



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 12:01 PM EDT

PDB ID : 7RF4 / pdb_00007rf4
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 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 : 2.27 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)

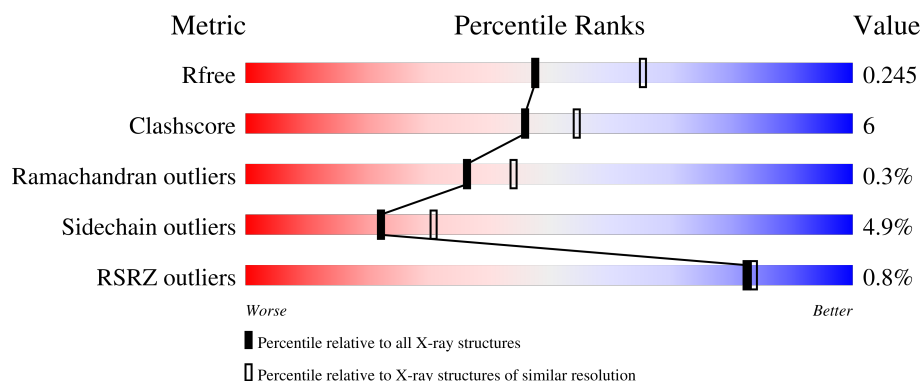
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

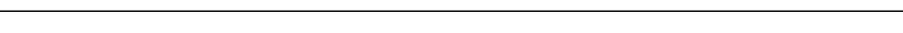
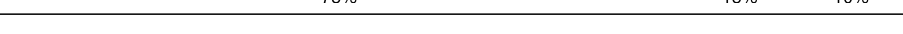
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 86% 11% .
1	a	344	 82% 14% .

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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 [i](#)

There are 37 unique types of molecules in this entry. The entry contains 103252 atoms, of which 51649 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	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

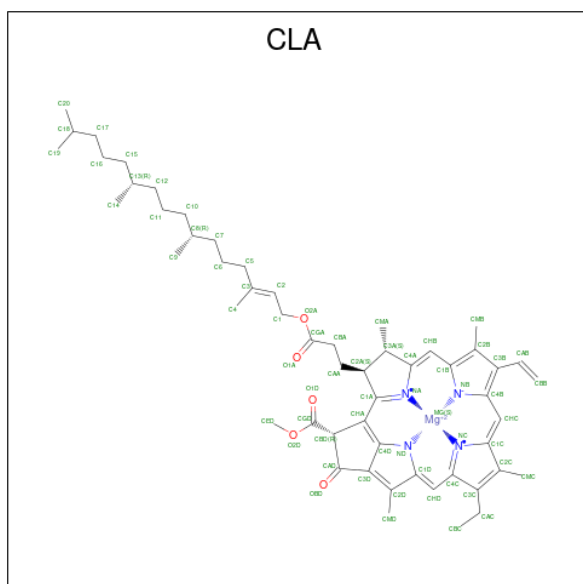
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 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	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	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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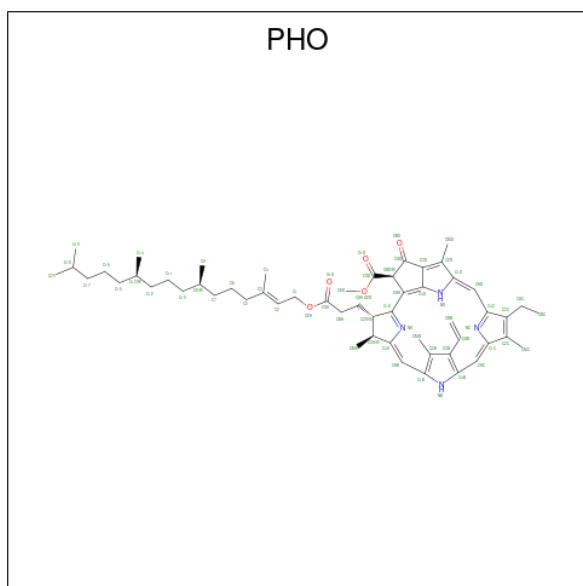
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

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

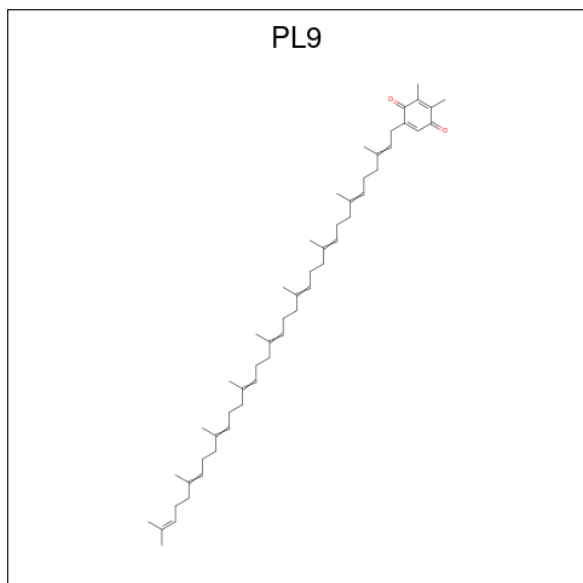


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

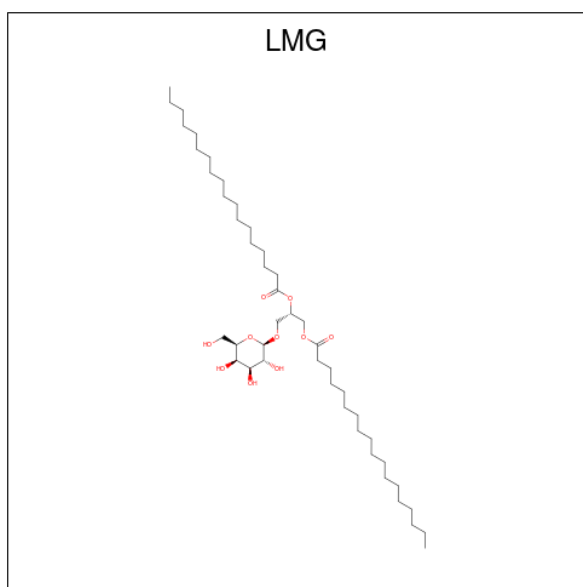
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 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
25	A	1	Total C H O 135 53 80 2	0	0
25	D	1	Total C H O 135 53 80 2	0	0
25	a	1	Total C H O 135 53 80 2	0	0
25	d	1	Total C H O 135 53 80 2	0	0

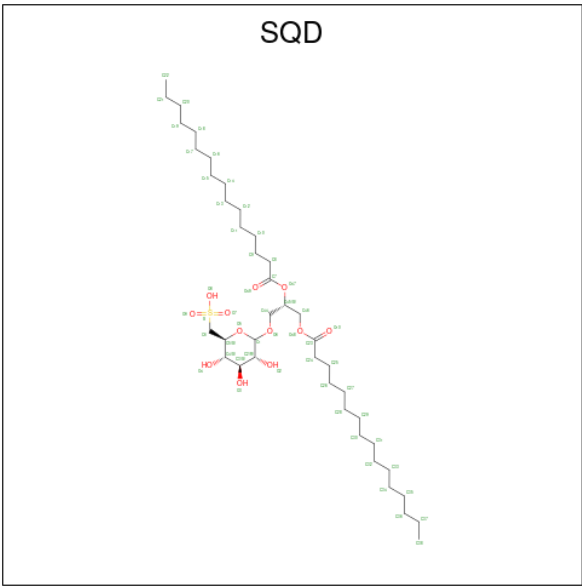
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

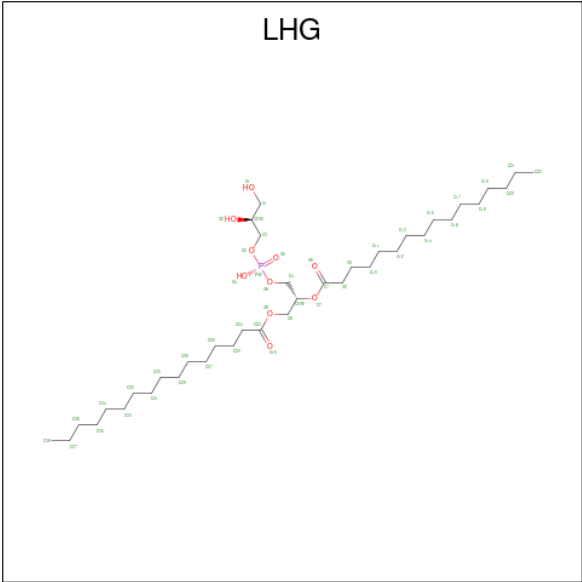
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



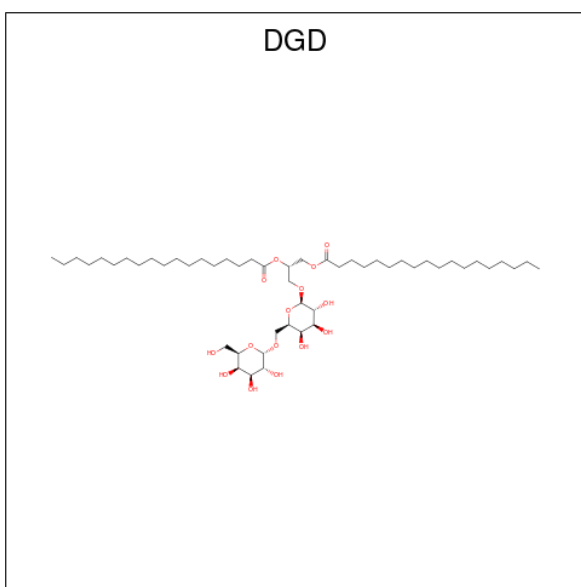
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			132	41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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



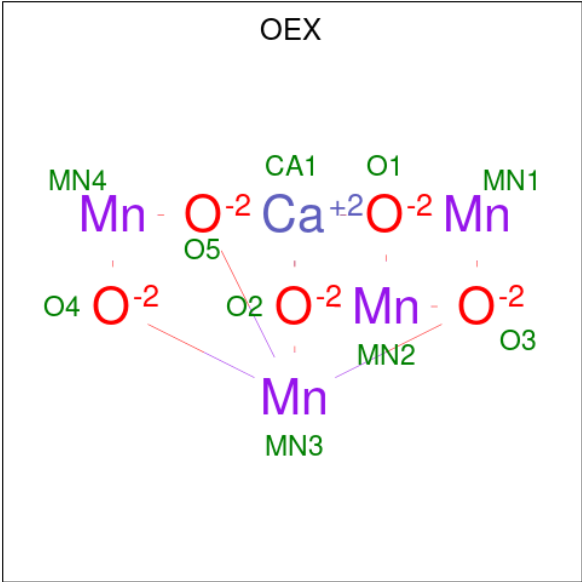
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	a	1	Total	C	H	O	P	0	0
			123	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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



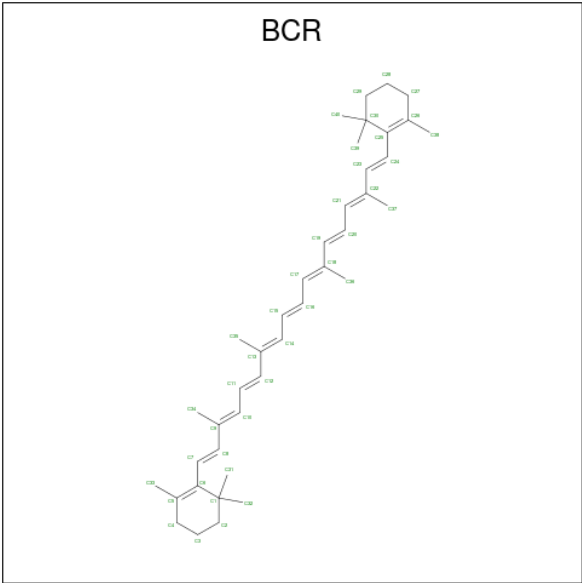
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



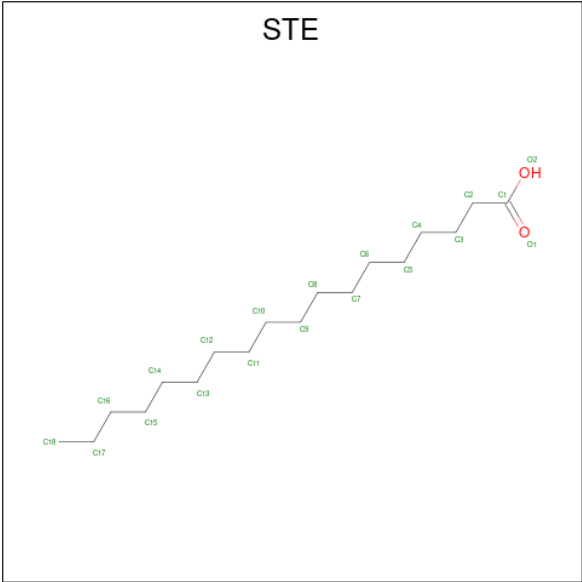
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	B	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	C	1	Total	C	H	0	0
			96	40	56		
31	D	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		
31	I	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	T	1	Total	C	H	0	0
			96	40	56		
31	Z	1	Total	C	H	0	0
			96	40	56		
31	a	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	d	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	t	1	Total	C	H	0	0
			96	40	56		
31	x	1	Total	C	H	0	0
			96	40	56		

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



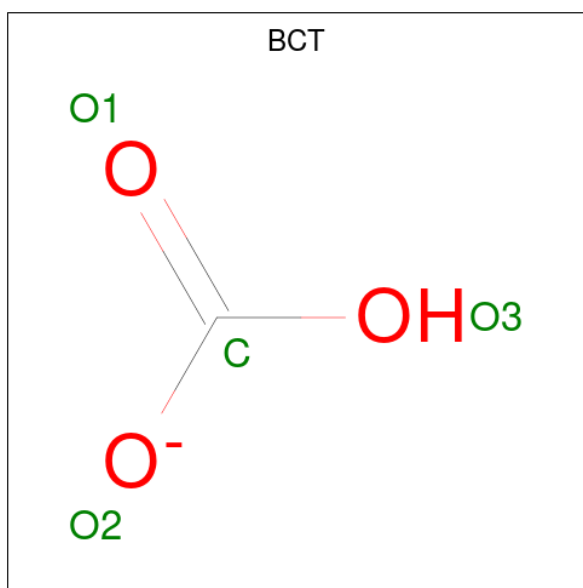
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	L	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	1	Total	C	H	O	0	0
			37	13	22	2		
32	M	1	Total	C	H		0	0
			26	10	16			

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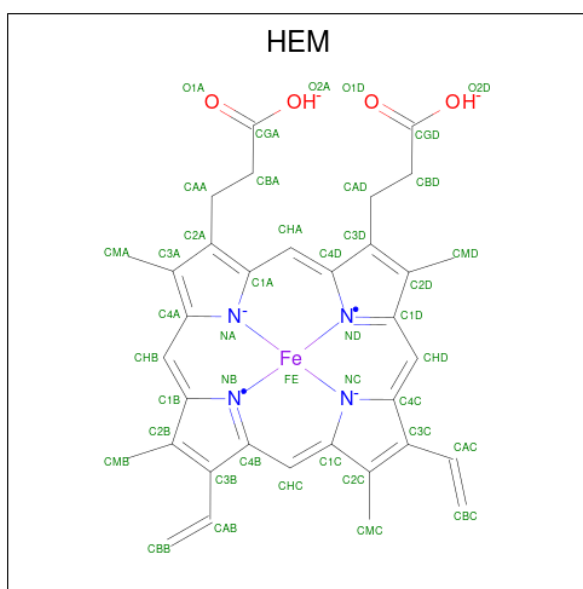
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total C H O 28 10 16 2	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	a	1	Total C H 41 15 26	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H 44 15 29	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	b	1	Total C H 41 14 27	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	x	1	Total C H O 55 18 35 2	0	0

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



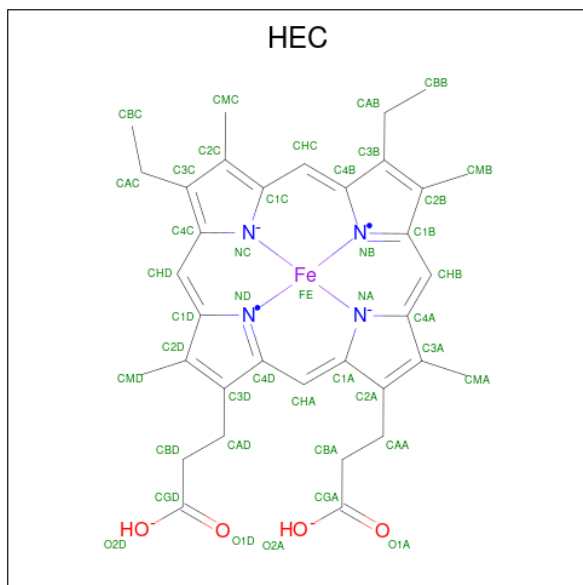
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- 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	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	V	1	Total	Na	0	0
			1	1		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	125	Total	O	0	0
			125	125		
37	B	135	Total	O	0	0
			135	135		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	119	Total 119	O 119	0	0
37	D	103	Total 103	O 103	0	0
37	E	20	Total 20	O 20	0	0
37	F	5	Total 5	O 5	0	0
37	H	22	Total 22	O 22	0	0
37	I	12	Total 12	O 12	0	0
37	J	11	Total 11	O 11	0	0
37	K	6	Total 6	O 6	0	0
37	L	9	Total 9	O 9	0	0
37	M	6	Total 6	O 6	0	0
37	O	68	Total 68	O 68	0	0
37	R	8	Total 8	O 8	0	0
37	T	7	Total 7	O 7	0	0
37	U	30	Total 30	O 30	0	0
37	V	49	Total 49	O 49	0	0
37	X	9	Total 9	O 9	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	6	Total 6	O 6	0	0
37	a	99	Total 99	O 99	0	0
37	b	114	Total 114	O 114	0	0
37	c	120	Total 120	O 120	0	0

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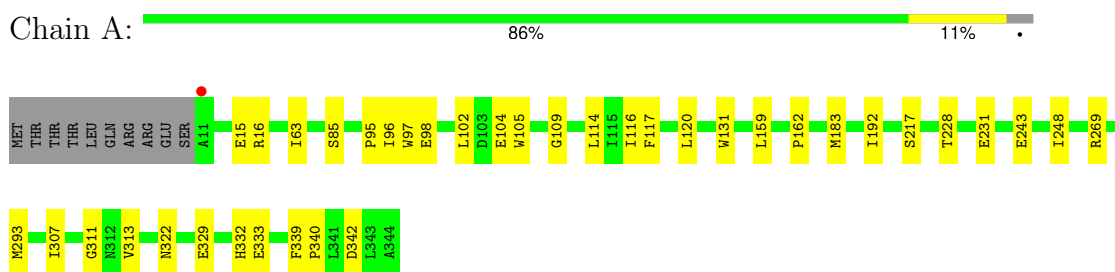
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	88	Total 88	O 88	0	0
37	e	18	Total 18	O 18	0	0
37	f	5	Total 5	O 5	0	0
37	h	22	Total 22	O 22	0	0
37	i	8	Total 8	O 8	0	0
37	j	9	Total 9	O 9	0	0
37	k	2	Total 2	O 2	0	0
37	l	11	Total 11	O 11	0	0
37	m	2	Total 2	O 2	0	0
37	o	70	Total 70	O 70	0	0
37	t	11	Total 11	O 11	0	0
37	u	35	Total 35	O 35	0	0
37	v	32	Total 32	O 32	0	0
37	x	7	Total 7	O 7	0	0
37	y	6	Total 6	O 6	0	0
37	z	11	Total 11	O 11	0	0

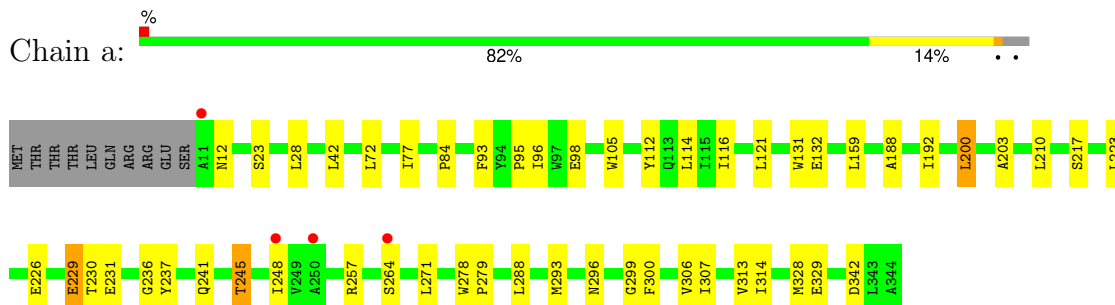
3 Residue-property plots [i](#)

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.

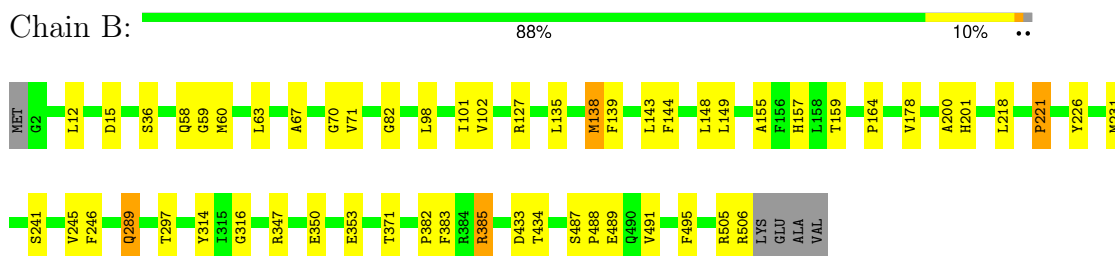
- Molecule 1: Photosystem II protein D1 1

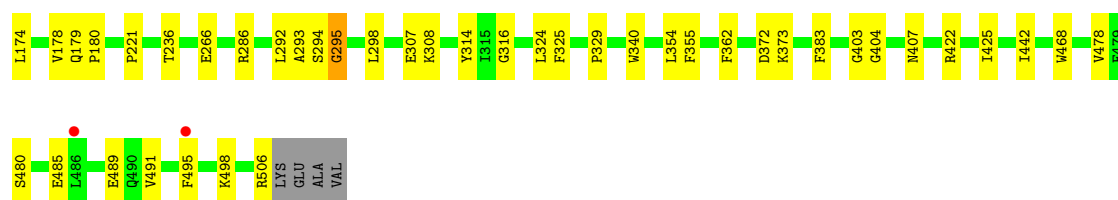


- Molecule 1: Photosystem II protein D1 1



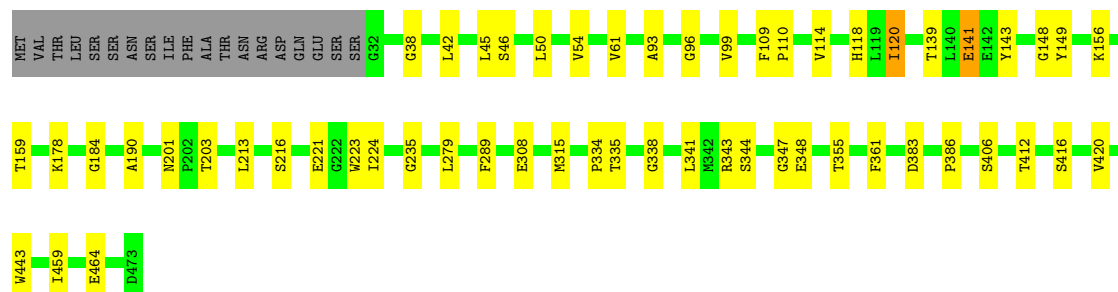
- Molecule 2: Photosystem II CP47 reaction center protein





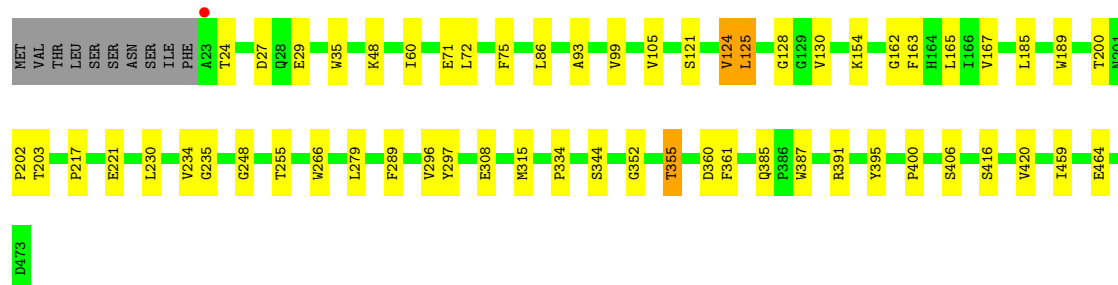
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 84% 12%



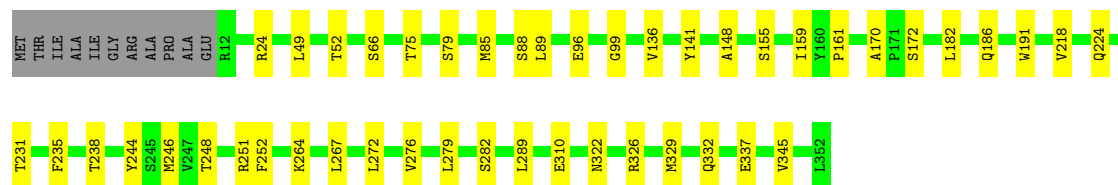
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12%



• Molecule 4: Photosystem II D2 protein

Chain D: 84% 13%



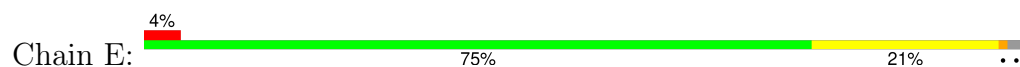
• Molecule 4: Photosystem II D2 protein

Chain d: 82% 14%

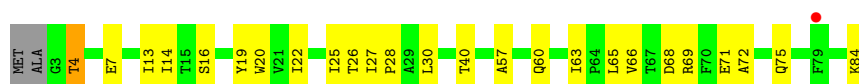




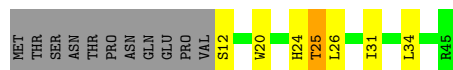
- Molecule 5: Cytochrome b559 subunit alpha



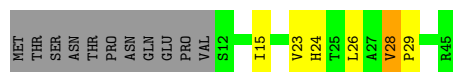
- Molecule 5: Cytochrome b559 subunit alpha



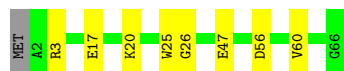
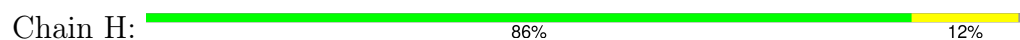
- Molecule 6: Cytochrome b559 subunit beta



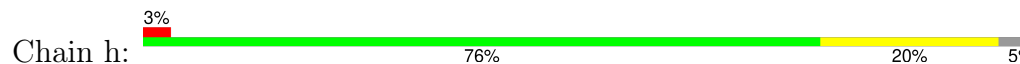
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



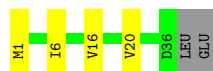
- Molecule 8: Photosystem II reaction center protein I





- Molecule 8: Photosystem II reaction center protein I

Chain i: 84% 11% 5%



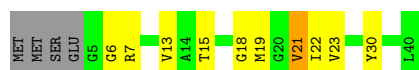
- Molecule 9: Photosystem II reaction center protein J

Chain J: 75% 15% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 65% 22% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 63% 15% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 52% 24% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 84% 16%

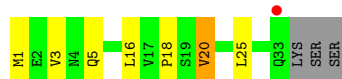
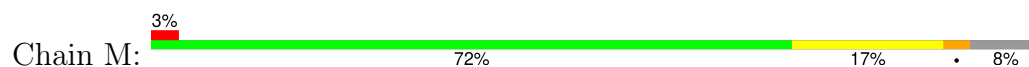


- Molecule 11: Photosystem II reaction center protein L

Chain l: 84% 14%



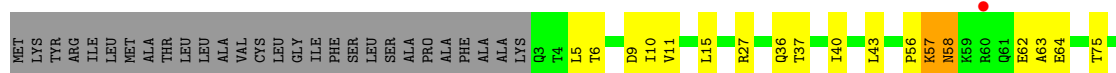
- Molecule 12: Photosystem II reaction center protein M



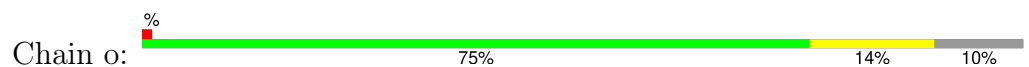
- Molecule 12: Photosystem II reaction center protein M



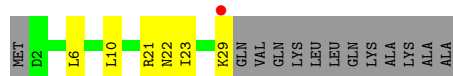
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

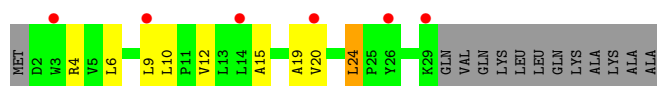


- Molecule 14: Photosystem II protein Y

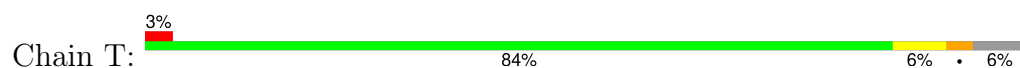


- Molecule 14: Photosystem II protein Y

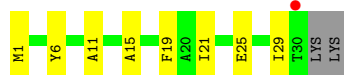




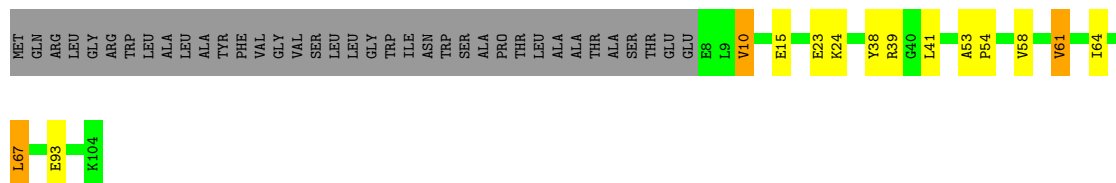
- Molecule 15: Photosystem II reaction center protein T



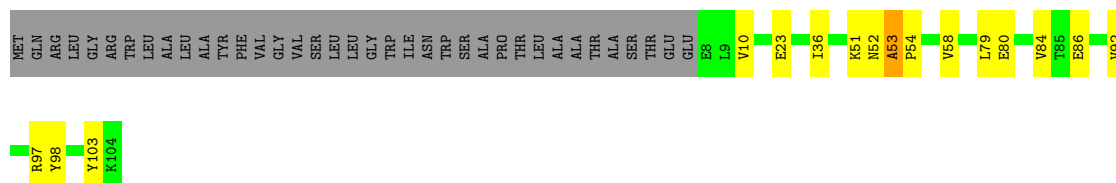
- Molecule 15: Photosystem II reaction center protein T



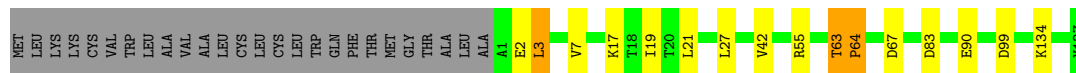
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein

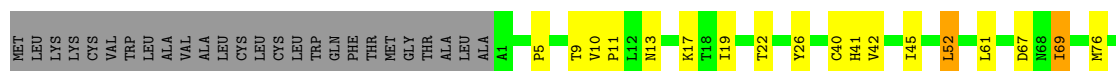


- Molecule 17: Cytochrome c-550

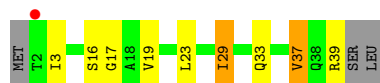


- Molecule 17: Cytochrome c-550

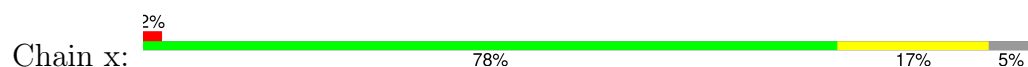




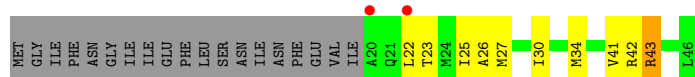
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



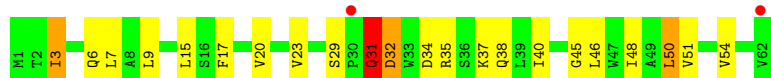
- Molecule 19: Photosystem II reaction center protein Ycf12



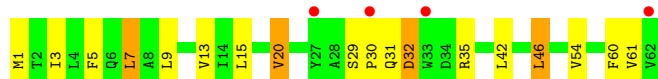
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.2 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.245	Depositor DCC
R_{free} test set	3275 reflections (0.52%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	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	103252	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/2707	0.70	0/3692
1	a	0.60	0/2704	0.68	0/3688
2	B	0.59	1/4161 (0.0%)	0.66	1/5669 (0.0%)
2	b	0.57	1/4118 (0.0%)	0.64	1/5611 (0.0%)
3	C	0.56	0/3547	0.64	0/4830
3	c	0.52	0/3619	0.63	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.58	0/2821	0.66	0/3844
5	E	0.49	0/688	0.54	0/940
5	e	0.44	0/683	0.54	0/932
6	F	0.47	0/284	0.59	0/387
6	f	0.46	0/284	0.59	0/387
7	H	0.57	0/523	0.62	0/713
7	h	0.50	0/511	0.60	0/697
8	I	0.57	0/293	0.70	0/396
8	i	0.56	0/293	0.57	0/396
9	J	0.50	0/263	0.61	0/356
9	j	0.44	0/263	0.59	0/356
10	K	0.44	0/303	0.53	0/416
10	k	0.41	0/303	0.52	0/416
11	L	0.60	0/311	0.59	0/422
11	l	0.63	0/303	0.58	0/412
12	M	0.62	0/249	0.60	0/341
12	m	0.62	0/244	0.74	0/334
13	O	0.55	0/1904	0.64	0/2585
13	o	0.58	0/1905	0.65	0/2583
14	R	0.37	0/227	0.51	0/313
14	r	0.32	0/227	0.44	0/313
15	T	0.66	0/257	0.70	0/349
15	t	0.58	0/255	0.63	0/346
16	U	0.54	0/785	0.61	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.61	1/785 (0.1%)	0.69	0/1064
17	V	0.55	0/1085	0.65	0/1473
17	v	0.49	0/1085	0.59	0/1473
18	X	0.48	0/284	0.53	0/384
18	x	0.43	0/289	0.54	0/391
19	Y	0.41	0/197	0.50	0/264
19	y	0.33	0/219	0.51	0/294
20	Z	0.38	0/490	0.50	0/669
20	z	0.34	0/488	0.45	0/666
All	All	0.56	3/42769 (0.0%)	0.64	2/58224 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	-8.47	1.47	1.51
16	u	103	TYR	CA-C	6.27	1.55	1.52
2	B	221	PRO	CA-C	-5.97	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	221	PRO	O-C-N	-6.56	118.29	121.31
2	B	221	PRO	O-C-N	-5.91	118.37	121.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	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	25	0
1	a	2619	2510	2510	36	0
2	B	4005	3873	3867	36	0
2	b	3978	3836	3836	41	0
3	C	3426	3355	3343	34	0
3	c	3500	3426	3426	33	0
4	D	2717	2621	2621	35	0
4	d	2723	2627	2627	32	0
5	E	666	651	651	17	0
5	e	664	648	648	16	0
6	F	275	282	282	5	0
6	f	275	282	282	3	0
7	H	510	532	532	4	0
7	h	498	518	518	6	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	4	0
9	j	257	268	268	7	0
10	K	293	305	305	6	0
10	k	293	305	305	7	0
11	L	304	316	316	6	0
11	l	296	304	304	1	0
12	M	256	269	269	4	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	30	0
13	o	1874	1846	1846	17	0
14	R	221	238	238	1	0
14	r	221	238	238	5	0
15	T	258	261	261	2	0
15	t	256	256	256	5	0
16	U	774	773	773	7	0
16	u	774	773	773	8	0
17	V	1064	1073	1073	8	0
17	v	1064	1073	1074	21	0
18	X	281	312	312	7	0
18	x	286	316	314	4	0
19	Y	196	217	217	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	8	0
20	Z	479	516	516	16	0
20	z	477	509	509	13	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	5	0
22	B	1035	1139	1139	21	0
22	C	839	922	922	18	0
22	D	195	216	216	4	0
22	a	130	144	144	1	0
22	b	1035	1139	1139	23	0
22	c	839	919	919	14	0
22	d	260	288	288	2	0
23	A	64	74	74	0	0
23	D	64	74	74	3	0
23	a	64	74	74	0	0
23	d	64	74	74	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	2	0
25	D	55	80	80	1	0
25	a	55	80	80	0	0
25	d	55	80	80	1	0
26	A	48	66	66	1	0
26	B	83	126	126	0	0
26	D	84	117	117	2	0
26	M	51	72	72	1	0
26	Y	48	66	66	1	0
26	b	55	86	86	1	0
26	c	134	181	181	4	0
26	d	44	58	58	0	0
26	m	51	72	71	2	0
27	A	91	135	135	3	0
27	B	54	78	77	0	0
27	D	36	45	44	1	0
27	L	49	65	64	4	0
27	a	54	78	78	0	0
27	f	41	48	47	1	0
27	t	36	56	56	1	0
28	A	49	74	74	4	0
28	D	145	215	215	9	0
28	L	49	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	49	74	74	5	0
28	d	88	125	125	3	0
28	e	42	57	57	0	0
28	l	49	74	74	1	0
29	A	66	96	96	1	0
29	C	186	246	244	6	0
29	H	62	82	81	0	0
29	c	186	245	242	6	0
29	h	62	82	82	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	120	168	168	7	0
31	C	40	56	56	3	0
31	D	40	56	56	3	0
31	H	40	56	56	0	0
31	I	40	56	56	1	0
31	K	80	112	112	0	0
31	T	40	56	56	1	0
31	Z	40	56	56	0	0
31	a	40	56	56	0	0
31	b	120	168	168	1	0
31	c	80	112	112	1	0
31	d	40	56	56	2	0
31	k	80	112	112	0	0
31	t	40	56	56	2	0
31	x	40	56	56	1	0
32	B	75	117	114	4	0
32	C	40	63	60	2	0
32	H	18	35	35	1	0
32	I	15	26	26	2	0
32	J	12	16	16	2	0
32	L	12	16	16	1	0
32	M	25	38	38	0	0
32	R	12	16	16	0	0
32	X	20	35	35	4	0
32	Z	8	12	12	0	0
32	a	27	42	42	0	0
32	b	111	197	191	7	0
32	c	32	51	51	1	0
32	d	37	61	61	5	0
32	j	12	16	16	2	0
32	l	18	35	35	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	t	24	36	36	1	0
32	x	20	35	35	1	0
33	D	4	1	1	0	0
33	a	4	1	1	0	0
34	F	43	30	30	4	0
34	f	43	30	30	5	0
35	V	43	32	30	0	0
35	v	43	32	31	6	0
36	V	1	0	0	0	0
37	A	125	0	0	5	0
37	B	135	0	0	8	0
37	C	119	0	0	4	0
37	D	103	0	0	5	0
37	E	20	0	0	4	0
37	F	5	0	0	1	0
37	H	22	0	0	2	0
37	I	12	0	0	0	0
37	J	11	0	0	1	0
37	K	6	0	0	1	0
37	L	9	0	0	2	0
37	M	6	0	0	1	0
37	O	68	0	0	5	0
37	R	8	0	0	0	0
37	T	7	0	0	1	0
37	U	30	0	0	1	0
37	V	49	0	0	2	0
37	X	9	0	0	2	0
37	Y	3	0	0	0	0
37	Z	6	0	0	1	0
37	a	99	0	0	7	0
37	b	114	0	0	4	0
37	c	120	0	0	5	0
37	d	88	0	0	2	0
37	e	18	0	0	2	0
37	f	5	0	0	0	0
37	h	22	0	0	4	0
37	i	8	0	0	0	0
37	j	9	0	0	0	0
37	k	2	0	0	0	0
37	l	11	0	0	0	0
37	m	2	0	0	0	0
37	o	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	t	11	0	0	0	0
37	u	35	0	0	2	0
37	v	32	0	0	2	0
37	x	7	0	0	0	0
37	y	6	0	0	3	0
37	z	11	0	0	3	0
All	All	51603	51649	51604	588	0

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 6.

The worst 5 of 588 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)
17:v:40:CYS:SG	35:v:201:HEC:CAC	2.10	1.40
16:u:36:ILE:O	37:u:201:HOH:O	1.82	0.97
34:F:101:HEM:O2A	37:F:201:HOH:O	1.82	0.96
17:v:40:CYS:SG	35:v:201:HEC:HAC	2.03	0.96
2:b:372:ASP:OD2	37:b:701:HOH:O	1.82	0.95

There are no symmetry-related clashes.

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%)	325 (98%)	7 (2%)	0	100	100
1	a	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	487 (97%)	13 (3%)	3 (1%)	21	25
3	C	442/461 (96%)	424 (96%)	17 (4%)	1 (0%)	43	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	53
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	61 (97%)	1 (2%)	1 (2%)	7	6
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	10	10
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	30	36
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	11
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	1
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	1
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	6
All	All	5231/5700 (92%)	5049 (96%)	165 (3%)	17 (0%)	36	44

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
20	Z	31	GLN
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%)	265 (98%)	5 (2%)	50	66
1	a	269/280 (96%)	256 (95%)	13 (5%)	23	32
2	B	408/407 (100%)	397 (97%)	11 (3%)	39	55
2	b	402/407 (99%)	387 (96%)	15 (4%)	30	43
3	C	346/362 (96%)	337 (97%)	9 (3%)	40	56
3	c	354/362 (98%)	340 (96%)	14 (4%)	28	40
4	D	276/283 (98%)	271 (98%)	5 (2%)	51	68
4	d	277/283 (98%)	264 (95%)	13 (5%)	23	33
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	37
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	17
6	F	28/39 (72%)	26 (93%)	2 (7%)	13	17
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	66
7	h	53/55 (96%)	47 (89%)	6 (11%)	5	6
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	4
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	50
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	37
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	19
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	7
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	7
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	31
13	o	207/228 (91%)	196 (95%)	11 (5%)	20	28
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	1
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	1
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	42
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	40
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	32
16	u	84/112 (75%)	80 (95%)	4 (5%)	23	32
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	18
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	23
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	8
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	8
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	7
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	10
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	3
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	8
All	All	4321/4654 (93%)	4110 (95%)	211 (5%)	22	31

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	29	GLU
5	e	66	VAL
17	v	107	LEU
3	c	125	LEU
4	d	182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	415	ASN
13	o	61	GLN
18	x	38	GLN
13	O	124	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
15	FME	t	1	15	8,9,10	1.49	1 (12%)	8,9,11	1.16	1 (12%)
12	FME	m	1	12	8,9,10	1.07	0	8,9,11	1.52	2 (25%)
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	0.76	0
8	FME	i	1	8	8,9,10	1.10	1 (12%)	8,9,11	1.13	0
15	FME	T	1	15	8,9,10	0.99	0	8,9,11	1.02	1 (12%)
12	FME	M	1	12	8,9,10	1.07	1 (12%)	8,9,11	0.96	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
15	FME	t	1	15	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	4/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.87	1.40	1.46
12	M	1	FME	CA-N	-2.24	1.43	1.46
8	I	1	FME	CA-N	-2.13	1.43	1.46
8	i	1	FME	CA-N	-2.13	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.98	127.41	122.82
12	m	1	FME	CB-CA-N	2.42	114.92	110.52
15	t	1	FME	CA-N-CN	-2.26	119.35	122.82
15	T	1	FME	CG-CB-CA	2.04	119.09	112.87

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

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 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 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$
32	STE	B	623	-	11,11,19	0.76	0	11,11,19	1.17	1 (9%)
32	STE	R	101	-	11,11,19	0.86	0	11,11,19	0.89	0
22	CLA	c	511	3	69,73,73	1.41	8 (11%)	82,113,113	1.49	5 (6%)
22	CLA	b	615	2	69,73,73	1.88	11 (15%)	82,113,113	1.29	9 (10%)
32	STE	C	518	-	11,11,19	0.98	1 (9%)	11,11,19	1.23	1 (9%)
27	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.79	10 (20%)
31	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	10 (17%)
32	STE	b	627	-	13,13,19	0.47	0	12,12,19	0.56	0
22	CLA	d	405	4	69,73,73	1.52	11 (15%)	82,113,113	1.22	6 (7%)
22	CLA	c	513	3	69,73,73	1.31	9 (13%)	82,113,113	1.20	7 (8%)
31	BCR	a	405	-	41,41,41	1.23	5 (12%)	56,56,56	1.44	9 (16%)
22	CLA	A	402	1	69,73,73	1.22	7 (10%)	82,113,113	1.48	12 (14%)
31	BCR	K	101	-	41,41,41	1.30	3 (7%)	56,56,56	1.23	6 (10%)
31	BCR	Z	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.34	5 (8%)
23	PHO	D	401	-	58,69,69	2.05	9 (15%)	55,99,99	1.46	8 (14%)
22	CLA	b	612	2	69,73,73	1.35	8 (11%)	82,113,113	1.52	13 (15%)
29	DGD	A	413	-	67,67,67	1.26	8 (11%)	81,81,81	1.37	11 (13%)
32	STE	X	101	-	19,19,19	0.71	1 (5%)	19,19,19	1.11	0
32	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMG	c	522	-	49,49,55	1.20	5 (10%)	57,57,63	1.42	7 (12%)
22	CLA	c	505	3	69,73,73	1.11	6 (8%)	82,113,113	1.30	7 (8%)
32	STE	t	104	-	9,9,19	0.58	0	8,8,19	0.45	0
22	CLA	B	609	2	69,73,73	1.27	7 (10%)	82,113,113	1.46	11 (13%)
31	BCR	b	618	-	41,41,41	1.56	4 (9%)	56,56,56	1.28	7 (12%)
31	BCR	I	101	-	41,41,41	1.24	5 (12%)	56,56,56	1.40	9 (16%)
22	CLA	a	404	1	69,73,73	1.38	10 (14%)	82,113,113	1.26	9 (10%)
32	STE	L	103	-	11,11,19	0.72	0	11,11,19	1.33	2 (18%)
22	CLA	A	403	37	69,73,73	1.45	11 (15%)	82,113,113	1.31	10 (12%)
22	CLA	C	507	37	69,73,73	1.19	5 (7%)	82,113,113	1.49	10 (12%)
32	STE	d	412	-	19,19,19	0.76	1 (5%)	19,19,19	0.93	0
26	LMG	A	409	-	48,48,55	1.19	3 (6%)	56,56,63	1.44	10 (17%)
22	CLA	b	602	2	69,73,73	1.34	9 (13%)	82,113,113	1.42	8 (9%)
31	BCR	b	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.29	5 (8%)
22	CLA	b	614	2	69,73,73	1.42	11 (15%)	82,113,113	1.42	11 (13%)
27	SQD	A	412	-	38,38,54	1.07	3 (7%)	40,40,65	1.39	4 (10%)
32	STE	b	624	-	14,14,19	0.35	0	13,13,19	1.01	0
22	CLA	B	607	37	69,73,73	1.43	10 (14%)	82,113,113	1.26	6 (7%)
32	STE	Z	102	-	7,7,19	0.52	0	6,6,19	0.29	0
22	CLA	C	503	3	69,73,73	1.40	10 (14%)	82,113,113	1.64	11 (13%)
32	STE	c	520	-	19,19,19	0.79	1 (5%)	19,19,19	0.89	0
26	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.35	7 (12%)
29	DGD	C	515	-	63,63,67	1.37	9 (14%)	77,77,81	1.35	11 (14%)
31	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.17	5 (8%)
23	PHO	a	403	-	58,69,69	1.95	11 (18%)	55,99,99	1.53	9 (16%)
22	CLA	C	501	3	69,73,73	1.63	11 (15%)	82,113,113	1.43	6 (7%)
29	DGD	h	101	-	63,63,67	1.11	4 (6%)	77,77,81	1.41	14 (18%)
32	STE	b	623	-	15,15,19	0.84	1 (6%)	15,15,19	0.87	0
32	STE	I	102	-	14,14,19	0.54	0	13,13,19	0.51	0
30	OEX	A	414	37,3,1	0,14,14	-	-	-	-	-
27	SQD	a	411	-	52,54,54	1.04	4 (7%)	62,65,65	1.68	11 (17%)
28	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.14	3 (5%)
26	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.39	8 (13%)
22	CLA	B	605	2	69,73,73	1.07	4 (5%)	82,113,113	1.33	10 (12%)
22	CLA	B	613	2	69,73,73	1.82	11 (15%)	82,113,113	1.21	8 (9%)
22	CLA	b	605	2	69,73,73	1.17	10 (14%)	82,113,113	1.50	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	512	3	69,73,73	1.37	11 (15%)	82,113,113	1.38	9 (10%)
22	CLA	b	604	2	69,73,73	1.21	7 (10%)	82,113,113	1.46	11 (13%)
22	CLA	B	610	37	69,73,73	1.34	9 (13%)	82,113,113	1.49	11 (13%)
22	CLA	b	609	2	69,73,73	1.49	10 (14%)	82,113,113	1.41	11 (13%)
32	STE	H	103	-	17,17,19	0.47	0	16,16,19	0.68	0
35	HEC	V	201	17	50,50,50	1.63	5 (10%)	68,82,82	1.52	15 (22%)
28	LHG	A	411	-	48,48,48	0.88	3 (6%)	51,54,54	1.26	6 (11%)
32	STE	b	626	-	9,9,19	0.52	0	8,8,19	0.52	0
26	LMG	d	410	-	44,44,55	1.27	5 (11%)	52,52,63	1.29	5 (9%)
32	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.30	1 (9%)
23	PHO	d	402	-	58,69,69	2.15	11 (18%)	55,99,99	1.73	11 (20%)
26	LMG	b	622	-	55,55,55	1.15	6 (10%)	63,63,63	1.38	7 (11%)
31	BCR	T	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.30	6 (10%)
29	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.53	12 (15%)
22	CLA	B	616	2	64,68,73	1.62	10 (15%)	76,107,113	1.43	8 (10%)
22	CLA	c	507	37	69,73,73	1.76	11 (15%)	82,113,113	1.48	12 (14%)
22	CLA	d	401	37	69,73,73	1.25	10 (14%)	82,113,113	1.33	11 (13%)
22	CLA	d	404	37	69,73,73	1.44	8 (11%)	82,113,113	1.66	13 (15%)
25	PL9	A	408	-	55,55,55	1.59	4 (7%)	68,69,69	1.53	11 (16%)
22	CLA	b	601	37	69,73,73	1.41	10 (14%)	82,113,113	1.39	9 (10%)
32	STE	l	102	-	17,17,19	0.44	0	16,16,19	0.83	0
27	SQD	t	102	-	35,35,54	1.13	2 (5%)	37,37,65	1.38	4 (10%)
32	STE	a	412	-	11,11,19	0.85	0	11,11,19	0.92	0
31	BCR	B	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.32	12 (14%)
32	STE	t	103	-	13,13,19	0.77	0	13,13,19	1.36	3 (23%)
27	SQD	L	101	-	47,49,54	0.97	2 (4%)	57,60,65	2.16	16 (28%)
26	LMG	B	626	-	55,55,55	1.23	7 (12%)	63,63,63	1.31	5 (7%)
32	STE	j	101	-	11,11,19	0.95	1 (9%)	11,11,19	0.85	0
25	PL9	D	407	-	55,55,55	1.46	8 (14%)	68,69,69	1.54	13 (19%)
26	LMG	c	519	-	37,37,55	1.41	7 (18%)	45,45,63	1.37	5 (11%)
27	SQD	B	622	-	52,54,54	1.01	3 (5%)	62,65,65	1.92	13 (20%)
33	BCT	D	402	21	3,3,3	1.03	0	2,3,3	3.61	2 (100%)
30	OEX	a	414	37,3,1	0,14,14	-	-	-	-	-
22	CLA	b	608	2	69,73,73	1.12	7 (10%)	82,113,113	1.33	7 (8%)
33	BCT	a	408	21	3,3,3	1.16	0	2,3,3	3.37	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	f	101	6,5	50,50,50	1.37	7 (14%)	67,82,82	1.25	5 (7%)
29	DGD	c	517	-	63,63,67	1.07	6 (9%)	77,77,81	1.53	13 (16%)
28	LHG	D	411	-	46,46,48	1.02	3 (6%)	49,52,54	1.23	4 (8%)
29	DGD	c	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.40	10 (12%)
32	STE	a	413	-	14,14,19	0.48	0	13,13,19	0.69	0
31	BCR	c	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	C	509	3	69,73,73	1.29	8 (11%)	82,113,113	1.32	9 (10%)
22	CLA	B	602	2	69,73,73	1.41	10 (14%)	82,113,113	1.38	11 (13%)
22	CLA	B	614	2	69,73,73	1.17	5 (7%)	82,113,113	1.28	9 (10%)
35	HEC	v	201	17	50,50,50	1.59	6 (12%)	68,82,82	1.59	13 (19%)
22	CLA	d	403	4	69,73,73	1.47	12 (17%)	82,113,113	1.24	8 (9%)
22	CLA	b	616	2	64,68,73	1.15	7 (10%)	76,107,113	1.53	11 (14%)
32	STE	b	621	-	19,19,19	0.72	0	19,19,19	0.99	1 (5%)
31	BCR	t	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.37	7 (12%)
31	BCR	d	406	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	8 (14%)
31	BCR	D	406	-	41,41,41	1.26	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	D	404	37	69,73,73	1.49	9 (13%)	82,113,113	1.26	7 (8%)
22	CLA	c	506	3	69,73,73	1.49	7 (10%)	82,113,113	1.36	9 (10%)
22	CLA	c	510	3	69,73,73	1.14	7 (10%)	82,113,113	1.23	8 (9%)
32	STE	B	620	-	16,16,19	0.78	0	16,16,19	0.96	0
32	STE	b	625	-	19,19,19	0.74	0	19,19,19	0.74	0
32	STE	x	102	-	19,19,19	0.71	0	19,19,19	1.13	2 (10%)
32	STE	M	103	-	9,9,19	0.65	0	8,8,19	0.46	0
29	DGD	C	516	-	63,63,67	1.25	9 (14%)	77,77,81	1.48	16 (20%)
31	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.23	5 (8%)
22	CLA	B	601	37	69,73,73	1.49	9 (13%)	82,113,113	1.32	6 (7%)
25	PL9	a	409	-	55,55,55	1.05	3 (5%)	68,69,69	1.65	15 (22%)
32	STE	B	624	-	17,17,19	0.68	0	17,17,19	0.99	0
27	SQD	D	409	-	34,36,54	1.02	3 (8%)	42,45,65	1.90	10 (23%)
22	CLA	b	603	2	69,73,73	1.32	8 (11%)	82,113,113	1.65	13 (15%)
31	BCR	C	514	-	41,41,41	1.28	2 (4%)	56,56,56	1.34	9 (16%)
28	LHG	a	410	-	48,48,48	0.91	1 (2%)	51,54,54	1.29	6 (11%)
22	CLA	A	405	1	58,62,73	1.31	9 (15%)	68,99,113	1.50	10 (14%)
34	HEM	F	101	6,5	50,50,50	1.45	4 (8%)	67,82,82	1.25	8 (11%)
22	CLA	B	604	2	69,73,73	1.46	9 (13%)	82,113,113	1.79	18 (21%)
26	LMG	D	412	-	31,31,55	1.03	3 (9%)	33,33,63	1.18	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	B	625	-	15,15,19	0.49	0	14,14,19	0.84	0
22	CLA	C	506	3	69,73,73	1.60	12 (17%)	82,113,113	1.24	8 (9%)
22	CLA	c	504	37	64,68,73	1.23	7 (10%)	76,107,113	1.21	8 (10%)
22	CLA	C	502	3	69,73,73	1.60	8 (11%)	82,113,113	1.36	10 (12%)
28	LHG	D	413	-	48,48,48	1.02	3 (6%)	51,54,54	1.37	6 (11%)
22	CLA	B	611	2	69,73,73	1.42	9 (13%)	82,113,113	1.63	12 (14%)
22	CLA	B	606	2	69,73,73	1.76	10 (14%)	82,113,113	1.26	10 (12%)
22	CLA	B	612	2	69,73,73	1.20	9 (13%)	82,113,113	1.45	9 (10%)
22	CLA	D	403	4	69,73,73	1.17	4 (5%)	82,113,113	1.17	5 (6%)
28	LHG	D	410	-	48,48,48	0.95	3 (6%)	51,54,54	1.24	6 (11%)
22	CLA	c	508	3	68,72,73	1.22	9 (13%)	80,111,113	1.26	10 (12%)
22	CLA	C	508	3	69,73,73	1.31	8 (11%)	82,113,113	1.44	14 (17%)
32	STE	c	523	-	11,11,19	0.84	0	11,11,19	1.23	1 (9%)
22	CLA	C	513	3	69,73,73	1.33	10 (14%)	82,113,113	1.50	10 (12%)
26	LMG	D	408	-	51,51,55	0.88	2 (3%)	59,59,63	1.28	6 (10%)
27	SQD	A	410	-	50,52,54	1.09	4 (8%)	60,63,65	2.04	15 (25%)
29	DGD	C	517	-	63,63,67	1.19	8 (12%)	77,77,81	1.56	12 (15%)
22	CLA	c	501	3	69,73,73	1.46	11 (15%)	82,113,113	1.49	8 (9%)
31	BCR	K	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	5 (8%)
22	CLA	b	610	37	69,73,73	1.71	9 (13%)	82,113,113	1.27	10 (12%)
25	PL9	d	407	-	55,55,55	1.56	10 (18%)	68,69,69	1.58	15 (22%)
22	CLA	b	611	2	69,73,73	1.20	5 (7%)	82,113,113	1.49	14 (17%)
22	CLA	b	607	37	69,73,73	1.33	13 (18%)	82,113,113	1.27	9 (10%)
22	CLA	B	603	2	69,73,73	1.21	9 (13%)	82,113,113	1.41	14 (17%)
22	CLA	c	509	3	69,73,73	1.40	9 (13%)	82,113,113	1.43	11 (13%)
22	CLA	C	510	3	69,73,73	1.33	12 (17%)	82,113,113	1.56	10 (12%)
26	LMG	Y	101	-	48,48,55	1.08	7 (14%)	56,56,63	1.25	6 (10%)
22	CLA	D	405	4	69,73,73	1.68	11 (15%)	82,113,113	1.22	9 (10%)
26	LMG	m	101	-	51,51,55	1.31	6 (11%)	59,59,63	1.39	8 (13%)
31	BCR	B	618	-	41,41,41	1.19	6 (14%)	56,56,56	1.32	6 (10%)
32	STE	M	102	-	14,14,19	0.86	0	14,14,19	0.93	0
22	CLA	C	512	3	69,73,73	1.29	7 (10%)	82,113,113	1.37	7 (8%)
22	CLA	b	613	2	69,73,73	1.45	11 (15%)	82,113,113	1.46	10 (12%)
23	PHO	A	404	-	58,69,69	1.77	11 (18%)	55,99,99	1.68	12 (21%)
29	DGD	c	516	-	63,63,67	1.30	8 (12%)	77,77,81	1.45	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	x	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.41	10 (17%)
32	STE	B	627	-	11,11,19	0.90	0	11,11,19	0.93	0
22	CLA	c	502	3	69,73,73	1.27	12 (17%)	82,113,113	1.40	13 (15%)
31	BCR	k	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.08	3 (5%)
32	STE	C	519	-	15,15,19	0.52	0	14,14,19	0.66	0
28	LHG	d	408	-	48,48,48	0.73	1 (2%)	51,54,54	1.21	4 (7%)
31	BCR	c	515	-	41,41,41	1.20	6 (14%)	56,56,56	1.31	8 (14%)
32	STE	C	520	-	11,11,19	0.75	0	11,11,19	1.22	0
22	CLA	a	402	1	69,73,73	1.36	9 (13%)	82,113,113	1.53	9 (10%)
26	LMG	B	621	-	26,26,55	1.09	2 (7%)	26,26,63	1.08	1 (3%)
32	STE	b	620	-	15,15,19	0.46	0	14,14,19	0.80	0
22	CLA	B	615	2	69,73,73	1.20	9 (13%)	82,113,113	1.31	5 (6%)
22	CLA	C	511	3	69,73,73	1.44	9 (13%)	82,113,113	1.41	3 (3%)
28	LHG	L	102	-	48,48,48	0.84	2 (4%)	51,54,54	1.18	4 (7%)
28	LHG	d	409	-	38,38,48	0.93	2 (5%)	41,44,54	1.23	5 (12%)
28	LHG	e	101	-	41,41,48	1.05	3 (7%)	44,47,54	1.31	4 (9%)
31	BCR	B	619	-	41,41,41	1.28	3 (7%)	56,56,56	1.51	11 (19%)
22	CLA	B	608	2	69,73,73	1.59	10 (14%)	82,113,113	1.16	11 (13%)
22	CLA	c	503	3	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	C	504	37	63,67,73	1.27	8 (12%)	74,105,113	1.30	8 (10%)
22	CLA	b	606	2	69,73,73	1.50	9 (13%)	82,113,113	1.54	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
32	STE	B	623	-	-	6/9/9/17	-
32	STE	R	101	-	-	4/9/9/17	-
22	CLA	c	511	3	-	14/39/115/115	-
22	CLA	b	615	2	-	11/39/115/115	-
32	STE	C	518	-	-	4/9/9/17	-
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
31	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	STE	b	627	-	-	7/11/11/17	-
22	CLA	d	405	4	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	513	3	-	9/39/115/115	-
31	BCR	a	405	-	-	3/29/63/63	0/2/2/2
22	CLA	A	402	1	-	5/39/115/115	-
31	BCR	K	101	-	-	12/29/63/63	0/2/2/2
31	BCR	Z	101	-	-	11/29/63/63	0/2/2/2
23	PHO	D	401	-	-	2/37/103/103	0/5/6/6
22	CLA	b	612	2	-	5/39/115/115	-
29	DGD	A	413	-	-	32/55/95/95	0/2/2/2
32	STE	X	101	-	-	13/17/17/17	-
32	STE	d	411	-	-	8/14/14/17	-
26	LMG	c	522	-	-	25/44/64/70	0/1/1/1
22	CLA	c	505	3	-	11/39/115/115	-
32	STE	t	104	-	-	3/7/7/17	-
22	CLA	B	609	2	-	6/39/115/115	-
31	BCR	b	618	-	-	1/29/63/63	0/2/2/2
31	BCR	I	101	-	-	5/29/63/63	0/2/2/2
22	CLA	a	404	1	-	8/39/115/115	-
32	STE	L	103	-	-	5/9/9/17	-
22	CLA	A	403	37	-	10/39/115/115	-
22	CLA	C	507	37	-	7/39/115/115	-
32	STE	d	412	-	-	9/17/17/17	-
26	LMG	A	409	-	-	18/43/63/70	0/1/1/1
22	CLA	b	602	2	-	13/39/115/115	-
31	BCR	b	617	-	-	9/29/63/63	0/2/2/2
22	CLA	b	614	2	-	16/39/115/115	-
27	SQD	A	412	-	-	19/39/39/69	-
32	STE	b	624	-	-	7/12/12/17	-
22	CLA	B	607	37	-	12/39/115/115	-
32	STE	Z	102	-	-	4/5/5/17	-
22	CLA	C	503	3	-	9/39/115/115	-
32	STE	c	520	-	-	7/17/17/17	-
26	LMG	c	521	-	-	22/43/63/70	0/1/1/1
29	DGD	C	515	-	-	23/51/91/95	0/2/2/2
31	BCR	H	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	a	403	-	-	4/37/103/103	0/5/6/6
22	CLA	C	501	3	-	2/39/115/115	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
32	STE	b	623	-	-	9/13/13/17	-
32	STE	I	102	-	-	4/12/12/17	-
27	SQD	a	411	-	-	21/49/69/69	0/1/1/1
28	LHG	l	101	-	-	16/53/53/53	-
26	LMG	M	101	-	-	20/46/66/70	0/1/1/1
22	CLA	B	605	2	-	13/39/115/115	-
22	CLA	B	613	2	-	11/39/115/115	-
22	CLA	b	605	2	-	15/39/115/115	-
22	CLA	c	512	3	-	20/39/115/115	-
22	CLA	b	604	2	-	10/39/115/115	-
22	CLA	B	610	37	-	10/39/115/115	-
22	CLA	b	609	2	-	14/39/115/115	-
32	STE	H	103	-	-	8/15/15/17	-
35	HEC	V	201	17	1/1/7/7	6/14/54/54	-
28	LHG	A	411	-	-	22/53/53/53	-
32	STE	b	626	-	-	4/7/7/17	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
32	STE	J	101	-	-	8/9/9/17	-
23	PHO	d	402	-	-	8/37/103/103	0/5/6/6
26	LMG	b	622	-	-	30/50/70/70	0/1/1/1
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
29	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	B	616	2	-	8/33/109/115	-
22	CLA	c	507	37	-	12/39/115/115	-
22	CLA	d	401	37	-	13/39/115/115	-
22	CLA	d	404	37	-	4/39/115/115	-
25	PL9	A	408	-	-	18/53/73/73	0/1/1/1
22	CLA	b	601	37	-	22/39/115/115	-
32	STE	l	102	-	-	7/15/15/17	-
27	SQD	t	102	-	-	15/37/37/69	-
32	STE	a	412	-	-	6/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	C	505	3	-	8/39/115/115	-
32	STE	t	103	-	-	4/11/11/17	-
27	SQD	L	101	-	-	29/44/64/69	0/1/1/1
26	LMG	B	626	-	-	35/50/70/70	0/1/1/1
32	STE	j	101	-	-	3/9/9/17	-
25	PL9	D	407	-	-	13/53/73/73	0/1/1/1
26	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	SQD	B	622	-	-	25/49/69/69	0/1/1/1
22	CLA	b	608	2	-	7/39/115/115	-
34	HEM	f	101	6,5	-	4/14/54/54	-
29	DGD	c	517	-	-	19/51/91/95	0/2/2/2
28	LHG	D	411	-	-	19/51/51/53	-
29	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	STE	a	413	-	-	8/12/12/17	-
31	BCR	c	514	-	-	8/29/63/63	0/2/2/2
22	CLA	C	509	3	-	15/39/115/115	-
22	CLA	B	614	2	-	19/39/115/115	-
22	CLA	B	602	2	-	9/39/115/115	-
35	HEC	v	201	17	1/1/7/7	6/14/54/54	-
22	CLA	d	403	4	-	11/39/115/115	-
22	CLA	b	616	2	-	10/33/109/115	-
32	STE	b	621	-	-	10/17/17/17	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
31	BCR	d	406	-	-	8/29/63/63	0/2/2/2
31	BCR	D	406	-	-	7/29/63/63	0/2/2/2
22	CLA	D	404	37	-	7/39/115/115	-
22	CLA	c	506	3	-	13/39/115/115	-
22	CLA	c	510	3	-	14/39/115/115	-
32	STE	B	620	-	-	5/14/14/17	-
32	STE	b	625	-	-	9/17/17/17	-
32	STE	x	102	-	-	13/17/17/17	-
32	STE	M	103	-	-	2/7/7/17	-
29	DGD	C	516	-	-	25/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	k	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	601	37	-	16/39/115/115	-
25	PL9	a	409	-	-	28/53/73/73	0/1/1/1
32	STE	B	624	-	-	11/15/15/17	-
27	SQD	D	409	-	-	13/28/48/69	0/1/1/1
22	CLA	b	603	2	-	10/39/115/115	-
31	BCR	C	514	-	-	6/29/63/63	0/2/2/2
28	LHG	a	410	-	-	21/53/53/53	-
22	CLA	A	405	1	-	5/26/102/115	-
34	HEM	F	101	6,5	-	3/14/54/54	-
22	CLA	B	604	2	-	14/39/115/115	-
26	LMG	D	412	-	-	19/33/33/70	-
32	STE	B	625	-	-	7/13/13/17	-
22	CLA	C	506	3	-	20/39/115/115	-
22	CLA	c	504	37	-	4/33/109/115	-
22	CLA	C	502	3	-	11/39/115/115	-
28	LHG	D	413	-	-	20/53/53/53	-
22	CLA	B	611	2	-	6/39/115/115	-
22	CLA	B	606	2	-	12/39/115/115	-
22	CLA	B	612	2	-	9/39/115/115	-
22	CLA	D	403	4	-	6/39/115/115	-
28	LHG	D	410	-	-	23/53/53/53	-
22	CLA	c	508	3	-	10/38/114/115	-
22	CLA	C	508	3	-	8/39/115/115	-
32	STE	c	523	-	-	6/9/9/17	-
22	CLA	C	513	3	-	9/39/115/115	-
26	LMG	D	408	-	-	15/46/66/70	0/1/1/1
27	SQD	A	410	-	-	20/47/67/69	0/1/1/1
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
22	CLA	c	501	3	-	10/39/115/115	-
31	BCR	K	102	-	-	9/29/63/63	0/2/2/2
22	CLA	b	610	37	-	6/39/115/115	-
25	PL9	d	407	-	-	16/53/73/73	0/1/1/1
22	CLA	b	611	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	607	37	-	15/39/115/115	-
22	CLA	B	603	2	-	16/39/115/115	-
22	CLA	c	509	3	-	8/39/115/115	-
22	CLA	C	510	3	-	8/39/115/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
22	CLA	D	405	4	-	13/39/115/115	-
26	LMG	m	101	-	-	24/46/66/70	0/1/1/1
31	BCR	B	618	-	-	10/29/63/63	0/2/2/2
32	STE	M	102	-	-	6/12/12/17	-
22	CLA	C	512	3	-	14/39/115/115	-
22	CLA	b	613	2	-	10/39/115/115	-
23	PHO	A	404	-	-	7/37/103/103	0/5/6/6
29	DGD	c	516	-	-	20/51/91/95	0/2/2/2
31	BCR	x	101	-	-	6/29/63/63	0/2/2/2
32	STE	B	627	-	-	6/9/9/17	-
22	CLA	c	502	3	-	10/39/115/115	-
31	BCR	k	101	-	-	12/29/63/63	0/2/2/2
32	STE	C	519	-	-	5/13/13/17	-
28	LHG	d	408	-	-	24/53/53/53	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
32	STE	C	520	-	-	4/9/9/17	-
22	CLA	a	402	1	-	2/39/115/115	-
26	LMG	B	621	-	-	12/22/22/70	-
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	B	615	2	-	8/39/115/115	-
22	CLA	C	511	3	-	6/39/115/115	-
28	LHG	L	102	-	-	23/53/53/53	-
28	LHG	d	409	-	-	10/43/43/53	-
28	LHG	e	101	-	-	24/46/46/53	-
31	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	B	608	2	-	11/39/115/115	-
22	CLA	c	503	3	-	7/39/115/115	-
22	CLA	C	504	37	-	8/32/108/115	-
22	CLA	b	606	2	-	5/39/115/115	-

The worst 5 of 971 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-ND	-10.84	1.84	2.05
22	b	610	CLA	MG-NB	-10.06	1.85	2.05
22	B	606	CLA	MG-NA	9.77	2.29	2.06
23	d	402	PHO	C1B-C2B	9.34	1.49	1.39
22	C	502	CLA	MG-NB	-8.85	1.88	2.05

The worst 5 of 1294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	9.53	111.03	106.68
22	c	511	CLA	C4A-NA-C1A	9.38	110.96	106.68
27	L	101	SQD	O6-C1-C2	9.32	122.43	108.27
22	C	511	CLA	C4A-NA-C1A	8.57	110.59	106.68
22	C	510	CLA	C4A-NA-C1A	8.41	110.52	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 2040 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C4B-C3B-CAB-CBB
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	C14-C13-C15-C16
22	C	507	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

121 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	511	CLA	2	0
22	b	615	CLA	3	0
27	f	102	SQD	1	0
32	b	627	STE	3	0
22	c	513	CLA	1	0
22	A	402	CLA	3	0
23	D	401	PHO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	413	DGD	1	0
32	X	101	STE	4	0
32	d	411	STE	2	0
26	c	522	LMG	1	0
22	B	609	CLA	2	0
31	b	618	BCR	1	0
31	I	101	BCR	1	0
32	L	103	STE	1	0
22	A	403	CLA	2	0
22	C	507	CLA	2	0
32	d	412	STE	4	0
26	A	409	LMG	1	0
22	b	602	CLA	2	0
22	b	614	CLA	3	0
32	b	624	STE	2	0
22	B	607	CLA	1	0
26	c	521	LMG	3	0
29	C	515	DGD	1	0
29	h	101	DGD	2	0
32	I	102	STE	2	0
28	l	101	LHG	1	0
26	M	101	LMG	1	0
22	B	605	CLA	3	0
22	B	613	CLA	2	0
22	b	605	CLA	4	0
22	c	512	CLA	2	0
22	b	604	CLA	1	0
22	B	610	CLA	2	0
22	b	609	CLA	3	0
32	H	103	STE	1	0
28	A	411	LHG	4	0
32	J	101	STE	2	0
23	d	402	PHO	2	0
26	b	622	LMG	1	0
31	T	101	BCR	1	0
22	B	616	CLA	1	0
22	d	404	CLA	1	0
25	A	408	PL9	2	0
22	b	601	CLA	1	0
27	t	102	SQD	1	0
31	B	617	BCR	1	0
22	C	505	CLA	2	0

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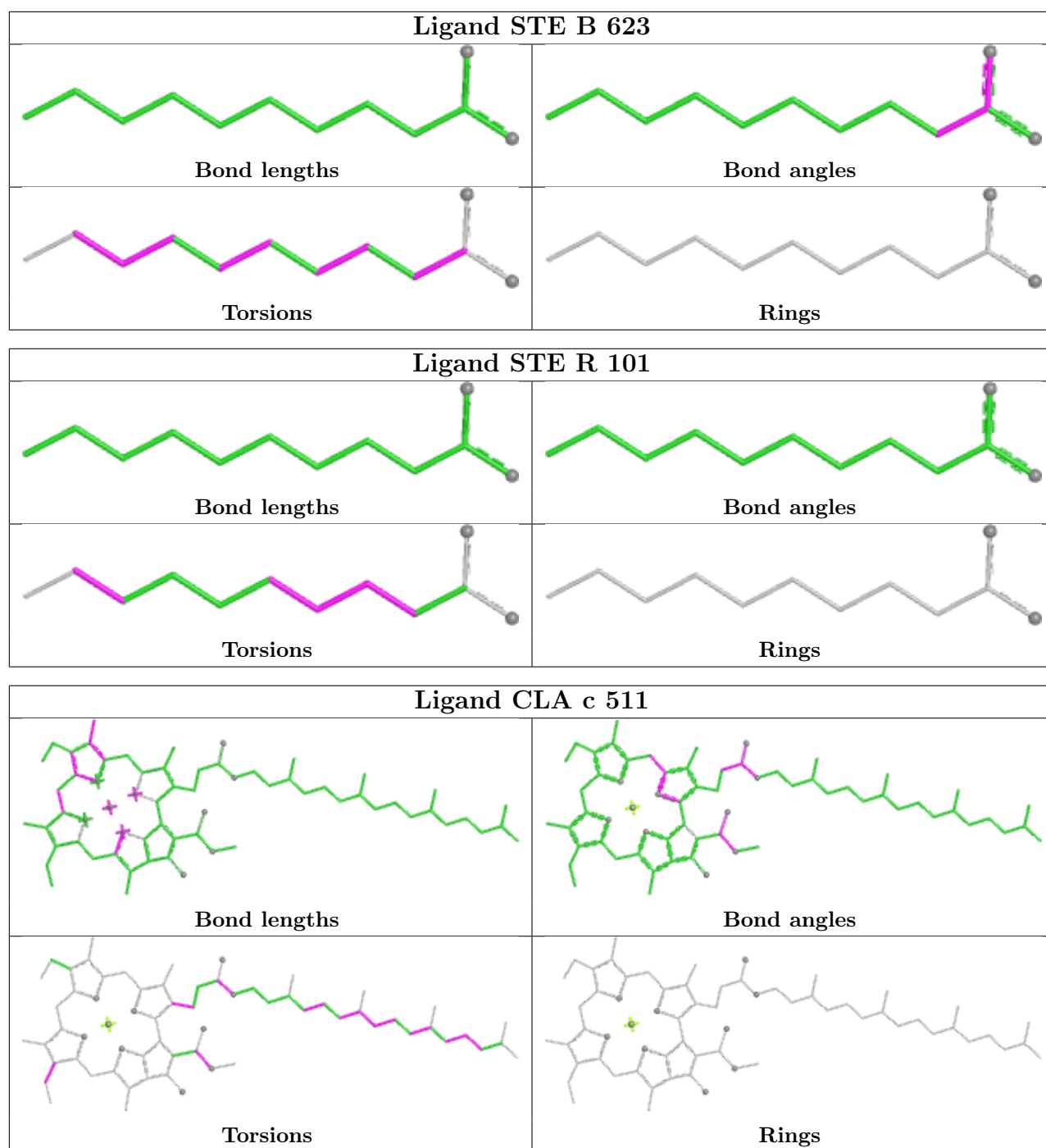
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	t	103	STE	1	0
27	L	101	SQD	4	0
32	j	101	STE	2	0
25	D	407	PL9	1	0
22	b	608	CLA	4	0
34	f	101	HEM	5	0
29	c	517	DGD	2	0
28	D	411	LHG	4	0
29	c	518	DGD	2	0
31	c	514	BCR	1	0
22	C	509	CLA	2	0
22	B	614	CLA	3	0
35	v	201	HEC	6	0
22	d	403	CLA	1	0
22	b	616	CLA	2	0
32	b	621	STE	2	0
31	t	101	BCR	2	0
31	d	406	BCR	2	0
31	D	406	BCR	3	0
22	c	506	CLA	1	0
22	c	510	CLA	1	0
32	B	620	STE	2	0
32	x	102	STE	1	0
29	C	516	DGD	5	0
22	B	601	CLA	1	0
27	D	409	SQD	1	0
31	C	514	BCR	3	0
28	a	410	LHG	5	0
34	F	101	HEM	4	0
22	B	604	CLA	4	0
26	D	412	LMG	1	0
22	C	506	CLA	1	0
22	c	504	CLA	1	0
28	D	413	LHG	4	0
22	B	611	CLA	1	0
22	B	606	CLA	2	0
22	B	612	CLA	1	0
22	D	403	CLA	4	0
28	D	410	LHG	1	0
22	c	508	CLA	2	0
22	C	508	CLA	3	0
32	c	523	STE	1	0

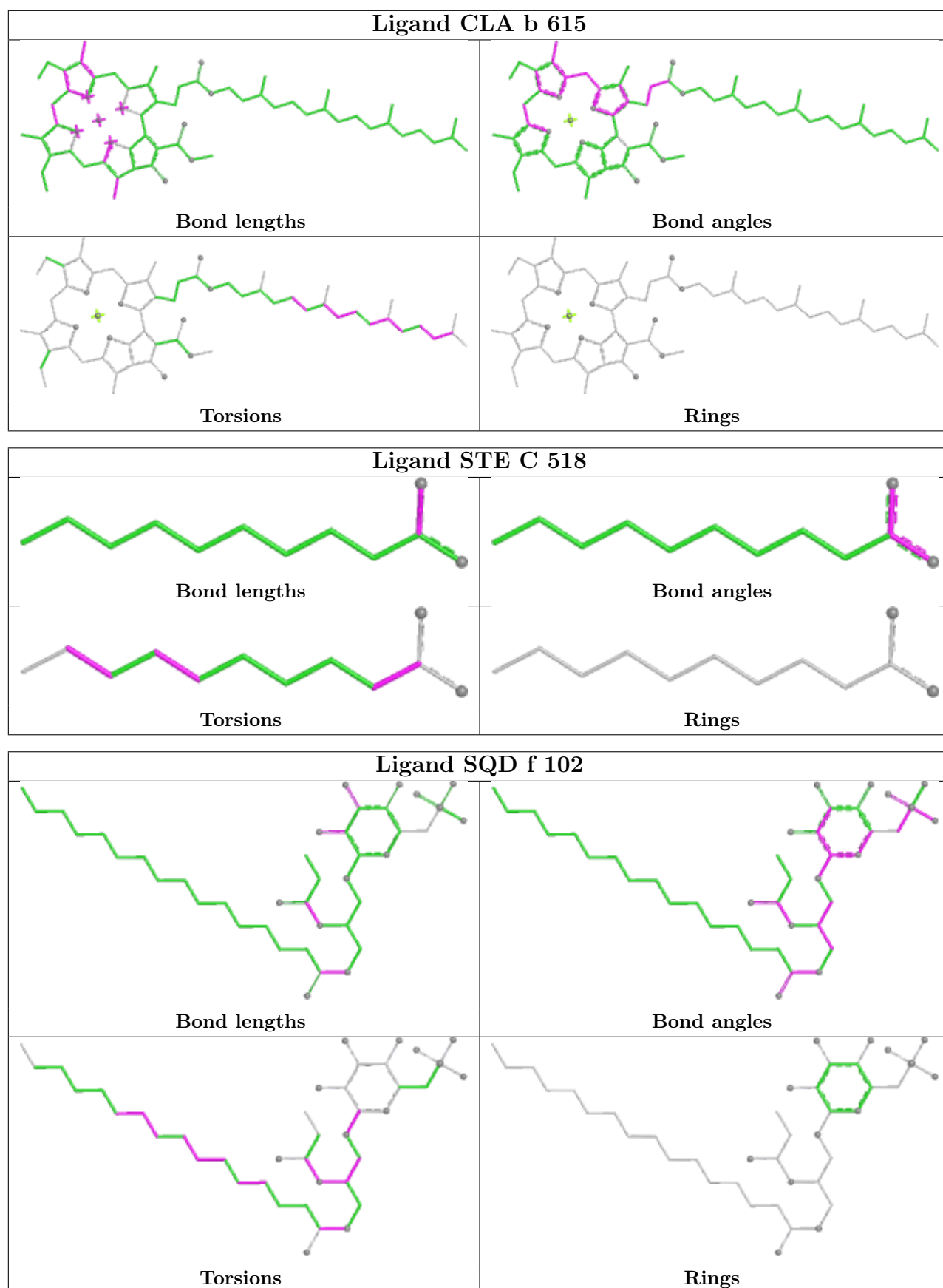
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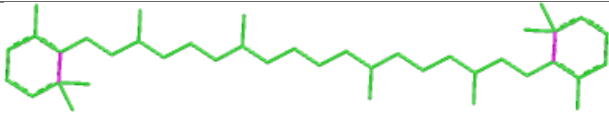
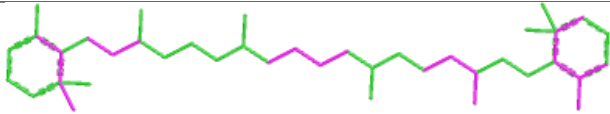
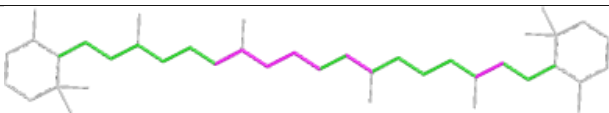
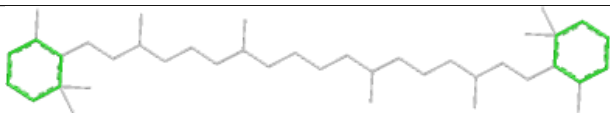
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	513	CLA	3	0
26	D	408	LMG	1	0
27	A	410	SQD	3	0
22	c	501	CLA	2	0
22	b	610	CLA	1	0
25	d	407	PL9	1	0
22	b	611	CLA	1	0
22	b	607	CLA	2	0
22	B	603	CLA	1	0
22	c	509	CLA	2	0
22	C	510	CLA	2	0
26	Y	101	LMG	1	0
26	m	101	LMG	2	0
31	B	618	BCR	4	0
22	b	613	CLA	1	0
29	c	516	DGD	2	0
31	x	101	BCR	1	0
32	B	627	STE	2	0
32	C	519	STE	2	0
28	d	408	LHG	1	0
22	a	402	CLA	1	0
22	B	615	CLA	1	0
22	C	511	CLA	3	0
28	L	102	LHG	1	0
28	d	409	LHG	2	0
31	B	619	BCR	2	0
22	B	608	CLA	2	0
22	c	503	CLA	3	0
22	C	504	CLA	1	0
22	b	606	CLA	1	0

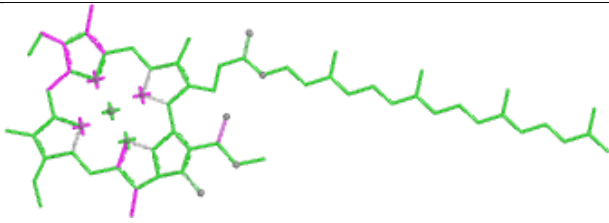
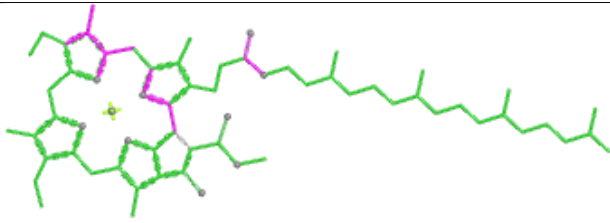
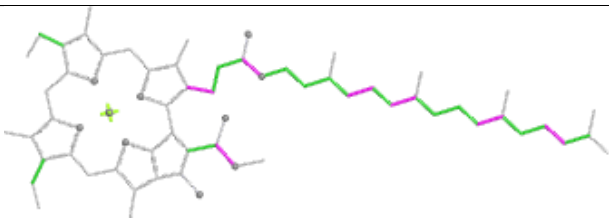
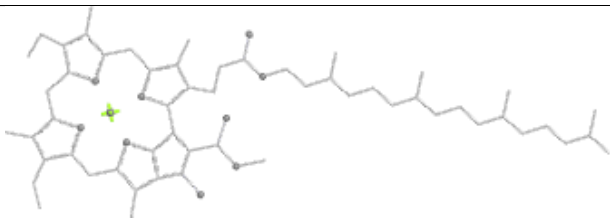
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

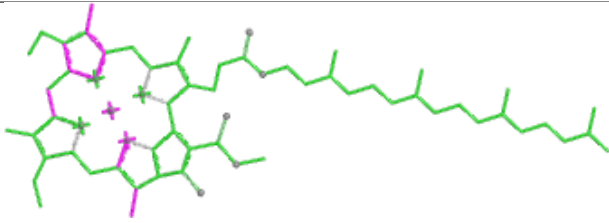
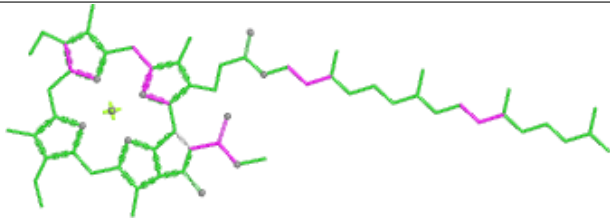
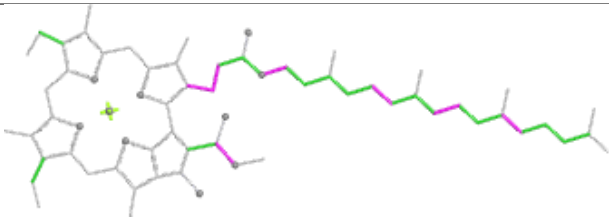
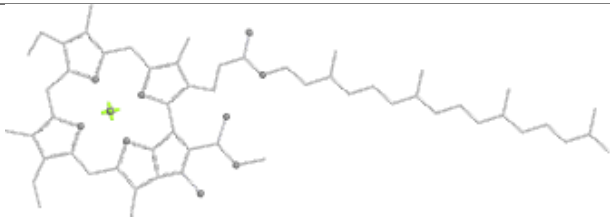


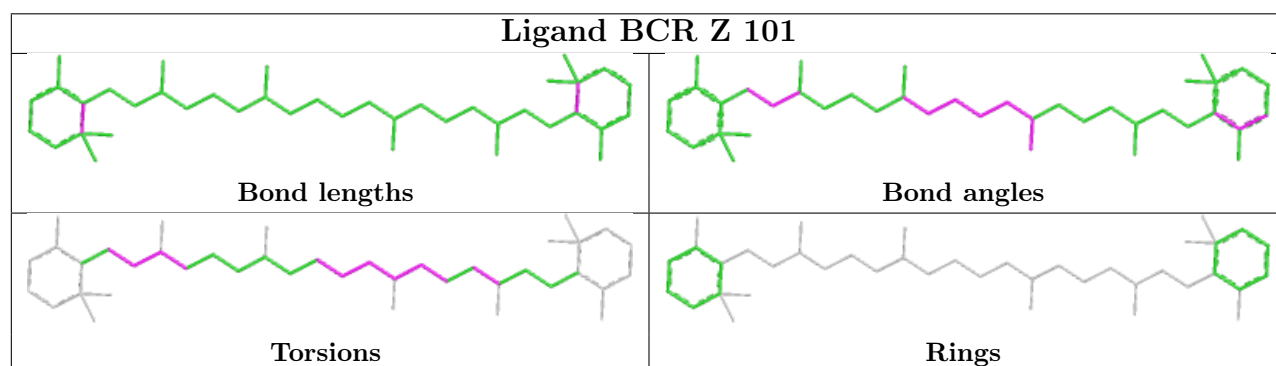
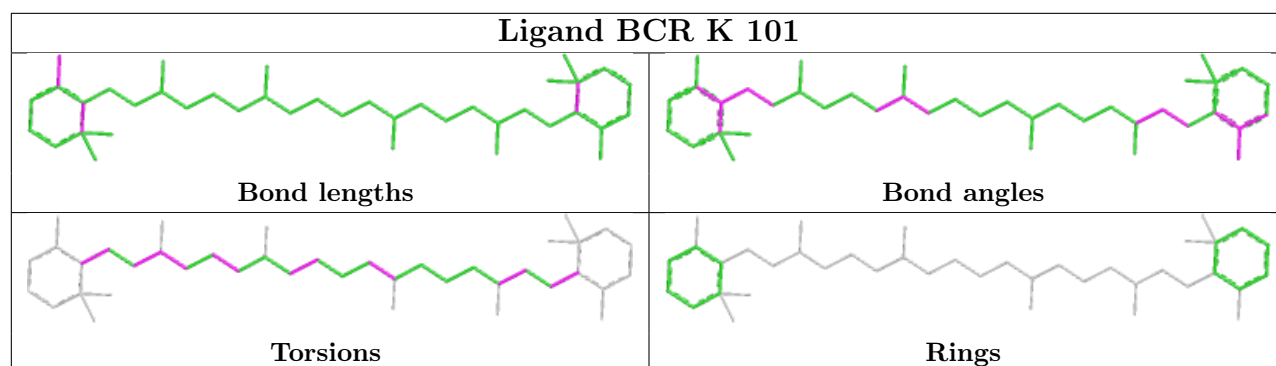
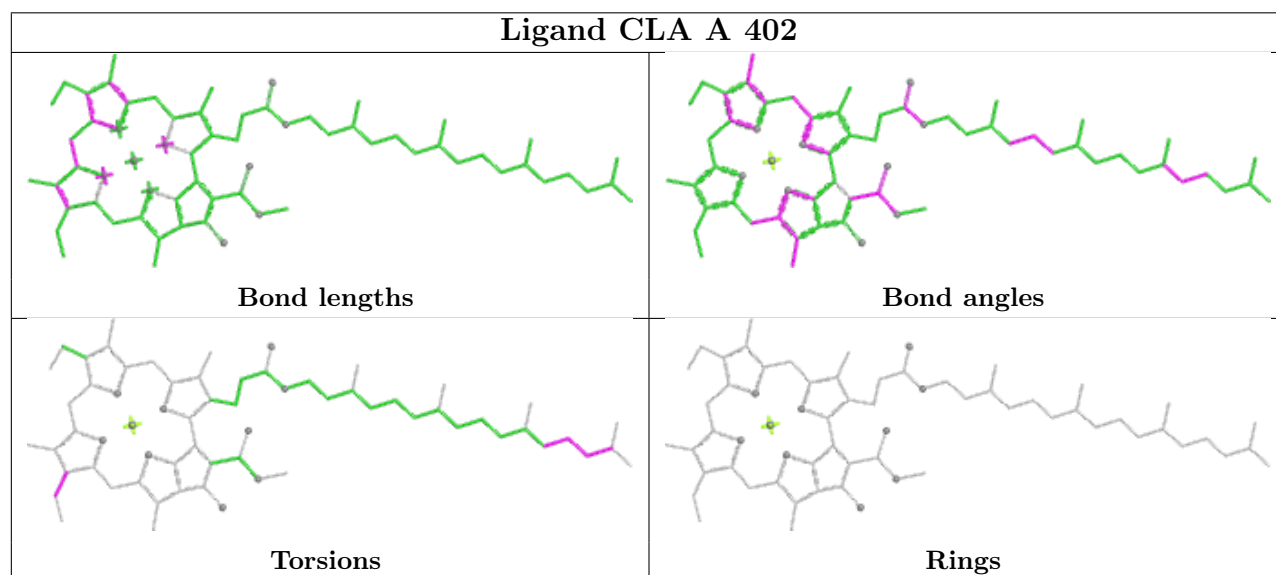
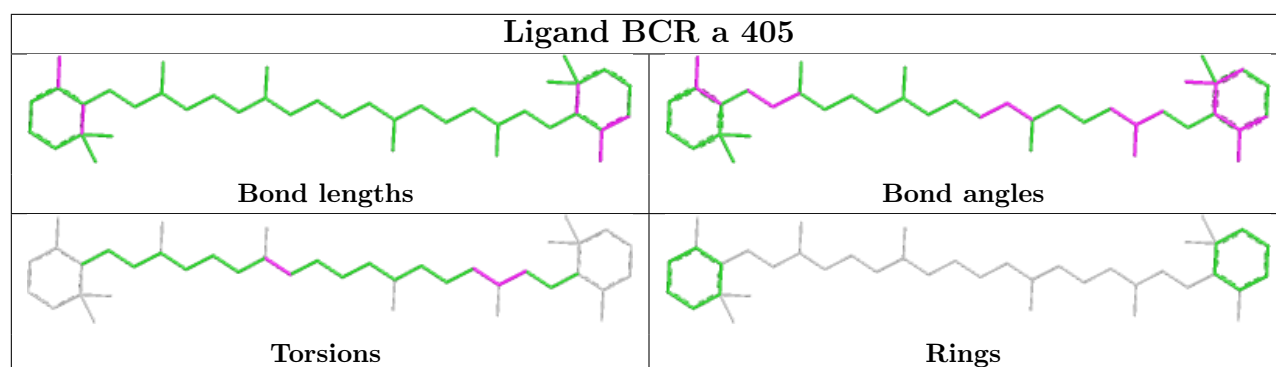


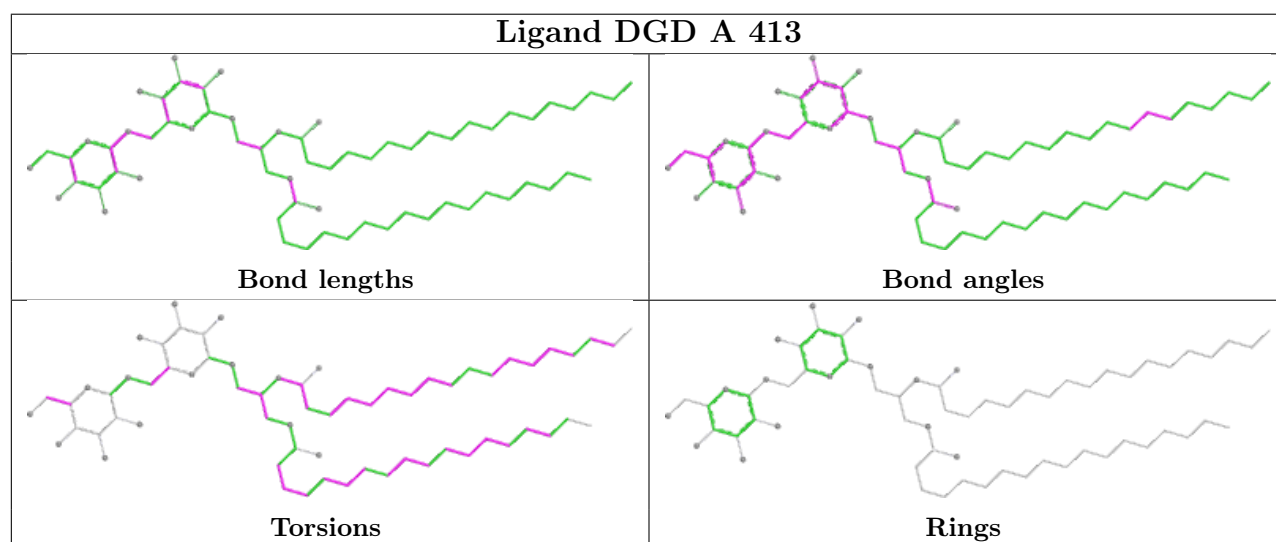
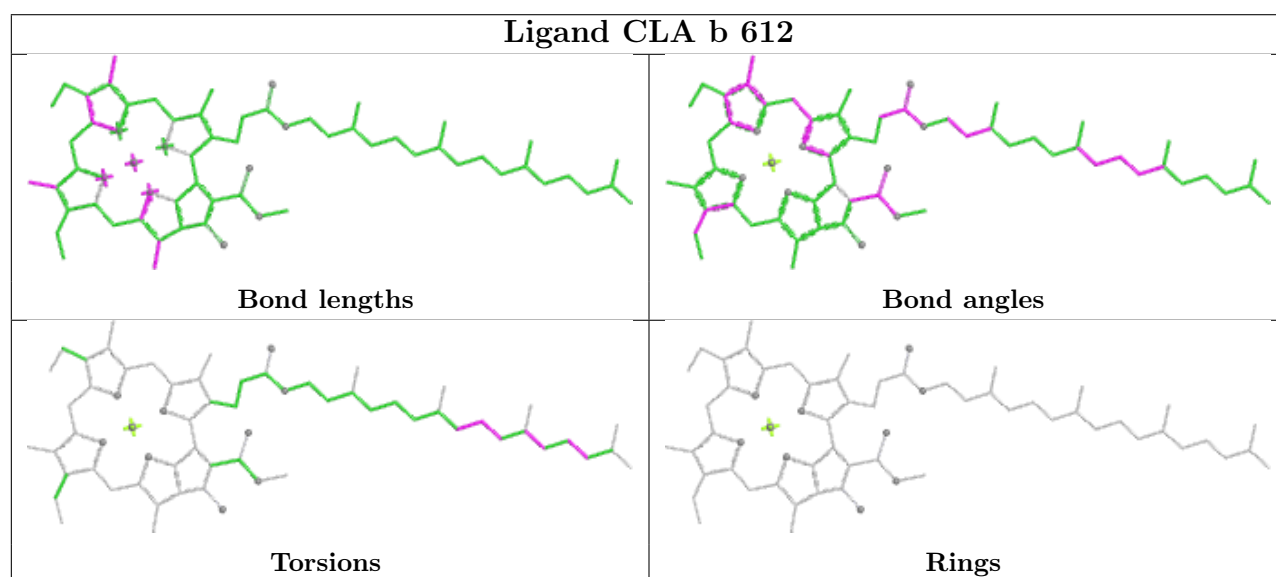
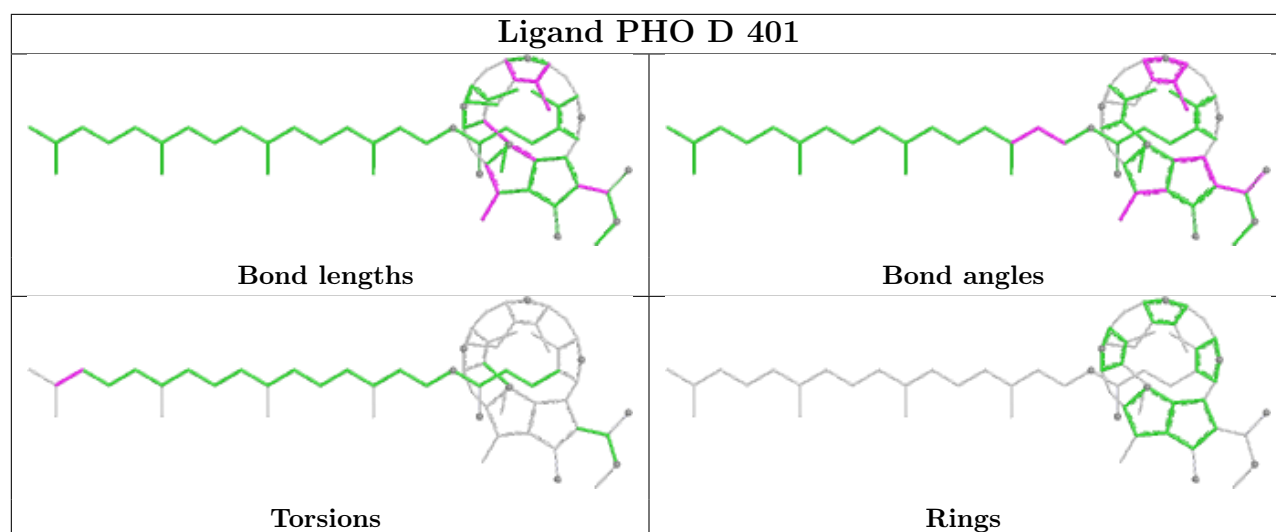
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

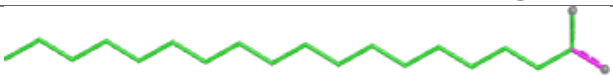
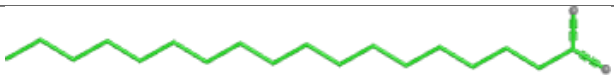
Ligand STE b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

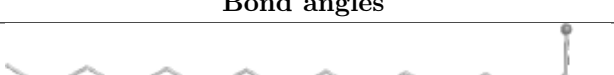
Ligand CLA d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

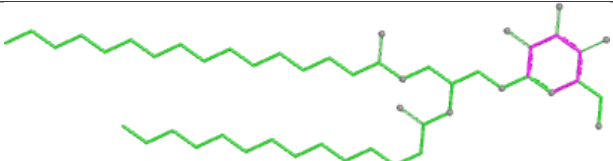
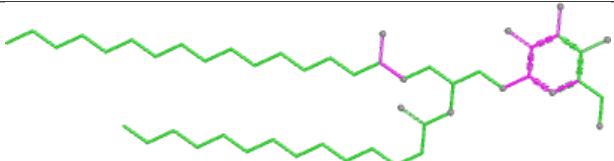
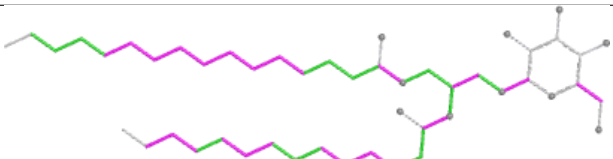
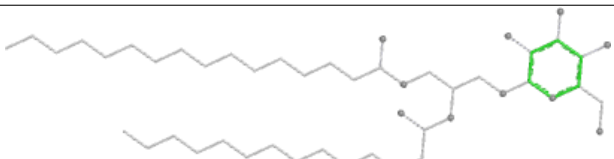
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

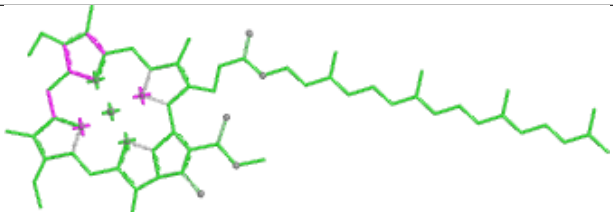
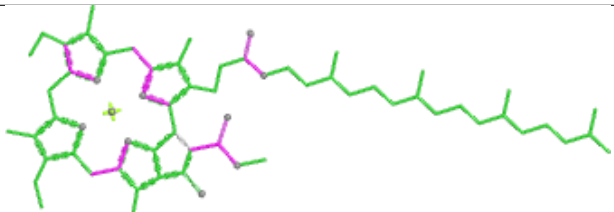
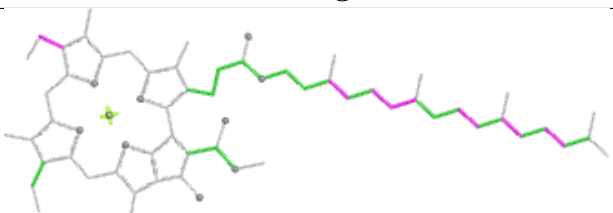
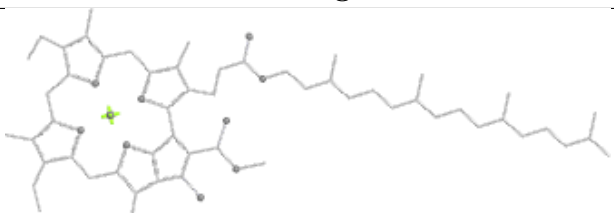




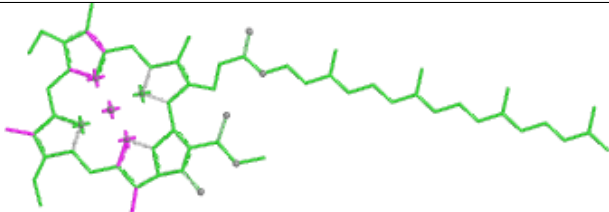
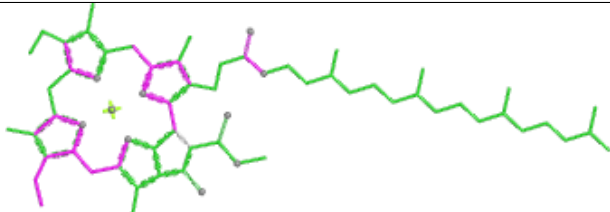
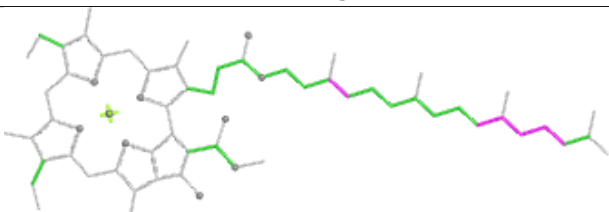
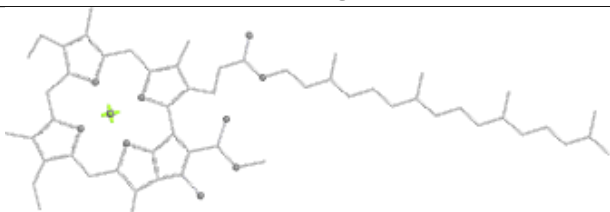
Ligand STE X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

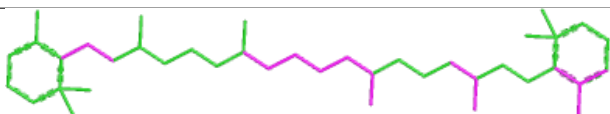
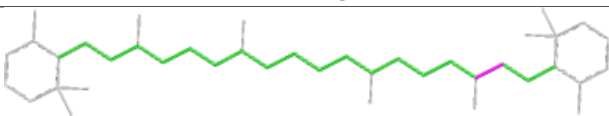
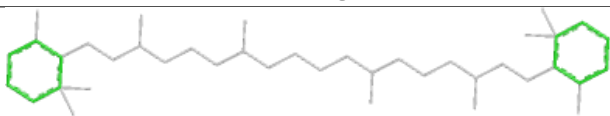
Ligand STE d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

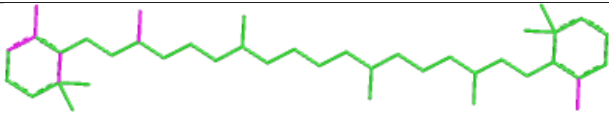
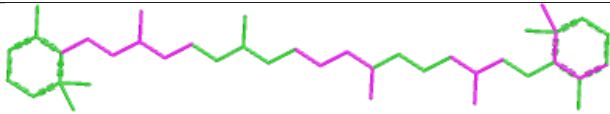
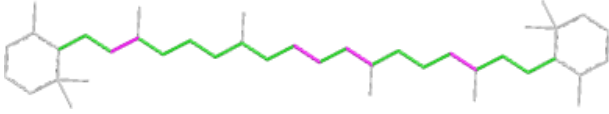
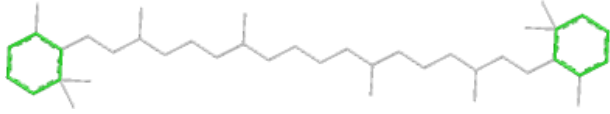
Ligand LMG c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

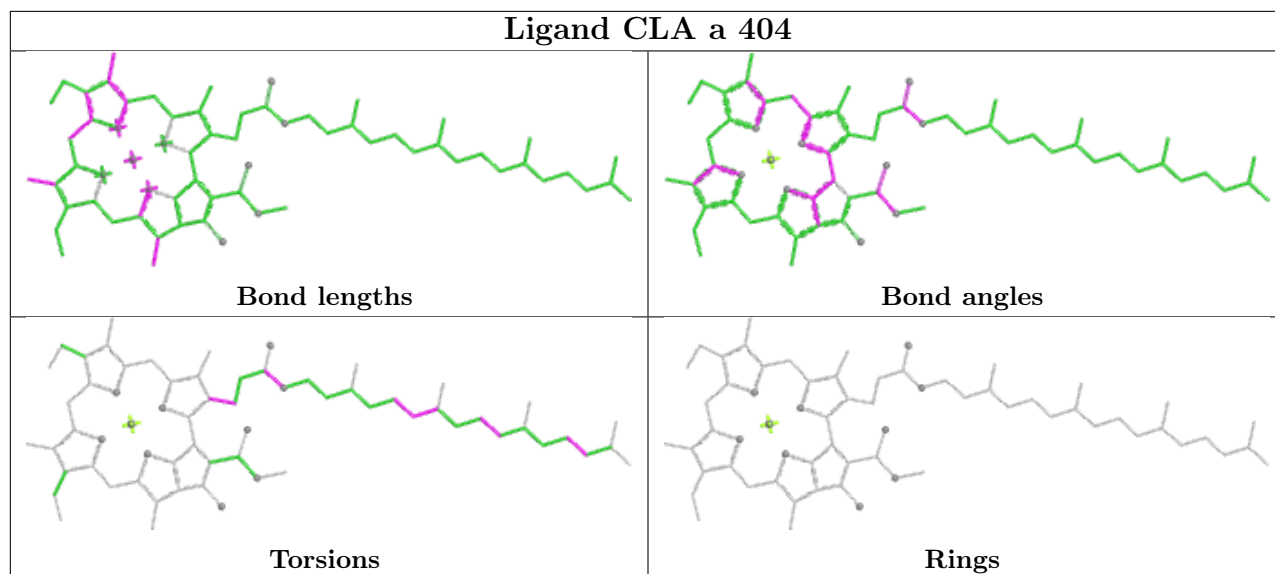
Ligand STE t 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

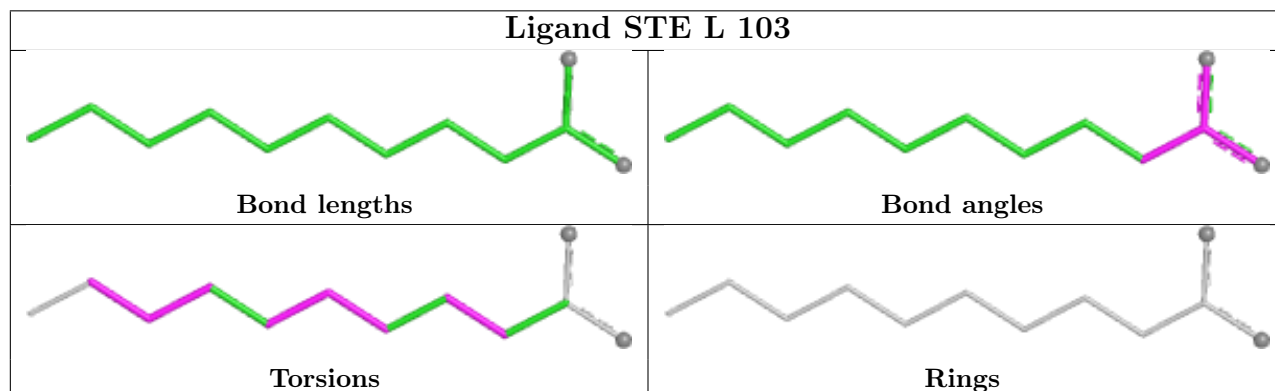
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

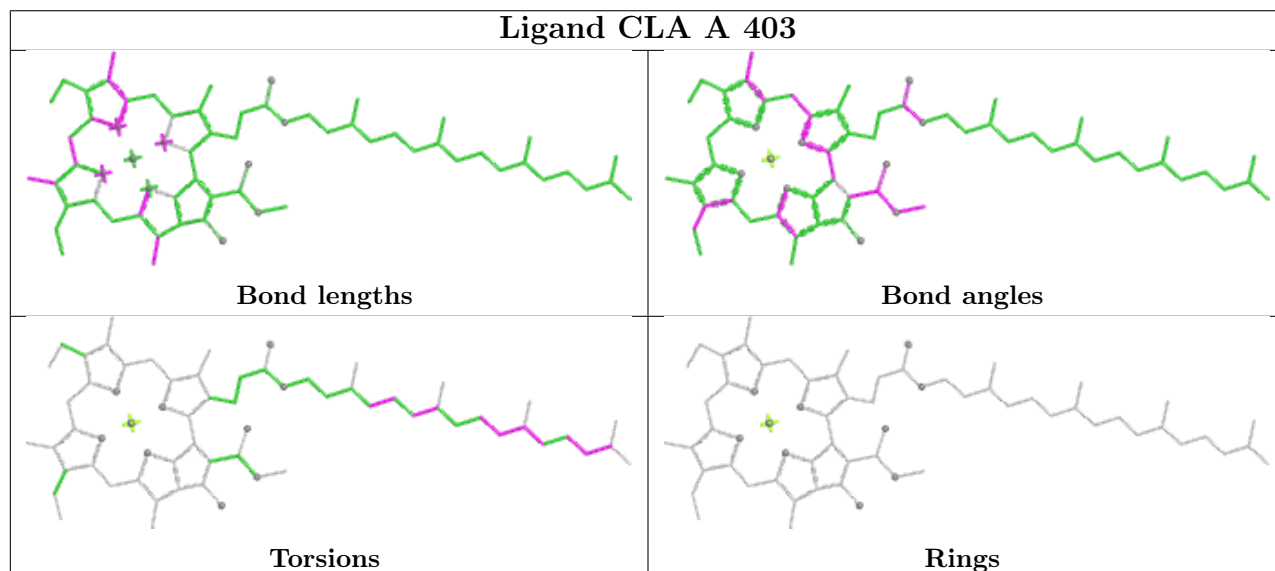
Ligand CLA a 404

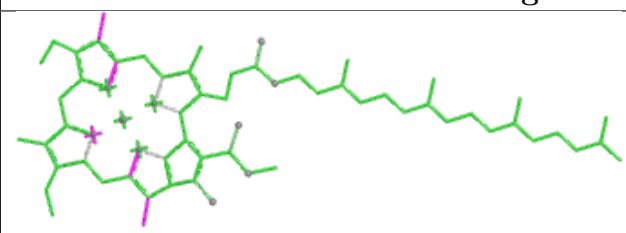
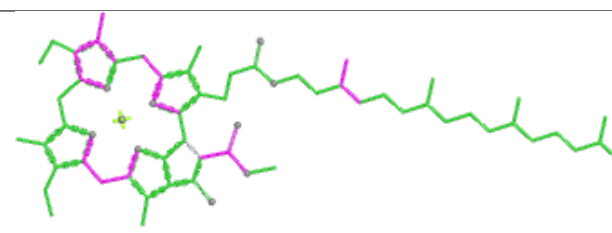
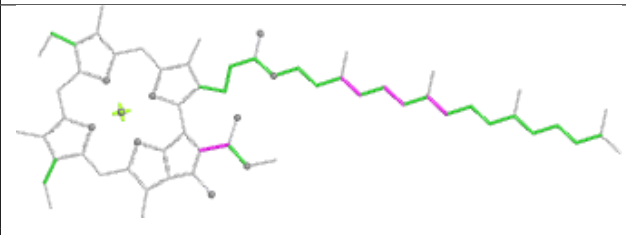
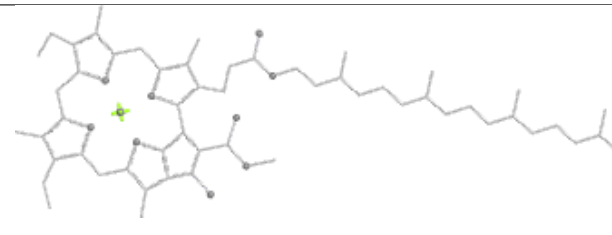


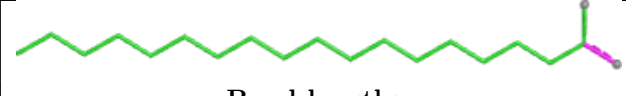
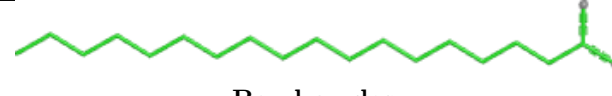
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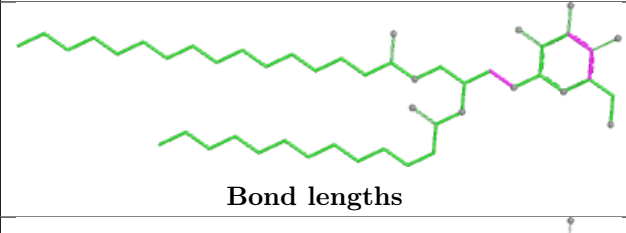
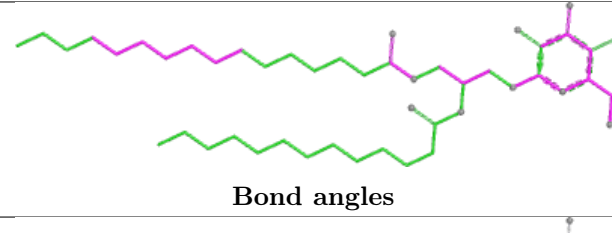


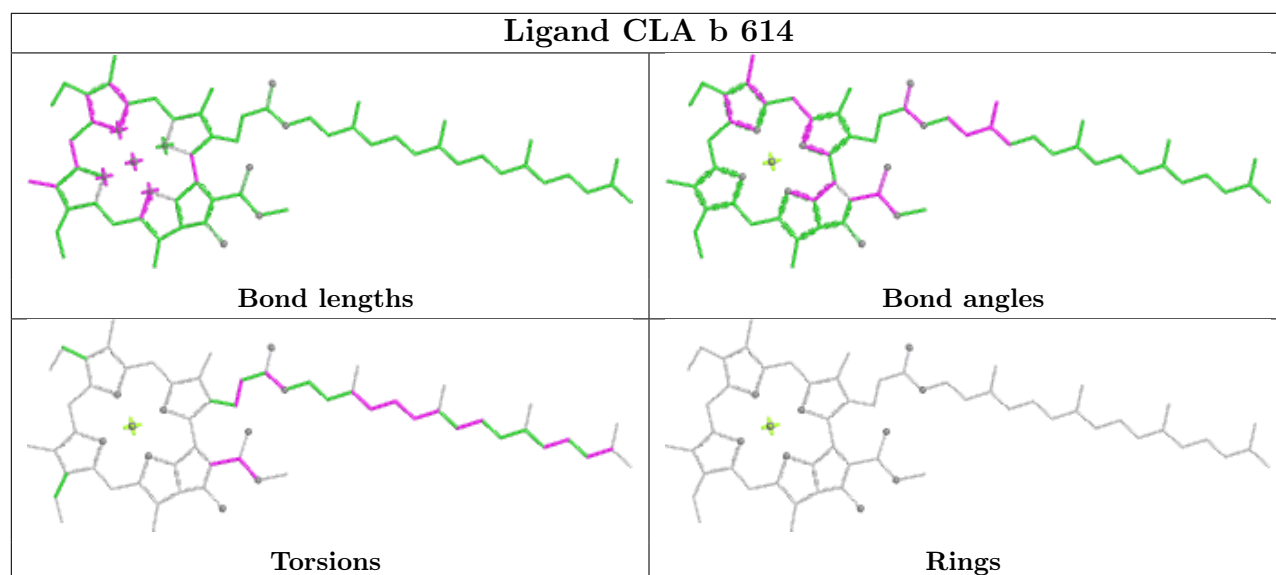
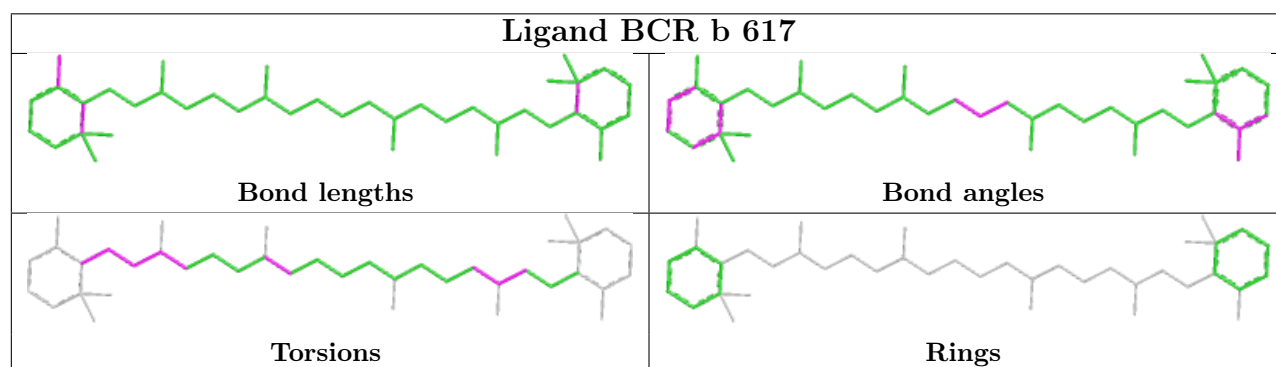
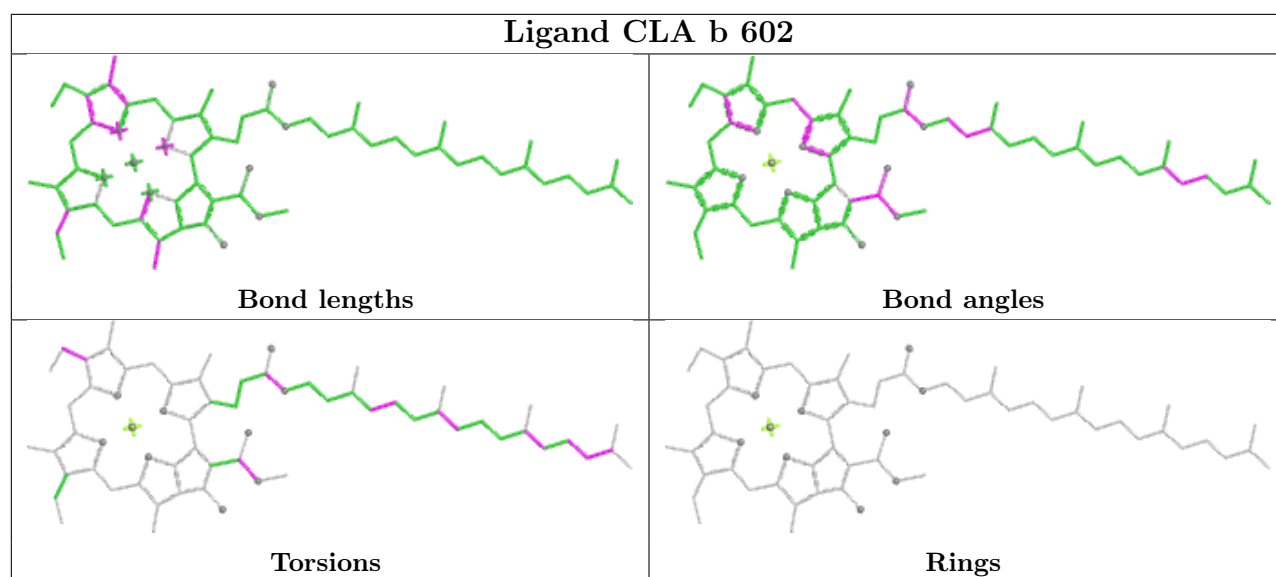
Ligand CLA A 403

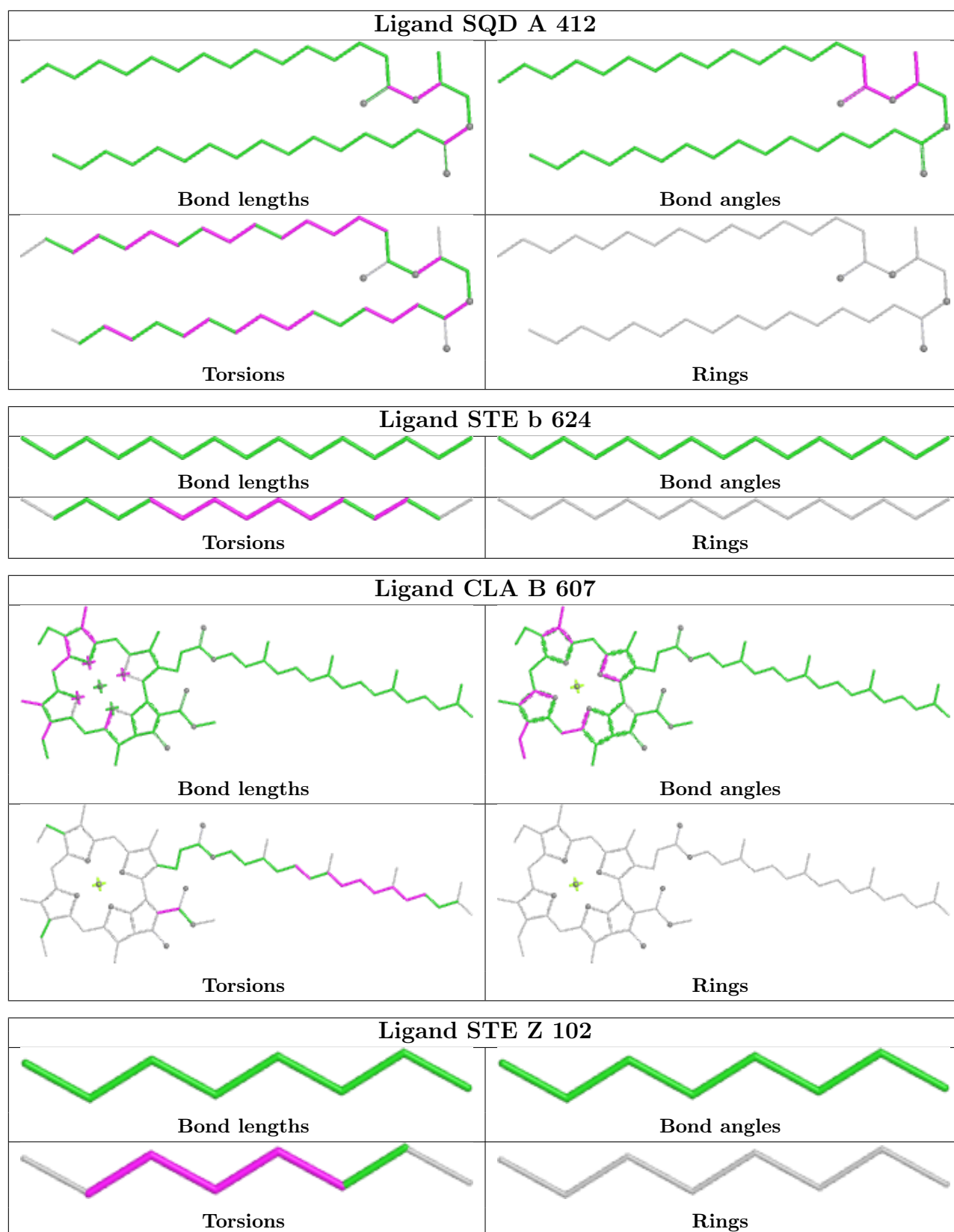


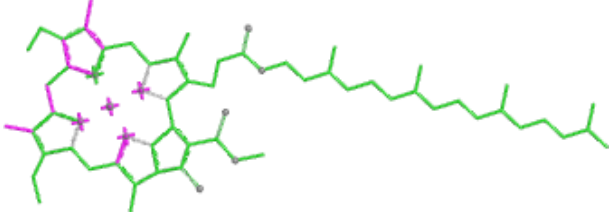
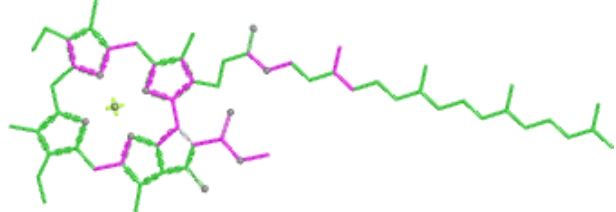
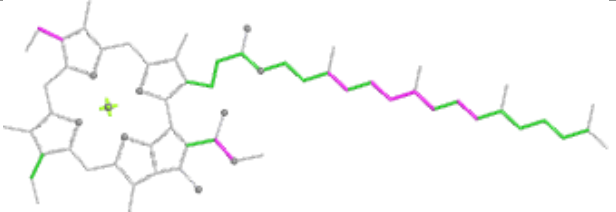
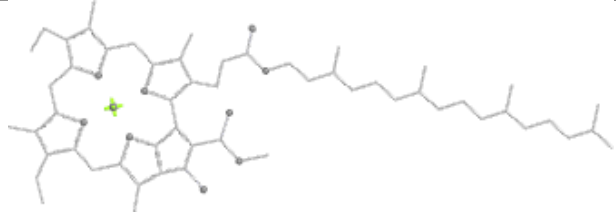
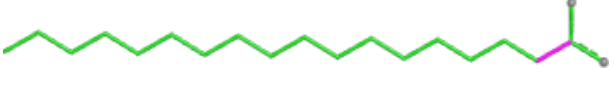
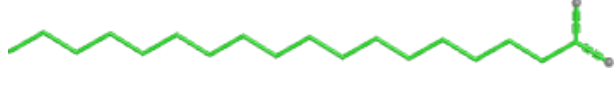
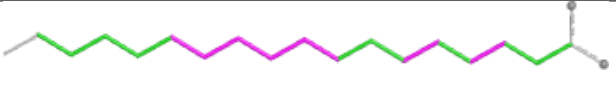
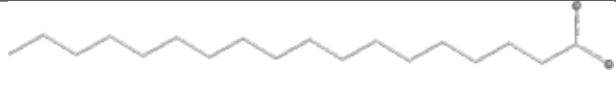
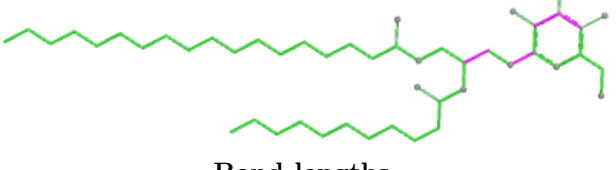
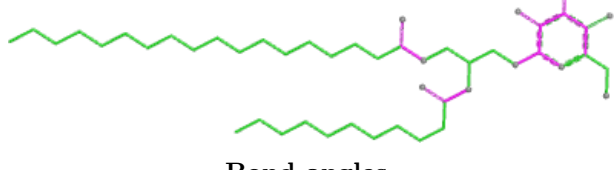
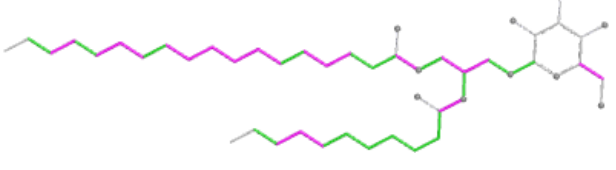
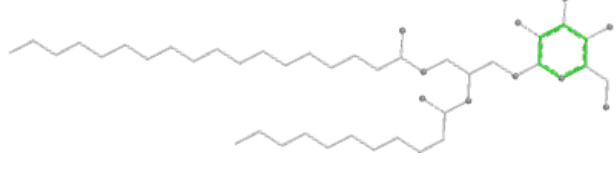
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

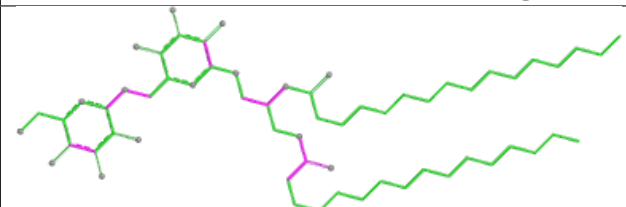
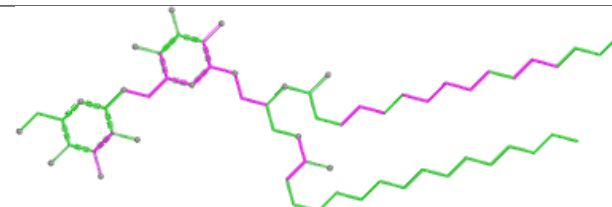
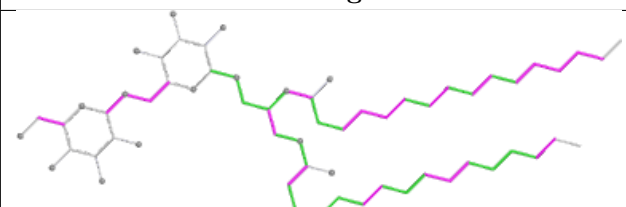
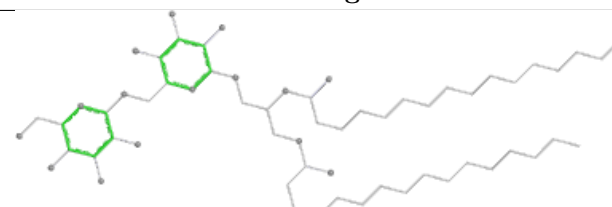
Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

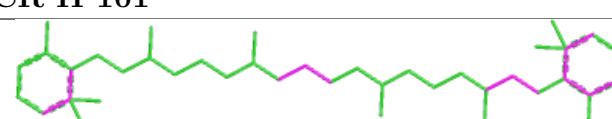
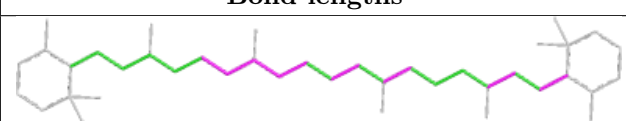
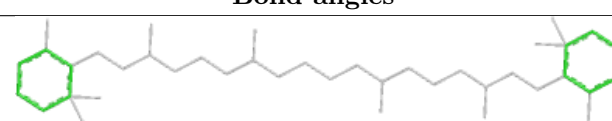
Ligand LMG A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

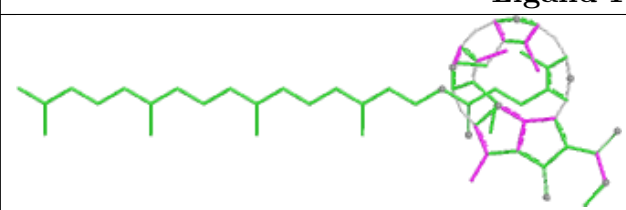
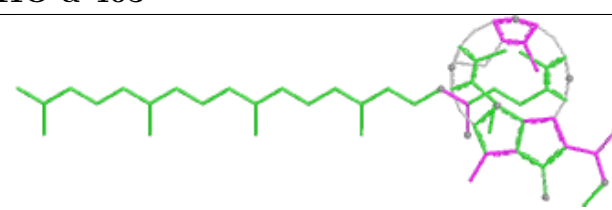
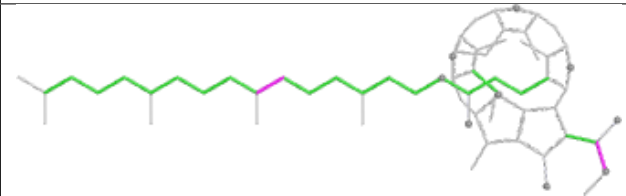
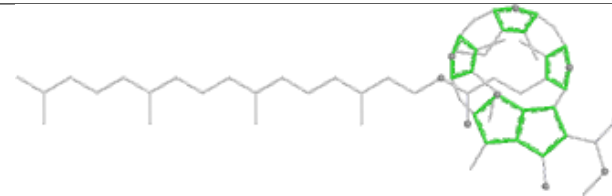


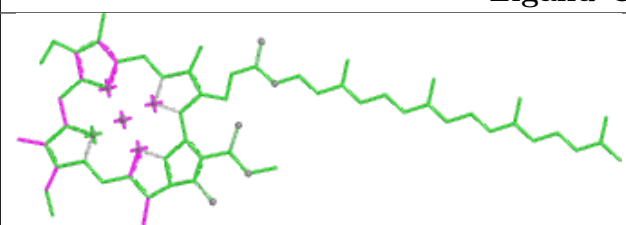
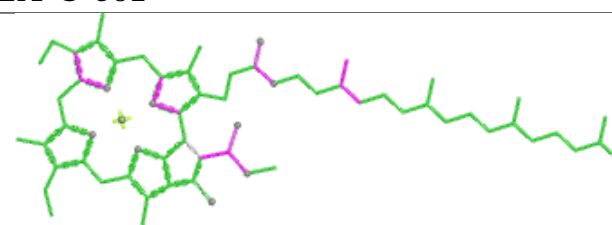
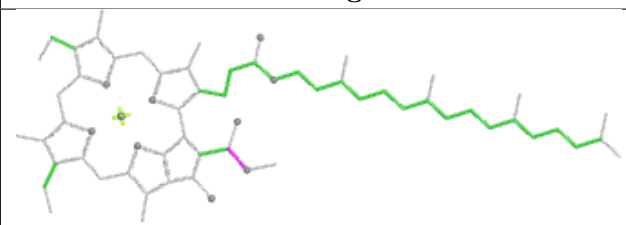
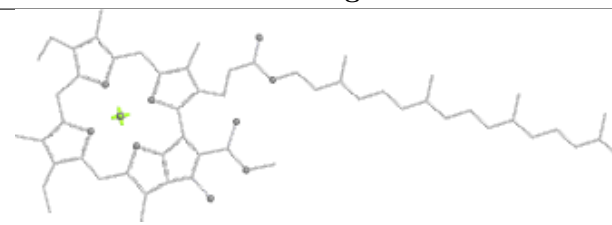


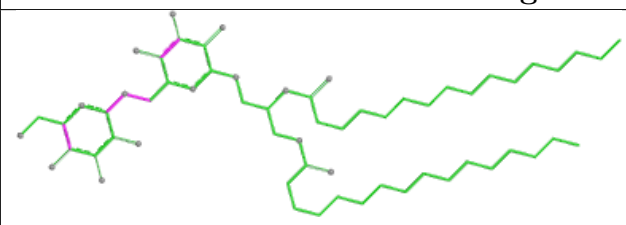
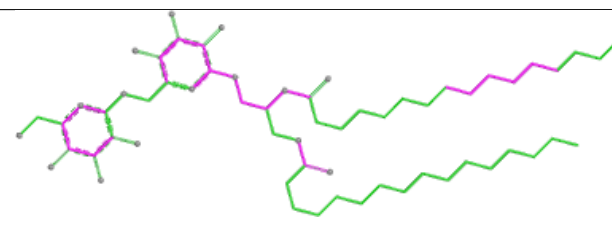
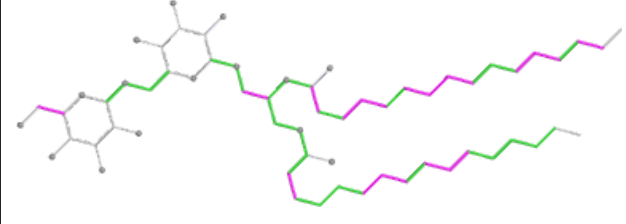
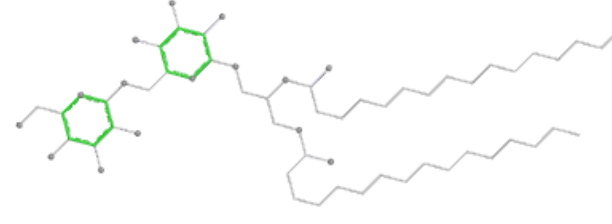
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

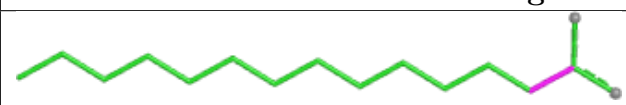
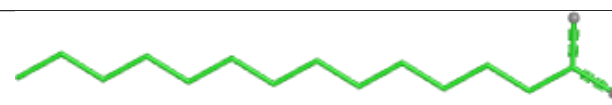
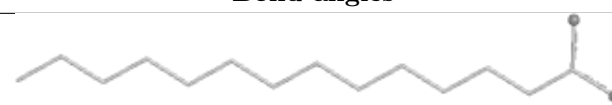
Ligand DGD C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

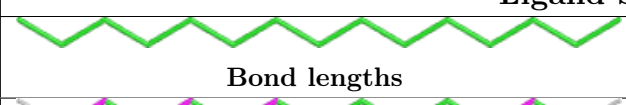
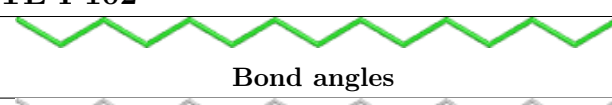
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

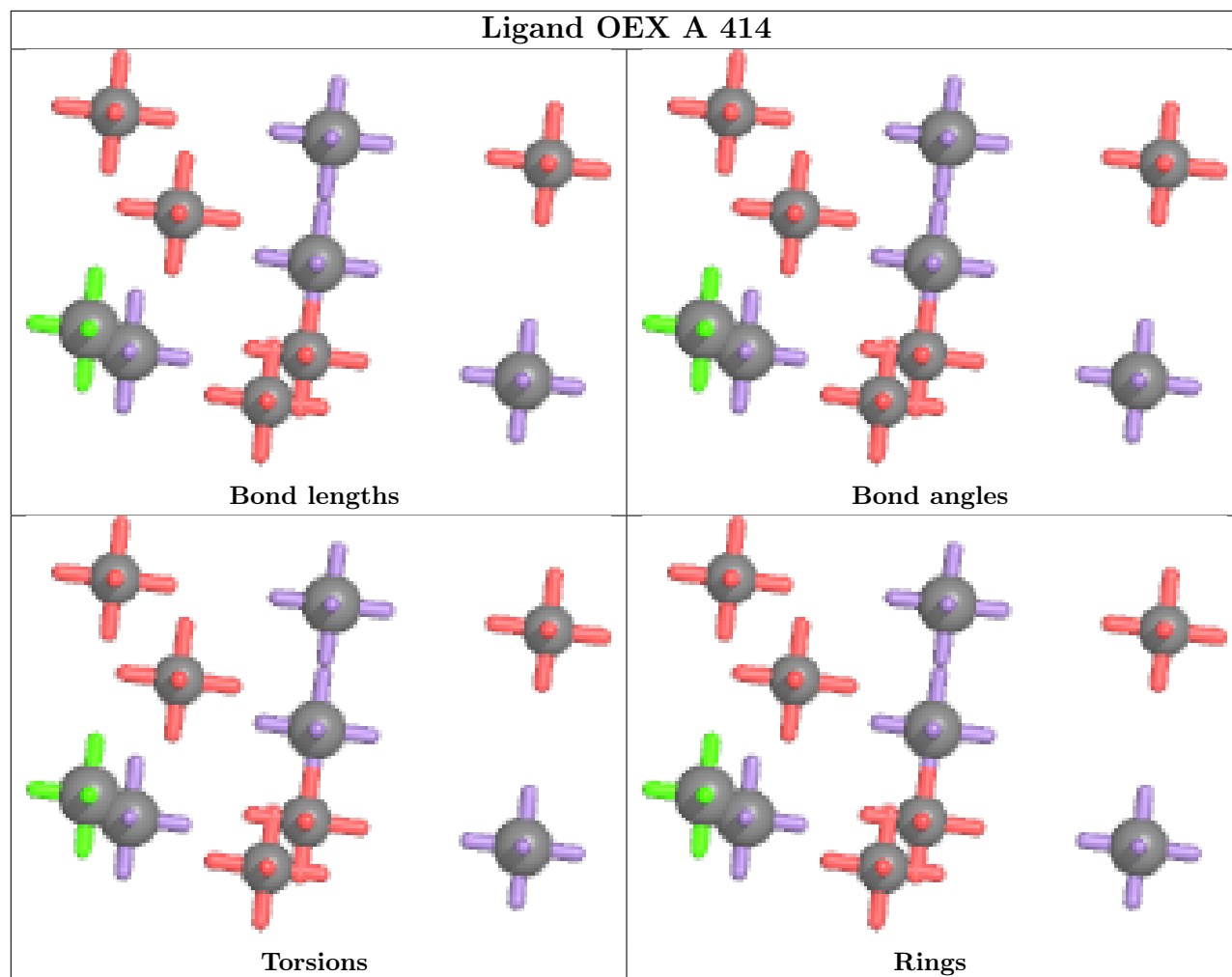
Ligand PHO a 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

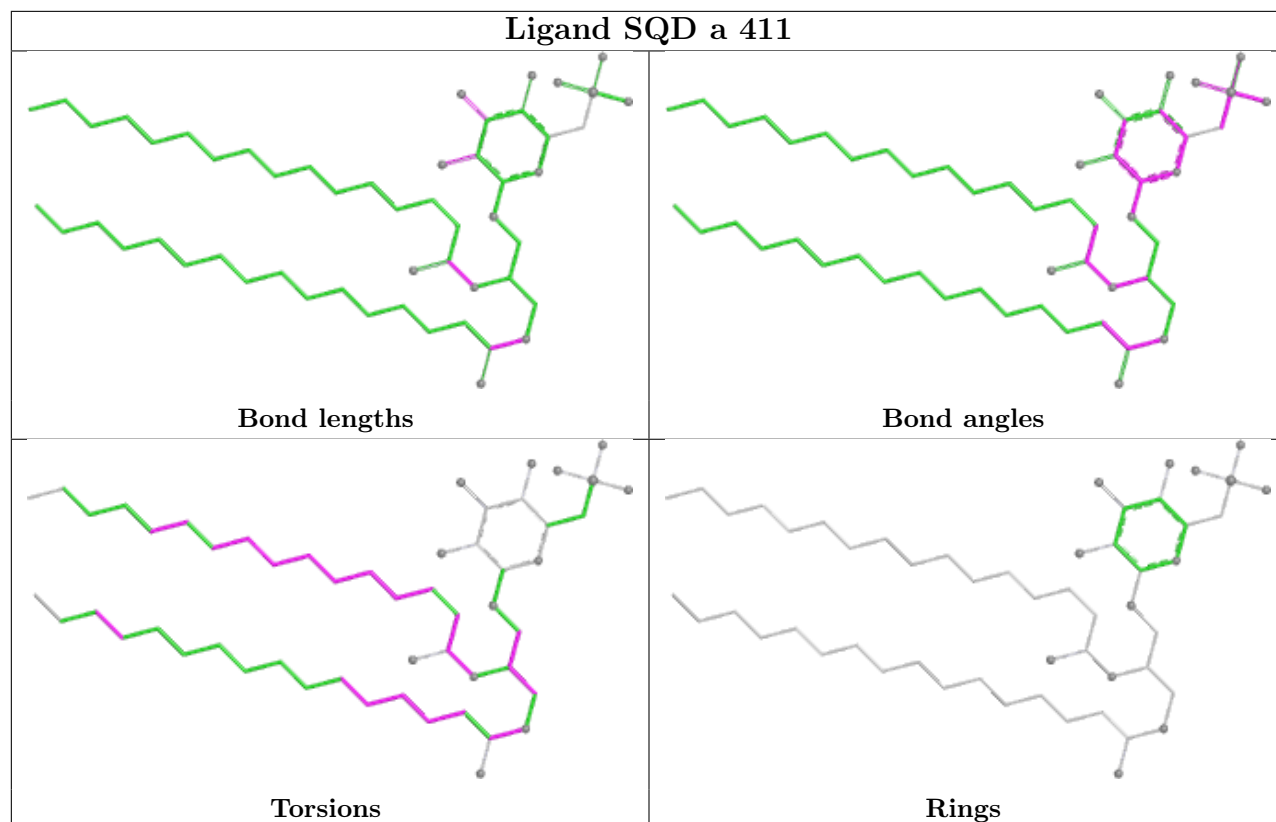
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

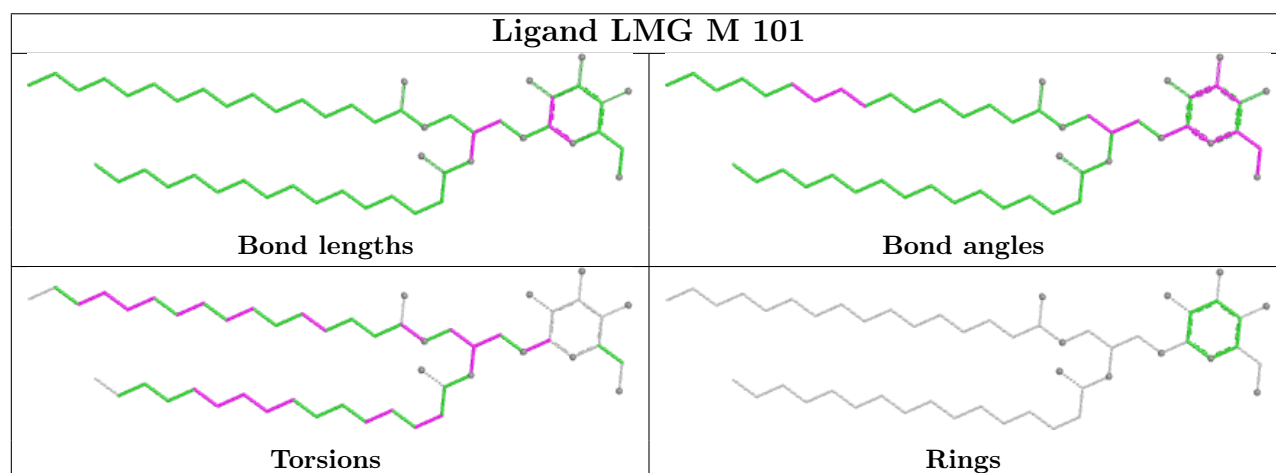
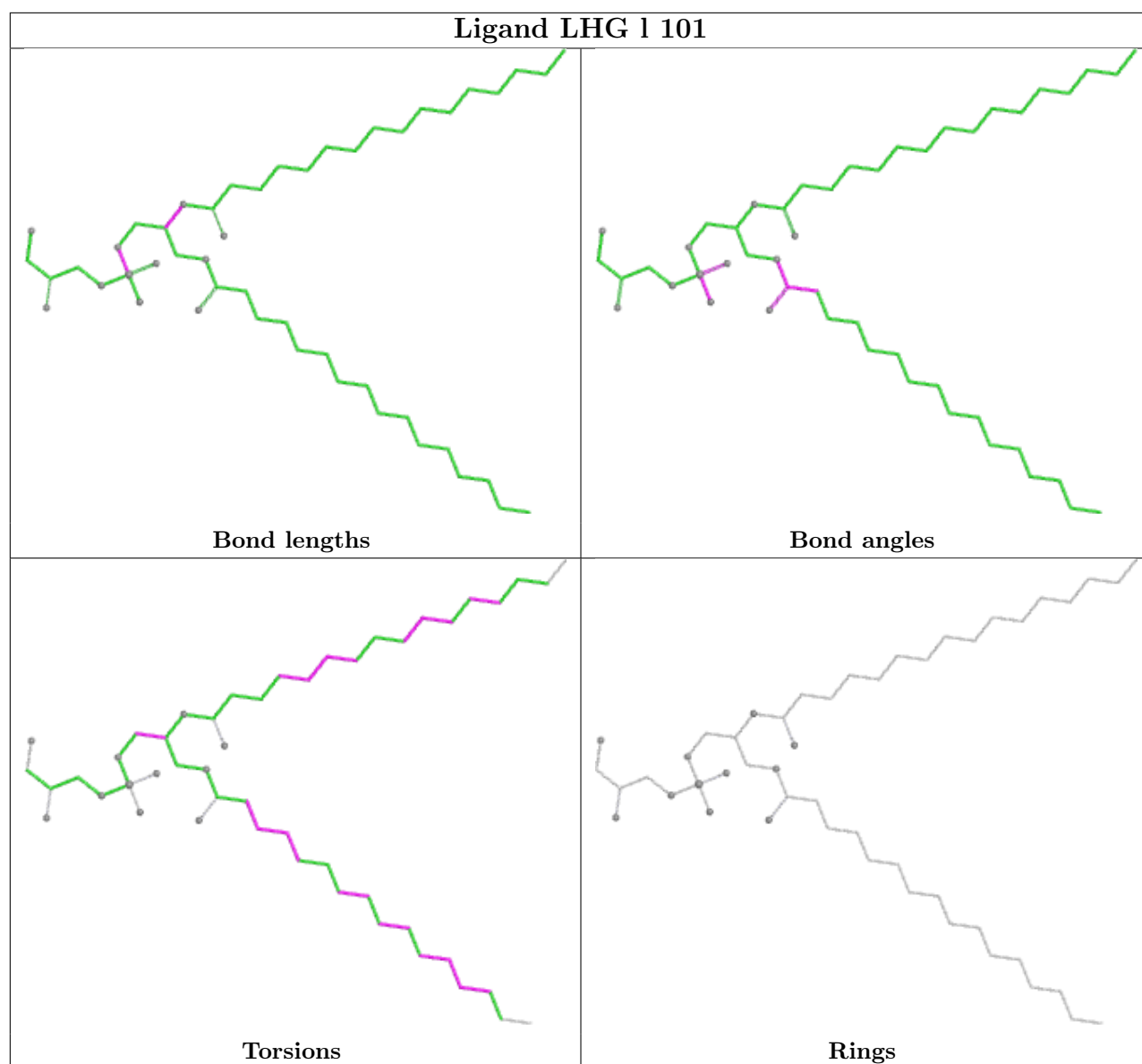
Ligand DGD h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

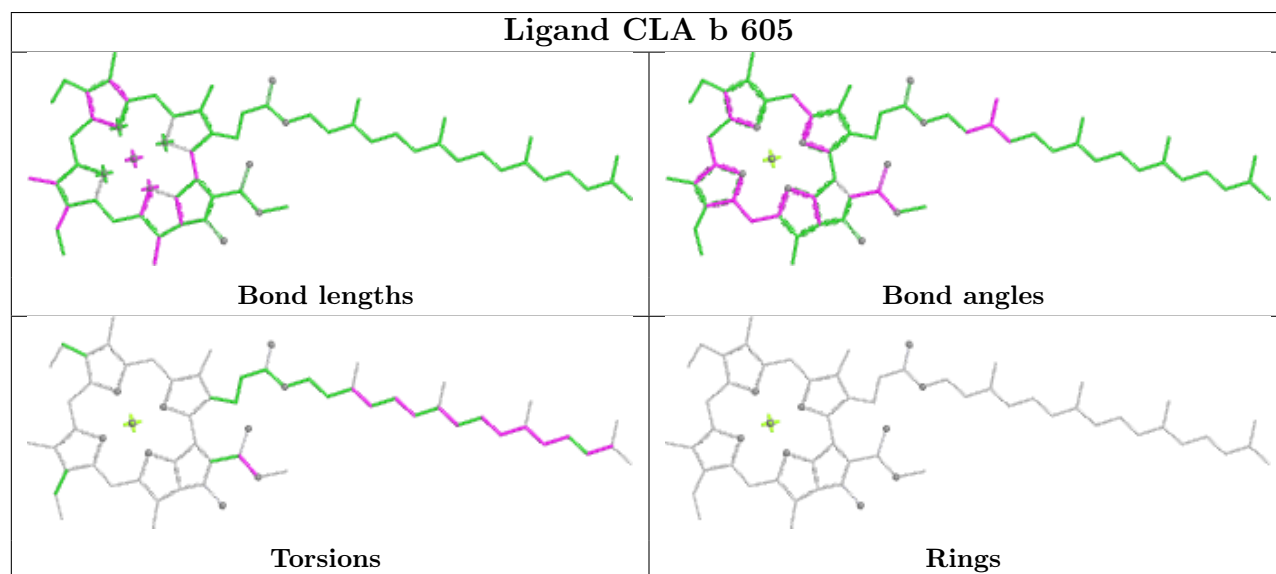
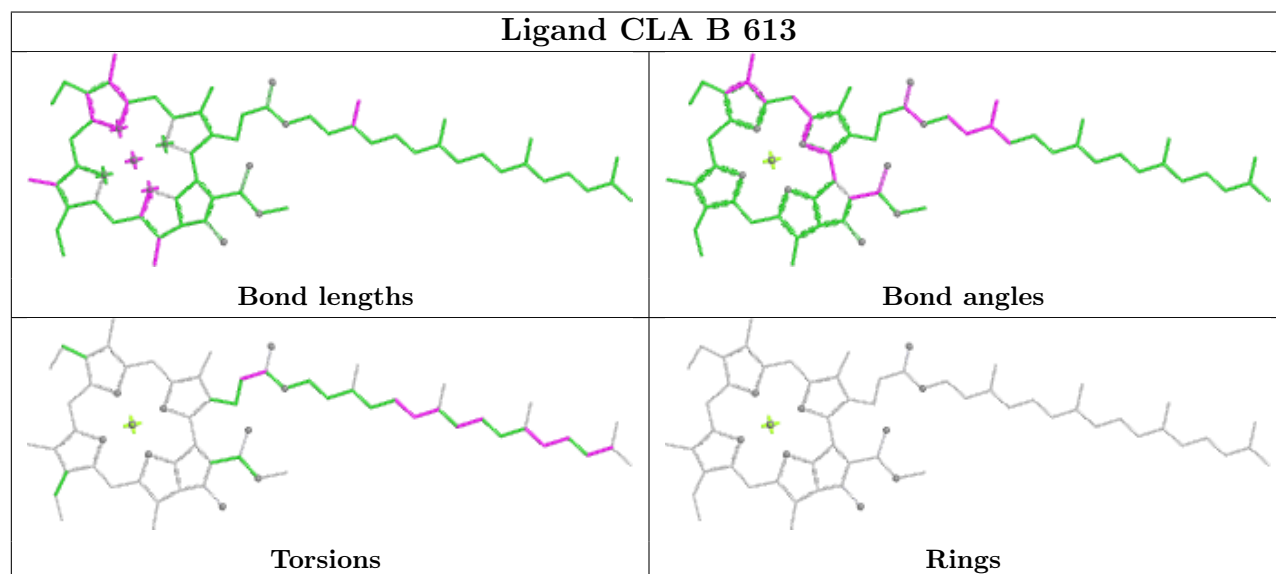
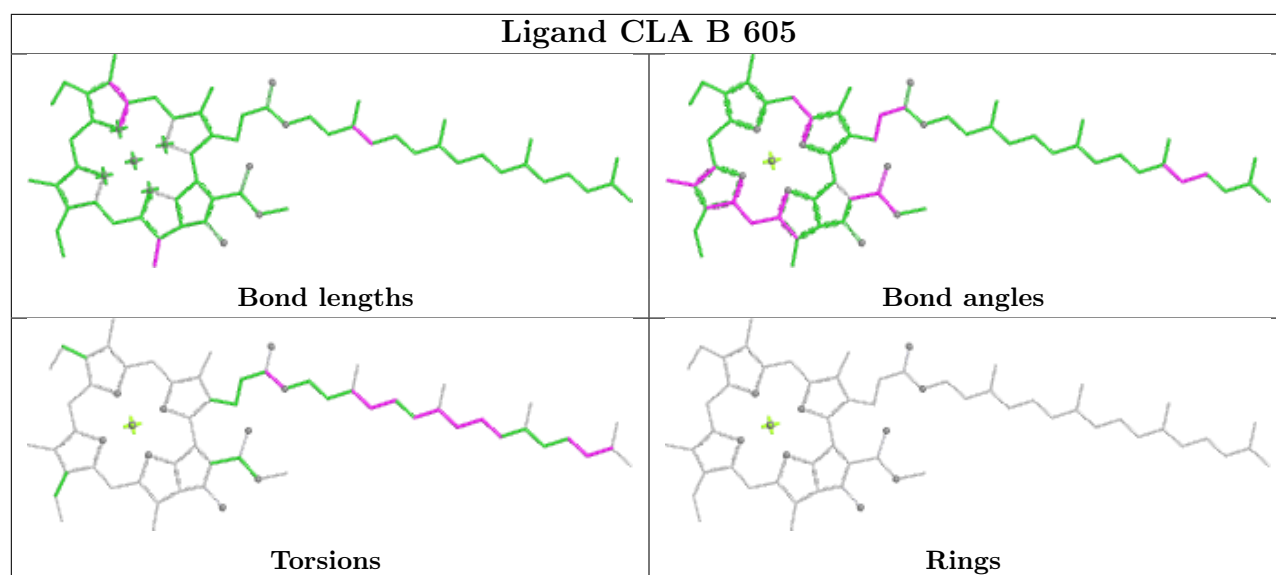
Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

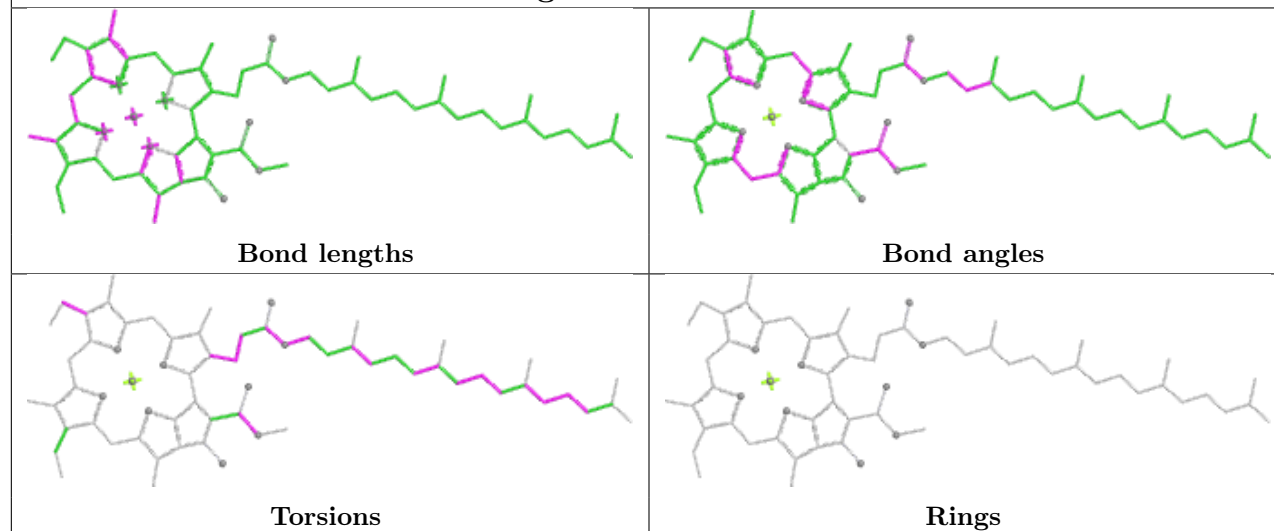
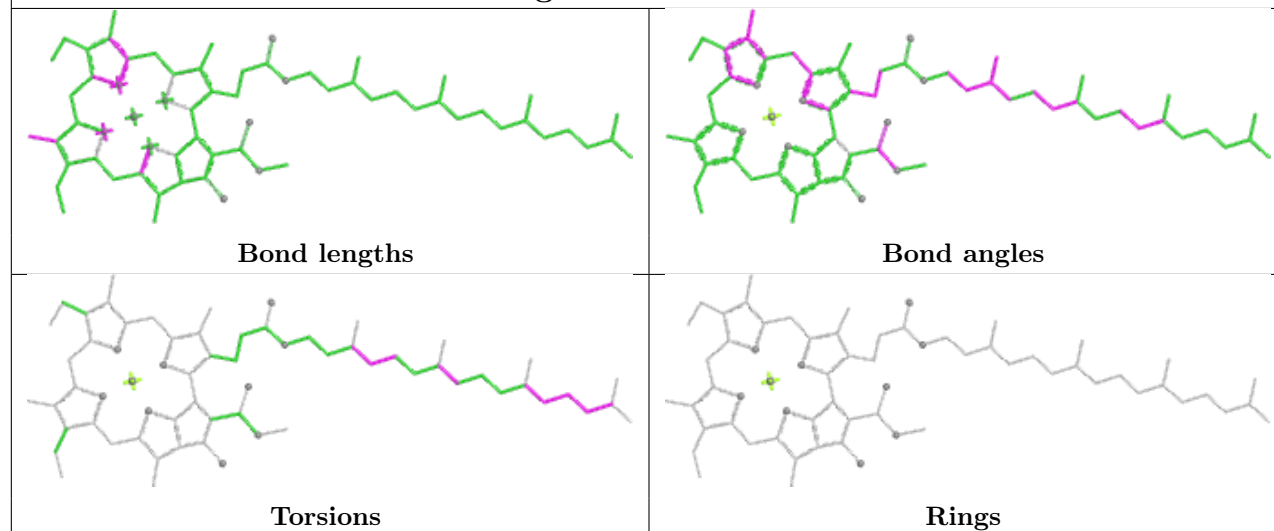
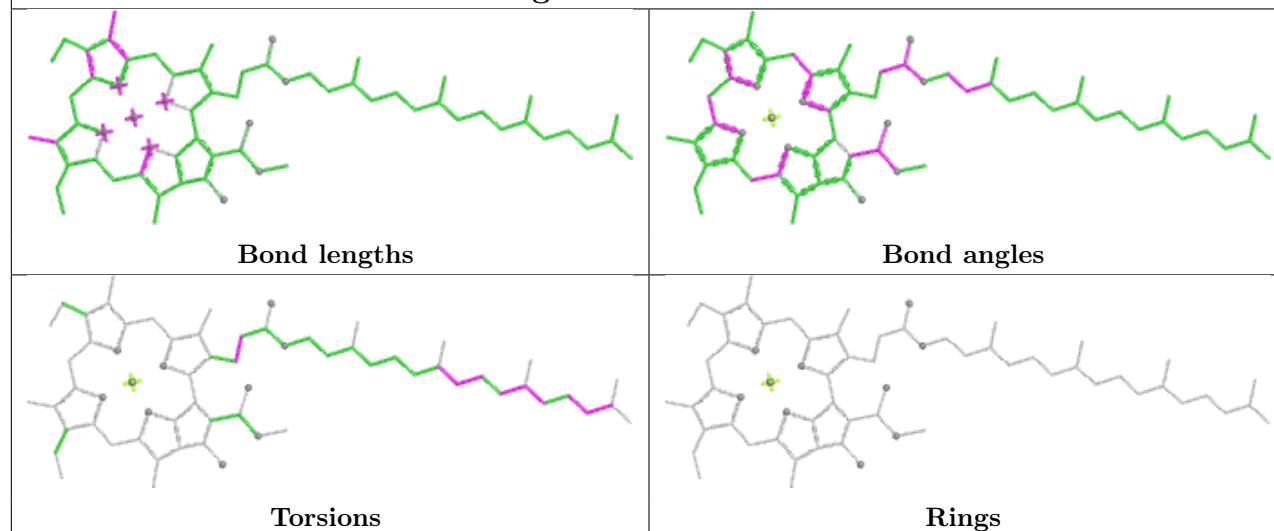
Ligand STE I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

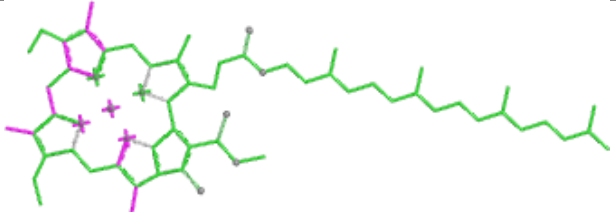
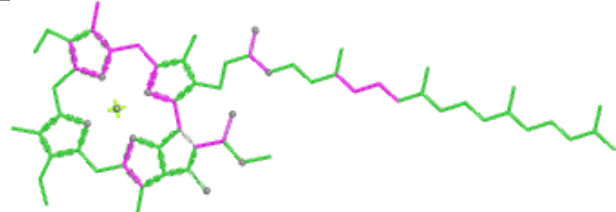
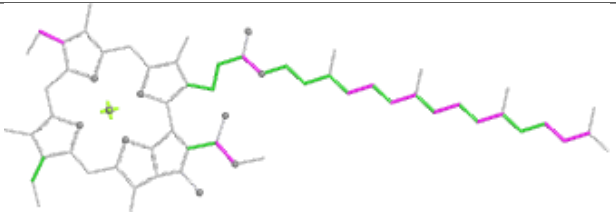
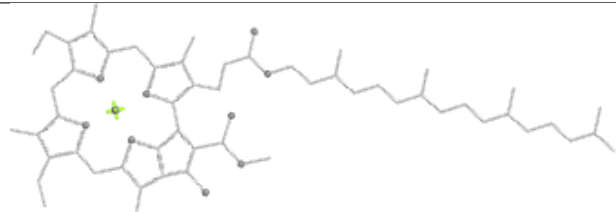


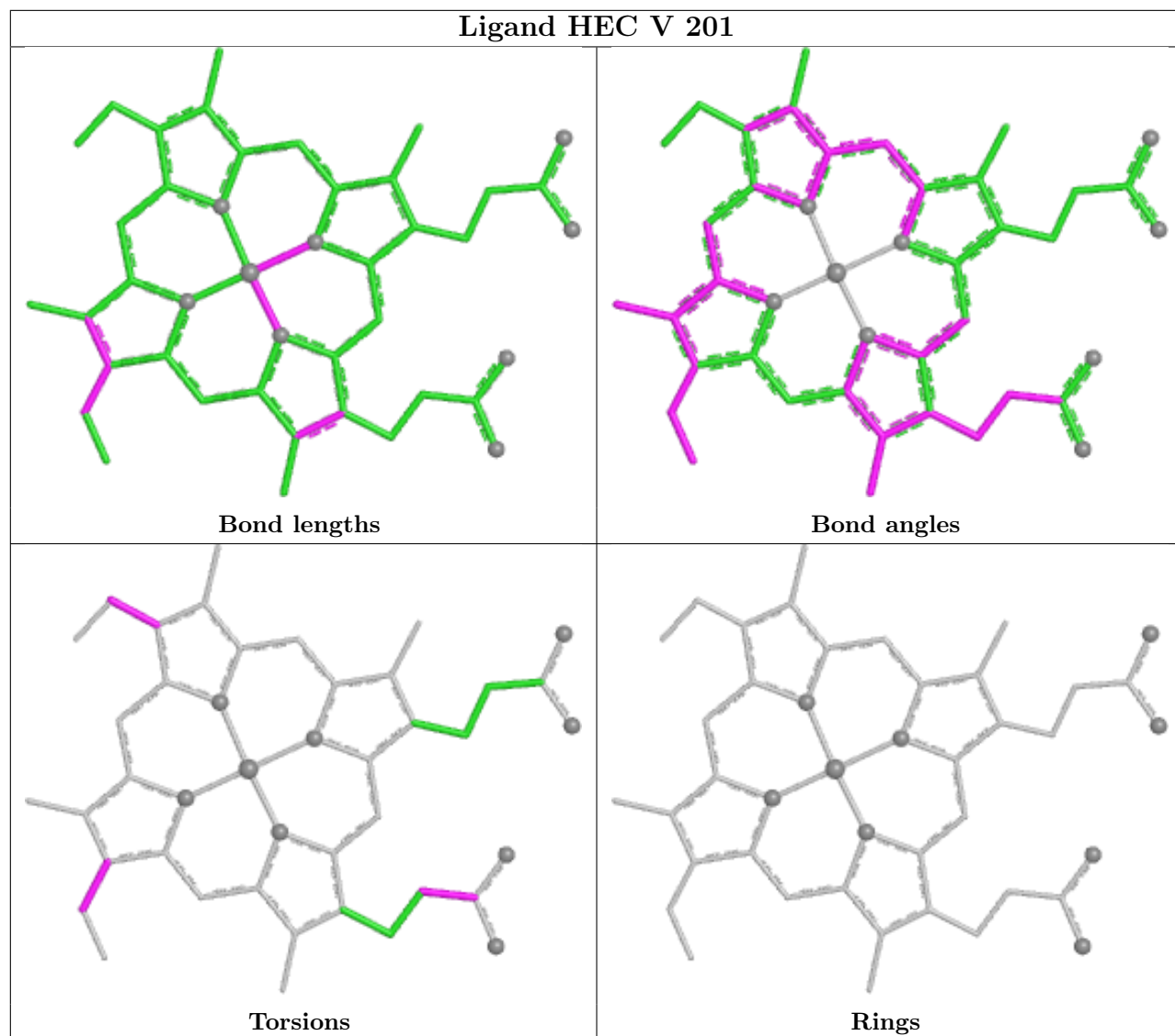


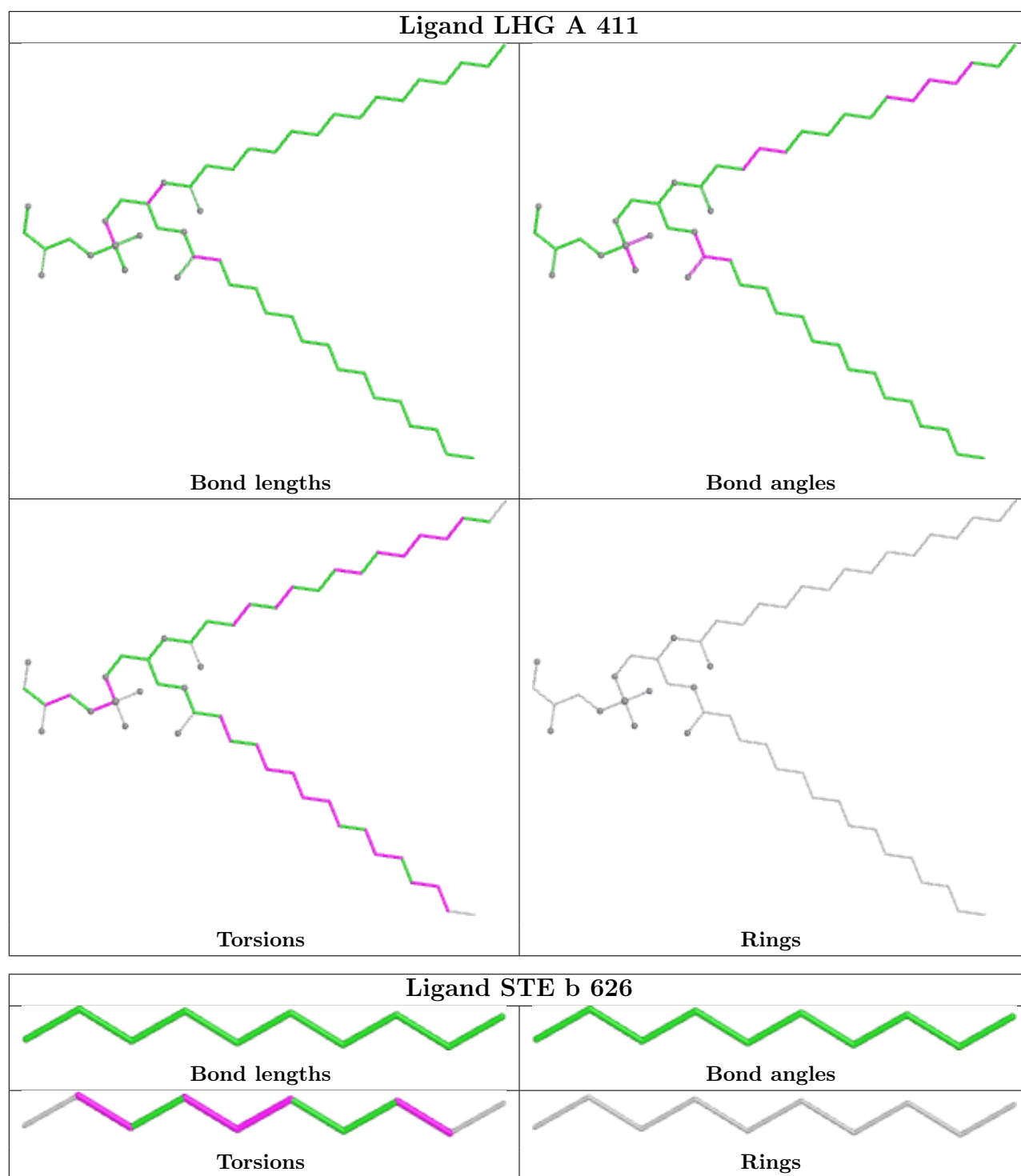


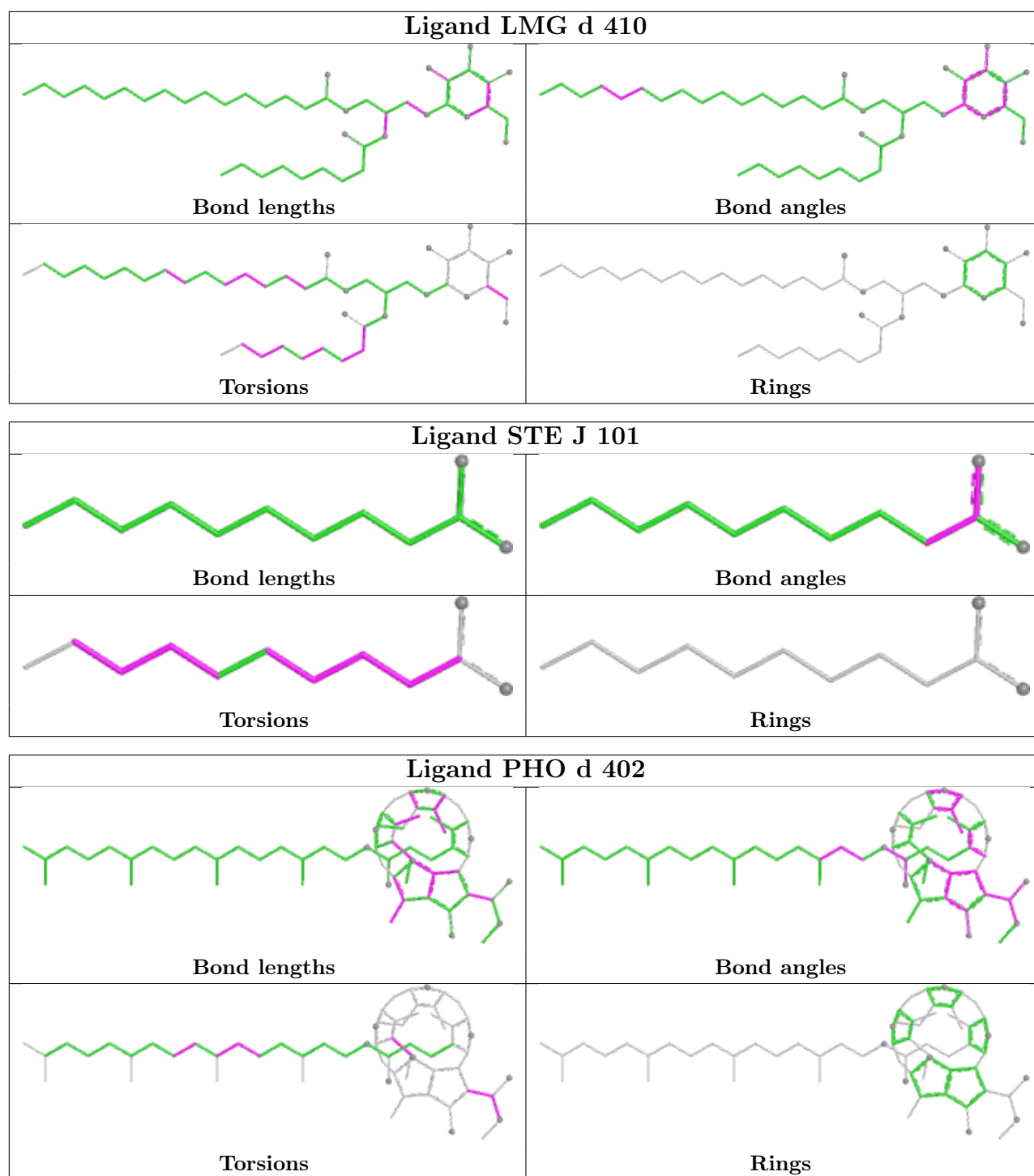


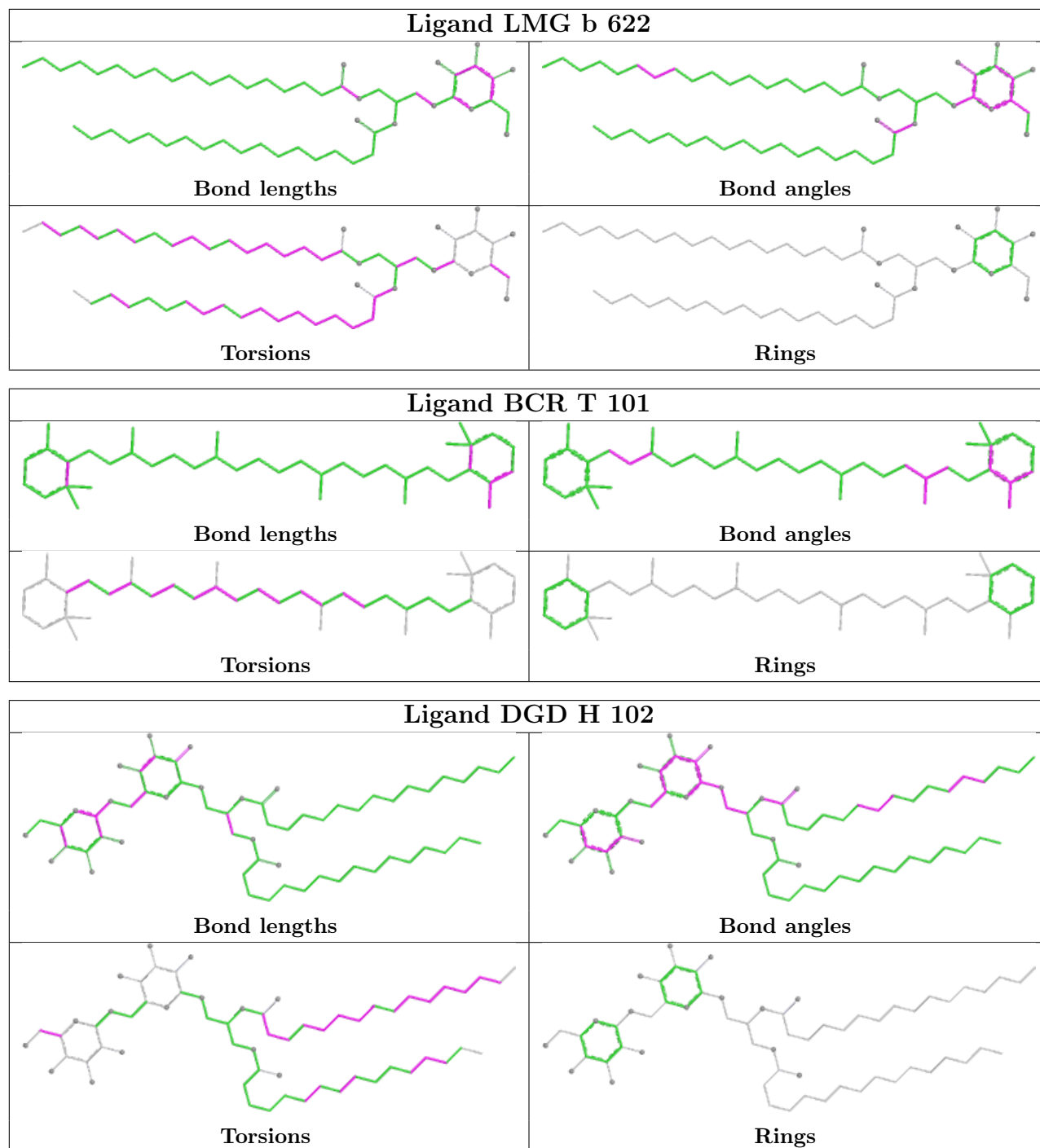
Ligand CLA c 512**Ligand CLA b 604****Ligand CLA B 610**

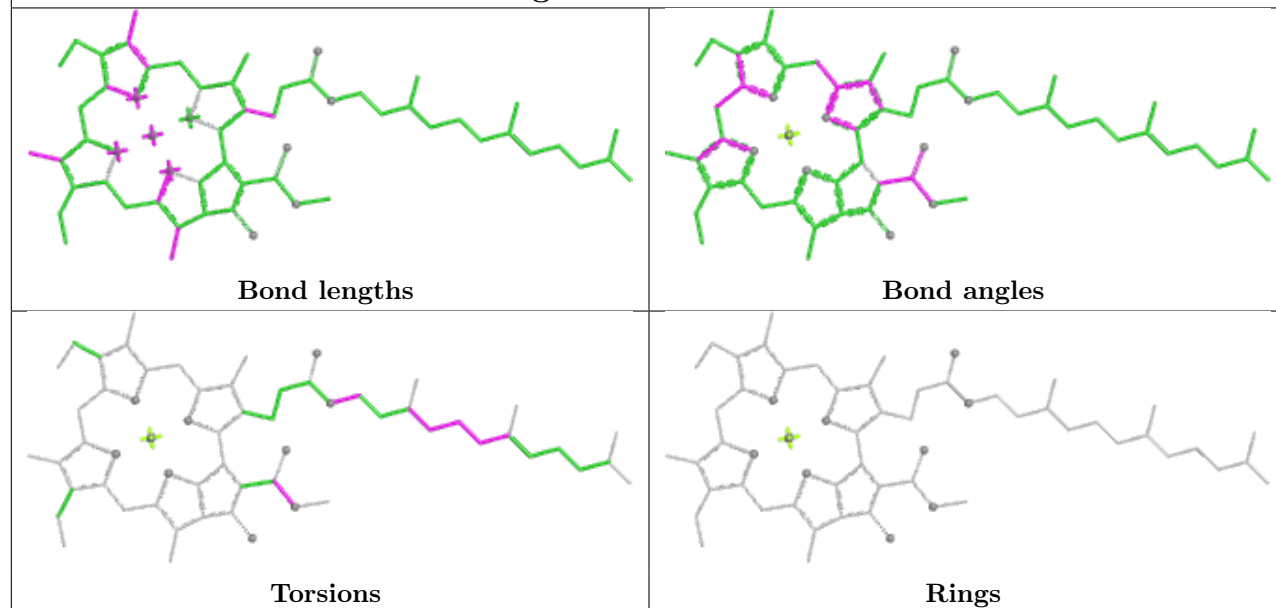
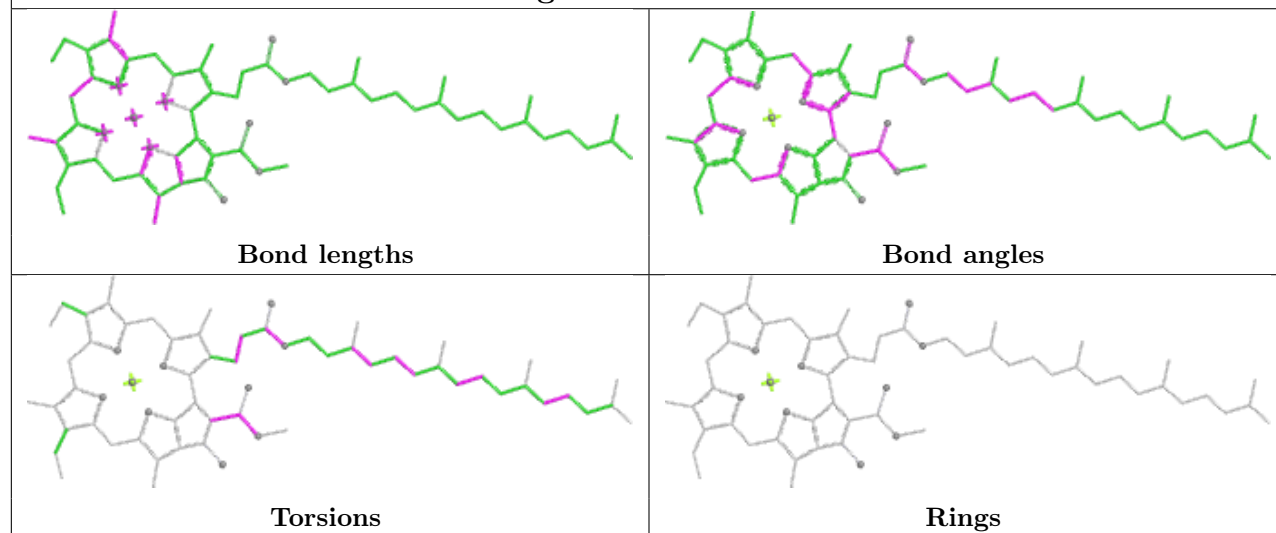
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

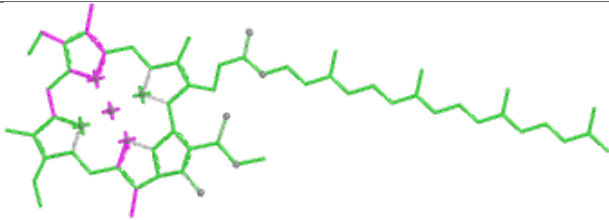
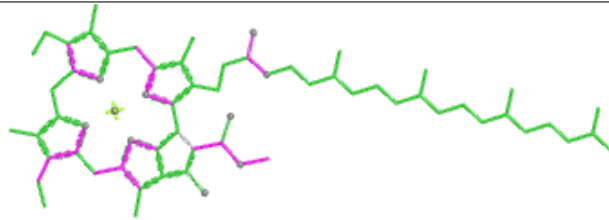
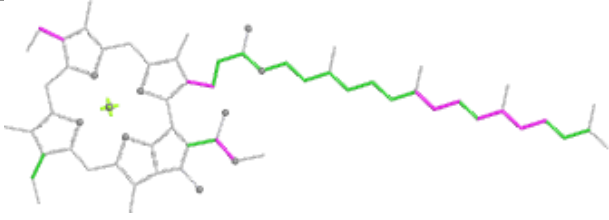
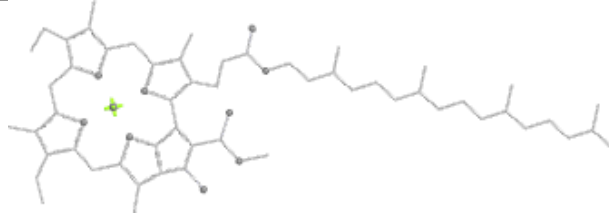


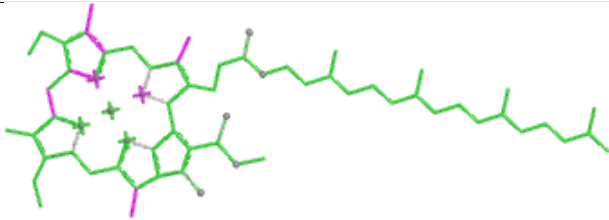
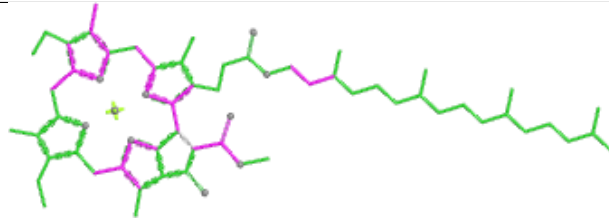
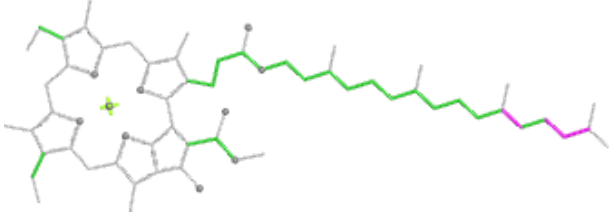
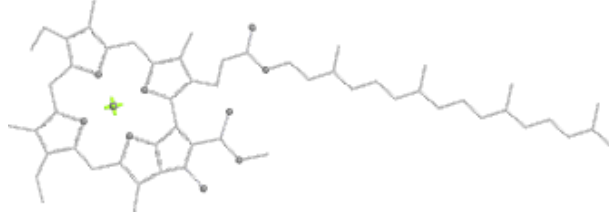


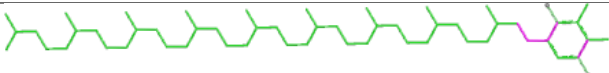
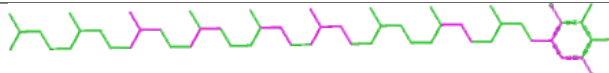
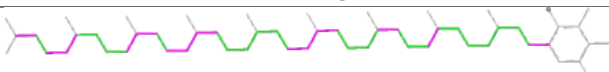


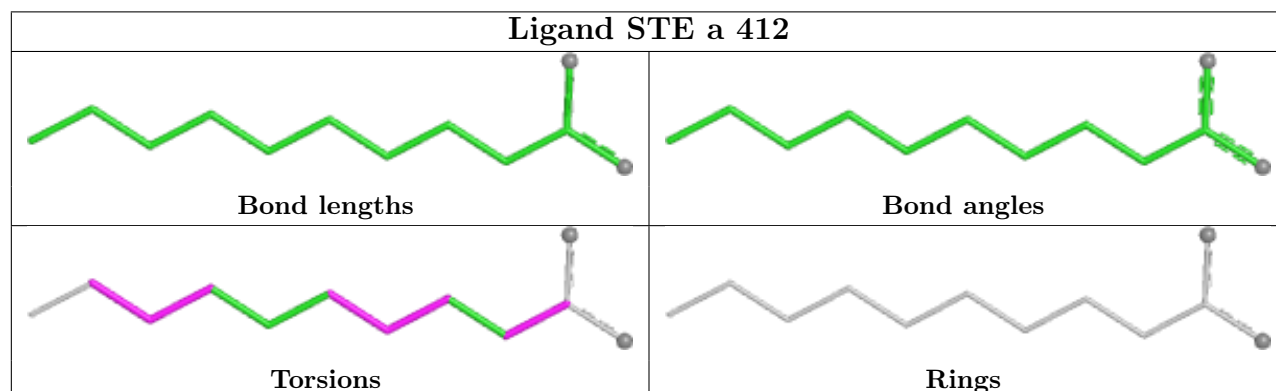
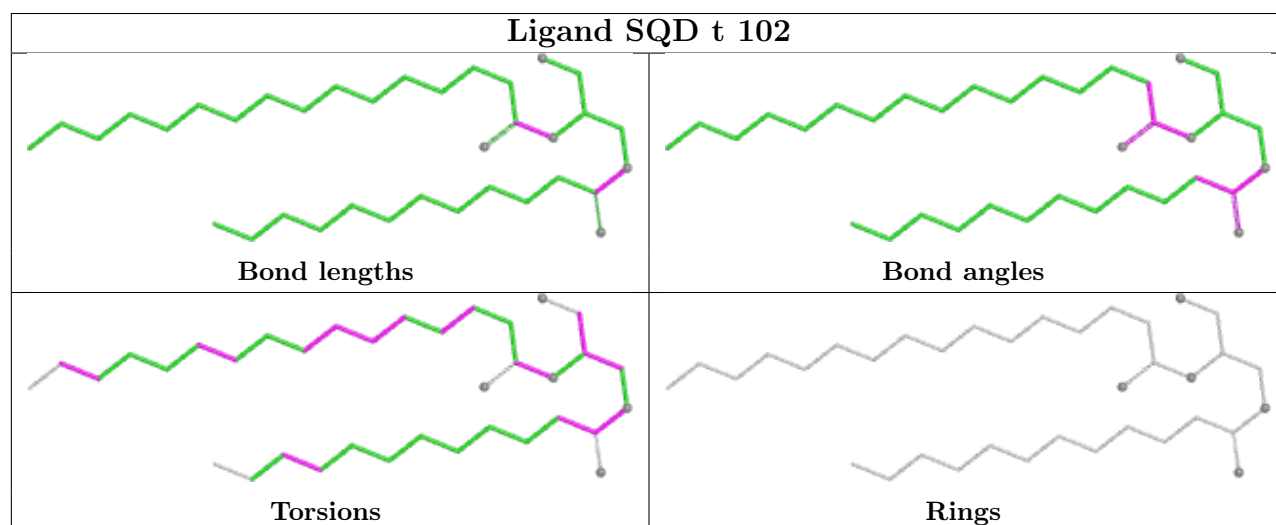
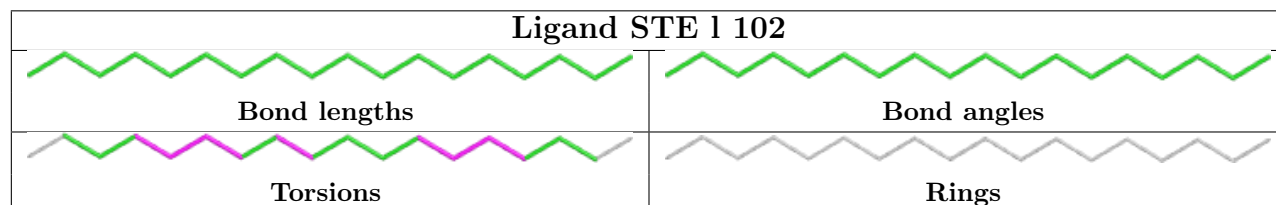
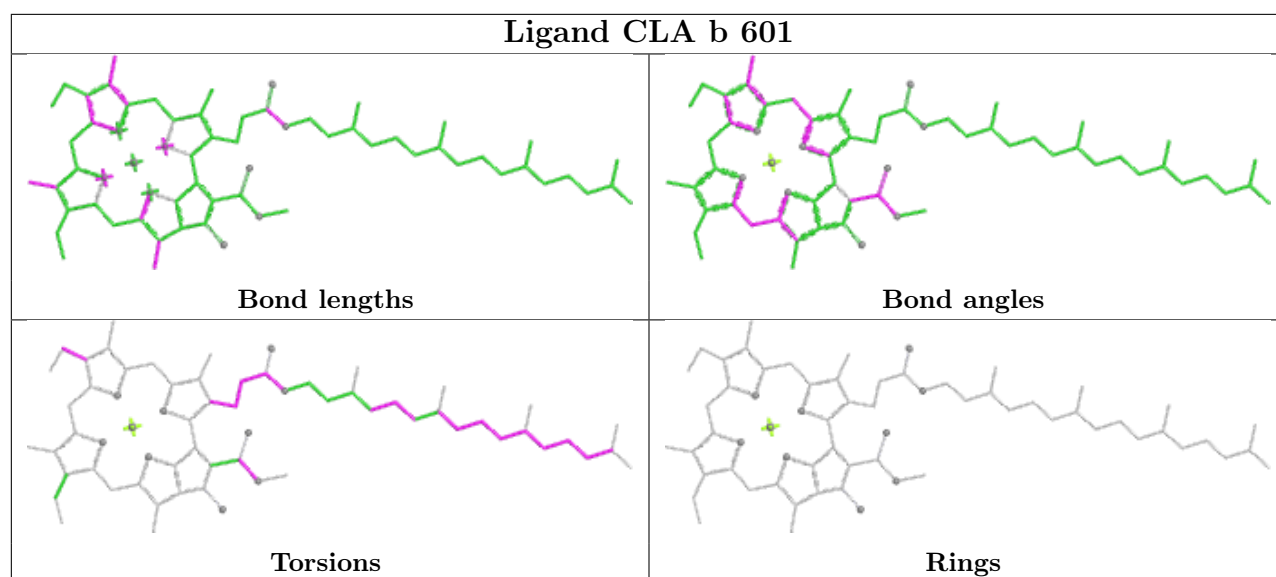


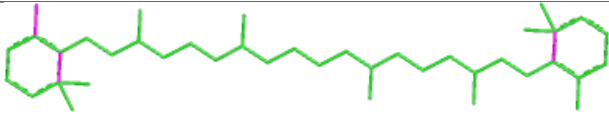
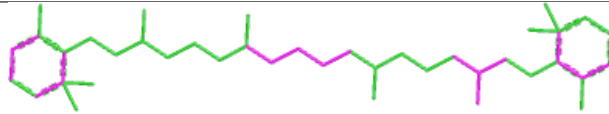
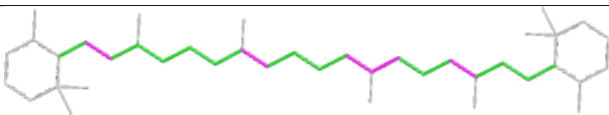
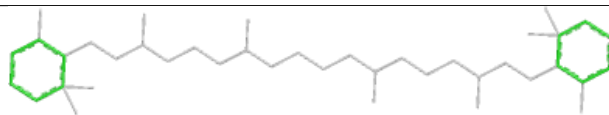
Ligand CLA B 616**Ligand CLA c 507**

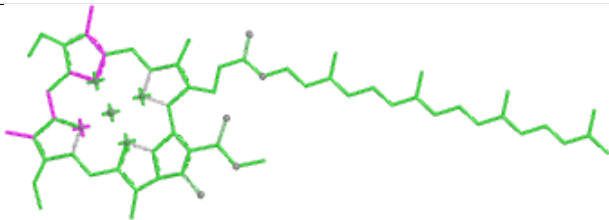
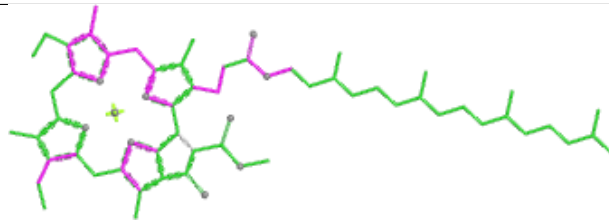
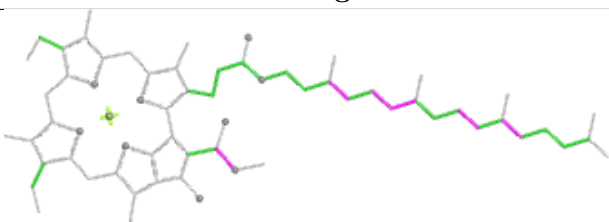
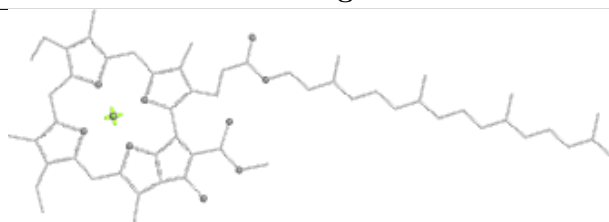
Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

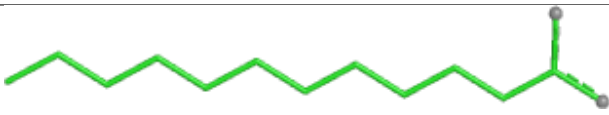
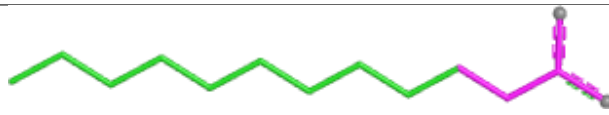
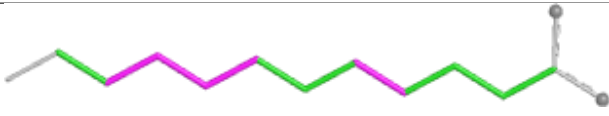
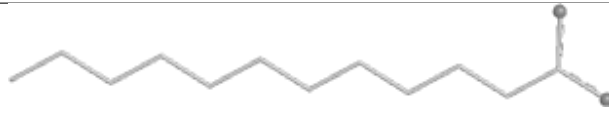
Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

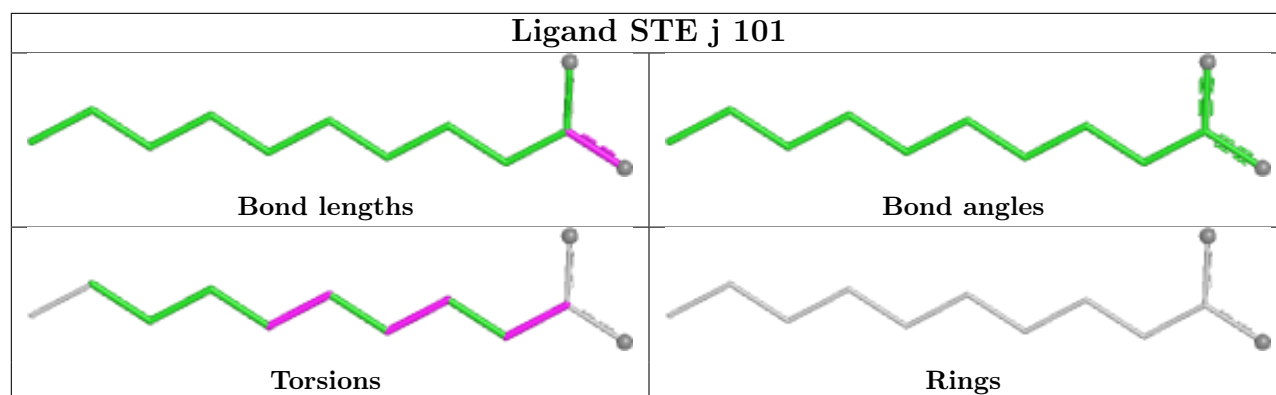
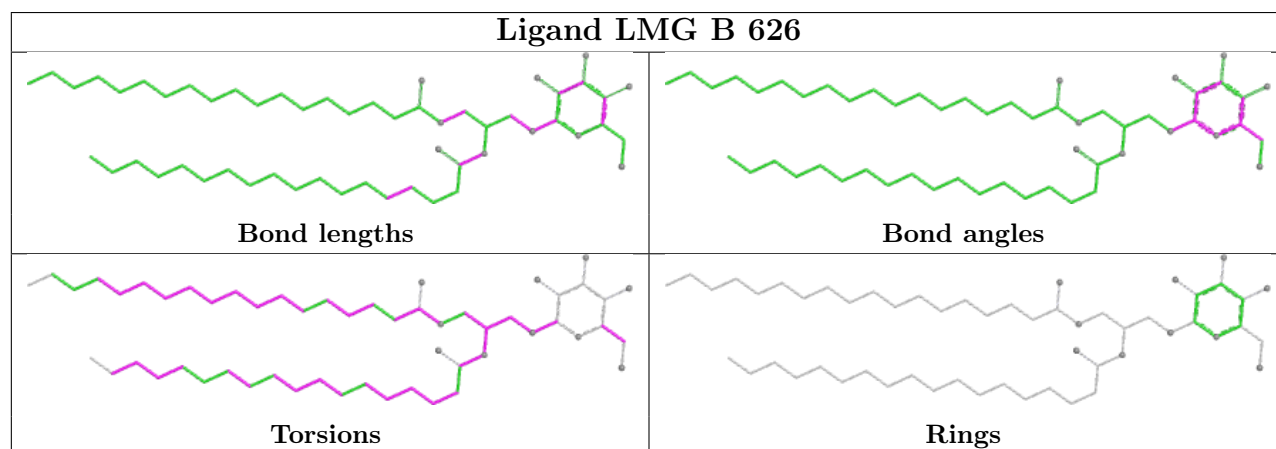
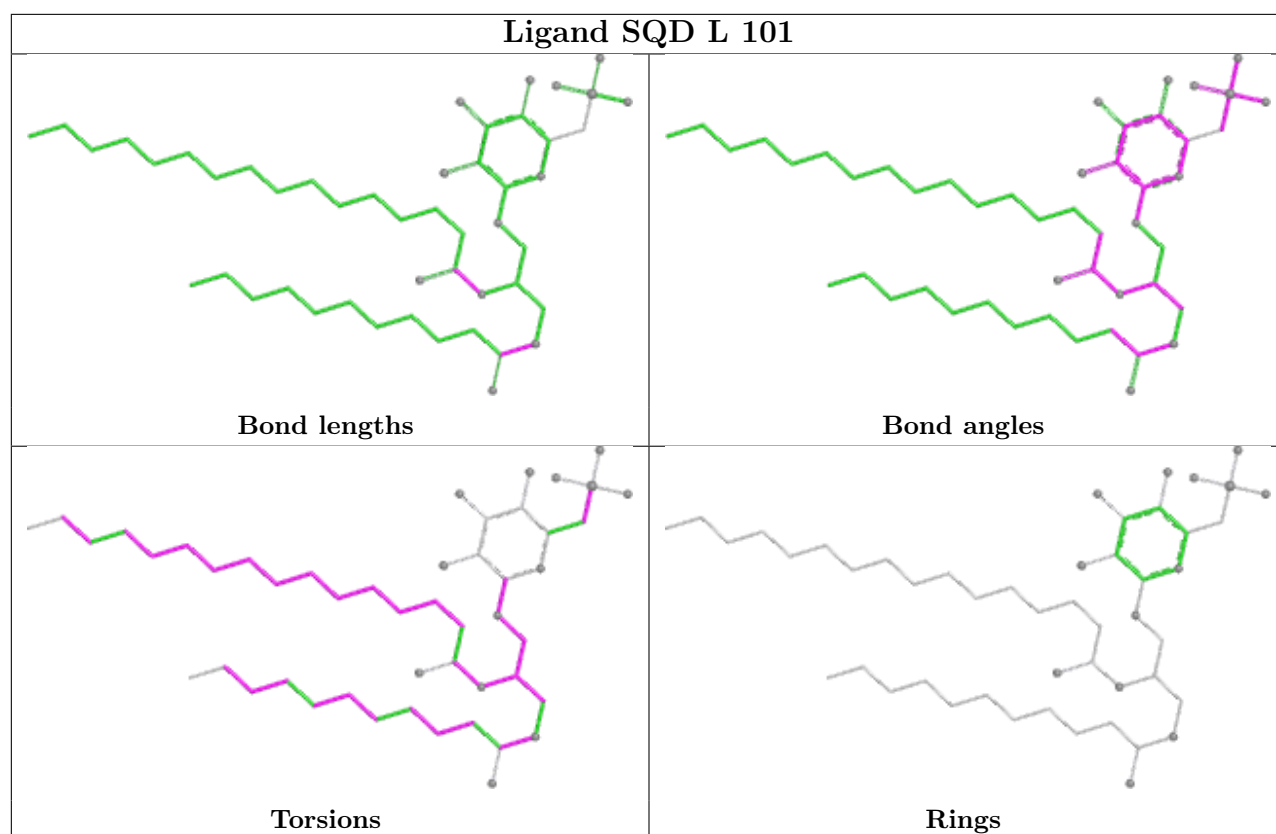
Ligand PL9 A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

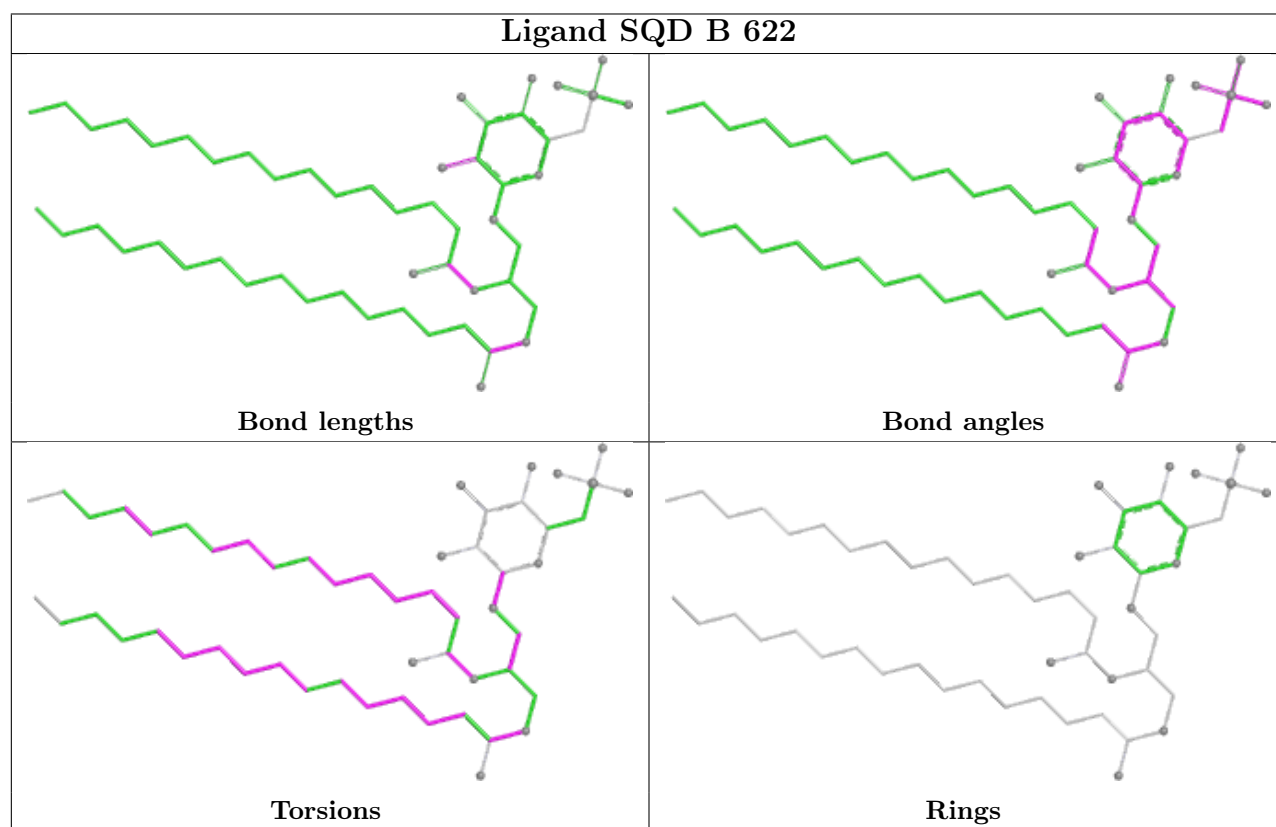
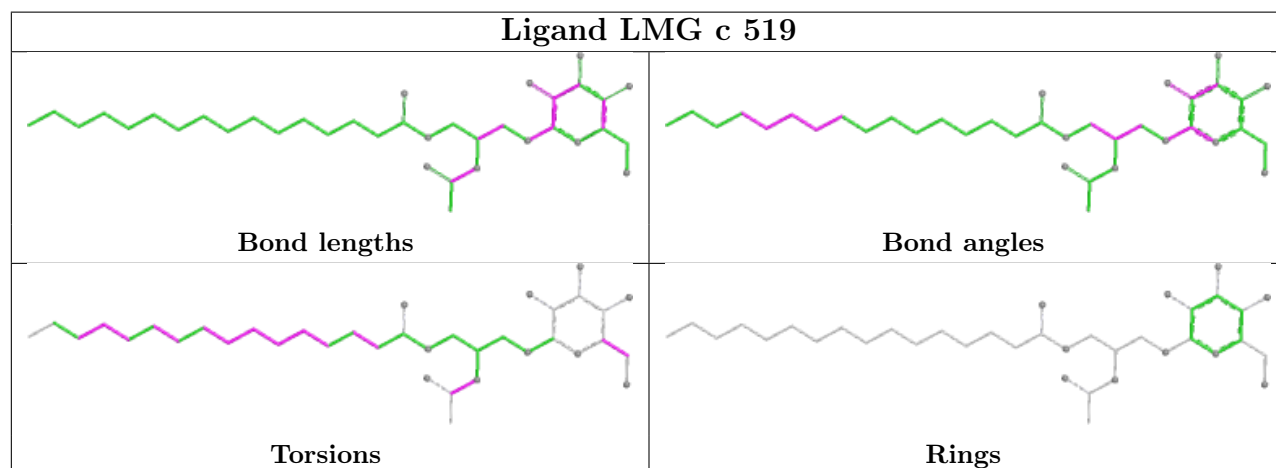
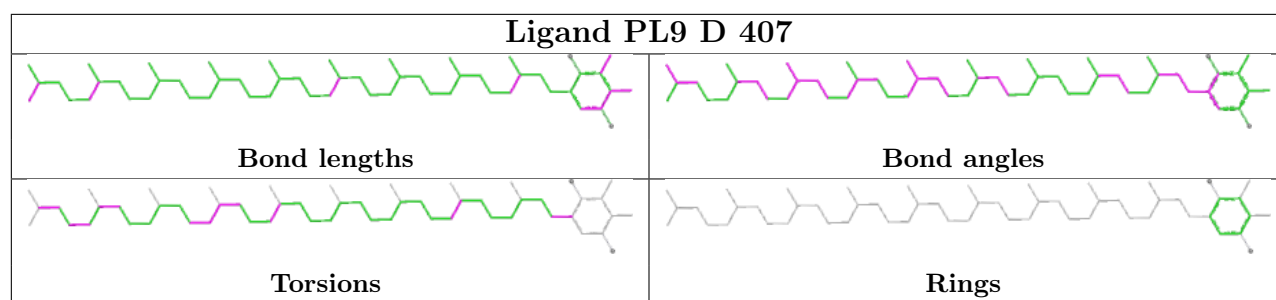


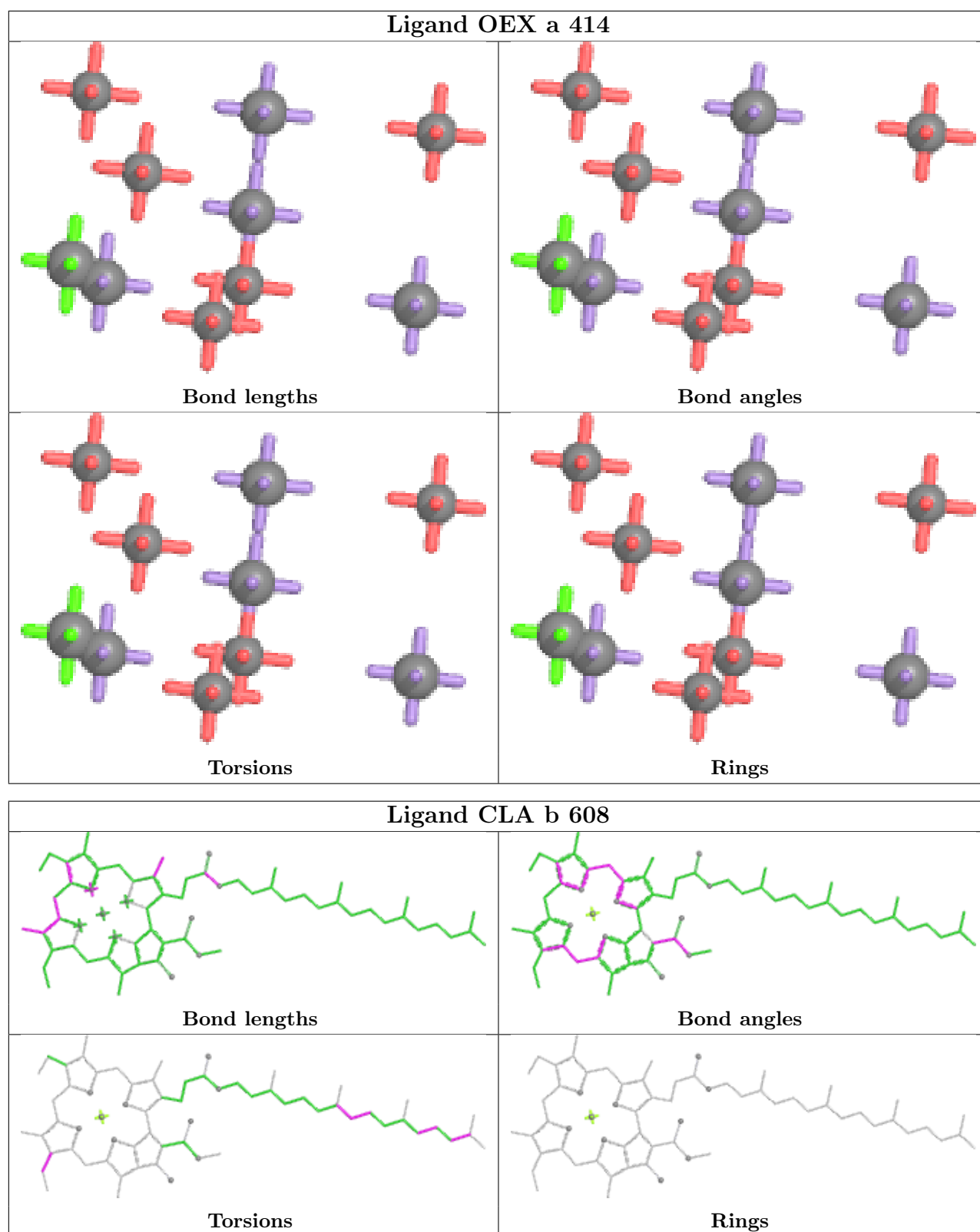
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

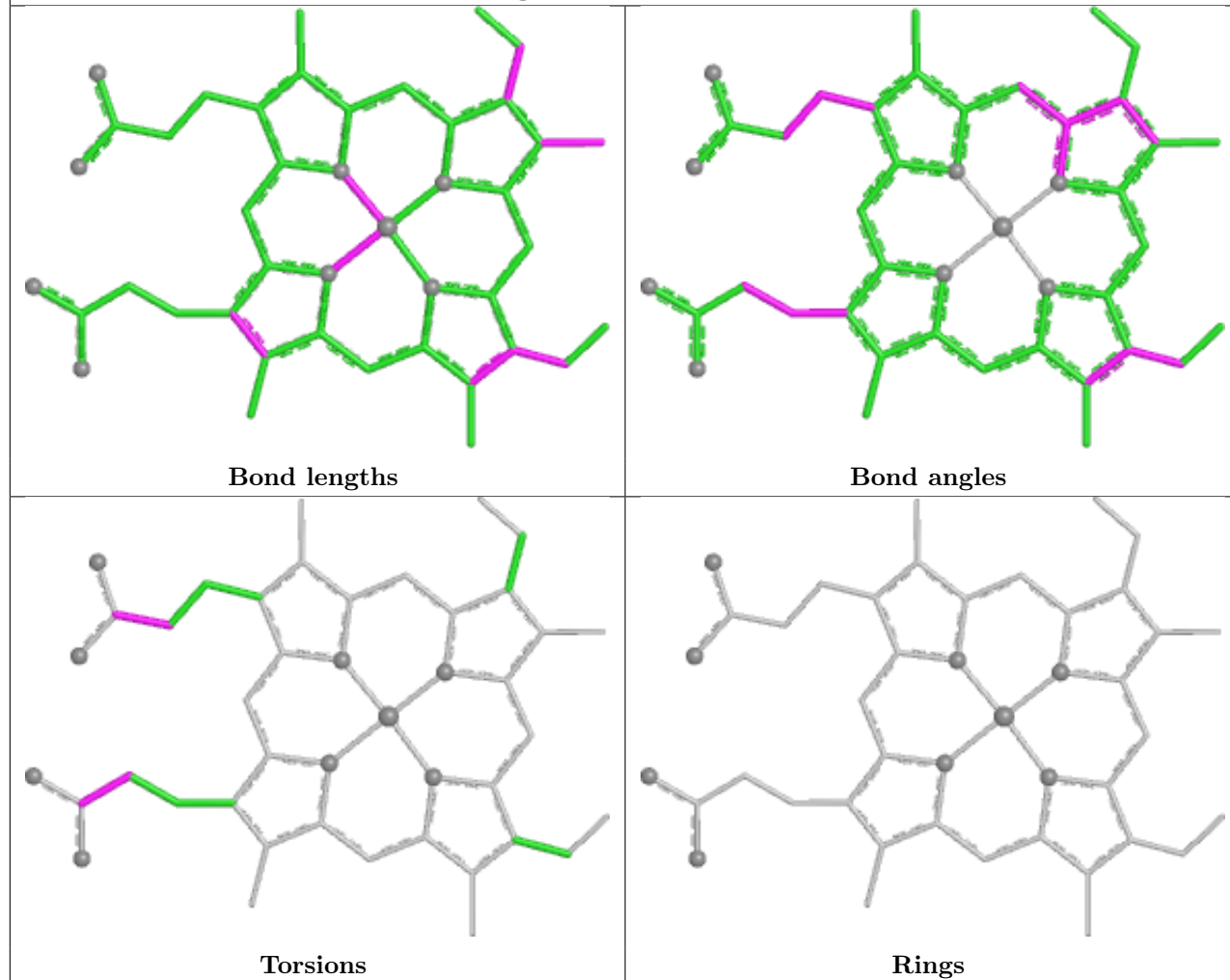
Ligand STE t 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



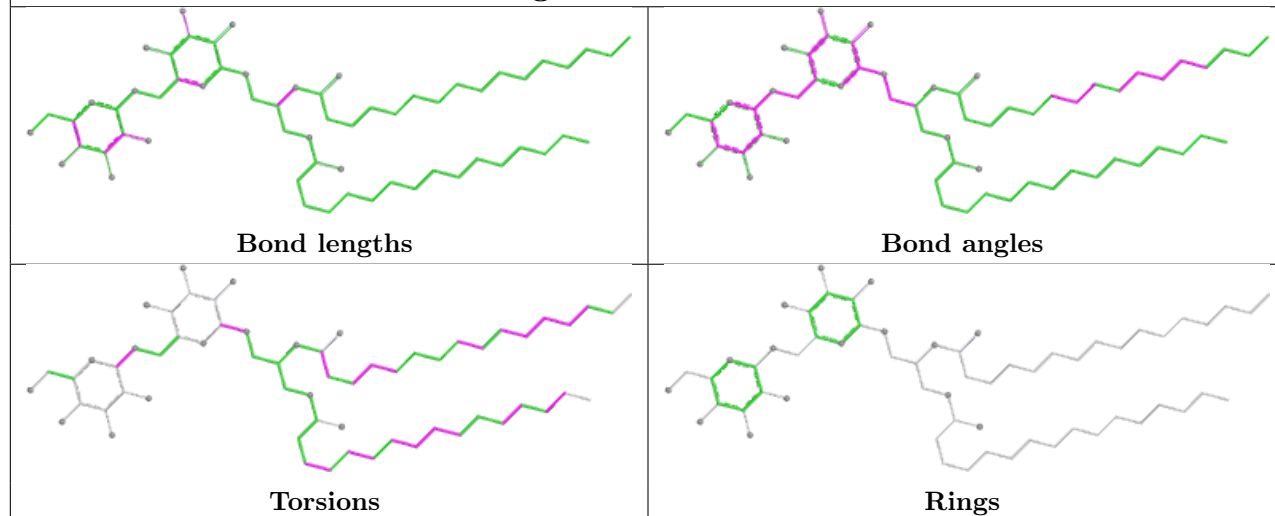


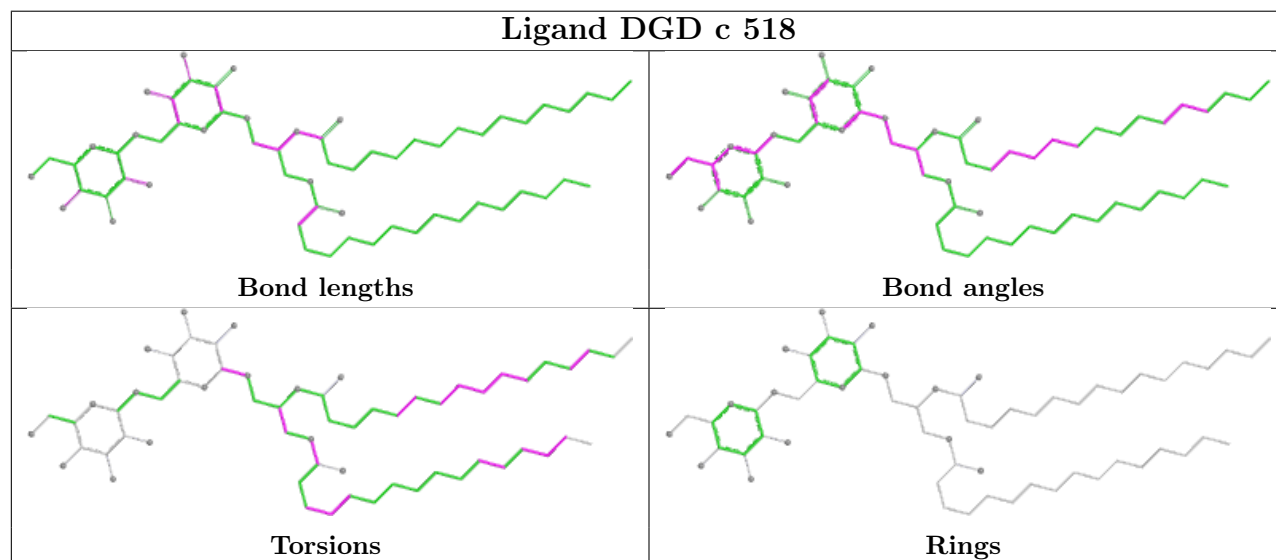
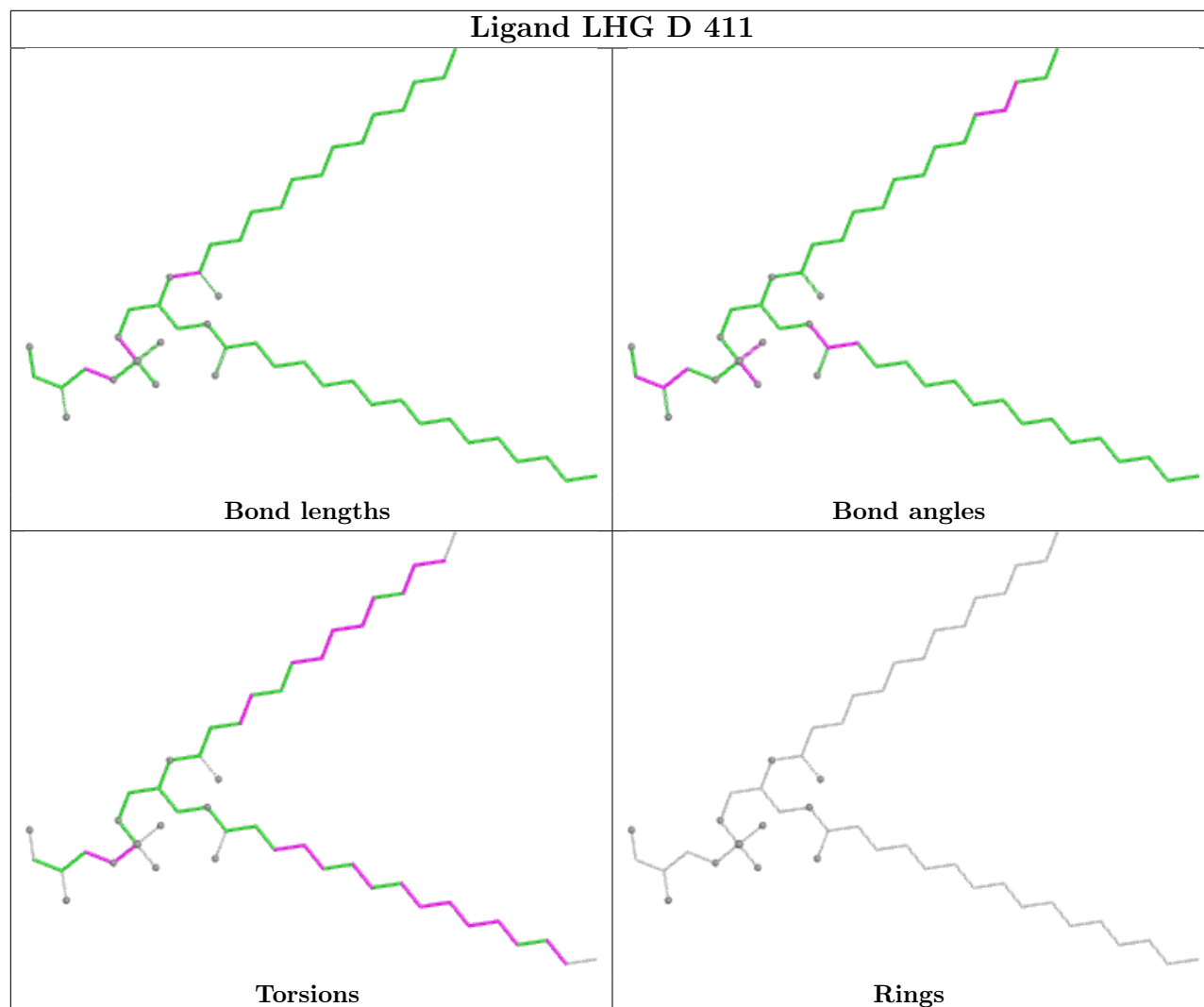


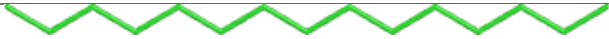
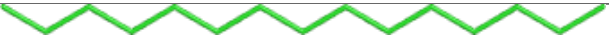
Ligand HEM f 101

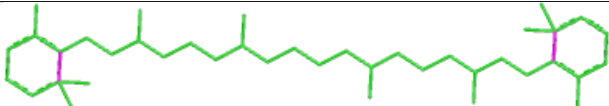
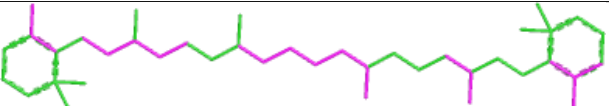
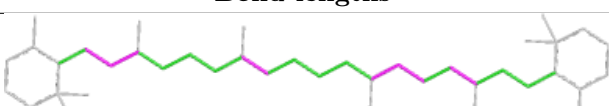
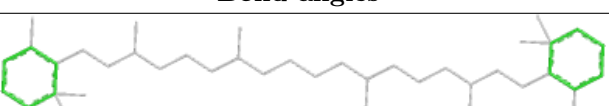


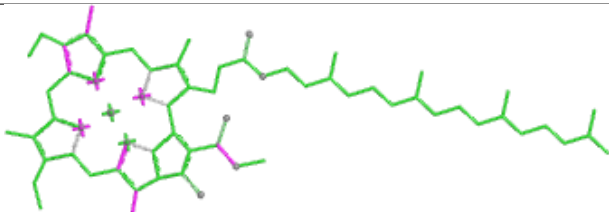
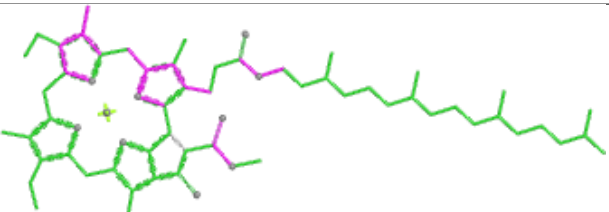
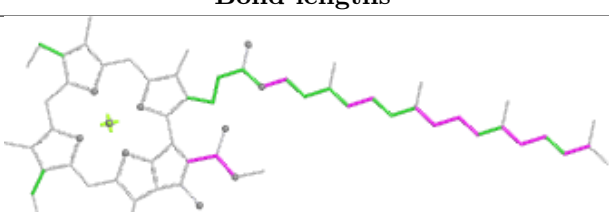
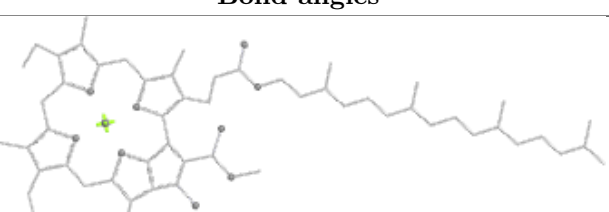
Ligand DGD c 517

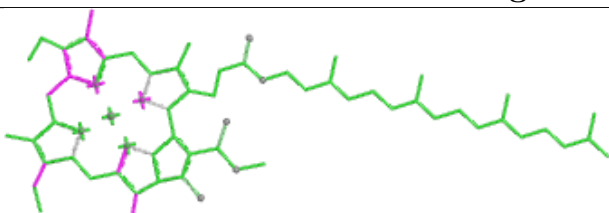
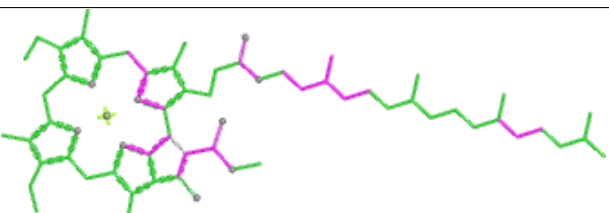
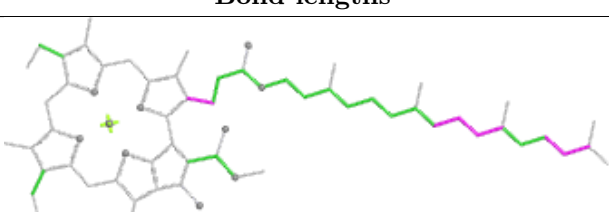
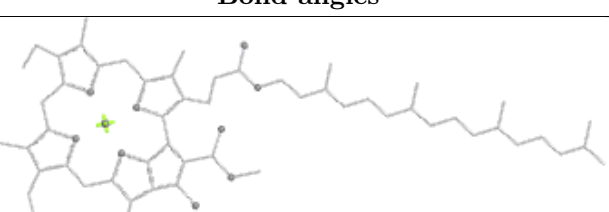




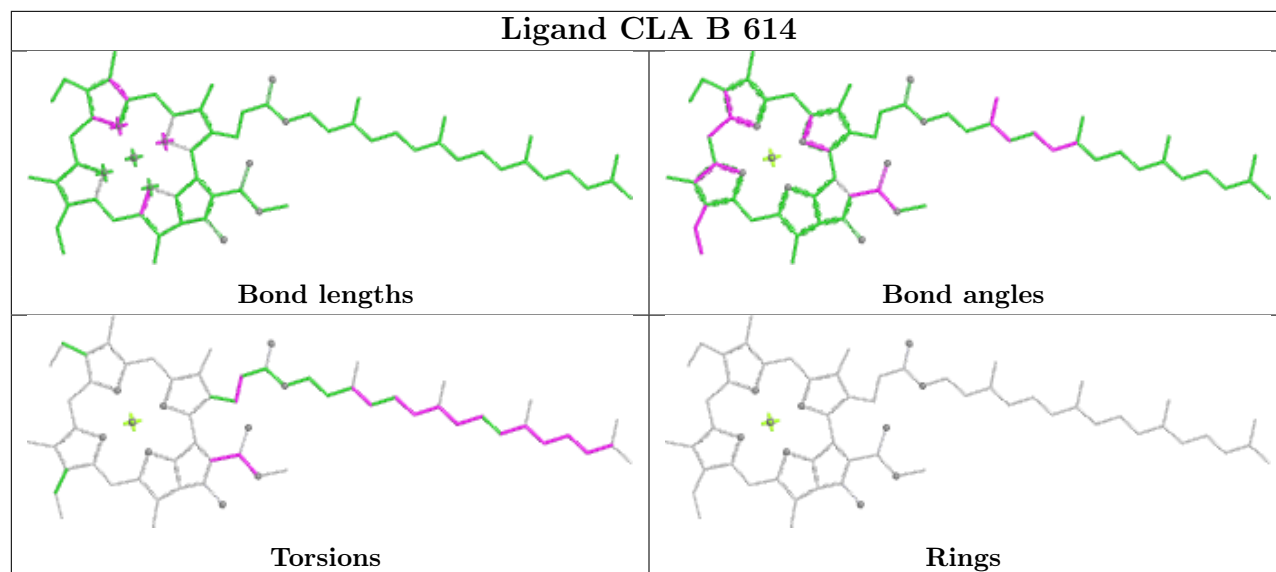
Ligand STE a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

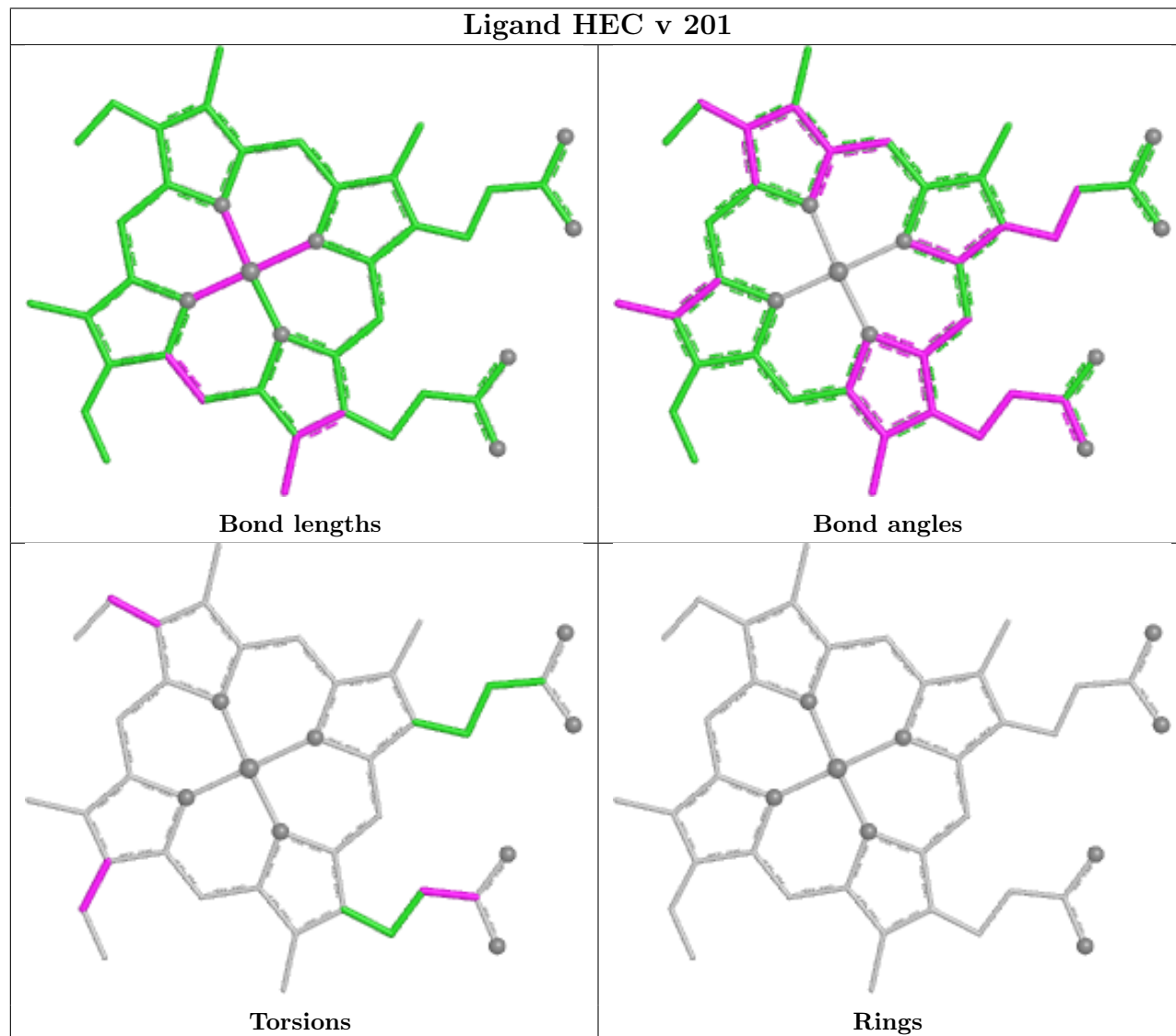
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

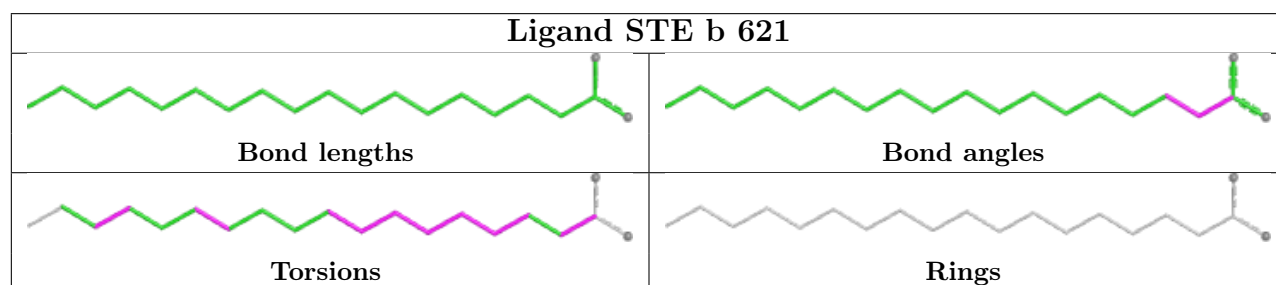
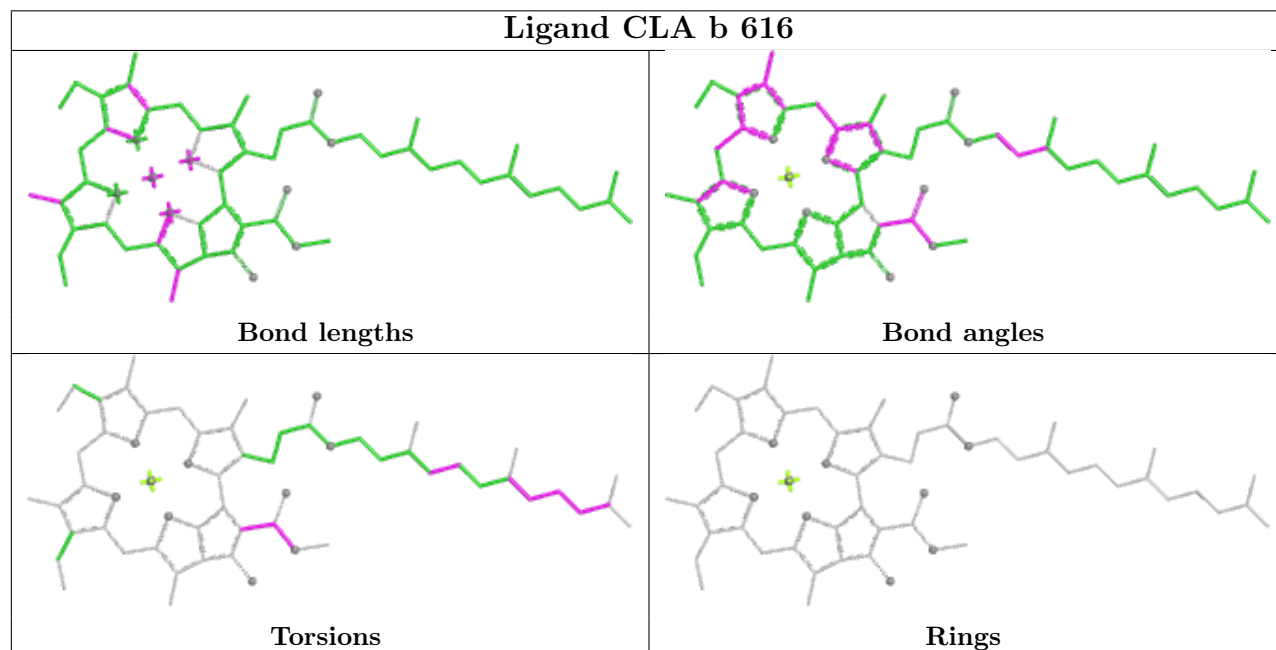
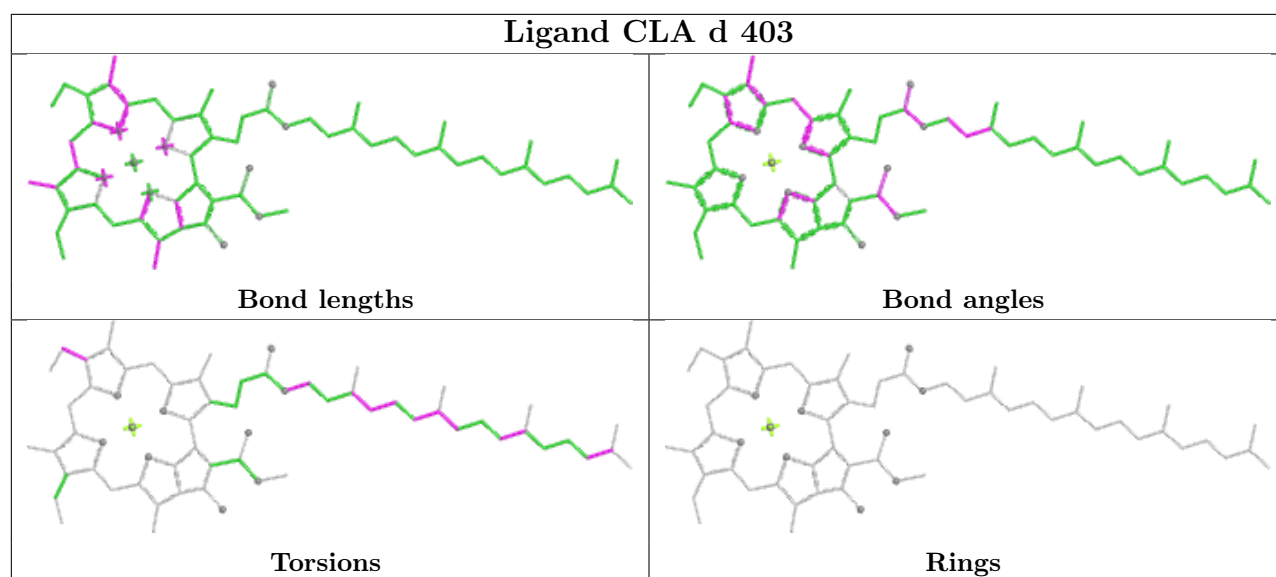
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

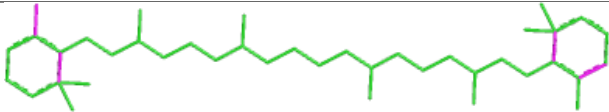
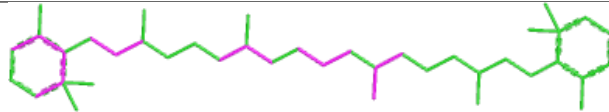
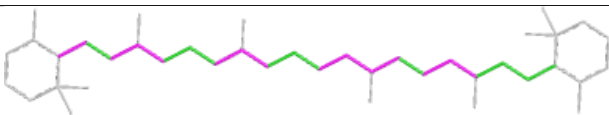
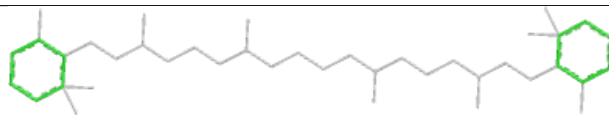
Ligand CLA B 614

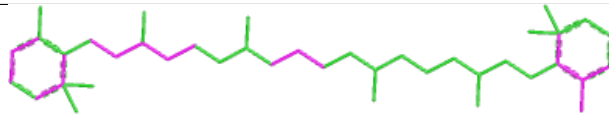
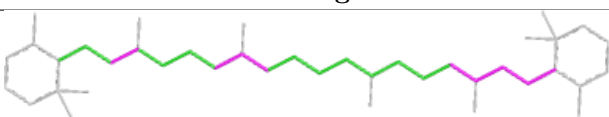
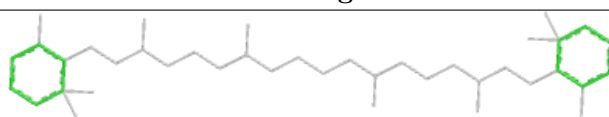


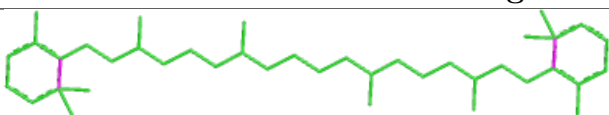
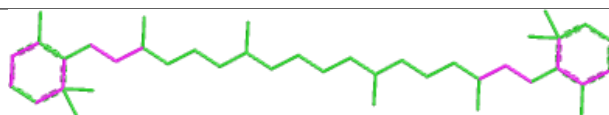
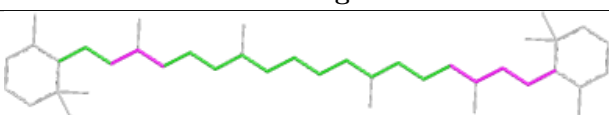
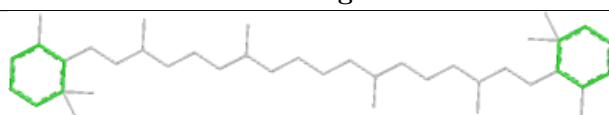
Ligand HEC v 201

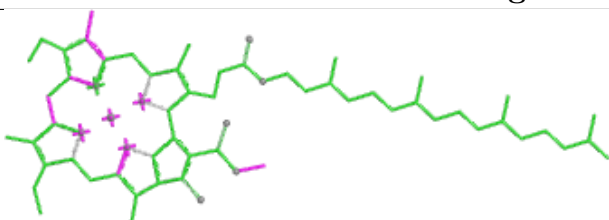
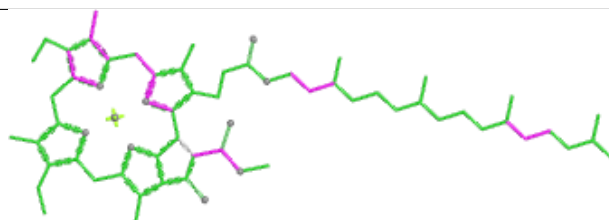
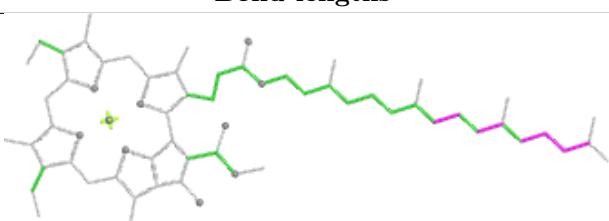
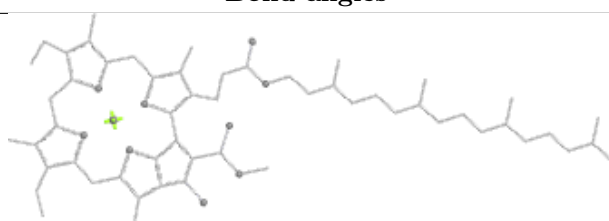


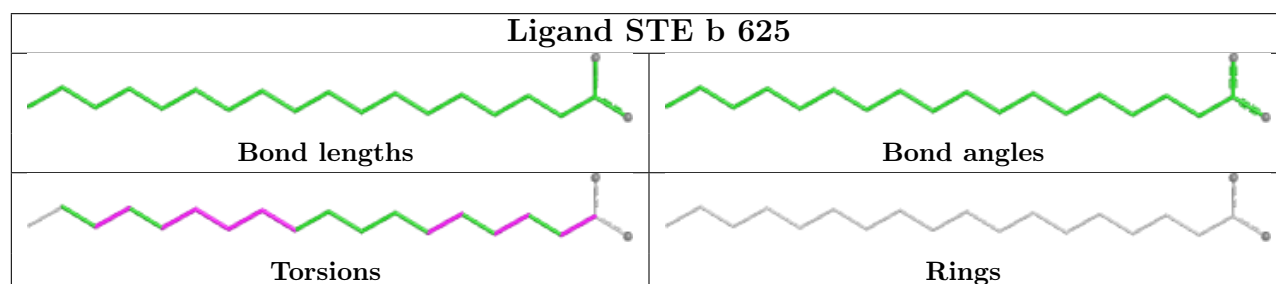
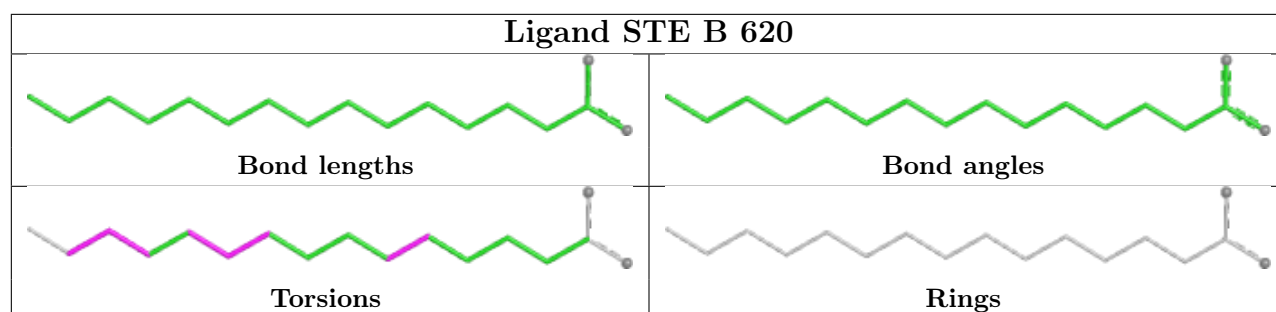
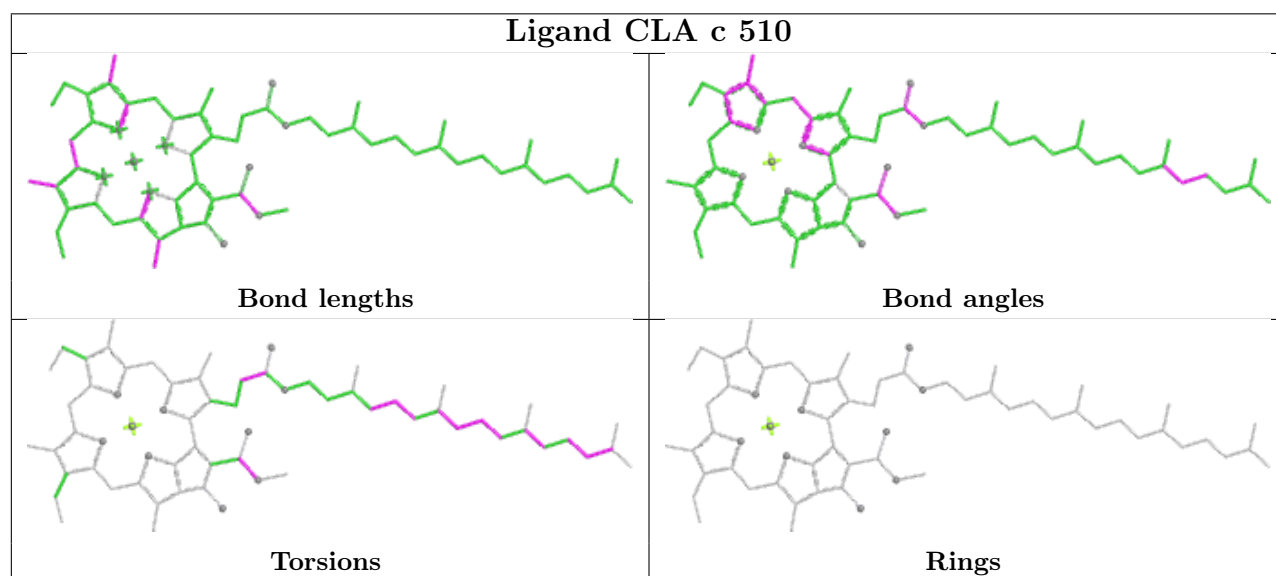
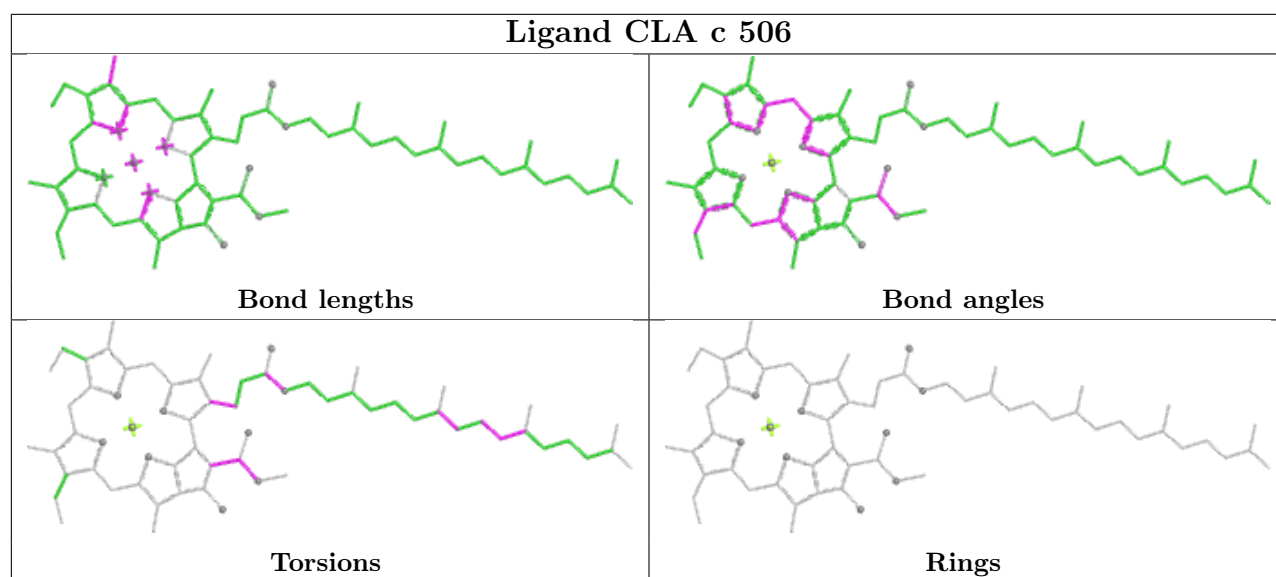


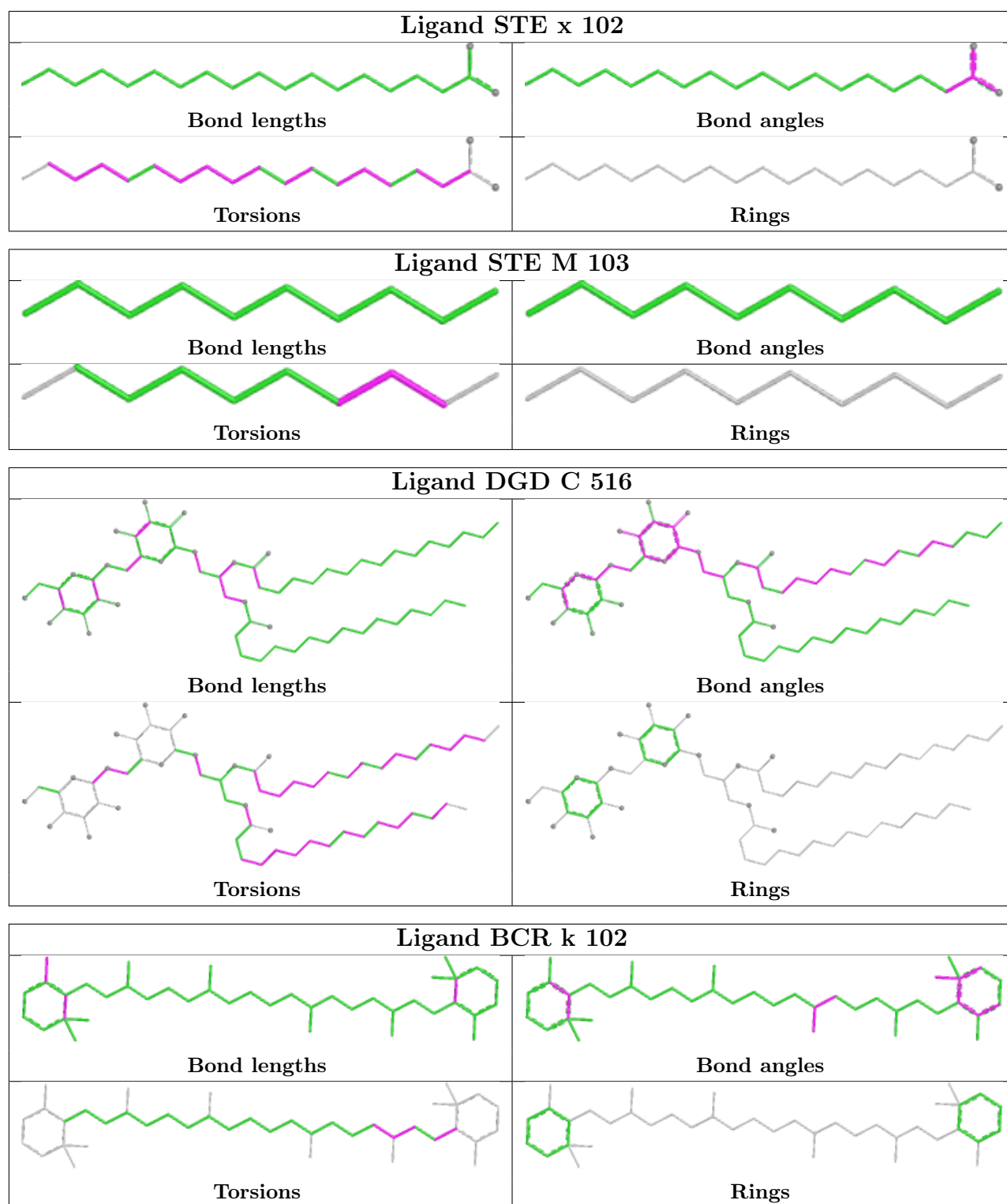
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

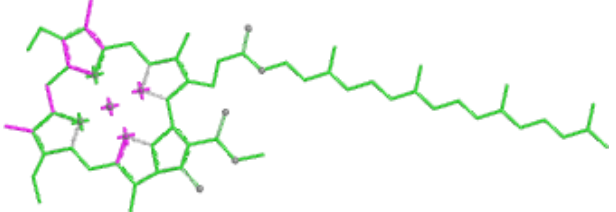
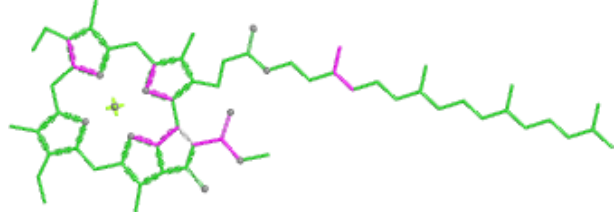
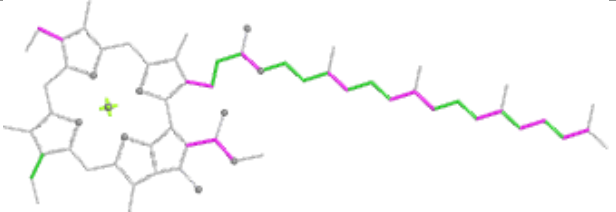
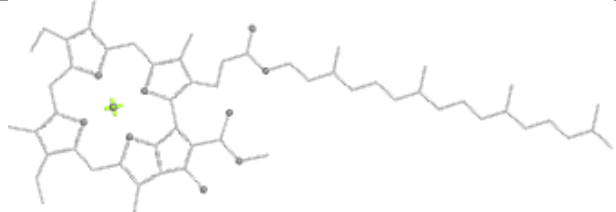
Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

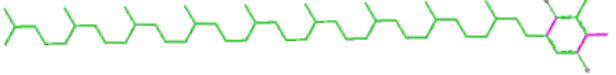
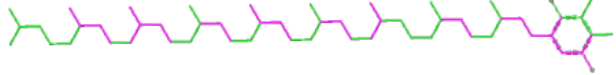
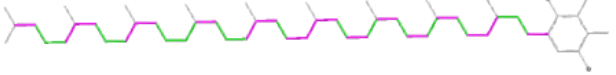
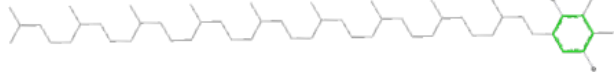
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

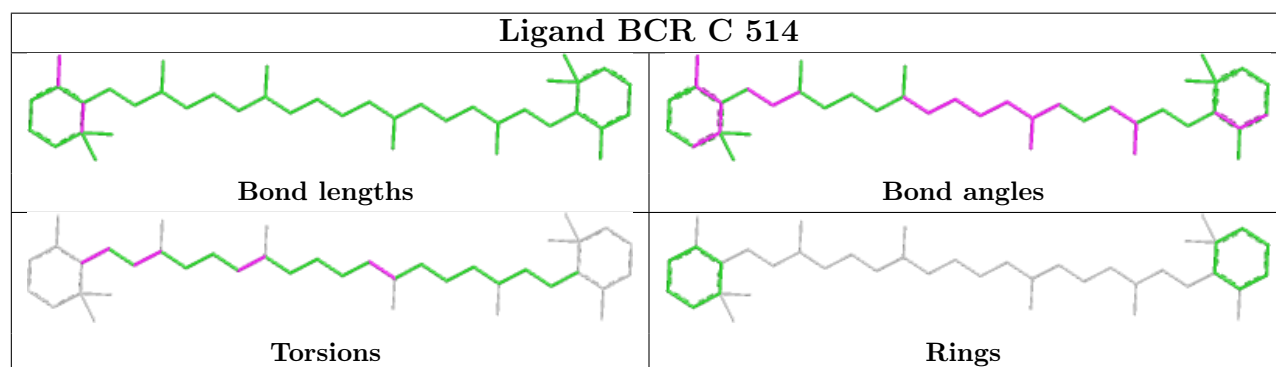
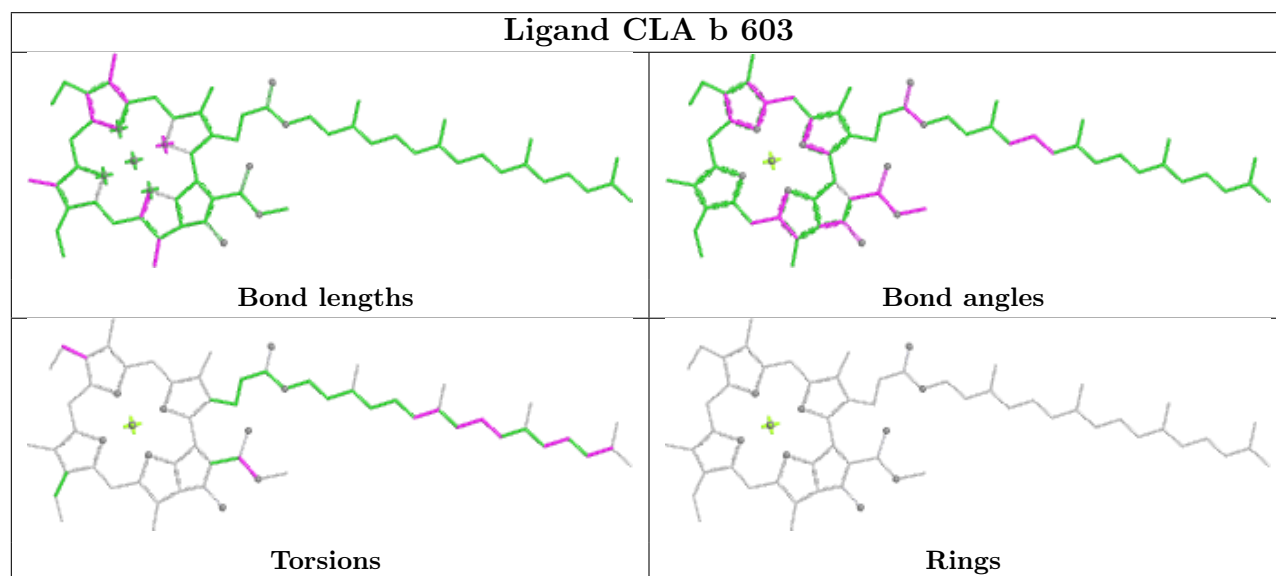
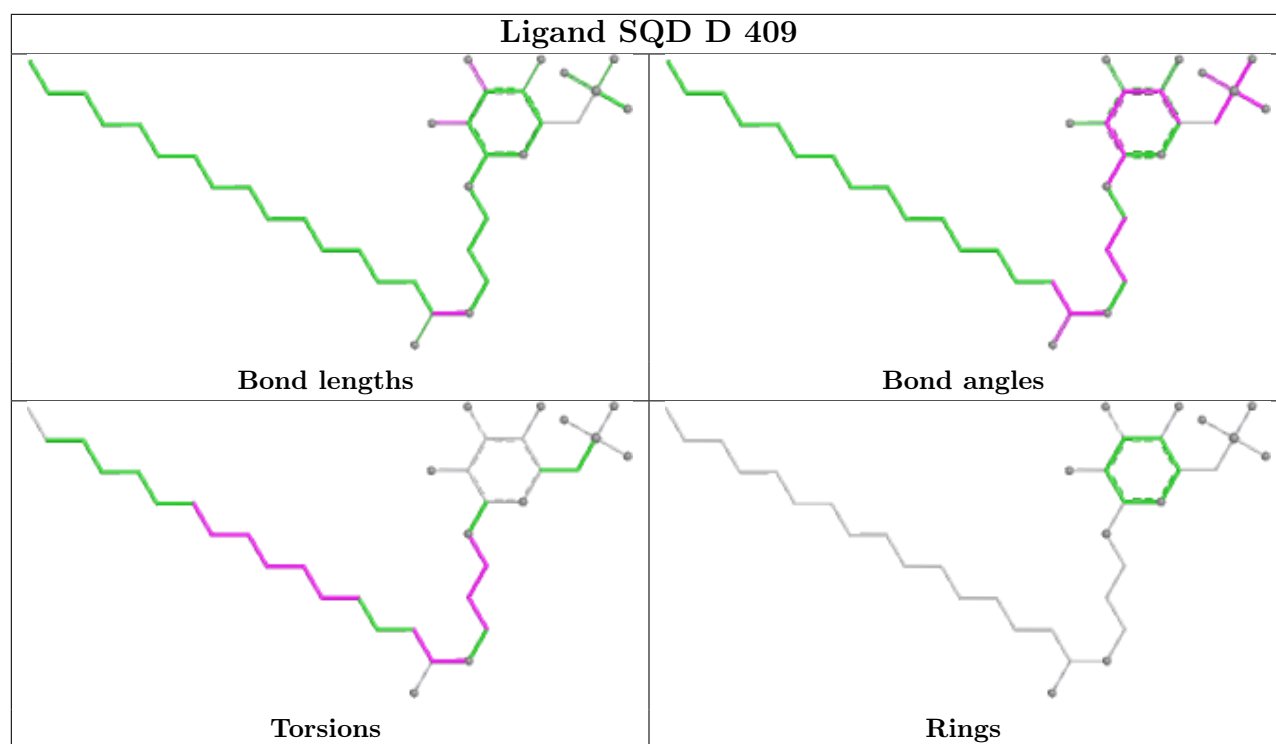


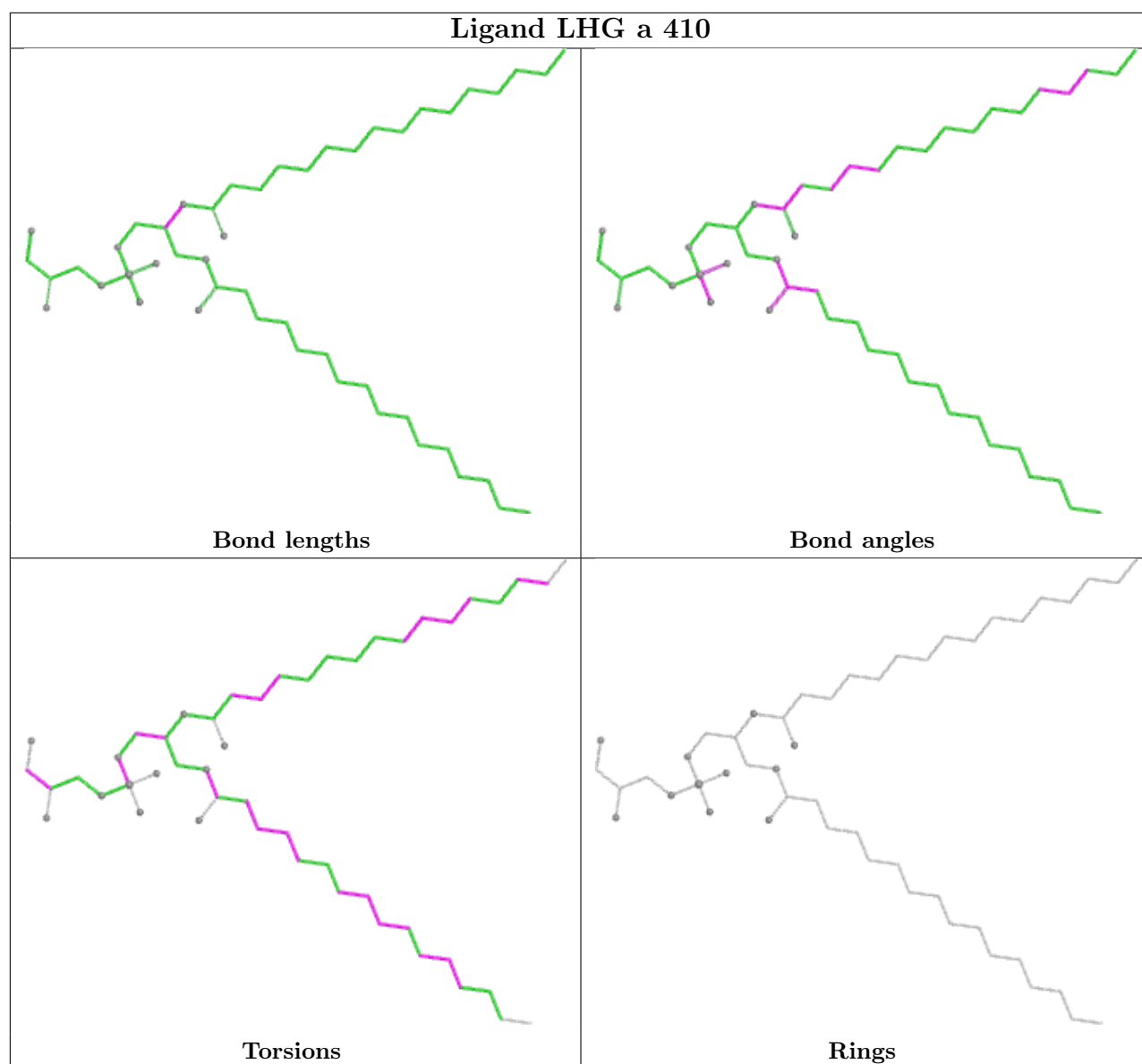


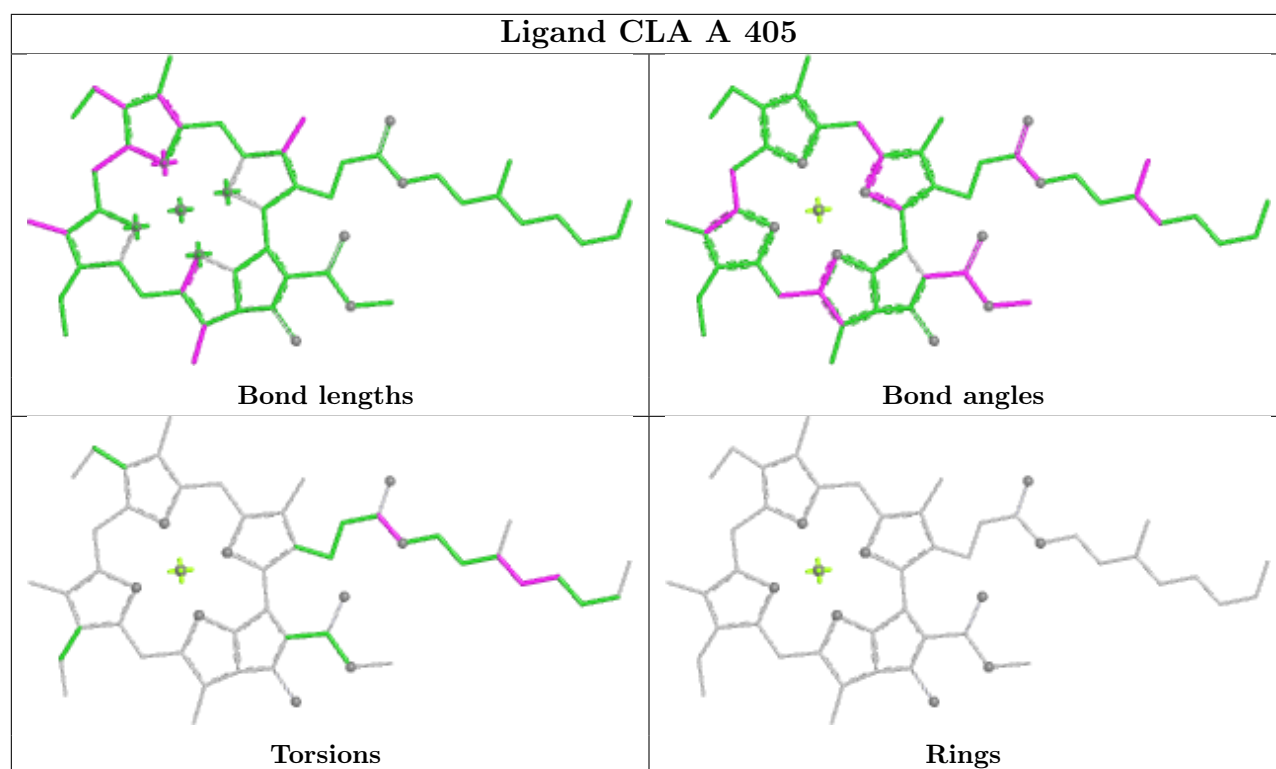
Ligand CLA B 601			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

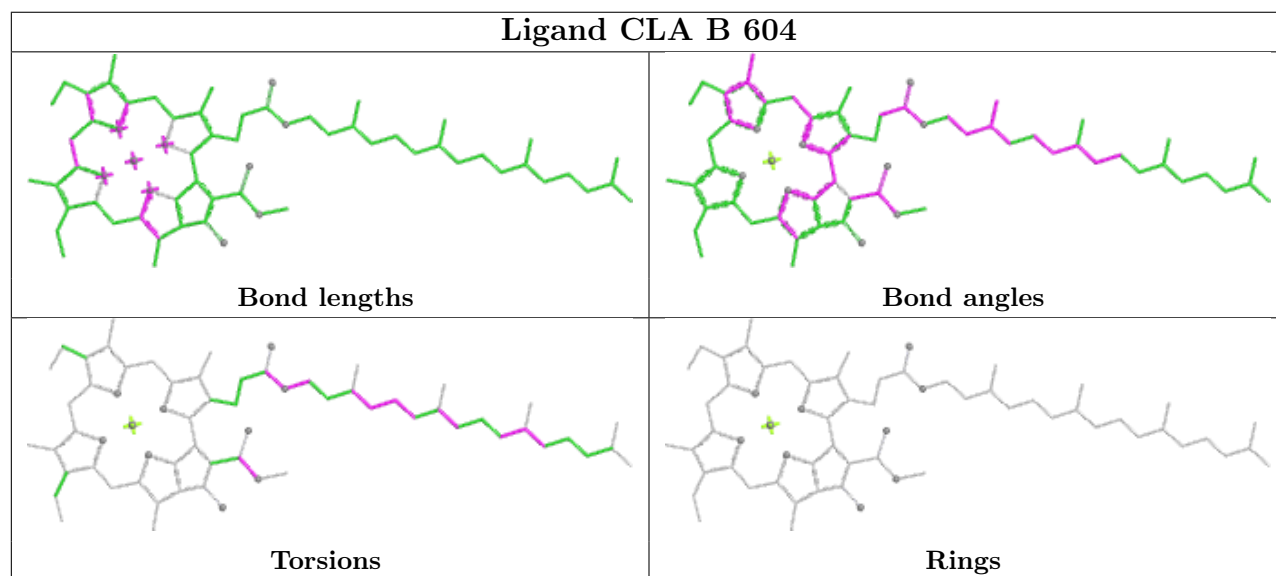
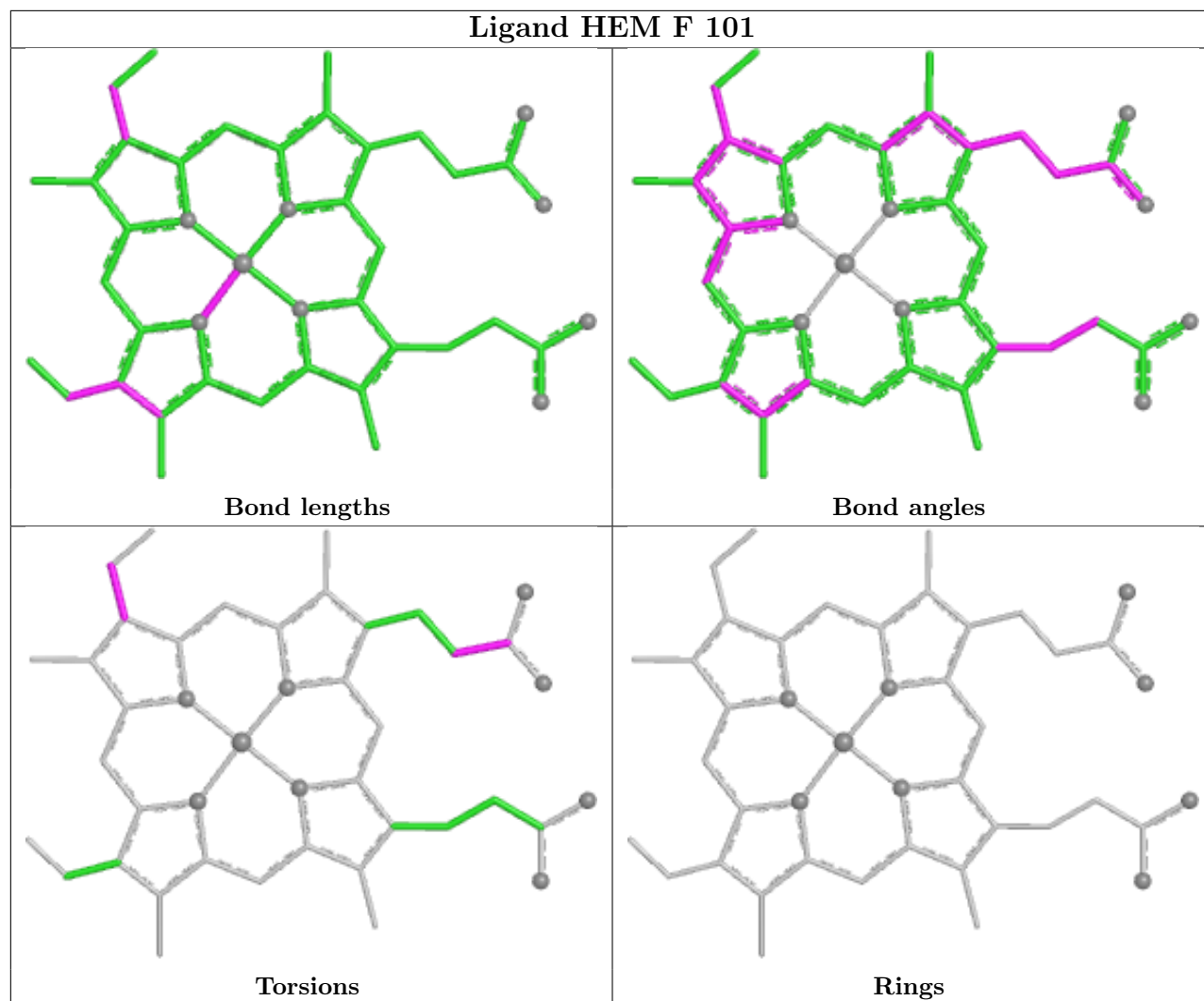
Ligand PL9 a 409			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

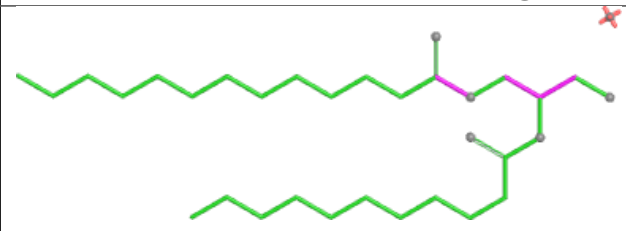
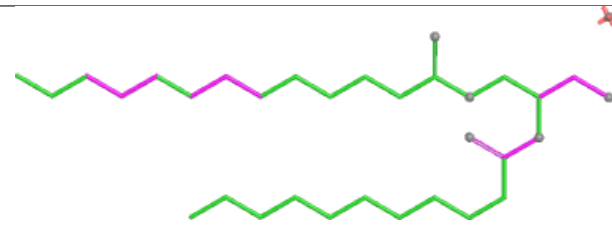
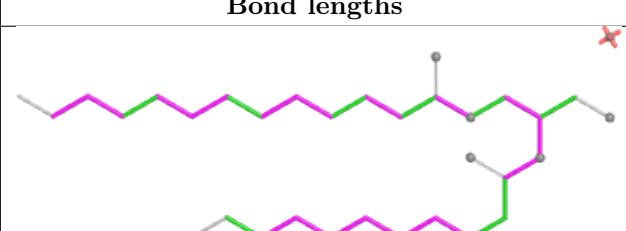
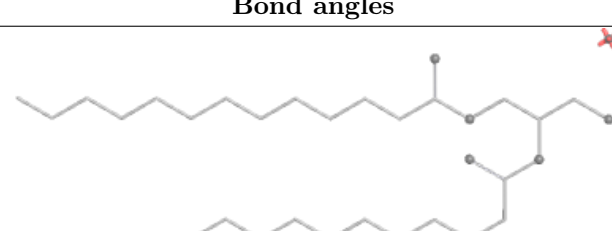
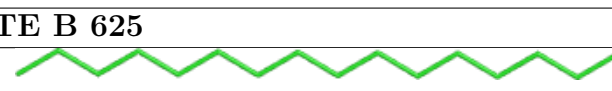
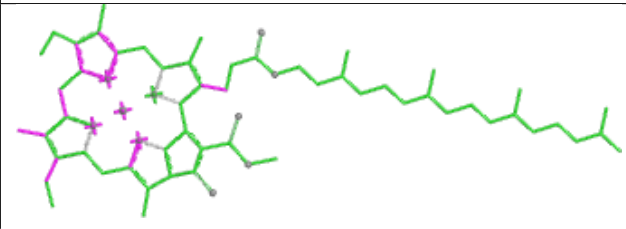
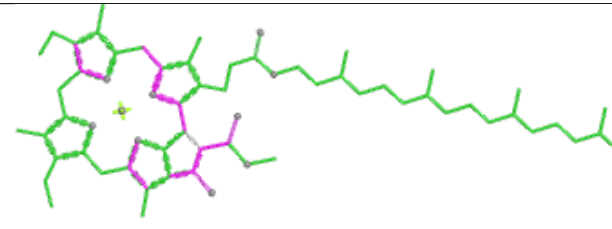
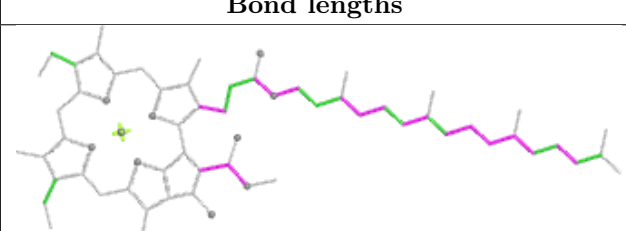
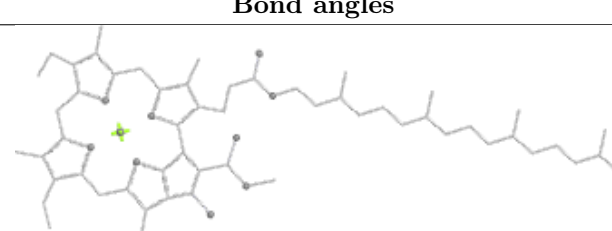
Ligand STE B 624			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

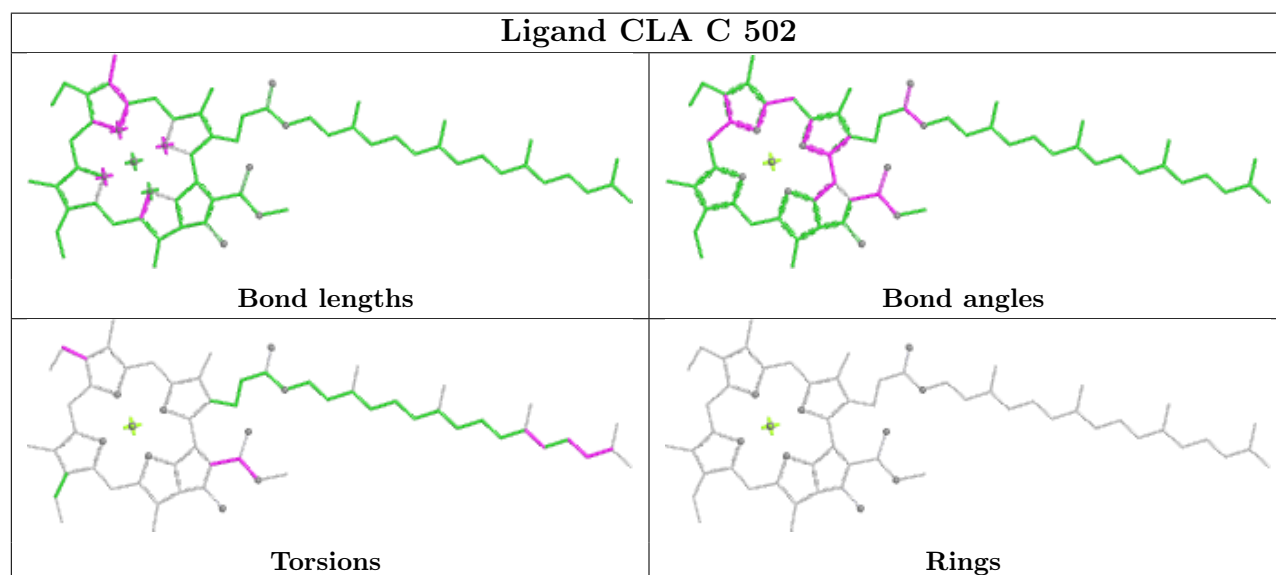
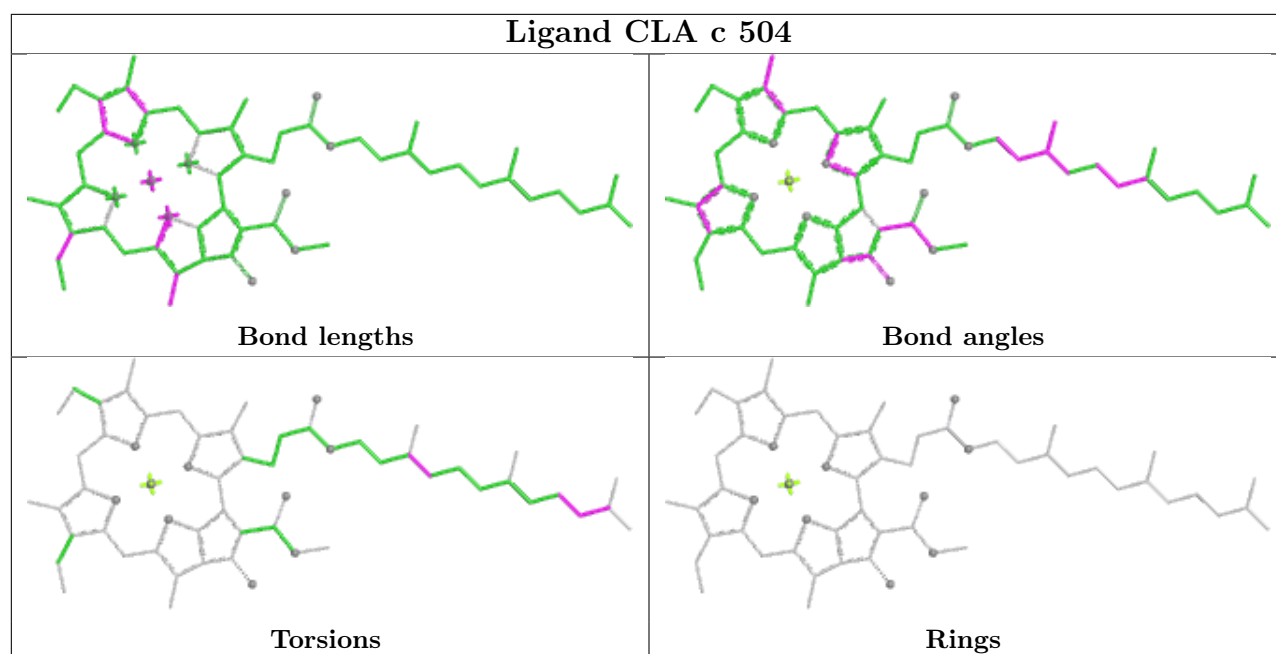


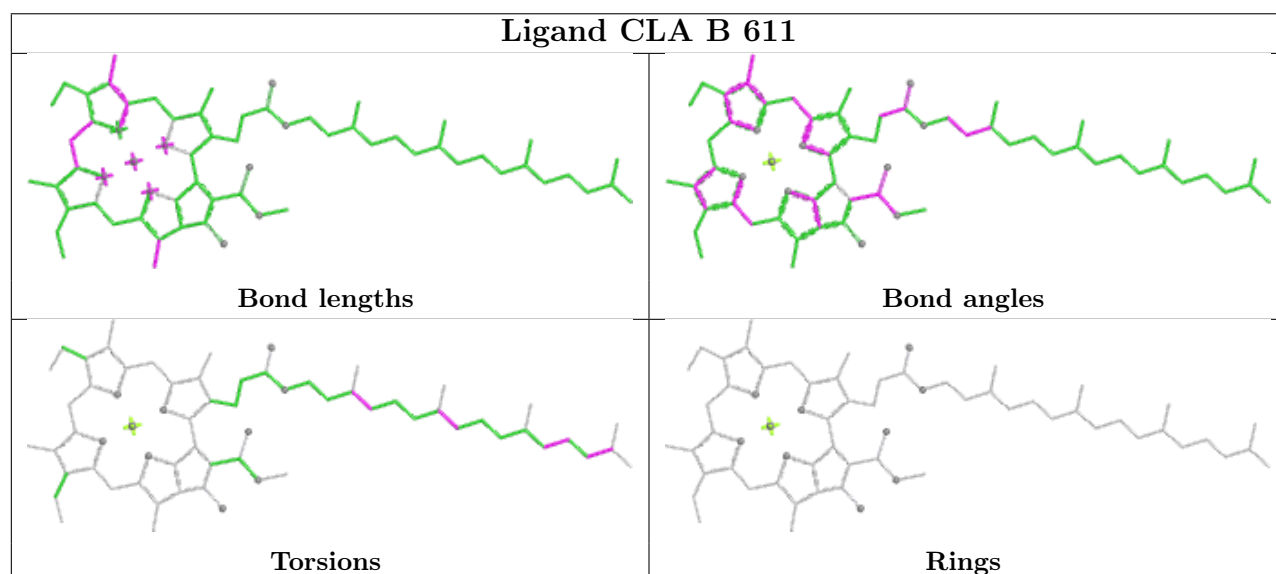
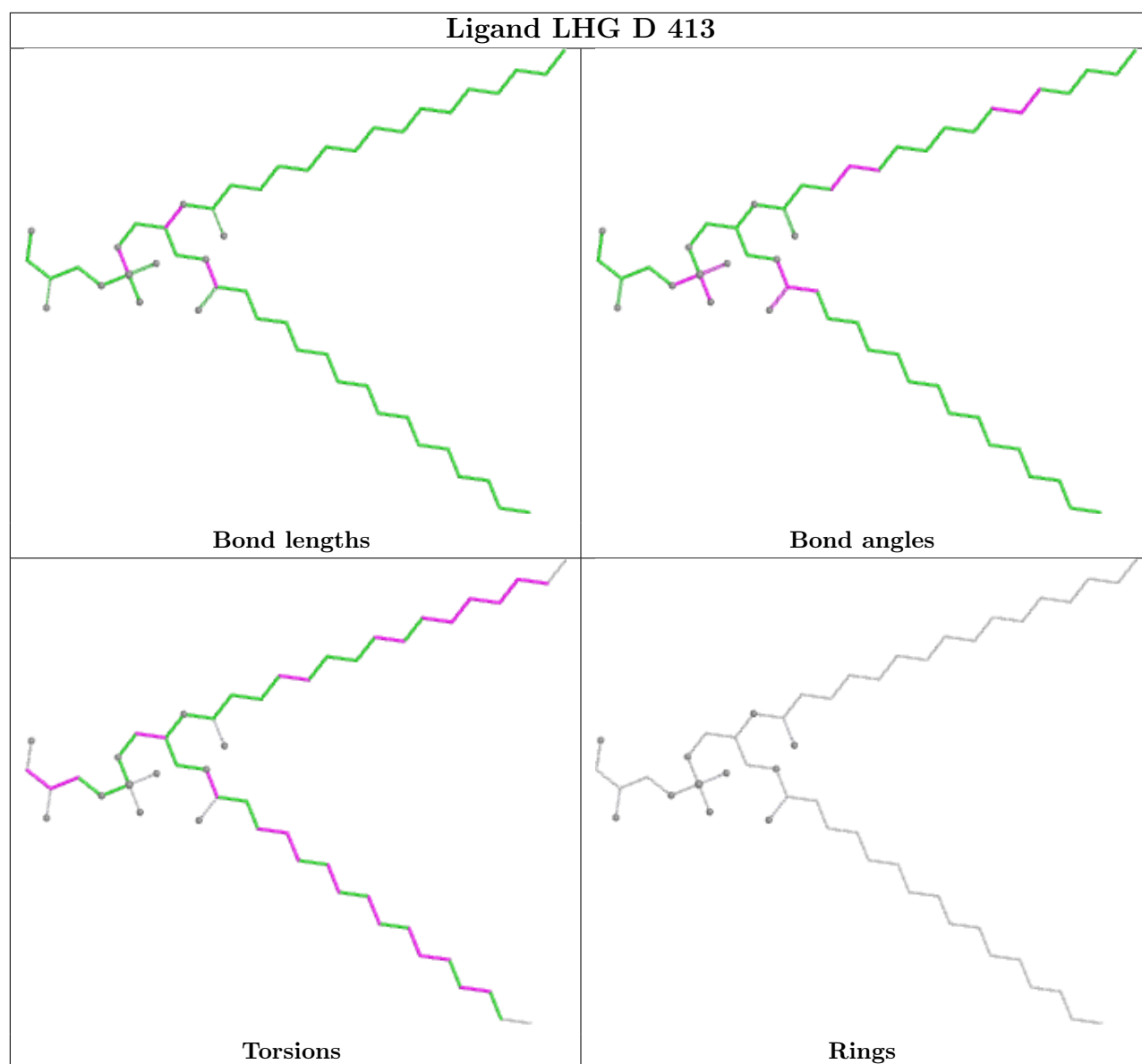


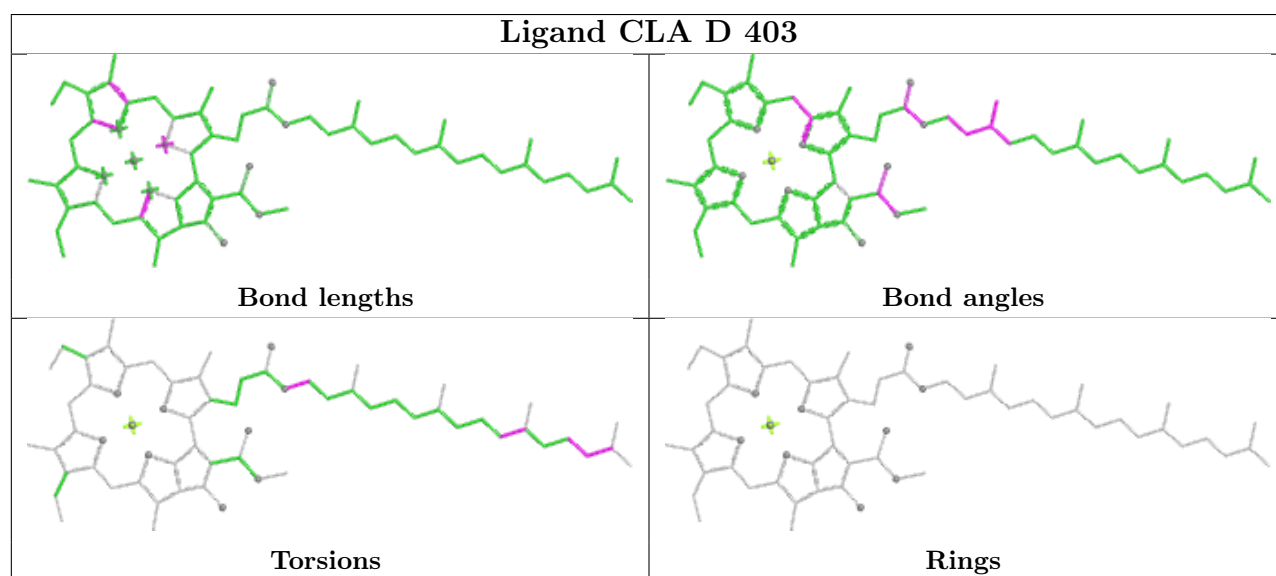
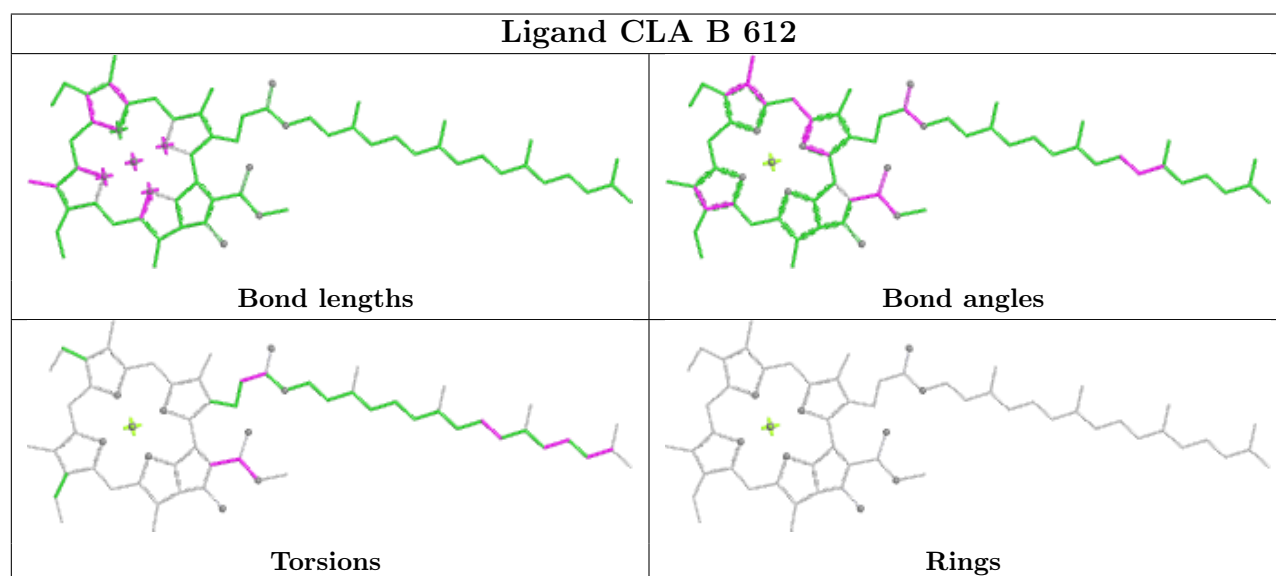
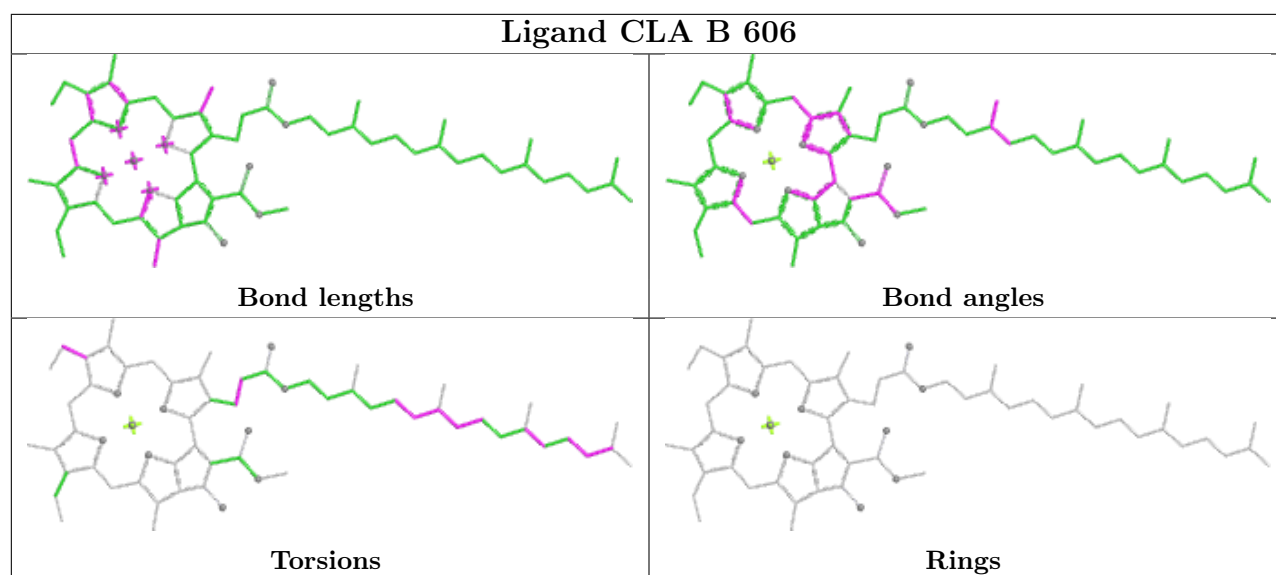


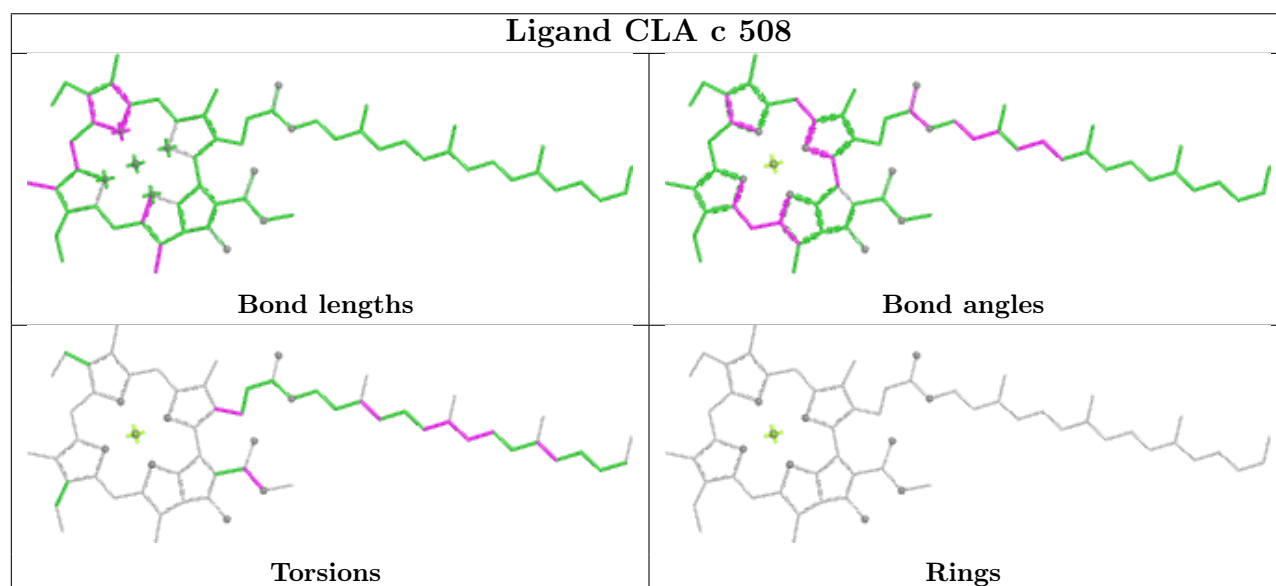
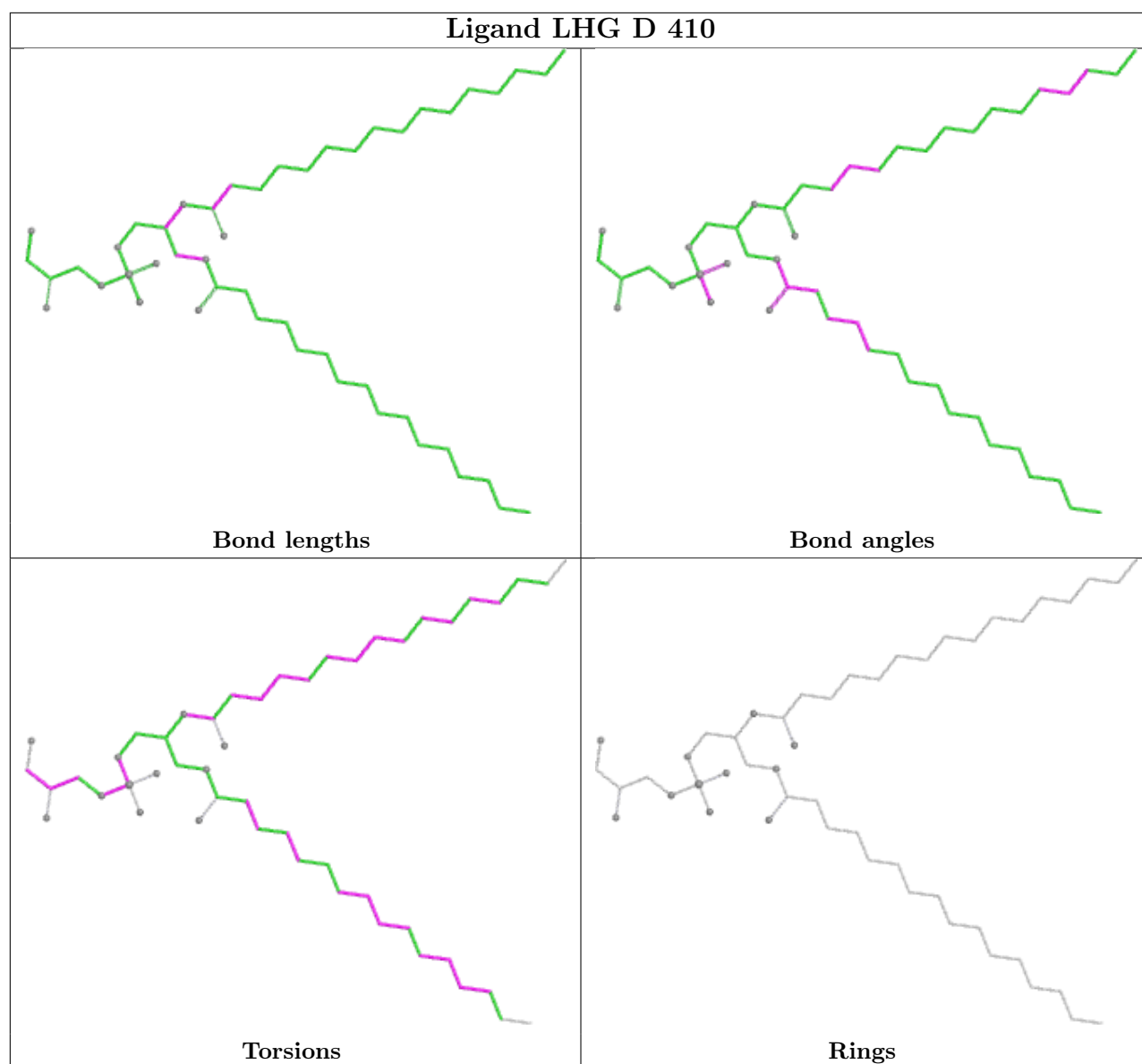


Ligand LMG D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

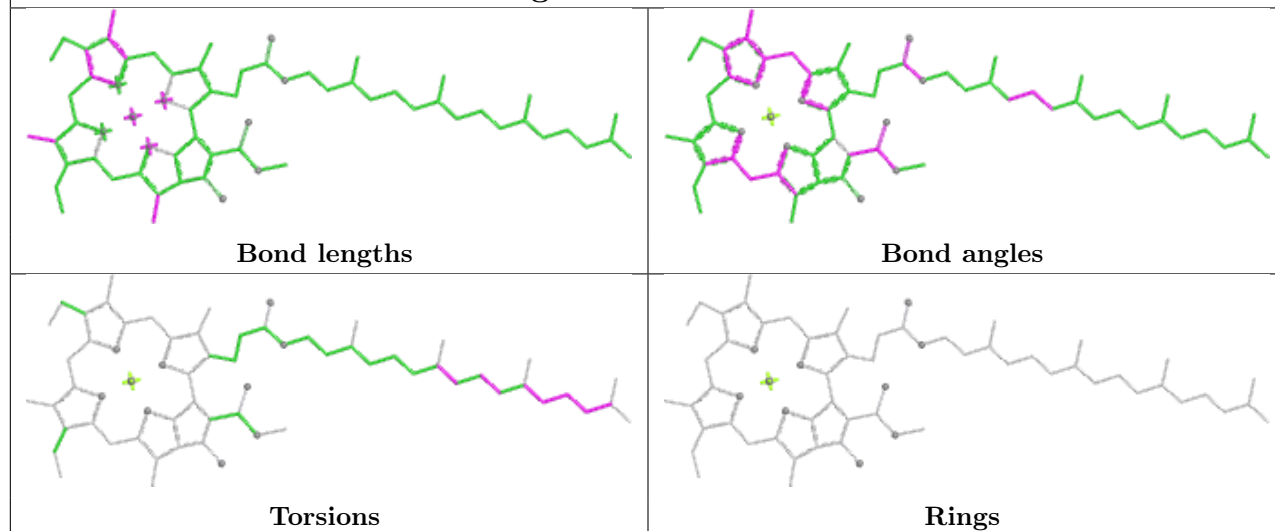




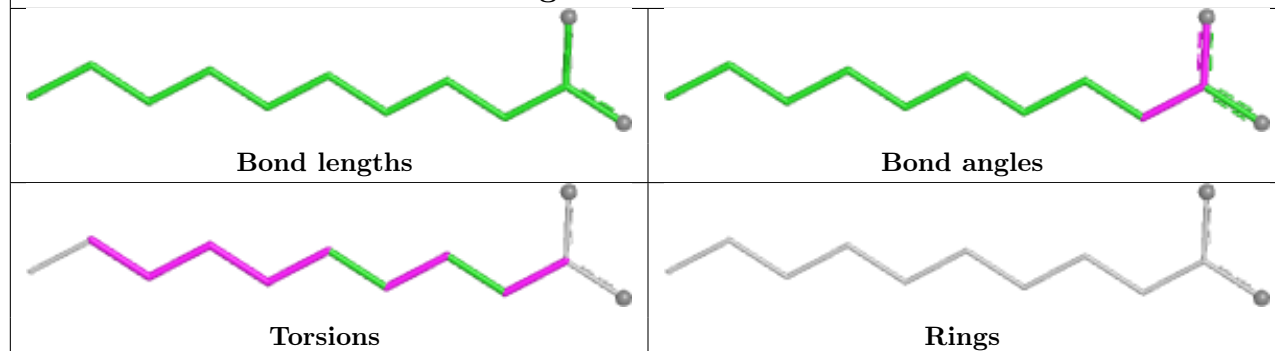




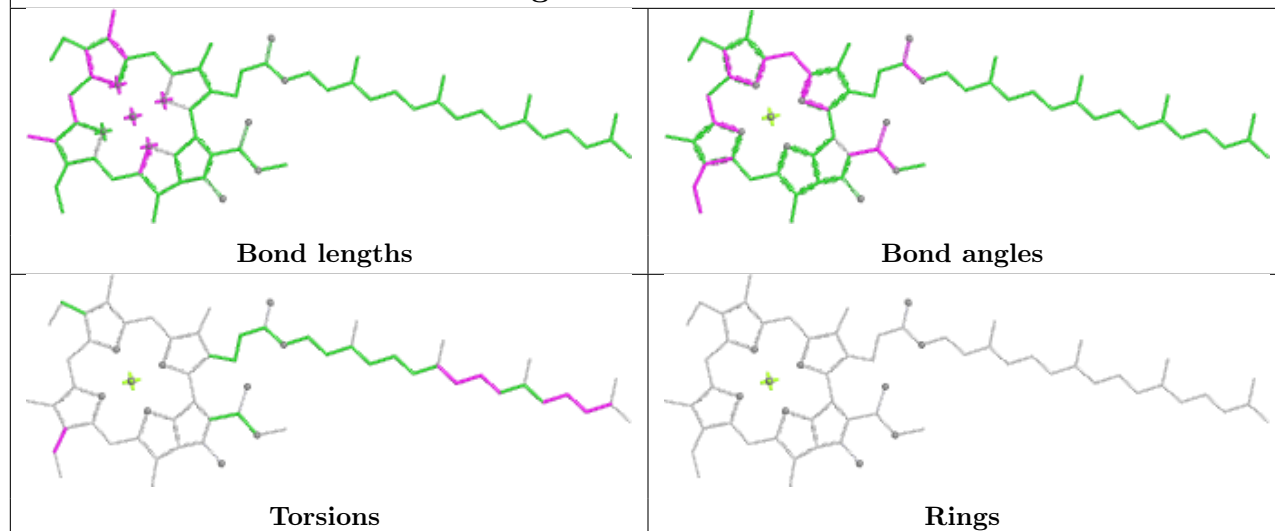
Ligand CLA C 508

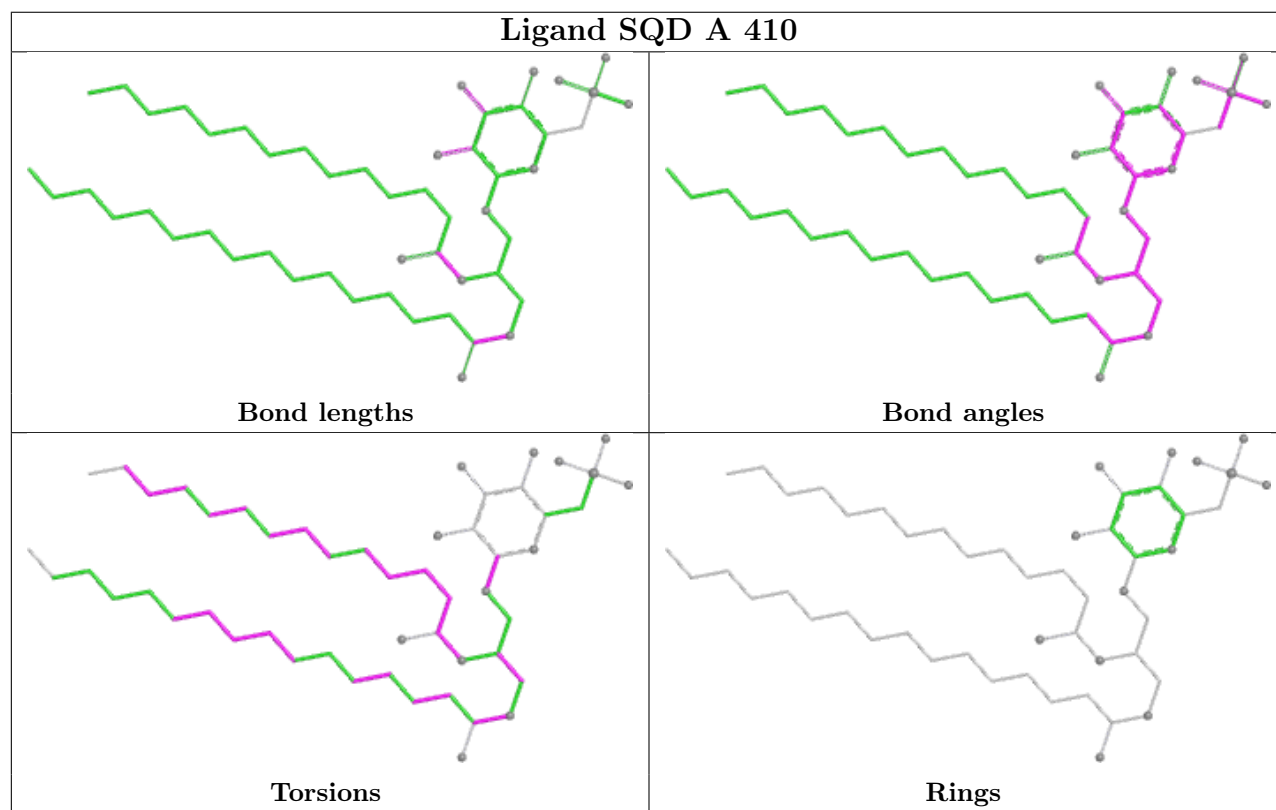
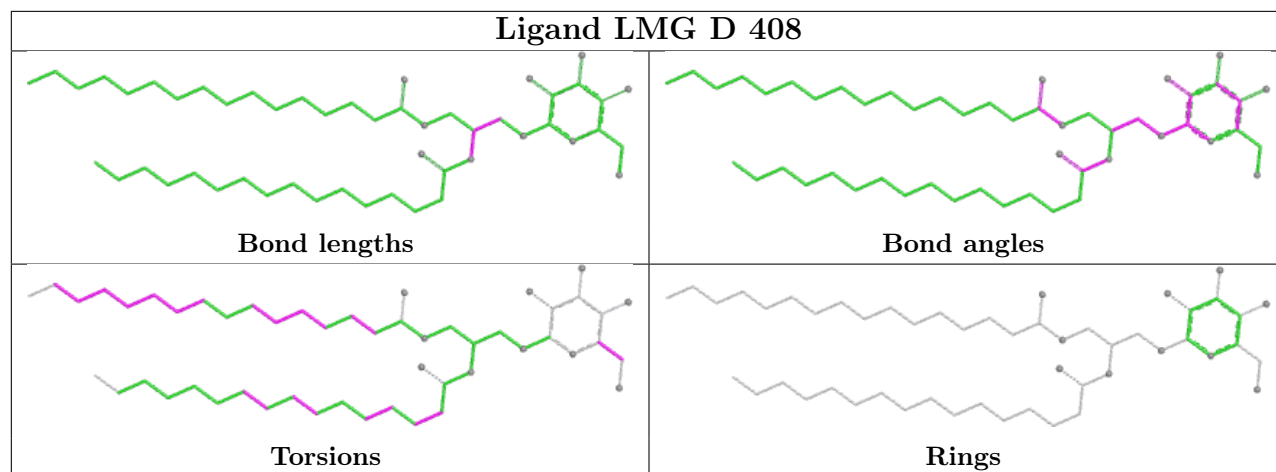


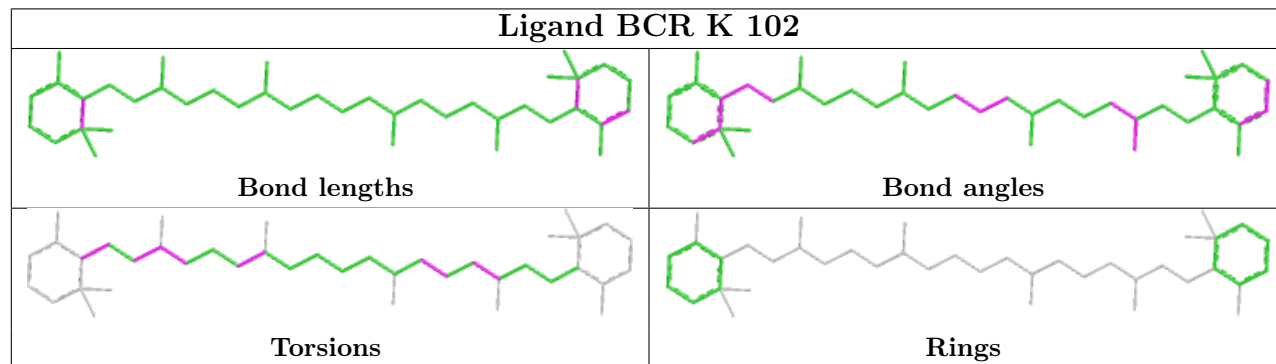
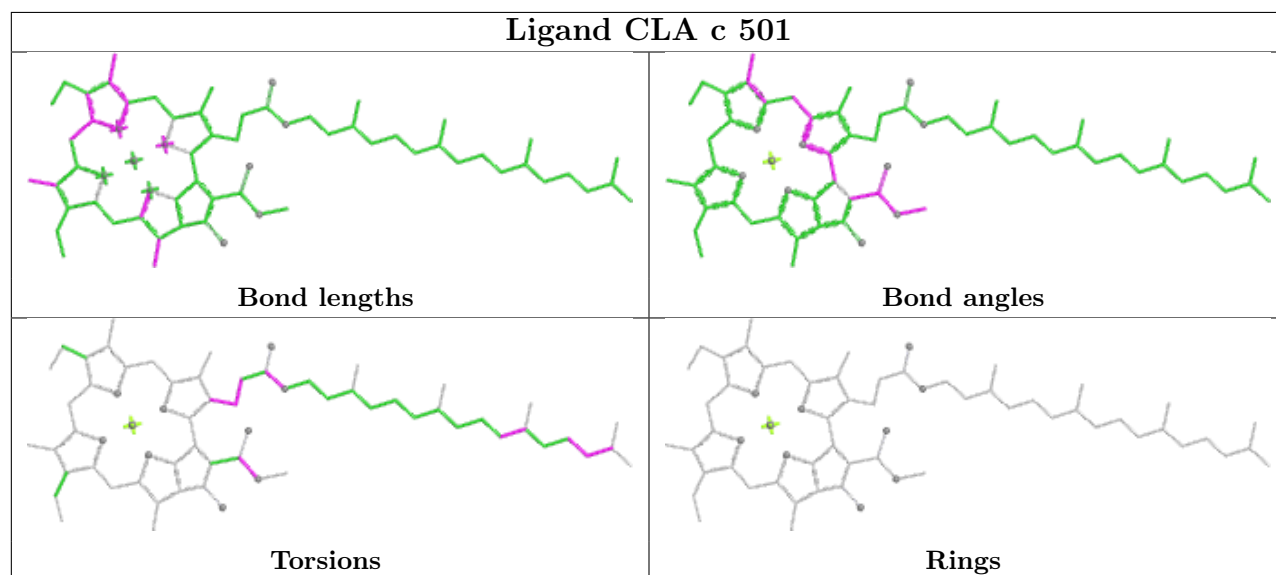
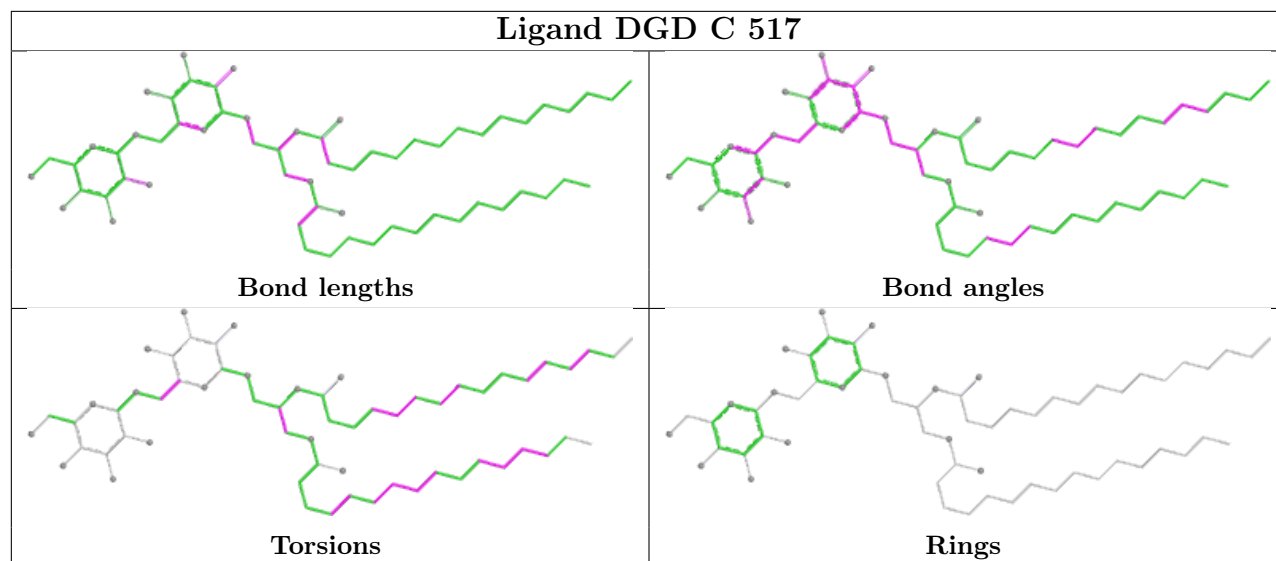
Ligand STE c 523

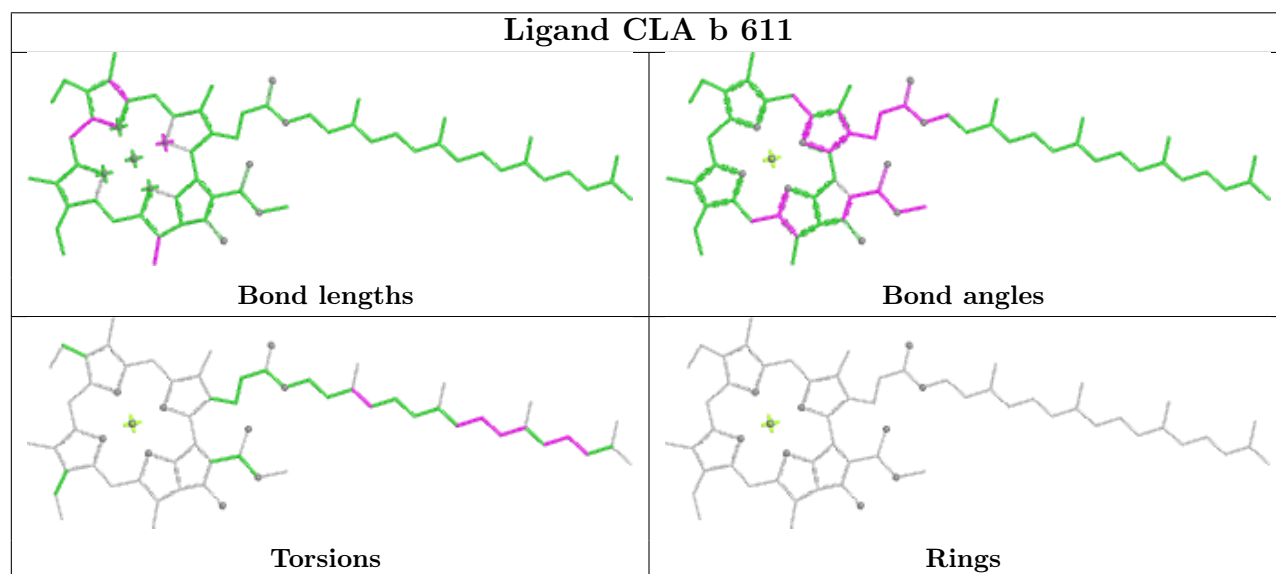
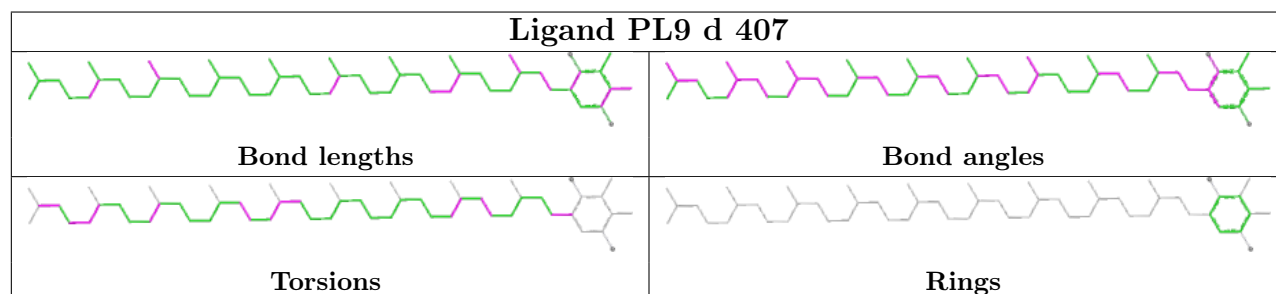
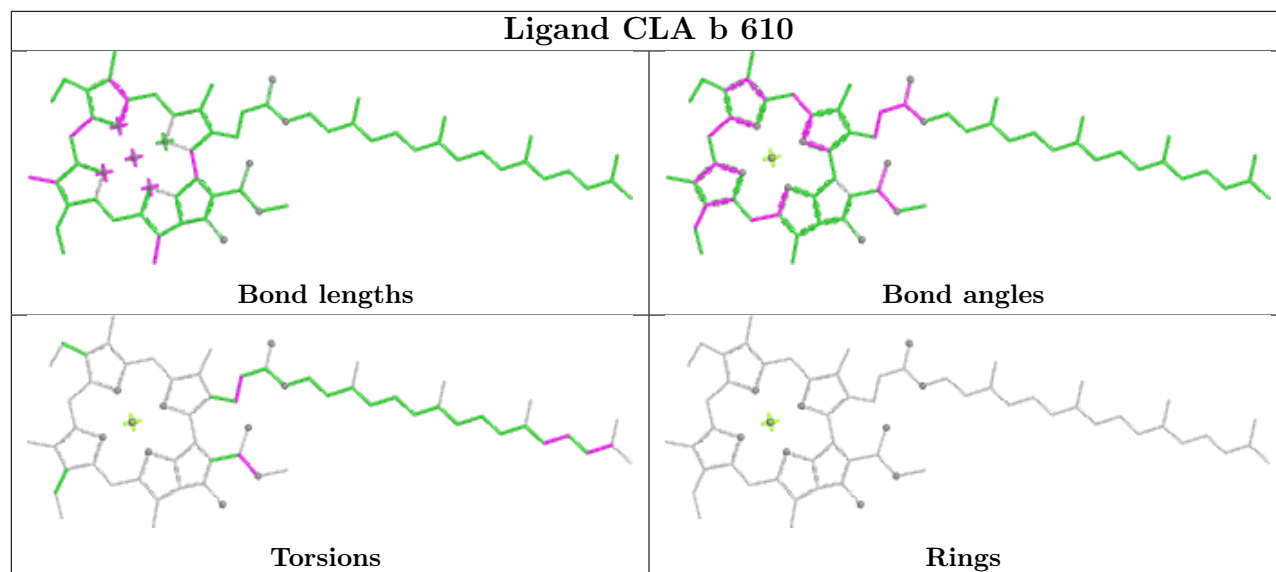


Ligand CLA C 513

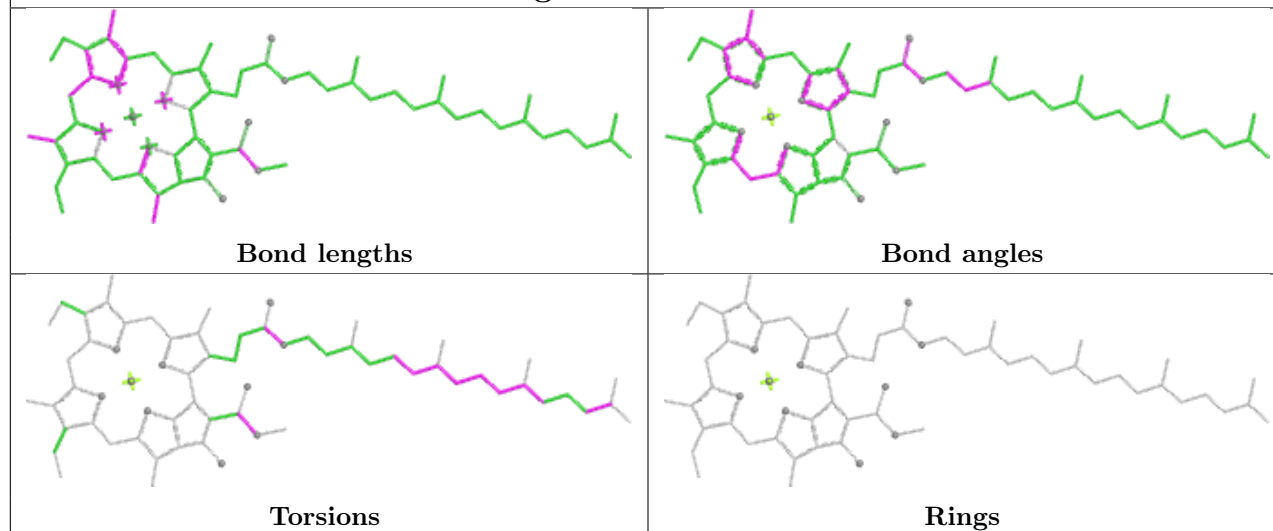




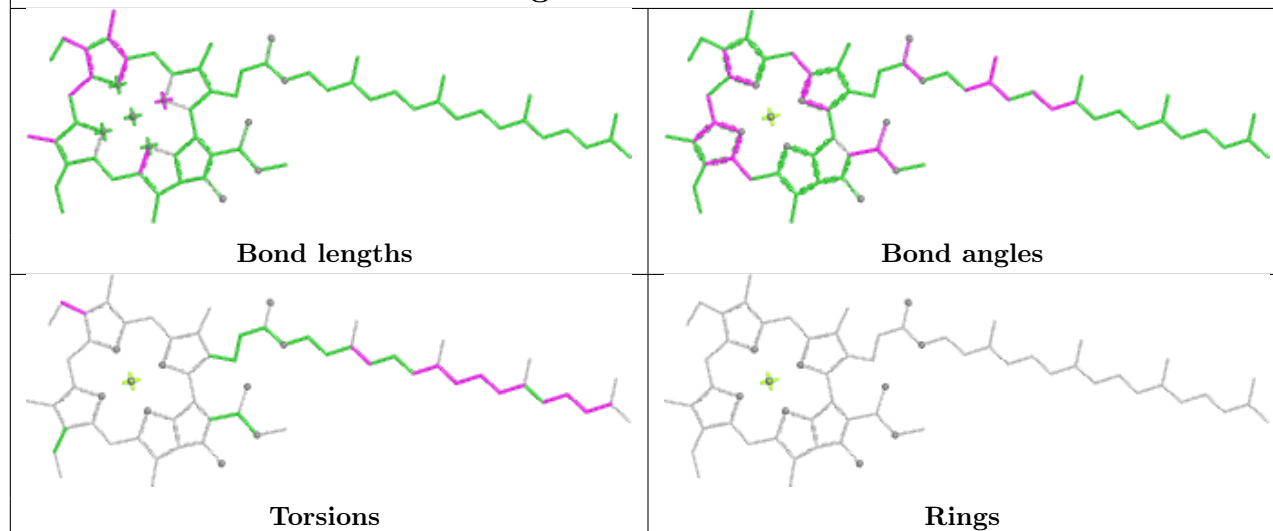




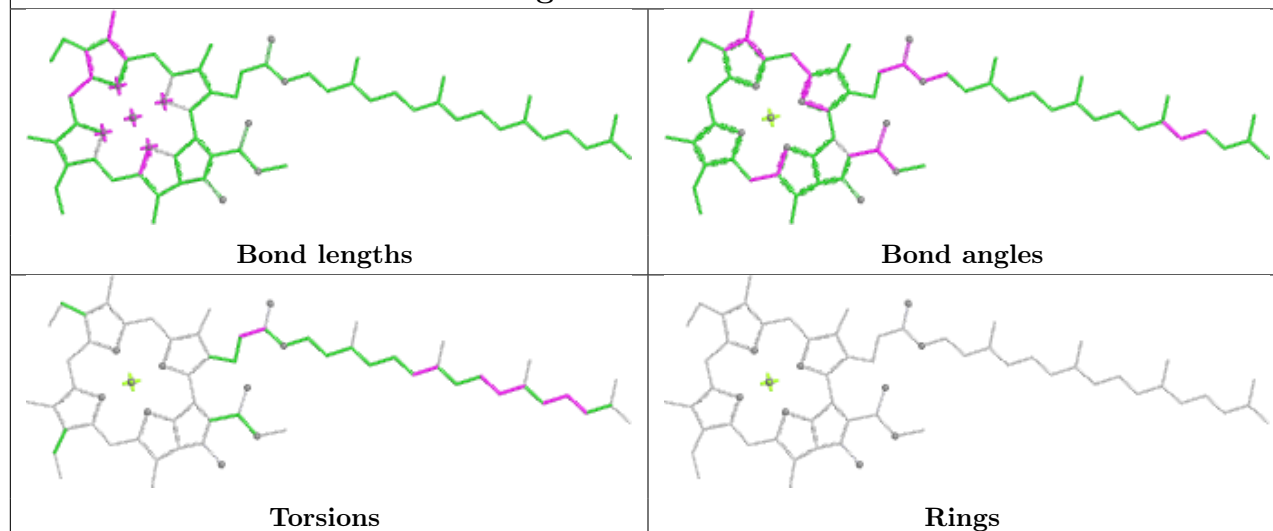
Ligand CLA b 607

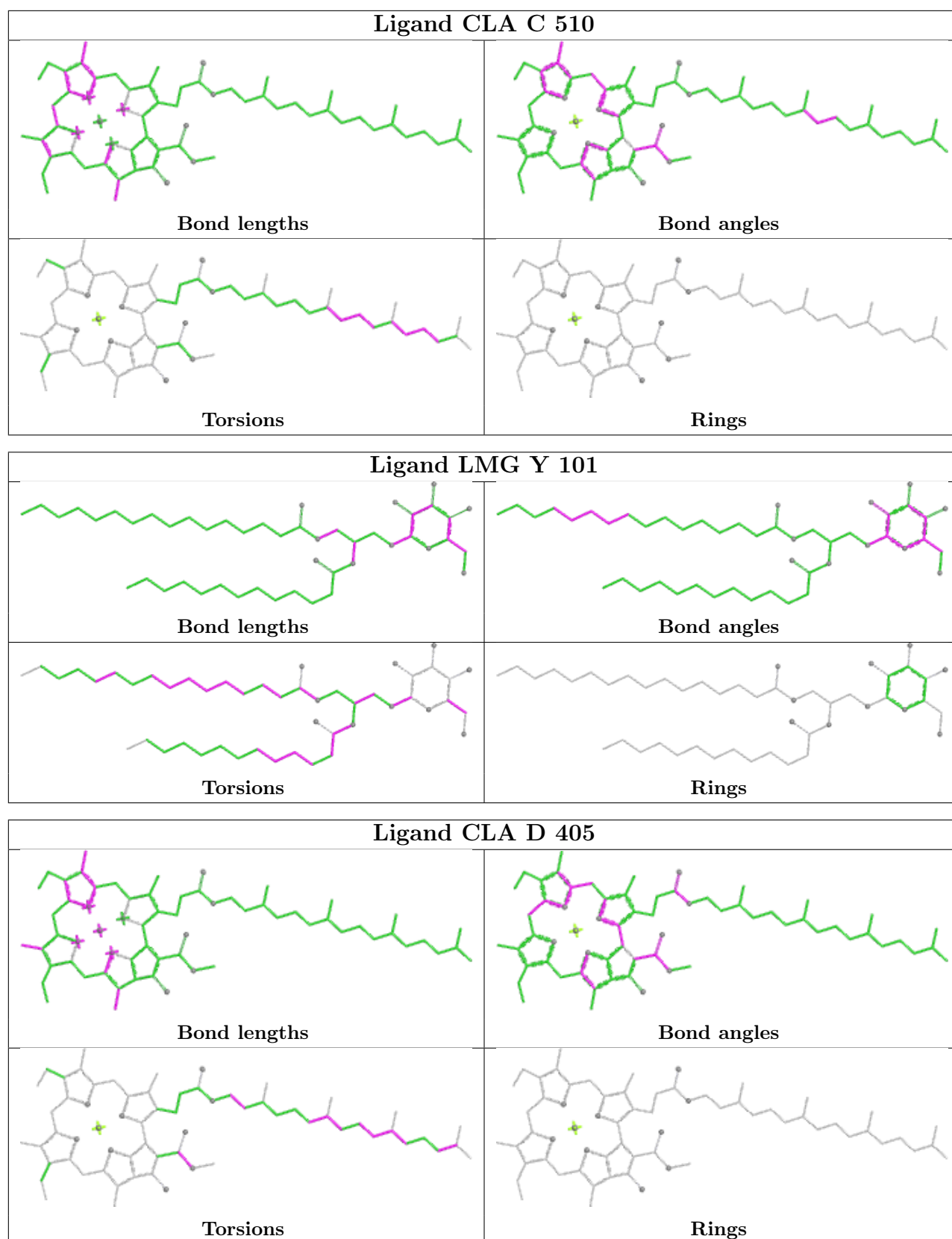


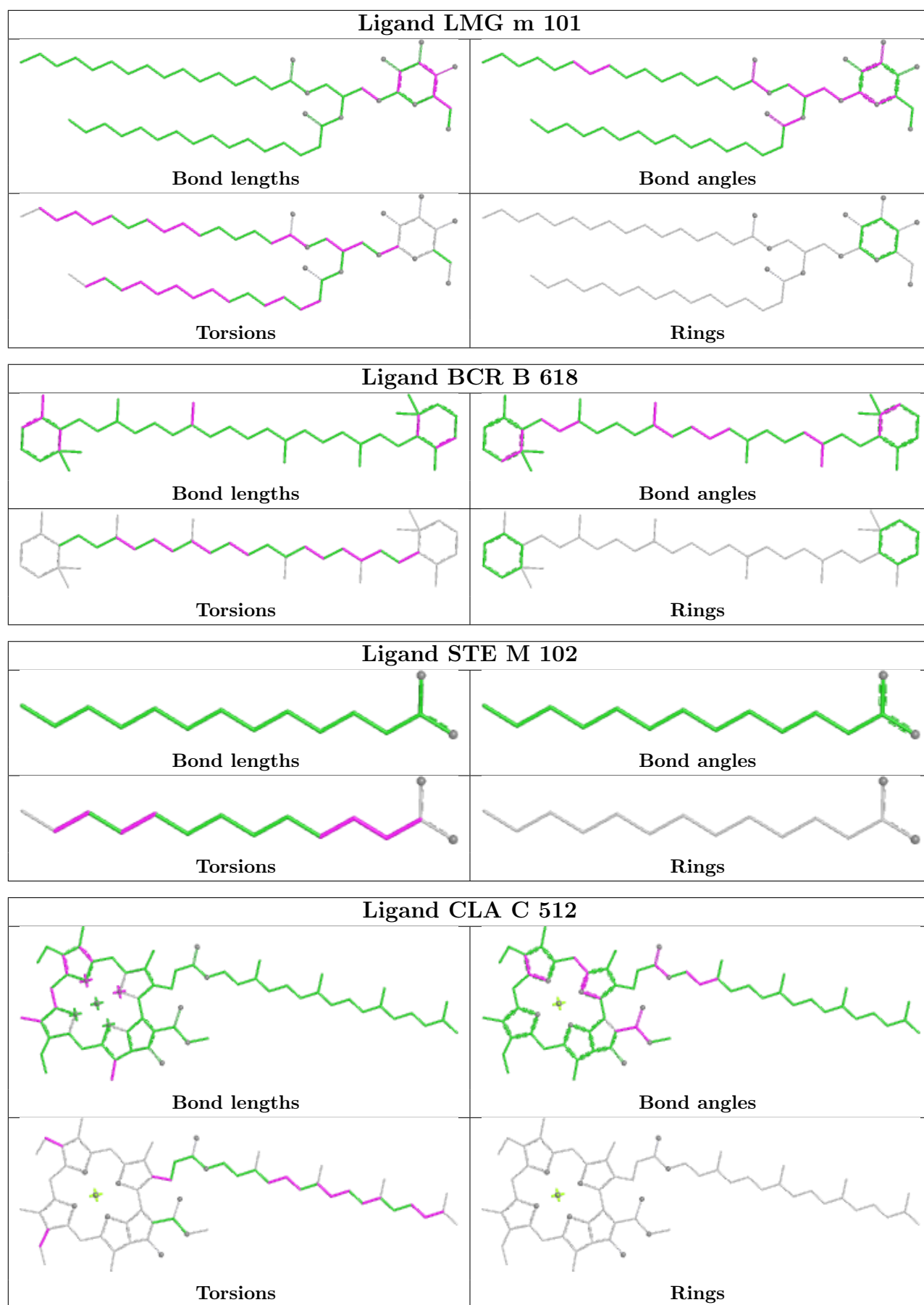
Ligand CLA B 603



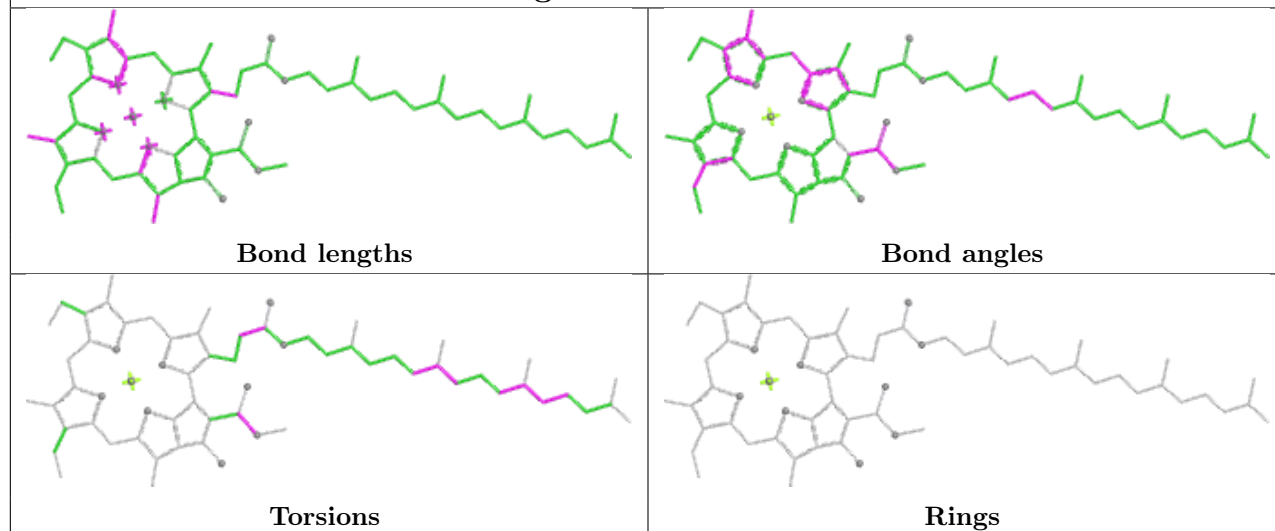
Ligand CLA c 509



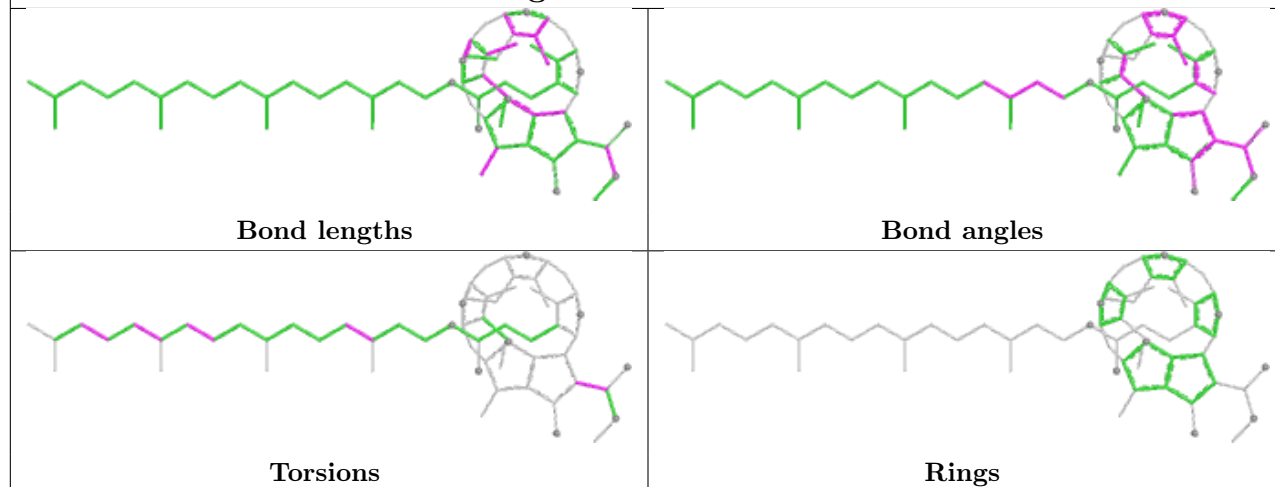




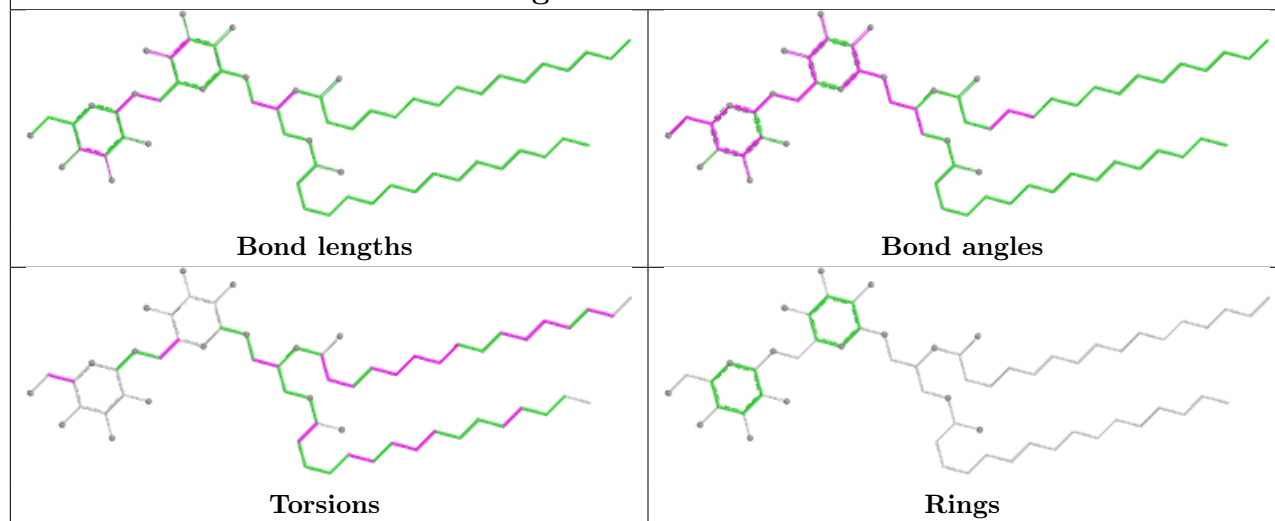
Ligand CLA b 613

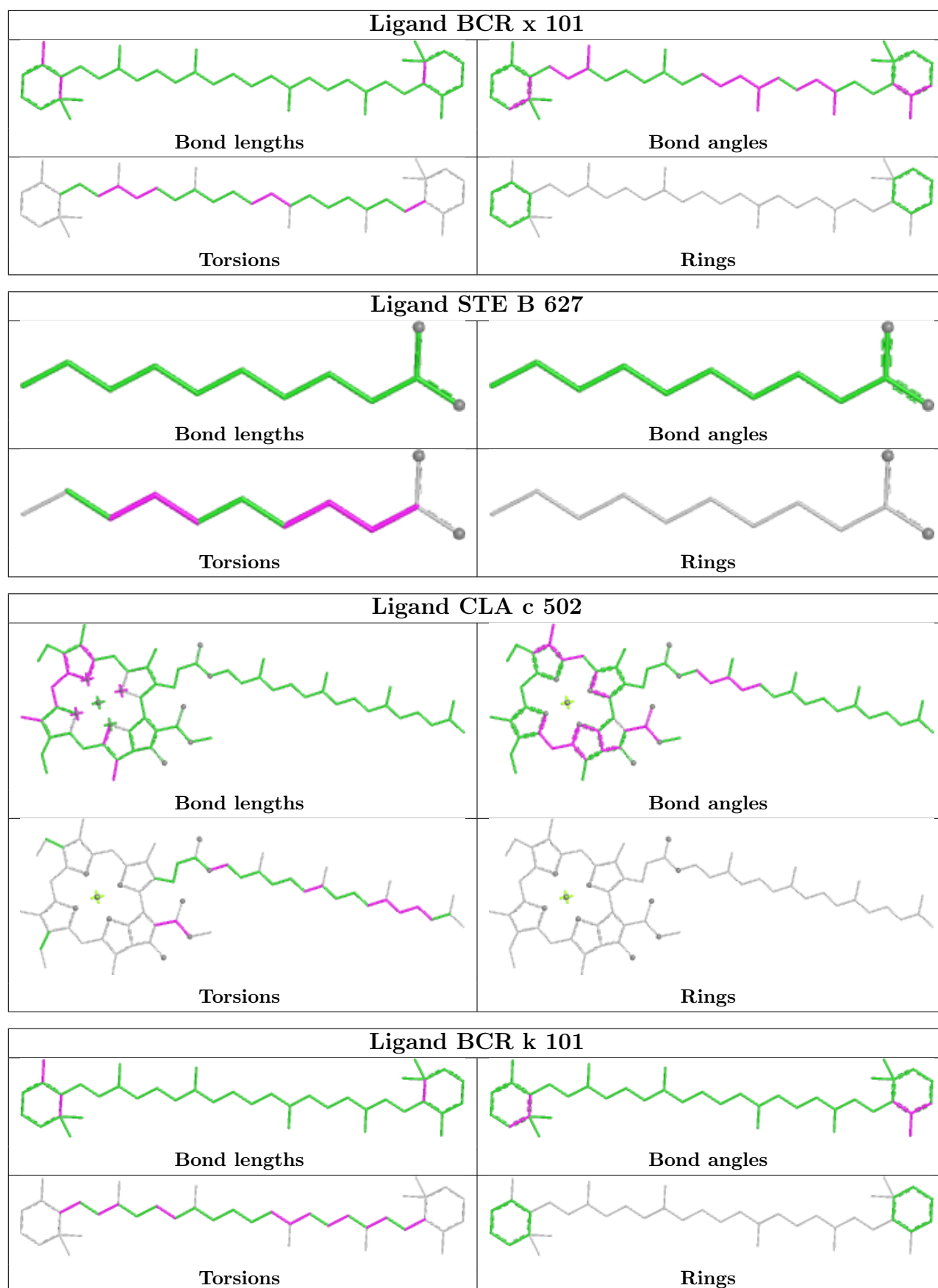


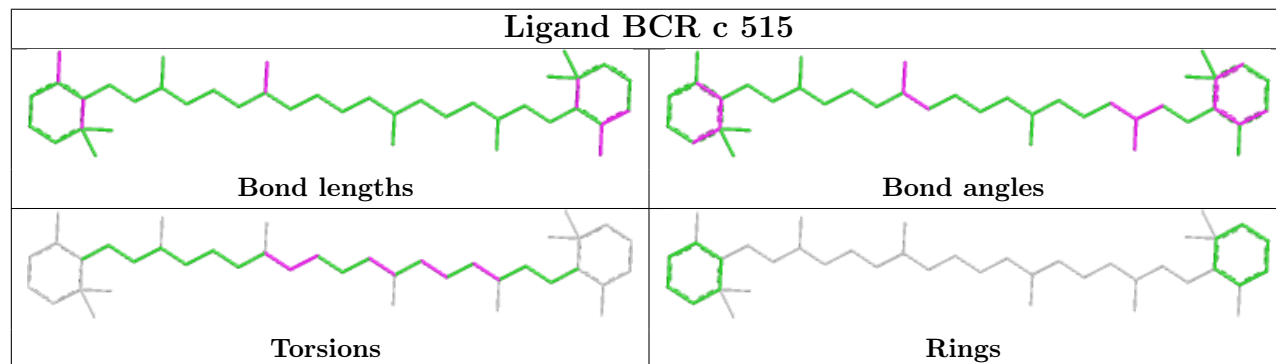
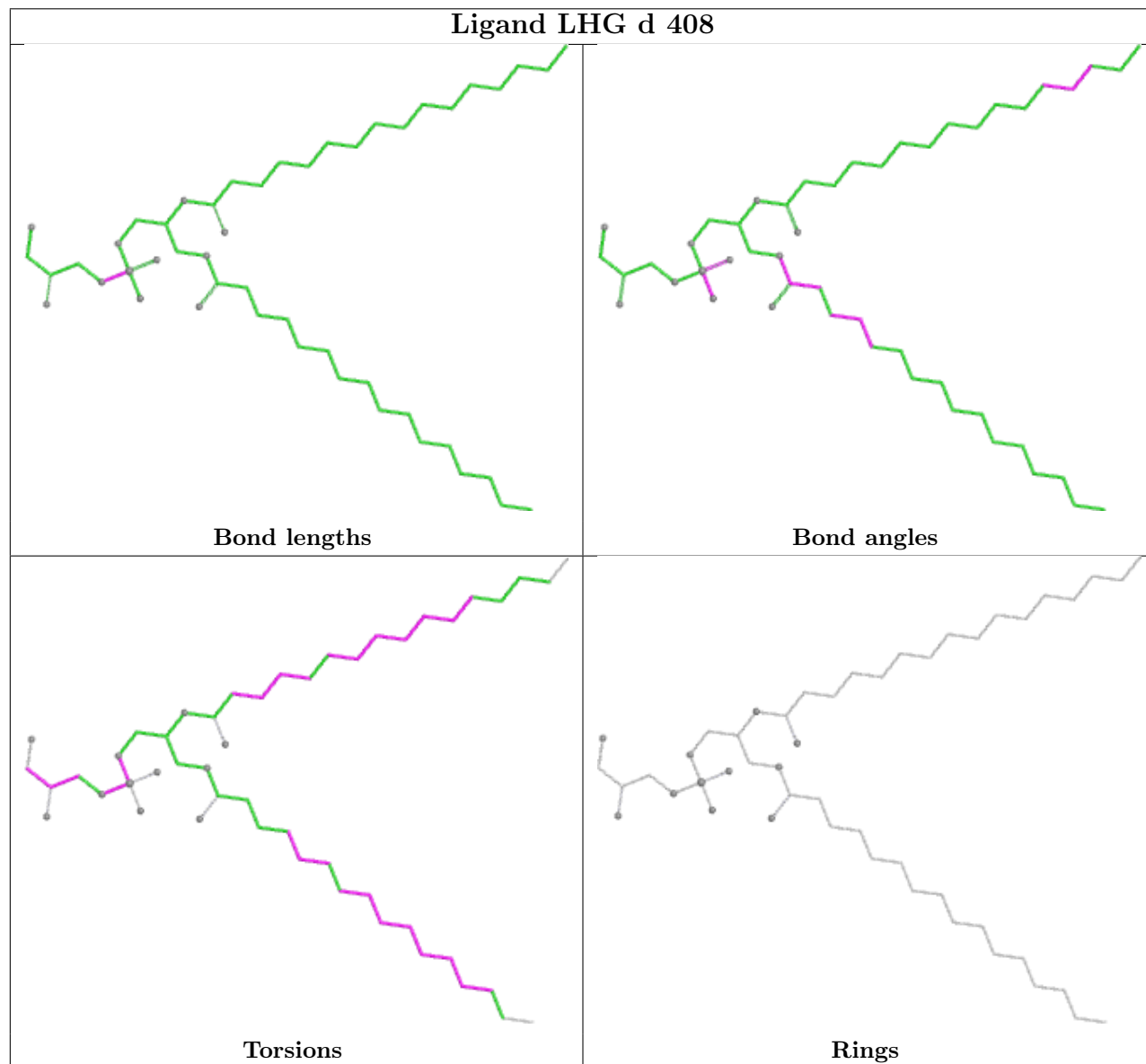
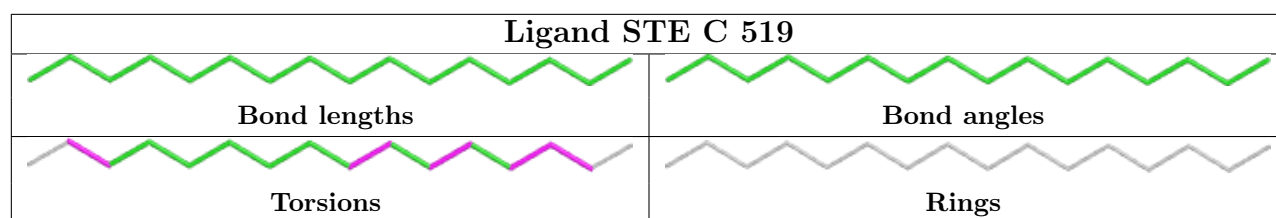
Ligand PHO A 404

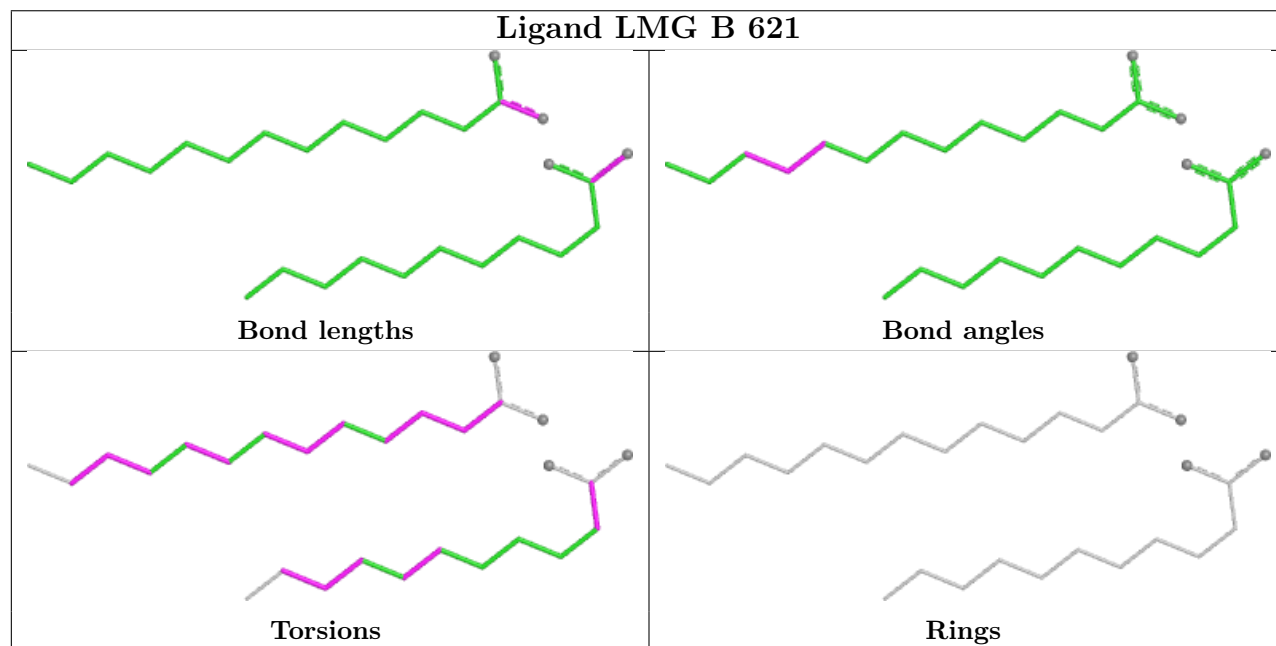
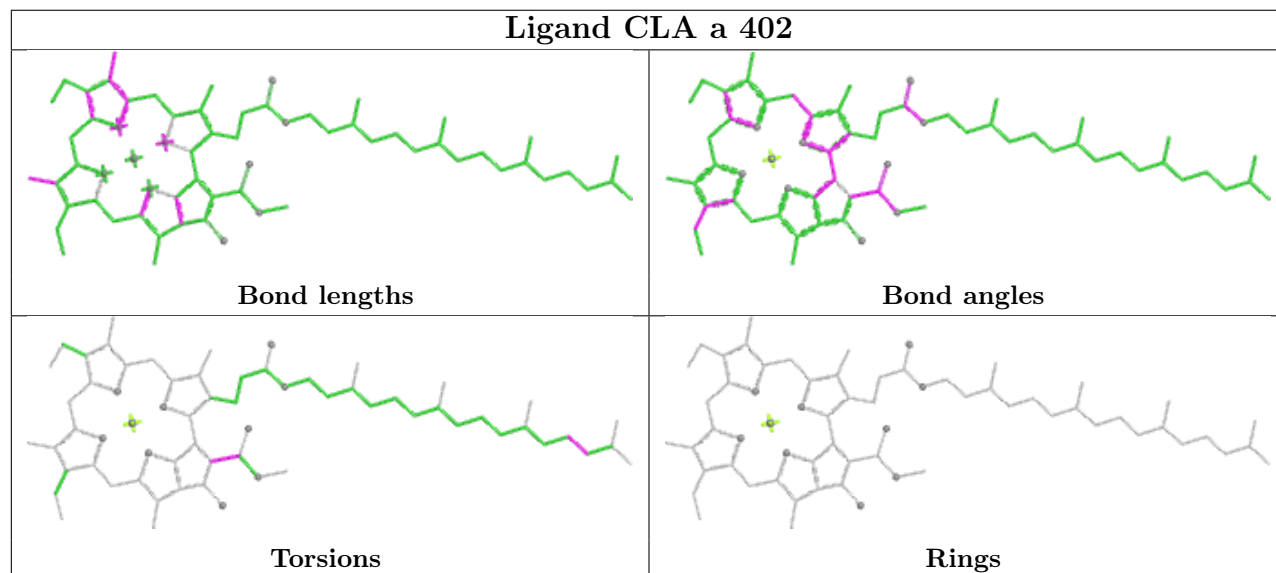
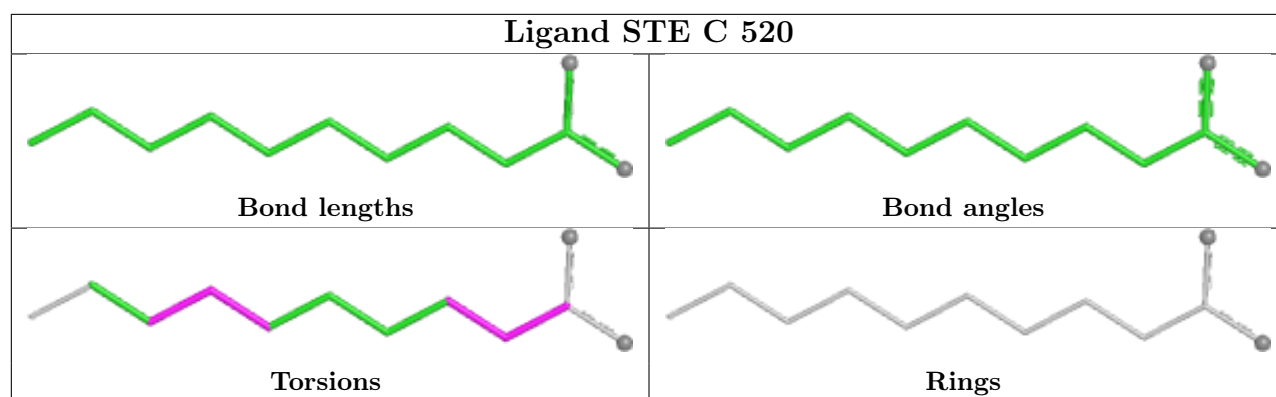


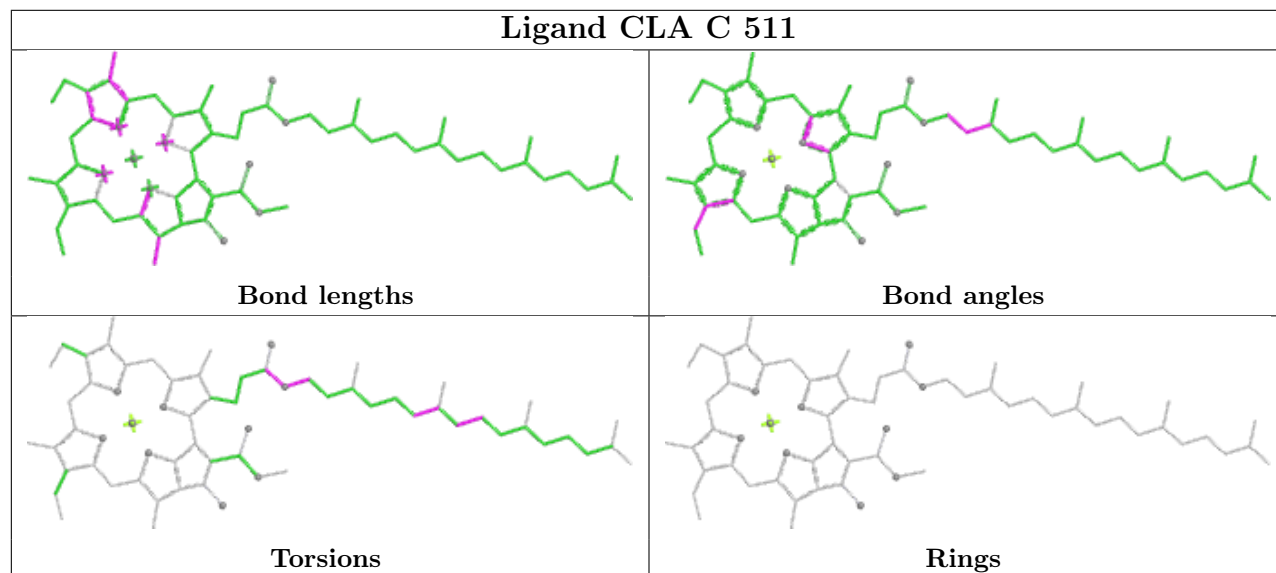
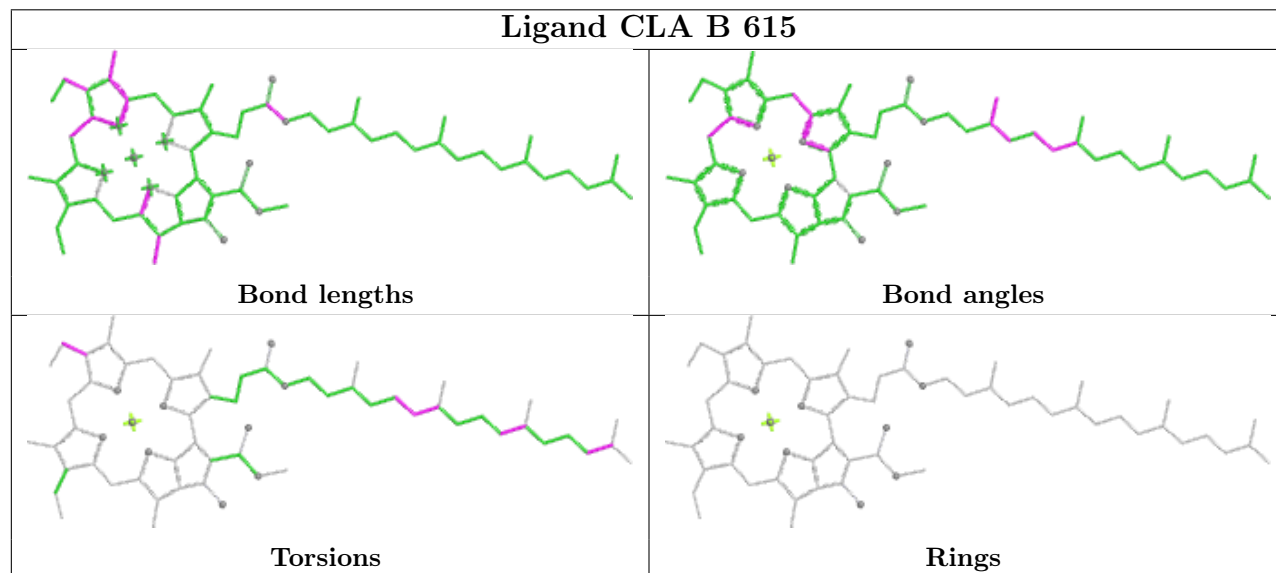
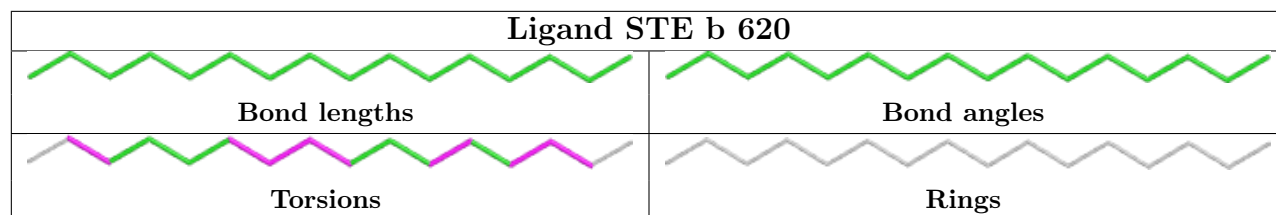
Ligand DGD c 516

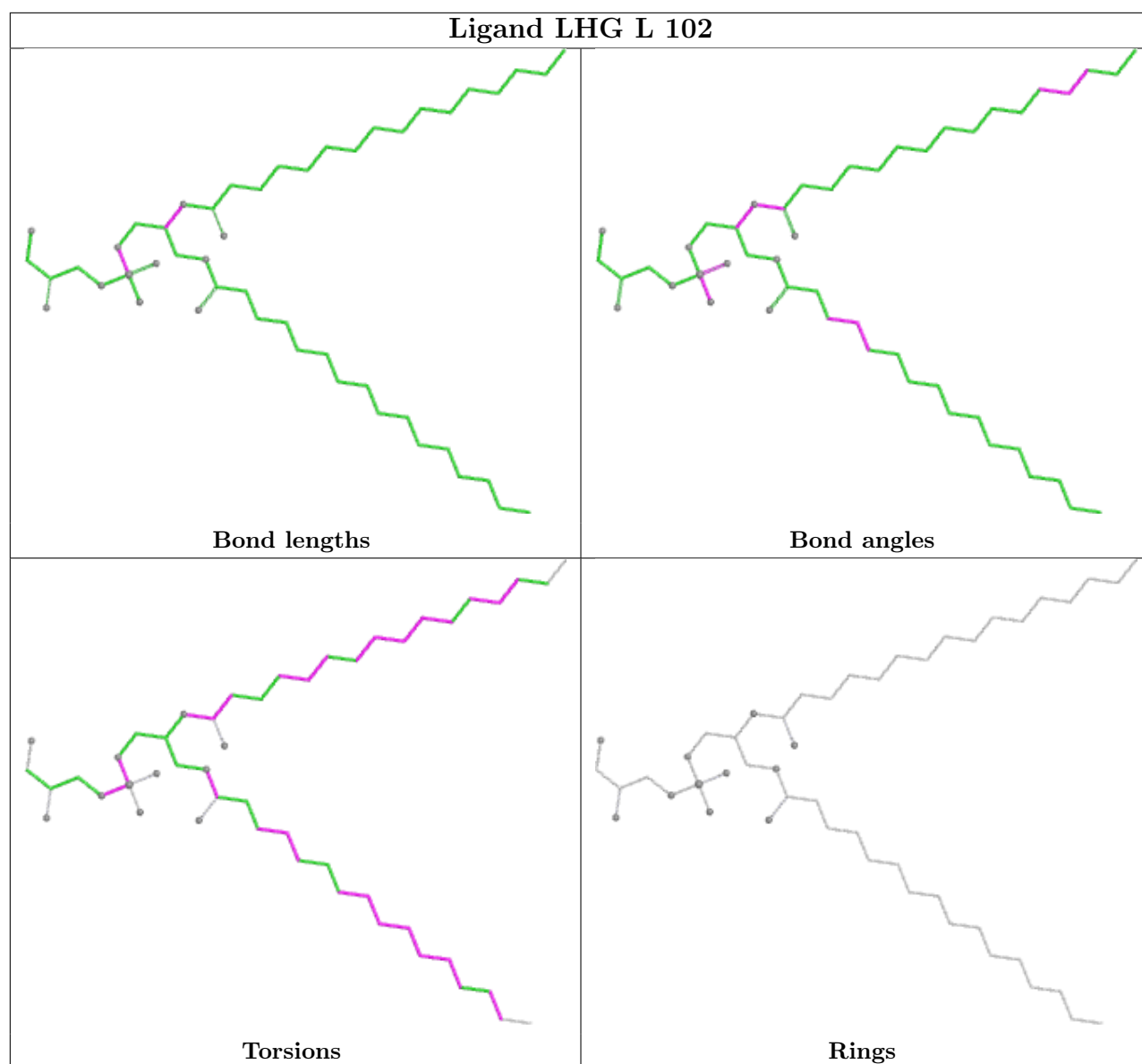


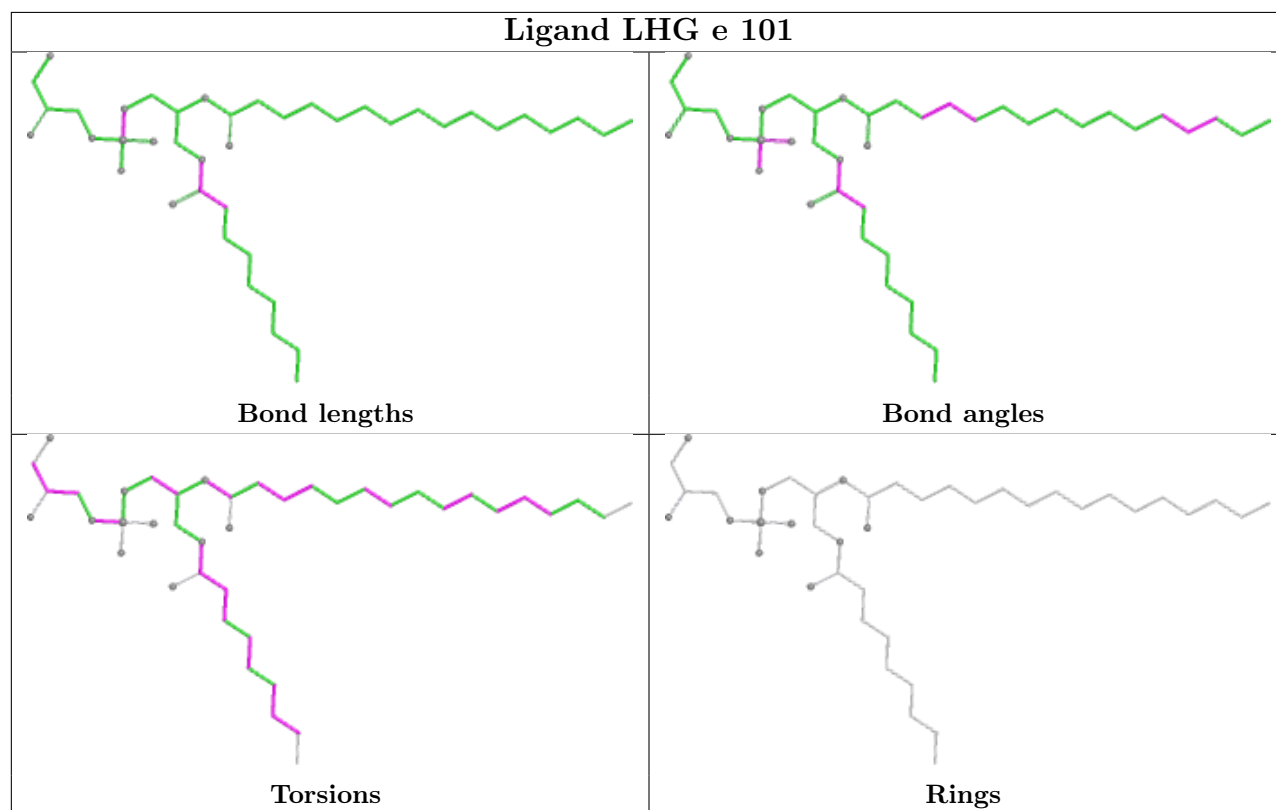
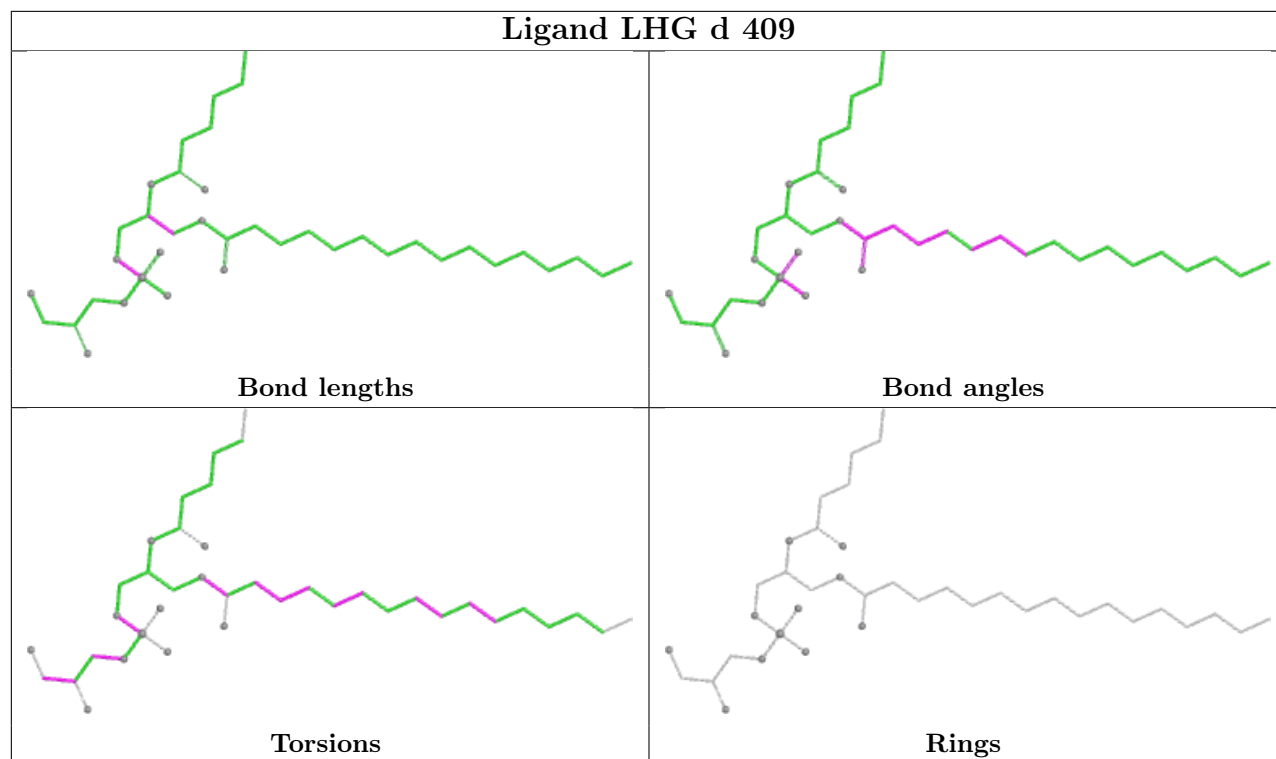


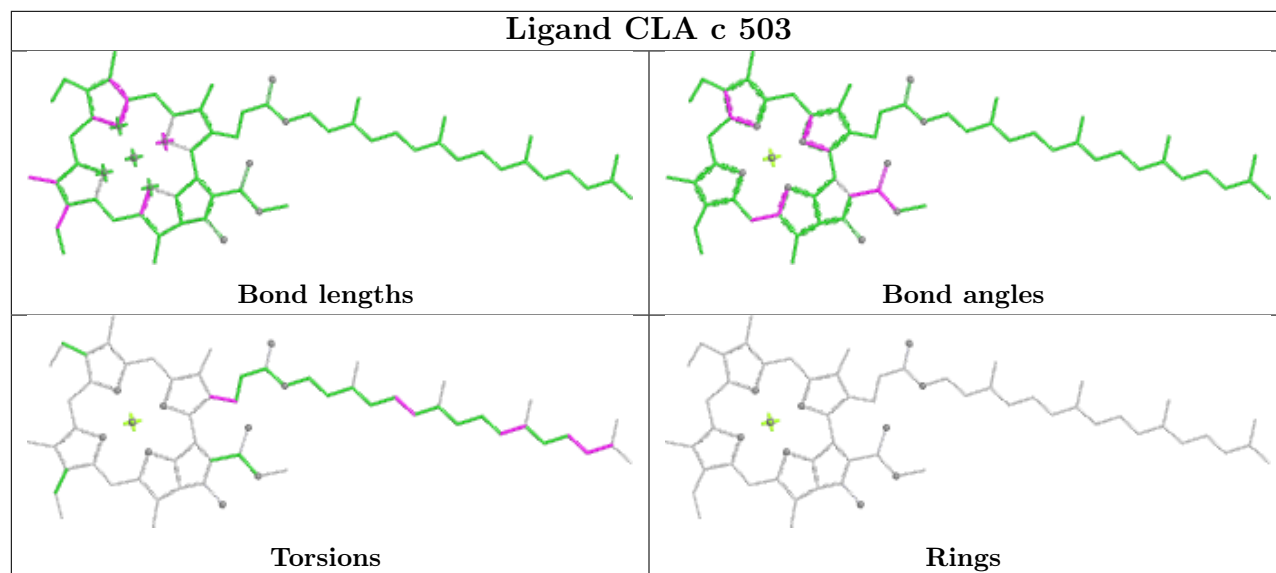
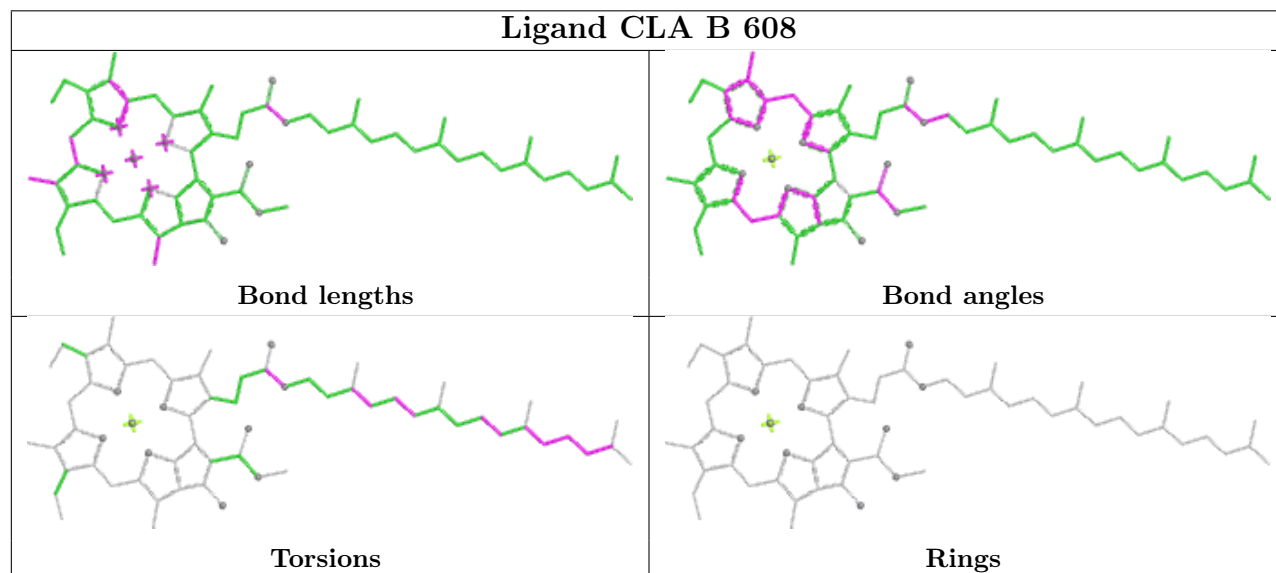
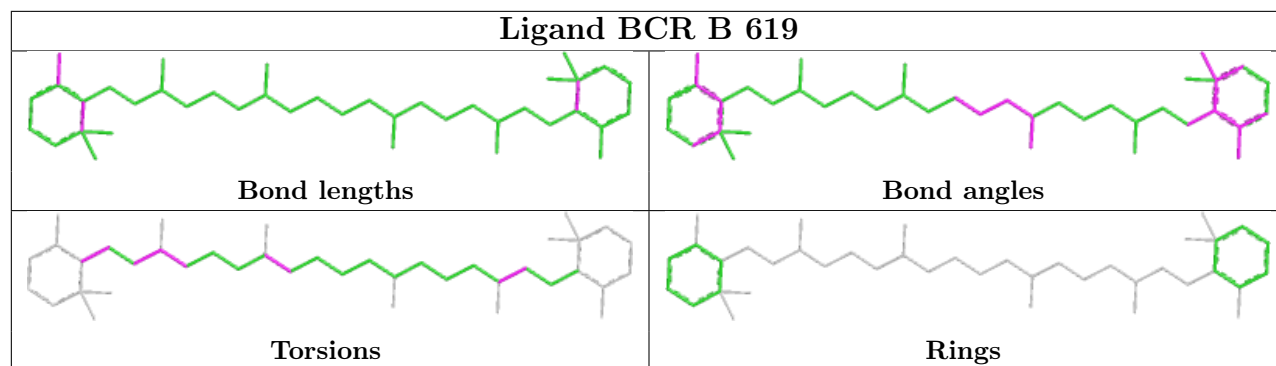


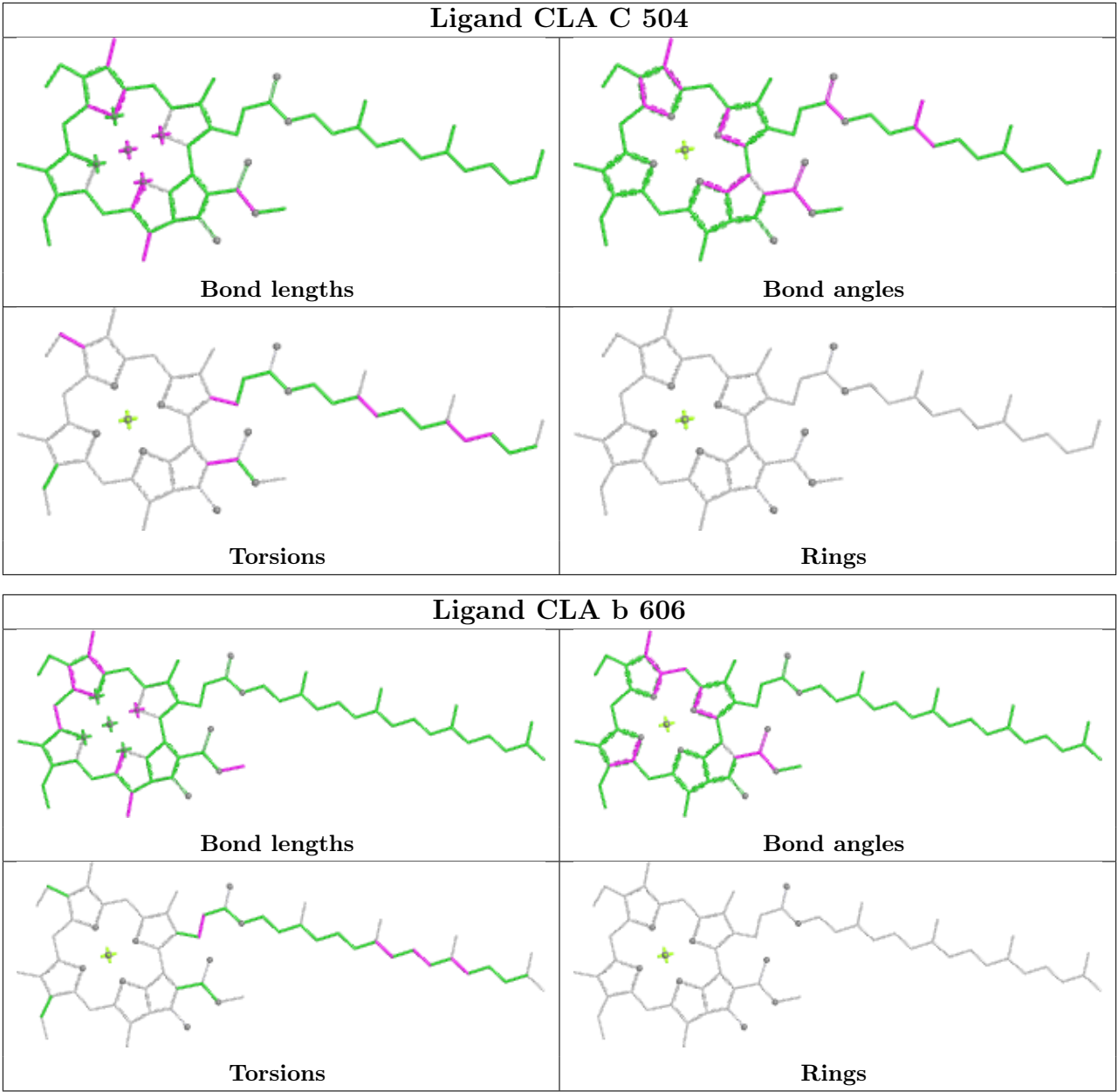












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.20

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%)	-0.55	1 (0%) 90 90	29, 38, 56, 86	0
1	a	334/344 (97%)	-0.44	4 (1%) 76 78	28, 40, 66, 86	0
2	B	505/510 (99%)	-0.40	0 100 100	22, 42, 70, 94	4 (0%)
2	b	505/510 (99%)	-0.29	4 (0%) 82 84	32, 46, 78, 112	0
3	C	442/461 (95%)	-0.36	0 100 100	22, 45, 63, 92	1 (0%)
3	c	451/461 (97%)	-0.25	1 (0%) 91 91	25, 50, 73, 105	2 (0%)
4	D	341/352 (96%)	-0.51	0 100 100	28, 39, 58, 89	0
4	d	341/352 (96%)	-0.37	0 100 100	28, 43, 69, 95	1 (0%)
5	E	82/84 (97%)	0.05	3 (3%) 45 47	35, 62, 78, 91	1 (1%)
5	e	82/84 (97%)	0.25	1 (1%) 76 78	46, 72, 89, 102	0
6	F	34/45 (75%)	-0.23	0 100 100	44, 53, 74, 88	0
6	f	34/45 (75%)	-0.10	0 100 100	51, 60, 89, 105	0
7	H	65/66 (98%)	-0.24	0 100 100	39, 51, 69, 75	0
7	h	63/66 (95%)	0.02	2 (3%) 50 52	48, 61, 72, 81	0
8	I	35/38 (92%)	-0.31	1 (2%) 53 55	40, 48, 75, 89	0
8	i	35/38 (92%)	-0.12	0 100 100	39, 51, 80, 92	0
9	J	36/40 (90%)	-0.13	0 100 100	43, 61, 87, 100	0
9	j	36/40 (90%)	0.06	0 100 100	48, 66, 99, 116	0
10	K	37/46 (80%)	-0.15	0 100 100	45, 62, 79, 86	0
10	k	37/46 (80%)	0.12	0 100 100	59, 67, 85, 91	0
11	L	37/37 (100%)	-0.59	0 100 100	31, 38, 71, 78	0
11	l	36/37 (97%)	-0.51	0 100 100	33, 41, 82, 92	0
12	M	32/36 (88%)	-0.37	1 (3%) 51 53	37, 44, 70, 82	0
12	m	31/36 (86%)	-0.45	0 100 100	36, 44, 62, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.20	2 (0%) 82 84	30, 52, 94, 132	1 (0%)
13	o	244/272 (89%)	-0.23	2 (0%) 82 84	30, 50, 90, 139	0
14	R	28/41 (68%)	0.65	1 (3%) 46 48	71, 81, 97, 101	0
14	r	28/41 (68%)	1.28	6 (21%) 2 2	88, 108, 129, 144	0
15	T	29/32 (90%)	-0.49	1 (3%) 48 50	32, 39, 68, 89	0
15	t	29/32 (90%)	-0.33	1 (3%) 48 50	36, 41, 85, 93	0
16	U	97/134 (72%)	-0.20	0 100 100	36, 54, 82, 102	0
16	u	97/134 (72%)	-0.27	0 100 100	39, 51, 66, 84	0
17	V	137/163 (84%)	-0.40	0 100 100	34, 50, 63, 81	0
17	v	137/163 (84%)	-0.17	0 100 100	40, 57, 81, 90	0
18	X	38/41 (92%)	-0.05	1 (2%) 57 59	50, 60, 83, 88	0
18	x	39/41 (95%)	0.07	1 (2%) 57 59	58, 67, 96, 110	0
19	Y	27/46 (58%)	0.84	2 (7%) 20 21	62, 84, 104, 114	0
19	y	30/46 (65%)	0.65	0 100 100	73, 89, 101, 113	0
20	Z	62/62 (100%)	0.55	2 (3%) 50 52	64, 80, 127, 137	0
20	z	62/62 (100%)	0.63	4 (6%) 25 26	71, 86, 124, 131	0
All	All	5293/5700 (92%)	-0.27	41 (0%) 82 84	22, 47, 85, 144	10 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	t	30	THR	4.9
13	o	58	ASN	4.6
20	z	33	TRP	4.2
7	h	64	ALA	3.6
18	x	40	SER	3.5

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
8	FME	I	1	10/11	0.92	0.11	46,58,68,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FME	T	1	10/11	0.94	0.10	31,58,77,77	0
12	FME	m	1	10/11	0.95	0.08	44,53,72,80	0
15	FME	t	1	10/11	0.95	0.08	34,54,68,69	0
12	FME	M	1	10/11	0.96	0.07	45,56,70,76	0
8	FME	i	1	10/11	0.97	0.07	42,55,68,74	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	d	412	20/20	0.75	0.18	40,68,83,90	0
32	STE	I	102	15/20	0.76	0.18	42,58,80,82	0
32	STE	B	625	16/20	0.78	0.16	40,64,82,85	0
32	STE	a	412	12/20	0.78	0.16	47,74,84,88	0
32	STE	H	103	18/20	0.78	0.16	52,77,88,89	0
32	STE	b	625	20/20	0.79	0.15	42,67,89,95	0
32	STE	b	624	15/20	0.79	0.17	50,66,87,92	0
32	STE	b	626	10/20	0.80	0.16	49,60,69,71	0
32	STE	c	523	12/20	0.80	0.13	55,74,88,90	0
28	LHG	A	411	49/49	0.80	0.14	45,84,111,116	0
32	STE	b	627	14/20	0.81	0.17	54,77,98,104	0
28	LHG	e	101	42/49	0.81	0.15	62,89,116,133	0
26	LMG	b	622	55/55	0.81	0.16	49,78,102,109	0
32	STE	L	103	12/20	0.82	0.17	48,66,88,88	0
32	STE	M	103	10/20	0.82	0.17	40,56,67,71	0
32	STE	B	624	18/20	0.82	0.14	52,72,90,94	0
26	LMG	c	521	48/55	0.83	0.14	34,77,102,106	0
27	SQD	A	412	39/54	0.83	0.14	45,66,96,103	0
32	STE	a	413	15/20	0.83	0.18	36,63,77,86	0
32	STE	c	520	20/20	0.83	0.12	42,64,85,89	0
32	STE	b	620	16/20	0.83	0.15	40,55,81,91	0
26	LMG	B	626	55/55	0.83	0.13	40,64,84,98	0
32	STE	x	102	20/20	0.83	0.14	50,66,80,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	C	518	12/20	0.84	0.14	39,57,68,69	0
25	PL9	A	408	55/55	0.84	0.14	32,67,92,100	0
32	STE	B	627	12/20	0.85	0.12	42,68,79,82	0
22	CLA	b	601	65/65	0.85	0.12	48,73,101,104	0
32	STE	C	519	16/20	0.85	0.14	47,62,75,75	0
32	STE	R	101	12/20	0.85	0.14	60,82,101,105	0
32	STE	t	104	10/20	0.85	0.14	43,60,72,77	0
26	LMG	c	519	37/55	0.85	0.12	45,69,89,99	0
32	STE	b	623	16/20	0.86	0.14	53,73,83,90	0
26	LMG	D	412	33/55	0.86	0.13	32,62,92,94	0
32	STE	J	101	12/20	0.86	0.13	49,65,72,74	0
32	STE	j	101	12/20	0.86	0.11	50,64,71,72	0
27	SQD	t	102	36/54	0.86	0.13	31,66,91,95	0
29	DGD	A	413	66/66	0.86	0.11	47,64,83,89	0
32	STE	B	620	17/20	0.87	0.12	37,60,76,76	0
25	PL9	a	409	55/55	0.87	0.14	41,72,95,100	0
26	LMG	B	621	28/55	0.87	0.13	36,52,67,73	0
32	STE	l	102	18/20	0.87	0.12	38,52,75,78	0
32	STE	b	621	20/20	0.87	0.11	42,60,79,84	0
22	CLA	B	601	65/65	0.87	0.11	40,70,93,104	0
32	STE	B	623	12/20	0.88	0.12	38,60,72,73	0
27	SQD	L	101	49/54	0.88	0.11	40,66,100,105	0
26	LMG	A	409	48/55	0.88	0.10	34,63,79,96	0
26	LMG	Y	101	48/55	0.88	0.11	52,75,93,102	0
32	STE	d	411	17/20	0.89	0.12	48,63,70,78	0
32	STE	Z	102	8/20	0.89	0.14	43,65,79,79	0
27	SQD	f	102	41/54	0.89	0.12	62,87,107,118	0
26	LMG	M	101	51/55	0.90	0.10	36,54,76,86	0
27	SQD	B	622	54/54	0.90	0.10	38,65,89,98	0
26	LMG	c	522	49/55	0.90	0.10	28,62,92,100	0
26	LMG	d	410	44/55	0.90	0.11	41,61,89,106	0
32	STE	t	103	14/20	0.90	0.10	43,57,69,70	0
26	LMG	m	101	51/55	0.90	0.10	39,58,78,87	0
32	STE	C	520	12/20	0.90	0.12	36,47,59,66	0
31	BCR	K	101	40/40	0.91	0.10	40,57,75,78	0
31	BCR	c	514	40/40	0.91	0.11	45,67,82,87	0
31	BCR	d	406	40/40	0.91	0.10	35,61,97,109	0
31	BCR	x	101	40/40	0.91	0.09	37,58,76,80	0
32	STE	X	101	20/20	0.91	0.10	39,56,75,81	0
27	SQD	a	411	54/54	0.91	0.10	47,69,98,106	0
22	CLA	c	512	65/65	0.91	0.11	42,63,90,104	0
22	CLA	C	513	65/65	0.91	0.10	41,63,99,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	BCR	B	619	40/40	0.92	0.09	29,49,73,84	0
31	BCR	C	514	40/40	0.92	0.10	29,46,59,77	0
27	SQD	D	409	36/54	0.92	0.11	51,77,96,105	0
31	BCR	Z	101	40/40	0.92	0.10	42,64,78,82	0
32	STE	M	102	15/20	0.92	0.09	38,53,63,66	0
22	CLA	c	513	65/65	0.92	0.11	47,77,104,108	0
29	DGD	H	102	62/66	0.92	0.09	33,51,66,72	0
31	BCR	k	101	40/40	0.92	0.10	46,68,84,90	0
29	DGD	c	518	62/66	0.92	0.10	35,62,87,98	0
31	BCR	H	101	40/40	0.93	0.08	35,52,66,74	0
29	DGD	C	516	62/66	0.93	0.09	31,54,103,124	0
31	BCR	K	102	40/40	0.93	0.10	39,58,71,71	0
31	BCR	T	101	40/40	0.93	0.07	32,46,58,65	0
22	CLA	c	506	65/65	0.93	0.10	35,57,100,103	0
31	BCR	b	617	40/40	0.93	0.08	32,48,65,66	0
31	BCR	b	619	40/40	0.93	0.09	30,55,81,85	0
29	DGD	c	517	62/66	0.93	0.08	38,60,95,104	0
31	BCR	c	515	40/40	0.93	0.09	33,53,70,76	0
28	LHG	d	409	39/49	0.93	0.09	32,52,69,75	0
29	DGD	h	101	62/66	0.93	0.09	34,52,67,70	0
31	BCR	k	102	40/40	0.93	0.11	46,63,76,78	0
31	BCR	B	618	40/40	0.93	0.08	29,45,60,67	0
27	SQD	A	410	52/54	0.93	0.09	37,66,96,101	0
26	LMG	D	408	51/55	0.93	0.11	32,65,89,99	0
31	BCR	D	406	40/40	0.93	0.09	34,51,88,99	0
22	CLA	c	511	65/65	0.94	0.10	43,63,80,86	0
29	DGD	C	517	62/66	0.94	0.08	31,53,79,87	0
31	BCR	I	101	40/40	0.94	0.07	27,40,50,54	0
22	CLA	C	512	65/65	0.94	0.10	39,61,93,102	0
22	CLA	b	606	65/65	0.94	0.08	28,46,80,92	0
28	LHG	D	411	47/49	0.94	0.10	28,53,83,89	0
28	LHG	a	410	49/49	0.94	0.11	39,57,79,91	0
31	BCR	a	405	40/40	0.94	0.07	24,39,58,59	0
31	BCR	B	617	40/40	0.94	0.08	30,45,64,65	0
31	BCR	b	618	40/40	0.94	0.07	29,44,60,62	0
22	CLA	c	503	65/65	0.94	0.08	34,49,61,67	0
22	CLA	C	510	65/65	0.94	0.07	29,48,65,73	0
22	CLA	c	508	64/65	0.94	0.09	37,55,93,115	0
33	BCT	a	408	4/4	0.94	0.09	34,44,53,64	0
22	CLA	c	502	65/65	0.95	0.08	32,48,68,72	0
22	CLA	C	503	65/65	0.95	0.07	31,47,57,61	0
22	CLA	c	504	60/65	0.95	0.07	35,51,84,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	504	59/65	0.95	0.08	32,48,87,92	0
22	CLA	C	506	65/65	0.95	0.08	30,50,89,98	0
22	CLA	c	509	65/65	0.95	0.09	30,53,72,80	0
22	CLA	c	510	65/65	0.95	0.07	35,50,66,84	0
22	CLA	C	508	65/65	0.95	0.08	30,49,107,117	0
22	CLA	C	509	65/65	0.95	0.08	30,50,68,77	0
22	CLA	B	606	65/65	0.95	0.08	30,45,78,92	0
22	CLA	d	405	65/65	0.95	0.08	32,54,94,107	0
23	PHO	D	401	64/64	0.95	0.06	26,40,50,54	0
23	PHO	d	402	64/64	0.95	0.07	28,43,55,68	0
22	CLA	C	511	65/65	0.95	0.08	32,59,76,80	0
25	PL9	D	407	55/55	0.95	0.07	26,39,54,62	0
22	CLA	B	614	65/65	0.95	0.08	26,46,80,96	0
25	PL9	d	407	55/55	0.95	0.07	24,40,53,63	0
22	CLA	B	615	65/65	0.95	0.08	27,42,67,84	0
31	BCR	t	101	40/40	0.95	0.06	27,44,59,62	0
29	DGD	C	515	62/66	0.95	0.10	27,47,83,98	0
22	CLA	a	404	65/65	0.95	0.09	24,44,87,96	0
22	CLA	B	616	60/65	0.95	0.10	23,43,89,97	0
22	CLA	C	502	65/65	0.95	0.07	28,47,68,78	0
22	CLA	b	608	65/65	0.95	0.08	31,48,71,77	0
22	CLA	b	609	65/65	0.95	0.08	31,52,71,79	0
22	CLA	b	614	65/65	0.95	0.08	25,43,80,87	0
22	CLA	b	615	65/65	0.95	0.08	27,46,66,74	0
22	CLA	b	616	60/65	0.95	0.09	31,49,92,99	0
36	NA	V	202	1/1	0.95	0.12	60,60,60,60	0
22	CLA	d	404	65/65	0.96	0.07	22,37,52,55	0
28	LHG	D	413	49/49	0.96	0.08	32,47,74,88	0
28	LHG	L	102	49/49	0.96	0.07	30,45,63,73	0
22	CLA	b	602	65/65	0.96	0.08	33,47,65,71	0
28	LHG	d	408	49/49	0.96	0.08	29,47,61,72	0
23	PHO	A	404	64/64	0.96	0.06	17,35,45,49	0
22	CLA	b	604	65/65	0.96	0.08	26,44,80,95	0
28	LHG	l	101	49/49	0.96	0.07	34,49,63,70	0
23	PHO	a	403	64/64	0.96	0.06	23,36,44,47	0
22	CLA	b	605	65/65	0.96	0.07	25,38,56,62	0
22	CLA	B	610	65/65	0.96	0.07	24,38,49,60	0
22	CLA	b	607	65/65	0.96	0.07	24,41,81,86	0
22	CLA	C	505	65/65	0.96	0.08	26,47,73,76	0
29	DGD	c	516	62/66	0.96	0.08	30,47,80,87	0
22	CLA	B	611	65/65	0.96	0.07	20,36,53,58	0
22	CLA	b	610	65/65	0.96	0.07	28,43,58,68	0

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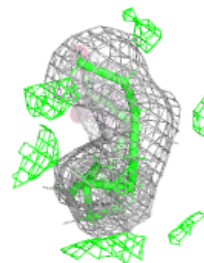
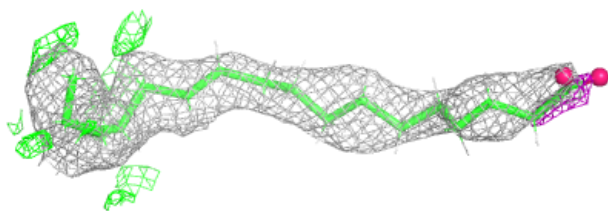
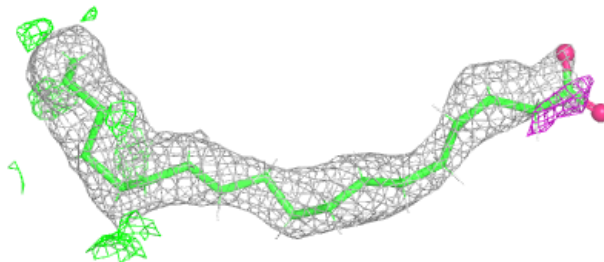
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	611	65/65	0.96	0.07	24,41,57,66	0
22	CLA	b	612	65/65	0.96	0.07	27,41,52,54	0
22	CLA	b	613	65/65	0.96	0.08	23,41,82,97	0
22	CLA	C	507	65/65	0.96	0.07	26,46,66,68	0
22	CLA	B	612	65/65	0.96	0.07	23,36,50,60	0
22	CLA	B	613	65/65	0.96	0.08	22,40,73,81	0
22	CLA	c	501	65/65	0.96	0.07	32,49,65,71	0
22	CLA	B	602	65/65	0.96	0.07	26,43,63,67	0
22	CLA	B	604	65/65	0.96	0.08	25,40,87,96	0
22	CLA	B	605	65/65	0.96	0.07	21,38,53,60	0
22	CLA	c	505	65/65	0.96	0.08	31,46,72,76	0
22	CLA	C	501	65/65	0.96	0.06	26,42,59,65	0
22	CLA	c	507	65/65	0.96	0.07	31,50,65,78	0
22	CLA	D	403	65/65	0.96	0.07	22,36,54,66	0
22	CLA	D	404	65/65	0.96	0.07	23,35,56,65	0
22	CLA	D	405	65/65	0.96	0.08	26,50,128,138	0
22	CLA	a	402	65/65	0.96	0.07	23,36,50,58	0
22	CLA	A	402	65/65	0.96	0.07	20,33,48,57	0
22	CLA	B	609	65/65	0.96	0.07	28,43,61,65	0
22	CLA	d	401	65/65	0.96	0.09	28,47,105,111	0
33	BCT	D	402	4/4	0.96	0.08	28,35,45,54	0
22	CLA	d	403	65/65	0.96	0.09	23,41,64,74	0
34	HEM	f	101	43/43	0.96	0.09	43,64,91,99	0
28	LHG	D	410	49/49	0.96	0.08	31,46,59,66	0
22	CLA	B	608	65/65	0.97	0.06	27,43,64,69	0
22	CLA	A	403	65/65	0.97	0.08	25,41,95,103	0
22	CLA	A	405	54/65	0.97	0.06	22,39,70,82	0
22	CLA	B	603	65/65	0.97	0.07	23,39,62,68	0
34	HEM	F	101	43/43	0.97	0.08	36,54,73,75	0
22	CLA	b	603	65/65	0.97	0.07	24,42,74,90	0
22	CLA	B	607	65/65	0.97	0.07	19,40,81,87	0
24	CL	A	407	1/1	0.98	0.03	37,37,37,37	0
24	CL	a	407	1/1	0.98	0.07	34,34,34,34	0
35	HEC	V	201	43/43	0.98	0.07	24,39,48,49	0
35	HEC	v	201	43/43	0.98	0.07	29,44,55,61	0
24	CL	A	406	1/1	0.98	0.04	36,36,36,36	0
24	CL	a	406	1/1	0.99	0.02	33,33,33,33	0
21	FE2	A	401	1/1	0.99	0.03	31,31,31,31	0
30	OEX	A	414	10/10	0.99	0.04	27,36,39,39	0
30	OEX	a	414	10/10	0.99	0.03	29,35,39,44	0
21	FE2	a	401	1/1	1.00	0.02	36,36,36,36	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.

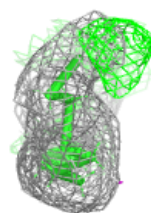
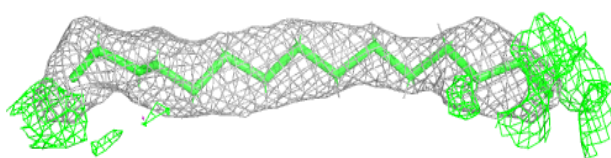
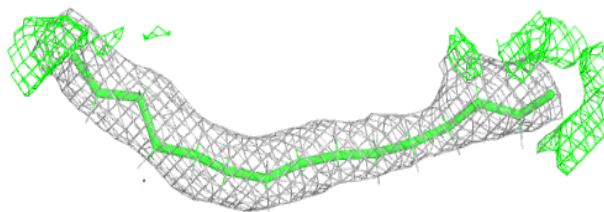
Electron density around STE d 412:

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

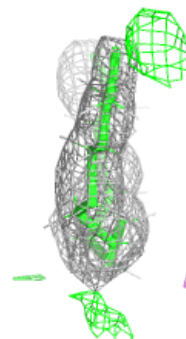
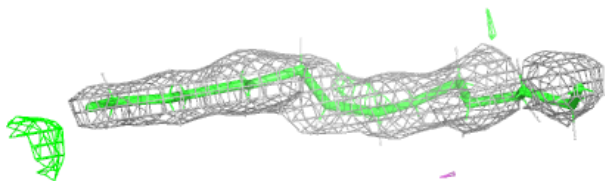
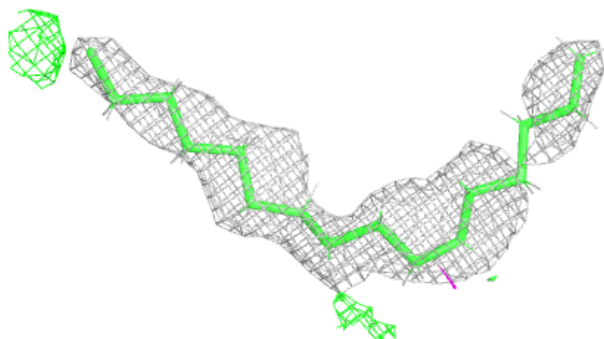


Electron density around STE I 102:

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

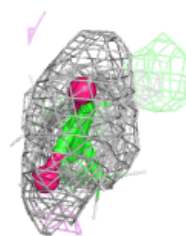
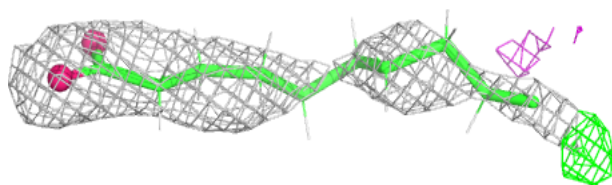
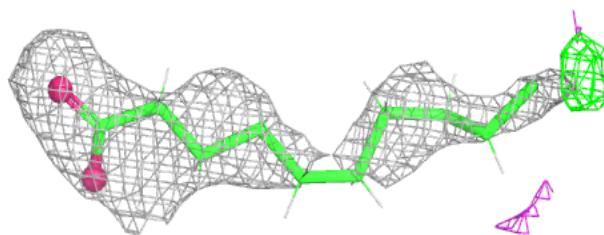
**Electron density around STE B 625:**

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

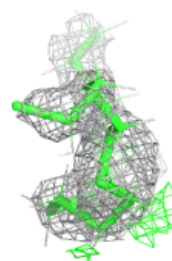
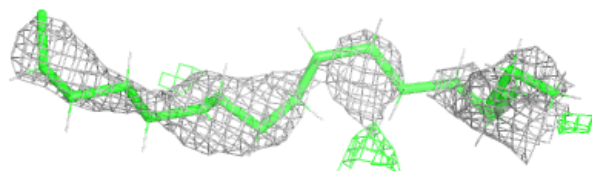
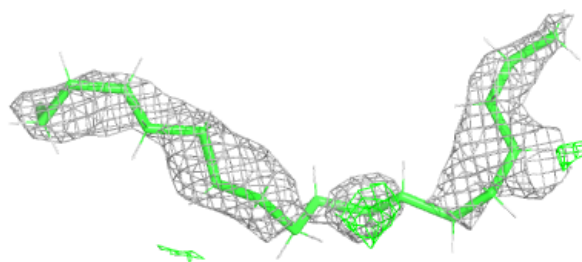


Electron density around STE a 412:

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

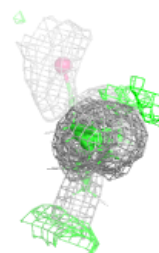
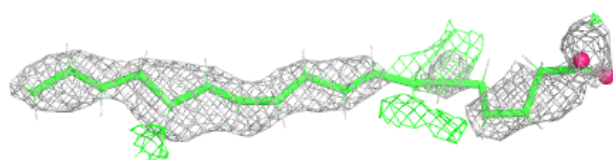
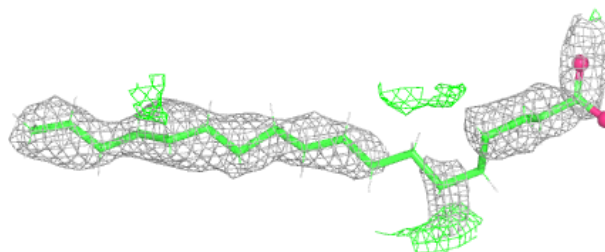
**Electron density around STE H 103:**

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

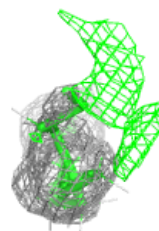
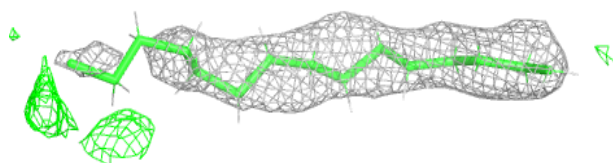
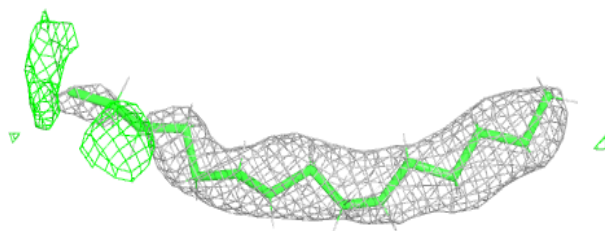


Electron density around STE b 625:

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

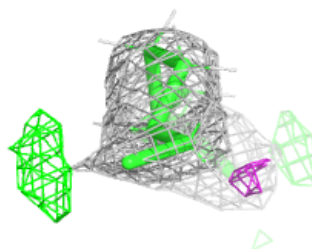
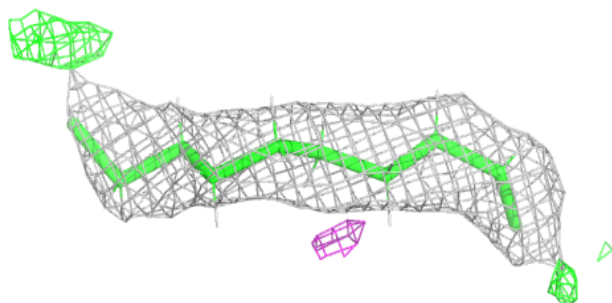
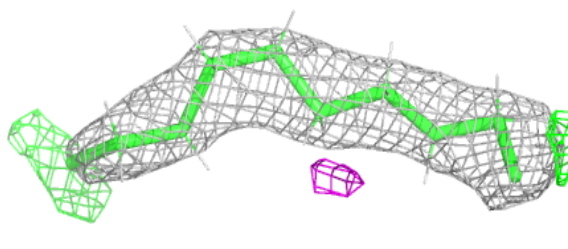
**Electron density around STE b 624:**

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

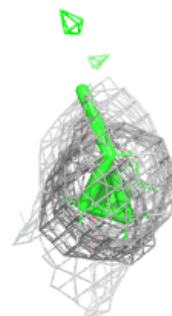
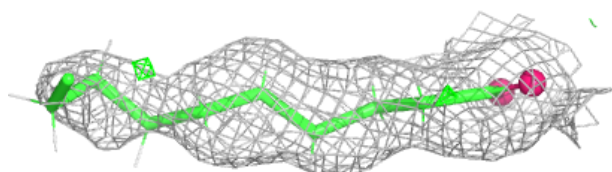
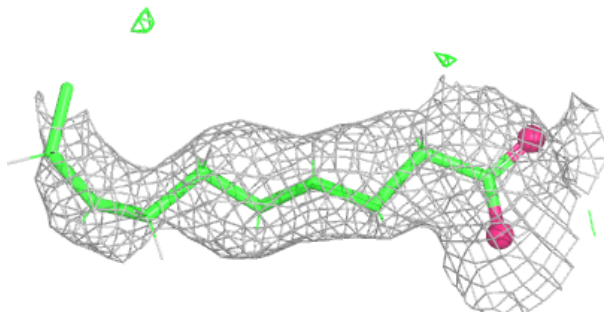


Electron density around STE b 626:

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

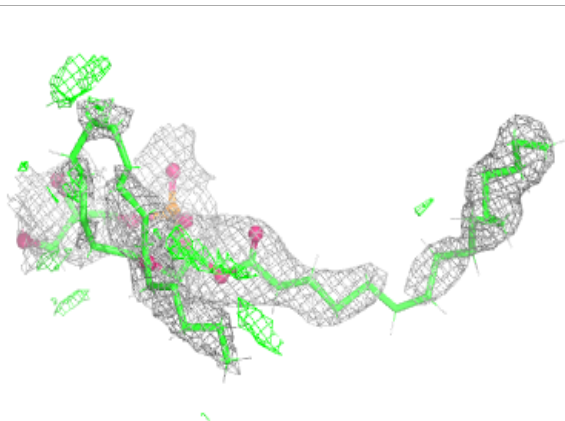
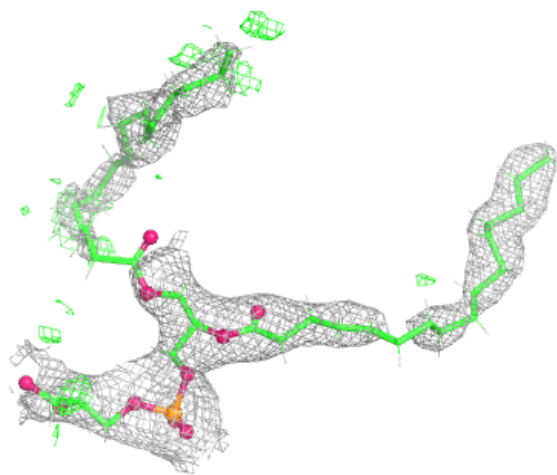
**Electron density around STE c 523:**

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



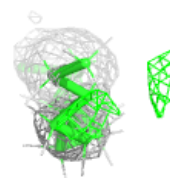
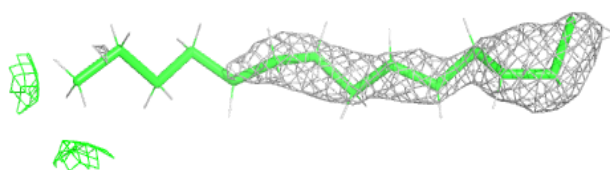
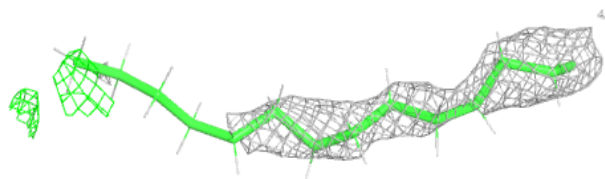
Electron density around LHG A 411:

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

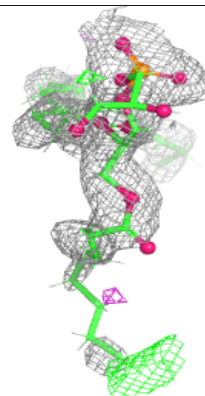
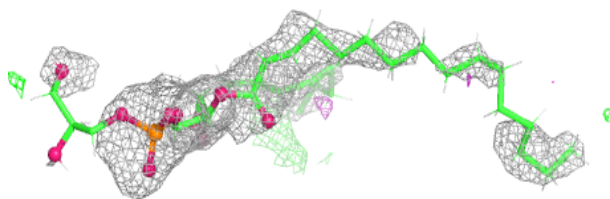
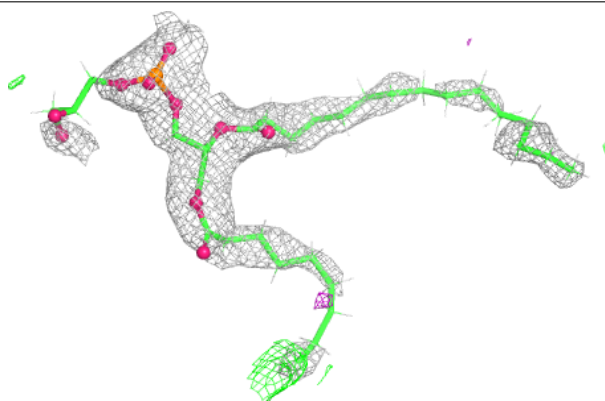


Electron density around STE b 627:

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

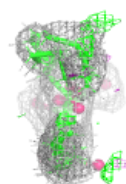
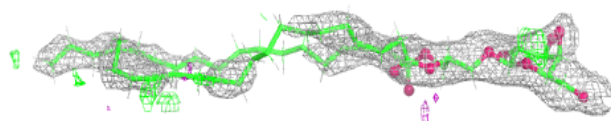
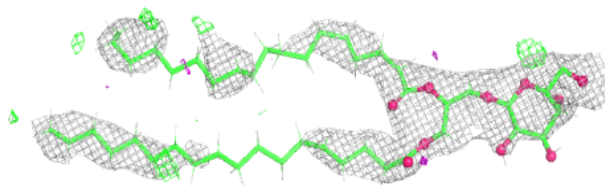
**Electron density around LHG e 101:**

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

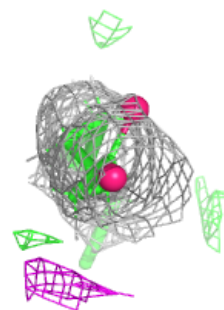
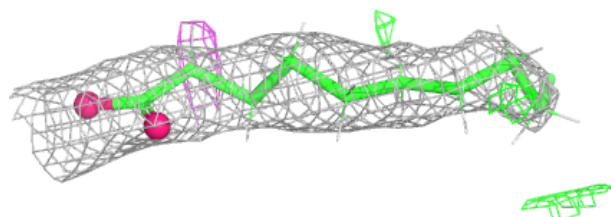
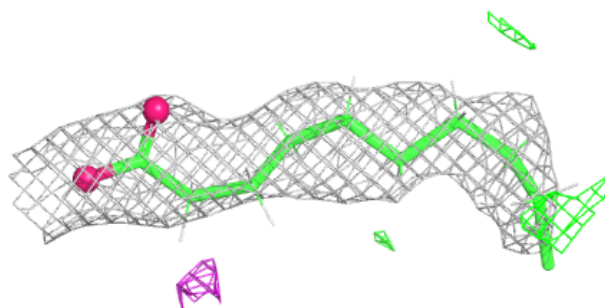


Electron density around LMG b 622:

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

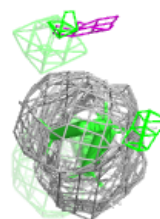
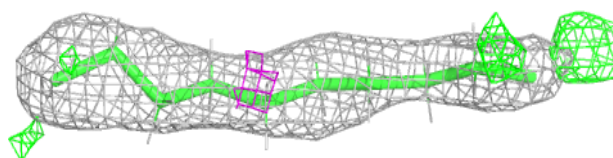
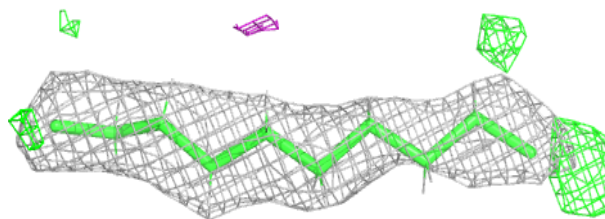
**Electron density around STE L 103:**

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

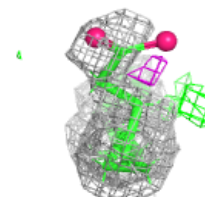
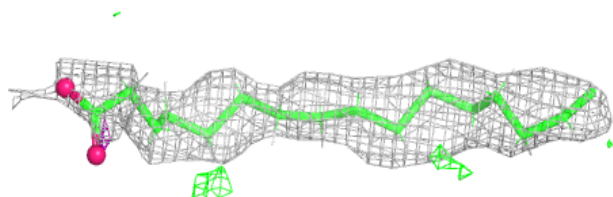
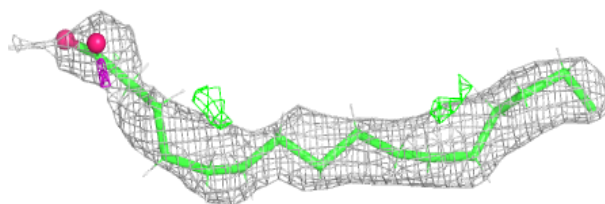


Electron density around STE M 103:

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

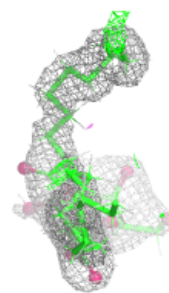
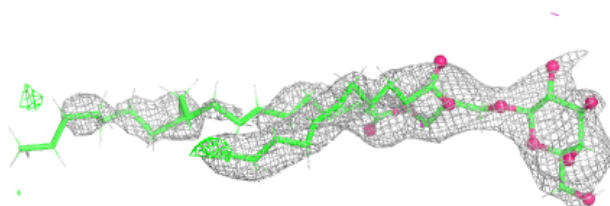
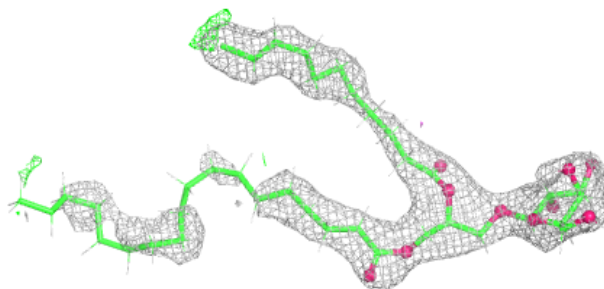
**Electron density around STE B 624:**

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



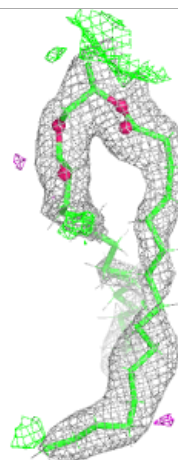
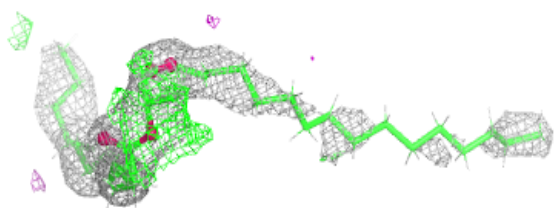
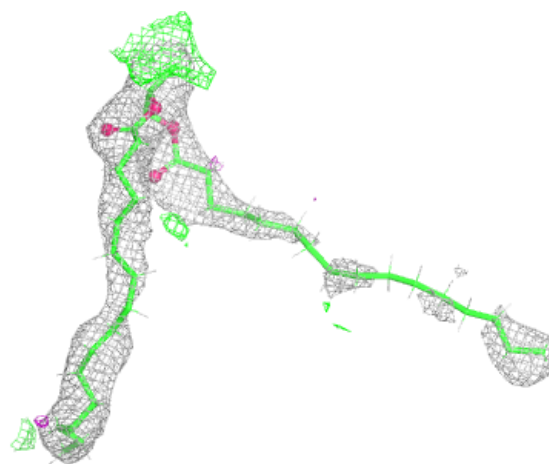
Electron density around LMG c 521:

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



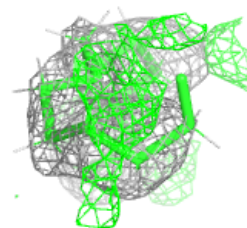
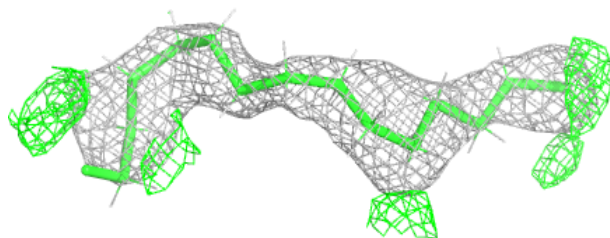
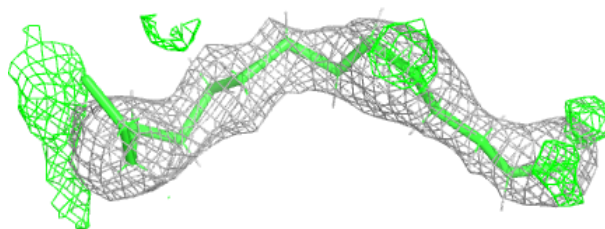
Electron density around SQD A 412:

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

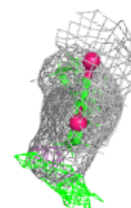
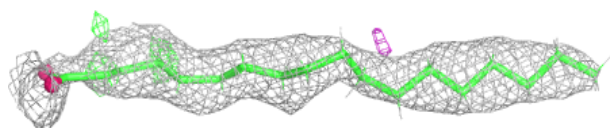
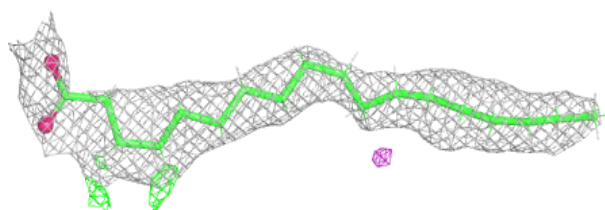


Electron density around STE a 413:

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

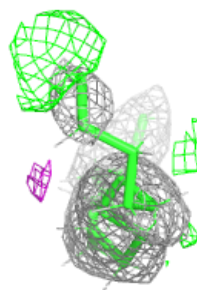
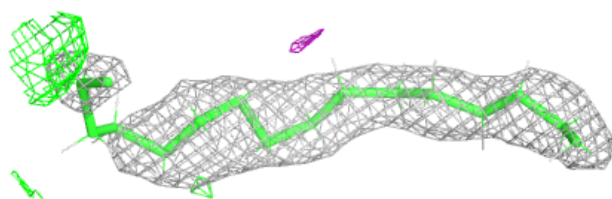
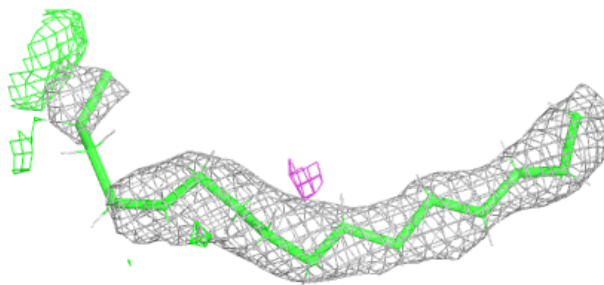
**Electron density around STE c 520:**

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

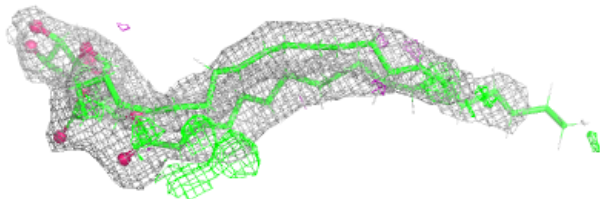
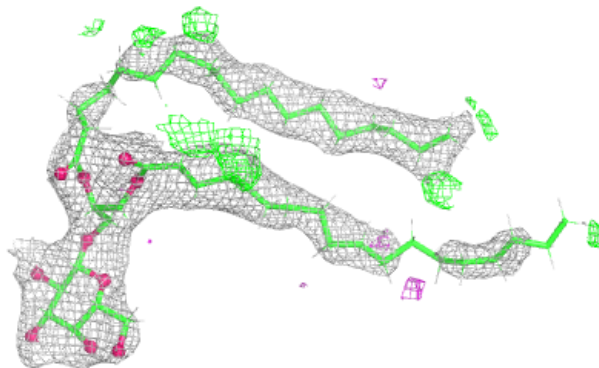


Electron density around STE b 620:

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

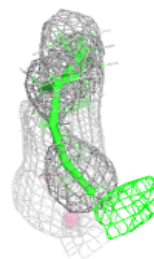
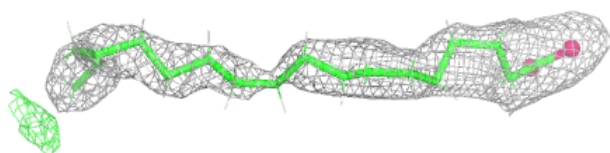
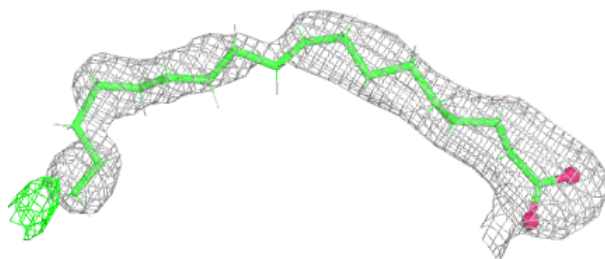
**Electron density around LMG B 626:**

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

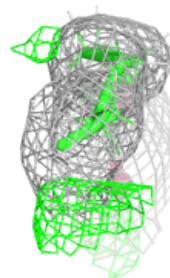
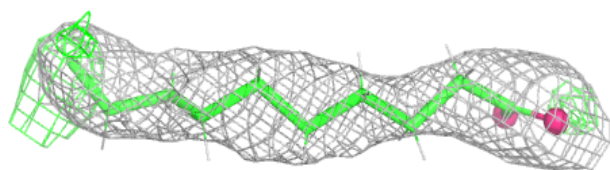
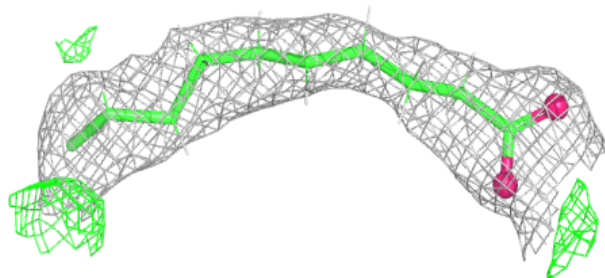


Electron density around STE x 102:

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

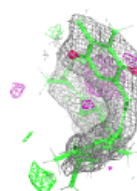
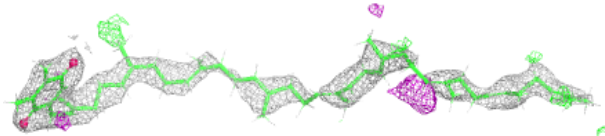
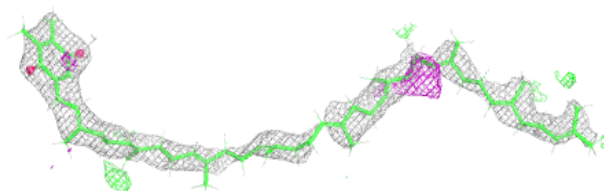
**Electron density around STE C 518:**

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

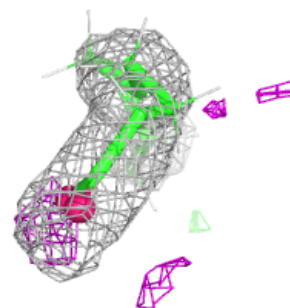
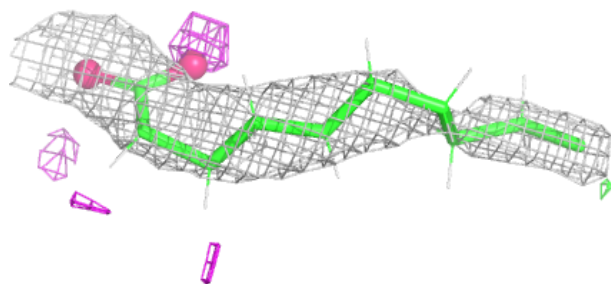
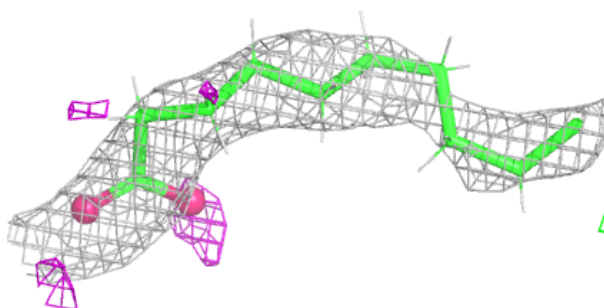


Electron density around PL9 A 408:

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

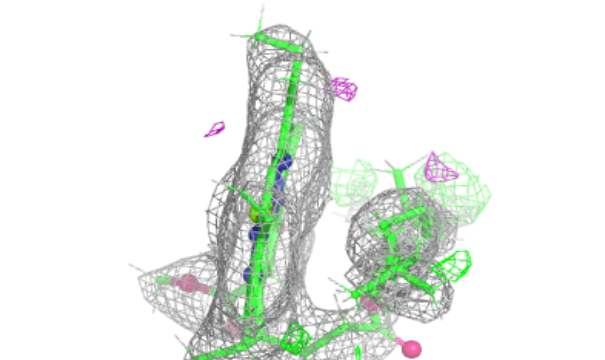
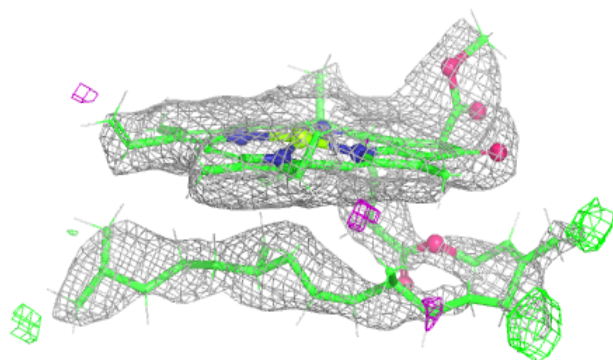
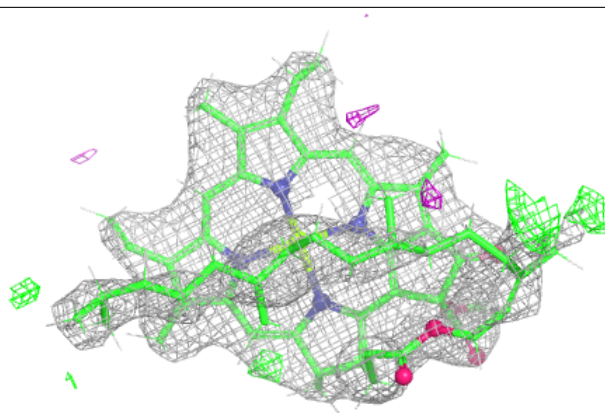
**Electron density around STE B 627:**

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

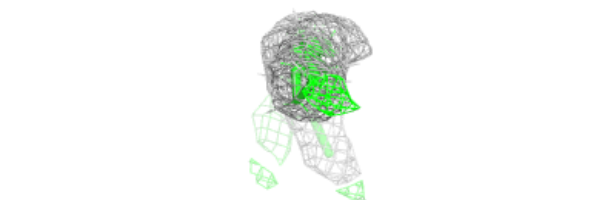
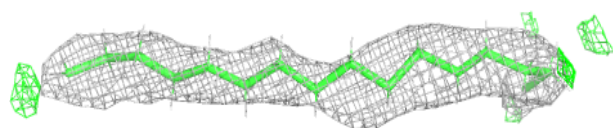
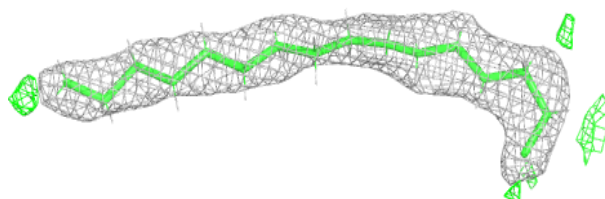


Electron density around CLA b 601:

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

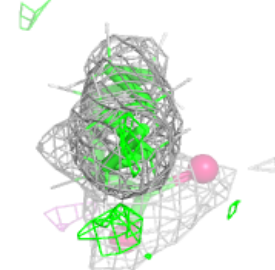
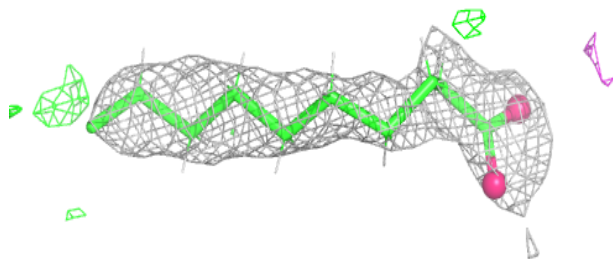
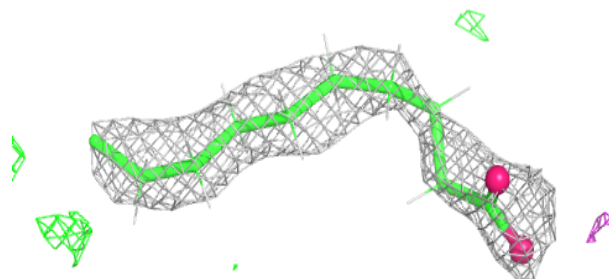
**Electron density around STE C 519:**

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

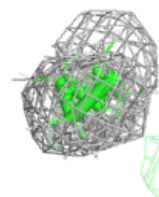
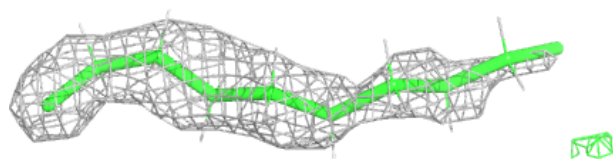
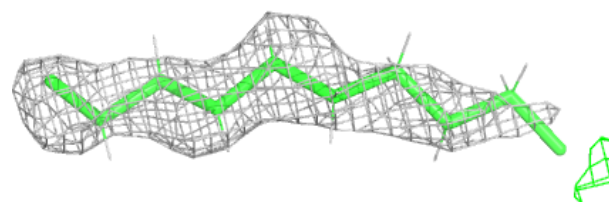


Electron density around STE R 101:

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

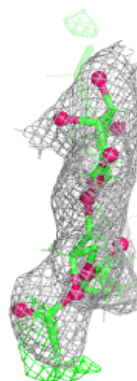
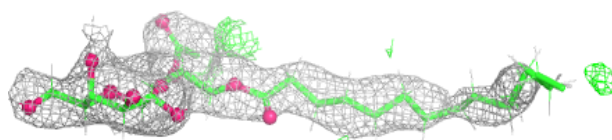
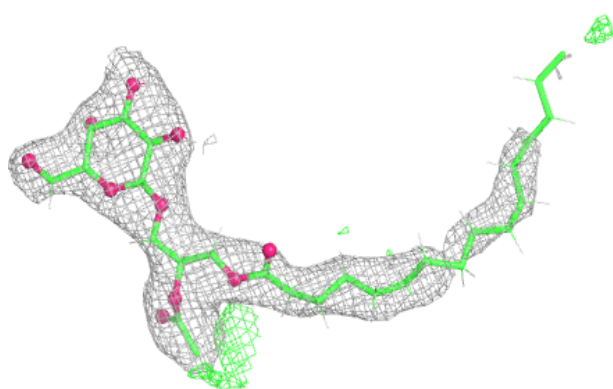
**Electron density around STE t 104:**

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

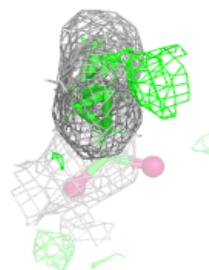
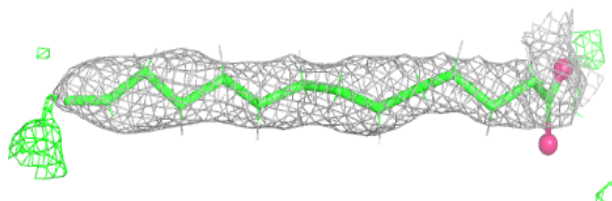
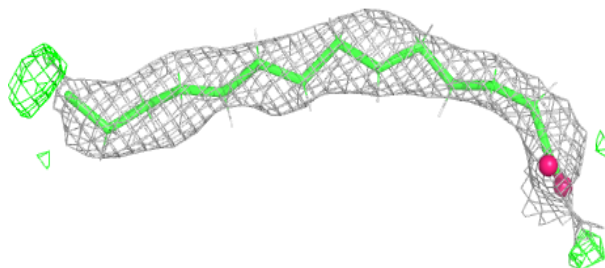


Electron density around LMG c 519:

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

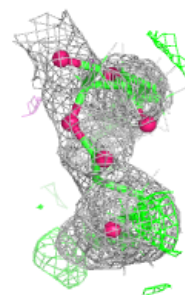
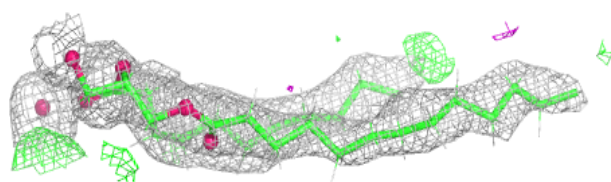
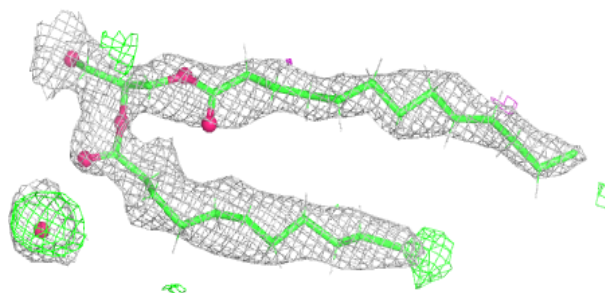
**Electron density around STE b 623:**

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

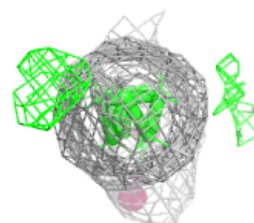
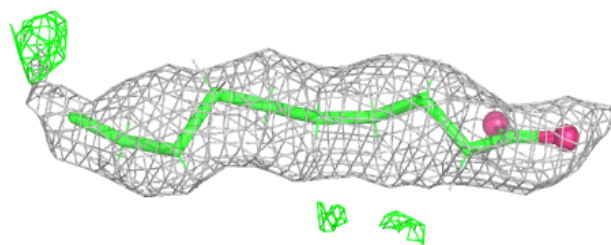
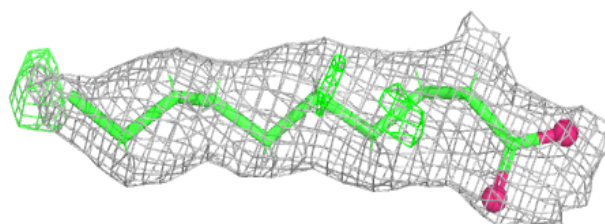


Electron density around LMG D 412:

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

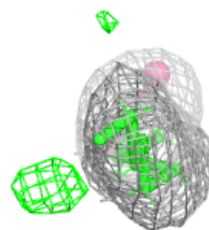
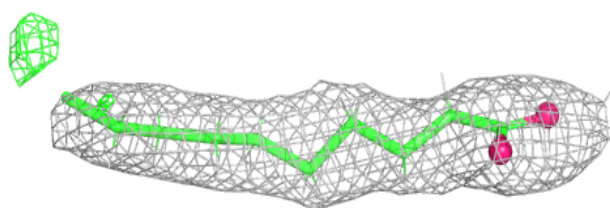
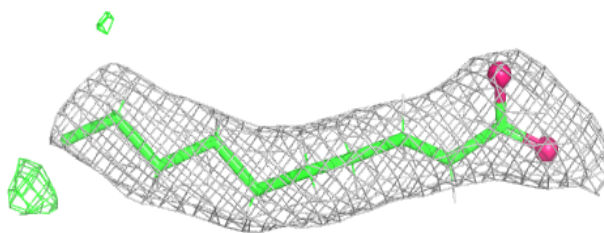
**Electron density around STE J 101:**

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



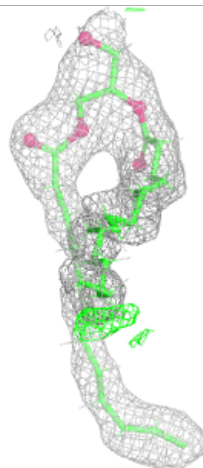
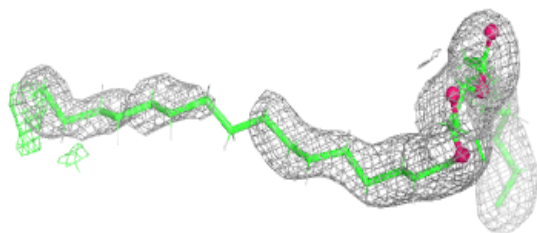
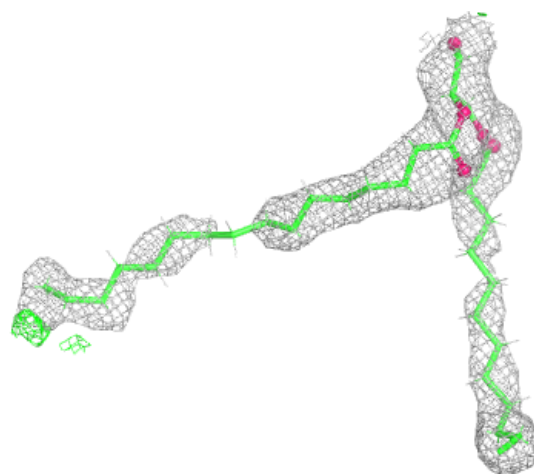
Electron density around STE j 101:

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



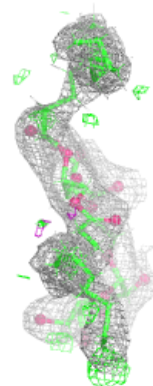
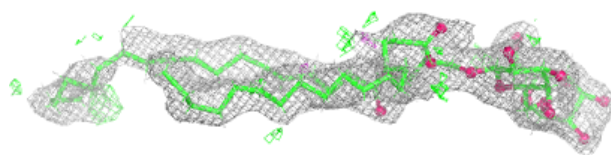
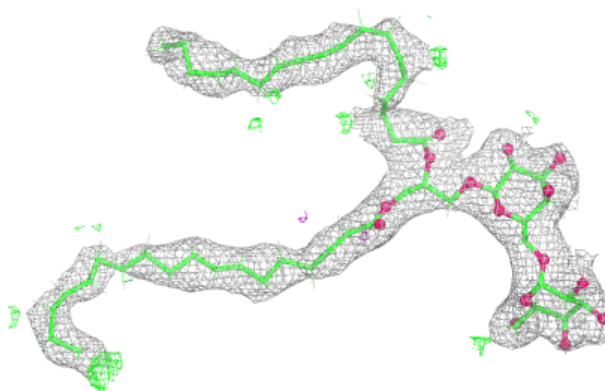
Electron density around SQD t 102:

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

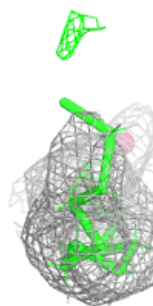
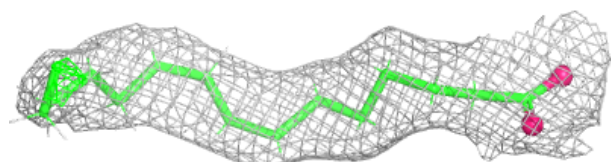
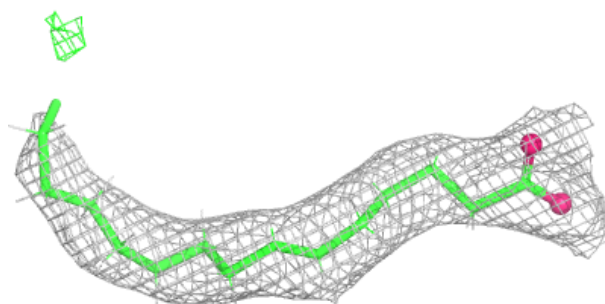


Electron density around DGD A 413:

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

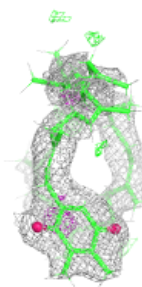
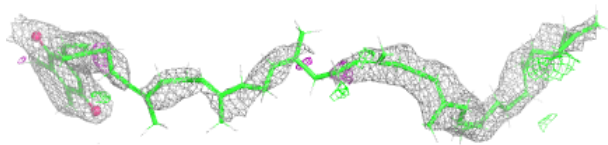
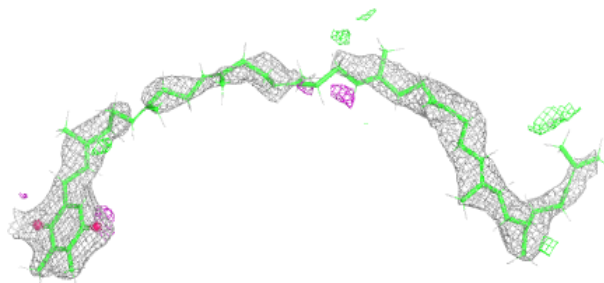
**Electron density around STE B 620:**

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

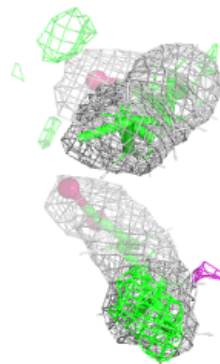
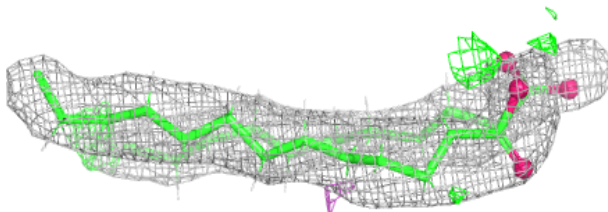
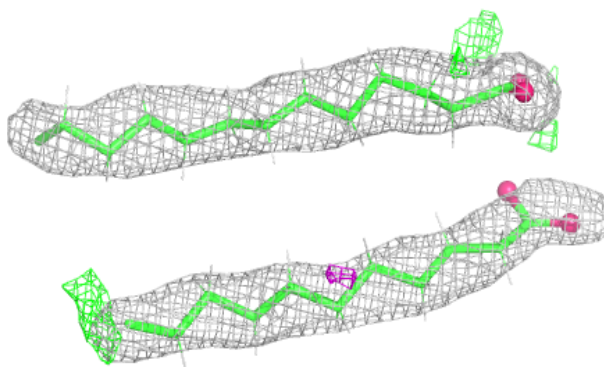


Electron density around PL9 a 409:

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

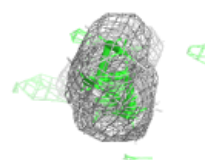
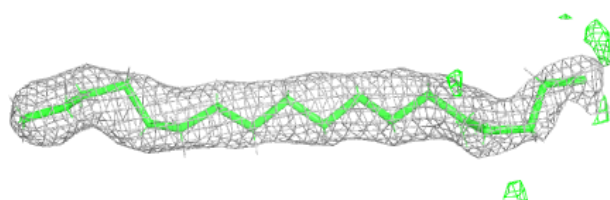
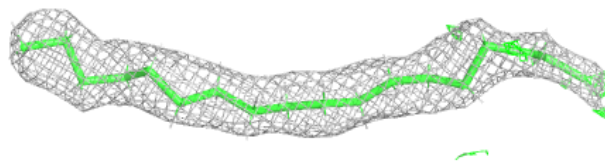
**Electron density around LMG B 621:**

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

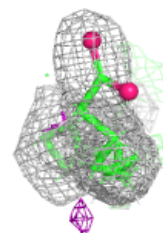
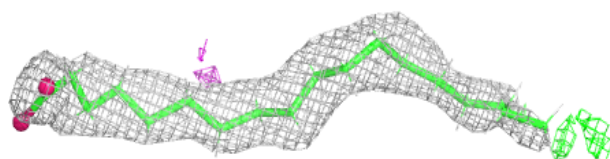
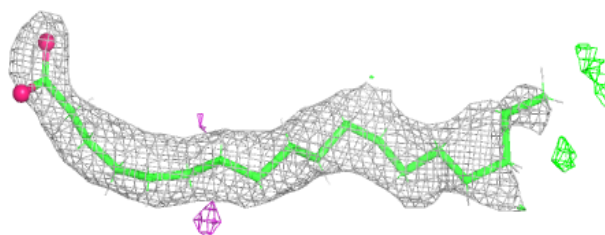


Electron density around STE l 102:

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

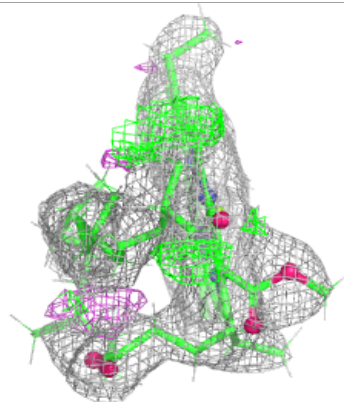
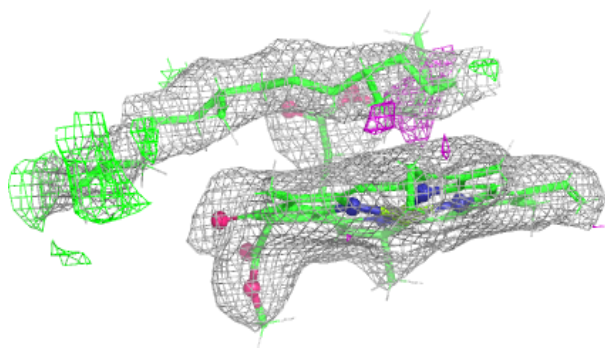
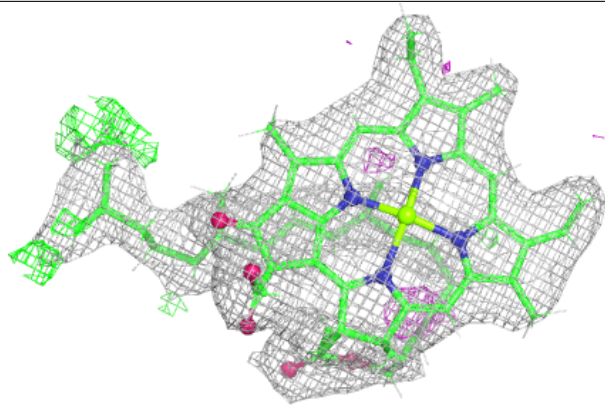
**Electron density around STE b 621:**

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

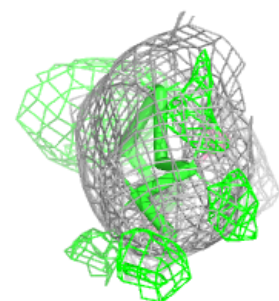
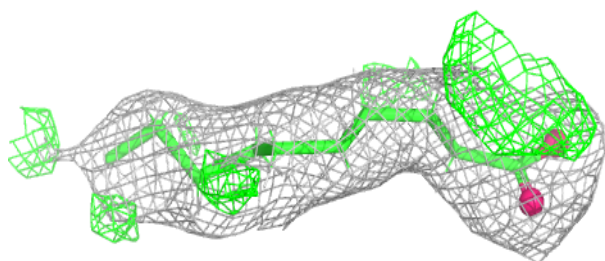
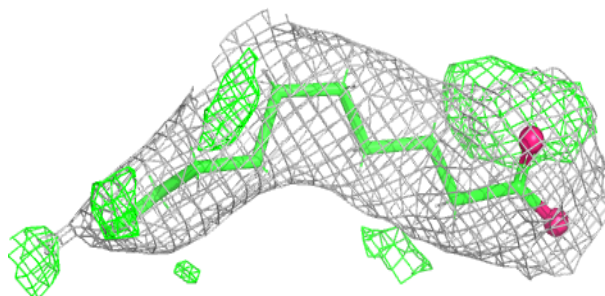


Electron density around CLA B 601:

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

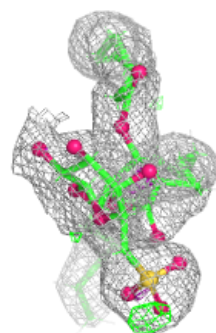
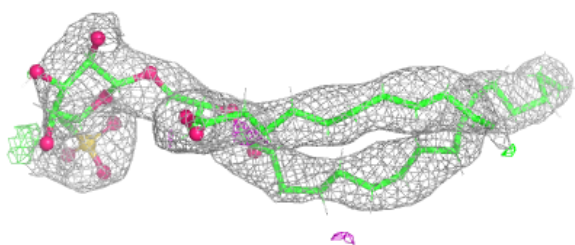
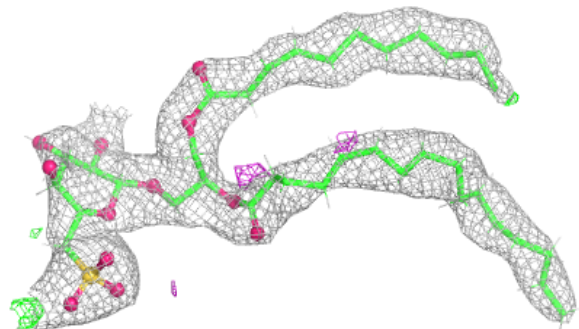
**Electron density around STE B 623:**

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

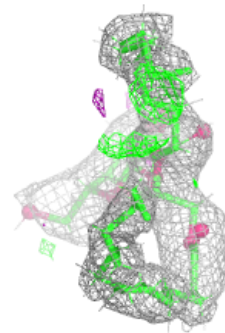
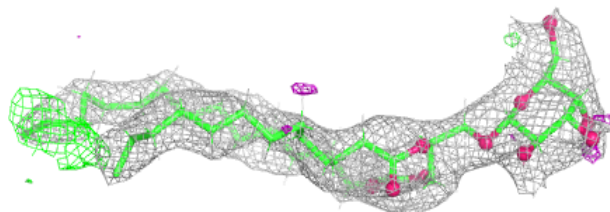
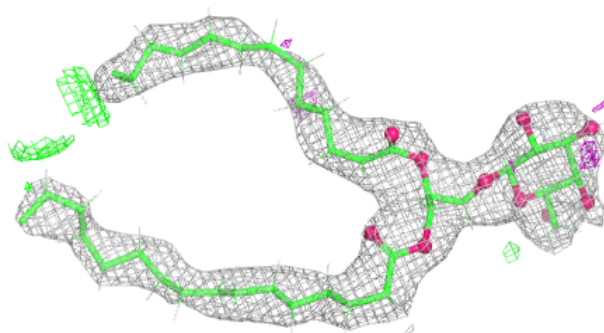


Electron density around SQD L 101:

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

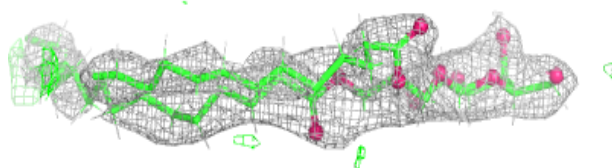
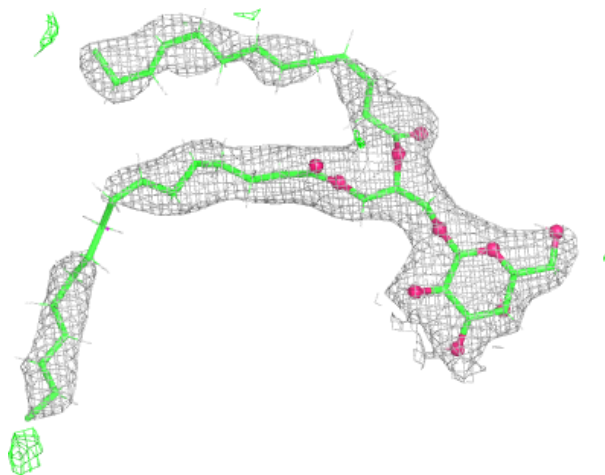
**Electron density around LMG A 409:**

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



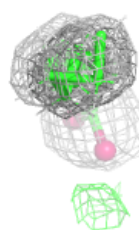
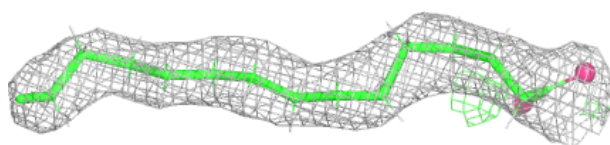
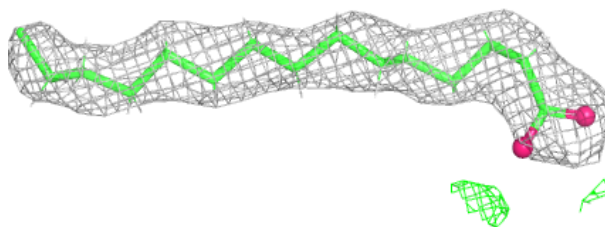
Electron density around LMG Y 101:

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

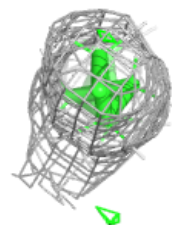
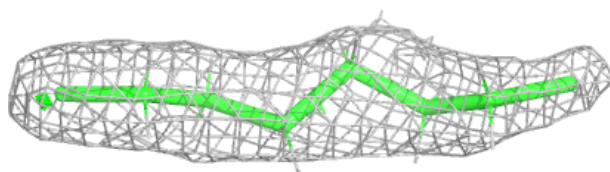
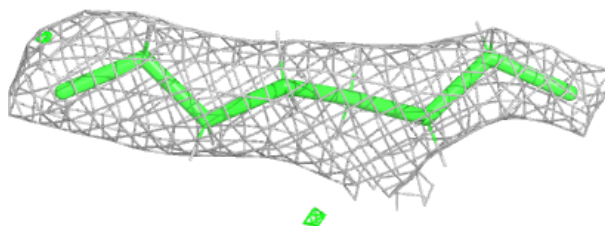


Electron density around STE d 411:

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

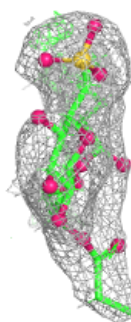
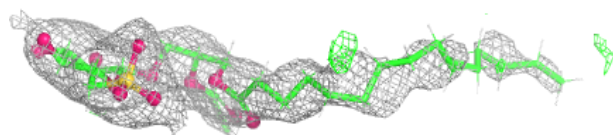
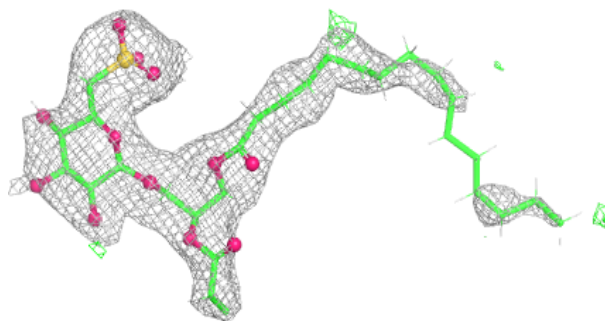
**Electron density around STE Z 102:**

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

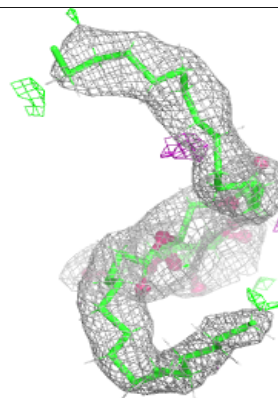
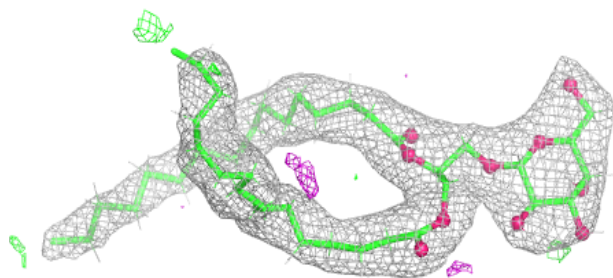
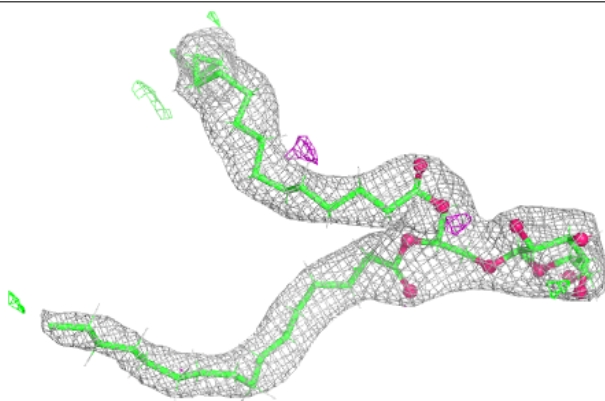


Electron density around SQD f 102:

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

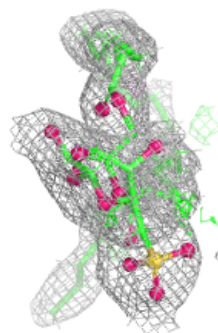
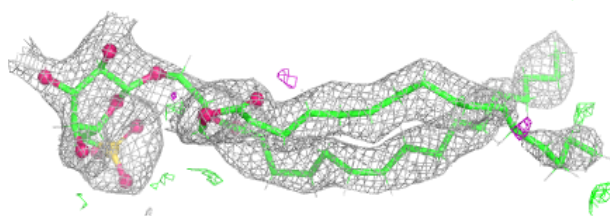
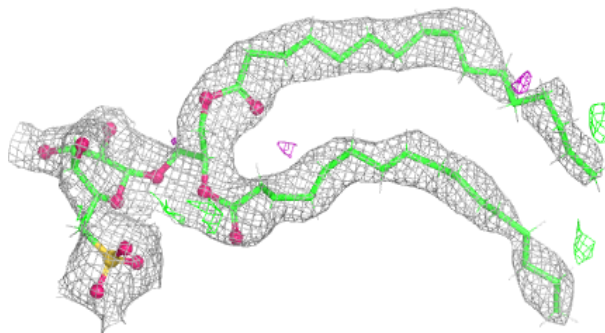
**Electron density around LMG M 101:**

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

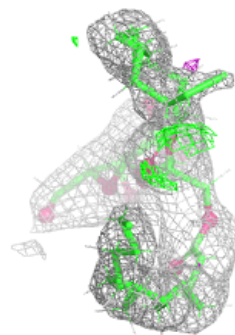
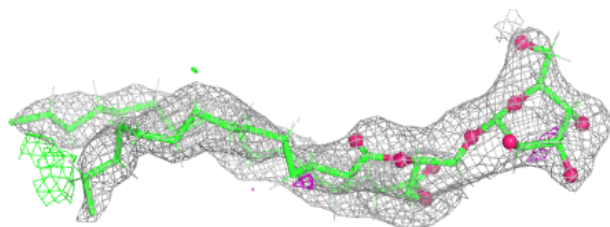
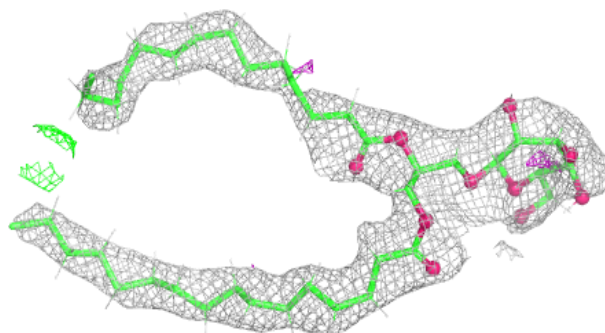


Electron density around SQD B 622:

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

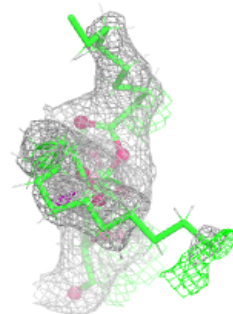
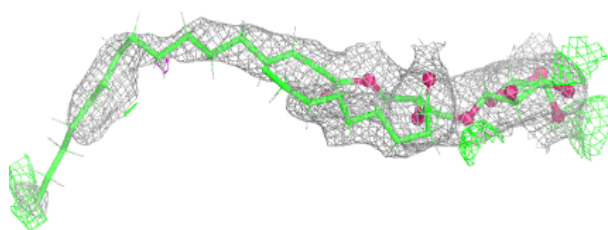
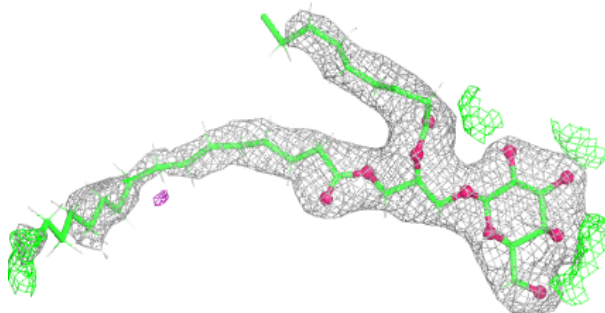
**Electron density around LMG c 522:**

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

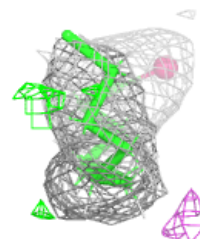
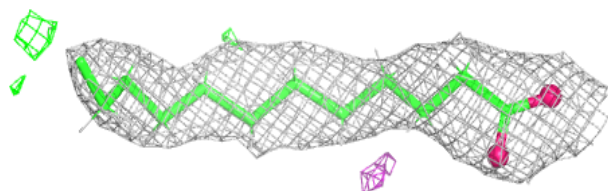
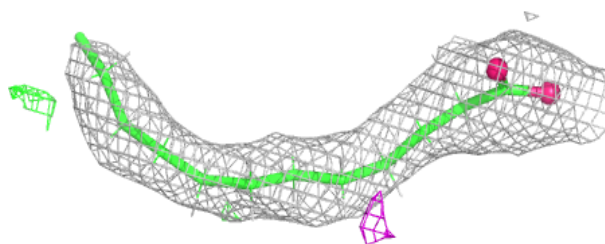


Electron density around LMG d 410:

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

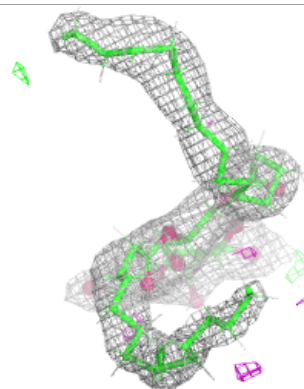
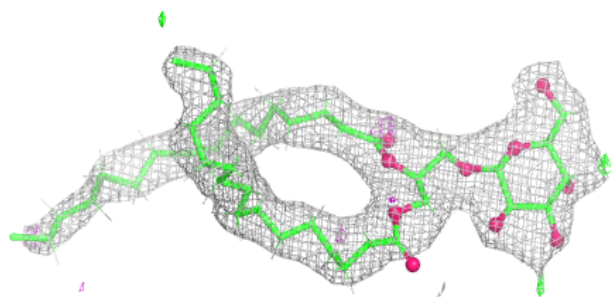
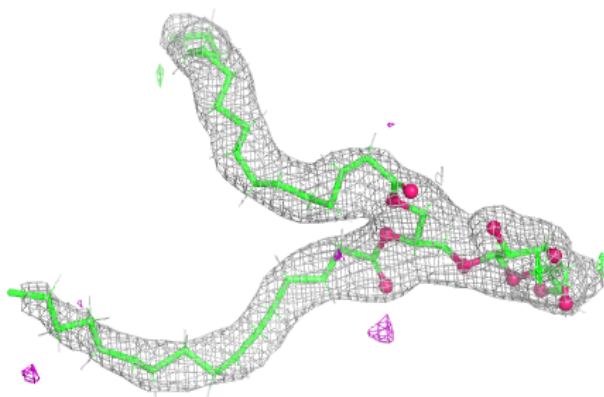
**Electron density around STE t 103:**

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

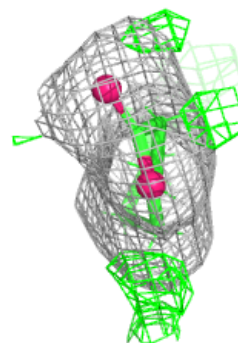
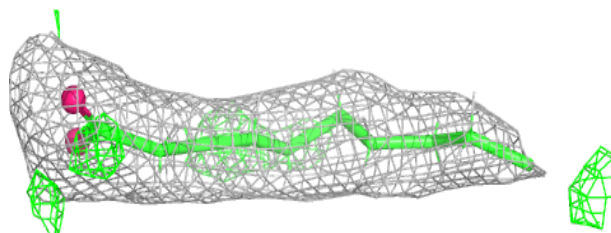
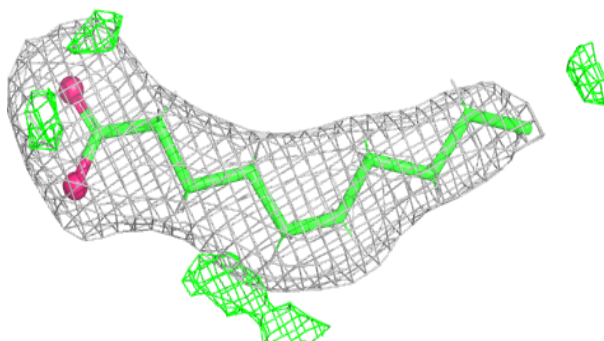


Electron density around LMG m 101:

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

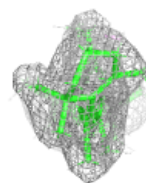
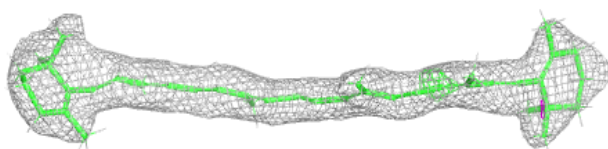
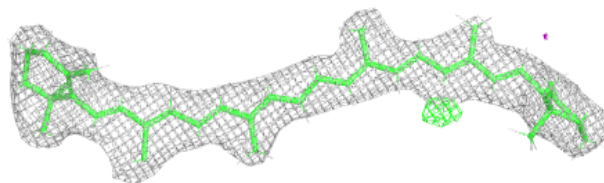
**Electron density around STE C 520:**

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

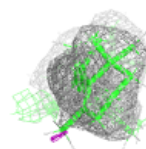
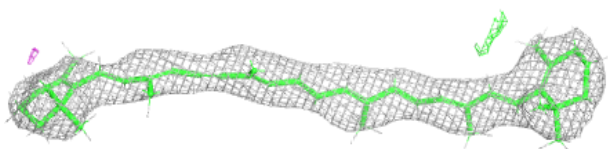
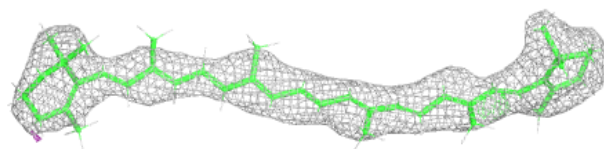


Electron density around BCR K 101:

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

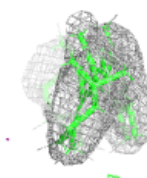
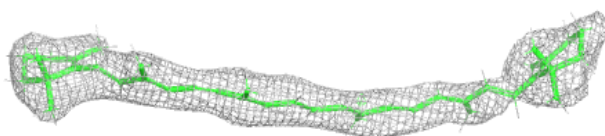
**Electron density around BCR c 514:**

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

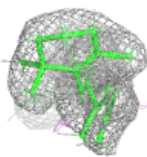
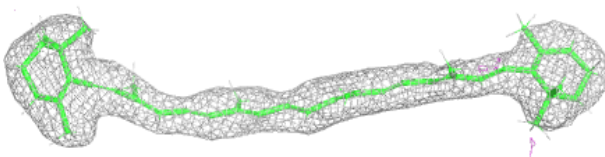
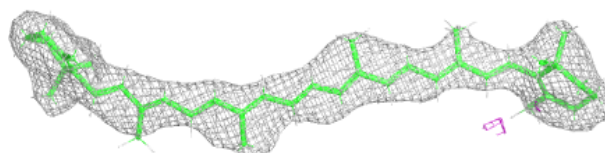


Electron density around BCR d 406:

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

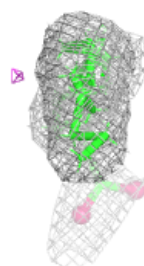
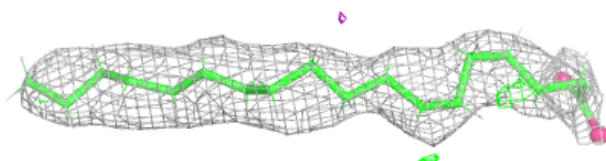
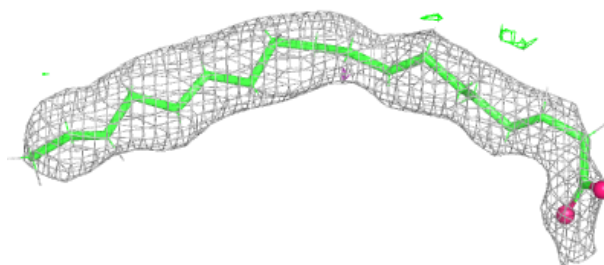
**Electron density around BCR x 101:**

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



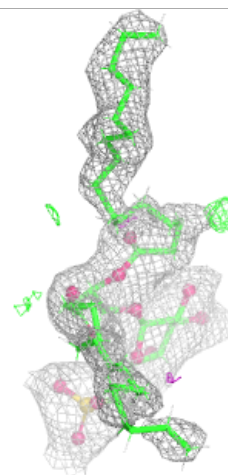
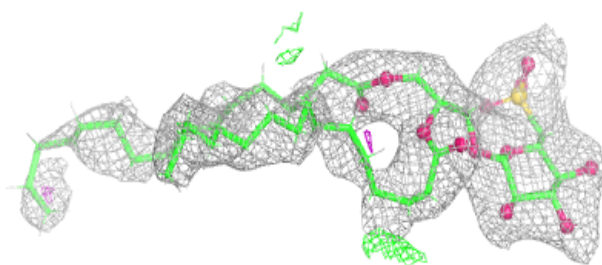
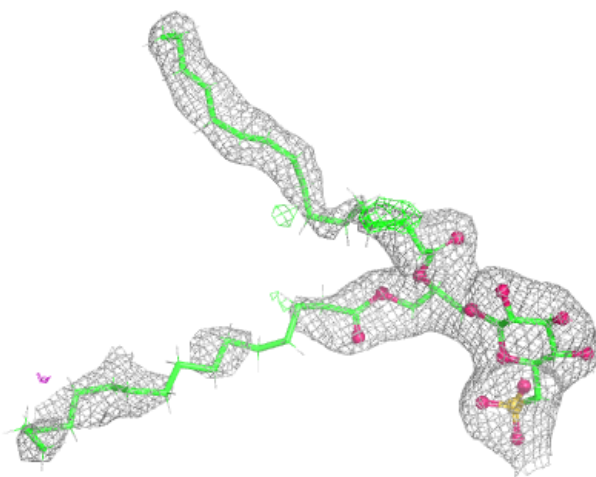
Electron density around STE X 101:

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



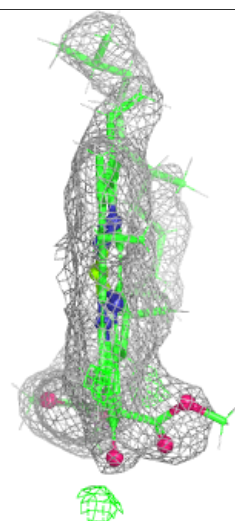
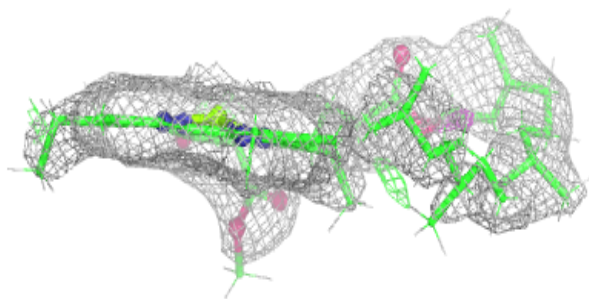
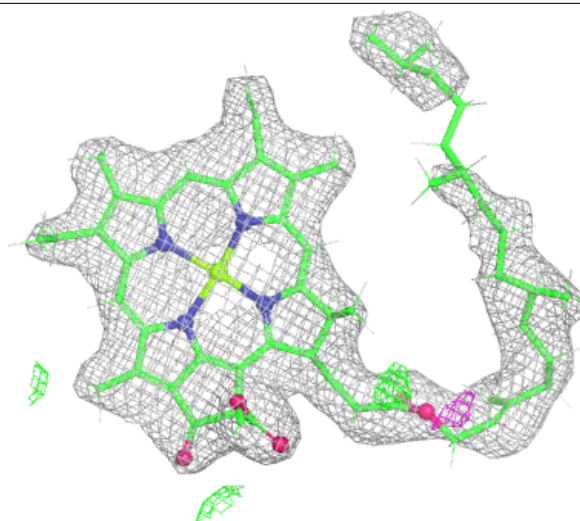
Electron density around SQD a 411:

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



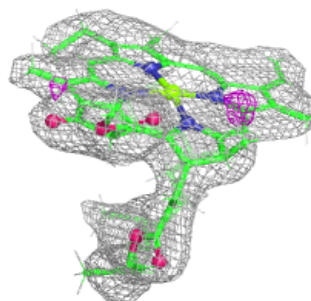
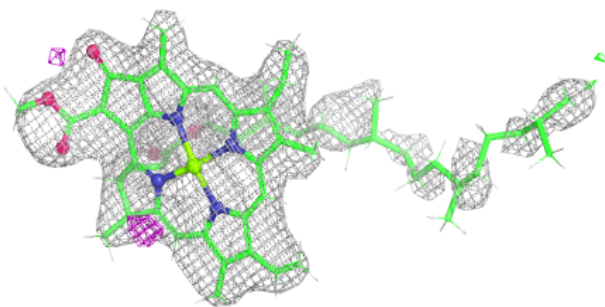
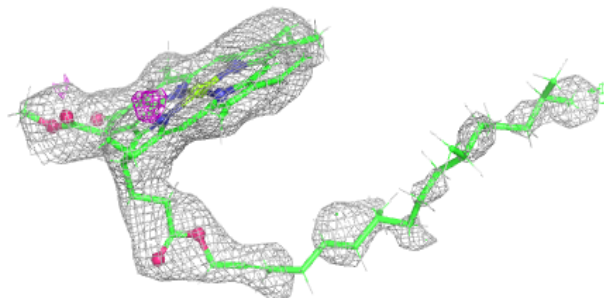
Electron density around CLA c 512:

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

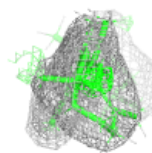
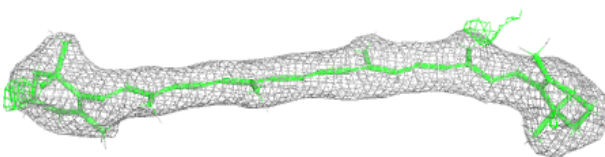
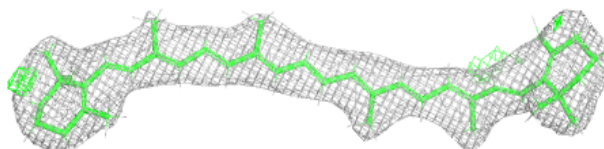


Electron density around CLA C 513:

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

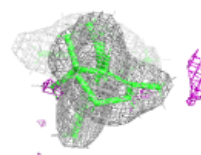
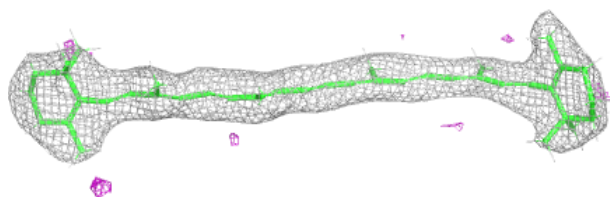
**Electron density around BCR B 619:**

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

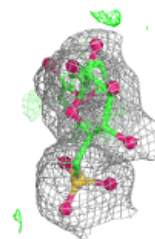
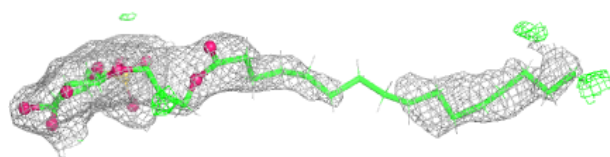
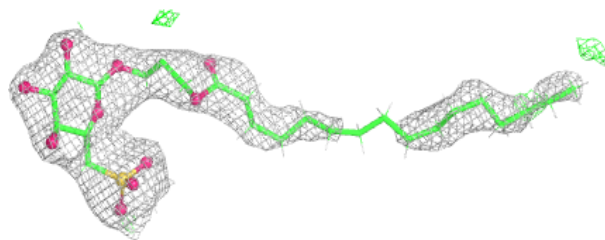


Electron density around BCR C 514:

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

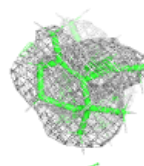
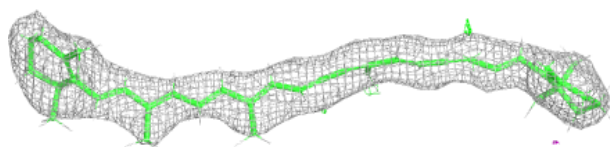
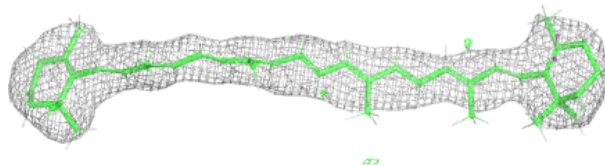
**Electron density around SQD D 409:**

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

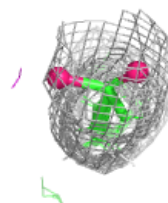
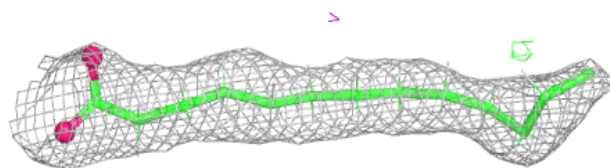
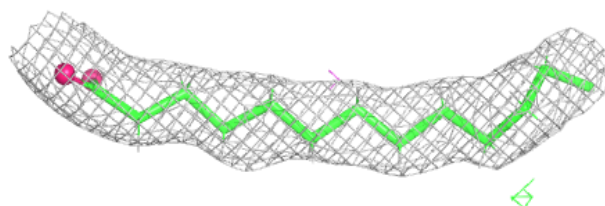


Electron density around BCR Z 101:

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

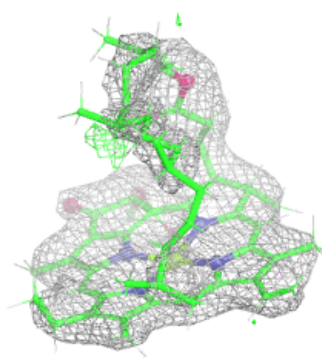
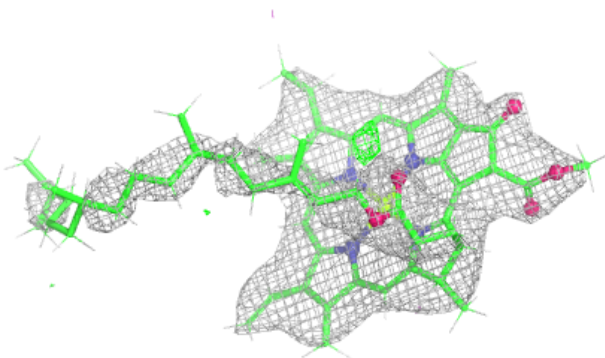
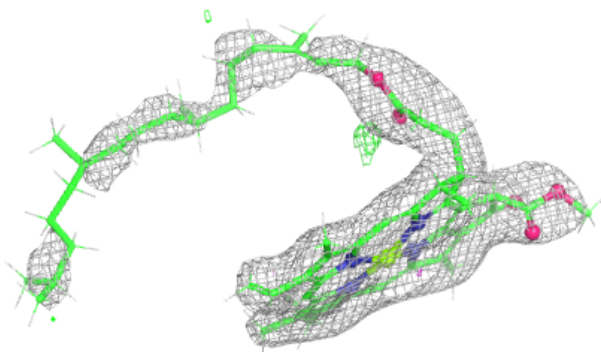
**Electron density around STE M 102:**

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

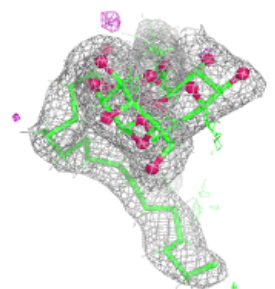
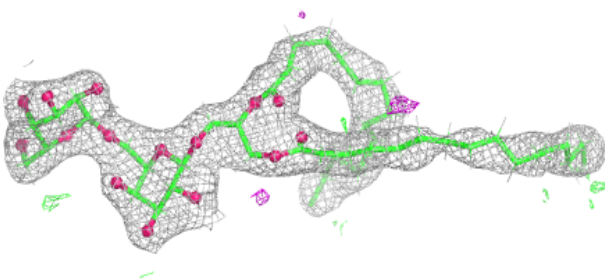
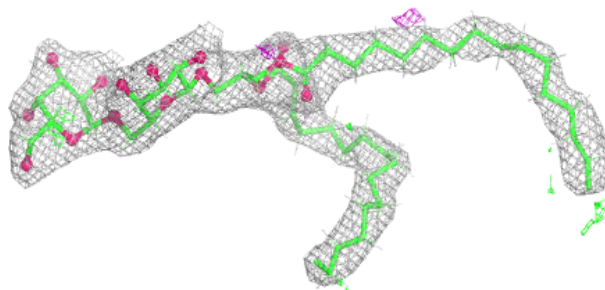


Electron density around CLA c 513:

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

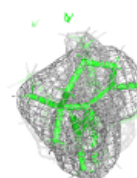
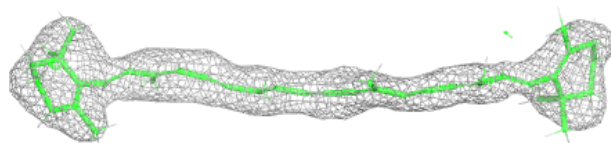
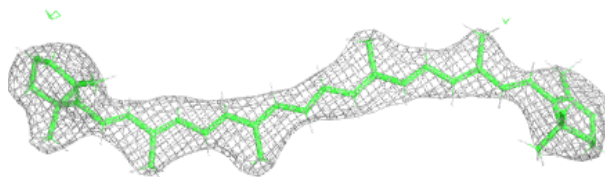
**Electron density around DGD H 102:**

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

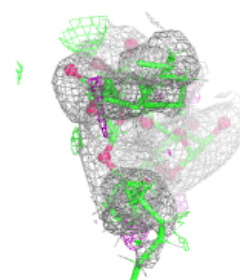
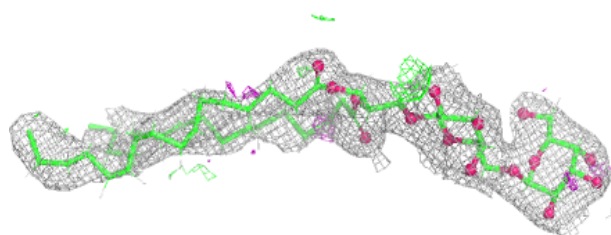
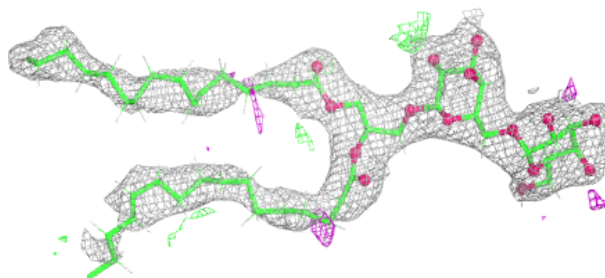


Electron density around BCR k 101:

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

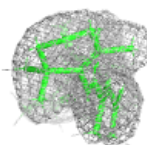
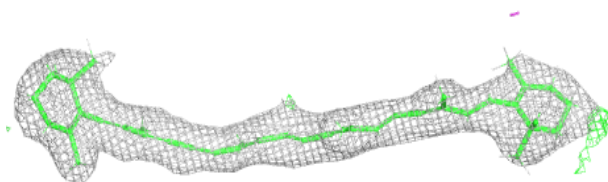
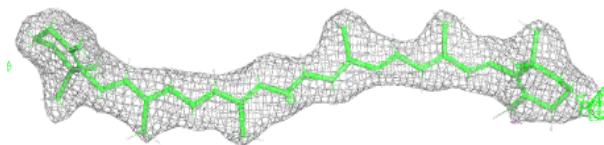
**Electron density around DGD c 518:**

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



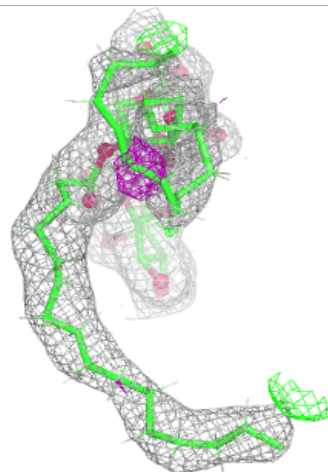
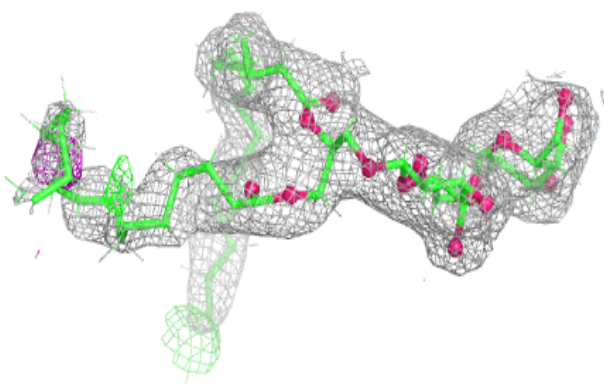
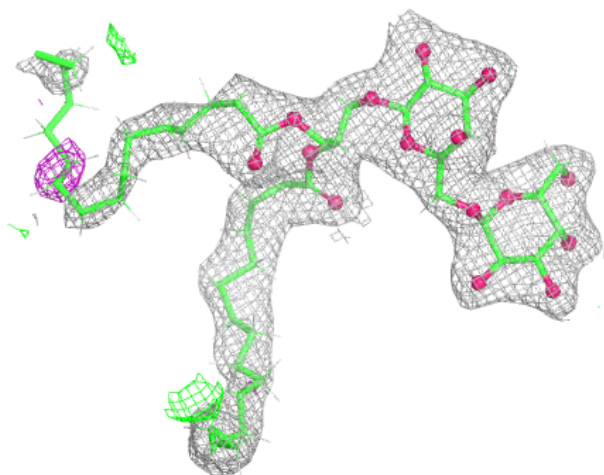
Electron density around BCR H 101:

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



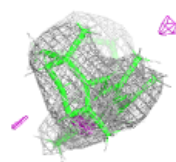
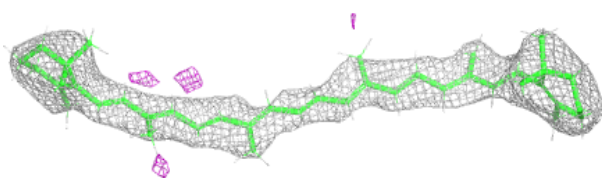
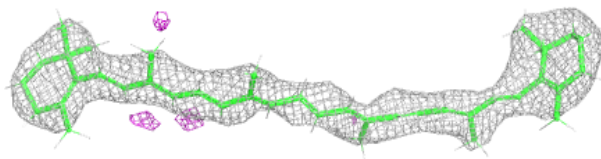
Electron density around DGD C 516:

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

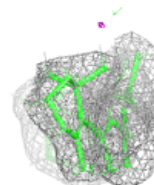
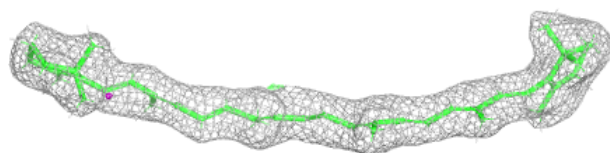
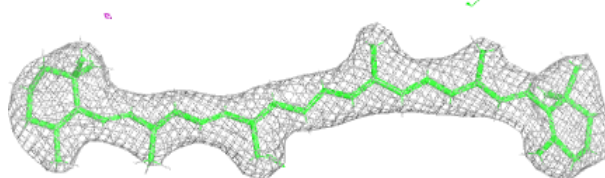


Electron density around BCR K 102:

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

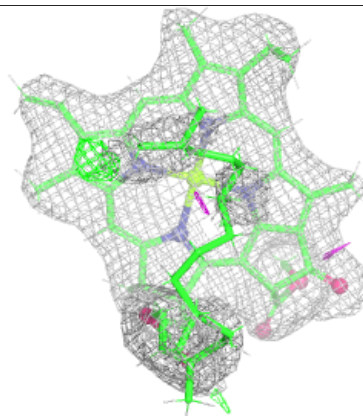
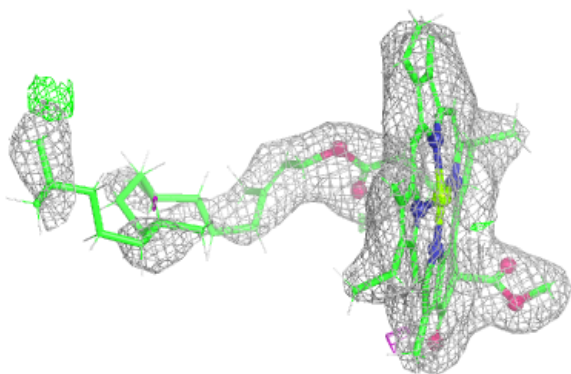
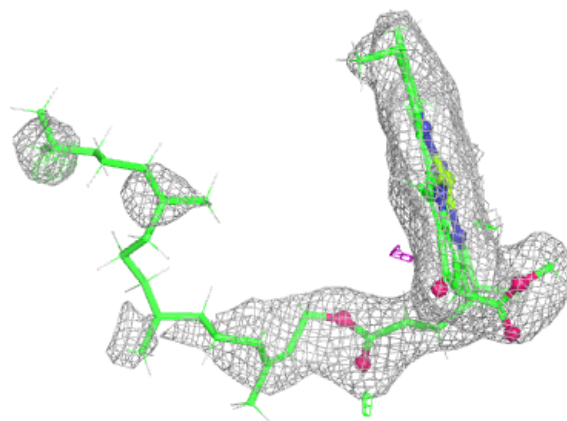
**Electron density around BCR T 101:**

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

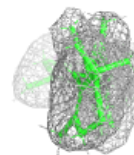
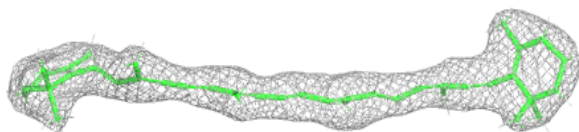


Electron density around CLA c 506:

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

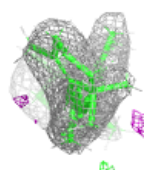
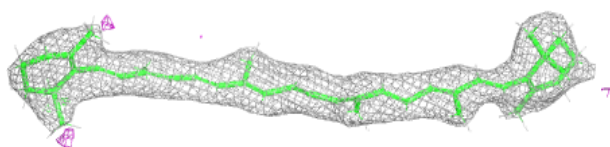
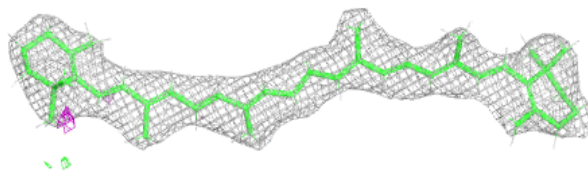
**Electron density around BCR b 617:**

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

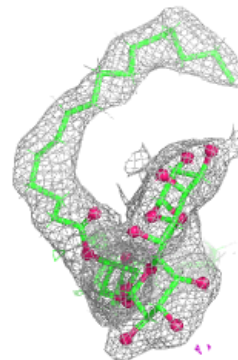
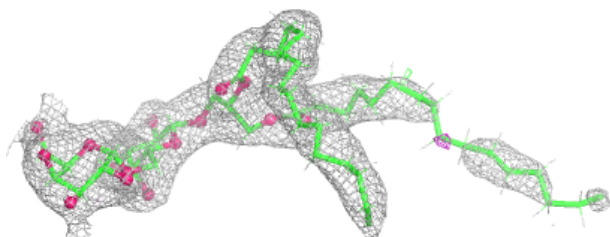
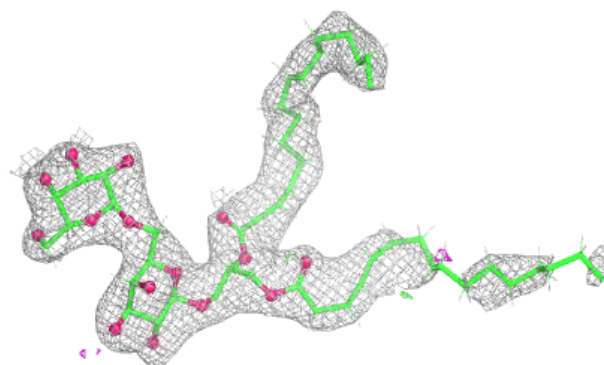


Electron density around BCR b 619:

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

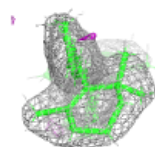
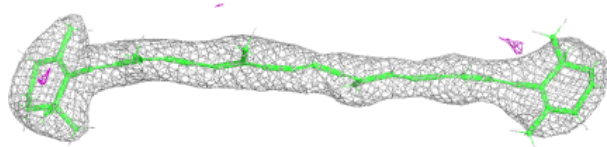
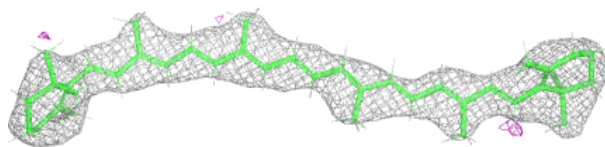
**Electron density around DGD c 517:**

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

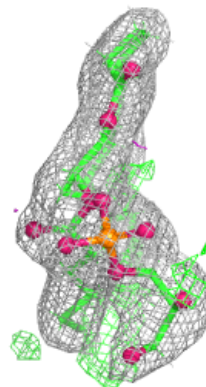
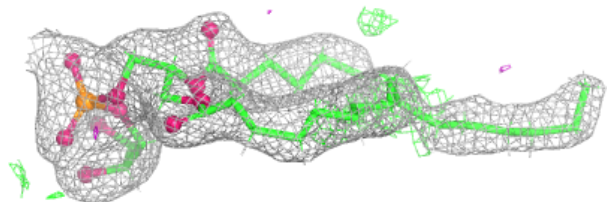
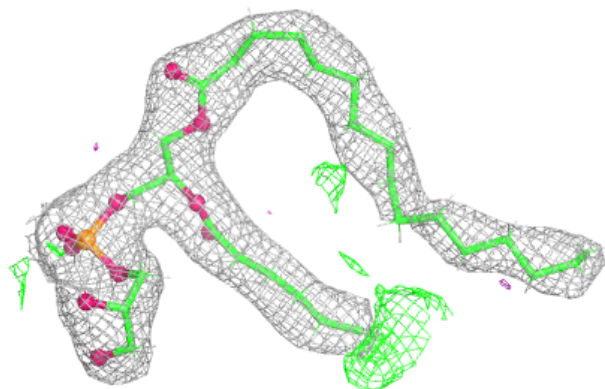


Electron density around BCR c 515:

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

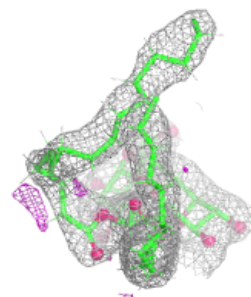
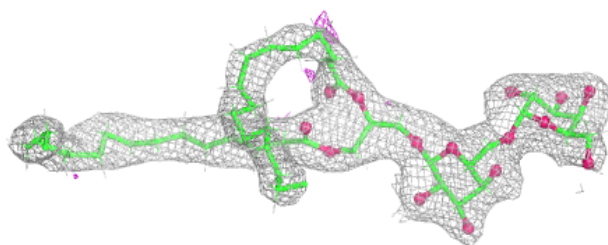
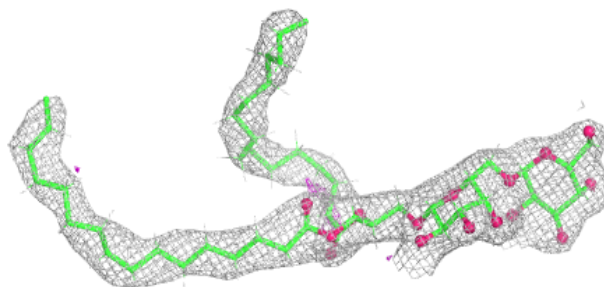
**Electron density around LHG d 409:**

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

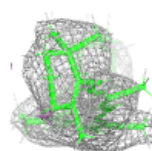
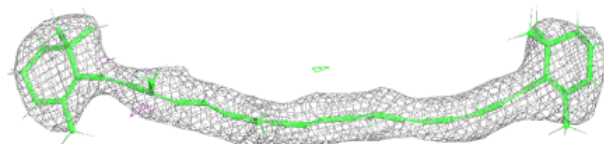


Electron density around DGD h 101:

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

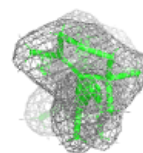
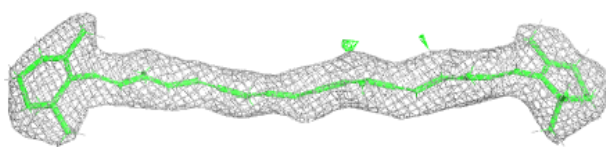
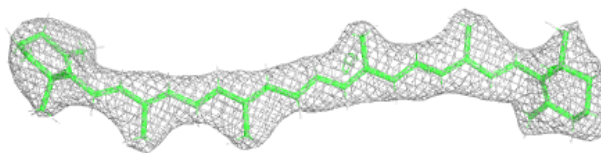
**Electron density around BCR k 102:**

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



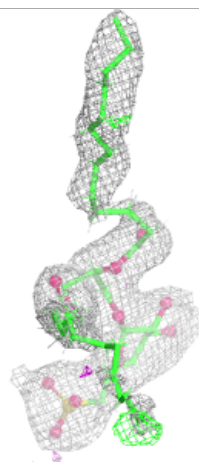
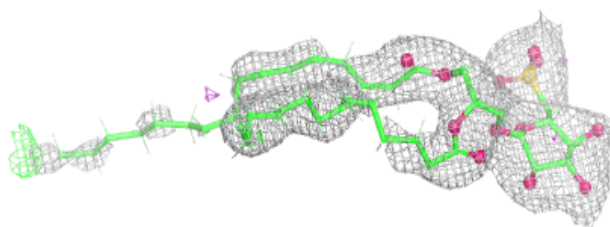
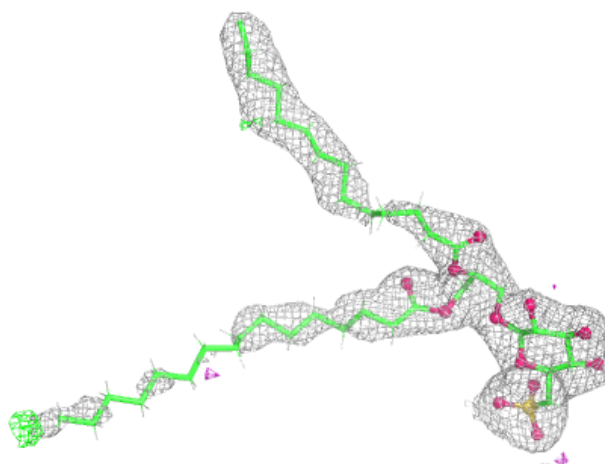
Electron density around BCR B 618:

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



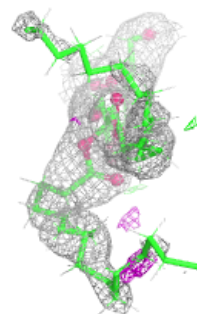
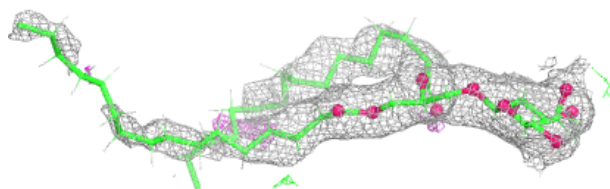
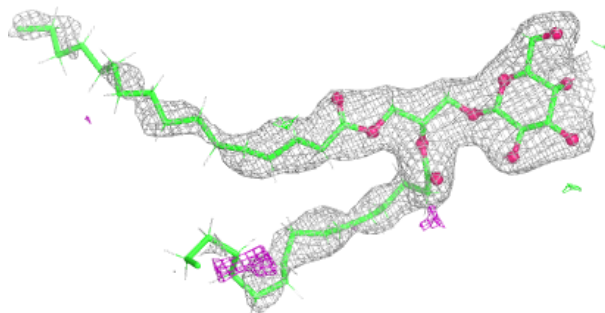
Electron density around SQD A 410:

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

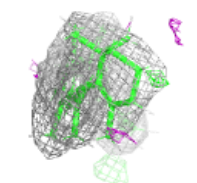
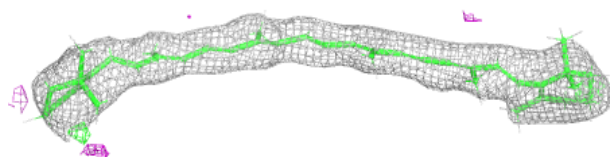
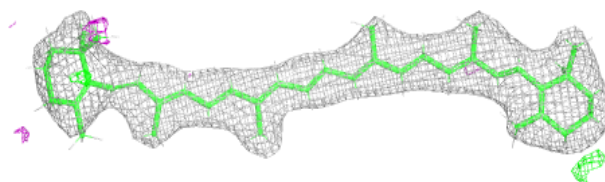


Electron density around LMG D 408:

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

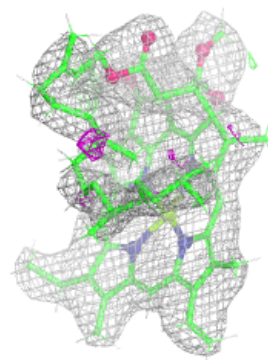
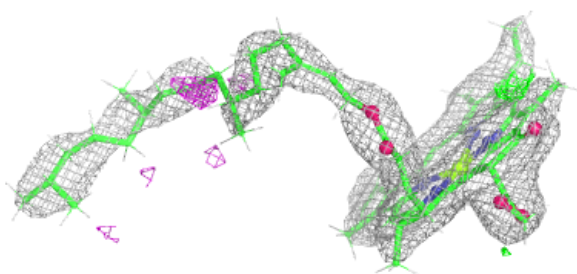
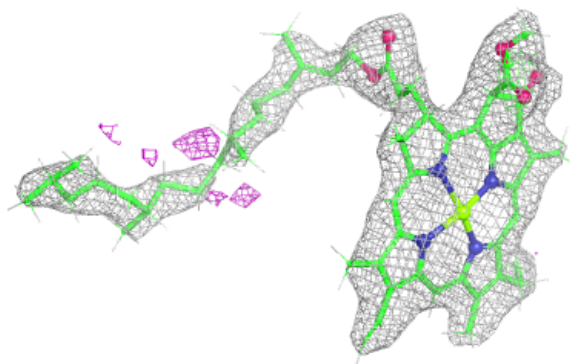
**Electron density around BCR D 406:**

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

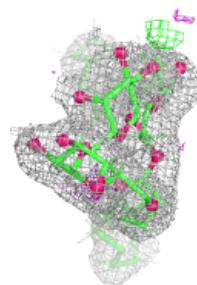
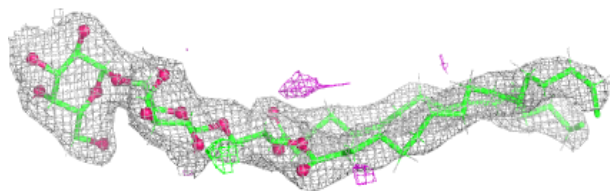
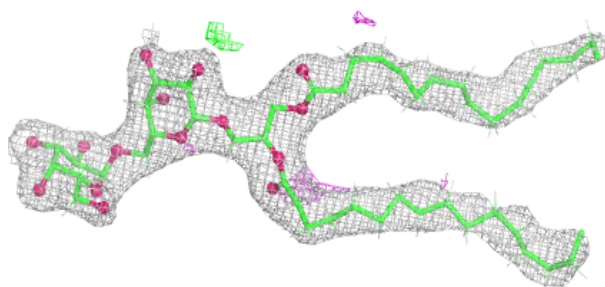


Electron density around CLA c 511:

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

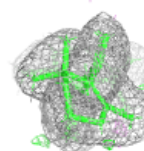
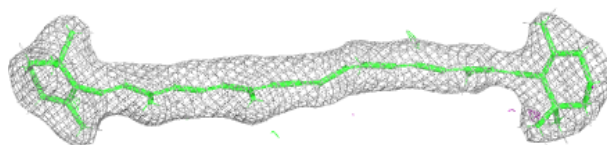
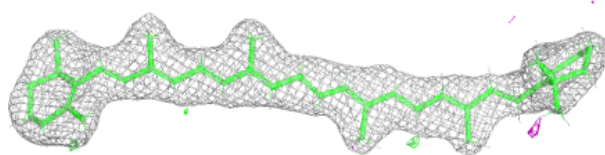
**Electron density around DGD C 517:**

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



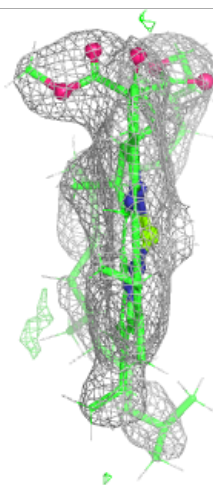
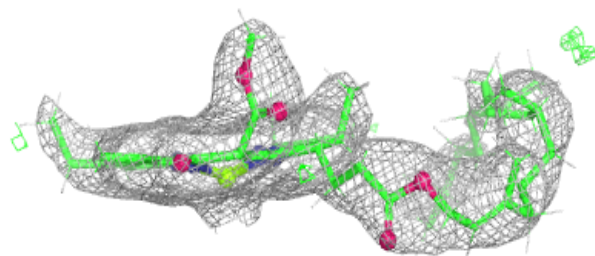
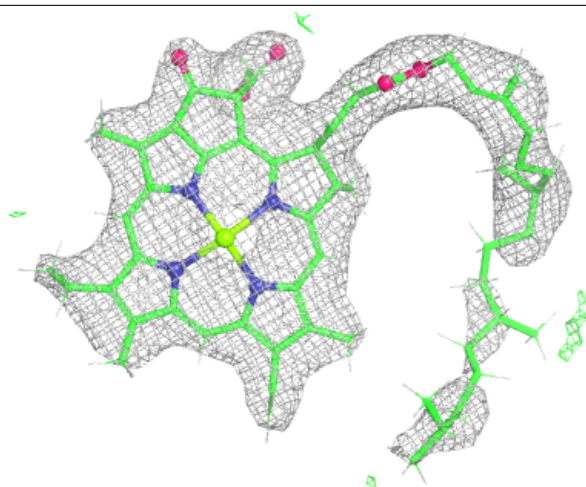
Electron density around BCR I 101:

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



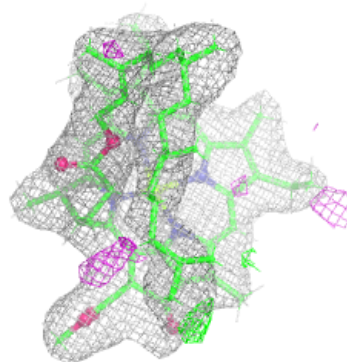
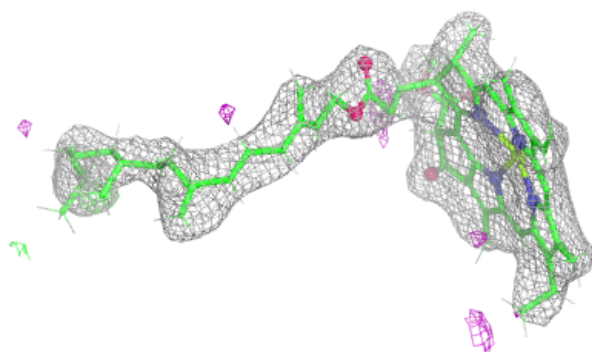
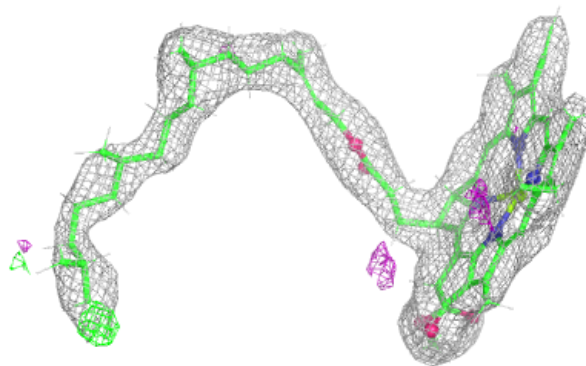
Electron density around CLA C 512:

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

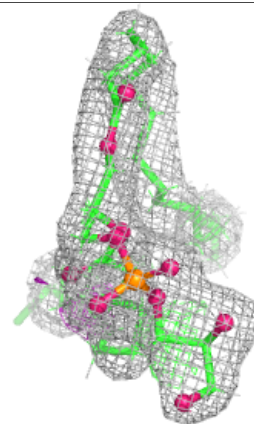
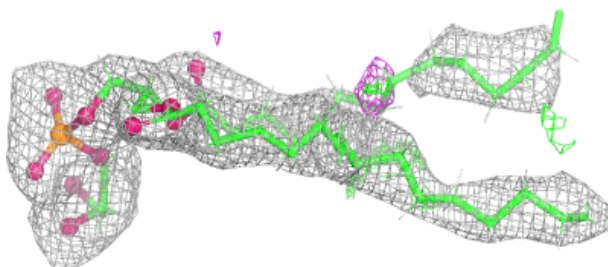
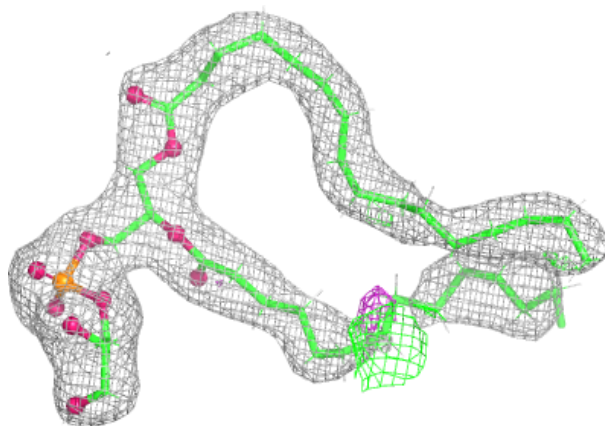


Electron density around CLA b 606:

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

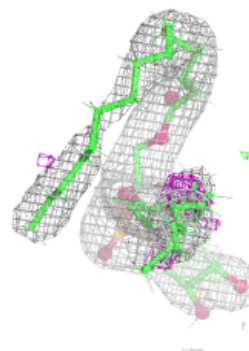
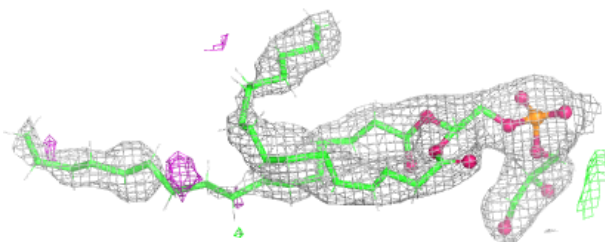
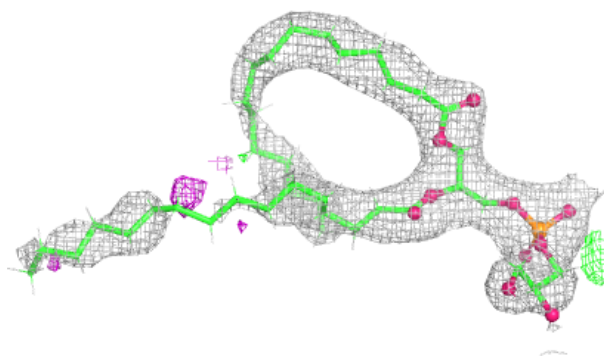
**Electron density around LHG D 411:**

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

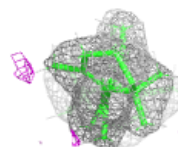
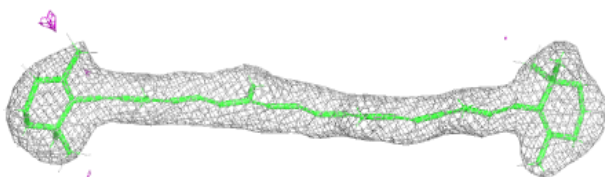
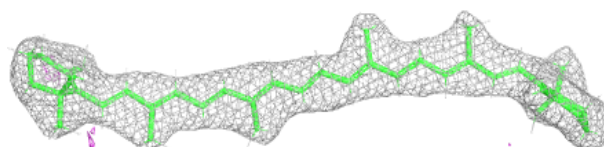


Electron density around LHG a 410:

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

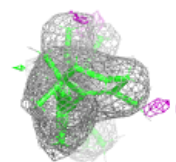
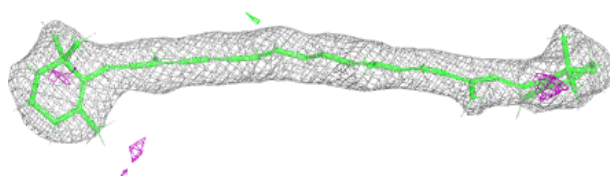
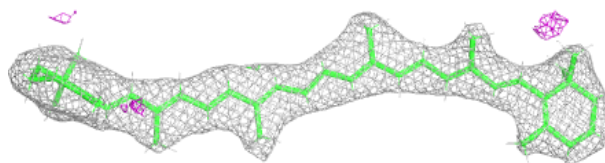
**Electron density around BCR a 405:**

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

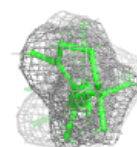
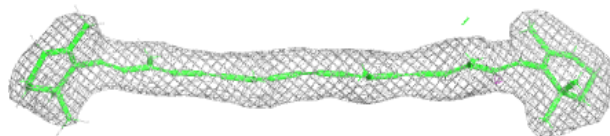
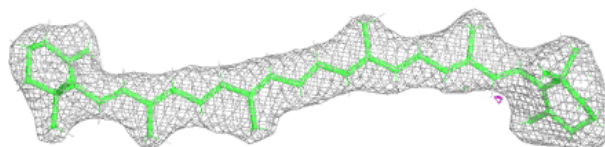


Electron density around BCR B 617:

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

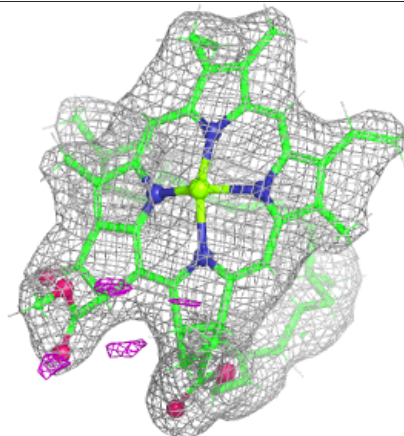
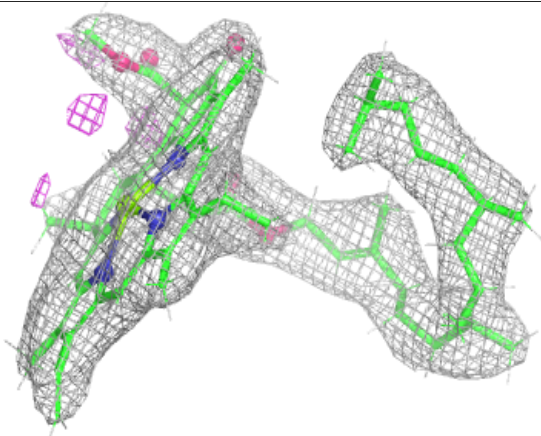
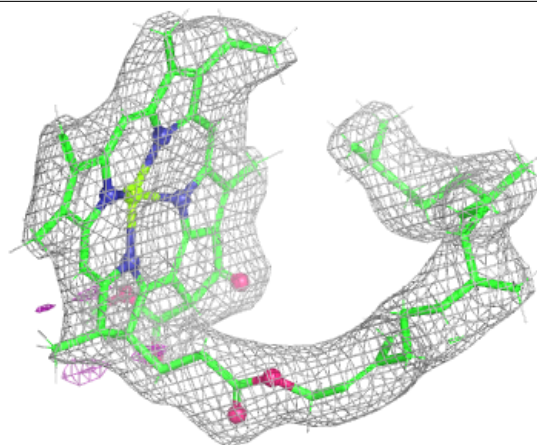
**Electron density around BCR b 618:**

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



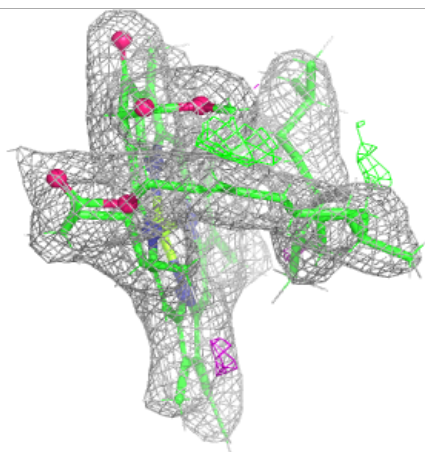
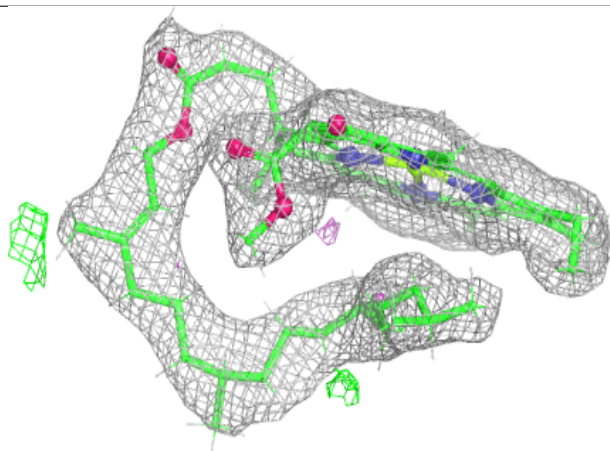
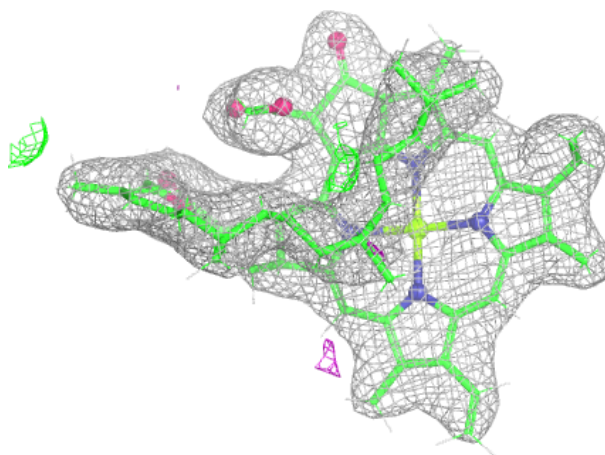
Electron density around CLA c 503:

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



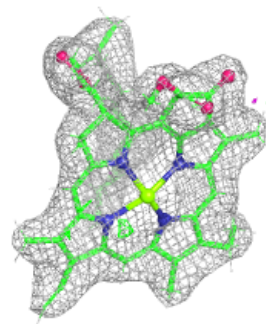
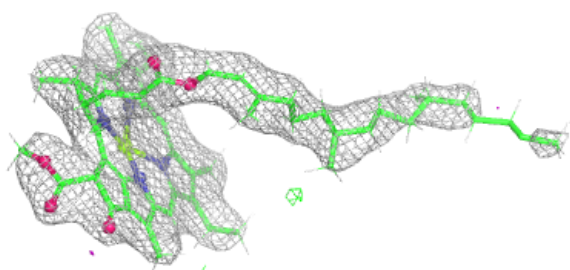
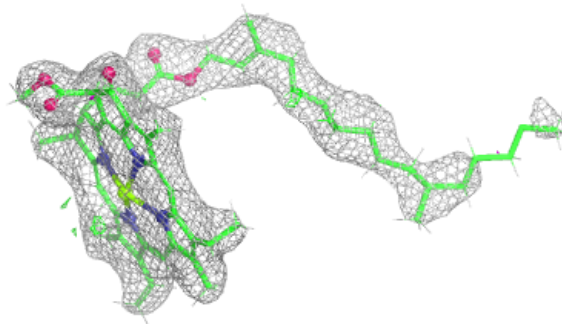
Electron density around CLA C 510:

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

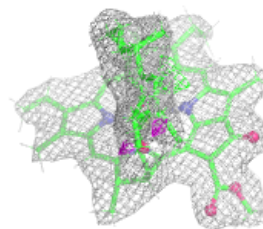
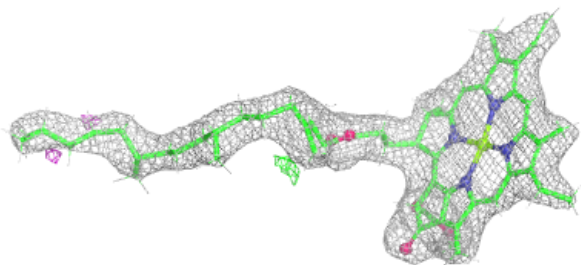
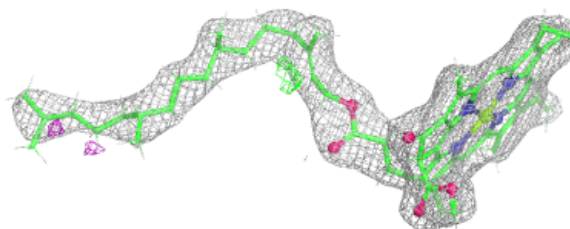


Electron density around CLA c 508:

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

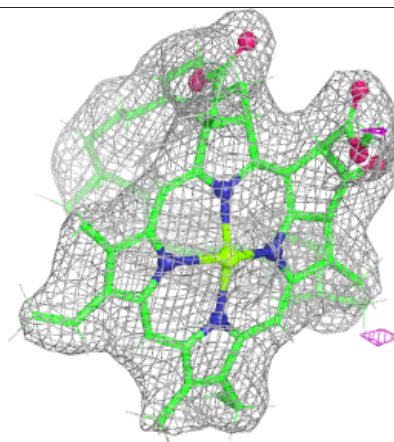
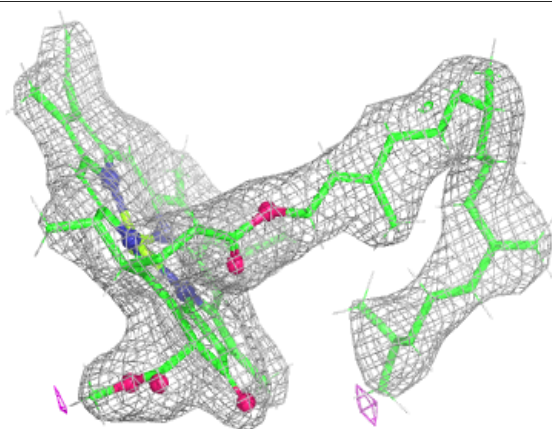
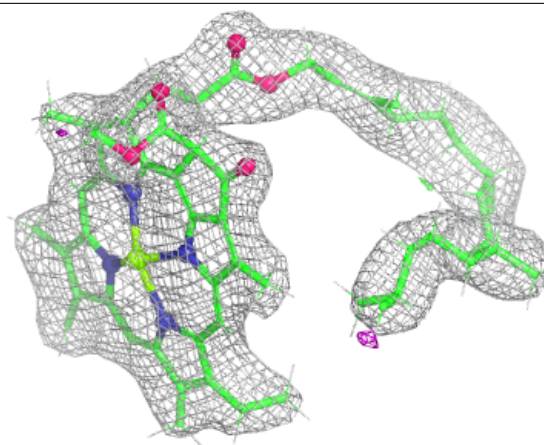
**Electron density around CLA c 502:**

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

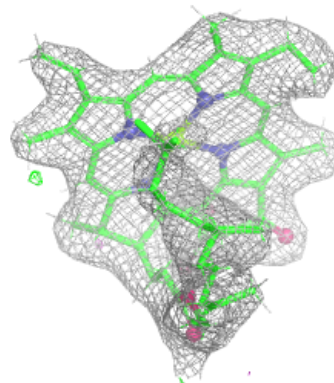
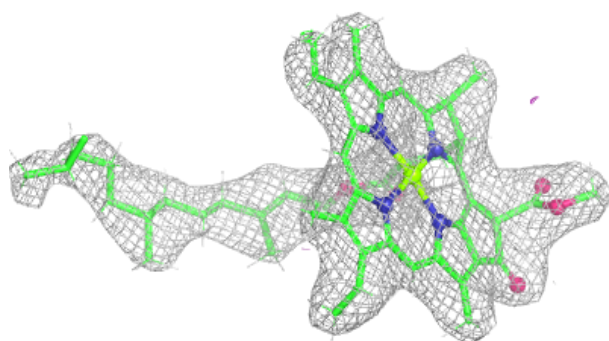
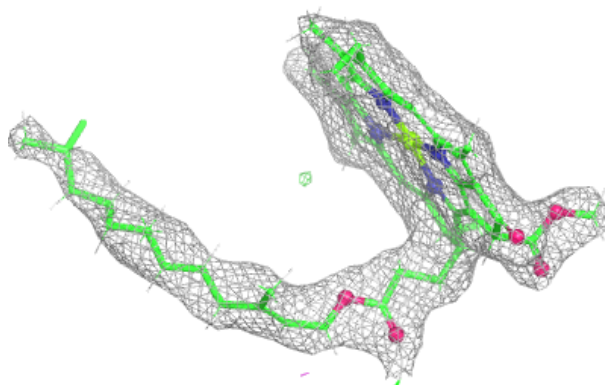


Electron density around CLA C 503:

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

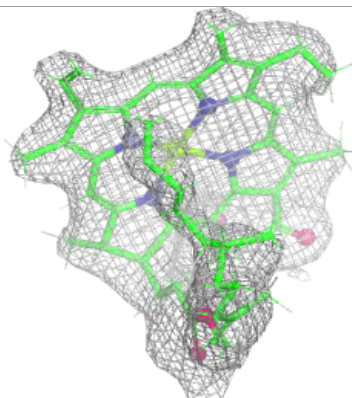
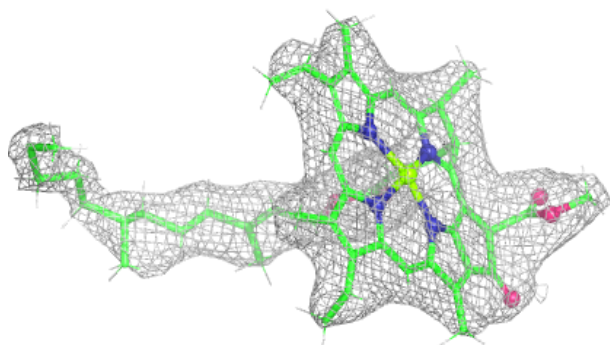
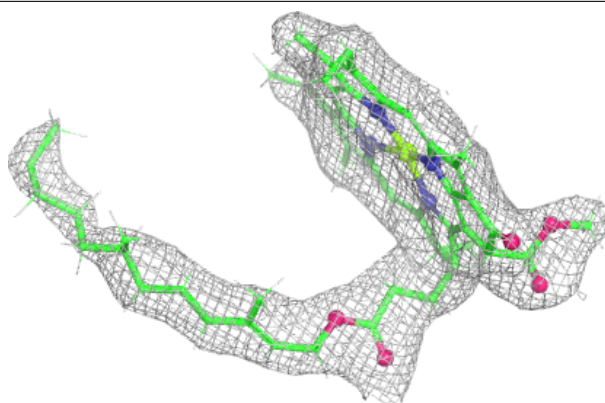
**Electron density around CLA c 504:**

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

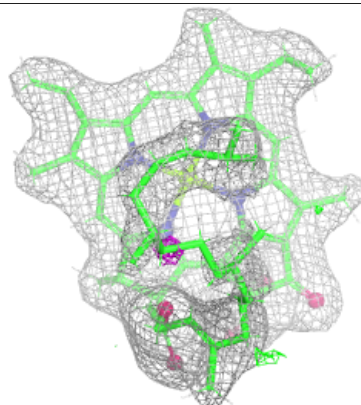
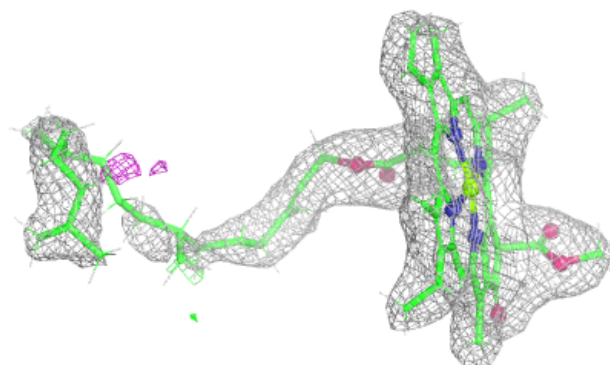
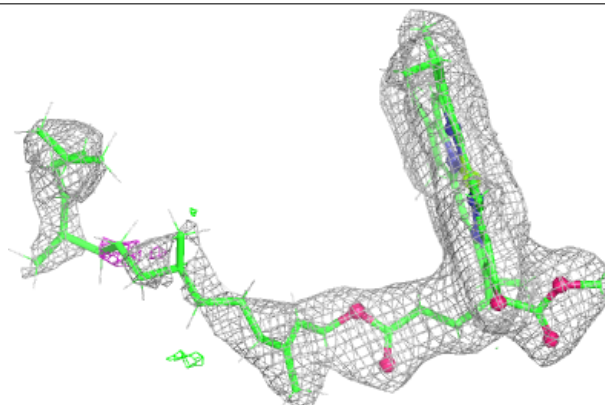


Electron density around CLA C 504:

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

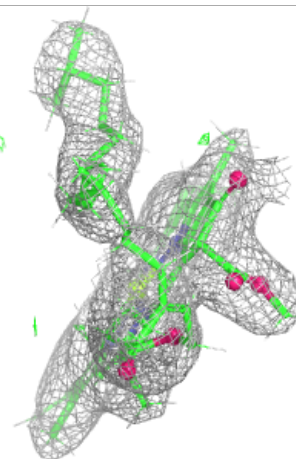
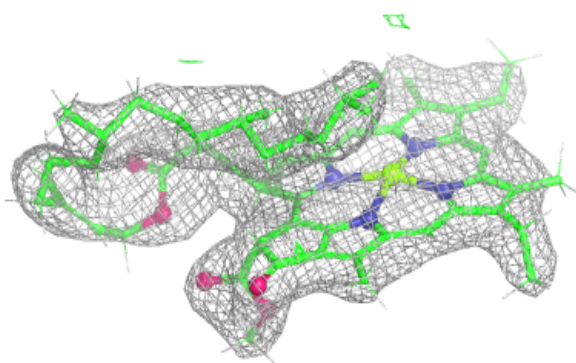
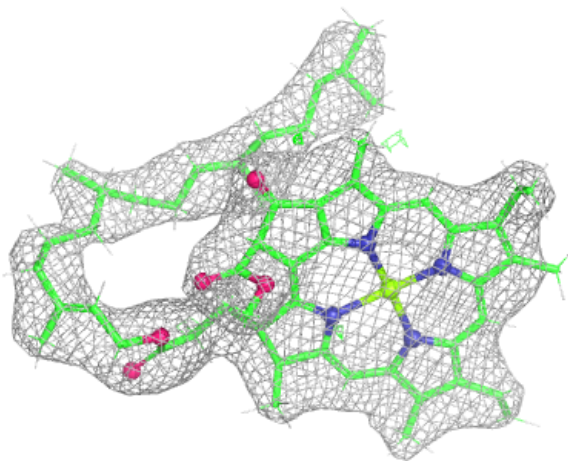
**Electron density around CLA C 506:**

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



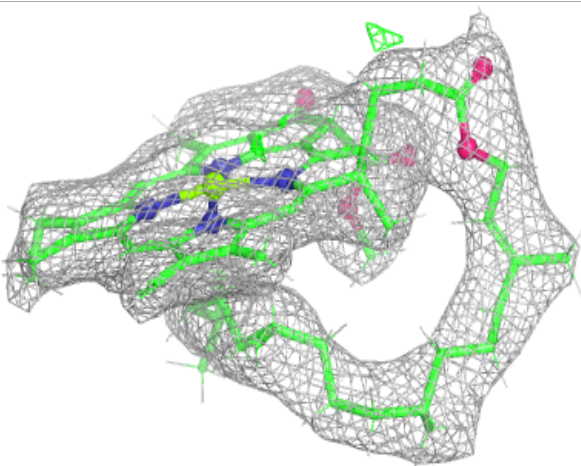
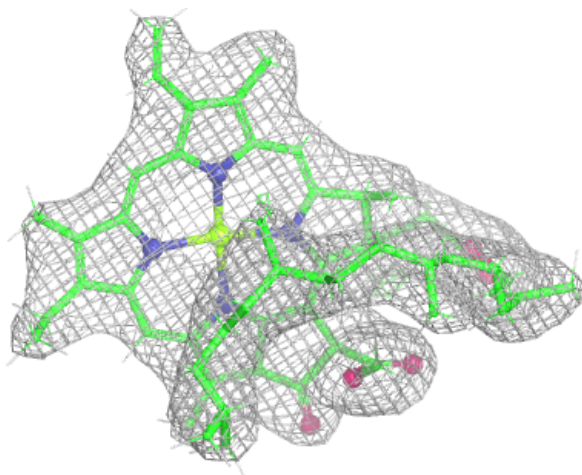
Electron density around CLA c 509:

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



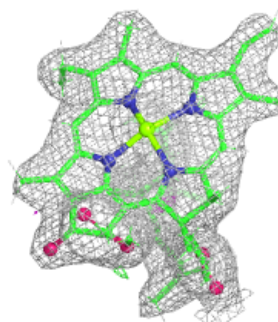
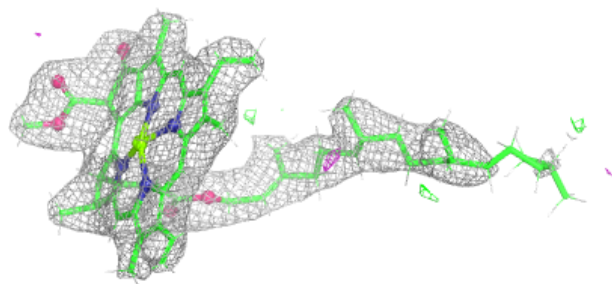
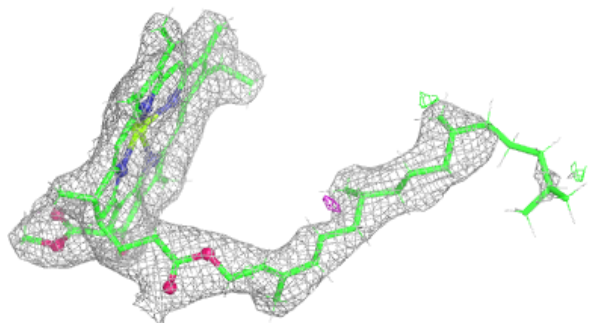
Electron density around CLA c 510:

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

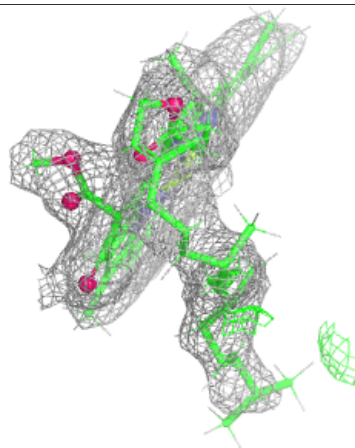
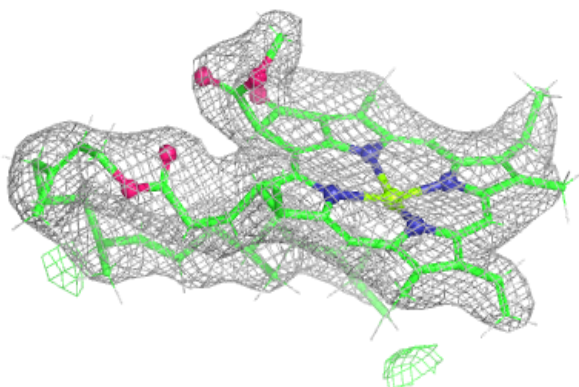
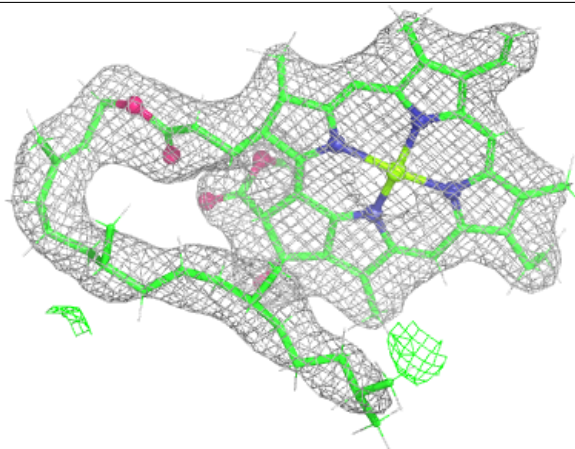


Electron density around CLA C 508:

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

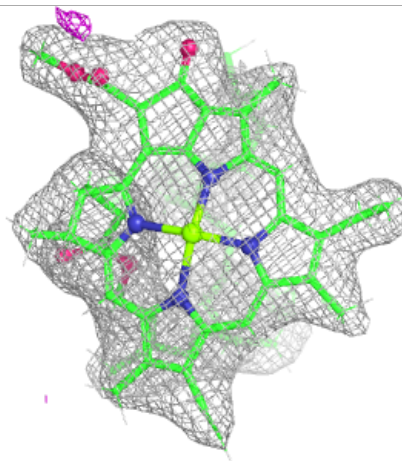
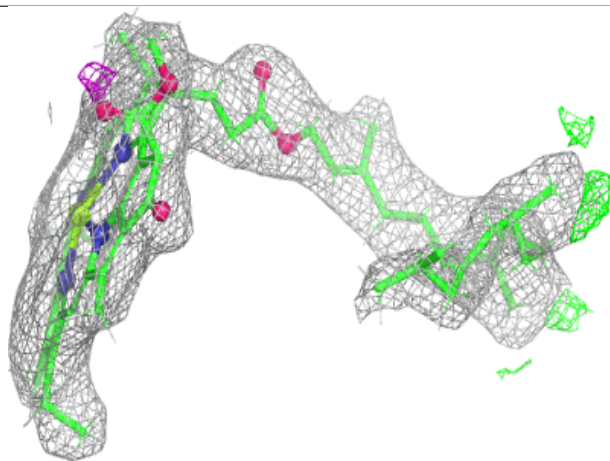
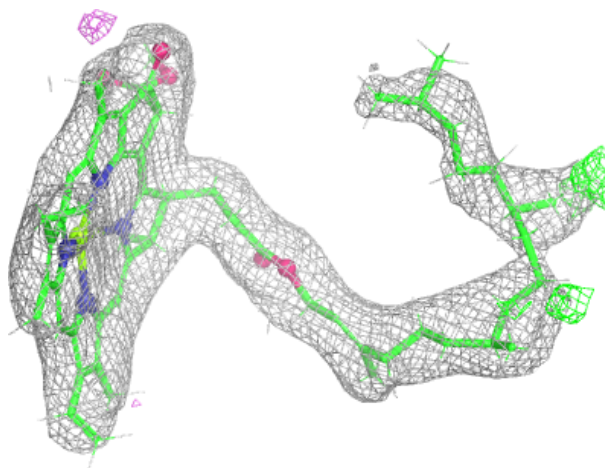
**Electron density around CLA C 509:**

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



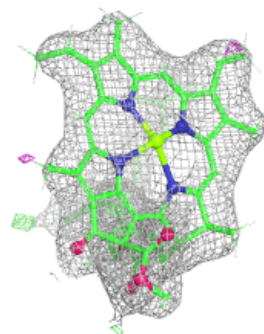
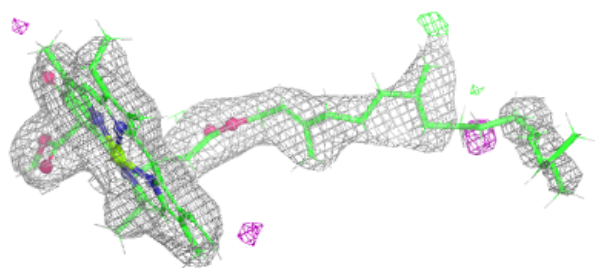
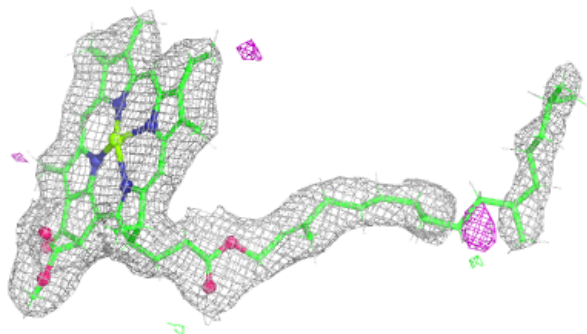
Electron density around CLA B 606:

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



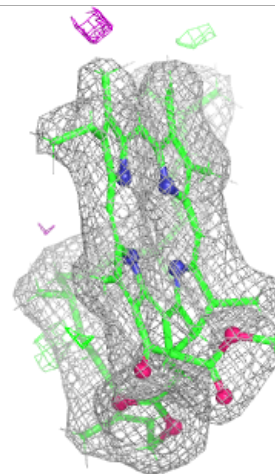
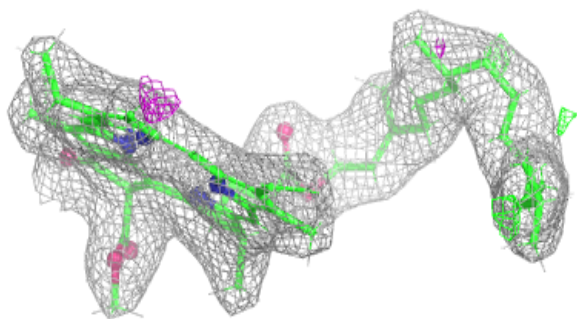
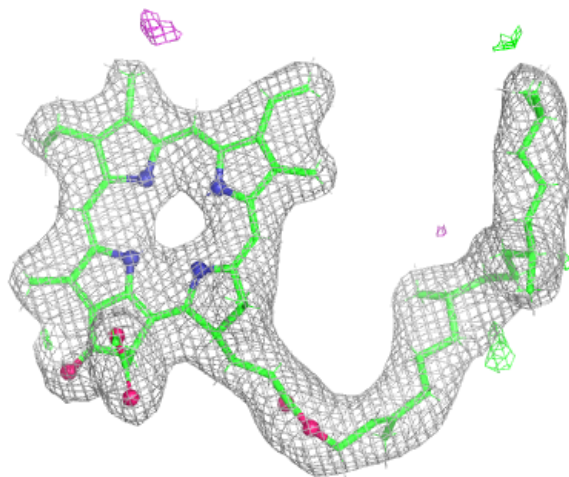
Electron density around CLA d 405:

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



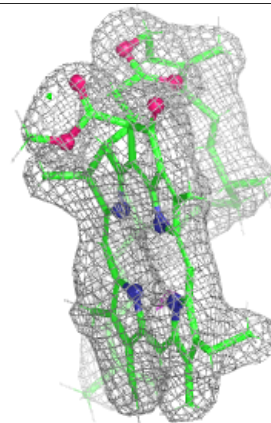
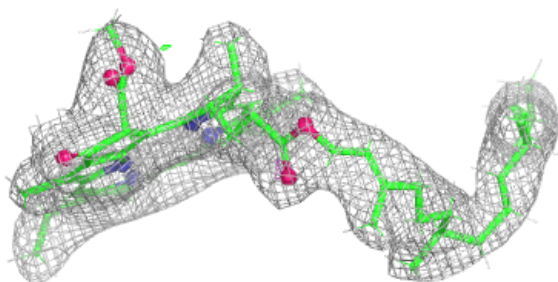
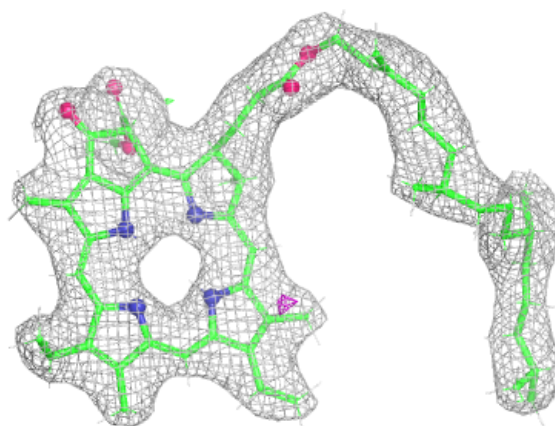
Electron density around PHO D 401:

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

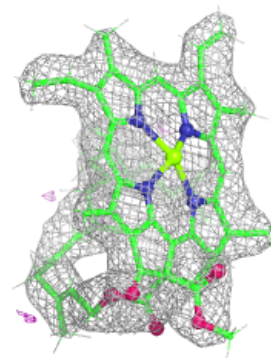
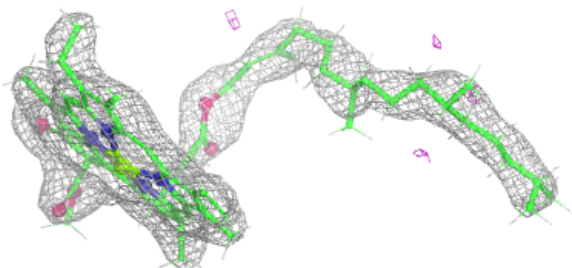
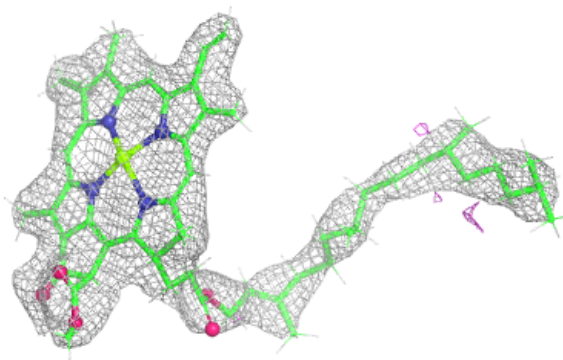


Electron density around PHO d 402:

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

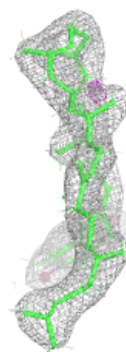
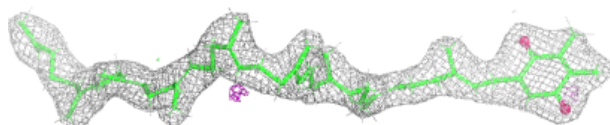
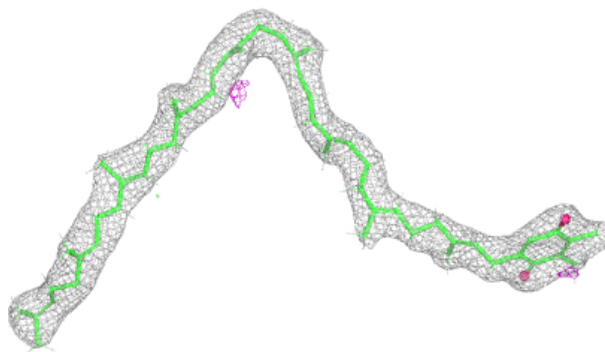
**Electron density around CLA C 511:**

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

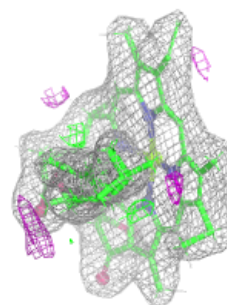
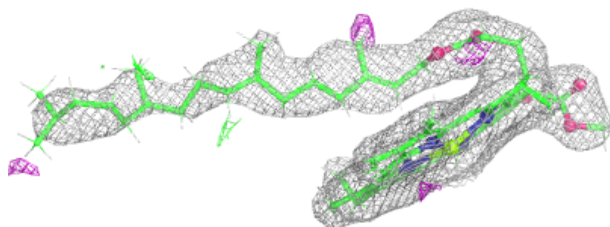
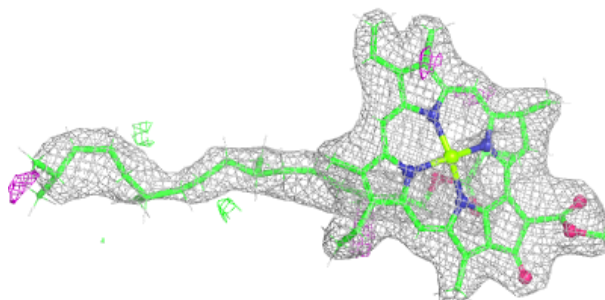


Electron density around PL9 D 407:

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

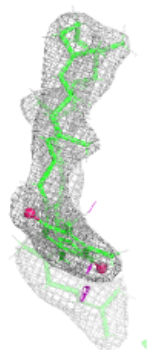
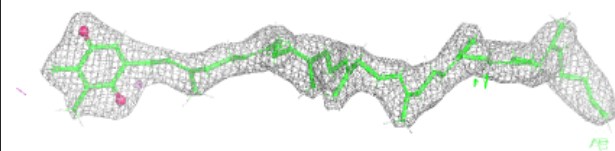
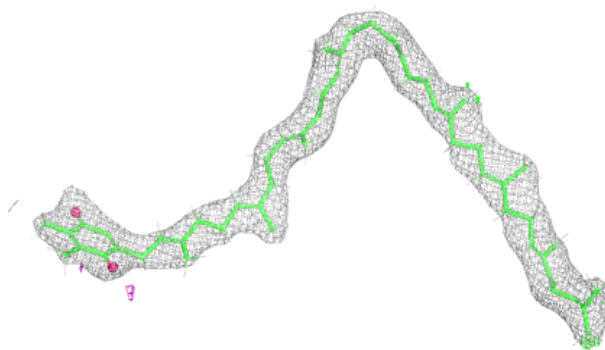
**Electron density around CLA B 614:**

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



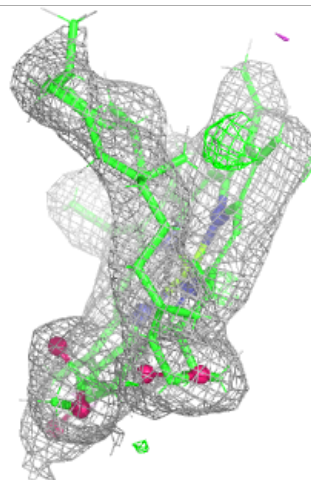
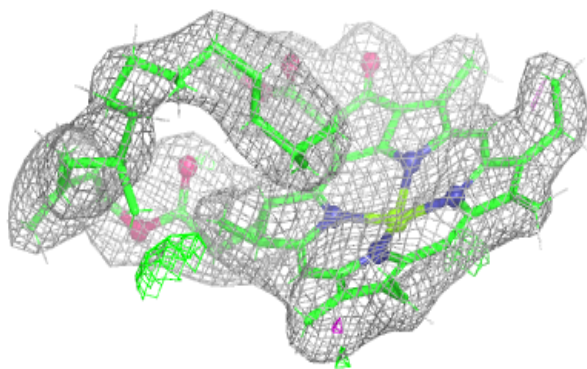
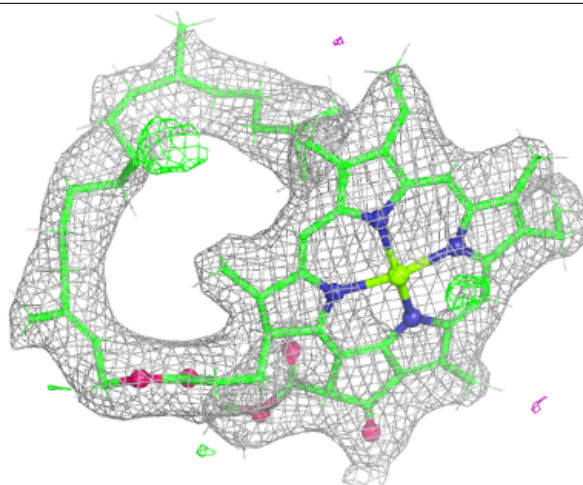
Electron density around PL9 d 407:

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



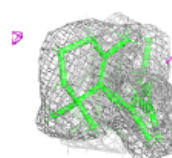
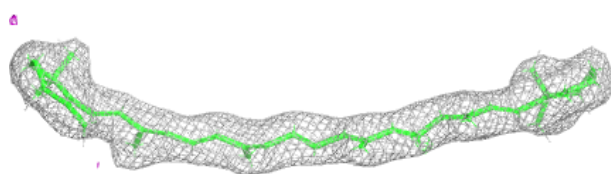
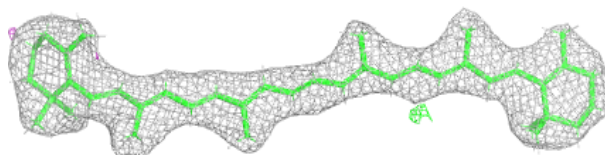
Electron density around CLA B 615:

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

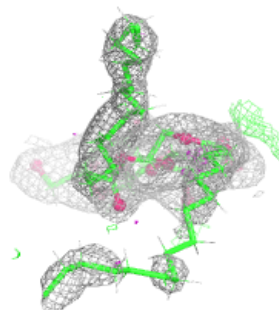
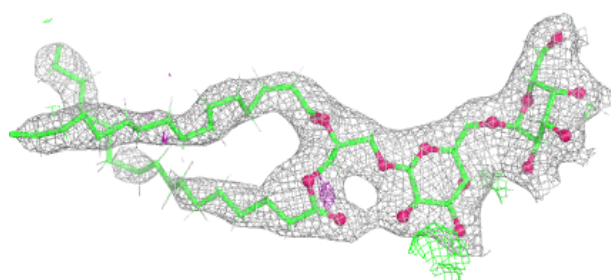
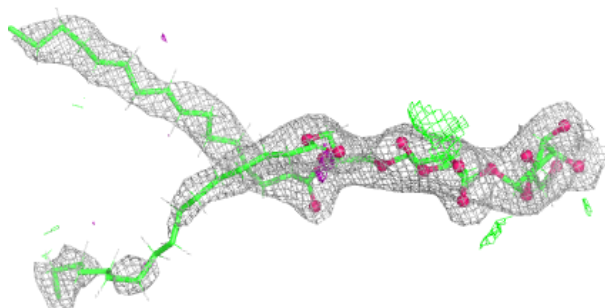


Electron density around BCR t 101:

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

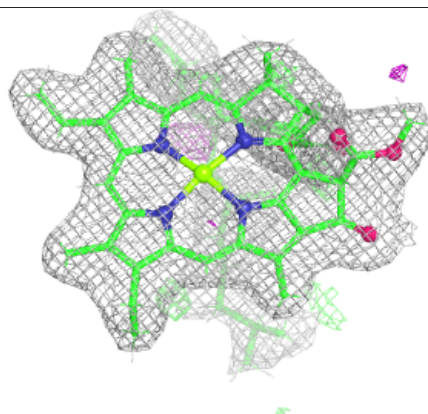
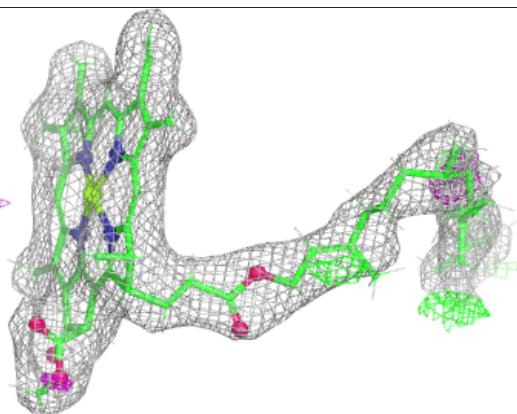
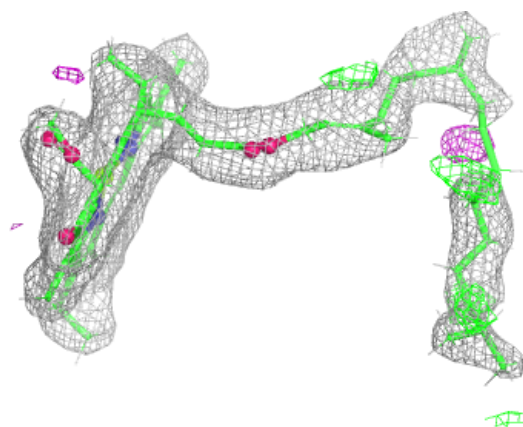
**Electron density around DGD C 515:**

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



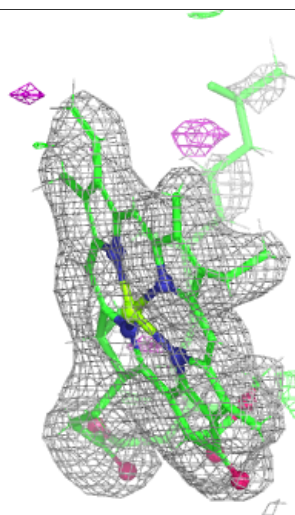
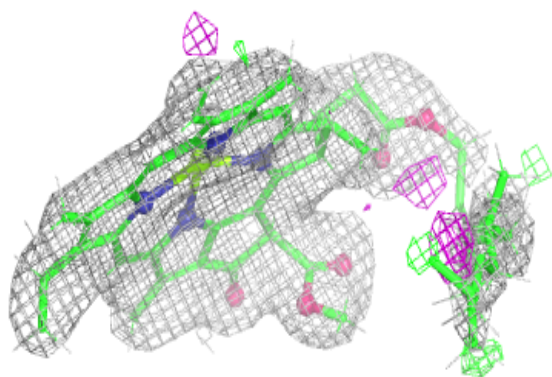
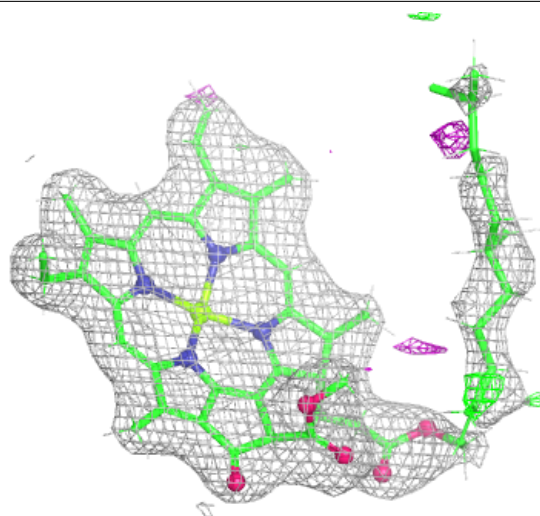
Electron density around CLA a 404:

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



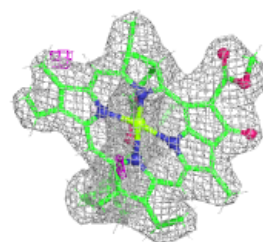
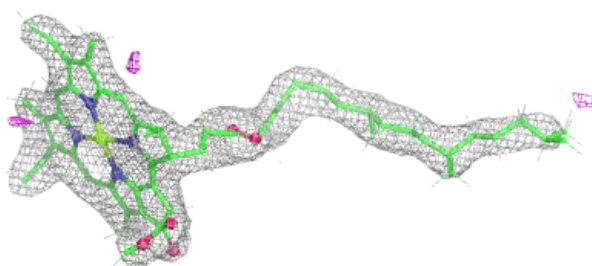
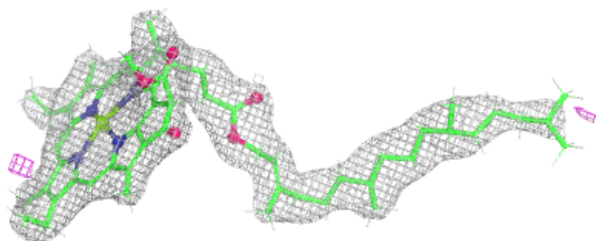
Electron density around CLA B 616:

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

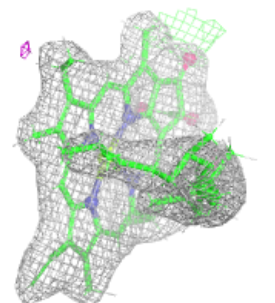
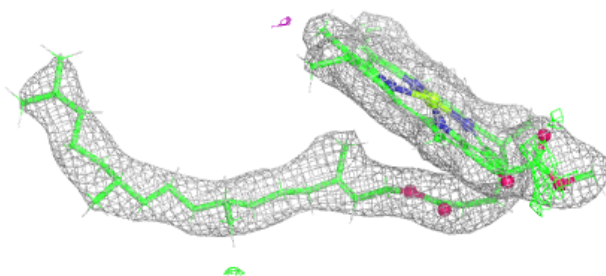
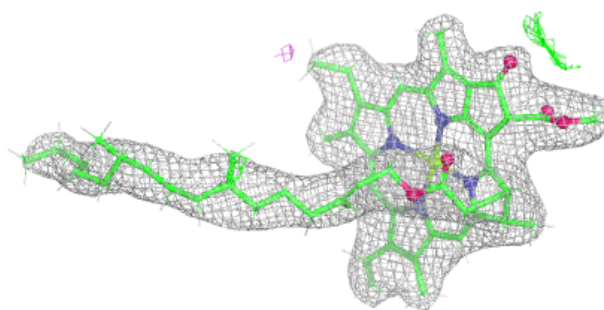


Electron density around CLA C 502:

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

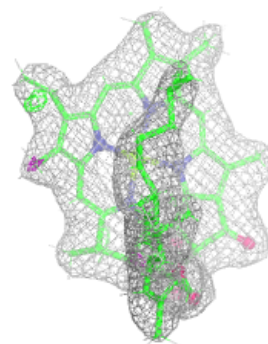
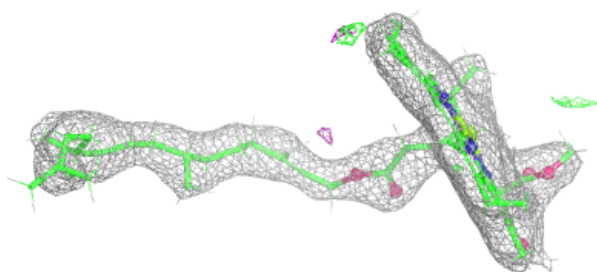
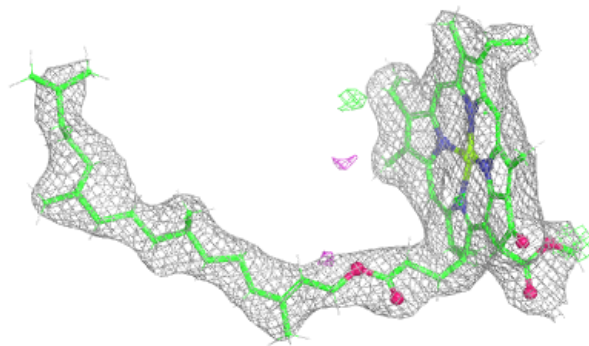
**Electron density around CLA b 608:**

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

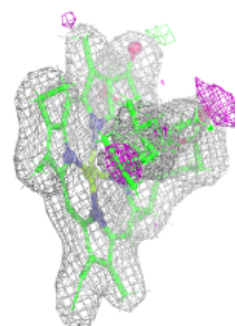
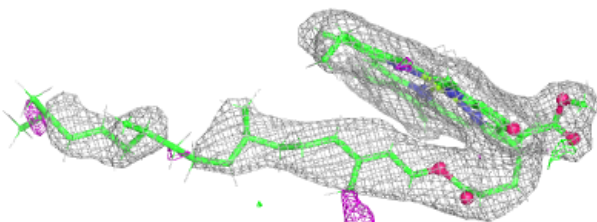
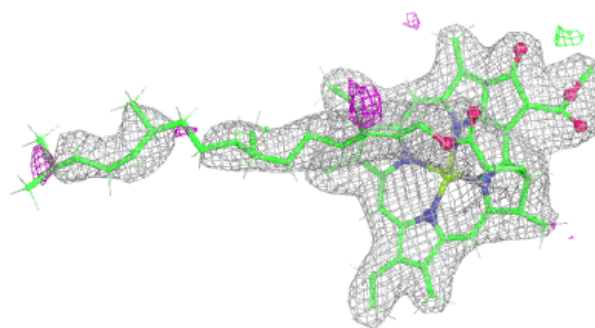


Electron density around CLA b 609:

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

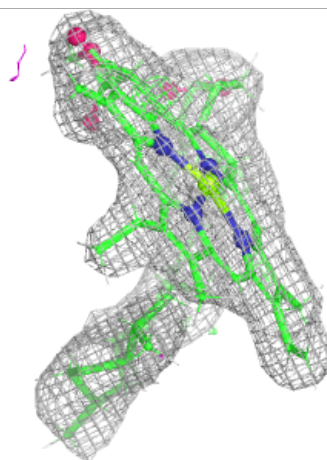
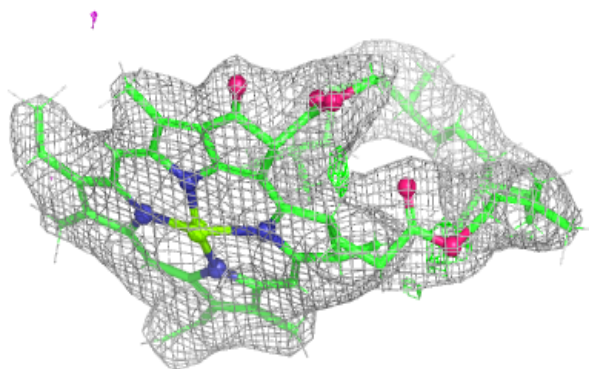
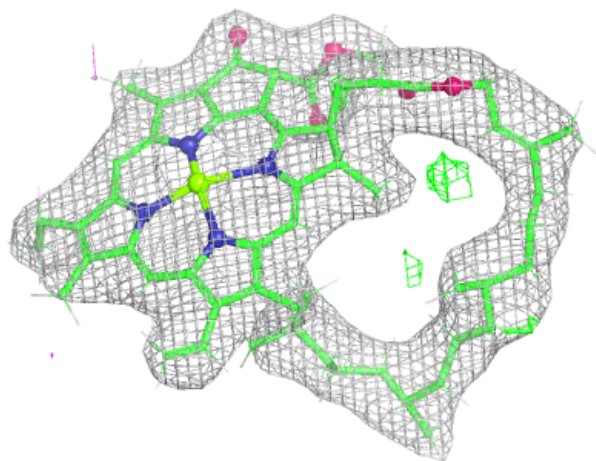
**Electron density around CLA b 614:**

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



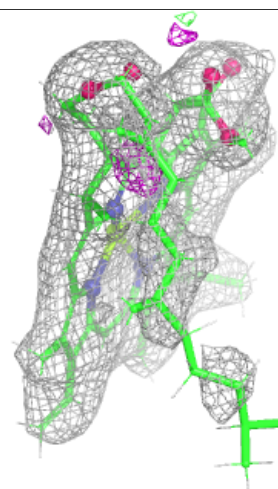
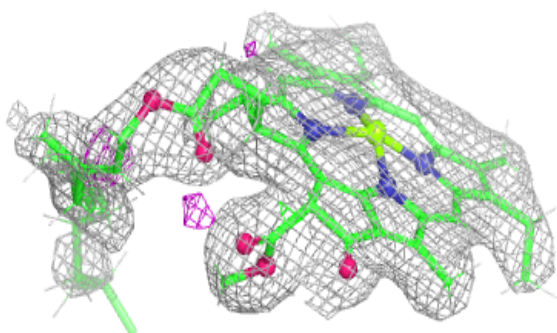
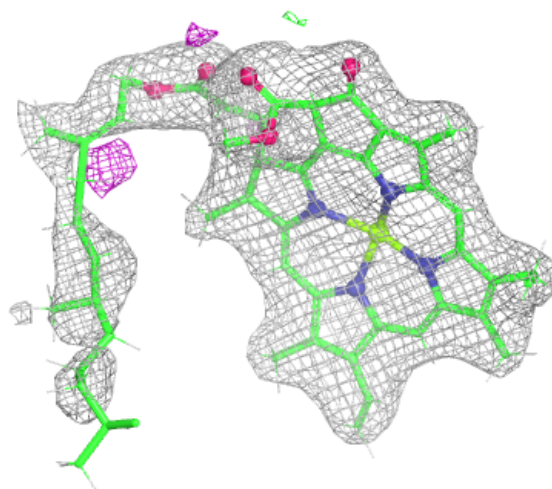
Electron density around CLA b 615:

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



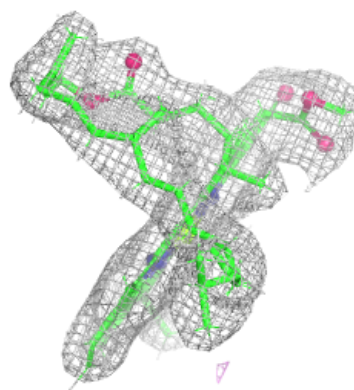
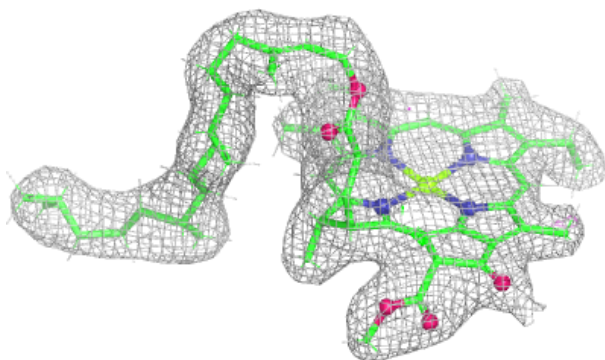
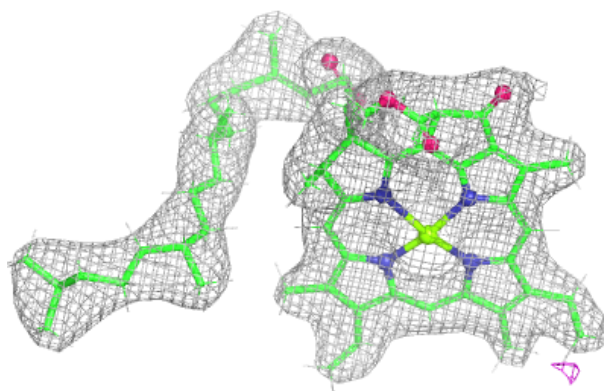
Electron density around CLA b 616:

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

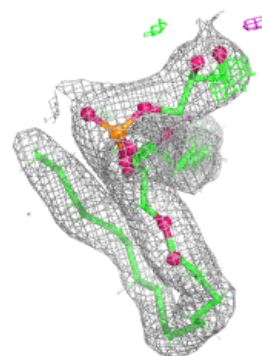
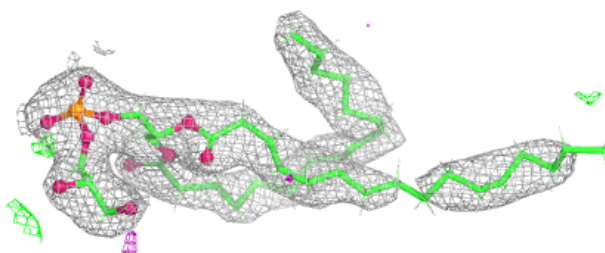
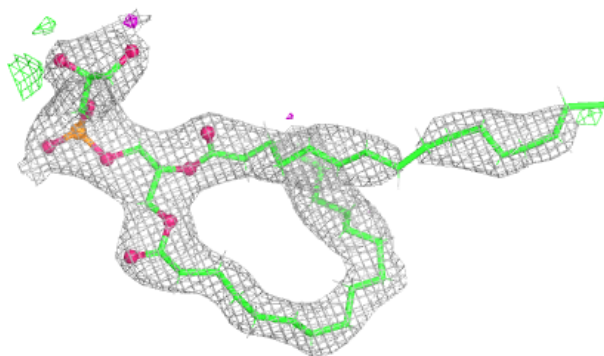


Electron density around CLA d 404:

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

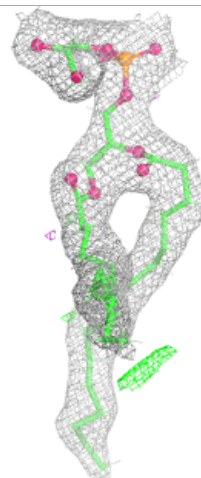
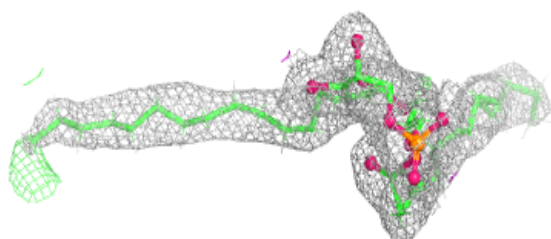
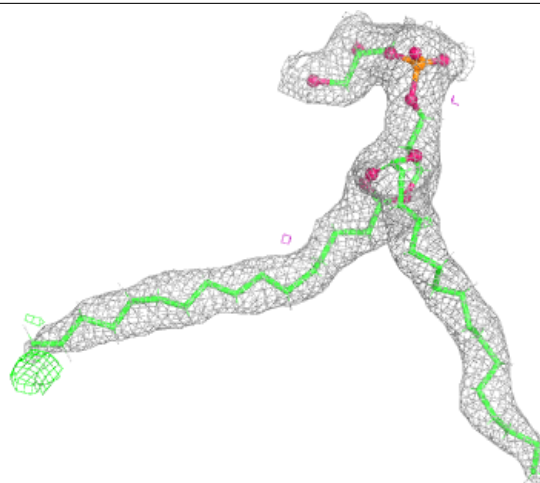
**Electron density around LHG D 413:**

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



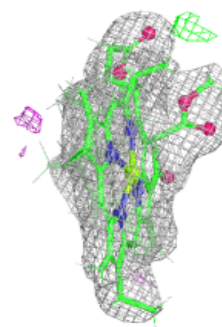
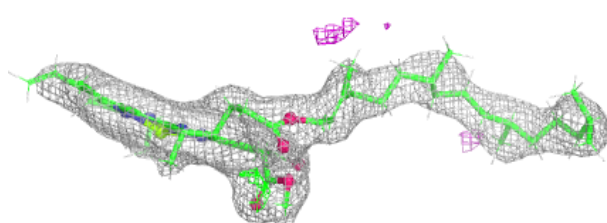
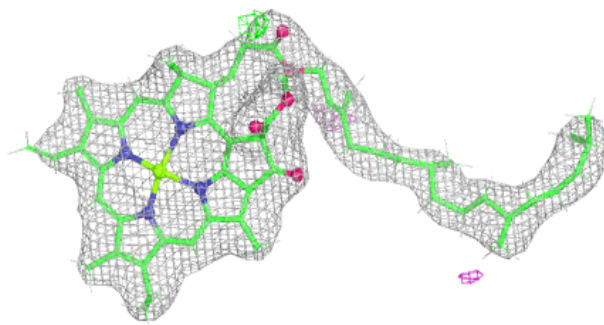
Electron density around LHG L 102:

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

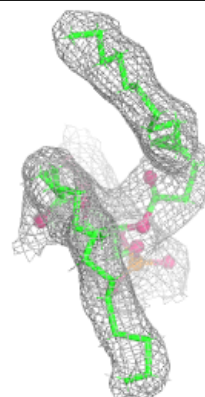
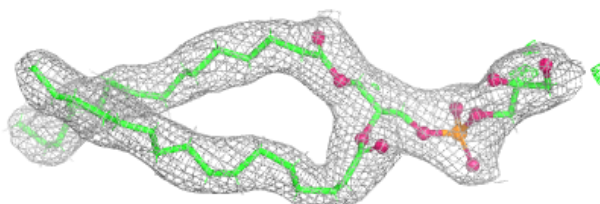
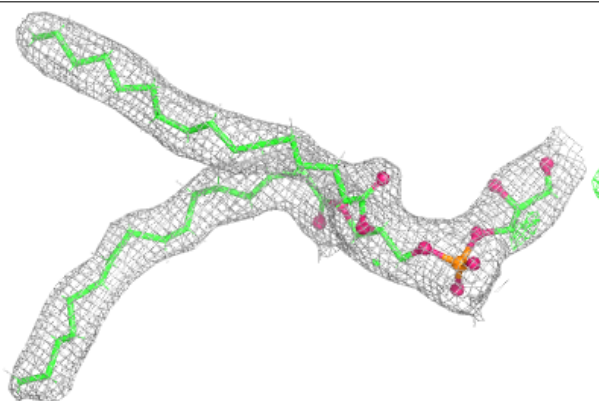


Electron density around CLA b 602:

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

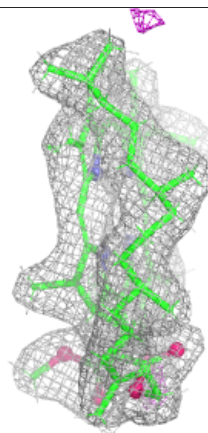
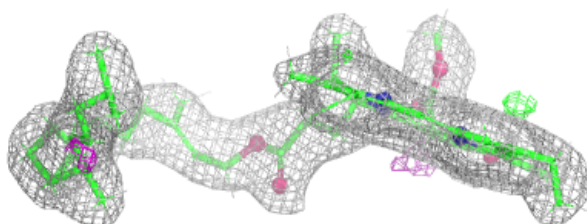
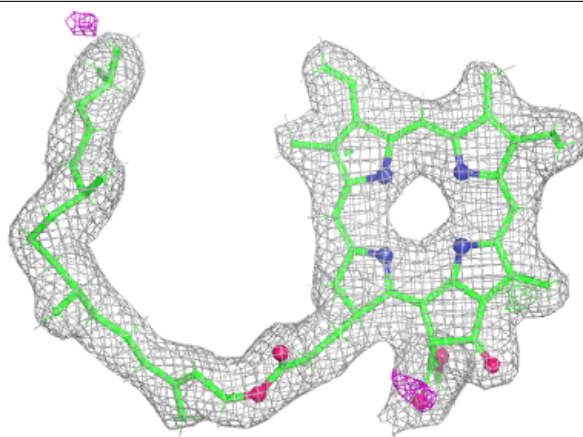
**Electron density around LHG d 408:**

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



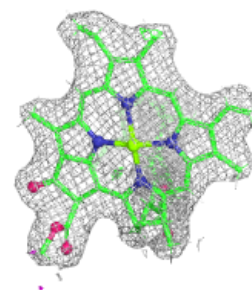
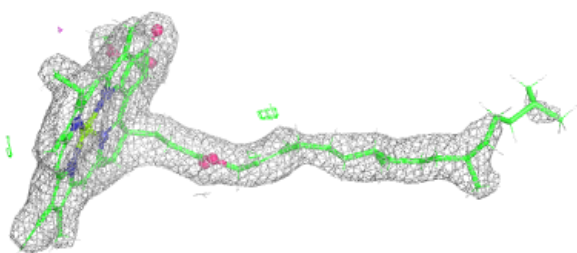
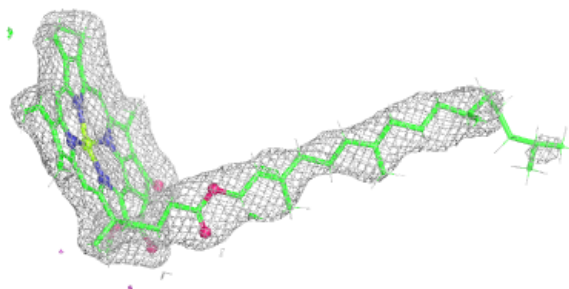
Electron density around PHO A 404:

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



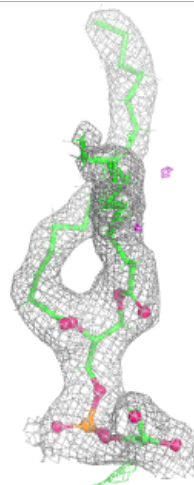
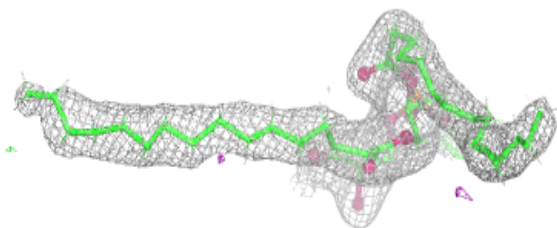
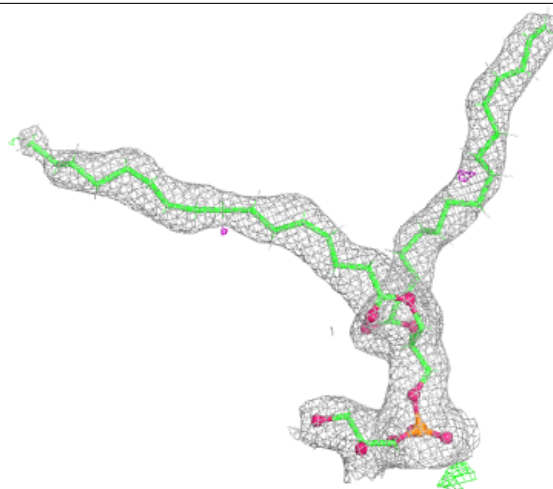
Electron density around CLA b 604:

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



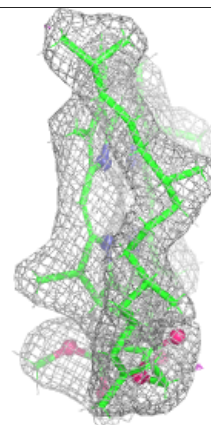
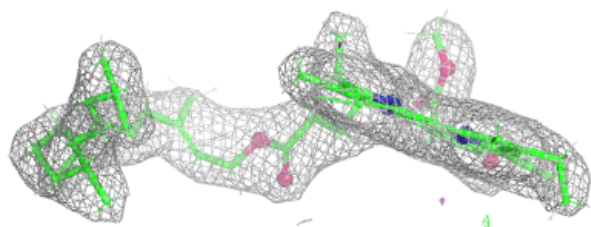
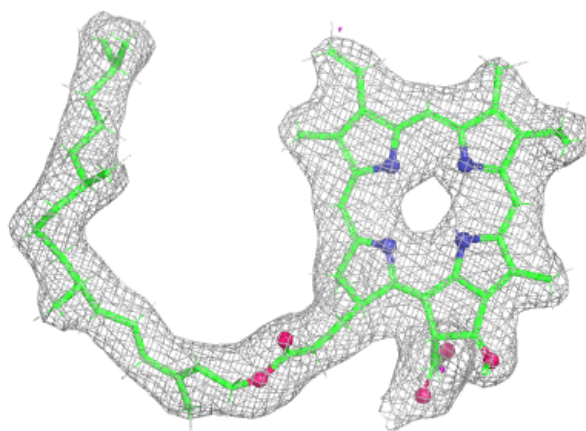
Electron density around LHG 1 101:

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

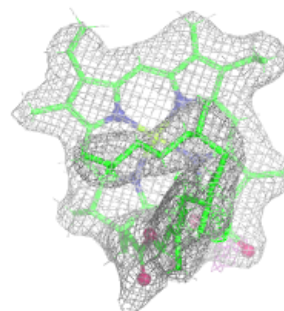
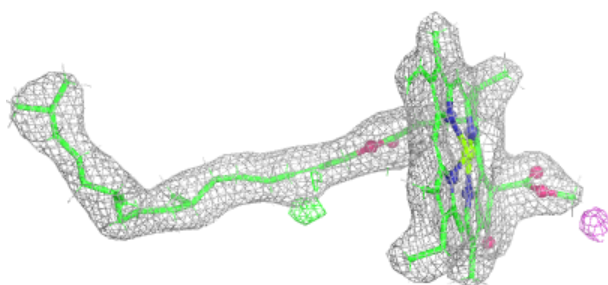
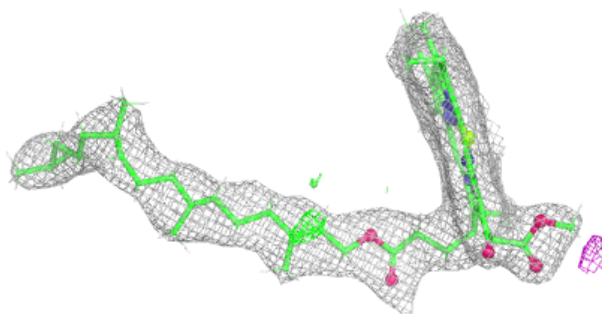


Electron density around PHO a 403:

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

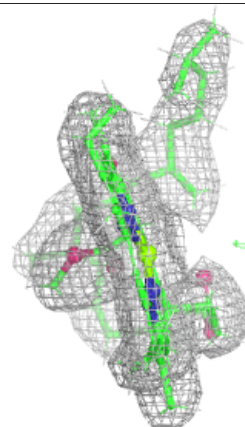
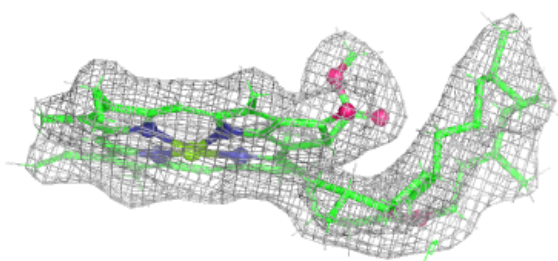
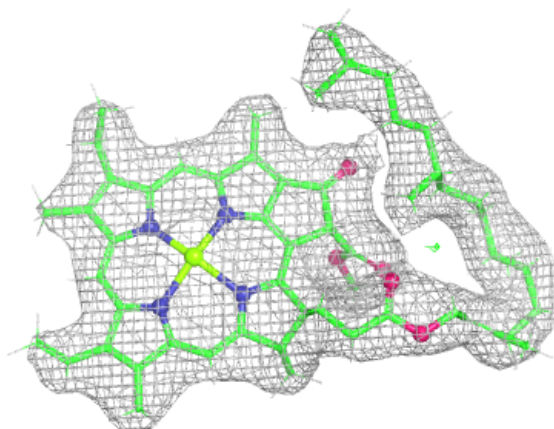
**Electron density around CLA b 605:**

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

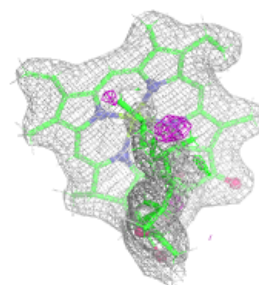
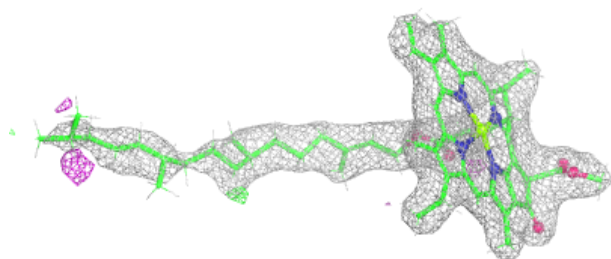
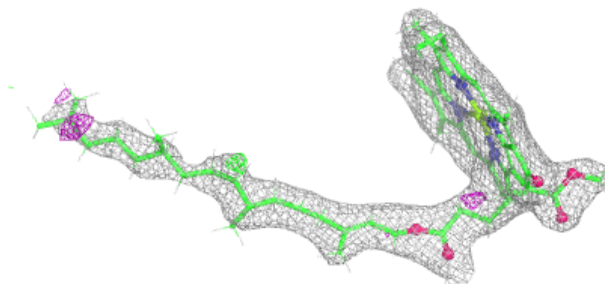


Electron density around CLA B 610:

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

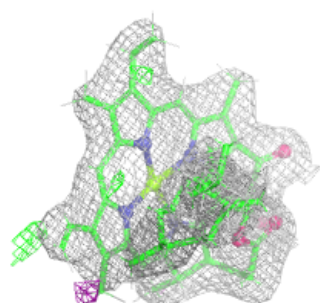
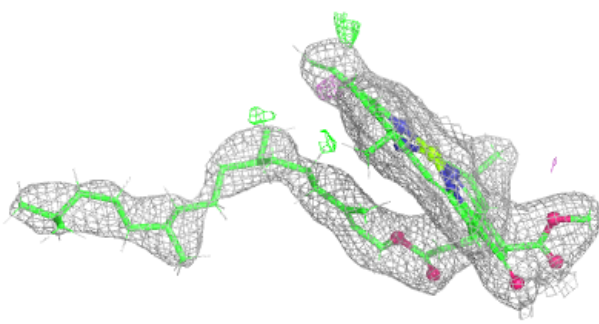
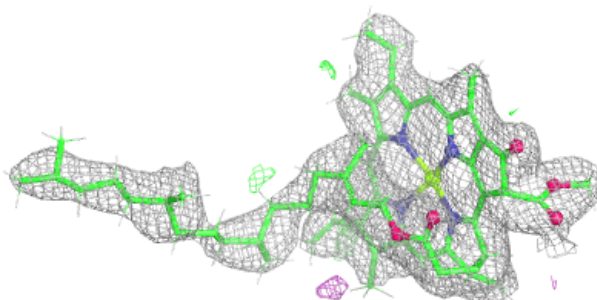
**Electron density around CLA b 607:**

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

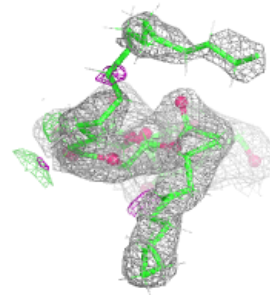
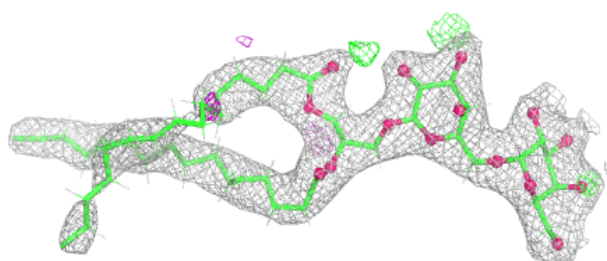
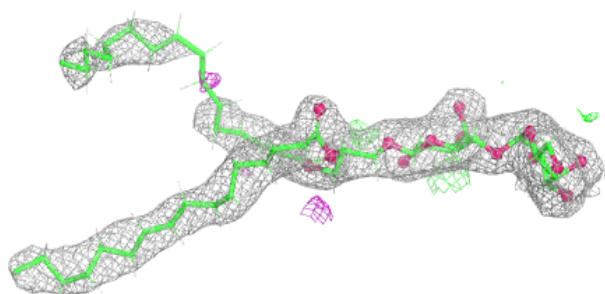


Electron density around CLA C 505:

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

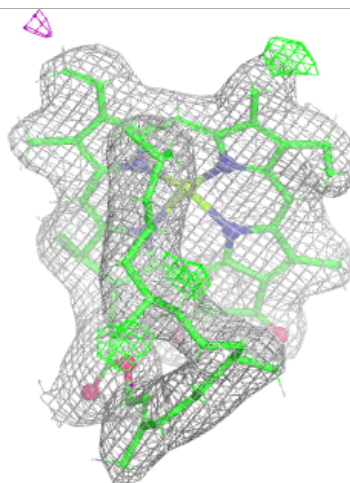
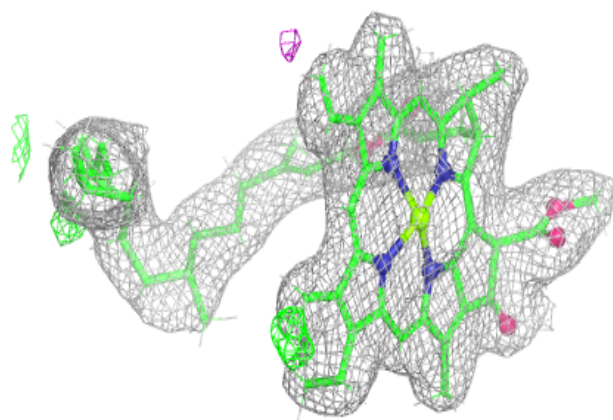
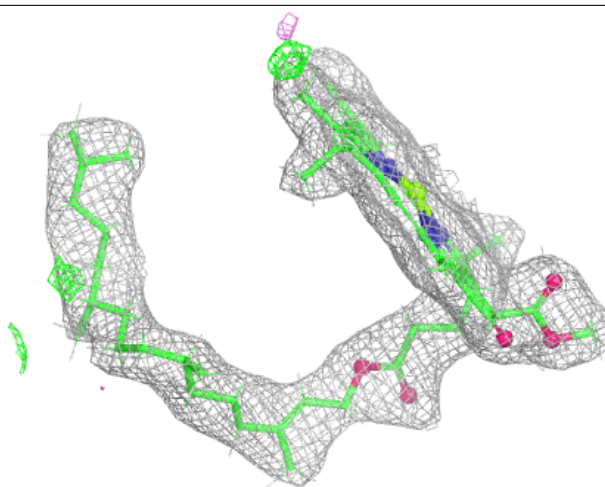
**Electron density around DGD c 516:**

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



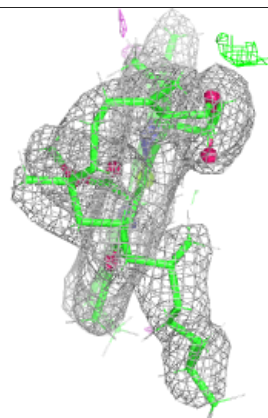
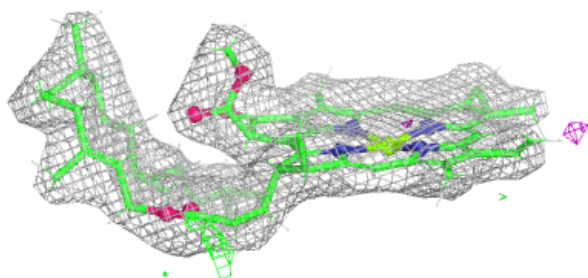
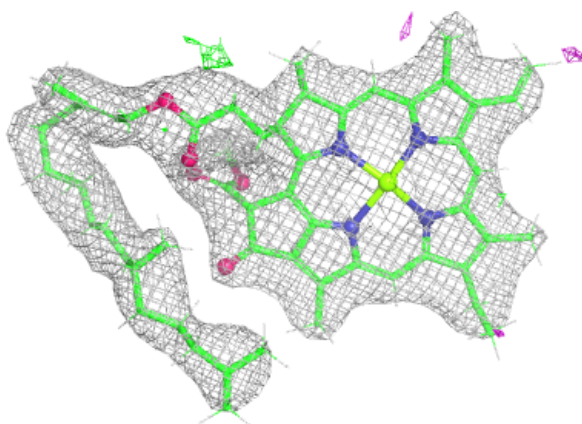
Electron density around CLA B 611:

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



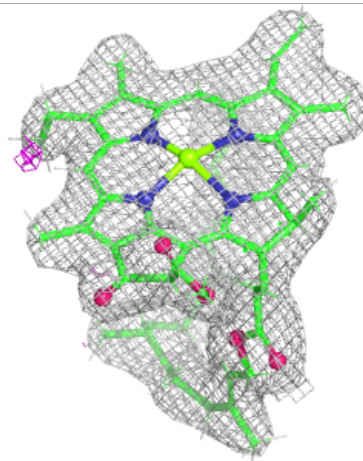
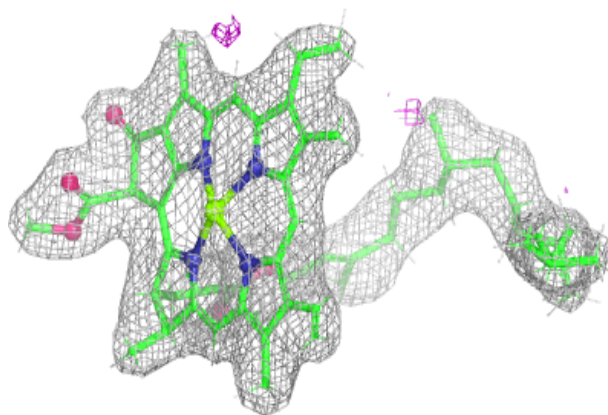
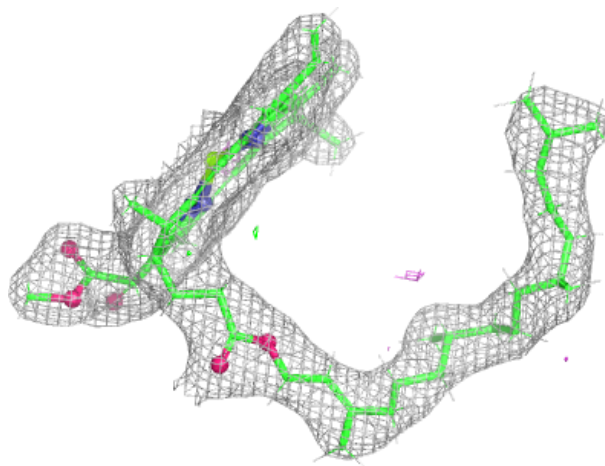
Electron density around CLA b 610:

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



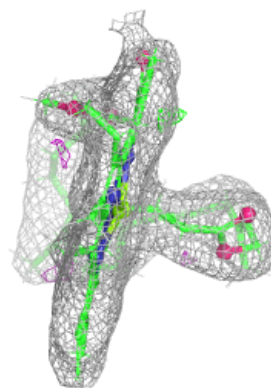
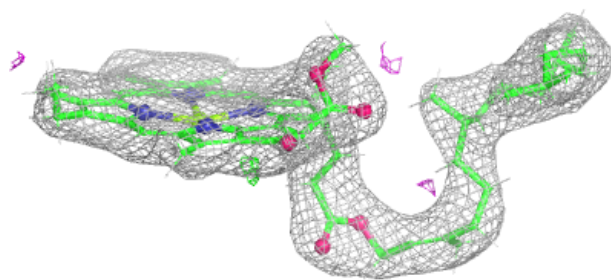
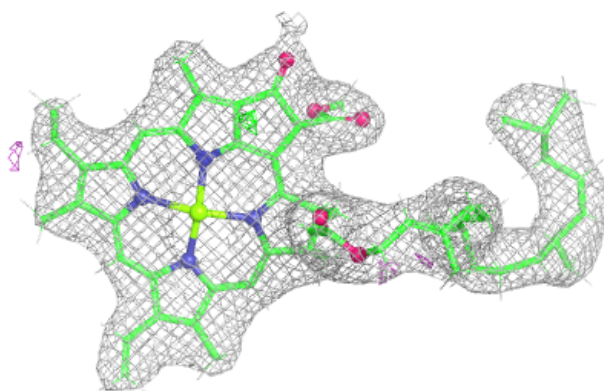
Electron density around CLA b 611:

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



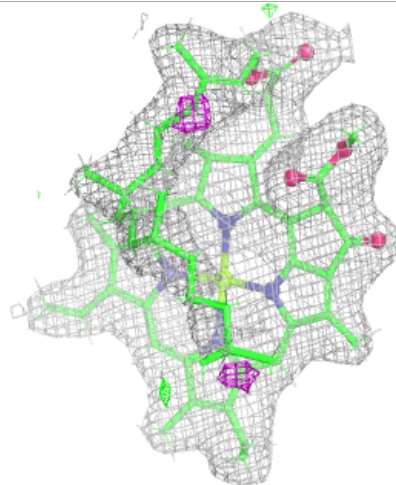
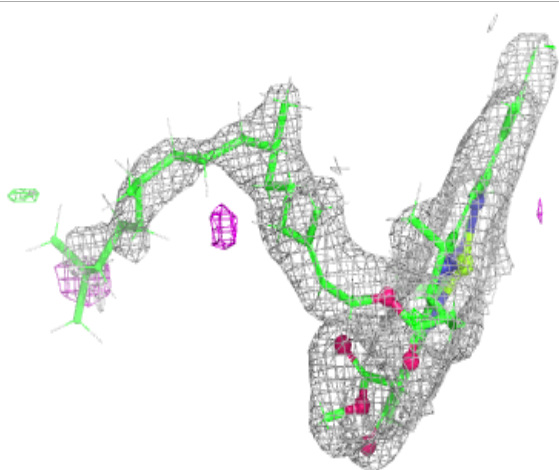
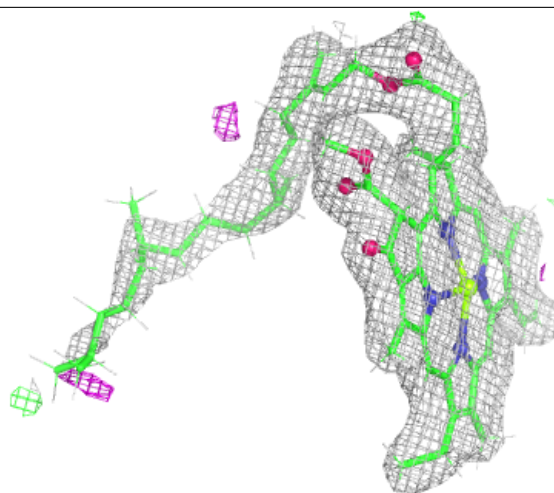
Electron density around CLA b 612:

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



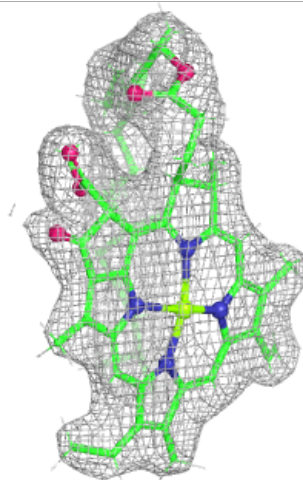
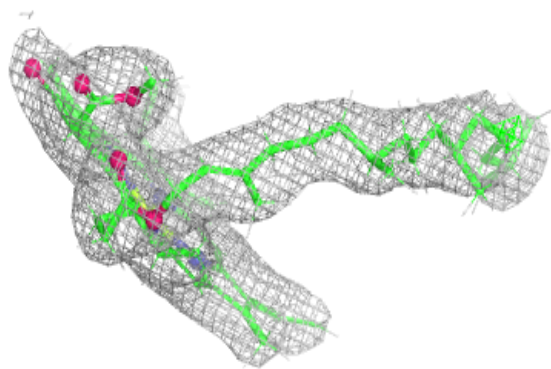
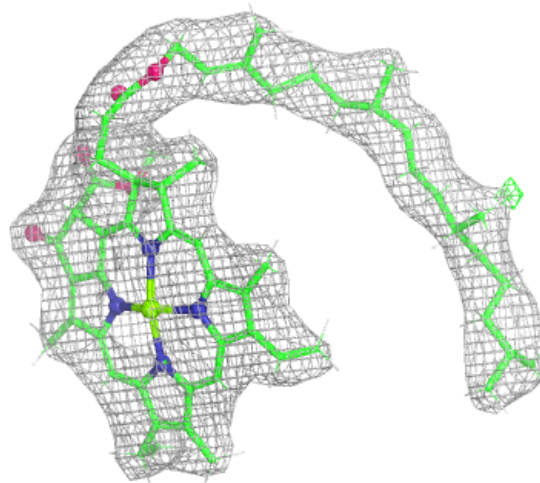
Electron density around CLA b 613:

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



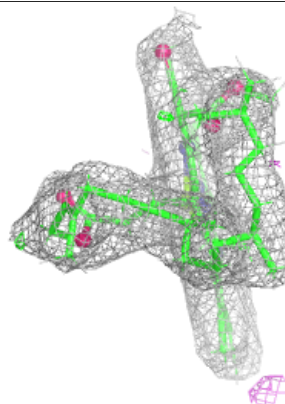
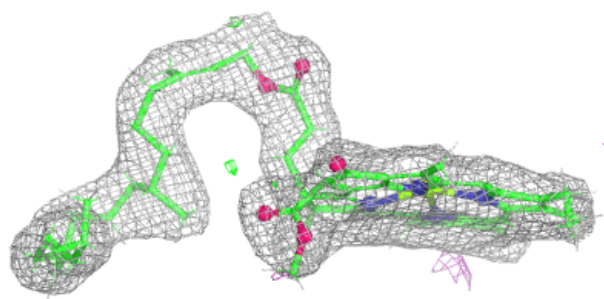
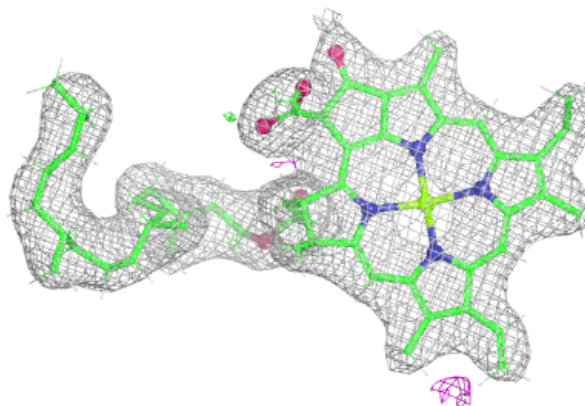
Electron density around CLA C 507:

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



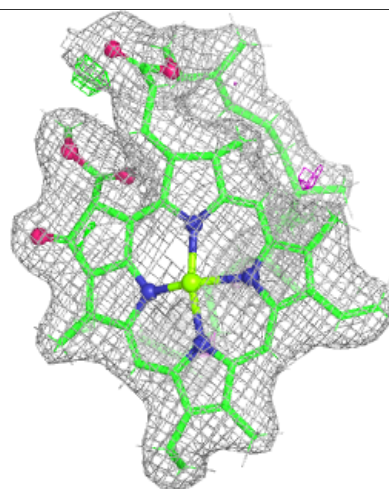
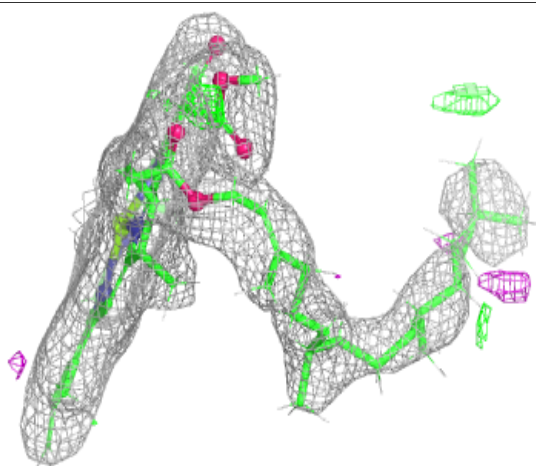
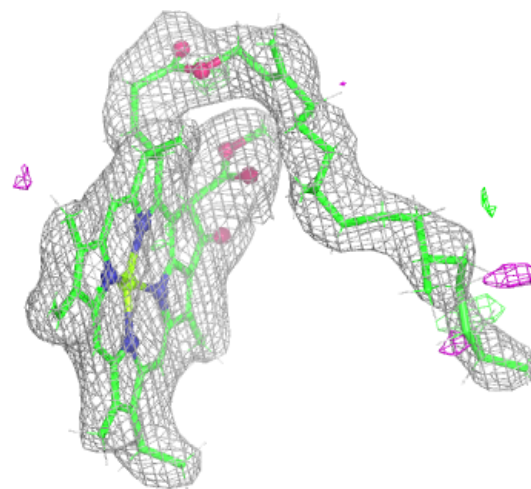
Electron density around CLA B 612:

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



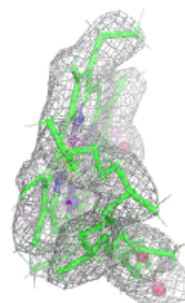
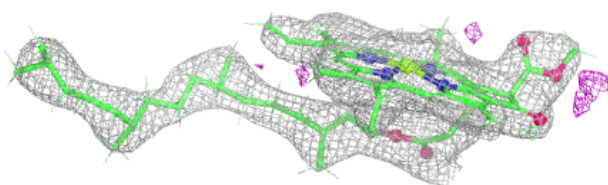
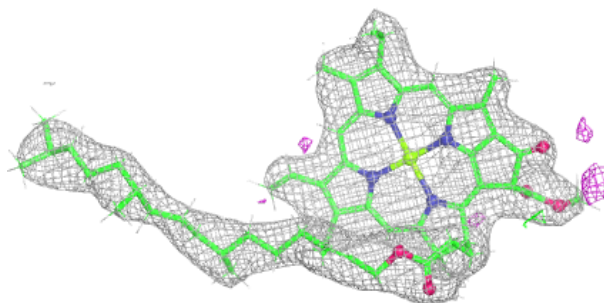
Electron density around CLA B 613:

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

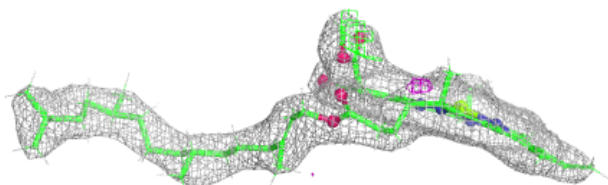
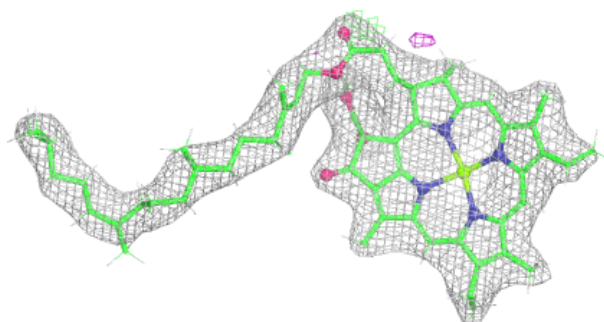


Electron density around CLA c 501:

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

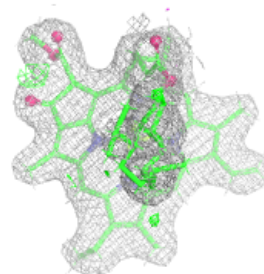
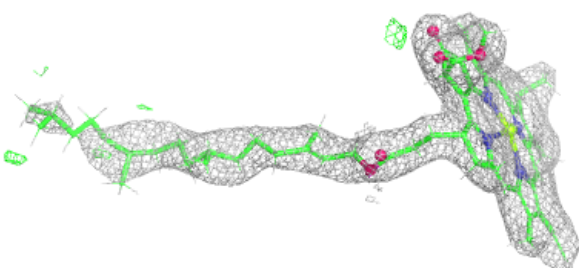
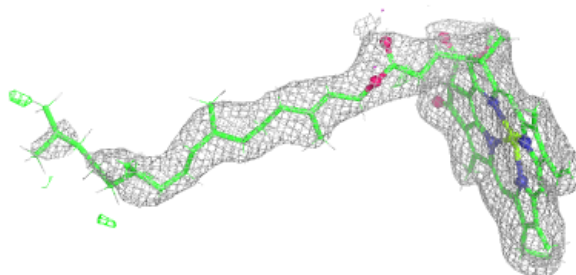
**Electron density around CLA B 602:**

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

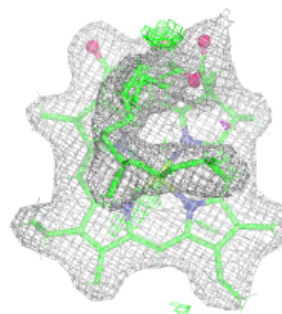
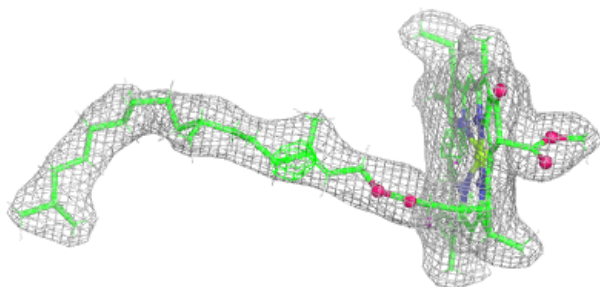
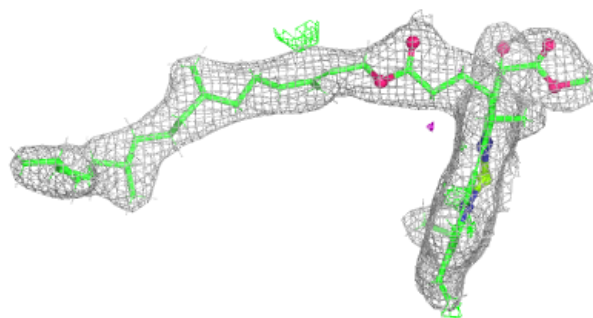


Electron density around CLA B 604:

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

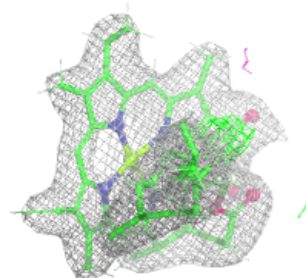
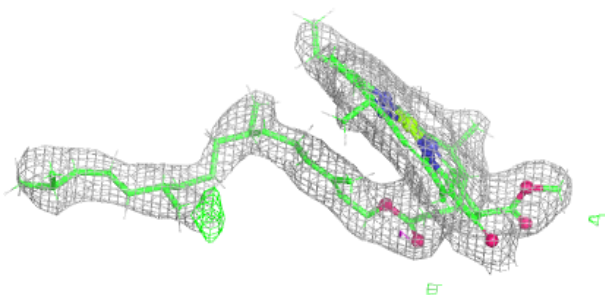
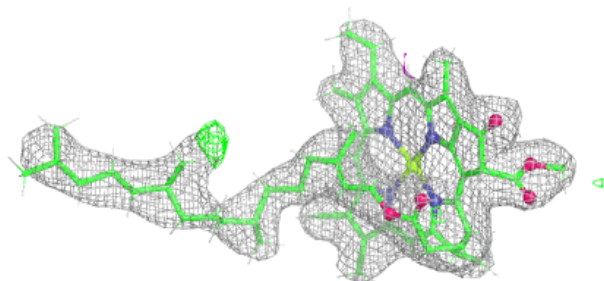
**Electron density around CLA B 605:**

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

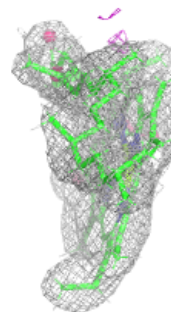
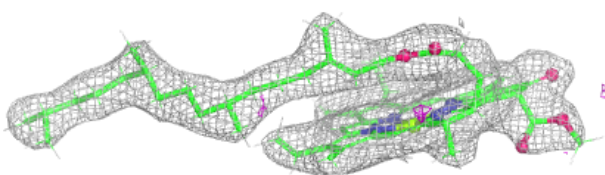
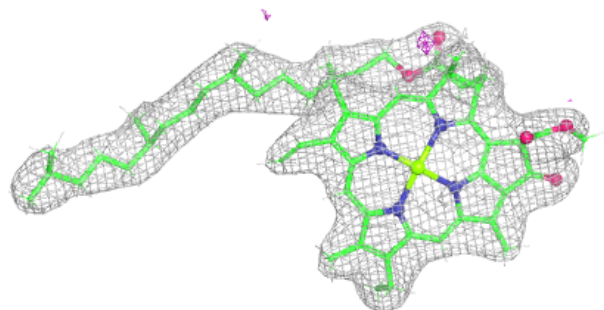


Electron density around CLA c 505:

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

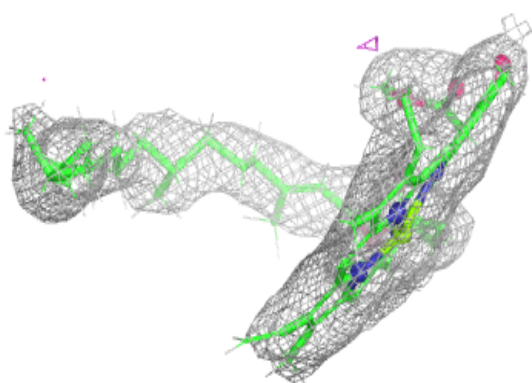
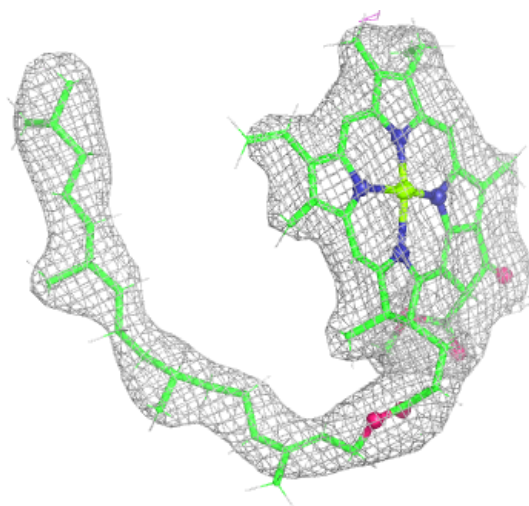
**Electron density around CLA C 501:**

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



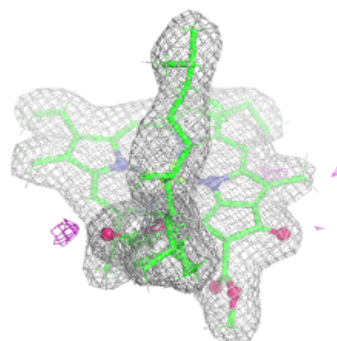
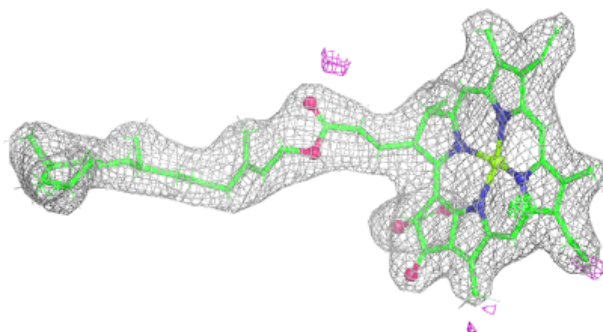
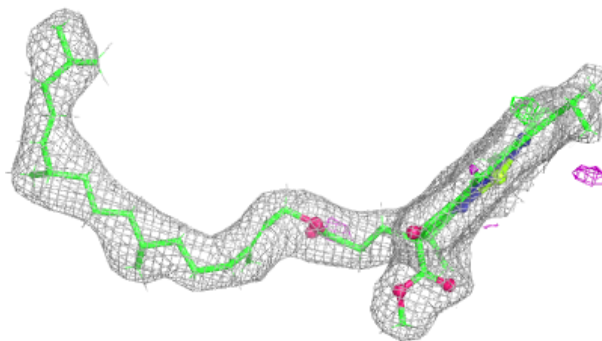
Electron density around CLA c 507:

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

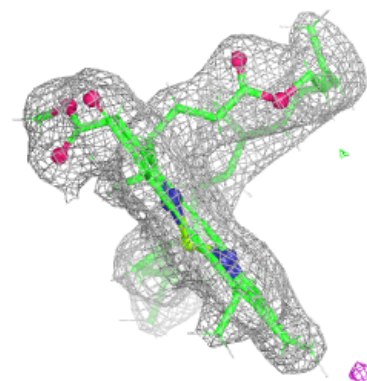
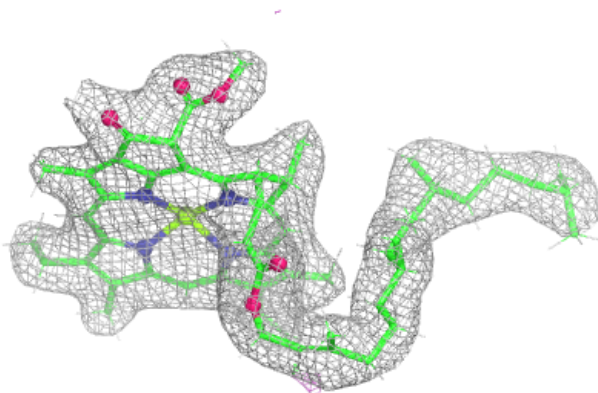
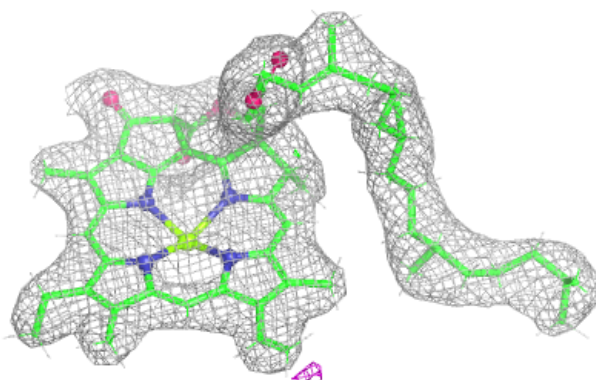


Electron density around CLA D 403:

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

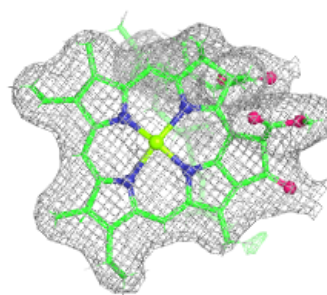
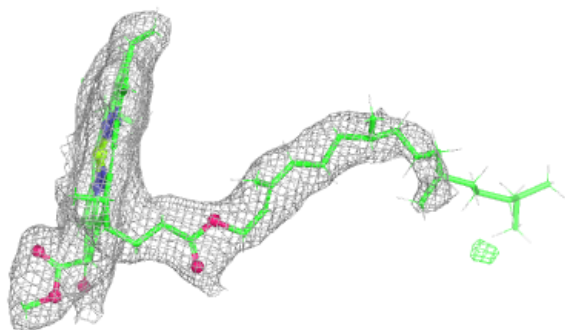
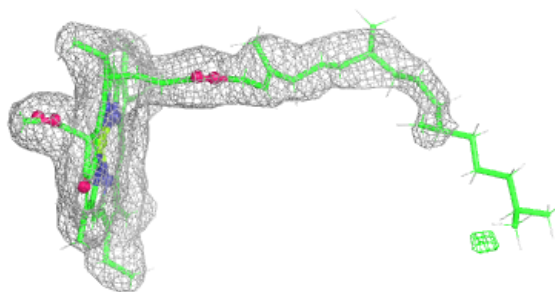
**Electron density around CLA D 404:**

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

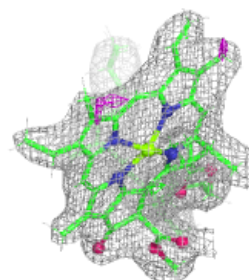
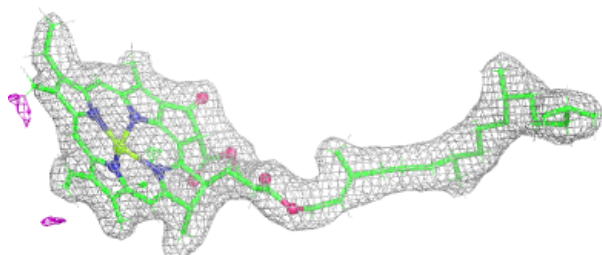
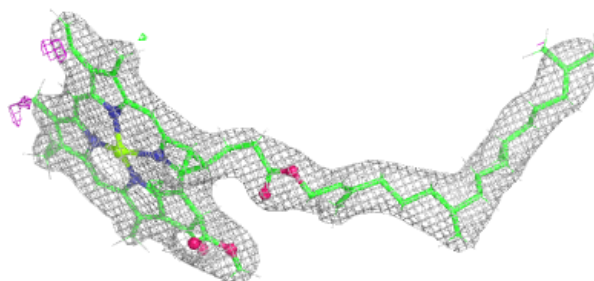


Electron density around CLA D 405:

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

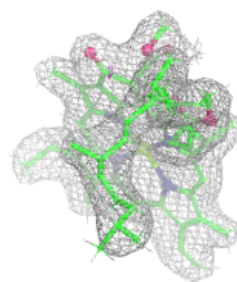
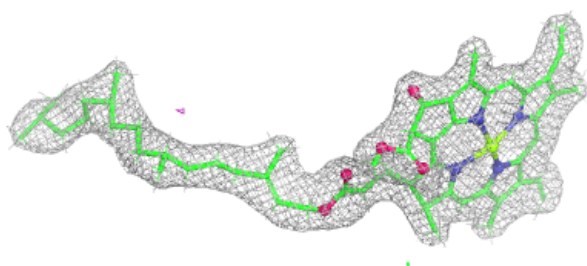
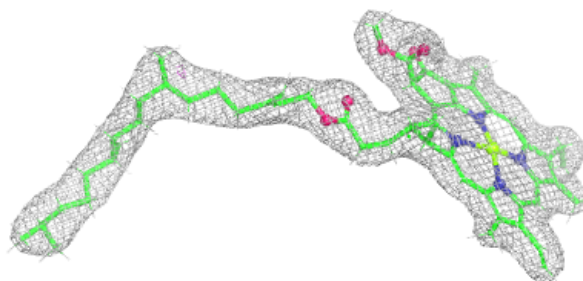
**Electron density around CLA a 402:**

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

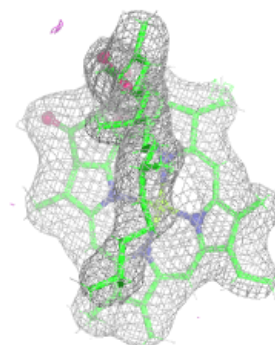
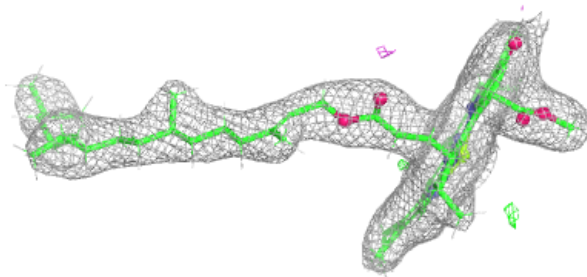
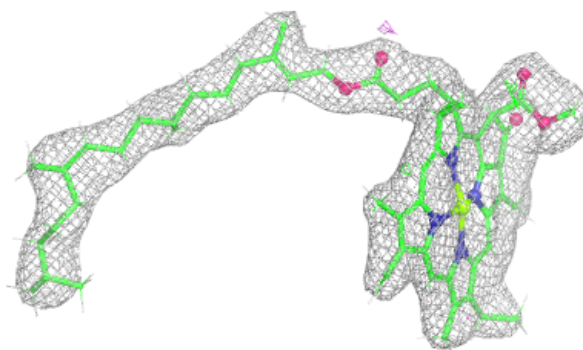


Electron density around CLA A 402:

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

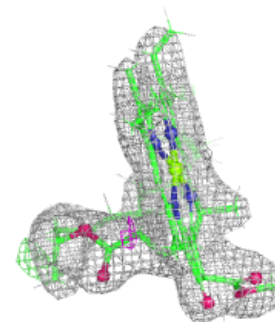
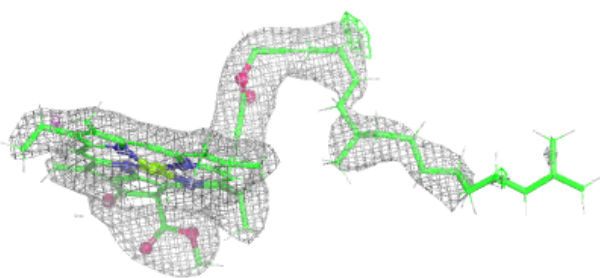
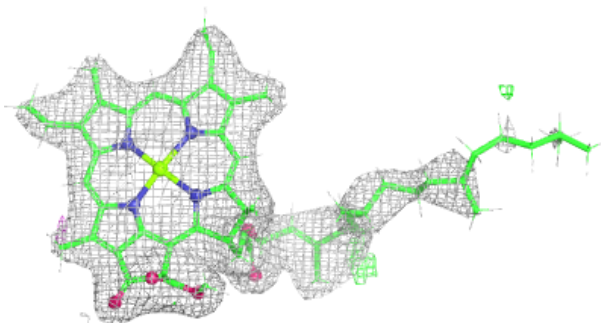
**Electron density around CLA B 609:**

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

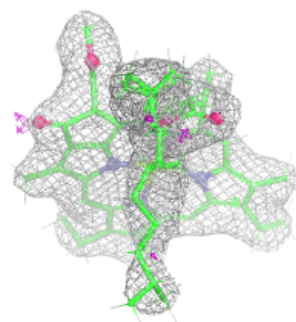
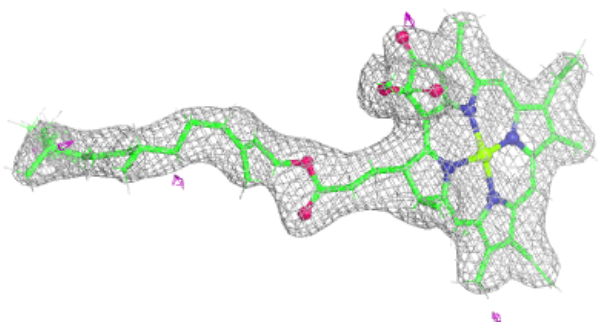
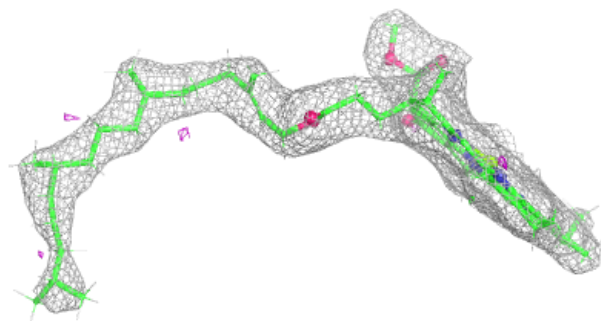


Electron density around CLA d 401:

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

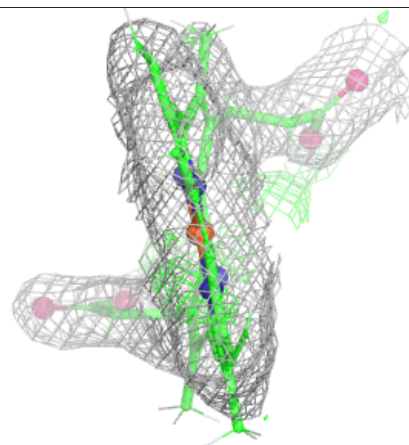
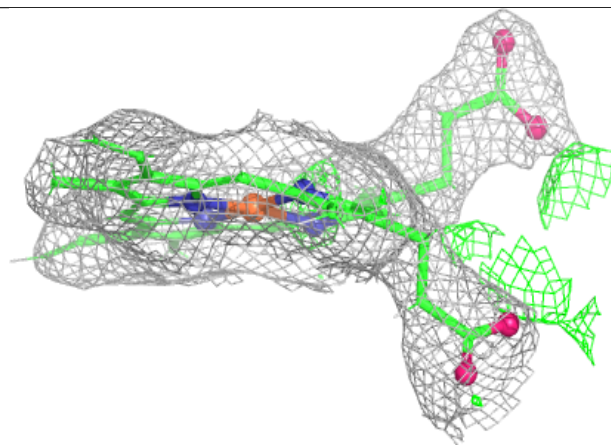
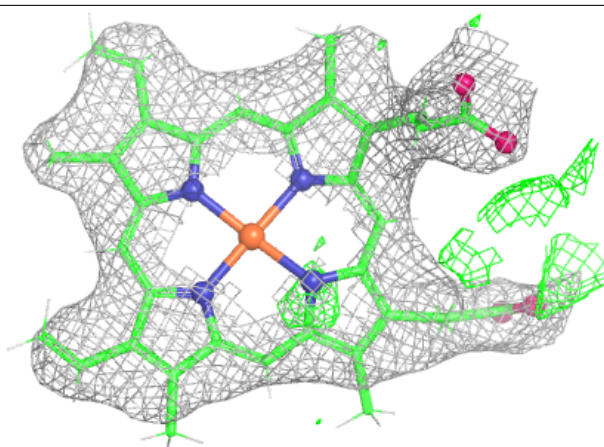
**Electron density around CLA d 403:**

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



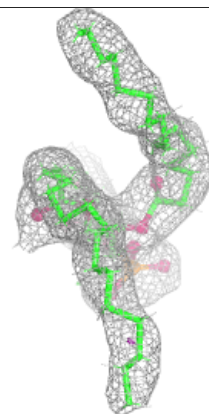
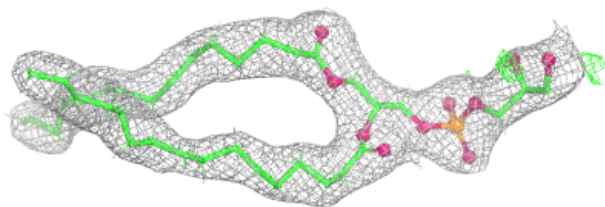
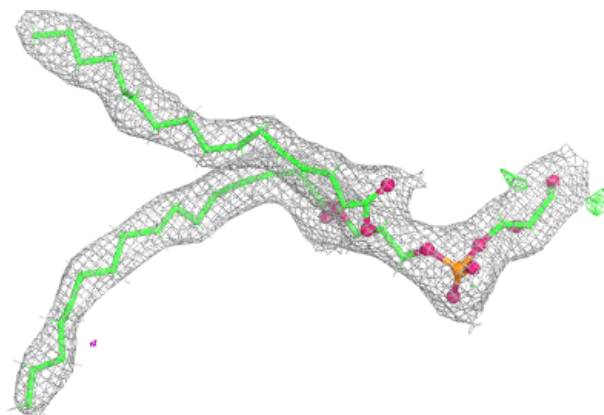
Electron density around HEM f 101:

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

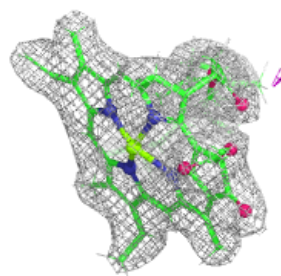
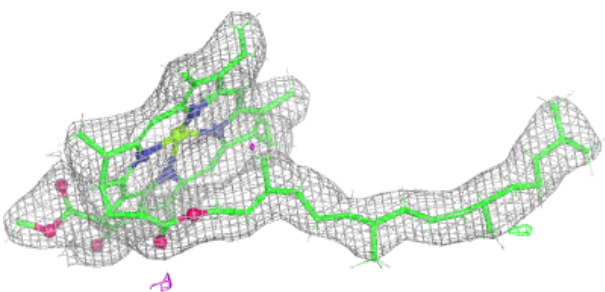
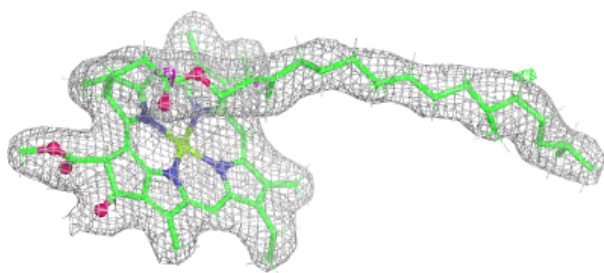


Electron density around LHG D 410:

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

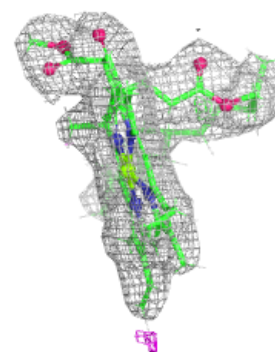
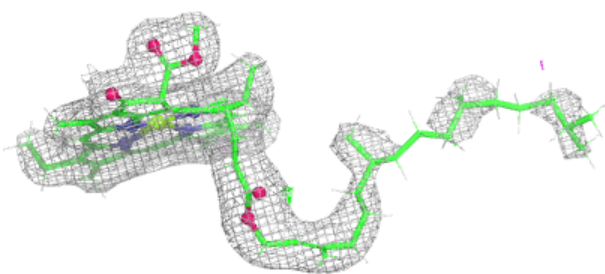
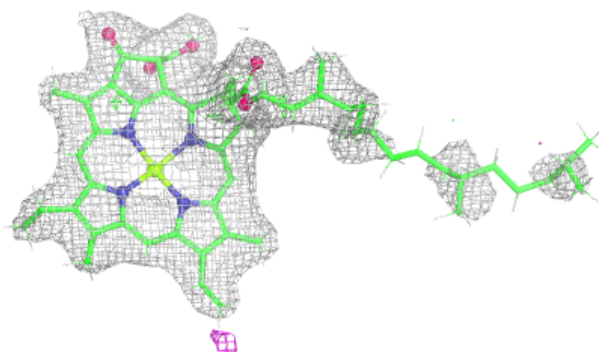
**Electron density around CLA B 608:**

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

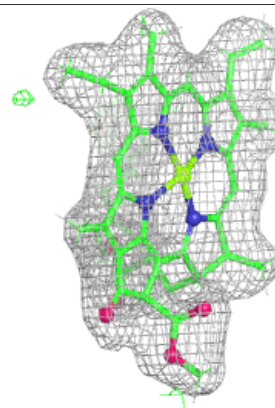
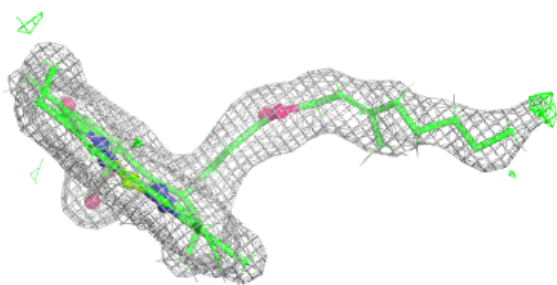
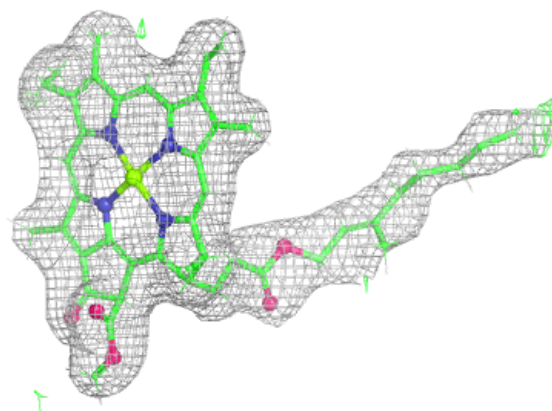


Electron density around CLA A 403:

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

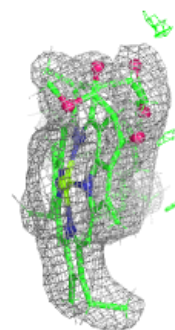
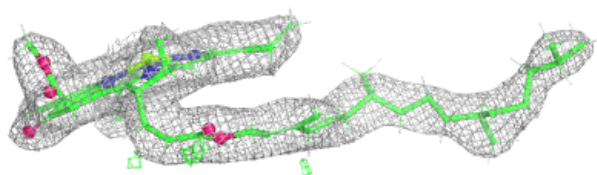
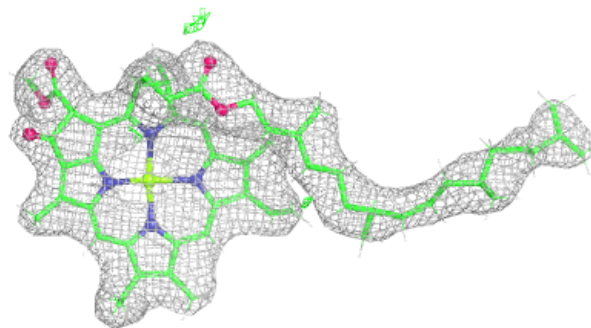
**Electron density around CLA A 405:**

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



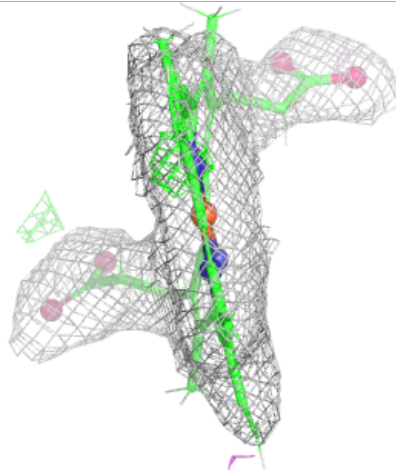
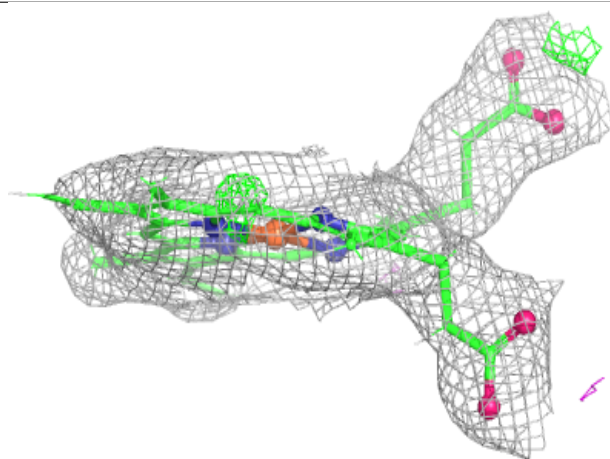
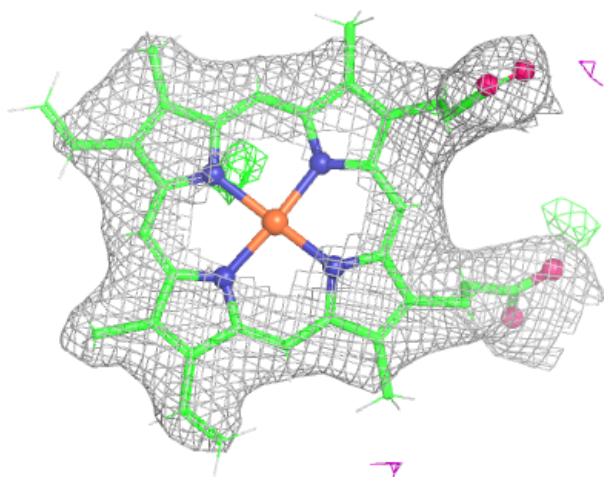
Electron density around CLA B 603:

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



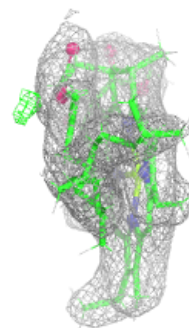
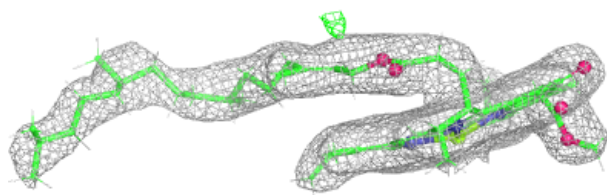
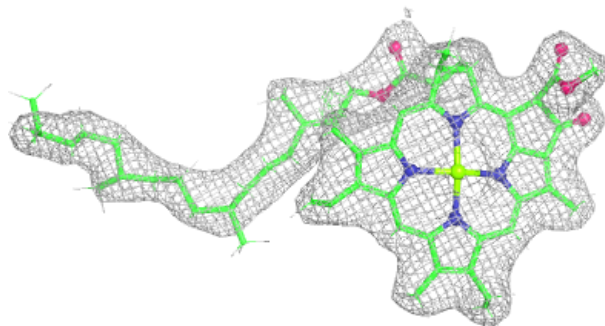
Electron density around HEM F 101:

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

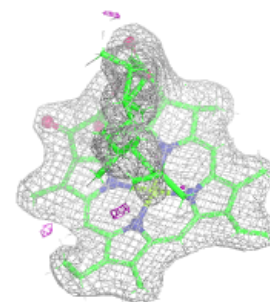
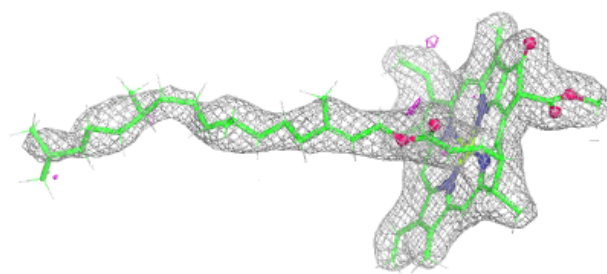
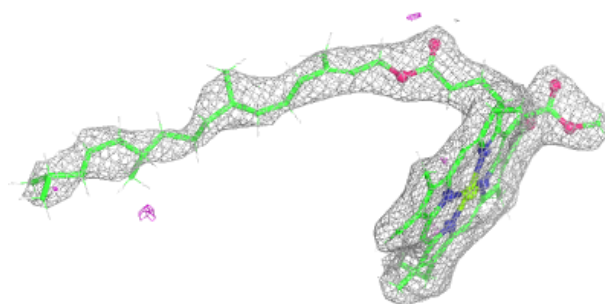


Electron density around CLA b 603:

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

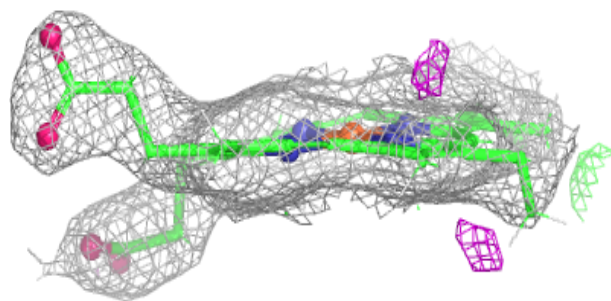
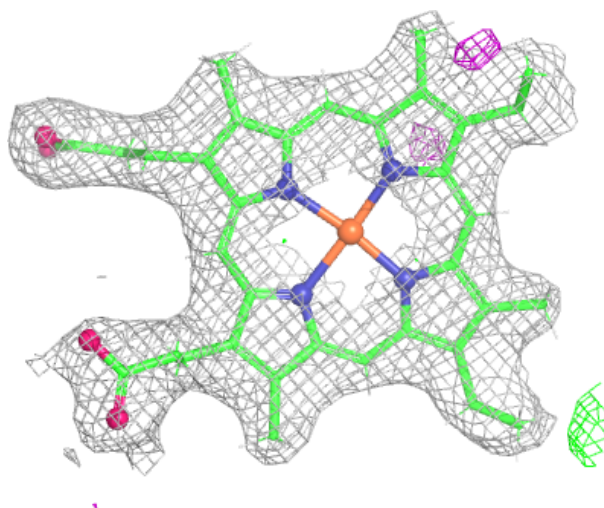
**Electron density around CLA B 607:**

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



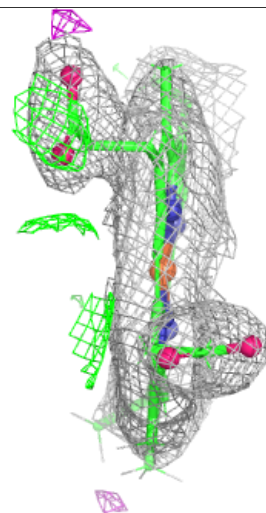
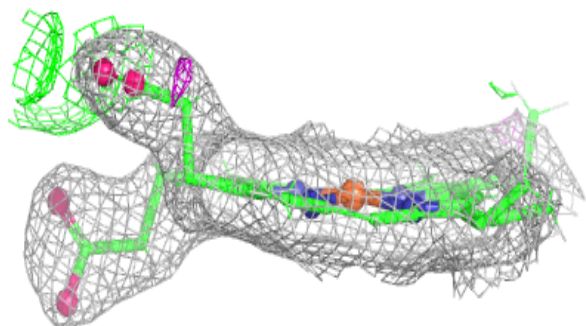
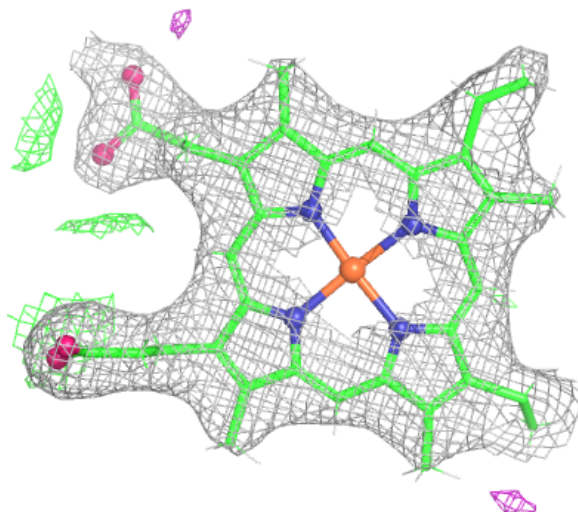
Electron density around HEC V 201:

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



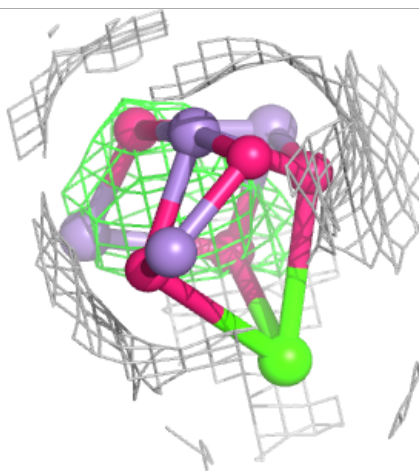
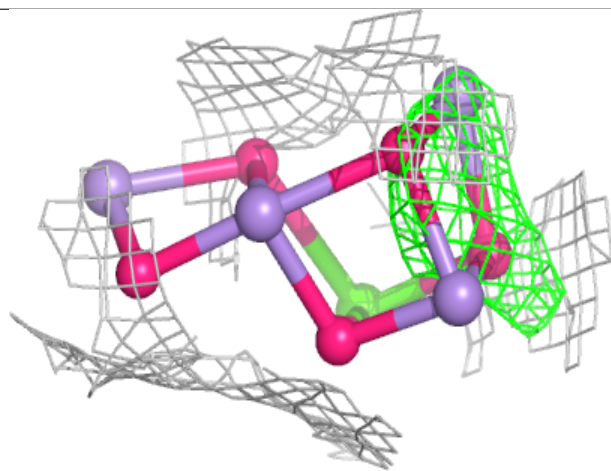
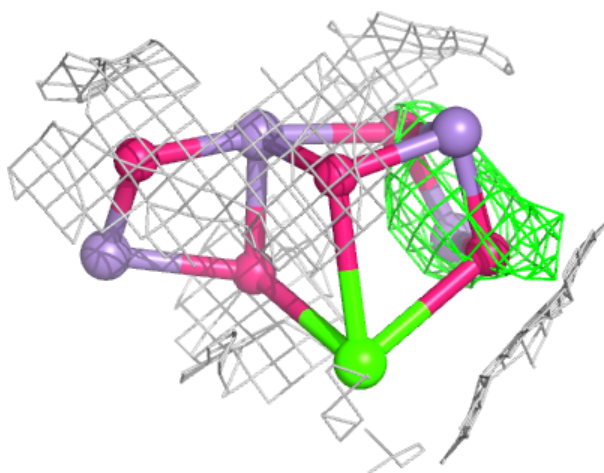
Electron density around HEC v 201:

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



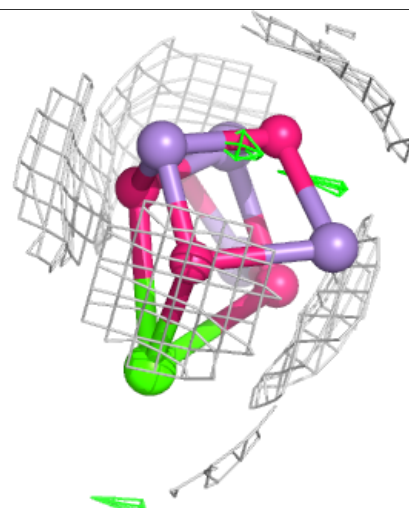
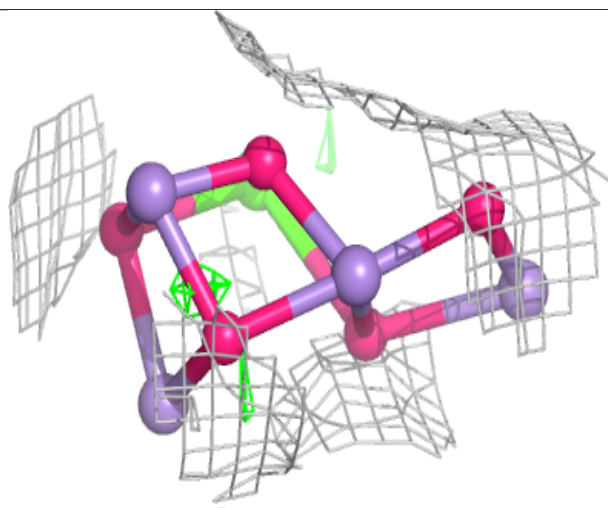
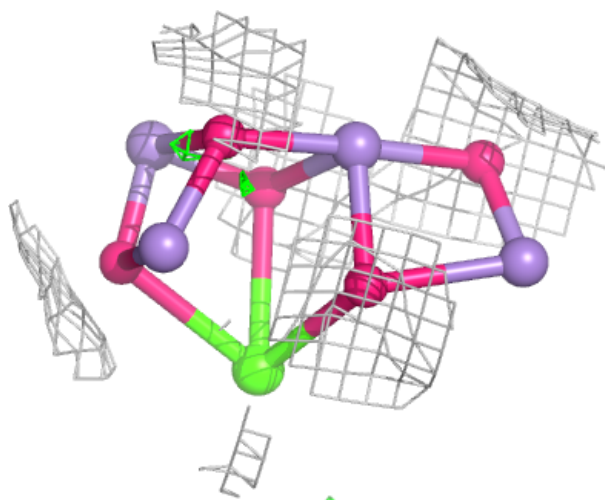
Electron density around OEX A 414:

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



Electron density around OEX 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.