



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:37 PM EDT

PDB ID : 6W1U / pdb_00006w1u
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)

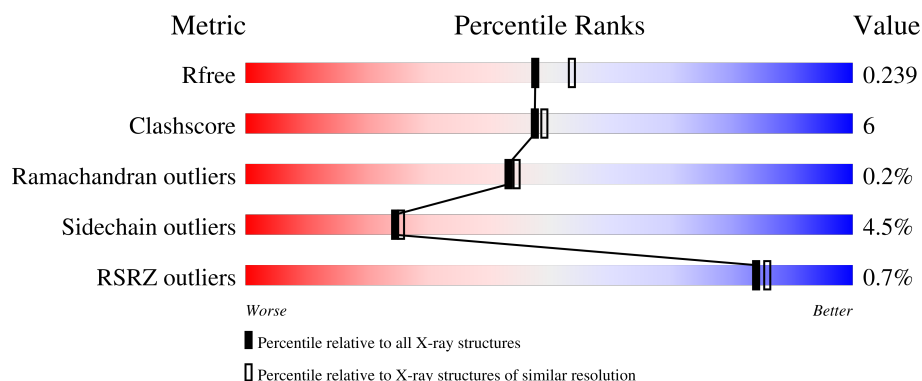
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

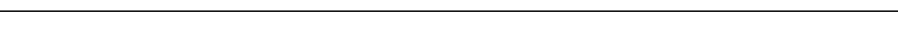
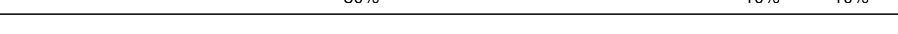
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	 86% 10% ..
1	a	344	 81% 15% ..

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CCP4 : 9.0.015 (Gargrove)
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
32	OEY	A	417[B]	-	-	X	-
35	HEC	F	101	X	-	-	-
35	HEC	V	201	X	-	-	-
35	HEC	e	101	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105950 atoms, of which 52556 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	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
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	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
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- 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
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	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
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	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			

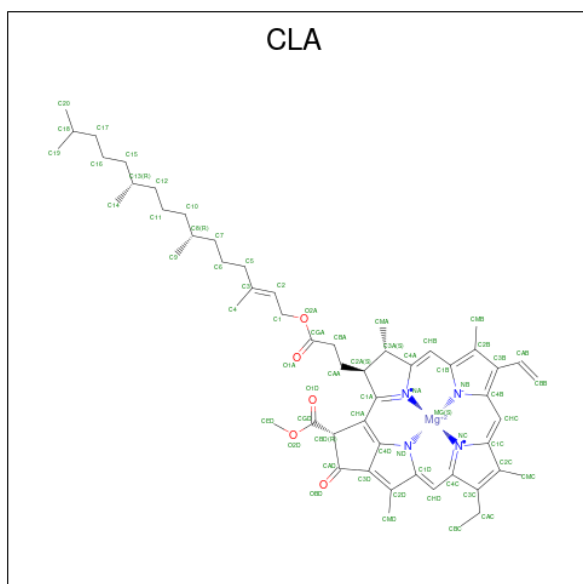
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	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		
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		

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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 117	C 49	H 58	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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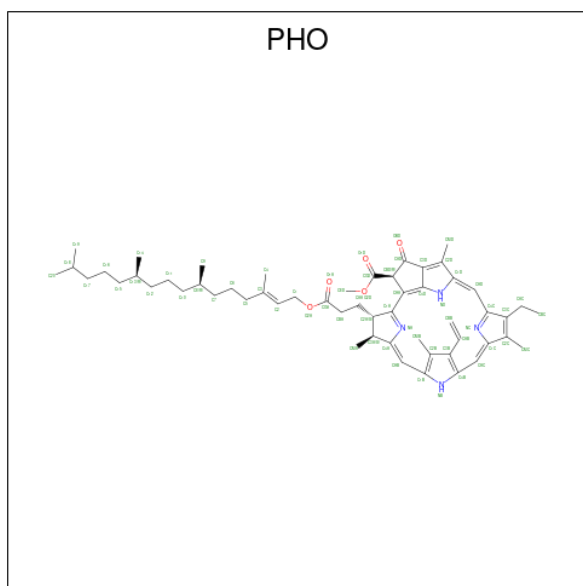
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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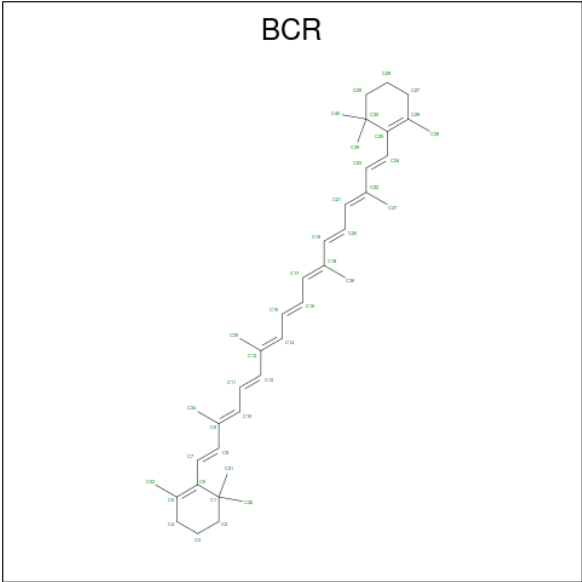
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	h	1	Total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

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



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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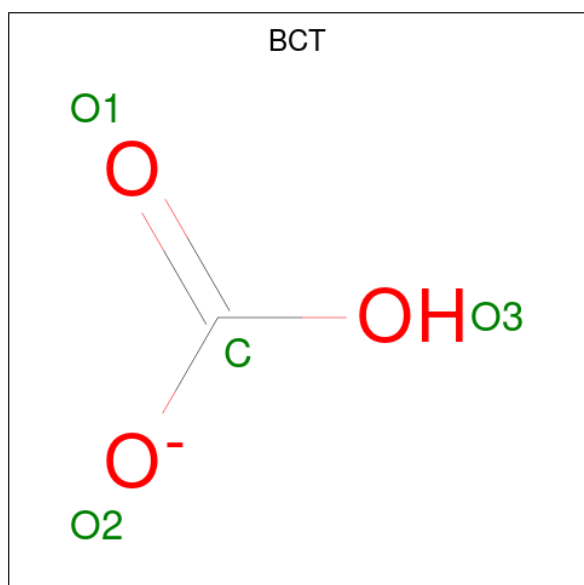
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40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

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

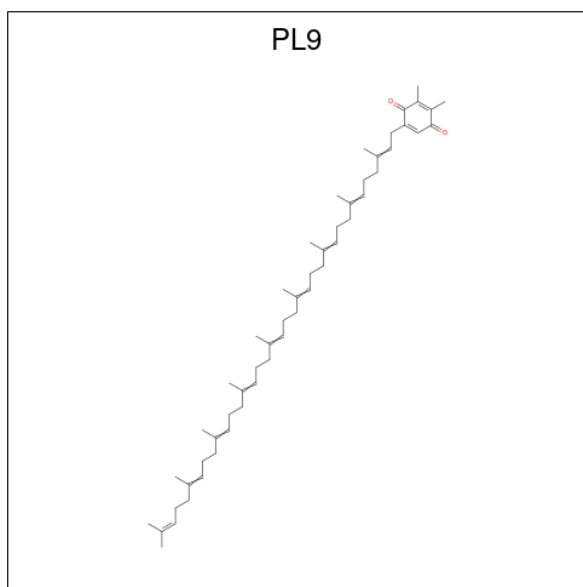
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



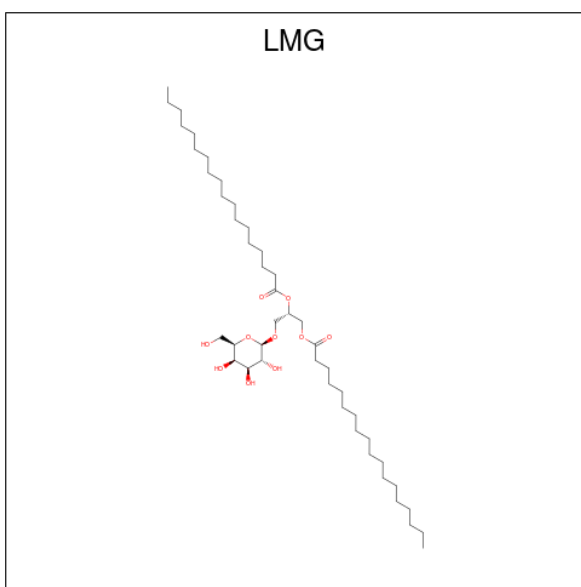
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

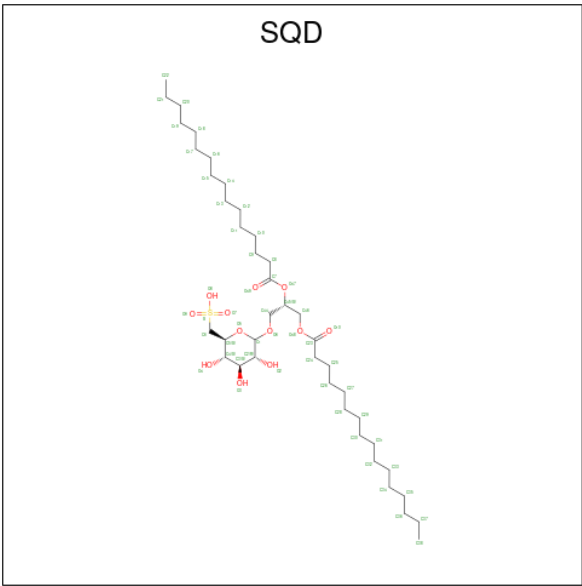
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			141	45	86	10		
28	C	1	Total	C	H	O	0	0
			111	38	63	10		
28	D	1	Total	C	H	O	0	0
			121	41	70	10		
28	D	1	Total	C	H	O	0	0
			78	27	45	6		
28	D	1	Total	C	H	O	0	0
			68	24	40	4		
28	M	1	Total	C	H	O	0	0
			121	41	70	10		
28	b	1	Total	C	H	O	0	0
			122	41	71	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			80	27	43	10		
28	c	1	Total	C	H	O	0	0
			116	38	68	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

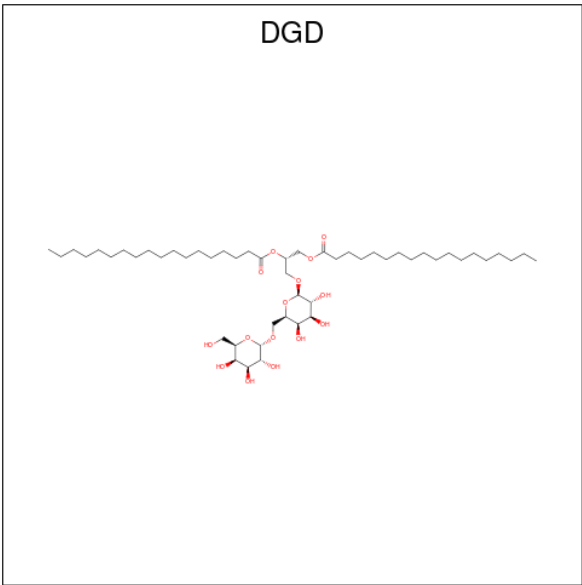
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



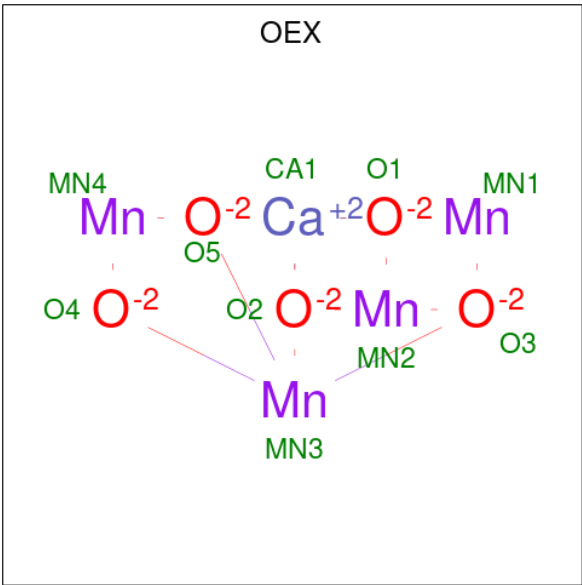
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			87	28	46	12	1		

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



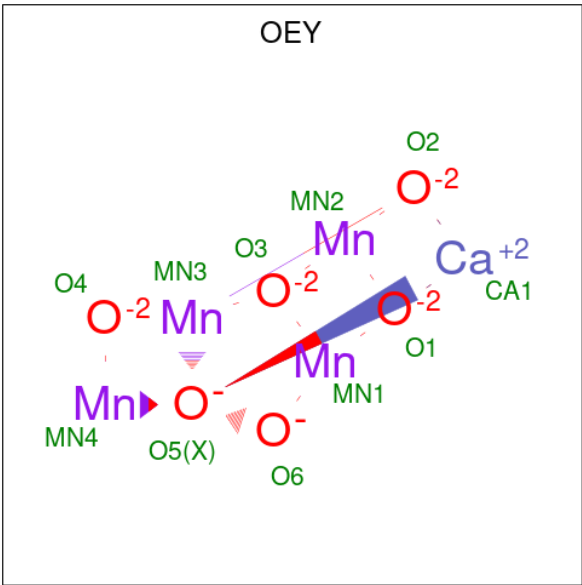
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			159	51	93	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			140	47	78	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			141	47	79	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	h	1	Total	C	H	O	0	0
			140	47	78	15		

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



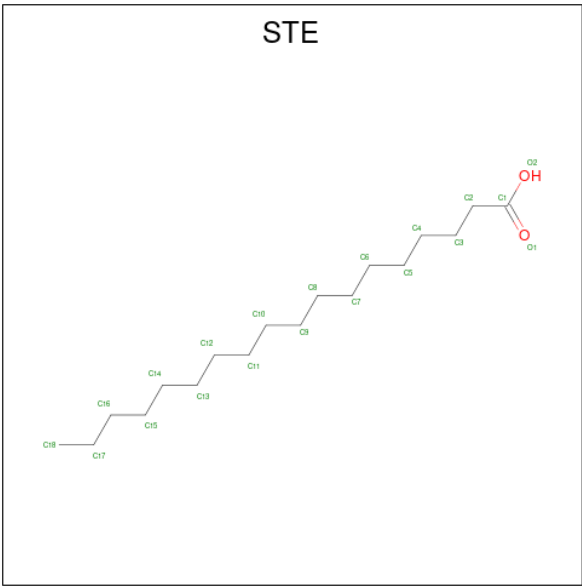
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H	O	0	0
			46	16	28	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H		0	0
			41	15	26			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			

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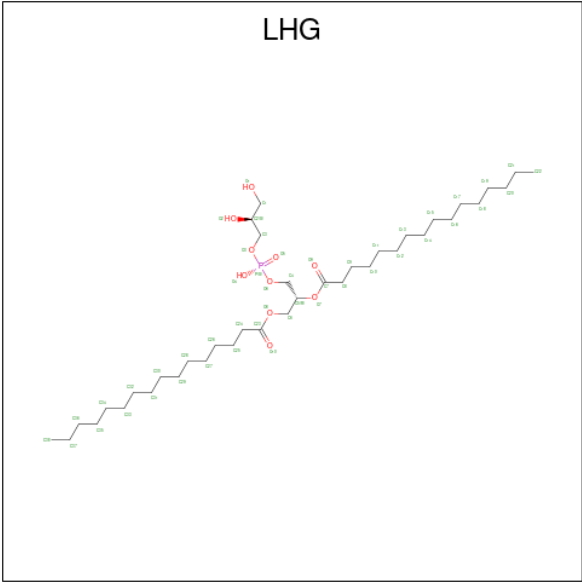
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total C H O 28 10 16 2	0	0
33	L	1	Total C H O 28 10 16 2	0	0
33	M	1	Total C H O 37 13 22 2	0	0
33	M	1	Total C H 26 10 16	0	0
33	T	1	Total C H 44 15 29	0	0
33	X	1	Total C H O 55 18 35 2	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H O 40 14 24 2	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H 26 10 16	0	0
33	c	1	Total C H O 28 10 16 2	0	0
33	c	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	h	1	Total C H 41 14 27	0	0
33	j	1	Total C H O 28 10 16 2	0	0

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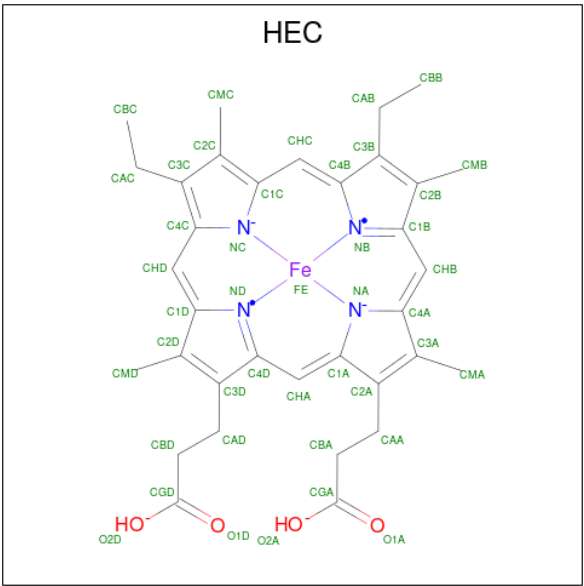
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	1	1	Total	C	H	0	0
			53	18	35		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	B	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
34	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
34	D	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
34	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	E	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
34	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
34	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	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
			73	34	1	30	4	4		
35	e	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
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	153	Total	O	0	8
			153	153		
36	B	216	Total	O	0	0
			216	216		
36	C	179	Total	O	0	0
			179	179		
36	D	131	Total	O	0	0
			131	131		
36	E	39	Total	O	0	0
			39	39		
36	F	7	Total	O	0	0
			7	7		
36	H	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	I	17	Total 17	O 17	0	0
36	J	19	Total 19	O 19	0	0
36	K	16	Total 16	O 16	0	0
36	L	9	Total 9	O 9	0	0
36	M	7	Total 7	O 7	0	0
36	O	101	Total 101	O 101	0	0
36	R	6	Total 6	O 6	0	0
36	T	10	Total 10	O 10	0	0
36	U	43	Total 43	O 43	0	0
36	V	62	Total 62	O 62	0	0
36	X	11	Total 11	O 11	0	0
36	Y	5	Total 5	O 5	0	0
36	Z	10	Total 10	O 10	0	0
36	a	137	Total 137	O 137	0	8
36	b	186	Total 186	O 186	0	0
36	c	179	Total 179	O 179	0	0
36	d	110	Total 110	O 110	0	0
36	e	29	Total 29	O 29	0	0
36	f	7	Total 7	O 7	0	0
36	h	31	Total 31	O 31	0	0
36	i	8	Total 8	O 8	0	0

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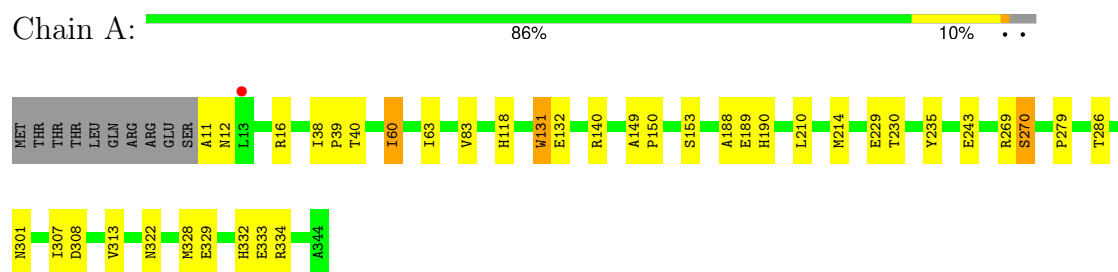
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	16	Total 16	O 16	0	0
36	k	7	Total 7	O 7	0	0
36	l	9	Total 9	O 9	0	0
36	m	7	Total 7	O 7	0	0
36	o	106	Total 106	O 106	0	0
36	r	6	Total 6	O 6	0	0
36	t	6	Total 6	O 6	0	0
36	u	56	Total 56	O 56	0	0
36	v	75	Total 75	O 75	0	0
36	x	12	Total 12	O 12	0	0
36	y	4	Total 4	O 4	0	0
36	z	11	Total 11	O 11	0	0

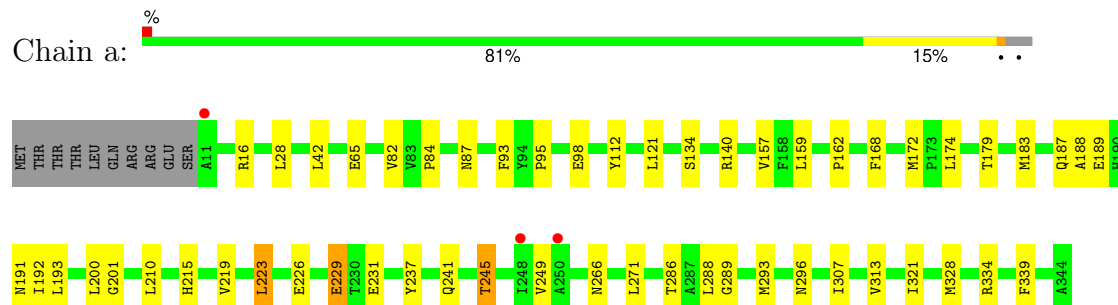
3 Residue-property plots [i](#)

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.

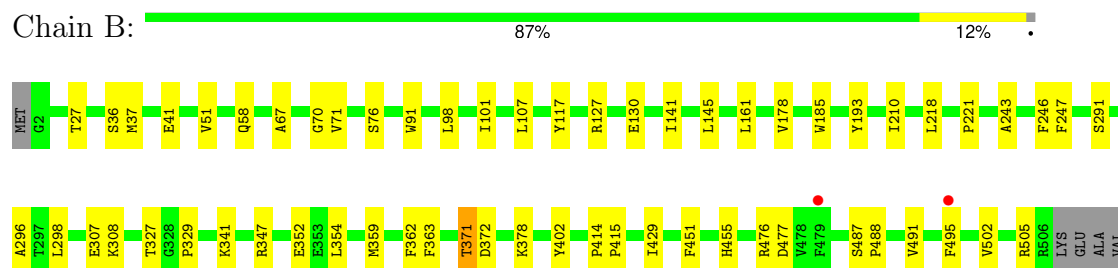
• Molecule 1: Photosystem II protein D1 1



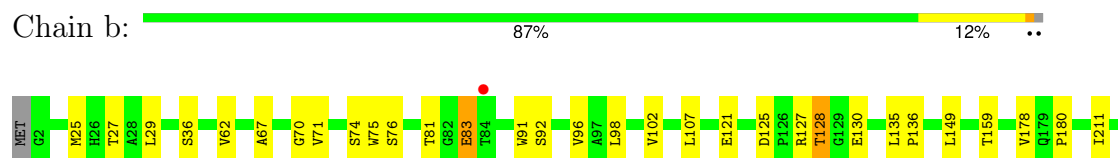
• Molecule 1: Photosystem II protein D1 1

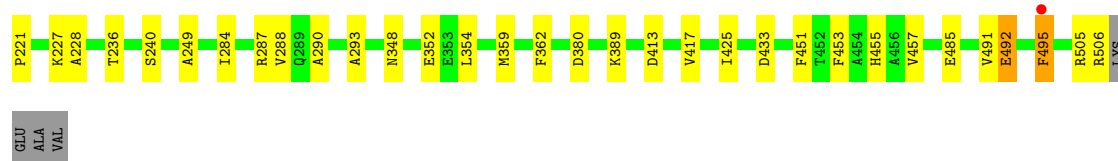


• Molecule 2: Photosystem II CP47 reaction center protein



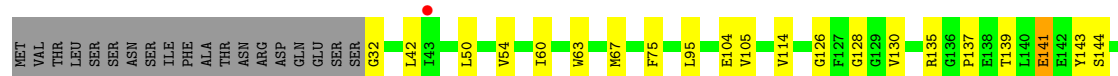
• Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 10%



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 12%



• Molecule 4: Photosystem II D2 protein

Chain D: 88% 8%

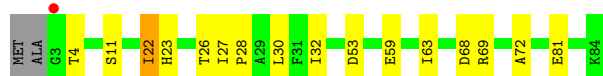
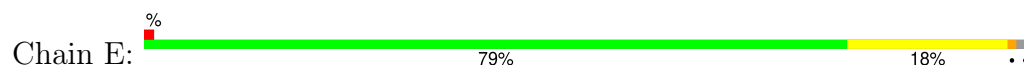


• Molecule 4: Photosystem II D2 protein

Chain d: 81% 16%



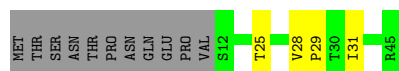
• Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



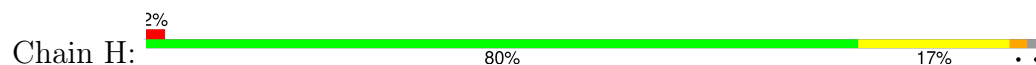
- Molecule 6: Cytochrome b559 subunit beta



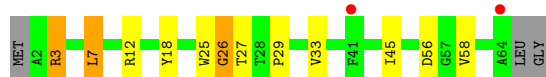
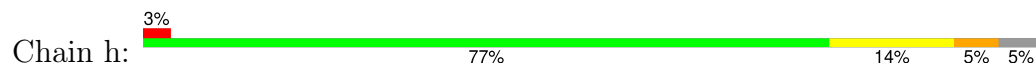
- Molecule 6: Cytochrome b559 subunit beta



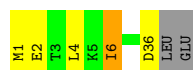
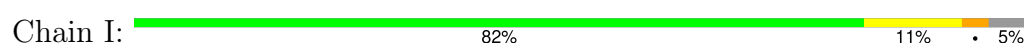
- Molecule 7: Photosystem II reaction center protein H



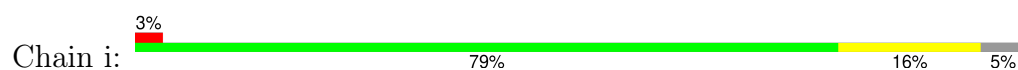
- Molecule 7: Photosystem II reaction center protein H



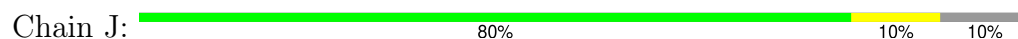
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



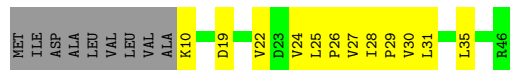
- Molecule 9: Photosystem II reaction center protein J



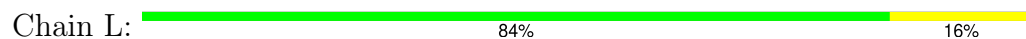
- Molecule 10: Photosystem II reaction center protein K



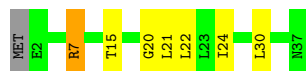
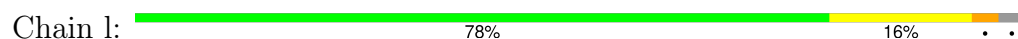
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 19% 8%



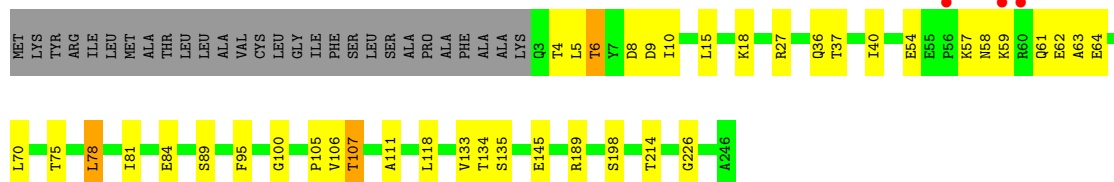
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 11% 11%



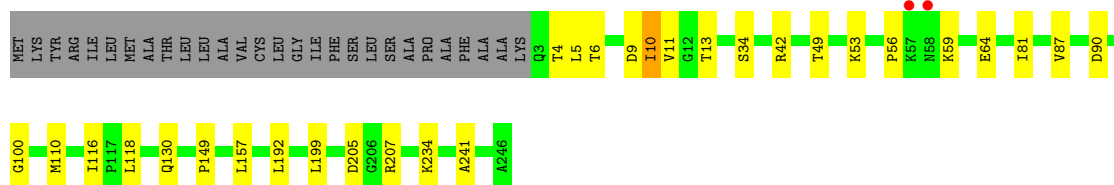
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  75% 14% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  79% 11% 10%

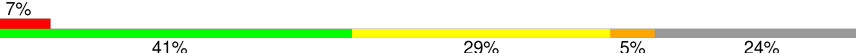


- Molecule 14: Photosystem II protein Y

Chain R:  2% 44% 32% 7% 17%



- Molecule 14: Photosystem II protein Y

Chain r:  7% 41% 29% 5% 24%



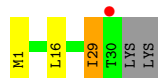
- Molecule 15: Photosystem II reaction center protein T

Chain T:  84% 9% 6%



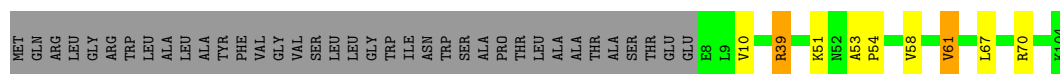
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 84% 6% 6%



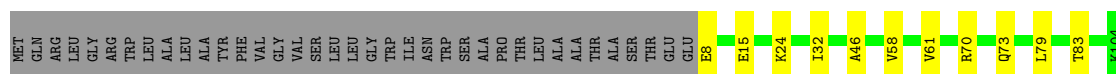
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 5% 28%



- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  64% 8% 28%



- Molecule 17: Cytochrome c-550

Chain V:  75% 7% 16%



- Molecule 17: Cytochrome c-550

Chain v:  72% 12% 16%

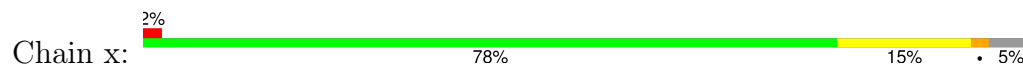


- Molecule 18: Photosystem II reaction center X protein

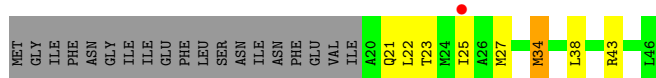
Chain X:  76% 15% 7%



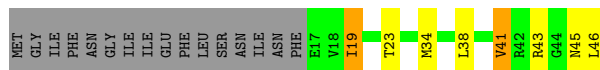
- Molecule 18: Photosystem II reaction center X protein



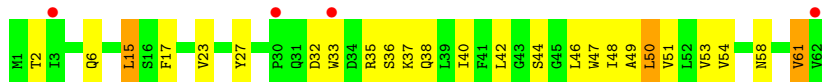
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 85.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.180 , 0.239 0.180 , 0.239	Depositor DCC
R_{free} test set	4171 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	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	0.96	EDS
Total number of atoms	105950	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	0/3187	0.68	1/4342 (0.0%)
1	a	0.54	0/3184	0.63	0/4338
2	B	0.60	0/4161	0.69	0/5669
2	b	0.58	0/4118	0.67	0/5611
3	C	0.58	0/3621	0.68	0/4930
3	c	0.54	0/3693	0.65	0/5026
4	D	0.64	0/2820	0.70	0/3840
4	d	0.61	0/2829	0.69	0/3852
5	E	0.52	0/688	0.64	0/940
5	e	0.47	0/683	0.64	0/932
6	F	0.53	0/284	0.55	0/387
6	f	0.44	0/284	0.61	0/387
7	H	0.59	0/523	0.71	0/713
7	h	0.51	0/511	0.62	0/697
8	I	0.56	0/293	0.64	0/396
8	i	0.56	0/293	0.62	0/396
9	J	0.49	0/263	0.58	0/356
9	j	0.48	0/263	0.62	0/356
10	K	0.50	0/303	0.61	0/416
10	k	0.43	0/303	0.56	0/416
11	L	0.63	0/311	0.66	0/422
11	l	0.63	0/303	0.60	0/412
12	M	0.57	0/249	0.70	0/341
12	m	0.67	0/244	0.69	0/334
13	O	0.57	0/1904	0.71	0/2585
13	o	0.58	0/1905	0.70	0/2583
14	R	0.41	0/277	0.57	0/380
14	r	0.36	0/245	0.45	0/336
15	T	0.62	0/257	0.77	0/349
15	t	0.61	0/255	0.59	0/346
16	U	0.53	0/785	0.65	0/1064
16	u	0.58	0/785	0.69	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.56	0/1085	0.66	0/1473
17	v	0.55	0/1085	0.67	0/1473
18	X	0.53	0/284	0.70	0/384
18	x	0.45	0/289	0.58	0/391
19	Y	0.46	0/197	0.57	0/264
19	y	0.40	0/219	0.53	0/294
20	Z	0.40	0/490	0.55	0/669
20	z	0.39	0/488	0.52	0/666
All	All	0.56	0/43961	0.66	1/59830 (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
1	A	0	1
1	a	0	1
17	V	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	TRP	CA-CB-CG	-5.12	103.88	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide
1	a	339[B]	PHE	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	3089	2942	2956	27	0
1	a	3086	2933	2947	36	0
2	B	4005	3859	3867	34	0
2	b	3978	3822	3836	44	0
3	C	3479	3397	3383	29	0
3	c	3553	3468	3466	37	0
4	D	2726	2624	2632	26	0
4	d	2732	2630	2638	35	0
5	E	666	650	651	11	0
5	e	664	647	648	18	0
6	F	275	281	282	5	0
6	f	275	281	282	9	0
7	H	510	532	532	12	0
7	h	498	518	518	11	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	2	0
9	j	257	268	268	8	0
10	K	293	305	305	10	0
10	k	293	305	305	4	0
11	L	304	316	316	5	0
11	l	296	304	304	4	0
12	M	256	269	269	7	0
12	m	251	267	267	5	0
13	O	1870	1828	1830	24	0
13	o	1874	1844	1846	15	0
14	R	271	298	298	8	0
14	r	240	253	249	8	0
15	T	258	261	261	2	0
15	t	256	256	256	2	0
16	U	774	772	773	6	0
16	u	774	772	773	6	0
17	V	1064	1068	1073	8	0
17	v	1064	1068	1074	13	0
18	X	281	312	312	5	0
18	x	286	316	314	4	0
19	Y	196	217	217	8	0
19	y	218	241	241	3	0
20	Z	479	516	516	14	0
20	z	477	509	509	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	249	264	264	5	0
22	B	1035	1139	1139	23	0
22	C	839	922	922	15	0
22	D	130	144	144	4	0
22	a	260	288	288	4	0
22	b	970	1067	1067	28	0
22	c	839	919	919	6	0
22	d	130	144	144	2	0
22	h	65	72	72	1	0
23	A	64	74	74	0	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	2	0
24	A	40	56	56	2	0
24	B	120	168	168	6	0
24	C	40	56	56	1	0
24	D	40	56	56	5	0
24	H	40	56	56	3	0
24	K	40	56	56	0	0
24	T	40	56	56	3	0
24	Y	40	56	56	2	0
24	Z	40	56	56	3	0
24	a	40	56	56	0	0
24	b	120	168	168	9	0
24	c	120	168	168	2	0
24	d	40	56	56	2	0
24	t	40	56	56	6	0
24	x	40	56	56	1	0
24	y	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	4	1	1	0	0
26	a	4	1	1	0	0
27	A	55	80	80	4	0
27	D	55	80	80	0	0
27	a	55	80	80	7	0
27	d	55	80	80	0	0
28	A	48	66	66	0	0
28	B	55	86	86	2	0
28	C	48	63	66	2	0
28	D	112	155	156	5	0
28	M	51	70	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	106	157	158	1	0
28	c	134	179	181	1	0
28	d	44	58	58	0	0
29	A	91	135	135	6	0
29	B	54	77	78	2	0
29	D	36	45	45	1	0
29	a	90	133	133	0	0
29	b	49	65	65	3	0
29	f	41	46	48	0	0
30	A	66	93	96	1	0
30	C	186	240	244	1	0
30	H	62	80	82	0	0
30	c	186	235	245	0	0
30	h	62	78	81	0	0
31	A	10	0	0	1	0
31	a	10	0	0	1	0
32	A	11	0	0	5	0
32	a	11	0	0	0	0
33	B	104	163	163	4	0
33	C	40	63	63	1	0
33	E	12	16	16	0	0
33	H	18	35	35	0	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	L	12	16	16	0	0
33	M	25	38	38	1	0
33	T	15	29	29	3	0
33	X	20	35	35	2	0
33	Z	8	12	12	1	0
33	a	22	32	32	1	0
33	b	82	141	141	3	0
33	c	32	51	51	1	0
33	d	57	96	96	5	0
33	h	14	27	27	2	0
33	j	12	16	16	1	0
33	l	18	35	35	1	0
34	B	49	73	74	1	0
34	D	145	210	215	4	0
34	E	49	72	74	0	0
34	d	137	193	199	3	0
34	e	42	55	57	0	0
34	l	49	73	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	43	32	32	3	0
35	V	43	30	31	1	0
35	e	43	32	32	7	0
35	v	43	30	31	5	0
36	A	153	0	0	3	0
36	B	216	0	0	0	0
36	C	179	0	0	1	0
36	D	131	0	0	4	0
36	E	39	0	0	0	0
36	F	7	0	0	0	0
36	H	23	0	0	1	0
36	I	17	0	0	1	0
36	J	19	0	0	1	0
36	K	16	0	0	0	0
36	L	9	0	0	1	0
36	M	7	0	0	3	0
36	O	101	0	0	7	0
36	R	6	0	0	1	0
36	T	10	0	0	0	0
36	U	43	0	0	3	0
36	V	62	0	0	3	0
36	X	11	0	0	1	0
36	Y	5	0	0	0	0
36	Z	10	0	0	1	0
36	a	137	0	0	4	0
36	b	186	0	0	5	0
36	c	179	0	0	8	0
36	d	110	0	0	0	0
36	e	29	0	0	3	0
36	f	7	0	0	1	0
36	h	31	0	0	4	0
36	i	8	0	0	0	0
36	j	16	0	0	2	0
36	k	7	0	0	0	0
36	l	9	0	0	0	0
36	m	7	0	0	1	0
36	o	106	0	0	4	0
36	r	6	0	0	2	0
36	t	6	0	0	0	0
36	u	56	0	0	1	0
36	v	75	0	0	1	0
36	x	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	4	0	0	0	0
36	z	11	0	0	1	0
All	All	53394	52556	52674	586	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 586 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	2.06	1.44
17:v:40:CYS:SG	35:v:201:HEC:HAC	1.97	1.03
13:o:9:ASP:OD2	36:o:301:HOH:O	1.76	1.02
14:r:32:GLN:O	36:r:101:HOH:O	1.79	0.97
3:c:315:MET:SD	36:c:751:HOH:O	2.21	0.97

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	391/344 (114%)	385 (98%)	6 (2%)	0	100	100
1	a	391/344 (114%)	381 (97%)	10 (3%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	8 (2%)	2 (0%)	30	28
3	c	459/461 (100%)	445 (97%)	13 (3%)	1 (0%)	43	44
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	55 (87%)	8 (13%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	7	4
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	14 (6%)	2 (1%)	16	12
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	28
14	R	32/41 (78%)	29 (91%)	2 (6%)	1 (3%)	3	1
14	r	27/41 (66%)	27 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	127 (94%)	7 (5%)	1 (1%)	18	15
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	2 (8%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	1
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
All	All	5372/5700 (94%)	5201 (97%)	158 (3%)	13 (0%)	43	44

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
17	V	64	PRO
3	c	416	SER
14	R	34	LEU

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	320/280 (114%)	313 (98%)	7 (2%)	45	53
1	a	319/280 (114%)	303 (95%)	16 (5%)	22	22
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	53
2	b	402/407 (99%)	386 (96%)	16 (4%)	28	29
3	C	353/362 (98%)	345 (98%)	8 (2%)	44	51
3	c	361/362 (100%)	347 (96%)	14 (4%)	28	31
4	D	277/283 (98%)	275 (99%)	2 (1%)	76	83
4	d	278/283 (98%)	266 (96%)	12 (4%)	26	27
5	E	72/73 (99%)	66 (92%)	6 (8%)	10	8
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	43
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	11
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	58
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	17
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	28
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	28
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	34
13	O	206/228 (90%)	194 (94%)	12 (6%)	18	16
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	27
14	R	28/33 (85%)	20 (71%)	8 (29%)	0	0
14	r	23/33 (70%)	17 (74%)	6 (26%)	0	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
16	U	84/112 (75%)	79 (94%)	5 (6%)	17	15
16	u	84/112 (75%)	82 (98%)	2 (2%)	43	49
17	V	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	v	117/138 (85%)	111 (95%)	6 (5%)	21	21
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
All	All	4444/4654 (96%)	4248 (96%)	196 (4%)	24	26

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	24	THR
6	f	23	VAL
3	c	104	GLU

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Mol	Chain	Res	Type
4	d	90	LEU
10	k	10	LYS

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

Mol	Chain	Res	Type
7	h	59	ASN
13	o	61	GLN
18	x	33	GLN
16	U	37	GLN
14	R	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.07	1 (12%)	8,9,11	1.30	1 (12%)
15	FME	t	1	15	8,9,10	1.22	1 (12%)	8,9,11	1.08	0
8	FME	i	1	8	8,9,10	0.91	0	8,9,11	1.44	2 (25%)
8	FME	I	1	8	8,9,10	1.18	1 (12%)	8,9,11	1.31	1 (12%)
15	FME	T	1	15	8,9,10	1.01	1 (12%)	8,9,11	1.37	1 (12%)
12	FME	M	1	12	8,9,10	0.89	0	8,9,11	1.02	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
15	FME	T	1	15	-	3/7/9/11	-
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	-3.07	1.42	1.46
8	I	1	FME	CA-N	-2.92	1.42	1.46
12	m	1	FME	CA-N	-2.32	1.43	1.46
15	T	1	FME	CA-N	-2.11	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.75	118.60	122.82
15	T	1	FME	O1-CN-N	-2.68	118.39	125.32
8	I	1	FME	CA-N-CN	-2.18	119.46	122.82
8	i	1	FME	C-CA-N	2.03	113.41	109.50
12	m	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	c	506	36	64,68,73	1.21	6 (9%)	76,107,113	1.38	14 (18%)
22	CLA	c	508	3	69,73,73	1.58	11 (15%)	82,113,113	1.36	9 (10%)
24	BCR	b	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.30	7 (12%)
23	PHO	A	404	-	58,69,69	1.84	9 (15%)	55,99,99	1.84	12 (21%)
34	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	1.23	5 (9%)
22	CLA	b	615	2	64,68,73	1.44	10 (15%)	76,107,113	1.51	8 (10%)
22	CLA	A	405	1	58,62,73	1.27	5 (8%)	68,99,113	1.32	11 (16%)
28	LMG	c	525	-	49,49,55	1.03	5 (10%)	57,57,63	1.34	5 (8%)
29	SQD	f	101	-	39,41,54	1.10	5 (12%)	49,52,65	1.91	12 (24%)
22	CLA	b	606	36	69,73,73	1.21	7 (10%)	82,113,113	1.45	8 (9%)
33	STE	Z	102	-	7,7,19	0.31	0	6,6,19	0.77	0
33	STE	C	521	-	15,15,19	0.48	0	14,14,19	0.67	0
30	DGD	c	521	-	63,63,67	1.09	4 (6%)	77,77,81	1.38	10 (12%)
22	CLA	C	510	3	69,73,73	1.14	7 (10%)	82,113,113	1.49	7 (8%)
22	CLA	C	511	3	69,73,73	1.23	10 (14%)	82,113,113	1.23	4 (4%)
24	BCR	H	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.49	10 (17%)
30	DGD	A	415	-	67,67,67	1.41	10 (14%)	81,81,81	1.44	12 (14%)
22	CLA	B	615	2	69,73,73	1.44	10 (14%)	82,113,113	1.45	15 (18%)
34	LHG	e	102	-	41,41,48	1.05	3 (7%)	44,47,54	1.40	5 (11%)
27	PL9	A	410	-	55,55,55	1.10	5 (9%)	68,69,69	1.70	14 (20%)
24	BCR	A	406	-	41,41,41	1.06	2 (4%)	56,56,56	1.48	8 (14%)
34	LHG	E	101	-	48,48,48	0.97	4 (8%)	51,54,54	1.21	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	503	3	69,73,73	1.02	5 (7%)	82,113,113	1.53	10 (12%)
34	LHG	d	408	-	38,38,48	0.80	1 (2%)	41,44,54	1.11	3 (7%)
28	LMG	c	522	-	37,37,55	1.33	6 (16%)	45,45,63	1.27	6 (13%)
27	PL9	a	410	-	55,55,55	1.13	5 (9%)	68,69,69	1.53	9 (13%)
34	LHG	D	412	-	48,48,48	0.97	2 (4%)	51,54,54	1.45	8 (15%)
22	CLA	B	610	2	69,73,73	1.25	10 (14%)	82,113,113	1.35	10 (12%)
28	LMG	C	519	-	48,48,55	1.14	4 (8%)	56,56,63	1.37	7 (12%)
33	STE	a	414	-	9,9,19	0.54	0	8,8,19	0.43	0
24	BCR	K	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	5 (8%)
30	DGD	c	520	-	63,63,67	1.07	4 (6%)	77,77,81	1.42	10 (12%)
33	STE	I	101	-	14,14,19	0.51	0	13,13,19	0.62	0
22	CLA	B	614	2	69,73,73	1.47	9 (13%)	82,113,113	1.33	13 (15%)
34	LHG	B	622	-	48,48,48	1.06	2 (4%)	51,54,54	1.10	2 (3%)
28	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.41	12 (20%)
22	CLA	d	402	4	69,73,73	1.45	9 (13%)	82,113,113	1.26	10 (12%)
22	CLA	C	502	3	69,73,73	1.43	10 (14%)	82,113,113	1.43	7 (8%)
22	CLA	c	504	3	69,73,73	1.33	8 (11%)	82,113,113	1.39	7 (8%)
24	BCR	Z	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.35	6 (10%)
33	STE	b	624	-	15,15,19	0.86	0	15,15,19	0.81	0
33	STE	C	520	-	11,11,19	0.88	0	11,11,19	1.01	0
33	STE	M	102	-	14,14,19	0.86	0	14,14,19	0.98	1 (7%)
33	STE	j	101	-	11,11,19	0.86	0	11,11,19	1.34	1 (9%)
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.87	0
24	BCR	c	518	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	8 (14%)
28	LMG	b	623	-	55,55,55	0.94	1 (1%)	63,63,63	1.50	10 (15%)
33	STE	B	625	-	11,11,19	0.97	1 (9%)	11,11,19	1.06	0
22	CLA	B	604	2	69,73,73	1.29	7 (10%)	82,113,113	1.41	13 (15%)
22	CLA	D	402	4	69,73,73	1.18	5 (7%)	82,113,113	1.32	6 (7%)
24	BCR	y	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.12	3 (5%)
28	LMG	D	411	-	26,26,55	0.76	1 (3%)	26,26,63	1.20	3 (11%)
22	CLA	B	616	2	69,73,73	1.22	9 (13%)	82,113,113	1.29	10 (12%)
22	CLA	b	601	2	69,73,73	1.11	8 (11%)	82,113,113	1.54	7 (8%)
33	STE	d	410	-	16,16,19	0.57	0	16,16,19	1.38	2 (12%)
22	CLA	B	602	36	69,73,73	1.34	8 (11%)	82,113,113	1.85	12 (14%)
22	CLA	D	403	4	69,73,73	1.58	12 (17%)	82,113,113	1.26	8 (9%)
33	STE	c	501	-	11,11,19	0.83	0	11,11,19	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	d	407	-	48,48,48	1.07	3 (6%)	51,54,54	1.26	6 (11%)
33	STE	B	621	-	16,16,19	0.63	0	16,16,19	1.31	2 (12%)
22	CLA	B	613	2	69,73,73	1.15	7 (10%)	82,113,113	1.43	8 (9%)
30	DGD	C	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.34	10 (12%)
29	SQD	D	407	-	34,36,54	0.96	1 (2%)	42,45,65	2.25	13 (30%)
24	BCR	Y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	8 (14%)
28	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.17	2 (6%)
33	STE	B	627	-	15,15,19	0.52	0	14,14,19	0.69	0
22	CLA	b	603	2	69,73,73	1.13	8 (11%)	82,113,113	1.57	15 (18%)
34	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.15	4 (7%)
24	BCR	c	517	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	6 (10%)
24	BCR	D	404	-	41,41,41	1.20	2 (4%)	56,56,56	1.26	5 (8%)
22	CLA	b	610	2	69,73,73	1.14	5 (7%)	82,113,113	1.41	12 (14%)
35	HEC	V	201	17	50,50,50	1.66	4 (8%)	68,82,82	1.48	11 (16%)
22	CLA	b	605	2	69,73,73	1.62	10 (14%)	82,113,113	1.78	18 (21%)
26	BCT	a	409	21	3,3,3	1.09	0	2,3,3	2.73	2 (100%)
22	CLA	B	607	2	69,73,73	1.35	7 (10%)	82,113,113	1.30	8 (9%)
30	DGD	h	102	-	63,63,67	1.15	7 (11%)	77,77,81	1.51	14 (18%)
22	CLA	C	504	3	69,73,73	1.47	9 (13%)	82,113,113	1.63	9 (10%)
22	CLA	C	512	3	69,73,73	1.64	11 (15%)	82,113,113	1.34	6 (7%)
22	CLA	c	507	3	69,73,73	1.20	7 (10%)	82,113,113	1.15	6 (7%)
27	PL9	d	405	-	55,55,55	1.65	7 (12%)	68,69,69	1.62	15 (22%)
28	LMG	c	524	-	48,48,55	1.13	3 (6%)	56,56,63	1.33	7 (12%)
22	CLA	C	503	3	69,73,73	1.24	5 (7%)	82,113,113	1.56	11 (13%)
29	SQD	a	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.82	10 (16%)
33	STE	B	626	-	17,17,19	0.67	0	17,17,19	1.08	0
22	CLA	A	402	1	69,73,73	1.23	7 (10%)	82,113,113	1.40	11 (13%)
22	CLA	A	411	36	69,73,73	1.29	9 (13%)	82,113,113	1.21	7 (8%)
22	CLA	c	505	3	69,73,73	1.36	7 (10%)	82,113,113	1.43	8 (9%)
24	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.36	6 (10%)
22	CLA	c	513	3	69,73,73	1.33	8 (11%)	82,113,113	1.36	5 (6%)
22	CLA	B	617	2	64,68,73	1.33	6 (9%)	76,107,113	1.73	16 (21%)
33	STE	E	102	-	11,11,19	0.87	0	11,11,19	1.24	1 (9%)
22	CLA	b	612	2	69,73,73	1.21	9 (13%)	82,113,113	1.45	11 (13%)
33	STE	B	624	-	13,13,19	0.68	0	13,13,19	1.39	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	606	2	69,73,73	1.13	7 (10%)	82,113,113	1.35	11 (13%)
24	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	6 (10%)
30	DGD	H	102	-	63,63,67	1.40	11 (17%)	77,77,81	1.46	15 (19%)
35	HEC	v	201	17	50,50,50	1.58	5 (10%)	68,82,82	1.47	9 (13%)
22	CLA	C	506	3	69,73,73	1.24	7 (10%)	82,113,113	1.19	5 (6%)
31	OEX	a	416[A]	1,36,3	0,14,14	-	-	-		
29	SQD	B	623	-	52,54,54	0.98	3 (5%)	62,65,65	1.79	10 (16%)
22	CLA	B	611	36	69,73,73	1.28	8 (11%)	82,113,113	1.65	12 (14%)
22	CLA	B	603	2	69,73,73	1.22	8 (11%)	82,113,113	1.40	9 (10%)
33	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.11	1 (9%)
23	PHO	a	404	-	58,69,69	1.88	10 (17%)	55,99,99	1.80	13 (23%)
28	LMG	D	406	-	51,51,55	0.89	3 (5%)	59,59,63	1.48	9 (15%)
33	STE	d	411	-	19,19,19	0.74	0	19,19,19	0.98	2 (10%)
22	CLA	c	510	3	68,72,73	1.39	9 (13%)	80,111,113	1.36	10 (12%)
22	CLA	B	605	2	69,73,73	1.41	7 (10%)	82,113,113	1.72	9 (10%)
22	CLA	b	608	2	69,73,73	1.23	6 (8%)	82,113,113	1.28	12 (14%)
33	STE	h	103	-	13,13,19	0.44	0	12,12,19	0.64	0
23	PHO	d	401	-	58,69,69	1.97	11 (18%)	55,99,99	1.51	10 (18%)
33	STE	L	101	-	11,11,19	0.79	0	11,11,19	1.51	2 (18%)
33	STE	d	412	-	19,19,19	0.64	0	19,19,19	1.02	1 (5%)
22	CLA	C	514	3	69,73,73	1.28	7 (10%)	82,113,113	1.22	6 (7%)
24	BCR	x	101	-	41,41,41	1.13	4 (9%)	56,56,56	1.36	8 (14%)
22	CLA	c	514	3	69,73,73	1.26	10 (14%)	82,113,113	1.46	7 (8%)
22	CLA	a	411	36	69,73,73	1.65	6 (8%)	82,113,113	1.24	6 (7%)
22	CLA	C	513	3	69,73,73	1.25	11 (15%)	82,113,113	1.33	12 (14%)
24	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	10 (17%)
22	CLA	b	609	36	69,73,73	1.45	5 (7%)	82,113,113	1.55	14 (17%)
34	LHG	d	406	-	48,48,48	1.04	3 (6%)	51,54,54	1.39	6 (11%)
22	CLA	h	101	36	69,73,73	1.38	9 (13%)	82,113,113	1.59	6 (7%)
22	CLA	B	608	36	69,73,73	1.32	9 (13%)	82,113,113	1.42	8 (9%)
22	CLA	b	611	2	69,73,73	1.08	8 (11%)	82,113,113	1.29	8 (9%)
22	CLA	B	612	2	69,73,73	1.45	9 (13%)	82,113,113	1.45	10 (12%)
35	HEC	e	101	6,5	50,50,50	1.70	9 (18%)	68,82,82	1.86	13 (19%)
33	STE	T	102	-	14,14,19	0.48	0	13,13,19	0.68	0
33	STE	a	415	-	11,11,19	0.83	0	11,11,19	1.13	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	b	622	-	19,19,19	0.68	0	19,19,19	1.11	1 (5%)
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.62	0
22	CLA	c	509	36	69,73,73	1.22	7 (10%)	82,113,113	1.35	8 (9%)
22	CLA	B	609	2	69,73,73	1.14	9 (13%)	82,113,113	1.43	12 (14%)
22	CLA	b	607	2	69,73,73	1.30	9 (13%)	82,113,113	1.34	10 (12%)
33	STE	C	522	-	11,11,19	0.74	0	11,11,19	1.31	2 (18%)
29	SQD	a	413	-	35,35,54	1.27	2 (5%)	37,37,65	1.51	6 (16%)
33	STE	c	523	-	19,19,19	0.82	0	19,19,19	0.82	0
32	OEY	a	417[B]	1,36,3	0,16,16	-	-	-		
24	BCR	b	616	-	41,41,41	1.23	5 (12%)	56,56,56	1.46	12 (21%)
22	CLA	c	511	3	69,73,73	1.42	7 (10%)	82,113,113	1.43	9 (10%)
31	OEX	A	416[A]	1,36,3	0,14,14	-	-	-		
22	CLA	c	515	3	69,73,73	1.34	10 (14%)	82,113,113	1.04	7 (8%)
24	BCR	C	515	-	41,41,41	1.32	4 (9%)	56,56,56	1.32	8 (14%)
28	LMG	A	412	-	48,48,55	1.05	2 (4%)	56,56,63	1.44	7 (12%)
33	STE	b	626	-	9,9,19	0.59	0	8,8,19	0.44	0
30	DGD	C	516	-	63,63,67	1.17	6 (9%)	77,77,81	1.41	17 (22%)
35	HEC	F	101	6,5	50,50,50	1.64	6 (12%)	68,82,82	1.45	12 (17%)
34	LHG	D	409	-	46,46,48	1.01	2 (4%)	49,52,54	1.36	2 (4%)
29	SQD	b	619	-	47,49,54	0.95	2 (4%)	57,60,65	2.07	14 (24%)
30	DGD	C	518	-	63,63,67	0.97	5 (7%)	77,77,81	1.31	7 (9%)
22	CLA	b	614	2	69,73,73	1.73	8 (11%)	82,113,113	1.52	12 (14%)
24	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	7 (12%)
22	CLA	C	508	36	69,73,73	1.42	7 (10%)	82,113,113	1.61	13 (15%)
22	CLA	C	505	36	63,67,73	1.32	7 (11%)	74,105,113	1.44	11 (14%)
22	CLA	A	403	36	69,73,73	1.30	10 (14%)	82,113,113	1.21	9 (10%)
33	STE	B	601	-	11,11,19	0.64	0	11,11,19	1.30	2 (18%)
28	LMG	B	629	-	55,55,55	1.48	6 (10%)	63,63,63	1.48	7 (11%)
29	SQD	A	414	-	38,38,54	1.08	3 (7%)	40,40,65	1.36	5 (12%)
24	BCR	T	101	-	41,41,41	1.09	4 (9%)	56,56,56	1.37	6 (10%)
24	BCR	B	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.42	11 (19%)
22	CLA	C	509	3	69,73,73	1.30	10 (14%)	82,113,113	1.60	12 (14%)
28	LMG	b	621	-	51,51,55	0.98	3 (5%)	59,59,63	1.47	10 (16%)
22	CLA	a	405	1	69,73,73	1.49	9 (13%)	82,113,113	1.38	7 (8%)
22	CLA	c	512	3	69,73,73	1.23	6 (8%)	82,113,113	1.21	7 (8%)
33	STE	X	101	-	19,19,19	0.67	0	19,19,19	1.31	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	B	628	-	14,14,19	0.43	0	13,13,19	0.88	0
22	CLA	b	604	2	69,73,73	1.14	5 (7%)	82,113,113	1.56	12 (14%)
22	CLA	a	402	1	69,73,73	1.32	8 (11%)	82,113,113	1.39	12 (14%)
26	BCT	A	409	21	3,3,3	1.12	0	2,3,3	3.38	2 (100%)
22	CLA	a	403	36	69,73,73	1.25	7 (10%)	82,113,113	1.21	8 (9%)
22	CLA	d	403	4	69,73,73	1.52	11 (15%)	82,113,113	1.31	9 (10%)
22	CLA	b	602	2	69,73,73	1.32	9 (13%)	82,113,113	1.60	19 (23%)
23	PHO	D	401	-	58,69,69	1.91	8 (13%)	55,99,99	1.36	9 (16%)
30	DGD	c	519	-	63,63,67	1.37	8 (12%)	77,77,81	1.43	15 (19%)
22	CLA	b	613	2	69,73,73	1.13	6 (8%)	82,113,113	1.23	10 (12%)
24	BCR	c	516	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
27	PL9	D	405	-	55,55,55	1.65	10 (18%)	68,69,69	1.71	13 (19%)
29	SQD	A	413	-	50,52,54	0.94	4 (8%)	60,63,65	1.94	10 (16%)
28	LMG	d	409	-	44,44,55	1.02	4 (9%)	52,52,63	1.41	7 (13%)
32	OXY	A	417[B]	1,36,3	0,16,16	-	-	-	-	-
33	STE	b	625	-	19,19,19	0.81	0	19,19,19	0.72	0
24	BCR	B	620	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	8 (14%)
33	STE	b	620	-	15,15,19	0.47	0	14,14,19	0.71	0
22	CLA	C	507	3	69,73,73	1.40	11 (15%)	82,113,113	1.17	5 (6%)
24	BCR	a	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.45	8 (14%)
33	STE	M	103	-	9,9,19	0.45	0	8,8,19	0.59	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
22	CLA	c	506	36	-	10/33/109/115	-
22	CLA	c	508	3	-	15/39/115/115	-
24	BCR	b	617	-	-	3/29/63/63	0/2/2/2
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
34	LHG	D	408	-	-	21/53/53/53	-
22	CLA	b	615	2	-	9/33/109/115	-
22	CLA	A	405	1	-	6/26/102/115	-
28	LMG	c	525	-	-	18/44/64/70	0/1/1/1
29	SQD	f	101	-	-	13/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	606	36	-	12/39/115/115	-
33	STE	Z	102	-	-	2/5/5/17	-
33	STE	C	521	-	-	5/13/13/17	-
30	DGD	c	521	-	-	13/51/91/95	0/2/2/2
22	CLA	C	510	3	-	6/39/115/115	-
22	CLA	C	511	3	-	8/39/115/115	-
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
30	DGD	A	415	-	-	21/55/95/95	0/2/2/2
22	CLA	B	615	2	-	12/39/115/115	-
34	LHG	e	102	-	-	23/46/46/53	-
27	PL9	A	410	-	-	19/53/73/73	0/1/1/1
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
34	LHG	E	101	-	-	27/53/53/53	-
22	CLA	c	503	3	-	5/39/115/115	-
34	LHG	d	408	-	-	15/43/43/53	-
28	LMG	c	522	-	-	9/31/51/70	0/1/1/1
27	PL9	a	410	-	-	17/53/73/73	0/1/1/1
34	LHG	D	412	-	-	17/53/53/53	-
22	CLA	B	610	2	-	6/39/115/115	-
28	LMG	C	519	-	-	19/43/63/70	0/1/1/1
33	STE	a	414	-	-	3/7/7/17	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
33	STE	I	101	-	-	4/12/12/17	-
22	CLA	B	614	2	-	10/39/115/115	-
34	LHG	B	622	-	-	20/53/53/53	-
28	LMG	M	101	-	-	19/46/66/70	0/1/1/1
22	CLA	d	402	4	-	9/39/115/115	-
22	CLA	C	502	3	-	2/39/115/115	-
22	CLA	c	504	3	-	5/39/115/115	-
24	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
33	STE	b	624	-	-	8/13/13/17	-
33	STE	C	520	-	-	3/9/9/17	-
33	STE	M	102	-	-	5/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	j	101	-	-	4/9/9/17	-
33	STE	l	102	-	-	7/15/15/17	-
24	BCR	c	518	-	-	8/29/63/63	0/2/2/2
28	LMG	b	623	-	-	20/50/70/70	0/1/1/1
33	STE	B	625	-	-	5/9/9/17	-
22	CLA	B	604	2	-	8/39/115/115	-
22	CLA	D	402	4	-	7/39/115/115	-
24	BCR	y	101	-	-	11/29/63/63	0/2/2/2
28	LMG	D	411	-	-	10/22/22/70	-
22	CLA	B	616	2	-	7/39/115/115	-
22	CLA	b	601	2	-	5/39/115/115	-
33	STE	d	410	-	-	9/14/14/17	-
22	CLA	B	602	36	-	17/39/115/115	-
22	CLA	D	403	4	-	7/39/115/115	-
33	STE	c	501	-	-	5/9/9/17	-
34	LHG	d	407	-	-	19/53/53/53	-
33	STE	B	621	-	-	6/14/14/17	-
22	CLA	B	613	2	-	7/39/115/115	-
30	DGD	C	517	-	-	18/51/91/95	0/2/2/2
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
24	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
28	LMG	D	410	-	-	15/33/33/70	-
33	STE	B	627	-	-	6/13/13/17	-
22	CLA	b	603	2	-	5/39/115/115	-
34	LHG	l	101	-	-	20/53/53/53	-
24	BCR	c	517	-	-	9/29/63/63	0/2/2/2
24	BCR	D	404	-	-	4/29/63/63	0/2/2/2
22	CLA	b	610	2	-	6/39/115/115	-
35	HEC	V	201	17	1/1/7/7	6/14/54/54	-
22	CLA	b	605	2	-	9/39/115/115	-
22	CLA	B	607	2	-	8/39/115/115	-
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
22	CLA	C	504	3	-	3/39/115/115	-
22	CLA	C	512	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	3	-	6/39/115/115	-
27	PL9	d	405	-	-	13/53/73/73	0/1/1/1
28	LMG	c	524	-	-	23/43/63/70	0/1/1/1
22	CLA	C	503	3	-	7/39/115/115	-
29	SQD	a	412	-	-	29/49/69/69	0/1/1/1
33	STE	B	626	-	-	8/15/15/17	-
22	CLA	A	402	1	-	3/39/115/115	-
22	CLA	A	411	36	-	9/39/115/115	-
22	CLA	c	505	3	-	2/39/115/115	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
22	CLA	c	513	3	-	11/39/115/115	-
22	CLA	B	617	2	-	7/33/109/115	-
33	STE	E	102	-	-	3/9/9/17	-
22	CLA	b	612	2	-	4/39/115/115	-
33	STE	B	624	-	-	3/11/11/17	-
22	CLA	B	606	2	-	8/39/115/115	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
35	HEC	v	201	17	1/1/7/7	4/14/54/54	-
22	CLA	C	506	3	-	13/39/115/115	-
29	SQD	B	623	-	-	21/49/69/69	0/1/1/1
22	CLA	B	611	36	-	5/39/115/115	-
22	CLA	B	603	2	-	4/39/115/115	-
33	STE	J	101	-	-	3/9/9/17	-
23	PHO	a	404	-	-	2/37/103/103	0/5/6/6
28	LMG	D	406	-	-	17/46/66/70	0/1/1/1
33	STE	d	411	-	-	10/17/17/17	-
22	CLA	c	510	3	-	9/38/114/115	-
22	CLA	B	605	2	-	11/39/115/115	-
22	CLA	b	608	2	-	7/39/115/115	-
33	STE	h	103	-	-	5/11/11/17	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
33	STE	L	101	-	-	5/9/9/17	-
33	STE	d	412	-	-	7/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	514	3	-	11/39/115/115	-
24	BCR	x	101	-	-	4/29/63/63	0/2/2/2
22	CLA	c	514	3	-	22/39/115/115	-
22	CLA	a	411	36	-	2/39/115/115	-
22	CLA	C	513	3	-	17/39/115/115	-
24	BCR	b	618	-	-	3/29/63/63	0/2/2/2
22	CLA	b	609	36	-	6/39/115/115	-
34	LHG	d	406	-	-	22/53/53/53	-
22	CLA	h	101	36	-	18/39/115/115	-
22	CLA	B	608	36	-	9/39/115/115	-
22	CLA	b	611	2	-	6/39/115/115	-
22	CLA	B	612	2	-	10/39/115/115	-
35	HEC	e	101	6,5	1/1/7/7	7/14/54/54	-
33	STE	T	102	-	-	7/12/12/17	-
33	STE	a	415	-	-	3/9/9/17	-
33	STE	b	622	-	-	11/17/17/17	-
33	STE	H	103	-	-	8/15/15/17	-
22	CLA	c	509	36	-	7/39/115/115	-
22	CLA	B	609	2	-	2/39/115/115	-
22	CLA	b	607	2	-	10/39/115/115	-
33	STE	C	522	-	-	3/9/9/17	-
29	SQD	a	413	-	-	21/37/37/69	-
33	STE	c	523	-	-	10/17/17/17	-
24	BCR	b	616	-	-	5/29/63/63	0/2/2/2
22	CLA	c	511	3	-	9/39/115/115	-
22	CLA	c	515	3	-	6/39/115/115	-
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
28	LMG	A	412	-	-	12/43/63/70	0/1/1/1
33	STE	b	626	-	-	5/7/7/17	-
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
35	HEC	F	101	6,5	1/1/7/7	6/14/54/54	-
34	LHG	D	409	-	-	26/51/51/53	-
29	SQD	b	619	-	-	19/44/64/69	0/1/1/1
30	DGD	C	518	-	-	15/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	614	2	-	9/39/115/115	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	C	508	36	-	10/39/115/115	-
22	CLA	C	505	36	-	8/32/108/115	-
22	CLA	A	403	36	-	9/39/115/115	-
33	STE	B	601	-	-	1/9/9/17	-
28	LMG	B	629	-	-	29/50/70/70	0/1/1/1
29	SQD	A	414	-	-	14/39/39/69	-
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
24	BCR	B	619	-	-	8/29/63/63	0/2/2/2
22	CLA	C	509	3	-	4/39/115/115	-
28	LMG	b	621	-	-	21/46/66/70	0/1/1/1
22	CLA	a	405	1	-	7/39/115/115	-
22	CLA	c	512	3	-	11/39/115/115	-
33	STE	X	101	-	-	10/17/17/17	-
33	STE	B	628	-	-	7/12/12/17	-
22	CLA	b	604	2	-	8/39/115/115	-
22	CLA	a	402	1	-	6/39/115/115	-
22	CLA	a	403	36	-	14/39/115/115	-
22	CLA	d	403	4	-	7/39/115/115	-
22	CLA	b	602	2	-	7/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
30	DGD	c	519	-	-	23/51/91/95	0/2/2/2
22	CLA	b	613	2	-	19/39/115/115	-
24	BCR	c	516	-	-	13/29/63/63	0/2/2/2
27	PL9	D	405	-	-	9/53/73/73	0/1/1/1
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
28	LMG	d	409	-	-	12/39/59/70	0/1/1/1
33	STE	b	625	-	-	6/17/17/17	-
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
33	STE	b	620	-	-	6/13/13/17	-
22	CLA	C	507	3	-	11/39/115/115	-
24	BCR	a	406	-	-	6/29/63/63	0/2/2/2
33	STE	M	103	-	-	2/7/7/17	-

The worst 5 of 868 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	MG-NB	9.21	2.24	2.05
22	a	411	CLA	MG-NA	8.98	2.27	2.06
22	C	512	CLA	MG-NA	8.92	2.27	2.06
22	b	605	CLA	MG-NA	8.78	2.27	2.06
23	d	401	PHO	C1B-C2B	8.65	1.49	1.39

The worst 5 of 1337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4A-NA-C1A	11.43	111.89	106.68
22	B	605	CLA	C4A-NA-C1A	10.71	111.56	106.68
22	b	605	CLA	C4A-NA-C1A	9.73	111.12	106.68
22	h	101	CLA	C4A-NA-C1A	9.72	111.11	106.68
22	C	504	CLA	C4A-NA-C1A	9.57	111.05	106.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	F	101	HEC	NA
35	V	201	HEC	NA
35	e	101	HEC	NA
35	v	201	HEC	NA

5 of 1750 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

117 monomers are involved in 209 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	506	CLA	2	0
22	c	508	CLA	1	0
24	b	617	BCR	5	0
22	b	615	CLA	2	0
28	c	525	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	606	CLA	1	0
33	Z	102	STE	1	0
33	C	521	STE	1	0
22	C	510	CLA	2	0
22	C	511	CLA	1	0
24	H	101	BCR	3	0
30	A	415	DGD	1	0
22	B	615	CLA	1	0
27	A	410	PL9	4	0
24	A	406	BCR	2	0
22	c	503	CLA	1	0
27	a	410	PL9	7	0
34	D	412	LHG	3	0
22	B	610	CLA	2	0
28	C	519	LMG	2	0
22	B	614	CLA	2	0
34	B	622	LHG	1	0
28	M	101	LMG	2	0
22	d	402	CLA	2	0
22	C	502	CLA	1	0
24	Z	101	BCR	3	0
33	M	102	STE	1	0
33	j	101	STE	1	0
33	l	102	STE	1	0
22	B	604	CLA	2	0
22	D	402	CLA	2	0
24	y	101	BCR	1	0
22	B	616	CLA	1	0
22	b	601	CLA	2	0
22	B	602	CLA	2	0
22	D	403	CLA	2	0
34	d	407	LHG	1	0
33	B	621	STE	2	0
22	B	613	CLA	1	0
30	C	517	DGD	1	0
29	D	407	SQD	1	0
24	Y	101	BCR	2	0
33	B	627	STE	1	0
22	b	603	CLA	3	0
24	c	517	BCR	2	0
24	D	404	BCR	5	0
35	V	201	HEC	1	0

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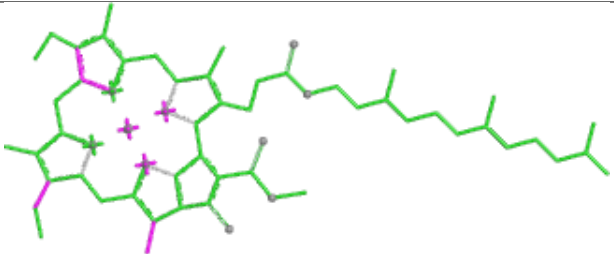
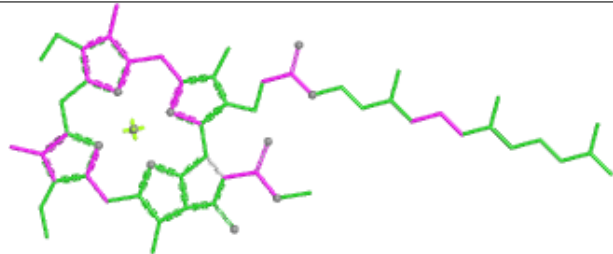
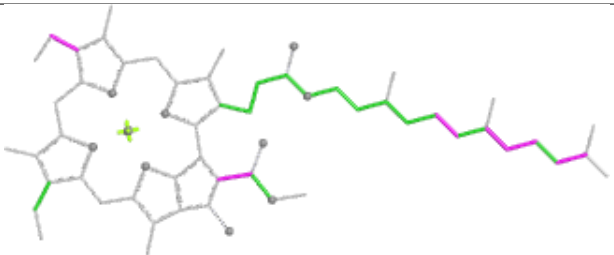
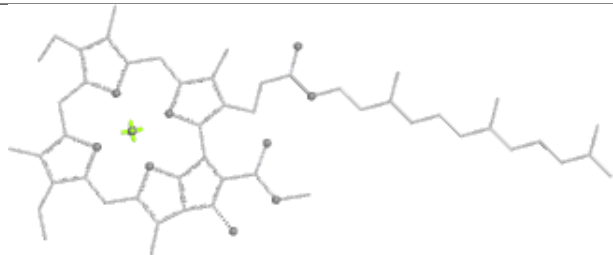
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	605	CLA	7	0
22	B	607	CLA	2	0
22	C	504	CLA	1	0
22	C	512	CLA	1	0
22	c	507	CLA	1	0
22	C	503	CLA	2	0
22	A	402	CLA	1	0
22	A	411	CLA	3	0
24	t	101	BCR	6	0
22	b	612	CLA	1	0
22	B	606	CLA	3	0
24	d	404	BCR	2	0
35	v	201	HEC	5	0
22	C	506	CLA	1	0
31	a	416[A]	OEX	1	0
29	B	623	SQD	2	0
22	B	603	CLA	3	0
23	a	404	PHO	1	0
28	D	406	LMG	5	0
33	d	411	STE	3	0
22	c	510	CLA	1	0
22	B	605	CLA	3	0
22	b	608	CLA	2	0
33	h	103	STE	2	0
23	d	401	PHO	2	0
33	d	412	STE	2	0
22	C	514	CLA	3	0
24	x	101	BCR	1	0
22	c	514	CLA	1	0
22	a	411	CLA	2	0
22	C	513	CLA	4	0
24	b	618	BCR	1	0
34	d	406	LHG	2	0
22	h	101	CLA	1	0
22	B	608	CLA	2	0
22	B	612	CLA	1	0
35	e	101	HEC	7	0
33	T	102	STE	3	0
33	a	415	STE	1	0
33	b	622	STE	2	0
22	c	509	CLA	1	0
22	B	609	CLA	4	0

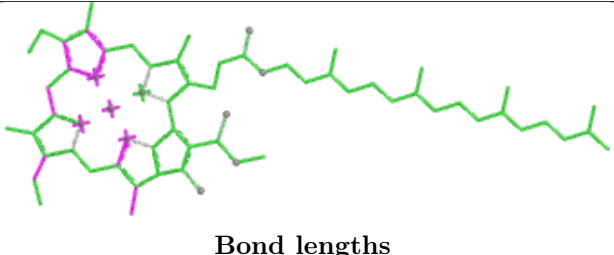
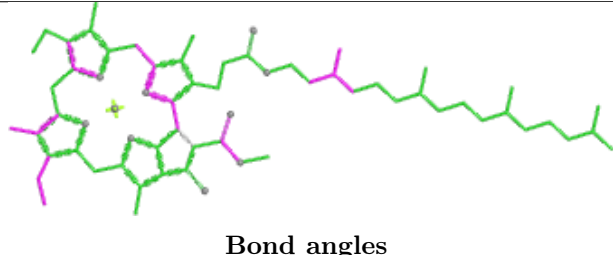
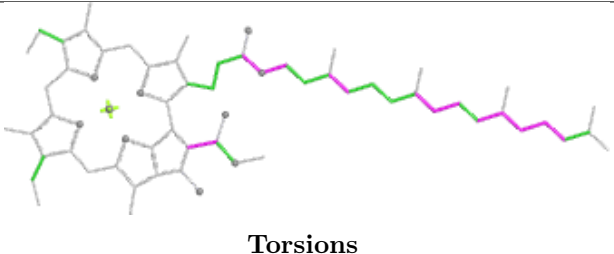
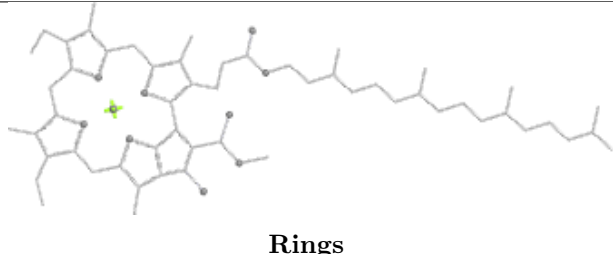
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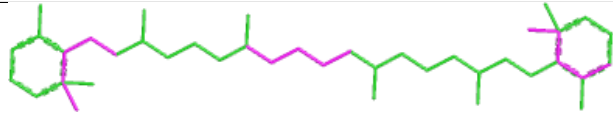
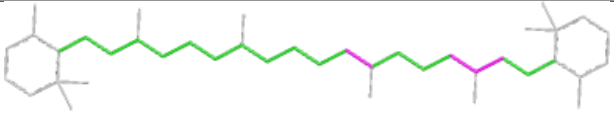
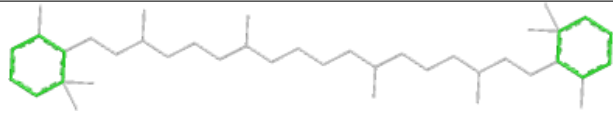
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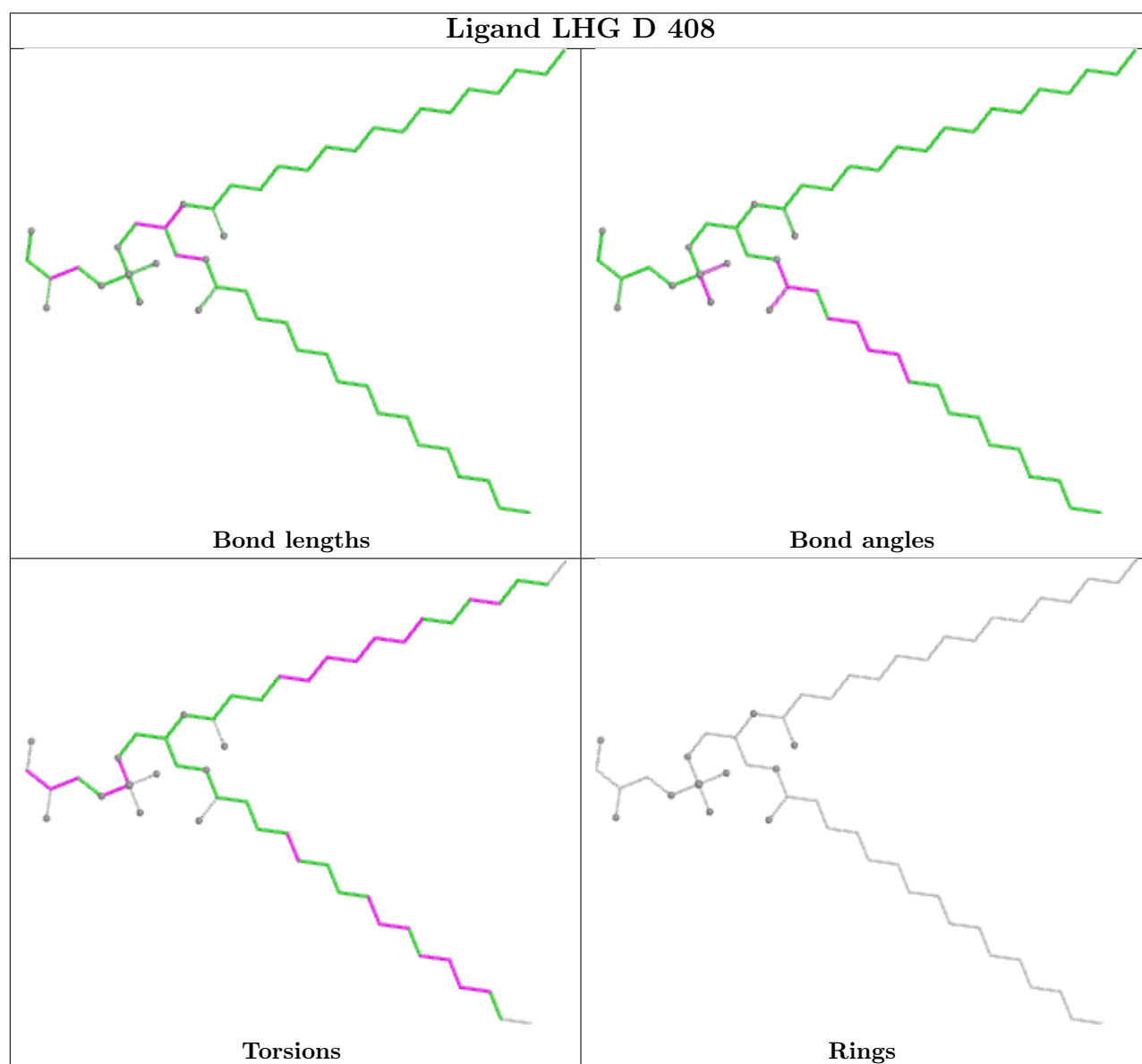
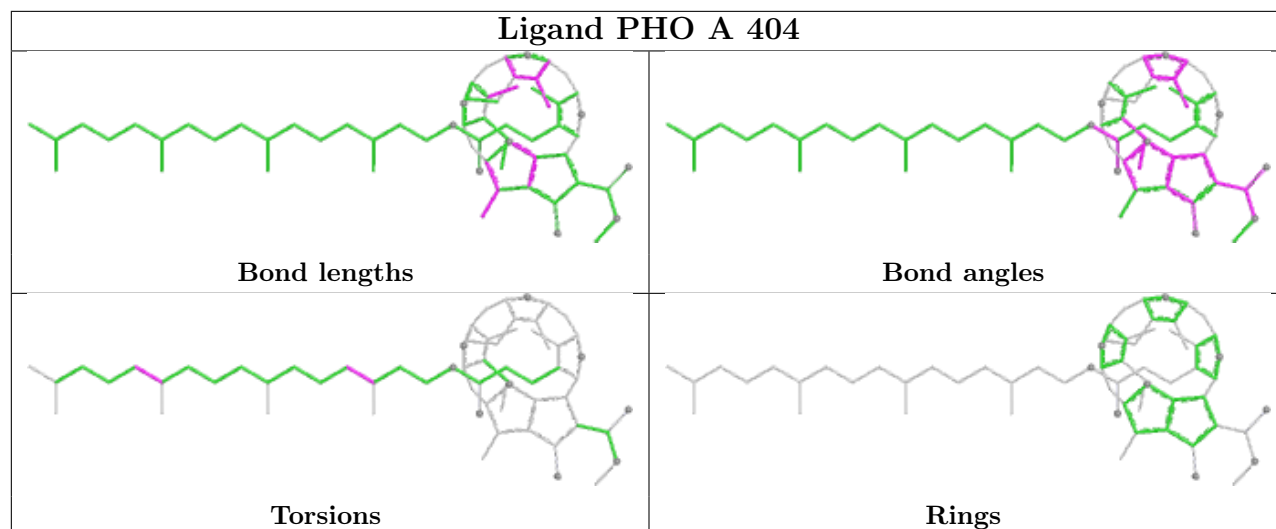
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	b	616	BCR	3	0
31	A	416[A]	OEX	1	0
24	C	515	BCR	1	0
33	b	626	STE	1	0
35	F	101	HEC	3	0
34	D	409	LHG	1	0
29	b	619	SQD	3	0
22	b	614	CLA	4	0
24	B	618	BCR	1	0
22	C	505	CLA	1	0
22	A	403	CLA	1	0
33	B	601	STE	1	0
28	B	629	LMG	2	0
29	A	414	SQD	4	0
24	T	101	BCR	3	0
24	B	619	BCR	3	0
22	C	509	CLA	1	0
28	b	621	LMG	1	0
22	a	405	CLA	1	0
33	X	101	STE	2	0
22	b	604	CLA	1	0
22	a	402	CLA	1	0
23	D	401	PHO	1	0
22	b	613	CLA	7	0
29	A	413	SQD	2	0
32	A	417[B]	OEY	5	0
24	B	620	BCR	2	0

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

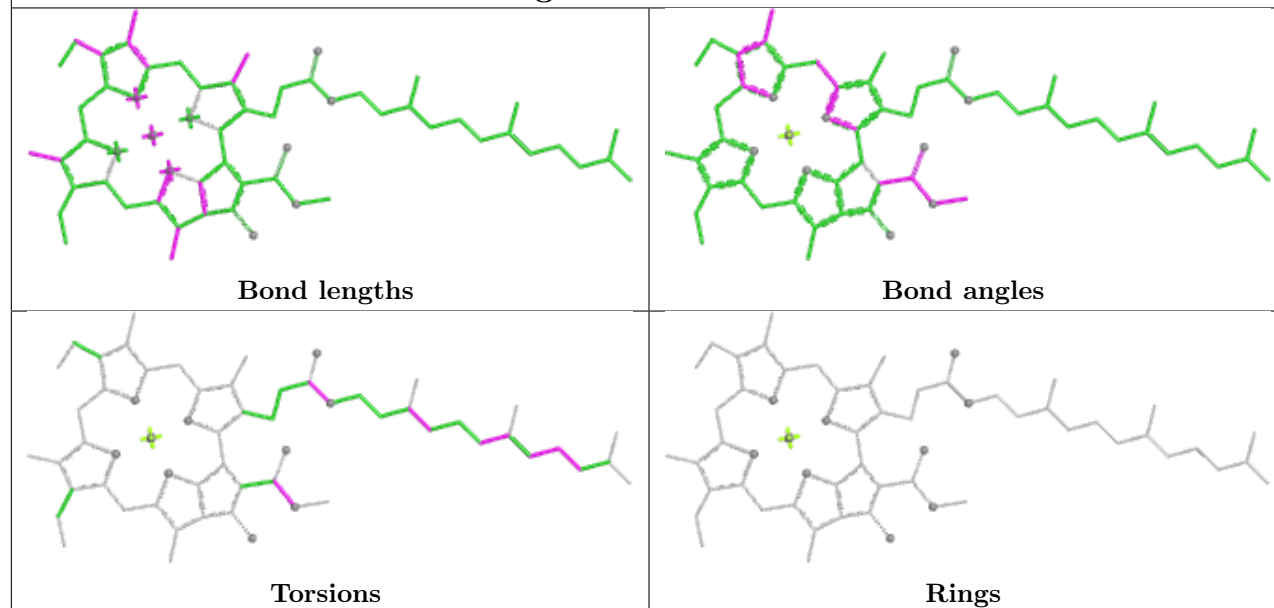
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

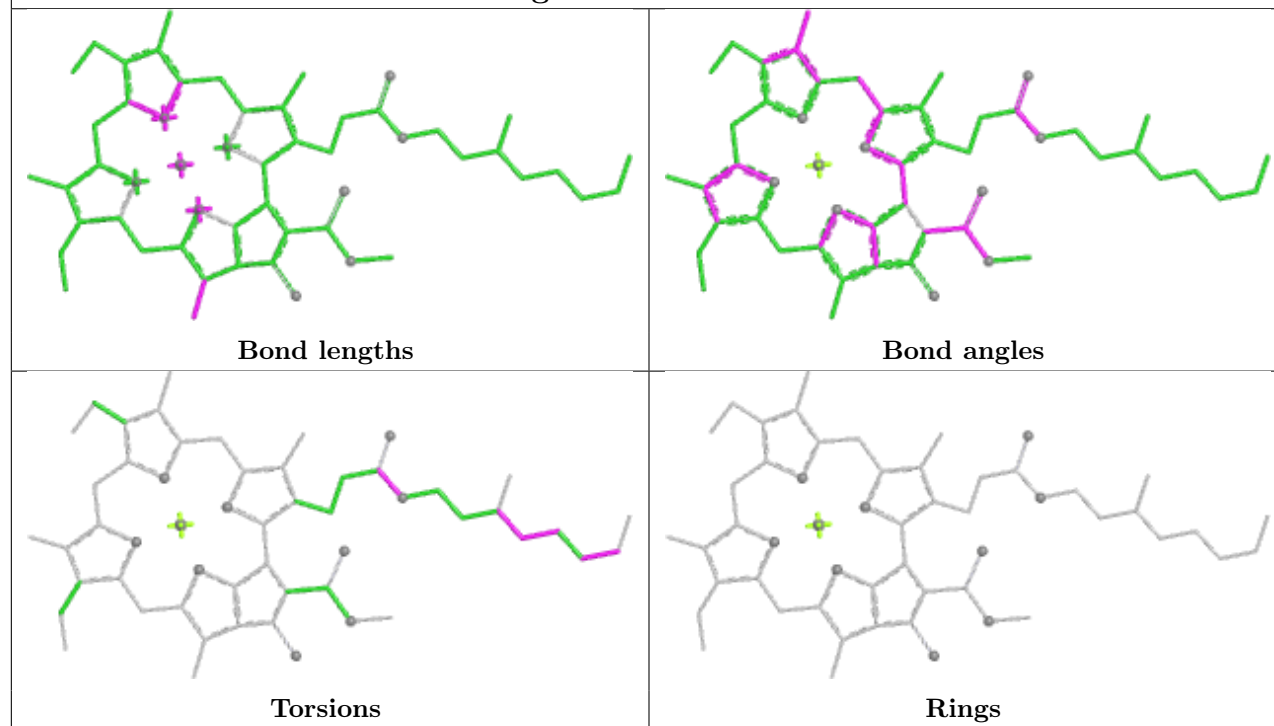
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

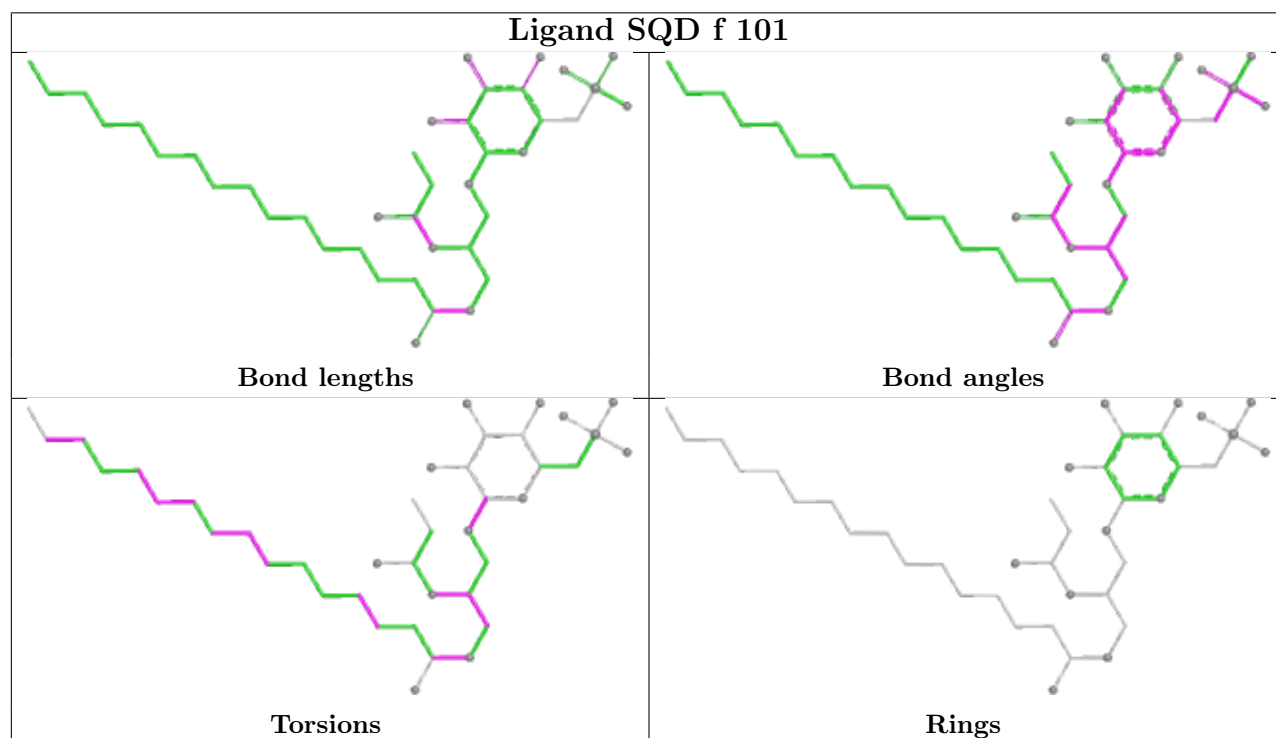
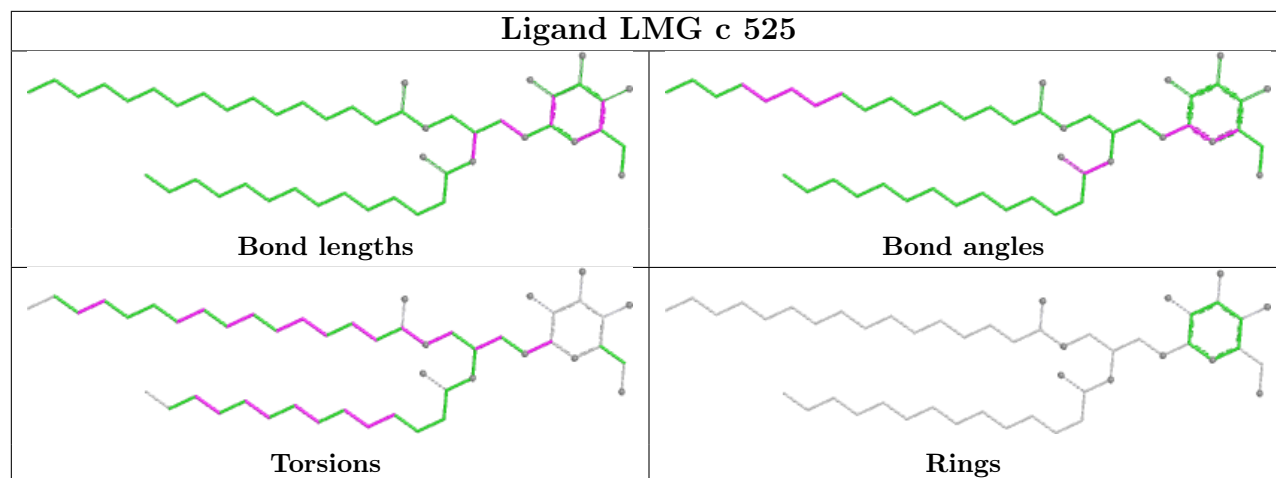


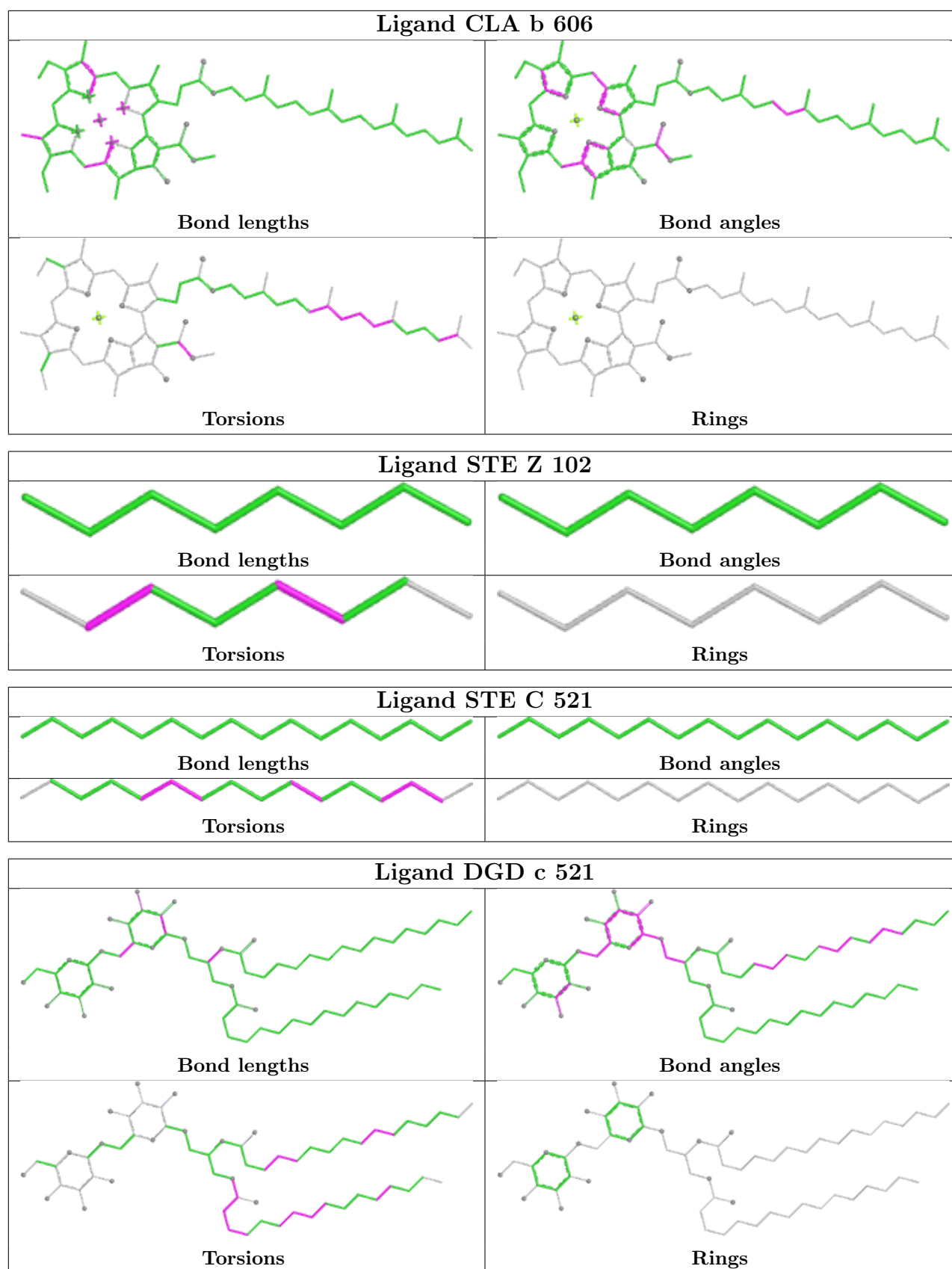
Ligand CLA b 615

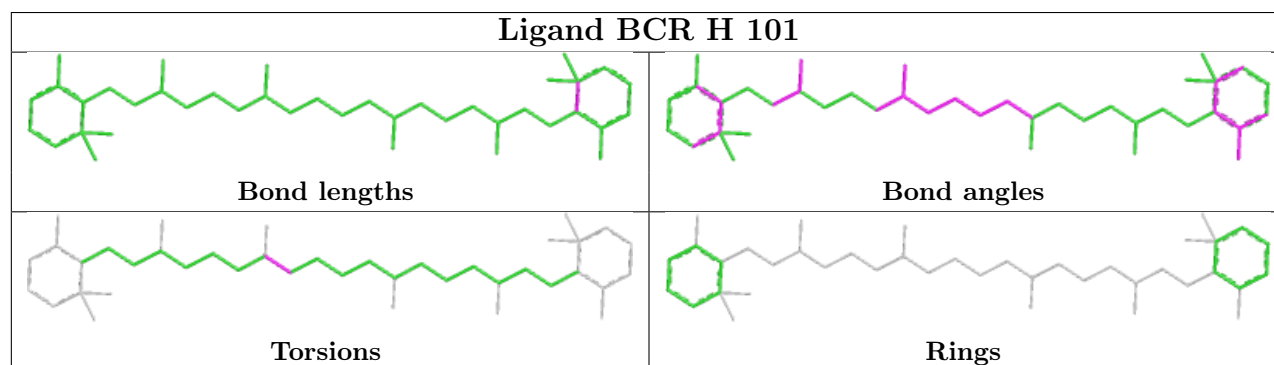
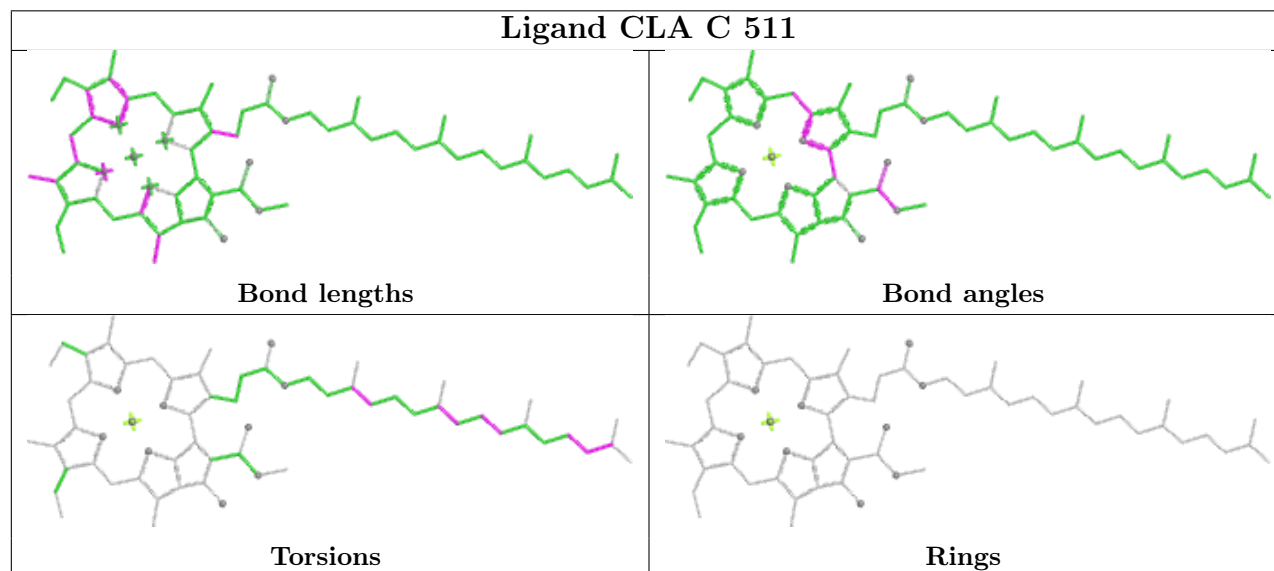
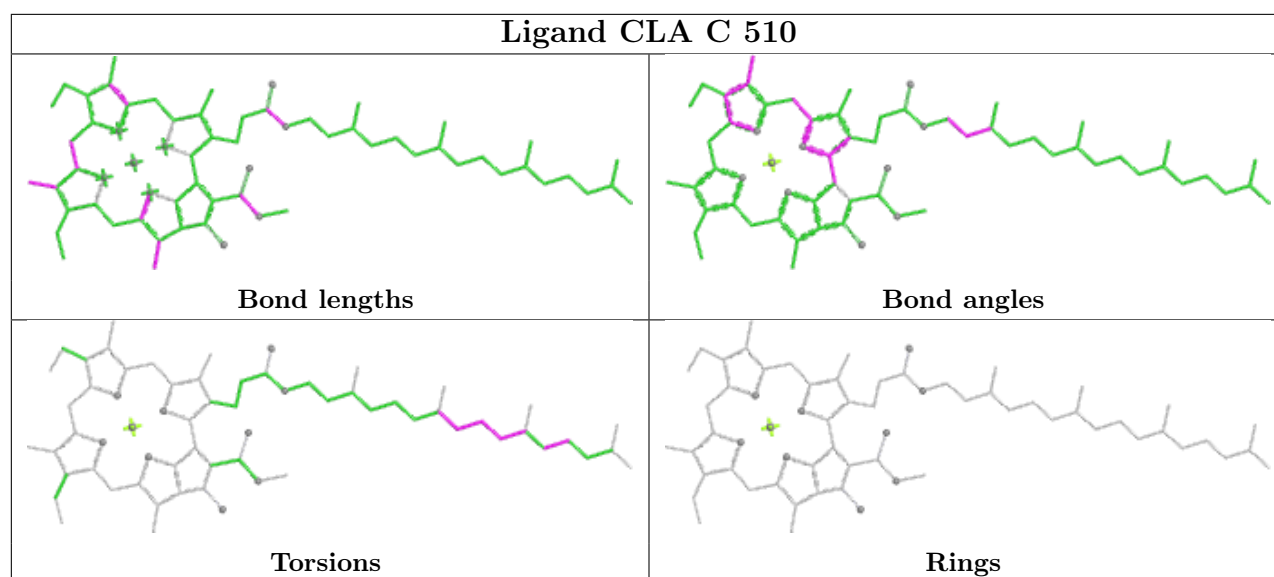


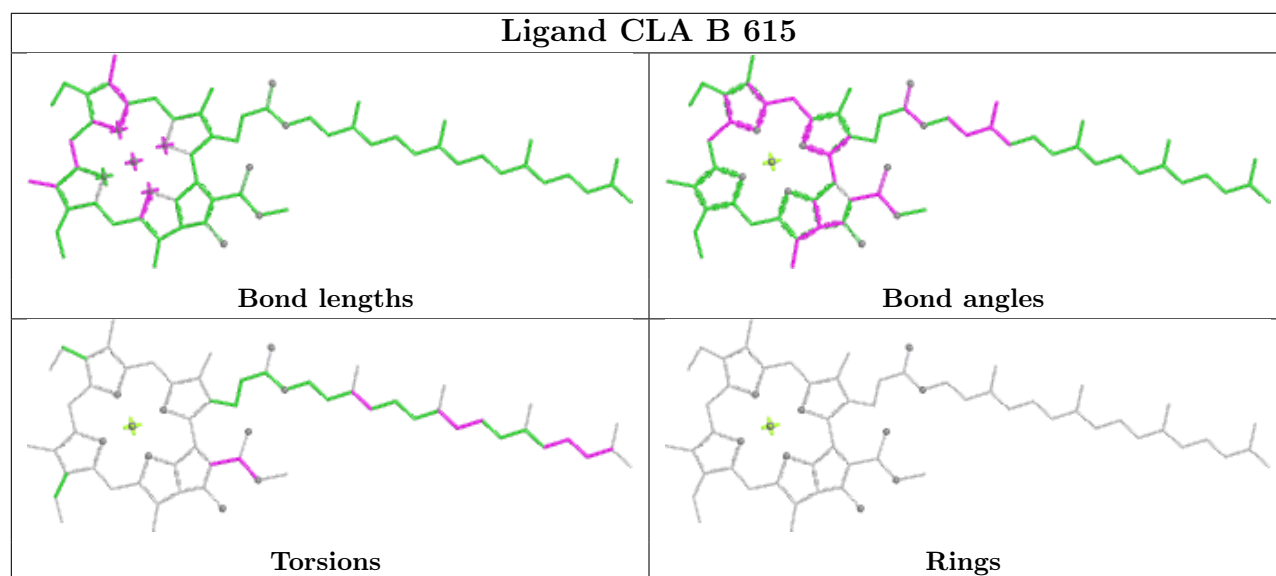
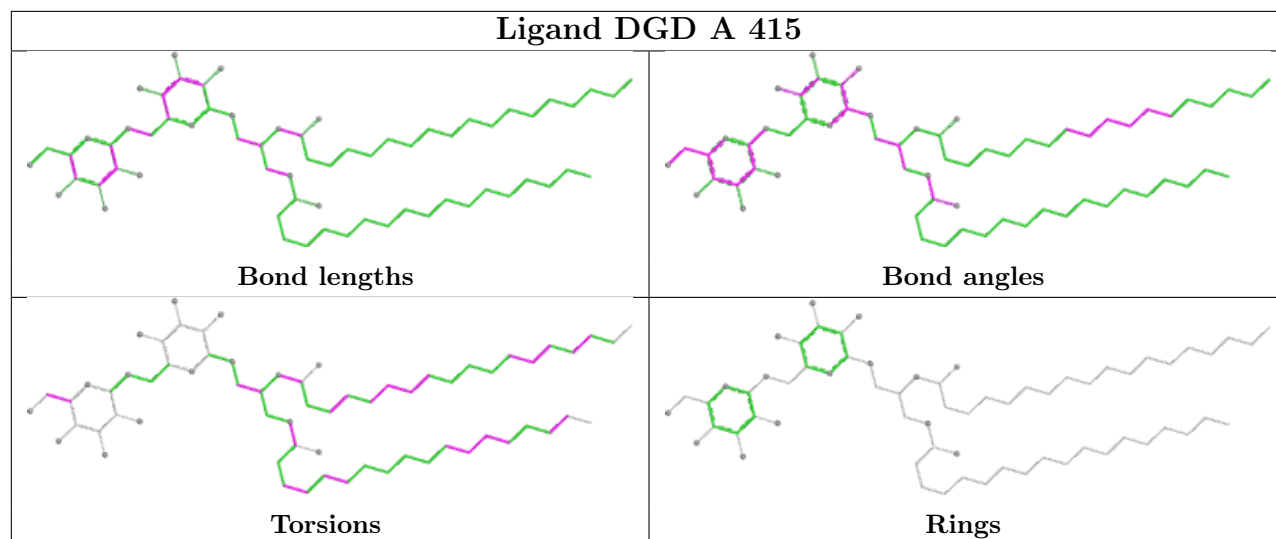
Ligand CLA A 405

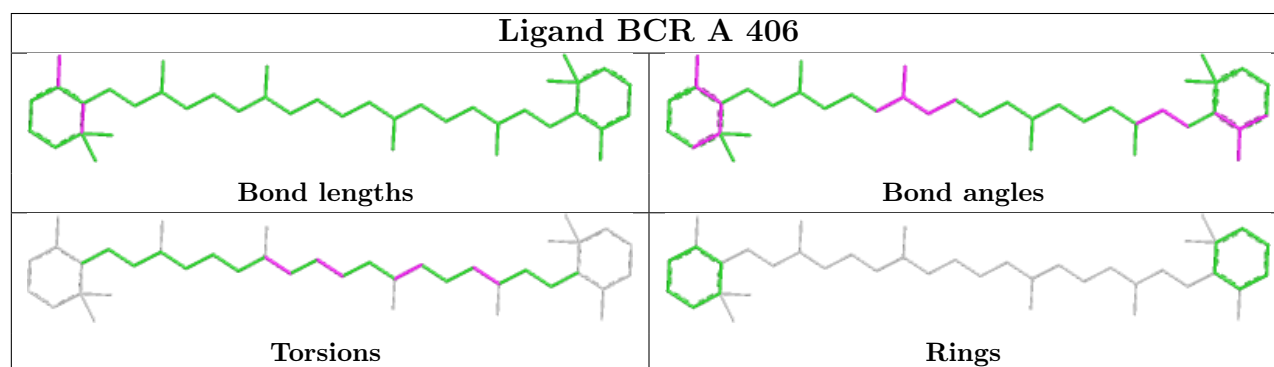
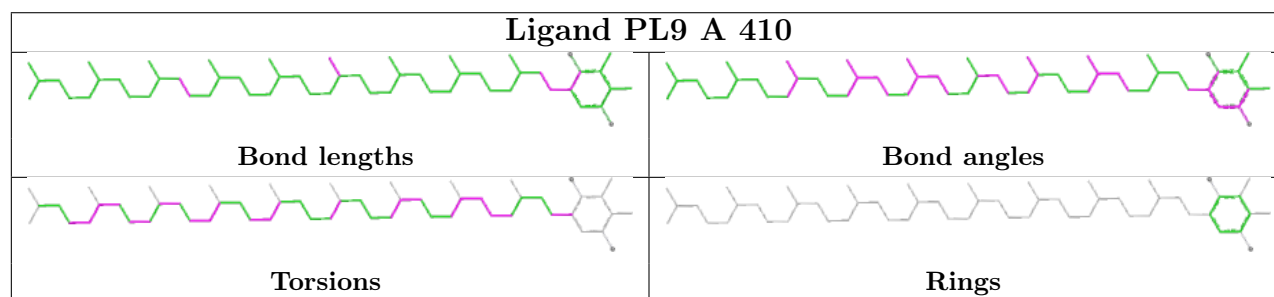
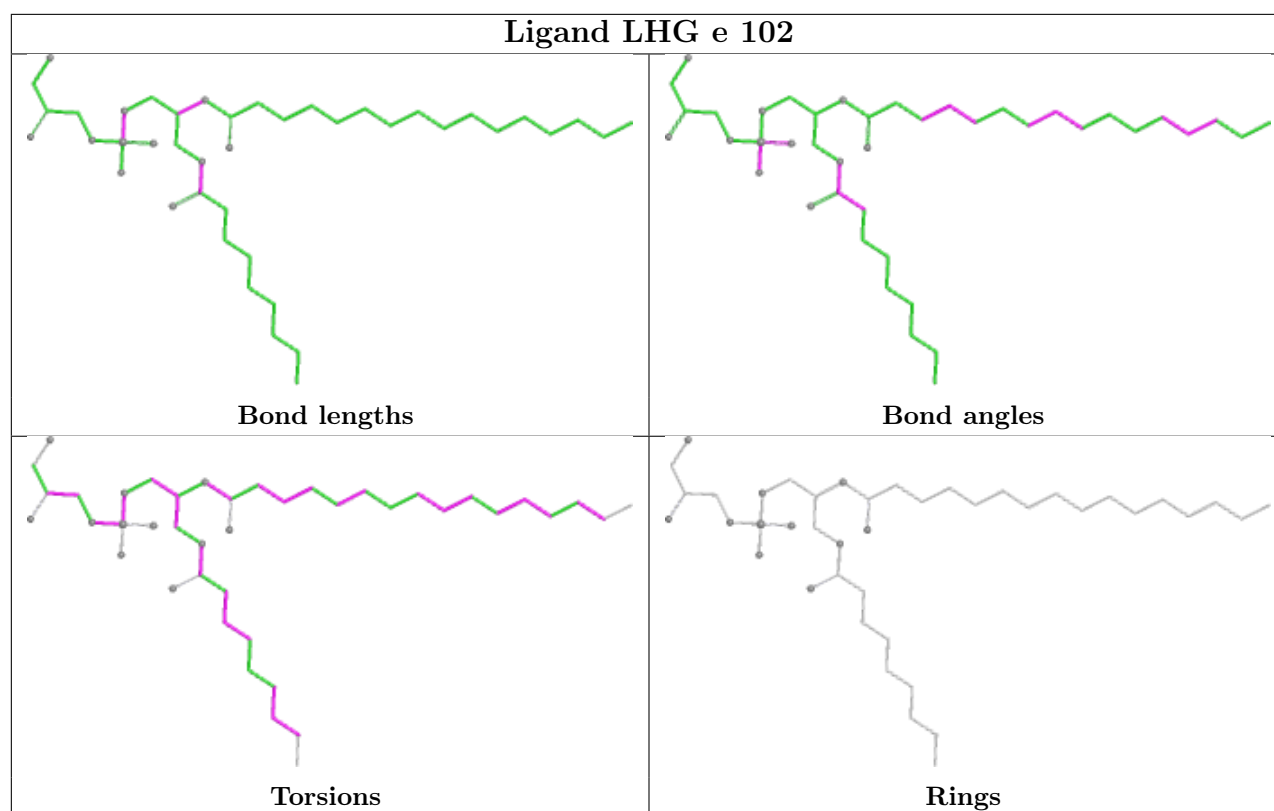


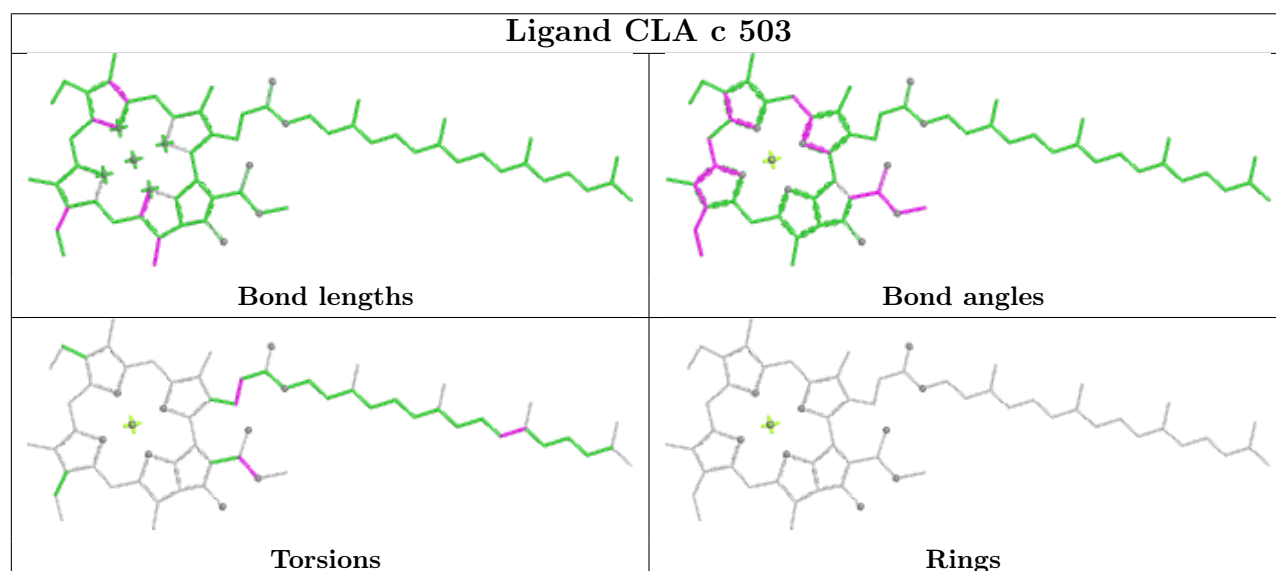
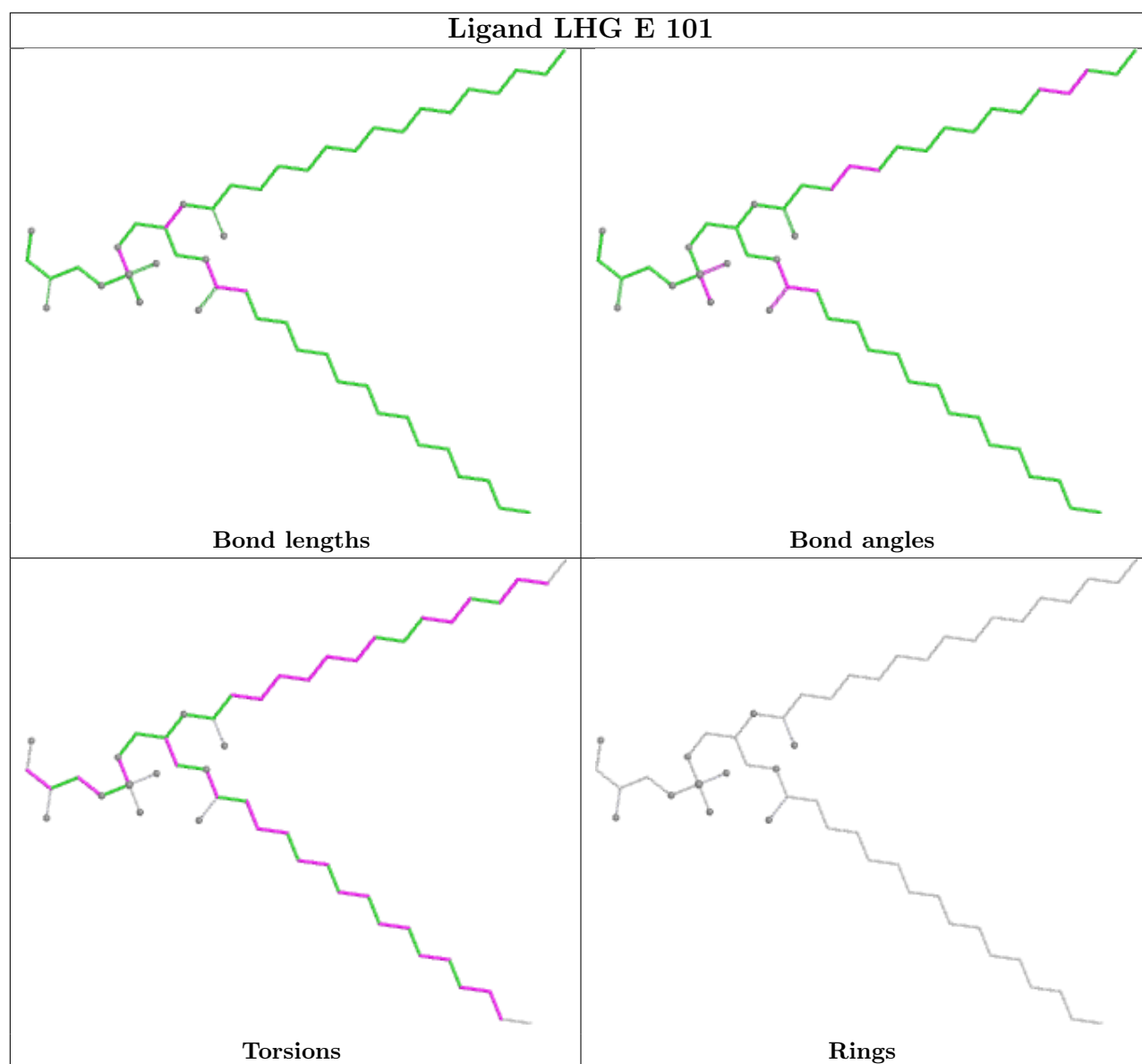




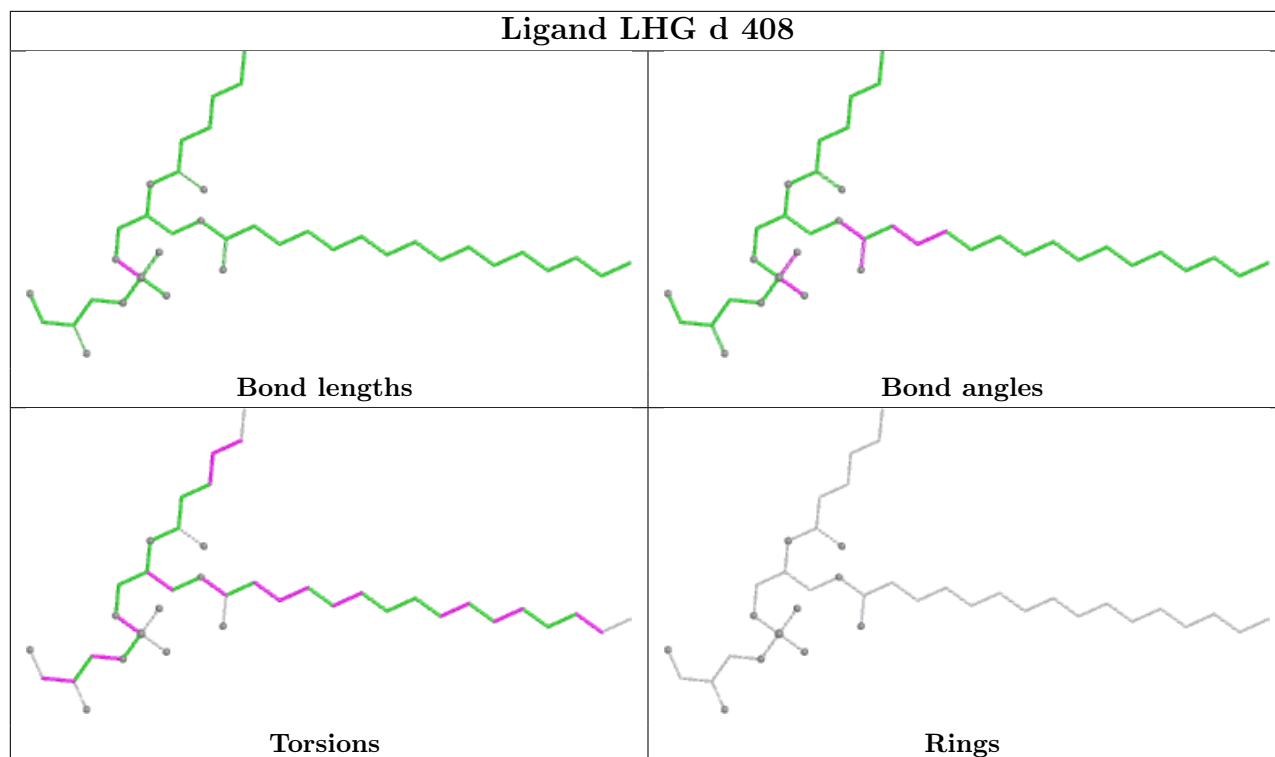




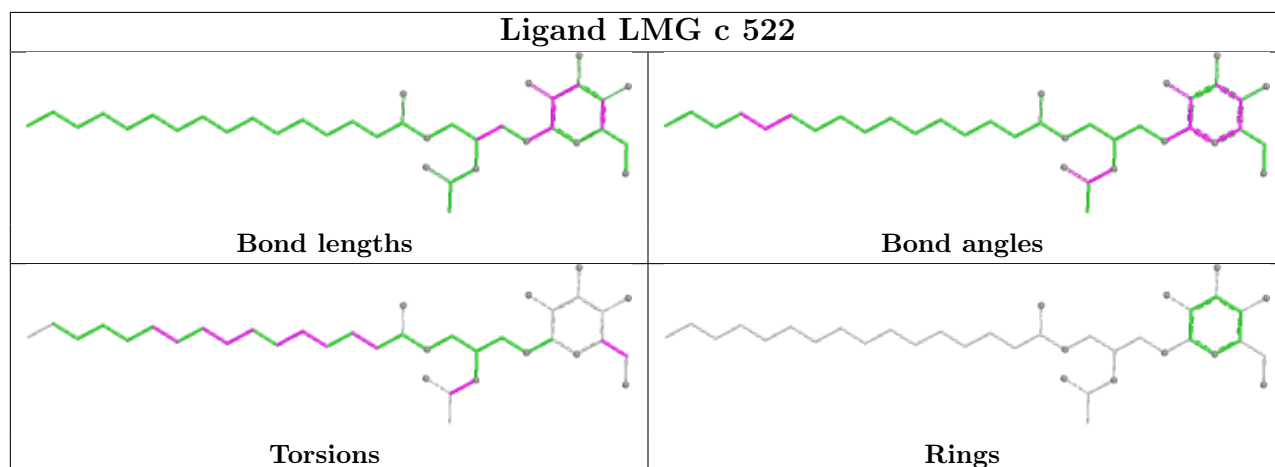




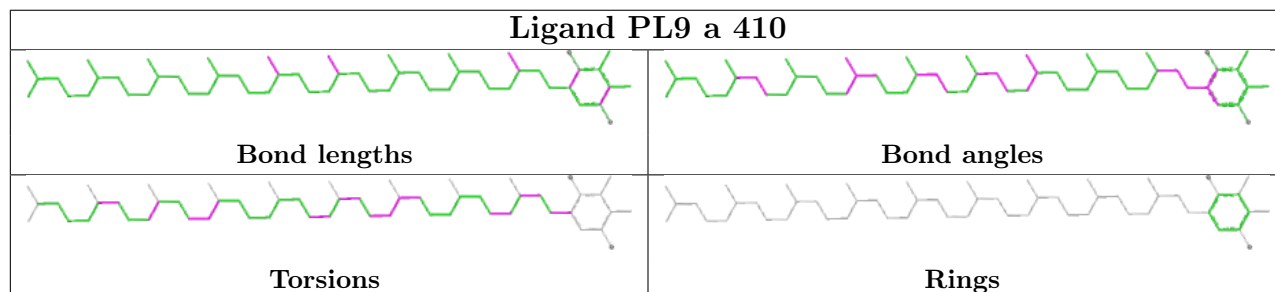
Ligand LHG d 408

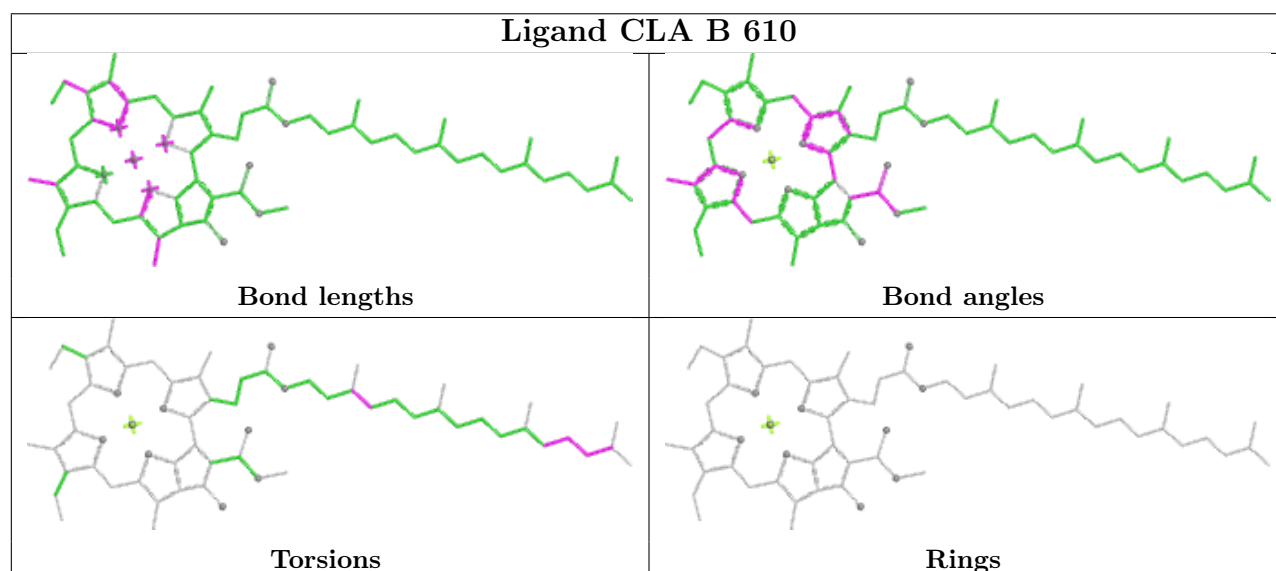
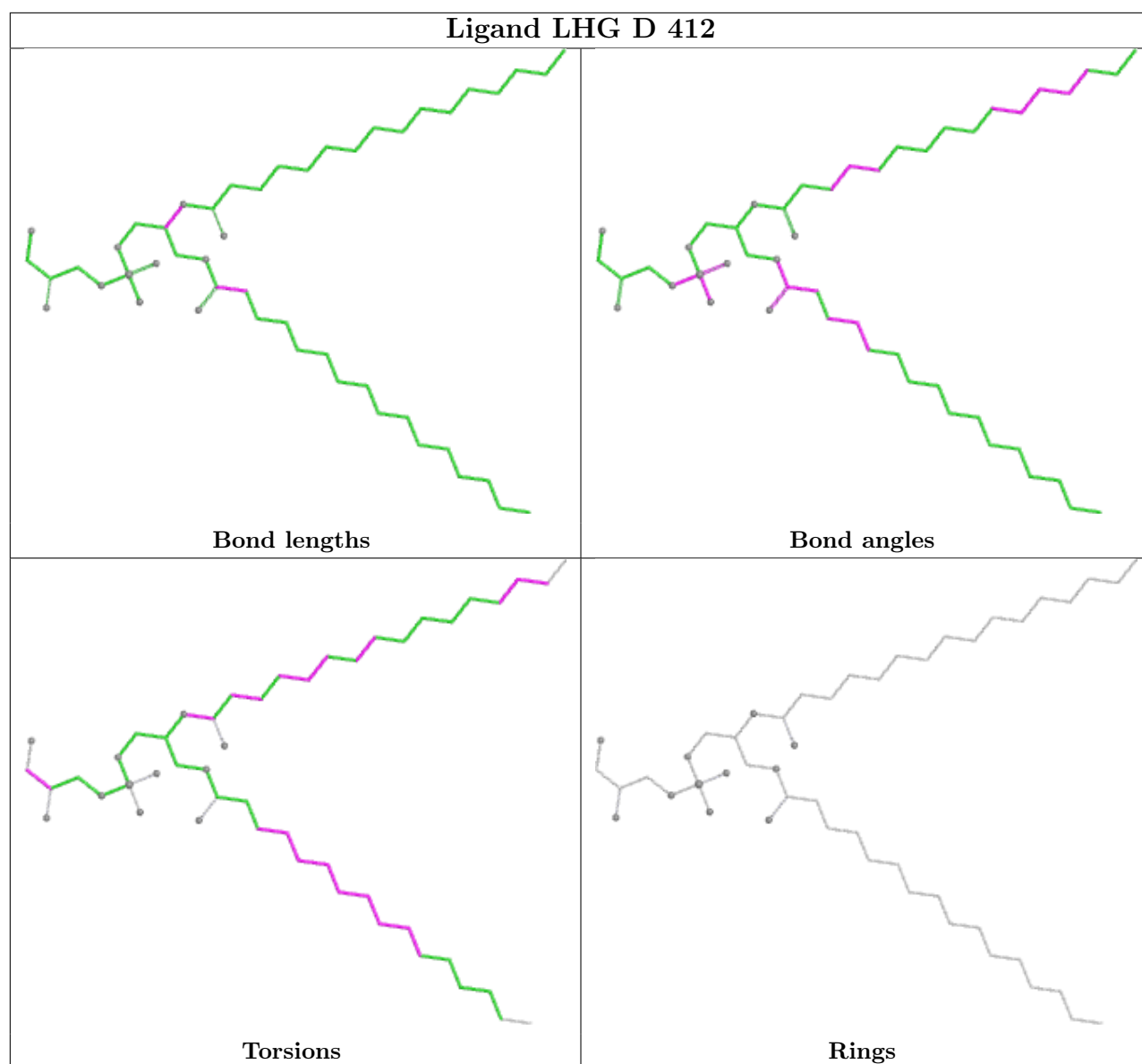


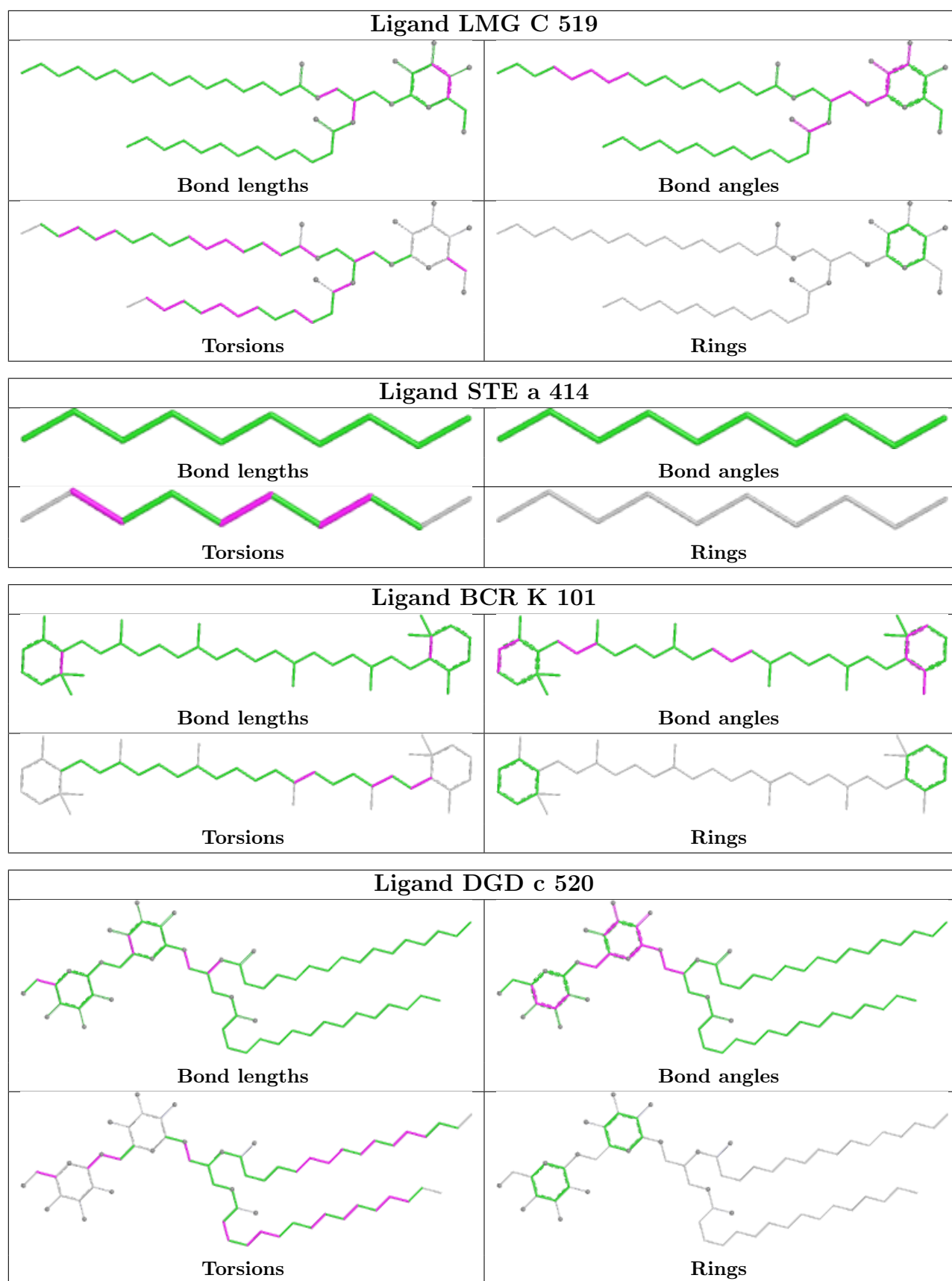
Ligand LMG c 522

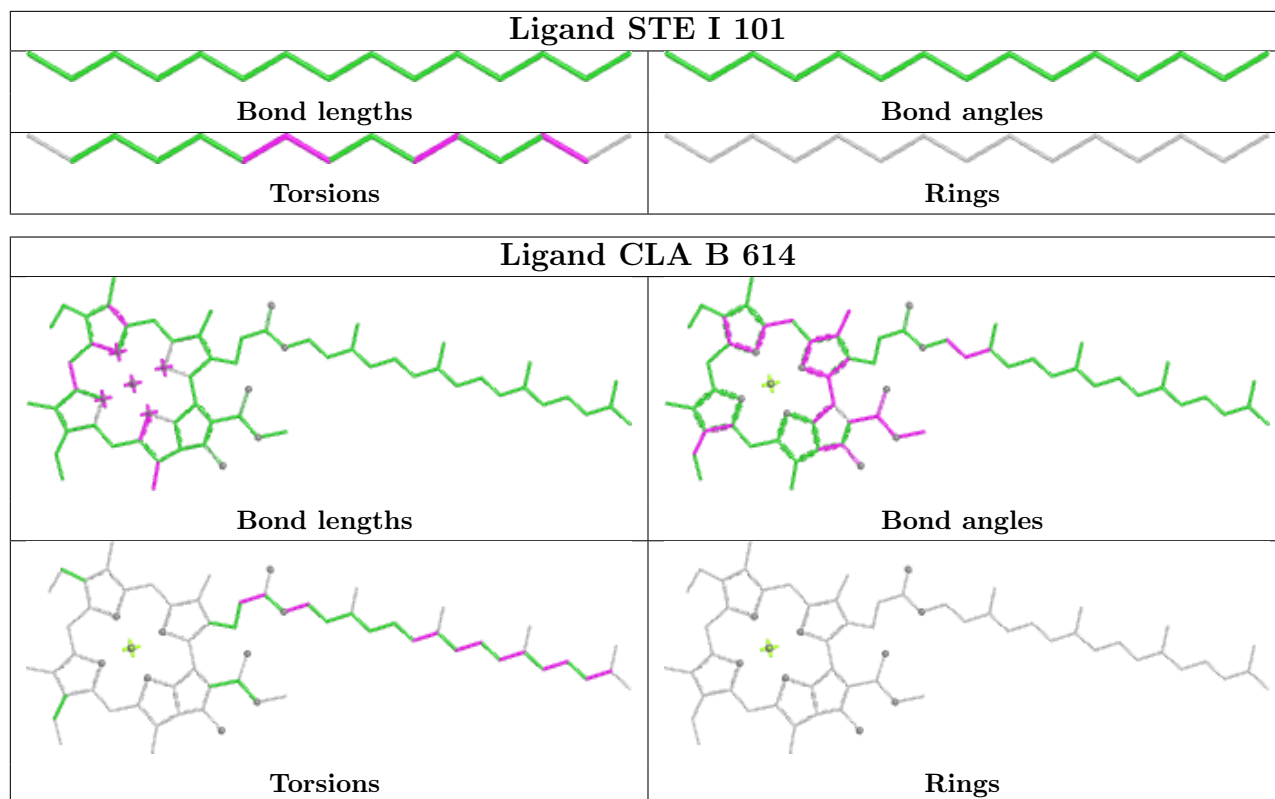


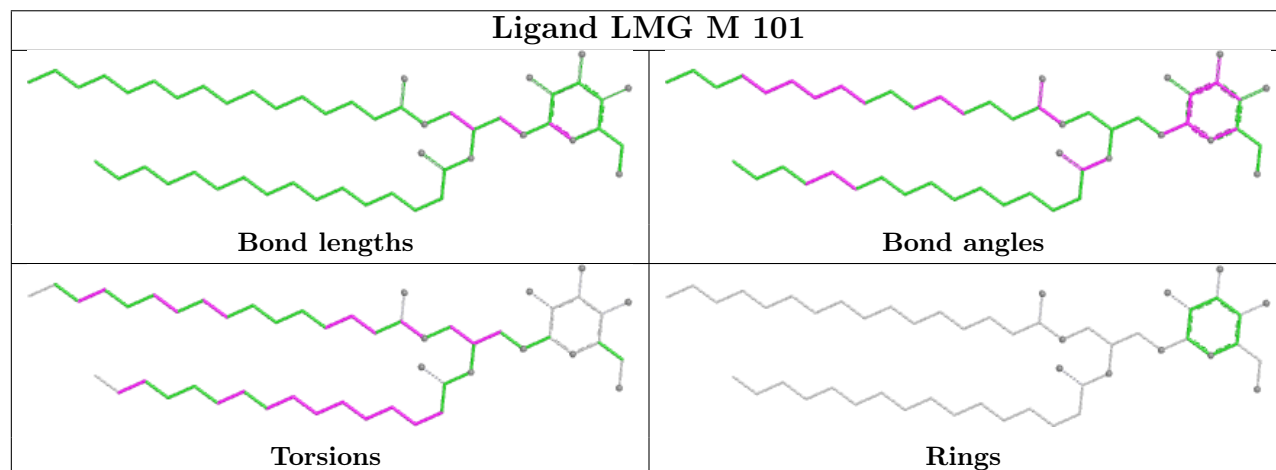
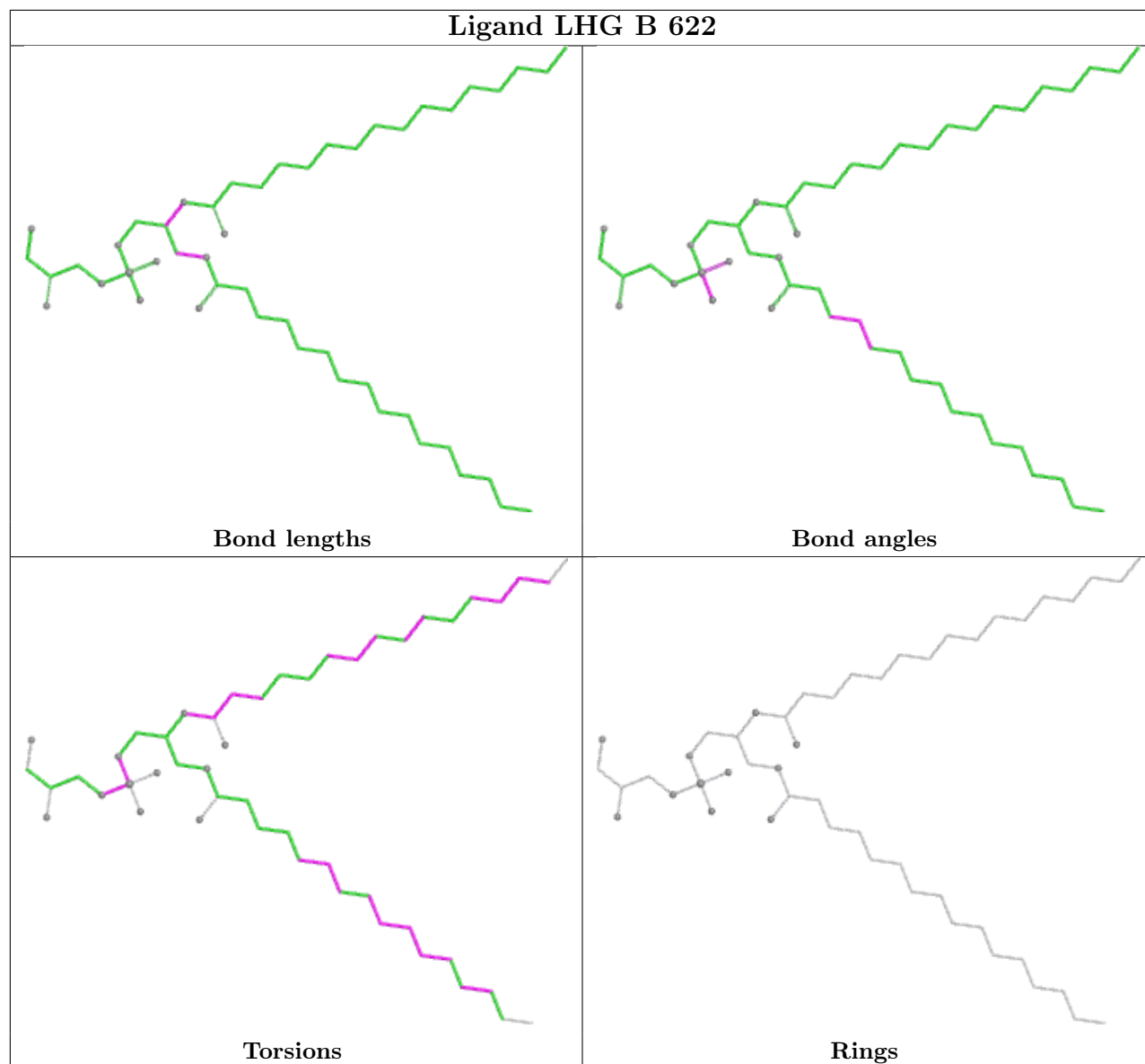
Ligand PL9 a 410



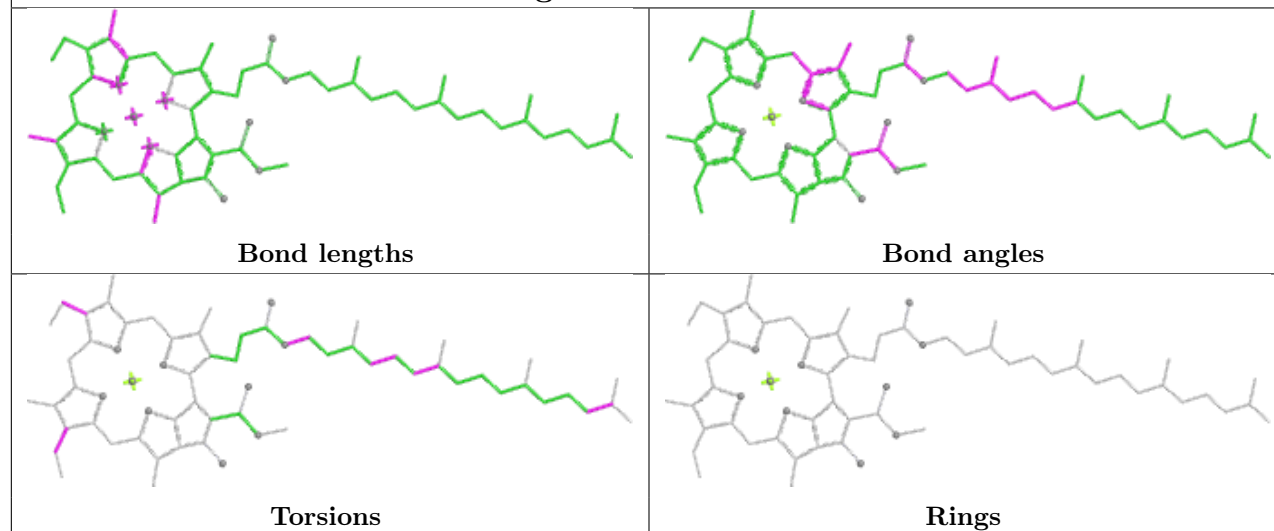




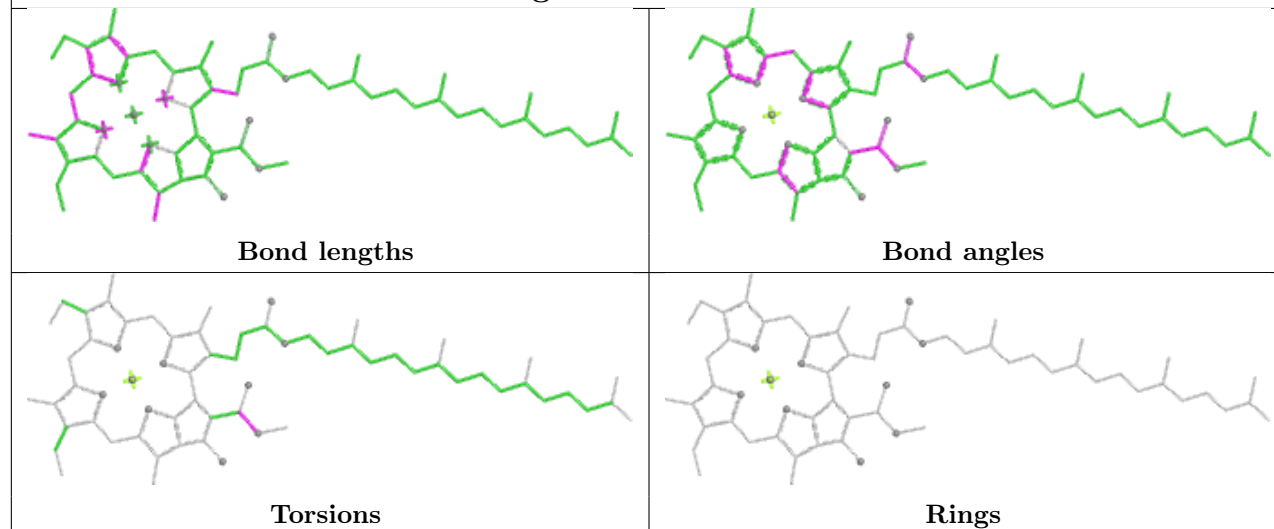




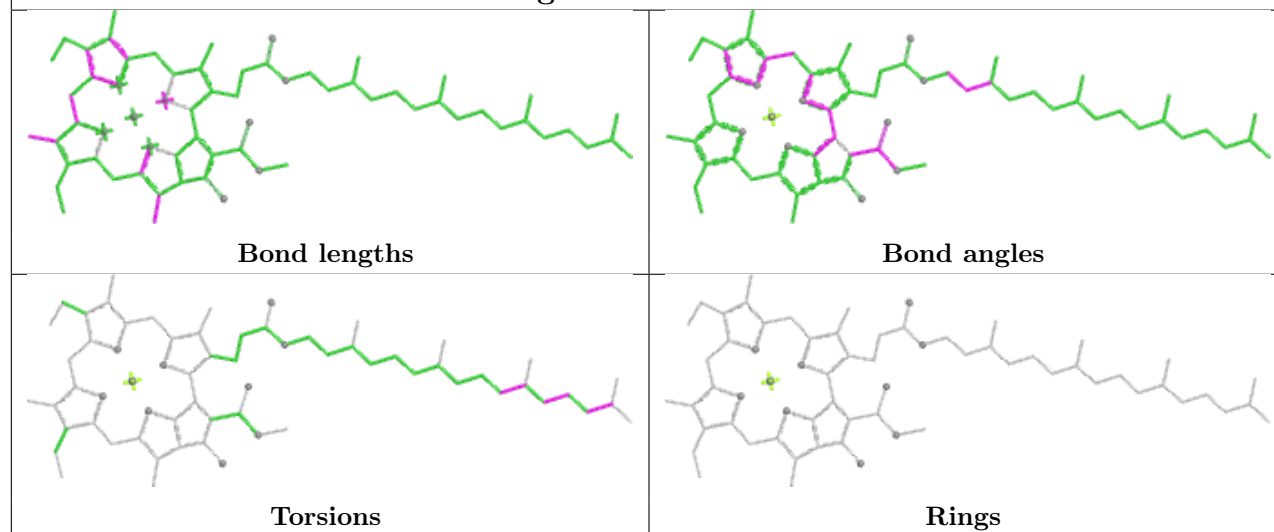
Ligand CLA d 402

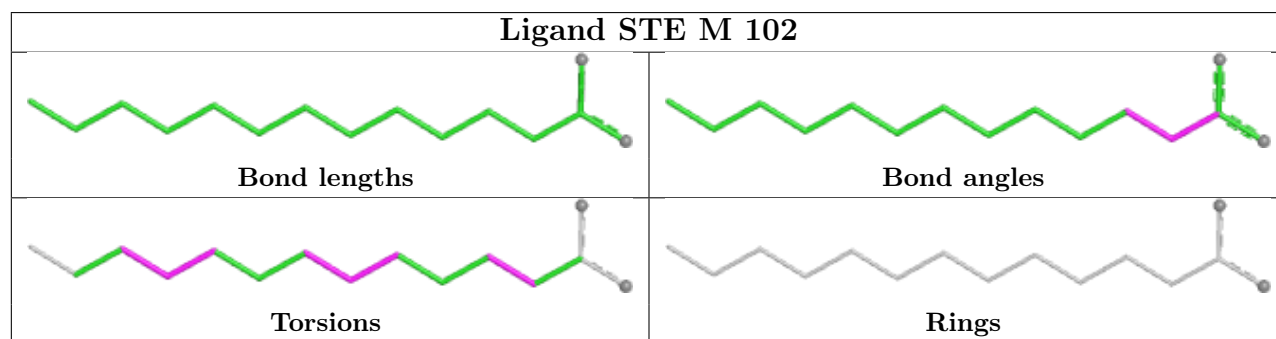
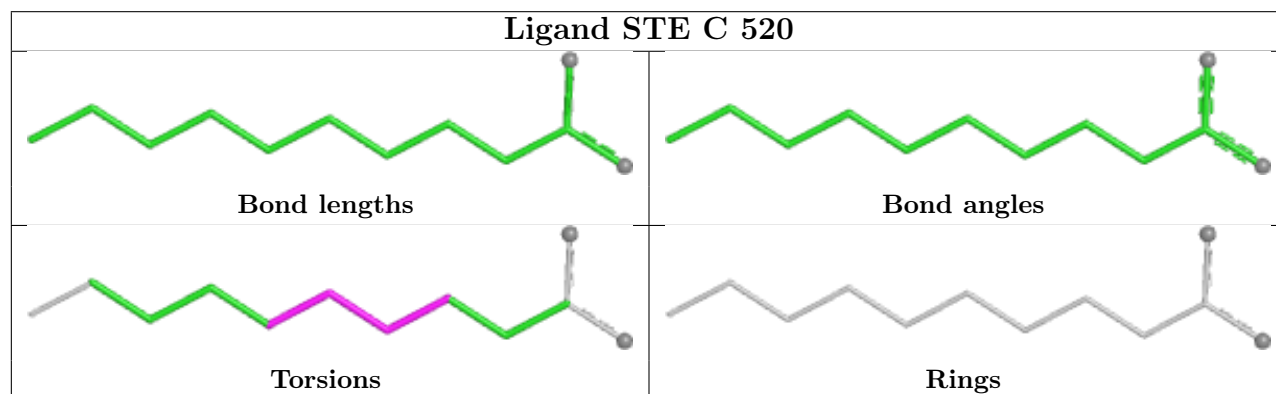
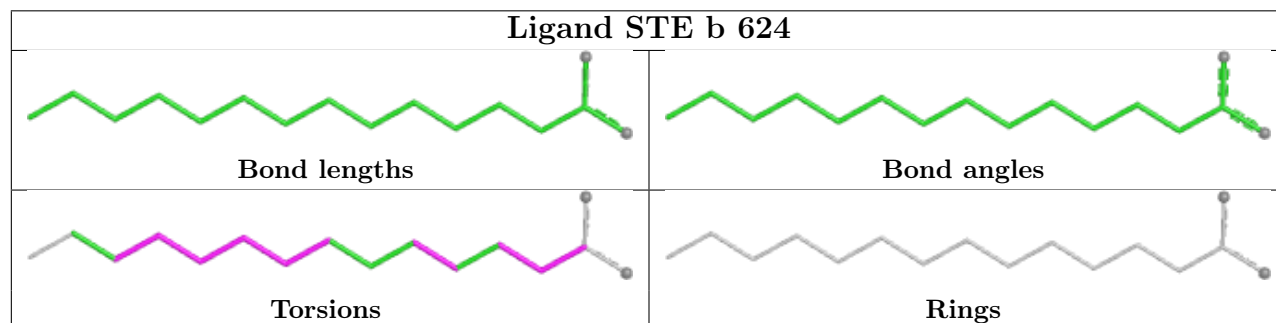
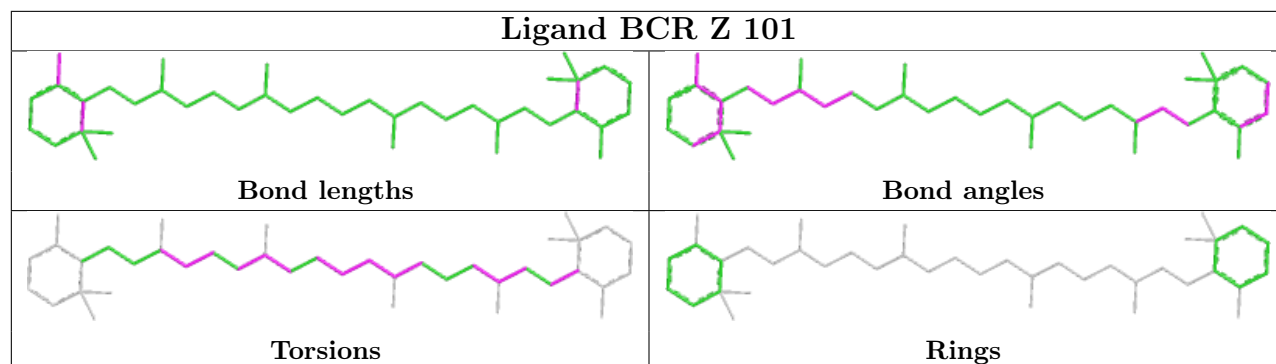


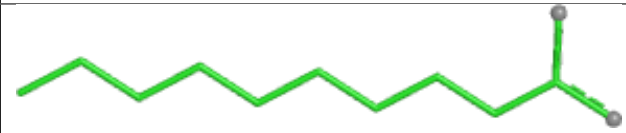
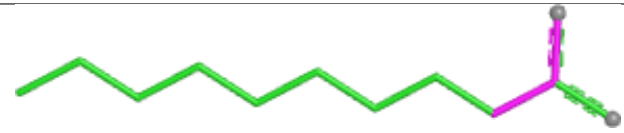
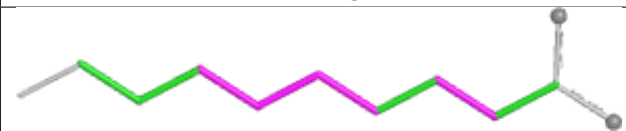
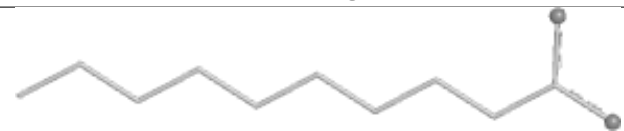
Ligand CLA C 502

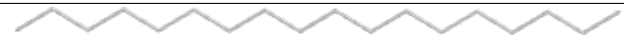


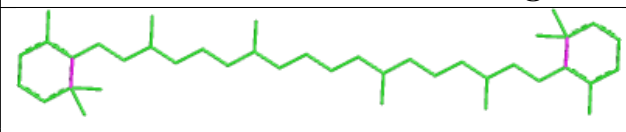
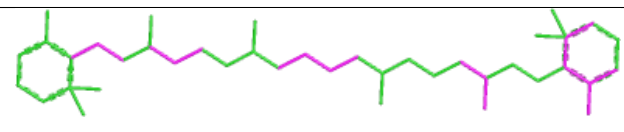
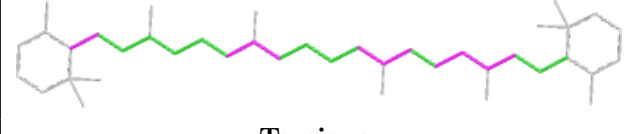
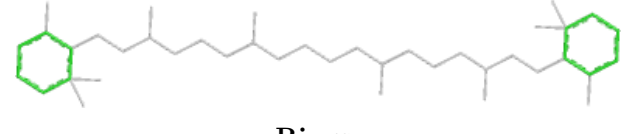
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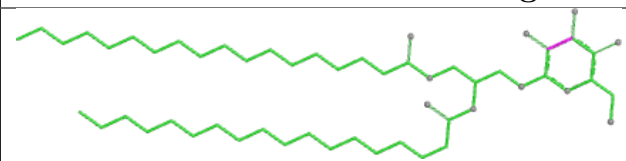
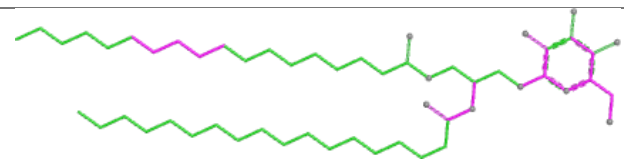
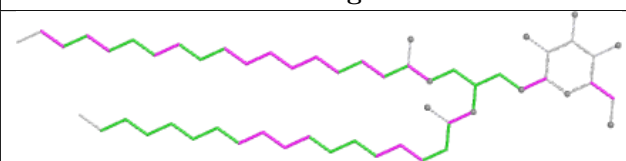
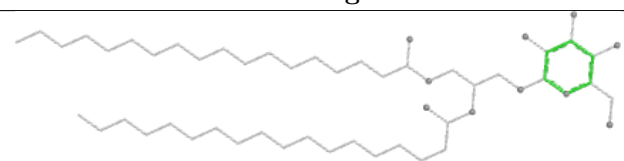


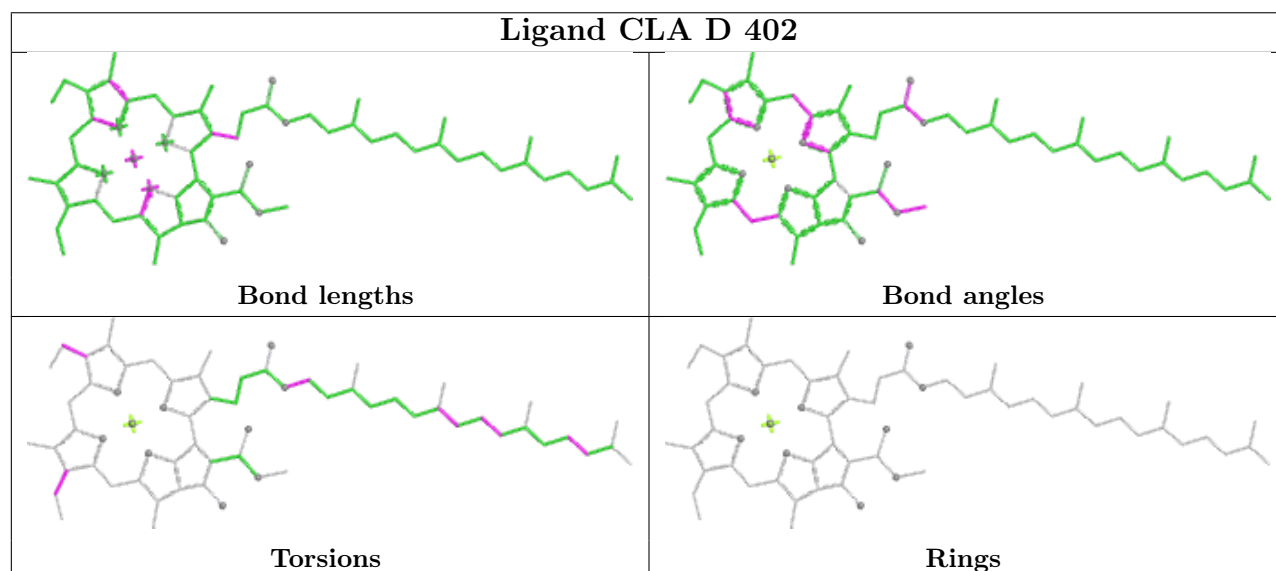
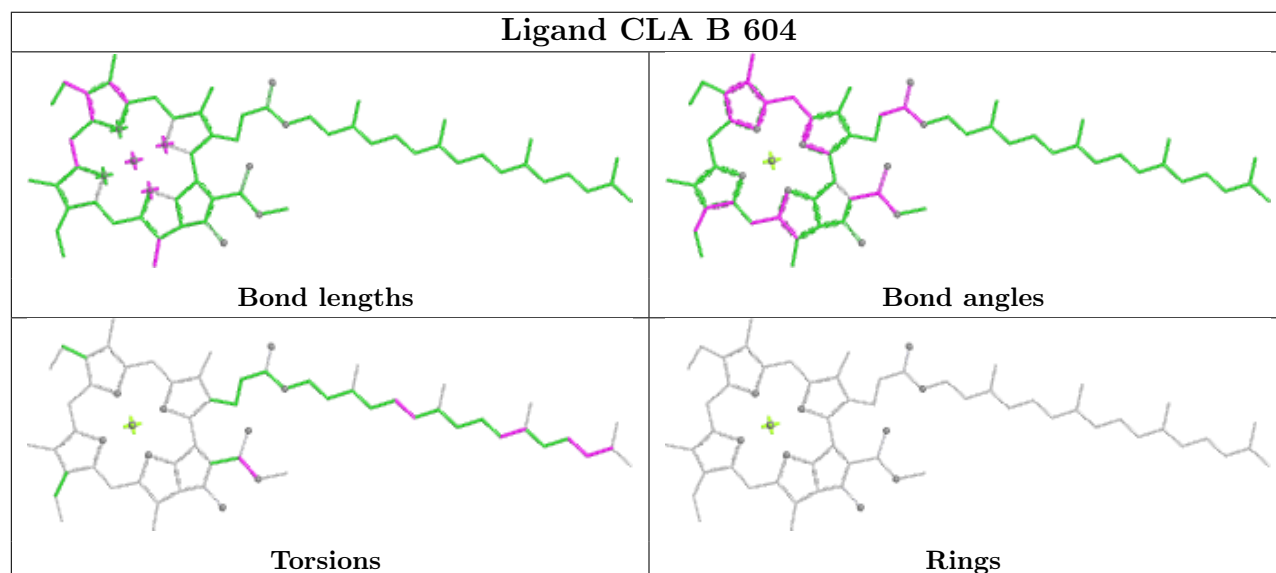
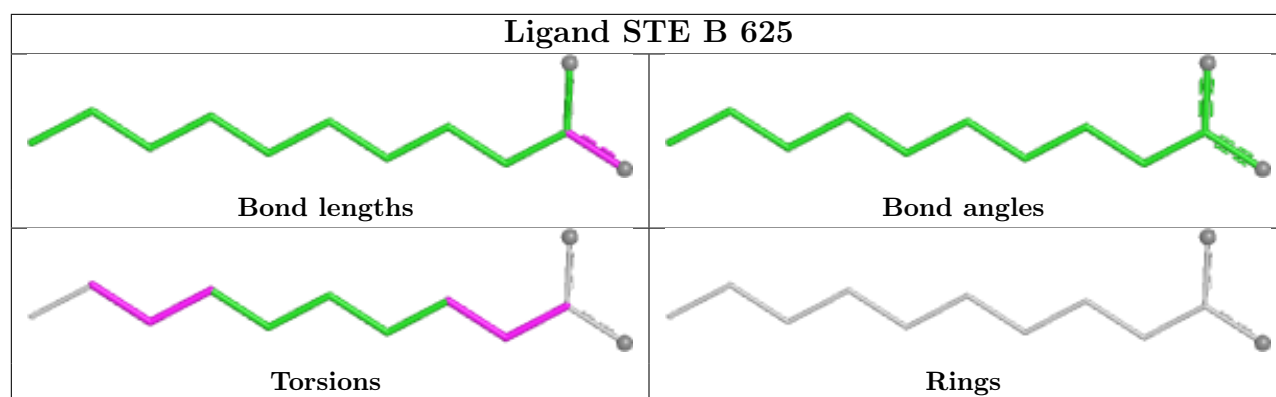


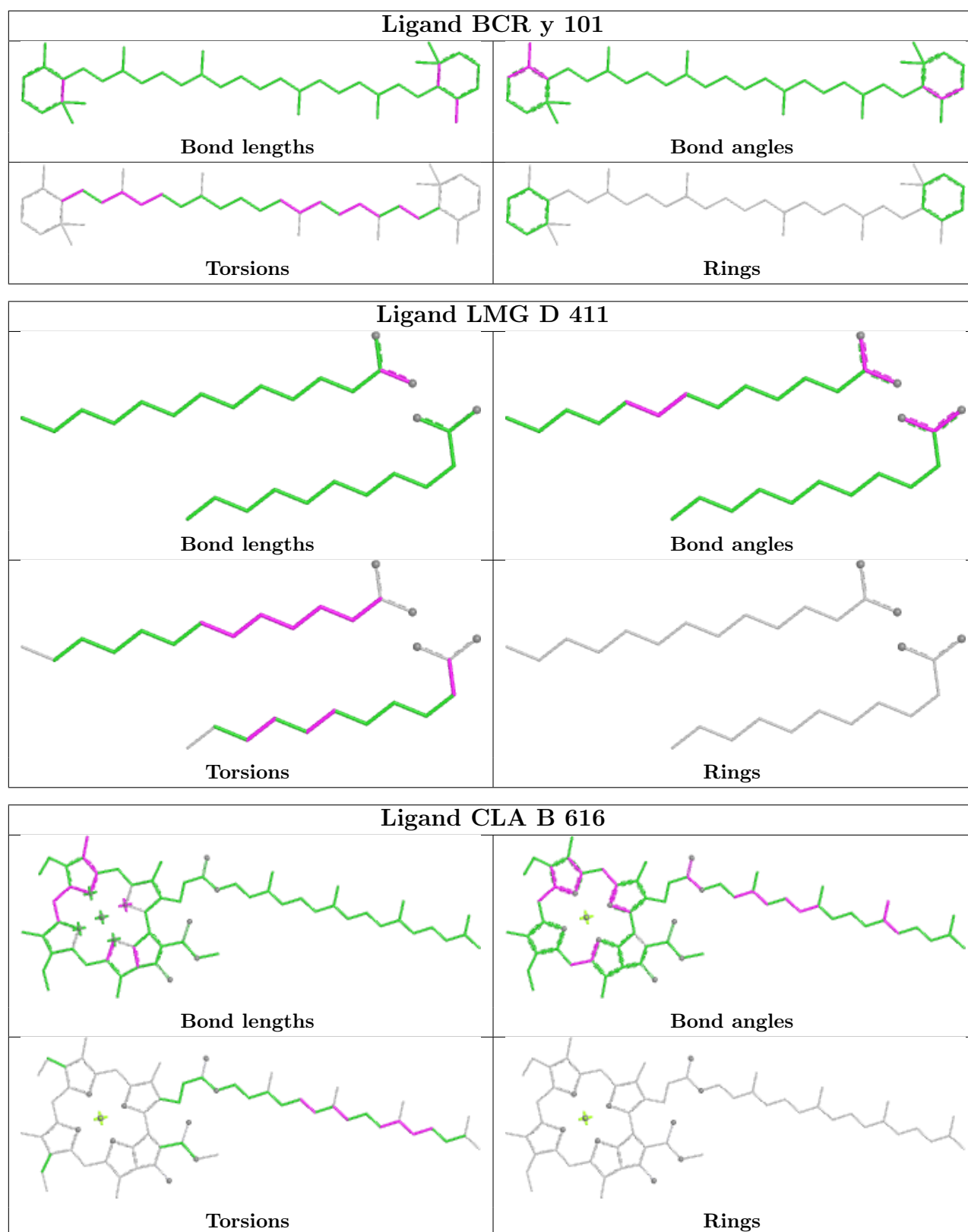
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

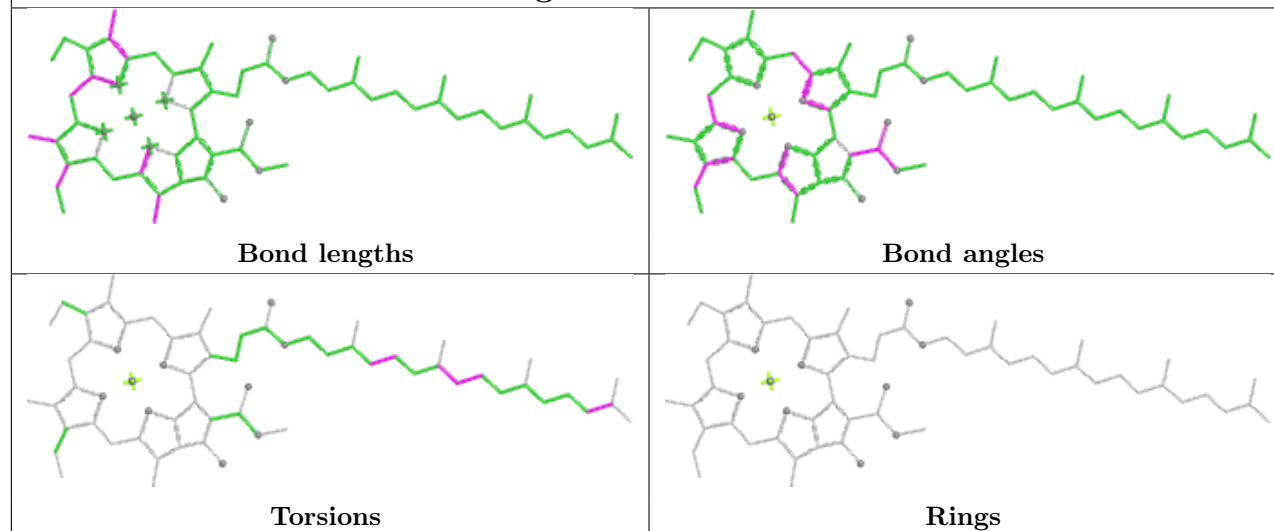
Ligand BCR c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

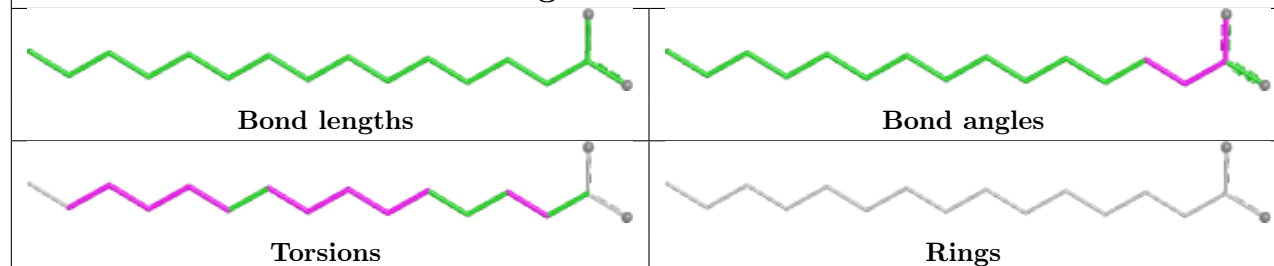




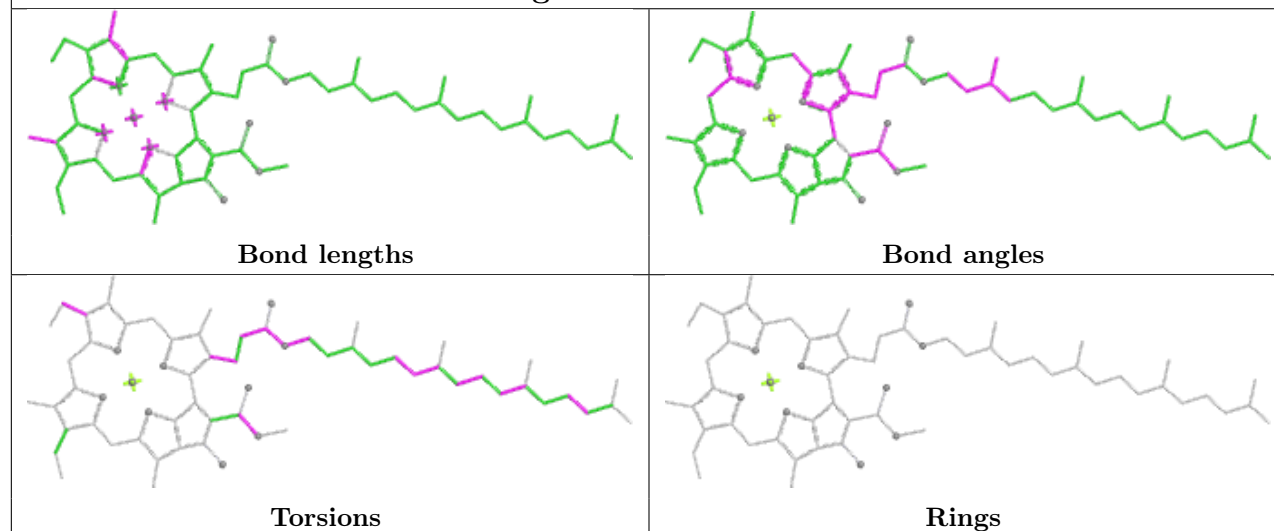
Ligand CLA b 601

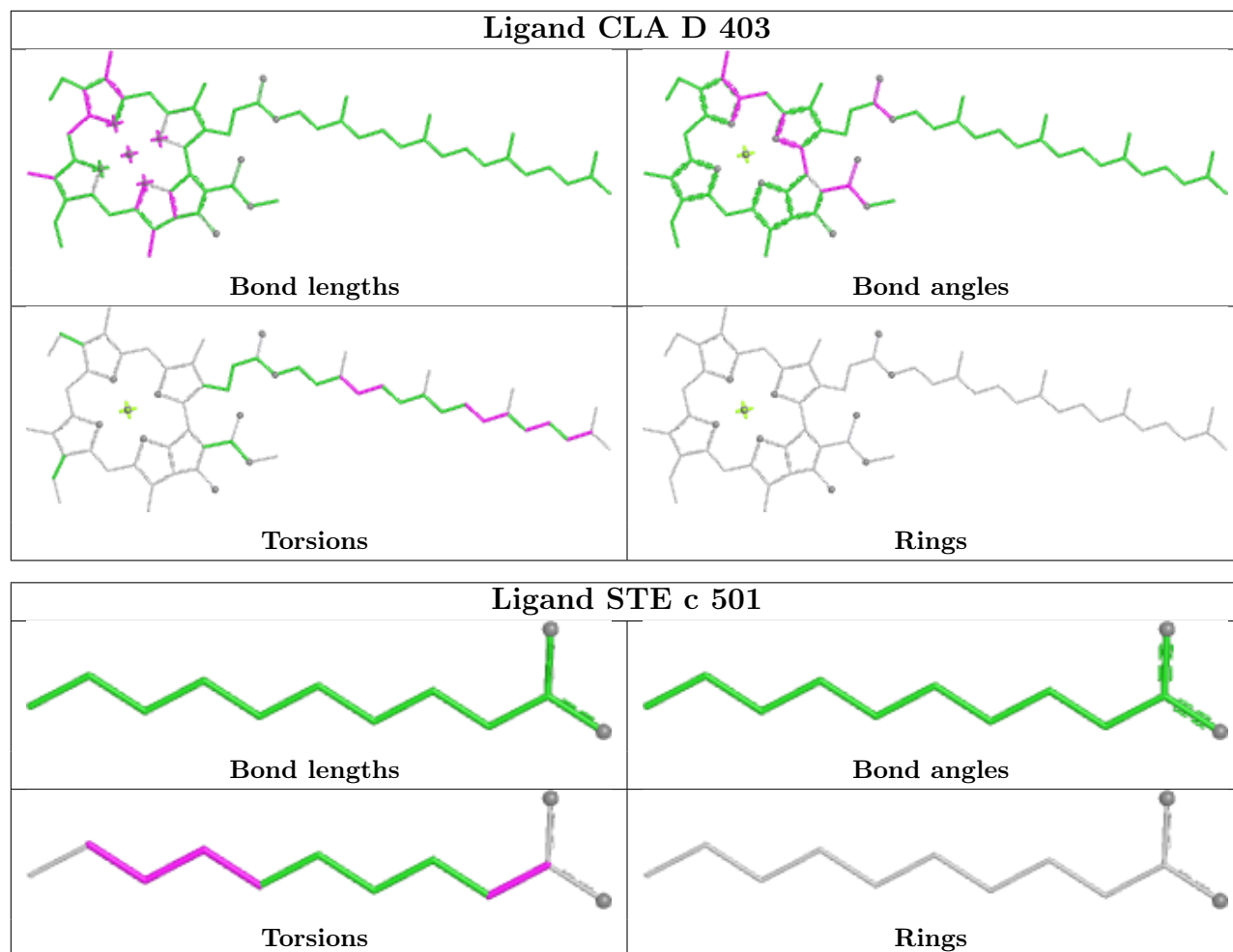


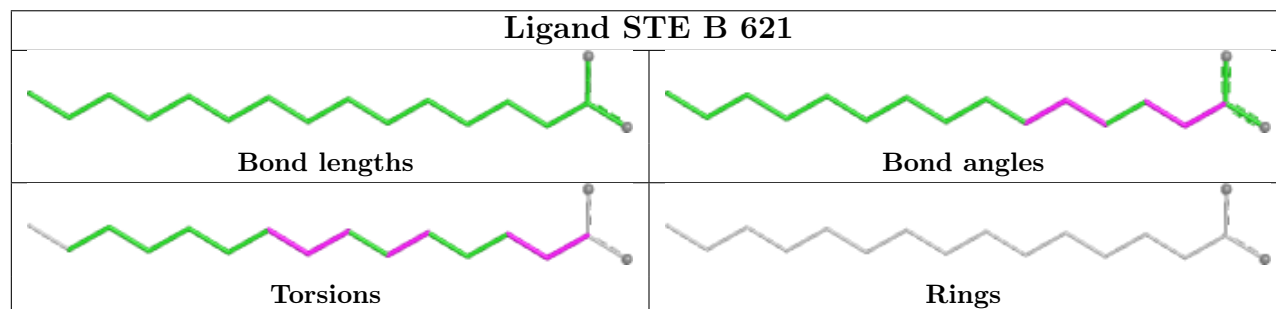
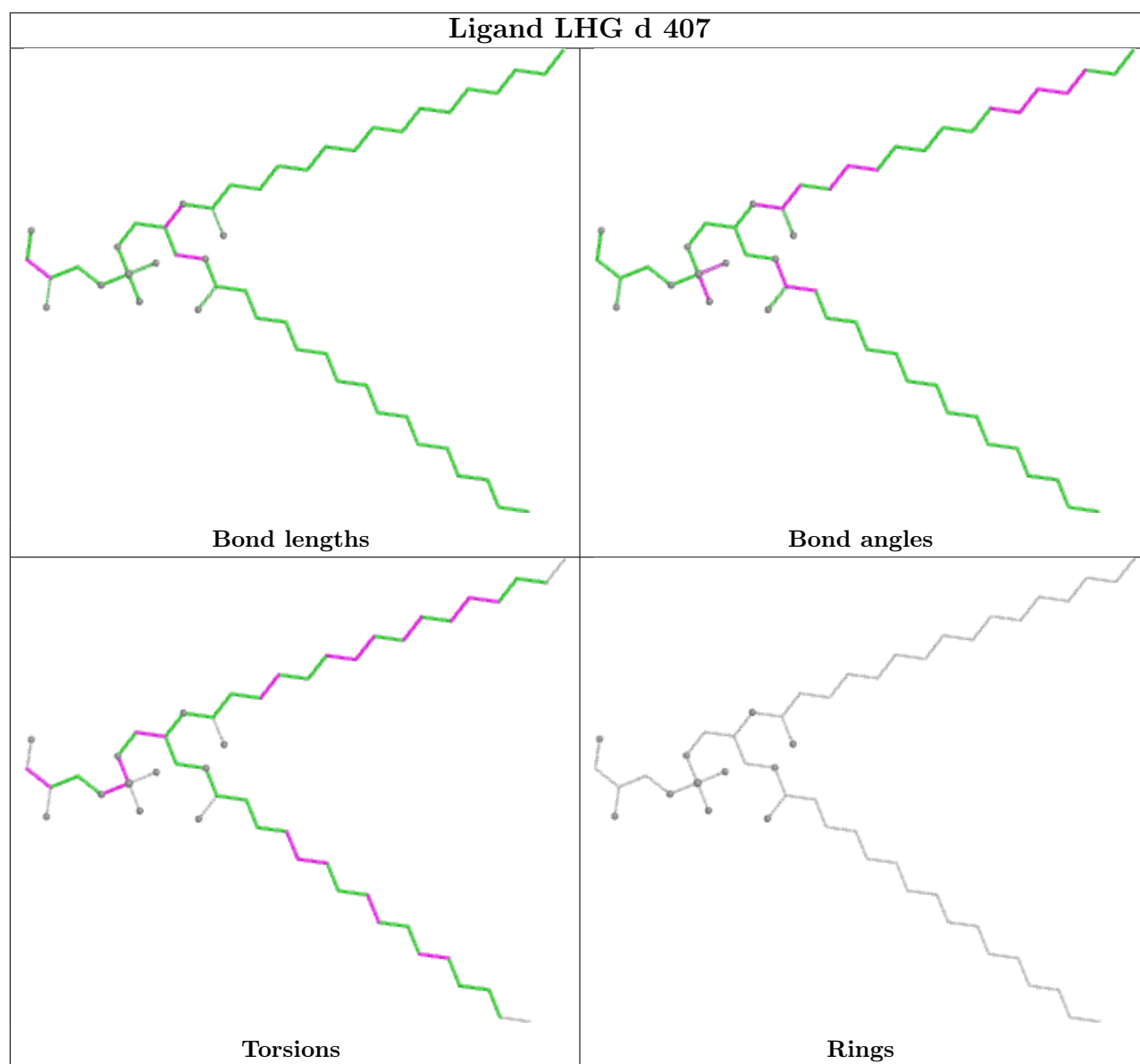
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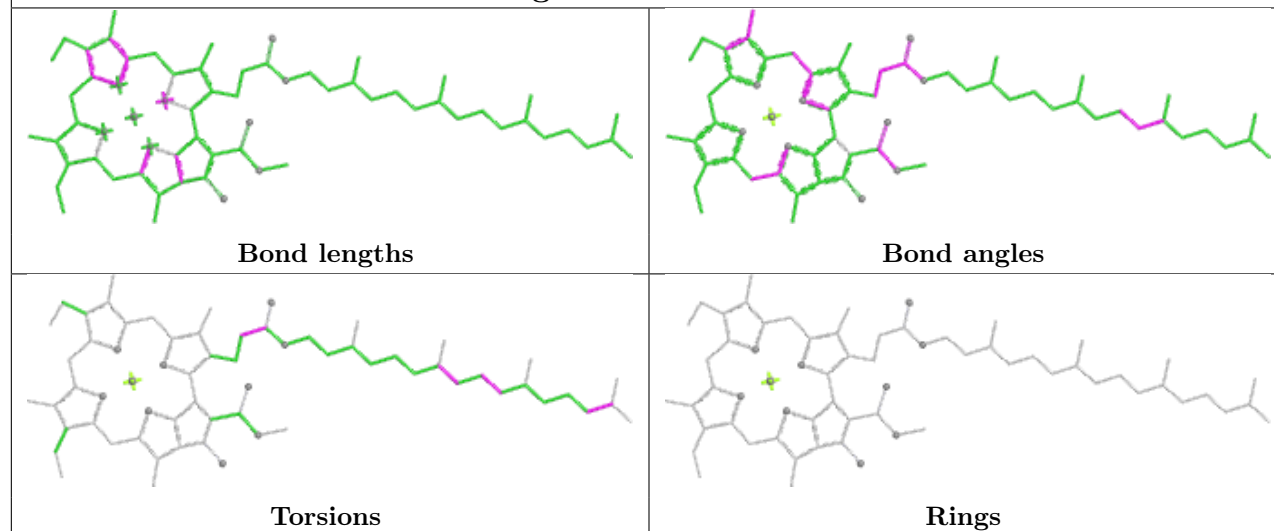
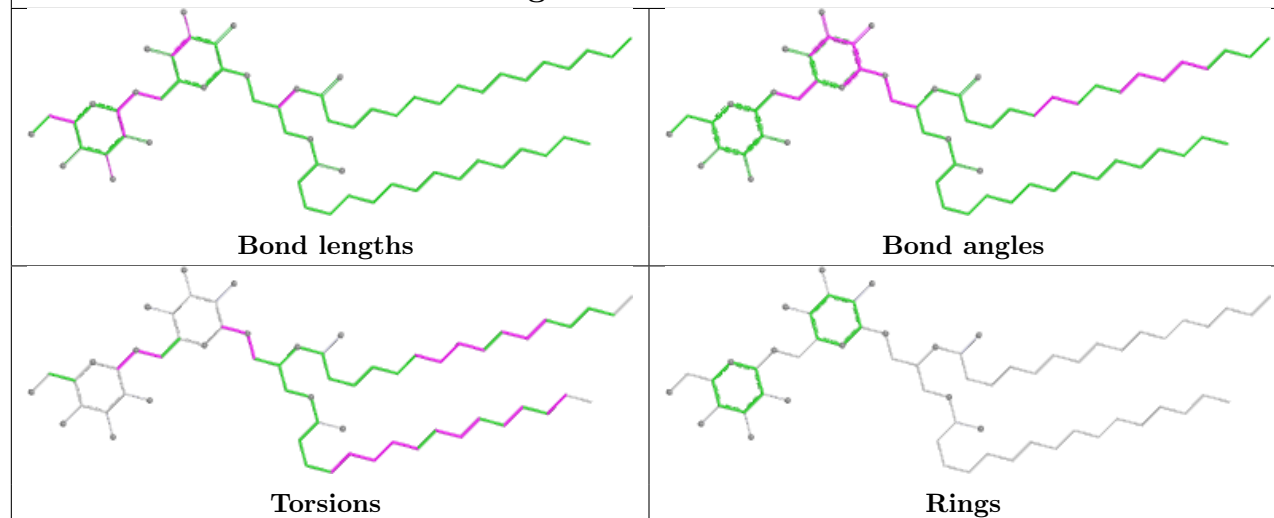


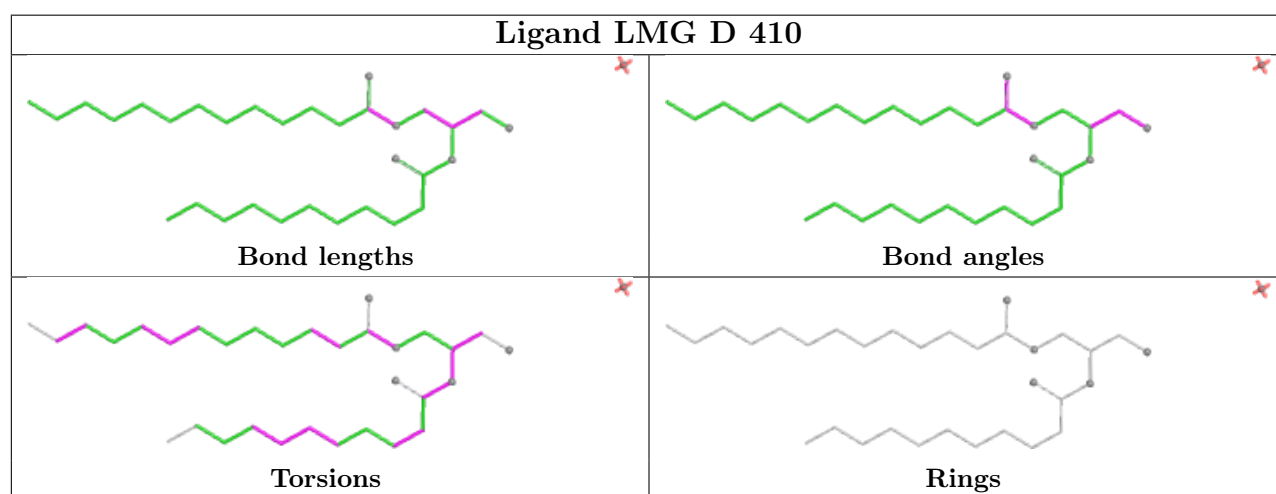
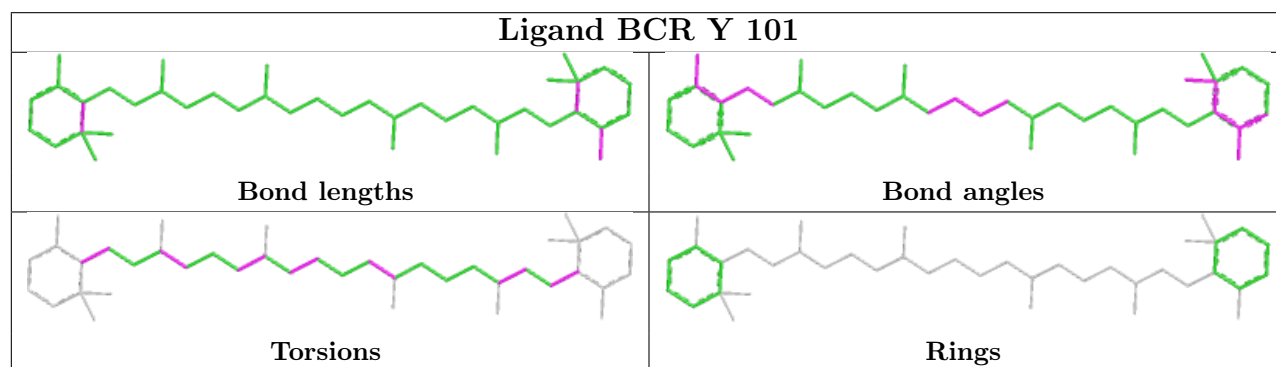
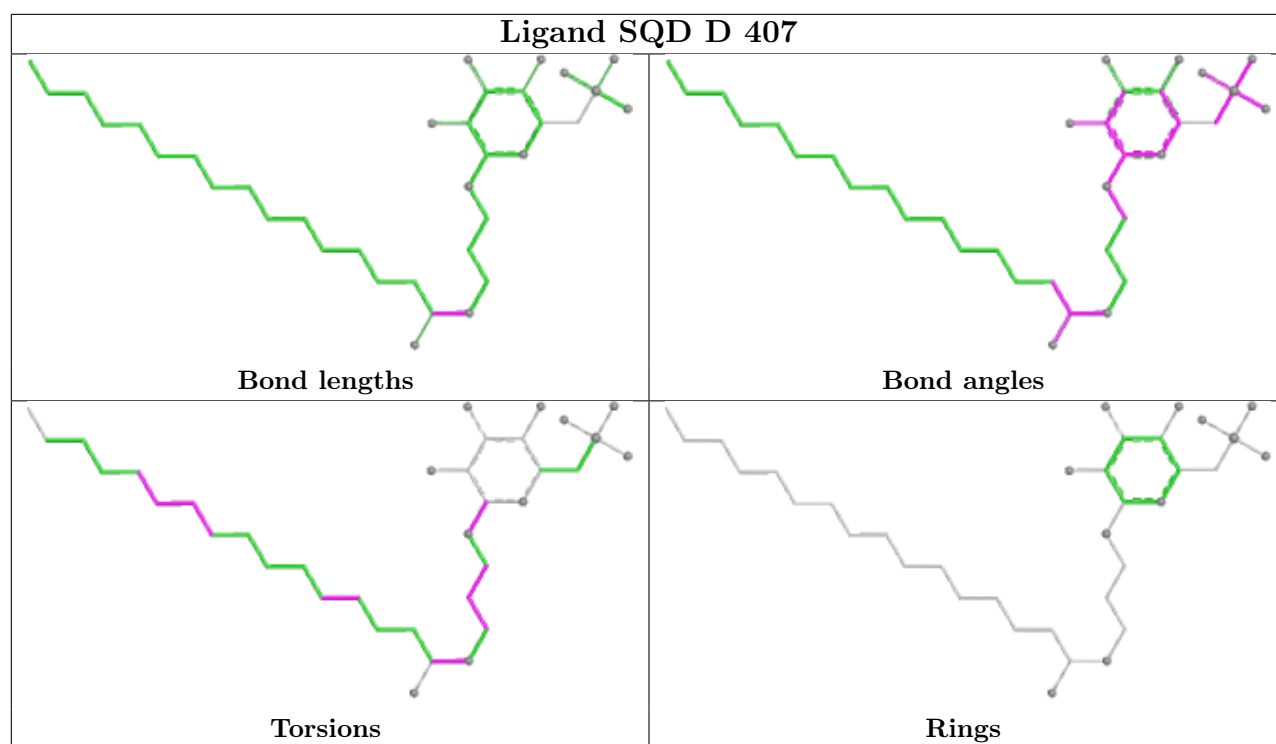
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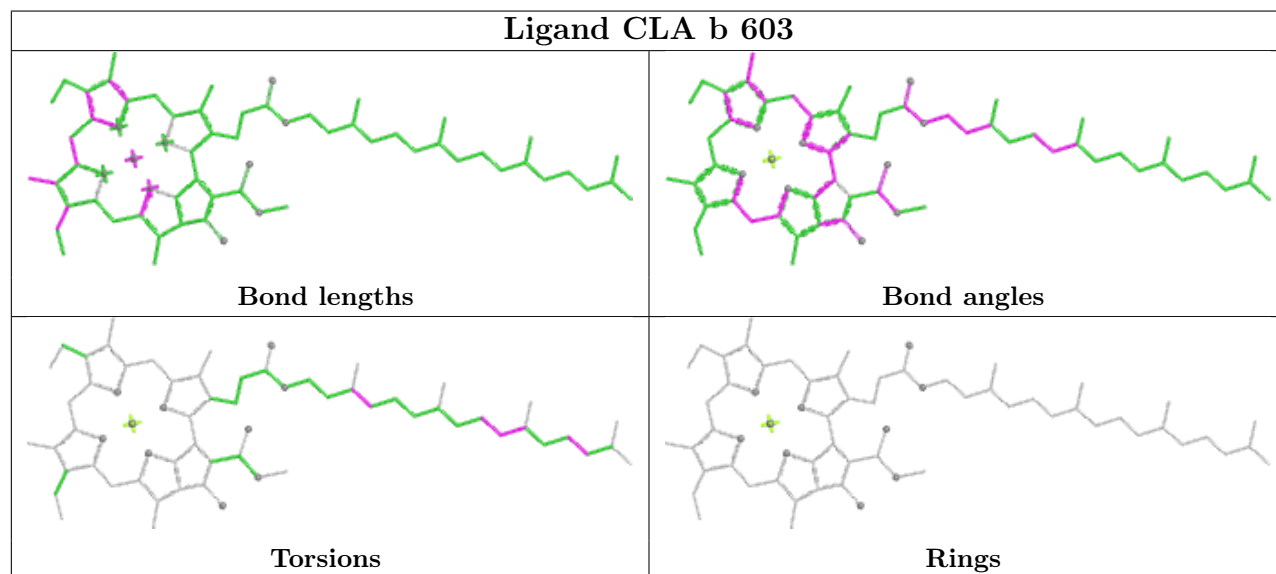
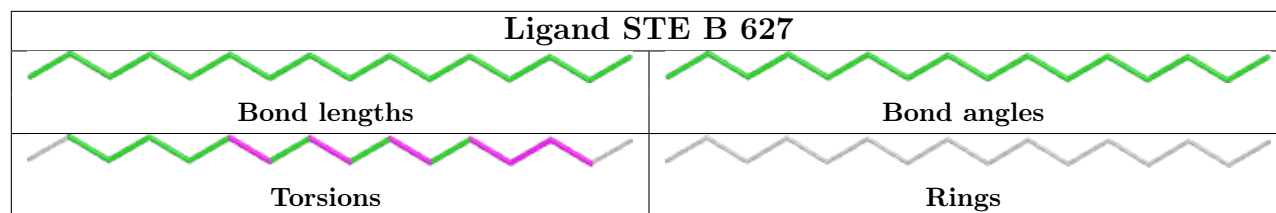




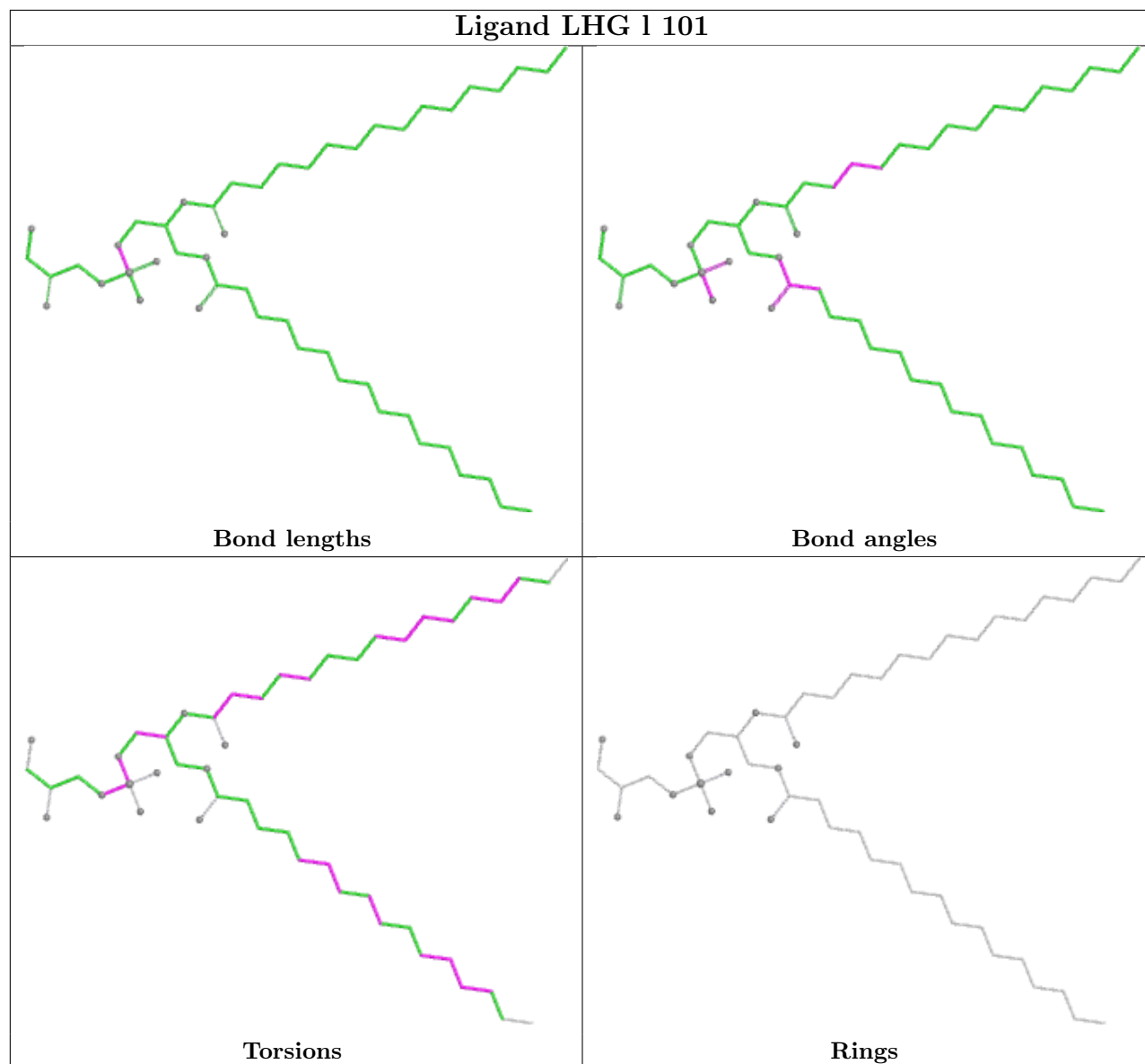


Ligand CLA B 613**Ligand DGD C 517**

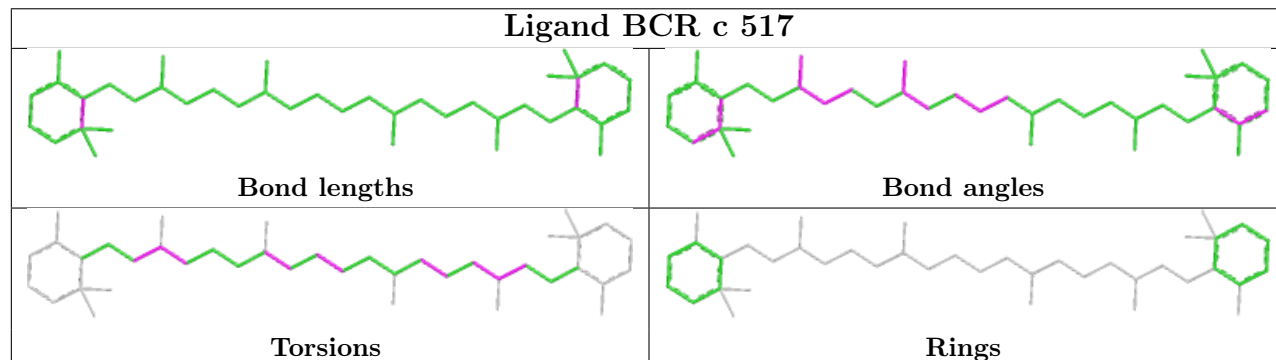


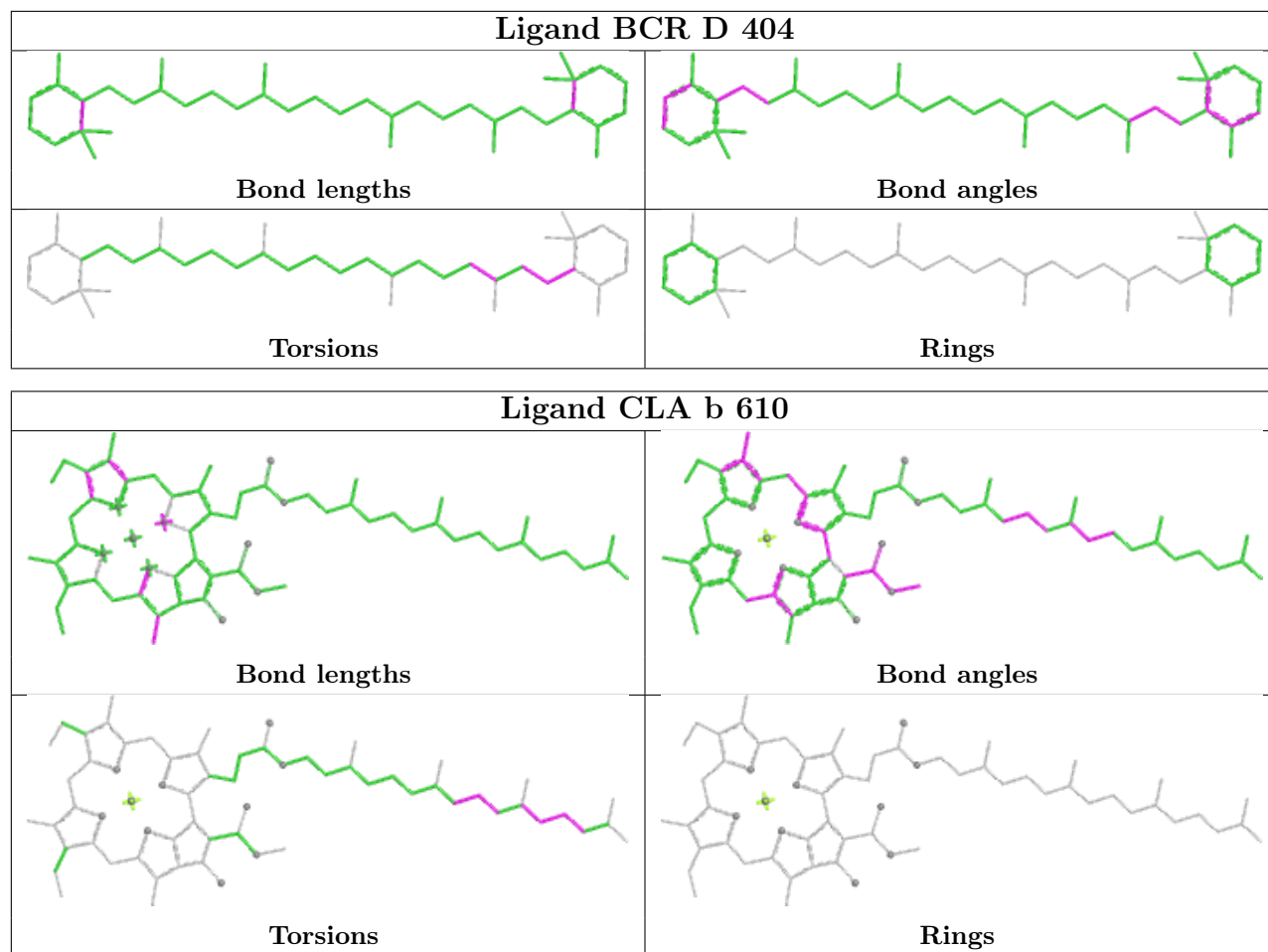


Ligand LHG l 101

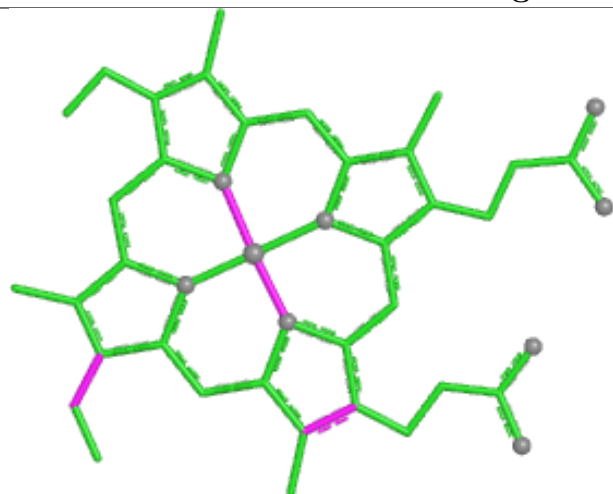


Ligand BCR c 517

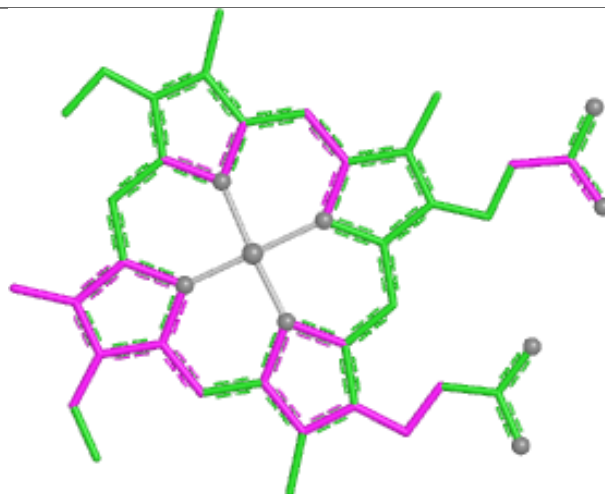




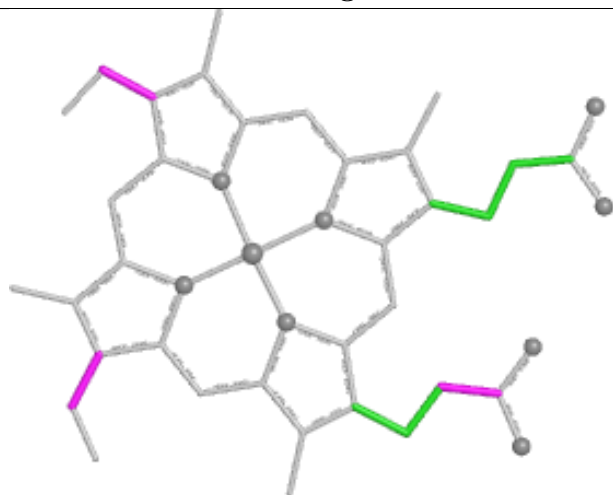
Ligand HEC V 201



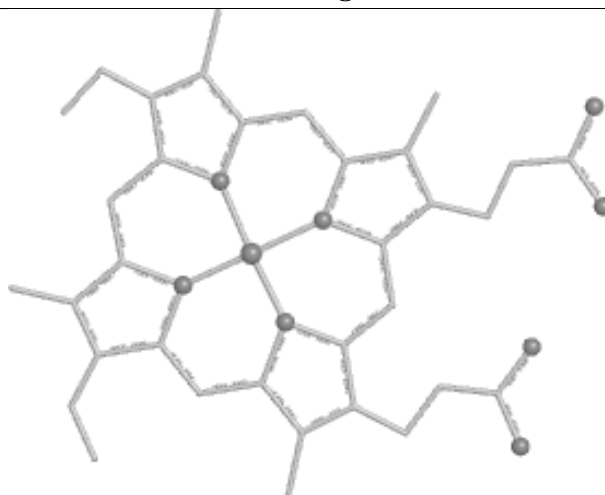
Bond lengths



Bond angles

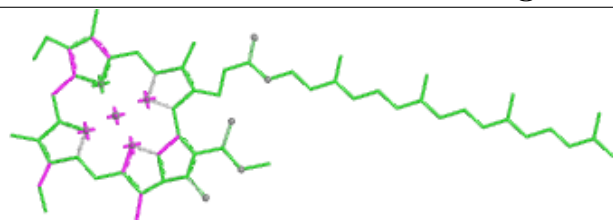


Torsions

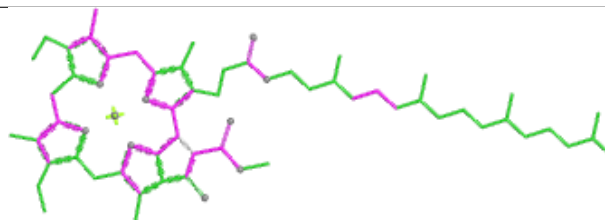


Rings

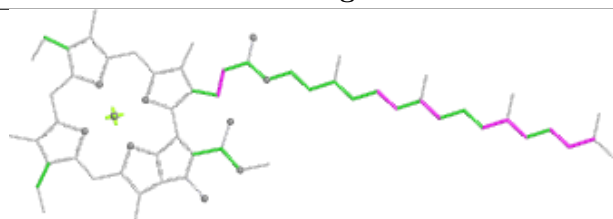
Ligand CLA b 605



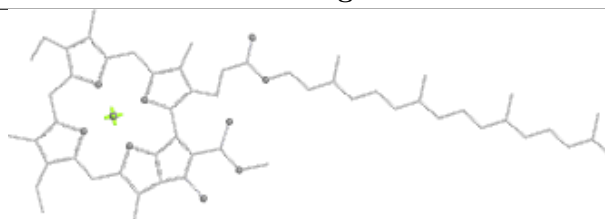
Bond lengths



Bond angles

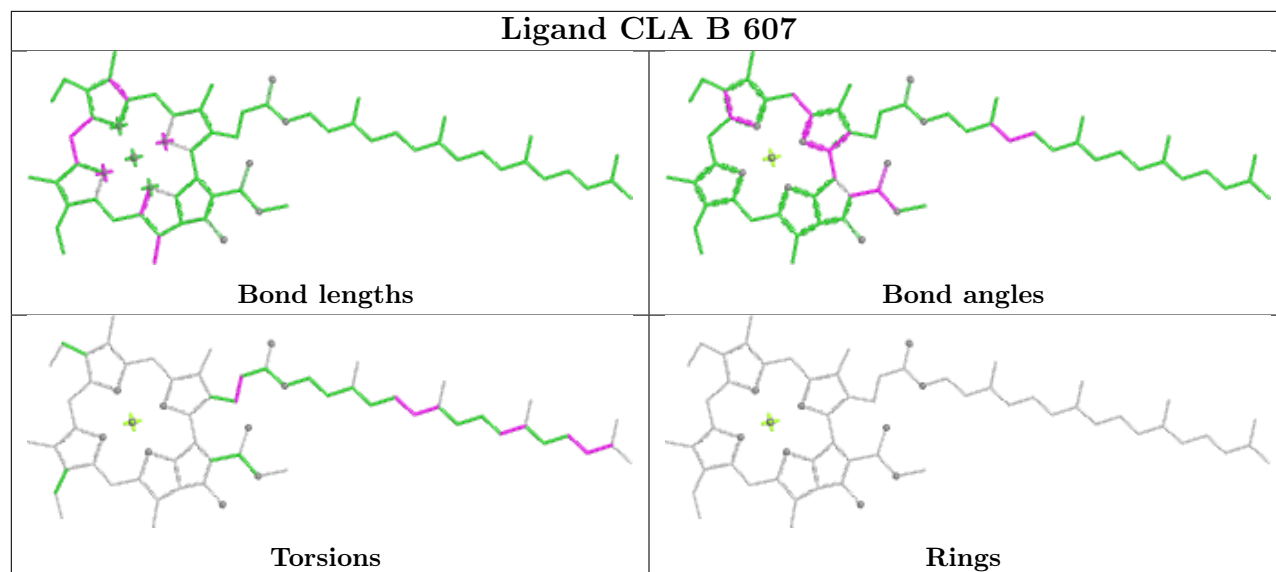


Torsions

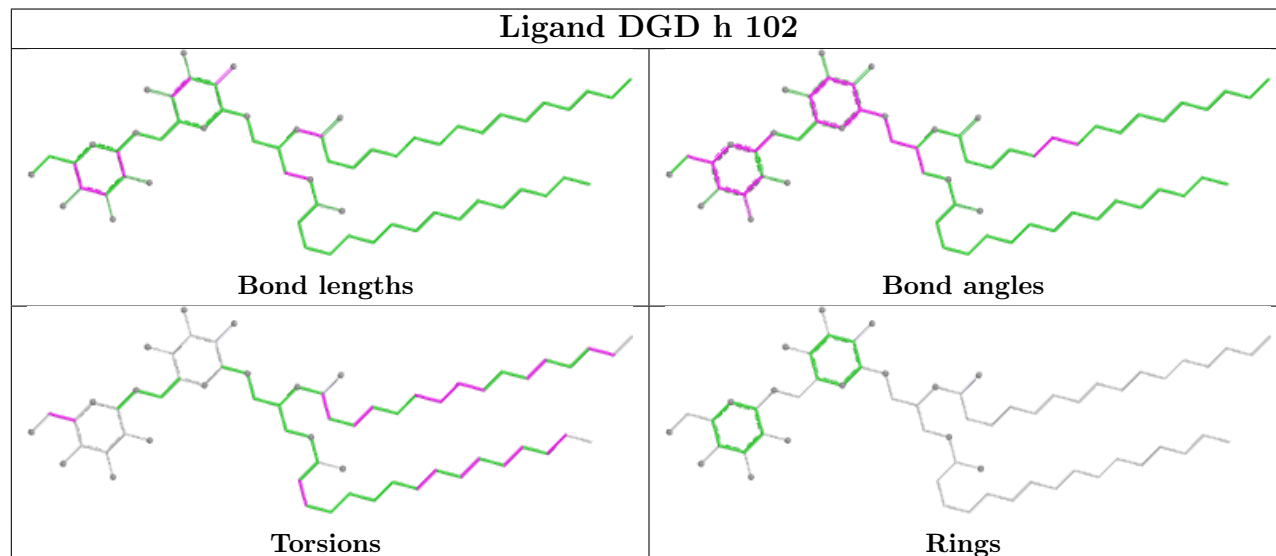


Rings

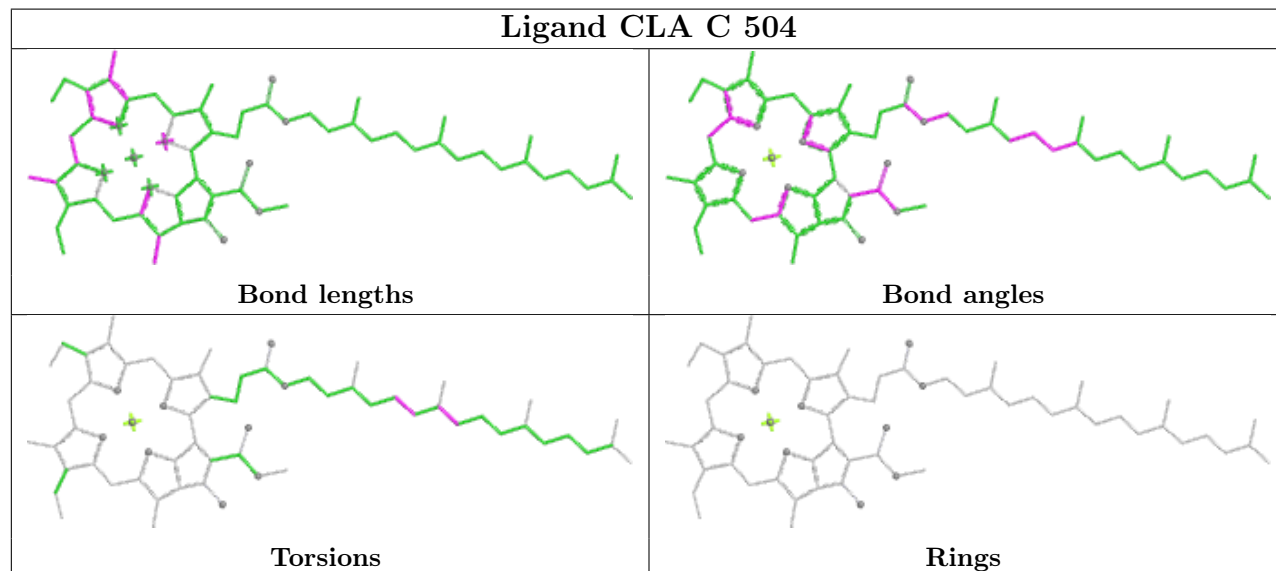
Ligand CLA B 607

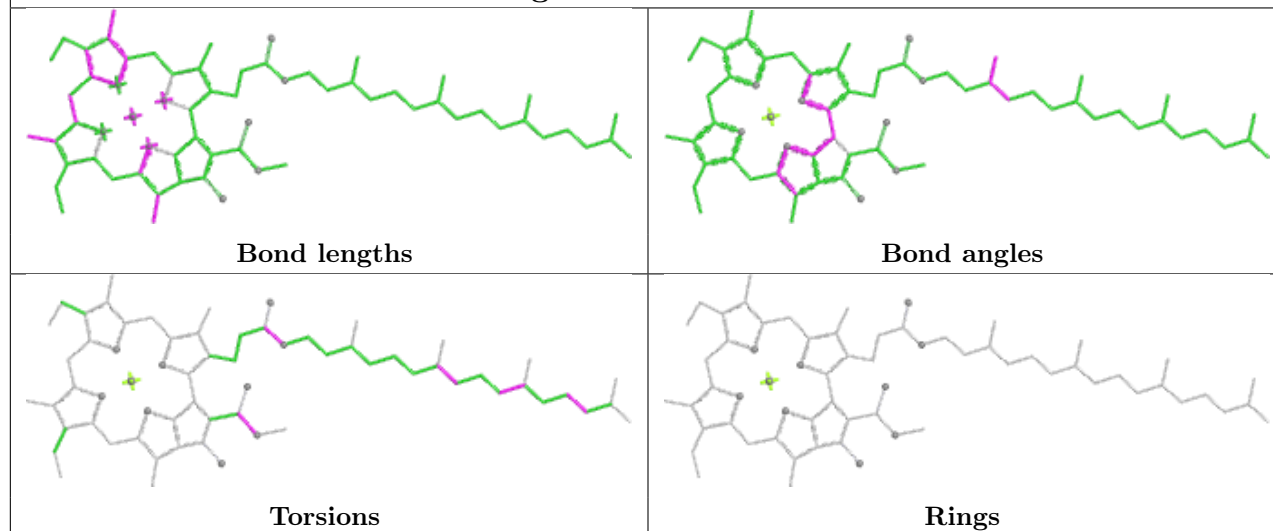
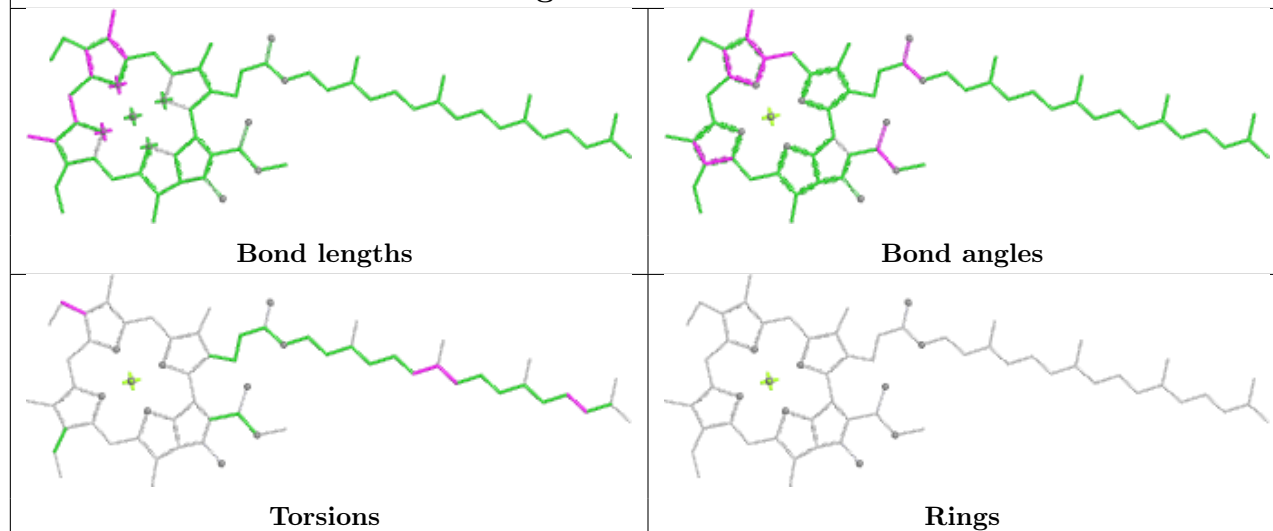
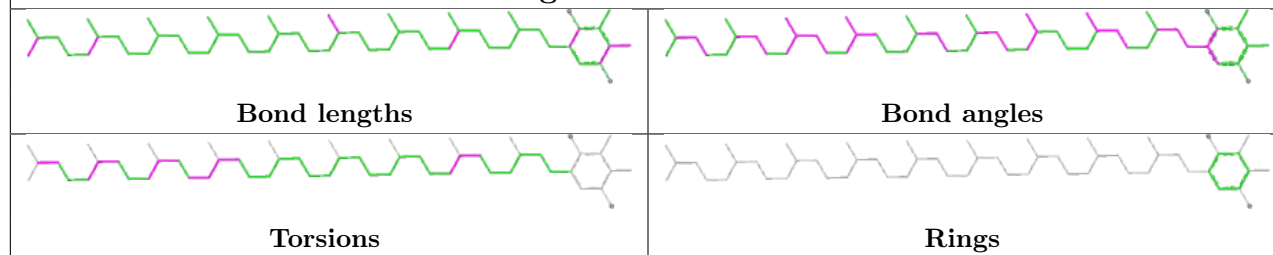


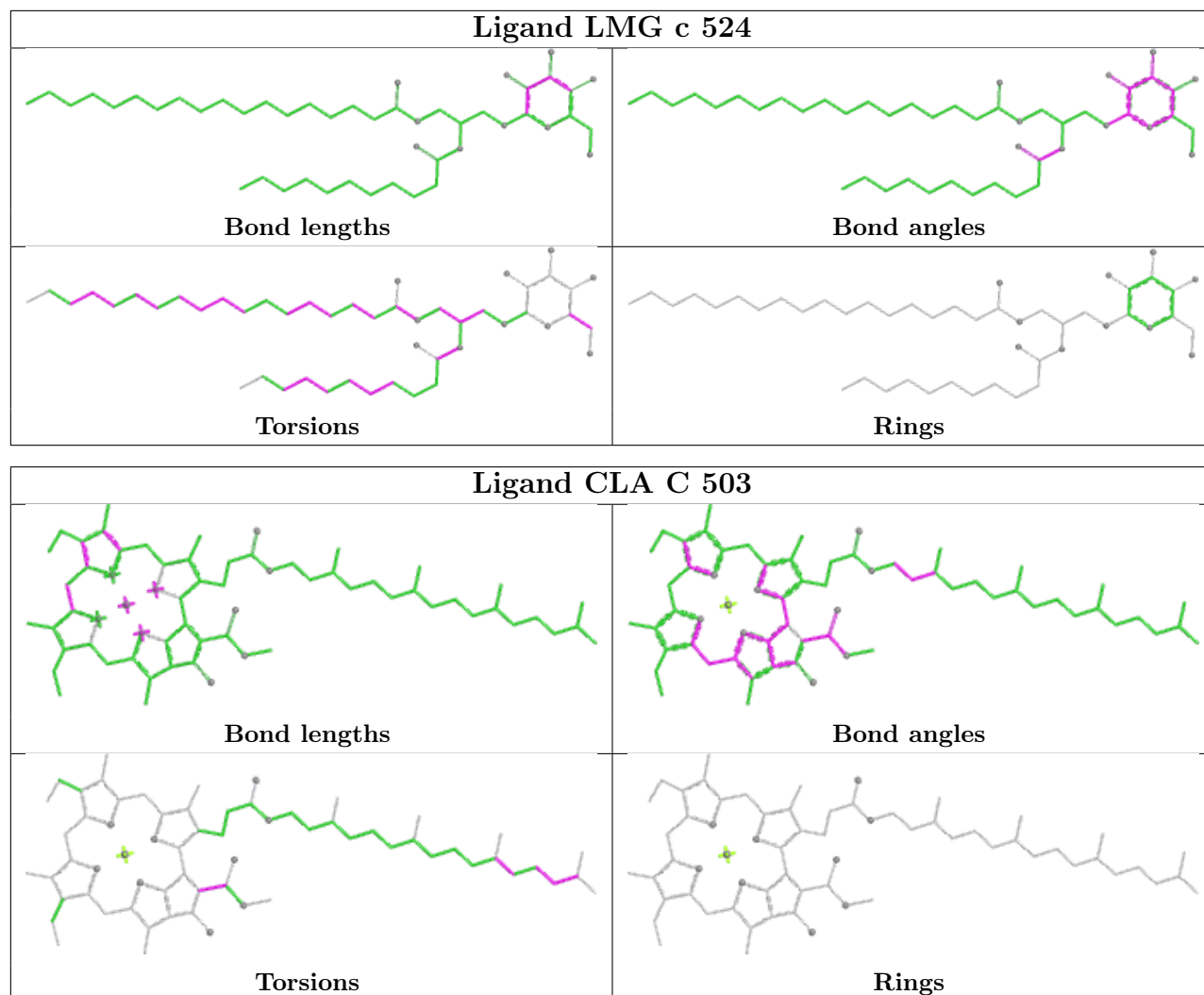
Ligand DGD h 102

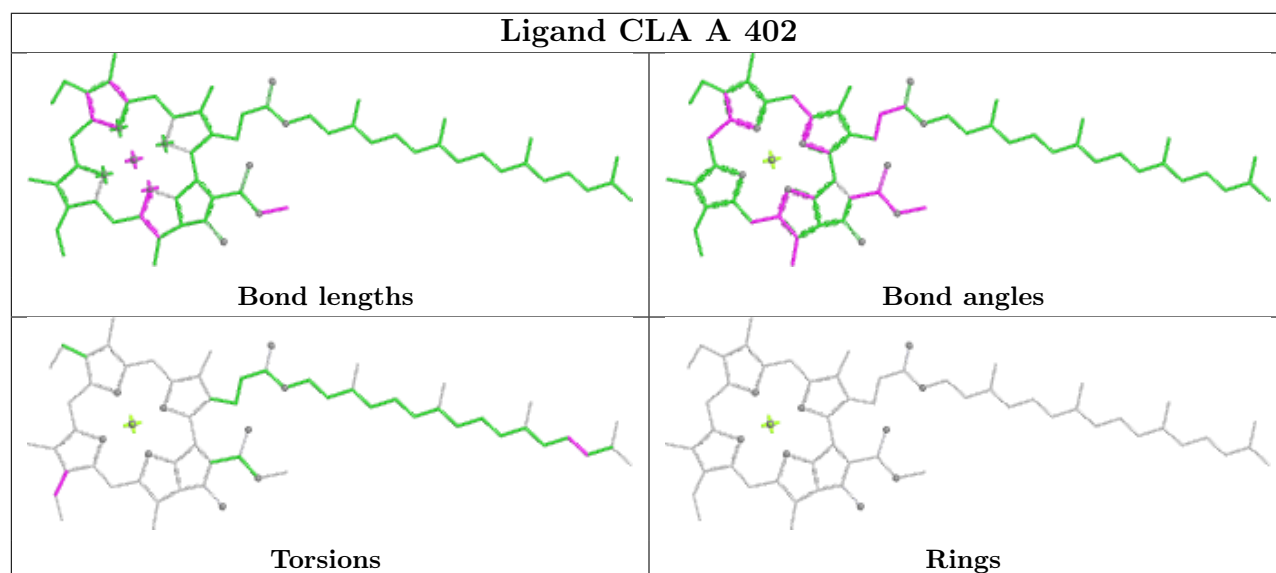
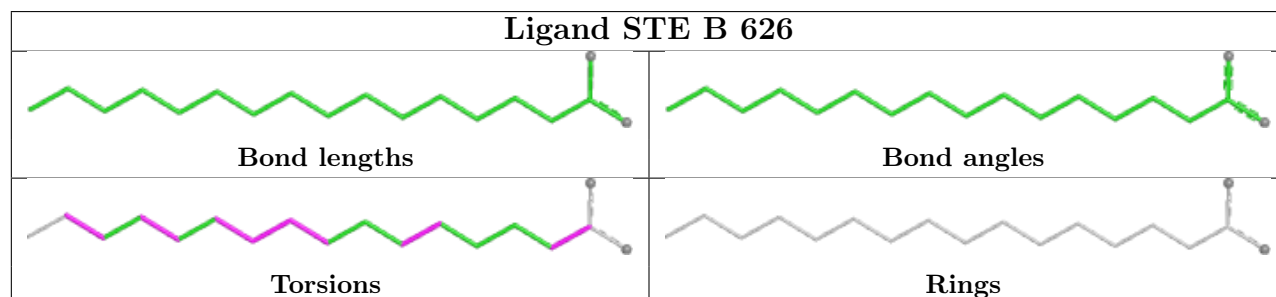
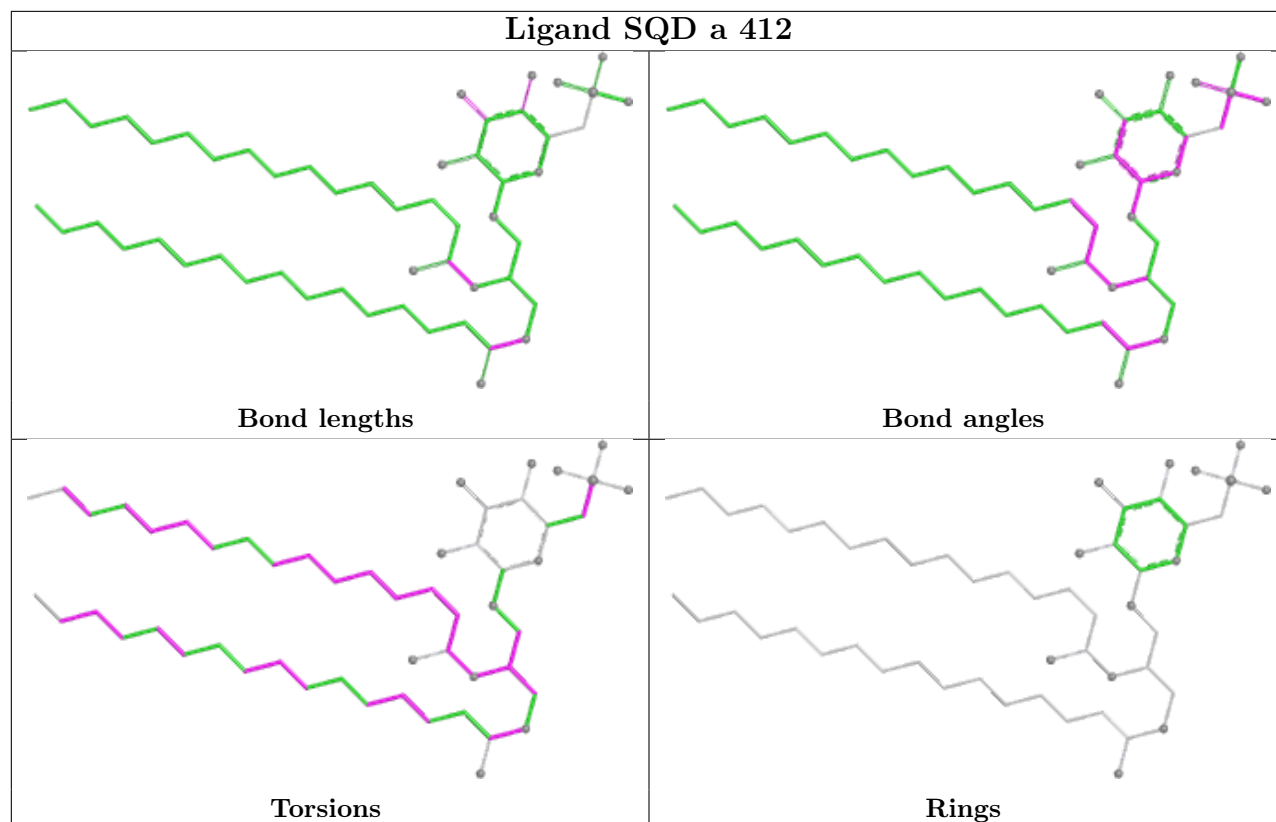


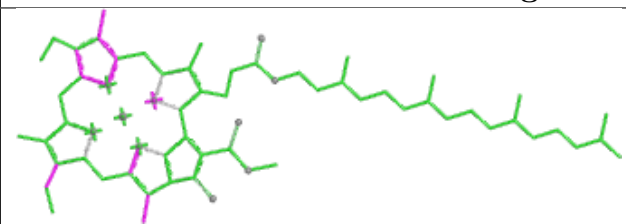
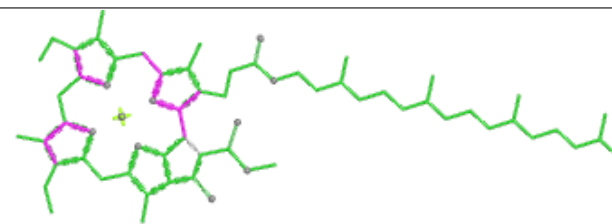
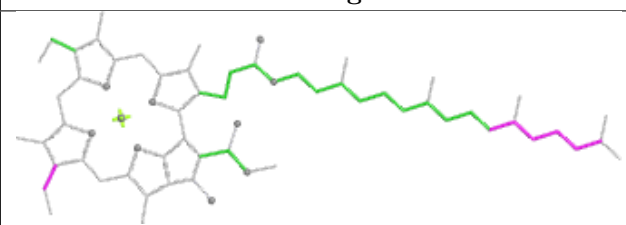
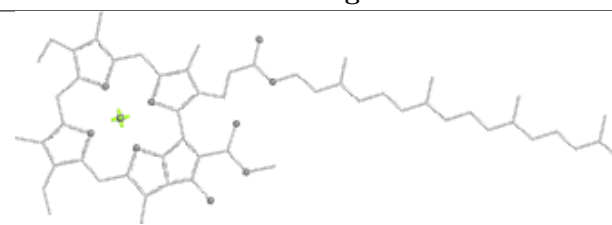
Ligand CLA C 504

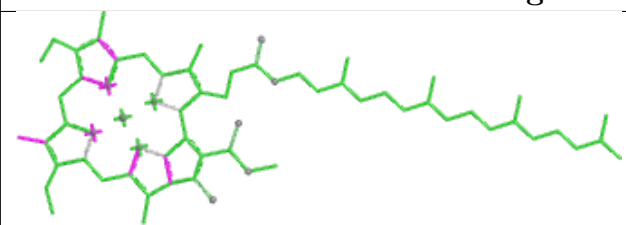
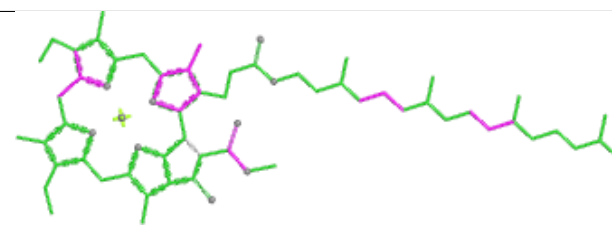
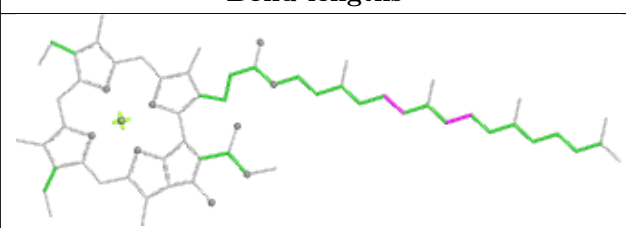
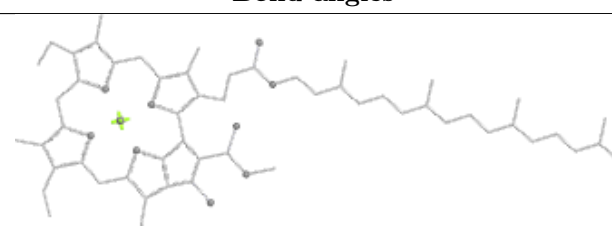


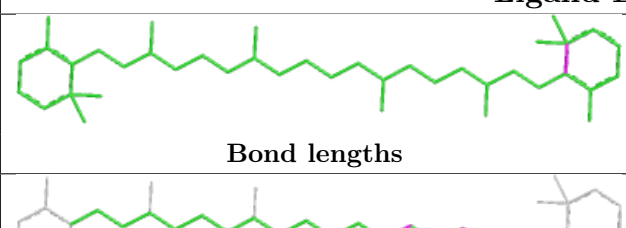
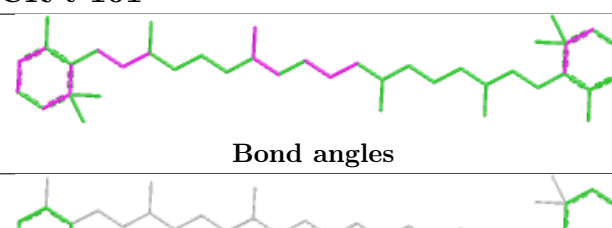
Ligand CLA C 512**Ligand CLA c 507****Ligand PL9 d 405**



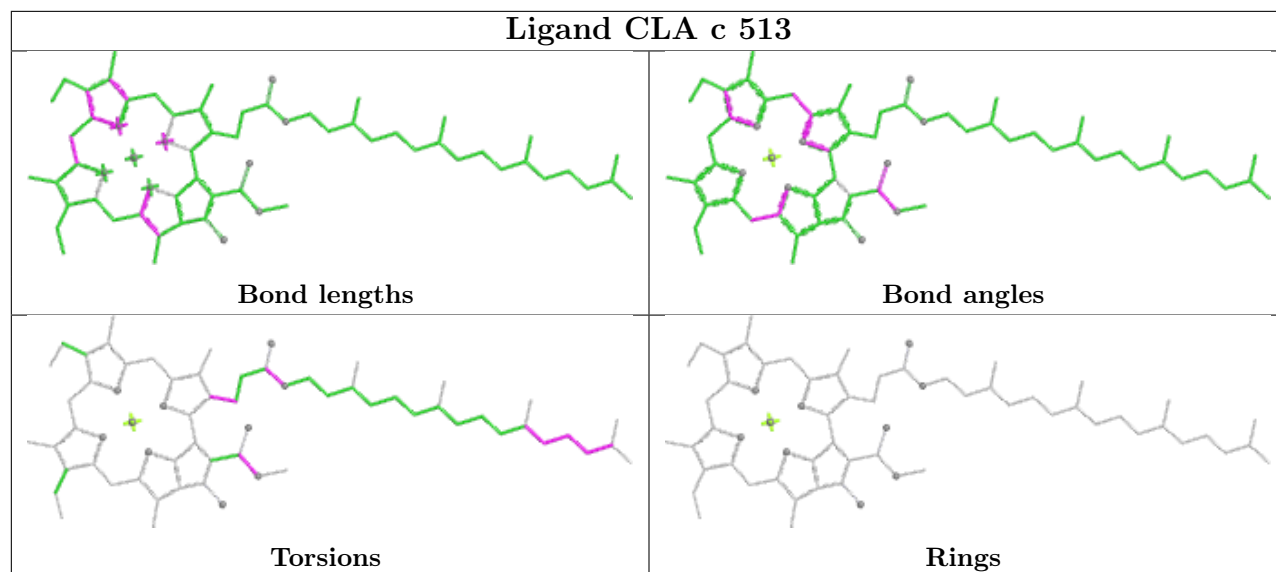


Ligand CLA A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

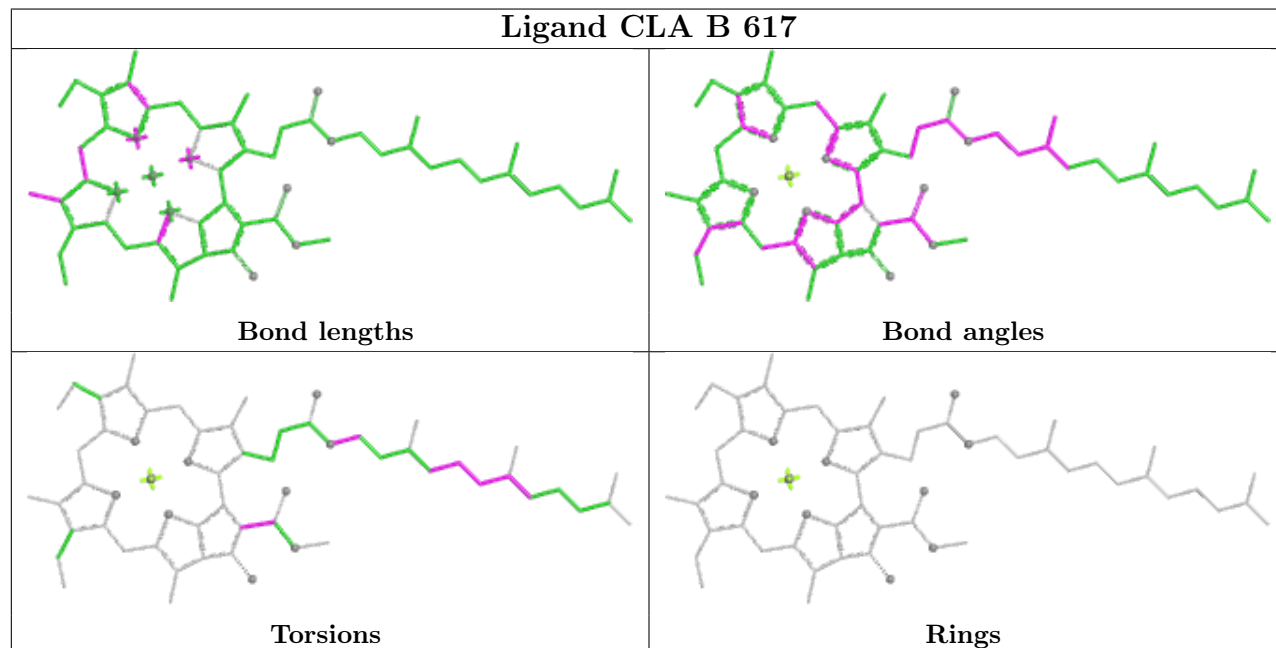
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

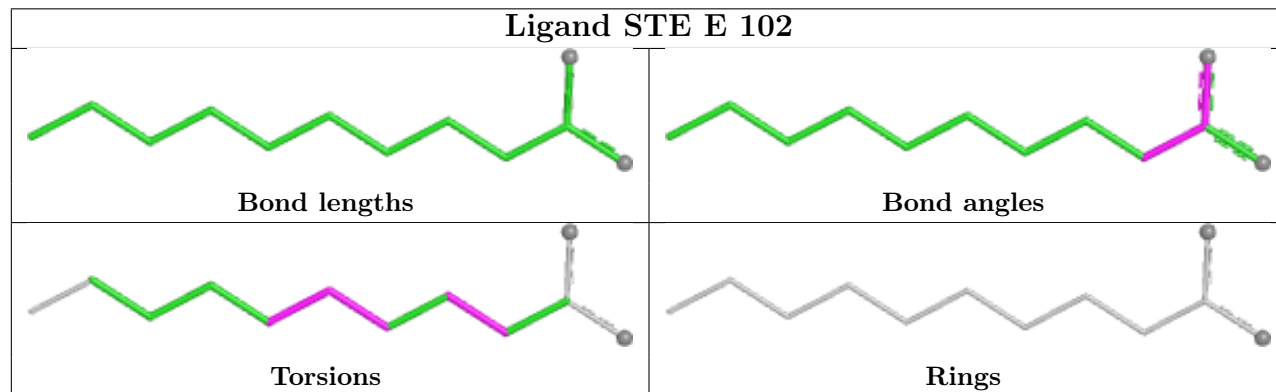
Ligand CLA c 513



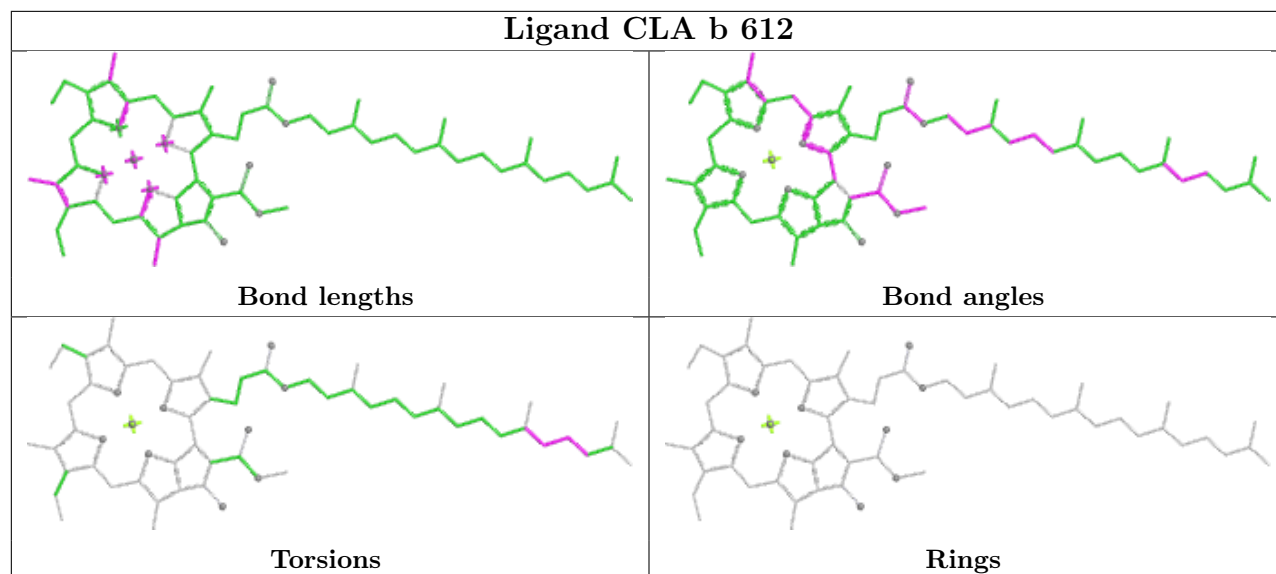
Ligand CLA B 617



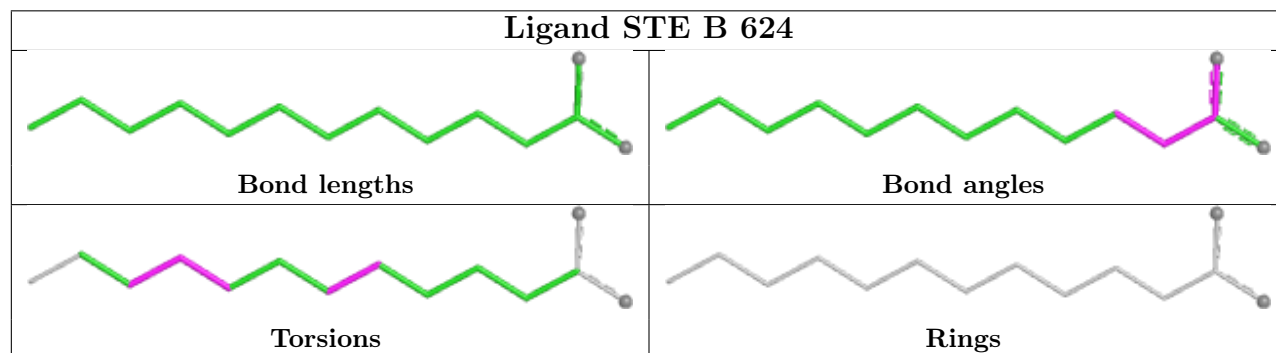
Ligand STE E 102



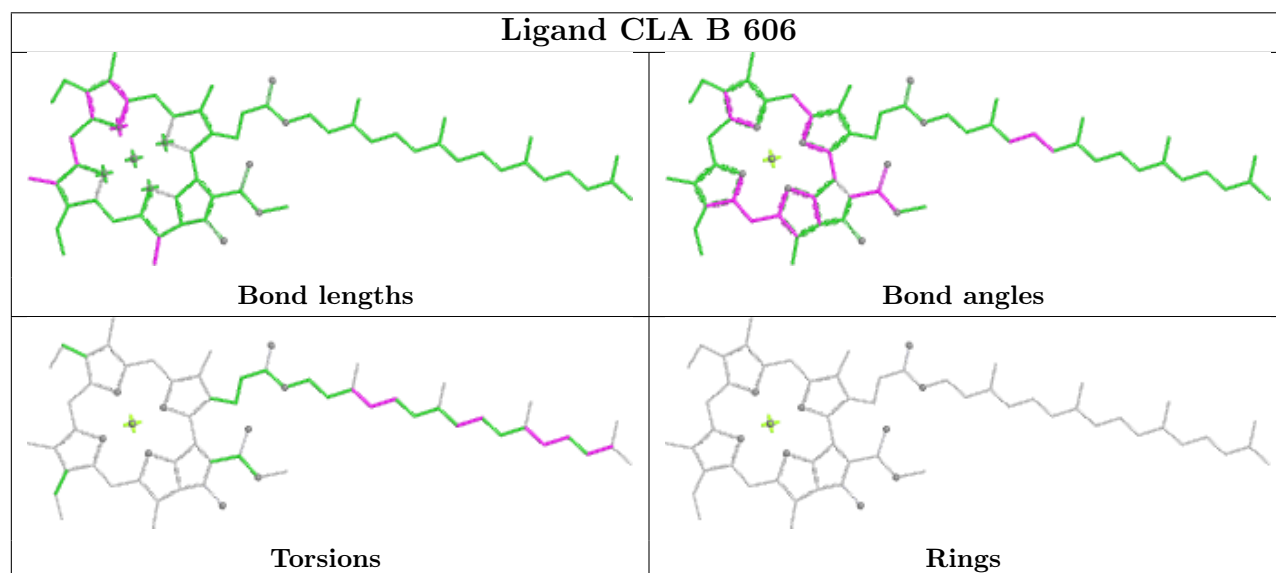
Ligand CLA b 612

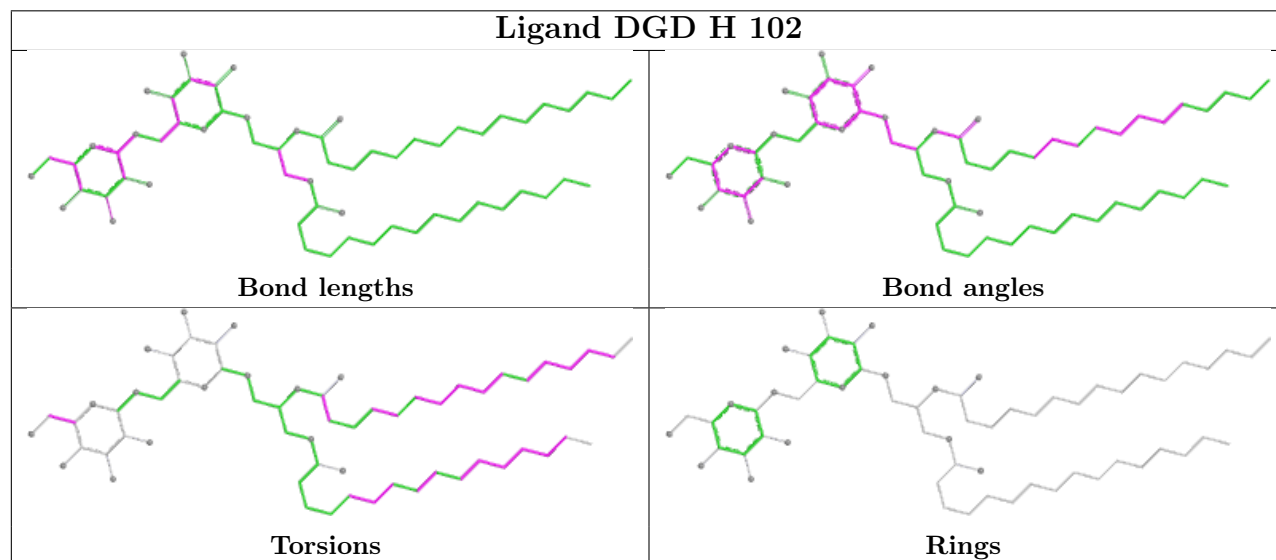
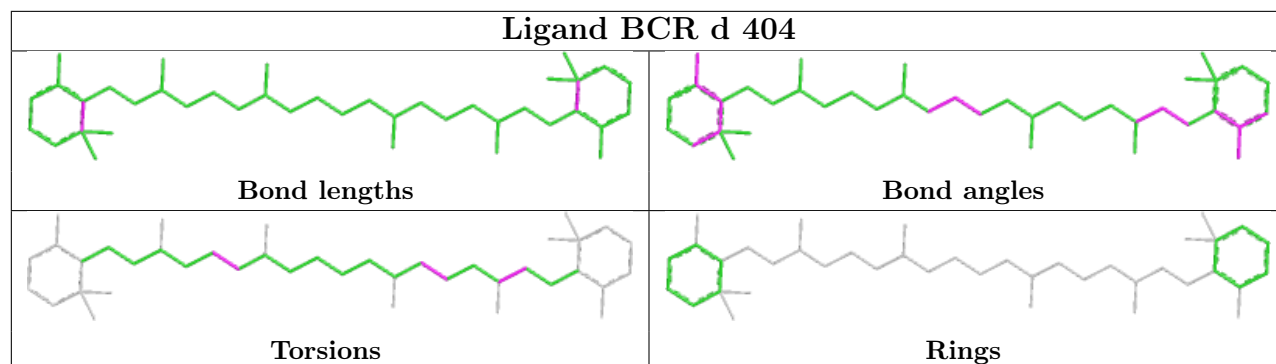


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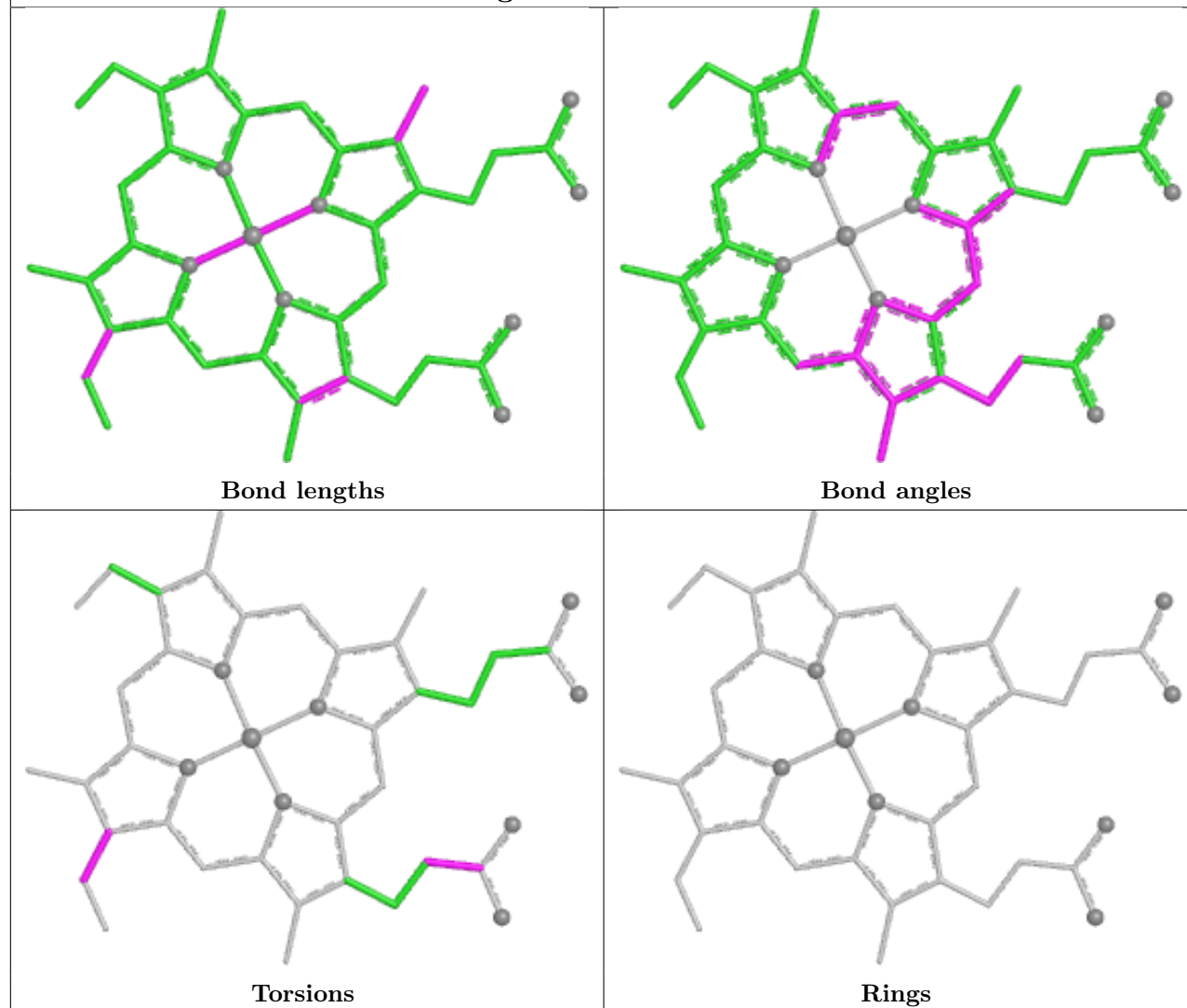


Ligand CLA B 606

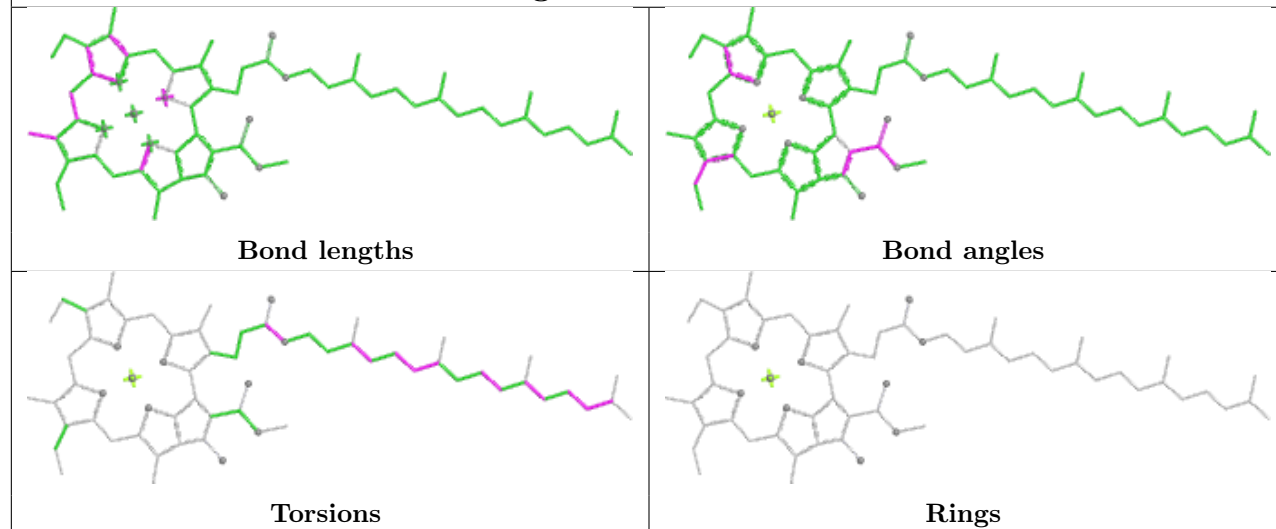


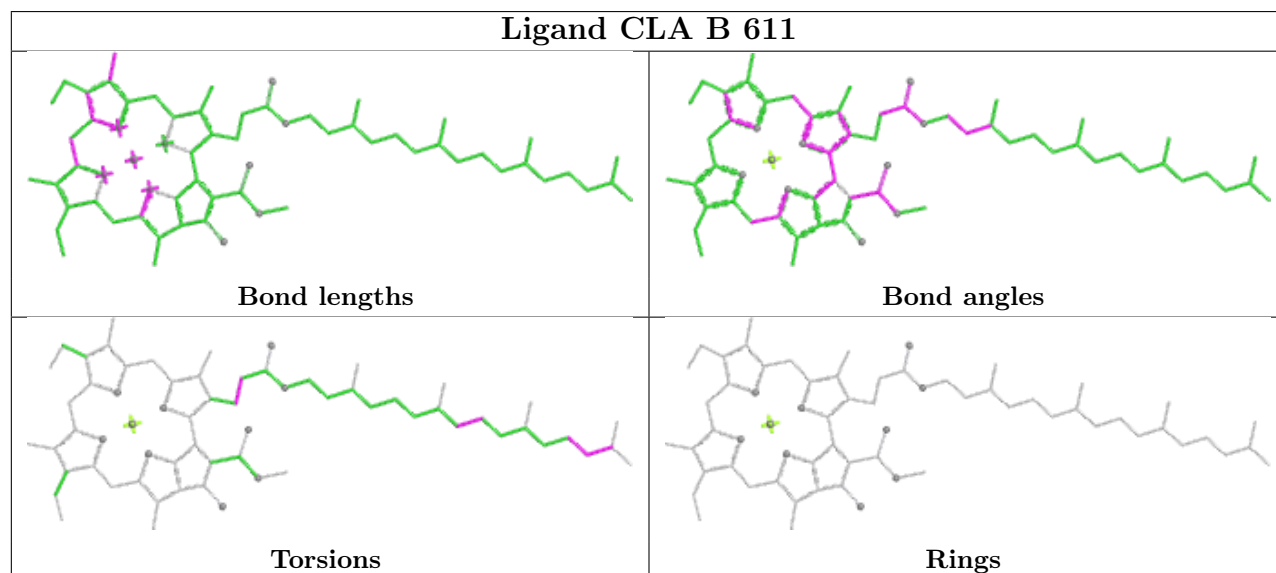
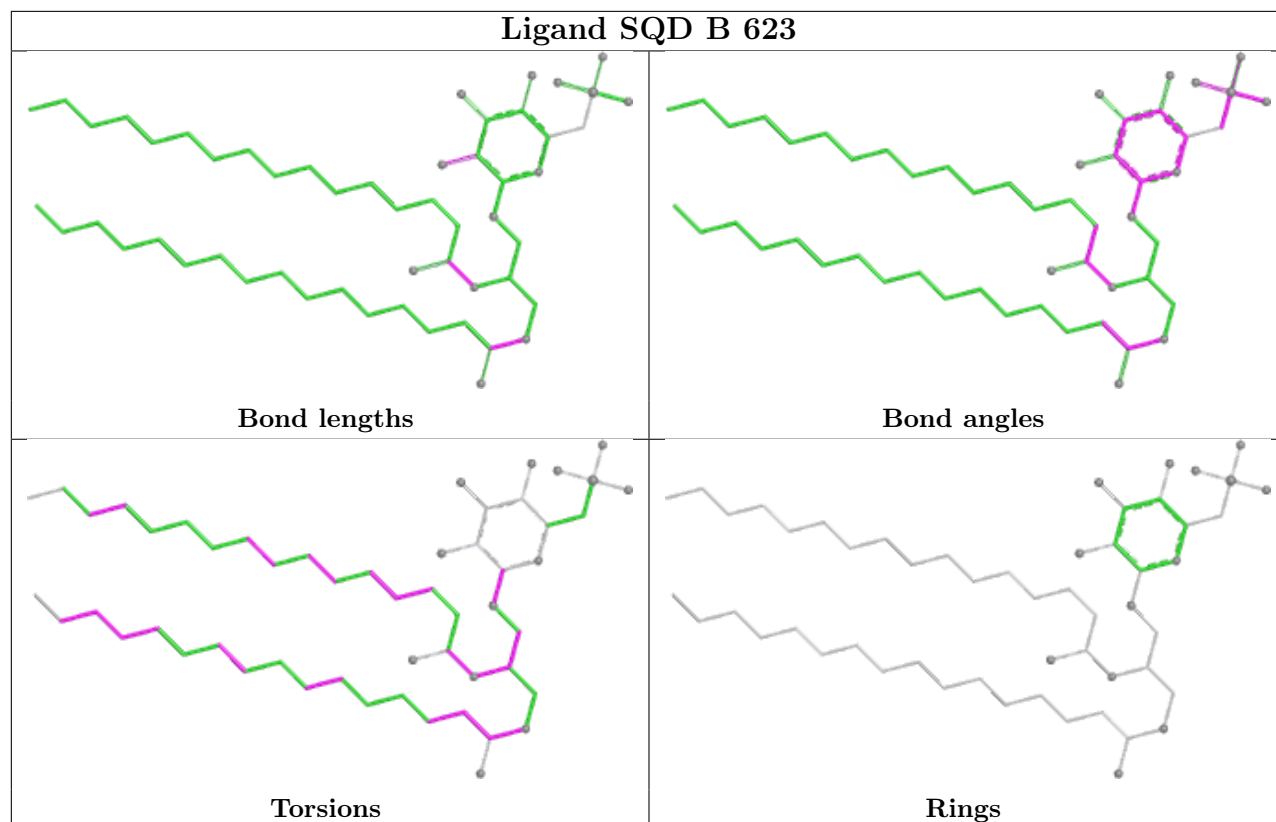


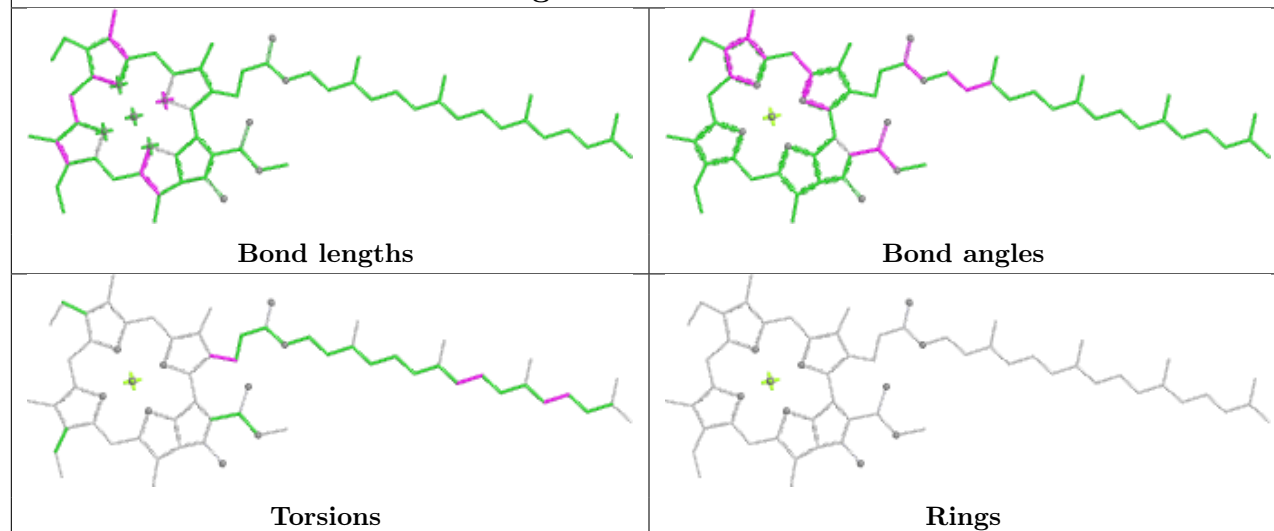
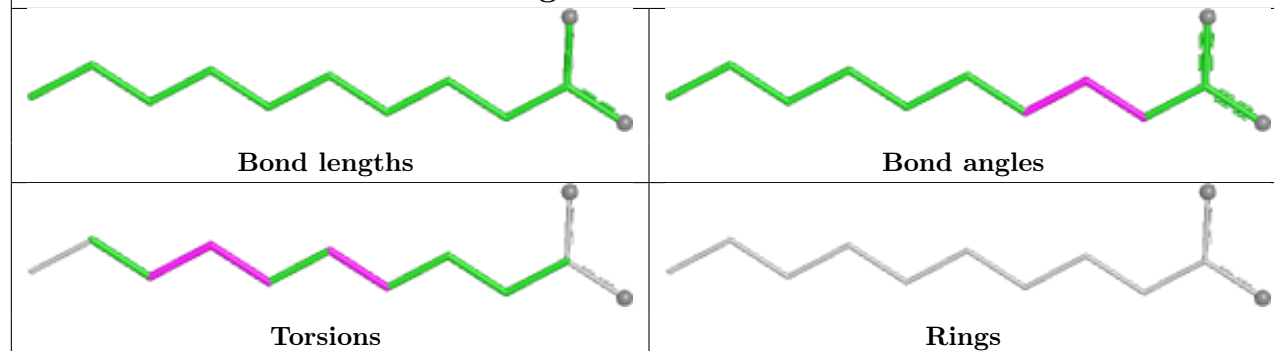
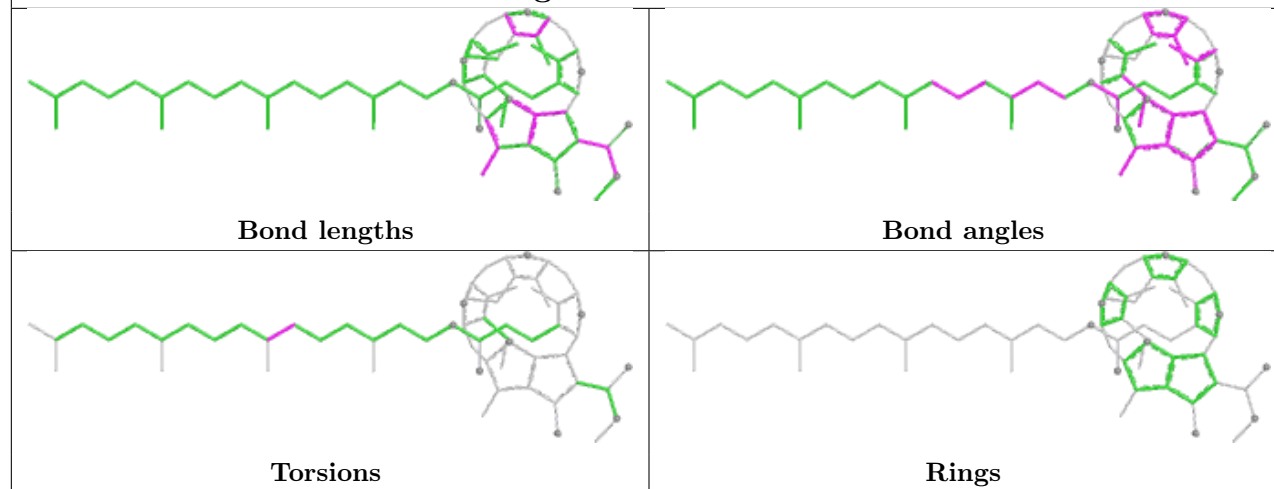
Ligand HEC v 201

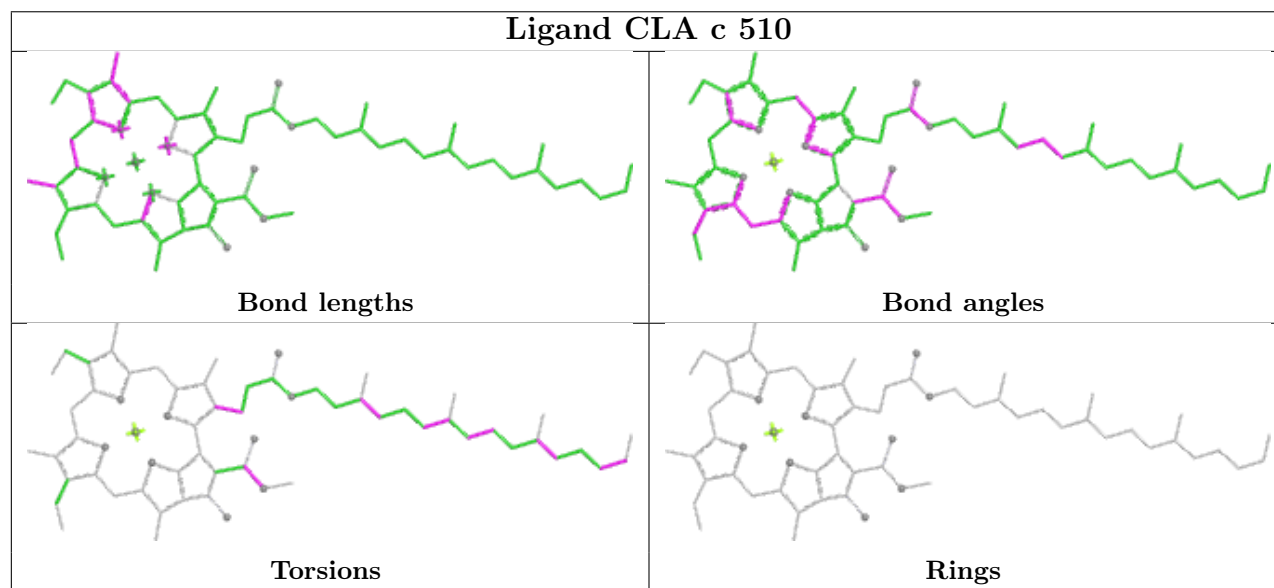
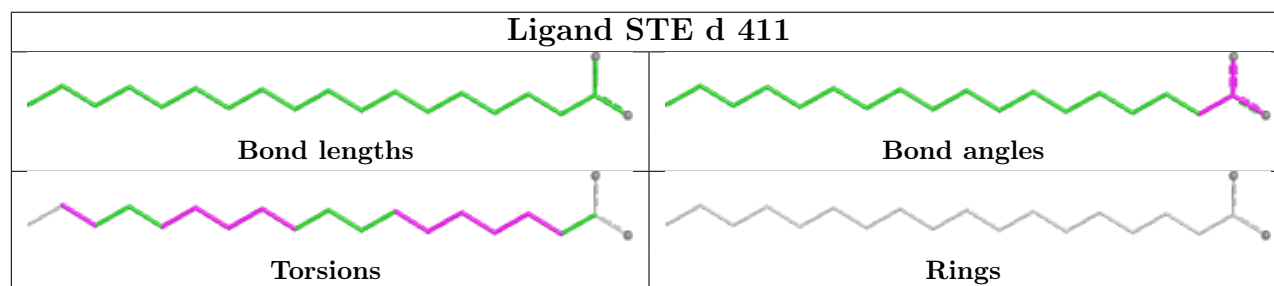
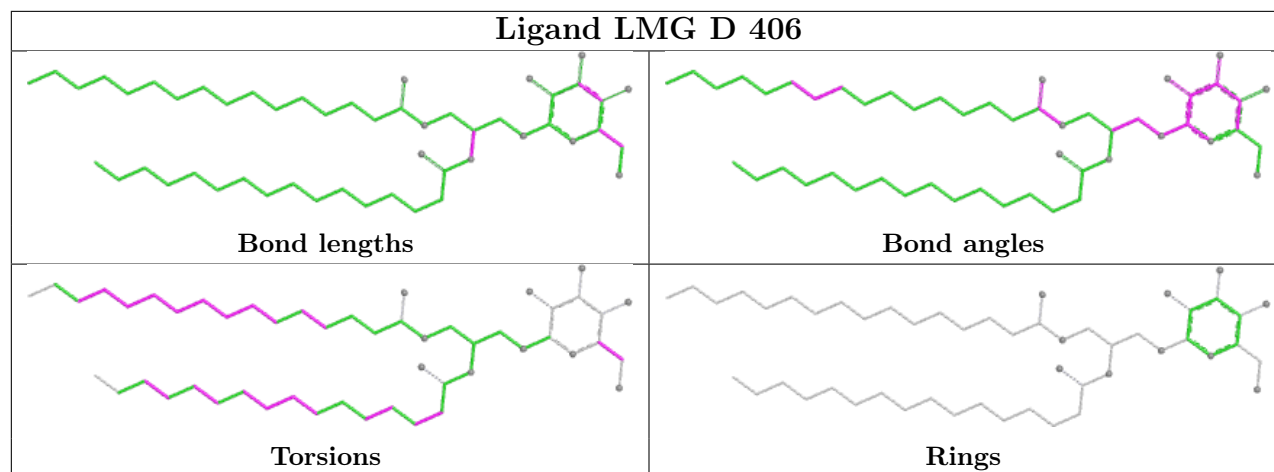


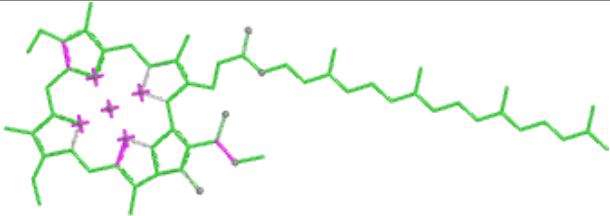
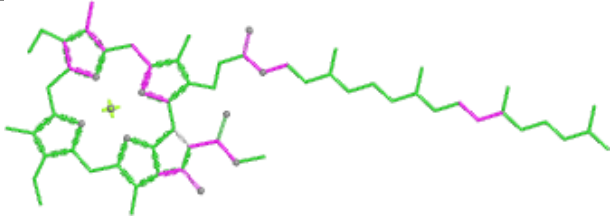
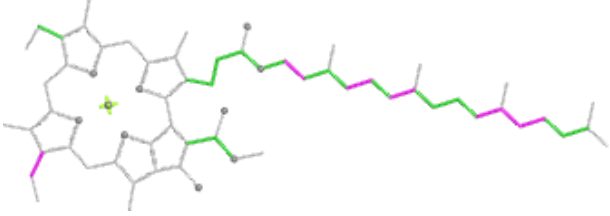
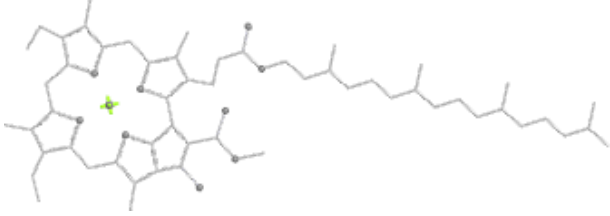
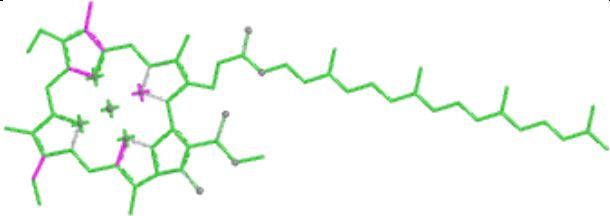
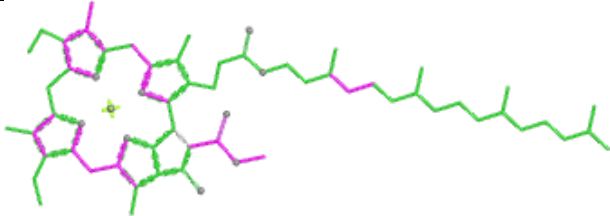
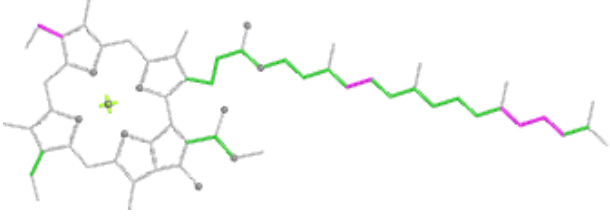
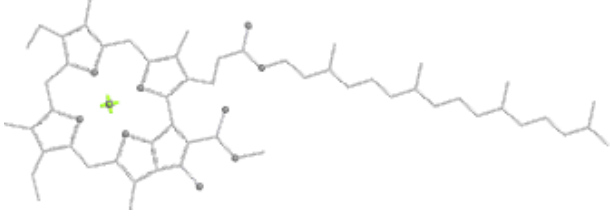
Ligand CLA C 506

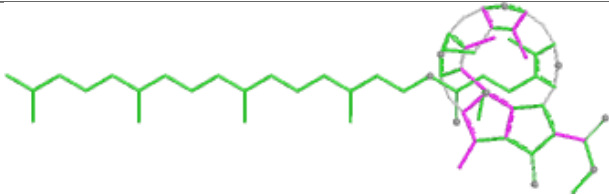
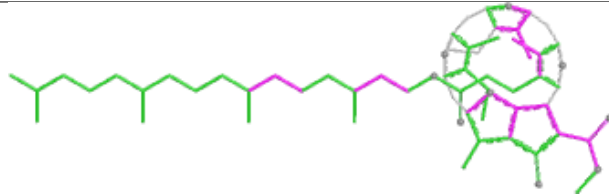
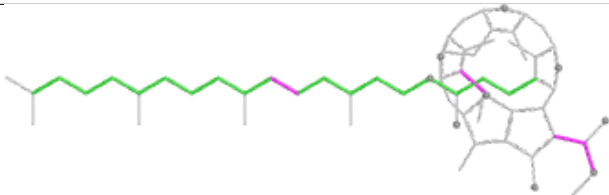
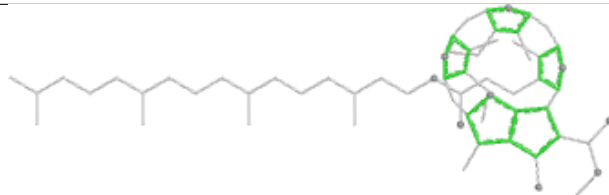


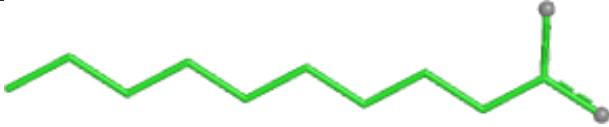
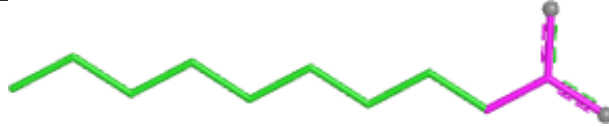
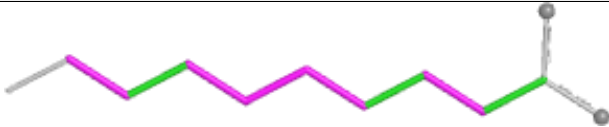
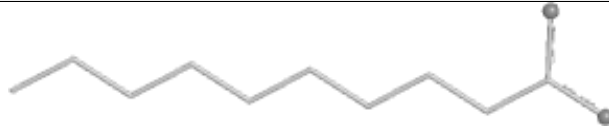


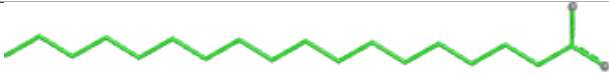
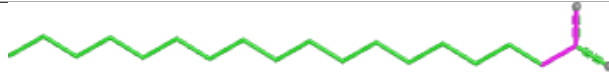
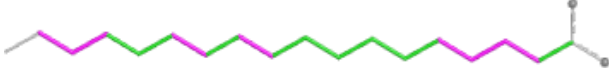
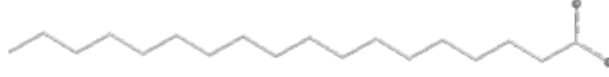
Ligand CLA B 603**Ligand STE J 101****Ligand PHO a 404**

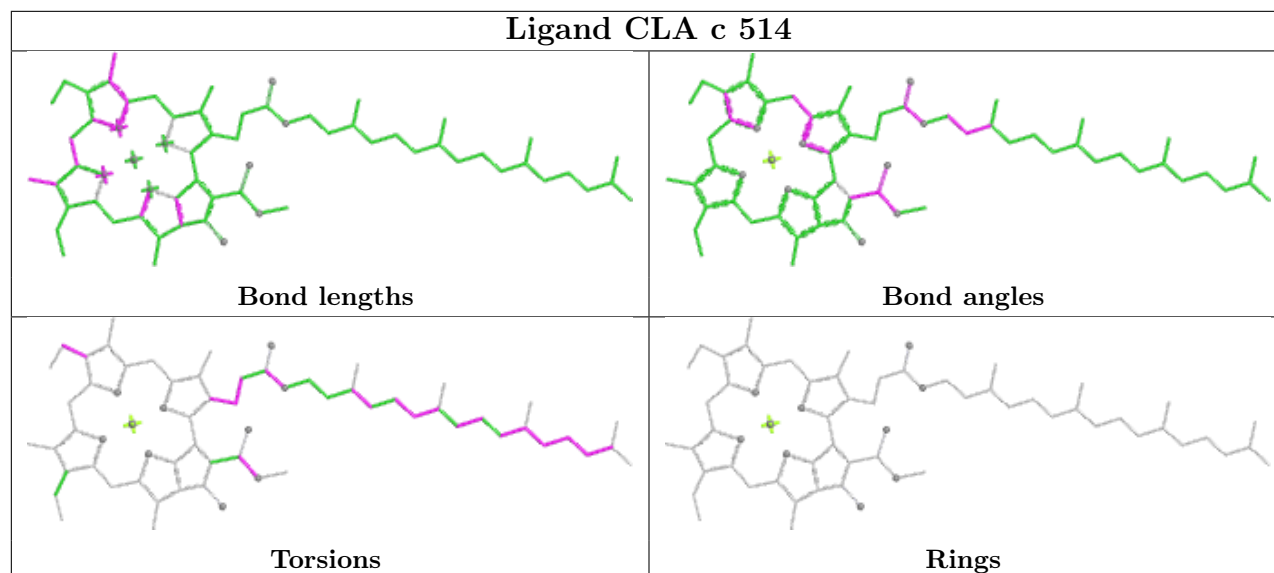
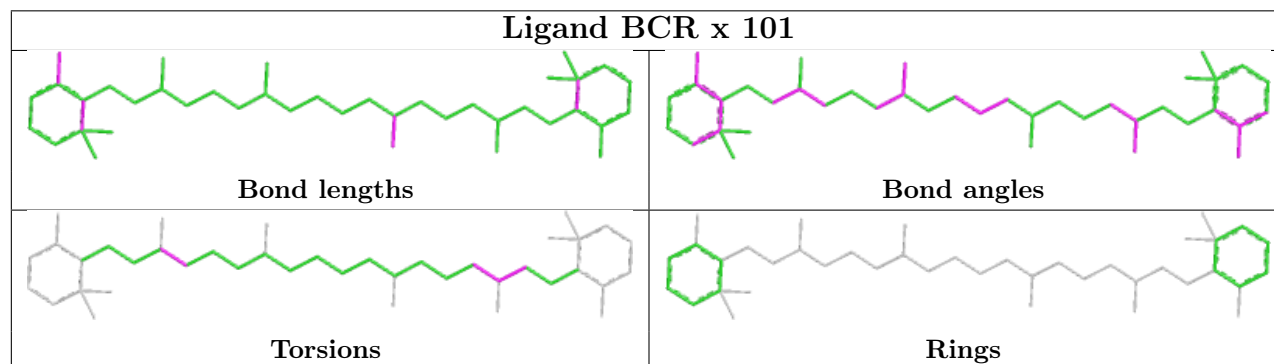
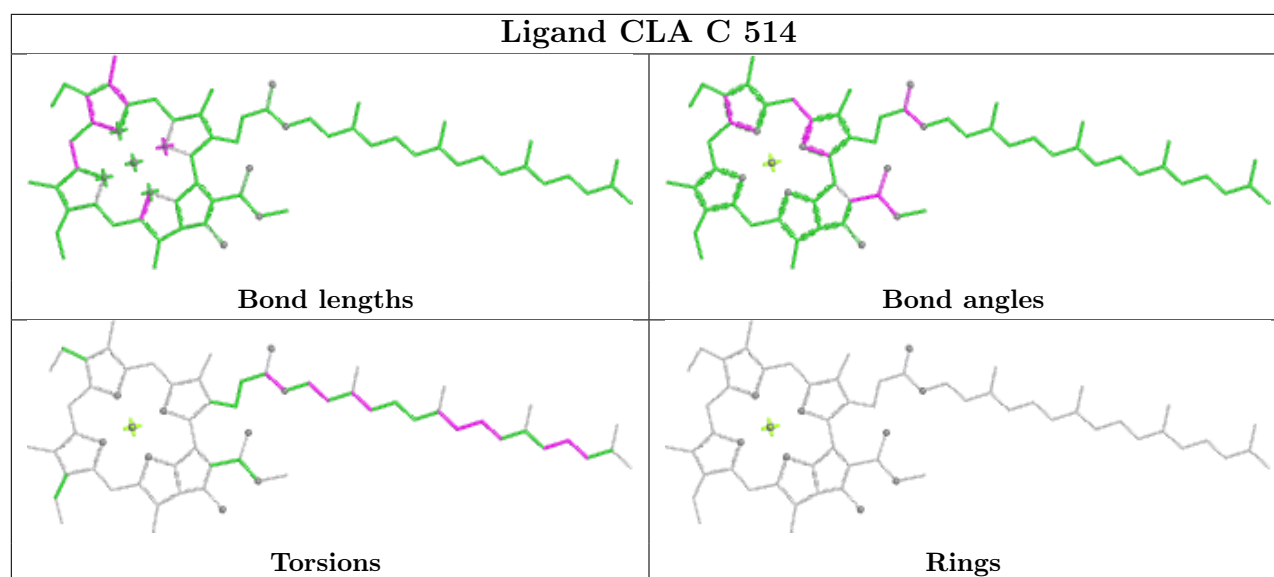


Ligand CLA B 605			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand CLA b 608			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand STE h 103			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	

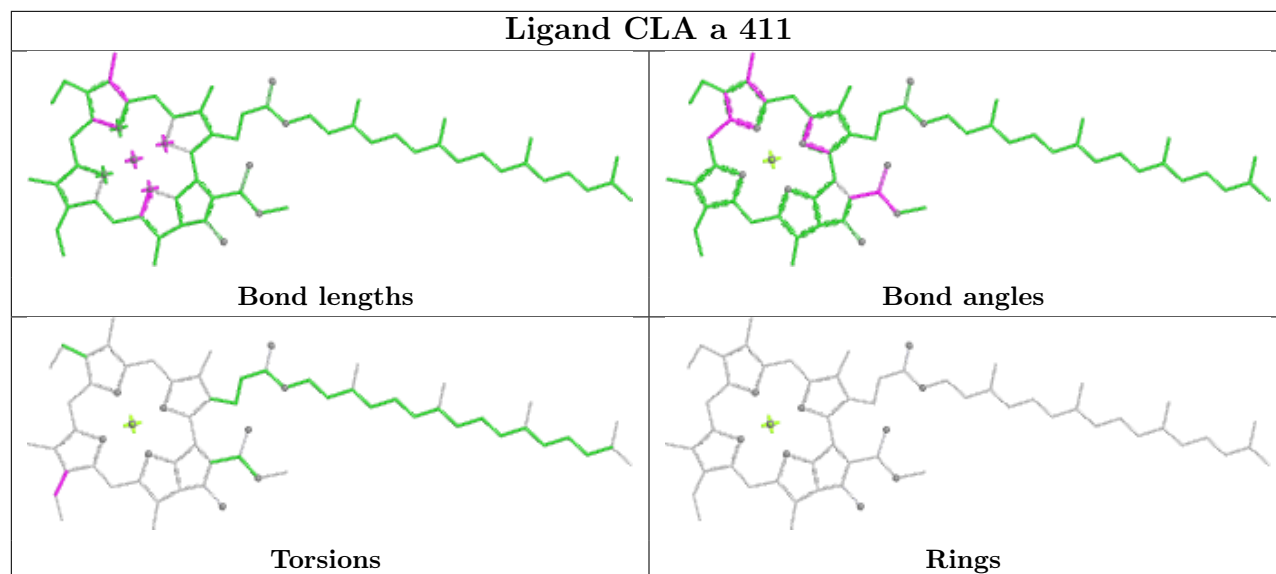
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE L 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

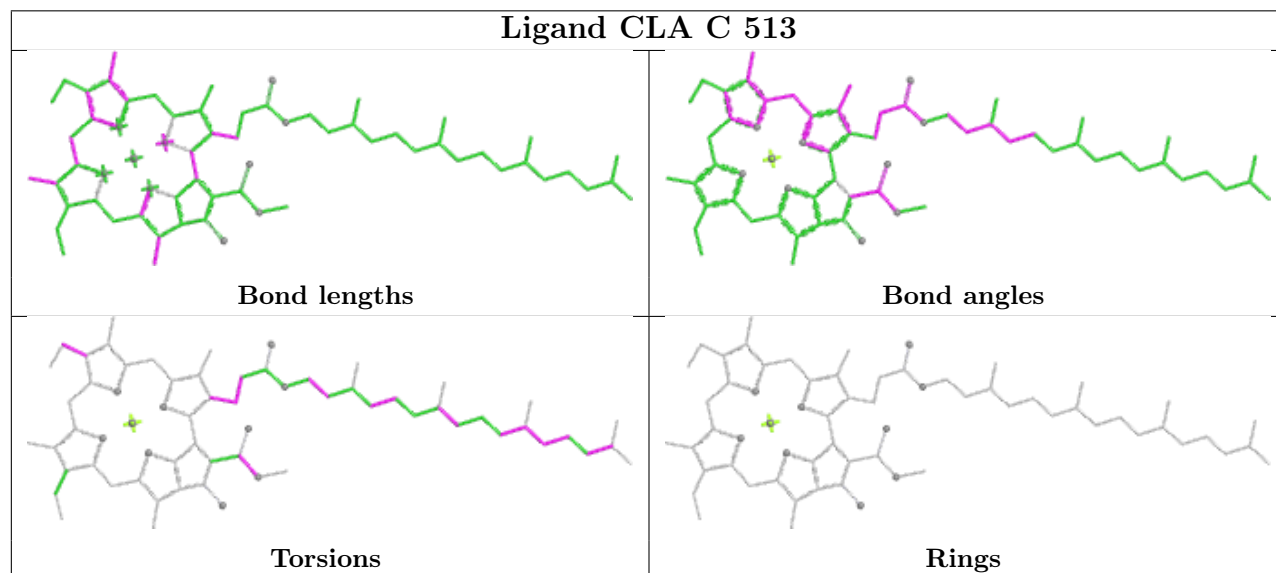
Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings



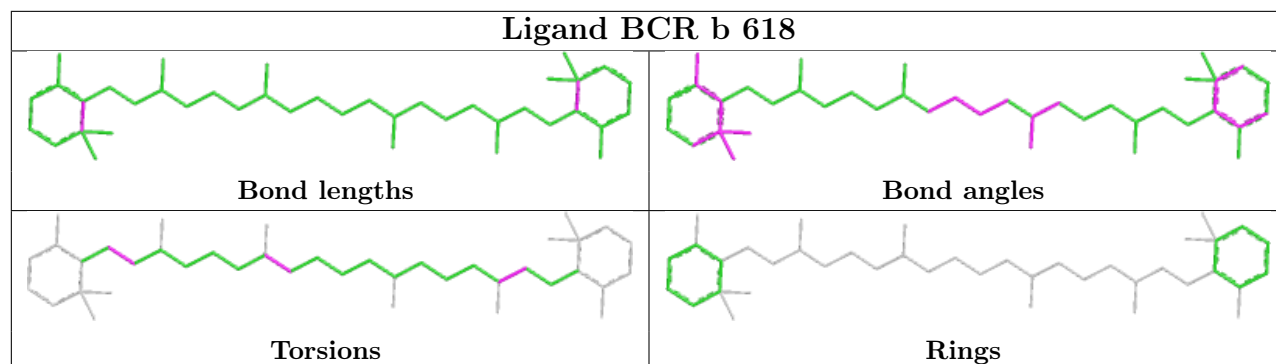
Ligand CLA a 411



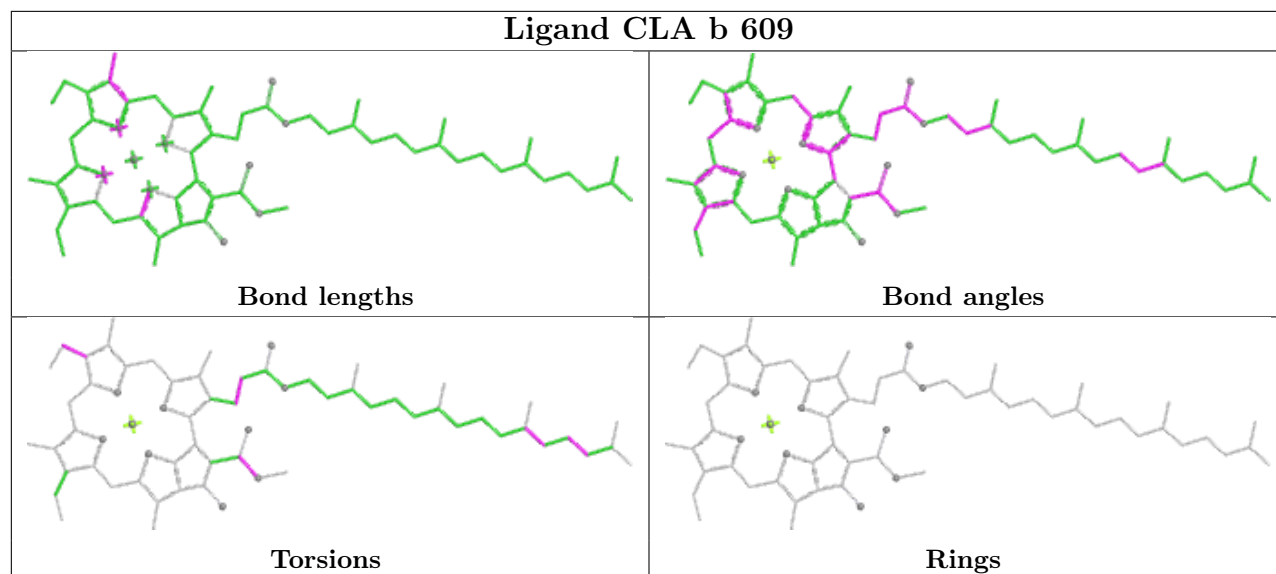
Ligand CLA C 513



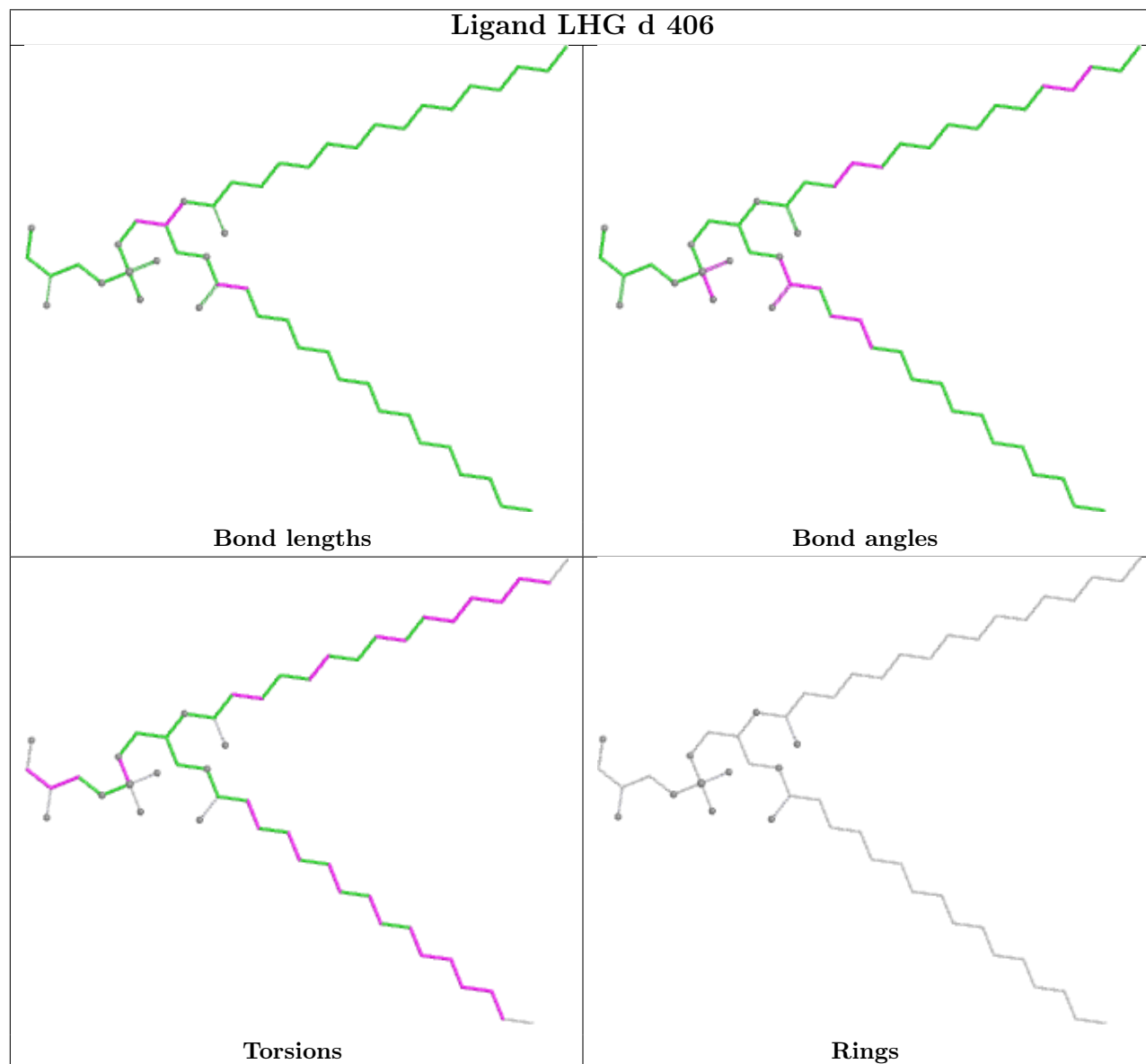
Ligand BCR b 618



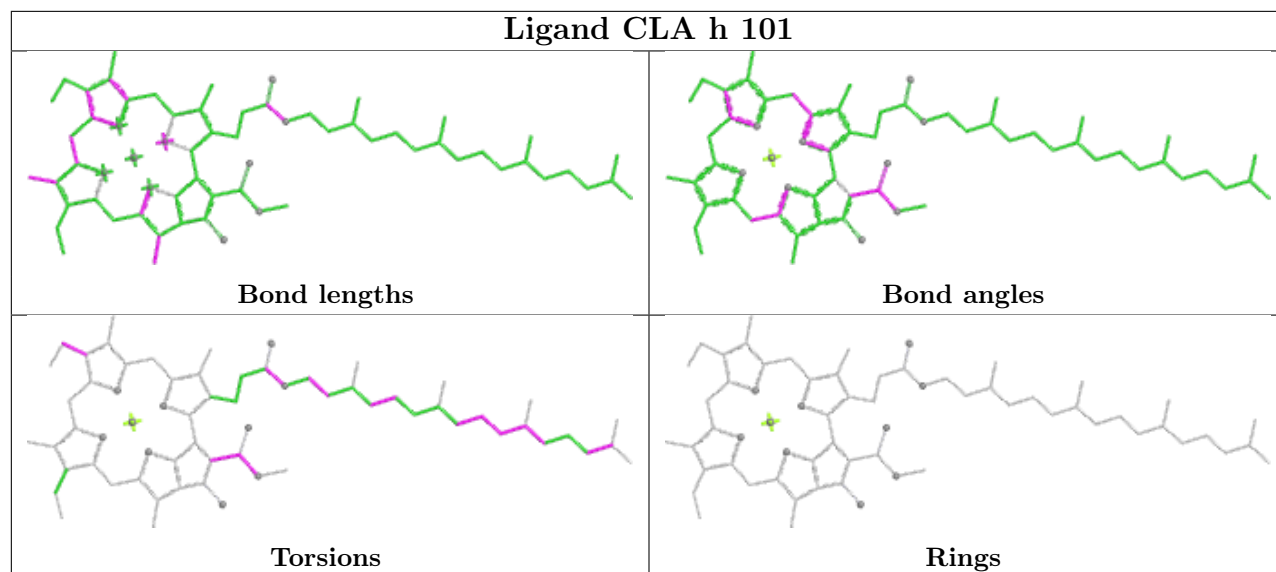
Ligand CLA b 609



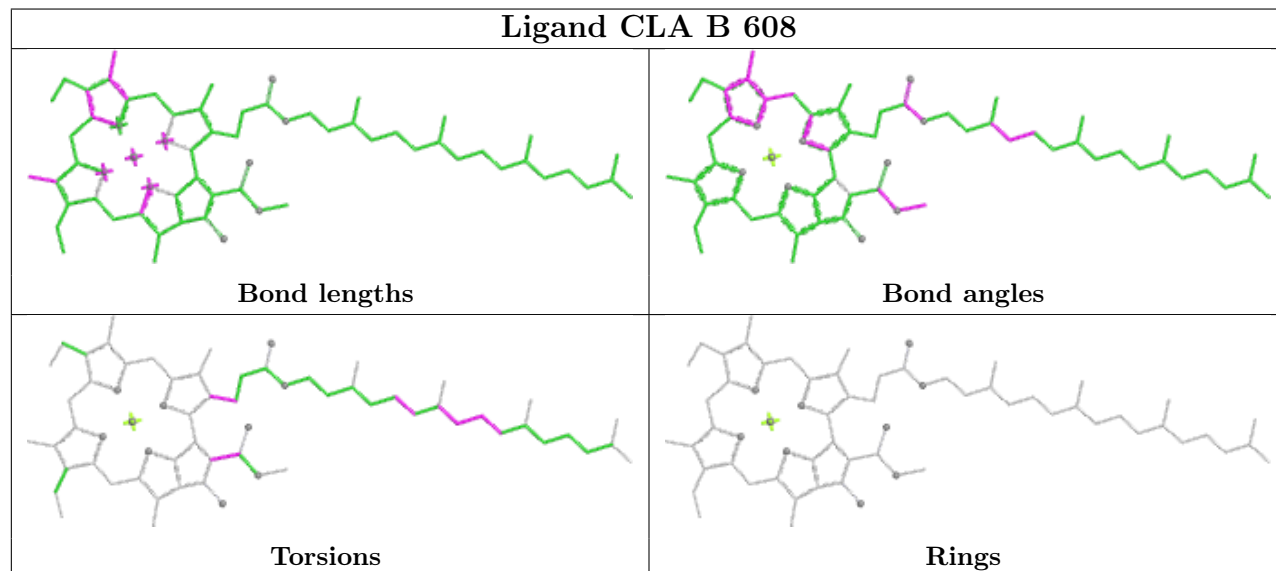
Ligand LHG d 406



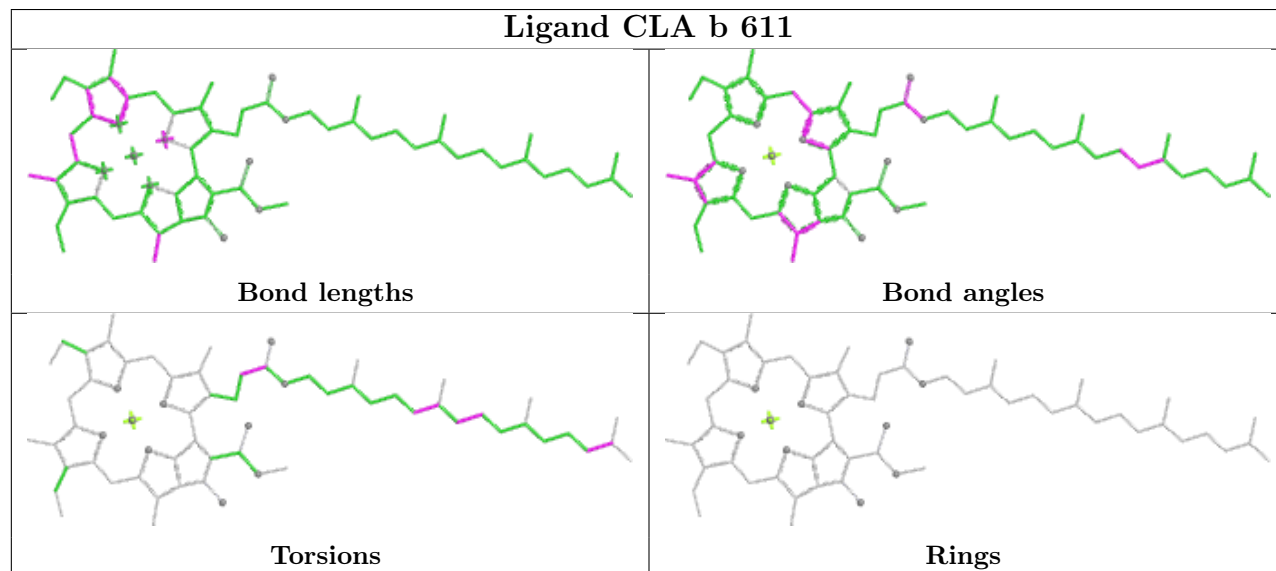
Ligand CLA h 101



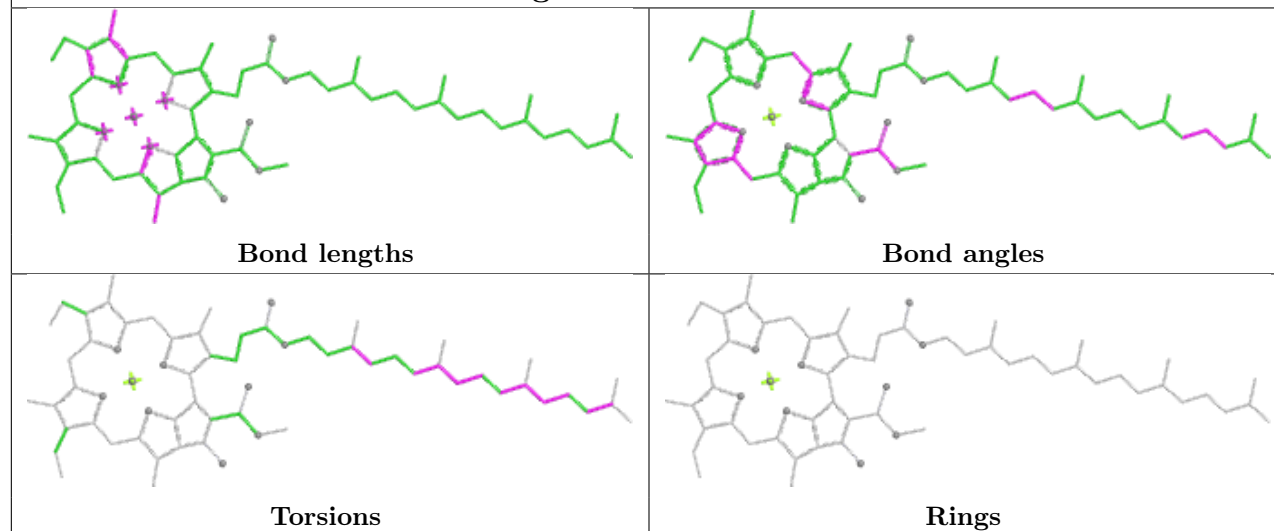
Ligand CLA B 608



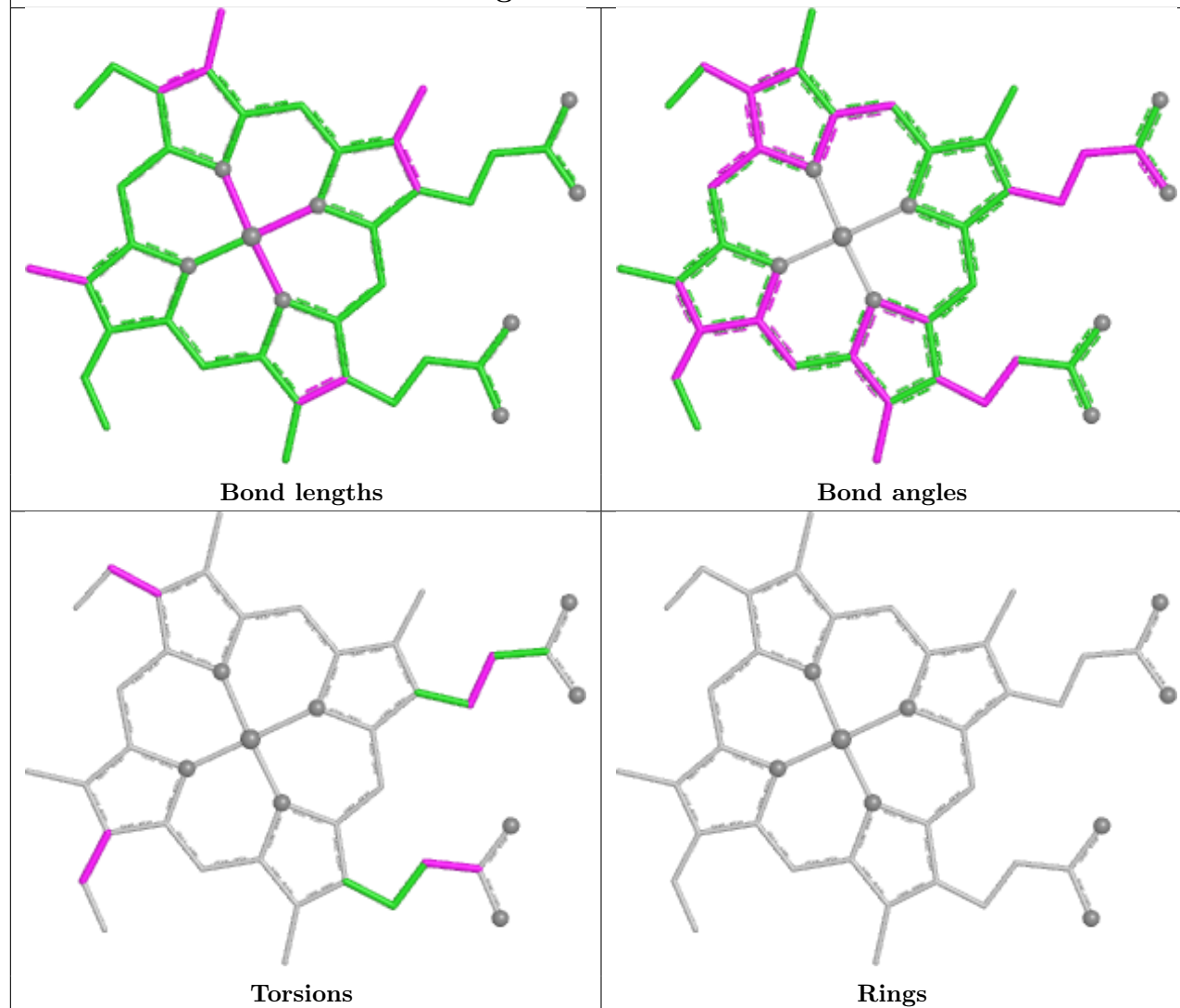
Ligand CLA b 611

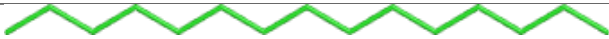
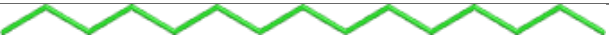


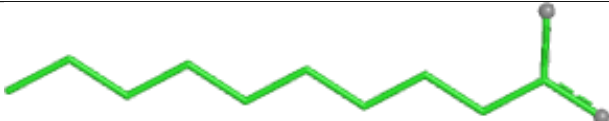
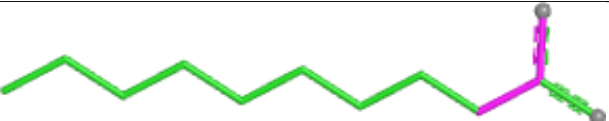
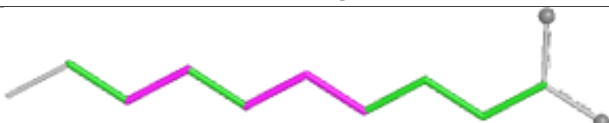
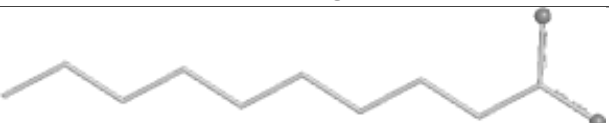
Ligand CLA B 612

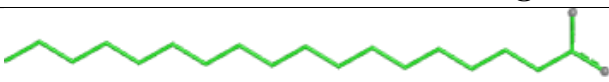
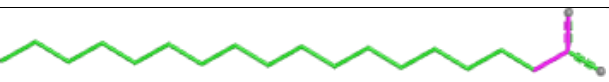
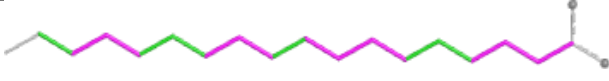
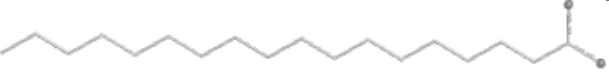


Ligand HEC e 101

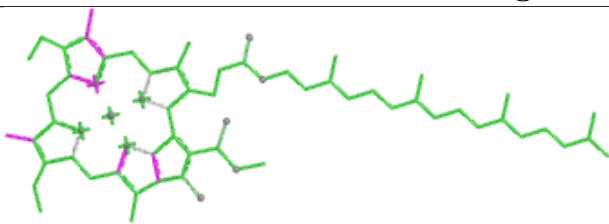
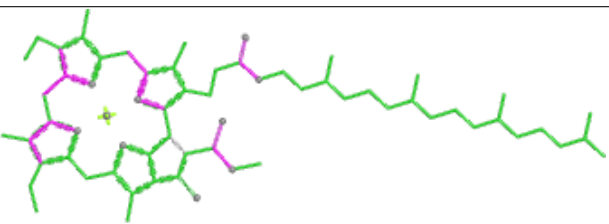
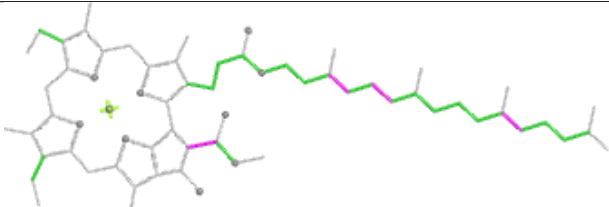
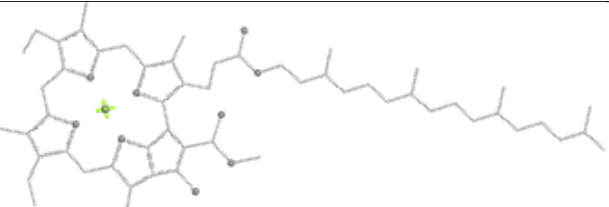


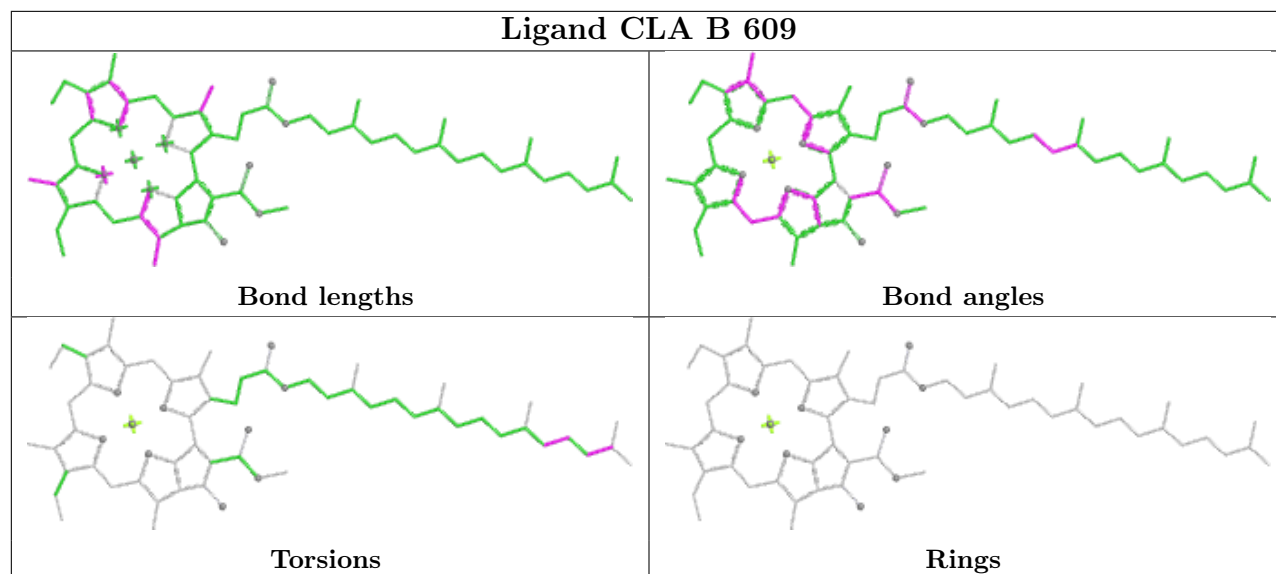
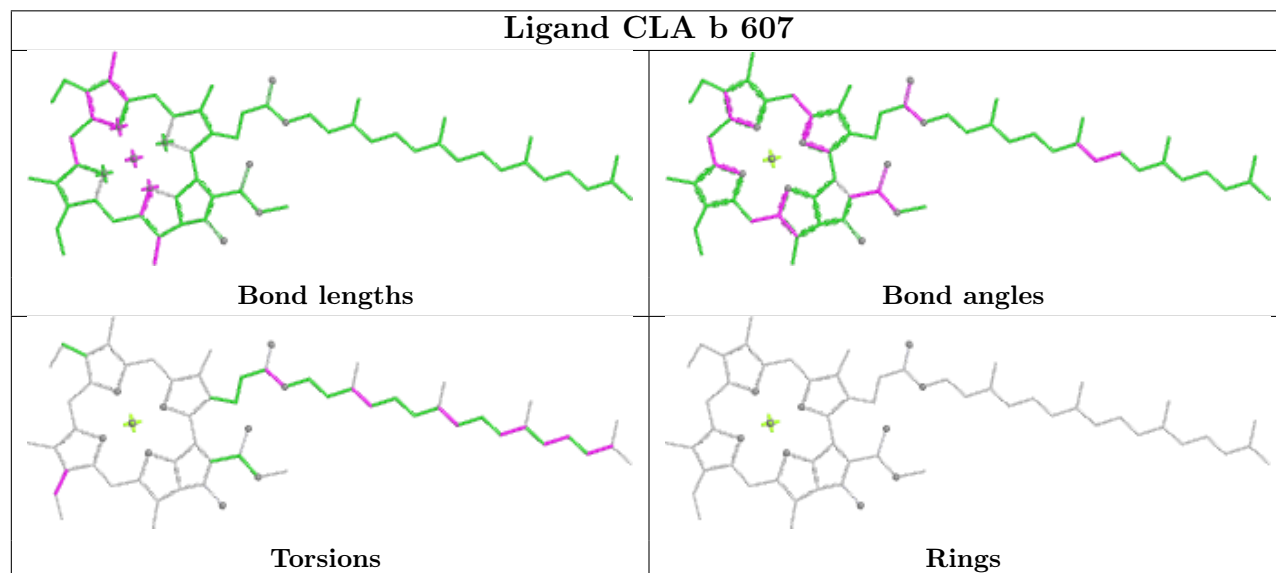
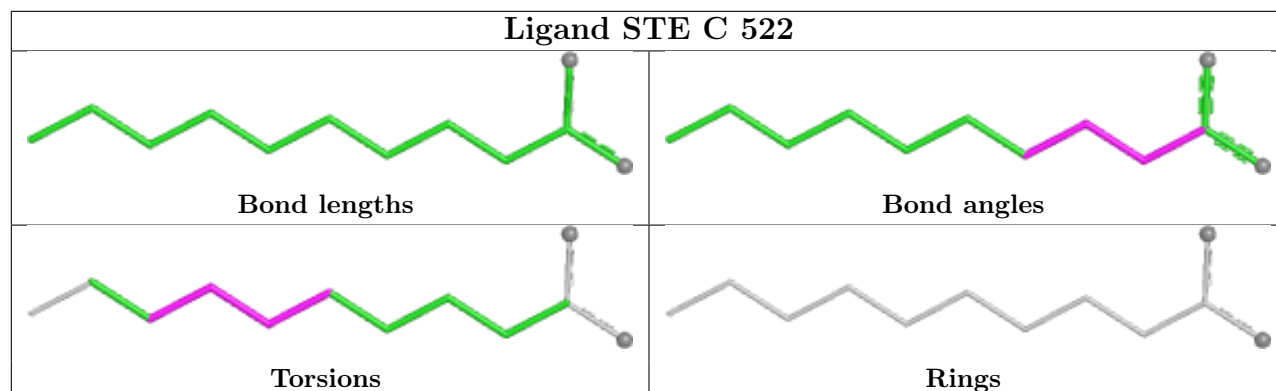
Ligand STE T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

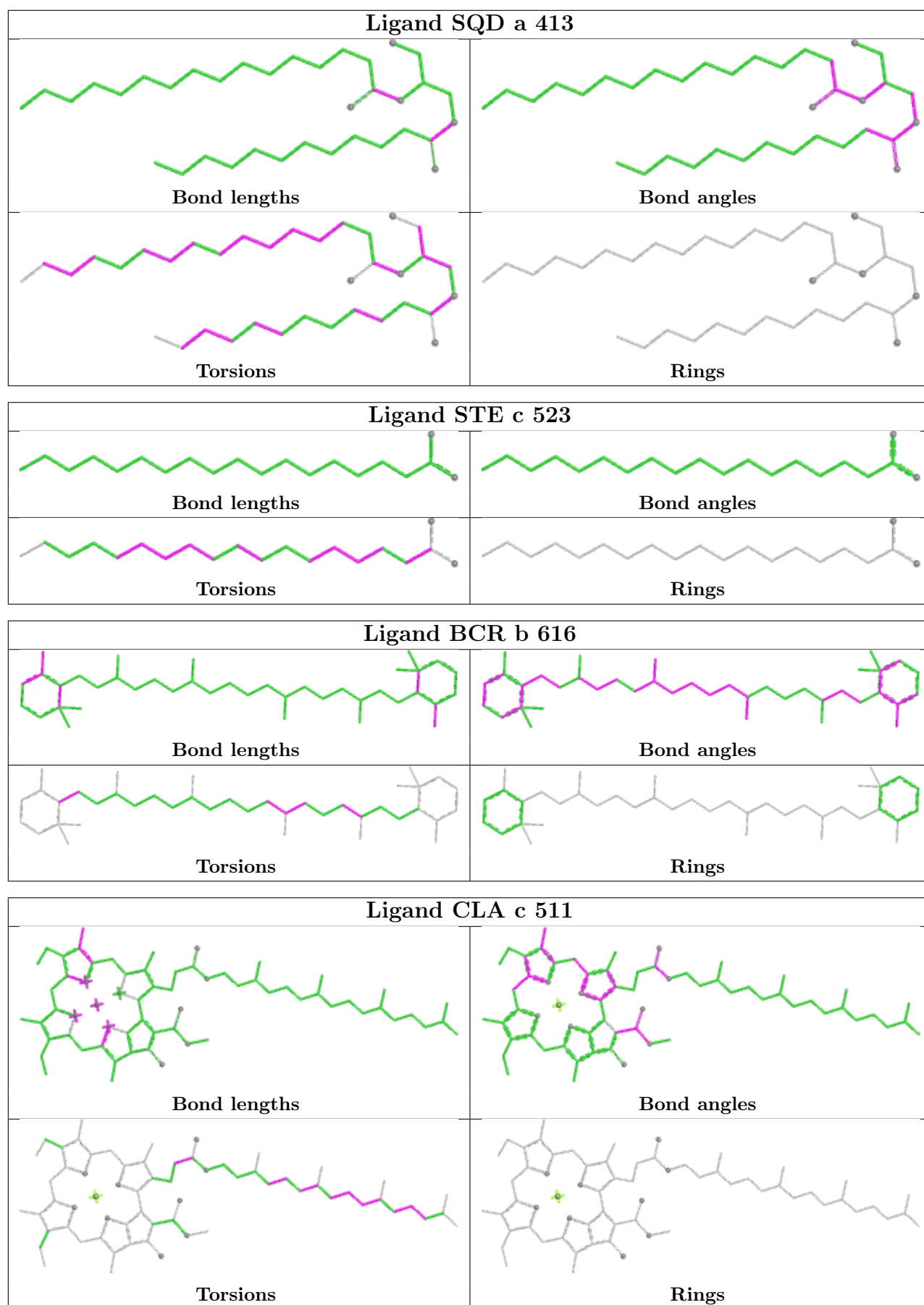
Ligand STE a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

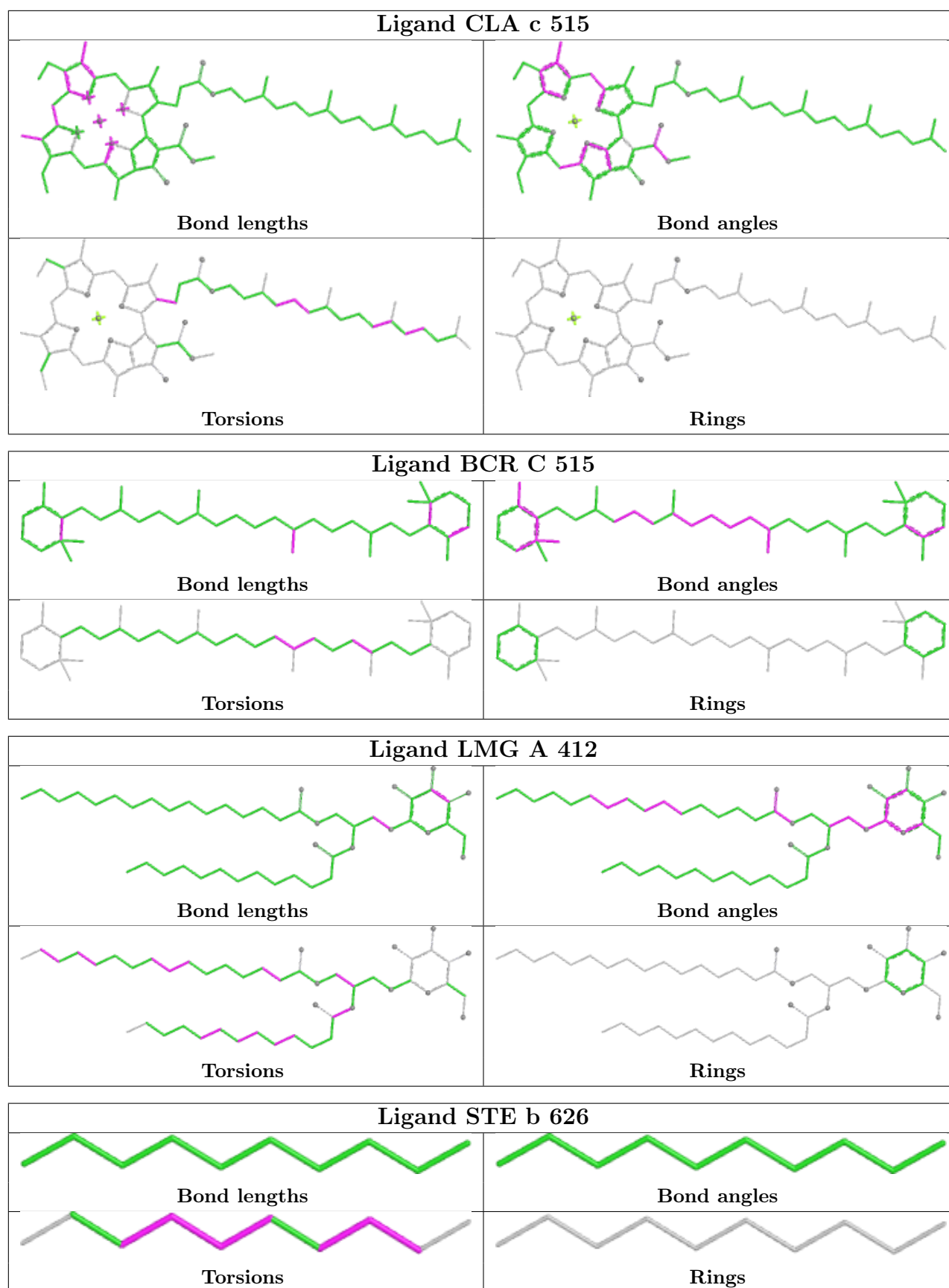
Ligand STE b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

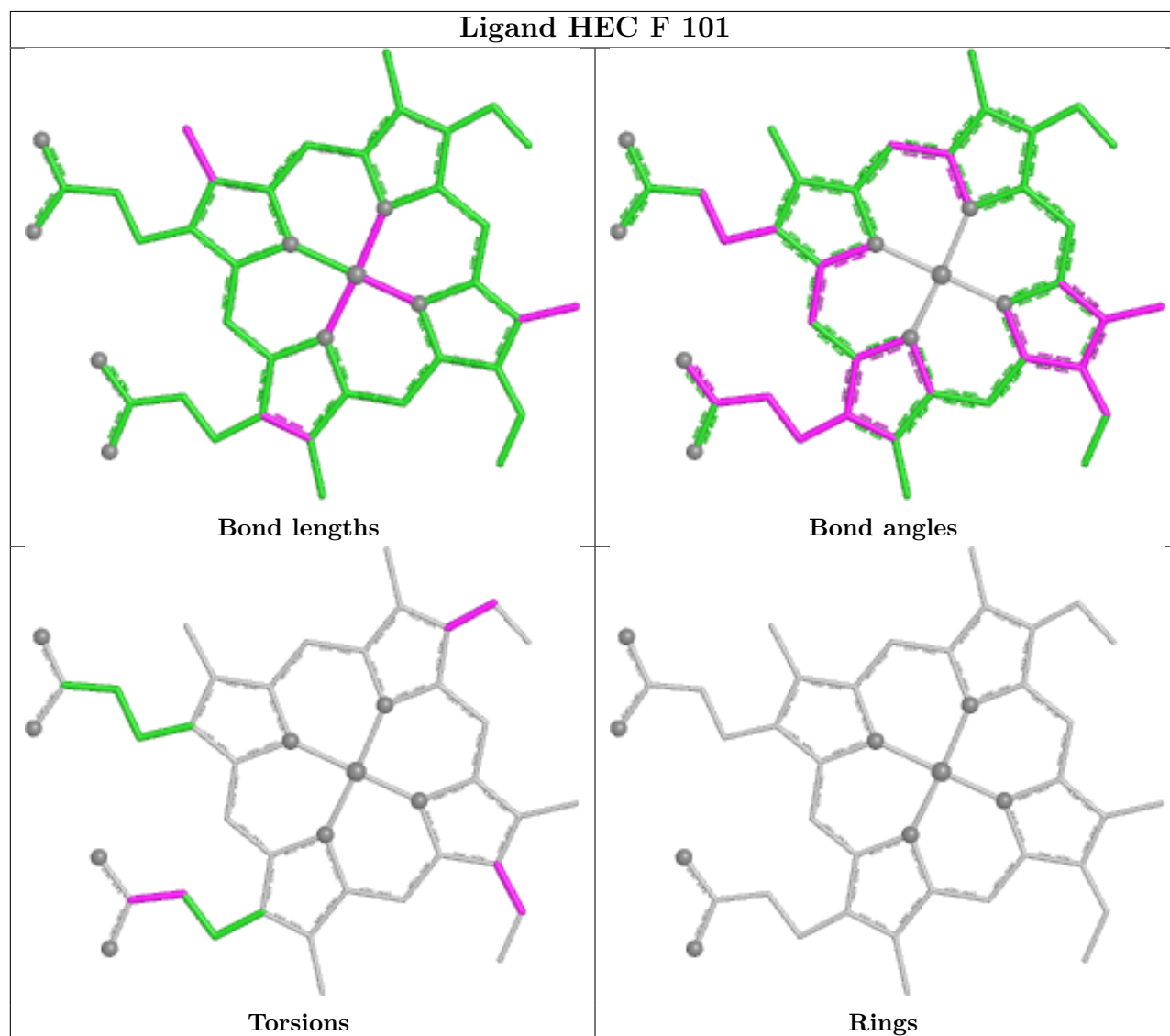
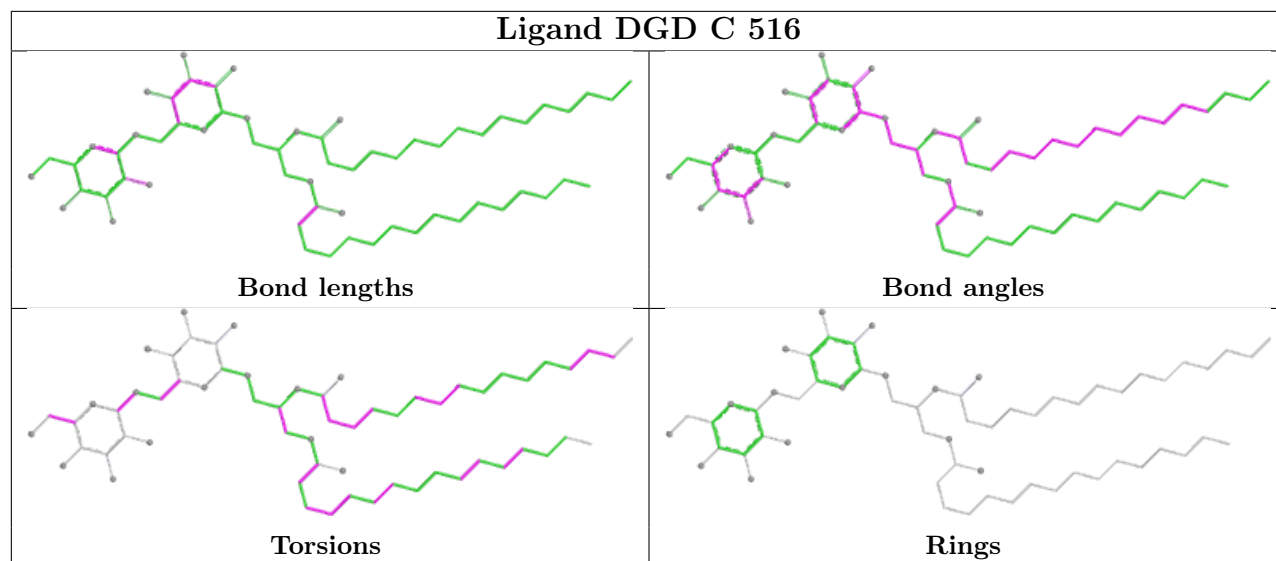
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

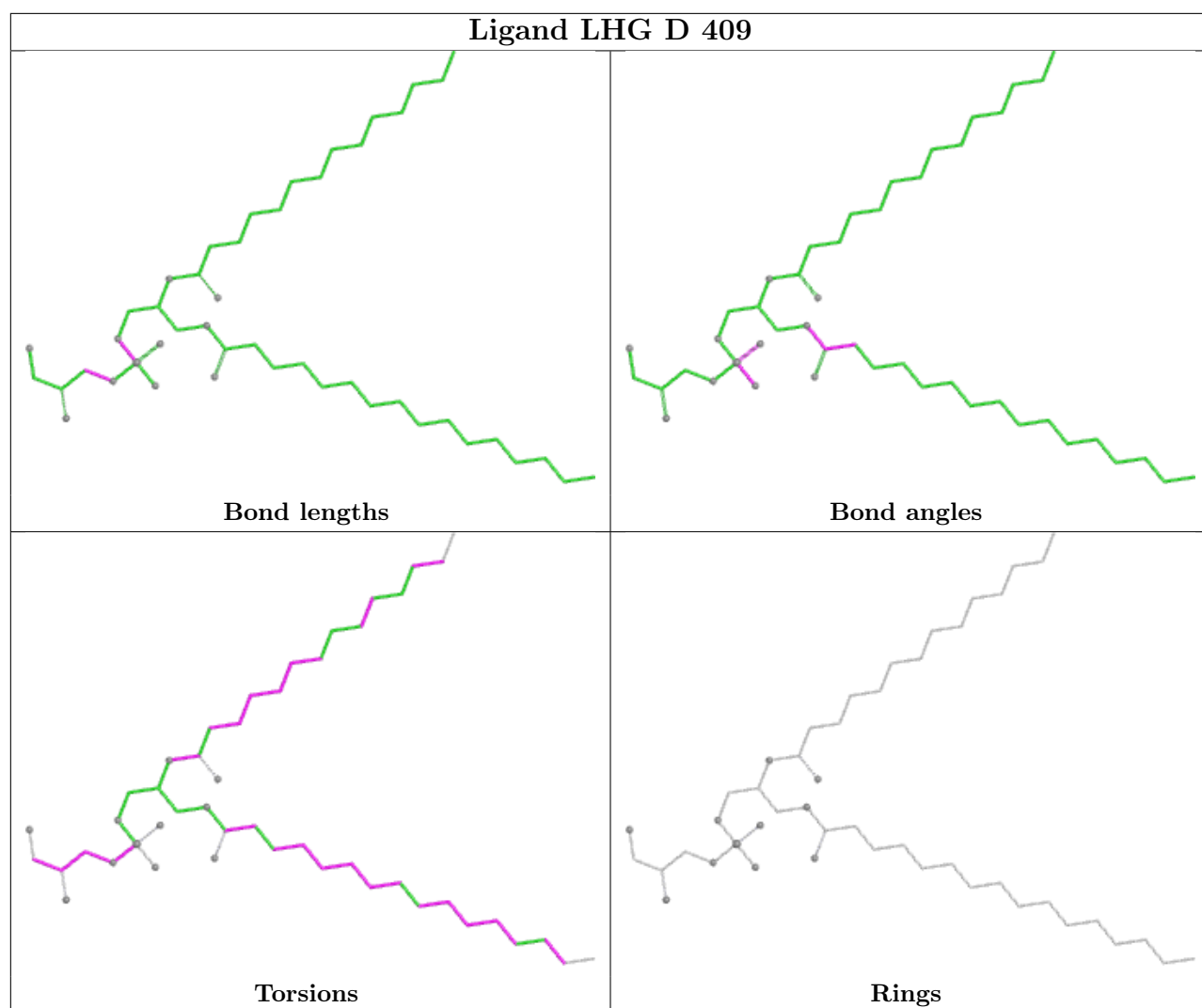
Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

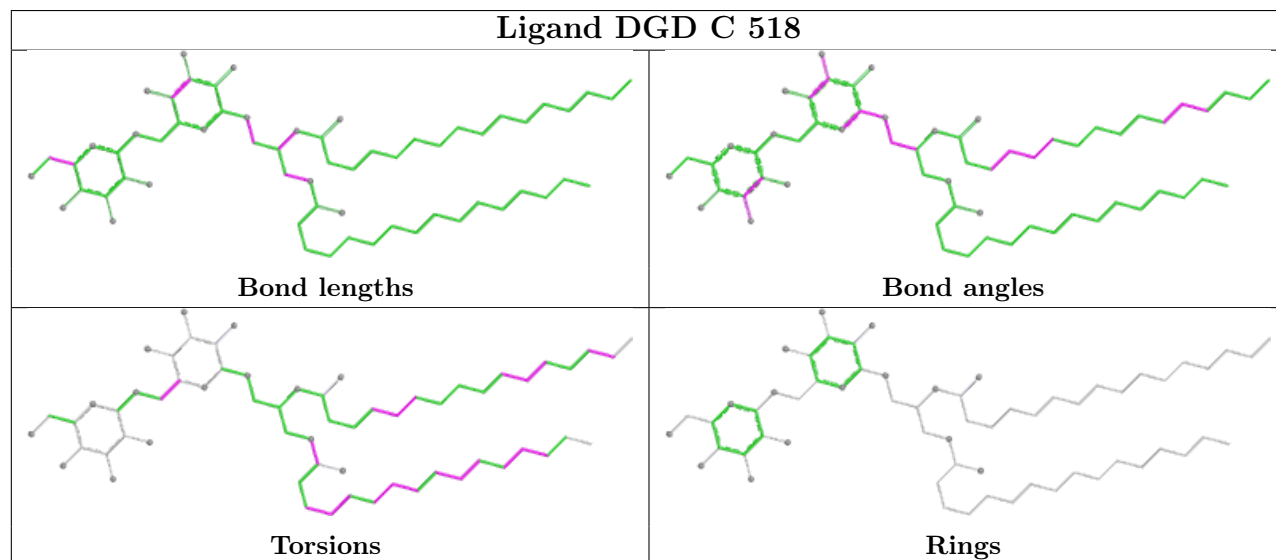
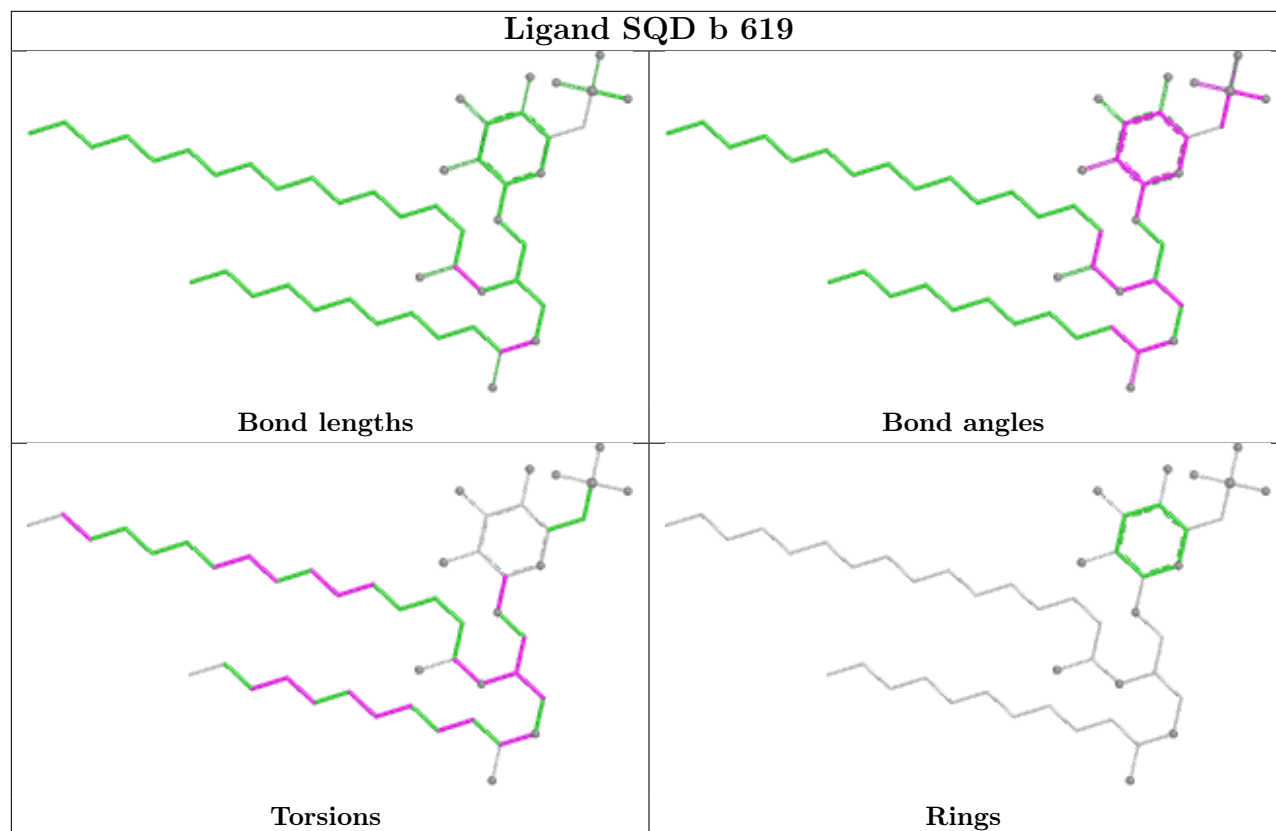
Ligand CLA B 609**Ligand CLA b 607****Ligand STE C 522**

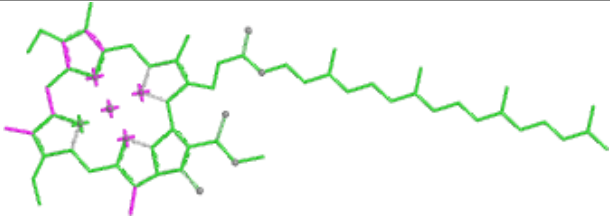
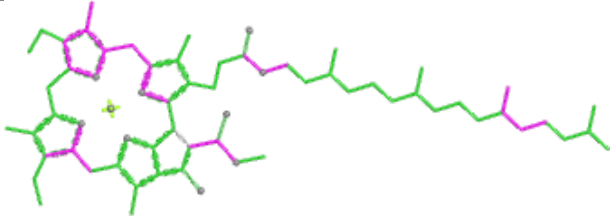
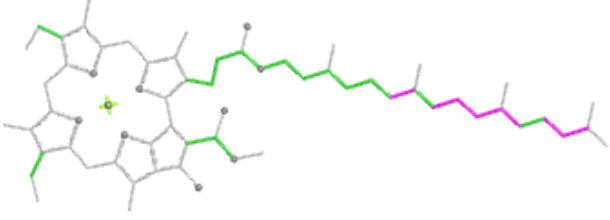
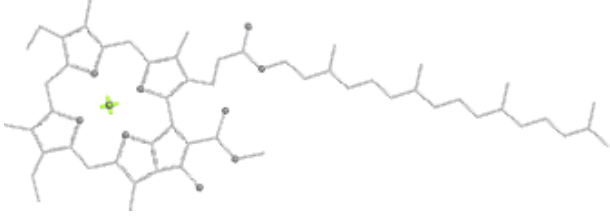
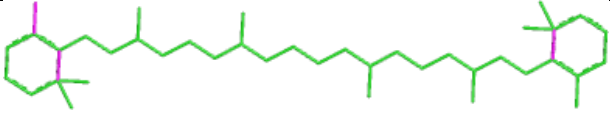
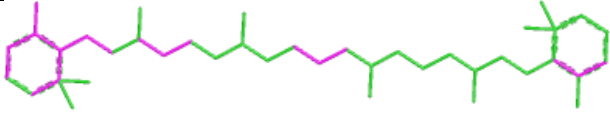
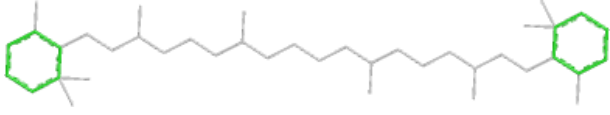
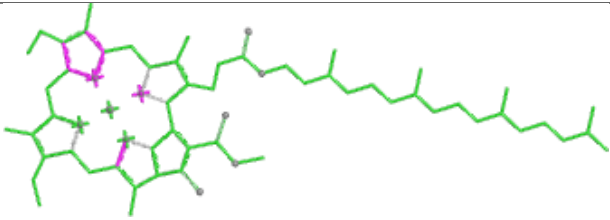
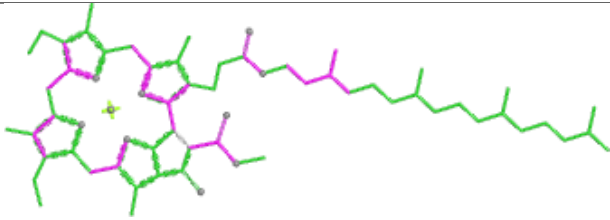
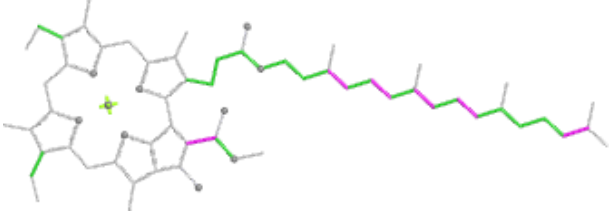
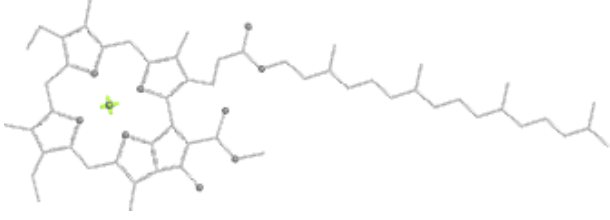




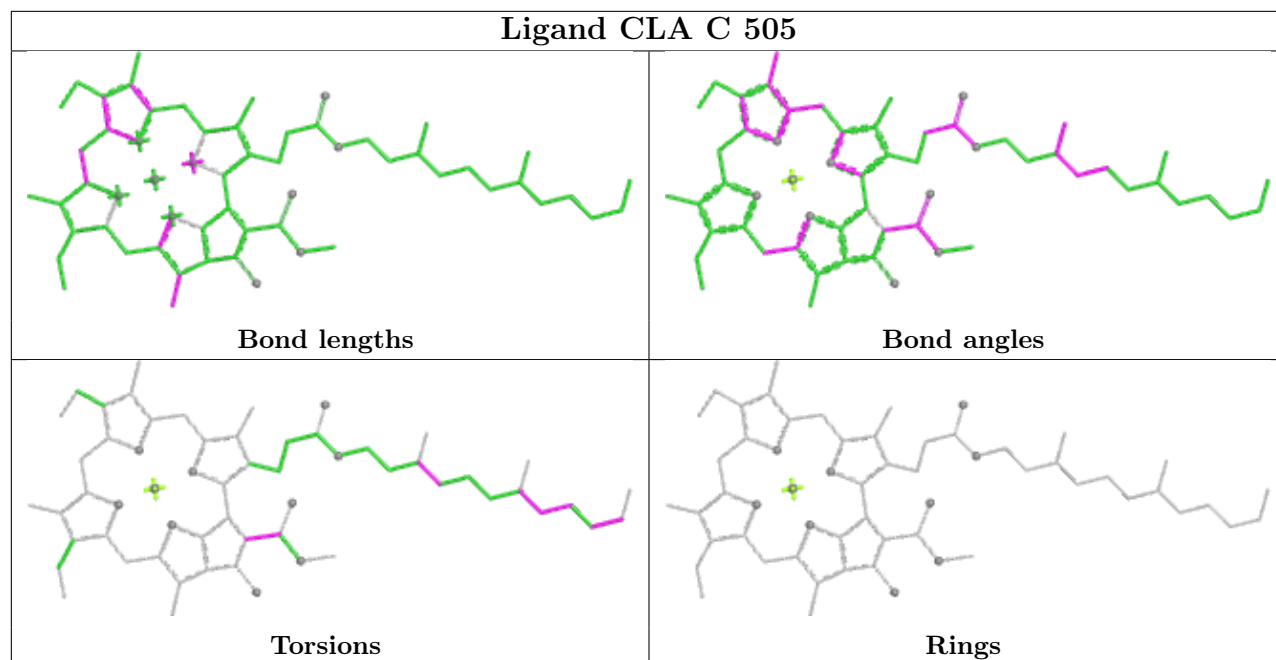




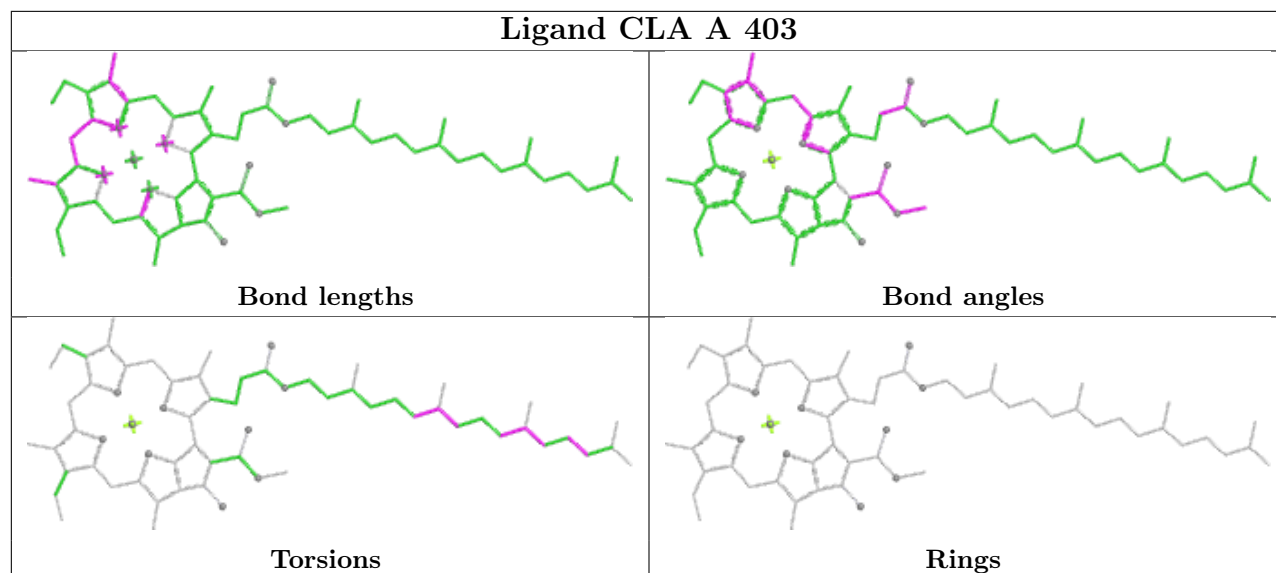


Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

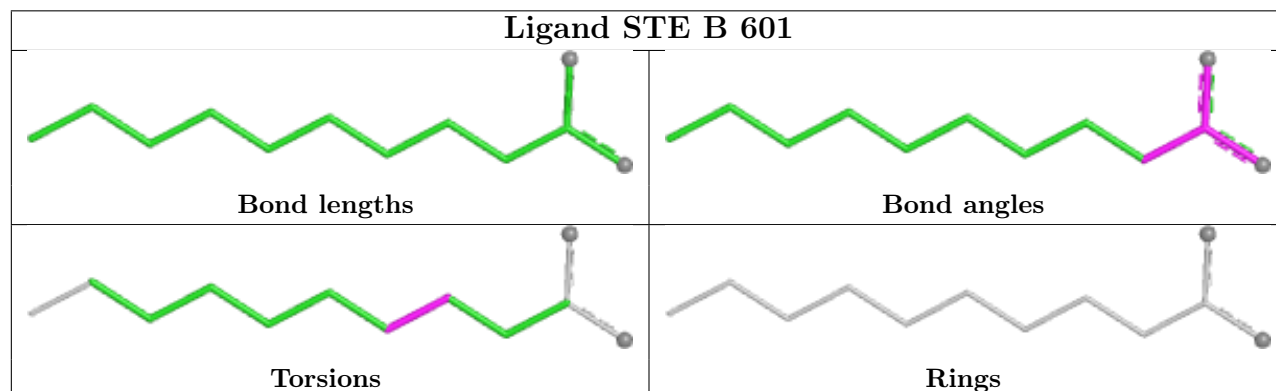
Ligand CLA C 505

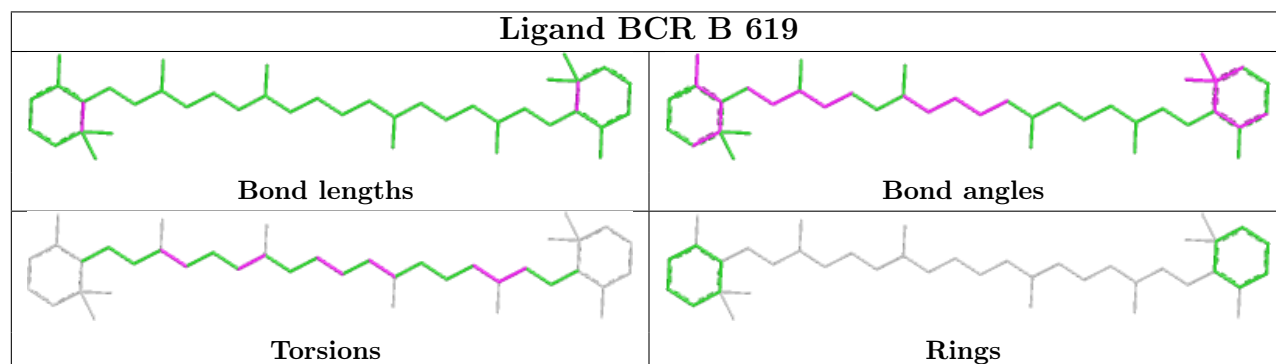
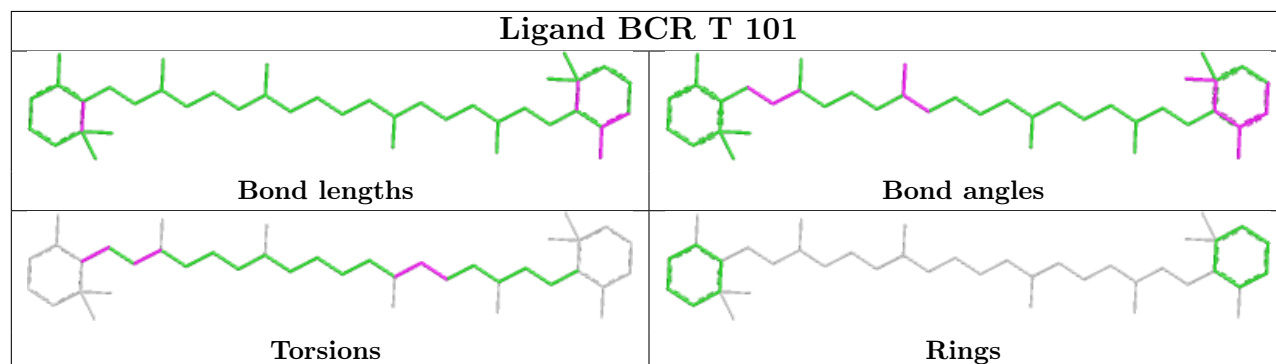
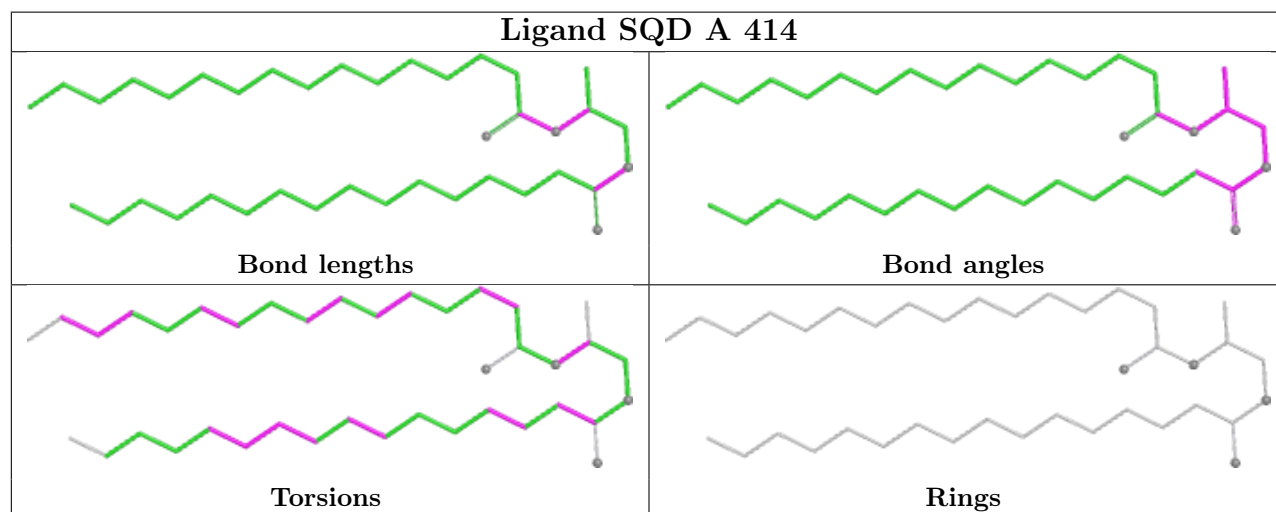
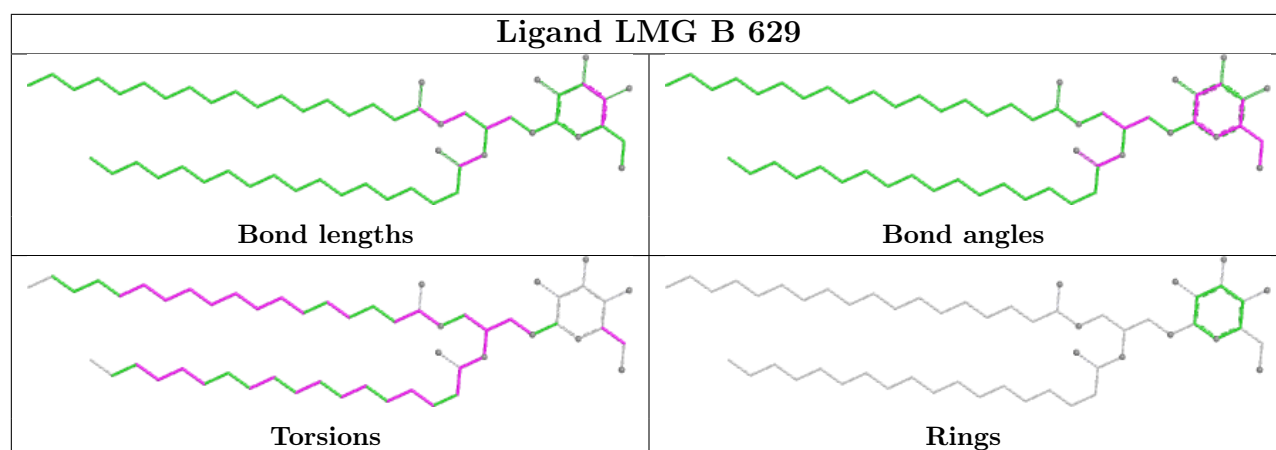


Ligand CLA A 403

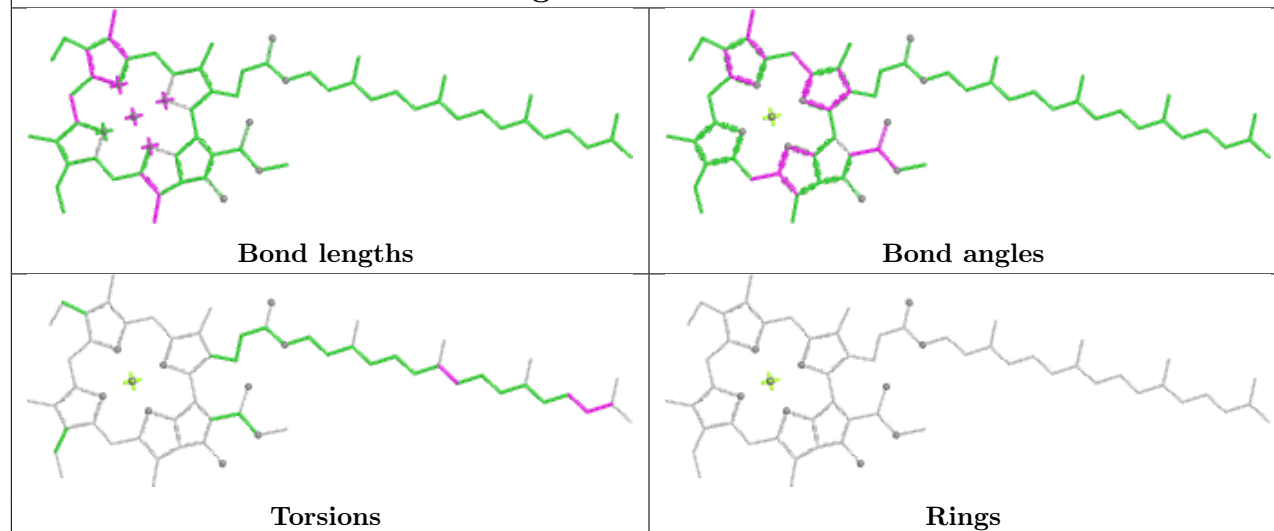


Ligand STE B 601

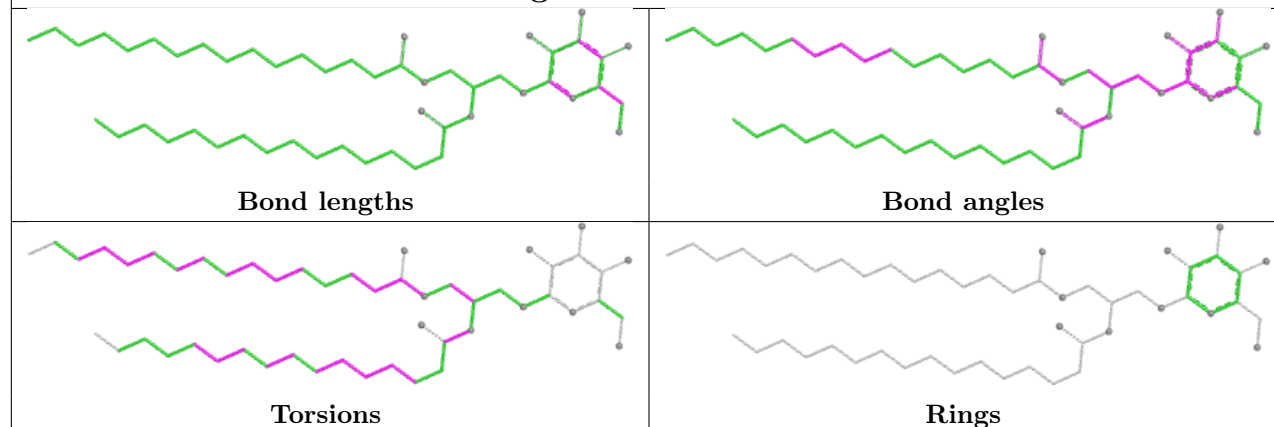




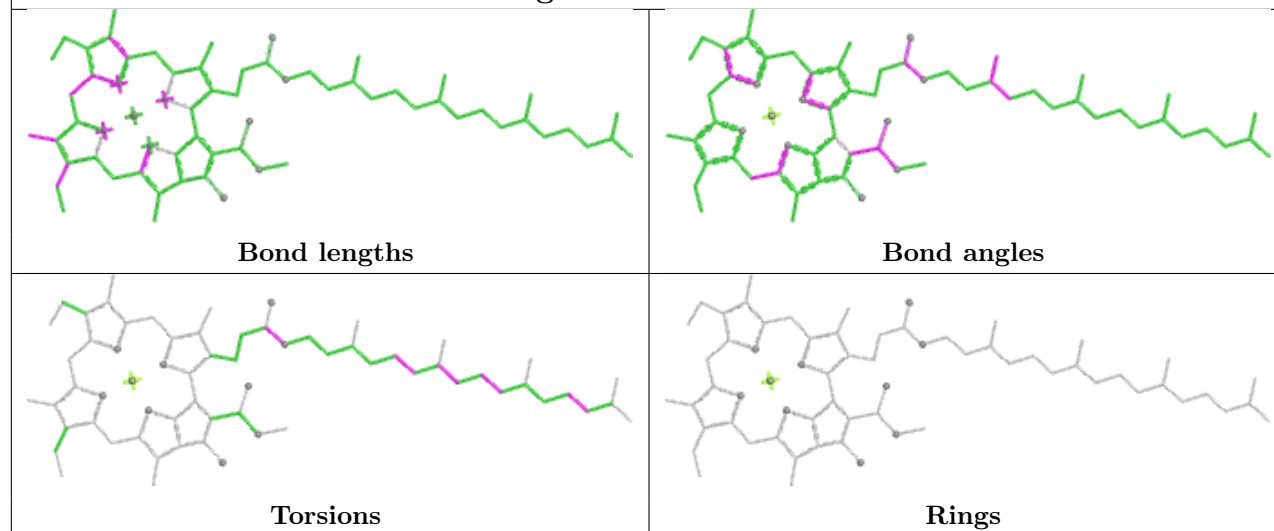
Ligand CLA C 509

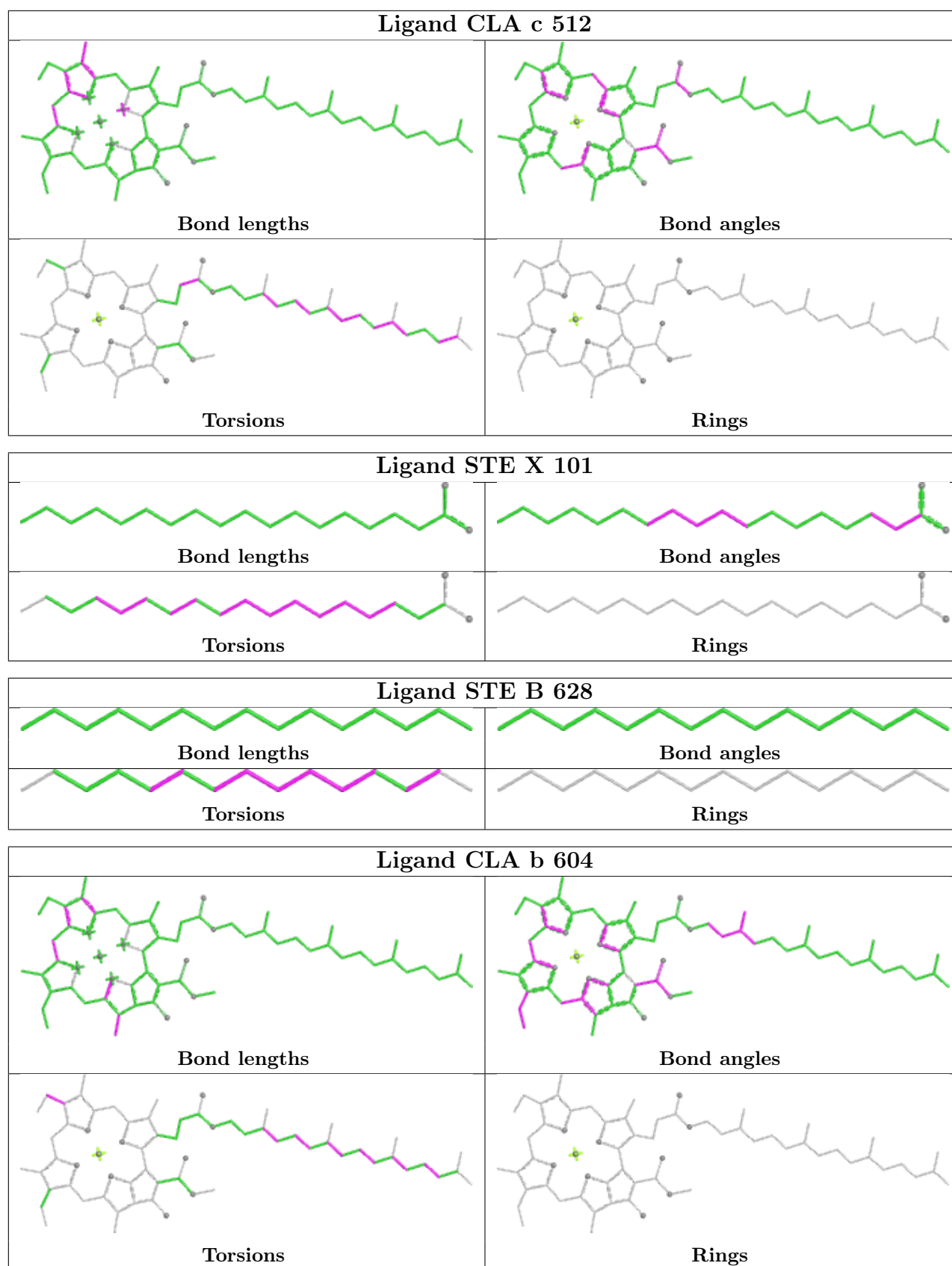


Ligand LMG b 621

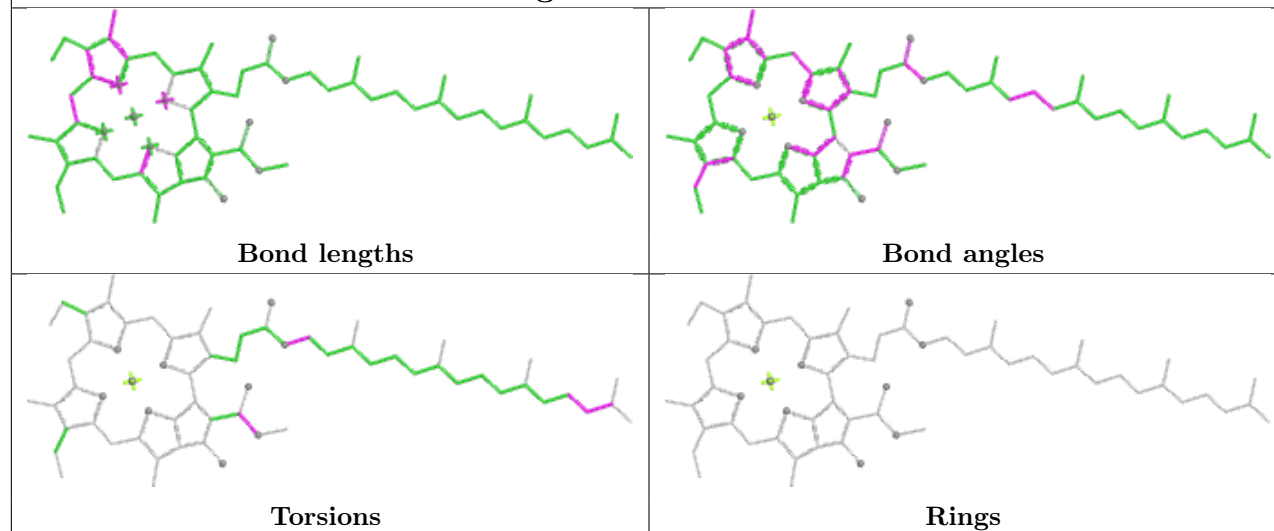


Ligand CLA a 405

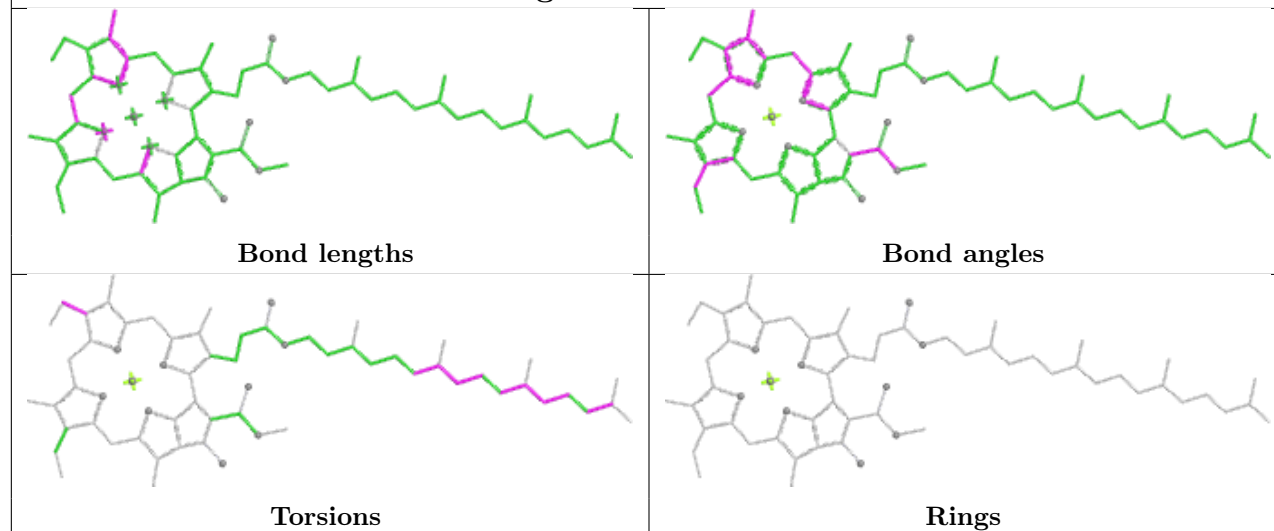




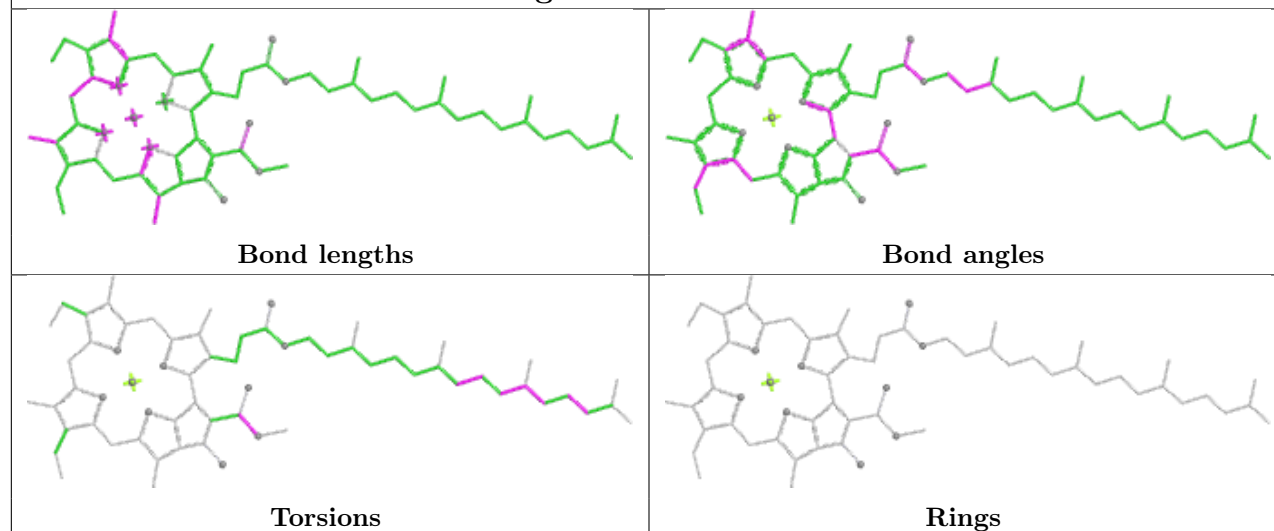
Ligand CLA a 402



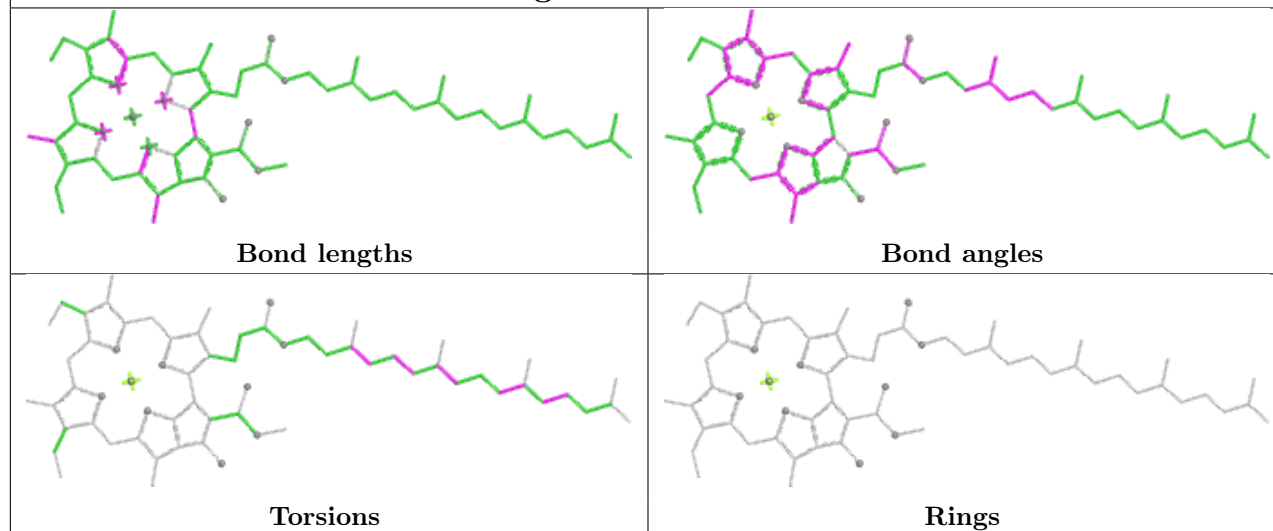
Ligand CLA a 403



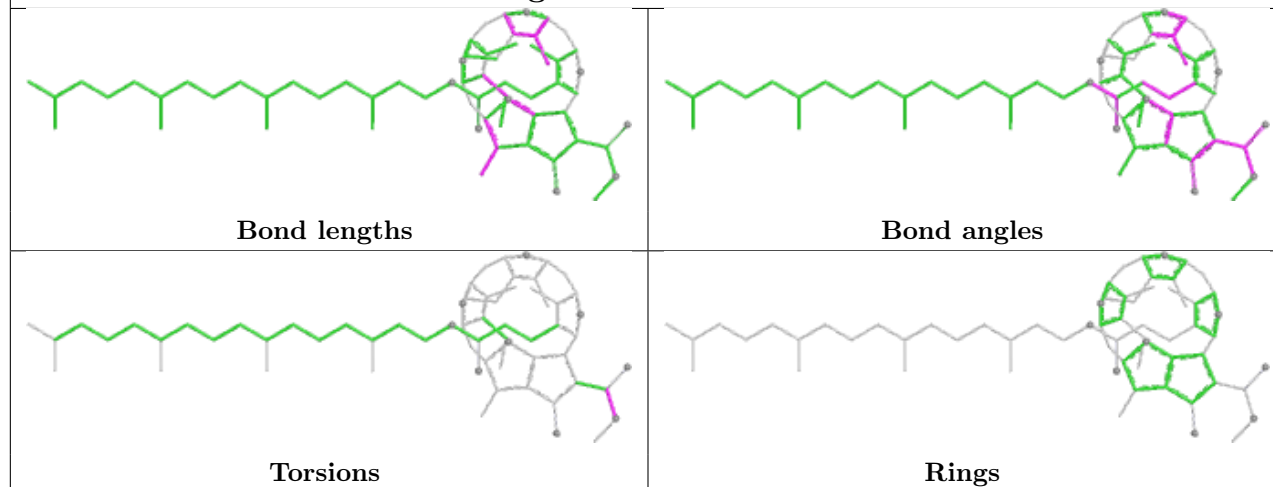
Ligand CLA d 403



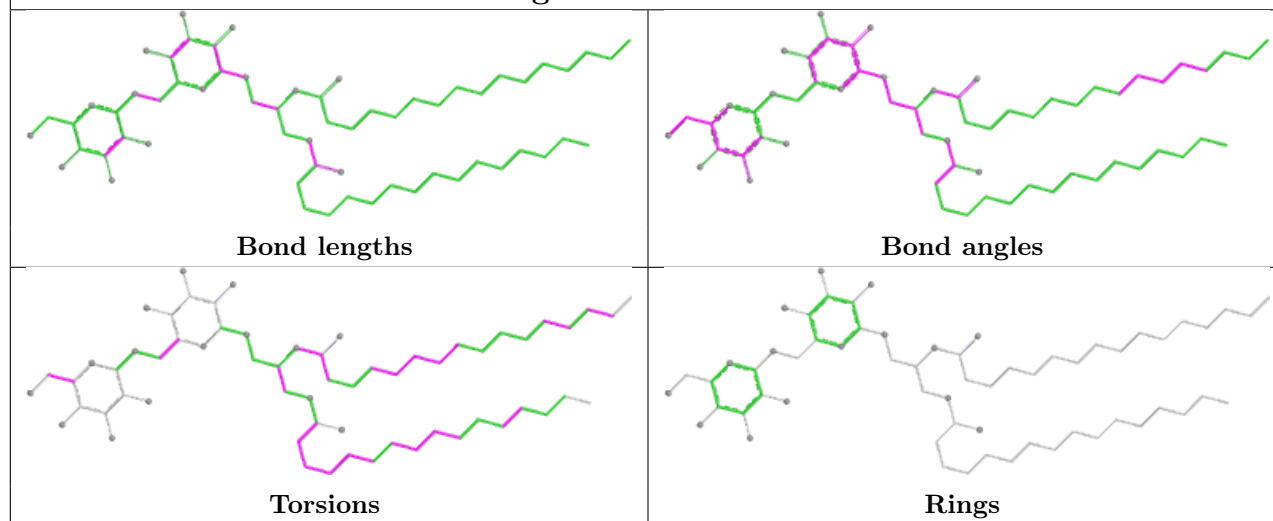
Ligand CLA b 602

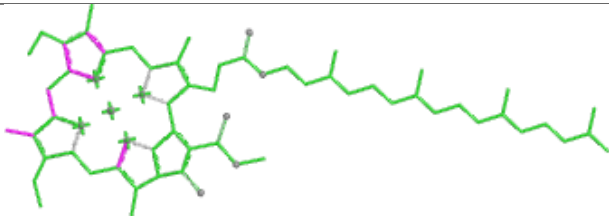
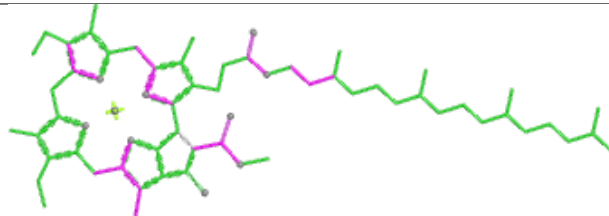
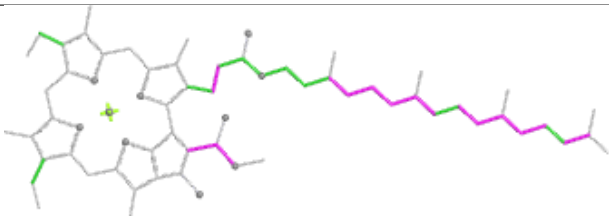
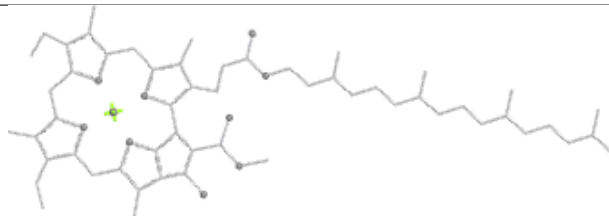


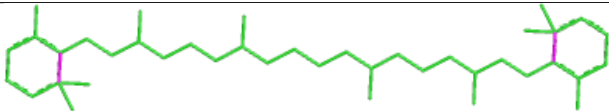
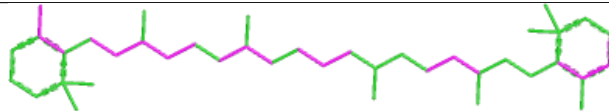
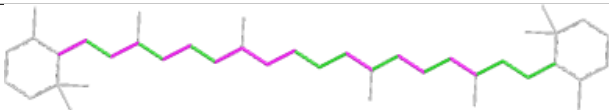
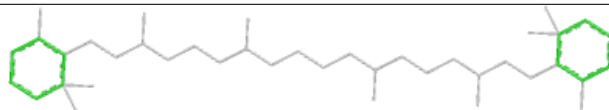
Ligand PHO D 401

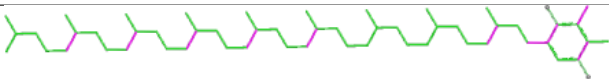
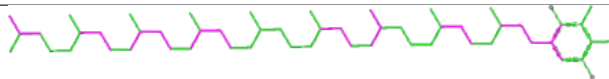
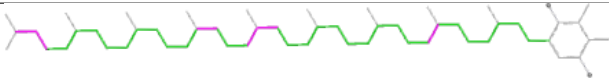


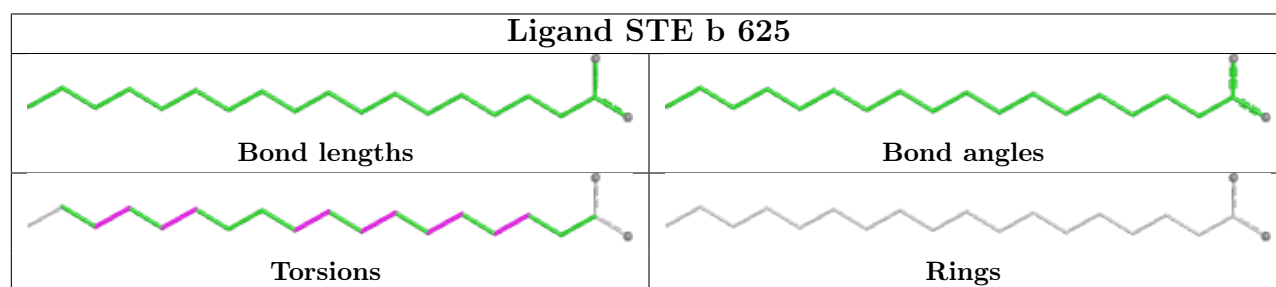
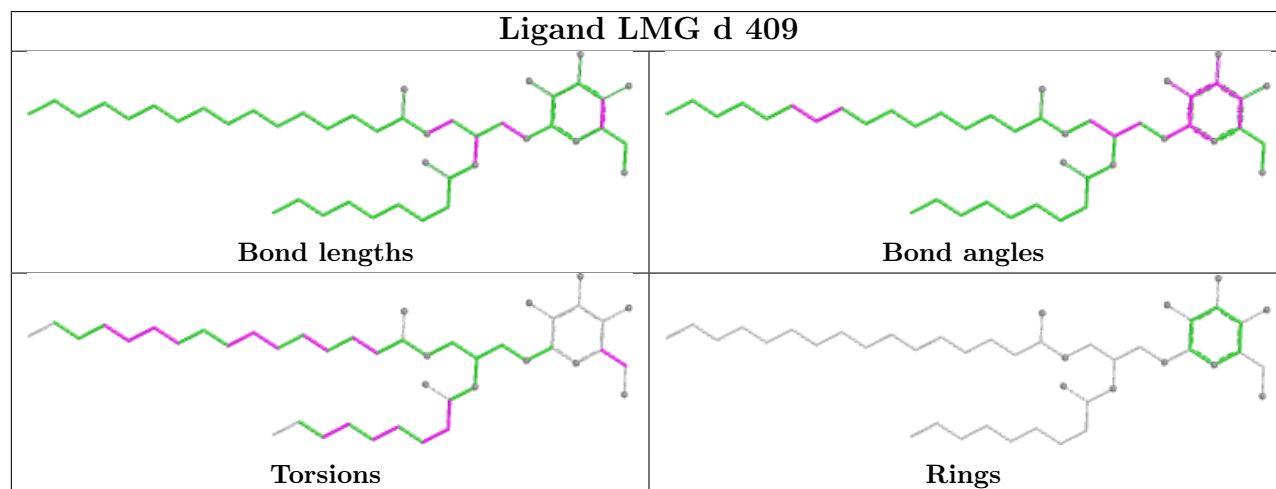
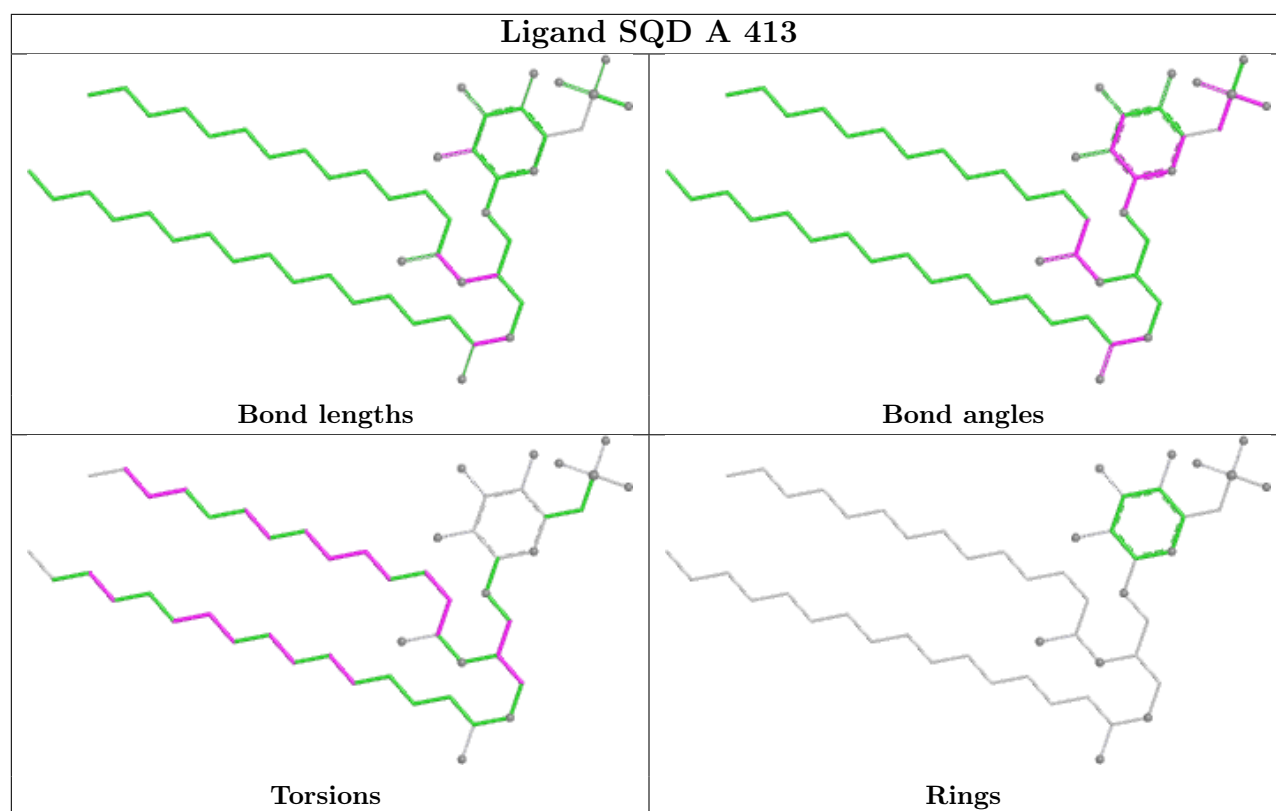
Ligand DGD c 519

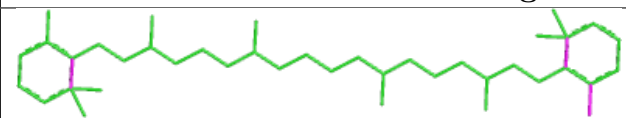
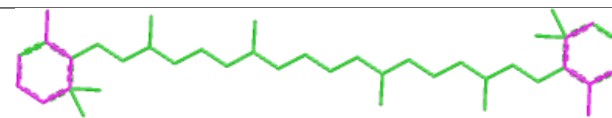
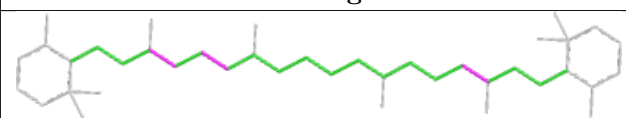
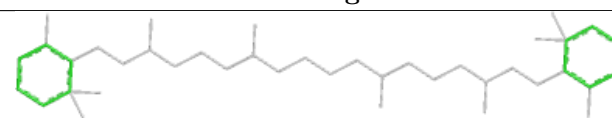


Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

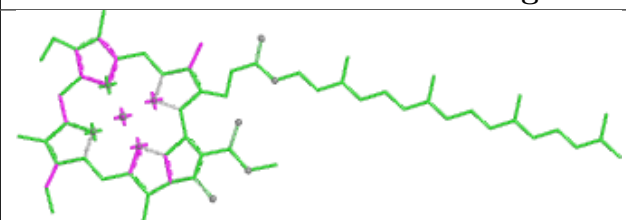
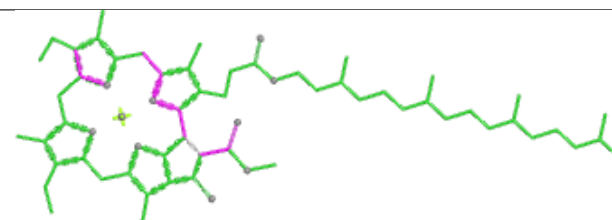
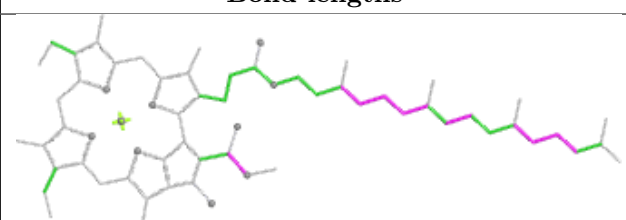
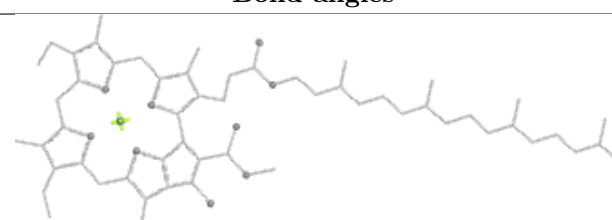
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

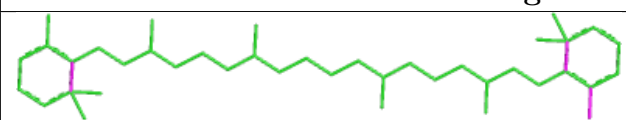
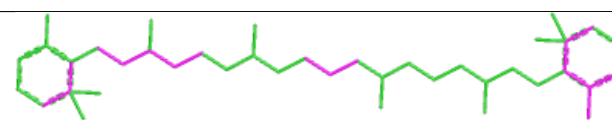
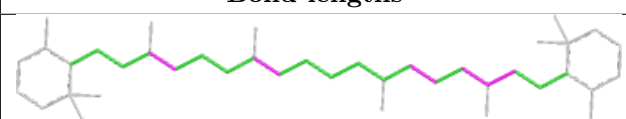
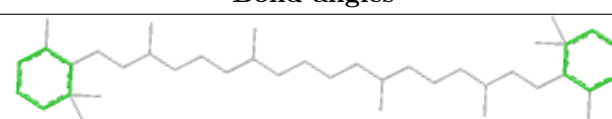
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

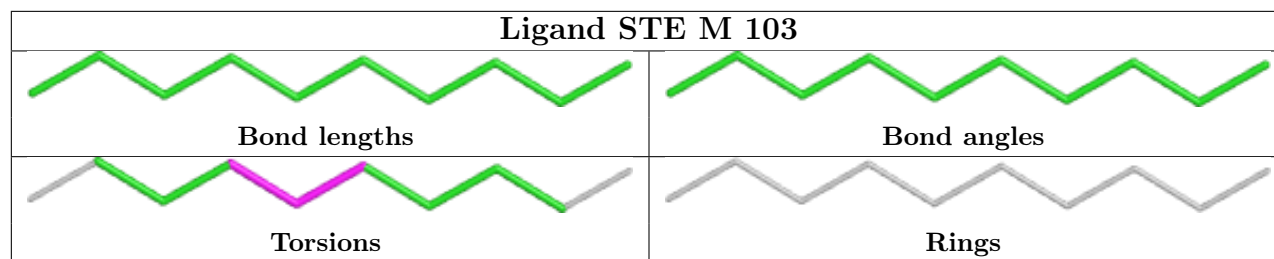


Ligand BCR B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	30:GLN	C	31:VAL	N	3.77

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.49	1 (0%) 90 91	13, 30, 48, 83	60 (17%)
1	a	334/344 (97%)	-0.39	3 (0%) 81 83	13, 32, 58, 87	60 (17%)
2	B	505/510 (99%)	-0.49	2 (0%) 88 90	19, 35, 65, 96	4 (0%)
2	b	505/510 (99%)	-0.35	2 (0%) 88 90	24, 39, 72, 105	0
3	C	442/461 (95%)	-0.42	1 (0%) 91 92	15, 38, 55, 78	7 (1%)
3	c	451/461 (97%)	-0.33	1 (0%) 91 92	15, 42, 64, 101	8 (1%)
4	D	341/352 (96%)	-0.65	0 100 100	16, 32, 48, 85	1 (0%)
4	d	341/352 (96%)	-0.46	0 100 100	17, 36, 57, 82	2 (0%)
5	E	82/84 (97%)	0.09	1 (1%) 76 78	30, 52, 69, 88	1 (1%)
5	e	82/84 (97%)	0.19	1 (1%) 76 78	40, 60, 79, 92	0
6	F	34/45 (75%)	-0.18	0 100 100	37, 43, 64, 84	0
6	f	34/45 (75%)	-0.03	0 100 100	40, 51, 77, 90	0
7	H	65/66 (98%)	-0.31	1 (1%) 72 74	31, 42, 63, 71	0
7	h	63/66 (95%)	0.01	2 (3%) 50 53	39, 50, 68, 78	0
8	I	35/38 (92%)	-0.36	0 100 100	34, 41, 73, 85	0
8	i	35/38 (92%)	-0.06	1 (2%) 53 56	32, 42, 80, 94	0
9	J	36/40 (90%)	-0.26	0 100 100	35, 51, 73, 95	0
9	j	36/40 (90%)	-0.01	0 100 100	36, 53, 91, 102	0
10	K	37/46 (80%)	-0.11	0 100 100	42, 53, 72, 74	0
10	k	37/46 (80%)	-0.01	0 100 100	44, 55, 73, 74	0
11	L	37/37 (100%)	-0.60	0 100 100	28, 33, 68, 75	0
11	l	36/37 (97%)	-0.58	0 100 100	26, 34, 80, 90	0
12	M	32/36 (88%)	-0.50	0 100 100	29, 38, 62, 73	0
12	m	31/36 (86%)	-0.50	0 100 100	28, 37, 56, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.23	3 (1%) 76 78	25, 44, 87, 140	1 (0%)
13	o	244/272 (89%)	-0.23	2 (0%) 82 84	28, 43, 83, 129	0
14	R	34/41 (82%)	0.57	1 (2%) 53 56	58, 71, 95, 110	0
14	r	31/41 (75%)	1.10	3 (9%) 13 14	67, 87, 105, 121	0
15	T	29/32 (90%)	-0.61	0 100 100	27, 33, 67, 86	0
15	t	29/32 (90%)	-0.38	1 (3%) 48 50	30, 35, 83, 94	0
16	U	97/134 (72%)	-0.28	0 100 100	32, 46, 69, 90	0
16	u	97/134 (72%)	-0.36	0 100 100	33, 43, 61, 83	0
17	V	137/163 (84%)	-0.41	0 100 100	31, 42, 59, 83	0
17	v	137/163 (84%)	-0.15	1 (0%) 84 86	33, 48, 72, 85	0
18	X	38/41 (92%)	-0.17	0 100 100	38, 51, 75, 83	0
18	x	39/41 (95%)	0.14	1 (2%) 57 60	47, 58, 88, 103	0
19	Y	27/46 (58%)	0.75	1 (3%) 45 47	54, 72, 90, 111	0
19	y	30/46 (65%)	0.49	0 100 100	63, 69, 90, 101	0
20	Z	62/62 (100%)	0.61	4 (6%) 25 26	53, 66, 112, 120	0
20	z	62/62 (100%)	0.53	2 (3%) 50 53	55, 71, 109, 124	0
All	All	5302/5700 (93%)	-0.31	35 (0%) 84 86	13, 40, 75, 140	144 (2%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	5.1
13	o	58	ASN	4.0
15	t	30	THR	3.7
20	Z	33	TRP	3.3
19	Y	25	ILE	3.3

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
12	FME	M	1	10/11	0.95	0.08	42,52,69,73	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	0.95	0.07	29,40,67,67	0
15	FME	t	1	10/11	0.95	0.07	27,43,73,73	0
8	FME	I	1	10/11	0.96	0.07	35,42,57,69	0
12	FME	m	1	10/11	0.96	0.07	32,49,65,76	0
8	FME	i	1	10/11	0.97	0.07	37,46,63,63	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
33	STE	b	626	10/20	0.74	0.17	43,58,68,71	0
33	STE	L	101	12/20	0.78	0.18	45,61,76,80	0
33	STE	H	103	18/20	0.79	0.16	49,70,84,84	0
33	STE	b	625	20/20	0.80	0.15	47,64,79,85	0
33	STE	h	103	14/20	0.80	0.17	50,65,88,91	0
33	STE	E	102	12/20	0.81	0.15	42,72,79,86	0
33	STE	d	412	20/20	0.81	0.14	39,63,81,82	0
28	LMG	B	629	55/55	0.81	0.14	35,58,81,93	0
34	LHG	E	101	49/49	0.81	0.13	46,74,98,118	0
28	LMG	b	623	55/55	0.82	0.16	49,77,101,110	0
33	STE	I	101	15/20	0.82	0.15	38,55,74,78	0
33	STE	a	414	10/20	0.83	0.14	34,65,74,75	0
28	LMG	c	524	48/55	0.83	0.14	47,71,106,116	0
33	STE	B	627	16/20	0.83	0.13	42,64,79,80	0
33	STE	B	601	12/20	0.84	0.14	44,63,83,88	0
33	STE	a	415	12/20	0.84	0.12	39,68,76,84	0
33	STE	c	501	12/20	0.84	0.11	45,66,83,85	0
34	LHG	e	102	42/49	0.84	0.14	61,78,99,119	0
33	STE	j	101	12/20	0.85	0.11	38,54,72,78	0
33	STE	B	628	15/20	0.85	0.15	39,62,75,80	0
29	SQD	a	413	36/54	0.85	0.13	31,61,87,90	0
28	LMG	D	410	33/55	0.86	0.12	33,53,78,93	0
30	DGD	A	415	66/66	0.86	0.11	41,62,85,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	STE	C	520	12/20	0.86	0.12	45,56,65,65	0
29	SQD	A	414	39/54	0.86	0.13	38,63,93,102	0
33	STE	b	622	20/20	0.86	0.12	39,58,75,78	0
33	STE	b	624	16/20	0.86	0.12	45,61,80,82	0
33	STE	B	626	18/20	0.86	0.12	39,63,82,84	0
33	STE	c	523	20/20	0.87	0.12	40,59,79,87	0
33	STE	b	620	16/20	0.87	0.13	35,50,75,81	0
28	LMG	A	412	48/55	0.88	0.10	36,54,79,101	0
28	LMG	c	525	49/55	0.88	0.11	35,54,95,112	0
33	STE	C	521	16/20	0.88	0.12	38,51,63,70	0
33	STE	B	621	17/20	0.88	0.10	35,49,69,71	0
33	STE	B	625	12/20	0.88	0.12	42,55,66,66	0
27	PL9	a	410	55/55	0.88	0.13	36,67,87,103	0
28	LMG	c	522	37/55	0.88	0.11	42,64,82,91	0
33	STE	B	624	14/20	0.89	0.10	32,49,66,66	0
22	CLA	h	101	65/65	0.89	0.10	37,64,87,99	0
27	PL9	A	410	55/55	0.89	0.12	35,65,88,95	0
33	STE	T	102	15/20	0.89	0.12	41,57,79,85	0
33	STE	l	102	18/20	0.89	0.12	33,50,77,89	0
33	STE	C	522	12/20	0.89	0.10	35,48,54,55	0
29	SQD	b	619	49/54	0.89	0.10	42,60,97,99	0
33	STE	Z	102	8/20	0.90	0.14	43,56,67,67	0
24	BCR	Z	101	40/40	0.90	0.11	38,56,69,70	0
33	STE	d	411	20/20	0.90	0.11	33,57,73,77	0
29	SQD	B	623	54/54	0.90	0.09	38,58,94,100	0
33	STE	J	101	12/20	0.90	0.10	45,60,72,73	0
28	LMG	b	621	51/55	0.90	0.10	29,51,77,92	0
33	STE	M	103	10/20	0.90	0.11	33,49,60,63	0
28	LMG	C	519	48/55	0.90	0.11	34,67,87,93	0
33	STE	X	101	20/20	0.90	0.10	27,50,73,76	0
24	BCR	c	516	40/40	0.91	0.09	43,58,71,73	0
26	BCT	a	409	4/4	0.91	0.10	26,33,40,48	0
24	BCR	Y	101	40/40	0.91	0.09	34,49,67,72	0
22	CLA	C	514	65/65	0.91	0.10	39,62,91,98	0
28	LMG	D	411	28/55	0.91	0.11	25,49,62,67	0
33	STE	M	102	15/20	0.92	0.10	34,48,62,68	0
29	SQD	f	101	41/54	0.92	0.12	47,78,110,116	0
33	STE	d	410	17/20	0.92	0.09	38,52,60,66	0
22	CLA	B	602	65/65	0.92	0.10	30,57,92,101	0
30	DGD	h	102	62/66	0.92	0.09	24,49,65,74	0
29	SQD	a	412	54/54	0.93	0.10	38,64,93,96	0
24	BCR	D	404	40/40	0.93	0.08	24,42,81,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	c	518	40/40	0.93	0.10	39,51,61,68	0
24	BCR	d	404	40/40	0.93	0.09	28,48,86,102	0
28	LMG	M	101	51/55	0.93	0.08	26,48,73,85	0
30	DGD	C	517	62/66	0.93	0.09	27,50,99,120	0
30	DGD	H	102	62/66	0.93	0.08	26,43,58,61	0
24	BCR	x	101	40/40	0.93	0.08	29,48,66,73	0
24	BCR	y	101	40/40	0.93	0.09	38,59,75,79	0
24	BCR	H	101	40/40	0.93	0.09	22,44,58,70	0
22	CLA	c	514	65/65	0.93	0.09	36,55,95,110	0
22	CLA	c	513	65/65	0.93	0.09	38,53,68,75	0
24	BCR	b	617	40/40	0.93	0.07	25,40,55,61	0
24	BCR	b	618	40/40	0.93	0.08	26,44,66,67	0
29	SQD	D	407	36/54	0.93	0.10	43,66,86,99	0
24	BCR	c	517	40/40	0.94	0.08	25,43,60,62	0
22	CLA	C	513	65/65	0.94	0.09	33,54,85,98	0
24	BCR	K	101	40/40	0.94	0.09	30,48,58,62	0
28	LMG	d	409	44/55	0.94	0.09	28,50,79,91	0
29	SQD	A	413	52/54	0.94	0.09	28,56,88,98	0
30	DGD	c	520	62/66	0.94	0.08	32,50,88,94	0
23	PHO	d	401	64/64	0.94	0.07	26,37,46,48	0
24	BCR	B	619	40/40	0.94	0.07	23,38,49,57	0
24	BCR	B	620	40/40	0.94	0.07	26,41,58,69	0
24	BCR	C	515	40/40	0.94	0.08	25,41,53,65	0
34	LHG	d	406	49/49	0.94	0.10	32,48,82,87	0
22	CLA	c	515	65/65	0.94	0.10	39,66,105,110	0
22	CLA	c	508	65/65	0.95	0.09	27,46,95,106	0
27	PL9	d	405	55/55	0.95	0.06	19,34,45,46	0
22	CLA	c	510	64/65	0.95	0.08	30,45,86,105	0
30	DGD	C	516	62/66	0.95	0.08	21,39,75,91	0
22	CLA	c	511	65/65	0.95	0.07	30,45,62,67	0
30	DGD	C	518	62/66	0.95	0.08	26,46,75,85	0
24	BCR	T	101	40/40	0.95	0.06	21,38,55,67	0
28	LMG	D	406	51/55	0.95	0.10	28,54,88,96	0
30	DGD	c	521	62/66	0.95	0.09	28,52,93,108	0
22	CLA	c	512	65/65	0.95	0.07	30,46,62,71	0
22	CLA	C	506	65/65	0.95	0.09	23,40,69,82	0
24	BCR	b	616	40/40	0.95	0.07	21,41,52,59	0
22	CLA	C	511	65/65	0.95	0.07	26,43,58,66	0
22	CLA	C	512	65/65	0.95	0.08	27,48,66,70	0
22	CLA	d	403	65/65	0.95	0.09	26,46,89,103	0
22	CLA	B	607	65/65	0.95	0.08	21,35,74,78	0
22	CLA	C	504	65/65	0.95	0.07	24,40,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	A	406	40/40	0.95	0.07	22,34,47,51	0
24	BCR	t	101	40/40	0.95	0.06	23,38,51,53	0
24	BCR	B	618	40/40	0.95	0.07	27,39,57,69	0
22	CLA	b	605	65/65	0.95	0.08	25,39,73,80	0
22	CLA	b	608	65/65	0.95	0.08	29,43,57,64	0
22	CLA	c	504	65/65	0.95	0.07	27,42,62,69	0
34	LHG	d	408	39/49	0.95	0.08	28,45,68,75	0
27	PL9	D	405	55/55	0.95	0.06	20,33,48,49	0
34	LHG	l	101	49/49	0.95	0.08	31,43,60,69	0
26	BCT	A	409	4/4	0.96	0.09	31,33,36,43	0
22	CLA	c	507	65/65	0.96	0.07	25,39,67,76	0
22	CLA	C	503	65/65	0.96	0.07	24,39,61,66	0
22	CLA	c	509	65/65	0.96	0.07	27,43,57,64	0
22	CLA	B	605	65/65	0.96	0.07	19,34,72,81	0
22	CLA	C	505	59/65	0.96	0.08	27,40,78,90	0
22	CLA	A	402	65/65	0.96	0.06	15,27,42,61	0
22	CLA	C	507	65/65	0.96	0.09	22,40,87,99	0
22	CLA	C	508	65/65	0.96	0.07	21,38,53,59	0
22	CLA	C	509	65/65	0.96	0.07	25,43,98,114	0
22	CLA	d	402	65/65	0.96	0.06	18,35,52,67	0
22	CLA	C	510	65/65	0.96	0.08	24,43,64,68	0
22	CLA	B	610	65/65	0.96	0.07	23,37,58,69	0
23	PHO	D	401	64/64	0.96	0.05	23,34,44,48	0
22	CLA	B	611	65/65	0.96	0.07	19,33,46,47	0
22	CLA	B	613	65/65	0.96	0.07	17,33,49,53	0
22	CLA	B	615	65/65	0.96	0.08	22,35,80,90	0
22	CLA	a	403	65/65	0.96	0.09	24,41,95,107	0
22	CLA	a	405	65/65	0.96	0.07	18,38,79,87	0
22	CLA	a	411	65/65	0.96	0.06	19,29,45,50	0
22	CLA	b	601	65/65	0.96	0.07	25,42,62,70	0
22	CLA	b	602	65/65	0.96	0.07	22,36,67,77	0
22	CLA	b	604	65/65	0.96	0.06	18,35,50,58	0
22	CLA	B	616	65/65	0.96	0.07	22,36,61,64	0
22	CLA	b	607	65/65	0.96	0.06	23,39,59,62	0
22	CLA	B	617	60/65	0.96	0.08	21,38,87,94	0
24	BCR	a	406	40/40	0.96	0.06	19,33,47,52	0
22	CLA	b	609	65/65	0.96	0.07	23,39,51,57	0
22	CLA	b	610	65/65	0.96	0.06	21,34,53,59	0
22	CLA	b	611	65/65	0.96	0.07	21,35,52,56	0
22	CLA	b	613	65/65	0.96	0.07	22,40,81,91	0
22	CLA	b	614	65/65	0.96	0.07	23,39,56,60	0
30	DGD	c	519	62/66	0.96	0.08	22,41,74,96	0

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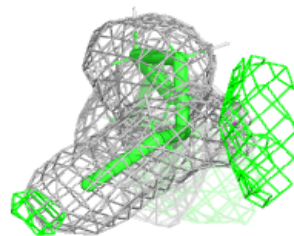
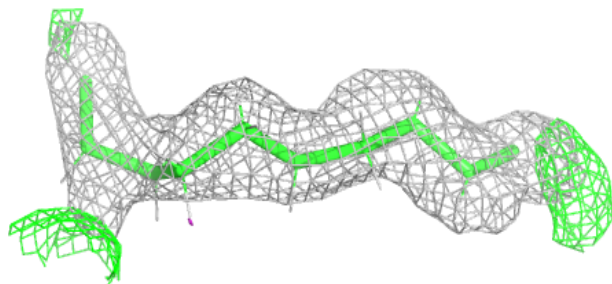
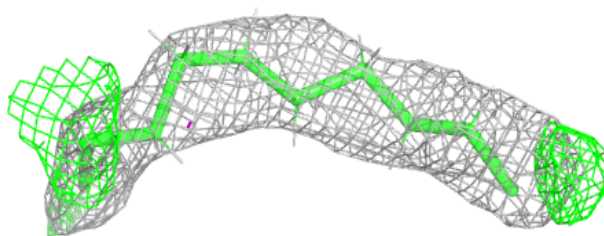
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LHG	D	408	49/49	0.96	0.07	18,41,53,59	0
34	LHG	D	409	47/49	0.96	0.09	27,48,87,104	0
34	LHG	D	412	49/49	0.96	0.08	27,43,71,77	0
22	CLA	b	615	60/65	0.96	0.08	26,42,84,93	0
22	CLA	c	503	65/65	0.96	0.06	22,40,53,61	0
22	CLA	C	502	65/65	0.96	0.07	20,34,53,55	0
22	CLA	c	505	65/65	0.96	0.07	30,43,53,59	0
22	CLA	c	506	60/65	0.96	0.07	29,42,79,84	0
22	CLA	a	402	65/65	0.97	0.05	18,29,47,59	0
22	CLA	B	603	65/65	0.97	0.06	22,37,54,60	0
22	CLA	B	612	65/65	0.97	0.06	21,32,51,52	0
23	PHO	A	404	64/64	0.97	0.05	18,28,37,39	0
22	CLA	B	604	65/65	0.97	0.06	17,34,61,63	0
23	PHO	a	404	64/64	0.97	0.05	17,31,42,45	0
22	CLA	B	614	65/65	0.97	0.07	18,31,67,71	0
22	CLA	A	405	54/65	0.97	0.06	18,33,61,69	0
22	CLA	b	603	65/65	0.97	0.07	17,37,85,98	0
22	CLA	B	606	65/65	0.97	0.07	21,33,47,52	0
34	LHG	B	622	49/49	0.97	0.06	25,41,56,64	0
22	CLA	A	411	65/65	0.97	0.06	16,27,54,64	0
22	CLA	b	606	65/65	0.97	0.07	19,36,71,78	0
22	CLA	B	608	65/65	0.97	0.07	17,34,65,74	0
22	CLA	B	609	65/65	0.97	0.06	21,36,57,63	0
22	CLA	A	403	65/65	0.97	0.07	22,36,90,100	0
34	LHG	d	407	49/49	0.97	0.07	25,42,55,61	0
22	CLA	D	402	65/65	0.97	0.06	13,30,52,59	0
22	CLA	D	403	65/65	0.97	0.07	21,42,102,116	0
22	CLA	b	612	65/65	0.97	0.06	19,33,72,90	0
35	HEC	F	101	43/43	0.97	0.08	26,44,64,66	0
35	HEC	e	101	43/43	0.97	0.08	36,52,72,81	0
35	HEC	V	201	43/43	0.98	0.06	21,31,44,53	0
35	HEC	v	201	43/43	0.98	0.07	25,37,45,48	0
25	CL	A	407	1/1	0.99	0.02	27,27,27,27	0
25	CL	a	407	1/1	0.99	0.04	28,28,28,28	0
25	CL	a	408	1/1	0.99	0.08	28,28,28,28	0
31	OEX	A	416[A]	10/10	0.99	0.03	25,30,31,31	10
31	OEX	a	416[A]	10/10	0.99	0.03	27,28,30,30	10
32	OEY	A	417[B]	11/11	0.99	0.03	21,27,31,34	11
32	OEY	a	417[B]	11/11	0.99	0.03	22,26,28,31	11
21	FE2	A	401	1/1	1.00	0.01	26,26,26,26	0
25	CL	A	408	1/1	1.00	0.04	28,28,28,28	0
21	FE2	a	401	1/1	1.00	0.01	34,34,34,34	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.

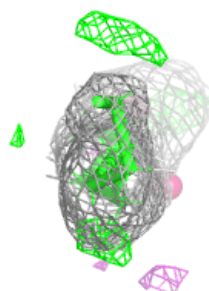
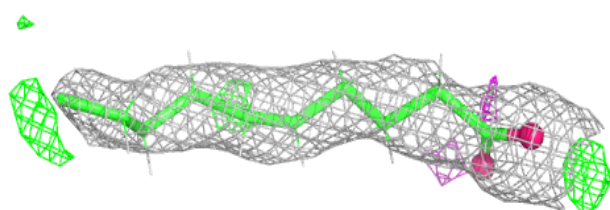
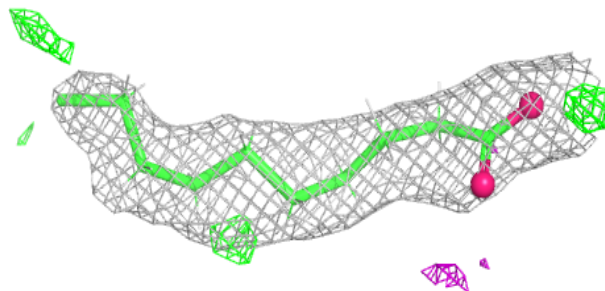
Electron density around STE b 626:

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

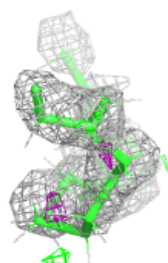
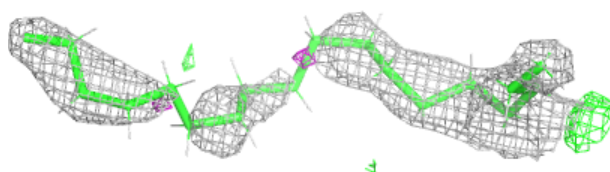
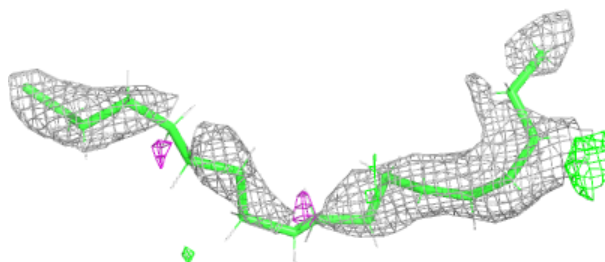


Electron density around STE L 101:

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

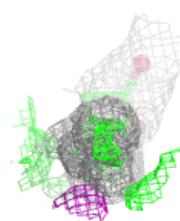
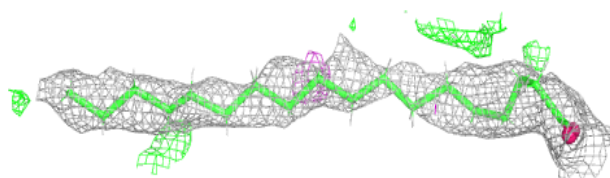
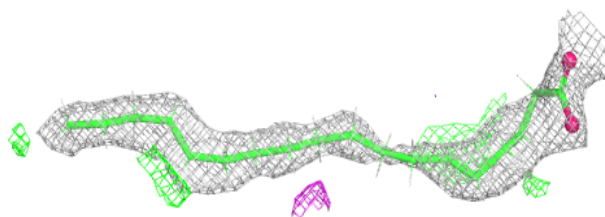
**Electron density around STE H 103:**

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

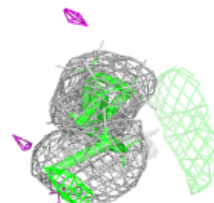
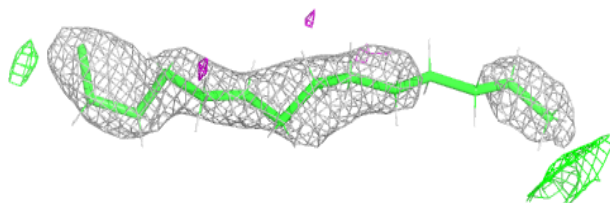
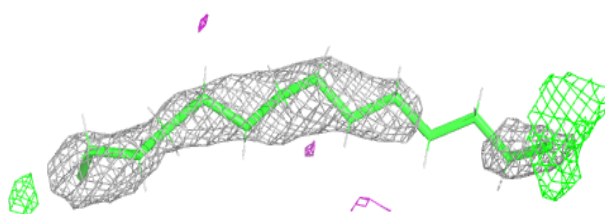


Electron density around STE b 625:

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

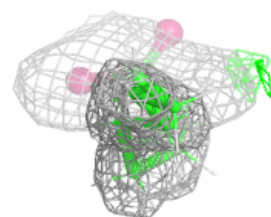
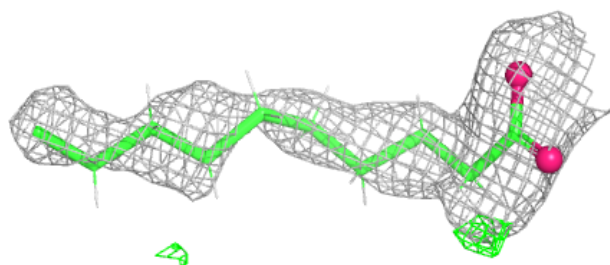
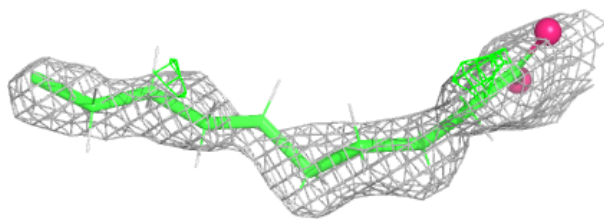
**Electron density around STE h 103:**

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

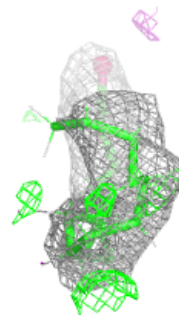
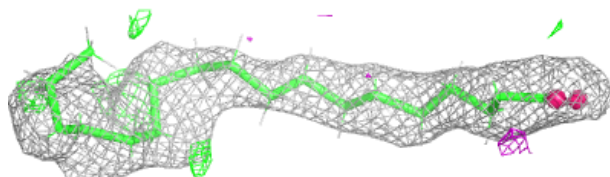
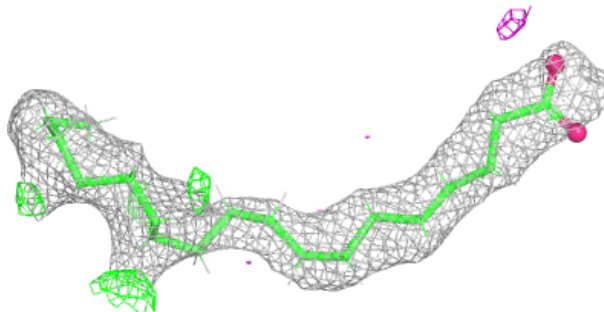


Electron density around STE E 102:

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

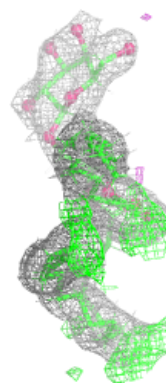
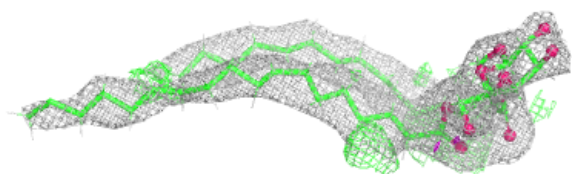
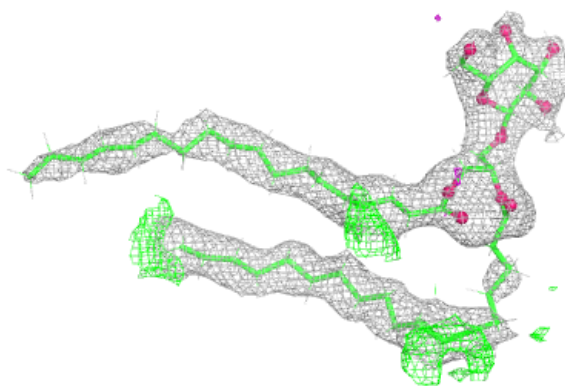
**Electron density around STE d 412:**

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



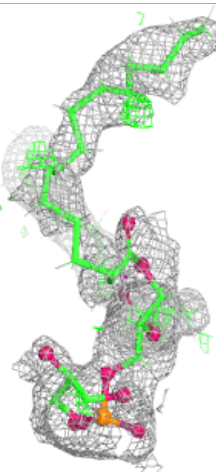
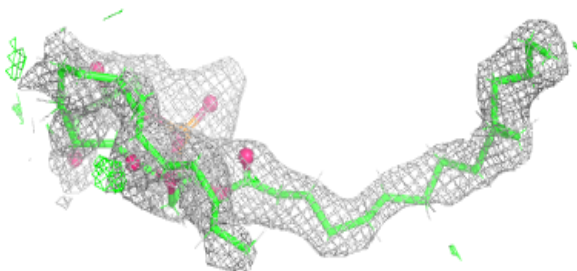
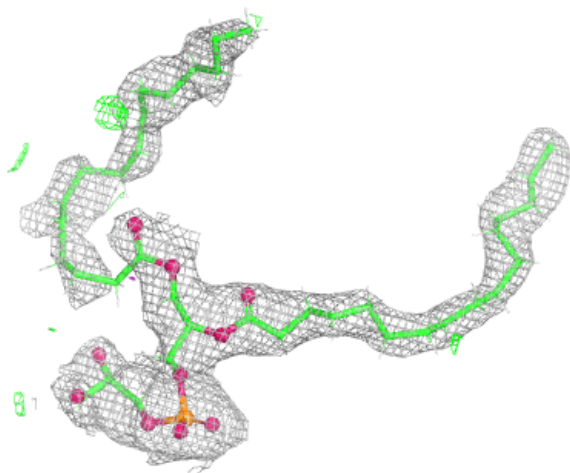
Electron density around LMG B 629:

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



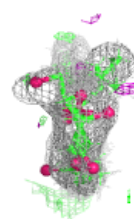
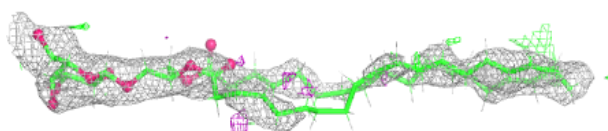
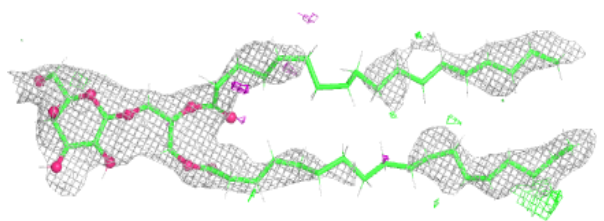
Electron density around LHG E 101:

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

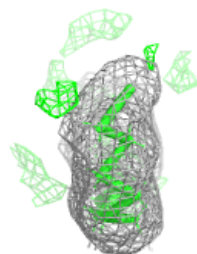
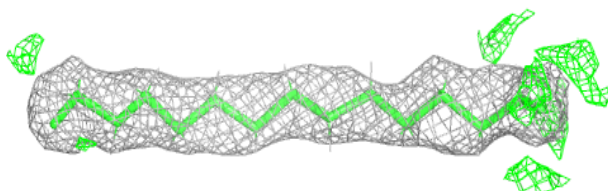
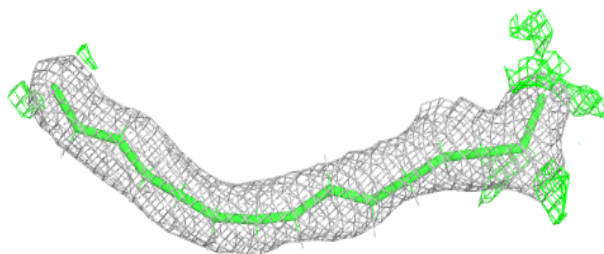


Electron density around LMG b 623:

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

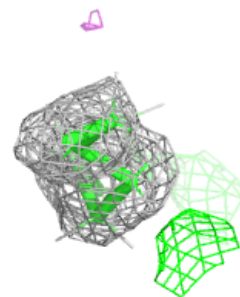
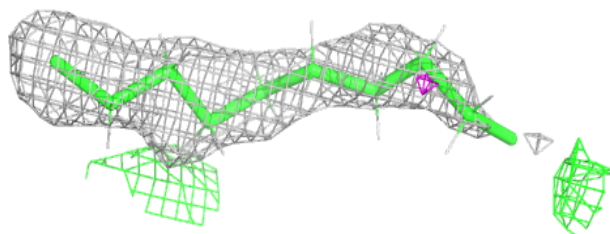
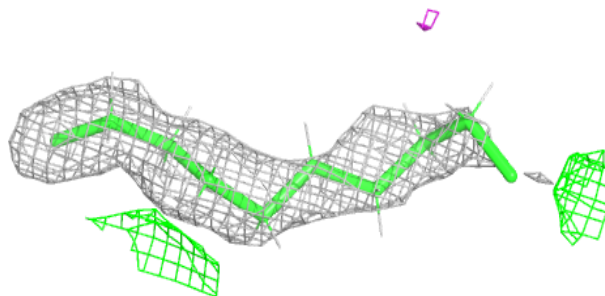
**Electron density around STE I 101:**

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

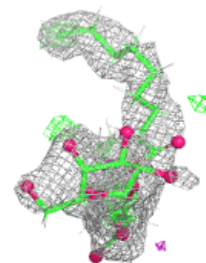
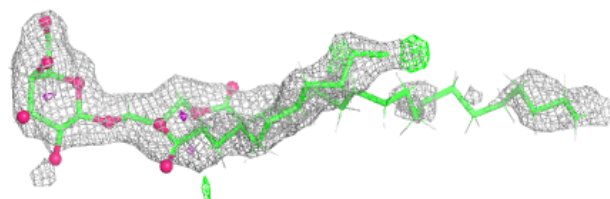
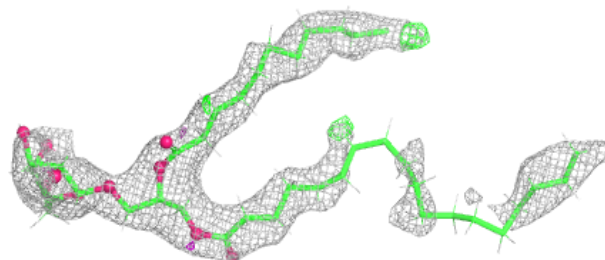


Electron density around STE a 414:

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

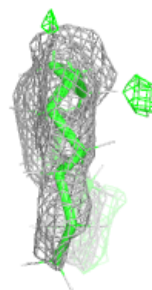
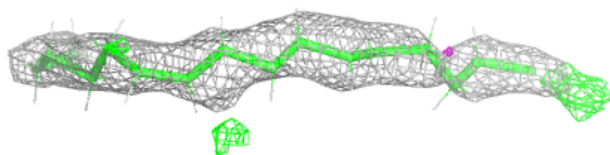
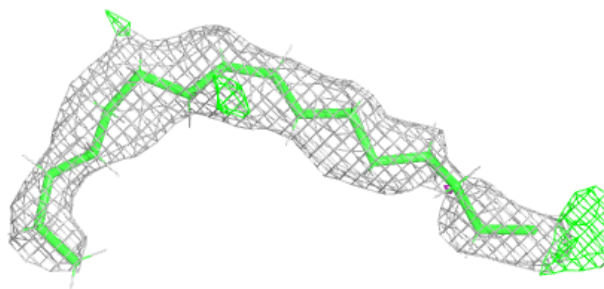
**Electron density around LMG c 524:**

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

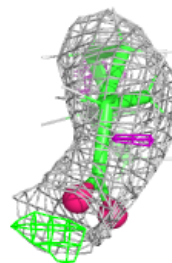
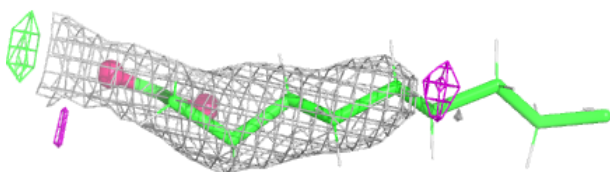
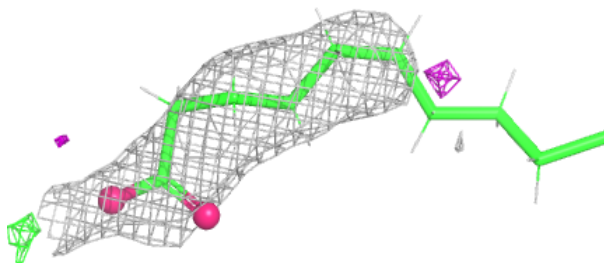


Electron density around STE B 627:

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

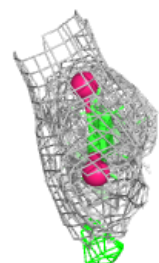
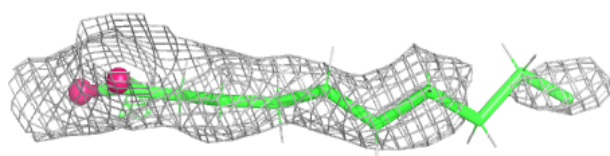
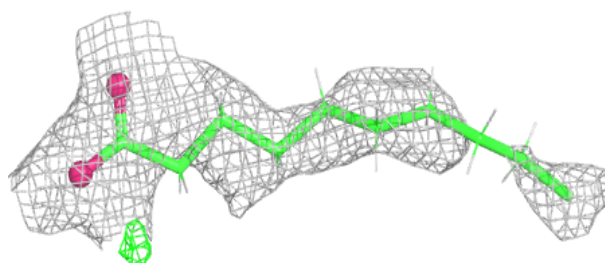
**Electron density around STE B 601:**

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

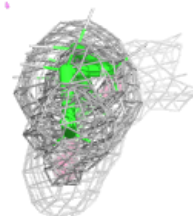
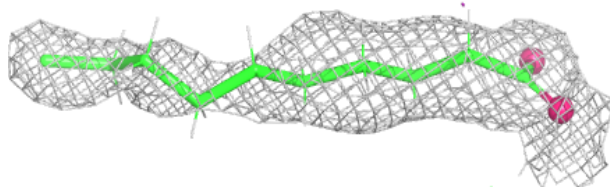
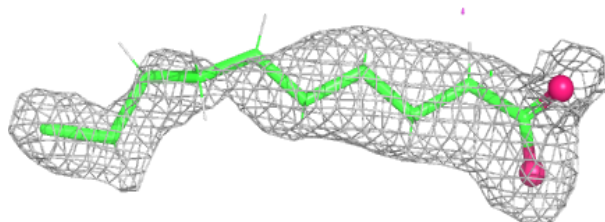


Electron density around STE a 415:

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

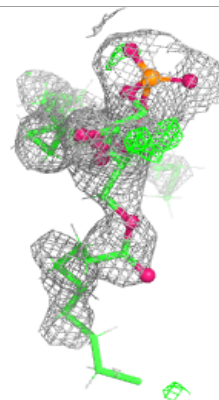
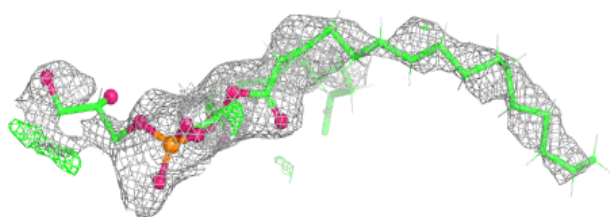
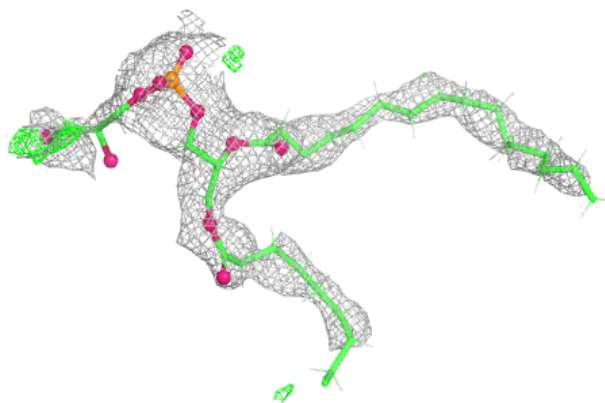
**Electron density around STE c 501:**

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

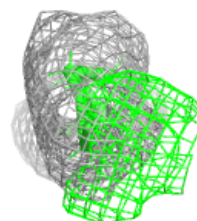
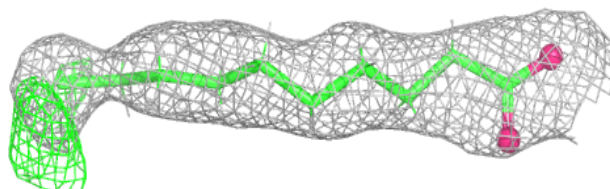
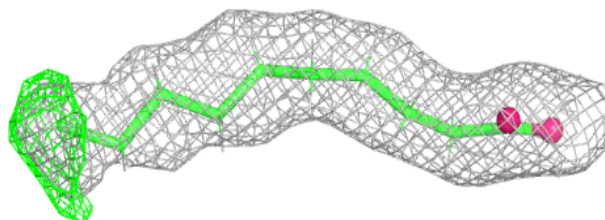


Electron density around LHG e 102:

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

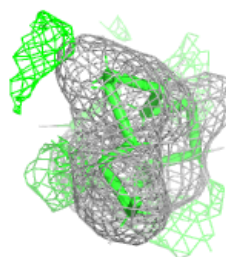
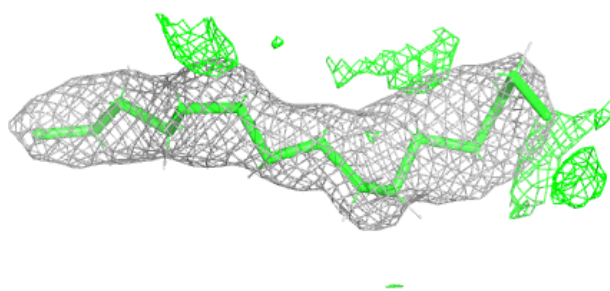
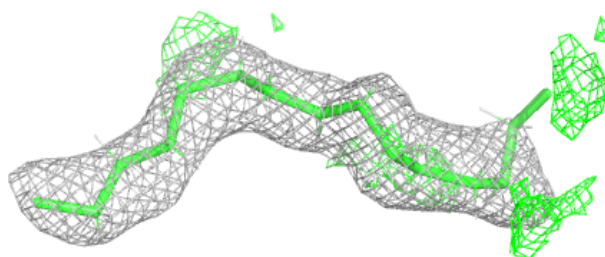
**Electron density around STE j 101:**

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



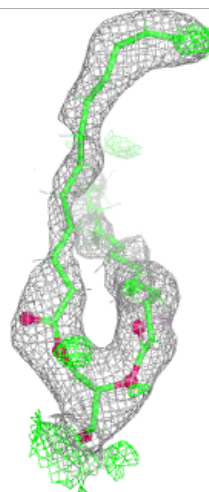
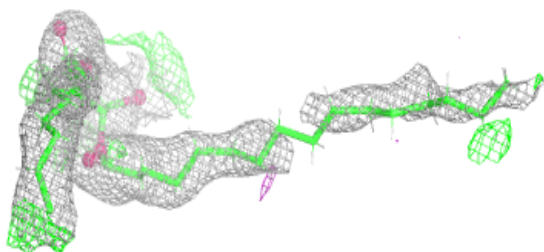
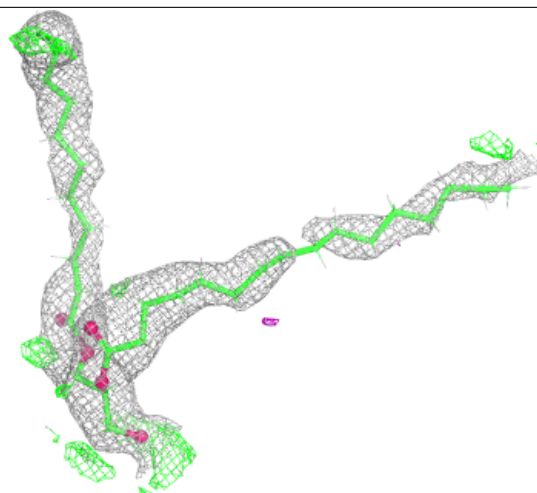
Electron density around STE B 628:

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



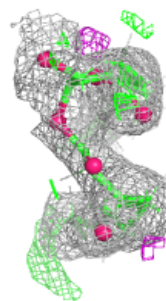
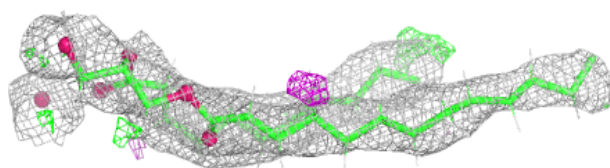
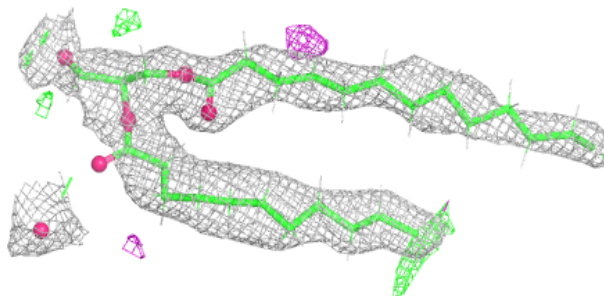
Electron density around SQD a 413:

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

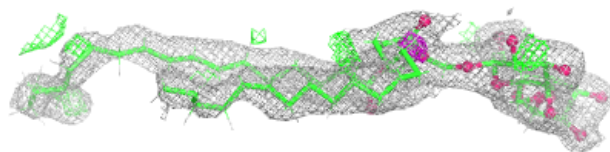
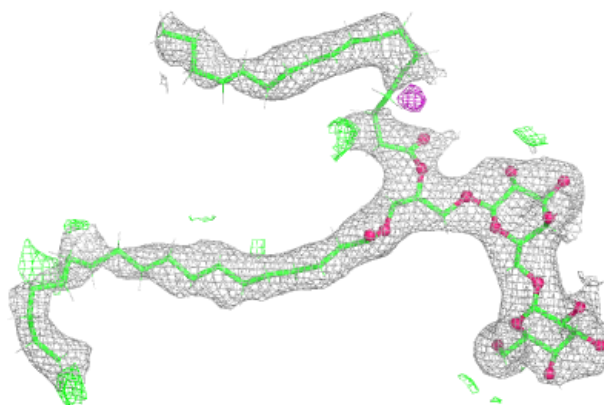


Electron density around LMG D 410:

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

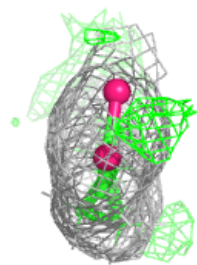
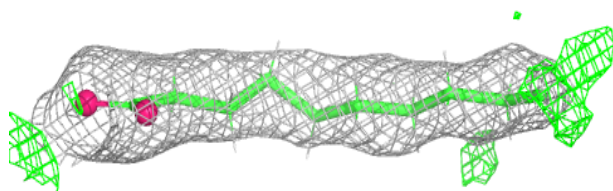
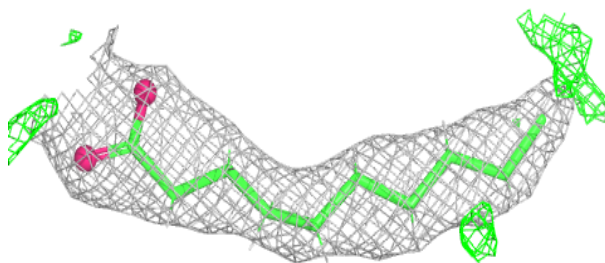
**Electron density around DGD A 415:**

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



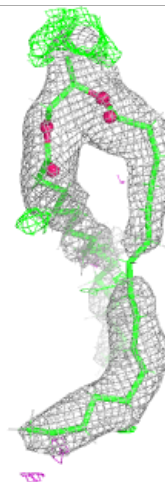
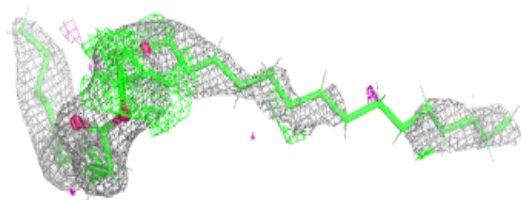
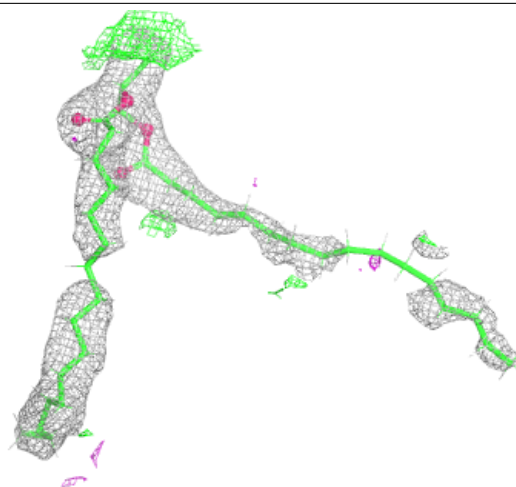
Electron density around STE C 520:

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



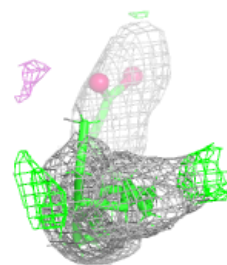
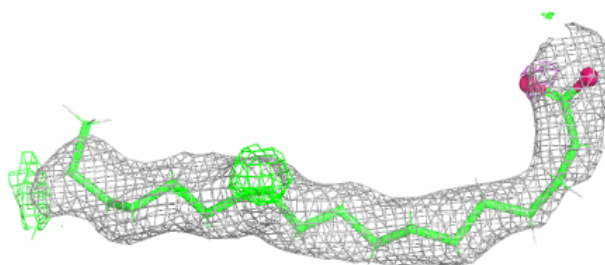
Electron density around SQD A 414:

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

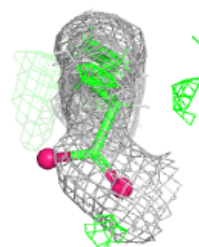
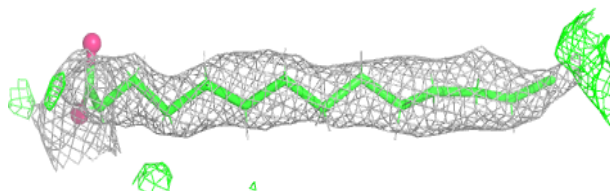
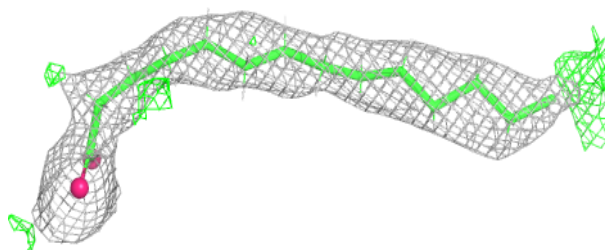


Electron density around STE b 622:

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

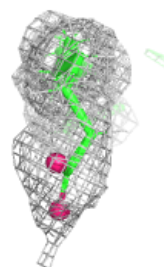
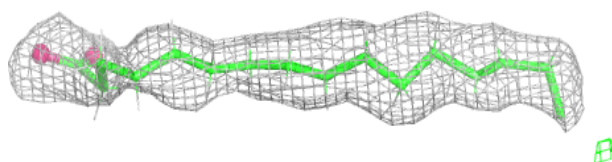
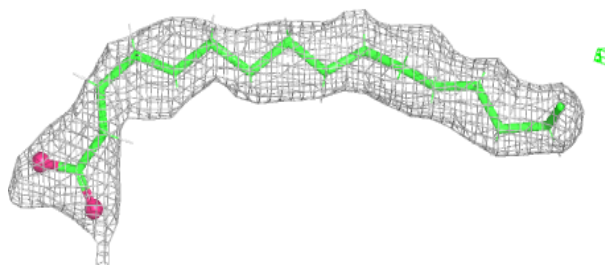
**Electron density around STE b 624:**

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

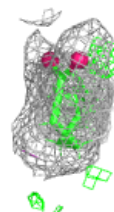
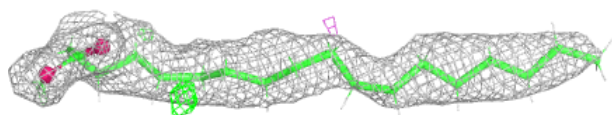
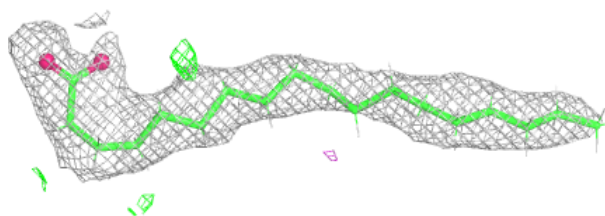


Electron density around STE B 626:

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

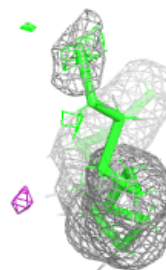
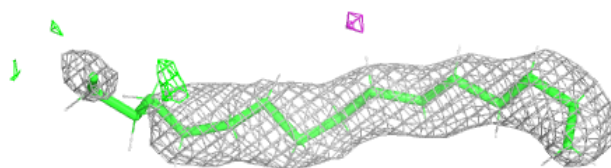
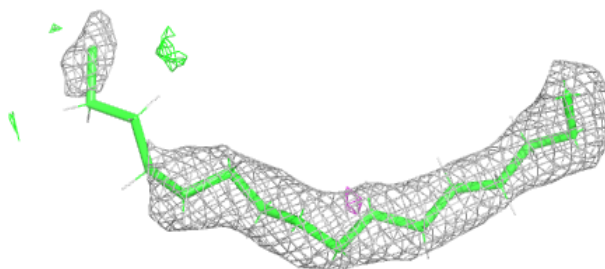
**Electron density around STE c 523:**

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

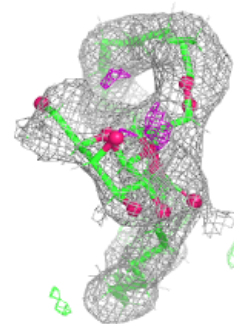
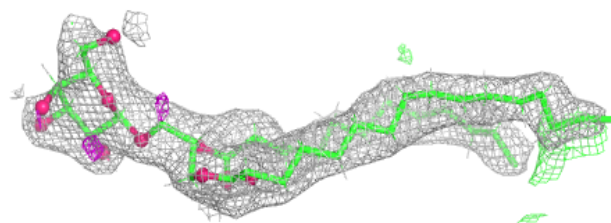
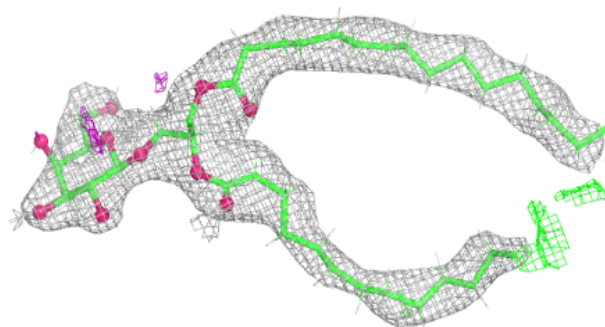


Electron density around STE b 620:

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

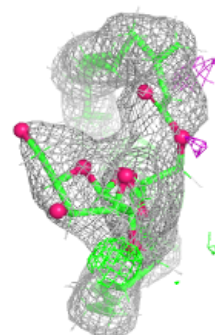
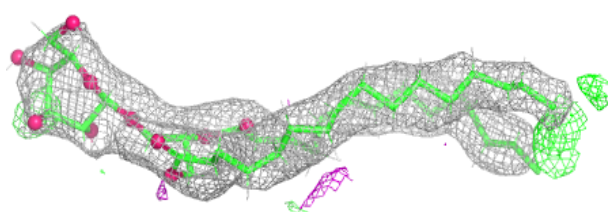
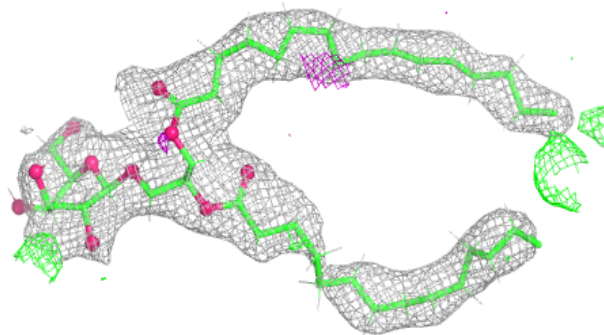
**Electron density around LMG A 412:**

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

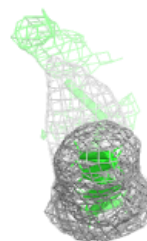
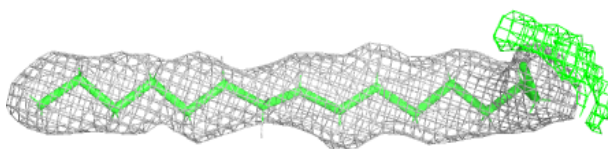
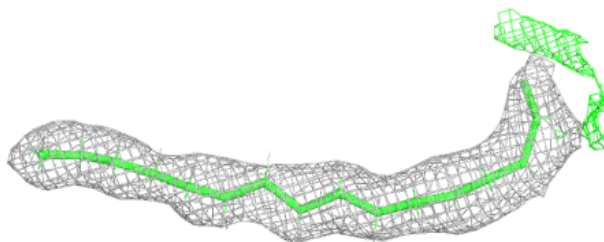


Electron density around LMG c 525:

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

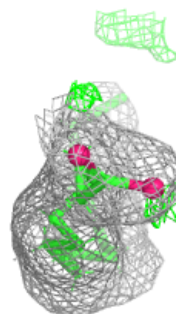
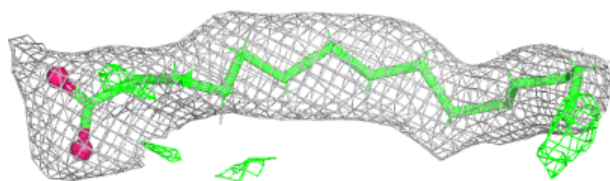
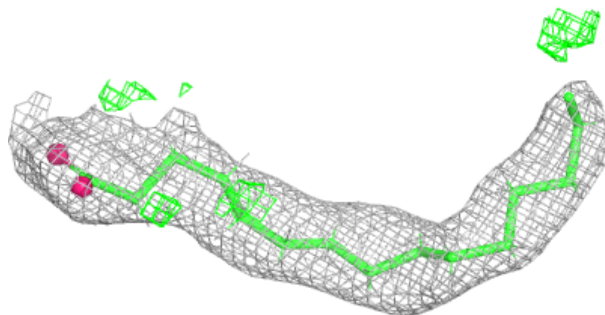
**Electron density around STE C 521:**

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

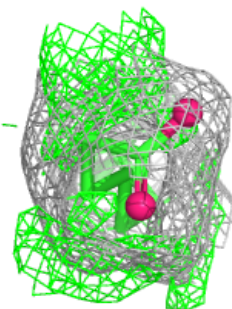
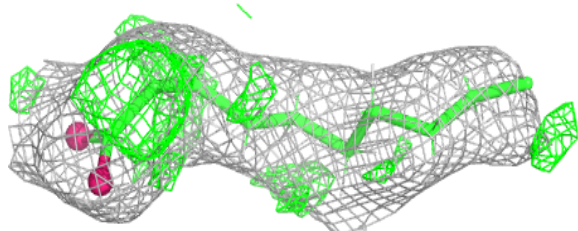
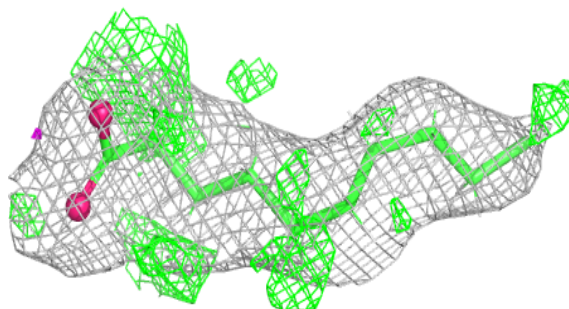


Electron density around STE B 621:

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

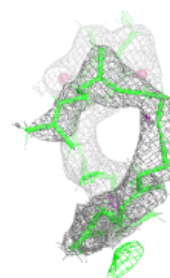
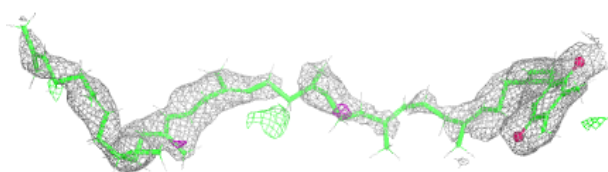
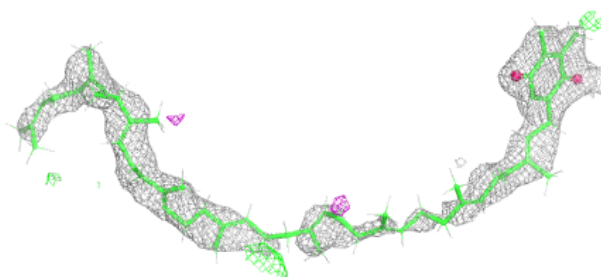
**Electron density around STE B 625:**

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

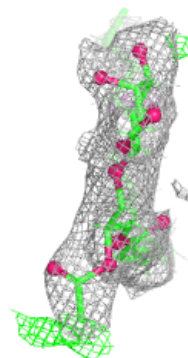
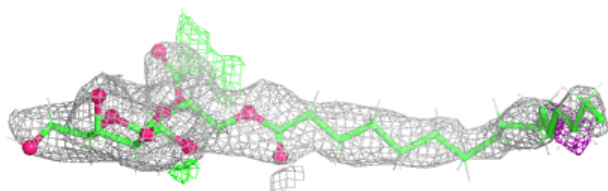
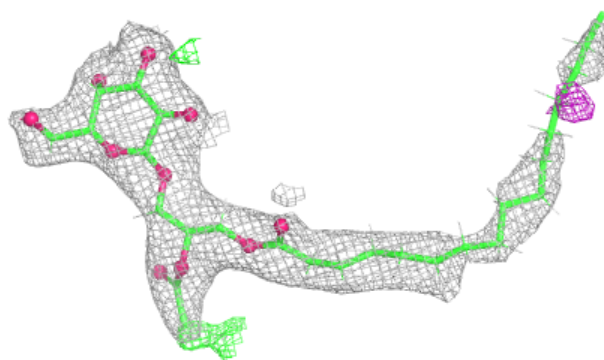


Electron density around PL9 a 410:

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

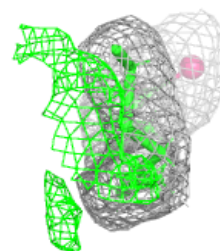
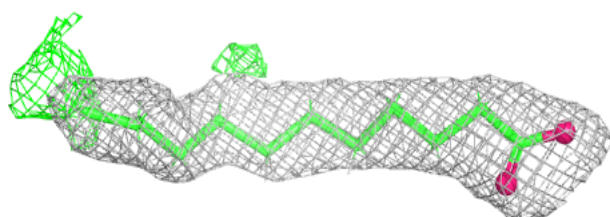
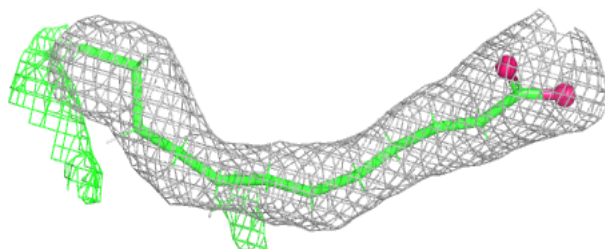
**Electron density around LMG c 522:**

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

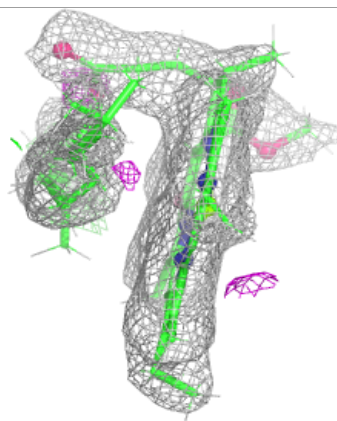
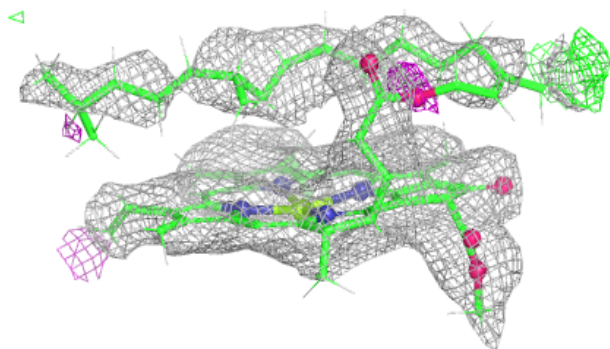
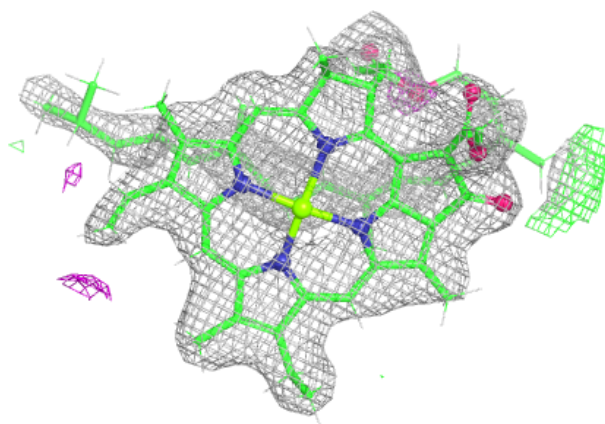


Electron density around STE B 624:

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

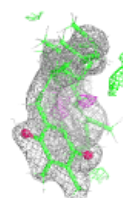
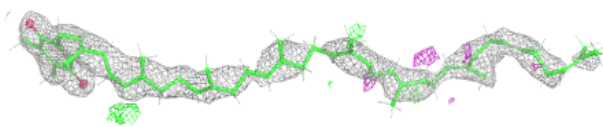
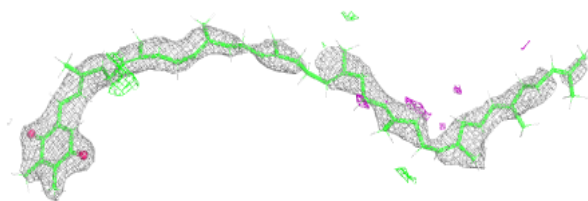
**Electron density around CLA h 101:**

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

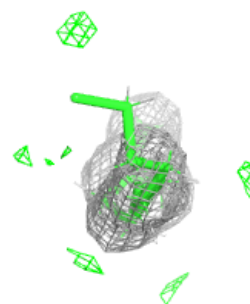
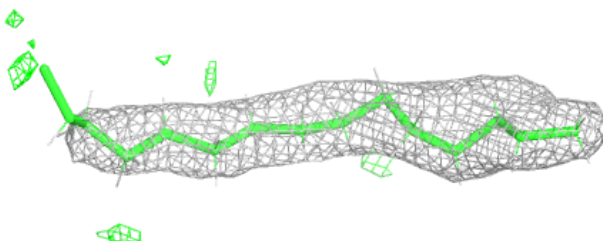
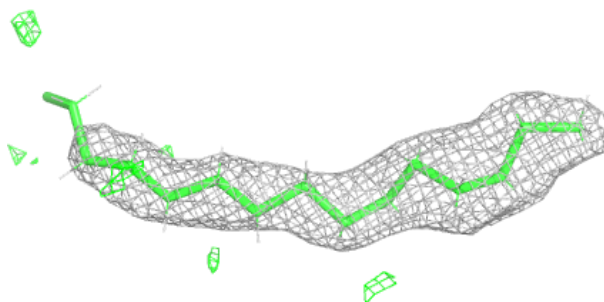


Electron density around PL9 A 410:

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

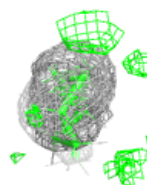
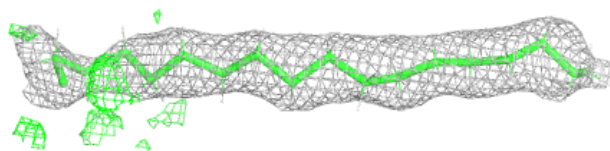
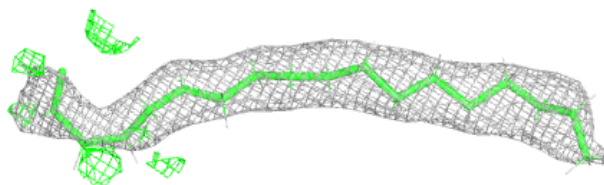
**Electron density around STE T 102:**

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

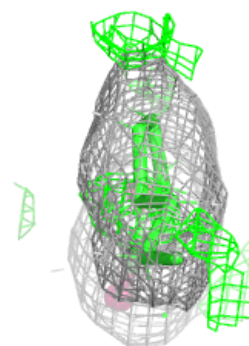
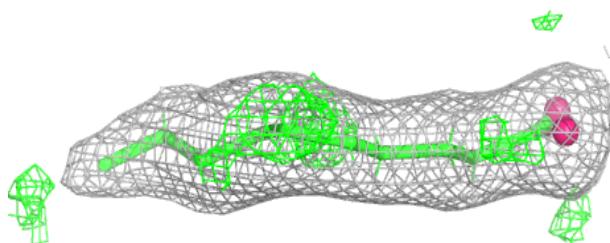
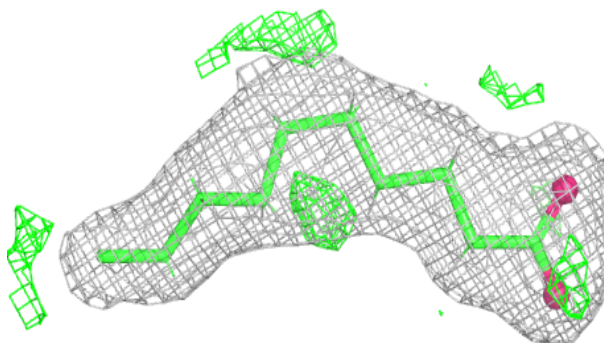


Electron density around STE I 102:

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

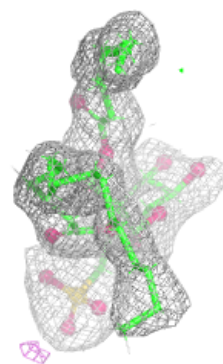
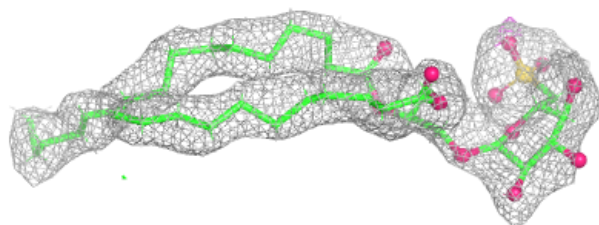
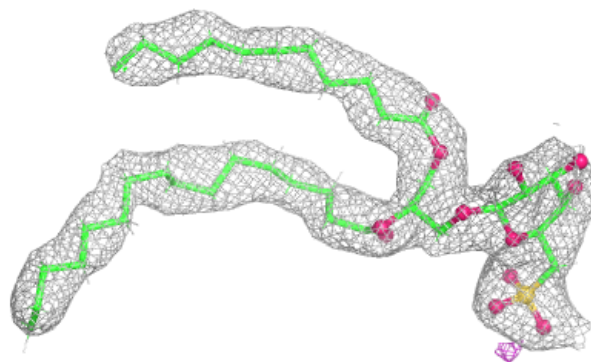
**Electron density around STE C 522:**

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

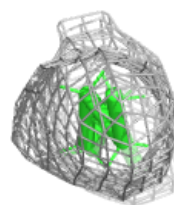
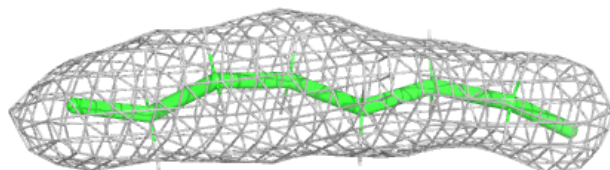
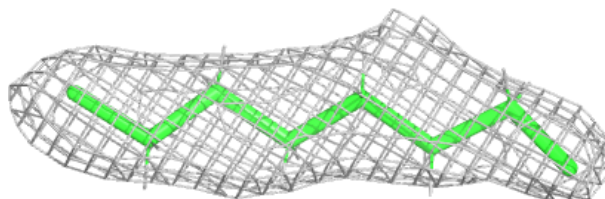


Electron density around SQD b 619:

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

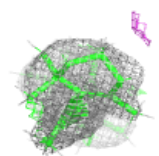
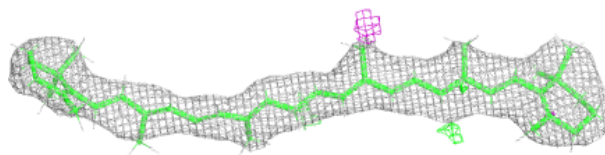
**Electron density around STE Z 102:**

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

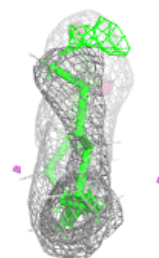
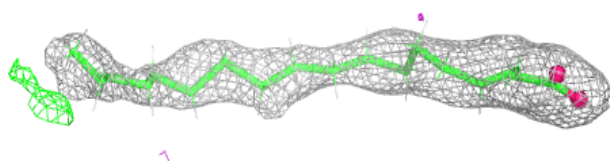
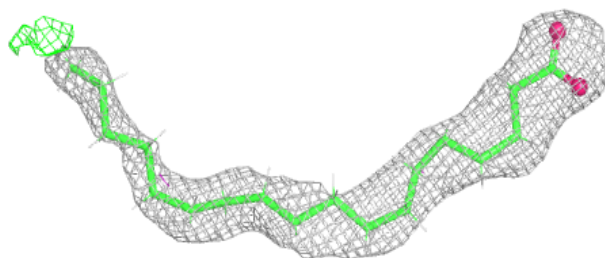


Electron density around BCR Z 101:

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

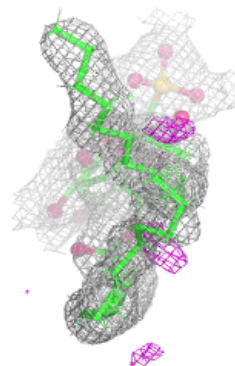
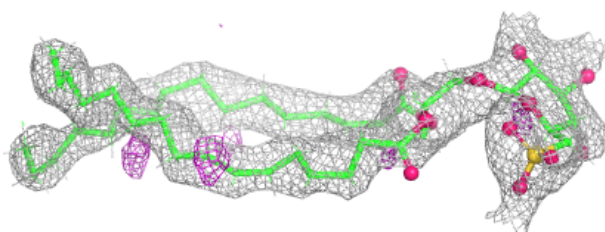
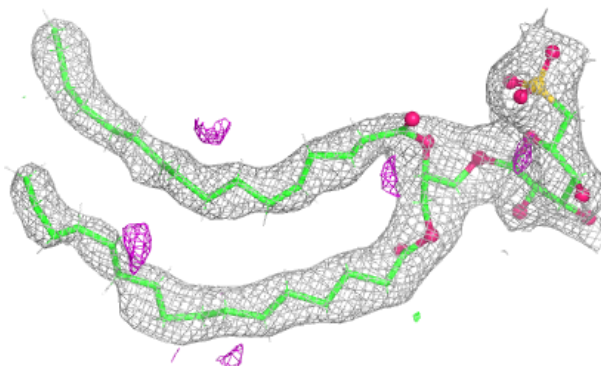
**Electron density around STE d 411:**

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

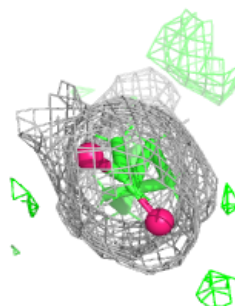
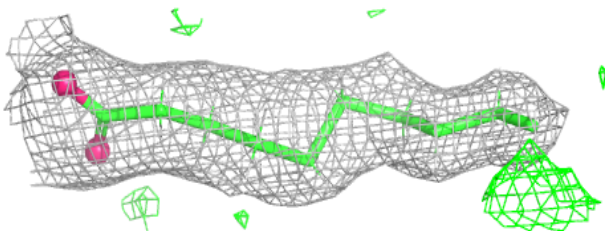
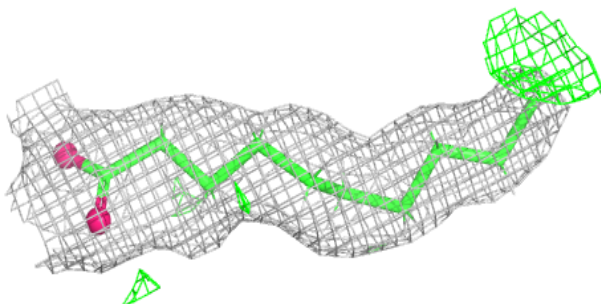


Electron density around SQD B 623:

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

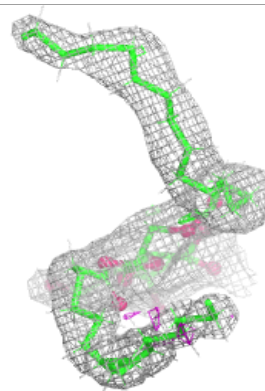
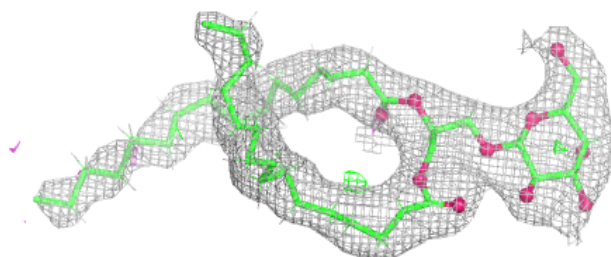
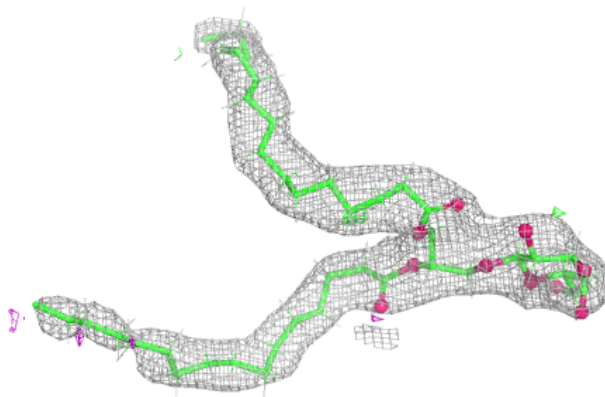
**Electron density around STE J 101:**

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

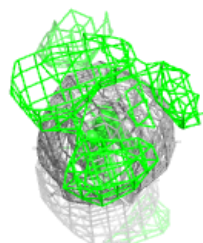
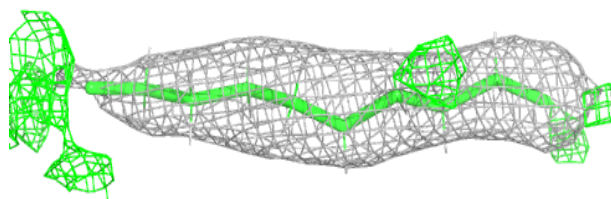
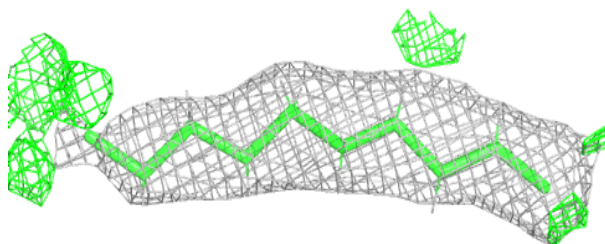


Electron density around LMG b 621:

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

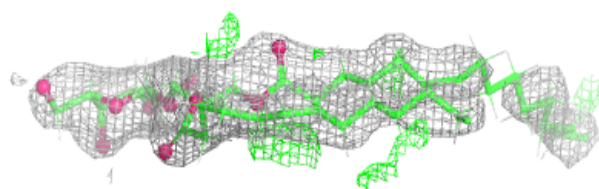
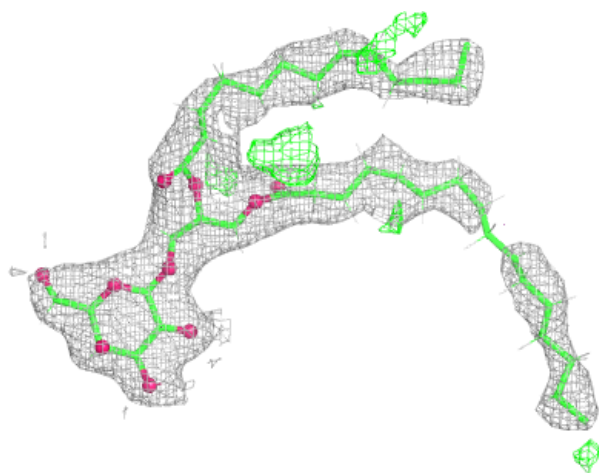
**Electron density around STE M 103:**

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



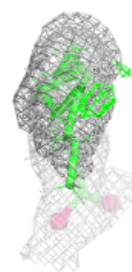
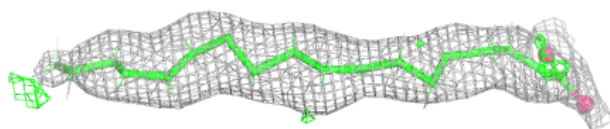
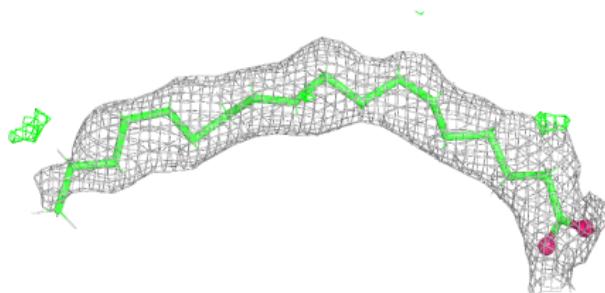
Electron density around LMG C 519:

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

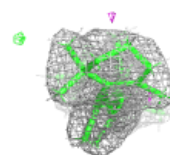
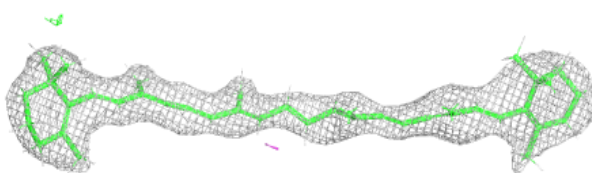
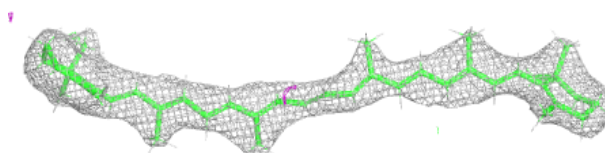


Electron density around STE X 101:

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

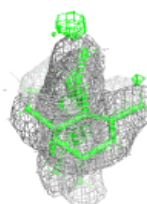
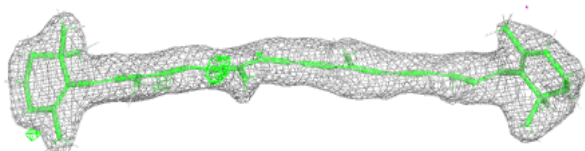
**Electron density around BCR c 516:**

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

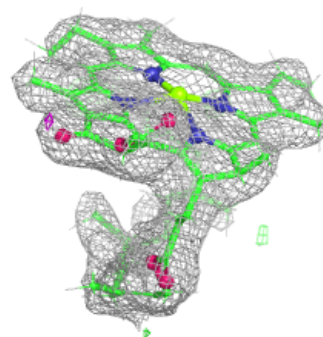
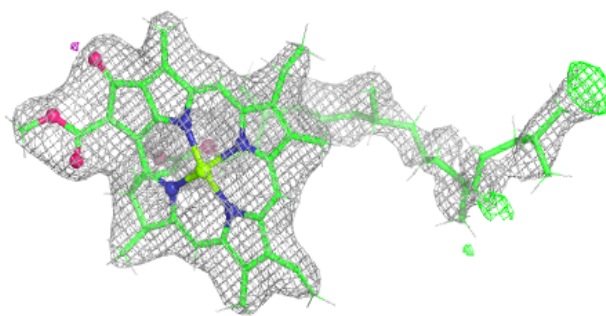
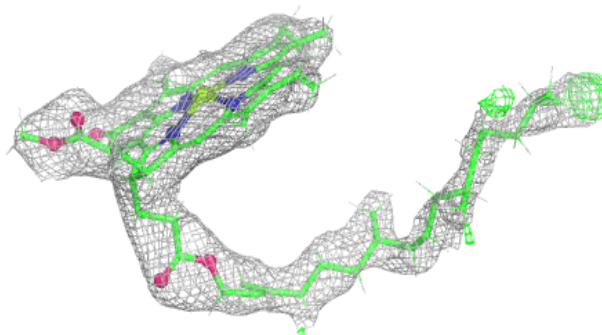


Electron density around BCR Y 101:

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

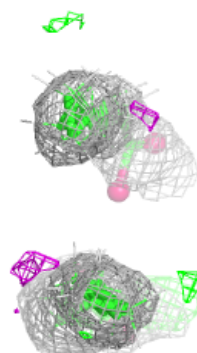
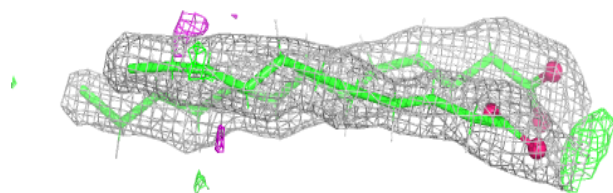
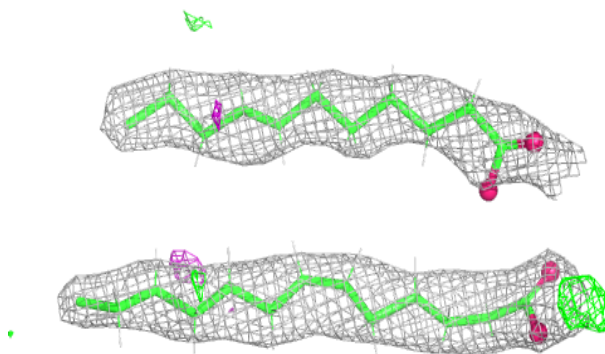
**Electron density around CLA C 514:**

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

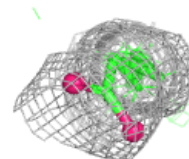
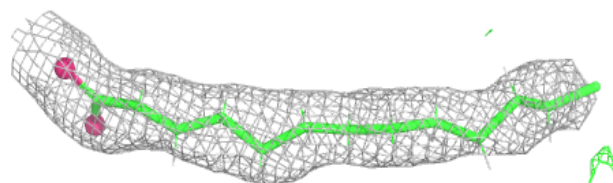
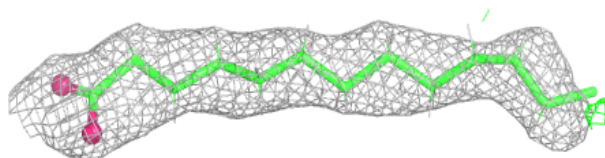


Electron density around LMG D 411:

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

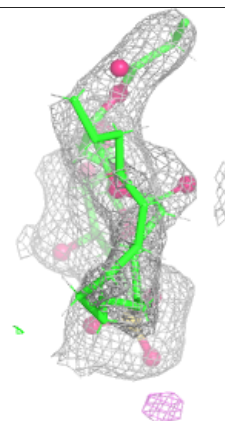
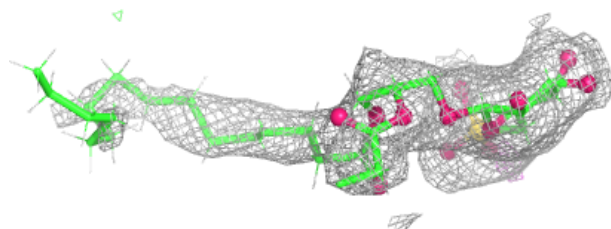
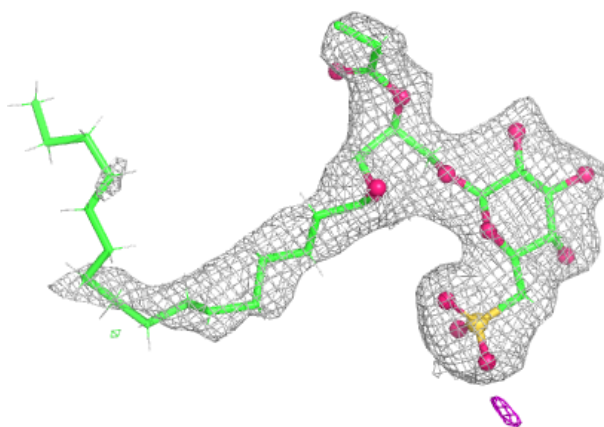
**Electron density around STE M 102:**

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

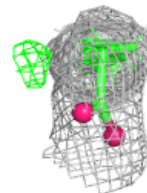
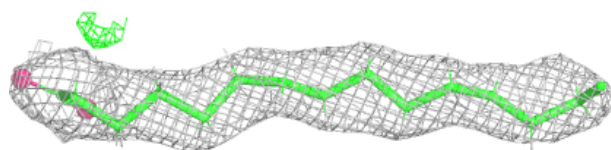
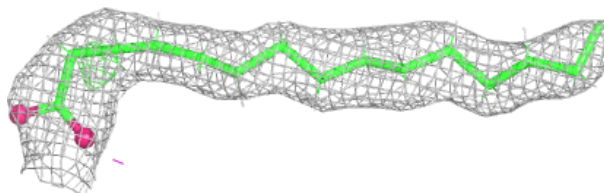


Electron density around SQD f 101:

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

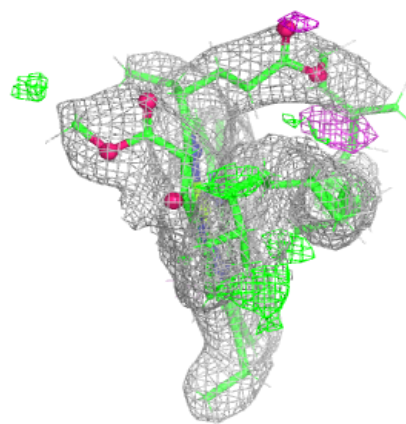
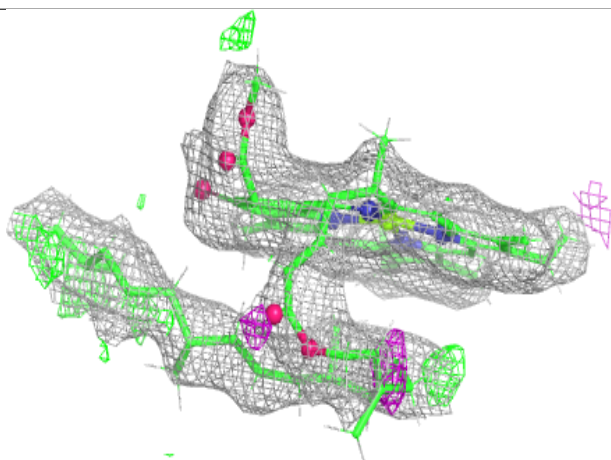
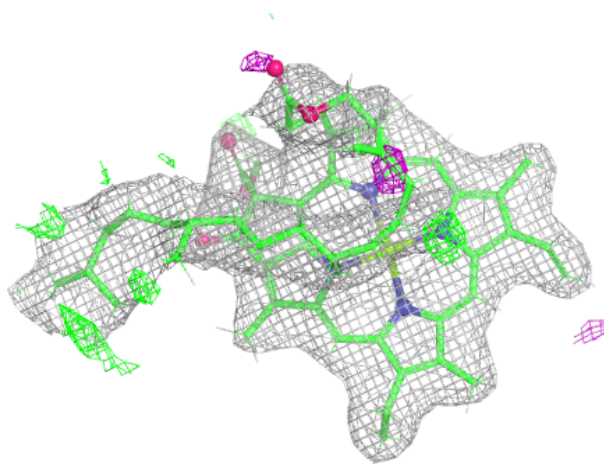
**Electron density around STE d 410:**

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



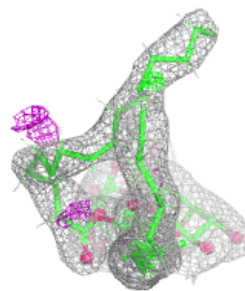
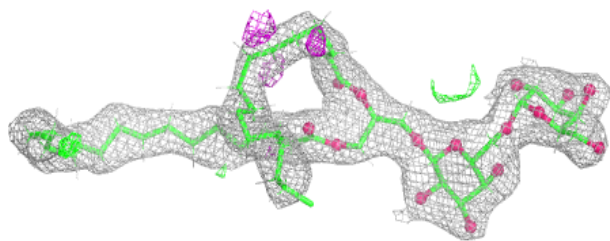
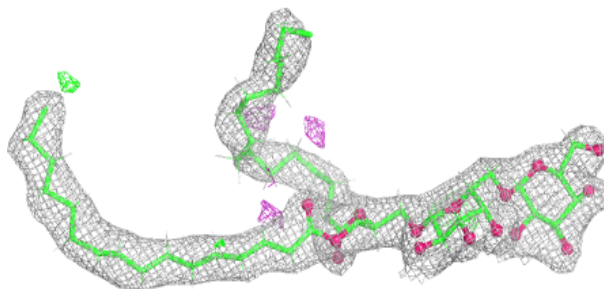
Electron density around CLA B 602:

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



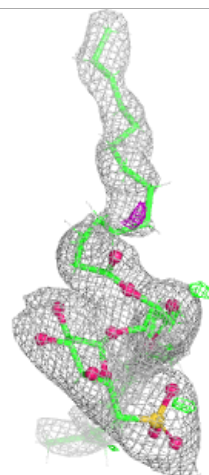
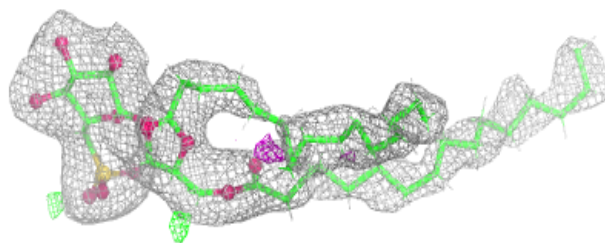
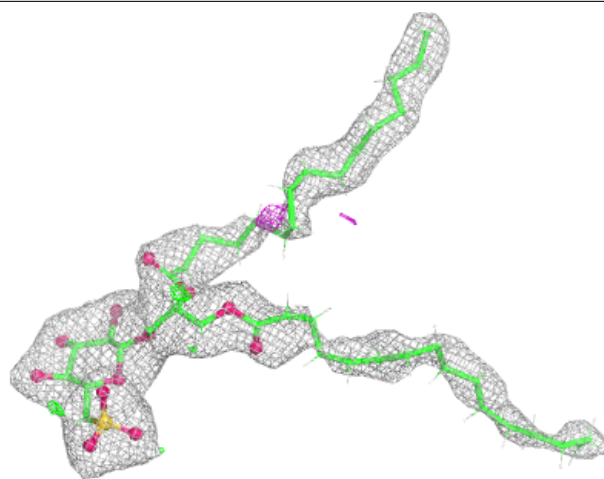
Electron density around DGD h 102:

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



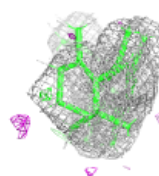
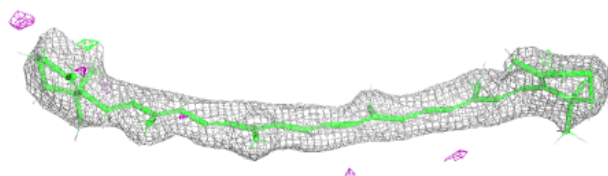
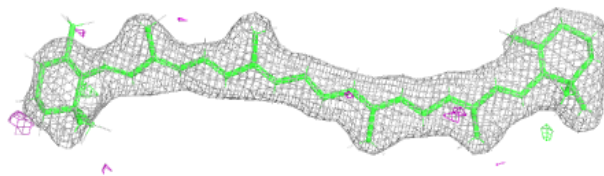
Electron density around SQD a 412:

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

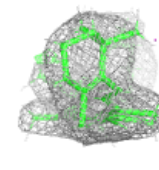
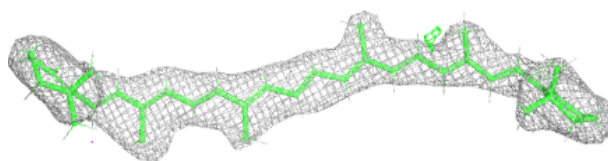
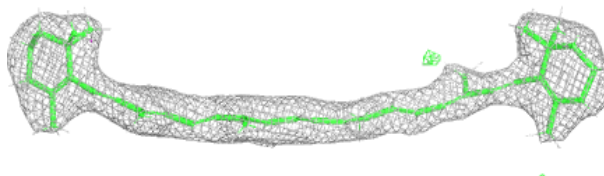


Electron density around BCR D 404:

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

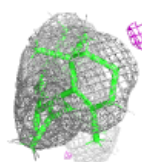
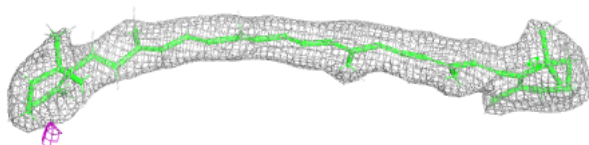
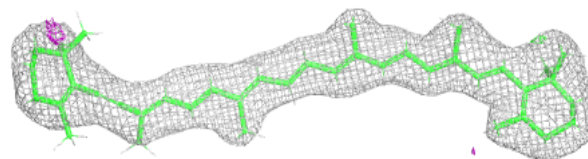
**Electron density around BCR c 518:**

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

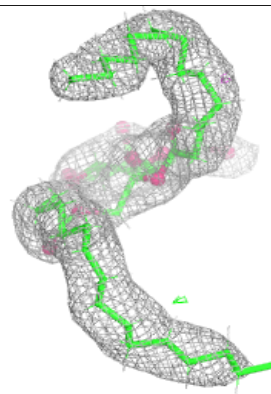
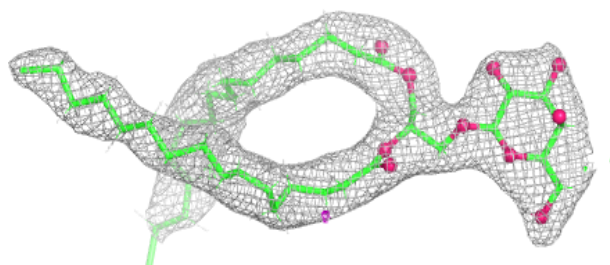
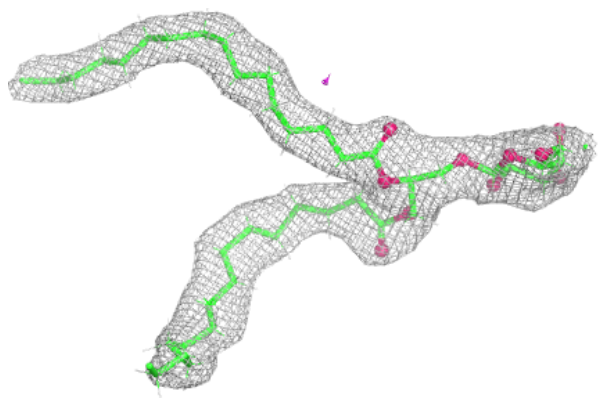


Electron density around BCR d 404:

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

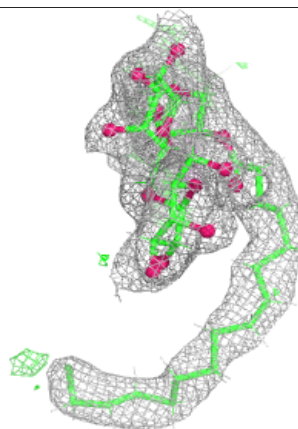
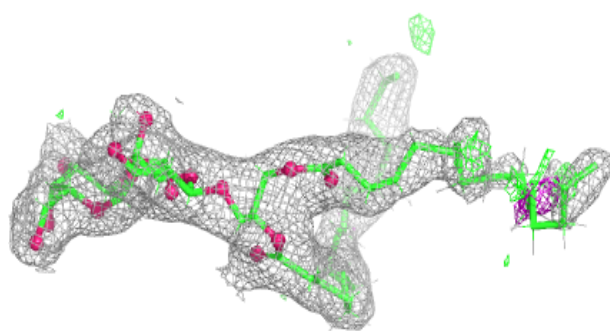
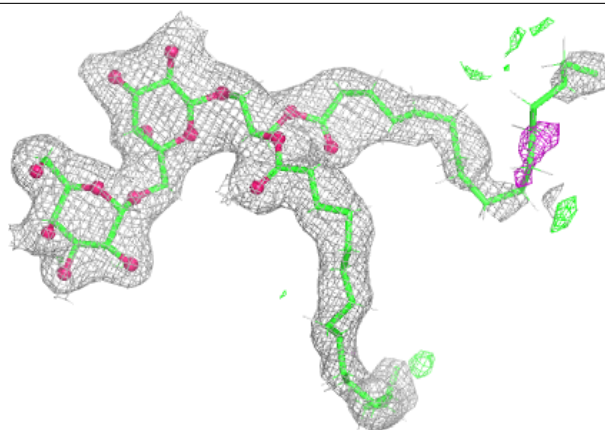
**Electron density around LMG M 101:**

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

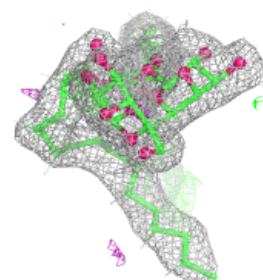
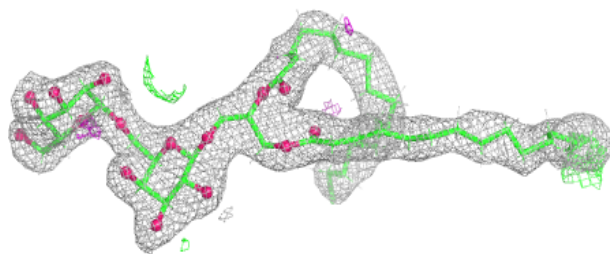


Electron density around DGD C 517:

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

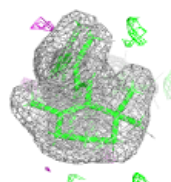
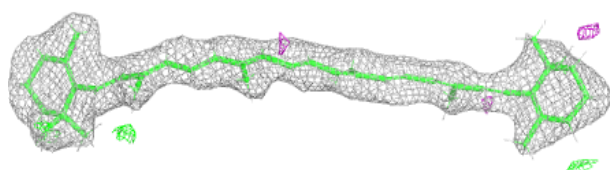
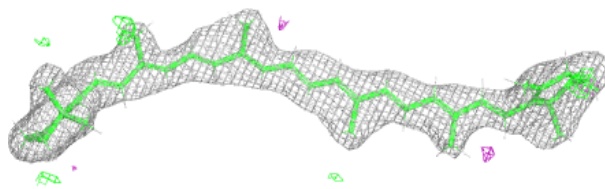
**Electron density around DGD H 102:**

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

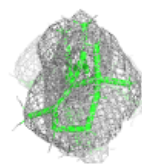
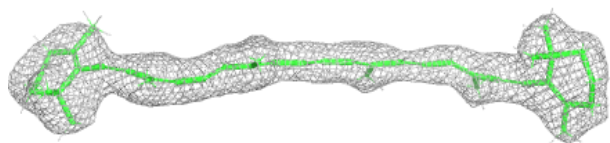
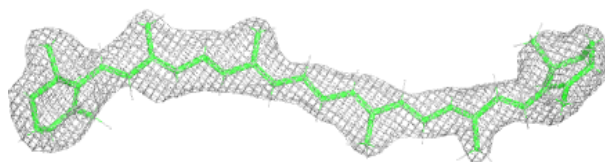


Electron density around BCR x 101:

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

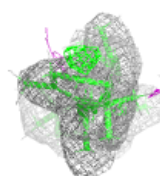
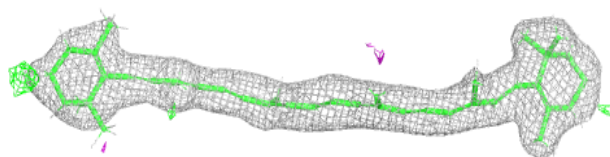
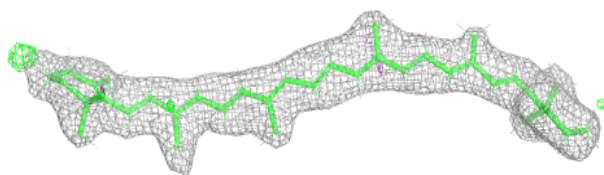
**Electron density around BCR y 101:**

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



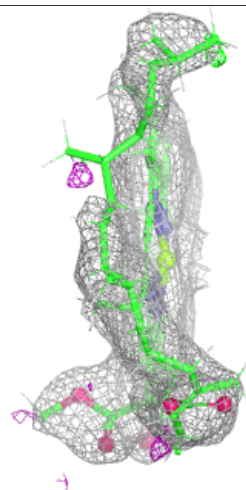
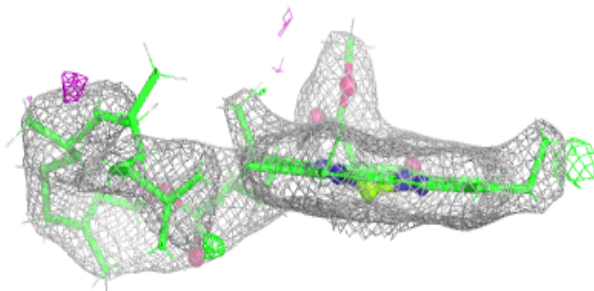
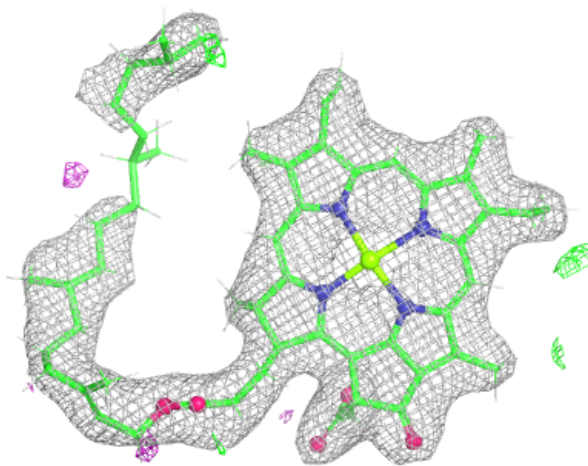
Electron density around BCR H 101:

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



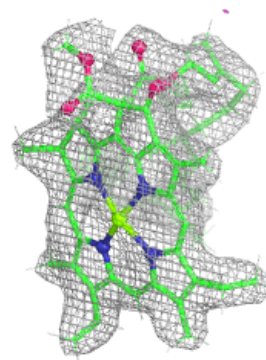
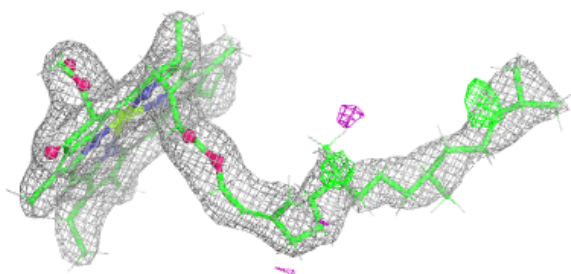
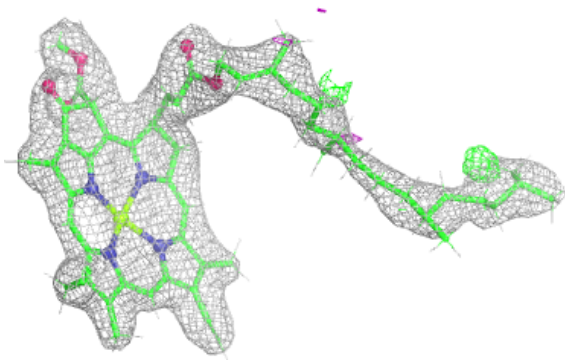
Electron density around CLA c 514:

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

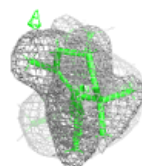
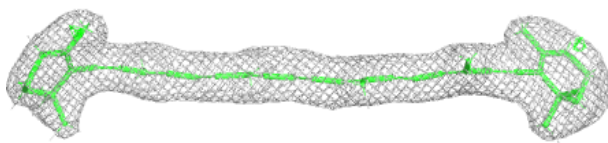
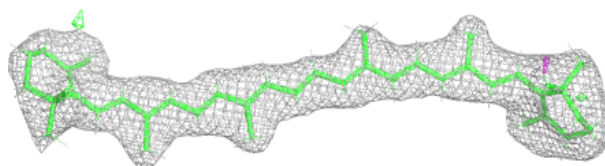


Electron density around CLA c 513:

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

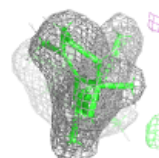
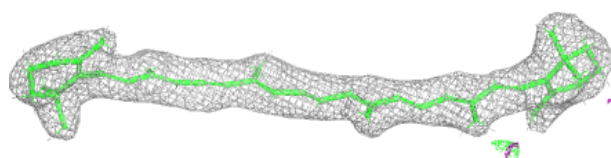
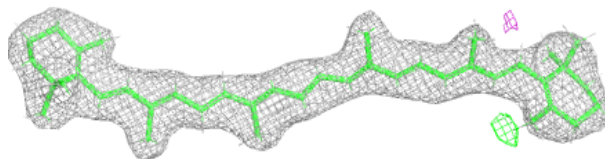
**Electron density around BCR b 617:**

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

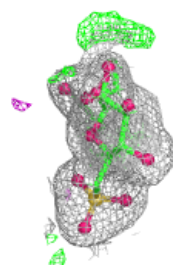
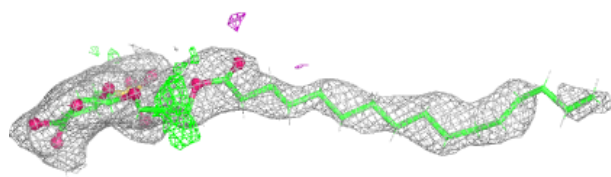
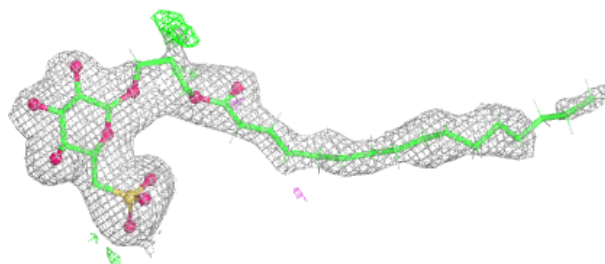


Electron density around BCR b 618:

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

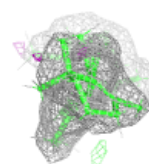
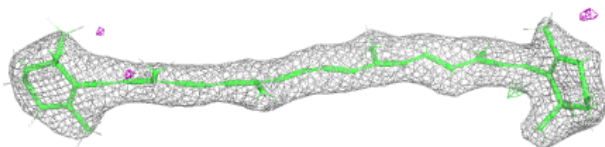
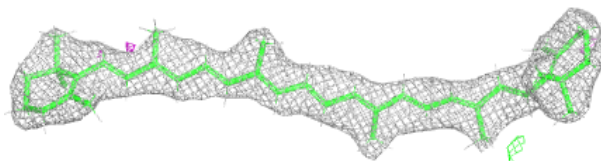
**Electron density around SQD D 407:**

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



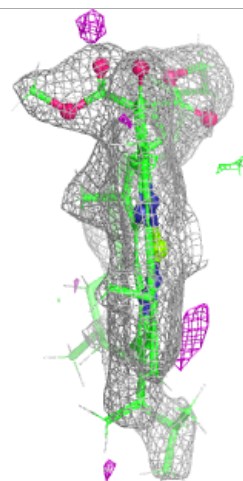
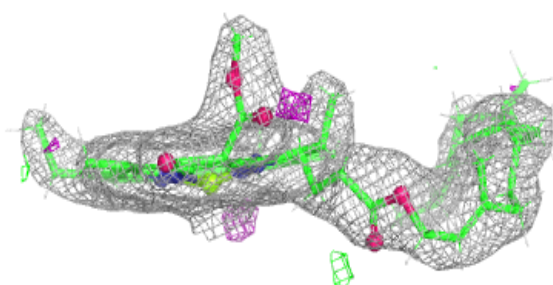
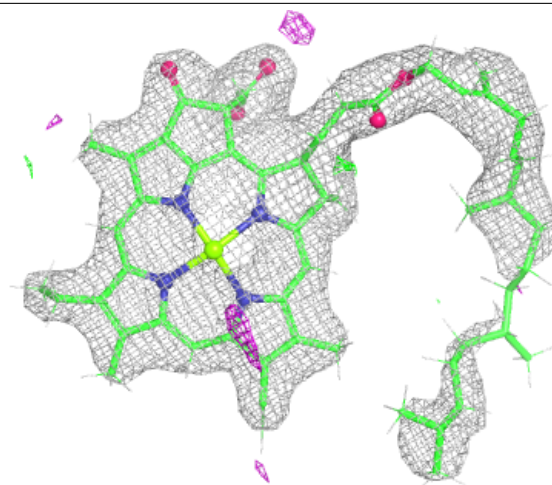
Electron density around BCR c 517:

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



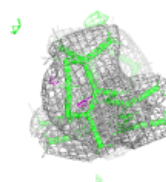
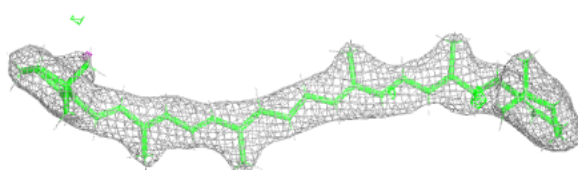
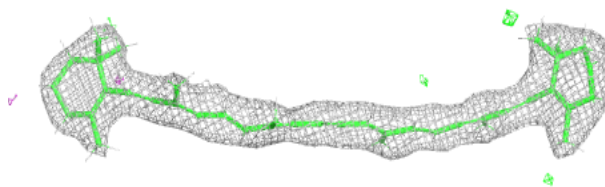
Electron density around CLA C 513:

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

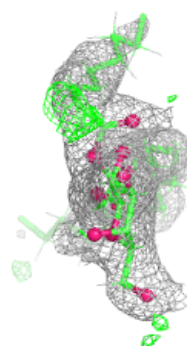
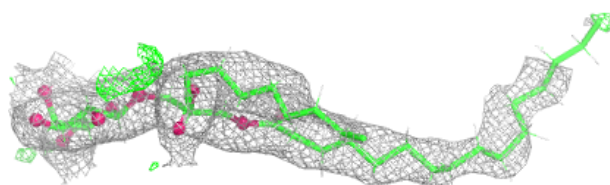
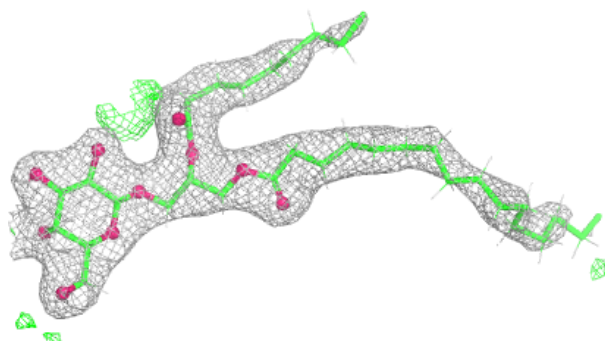


Electron density around BCR K 101:

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

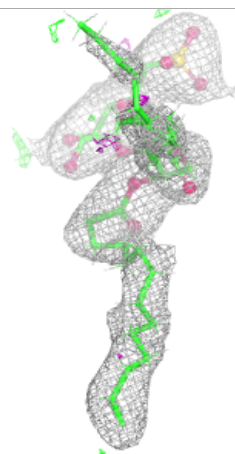
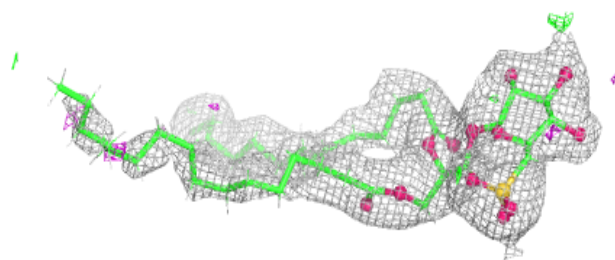
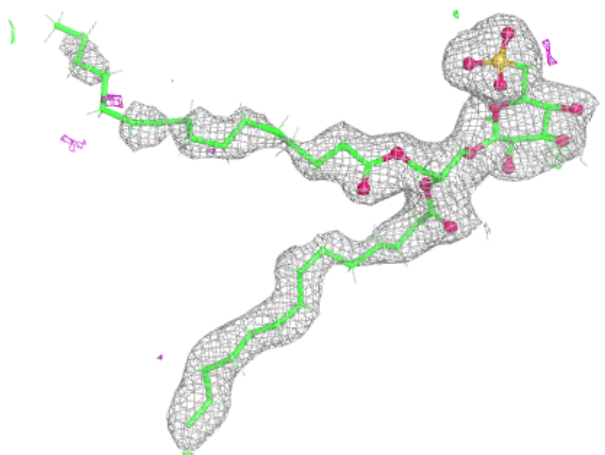
**Electron density around LMG d 409:**

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



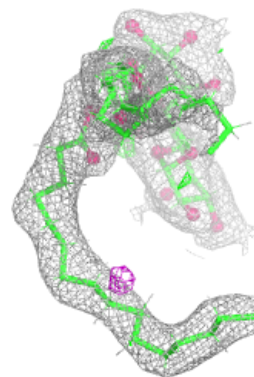
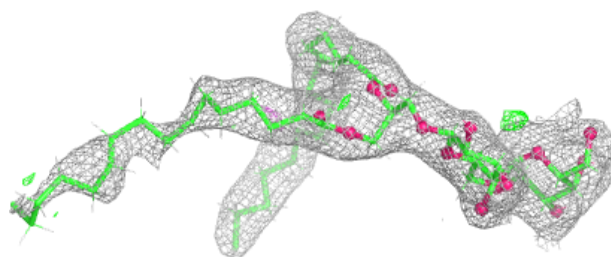
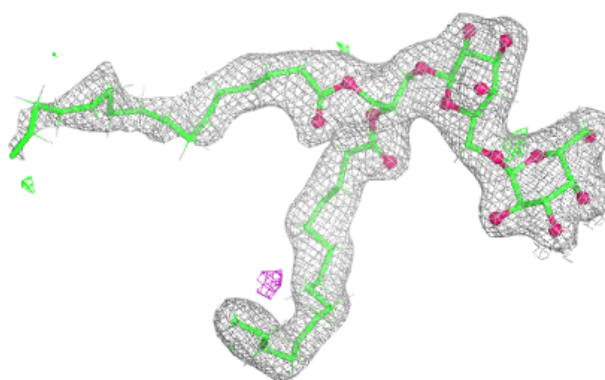
Electron density around SQD A 413:

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

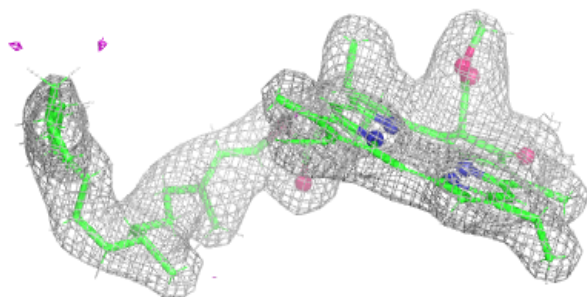
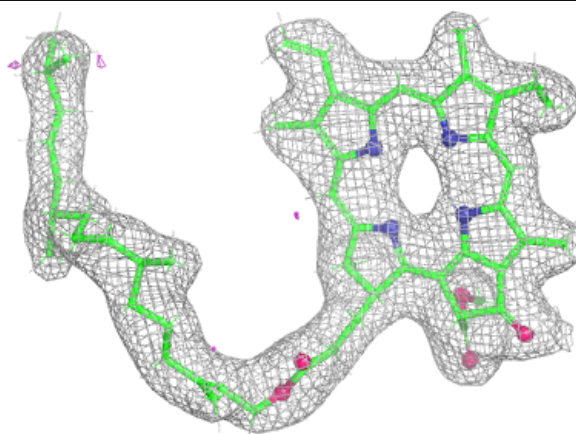


Electron density around DGD c 520:

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

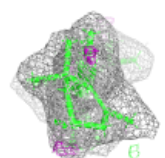
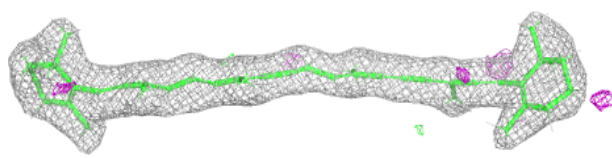
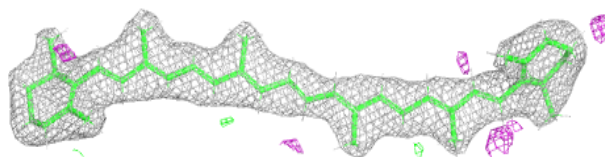
**Electron density around PHO d 401:**

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

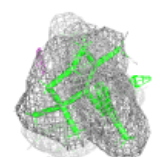
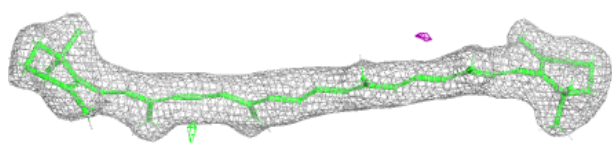
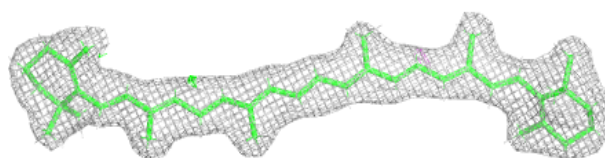


Electron density around BCR B 619:

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

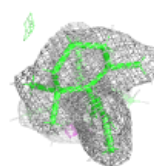
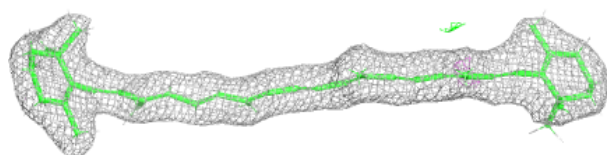
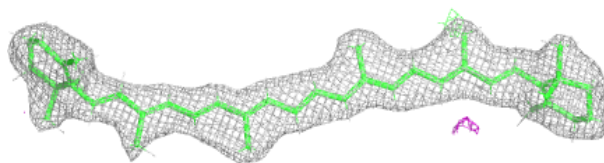
**Electron density around BCR B 620:**

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

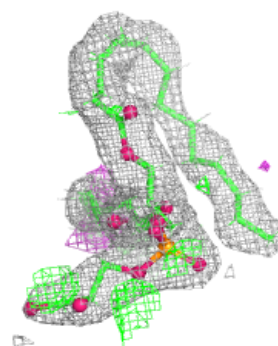
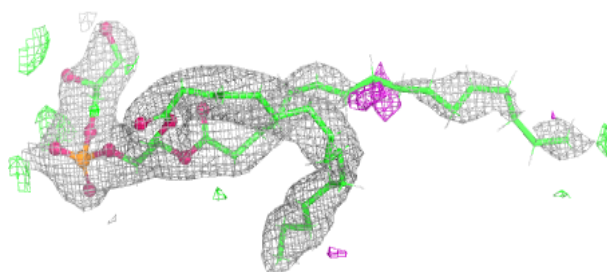
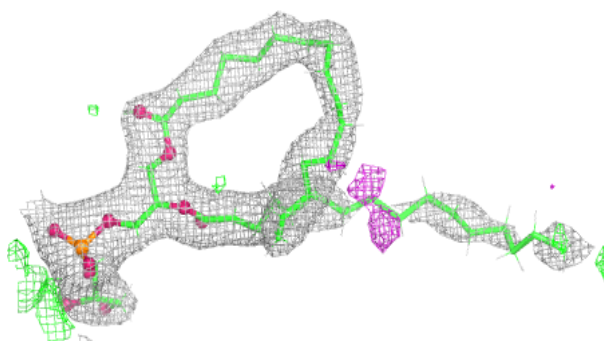


Electron density around BCR C 515:

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

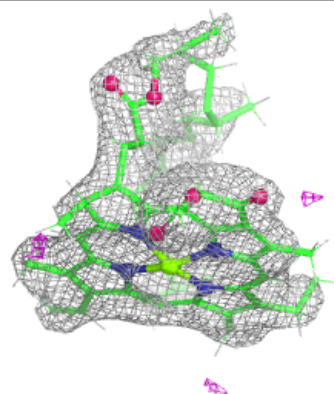
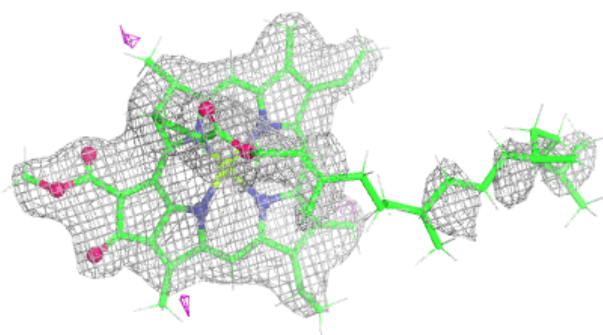
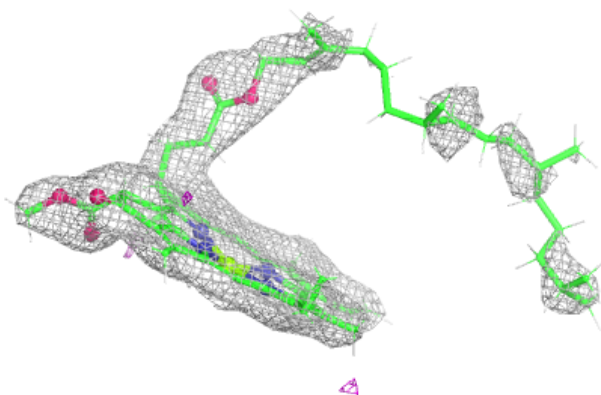
**Electron density around LHG d 406:**

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

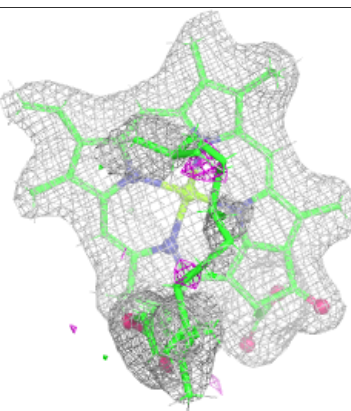
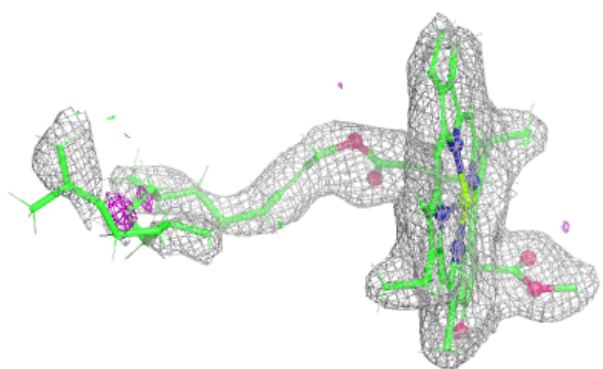
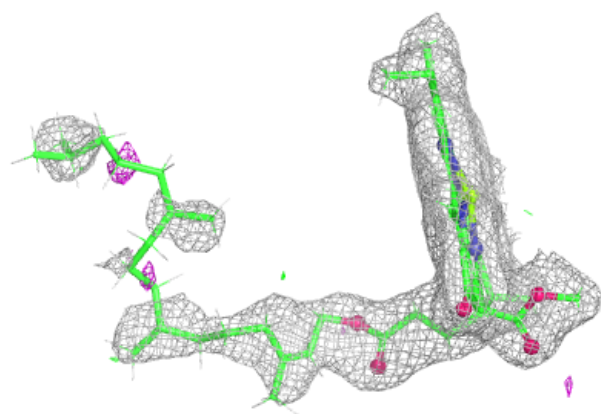


Electron density around CLA c 515:

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

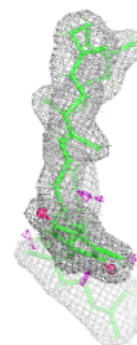
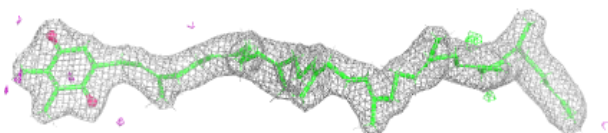
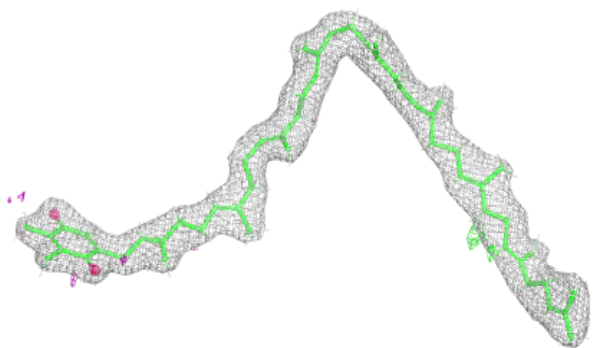
**Electron density around CLA c 508:**

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

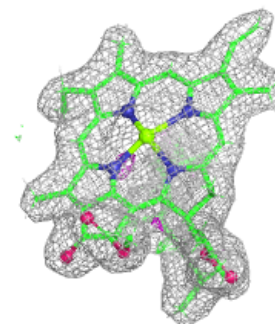
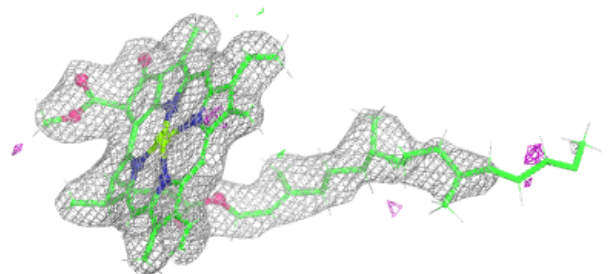
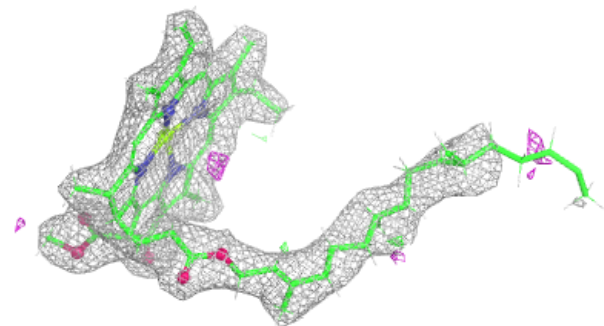


Electron density around PL9 d 405:

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

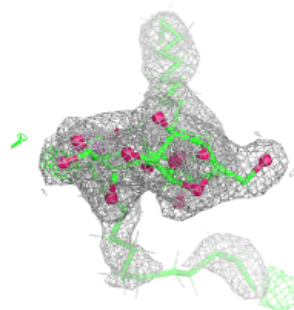
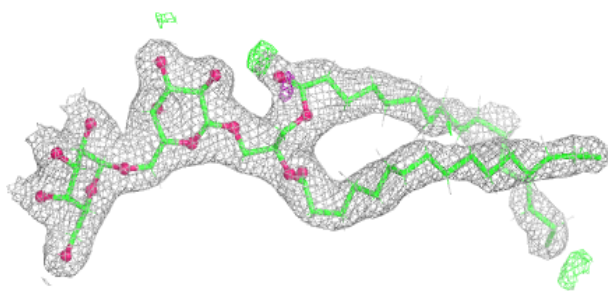
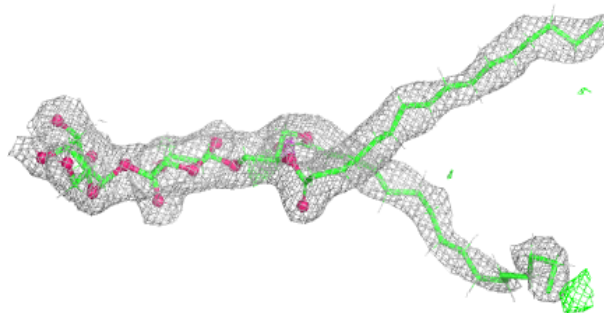
**Electron density around CLA c 510:**

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



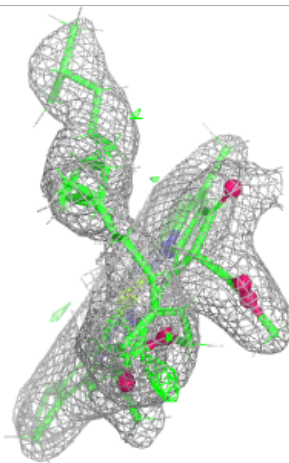
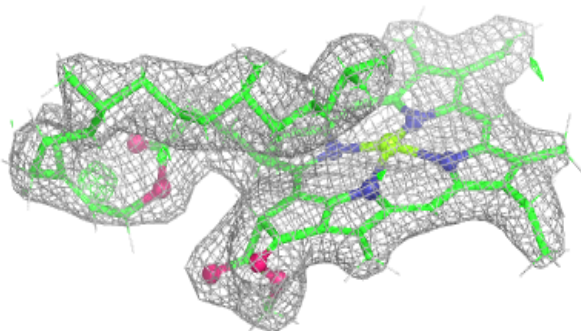
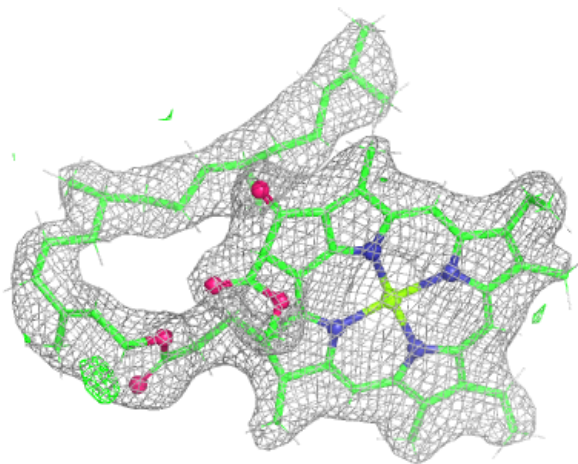
Electron density around DGD C 516:

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



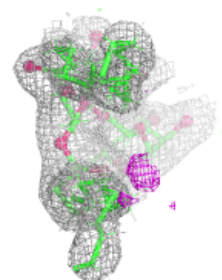
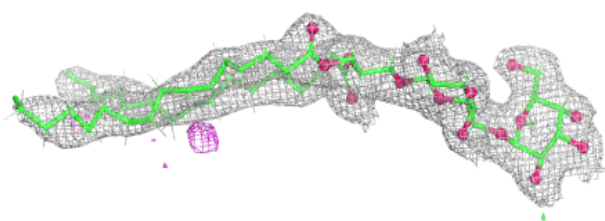
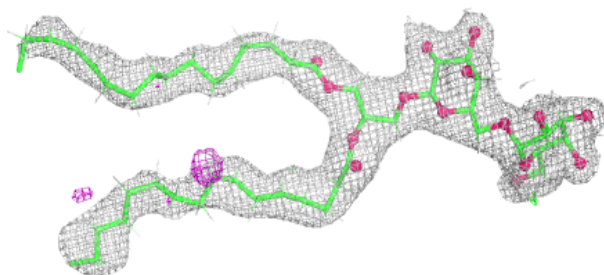
Electron density around CLA c 511:

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

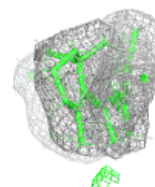
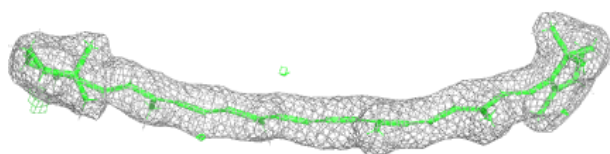
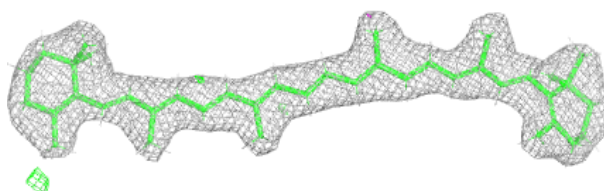


Electron density around DGD C 518:

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

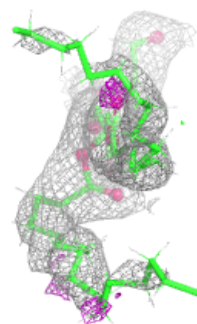
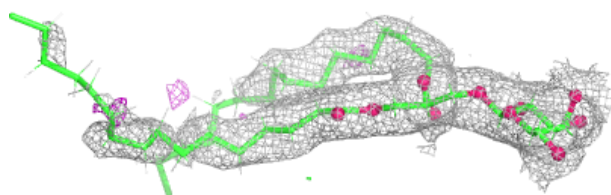
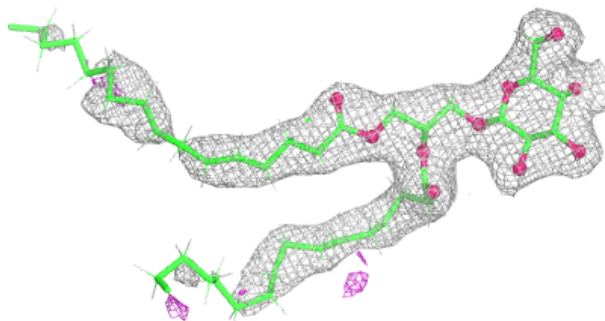
**Electron density around BCR T 101:**

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

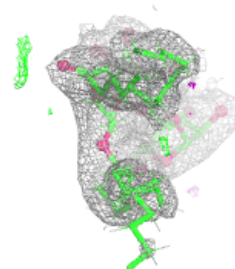
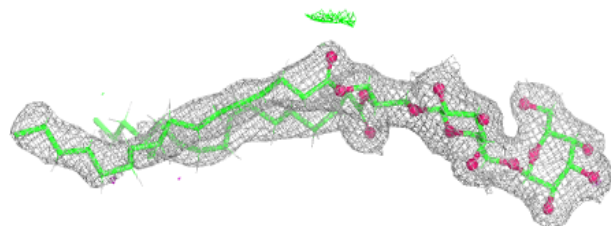
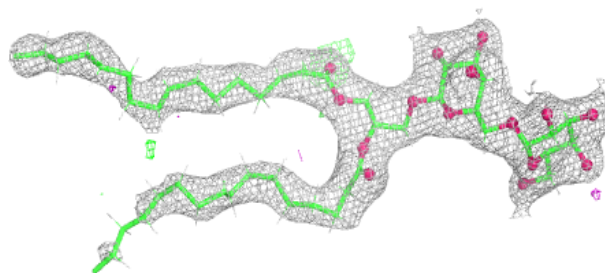


Electron density around LMG D 406:

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

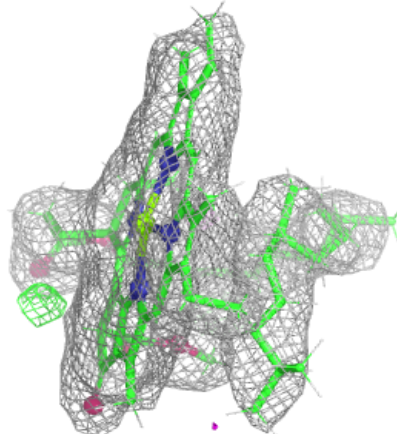
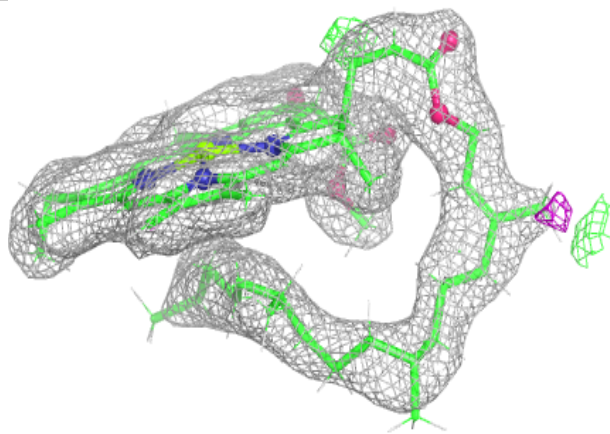
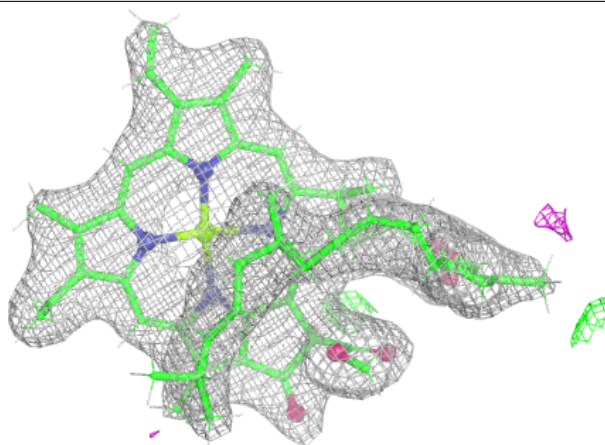
**Electron density around DGD c 521:**

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



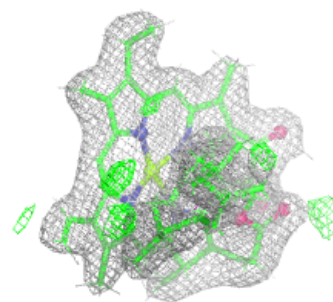
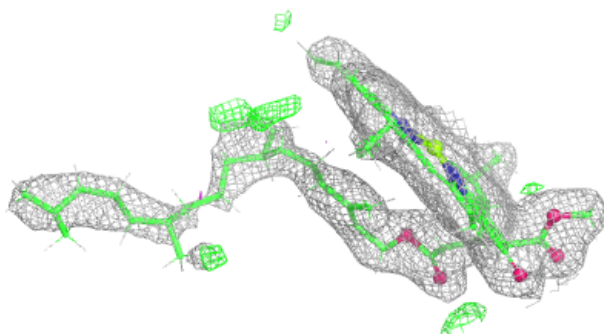
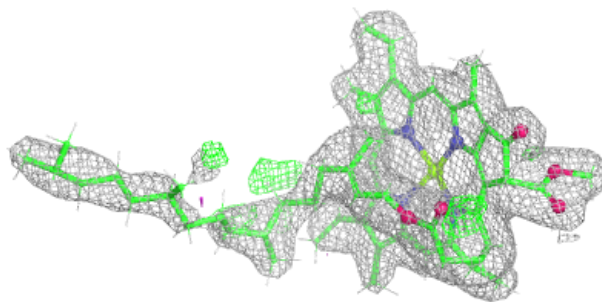
Electron density around CLA c 512:

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

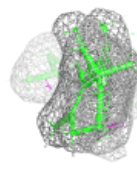
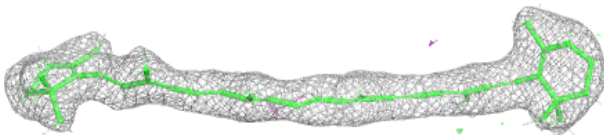
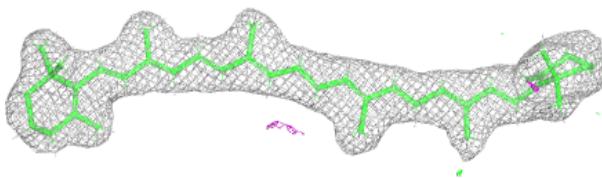


Electron density around CLA C 506:

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

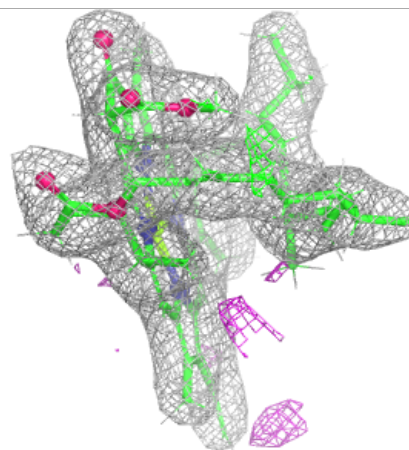
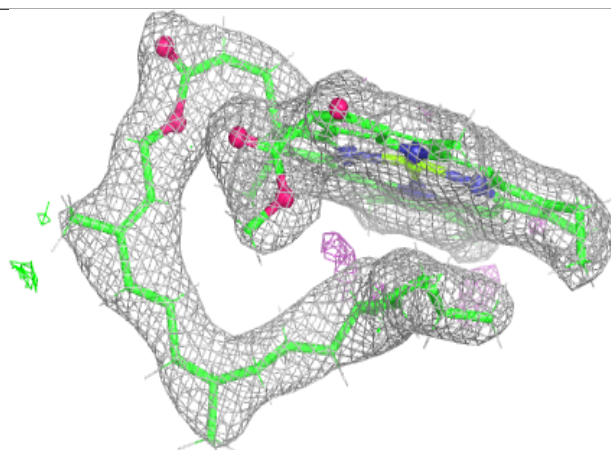
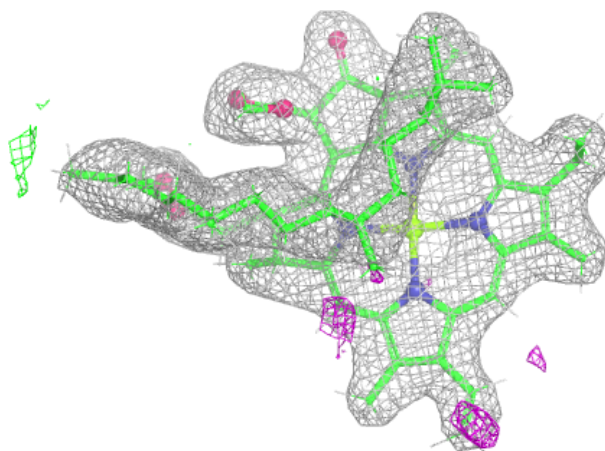
**Electron density around BCR b 616:**

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



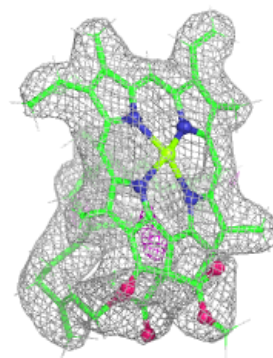
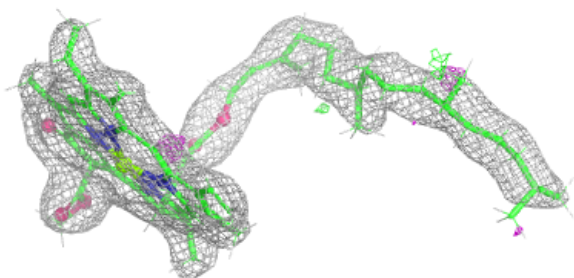
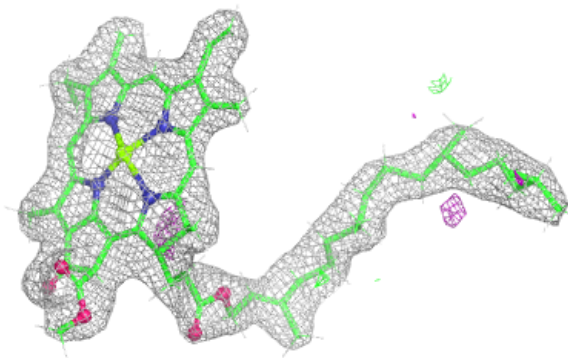
Electron density around CLA C 511:

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

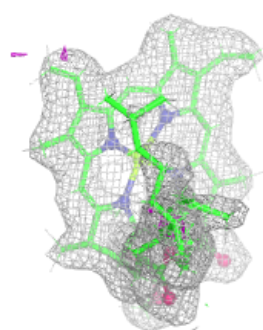
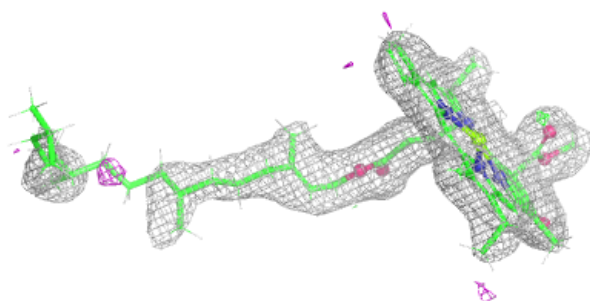
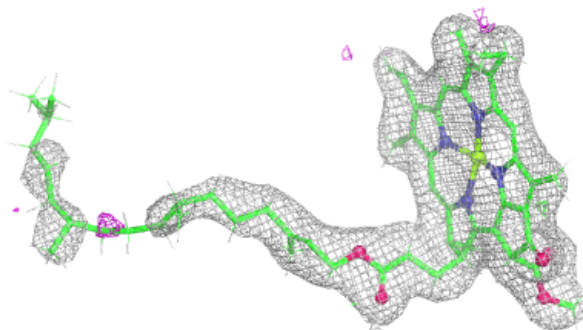


Electron density around CLA C 512:

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

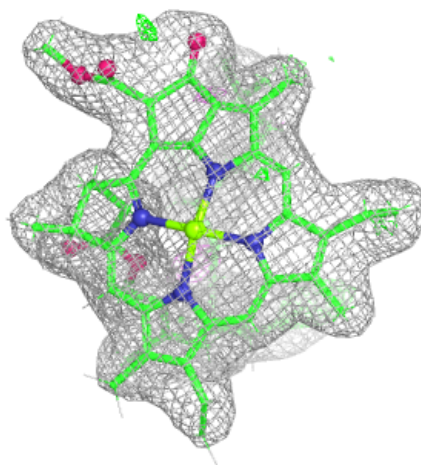
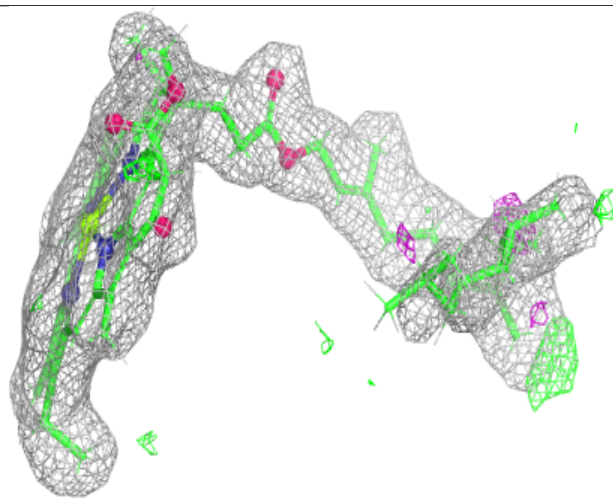
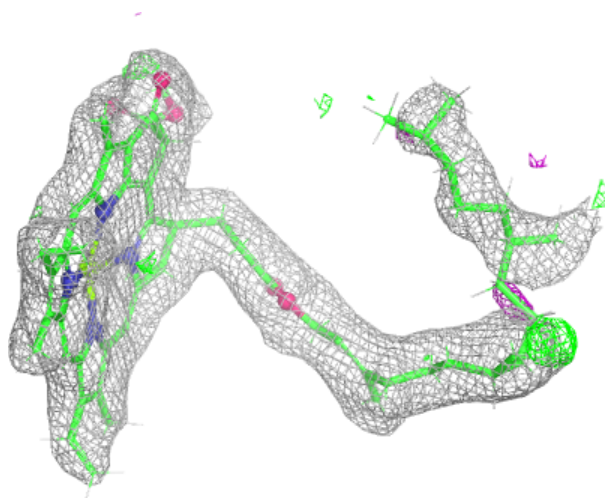
**Electron density around CLA d 403:**

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



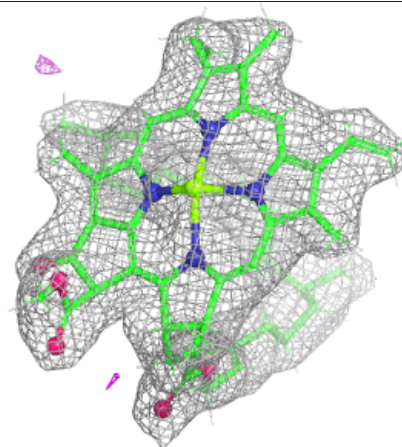
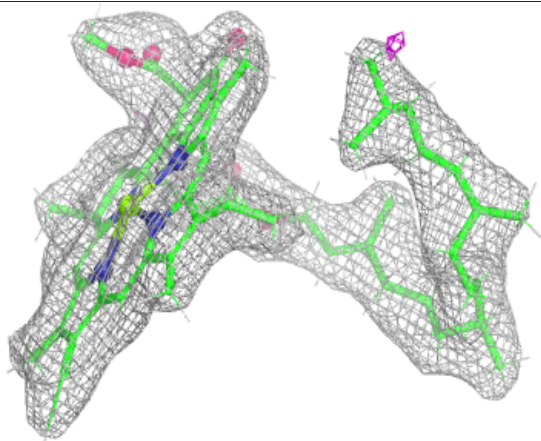
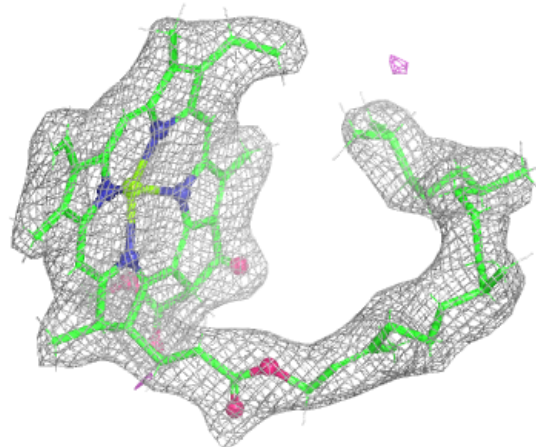
Electron density around CLA B 607:

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

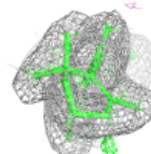
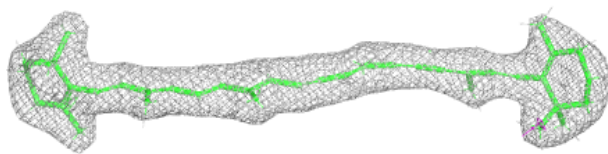
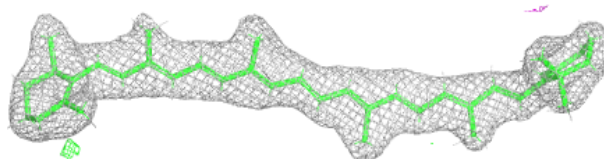


Electron density around CLA C 504:

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

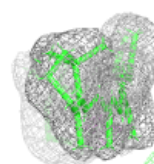
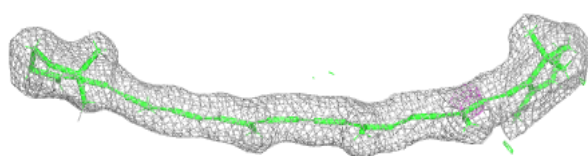
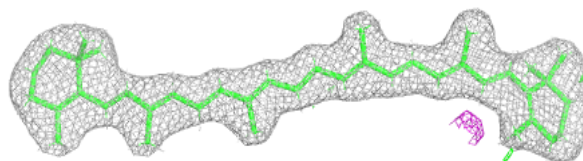
**Electron density around BCR A 406:**

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

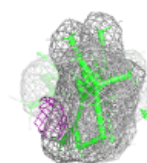
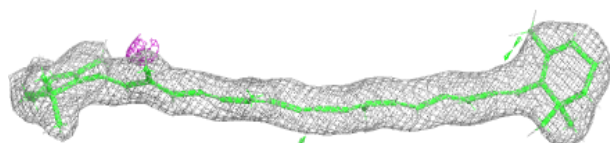
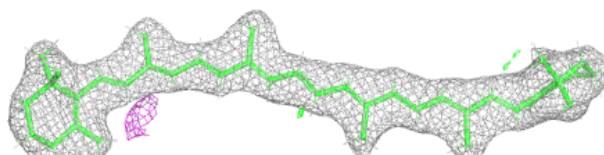


Electron density around BCR t 101:

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

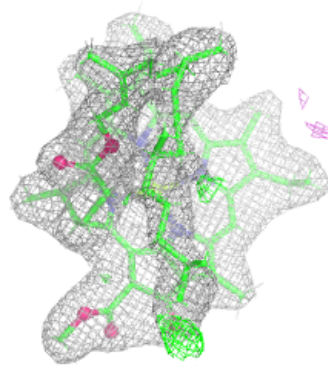
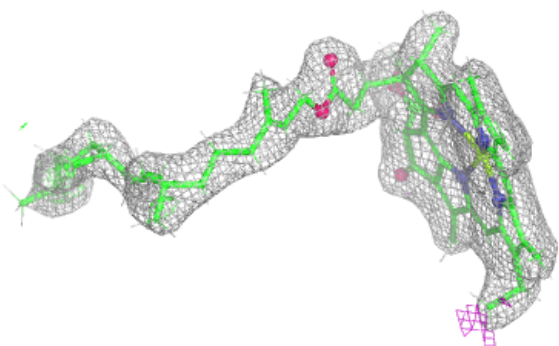
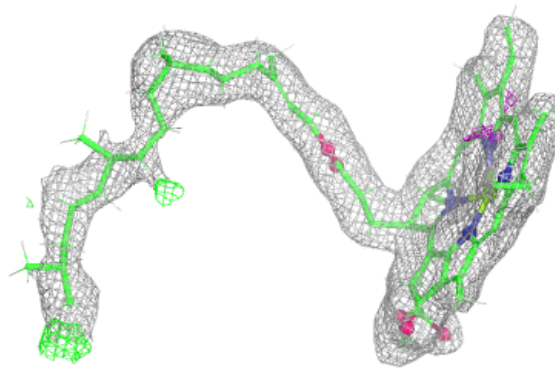
**Electron density around BCR B 618:**

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

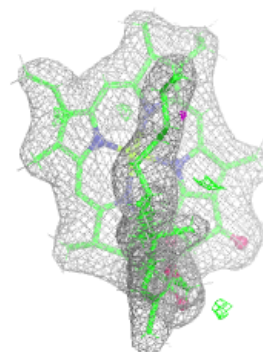
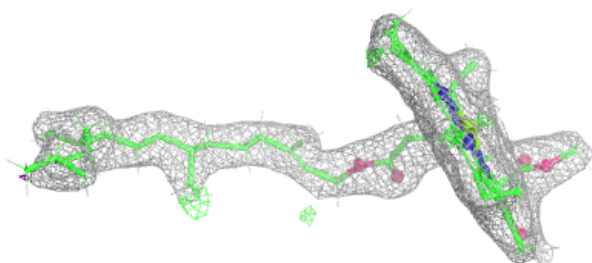
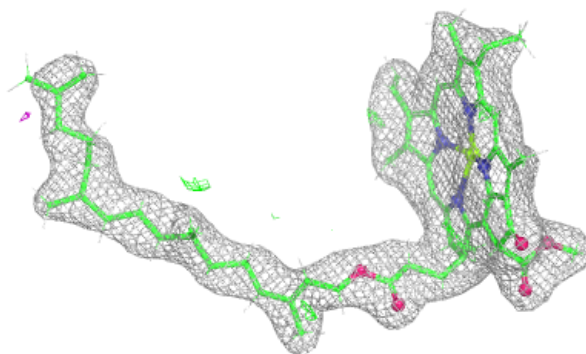


Electron density around CLA b 605:

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

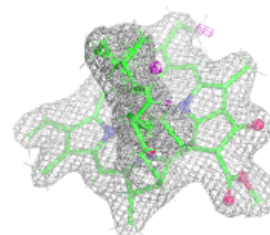
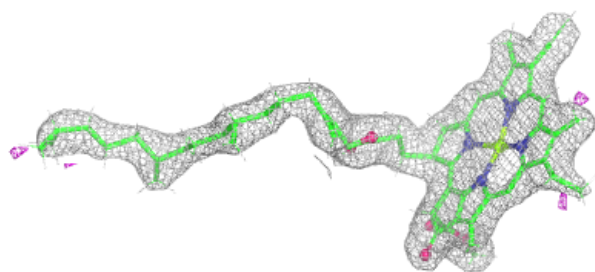
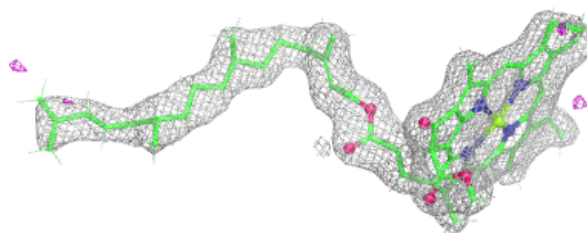
**Electron density around CLA b 608:**

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

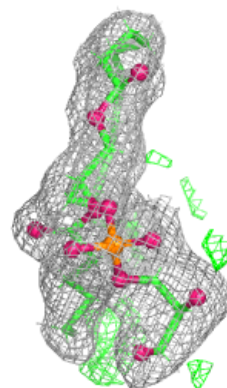
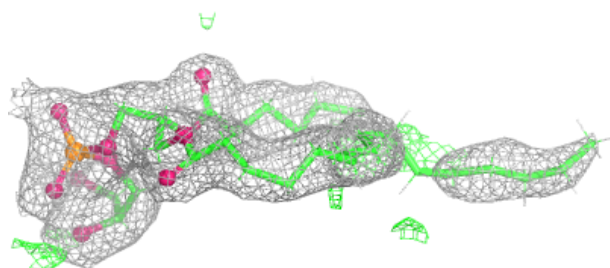
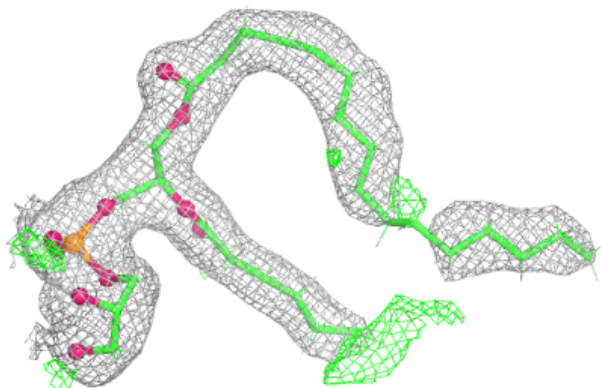


Electron density around CLA c 504:

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

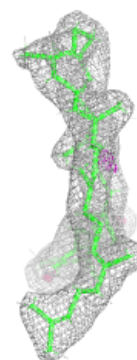
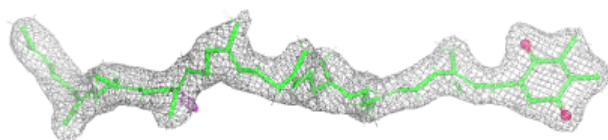
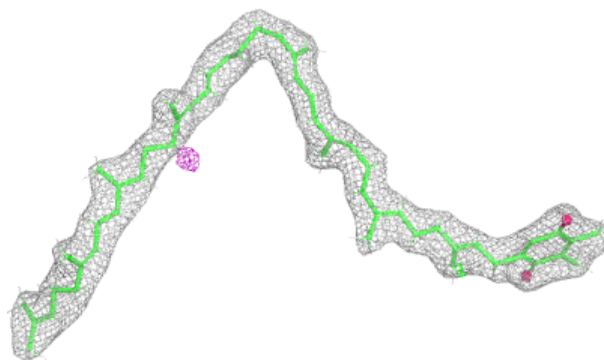
**Electron density around LHG d 408:**

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



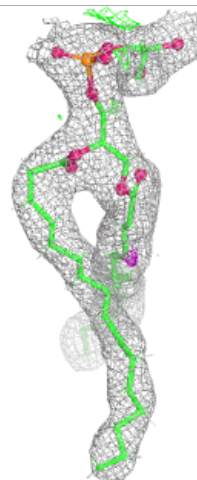
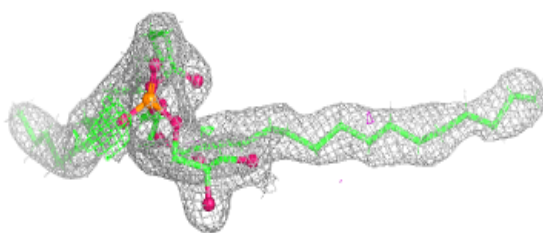
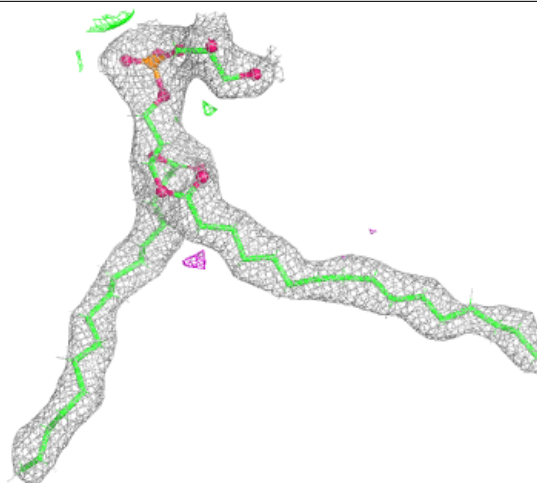
Electron density around PL9 D 405:

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



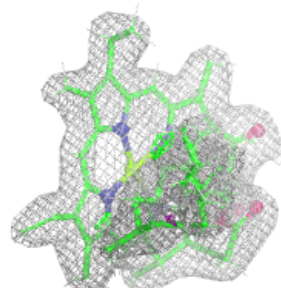
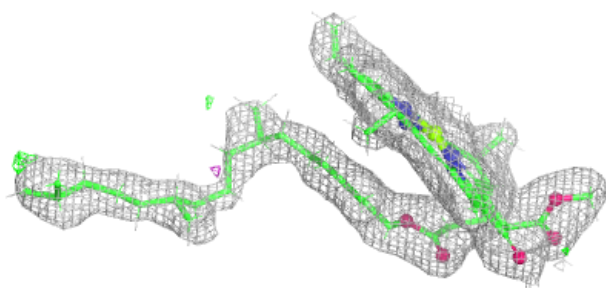
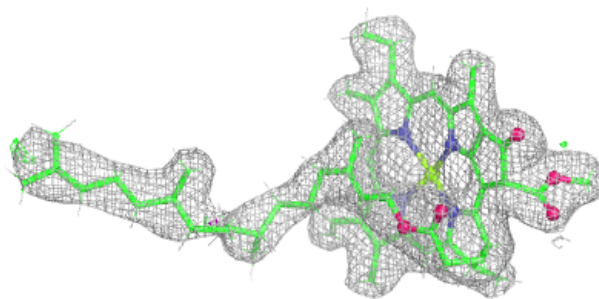
Electron density around LHG 1 101:

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

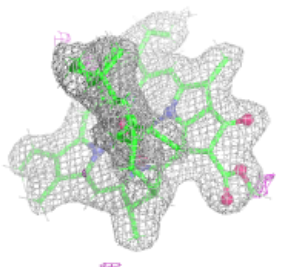
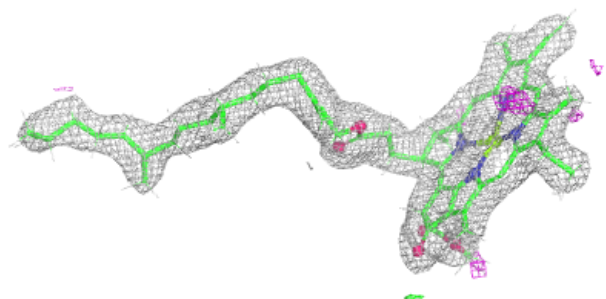
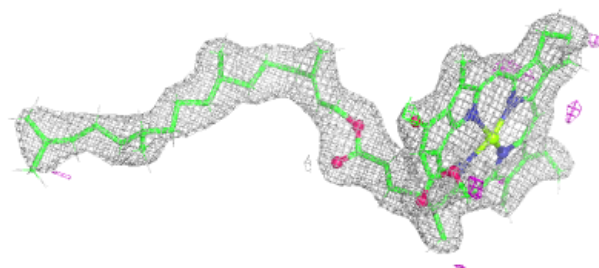


Electron density around CLA c 507:

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

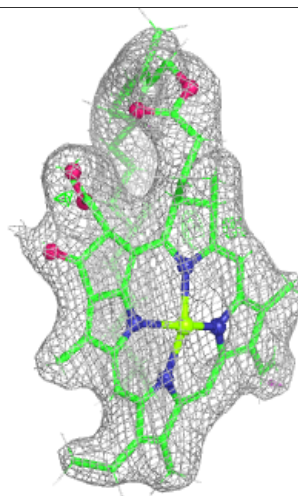
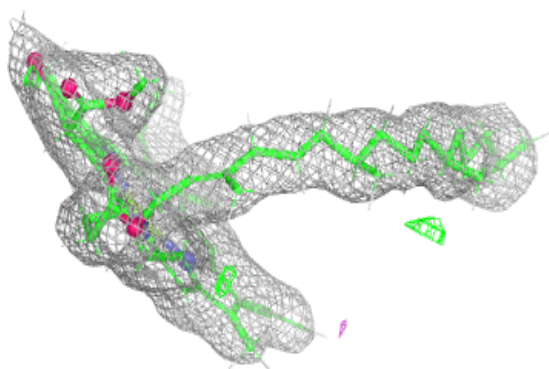
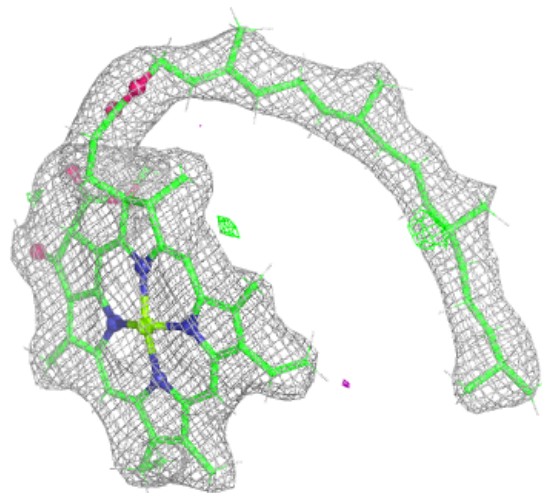
**Electron density around CLA C 503:**

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



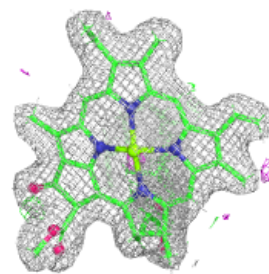
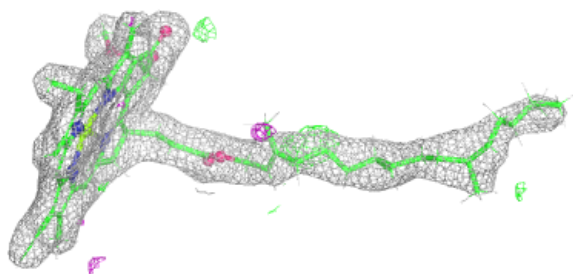
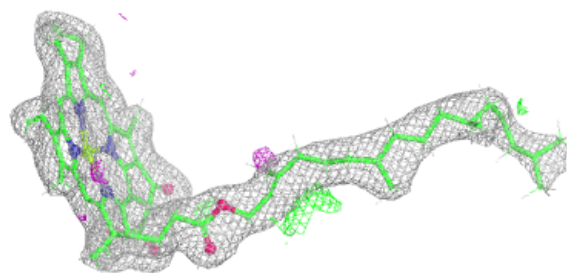
Electron density around CLA c 509:

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

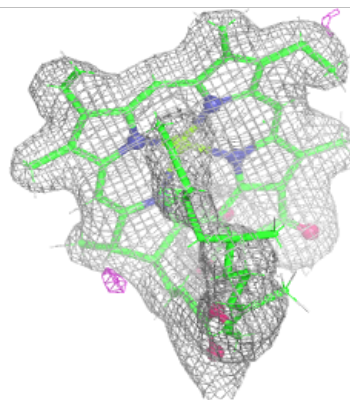
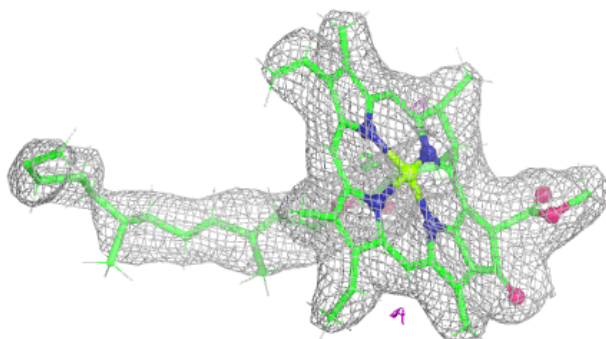
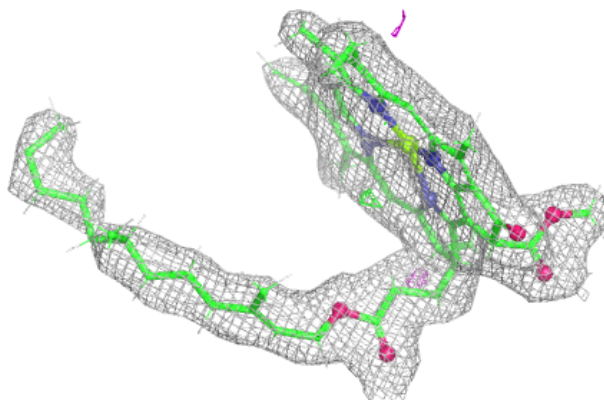


Electron density around CLA B 605:

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

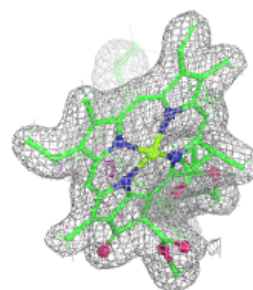
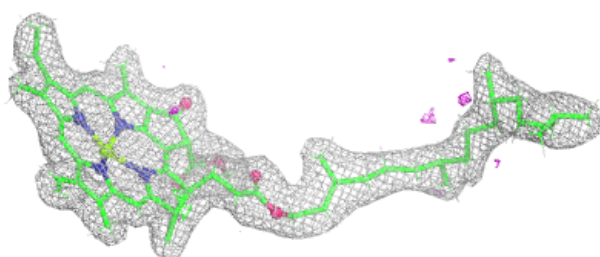
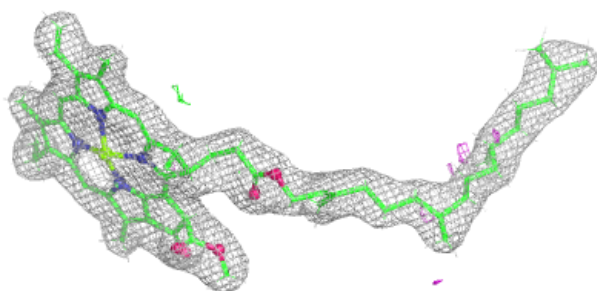
**Electron density around CLA C 505:**

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

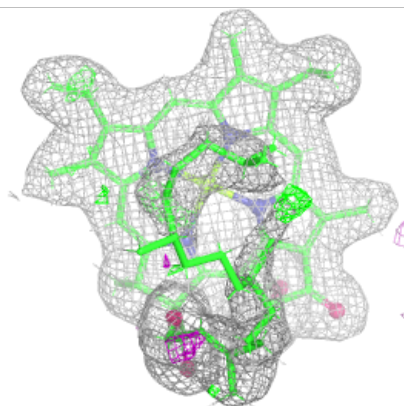
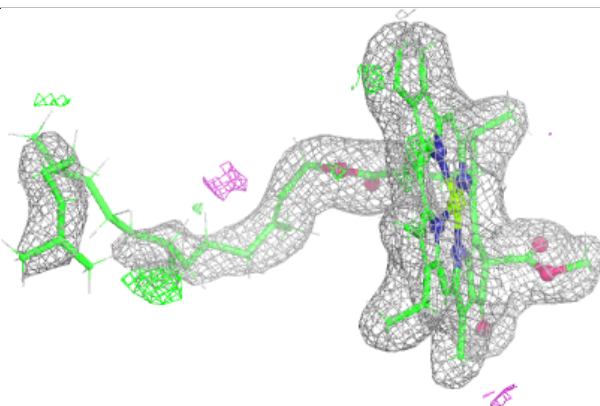
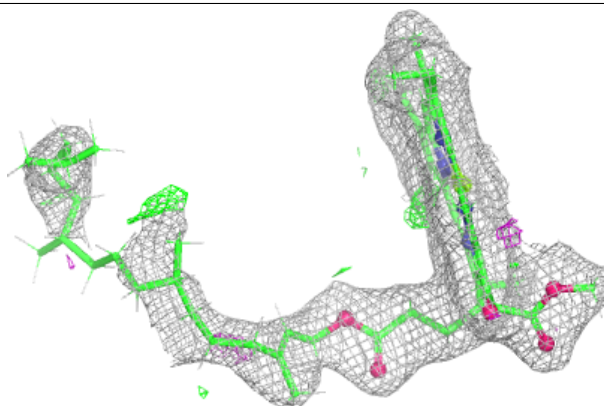


Electron density around CLA A 402:

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

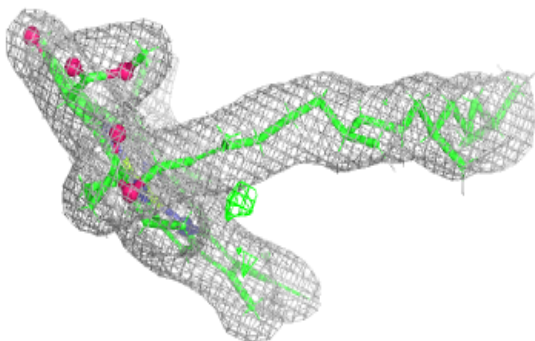
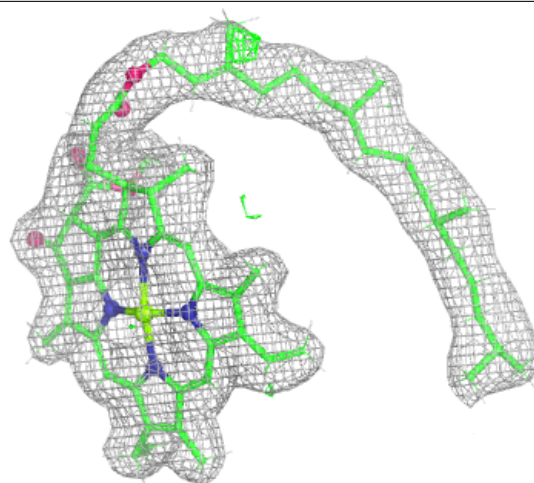
**Electron density around CLA C 507:**

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



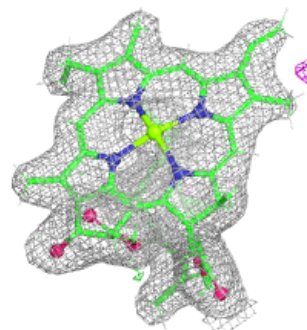
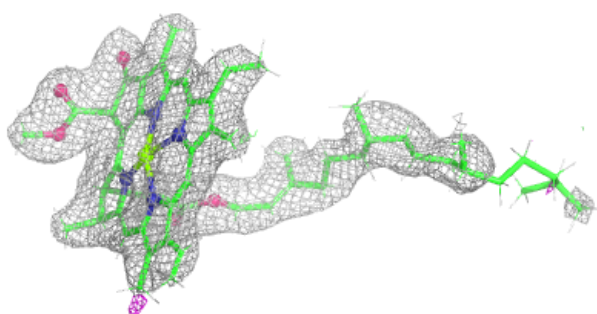
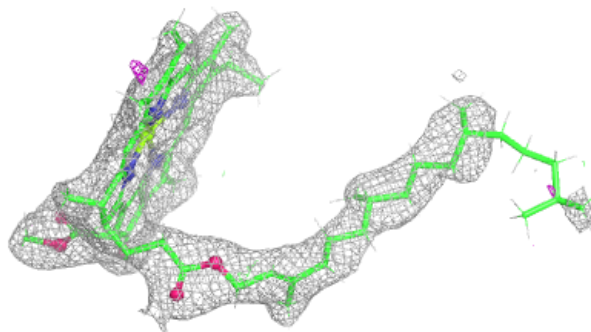
Electron density around CLA C 508:

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

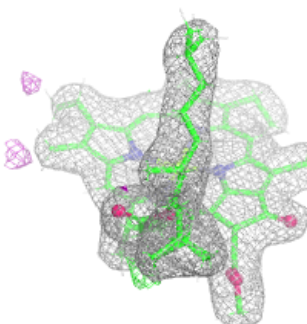
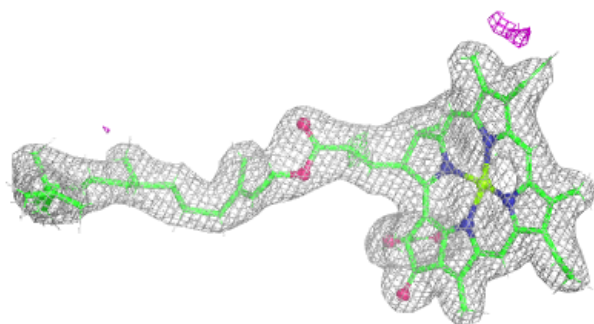
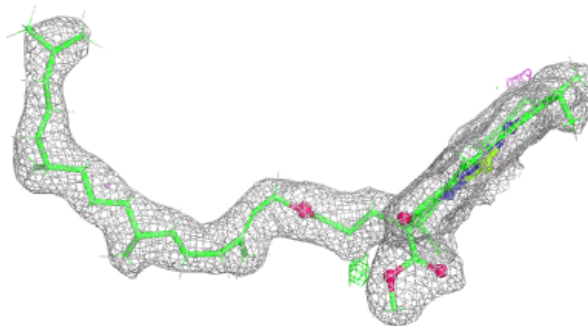


Electron density around CLA C 509:

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

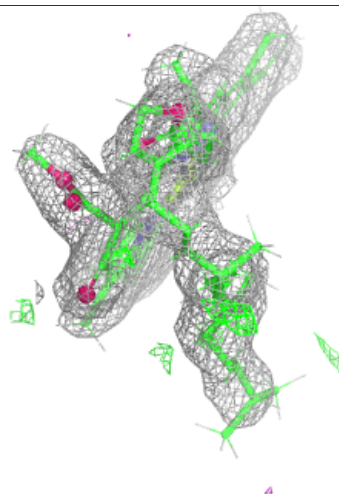
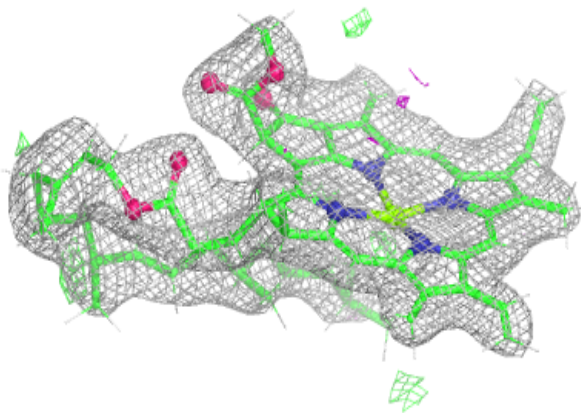
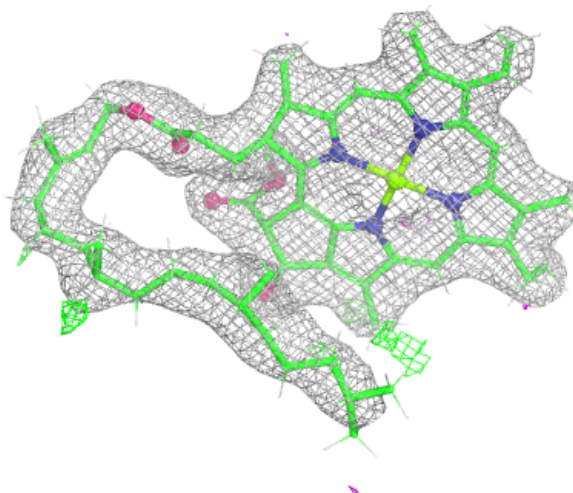
**Electron density around CLA d 402:**

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



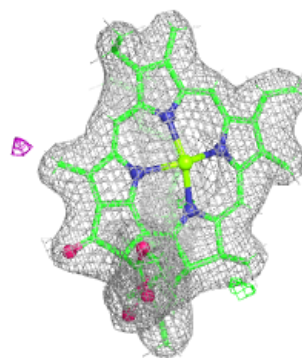
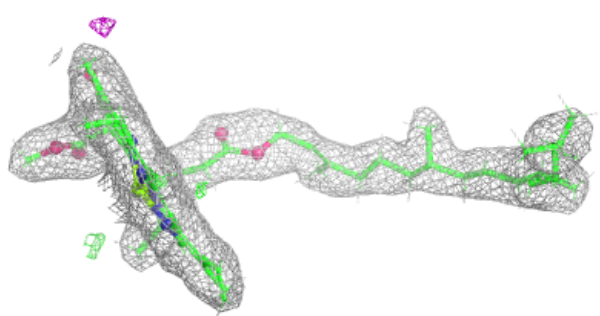
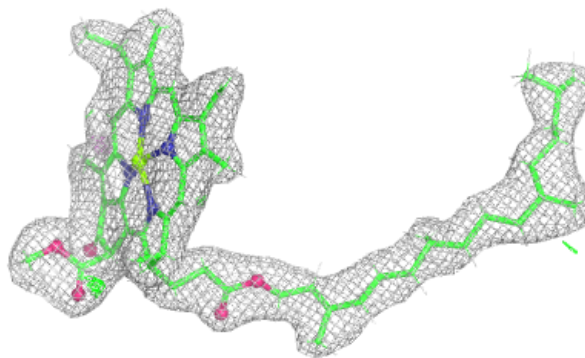
Electron density around CLA C 510:

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



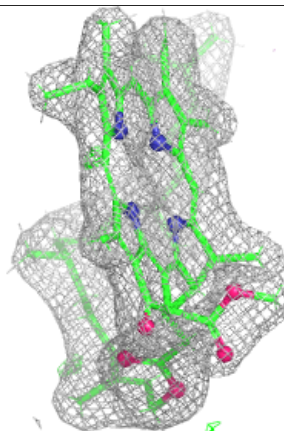
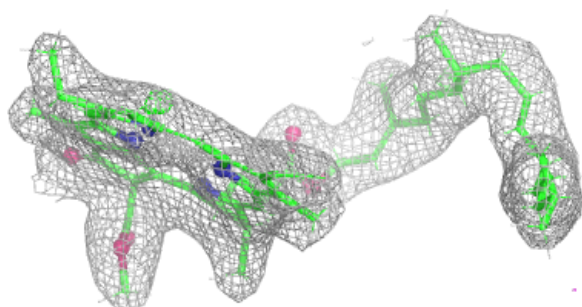
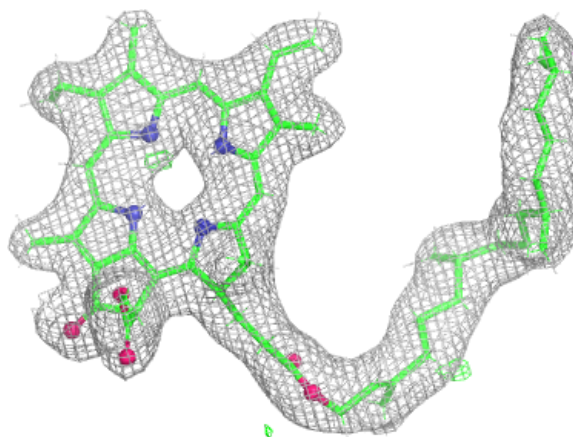
Electron density around CLA B 610:

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



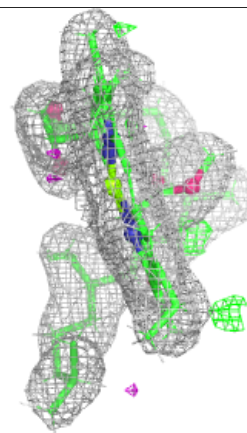
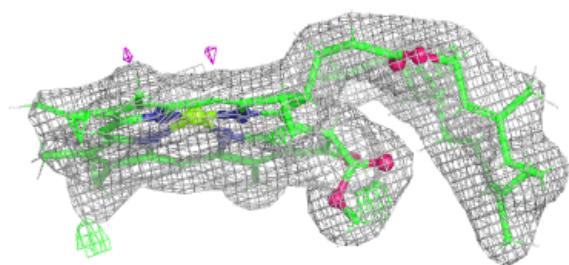
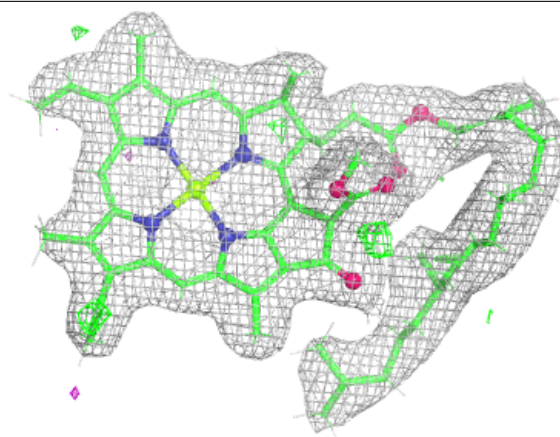
Electron density around PHO D 401:

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



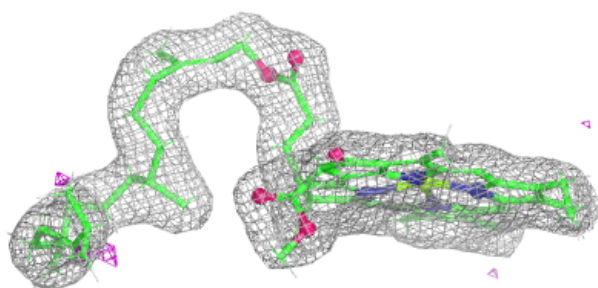
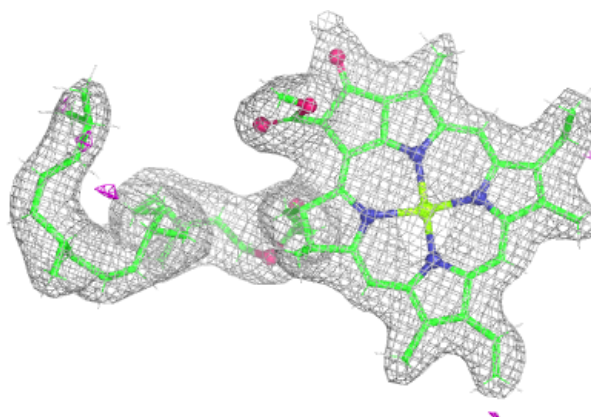
Electron density around CLA B 611:

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

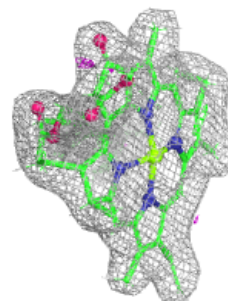
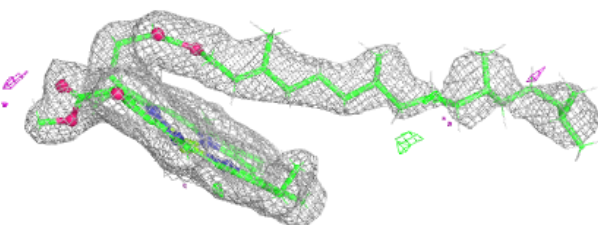
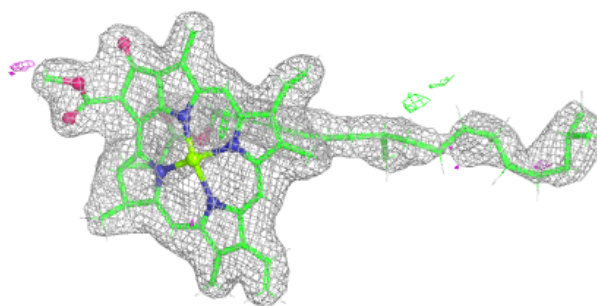


Electron density around CLA B 613:

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

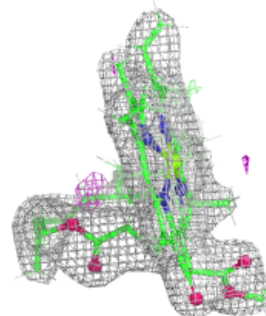
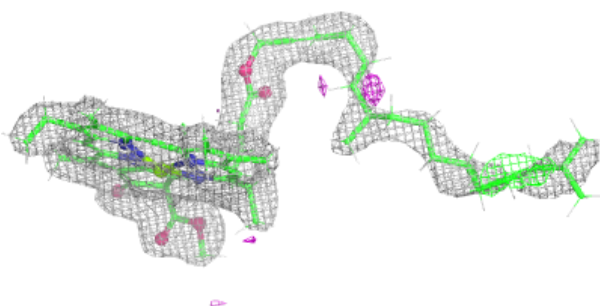
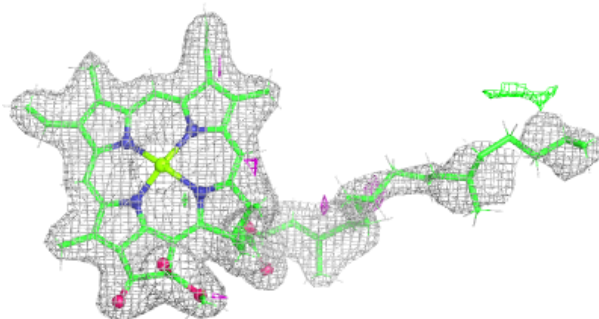
**Electron density around CLA B 615:**

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

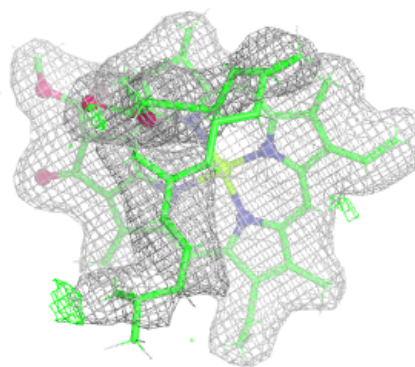
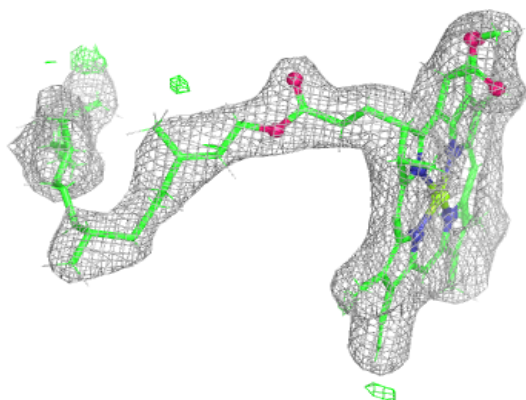
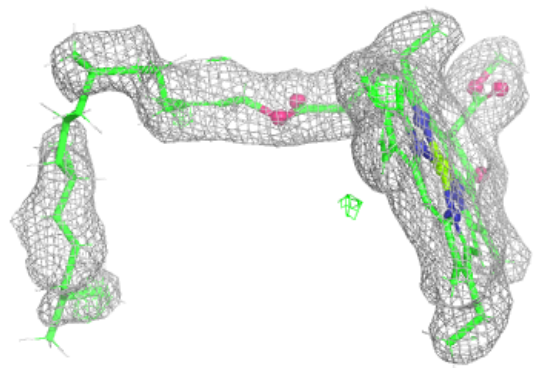


Electron density around CLA a 403:

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

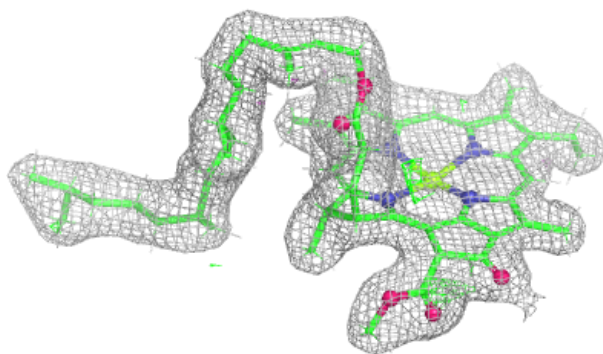
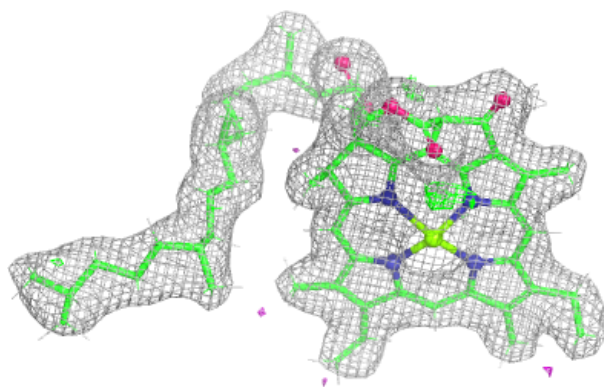
**Electron density around CLA a 405:**

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

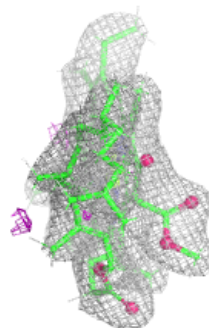
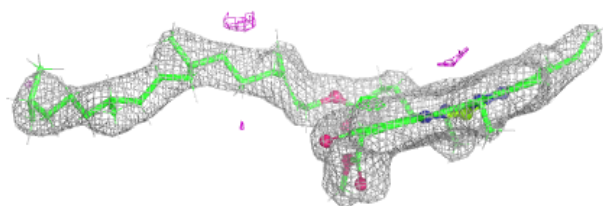
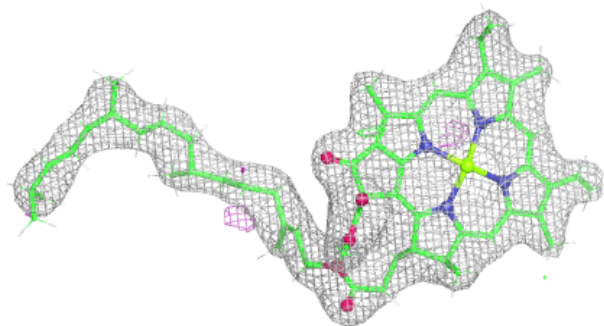


Electron density around CLA a 411:

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

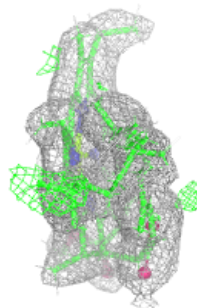
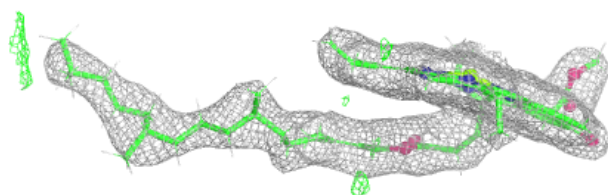
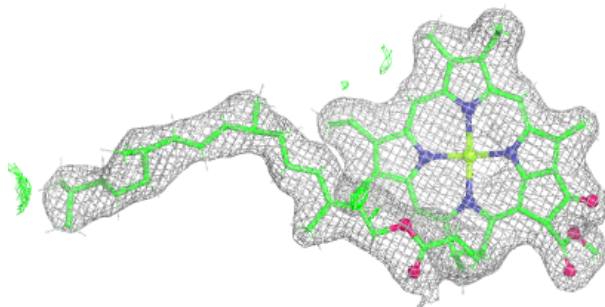
**Electron density around CLA b 601:**

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

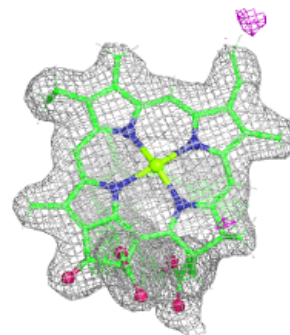
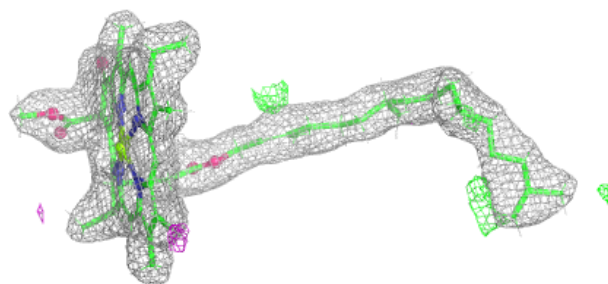
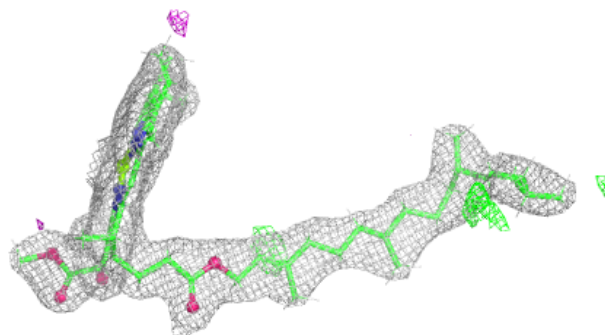


Electron density around CLA b 602:

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

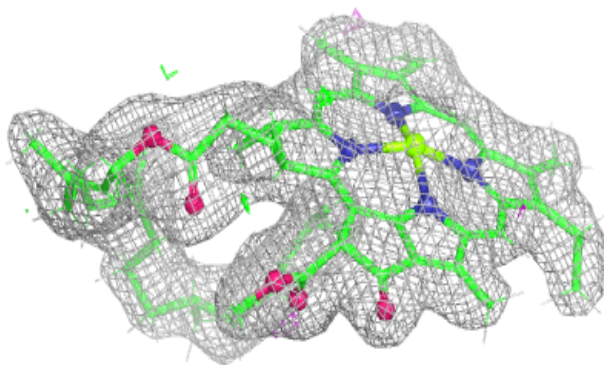
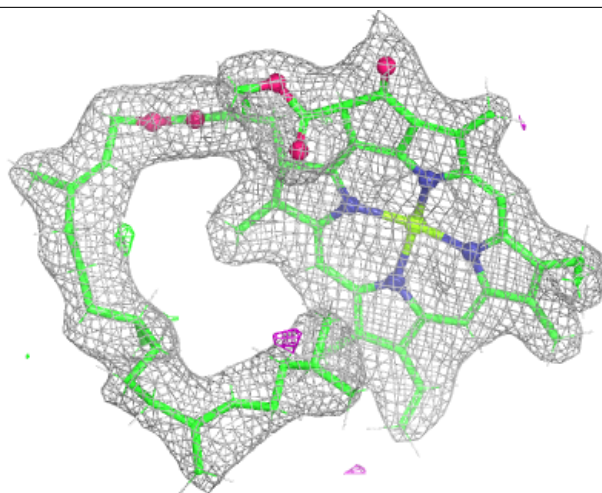
**Electron density around CLA b 604:**

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



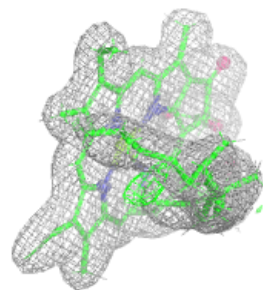
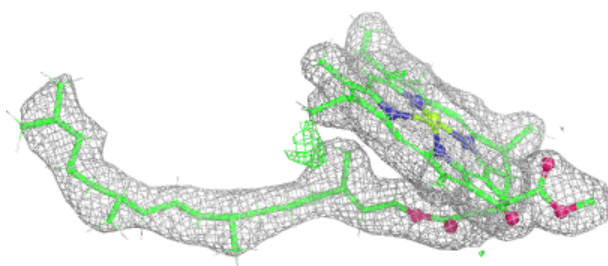
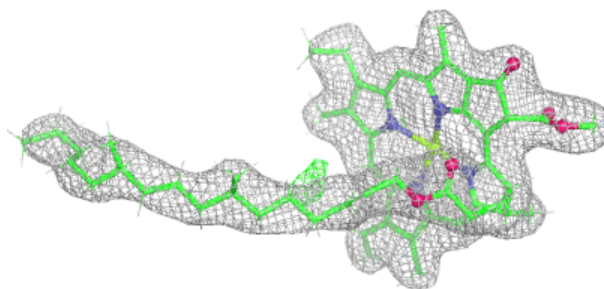
Electron density around CLA B 616:

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



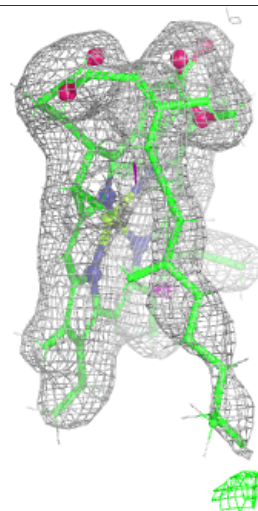
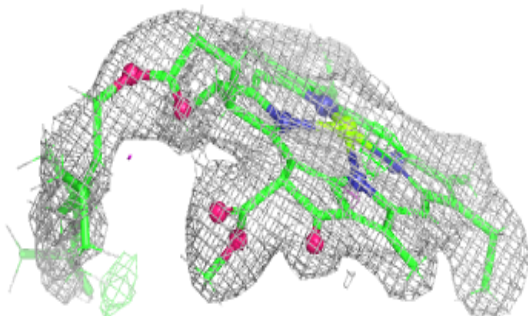
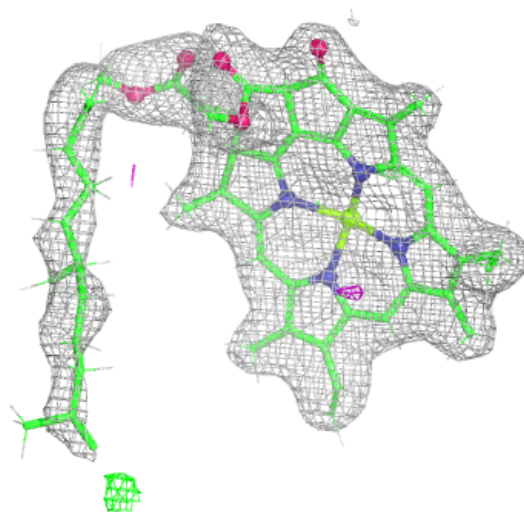
Electron density around CLA b 607:

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



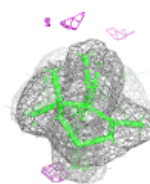
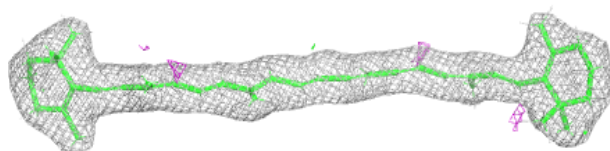
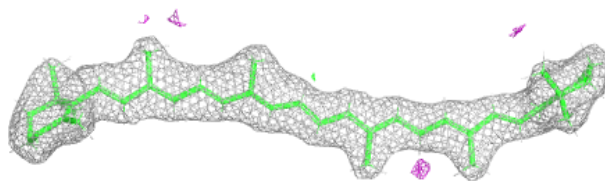
Electron density around CLA B 617:

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

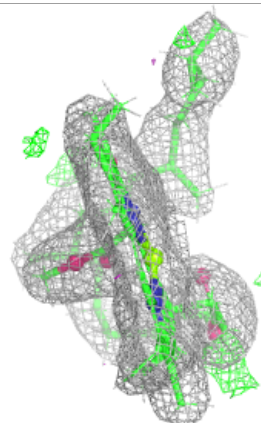
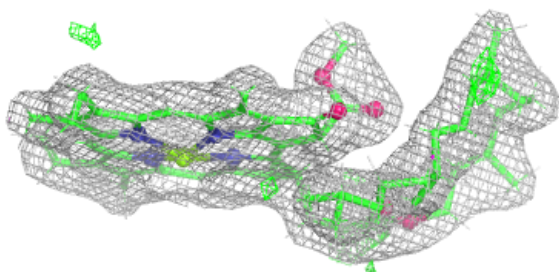
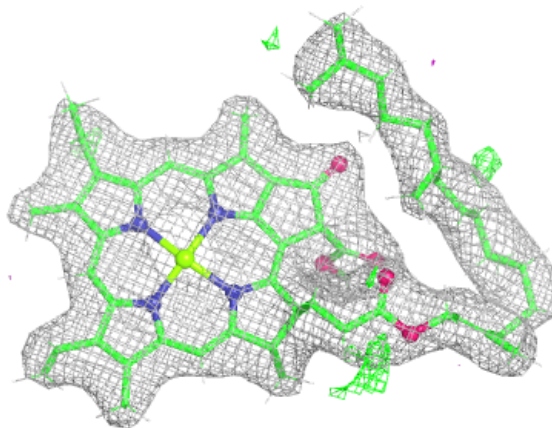


Electron density around BCR a 406:

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

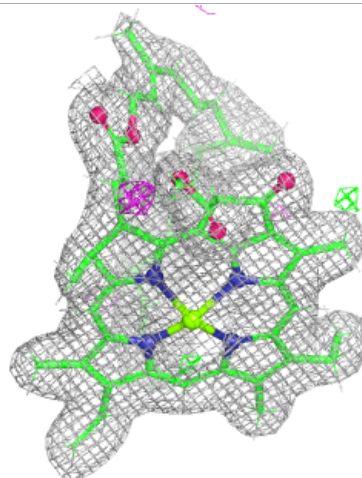
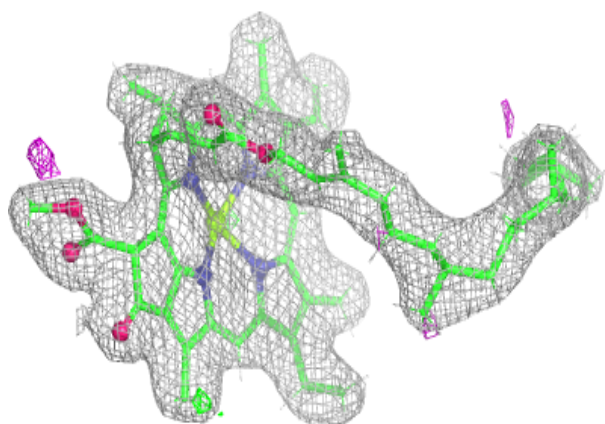
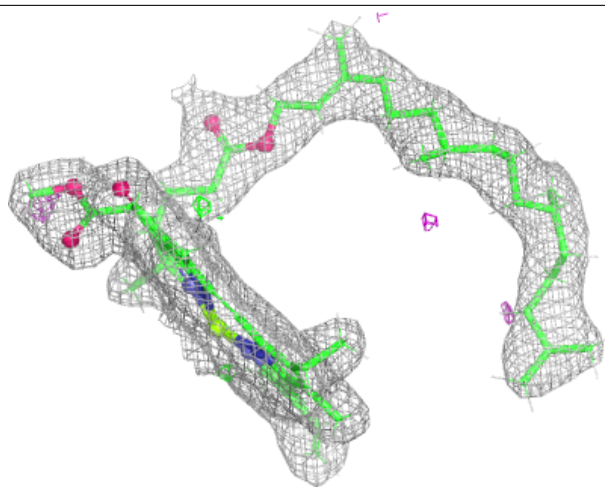
**Electron density around CLA b 609:**

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



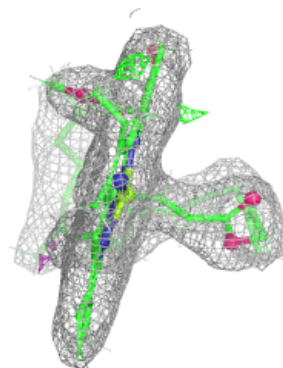
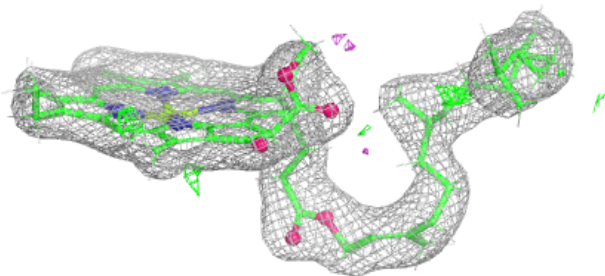
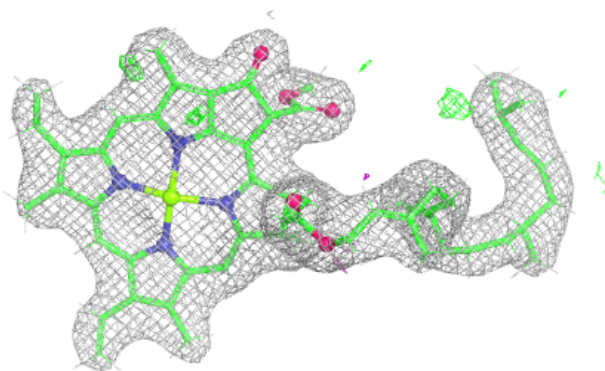
Electron density around CLA b 610:

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

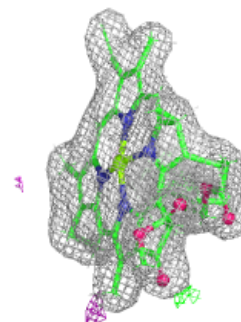
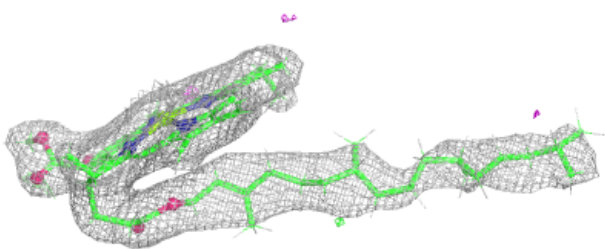
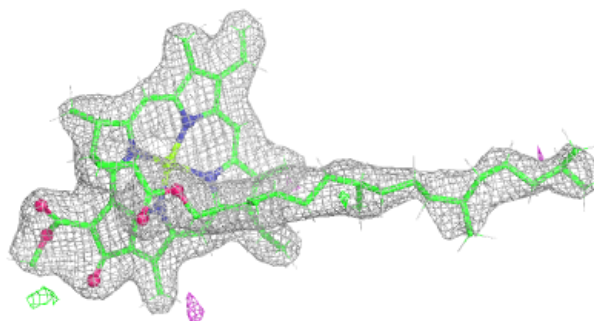


Electron density around CLA b 611:

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

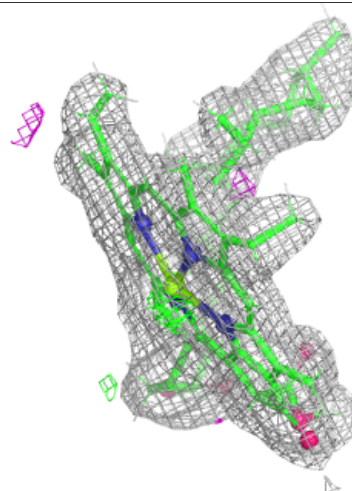
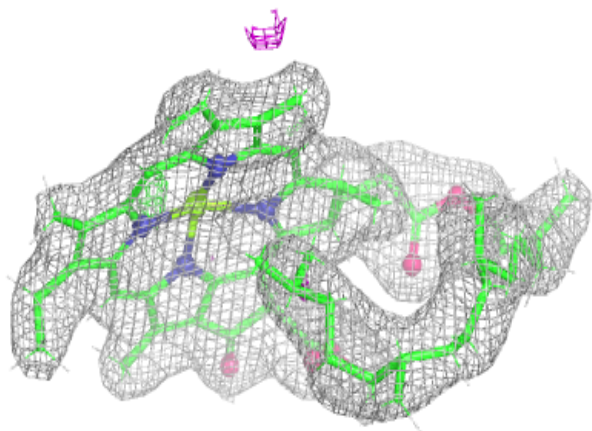
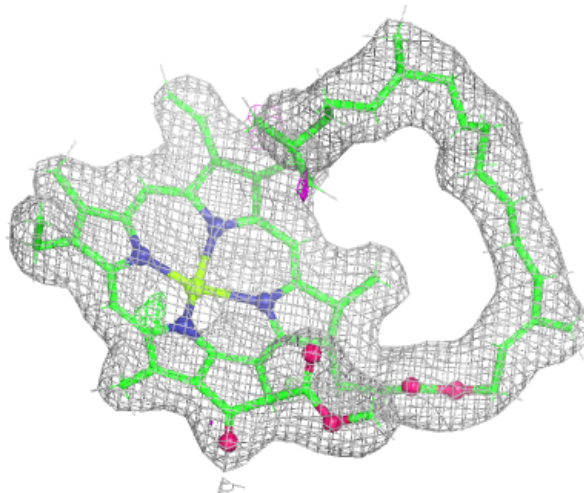
**Electron density around CLA b 613:**

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



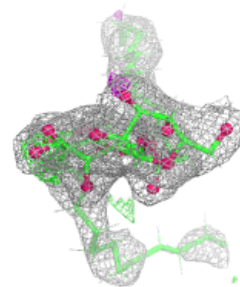
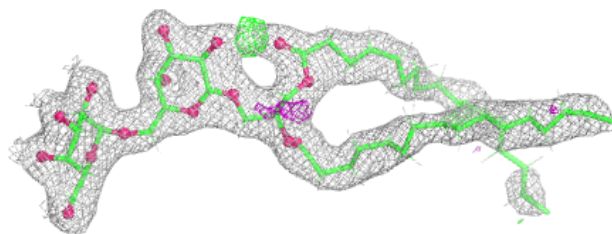
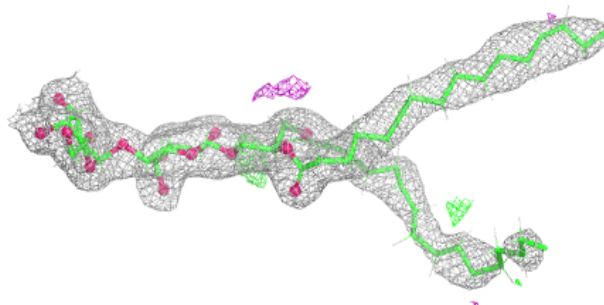
Electron density around CLA b 614:

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

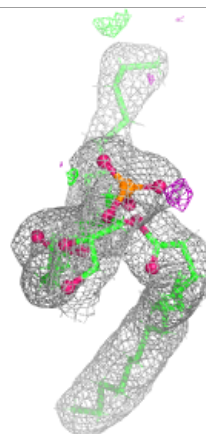
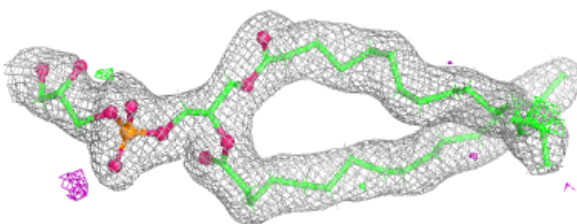
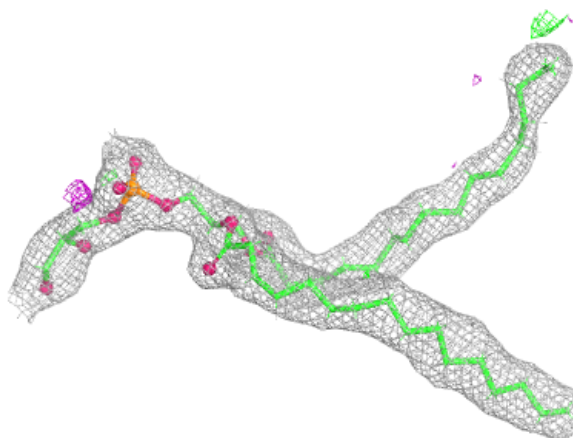


Electron density around DGD c 519:

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

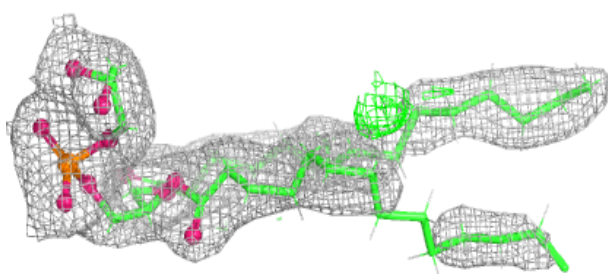
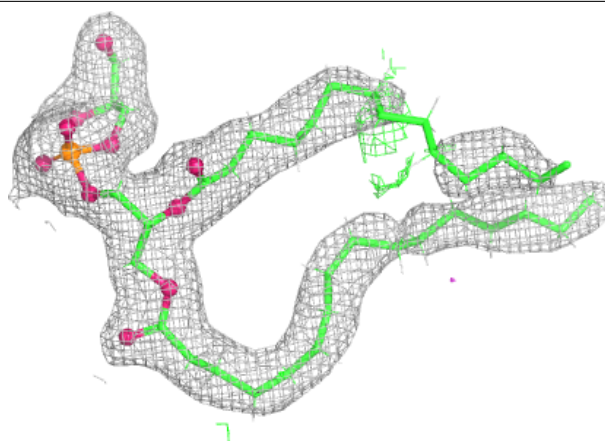
**Electron density around LHG D 408:**

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

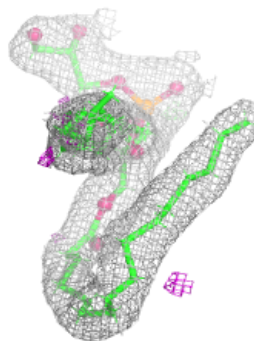
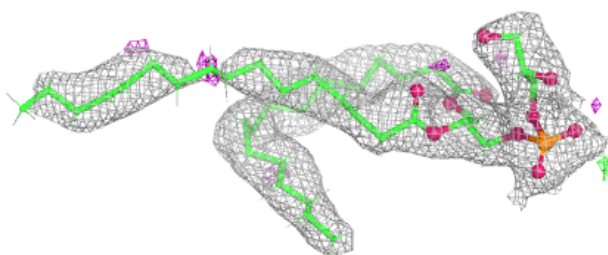
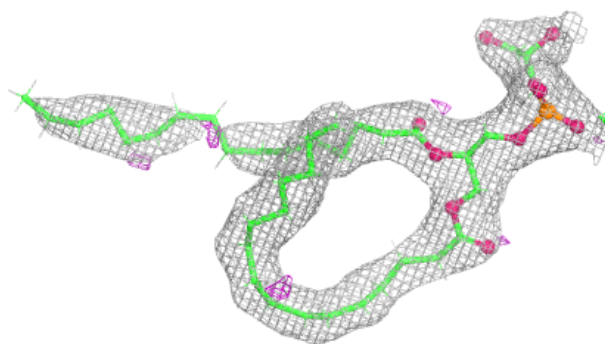


Electron density around LHG D 409:

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

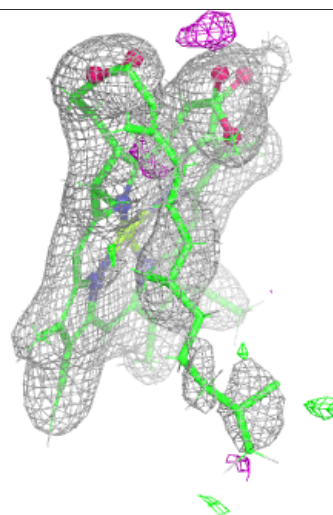
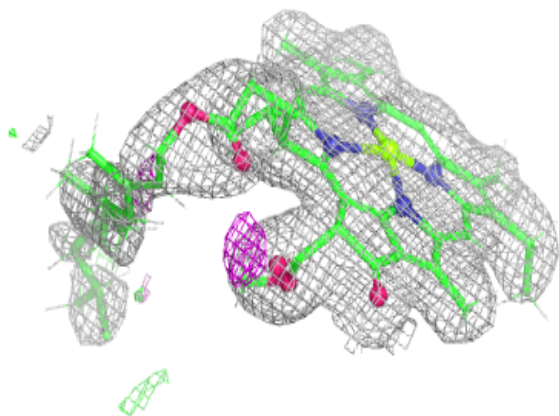
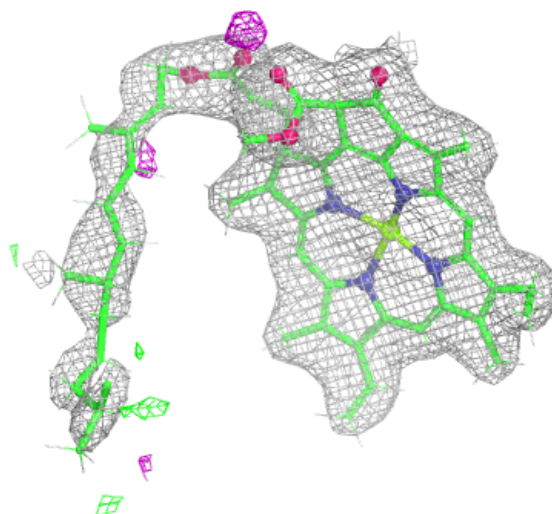
**Electron density around LHG D 412:**

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



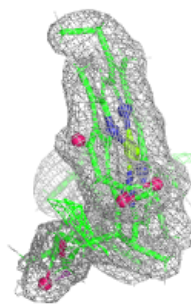
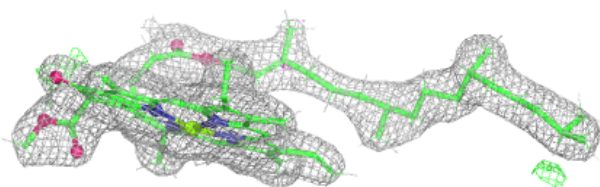
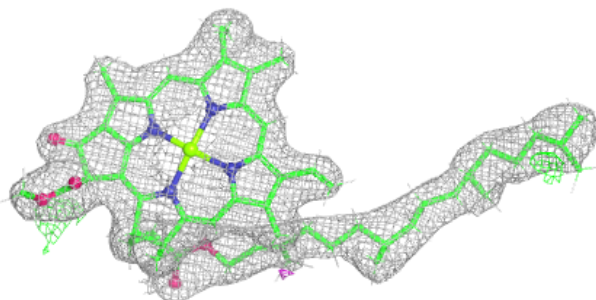
Electron density around CLA b 615:

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

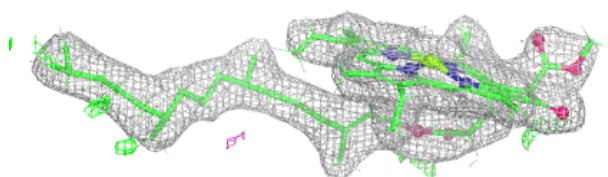
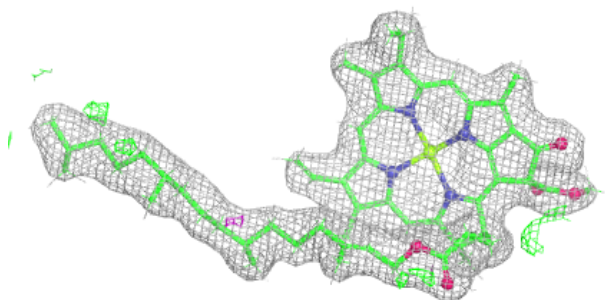


Electron density around CLA c 503:

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

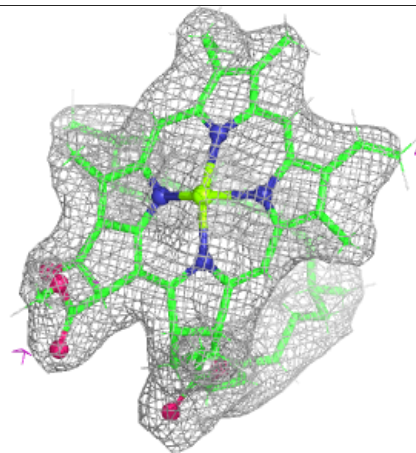
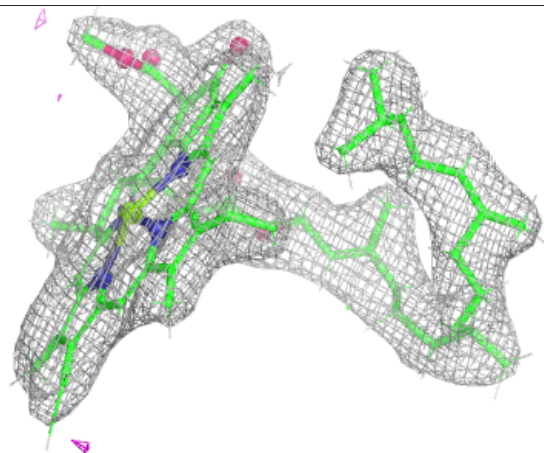
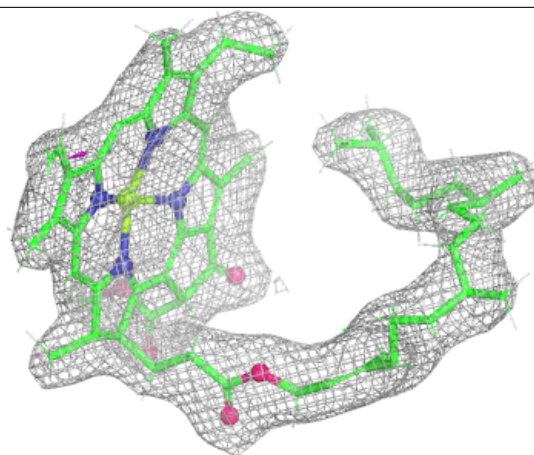
**Electron density around CLA C 502:**

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

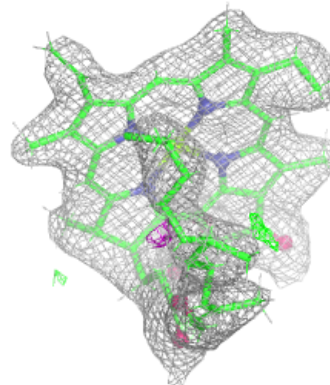
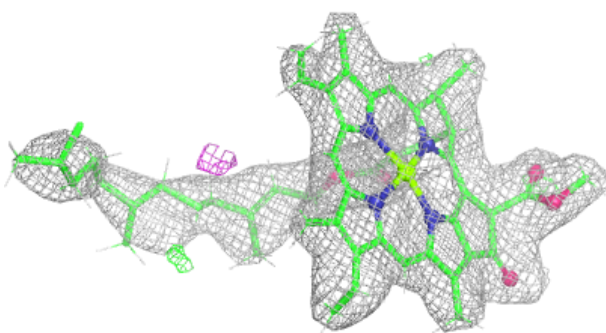
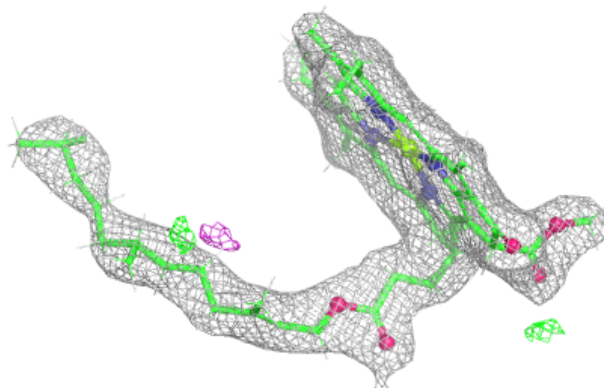


Electron density around CLA c 505:

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

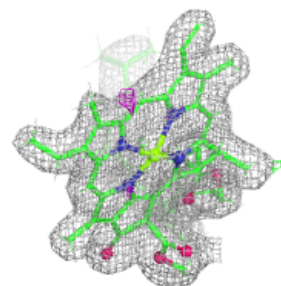
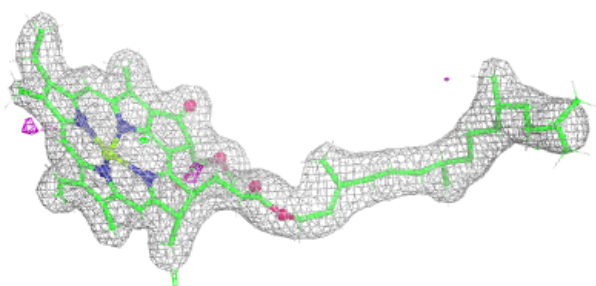
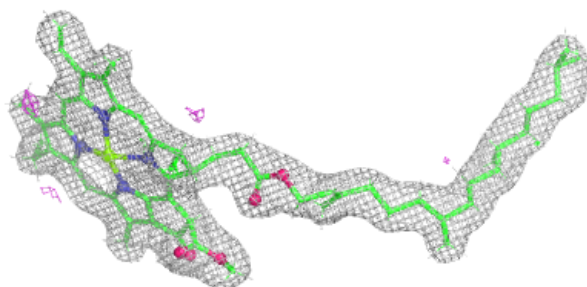
**Electron density around CLA c 506:**

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

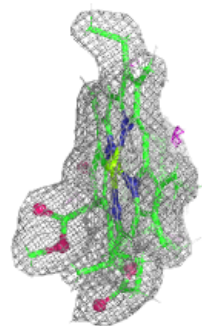
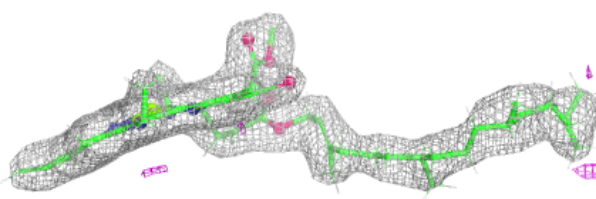
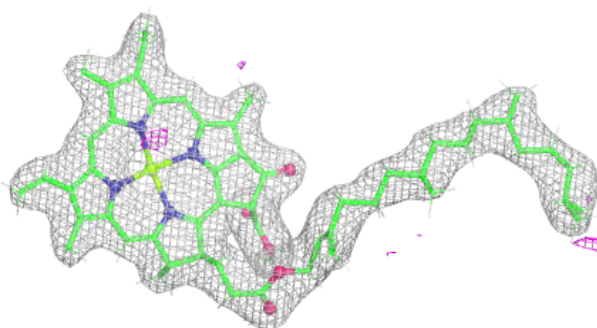


Electron density around CLA a 402:

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

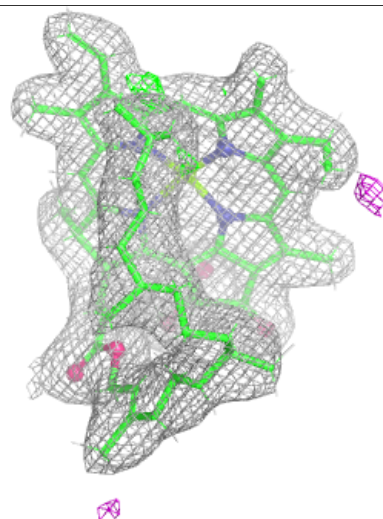
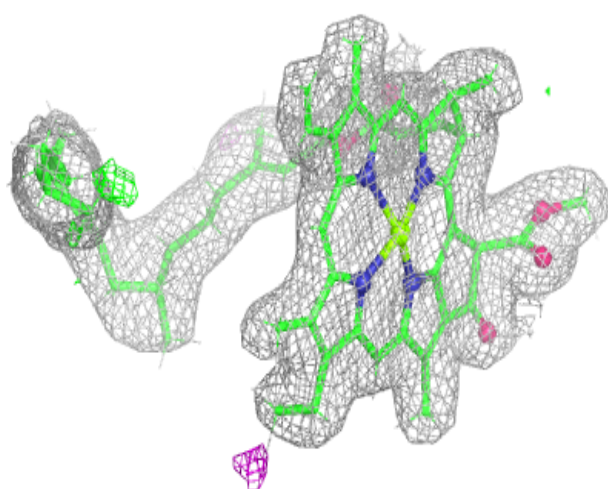
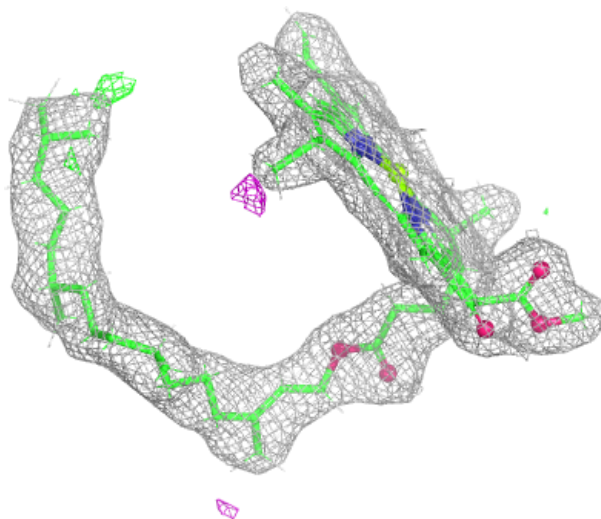
**Electron density around CLA B 603:**

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



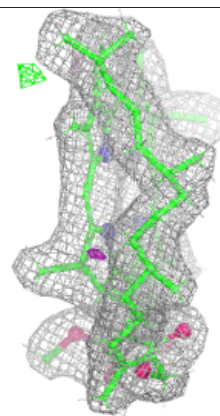
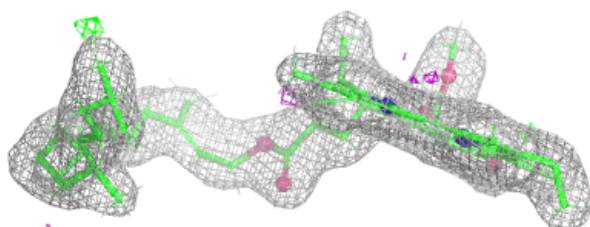
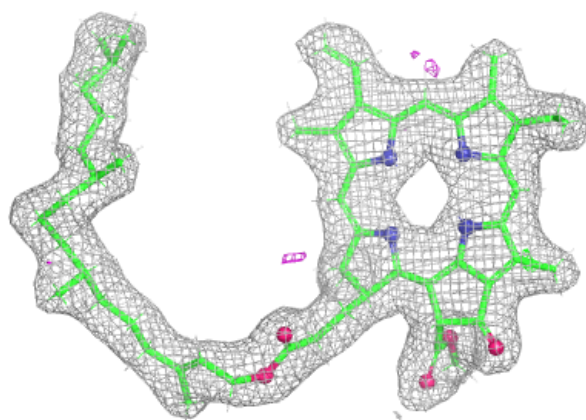
Electron density around CLA B 612:

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

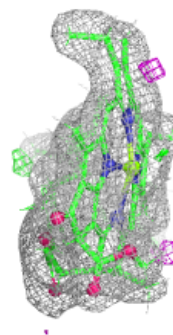
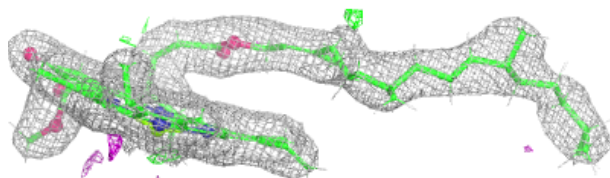
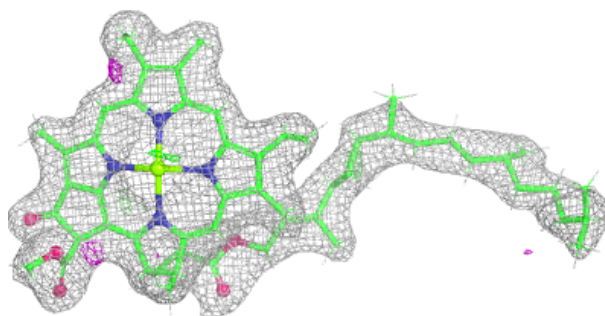


Electron density around PHO A 404:

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

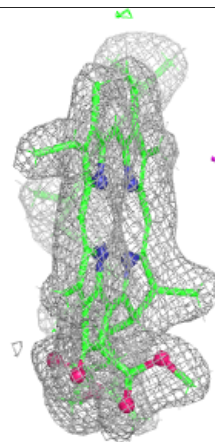
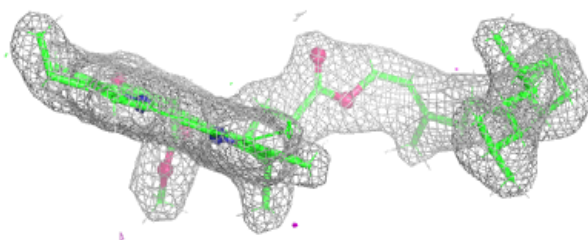
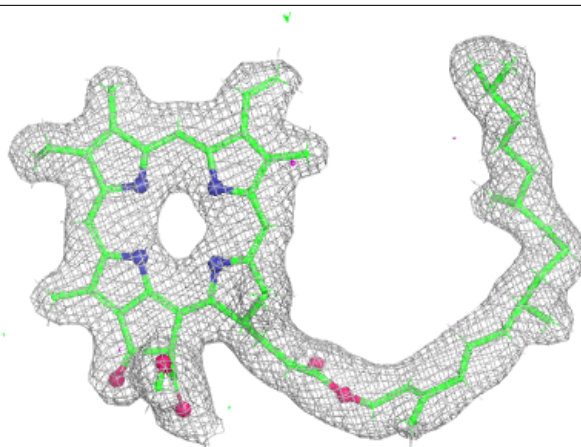
**Electron density around CLA B 604:**

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



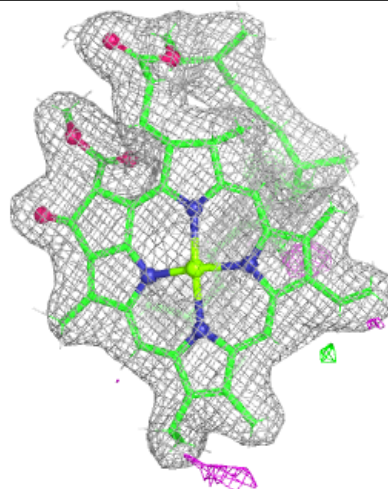
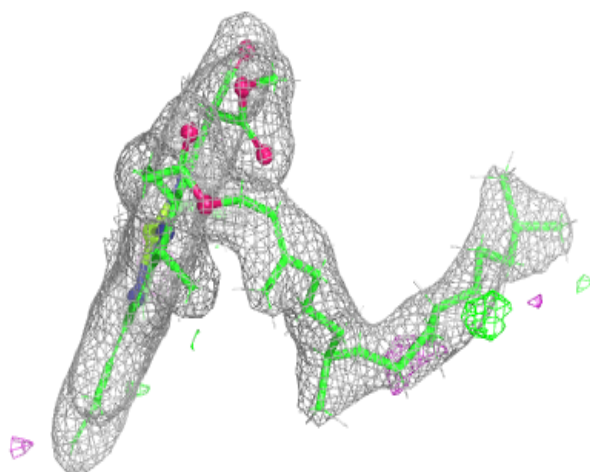
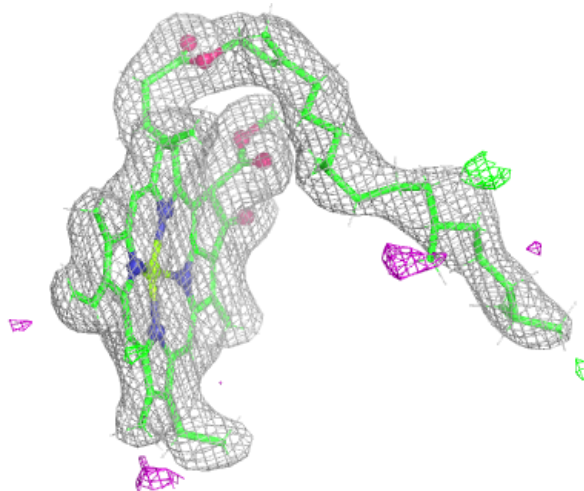
Electron density around PHO a 404:

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



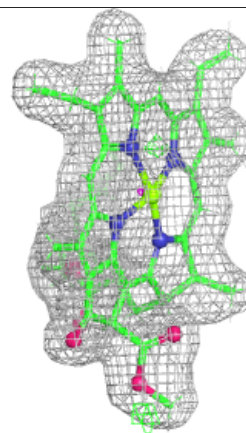
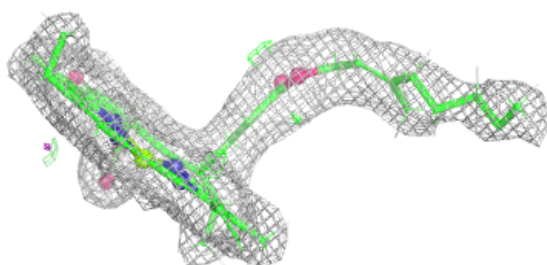
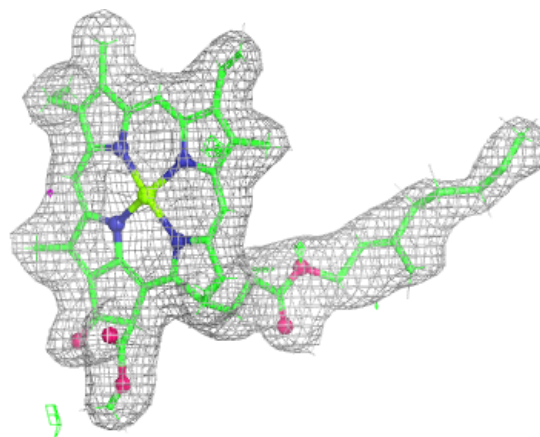
Electron density around CLA B 614:

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



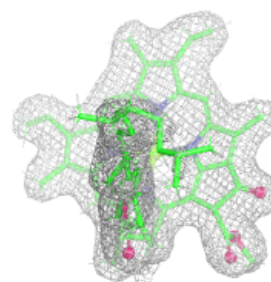
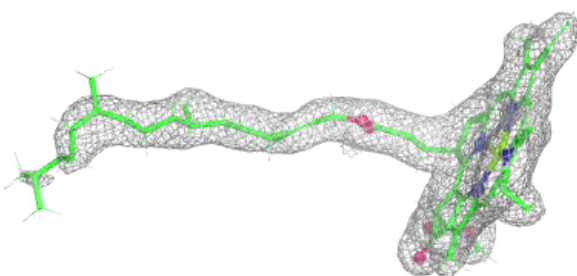
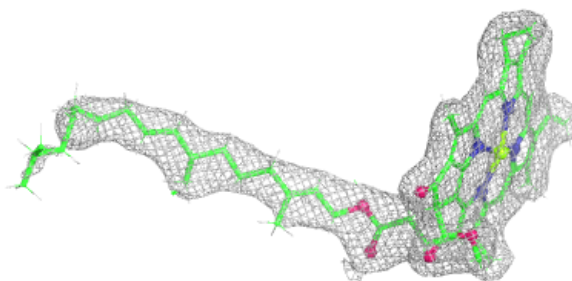
Electron density around CLA A 405:

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

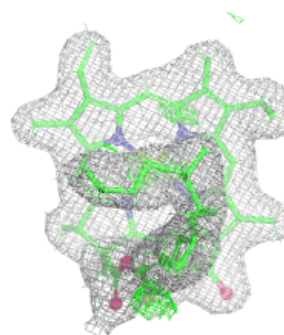
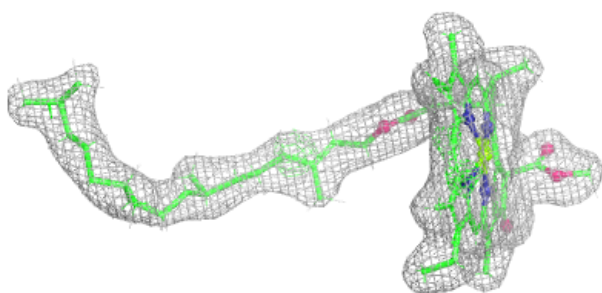
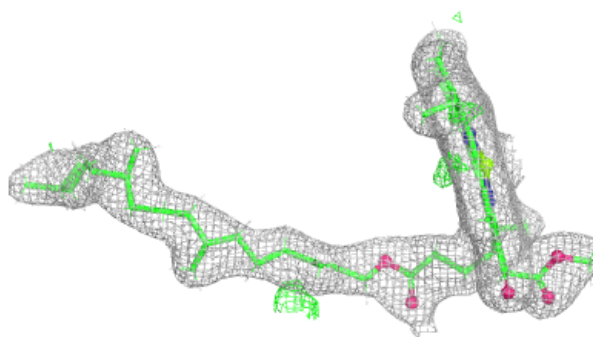


Electron density around CLA b 603:

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

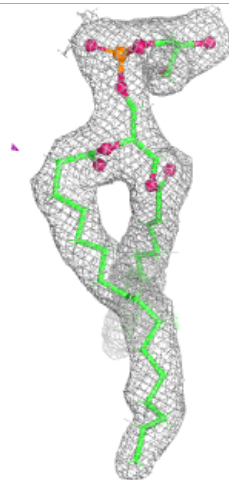
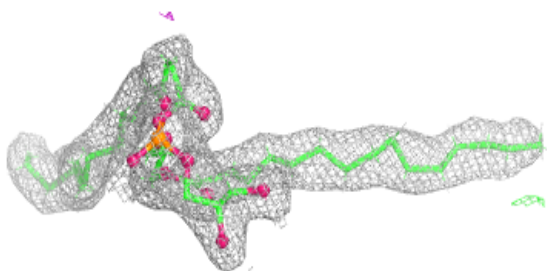
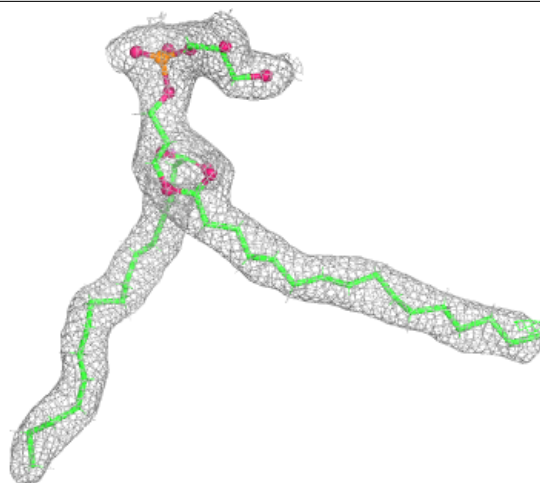
**Electron density around CLA B 606:**

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



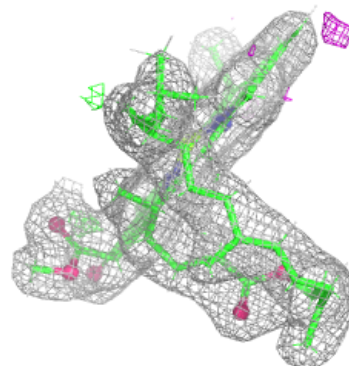
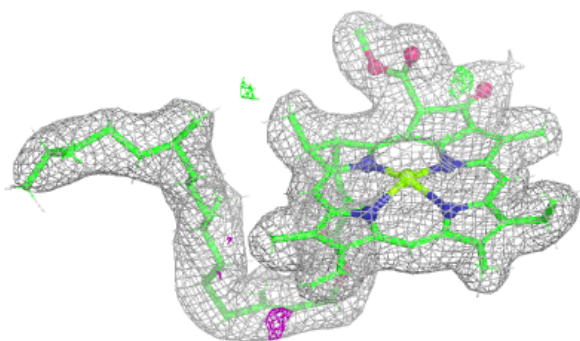
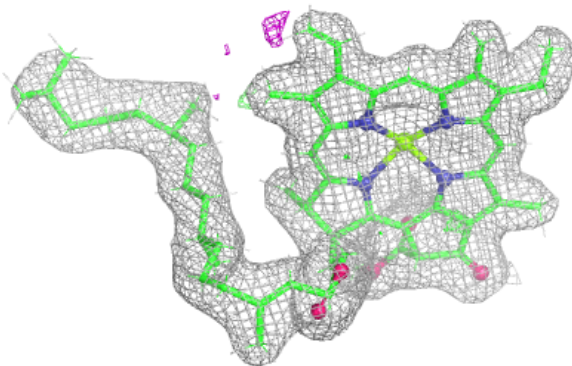
Electron density around LHG B 622:

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

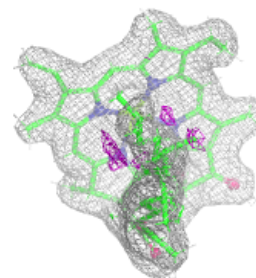
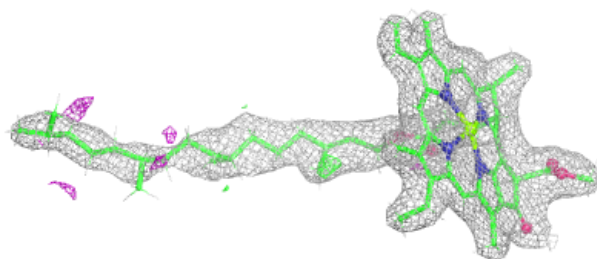
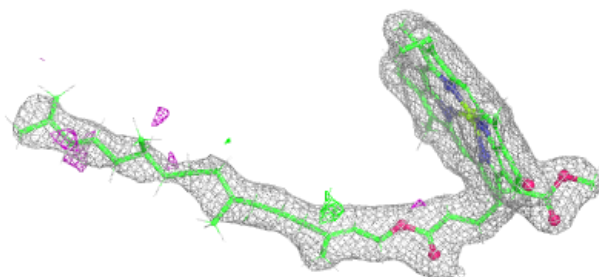


Electron density around CLA A 411:

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

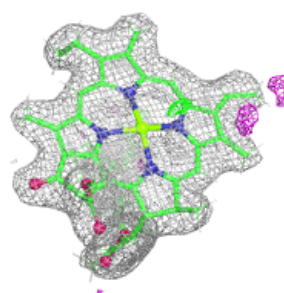
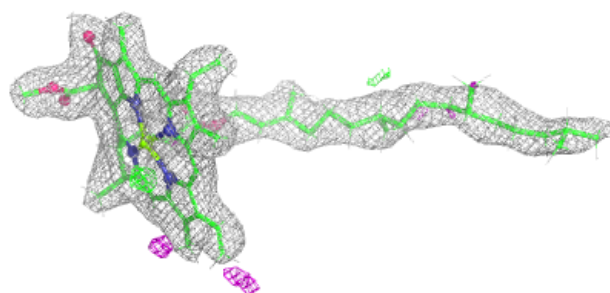
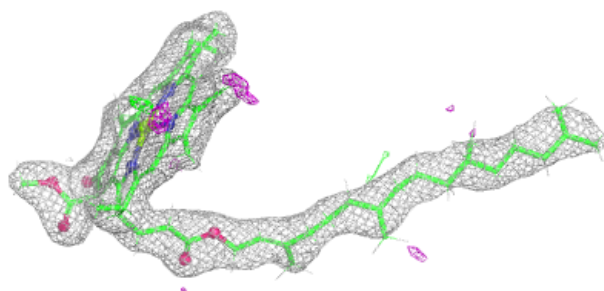
**Electron density around CLA b 606:**

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

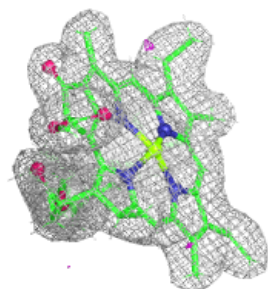
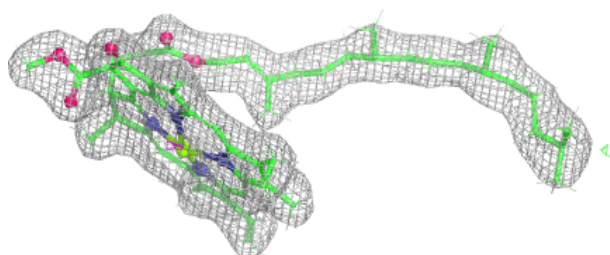
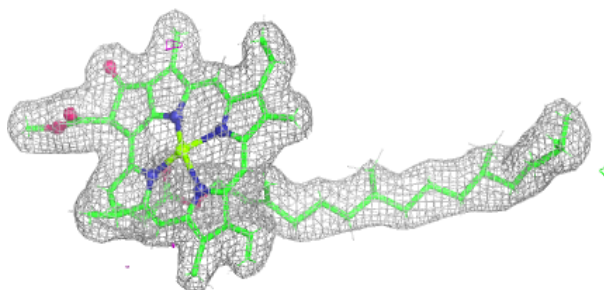


Electron density around CLA B 608:

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

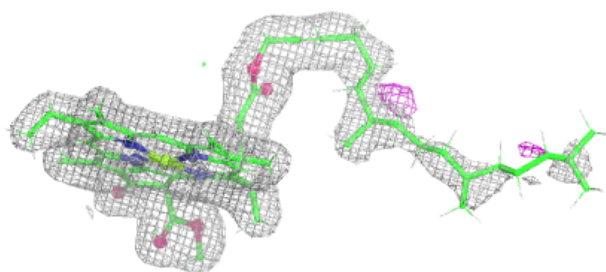
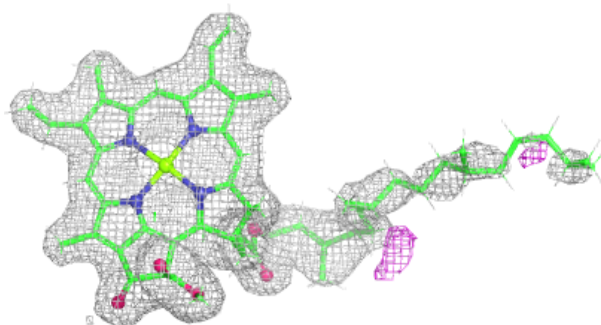
**Electron density around CLA B 609:**

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

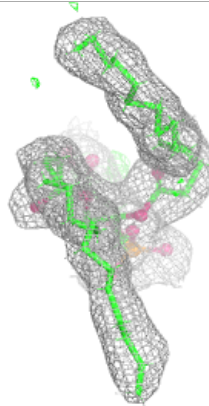
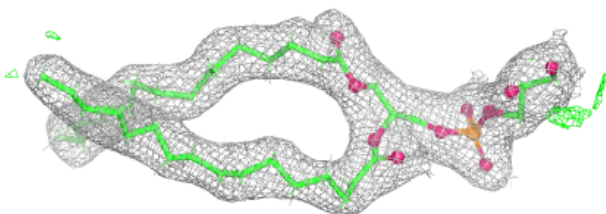
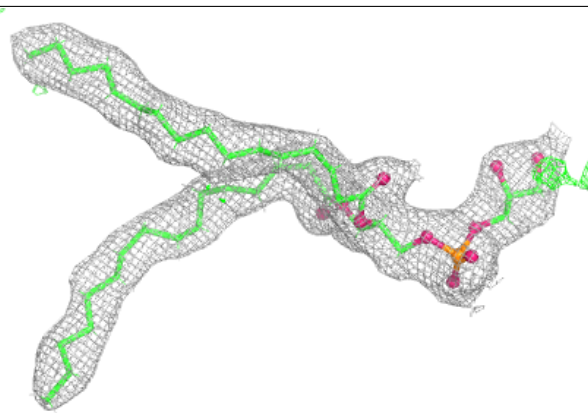


Electron density around CLA A 403:

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

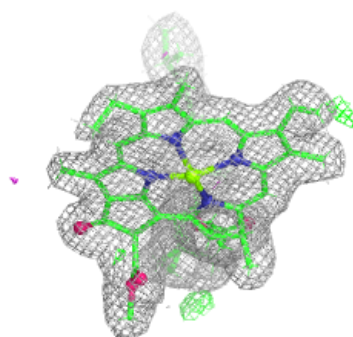
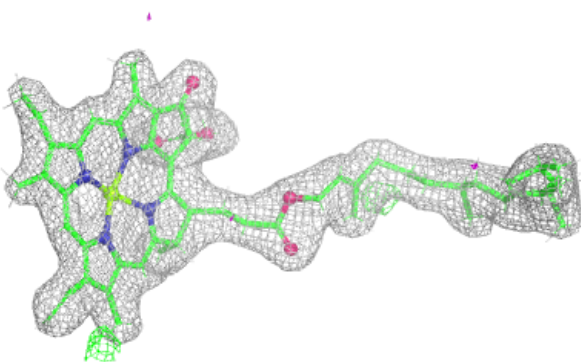
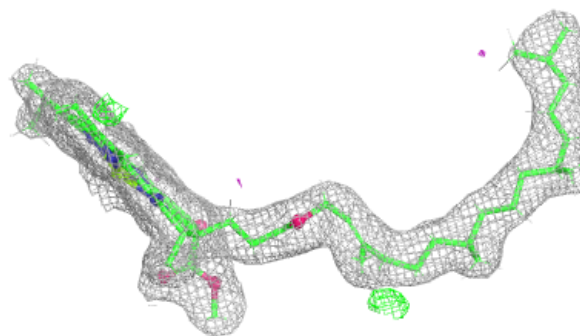
**Electron density around LHG d 407:**

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

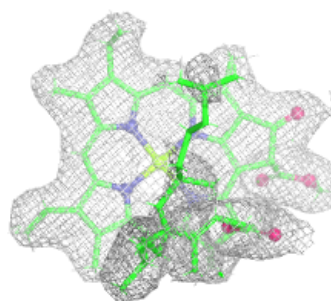
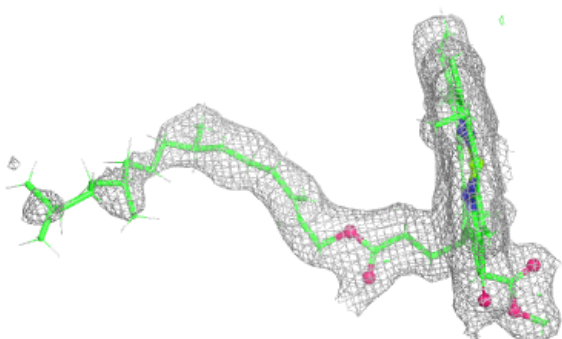
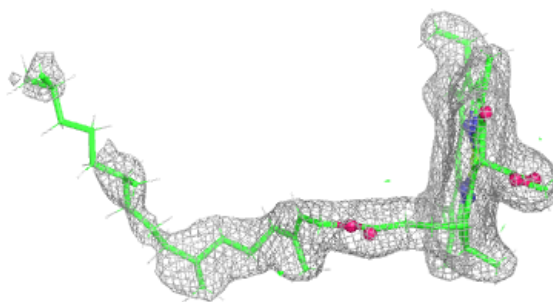


Electron density around CLA D 402:

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

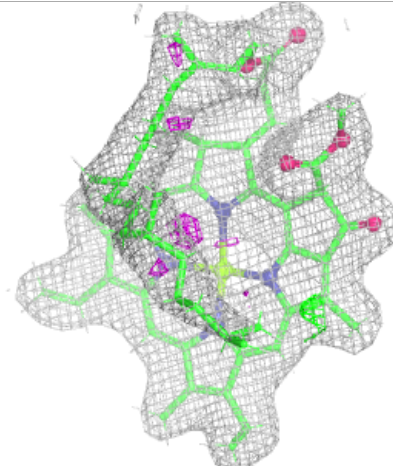
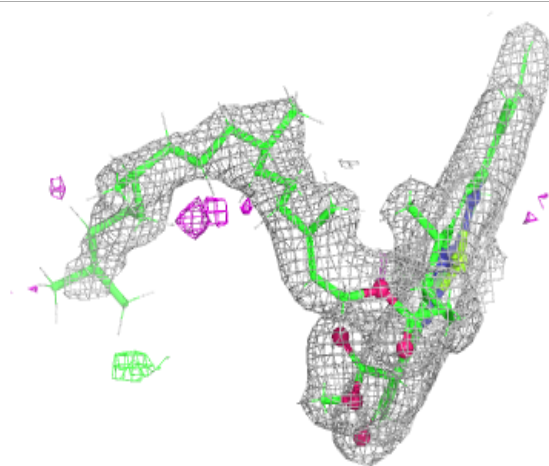
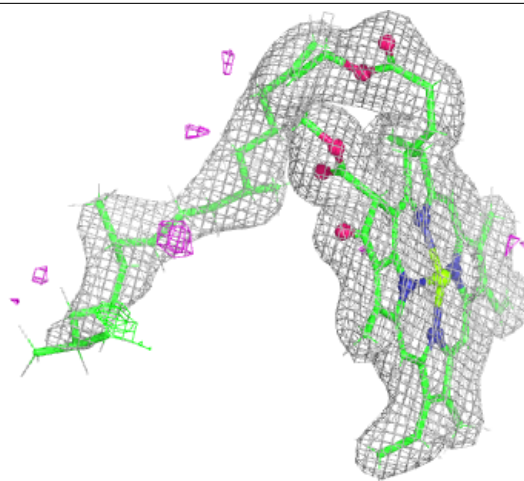
**Electron density around CLA D 403:**

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



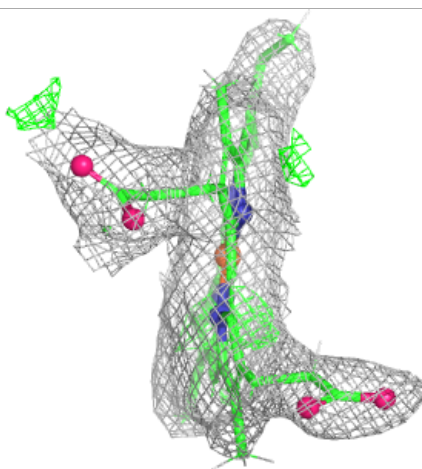
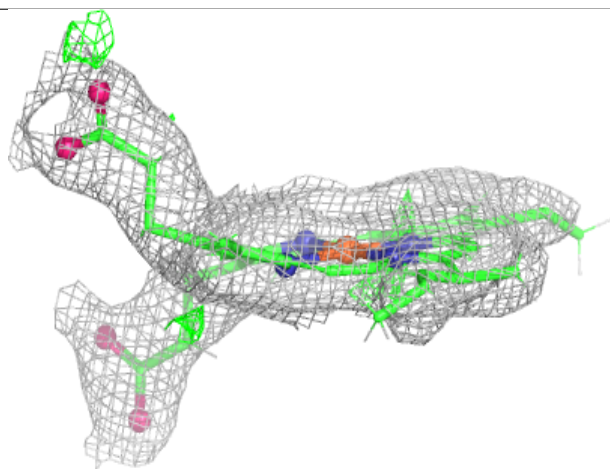
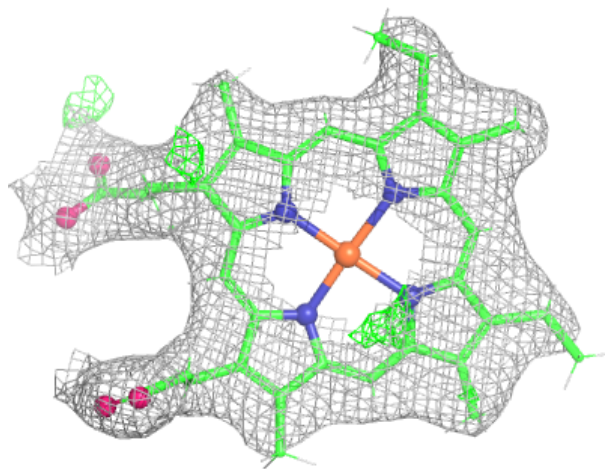
Electron density around CLA b 612:

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



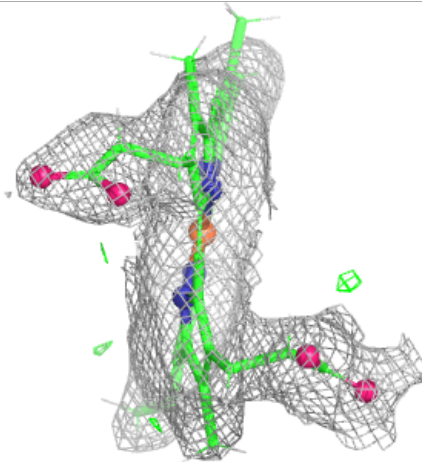
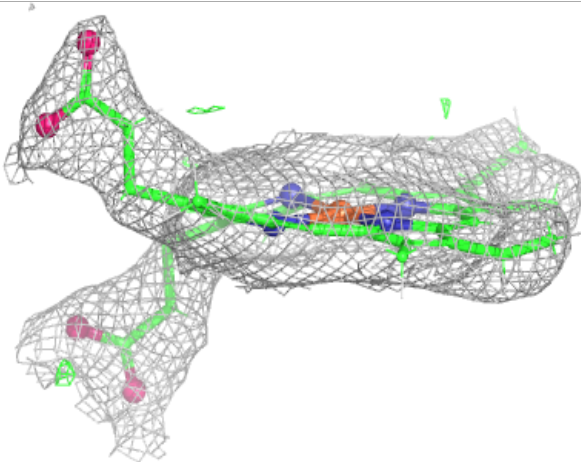
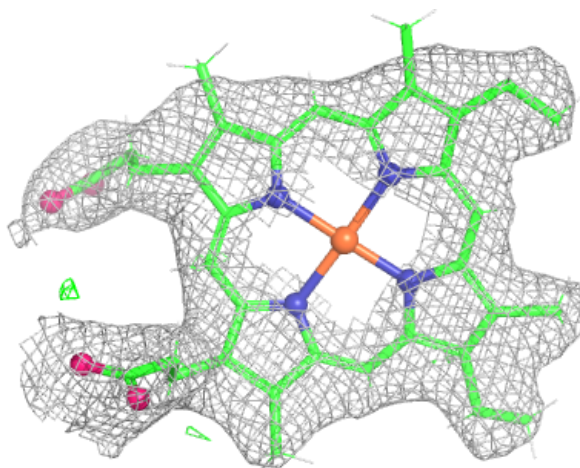
Electron density around HEC F 101:

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



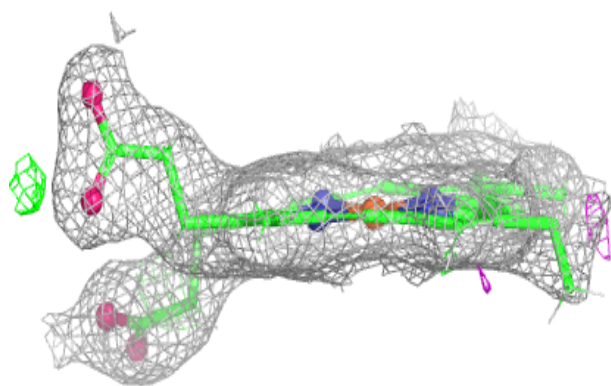
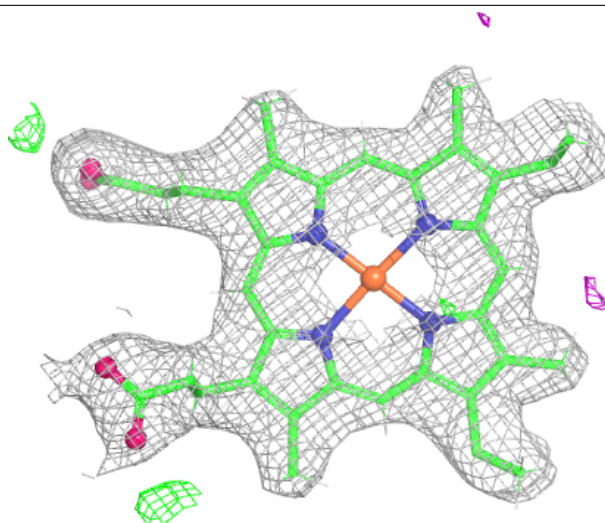
Electron density around HEC e 101:

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



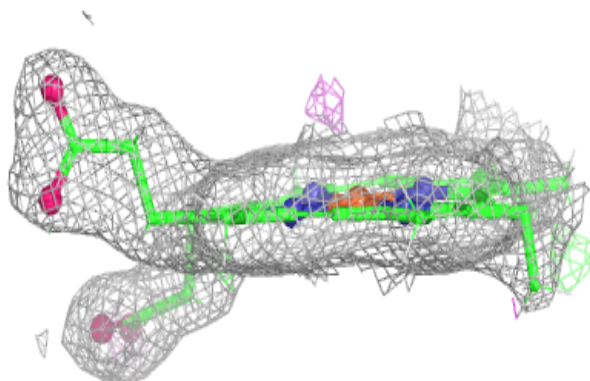
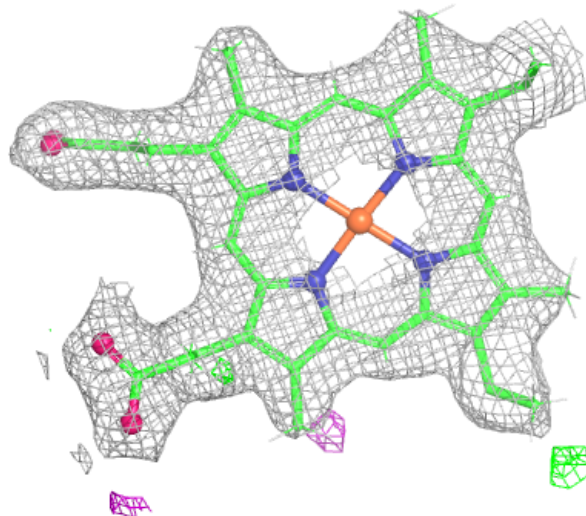
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.