



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 09:13 AM UTC

PDB ID : 6W1R / pdb_00006w1r
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.23 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

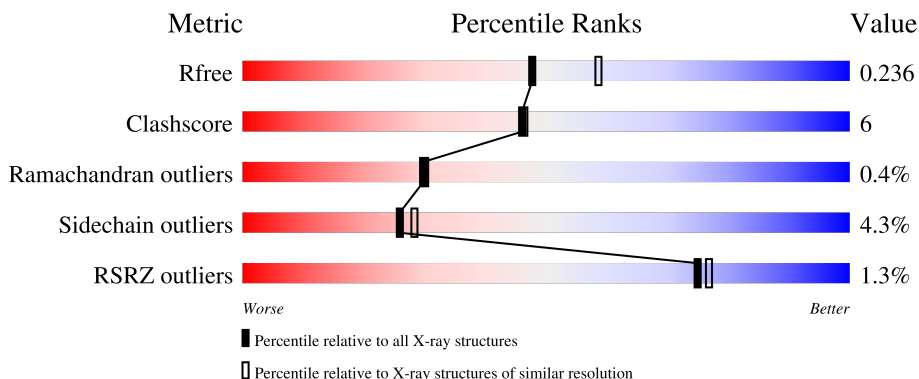
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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

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

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CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	506	 86% 13% .
2	b	506	 87% 12% .
3	C	461	 81% 14% .
3	c	461	 83% 14% ..
4	D	352	 85% 11% ..
4	d	352	 83% 14% ..
5	E	84	 75% 21% ..
5	e	84	 73% 24% ..
6	F	45	 60% 13% . 24%
6	f	45	 58% 13% . 24%
7	H	66	 86% 12% .
7	h	66	 77% 18% 5%
8	I	38	 84% 11% 5%
8	i	38	 79% 16% 5%
9	J	40	 78% 10% . 10%
9	j	40	 72% 18% 10%
10	K	46	 63% 15% . 20%
10	k	46	 52% 26% . 20%
11	L	37	 86% 14%
11	l	37	 86% 11% .
12	M	36	 64% 22% 6% 8%
12	m	36	 72% 17% 11%
13	O	272	 75% 12% . 10%
13	o	272	 77% 12% . 10%
14	R	40	 20% 65% 18% . 15%

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Mol	Chain	Length	Quality of chain
14	r	40	
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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	409	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
34	BCT	D	403	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105311 atoms, of which 52566 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

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

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

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

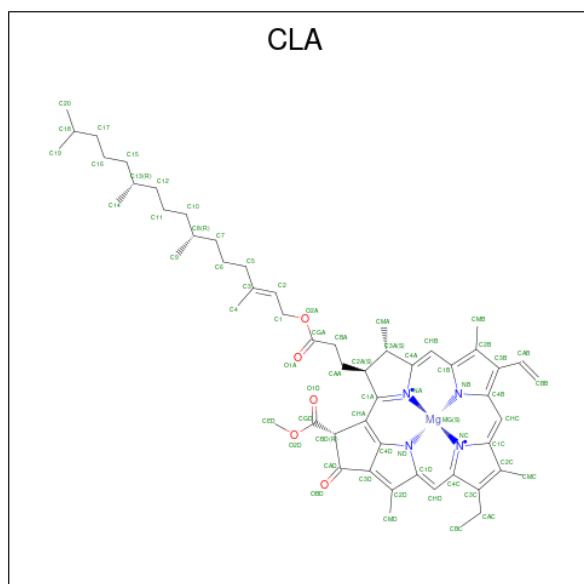
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	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: $C_{55}H_{72}MgN_4O_5$).



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

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

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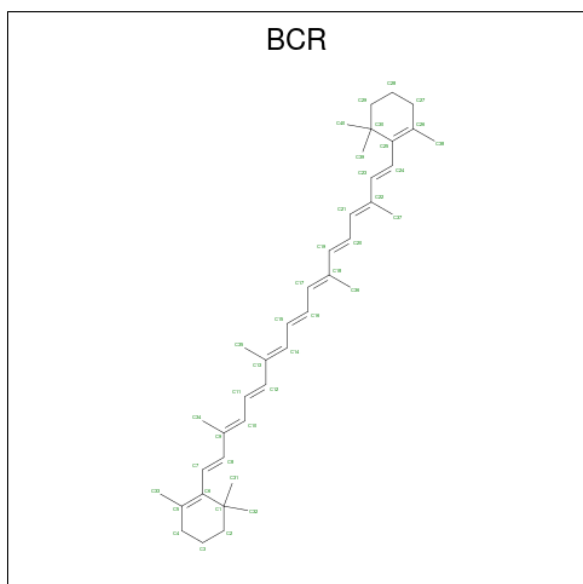
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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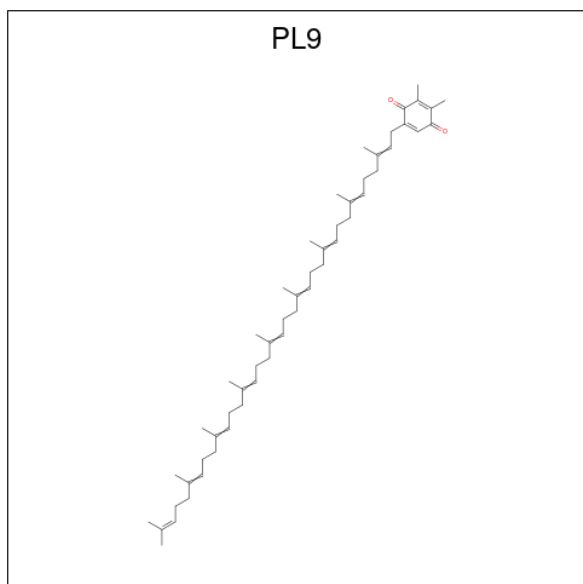
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	H	0	0
			96	40	56		
23	D	1	Total	C	H	0	0
			96	40	56		
23	K	1	Total	C	H	0	0
			96	40	56		
23	K	1	Total	C	H	0	0
			96	40	56		
23	T	1	Total	C	H	0	0
			96	40	56		
23	X	1	Total	C	H	0	0
			96	40	56		
23	a	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	c	1	Total	C	H	0	0
			96	40	56		
23	c	1	Total	C	H	0	0
			96	40	56		
23	d	1	Total	C	H	0	0
			96	40	56		
23	h	1	Total	C	H	0	0
			96	40	56		
23	k	1	Total	C	H	0	0
			96	40	56		
23	k	1	Total	C	H	0	0
			96	40	56		
23	t	1	Total	C	H	0	0
			96	40	56		

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

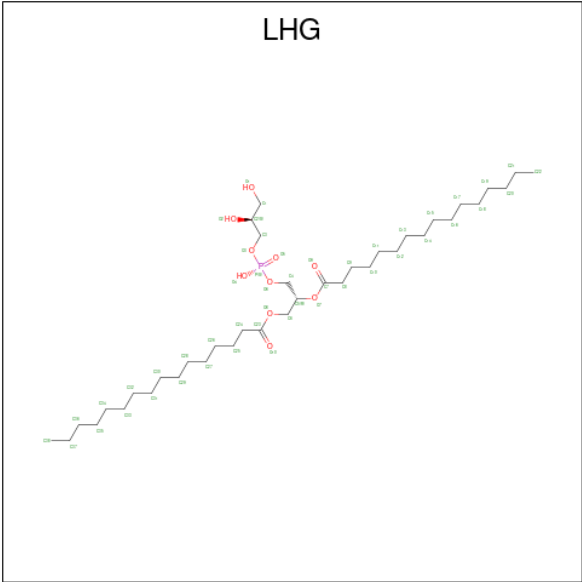
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



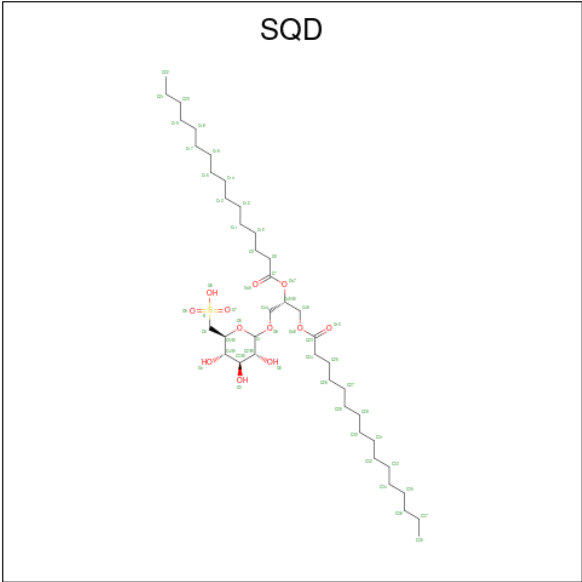
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			135	53	80	2		
25	D	1	Total	C	H	O	0	0
			135	53	80	2		
25	a	1	Total	C	H	O	0	0
			135	53	80	2		
25	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



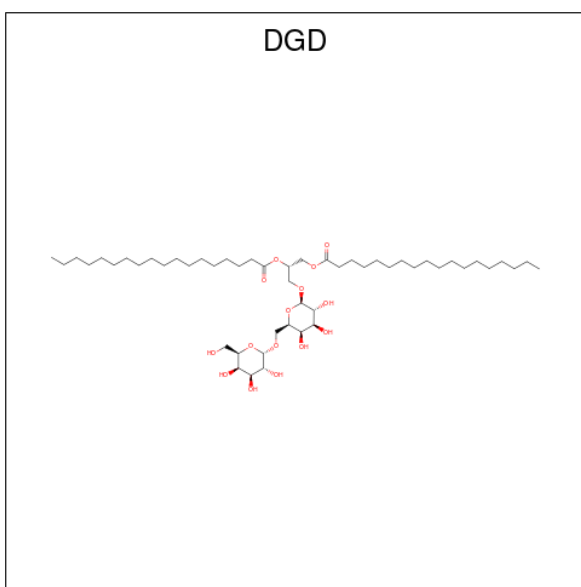
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
26	A	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
26	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	a	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
26	d	1	Total	C	H	O	P	0	0
			89	28	50	10	1		
26	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
26	l	1	Total	C	H	O	P	0	0
			121	38	72	10	1		

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



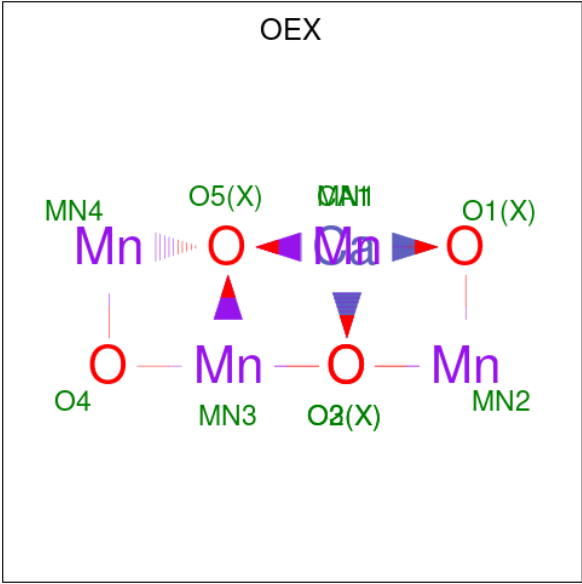
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			130	41	76	12	1		
27	a	1	Total	C	H	O		0	0
			92	31	56	5			
27	d	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



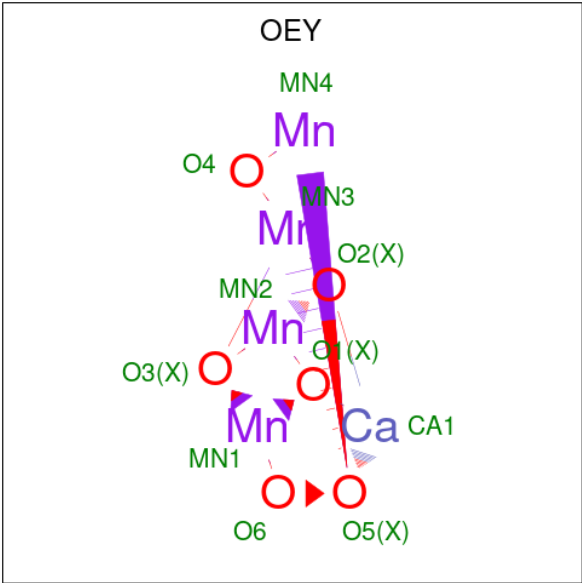
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			160	51	94	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			142	47	80	15		
28	C	1	Total	C	H	O	0	0
			141	47	79	15		
28	H	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	h	1	Total	C	H	O	0	0
			141	47	79	15		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



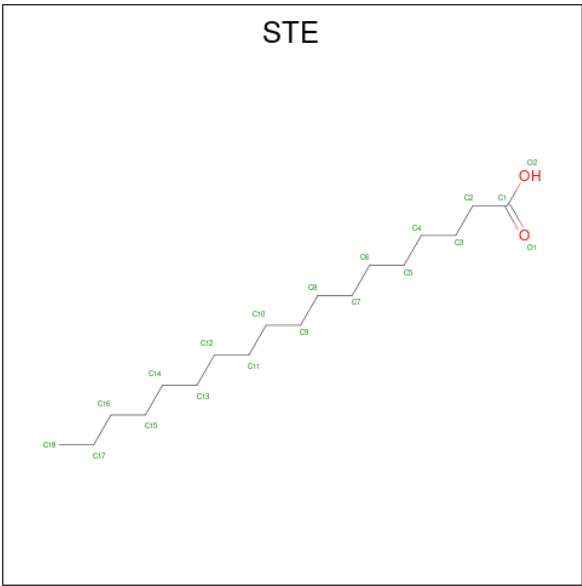
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			43	15	26	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		
31	B	1	Total	C	H		0	0
			47	16	31			
31	B	1	Total	C	H		0	0
			41	15	26			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	C	1	Total	C	H		0	0
			47	16	31			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	D	1	Total	C	H	O	0	0
			55	18	35	2		
31	H	1	Total	C	H		0	0
			53	18	35			
31	I	1	Total	C	H		0	0
			41	15	26			
31	J	1	Total	C	H	O	0	0
			28	10	16	2		

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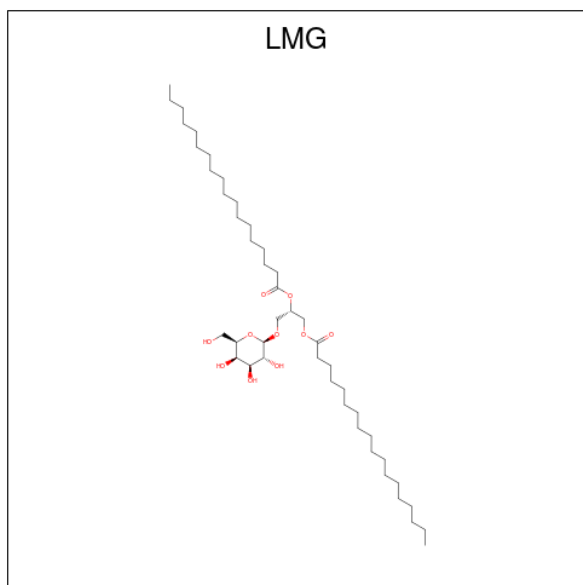
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	L	1	Total C H O 28 10 16 2	0	0
31	M	1	Total C H O 37 13 22 2	0	0
31	M	1	Total C H 26 10 16	0	0
31	M	1	Total C H 53 18 35	0	0
31	R	1	Total C H O 28 10 16 2	0	0
31	T	1	Total C H 47 16 31	0	0
31	T	1	Total C H 44 15 29	0	0
31	Z	1	Total C H 20 8 12	0	0
31	a	1	Total C H 26 10 16	0	0
31	a	1	Total C H O 28 10 16 2	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H O 40 14 24 2	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	c	1	Total C H O 28 10 16 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	h	1	Total C H 41 14 27	0	0
31	j	1	Total C H O 28 10 16 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



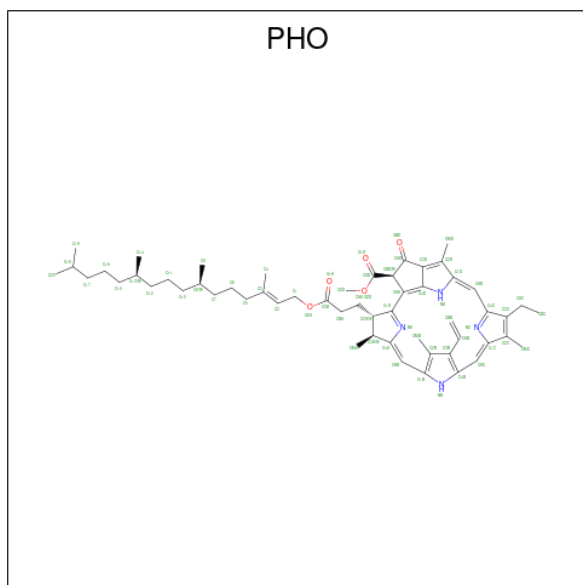
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			122	41	71	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		
32	D	1	Total	C	H	O	0	0
			68	24	40	4		
32	M	1	Total	C	H	O	0	0
			122	41	71	10		
32	Y	1	Total	C	H	O	0	0
			113	38	65	10		
32	a	1	Total	C	H	O	0	0
			140	45	85	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			80	27	43	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		

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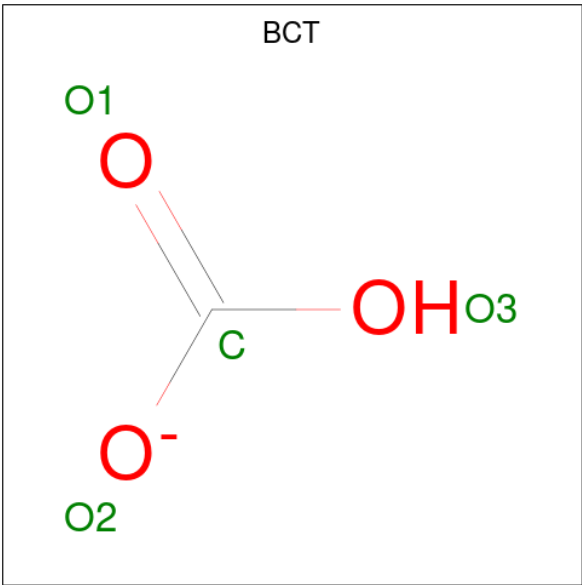
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			116	39	67	10		
32	d	1	Total	C	H	O	0	0
			101	34	57	10		
32	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



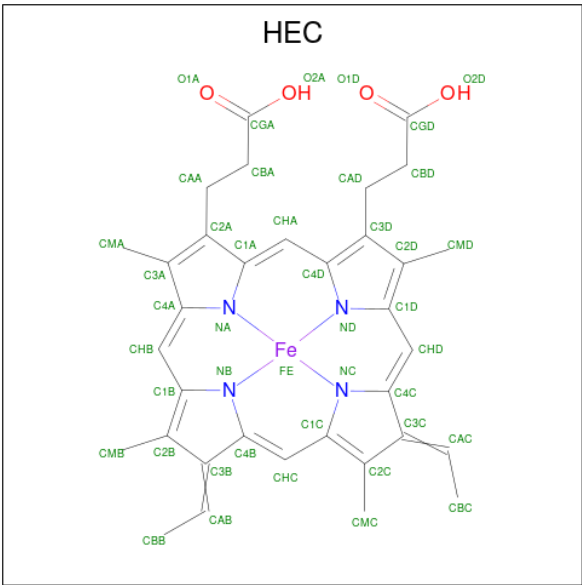
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	f	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	119	Total	O	0	8
			119	119		
36	B	148	Total	O	0	0
			148	148		
36	C	118	Total	O	0	0
			118	118		
36	D	98	Total	O	0	0
			98	98		
36	E	21	Total	O	0	0
			21	21		
36	F	2	Total	O	0	0
			2	2		
36	H	26	Total	O	0	0
			26	26		
36	I	7	Total	O	0	0
			7	7		
36	J	6	Total	O	0	0
			6	6		
36	K	4	Total	O	0	0
			4	4		
36	L	9	Total	O	0	0
			9	9		
36	M	3	Total	O	0	0
			3	3		
36	O	71	Total	O	0	0
			71	71		
36	R	1	Total	O	0	0
			1	1		
36	T	2	Total	O	0	0
			2	2		
36	U	31	Total	O	0	0
			31	31		
36	V	51	Total	O	0	0
			51	51		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	9	Total O 9 9	0	0
36	Y	4	Total O 4 4	0	0
36	Z	2	Total O 2 2	0	0
36	a	114	Total O 114 114	0	8
36	b	126	Total O 126 126	0	0
36	c	122	Total O 122 122	0	0
36	d	94	Total O 94 94	0	0
36	e	13	Total O 13 13	0	0
36	f	2	Total O 2 2	0	0
36	h	21	Total O 21 21	0	0
36	i	8	Total O 8 8	0	0
36	j	8	Total O 8 8	0	0
36	k	6	Total O 6 6	0	0
36	l	8	Total O 8 8	0	0
36	m	7	Total O 7 7	0	0
36	o	67	Total O 67 67	0	0
36	r	1	Total O 1 1	0	0
36	t	5	Total O 5 5	0	0
36	u	41	Total O 41 41	0	0
36	v	31	Total O 31 31	0	0
36	x	9	Total O 9 9	0	0

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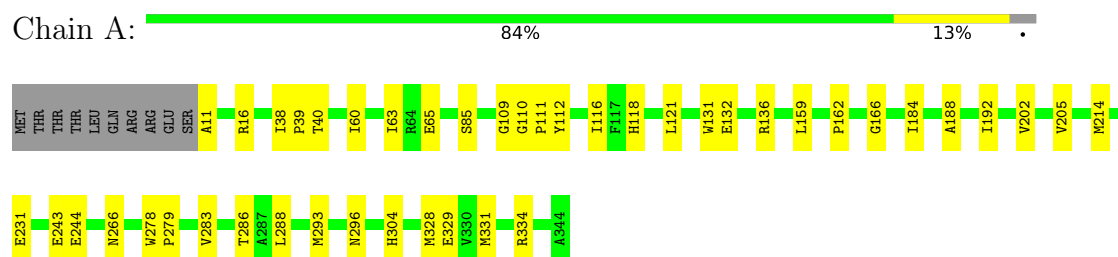
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	y	1	Total	O	0	0
			1	1		
36	z	1	Total	O	0	0
			1	1		

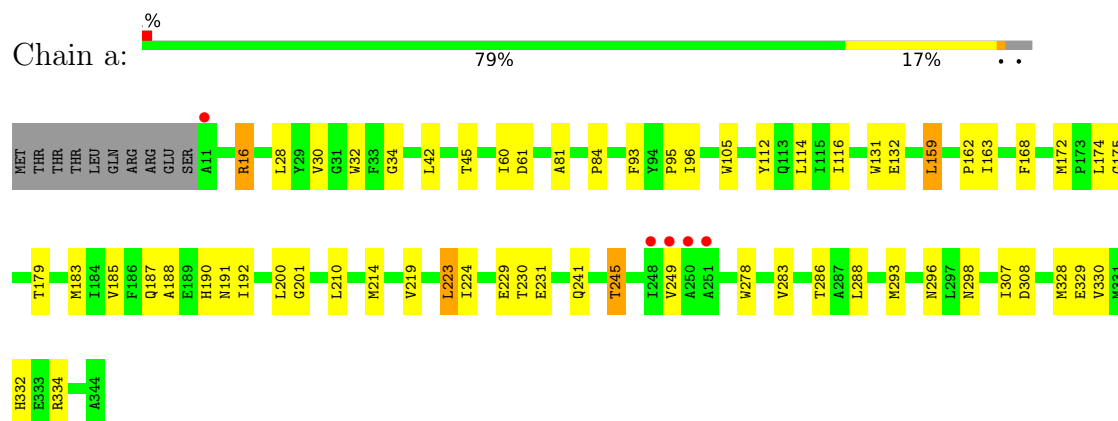
3 Residue-property plots

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.

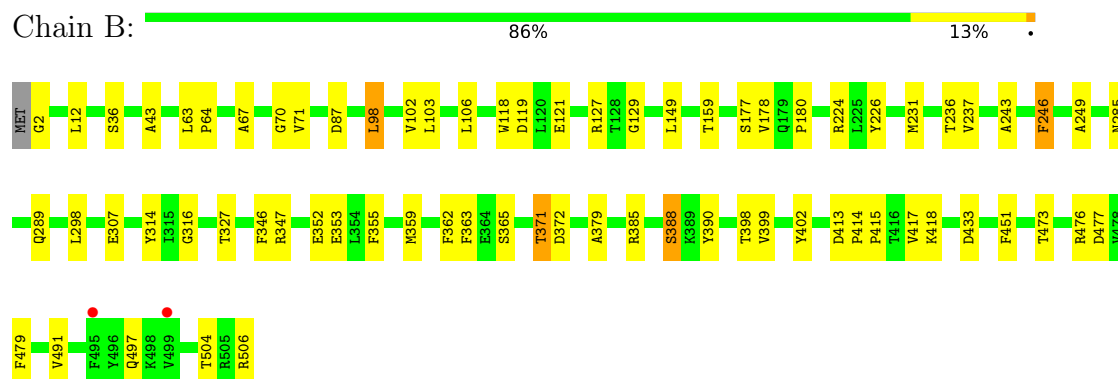
• Molecule 1: Photosystem II protein D1 1



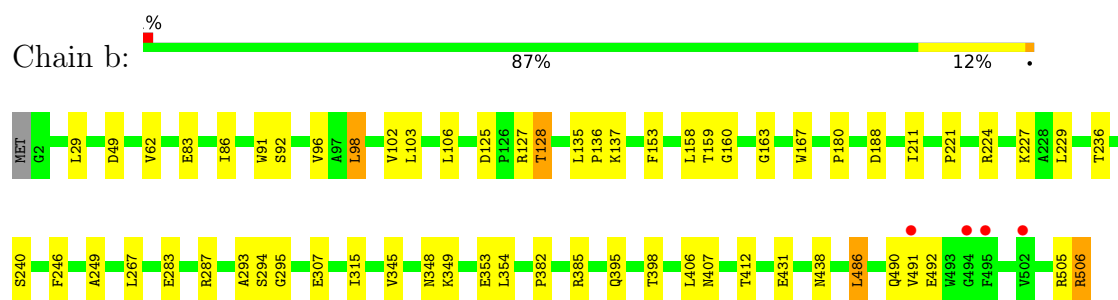
• Molecule 1: Photosystem II protein D1 1



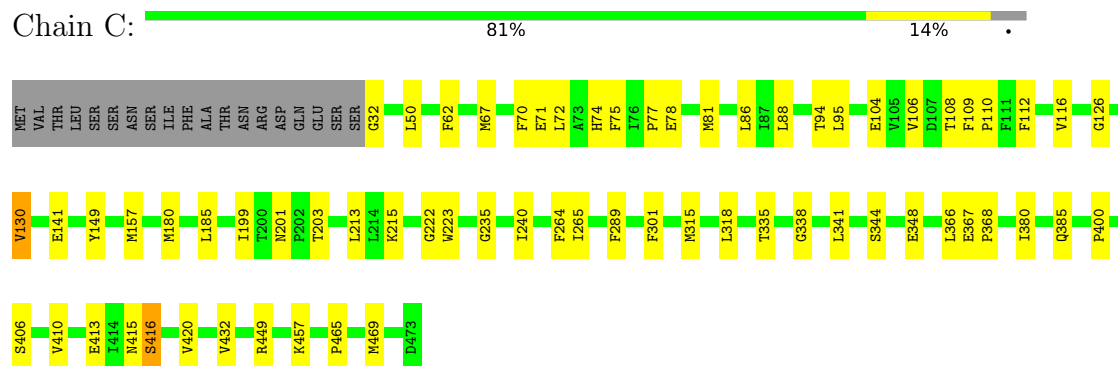
• Molecule 2: Photosystem II CP47 reaction center protein



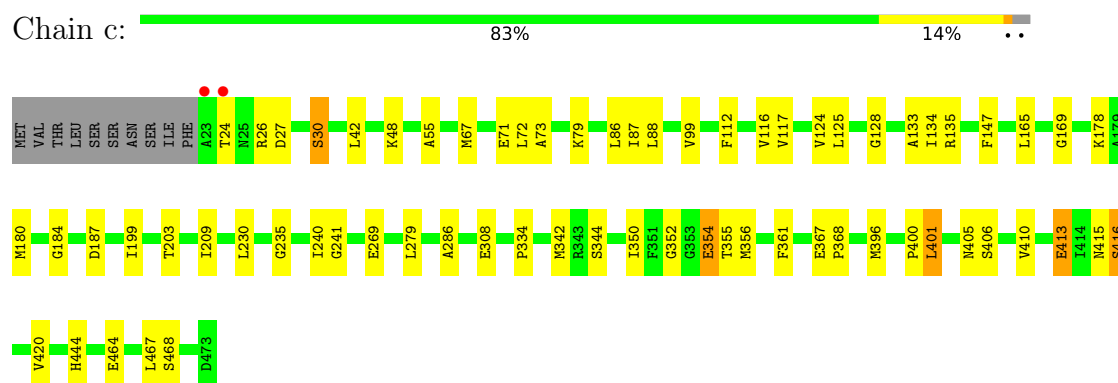
• Molecule 2: Photosystem II CP47 reaction center protein



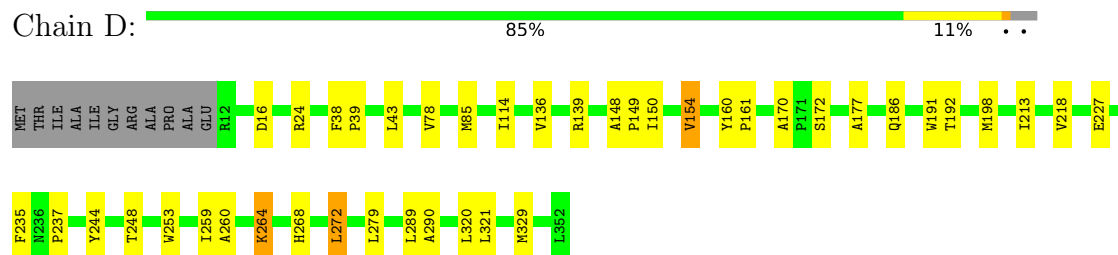
• Molecule 3: Photosystem II CP43 reaction center protein



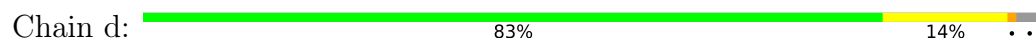
• Molecule 3: Photosystem II CP43 reaction center protein

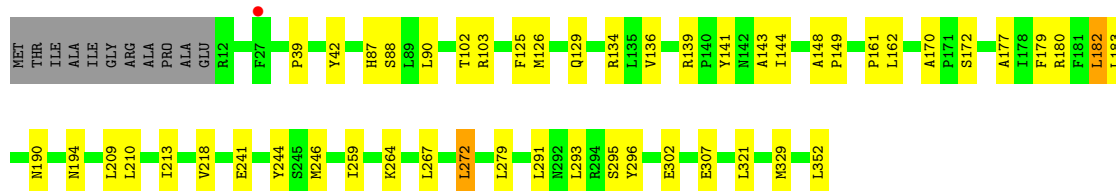


• Molecule 4: Photosystem II D2 protein

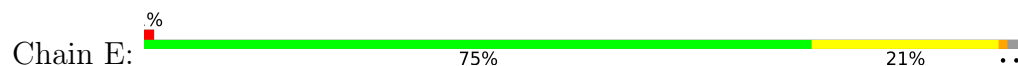


• Molecule 4: Photosystem II D2 protein

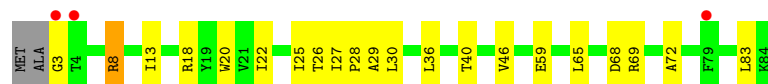
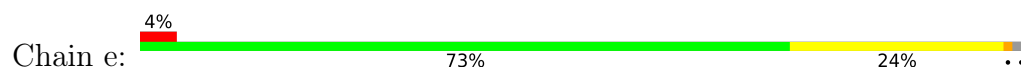




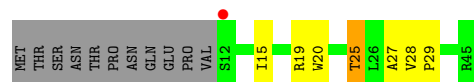
• Molecule 5: Cytochrome b559 subunit alpha



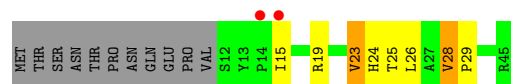
• Molecule 5: Cytochrome b559 subunit alpha



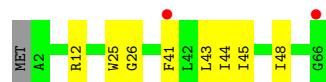
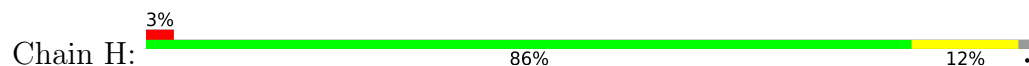
• Molecule 6: Cytochrome b559 subunit beta



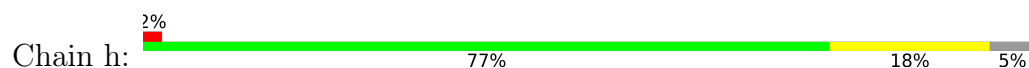
• Molecule 6: Cytochrome b559 subunit beta



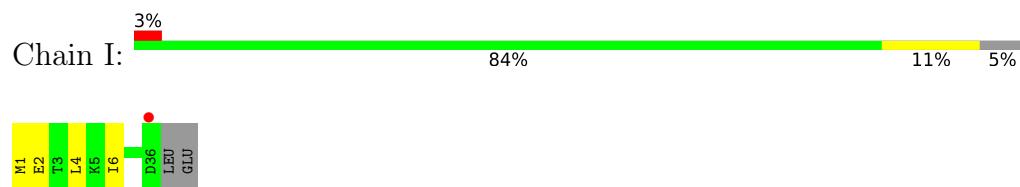
• Molecule 7: Photosystem II reaction center protein H



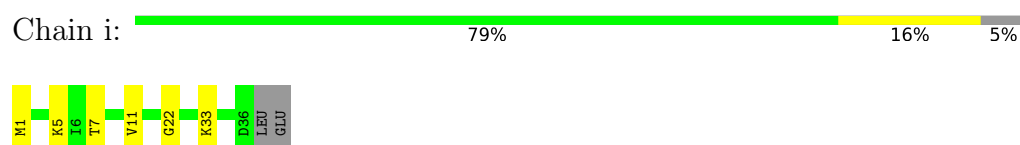
• Molecule 7: Photosystem II reaction center protein H



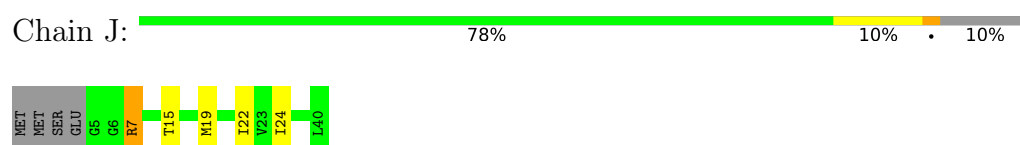
- Molecule 8: Photosystem II reaction center protein I



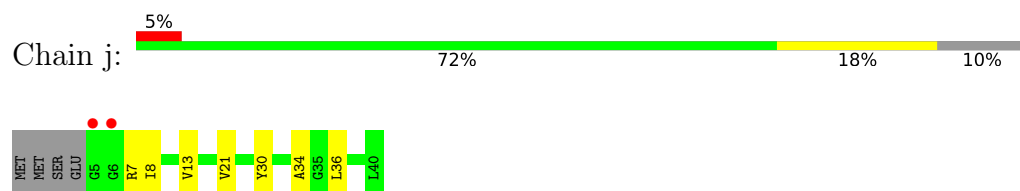
- Molecule 8: Photosystem II reaction center protein I



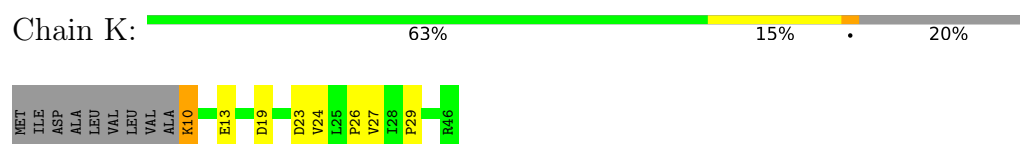
- Molecule 9: Photosystem II reaction center protein J



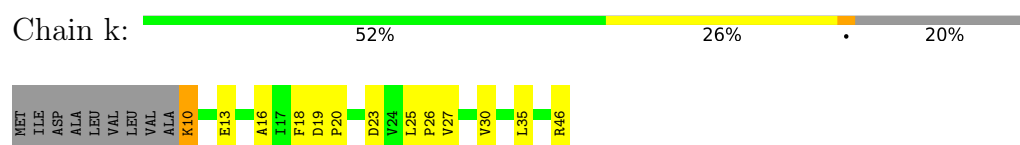
- Molecule 9: Photosystem II reaction center protein J



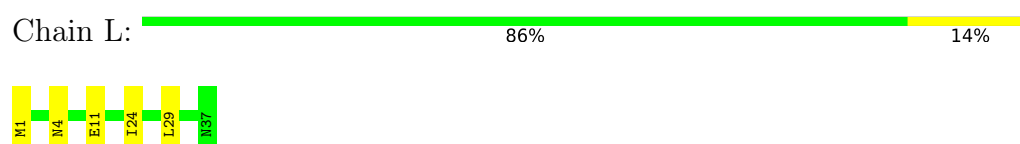
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 64% 22% 6% 8%



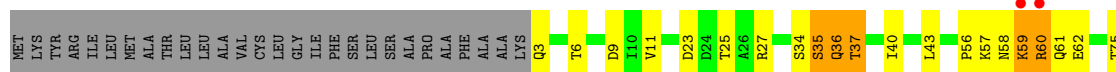
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 17% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  % 75% 12% . 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  % 77% 12% . 10%

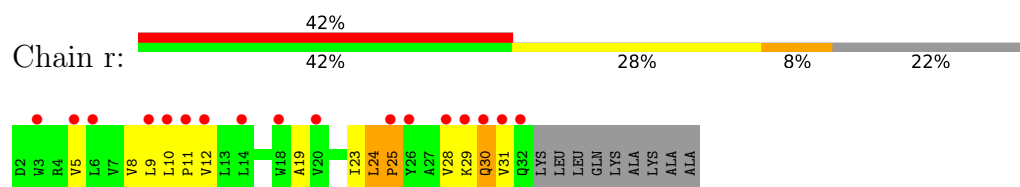


- Molecule 14: Photosystem II protein Y

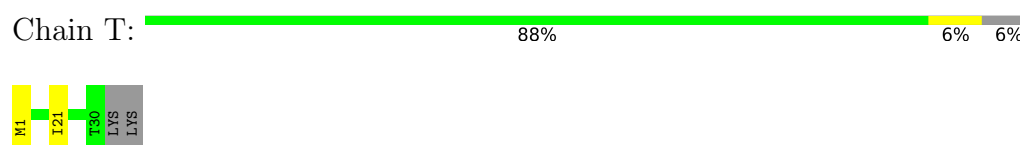
Chain R:  20% 65% 18% . 15%



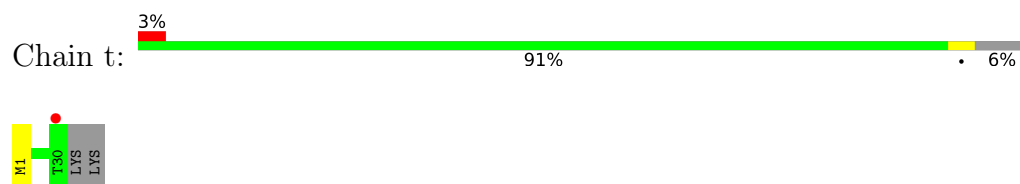
- Molecule 14: Photosystem II protein Y



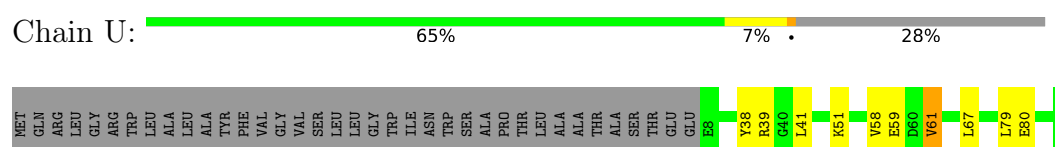
- Molecule 15: Photosystem II reaction center protein T



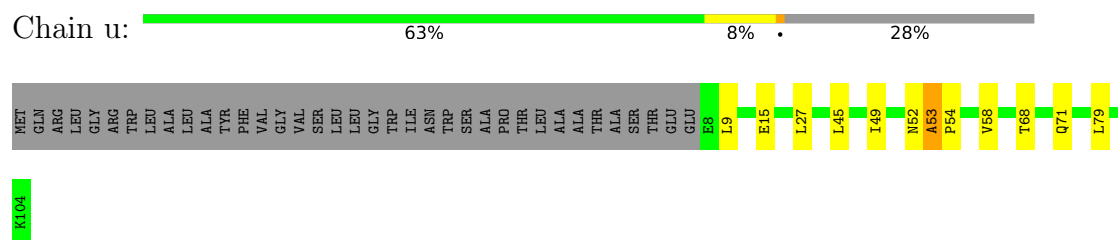
- Molecule 15: Photosystem II reaction center protein T



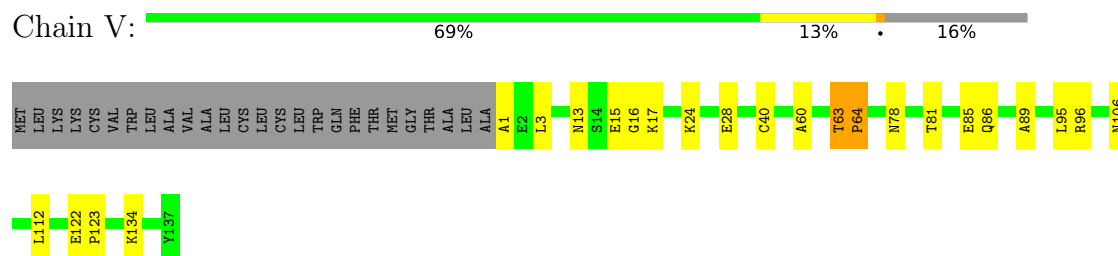
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein

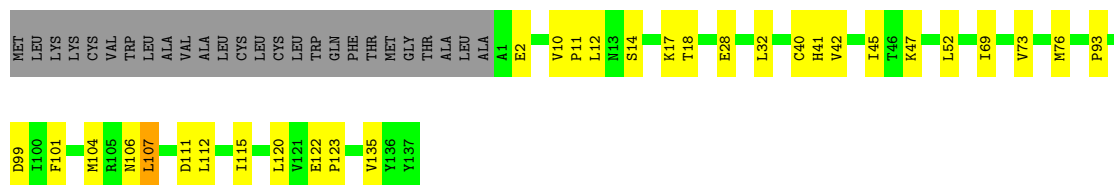


- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550

Chain v:  65% 18% 16%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  76% 17% 7%

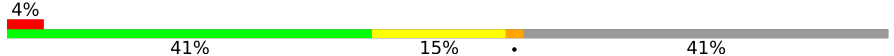


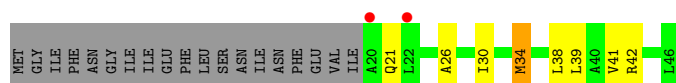
- Molecule 18: Photosystem II reaction center X protein

Chain x:  80% 15% 5%



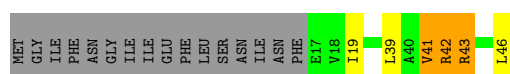
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  41% 15% 41%



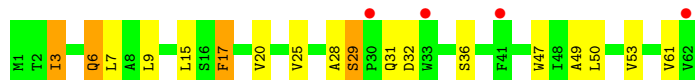
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  52% 7% 35%



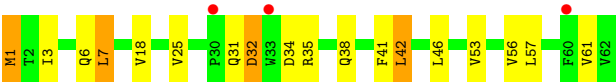
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  71% 23% 6%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  71% 23% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.0 (33.70-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.172 , 0.235 0.173 , 0.236	Depositor DCC
R_{free} test set	3445 reflections (0.55%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105311	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3187	0.63	0/4342
1	a	0.51	0/3184	0.61	0/4338
2	B	0.60	1/4161 (0.0%)	0.68	0/5669
2	b	0.56	0/4118	0.67	0/5611
3	C	0.58	0/3621	0.67	0/4930
3	c	0.52	0/3693	0.64	0/5026
4	D	0.62	0/2820	0.69	0/3840
4	d	0.58	0/2829	0.67	0/3852
5	E	0.48	0/688	0.60	0/940
5	e	0.42	0/683	0.62	0/932
6	F	0.45	0/284	0.61	0/387
6	f	0.49	0/284	0.67	0/387
7	H	0.55	0/523	0.63	0/713
7	h	0.51	0/511	0.61	0/697
8	I	0.56	0/293	0.74	0/396
8	i	0.58	0/293	0.61	0/396
9	J	0.47	0/263	0.60	0/356
9	j	0.48	0/263	0.61	0/356
10	K	0.44	0/303	0.59	0/416
10	k	0.48	0/303	0.59	0/416
11	L	0.65	0/311	0.70	0/422
11	l	0.64	0/303	0.61	0/412
12	M	0.64	0/249	0.69	0/341
12	m	0.64	0/244	0.75	0/334
13	O	0.57	0/1904	0.71	0/2585
13	o	0.59	0/1905	0.68	0/2583
14	R	0.41	0/277	0.54	0/380
14	r	0.33	0/246	0.44	0/339
15	T	0.68	0/257	0.72	0/349
15	t	0.62	0/255	0.70	0/346
16	U	0.51	0/785	0.63	0/1064
16	u	0.58	0/785	0.71	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.57	0/1085	0.69	0/1473
17	v	0.51	0/1085	0.66	0/1473
18	X	0.46	0/284	0.59	0/384
18	x	0.40	0/289	0.53	0/391
19	Y	0.51	0/197	0.57	0/264
19	y	0.38	0/219	0.55	0/294
20	Z	0.39	0/490	0.53	0/669
20	z	0.36	0/488	0.52	0/666
All	All	0.55	1/43962 (0.0%)	0.65	0/59833

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	GLY	C-N	-6.16	1.20	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3089	2942	2956	33	0
1	a	3086	2933	2947	40	0
2	B	4005	3859	3867	52	0
2	b	3978	3822	3836	36	0
3	C	3479	3397	3383	41	0
3	c	3553	3468	3466	41	0
4	D	2726	2624	2632	34	0
4	d	2732	2630	2638	31	0
5	E	666	650	651	16	0
5	e	664	647	648	17	0
6	F	275	281	282	6	0
6	f	275	281	282	6	0
7	H	510	532	532	8	0
7	h	498	518	518	6	0
8	I	296	311	311	1	0
8	i	296	311	311	3	0
9	J	257	268	268	4	0
9	j	257	268	268	4	0
10	K	293	305	305	4	0
10	k	293	305	305	10	0
11	L	304	316	316	5	0
11	l	296	304	304	0	0
12	M	256	269	269	10	0
12	m	251	267	267	3	0
13	O	1870	1828	1830	22	0
13	o	1874	1844	1846	16	0
14	R	271	298	298	6	0
14	r	240	253	250	8	0
15	T	258	261	261	1	0
15	t	256	256	256	0	0
16	U	774	772	773	4	0
16	u	774	772	773	10	0
17	V	1064	1068	1073	22	0
17	v	1064	1068	1073	19	0
18	X	281	312	312	5	0
18	x	286	316	314	4	0
19	Y	196	217	217	5	0
19	y	218	241	241	6	0
20	Z	479	516	516	10	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	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	970	1067	1067	19	0
22	C	839	922	922	12	0
22	D	130	144	144	6	0
22	H	65	72	72	4	0
22	a	260	288	288	3	0
22	b	1035	1139	1139	18	0
22	c	839	919	919	12	0
22	d	130	144	144	1	0
23	A	40	56	56	1	0
23	B	120	168	168	8	0
23	C	80	112	112	4	0
23	D	40	56	56	4	0
23	K	80	112	112	3	0
23	T	40	56	56	1	0
23	X	40	56	56	5	0
23	a	40	56	56	0	0
23	b	120	168	168	4	0
23	c	80	112	112	6	0
23	d	40	56	56	2	0
23	h	40	56	56	0	0
23	k	80	112	112	5	0
23	t	40	56	56	4	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	5	0
25	D	55	80	80	2	0
25	a	55	80	80	2	0
25	d	55	80	80	0	0
26	A	96	138	141	2	0
26	D	98	145	148	4	0
26	L	49	73	74	2	0
26	a	49	73	74	2	0
26	d	88	122	125	0	0
26	e	42	55	57	0	0
26	l	49	72	74	0	0
27	A	91	135	135	2	0
27	B	54	77	78	1	0
27	F	36	45	45	1	0
27	L	49	65	65	1	0
27	a	90	132	133	1	0
27	d	41	48	48	2	0
28	A	66	94	96	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	C	186	241	245	0	0
28	H	62	79	82	0	0
28	c	186	237	244	1	0
28	h	62	79	82	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	1	0
30	a	11	0	0	0	0
31	B	90	143	140	1	0
31	C	40	63	60	0	0
31	D	20	35	35	1	0
31	H	18	35	35	1	0
31	I	15	26	26	0	0
31	J	12	16	16	0	0
31	L	12	16	16	0	0
31	M	43	73	73	2	0
31	R	12	16	16	0	0
31	T	31	60	54	0	0
31	Z	8	12	12	1	0
31	a	22	32	32	0	0
31	b	66	110	110	2	0
31	c	32	51	51	1	0
31	d	57	96	96	10	0
31	h	14	27	27	2	0
31	j	12	16	16	1	0
31	t	14	20	20	0	0
32	C	48	66	66	1	0
32	D	112	156	156	0	0
32	M	51	71	72	2	0
32	Y	48	65	66	0	0
32	a	55	85	86	3	0
32	b	55	86	86	1	0
32	c	134	179	181	0	0
32	d	44	57	58	0	0
32	m	51	72	72	2	0
33	D	128	148	148	4	0
33	a	64	74	74	2	0
33	d	64	74	74	2	0
34	D	4	1	1	2	0
34	a	4	1	1	0	0
35	F	43	32	32	7	0
35	V	43	30	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	43	32	32	7	0
35	v	43	30	30	2	0
36	A	119	0	0	5	0
36	B	148	0	0	3	0
36	C	118	0	0	3	0
36	D	98	0	0	0	0
36	E	21	0	0	2	0
36	F	2	0	0	0	0
36	H	26	0	0	0	0
36	I	7	0	0	0	0
36	J	6	0	0	0	0
36	K	4	0	0	0	0
36	L	9	0	0	0	0
36	M	3	0	0	0	0
36	O	71	0	0	1	0
36	R	1	0	0	0	0
36	T	2	0	0	0	0
36	U	31	0	0	1	0
36	V	51	0	0	3	0
36	X	9	0	0	1	0
36	Y	4	0	0	1	0
36	Z	2	0	0	0	0
36	a	114	0	0	2	0
36	b	126	0	0	1	0
36	c	122	0	0	0	0
36	d	94	0	0	0	0
36	e	13	0	0	1	0
36	f	2	0	0	0	0
36	h	21	0	0	1	0
36	i	8	0	0	1	0
36	j	8	0	0	2	0
36	k	6	0	0	0	0
36	l	8	0	0	0	0
36	m	7	0	0	0	0
36	o	67	0	0	1	0
36	r	1	0	0	0	0
36	t	5	0	0	0	0
36	u	41	0	0	3	0
36	v	31	0	0	2	0
36	x	9	0	0	0	0
36	y	1	0	0	0	0
36	z	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52745	52566	52662	607	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 607 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:40:CYS:SG	35:V:201:HEC:CAC	2.02	1.46
35:F:101:HEC:HBC3	35:F:101:HEC:HHD	1.47	0.95
17:V:40:CYS:SG	35:V:201:HEC:HAC	2.06	0.94
13:O:59:LYS:O	13:O:61:GLN:N	2.07	0.88
13:O:6:THR:HG22	13:O:9:ASP:OD2	1.74	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/344 (114%)	379 (97%)	12 (3%)	0	100	100
1	a	391/344 (114%)	381 (97%)	10 (3%)	0	100	100
2	B	508/506 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/506 (99%)	486 (97%)	15 (3%)	2 (0%)	30	30
3	C	450/461 (98%)	438 (97%)	11 (2%)	1 (0%)	43	48
3	c	459/461 (100%)	445 (97%)	13 (3%)	1 (0%)	43	48
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	75 (94%)	4 (5%)	1 (1%)	9	5
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%)	56 (89%)	7 (11%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	223 (92%)	13 (5%)	7 (3%)	3	1
13	o	242/272 (89%)	229 (95%)	12 (5%)	1 (0%)	30	30
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	0
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%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	89 (94%)	5 (5%)	1 (1%)	11	7
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	16
17	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	24 (86%)	2 (7%)	2 (7%)	1	0
20	Z	60/62 (97%)	48 (80%)	12 (20%)	0	100	100
20	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5374/5690 (94%)	5161 (96%)	192 (4%)	21 (0%)	30	30

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	36	GLN
13	O	59	LYS
13	O	60	ARG
13	O	62	GLU
17	V	64	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/280 (114%)	315 (98%)	5 (2%)	55	65
1	a	319/280 (114%)	306 (96%)	13 (4%)	27	30
2	B	408/404 (101%)	399 (98%)	9 (2%)	45	54
2	b	402/404 (100%)	389 (97%)	13 (3%)	34	40
3	C	353/362 (98%)	342 (97%)	11 (3%)	35	41
3	c	361/362 (100%)	343 (95%)	18 (5%)	22	22
4	D	277/283 (98%)	270 (98%)	7 (2%)	42	50
4	d	278/283 (98%)	266 (96%)	12 (4%)	26	28
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	45
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	45
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	36
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	5
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	41
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	29
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	2
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	195 (95%)	11 (5%)	20	20
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	R	28/32 (88%)	25 (89%)	3 (11%)	6	3
14	r	23/32 (72%)	18 (78%)	5 (22%)	1	0
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	79 (94%)	5 (6%)	17	16
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
17	V	117/138 (85%)	115 (98%)	2 (2%)	53	63
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	28
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	40
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	3
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	z	51/52 (98%)	42 (82%)	9 (18%)	2	0
All	All	4444/4646 (96%)	4253 (96%)	191 (4%)	26	28

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	396	MET
9	j	7	ARG
3	c	468	SER
4	d	321	LEU
11	l	2	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	58	ASN
13	o	61	GLN
20	z	31	GLN
13	O	155	ASN
13	O	132	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	1.04	1 (12%)	8,9,11	1.34	2 (25%)
8	FME	I	1	8	8,9,10	1.04	1 (12%)	8,9,11	1.05	0
15	FME	t	1	15	8,9,10	1.34	1 (12%)	8,9,11	0.74	0
8	FME	i	1	8	8,9,10	1.16	1 (12%)	8,9,11	0.78	0
15	FME	T	1	15	8,9,10	1.07	0	8,9,11	1.39	1 (12%)
12	FME	M	1	12	8,9,10	0.90	0	8,9,11	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' 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	-	2/7/9/11	-

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.08	1.42	1.46
12	m	1	FME	CA-N	-2.34	1.43	1.46
8	i	1	FME	CA-N	-2.21	1.43	1.46
8	I	1	FME	CA-N	-2.03	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	2.90	127.29	122.82
12	m	1	FME	CA-N-CN	-2.35	119.21	122.82
12	m	1	FME	CB-CA-N	2.19	114.50	110.52

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
32	LMG	d	408	-	44,44,55	1.05	4 (9%)	52,52,63	1.27	5 (9%)
23	BCR	h	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.36	8 (14%)
28	DGD	h	102	-	63,63,67	1.27	9 (14%)	77,77,81	1.40	9 (11%)
22	CLA	b	606	-	69,73,73	1.34	8 (11%)	82,113,113	1.58	9 (10%)
22	CLA	d	403	-	69,73,73	1.36	10 (14%)	82,113,113	1.25	7 (8%)
31	STE	M	102	-	14,14,19	0.86	0	14,14,19	0.93	0
26	LHG	A	412	-	48,48,48	0.86	2 (4%)	51,54,54	1.19	5 (9%)
31	STE	b	624	-	9,9,19	0.49	0	8,8,19	0.50	0
28	DGD	c	518	-	63,63,67	1.09	3 (4%)	77,77,81	1.23	4 (5%)
23	BCR	a	406	-	41,41,41	1.07	3 (7%)	56,56,56	1.33	5 (8%)
23	BCR	B	619	-	41,41,41	1.11	3 (7%)	56,56,56	1.55	13 (23%)
30	OEY	a	419[B]	36,1,3	0,16,16	-	-	-	-	-
31	STE	B	625	-	14,14,19	0.48	0	13,13,19	0.78	0
23	BCR	D	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.29	7 (12%)
31	STE	B	623	-	17,17,19	0.72	0	17,17,19	1.02	1 (5%)
31	STE	I	101	-	14,14,19	0.67	0	13,13,19	0.43	0
22	CLA	a	405	-	69,73,73	1.37	11 (15%)	82,113,113	1.14	7 (8%)
22	CLA	b	615	-	69,73,73	1.48	11 (15%)	82,113,113	1.27	8 (9%)
32	LMG	b	621	-	55,55,55	0.94	2 (3%)	63,63,63	1.53	10 (15%)
29	OEX	A	415[A]	36,1,3	0,15,15	-	-	-	-	-
22	CLA	C	510	-	69,73,73	1.36	11 (15%)	82,113,113	1.28	5 (6%)
28	DGD	c	517	-	63,63,67	1.38	8 (12%)	77,77,81	1.42	11 (14%)
22	CLA	B	614	-	69,73,73	1.44	7 (10%)	82,113,113	1.20	9 (10%)
22	CLA	B	612	-	69,73,73	1.38	10 (14%)	82,113,113	1.40	8 (9%)
22	CLA	b	602	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	7 (8%)
31	STE	B	601	-	11,11,19	0.75	0	11,11,19	1.09	1 (9%)
31	STE	L	103	-	11,11,19	0.80	0	11,11,19	1.18	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	F	102	-	34,36,54	1.03	3 (8%)	42,45,65	1.78	9 (21%)
31	STE	M	103	-	9,9,19	0.56	0	8,8,19	0.52	0
22	CLA	B	613	-	69,73,73	1.57	7 (10%)	82,113,113	1.35	9 (10%)
22	CLA	c	507	-	69,73,73	1.35	8 (11%)	82,113,113	1.23	9 (10%)
23	BCR	K	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.32	9 (16%)
22	CLA	B	609	-	69,73,73	1.35	8 (11%)	82,113,113	1.54	7 (8%)
31	STE	b	623	-	19,19,19	0.79	0	19,19,19	0.79	1 (5%)
22	CLA	B	611	-	69,73,73	1.22	6 (8%)	82,113,113	1.29	6 (7%)
31	STE	B	620	-	16,16,19	0.79	1 (6%)	16,16,19	0.94	1 (6%)
23	BCR	B	617	-	41,41,41	1.08	3 (7%)	56,56,56	1.55	11 (19%)
33	PHO	a	404	-	58,69,69	2.03	6 (10%)	55,99,99	1.45	11 (20%)
35	HEC	v	201	17	46,50,50	1.84	5 (10%)	58,82,82	1.85	9 (15%)
22	CLA	b	608	-	69,73,73	1.53	11 (15%)	82,113,113	1.29	7 (8%)
22	CLA	c	513	-	69,73,73	1.26	9 (13%)	82,113,113	1.46	9 (10%)
32	LMG	C	516	-	48,48,55	1.20	3 (6%)	56,56,63	1.54	9 (16%)
26	LHG	d	407	-	38,38,48	1.05	2 (5%)	41,44,54	1.17	2 (4%)
31	STE	Z	101	-	7,7,19	0.53	0	6,6,19	0.34	0
32	LMG	c	523	-	49,49,55	1.06	5 (10%)	57,57,63	1.31	4 (7%)
32	LMG	D	411	-	26,26,55	1.02	1 (3%)	26,26,63	1.20	2 (7%)
31	STE	d	412	-	19,19,19	0.66	0	19,19,19	0.90	1 (5%)
22	CLA	c	512	3	69,73,73	1.51	8 (11%)	82,113,113	1.39	7 (8%)
22	CLA	H	101	36	69,73,73	1.46	9 (13%)	82,113,113	1.36	8 (9%)
26	LHG	l	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	7 (13%)
22	CLA	C	502	-	69,73,73	1.12	7 (10%)	82,113,113	1.34	10 (12%)
22	CLA	C	509	-	69,73,73	1.31	11 (15%)	82,113,113	1.40	11 (13%)
33	PHO	d	401	-	58,69,69	2.12	10 (17%)	55,99,99	1.67	9 (16%)
22	CLA	B	604	-	69,73,73	1.48	9 (13%)	82,113,113	1.87	13 (15%)
27	SQD	A	411	-	50,52,54	1.10	6 (12%)	60,63,65	2.10	15 (25%)
31	STE	T	102	-	15,15,19	0.48	0	14,14,19	0.82	0
25	PL9	A	408	-	55,55,55	1.61	12 (21%)	68,69,69	1.71	16 (23%)
25	PL9	d	405	-	55,55,55	1.52	6 (10%)	68,69,69	1.59	12 (17%)
31	STE	C	521	-	15,15,19	0.56	0	14,14,19	0.52	0
31	STE	C	522	-	11,11,19	0.96	1 (9%)	11,11,19	1.02	0
26	LHG	e	101	-	41,41,48	1.13	4 (9%)	44,47,54	1.27	3 (6%)
35	HEC	f	101	5,6	46,50,50	1.81	7 (15%)	58,82,82	2.00	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	402	-	69,73,73	1.38	12 (17%)	82,113,113	1.48	11 (13%)
22	CLA	b	601	36	69,73,73	1.44	10 (14%)	82,113,113	1.55	10 (12%)
22	CLA	b	614	-	69,73,73	1.25	9 (13%)	82,113,113	1.27	7 (8%)
31	STE	a	416	-	11,11,19	0.89	0	11,11,19	1.17	1 (9%)
32	LMG	m	101	-	51,51,55	1.17	4 (7%)	59,59,63	1.60	9 (15%)
31	STE	c	501	-	11,11,19	0.84	0	11,11,19	1.00	0
32	LMG	M	101	-	51,51,55	0.87	1 (1%)	59,59,63	1.37	10 (16%)
33	PHO	D	401	-	58,69,69	1.75	11 (18%)	55,99,99	1.43	9 (16%)
22	CLA	c	503	-	69,73,73	1.49	8 (11%)	82,113,113	1.38	14 (17%)
22	CLA	C	511	3	69,73,73	1.50	10 (14%)	82,113,113	1.18	5 (6%)
32	LMG	D	410	-	31,31,55	1.26	4 (12%)	33,33,63	1.16	3 (9%)
35	HEC	F	101	5,6	46,50,50	1.84	5 (10%)	58,82,82	1.78	8 (13%)
22	CLA	D	405	-	69,73,73	1.36	8 (11%)	82,113,113	1.24	7 (8%)
31	STE	B	624	-	15,15,19	0.60	0	14,14,19	0.50	0
23	BCR	b	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.40	8 (14%)
22	CLA	c	509	-	68,72,73	1.48	11 (16%)	80,111,113	1.36	7 (8%)
22	CLA	b	603	-	69,73,73	1.30	8 (11%)	82,113,113	1.47	11 (13%)
23	BCR	X	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.37	8 (14%)
23	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.10	4 (7%)
31	STE	j	101	-	11,11,19	0.75	0	11,11,19	1.39	2 (18%)
23	BCR	k	102	-	41,41,41	1.07	3 (7%)	56,56,56	1.20	6 (10%)
27	SQD	A	413	-	38,38,54	1.10	4 (10%)	40,40,65	1.40	4 (10%)
31	STE	H	103	-	17,17,19	0.49	0	16,16,19	0.69	0
32	LMG	c	520	-	37,37,55	1.12	4 (10%)	45,45,63	1.38	7 (15%)
22	CLA	c	511	-	69,73,73	1.35	7 (10%)	82,113,113	1.47	7 (8%)
22	CLA	A	409	36	69,73,73	1.04	4 (5%)	82,113,113	1.38	9 (10%)
27	SQD	B	621	-	52,54,54	0.94	2 (3%)	62,65,65	2.15	16 (25%)
31	STE	h	103	-	13,13,19	0.45	0	12,12,19	0.62	0
23	BCR	t	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.49	10 (17%)
32	LMG	c	522	-	48,48,55	1.20	4 (8%)	56,56,63	1.26	6 (10%)
22	CLA	b	610	36	69,73,73	1.11	6 (8%)	82,113,113	1.40	12 (14%)
23	BCR	b	618	-	41,41,41	1.29	3 (7%)	56,56,56	1.34	7 (12%)
31	STE	b	620	-	19,19,19	0.86	1 (5%)	19,19,19	0.93	0
23	BCR	T	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.25	4 (7%)
22	CLA	C	513	-	69,73,73	1.35	11 (15%)	82,113,113	1.50	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	504	-	69,73,73	1.20	6 (8%)	82,113,113	1.32	5 (6%)
32	LMG	D	408	-	51,51,55	0.99	3 (5%)	59,59,63	1.46	7 (11%)
31	STE	d	411	-	19,19,19	0.63	0	19,19,19	1.07	2 (10%)
22	CLA	B	602	-	69,73,73	1.26	8 (11%)	82,113,113	1.36	10 (12%)
23	BCR	A	405	-	41,41,41	1.15	1 (2%)	56,56,56	1.43	8 (14%)
27	SQD	a	414	-	35,35,54	1.13	2 (5%)	37,37,65	1.32	3 (8%)
22	CLA	b	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.41	14 (17%)
22	CLA	C	503	-	69,73,73	1.37	9 (13%)	82,113,113	1.52	9 (10%)
27	SQD	a	413	-	52,54,54	0.94	4 (7%)	62,65,65	1.93	11 (17%)
28	DGD	C	517	-	63,63,67	1.42	10 (15%)	77,77,81	1.37	13 (16%)
22	CLA	c	502	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	9 (10%)
29	OEX	a	418[A]	36,1,3	0,15,15	-	-	-		
31	STE	T	103	-	14,14,19	0.53	0	13,13,19	0.71	0
22	CLA	c	505	36	64,68,73	1.31	7 (10%)	76,107,113	1.40	15 (19%)
22	CLA	c	506	-	69,73,73	1.23	7 (10%)	82,113,113	1.54	12 (14%)
35	HEC	V	201	17	46,50,50	1.77	7 (15%)	58,82,82	1.95	6 (10%)
31	STE	J	101	-	11,11,19	0.77	0	11,11,19	1.30	2 (18%)
32	LMG	Y	101	-	48,48,55	1.20	6 (12%)	56,56,63	1.21	5 (8%)
33	PHO	D	402	-	58,69,69	1.89	11 (18%)	55,99,99	1.56	10 (18%)
22	CLA	B	603	-	69,73,73	1.23	9 (13%)	82,113,113	1.37	10 (12%)
22	CLA	A	404	-	58,62,73	1.33	8 (13%)	68,99,113	1.28	6 (8%)
31	STE	D	413	-	19,19,19	0.66	0	19,19,19	1.06	0
22	CLA	b	612	-	69,73,73	1.34	9 (13%)	82,113,113	1.43	11 (13%)
30	OXY	A	416[B]	36,1,3	0,16,16	-	-	-		
22	CLA	b	607	36	69,73,73	1.50	9 (13%)	82,113,113	1.41	11 (13%)
22	CLA	C	512	-	69,73,73	1.58	8 (11%)	82,113,113	1.32	11 (13%)
31	STE	b	622	-	15,15,19	1.02	1 (6%)	15,15,19	1.14	2 (13%)
22	CLA	B	605	-	69,73,73	1.37	9 (13%)	82,113,113	1.17	9 (10%)
31	STE	B	622	-	11,11,19	0.91	1 (9%)	11,11,19	1.27	1 (9%)
34	BCT	a	409	21	3,3,3	1.59	0	2,3,3	3.76	2 (100%)
26	LHG	d	406	-	48,48,48	0.82	2 (4%)	51,54,54	1.18	2 (3%)
23	BCR	K	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	8 (14%)
31	STE	a	415	-	9,9,19	0.56	0	8,8,19	0.55	0
22	CLA	C	508	-	69,73,73	1.24	5 (7%)	82,113,113	1.24	9 (10%)
27	SQD	L	101	-	47,49,54	0.94	2 (4%)	57,60,65	2.46	19 (33%)
22	CLA	c	514	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	c	516	-	41,41,41	1.19	4 (9%)	56,56,56	1.53	9 (16%)
22	CLA	a	411	36	69,73,73	1.44	7 (10%)	82,113,113	1.28	9 (10%)
22	CLA	C	506	-	69,73,73	1.49	9 (13%)	82,113,113	1.38	9 (10%)
22	CLA	D	404	-	69,73,73	1.43	9 (13%)	82,113,113	1.35	11 (13%)
25	PL9	D	407	-	55,55,55	1.20	5 (9%)	68,69,69	1.82	18 (26%)
22	CLA	b	609	-	69,73,73	1.48	8 (11%)	82,113,113	1.45	10 (12%)
25	PL9	a	410	-	55,55,55	0.94	2 (3%)	68,69,69	1.59	11 (16%)
26	LHG	a	412	-	48,48,48	1.11	5 (10%)	51,54,54	1.44	9 (17%)
31	STE	c	521	-	19,19,19	0.81	1 (5%)	19,19,19	0.70	0
23	BCR	c	515	-	41,41,41	1.03	3 (7%)	56,56,56	1.30	10 (17%)
22	CLA	B	615	-	69,73,73	1.50	10 (14%)	82,113,113	1.48	6 (7%)
28	DGD	c	519	-	63,63,67	1.11	7 (11%)	77,77,81	1.37	13 (16%)
23	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.17	6 (10%)
22	CLA	A	403	36	69,73,73	1.45	9 (13%)	82,113,113	1.28	10 (12%)
27	SQD	d	409	-	39,41,54	1.14	3 (7%)	49,52,65	1.88	13 (26%)
22	CLA	C	504	36	63,67,73	1.58	10 (15%)	74,105,113	1.38	12 (16%)
22	CLA	b	613	-	69,73,73	1.28	6 (8%)	82,113,113	1.20	7 (8%)
22	CLA	b	616	-	64,68,73	1.20	9 (14%)	76,107,113	1.40	12 (15%)
26	LHG	D	412	-	48,48,48	0.99	4 (8%)	51,54,54	1.36	7 (13%)
28	DGD	C	519	-	63,63,67	1.16	9 (14%)	77,77,81	1.38	7 (9%)
26	LHG	D	409	-	48,48,48	1.34	5 (10%)	51,54,54	1.27	7 (13%)
28	DGD	H	102	-	63,63,67	1.30	7 (11%)	77,77,81	1.34	8 (10%)
31	STE	t	102	-	13,13,19	0.74	0	13,13,19	1.24	2 (15%)
31	STE	d	410	-	16,16,19	0.72	1 (6%)	16,16,19	1.41	2 (12%)
31	STE	C	520	-	11,11,19	0.97	1 (9%)	11,11,19	1.17	1 (9%)
34	BCT	D	403	21	3,3,3	1.03	0	2,3,3	3.04	1 (50%)
22	CLA	c	508	36	69,73,73	1.67	7 (10%)	82,113,113	1.43	10 (12%)
22	CLA	b	604	-	69,73,73	1.28	8 (11%)	82,113,113	1.81	15 (18%)
28	DGD	A	414	-	67,67,67	1.41	10 (14%)	81,81,81	1.41	13 (16%)
22	CLA	B	608	-	69,73,73	1.31	9 (13%)	82,113,113	1.50	13 (15%)
31	STE	R	101	-	11,11,19	0.95	0	11,11,19	0.83	0
22	CLA	a	403	36	69,73,73	1.48	11 (15%)	82,113,113	1.37	8 (9%)
22	CLA	a	402	-	69,73,73	1.48	11 (15%)	82,113,113	1.14	8 (9%)
23	BCR	C	514	-	41,41,41	1.30	4 (9%)	56,56,56	1.27	6 (10%)
28	DGD	C	518	-	63,63,67	1.11	4 (6%)	77,77,81	1.36	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	C	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	8 (14%)
22	CLA	c	510	-	69,73,73	1.25	8 (11%)	82,113,113	1.51	8 (9%)
31	STE	M	104	-	17,17,19	0.37	0	16,16,19	0.88	0
26	LHG	L	102	-	48,48,48	0.78	2 (4%)	51,54,54	1.17	2 (3%)
23	BCR	B	618	-	41,41,41	1.08	3 (7%)	56,56,56	1.43	9 (16%)
22	CLA	C	507	36	69,73,73	1.42	10 (14%)	82,113,113	1.52	6 (7%)
22	CLA	B	606	-	69,73,73	1.47	8 (11%)	82,113,113	1.34	9 (10%)
22	CLA	d	402	-	69,73,73	1.11	6 (8%)	82,113,113	1.12	8 (9%)
26	LHG	A	410	-	46,46,48	1.21	5 (10%)	49,52,54	1.18	4 (8%)
32	LMG	a	417	-	55,55,55	1.59	10 (18%)	63,63,63	1.50	11 (17%)
22	CLA	B	616	-	64,68,73	1.49	9 (14%)	76,107,113	1.52	6 (7%)
22	CLA	b	605	-	69,73,73	1.15	7 (10%)	82,113,113	1.49	9 (10%)
22	CLA	B	607	36	69,73,73	1.27	6 (8%)	82,113,113	1.46	7 (8%)
23	BCR	b	617	-	41,41,41	1.01	3 (7%)	56,56,56	1.31	8 (14%)
22	CLA	C	501	-	69,73,73	1.43	11 (15%)	82,113,113	1.28	9 (10%)
22	CLA	B	610	36	69,73,73	1.28	9 (13%)	82,113,113	1.33	9 (10%)
22	CLA	C	505	-	69,73,73	1.41	6 (8%)	82,113,113	1.32	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	d	408	-	-	12/39/59/70	0/1/1/1
23	BCR	h	101	-	-	8/29/63/63	0/2/2/2
28	DGD	h	102	-	-	15/51/91/95	0/2/2/2
22	CLA	b	606	-	1/1/20/20	2/39/115/115	-
22	CLA	d	403	-	-	8/39/115/115	-
31	STE	M	102	-	-	9/12/12/17	-
26	LHG	A	412	-	-	27/53/53/53	-
31	STE	b	624	-	-	2/7/7/17	-
28	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	BCR	a	406	-	-	7/29/63/63	0/2/2/2
23	BCR	B	619	-	-	6/29/63/63	0/2/2/2
31	STE	B	625	-	-	7/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	D	406	-	-	4/29/63/63	0/2/2/2
31	STE	B	623	-	-	10/15/15/17	-
31	STE	I	101	-	-	4/12/12/17	-
22	CLA	a	405	-	1/1/20/20	9/39/115/115	-
22	CLA	b	615	-	1/1/20/20	3/39/115/115	-
32	LMG	b	621	-	-	25/50/70/70	0/1/1/1
22	CLA	C	510	-	1/1/20/20	6/39/115/115	-
28	DGD	c	517	-	-	29/51/91/95	0/2/2/2
22	CLA	B	614	-	1/1/20/20	13/39/115/115	-
22	CLA	B	612	-	1/1/20/20	7/39/115/115	-
22	CLA	b	602	-	-	6/39/115/115	-
31	STE	B	601	-	-	7/9/9/17	-
31	STE	L	103	-	-	4/9/9/17	-
27	SQD	F	102	-	-	14/28/48/69	0/1/1/1
31	STE	M	103	-	-	2/7/7/17	-
22	CLA	B	613	-	1/1/20/20	11/39/115/115	-
22	CLA	c	507	-	1/1/20/20	13/39/115/115	-
23	BCR	K	101	-	-	8/29/63/63	0/2/2/2
22	CLA	B	609	-	-	2/39/115/115	-
31	STE	b	623	-	-	11/17/17/17	-
22	CLA	B	611	-	1/1/20/20	4/39/115/115	-
31	STE	B	620	-	-	9/14/14/17	-
23	BCR	B	617	-	-	9/29/63/63	0/2/2/2
33	PHO	a	404	-	-	4/37/103/103	0/5/6/6
35	HEC	v	201	17	-	6/14/54/54	-
22	CLA	b	608	-	1/1/20/20	7/39/115/115	-
22	CLA	c	513	-	1/1/20/20	19/39/115/115	-
32	LMG	C	516	-	-	19/43/63/70	0/1/1/1
26	LHG	d	407	-	-	14/43/43/53	-
31	STE	Z	101	-	-	2/5/5/17	-
32	LMG	c	523	-	-	22/44/64/70	0/1/1/1
32	LMG	D	411	-	-	9/22/22/70	-
31	STE	d	412	-	-	11/17/17/17	-
22	CLA	c	512	3	1/1/20/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	101	36	1/1/20/20	18/39/115/115	-
26	LHG	l	101	-	-	14/53/53/53	-
22	CLA	C	502	-	1/1/20/20	9/39/115/115	-
22	CLA	C	509	-	1/1/20/20	11/39/115/115	-
33	PHO	d	401	-	-	10/37/103/103	0/5/6/6
22	CLA	B	604	-	1/1/20/20	9/39/115/115	-
27	SQD	A	411	-	-	23/47/67/69	0/1/1/1
31	STE	T	102	-	-	10/13/13/17	-
25	PL9	A	408	-	-	20/53/73/73	0/1/1/1
25	PL9	d	405	-	-	15/53/73/73	0/1/1/1
31	STE	C	521	-	-	6/13/13/17	-
31	STE	C	522	-	-	1/9/9/17	-
26	LHG	e	101	-	-	24/46/46/53	-
35	HEC	f	101	5,6	-	6/14/54/54	-
22	CLA	A	402	-	1/1/20/20	9/39/115/115	-
22	CLA	b	601	36	1/1/20/20	22/39/115/115	-
22	CLA	b	614	-	1/1/20/20	16/39/115/115	-
31	STE	a	416	-	-	4/9/9/17	-
32	LMG	m	101	-	-	21/46/66/70	0/1/1/1
31	STE	c	501	-	-	7/9/9/17	-
32	LMG	M	101	-	-	25/46/66/70	0/1/1/1
33	PHO	D	401	-	-	5/37/103/103	0/5/6/6
22	CLA	c	503	-	1/1/20/20	7/39/115/115	-
22	CLA	C	511	3	1/1/20/20	8/39/115/115	-
32	LMG	D	410	-	-	13/33/33/70	-
35	HEC	F	101	5,6	-	5/14/54/54	-
22	CLA	D	405	-	1/1/20/20	12/39/115/115	-
31	STE	B	624	-	-	10/13/13/17	-
23	BCR	b	619	-	-	8/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/19/20	3/38/114/115	-
22	CLA	b	603	-	1/1/20/20	4/39/115/115	-
23	BCR	X	101	-	-	6/29/63/63	0/2/2/2
23	BCR	k	101	-	-	9/29/63/63	0/2/2/2
31	STE	j	101	-	-	4/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	k	102	-	-	9/29/63/63	0/2/2/2
27	SQD	A	413	-	-	18/39/39/69	-
31	STE	H	103	-	-	8/15/15/17	-
32	LMG	c	520	-	-	7/31/51/70	0/1/1/1
22	CLA	c	511	-	1/1/20/20	10/39/115/115	-
22	CLA	A	409	36	1/1/20/20	5/39/115/115	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
31	STE	h	103	-	-	6/11/11/17	-
23	BCR	t	101	-	-	6/29/63/63	0/2/2/2
32	LMG	c	522	-	-	25/43/63/70	0/1/1/1
22	CLA	b	610	36	1/1/20/20	7/39/115/115	-
23	BCR	b	618	-	-	4/29/63/63	0/2/2/2
31	STE	b	620	-	-	9/17/17/17	-
23	BCR	T	101	-	-	10/29/63/63	0/2/2/2
22	CLA	C	513	-	1/1/20/20	9/39/115/115	-
22	CLA	c	504	-	1/1/20/20	5/39/115/115	-
32	LMG	D	408	-	-	15/46/66/70	0/1/1/1
31	STE	d	411	-	-	11/17/17/17	-
22	CLA	B	602	-	1/1/20/20	8/39/115/115	-
23	BCR	A	405	-	-	9/29/63/63	0/2/2/2
27	SQD	a	414	-	-	16/37/37/69	-
22	CLA	b	611	-	1/1/20/20	7/39/115/115	-
22	CLA	C	503	-	1/1/20/20	2/39/115/115	-
27	SQD	a	413	-	-	25/49/69/69	0/1/1/1
28	DGD	C	517	-	-	19/51/91/95	0/2/2/2
22	CLA	c	502	-	1/1/20/20	5/39/115/115	-
31	STE	T	103	-	-	8/12/12/17	-
22	CLA	c	505	36	1/1/19/20	5/33/109/115	-
22	CLA	c	506	-	1/1/20/20	11/39/115/115	-
35	HEC	V	201	17	-	6/14/54/54	-
31	STE	J	101	-	-	2/9/9/17	-
32	LMG	Y	101	-	-	23/43/63/70	0/1/1/1
33	PHO	D	402	-	-	4/37/103/103	0/5/6/6
22	CLA	B	603	-	1/1/20/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	404	-	1/1/17/20	2/26/102/115	-
31	STE	D	413	-	-	12/17/17/17	-
22	CLA	b	612	-	1/1/20/20	4/39/115/115	-
22	CLA	b	607	36	1/1/20/20	10/39/115/115	-
22	CLA	C	512	-	1/1/20/20	10/39/115/115	-
31	STE	b	622	-	-	6/13/13/17	-
22	CLA	B	605	-	1/1/20/20	14/39/115/115	-
31	STE	B	622	-	-	7/9/9/17	-
26	LHG	d	406	-	-	23/53/53/53	-
23	BCR	K	102	-	-	11/29/63/63	0/2/2/2
31	STE	a	415	-	-	3/7/7/17	-
22	CLA	C	508	-	-	6/39/115/115	-
27	SQD	L	101	-	-	18/44/64/69	0/1/1/1
22	CLA	c	514	-	1/1/20/20	8/39/115/115	-
23	BCR	c	516	-	-	5/29/63/63	0/2/2/2
22	CLA	a	411	36	1/1/20/20	3/39/115/115	-
22	CLA	C	506	-	1/1/20/20	12/39/115/115	-
22	CLA	D	404	-	-	10/39/115/115	-
25	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	609	-	-	7/39/115/115	-
25	PL9	a	410	-	-	19/53/73/73	0/1/1/1
26	LHG	a	412	-	-	20/53/53/53	-
31	STE	c	521	-	-	10/17/17/17	-
23	BCR	c	515	-	-	8/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	9/39/115/115	-
28	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	BCR	d	404	-	-	4/29/63/63	0/2/2/2
22	CLA	A	403	36	1/1/20/20	9/39/115/115	-
27	SQD	d	409	-	-	13/36/56/69	0/1/1/1
22	CLA	C	504	36	1/1/18/20	5/32/108/115	-
22	CLA	b	613	-	1/1/20/20	6/39/115/115	-
22	CLA	b	616	-	1/1/19/20	9/33/109/115	-
26	LHG	D	412	-	-	15/53/53/53	-
28	DGD	C	519	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	D	409	-	-	22/53/53/53	-
28	DGD	H	102	-	-	17/51/91/95	0/2/2/2
31	STE	t	102	-	-	4/11/11/17	-
31	STE	d	410	-	-	12/14/14/17	-
31	STE	C	520	-	-	3/9/9/17	-
22	CLA	c	508	36	1/1/20/20	12/39/115/115	-
22	CLA	b	604	-	1/1/20/20	9/39/115/115	-
28	DGD	A	414	-	-	27/55/95/95	0/2/2/2
22	CLA	B	608	-	1/1/20/20	3/39/115/115	-
31	STE	R	101	-	-	3/9/9/17	-
22	CLA	a	403	36	-	10/39/115/115	-
22	CLA	a	402	-	1/1/20/20	5/39/115/115	-
23	BCR	C	514	-	-	5/29/63/63	0/2/2/2
28	DGD	C	518	-	-	21/51/91/95	0/2/2/2
23	BCR	C	515	-	-	11/29/63/63	0/2/2/2
22	CLA	c	510	-	1/1/20/20	11/39/115/115	-
31	STE	M	104	-	-	7/15/15/17	-
26	LHG	L	102	-	-	16/53/53/53	-
23	BCR	B	618	-	-	3/29/63/63	0/2/2/2
22	CLA	C	507	36	1/1/20/20	5/39/115/115	-
22	CLA	B	606	-	1/1/20/20	9/39/115/115	-
22	CLA	d	402	-	-	8/39/115/115	-
26	LHG	A	410	-	-	23/51/51/53	-
32	LMG	a	417	-	-	30/50/70/70	0/1/1/1
22	CLA	B	616	-	1/1/19/20	9/33/109/115	-
22	CLA	b	605	-	1/1/20/20	5/39/115/115	-
22	CLA	B	607	36	1/1/20/20	13/39/115/115	-
23	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	2/39/115/115	-
22	CLA	B	610	36	1/1/20/20	6/39/115/115	-
22	CLA	C	505	-	1/1/20/20	8/39/115/115	-

The worst 5 of 921 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	404	PHO	C1B-C2B	10.14	1.50	1.39
33	d	401	PHO	C1B-C2B	9.39	1.49	1.39
22	c	508	CLA	MG-NB	-8.38	1.89	2.05
33	D	402	PHO	C1B-C2B	8.23	1.48	1.39
22	c	503	CLA	MG-NB	-8.19	1.89	2.05

The worst 5 of 1277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O6-C1-C2	11.79	126.19	108.27
22	B	604	CLA	C4A-NA-C1A	11.68	112.01	106.68
22	b	604	CLA	C4A-NA-C1A	10.41	111.43	106.68
35	V	201	HEC	CBB-CAB-C3B	-10.03	107.39	127.43
35	v	201	HEC	CBB-CAB-C3B	-9.31	108.83	127.43

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	409	CLA	ND
22	B	602	CLA	ND

5 of 1842 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C14-C13-C15-C16
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CHA-CBD-CGD-O2D
22	B	616	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

110 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	606	CLA	4	0
26	A	412	LHG	2	0
23	B	619	BCR	3	0
31	B	625	STE	1	0
23	D	406	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	615	CLA	2	0
32	b	621	LMG	1	0
22	B	614	CLA	1	0
22	B	612	CLA	2	0
22	b	602	CLA	1	0
27	F	102	SQD	1	0
22	B	613	CLA	1	0
22	c	507	CLA	1	0
23	K	101	BCR	2	0
22	B	609	CLA	2	0
23	B	617	BCR	2	0
33	a	404	PHO	2	0
35	v	201	HEC	2	0
32	C	516	LMG	1	0
31	Z	101	STE	1	0
31	d	412	STE	5	0
22	c	512	CLA	3	0
22	H	101	CLA	4	0
22	C	509	CLA	1	0
33	d	401	PHO	2	0
22	B	604	CLA	7	0
27	A	411	SQD	1	0
25	A	408	PL9	5	0
35	f	101	HEC	7	0
22	A	402	CLA	2	0
22	b	601	CLA	1	0
22	b	614	CLA	2	0
32	m	101	LMG	2	0
32	M	101	LMG	2	0
33	D	401	PHO	1	0
22	c	503	CLA	2	0
22	C	511	CLA	2	0
35	F	101	HEC	7	0
22	D	405	CLA	2	0
23	b	619	BCR	1	0
22	c	509	CLA	1	0
23	X	101	BCR	5	0
23	k	101	BCR	2	0
31	j	101	STE	1	0
23	k	102	BCR	3	0
27	A	413	SQD	1	0
31	H	103	STE	1	0

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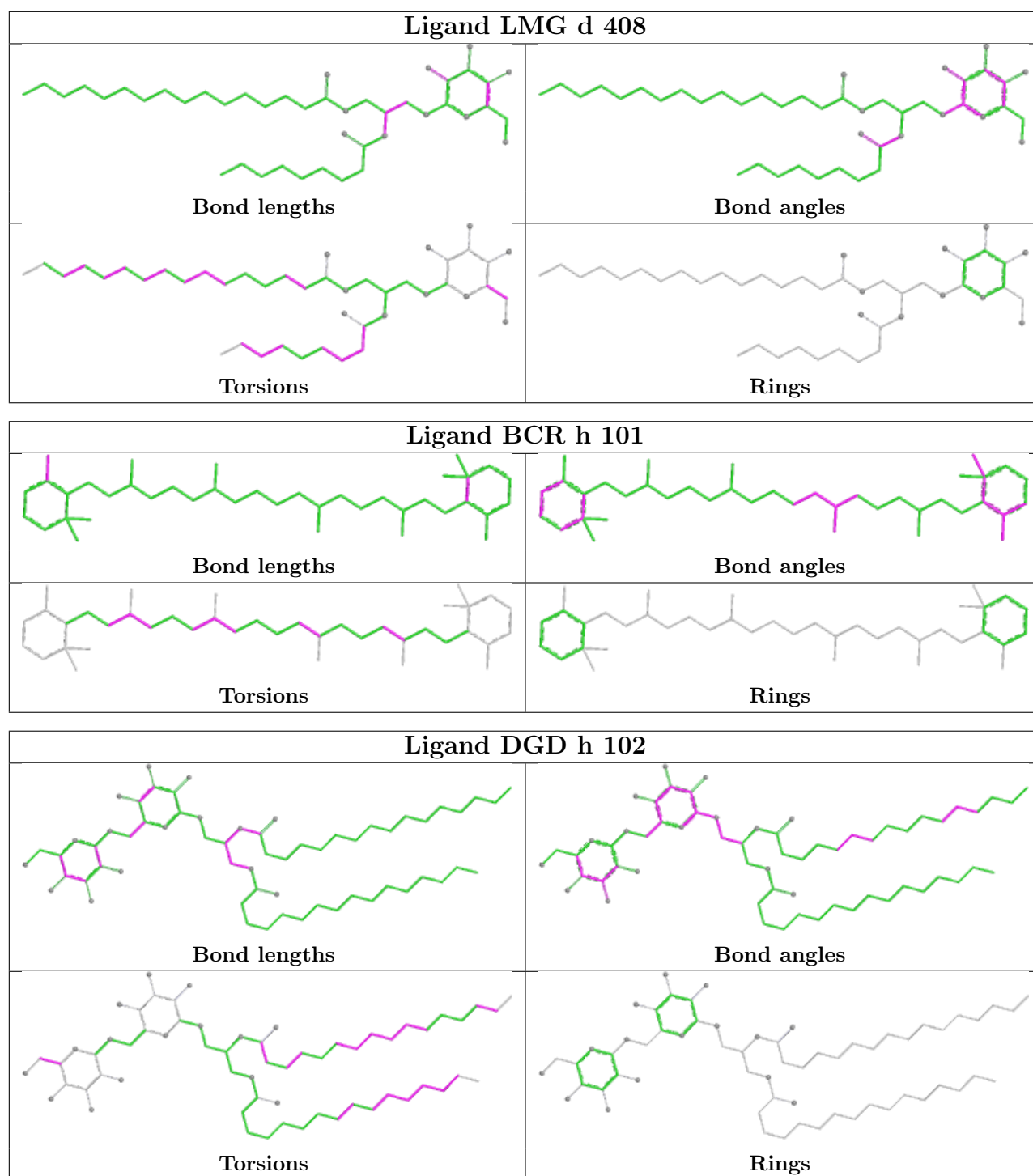
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	511	CLA	1	0
22	A	409	CLA	3	0
27	B	621	SQD	1	0
31	h	103	STE	2	0
23	t	101	BCR	4	0
23	b	618	BCR	1	0
31	b	620	STE	1	0
23	T	101	BCR	1	0
22	C	513	CLA	1	0
31	d	411	STE	1	0
23	A	405	BCR	1	0
27	a	414	SQD	1	0
22	c	502	CLA	1	0
22	c	506	CLA	1	0
35	V	201	HEC	5	0
33	D	402	PHO	3	0
22	B	603	CLA	1	0
31	D	413	STE	1	0
30	A	416[B]	OEY	1	0
22	b	607	CLA	3	0
22	C	512	CLA	1	0
31	b	622	STE	1	0
22	B	605	CLA	4	0
23	K	102	BCR	1	0
27	L	101	SQD	1	0
22	c	514	CLA	2	0
23	c	516	BCR	4	0
22	a	411	CLA	3	0
22	C	506	CLA	3	0
22	D	404	CLA	4	0
25	D	407	PL9	2	0
22	b	609	CLA	1	0
25	a	410	PL9	2	0
26	a	412	LHG	2	0
31	c	521	STE	1	0
23	c	515	BCR	2	0
28	c	519	DGD	1	0
23	d	404	BCR	2	0
22	A	403	CLA	3	0
27	d	409	SQD	2	0
22	b	613	CLA	5	0
22	b	616	CLA	1	0

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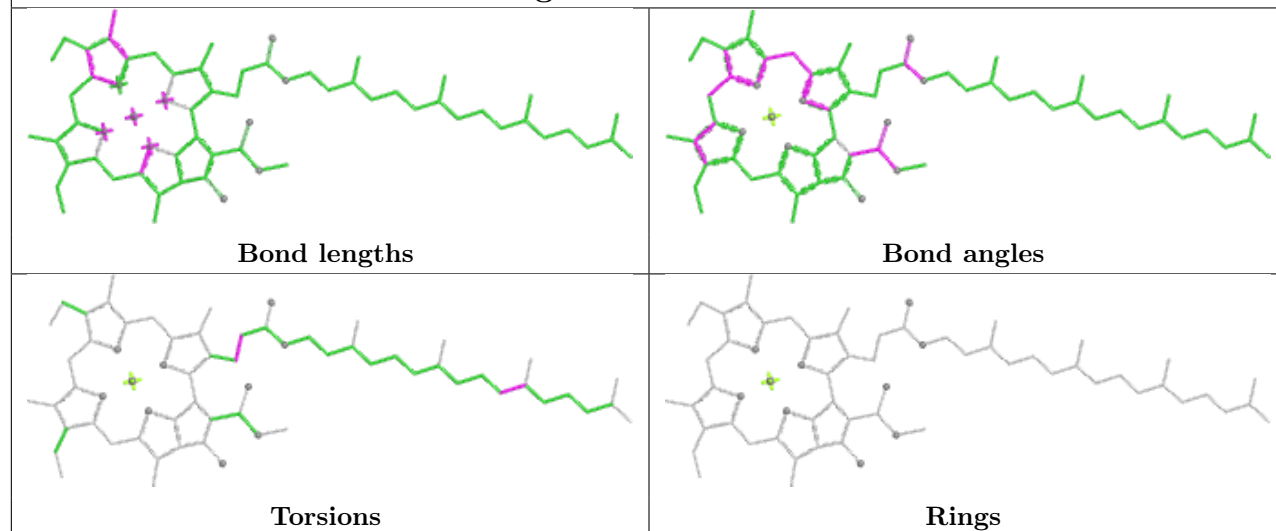
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	412	LHG	3	0
26	D	409	LHG	1	0
31	d	410	STE	4	0
34	D	403	BCT	2	0
22	c	508	CLA	1	0
22	b	604	CLA	2	0
28	A	414	DGD	3	0
22	B	608	CLA	2	0
23	C	514	BCR	3	0
23	C	515	BCR	1	0
31	M	104	STE	2	0
26	L	102	LHG	2	0
23	B	618	BCR	3	0
22	B	606	CLA	1	0
22	d	402	CLA	1	0
32	a	417	LMG	3	0
22	b	605	CLA	1	0
23	b	617	BCR	2	0
22	C	501	CLA	2	0
22	B	610	CLA	1	0
22	C	505	CLA	2	0

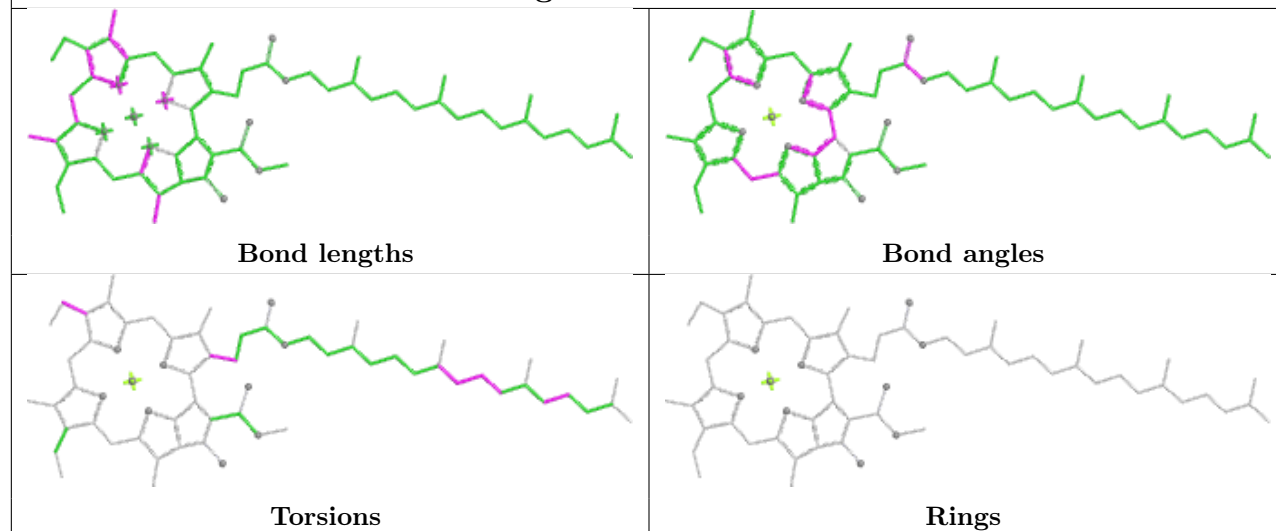
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



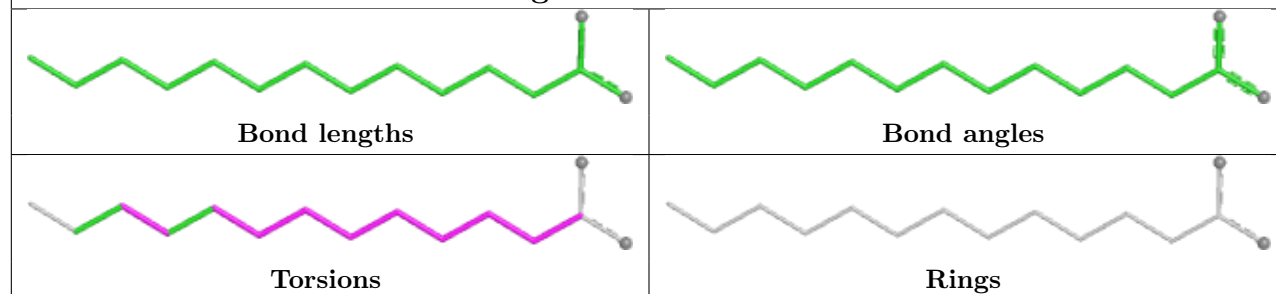
Ligand CLA b 606

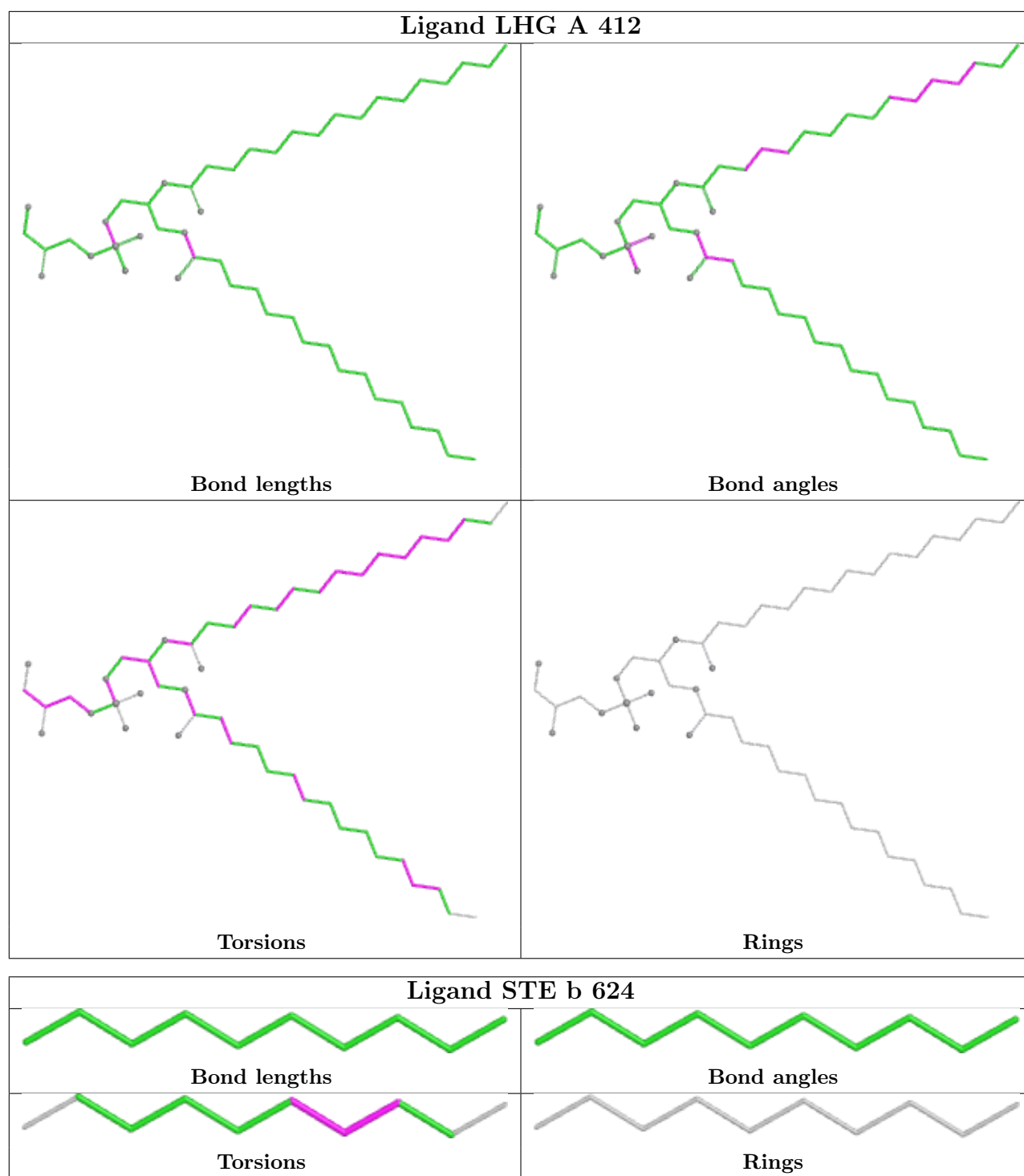


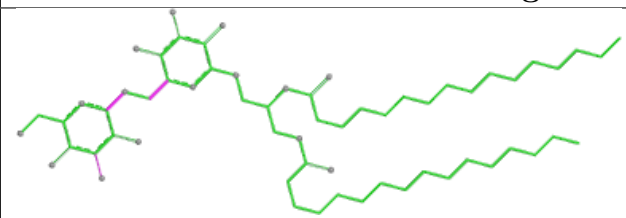
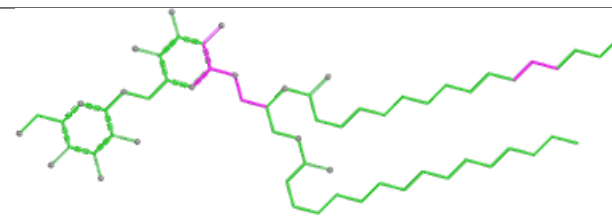
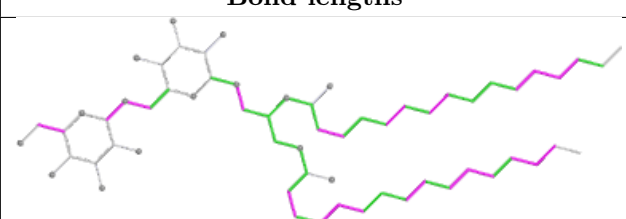
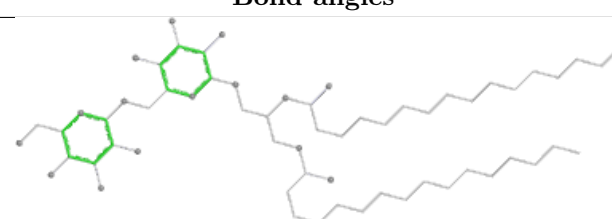
Ligand CLA d 403

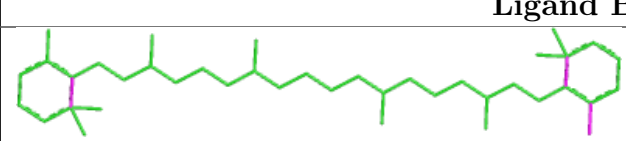
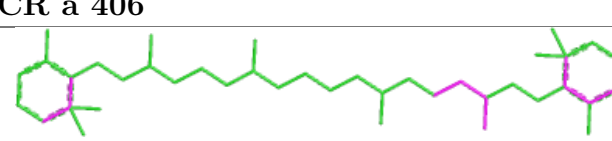
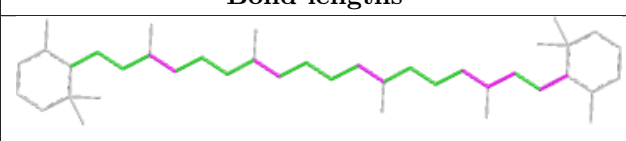
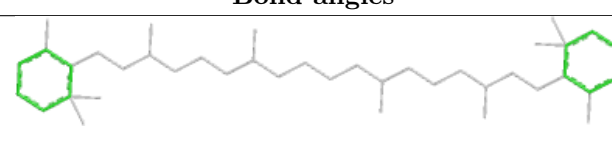


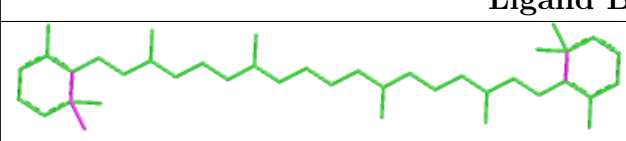
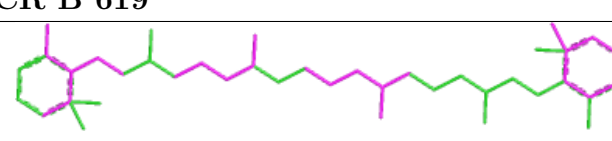
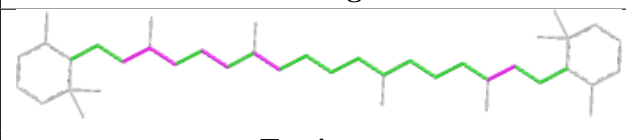
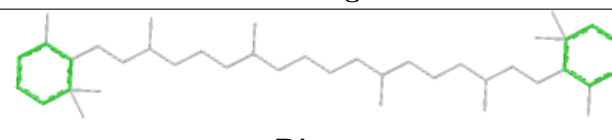
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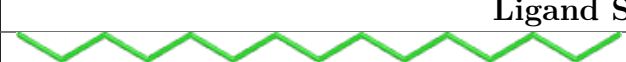
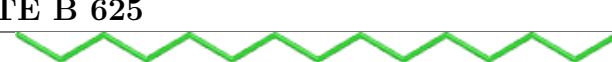
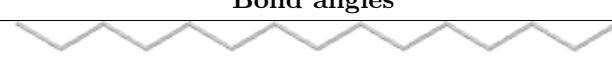


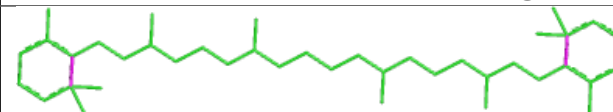
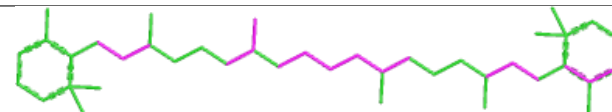
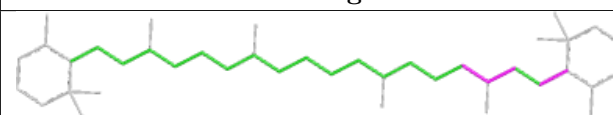
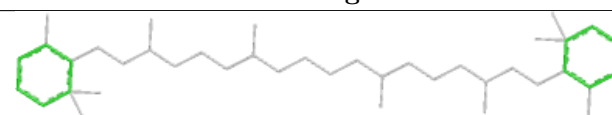


Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

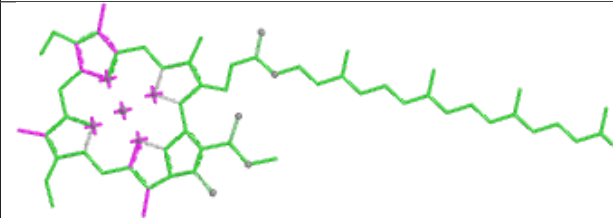
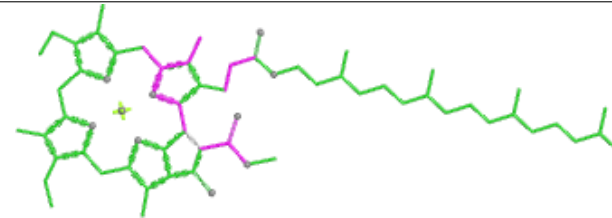
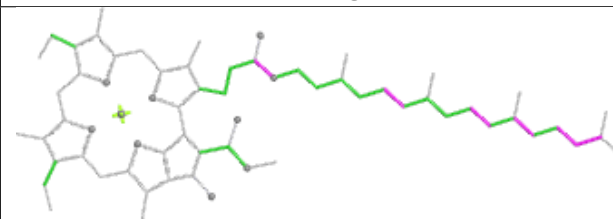
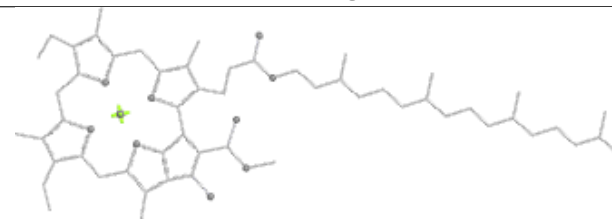
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

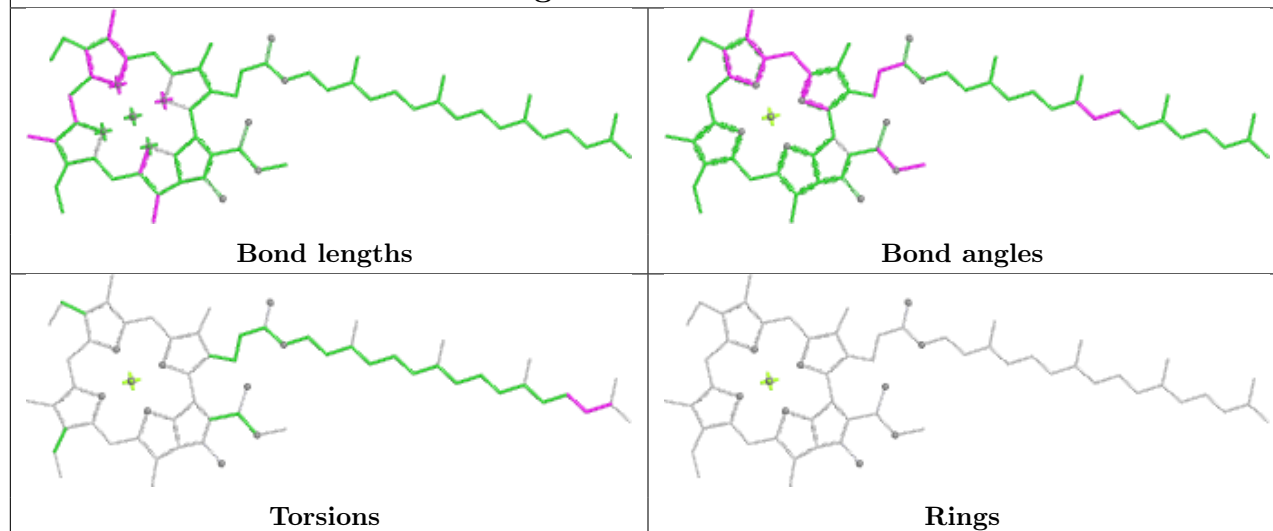
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

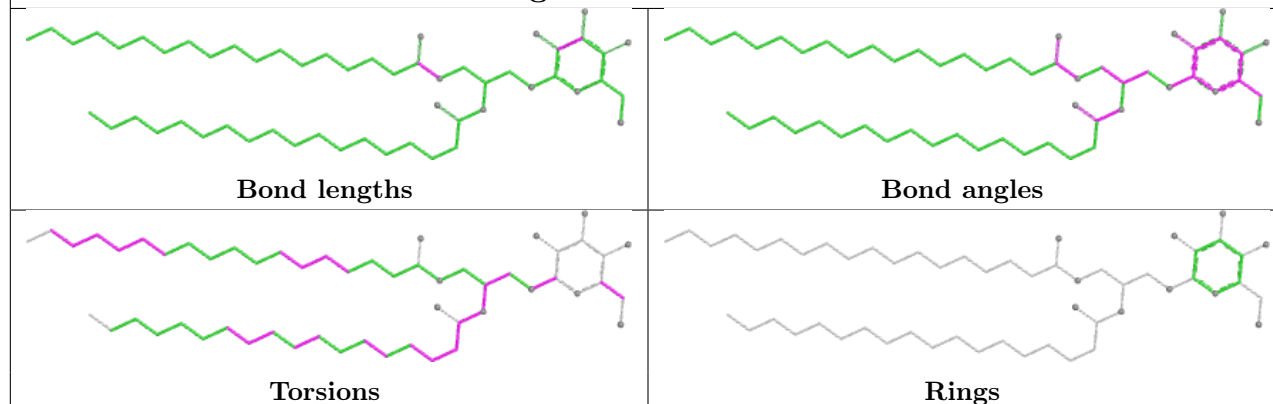
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

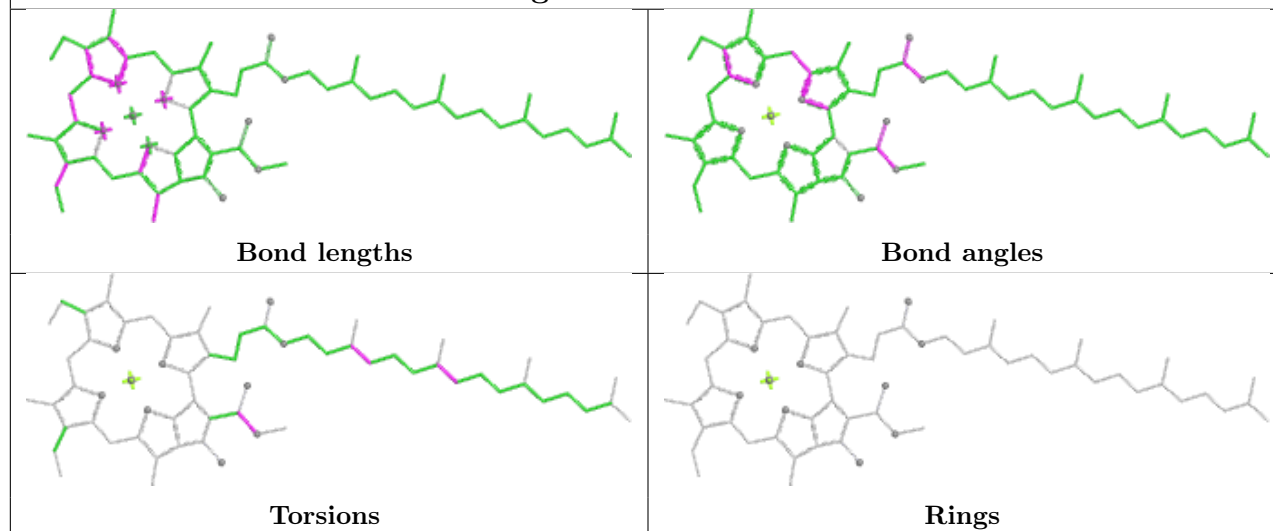
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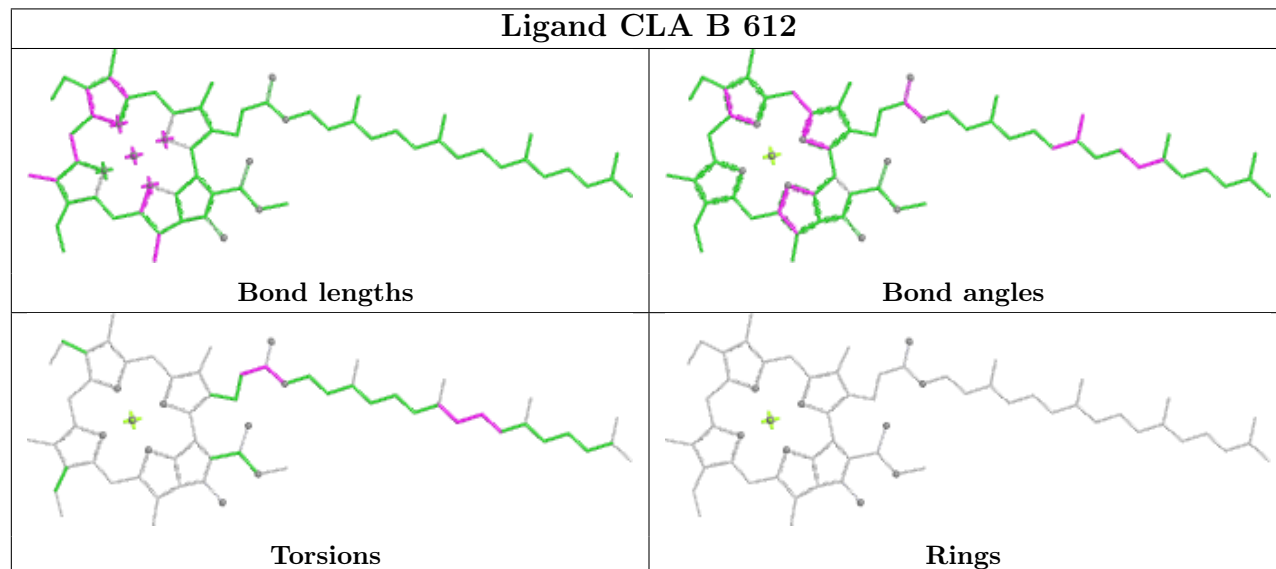
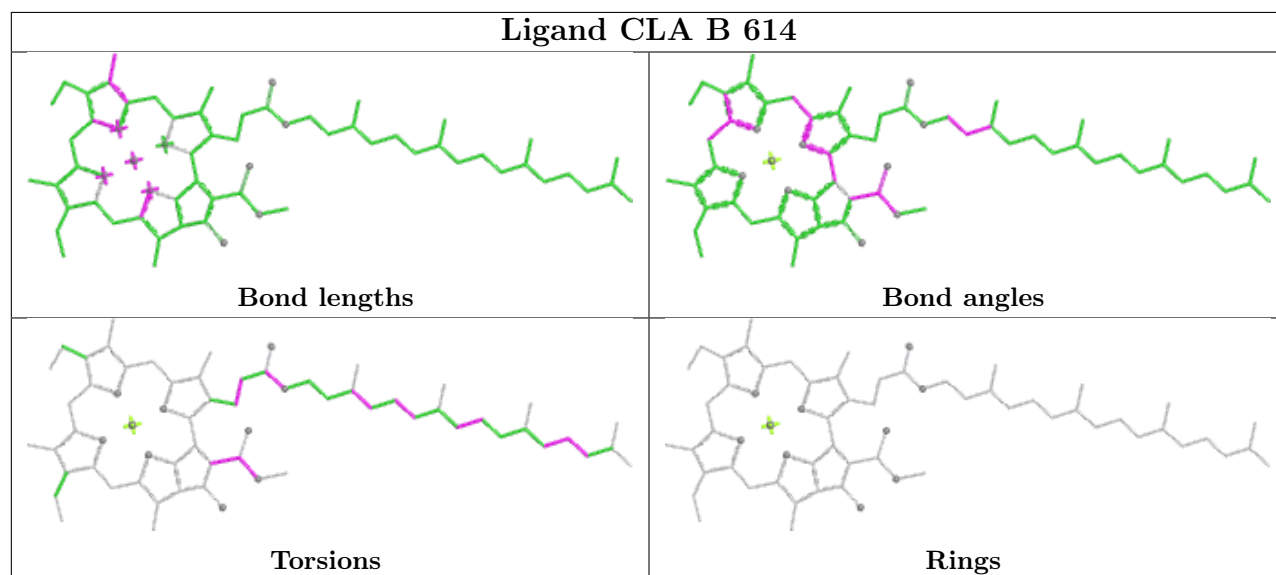
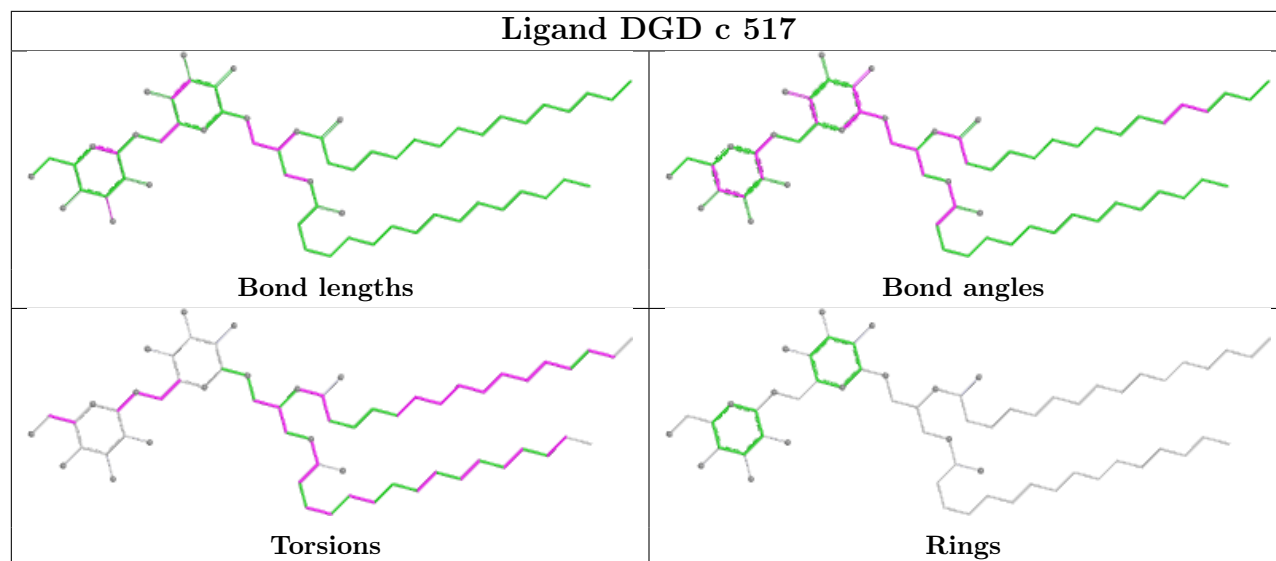


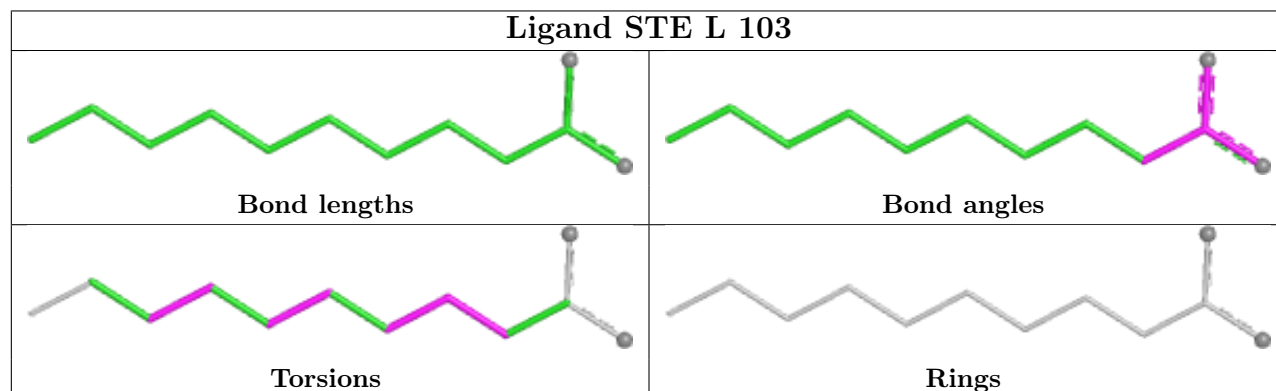
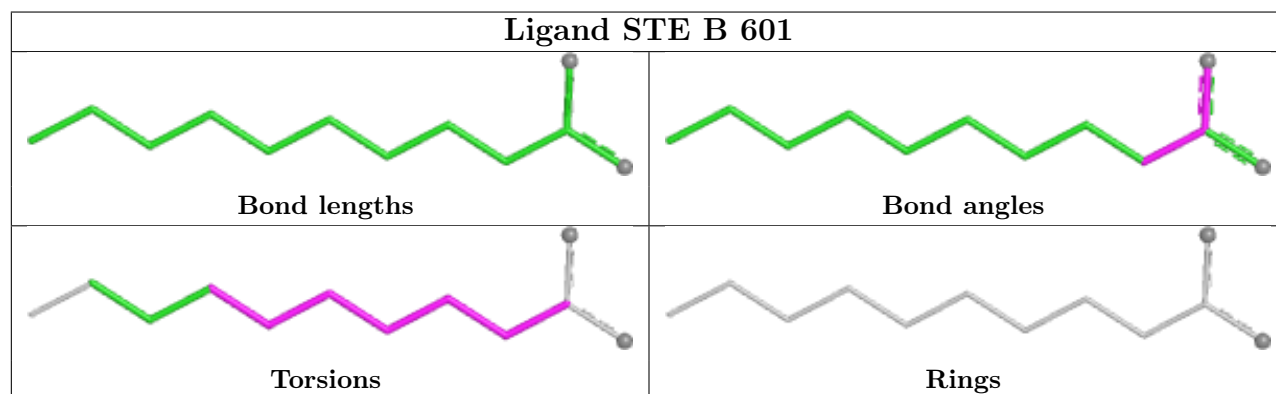
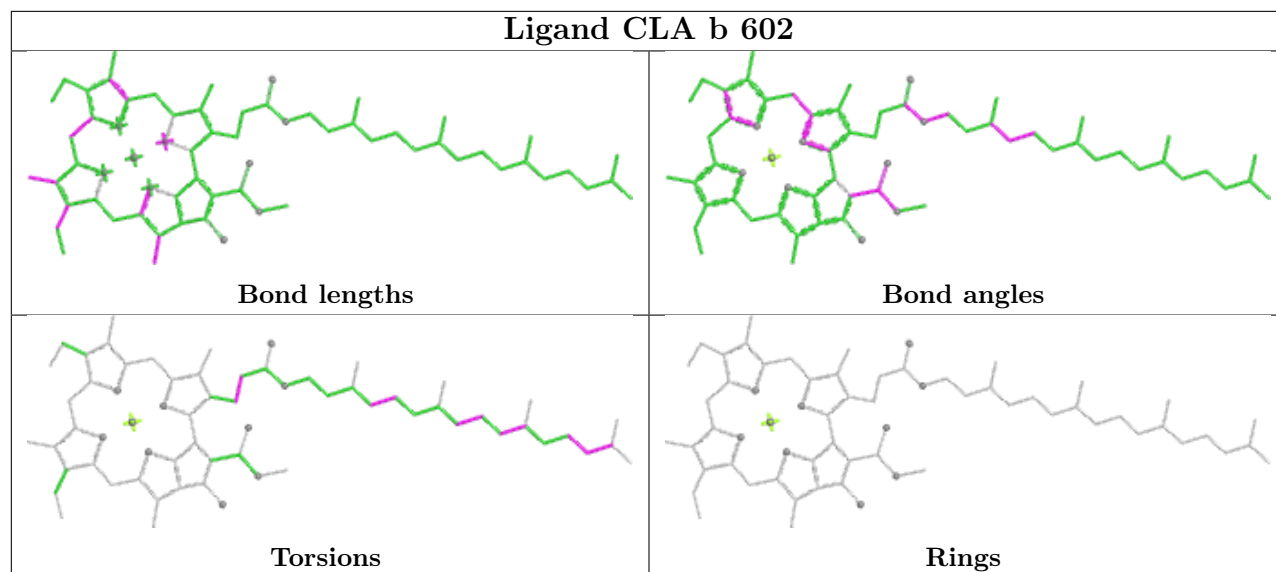
Ligand LMG b 621

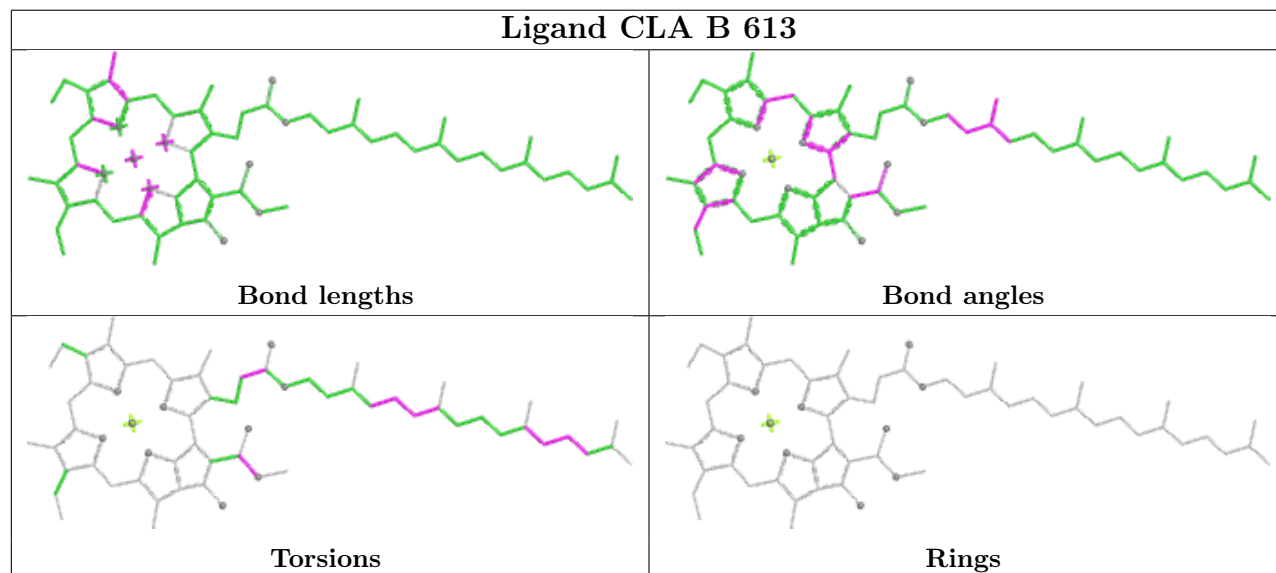
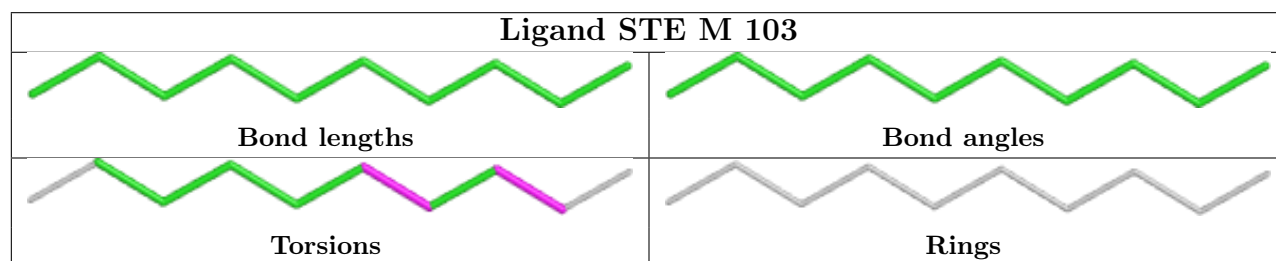
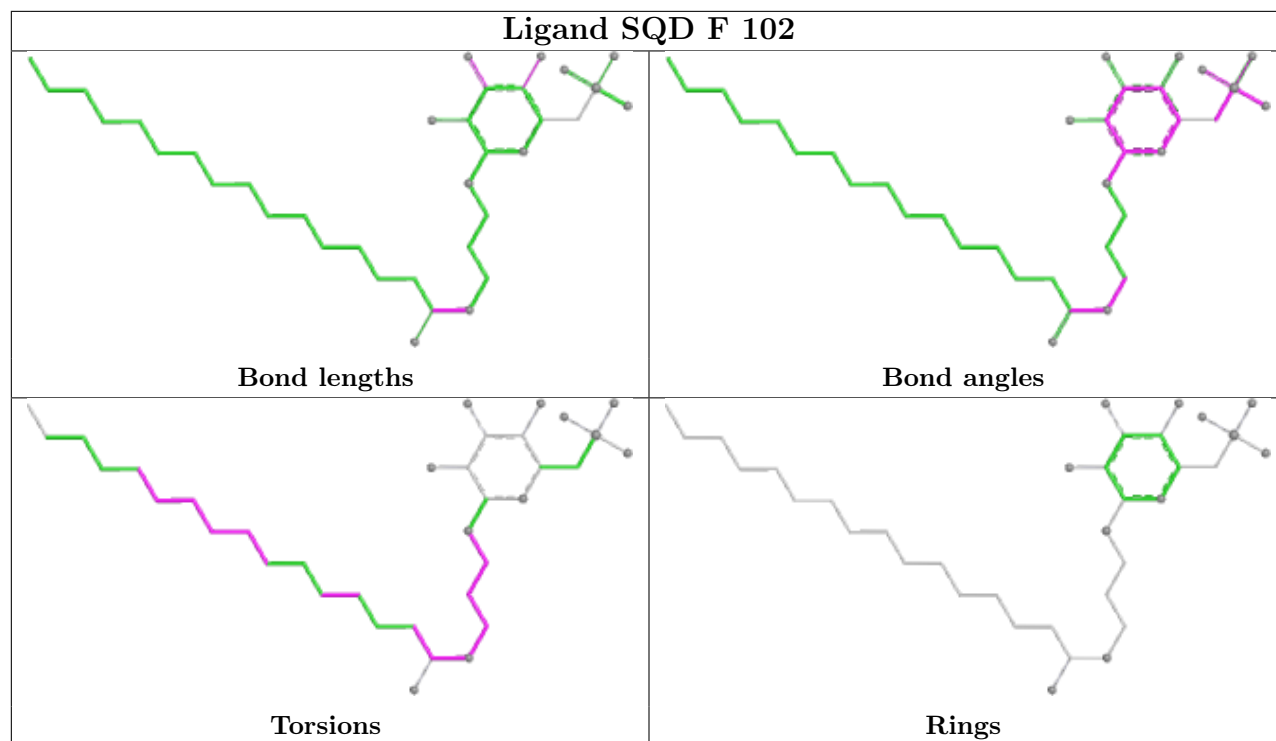


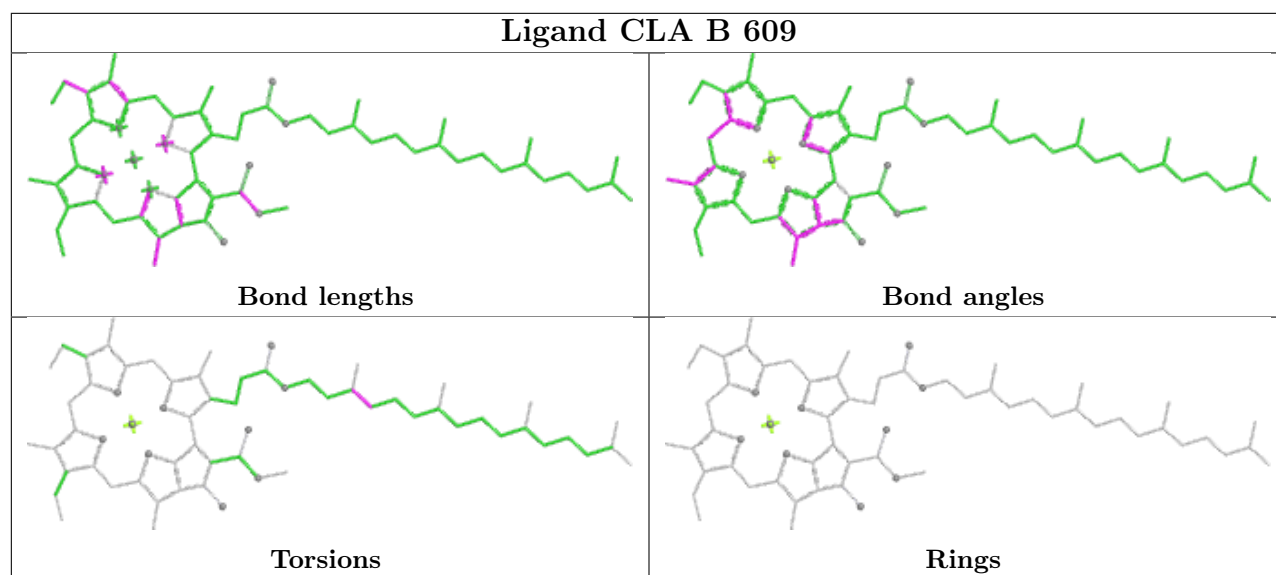
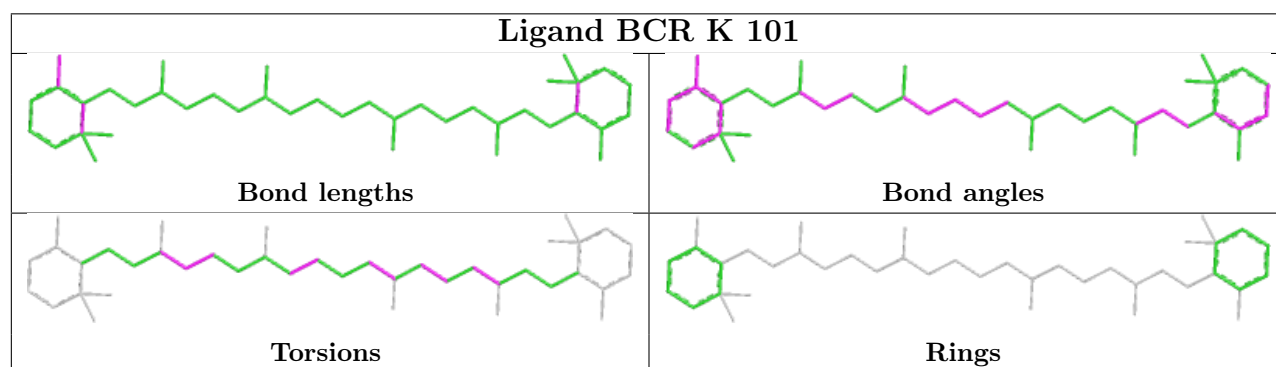
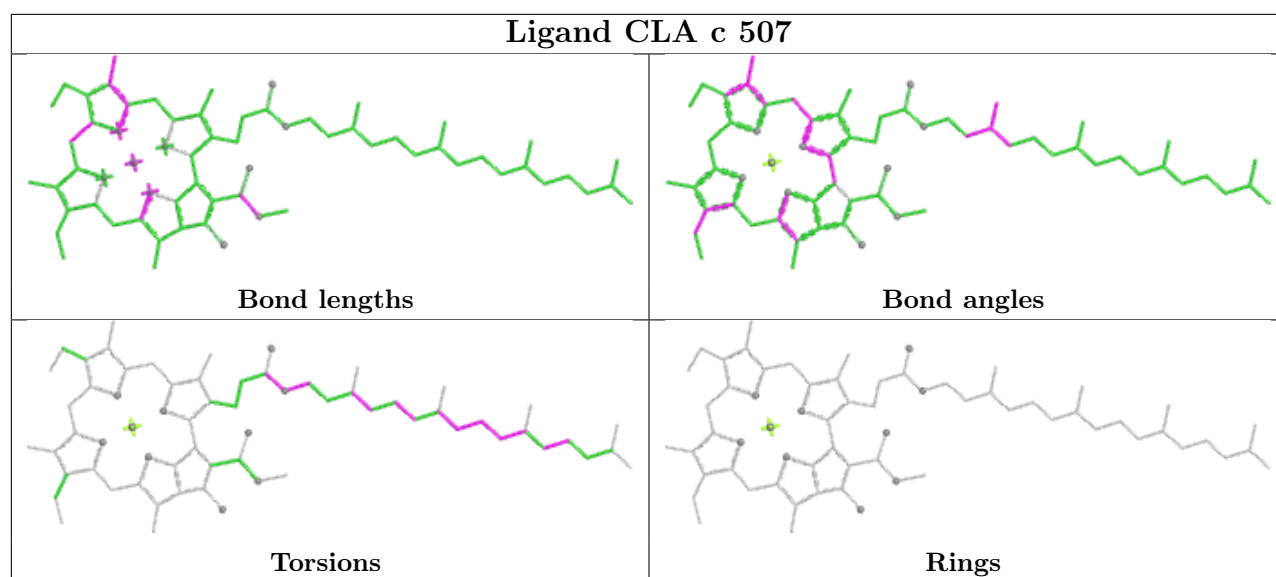
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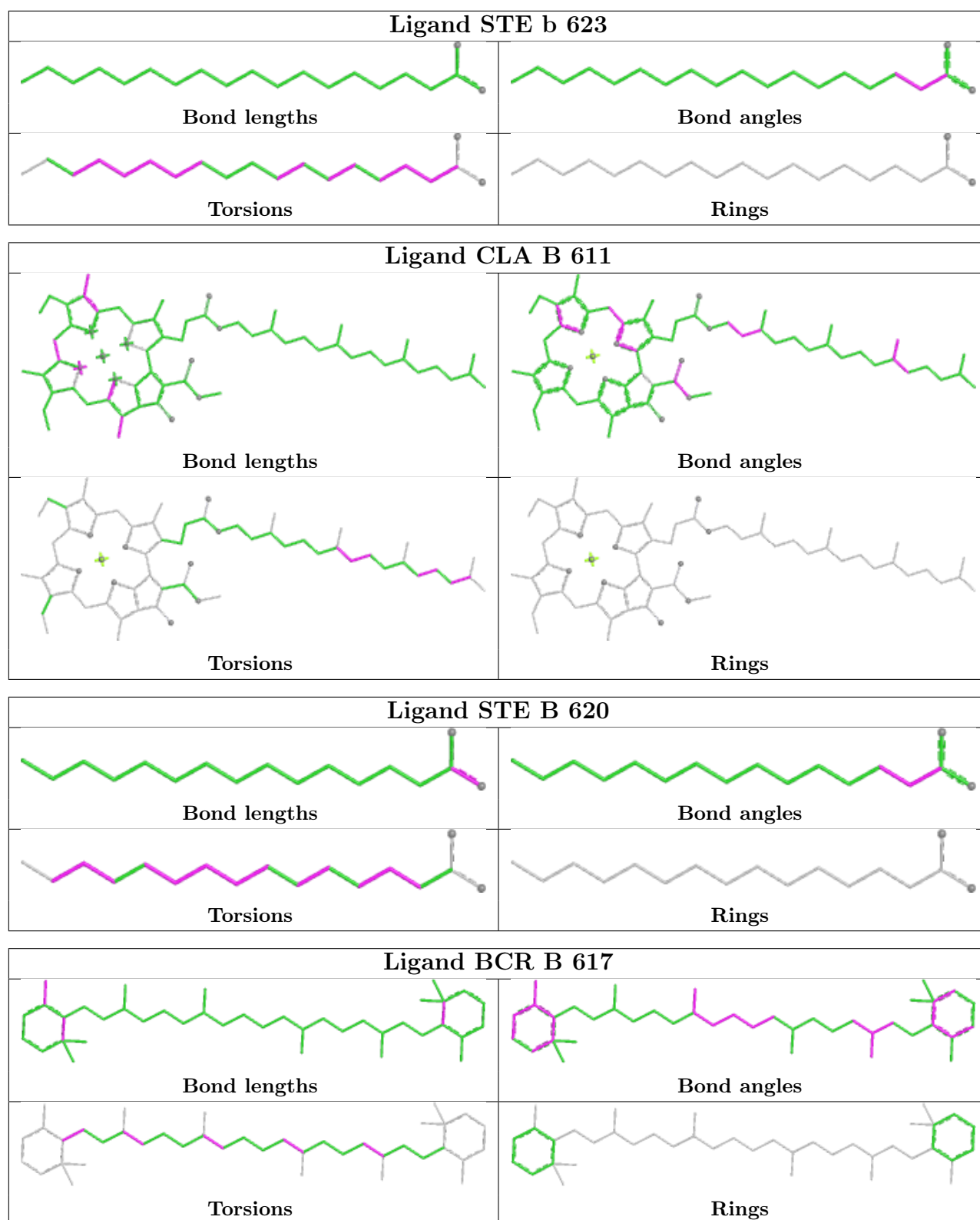




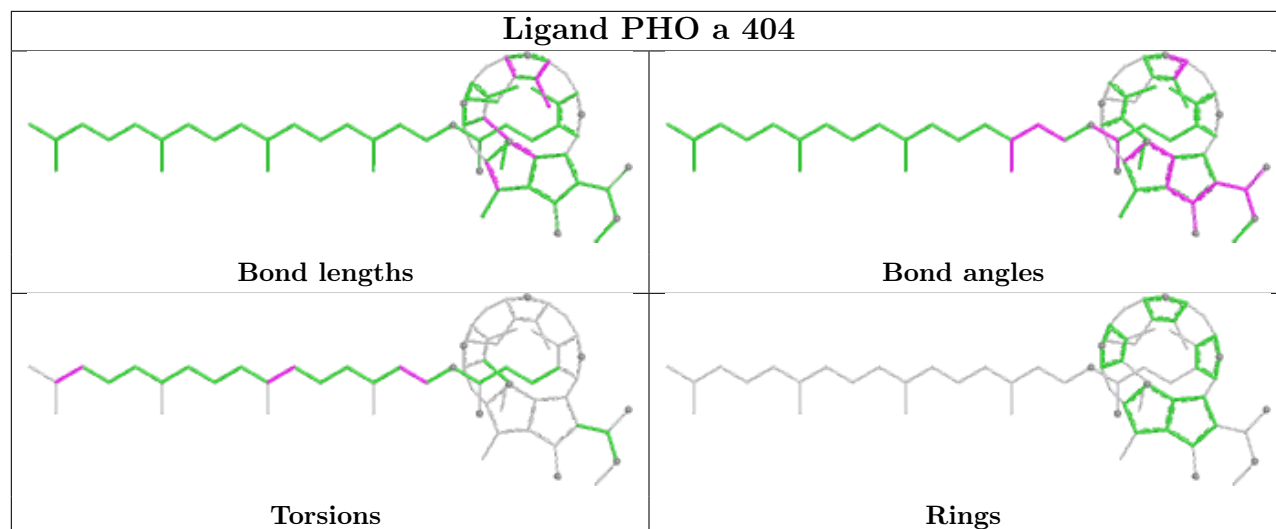




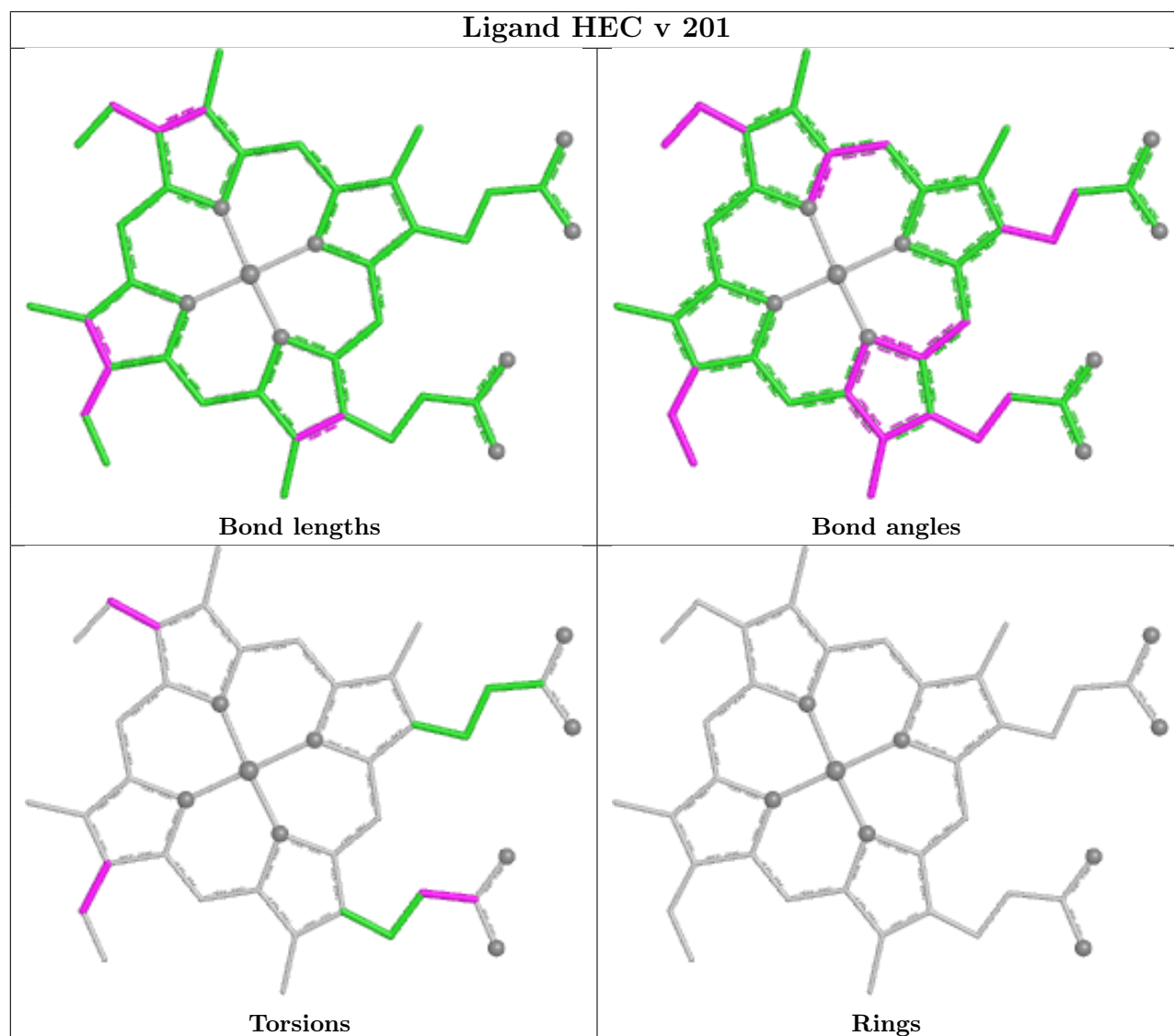


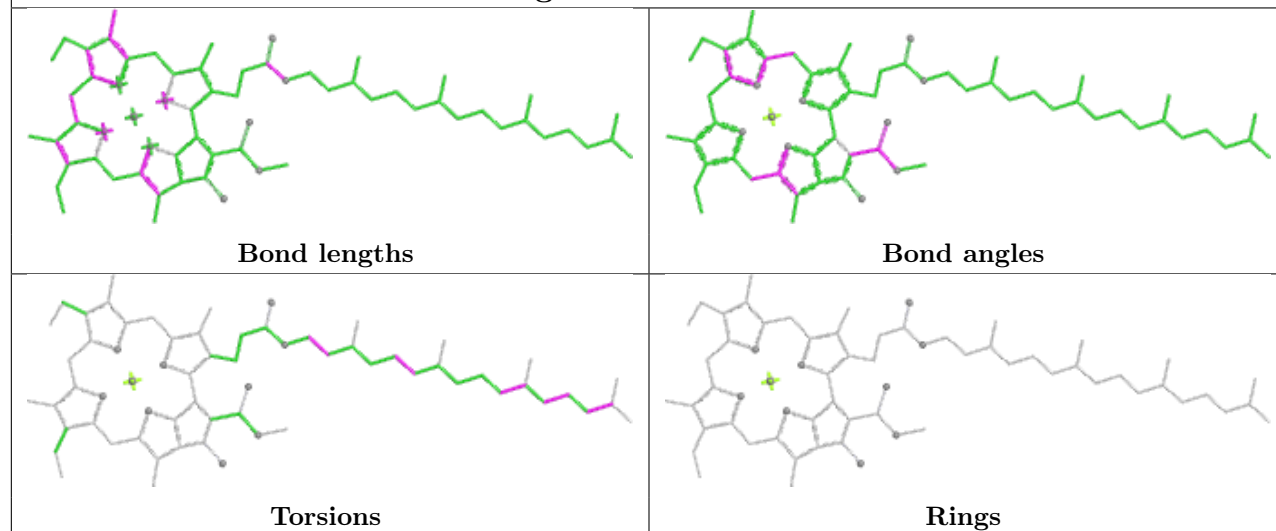
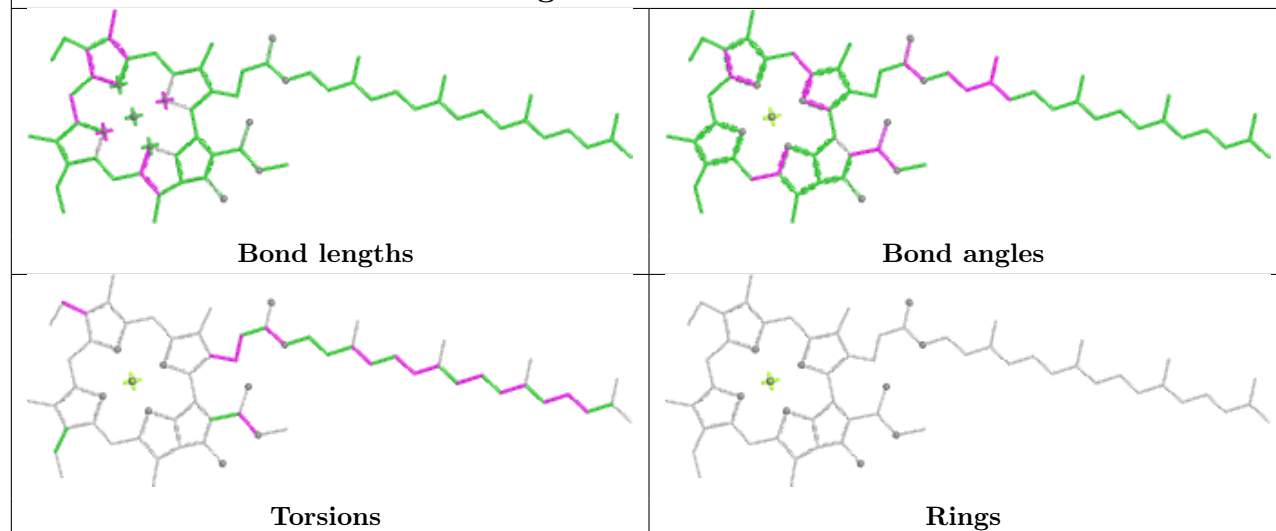
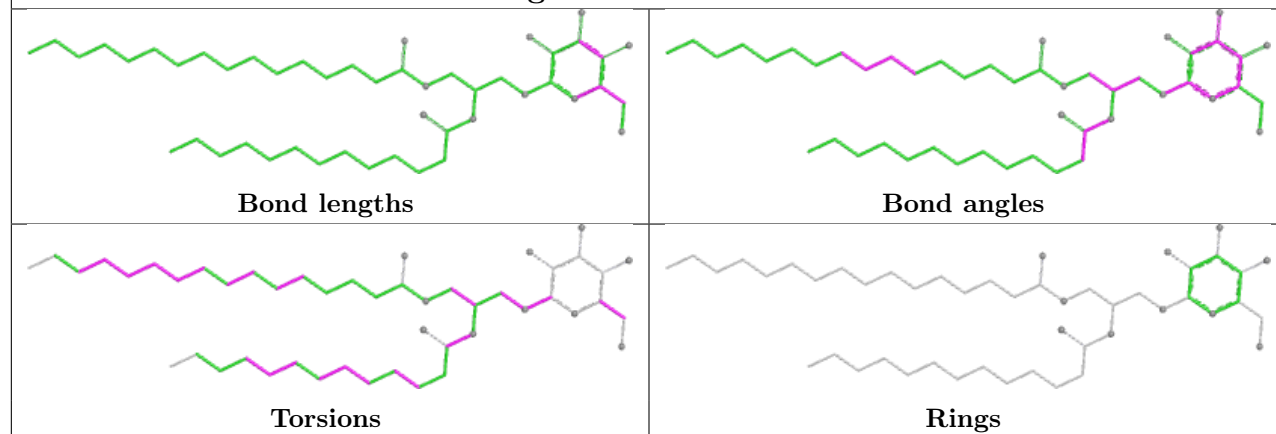


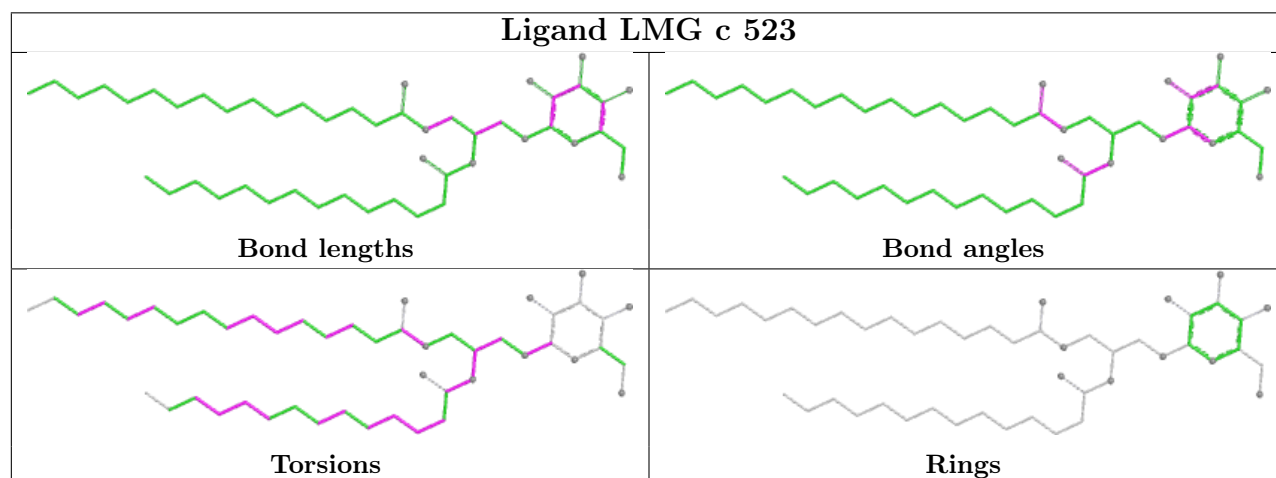
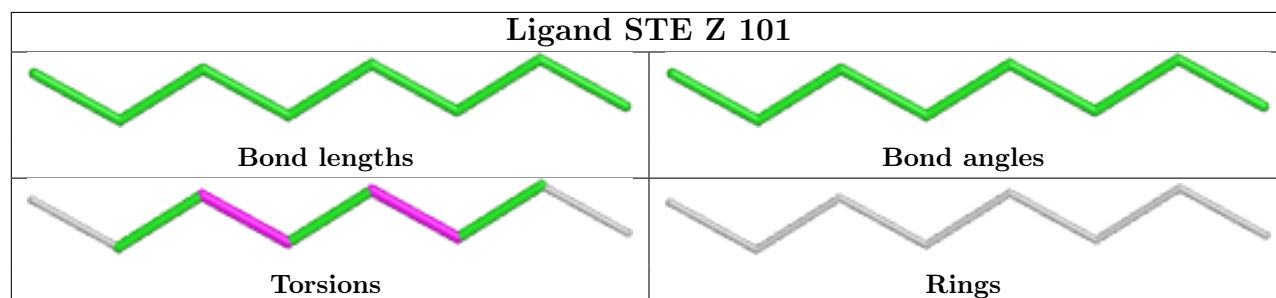
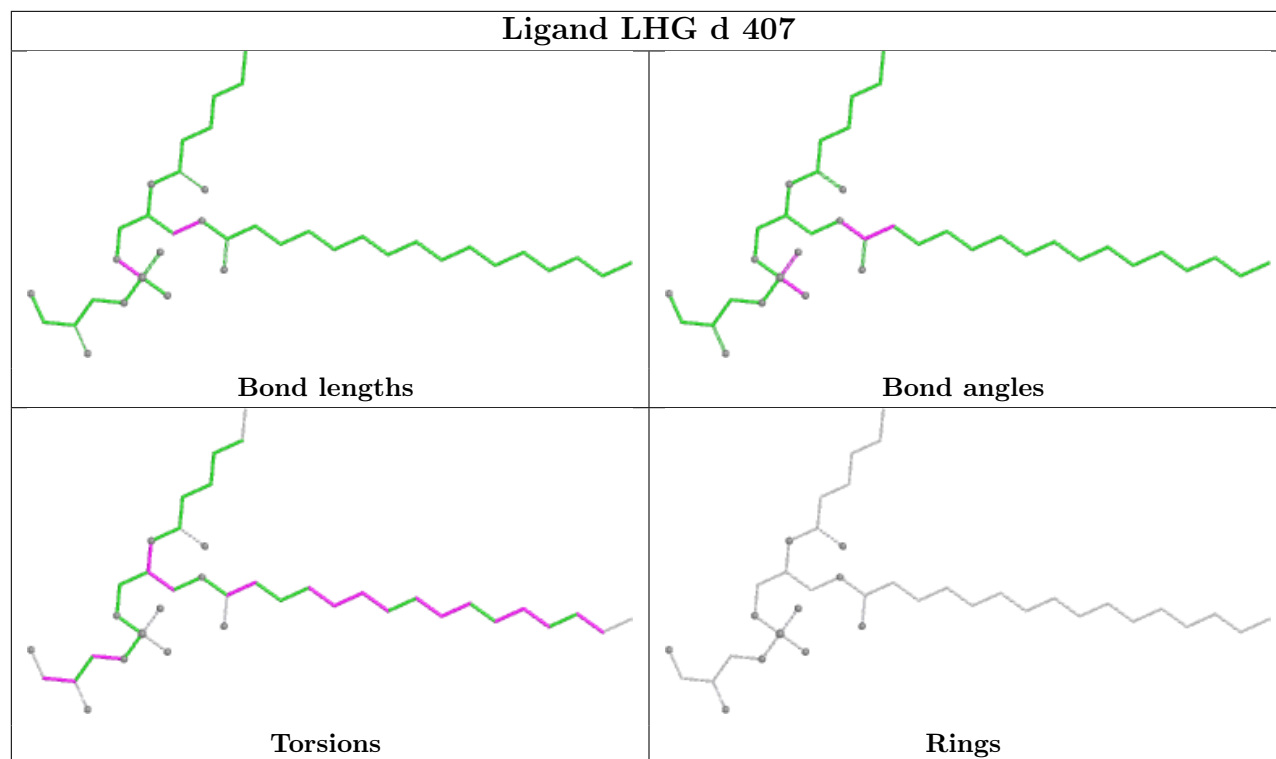
Ligand PHO a 404

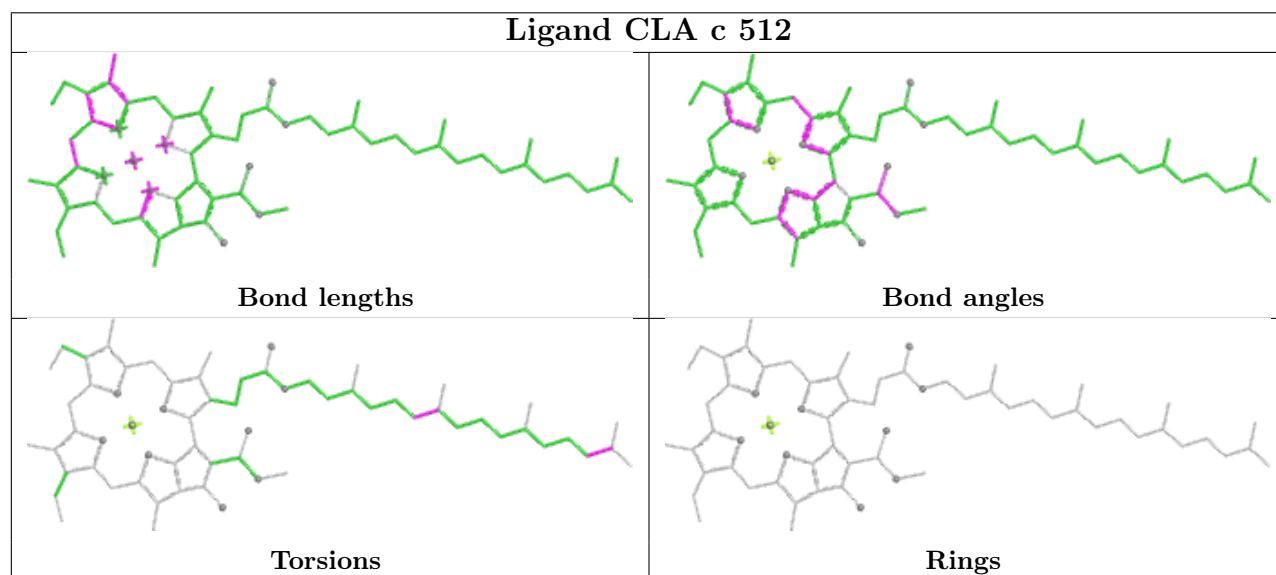
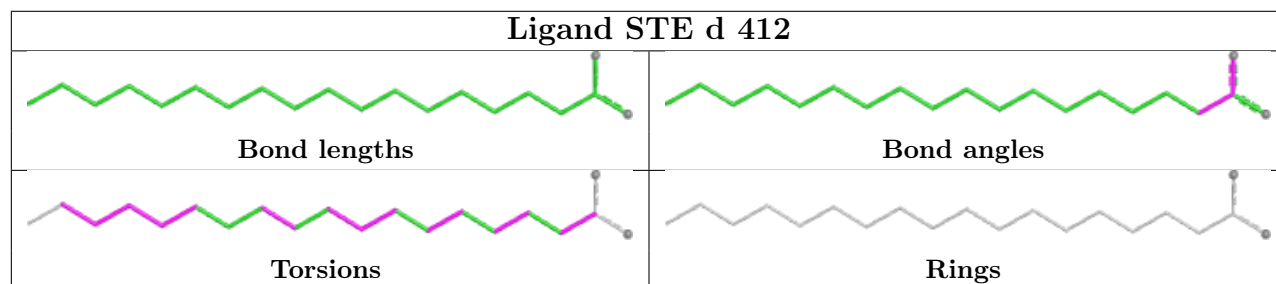
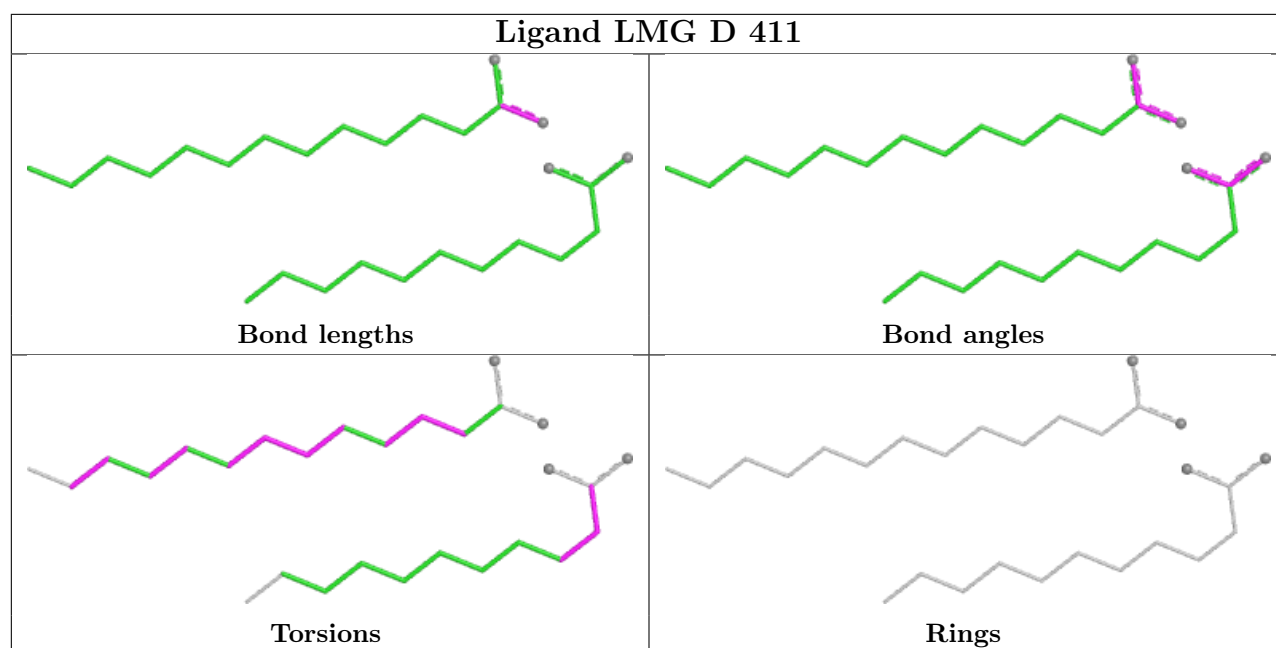


Ligand HEC v 201

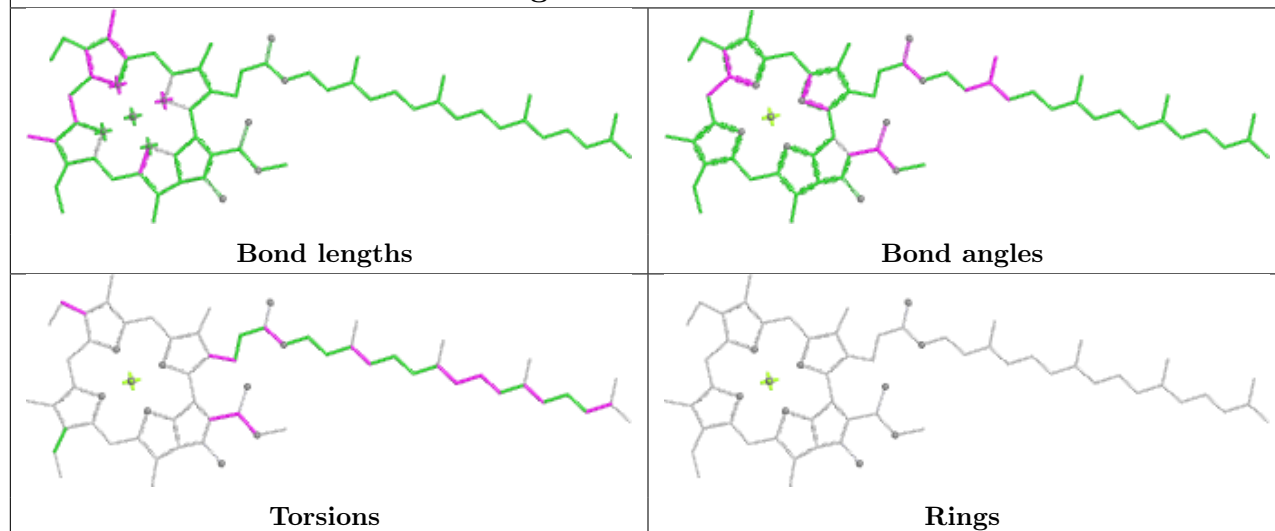


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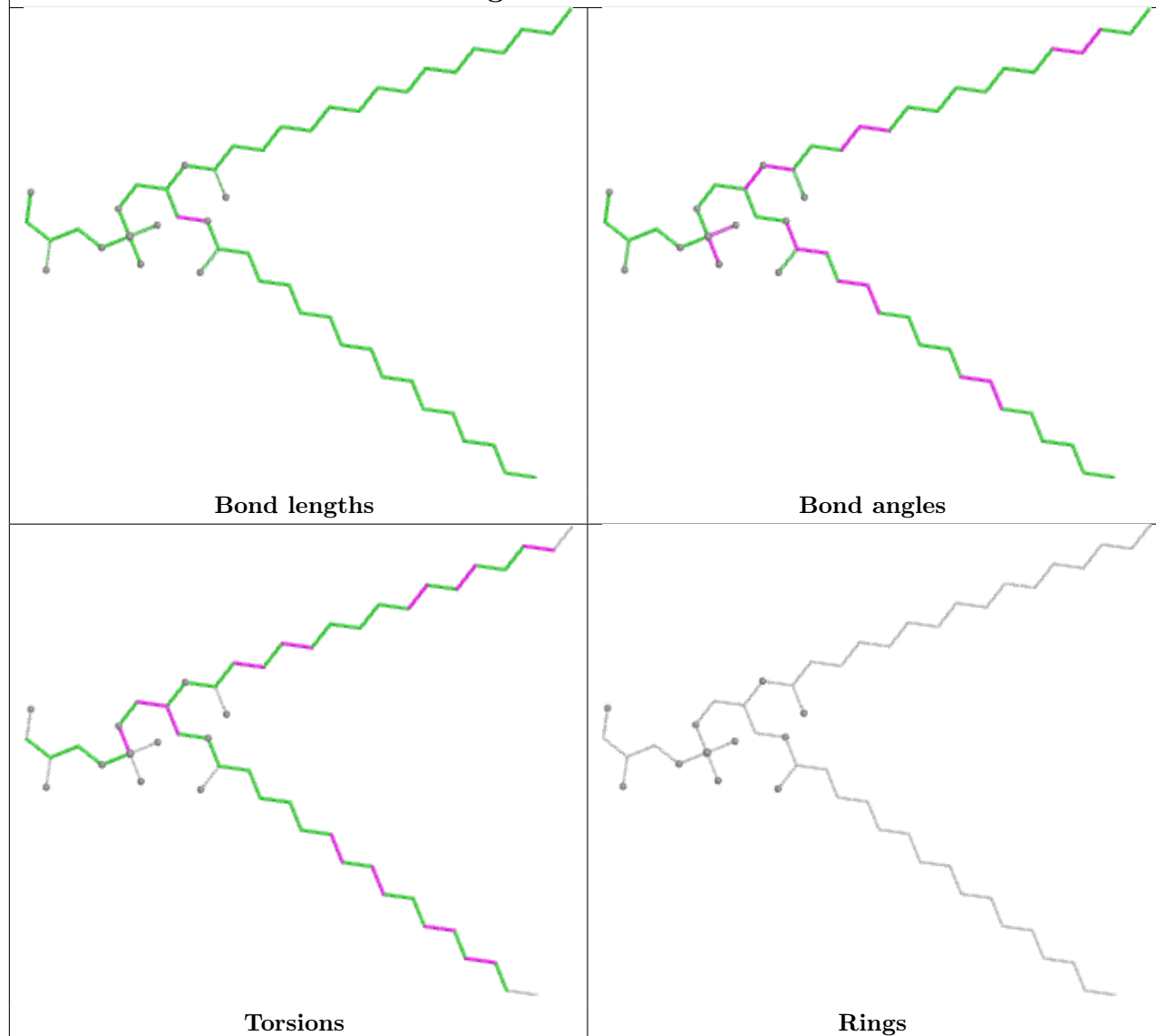


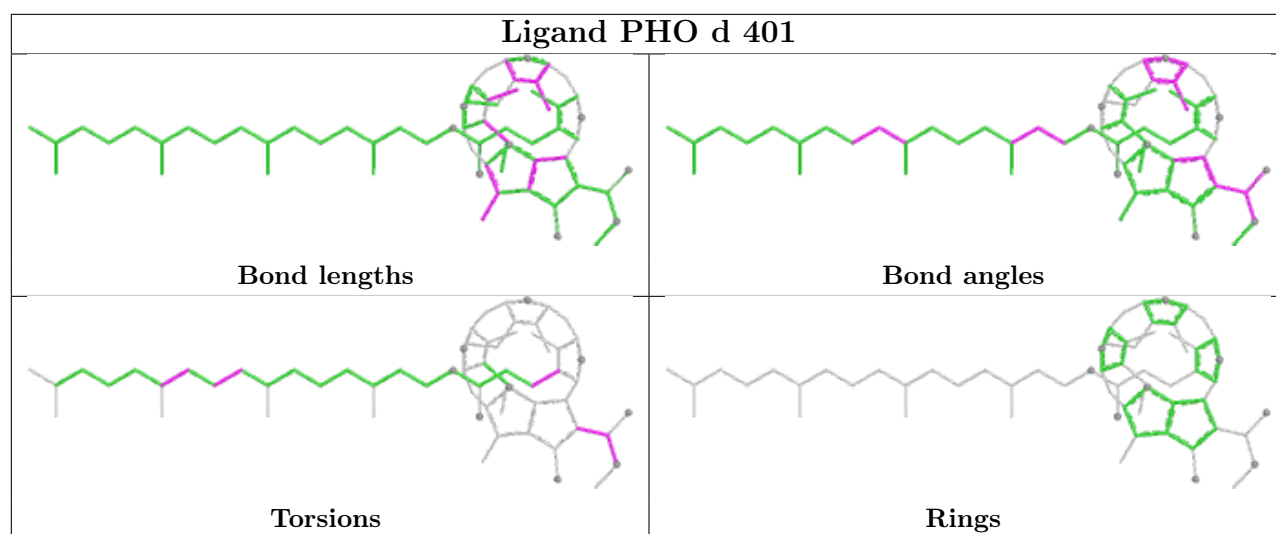
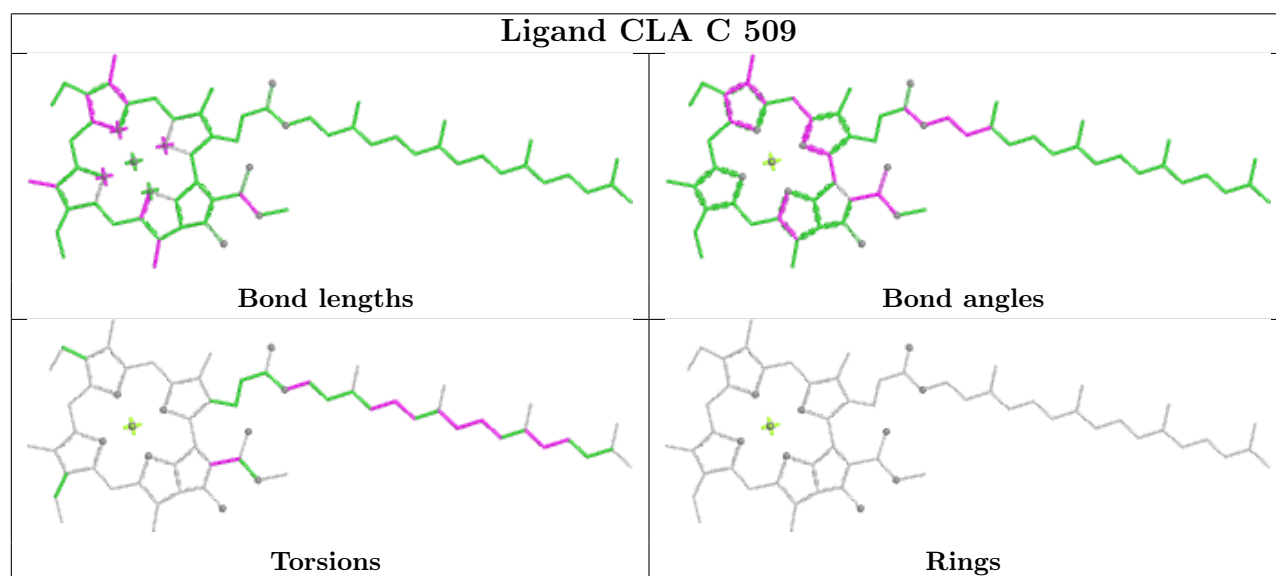
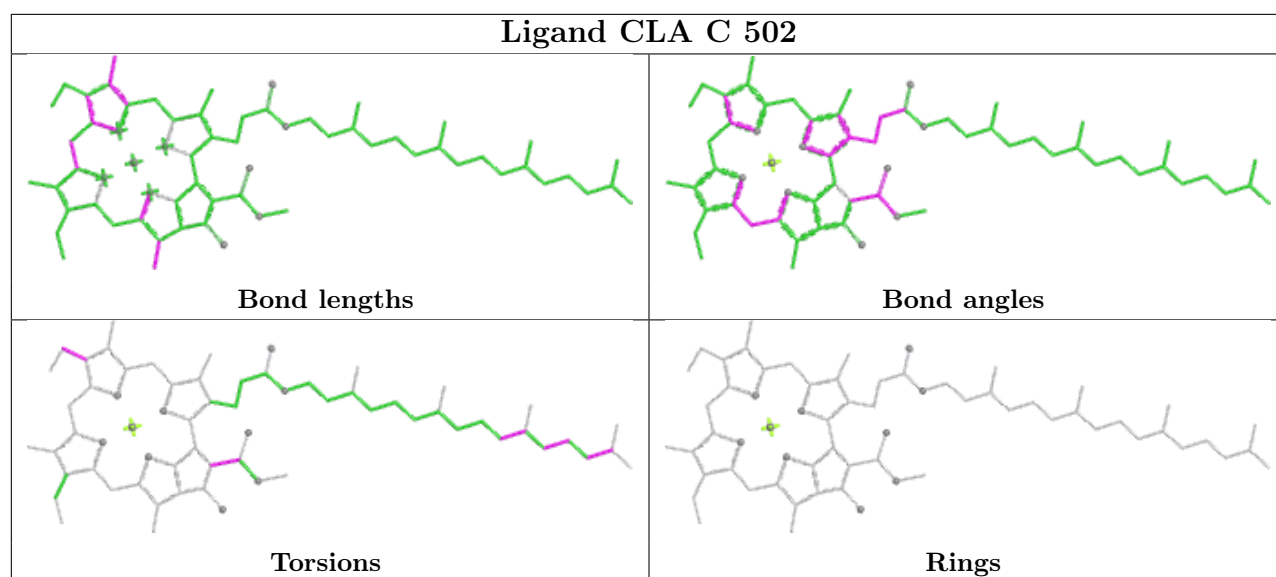


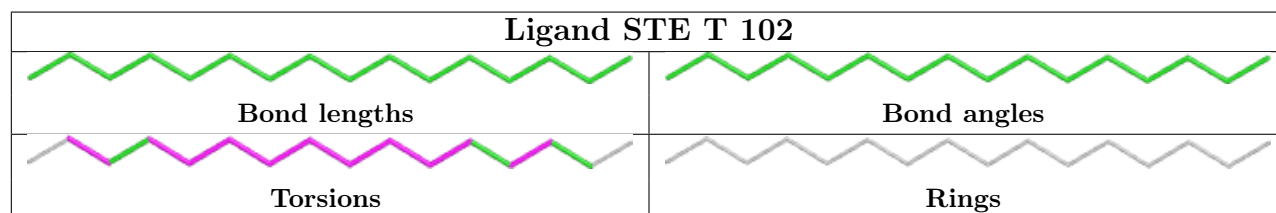
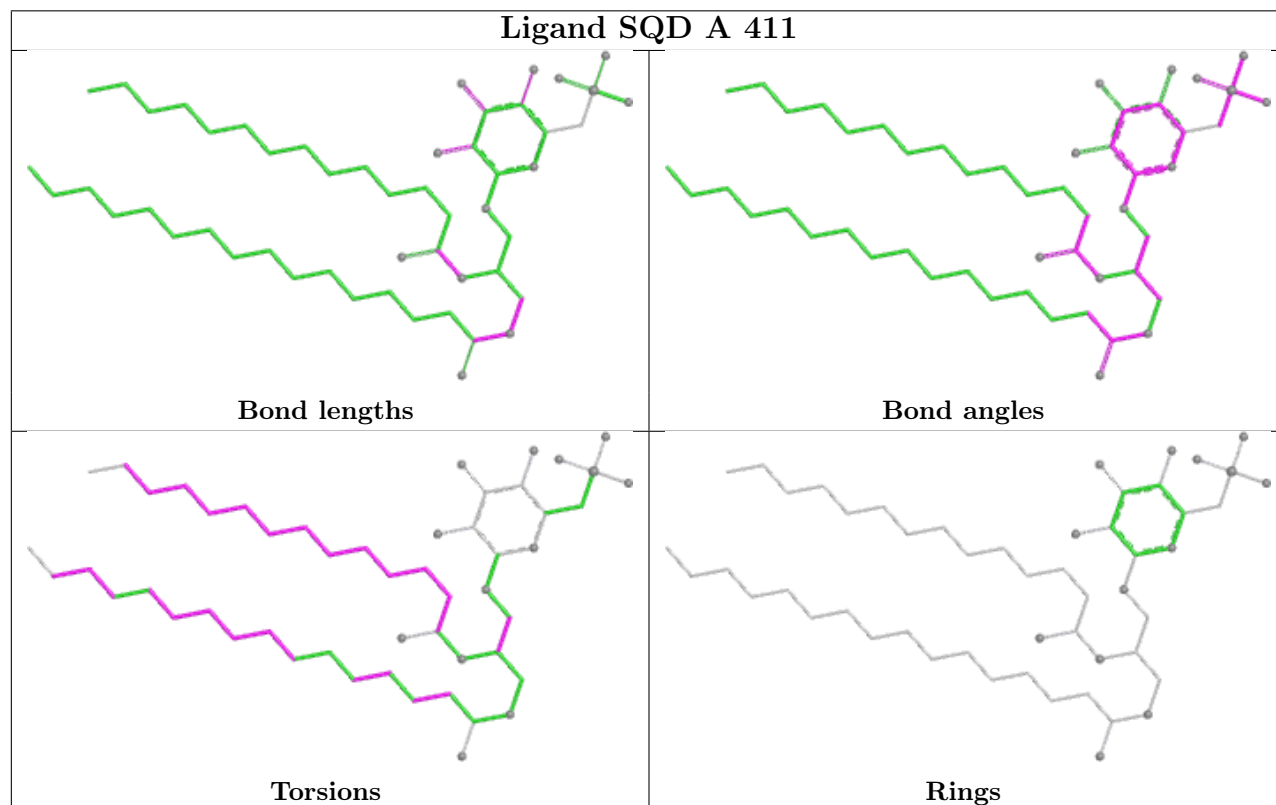
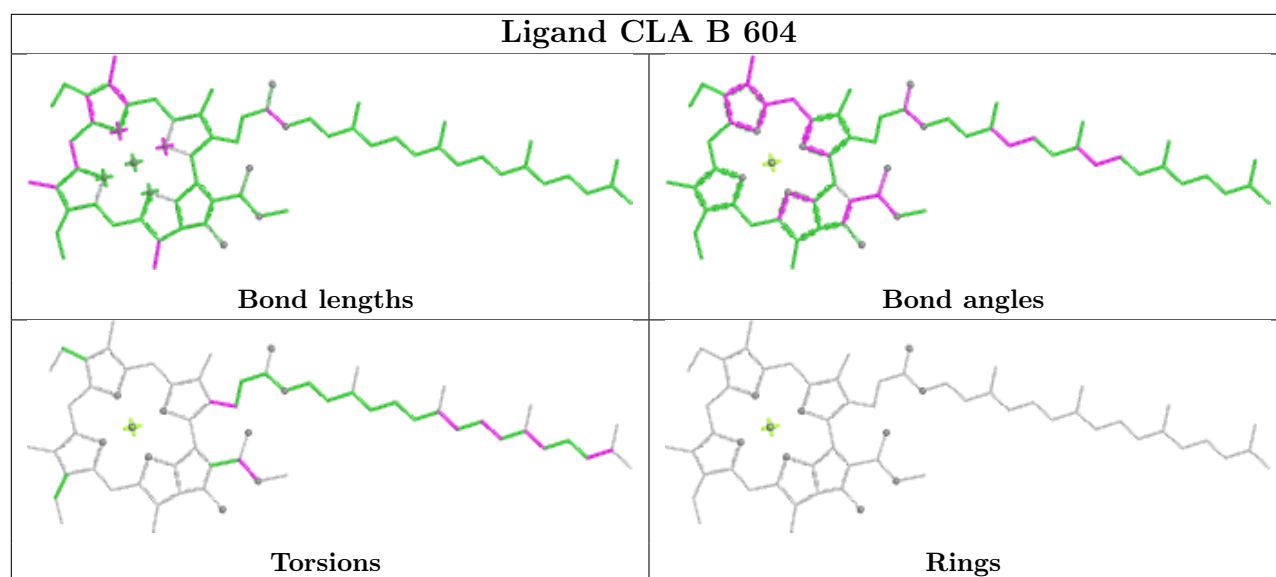
Ligand CLA H 101

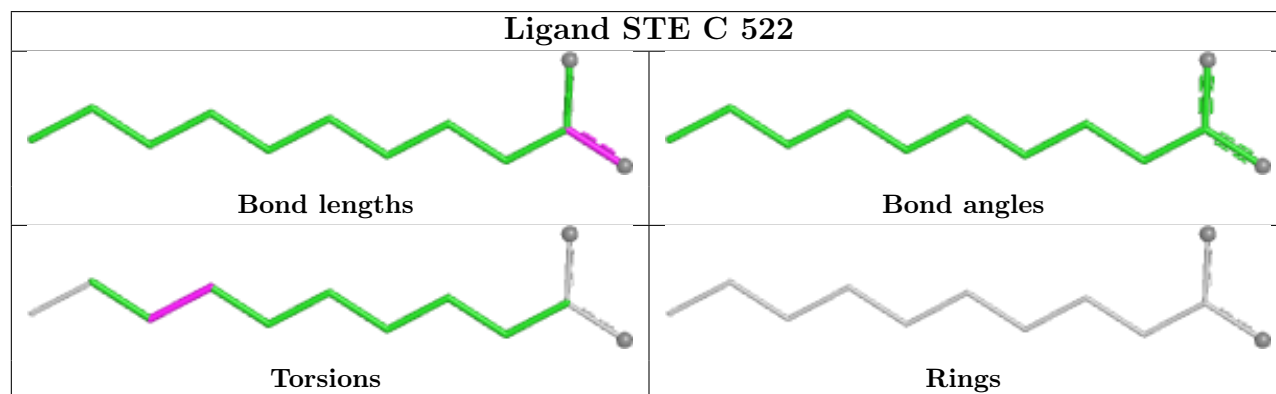
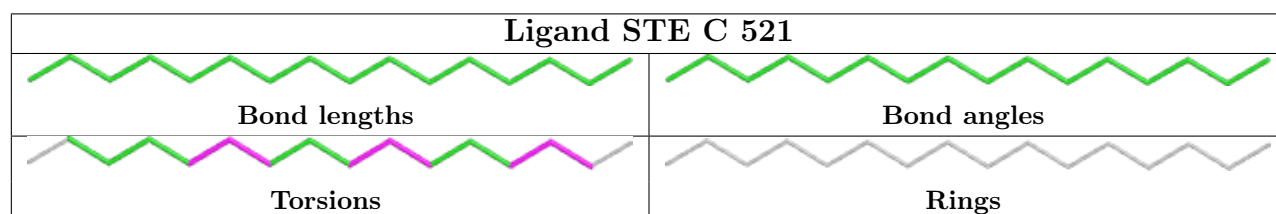
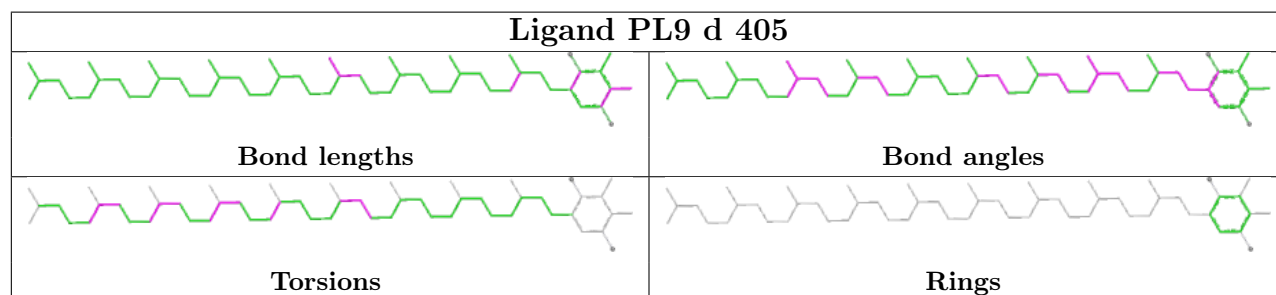
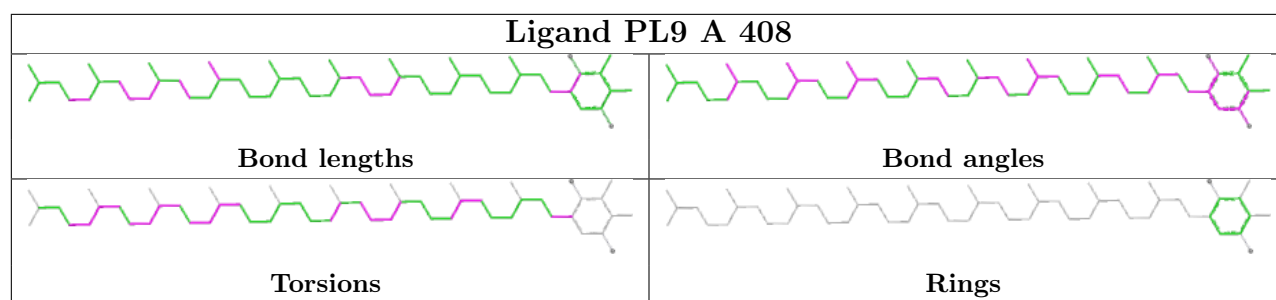


Ligand LHG 1 101

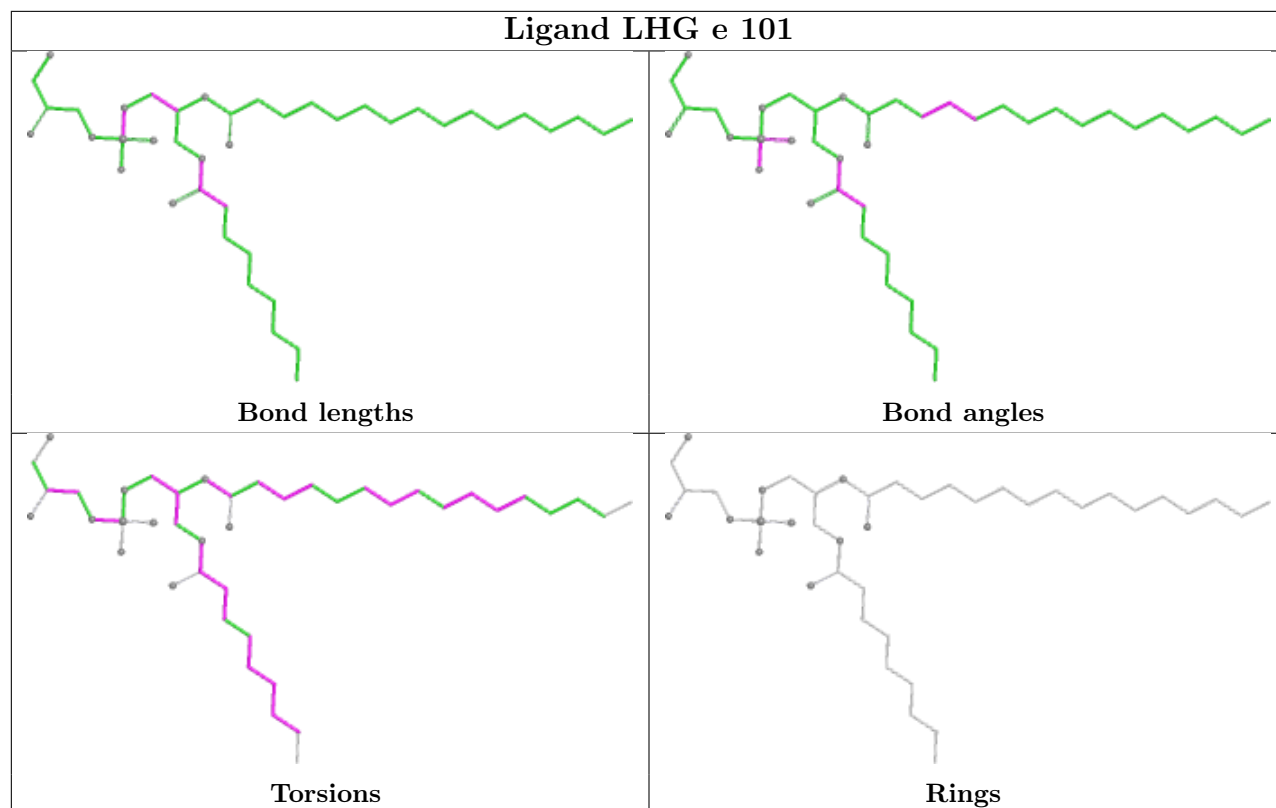




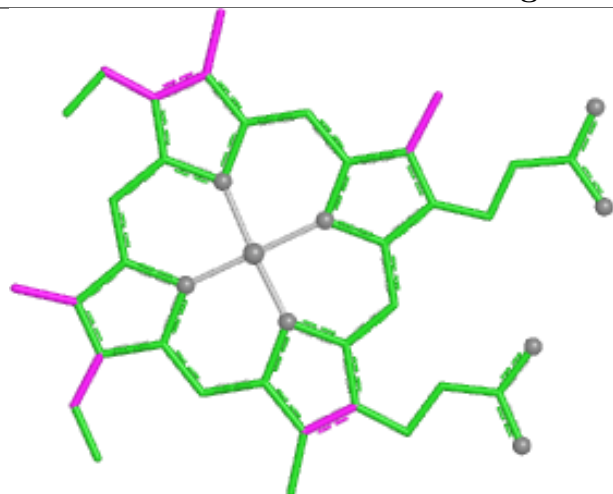




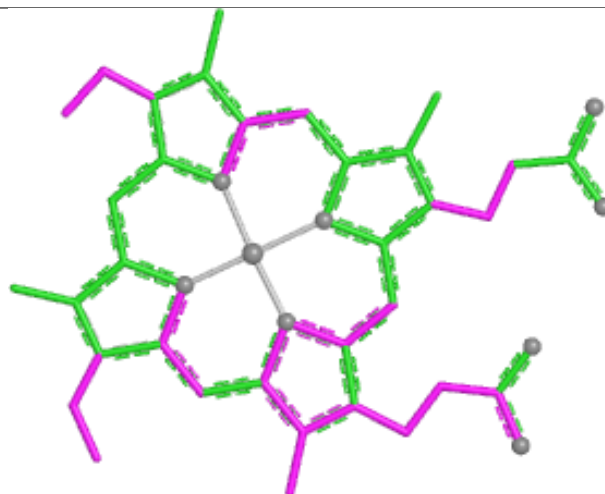
Ligand LHG e 101



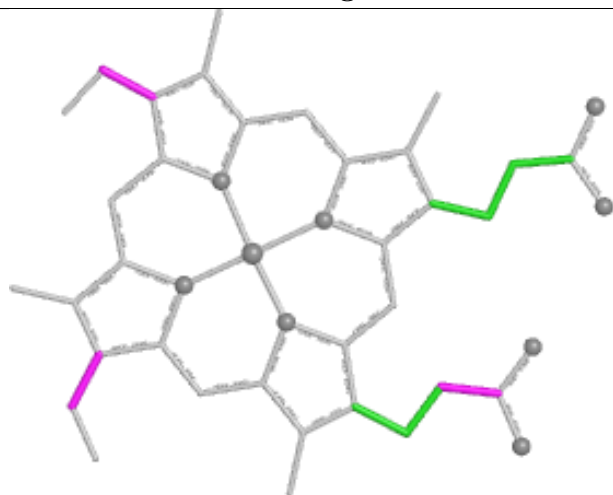
Ligand HEC f 101



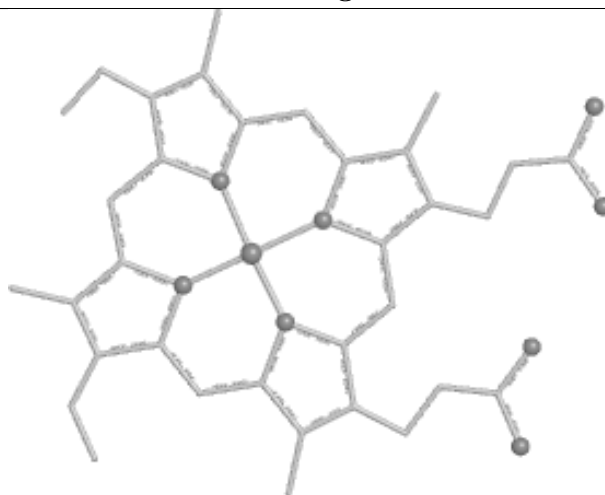
Bond lengths



Bond angles

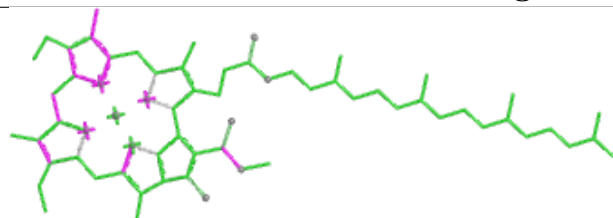


Torsions

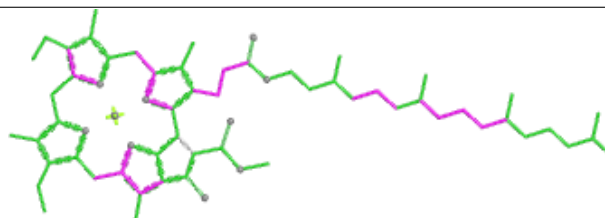


Rings

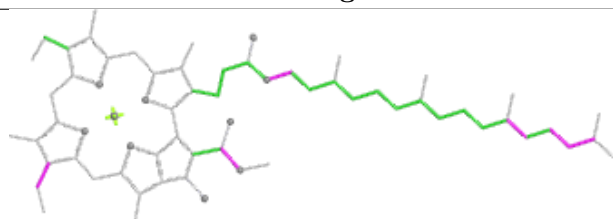
Ligand CLA A 402



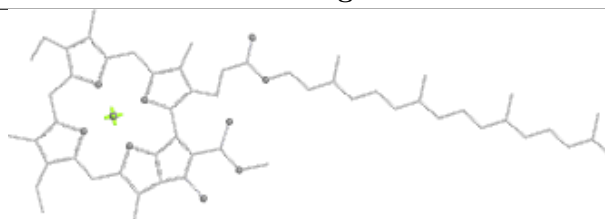
Bond lengths



Bond angles

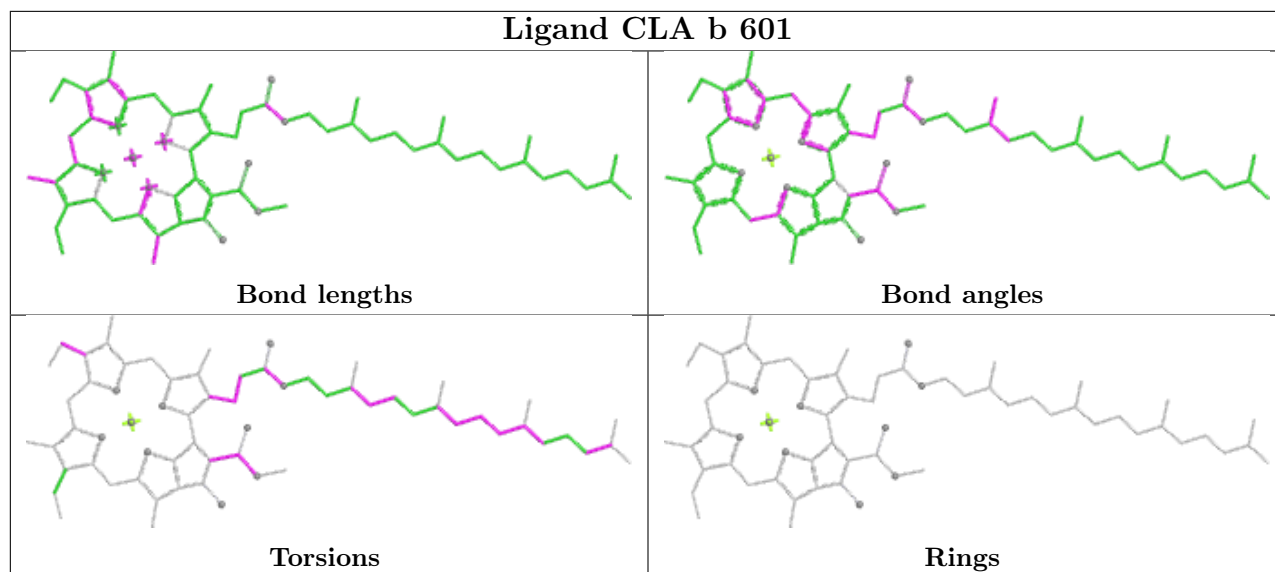


Torsions

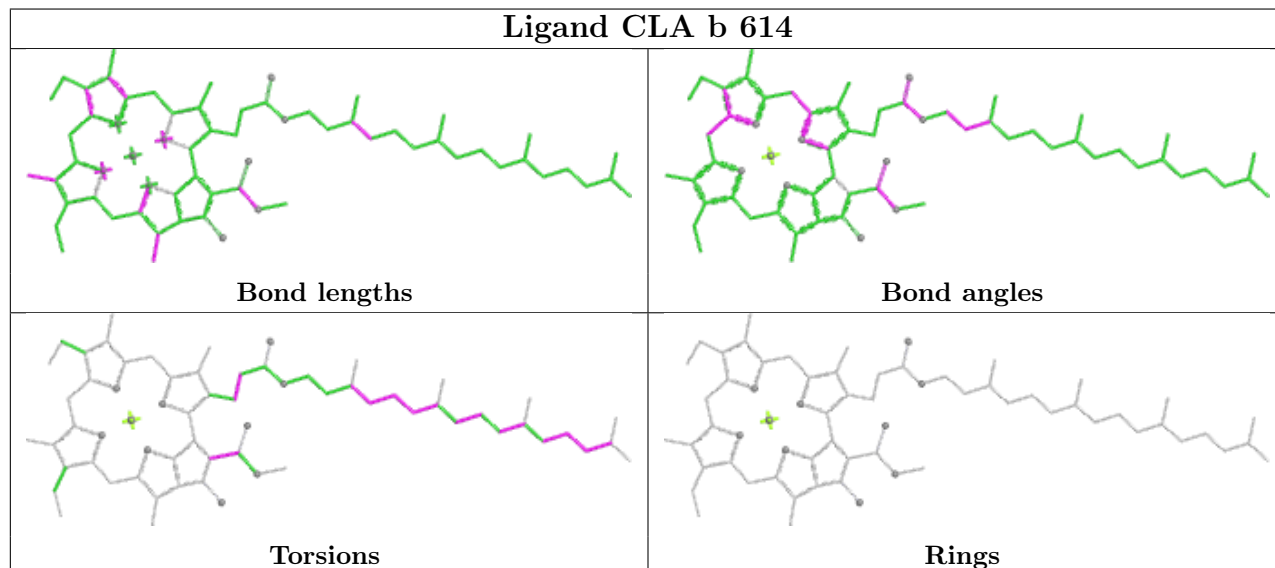


Rings

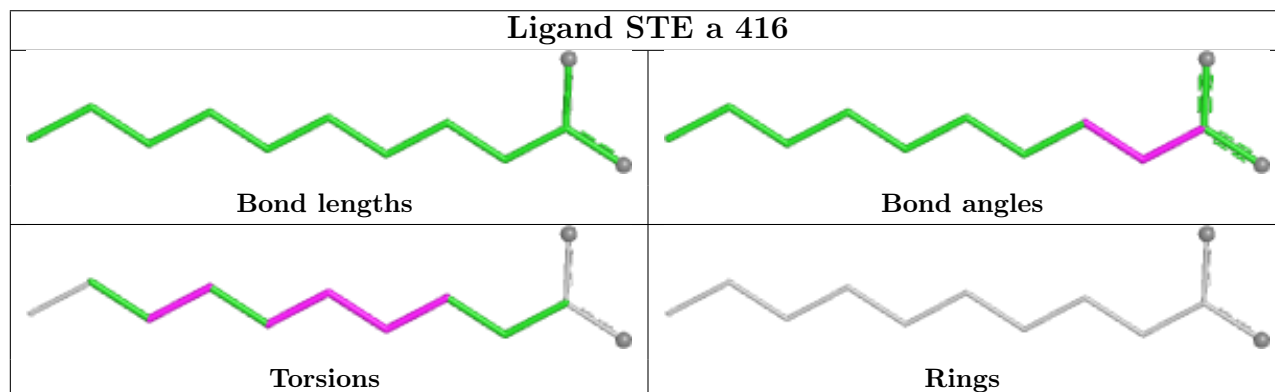
Ligand CLA b 601

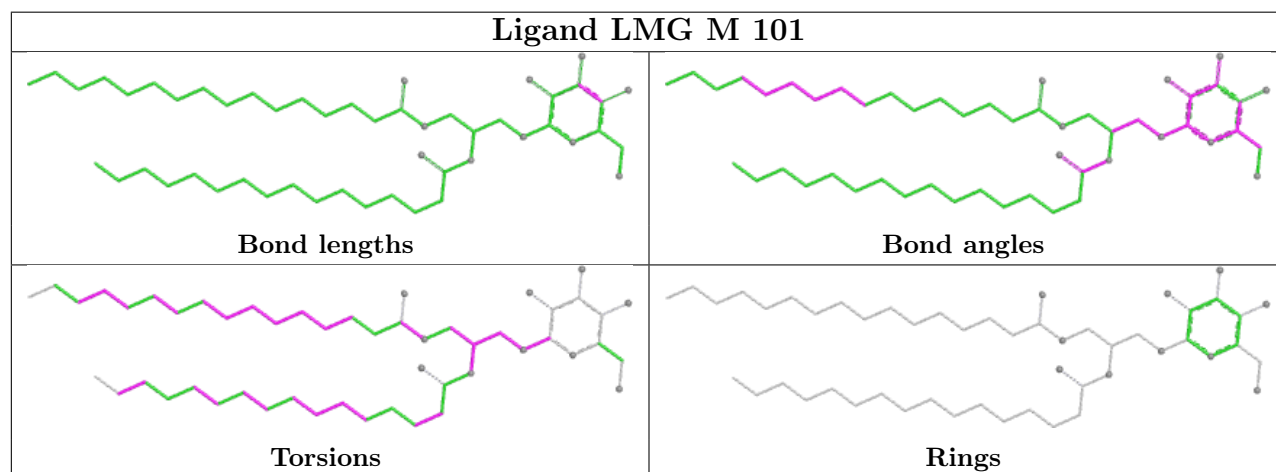
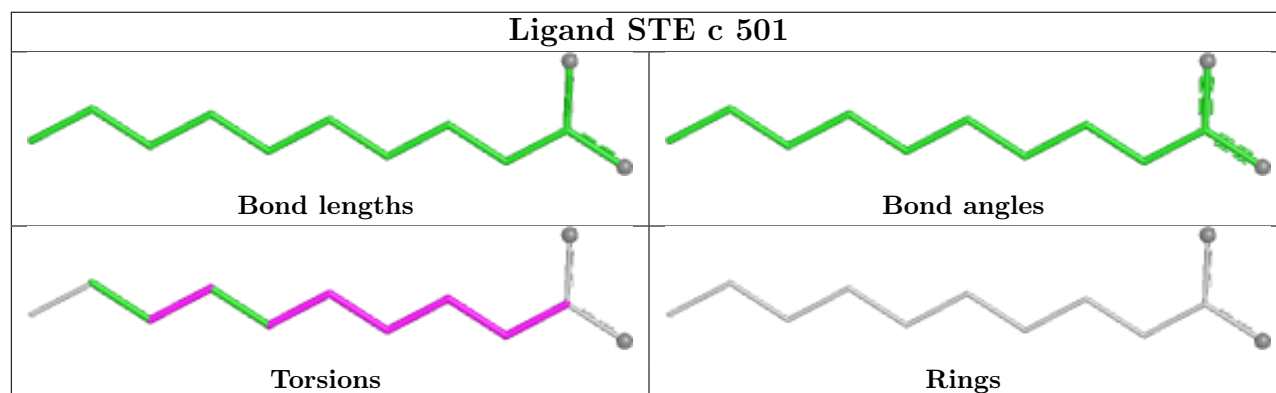
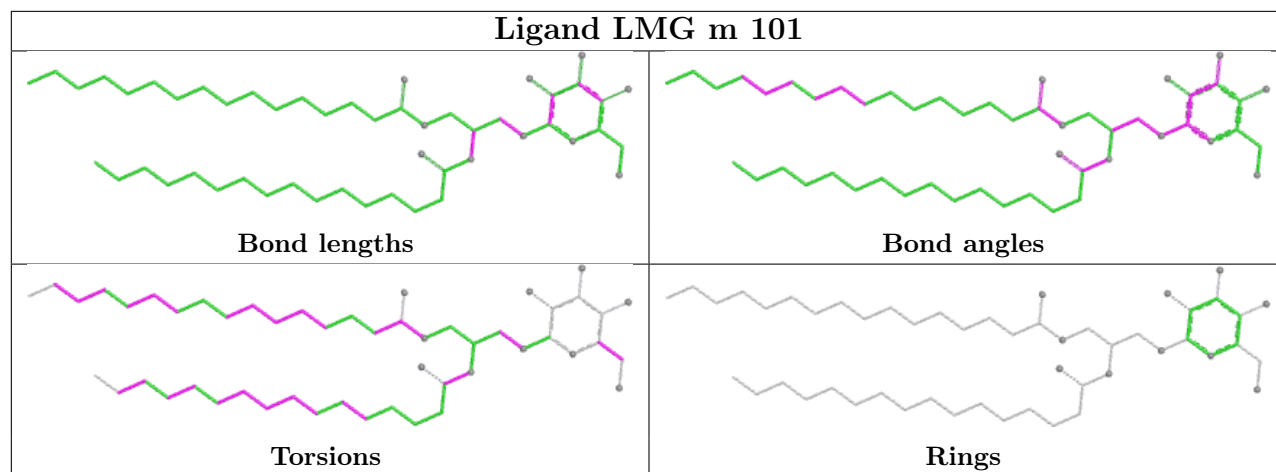


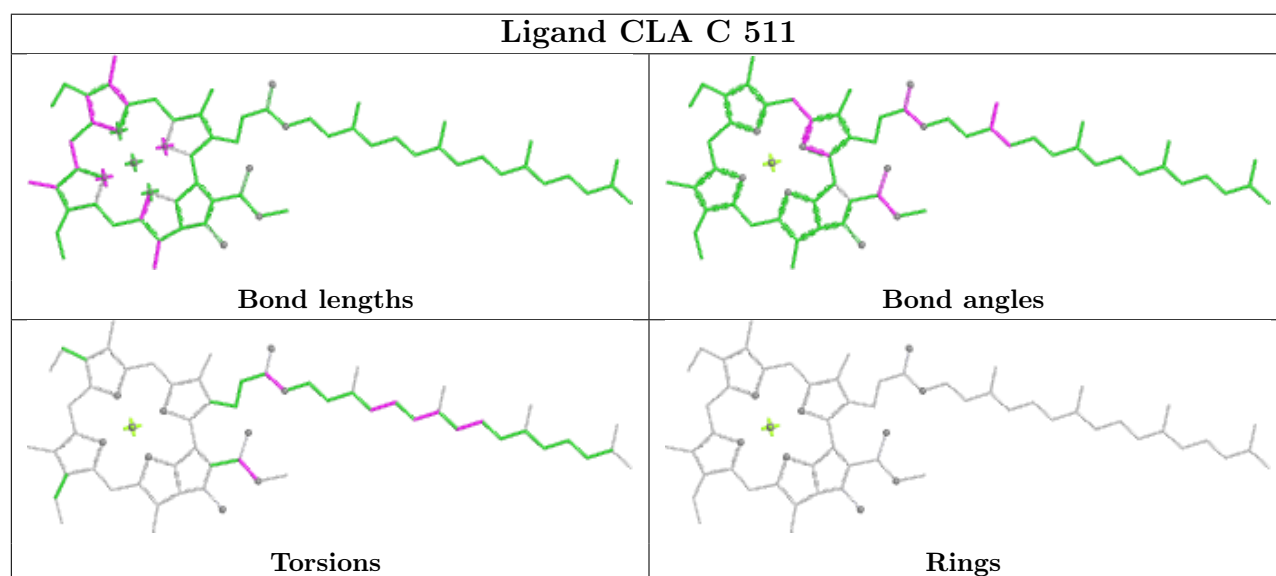
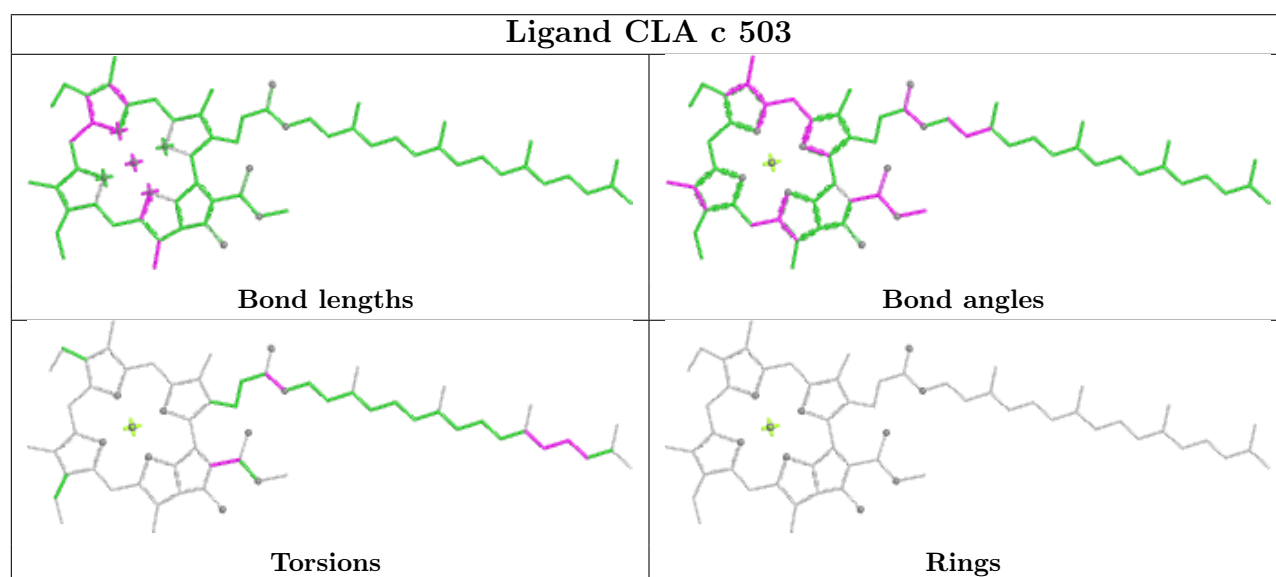
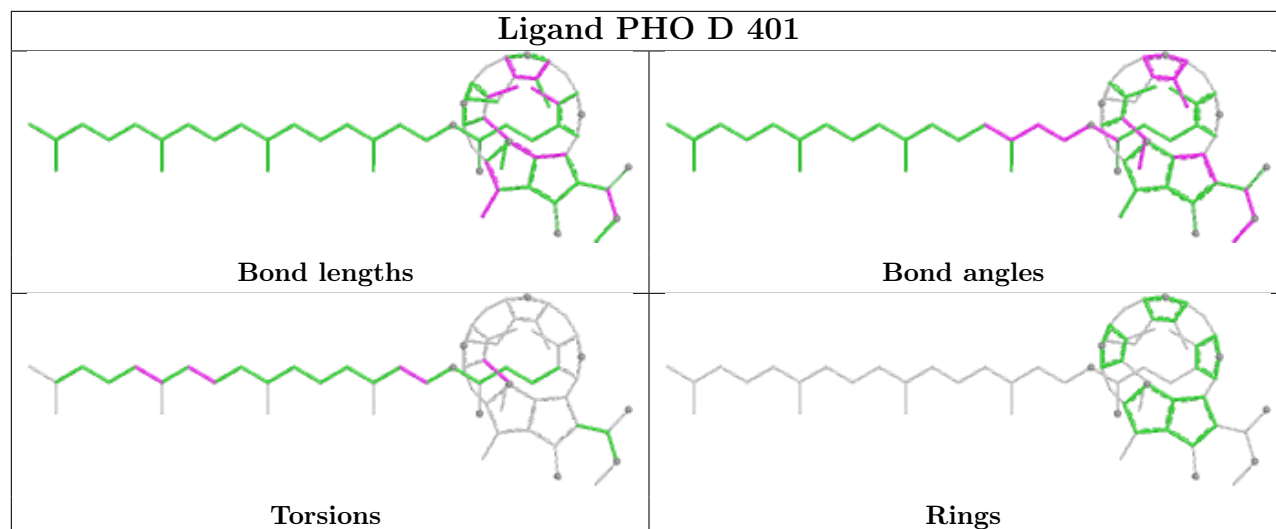
Ligand CLA b 614

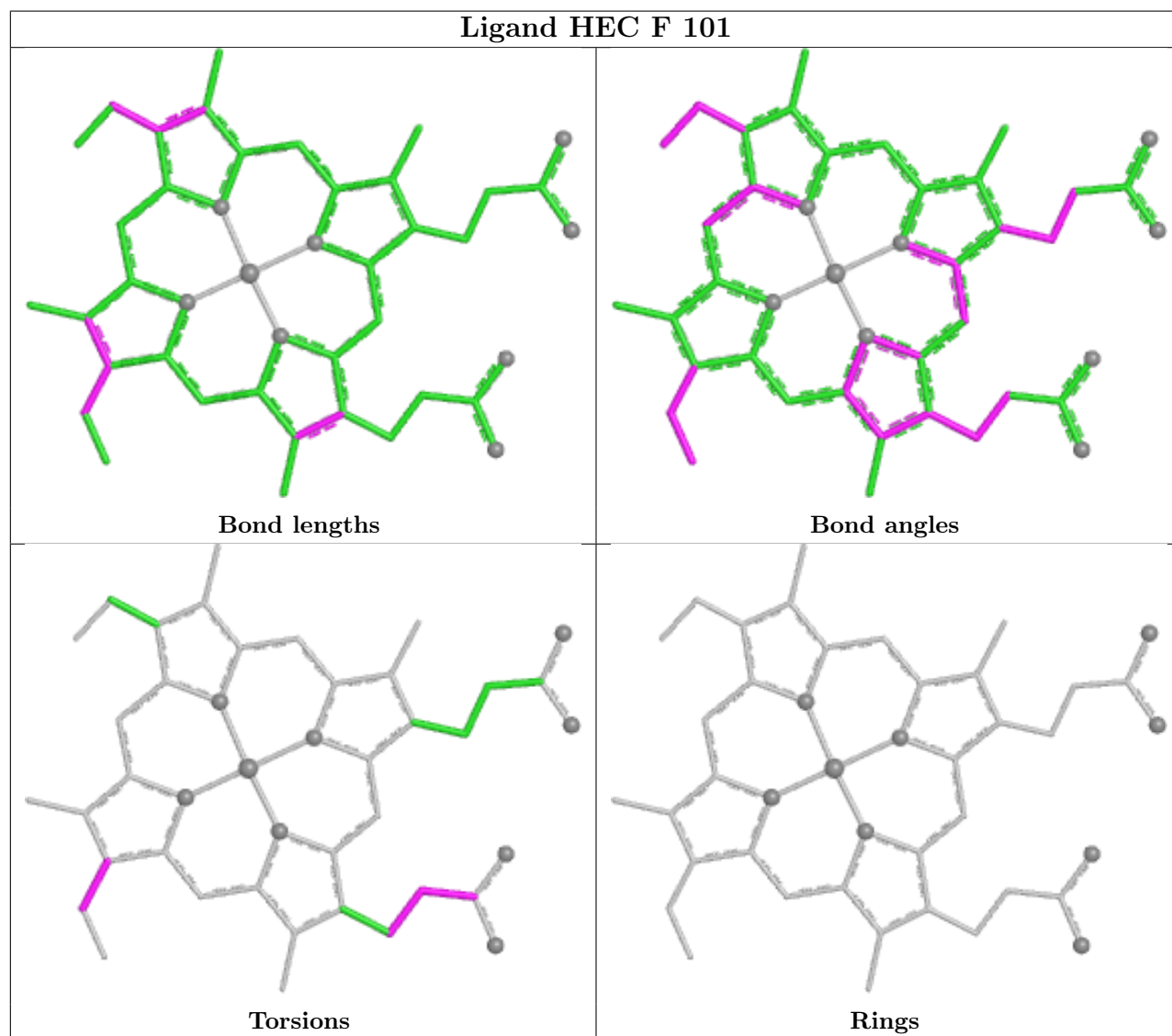
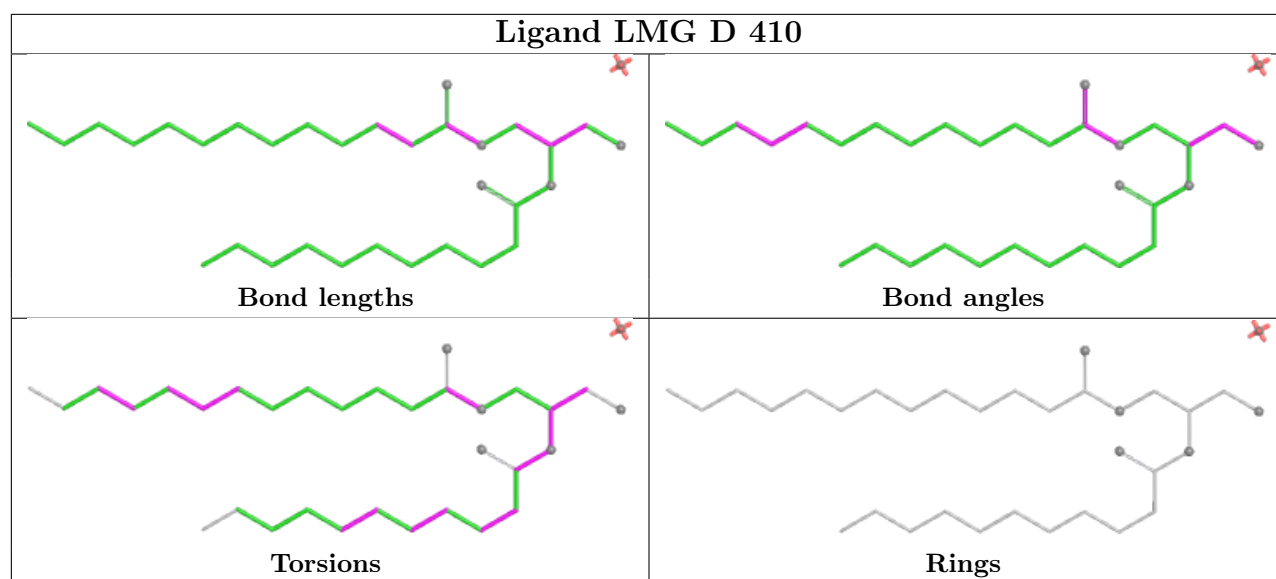


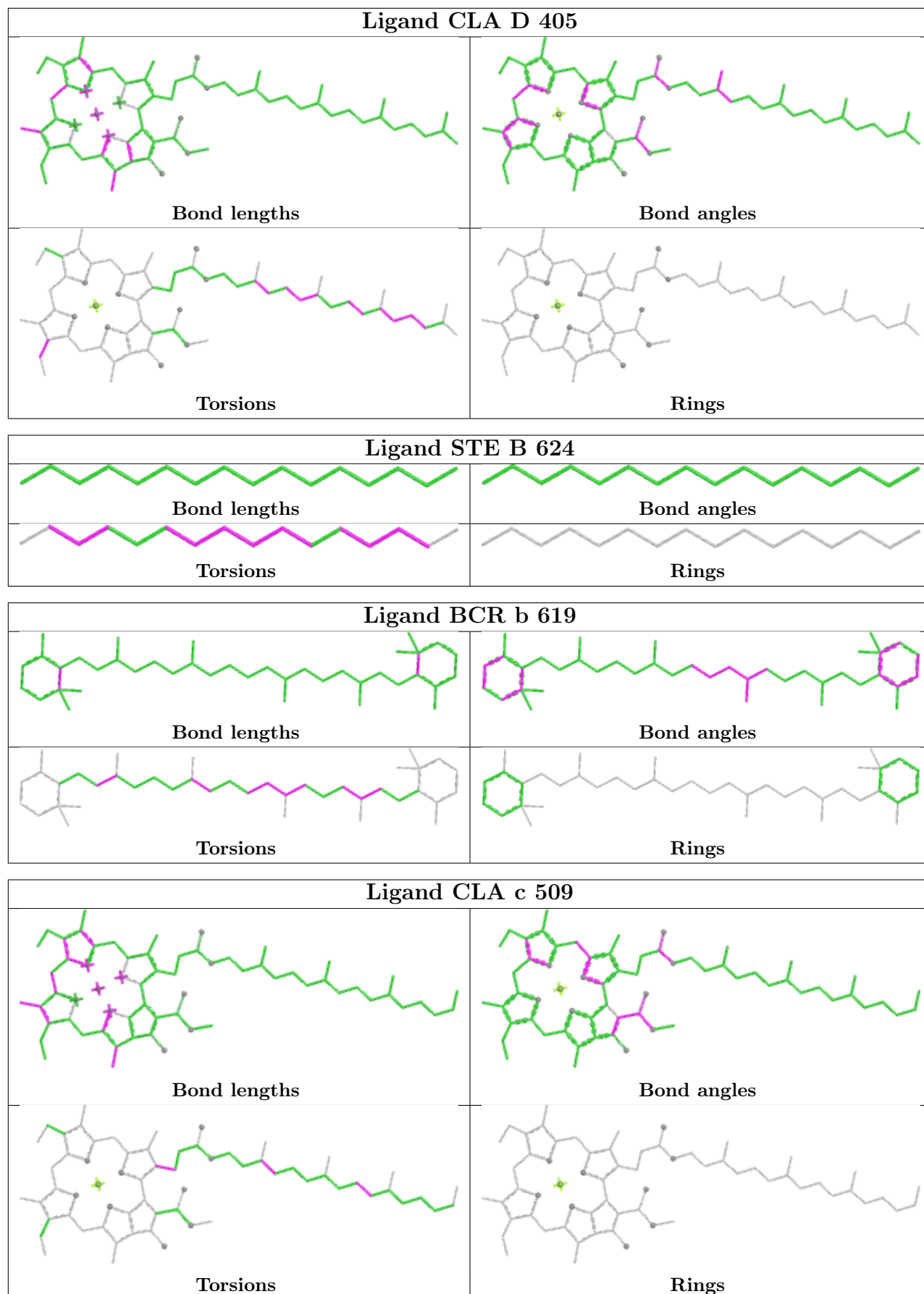
Ligand STE a 416

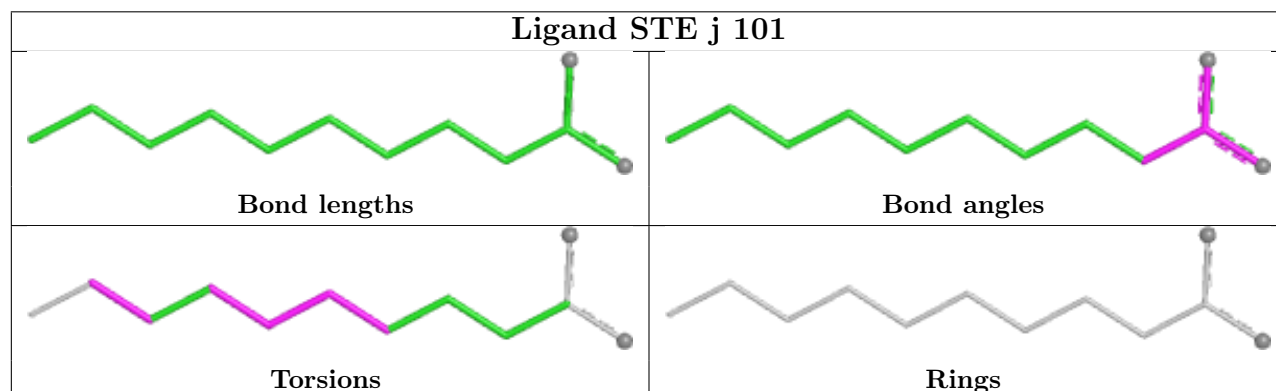
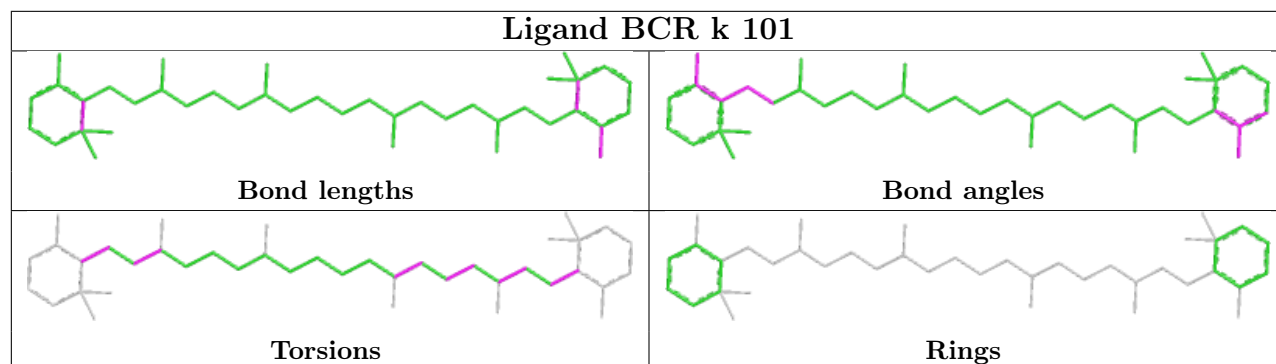
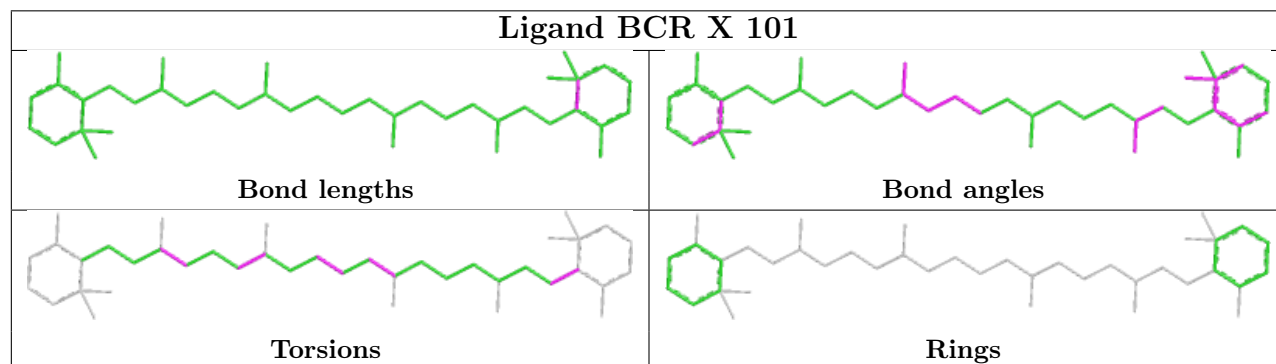
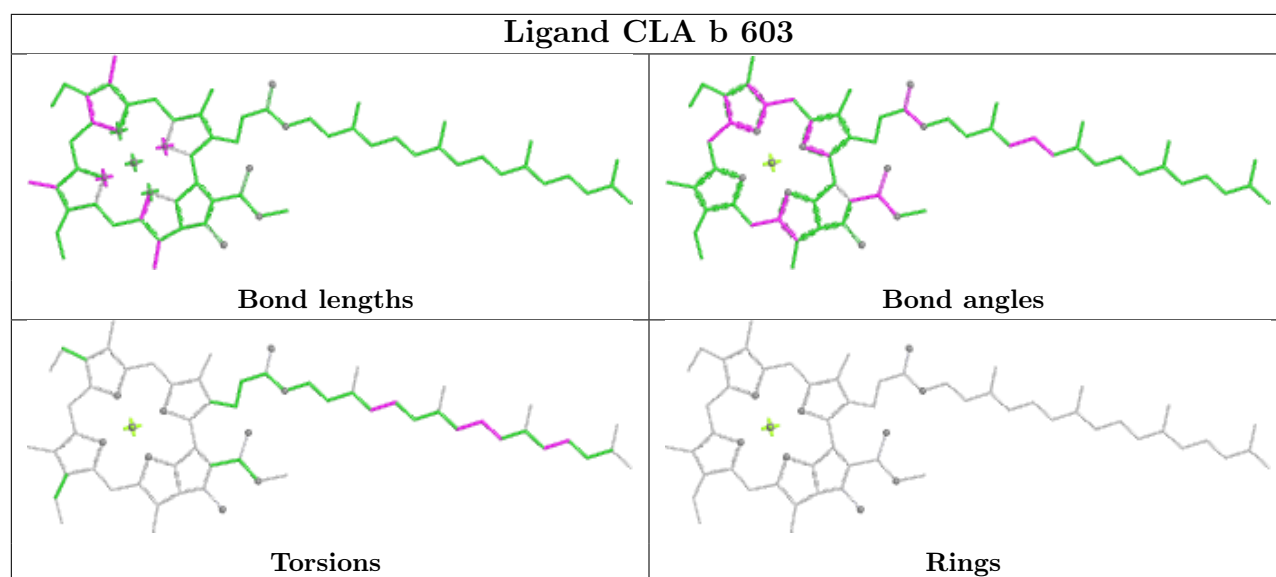


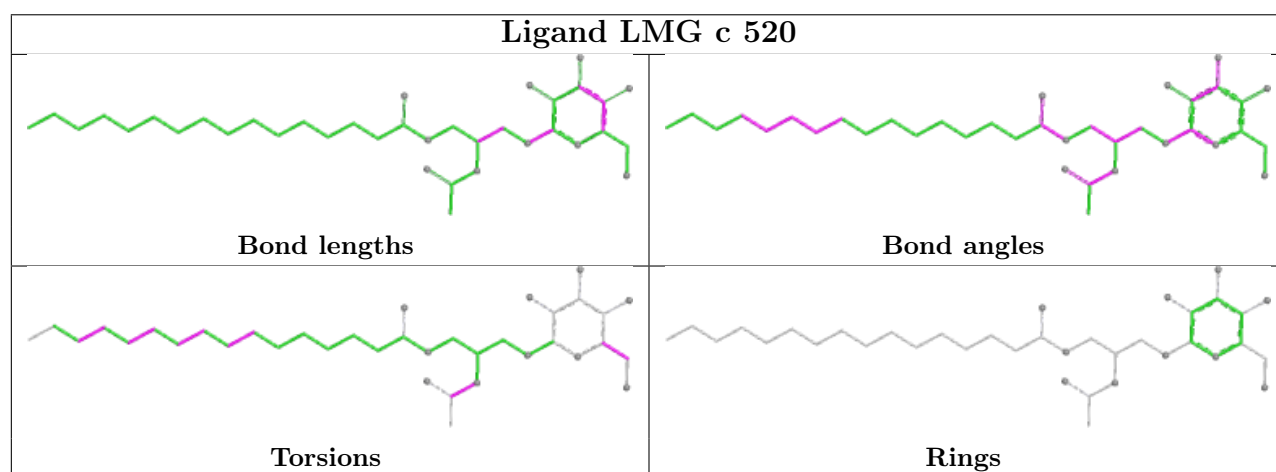
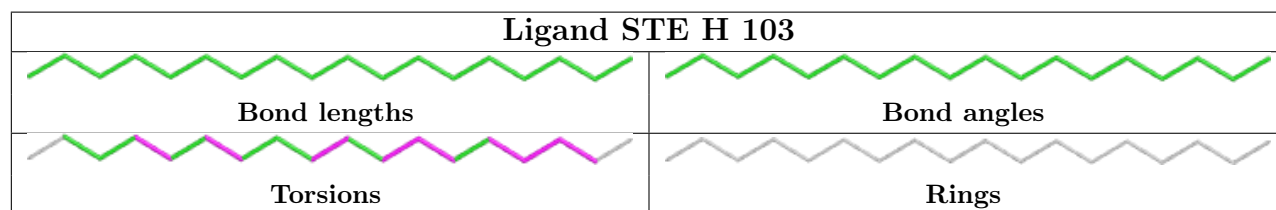
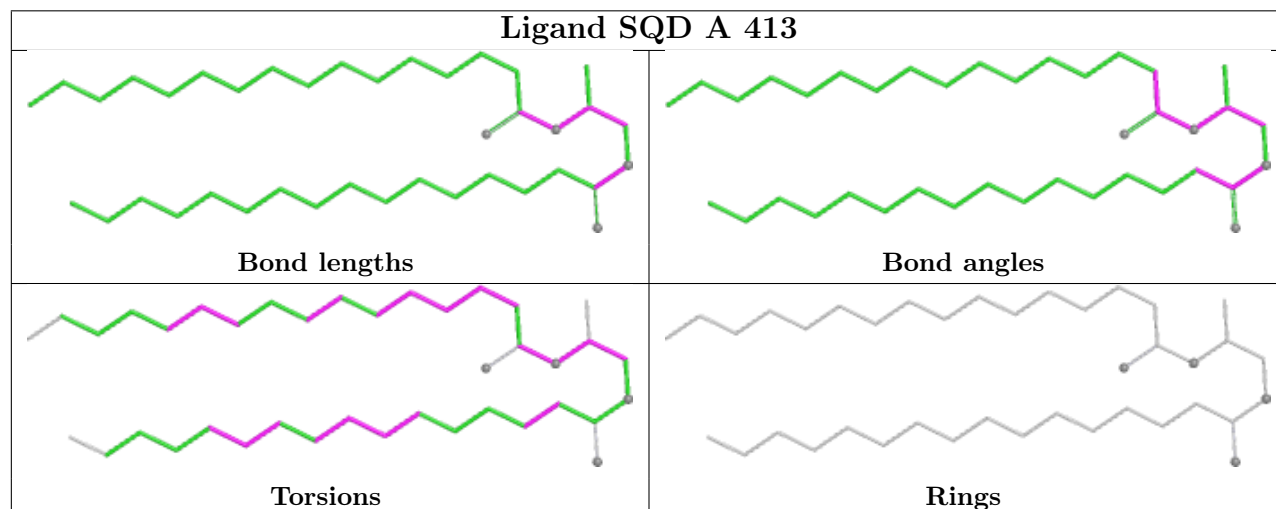
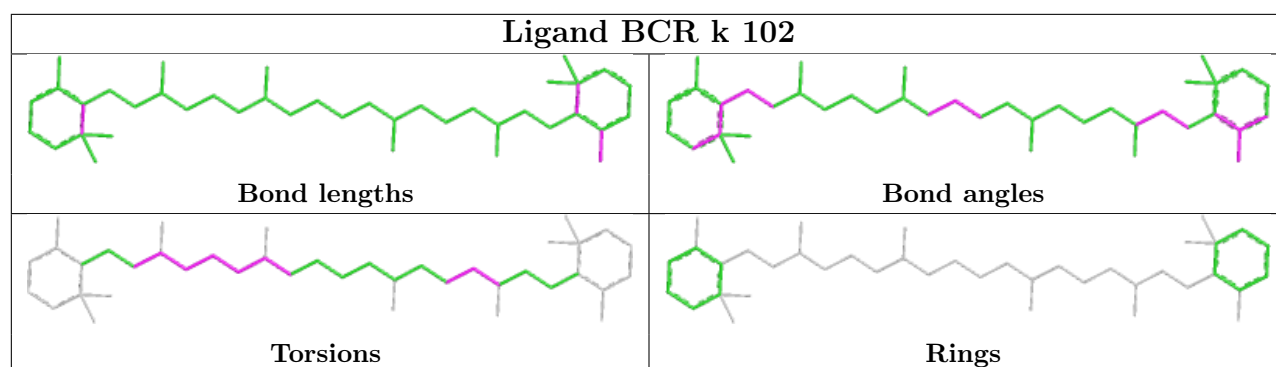


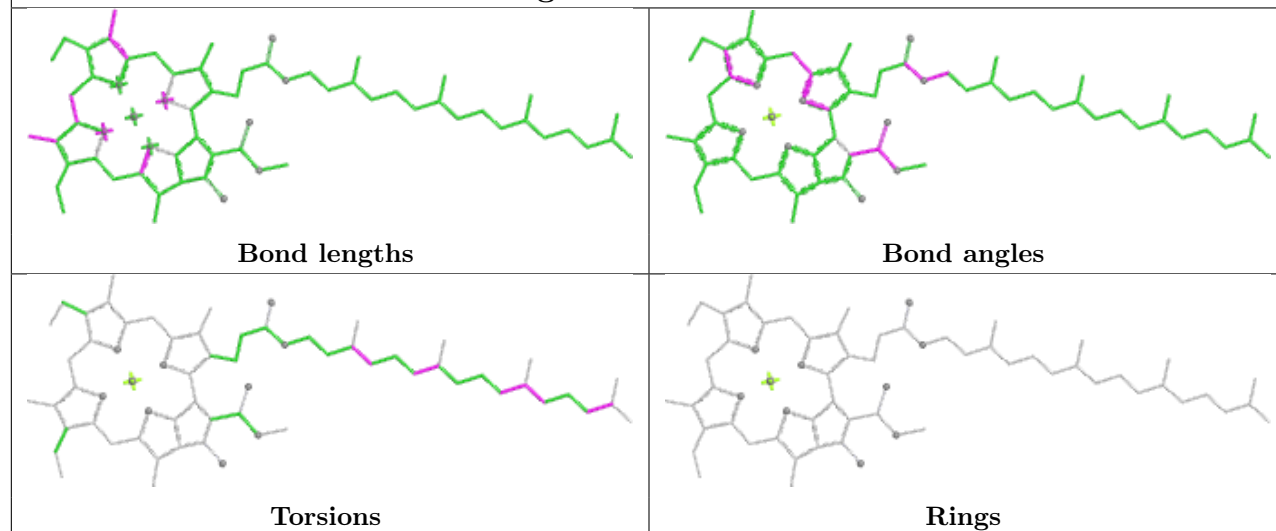
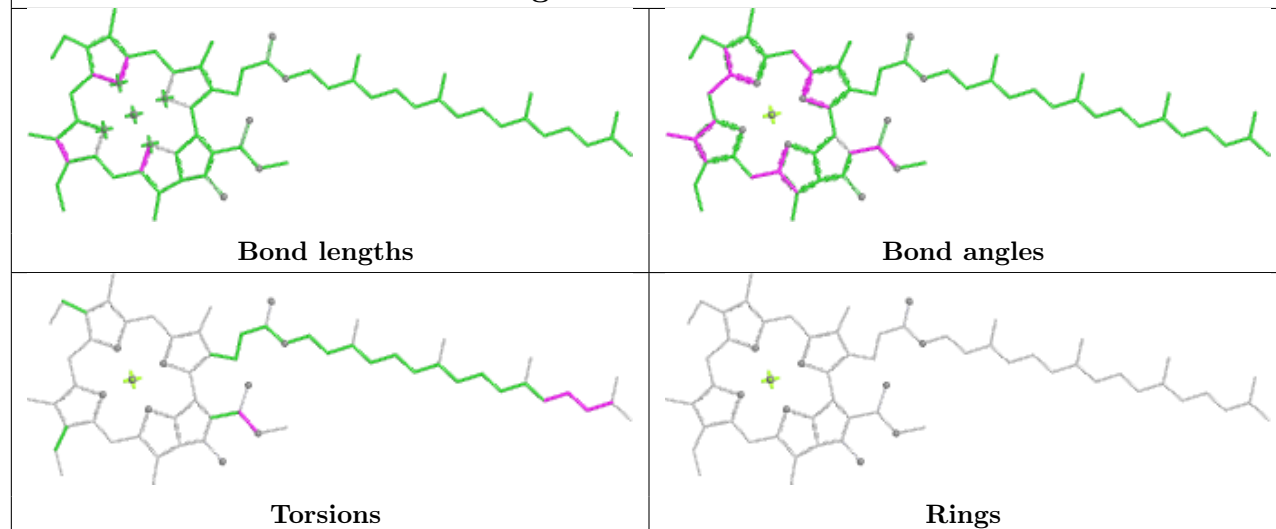


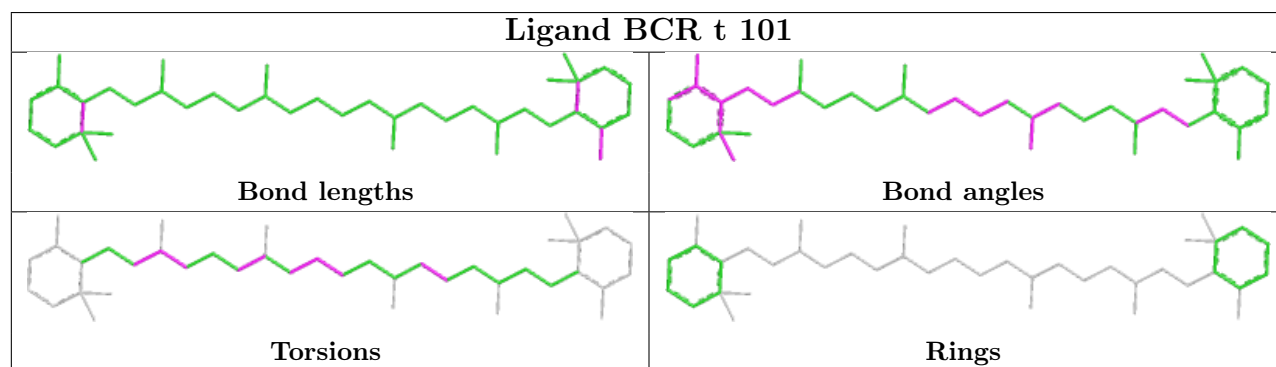
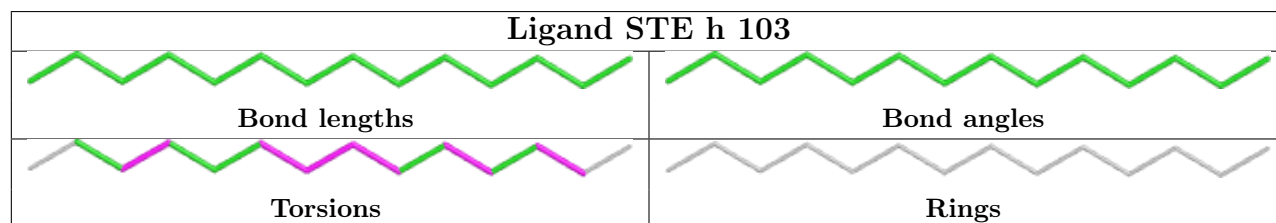
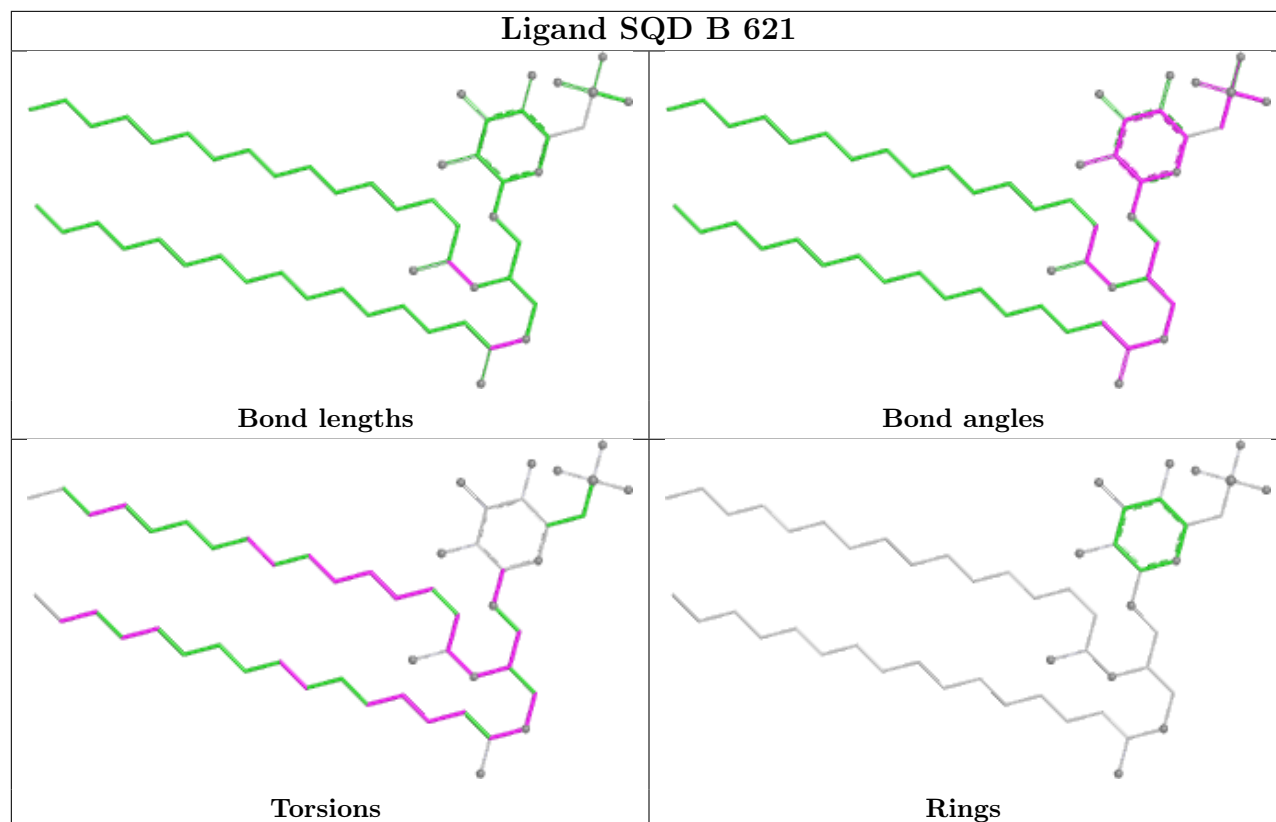


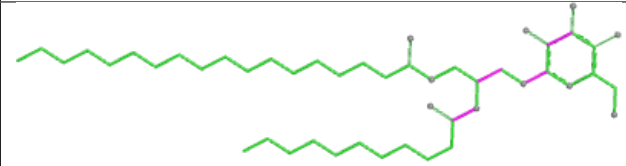
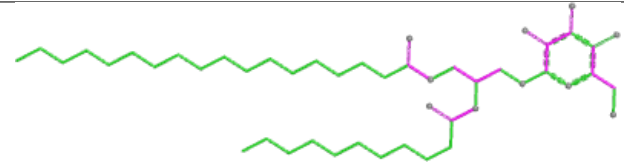
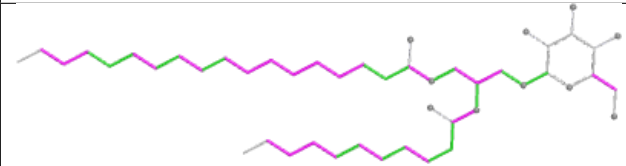
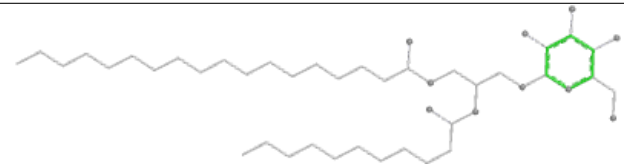
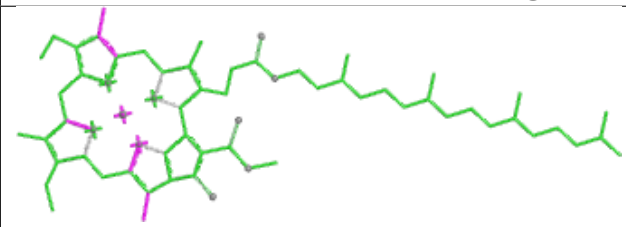
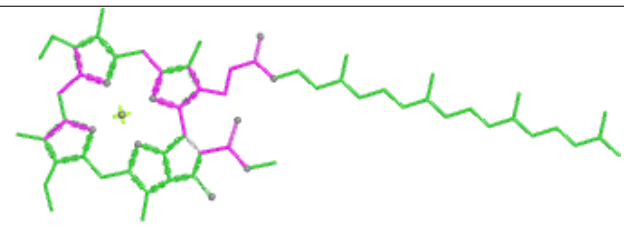
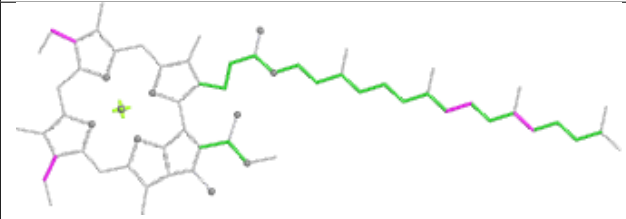
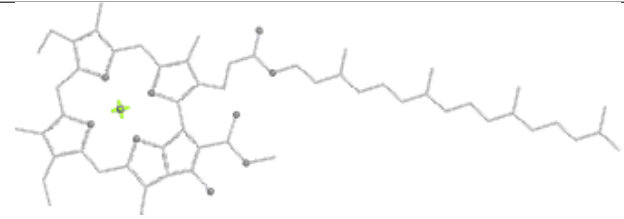
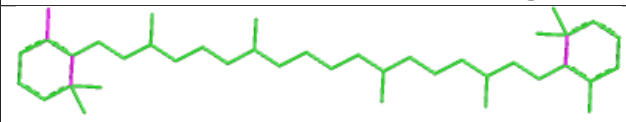
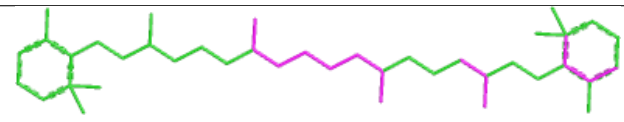
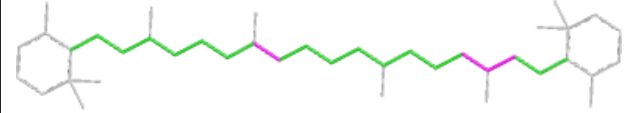
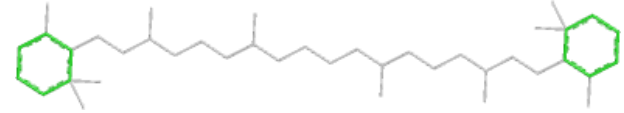
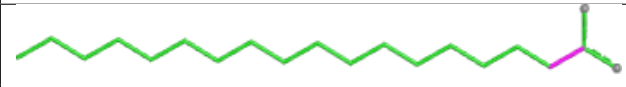
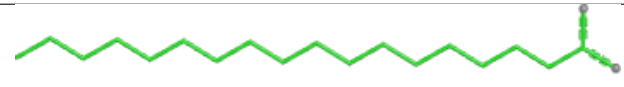
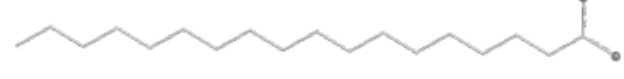


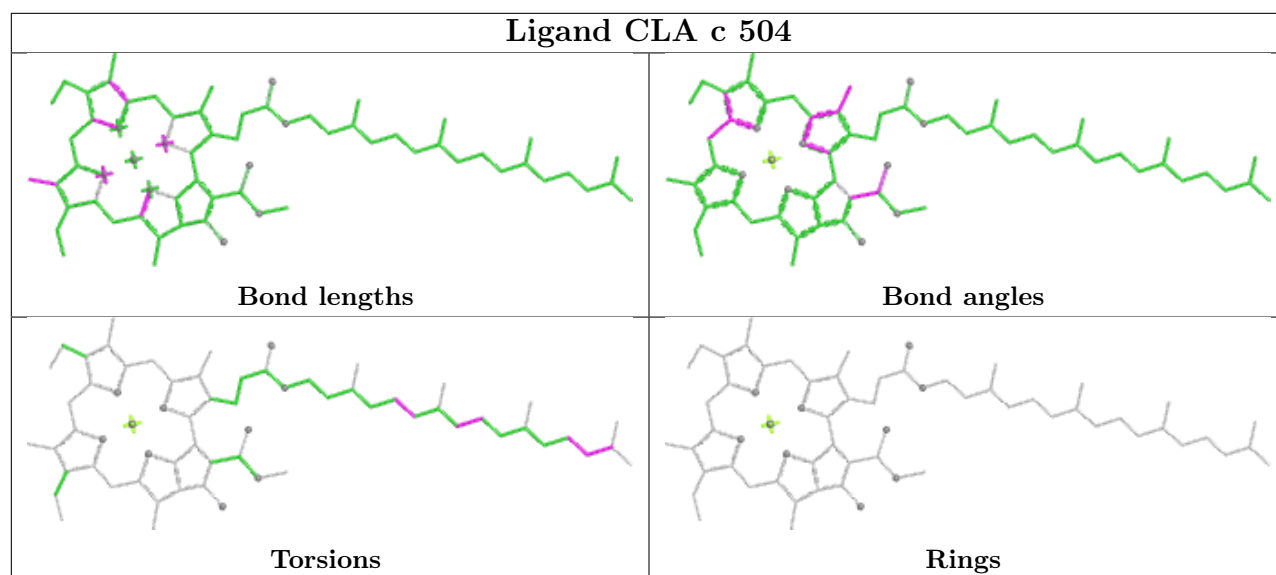
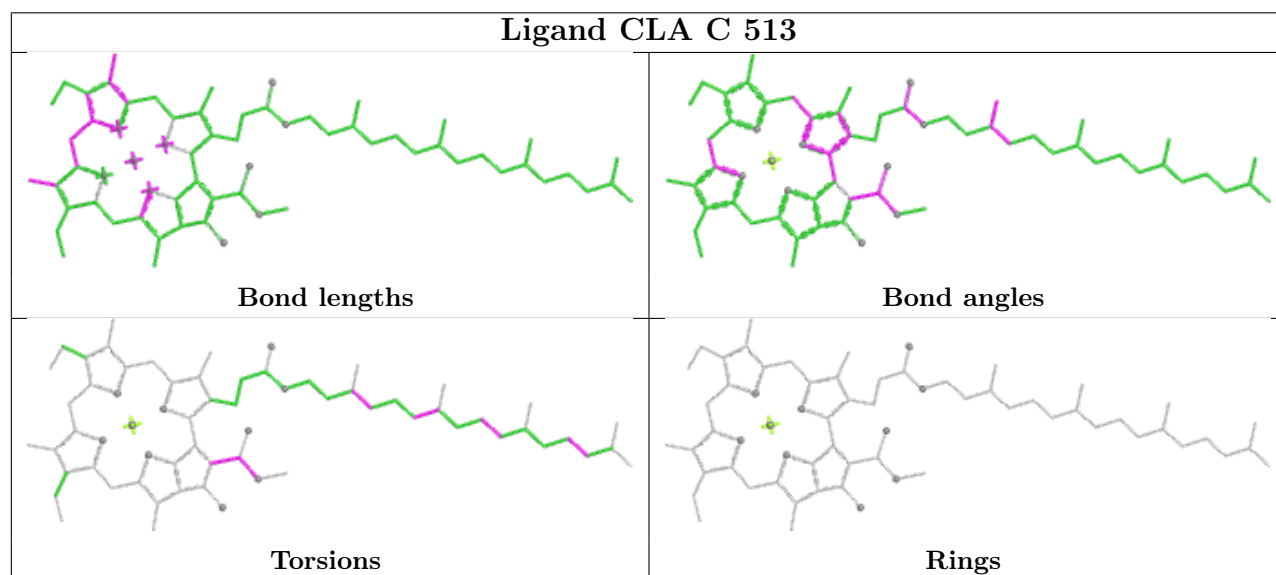
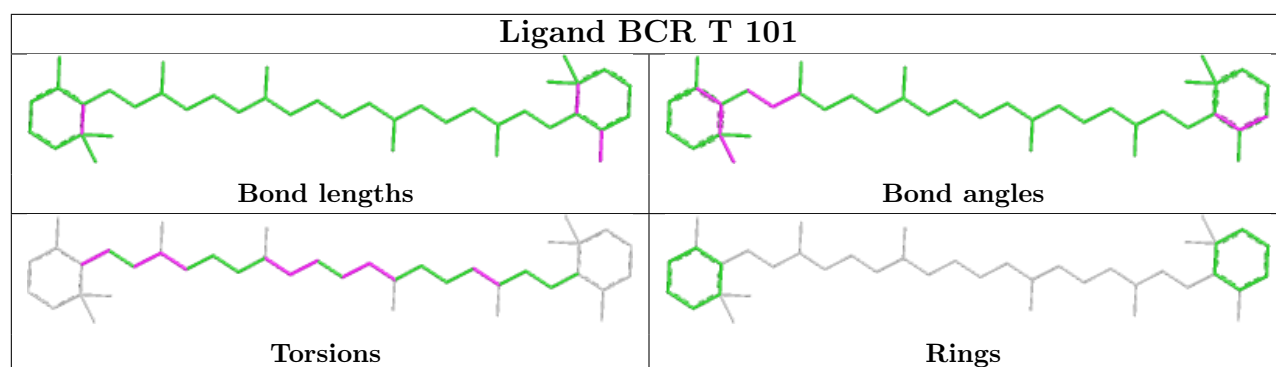


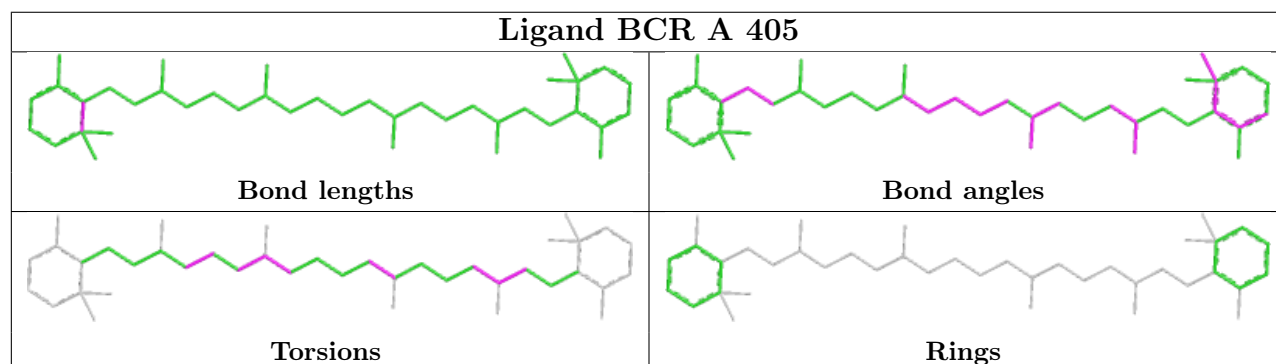
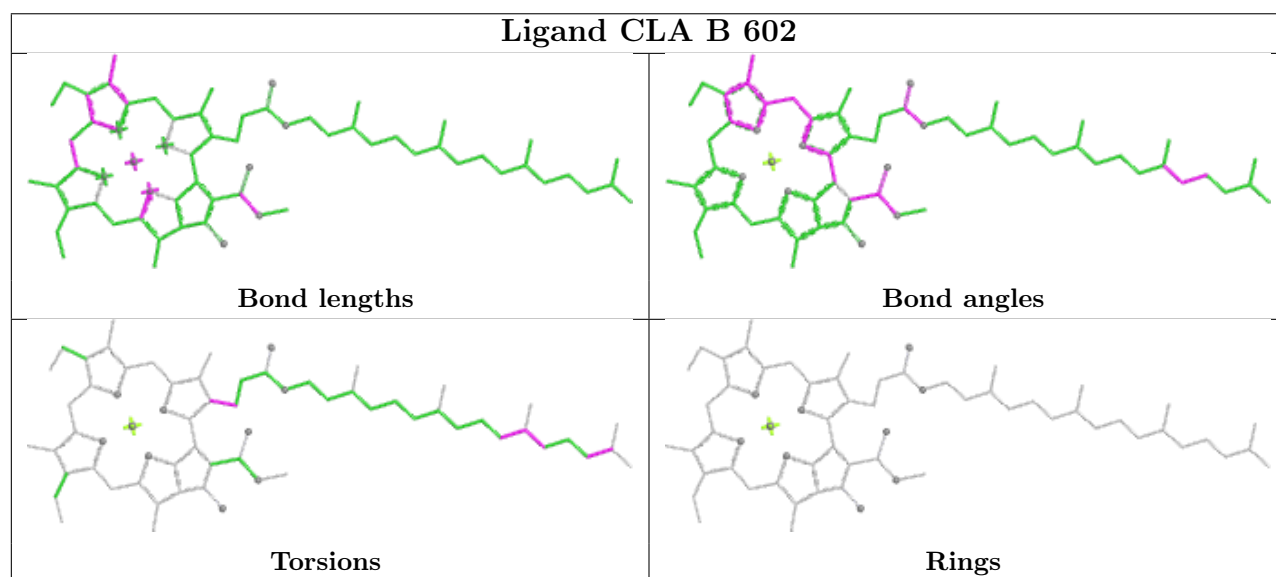
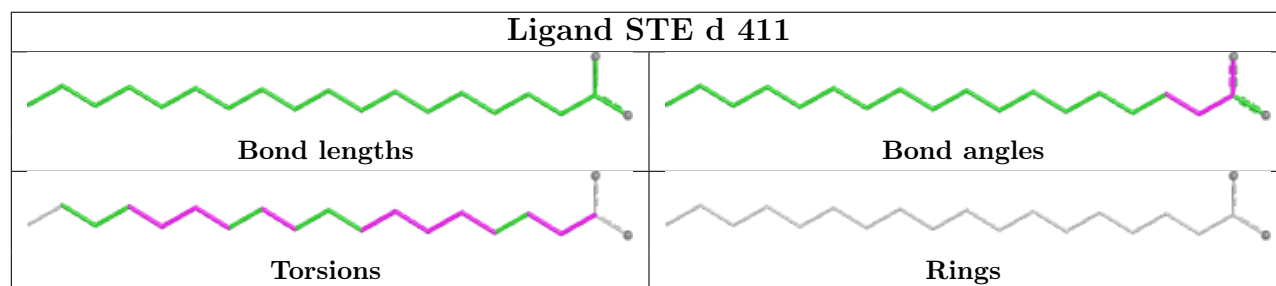
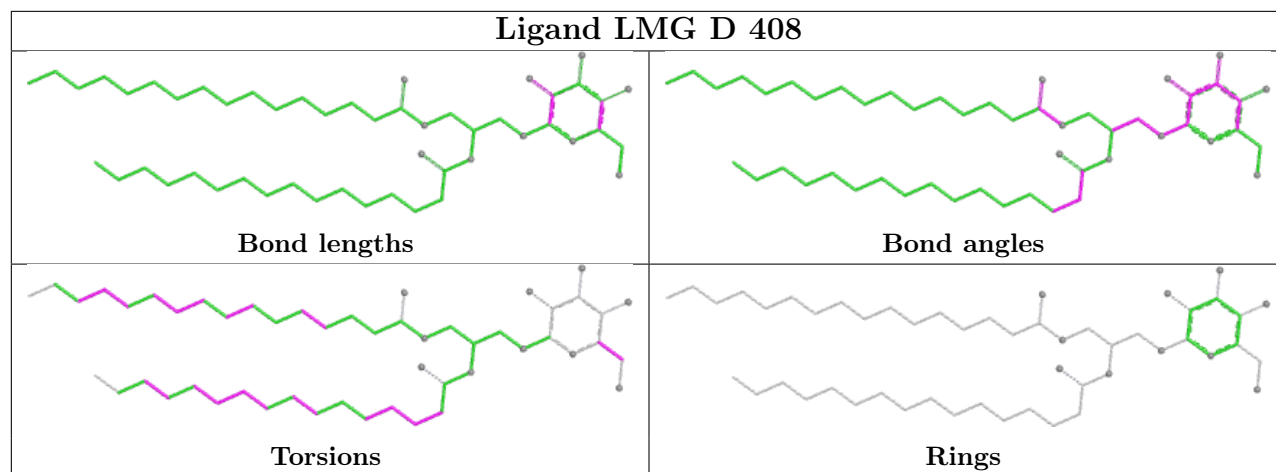


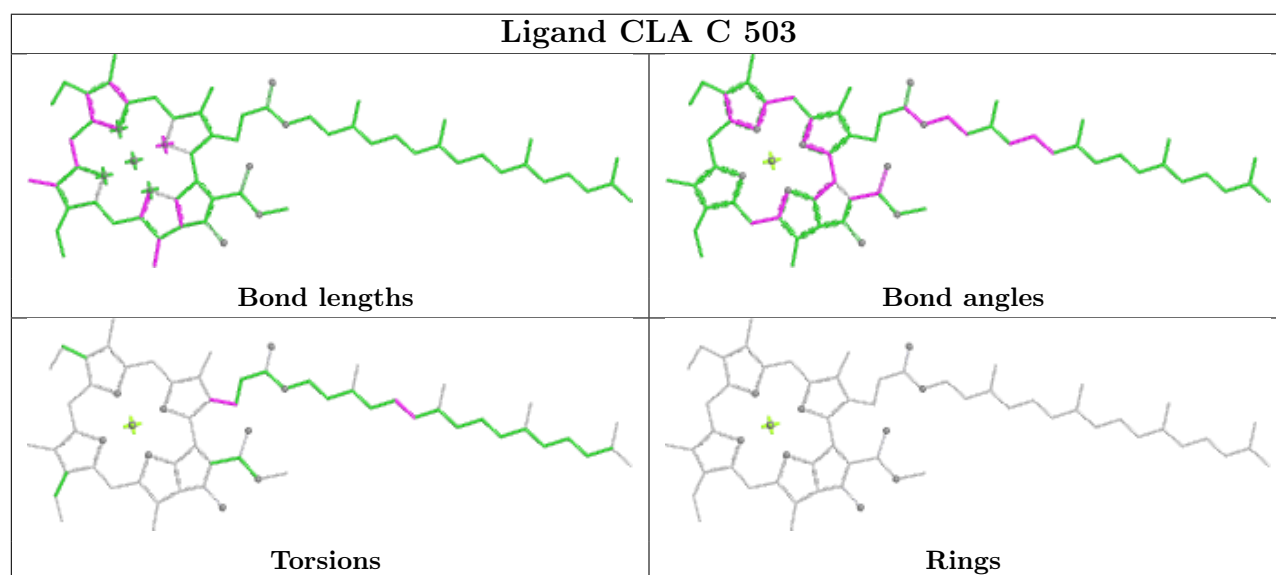
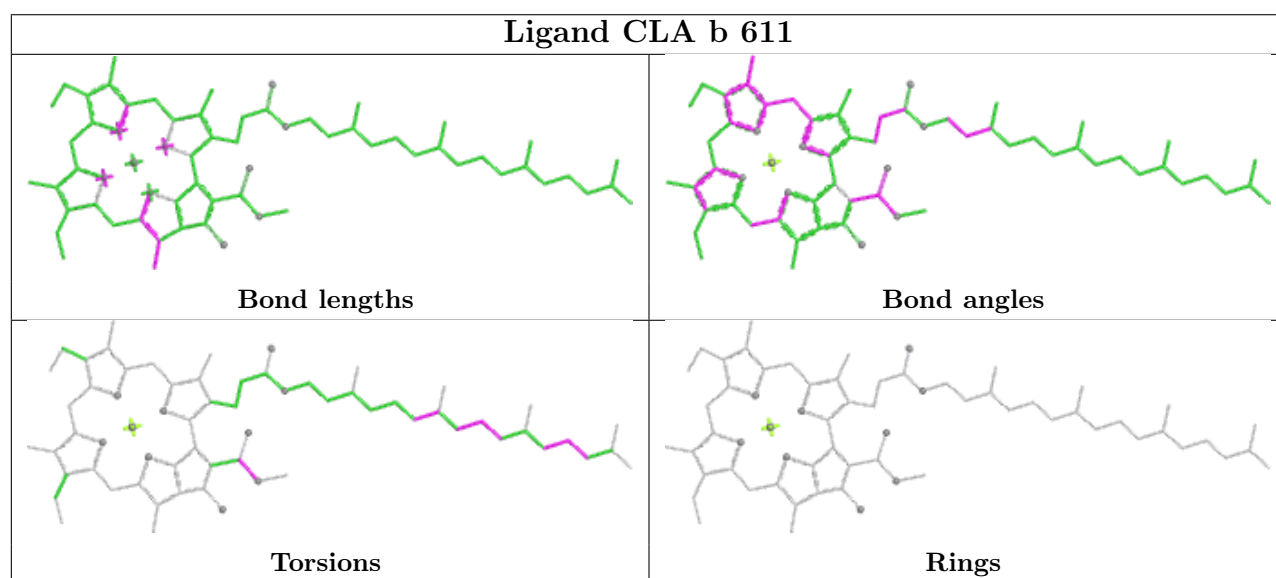
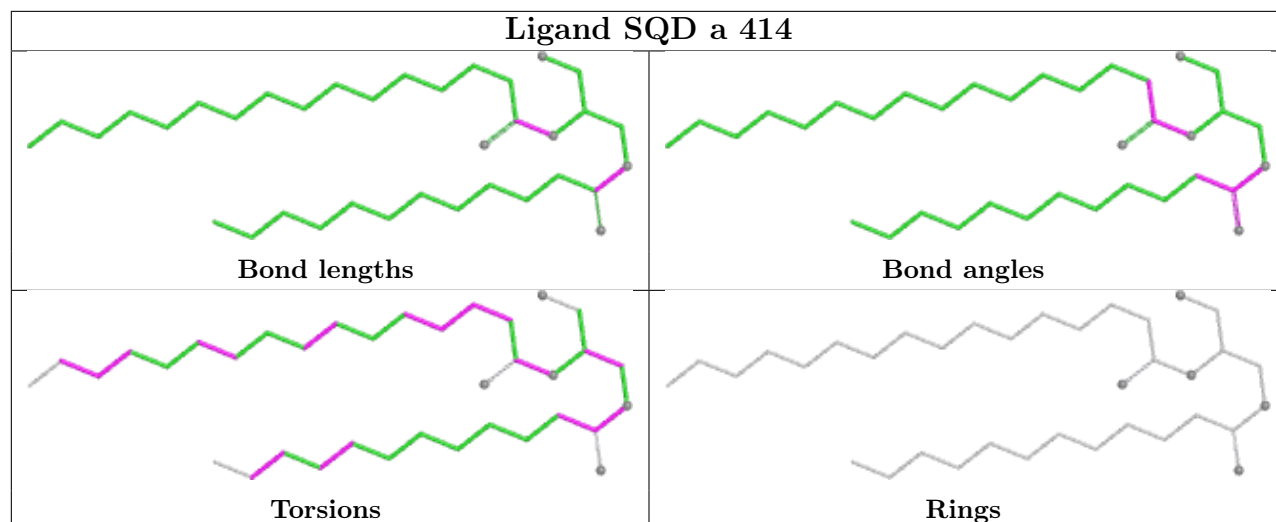
Ligand CLA c 511**Ligand CLA A 409**

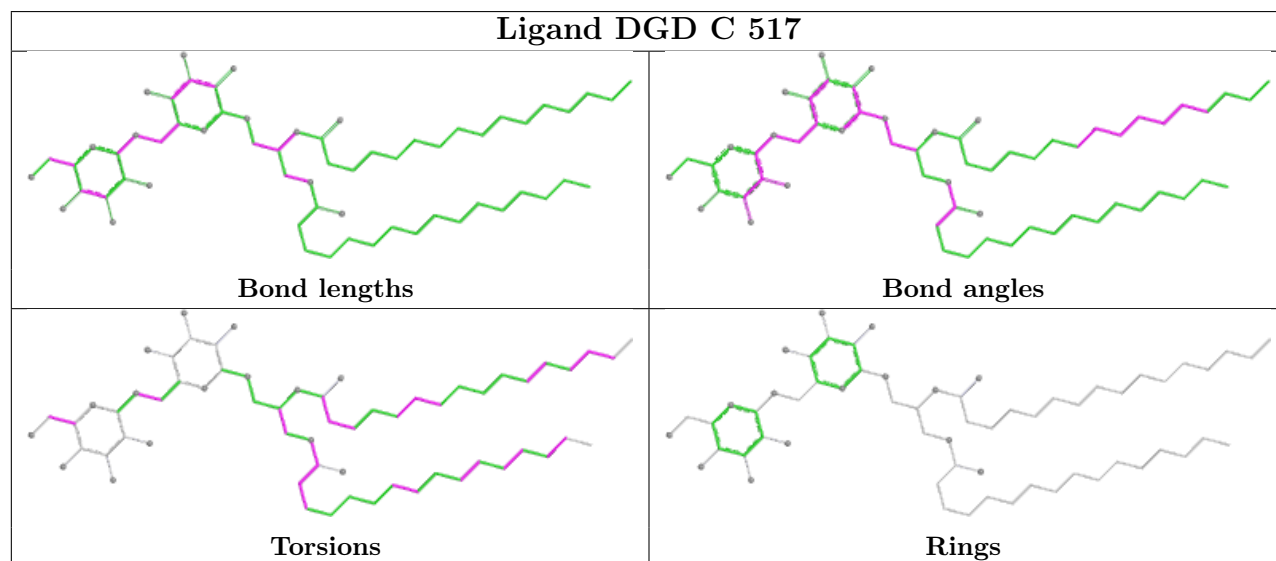
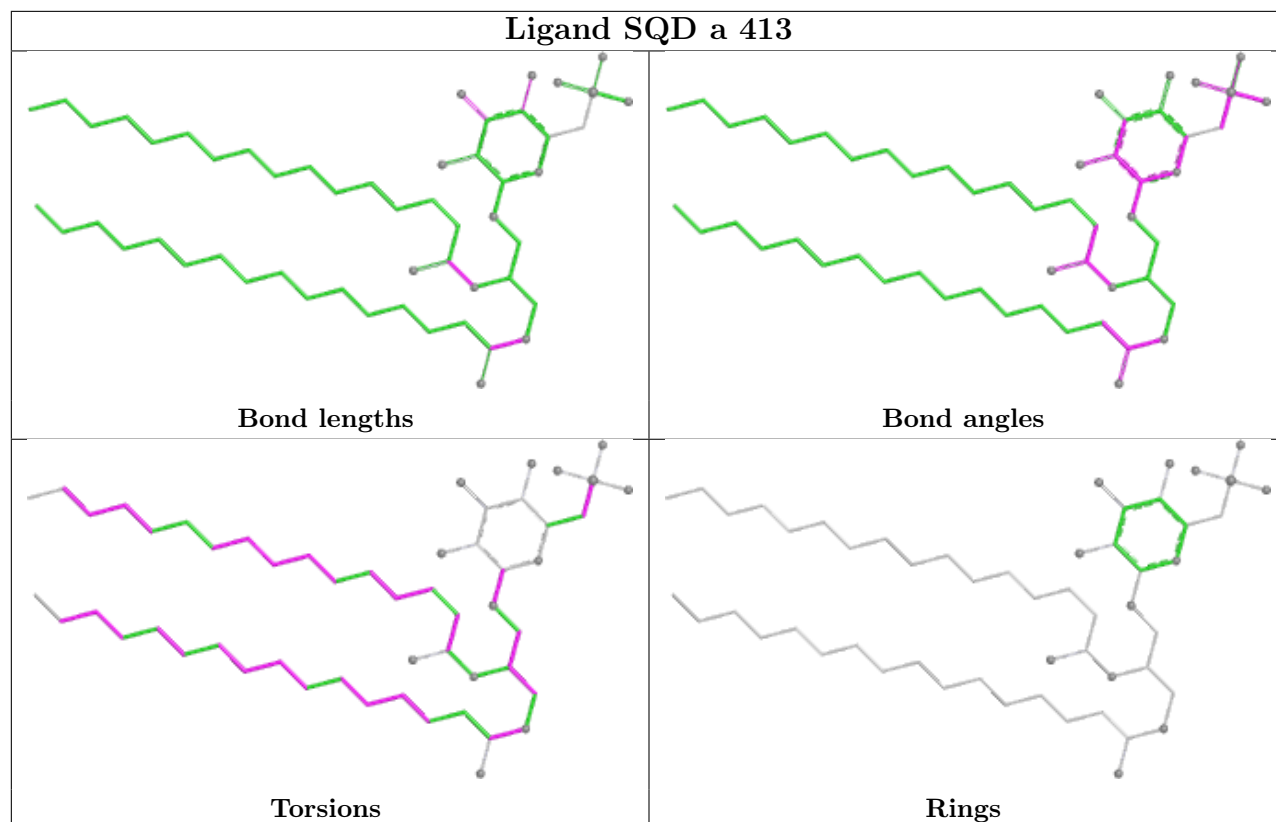


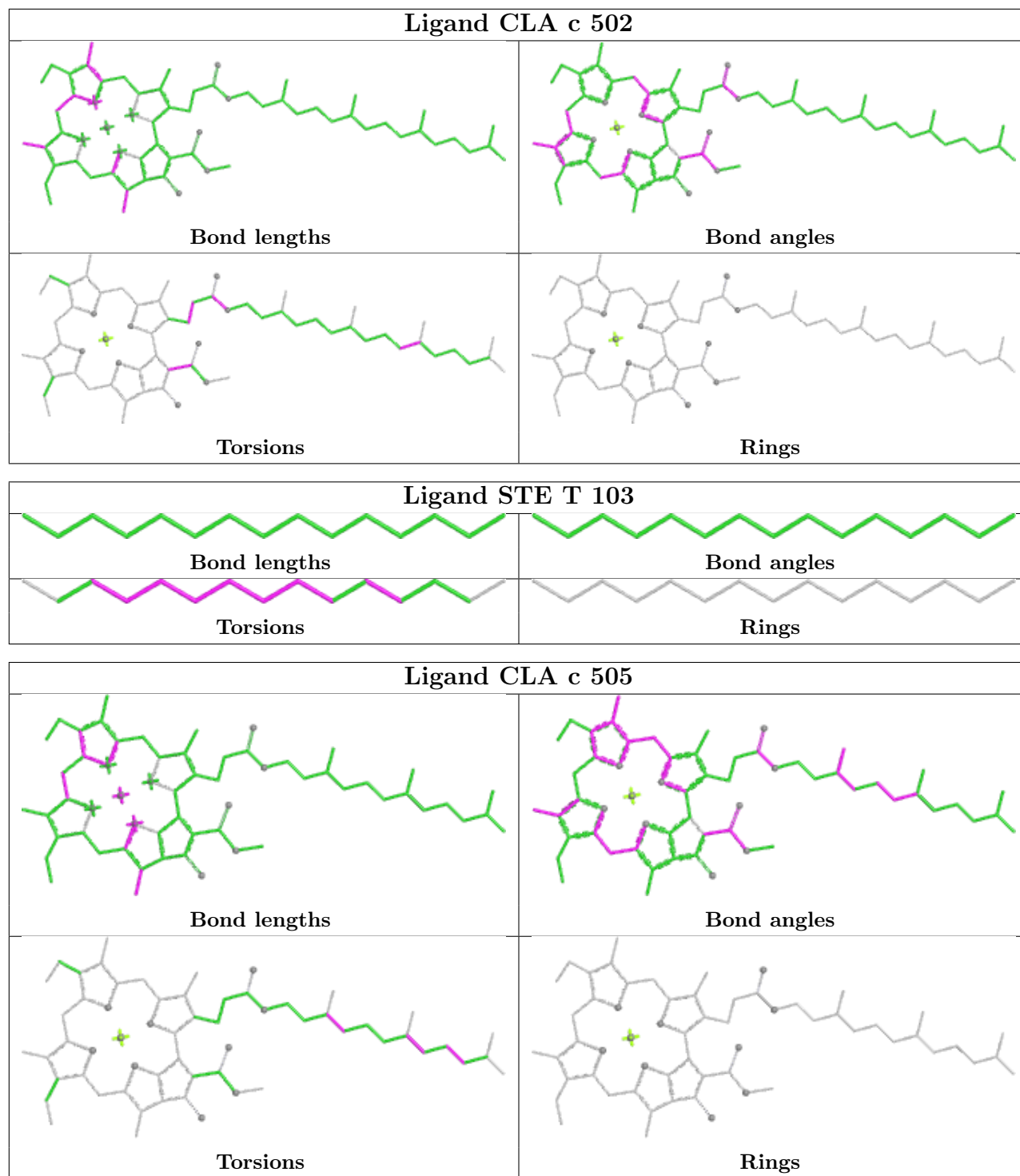
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 610	
 Bond lengths	 Bond angles
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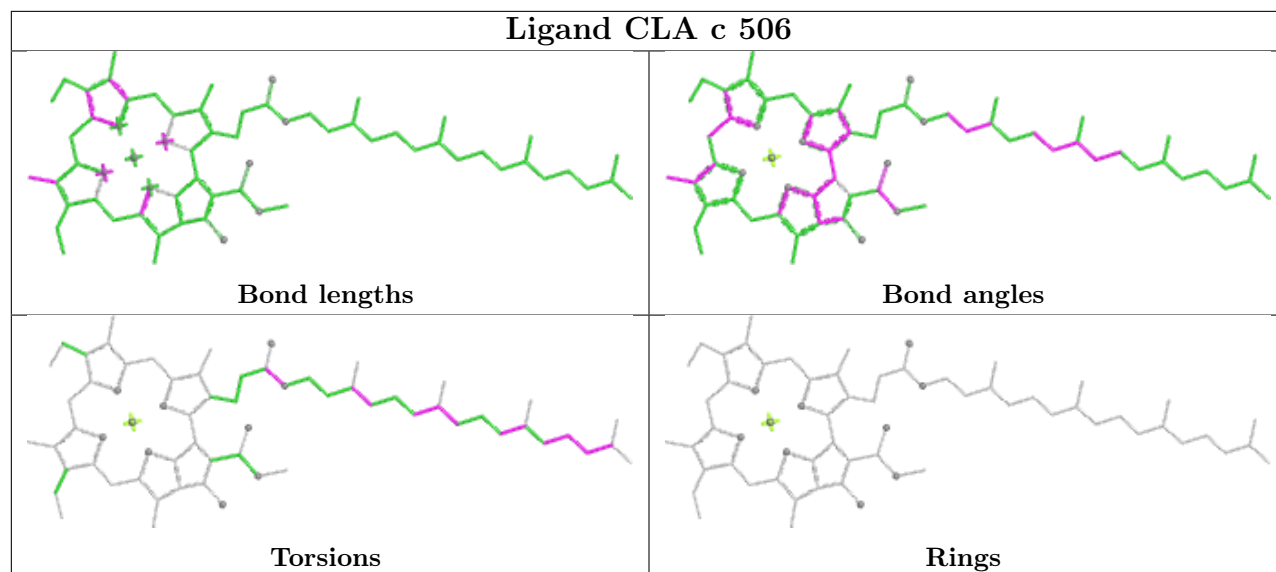




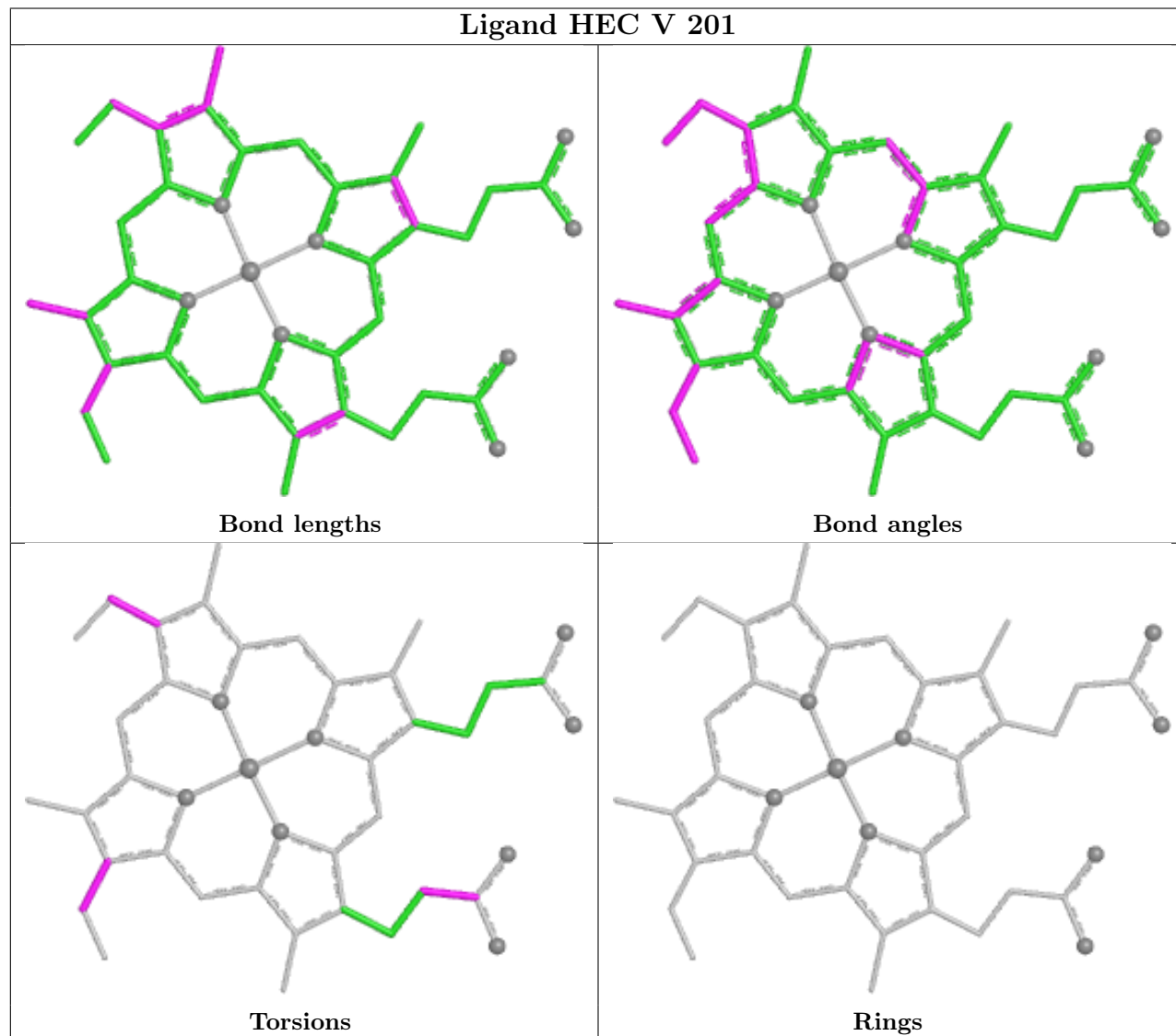


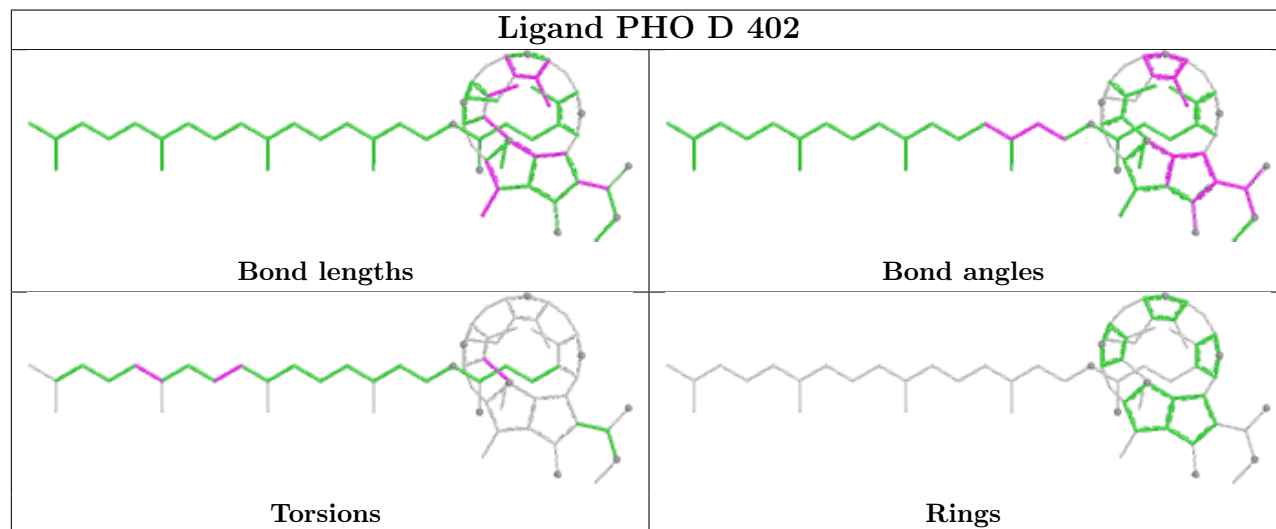
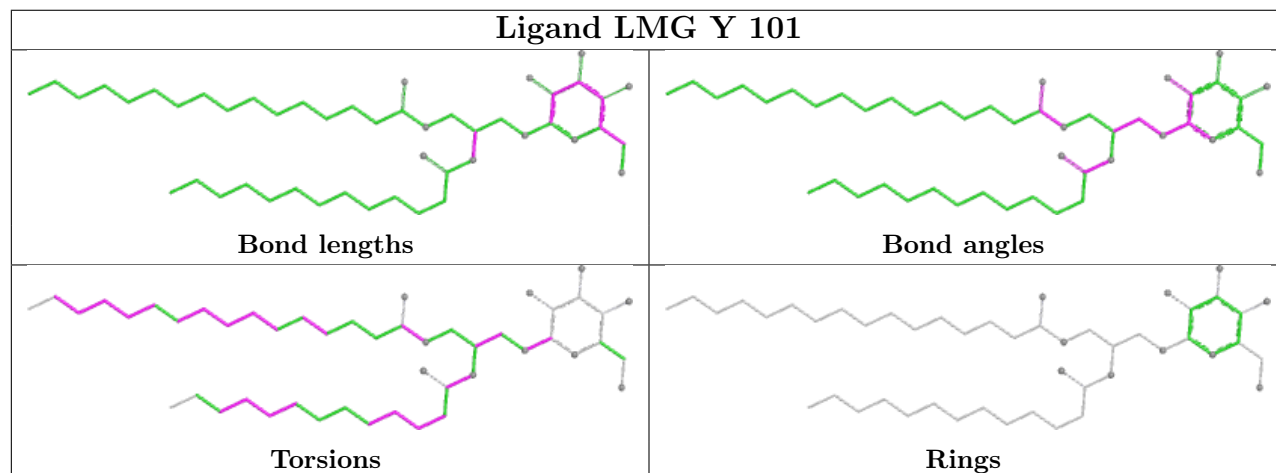
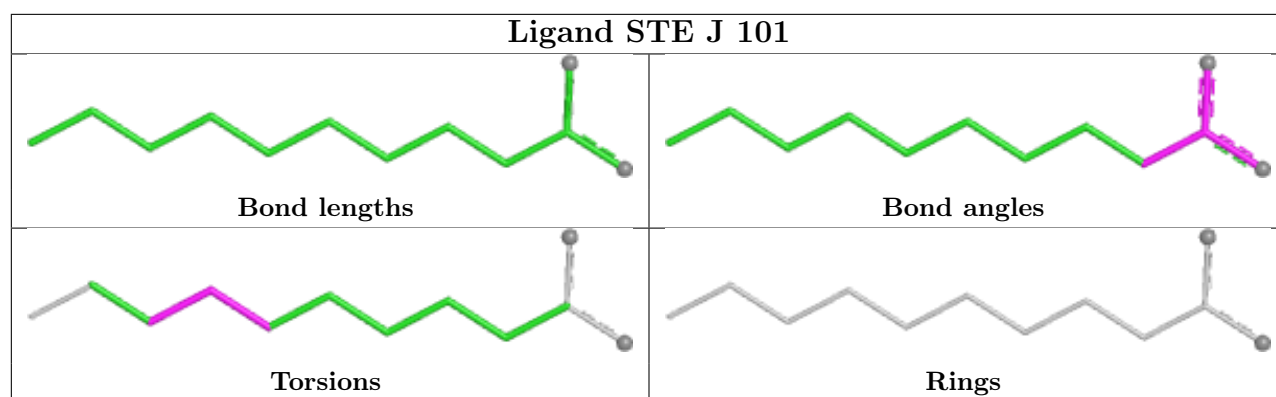


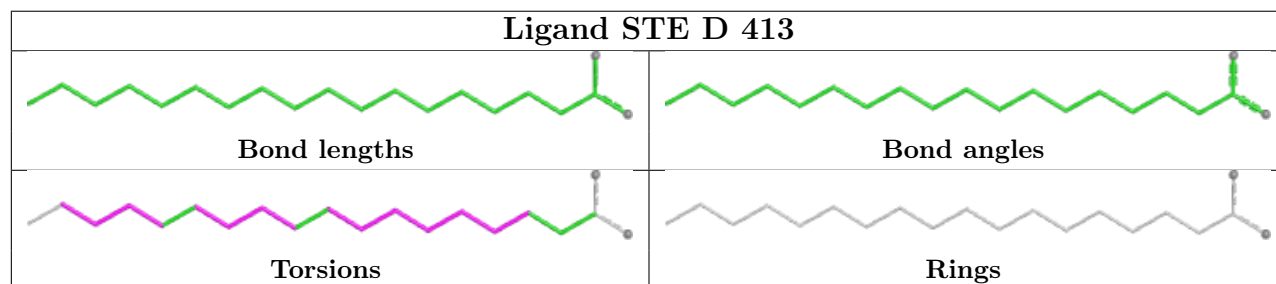
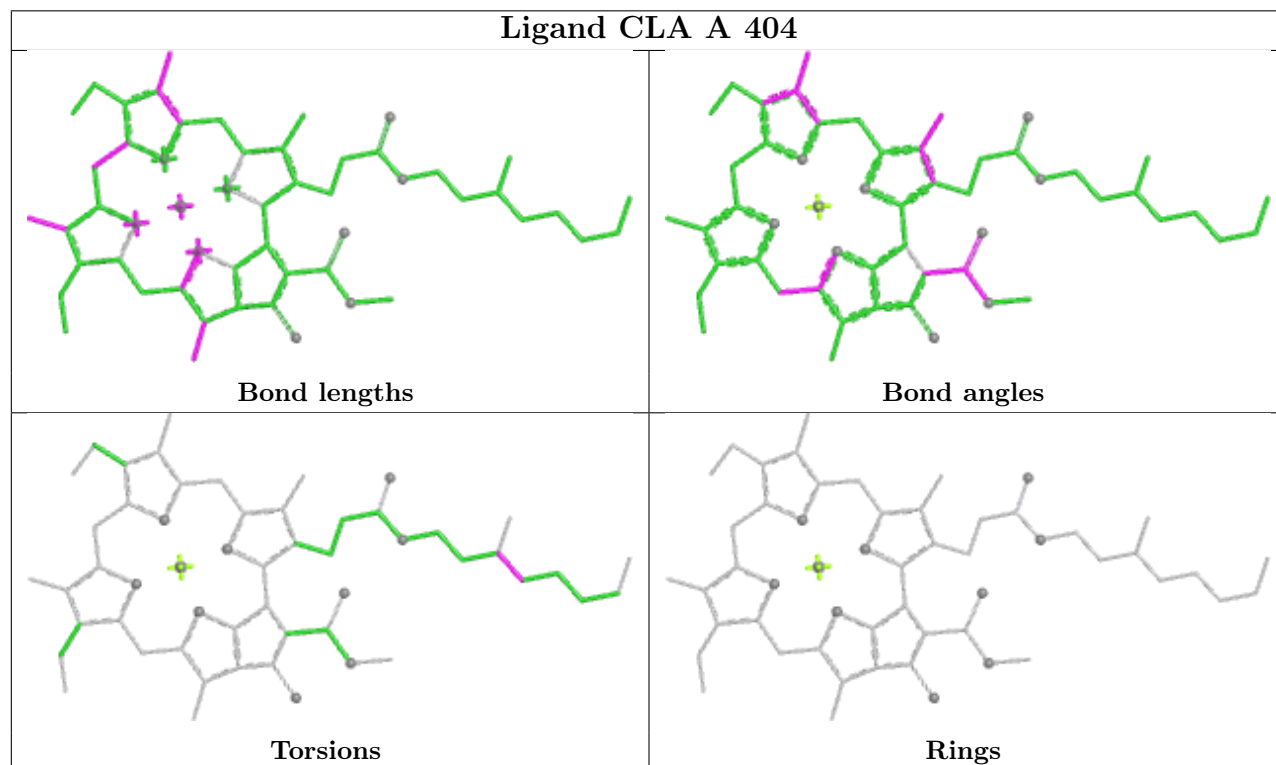
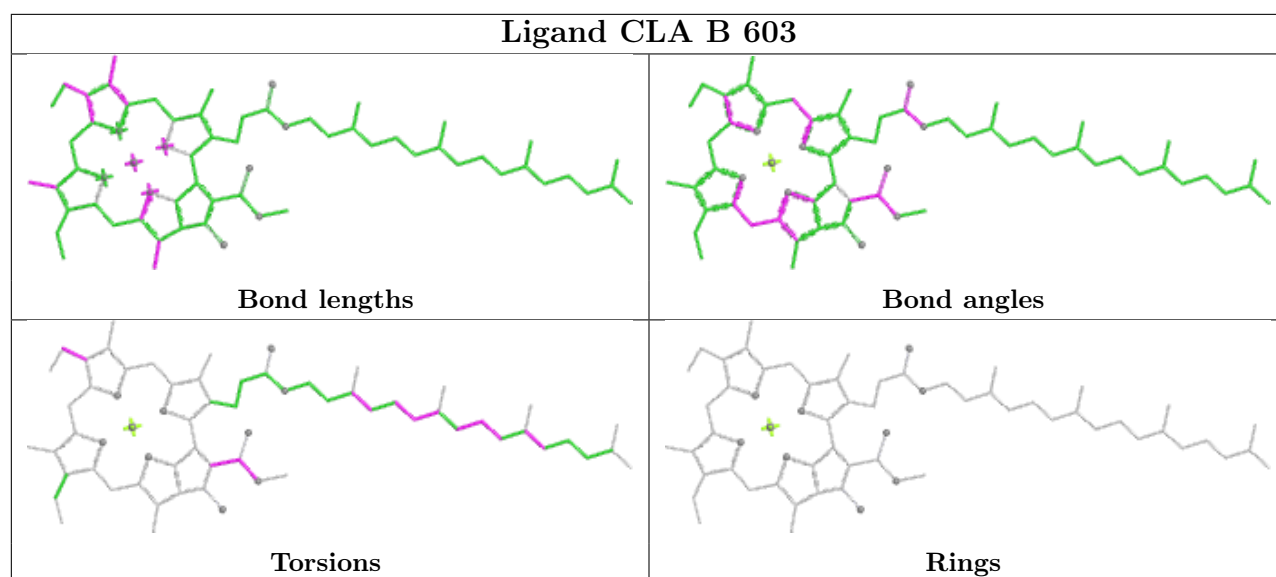
Ligand CLA c 506

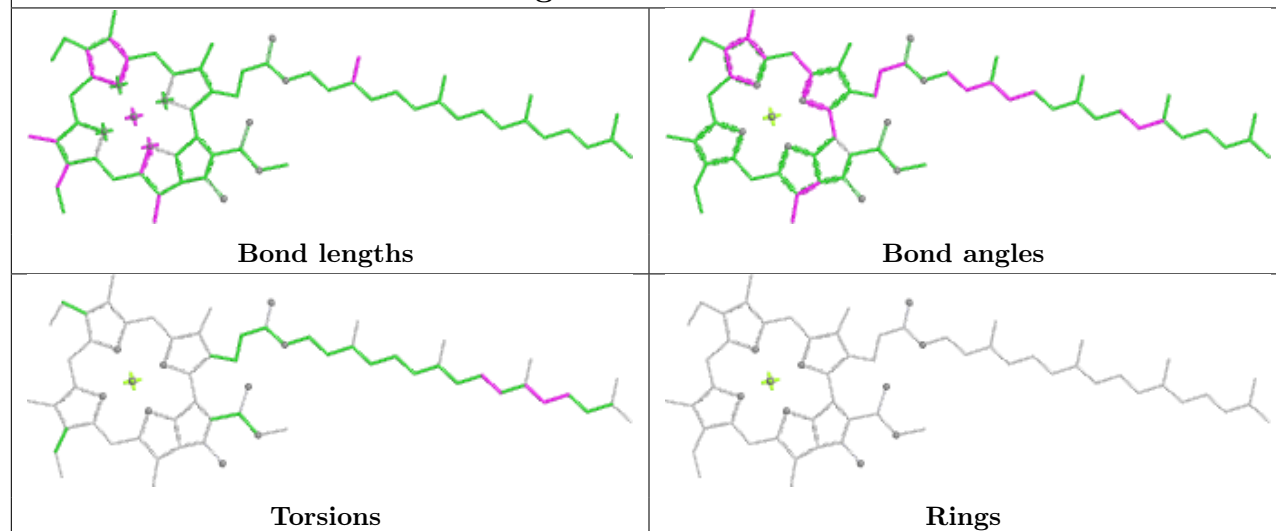
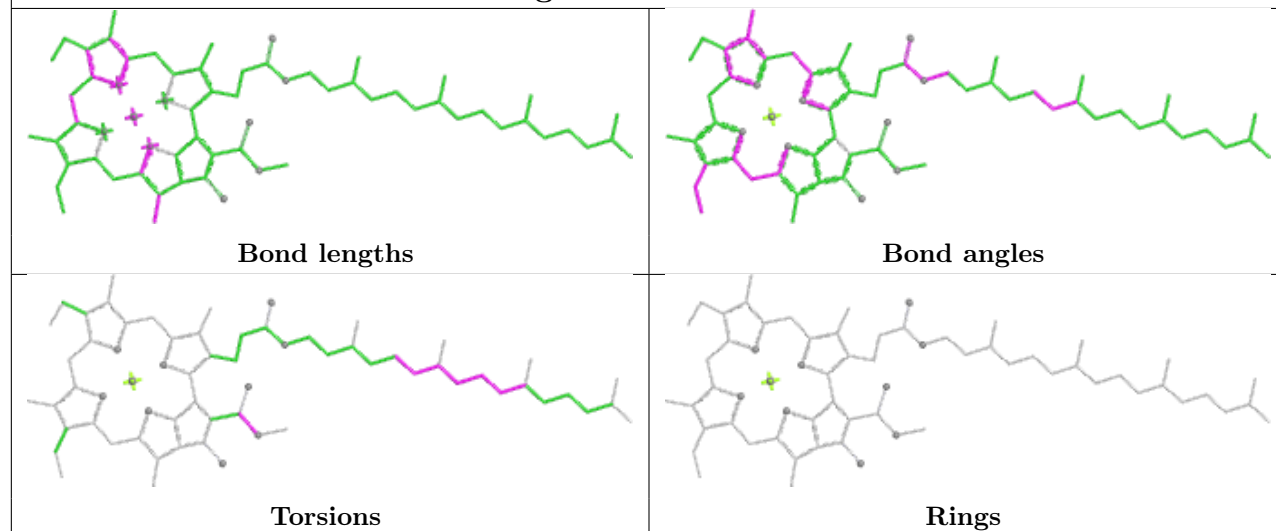
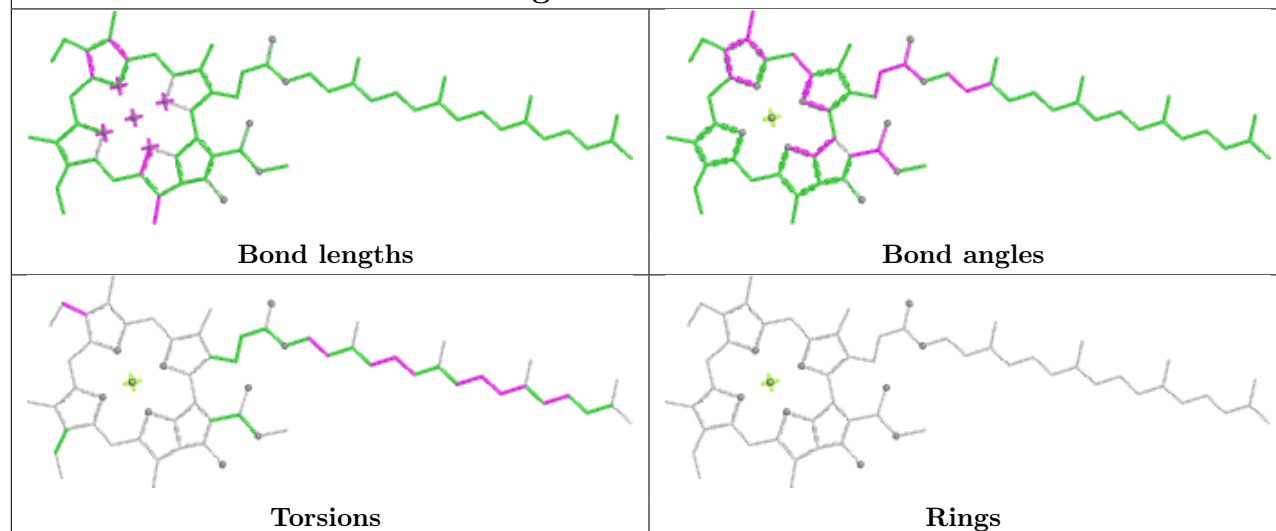


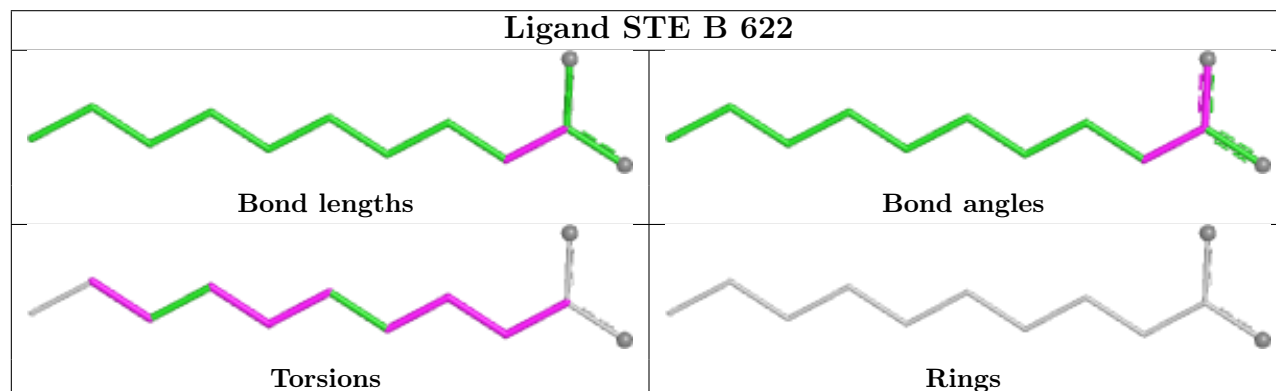
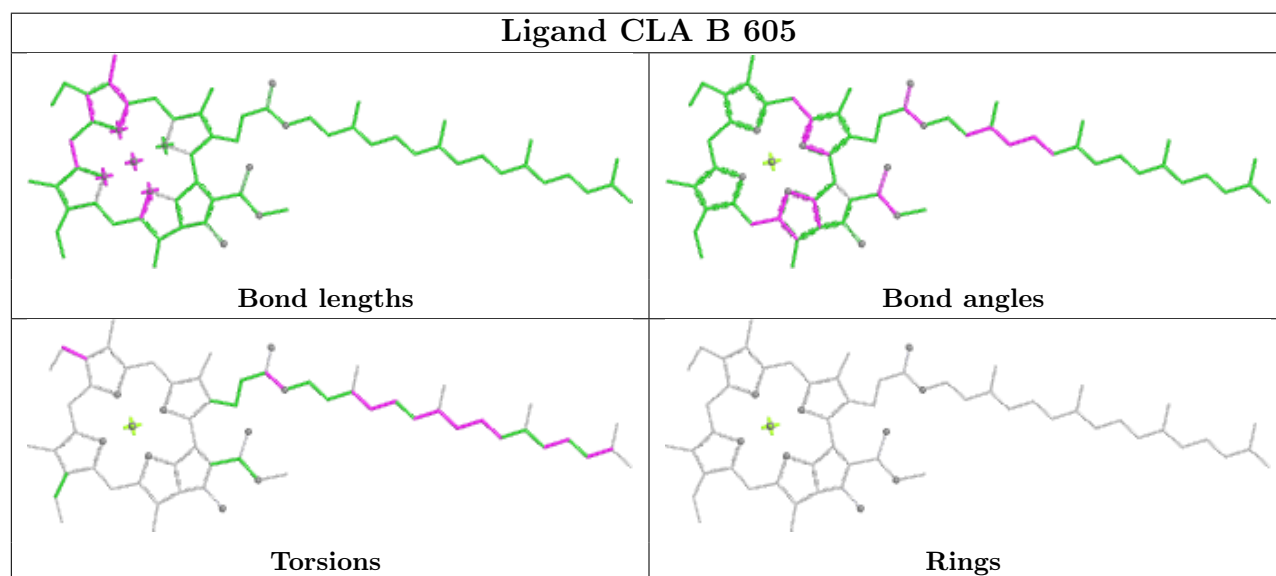
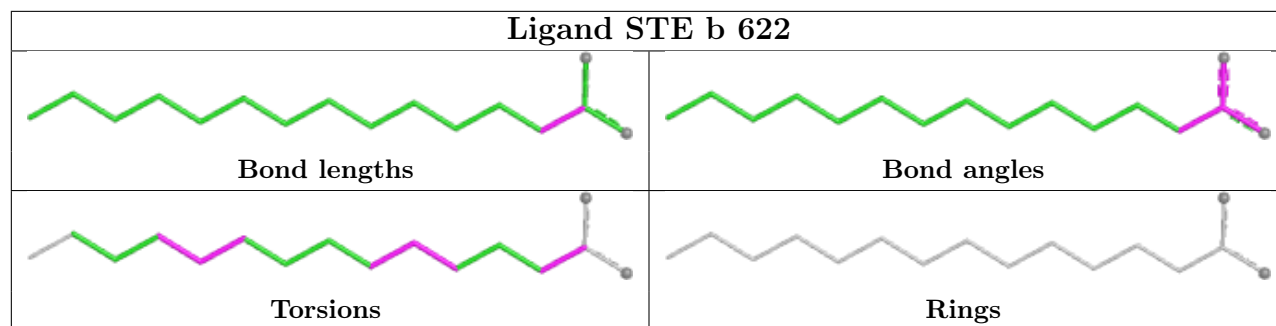
Ligand HEC V 201



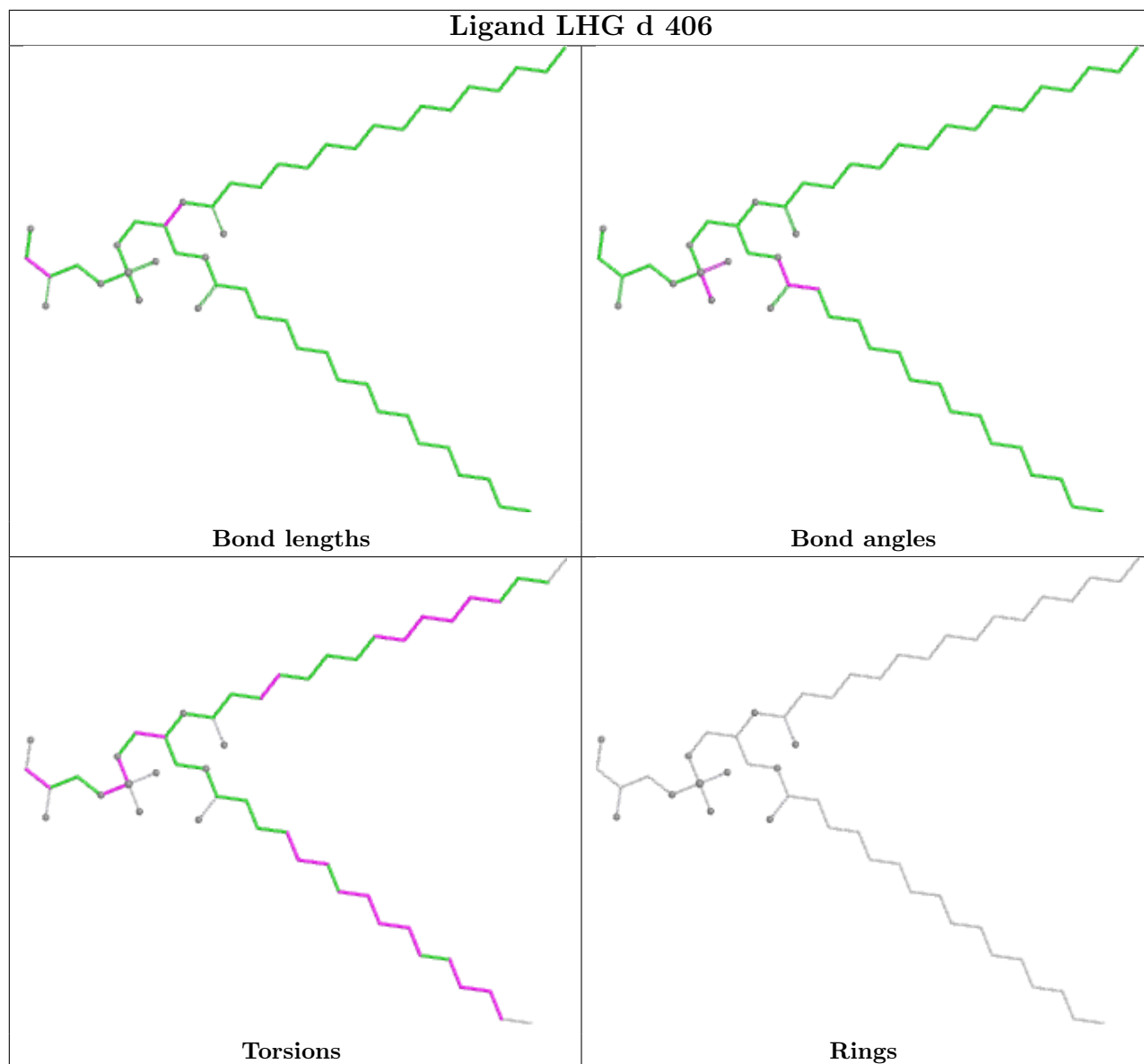




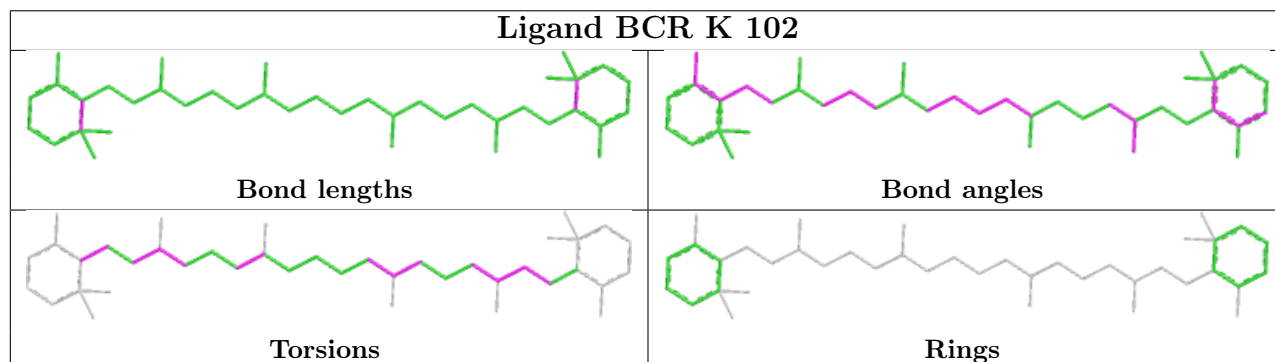
Ligand CLA b 612**Ligand CLA b 607****Ligand CLA C 512**

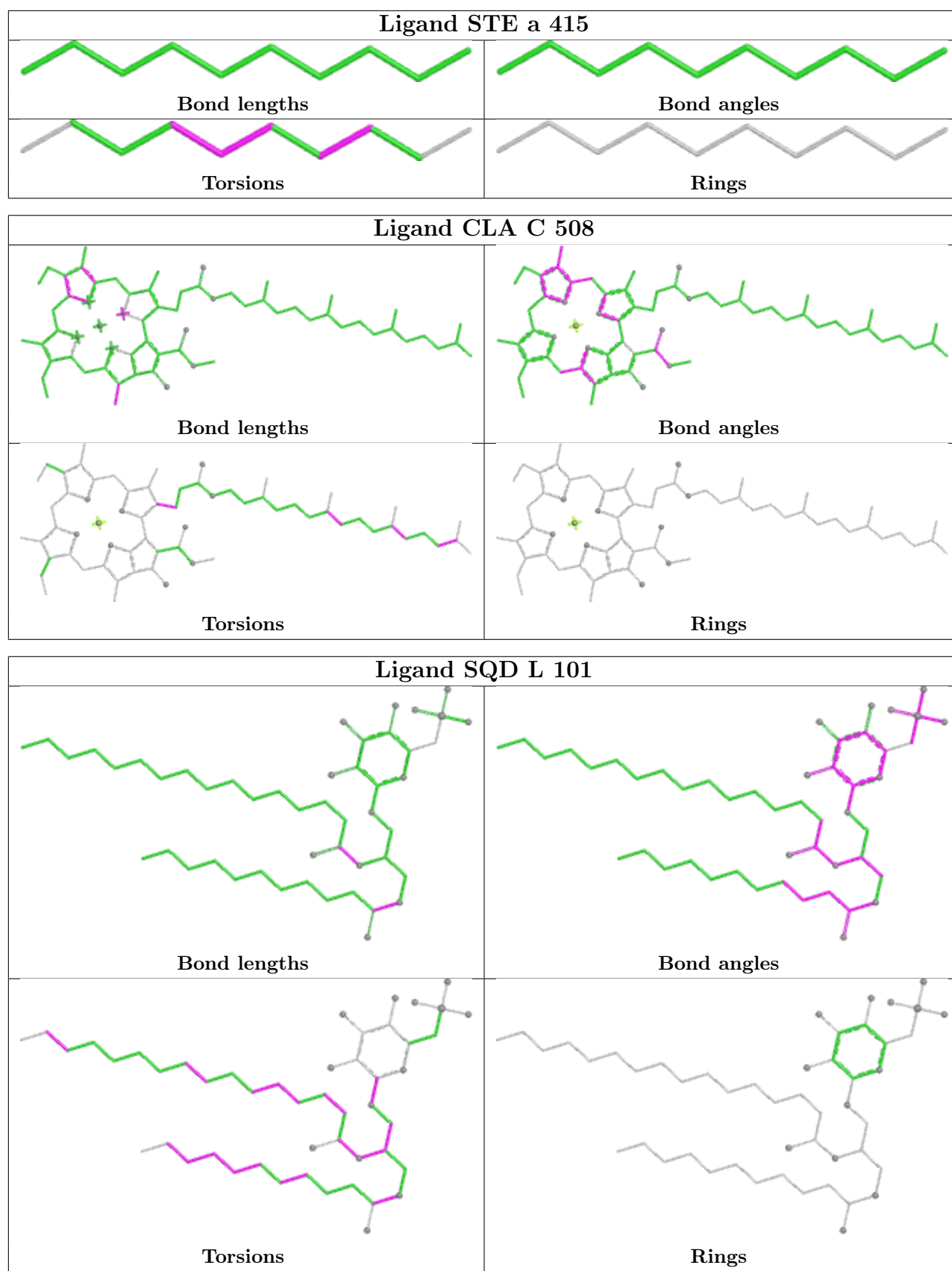


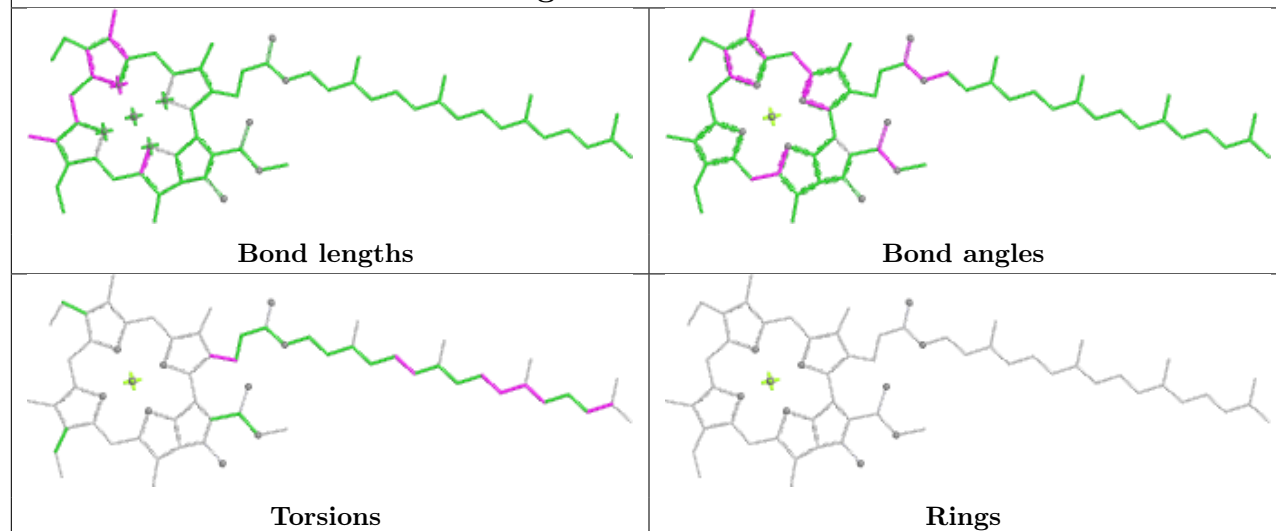
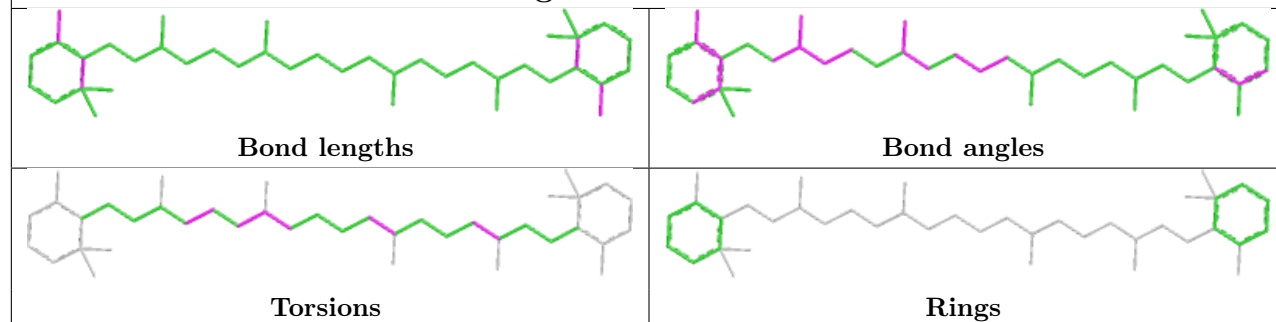
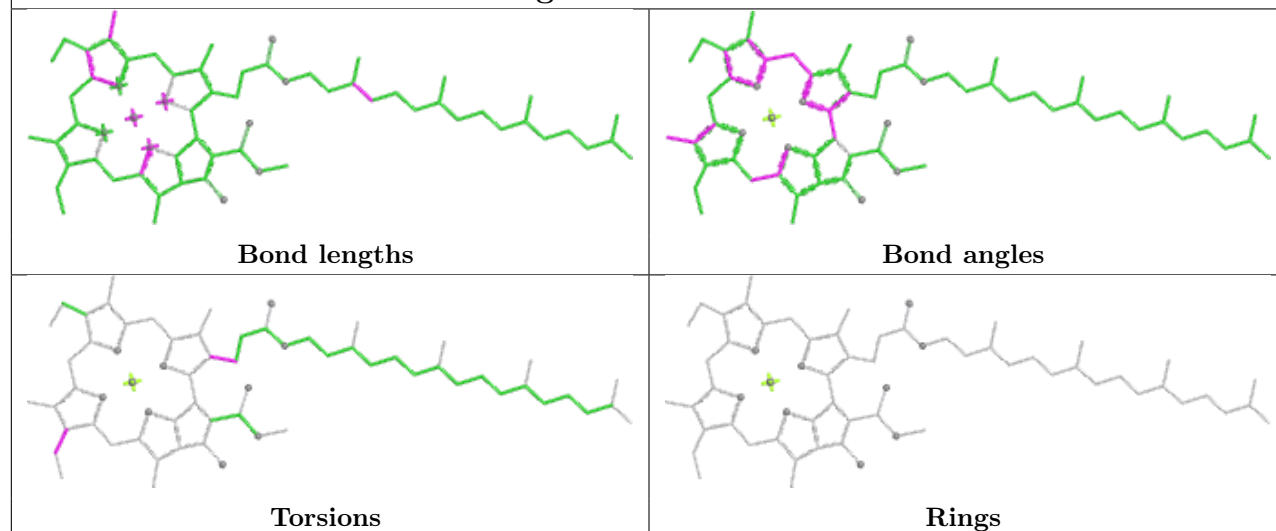
Ligand LHG d 406

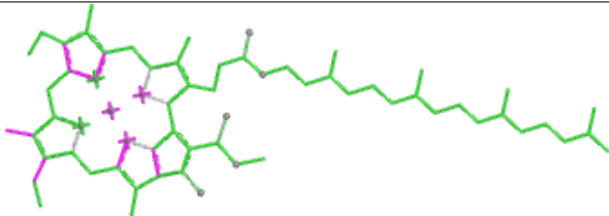
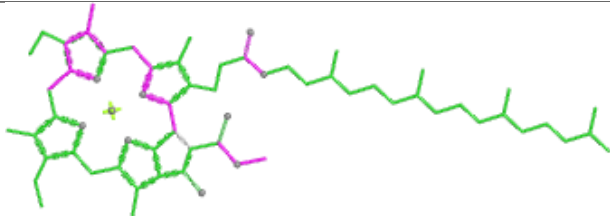
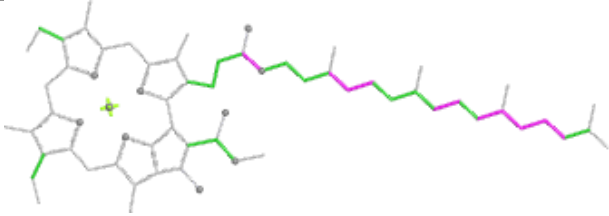
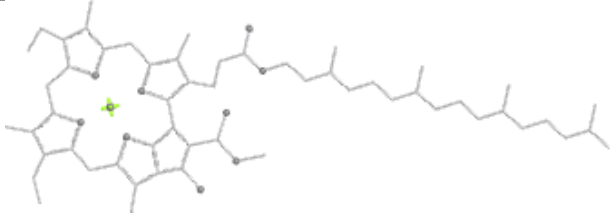
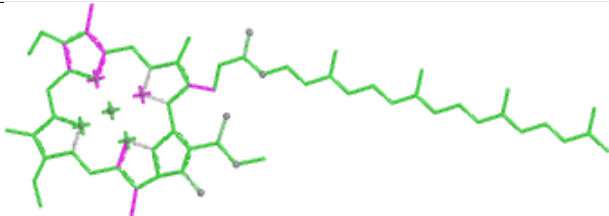
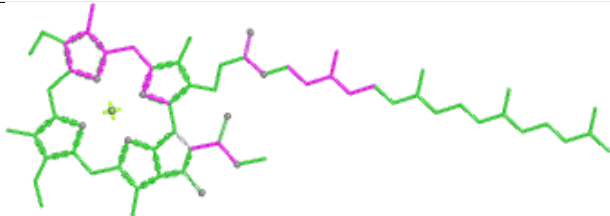
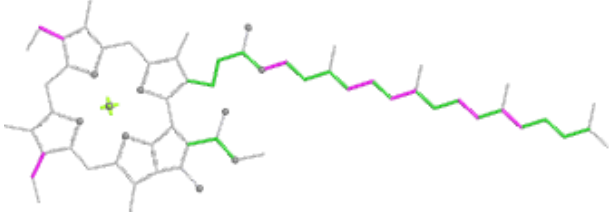
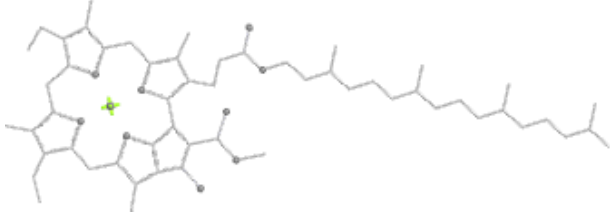
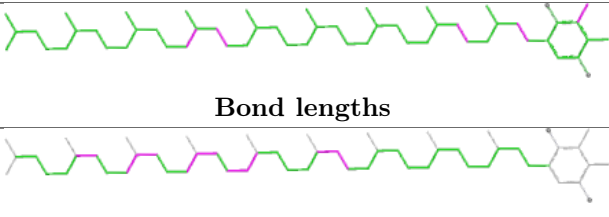
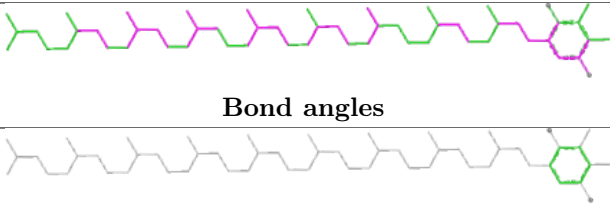


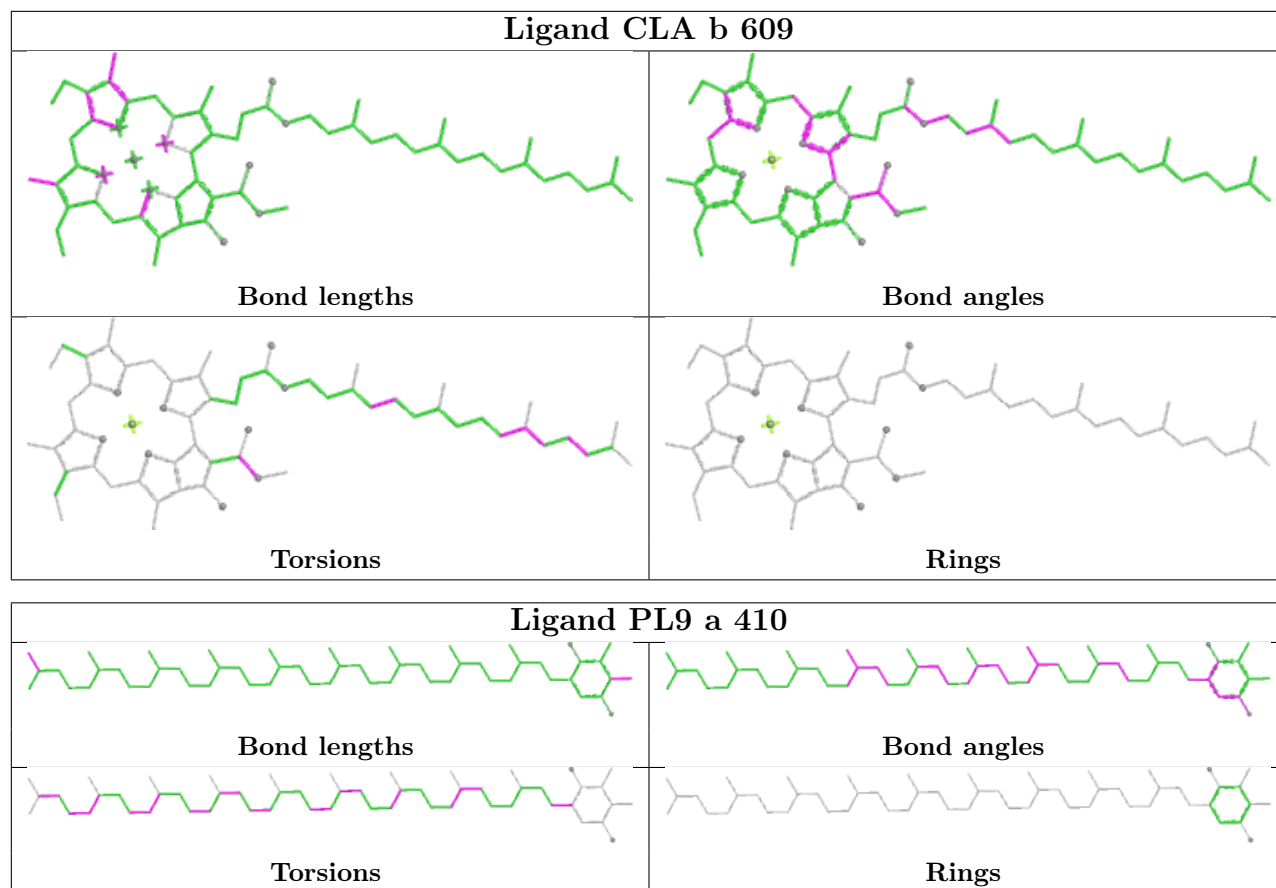
Ligand BCR K 102

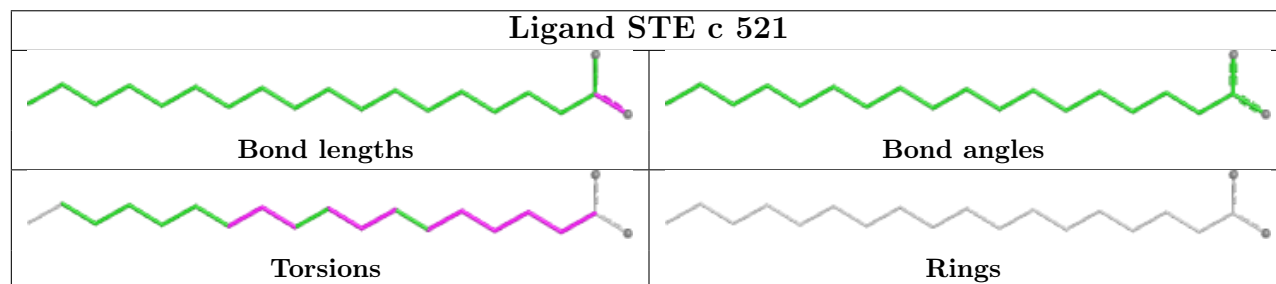
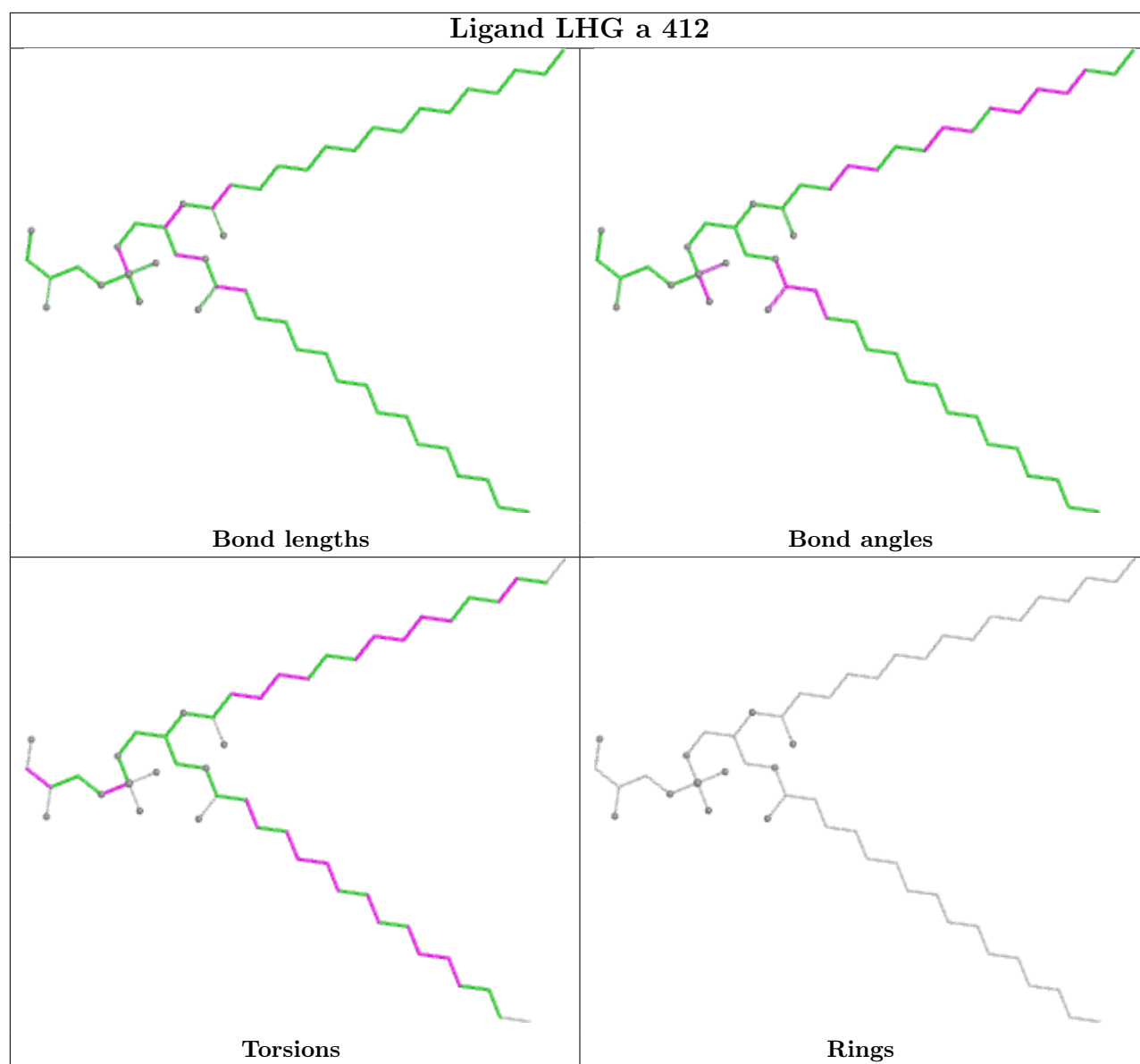


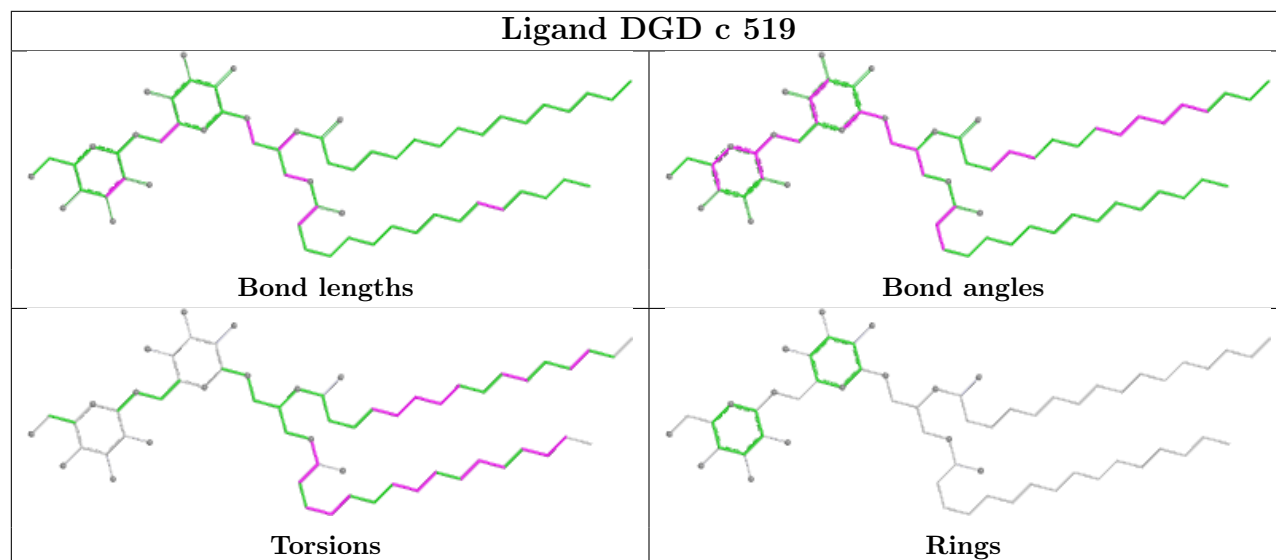
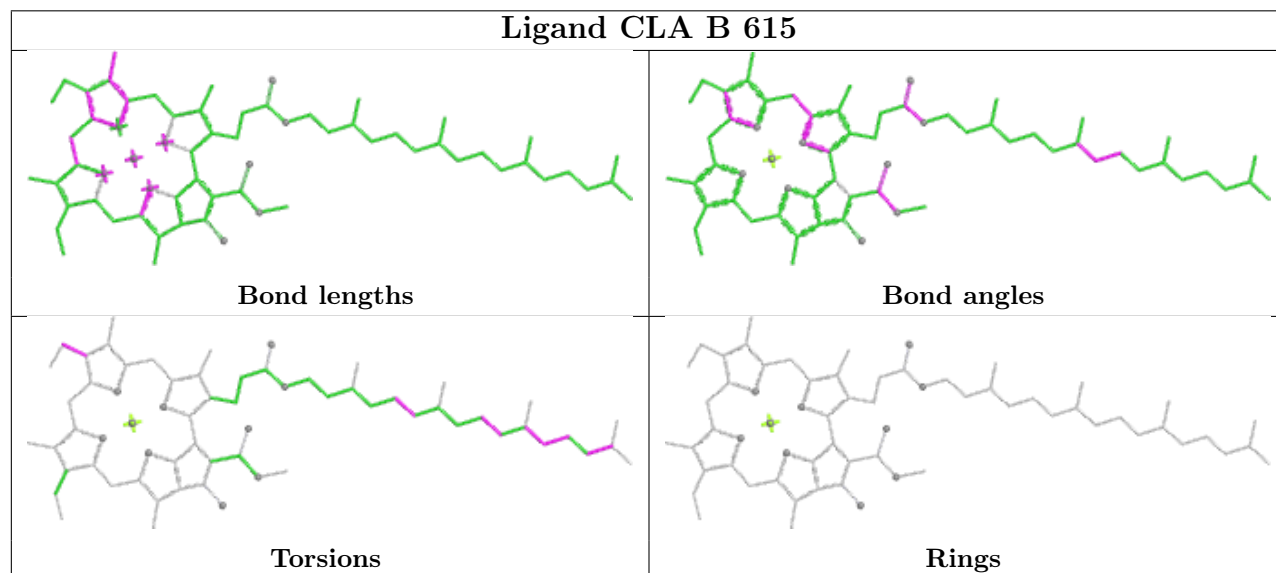
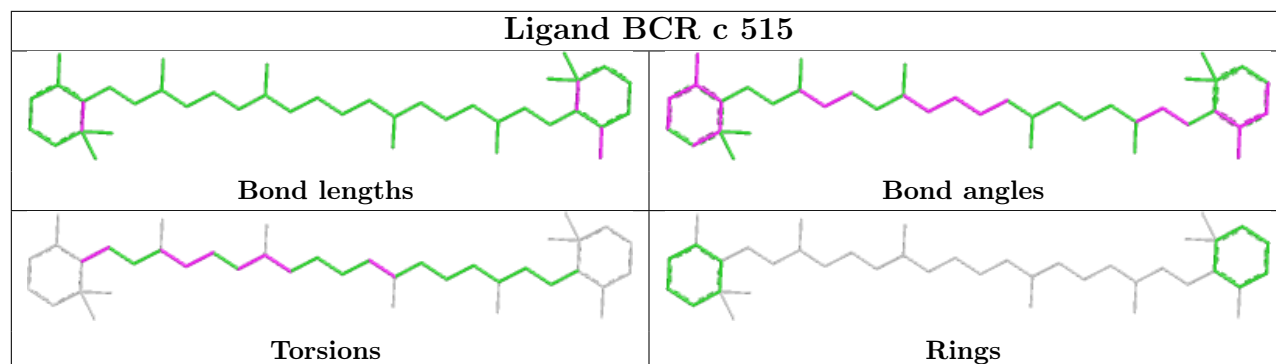


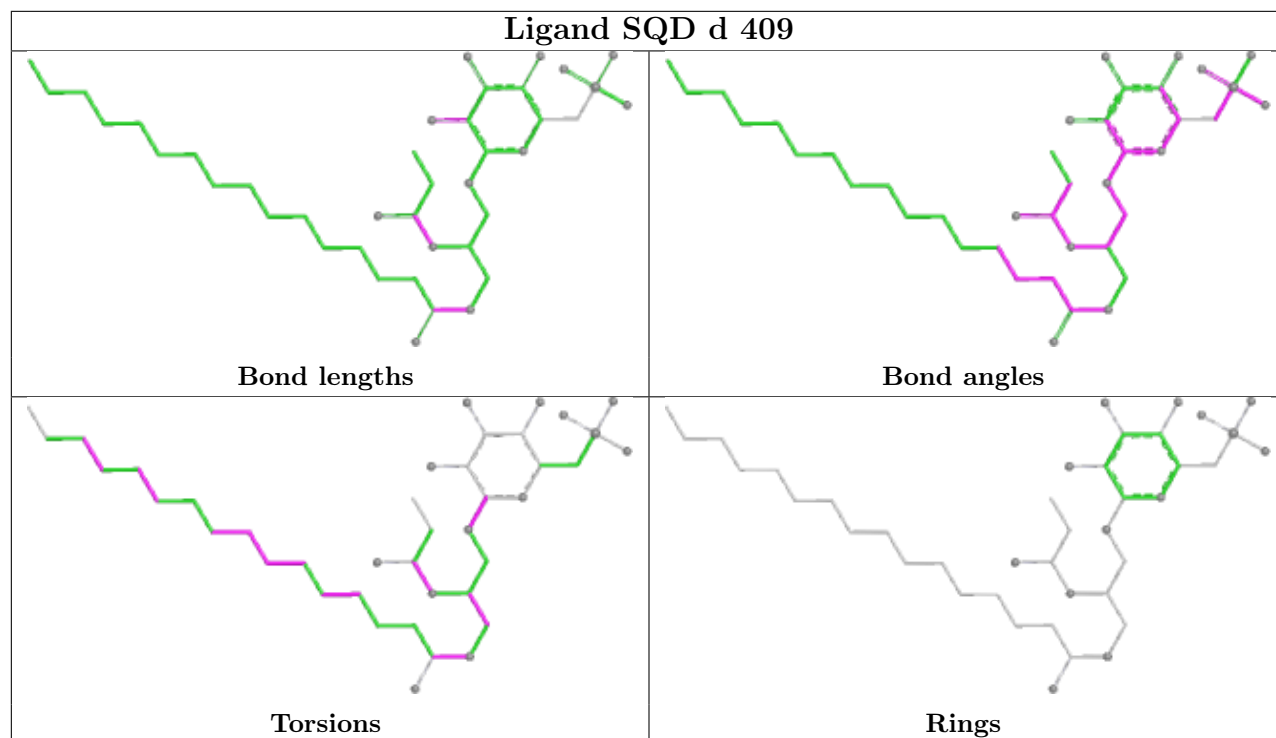
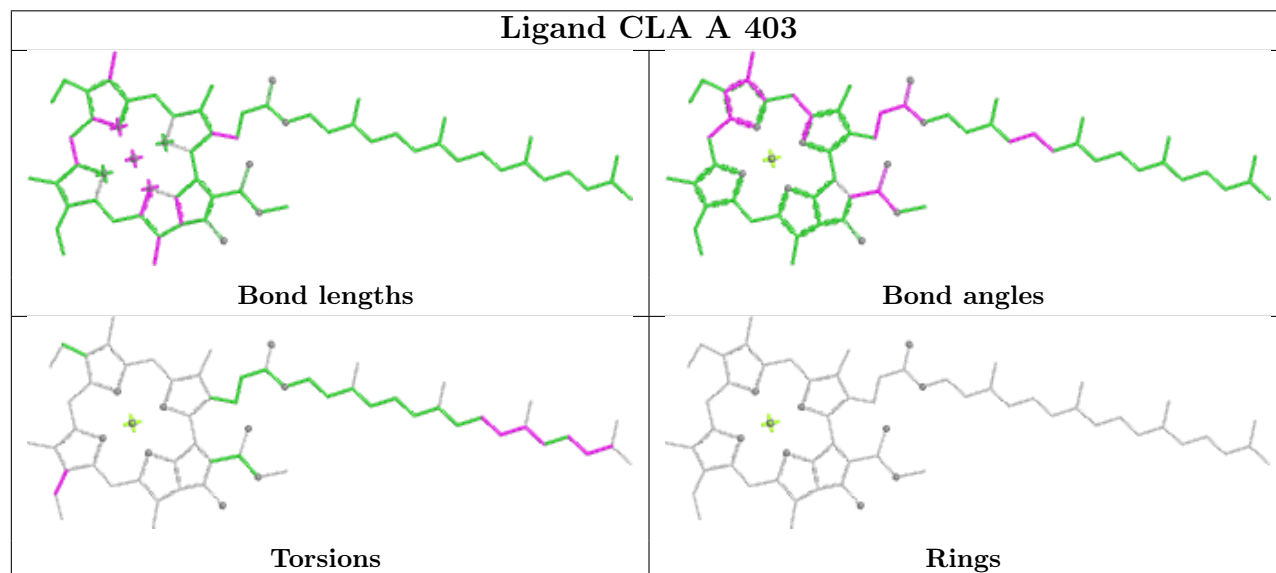
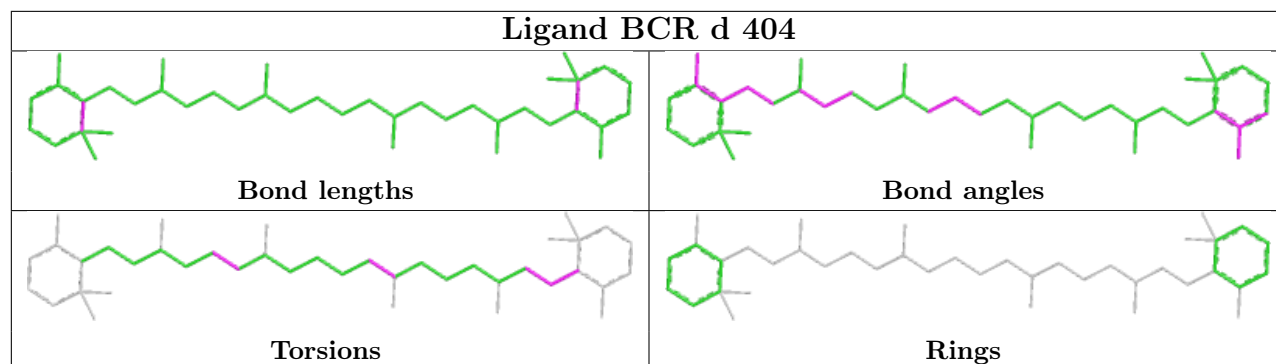
Ligand CLA c 514**Ligand BCR c 516****Ligand CLA a 411**

Ligand CLA C 506	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand CLA D 404	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand PL9 D 407	
	
Bond lengths	
	Bond angles
Torsions	
	Rings

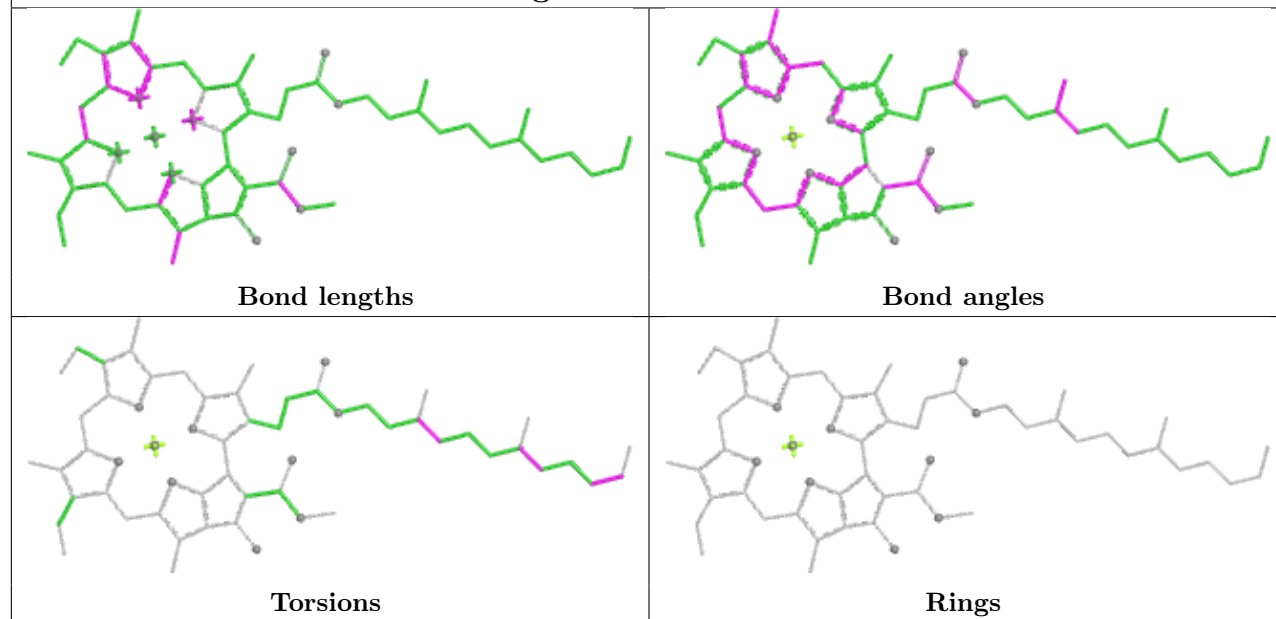




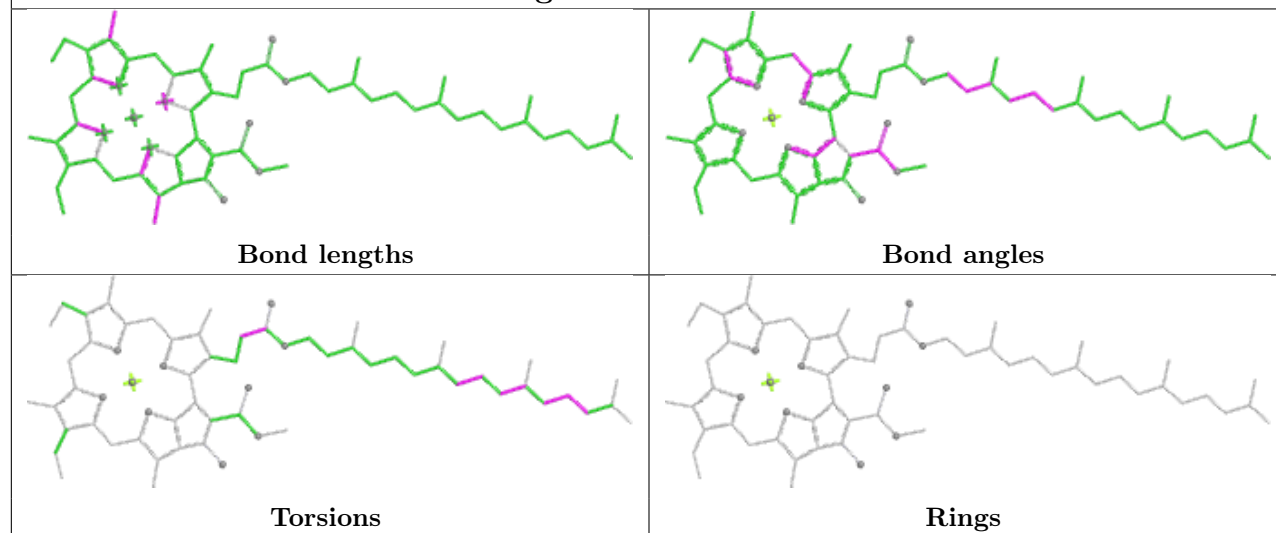


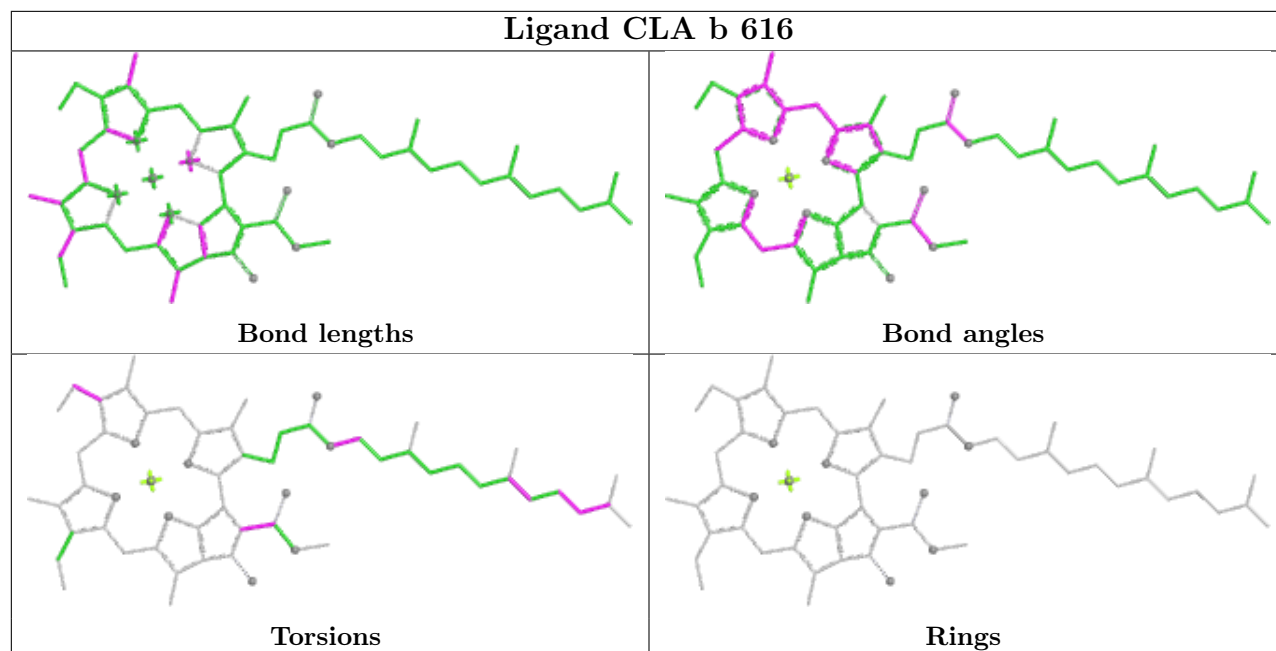


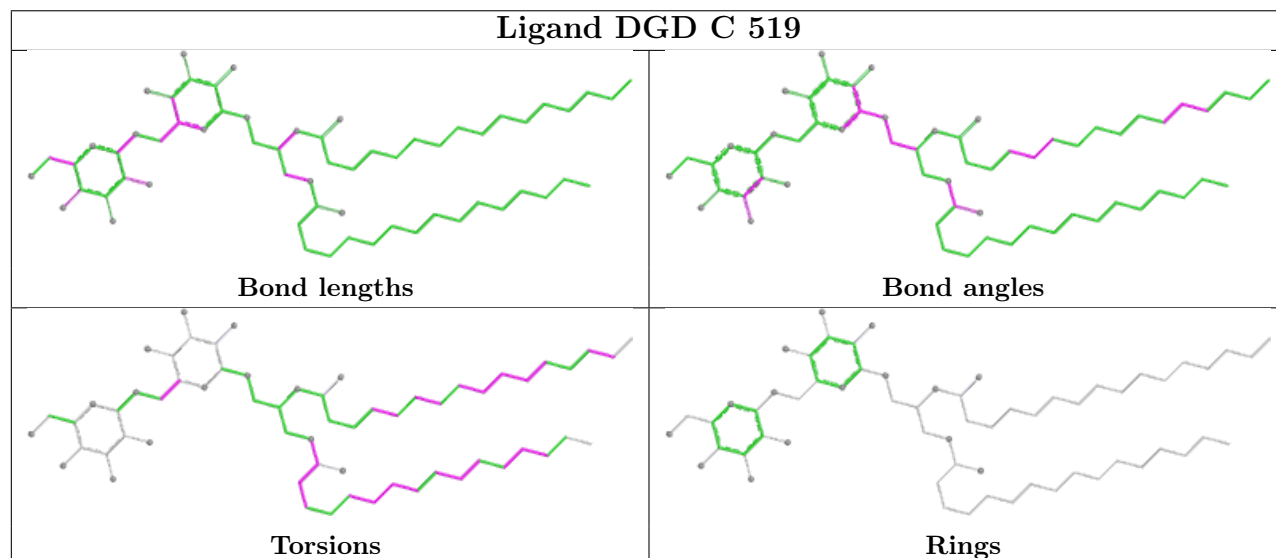
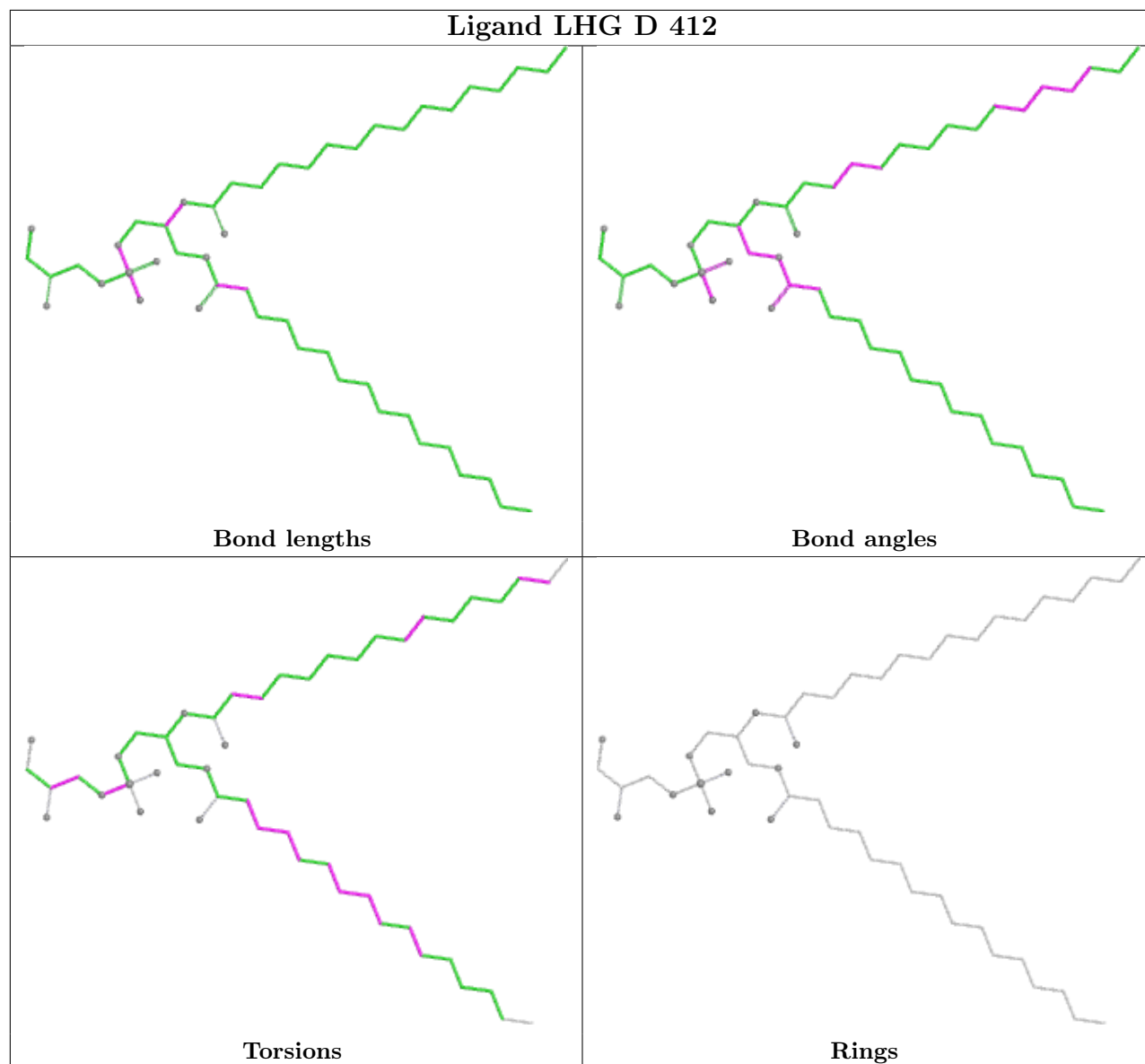
Ligand CLA C 504

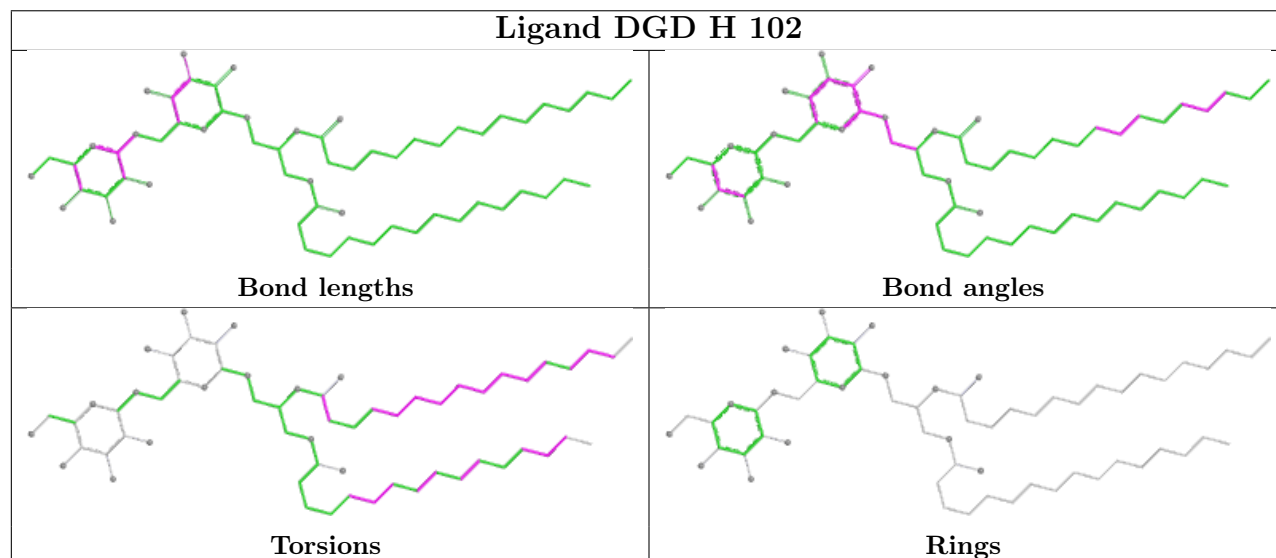
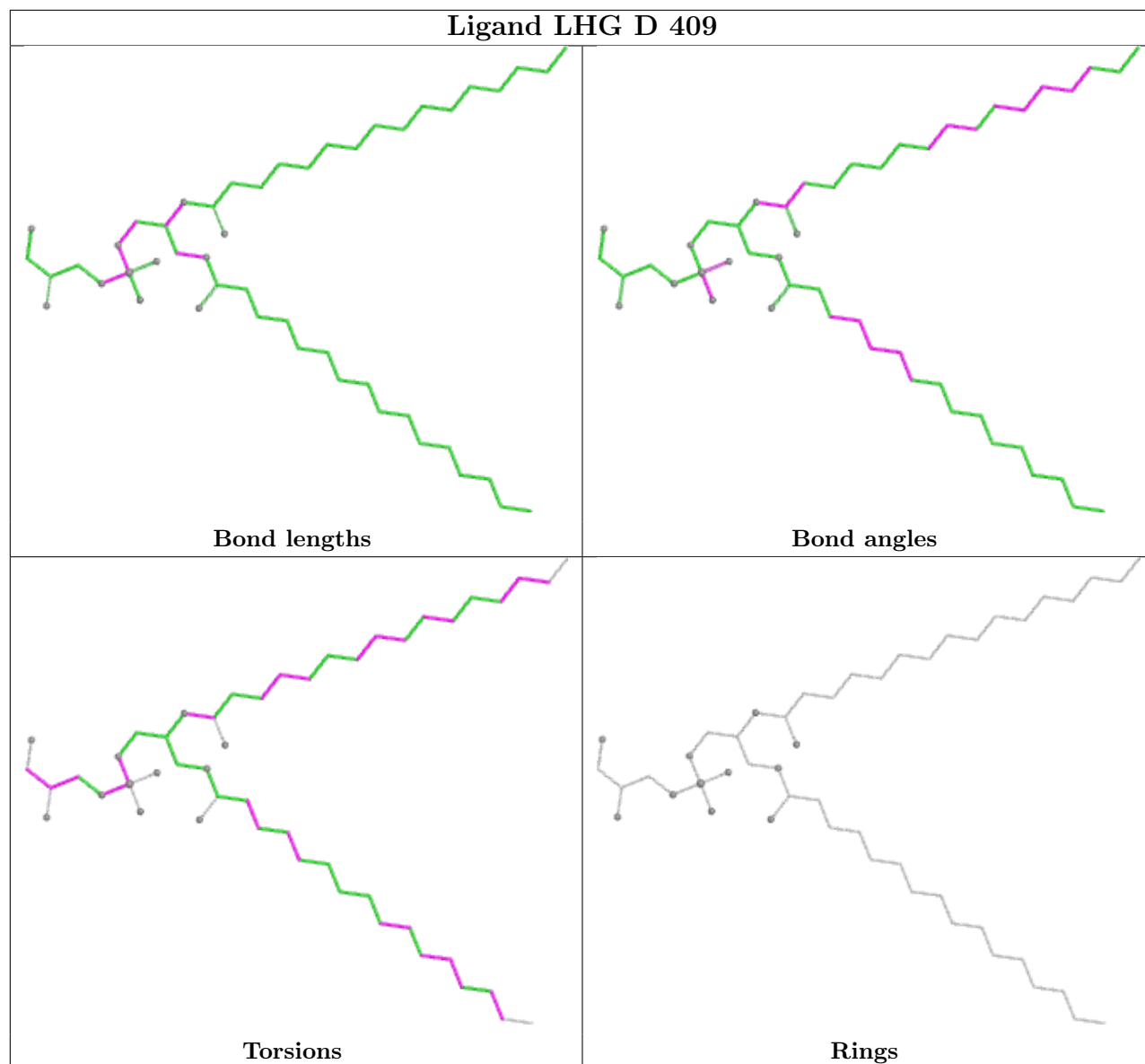


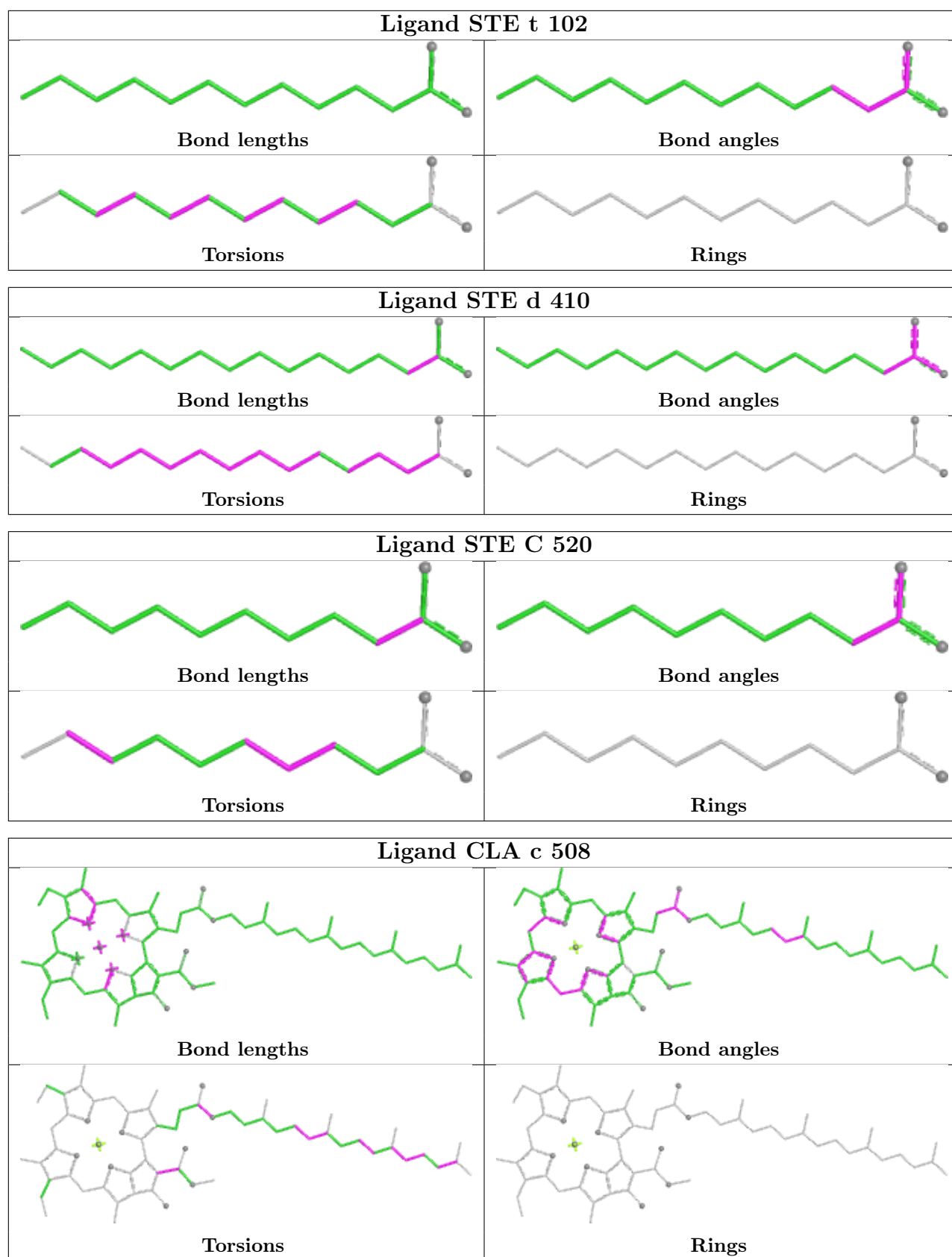
Ligand CLA b 613



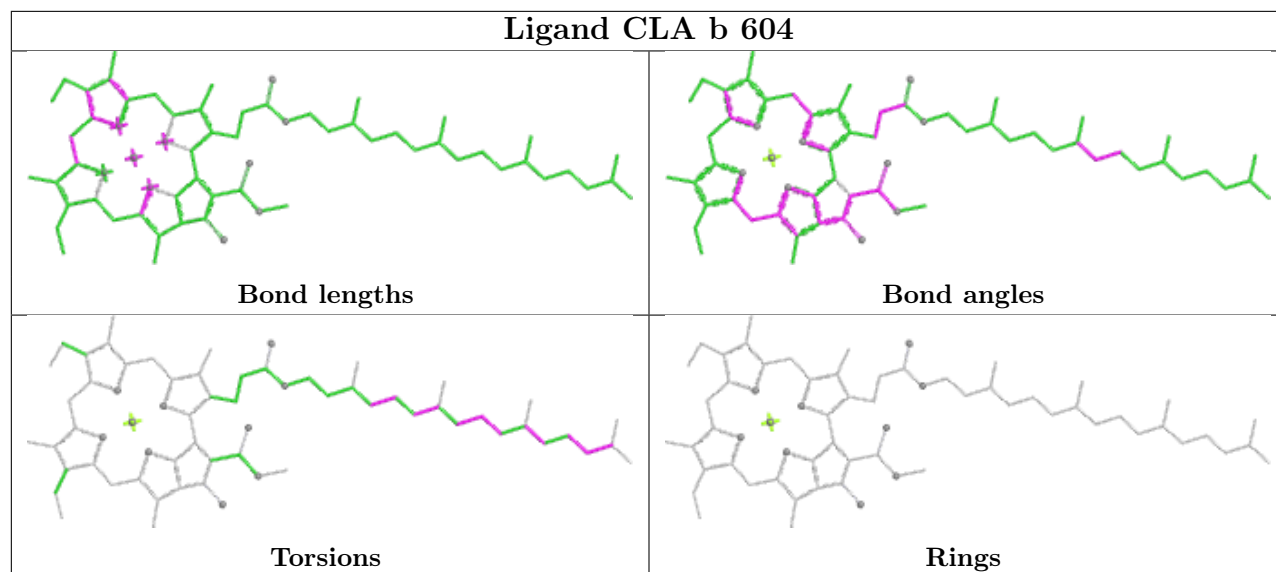




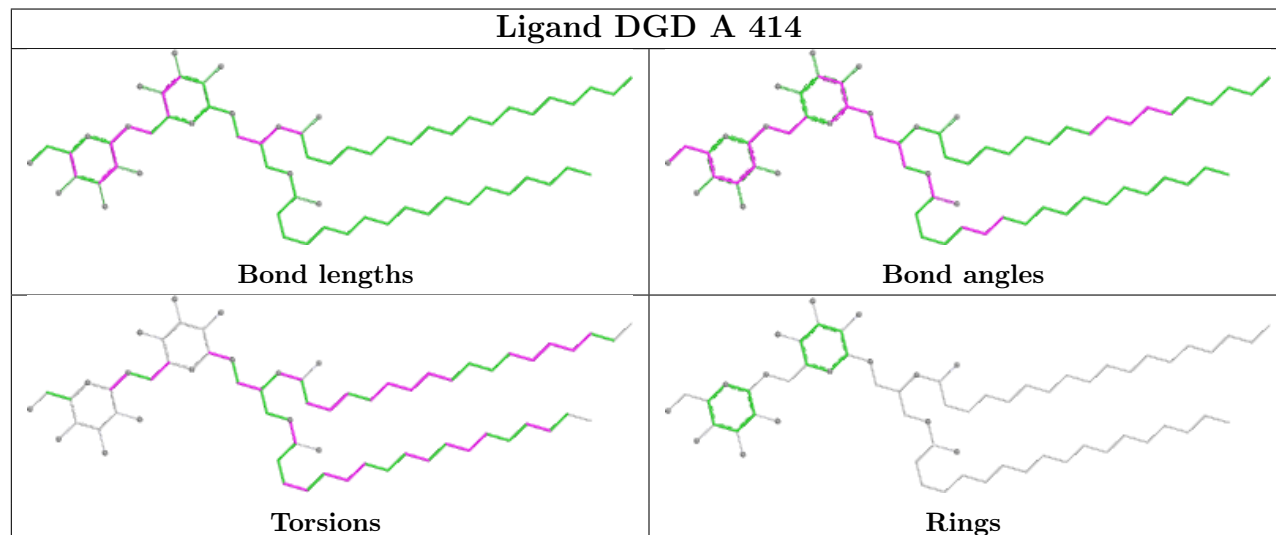




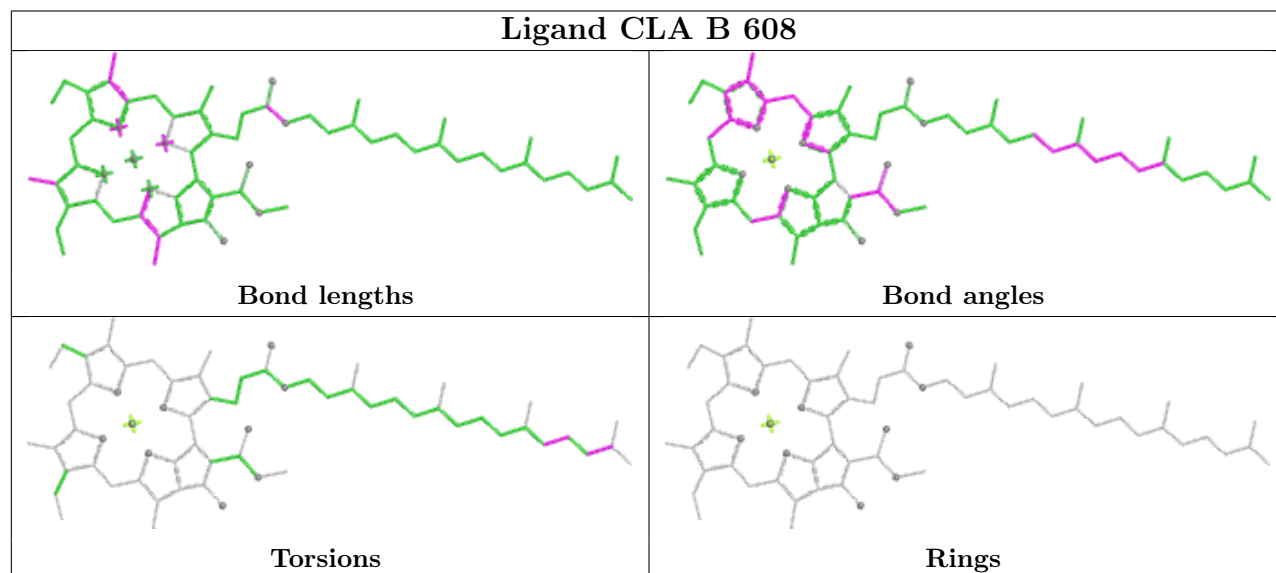
Ligand CLA b 604

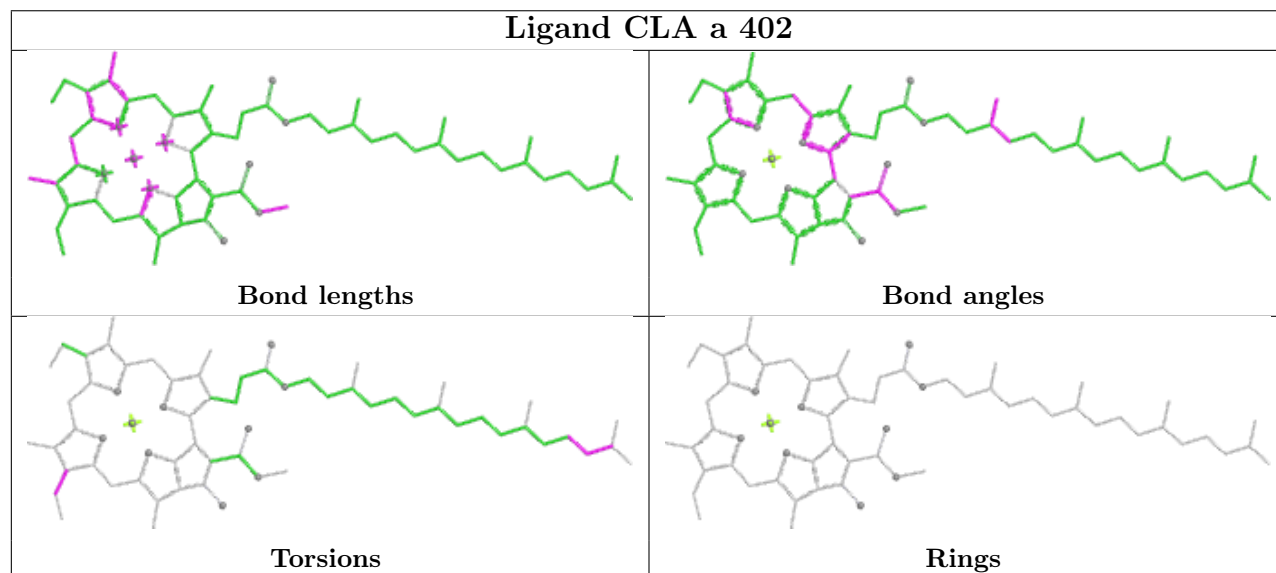
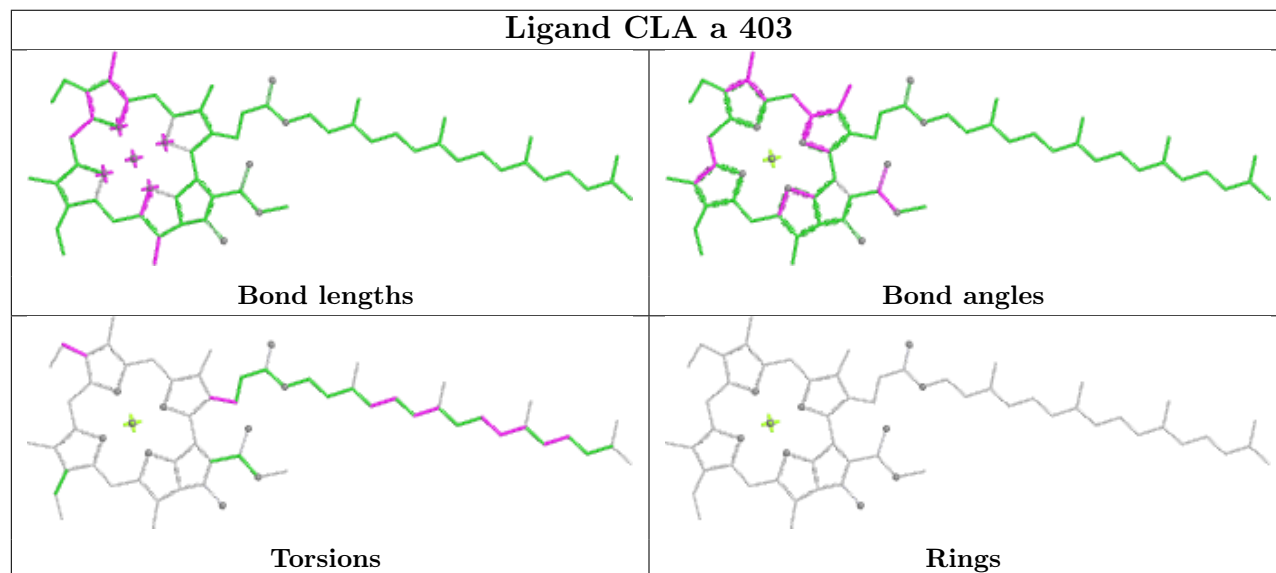
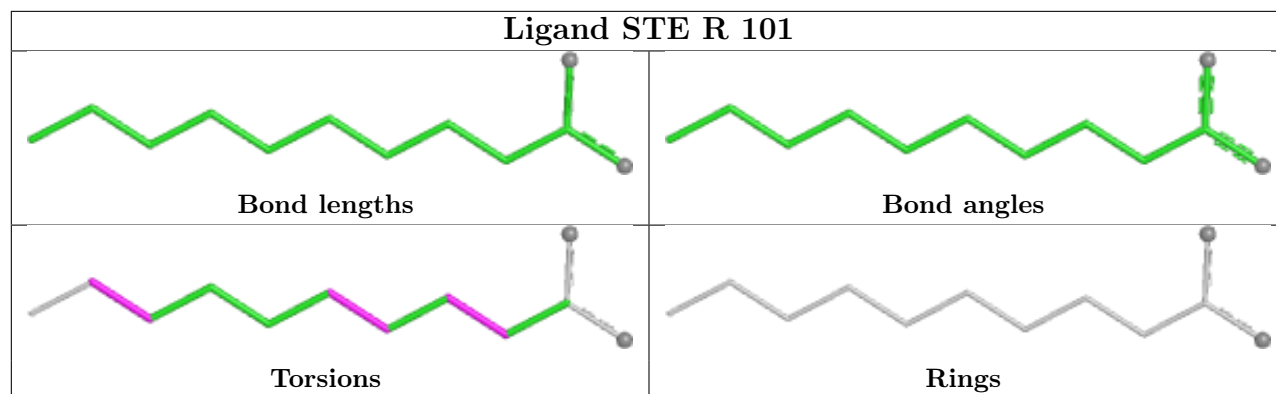


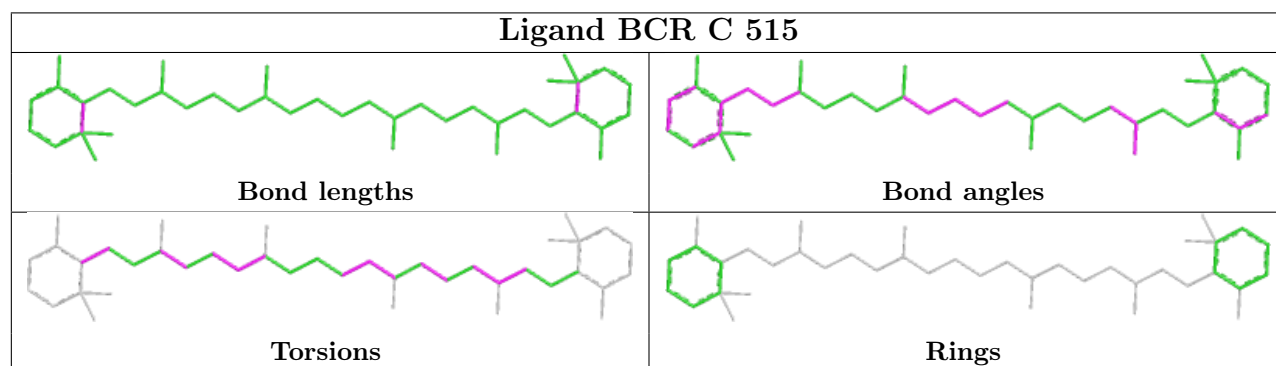
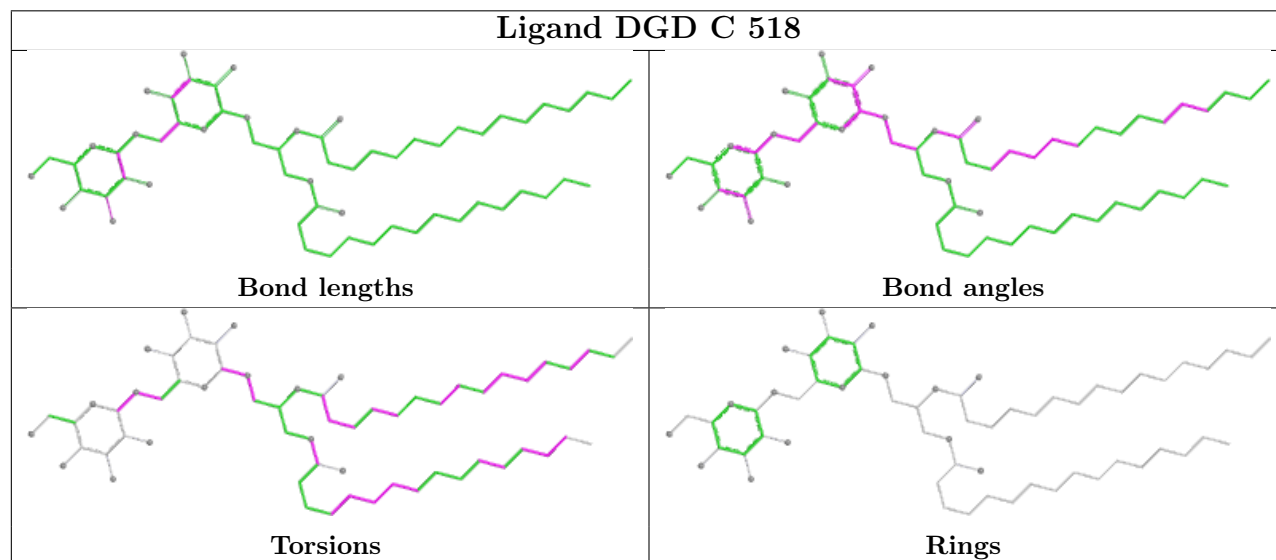
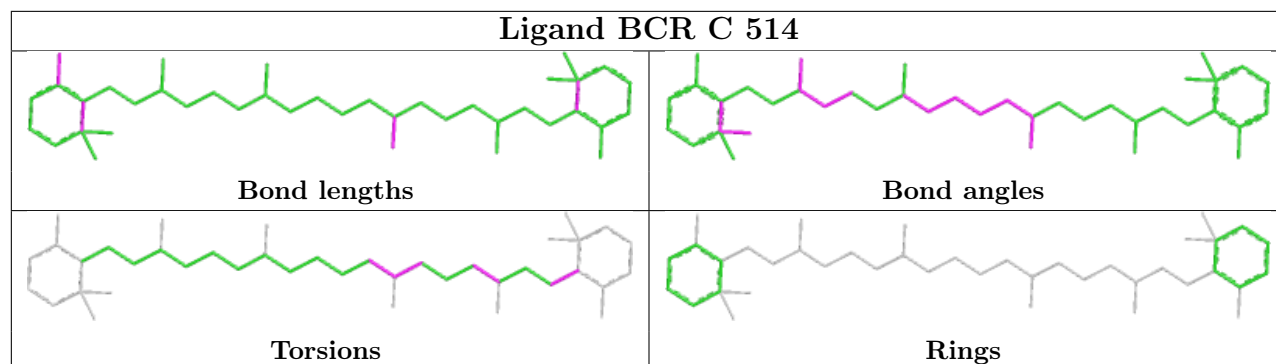
Ligand DGD A 414

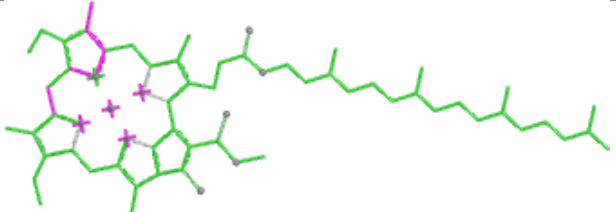
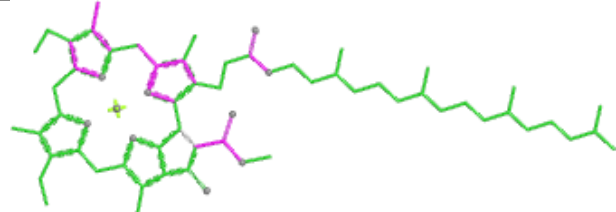
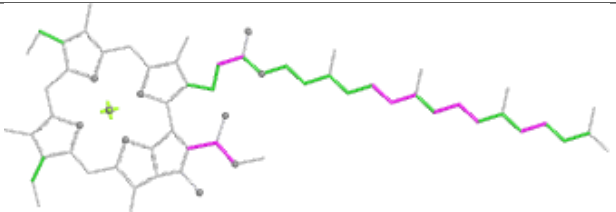
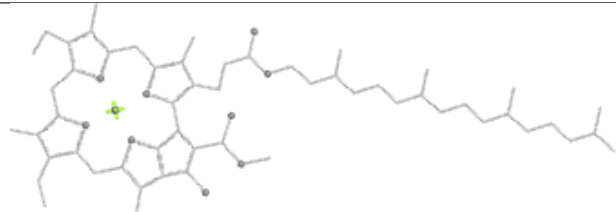


Ligand CLA B 608



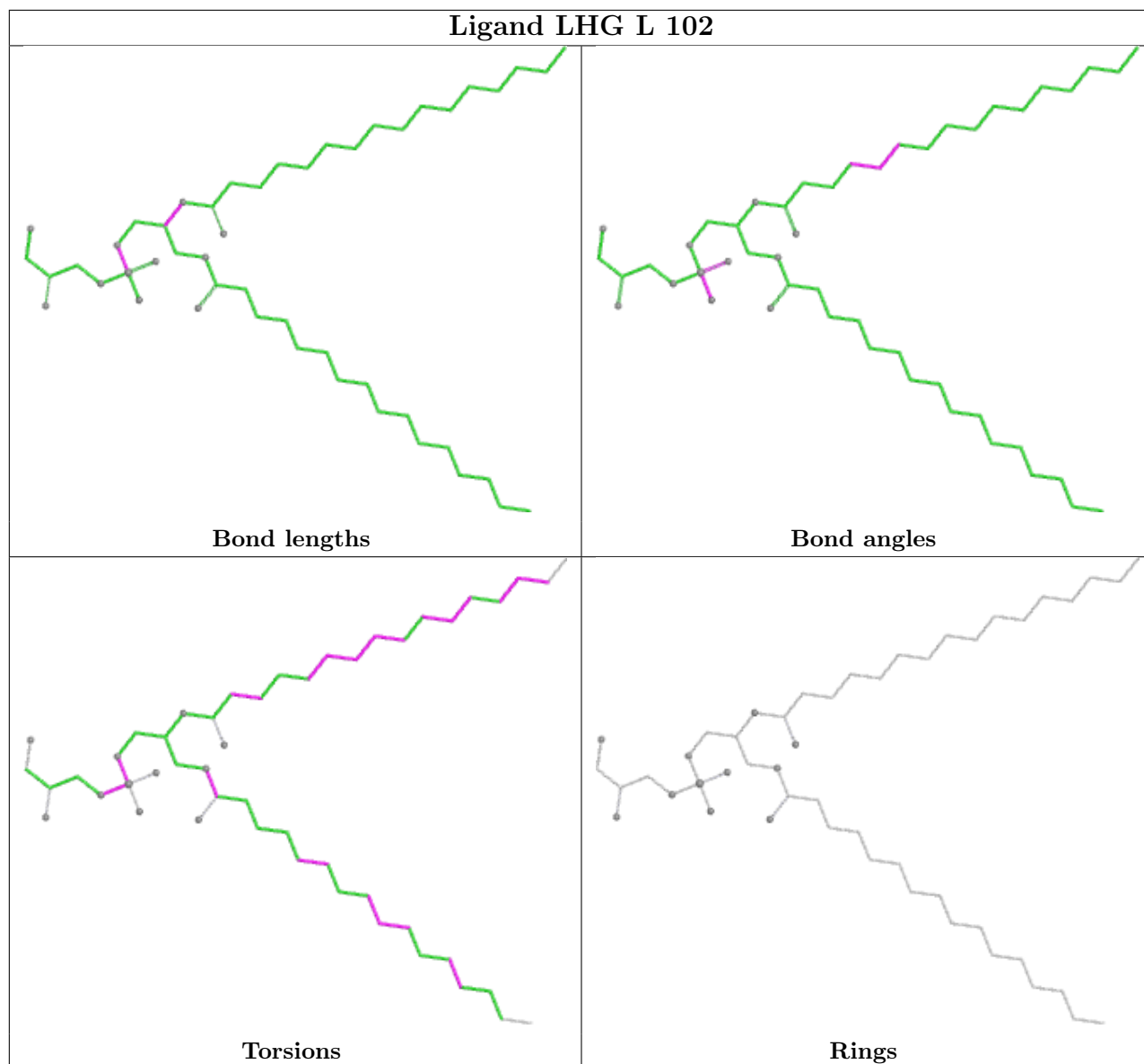




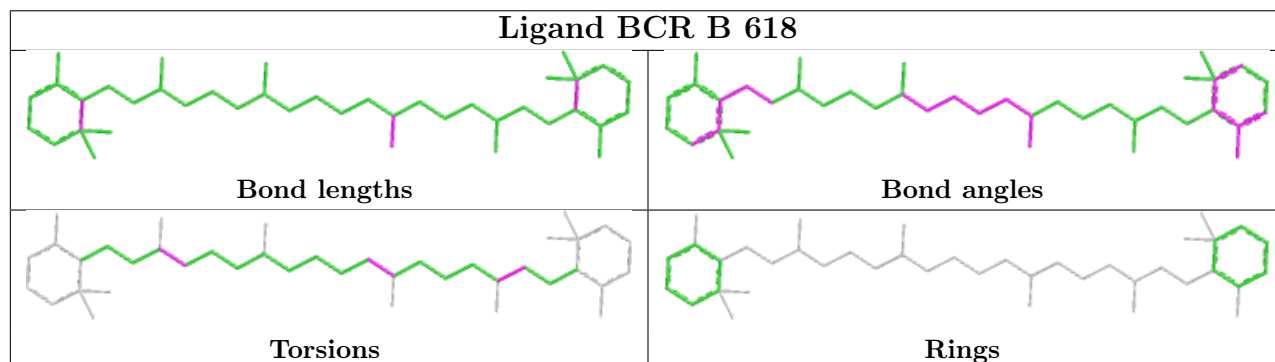
Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

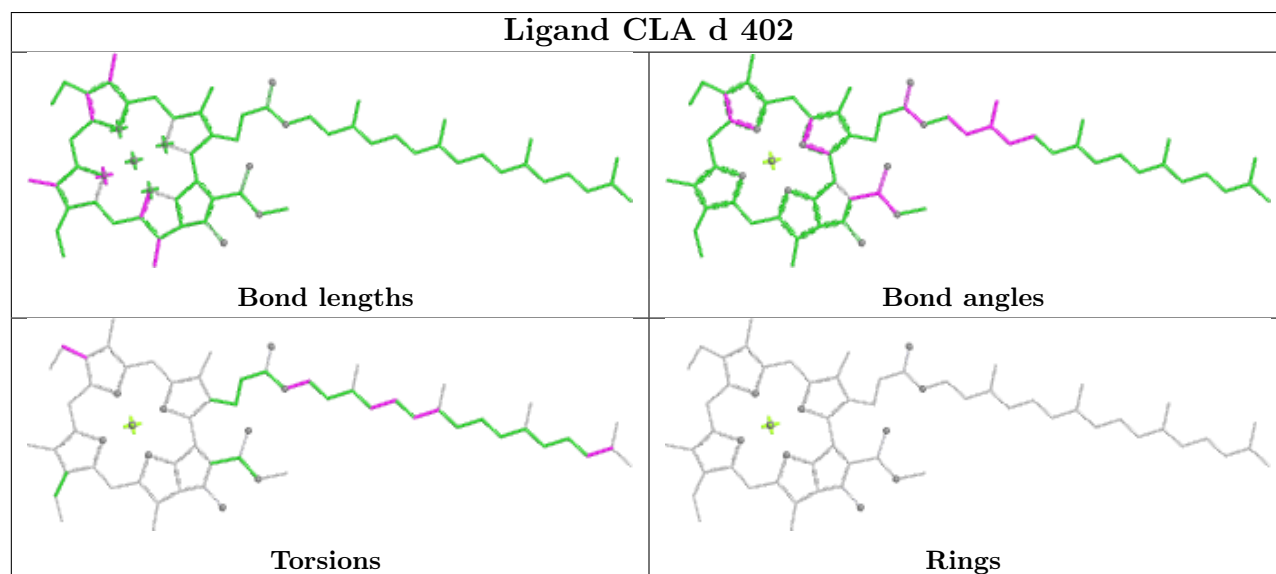
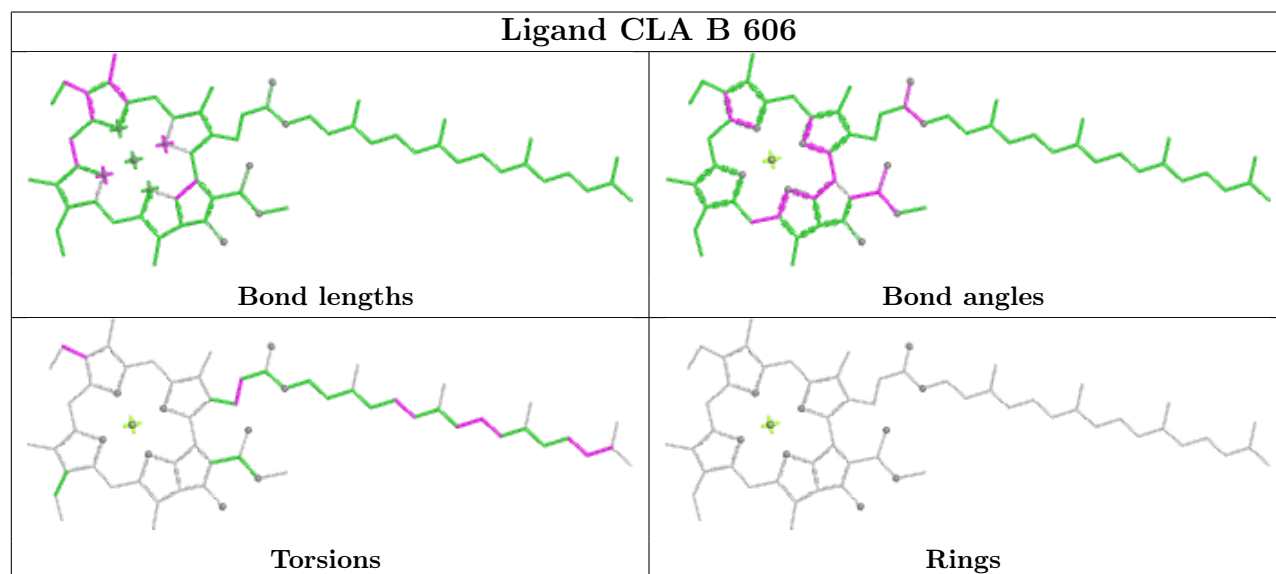
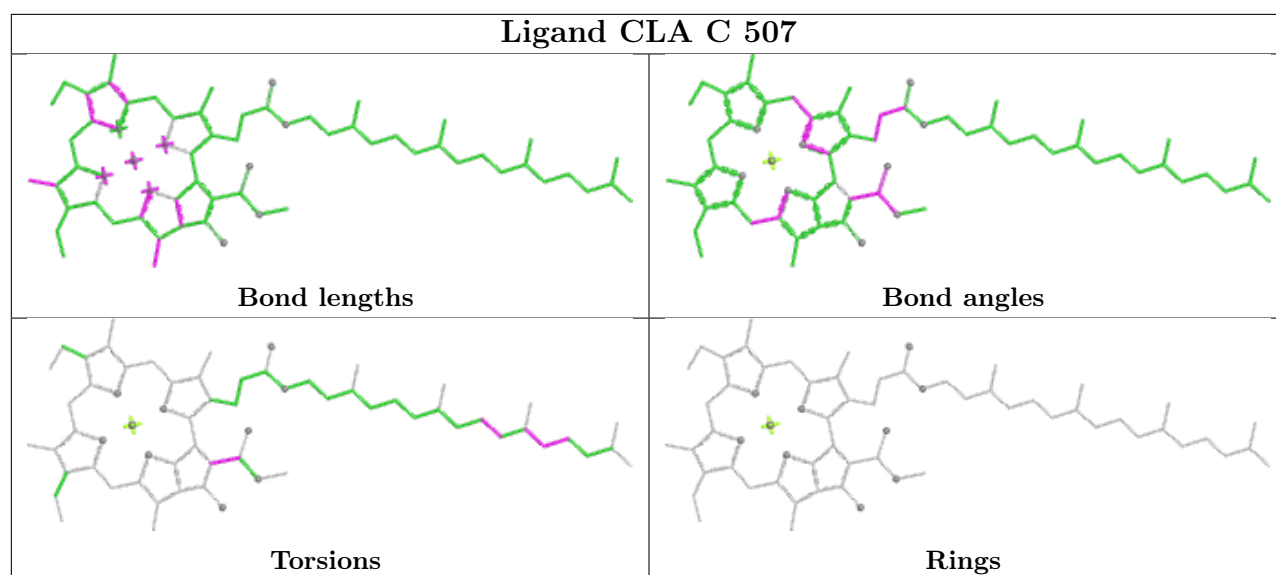
Ligand STE M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

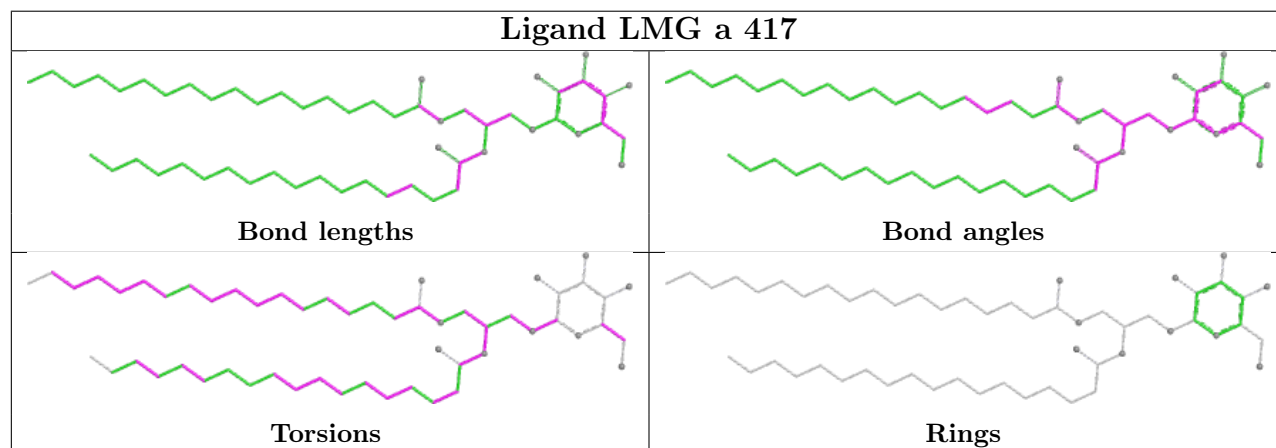
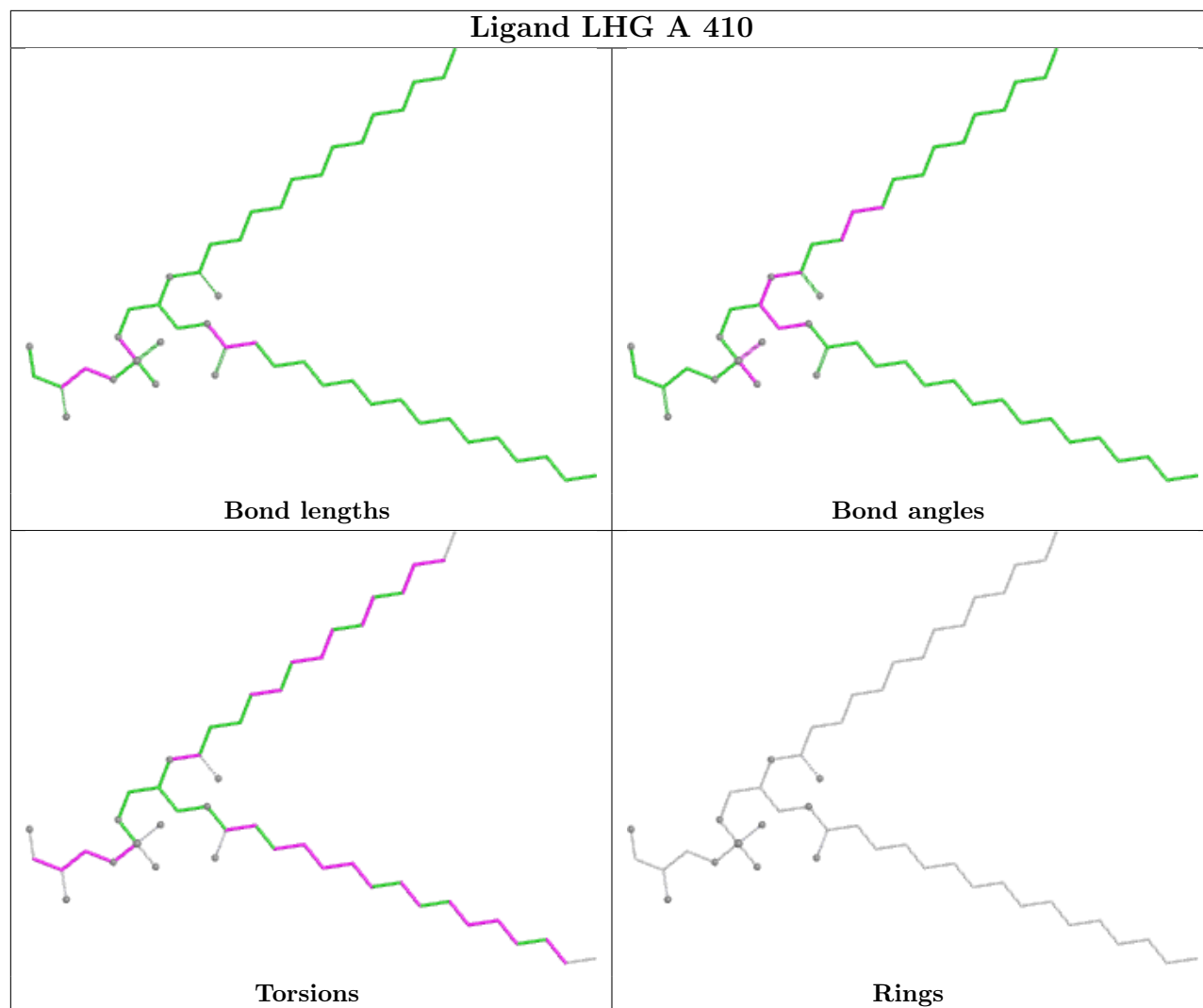
Ligand LHG L 102

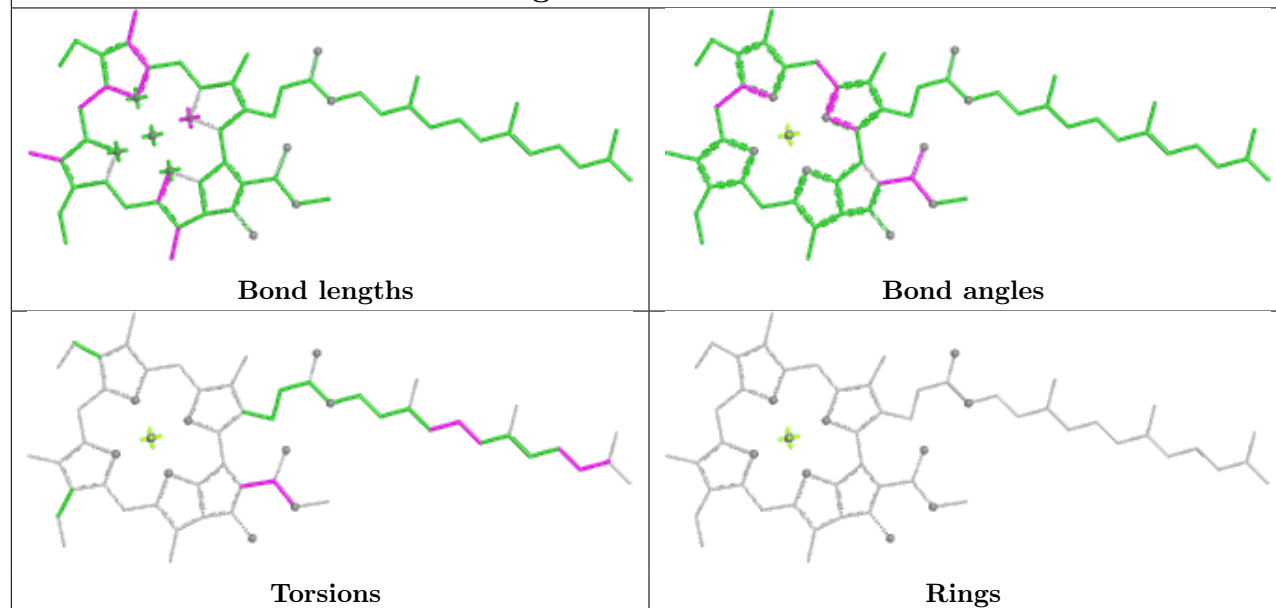
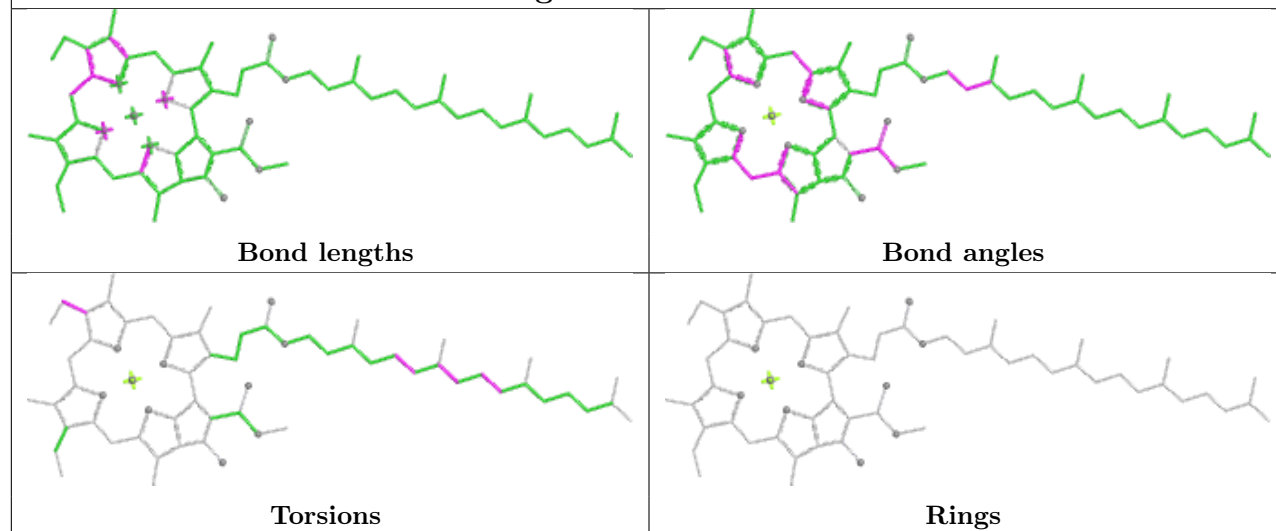


Ligand BCR B 618

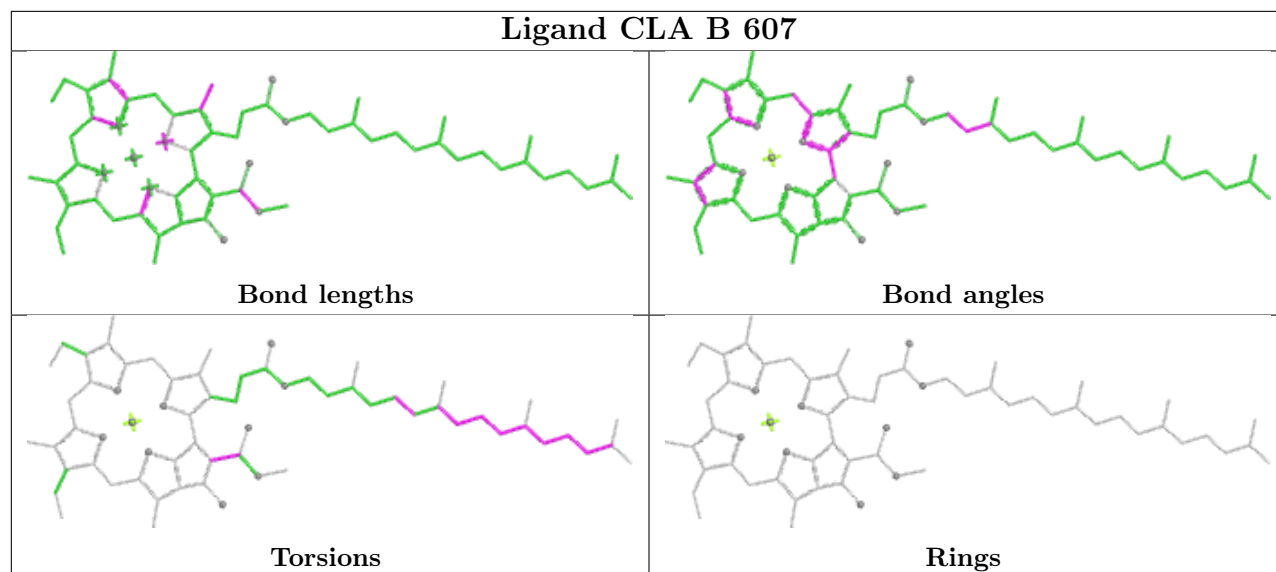




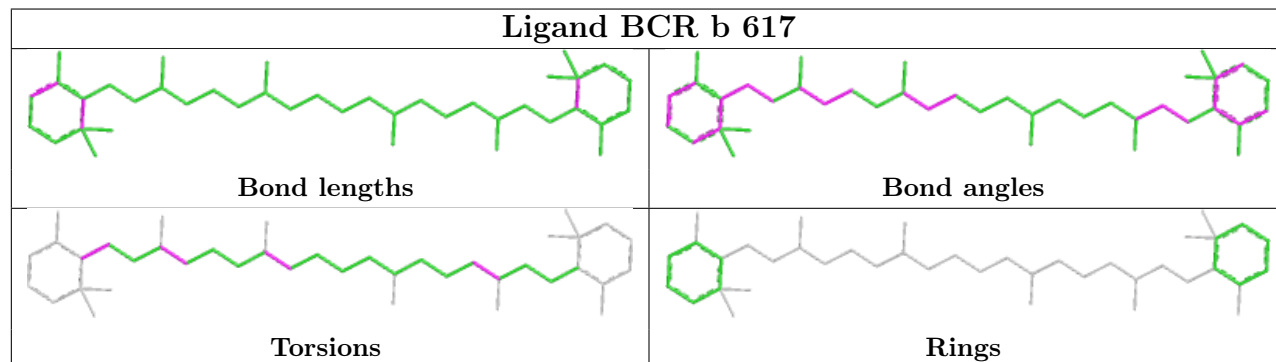


Ligand CLA B 616**Ligand CLA b 605**

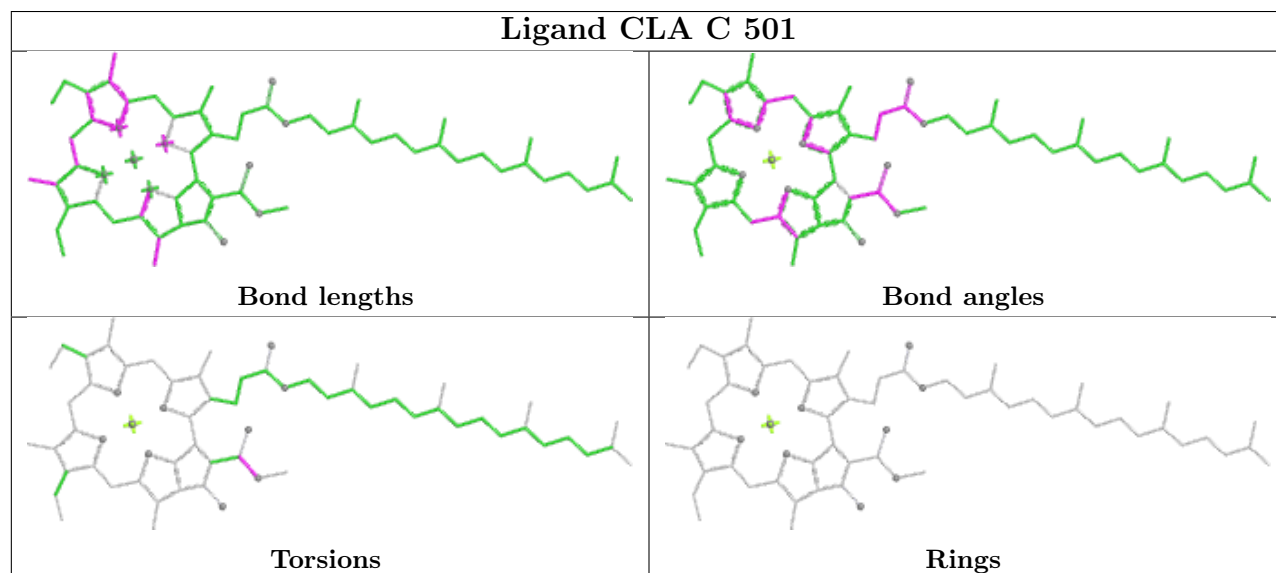
Ligand CLA B 607

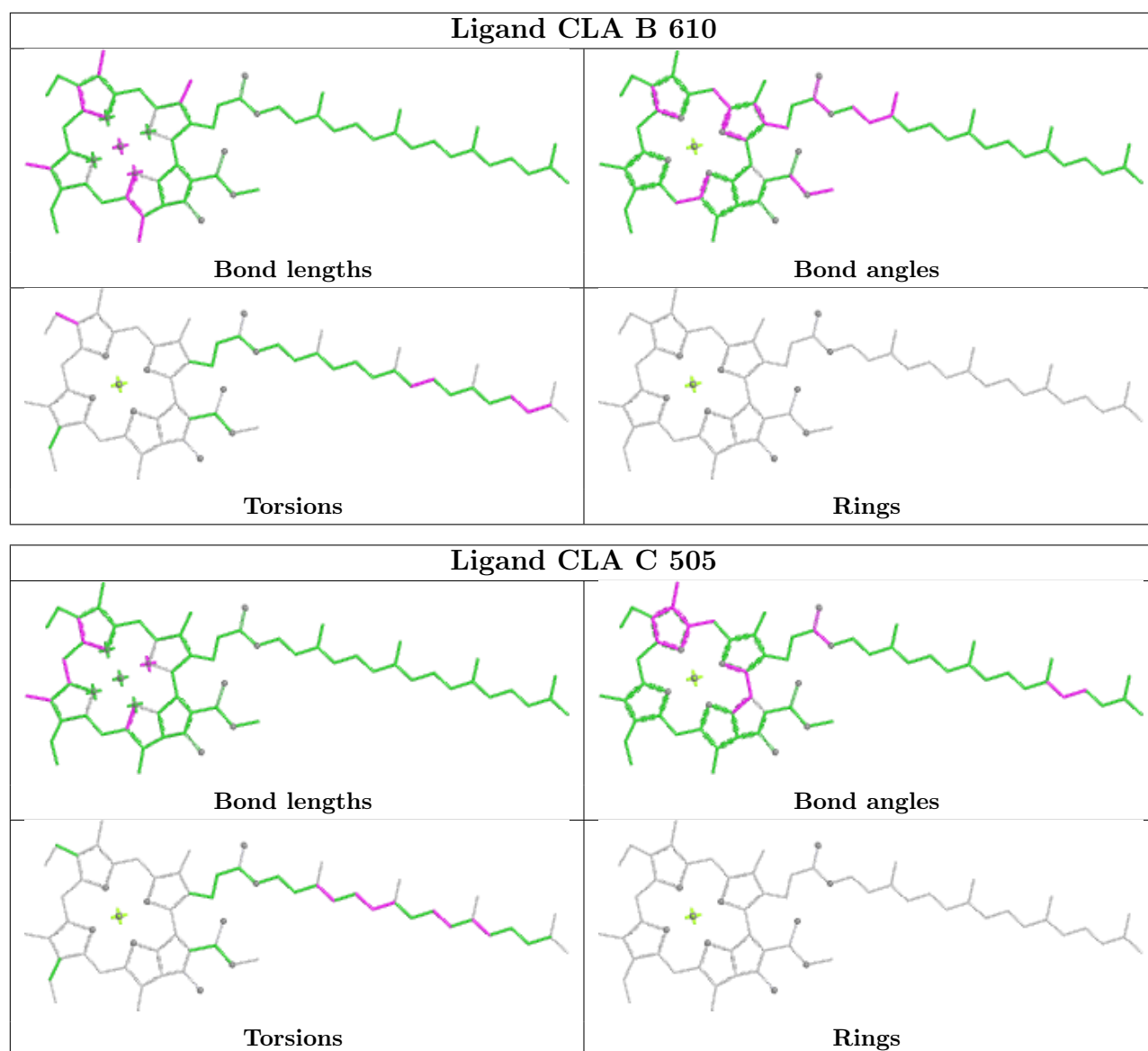


Ligand BCR b 617



Ligand CLA C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.52	0 100 100	17, 36, 61, 87	60 (17%)
1	a	334/344 (97%)	-0.42	5 (1%) 72 73	17, 38, 68, 87	60 (17%)
2	B	505/506 (99%)	-0.47	2 (0%) 88 90	21, 41, 74, 111	4 (0%)
2	b	505/506 (99%)	-0.38	4 (0%) 82 84	31, 44, 82, 120	0
3	C	442/461 (95%)	-0.45	0 100 100	18, 45, 64, 89	7 (1%)
3	c	451/461 (97%)	-0.36	2 (0%) 88 90	18, 48, 73, 111	8 (1%)
4	D	341/352 (96%)	-0.61	0 100 100	20, 38, 59, 98	1 (0%)
4	d	341/352 (96%)	-0.50	1 (0%) 90 91	20, 42, 69, 92	2 (0%)
5	E	82/84 (97%)	0.04	1 (1%) 76 78	36, 62, 85, 91	1 (1%)
5	e	82/84 (97%)	0.20	3 (3%) 45 45	45, 73, 92, 109	0
6	F	34/45 (75%)	-0.15	1 (2%) 53 54	43, 53, 81, 104	0
6	f	34/45 (75%)	-0.03	2 (5%) 28 26	49, 58, 101, 116	0
7	H	65/66 (98%)	-0.26	2 (3%) 51 51	40, 51, 71, 81	0
7	h	63/66 (95%)	0.00	1 (1%) 70 72	50, 62, 76, 86	0
8	I	35/38 (92%)	-0.39	1 (2%) 53 54	39, 47, 80, 94	0
8	i	35/38 (92%)	-0.30	0 100 100	39, 48, 87, 90	0
9	J	36/40 (90%)	-0.10	0 100 100	42, 58, 88, 107	0
9	j	36/40 (90%)	-0.02	2 (5%) 30 28	46, 62, 96, 117	0
10	K	37/46 (80%)	-0.06	0 100 100	53, 64, 88, 94	0
10	k	37/46 (80%)	0.01	0 100 100	57, 67, 88, 91	0
11	L	37/37 (100%)	-0.62	0 100 100	33, 37, 74, 81	0
11	l	36/37 (97%)	-0.57	0 100 100	28, 39, 82, 93	0
12	M	32/36 (88%)	-0.45	1 (3%) 51 51	33, 42, 68, 84	0
12	m	31/36 (86%)	-0.51	0 100 100	33, 42, 63, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.30	2 (0%) 82 84	29, 49, 95, 136	1 (0%)
13	o	244/272 (89%)	-0.33	2 (0%) 82 84	30, 49, 89, 136	0
14	R	34/40 (85%)	1.54	8 (23%) 2 1	83, 102, 117, 120	0
14	r	31/40 (77%)	2.10	17 (54%) 0 0	92, 128, 144, 151	0
15	T	29/32 (90%)	-0.56	0 100 100	33, 39, 72, 87	0
15	t	29/32 (90%)	-0.43	1 (3%) 48 48	34, 41, 86, 89	0
16	U	97/134 (72%)	-0.34	0 100 100	39, 52, 74, 103	0
16	u	97/134 (72%)	-0.42	0 100 100	38, 49, 66, 92	0
17	V	137/163 (84%)	-0.47	0 100 100	34, 49, 64, 81	0
17	v	137/163 (84%)	-0.24	0 100 100	41, 55, 81, 86	0
18	X	38/41 (92%)	-0.08	0 100 100	49, 64, 85, 92	0
18	x	39/41 (95%)	0.27	1 (2%) 57 58	56, 73, 101, 117	0
19	Y	27/46 (58%)	0.82	2 (7%) 20 18	64, 85, 97, 112	0
19	y	30/46 (65%)	0.53	0 100 100	68, 82, 99, 106	0
20	Z	62/62 (100%)	0.51	4 (6%) 25 23	60, 81, 126, 137	0
20	z	62/62 (100%)	0.54	3 (4%) 35 34	67, 78, 117, 134	0
All	All	5302/5690 (93%)	-0.32	68 (1%) 75 77	17, 46, 87, 151	144 (2%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	5.5
14	r	14	LEU	4.4
14	R	35	LEU	4.4
14	r	32	GLN	4.3
13	o	58	ASN	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.94	0.09	48,61,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.95	0.07	46,59,70,75	0
12	FME	m	1	10/11	0.95	0.08	40,57,76,89	0
15	FME	T	1	10/11	0.95	0.07	36,48,68,68	0
15	FME	t	1	10/11	0.95	0.08	34,48,77,77	0
12	FME	M	1	10/11	0.96	0.08	47,57,75,77	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
31	STE	H	103	18/20	0.74	0.19	56,85,97,102	0
31	STE	d	412	20/20	0.76	0.17	53,75,97,103	0
26	LHG	A	412	49/49	0.77	0.16	46,87,119,124	0
31	STE	b	624	10/20	0.78	0.15	41,58,71,73	0
26	LHG	e	101	42/49	0.78	0.16	60,94,114,125	0
31	STE	I	101	15/20	0.80	0.16	43,64,86,87	0
31	STE	R	101	12/20	0.80	0.20	68,87,105,110	0
32	LMG	c	522	48/55	0.80	0.16	42,81,110,115	0
22	CLA	b	601	65/65	0.82	0.13	52,76,101,103	0
31	STE	b	622	16/20	0.82	0.15	44,66,87,93	0
32	LMG	b	621	55/55	0.82	0.16	50,79,102,113	0
31	STE	b	623	20/20	0.82	0.15	44,66,96,98	0
31	STE	L	103	12/20	0.83	0.16	55,70,86,96	0
25	PL9	A	408	55/55	0.83	0.16	42,71,90,93	0
31	STE	T	102	16/20	0.83	0.15	40,55,78,91	0
31	STE	h	103	14/20	0.83	0.17	57,74,88,95	0
32	LMG	D	410	33/55	0.83	0.14	42,60,95,106	0
31	STE	a	416	12/20	0.83	0.13	35,72,80,82	0
31	STE	B	624	16/20	0.83	0.14	40,64,83,86	0
31	STE	B	625	15/20	0.84	0.19	43,66,83,92	0
32	LMG	a	417	55/55	0.84	0.14	39,61,90,107	0
31	STE	a	415	10/20	0.85	0.14	33,67,81,83	0
31	STE	C	522	12/20	0.85	0.14	40,56,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	STE	j	101	12/20	0.85	0.12	47,65,78,79	0
28	DGD	A	414	66/66	0.85	0.11	43,67,92,99	0
31	STE	C	520	12/20	0.85	0.13	45,63,73,76	0
31	STE	T	103	15/20	0.85	0.15	40,62,91,93	0
31	STE	c	501	12/20	0.85	0.11	44,72,81,86	0
31	STE	C	521	16/20	0.86	0.13	46,61,71,77	0
31	STE	B	623	18/20	0.86	0.12	45,65,90,95	0
31	STE	b	620	20/20	0.86	0.12	44,61,82,88	0
31	STE	c	521	20/20	0.86	0.13	45,65,94,110	0
31	STE	d	411	20/20	0.86	0.12	49,67,82,86	0
31	STE	Z	101	8/20	0.86	0.14	42,63,77,77	0
27	SQD	d	409	41/54	0.87	0.13	59,95,120,123	0
32	LMG	Y	101	48/55	0.87	0.12	50,77,102,109	0
25	PL9	a	410	55/55	0.87	0.14	43,76,96,103	0
31	STE	B	601	12/20	0.87	0.14	56,74,93,94	0
27	SQD	A	413	39/54	0.87	0.13	45,70,99,104	0
31	STE	M	103	10/20	0.88	0.14	40,54,63,72	0
32	LMG	D	411	28/55	0.88	0.12	35,54,68,74	0
31	STE	t	102	14/20	0.88	0.12	39,51,63,69	0
31	STE	B	622	12/20	0.89	0.12	35,58,68,76	0
32	LMG	C	516	48/55	0.89	0.11	37,60,85,102	0
27	SQD	a	414	36/54	0.89	0.12	24,66,100,107	0
32	LMG	c	520	37/55	0.89	0.10	49,70,89,90	0
22	CLA	H	101	65/65	0.89	0.10	43,68,99,105	0
32	LMG	c	523	49/55	0.89	0.11	37,62,105,119	0
22	CLA	C	513	65/65	0.90	0.11	51,69,108,113	0
27	SQD	L	101	49/54	0.90	0.10	42,64,97,117	0
31	STE	M	102	15/20	0.90	0.12	43,60,73,74	0
23	BCR	h	101	40/40	0.90	0.10	41,63,87,90	0
31	STE	B	620	17/20	0.90	0.11	39,56,72,81	0
31	STE	D	413	20/20	0.91	0.10	38,56,85,86	0
32	LMG	M	101	51/55	0.91	0.09	34,54,82,89	0
28	DGD	C	518	62/66	0.91	0.10	38,59,101,119	0
23	BCR	K	101	40/40	0.91	0.11	45,63,78,89	0
23	BCR	c	515	40/40	0.91	0.10	46,65,82,84	0
27	SQD	B	621	54/54	0.91	0.09	41,64,93,101	0
27	SQD	F	102	36/54	0.91	0.10	53,78,93,101	0
31	STE	d	410	17/20	0.91	0.11	44,60,69,76	0
32	LMG	m	101	51/55	0.91	0.10	31,58,83,98	0
23	BCR	X	101	40/40	0.92	0.09	34,54,70,73	0
22	CLA	c	514	65/65	0.92	0.10	47,72,110,119	0
31	STE	M	104	18/20	0.92	0.10	37,51,85,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	BCR	d	404	40/40	0.92	0.10	36,56,96,97	0
23	BCR	K	102	40/40	0.92	0.09	42,61,76,76	0
28	DGD	h	102	62/66	0.92	0.09	37,53,67,76	0
31	STE	J	101	12/20	0.92	0.10	48,64,78,79	0
27	SQD	a	413	54/54	0.92	0.10	47,66,94,98	0
23	BCR	b	617	40/40	0.93	0.07	31,49,60,63	0
32	LMG	D	408	51/55	0.93	0.11	33,65,95,99	0
23	BCR	k	101	40/40	0.93	0.09	40,67,80,83	0
23	BCR	D	406	40/40	0.93	0.09	33,49,89,93	0
28	DGD	c	518	62/66	0.93	0.09	37,57,94,108	0
32	LMG	d	408	44/55	0.93	0.10	36,61,95,103	0
22	CLA	c	513	65/65	0.93	0.10	47,65,103,110	0
22	CLA	c	510	65/65	0.94	0.09	32,54,72,73	0
23	BCR	A	405	40/40	0.94	0.07	26,40,48,51	0
23	BCR	k	102	40/40	0.94	0.10	40,58,70,72	0
23	BCR	t	101	40/40	0.94	0.06	25,43,56,57	0
23	BCR	B	617	40/40	0.94	0.07	29,46,63,67	0
23	BCR	B	618	40/40	0.94	0.07	30,43,56,61	0
23	BCR	b	618	40/40	0.94	0.07	26,46,60,67	0
28	DGD	H	102	62/66	0.94	0.08	31,51,65,77	0
28	DGD	c	517	62/66	0.94	0.09	28,46,79,95	0
26	LHG	a	412	49/49	0.94	0.09	33,53,75,84	0
28	DGD	c	519	62/66	0.94	0.09	31,59,86,90	0
23	BCR	b	619	40/40	0.94	0.08	34,53,64,73	0
27	SQD	A	411	52/54	0.94	0.10	41,66,102,108	0
23	BCR	C	514	40/40	0.94	0.08	30,47,59,73	0
22	CLA	C	512	65/65	0.94	0.10	41,62,105,110	0
34	BCT	a	409	4/4	0.94	0.09	32,35,48,57	0
22	CLA	c	506	65/65	0.95	0.08	30,49,70,81	0
28	DGD	C	519	62/66	0.95	0.08	29,55,84,94	0
22	CLA	c	507	65/65	0.95	0.09	33,54,91,108	0
22	CLA	c	509	64/65	0.95	0.09	36,53,103,122	0
23	BCR	c	516	40/40	0.95	0.08	31,50,77,78	0
22	CLA	B	606	65/65	0.95	0.07	20,41,72,78	0
22	CLA	c	511	65/65	0.95	0.08	35,54,72,75	0
22	CLA	c	512	65/65	0.95	0.09	40,61,79,85	0
22	CLA	C	503	65/65	0.95	0.07	35,51,62,64	0
22	CLA	C	510	65/65	0.95	0.07	31,52,70,74	0
22	CLA	d	403	65/65	0.95	0.09	32,55,102,112	0
22	CLA	a	405	65/65	0.95	0.08	22,40,94,108	0
26	LHG	A	410	47/49	0.95	0.09	34,53,93,105	0
22	CLA	C	511	65/65	0.95	0.08	38,56,75,80	0

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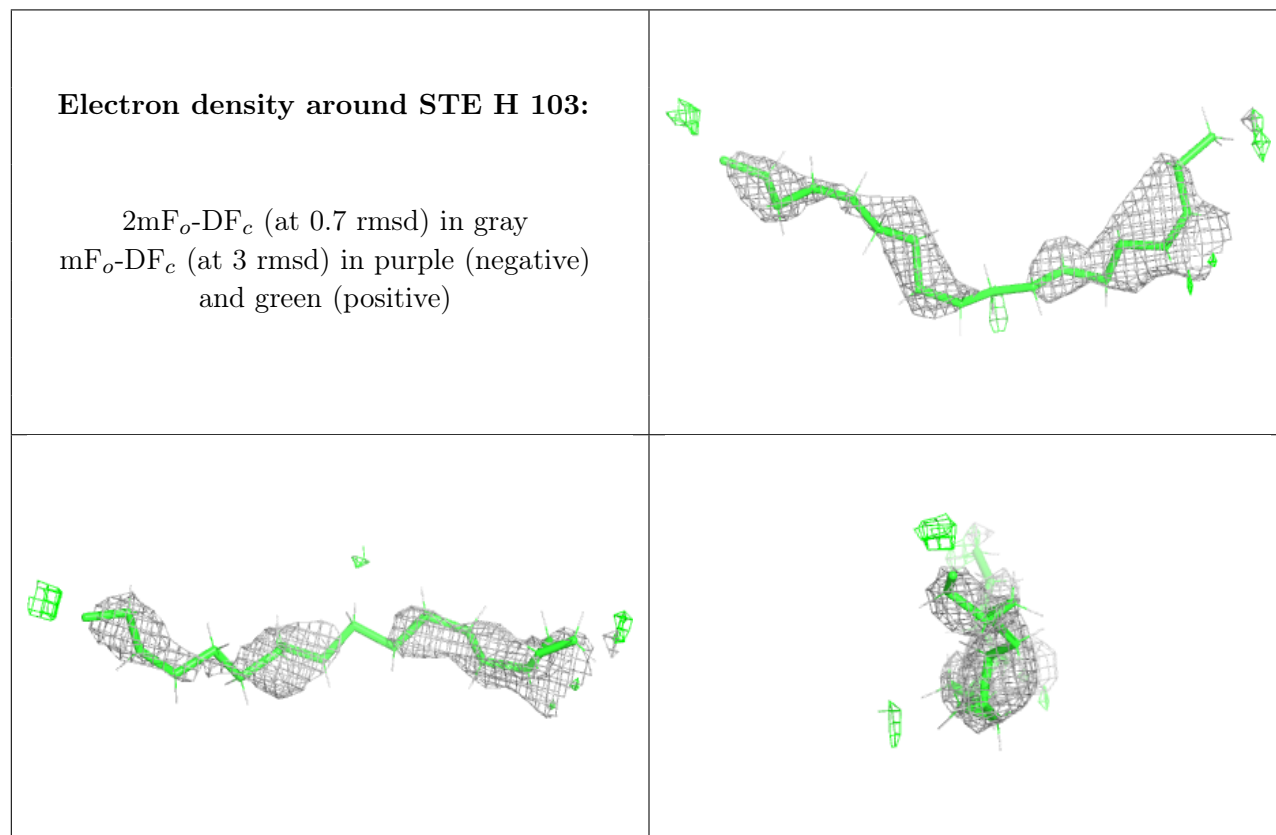
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	602	65/65	0.95	0.08	29,47,70,76	0
26	LHG	d	407	39/49	0.95	0.08	35,53,78,84	0
23	BCR	B	619	40/40	0.95	0.07	28,47,61,74	0
26	LHG	l	101	49/49	0.95	0.08	34,51,60,72	0
22	CLA	b	605	65/65	0.95	0.07	29,41,60,66	0
23	BCR	C	515	40/40	0.95	0.09	45,60,79,83	0
22	CLA	b	606	65/65	0.95	0.07	30,45,78,87	0
22	CLA	b	609	65/65	0.95	0.08	32,51,76,78	0
22	CLA	b	615	65/65	0.95	0.07	30,46,67,79	0
23	BCR	T	101	40/40	0.95	0.07	27,46,64,66	0
22	CLA	b	616	60/65	0.95	0.09	33,50,91,95	0
23	BCR	a	406	40/40	0.95	0.06	24,37,48,58	0
22	CLA	c	504	65/65	0.95	0.07	35,50,61,64	0
33	PHO	d	401	64/64	0.95	0.07	27,44,54,62	0
34	BCT	D	403	4/4	0.95	0.07	33,37,44,45	0
28	DGD	C	517	62/66	0.95	0.09	27,42,78,88	0
26	LHG	D	412	49/49	0.96	0.08	34,48,69,76	0
26	LHG	L	102	49/49	0.96	0.07	30,47,62,69	0
22	CLA	B	602	65/65	0.96	0.07	27,41,68,77	0
22	CLA	B	609	65/65	0.96	0.08	28,46,66,74	0
22	CLA	B	610	65/65	0.96	0.06	22,36,47,54	0
22	CLA	D	404	65/65	0.96	0.07	19,33,58,67	0
22	CLA	D	405	65/65	0.96	0.07	24,45,110,127	0
22	CLA	d	402	65/65	0.96	0.07	25,40,65,80	0
22	CLA	B	612	65/65	0.96	0.06	24,37,51,56	0
22	CLA	a	402	65/65	0.96	0.06	22,34,48,60	0
22	CLA	a	403	65/65	0.96	0.08	29,45,101,111	0
22	CLA	B	615	65/65	0.96	0.08	26,43,65,70	0
22	CLA	a	411	65/65	0.96	0.07	21,37,47,52	0
22	CLA	B	616	60/65	0.96	0.09	27,46,107,121	0
22	CLA	C	501	65/65	0.96	0.07	28,42,53,62	0
22	CLA	b	603	65/65	0.96	0.07	25,43,77,92	0
22	CLA	C	502	65/65	0.96	0.07	32,48,65,66	0
22	CLA	B	604	65/65	0.96	0.07	22,37,79,93	0
22	CLA	b	608	65/65	0.96	0.07	29,48,70,87	0
22	CLA	C	504	59/65	0.96	0.08	33,47,84,103	0
22	CLA	b	610	65/65	0.96	0.07	27,43,56,64	0
22	CLA	b	611	65/65	0.96	0.06	20,39,63,71	0
22	CLA	b	612	65/65	0.96	0.07	22,39,54,60	0
22	CLA	b	613	65/65	0.96	0.07	22,41,82,90	0
22	CLA	b	614	65/65	0.96	0.07	29,43,84,94	0
22	CLA	C	505	65/65	0.96	0.07	27,47,70,73	0

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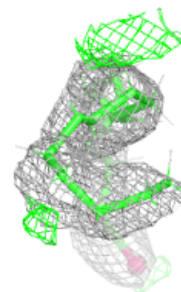
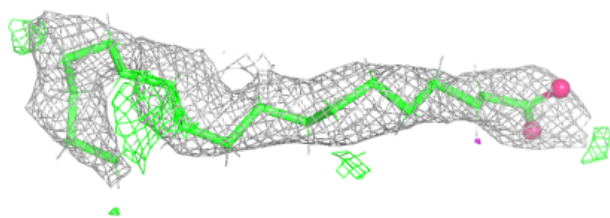
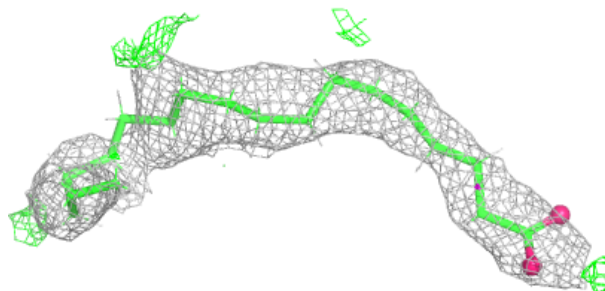
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	506	65/65	0.96	0.08	28,48,91,99	0
22	CLA	c	502	65/65	0.96	0.07	29,44,56,62	0
22	CLA	c	503	65/65	0.96	0.07	35,47,65,71	0
22	CLA	C	507	65/65	0.96	0.07	30,48,65,71	0
22	CLA	c	505	60/65	0.96	0.07	37,54,82,90	0
22	CLA	C	508	65/65	0.96	0.08	30,51,113,130	0
25	PL9	D	407	55/55	0.96	0.07	25,39,51,66	0
22	CLA	C	509	65/65	0.96	0.08	29,50,70,77	0
33	PHO	D	401	64/64	0.96	0.06	21,34,45,48	0
33	PHO	D	402	64/64	0.96	0.06	26,37,46,47	0
33	PHO	a	404	64/64	0.96	0.06	24,34,44,44	0
25	PL9	d	405	55/55	0.96	0.06	26,40,51,54	0
22	CLA	c	508	65/65	0.96	0.07	33,48,64,75	0
22	CLA	B	605	65/65	0.96	0.07	25,37,51,53	0
22	CLA	b	607	65/65	0.97	0.07	22,43,71,75	0
22	CLA	A	403	65/65	0.97	0.09	24,40,103,110	0
22	CLA	B	613	65/65	0.97	0.07	21,38,77,88	0
22	CLA	B	614	65/65	0.97	0.08	24,41,87,101	0
22	CLA	A	404	54/65	0.97	0.06	21,36,64,77	0
26	LHG	D	409	49/49	0.97	0.07	26,43,55,62	0
22	CLA	A	409	65/65	0.97	0.06	23,34,56,61	0
22	CLA	B	607	65/65	0.97	0.07	22,35,71,80	0
22	CLA	B	608	65/65	0.97	0.06	23,39,63,69	0
26	LHG	d	406	49/49	0.97	0.07	30,46,60,68	0
22	CLA	A	402	65/65	0.97	0.06	18,33,51,69	0
22	CLA	b	604	65/65	0.97	0.07	28,41,91,114	0
22	CLA	B	603	65/65	0.97	0.07	23,38,66,74	0
22	CLA	B	611	65/65	0.97	0.05	23,34,51,51	0
35	HEC	F	101	43/43	0.97	0.08	40,57,70,79	0
35	HEC	f	101	43/43	0.97	0.09	48,65,89,92	0
35	HEC	V	201	43/43	0.98	0.06	28,37,45,54	0
35	HEC	v	201	43/43	0.98	0.06	30,41,55,57	0
24	CL	A	407	1/1	0.99	0.07	36,36,36,36	0
24	CL	a	407	1/1	0.99	0.04	32,32,32,32	0
29	OEX	A	415[A]	10/10	0.99	0.03	36,38,42,43	10
29	OEX	a	418[A]	10/10	0.99	0.03	33,39,42,43	10
30	OEY	a	419[B]	11/11	0.99	0.03	18,23,28,29	11
24	CL	a	408	1/1	0.99	0.08	34,34,34,34	0
24	CL	A	406	1/1	0.99	0.04	34,34,34,34	0
30	OEY	A	416[B]	11/11	1.00	0.03	18,23,28,28	11
21	FE2	a	401	1/1	1.00	0.02	38,38,38,38	0
21	FE2	A	401	1/1	1.00	0.04	37,37,37,37	0

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



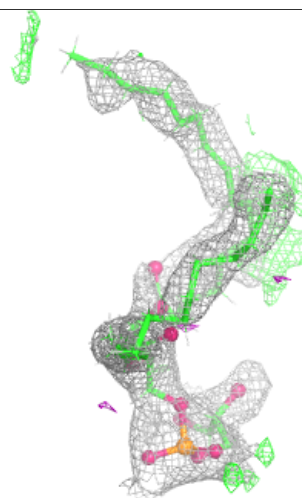
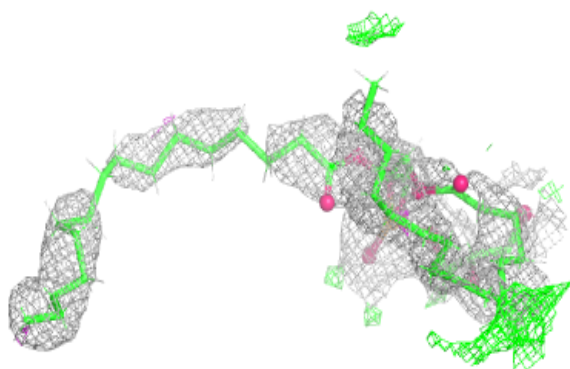
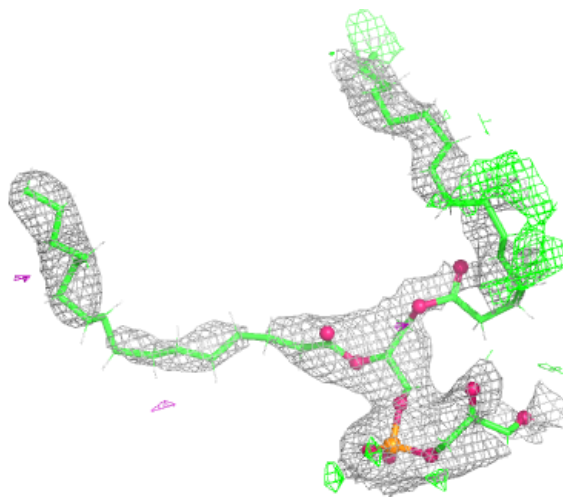
Electron density around STE d 412:

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



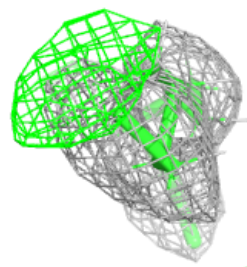
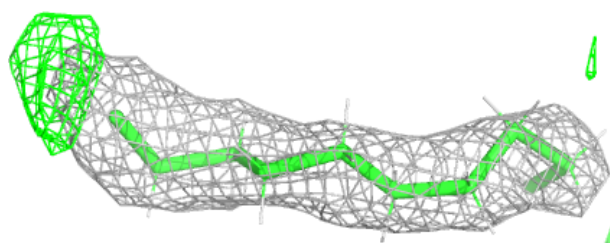
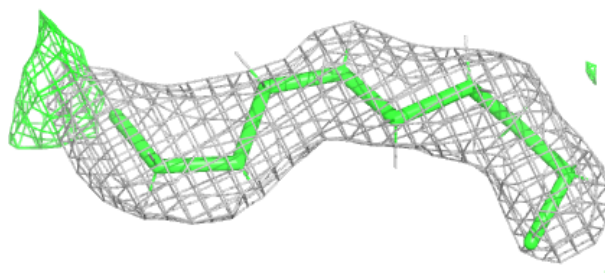
Electron density around LHG A 412:

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

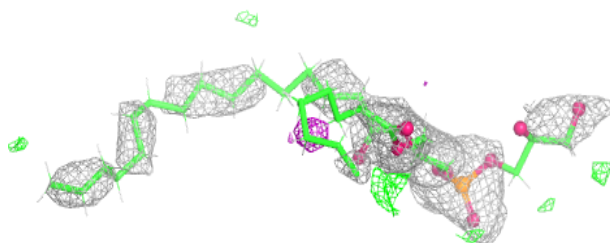
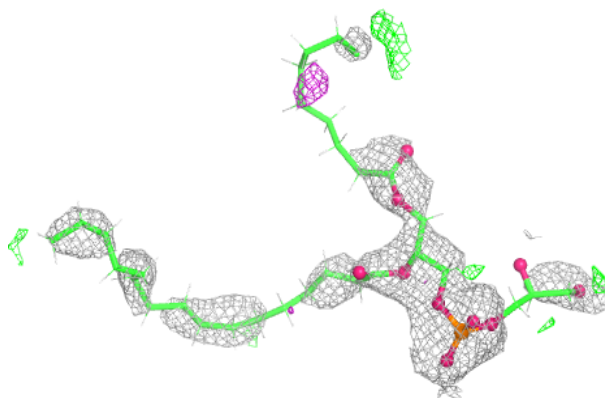


Electron density around STE b 624:

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

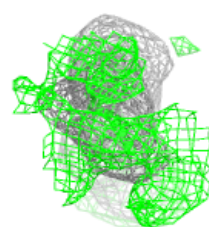
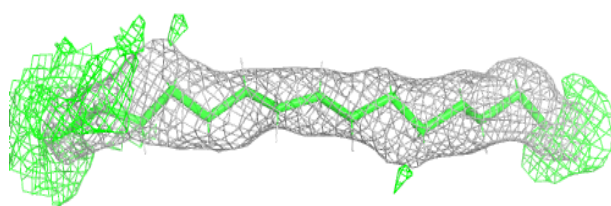
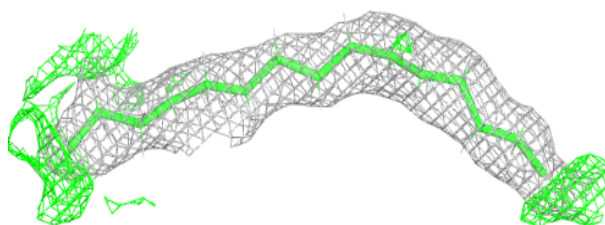
**Electron density around LHG e 101:**

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

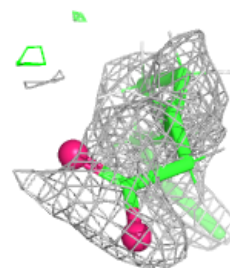
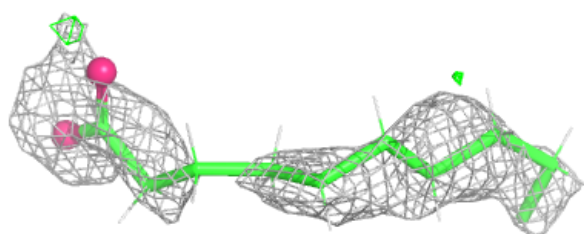
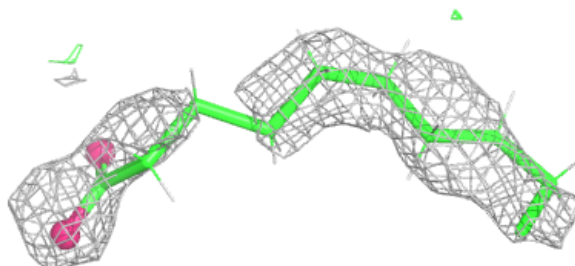


Electron density around STE I 101:

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

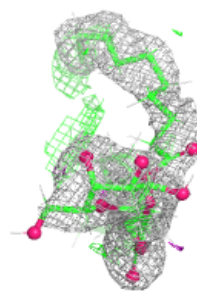
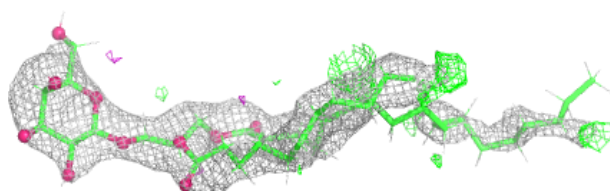
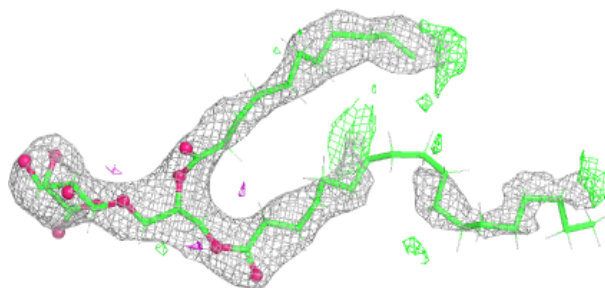
**Electron density around STE R 101:**

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

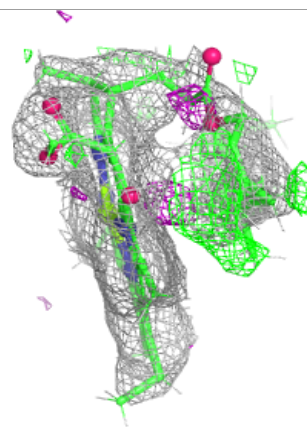
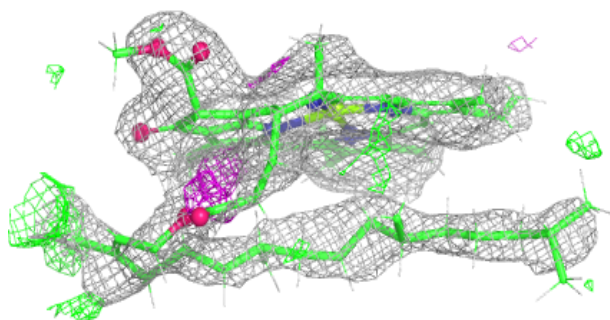
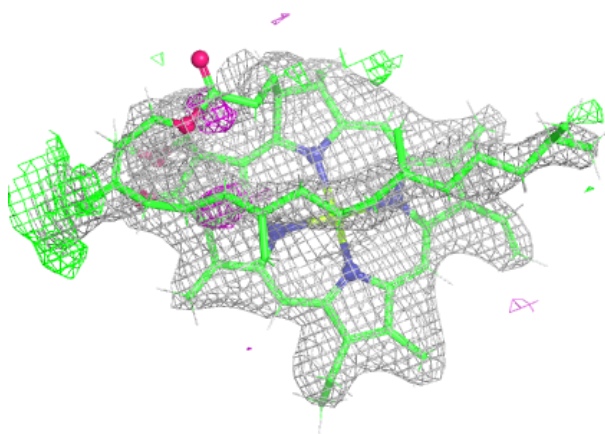


Electron density around LMG c 522:

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

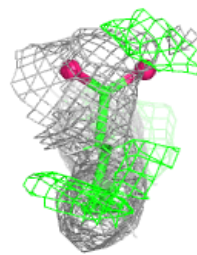
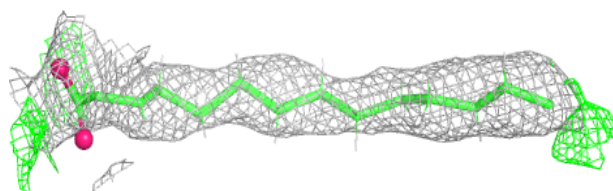
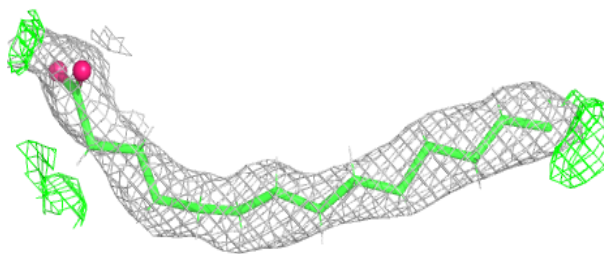
**Electron density around CLA b 601:**

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

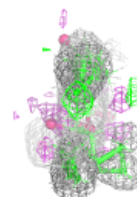
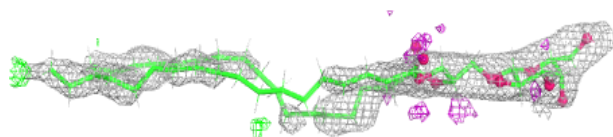
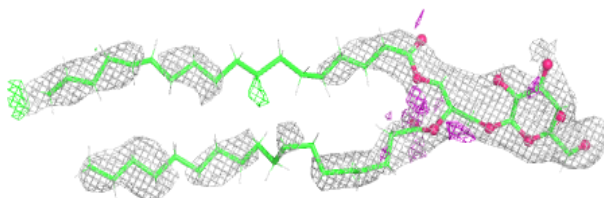


Electron density around STE b 622:

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and green (positive)

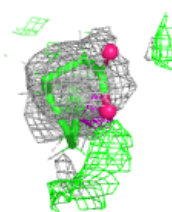
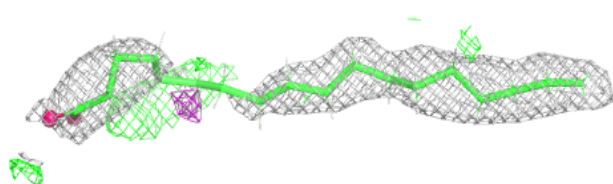
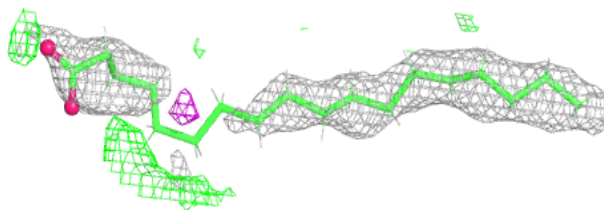
**Electron density around LMG b 621:**

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

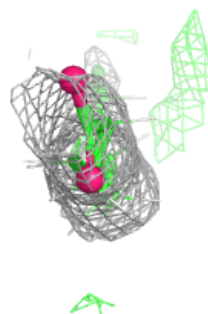
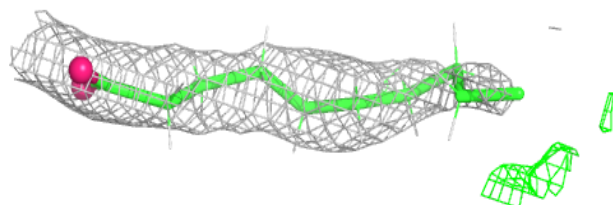
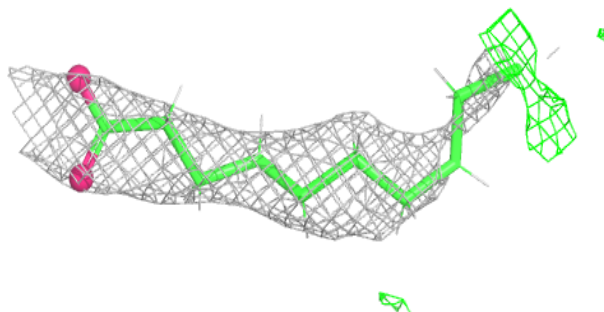


Electron density around STE b 623:

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

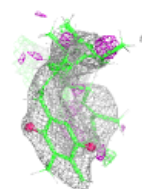
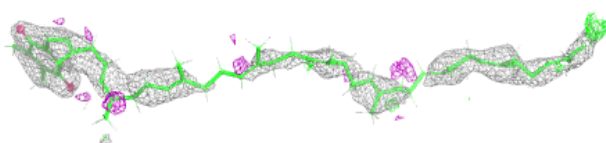
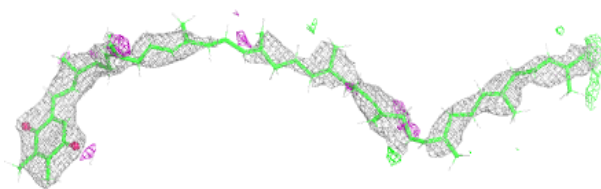
**Electron density around STE L 103:**

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

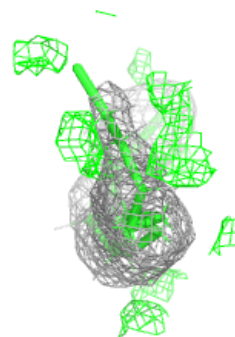
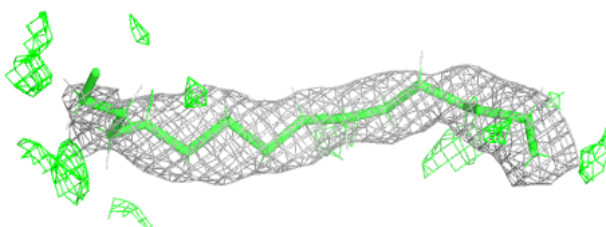
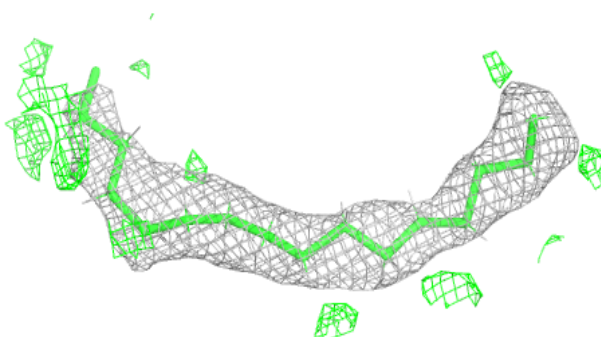


Electron density around PL9 A 408:

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

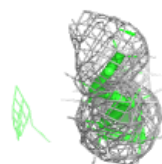
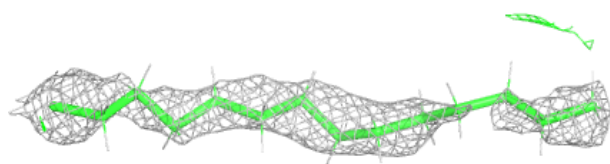
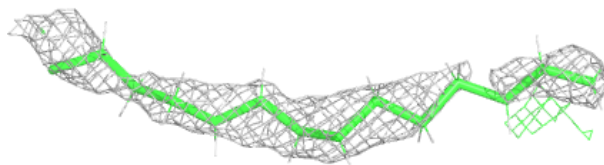
**Electron density around STE T 102:**

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

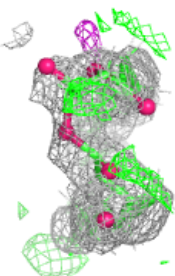
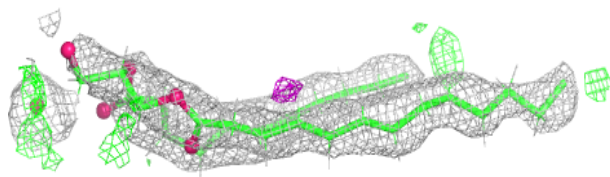
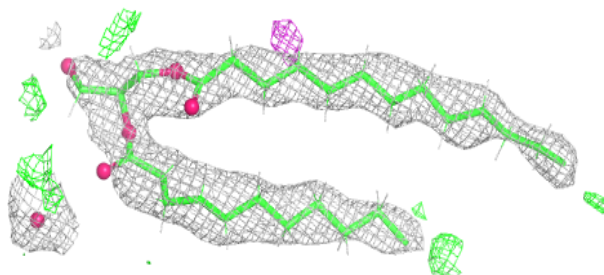


Electron density around STE h 103:

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

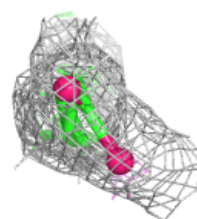
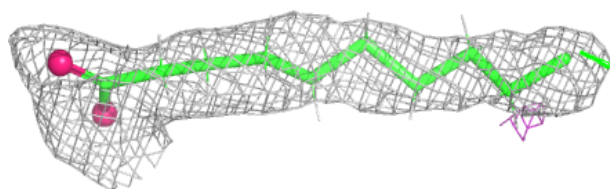
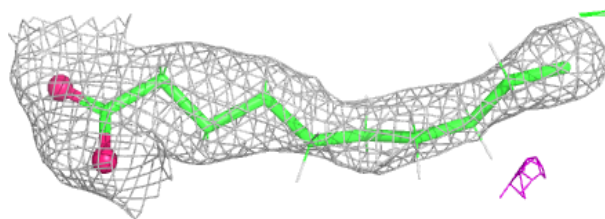
**Electron density around LMG D 410:**

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

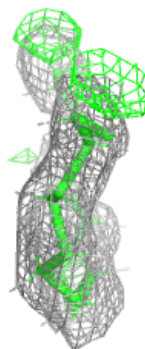
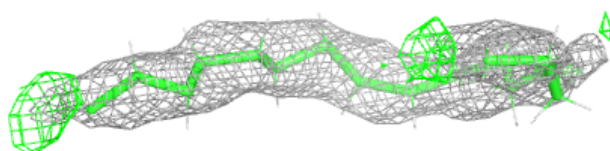
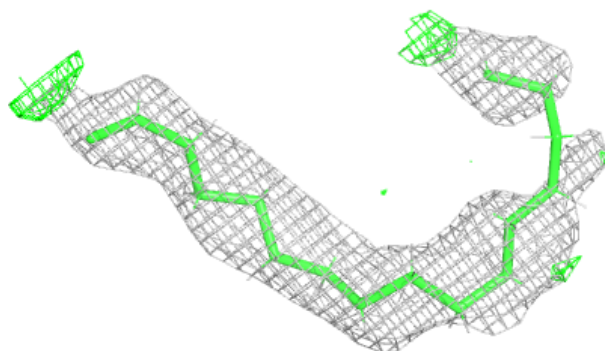


Electron density around STE a 416:

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

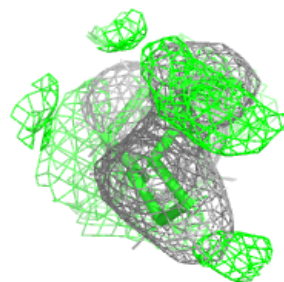
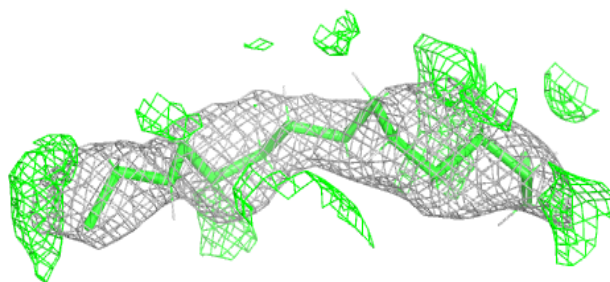
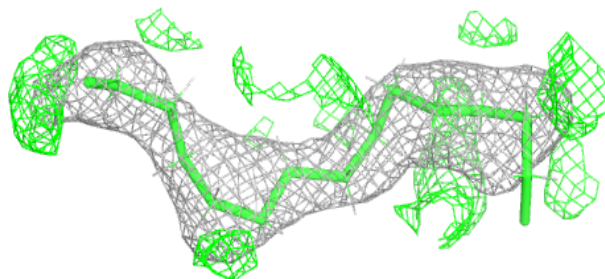
**Electron density around STE B 624:**

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

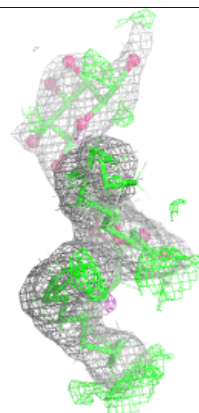
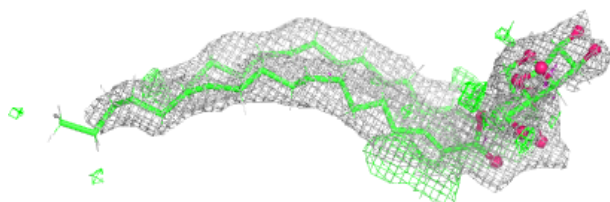
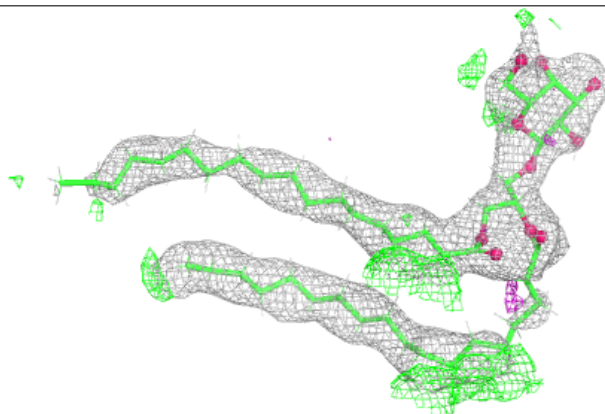


Electron density around STE B 625:

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

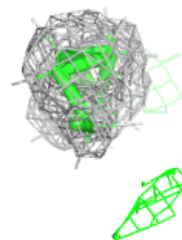
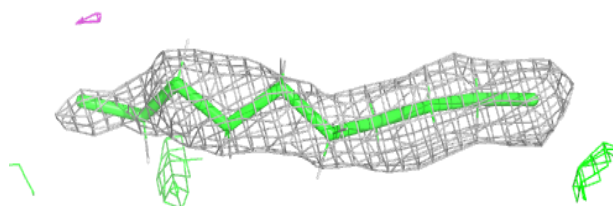
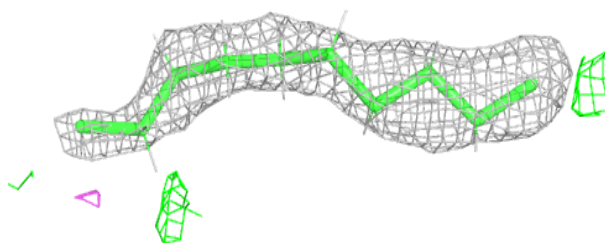
**Electron density around LMG a 417:**

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

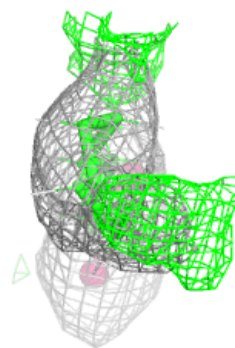
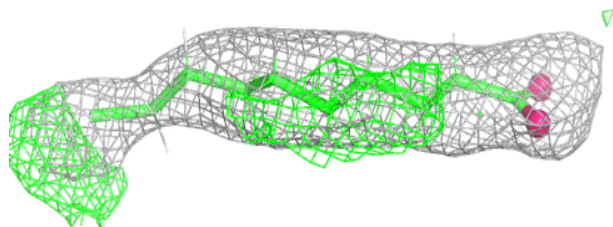
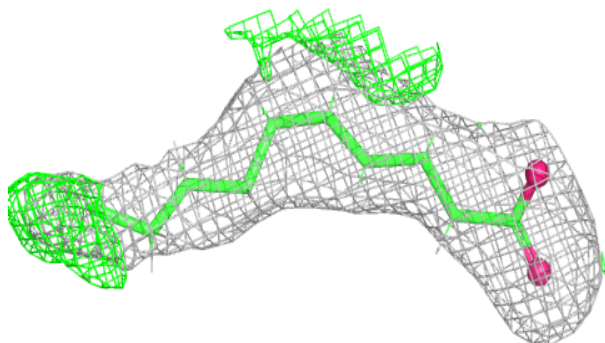


Electron density around STE a 415:

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

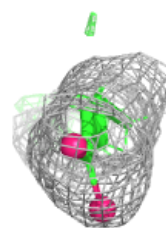
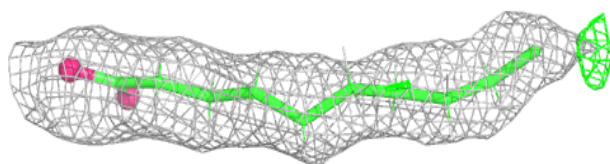
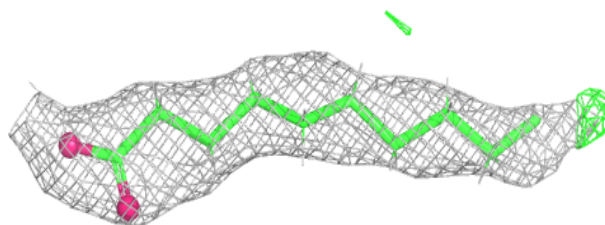
**Electron density around STE C 522:**

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

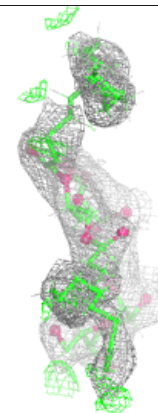
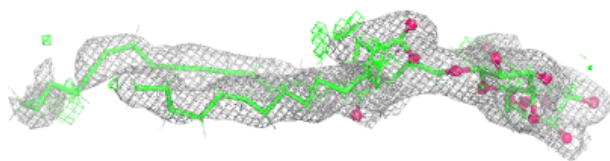
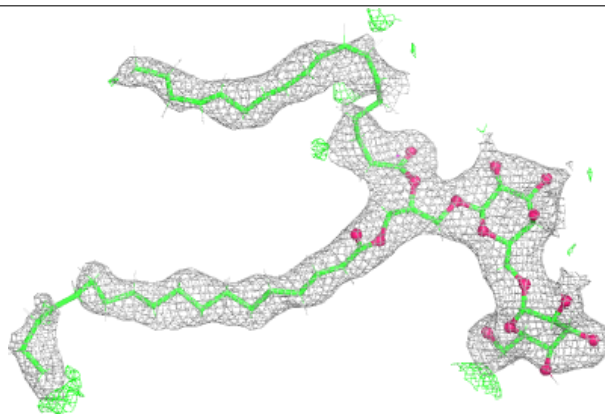


Electron density around STE j 101:

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

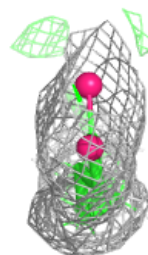
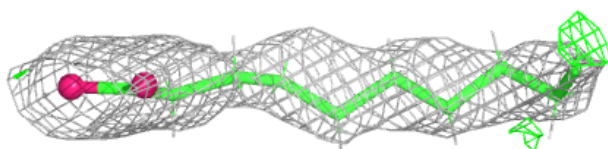
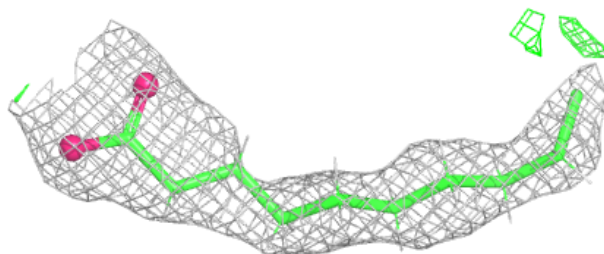
**Electron density around DGD A 414:**

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

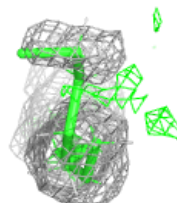
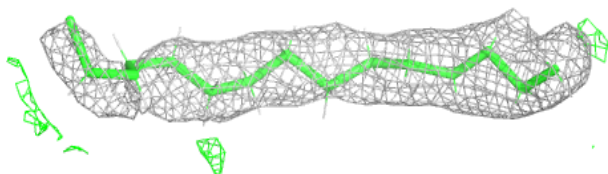
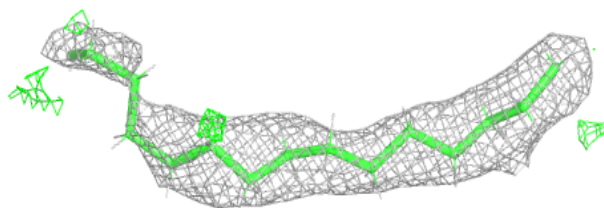


Electron density around STE C 520:

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

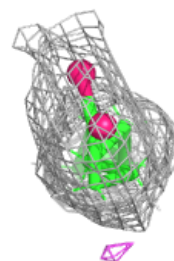
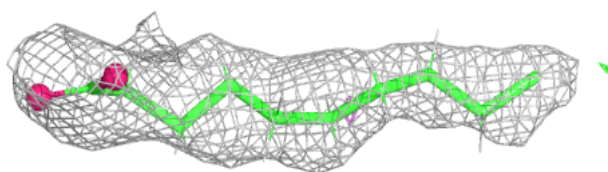
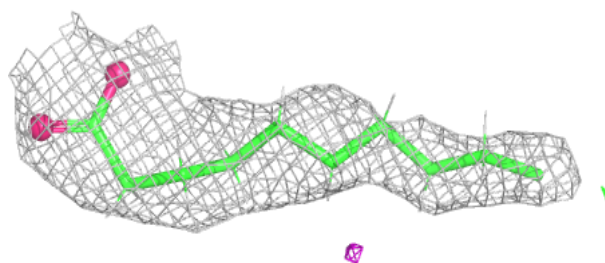
**Electron density around STE T 103:**

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

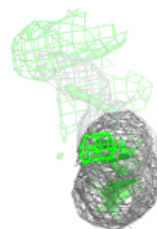
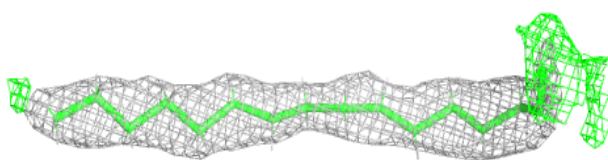
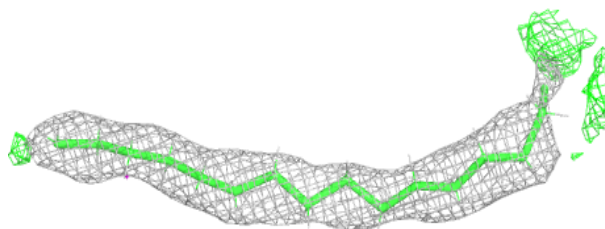


Electron density around STE c 501:

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

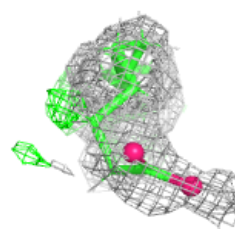
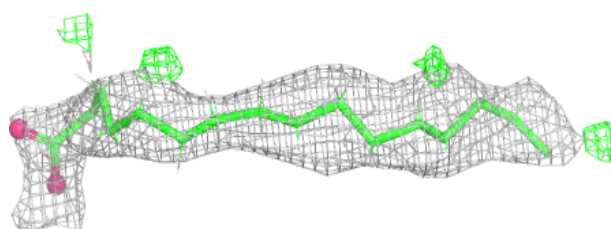
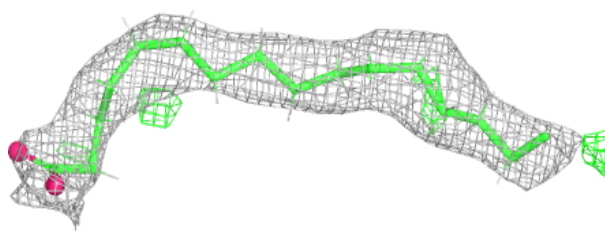
**Electron density around STE C 521:**

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

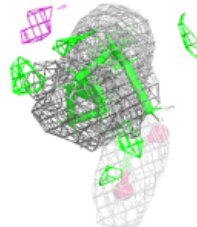
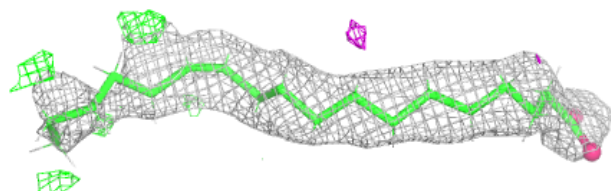
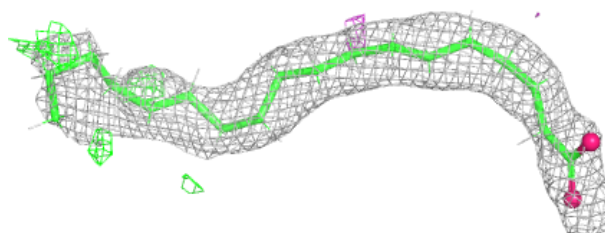


Electron density around STE B 623:

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

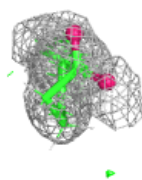
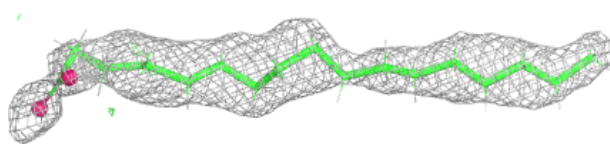
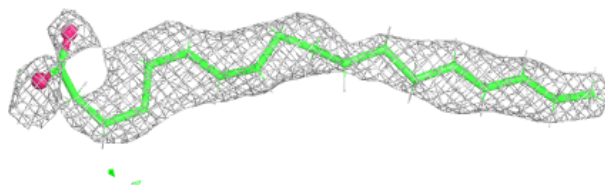
**Electron density around STE b 620:**

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

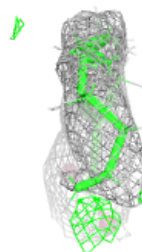
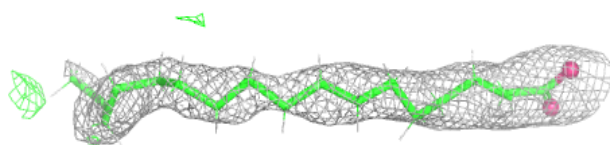
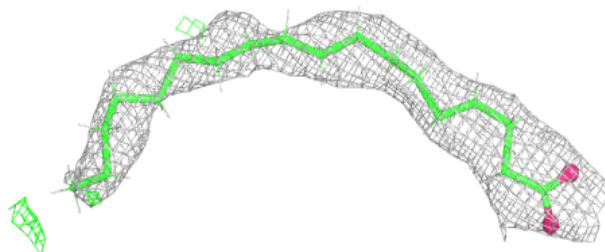


Electron density around STE c 521:

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

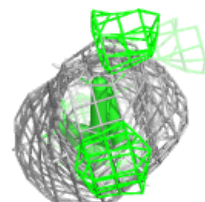
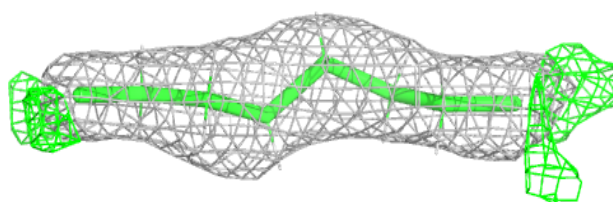
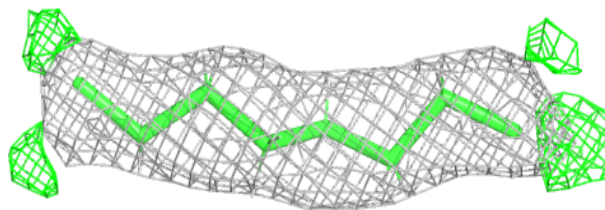
**Electron density around STE d 411:**

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

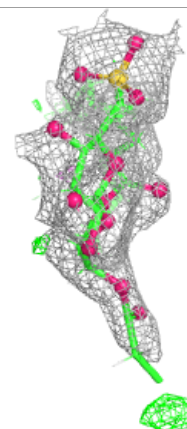
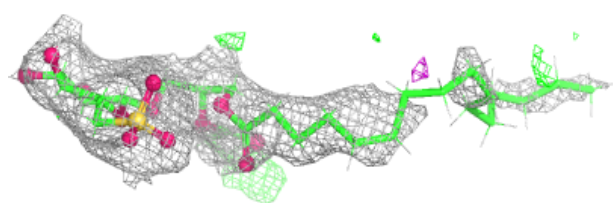
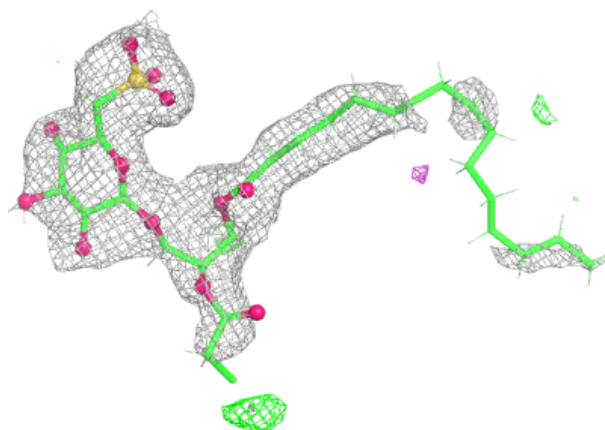


Electron density around STE Z 101:

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

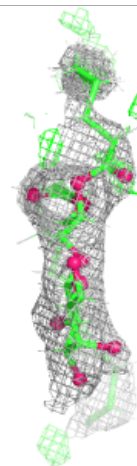
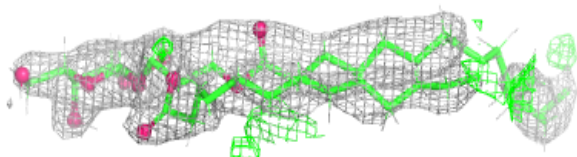
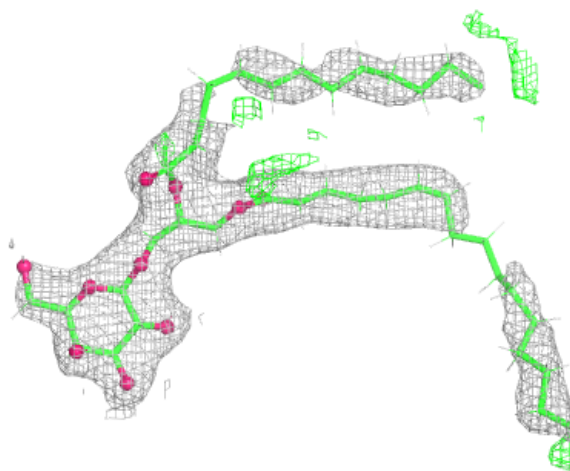
**Electron density around SQD d 409:**

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



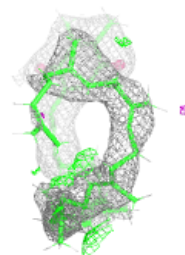
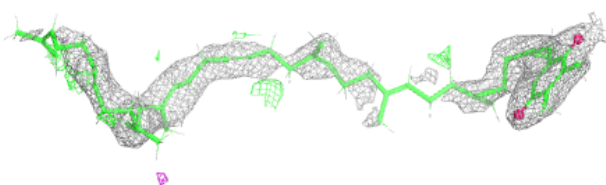
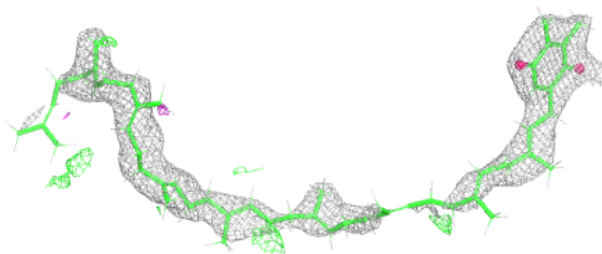
Electron density around LMG Y 101:

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

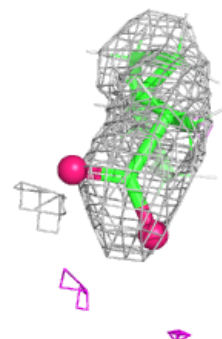
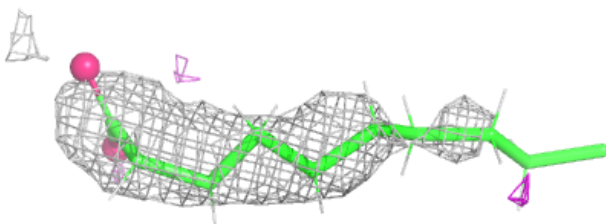
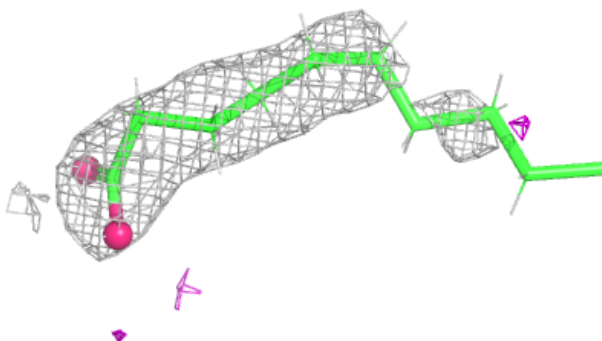


Electron density around PL9 a 410:

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

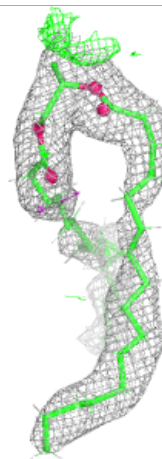
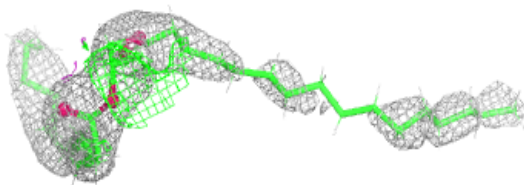
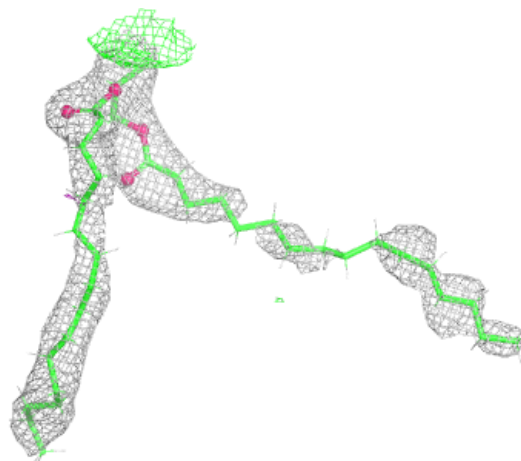
**Electron density around STE B 601:**

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



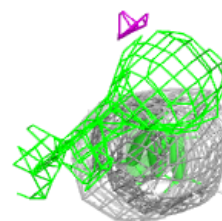
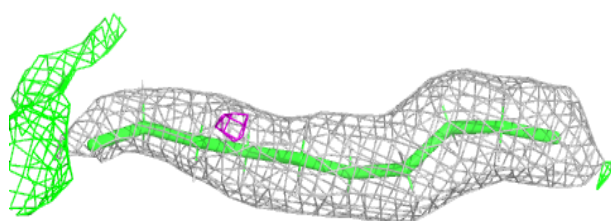
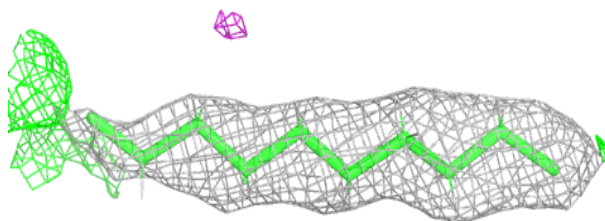
Electron density around SQD A 413:

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

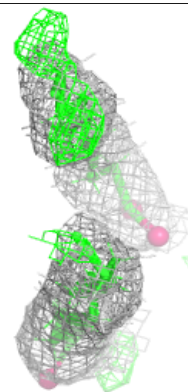
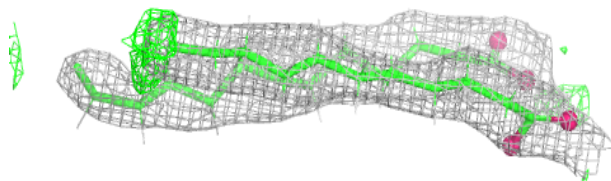
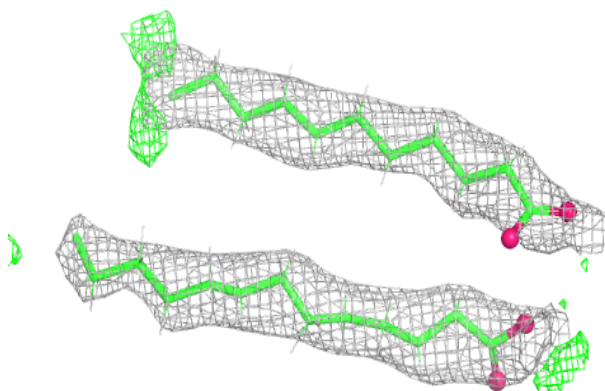


Electron density around STE M 103:

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

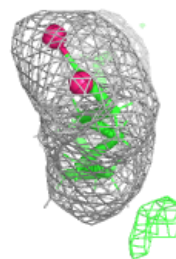
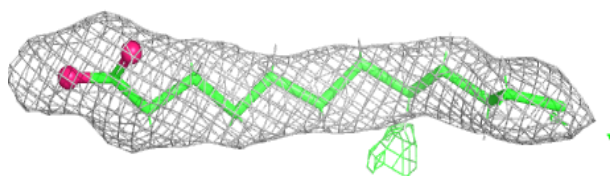
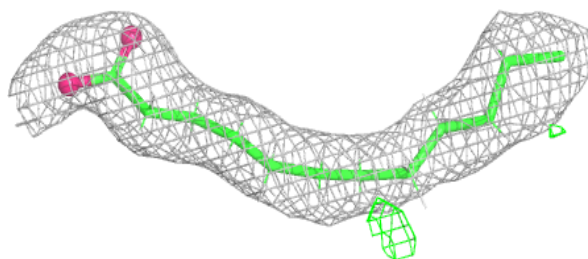
**Electron density around LMG D 411:**

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

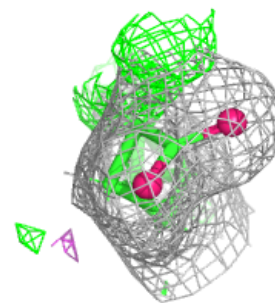
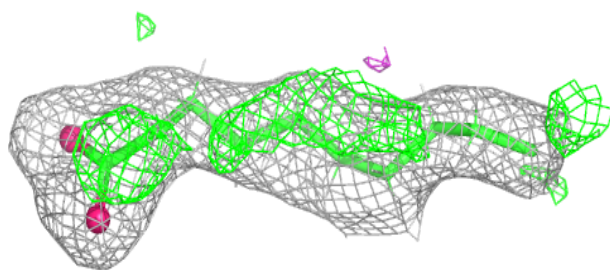
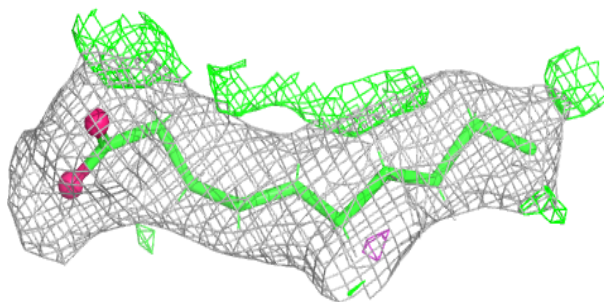


Electron density around STE t 102:

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

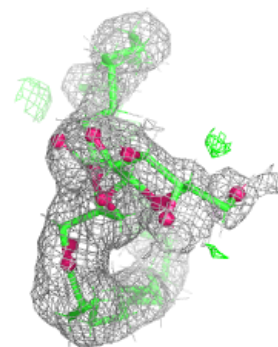
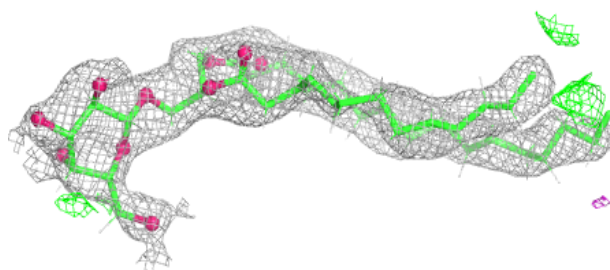
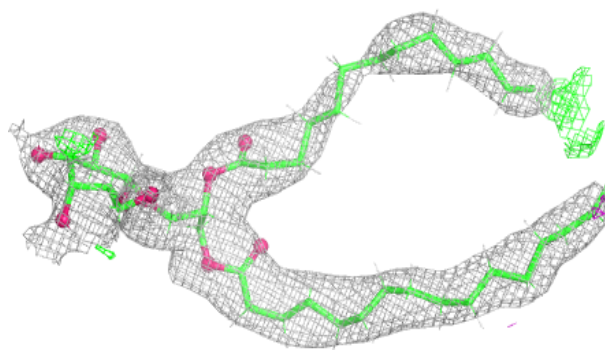
**Electron density around STE B 622:**

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



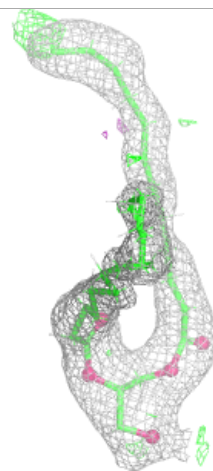
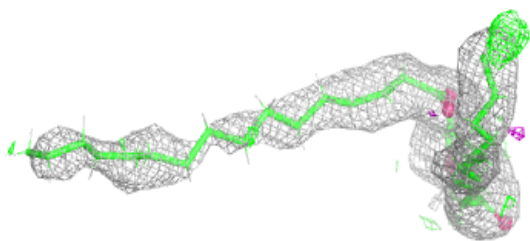
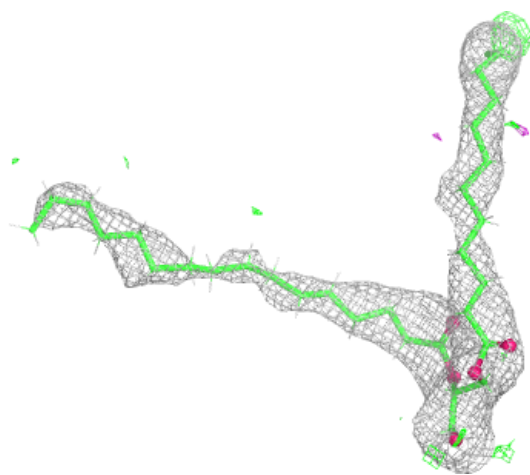
Electron density around LMG C 516:

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



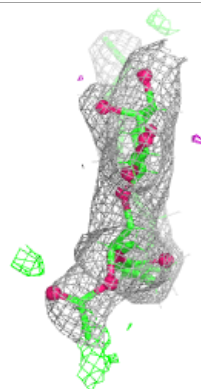
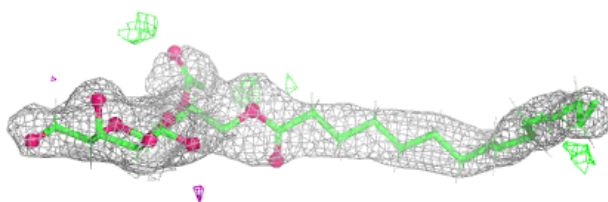
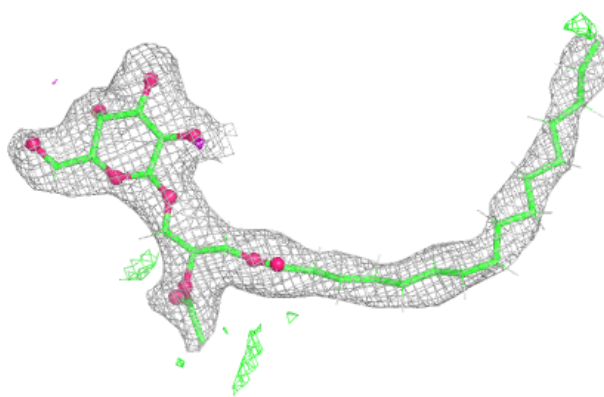
Electron density around SQD a 414:

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



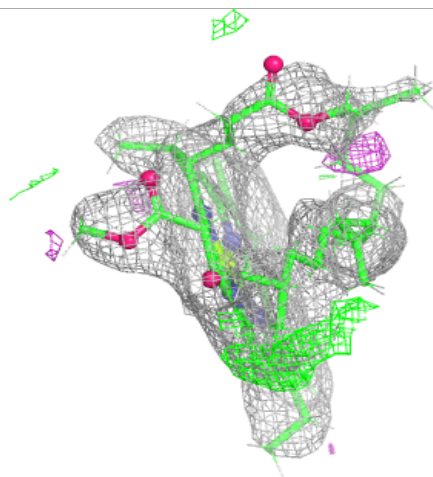
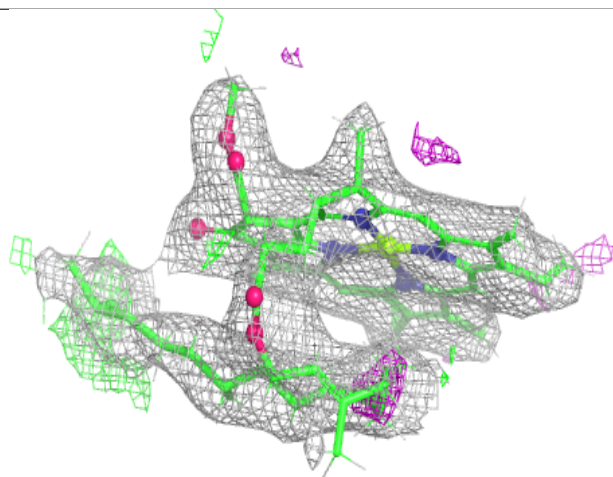
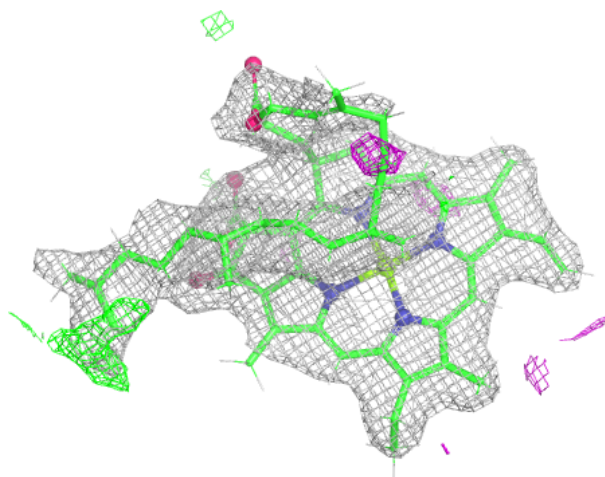
Electron density around LMG c 520:

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



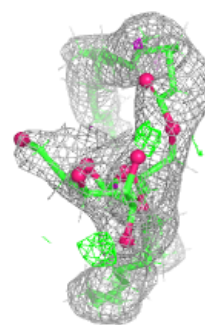
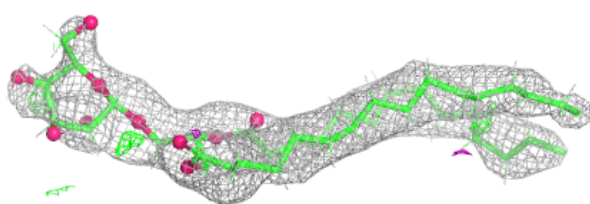
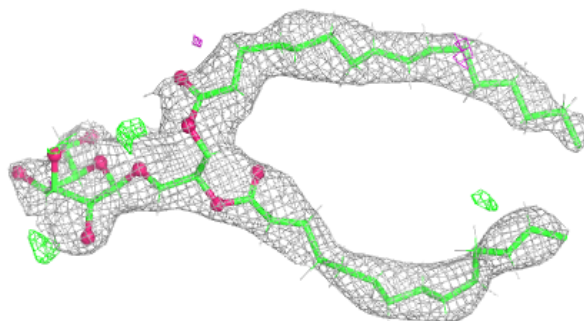
Electron density around CLA H 101:

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

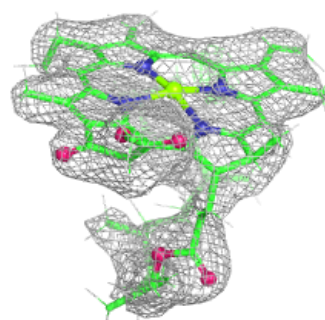
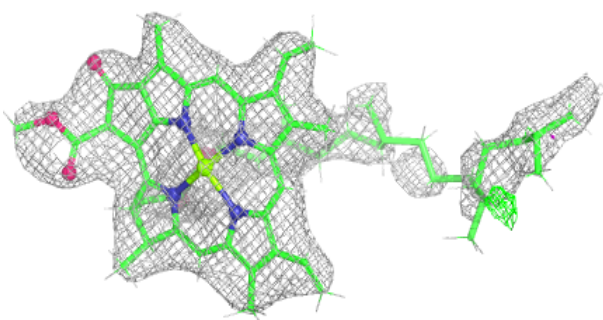
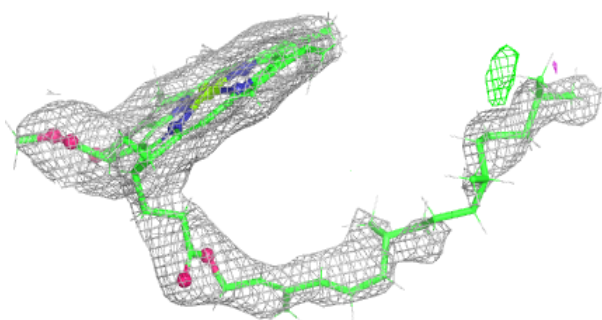


Electron density around LMG c 523:

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

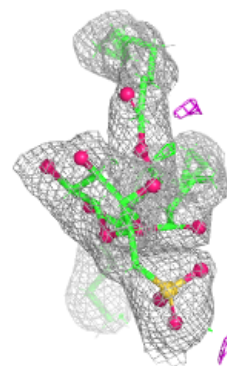
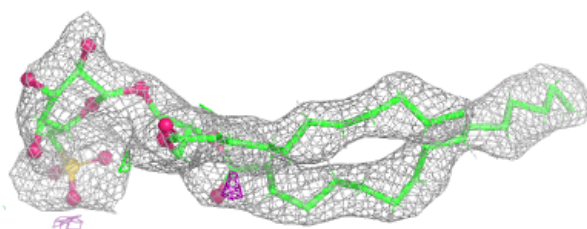
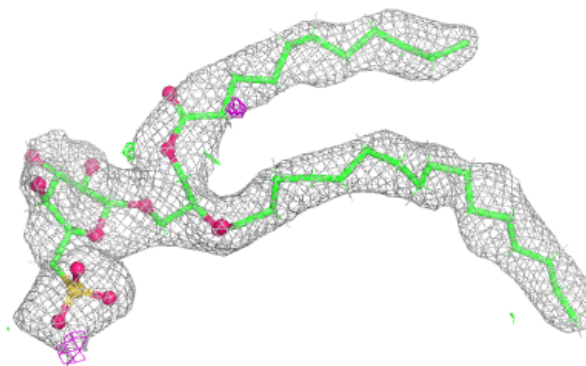
**Electron density around CLA C 513:**

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

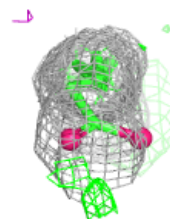
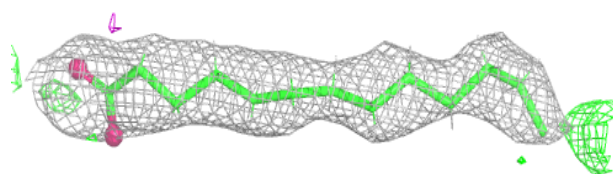
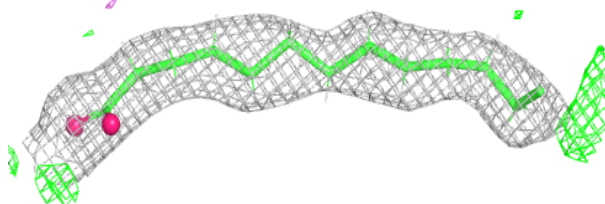


Electron density around SQD L 101:

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

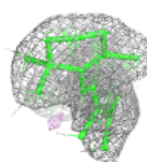
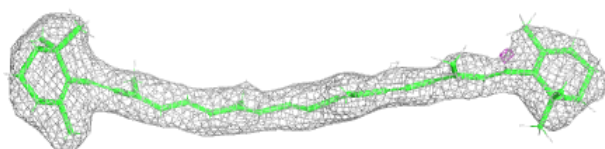
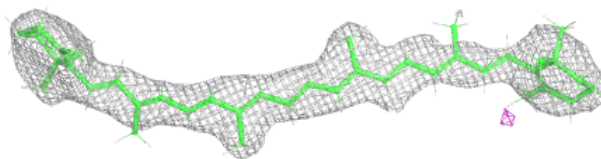
**Electron density around STE M 102:**

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

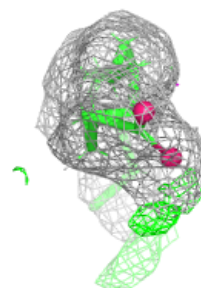
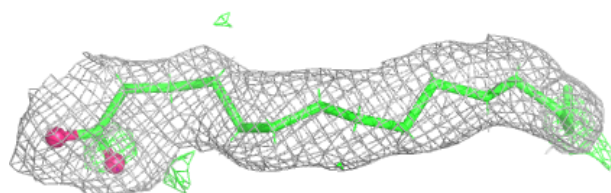
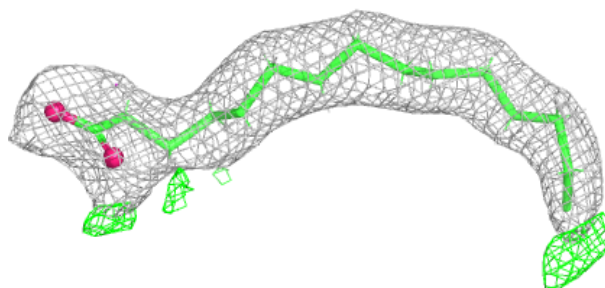


Electron density around BCR h 101:

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

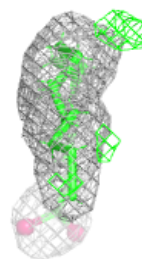
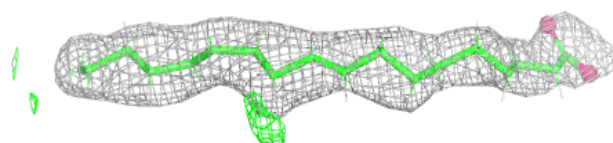
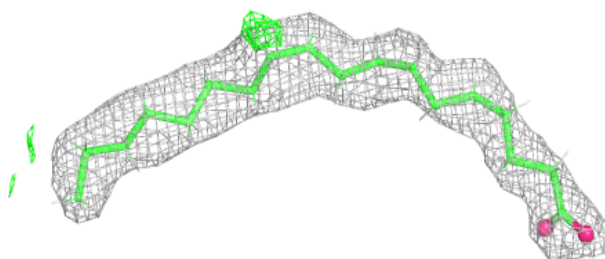
**Electron density around STE B 620:**

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

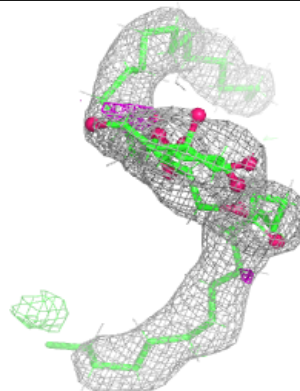
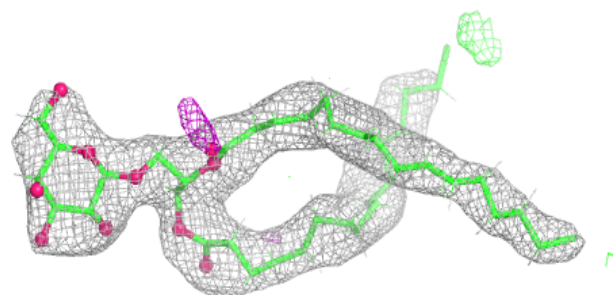
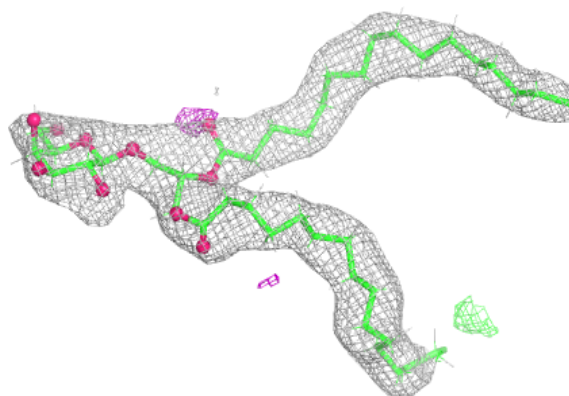


Electron density around STE D 413:

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

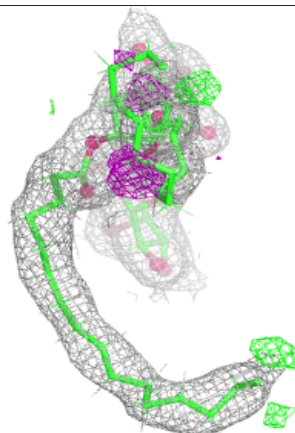
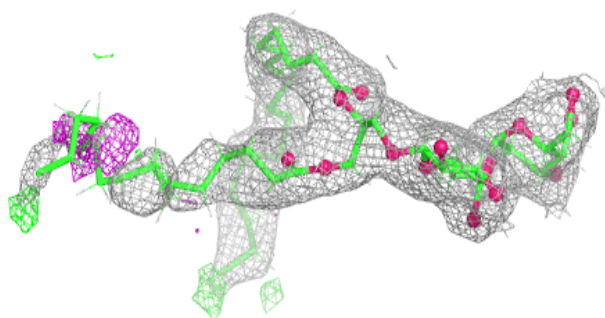
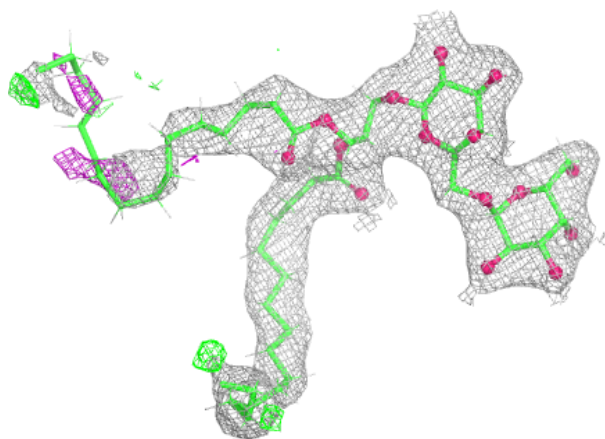
**Electron density around LMG M 101:**

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

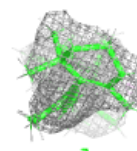
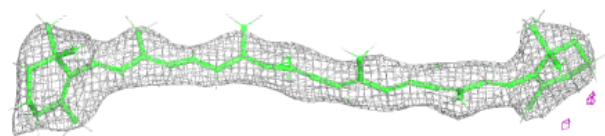


Electron density around DGD C 518:

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

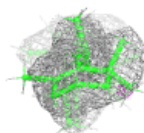
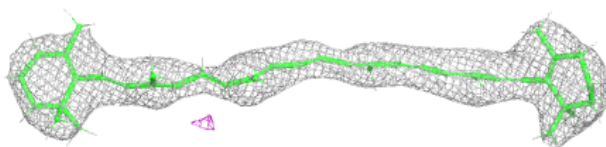
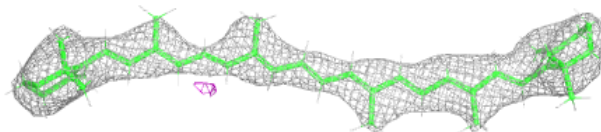
**Electron density around BCR K 101:**

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

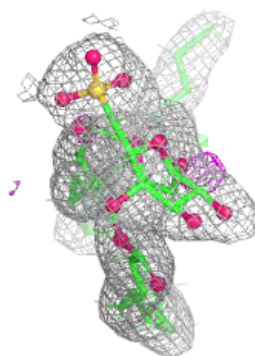
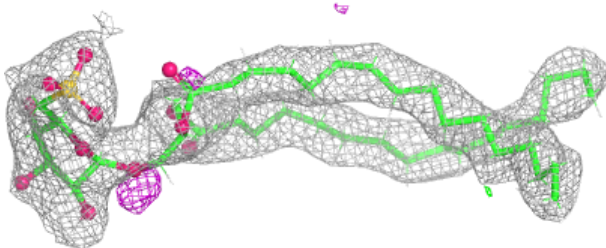
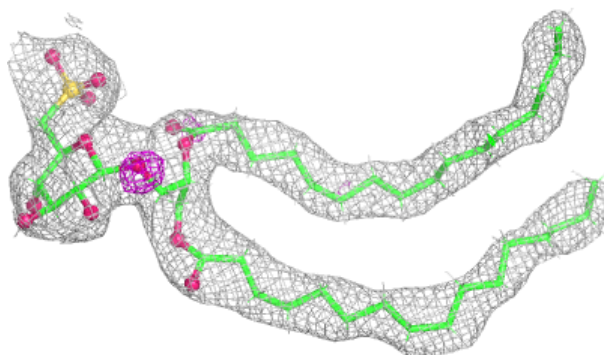


Electron density around BCR c 515:

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

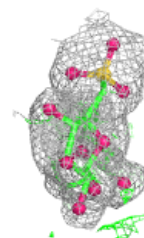
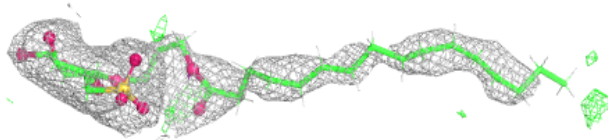
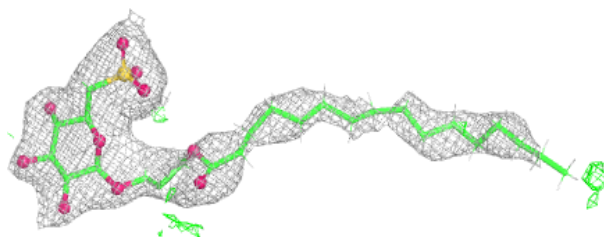
**Electron density around SQD B 621:**

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

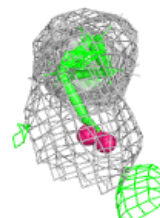
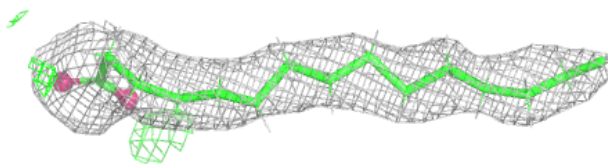
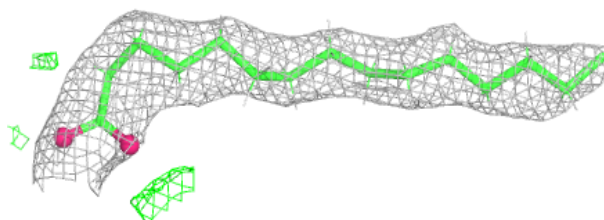


Electron density around SQD F 102:

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

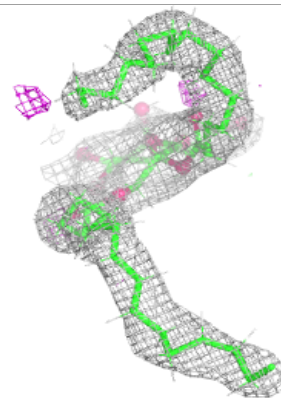
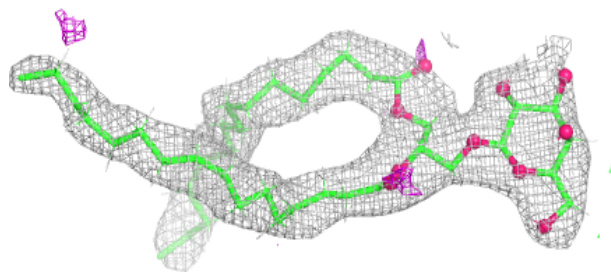
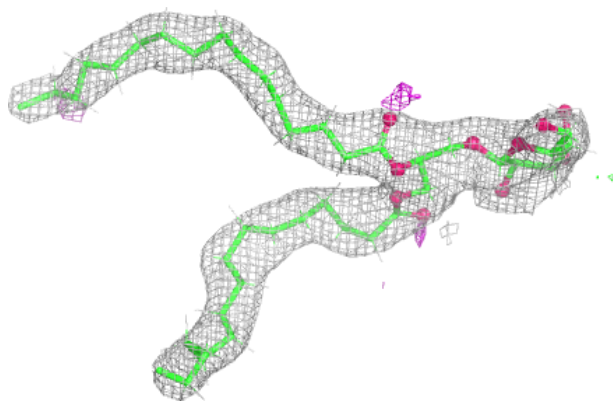
**Electron density around STE d 410:**

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

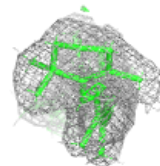
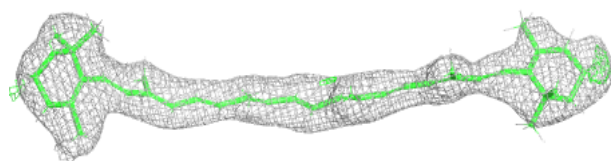
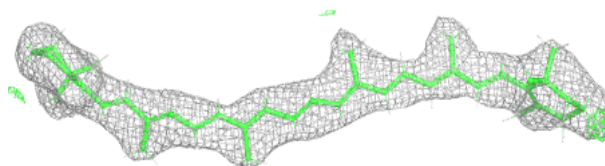


Electron density around LMG m 101:

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

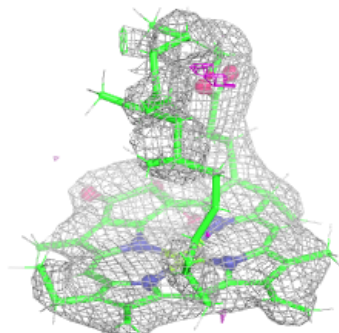
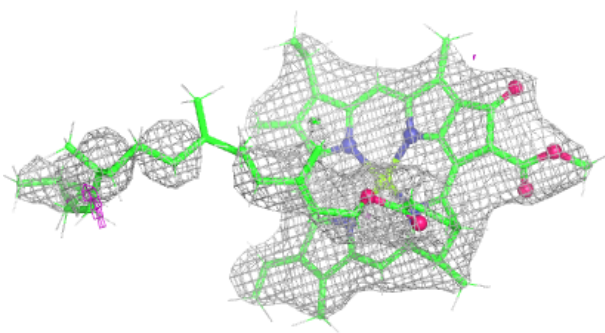
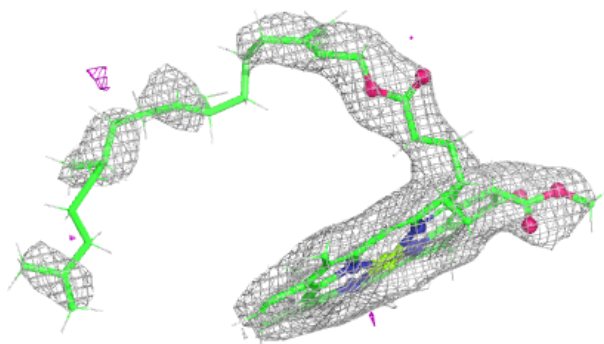
**Electron density around BCR X 101:**

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

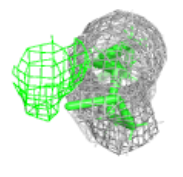
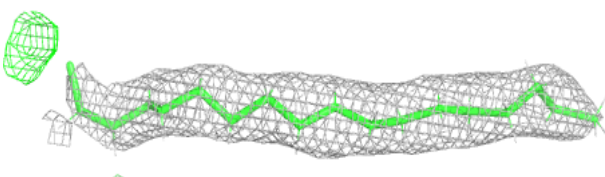
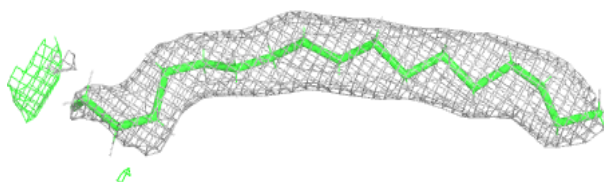


Electron density around CLA c 514:

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

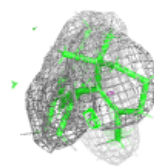
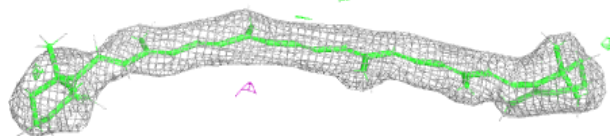
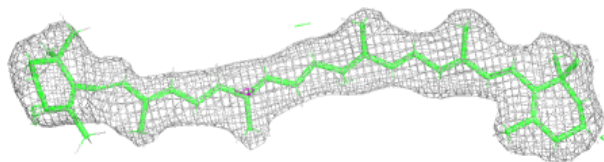
**Electron density around STE M 104:**

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

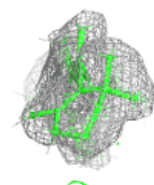
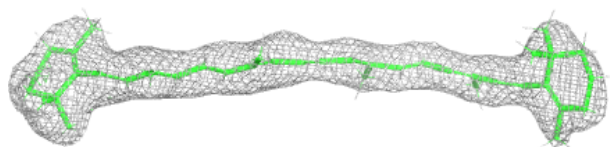


Electron density around BCR d 404:

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

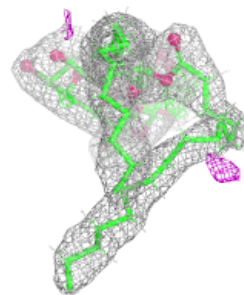
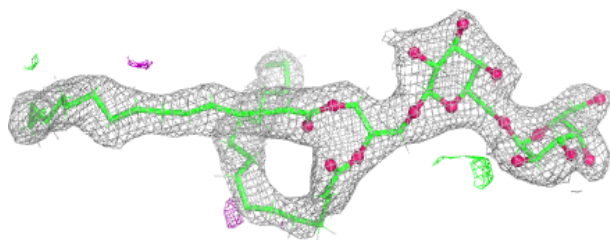
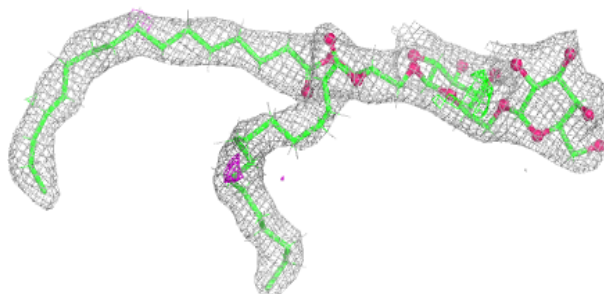
**Electron density around BCR K 102:**

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

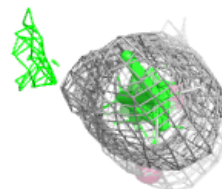
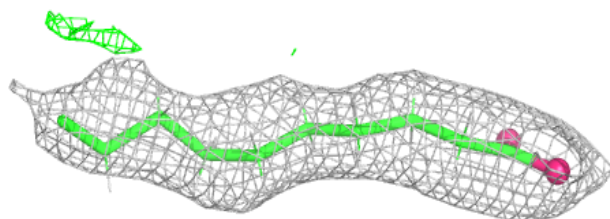
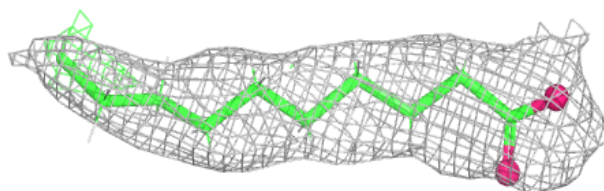


Electron density around DGD h 102:

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

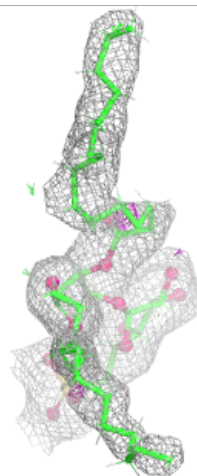
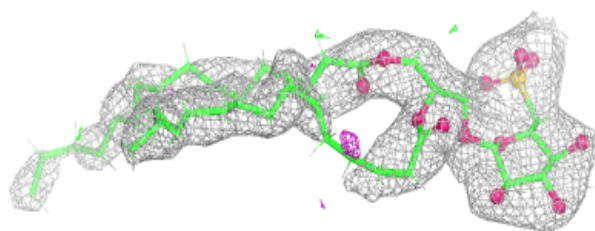
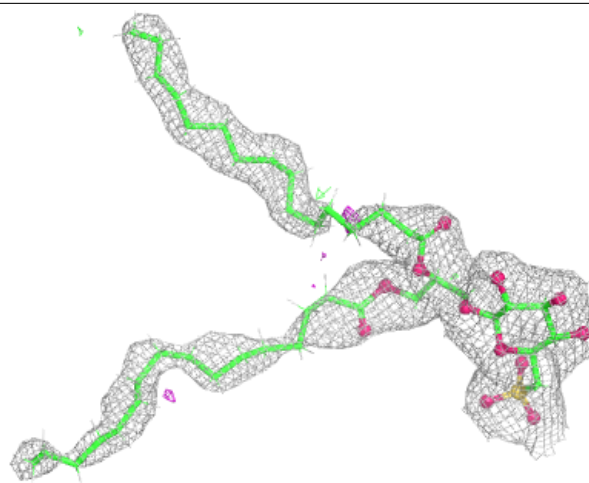
**Electron density around STE J 101:**

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



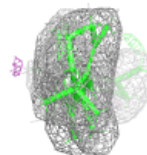
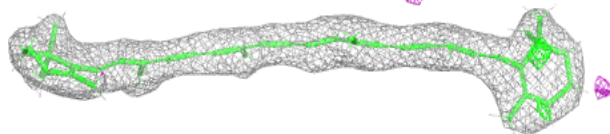
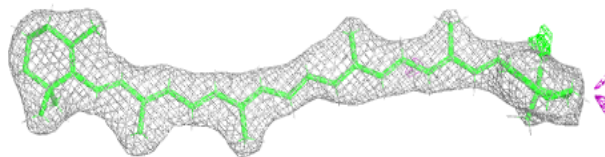
Electron density around SQD a 413:

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

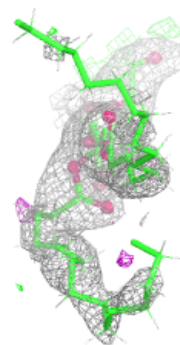
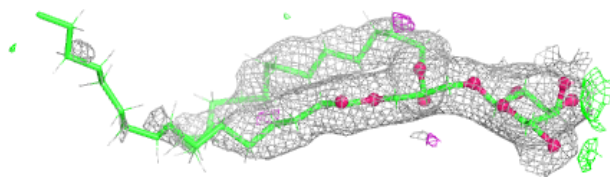
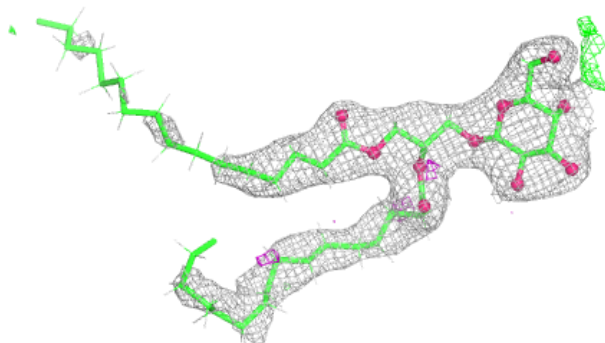


Electron density around BCR b 617:

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

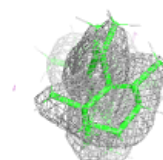
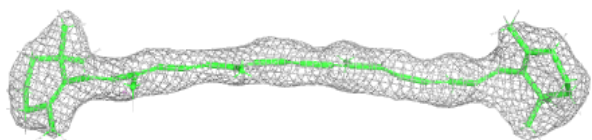
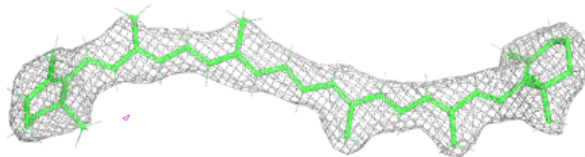
**Electron density around LMG D 408:**

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

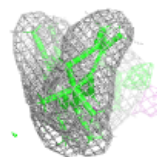
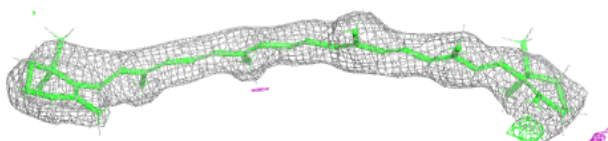


Electron density around BCR k 101:

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

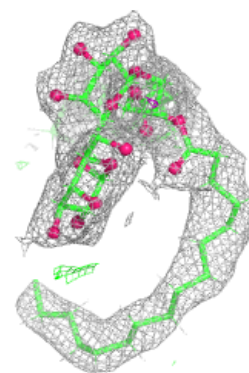
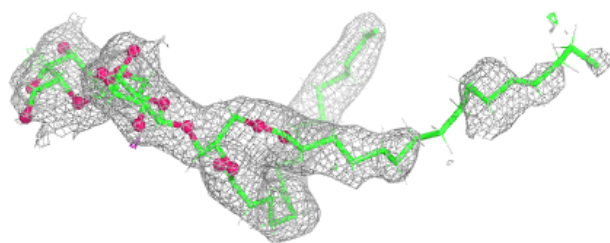
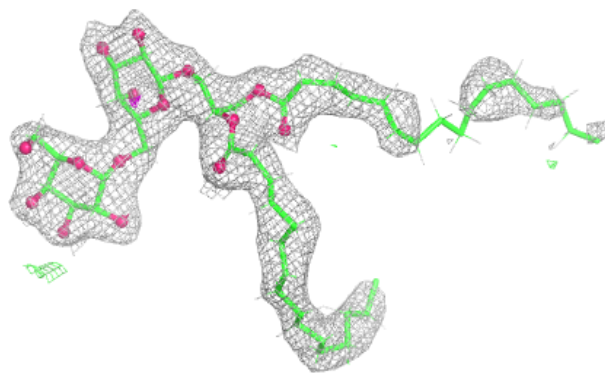
**Electron density around BCR D 406:**

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

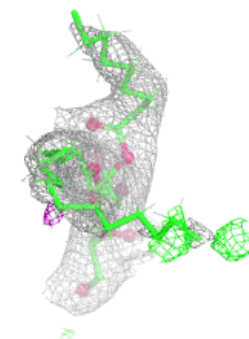
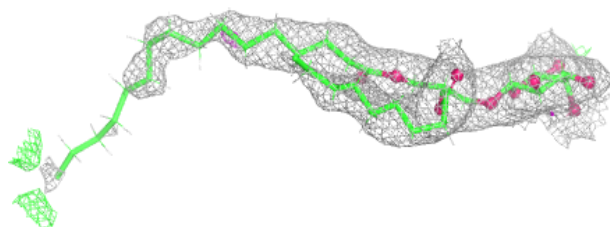
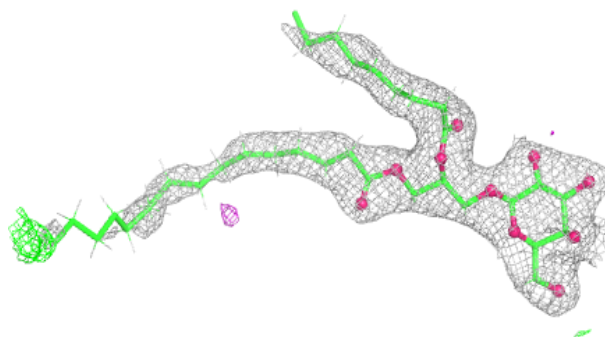


Electron density around DGD c 518:

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

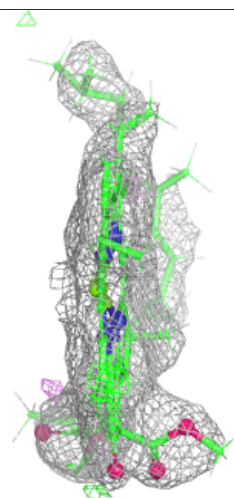
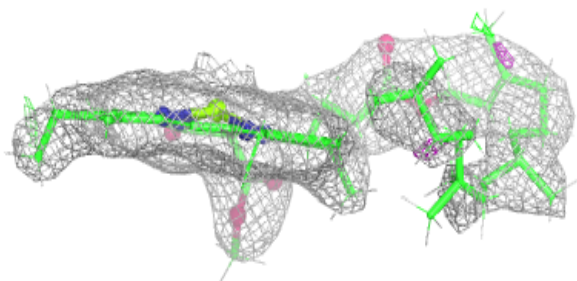
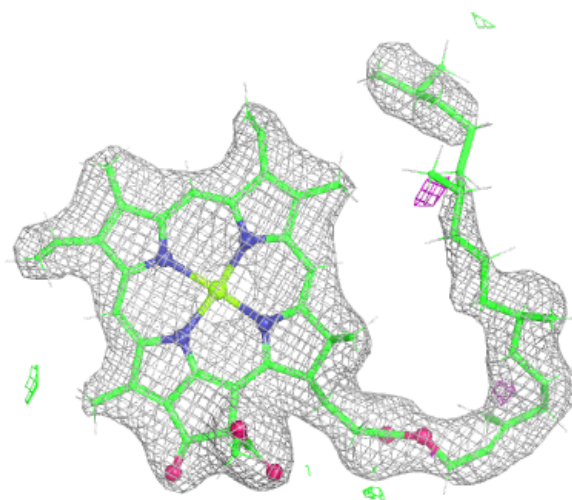
**Electron density around LMG d 408:**

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



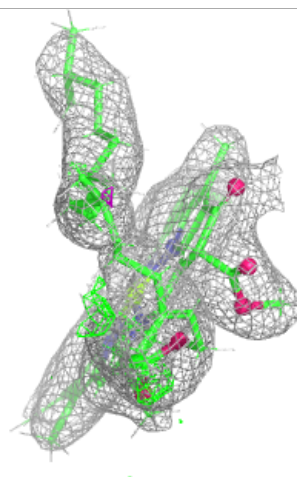
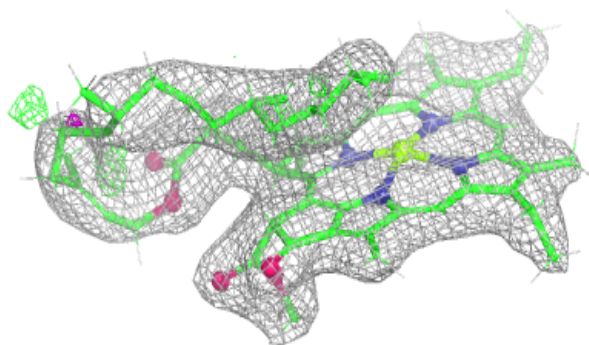
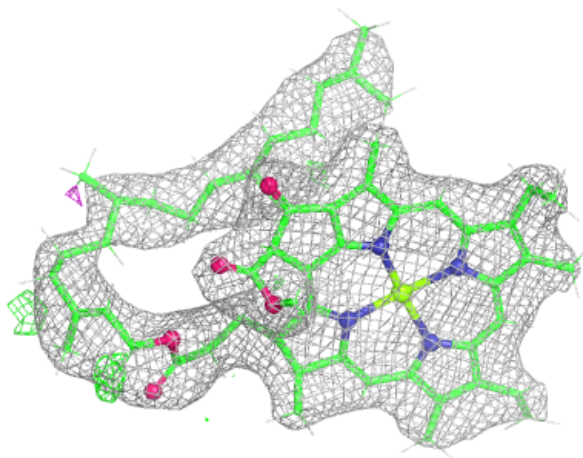
Electron density around CLA c 513:

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



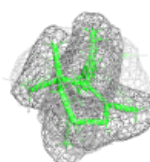
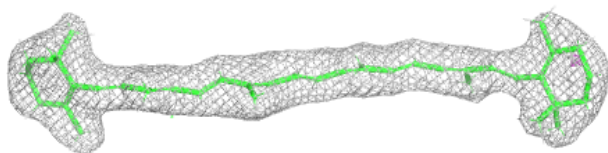
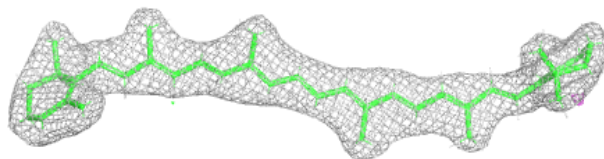
Electron density around CLA c 510:

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

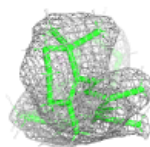
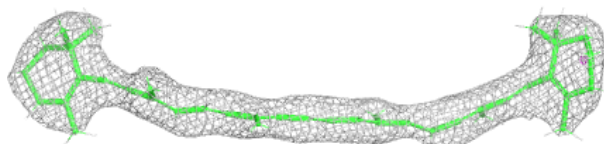


Electron density around BCR A 405:

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

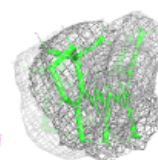
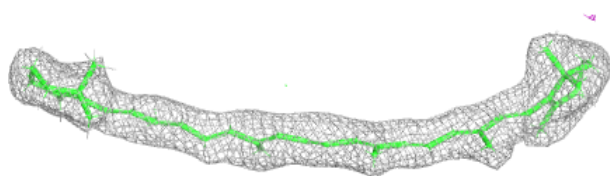
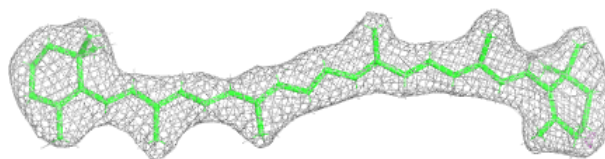
**Electron density around BCR k 102:**

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

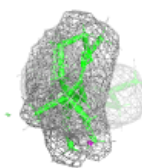
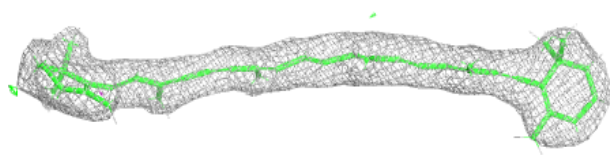
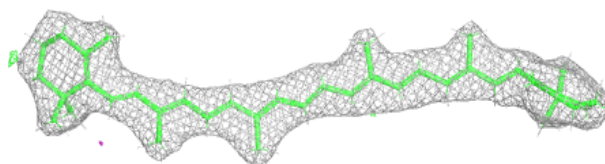


Electron density around BCR t 101:

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

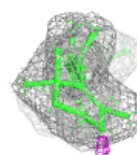
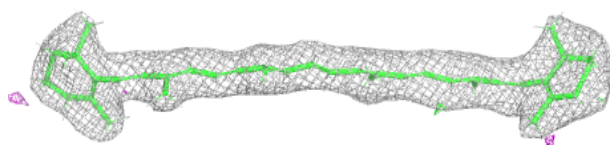
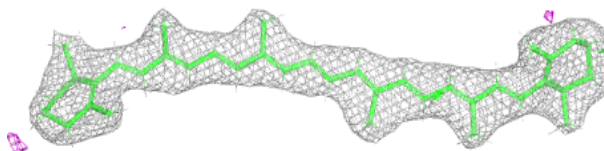
**Electron density around BCR B 617:**

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

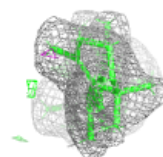
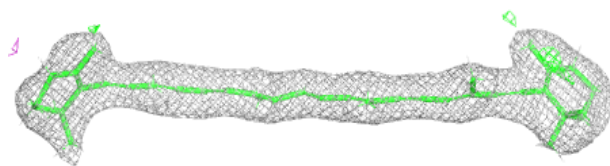
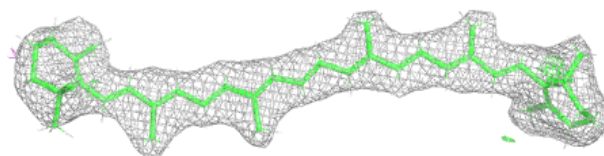


Electron density around BCR B 618:

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

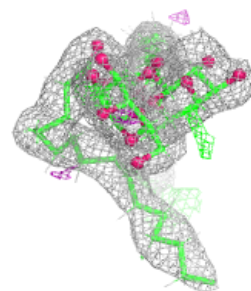
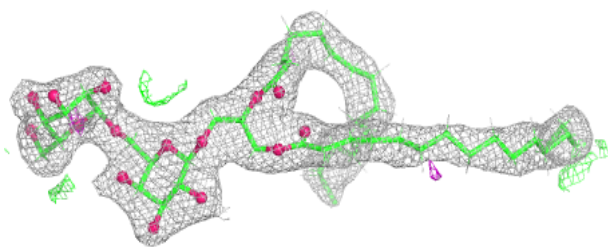
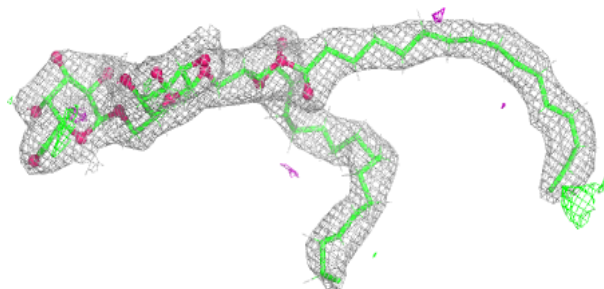
**Electron density around BCR b 618:**

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

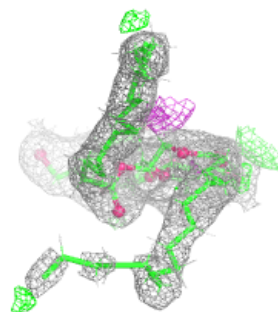
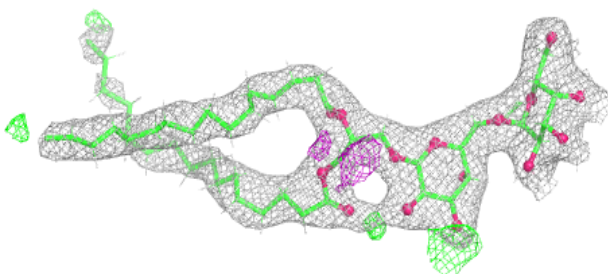
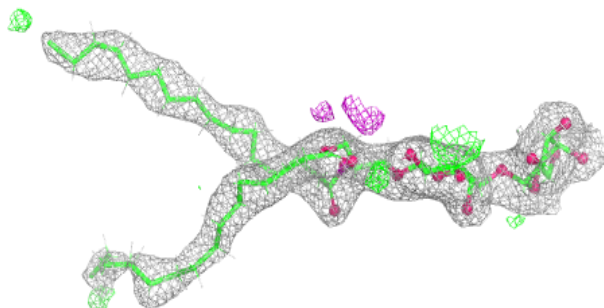


Electron density around DGD H 102:

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

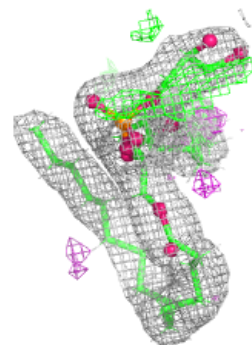
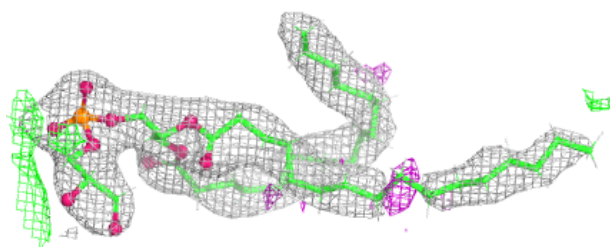
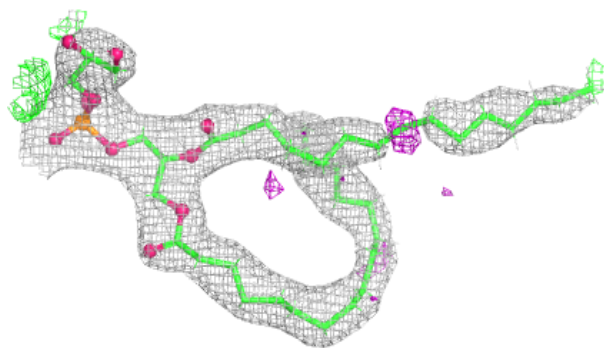
**Electron density around DGD c 517:**

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

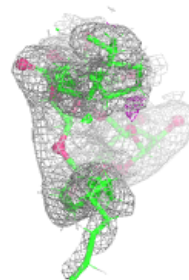
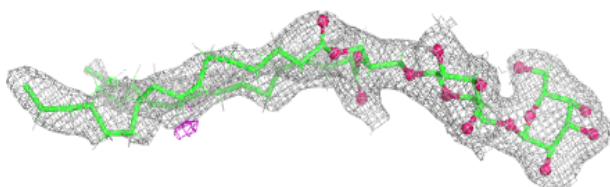
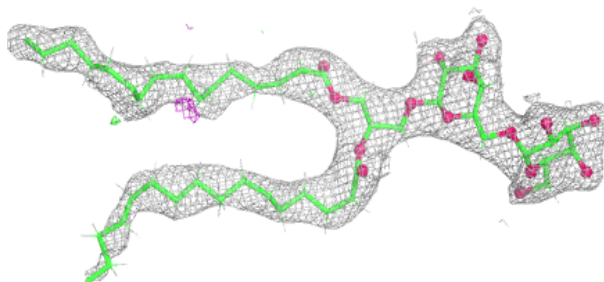


Electron density around LHG a 412:

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

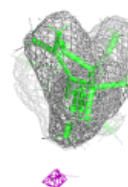
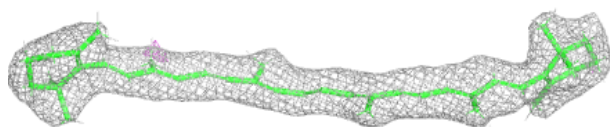
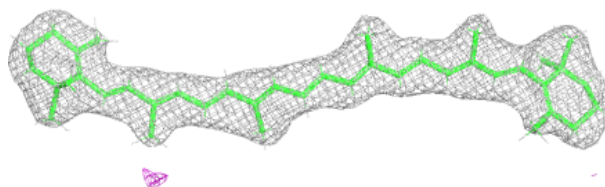
**Electron density around DGD c 519:**

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

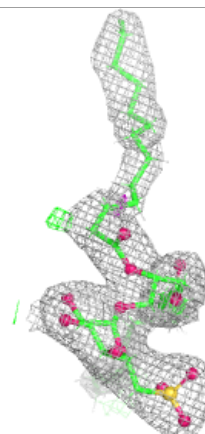
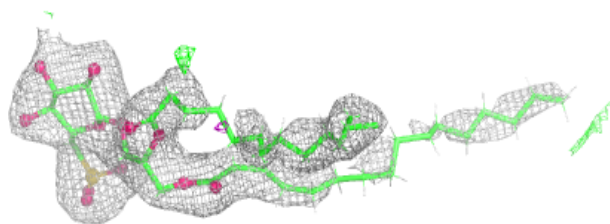
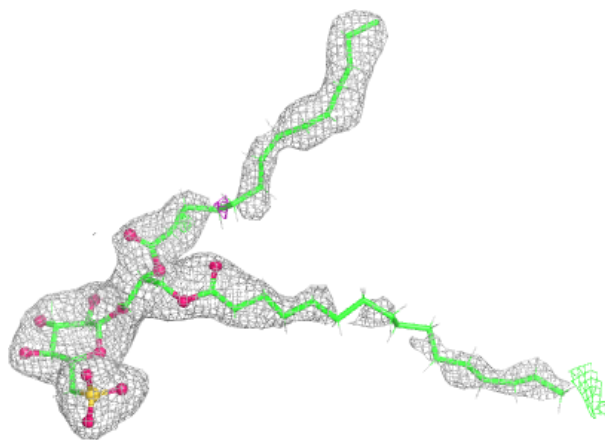


Electron density around BCR b 619:

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

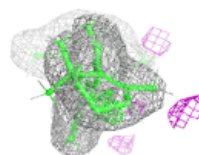
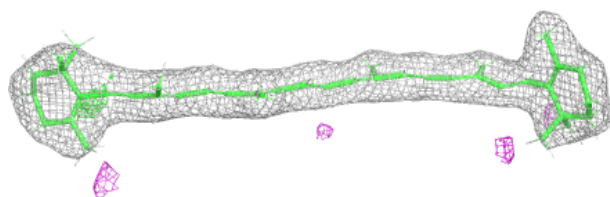
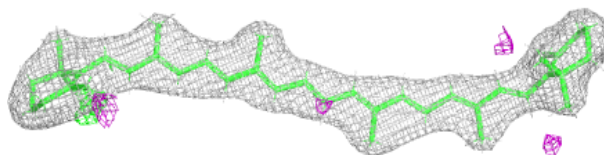
**Electron density around SQD A 411:**

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



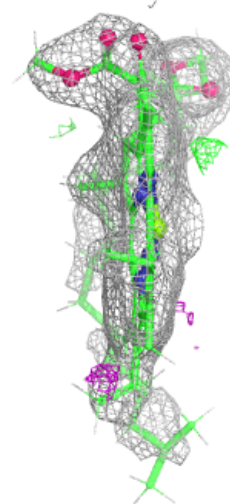
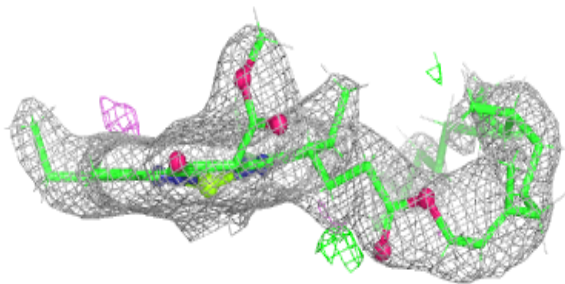
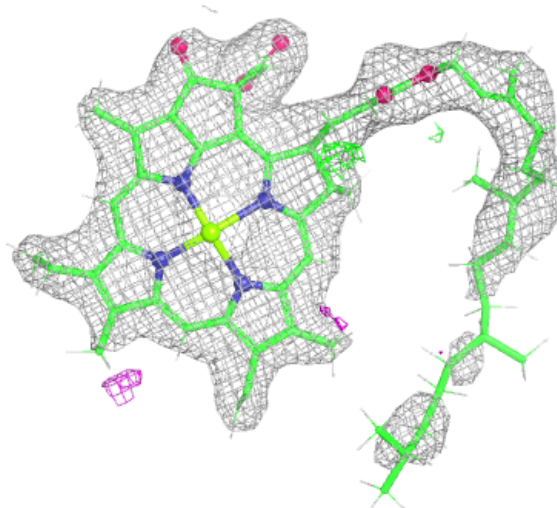
Electron density around BCR C 514:

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



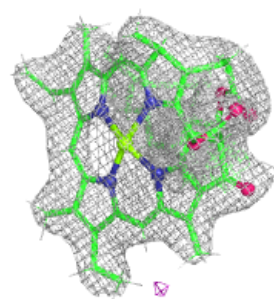
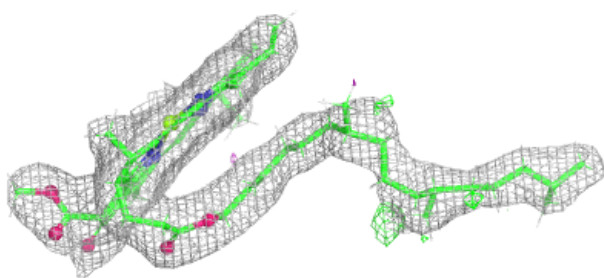
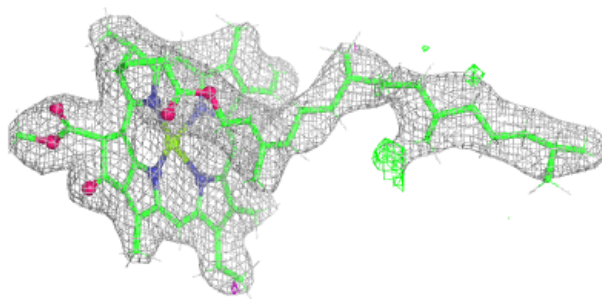
Electron density around CLA C 512:

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

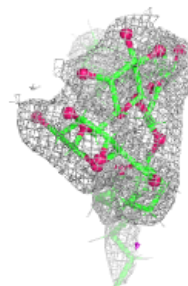
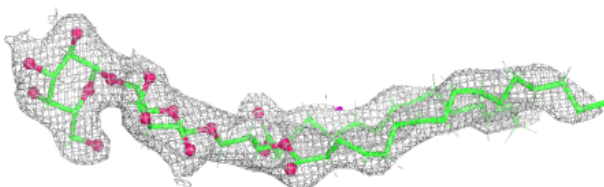
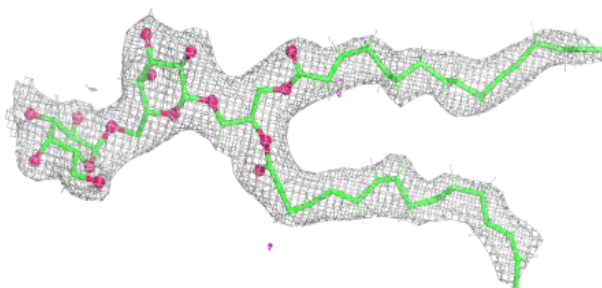


Electron density around CLA c 506:

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

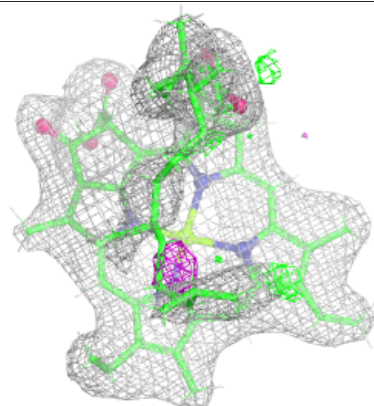
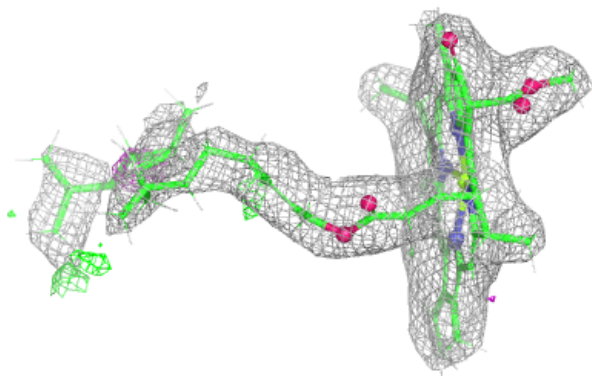
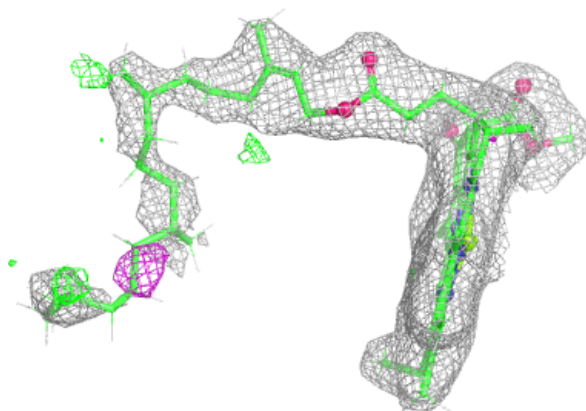
**Electron density around DGD C 519:**

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

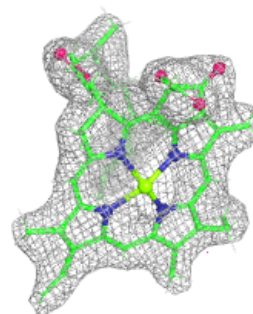
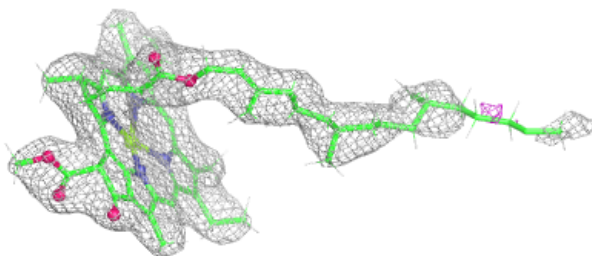
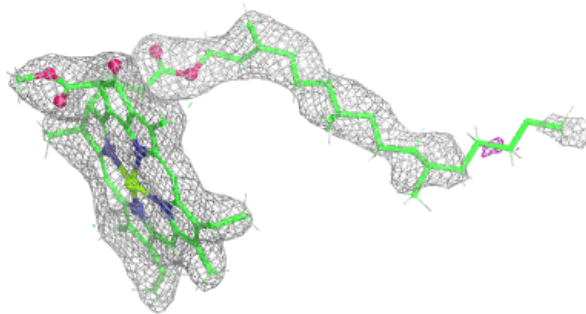


Electron density around CLA c 507:

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

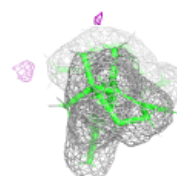
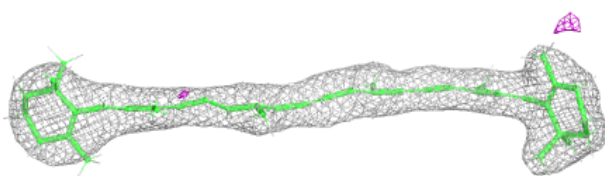
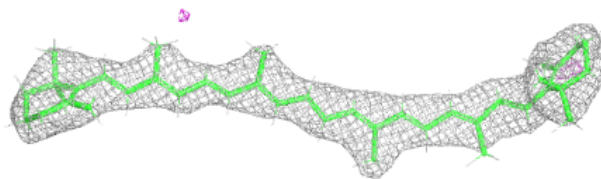
**Electron density around CLA c 509:**

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



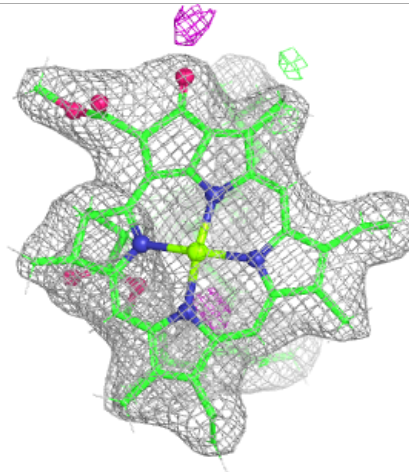
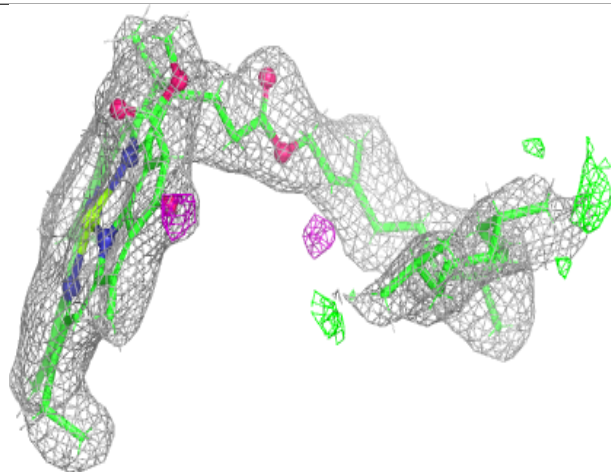
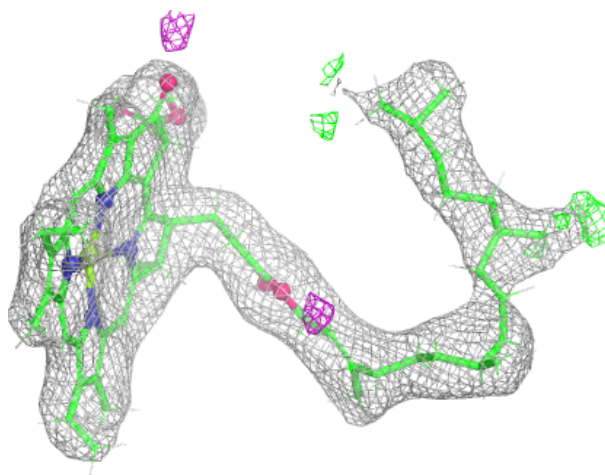
Electron density around BCR c 516:

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



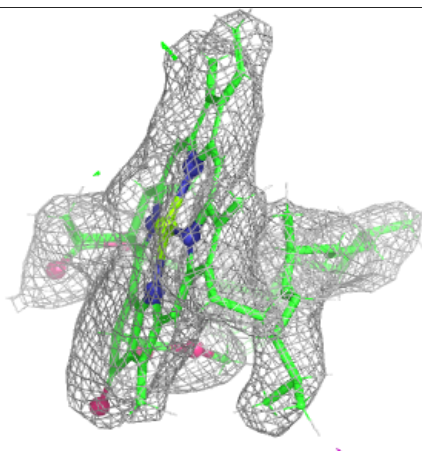
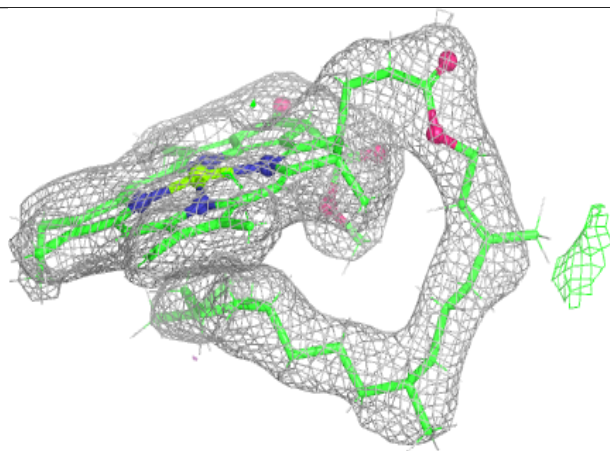
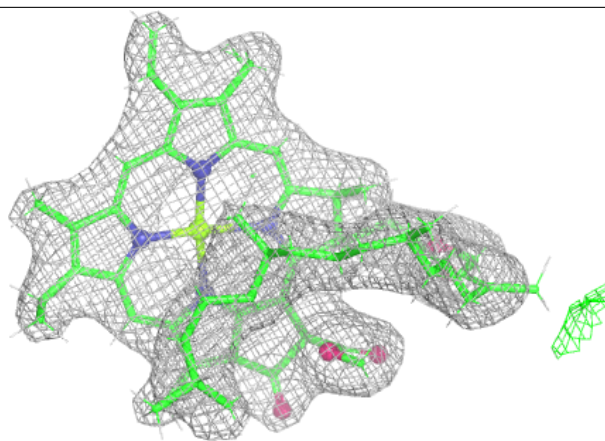
Electron density around CLA B 606:

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



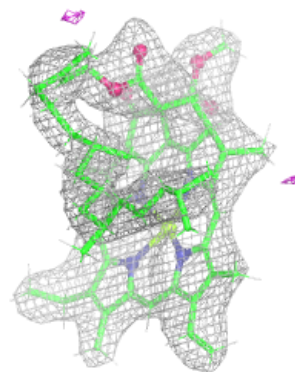
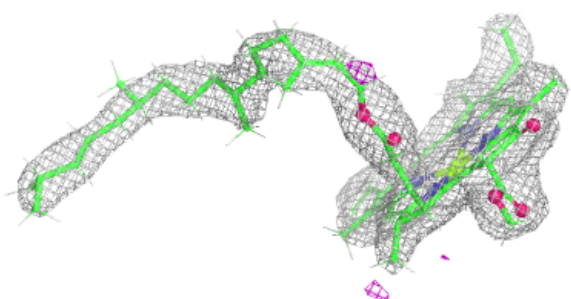
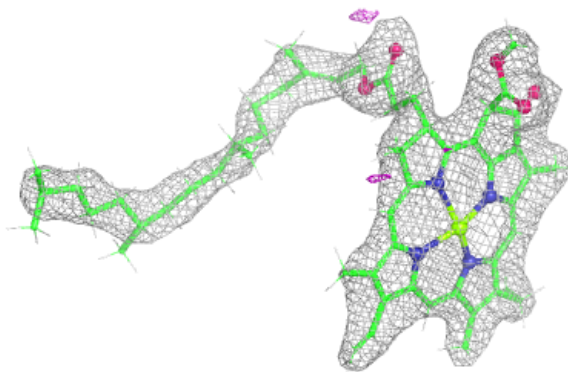
Electron density around CLA c 511:

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



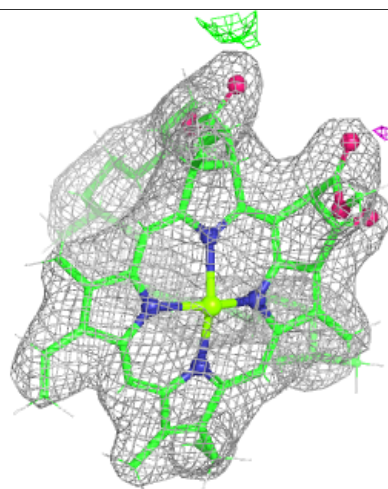
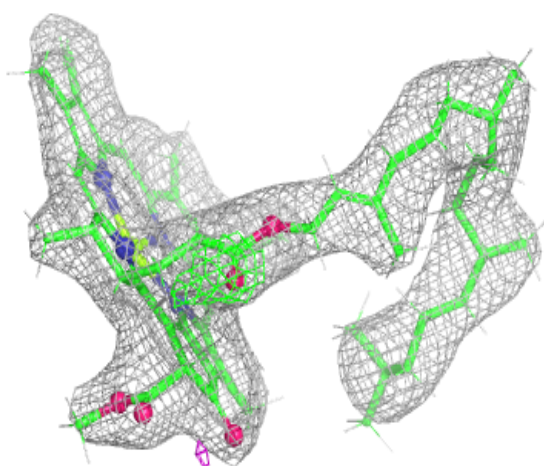
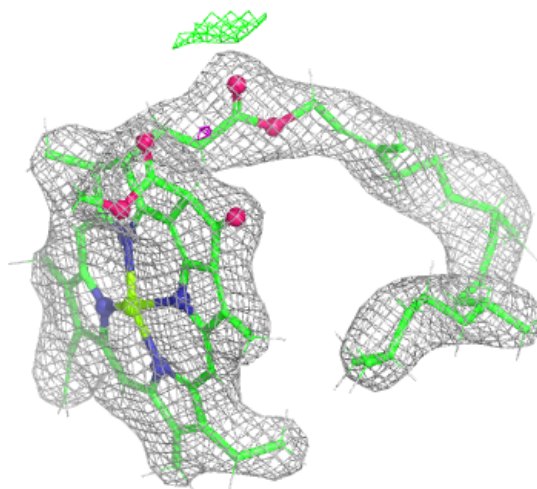
Electron density around CLA c 512:

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



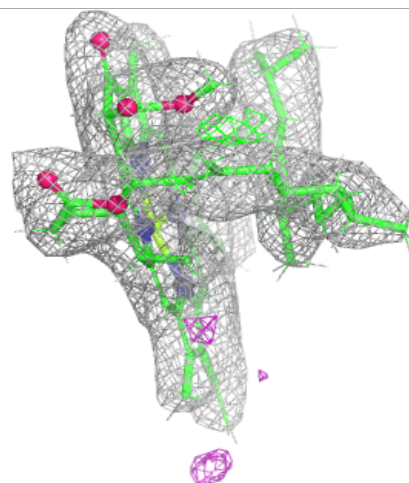
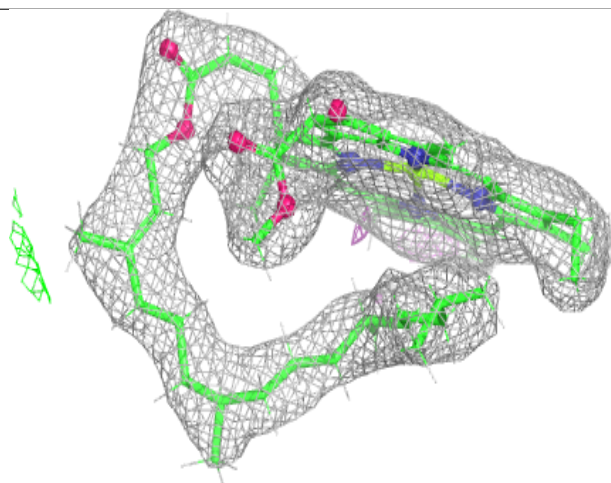
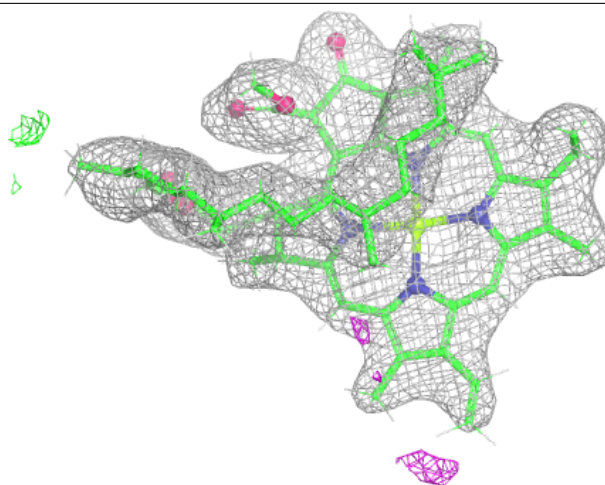
Electron density around CLA C 503:

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



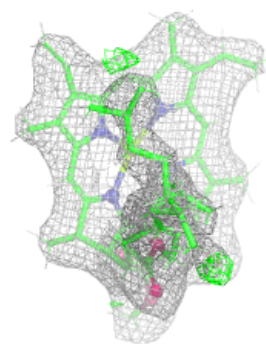
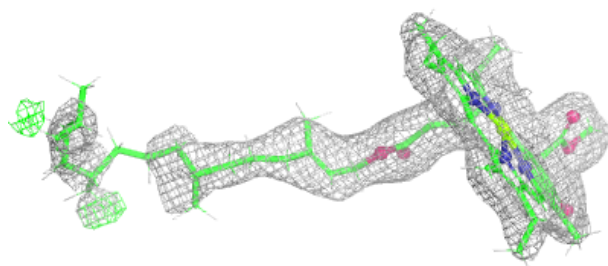
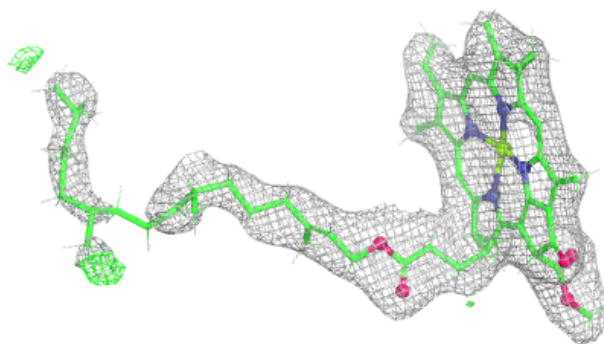
Electron density around CLA C 510:

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

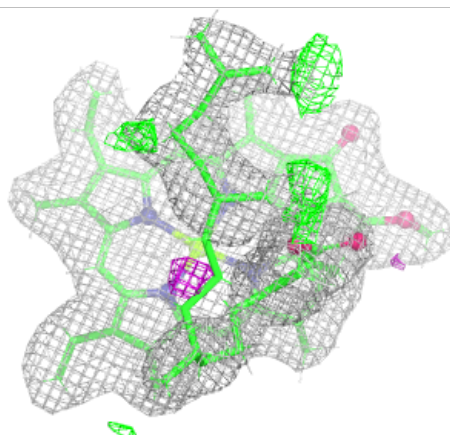
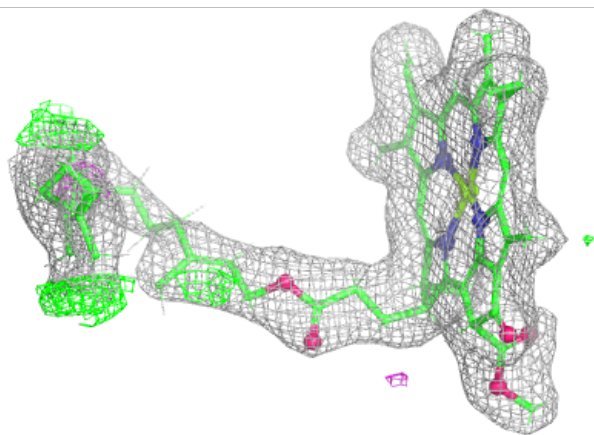
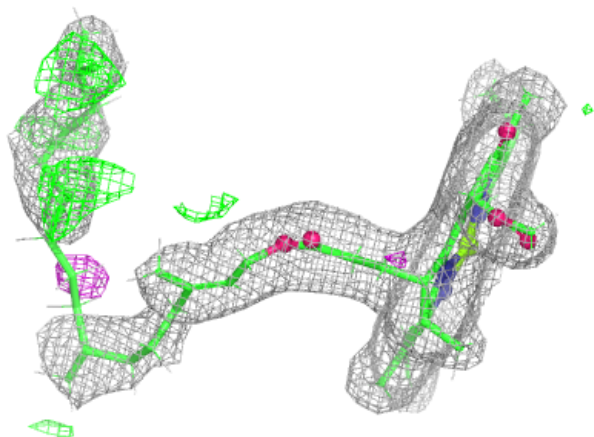


Electron density around CLA d 403:

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

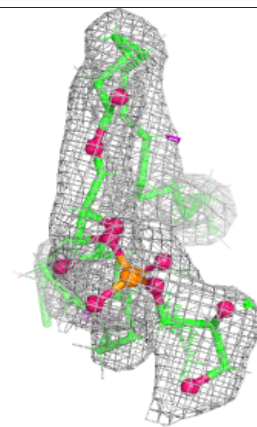
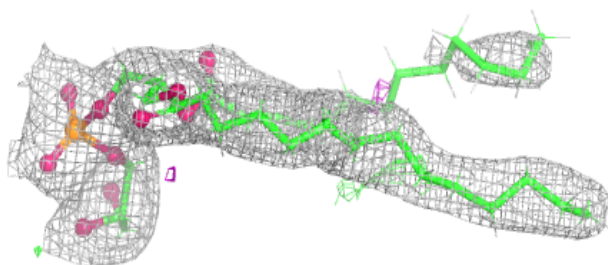
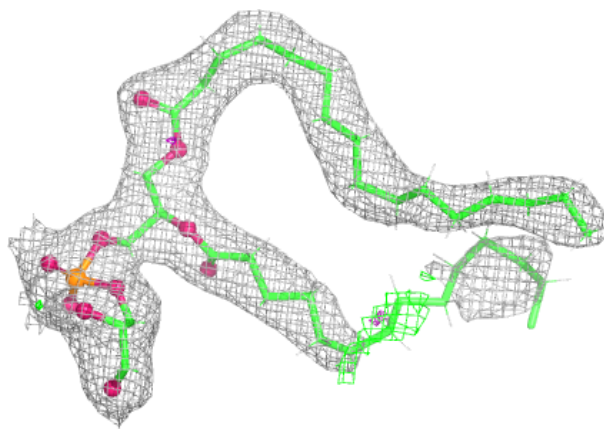
**Electron density around CLA a 405:**

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

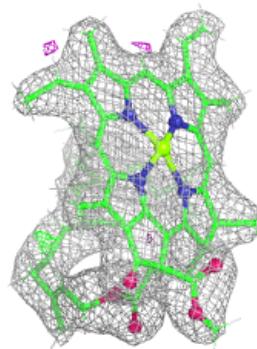
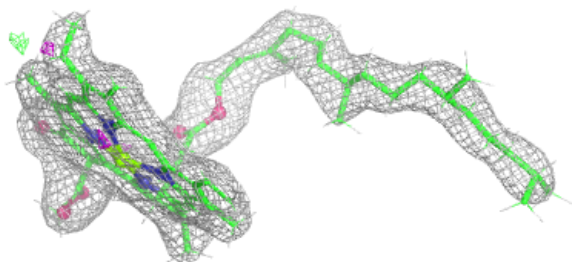
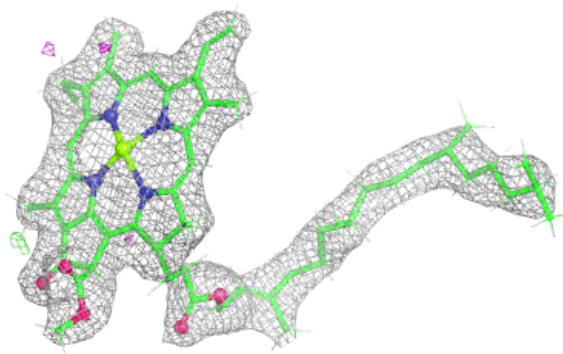


Electron density around LHG A 410:

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

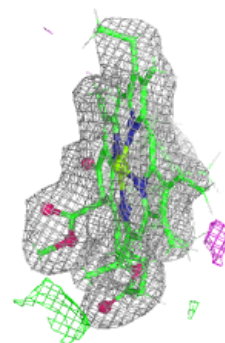
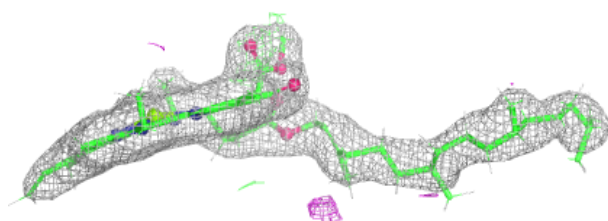
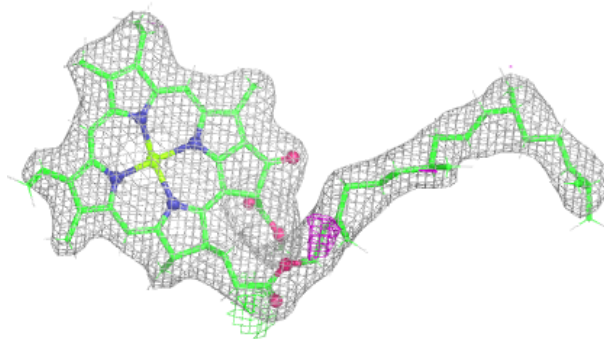
**Electron density around CLA C 511:**

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

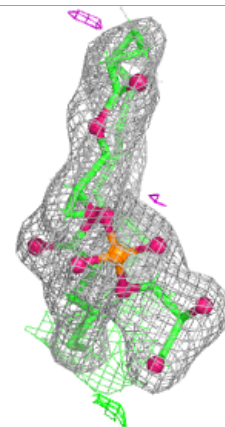
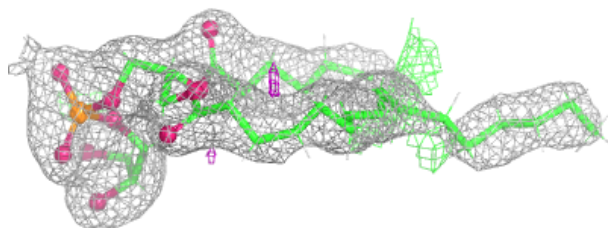
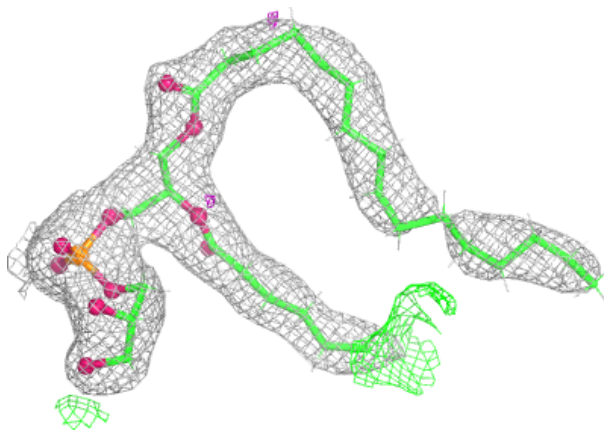


Electron density around CLA b 602:

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

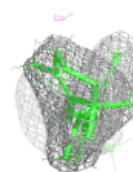
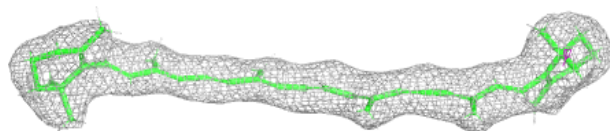
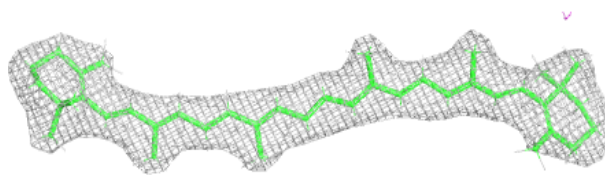
**Electron density around LHG d 407:**

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



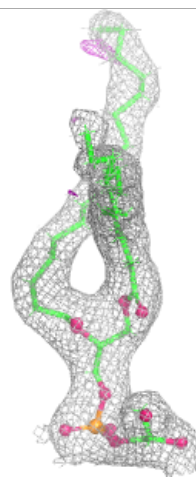
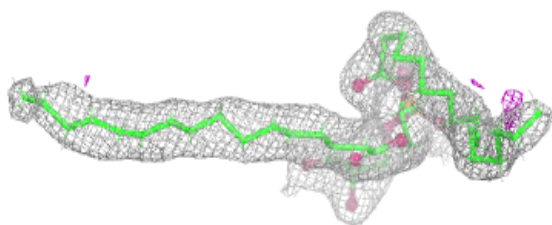
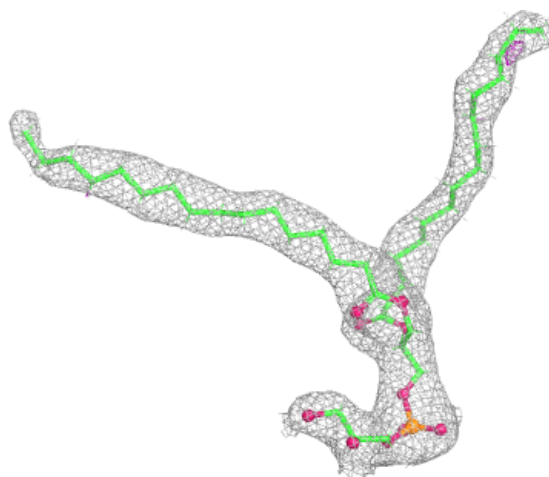
Electron density around BCR B 619:

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



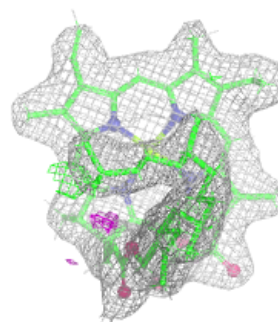
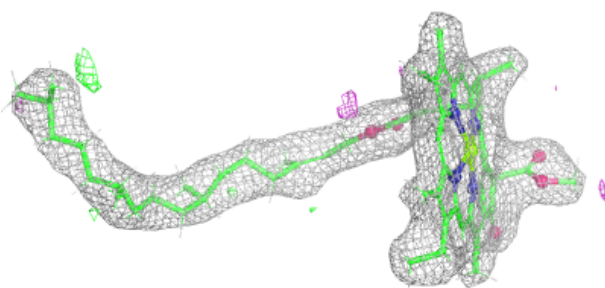
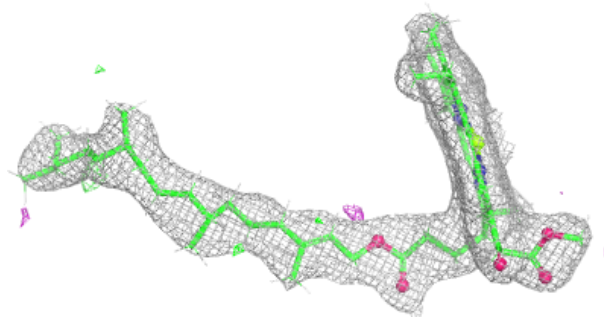
Electron density around LHG 1 101:

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

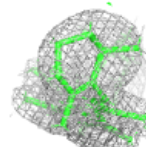
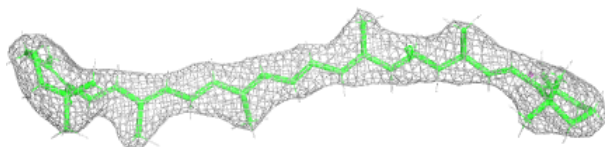
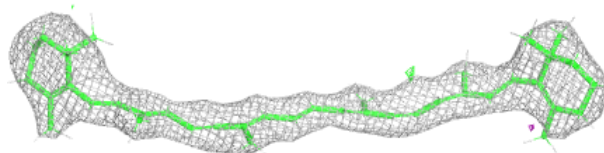


Electron density around CLA b 605:

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

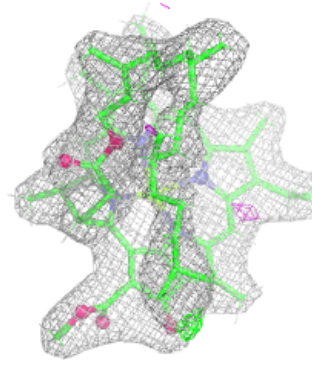
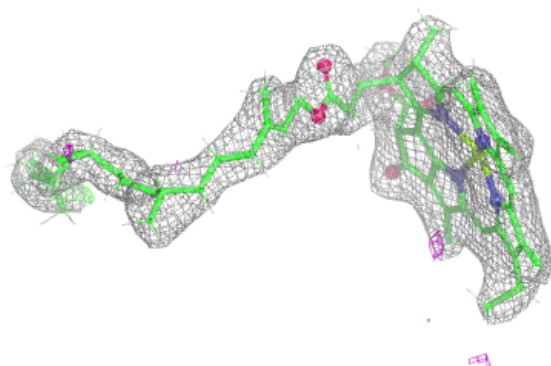
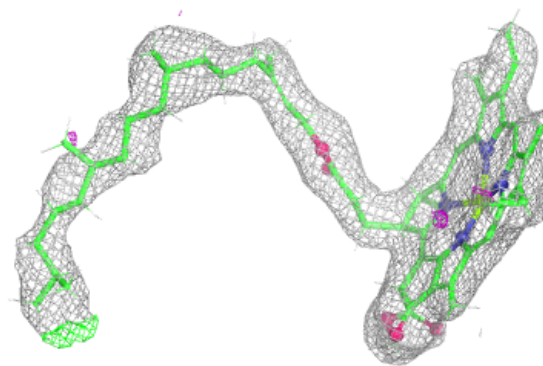
**Electron density around BCR C 515:**

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

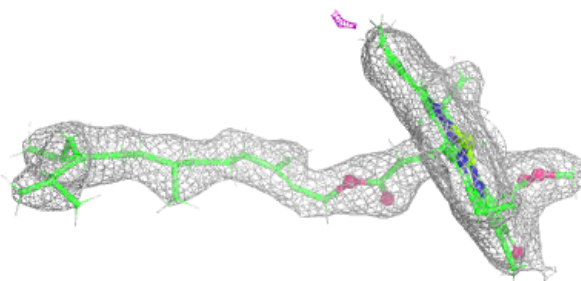
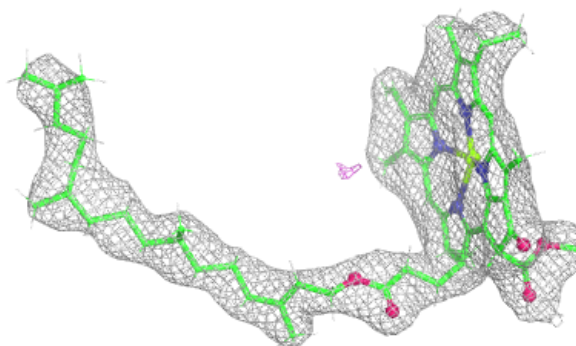


Electron density around CLA b 606:

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

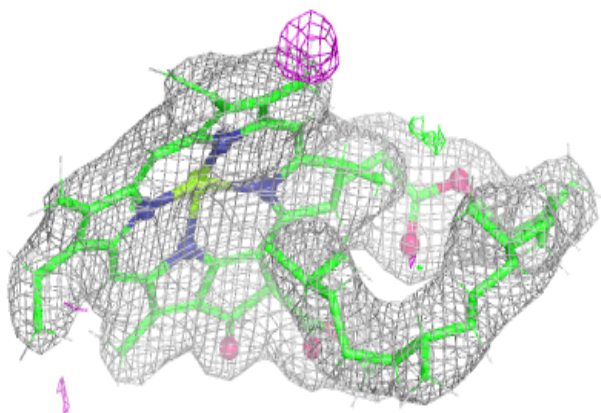
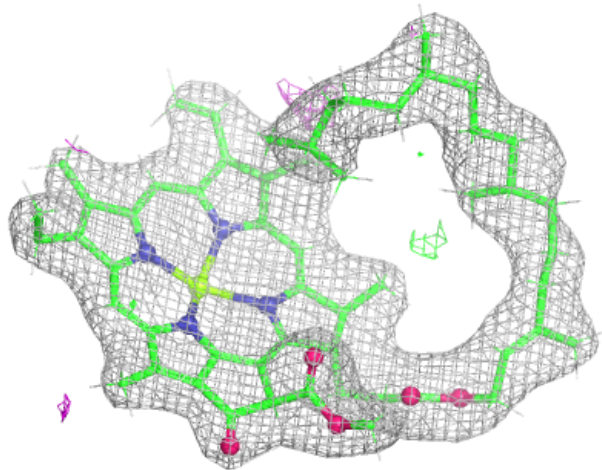
**Electron density around CLA b 609:**

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



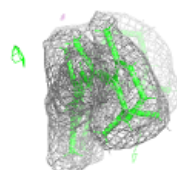
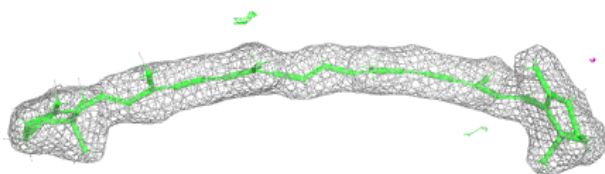
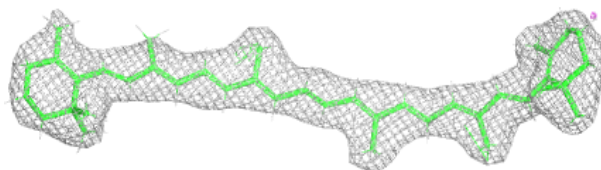
Electron density around CLA b 615:

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



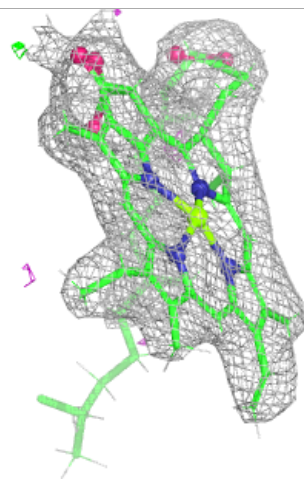
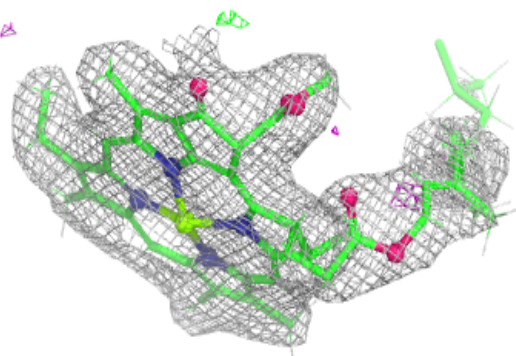
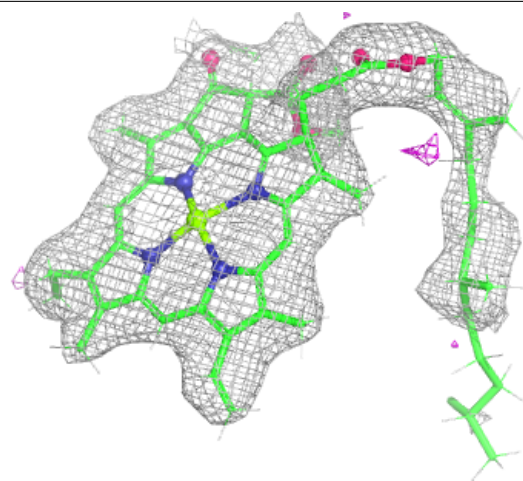
Electron density around BCR T 101:

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



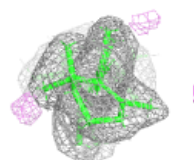
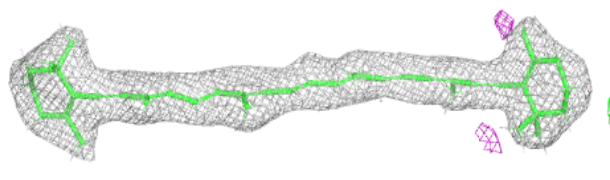
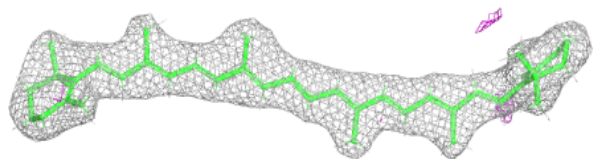
Electron density around CLA b 616:

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



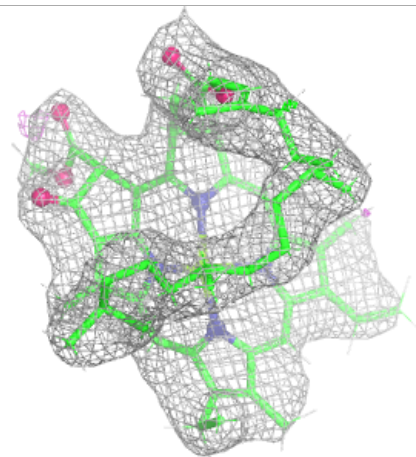
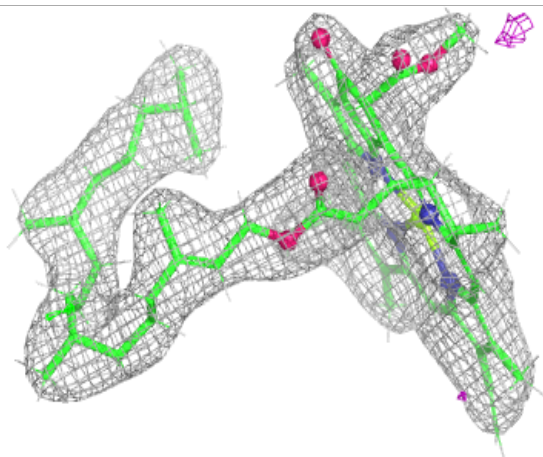
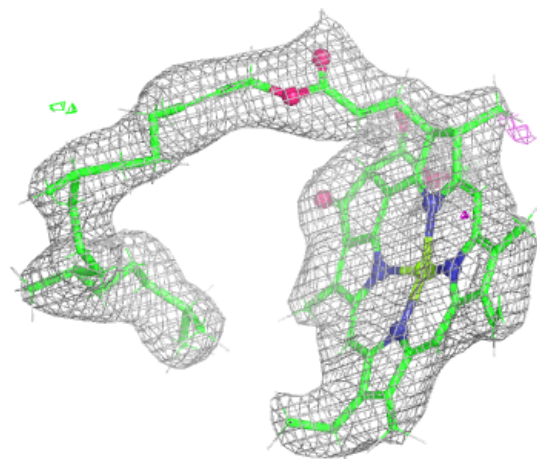
Electron density around BCR a 406:

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



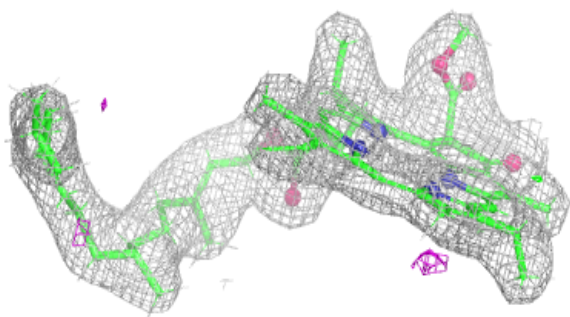
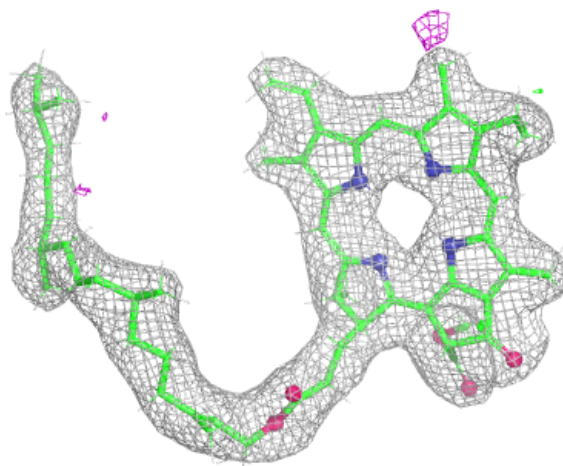
Electron density around CLA c 504:

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



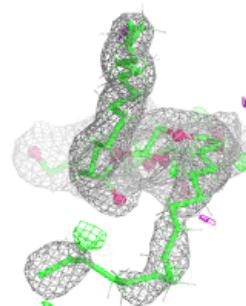
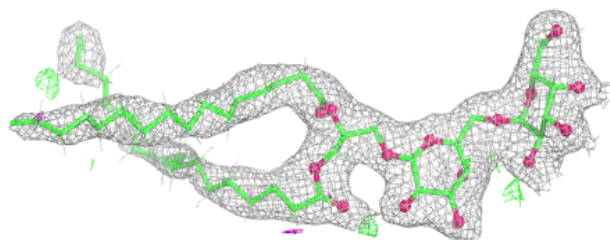
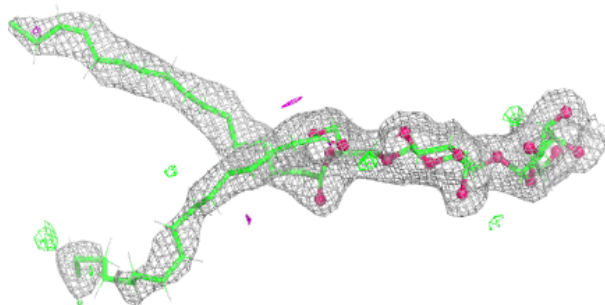
Electron density around PHO d 401:

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

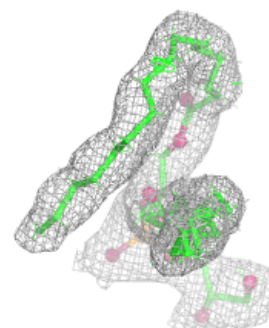
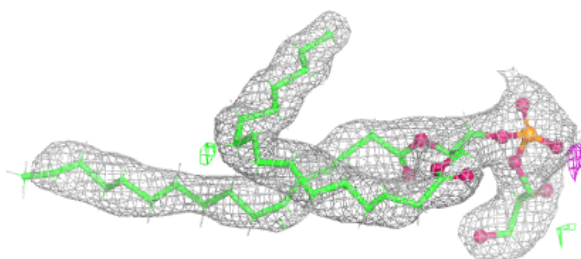
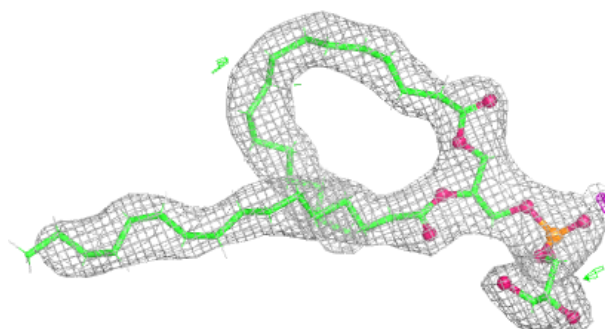


Electron density around DGD C 517:

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

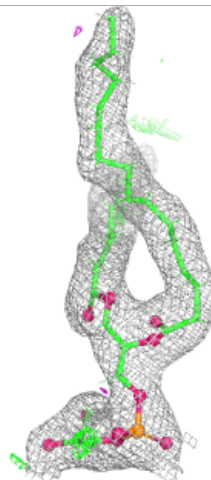
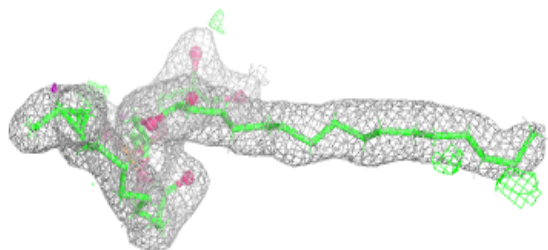
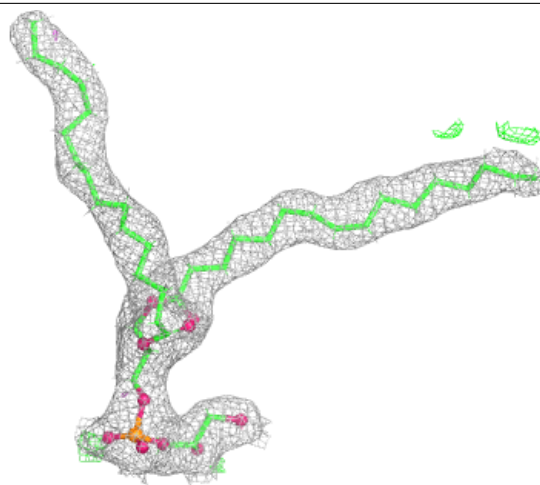
**Electron density around LHG D 412:**

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



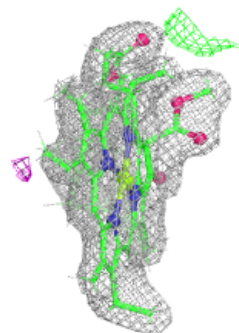
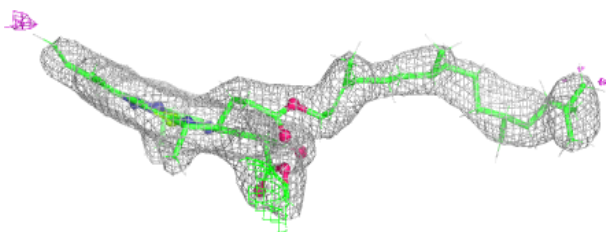
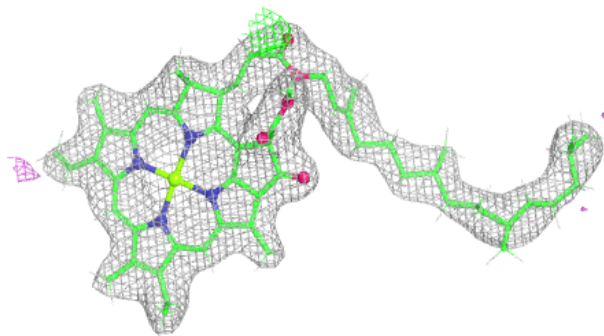
Electron density around LHG L 102:

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

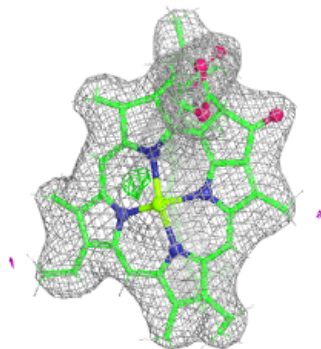
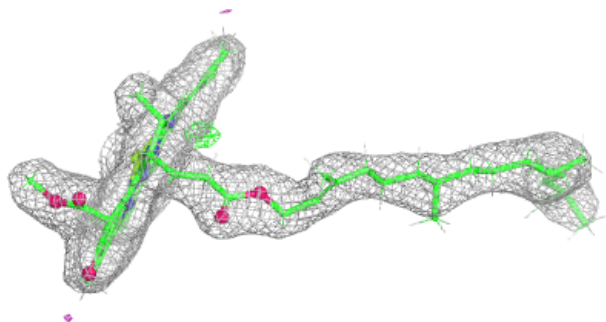
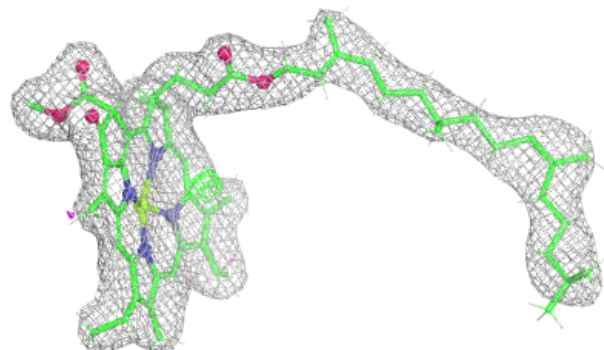


Electron density around CLA B 602:

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

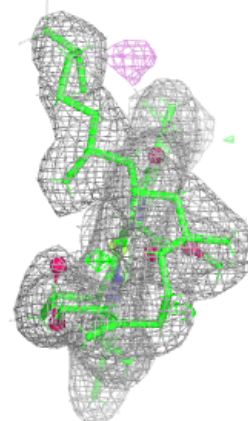
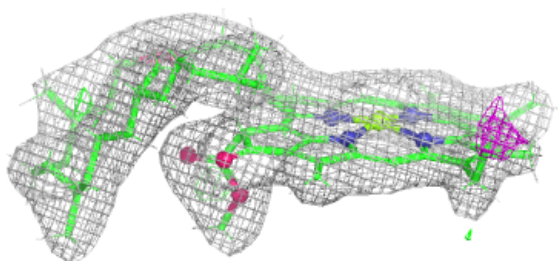
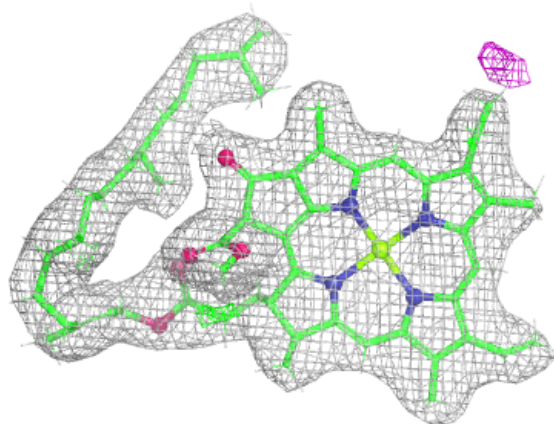
**Electron density around CLA B 609:**

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

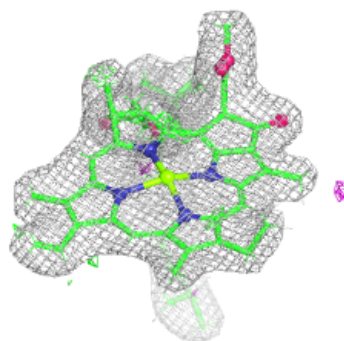
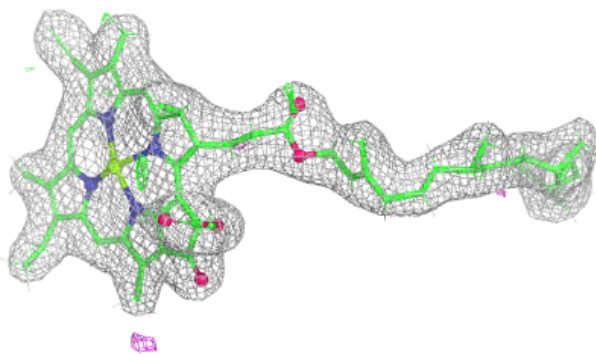
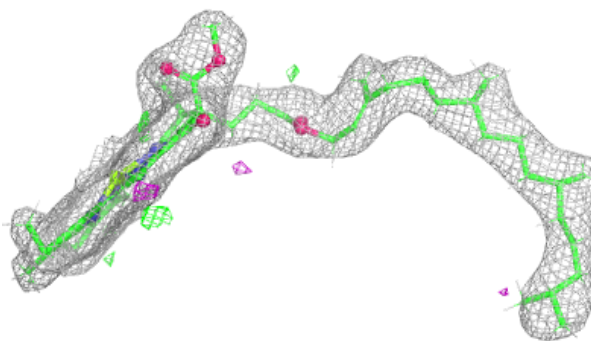


Electron density around CLA B 610:

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

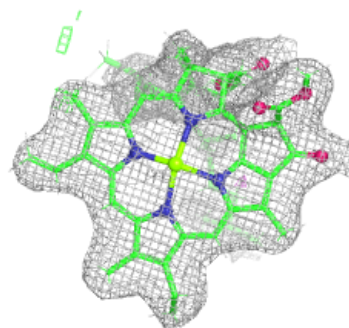
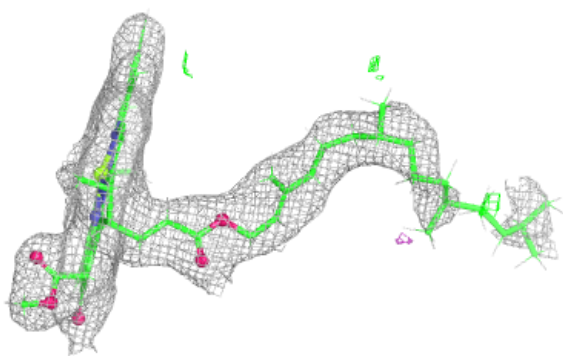
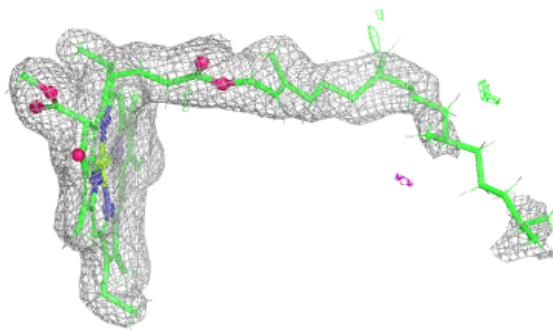
**Electron density around CLA D 404:**

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

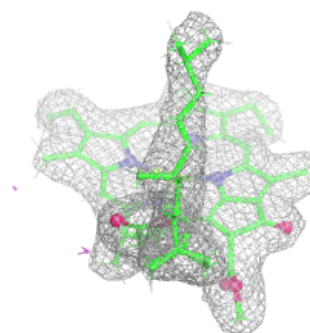
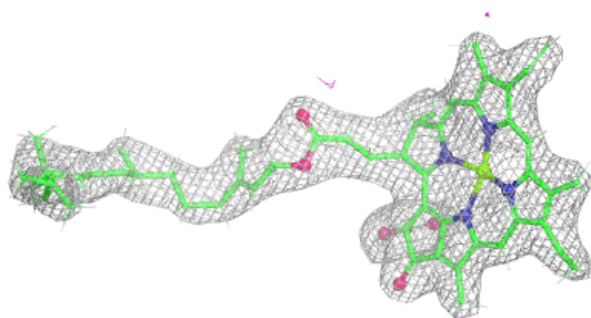
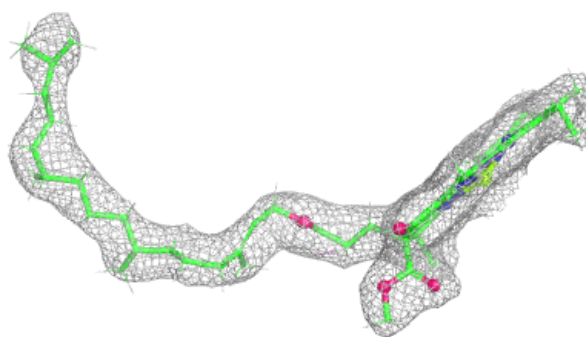


Electron density around CLA D 405:

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

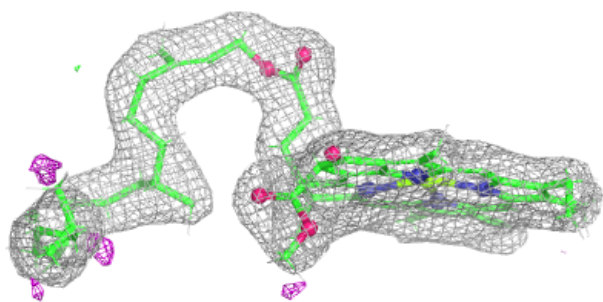
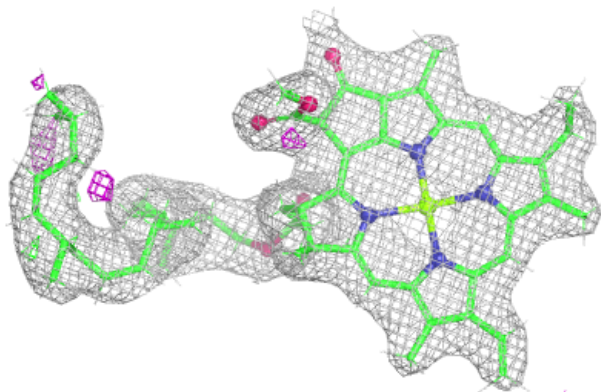
**Electron density around CLA d 402:**

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

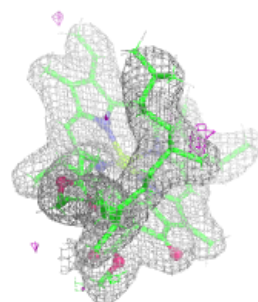
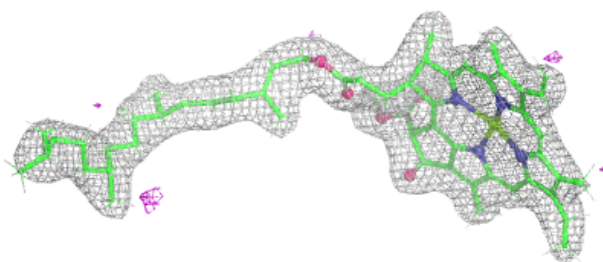
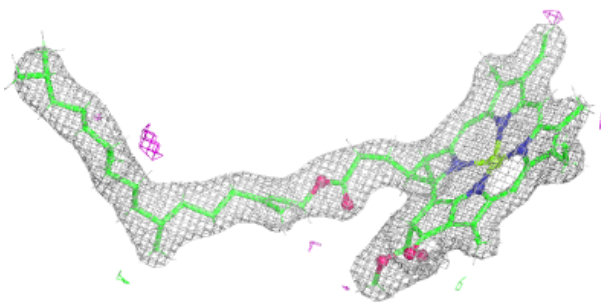


Electron density around CLA B 612:

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

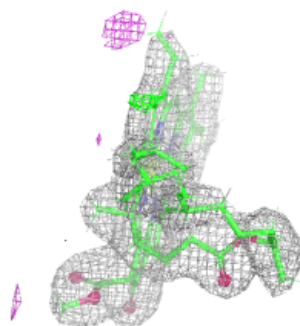
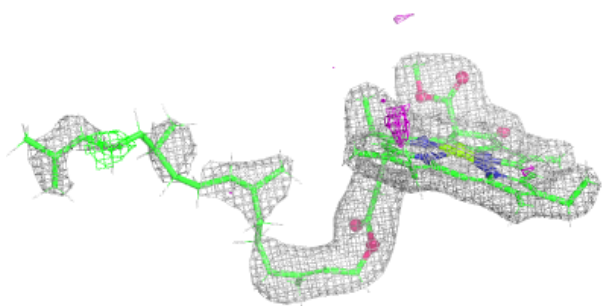
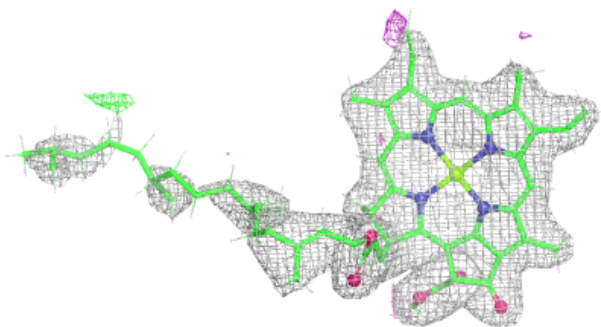
**Electron density around CLA a 402:**

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



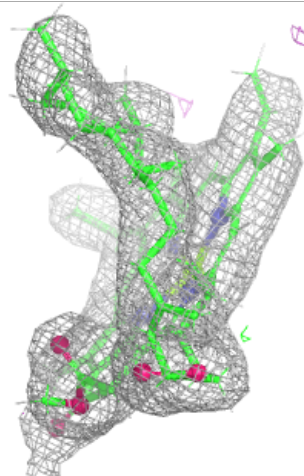
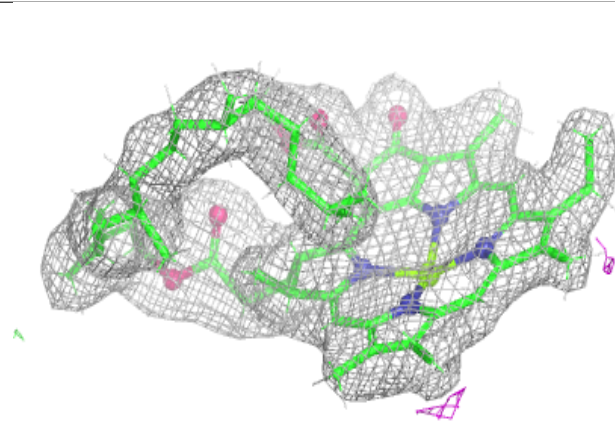
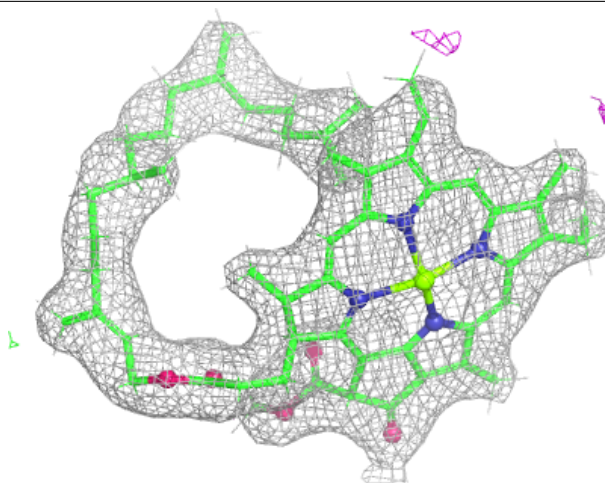
Electron density around CLA a 403:

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



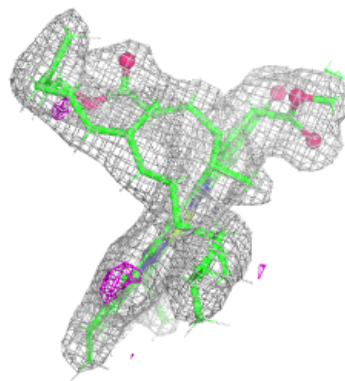
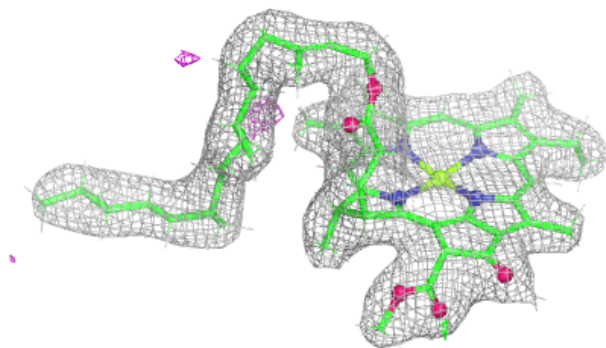
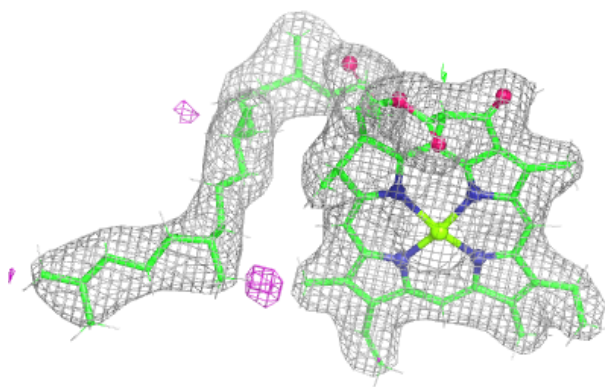
Electron density around CLA B 615:

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



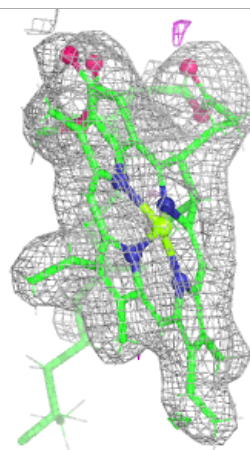
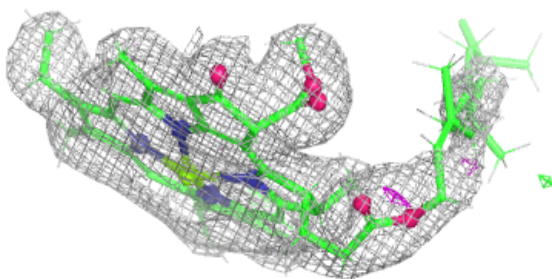
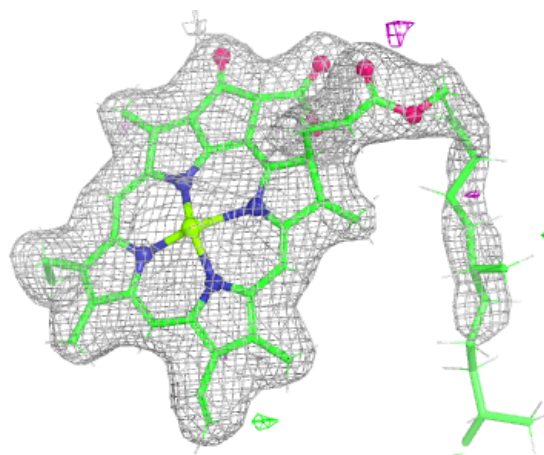
Electron density around CLA a 411:

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



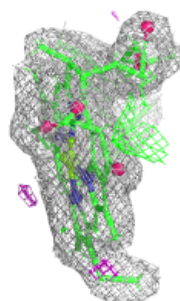
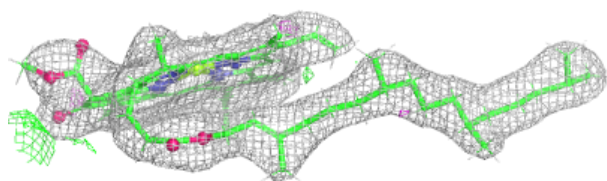
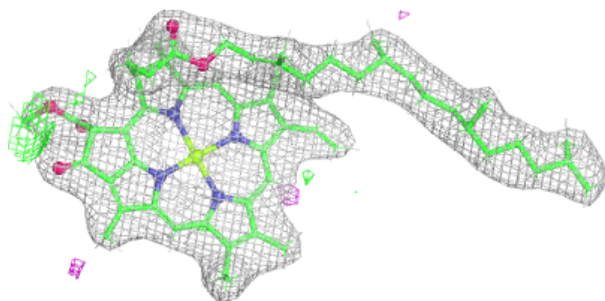
Electron density around CLA B 616:

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

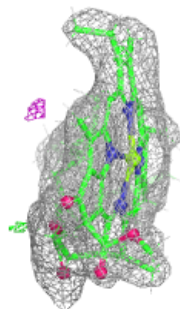
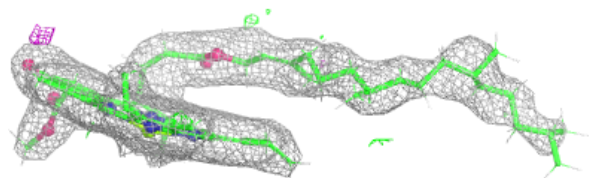
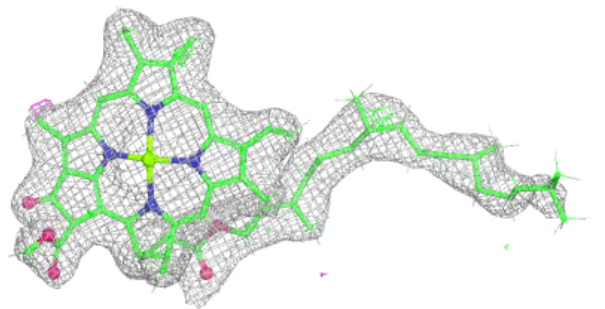


Electron density around CLA C 501:

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

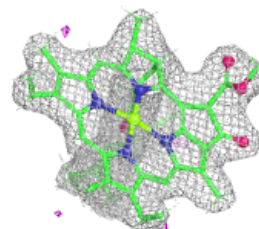
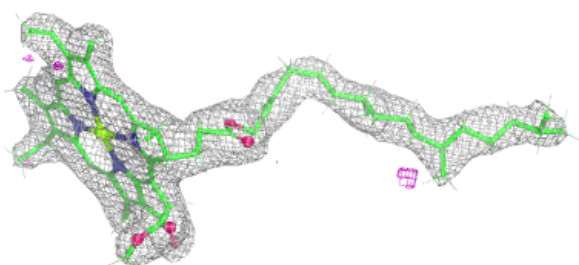
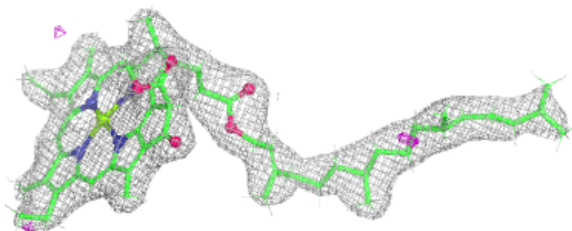
**Electron density around CLA b 603:**

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

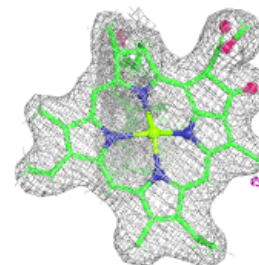
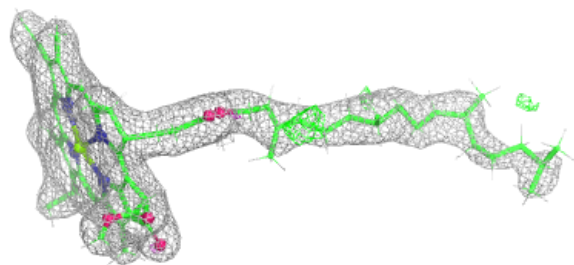
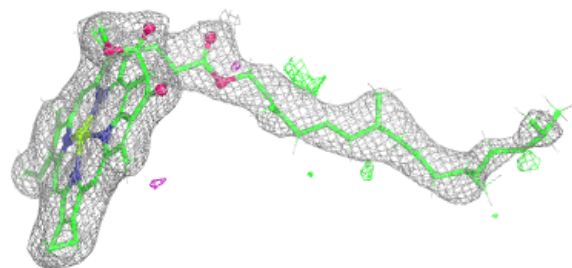


Electron density around CLA C 502:

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

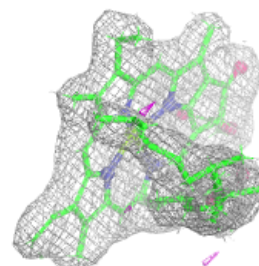
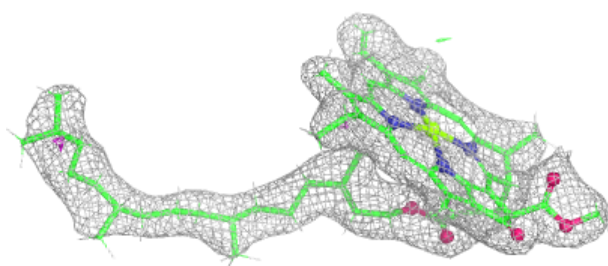
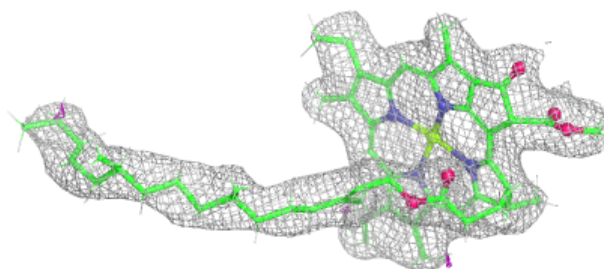
**Electron density around CLA B 604:**

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

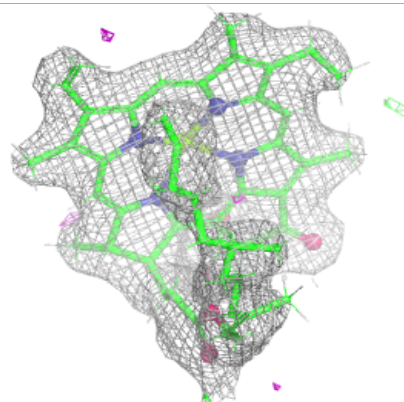
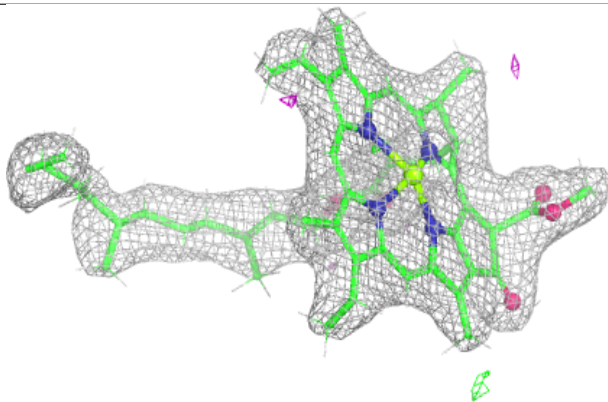
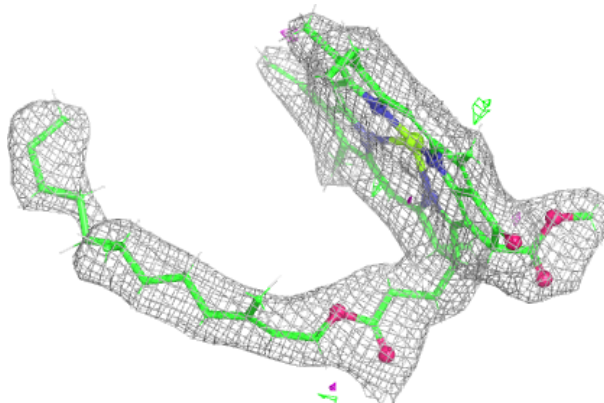


Electron density around CLA b 608:

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

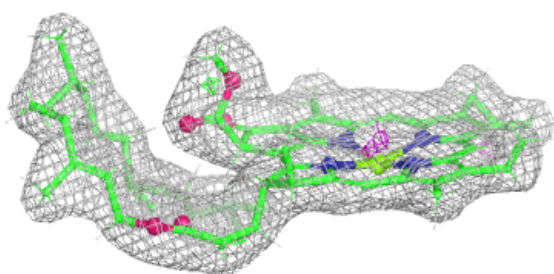
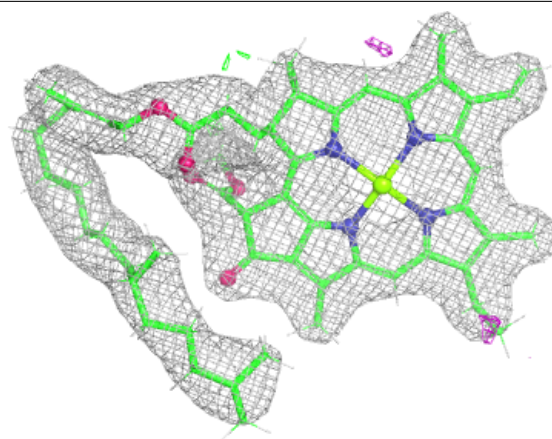
**Electron density around CLA C 504:**

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



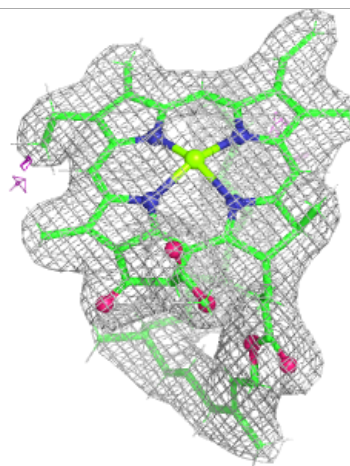
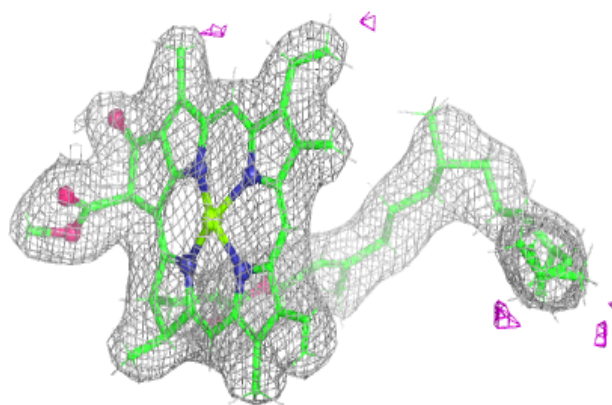
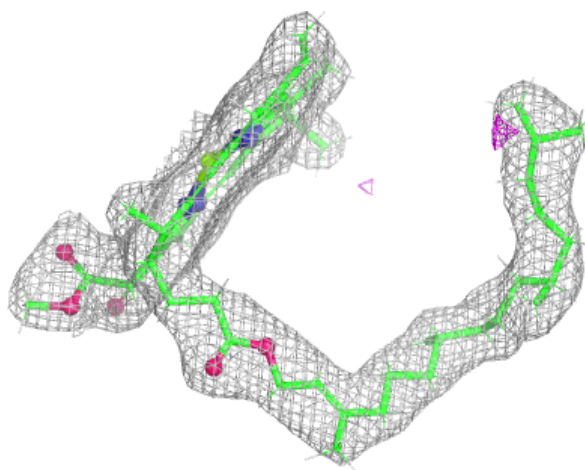
Electron density around CLA b 610:

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



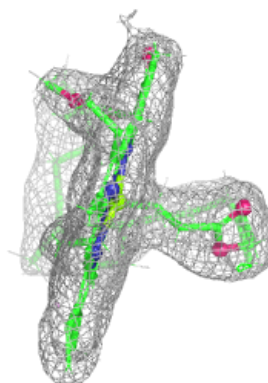
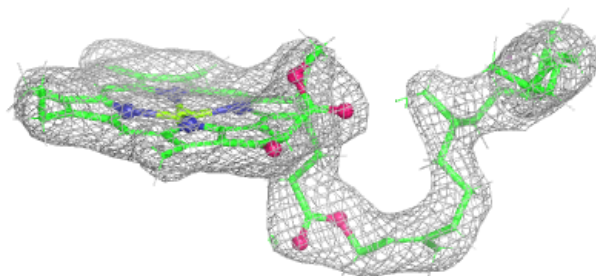
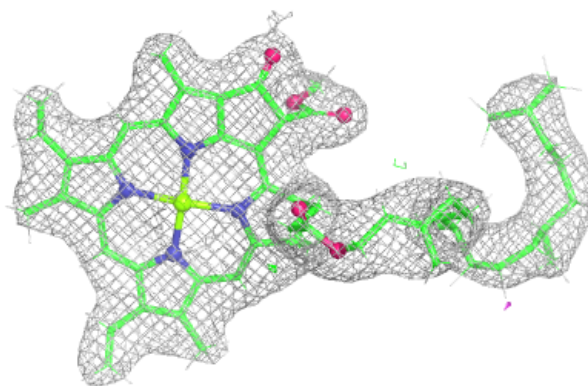
Electron density around CLA b 611:

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



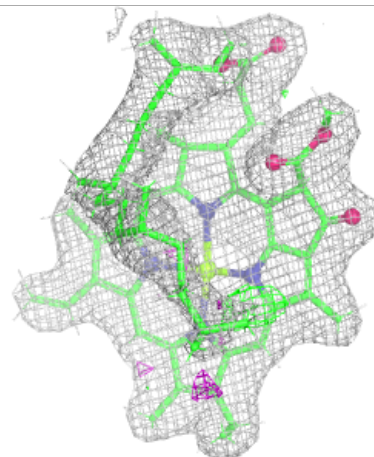
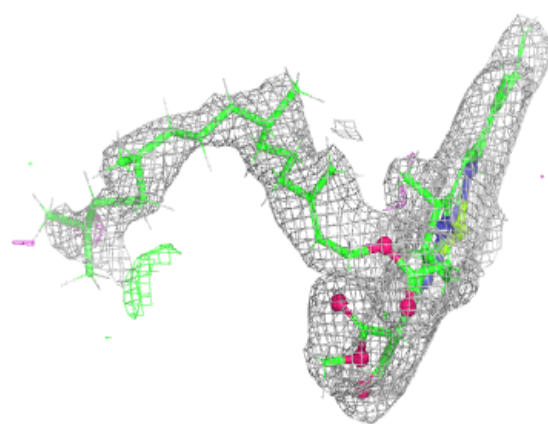
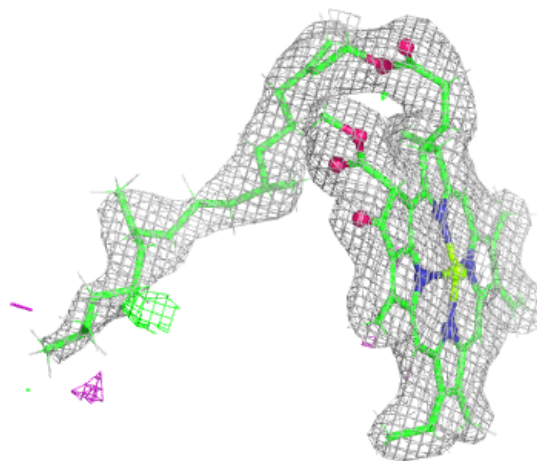
Electron density around CLA b 612:

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



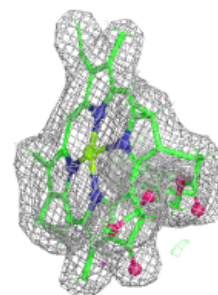
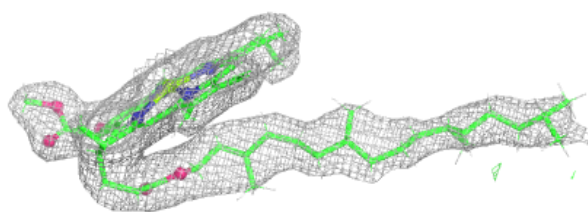
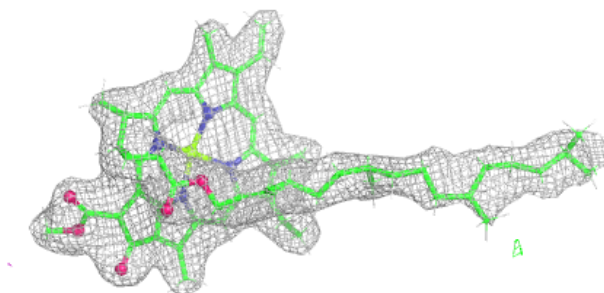
Electron density around CLA b 613:

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

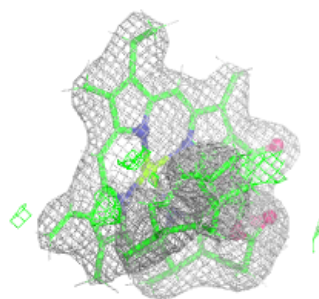
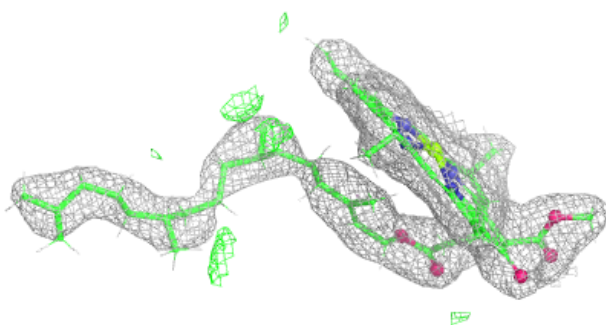
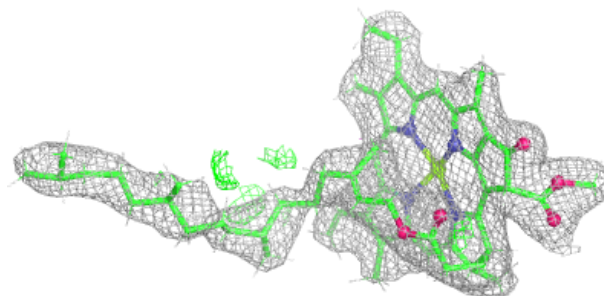


Electron density around CLA b 614:

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

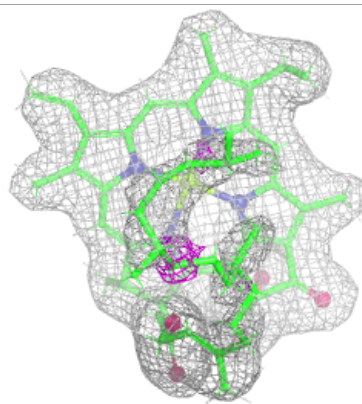
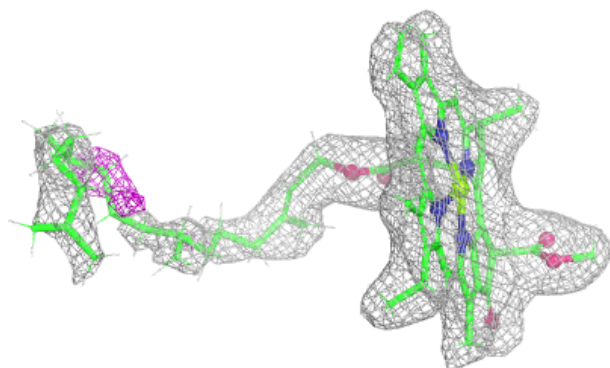
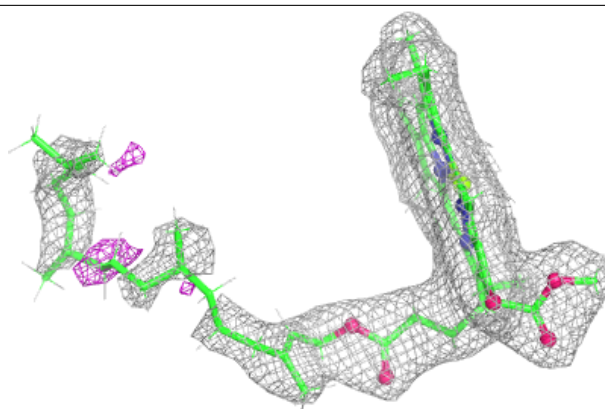
**Electron density around CLA C 505:**

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

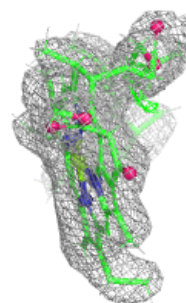
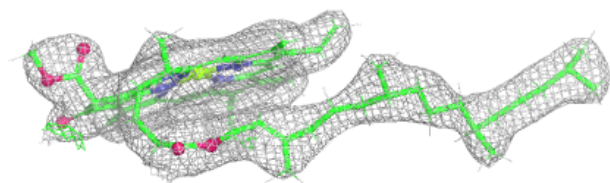
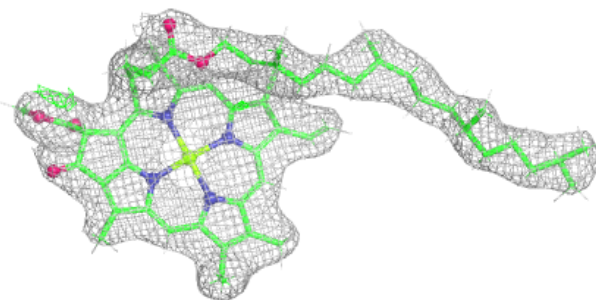


Electron density around CLA C 506:

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

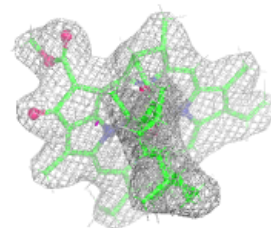
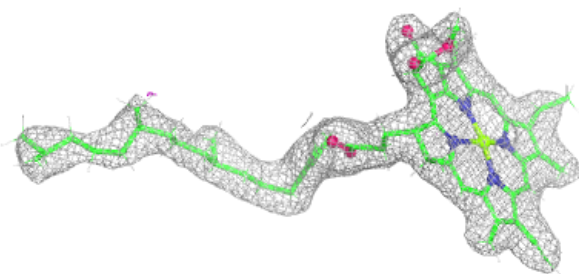
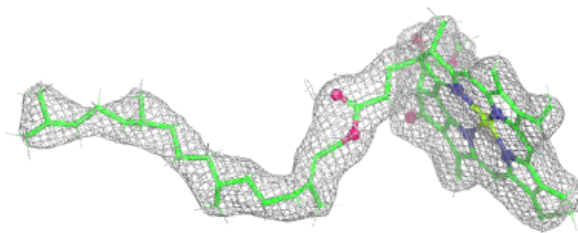
**Electron density around CLA c 502:**

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



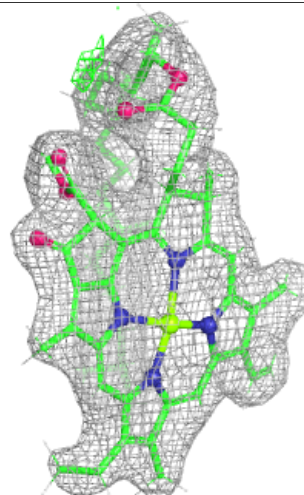
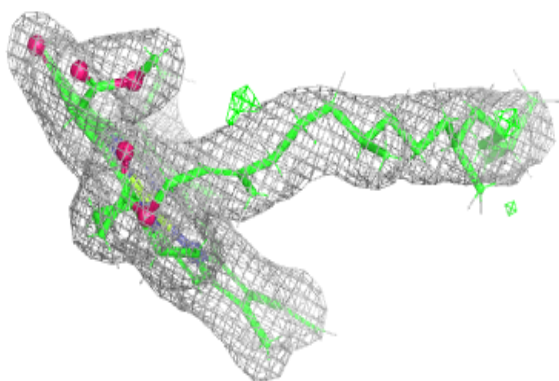
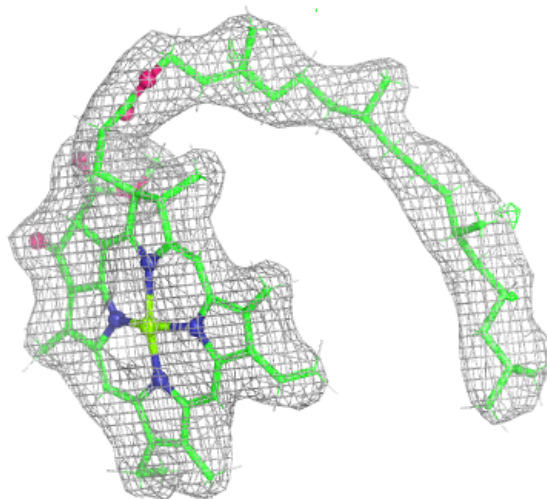
Electron density around CLA c 503:

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



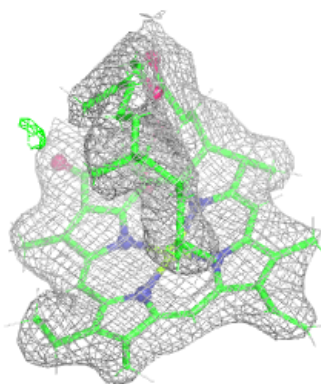
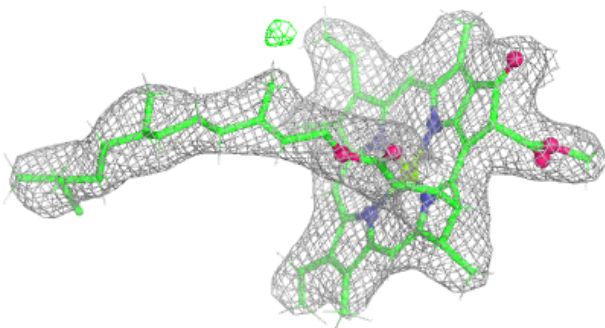
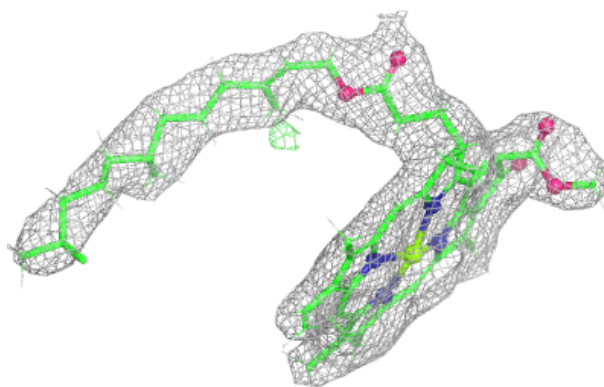
Electron density around CLA C 507:

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

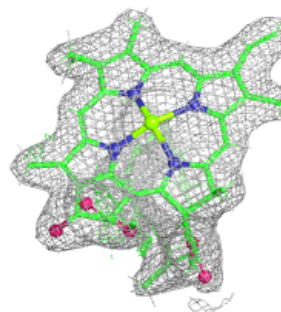
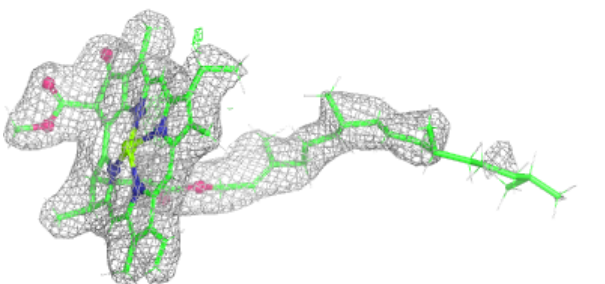
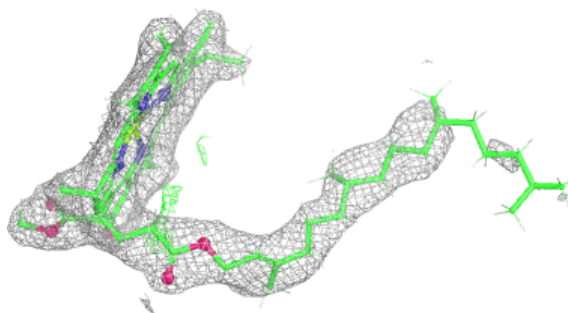


Electron density around CLA c 505:

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

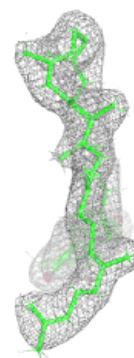
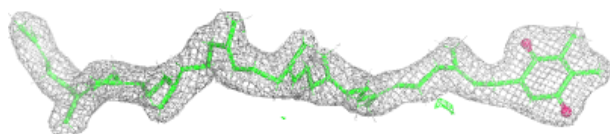
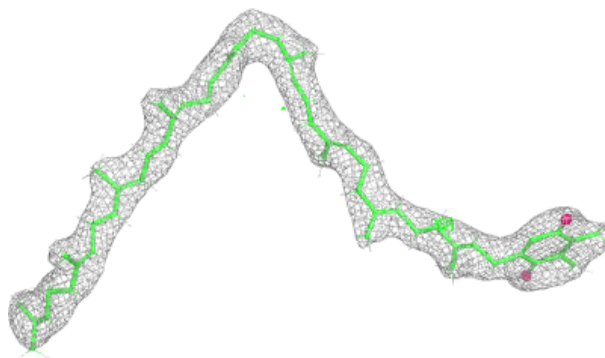
**Electron density around CLA C 508:**

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



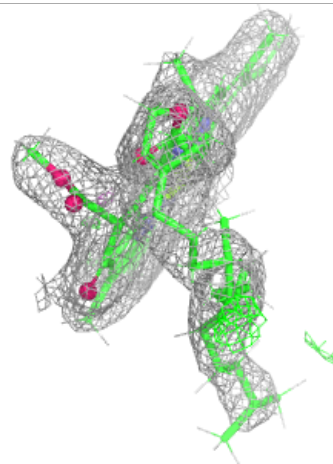
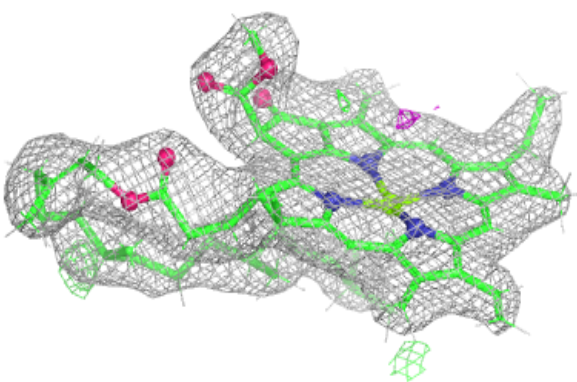
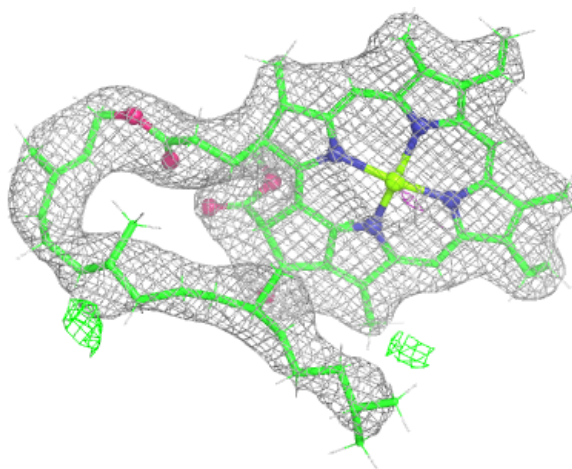
Electron density around PL9 D 407:

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



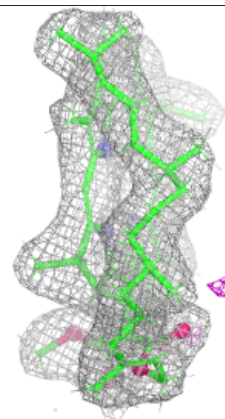
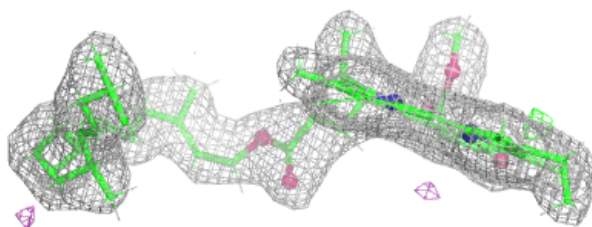
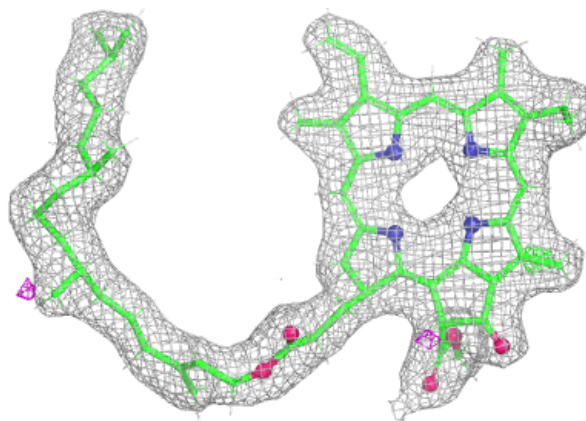
Electron density around CLA C 509:

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



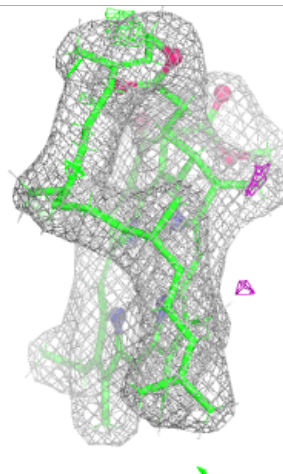
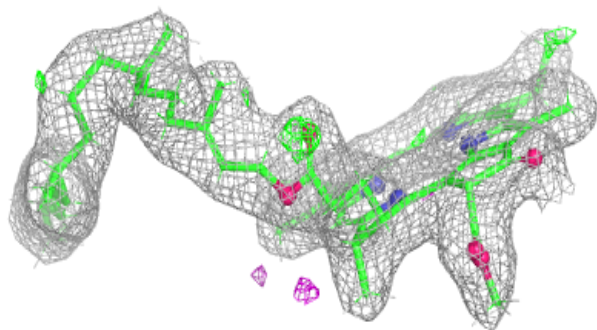
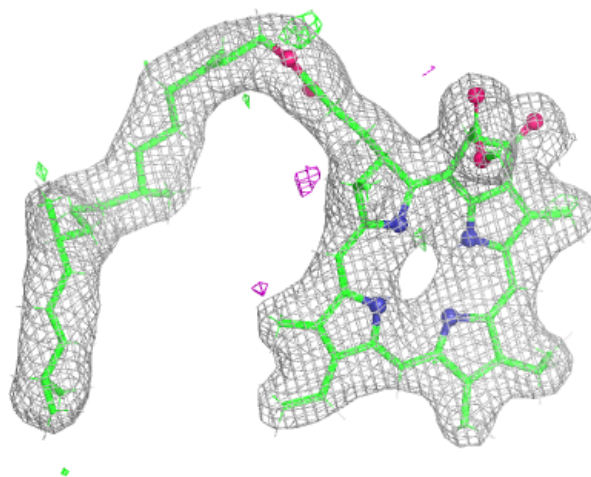
Electron density around PHO D 401:

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



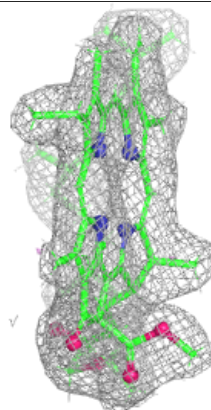
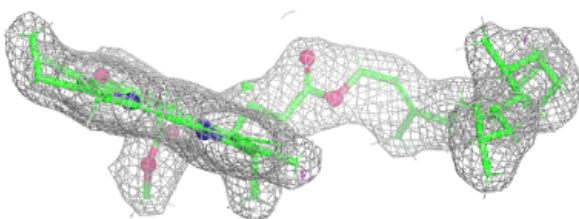
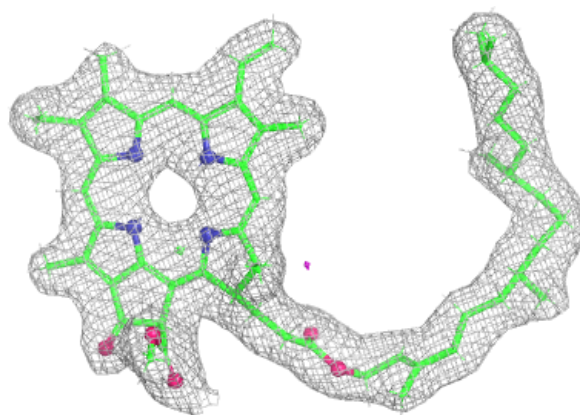
Electron density around PHO D 402:

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

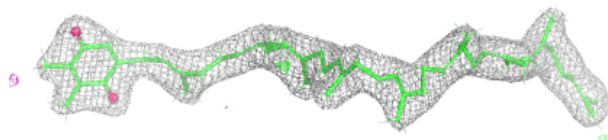
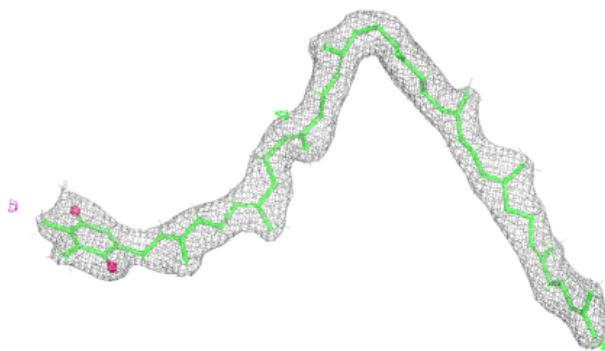


Electron density around PHO a 404:

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

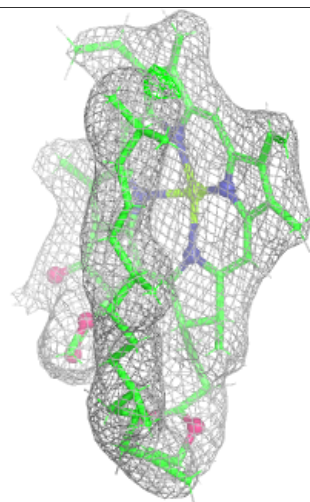
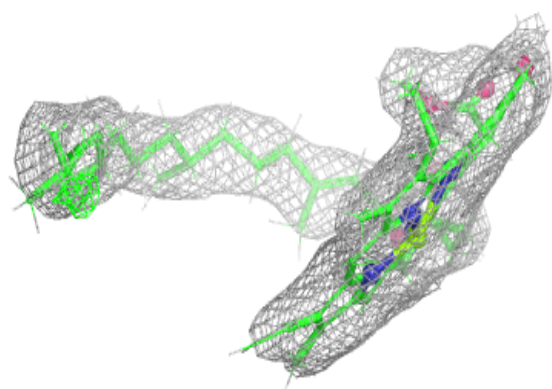
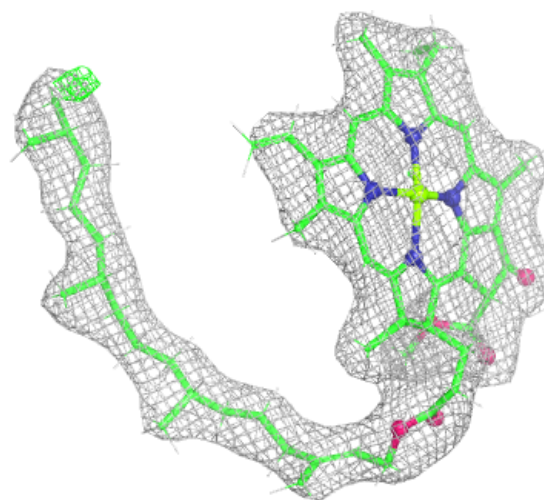
**Electron density around PL9 d 405:**

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



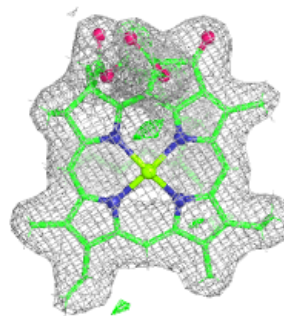
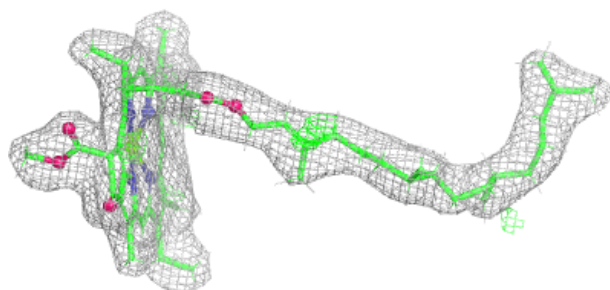
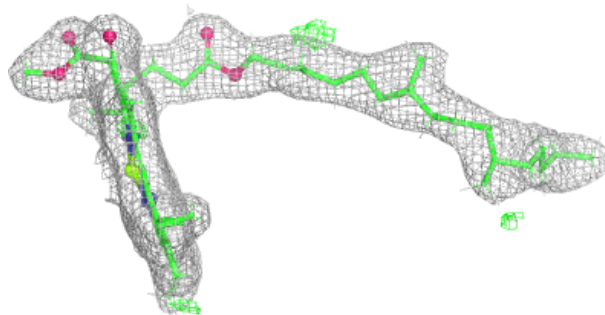
Electron density around CLA c 508:

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

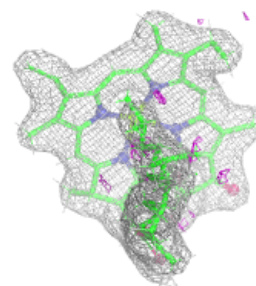
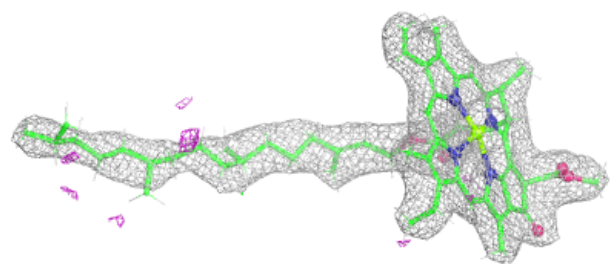
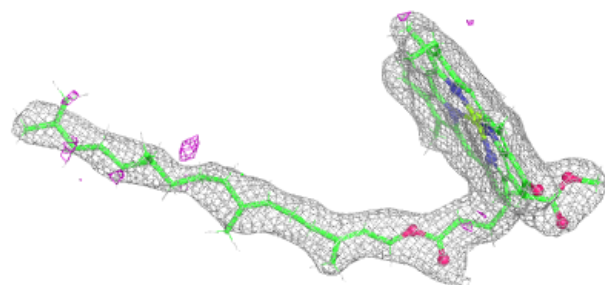


Electron density around CLA B 605:

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

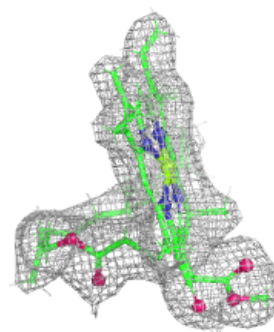
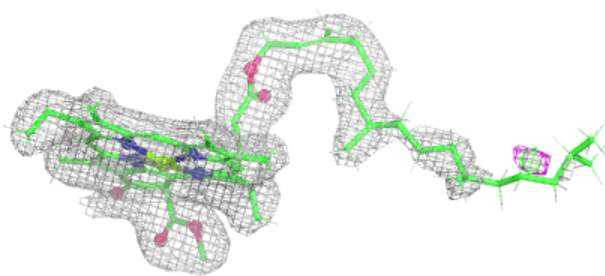
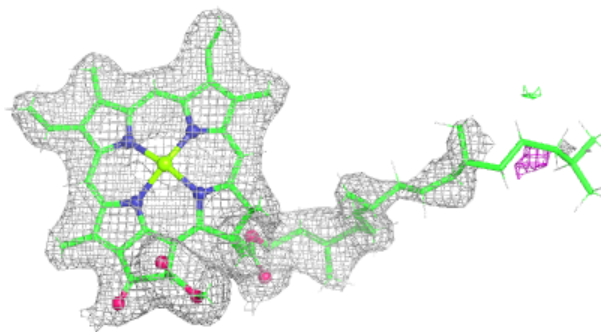
**Electron density around CLA b 607:**

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



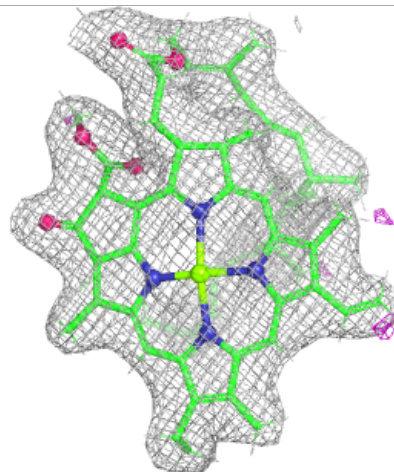
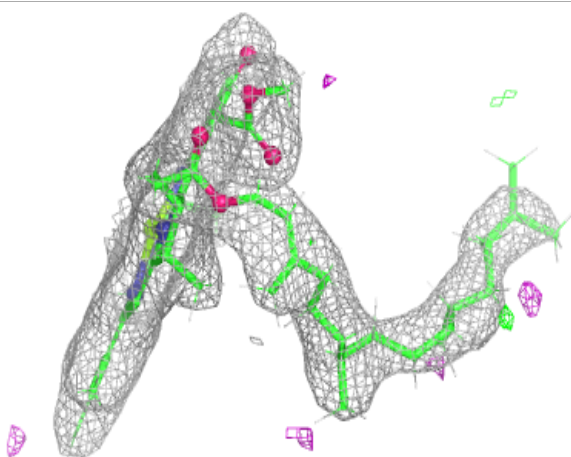
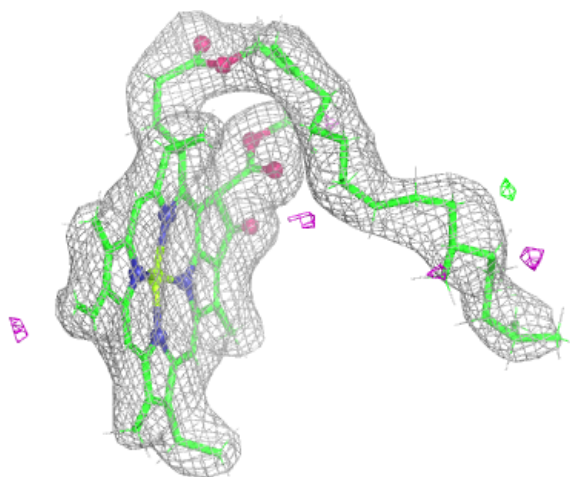
Electron density around CLA A 403:

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



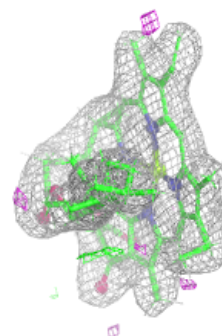
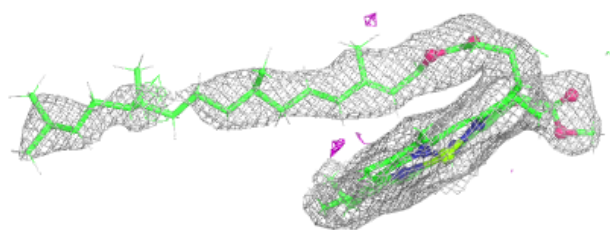
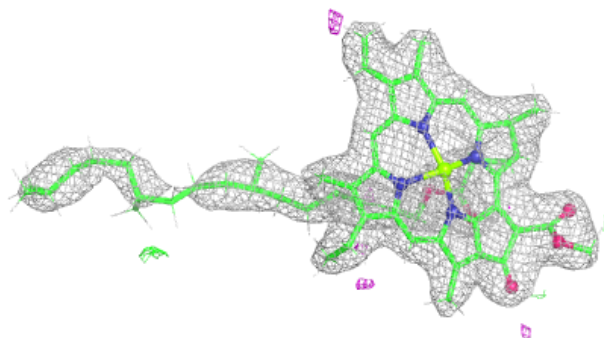
Electron density around CLA B 613:

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

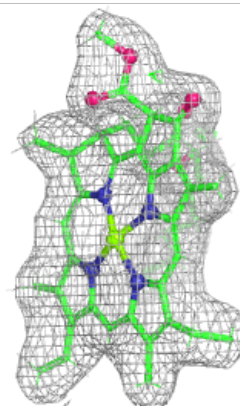
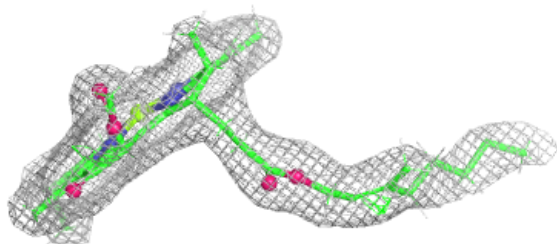
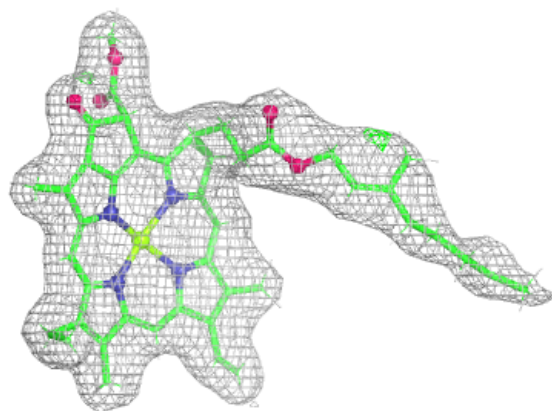


Electron density around CLA B 614:

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

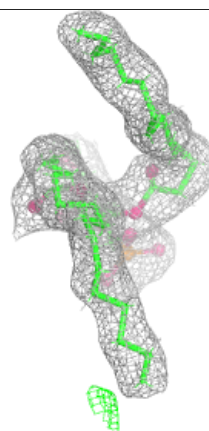
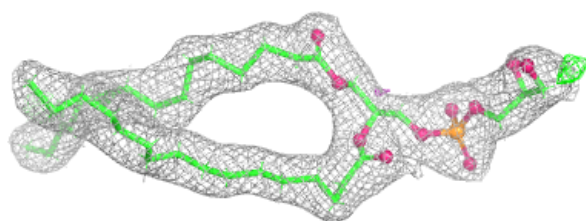
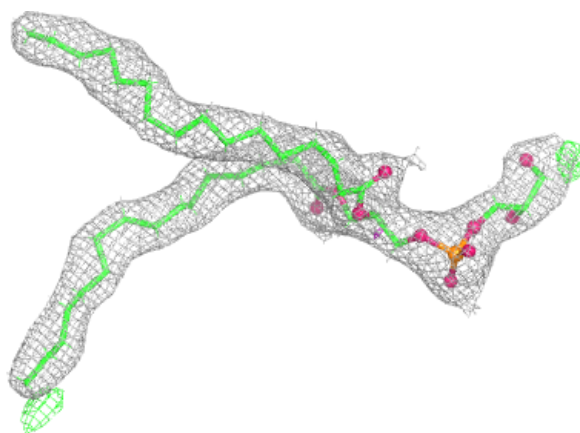
**Electron density around CLA A 404:**

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

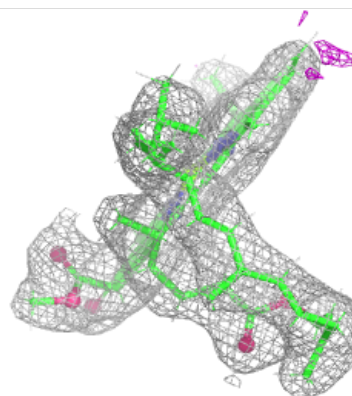
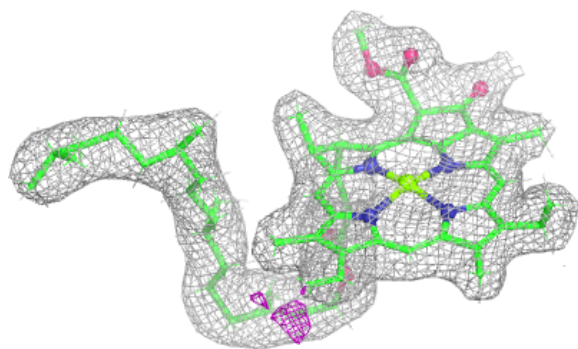
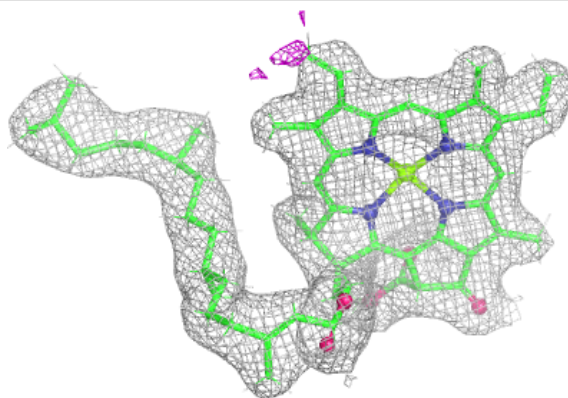


Electron density around LHG D 409:

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

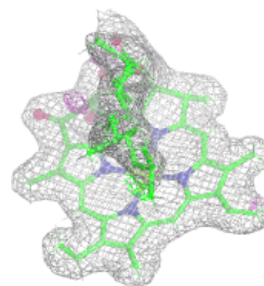
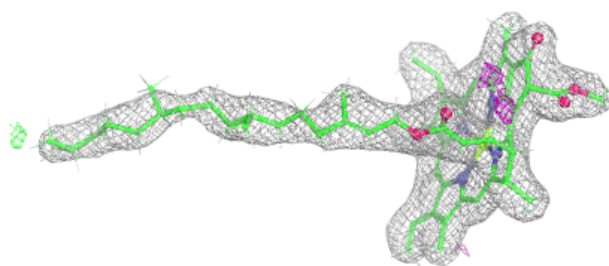
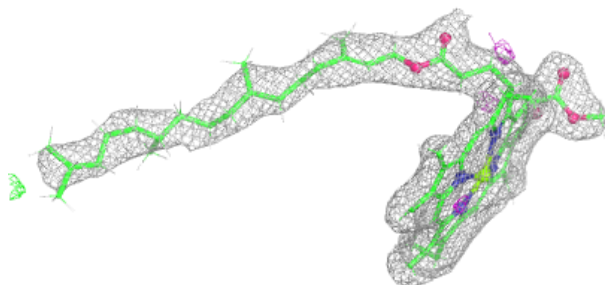
**Electron density around CLA A 409:**

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

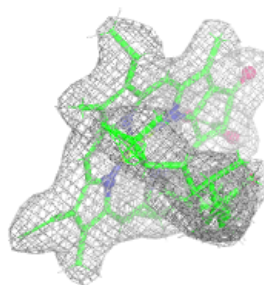
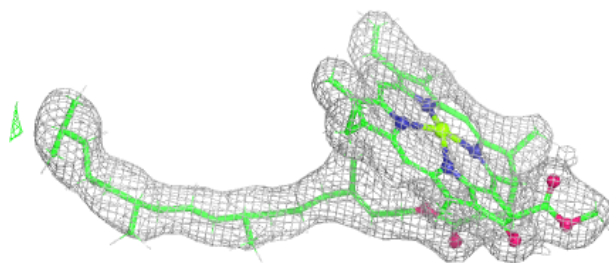
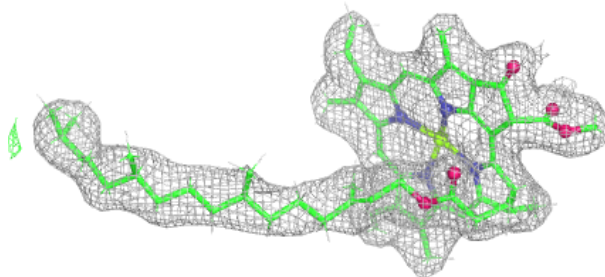


Electron density around CLA B 607:

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

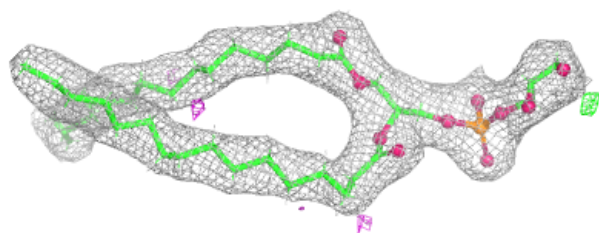
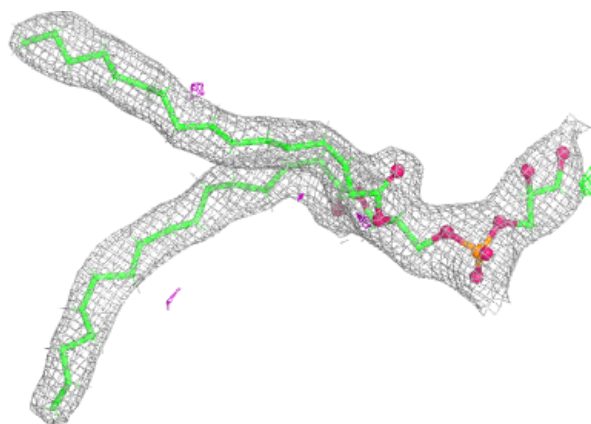
**Electron density around CLA B 608:**

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

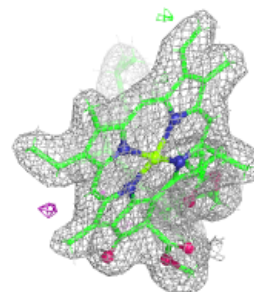
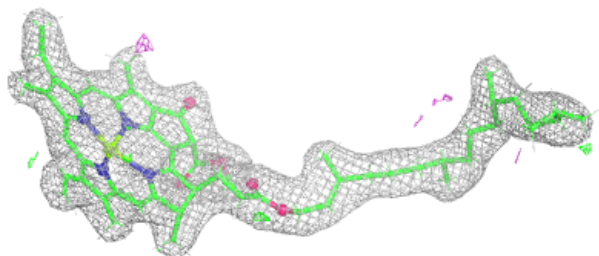
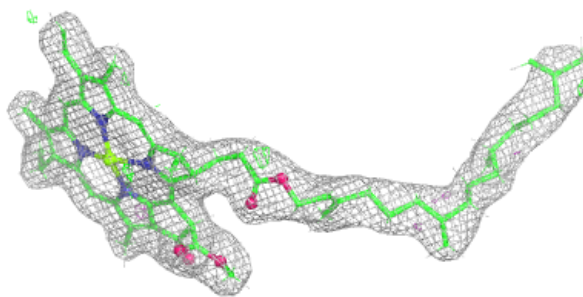


Electron density around LHG d 406:

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

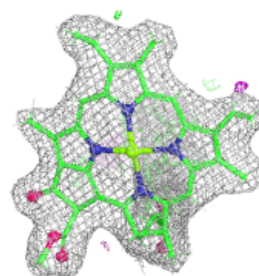
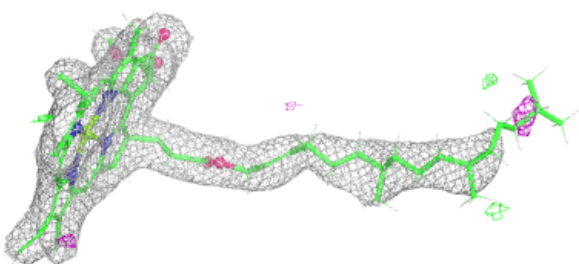
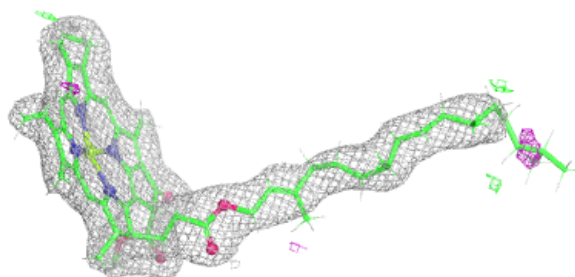
**Electron density around CLA A 402:**

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

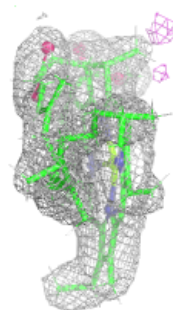
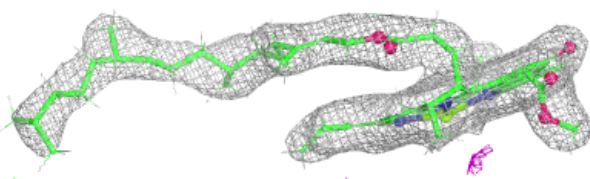
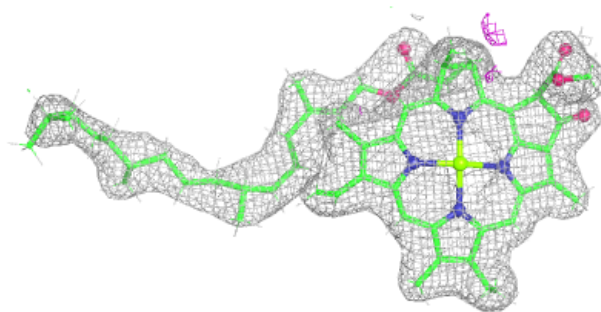


Electron density around CLA b 604:

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

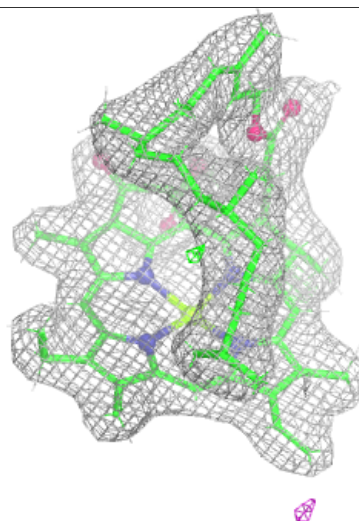
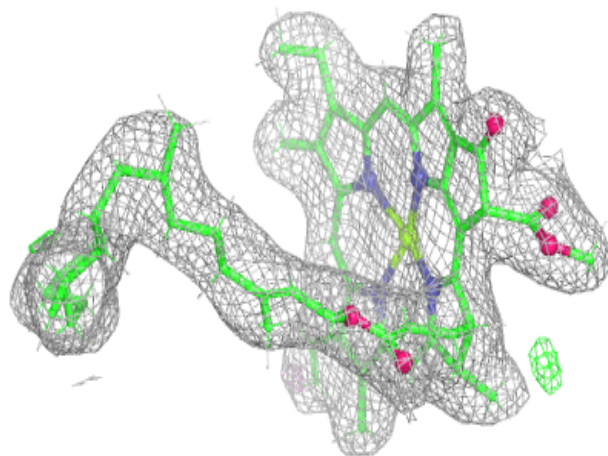
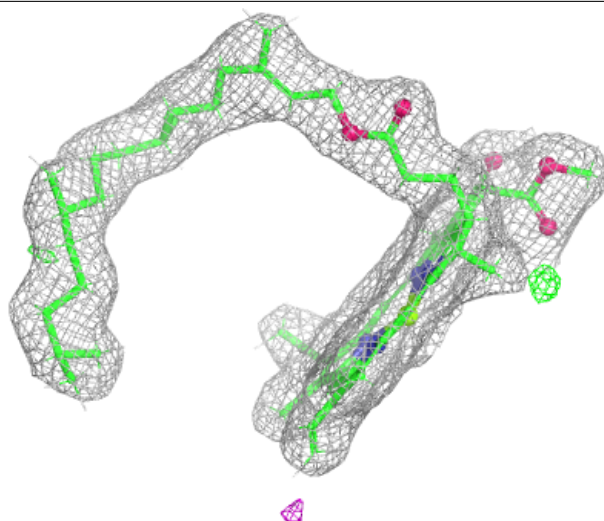
**Electron density around CLA B 603:**

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



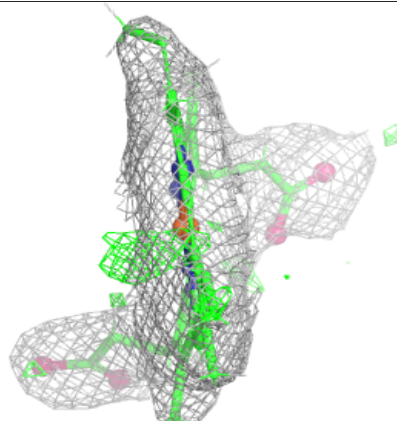
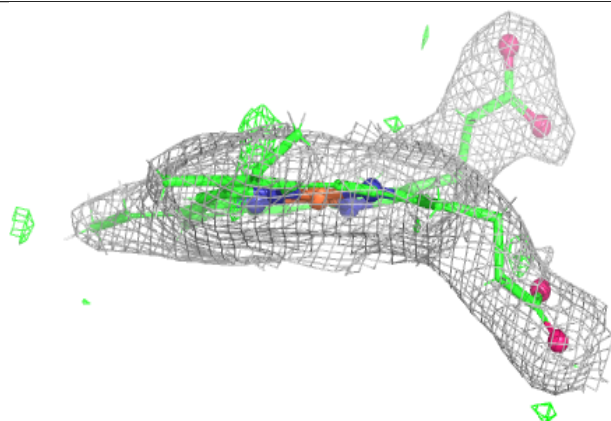
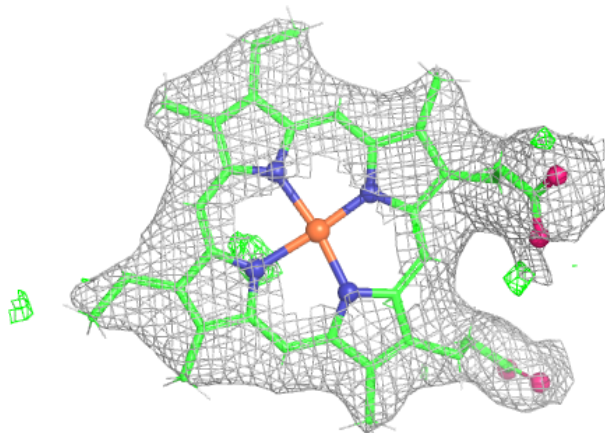
Electron density around CLA B 611:

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



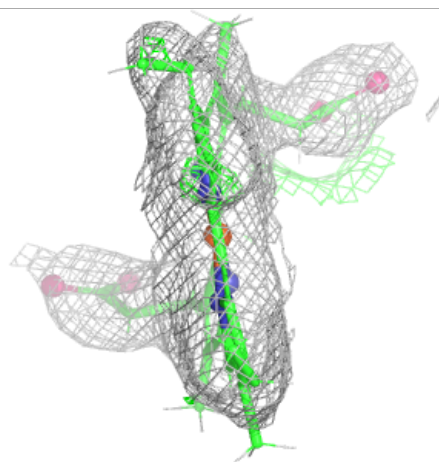
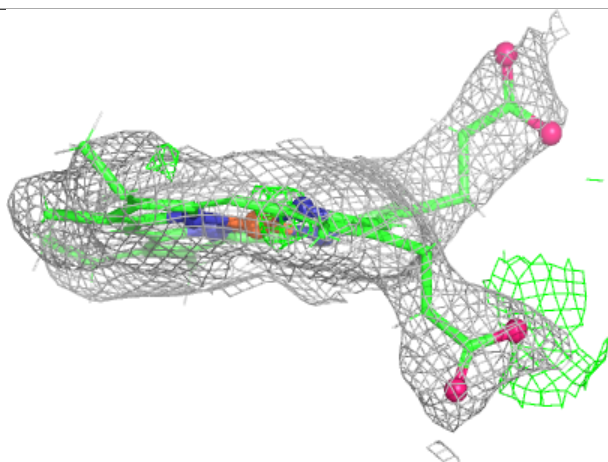
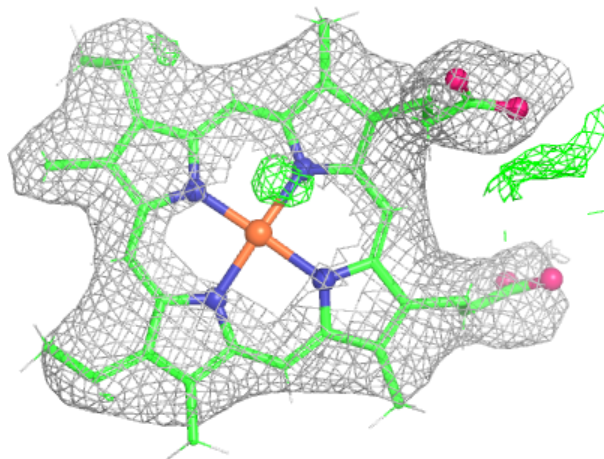
Electron density around HEC F 101:

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



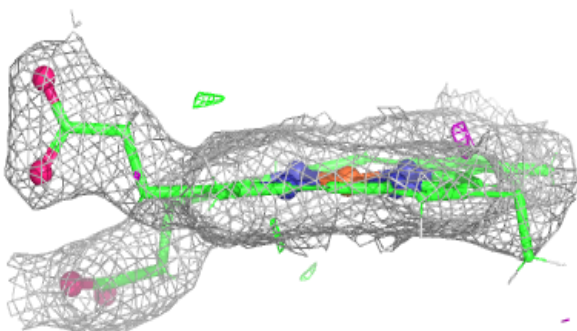
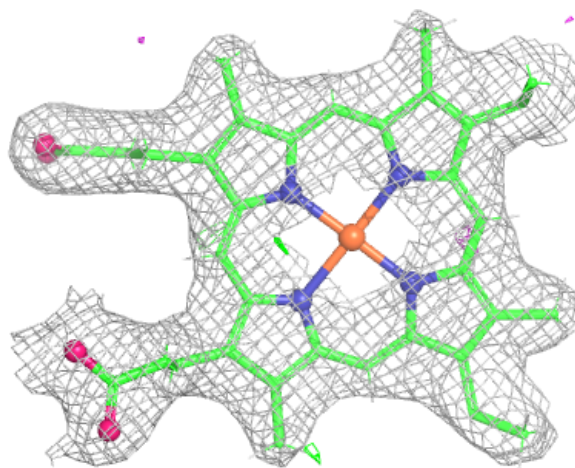
Electron density around HEC f 101:

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



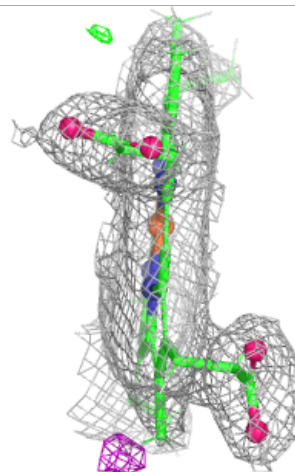
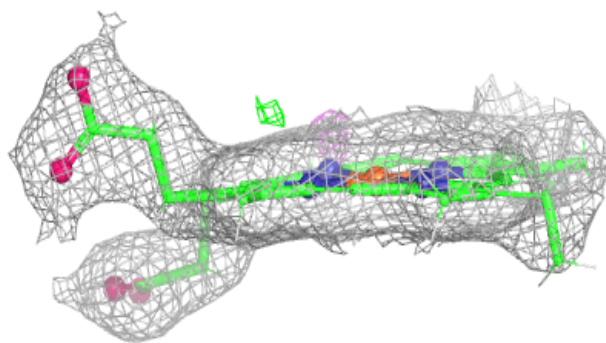
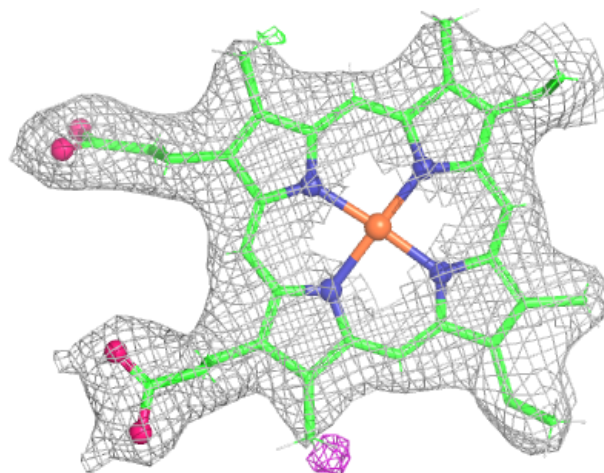
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.