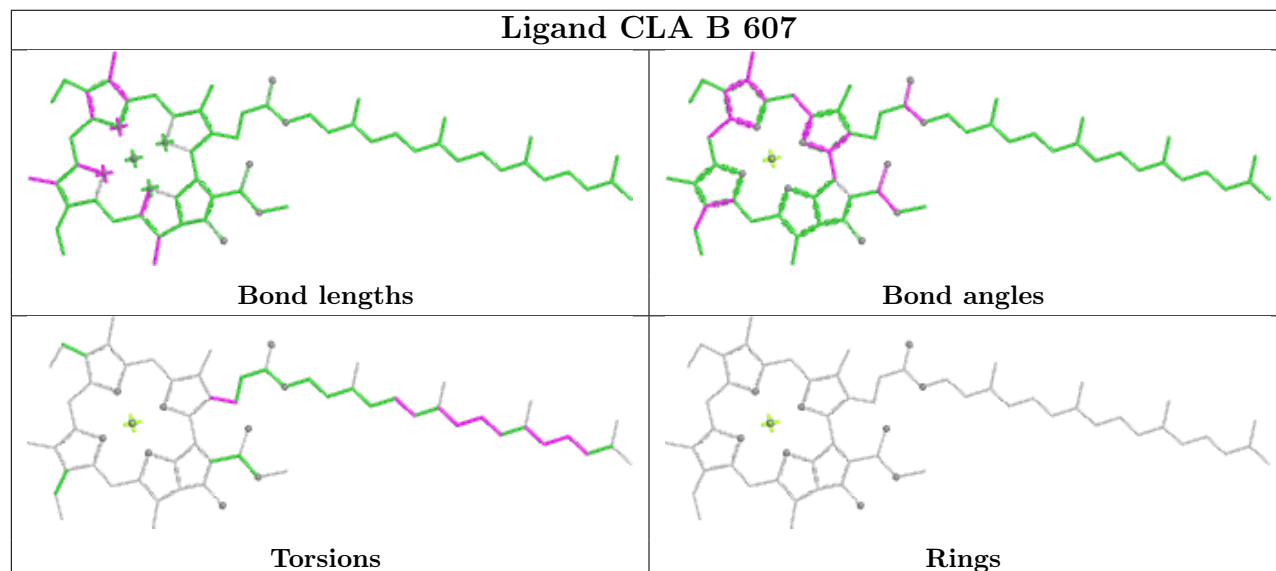
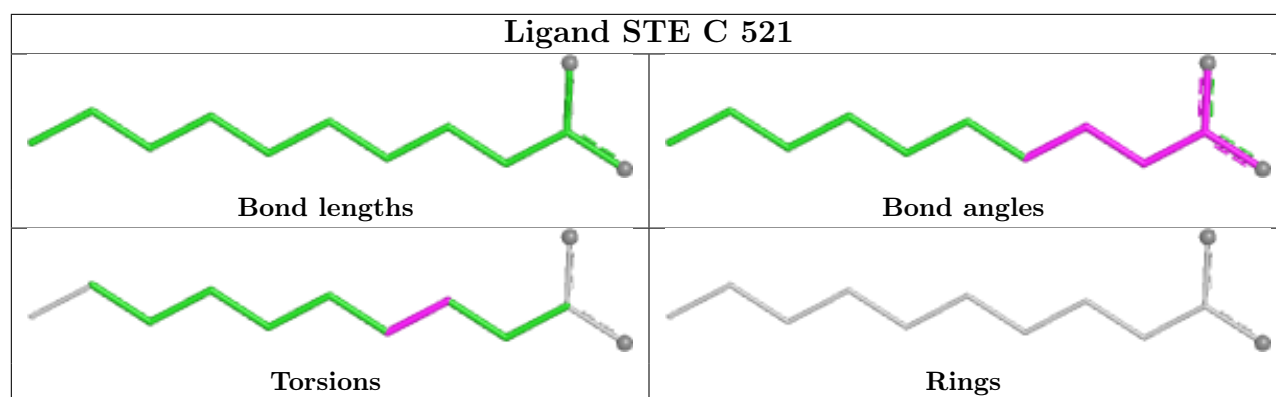
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

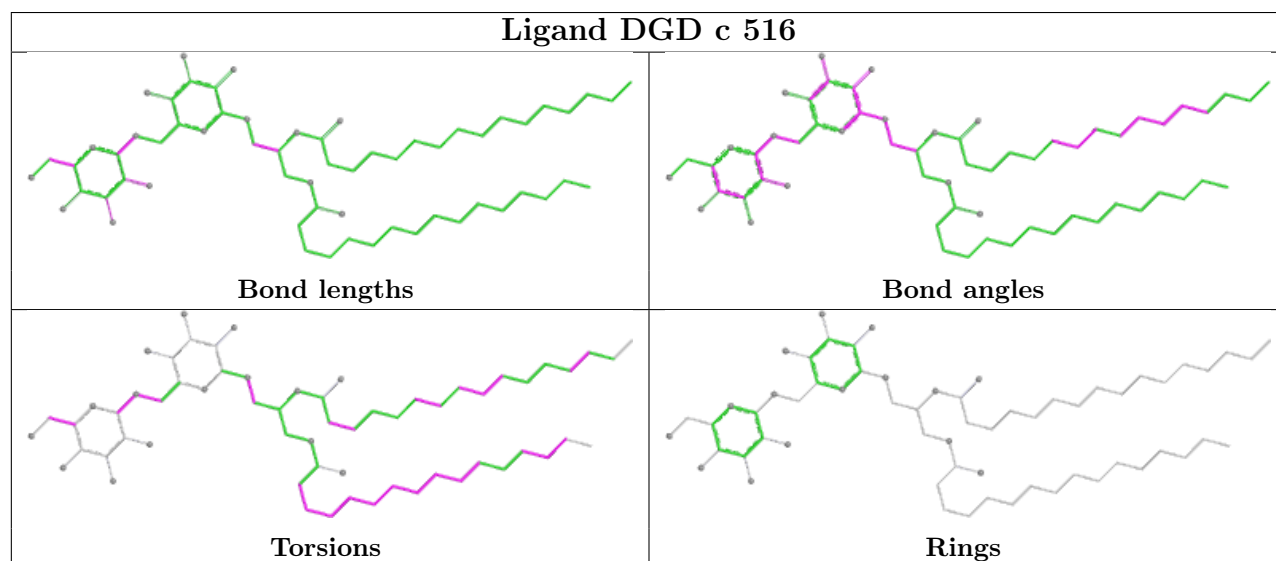
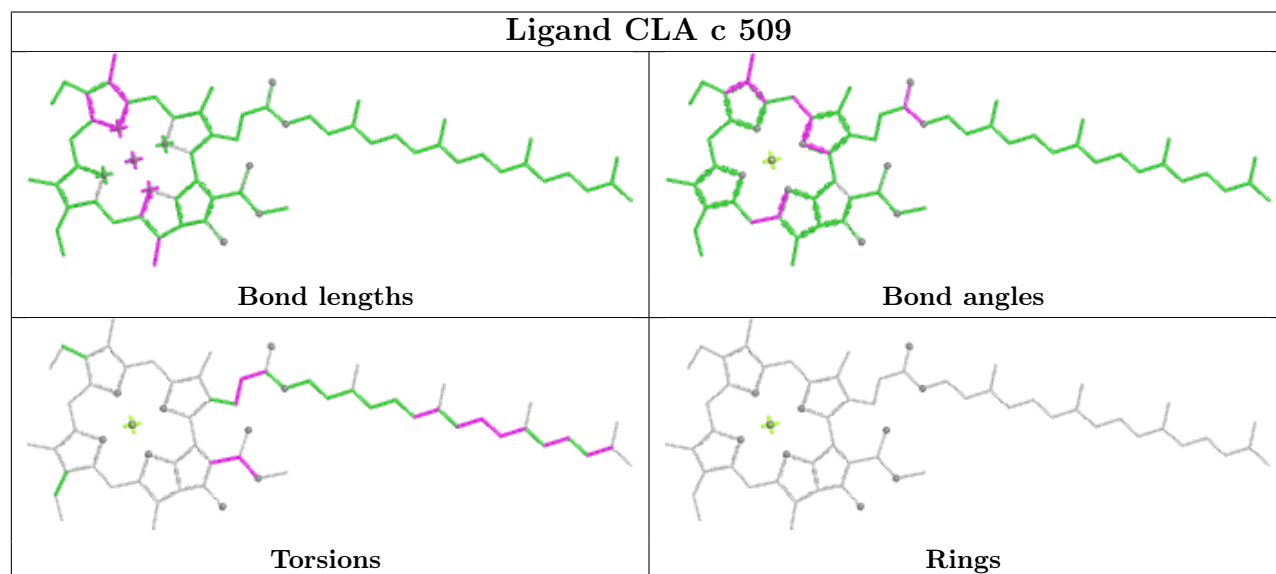
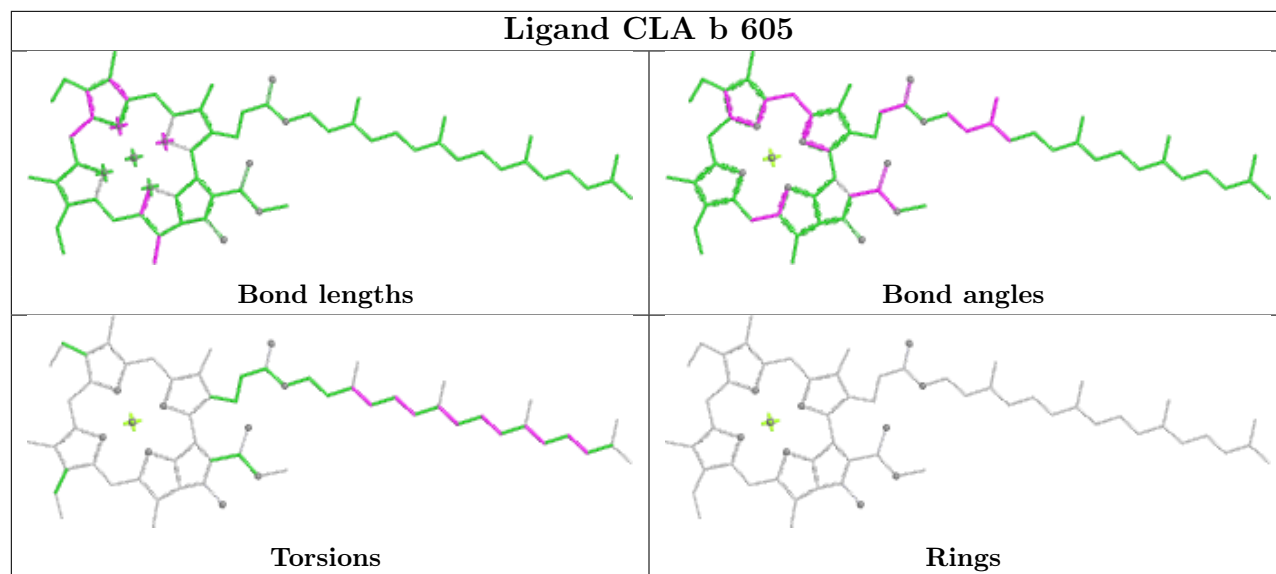
Ligand PL9 A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

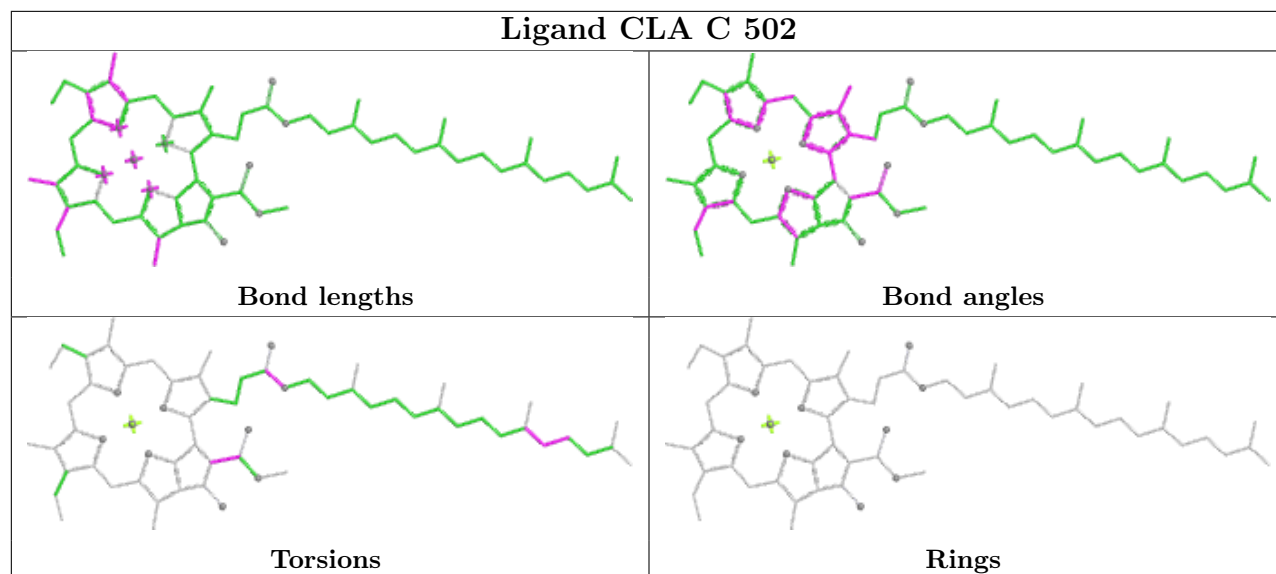
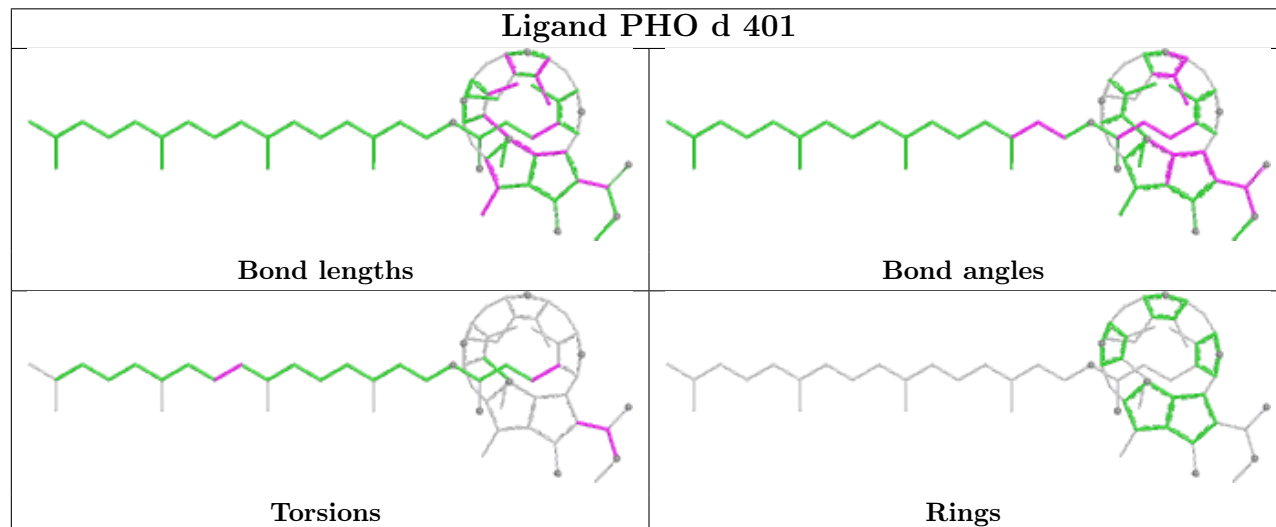
Ligand CLA b 612**Ligand STE b 624****Ligand DGD H 102**

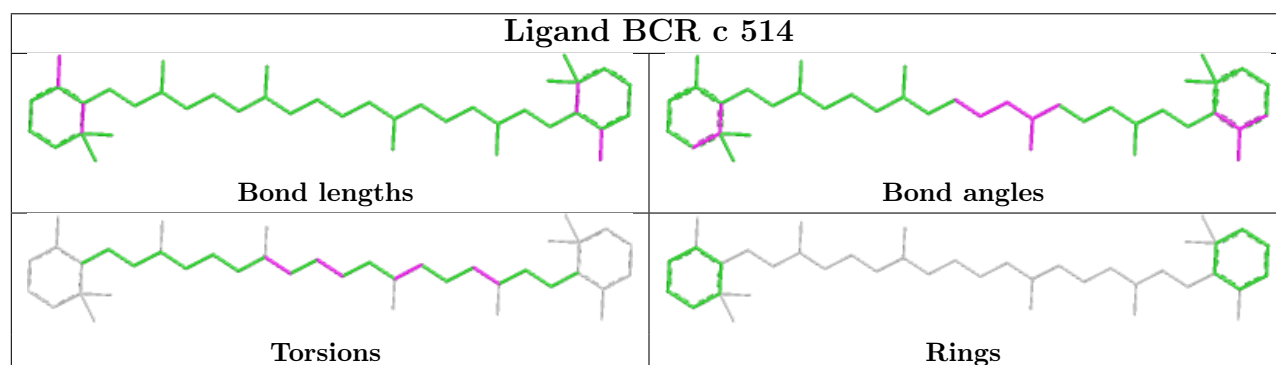
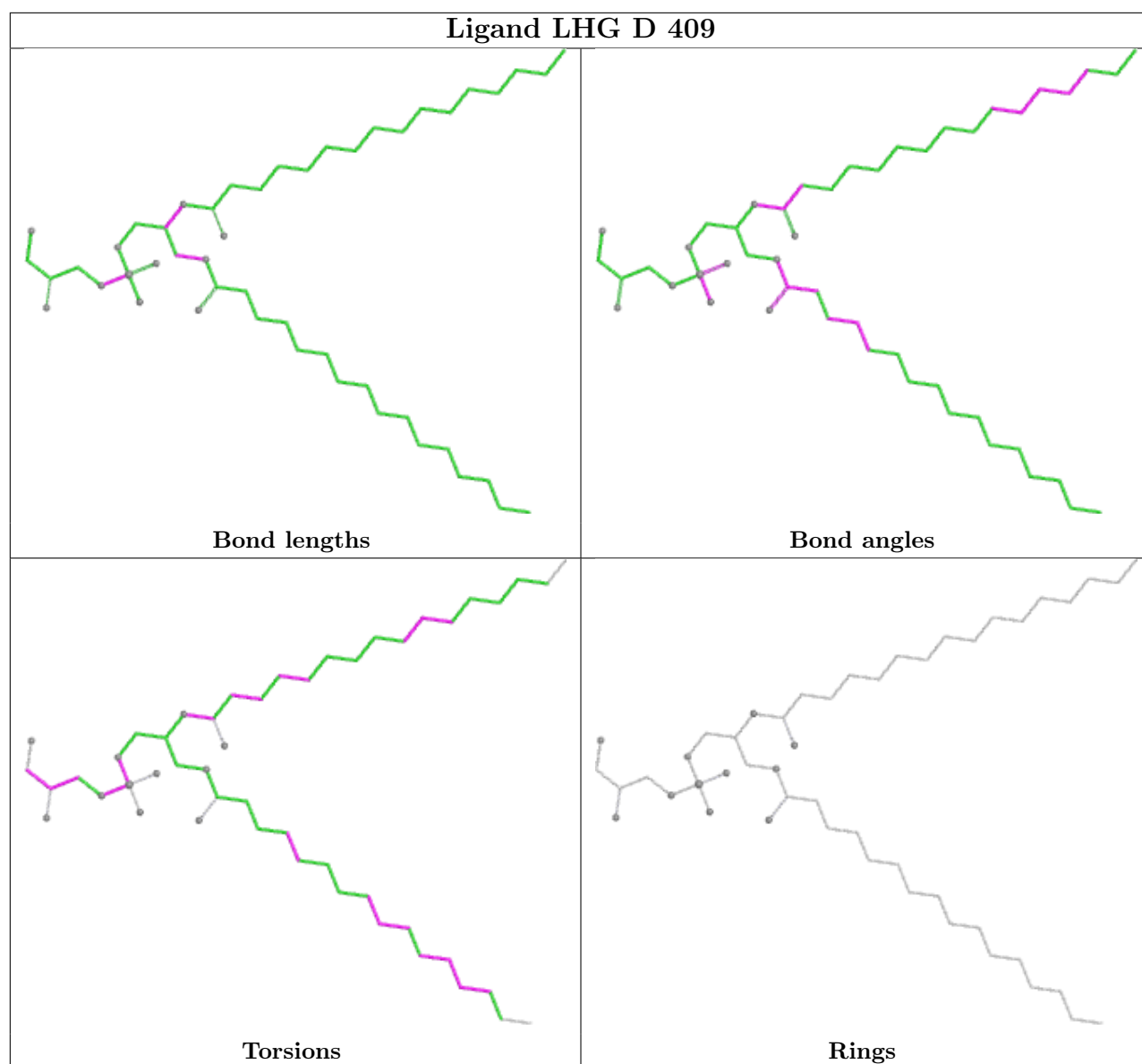


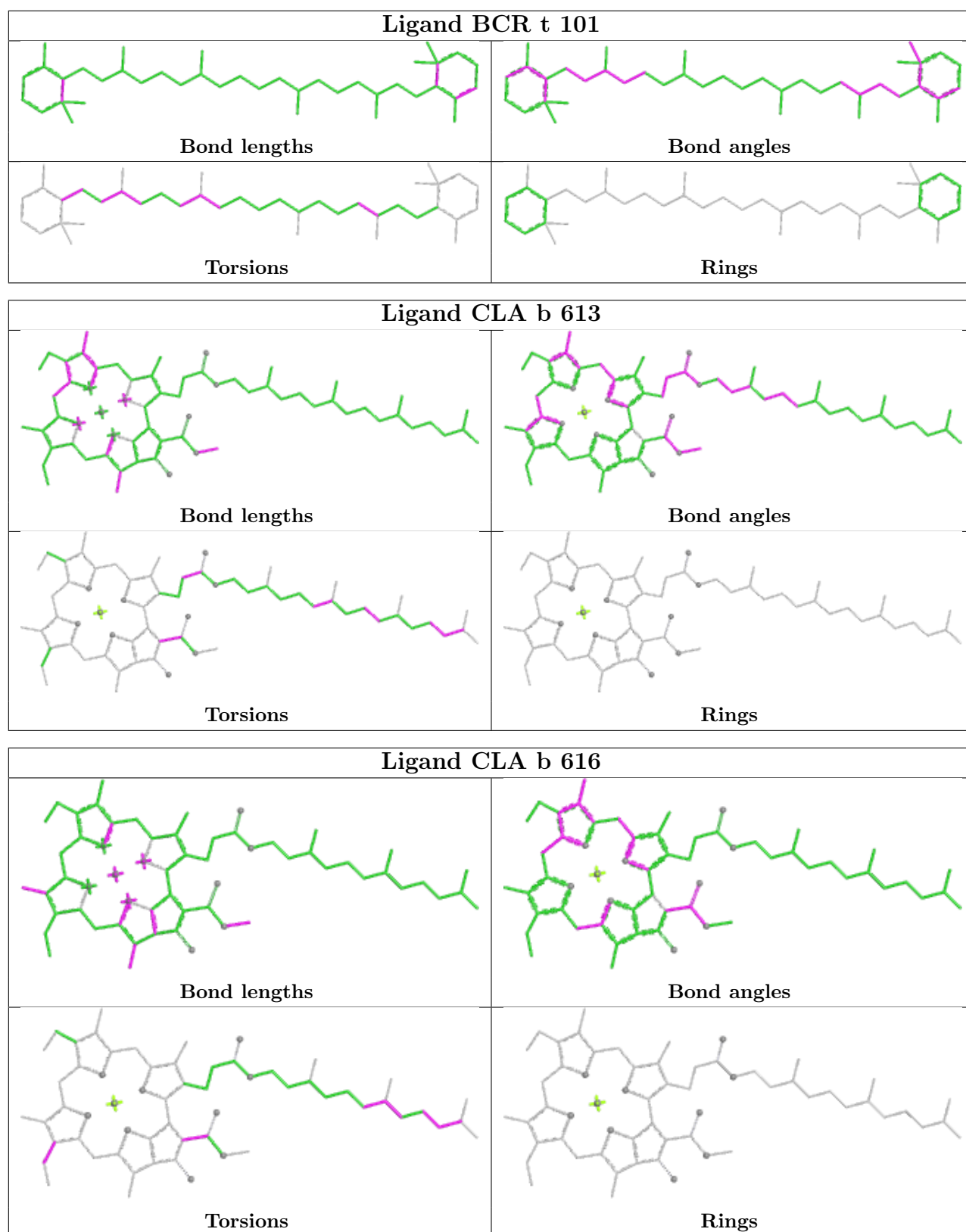


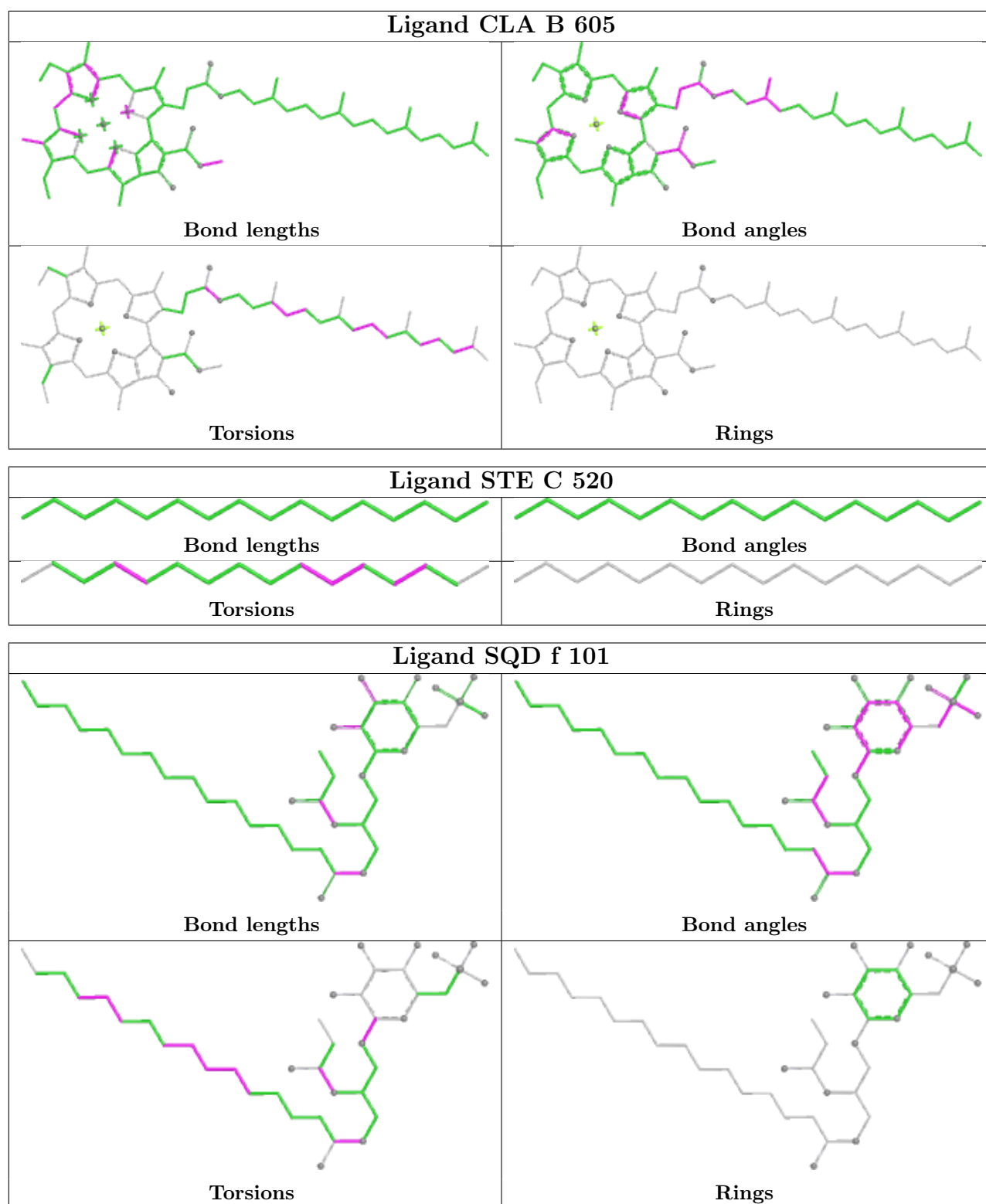


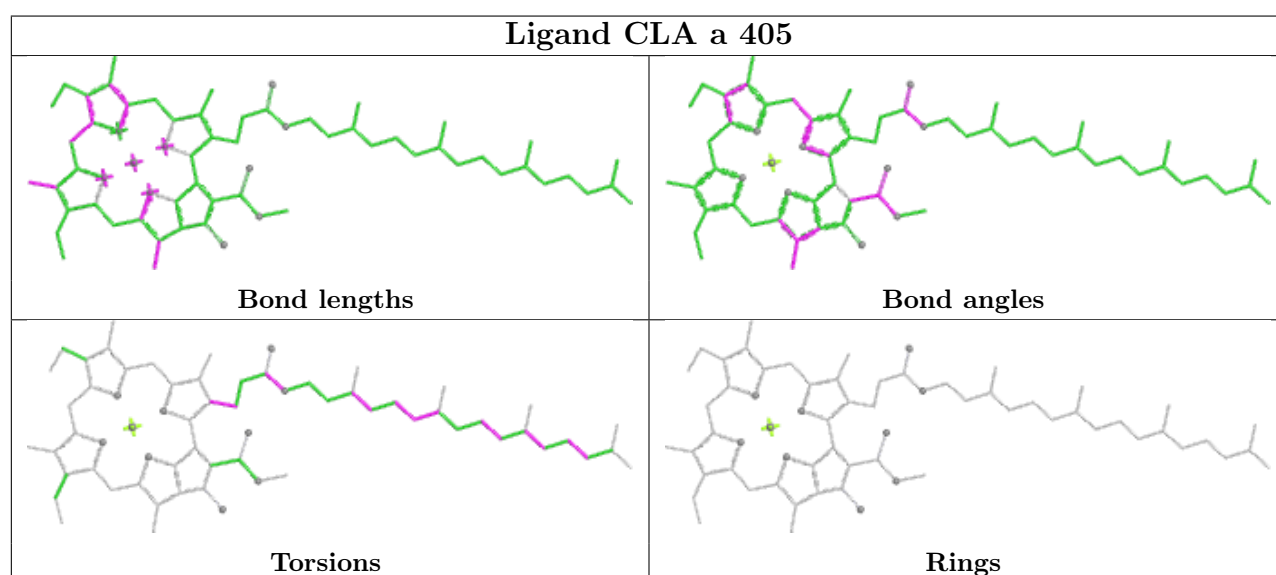
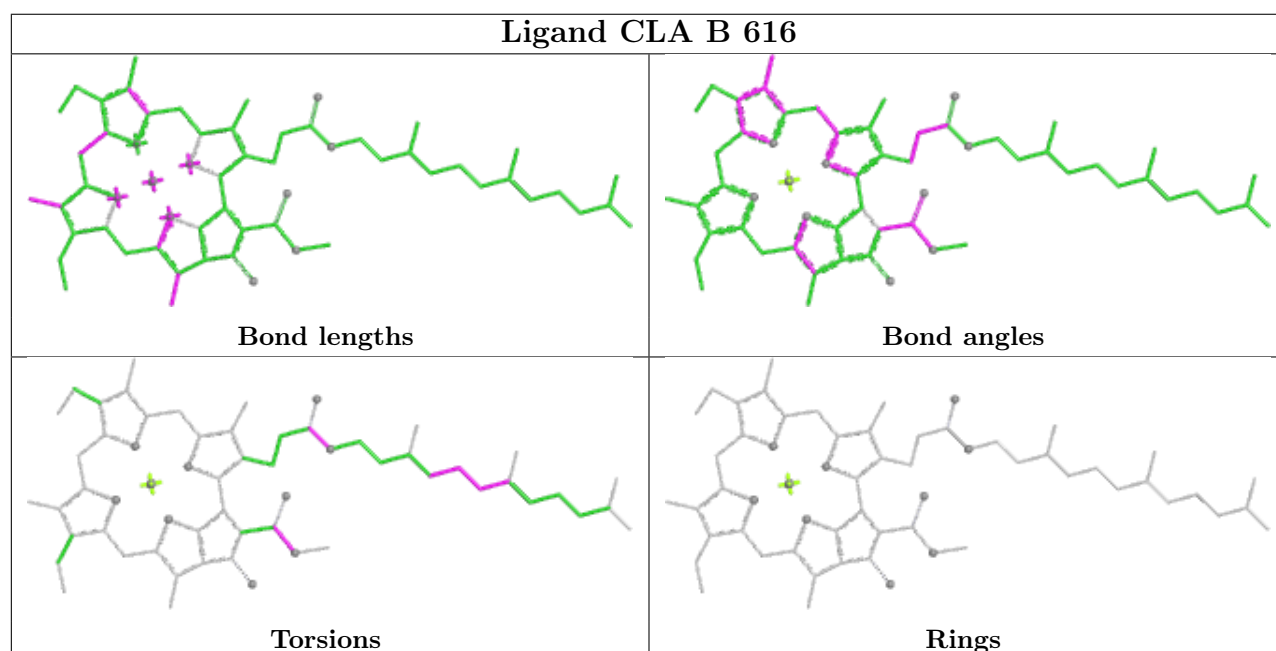
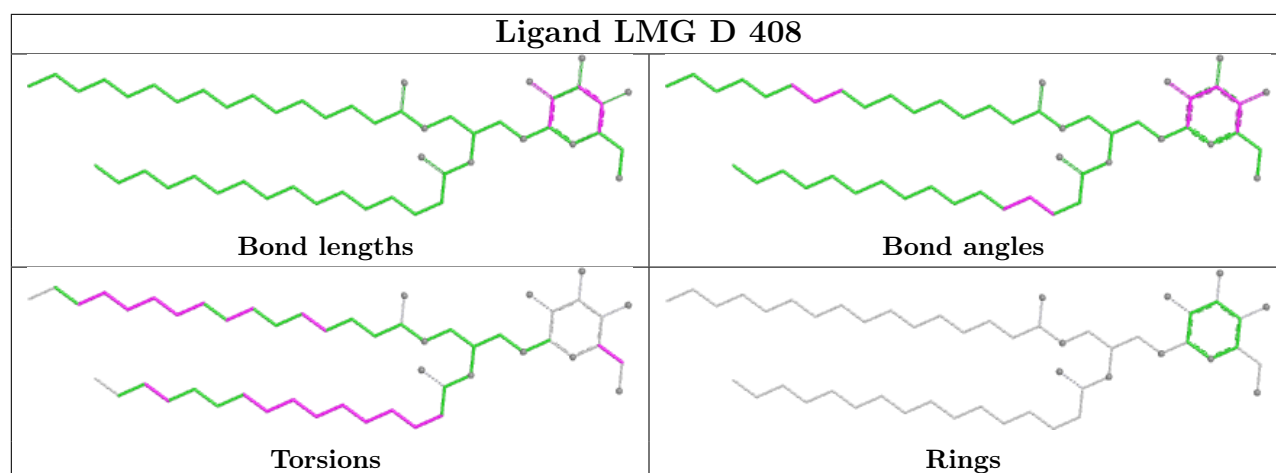


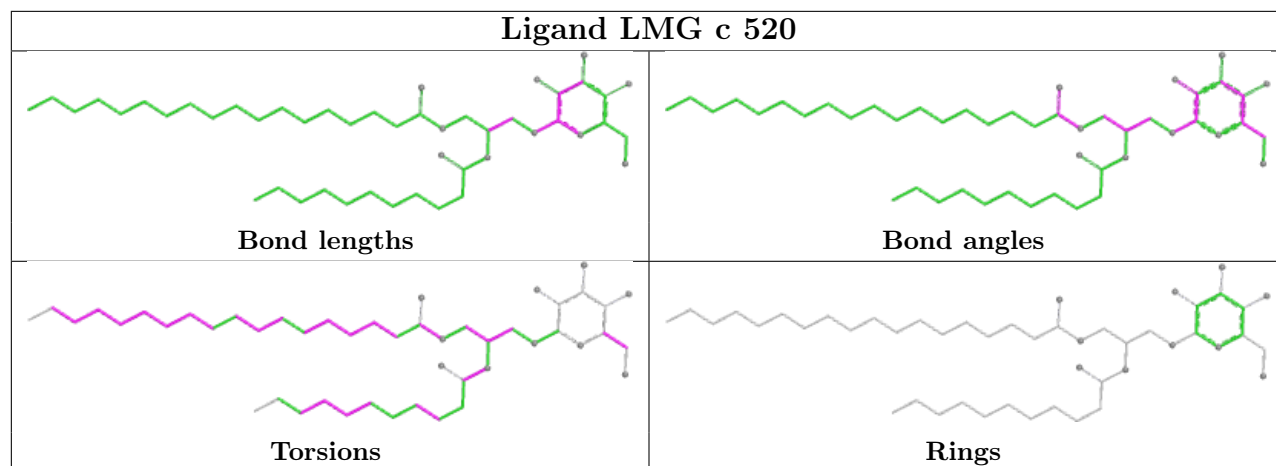
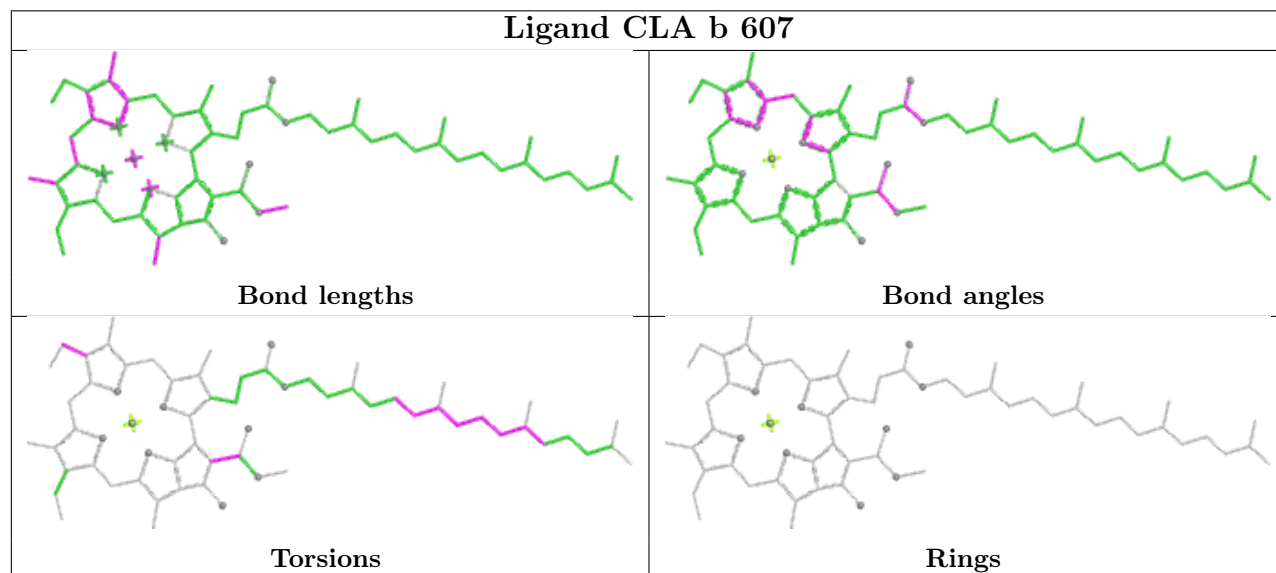
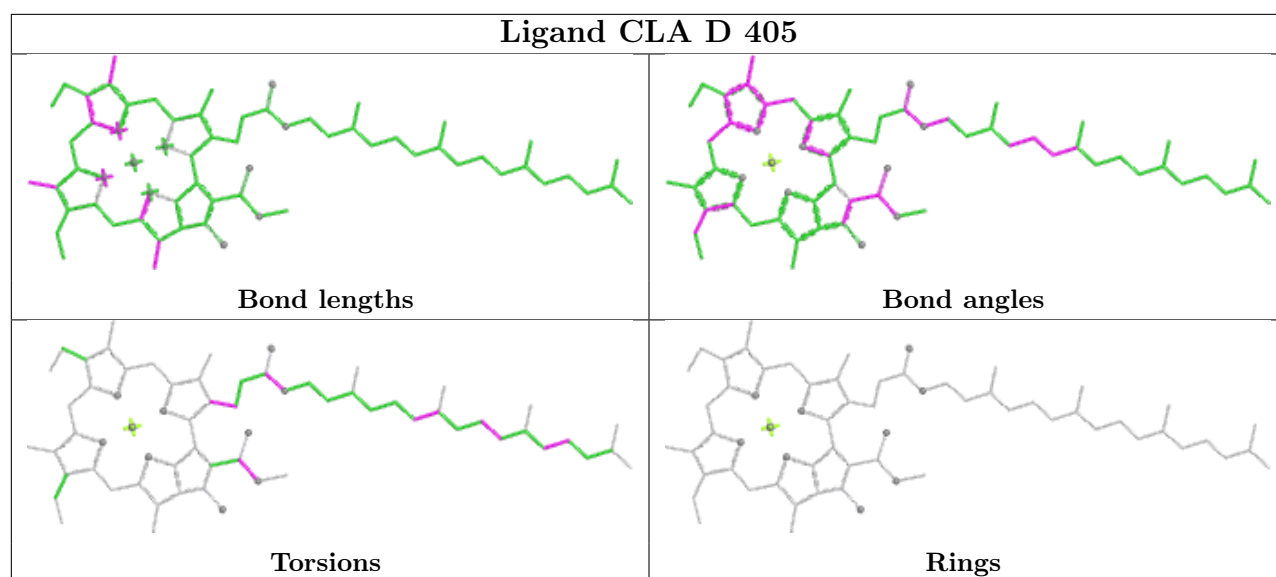
Ligand CLA C 502**Ligand PHO d 401**

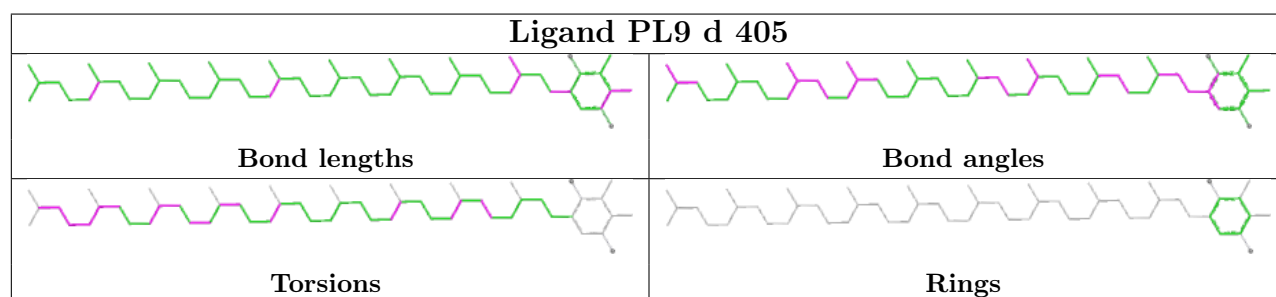
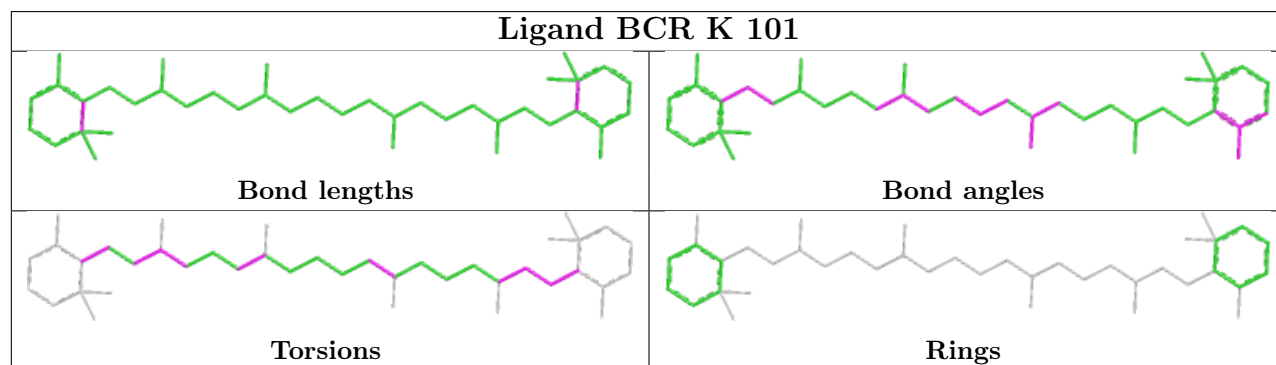
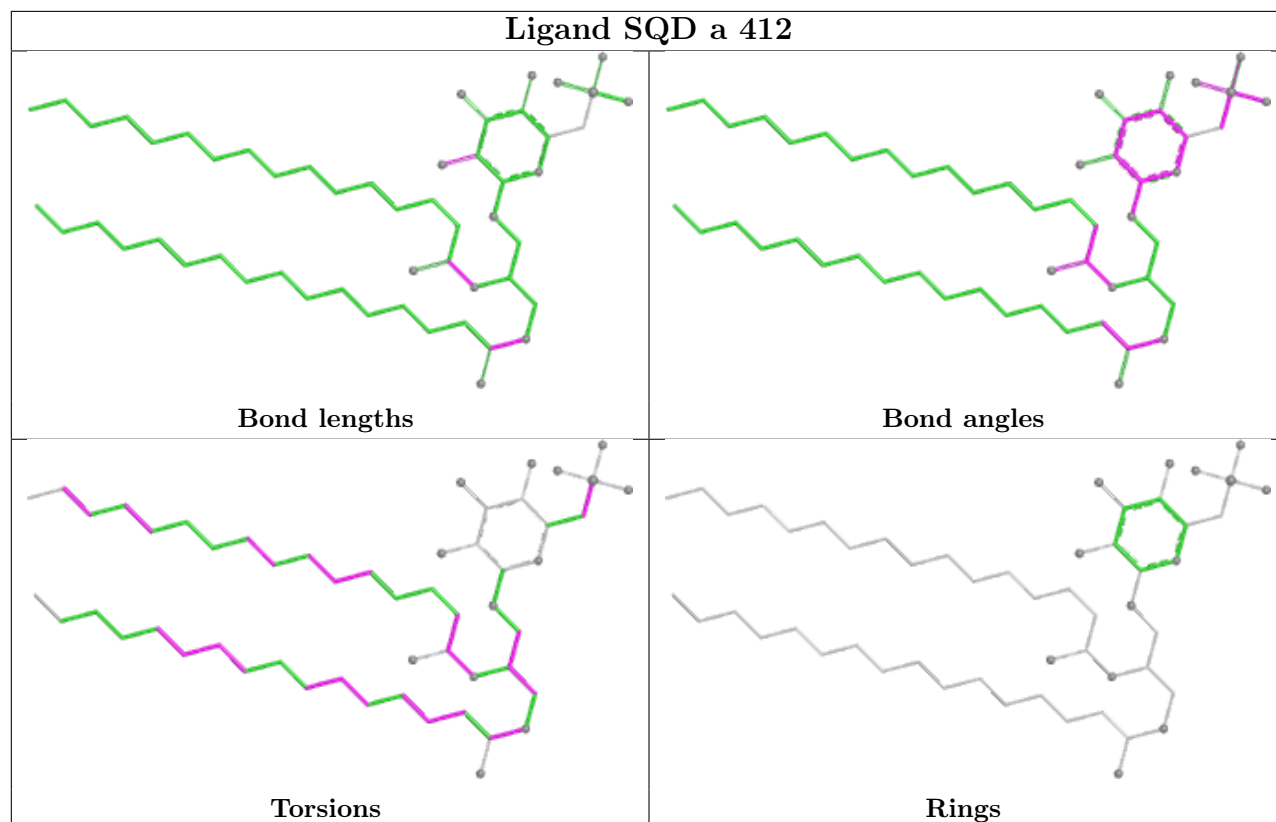


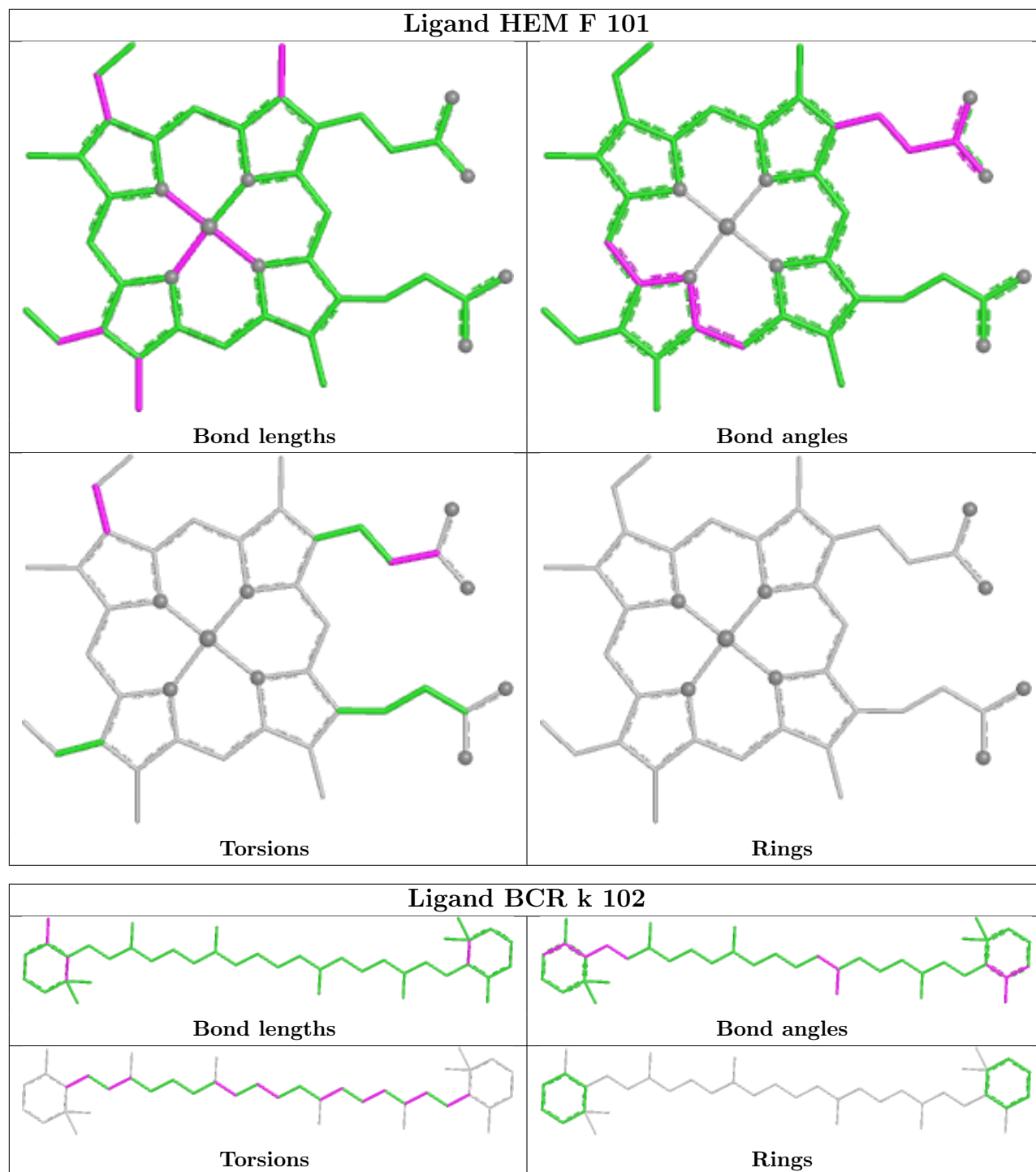




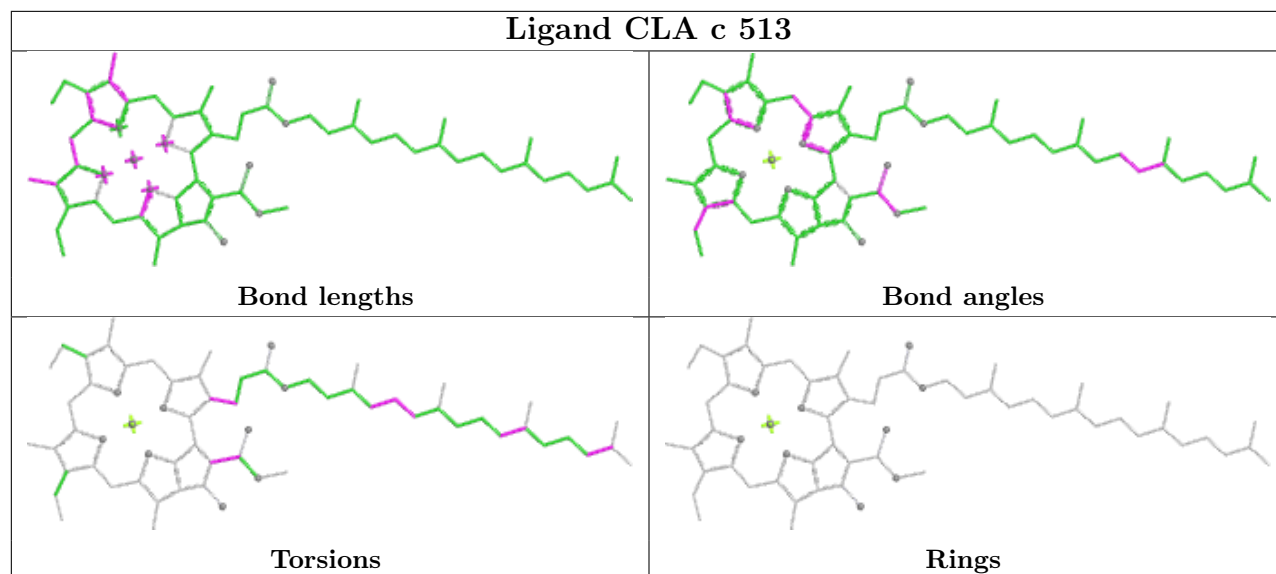




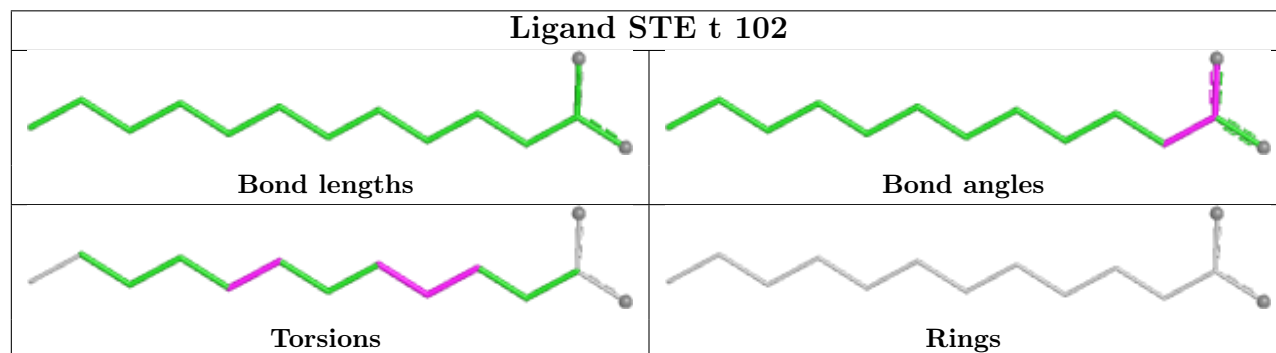




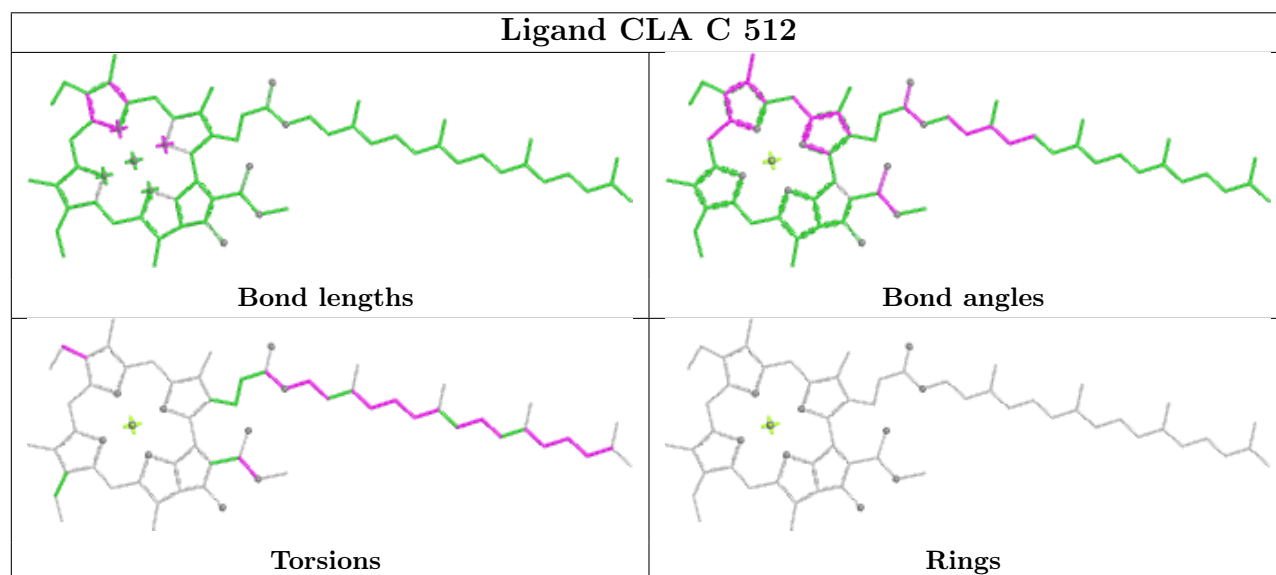
Ligand CLA c 513

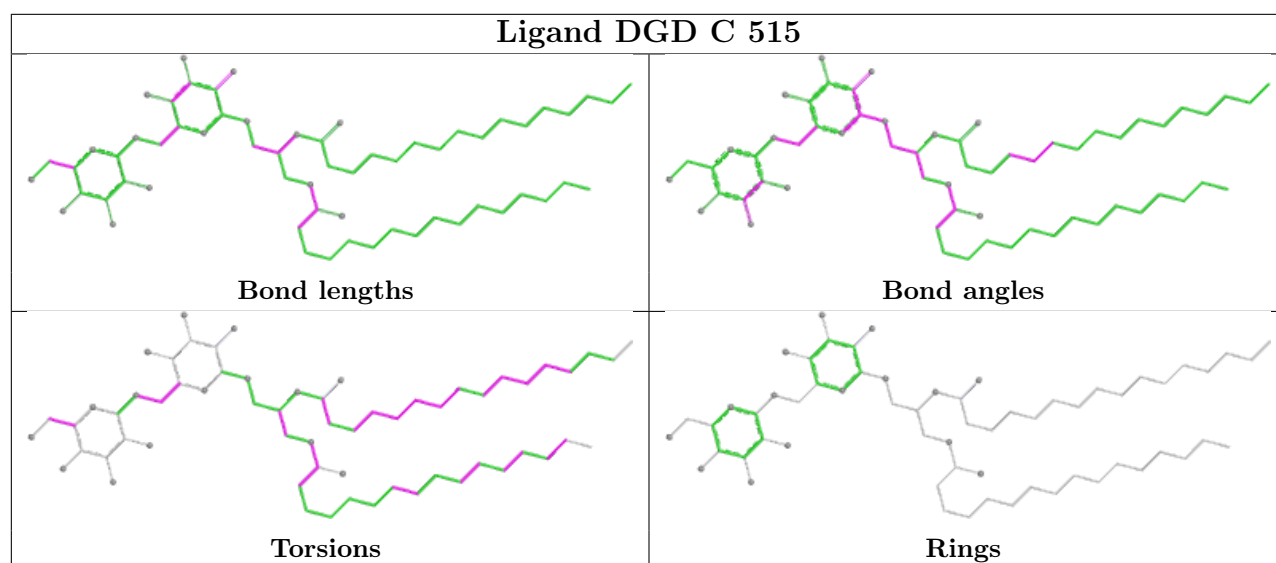
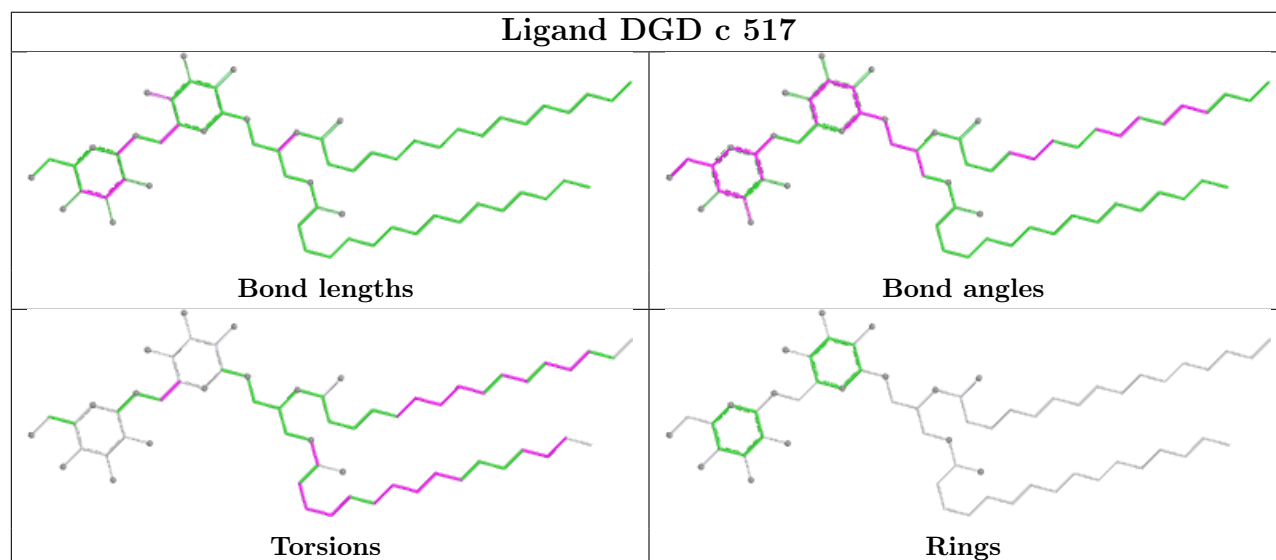
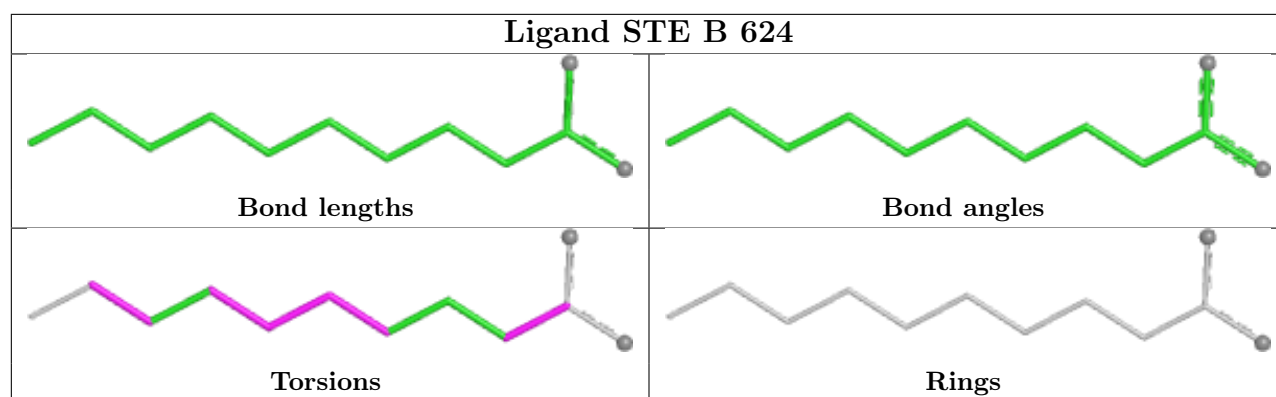


Ligand STE t 102

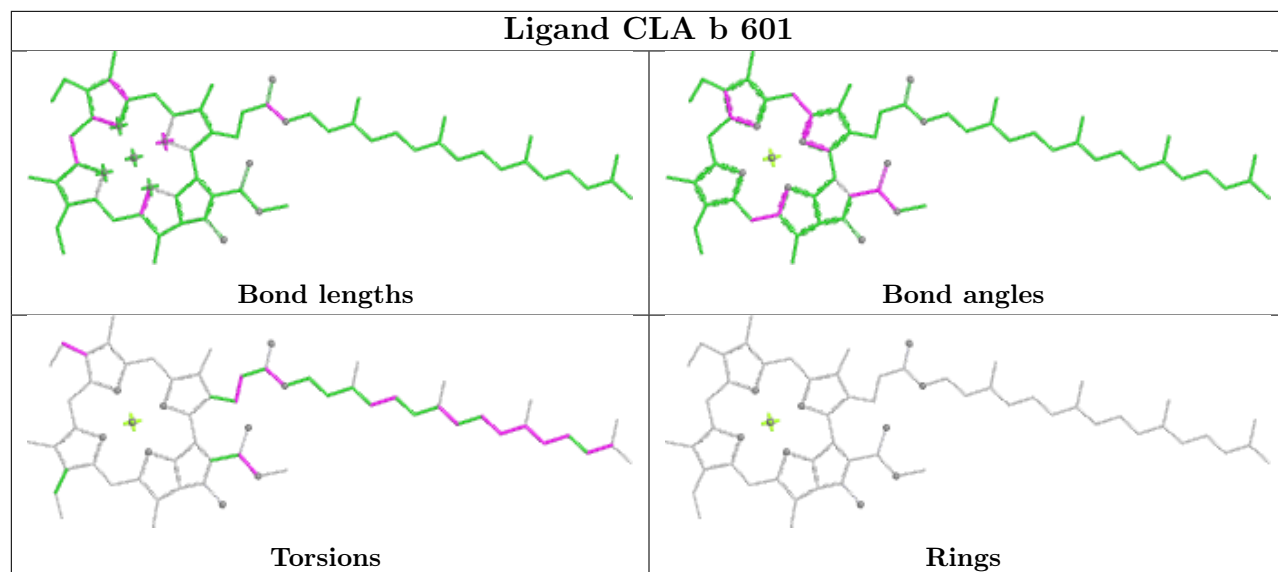


Ligand CLA C 512

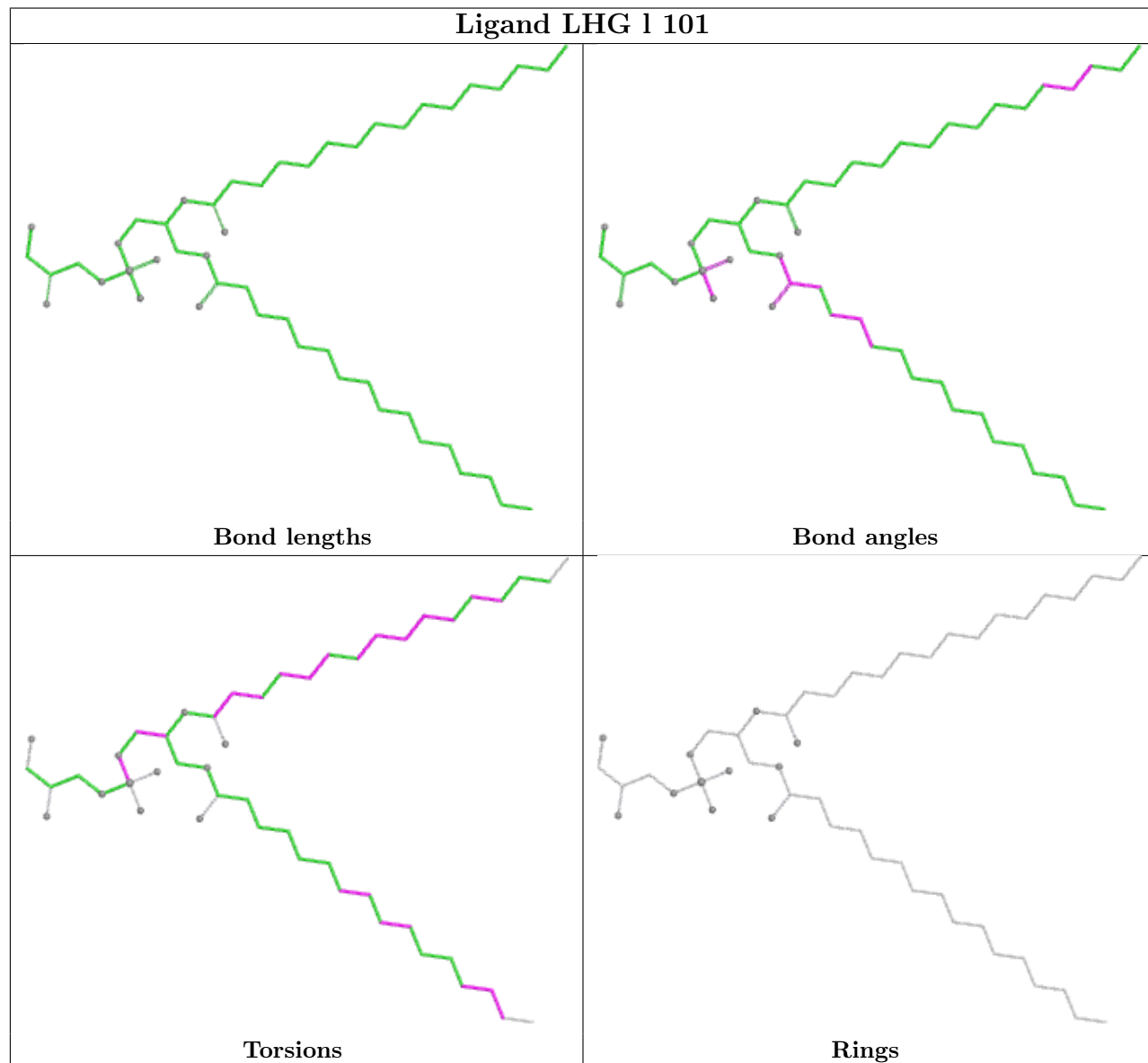


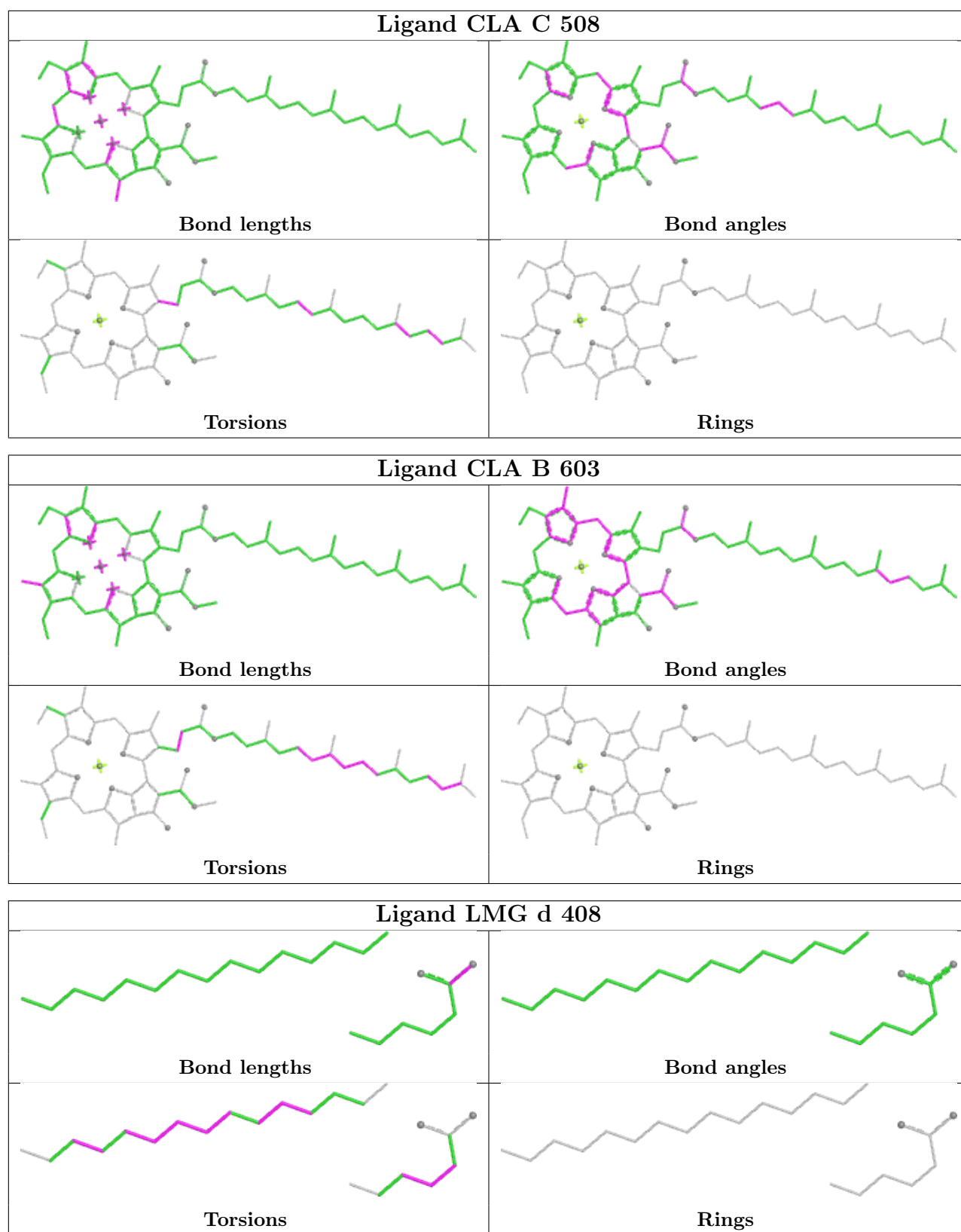


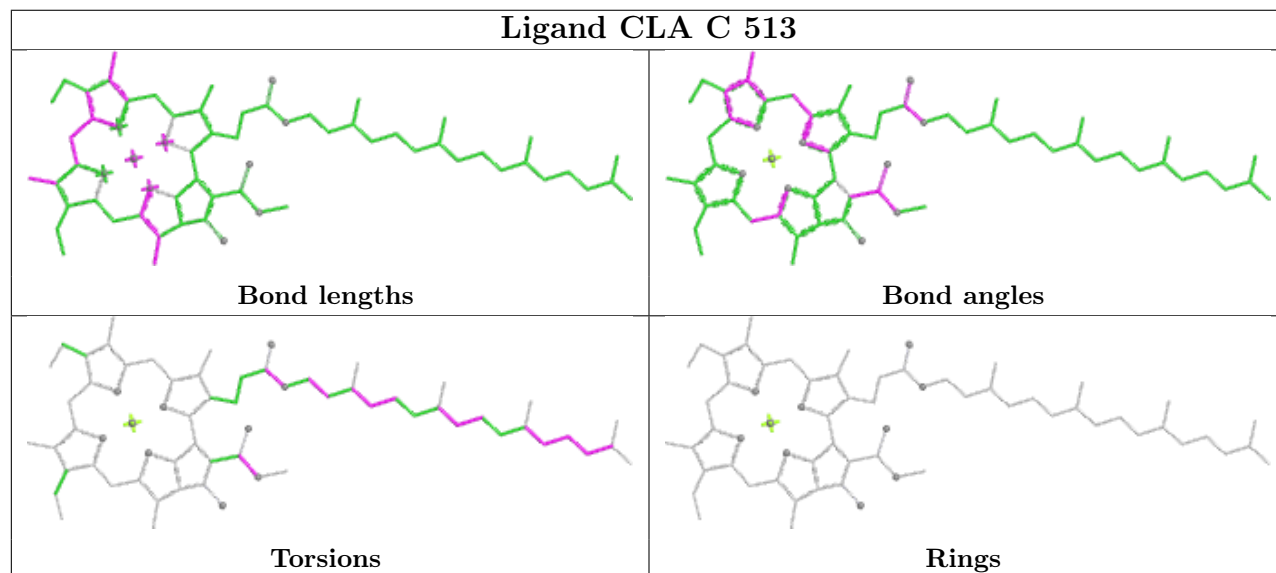
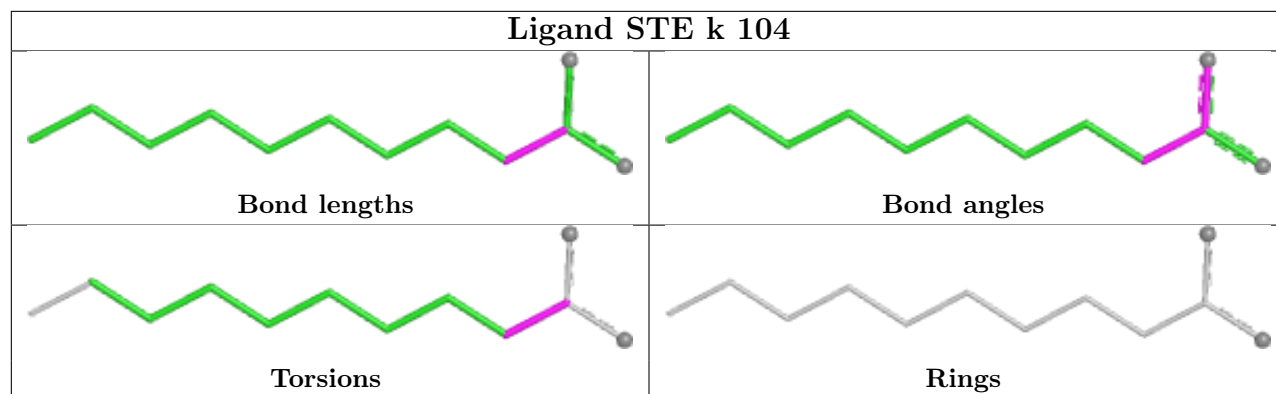
Ligand CLA b 601



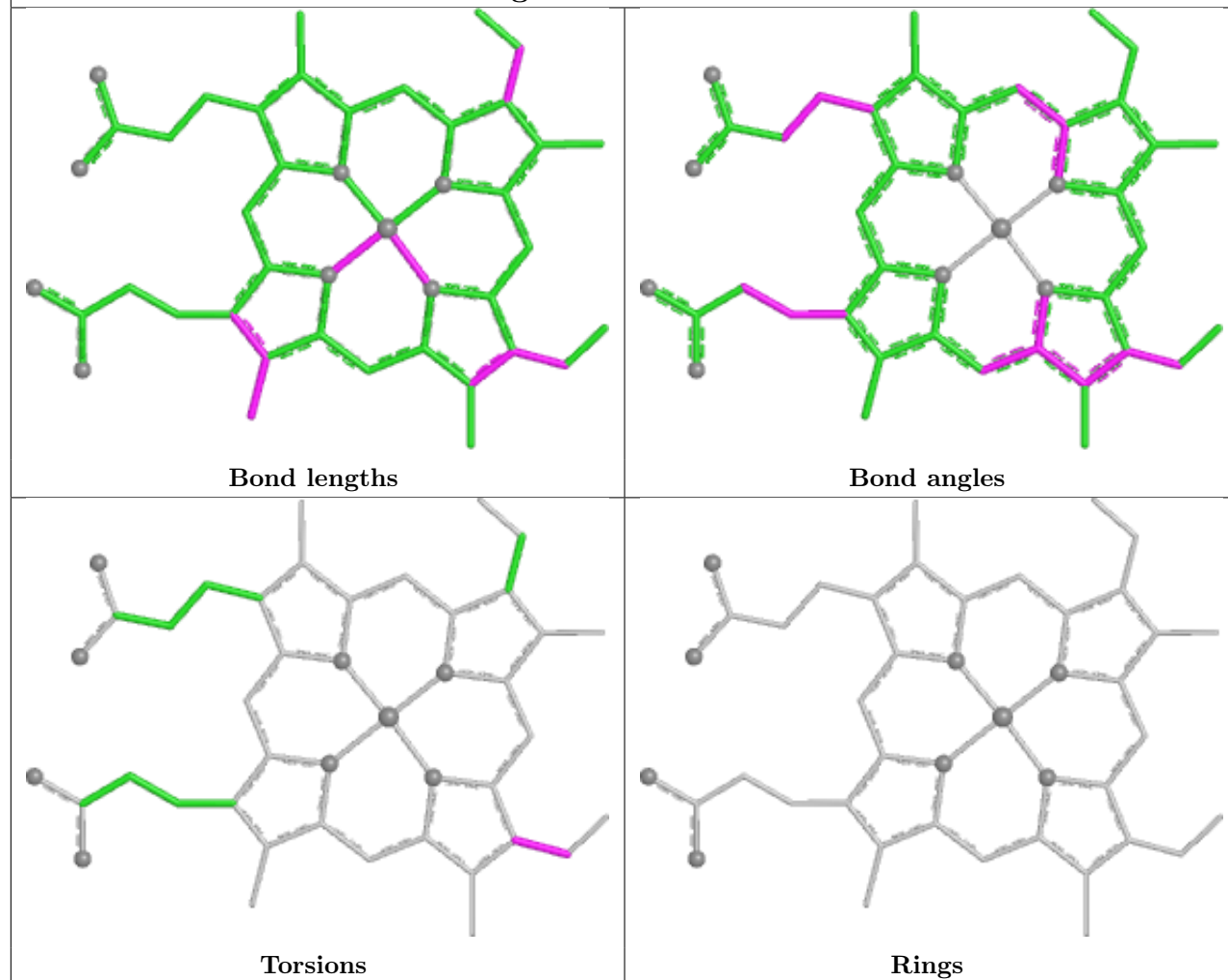
Ligand LHG 1 101



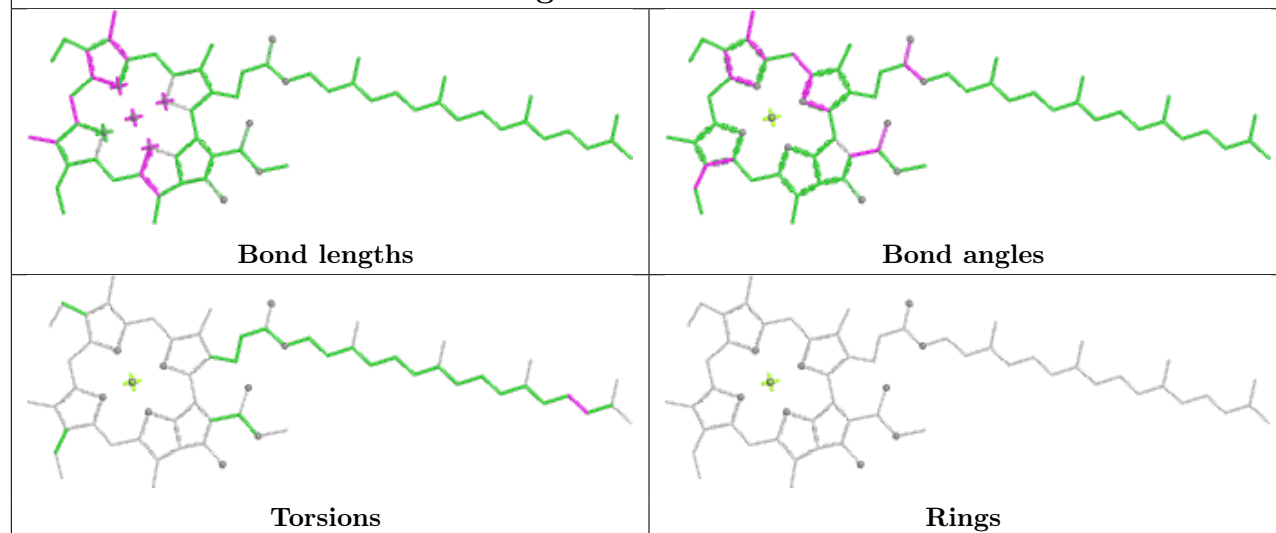




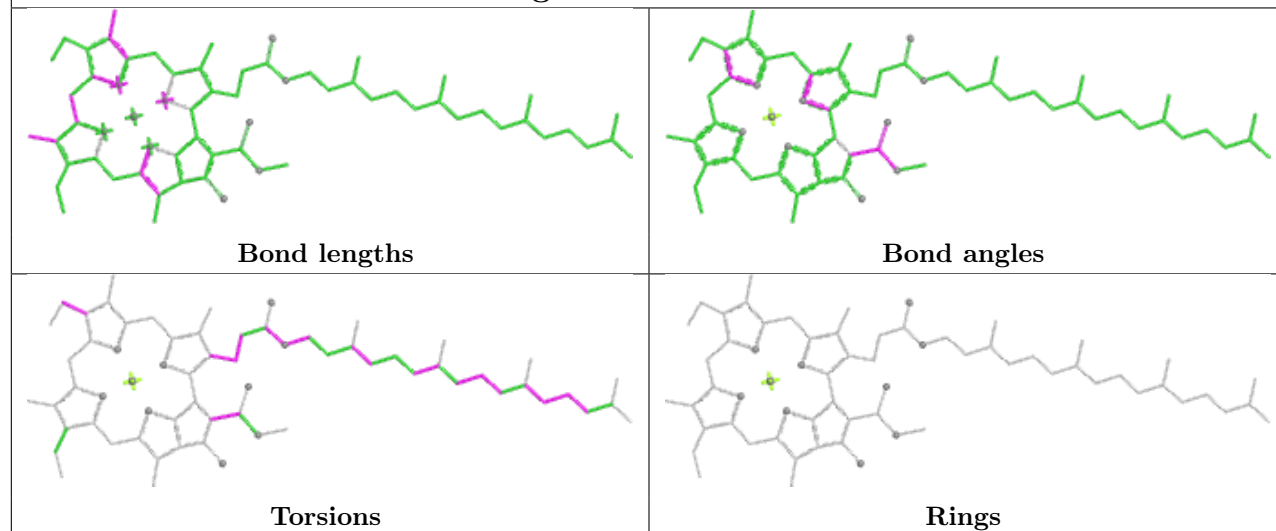
Ligand HEM e 101



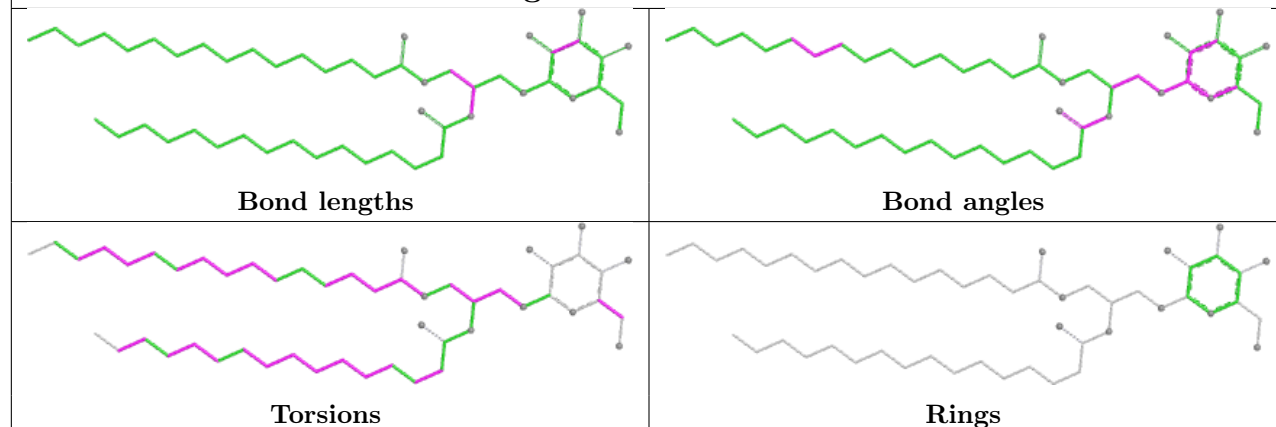
Ligand CLA a 402



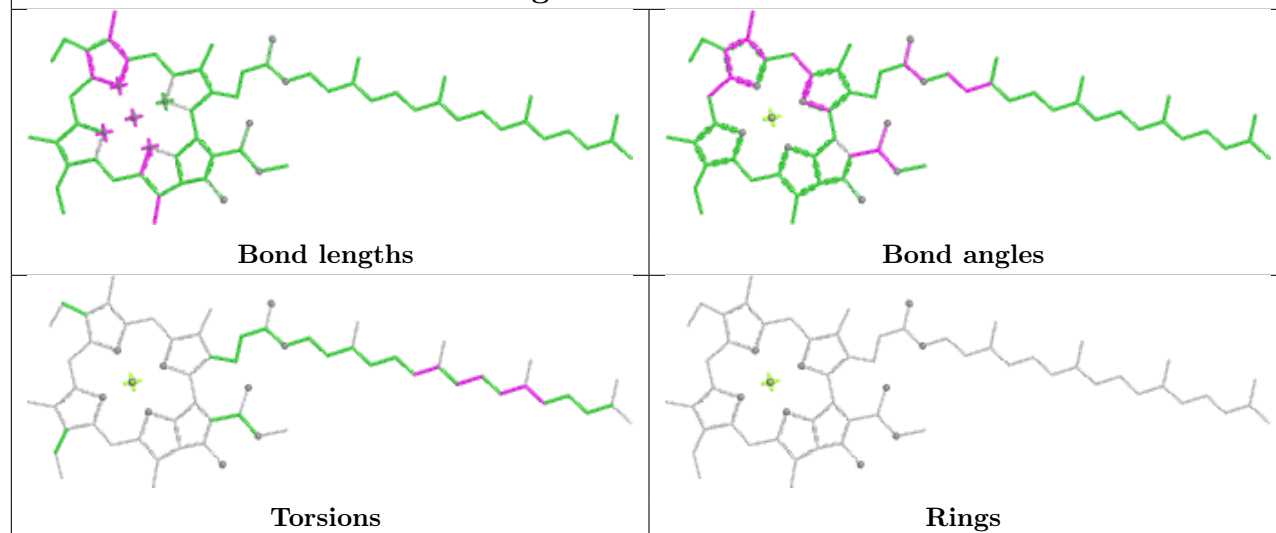
Ligand CLA B 601

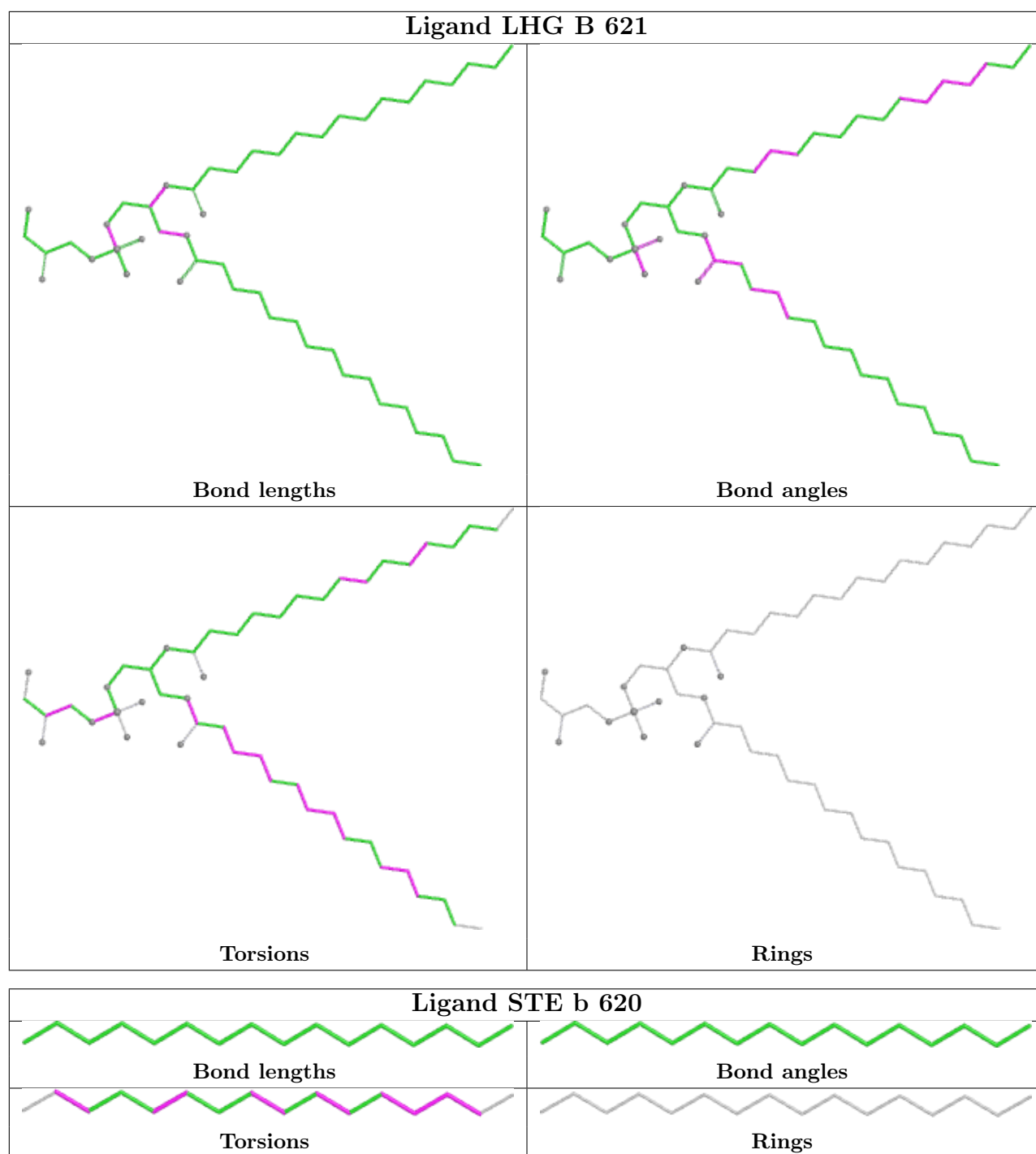


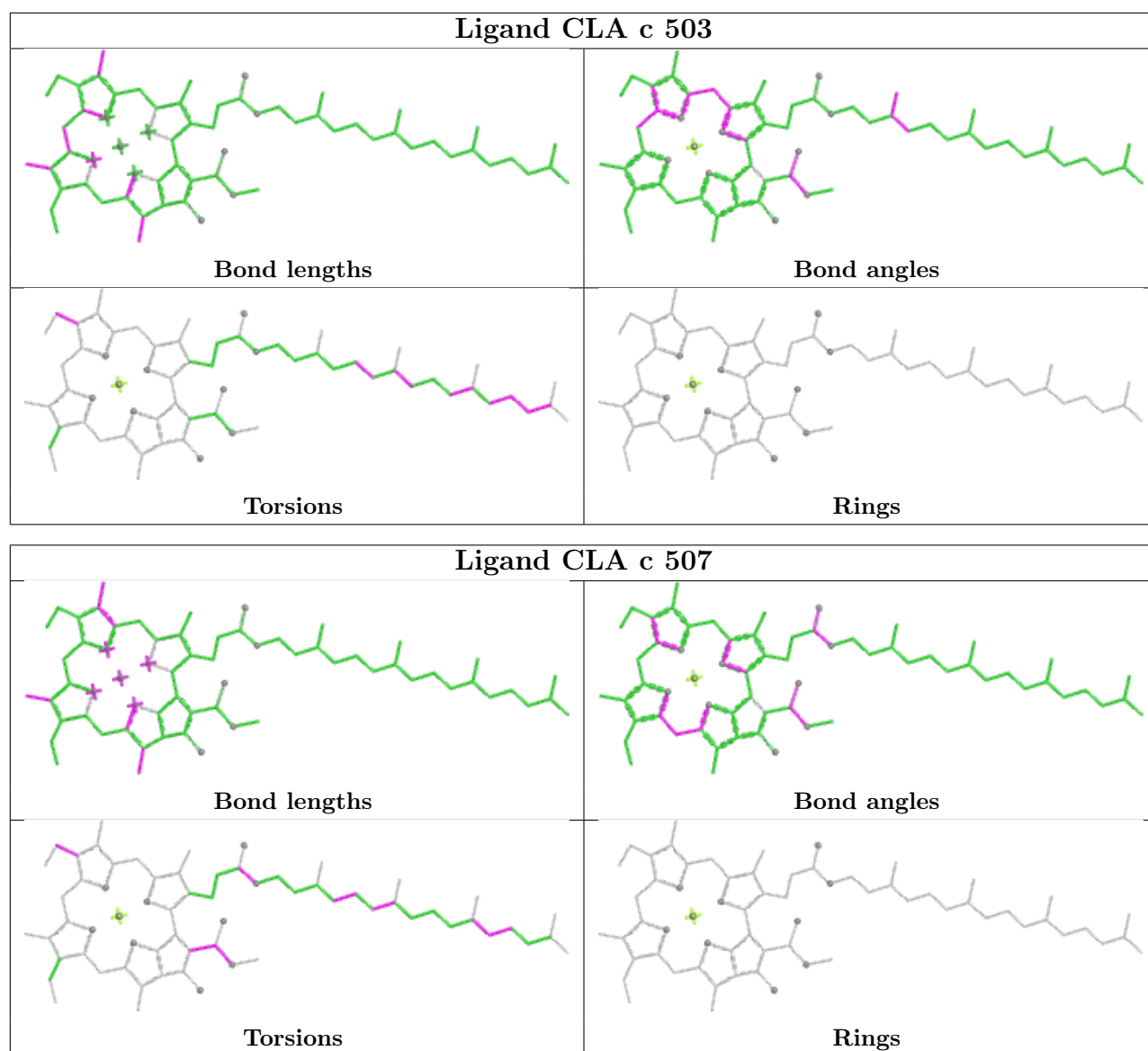
Ligand LMG M 101



Ligand CLA A 403







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%)	-0.64	2 (0%) 85 86	27, 34, 52, 87	0
1	a	334/344 (97%)	-0.51	2 (0%) 85 86	27, 36, 61, 82	0
2	B	505/510 (99%)	-0.48	0 100 100	19, 38, 66, 92	4 (0%)
2	b	505/510 (99%)	-0.33	2 (0%) 88 89	30, 42, 73, 116	0
3	C	442/461 (95%)	-0.41	0 100 100	18, 42, 58, 84	1 (0%)
3	c	451/461 (97%)	-0.31	1 (0%) 91 92	22, 46, 65, 101	2 (0%)
4	D	341/352 (96%)	-0.61	0 100 100	26, 36, 52, 87	0
4	d	341/352 (96%)	-0.45	0 100 100	27, 40, 62, 93	1 (0%)
5	E	82/84 (97%)	0.07	3 (3%) 45 45	33, 57, 71, 90	1 (1%)
5	e	82/84 (97%)	0.28	3 (3%) 45 45	45, 64, 80, 98	0
6	F	34/45 (75%)	-0.22	0 100 100	44, 49, 65, 85	0
6	f	34/45 (75%)	0.01	1 (2%) 53 54	47, 56, 84, 93	0
7	H	65/66 (98%)	-0.33	1 (1%) 72 73	37, 46, 61, 79	0
7	h	63/66 (95%)	0.02	3 (4%) 35 35	44, 57, 67, 75	0
8	I	35/38 (92%)	-0.32	1 (2%) 53 54	38, 45, 71, 82	0
8	i	35/38 (92%)	-0.19	1 (2%) 53 54	37, 45, 83, 91	0
9	J	36/40 (90%)	-0.08	1 (2%) 55 55	41, 55, 81, 92	0
9	j	36/40 (90%)	0.08	2 (5%) 30 28	44, 58, 93, 106	0
10	K	37/46 (80%)	-0.09	0 100 100	49, 57, 78, 83	0
10	k	37/46 (80%)	0.05	0 100 100	52, 61, 74, 82	0
11	L	37/37 (100%)	-0.62	0 100 100	30, 36, 65, 71	0
11	l	36/37 (97%)	-0.48	0 100 100	30, 37, 72, 92	0
12	M	32/36 (88%)	-0.41	1 (3%) 51 51	32, 41, 60, 77	0
12	m	31/36 (86%)	-0.45	0 100 100	32, 41, 57, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.22	4 (1%) 70 71	29, 48, 85, 133	1 (0%)
13	o	244/272 (89%)	-0.25	4 (1%) 70 71	31, 45, 86, 140	0
14	R	28/41 (68%)	0.71	1 (3%) 46 46	62, 76, 87, 100	0
14	r	28/41 (68%)	1.41	9 (32%) 1 0	76, 98, 118, 140	0
15	T	29/32 (90%)	-0.53	0 100 100	32, 38, 65, 77	0
15	t	29/32 (90%)	-0.26	1 (3%) 48 48	32, 39, 76, 95	0
16	U	97/134 (72%)	-0.23	0 100 100	37, 49, 77, 87	0
16	u	97/134 (72%)	-0.32	0 100 100	35, 46, 61, 90	0
17	V	137/163 (84%)	-0.41	0 100 100	34, 46, 61, 76	0
17	v	137/163 (84%)	-0.17	0 100 100	38, 52, 72, 85	0
18	X	38/41 (92%)	-0.13	0 100 100	45, 56, 71, 81	0
18	x	39/41 (95%)	0.19	2 (5%) 33 32	53, 65, 94, 106	0
19	Y	27/46 (58%)	1.00	4 (14%) 5 5	56, 75, 98, 101	0
19	y	30/46 (65%)	0.66	0 100 100	65, 80, 99, 109	0
20	Z	62/62 (100%)	0.64	3 (4%) 35 35	57, 74, 117, 127	0
20	z	62/62 (100%)	0.73	5 (8%) 18 16	60, 78, 116, 129	0
All	All	5293/5700 (92%)	-0.31	57 (1%) 78 79	18, 44, 78, 140	10 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.8
15	t	30	THR	5.4
18	x	40	SER	4.4
7	H	66	GLY	3.9
19	Y	20	ALA	3.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	T	1	10/11	0.94	0.08	31,46,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FME	t	1	10/11	0.94	0.09	36,48,66,66	0
12	FME	M	1	10/11	0.95	0.10	41,50,67,78	0
8	FME	i	1	10/11	0.96	0.07	45,54,66,70	0
12	FME	m	1	10/11	0.96	0.07	34,46,59,71	0
8	FME	I	1	10/11	0.97	0.06	41,52,63,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
32	STE	H	103	18/20	0.70	0.19	47,75,87,88	0
32	STE	a	415	12/20	0.75	0.17	55,69,75,77	0
32	STE	k	104	12/20	0.75	0.14	50,66,81,84	0
32	STE	b	624	16/20	0.76	0.16	51,66,80,83	0
32	STE	b	626	10/20	0.76	0.15	43,55,61,65	0
32	STE	I	101	15/20	0.76	0.17	45,59,81,82	0
28	LHG	E	101	49/49	0.77	0.16	54,79,113,119	0
32	STE	B	626	16/20	0.77	0.16	47,64,76,87	0
27	LMG	b	622	55/55	0.78	0.17	49,75,94,103	0
32	STE	E	102	12/20	0.78	0.18	53,75,86,89	0
32	STE	C	520	16/20	0.79	0.14	42,56,79,79	0
32	STE	b	625	20/20	0.79	0.14	42,65,80,84	0
27	LMG	c	520	48/55	0.80	0.15	41,73,104,109	0
27	LMG	d	408	23/55	0.81	0.17	43,66,82,84	0
27	LMG	D	410	33/55	0.81	0.14	38,56,80,83	0
28	LHG	e	102	42/49	0.81	0.14	58,82,104,116	0
32	STE	b	620	16/20	0.81	0.15	35,53,66,76	0
32	STE	c	519	20/20	0.82	0.13	43,61,86,98	0
29	SQD	a	413	36/54	0.82	0.14	31,64,84,89	0
32	STE	M	104	15/20	0.83	0.15	44,60,84,86	0
32	STE	B	627	12/20	0.83	0.16	51,65,84,84	0
32	STE	m	102	12/20	0.83	0.16	51,64,80,84	0
32	STE	J	101	12/20	0.84	0.14	46,60,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	B	623	44/66	0.84	0.13	39,56,75,85	0
32	STE	x	102	20/20	0.84	0.12	36,60,76,80	0
22	CLA	b	601	65/65	0.85	0.12	44,68,89,105	0
30	DGD	A	414	66/66	0.85	0.12	42,65,81,89	0
26	PL9	A	409	55/55	0.85	0.14	37,69,85,88	0
27	LMG	C	518	48/55	0.85	0.13	40,74,93,101	0
29	SQD	A	413	39/54	0.85	0.13	42,60,87,91	0
32	STE	j	101	12/20	0.86	0.12	42,60,73,77	0
32	STE	C	521	12/20	0.86	0.12	37,48,57,59	0
29	SQD	f	101	41/54	0.86	0.14	62,86,110,115	0
32	STE	d	410	17/20	0.86	0.13	42,58,69,78	0
27	LMG	A	410	48/55	0.87	0.11	41,57,75,87	0
32	STE	B	625	18/20	0.87	0.11	43,59,73,74	0
32	STE	B	624	12/20	0.88	0.11	41,57,67,77	0
27	LMG	D	411	28/55	0.88	0.12	33,52,63,64	0
32	STE	M	103	10/20	0.88	0.13	38,48,56,65	0
26	PL9	a	410	55/55	0.88	0.12	40,66,87,94	0
27	LMG	c	518	37/55	0.88	0.11	44,65,82,88	0
29	SQD	L	101	49/54	0.89	0.10	41,59,89,101	0
32	STE	C	519	12/20	0.89	0.12	42,57,69,73	0
32	STE	b	621	20/20	0.89	0.10	40,56,70,73	0
27	LMG	a	414	49/55	0.89	0.11	37,58,84,101	0
24	BCR	k	101	40/40	0.89	0.11	42,60,76,77	0
32	STE	t	103	10/20	0.89	0.12	32,61,69,71	0
29	SQD	B	622	54/54	0.89	0.10	36,61,87,102	0
32	STE	l	102	18/20	0.90	0.12	36,53,83,90	0
32	STE	B	620	17/20	0.90	0.10	36,50,66,67	0
24	BCR	Z	101	40/40	0.90	0.10	40,58,72,79	0
22	CLA	B	601	65/65	0.90	0.10	36,63,90,96	0
24	BCR	K	101	40/40	0.91	0.10	43,57,72,82	0
32	STE	M	102	15/20	0.91	0.11	38,51,67,67	0
27	LMG	M	101	51/55	0.91	0.09	32,52,68,73	0
22	CLA	C	513	65/65	0.91	0.10	42,63,92,95	0
24	BCR	d	404	40/40	0.91	0.11	36,54,84,98	0
30	DGD	C	516	62/66	0.91	0.10	35,55,105,118	0
24	BCR	D	406	40/40	0.91	0.10	31,46,83,87	0
32	STE	t	102	14/20	0.91	0.09	36,53,59,60	0
24	BCR	k	102	40/40	0.91	0.10	45,65,75,78	0
29	SQD	a	412	54/54	0.91	0.10	45,65,85,89	0
24	BCR	x	101	40/40	0.92	0.09	38,57,78,80	0
30	DGD	h	101	62/66	0.92	0.09	30,51,63,69	0
32	STE	D	412	20/20	0.92	0.09	32,53,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMG	m	101	51/55	0.92	0.09	35,54,68,80	0
29	SQD	F	102	36/54	0.92	0.10	44,73,93,97	0
24	BCR	b	617	40/40	0.93	0.08	28,47,58,59	0
28	LHG	b	623	49/49	0.93	0.10	34,52,68,73	0
27	LMG	D	408	51/55	0.93	0.11	29,58,82,92	0
29	SQD	A	412	52/54	0.93	0.10	33,59,86,89	0
24	BCR	b	619	40/40	0.93	0.08	32,49,67,74	0
24	BCR	B	617	40/40	0.93	0.08	27,42,58,64	0
24	BCR	B	619	40/40	0.93	0.08	28,46,64,68	0
24	BCR	C	514	40/40	0.93	0.09	28,44,57,62	0
24	BCR	k	103	40/40	0.93	0.10	44,58,69,74	0
22	CLA	C	512	65/65	0.93	0.10	37,55,85,90	0
24	BCR	H	101	40/40	0.93	0.08	31,48,62,70	0
22	CLA	c	512	65/65	0.93	0.10	46,59,87,93	0
27	LMG	d	409	44/55	0.93	0.10	36,56,83,89	0
22	CLA	c	513	65/65	0.93	0.10	43,67,103,109	0
30	DGD	C	517	62/66	0.93	0.10	30,53,74,86	0
30	DGD	c	516	62/66	0.93	0.09	33,56,93,101	0
22	CLA	c	503	65/65	0.94	0.09	37,48,61,71	0
24	BCR	B	618	40/40	0.94	0.07	26,39,53,56	0
22	CLA	c	505	65/65	0.94	0.09	30,44,71,73	0
22	CLA	c	506	65/65	0.94	0.10	30,54,99,106	0
22	CLA	c	509	65/65	0.94	0.09	36,51,70,74	0
22	CLA	c	511	65/65	0.94	0.09	40,55,73,77	0
22	CLA	B	606	65/65	0.94	0.08	24,39,76,81	0
24	BCR	K	102	40/40	0.94	0.09	40,55,71,75	0
24	BCR	T	101	40/40	0.94	0.07	29,43,62,64	0
22	CLA	b	606	65/65	0.94	0.08	28,43,75,79	0
30	DGD	C	515	62/66	0.94	0.09	23,43,80,92	0
24	BCR	A	406	40/40	0.94	0.07	26,38,50,52	0
28	LHG	d	407	39/49	0.94	0.08	34,50,70,73	0
30	DGD	H	102	62/66	0.94	0.08	31,47,60,62	0
24	BCR	b	618	40/40	0.94	0.07	29,42,53,59	0
30	DGD	c	517	62/66	0.94	0.09	32,54,90,96	0
28	LHG	A	411	47/49	0.95	0.09	31,51,76,89	0
28	LHG	B	621	49/49	0.95	0.08	31,47,65,80	0
24	BCR	c	514	40/40	0.95	0.08	30,45,60,69	0
22	CLA	C	505	65/65	0.95	0.08	26,43,71,76	0
22	CLA	a	405	65/65	0.95	0.08	21,38,87,98	0
22	CLA	C	506	65/65	0.95	0.09	27,49,99,103	0
28	LHG	l	101	49/49	0.95	0.08	25,47,57,73	0
22	CLA	d	403	65/65	0.95	0.08	36,53,90,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	t	101	40/40	0.95	0.06	27,42,57,58	0
23	PHO	d	401	64/64	0.95	0.06	29,42,51,60	0
22	CLA	b	602	65/65	0.95	0.08	27,47,66,77	0
26	PL9	D	407	55/55	0.95	0.07	24,37,51,53	0
22	CLA	C	508	65/65	0.95	0.08	33,47,100,108	0
26	PL9	d	405	55/55	0.95	0.07	24,38,48,52	0
22	CLA	b	609	65/65	0.95	0.08	31,48,72,76	0
22	CLA	b	615	65/65	0.95	0.07	27,42,65,68	0
22	CLA	b	616	60/65	0.95	0.09	28,47,91,95	0
22	CLA	c	502	65/65	0.95	0.07	31,49,64,70	0
22	CLA	C	509	65/65	0.95	0.09	26,49,67,72	0
22	CLA	c	504	60/65	0.95	0.08	34,49,80,87	0
22	CLA	C	510	65/65	0.95	0.07	30,46,68,74	0
30	DGD	c	515	62/66	0.95	0.09	26,45,79,86	0
22	CLA	C	511	65/65	0.95	0.08	35,52,66,77	0
22	CLA	c	507	65/65	0.95	0.08	30,48,66,67	0
24	BCR	a	406	40/40	0.95	0.06	22,38,51,55	0
22	CLA	c	508	64/65	0.95	0.09	29,45,85,98	0
22	CLA	B	616	60/65	0.95	0.09	28,44,86,98	0
22	CLA	c	510	65/65	0.95	0.08	31,50,66,74	0
33	BCT	D	402	4/4	0.95	0.07	28,32,35,42	0
22	CLA	B	605	65/65	0.96	0.07	23,35,52,55	0
22	CLA	A	403	65/65	0.96	0.08	22,37,83,96	0
22	CLA	B	609	65/65	0.96	0.07	28,39,58,68	0
22	CLA	B	610	65/65	0.96	0.07	21,36,46,49	0
22	CLA	B	613	65/65	0.96	0.07	21,37,68,77	0
22	CLA	D	403	65/65	0.96	0.07	21,33,56,65	0
22	CLA	D	404	65/65	0.96	0.06	22,33,50,57	0
22	CLA	D	405	65/65	0.96	0.08	25,47,98,106	0
22	CLA	d	402	65/65	0.96	0.07	23,36,60,64	0
22	CLA	a	403	65/65	0.96	0.09	26,43,91,102	0
23	PHO	A	404	64/64	0.96	0.06	19,31,42,44	0
23	PHO	D	401	64/64	0.96	0.06	23,35,45,49	0
23	PHO	a	404	64/64	0.96	0.06	22,34,42,44	0
22	CLA	B	614	65/65	0.96	0.08	25,40,76,85	0
22	CLA	a	411	65/65	0.96	0.07	23,34,52,56	0
22	CLA	B	615	65/65	0.96	0.08	28,40,71,75	0
22	CLA	A	402	65/65	0.96	0.06	21,31,44,62	0
22	CLA	b	603	65/65	0.96	0.07	24,40,68,75	0
22	CLA	b	604	65/65	0.96	0.07	25,41,77,86	0
22	CLA	b	605	65/65	0.96	0.07	23,38,51,57	0
28	LHG	L	102	49/49	0.96	0.07	29,43,57,69	0

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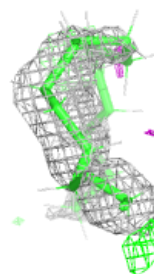
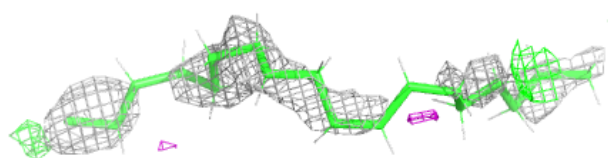
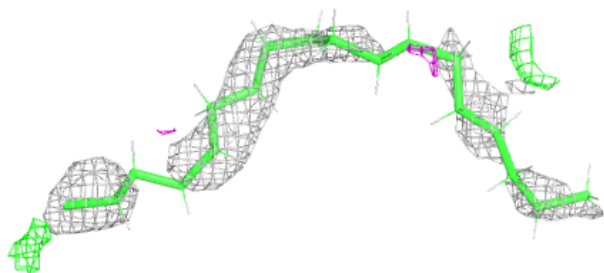
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	501	65/65	0.96	0.07	23,37,53,58	0
28	LHG	d	406	49/49	0.96	0.07	27,44,56,65	0
22	CLA	b	607	65/65	0.96	0.08	22,39,66,74	0
22	CLA	b	608	65/65	0.96	0.07	30,46,66,76	0
22	CLA	C	502	65/65	0.96	0.07	33,45,64,76	0
22	CLA	b	610	65/65	0.96	0.08	27,40,51,61	0
22	CLA	b	611	65/65	0.96	0.06	22,35,55,64	0
22	CLA	b	612	65/65	0.96	0.07	21,37,49,59	0
22	CLA	b	613	65/65	0.96	0.07	25,38,75,78	0
22	CLA	b	614	65/65	0.96	0.08	27,42,77,88	0
22	CLA	C	503	65/65	0.96	0.07	33,46,56,58	0
22	CLA	C	504	59/65	0.96	0.07	29,47,84,88	0
22	CLA	c	501	65/65	0.96	0.07	28,45,56,61	0
22	CLA	B	602	65/65	0.96	0.07	26,41,57,65	0
22	CLA	B	603	65/65	0.96	0.07	20,36,62,63	0
22	CLA	C	507	65/65	0.96	0.07	28,46,61,63	0
22	CLA	B	604	65/65	0.96	0.07	24,36,70,78	0
33	BCT	a	409	4/4	0.96	0.08	33,34,45,51	0
34	HEM	e	101	43/43	0.96	0.09	48,59,78,79	0
22	CLA	B	612	65/65	0.97	0.06	22,35,49,58	0
22	CLA	a	402	65/65	0.97	0.06	22,33,46,56	0
22	CLA	B	608	65/65	0.97	0.06	25,37,55,61	0
28	LHG	D	409	49/49	0.97	0.07	25,43,55,61	0
22	CLA	A	405	54/65	0.97	0.06	22,37,67,72	0
22	CLA	B	607	65/65	0.97	0.07	20,36,61,68	0
34	HEM	F	101	43/43	0.97	0.08	40,49,68,72	0
22	CLA	B	611	65/65	0.97	0.05	21,33,52,55	0
25	CL	A	407	1/1	0.98	0.04	34,34,34,34	0
35	HEC	V	201	43/43	0.98	0.07	27,37,46,49	0
35	HEC	v	201	43/43	0.98	0.06	33,41,51,58	0
25	CL	a	408	1/1	0.99	0.09	32,32,32,32	0
31	OEX	A	415	10/10	0.99	0.03	26,29,33,36	0
31	OEX	a	416	10/10	0.99	0.03	24,30,33,33	0
25	CL	A	408	1/1	0.99	0.04	30,30,30,30	0
25	CL	a	407	1/1	0.99	0.03	32,32,32,32	0
21	FE2	A	401	1/1	1.00	0.01	29,29,29,29	0
21	FE2	a	401	1/1	1.00	0.01	37,37,37,37	0

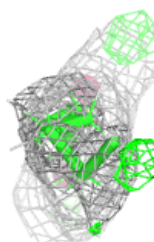
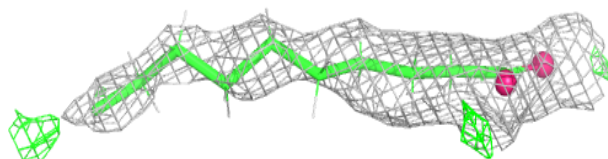
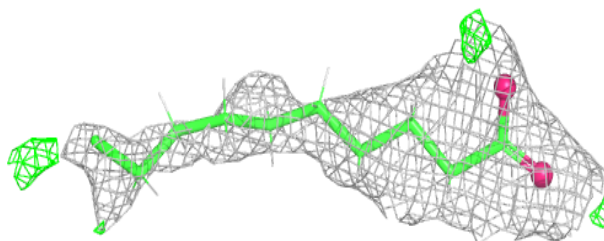
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

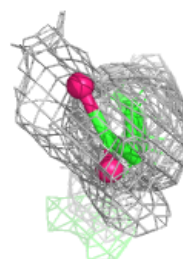
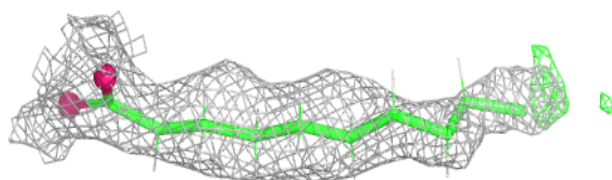
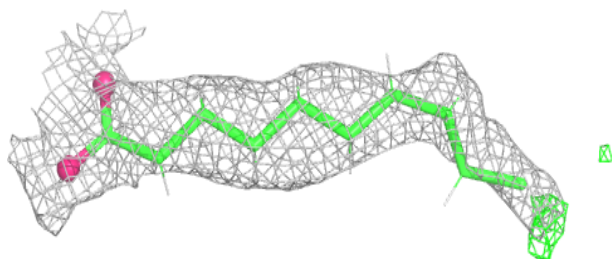
**Electron density around STE a 415:**

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

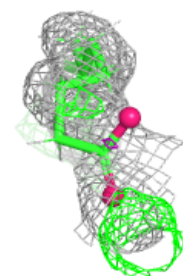
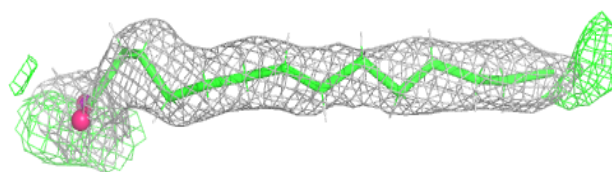
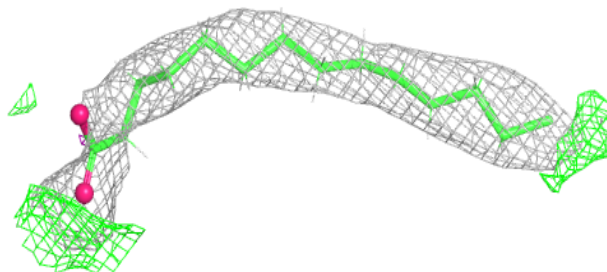


Electron density around STE k 104:

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

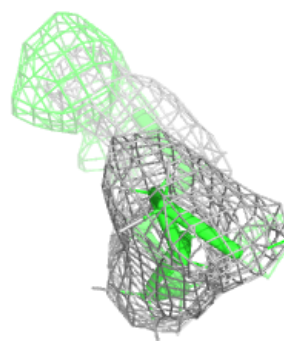
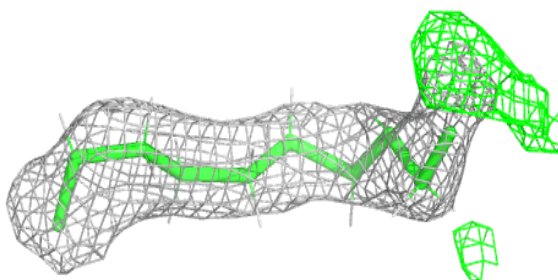
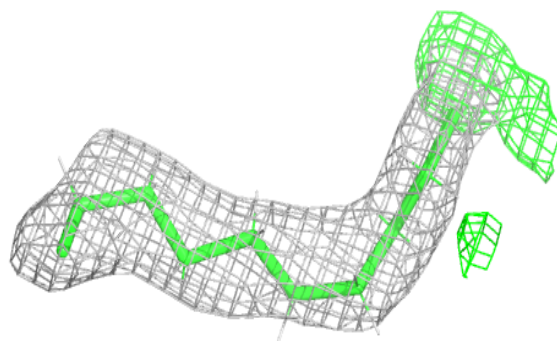
**Electron density around STE b 624:**

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

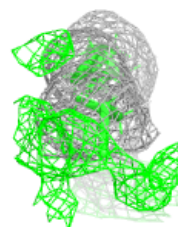
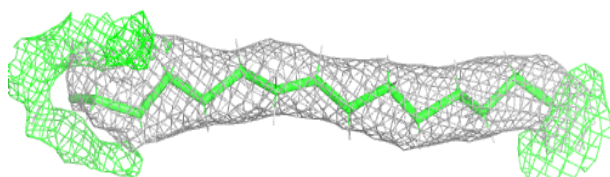
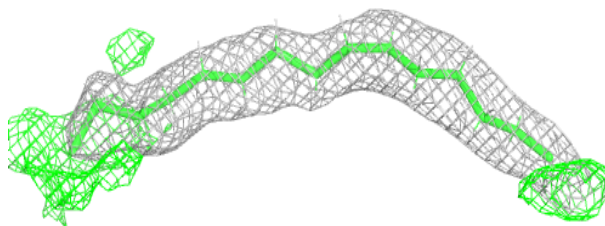


Electron density around STE b 626:

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

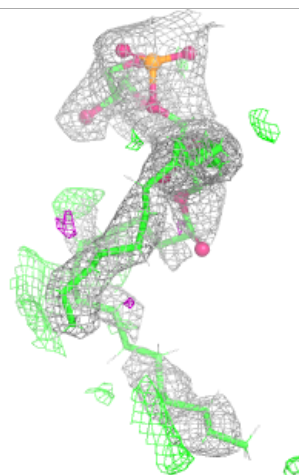
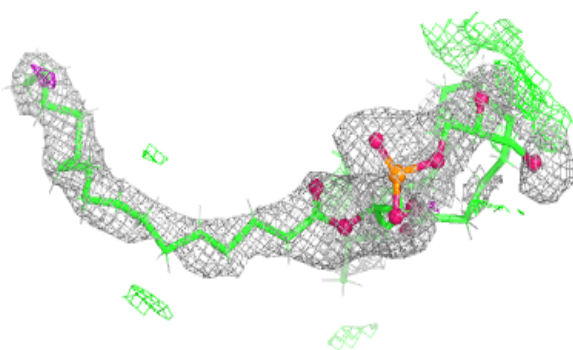
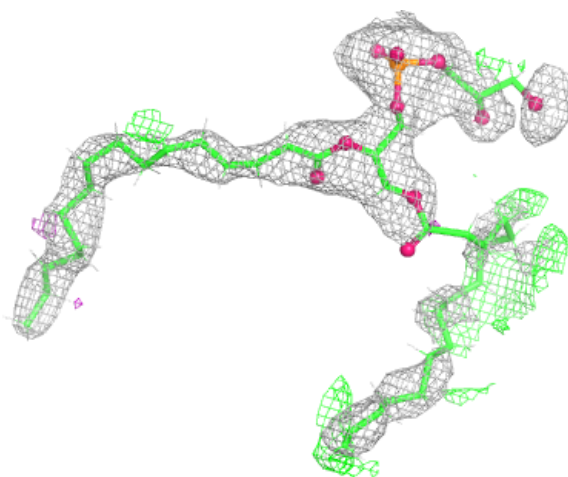
**Electron density around STE I 101:**

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



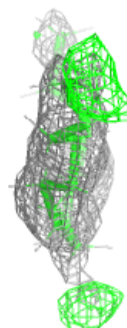
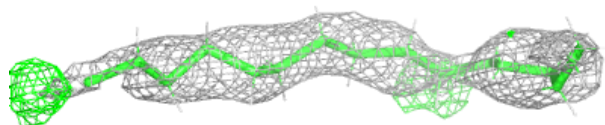
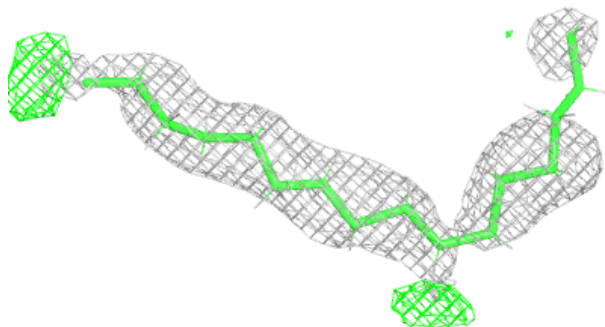
Electron density around LHG E 101:

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

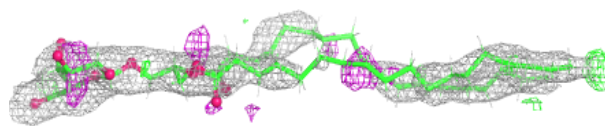
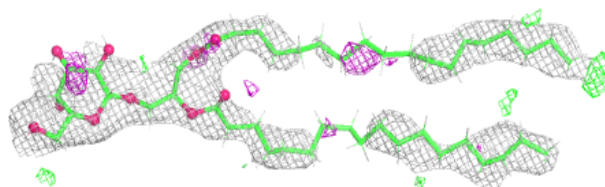


Electron density around STE B 626:

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

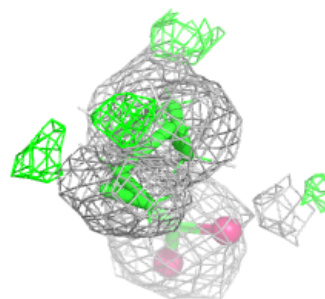
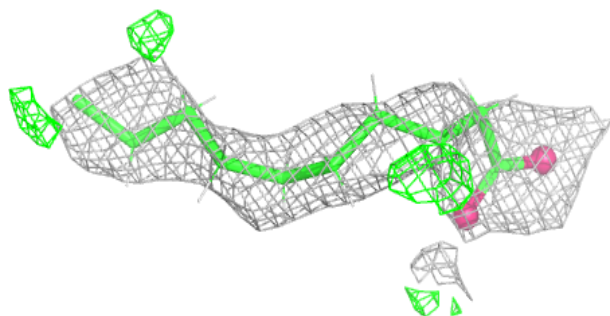
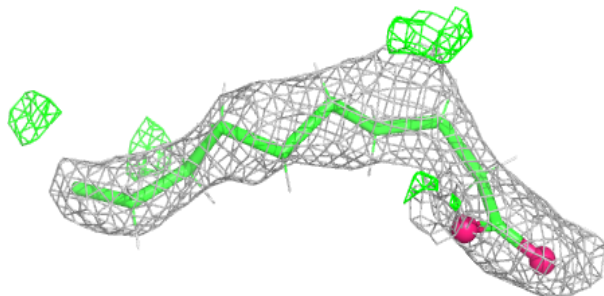
**Electron density around LMG b 622:**

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

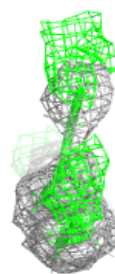
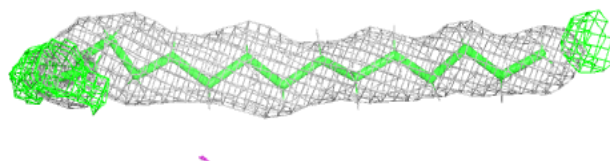
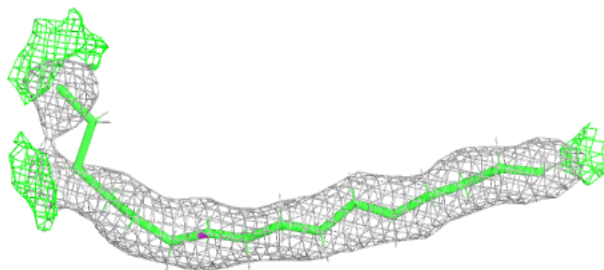


Electron density around STE E 102:

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

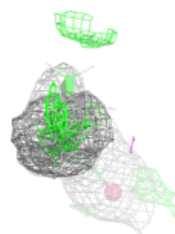
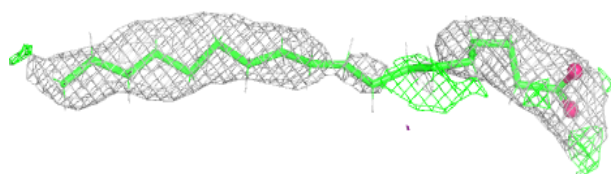
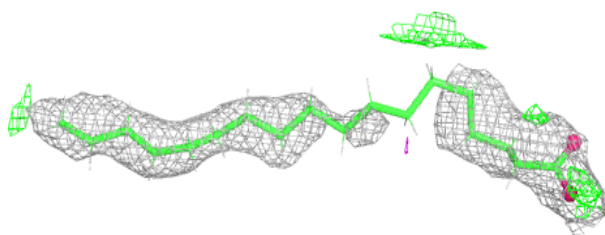
**Electron density around STE C 520:**

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

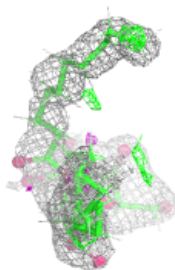
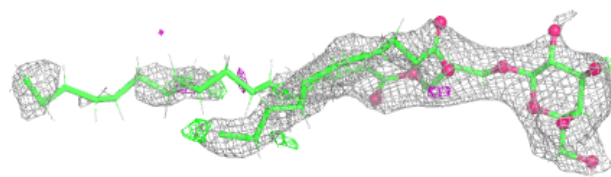
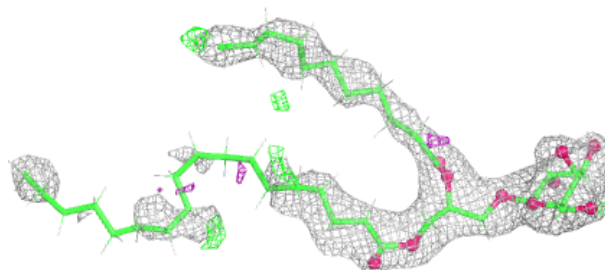


Electron density around STE b 625:

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

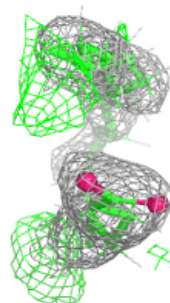
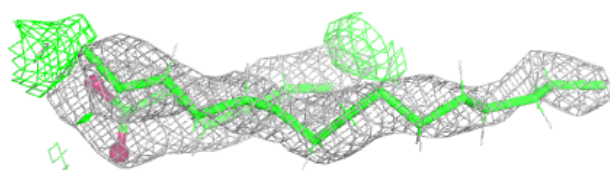
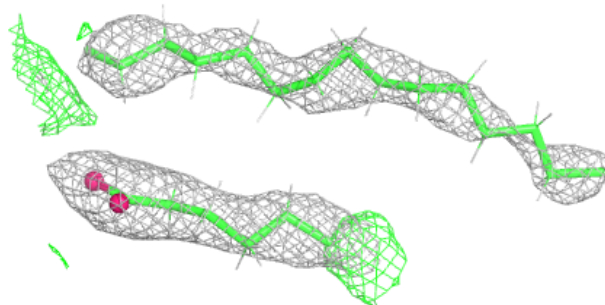
**Electron density around LMG c 520:**

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

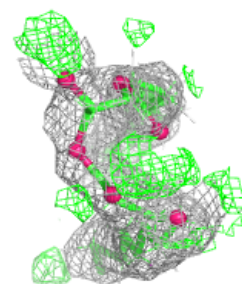
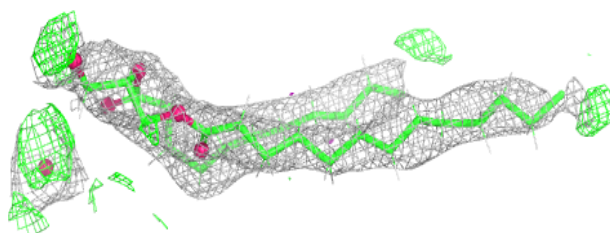
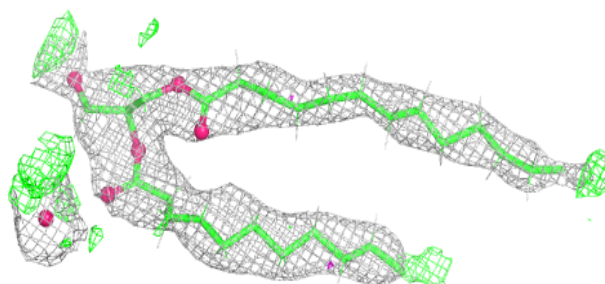


Electron density around LMG d 408:

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

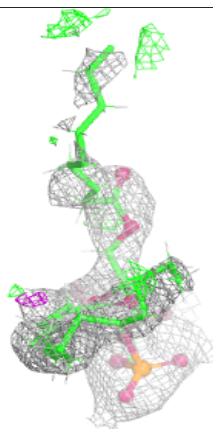
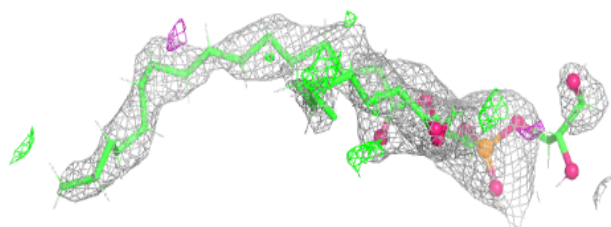
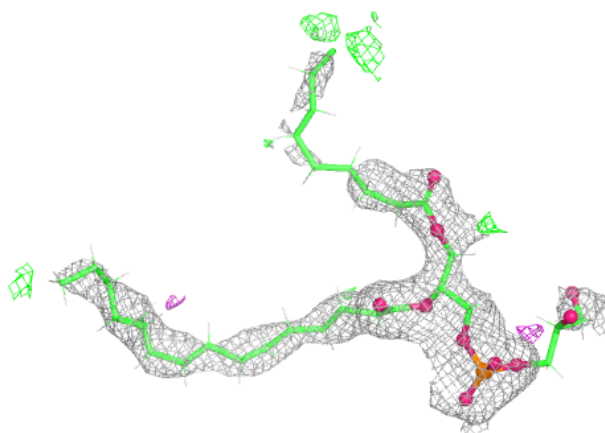
**Electron density around LMG D 410:**

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

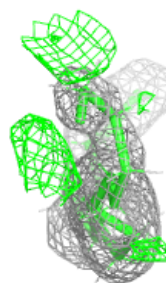
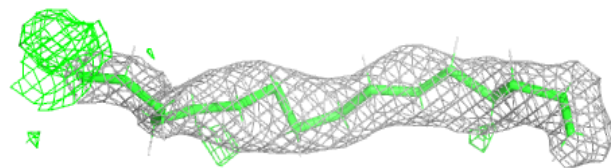
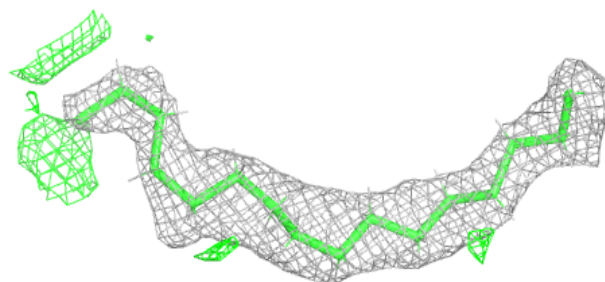


Electron density around LHG e 102:

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

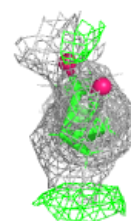
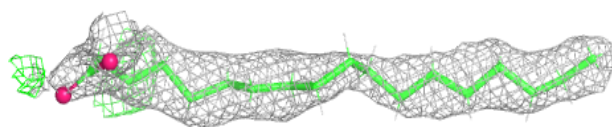
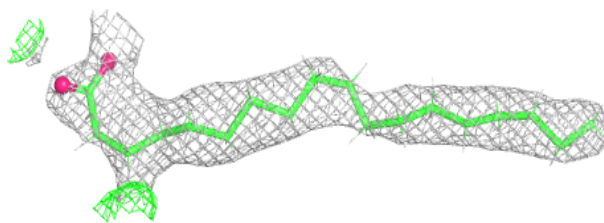
**Electron density around STE b 620:**

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



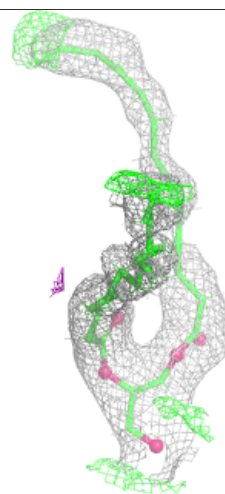
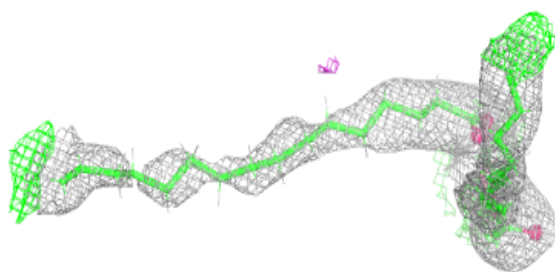
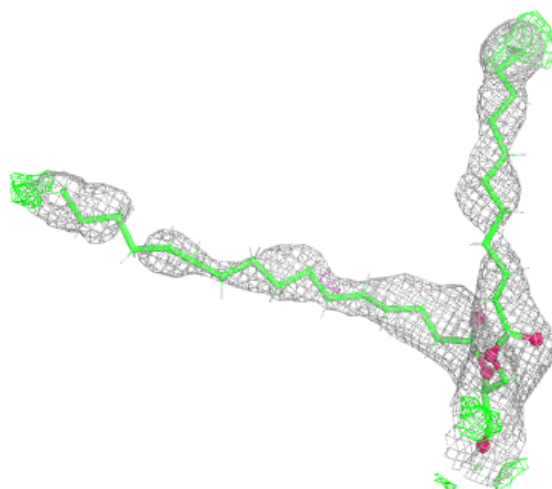
Electron density around STE c 519:

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



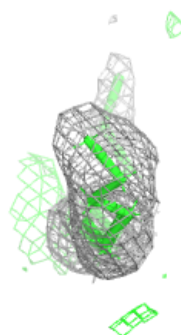
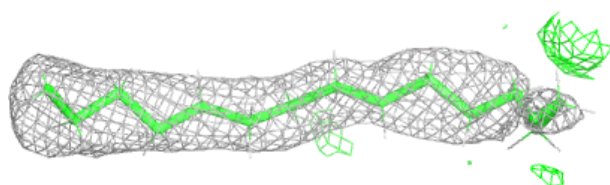
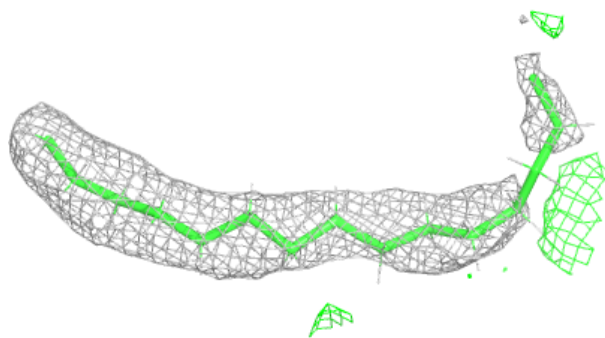
Electron density around SQD a 413:

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

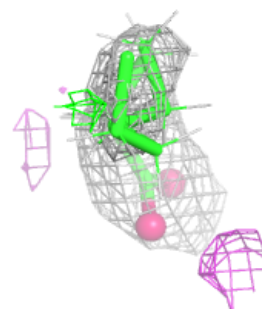
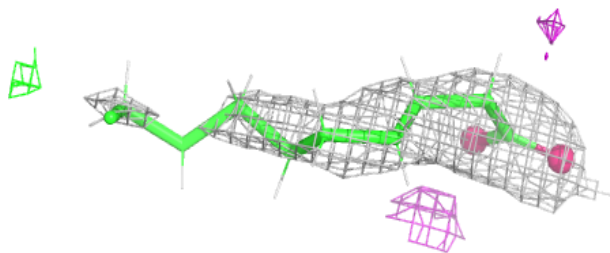
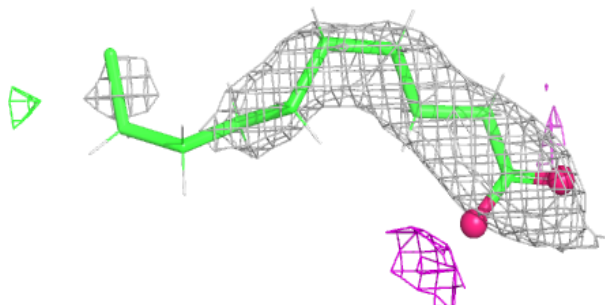


Electron density around STE M 104:

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

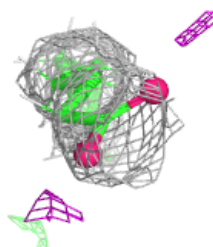
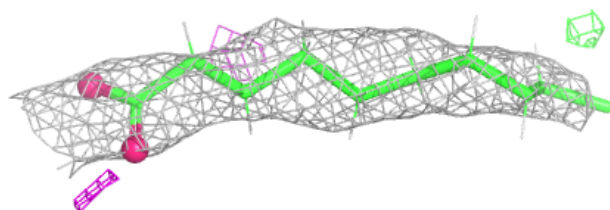
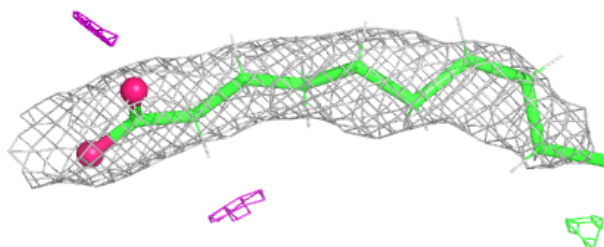
**Electron density around STE B 627:**

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

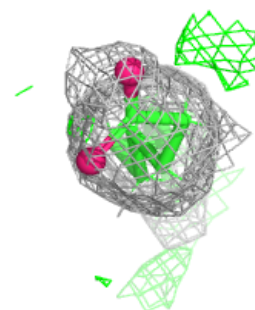
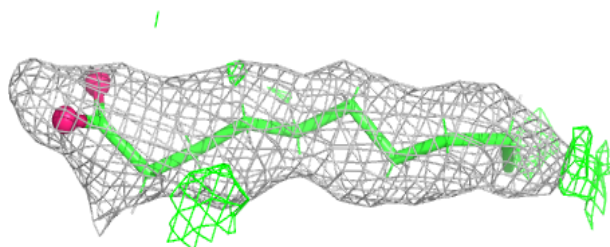
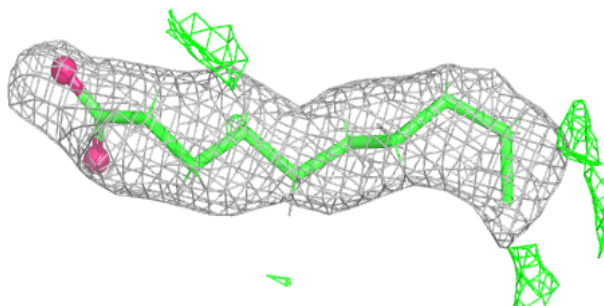


Electron density around STE m 102:

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

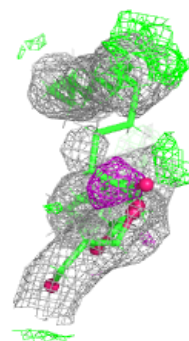
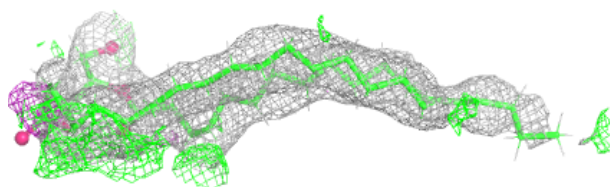
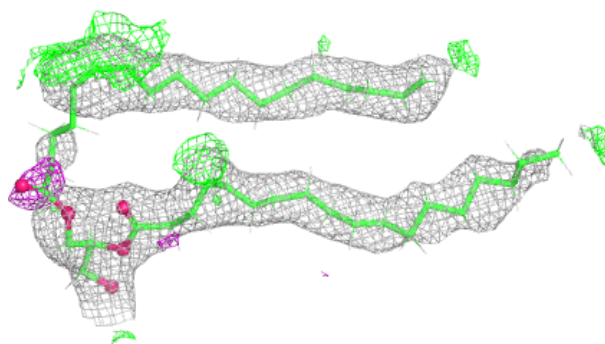
**Electron density around STE J 101:**

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

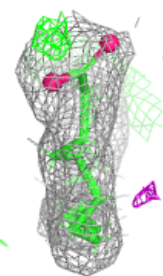
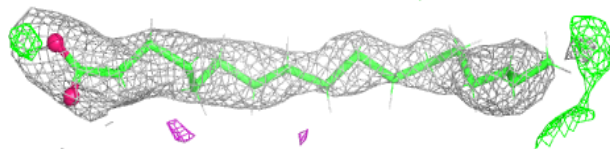
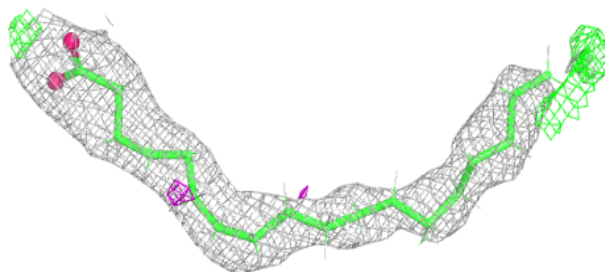


Electron density around DGD B 623:

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

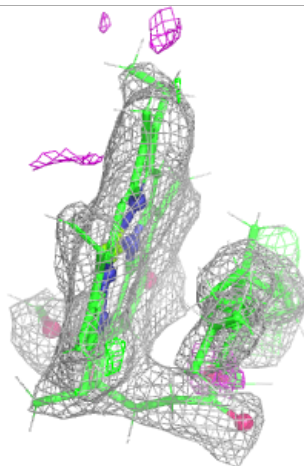
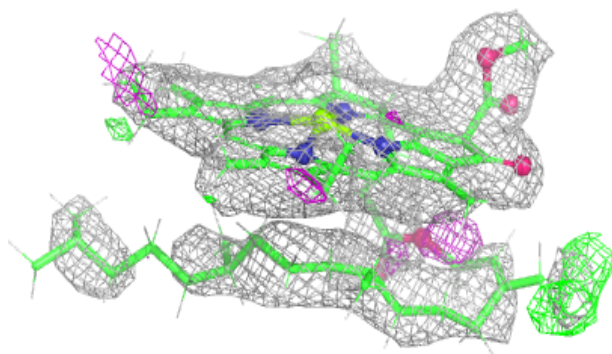
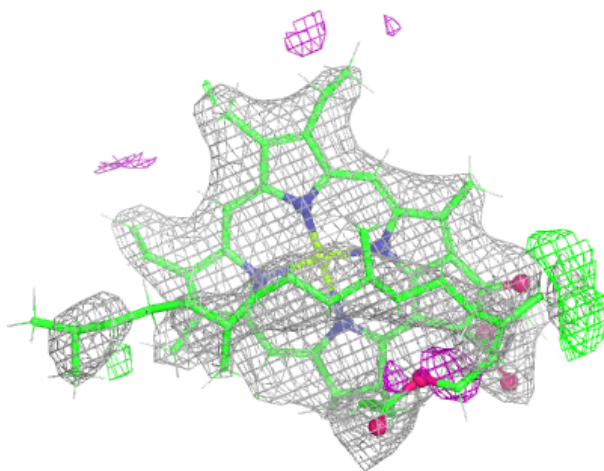
**Electron density around STE x 102:**

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



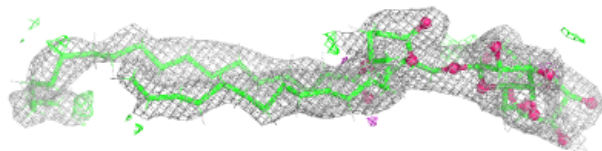
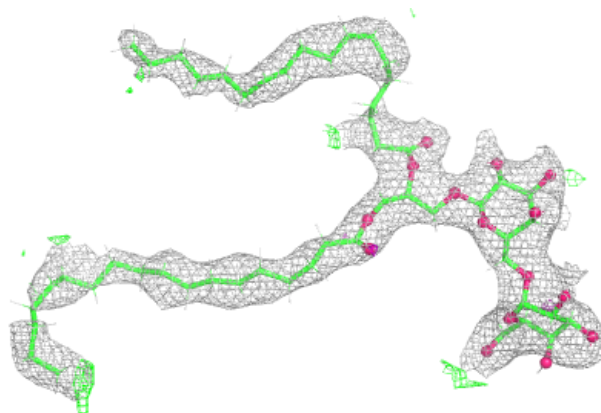
Electron density around CLA b 601:

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

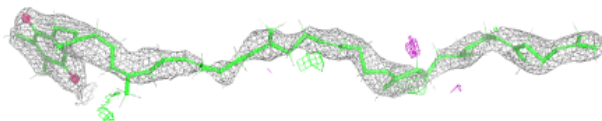
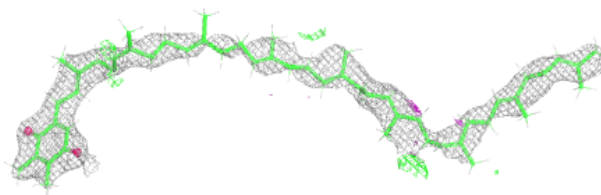


Electron density around DGD A 414:

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

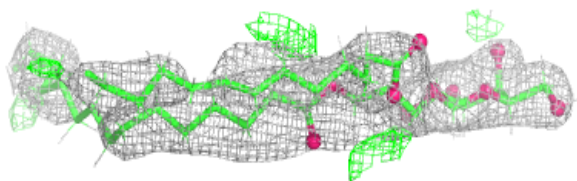
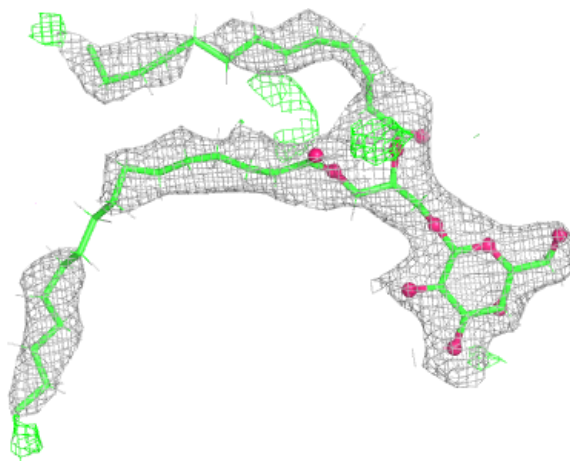
**Electron density around PL9 A 409:**

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



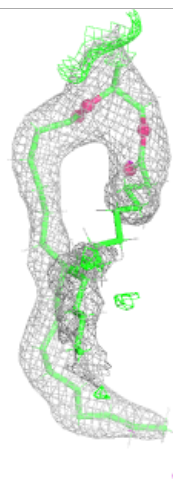
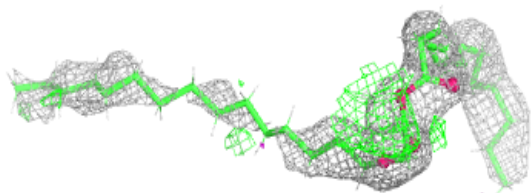
Electron density around LMG C 518:

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



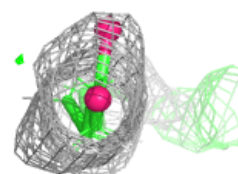
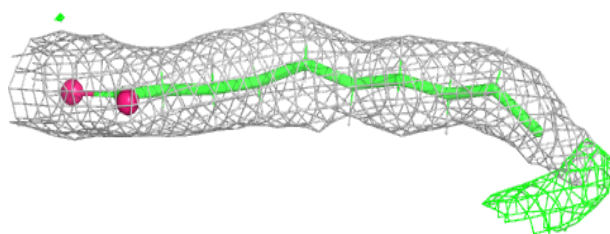
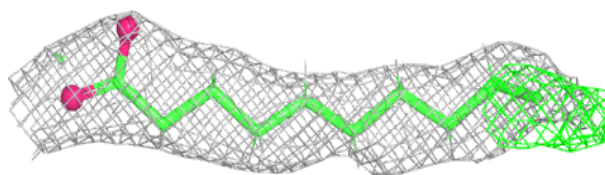
Electron density around SQD A 413:

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

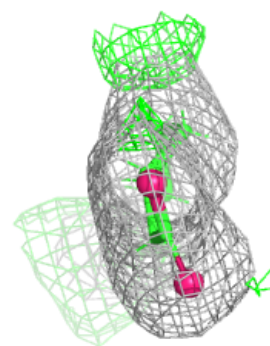
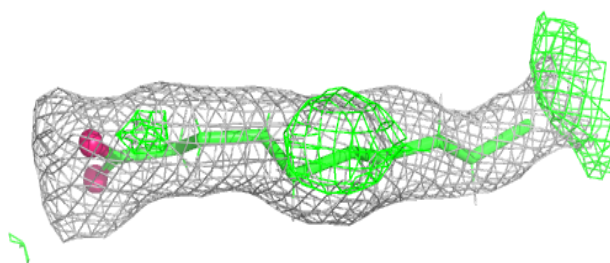
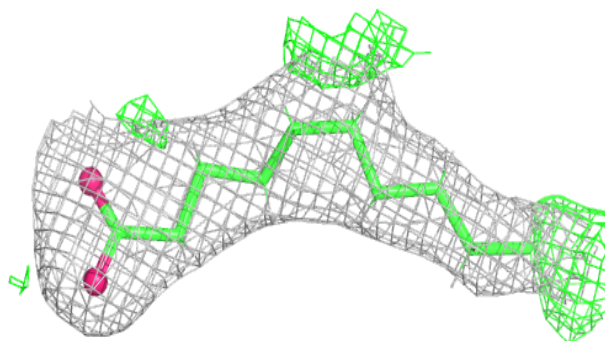


Electron density around STE j 101:

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

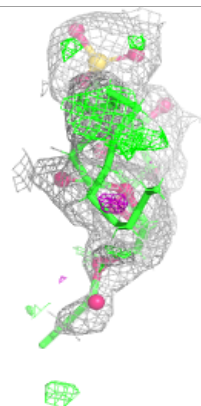
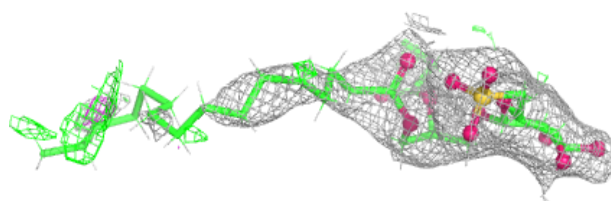
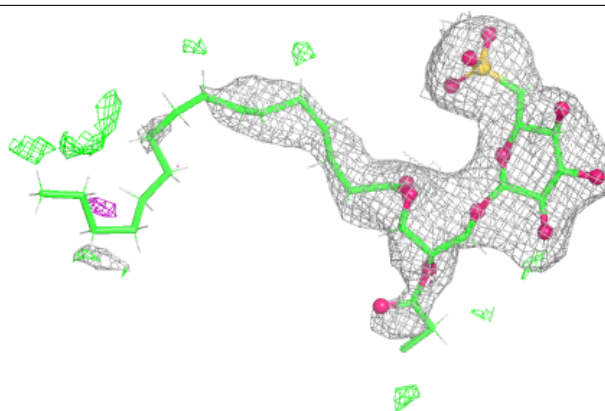
**Electron density around STE C 521:**

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

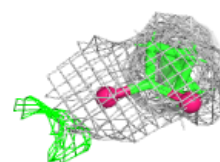
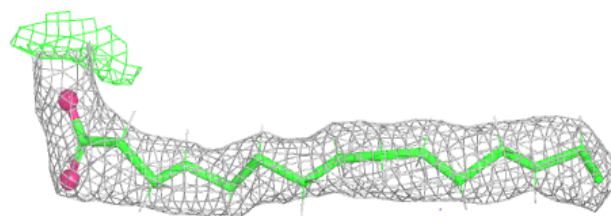


Electron density around SQD f 101:

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

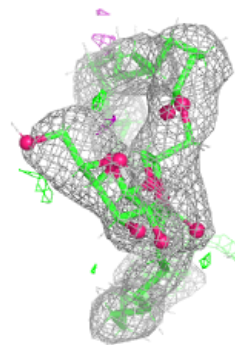
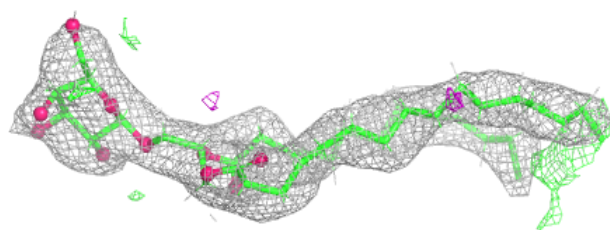
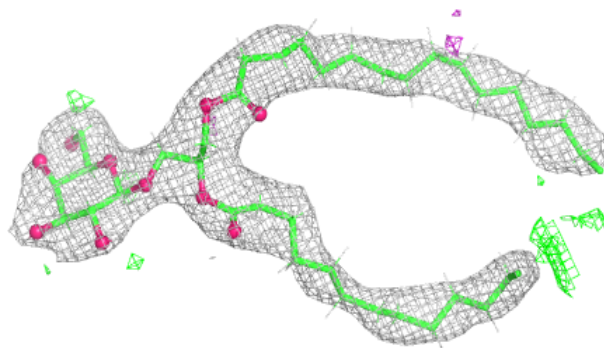
**Electron density around STE d 410:**

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

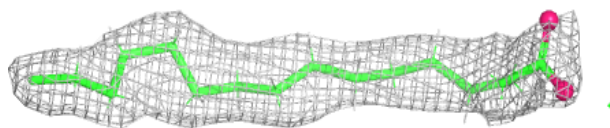
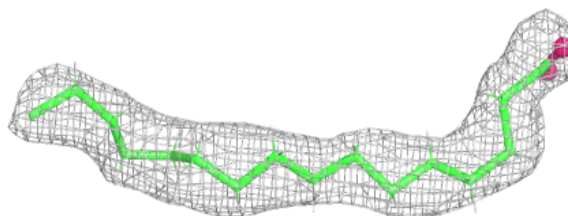


Electron density around LMG A 410:

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

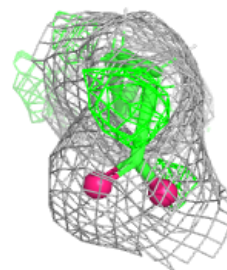
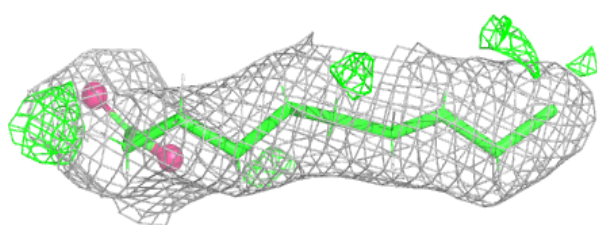
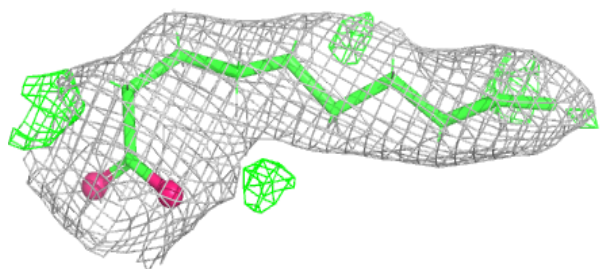
**Electron density around STE B 625:**

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

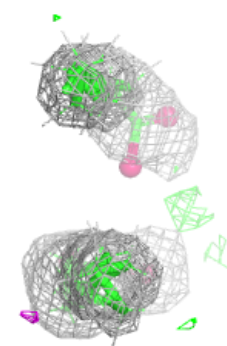
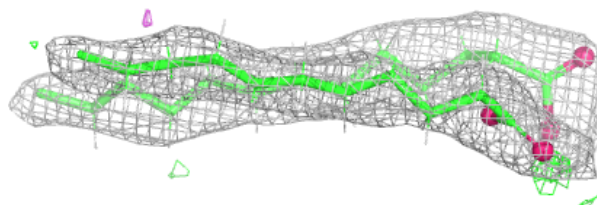
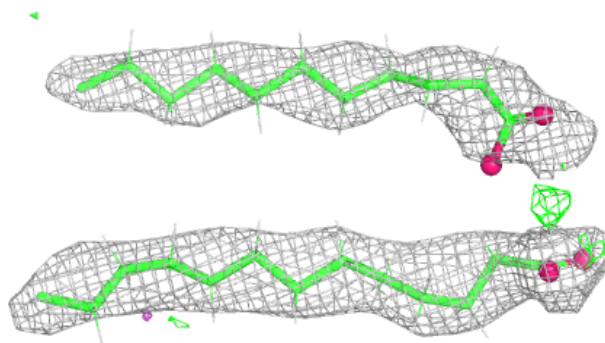


Electron density around STE B 624:

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

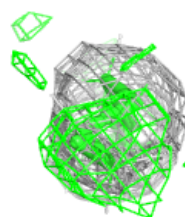
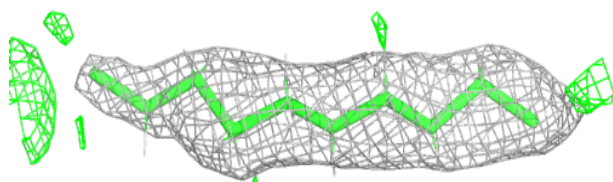
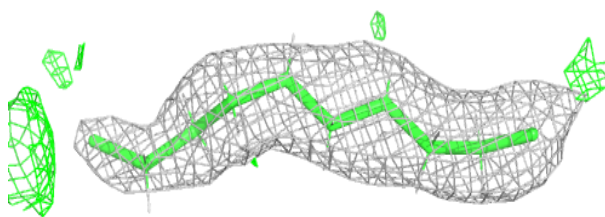
**Electron density around LMG D 411:**

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

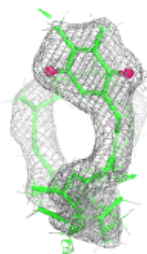
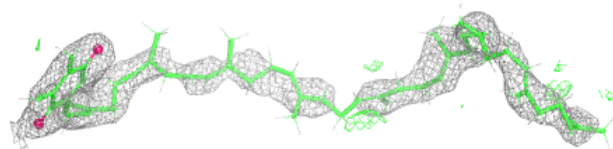
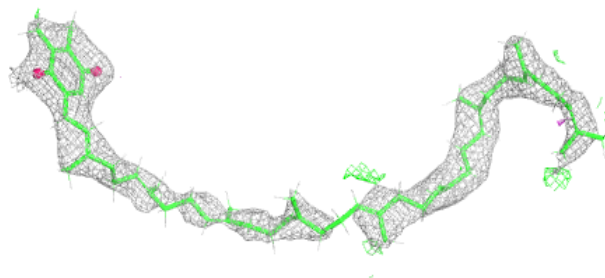


Electron density around STE M 103:

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

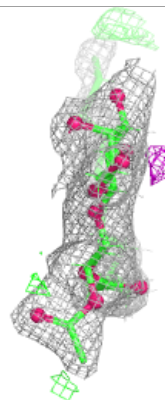
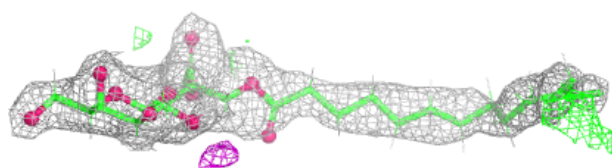
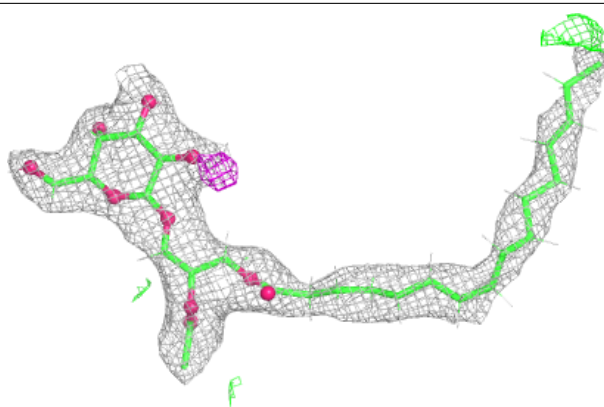
**Electron density around PL9 a 410:**

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

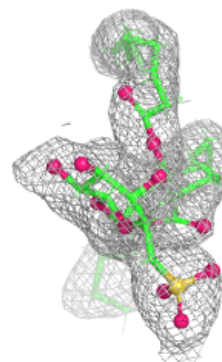
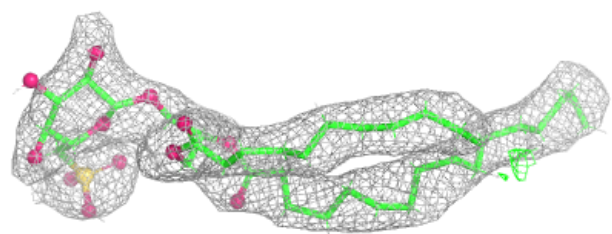
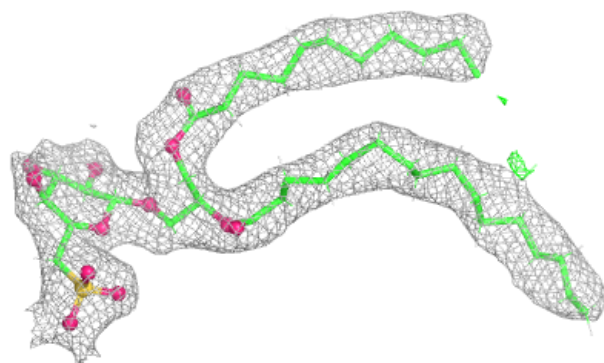


Electron density around LMG c 518:

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

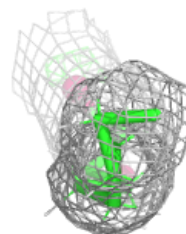
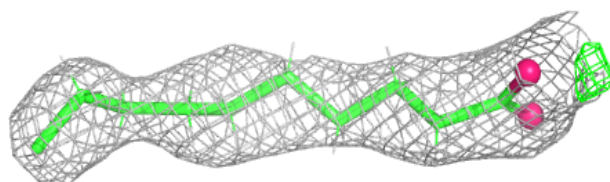
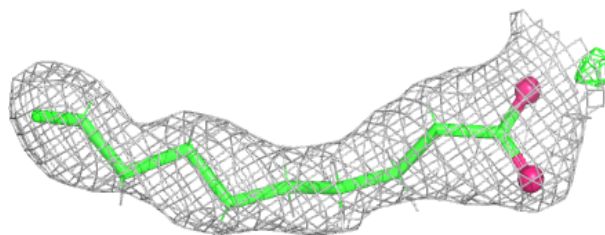
**Electron density around SQD L 101:**

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

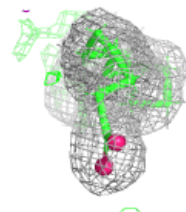
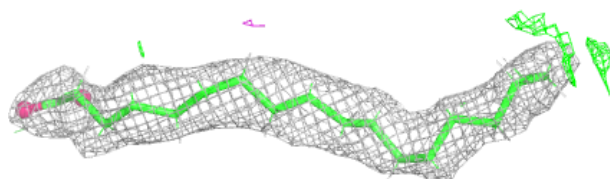
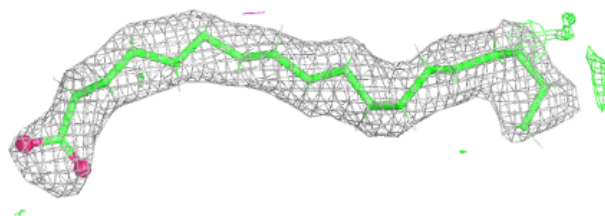


Electron density around STE C 519:

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

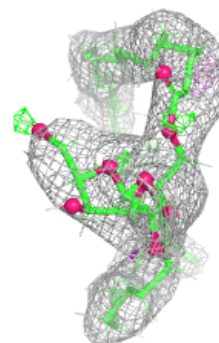
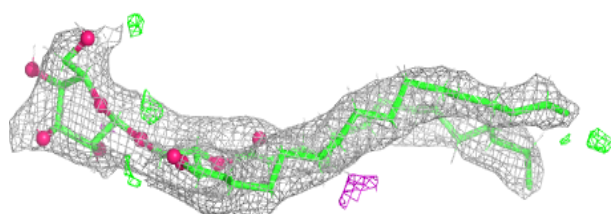
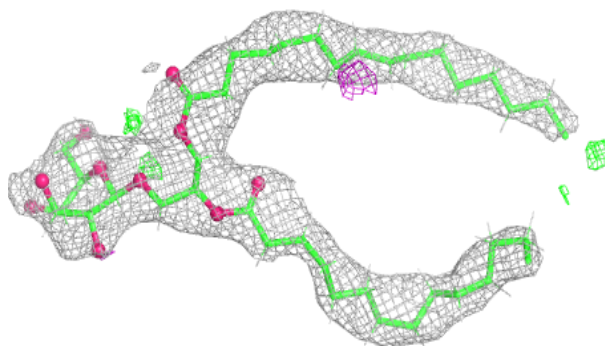
**Electron density around STE b 621:**

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

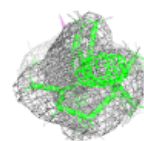
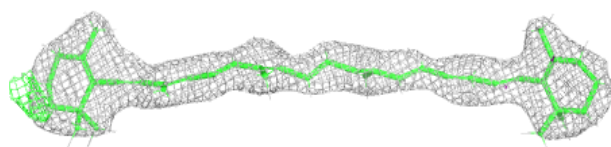


Electron density around LMG a 414:

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

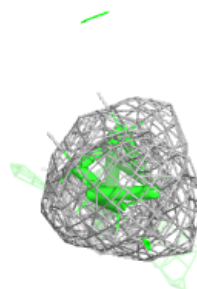
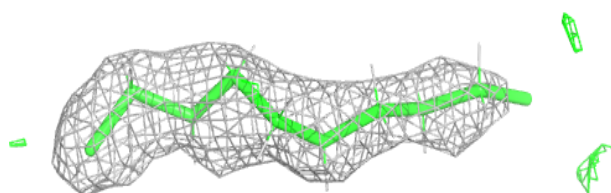
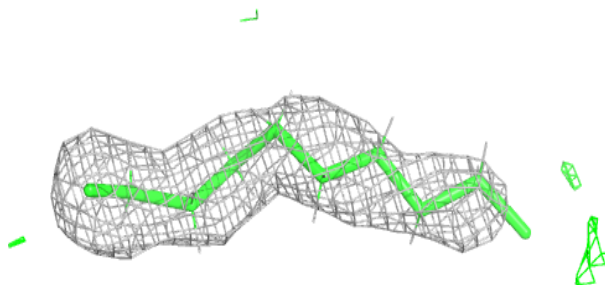
**Electron density around BCR k 101:**

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

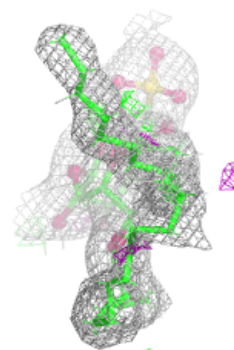
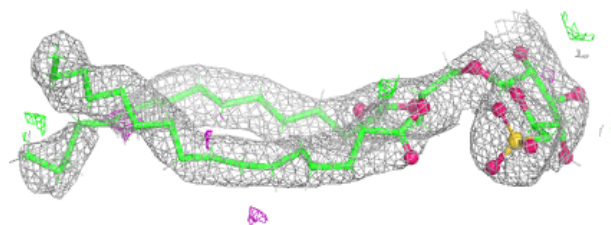
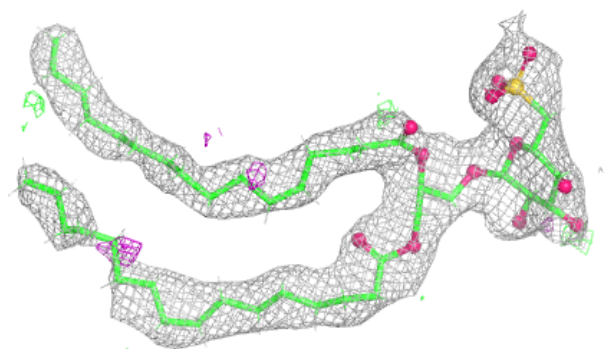


Electron density around STE t 103:

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

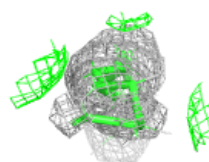
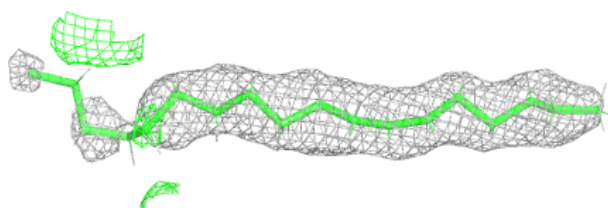
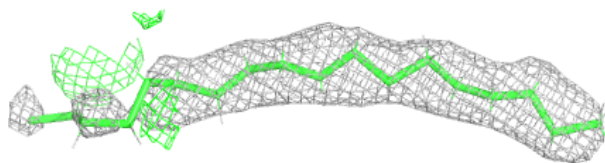
**Electron density around SQD B 622:**

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

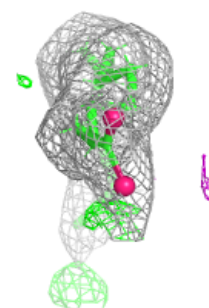
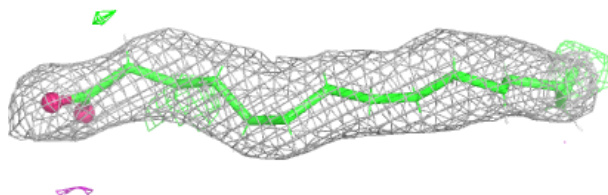
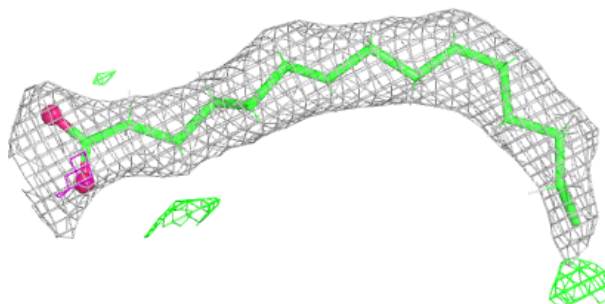


Electron density around STE I 102:

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

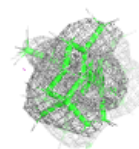
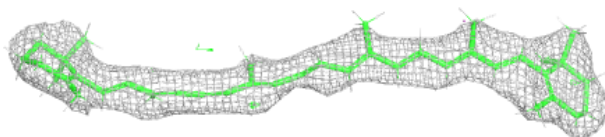
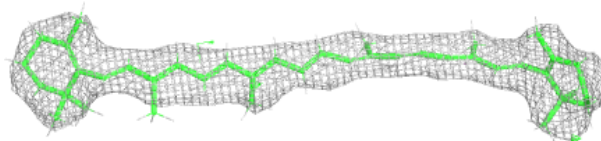
**Electron density around STE B 620:**

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

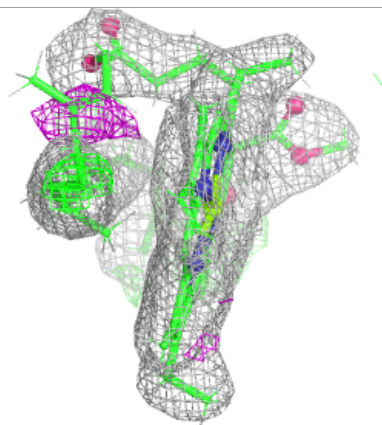
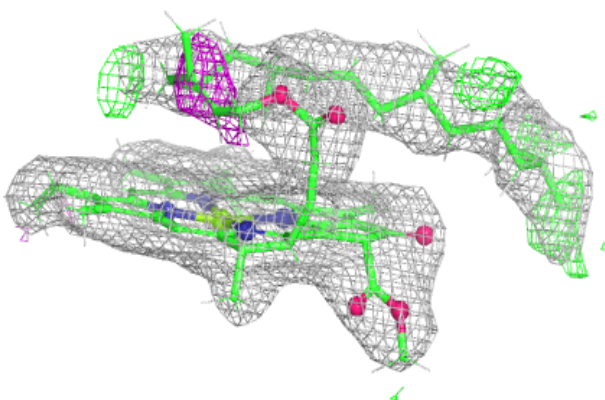
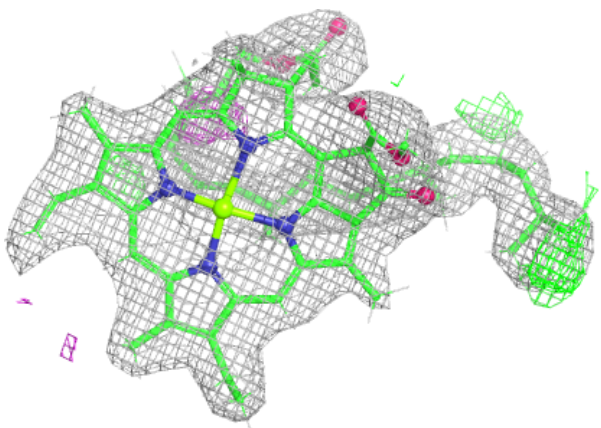


Electron density around BCR Z 101:

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

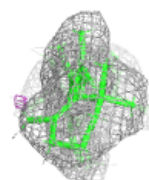
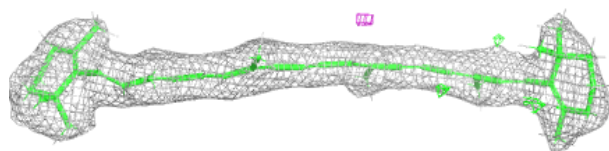
**Electron density around CLA B 601:**

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

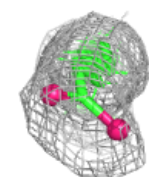
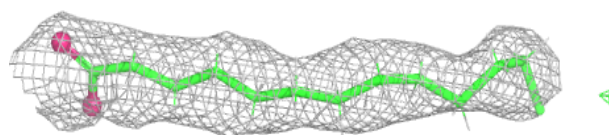
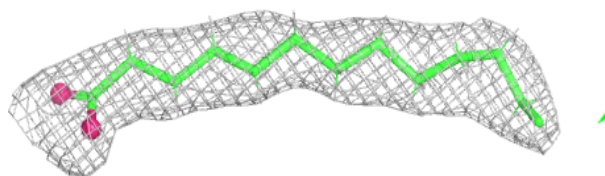


Electron density around BCR K 101:

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

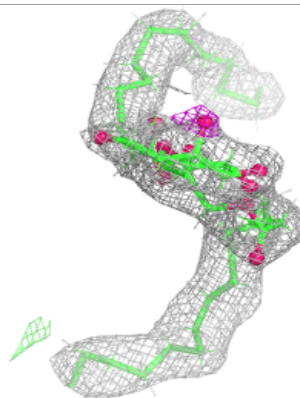
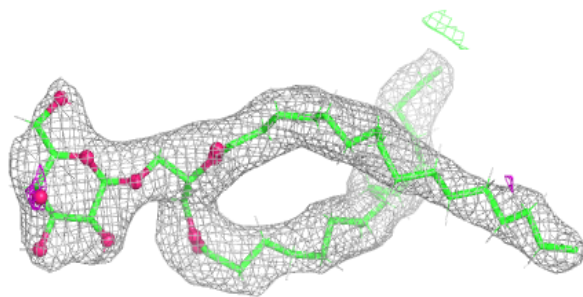
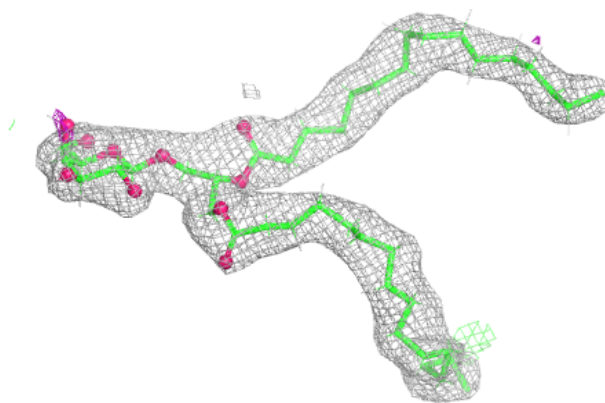
**Electron density around STE M 102:**

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

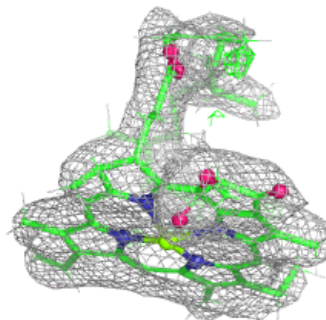
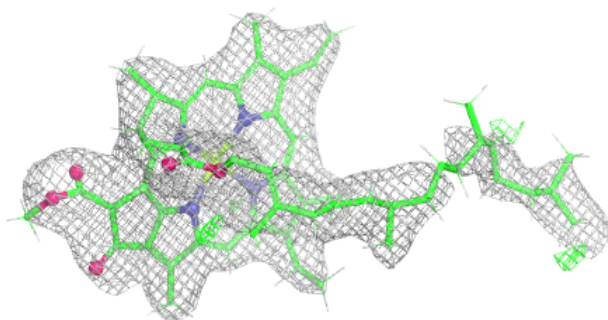
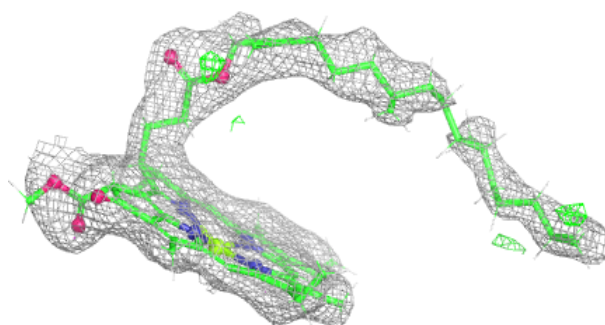


Electron density around LMG M 101:

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

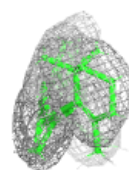
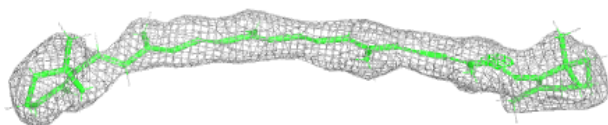
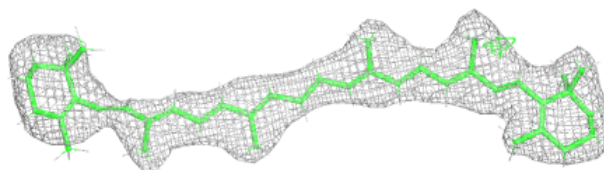
**Electron density around CLA C 513:**

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

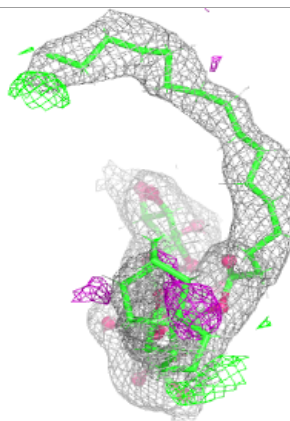
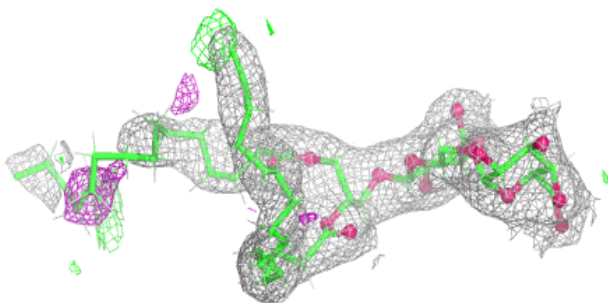
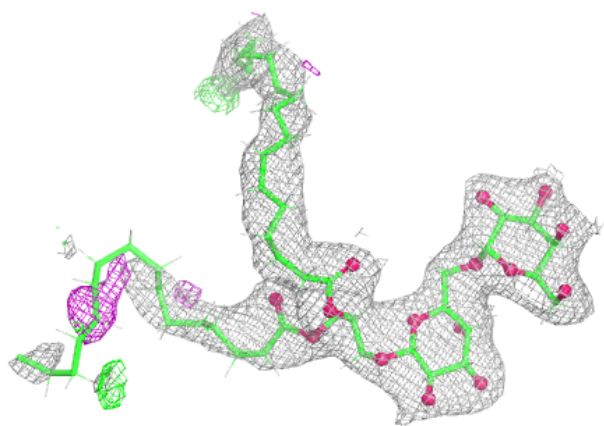


Electron density around BCR d 404:

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

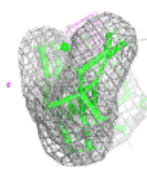
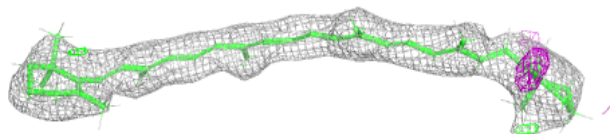
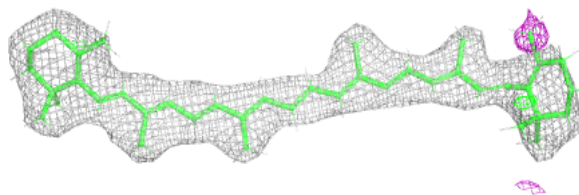
**Electron density around DGD C 516:**

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

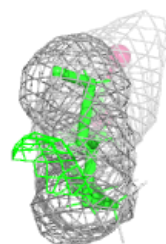
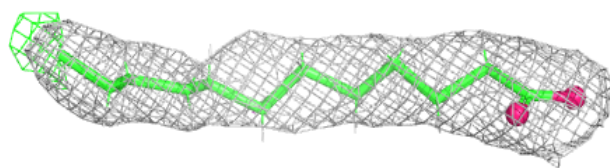
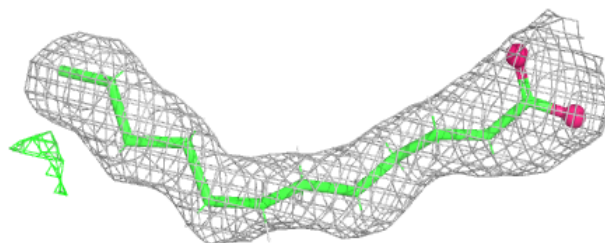


Electron density around BCR D 406:

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

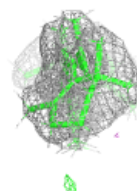
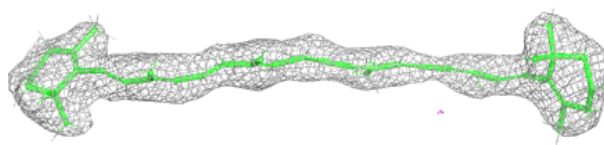
**Electron density around STE t 102:**

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



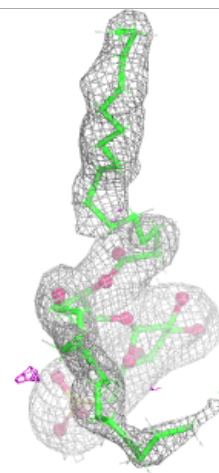
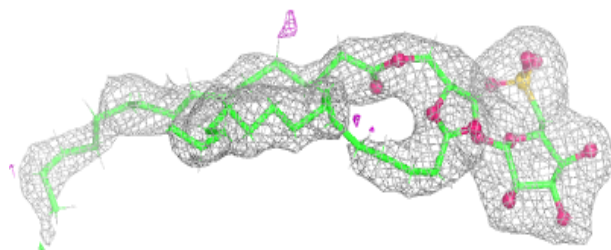
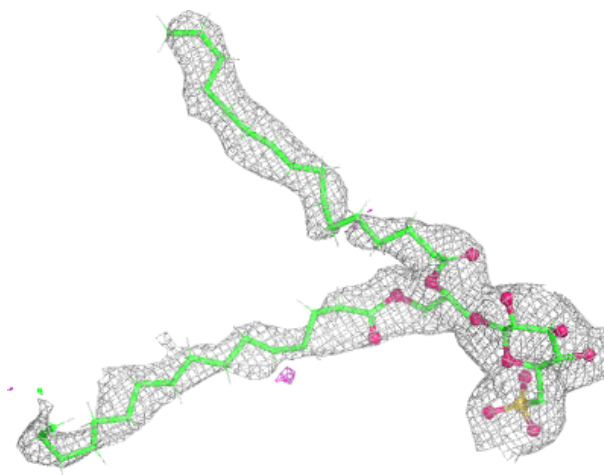
Electron density around BCR k 102:

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



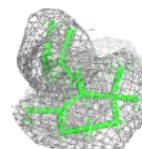
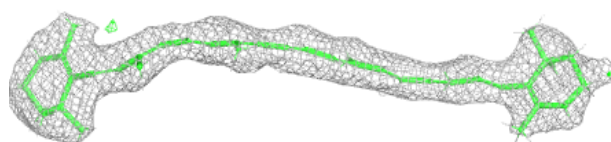
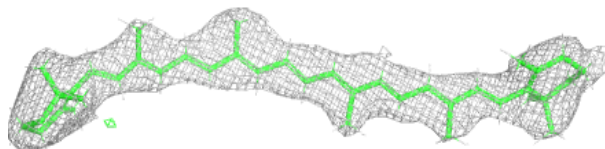
Electron density around SQD a 412:

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

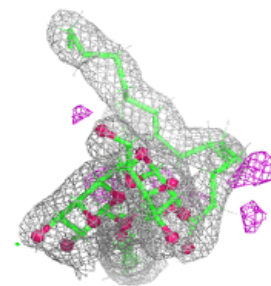
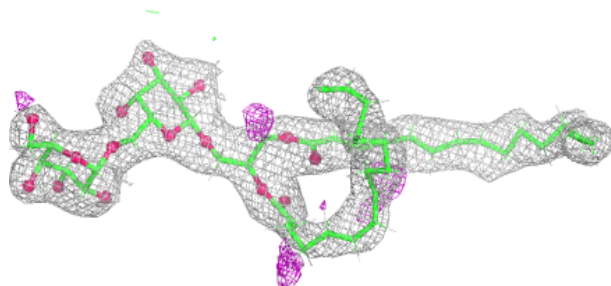
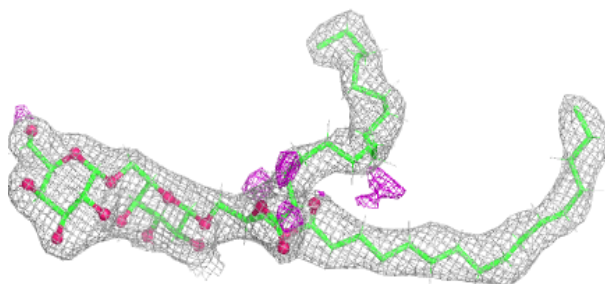


Electron density around BCR x 101:

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

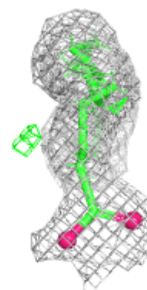
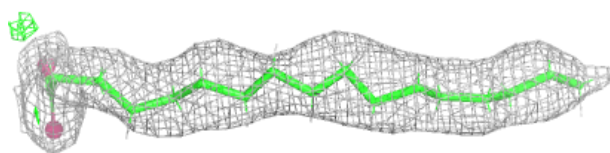
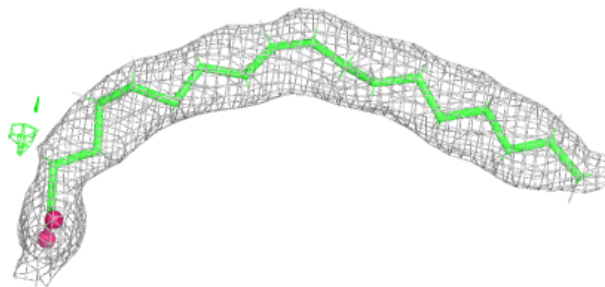
**Electron density around DGD h 101:**

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

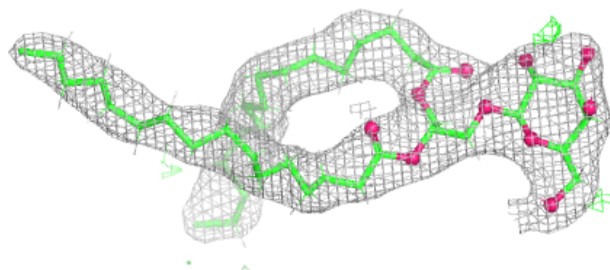
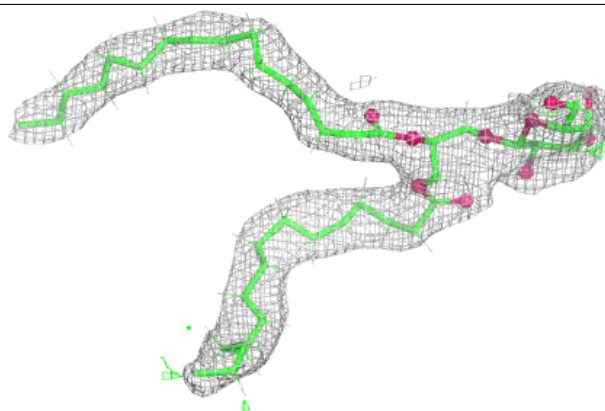


Electron density around STE D 412:

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

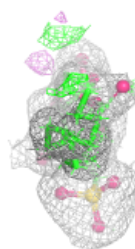
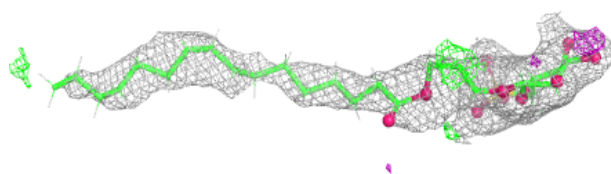
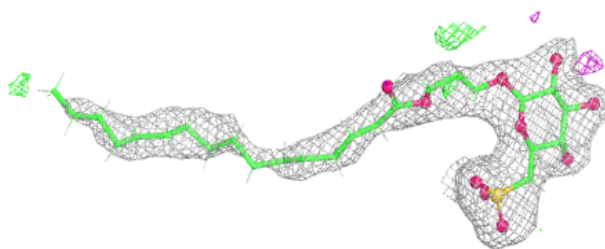
**Electron density around LMG m 101:**

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

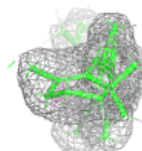
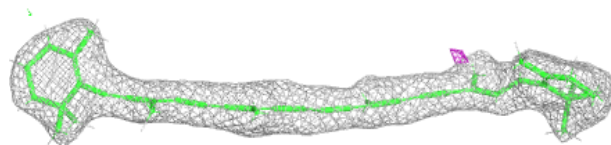


Electron density around SQD F 102:

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

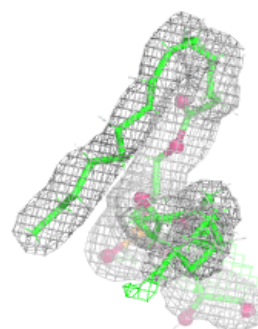
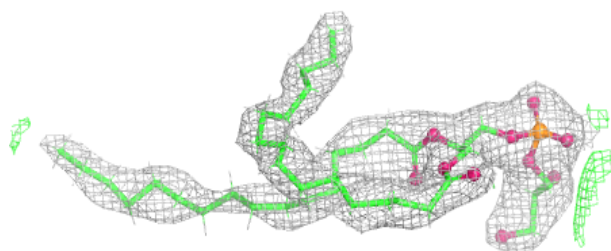
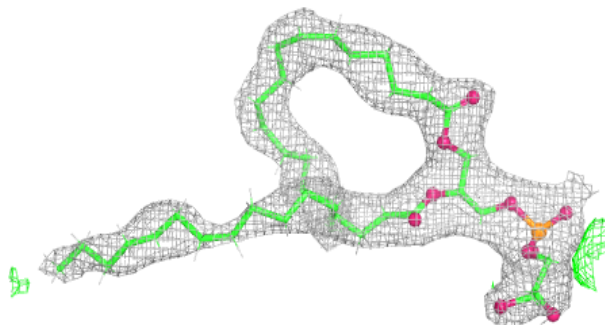
**Electron density around BCR b 617:**

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

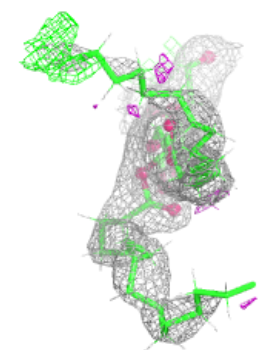
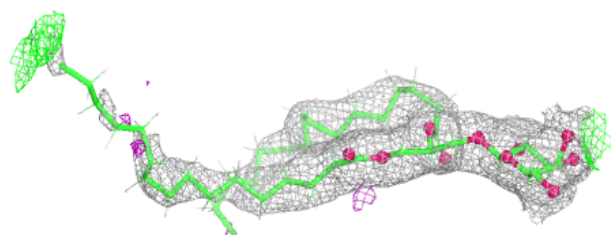
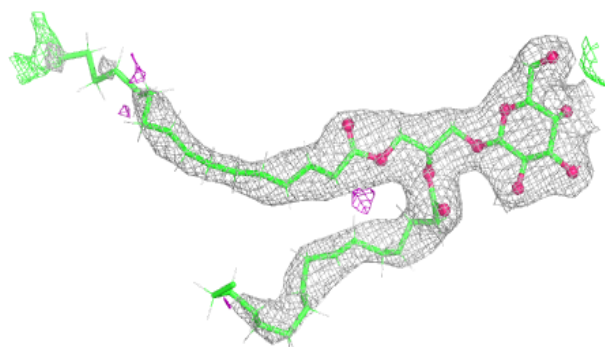


Electron density around LHG b 623:

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

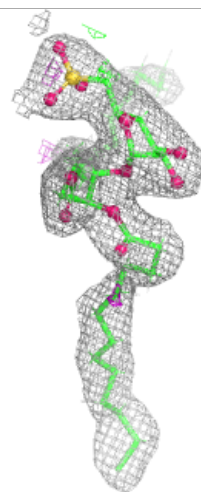
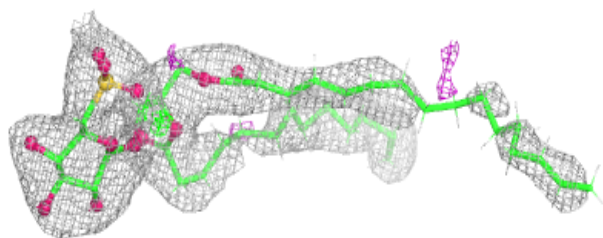
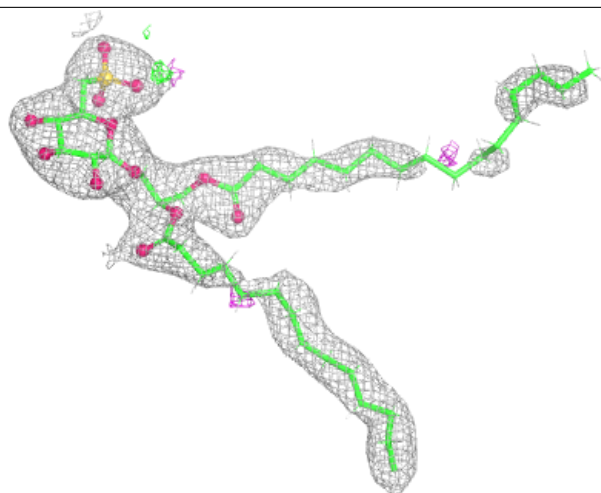
**Electron density around LMG D 408:**

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



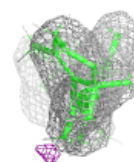
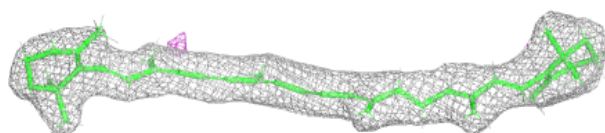
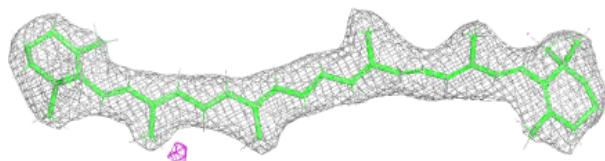
Electron density around SQD A 412:

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

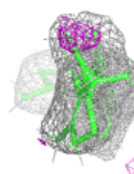
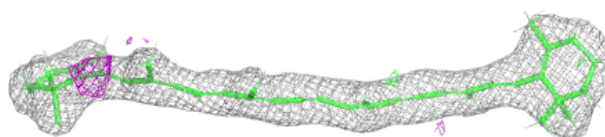
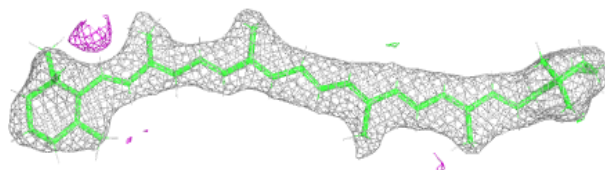


Electron density around BCR b 619:

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

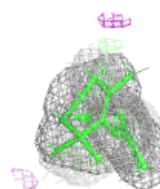
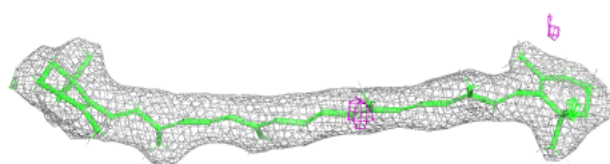
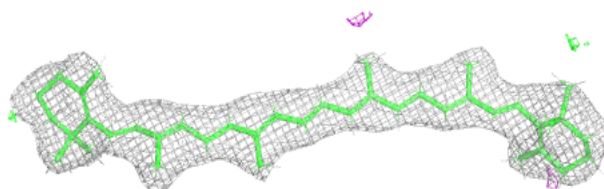
**Electron density around BCR B 617:**

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

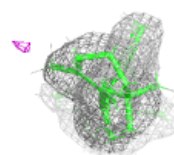
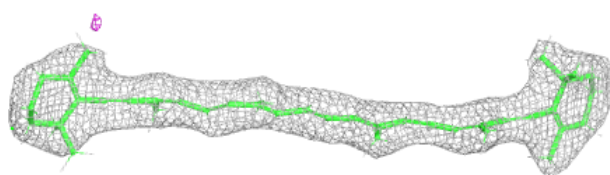
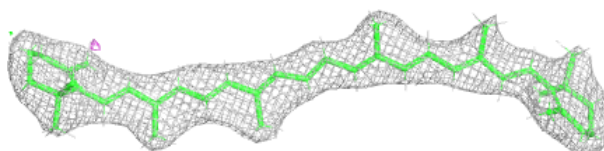


Electron density around BCR B 619:

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

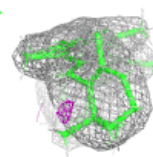
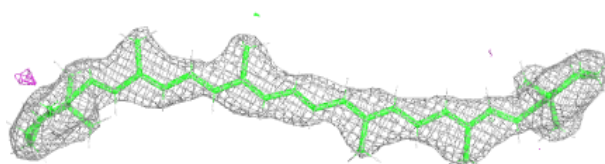
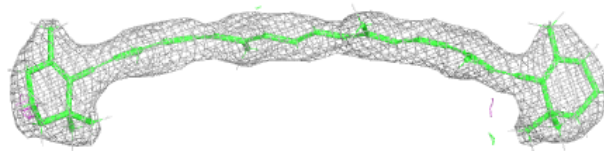
**Electron density around BCR C 514:**

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



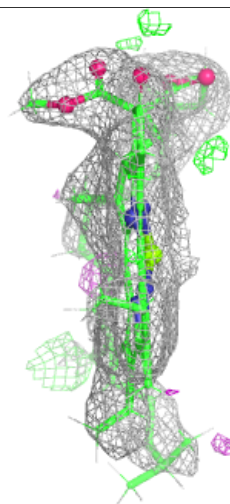
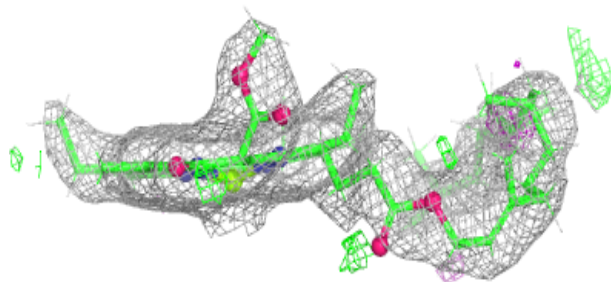
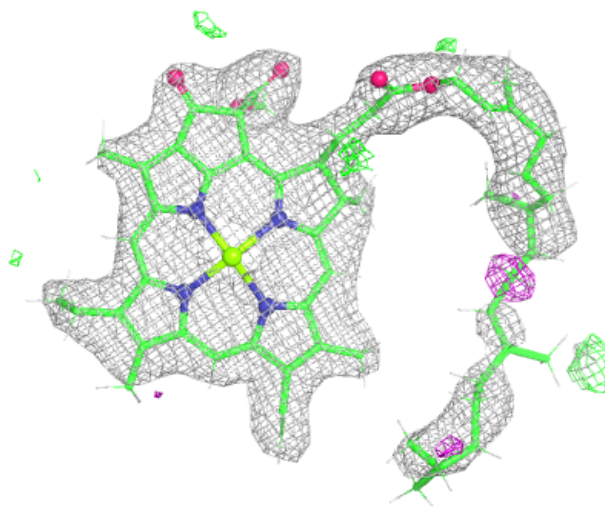
Electron density around BCR k 103:

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



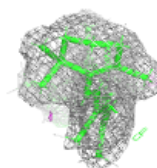
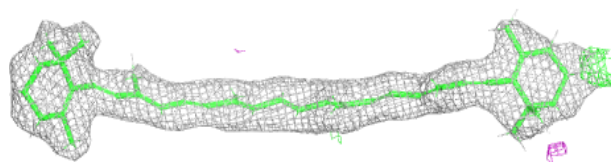
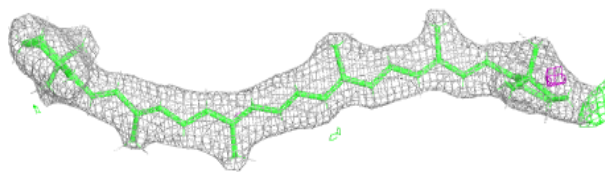
Electron density around CLA C 512:

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



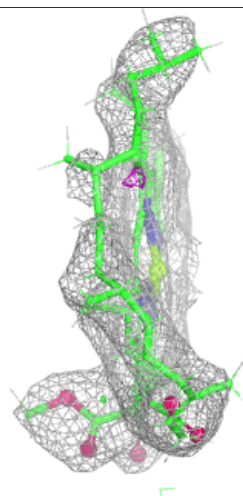
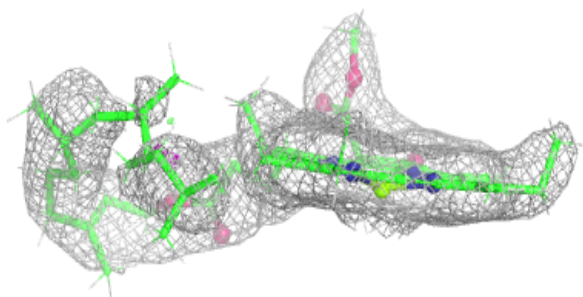
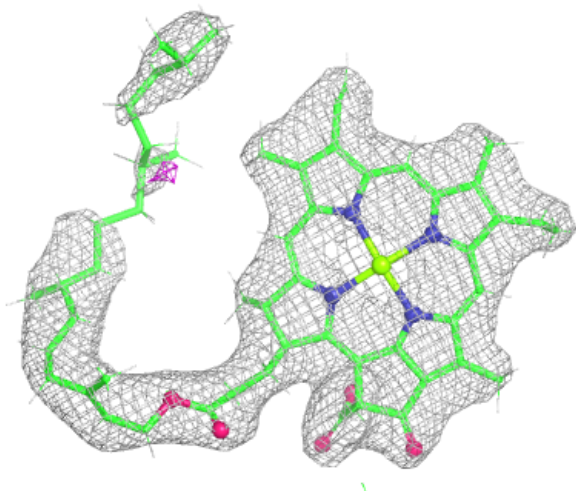
Electron density around BCR H 101:

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



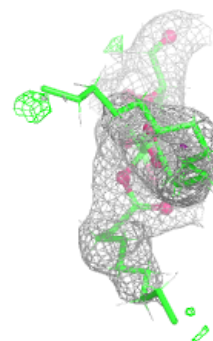
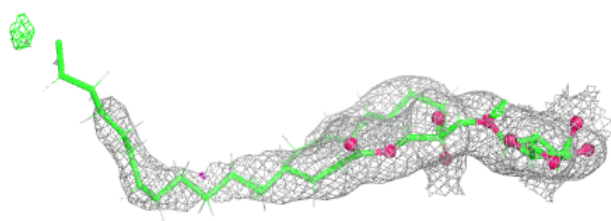
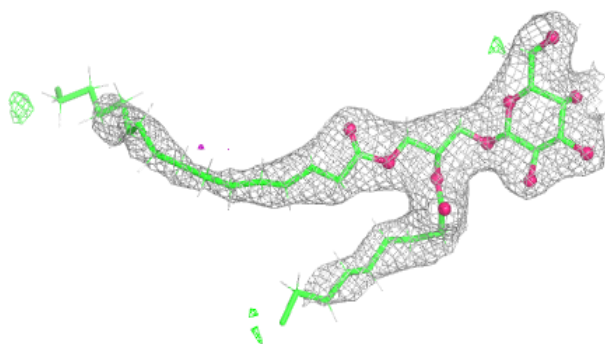
Electron density around CLA c 512:

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

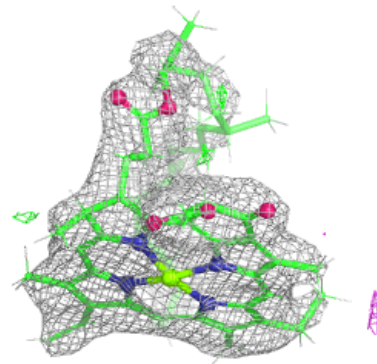
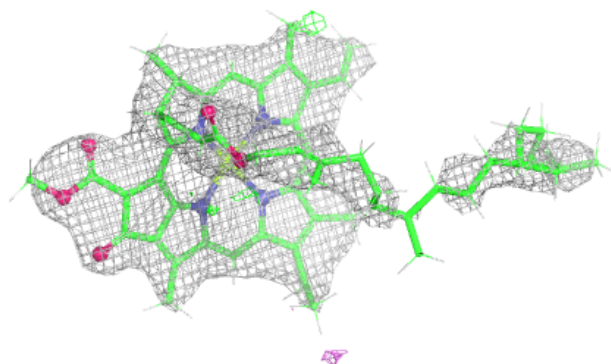
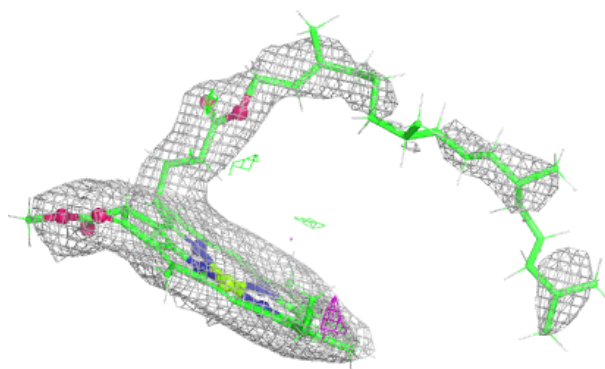


Electron density around LMG d 409:

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

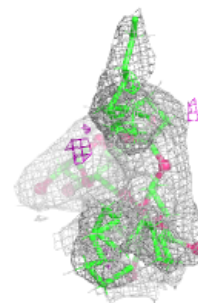
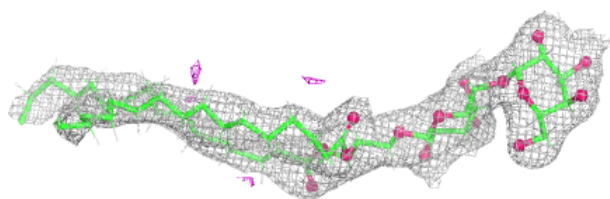
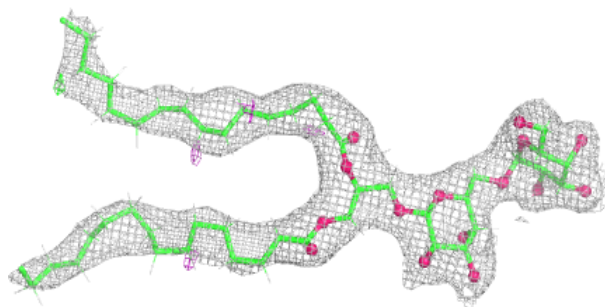
**Electron density around CLA c 513:**

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

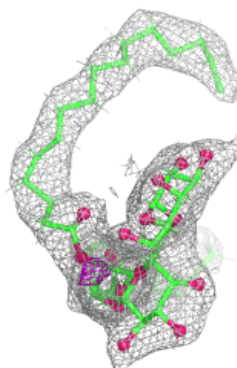
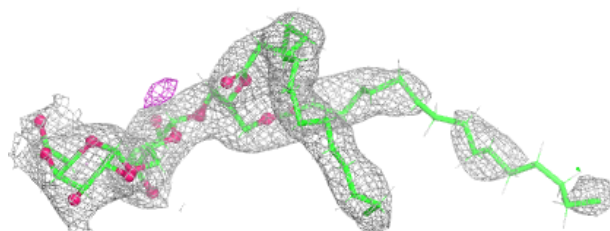
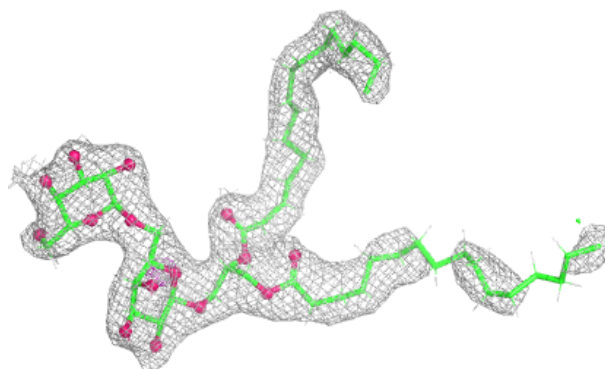


Electron density around DGD C 517:

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

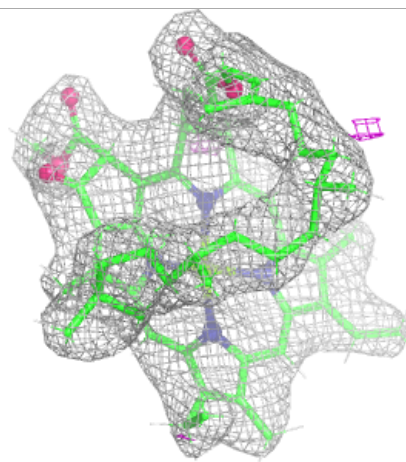
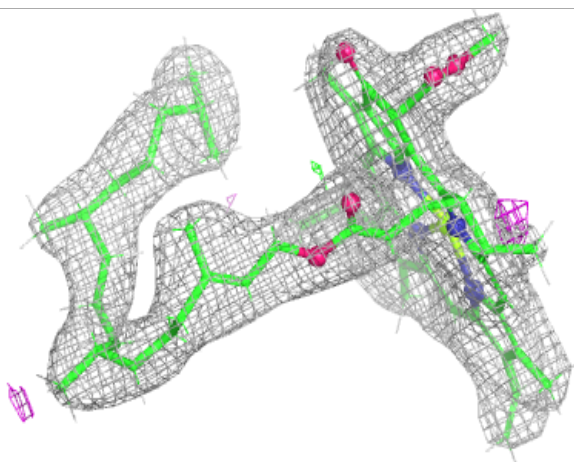
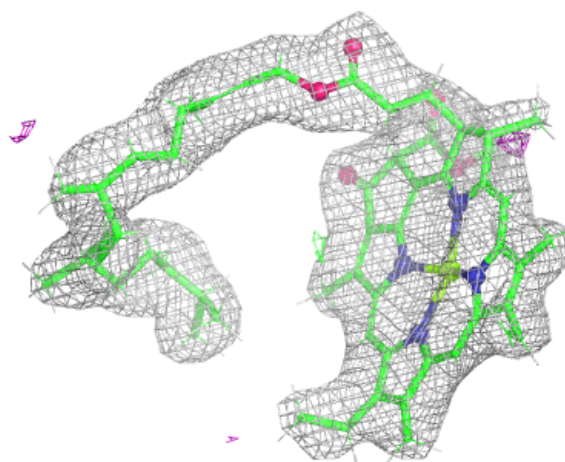
**Electron density around DGD c 516:**

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



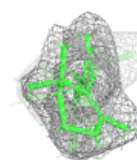
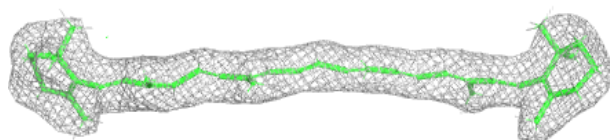
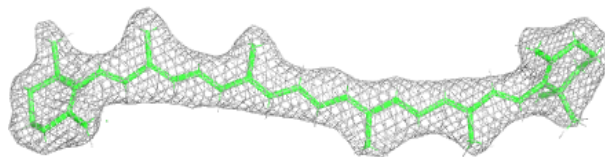
Electron density around CLA c 503:

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

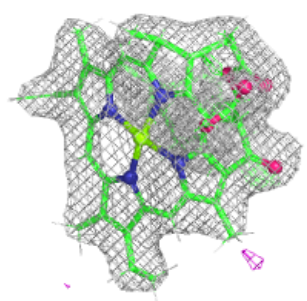
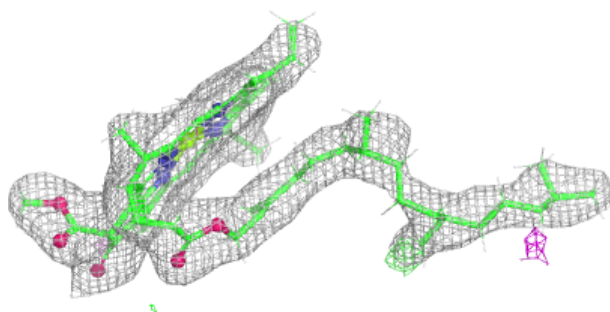
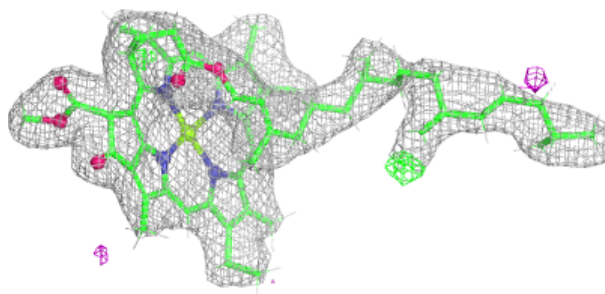


Electron density around BCR B 618:

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

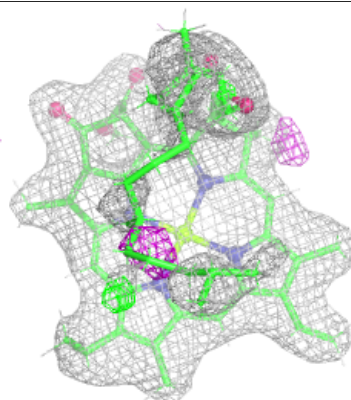
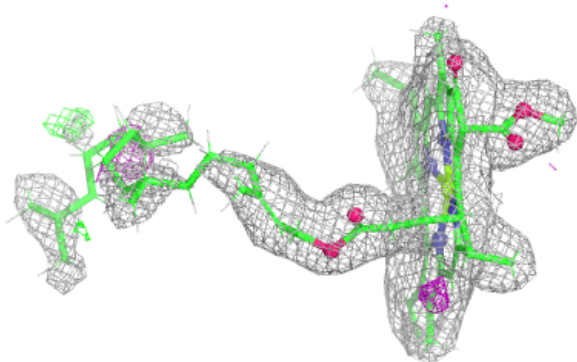
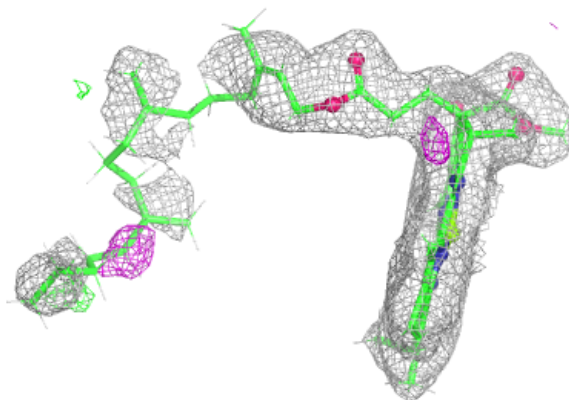
**Electron density around CLA c 505:**

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



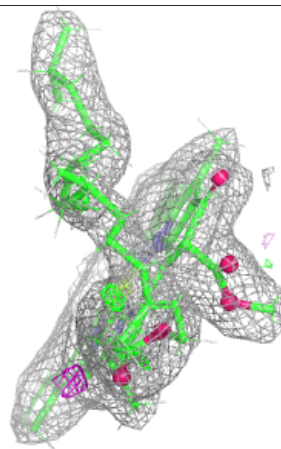
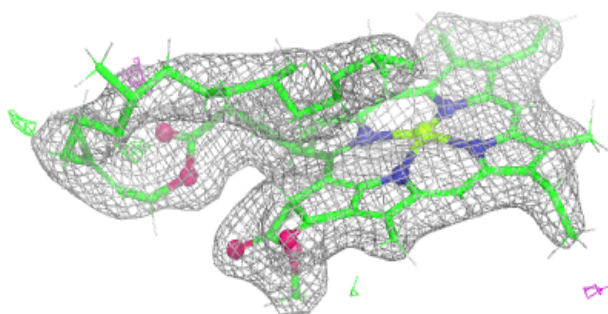
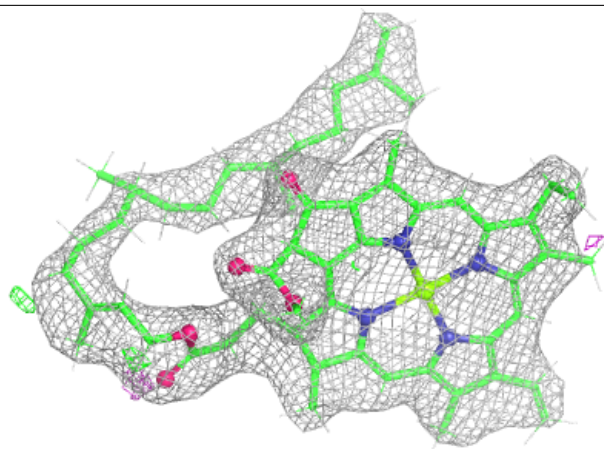
Electron density around CLA c 506:

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

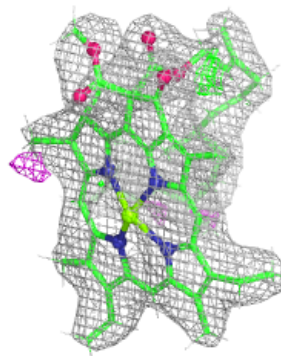
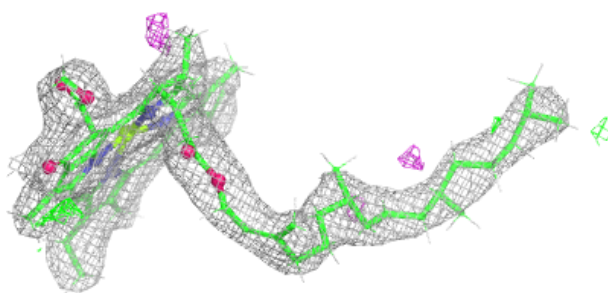
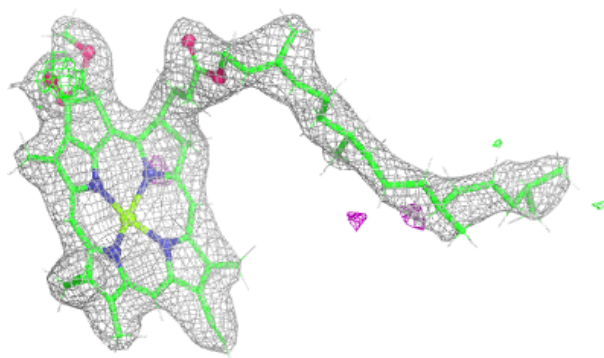


Electron density around CLA c 509:

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

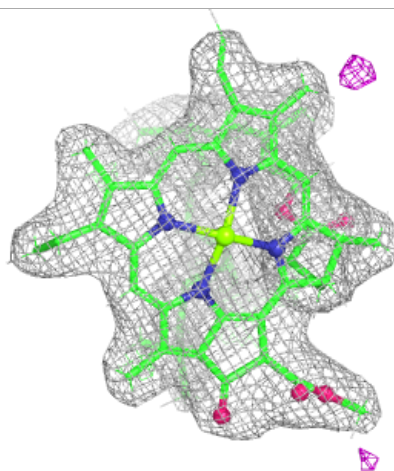
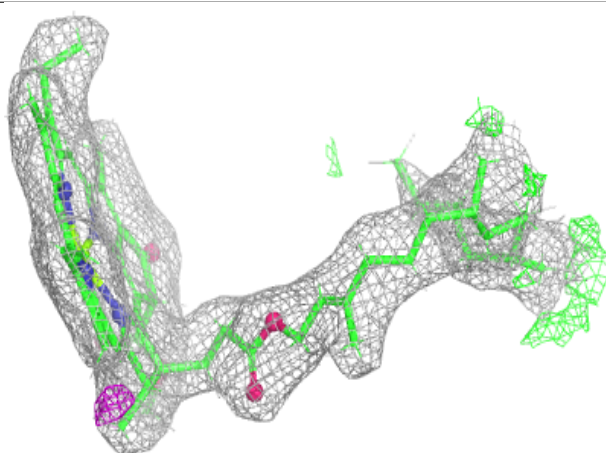
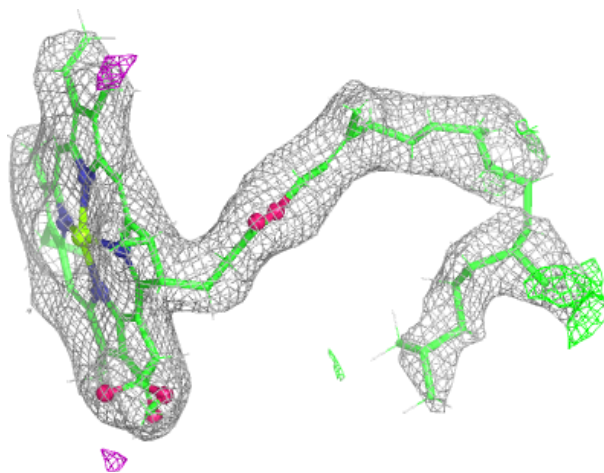
**Electron density around CLA c 511:**

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



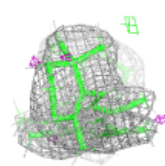
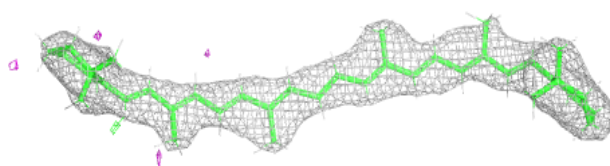
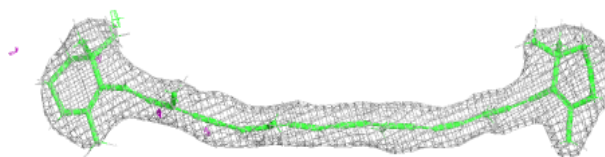
Electron density around CLA B 606:

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

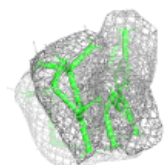
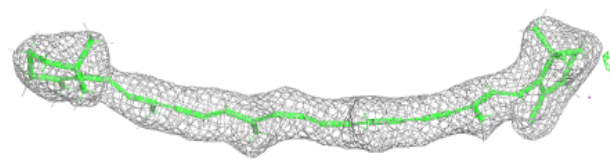
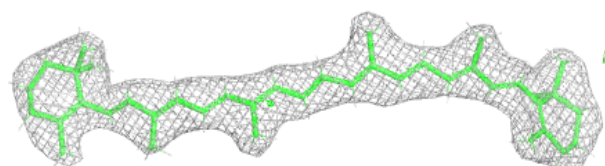


Electron density around BCR K 102:

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

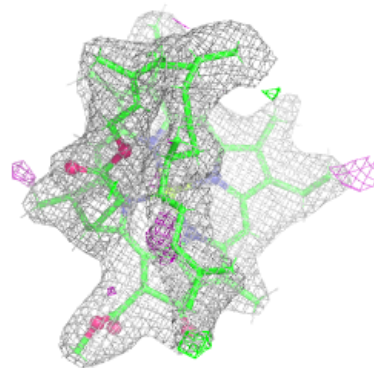
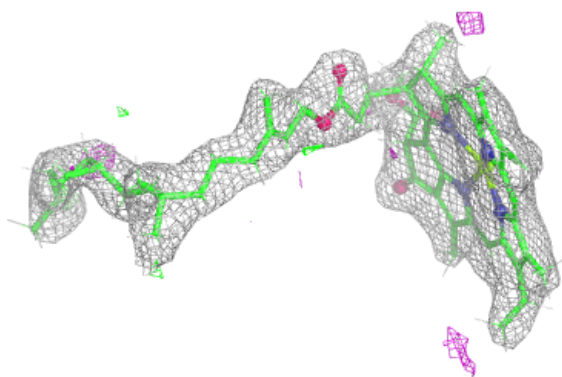
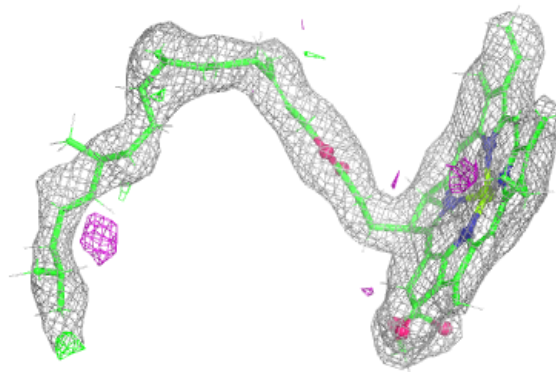
**Electron density around BCR T 101:**

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

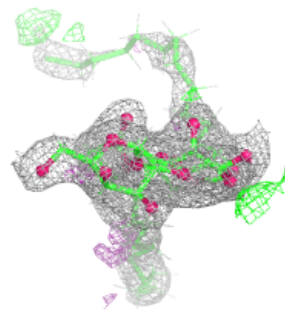
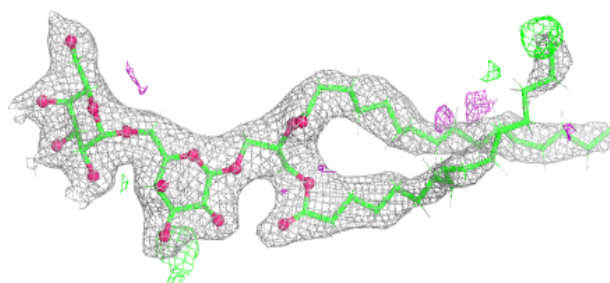
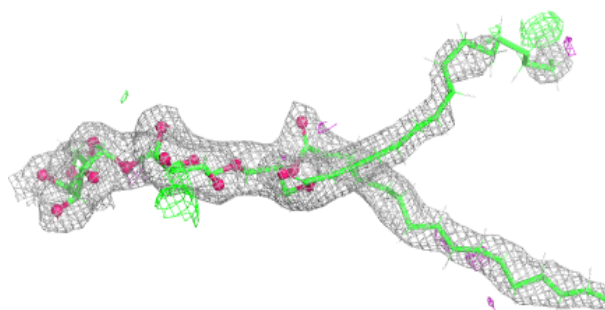


Electron density around CLA b 606:

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

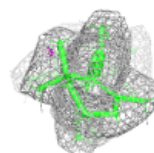
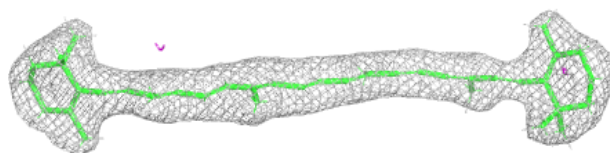
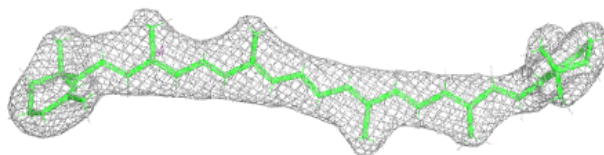
**Electron density around DGD C 515:**

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

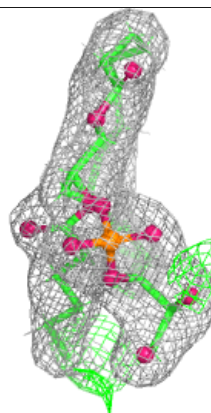
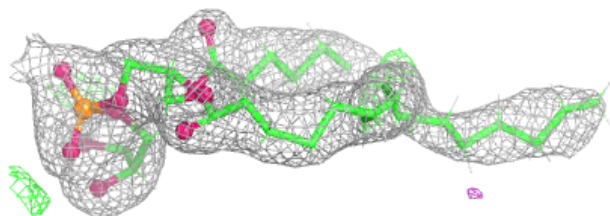
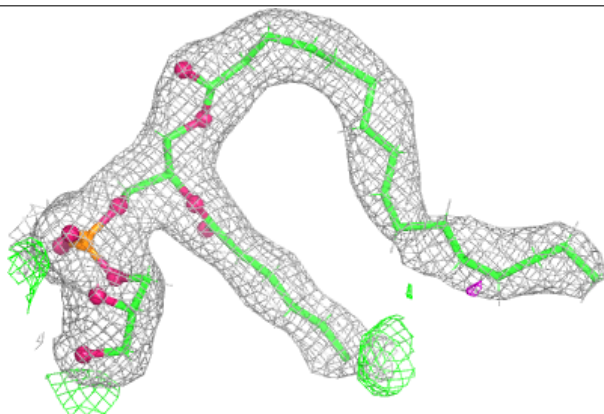


Electron density around BCR A 406:

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

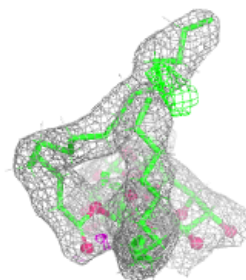
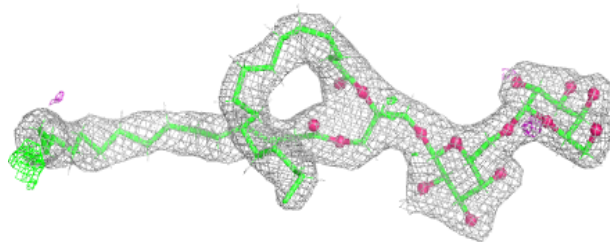
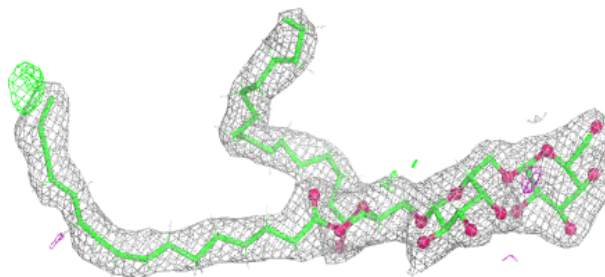
**Electron density around LHG d 407:**

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

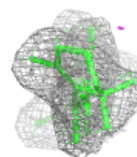
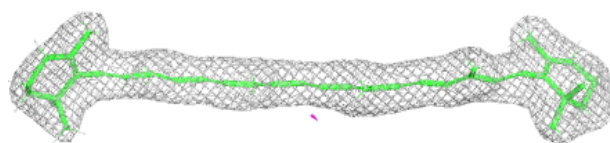
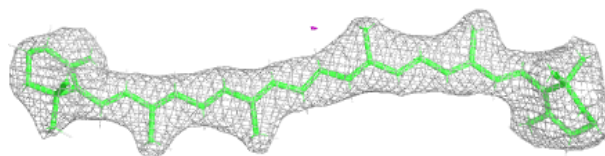


Electron density around DGD H 102:

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

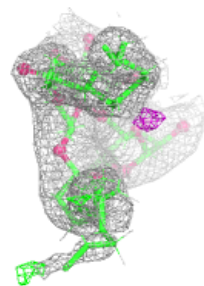
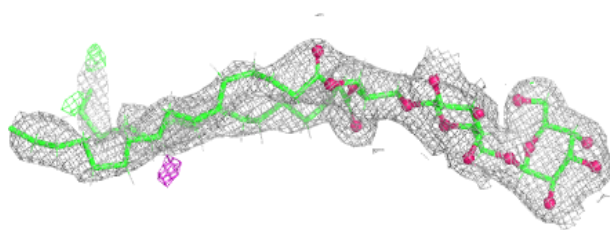
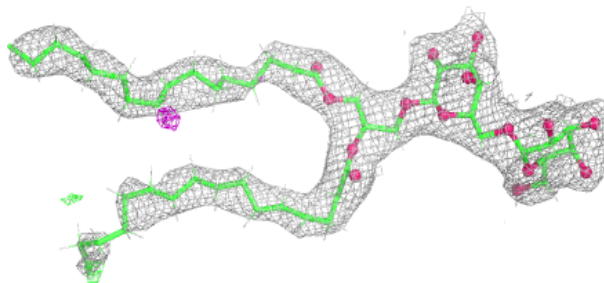
**Electron density around BCR b 618:**

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



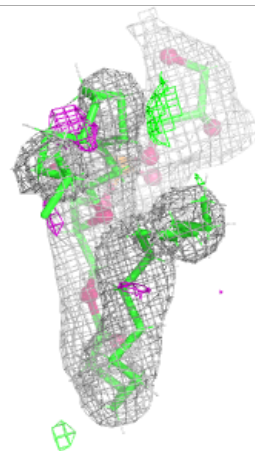
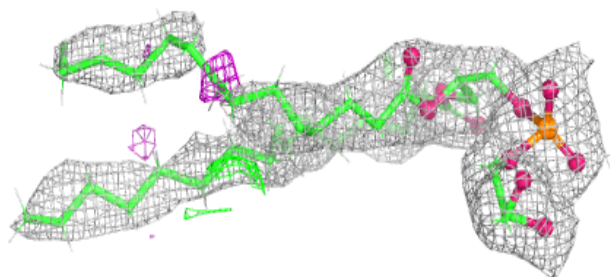
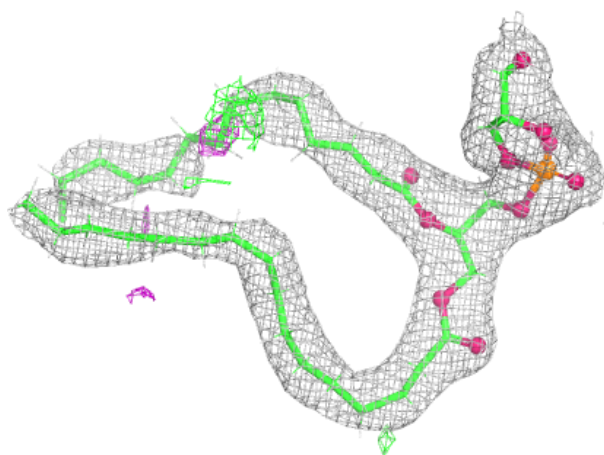
Electron density around DGD c 517:

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



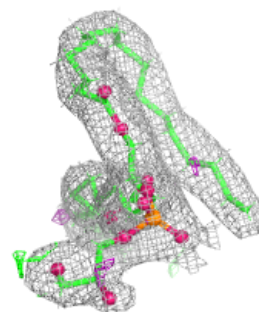
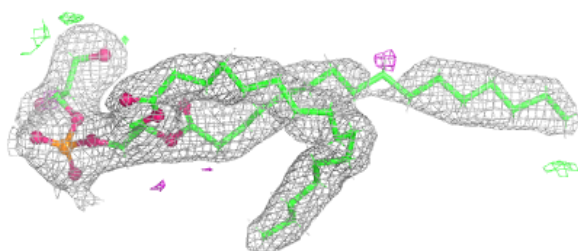
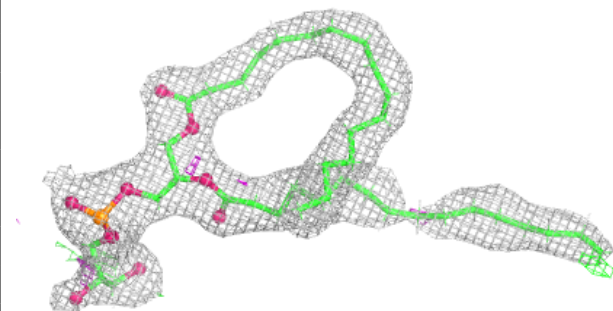
Electron density around LHG A 411:

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

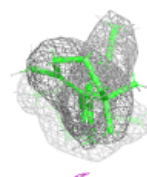
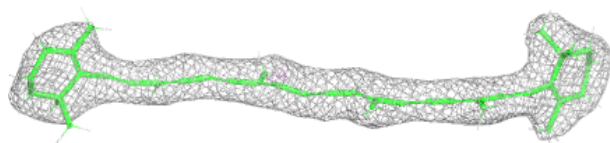
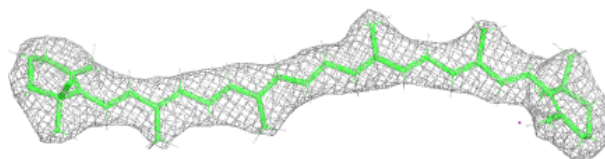


Electron density around LHG B 621:

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

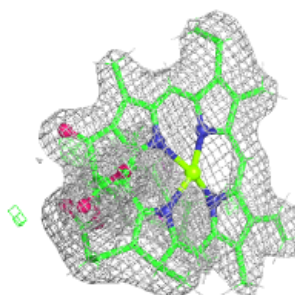
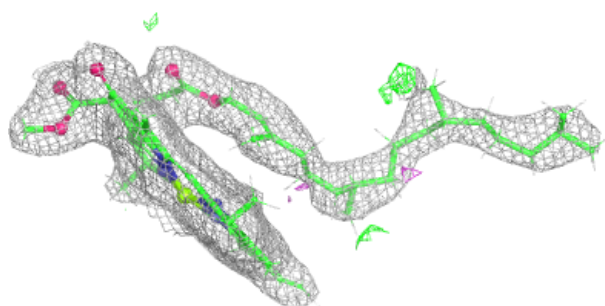
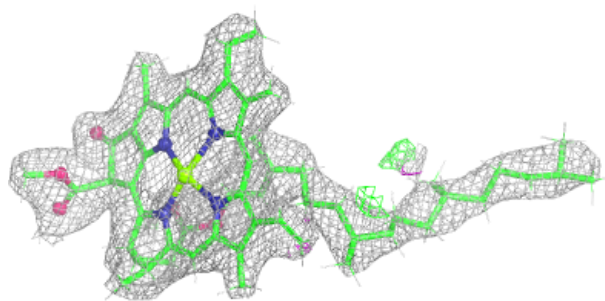
**Electron density around BCR c 514:**

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

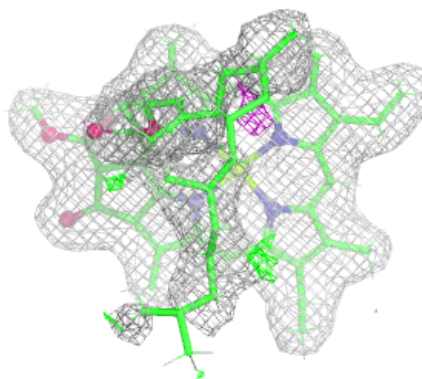
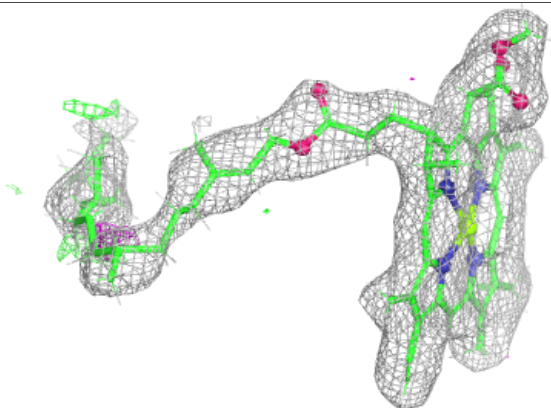
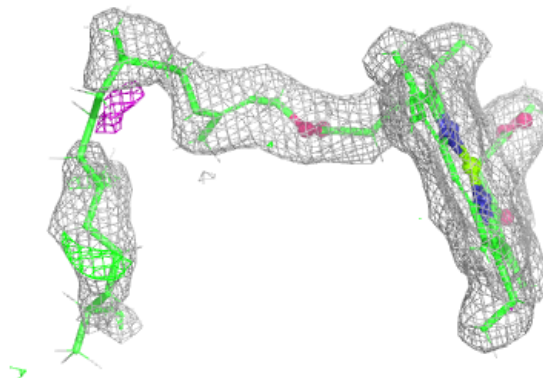


Electron density around CLA C 505:

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

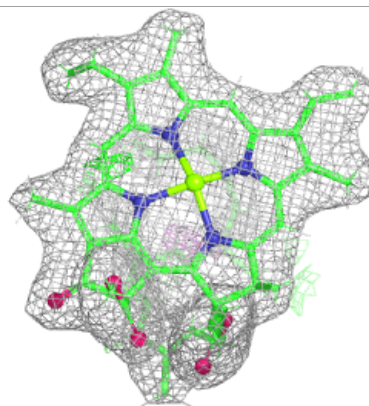
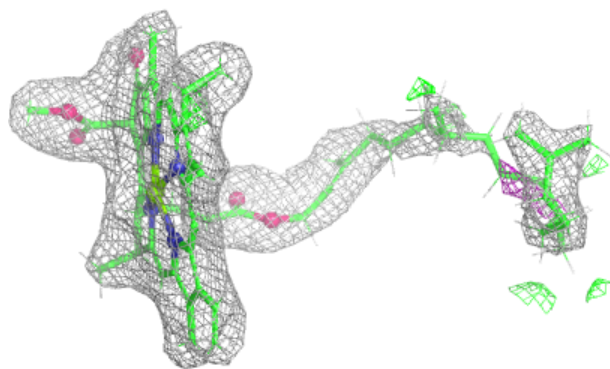
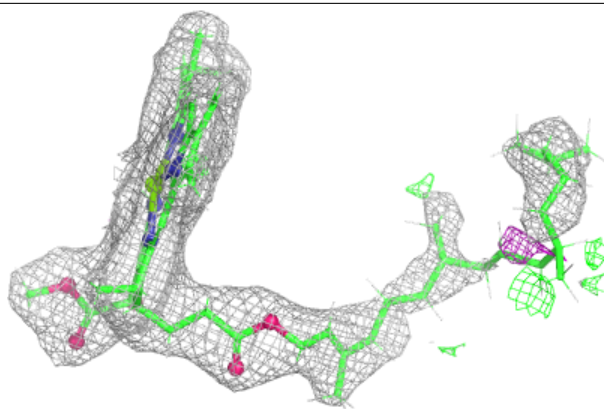
**Electron density around CLA a 405:**

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



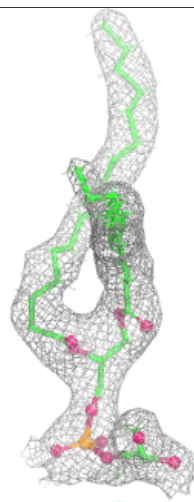
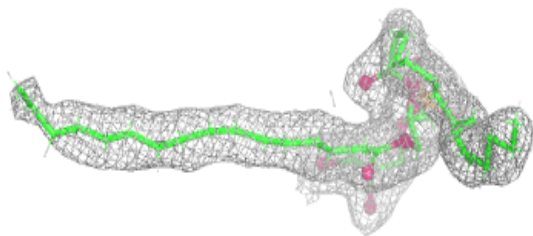
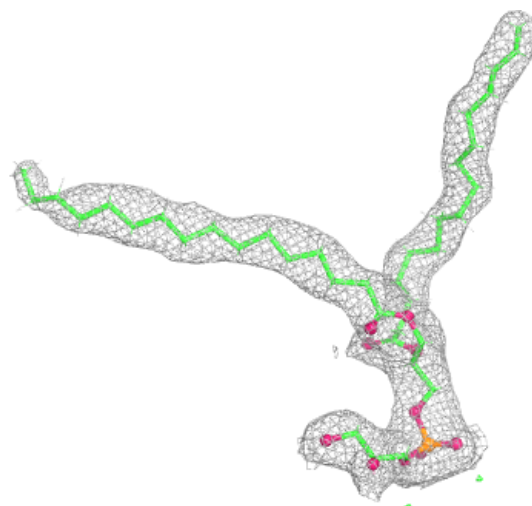
Electron density around CLA C 506:

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



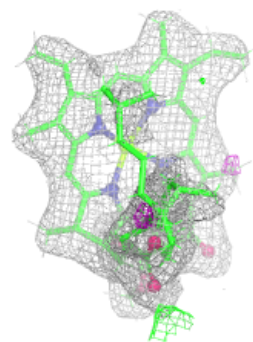
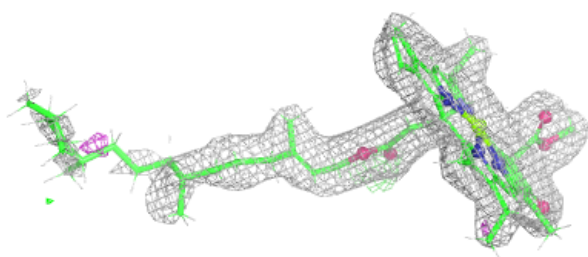
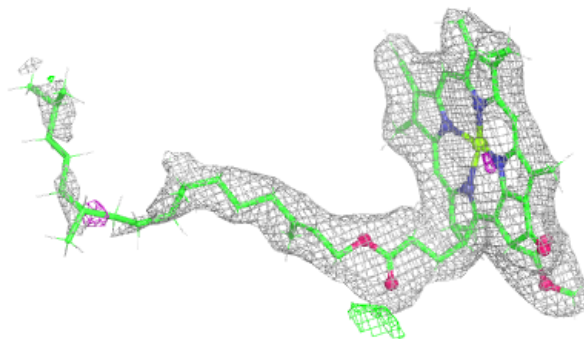
Electron density around LHG 1 101:

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

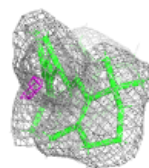
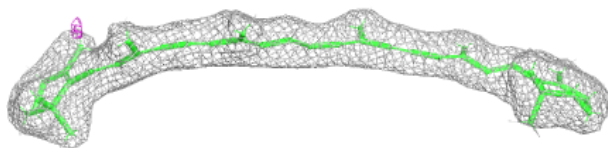
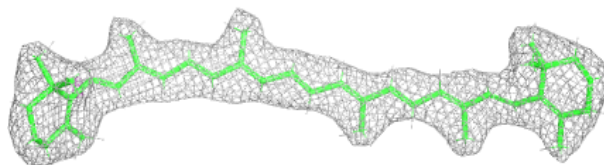


Electron density around CLA d 403:

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

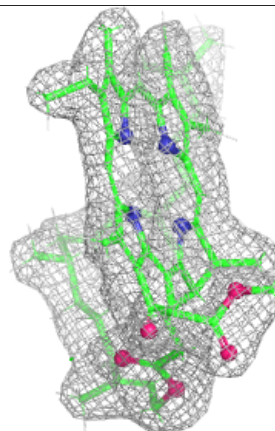
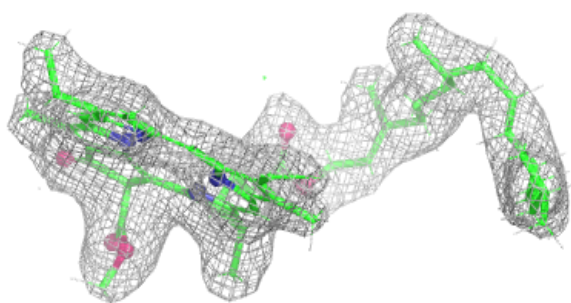
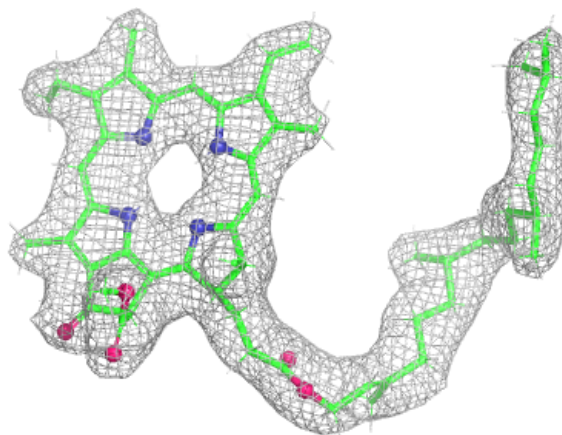
**Electron density around BCR t 101:**

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

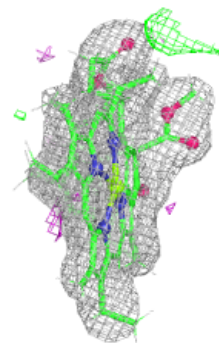
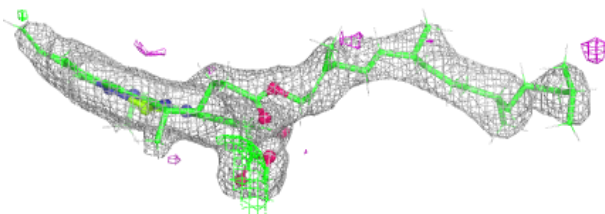
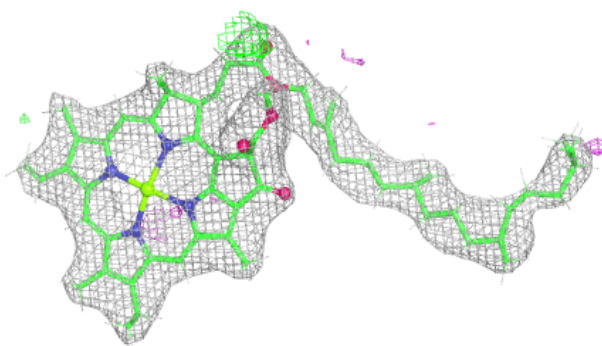


Electron density around PHO d 401:

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

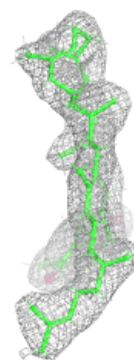
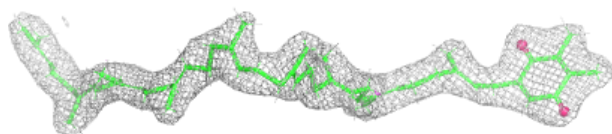
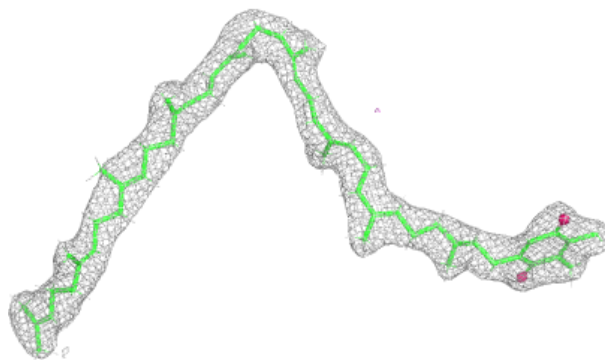
**Electron density around CLA b 602:**

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

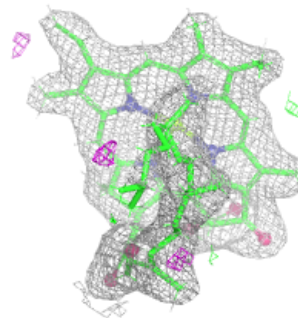
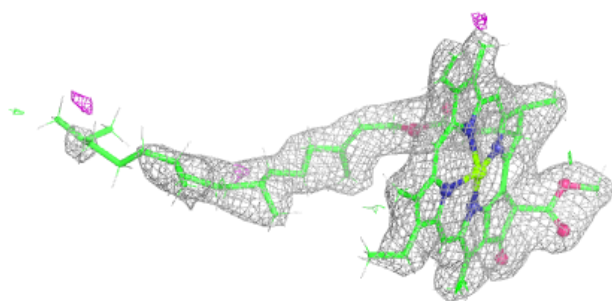
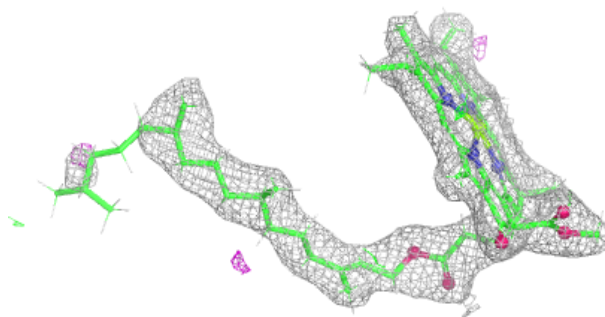


Electron density around PL9 D 407:

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

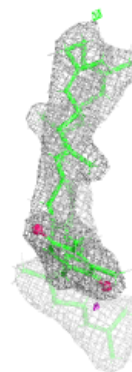
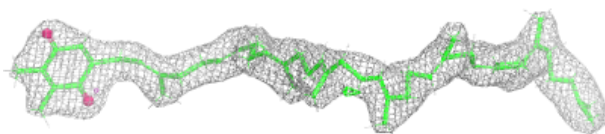
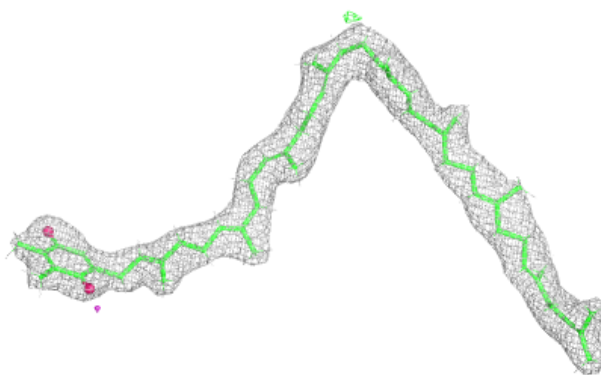
**Electron density around CLA C 508:**

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

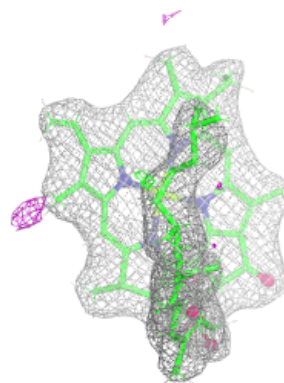
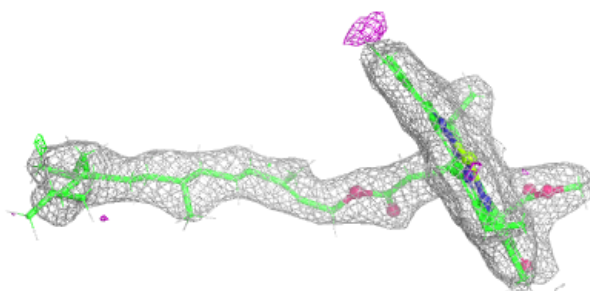
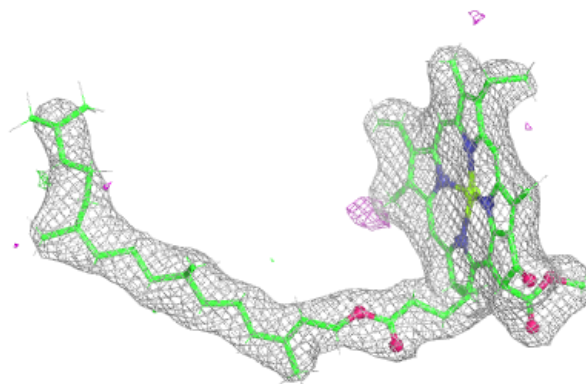


Electron density around PL9 d 405:

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

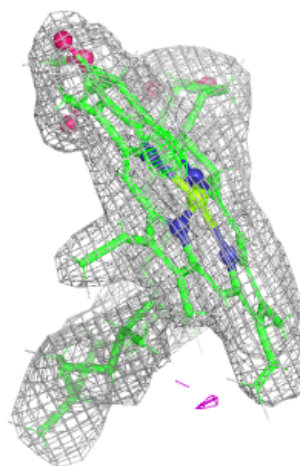
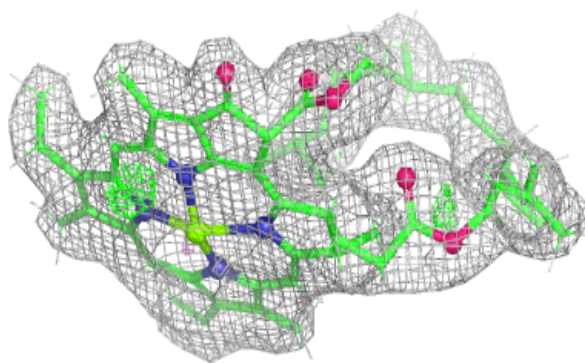
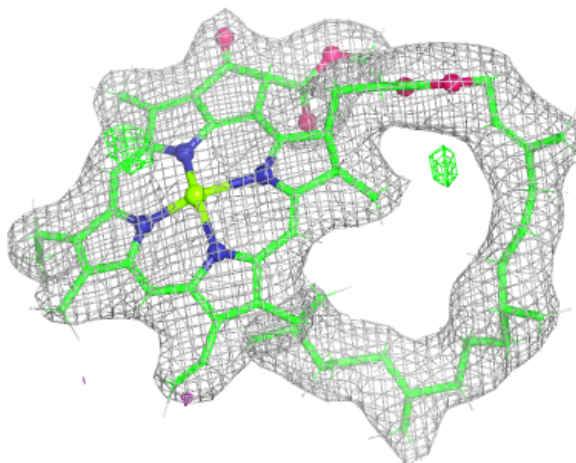
**Electron density around CLA b 609:**

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



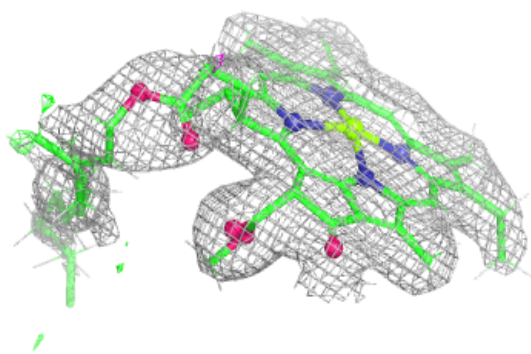
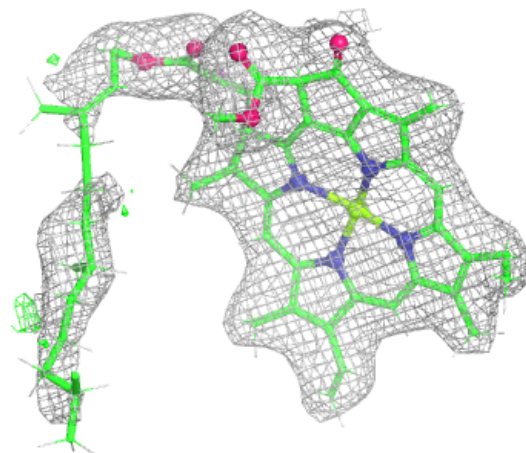
Electron density around CLA b 615:

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



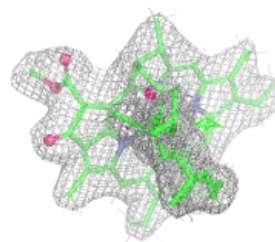
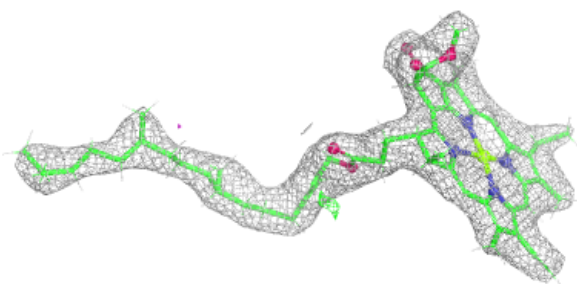
Electron density around CLA b 616:

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



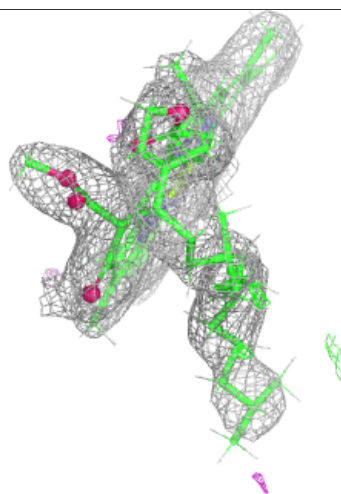
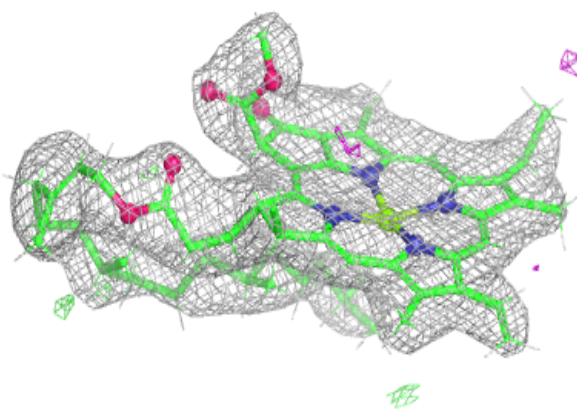
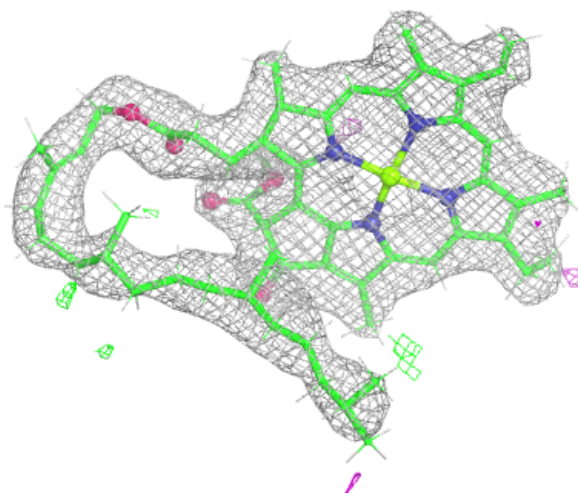
Electron density around CLA c 502:

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



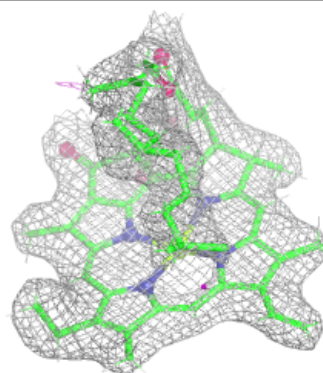
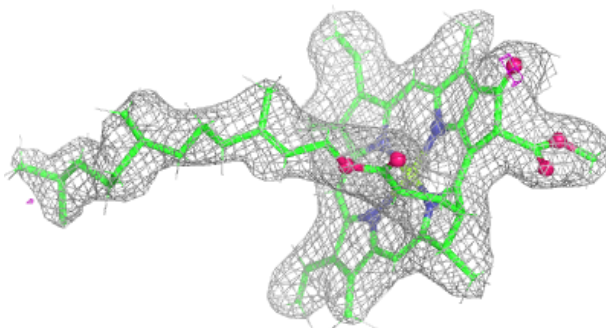
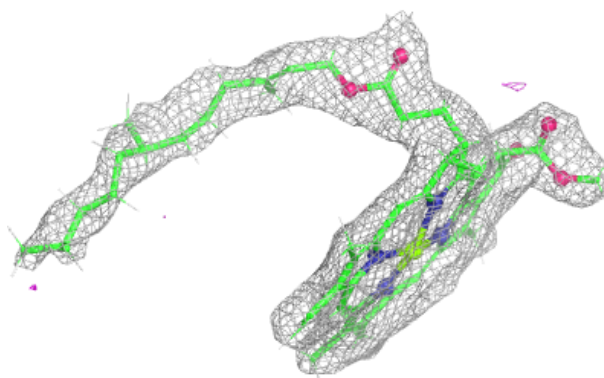
Electron density around CLA C 509:

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



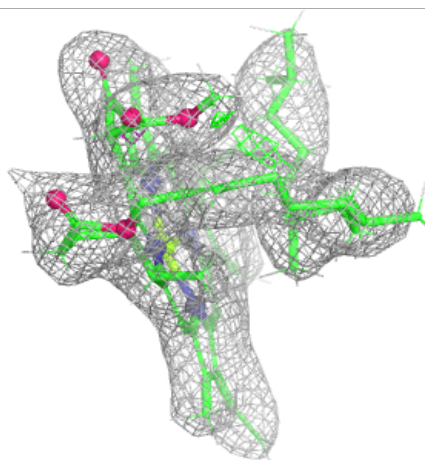
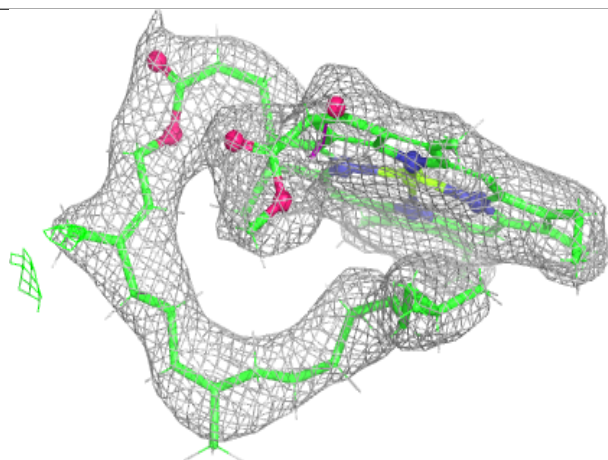
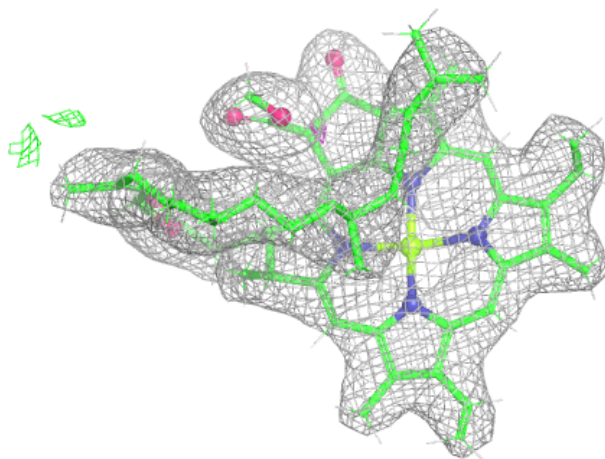
Electron density around CLA c 504:

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



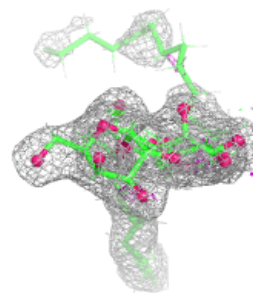
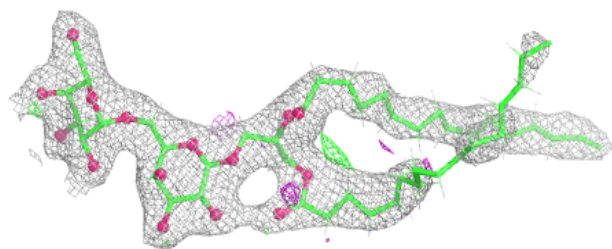
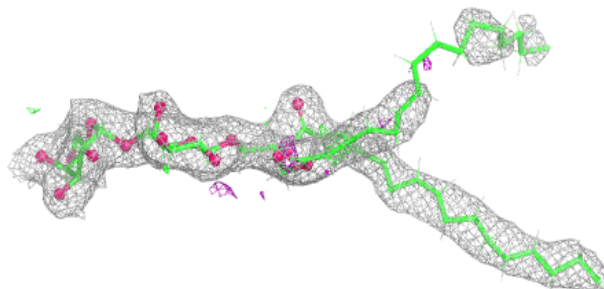
Electron density around CLA C 510:

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

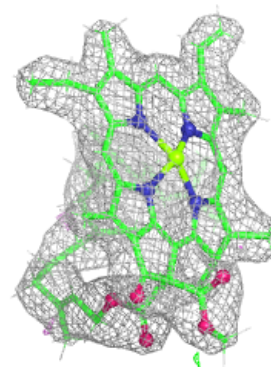
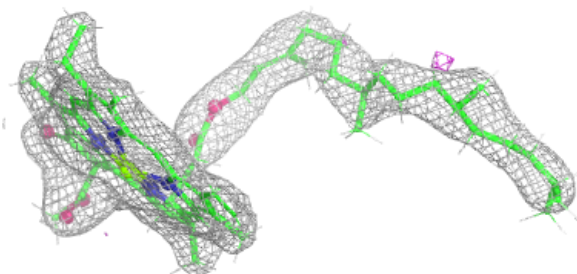
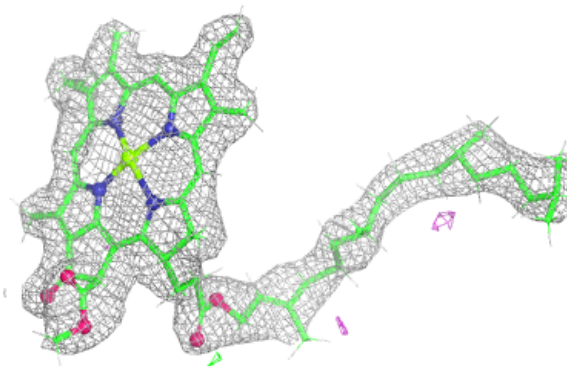


Electron density around DGD c 515:

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

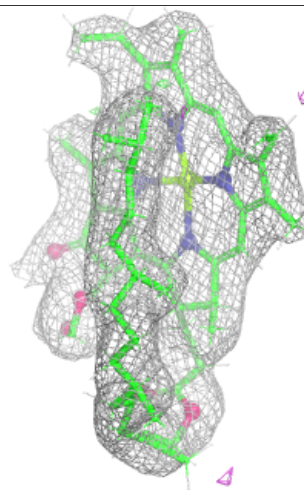
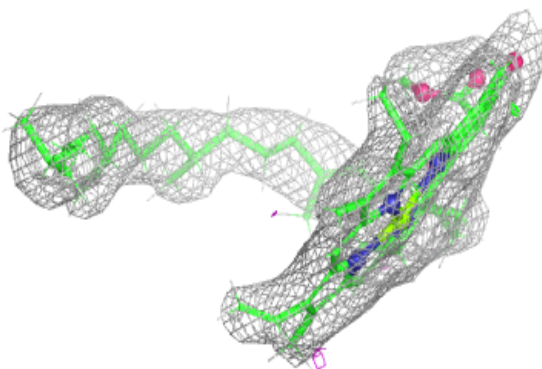
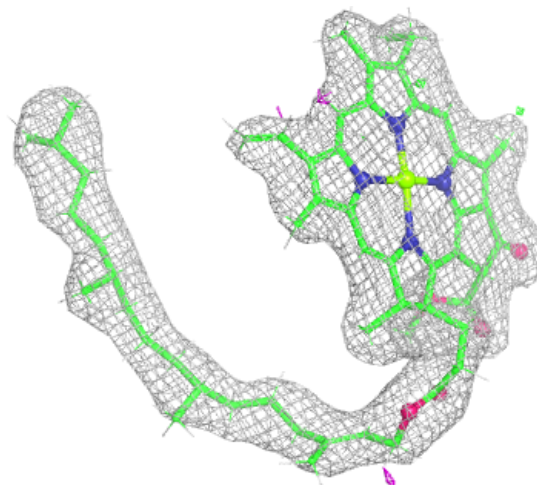
**Electron density around CLA C 511:**

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



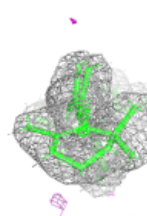
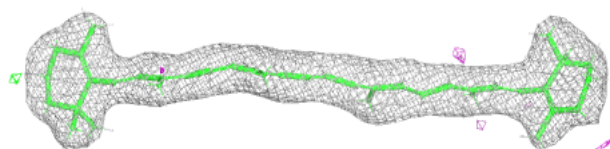
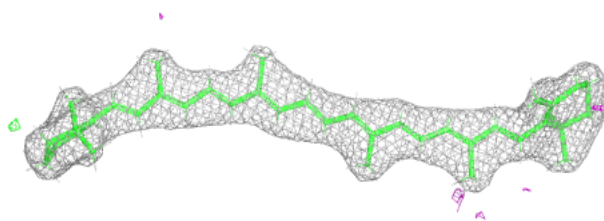
Electron density around CLA c 507:

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

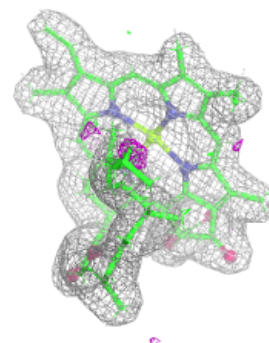
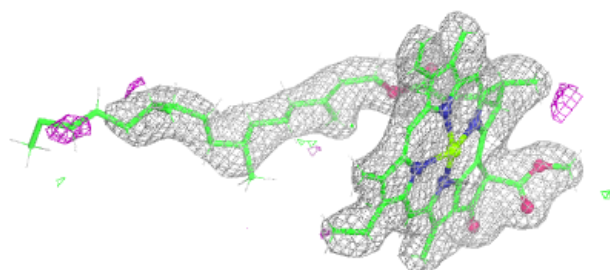
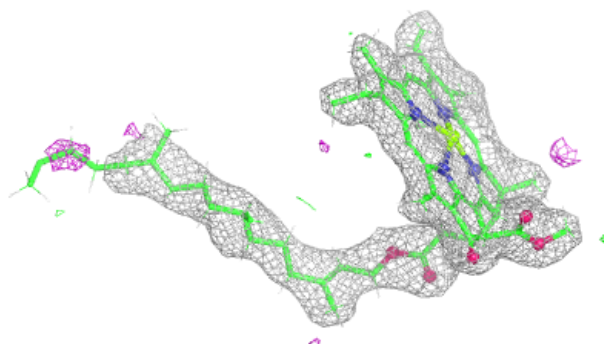


Electron density around BCR a 406:

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

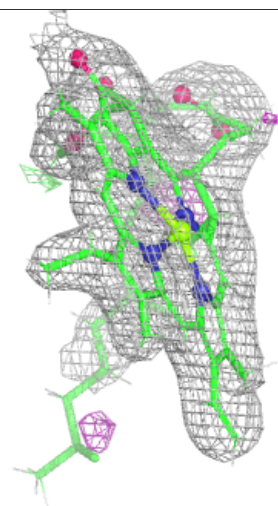
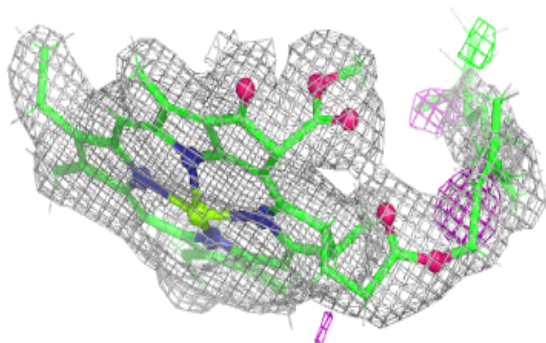
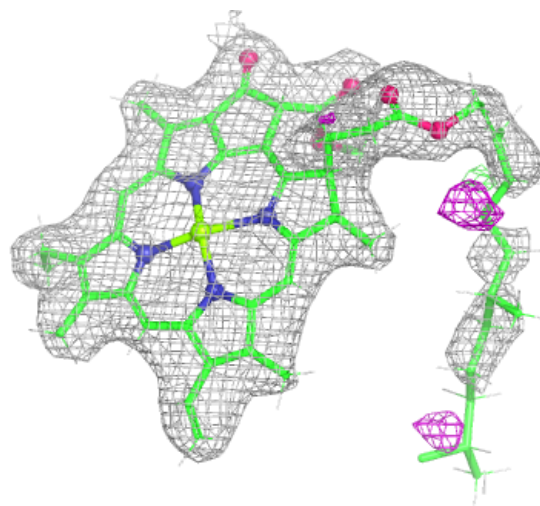
**Electron density around CLA c 508:**

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



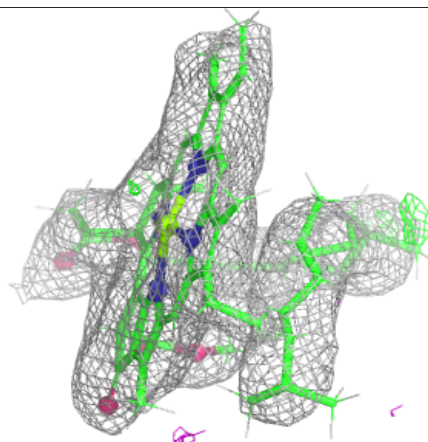
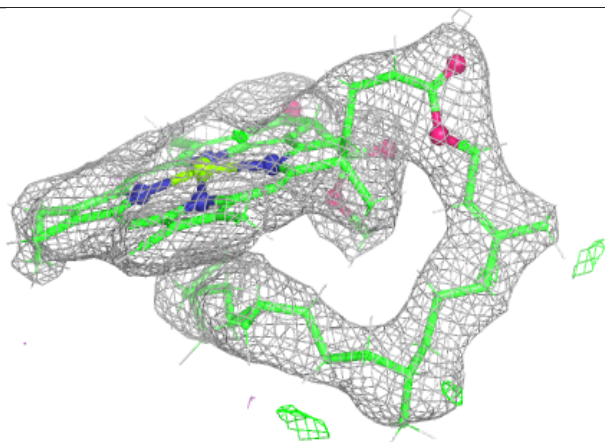
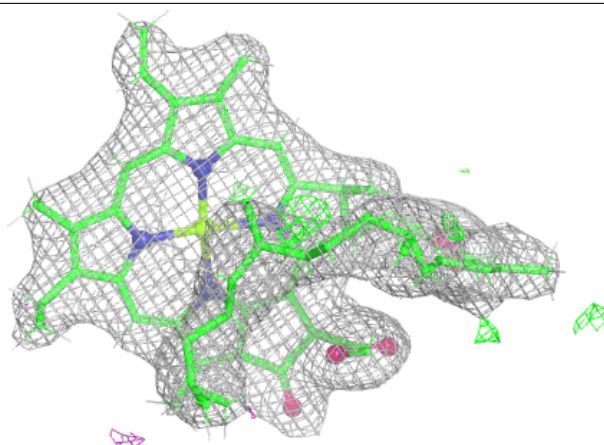
Electron density around CLA B 616:

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



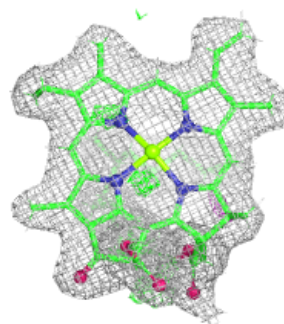
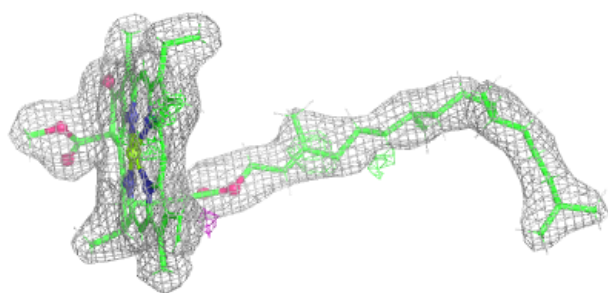
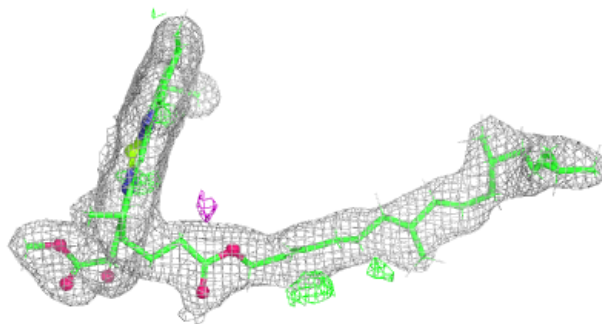
Electron density around CLA c 510:

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

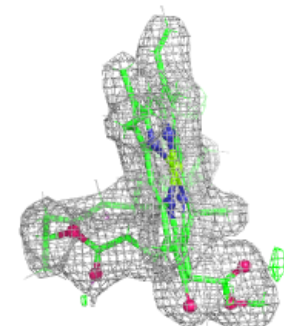
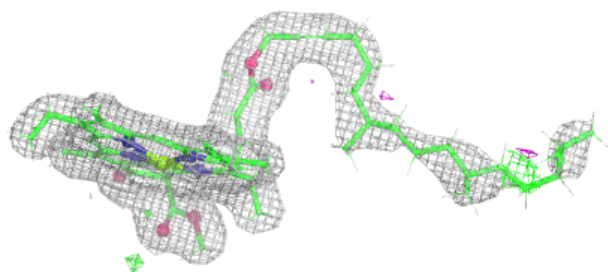
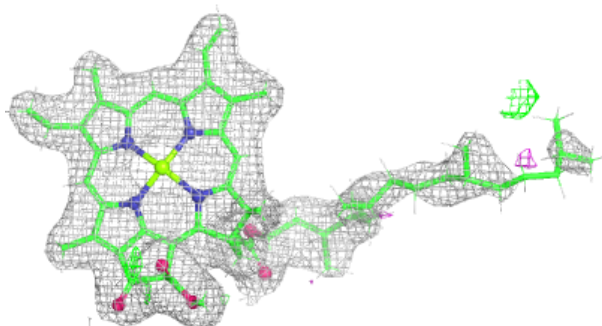


Electron density around CLA B 605:

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

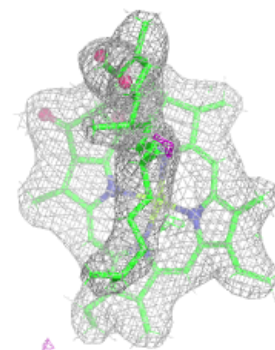
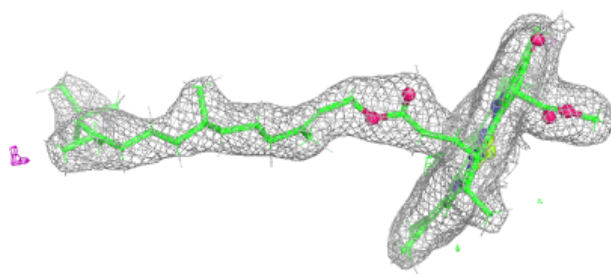
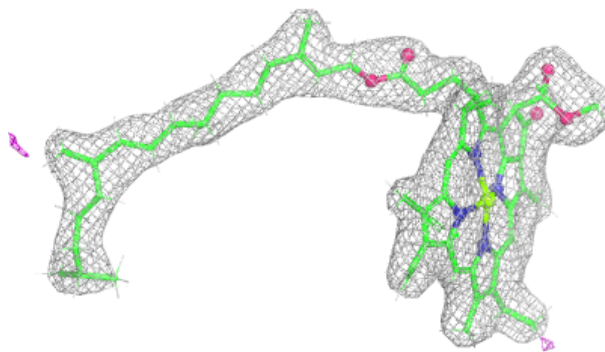
**Electron density around CLA A 403:**

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

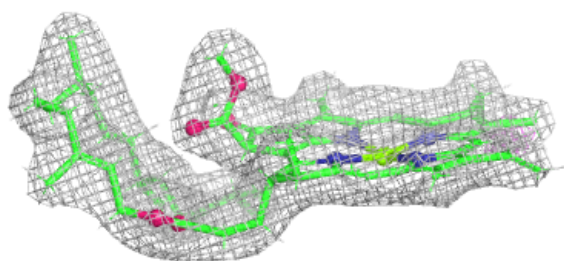
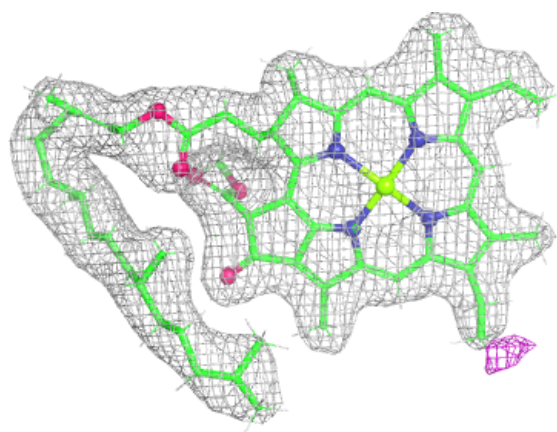


Electron density around CLA B 609:

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

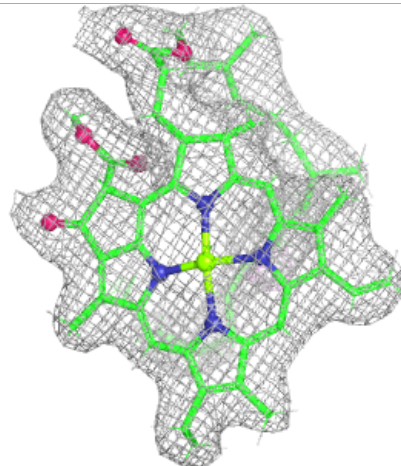
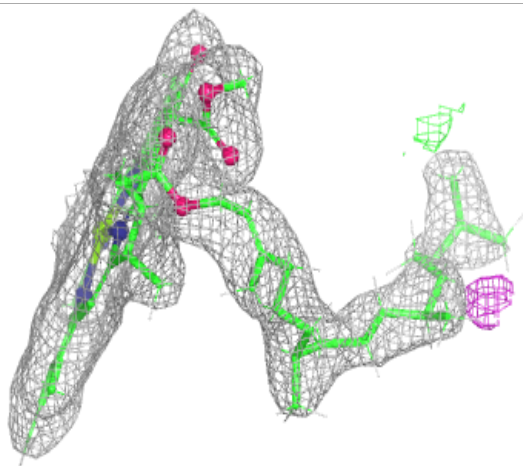
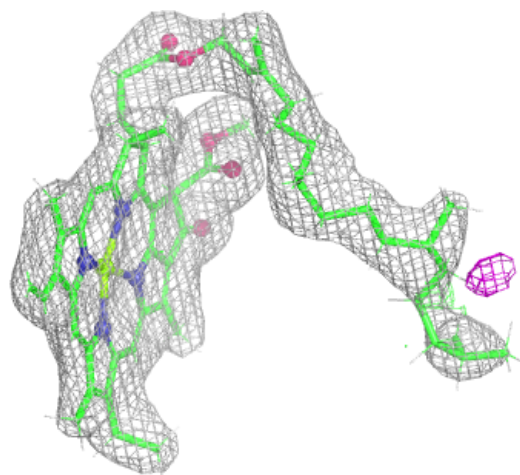
**Electron density around CLA B 610:**

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



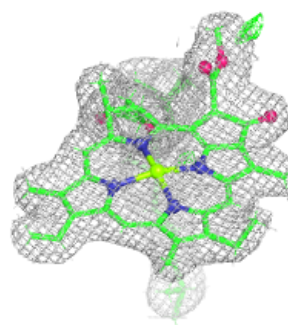
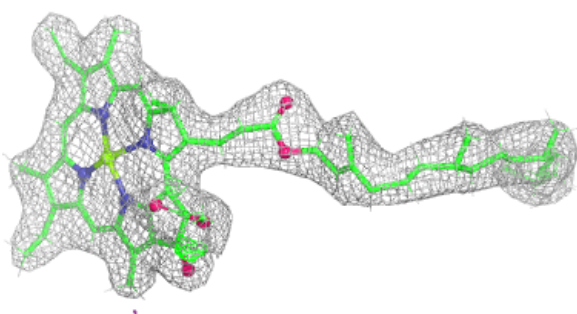
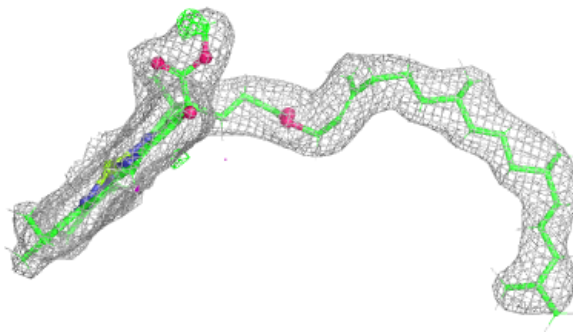
Electron density around CLA B 613:

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

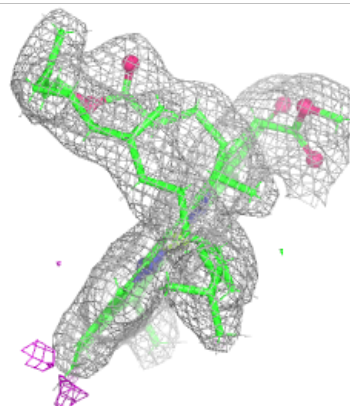
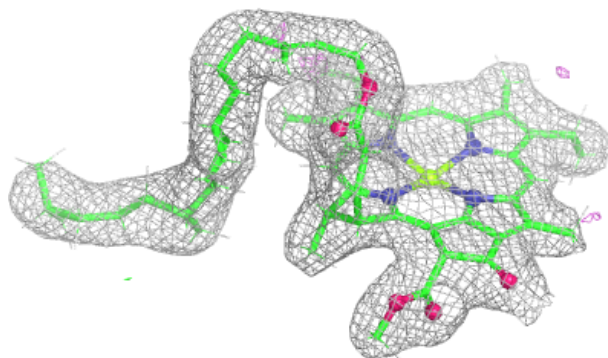
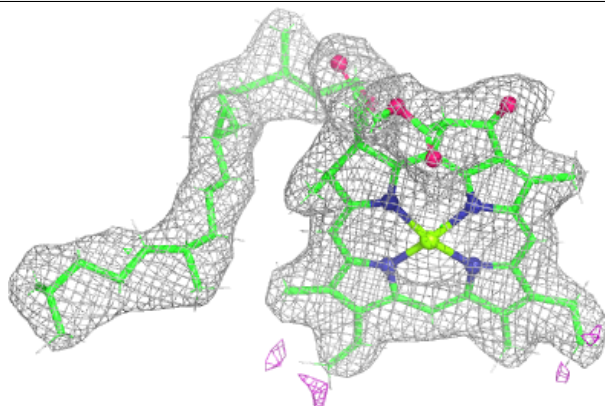


Electron density around CLA D 403:

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

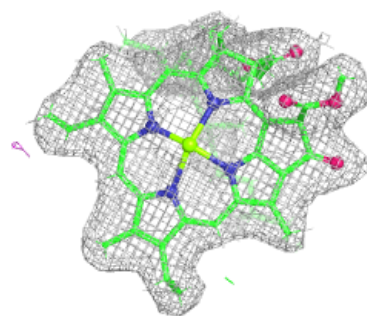
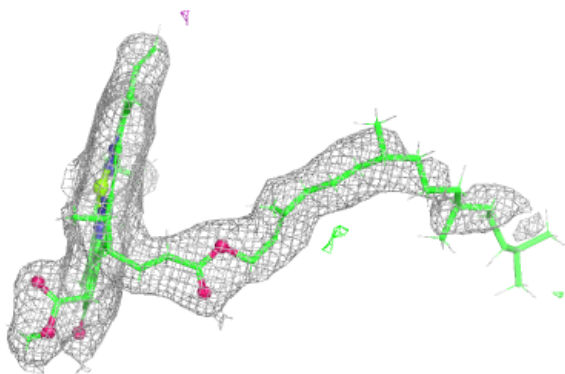
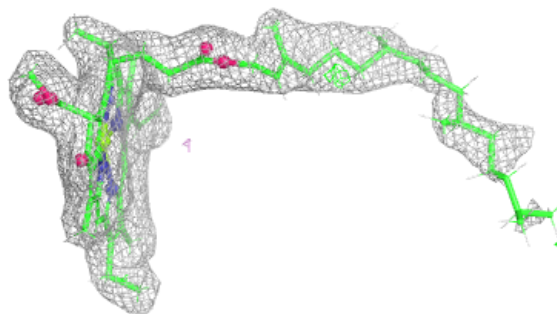
**Electron density around CLA D 404:**

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

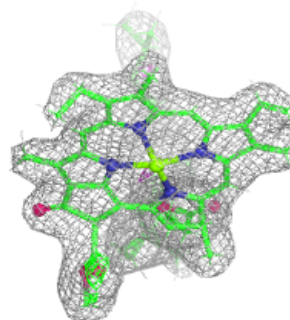
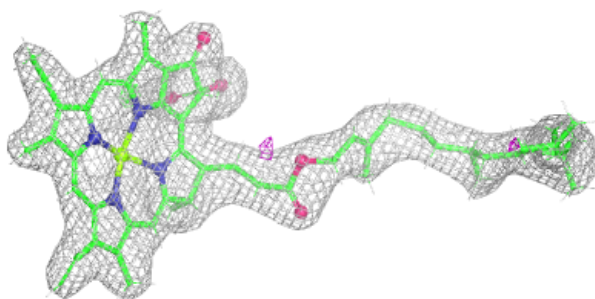
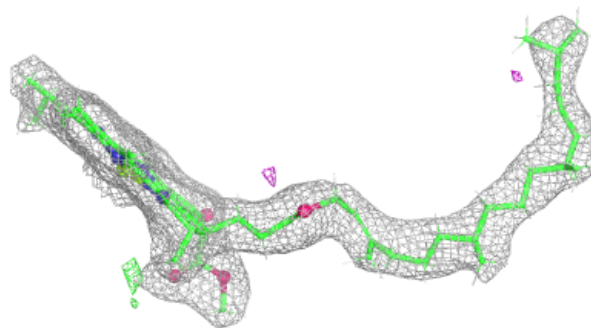


Electron density around CLA D 405:

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

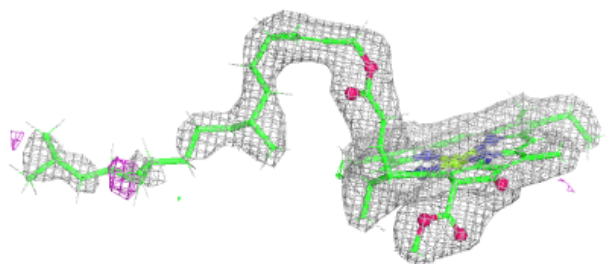
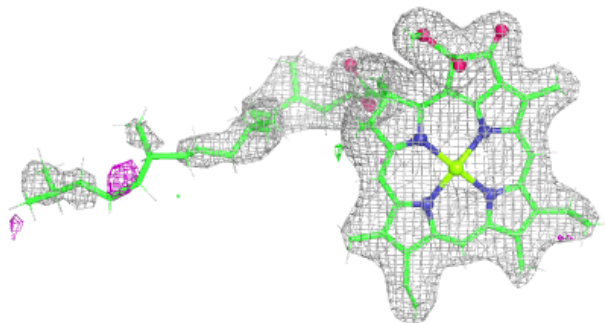
**Electron density around CLA d 402:**

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

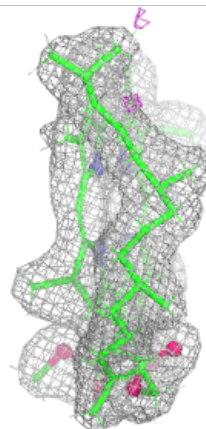
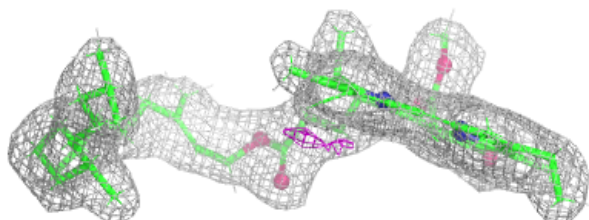
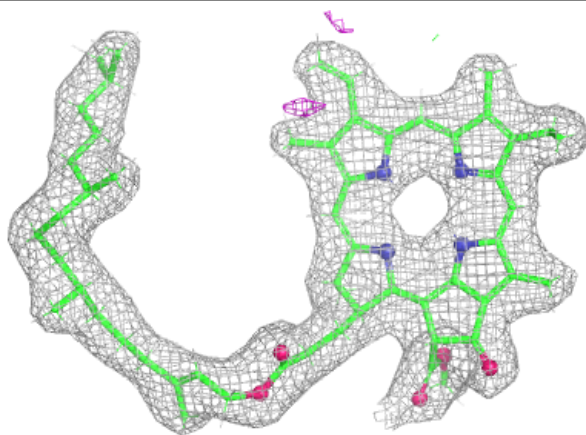


Electron density around CLA a 403:

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

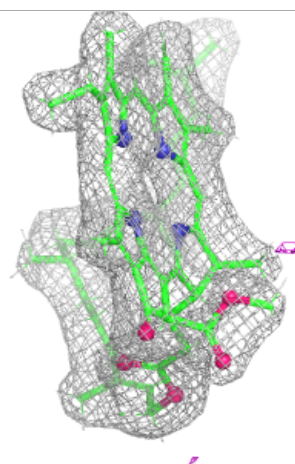
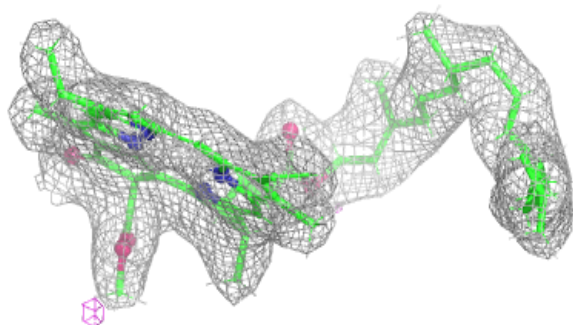
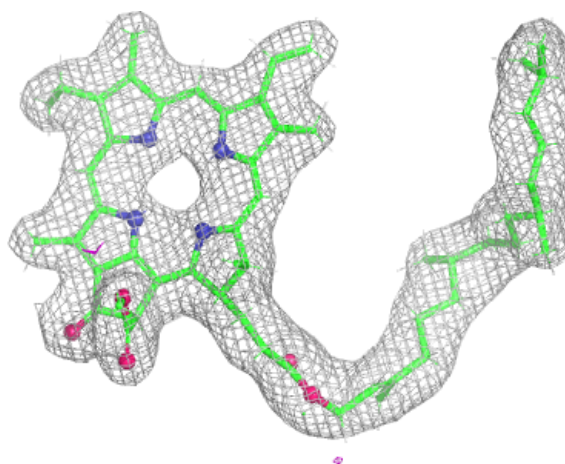
**Electron density around PHO A 404:**

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



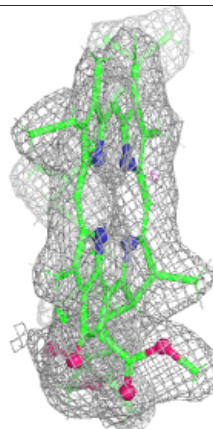
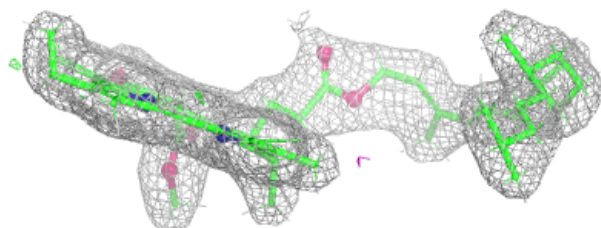
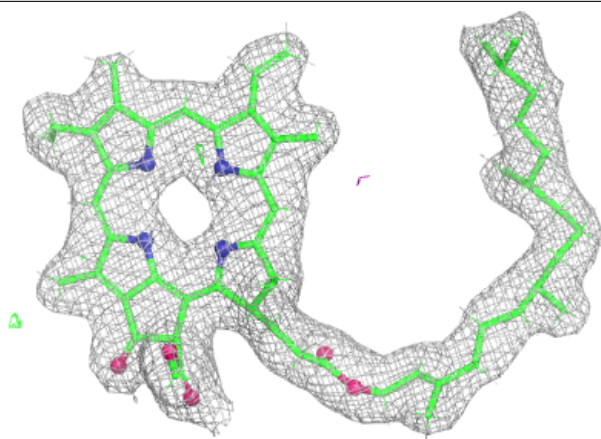
Electron density around PHO D 401:

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



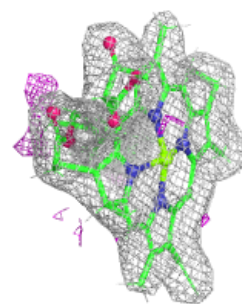
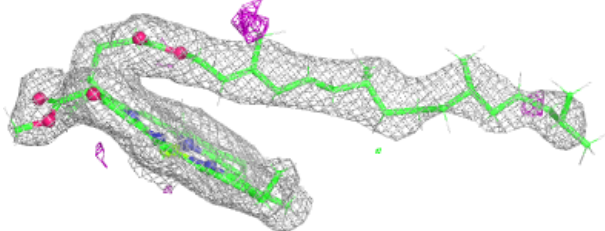
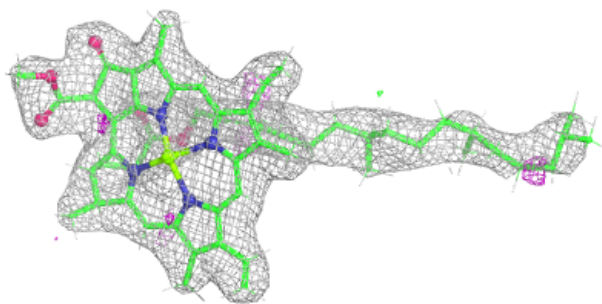
Electron density around PHO a 404:

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

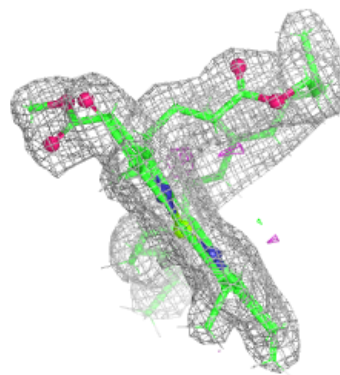
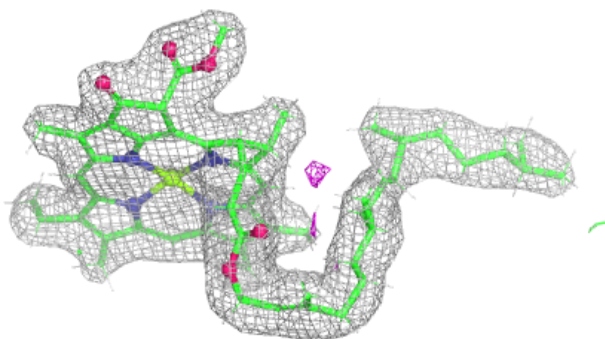
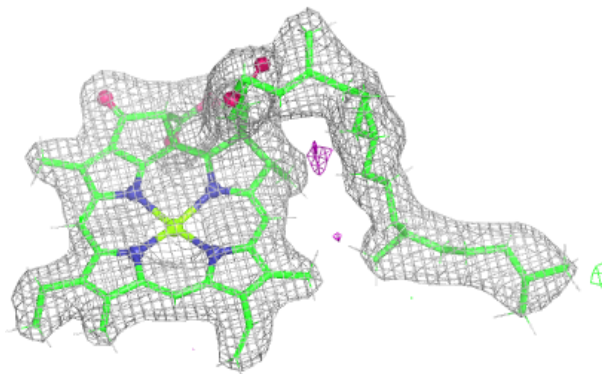


Electron density around CLA B 614:

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

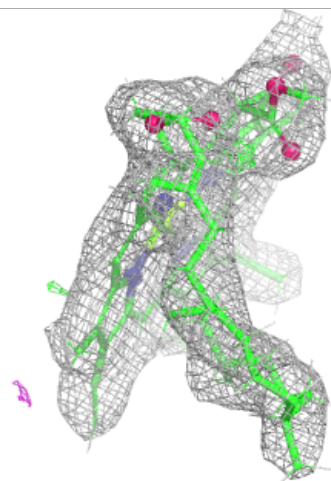
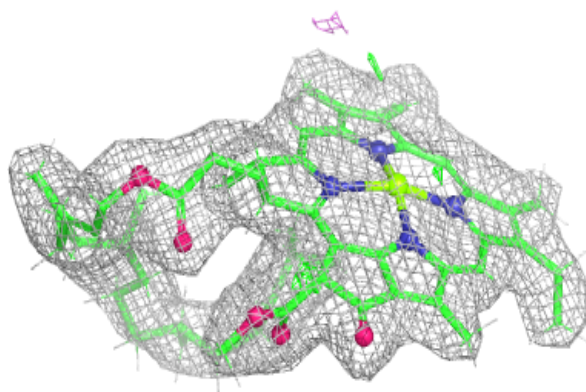
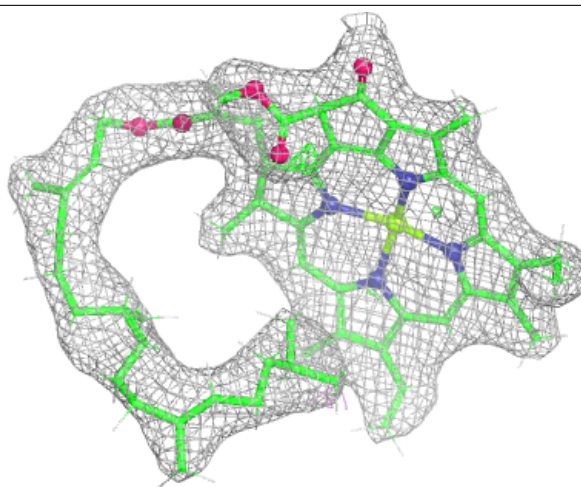
**Electron density around CLA a 411:**

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



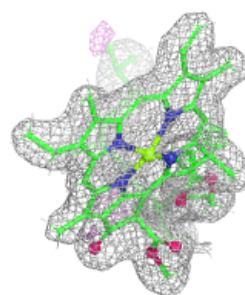
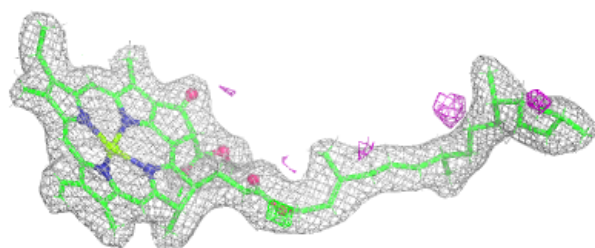
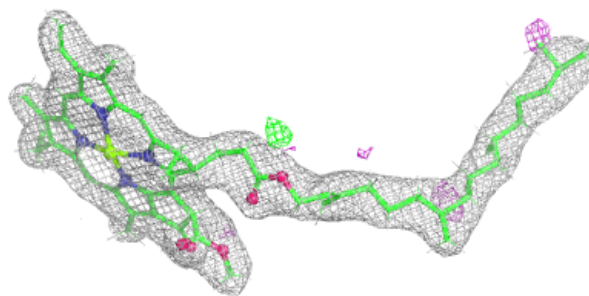
Electron density around CLA B 615:

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

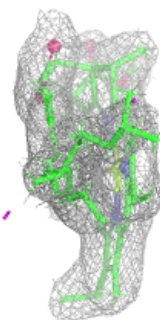
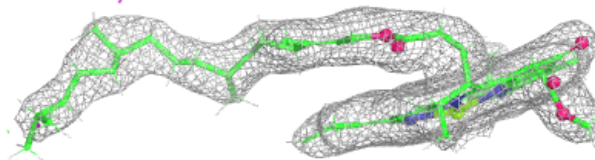
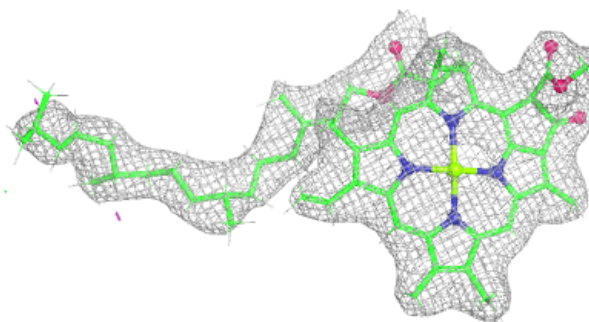


Electron density around CLA A 402:

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

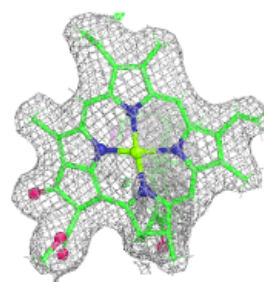
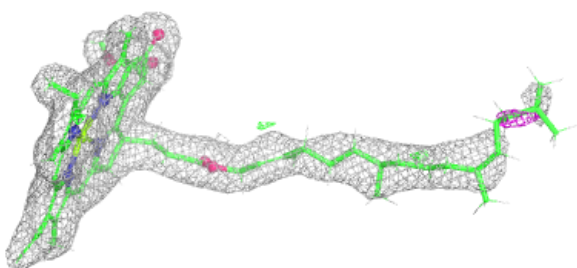
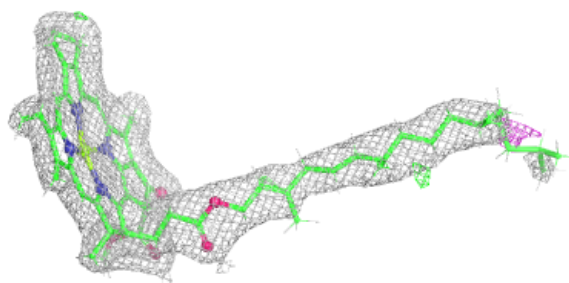
**Electron density around CLA b 603:**

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

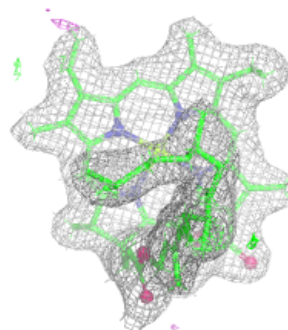
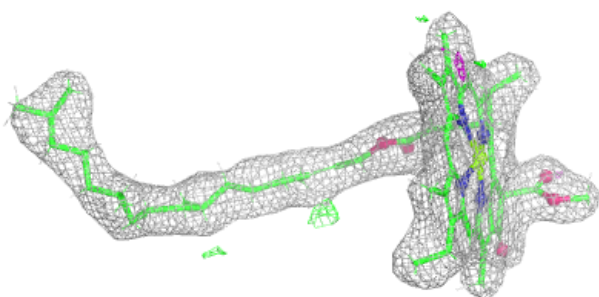
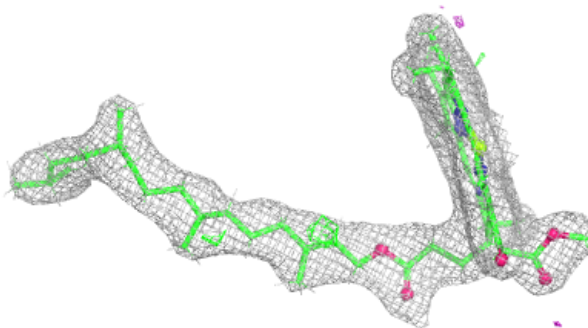


Electron density around CLA b 604:

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

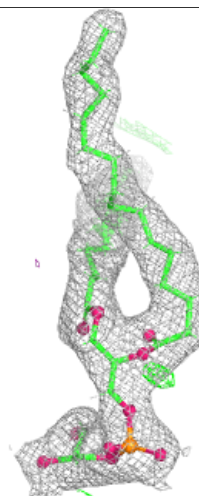
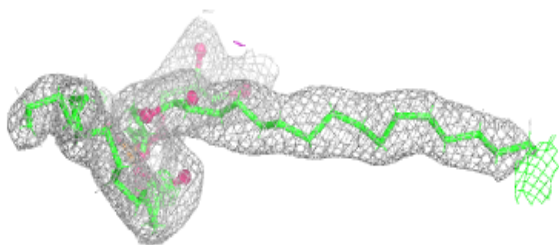
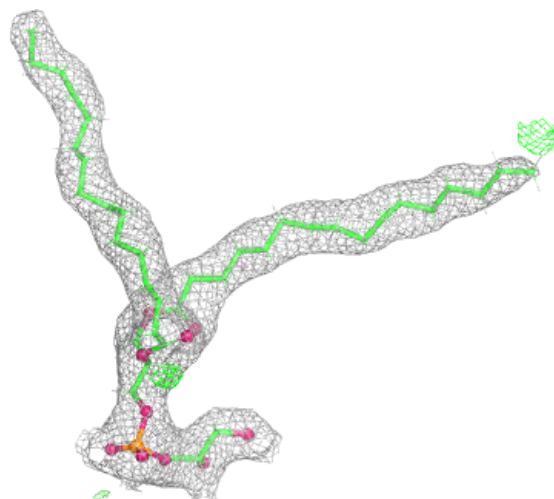
**Electron density around CLA b 605:**

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



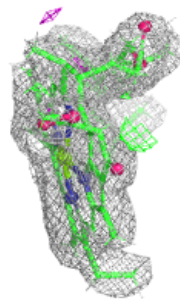
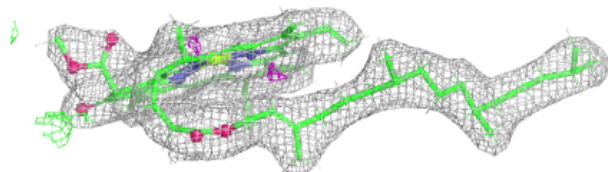
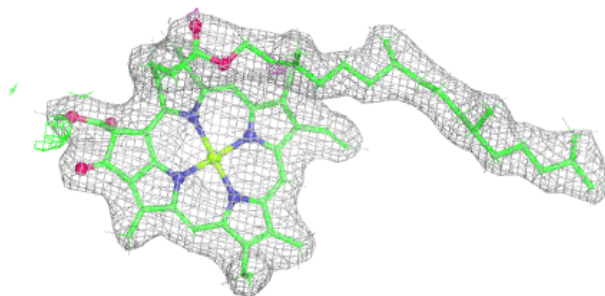
Electron density around LHG L 102:

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

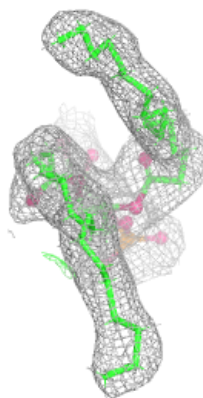
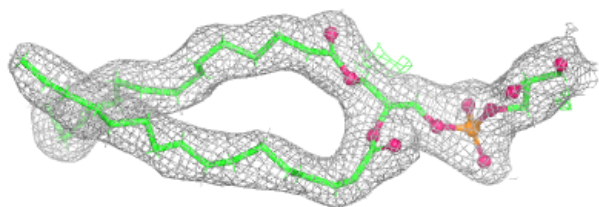
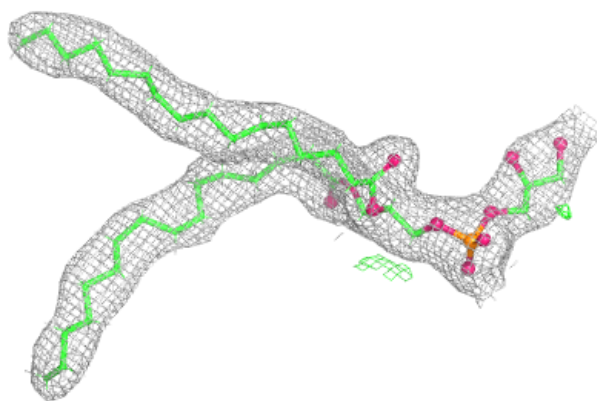


Electron density around CLA C 501:

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

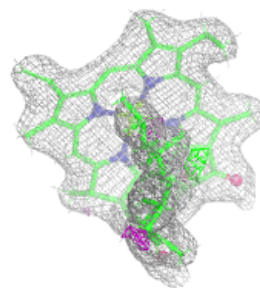
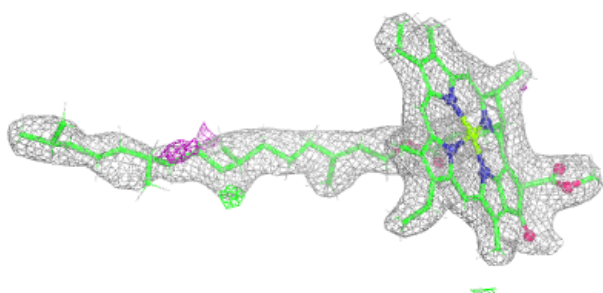
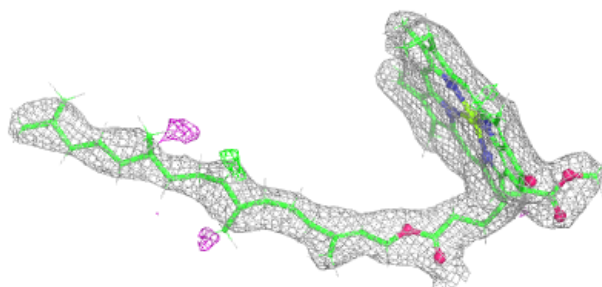
**Electron density around LHG d 406:**

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

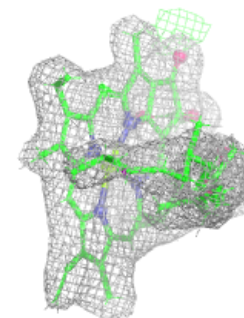
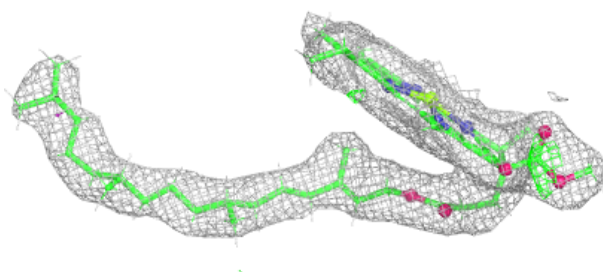
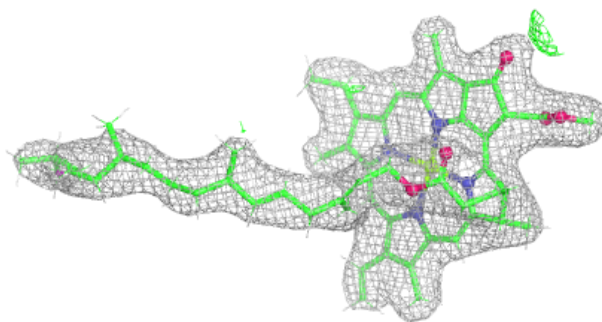


Electron density around CLA b 607:

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

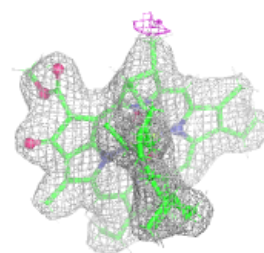
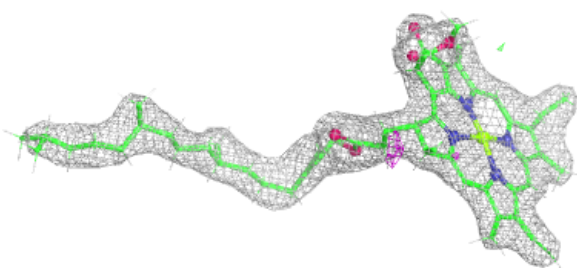
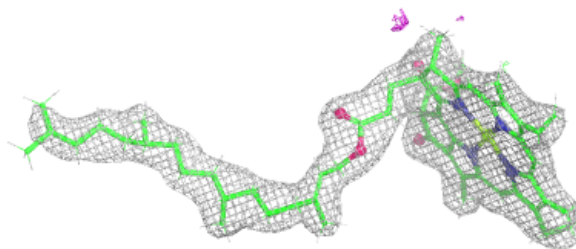
**Electron density around CLA b 608:**

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



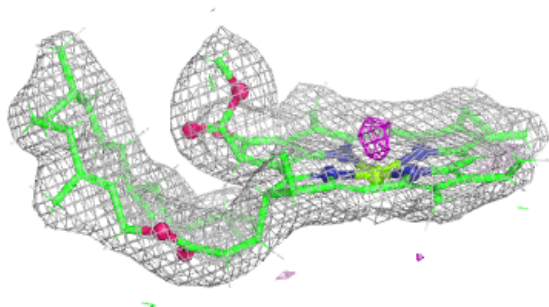
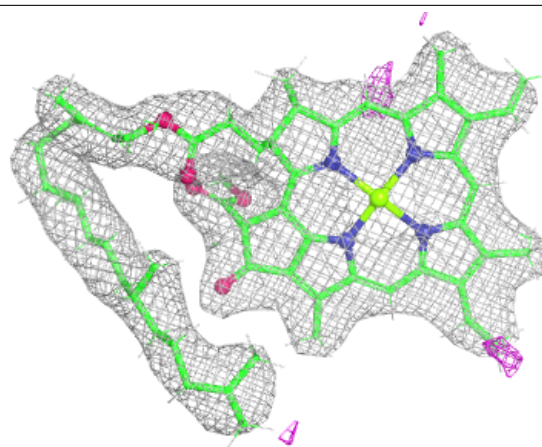
Electron density around CLA C 502:

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



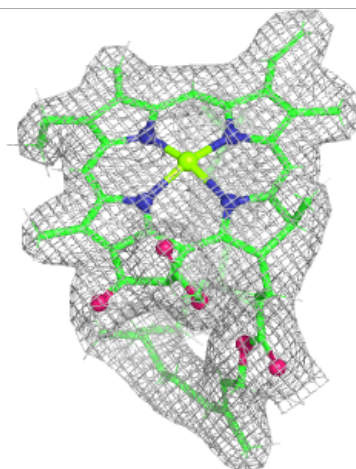
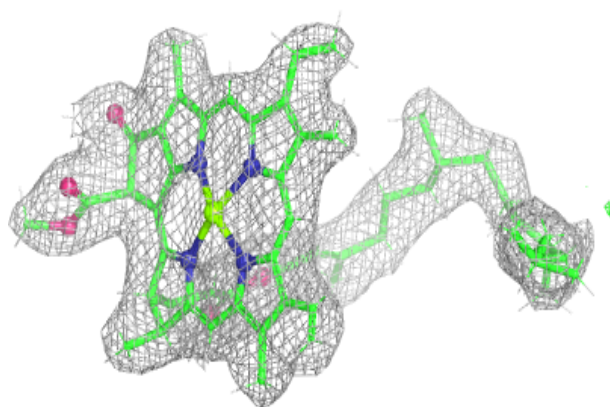
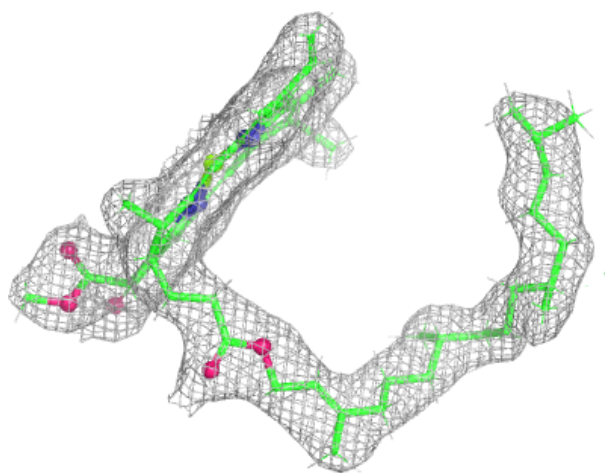
Electron density around CLA b 610:

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



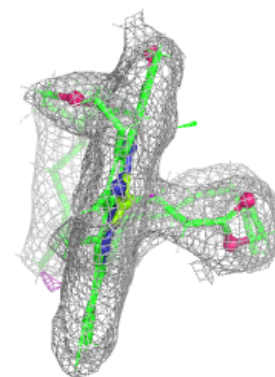
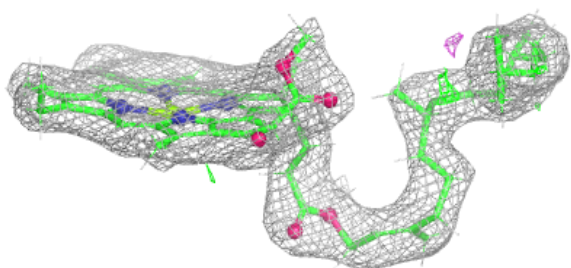
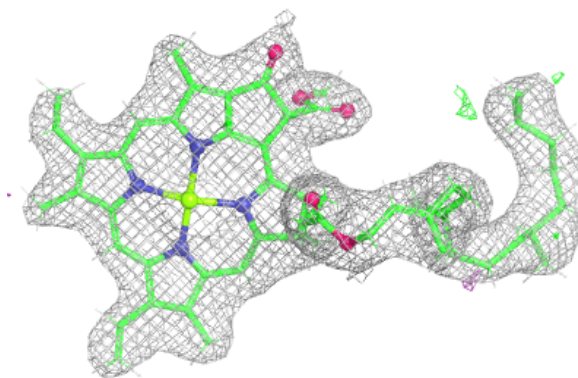
Electron density around CLA b 611:

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



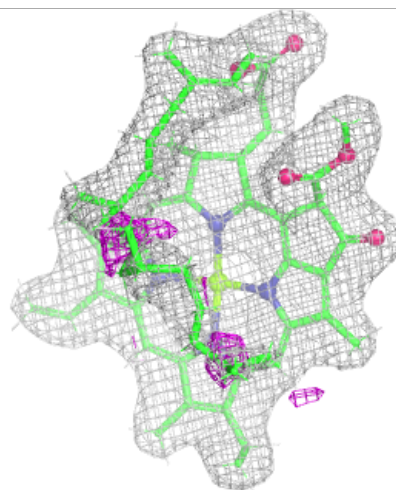
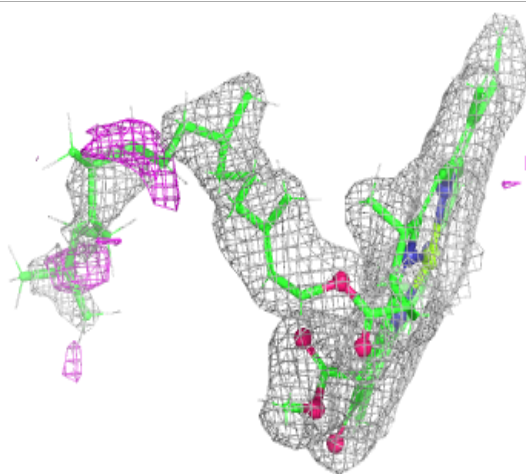
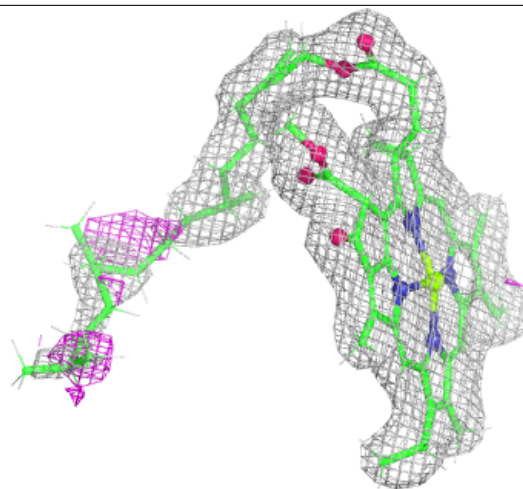
Electron density around CLA b 612:

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



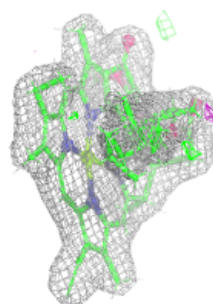
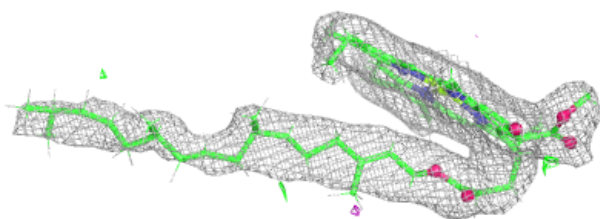
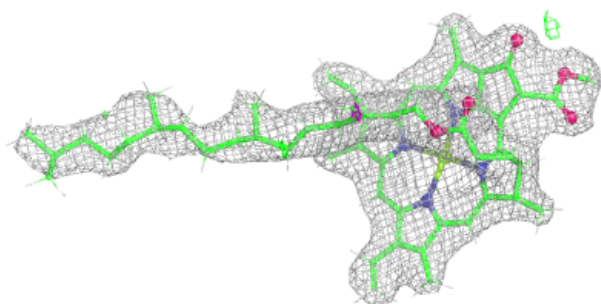
Electron density around CLA b 613:

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



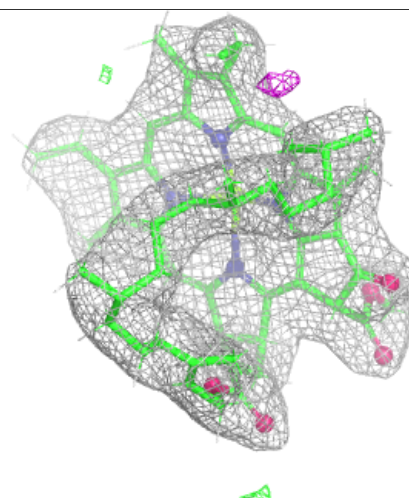
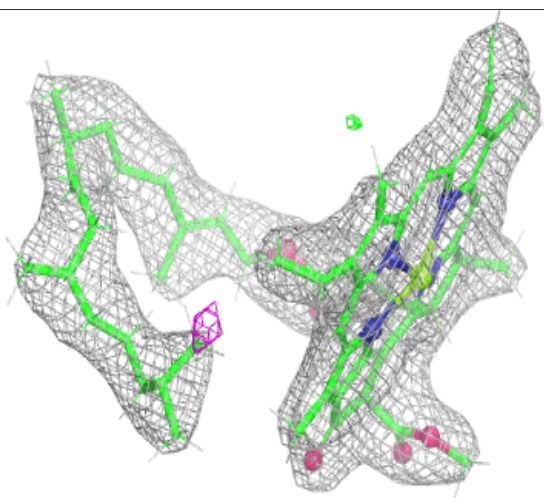
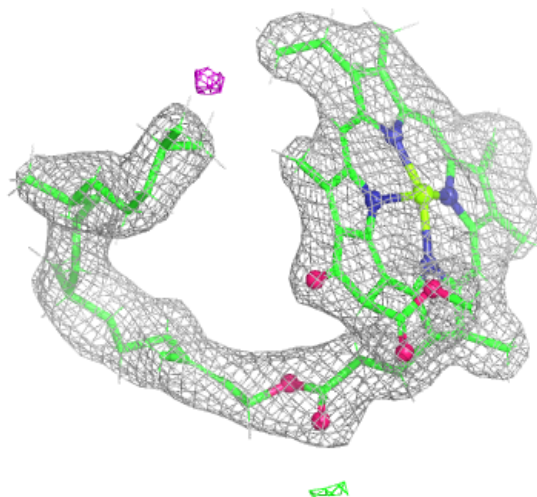
Electron density around CLA b 614:

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



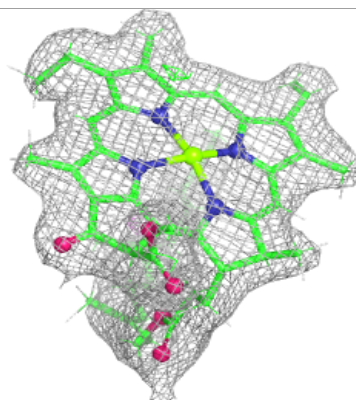
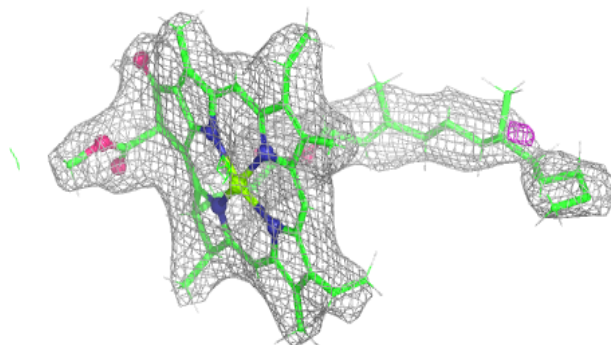
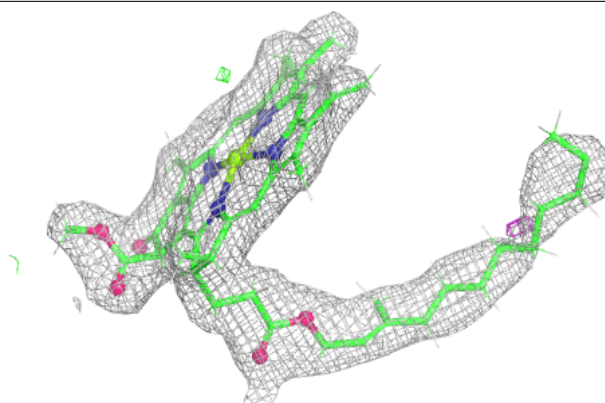
Electron density around CLA C 503:

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

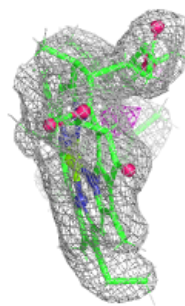
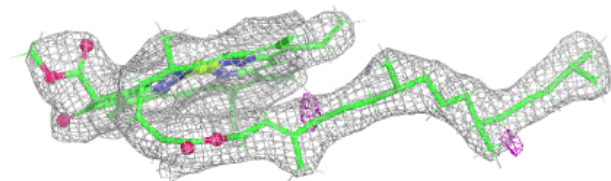
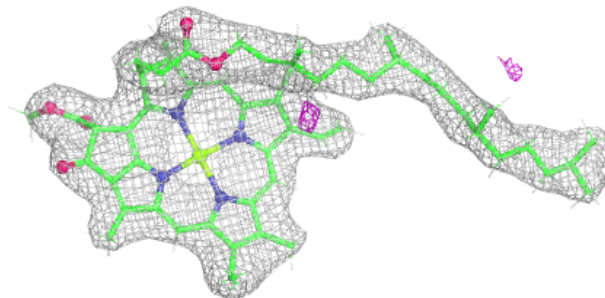


Electron density around CLA C 504:

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

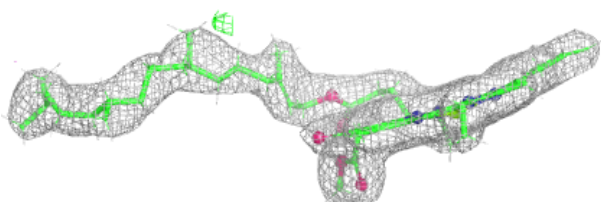
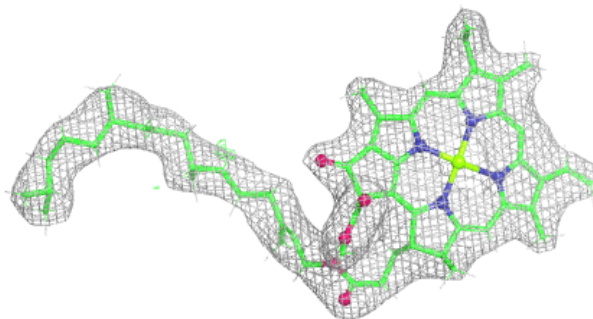
**Electron density around CLA c 501:**

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

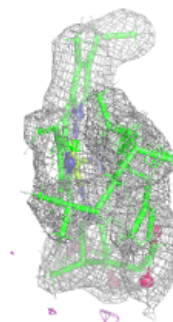
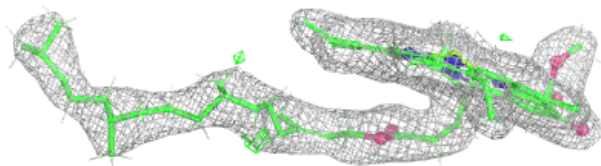
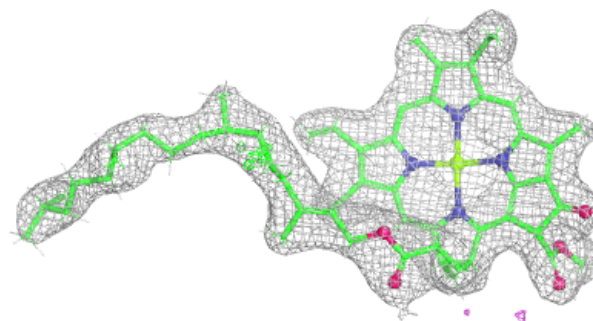


Electron density around CLA B 602:

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

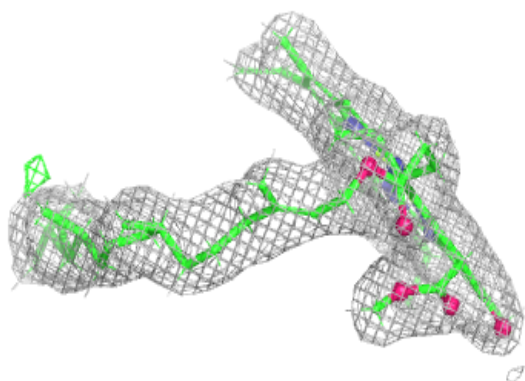
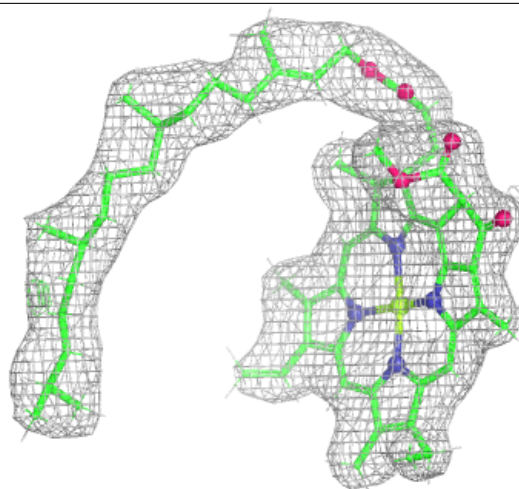
**Electron density around CLA B 603:**

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



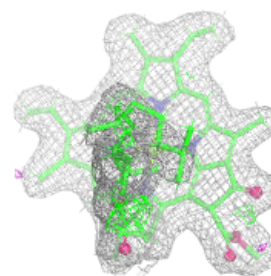
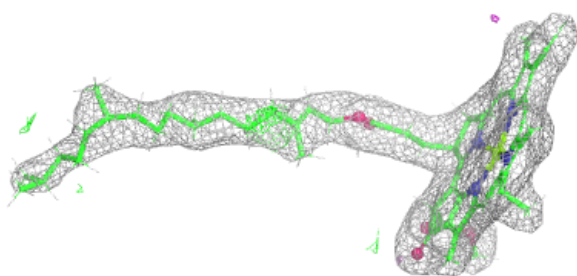
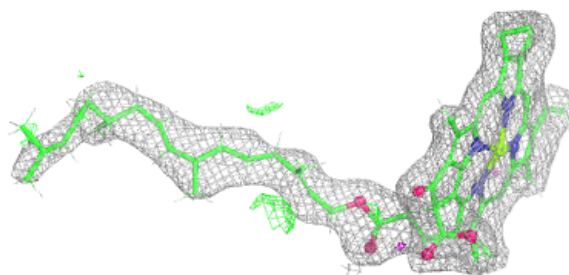
Electron density around CLA C 507:

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



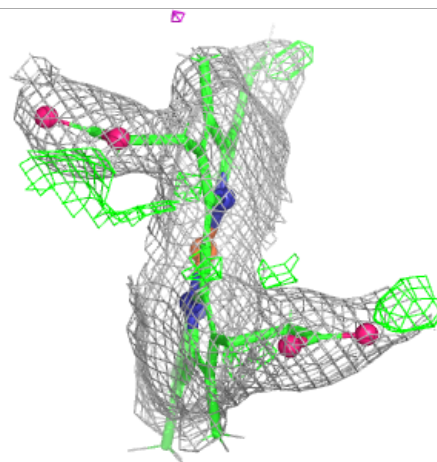
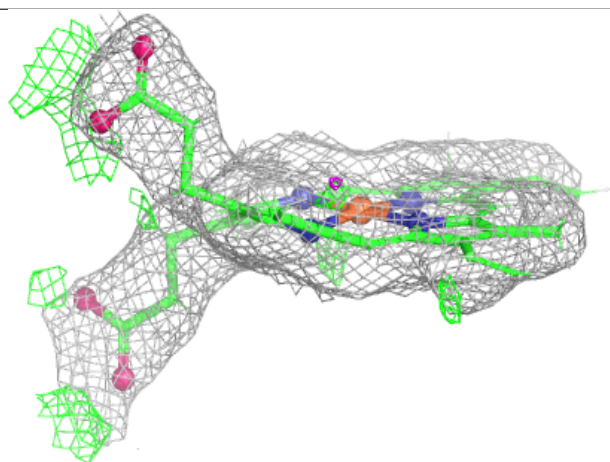
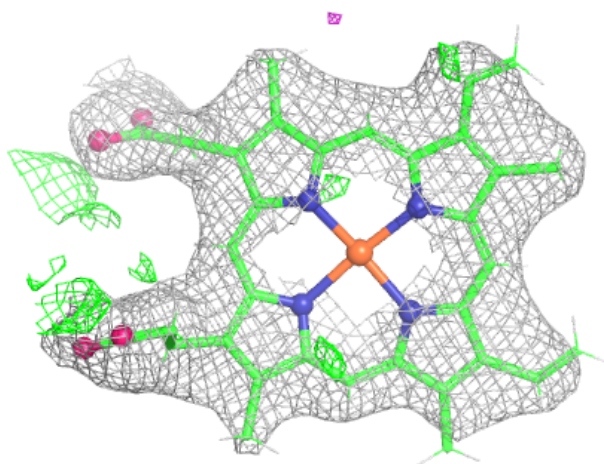
Electron density around CLA B 604:

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



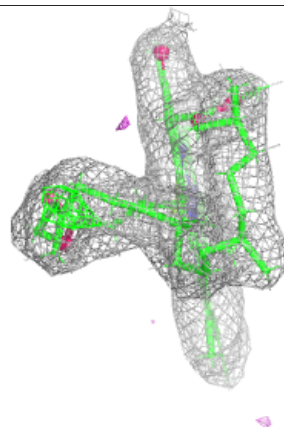
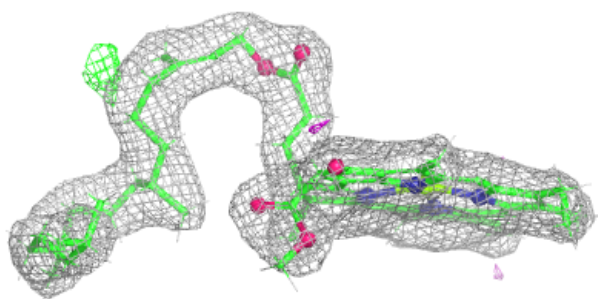
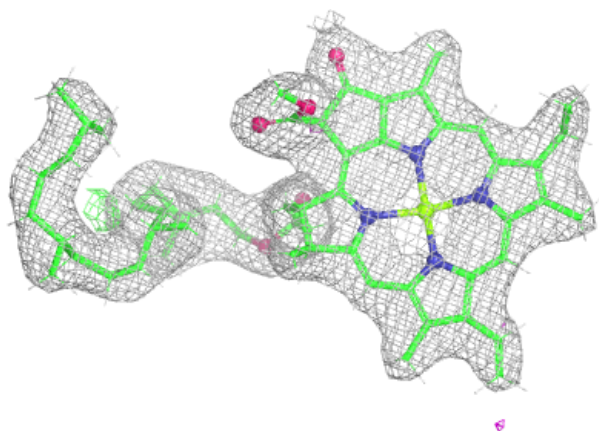
Electron density around HEM e 101:

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

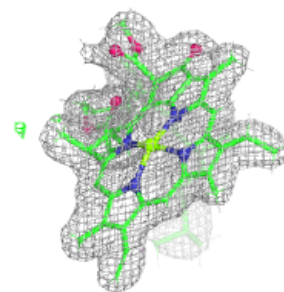
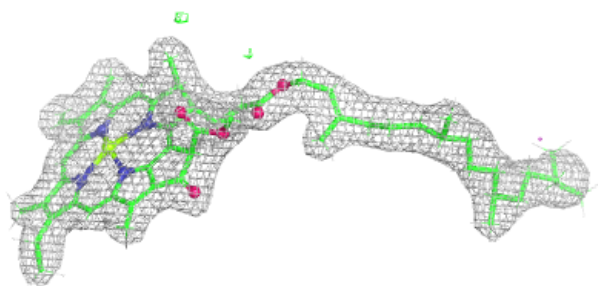
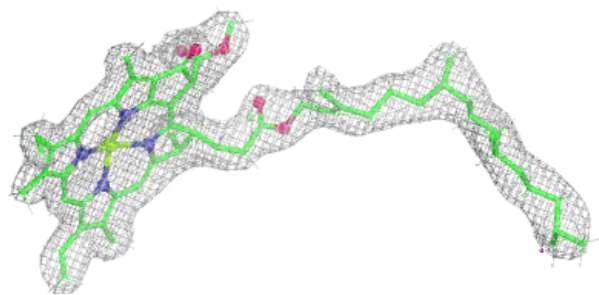


Electron density around CLA B 612:

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

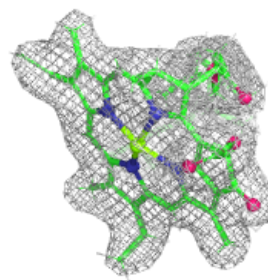
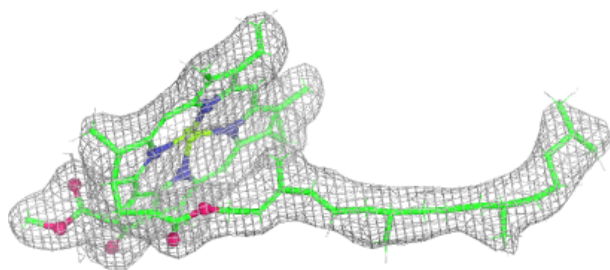
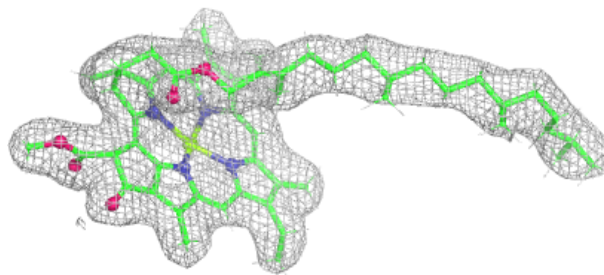
**Electron density around CLA a 402:**

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

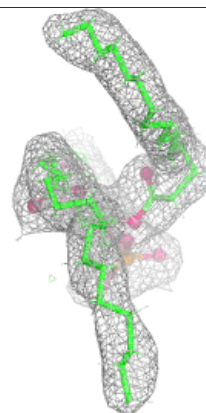
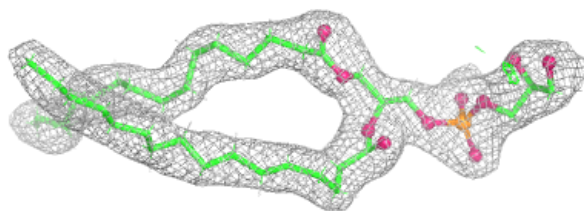
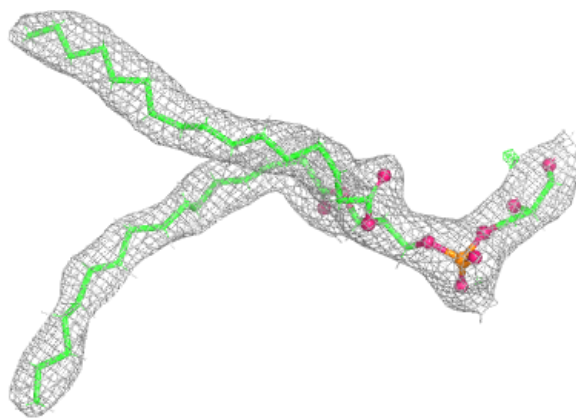


Electron density around CLA B 608:

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

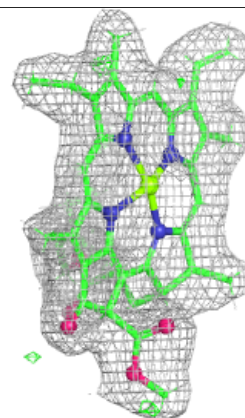
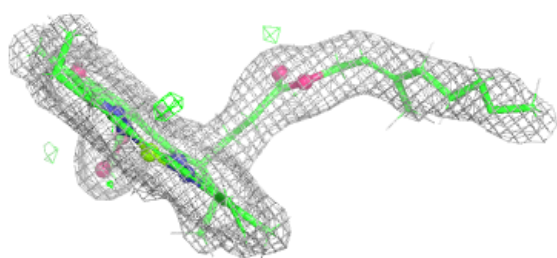
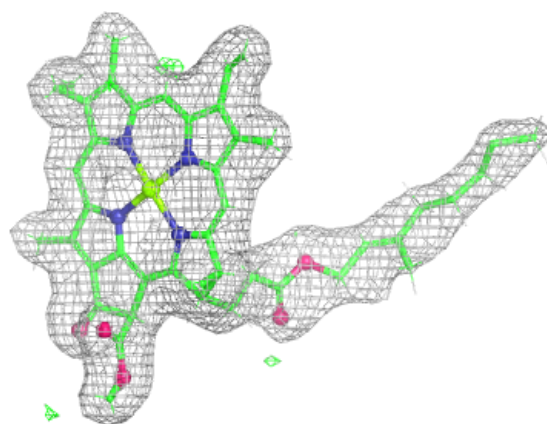
**Electron density around LHG D 409:**

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

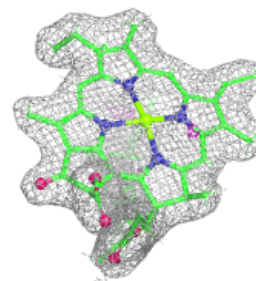
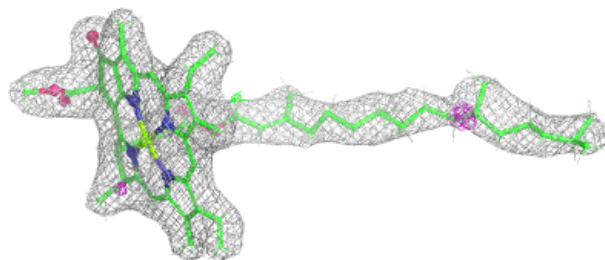
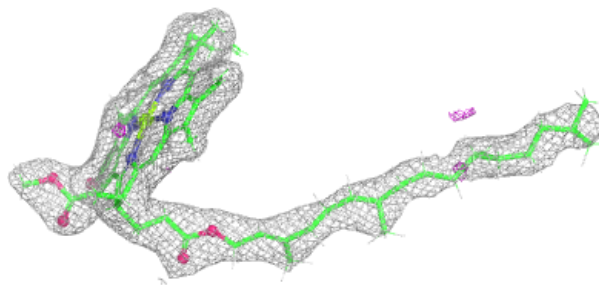


Electron density around CLA A 405:

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

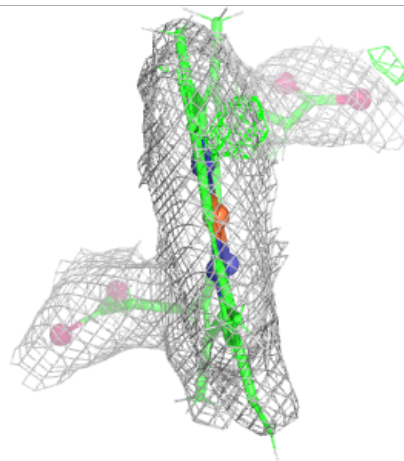
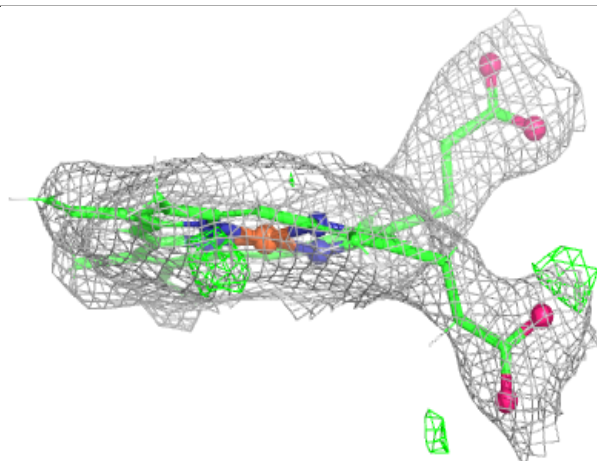
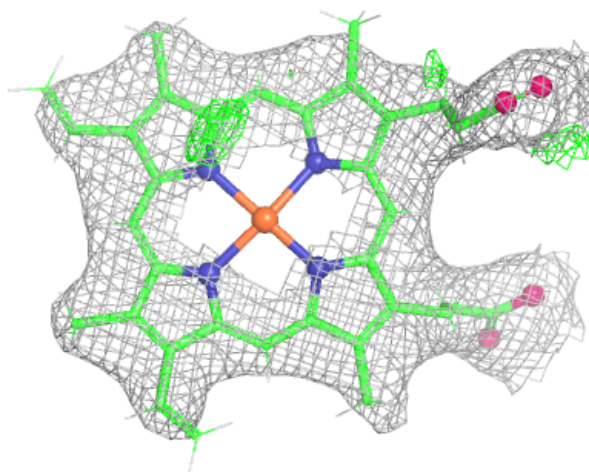
**Electron density around CLA B 607:**

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



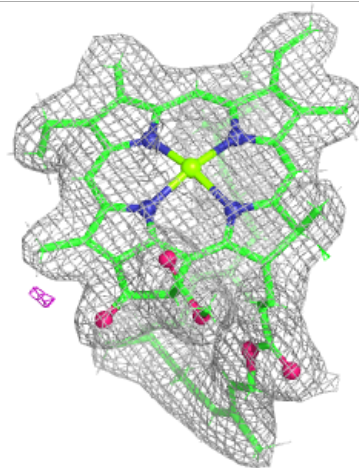
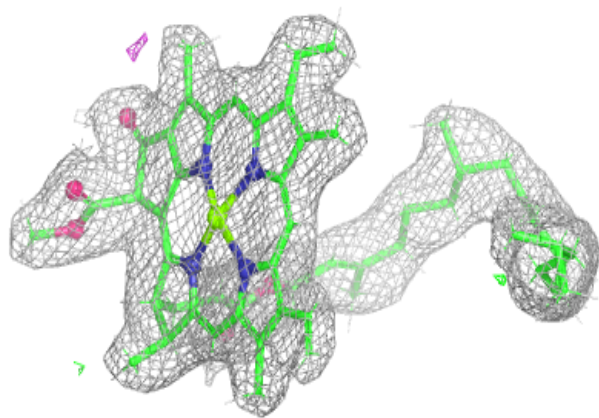
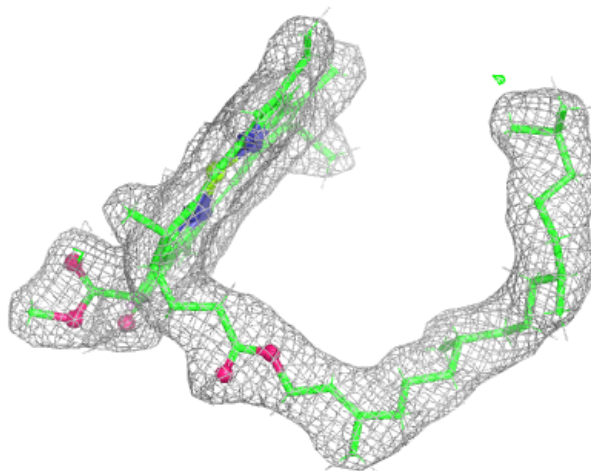
Electron density around HEM F 101:

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



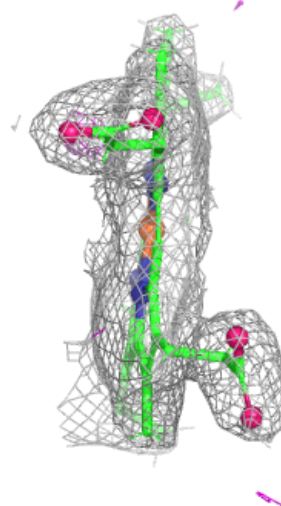
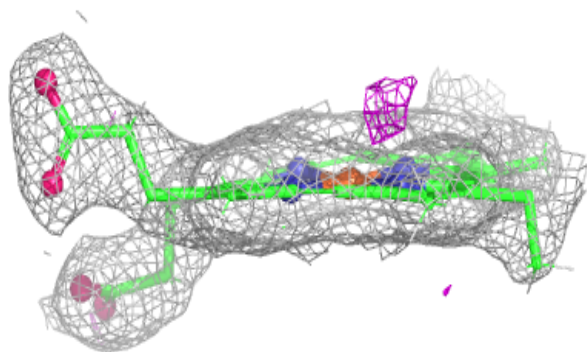
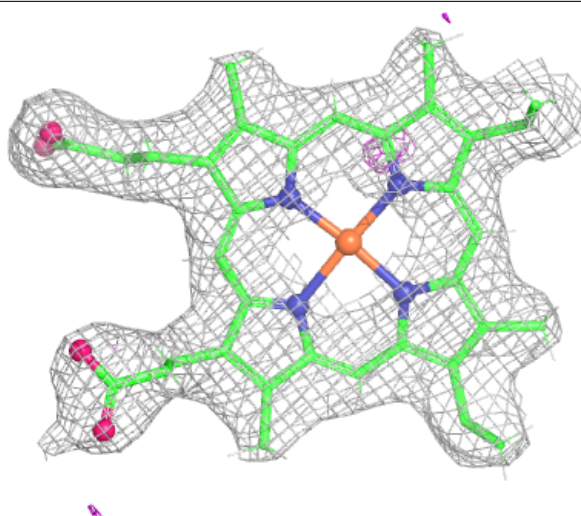
Electron density around CLA B 611:

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



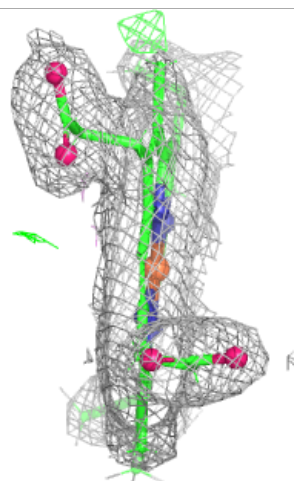
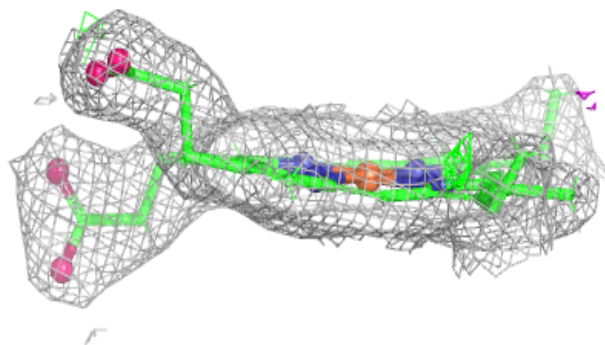
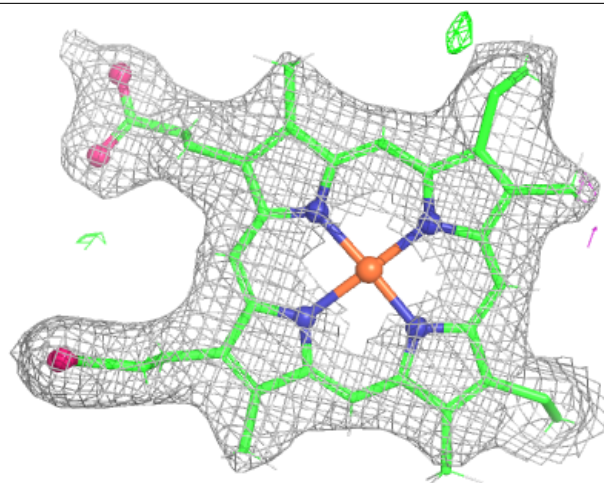
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.