



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 06:36 PM EDT

PDB ID : 7RF7 / pdb_00007rf7
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

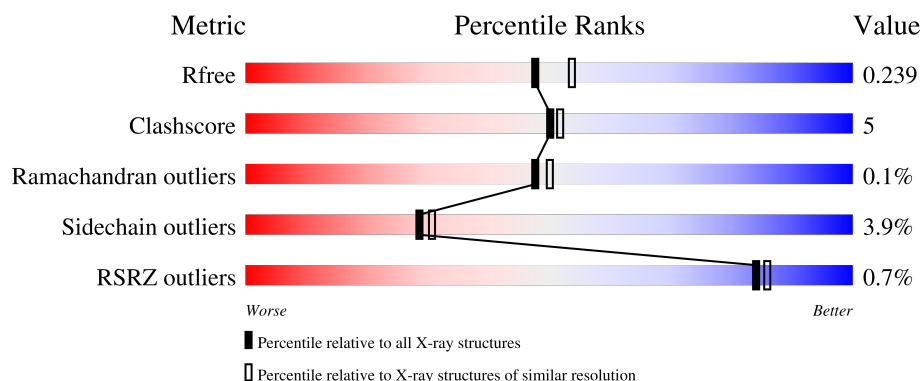
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	 88% 9% .
1	a	344	 83% 13% .

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

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

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

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

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106082 atoms, of which 52760 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

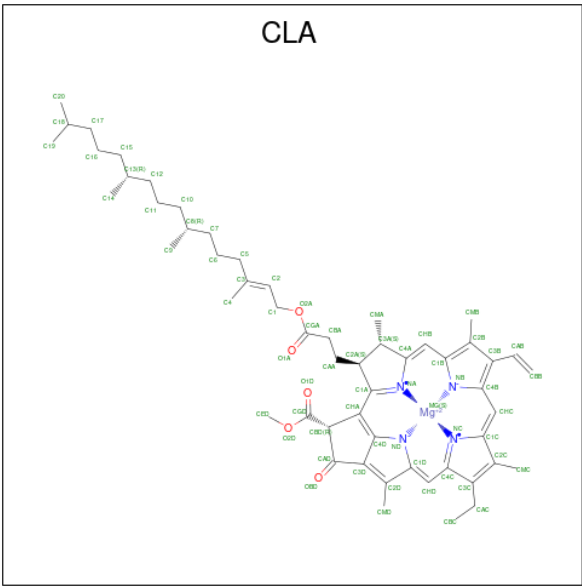
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- 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: C₅₅H₇₂MgN₄O₅).



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
			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		

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



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

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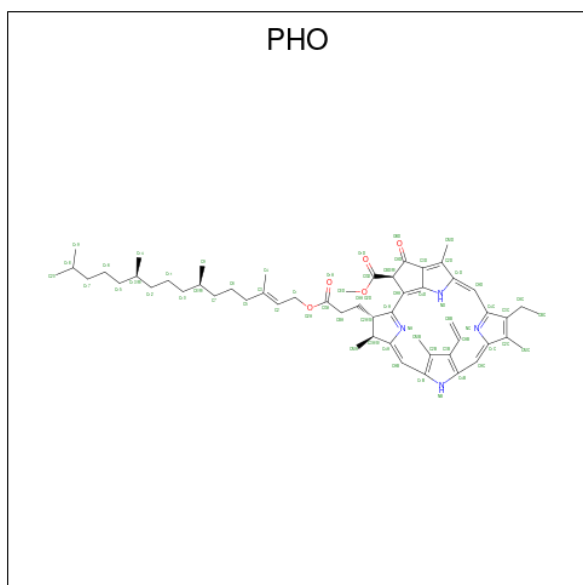
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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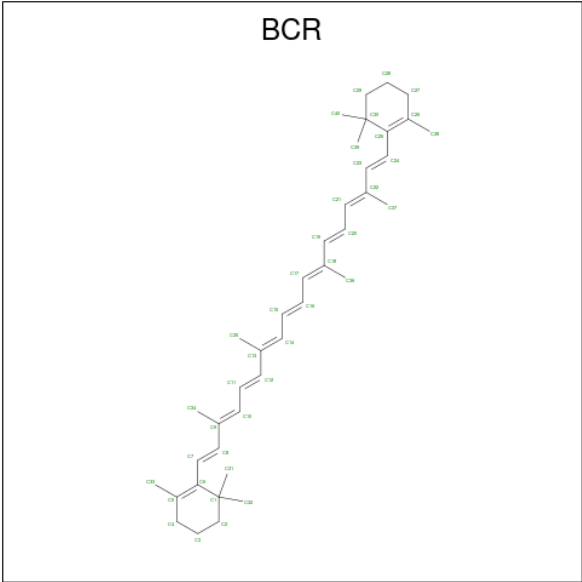
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

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



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

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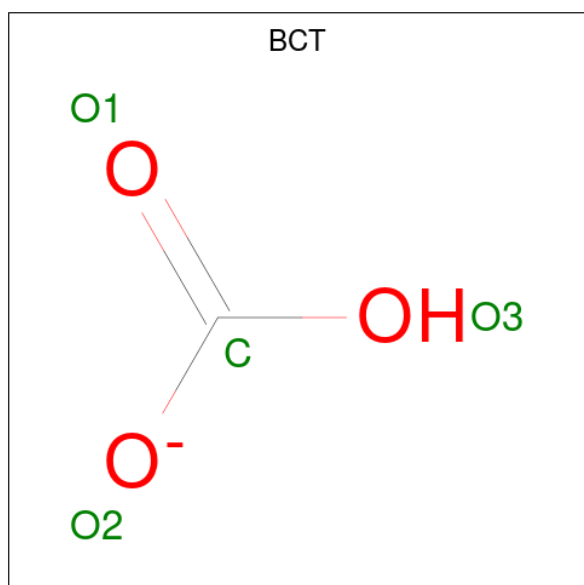
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

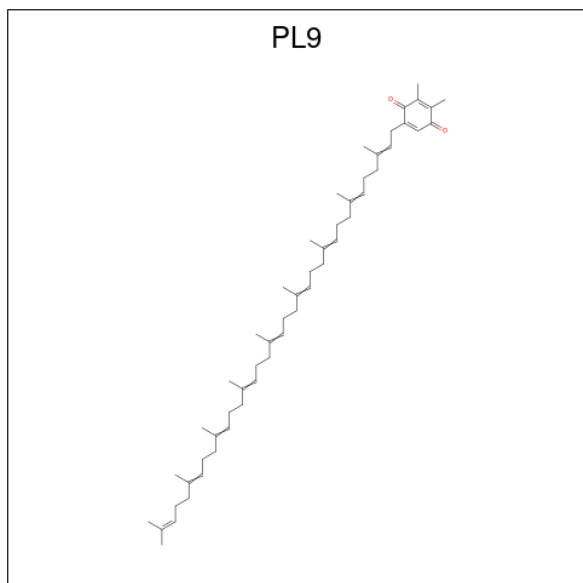
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



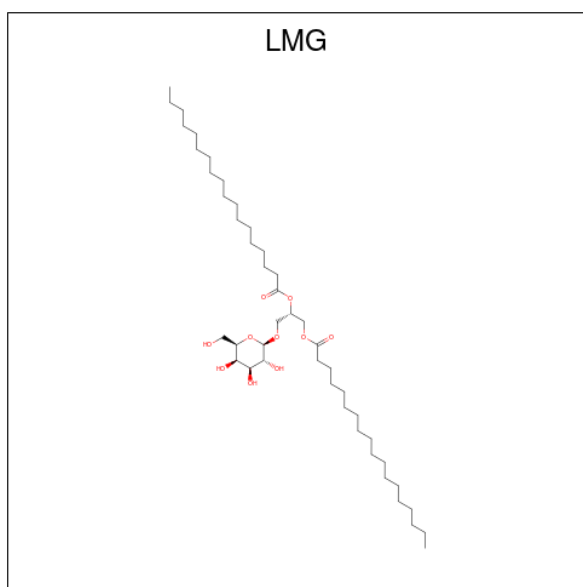
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

- 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: $C_{53}H_{80}O_2$).



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

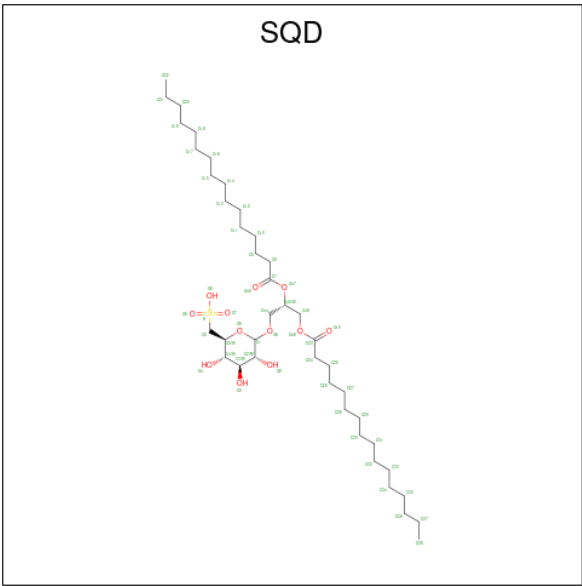
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

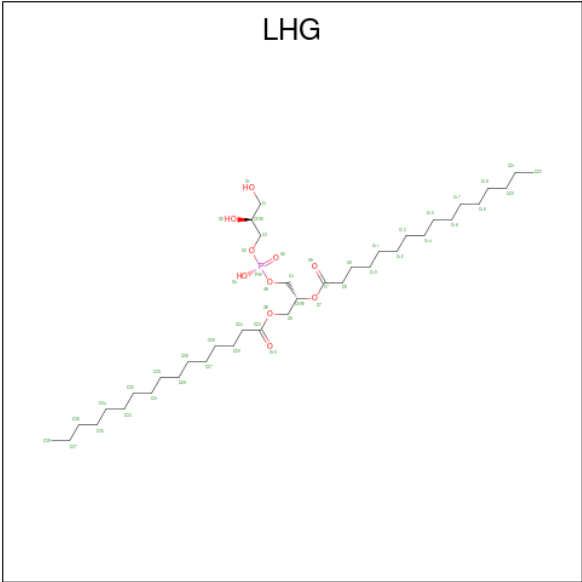
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



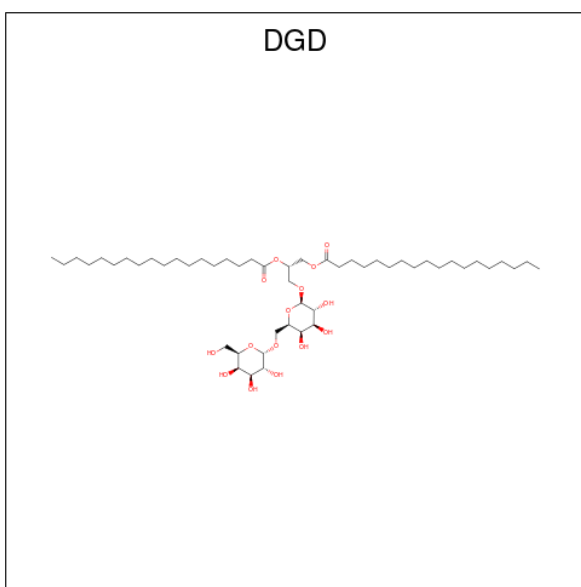
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



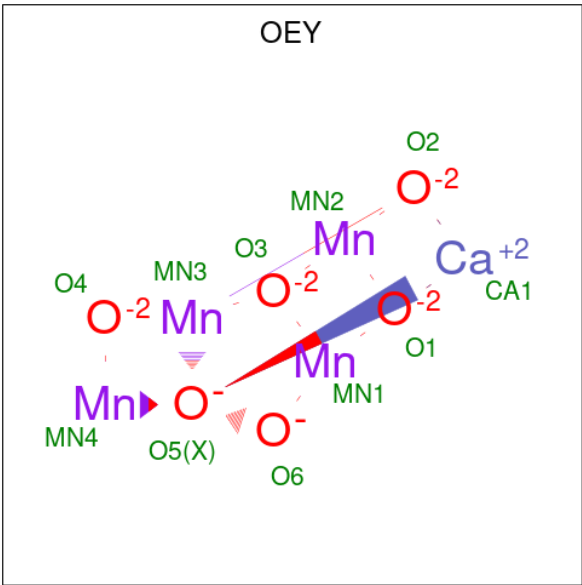
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	d	1	Total	C	H	O	P	0	0
			123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

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



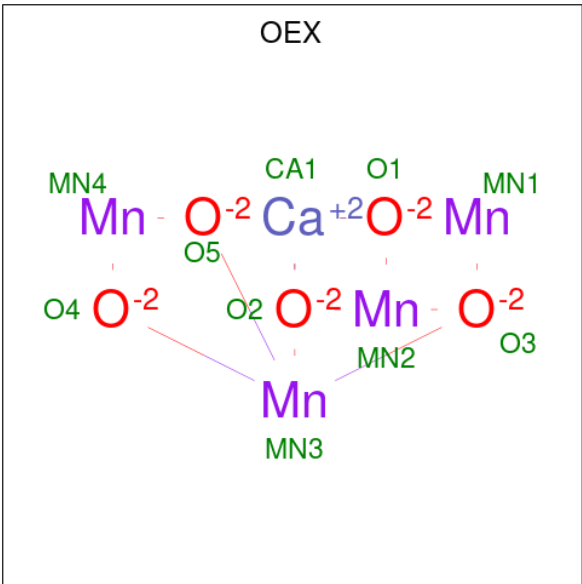
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total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

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

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



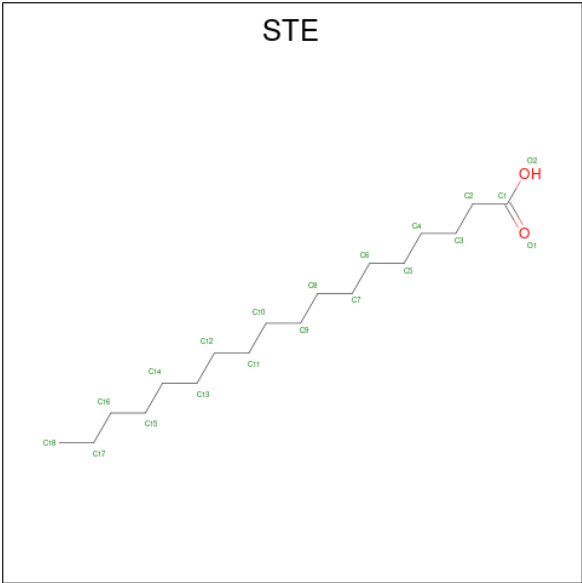
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 34 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



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

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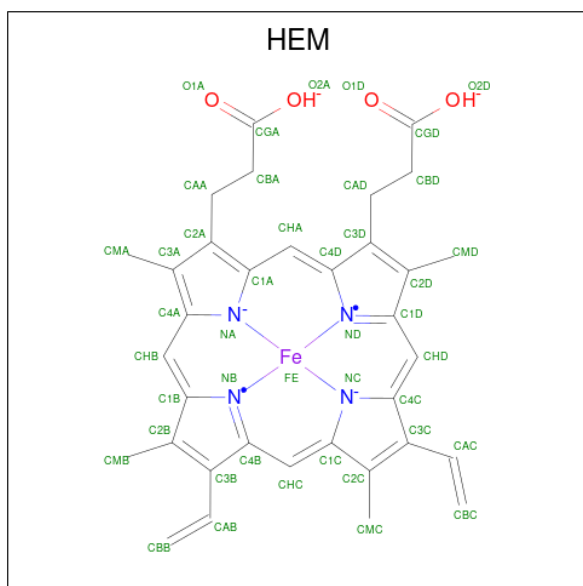
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	1	Total C H O 28 10 16 2	0	0
34	L	1	Total C H O 28 10 16 2	0	0
34	M	1	Total C H O 37 13 22 2	0	0
34	M	1	Total C H 26 10 16	0	0
34	R	1	Total C H O 28 10 16 2	0	0
34	T	1	Total C H 44 15 29	0	0
34	X	1	Total C H O 55 18 35 2	0	0
34	Z	1	Total C H 20 8 12	0	0
34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

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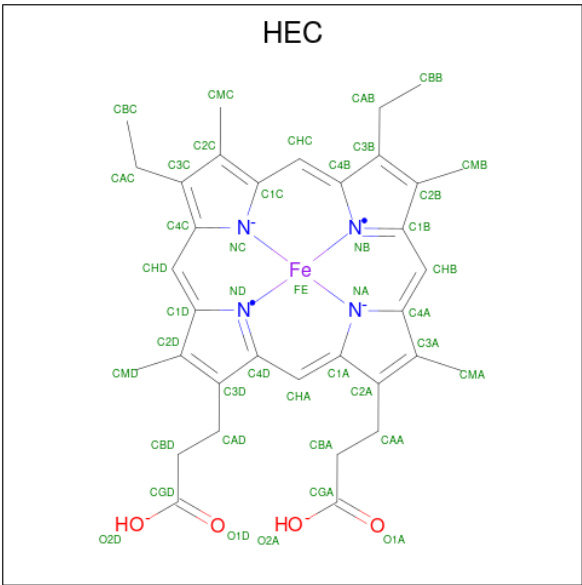
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	h	1	Total	C	H	0	0
			41	14	27		
34	j	1	Total	C	H	O	0
			28	10	16	2	
34	l	1	Total	C	H	0	0
			53	18	35		
34	t	1	Total	C	H	O	0
			34	12	20	2	

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



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	151	Total	O	0	8
			151	151		
37	B	204	Total	O	0	0
			204	204		
37	C	173	Total	O	0	0
			173	173		
37	D	131	Total	O	0	0
			131	131		
37	E	33	Total	O	0	0
			33	33		
37	F	8	Total	O	0	0
			8	8		
37	H	34	Total	O	0	0
			34	34		
37	I	17	Total	O	0	0
			17	17		
37	J	24	Total	O	0	0
			24	24		
37	K	15	Total	O	0	0
			15	15		

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

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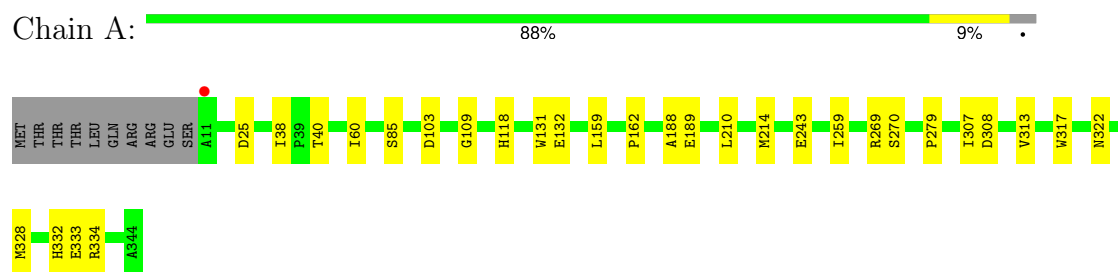
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	7	Total 7	O 7	0	0
37	o	100	Total 100	O 100	0	0
37	r	7	Total 7	O 7	0	0
37	t	8	Total 8	O 8	0	0
37	u	48	Total 48	O 48	0	0
37	v	59	Total 59	O 59	0	0
37	x	11	Total 11	O 11	0	0
37	y	4	Total 4	O 4	0	0
37	z	12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

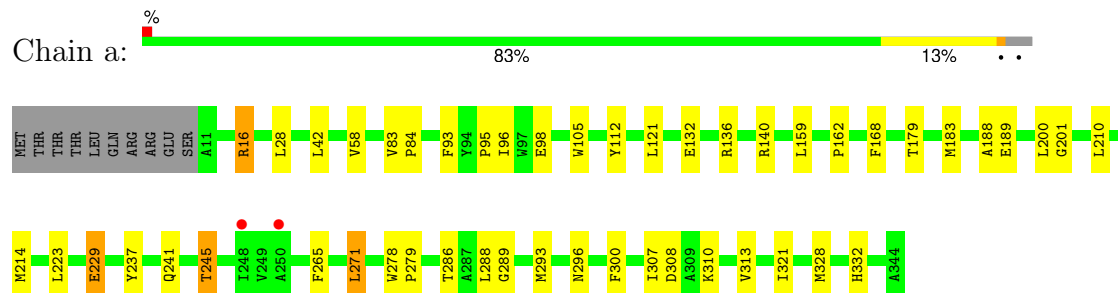
3 Residue-property plots

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

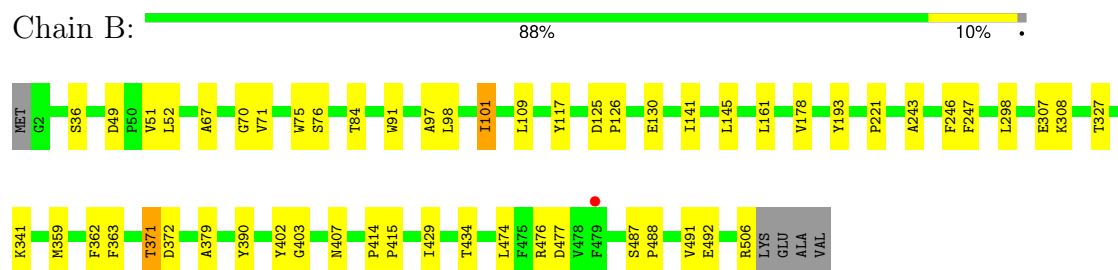
- Molecule 1: Photosystem II protein D1 1



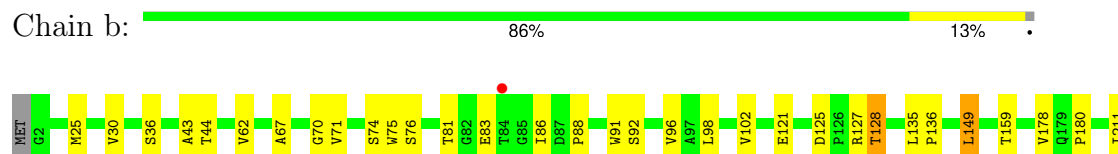
- Molecule 1: Photosystem II protein D1 1

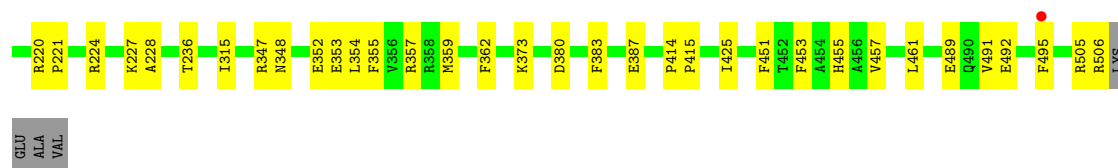


- Molecule 2: Photosystem II CP47 reaction center protein



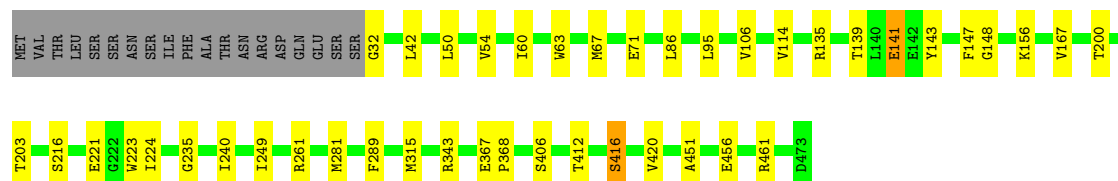
- Molecule 2: Photosystem II CP47 reaction center protein





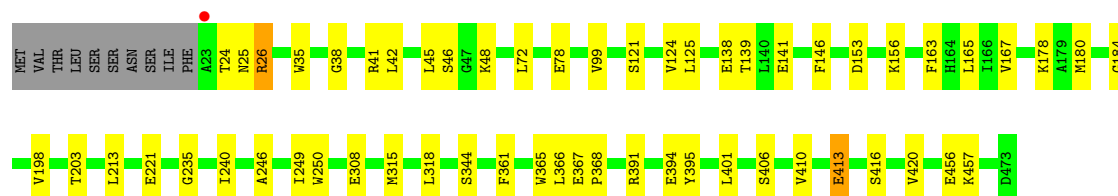
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 9% .



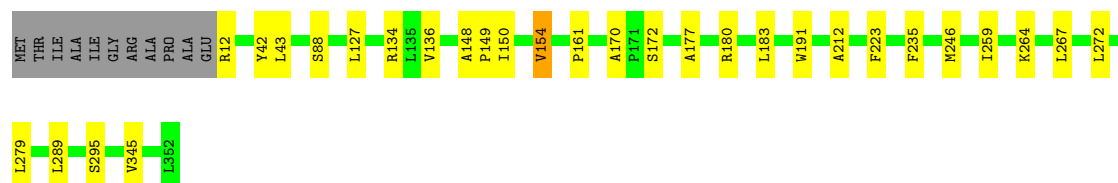
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12% .



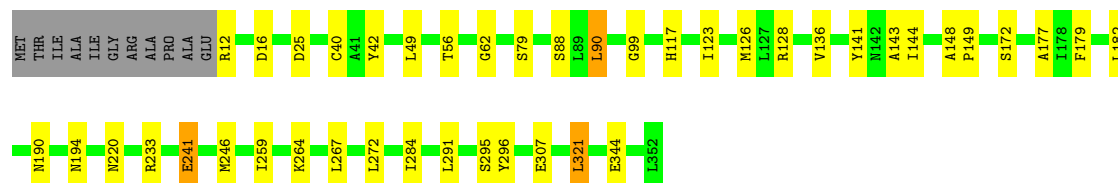
- Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .



- Molecule 4: Photosystem II D2 protein

Chain d: 85% 11% . .

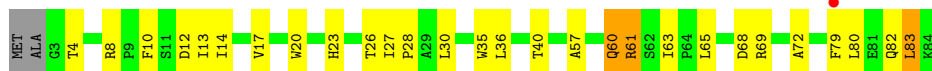


- Molecule 5: Cytochrome b559 subunit alpha

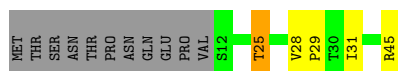
Chain E: 81% 17% .



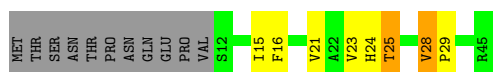
- Molecule 5: Cytochrome b559 subunit alpha



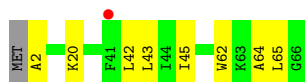
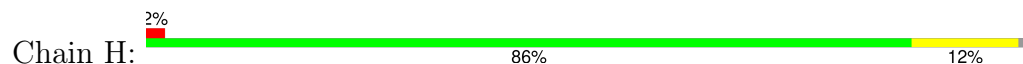
- Molecule 6: Cytochrome b559 subunit beta



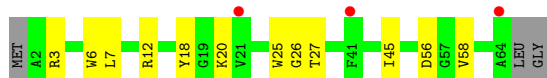
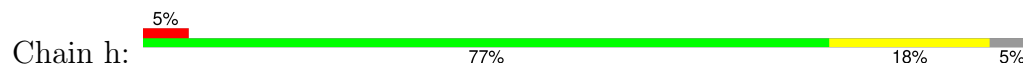
- Molecule 6: Cytochrome b559 subunit beta



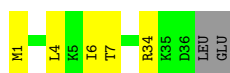
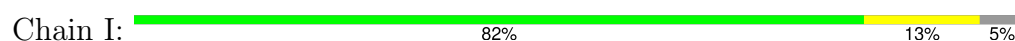
- Molecule 7: Photosystem II reaction center protein H



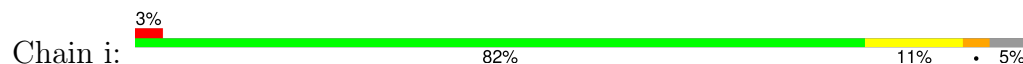
- Molecule 7: Photosystem II reaction center protein H

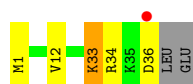


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





• Molecule 9: Photosystem II reaction center protein J

Chain J: 80% 10% 10%



• Molecule 9: Photosystem II reaction center protein J

Chain j: 65% 25% 10%



• Molecule 10: Photosystem II reaction center protein K

Chain K: 67% 11% 20%



• Molecule 10: Photosystem II reaction center protein K

Chain k: 48% 33% 20%



• Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 11%



• Molecule 11: Photosystem II reaction center protein L

Chain l: 81% 14% 5% 2%



• Molecule 12: Photosystem II reaction center protein M

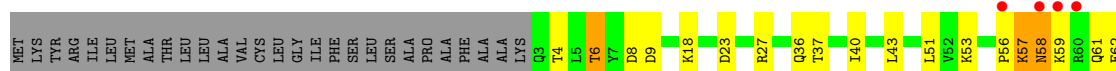
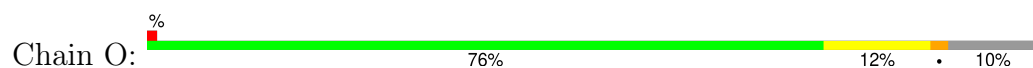
Chain M: 69% 22% 8%



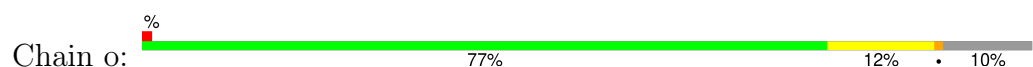
- Molecule 12: Photosystem II reaction center protein M



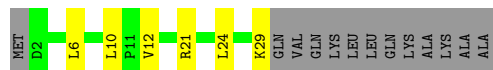
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



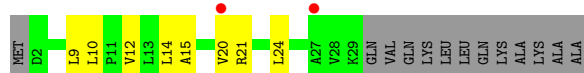
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



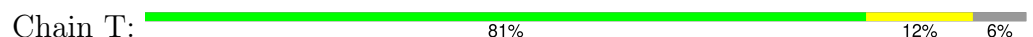
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y

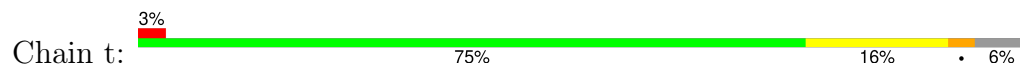


- Molecule 15: Photosystem II reaction center protein T

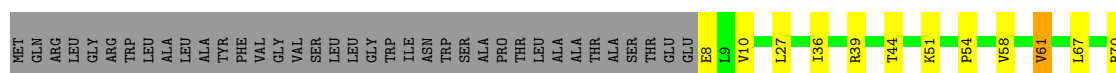




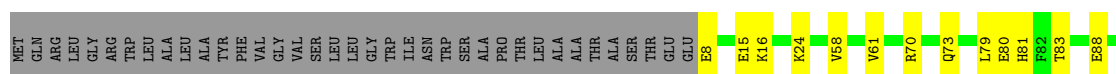
- Molecule 15: Photosystem II reaction center protein T



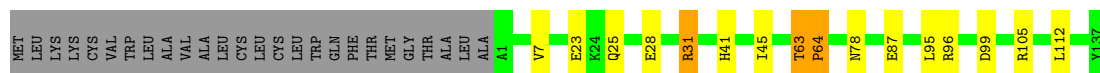
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 17: Cytochrome c-550

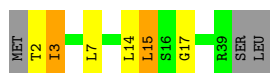


- Molecule 17: Cytochrome c-550



- Molecule 18: Photosystem II reaction center X protein

Chain X:  78% 10% 5% 7%

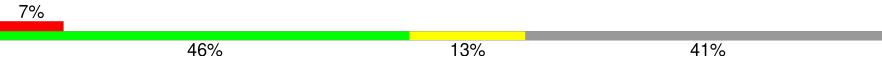


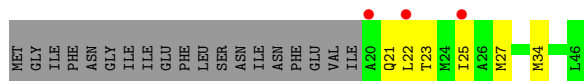
- Molecule 18: Photosystem II reaction center X protein

Chain x:  2% 71% 22% 5%

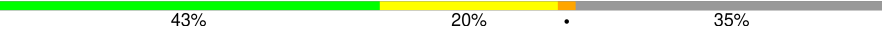


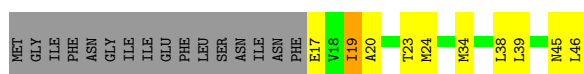
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  7% 46% 13% 41%



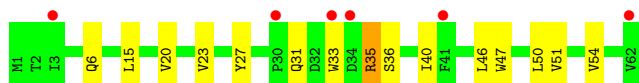
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  43% 20% 35%



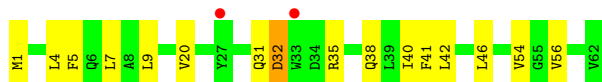
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  10% 76% 23%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  3% 74% 24%



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 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.239 0.186 , 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 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	106082	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: STE, BCR, LMG, LHG, OEY, HEM, FME, OEX, PL9, FE2, DGD, SQD, BCT, HEC, CL, PHO, 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	1/3227 (0.0%)	0.61	0/4397
1	a	0.48	0/3224	0.57	0/4393
2	B	0.59	2/4161 (0.0%)	0.65	4/5669 (0.1%)
2	b	0.53	0/4118	0.60	0/5611
3	C	0.52	0/3647	0.61	0/4965
3	c	0.48	0/3719	0.58	0/5061
4	D	0.58	0/2825	0.64	0/3847
4	d	0.54	0/2834	0.62	0/3859
5	E	0.47	0/688	0.57	0/940
5	e	0.43	0/683	0.57	0/932
6	F	0.46	0/284	0.50	0/387
6	f	0.39	0/284	0.57	0/387
7	H	0.54	0/523	0.63	0/713
7	h	0.48	0/511	0.59	0/697
8	I	0.50	0/293	0.56	0/396
8	i	0.51	0/293	0.53	0/396
9	J	0.44	0/263	0.56	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.43	0/303	0.54	0/416
10	k	0.39	0/303	0.49	0/416
11	L	0.57	0/311	0.61	0/422
11	l	0.57	0/303	0.54	0/412
12	M	0.52	0/249	0.62	0/341
12	m	0.61	0/244	0.61	0/334
13	O	0.51	0/1904	0.65	0/2585
13	o	0.52	0/1905	0.61	0/2583
14	R	0.31	0/227	0.42	0/313
14	r	0.30	0/227	0.39	0/313
15	T	0.57	0/257	0.69	0/349
15	t	0.55	0/255	0.53	0/346
16	U	0.47	0/785	0.57	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.55	0/785	0.60	0/1064
17	V	0.53	0/1085	0.59	0/1473
17	v	0.50	0/1085	0.58	0/1473
18	X	0.46	0/284	0.61	0/384
18	x	0.40	0/289	0.50	0/391
19	Y	0.41	0/197	0.48	0/264
19	y	0.35	0/219	0.48	0/294
20	Z	0.39	0/490	0.49	0/669
20	z	0.34	0/488	0.44	0/666
All	All	0.52	3/44035 (0.0%)	0.60	4/59934 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PRO	CA-C	-14.99	1.42	1.52
1	A	38	ILE	CA-CB	12.88	1.61	1.54
2	B	221	PRO	C-O	5.72	1.29	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	PRO	O-C-N	-14.12	114.51	121.15
2	B	221	PRO	CA-C-O	5.14	124.79	120.73
2	B	221	PRO	CA-C-N	5.03	124.94	119.76
2	B	221	PRO	C-N-CA	5.03	124.94	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	2985	2963	21	0
1	a	3110	2976	2954	31	0
2	B	4005	3873	3867	33	0
2	b	3978	3836	3836	49	0
3	C	3509	3432	3409	28	0
3	c	3583	3503	3492	39	0
4	D	2731	2637	2637	21	0
4	d	2737	2643	2643	30	0
5	E	666	651	651	8	0
5	e	664	648	648	24	0
6	F	275	282	282	4	0
6	f	275	282	282	6	0
7	H	510	532	532	7	0
7	h	498	518	518	9	0
8	I	296	311	311	1	0
8	i	296	311	311	3	0
9	J	257	268	268	3	0
9	j	257	268	268	6	0
10	K	293	305	305	6	0
10	k	293	305	305	8	0
11	L	304	316	316	3	0
11	l	296	304	304	3	0
12	M	256	269	269	7	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	28	0
13	o	1874	1846	1846	20	0
14	R	221	238	238	1	0
14	r	221	238	238	3	0
15	T	258	261	261	2	0
15	t	256	256	256	5	0
16	U	774	773	773	7	0
16	u	774	773	773	5	0
17	V	1064	1071	1073	11	0
17	v	1064	1071	1073	19	0
18	X	281	312	312	4	0
18	x	286	316	314	10	0
19	Y	196	217	217	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	7	0
20	Z	479	516	516	7	0
20	z	477	509	509	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	249	264	264	1	0
22	B	1035	1139	1139	15	0
22	C	839	922	922	14	0
22	D	130	144	144	2	0
22	a	260	288	288	4	0
22	b	1035	1139	1139	20	0
22	c	839	919	919	7	0
22	d	130	144	144	0	0
23	A	64	74	74	1	0
23	D	64	74	74	1	0
23	d	128	148	148	1	0
24	A	40	56	56	0	0
24	B	120	168	168	2	0
24	C	40	56	56	2	0
24	D	40	56	56	1	0
24	H	40	56	56	1	0
24	K	80	112	112	0	0
24	T	40	56	56	1	0
24	Y	40	56	56	0	0
24	a	40	56	56	0	0
24	b	120	168	168	4	0
24	c	80	112	112	1	0
24	d	40	56	56	2	0
24	k	80	112	112	1	0
24	t	40	56	56	4	0
24	x	40	56	56	0	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	2	0
27	d	55	80	80	0	0
28	A	48	66	66	2	0
28	C	48	66	66	1	0
28	D	112	157	157	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	M	51	72	71	1	0
28	a	55	86	86	3	0
28	b	106	158	158	1	0
28	c	134	181	181	7	0
28	d	44	58	58	0	0
29	A	91	135	134	4	0
29	B	54	78	78	1	0
29	D	36	46	46	1	0
29	a	90	133	133	1	0
29	b	49	65	65	1	0
29	f	41	48	48	2	0
30	A	49	74	74	0	0
30	B	98	148	148	1	0
30	D	96	141	141	4	0
30	d	137	199	199	5	0
30	e	42	57	57	1	0
30	l	49	74	74	0	0
31	A	66	96	96	4	0
31	C	186	246	244	1	0
31	H	62	82	82	0	0
31	c	186	246	244	4	0
31	h	62	82	80	1	0
32	A	11	0	0	2	0
32	a	11	0	0	2	0
33	A	10	0	0	0	0
33	a	10	0	0	0	0
34	B	75	117	117	4	0
34	C	40	63	63	1	0
34	H	18	35	35	1	0
34	I	15	26	26	2	0
34	J	12	16	16	0	0
34	L	12	16	16	1	0
34	M	25	38	38	2	0
34	R	12	16	16	1	0
34	T	15	29	29	1	0
34	X	20	35	35	2	0
34	Z	8	12	12	1	0
34	a	37	58	58	4	0
34	b	82	141	141	8	0
34	c	32	51	51	2	0
34	d	57	96	96	4	0
34	h	14	27	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	j	12	16	16	2	0
34	l	18	35	35	2	0
34	t	14	20	20	0	0
35	F	43	30	30	3	0
35	e	43	30	30	6	0
36	V	43	30	30	0	0
36	v	43	30	30	3	0
37	A	151	0	0	7	0
37	B	204	0	0	5	0
37	C	173	0	0	4	0
37	D	131	0	0	2	0
37	E	33	0	0	1	0
37	F	8	0	0	0	0
37	H	34	0	0	2	0
37	I	17	0	0	0	0
37	J	24	0	0	1	0
37	K	15	0	0	1	0
37	L	10	0	0	1	0
37	M	8	0	0	3	0
37	O	86	0	0	10	0
37	R	4	0	0	1	0
37	T	8	0	0	0	0
37	U	34	0	0	3	0
37	V	64	0	0	5	1
37	X	15	0	0	1	0
37	Y	3	0	0	0	0
37	Z	10	0	0	1	0
37	a	132	0	0	5	0
37	b	172	0	0	11	0
37	c	157	0	0	16	0
37	d	110	0	0	3	0
37	e	28	0	0	6	0
37	f	6	0	0	0	0
37	h	20	0	0	3	0
37	i	11	0	0	0	0
37	j	8	0	0	2	0
37	k	5	0	0	1	0
37	l	8	0	0	0	0
37	m	7	0	0	3	0
37	o	100	0	0	5	0
37	r	7	0	0	1	0
37	t	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	u	48	0	0	0	1
37	v	59	0	0	7	0
37	x	11	0	0	7	0
37	y	4	0	0	3	0
37	z	12	0	0	0	0
All	All	53322	52760	52670	552	1

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

The worst 5 of 552 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	36:v:201:HEC:CAC	2.03	1.47
19:y:17:GLU:N	37:y:101:HOH:O	1.87	1.07
2:b:353:GLU:HA	37:b:701:HOH:O	1.55	1.05
5:e:36:LEU:C	37:e:201:HOH:O	2.00	1.03
2:b:352:GLU:C	37:b:701:HOH:O	1.98	1.03

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:V:332:HOH:O	37:u:244:HOH:O[3_457]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	36	36
1	a	397/344 (115%)	388 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	454/461 (98%)	444 (98%)	9 (2%)	1 (0%)	43	44
3	c	463/461 (100%)	452 (98%)	10 (2%)	1 (0%)	43	44
4	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	10	7
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
All	All	5387/5700 (94%)	5241 (97%)	139 (3%)	7 (0%)	48	50

5 of 7 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	321 (99%)	3 (1%)	70	78
1	a	323/280 (115%)	311 (96%)	12 (4%)	30	33
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	53
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	45
3	C	356/362 (98%)	348 (98%)	8 (2%)	45	53
3	c	364/362 (101%)	354 (97%)	10 (3%)	39	45
4	D	277/283 (98%)	273 (99%)	4 (1%)	59	67
4	d	278/283 (98%)	268 (96%)	10 (4%)	31	34
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	11
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	17
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	6
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
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%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
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%)	197 (95%)	10 (5%)	23	23
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	0
14	r	22/33 (67%)	18 (82%)	4 (18%)	2	1
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%)	78 (93%)	6 (7%)	13	11
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	34
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	46
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	35
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	5
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%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4451/4654 (96%)	4280 (96%)	171 (4%)	28	32

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	321	LEU
13	o	115	ARG
5	e	65	LEU
10	k	19	ASP
14	r	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
16	u	37	GLN
6	f	44	GLN
13	o	61	GLN
17	v	106	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	1.00	1 (12%)	8,9,11	1.28	1 (12%)
8	FME	i	1	8	8,9,10	0.92	0	8,9,11	1.44	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	FME	T	1	15	8,9,10	1.04	0	8,9,11	1.13	1 (12%)
15	FME	t	1	15	8,9,10	1.11	1 (12%)	8,9,11	1.11	0
12	FME	M	1	12	8,9,10	0.87	0	8,9,11	0.80	0
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.13	1 (12%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.79	1.42	1.46
15	t	1	FME	CA-N	-2.46	1.43	1.46
12	m	1	FME	CA-N	-2.06	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.15	117.98	122.82
12	m	1	FME	CB-CA-N	2.22	114.56	110.52
8	I	1	FME	CA-N-CN	-2.05	119.67	122.82
15	T	1	FME	O1-CN-N	-2.00	120.14	125.32

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no 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	505	3	69,73,73	1.28	8 (11%)	82,113,113	1.24	8 (9%)
28	LMG	D	411	-	26,26,55	0.64	0	26,26,63	1.23	2 (7%)
22	CLA	C	511	3	69,73,73	1.60	10 (14%)	82,113,113	1.32	3 (3%)
24	BCR	C	514	-	41,41,41	1.31	4 (9%)	56,56,56	1.36	6 (10%)
22	CLA	b	602	2	69,73,73	1.11	9 (13%)	82,113,113	1.54	8 (9%)
24	BCR	k	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
31	DGD	C	515	-	63,63,67	1.11	3 (4%)	77,77,81	1.39	12 (15%)
22	CLA	B	607	37	69,73,73	1.25	10 (14%)	82,113,113	1.43	11 (13%)
34	STE	H	103	-	17,17,19	0.45	0	16,16,19	0.68	0
34	STE	b	621	-	15,15,19	0.41	0	14,14,19	0.78	0
28	LMG	a	416	-	55,55,55	1.21	5 (9%)	63,63,63	1.49	7 (11%)
34	STE	d	412	-	19,19,19	0.77	0	19,19,19	1.00	1 (5%)
36	HEC	V	201	17	50,50,50	1.60	4 (8%)	68,82,82	1.48	13 (19%)
31	DGD	c	518	-	63,63,67	1.02	3 (4%)	77,77,81	1.38	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	A	404	-	58,69,69	1.80	10 (17%)	55,99,99	1.76	11 (20%)
24	BCR	H	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.33	9 (16%)
34	STE	d	413	-	19,19,19	0.60	0	19,19,19	1.09	1 (5%)
30	LHG	e	102	-	41,41,48	1.06	4 (9%)	44,47,54	1.38	5 (11%)
34	STE	d	411	-	16,16,19	0.53	0	16,16,19	1.43	4 (25%)
23	PHO	d	402	-	58,69,69	2.03	10 (17%)	55,99,99	1.52	9 (16%)
28	LMG	b	624	-	55,55,55	0.88	2 (3%)	63,63,63	1.50	10 (15%)
28	LMG	c	519	-	37,37,55	1.22	5 (13%)	45,45,63	1.35	7 (15%)
29	SQD	D	407	-	34,36,54	0.96	2 (5%)	42,45,65	2.21	12 (28%)
34	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.21	1 (9%)
24	BCR	K	102	-	41,41,41	1.13	4 (9%)	56,56,56	1.19	7 (12%)
22	CLA	d	404	4	69,73,73	1.42	11 (15%)	82,113,113	1.24	11 (13%)
30	LHG	A	414	-	48,48,48	0.87	3 (6%)	51,54,54	1.21	4 (7%)
24	BCR	b	618	-	41,41,41	1.29	4 (9%)	56,56,56	1.26	7 (12%)
22	CLA	B	606	2	69,73,73	1.38	6 (8%)	82,113,113	1.22	6 (7%)
34	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.62	0
24	BCR	x	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	7 (12%)
29	SQD	a	411	-	52,54,54	1.01	4 (7%)	62,65,65	1.75	11 (17%)
34	STE	h	102	-	13,13,19	0.44	0	12,12,19	0.64	0
22	CLA	b	601	37	69,73,73	1.37	8 (11%)	82,113,113	1.60	8 (9%)
22	CLA	c	504	37	64,68,73	1.28	6 (9%)	76,107,113	1.22	11 (14%)
28	LMG	A	412	-	48,48,55	1.06	3 (6%)	56,56,63	1.35	7 (12%)
22	CLA	B	615	2	69,73,73	1.23	12 (17%)	82,113,113	1.30	10 (12%)
22	CLA	D	403	4	69,73,73	1.52	11 (15%)	82,113,113	1.31	12 (14%)
22	CLA	B	611	2	69,73,73	1.41	10 (14%)	82,113,113	1.48	13 (15%)
28	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.32	7 (12%)
24	BCR	B	618	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	C	504	37	63,67,73	1.25	9 (14%)	74,105,113	1.28	11 (14%)
22	CLA	b	604	2	69,73,73	1.04	6 (8%)	82,113,113	1.51	11 (13%)
22	CLA	B	603	2	69,73,73	1.24	7 (10%)	82,113,113	1.44	12 (14%)
22	CLA	b	612	2	69,73,73	1.10	6 (8%)	82,113,113	1.30	9 (10%)
31	DGD	A	416	-	67,67,67	1.27	9 (13%)	81,81,81	1.44	11 (13%)
34	STE	Z	101	-	7,7,19	0.34	0	6,6,19	0.69	0
33	OEX	a	417[A]	37,3,1	0,14,14	-	-	-	-	-
24	BCR	A	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	a	409	-	55,55,55	1.24	7 (12%)	68,69,69	1.54	12 (17%)
30	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	4 (7%)
22	CLA	c	513	3	69,73,73	1.36	9 (13%)	82,113,113	1.15	8 (9%)
24	BCR	T	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.27	4 (7%)
22	CLA	d	403	4	69,73,73	1.39	9 (13%)	82,113,113	1.31	8 (9%)
22	CLA	A	411	37	69,73,73	1.23	9 (13%)	82,113,113	1.28	7 (8%)
28	LMG	d	410	-	44,44,55	1.05	2 (4%)	52,52,63	1.36	8 (15%)
34	STE	X	101	-	19,19,19	0.67	0	19,19,19	1.32	3 (15%)
24	BCR	a	405	-	41,41,41	1.11	3 (7%)	56,56,56	1.39	9 (16%)
34	STE	B	627	-	11,11,19	0.81	0	11,11,19	0.84	0
34	STE	C	519	-	11,11,19	0.75	0	11,11,19	1.17	1 (9%)
31	DGD	C	516	-	63,63,67	1.25	8 (12%)	77,77,81	1.34	9 (11%)
34	STE	T	102	-	14,14,19	0.41	0	13,13,19	0.83	0
22	CLA	a	404	1	69,73,73	1.42	10 (14%)	82,113,113	1.40	6 (7%)
22	CLA	a	403	37	69,73,73	1.29	7 (10%)	82,113,113	1.30	11 (13%)
22	CLA	c	506	3	69,73,73	1.35	9 (13%)	82,113,113	1.37	11 (13%)
22	CLA	C	502	3	69,73,73	1.17	6 (8%)	82,113,113	1.48	10 (12%)
23	PHO	d	401	-	58,69,69	1.86	11 (18%)	55,99,99	1.58	10 (18%)
24	BCR	c	515	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	4 (7%)
22	CLA	C	507	37	69,73,73	1.37	7 (10%)	82,113,113	1.56	12 (14%)
22	CLA	b	603	2	69,73,73	1.34	8 (11%)	82,113,113	1.51	13 (15%)
22	CLA	c	508	3	68,72,73	1.32	9 (13%)	80,111,113	1.33	11 (13%)
24	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.31	7 (12%)
22	CLA	a	410	37	69,73,73	1.49	5 (7%)	82,113,113	1.33	5 (6%)
22	CLA	C	510	3	69,73,73	1.26	11 (15%)	82,113,113	1.21	4 (4%)
34	STE	B	625	-	17,17,19	0.66	0	17,17,19	1.12	1 (5%)
24	BCR	d	405	-	41,41,41	1.25	3 (7%)	56,56,56	1.21	6 (10%)
22	CLA	c	502	3	69,73,73	1.28	8 (11%)	82,113,113	1.46	8 (9%)
29	SQD	A	413	-	50,52,54	0.96	4 (8%)	60,63,65	1.83	12 (20%)
22	CLA	b	615	2	69,73,73	1.54	8 (11%)	82,113,113	1.45	8 (9%)
36	HEC	v	201	17	50,50,50	1.60	6 (12%)	68,82,82	1.40	9 (13%)
24	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.08	4 (7%)
22	CLA	c	507	37	69,73,73	1.26	3 (4%)	82,113,113	1.31	8 (9%)
35	HEM	e	101	5,6	50,50,50	1.47	10 (20%)	67,82,82	1.39	11 (16%)
22	CLA	c	505	3	69,73,73	1.16	6 (8%)	82,113,113	1.13	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCT	a	408	21	3,3,3	1.33	0	2,3,3	2.71	1 (50%)
22	CLA	C	512	3	69,73,73	1.19	9 (13%)	82,113,113	1.24	9 (10%)
22	CLA	c	510	3	69,73,73	1.38	8 (11%)	82,113,113	1.30	8 (9%)
35	HEM	F	101	5,6	50,50,50	1.36	6 (12%)	67,82,82	1.25	7 (10%)
29	SQD	b	620	-	47,49,54	0.94	4 (8%)	57,60,65	2.11	16 (28%)
22	CLA	C	506	3	69,73,73	1.35	10 (14%)	82,113,113	1.17	8 (9%)
22	CLA	b	608	2	69,73,73	1.22	9 (13%)	82,113,113	1.25	6 (7%)
22	CLA	B	605	2	69,73,73	1.11	7 (10%)	82,113,113	1.22	8 (9%)
32	OEY	A	417[B]	37,3,1	0,16,16	-	-	-	-	-
31	DGD	C	517	-	63,63,67	0.92	4 (6%)	77,77,81	1.32	7 (9%)
30	LHG	d	409	-	38,38,48	0.73	1 (2%)	41,44,54	1.15	3 (7%)
28	LMG	C	518	-	48,48,55	1.16	5 (10%)	56,56,63	1.34	6 (10%)
22	CLA	B	613	2	69,73,73	1.41	13 (18%)	82,113,113	1.39	8 (9%)
24	BCR	t	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.37	8 (14%)
31	DGD	c	517	-	63,63,67	0.99	4 (6%)	77,77,81	1.42	10 (12%)
34	STE	b	625	-	15,15,19	0.76	0	15,15,19	0.98	1 (6%)
22	CLA	A	402	1	69,73,73	1.27	8 (11%)	82,113,113	1.40	10 (12%)
33	OEX	A	418[A]	37,3,1	0,14,14	-	-	-	-	-
31	DGD	h	101	-	63,63,67	1.04	4 (6%)	77,77,81	1.48	11 (14%)
30	LHG	B	622	-	48,48,48	0.91	3 (6%)	51,54,54	1.42	8 (15%)
34	STE	J	101	-	11,11,19	0.68	0	11,11,19	1.38	1 (9%)
22	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.52	11 (13%)
32	OEY	a	418[B]	37,3,1	0,16,16	-	-	-	-	-
24	BCR	D	404	-	41,41,41	1.24	2 (4%)	56,56,56	1.14	4 (7%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.33	8 (14%)
22	CLA	C	513	3	69,73,73	1.25	7 (10%)	82,113,113	1.22	6 (7%)
30	LHG	D	409	-	46,46,48	1.00	3 (6%)	49,52,54	1.35	3 (6%)
29	SQD	a	412	-	35,35,54	1.12	2 (5%)	37,37,65	1.46	4 (10%)
34	STE	I	101	-	14,14,19	0.48	0	13,13,19	0.60	0
22	CLA	A	405	1	58,62,73	1.25	8 (13%)	68,99,113	1.36	12 (17%)
22	CLA	c	512	3	69,73,73	1.24	9 (13%)	82,113,113	1.43	7 (8%)
22	CLA	b	611	2	69,73,73	1.07	4 (5%)	82,113,113	1.36	10 (12%)
30	LHG	B	621	-	48,48,48	1.02	2 (4%)	51,54,54	1.11	3 (5%)
27	PL9	d	406	-	55,55,55	1.69	7 (12%)	68,69,69	1.64	14 (20%)
29	SQD	B	623	-	52,54,54	0.96	3 (5%)	62,65,65	1.73	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	STE	C	521	-	11,11,19	0.61	0	11,11,19	1.58	2 (18%)
30	LHG	d	408	-	48,48,48	0.97	3 (6%)	51,54,54	1.21	4 (7%)
28	LMG	M	101	-	51,51,55	1.07	6 (11%)	59,59,63	1.43	9 (15%)
22	CLA	a	402	1	69,73,73	1.32	8 (11%)	82,113,113	1.40	10 (12%)
22	CLA	B	614	2	69,73,73	1.35	8 (11%)	82,113,113	1.41	11 (13%)
22	CLA	B	612	2	69,73,73	1.10	6 (8%)	82,113,113	1.44	9 (10%)
22	CLA	B	608	2	69,73,73	1.16	7 (10%)	82,113,113	1.45	13 (15%)
34	STE	c	520	-	19,19,19	0.69	0	19,19,19	1.04	1 (5%)
22	CLA	c	503	3	69,73,73	1.32	9 (13%)	82,113,113	1.37	5 (6%)
28	LMG	c	522	-	49,49,55	0.96	2 (4%)	57,57,63	1.32	4 (7%)
34	STE	a	414	-	11,11,19	0.86	0	11,11,19	1.00	0
24	BCR	b	617	-	41,41,41	1.20	4 (9%)	56,56,56	1.41	9 (16%)
22	CLA	c	509	3	69,73,73	1.30	6 (8%)	82,113,113	1.33	9 (10%)
26	BCT	A	409	21	3,3,3	1.19	0	2,3,3	3.30	1 (50%)
31	DGD	c	516	-	63,63,67	1.25	11 (17%)	77,77,81	1.44	14 (18%)
34	STE	B	624	-	11,11,19	0.96	1 (9%)	11,11,19	1.36	2 (18%)
34	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.27	1 (7%)
29	SQD	f	101	-	39,41,54	1.12	5 (12%)	49,52,65	1.94	10 (20%)
22	CLA	c	511	3	69,73,73	1.33	10 (14%)	82,113,113	1.38	5 (6%)
34	STE	L	101	-	11,11,19	0.76	0	11,11,19	1.58	2 (18%)
22	CLA	C	503	3	69,73,73	1.38	11 (15%)	82,113,113	1.55	9 (10%)
24	BCR	K	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.31	8 (14%)
27	PL9	D	405	-	55,55,55	1.69	10 (18%)	68,69,69	1.69	14 (20%)
22	CLA	C	509	3	69,73,73	1.08	7 (10%)	82,113,113	1.54	7 (8%)
24	BCR	B	617	-	41,41,41	1.22	3 (7%)	56,56,56	1.29	6 (10%)
22	CLA	B	601	37	69,73,73	1.30	7 (10%)	82,113,113	1.65	10 (12%)
34	STE	M	102	-	14,14,19	0.80	0	14,14,19	1.02	1 (7%)
22	CLA	B	616	2	64,68,73	1.32	8 (12%)	76,107,113	1.73	14 (18%)
22	CLA	b	614	2	69,73,73	1.13	5 (7%)	82,113,113	1.27	8 (9%)
22	CLA	D	402	4	69,73,73	1.20	5 (7%)	82,113,113	1.31	10 (12%)
22	CLA	B	609	2	69,73,73	1.24	7 (10%)	82,113,113	1.38	7 (8%)
34	STE	a	415	-	14,14,19	0.42	0	13,13,19	0.86	0
22	CLA	b	605	2	69,73,73	1.15	7 (10%)	82,113,113	1.49	10 (12%)
30	LHG	d	407	-	48,48,48	0.98	3 (6%)	51,54,54	1.37	7 (13%)
34	STE	b	626	-	19,19,19	0.69	0	19,19,19	0.84	0

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	1.58	9 (13%)	82,113,113	1.82	17 (20%)
28	LMG	b	622	-	51,51,55	1.02	5 (9%)	59,59,63	1.47	7 (11%)
22	CLA	A	403	37	69,73,73	1.27	10 (14%)	82,113,113	1.15	6 (7%)
22	CLA	b	607	37	69,73,73	1.25	7 (10%)	82,113,113	1.49	8 (9%)
22	CLA	B	610	37	69,73,73	1.16	6 (8%)	82,113,113	1.54	10 (12%)
31	DGD	H	102	-	63,63,67	1.23	7 (11%)	77,77,81	1.47	12 (15%)
22	CLA	c	501	3	69,73,73	1.03	5 (7%)	82,113,113	1.44	9 (10%)
28	LMG	D	406	-	51,51,55	0.88	2 (3%)	59,59,63	1.43	9 (15%)
22	CLA	b	609	2	69,73,73	1.23	8 (11%)	82,113,113	1.32	8 (9%)
34	STE	b	627	-	9,9,19	0.51	0	8,8,19	0.56	0
22	CLA	B	602	2	69,73,73	1.28	9 (13%)	82,113,113	1.39	11 (13%)
34	STE	l	102	-	17,17,19	0.32	0	16,16,19	1.00	0
34	STE	C	520	-	15,15,19	0.40	0	14,14,19	0.80	0
22	CLA	b	613	2	69,73,73	1.20	8 (11%)	82,113,113	1.53	10 (12%)
24	BCR	Y	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	4 (7%)
34	STE	a	413	-	9,9,19	0.52	0	8,8,19	0.52	0
30	LHG	D	408	-	48,48,48	1.09	4 (8%)	51,54,54	1.30	7 (13%)
22	CLA	B	604	2	69,73,73	1.46	6 (8%)	82,113,113	1.57	9 (10%)
28	LMG	D	410	-	31,31,55	0.91	2 (6%)	33,33,63	1.17	2 (6%)
34	STE	B	620	-	16,16,19	0.66	0	16,16,19	1.10	0
22	CLA	b	616	2	64,68,73	1.42	9 (14%)	76,107,113	1.40	9 (11%)
34	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.69	0
27	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	1.81	15 (22%)
23	PHO	D	401	-	58,69,69	1.93	8 (13%)	55,99,99	1.48	11 (20%)
34	STE	b	623	-	19,19,19	0.65	0	19,19,19	1.11	2 (10%)
34	STE	c	523	-	11,11,19	0.80	0	11,11,19	0.91	0
34	STE	R	101	-	11,11,19	0.89	0	11,11,19	0.77	0
29	SQD	A	415	-	38,38,54	1.01	3 (7%)	40,40,65	1.28	5 (12%)
22	CLA	C	501	3	69,73,73	1.31	7 (10%)	82,113,113	1.49	8 (9%)
24	BCR	c	514	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	6 (10%)
22	CLA	b	610	37	69,73,73	1.31	6 (8%)	82,113,113	1.44	13 (15%)

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	505	3	-	12/39/115/115	-
28	LMG	D	411	-	-	10/22/22/70	-
22	CLA	C	511	3	-	12/39/115/115	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
22	CLA	b	602	2	-	7/39/115/115	-
24	BCR	k	102	-	-	7/29/63/63	0/2/2/2
31	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	B	607	37	-	8/39/115/115	-
34	STE	H	103	-	-	11/15/15/17	-
34	STE	b	621	-	-	5/13/13/17	-
28	LMG	a	416	-	-	25/50/70/70	0/1/1/1
34	STE	d	412	-	-	10/17/17/17	-
36	HEC	V	201	17	1/1/7/7	5/14/54/54	-
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
34	STE	d	413	-	-	9/17/17/17	-
30	LHG	e	102	-	-	26/46/46/53	-
34	STE	d	411	-	-	9/14/14/17	-
23	PHO	d	402	-	-	7/37/103/103	0/5/6/6
28	LMG	b	624	-	-	28/50/70/70	0/1/1/1
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
34	STE	j	101	-	-	4/9/9/17	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	d	404	4	-	8/39/115/115	-
30	LHG	A	414	-	-	29/53/53/53	-
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
22	CLA	B	606	2	-	10/39/115/115	-
34	STE	B	626	-	-	10/13/13/17	-
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2
29	SQD	a	411	-	-	25/49/69/69	0/1/1/1
34	STE	h	102	-	-	5/11/11/17	-
22	CLA	b	601	37	-	18/39/115/115	-
22	CLA	c	504	37	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	A	412	-	-	18/43/63/70	0/1/1/1
22	CLA	B	615	2	-	7/39/115/115	-
22	CLA	D	403	4	-	9/39/115/115	-
22	CLA	B	611	2	-	6/39/115/115	-
28	LMG	c	521	-	-	24/43/63/70	0/1/1/1
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
22	CLA	C	504	37	-	8/32/108/115	-
22	CLA	b	604	2	-	4/39/115/115	-
22	CLA	B	603	2	-	10/39/115/115	-
22	CLA	b	612	2	-	6/39/115/115	-
31	DGD	A	416	-	-	24/55/95/95	0/2/2/2
34	STE	Z	101	-	-	3/5/5/17	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
27	PL9	a	409	-	-	23/53/73/73	0/1/1/1
30	LHG	l	101	-	-	18/53/53/53	-
22	CLA	c	513	3	-	7/39/115/115	-
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
22	CLA	d	403	4	-	8/39/115/115	-
22	CLA	A	411	37	-	10/39/115/115	-
28	LMG	d	410	-	-	12/39/59/70	0/1/1/1
34	STE	X	101	-	-	9/17/17/17	-
24	BCR	a	405	-	-	2/29/63/63	0/2/2/2
34	STE	B	627	-	-	6/9/9/17	-
34	STE	C	519	-	-	5/9/9/17	-
31	DGD	C	516	-	-	19/51/91/95	0/2/2/2
34	STE	T	102	-	-	7/12/12/17	-
22	CLA	a	404	1	-	6/39/115/115	-
22	CLA	a	403	37	-	13/39/115/115	-
22	CLA	c	506	3	-	14/39/115/115	-
22	CLA	C	502	3	-	5/39/115/115	-
23	PHO	d	401	-	-	4/37/103/103	0/5/6/6
24	BCR	c	515	-	-	7/29/63/63	0/2/2/2
22	CLA	C	507	37	-	8/39/115/115	-
22	CLA	b	603	2	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	508	3	-	14/38/114/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	a	410	37	-	3/39/115/115	-
22	CLA	C	510	3	-	9/39/115/115	-
34	STE	B	625	-	-	9/15/15/17	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
22	CLA	c	502	3	-	5/39/115/115	-
29	SQD	A	413	-	-	15/47/67/69	0/1/1/1
22	CLA	b	615	2	-	10/39/115/115	-
36	HEC	v	201	17	1/1/7/7	4/14/54/54	-
24	BCR	k	101	-	-	8/29/63/63	0/2/2/2
22	CLA	c	507	37	-	7/39/115/115	-
35	HEM	e	101	5,6	-	5/14/54/54	-
22	CLA	c	505	3	-	7/39/115/115	-
22	CLA	C	512	3	-	15/39/115/115	-
22	CLA	c	510	3	-	12/39/115/115	-
35	HEM	F	101	5,6	-	3/14/54/54	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
22	CLA	C	506	3	-	9/39/115/115	-
22	CLA	b	608	2	-	7/39/115/115	-
22	CLA	B	605	2	-	11/39/115/115	-
31	DGD	C	517	-	-	15/51/91/95	0/2/2/2
30	LHG	d	409	-	-	18/43/43/53	-
28	LMG	C	518	-	-	21/43/63/70	0/1/1/1
22	CLA	B	613	2	-	10/39/115/115	-
24	BCR	t	101	-	-	5/29/63/63	0/2/2/2
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
34	STE	b	625	-	-	4/13/13/17	-
22	CLA	A	402	1	-	3/39/115/115	-
31	DGD	h	101	-	-	16/51/91/95	0/2/2/2
30	LHG	B	622	-	-	22/53/53/53	-
34	STE	J	101	-	-	2/9/9/17	-
22	CLA	C	508	3	-	4/39/115/115	-
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	619	-	-	3/29/63/63	0/2/2/2
22	CLA	C	513	3	-	10/39/115/115	-
30	LHG	D	409	-	-	26/51/51/53	-
29	SQD	a	412	-	-	14/37/37/69	-
34	STE	I	101	-	-	6/12/12/17	-
22	CLA	A	405	1	-	6/26/102/115	-
22	CLA	c	512	3	-	22/39/115/115	-
22	CLA	b	611	2	-	6/39/115/115	-
30	LHG	B	621	-	-	26/53/53/53	-
27	PL9	d	406	-	-	12/53/73/73	0/1/1/1
29	SQD	B	623	-	-	22/49/69/69	0/1/1/1
34	STE	C	521	-	-	5/9/9/17	-
30	LHG	d	408	-	-	22/53/53/53	-
28	LMG	M	101	-	-	18/46/66/70	0/1/1/1
22	CLA	a	402	1	-	6/39/115/115	-
22	CLA	B	614	2	-	11/39/115/115	-
22	CLA	B	612	2	-	9/39/115/115	-
22	CLA	B	608	2	-	1/39/115/115	-
34	STE	c	520	-	-	10/17/17/17	-
22	CLA	c	503	3	-	3/39/115/115	-
28	LMG	c	522	-	-	19/44/64/70	0/1/1/1
34	STE	a	414	-	-	5/9/9/17	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	c	509	3	-	11/39/115/115	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
34	STE	B	624	-	-	3/9/9/17	-
34	STE	t	102	-	-	5/11/11/17	-
29	SQD	f	101	-	-	15/36/56/69	0/1/1/1
22	CLA	c	511	3	-	13/39/115/115	-
34	STE	L	101	-	-	4/9/9/17	-
22	CLA	C	503	3	-	3/39/115/115	-
24	BCR	K	101	-	-	14/29/63/63	0/2/2/2
27	PL9	D	405	-	-	10/53/73/73	0/1/1/1
22	CLA	C	509	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	B	601	37	-	21/39/115/115	-
34	STE	M	102	-	-	4/12/12/17	-
22	CLA	B	616	2	-	8/33/109/115	-
22	CLA	b	614	2	-	18/39/115/115	-
22	CLA	D	402	4	-	11/39/115/115	-
22	CLA	B	609	2	-	7/39/115/115	-
34	STE	a	415	-	-	7/12/12/17	-
22	CLA	b	605	2	-	12/39/115/115	-
30	LHG	d	407	-	-	22/53/53/53	-
34	STE	b	626	-	-	5/17/17/17	-
22	CLA	b	606	2	-	12/39/115/115	-
28	LMG	b	622	-	-	24/46/66/70	0/1/1/1
22	CLA	A	403	37	-	11/39/115/115	-
22	CLA	b	607	37	-	14/39/115/115	-
22	CLA	B	610	37	-	7/39/115/115	-
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	c	501	3	-	5/39/115/115	-
28	LMG	D	406	-	-	16/46/66/70	0/1/1/1
22	CLA	b	609	2	-	6/39/115/115	-
34	STE	b	627	-	-	5/7/7/17	-
22	CLA	B	602	2	-	6/39/115/115	-
34	STE	l	102	-	-	9/15/15/17	-
34	STE	C	520	-	-	5/13/13/17	-
22	CLA	b	613	2	-	4/39/115/115	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
34	STE	a	413	-	-	3/7/7/17	-
30	LHG	D	408	-	-	25/53/53/53	-
22	CLA	B	604	2	-	10/39/115/115	-
28	LMG	D	410	-	-	14/33/33/70	-
34	STE	B	620	-	-	8/14/14/17	-
22	CLA	b	616	2	-	13/33/109/115	-
34	STE	M	103	-	-	1/7/7/17	-
27	PL9	A	410	-	-	22/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
34	STE	b	623	-	-	11/17/17/17	-
34	STE	c	523	-	-	5/9/9/17	-
34	STE	R	101	-	-	4/9/9/17	-
29	SQD	A	415	-	-	12/39/39/69	-
22	CLA	C	501	3	-	1/39/115/115	-
24	BCR	c	514	-	-	6/29/63/63	0/2/2/2
22	CLA	b	610	37	-	7/39/115/115	-

The worst 5 of 862 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	9.23	1.49	1.39
22	b	606	CLA	MG-NA	8.45	2.26	2.06
22	C	511	CLA	MG-NA	8.43	2.26	2.06
23	d	402	PHO	C3B-C4B	8.34	1.49	1.41
23	D	401	PHO	C3B-C4B	8.24	1.49	1.41

The worst 5 of 1254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	10.58	111.51	106.68
22	B	601	CLA	C4A-NA-C1A	10.46	111.45	106.68
29	b	620	SQD	O6-C1-C2	9.54	122.76	108.27
22	b	601	CLA	C4A-NA-C1A	9.38	110.96	106.68
22	B	604	CLA	C4A-NA-C1A	9.28	110.91	106.68

All (2) chirality outliers are listed below:

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

5 of 1837 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
22	B	601	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

119 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	505	CLA	1	0
28	D	411	LMG	1	0
22	C	511	CLA	2	0
24	C	514	BCR	2	0
22	b	602	CLA	1	0
22	B	607	CLA	1	0
34	H	103	STE	1	0
34	b	621	STE	3	0
28	a	416	LMG	3	0
34	d	412	STE	2	0
31	c	518	DGD	2	0
23	A	404	PHO	1	0
24	H	101	BCR	1	0
34	d	413	STE	2	0
30	e	102	LHG	1	0
23	d	402	PHO	1	0
29	D	407	SQD	1	0
34	j	101	STE	2	0
24	b	618	BCR	2	0
22	B	606	CLA	2	0
34	h	102	STE	3	0
22	b	601	CLA	2	0
28	A	412	LMG	2	0
22	D	403	CLA	2	0
22	B	611	CLA	1	0
28	c	521	LMG	1	0
24	B	618	BCR	1	0
22	b	604	CLA	2	0
22	B	603	CLA	3	0
22	b	612	CLA	2	0
31	A	416	DGD	4	0
34	Z	101	STE	1	0
27	a	409	PL9	2	0
22	c	513	CLA	1	0
24	T	101	BCR	1	0
22	A	411	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	101	STE	2	0
34	B	627	STE	1	0
31	C	516	DGD	1	0
34	T	102	STE	1	0
22	a	404	CLA	3	0
22	c	506	CLA	1	0
22	C	502	CLA	1	0
24	c	515	BCR	1	0
24	B	619	BCR	1	0
22	a	410	CLA	1	0
24	d	405	BCR	2	0
29	A	413	SQD	3	0
22	b	615	CLA	4	0
36	v	201	HEC	3	0
24	k	101	BCR	1	0
22	c	507	CLA	1	0
35	e	101	HEM	6	0
22	c	505	CLA	1	0
22	C	512	CLA	3	0
35	F	101	HEM	3	0
29	b	620	SQD	1	0
22	C	506	CLA	1	0
32	A	417[B]	OEY	2	0
30	d	409	LHG	1	0
28	C	518	LMG	1	0
22	B	613	CLA	1	0
24	t	101	BCR	4	0
31	c	517	DGD	3	0
31	h	101	DGD	1	0
30	B	622	LHG	1	0
22	C	508	CLA	1	0
32	a	418[B]	OEY	2	0
24	D	404	BCR	1	0
22	C	513	CLA	2	0
30	D	409	LHG	3	0
29	a	412	SQD	1	0
34	I	101	STE	2	0
22	c	512	CLA	1	0
29	B	623	SQD	1	0
30	d	408	LHG	2	0
28	M	101	LMG	1	0
22	B	614	CLA	2	0

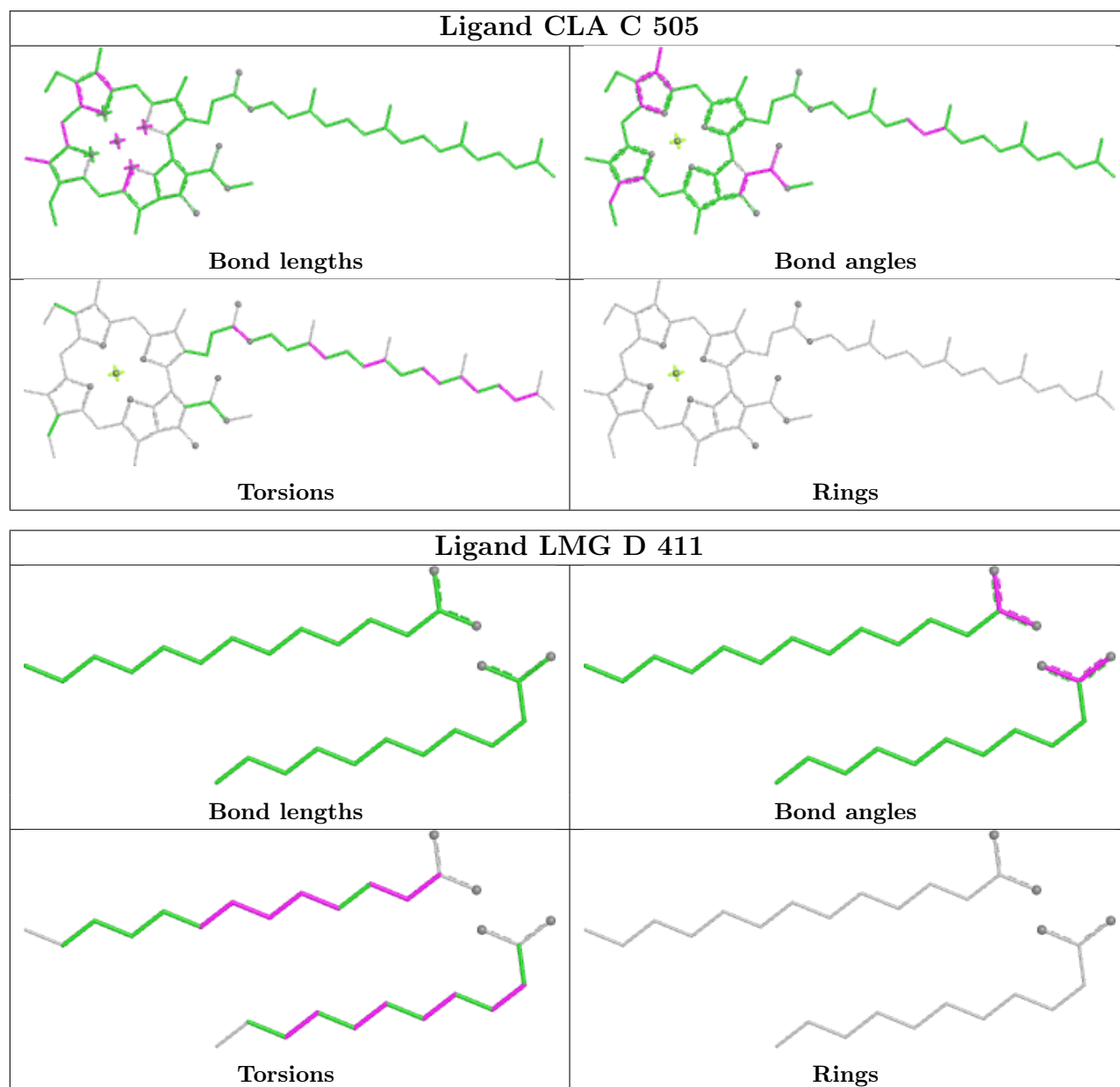
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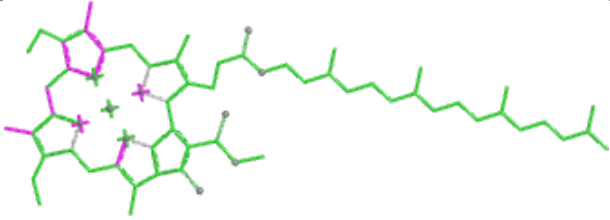
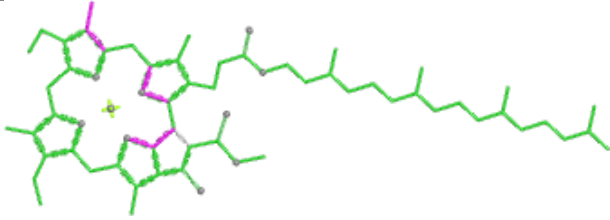
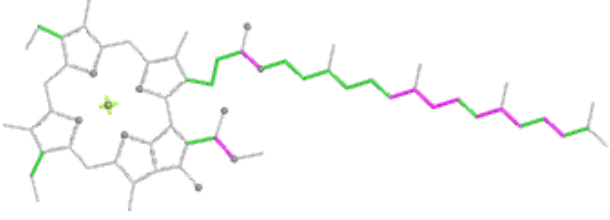
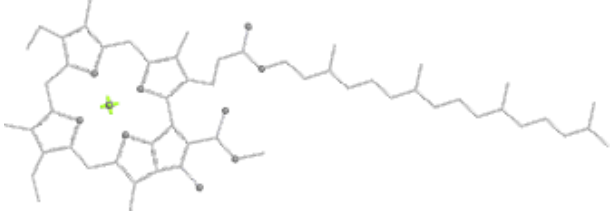
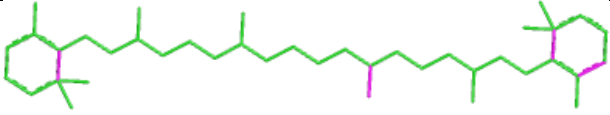
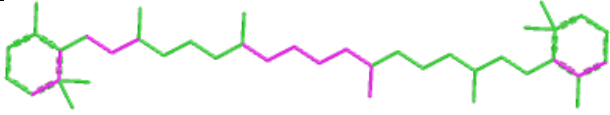
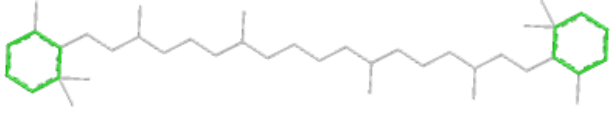
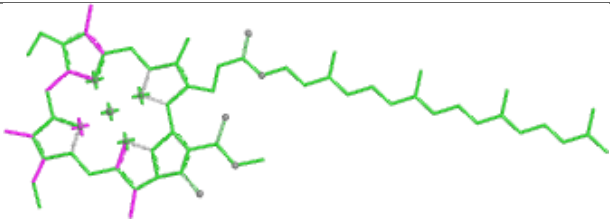
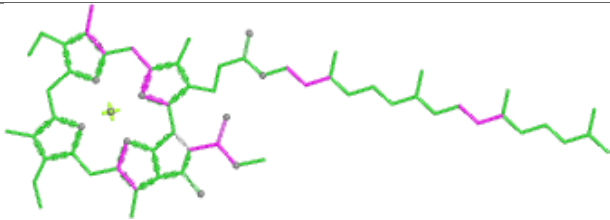
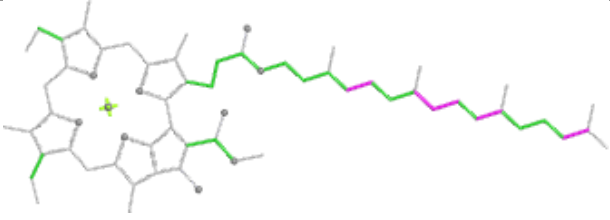
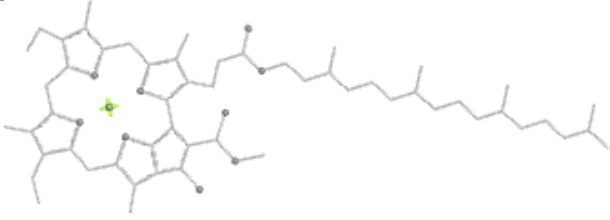
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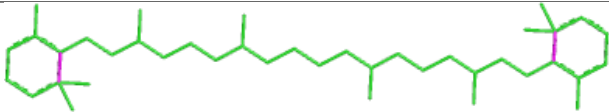
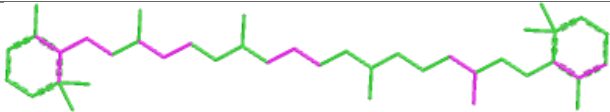
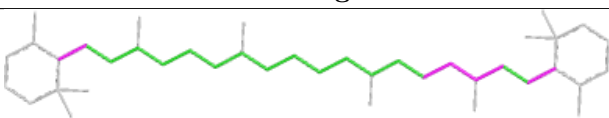
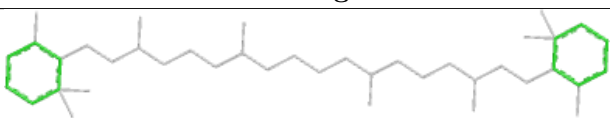
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	608	CLA	3	0
34	c	520	STE	2	0
22	c	503	CLA	1	0
28	c	522	LMG	6	0
34	a	414	STE	4	0
24	b	617	BCR	2	0
34	B	624	STE	2	0
29	f	101	SQD	2	0
22	c	511	CLA	2	0
34	L	101	STE	1	0
22	C	503	CLA	1	0
22	C	509	CLA	3	0
22	B	601	CLA	1	0
34	M	102	STE	1	0
22	b	614	CLA	4	0
22	B	609	CLA	2	0
22	b	605	CLA	2	0
30	d	407	LHG	2	0
34	b	626	STE	1	0
22	b	606	CLA	2	0
28	b	622	LMG	1	0
22	b	607	CLA	1	0
22	c	501	CLA	2	0
28	D	406	LMG	2	0
22	b	609	CLA	1	0
34	b	627	STE	1	0
22	B	602	CLA	2	0
34	l	102	STE	2	0
34	C	520	STE	1	0
30	D	408	LHG	1	0
22	B	604	CLA	1	0
34	B	620	STE	1	0
22	b	616	CLA	1	0
34	M	103	STE	1	0
27	A	410	PL9	4	0
23	D	401	PHO	1	0
34	b	623	STE	3	0
34	R	101	STE	1	0
29	A	415	SQD	1	0
22	C	501	CLA	1	0
22	b	610	CLA	1	0

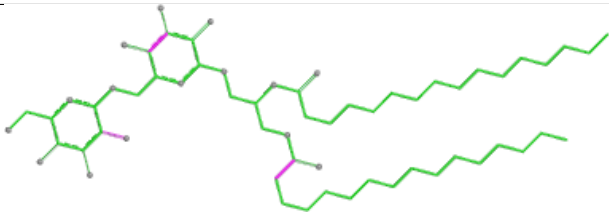
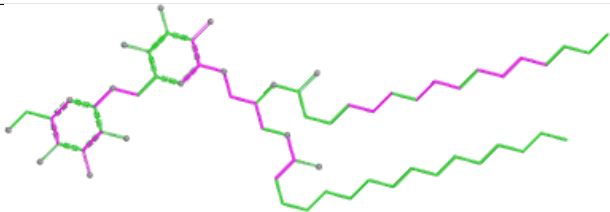
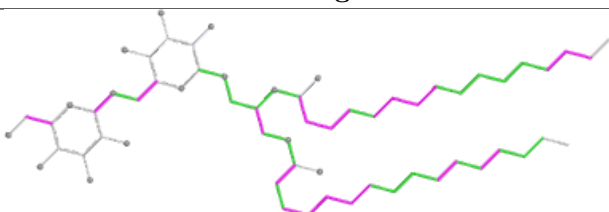
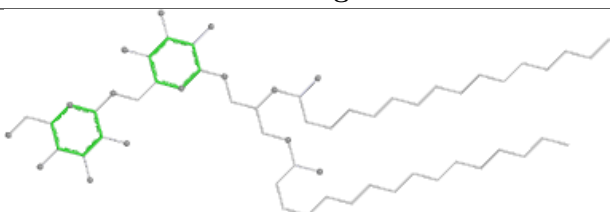
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

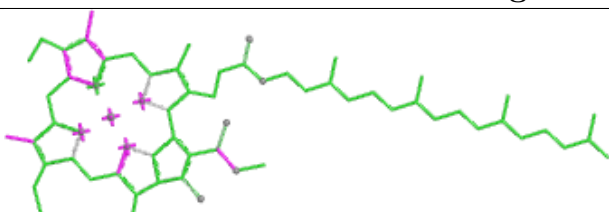
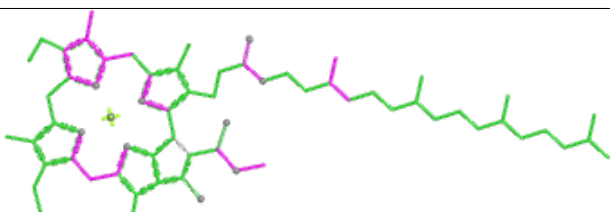
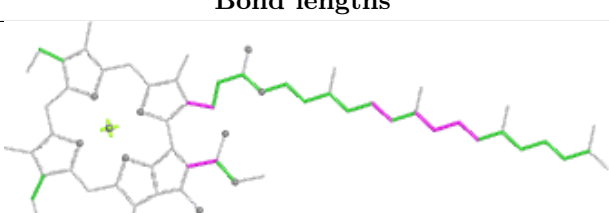
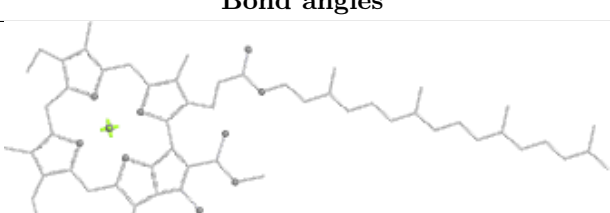
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

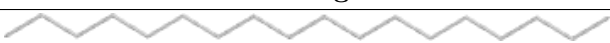


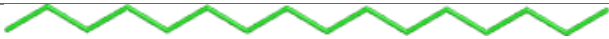
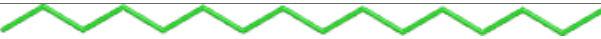
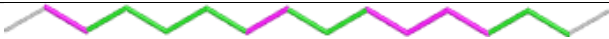
Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

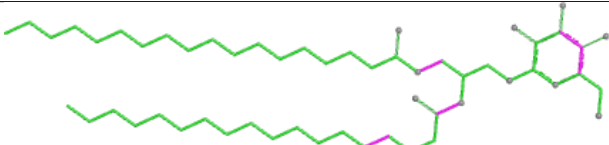
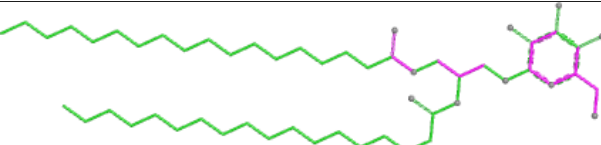
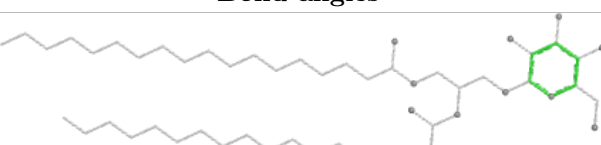
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

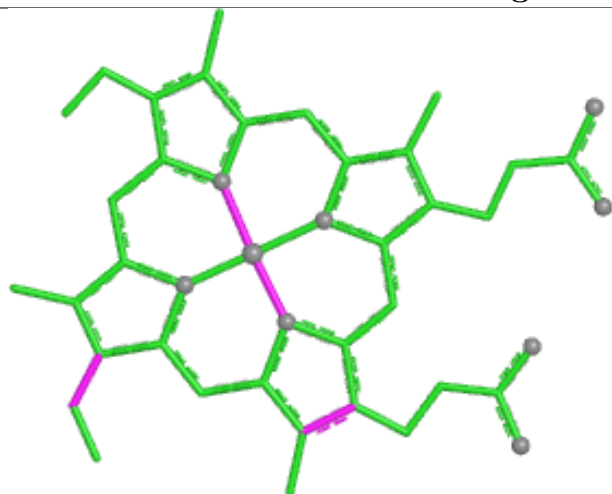
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

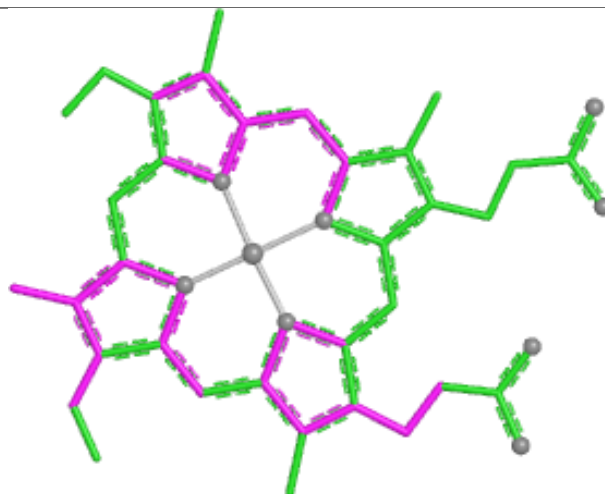
Ligand LMG a 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

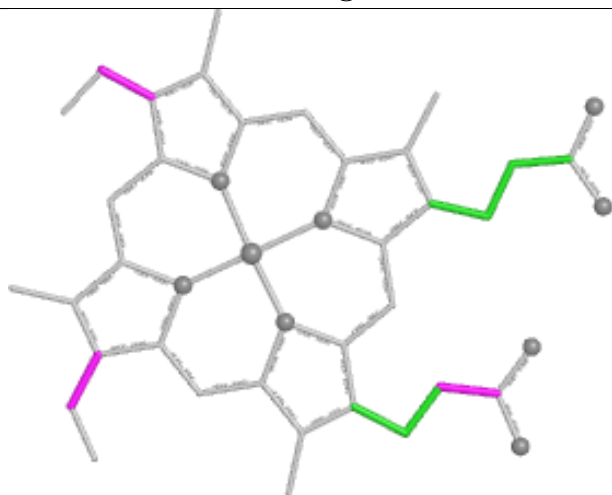
Ligand HEC V 201



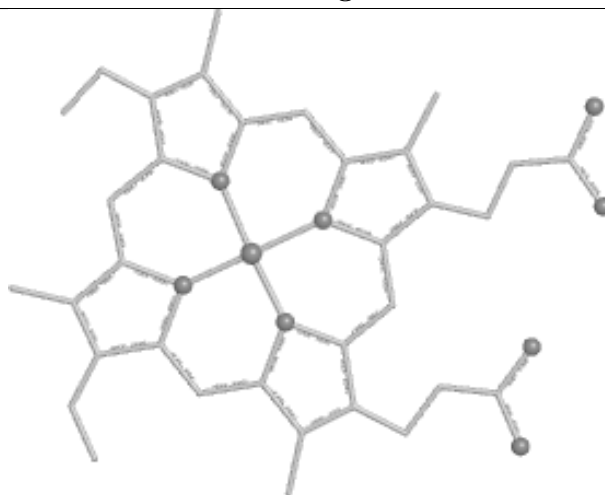
Bond lengths



Bond angles

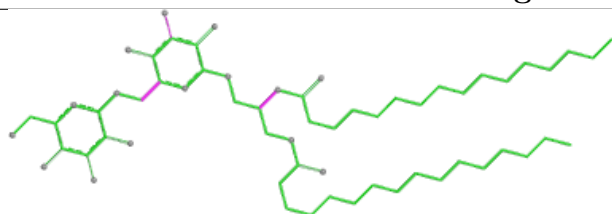


Torsions

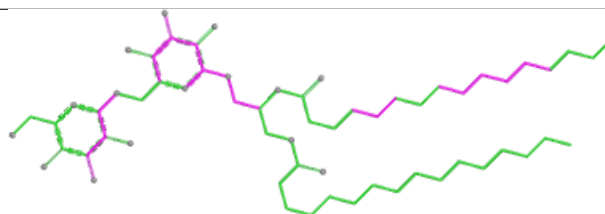


Rings

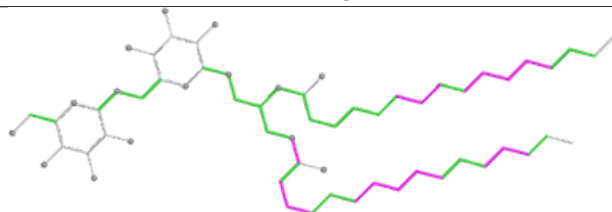
Ligand DGD c 518



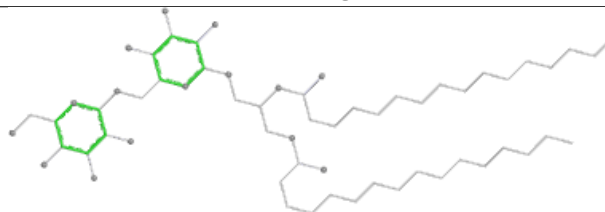
Bond lengths



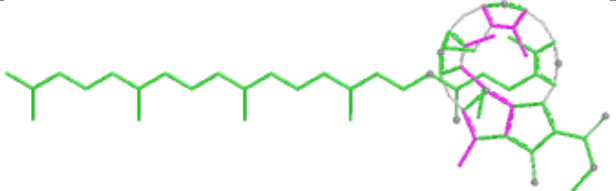
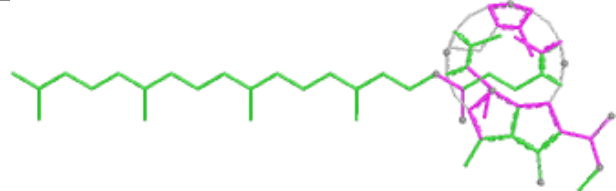
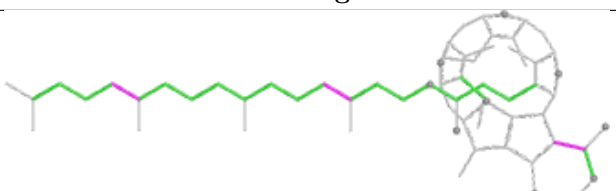
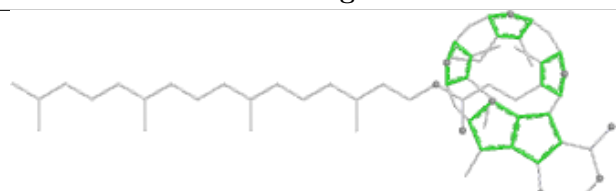
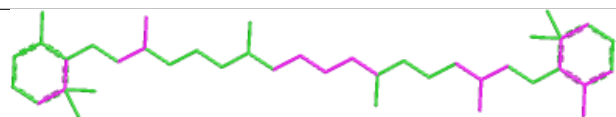
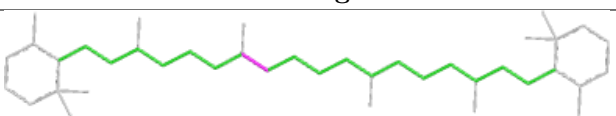
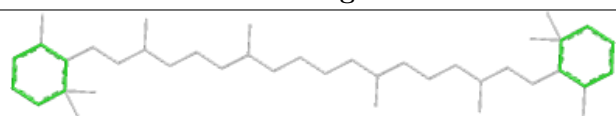
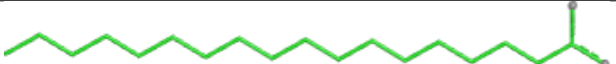
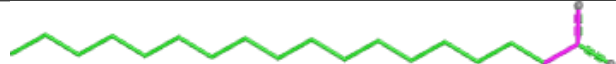
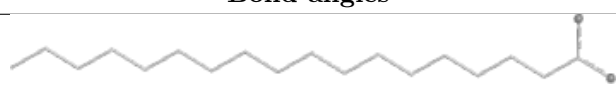
Bond angles

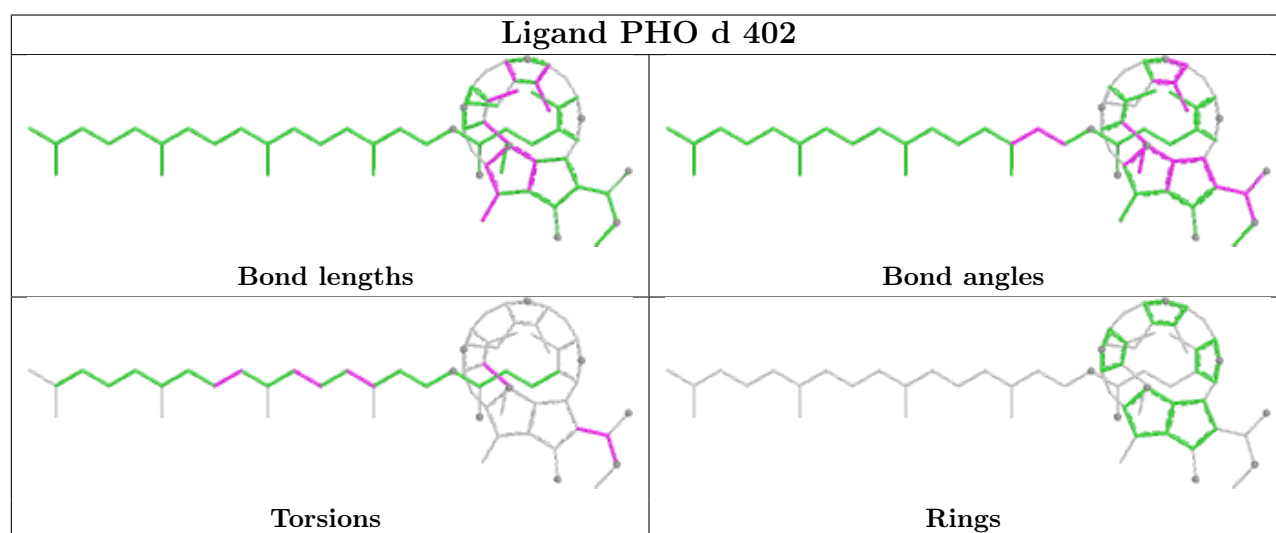
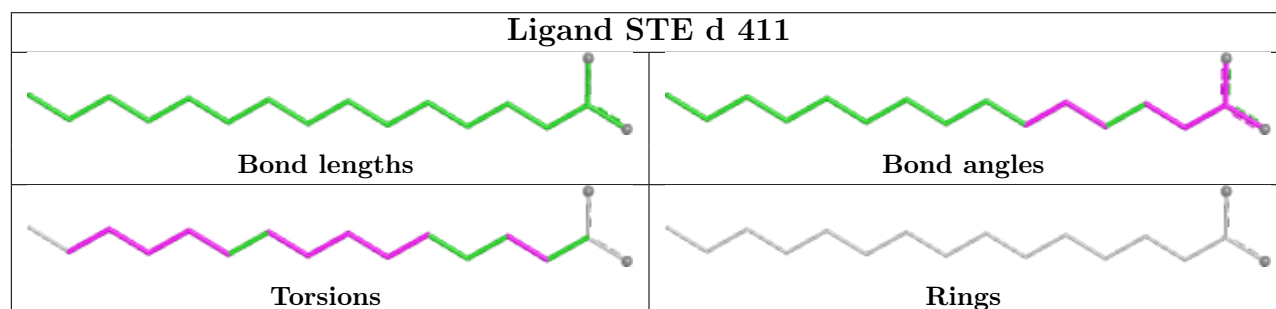
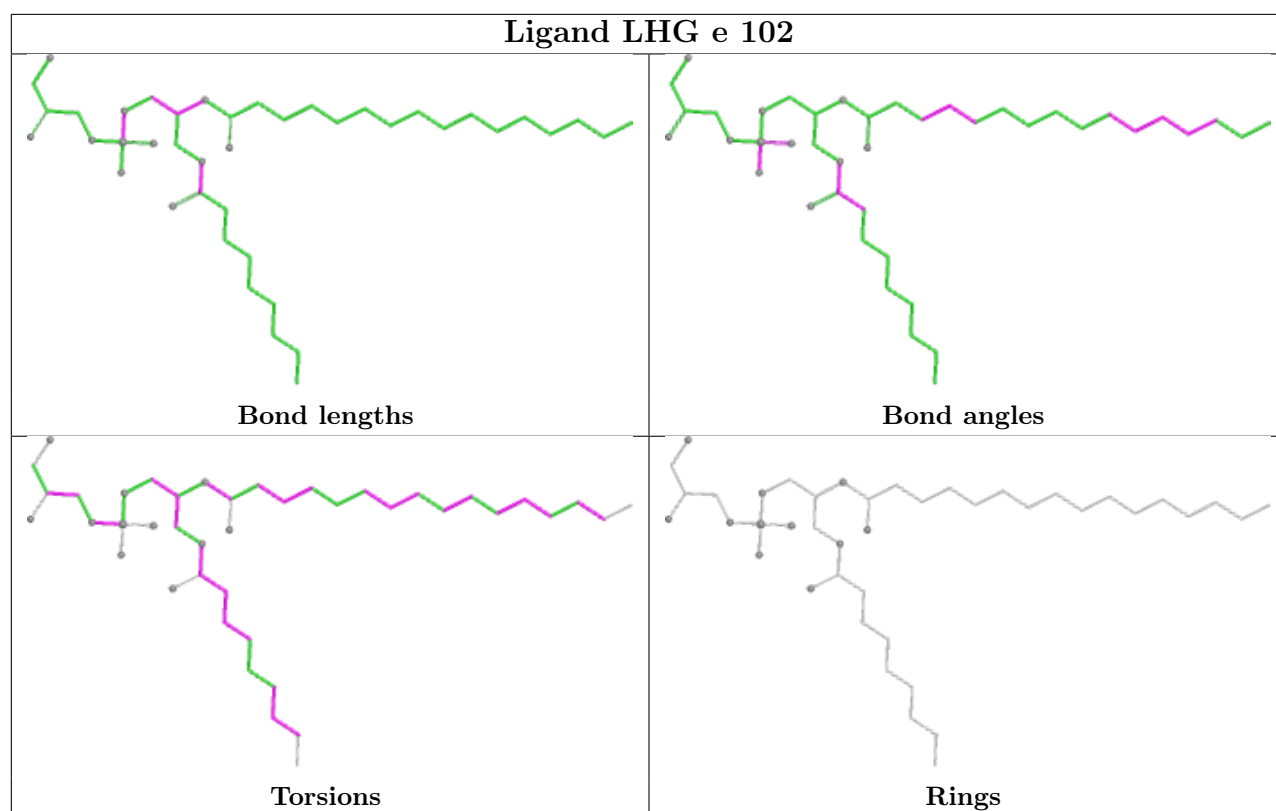


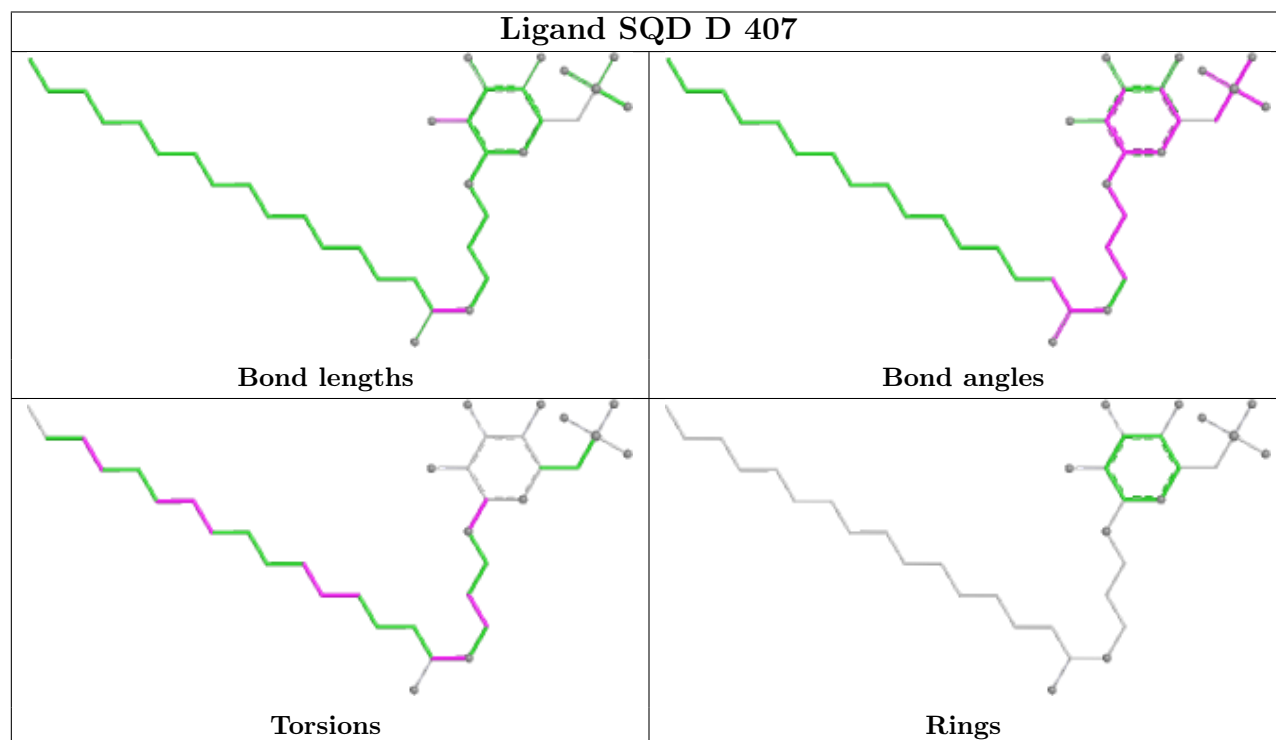
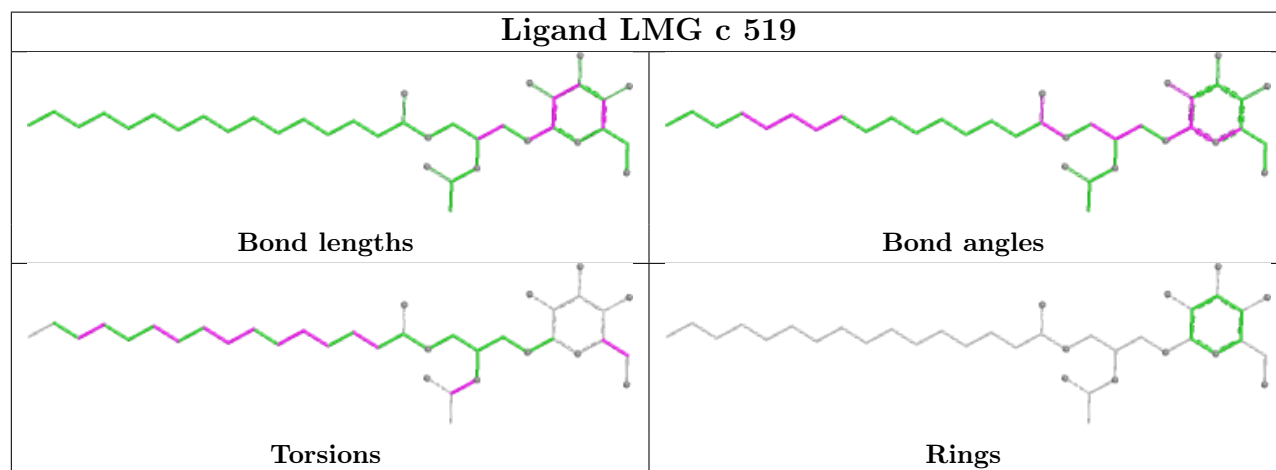
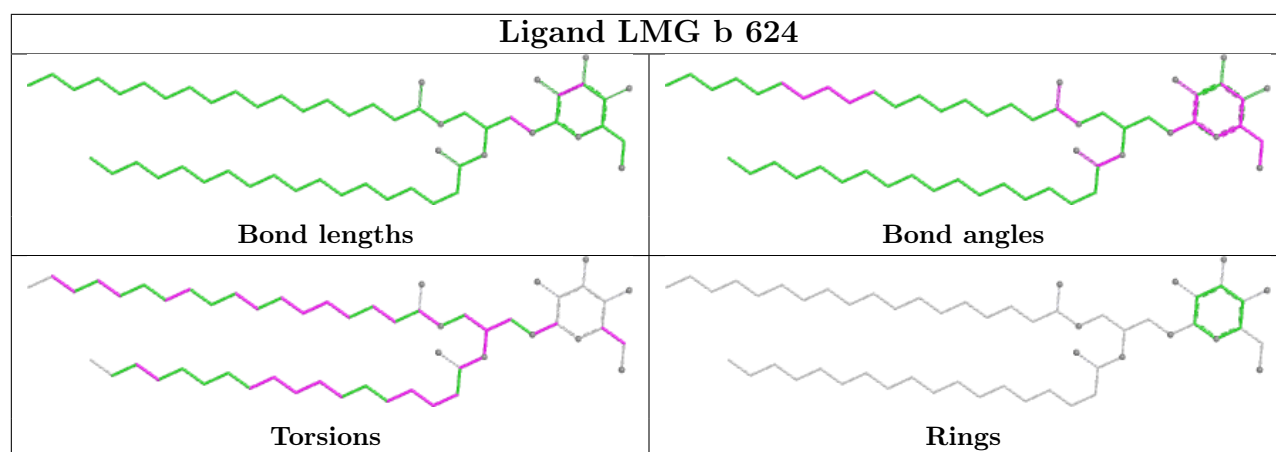
Torsions

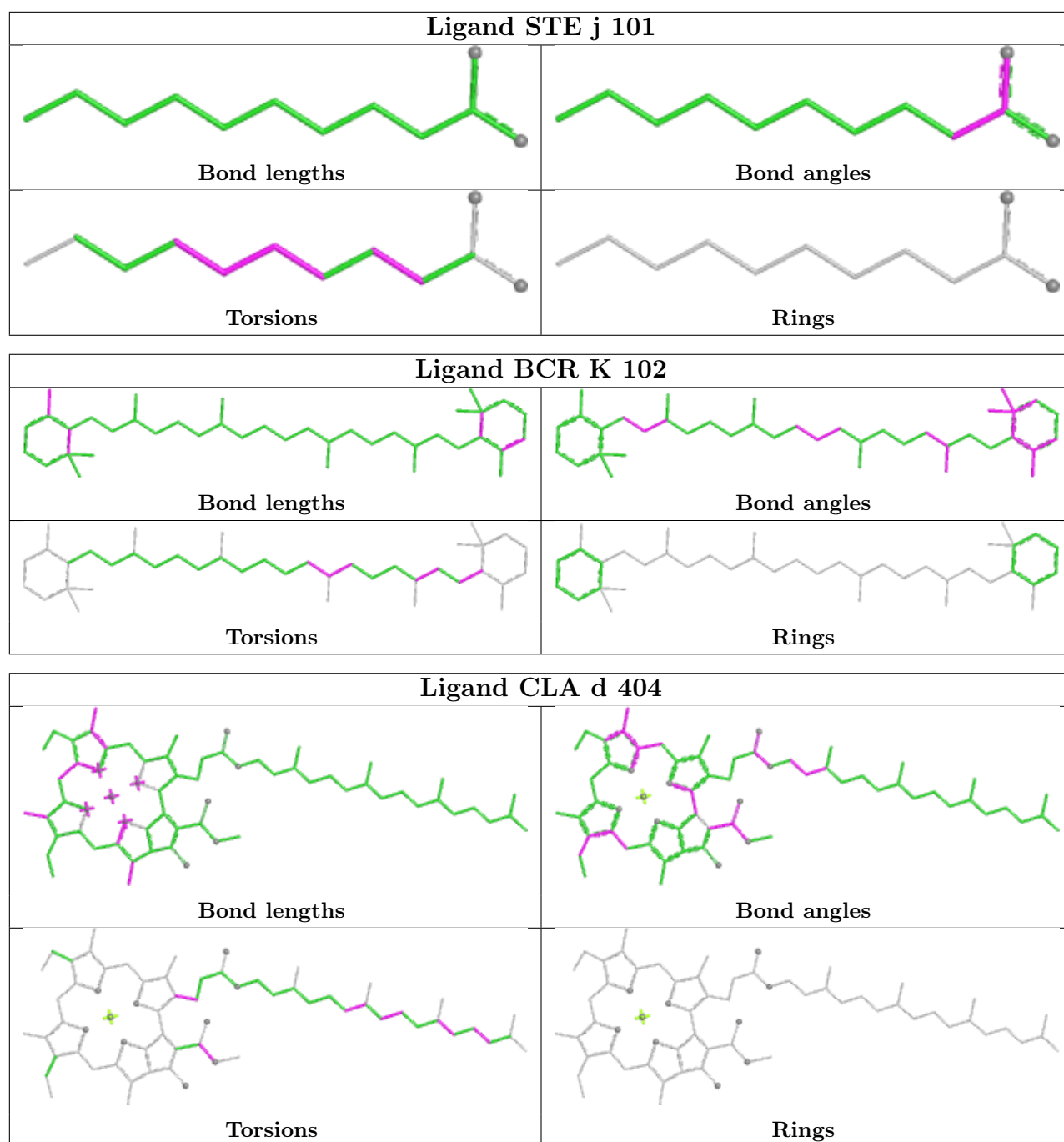


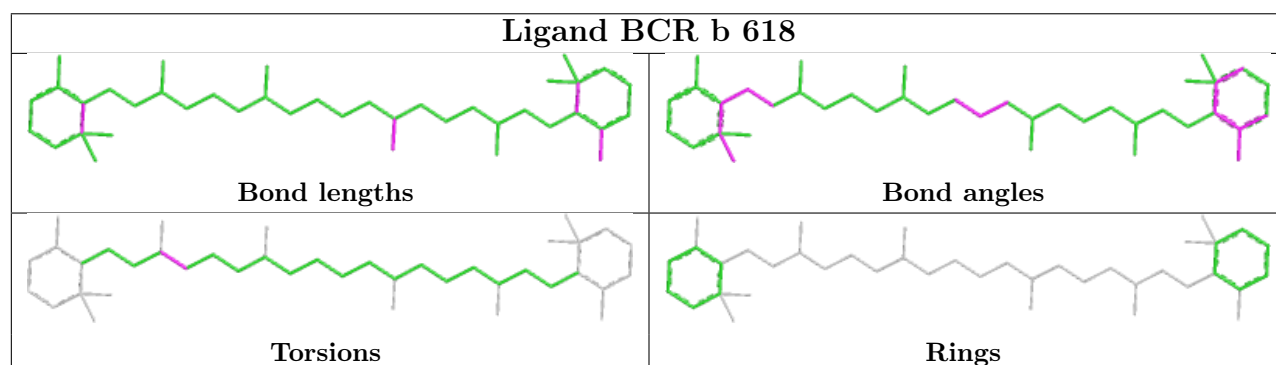
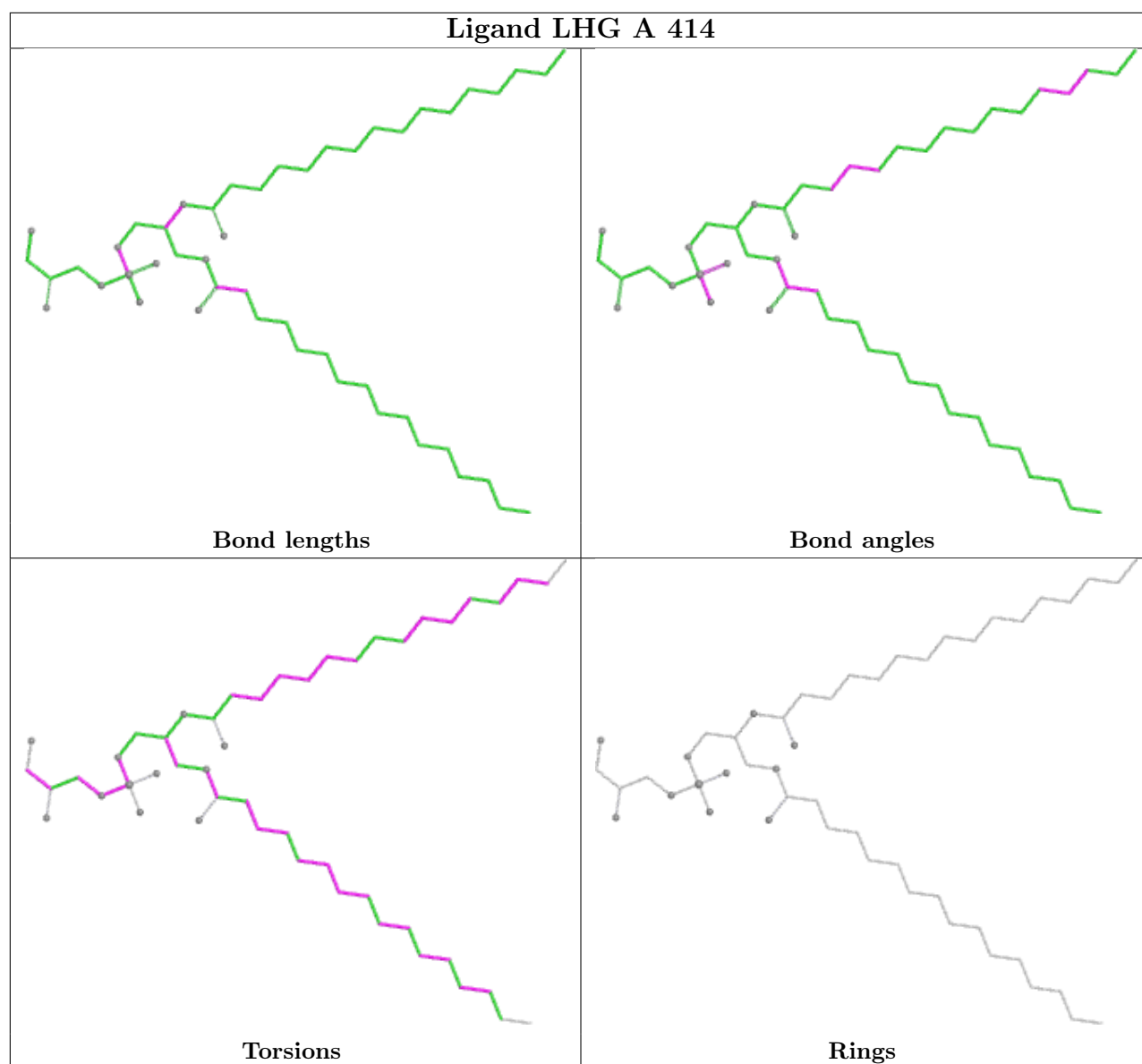
Rings

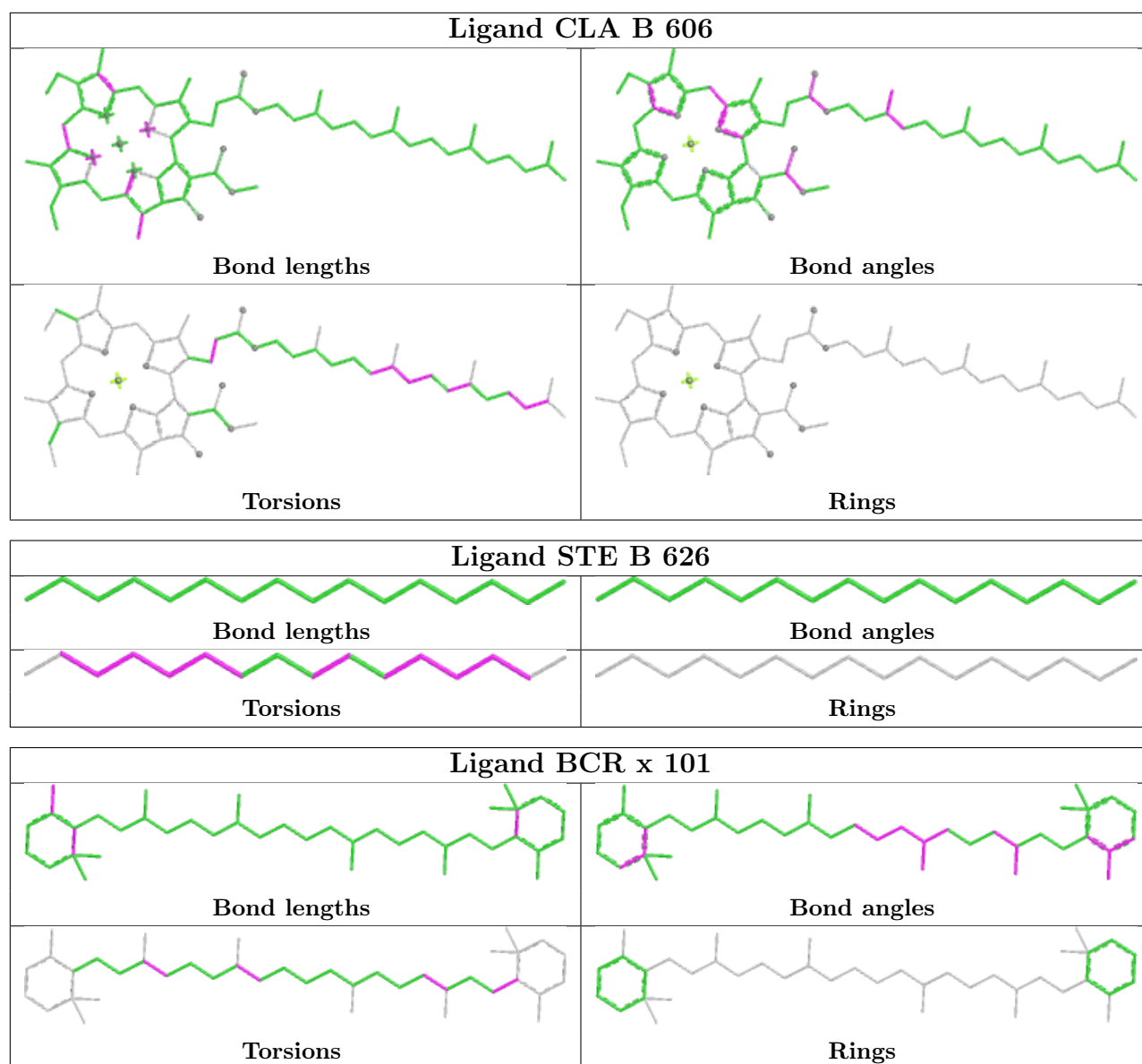
Ligand PHO A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE d 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

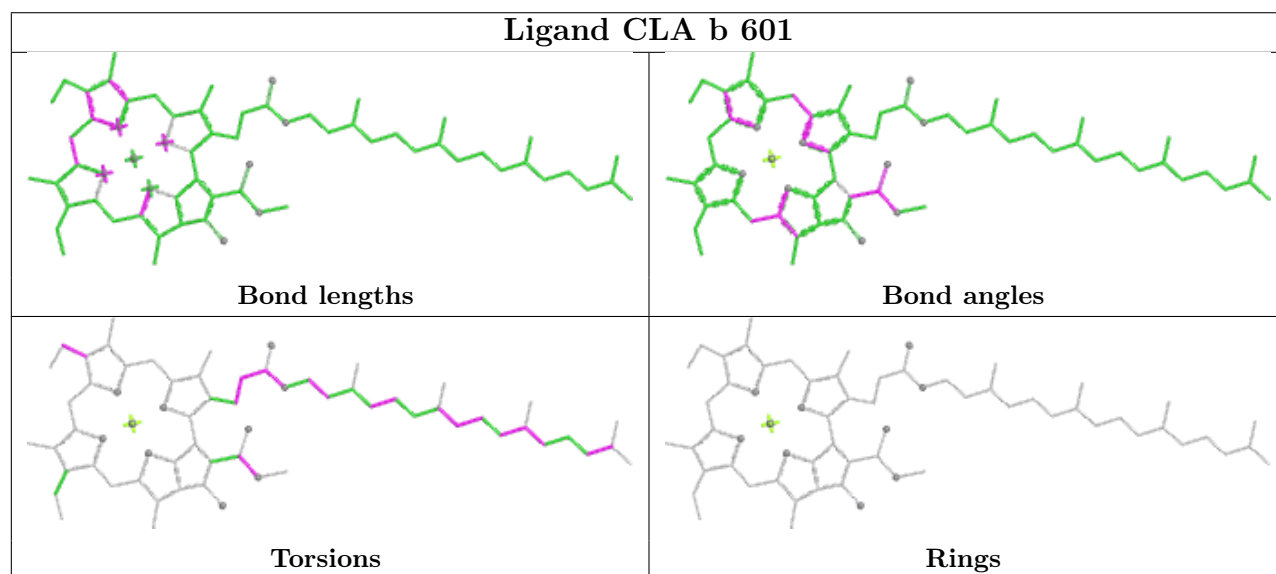
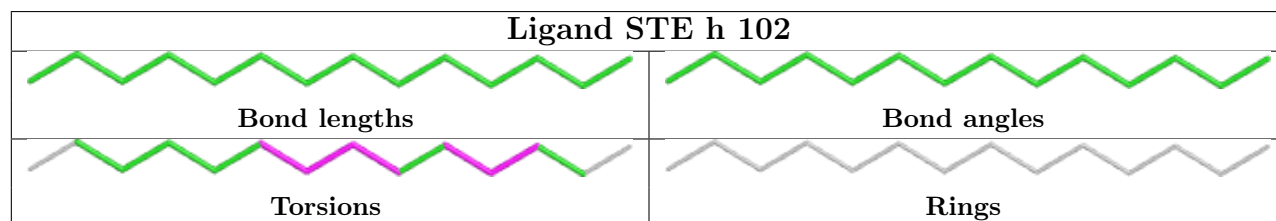
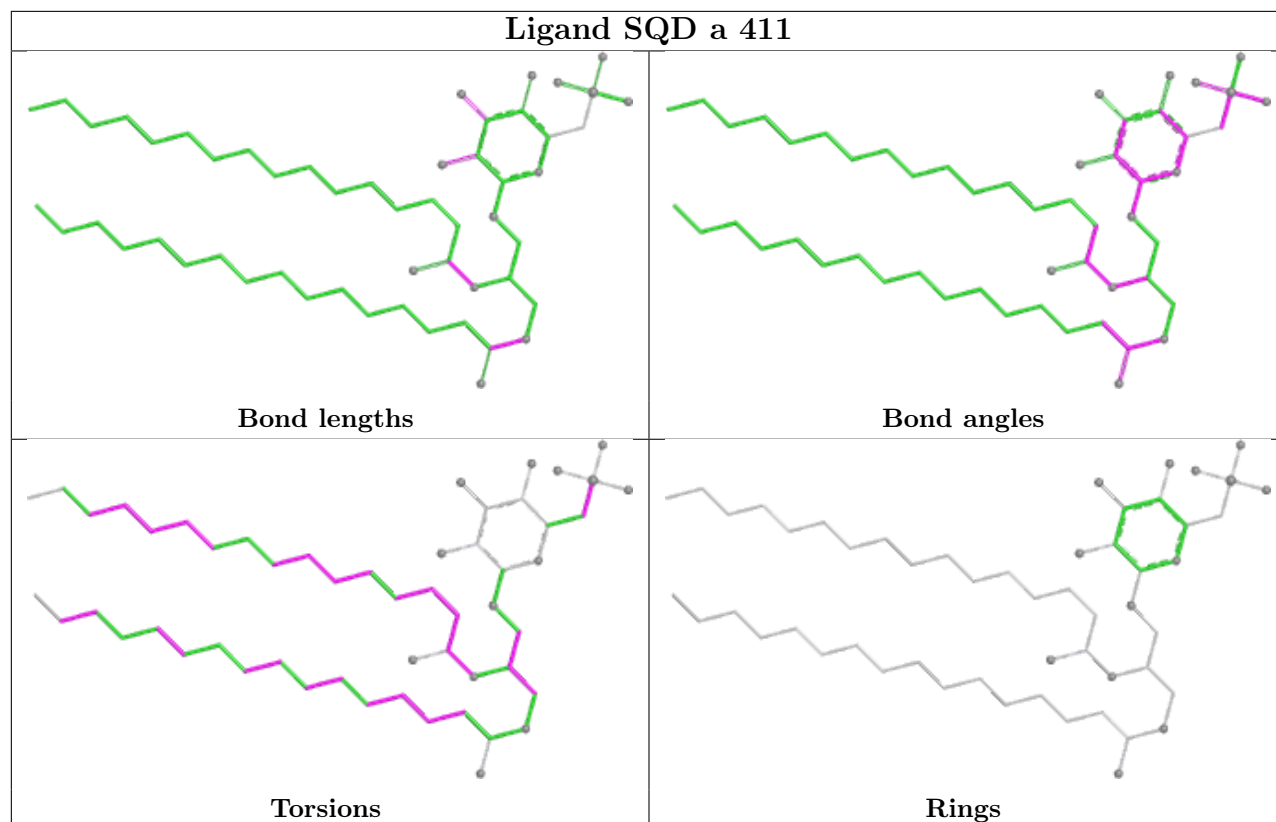


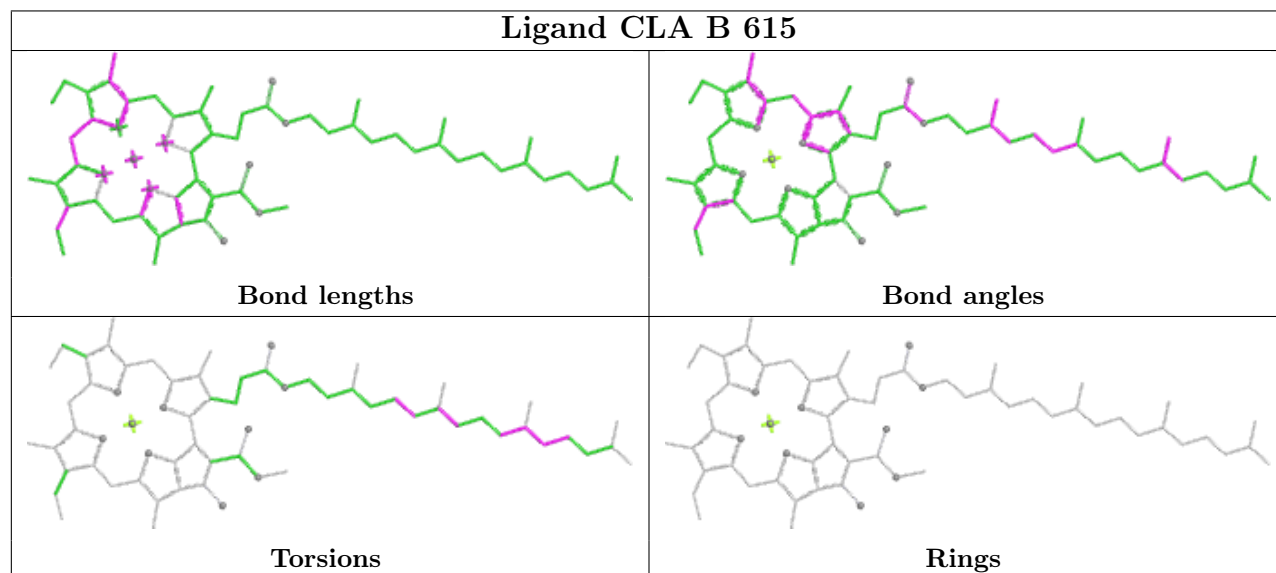
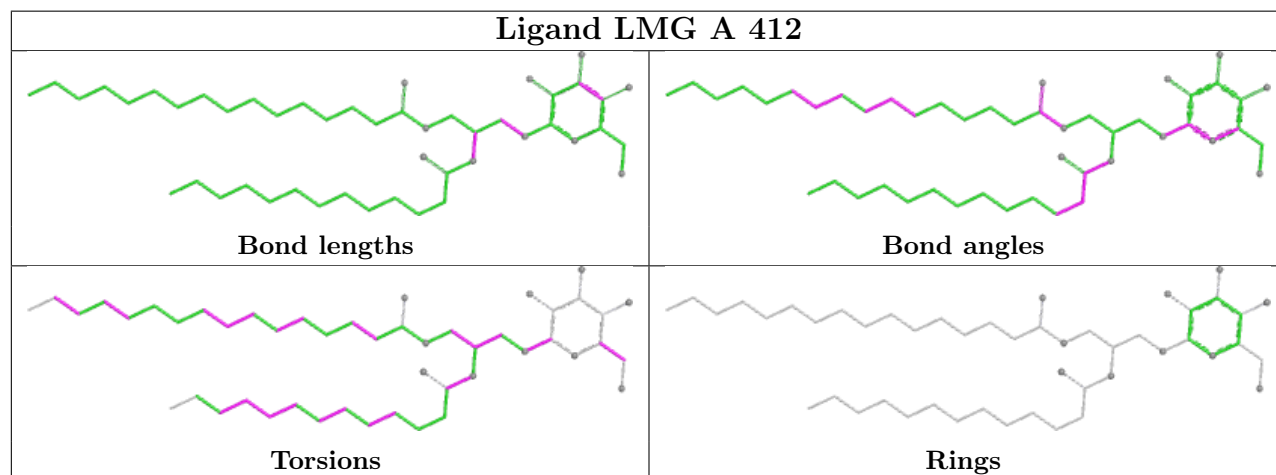
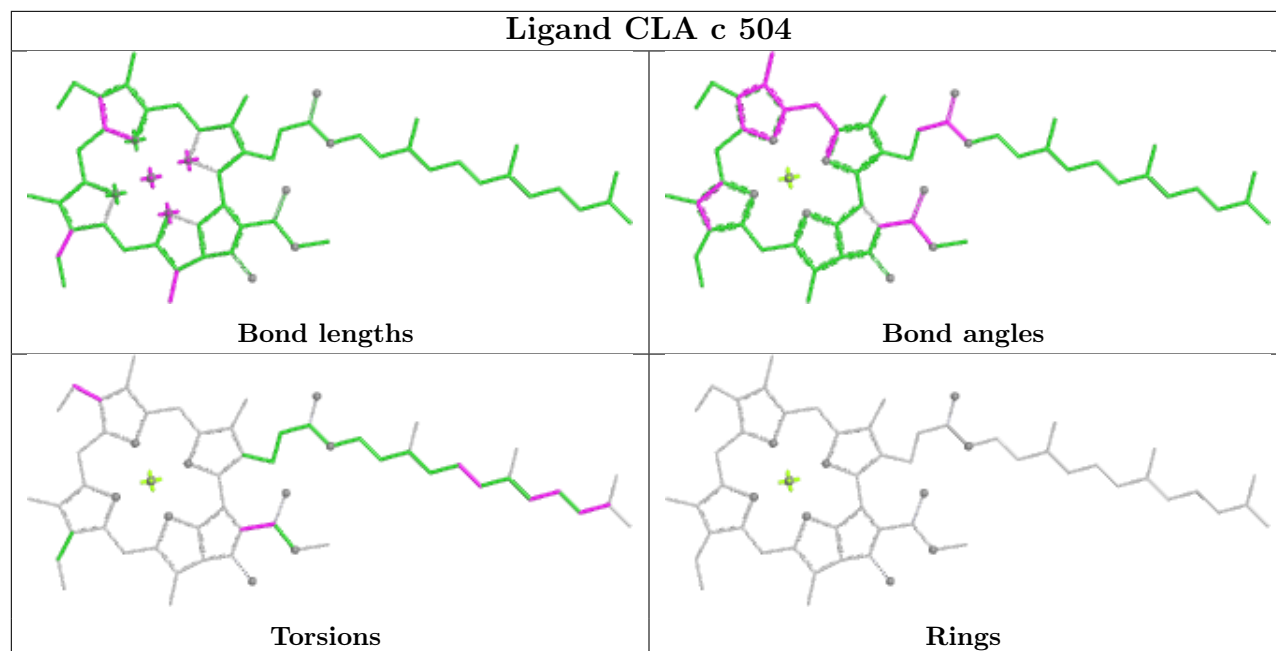


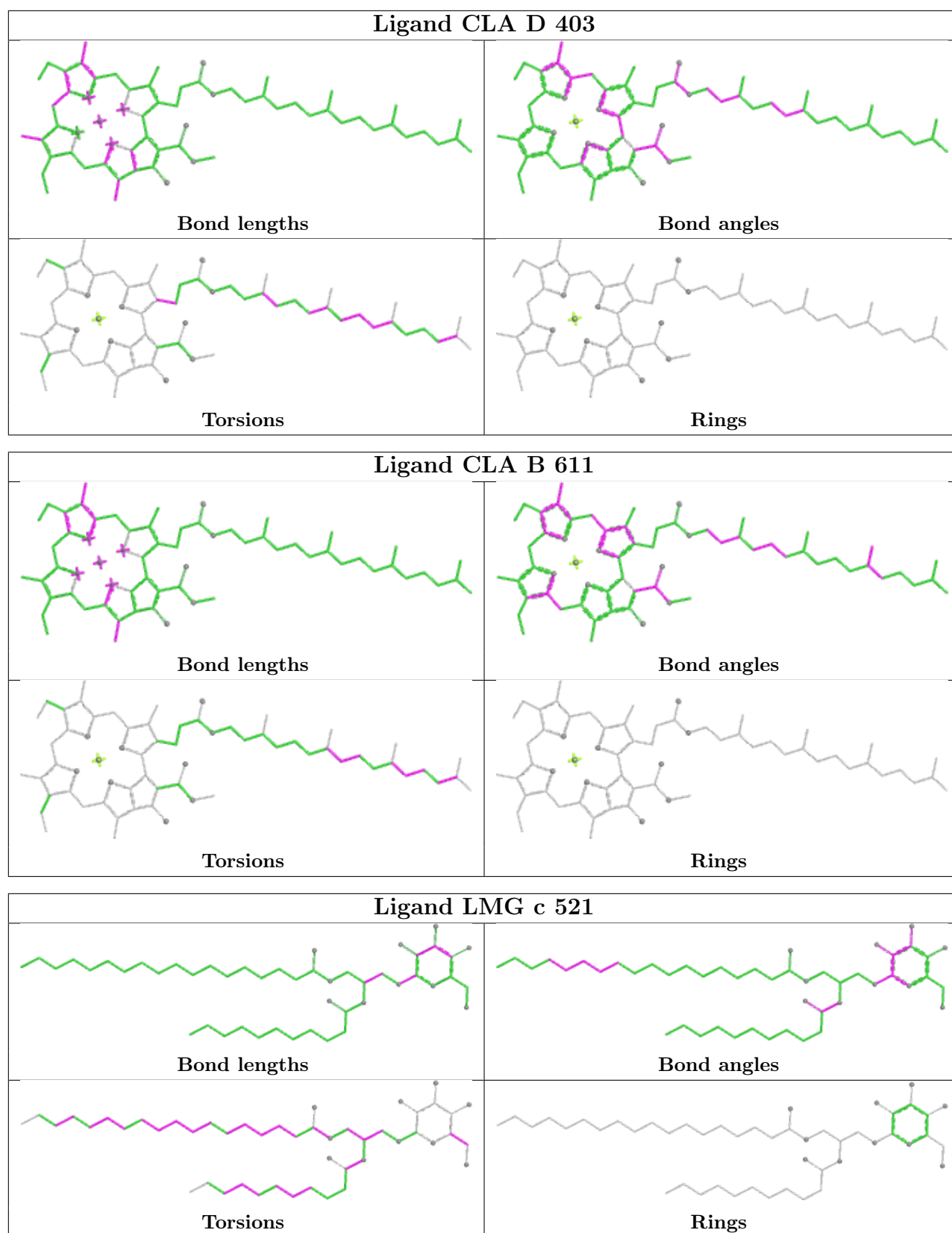


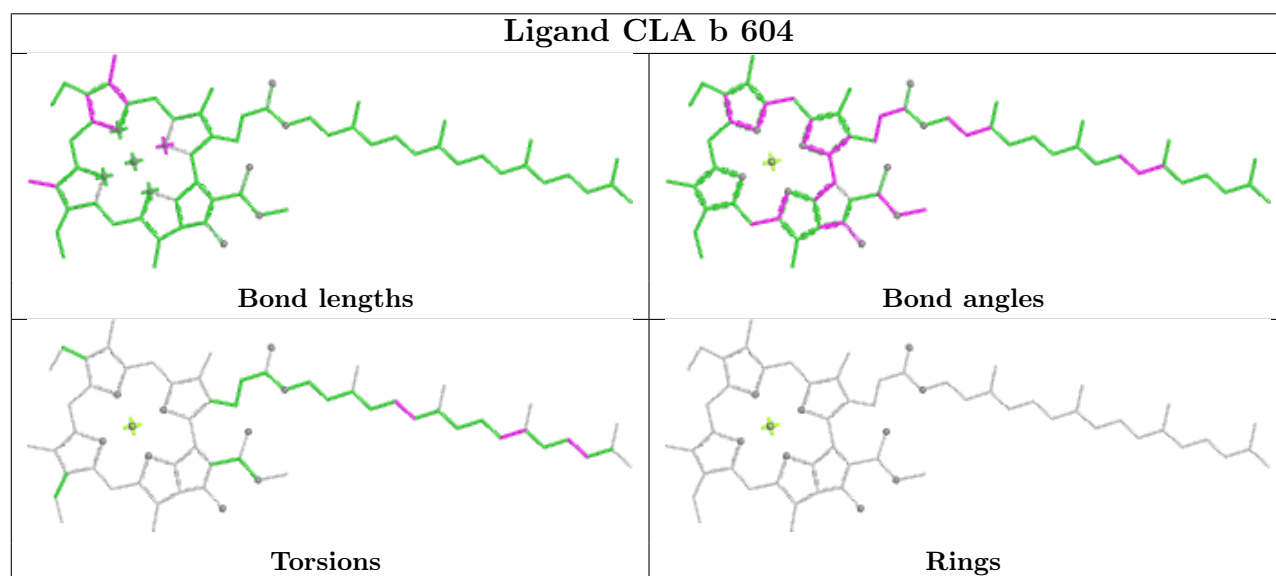
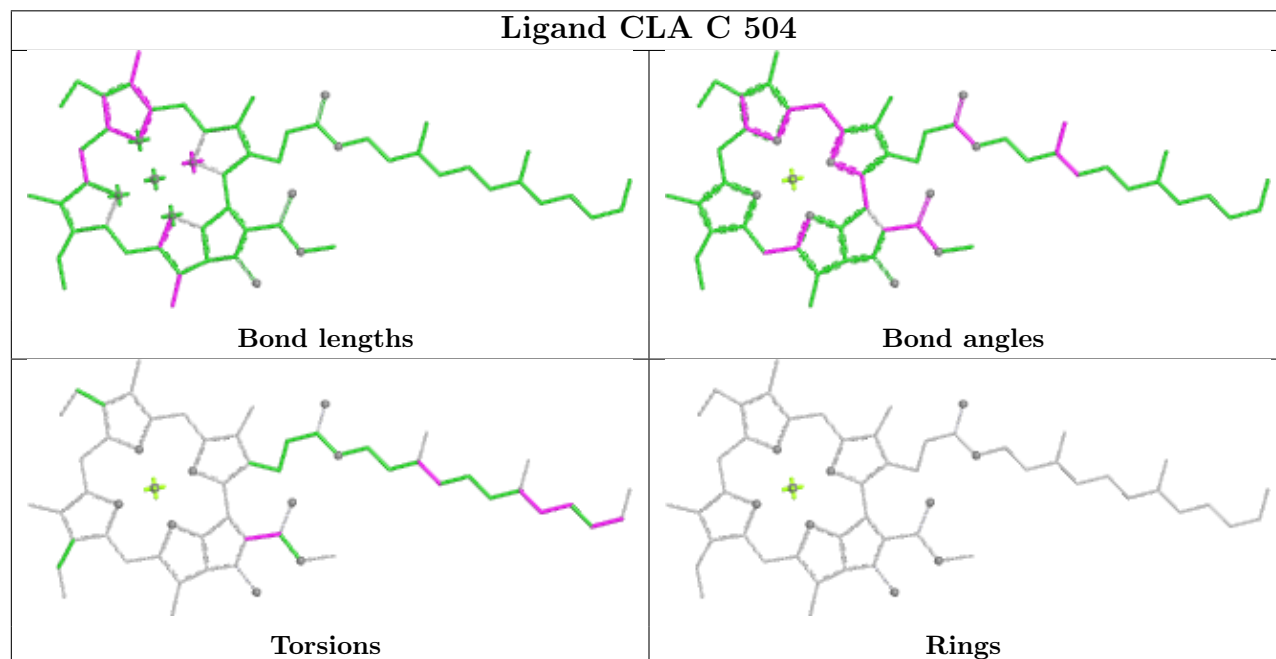
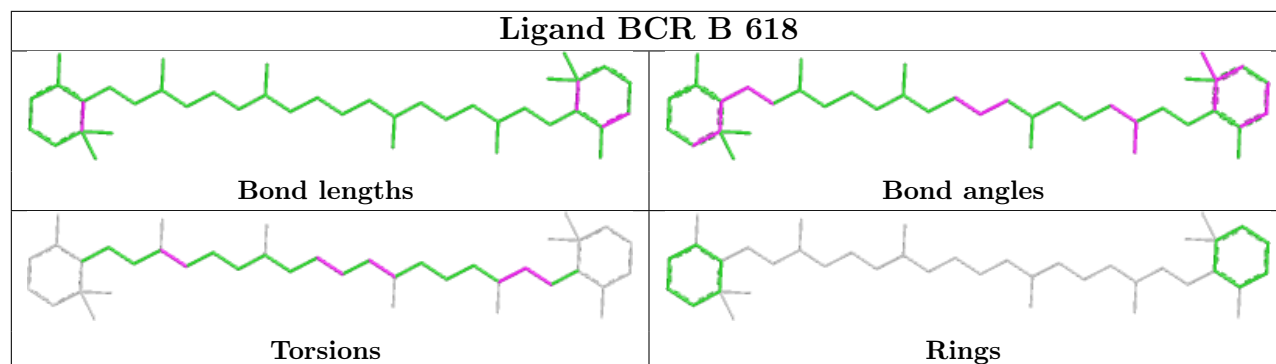


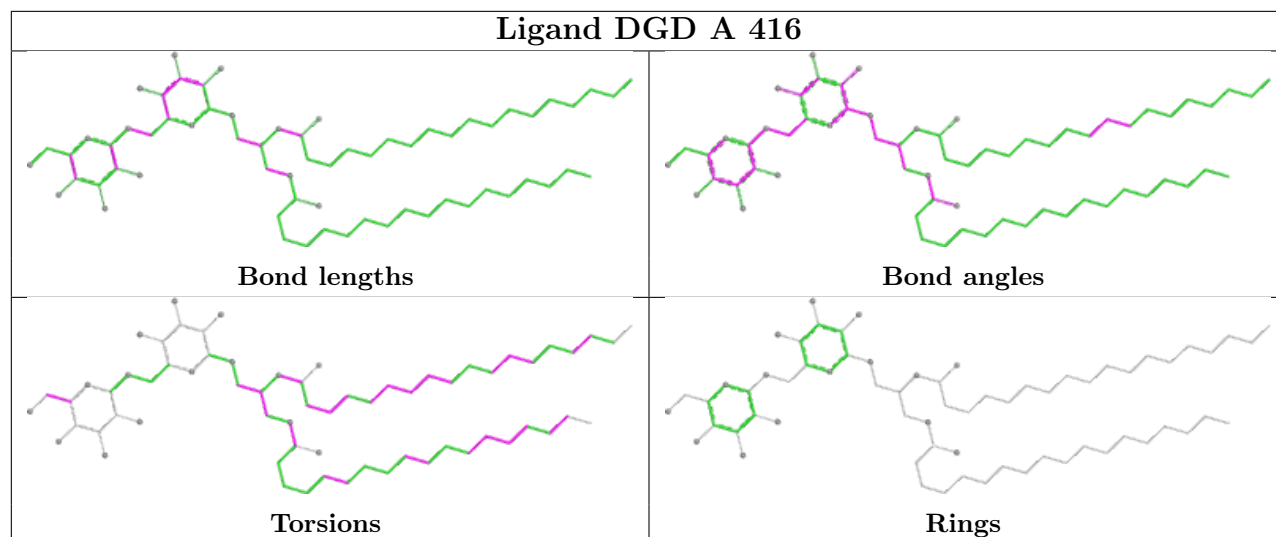
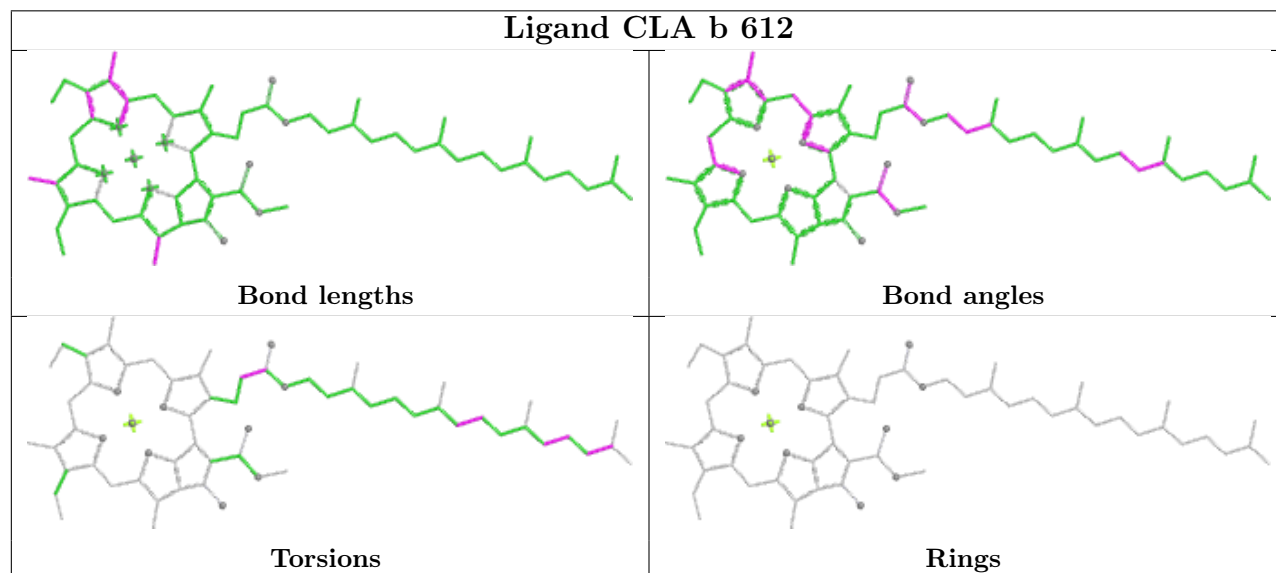
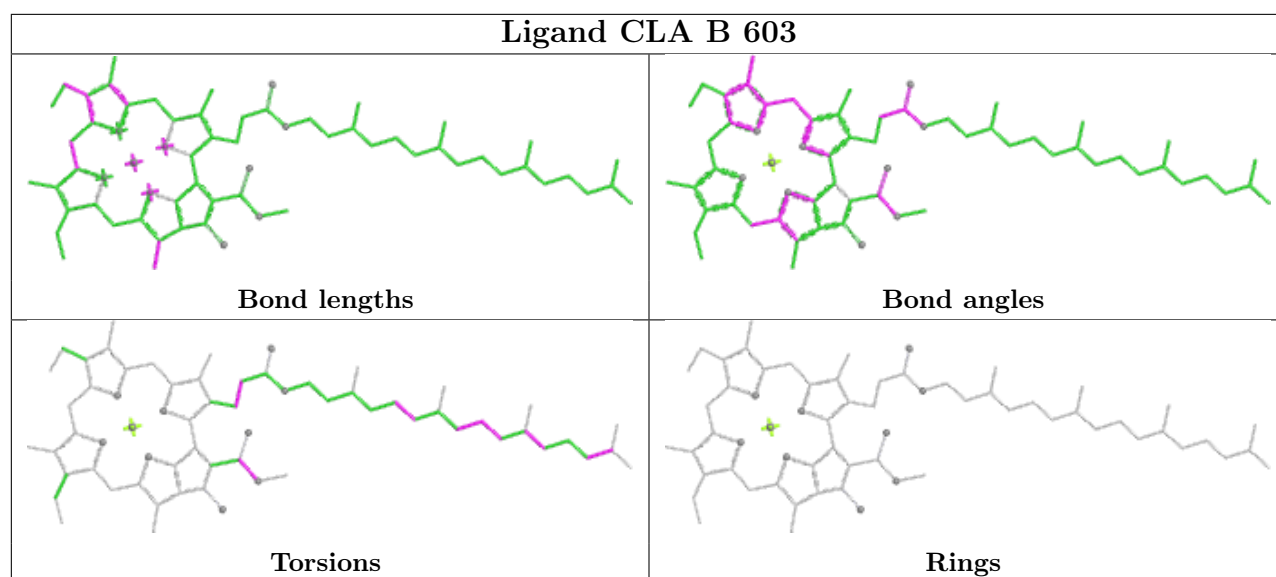


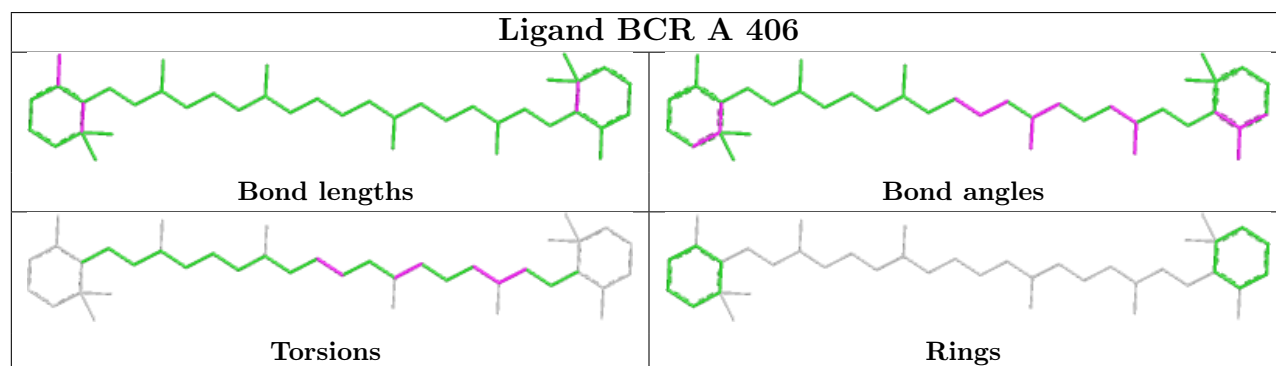
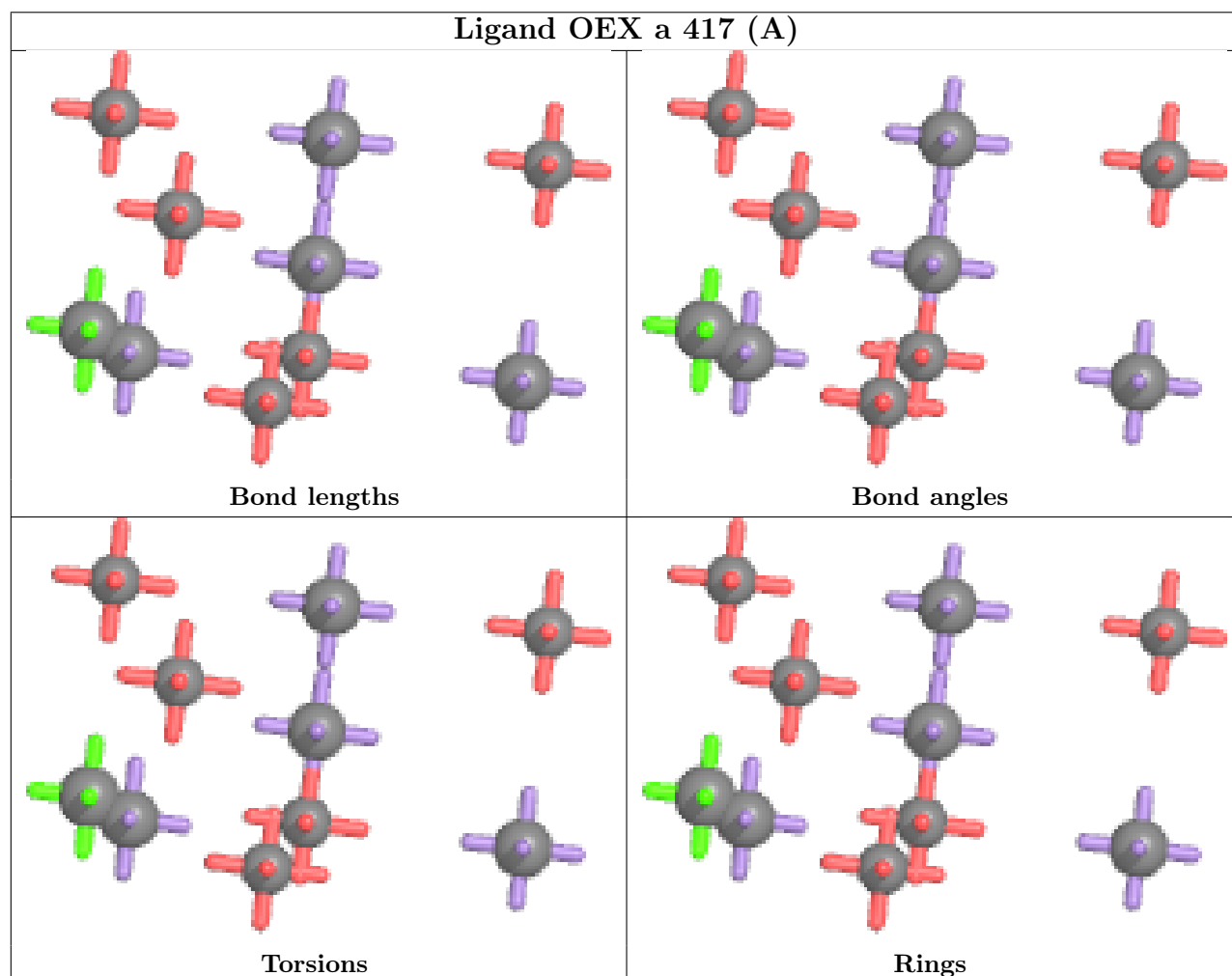
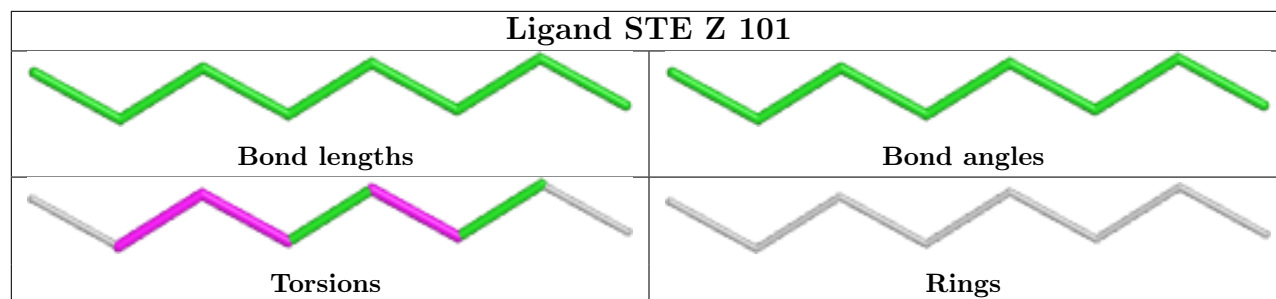


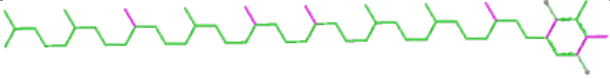
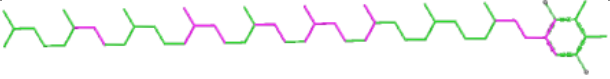
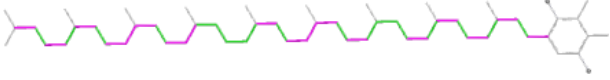
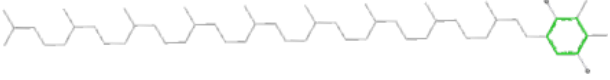


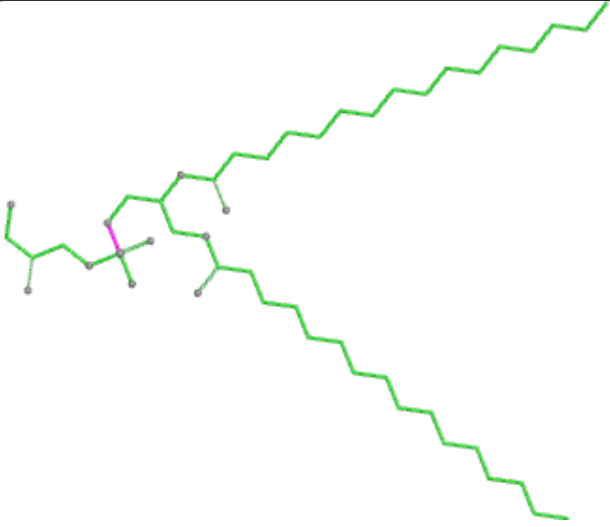
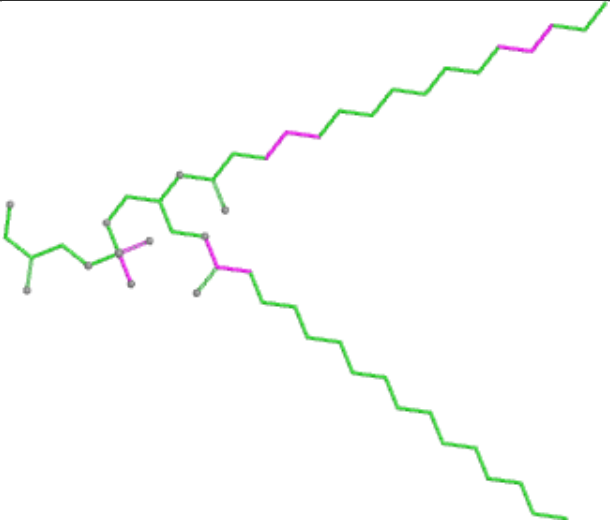
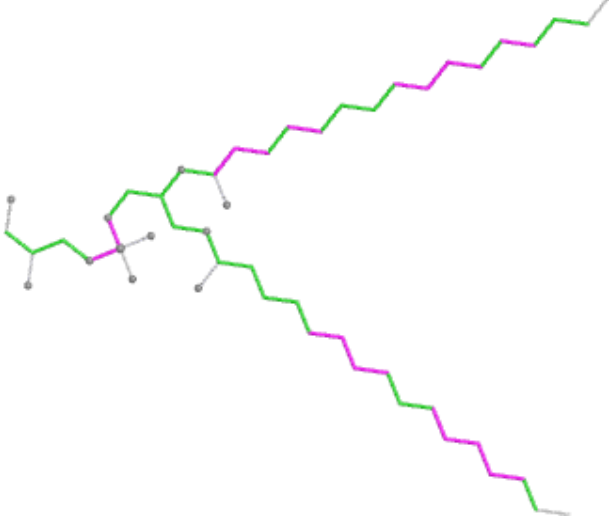
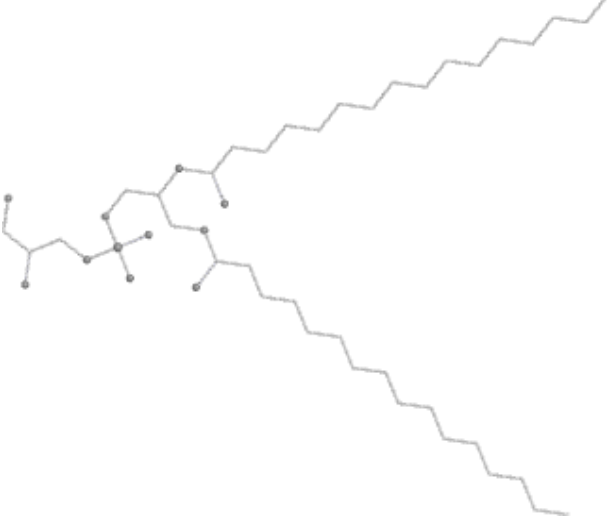


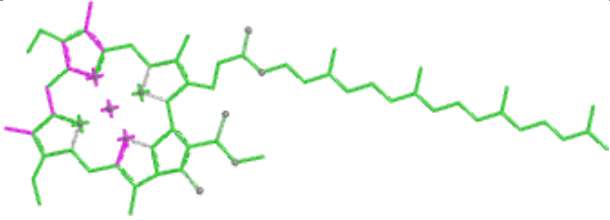
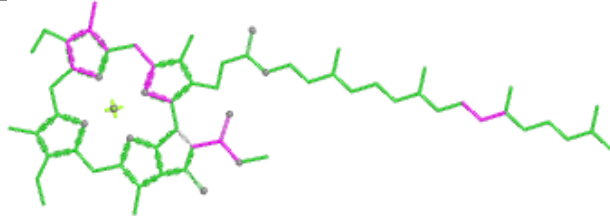
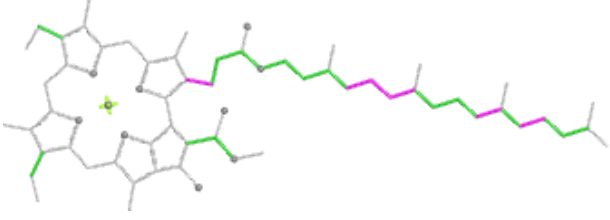
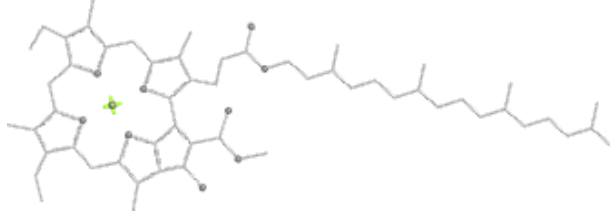
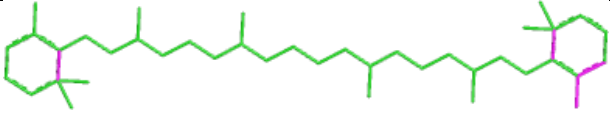
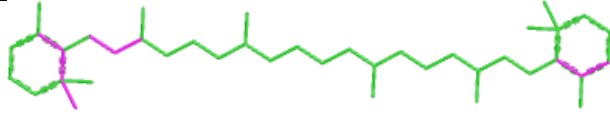
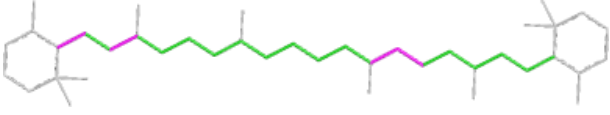
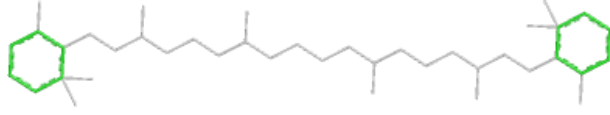
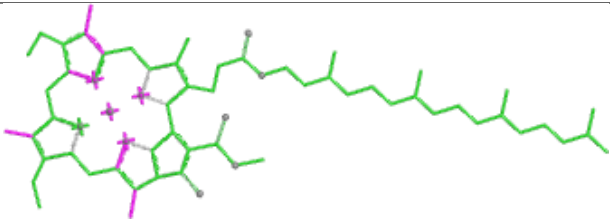
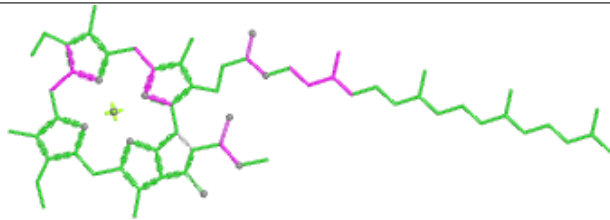
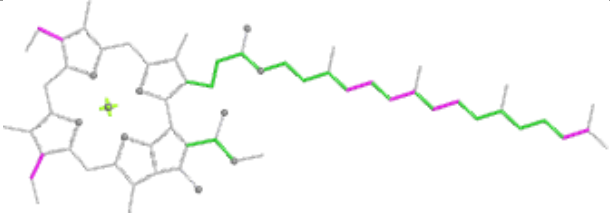
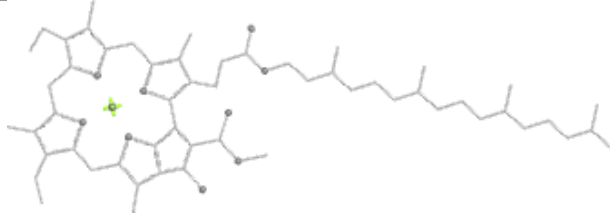


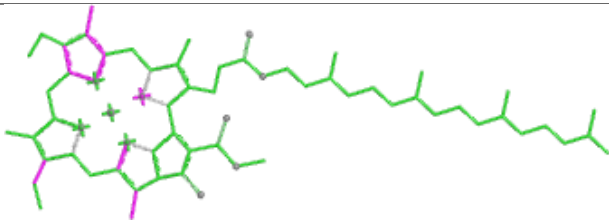
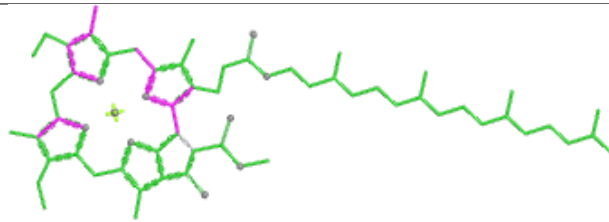
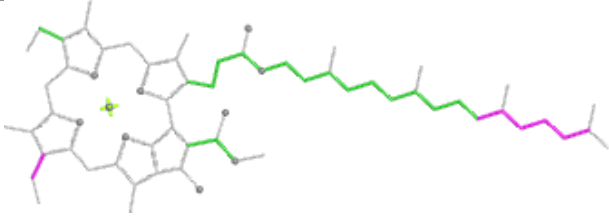
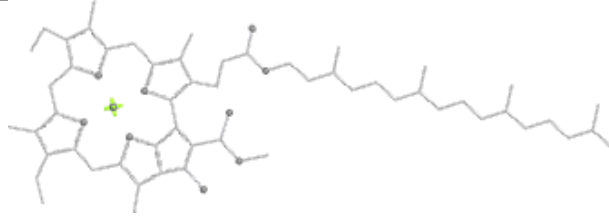


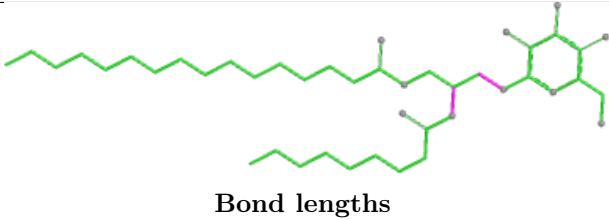
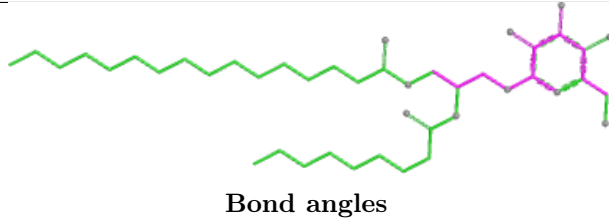
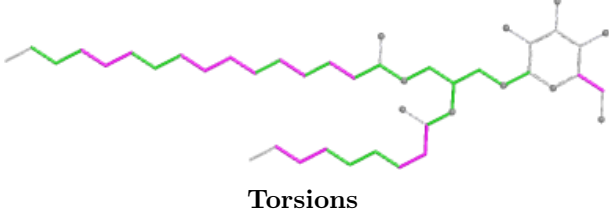
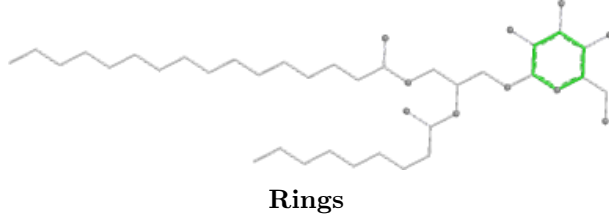


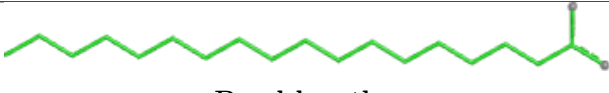
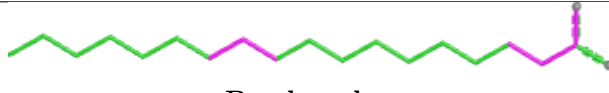
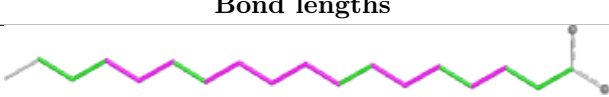
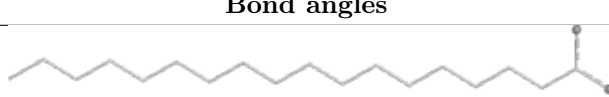
Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

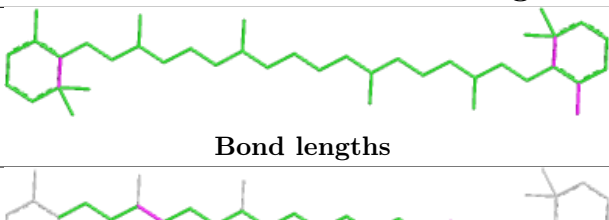
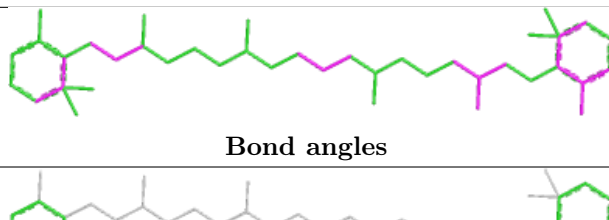
Ligand LHG l 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

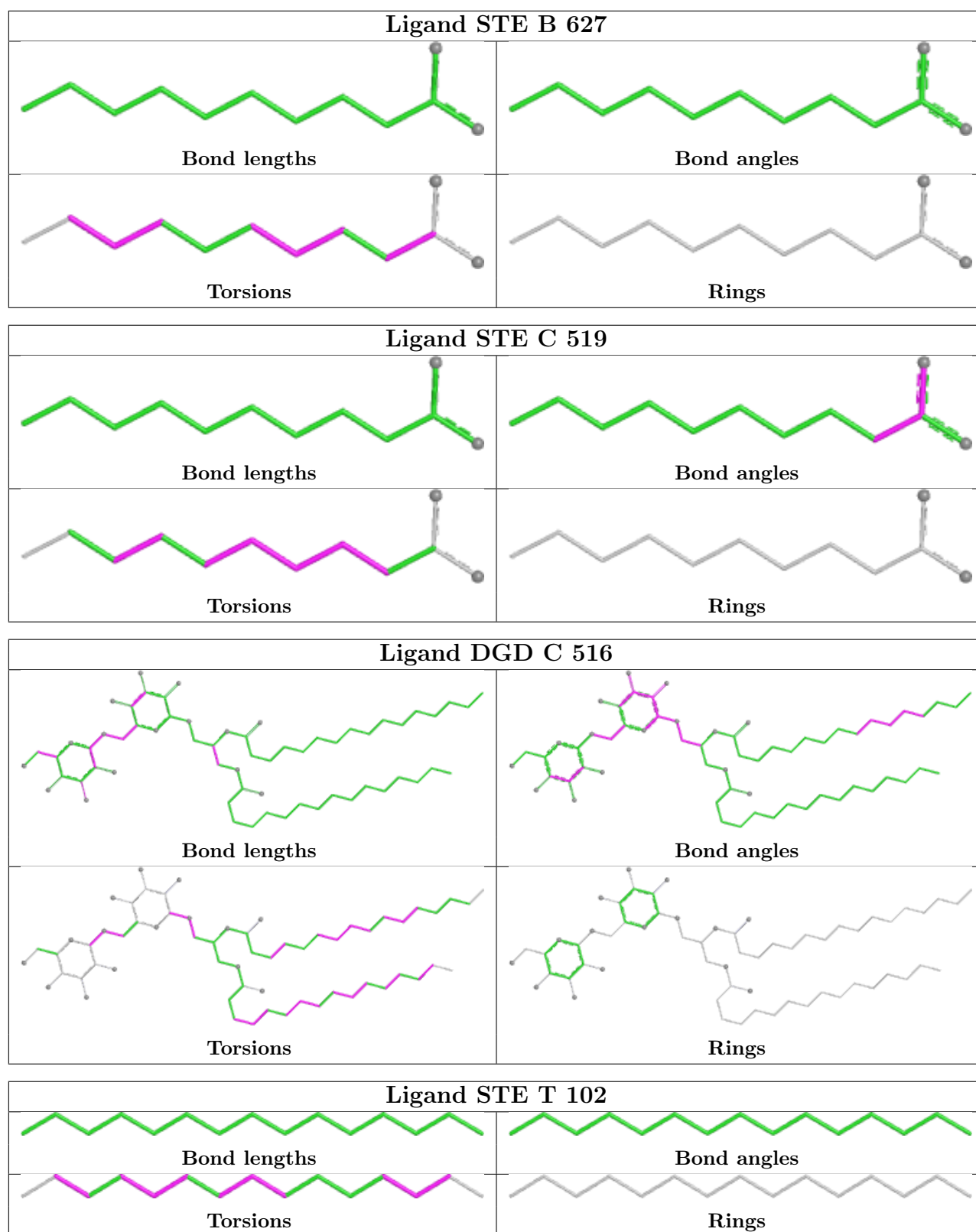
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA d 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

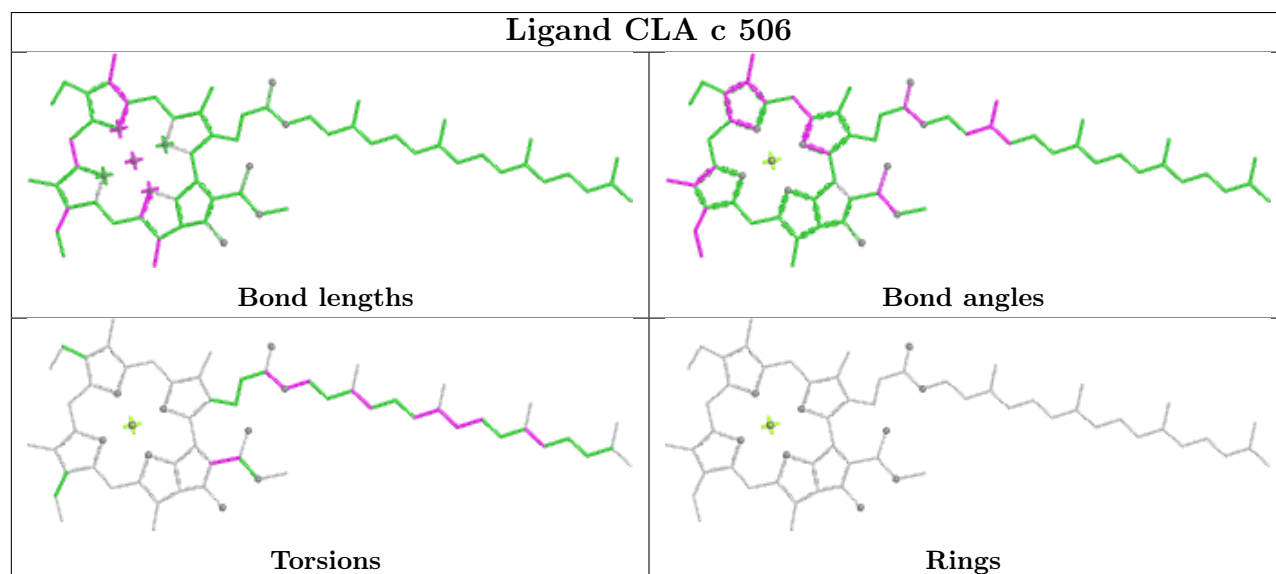
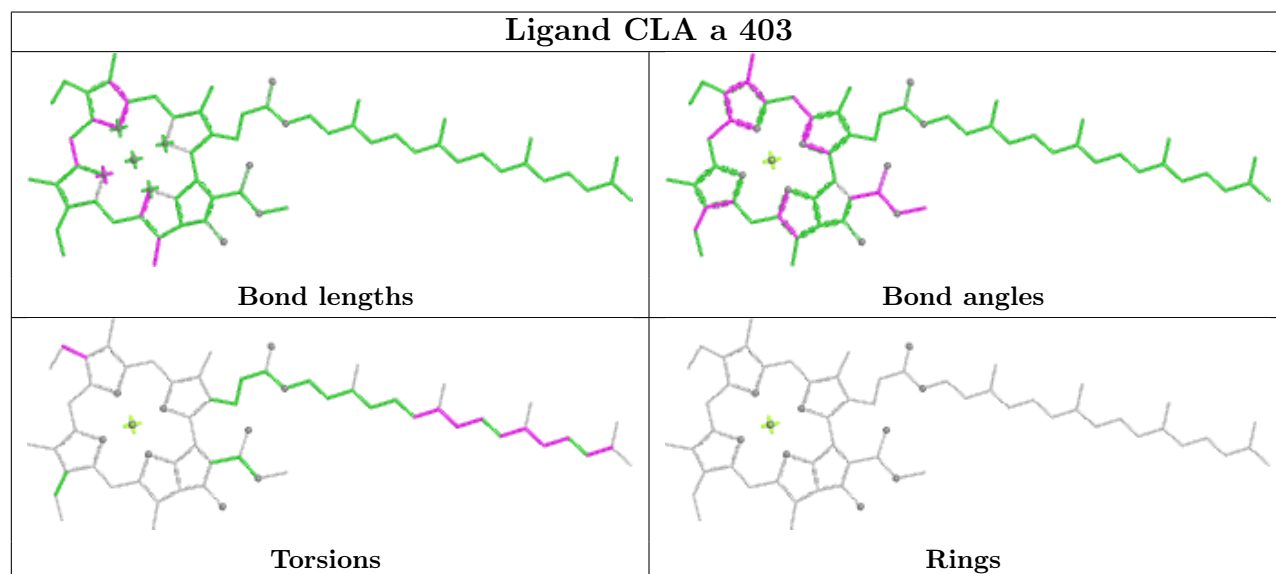
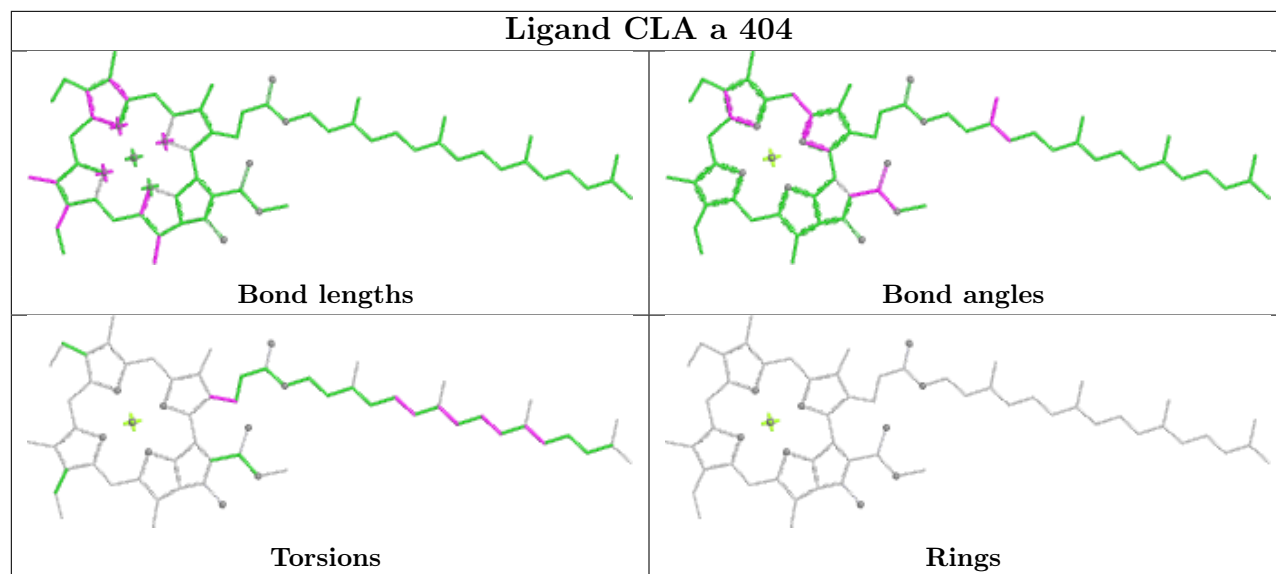
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Bond lengths	Bond angles
	
Torsions	Rings

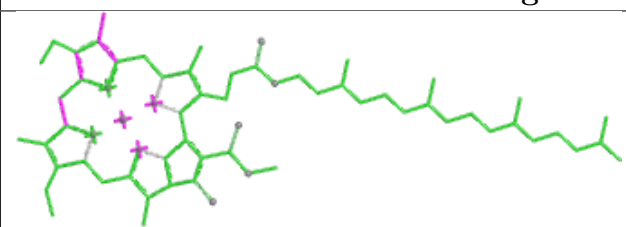
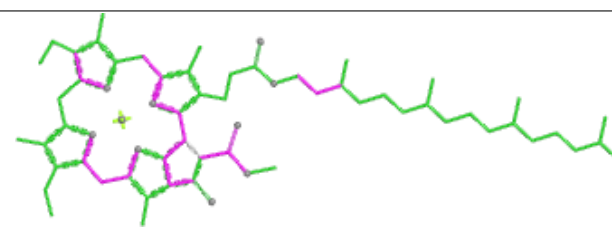
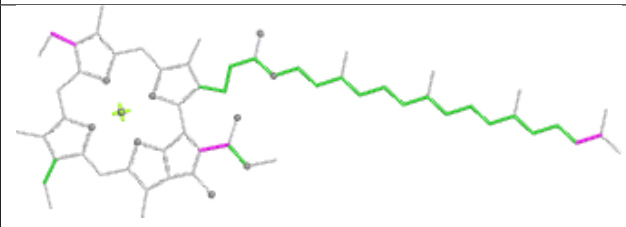
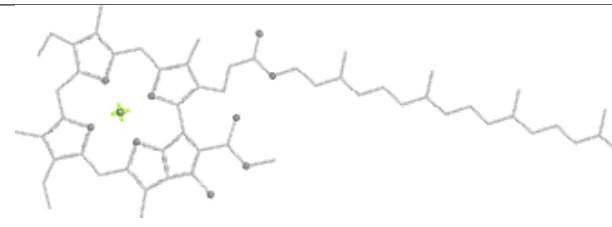
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

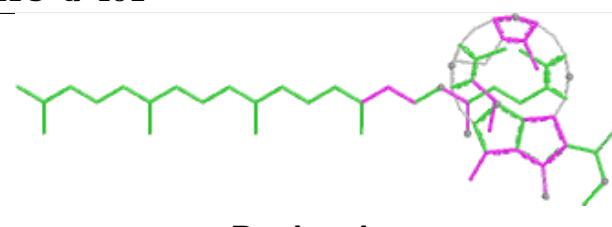
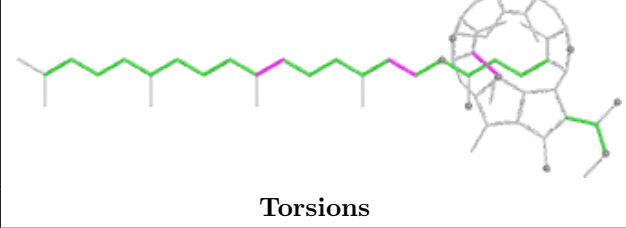
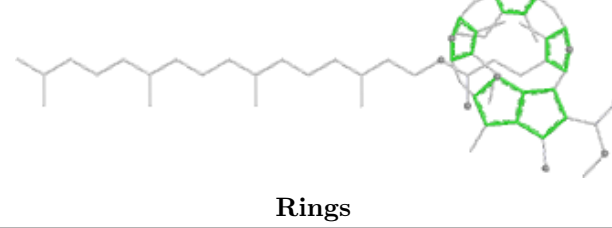
Ligand STE X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

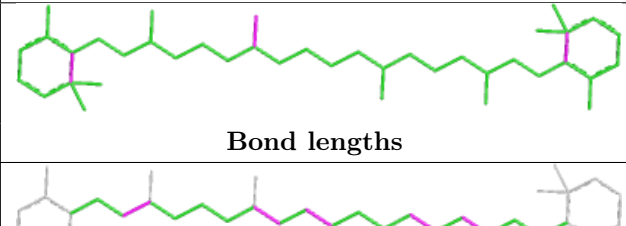
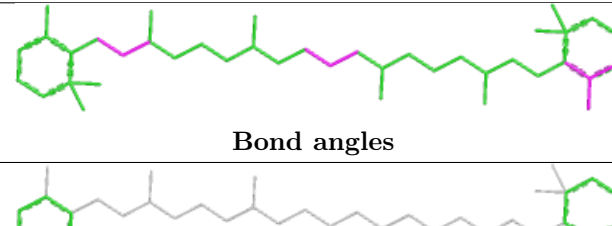
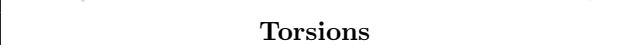
Ligand BCR a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

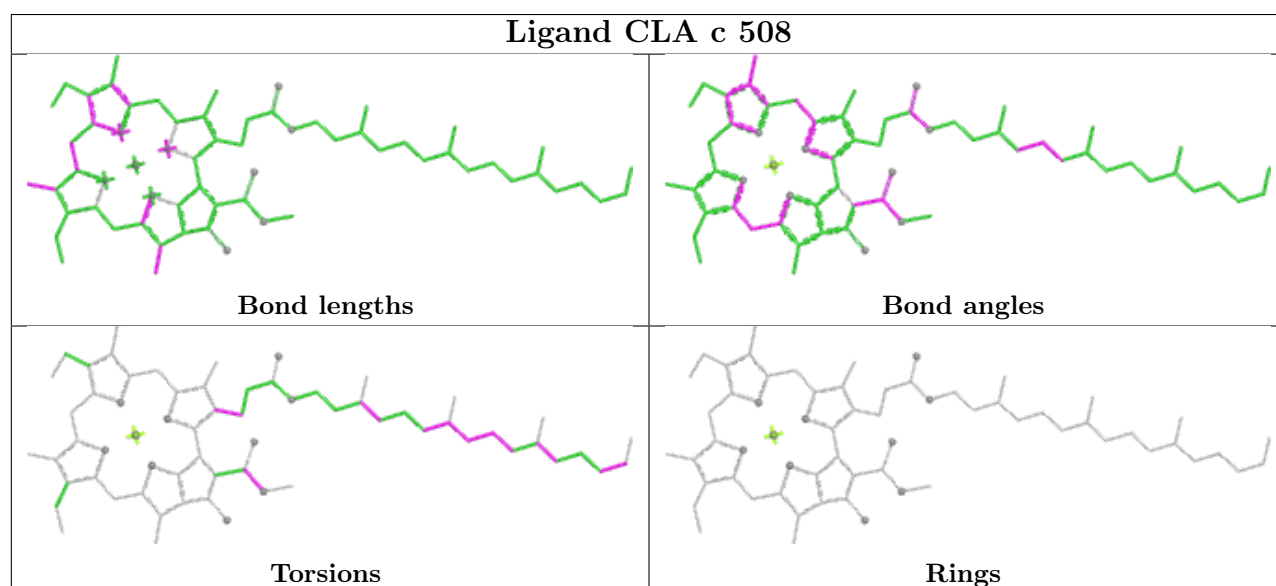
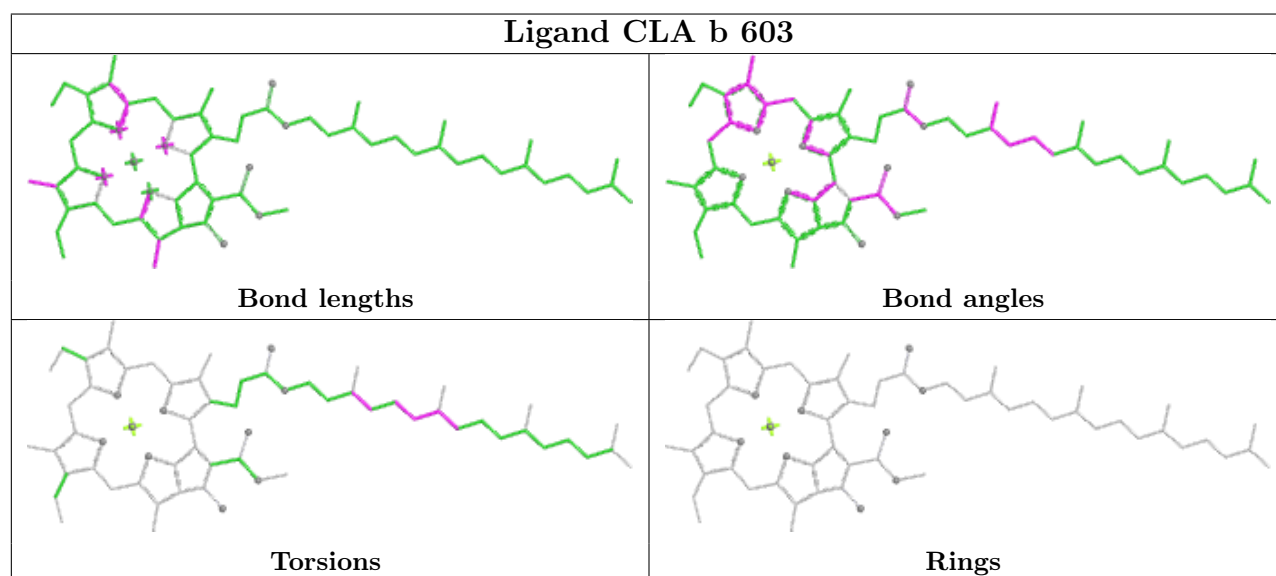
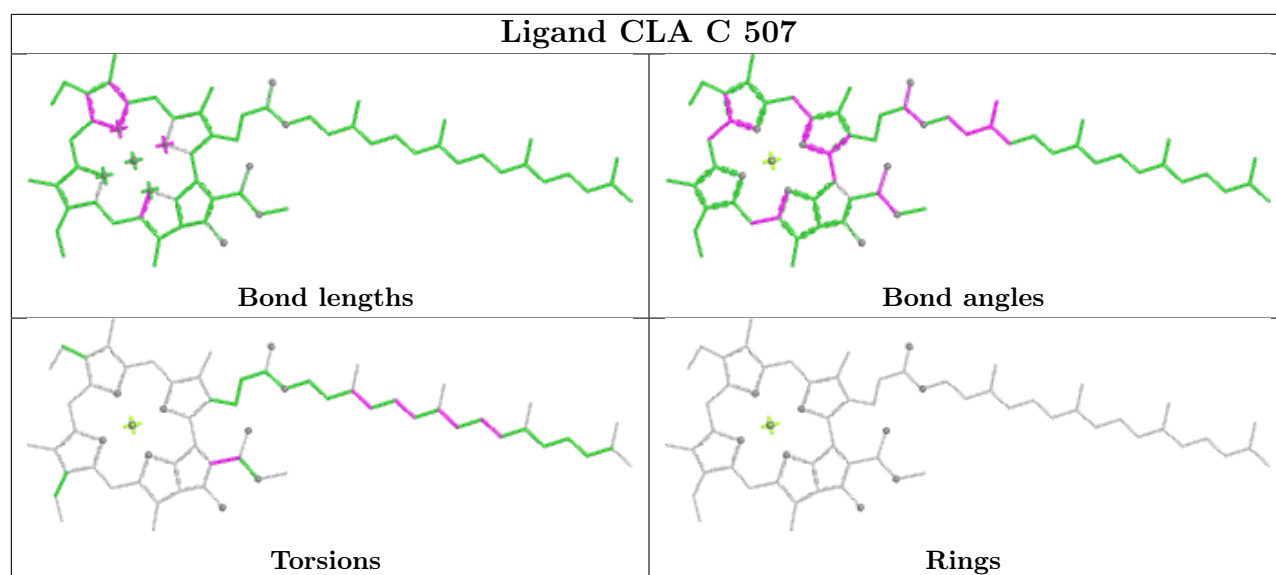


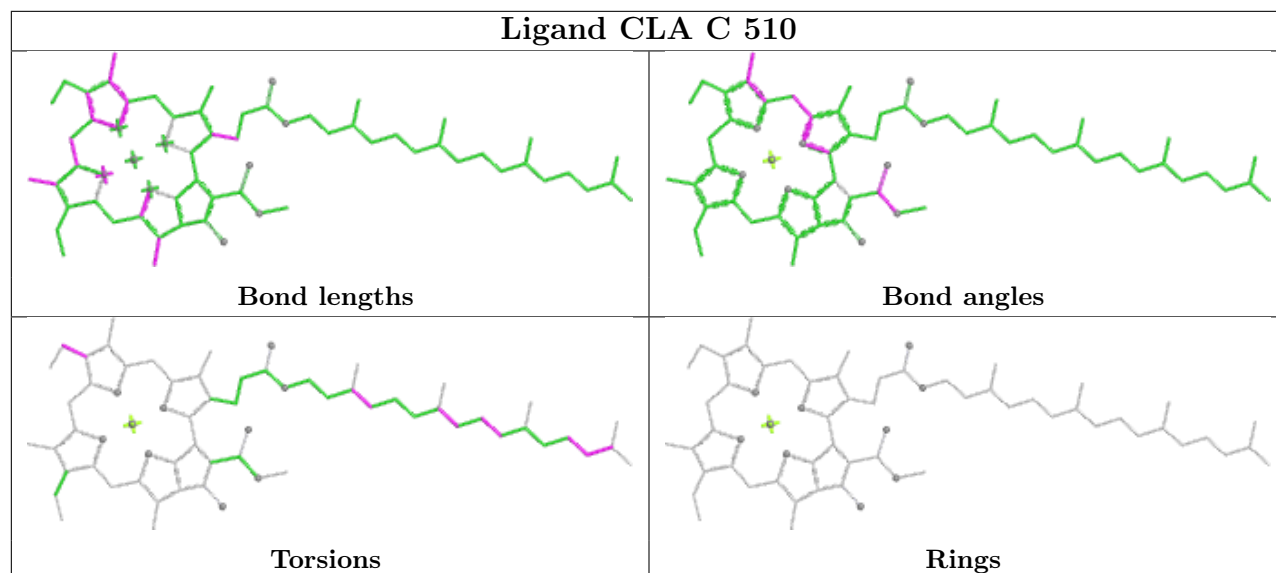
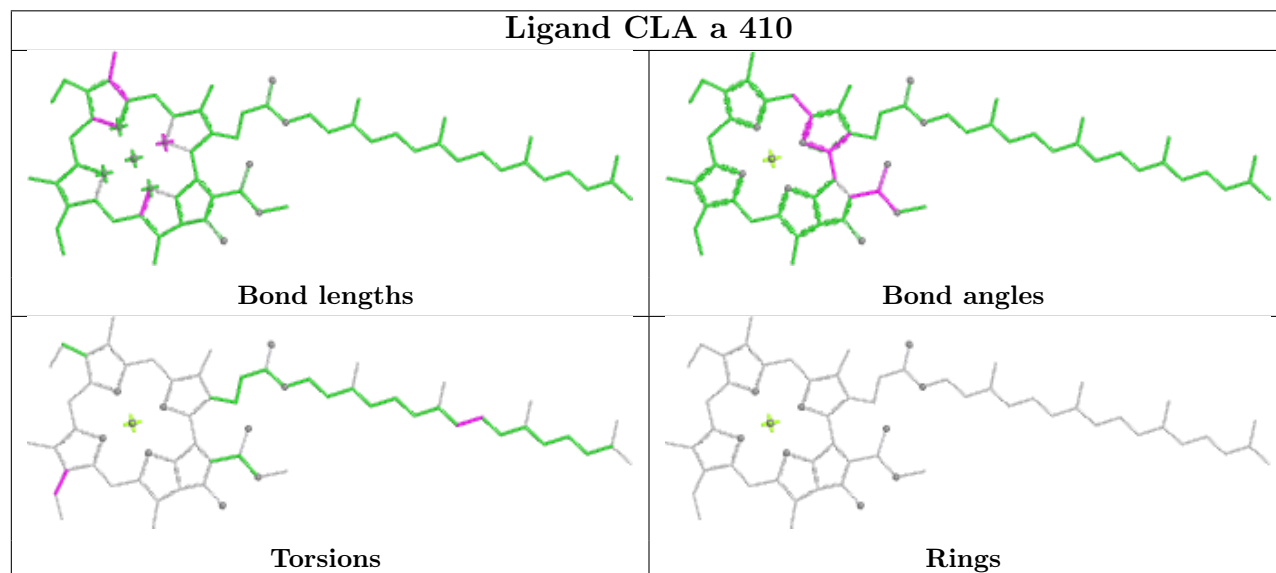
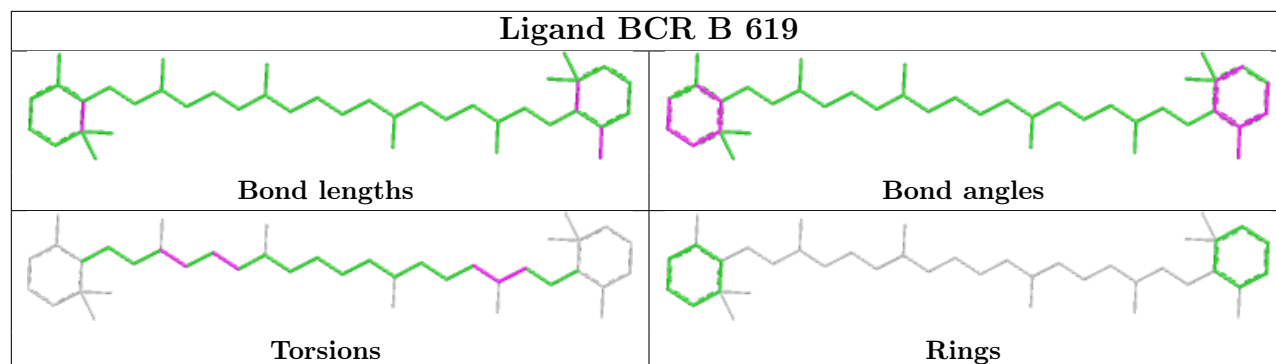


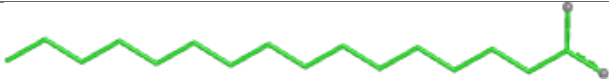
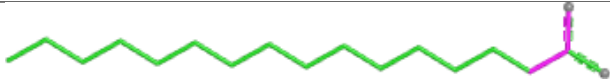
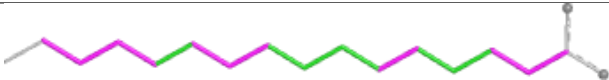
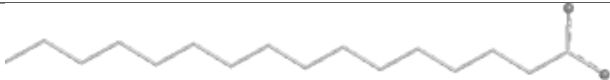
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

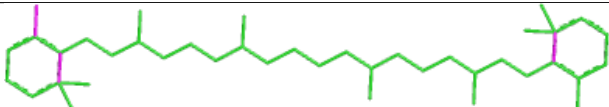
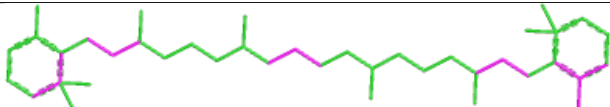
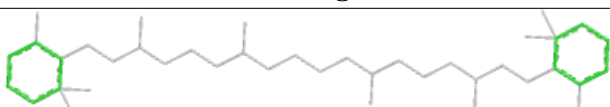
Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

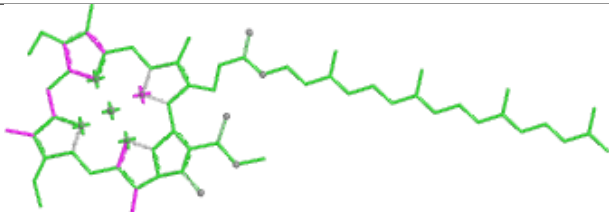
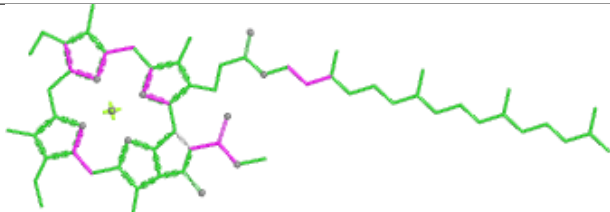
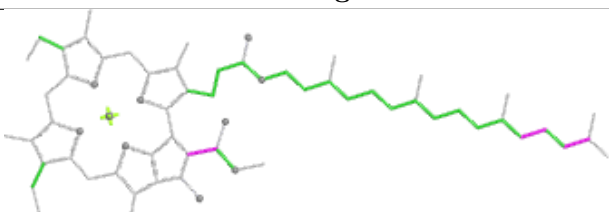
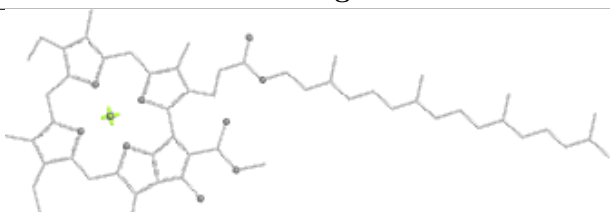
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Bond lengths	Bond angles
	
Torsions	Rings

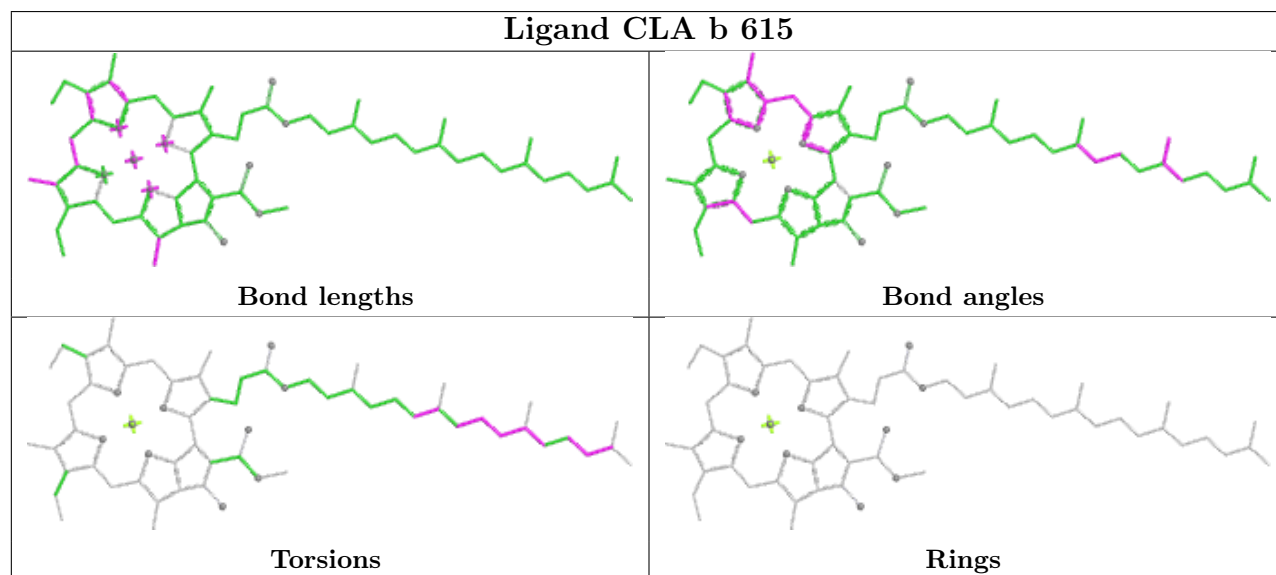
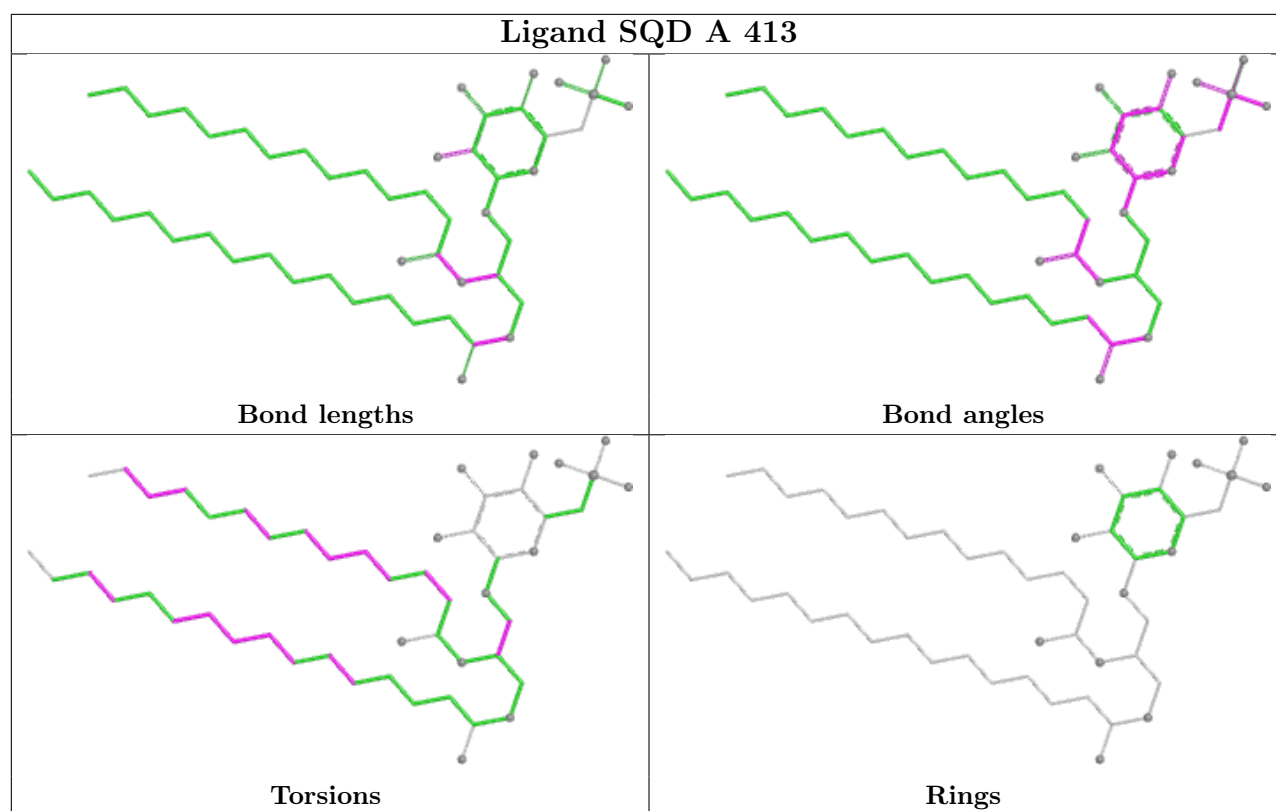




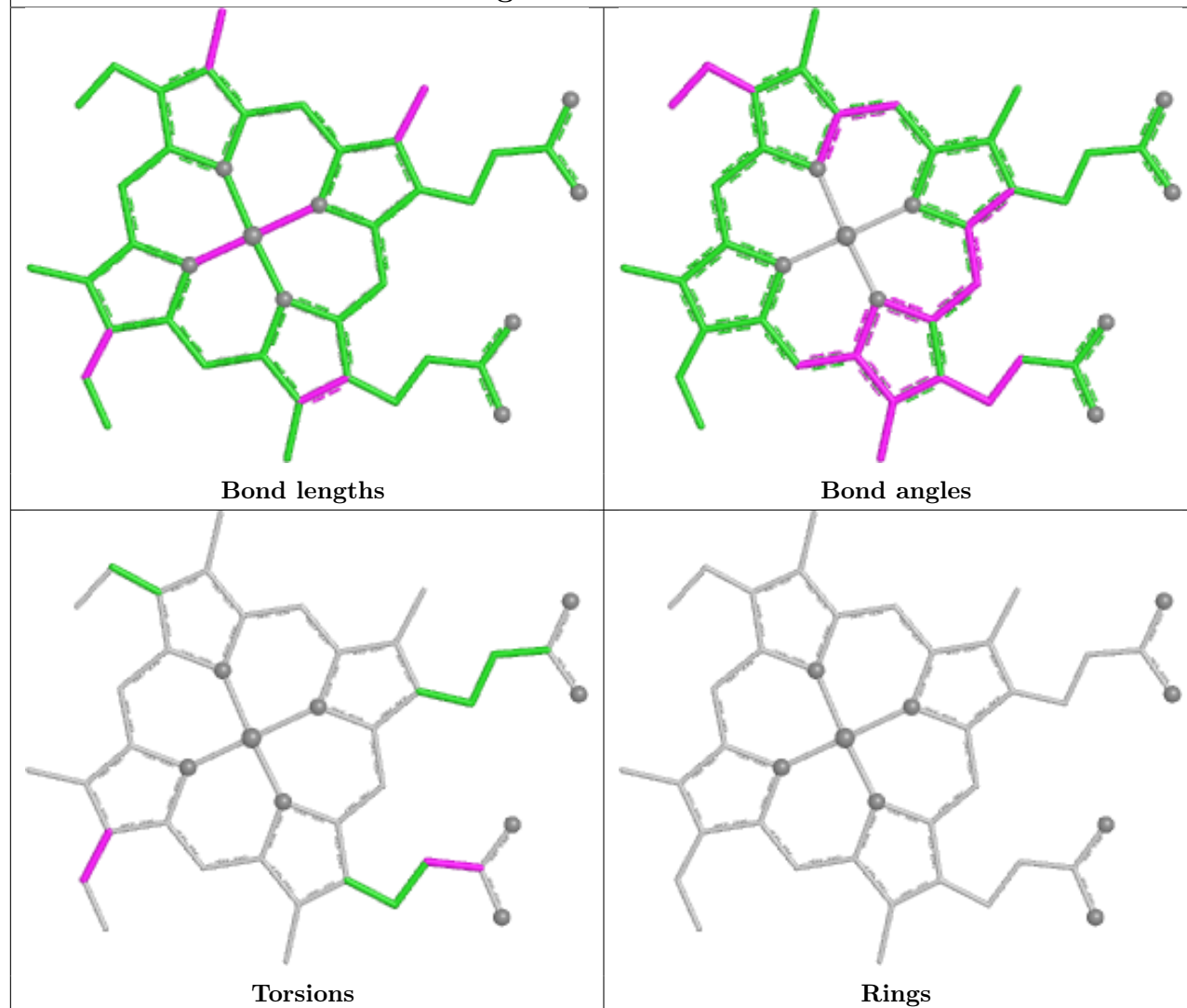
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

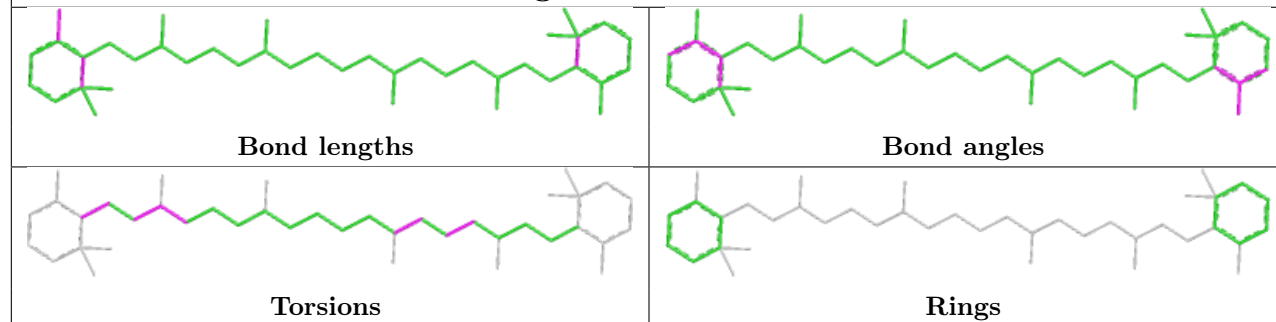
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings



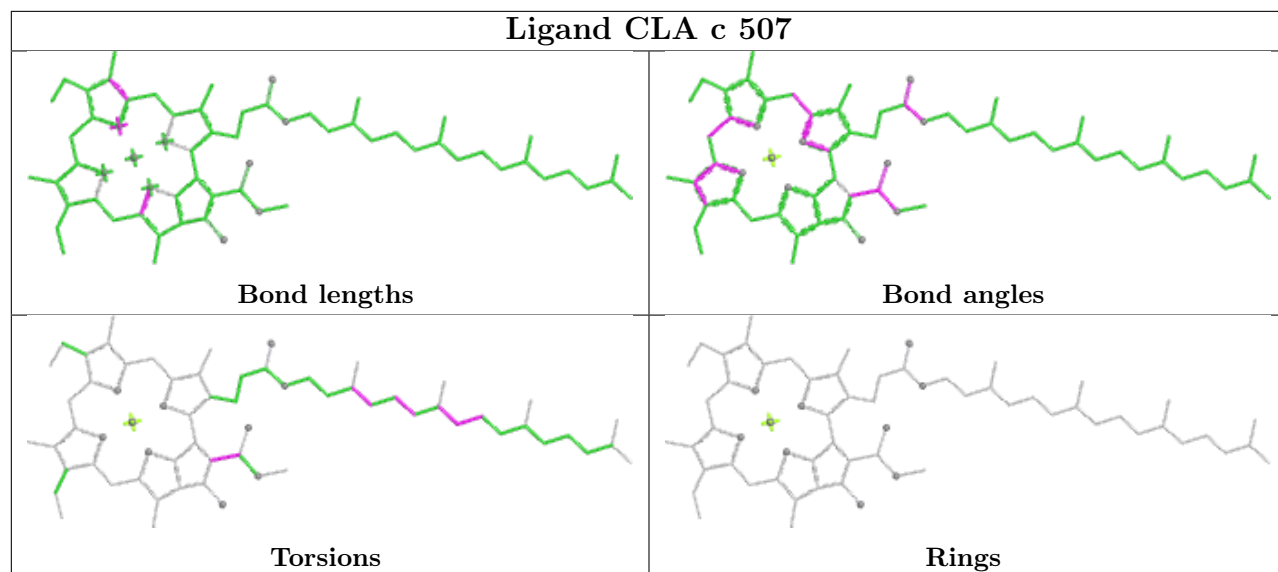
Ligand HEC v 201



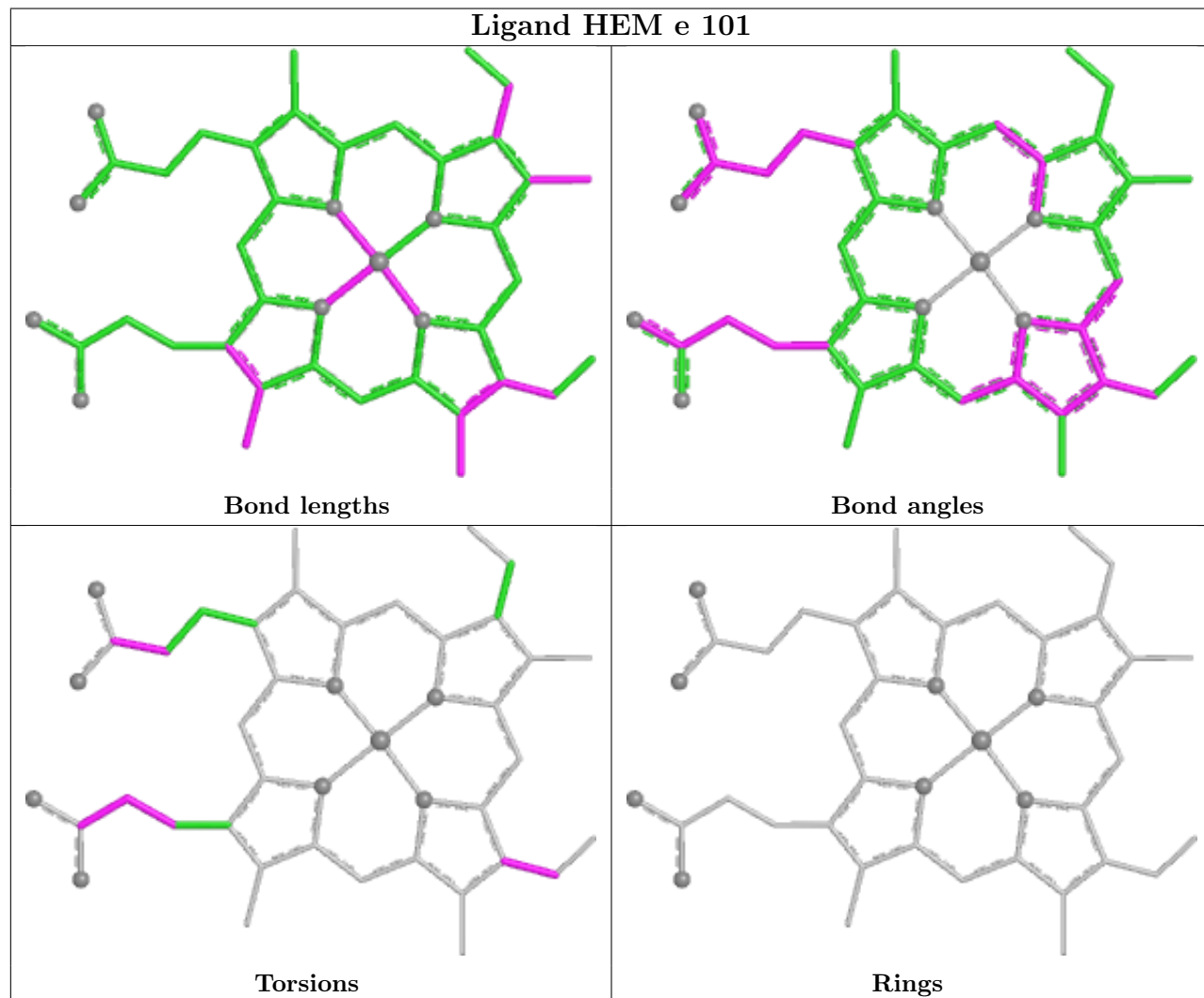
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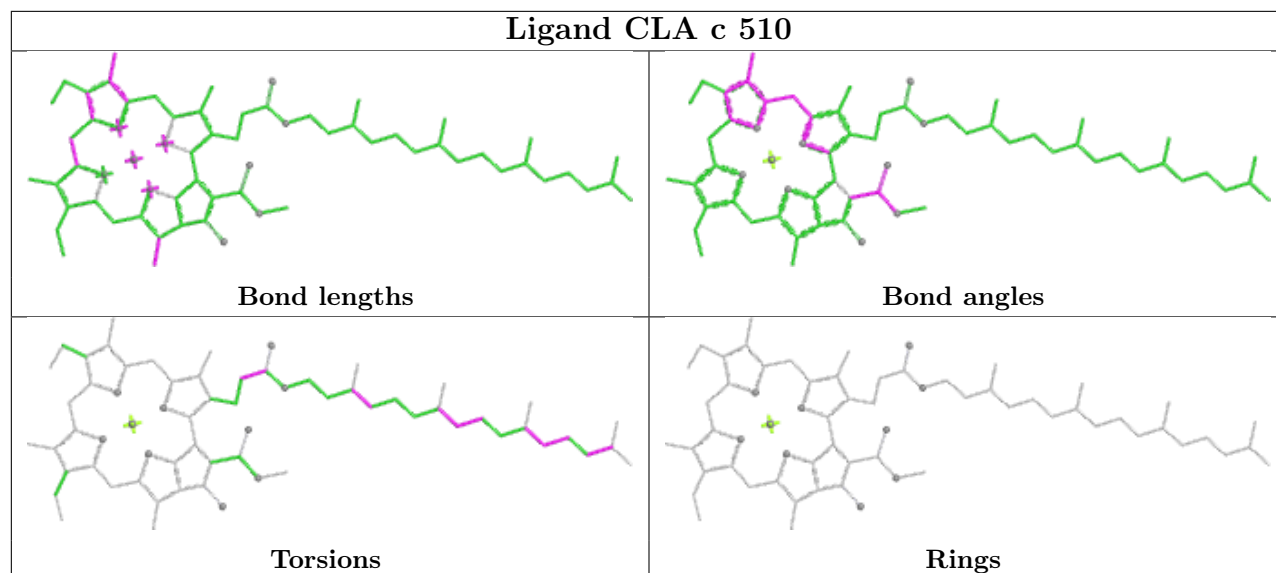
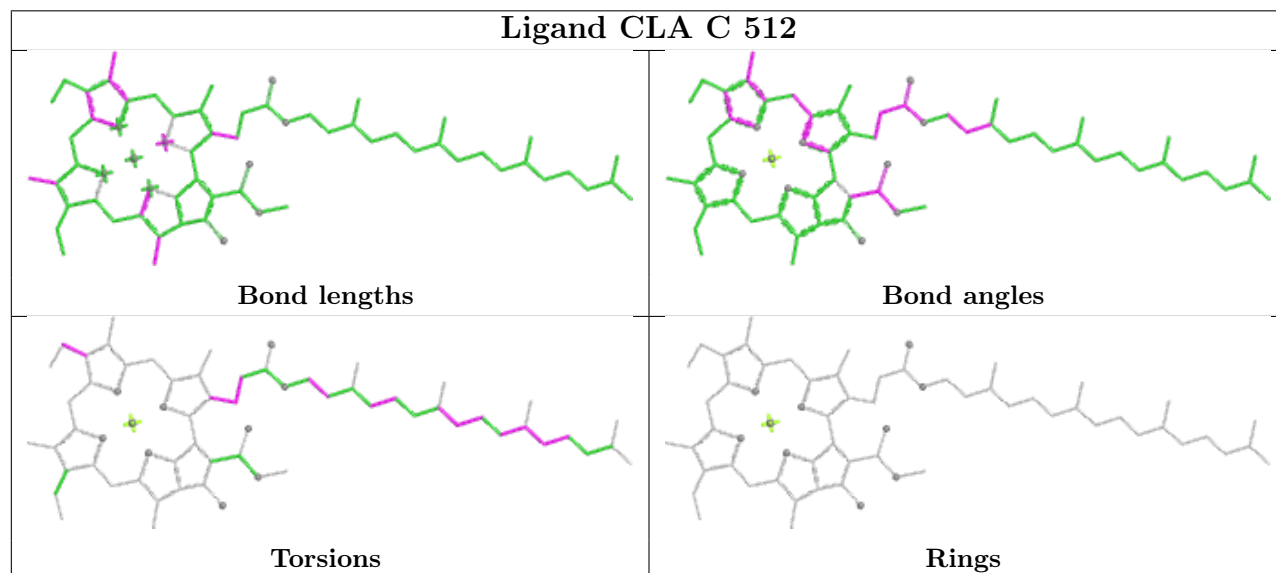
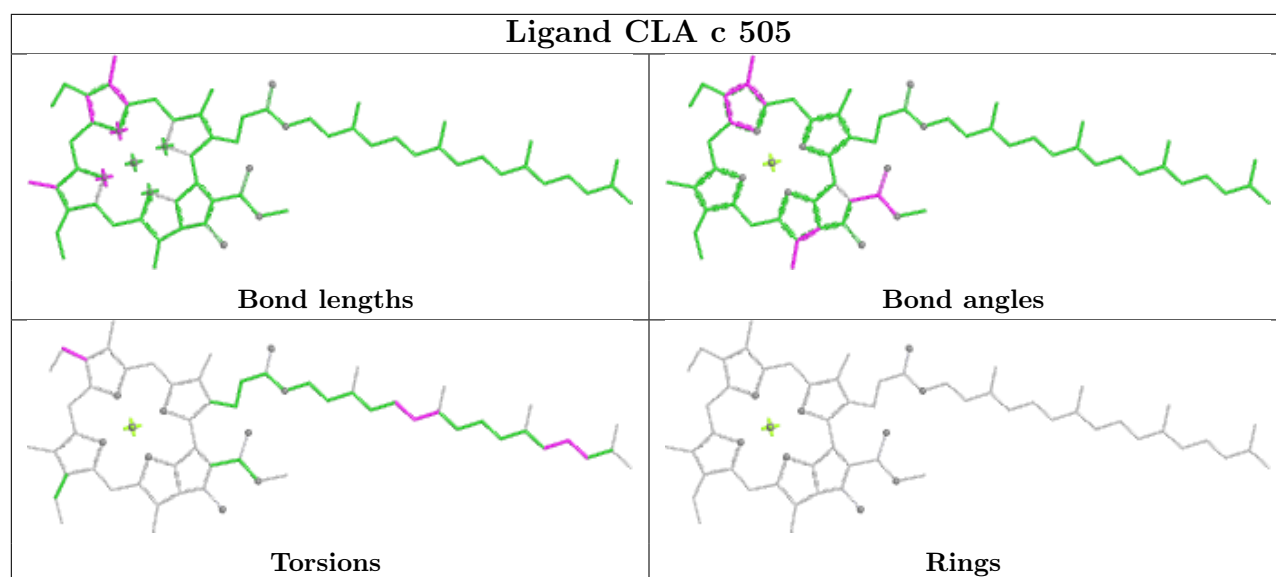


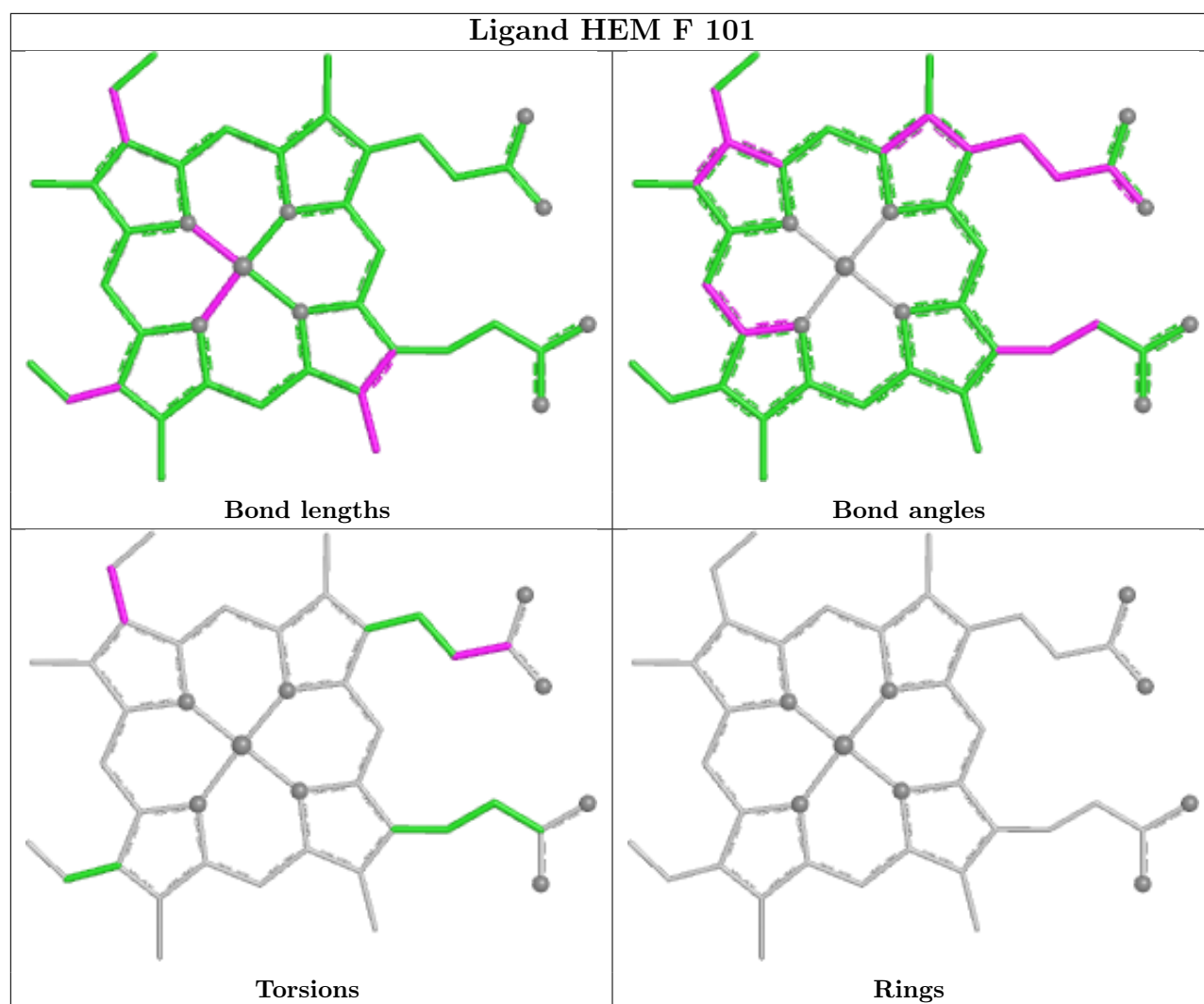
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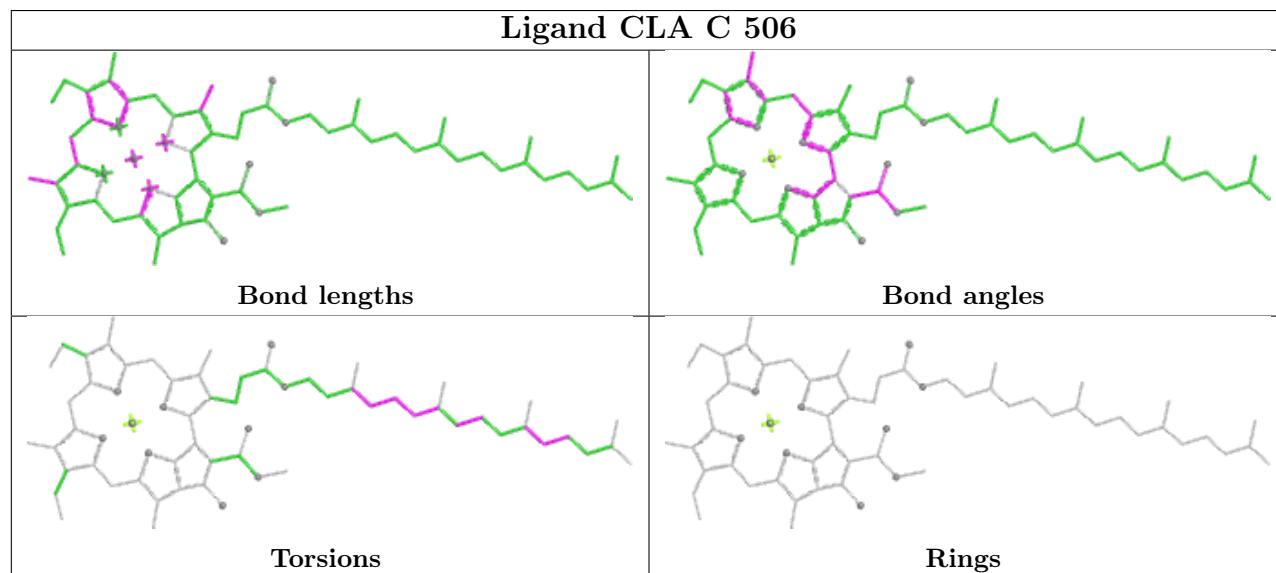
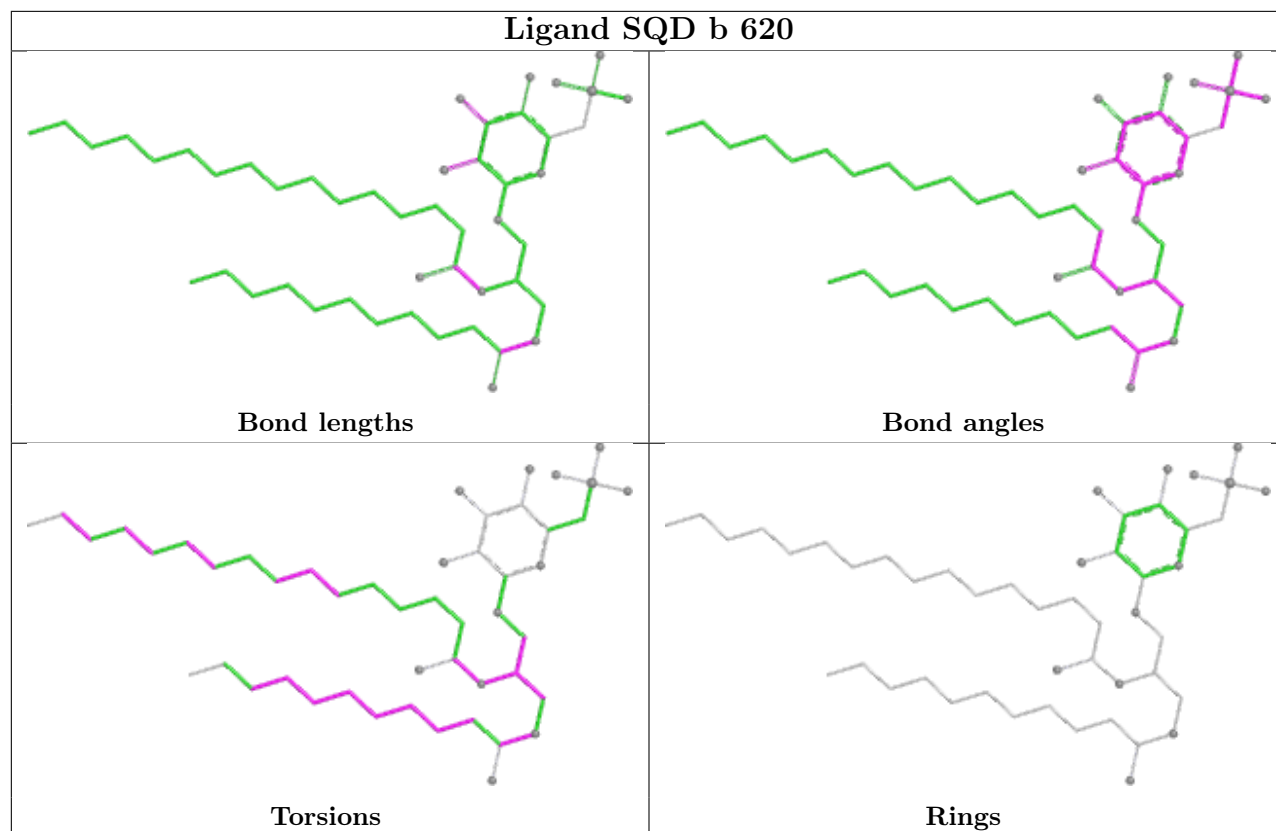


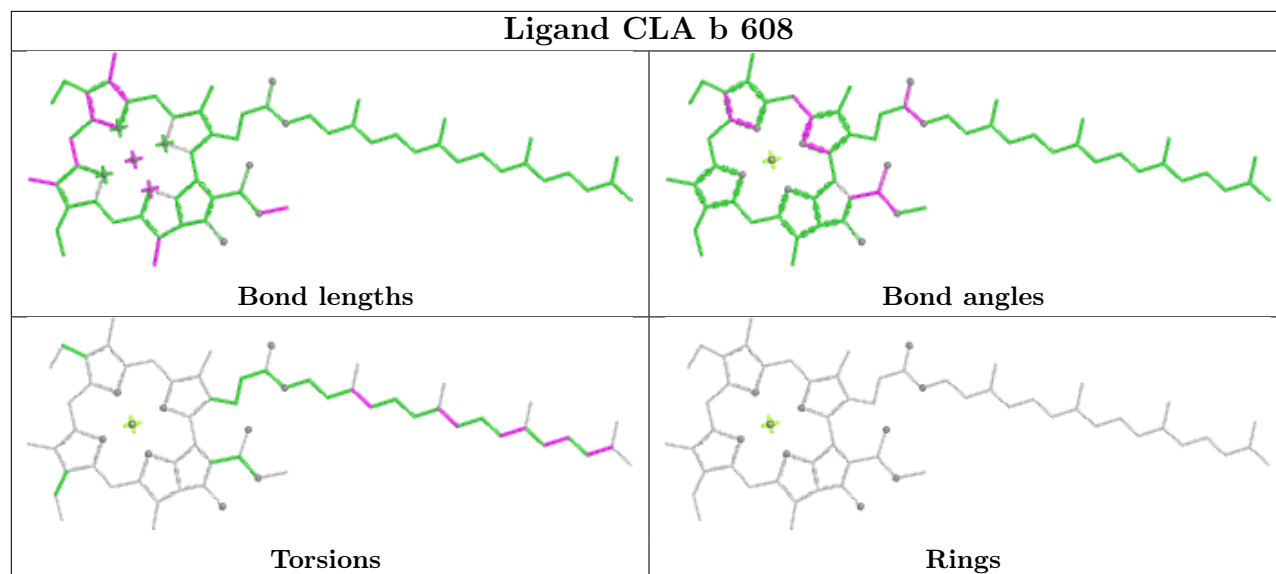
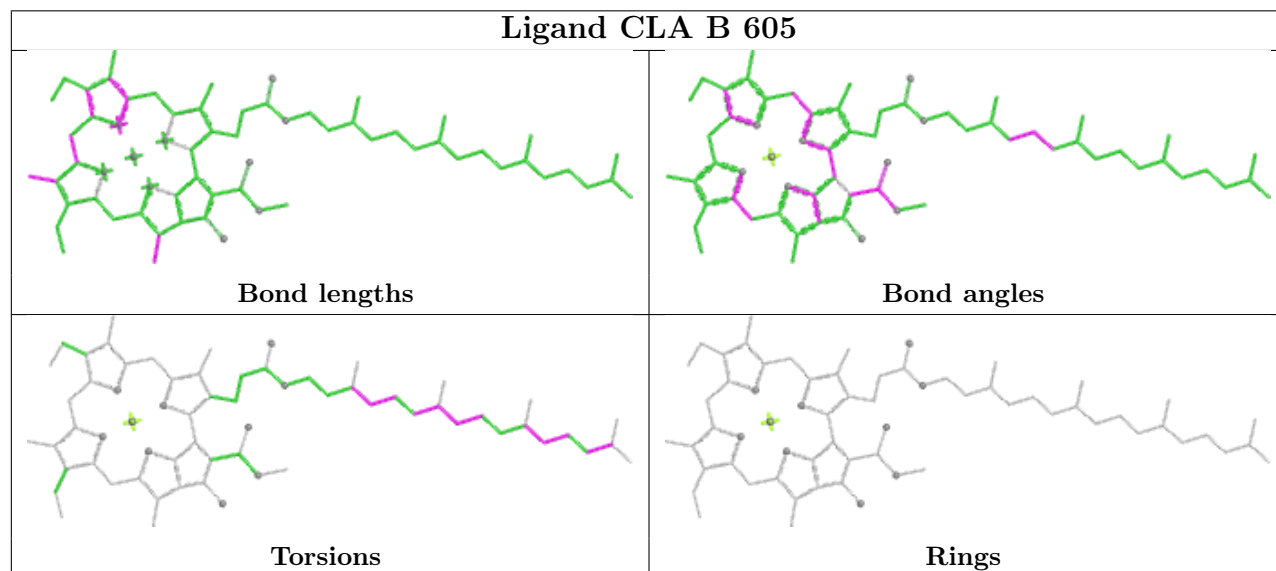
Ligand HEM e 101



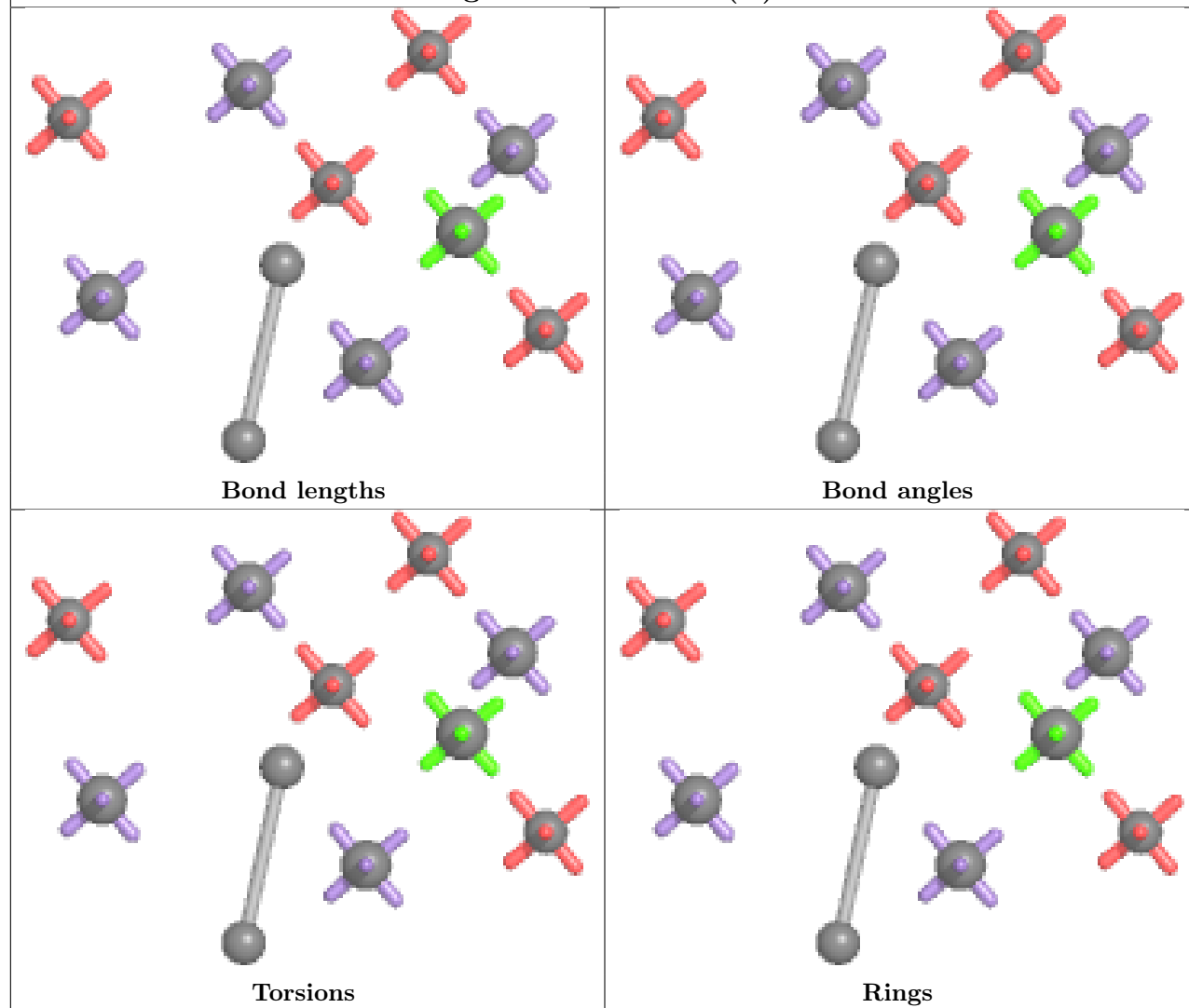




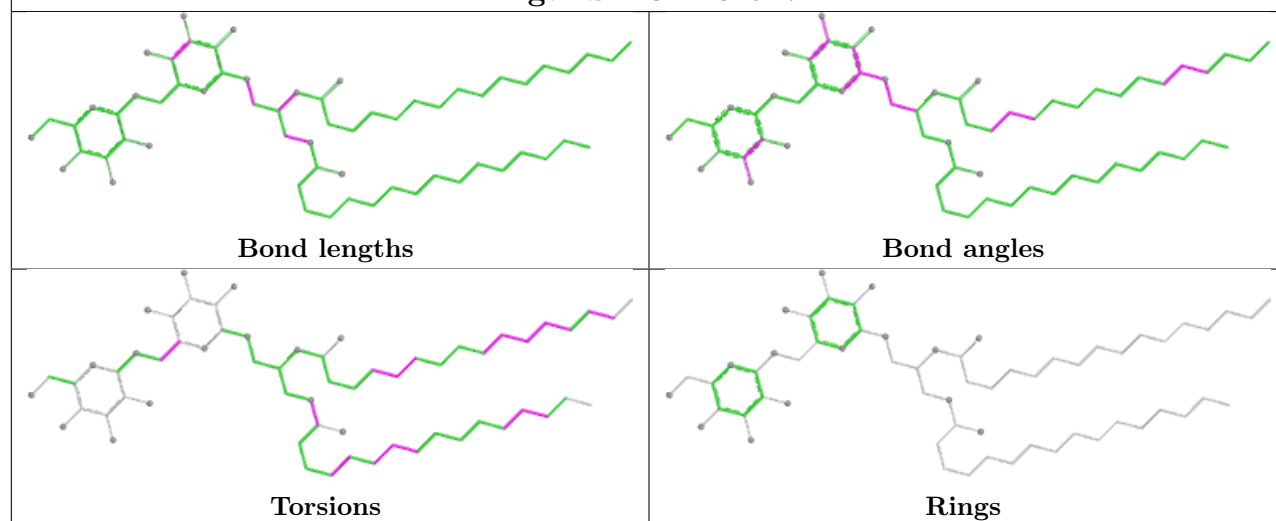


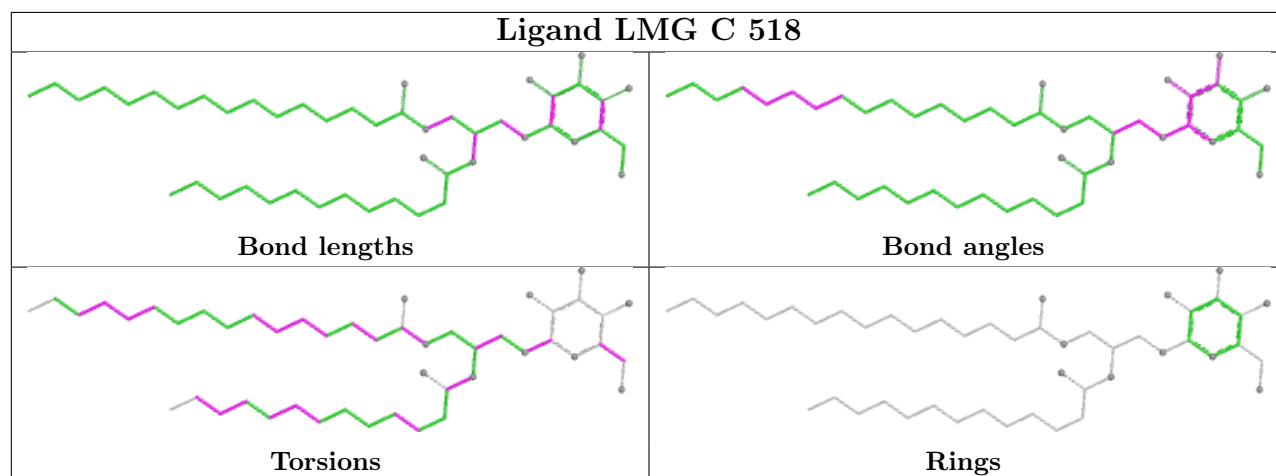
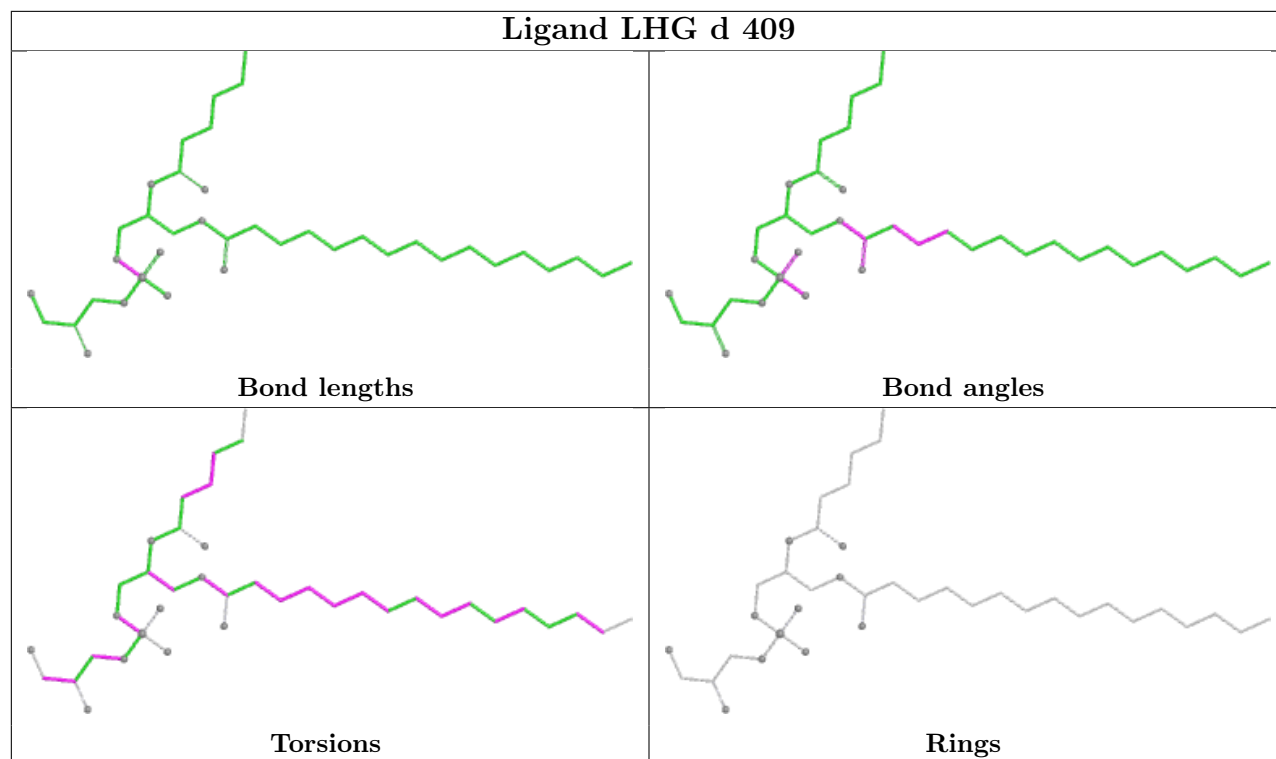
Ligand CLA b 608**Ligand CLA B 605**

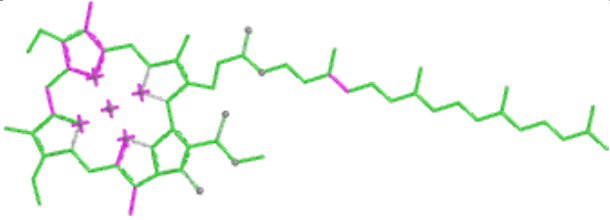
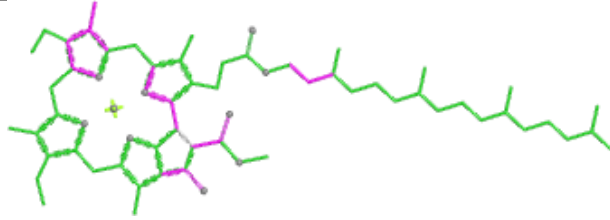
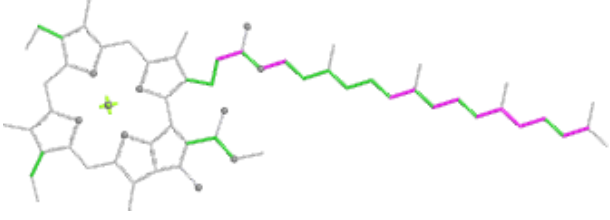
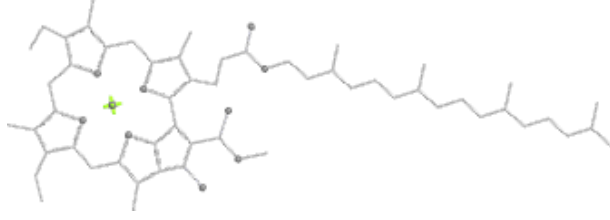
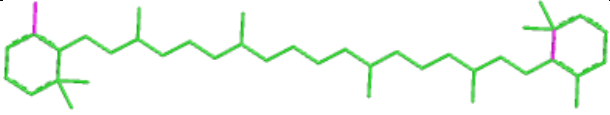
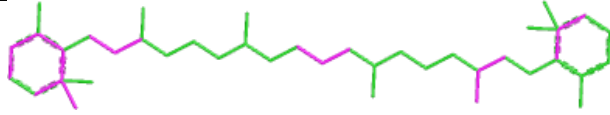
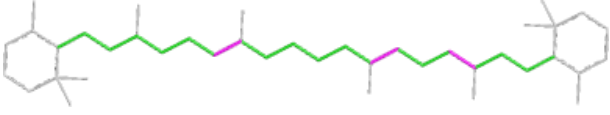
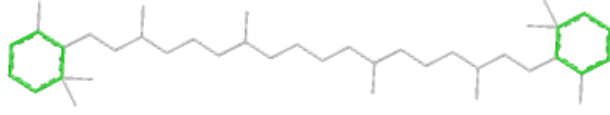
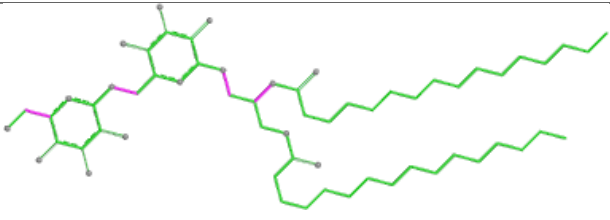
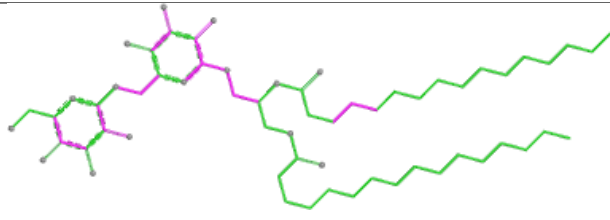
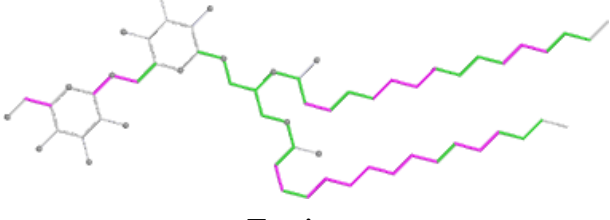
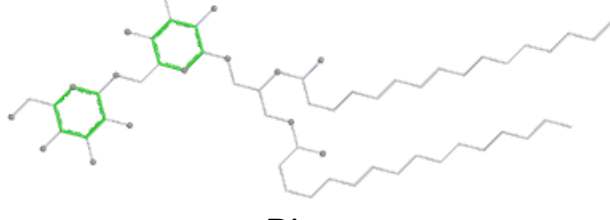
Ligand OEY A 417 (B)

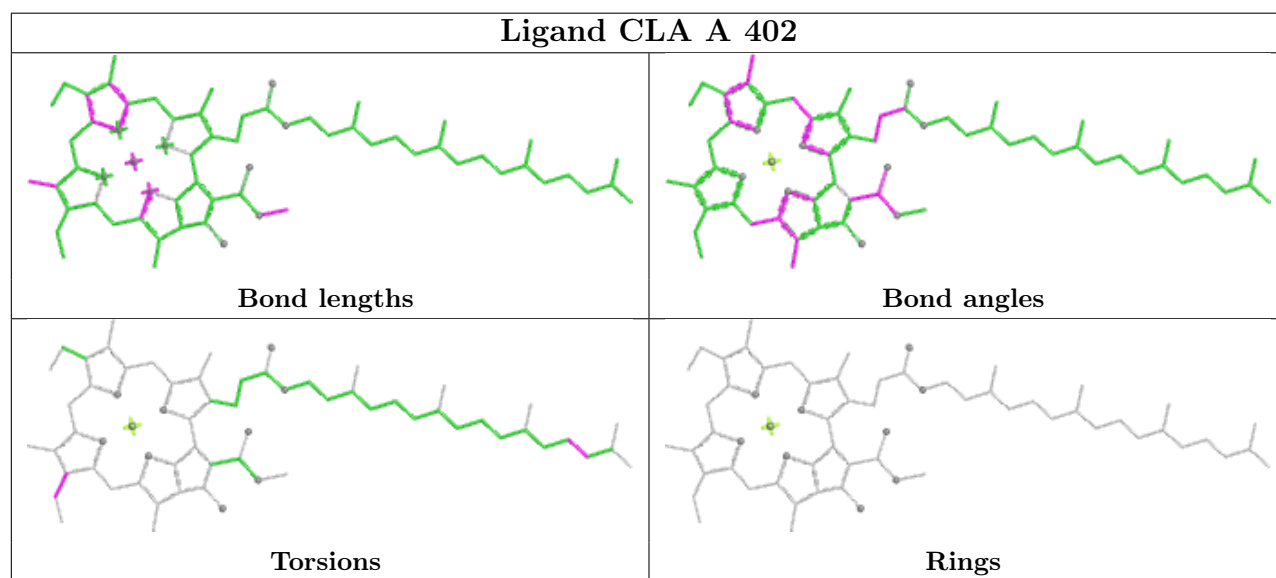
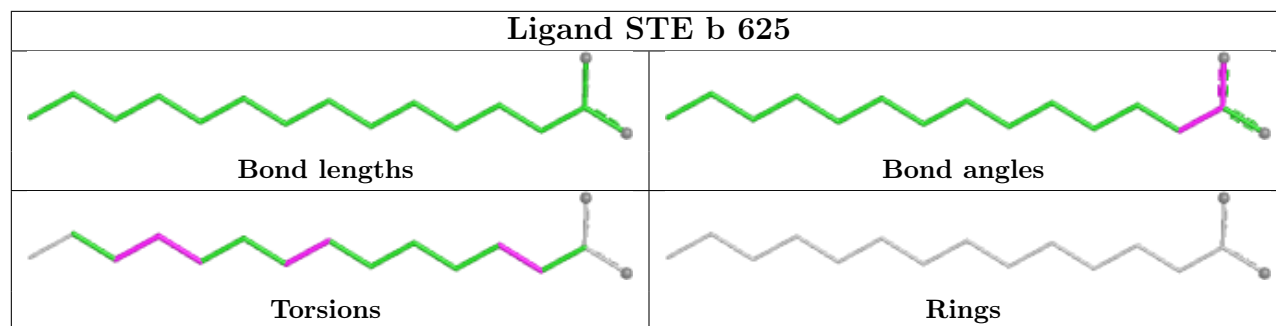


Ligand DGD C 517

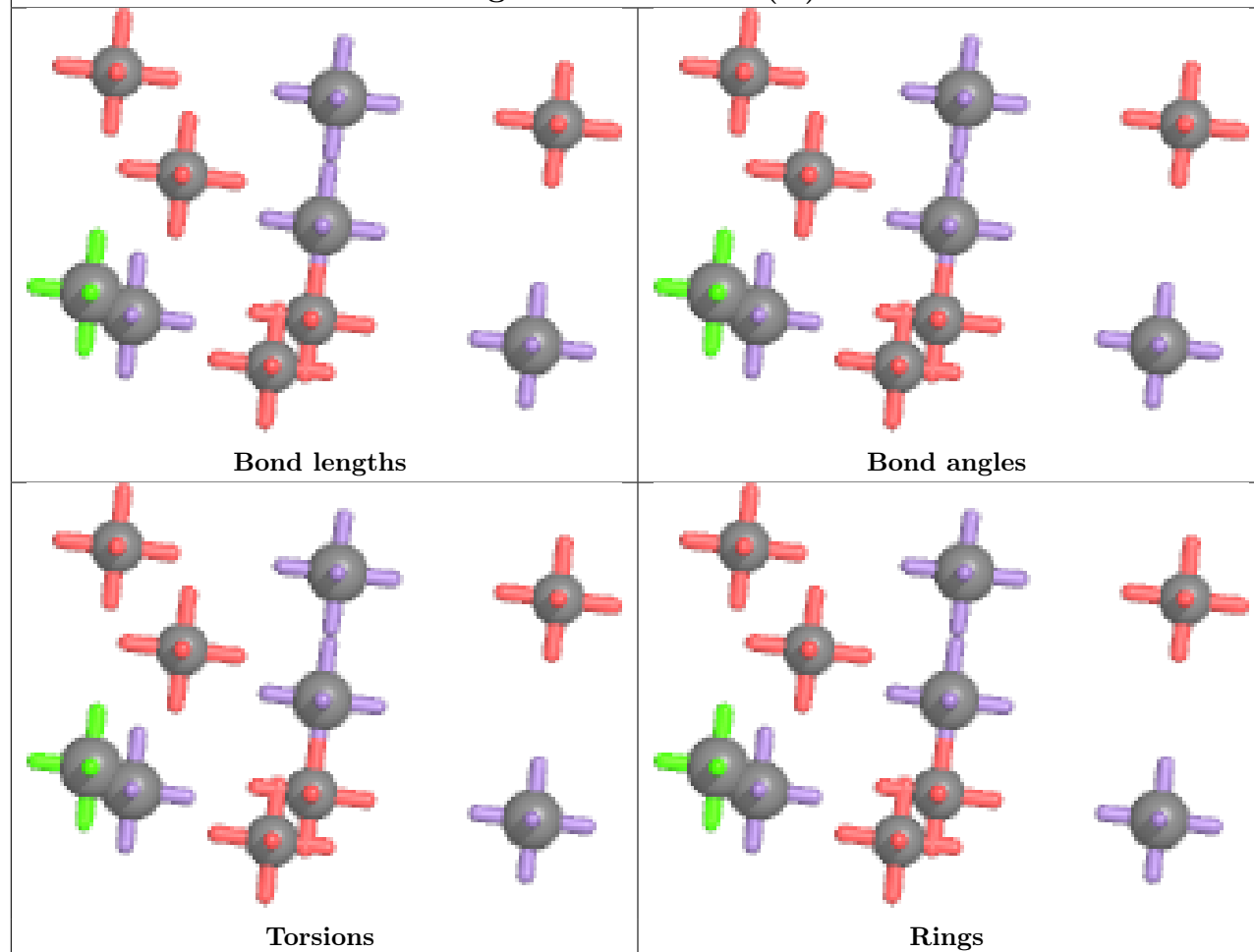




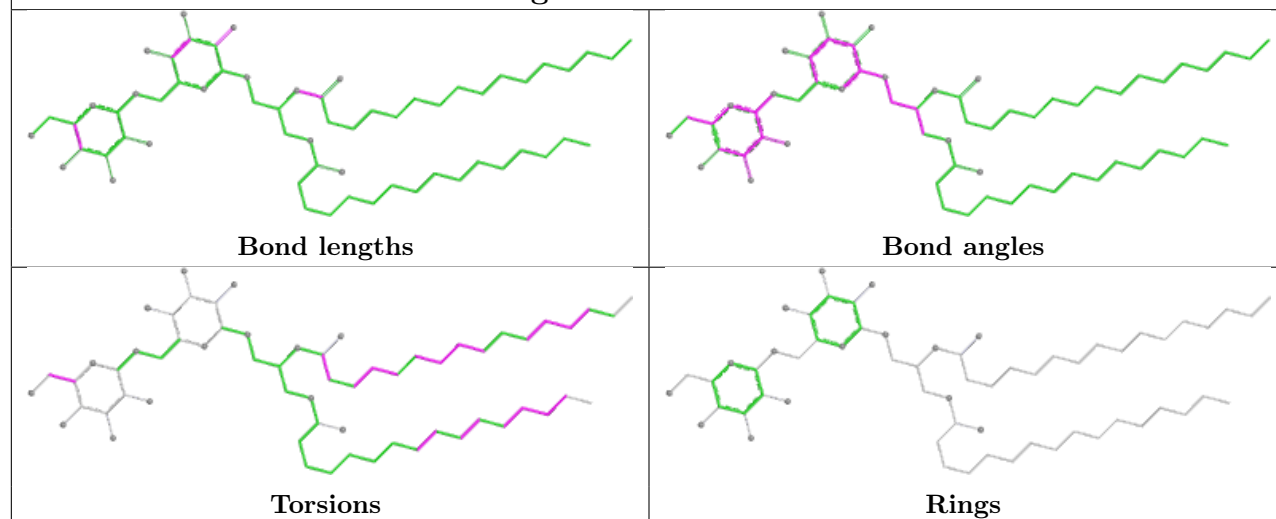
Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

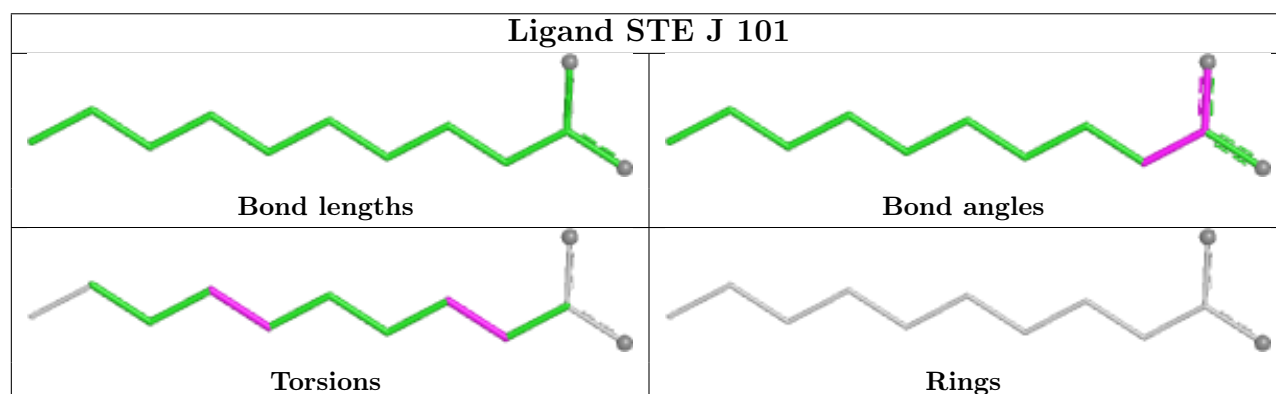
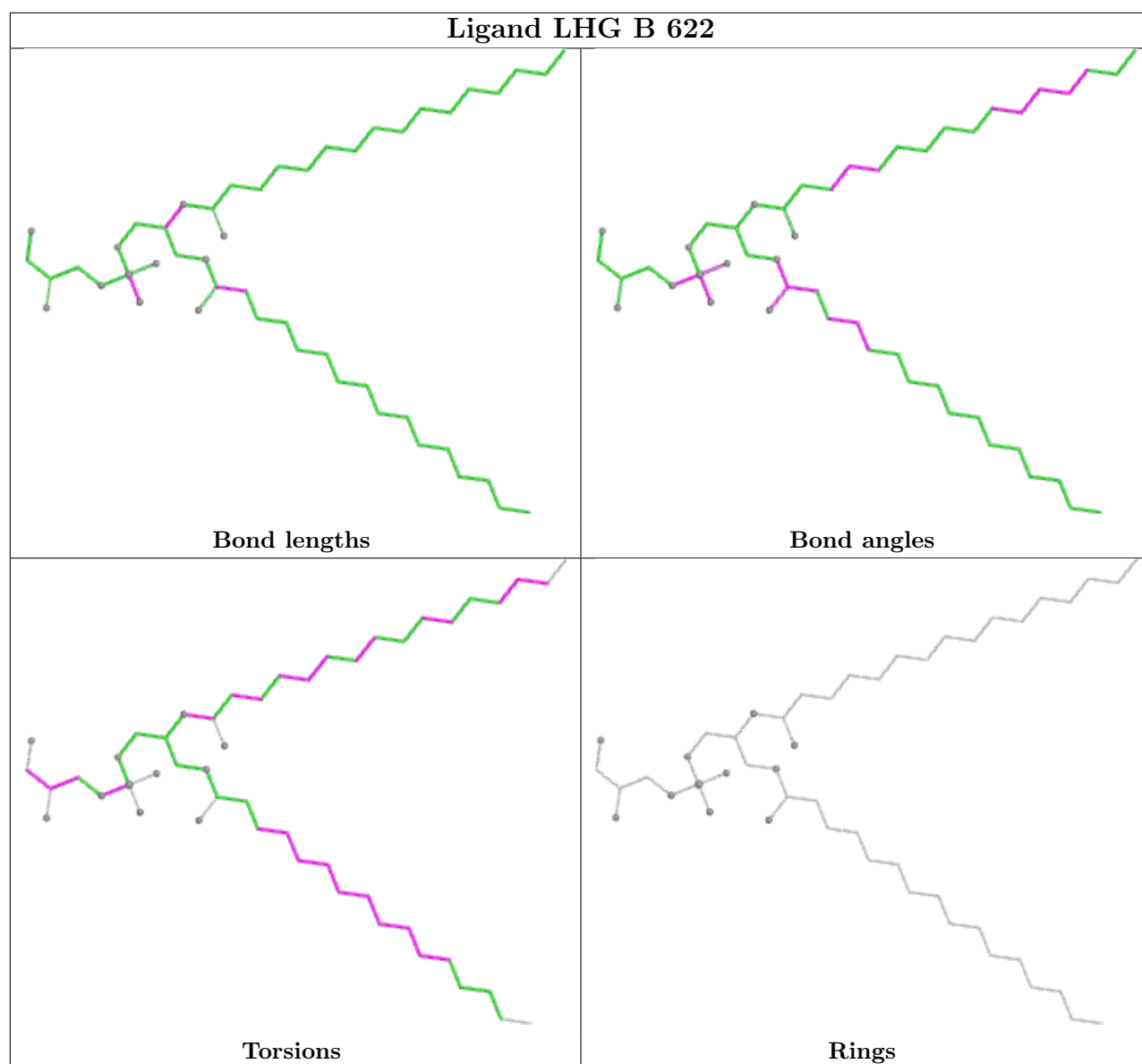


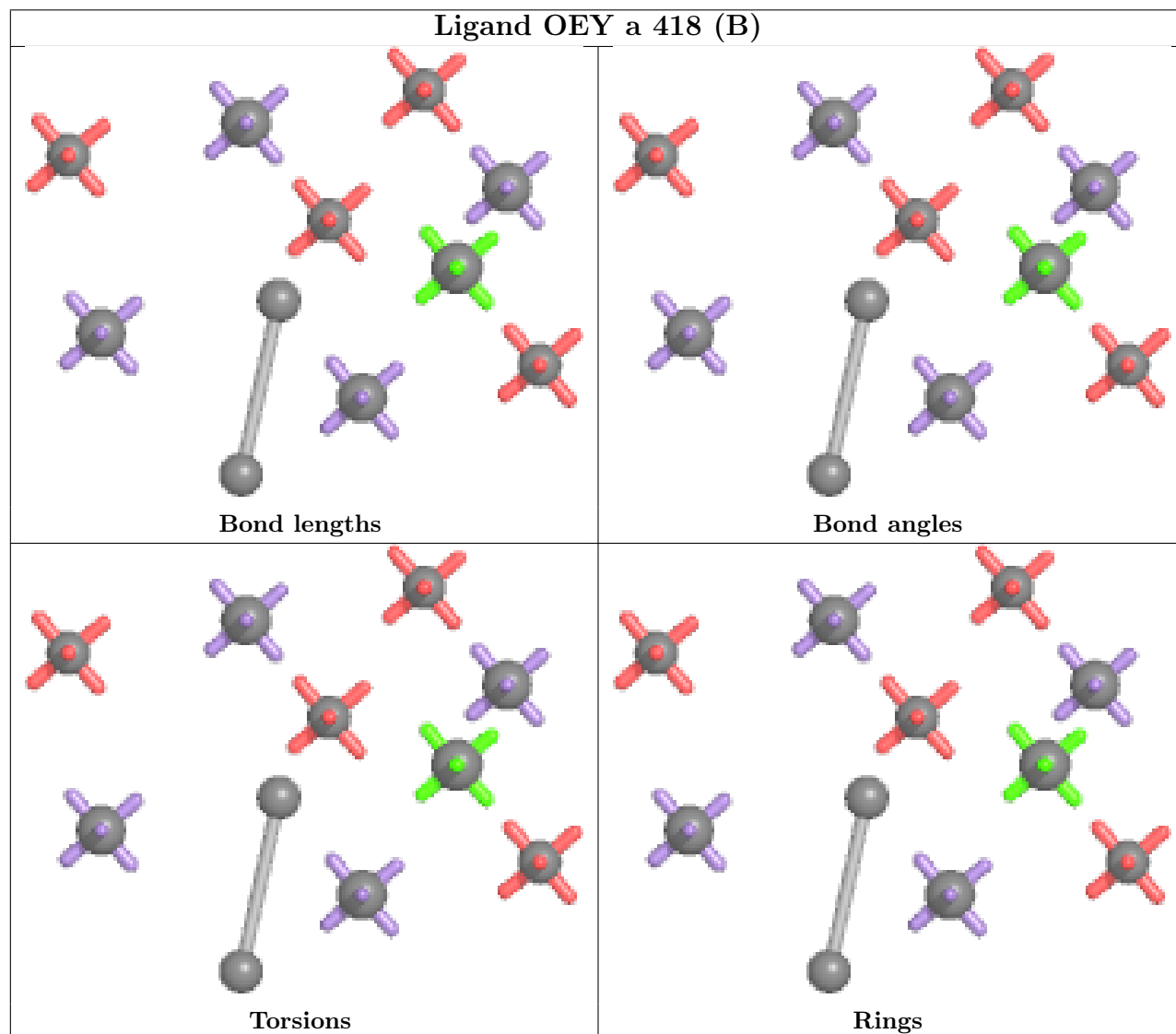
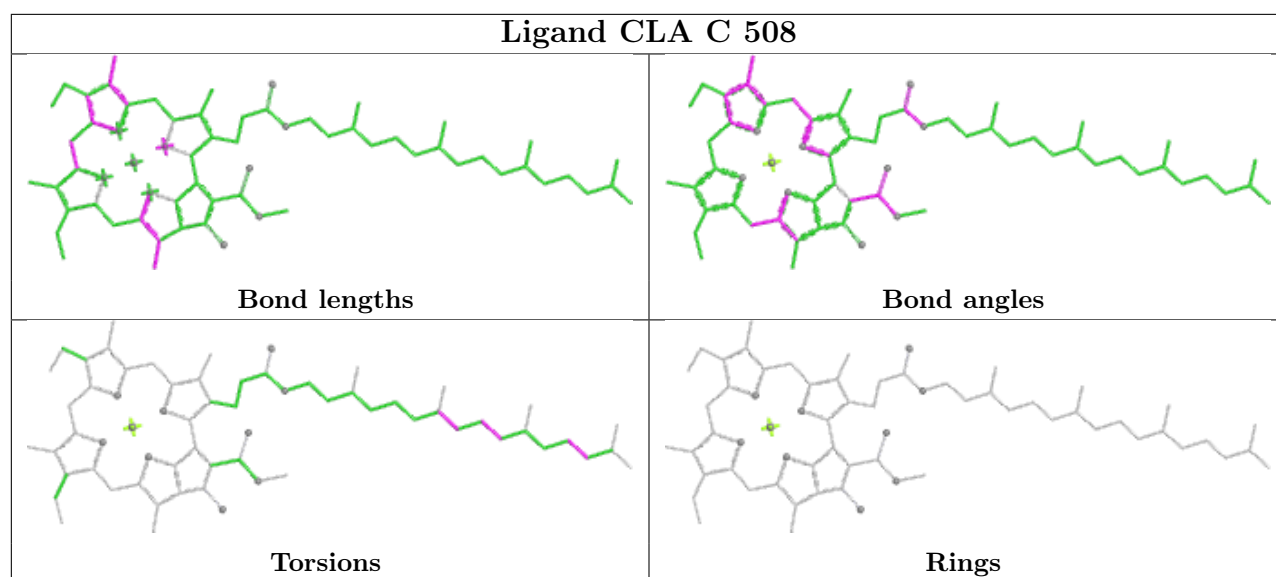
Ligand OEX A 418 (A)

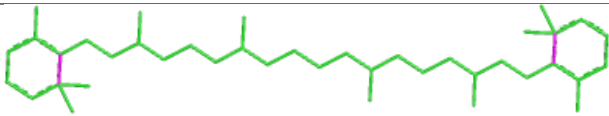
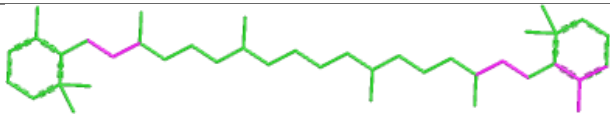
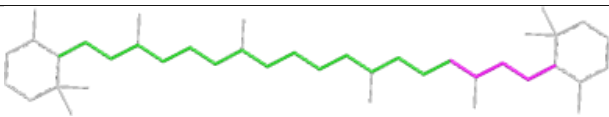
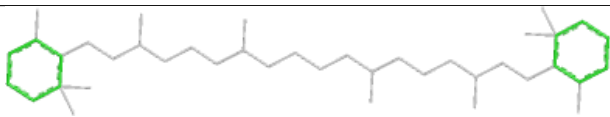


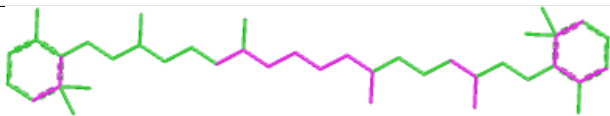
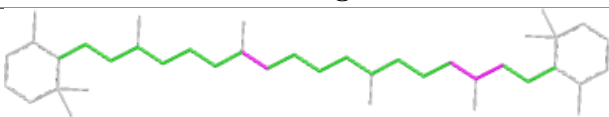
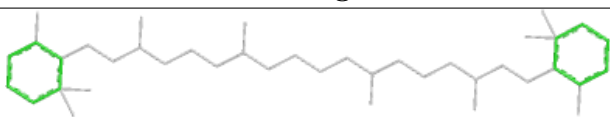
Ligand DGD h 101

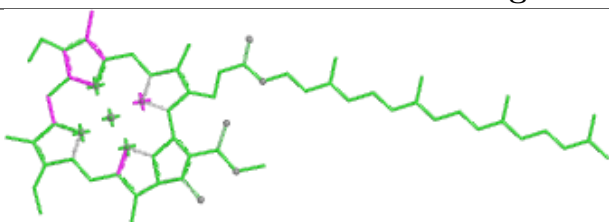
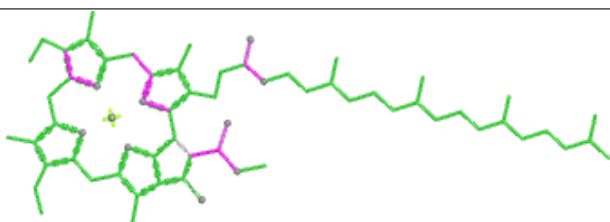
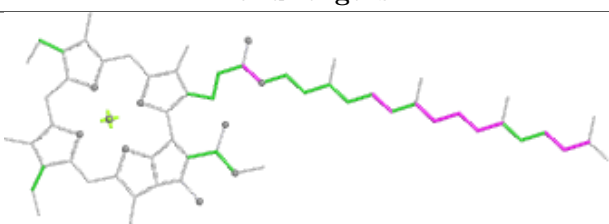
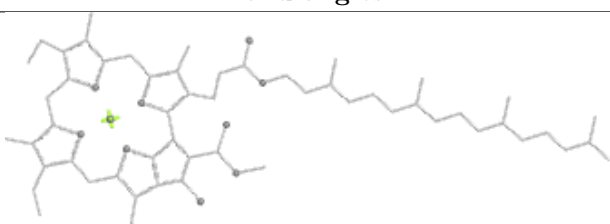


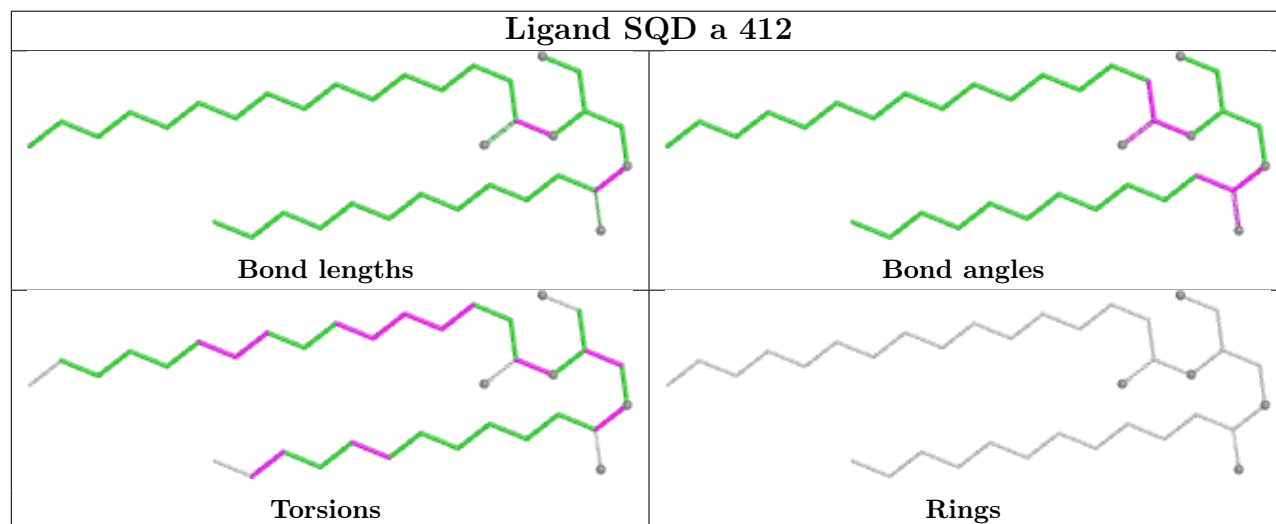
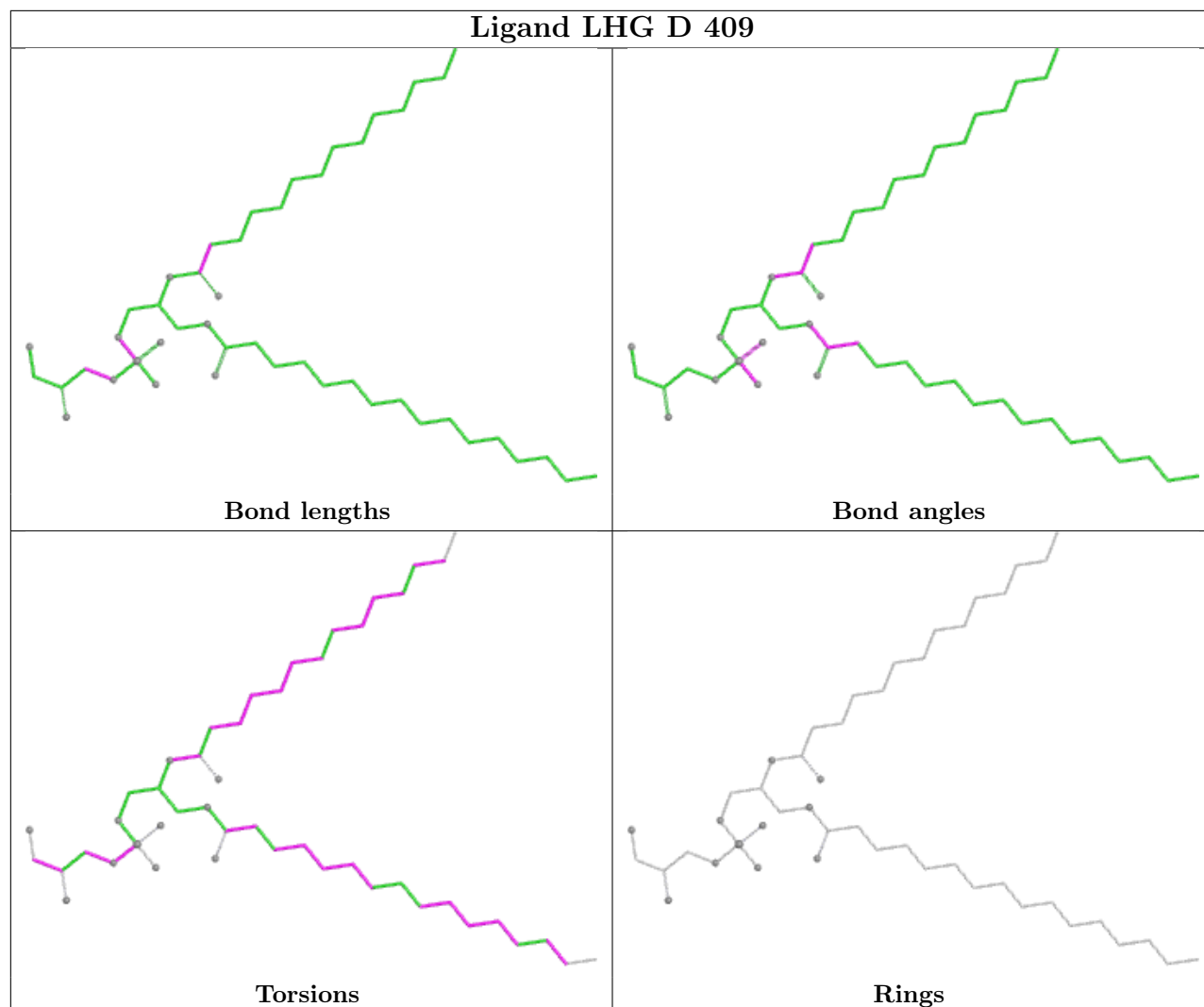


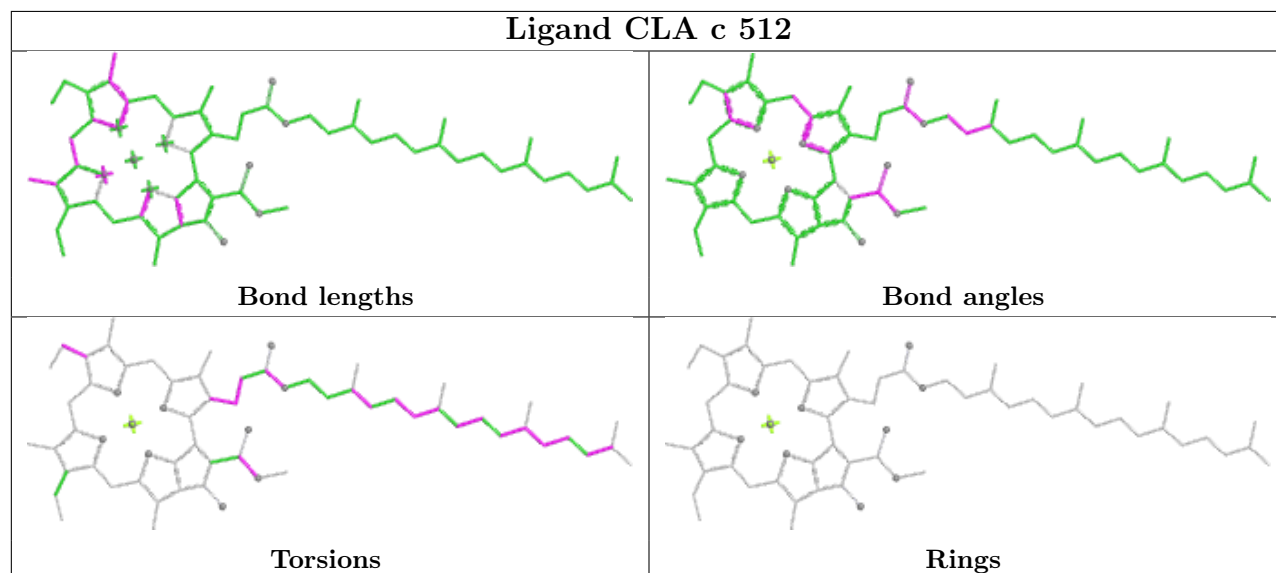
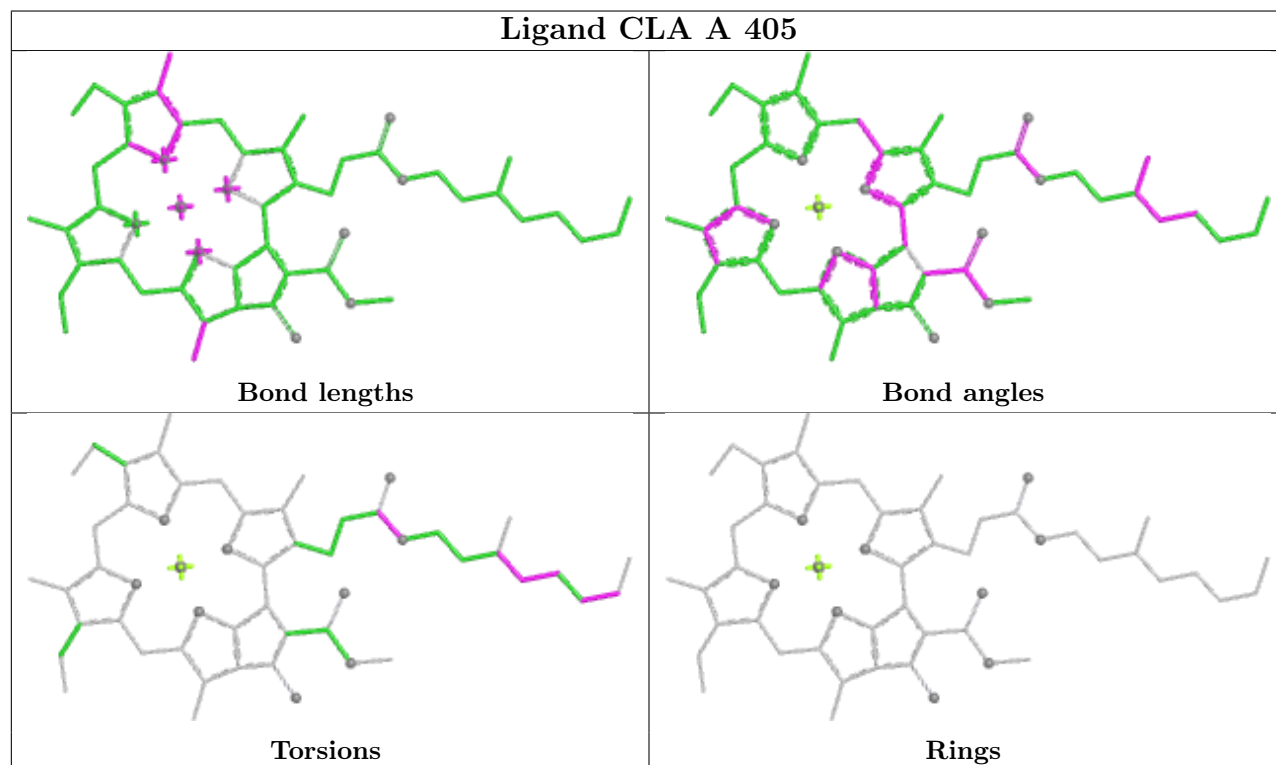
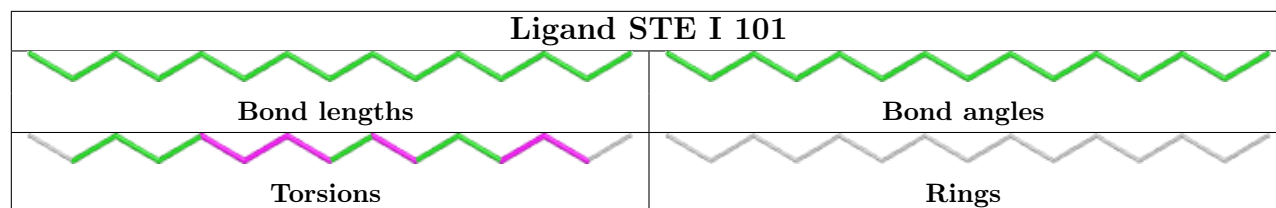


Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

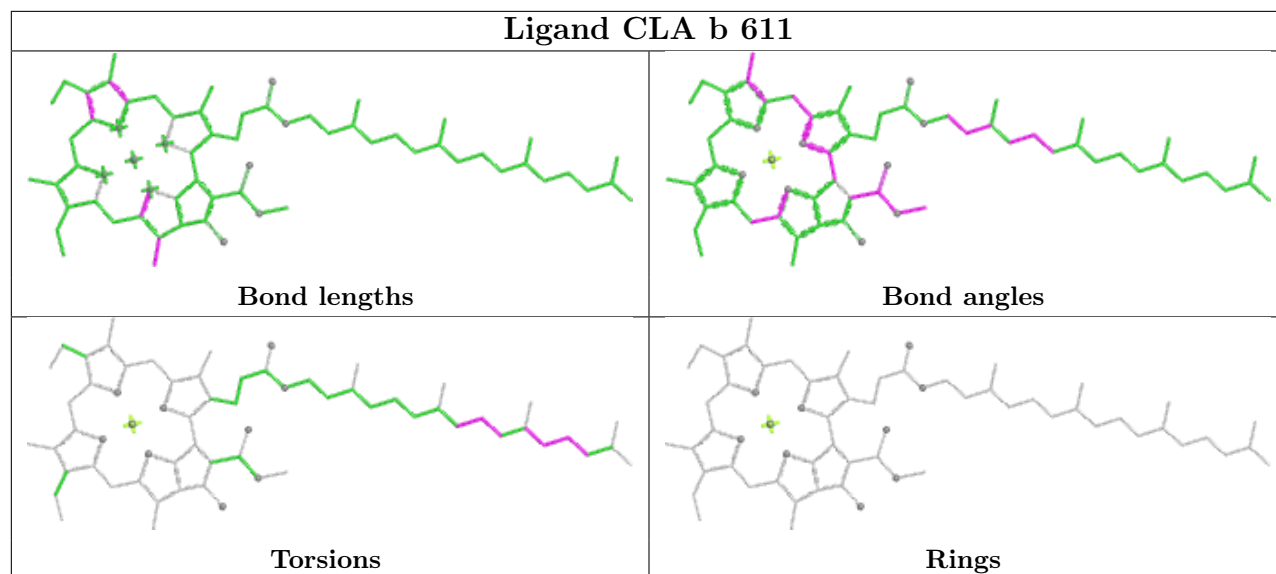
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

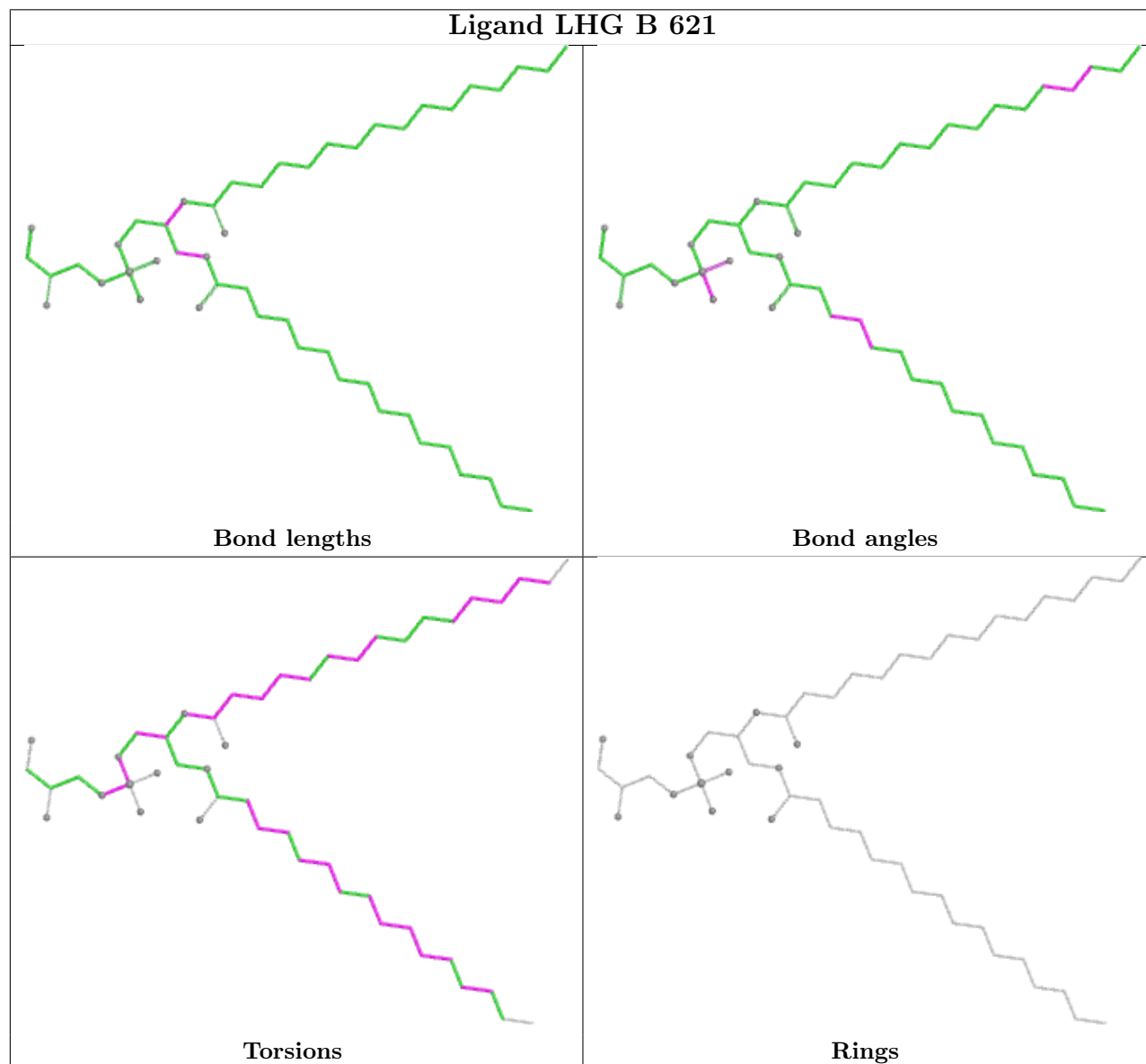


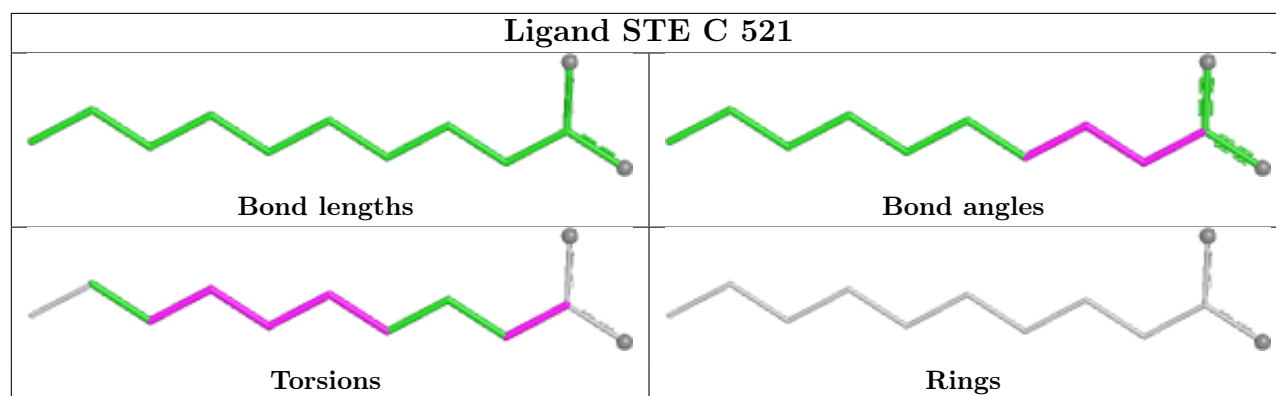
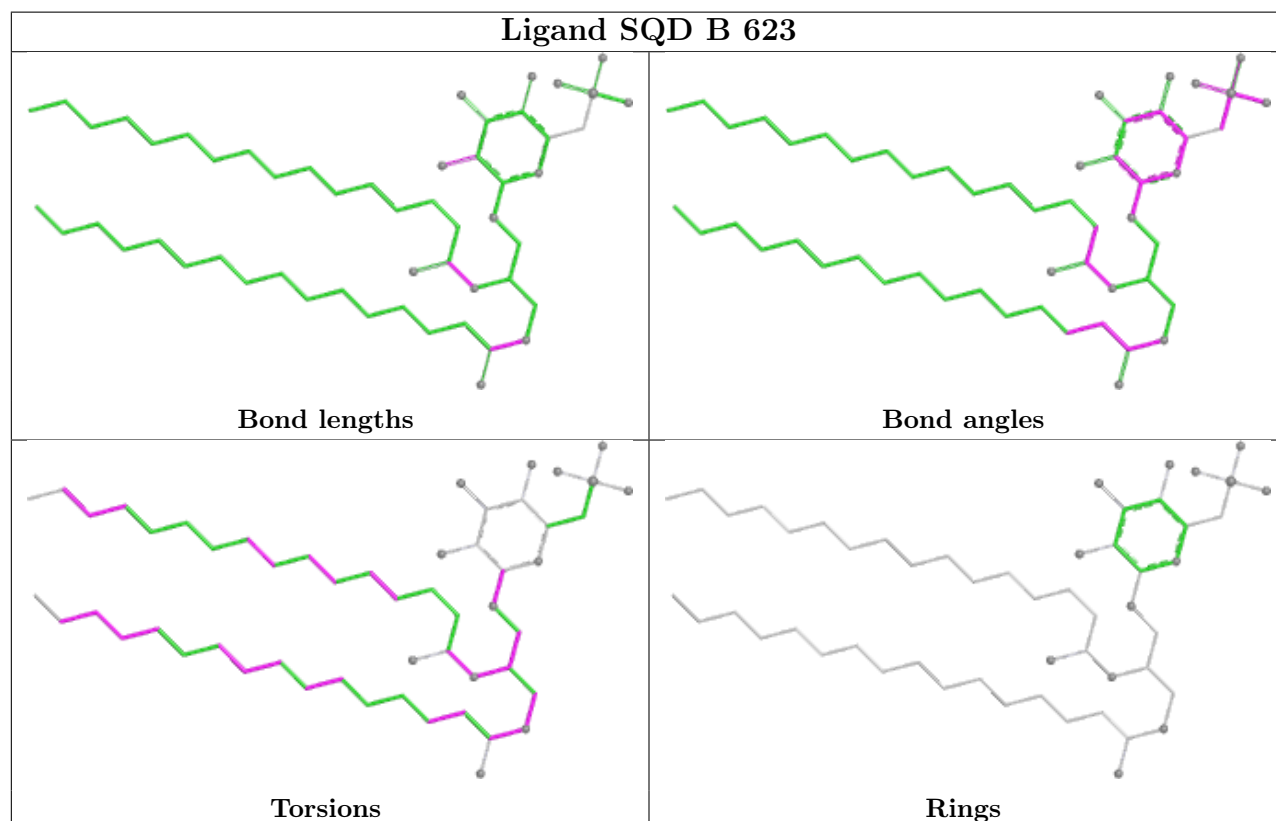
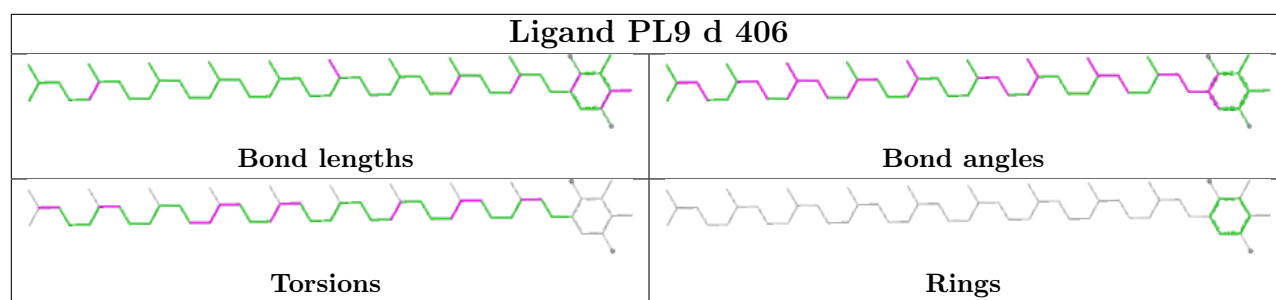


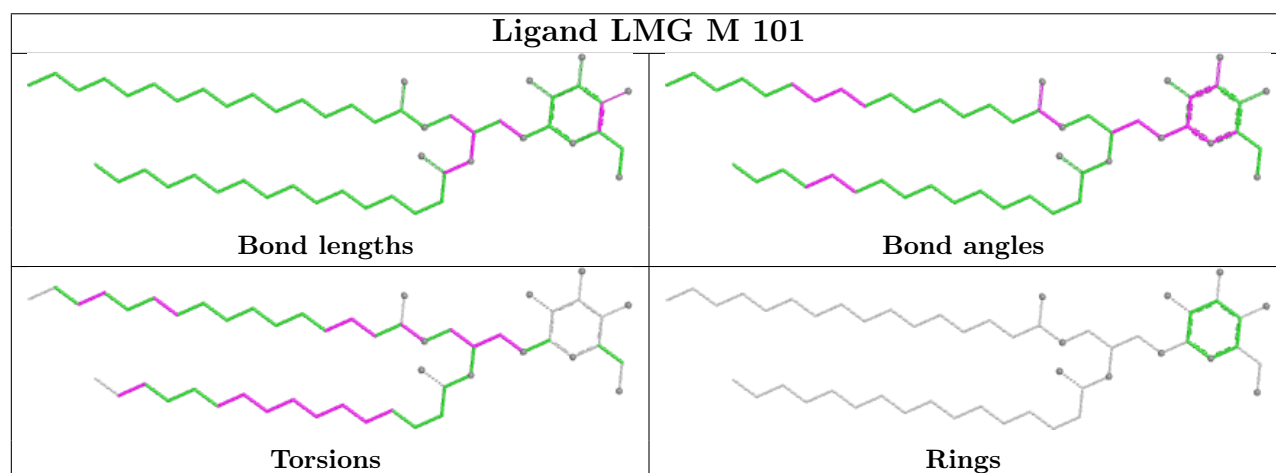
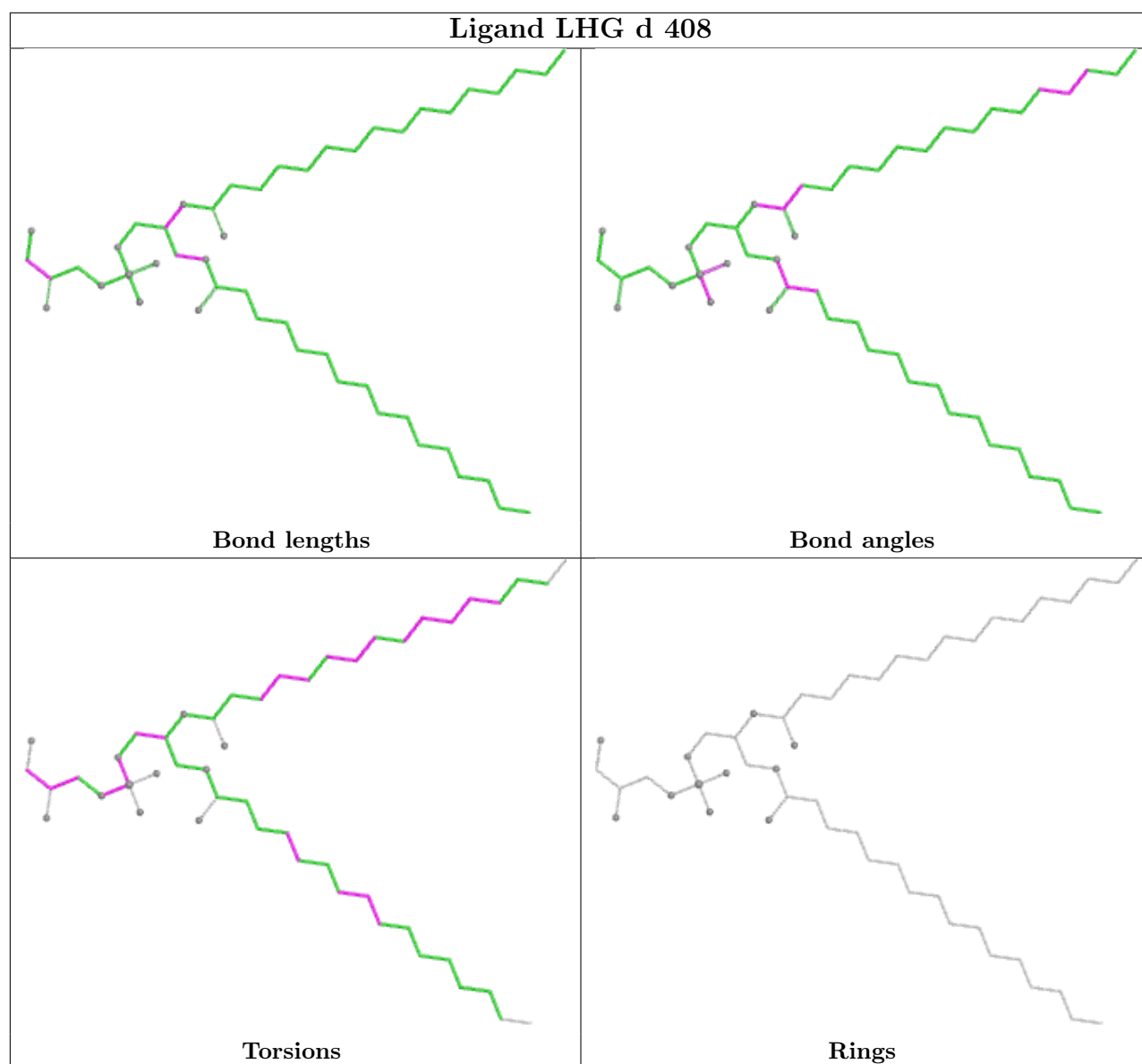
Ligand CLA b 611

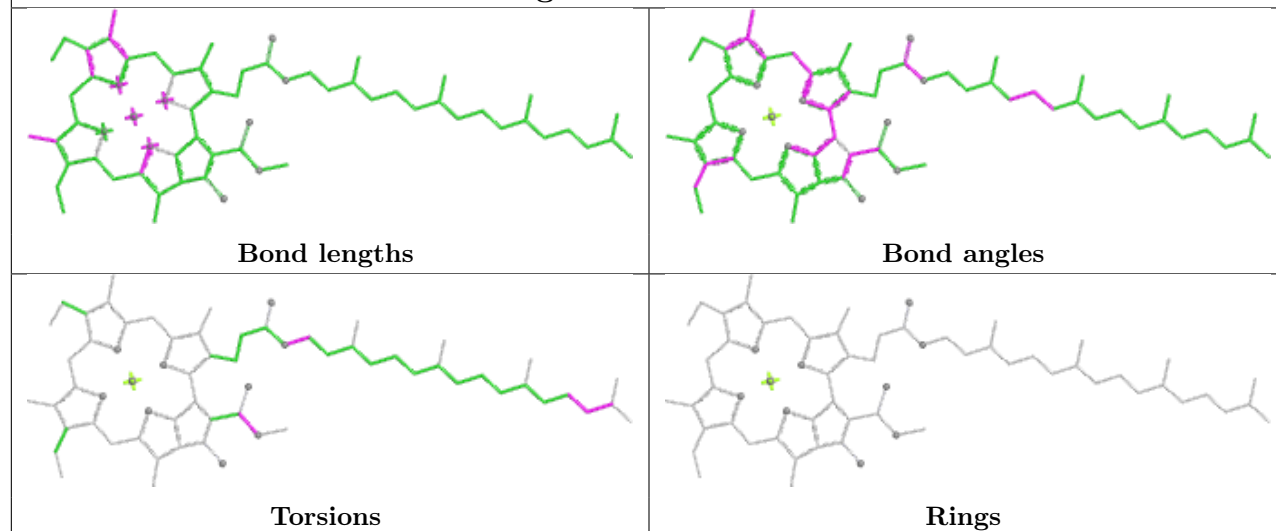
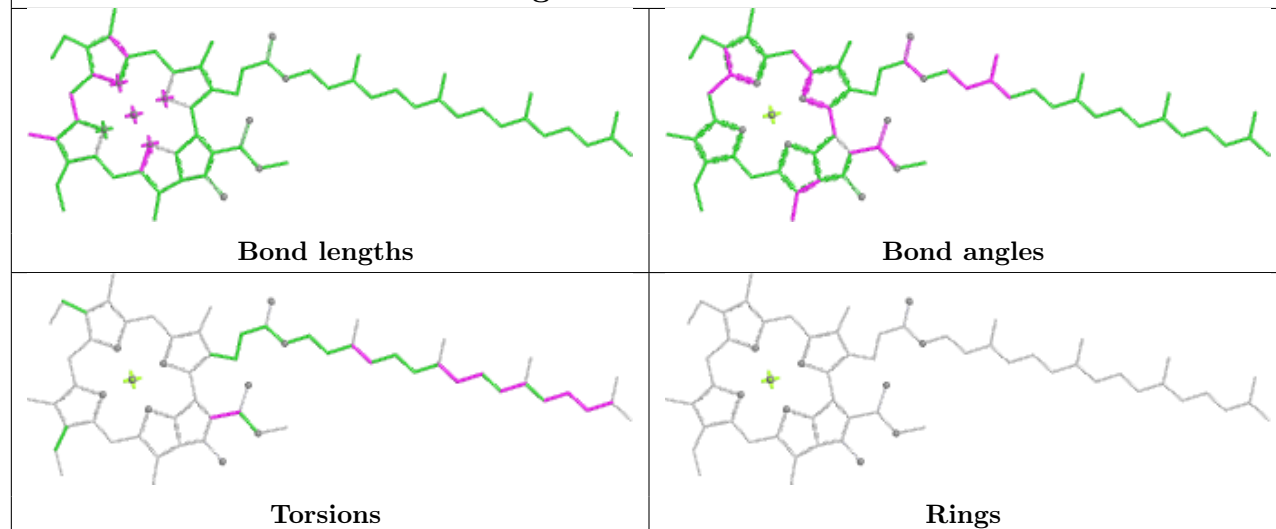
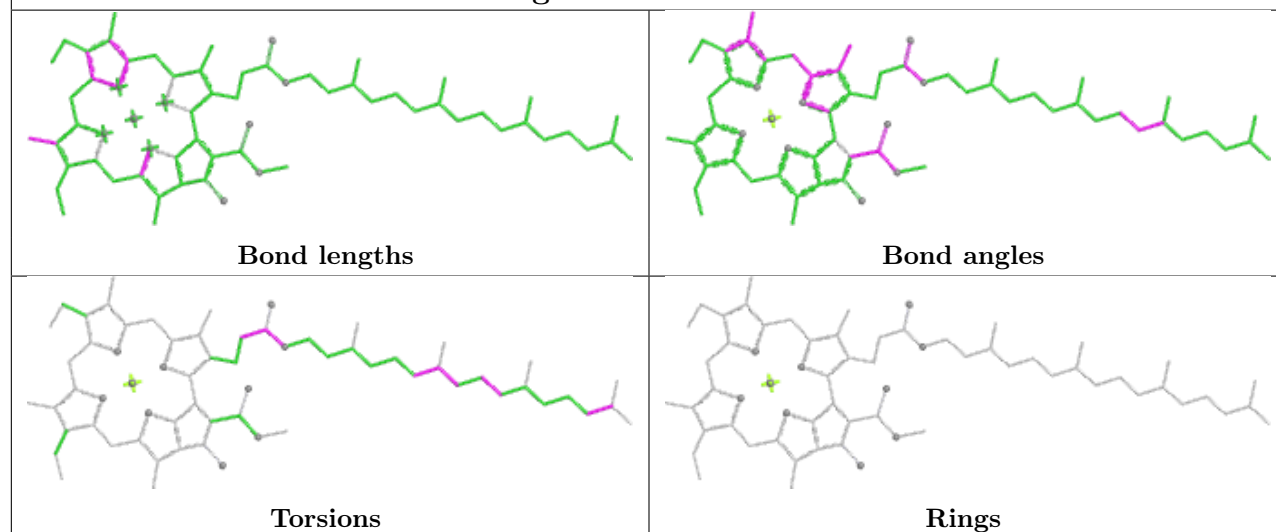


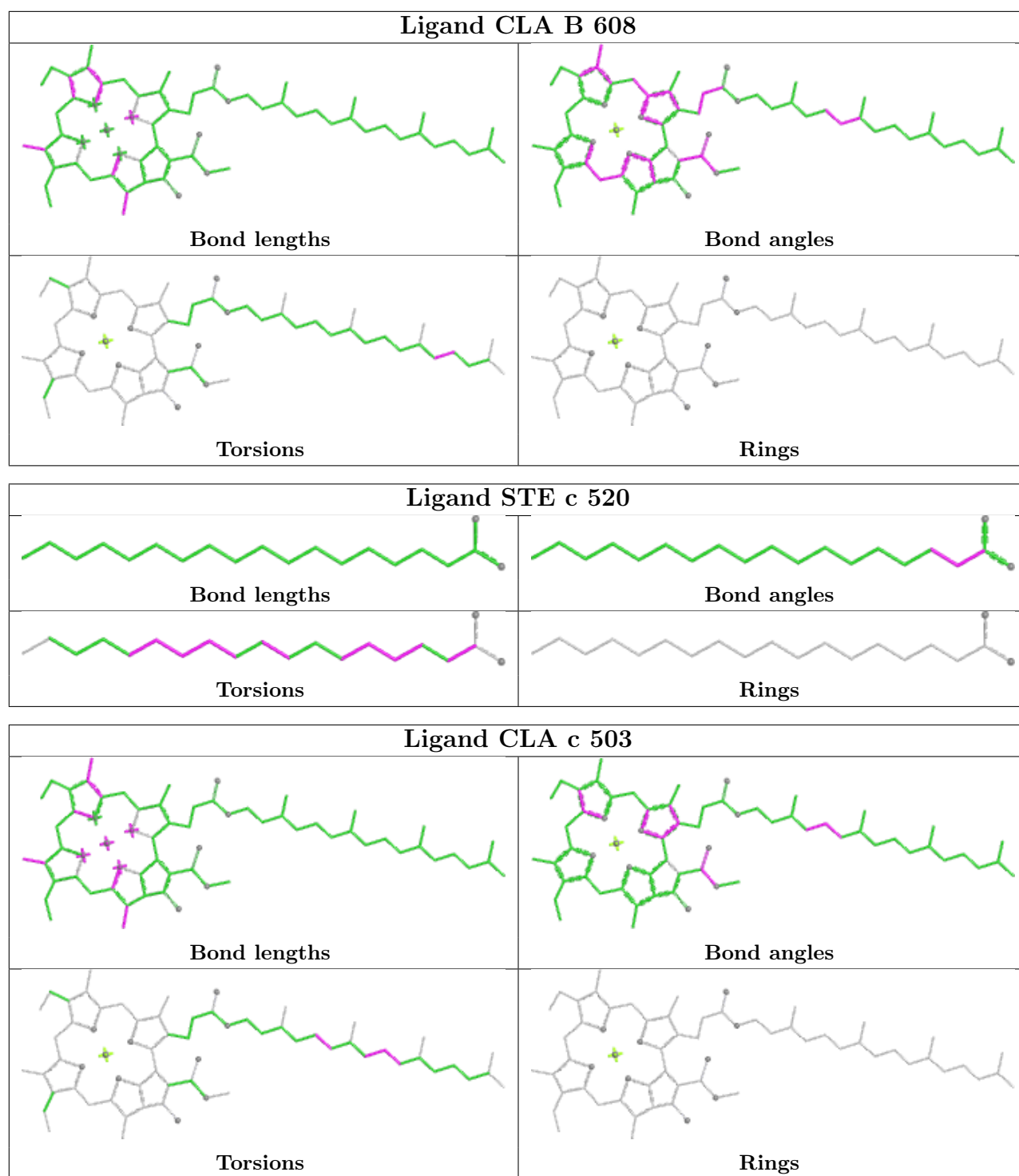
Ligand LHG B 621

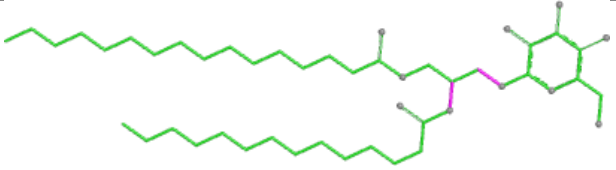
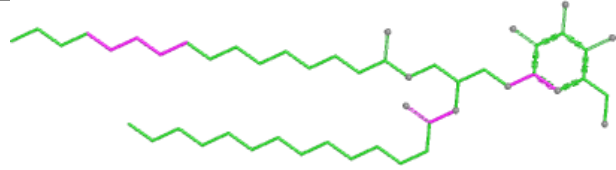
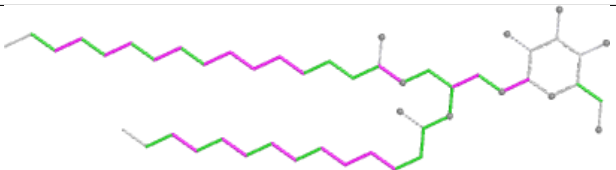
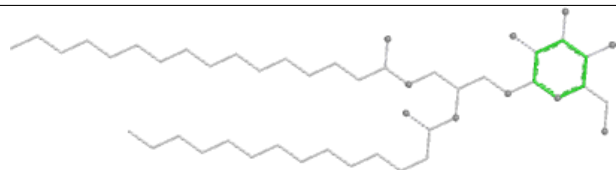


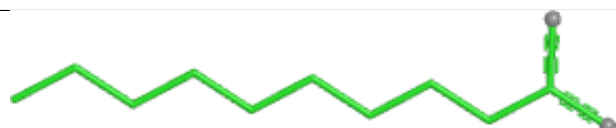
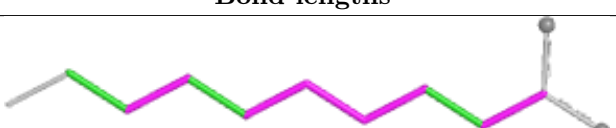
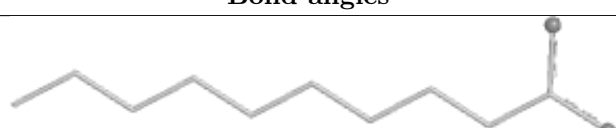


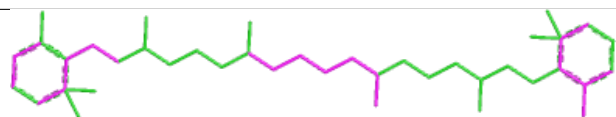
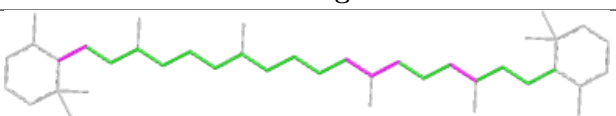
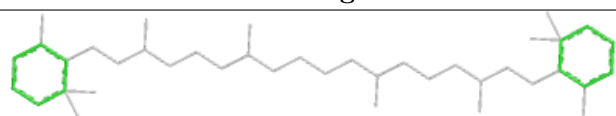


Ligand CLA a 402**Ligand CLA B 614****Ligand CLA B 612**

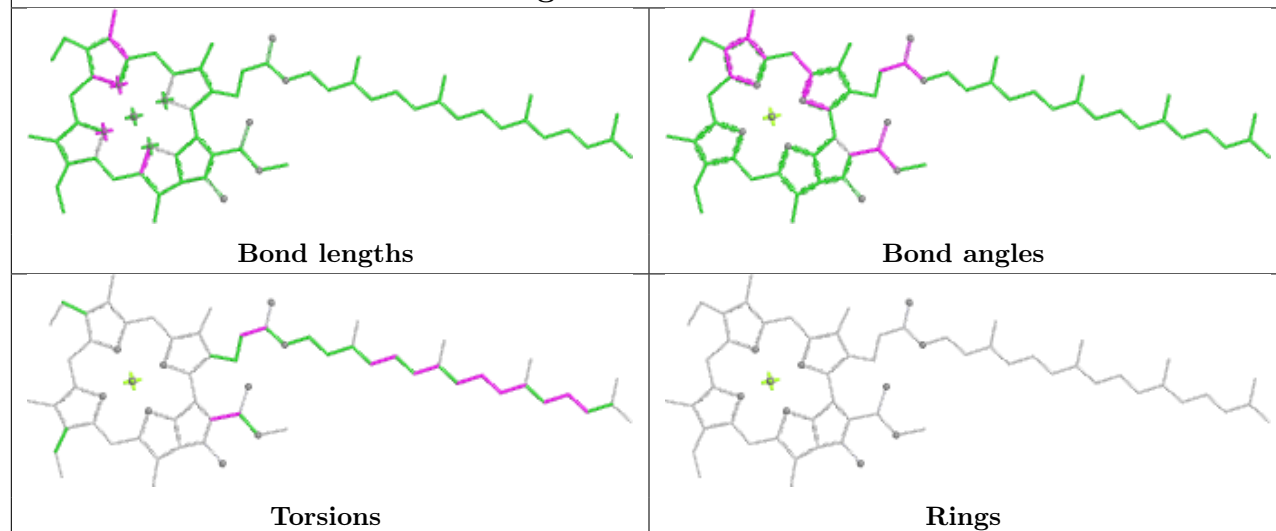


Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

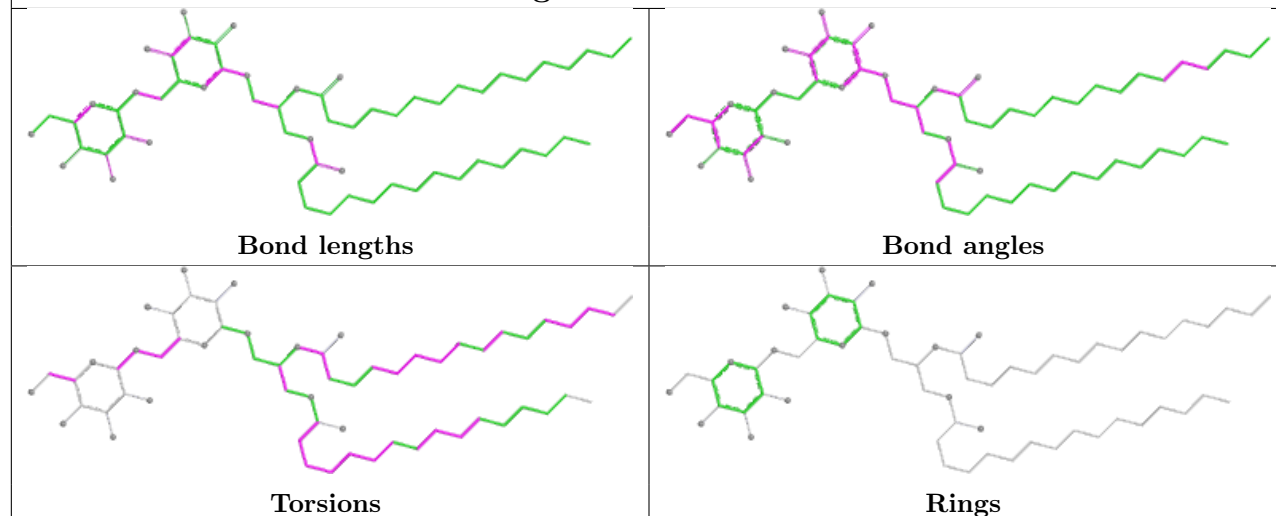
Ligand STE a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

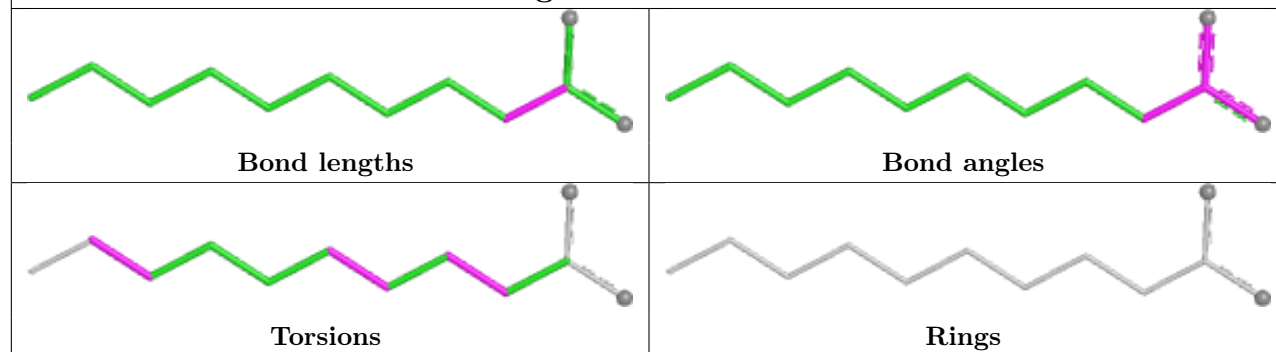
Ligand CLA c 509

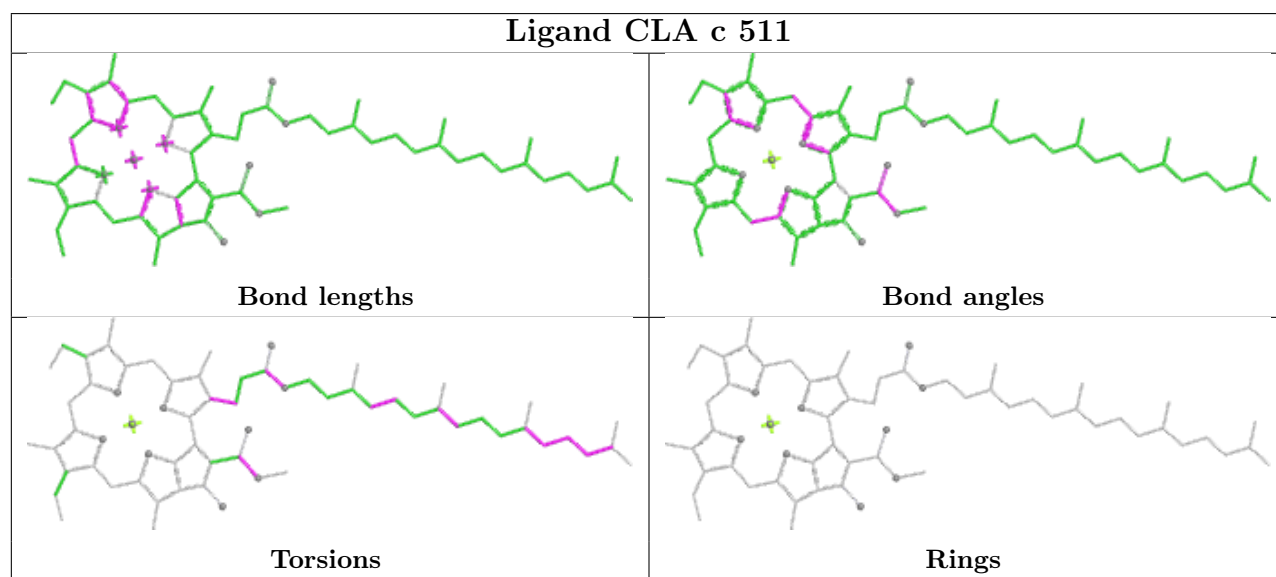
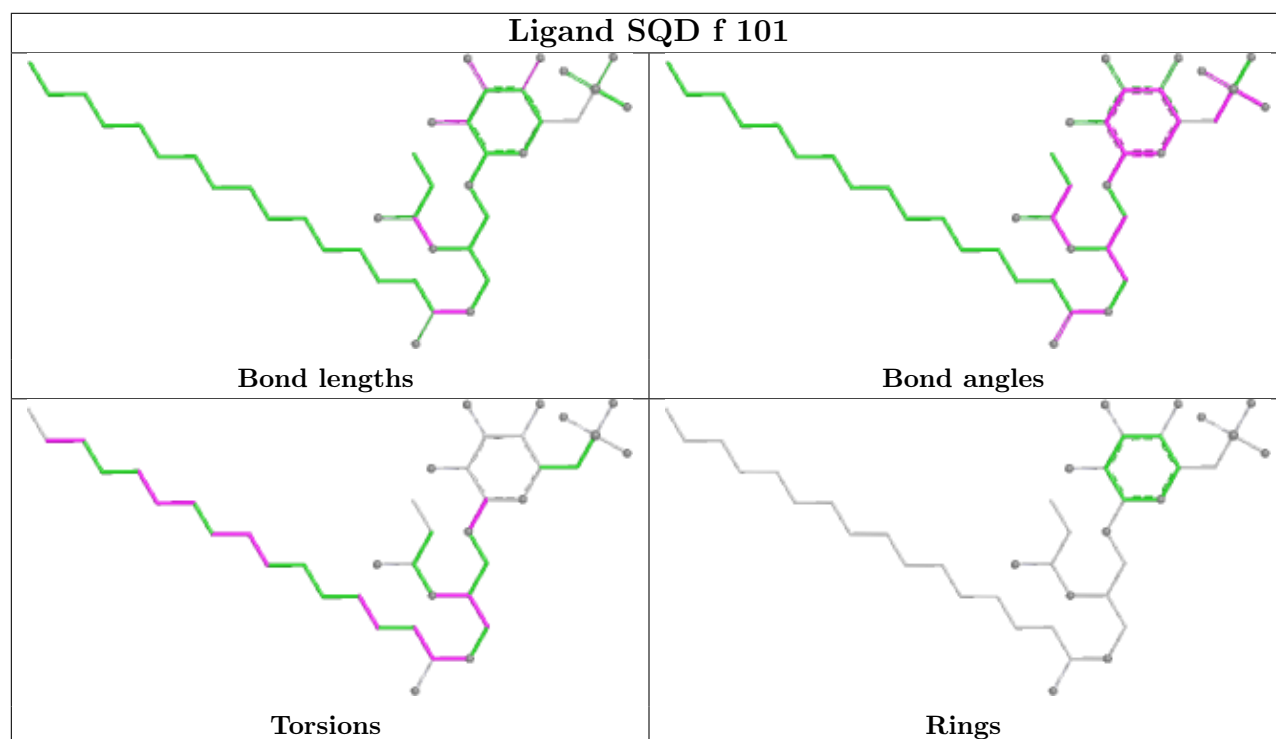
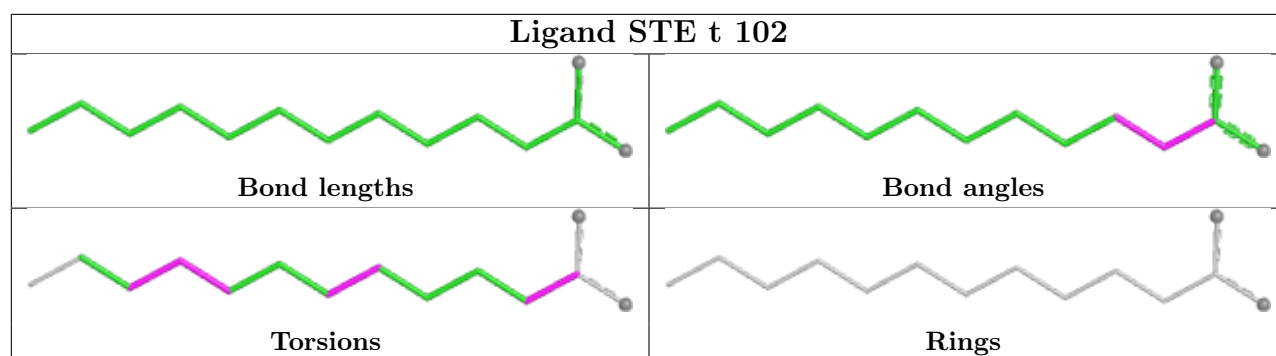


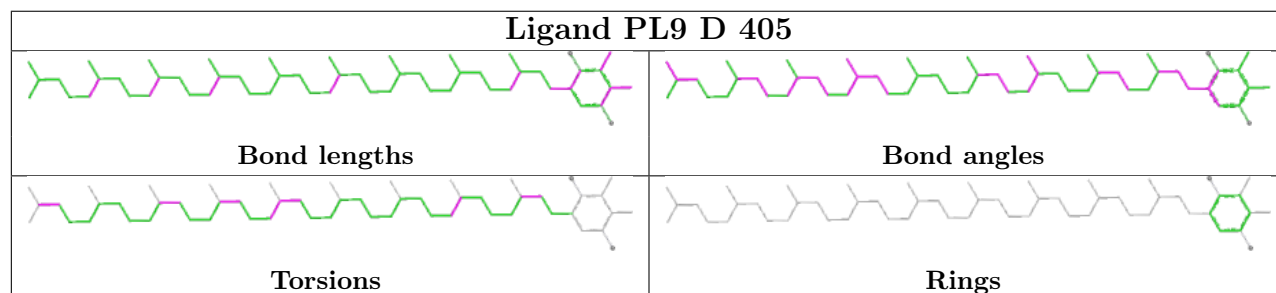
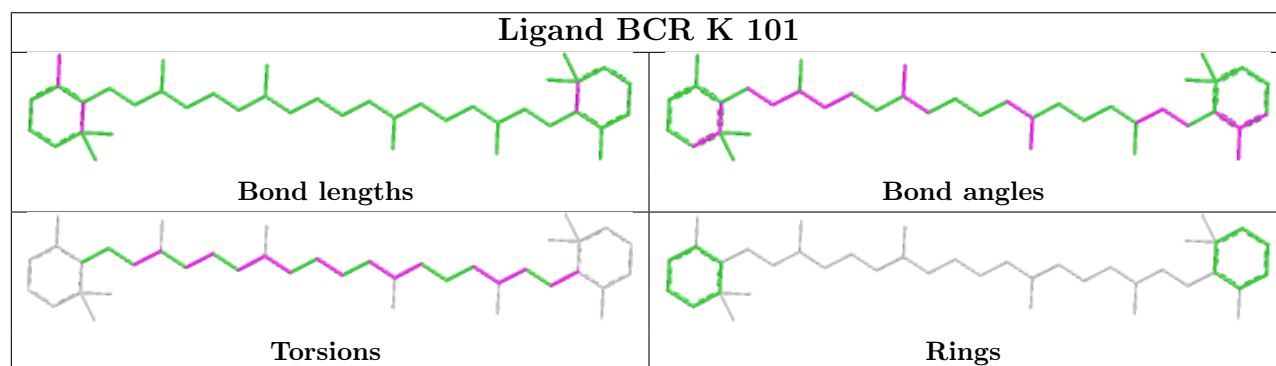
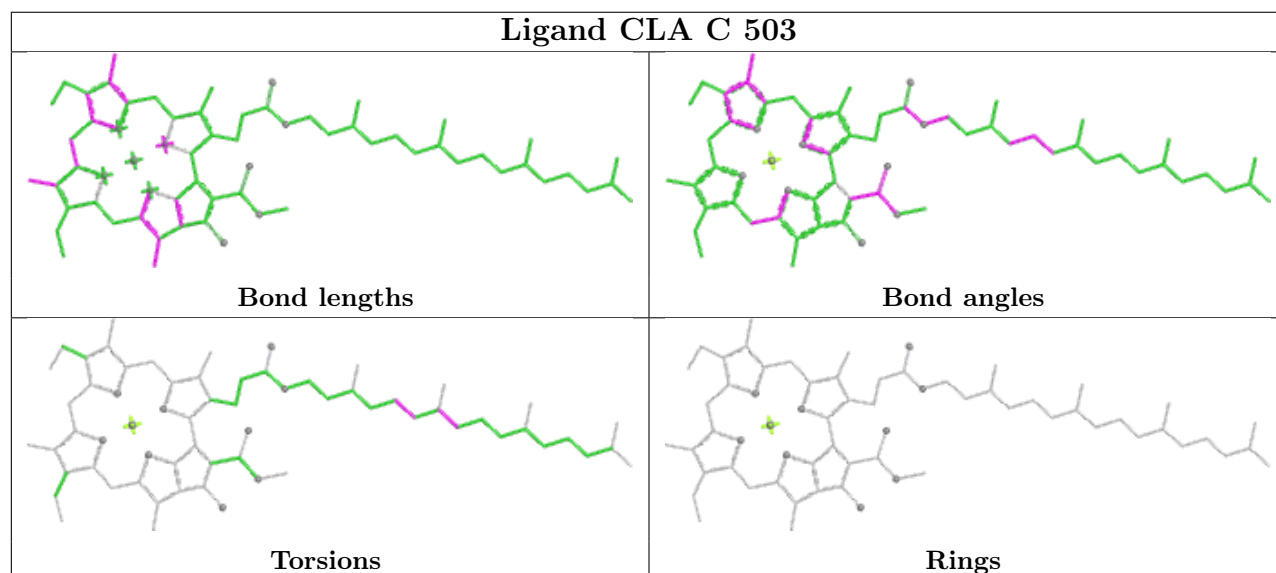
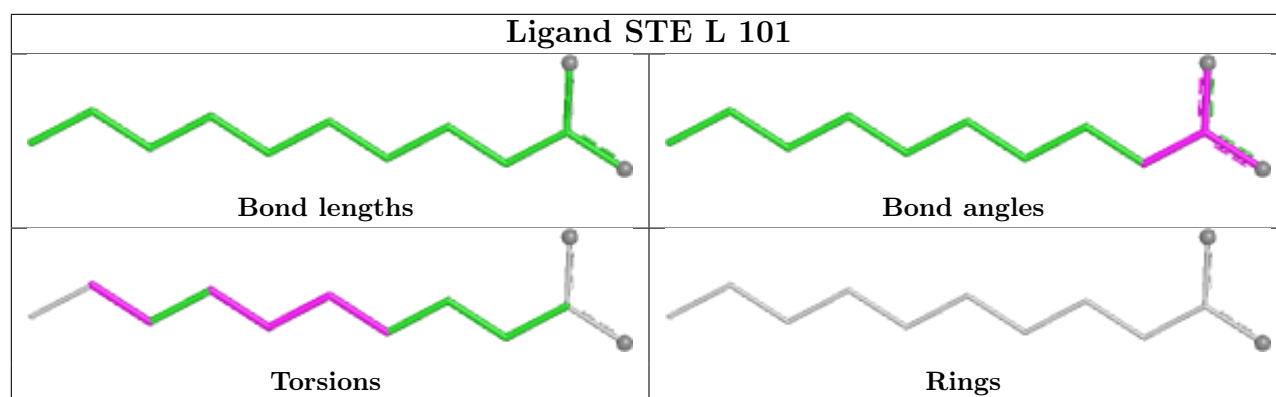
Ligand DGD c 516

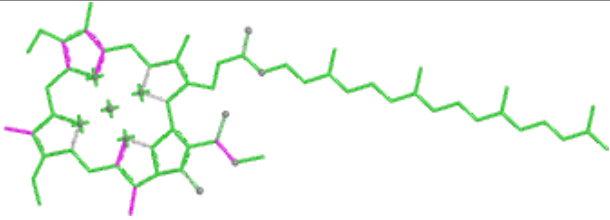
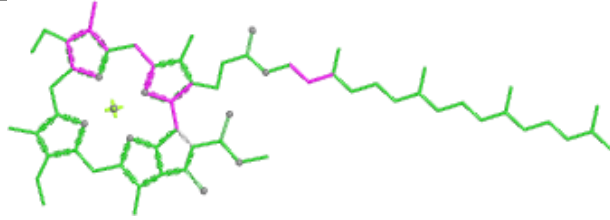
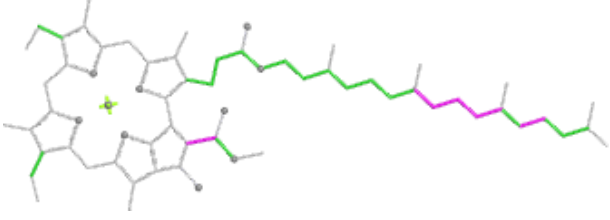
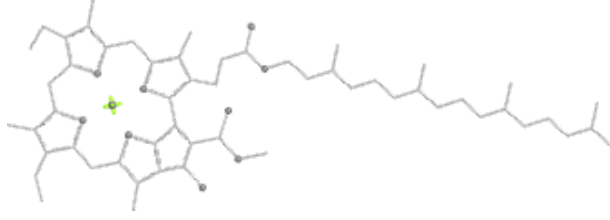
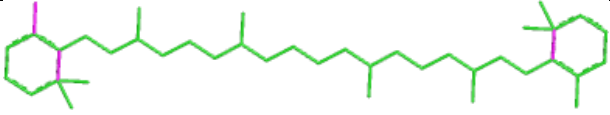
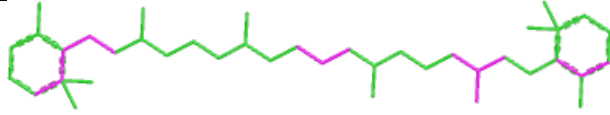
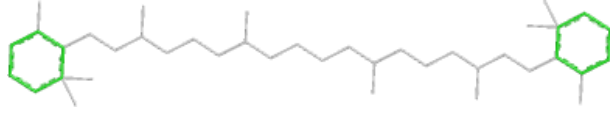
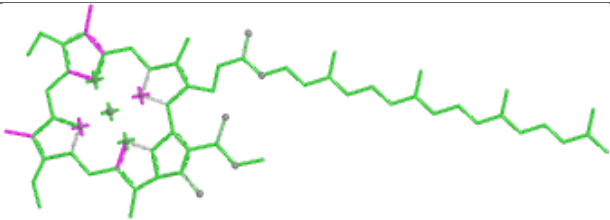
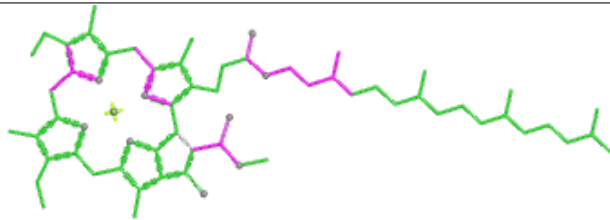
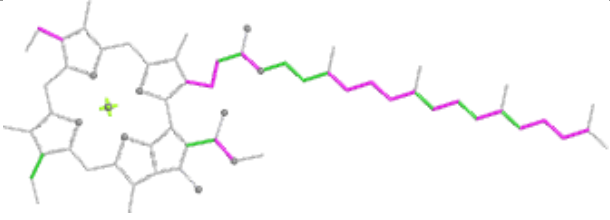
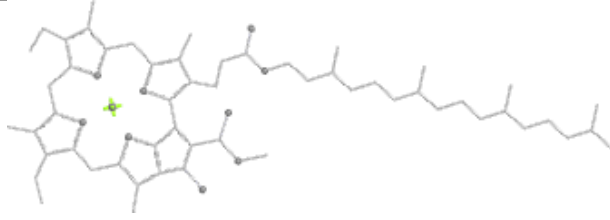


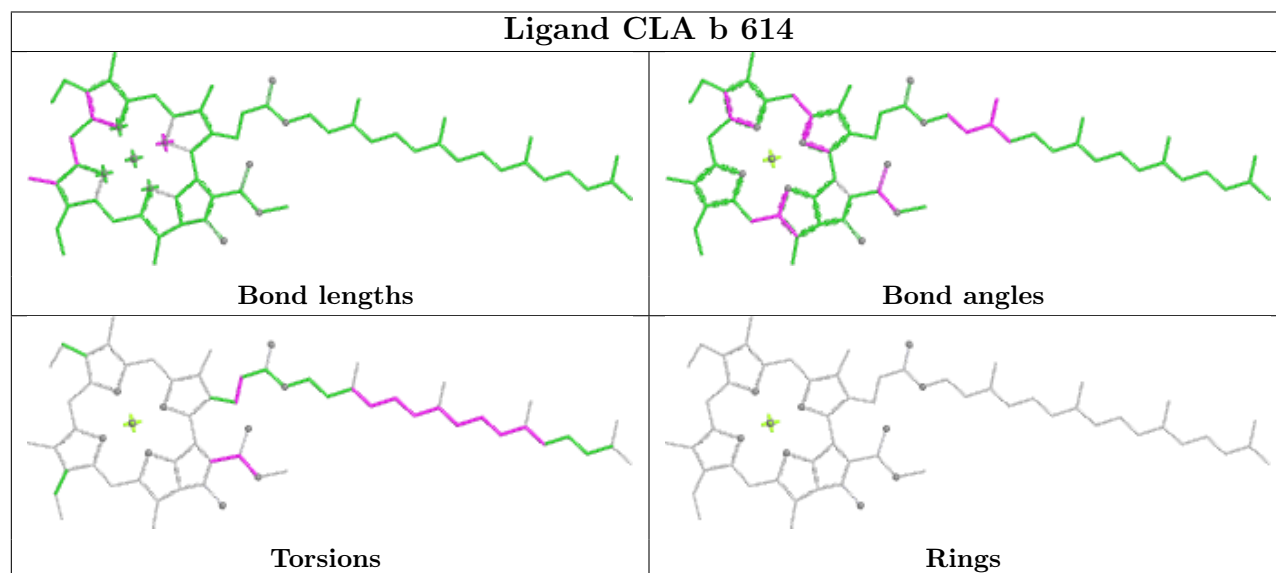
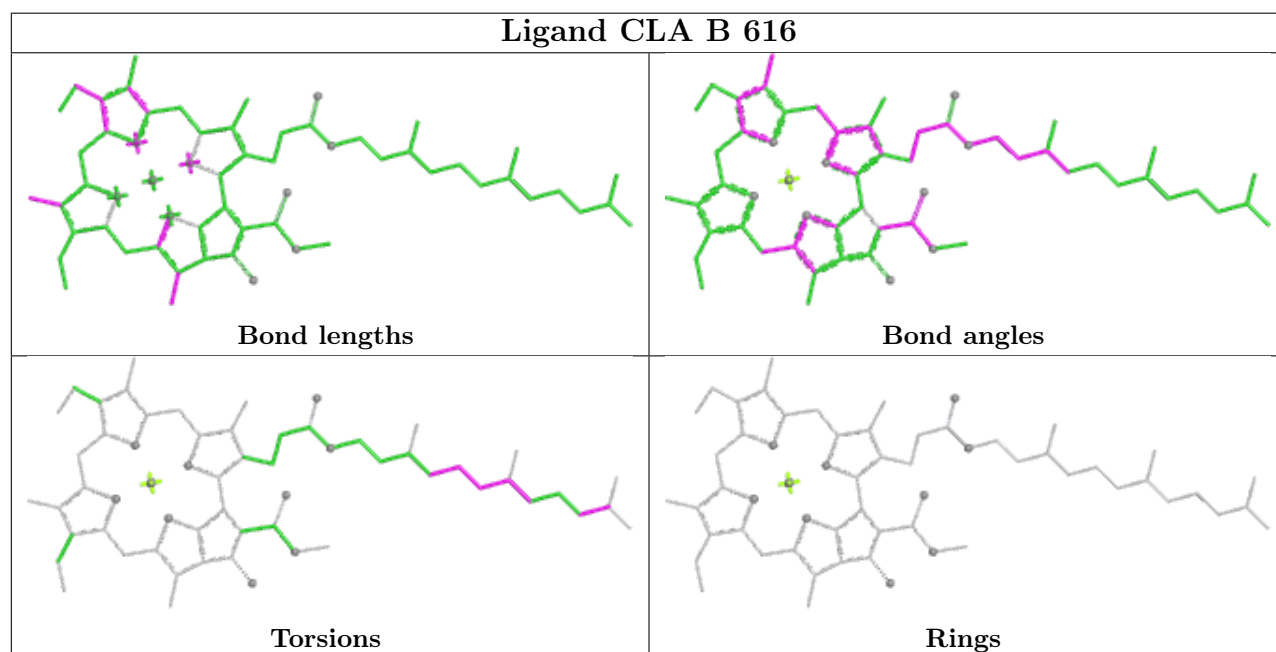
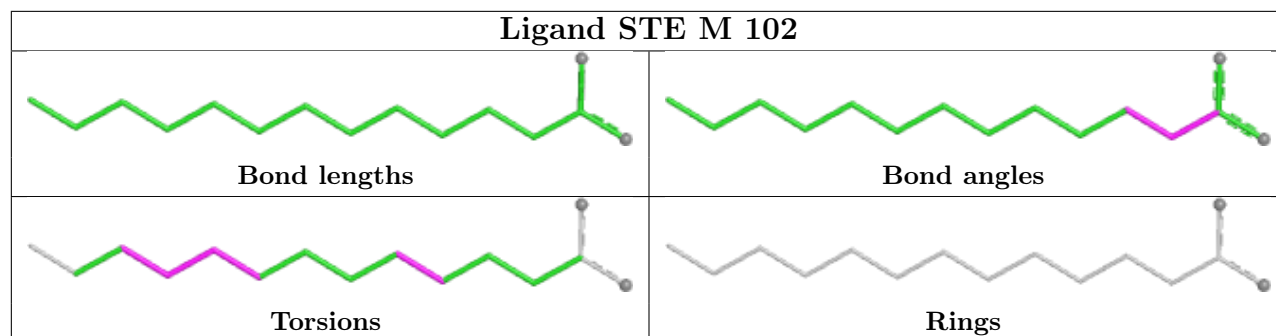
Ligand STE B 624

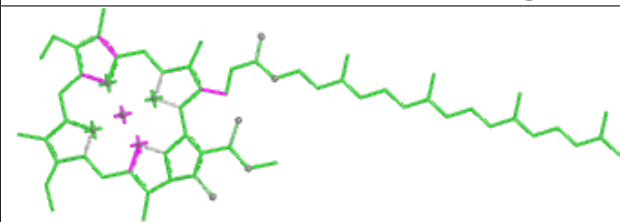
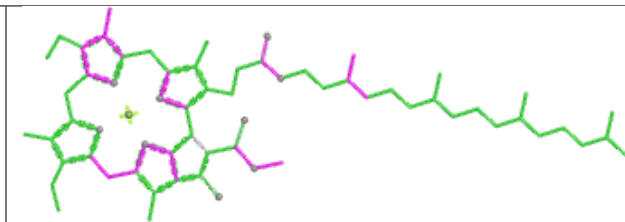
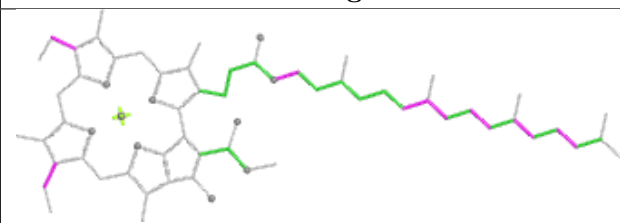
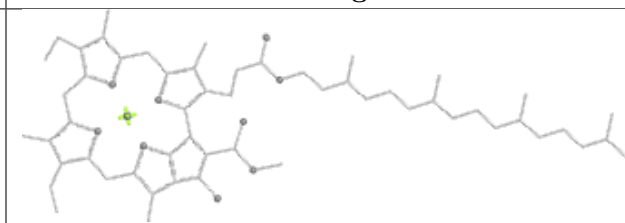


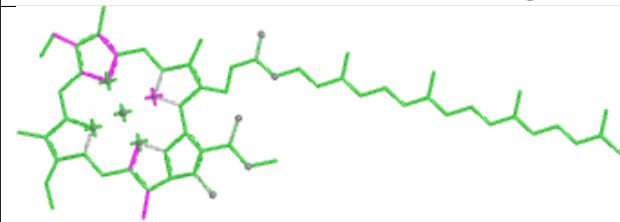
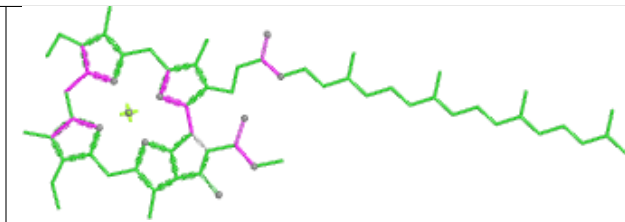
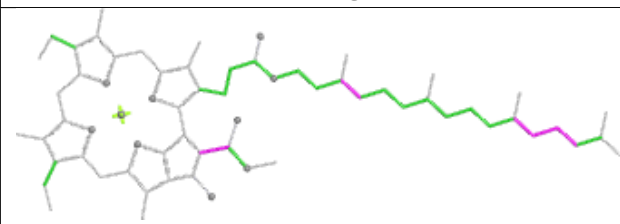
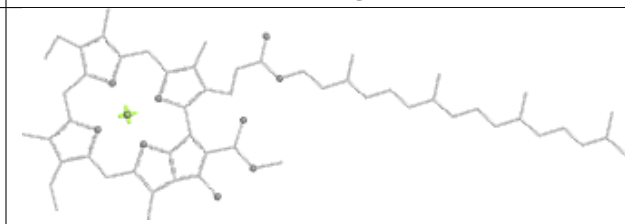


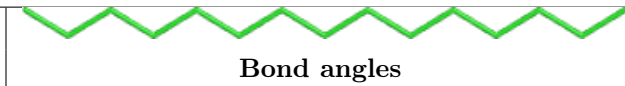


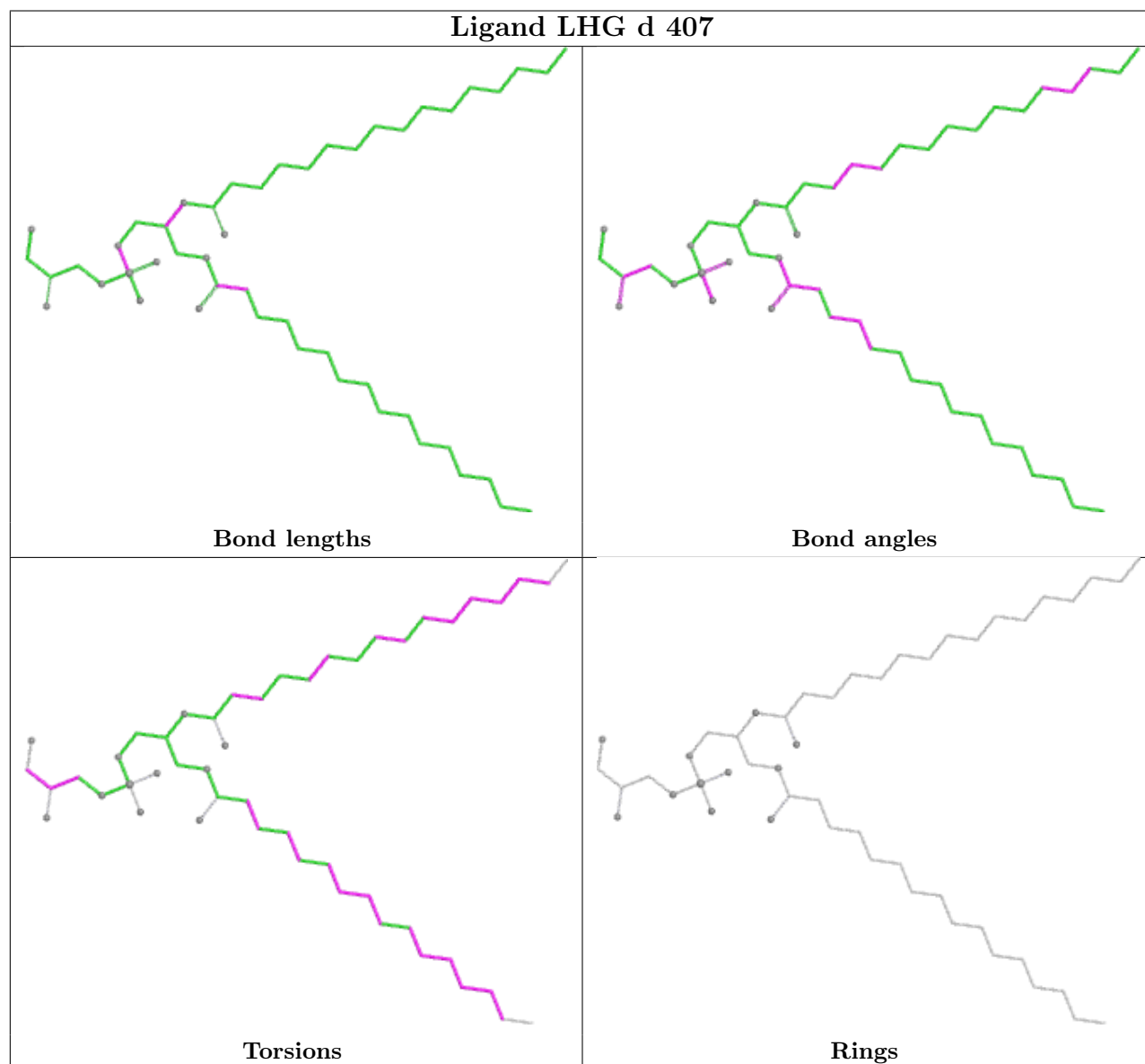
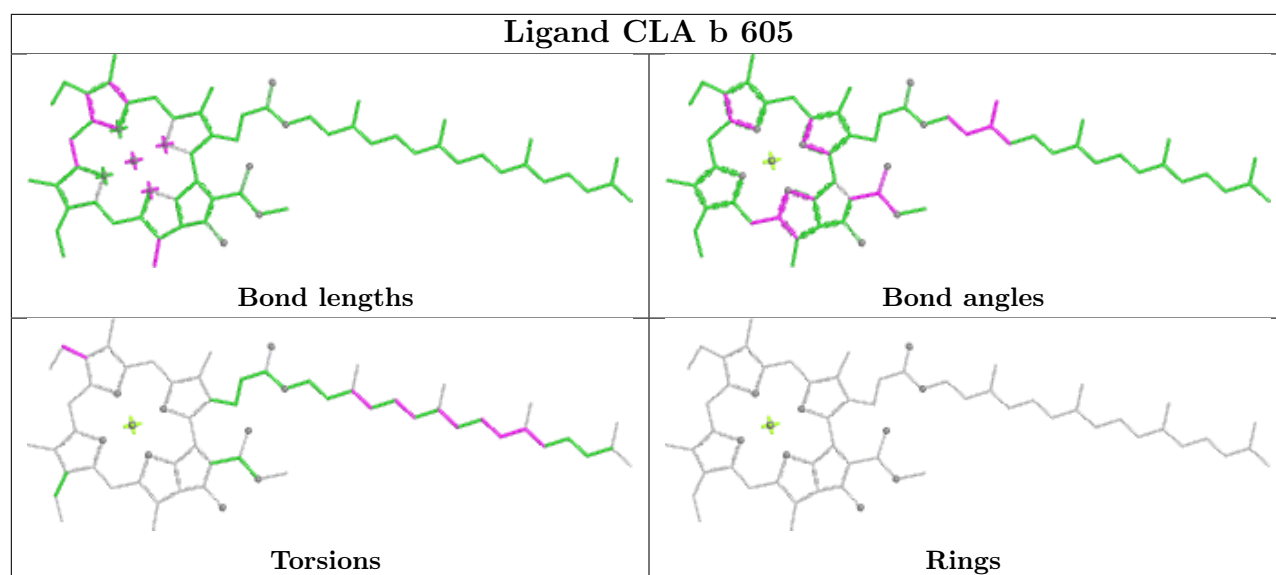
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

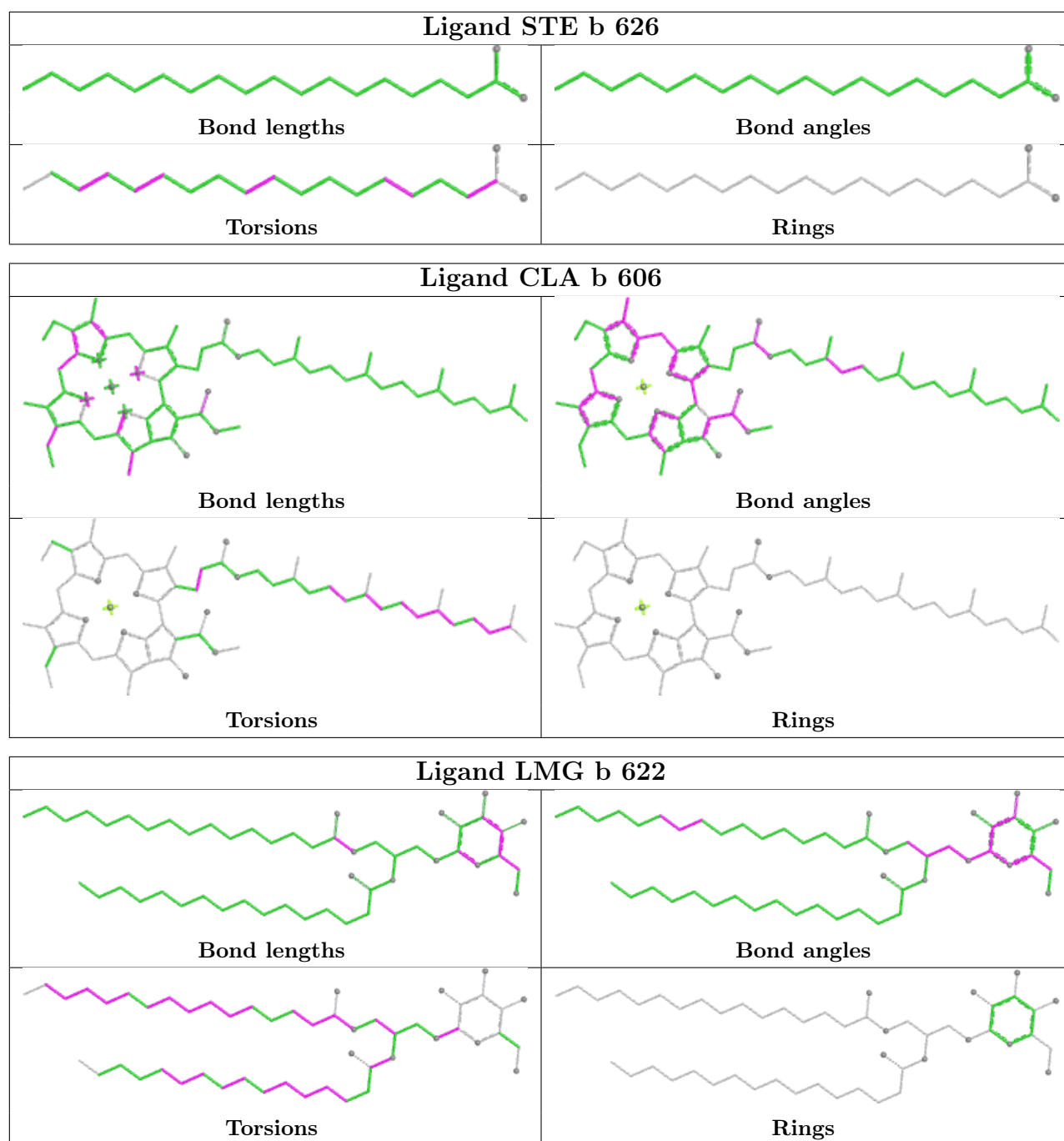


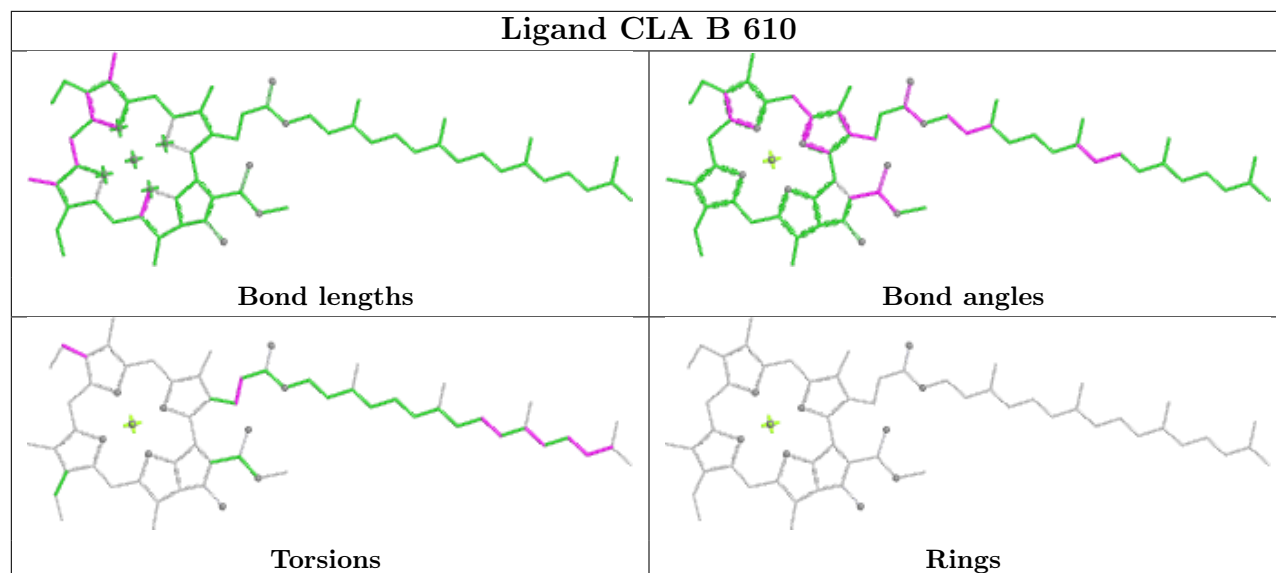
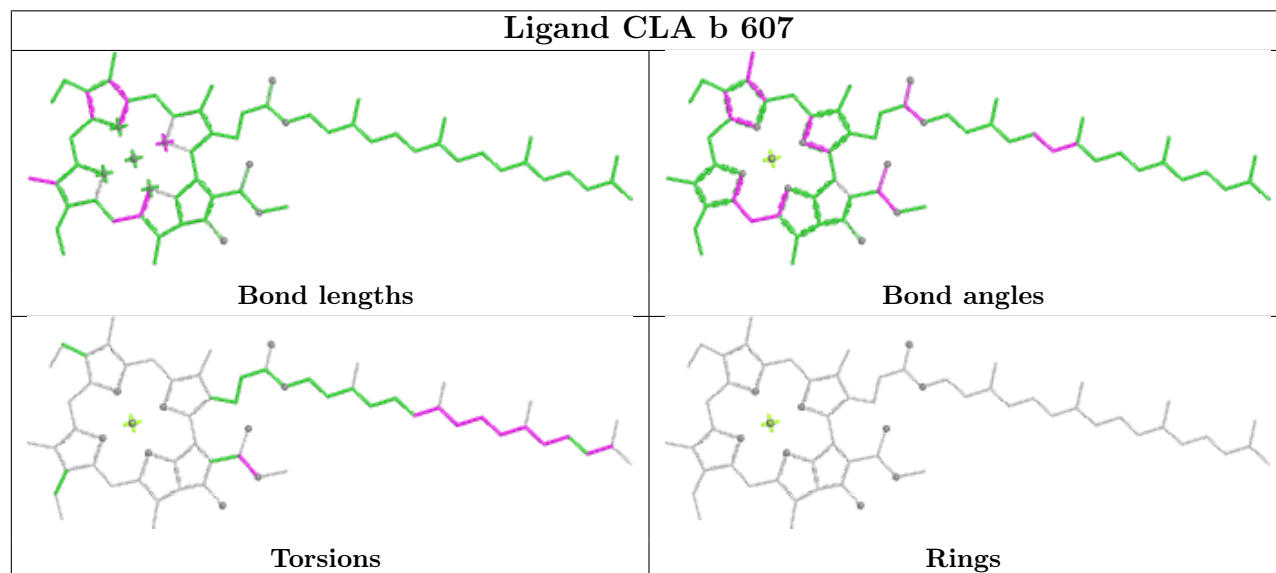
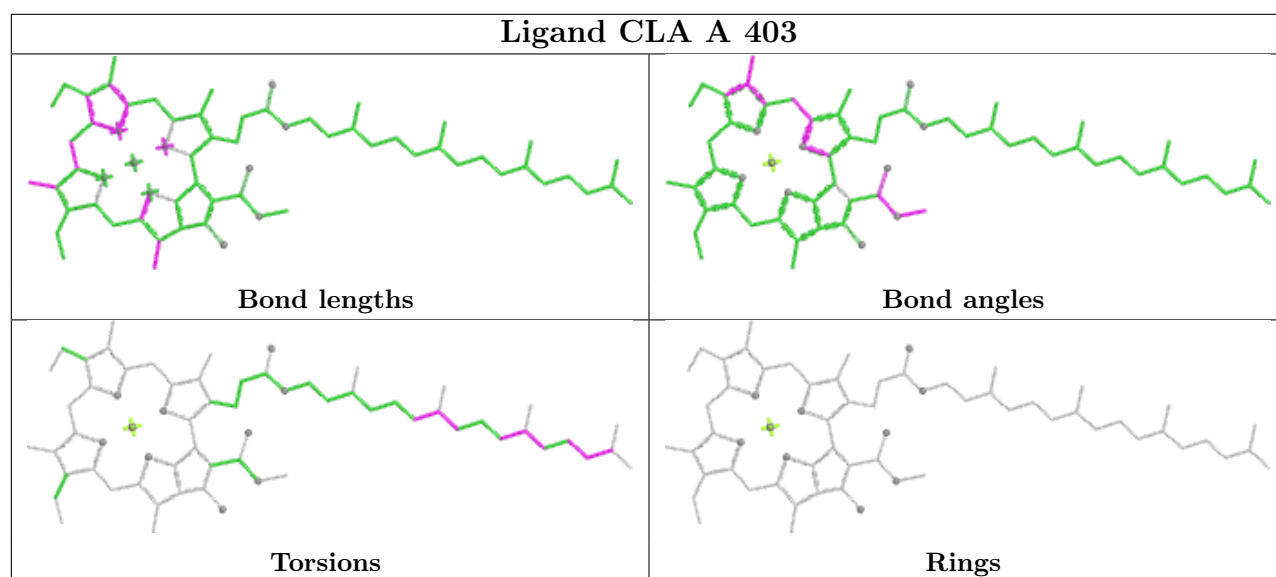
Ligand CLA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

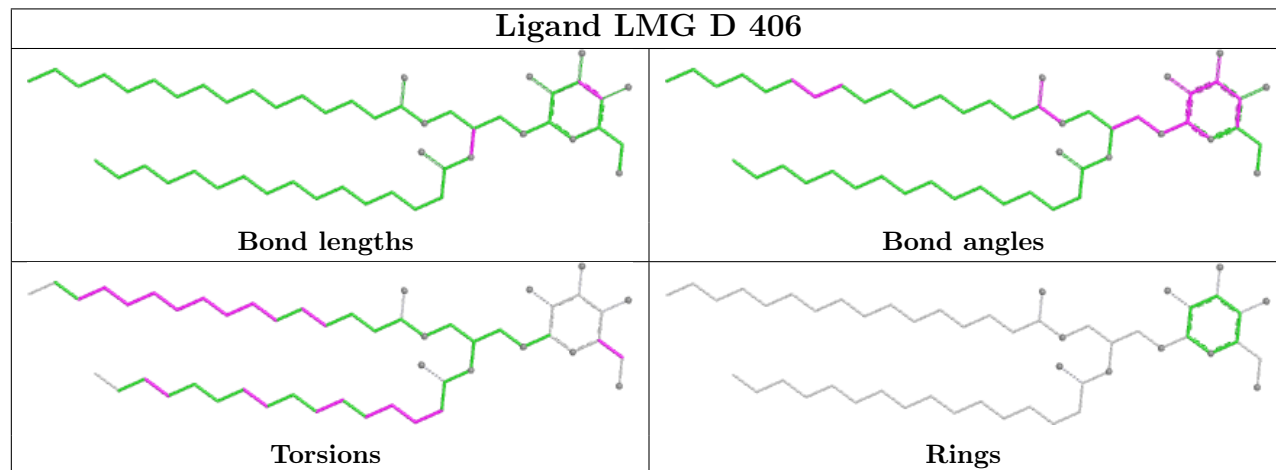
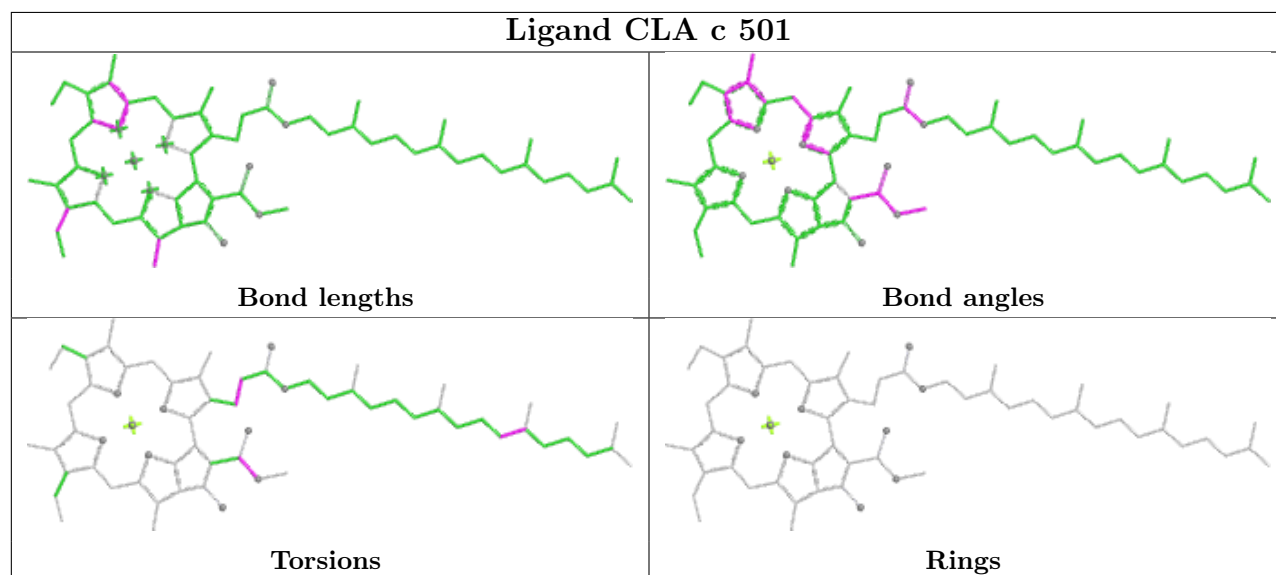
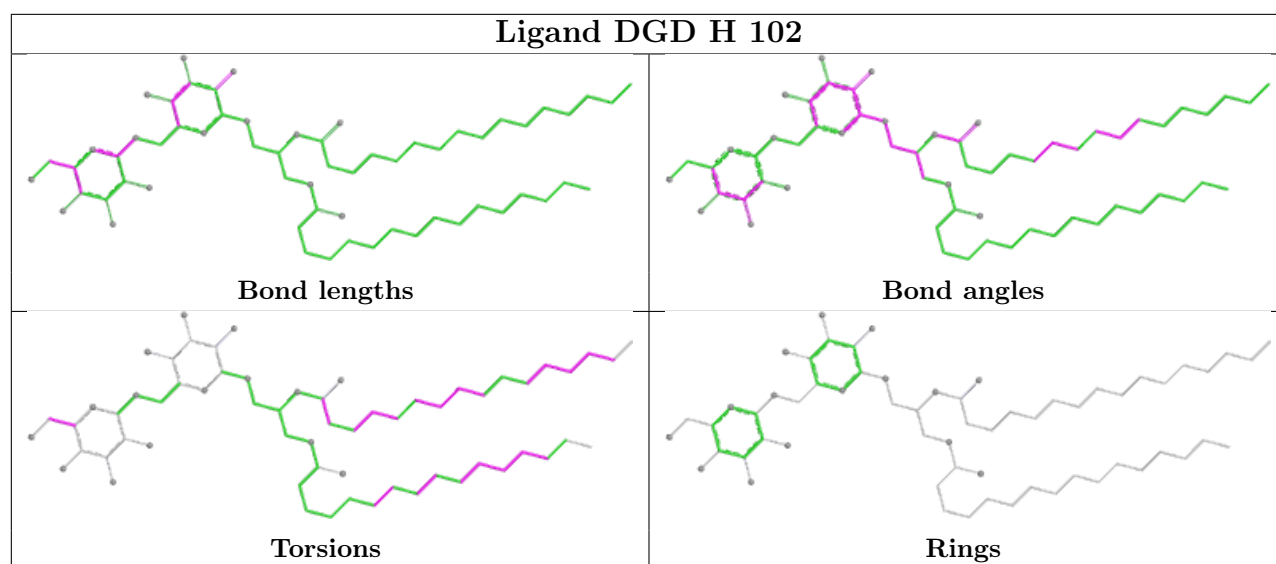
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

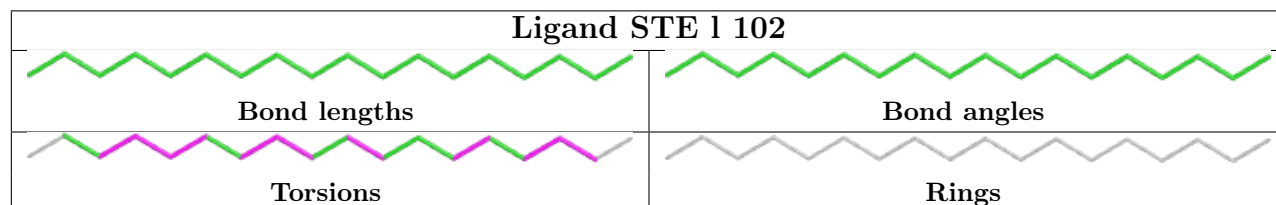
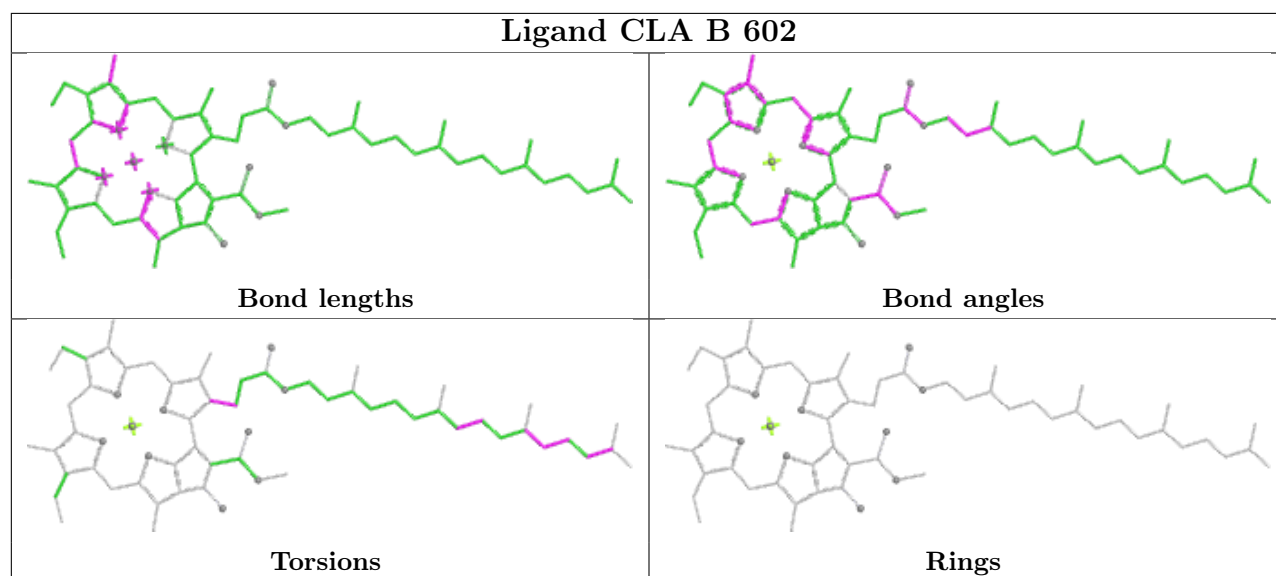
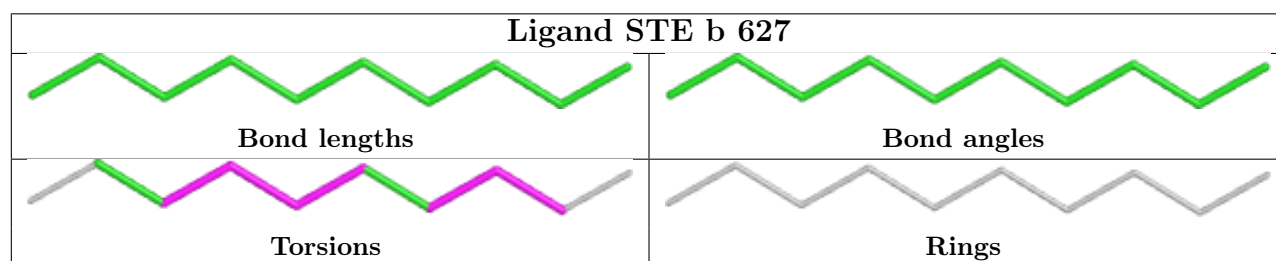
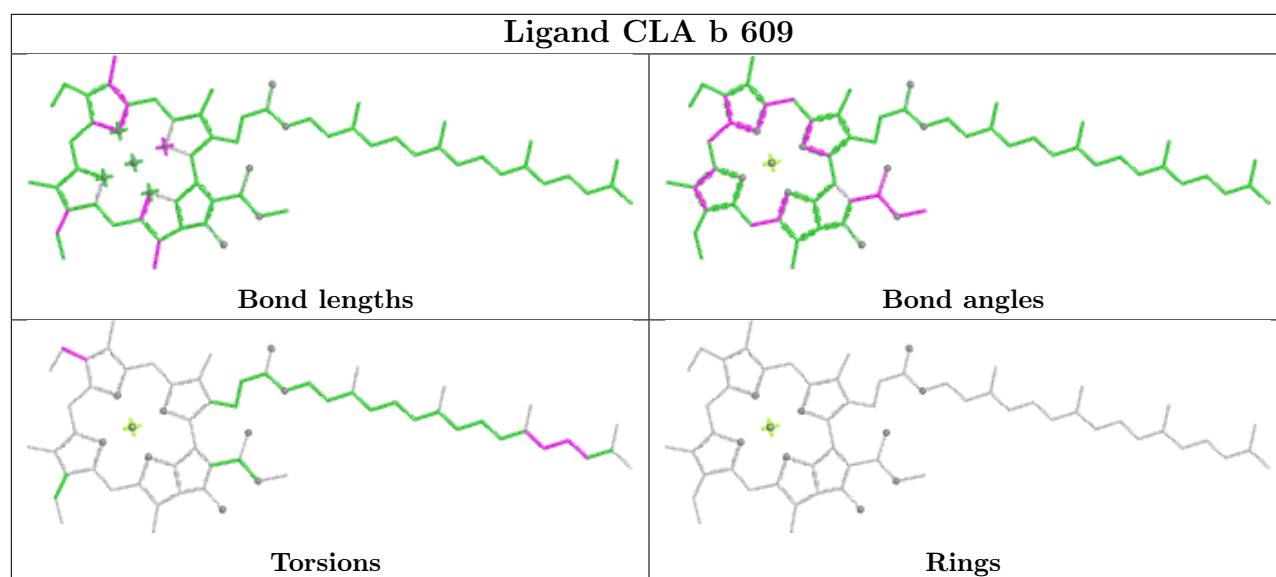
Ligand STE a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

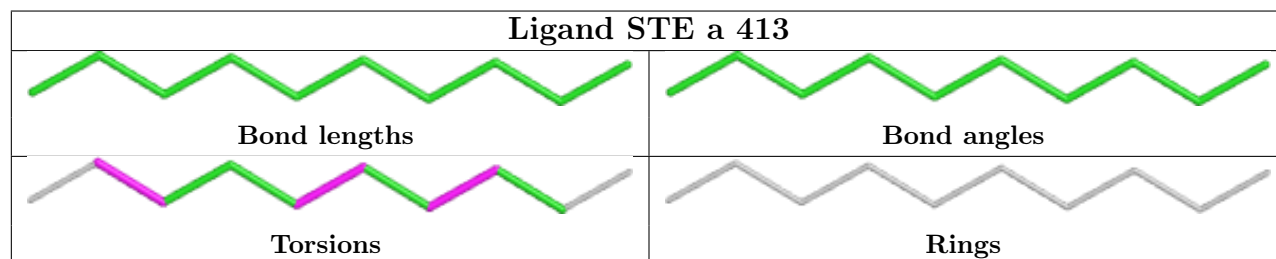
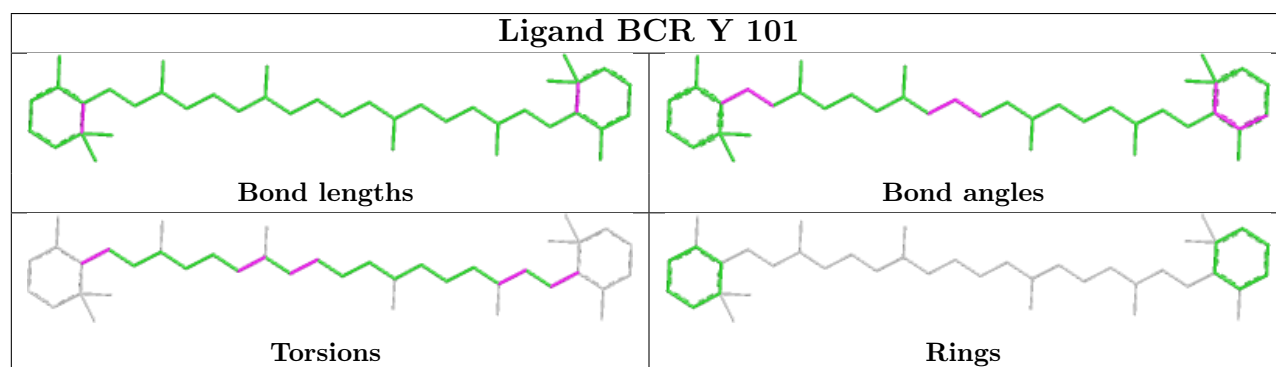
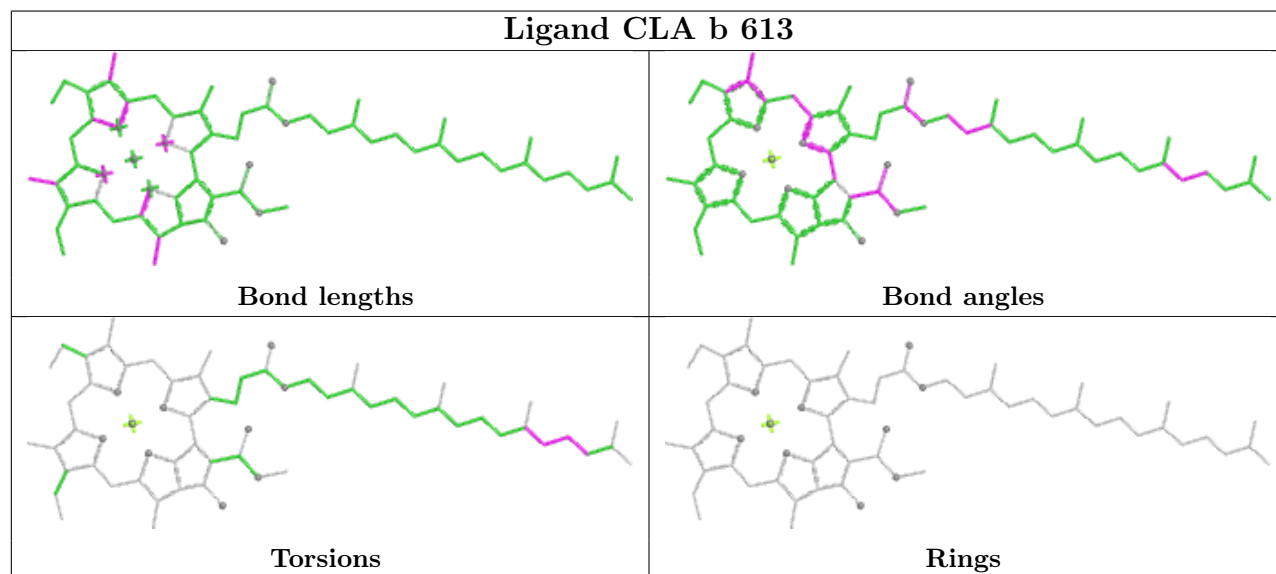
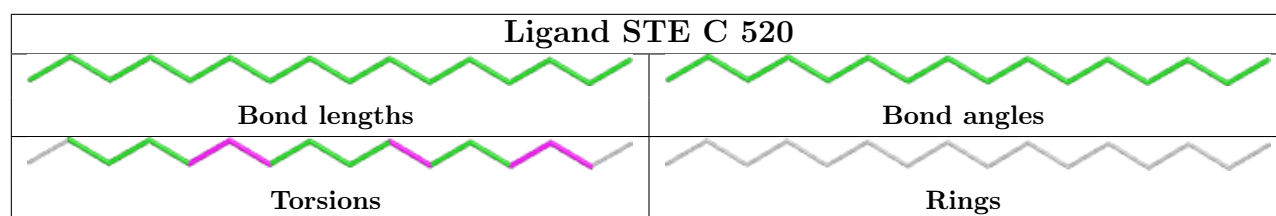


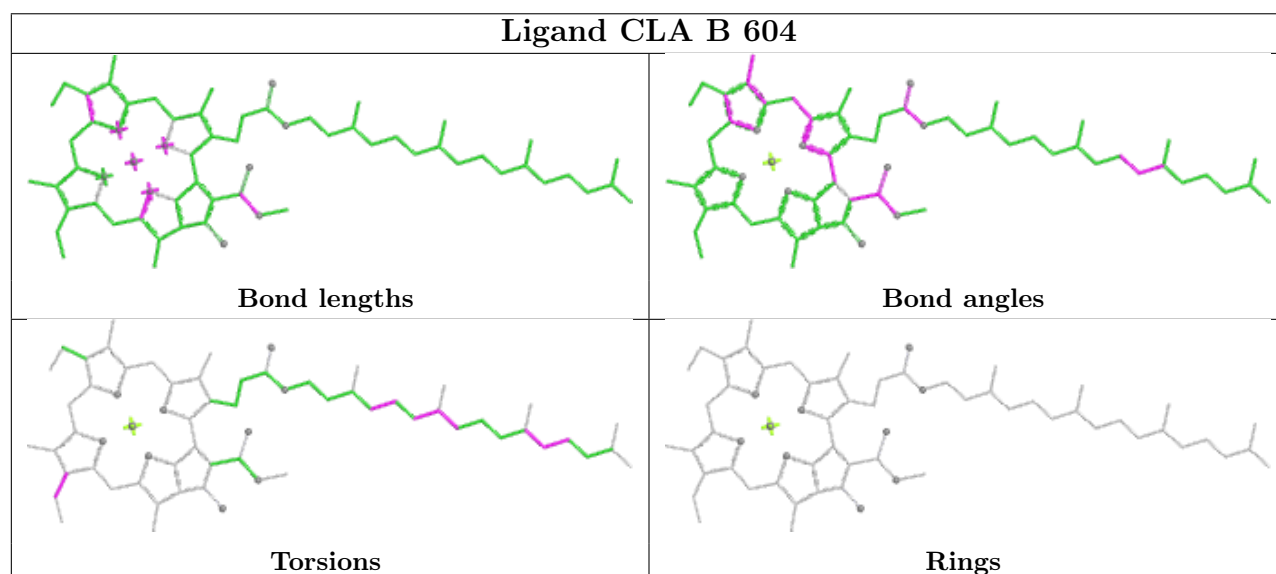
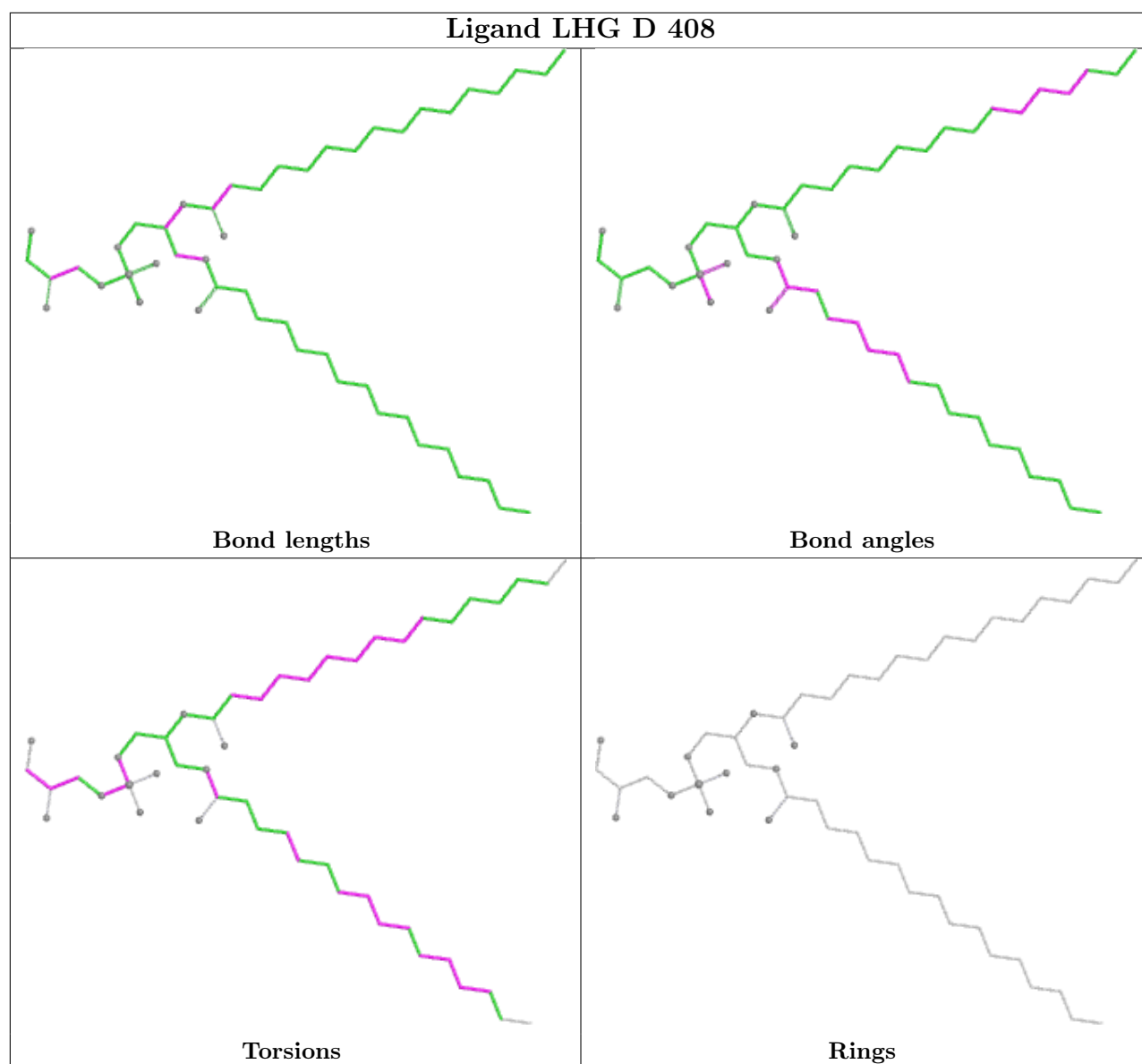


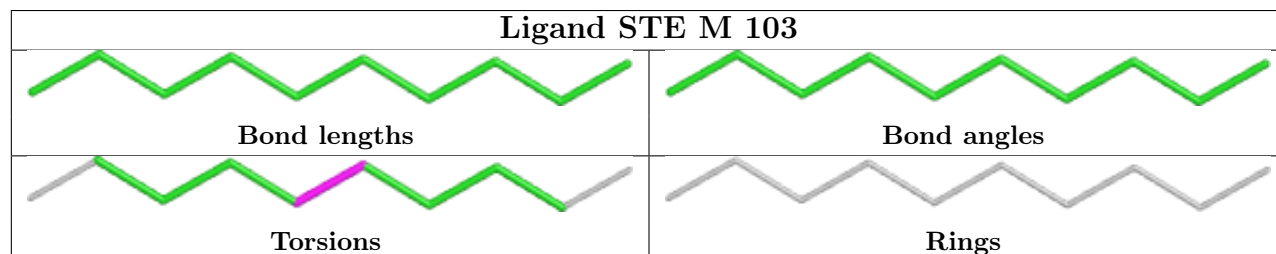
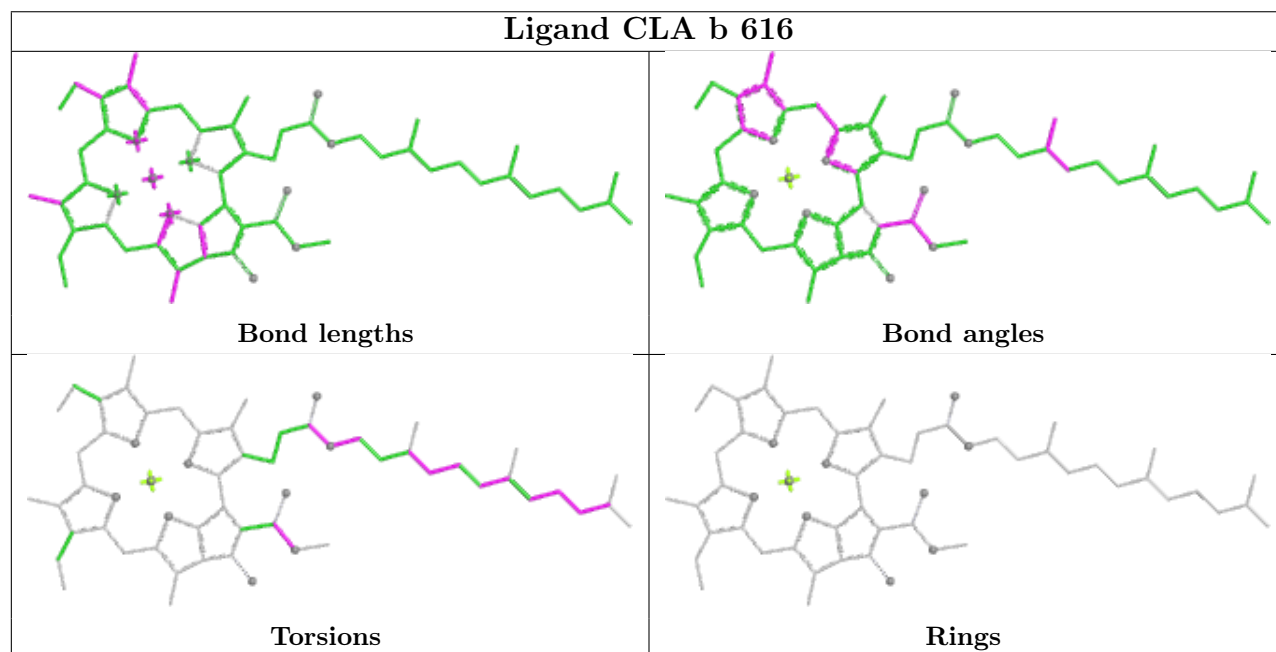
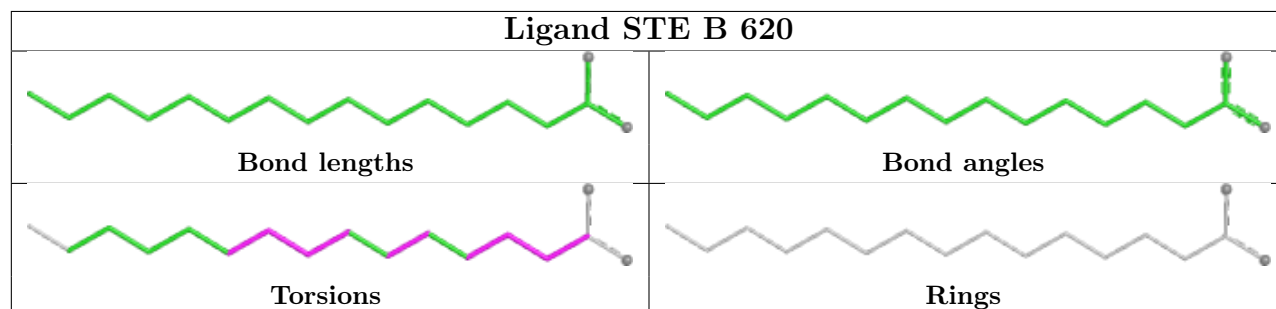
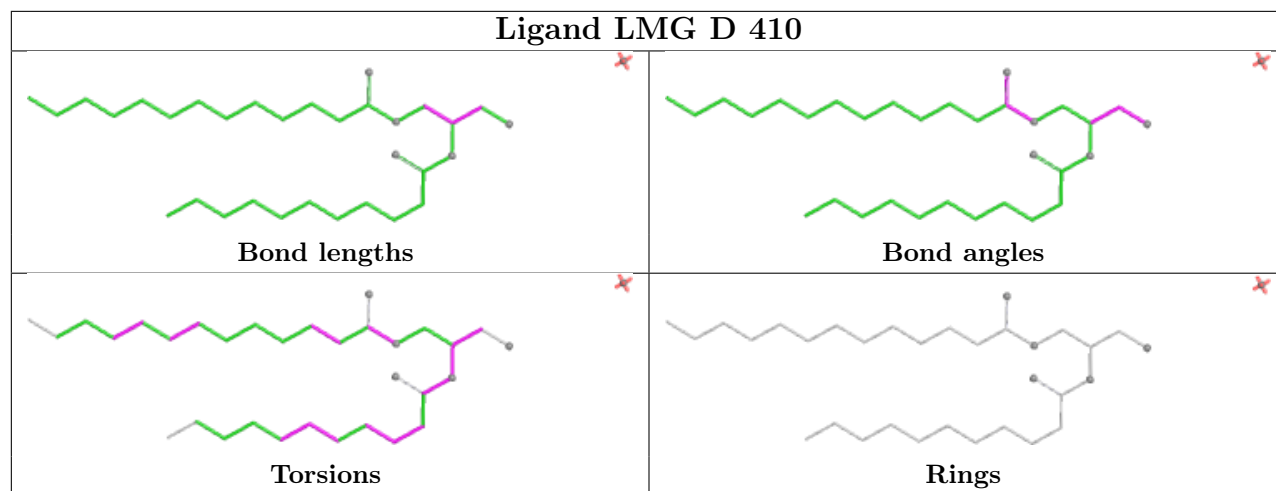


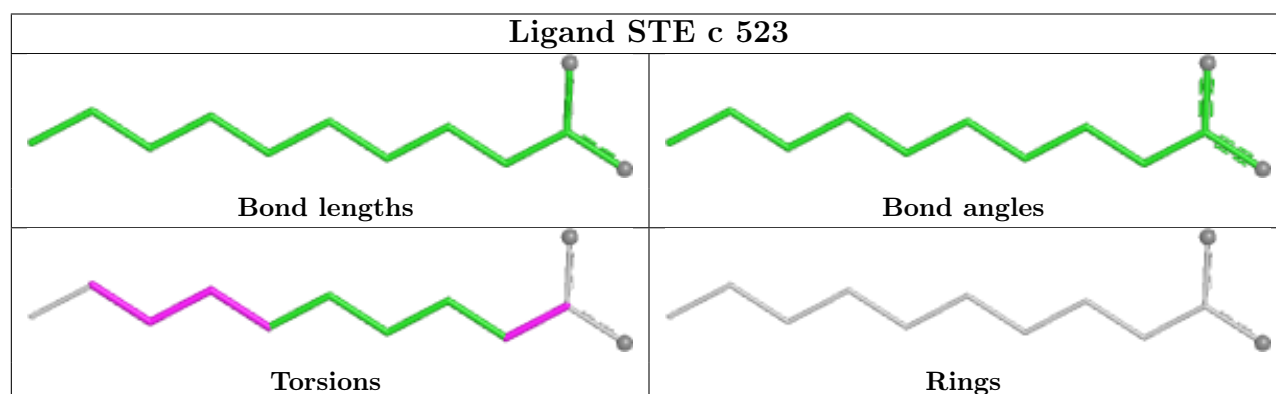
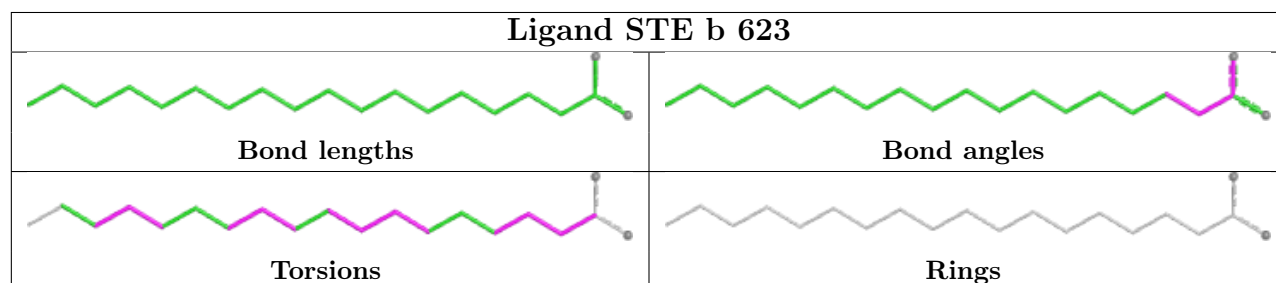
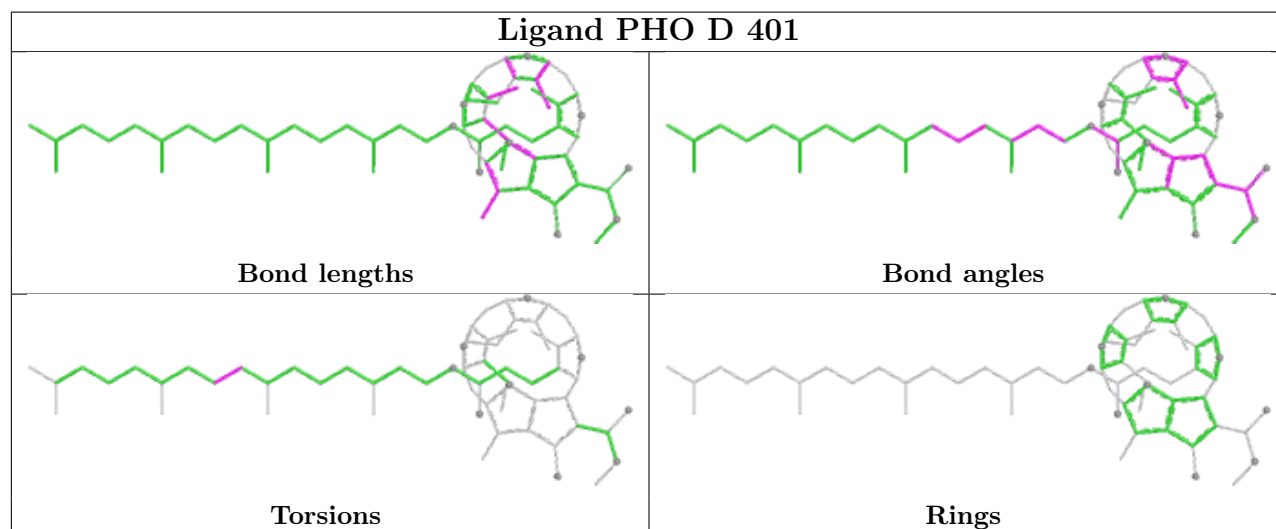
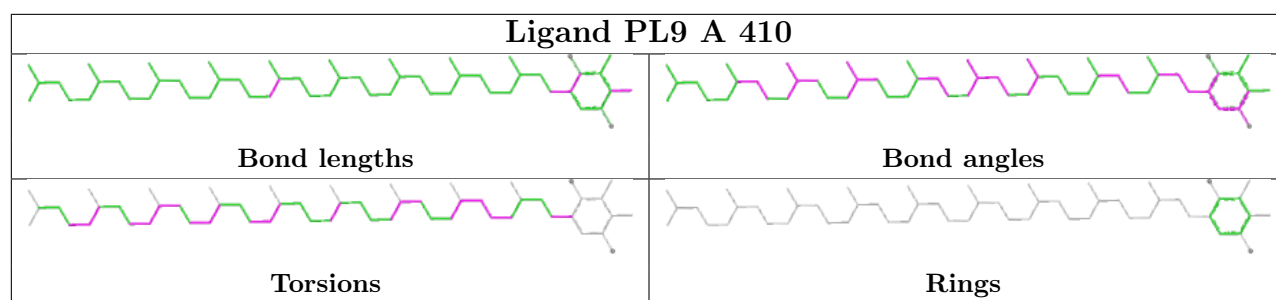


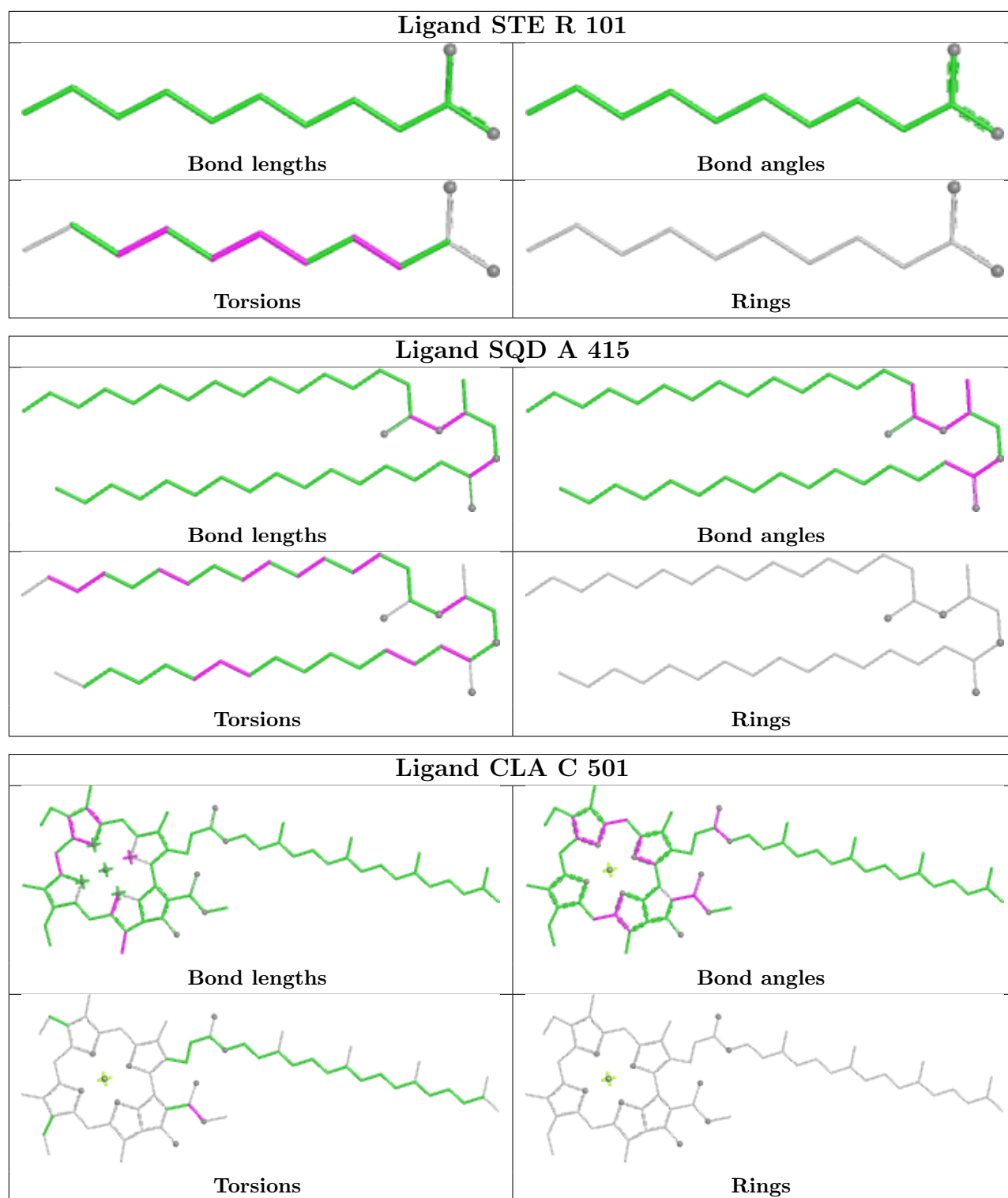


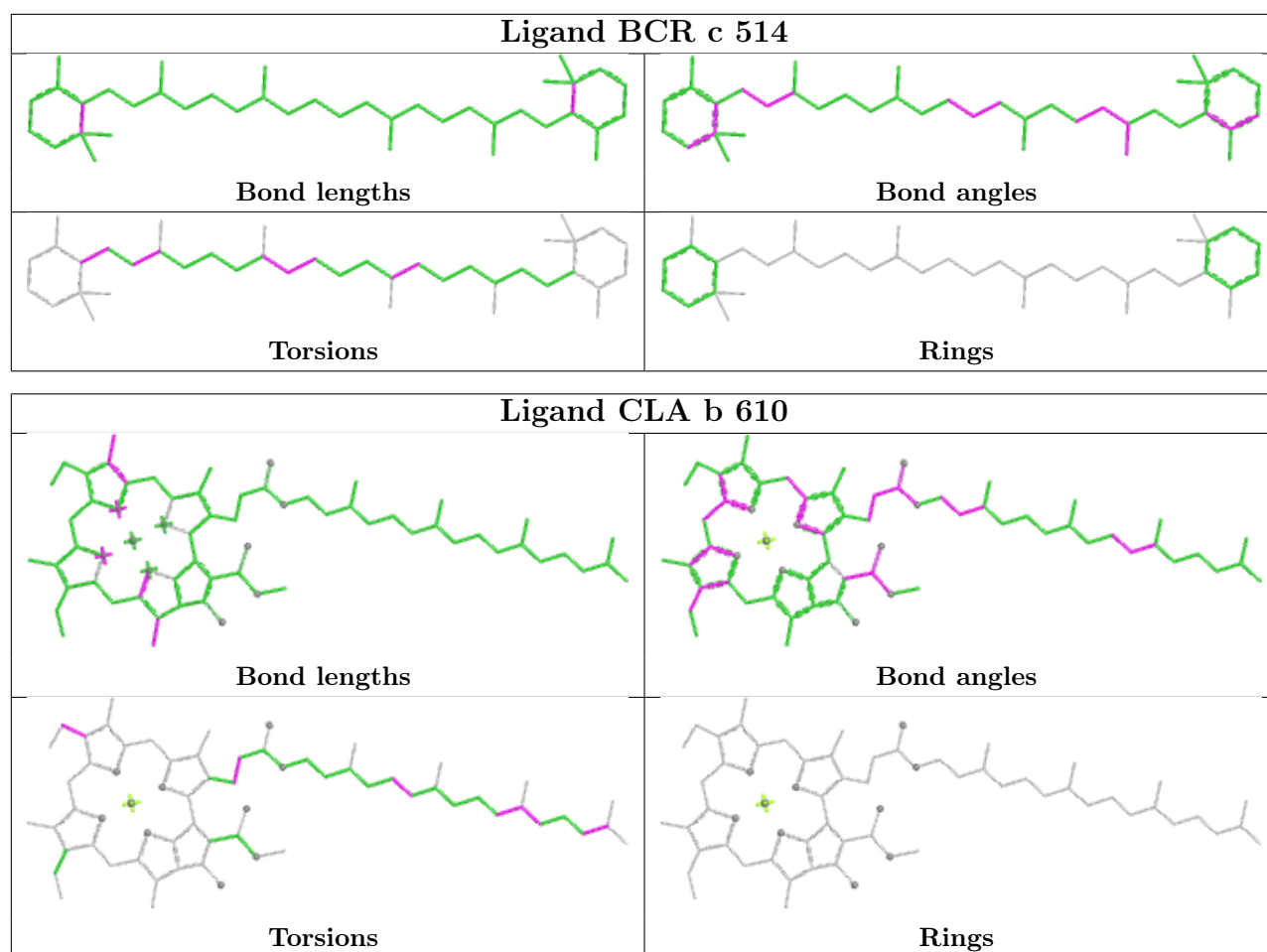












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	-0.50	1 (0%) 90 91	13, 30, 47, 79	64 (19%)
1	a	334/344 (97%)	-0.40	2 (0%) 85 87	13, 32, 57, 78	64 (19%)
2	B	505/510 (99%)	-0.43	1 (0%) 91 92	19, 35, 62, 87	4 (0%)
2	b	505/510 (99%)	-0.29	2 (0%) 88 90	25, 38, 70, 102	0
3	C	442/461 (95%)	-0.37	0 100 100	15, 38, 53, 76	11 (2%)
3	c	451/461 (97%)	-0.28	1 (0%) 91 92	14, 42, 62, 94	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	16, 33, 47, 78	2 (0%)
4	d	341/352 (96%)	-0.42	0 100 100	15, 36, 57, 81	3 (0%)
5	E	82/84 (97%)	0.14	0 100 100	31, 52, 66, 83	1 (1%)
5	e	82/84 (97%)	0.30	1 (1%) 76 78	41, 59, 76, 91	0
6	F	34/45 (75%)	-0.15	0 100 100	37, 44, 60, 80	0
6	f	34/45 (75%)	0.09	0 100 100	42, 52, 75, 88	0
7	H	65/66 (98%)	-0.21	1 (1%) 72 74	32, 43, 58, 70	0
7	h	63/66 (95%)	0.05	3 (4%) 35 38	39, 50, 64, 69	0
8	I	35/38 (92%)	-0.32	0 100 100	35, 41, 68, 82	0
8	i	35/38 (92%)	-0.02	1 (2%) 53 56	33, 43, 78, 87	0
9	J	36/40 (90%)	-0.15	0 100 100	36, 52, 72, 95	0
9	j	36/40 (90%)	0.04	0 100 100	37, 54, 84, 97	0
10	K	37/46 (80%)	-0.08	0 100 100	41, 53, 70, 74	0
10	k	37/46 (80%)	0.12	0 100 100	46, 56, 72, 76	0
11	L	37/37 (100%)	-0.53	0 100 100	27, 33, 64, 69	0
11	l	36/37 (97%)	-0.55	0 100 100	27, 34, 73, 87	0
12	M	32/36 (88%)	-0.47	0 100 100	29, 38, 59, 71	0
12	m	31/36 (86%)	-0.47	0 100 100	30, 38, 54, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.16	4 (1%) 70 73	26, 45, 85, 140	1 (0%)
13	o	244/272 (89%)	-0.15	2 (0%) 82 84	27, 44, 81, 124	0
14	R	28/41 (68%)	0.65	0 100 100	58, 68, 83, 92	0
14	r	28/41 (68%)	1.02	2 (7%) 22 23	65, 83, 103, 113	0
15	T	29/32 (90%)	-0.55	0 100 100	28, 34, 61, 81	0
15	t	29/32 (90%)	-0.32	1 (3%) 48 50	31, 35, 82, 95	0
16	U	97/134 (72%)	-0.21	0 100 100	34, 46, 70, 84	0
16	u	97/134 (72%)	-0.32	0 100 100	32, 42, 59, 80	0
17	V	137/163 (84%)	-0.33	0 100 100	32, 42, 57, 77	0
17	v	137/163 (84%)	-0.09	1 (0%) 84 86	34, 49, 68, 78	0
18	X	38/41 (92%)	-0.09	0 100 100	40, 51, 70, 76	0
18	x	39/41 (95%)	0.24	1 (2%) 57 60	48, 59, 84, 97	0
19	Y	27/46 (58%)	0.89	3 (11%) 10 10	52, 73, 94, 100	0
19	y	30/46 (65%)	0.63	0 100 100	62, 72, 87, 96	0
20	Z	62/62 (100%)	0.72	6 (9%) 13 14	54, 67, 108, 114	0
20	z	62/62 (100%)	0.68	2 (3%) 50 53	56, 73, 109, 124	0
All	All	5293/5700 (92%)	-0.26	35 (0%) 84 86	13, 40, 72, 140	162 (3%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.4
15	t	30	THR	4.4
18	x	40	SER	3.5
13	O	60	ARG	3.4
2	b	495	PHE	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
15	FME	t	1	10/11	0.94	0.07	29,43,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.95	0.07	40,49,68,70	0
12	FME	m	1	10/11	0.96	0.07	33,47,63,74	0
15	FME	T	1	10/11	0.96	0.07	29,41,62,62	0
8	FME	I	1	10/11	0.96	0.08	34,41,49,59	0
8	FME	i	1	10/11	0.97	0.07	35,44,57,58	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
34	STE	b	627	10/20	0.73	0.19	44,59,69,70	0
34	STE	L	101	12/20	0.77	0.18	46,59,75,80	0
34	STE	I	101	15/20	0.77	0.17	39,56,70,70	0
34	STE	h	102	14/20	0.77	0.17	47,62,75,78	0
34	STE	H	103	18/20	0.78	0.16	48,66,76,79	0
34	STE	j	101	12/20	0.78	0.13	42,56,70,73	0
34	STE	b	626	20/20	0.79	0.14	44,62,74,79	0
34	STE	d	413	20/20	0.80	0.14	42,62,76,76	0
30	LHG	A	414	49/49	0.80	0.13	47,70,98,111	0
28	LMG	b	624	55/55	0.80	0.16	50,72,91,96	0
28	LMG	a	416	55/55	0.81	0.13	38,56,75,80	0
29	SQD	a	412	36/54	0.81	0.14	33,59,78,86	0
34	STE	c	523	12/20	0.81	0.12	49,64,81,82	0
34	STE	a	413	10/20	0.82	0.14	37,60,68,72	0
34	STE	a	414	12/20	0.82	0.13	50,64,74,78	0
34	STE	B	626	16/20	0.82	0.13	45,63,72,75	0
28	LMG	c	521	48/55	0.82	0.14	47,69,94,103	0
29	SQD	A	415	39/54	0.83	0.14	37,59,88,94	0
30	LHG	e	102	42/49	0.83	0.14	57,79,100,109	0
34	STE	R	101	12/20	0.84	0.15	51,75,78,85	0
34	STE	b	621	16/20	0.84	0.13	35,49,65,75	0
31	DGD	A	416	66/66	0.85	0.11	41,61,75,79	0
34	STE	c	520	20/20	0.85	0.12	43,57,79,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	LMG	D	410	33/55	0.85	0.13	36,55,74,80	0
34	STE	a	415	15/20	0.85	0.16	42,58,69,74	0
34	STE	B	627	12/20	0.85	0.14	44,59,76,79	0
34	STE	C	520	16/20	0.85	0.12	36,52,62,69	0
34	STE	b	625	16/20	0.86	0.12	45,62,72,74	0
28	LMG	A	412	48/55	0.86	0.10	36,55,74,89	0
34	STE	B	625	18/20	0.86	0.12	38,57,69,74	0
34	STE	C	519	12/20	0.86	0.12	46,56,66,67	0
34	STE	B	620	17/20	0.87	0.10	36,50,62,62	0
34	STE	T	102	15/20	0.87	0.12	41,56,70,76	0
34	STE	Z	101	8/20	0.87	0.17	46,57,66,66	0
28	LMG	c	522	49/55	0.87	0.10	37,55,79,96	0
28	LMG	c	519	37/55	0.87	0.12	39,61,75,81	0
34	STE	B	624	12/20	0.88	0.12	44,55,64,66	0
27	PL9	A	410	55/55	0.88	0.12	34,63,84,90	0
34	STE	C	521	12/20	0.88	0.11	34,47,54,58	0
34	STE	d	412	20/20	0.88	0.11	36,55,71,73	0
34	STE	b	623	20/20	0.88	0.11	39,55,69,79	0
22	CLA	b	601	65/65	0.88	0.11	42,65,85,91	0
28	LMG	C	518	48/55	0.88	0.12	36,65,86,89	0
34	STE	l	102	18/20	0.88	0.12	34,47,72,80	0
29	SQD	b	620	49/54	0.89	0.09	38,57,85,89	0
27	PL9	a	409	55/55	0.89	0.12	37,66,80,89	0
34	STE	J	101	12/20	0.89	0.11	45,59,70,72	0
34	STE	X	101	20/20	0.89	0.10	31,48,62,64	0
34	STE	t	102	14/20	0.89	0.10	33,52,62,65	0
24	BCR	c	514	40/40	0.90	0.10	43,59,70,72	0
29	SQD	f	101	41/54	0.90	0.12	49,76,94,100	0
22	CLA	B	601	65/65	0.90	0.10	30,59,82,94	0
34	STE	M	103	10/20	0.90	0.10	35,48,55,58	0
24	BCR	K	101	40/40	0.90	0.11	41,55,70,71	0
28	LMG	b	622	51/55	0.90	0.10	29,50,68,80	0
29	SQD	B	623	54/54	0.90	0.09	40,57,86,96	0
24	BCR	Y	101	40/40	0.90	0.10	35,50,68,71	0
28	LMG	D	411	28/55	0.91	0.10	28,48,59,61	0
29	SQD	D	407	36/54	0.91	0.11	44,68,83,94	0
28	LMG	M	101	51/55	0.91	0.09	29,47,70,84	0
22	CLA	C	513	65/65	0.91	0.09	40,60,87,89	0
34	STE	M	102	15/20	0.91	0.10	34,48,63,63	0
34	STE	d	411	17/20	0.91	0.10	40,54,61,61	0
31	DGD	h	101	62/66	0.92	0.09	24,47,62,66	0
29	SQD	a	411	54/54	0.92	0.10	41,61,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	d	405	40/40	0.92	0.10	32,51,85,98	0
24	BCR	k	101	40/40	0.92	0.10	42,61,73,75	0
28	LMG	d	410	44/55	0.92	0.09	31,50,73,88	0
24	BCR	x	101	40/40	0.92	0.09	31,51,66,74	0
26	BCT	a	408	4/4	0.92	0.10	26,32,39,46	0
24	BCR	H	101	40/40	0.92	0.09	26,44,57,61	0
31	DGD	C	516	62/66	0.92	0.09	30,48,91,108	0
22	CLA	c	513	65/65	0.93	0.10	39,68,104,108	0
31	DGD	H	102	62/66	0.93	0.08	26,41,58,63	0
31	DGD	c	517	62/66	0.93	0.08	33,51,82,89	0
24	BCR	B	618	40/40	0.93	0.07	24,37,49,55	0
24	BCR	B	619	40/40	0.93	0.08	29,41,54,60	0
24	BCR	k	102	40/40	0.93	0.10	39,54,66,67	0
24	BCR	D	404	40/40	0.93	0.09	25,43,76,85	0
22	CLA	C	512	65/65	0.93	0.10	33,53,82,92	0
22	CLA	c	511	65/65	0.93	0.10	39,52,71,74	0
22	CLA	c	512	65/65	0.93	0.10	39,57,86,92	0
30	LHG	d	407	49/49	0.93	0.11	32,50,70,76	0
24	BCR	b	618	40/40	0.93	0.08	25,39,57,61	0
24	BCR	b	619	40/40	0.93	0.08	28,45,65,68	0
22	CLA	c	506	65/65	0.94	0.10	30,48,87,97	0
30	LHG	d	409	39/49	0.94	0.09	28,46,69,71	0
24	BCR	C	514	40/40	0.94	0.08	25,41,53,63	0
22	CLA	c	508	64/65	0.94	0.09	30,45,85,96	0
31	DGD	C	515	62/66	0.94	0.09	22,40,74,80	0
29	SQD	A	413	52/54	0.94	0.09	29,55,82,90	0
31	DGD	C	517	62/66	0.94	0.08	25,45,68,74	0
28	LMG	D	406	51/55	0.94	0.10	28,50,76,88	0
24	BCR	c	515	40/40	0.94	0.08	27,43,56,61	0
23	PHO	d	402	64/64	0.94	0.07	27,38,48,50	0
24	BCR	B	617	40/40	0.94	0.07	28,39,55,60	0
24	BCR	K	102	40/40	0.94	0.09	32,48,61,64	0
24	BCR	T	101	40/40	0.94	0.06	22,39,54,62	0
22	CLA	C	511	65/65	0.94	0.08	28,49,64,66	0
24	BCR	b	617	40/40	0.94	0.07	23,41,53,57	0
22	CLA	C	505	65/65	0.95	0.09	24,39,69,74	0
22	CLA	C	506	65/65	0.95	0.09	23,42,82,89	0
22	CLA	c	509	65/65	0.95	0.08	32,46,62,68	0
22	CLA	C	507	65/65	0.95	0.07	22,40,52,57	0
22	CLA	C	509	65/65	0.95	0.08	26,43,64,72	0
22	CLA	C	510	65/65	0.95	0.07	25,42,58,62	0
24	BCR	t	101	40/40	0.95	0.06	24,39,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	d	404	65/65	0.95	0.09	27,46,81,87	0
22	CLA	B	606	65/65	0.95	0.08	24,36,74,79	0
24	BCR	A	406	40/40	0.95	0.07	23,35,45,47	0
30	LHG	B	622	49/49	0.95	0.09	27,45,65,70	0
30	LHG	D	409	47/49	0.95	0.09	27,48,73,88	0
27	PL9	D	405	55/55	0.95	0.06	21,33,46,47	0
22	CLA	C	502	65/65	0.95	0.07	28,39,61,73	0
27	PL9	d	406	55/55	0.95	0.06	22,34,42,44	0
30	LHG	l	101	49/49	0.95	0.08	31,43,57,64	0
22	CLA	C	503	65/65	0.95	0.07	26,41,51,57	0
22	CLA	C	504	59/65	0.95	0.08	28,40,76,84	0
22	CLA	b	602	65/65	0.95	0.08	28,42,60,61	0
22	CLA	b	606	65/65	0.95	0.08	27,39,69,74	0
22	CLA	b	609	65/65	0.95	0.08	29,45,60,68	0
31	DGD	c	516	62/66	0.95	0.08	22,41,70,78	0
22	CLA	b	614	65/65	0.95	0.08	24,41,73,77	0
31	DGD	c	518	62/66	0.95	0.08	30,49,77,88	0
22	CLA	b	616	60/65	0.95	0.08	26,42,85,88	0
22	CLA	c	502	65/65	0.95	0.07	29,41,61,65	0
22	CLA	c	503	65/65	0.95	0.07	30,43,53,62	0
24	BCR	a	405	40/40	0.95	0.06	22,33,46,49	0
22	CLA	c	504	60/65	0.95	0.08	29,42,80,83	0
22	CLA	c	505	65/65	0.95	0.07	26,39,64,73	0
22	CLA	a	404	65/65	0.96	0.08	20,37,74,79	0
23	PHO	A	404	64/64	0.96	0.05	18,28,36,40	0
23	PHO	D	401	64/64	0.96	0.06	22,34,43,48	0
23	PHO	d	401	64/64	0.96	0.06	18,32,39,48	0
22	CLA	a	410	65/65	0.96	0.06	20,29,47,54	0
22	CLA	B	616	60/65	0.96	0.09	22,38,79,86	0
22	CLA	C	501	65/65	0.96	0.07	22,36,50,53	0
22	CLA	b	603	65/65	0.96	0.07	23,36,68,70	0
22	CLA	b	605	65/65	0.96	0.06	21,35,49,52	0
22	CLA	B	603	65/65	0.96	0.07	16,34,59,61	0
22	CLA	b	607	65/65	0.96	0.08	20,36,67,71	0
22	CLA	b	608	65/65	0.96	0.07	25,41,58,61	0
22	CLA	B	604	65/65	0.96	0.07	20,34,66,70	0
22	CLA	b	610	65/65	0.96	0.07	24,39,48,56	0
22	CLA	b	611	65/65	0.96	0.07	22,34,54,60	0
22	CLA	b	612	65/65	0.96	0.07	20,34,51,54	0
22	CLA	A	402	65/65	0.96	0.07	16,27,41,55	0
22	CLA	b	615	65/65	0.96	0.07	26,40,56,60	0
22	CLA	B	607	65/65	0.96	0.07	18,34,60,69	0

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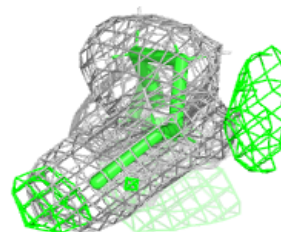
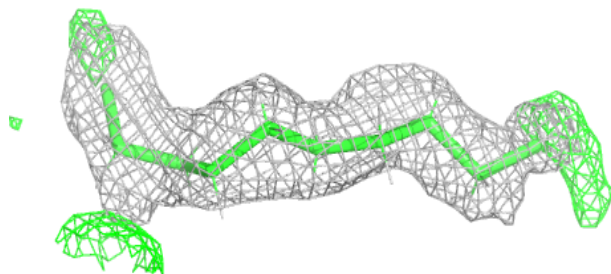
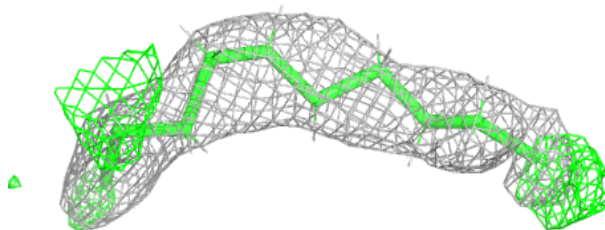
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	c	501	65/65	0.96	0.07	23,41,52,56	0
22	CLA	B	609	65/65	0.96	0.07	23,37,61,73	0
30	LHG	B	621	49/49	0.96	0.07	27,42,59,64	0
22	CLA	B	610	65/65	0.96	0.07	20,34,46,47	0
30	LHG	D	408	49/49	0.96	0.07	21,40,51,57	0
22	CLA	C	508	65/65	0.96	0.08	27,43,95,106	0
22	CLA	B	611	65/65	0.96	0.06	22,32,51,54	0
30	LHG	d	408	49/49	0.96	0.07	26,42,52,57	0
22	CLA	B	612	65/65	0.96	0.07	19,34,46,50	0
22	CLA	c	507	65/65	0.96	0.07	27,44,59,61	0
22	CLA	B	613	65/65	0.96	0.07	19,32,63,67	0
26	BCT	A	409	4/4	0.96	0.08	31,32,33,40	0
22	CLA	B	614	65/65	0.96	0.08	21,37,73,79	0
22	CLA	c	510	65/65	0.96	0.07	32,47,64,67	0
22	CLA	B	615	65/65	0.96	0.07	23,36,61,64	0
22	CLA	D	403	65/65	0.96	0.07	24,43,100,108	0
22	CLA	a	403	65/65	0.96	0.08	23,41,91,95	0
22	CLA	d	403	65/65	0.96	0.07	20,35,57,67	0
22	CLA	A	405	54/65	0.97	0.06	18,33,58,67	0
22	CLA	A	411	65/65	0.97	0.06	18,27,56,59	0
22	CLA	B	605	65/65	0.97	0.06	21,32,46,53	0
22	CLA	D	402	65/65	0.97	0.06	13,30,54,60	0
22	CLA	b	613	65/65	0.97	0.07	18,34,72,79	0
22	CLA	b	604	65/65	0.97	0.07	18,35,71,83	0
22	CLA	A	403	65/65	0.97	0.08	21,35,85,91	0
22	CLA	a	402	65/65	0.97	0.05	18,30,47,60	0
22	CLA	B	602	65/65	0.97	0.06	23,36,55,60	0
22	CLA	B	608	65/65	0.97	0.06	22,35,54,62	0
35	HEM	F	101	43/43	0.97	0.08	32,45,60,66	0
35	HEM	e	101	43/43	0.97	0.08	40,51,71,74	0
25	CL	a	406	1/1	0.98	0.04	28,28,28,28	0
36	HEC	V	201	43/43	0.98	0.06	23,33,44,47	0
36	HEC	v	201	43/43	0.98	0.07	25,37,47,49	0
32	OEY	A	417[B]	11/11	0.99	0.03	20,26,30,32	11
33	OEX	A	418[A]	10/10	0.99	0.03	29,31,35,35	10
33	OEX	a	417[A]	10/10	0.99	0.03	26,32,35,35	10
25	CL	A	407	1/1	0.99	0.03	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.07	28,28,28,28	0
25	CL	A	408	1/1	0.99	0.04	28,28,28,28	0
32	OEY	a	418[B]	11/11	1.00	0.02	22,25,29,31	11
21	FE2	a	401	1/1	1.00	0.02	32,32,32,32	0
21	FE2	A	401	1/1	1.00	0.01	27,27,27,27	0

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

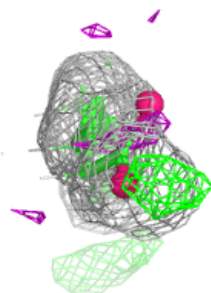
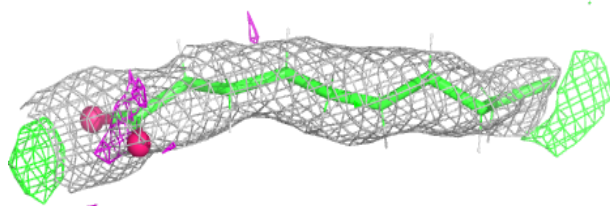
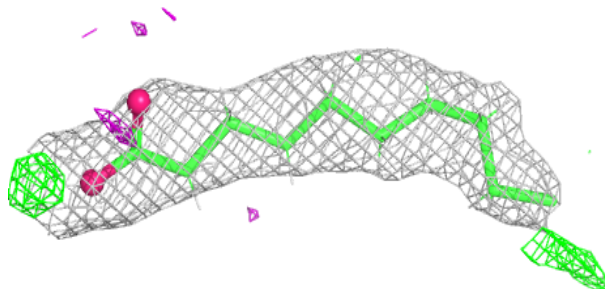
Electron density around STE b 627:

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

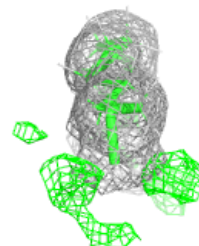
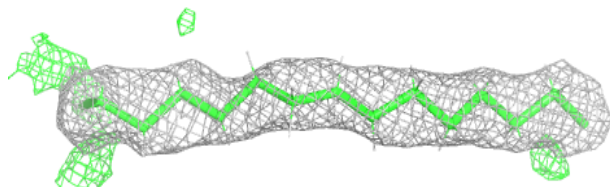
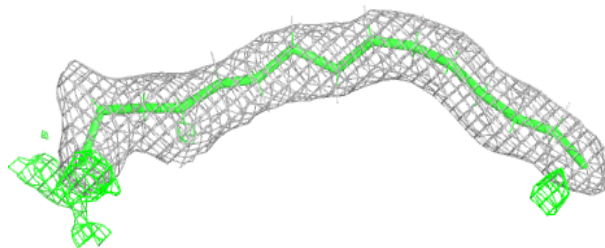


Electron density around STE L 101:

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

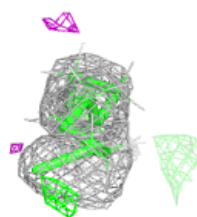
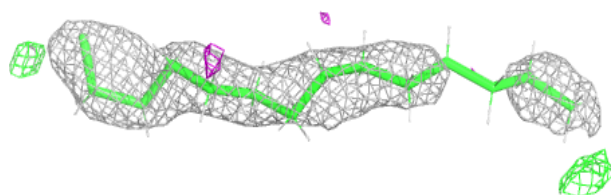
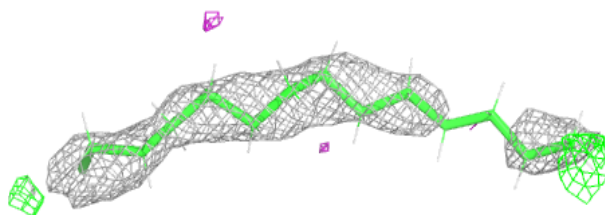
**Electron density around STE I 101:**

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

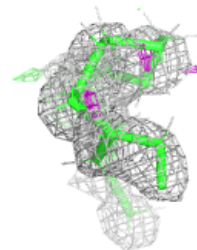
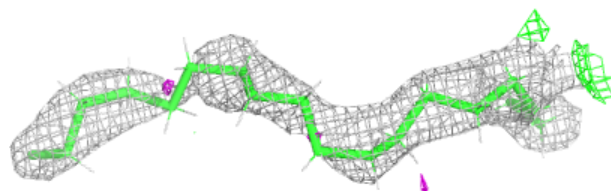
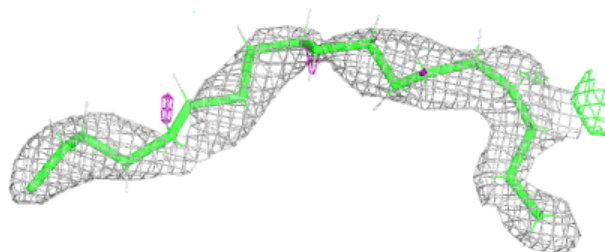


Electron density around STE h 102:

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and green (positive)

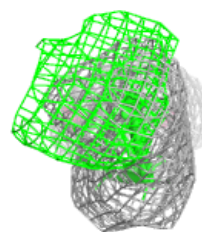
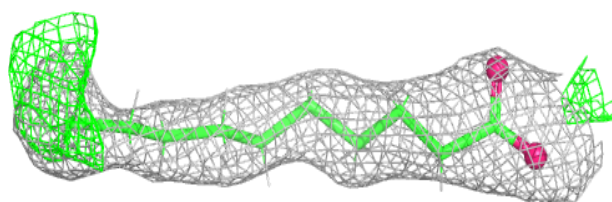
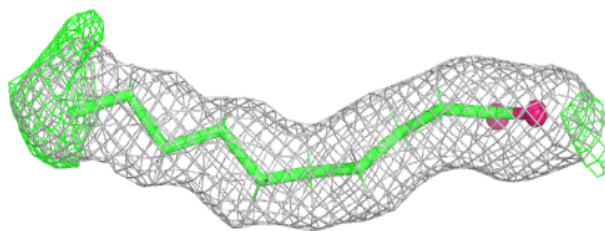
**Electron density around STE H 103:**

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and green (positive)

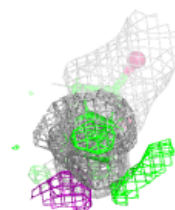
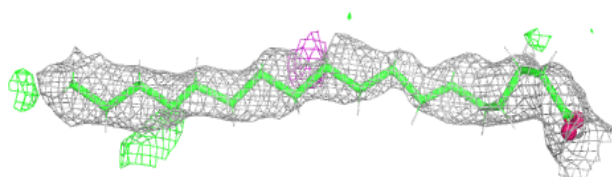
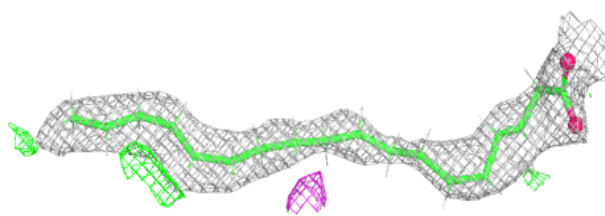


Electron density around STE j 101:

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

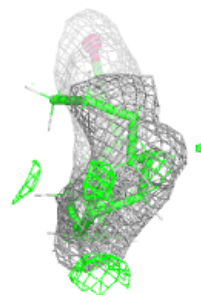
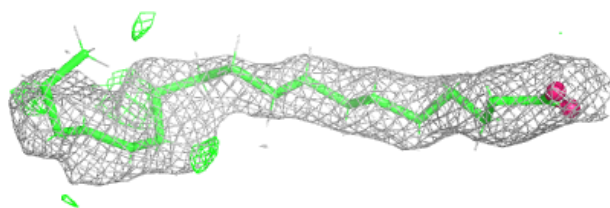
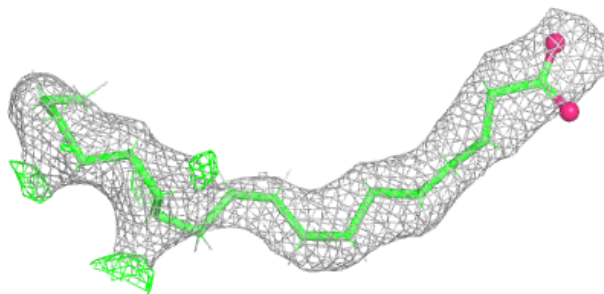
**Electron density around STE b 626:**

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and green (positive)



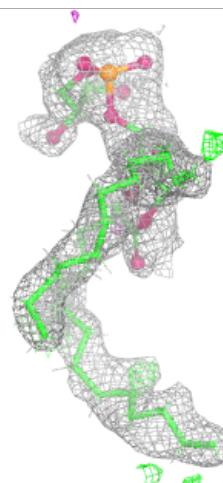
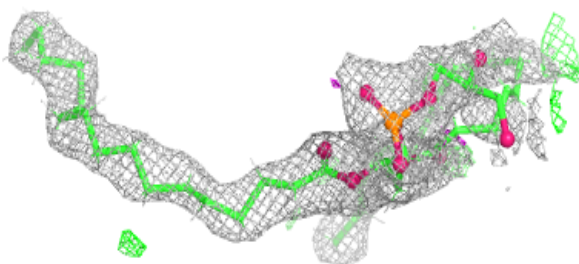
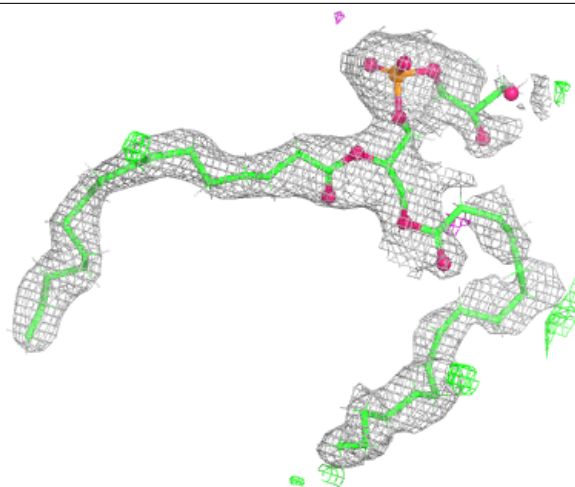
Electron density around STE d 413:

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



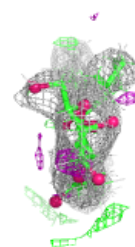
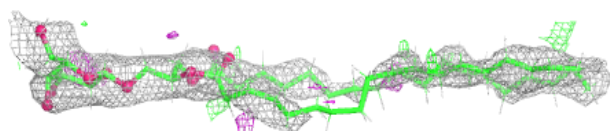
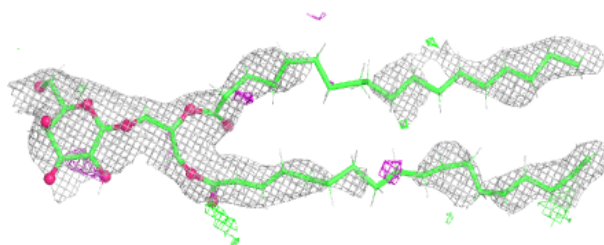
Electron density around LHG A 414:

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

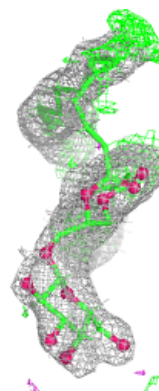
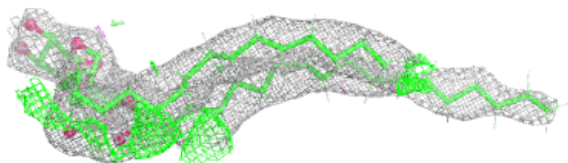
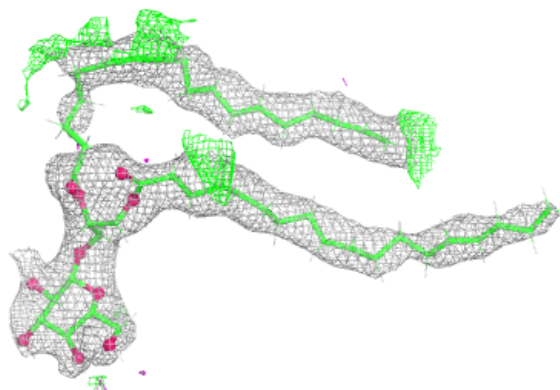


Electron density around LMG b 624:

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

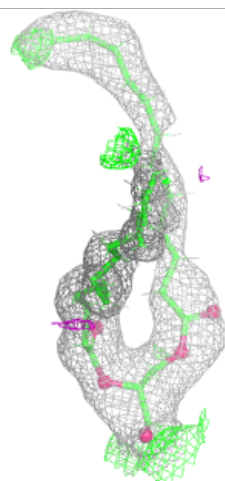
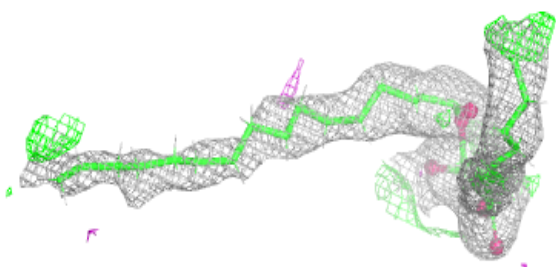
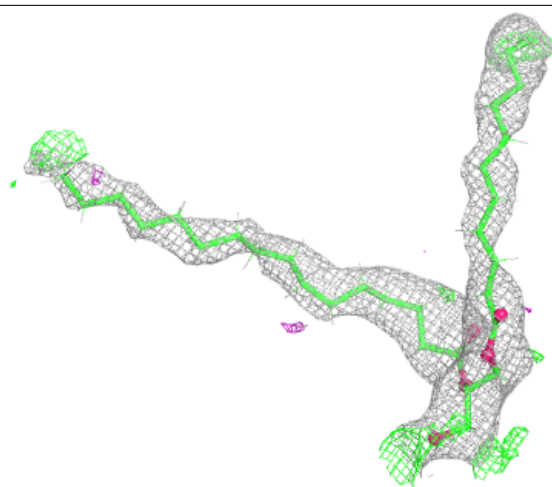
**Electron density around LMG a 416:**

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



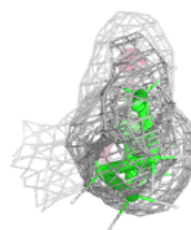
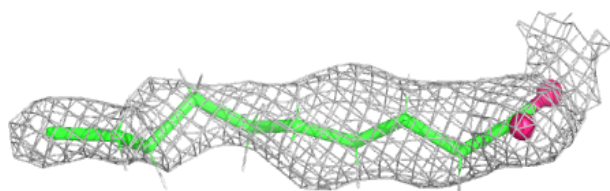
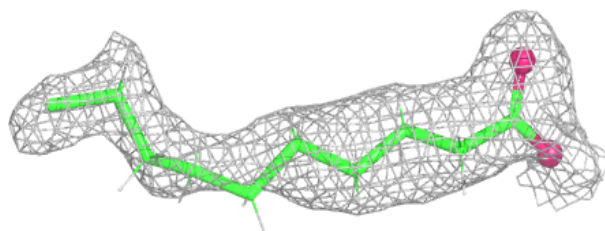
Electron density around SQD a 412:

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and green (positive)

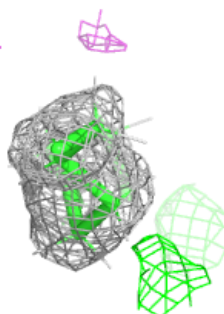
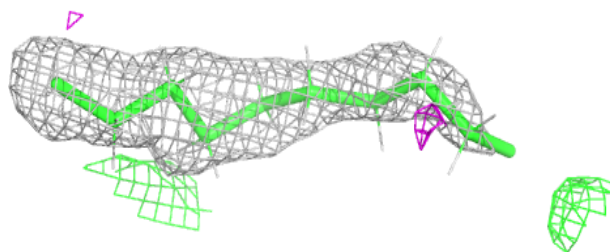
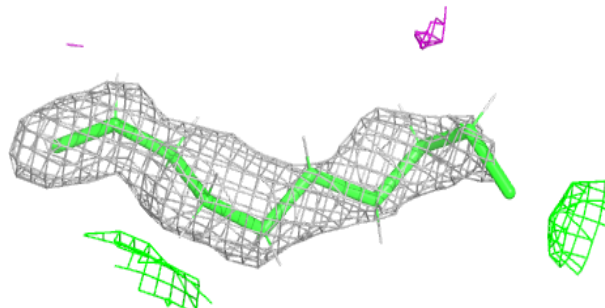


Electron density around STE c 523:

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and green (positive)

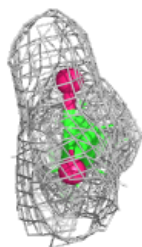
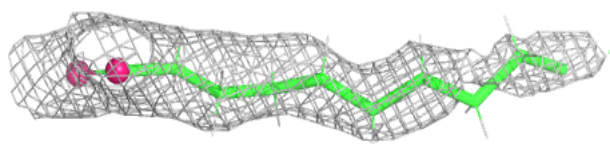
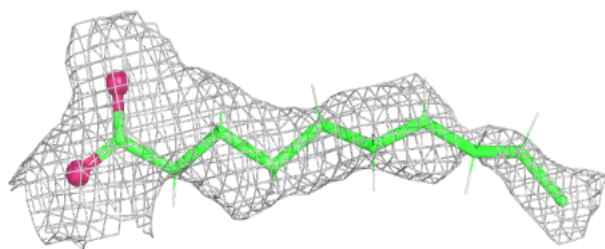
**Electron density around STE a 413:**

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

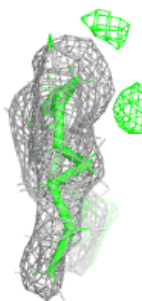
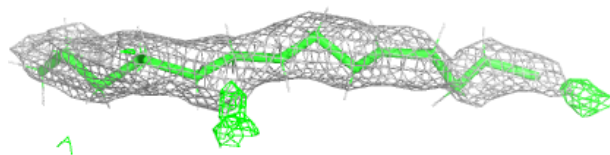
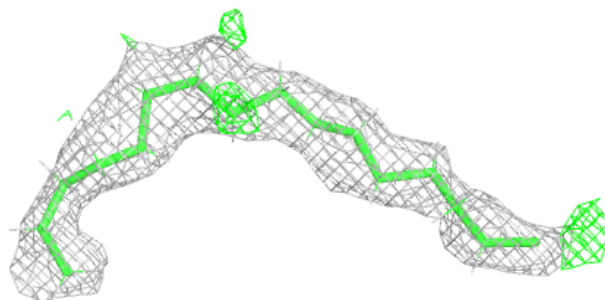


Electron density around STE a 414:

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

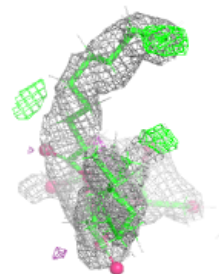
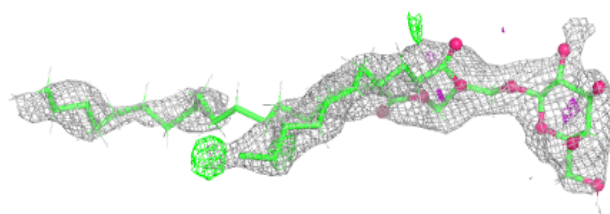
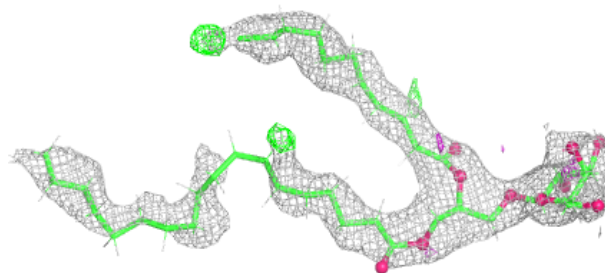
**Electron density around STE B 626:**

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



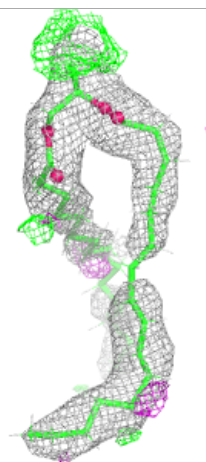
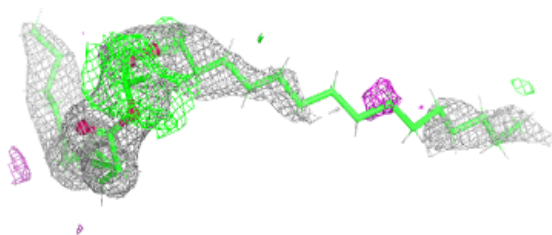
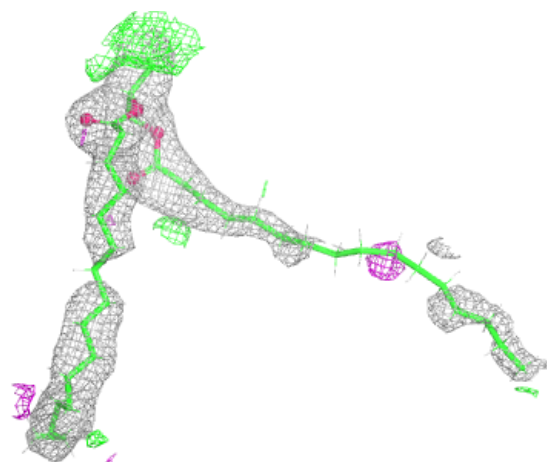
Electron density around LMG c 521:

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and green (positive)



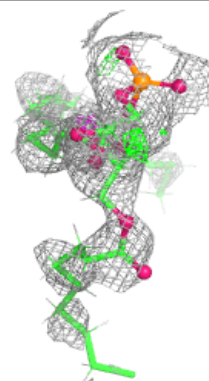
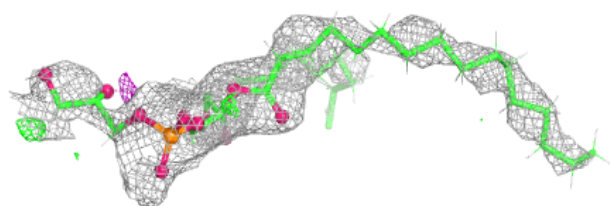
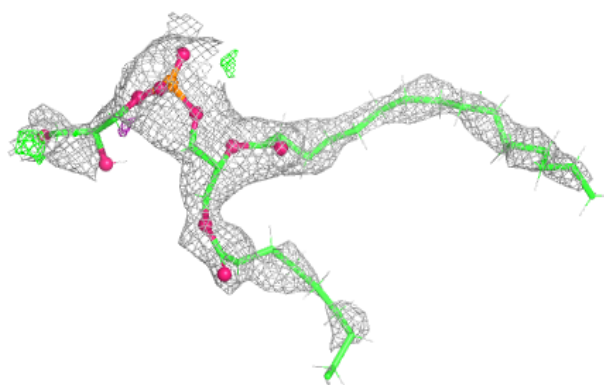
Electron density around SQD A 415:

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and green (positive)

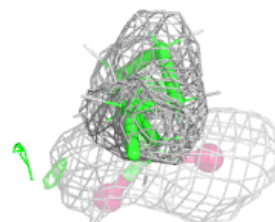
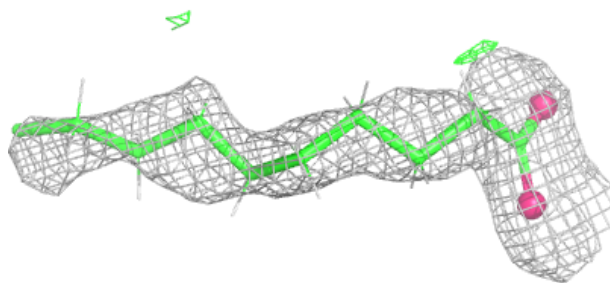
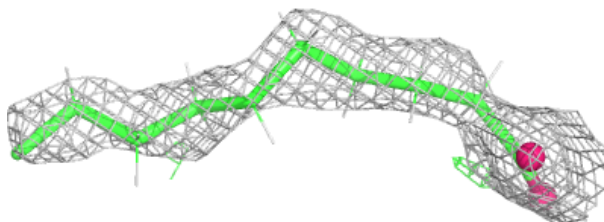


Electron density around LHG e 102:

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and green (positive)

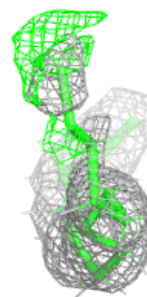
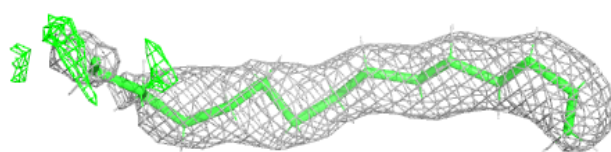
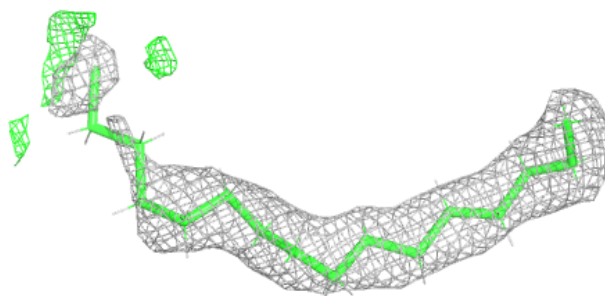
**Electron density around STE R 101:**

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

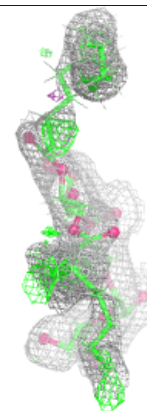
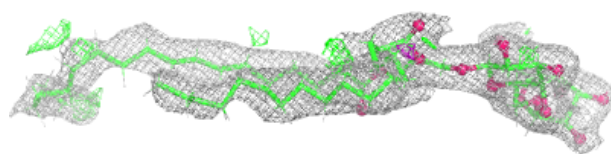
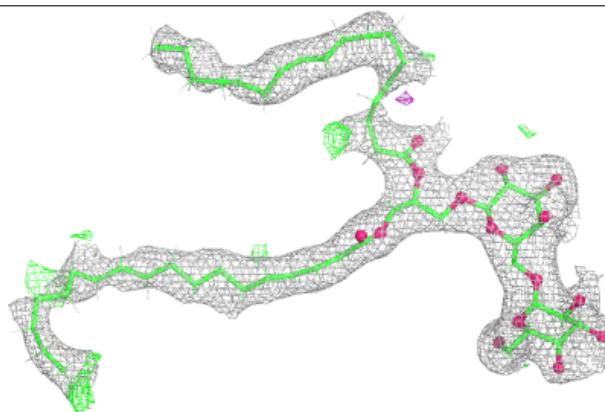


Electron density around STE b 621:

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

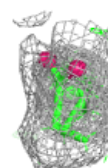
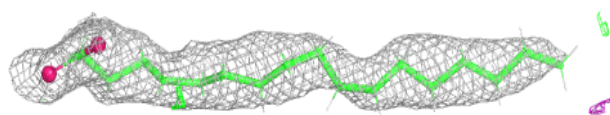
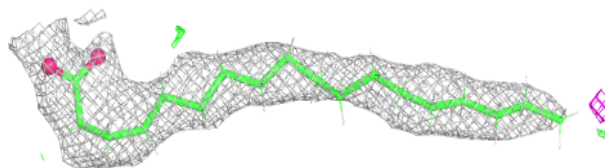
**Electron density around DGD A 416:**

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

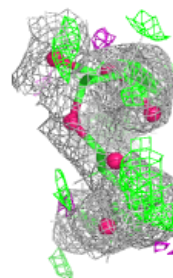
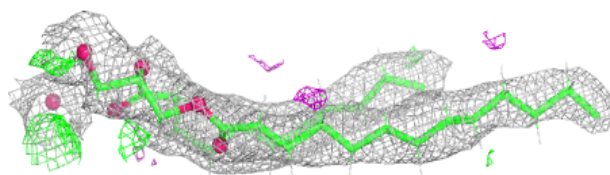
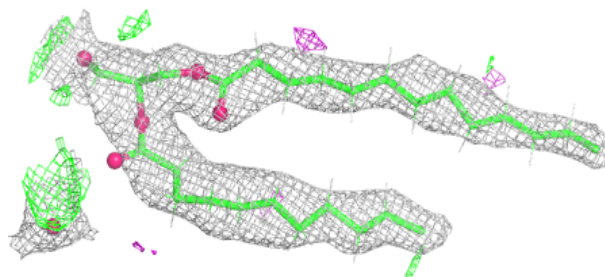


Electron density around STE c 520:

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

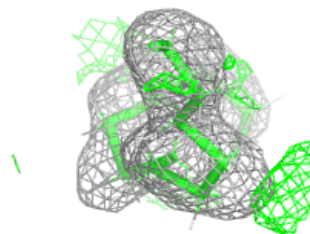
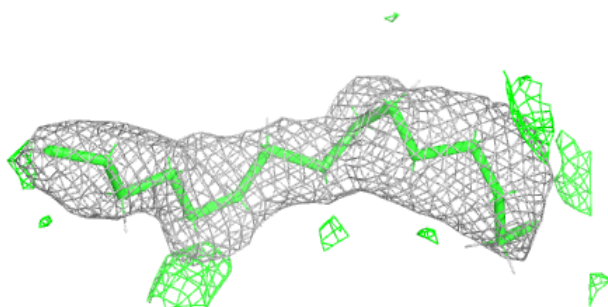
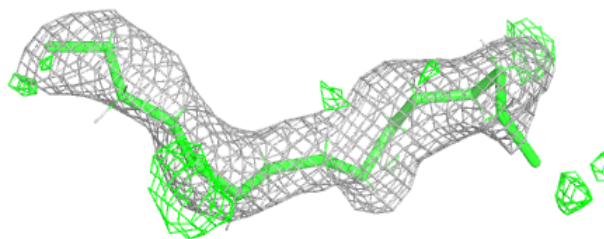
**Electron density around LMG D 410:**

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

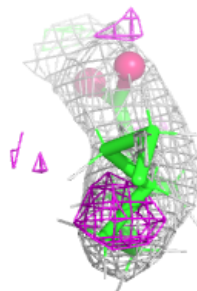
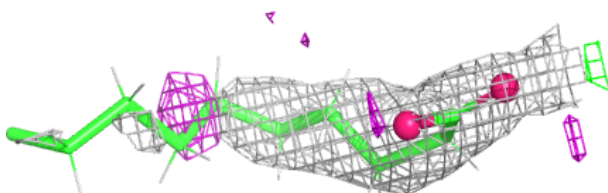
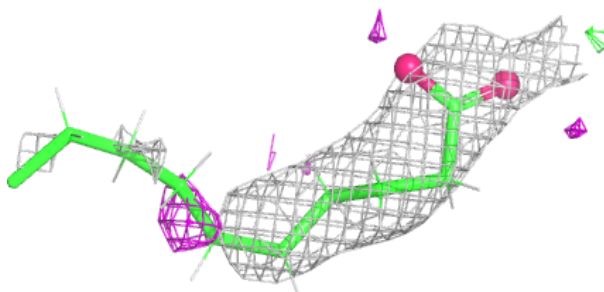


Electron density around STE a 415:

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

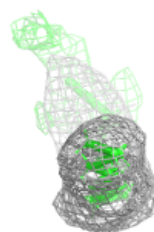
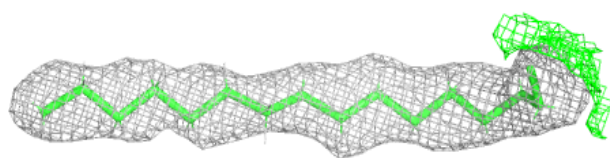
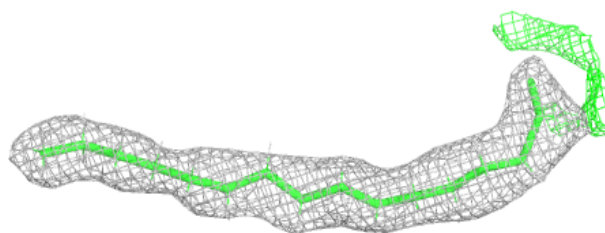
**Electron density around STE B 627:**

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

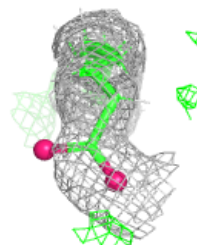
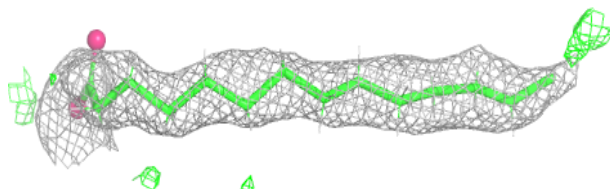
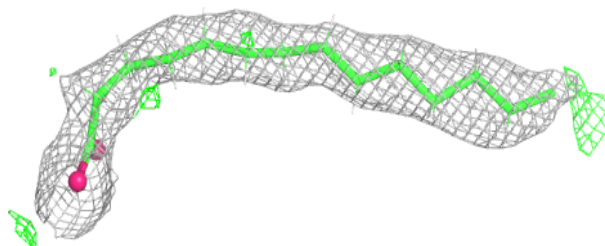


Electron density around STE C 520:

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

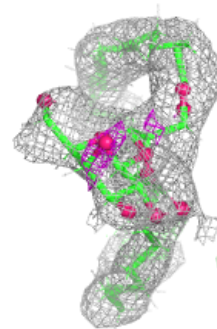
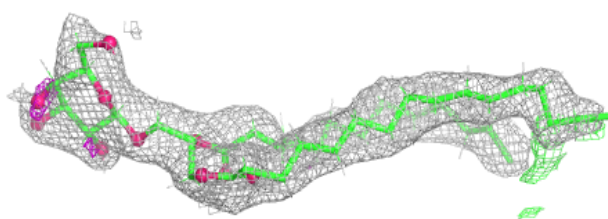
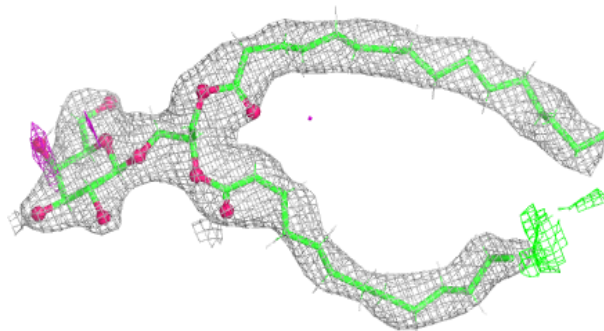
**Electron density around STE b 625:**

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

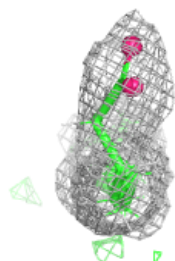
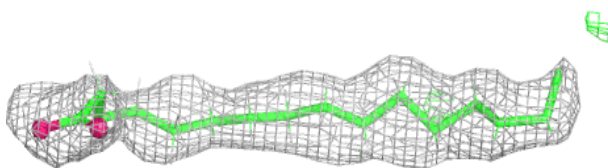
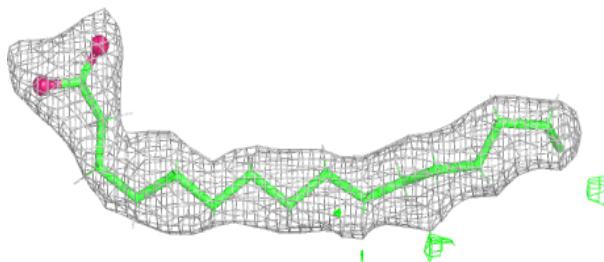


Electron density around LMG A 412:

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

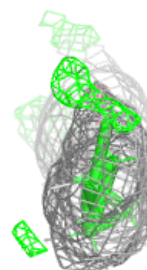
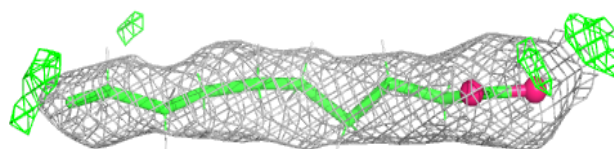
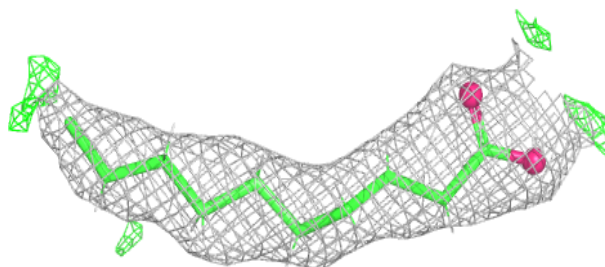
**Electron density around STE B 625:**

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

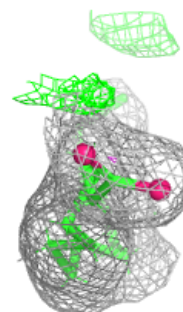
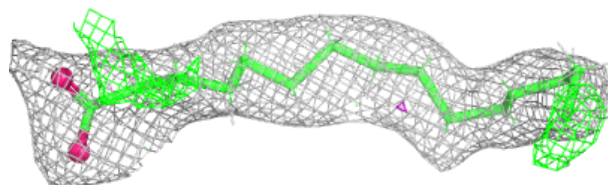
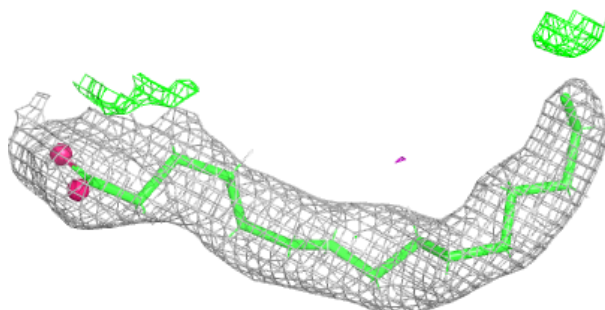


Electron density around STE C 519:

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

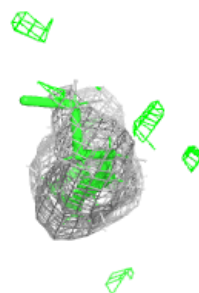
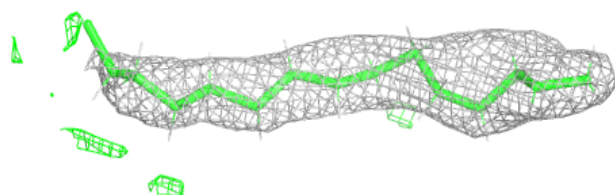
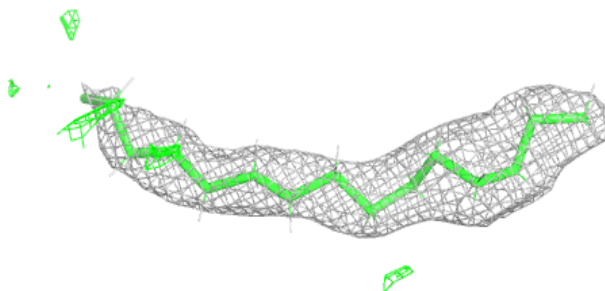
**Electron density around STE B 620:**

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

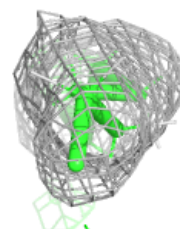
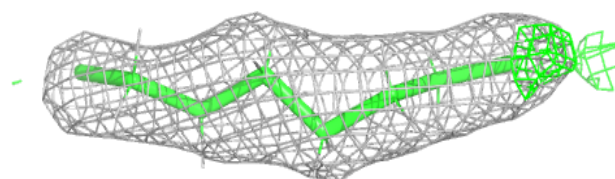
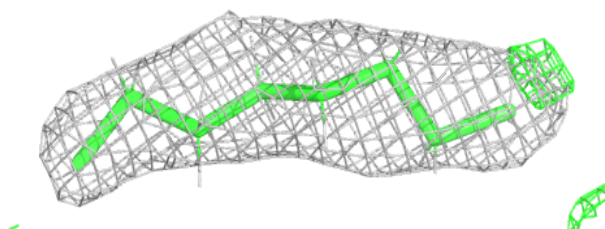


Electron density around STE T 102:

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

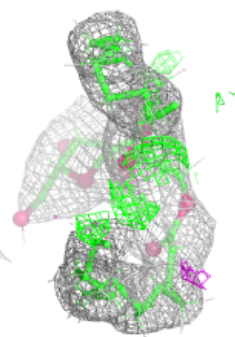
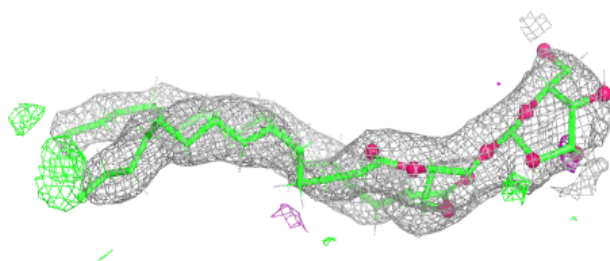
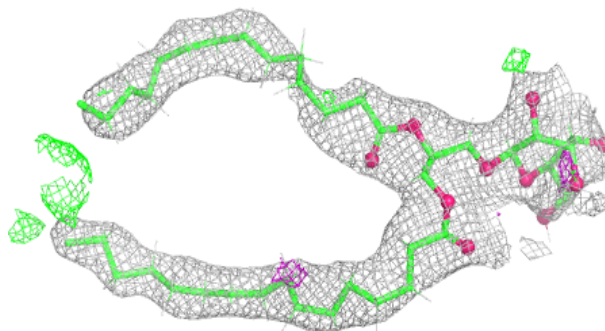
**Electron density around STE Z 101:**

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

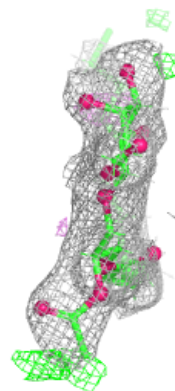
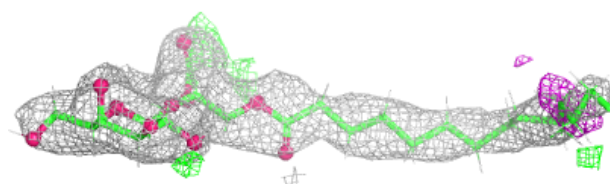
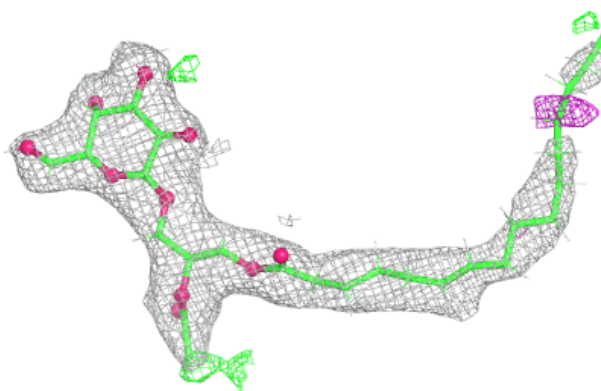


Electron density around LMG c 522:

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

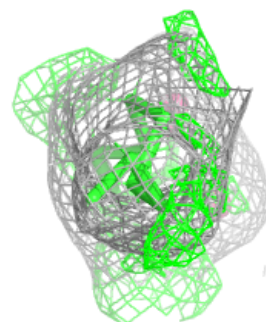
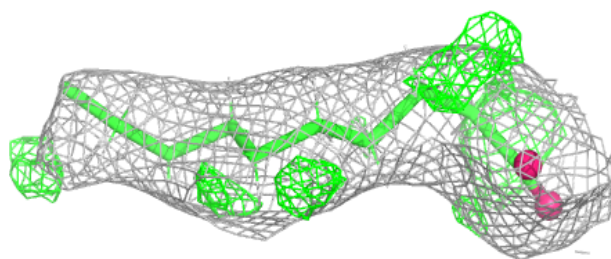
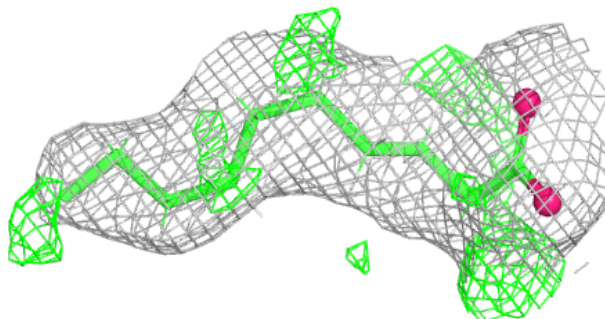
**Electron density around LMG c 519:**

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

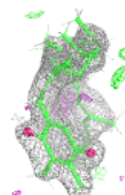
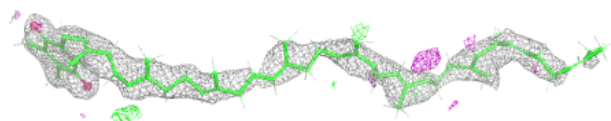
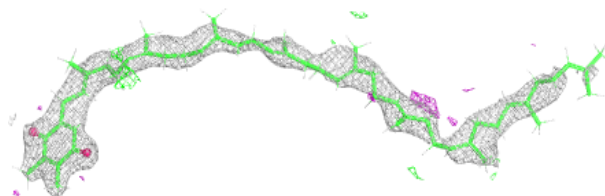


Electron density around STE B 624:

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

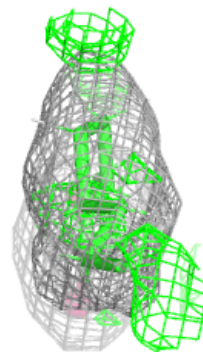
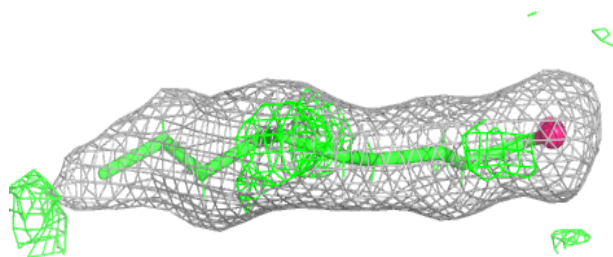
**Electron density around PL9 A 410:**

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

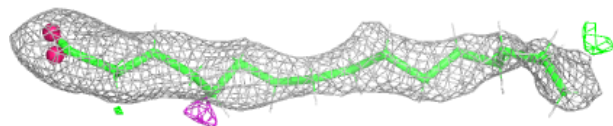
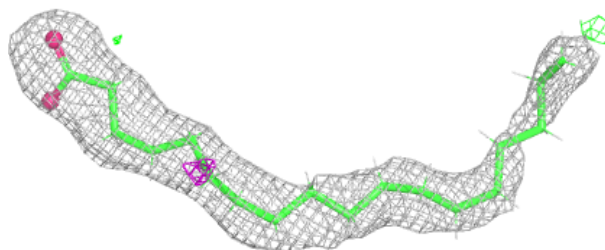


Electron density around STE C 521:

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

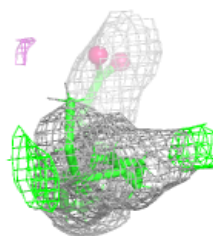
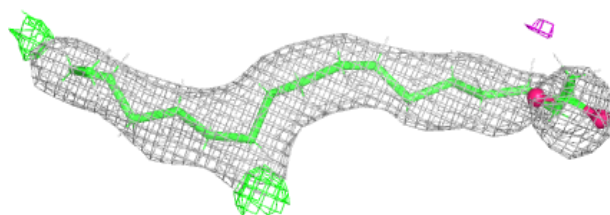
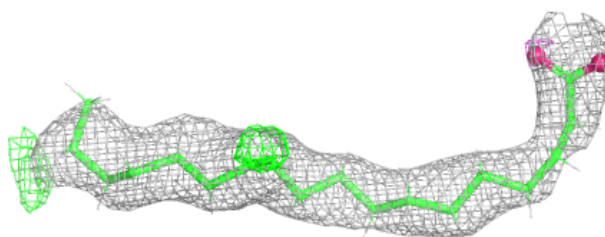
**Electron density around STE d 412:**

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

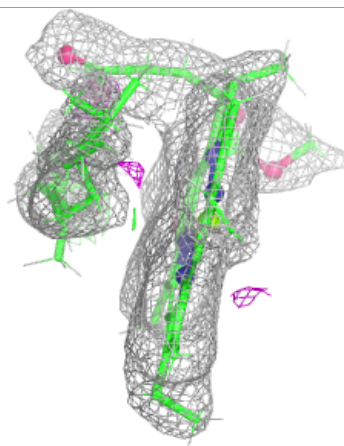
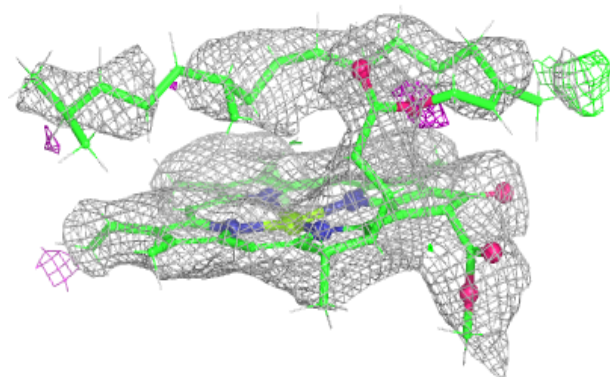
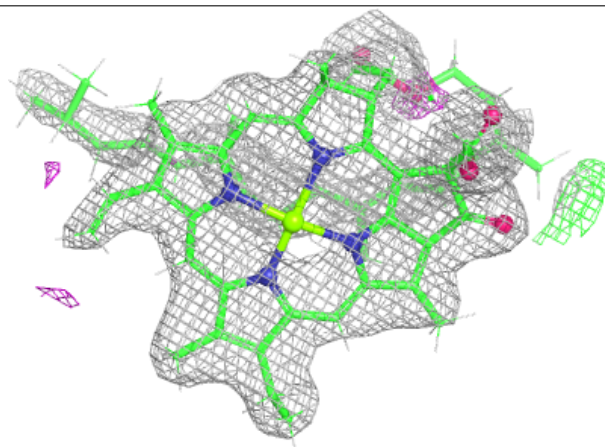


Electron density around STE b 623:

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

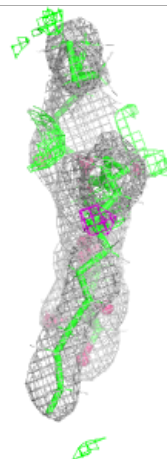
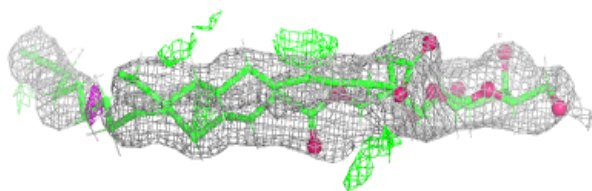
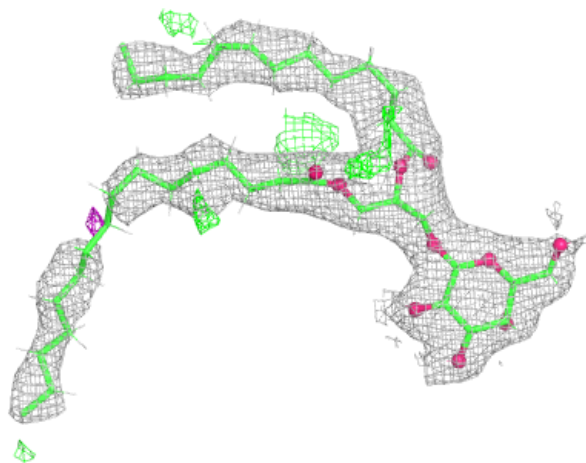
**Electron density around CLA b 601:**

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



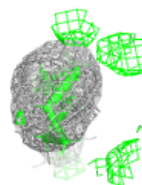
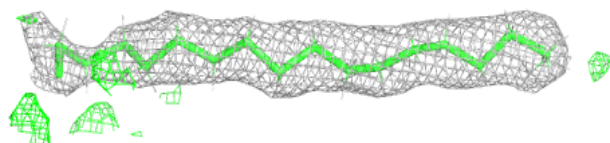
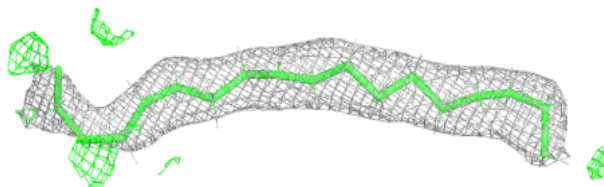
Electron density around LMG C 518:

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

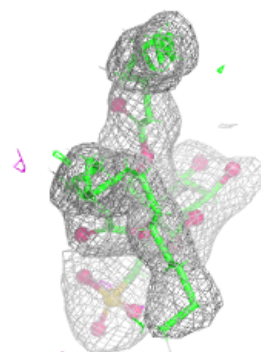
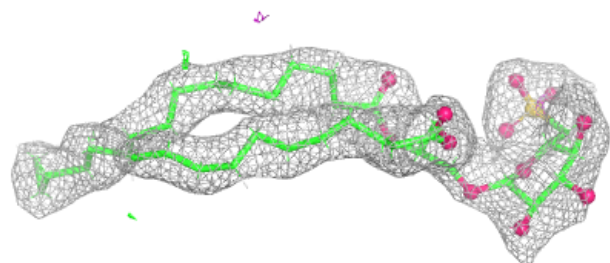
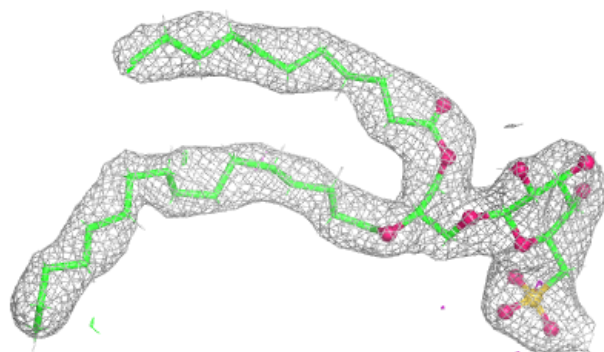


Electron density around STE l 102:

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

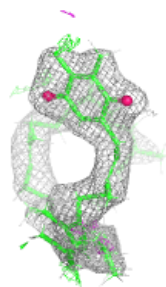
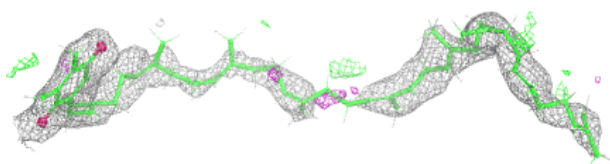
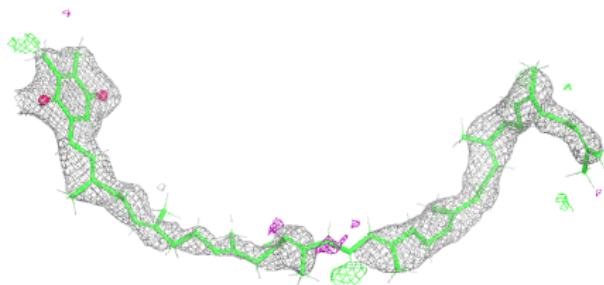
**Electron density around SQD b 620:**

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

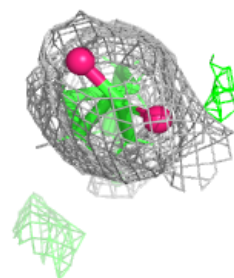
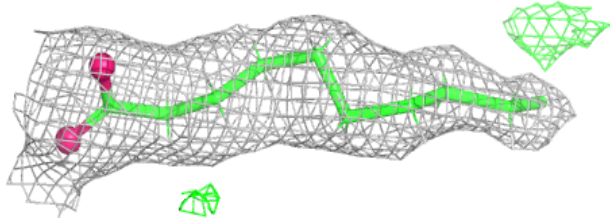
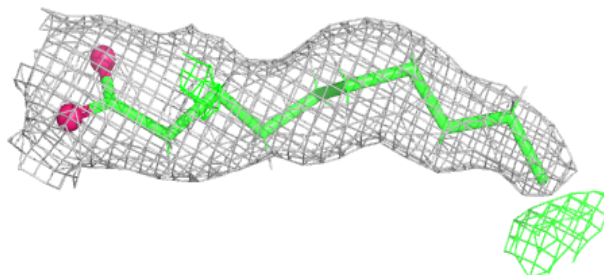


Electron density around PL9 a 409:

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

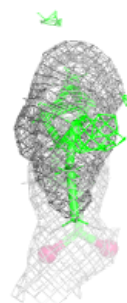
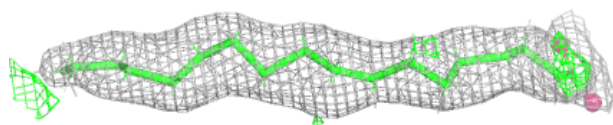
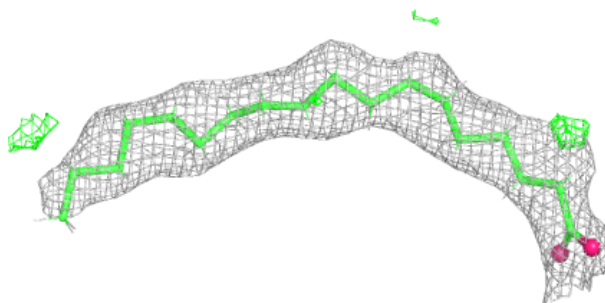
**Electron density around STE J 101:**

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

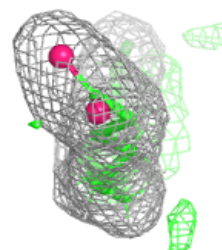
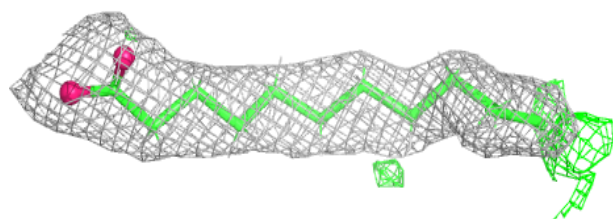
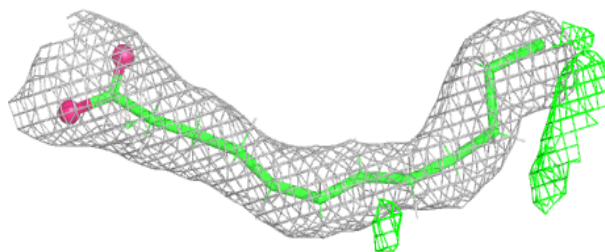


Electron density around STE X 101:

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

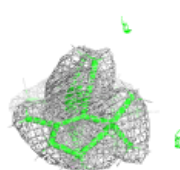
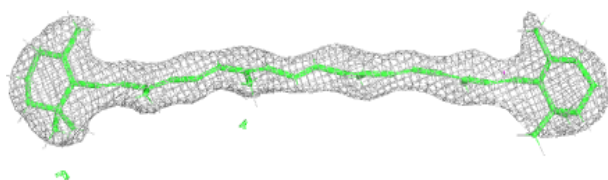
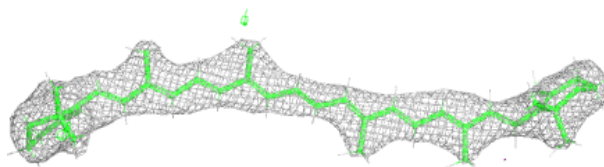
**Electron density around STE t 102:**

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

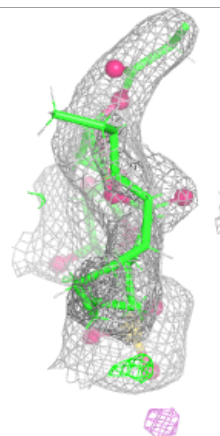
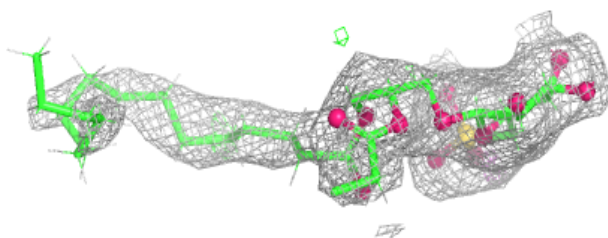
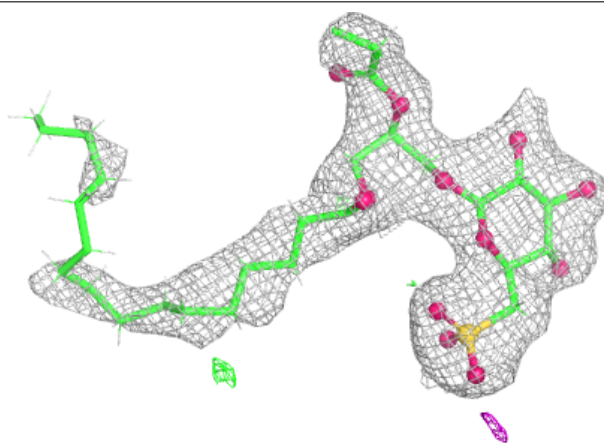


Electron density around BCR c 514:

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

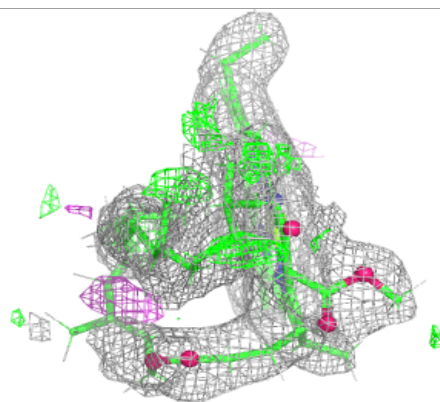
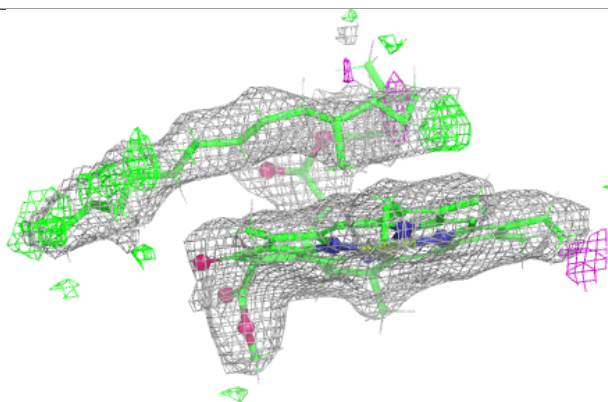
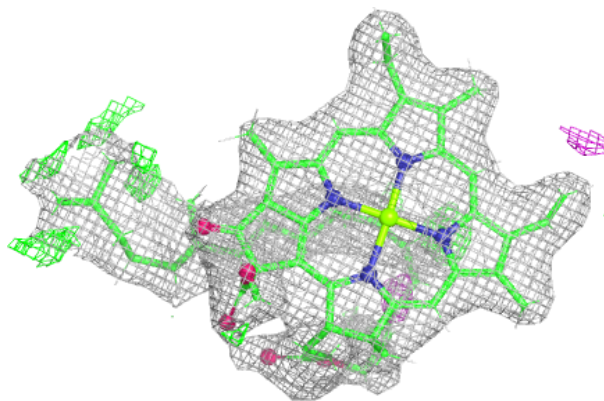
**Electron density around SQD f 101:**

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

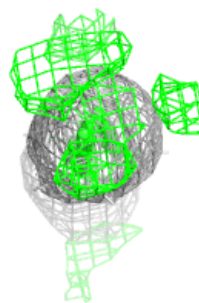
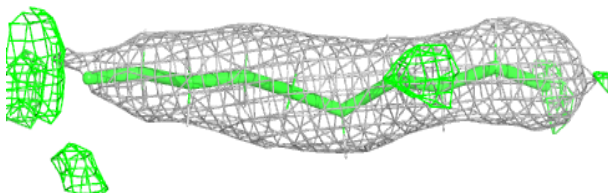
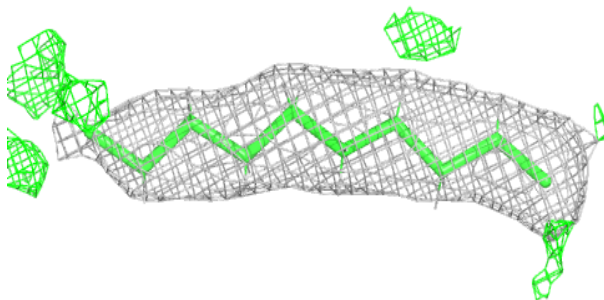


Electron density around CLA B 601:

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

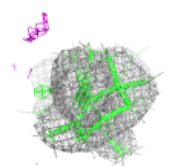
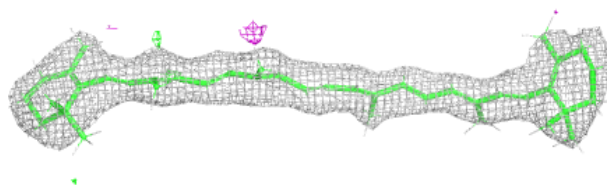
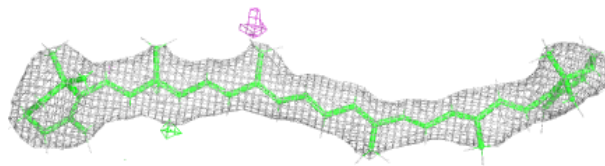
**Electron density around STE M 103:**

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

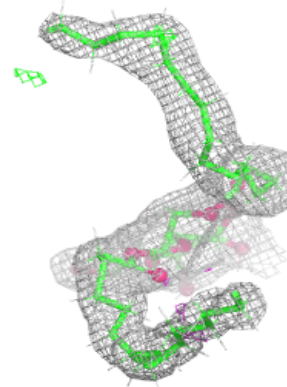
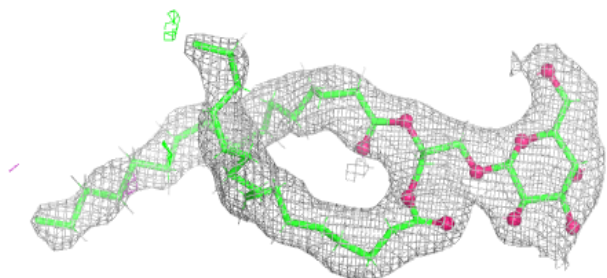
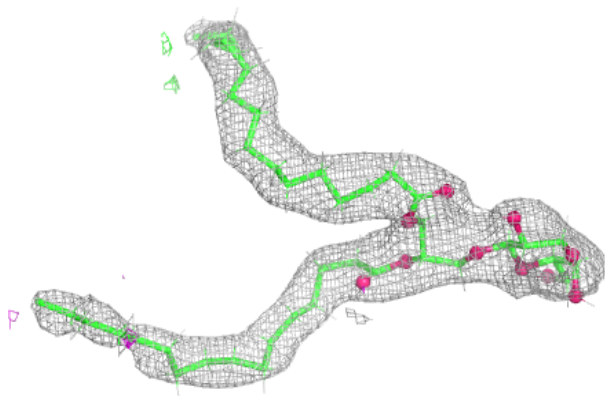


Electron density around BCR K 101:

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

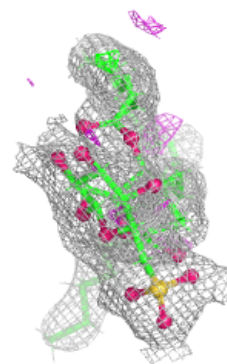
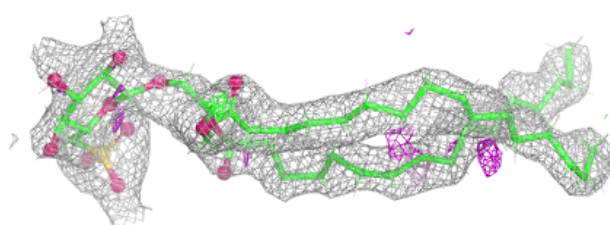
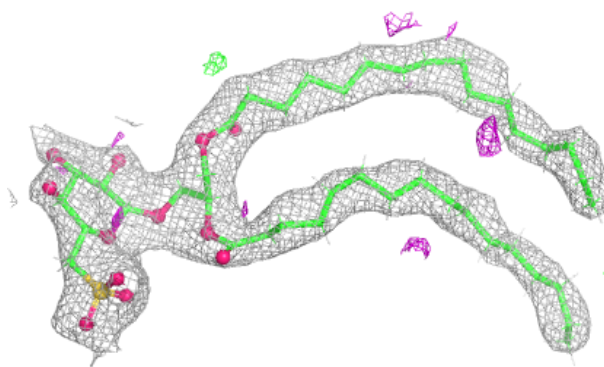
**Electron density around LMG b 622:**

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

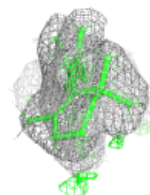
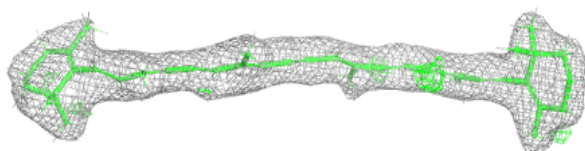
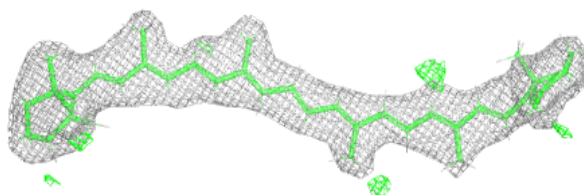


Electron density around SQD B 623:

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

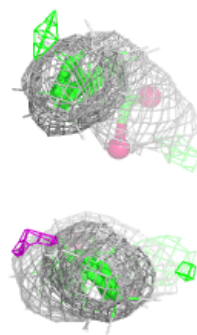
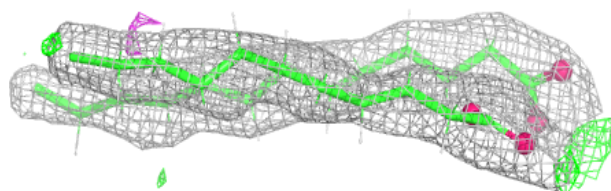
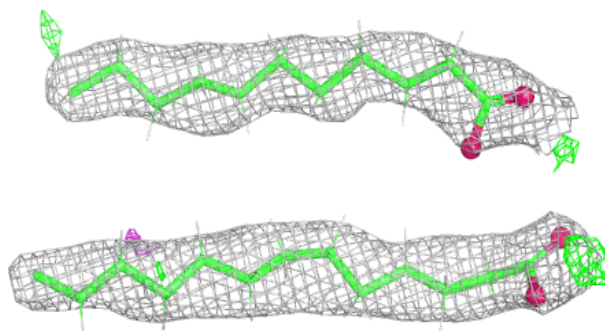
**Electron density around BCR Y 101:**

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

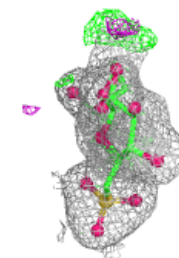
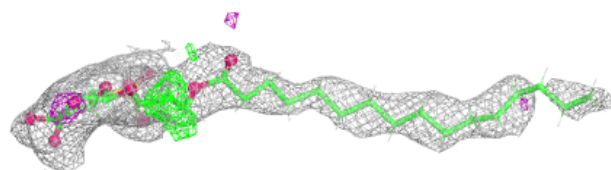
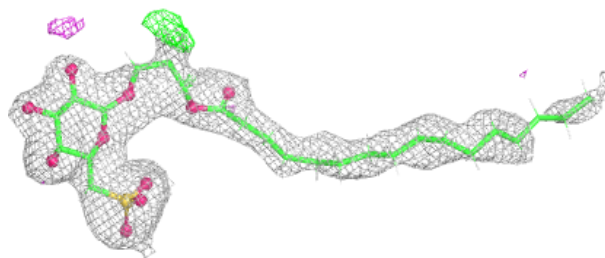


Electron density around LMG D 411:

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

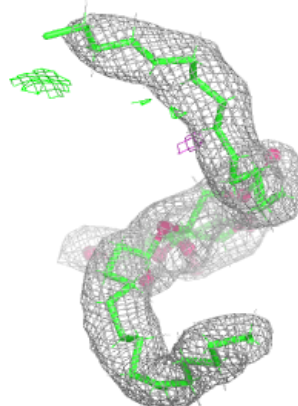
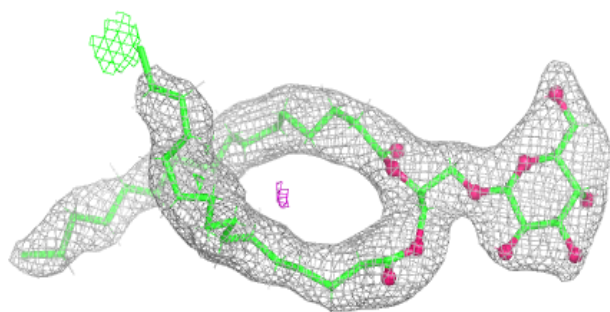
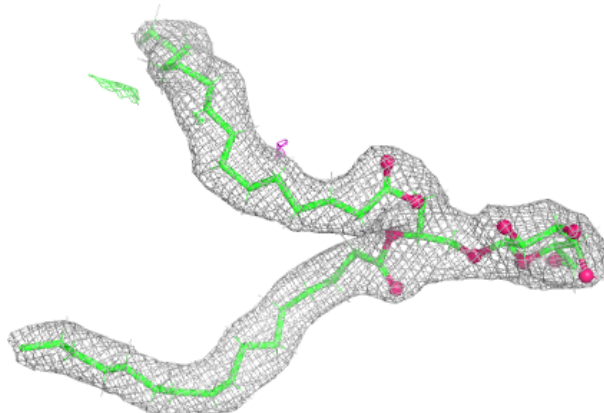
**Electron density around SQD D 407:**

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

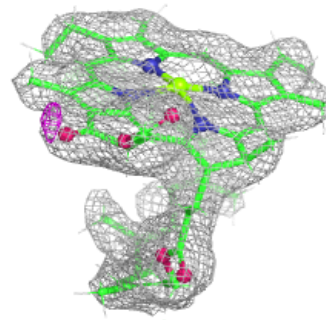
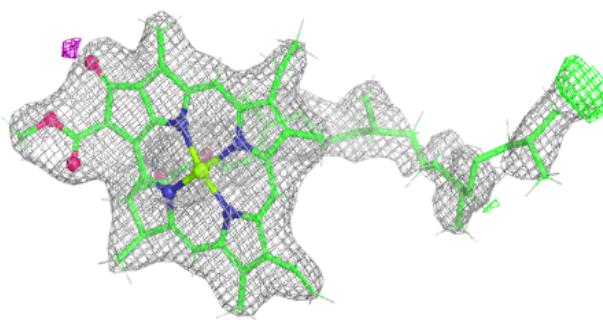
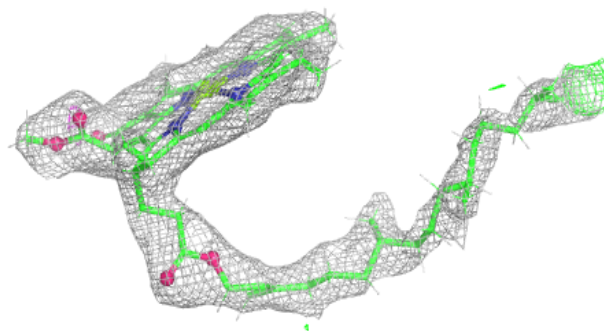


Electron density around LMG M 101:

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

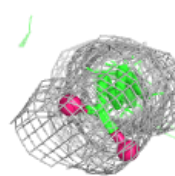
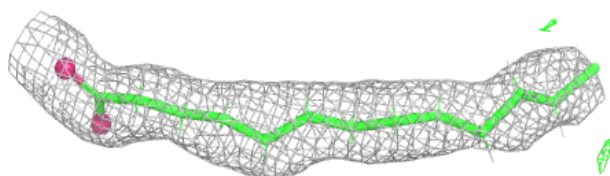
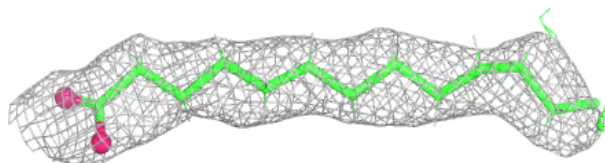
**Electron density around CLA C 513:**

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

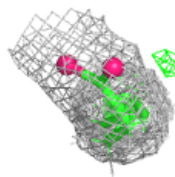
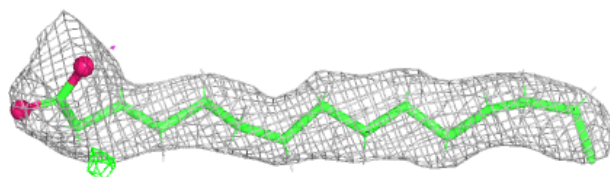
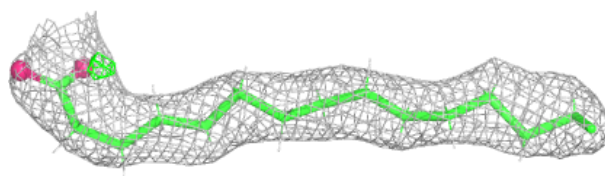


Electron density around STE M 102:

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

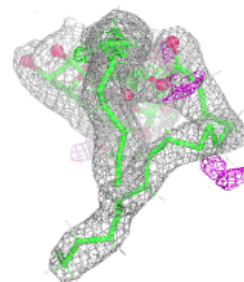
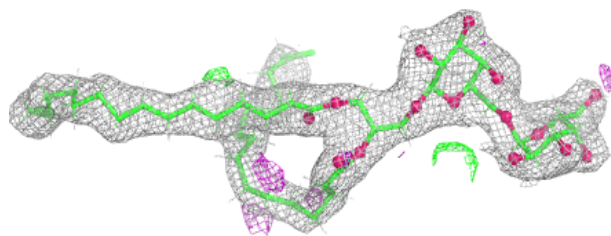
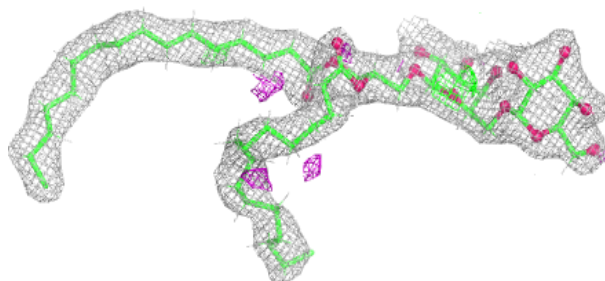
**Electron density around STE d 411:**

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



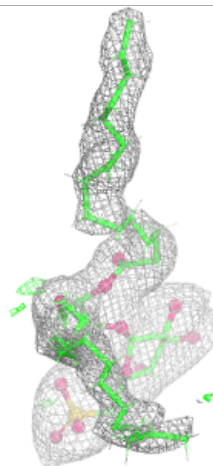
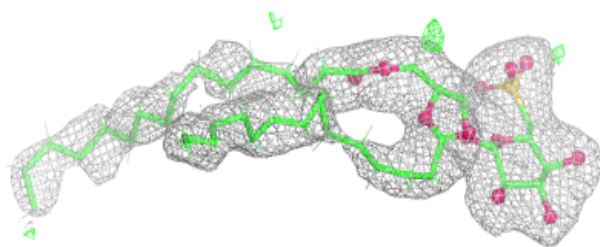
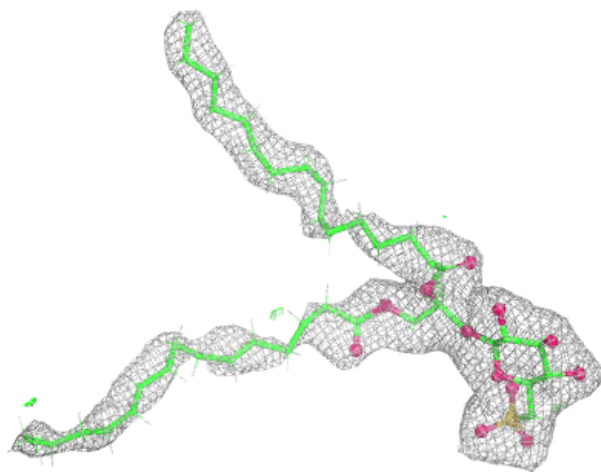
Electron density around DGD h 101:

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



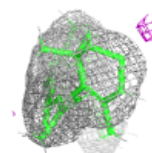
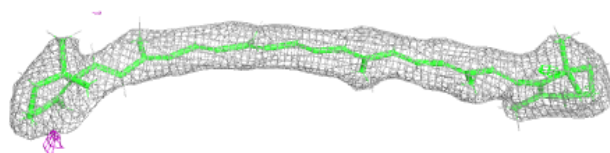
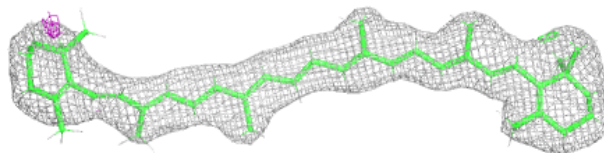
Electron density around SQD a 411:

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

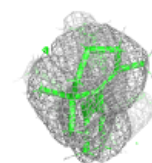
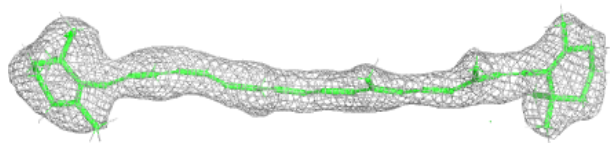


Electron density around BCR d 405:

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

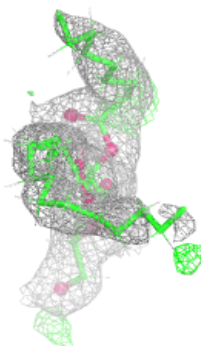
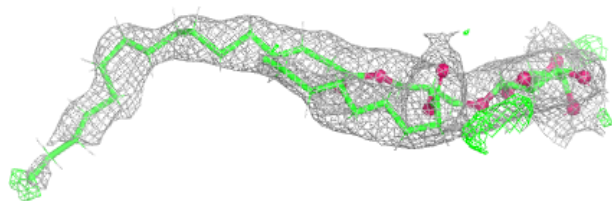
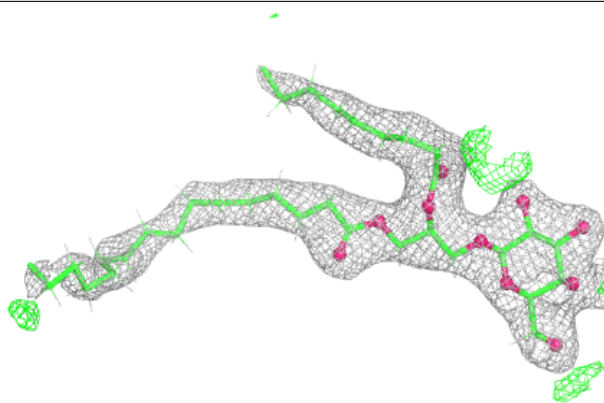
**Electron density around BCR k 101:**

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

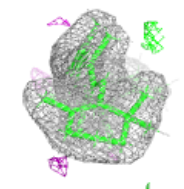
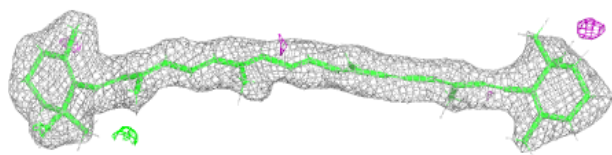
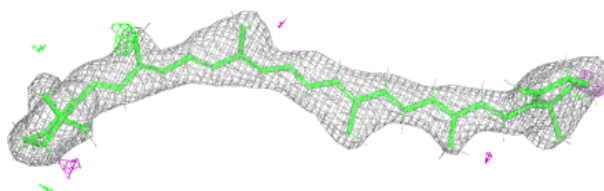


Electron density around LMG d 410:

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

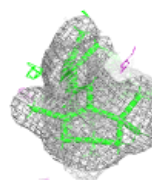
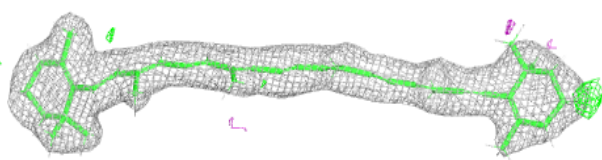
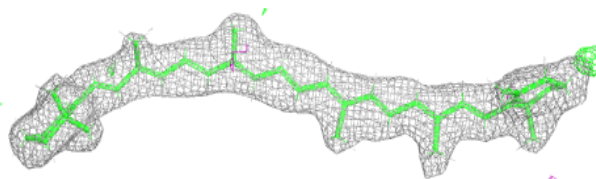
**Electron density around BCR x 101:**

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

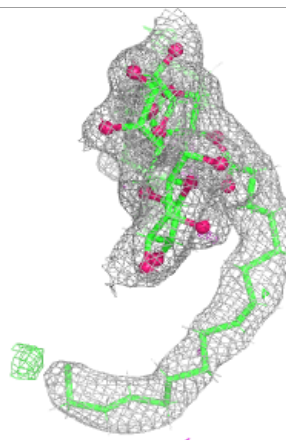
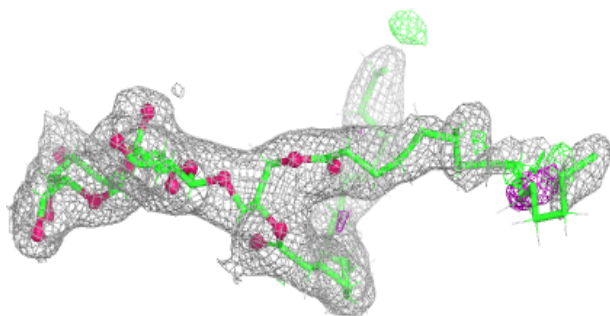
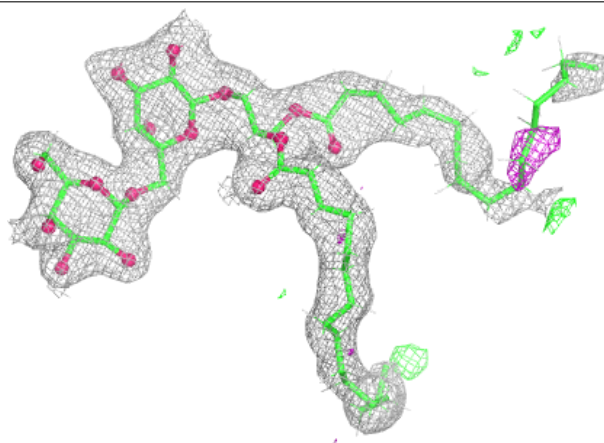


Electron density around BCR H 101:

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

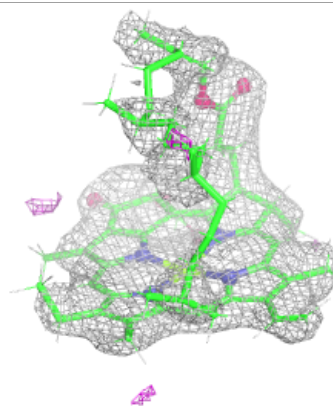
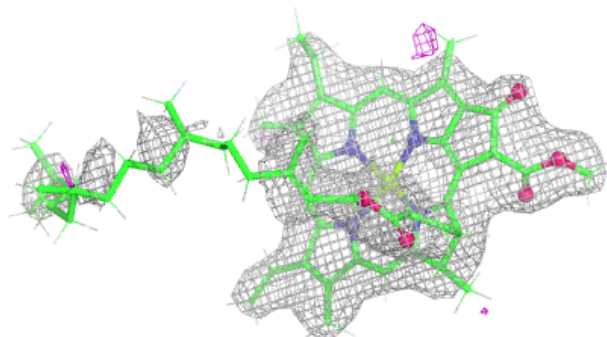
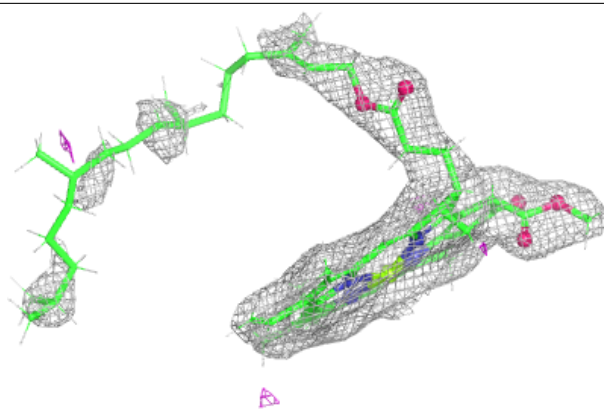
**Electron density around DGD C 516:**

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

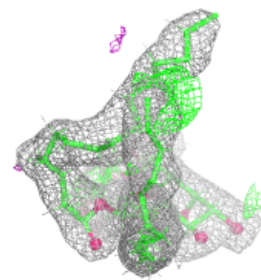
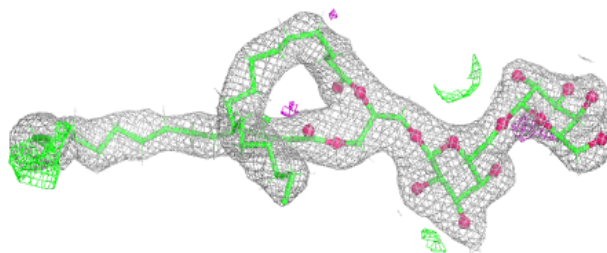
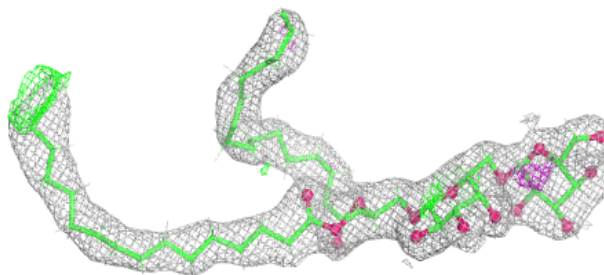


Electron density around CLA c 513:

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

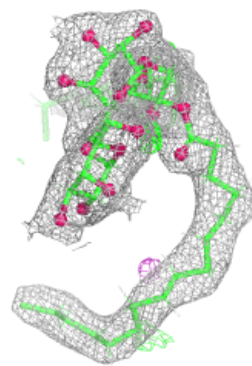
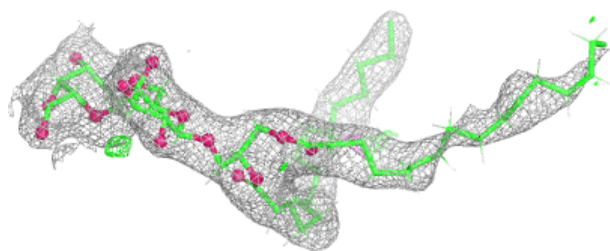
**Electron density around DGD H 102:**

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

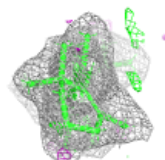
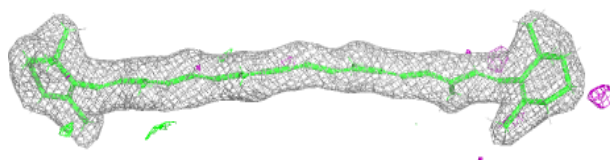
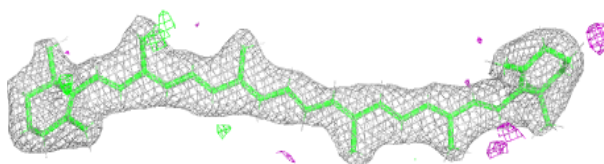


Electron density around DGD c 517:

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

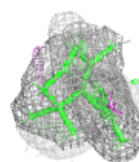
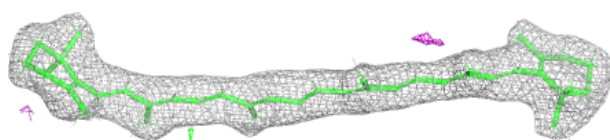
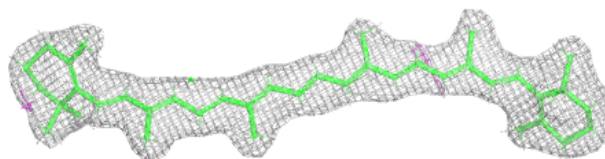
**Electron density around BCR B 618:**

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

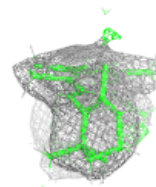
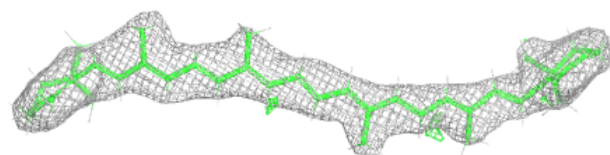
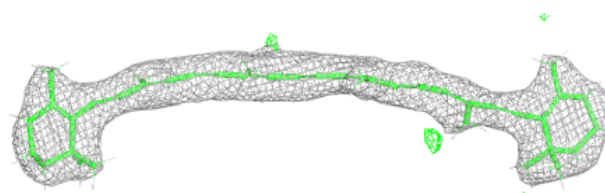


Electron density around BCR B 619:

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

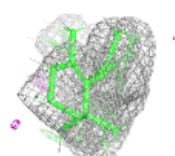
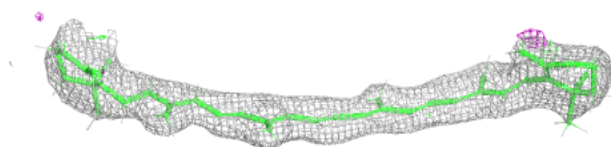
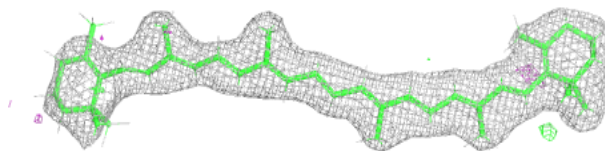
**Electron density around BCR k 102:**

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



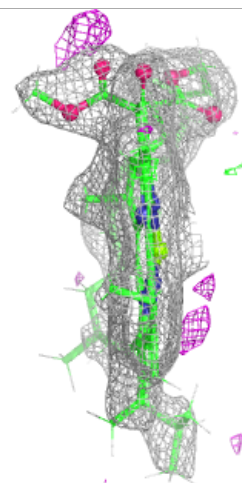
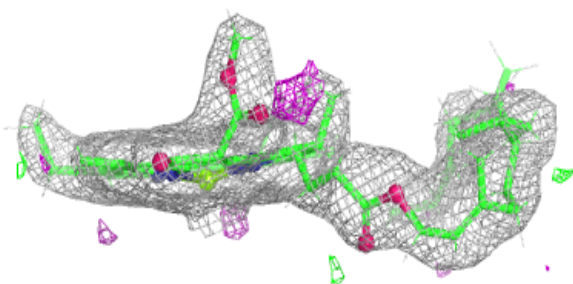
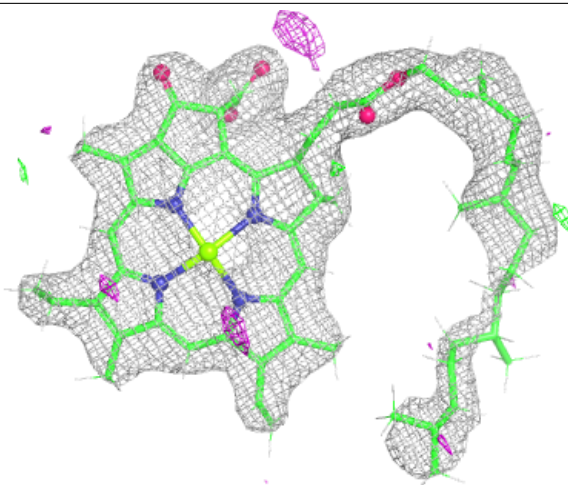
Electron density around BCR D 404:

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



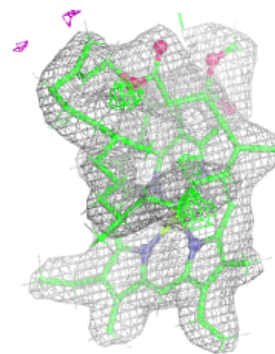
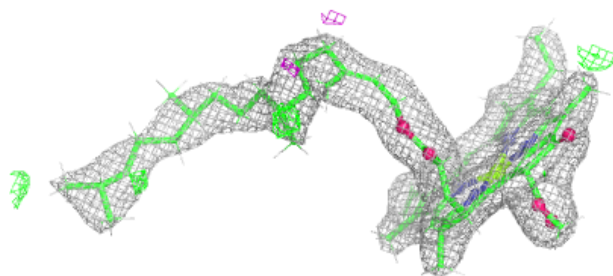
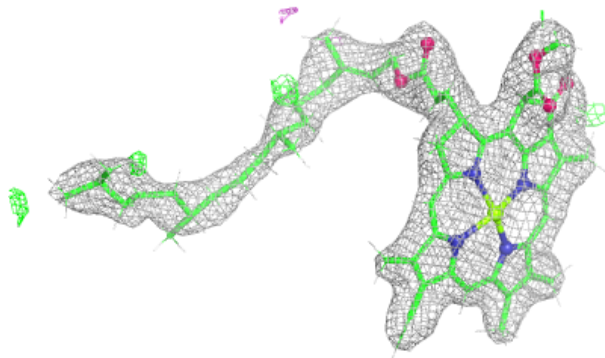
Electron density around CLA C 512:

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



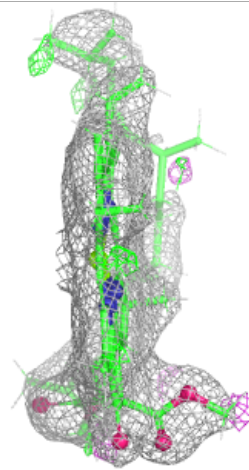
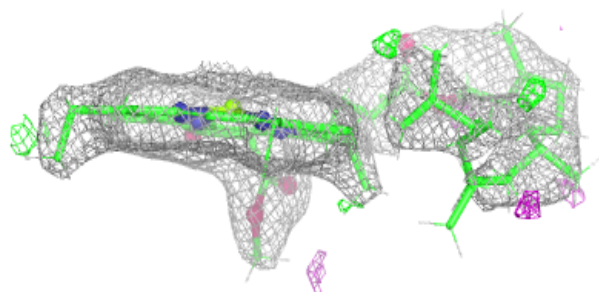
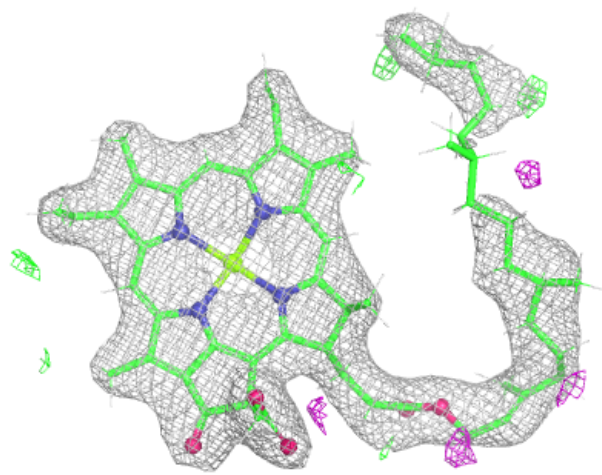
Electron density around CLA c 511:

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



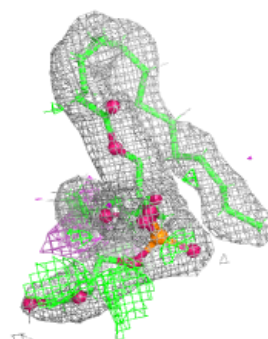
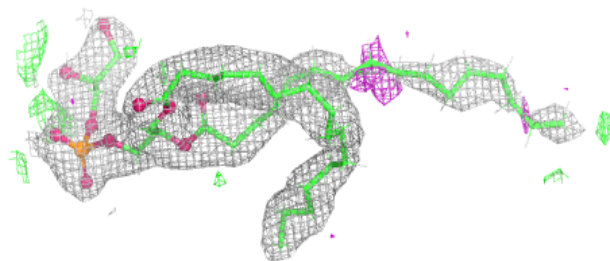
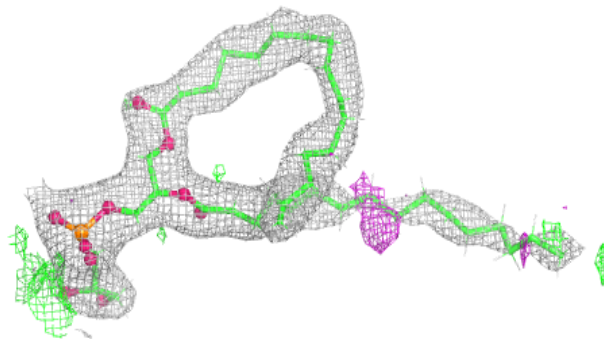
Electron density around CLA c 512:

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

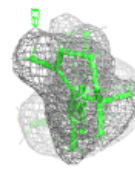
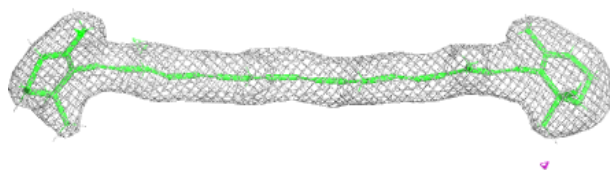
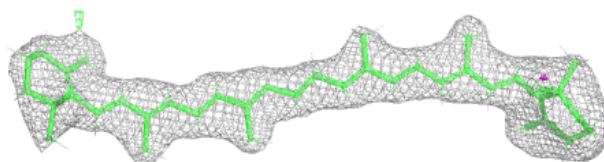


Electron density around LHG d 407:

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

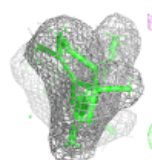
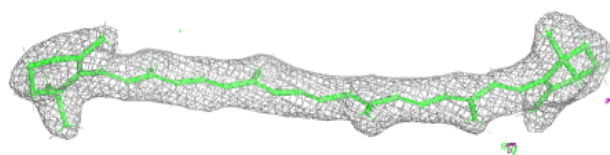
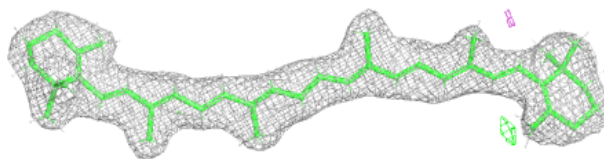
**Electron density around BCR b 618:**

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

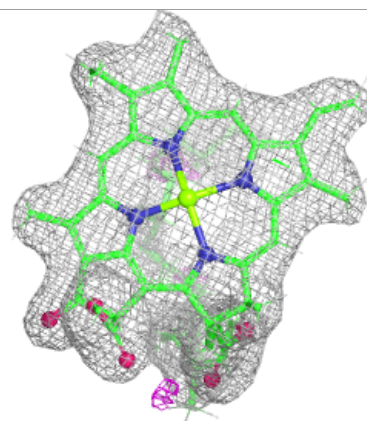
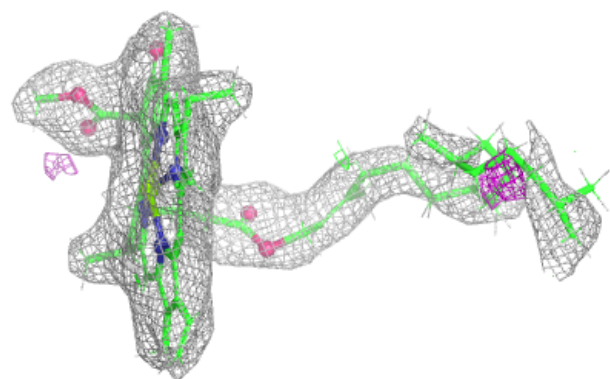
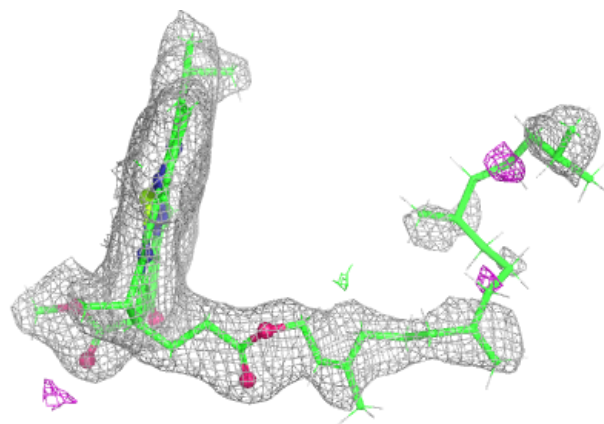


Electron density around BCR b 619:

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

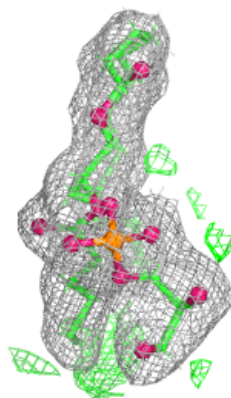
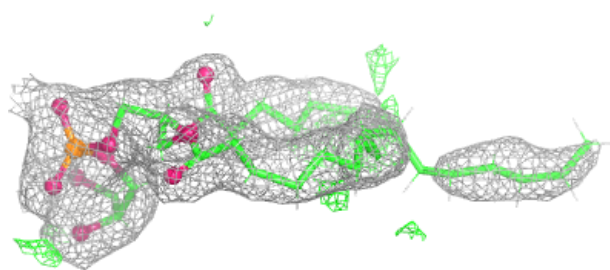
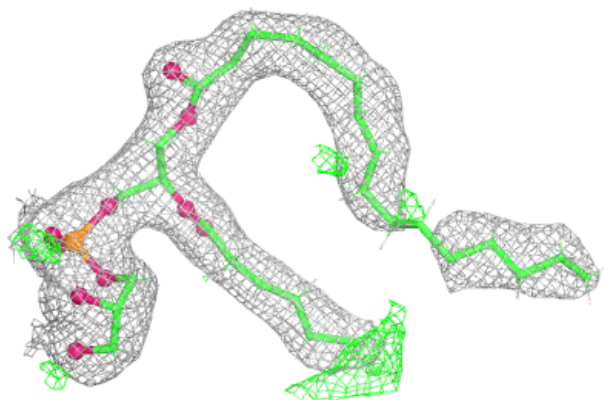
**Electron density around CLA c 506:**

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

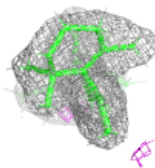
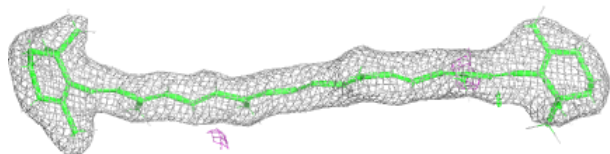
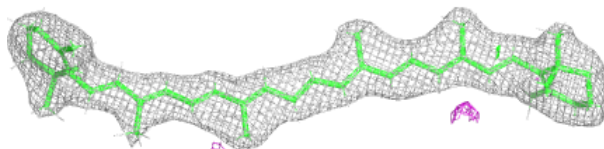


Electron density around LHG d 409:

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

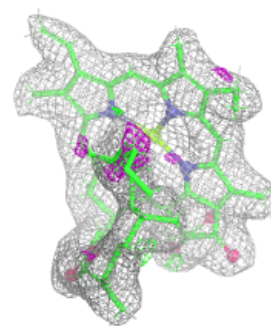
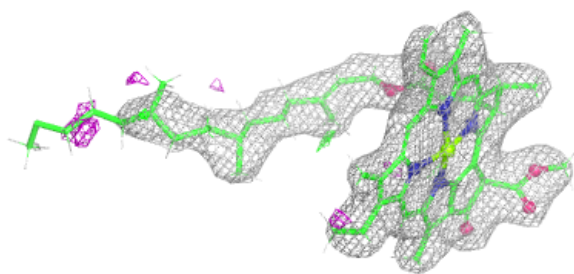
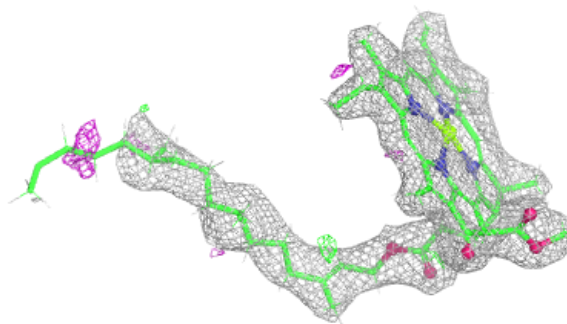
**Electron density around BCR C 514:**

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

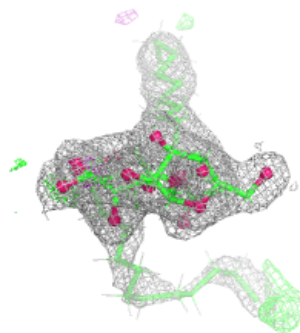
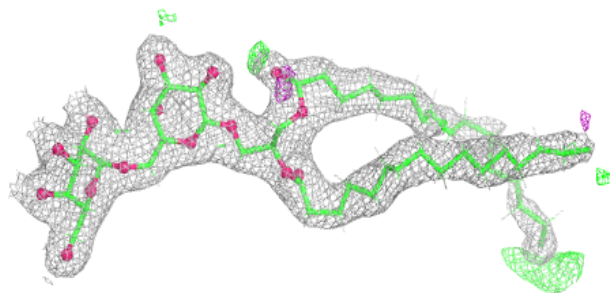
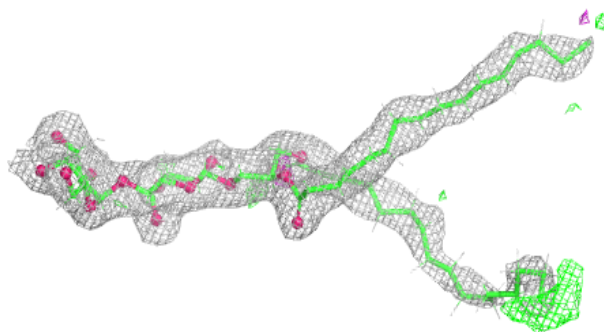


Electron density around CLA c 508:

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

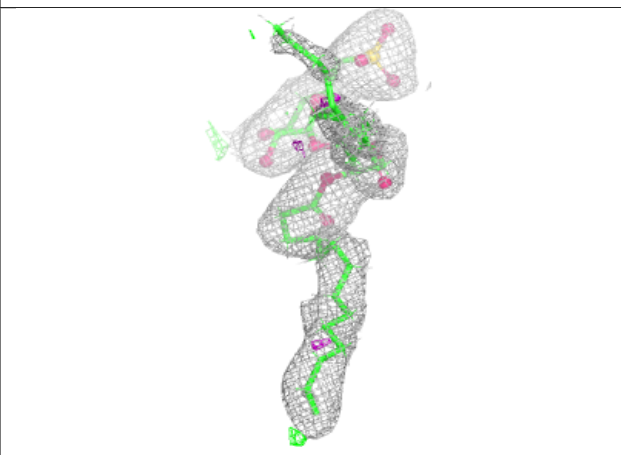
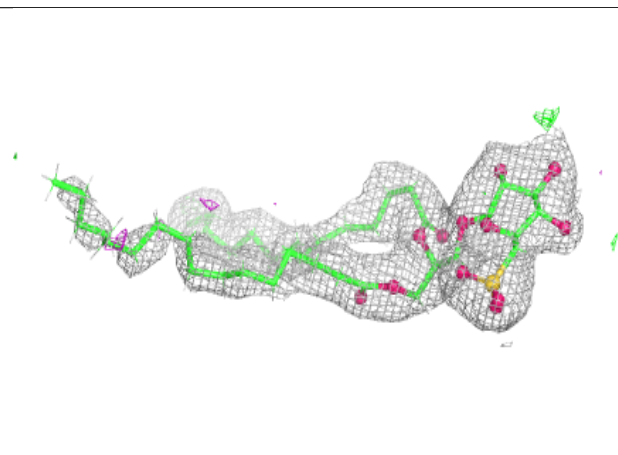
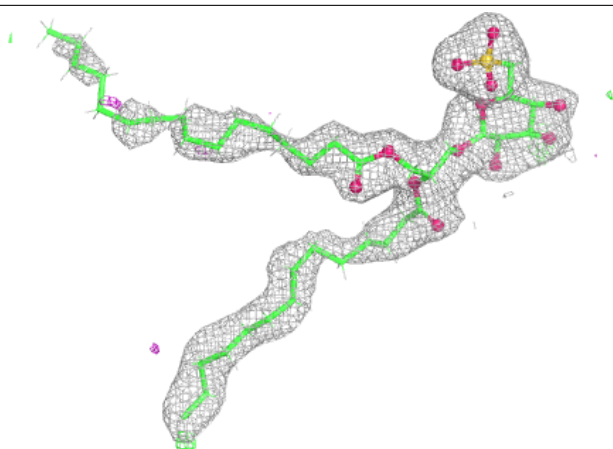
**Electron density around DGD C 515:**

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

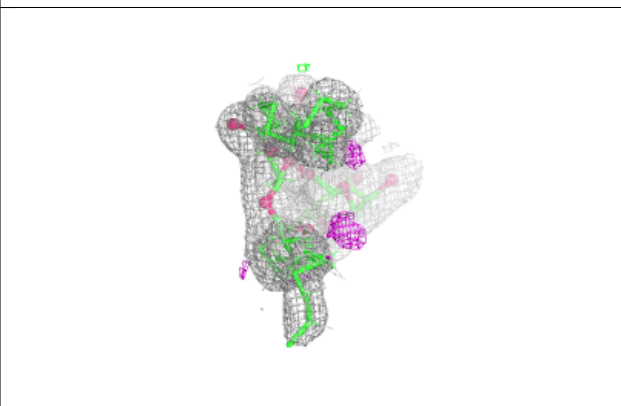
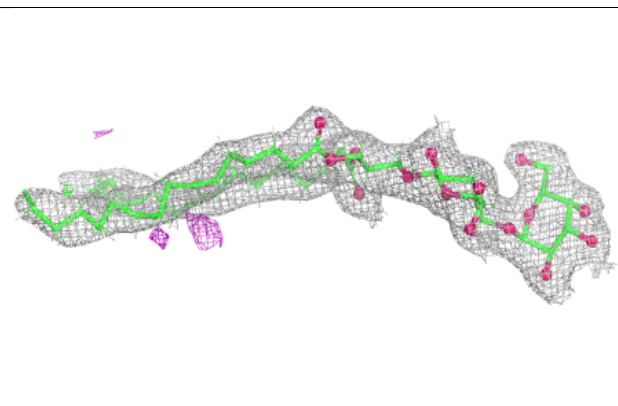
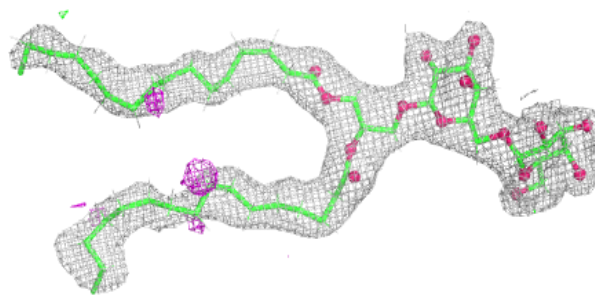


Electron density around SQD A 413:

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

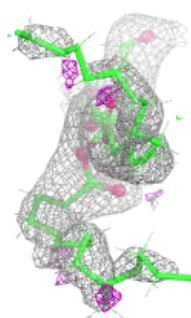
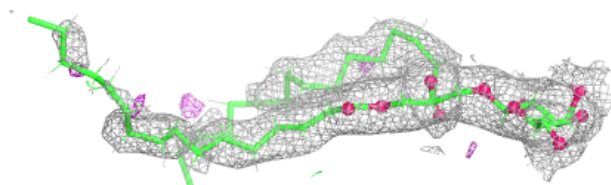
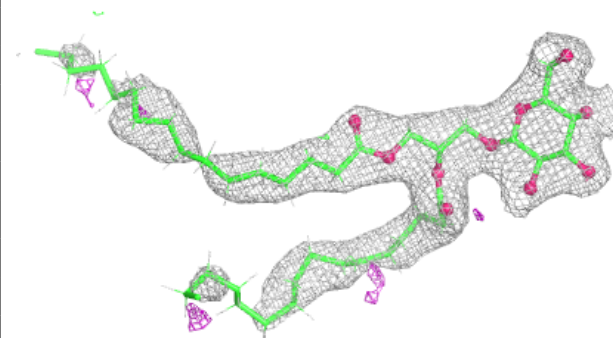
**Electron density around DGD C 517:**

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

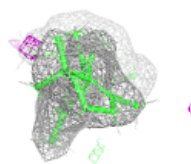
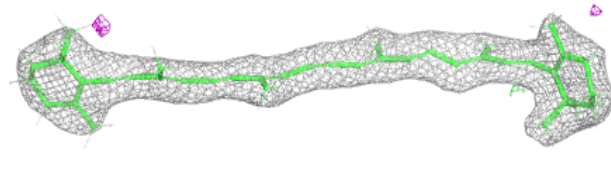
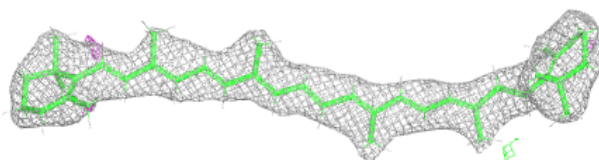


Electron density around LMG D 406:

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

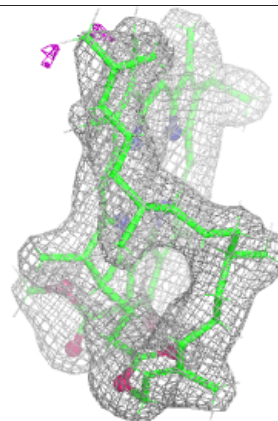
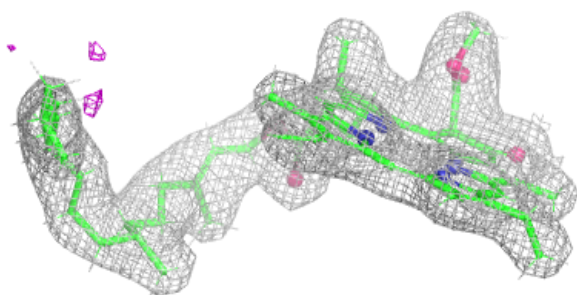
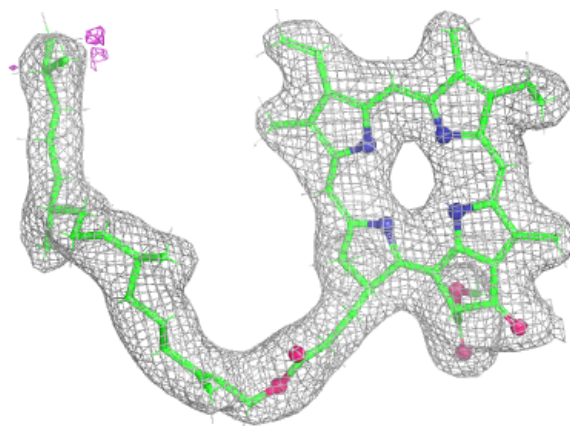
**Electron density around BCR c 515:**

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

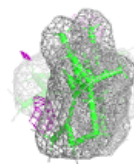
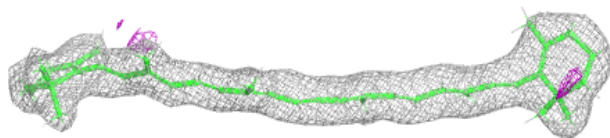
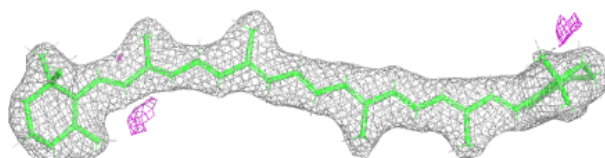


Electron density around PHO d 402:

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

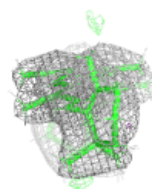
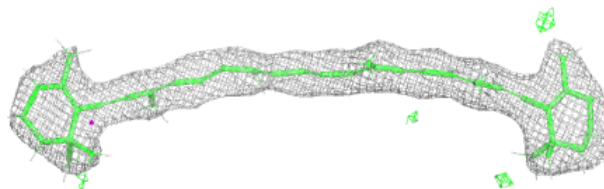
**Electron density around BCR B 617:**

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

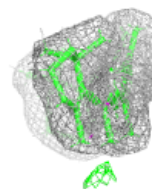
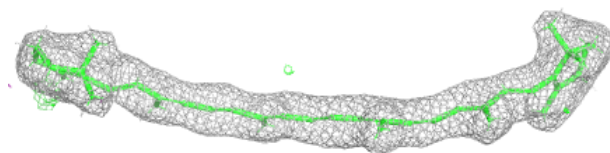
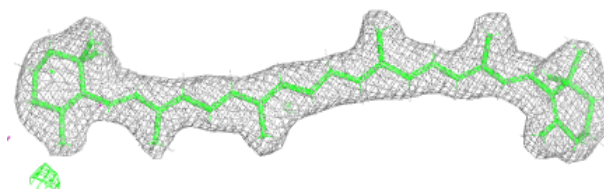


Electron density around BCR K 102:

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

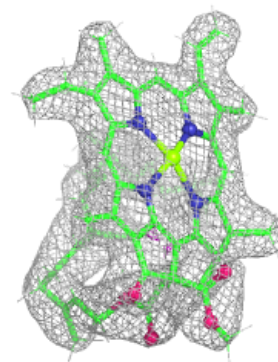
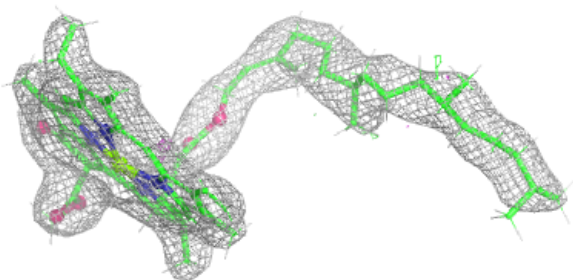
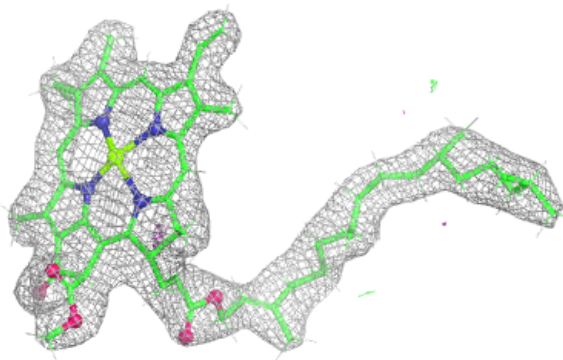
**Electron density around BCR T 101:**

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

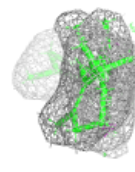
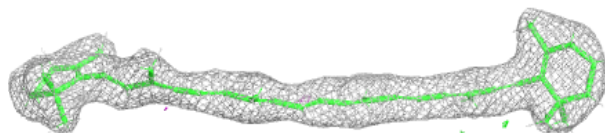
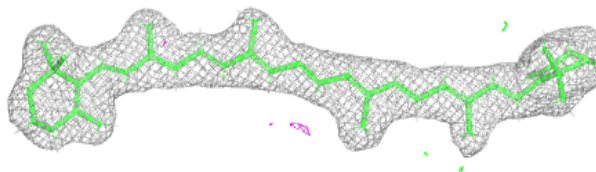


Electron density around CLA C 511:

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

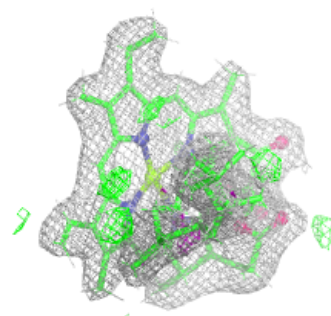
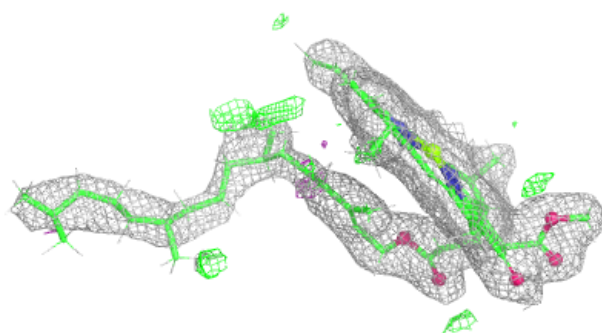
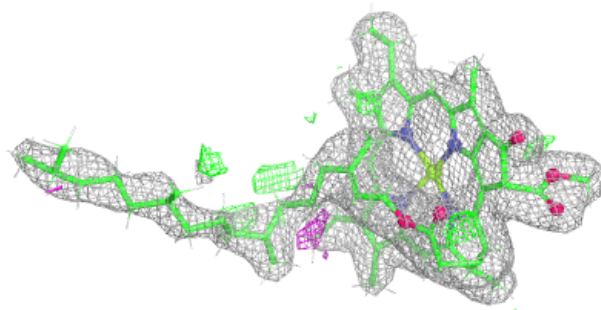
**Electron density around BCR b 617:**

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

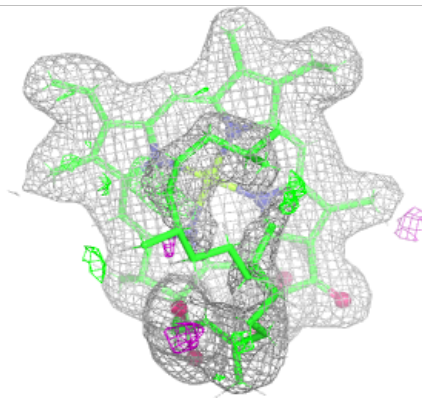
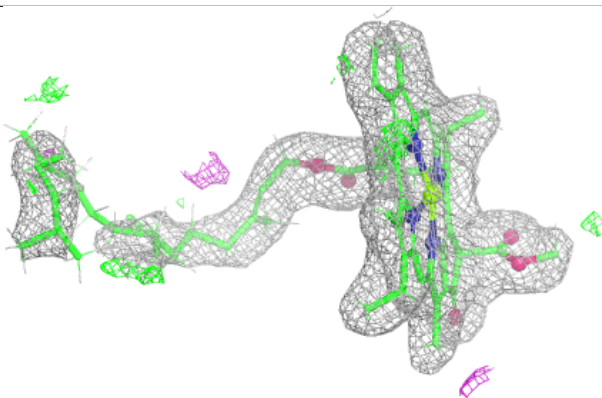
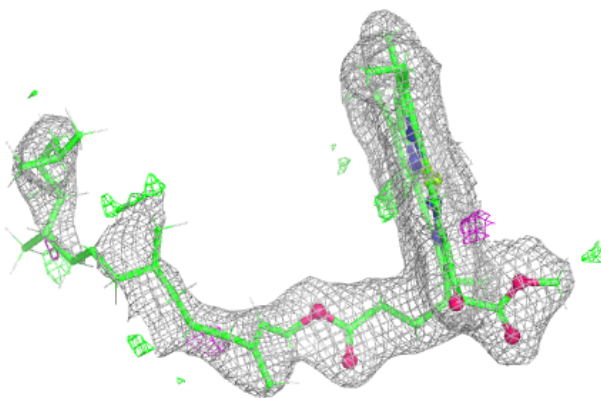


Electron density around CLA C 505:

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

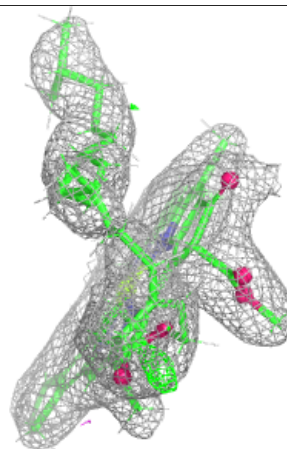
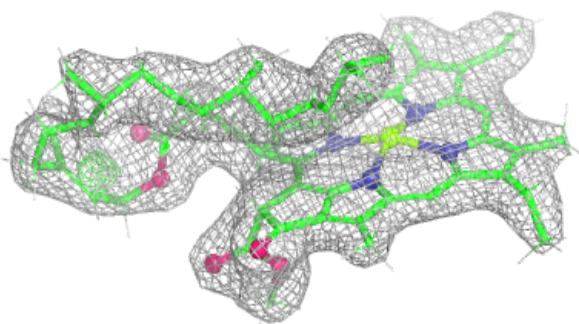
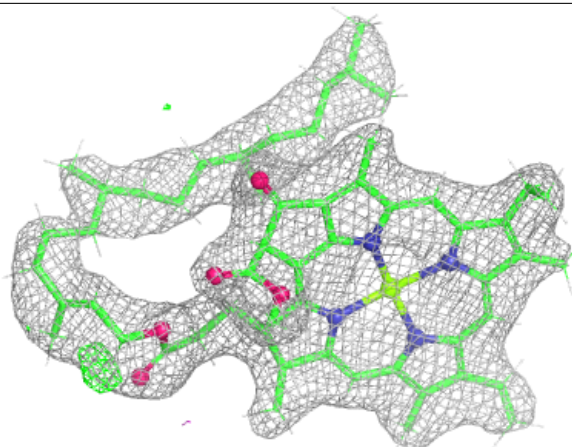
**Electron density around CLA C 506:**

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



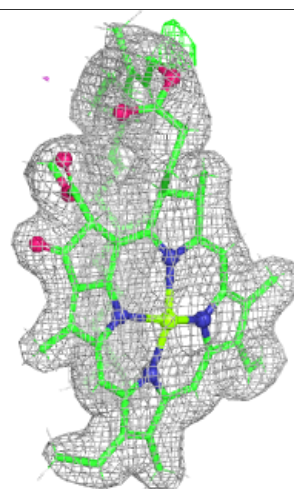
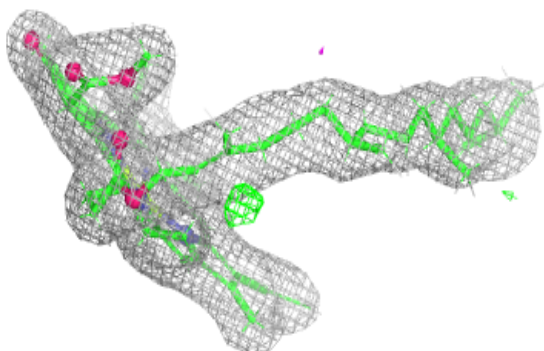
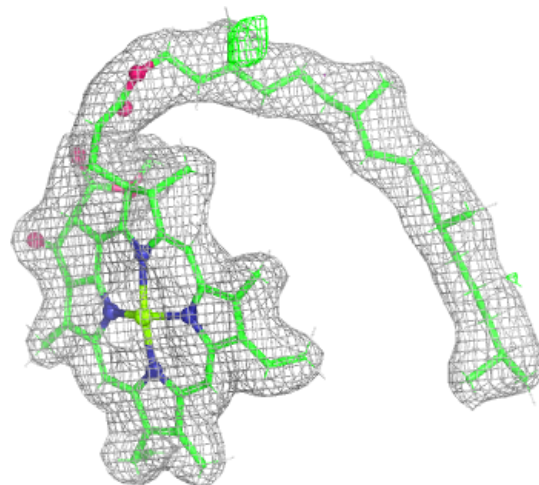
Electron density around CLA c 509:

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



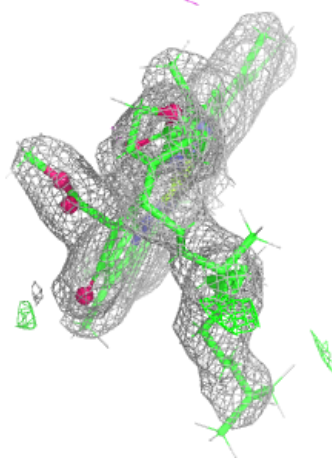
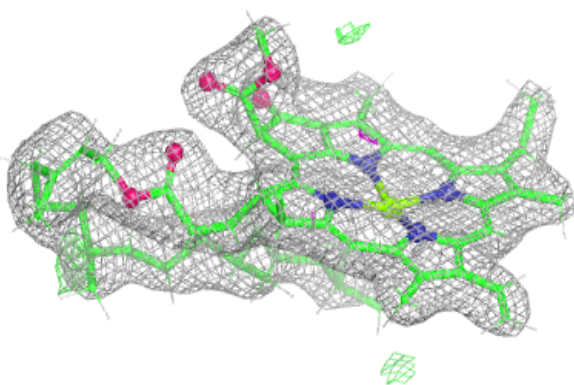
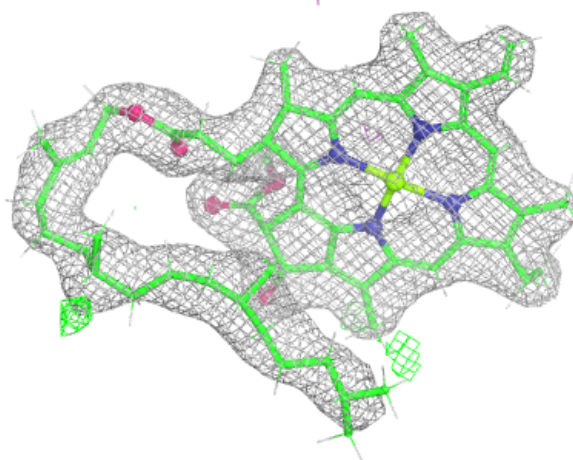
Electron density around CLA C 507:

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



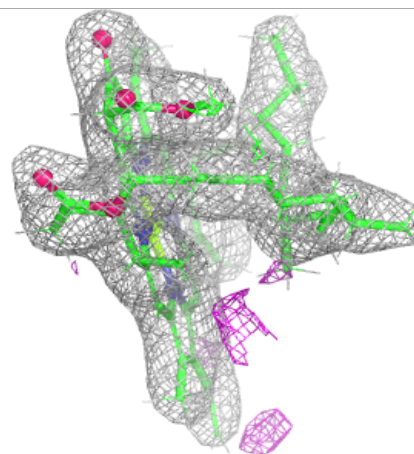
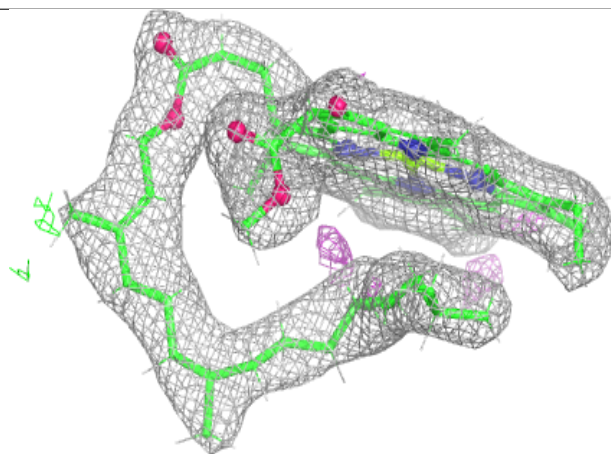
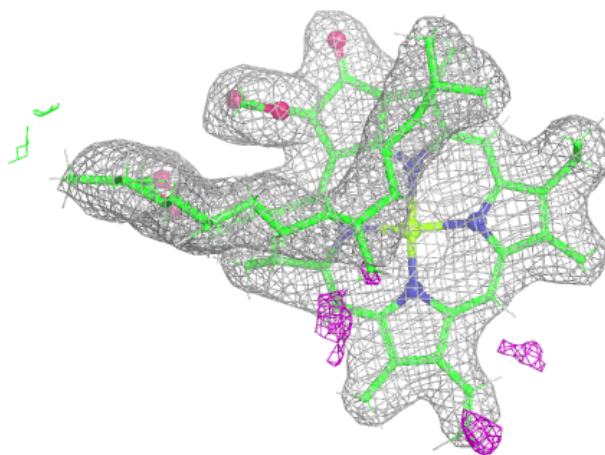
Electron density around CLA C 509:

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



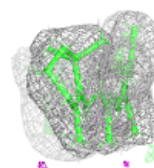
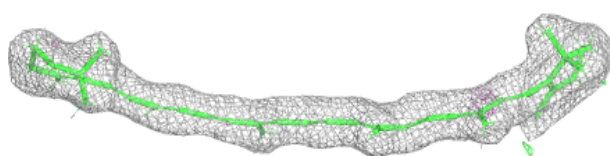
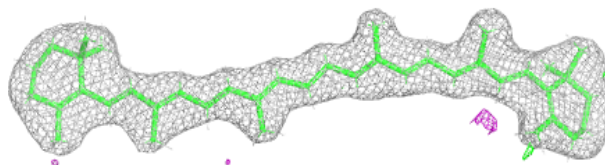
Electron density around CLA C 510:

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

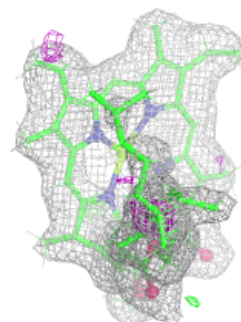
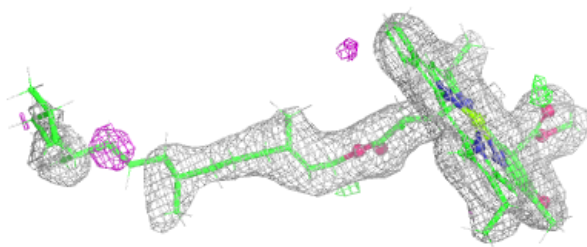
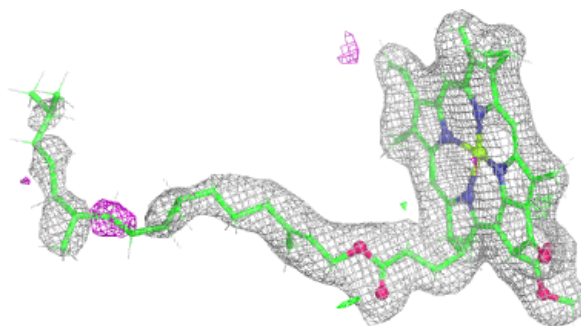


Electron density around BCR t 101:

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

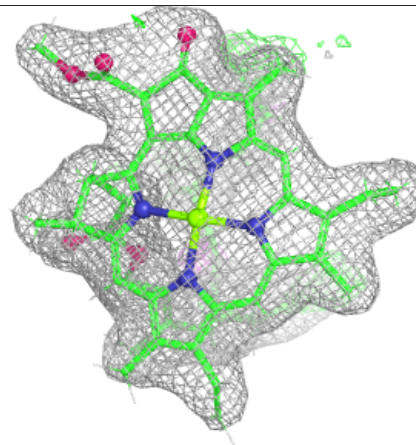
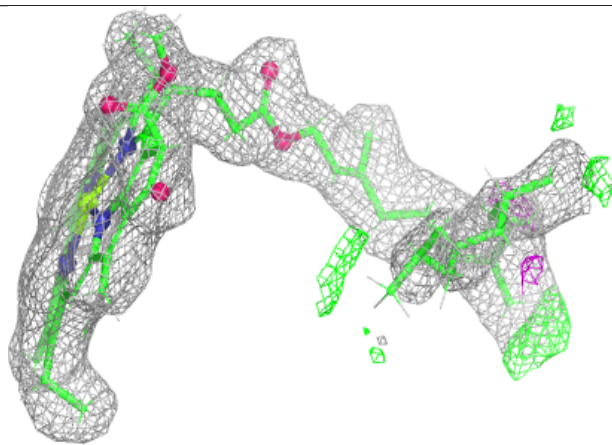
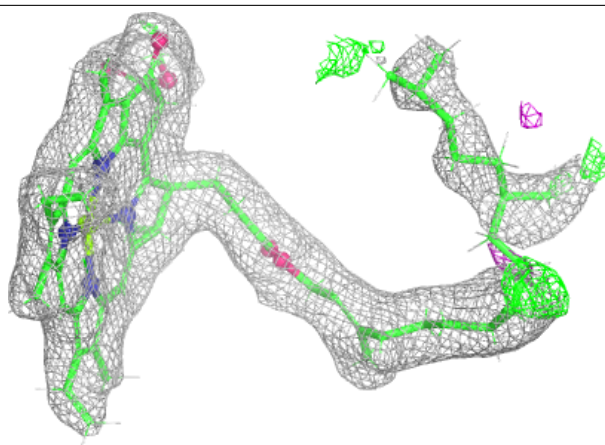
**Electron density around CLA d 404:**

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

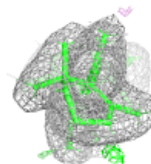
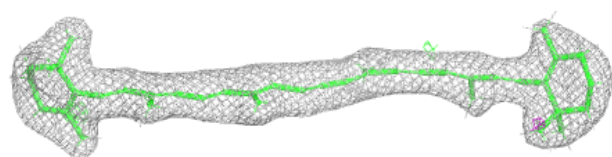
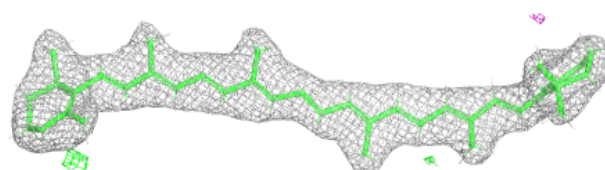


Electron density around CLA B 606:

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

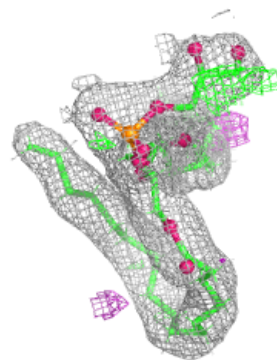
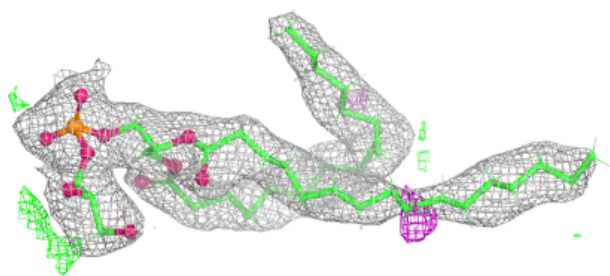
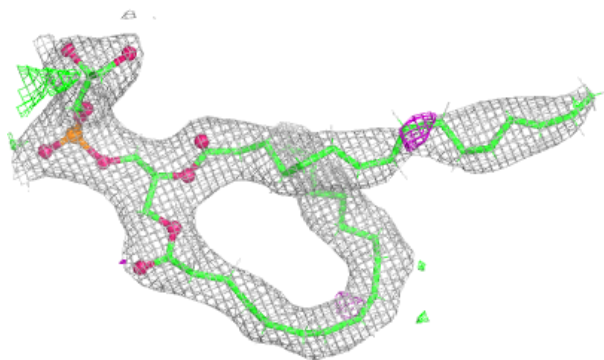
**Electron density around BCR A 406:**

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

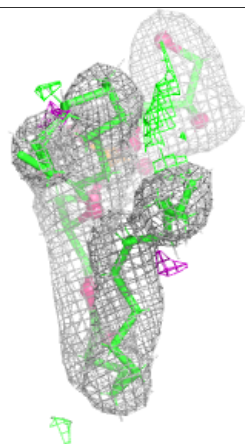
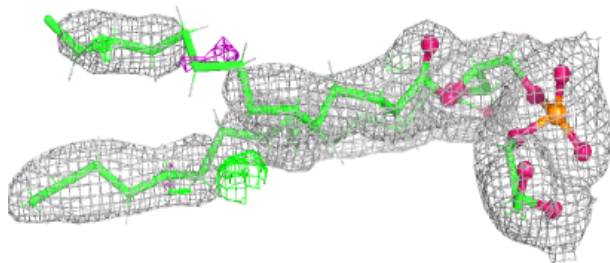
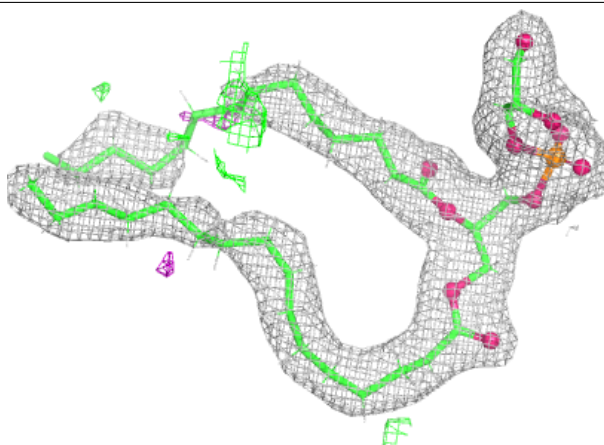


Electron density around LHG B 622:

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

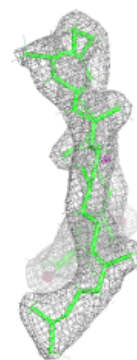
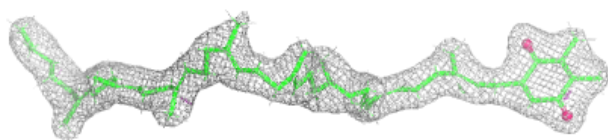
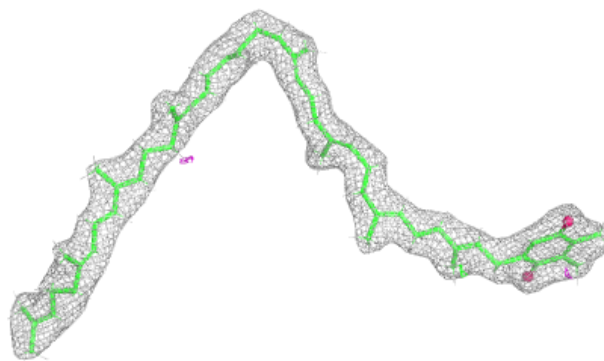
**Electron density around LHG D 409:**

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

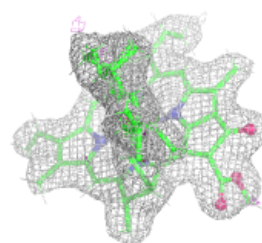
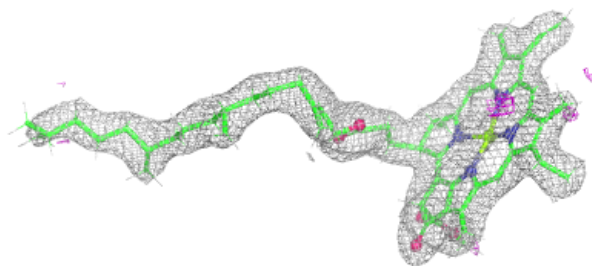
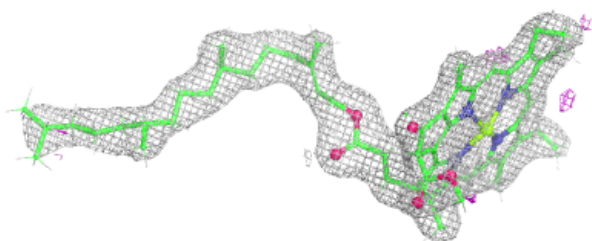


Electron density around PL9 D 405:

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

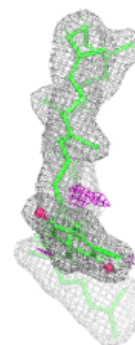
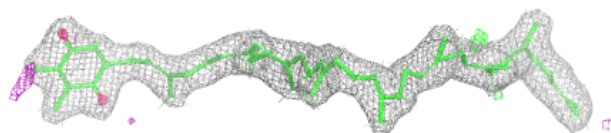
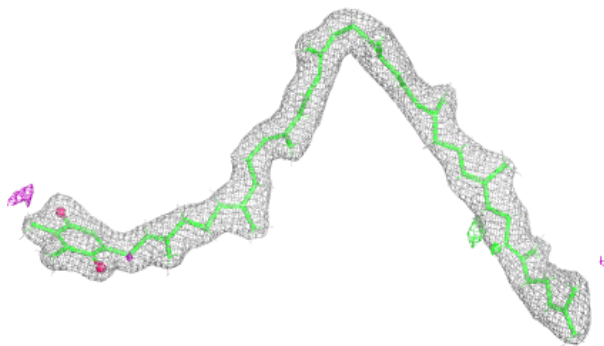
**Electron density around CLA C 502:**

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



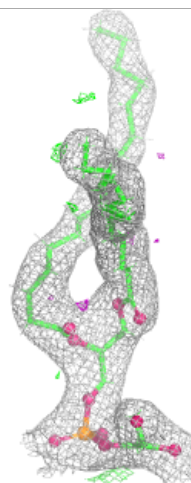
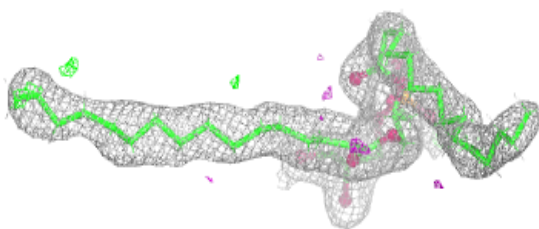
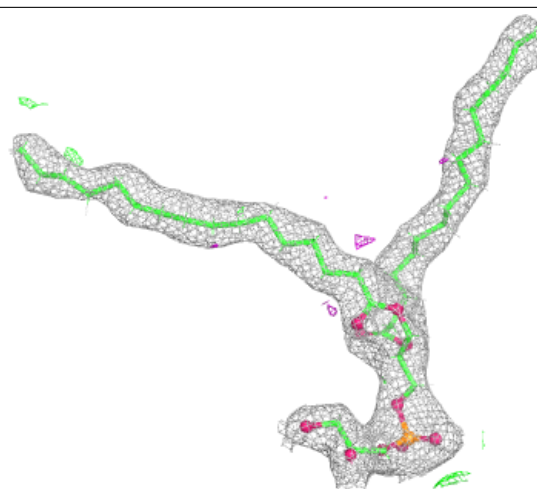
Electron density around PL9 d 406:

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



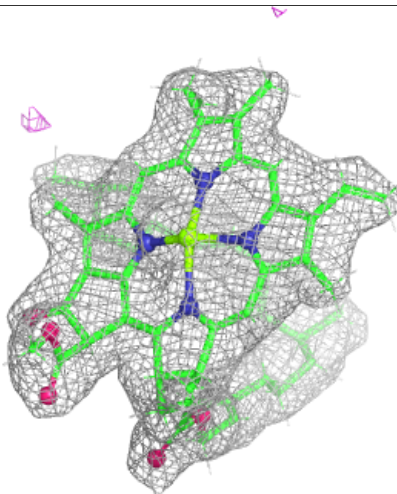
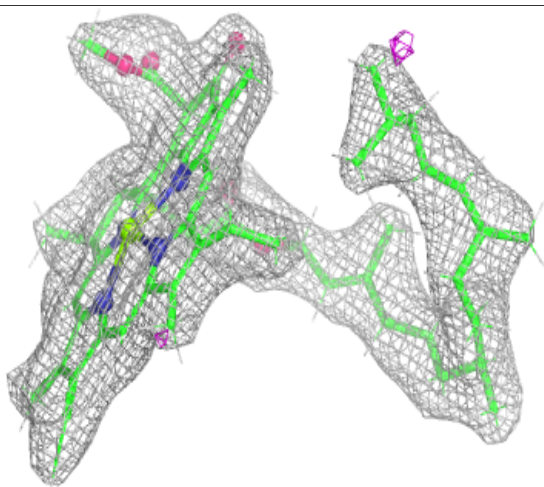
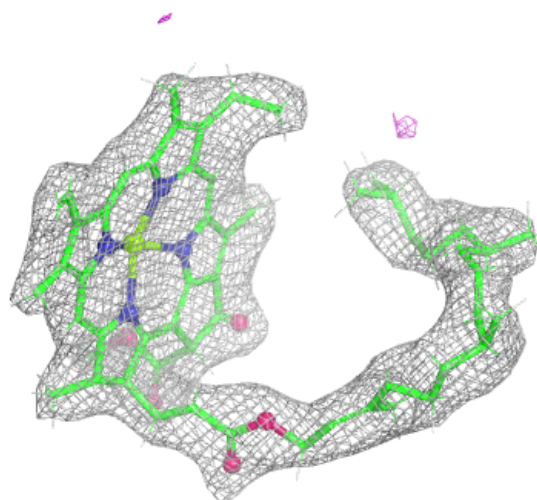
Electron density around LHG 1 101:

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



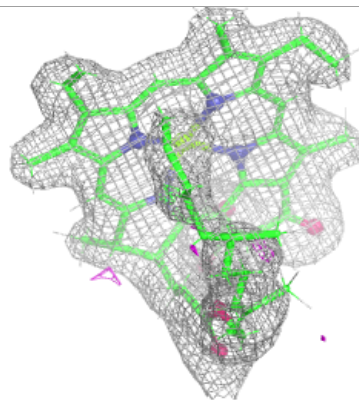
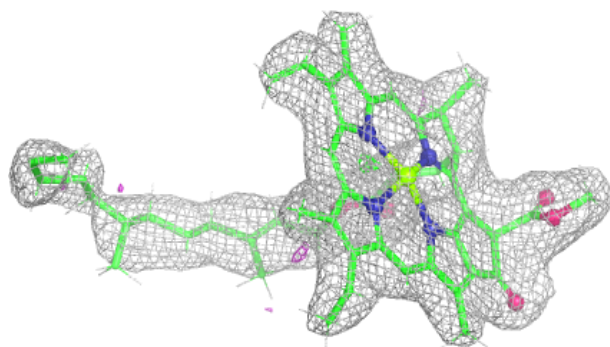
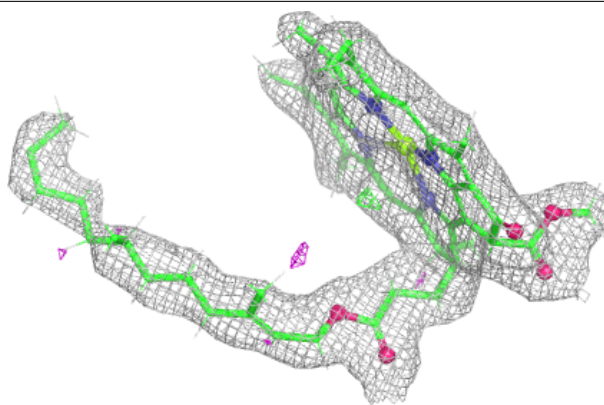
Electron density around CLA C 503:

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

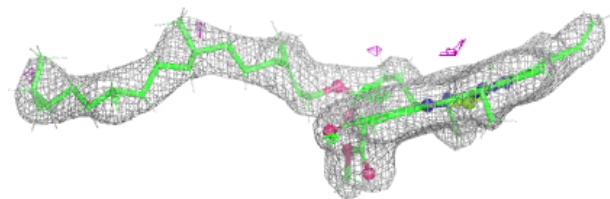
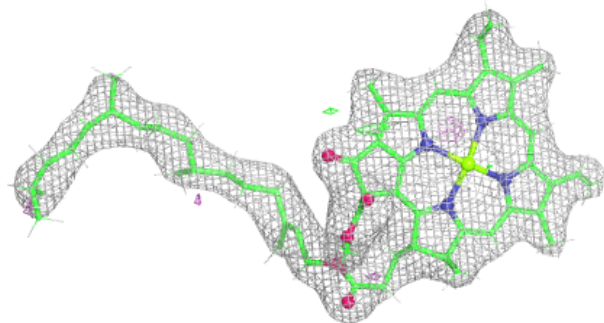


Electron density around CLA C 504:

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

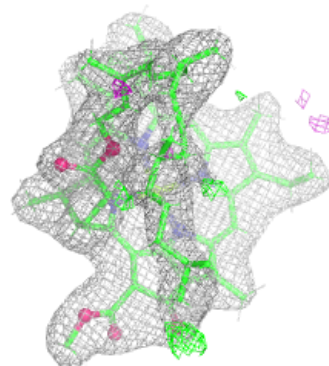
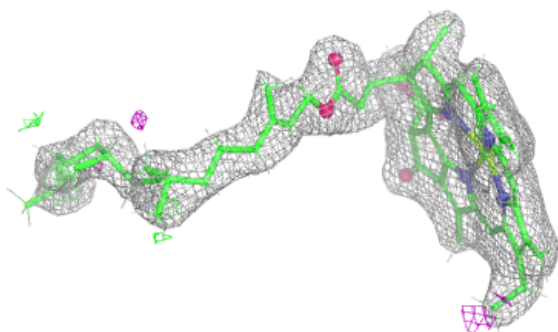
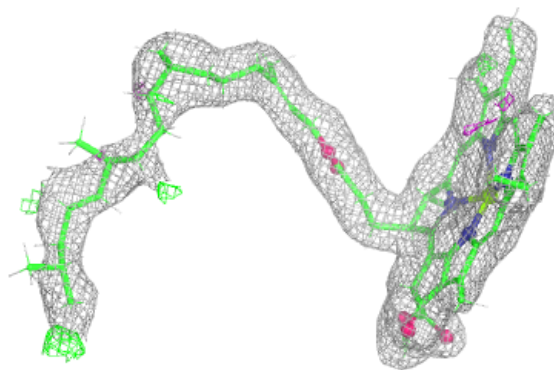
**Electron density around CLA b 602:**

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

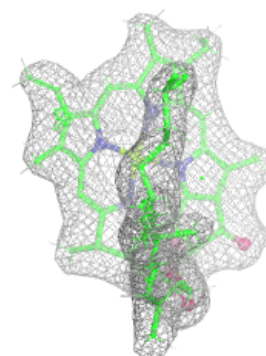
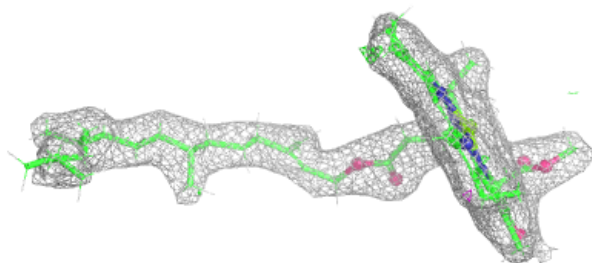
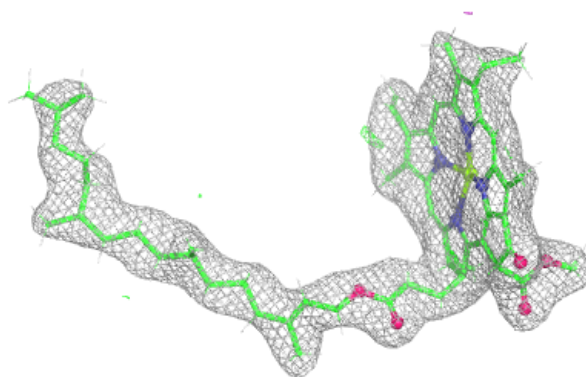


Electron density around CLA b 606:

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

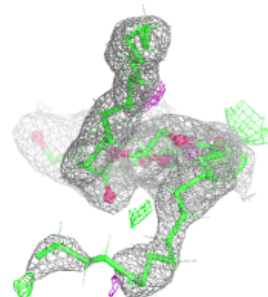
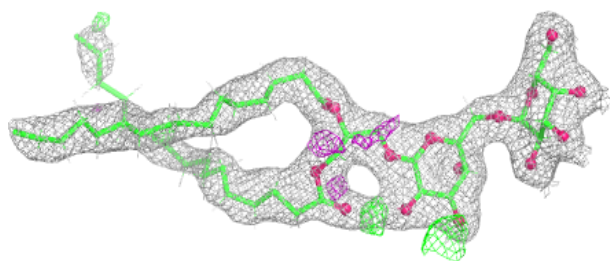
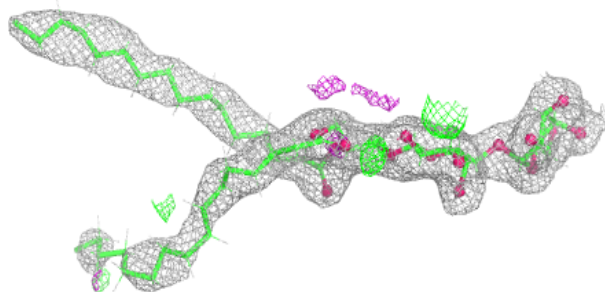
**Electron density around CLA b 609:**

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

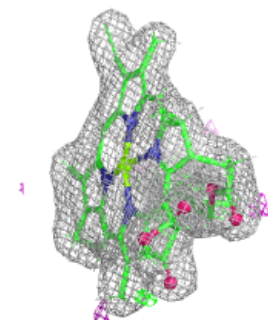
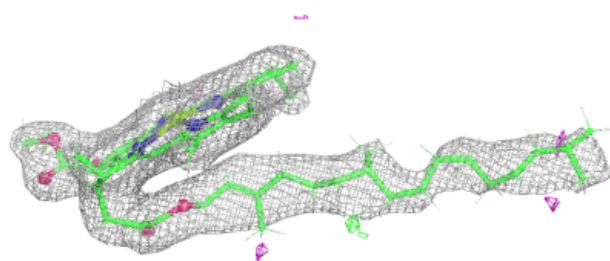
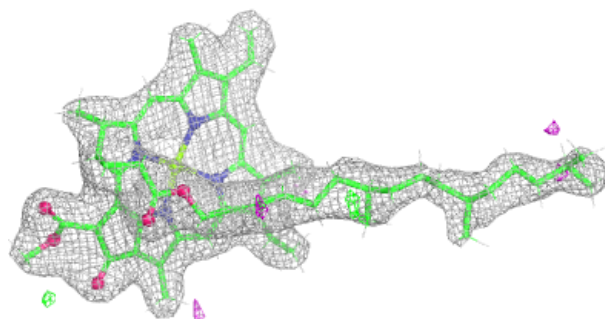


Electron density around DGD c 516:

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

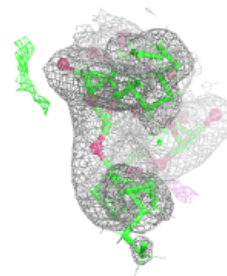
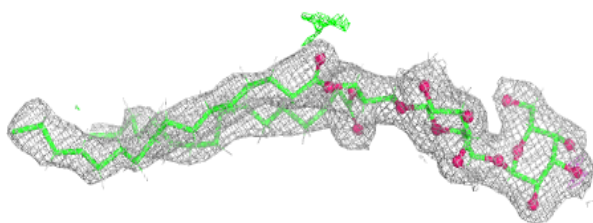
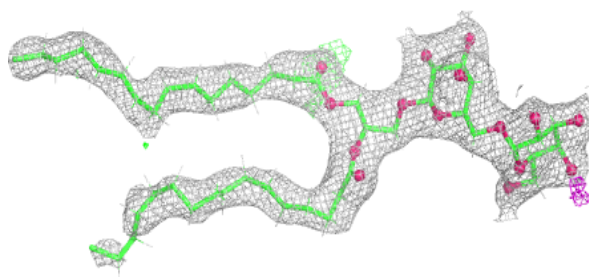
**Electron density around CLA b 614:**

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



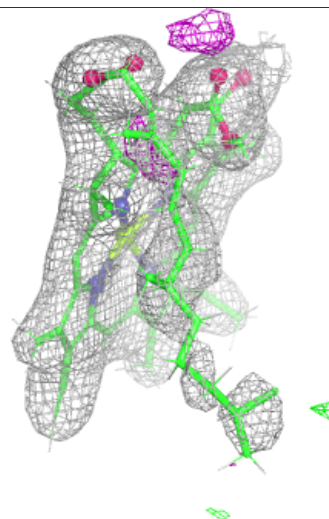
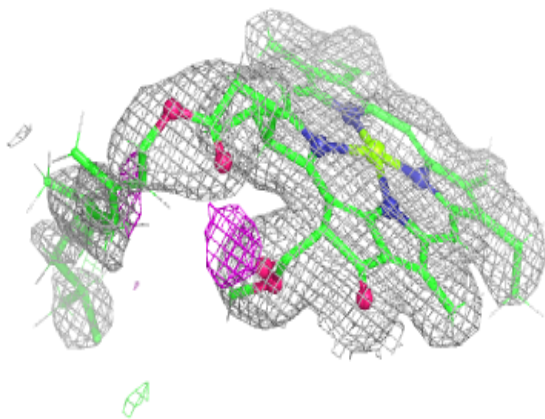
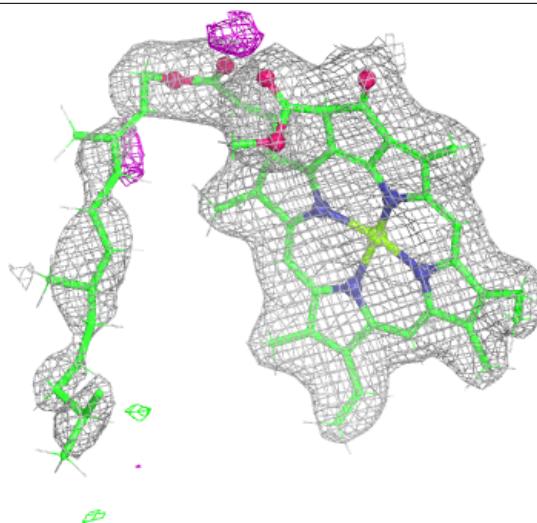
Electron density around DGD c 518:

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



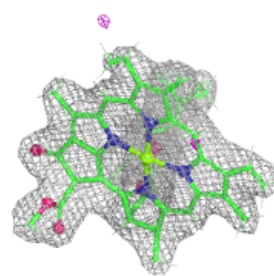
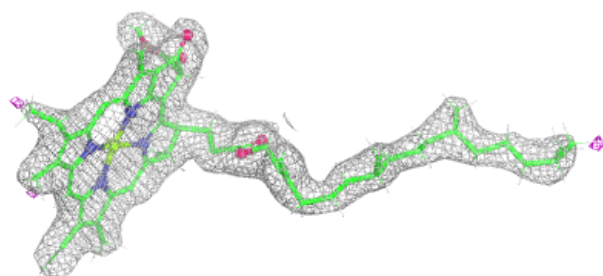
Electron density around CLA b 616:

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



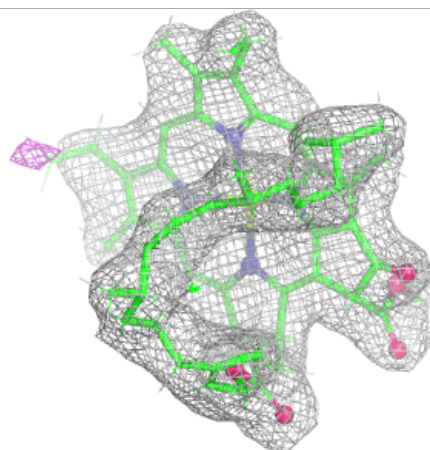
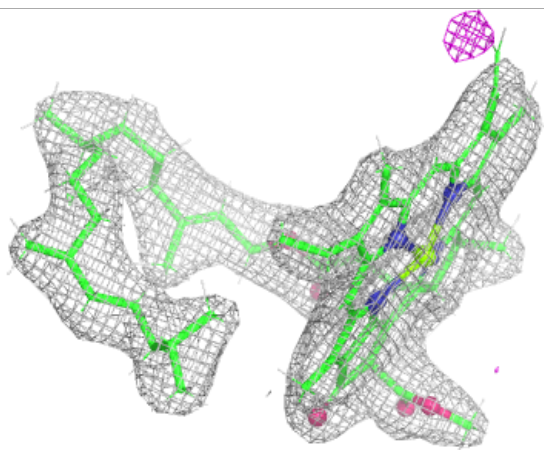
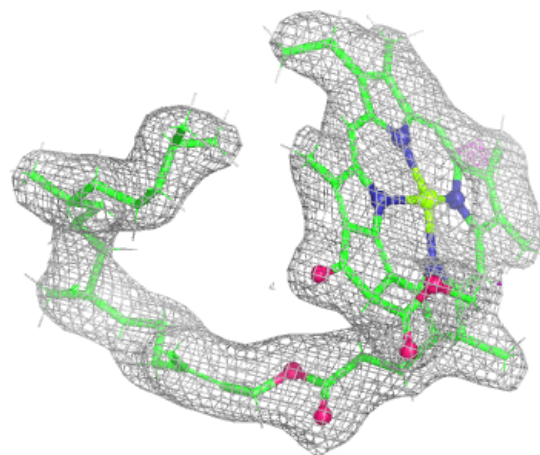
Electron density around CLA c 502:

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

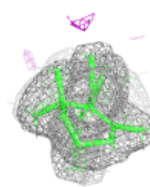
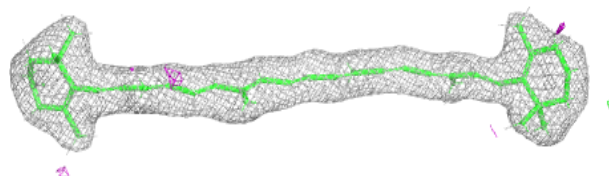
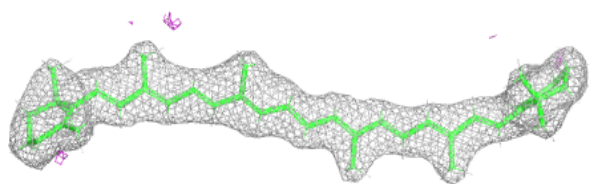


Electron density around CLA c 503:

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

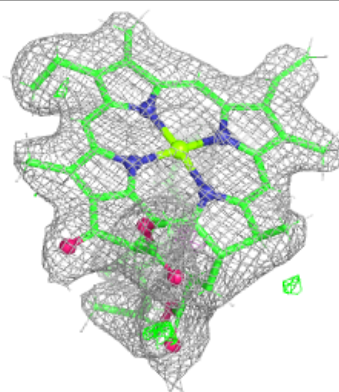
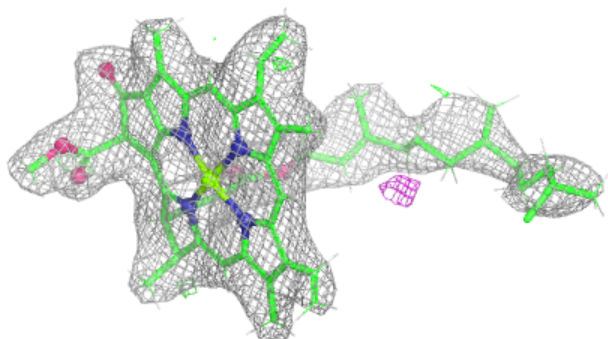
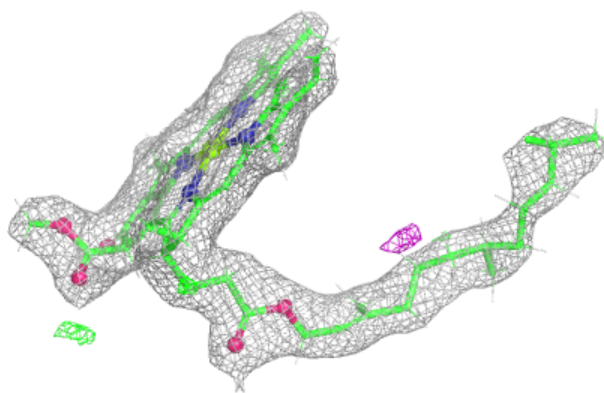
**Electron density around BCR a 405:**

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

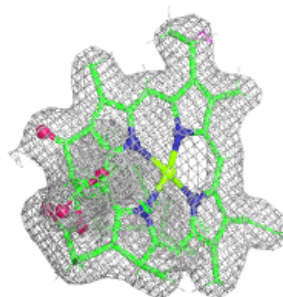
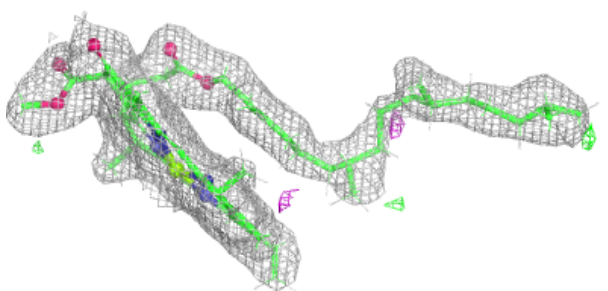
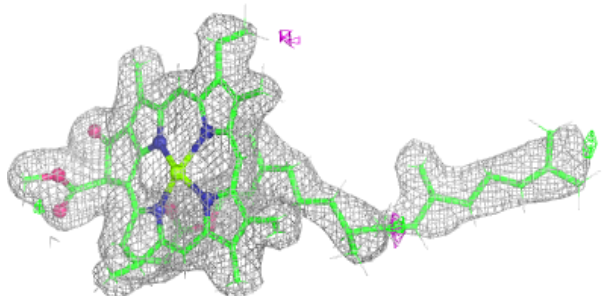


Electron density around CLA c 504:

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

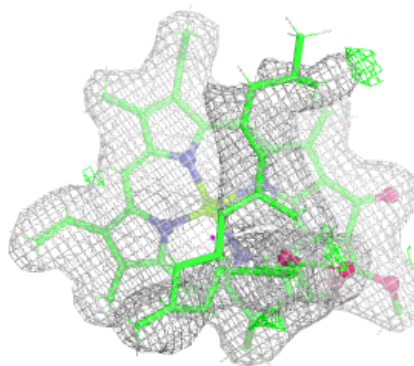
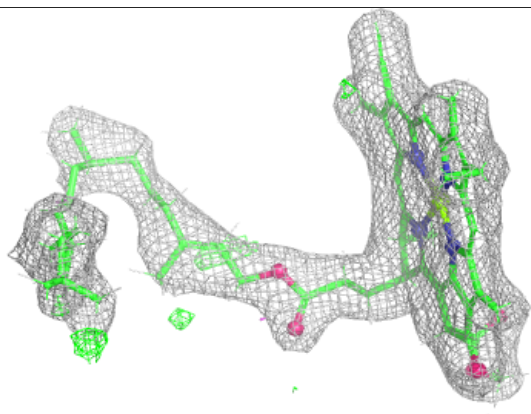
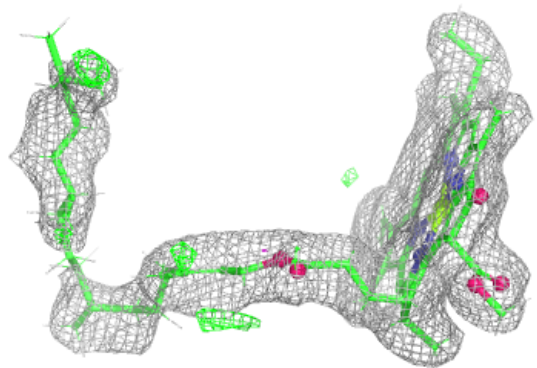
**Electron density around CLA c 505:**

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



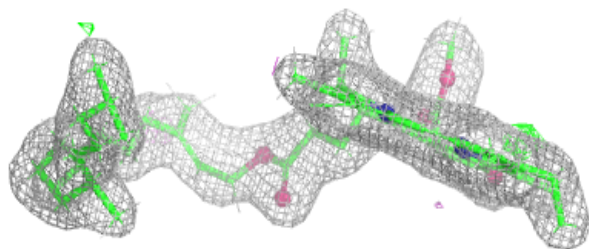
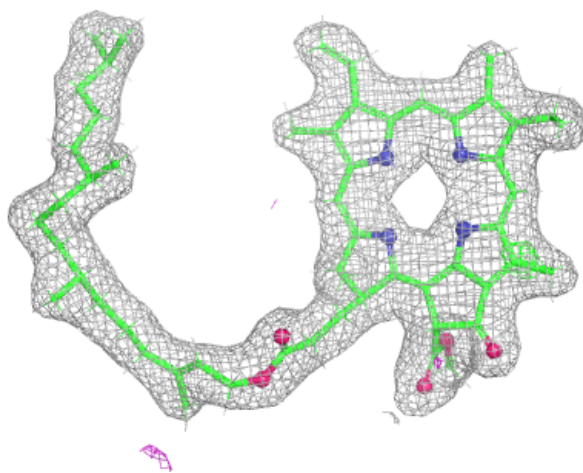
Electron density around CLA a 404:

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



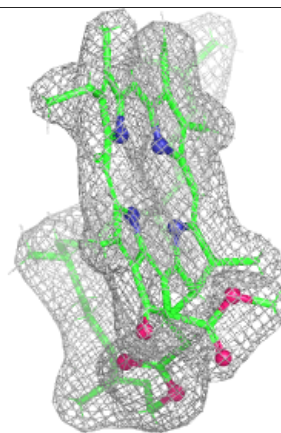
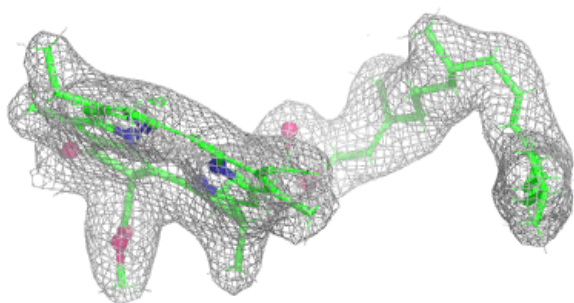
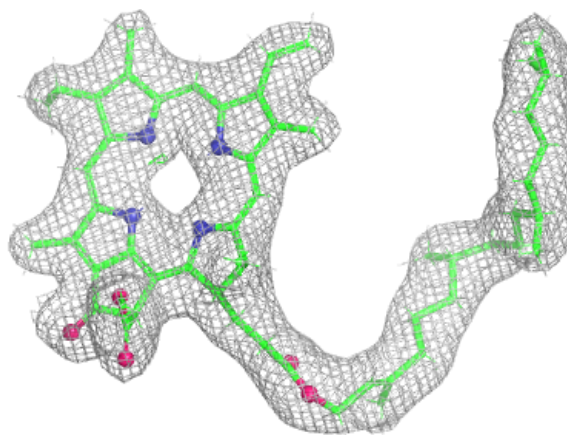
Electron density around PHO A 404:

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



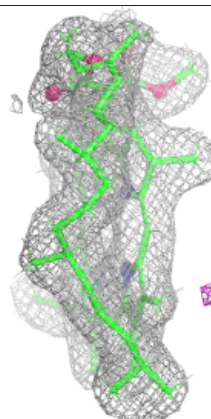
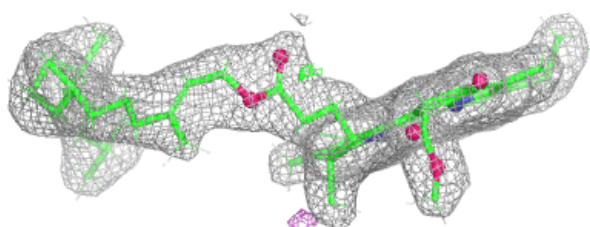
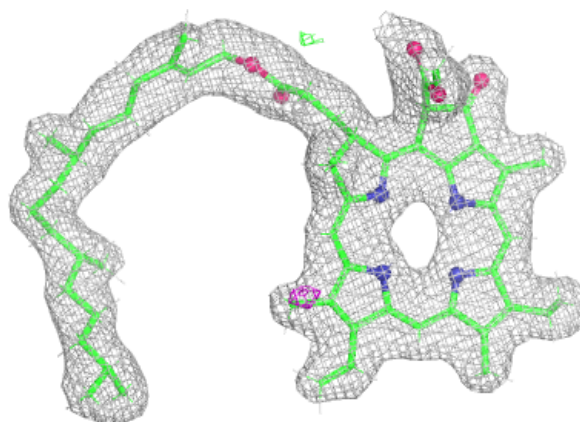
Electron density around PHO D 401:

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

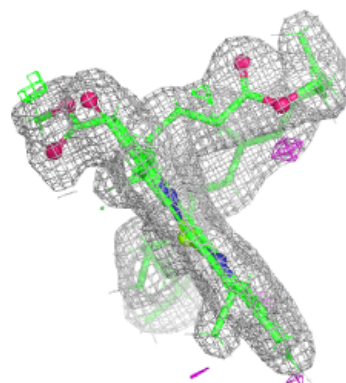
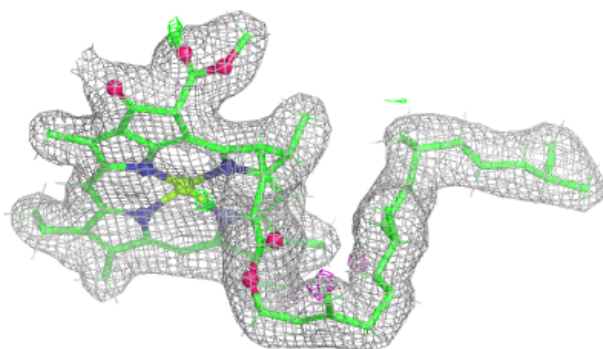
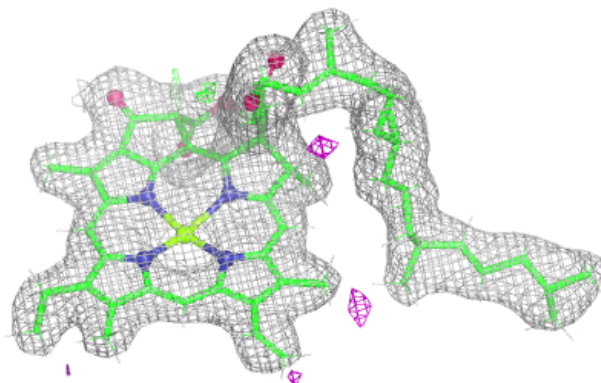


Electron density around PHO d 401:

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

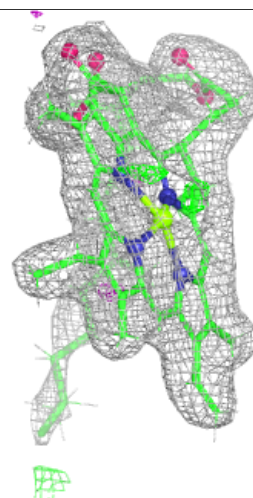
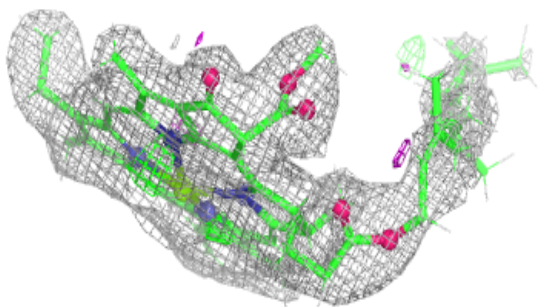
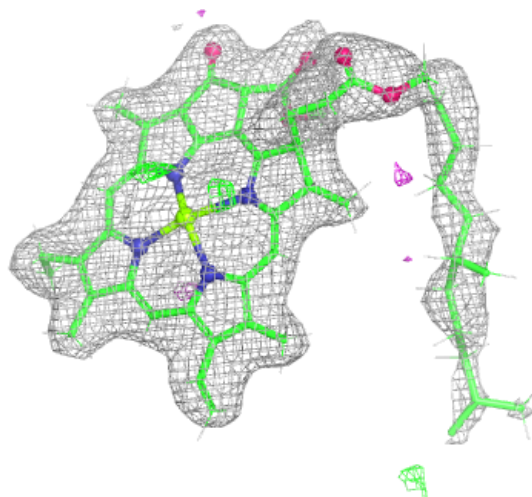
**Electron density around CLA a 410:**

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



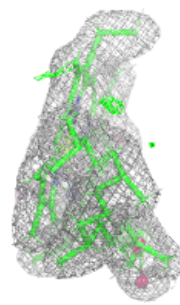
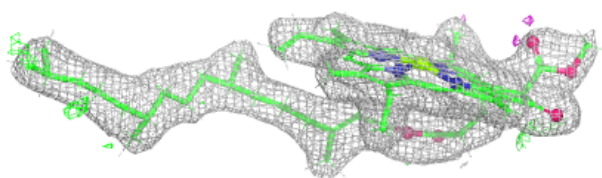
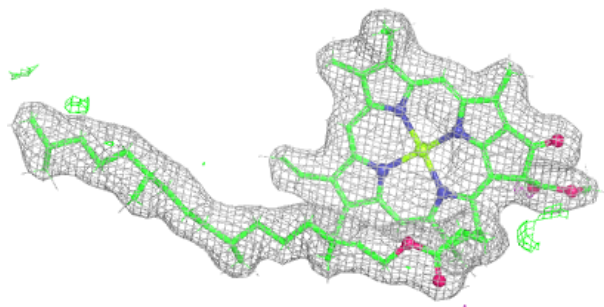
Electron density around CLA B 616:

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

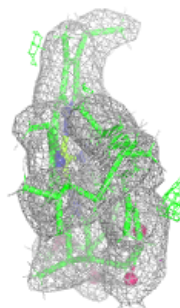
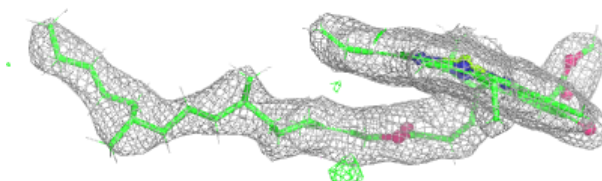
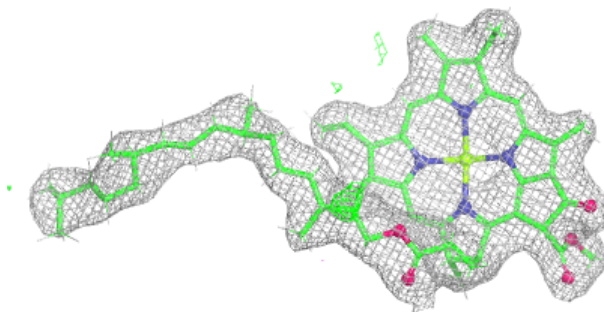


Electron density around CLA C 501:

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

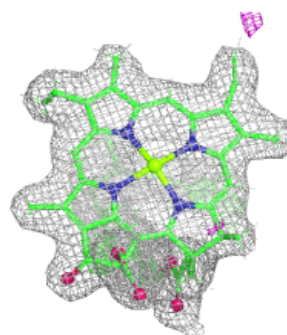
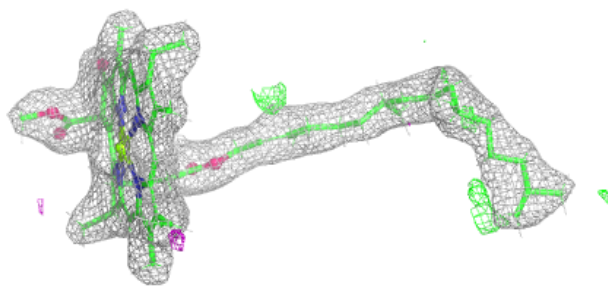
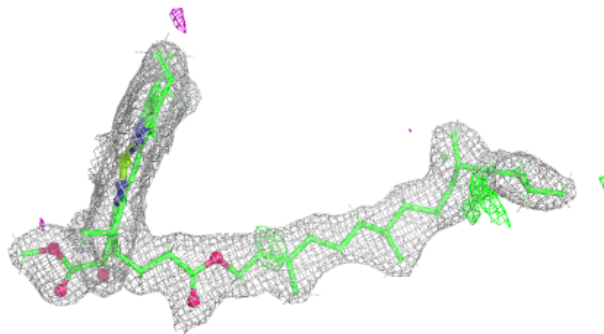
**Electron density around CLA b 603:**

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

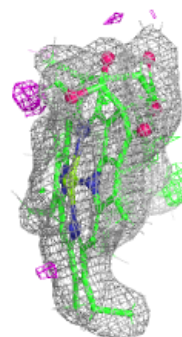
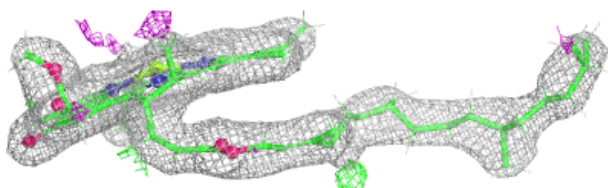
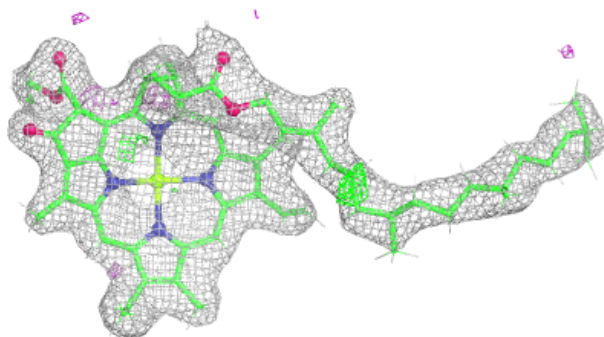


Electron density around CLA b 605:

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

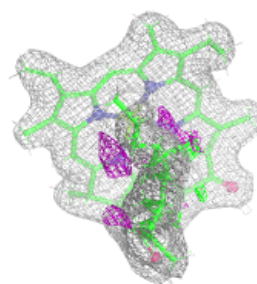
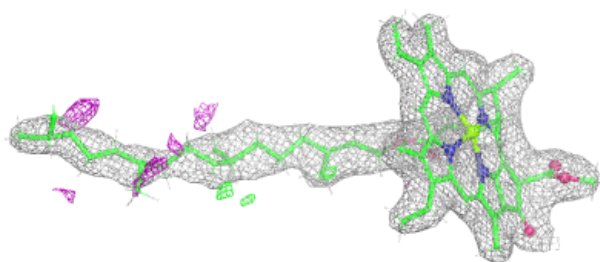
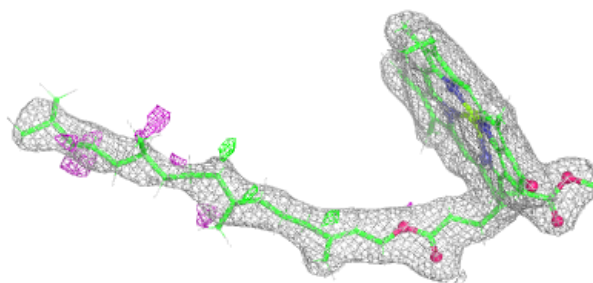
**Electron density around CLA B 603:**

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

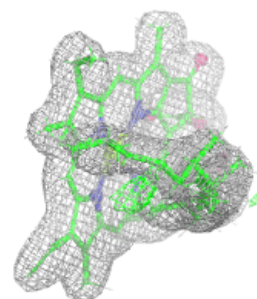
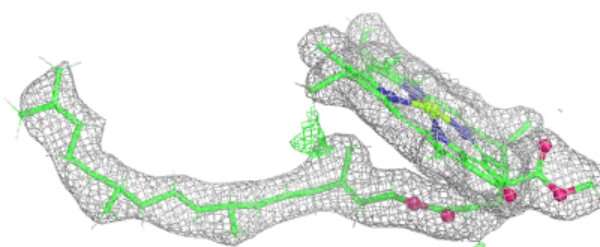
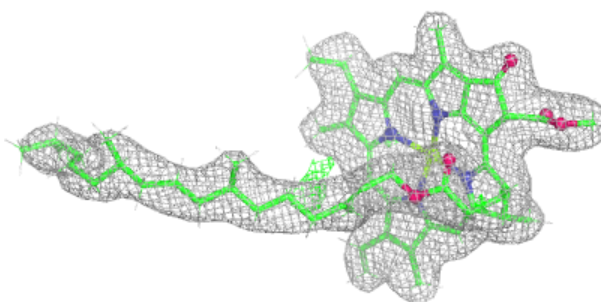


Electron density around CLA b 607:

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

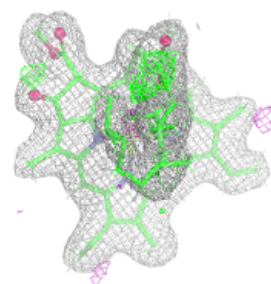
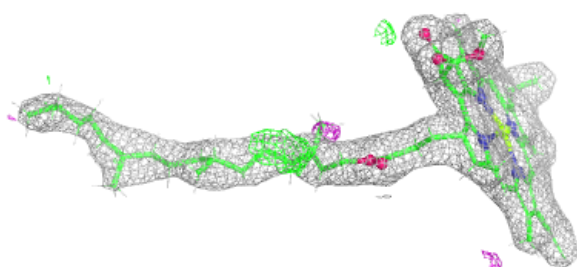
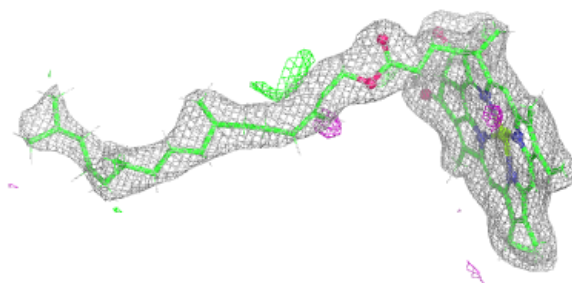
**Electron density around CLA b 608:**

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

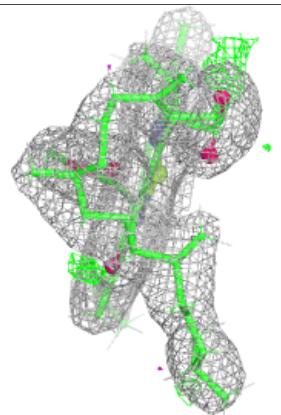
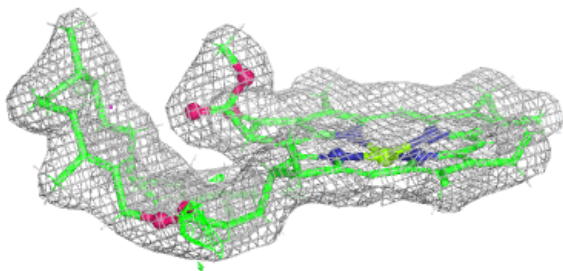
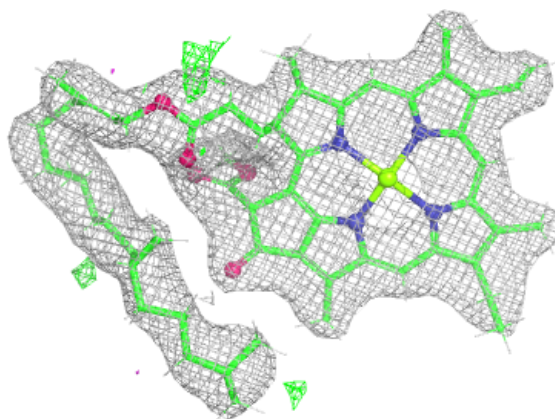


Electron density around CLA B 604:

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

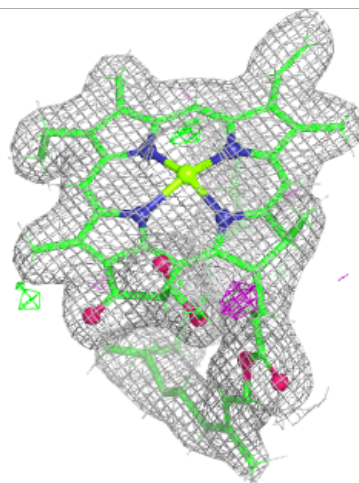
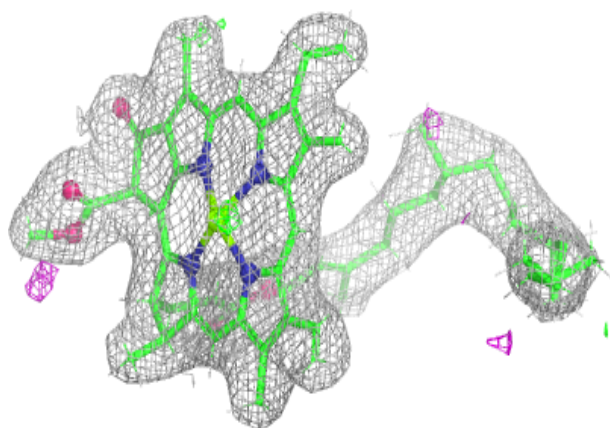
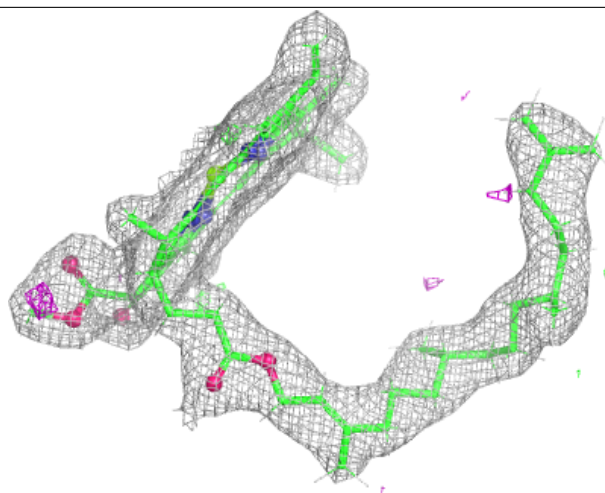
**Electron density around CLA b 610:**

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



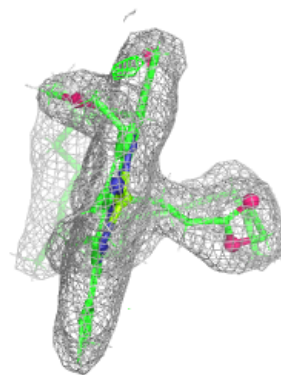
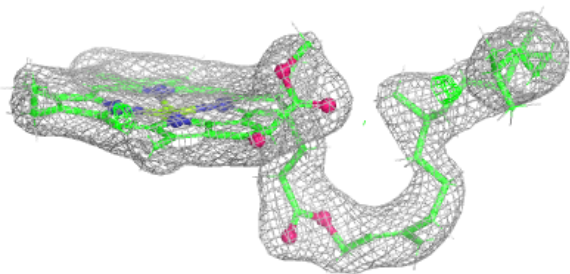
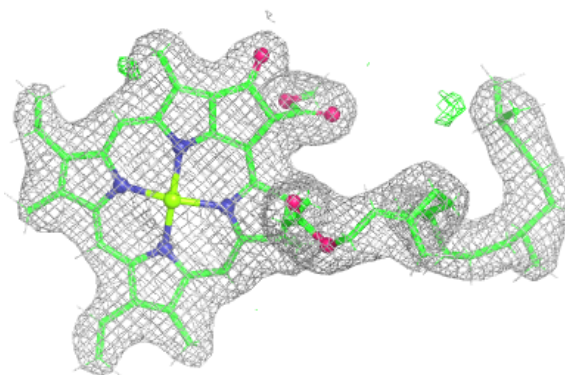
Electron density around CLA b 611:

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

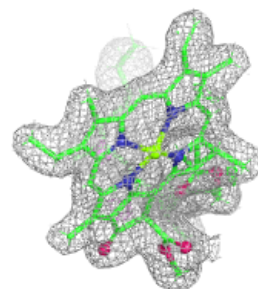
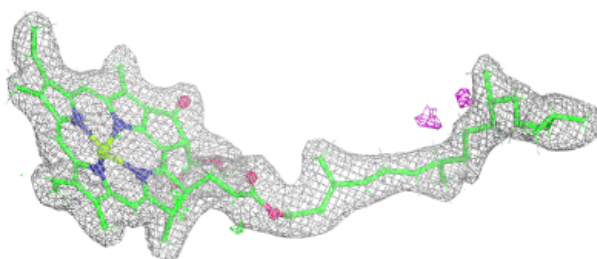
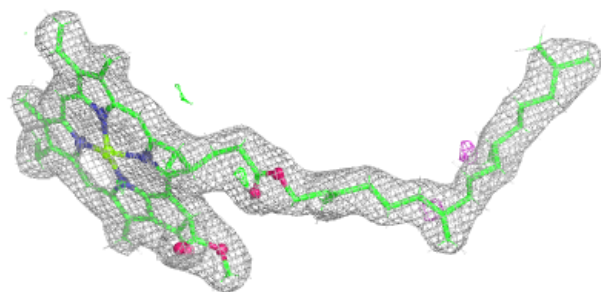


Electron density around CLA b 612:

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

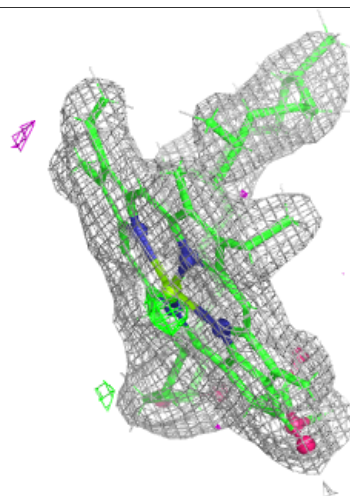
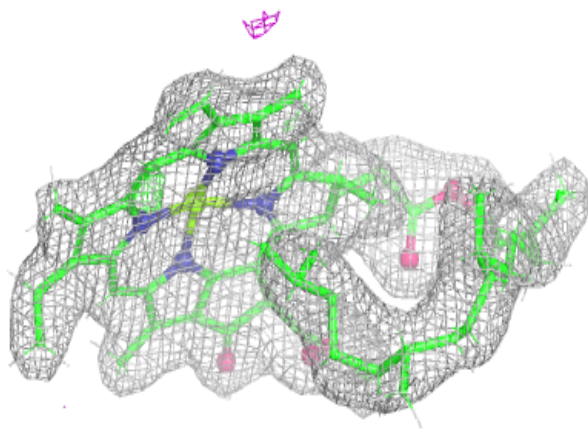
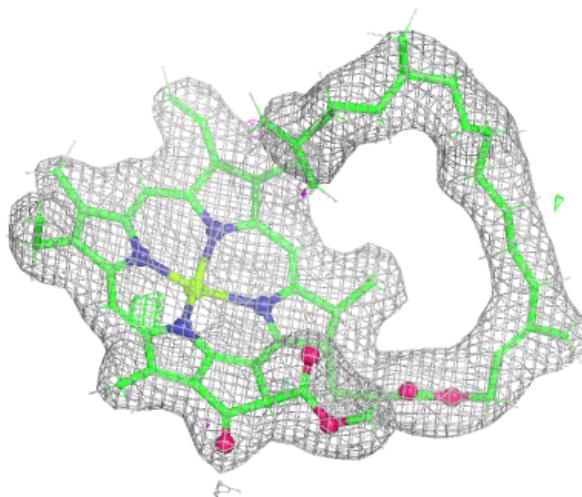
**Electron density around CLA A 402:**

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



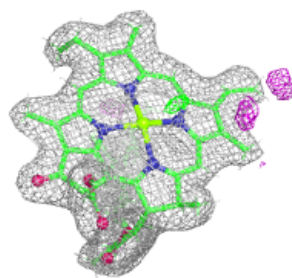
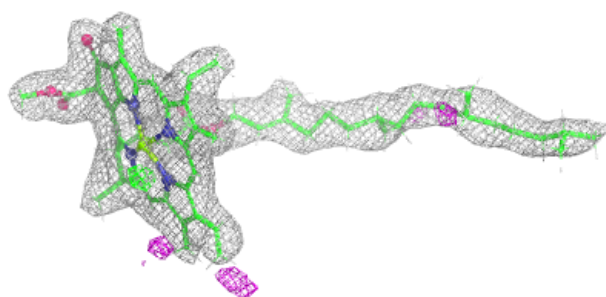
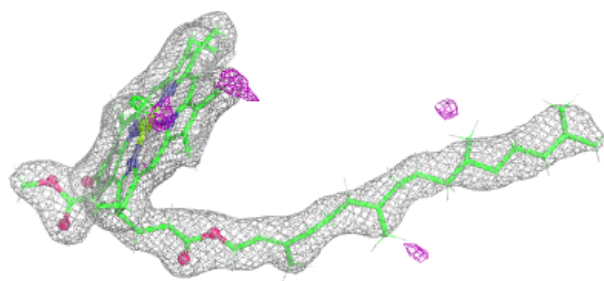
Electron density around CLA b 615:

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

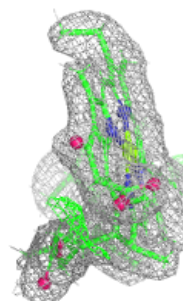
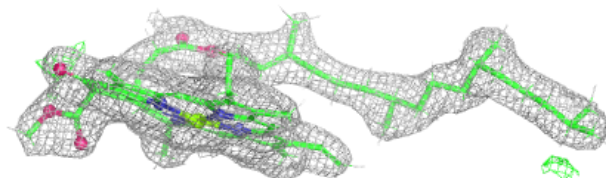
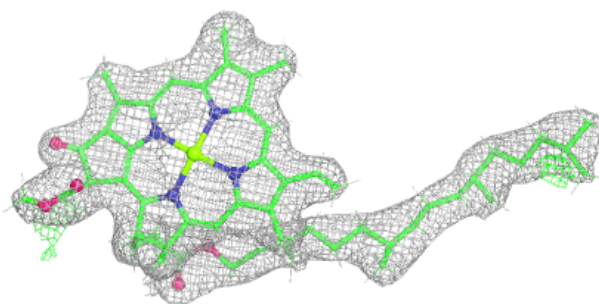


Electron density around CLA B 607:

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

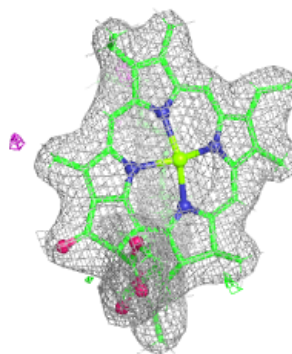
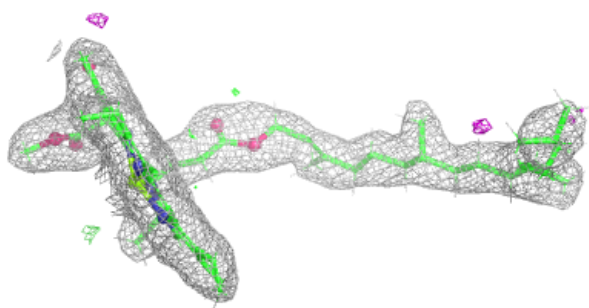
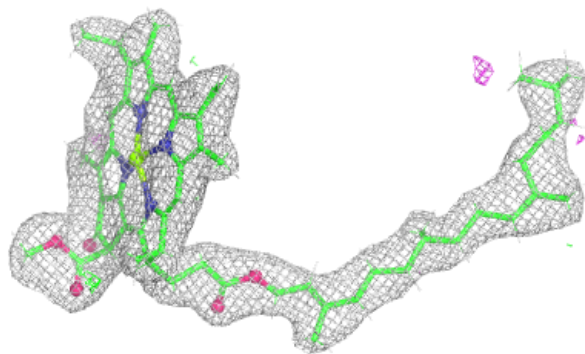
**Electron density around CLA c 501:**

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



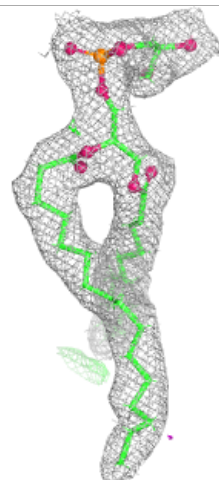
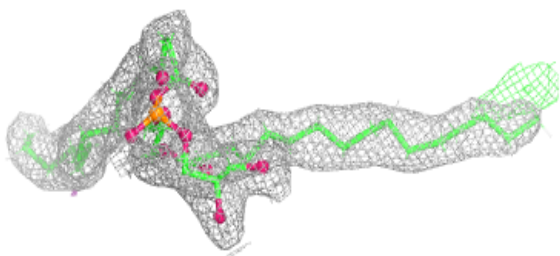
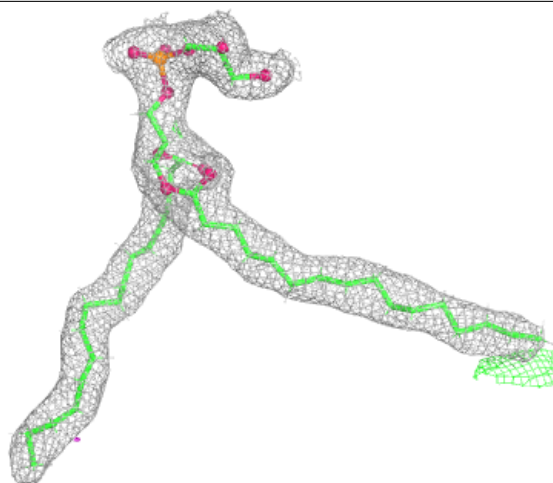
Electron density around CLA B 609:

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



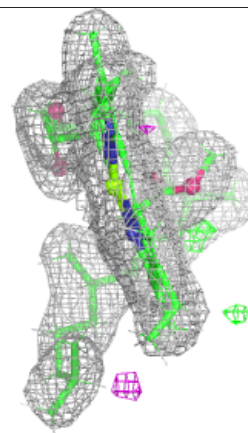
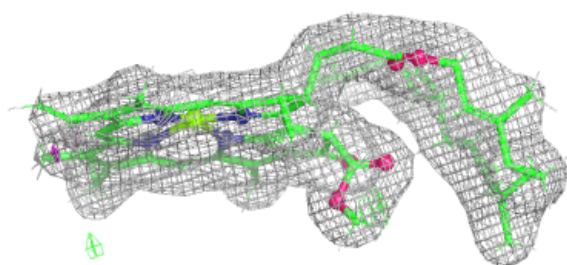
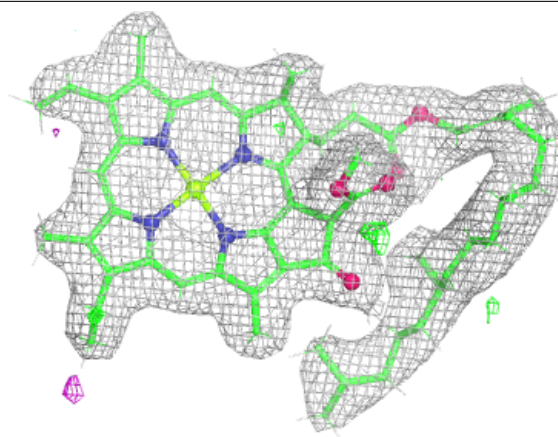
Electron density around LHG B 621:

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



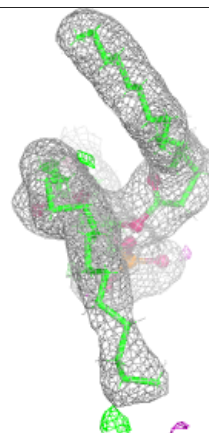
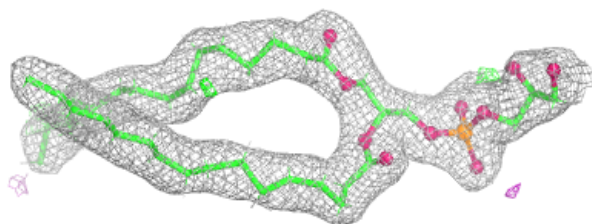
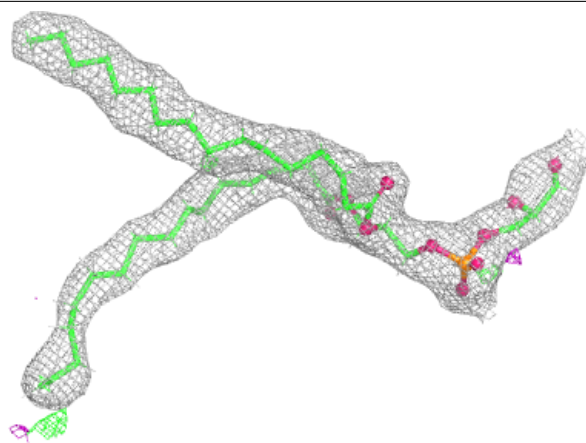
Electron density around CLA B 610:

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



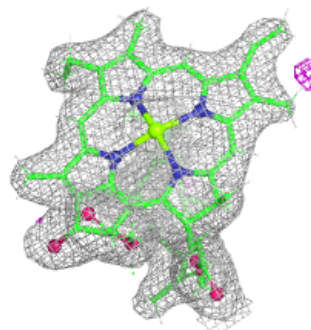
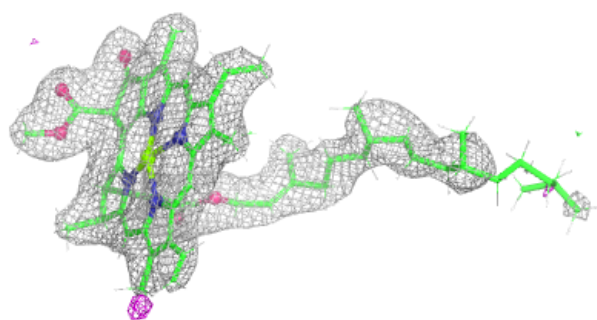
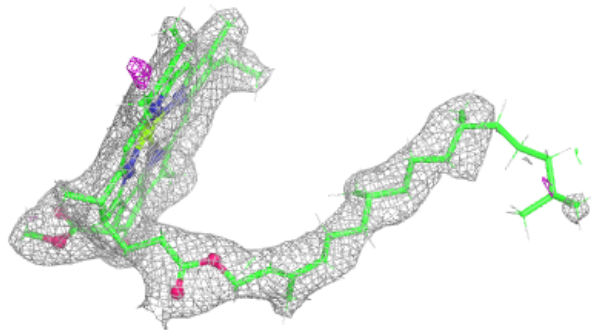
Electron density around LHG D 408:

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



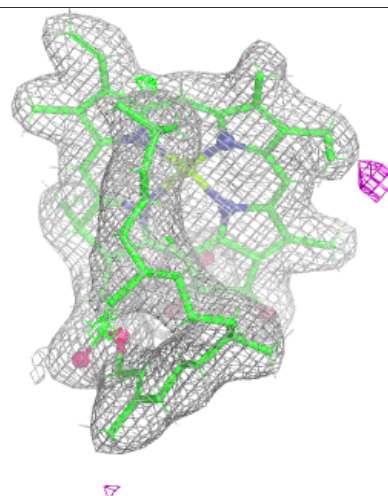
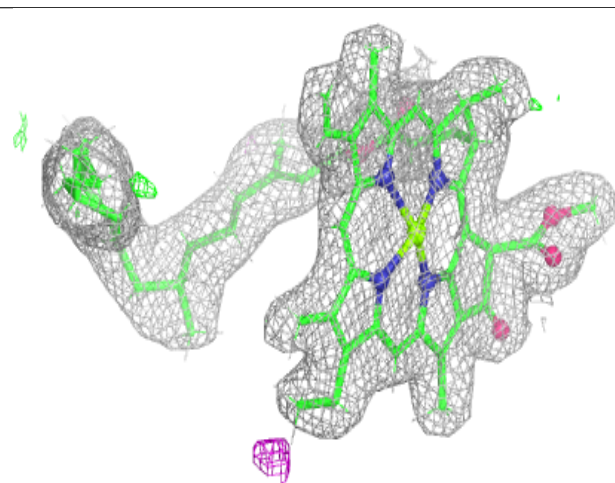
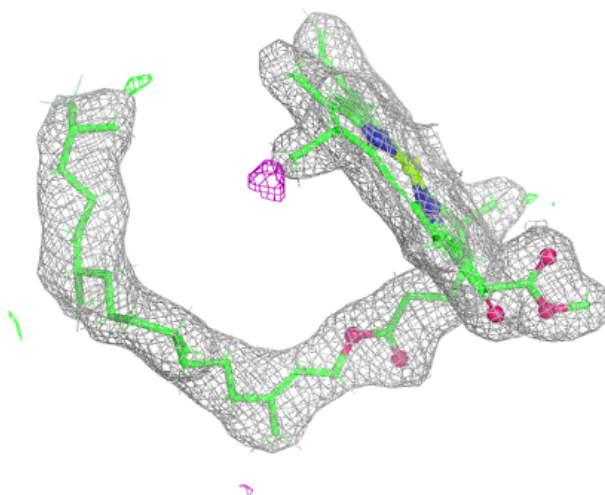
Electron density around CLA C 508:

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



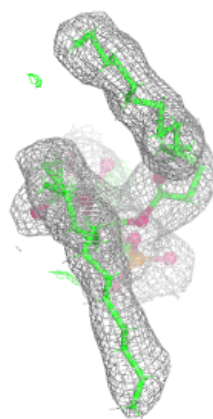
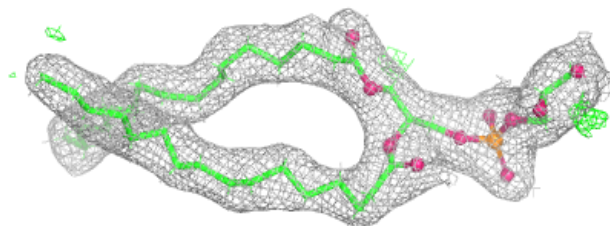
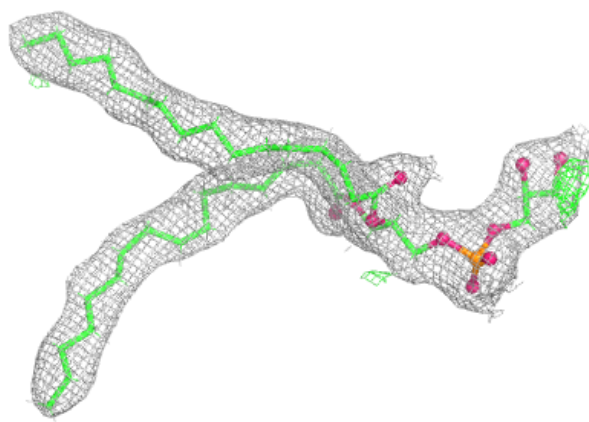
Electron density around CLA B 611:

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



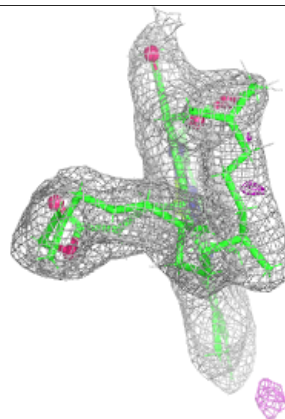
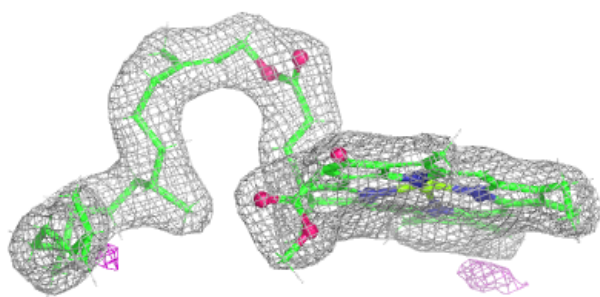
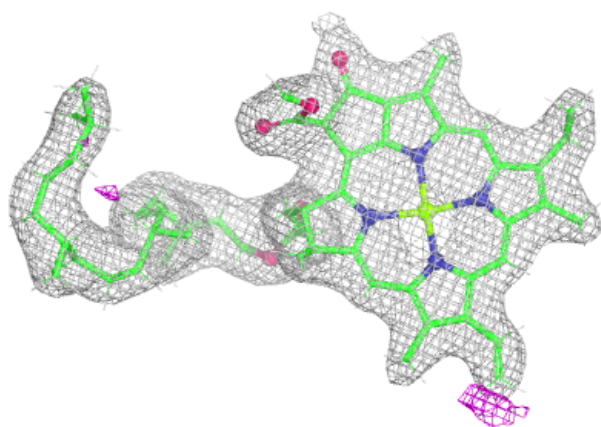
Electron density around LHG d 408:

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



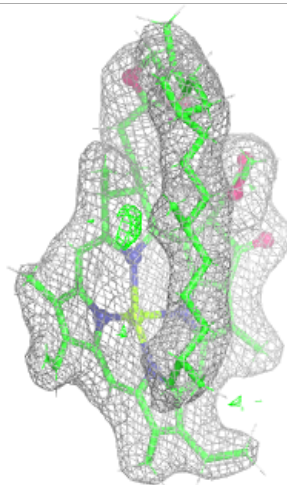
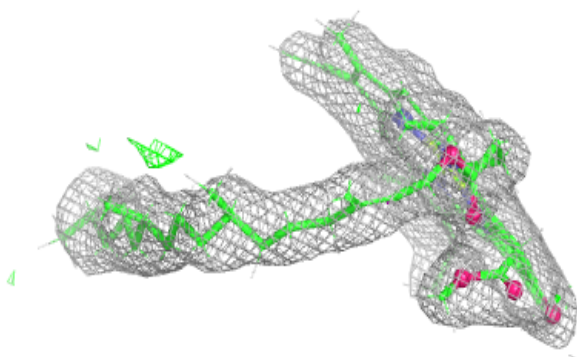
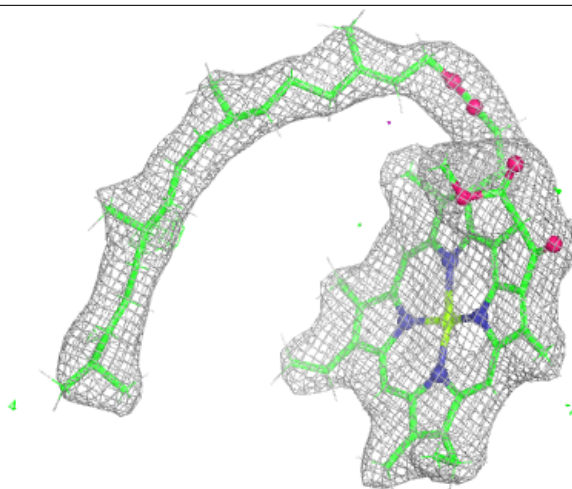
Electron density around CLA B 612:

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



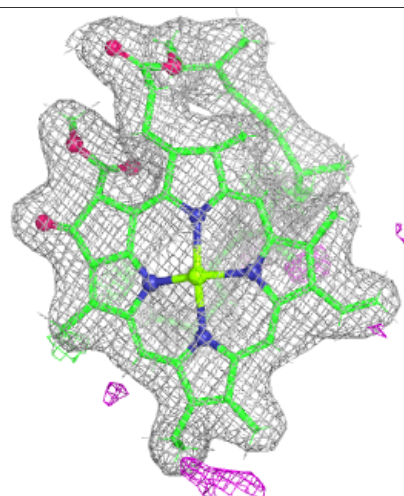
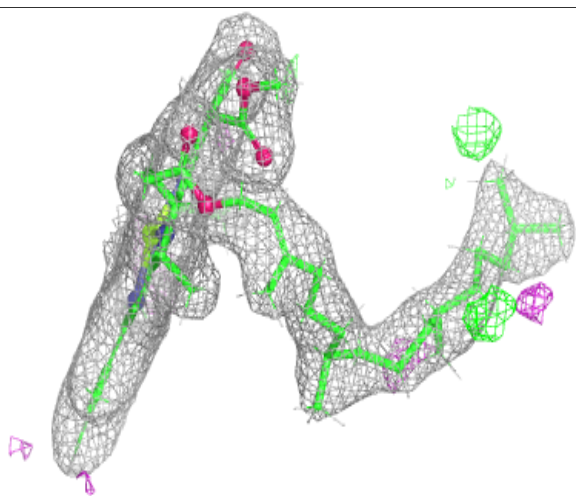
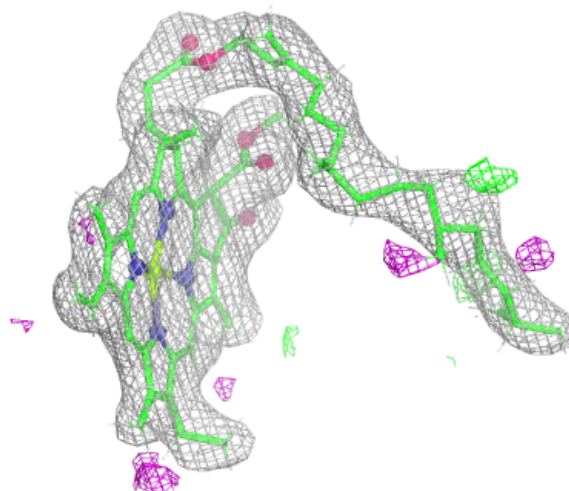
Electron density around CLA c 507:

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



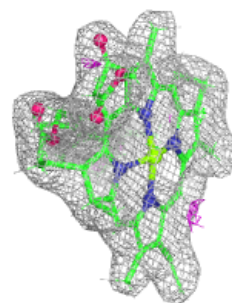
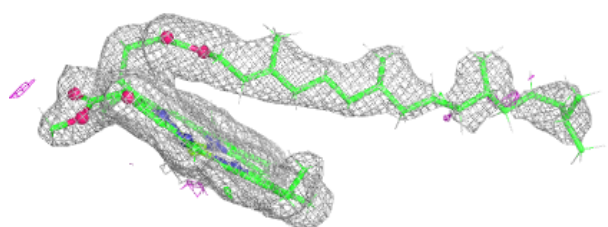
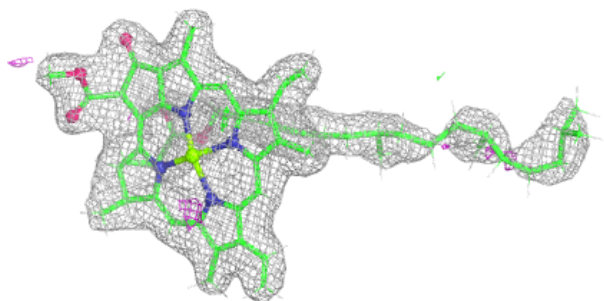
Electron density around CLA B 613:

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



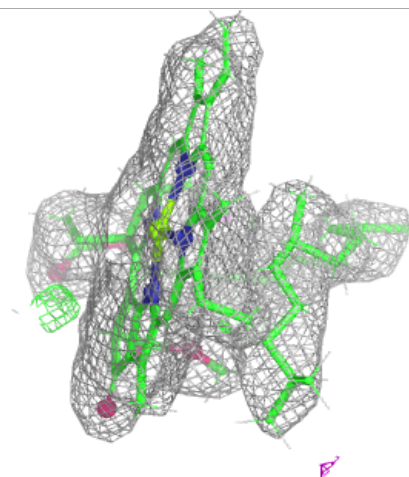
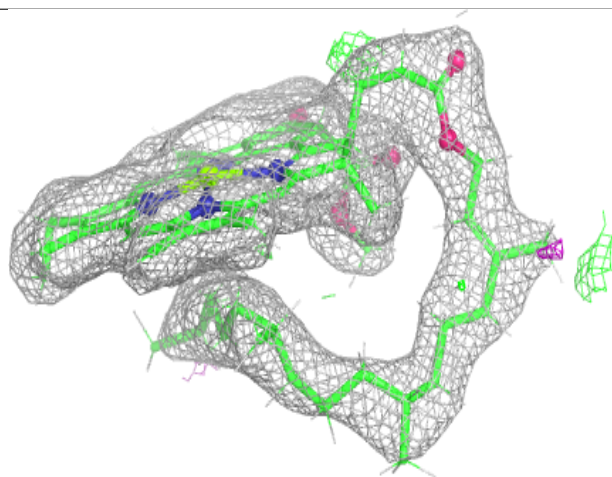
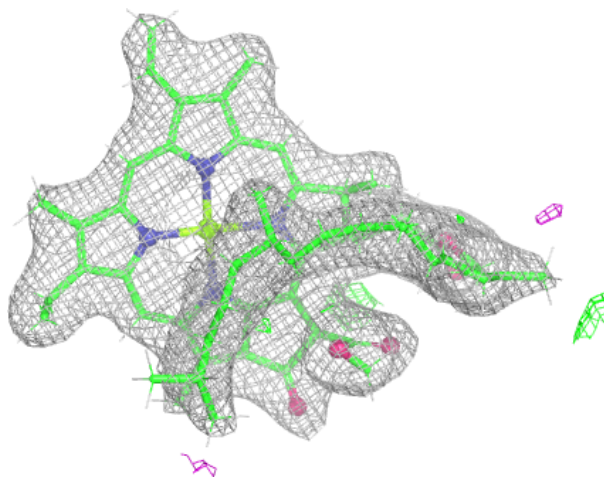
Electron density around CLA B 614:

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



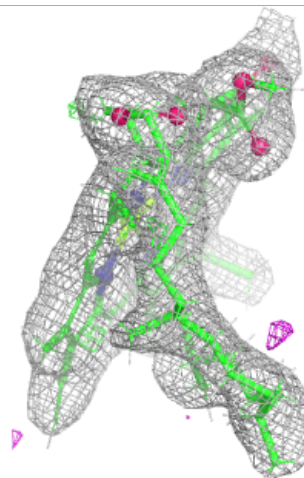
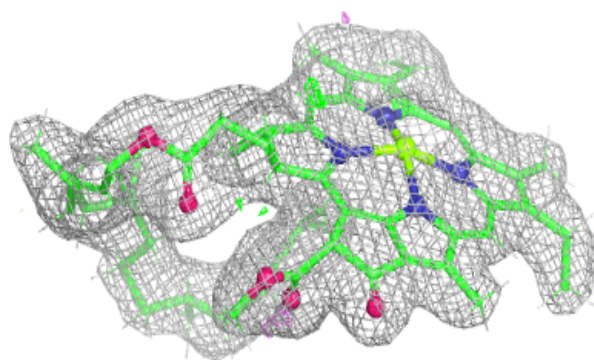
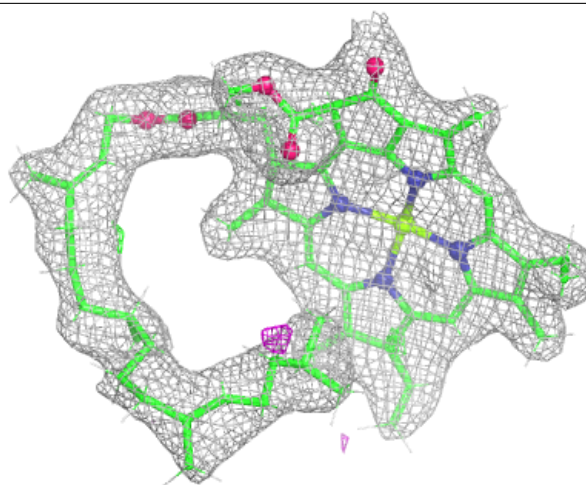
Electron density around CLA c 510:

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



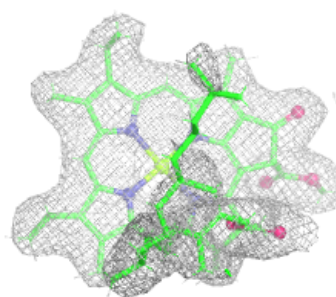
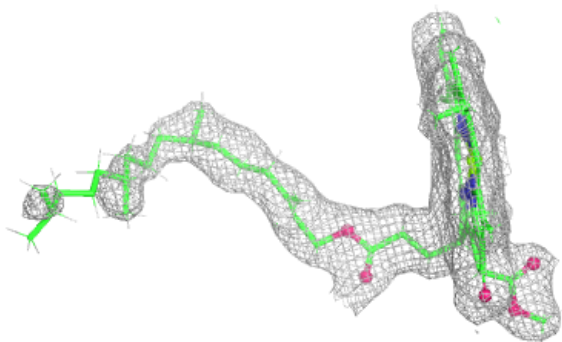
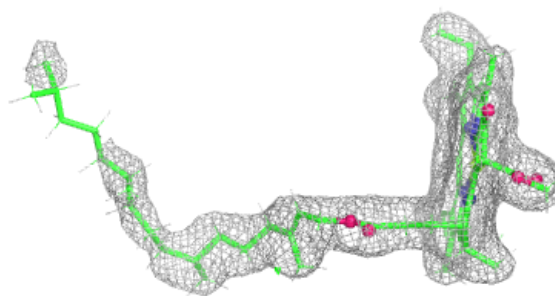
Electron density around CLA B 615:

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

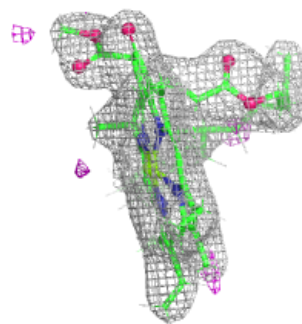
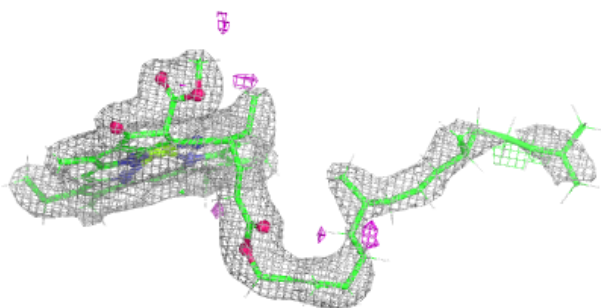
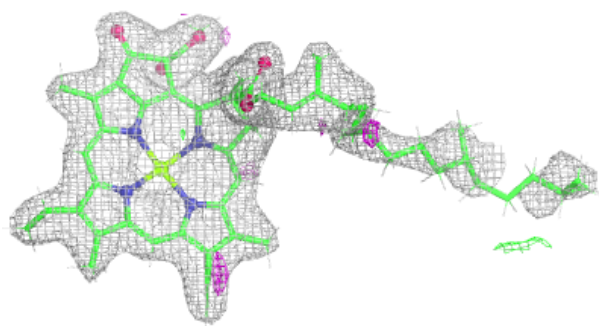


Electron density around CLA D 403:

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

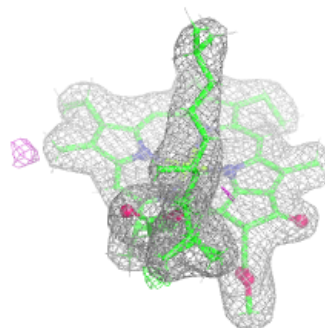
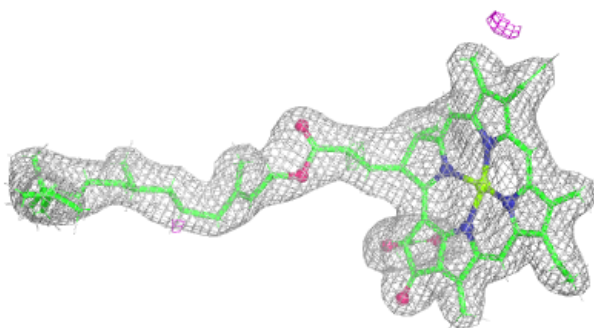
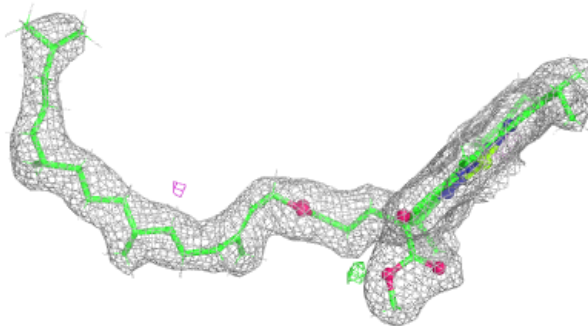
**Electron density around CLA a 403:**

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



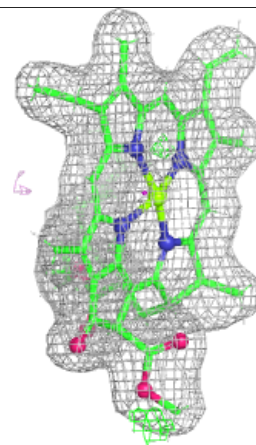
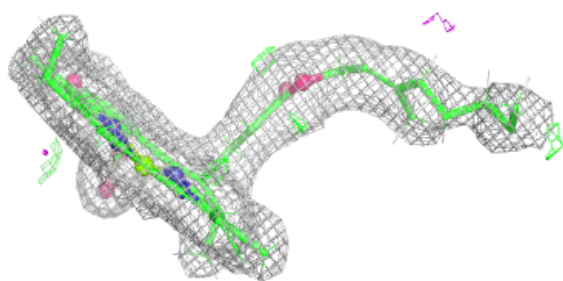
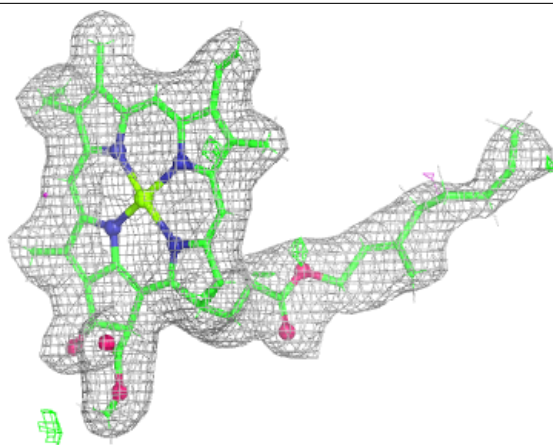
Electron density around CLA d 403:

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



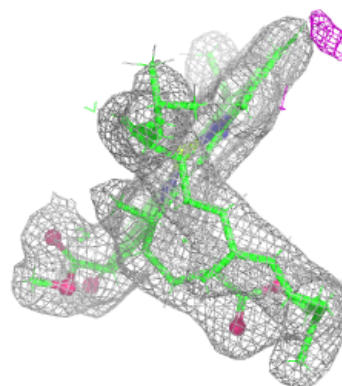
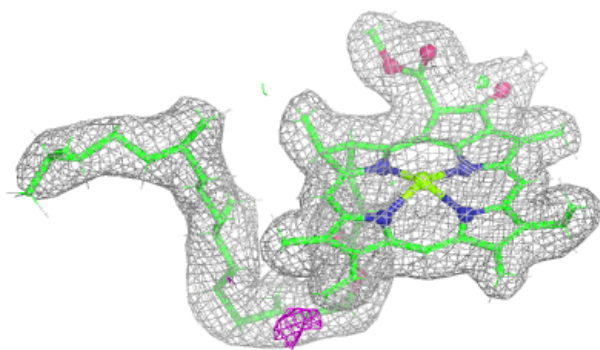
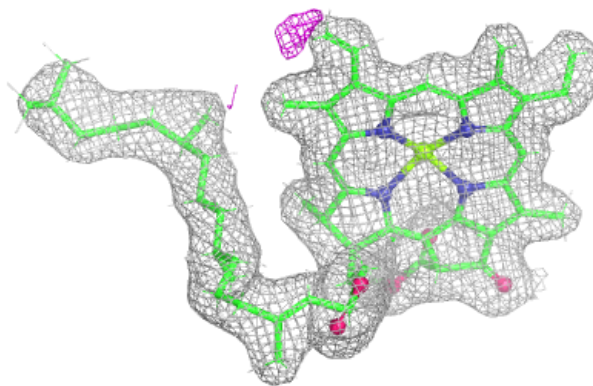
Electron density around CLA A 405:

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

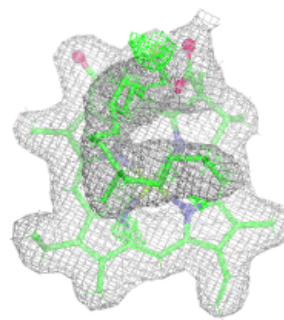
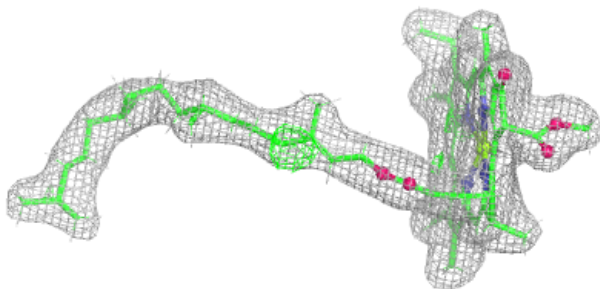
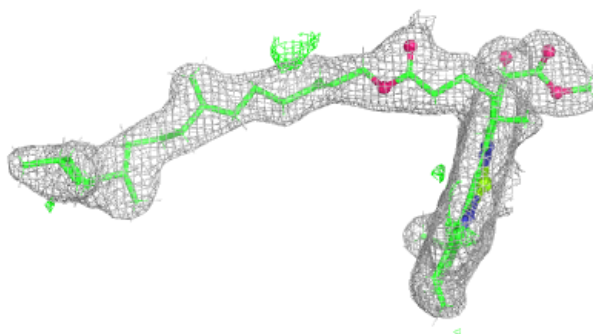


Electron density around CLA A 411:

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

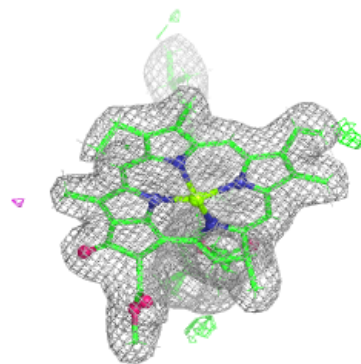
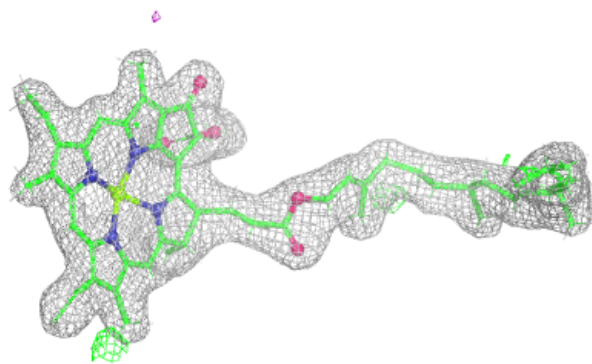
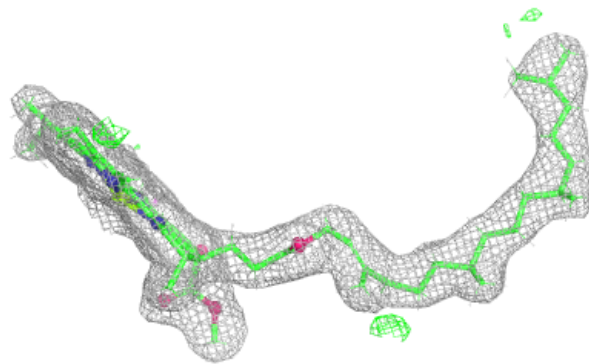
**Electron density around CLA B 605:**

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



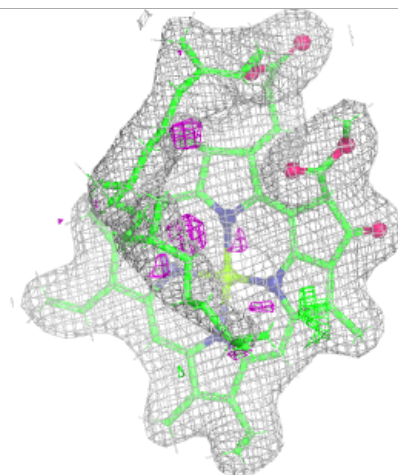
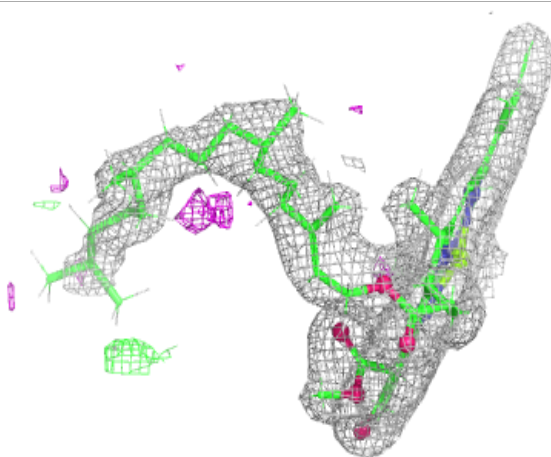
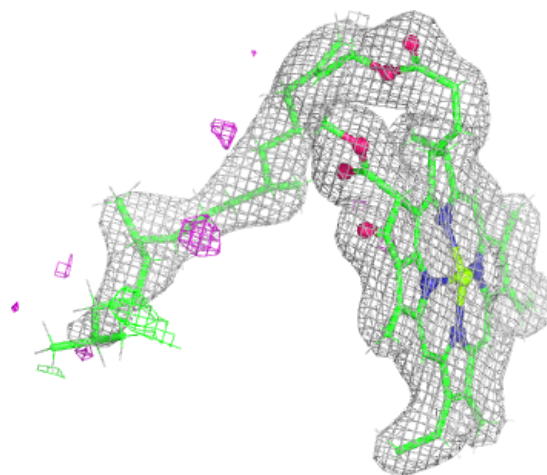
Electron density around CLA D 402:

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



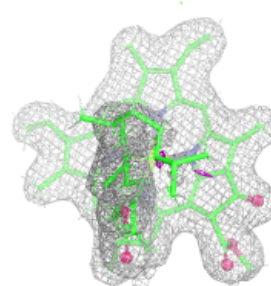
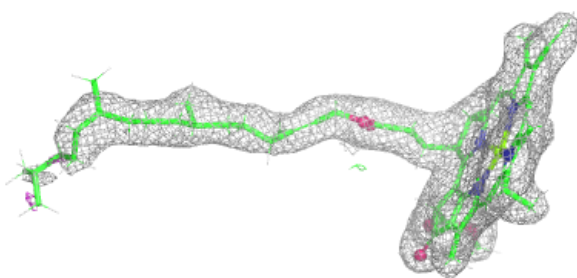
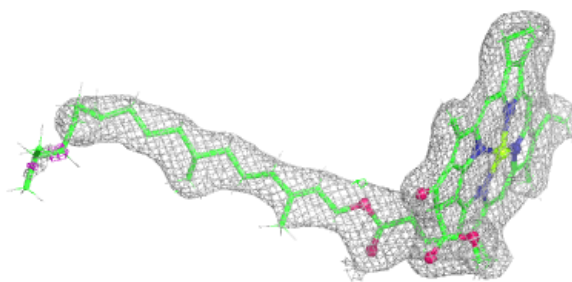
Electron density around CLA b 613:

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

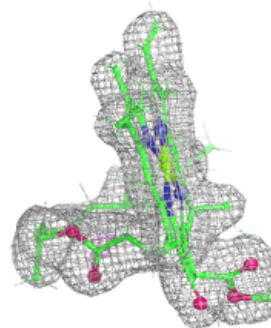
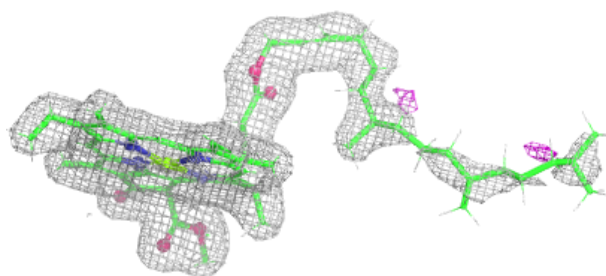
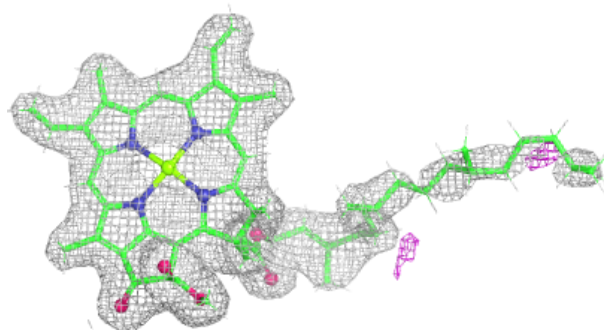


Electron density around CLA b 604:

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

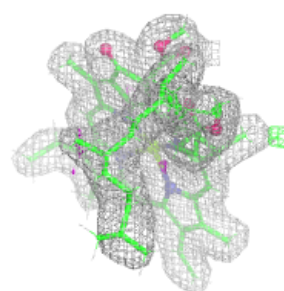
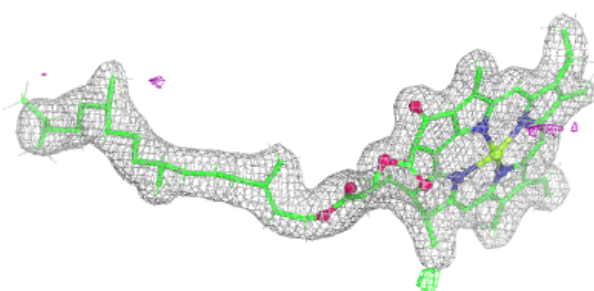
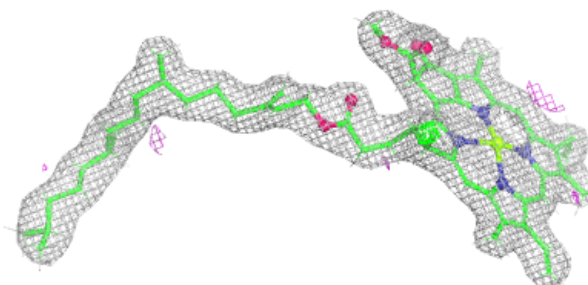
**Electron density around CLA A 403:**

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

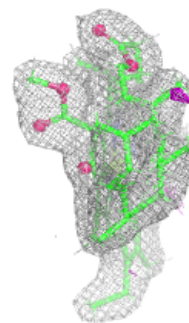
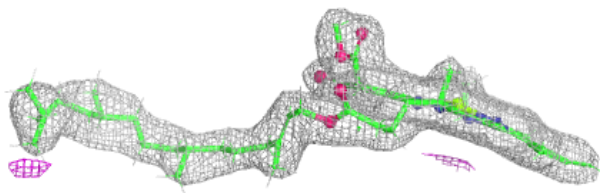
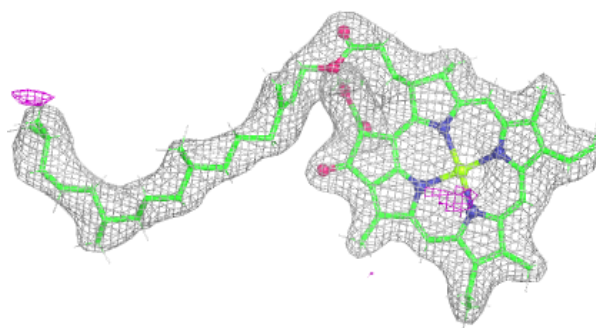


Electron density around CLA a 402:

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

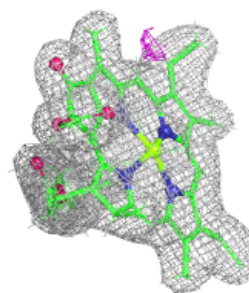
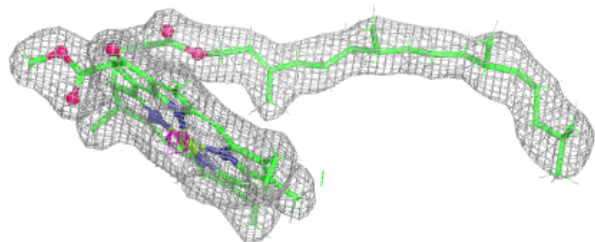
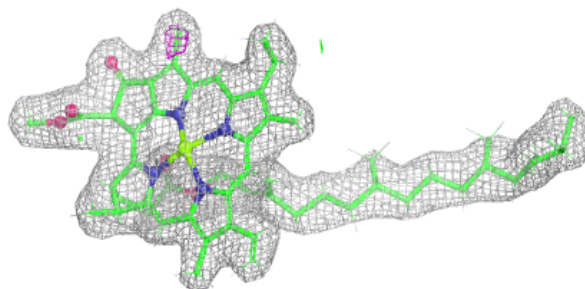
**Electron density around CLA B 602:**

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



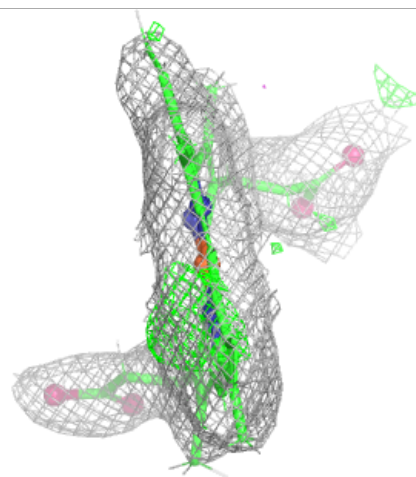
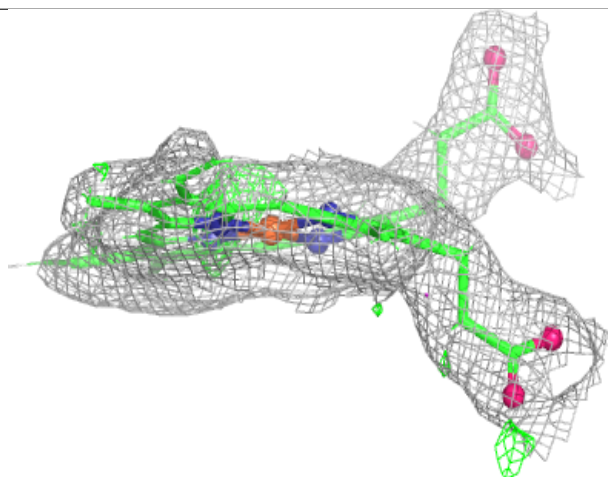
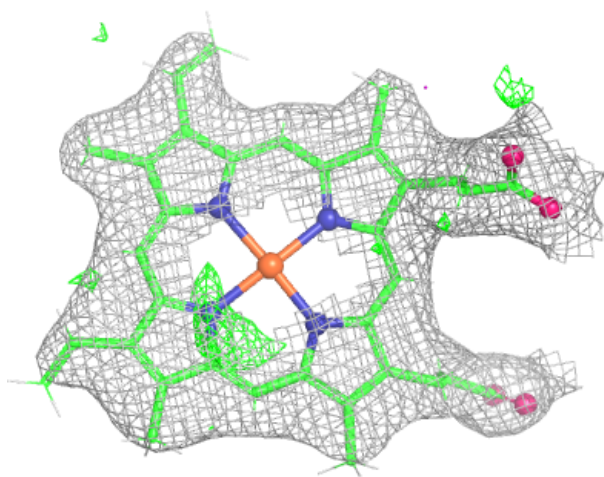
Electron density around CLA B 608:

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



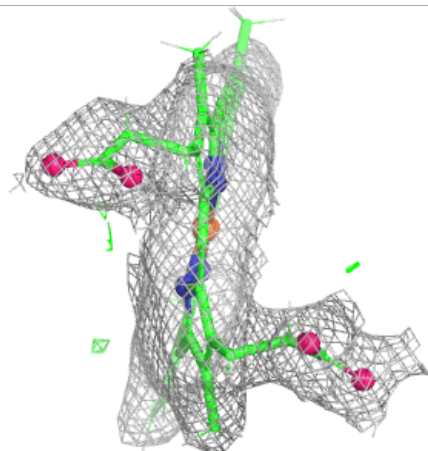
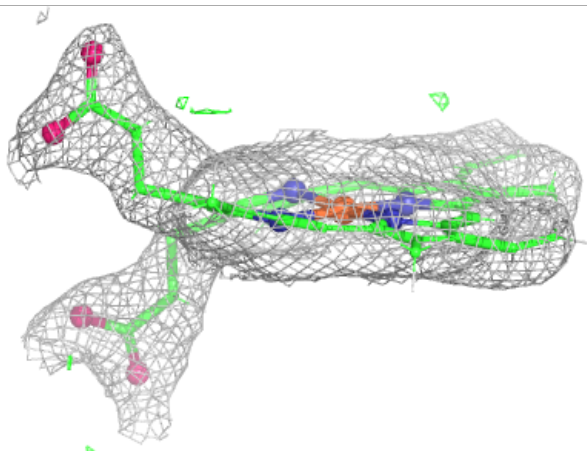
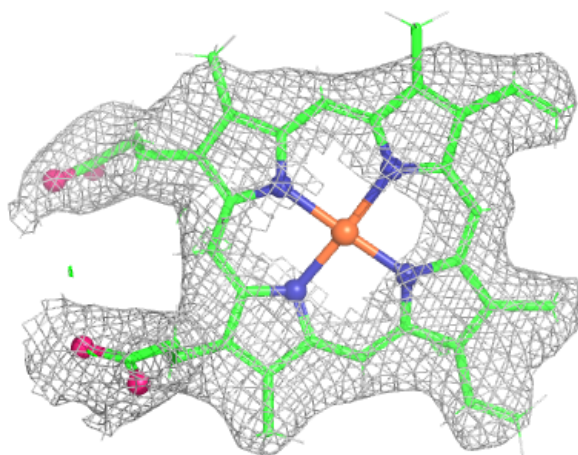
Electron density around HEM F 101:

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



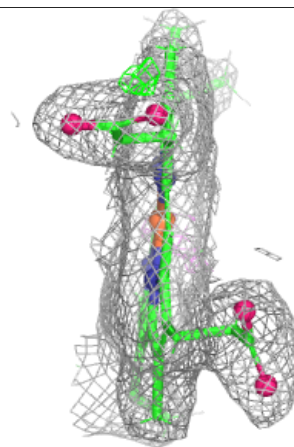
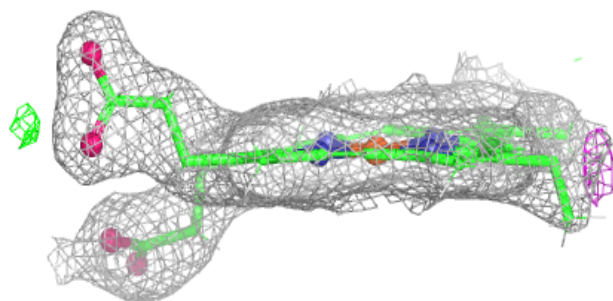
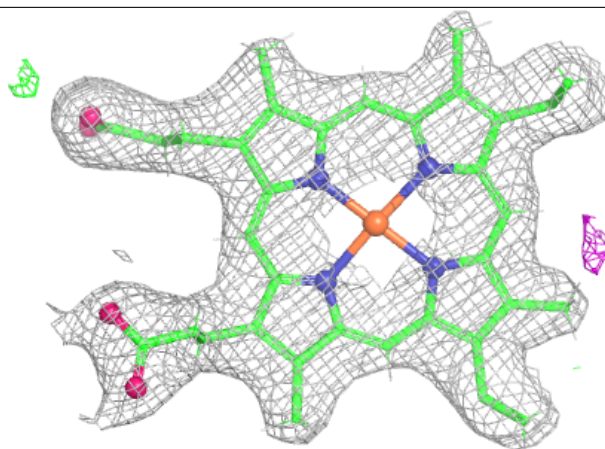
Electron density around HEM e 101:

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



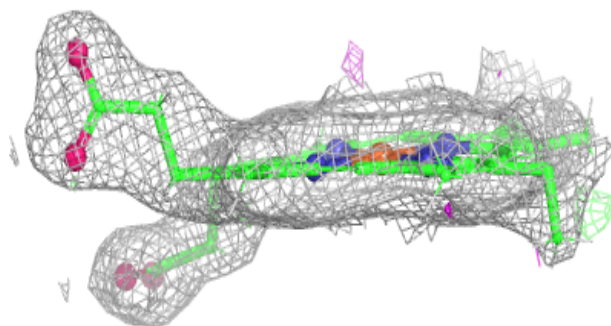
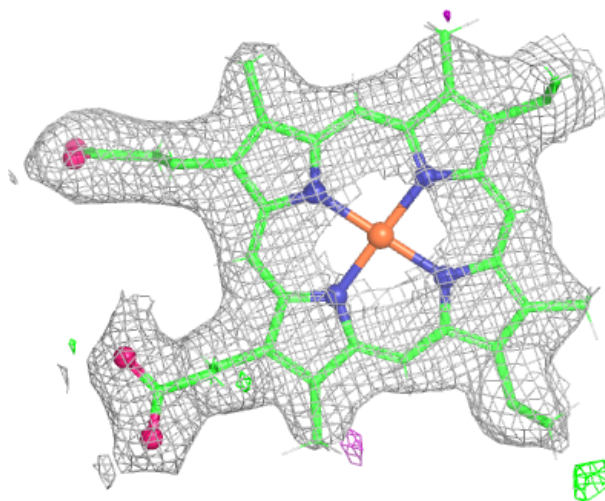
Electron density around HEC V 201:

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



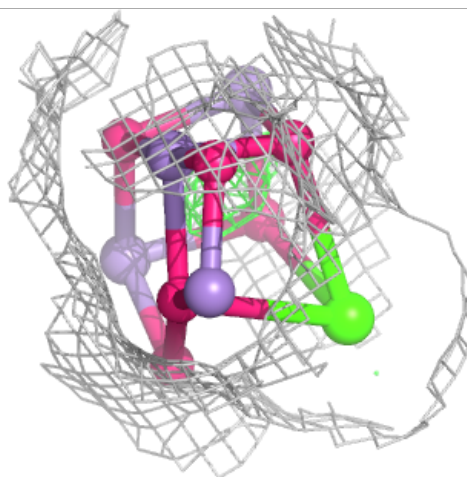
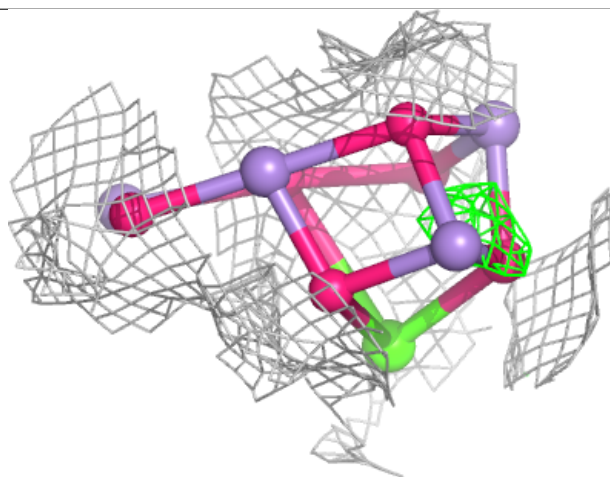
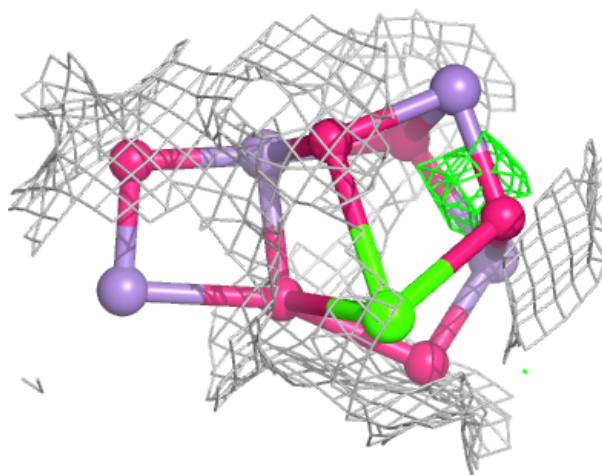
Electron density around HEC v 201:

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



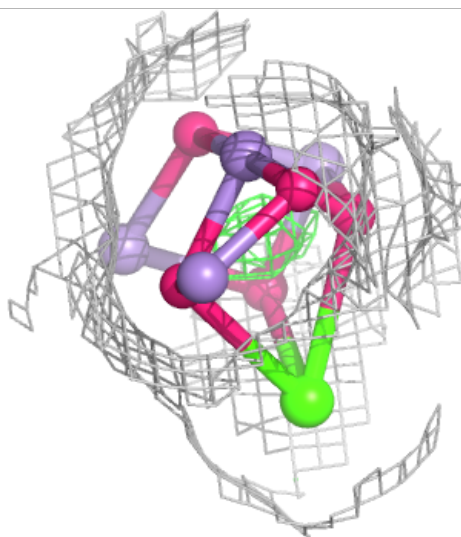
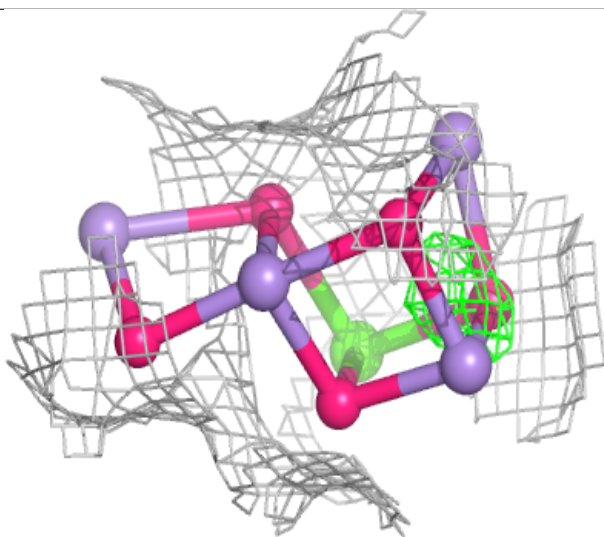
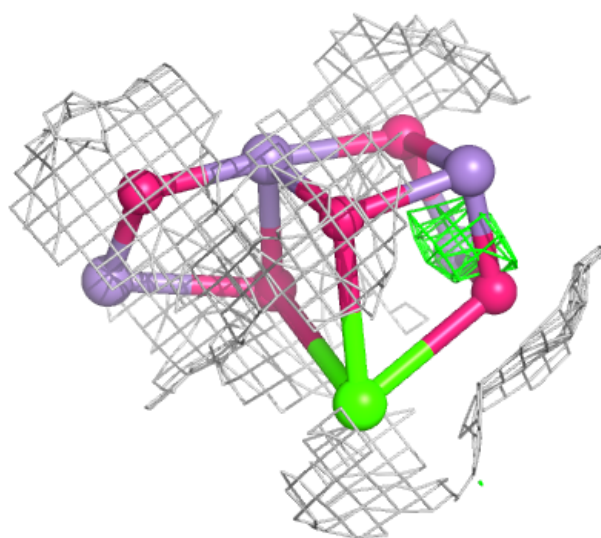
Electron density around OEY A 417 (B):

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



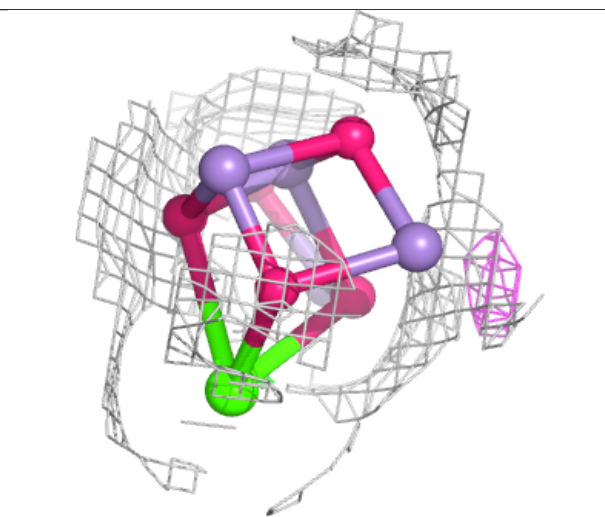
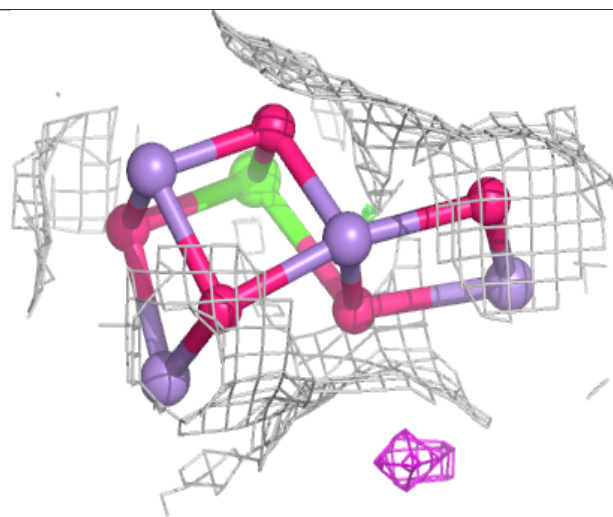
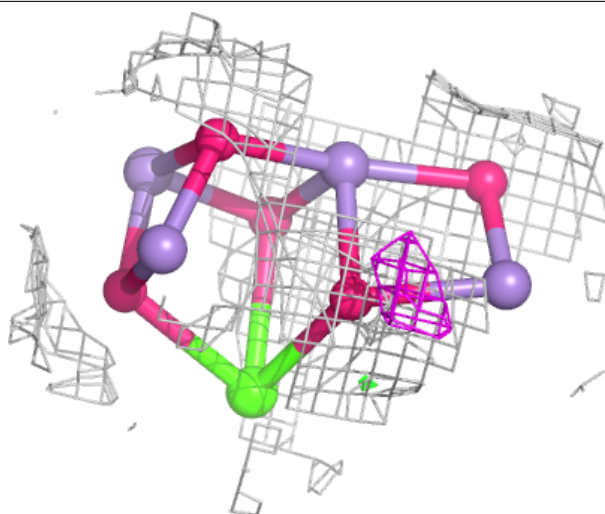
Electron density around OEX A 418 (A):

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



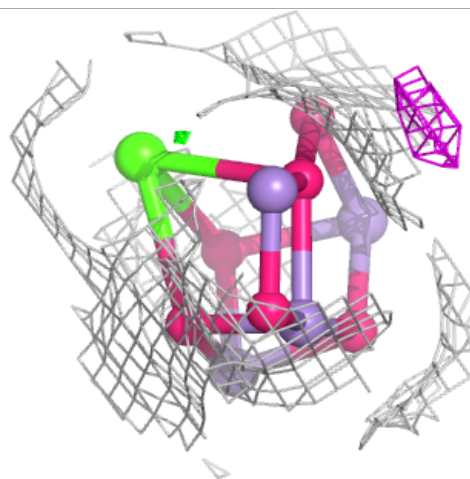
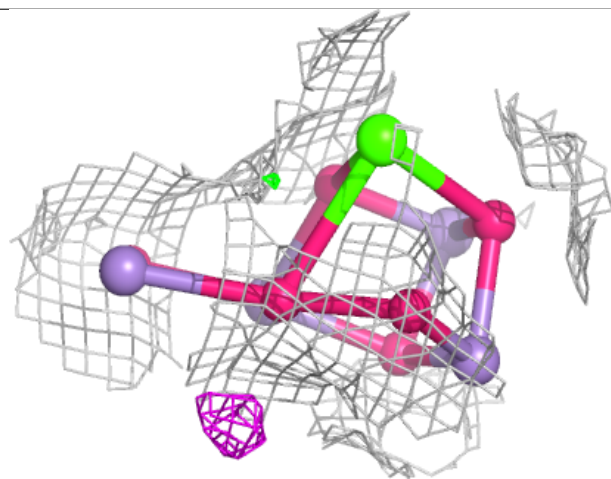
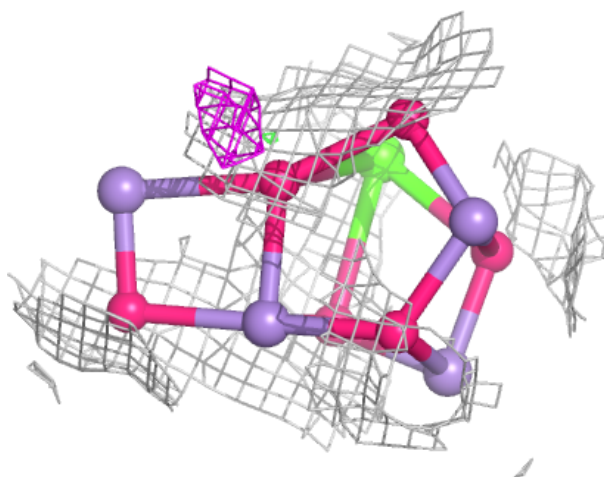
Electron density around OEX a 417 (A):

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



Electron density around OEY a 418 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.