



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:47 PM EDT

PDB ID : 7RF1 / pdb_00007rf1
Title : RT XFEL structure of Photosystem II averaged across all S-states at 1.89 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 1.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

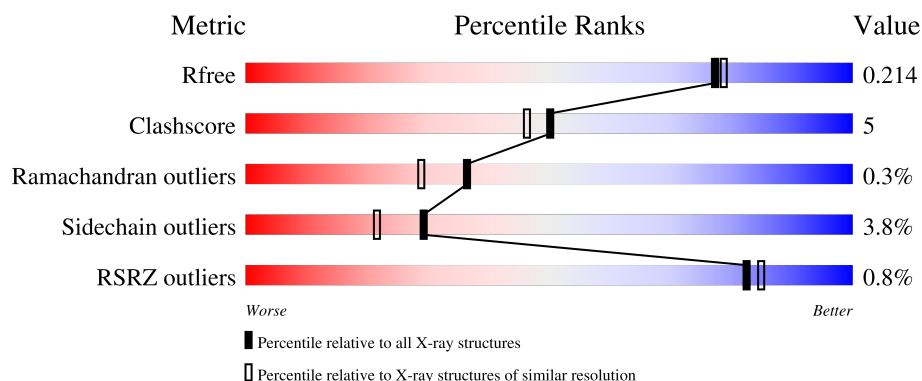
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

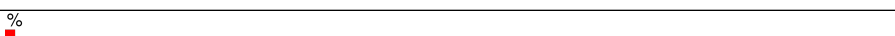
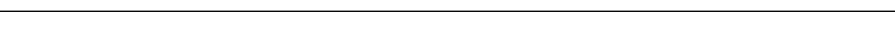
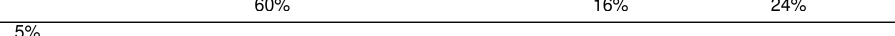
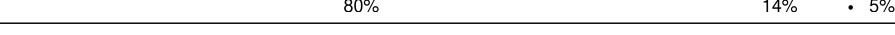
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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

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

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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

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
27	STE	A	417	-	-	X	-
27	STE	b	624	-	-	X	-
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 104284 atoms, of which 51760 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5140	1717	2518	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7824	2614	3840	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6775	2248	3350	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			598	204	305	43			

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 14 is a protein called Photosystem II reaction center protein T.

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

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 15 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 16 is a protein called Cytochrome c-550.

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

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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 Z.

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

- Molecule 20 is a protein called Photosystem II protein Y.

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

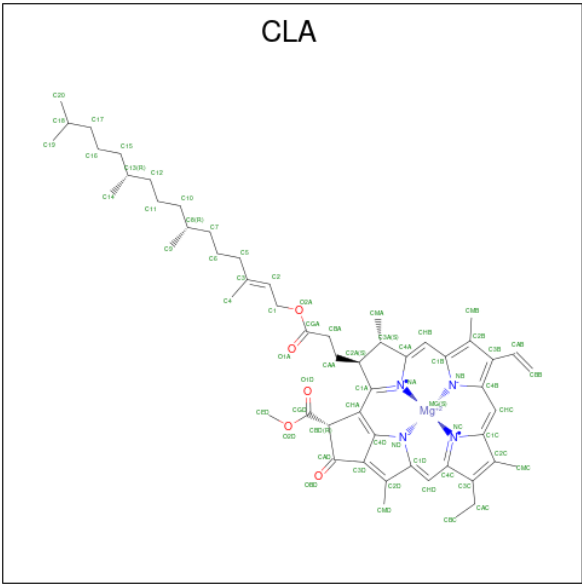
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	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
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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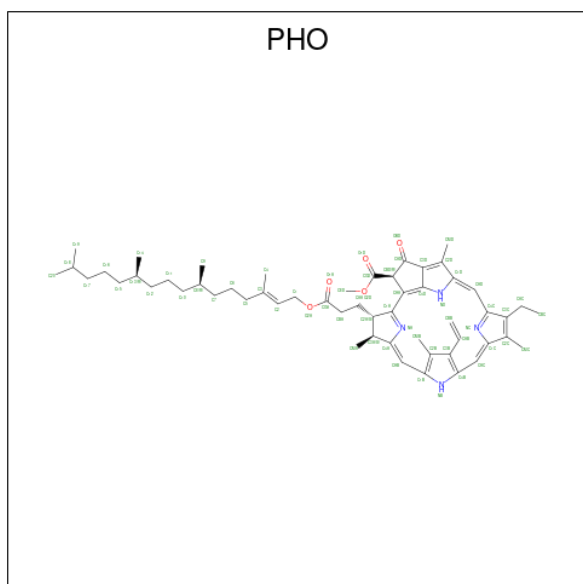
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

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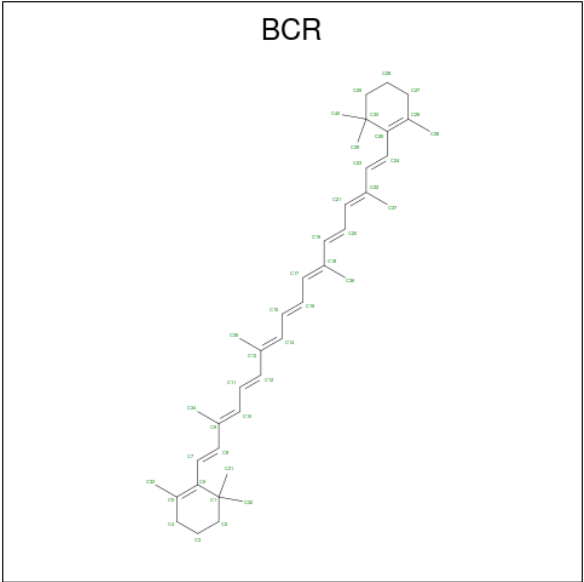
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	h	1	Total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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



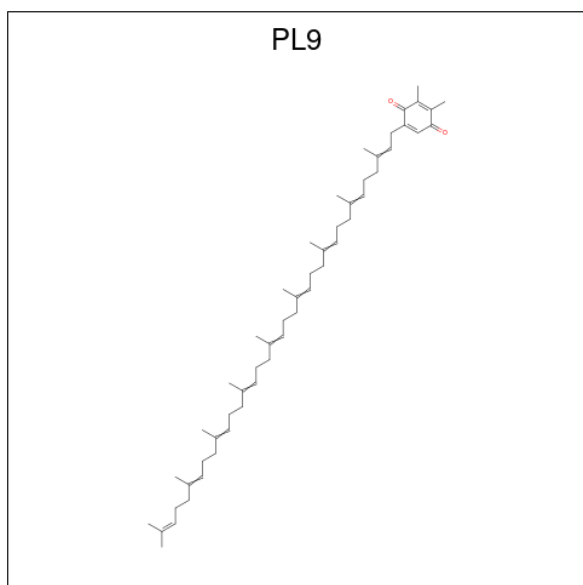
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total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

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

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



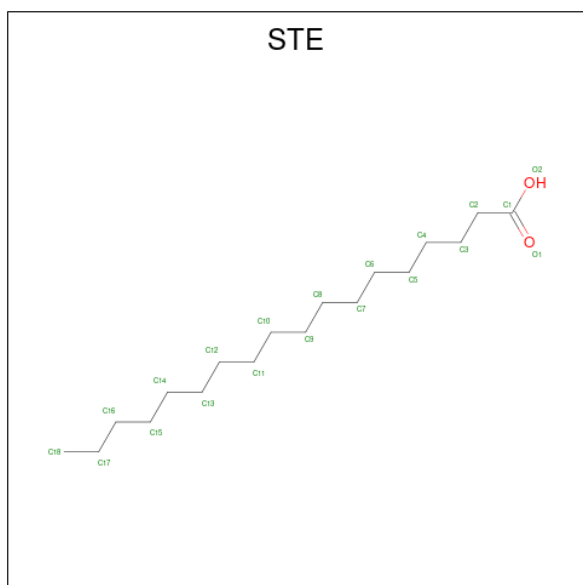
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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

- Molecule 27 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C			0	0
			9	9				
27	A	1	Total	C			0	0
			8	8				
27	A	1	Total	C	H		0	0
			52	17	35			
27	A	1	Total	C			0	0
			11	11				
27	B	1	Total	C	H	O	0	0
			43	15	26	2		
27	B	1	Total	C	H	O	0	0
			28	10	16	2		
27	B	1	Total	C	H		0	0
			41	15	26			
27	C	1	Total	C	H	O	0	0
			35	12	21	2		
27	C	1	Total	C	H		0	0
			15	5	10			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 7 7	0	0
27	C	1	Total C H O 28 10 16 2	0	0
27	C	1	Total C H 47 16 31	0	0
27	C	1	Total C 8 8	0	0
27	C	1	Total C 14 14	0	0
27	C	1	Total C H 43 14 29	0	0
27	D	1	Total C H O 55 18 35 2	0	0
27	D	1	Total C 9 9	0	0
27	E	1	Total C H O 28 10 16 2	0	0
27	E	1	Total C 12 12	0	0
27	E	1	Total C H O 55 18 35 2	0	0
27	H	1	Total C H 53 18 35	0	0
27	I	1	Total C H 41 15 26	0	0
27	I	1	Total C H O 45 15 28 2	0	0
27	J	1	Total C H O 28 10 16 2	0	0
27	M	1	Total C H O 37 13 22 2	0	0
27	M	1	Total C H 26 10 16	0	0
27	T	1	Total C H 46 16 30	0	0
27	Z	1	Total C H 52 17 35	0	0
27	a	1	Total C H 26 10 16	0	0
27	a	1	Total C H O 28 10 16 2	0	0

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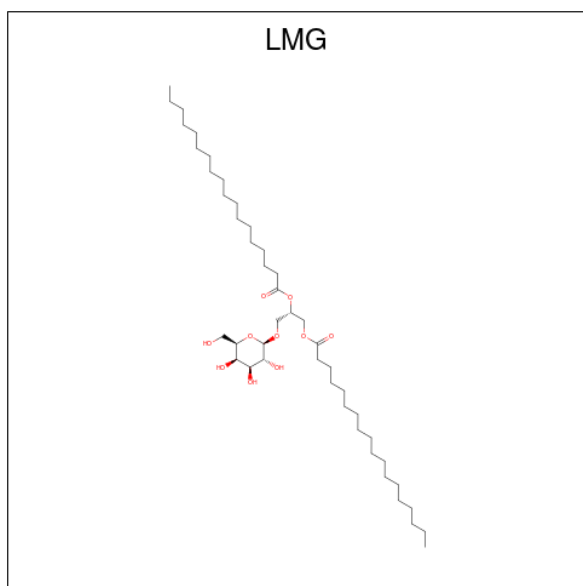
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C H O 55 18 35 2	0	0
27	b	1	Total C O 20 18 2	0	0
27	b	1	Total C H O 40 14 24 2	0	0
27	b	1	Total C H 26 10 16	0	0
27	b	1	Total C 11 11	0	0
27	c	1	Total C H 37 13 24	0	0
27	c	1	Total C H 53 18 35	0	0
27	d	1	Total C H O 43 15 26 2	0	0
27	d	1	Total C H O 28 10 16 2	0	0
27	d	1	Total C 10 10	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C 8 8	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C O 13 11 2	0	0
27	i	1	Total C O 12 10 2	0	0
27	i	1	Total C H 18 6 12	0	0
27	j	1	Total C H O 28 10 16 2	0	0
27	j	1	Total C 16 16	0	0
27	l	1	Total C H 53 18 35	0	0
27	m	1	Total C H O 28 10 16 2	0	0
27	m	1	Total C H 44 15 29	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	t	1	Total	C	H	O	0	0
			34	12	20	2		
27	t	1	Total	C	H	O	0	0
			46	16	28	2		
27	x	1	Total	C	H	O	0	0
			55	18	35	2		
27	z	1	Total	C	H		0	0
			24	9	15			

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



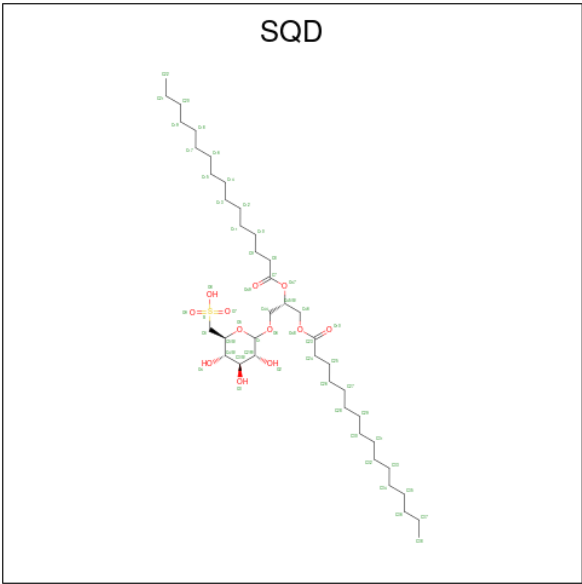
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			109	35	64	10		
28	C	1	Total	C	H	O	0	0
			83	26	47	10		
28	C	1	Total	C	H	O	0	0
			114	38	66	10		
28	D	1	Total	C	H	O	0	0
			124	40	74	10		
28	D	1	Total	C	H	O	0	0
			123	41	72	10		
28	M	1	Total	C	H	O	0	0
			123	41	72	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	a	1	Total	C	H	O	0	0
			141	45	86	10		
28	b	1	Total	C	O		0	0
			24	20	4			
28	b	1	Total	C	H	O	0	0
			123	41	72	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			75	25	45	5		
28	c	1	Total	C	H	O	0	0
			110	36	64	10		
28	c	1	Total	C	H	O	0	0
			117	38	69	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

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



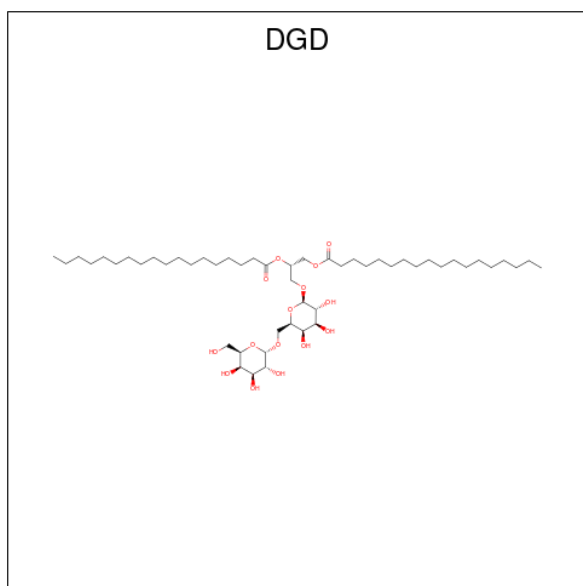
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	O	S		0	0
			54	41	12	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	O	S		0	0
			54	41	12	1			
29	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
29	l	1	Total	C	H	O	S	0	0
			131	41	77	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



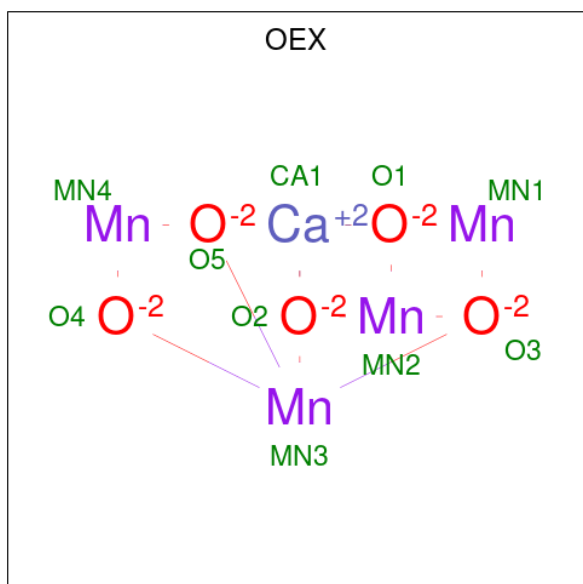
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O		0	0
			162	51	96	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	C	1	Total	C	H	O		0	0
			144	47	82	15			
30	H	1	Total	C	H	O		0	0
			144	47	82	15			

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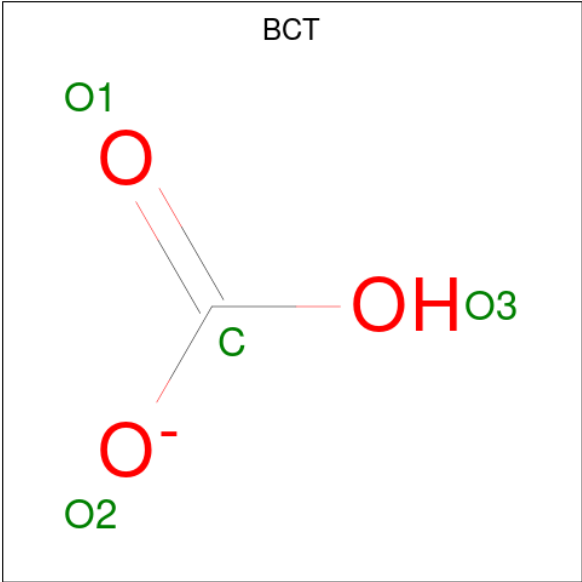
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



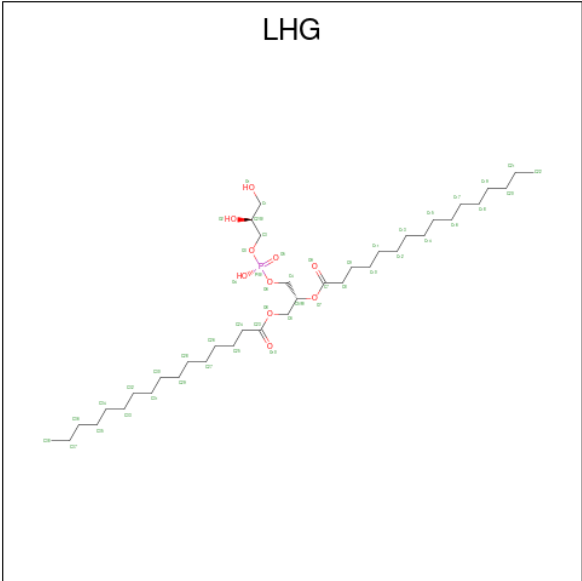
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



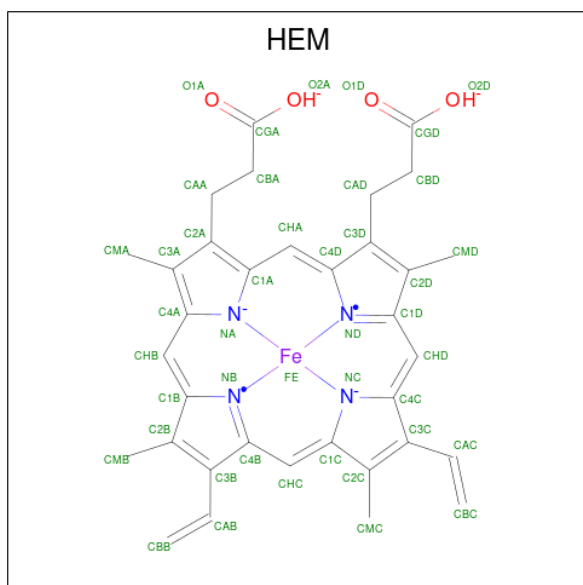
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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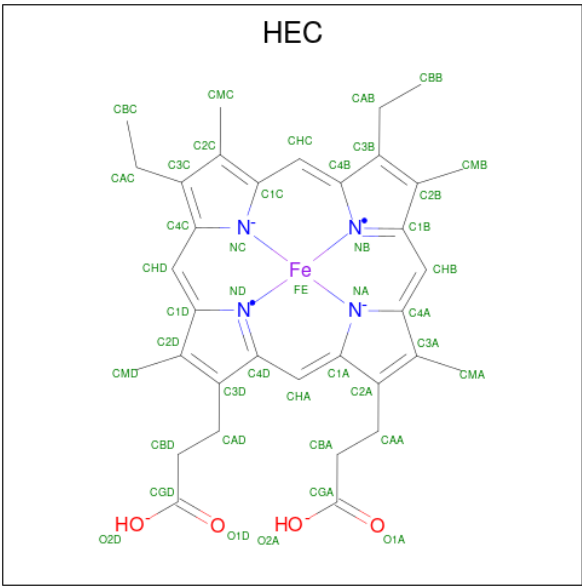
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	d	1	Total	C	H	O	P	0	0
			123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

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	202	Total	O	0	0
			202	202		
36	C	180	Total	O	0	0
			180	180		
36	D	137	Total	O	0	0
			137	137		
36	E	20	Total	O	0	0
			20	20		
36	F	11	Total	O	0	0
			11	11		
36	H	26	Total	O	0	0
			26	26		
36	I	9	Total	O	0	0
			9	9		
36	J	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	K	4	Total 4	O 4	0	0
36	L	10	Total 10	O 10	0	0
36	M	7	Total 7	O 7	0	0
36	O	104	Total 104	O 104	0	0
36	T	9	Total 9	O 9	0	0
36	U	45	Total 45	O 45	0	0
36	V	82	Total 82	O 82	0	0
36	Y	1	Total 1	O 1	0	0
36	X	12	Total 12	O 12	0	0
36	a	115	Total 115	O 115	0	0
36	b	200	Total 200	O 200	0	0
36	c	171	Total 171	O 171	0	0
36	d	125	Total 125	O 125	0	0
36	e	10	Total 10	O 10	0	0
36	f	10	Total 10	O 10	0	0
36	h	23	Total 23	O 23	0	0
36	i	5	Total 5	O 5	0	0
36	j	6	Total 6	O 6	0	0
36	k	5	Total 5	O 5	0	0
36	l	15	Total 15	O 15	0	0
36	m	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	o	110	Total 110	O 110	0	0
36	t	12	Total 12	O 12	0	0
36	u	61	Total 61	O 61	0	0
36	v	59	Total 59	O 59	0	0
36	y	2	Total 2	O 2	0	0
36	x	7	Total 7	O 7	0	0
36	z	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

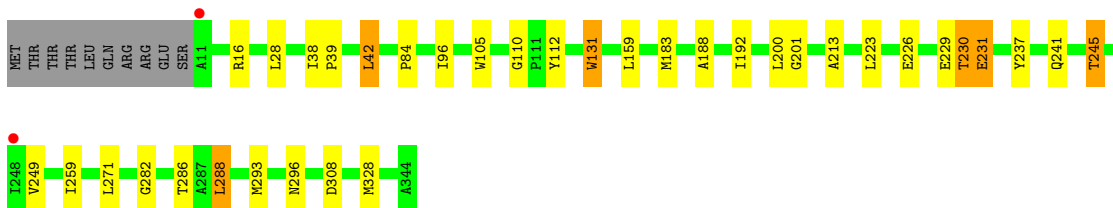
- Molecule 1: Photosystem II protein D1 1

Chain A: 



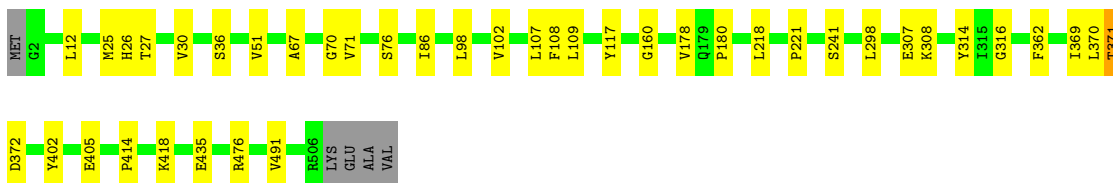
- Molecule 1: Photosystem II protein D1 1

Chain a: 



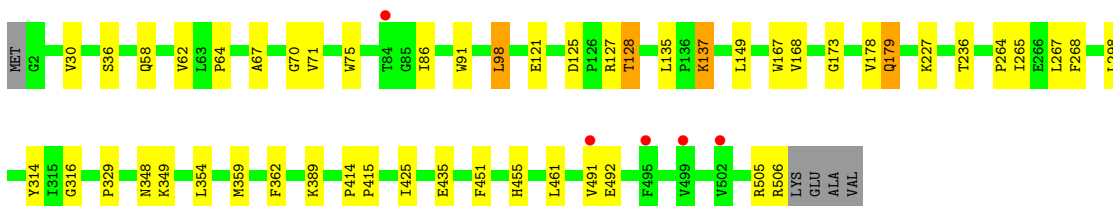
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

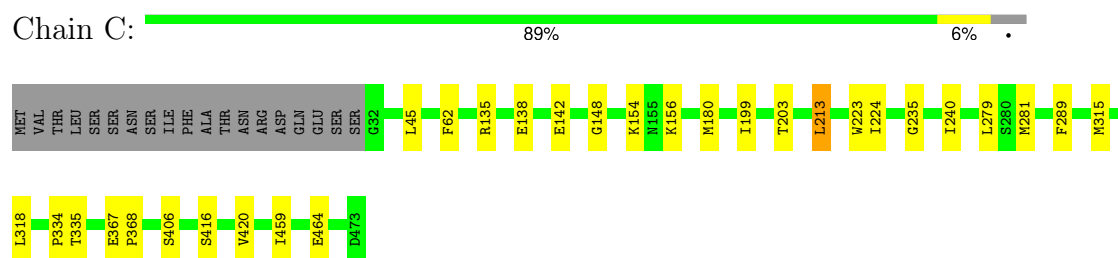


- Molecule 2: Photosystem II CP47 reaction center protein

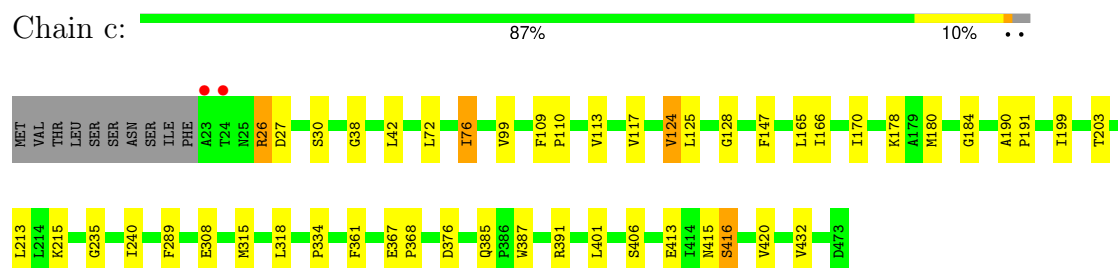
Chain b: 



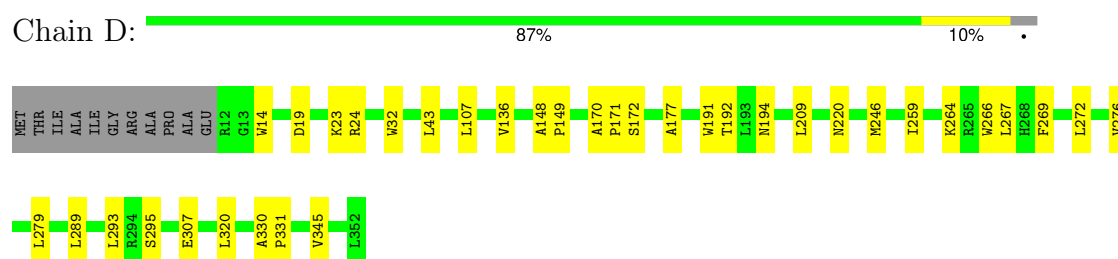
- Molecule 3: Photosystem II CP43 reaction center protein



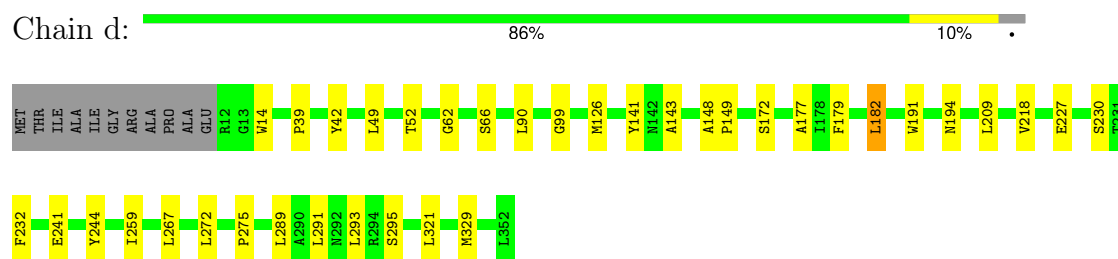
- Molecule 3: Photosystem II CP43 reaction center protein



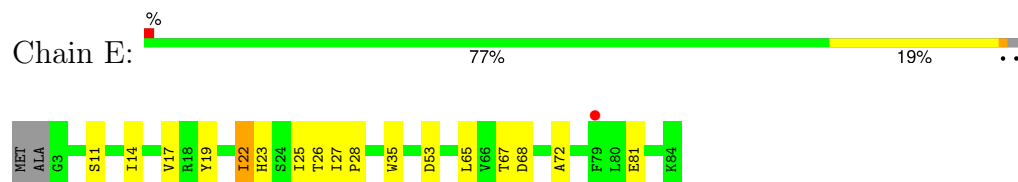
- Molecule 4: Photosystem II D2 protein



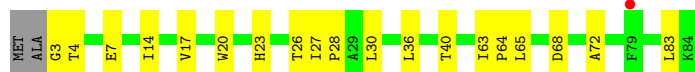
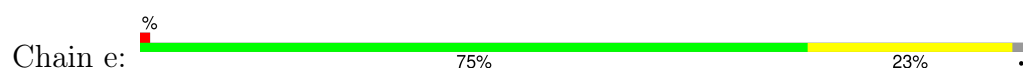
- Molecule 4: Photosystem II D2 protein



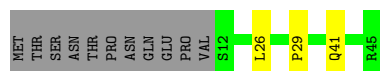
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



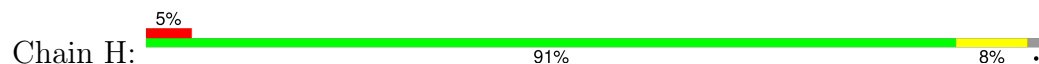
- Molecule 6: Cytochrome b559 subunit beta



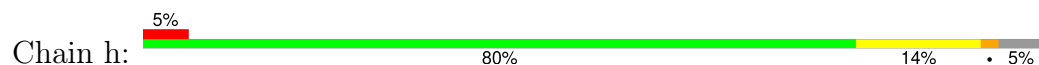
- Molecule 6: Cytochrome b559 subunit beta



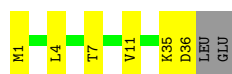
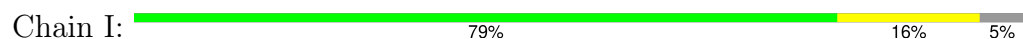
- Molecule 7: Photosystem II reaction center protein H



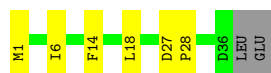
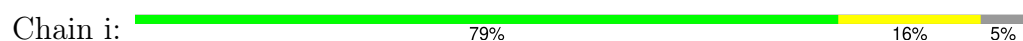
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

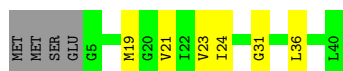


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

Chain J:  75% 15% 10%



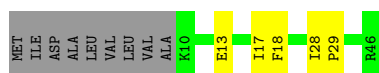
- Molecule 9: Photosystem II reaction center protein J

Chain j:  72% 15% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  70% 11% 20%

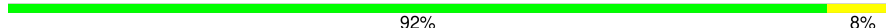


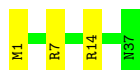
- Molecule 10: Photosystem II reaction center protein K

Chain k:  52% 28% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 8%



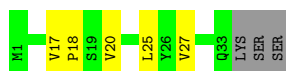
- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 11% 5% 3%



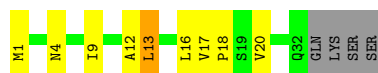
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%



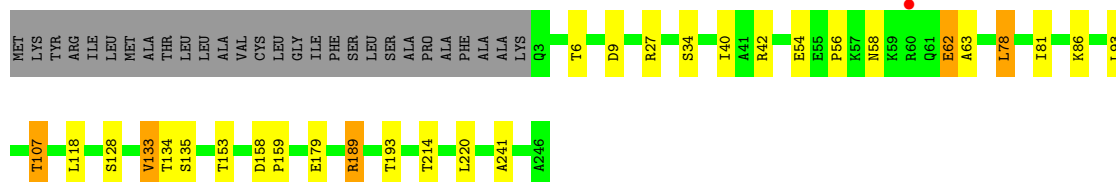
- Molecule 12: Photosystem II reaction center protein M

Chain m:  64% 22% • 11%



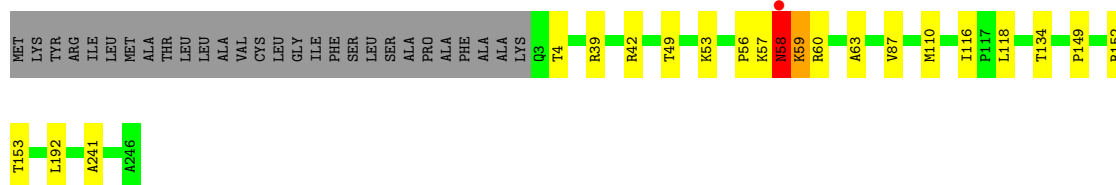
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 9% • 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  82% 7% 10%



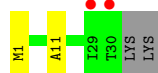
- Molecule 14: Photosystem II reaction center protein T

Chain T:  6% 84% 9% 6%



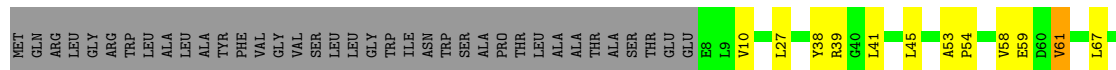
- Molecule 14: Photosystem II reaction center protein T

Chain t:  6% 88% 6% 6%



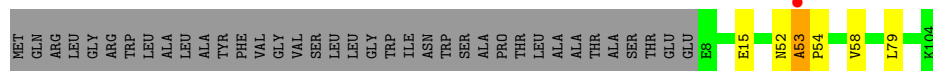
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  63% 9% • 28%

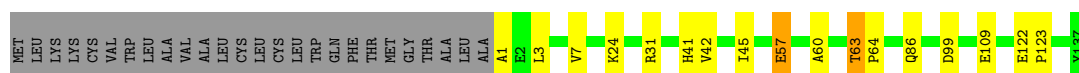




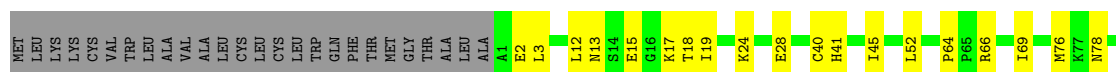
- Molecule 15: Photosystem II 12 kDa extrinsic protein



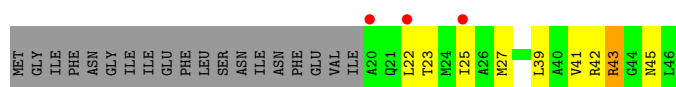
- Molecule 16: Cytochrome c-550



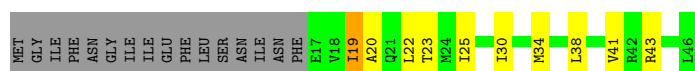
- Molecule 16: Cytochrome c-550



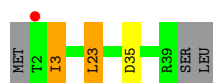
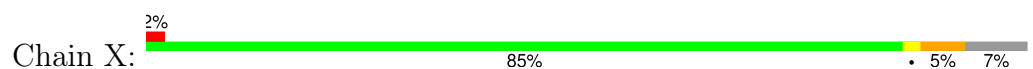
- Molecule 17: Photosystem II reaction center protein Ycf12



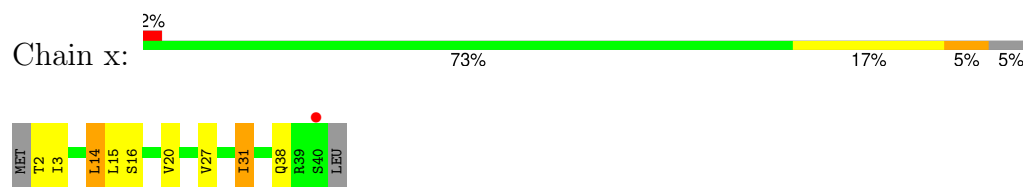
- Molecule 17: Photosystem II reaction center protein Ycf12



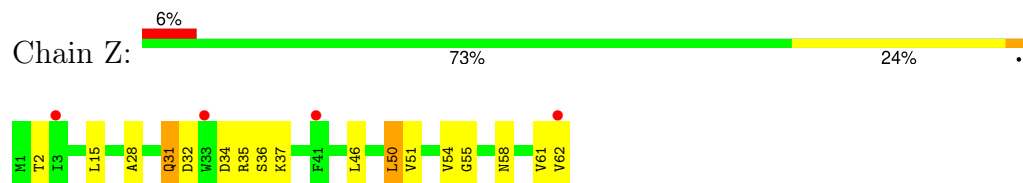
- Molecule 18: Photosystem II reaction center X protein



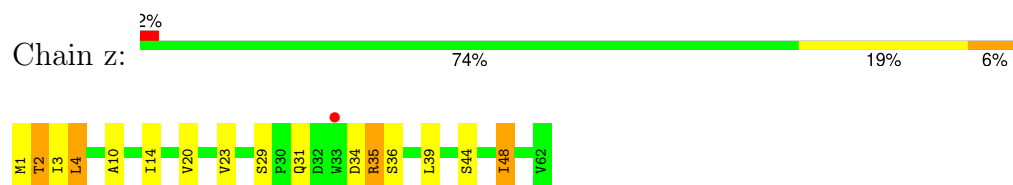
- Molecule 18: Photosystem II reaction center X protein



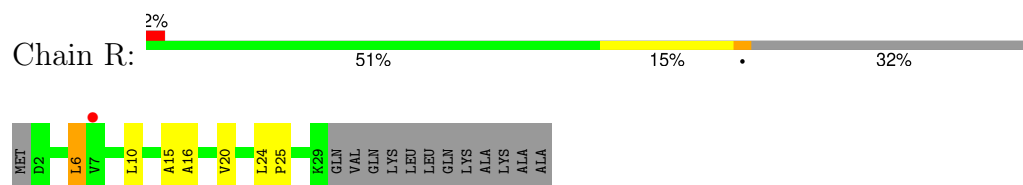
- Molecule 19: Photosystem II reaction center protein Z



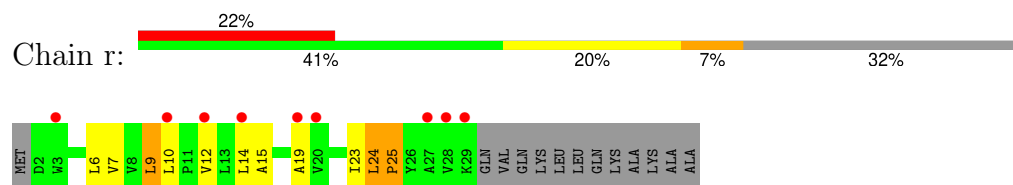
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 221.60Å 307.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 1.89 33.67 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.67-1.89) 89.2 (33.67-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.214 0.171 , 0.214	Depositor DCC
R_{free} test set	5621 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	104284	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: FME, DGD, FE2, PHO, HEM, OEX, HEC, LHG, PL9, CL, BCR, STE, SQD, BCT, LMG, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/2707 (0.0%)	0.68	0/3692
1	a	0.58	1/2704 (0.0%)	0.70	2/3688 (0.1%)
2	B	0.54	1/4161 (0.0%)	0.62	0/5669
2	b	0.52	0/4127	0.60	0/5623
3	C	0.52	0/3546	0.61	0/4828
3	c	0.48	0/3619	0.58	0/4926
4	D	0.59	0/2812	0.63	0/3832
4	d	0.53	0/2821	0.62	0/3844
5	E	0.53	0/688	0.59	0/940
5	e	0.45	0/683	0.57	0/932
6	F	0.59	0/284	0.64	0/387
6	f	0.55	0/284	0.66	0/387
7	H	0.67	0/523	0.69	0/713
7	h	0.54	0/511	0.65	0/697
8	I	0.63	0/293	0.63	0/396
8	i	0.64	0/293	0.65	0/396
9	J	0.48	0/263	0.59	0/356
9	j	0.55	0/263	0.54	0/356
10	K	0.47	0/303	0.66	0/416
10	k	0.57	1/303 (0.3%)	0.55	0/416
11	L	0.72	0/311	0.74	0/422
11	l	0.64	0/303	0.68	0/412
12	M	0.64	0/249	0.71	0/341
12	m	0.68	0/244	0.71	0/334
13	O	0.62	0/1904	0.69	0/2585
13	o	0.61	0/1905	0.69	0/2583
14	T	0.69	0/257	0.74	0/349
14	t	0.70	0/255	0.67	0/346
15	U	0.53	0/785	0.63	0/1064
15	u	0.62	0/785	0.73	0/1064
16	V	0.62	0/1085	0.69	1/1473 (0.1%)
16	v	0.57	0/1085	0.66	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.46	0/197	0.58	0/264
17	y	0.42	0/219	0.56	0/294
18	X	0.48	0/284	0.60	0/384
18	x	0.42	0/289	0.52	0/391
19	Z	0.43	0/490	0.58	0/669
19	z	0.55	1/488 (0.2%)	0.56	0/666
20	R	0.35	0/227	0.54	0/313
20	r	0.33	0/227	0.44	0/313
All	All	0.56	5/42777 (0.0%)	0.64	3/58234 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1
15	u	0	1
16	V	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	13.22	1.61	1.54
19	z	23	VAL	CA-CB	-7.81	1.50	1.54
1	a	110	GLY	CA-C	6.98	1.56	1.51
10	k	28	ILE	CA-CB	-6.30	1.50	1.54
2	B	221	PRO	CA-C	6.26	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	110	GLY	O-C-N	12.76	125.66	121.07
1	a	131	TRP	CA-CB-CG	-5.03	104.05	113.60
16	V	63	THR	C-N-CD	-5.00	104.49	125.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain
15	u	52	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2518	2519	14	0
1	a	2619	2510	2510	21	0
2	B	4005	3873	3867	22	0
2	b	3984	3840	3842	42	0
3	C	3425	3350	3339	19	0
3	c	3500	3426	3426	31	0
4	D	2717	2621	2621	28	0
4	d	2723	2627	2627	21	0
5	E	666	651	651	11	0
5	e	664	648	648	16	0
6	F	275	282	282	2	0
6	f	275	282	282	8	0
7	H	510	532	532	4	0
7	h	498	518	518	6	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	7	0
9	j	257	268	268	6	0
10	K	293	305	305	2	0
10	k	293	305	305	6	0
11	L	304	316	316	2	0
11	l	296	304	304	4	0
12	M	256	269	269	3	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	17	0
13	o	1874	1846	1846	10	0
14	T	258	261	261	1	0
14	t	256	256	256	1	0
15	U	774	773	773	7	0
15	u	774	773	773	6	0
16	V	1064	1073	1073	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	v	1064	1073	1073	18	0
17	Y	196	217	217	5	0
17	y	218	241	241	6	0
18	X	281	312	312	3	0
18	x	286	316	314	4	0
19	Z	479	516	516	8	0
19	z	477	509	509	9	0
20	R	221	238	238	4	0
20	r	221	238	238	7	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	3	0
23	B	1035	1139	1139	14	0
23	C	839	922	922	20	0
23	D	195	216	216	4	0
23	a	260	288	288	2	0
23	b	970	1067	1067	18	0
23	c	839	919	919	19	0
23	d	130	144	144	3	0
23	h	65	72	72	2	0
24	A	64	74	74	3	0
24	D	64	74	74	1	0
24	a	64	74	74	1	0
24	d	64	74	74	1	0
25	A	40	56	56	0	0
25	B	120	168	168	8	0
25	C	120	168	168	4	0
25	D	40	56	56	6	0
25	H	40	56	56	3	0
25	K	40	56	56	3	0
25	T	40	56	56	4	0
25	a	40	56	56	3	0
25	b	120	168	168	6	0
25	c	80	112	112	7	0
25	d	40	56	56	2	0
25	k	80	112	112	1	0
25	t	40	56	56	4	0
25	x	40	56	56	3	0
26	A	55	80	80	0	0
26	D	55	80	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	a	55	80	80	2	0
26	d	55	80	80	0	0
27	A	45	35	83	11	0
27	B	44	68	68	1	0
27	C	90	107	152	5	0
27	D	29	35	52	2	0
27	E	44	51	74	6	0
27	H	18	35	35	0	0
27	I	32	54	52	2	0
27	J	12	16	16	2	0
27	M	25	38	38	0	0
27	T	16	30	31	0	0
27	Z	17	35	33	0	0
27	a	22	32	32	0	0
27	b	77	75	131	14	0
27	c	31	59	57	1	0
27	d	39	42	61	4	0
27	e	39	0	67	5	0
27	i	18	12	24	3	0
27	j	28	16	44	4	0
27	l	18	35	35	3	0
27	m	27	45	45	0	0
27	t	32	48	48	0	0
27	x	20	35	35	1	0
27	z	9	15	14	0	0
28	A	48	66	66	2	0
28	B	45	64	60	1	0
28	C	84	113	106	3	0
28	D	101	146	142	5	0
28	M	51	72	71	0	0
28	a	55	86	86	1	0
28	b	130	158	179	14	0
28	c	173	246	240	3	0
28	d	44	58	58	1	0
29	A	106	70	149	12	0
29	F	36	45	45	2	0
29	a	108	77	156	10	0
29	b	49	64	65	1	0
29	f	41	48	49	2	0
29	l	54	77	78	0	0
30	A	66	96	96	7	0
30	C	186	246	245	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	62	82	80	1	0
30	c	186	246	242	4	0
30	h	62	82	80	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	D	4	1	1	0	0
32	a	4	1	1	0	0
33	D	145	215	215	4	0
33	E	49	74	74	4	0
33	L	49	74	74	0	0
33	a	42	57	57	1	0
33	d	137	199	199	7	0
33	l	49	74	74	1	0
34	F	43	30	30	2	0
34	f	43	30	30	7	0
35	V	43	32	30	0	0
35	v	43	32	30	3	0
36	A	144	0	0	2	0
36	B	202	0	0	2	0
36	C	180	0	0	2	0
36	D	137	0	0	4	0
36	E	20	0	0	0	0
36	F	11	0	0	0	0
36	H	26	0	0	0	0
36	I	9	0	0	1	0
36	J	13	0	0	1	0
36	K	4	0	0	0	0
36	L	10	0	0	0	0
36	M	7	0	0	0	0
36	O	104	0	0	3	0
36	T	9	0	0	0	0
36	U	45	0	0	2	0
36	V	82	0	0	1	0
36	X	12	0	0	0	0
36	Y	1	0	0	0	0
36	a	115	0	0	2	0
36	b	200	0	0	1	0
36	c	171	0	0	4	0
36	d	125	0	0	1	0
36	e	10	0	0	1	0
36	f	10	0	0	1	0
36	h	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	i	5	0	0	0	0
36	j	6	0	0	1	0
36	k	5	0	0	2	0
36	l	15	0	0	0	0
36	m	7	0	0	0	0
36	o	110	0	0	0	0
36	t	12	0	0	0	0
36	u	61	0	0	0	0
36	v	59	0	0	1	0
36	x	7	0	0	0	0
36	y	2	0	0	0	0
36	z	1	0	0	0	0
All	All	52524	51760	52200	549	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 5.

The worst 5 of 549 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)
16:v:40:CYS:SG	35:v:201:HEC:CAC	2.05	1.45
2:b:267:LEU:HD13	28:b:619:LMG:C2	1.94	0.98
2:b:267:LEU:HD22	28:b:619:LMG:C1	1.95	0.96
28:C:517:LMG:HO4	28:C:517:LMG:HO5	1.17	0.93
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.50	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	328 (99%)	3 (1%)	1 (0%)	36	29
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	493 (98%)	10 (2%)	1 (0%)	43	36
3	C	442/461 (96%)	432 (98%)	9 (2%)	1 (0%)	43	36
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	36
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	10 (4%)	2 (1%)	16	8
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	16	8
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	4
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	10
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	2
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	0	1 (4%)	2	0
All	All	5232/5700 (92%)	5089 (97%)	129 (2%)	14 (0%)	36	29

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	o	58	ASN
15	u	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	87
1	a	269/280 (96%)	256 (95%)	13 (5%)	23	15
2	B	408/407 (100%)	400 (98%)	8 (2%)	48	46
2	b	403/407 (99%)	392 (97%)	11 (3%)	39	34
3	C	346/362 (96%)	341 (99%)	5 (1%)	59	59
3	c	354/362 (98%)	340 (96%)	14 (4%)	28	20
4	D	276/283 (98%)	273 (99%)	3 (1%)	65	67
4	d	277/283 (98%)	267 (96%)	10 (4%)	31	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	7
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	19
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	47
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	6
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	8
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	29
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	19
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	4
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	26
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	31
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	23
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	23
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	14
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	25
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	21
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	80 (95%)	4 (5%)	23	15
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	63
16	V	117/138 (85%)	111 (95%)	6 (5%)	21	13
16	v	117/138 (85%)	108 (92%)	9 (8%)	12	5
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	2
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	8
18	x	31/34 (91%)	26 (84%)	5 (16%)	2	1
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	22/33 (67%)	21 (96%)	1 (4%)	24	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	r	22/33 (67%)	18 (82%)	4 (18%)	2	0
All	All	4322/4654 (93%)	4157 (96%)	165 (4%)	29	21

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	7	LEU
16	v	106	ASN
9	j	21	VAL
13	o	39	ARG
18	x	2	THR

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

Mol	Chain	Res	Type
5	e	74	GLN
13	o	196	GLN
5	e	82	GLN
13	o	36	GLN
16	v	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.91	1 (12%)	8,9,11	1.42	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	1.01	0	8,9,11	1.34	1 (12%)
12	FME	M	1	12	8,9,10	0.86	0	8,9,11	0.99	0
14	FME	t	1	14	8,9,10	1.27	1 (12%)	8,9,11	1.27	1 (12%)
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.93	0
14	FME	T	1	14	8,9,10	0.91	0	8,9,11	1.35	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.90	1.42	1.46
12	m	1	FME	CA-N	-2.04	1.43	1.46
8	I	1	FME	CA-N	-2.01	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.88	118.39	122.82
14	t	1	FME	CB-CA-N	2.60	115.25	110.52
8	i	1	FME	CA-N-CN	-2.47	119.02	122.82
14	T	1	FME	O1-CN-N	-2.07	119.96	125.32

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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
23	CLA	c	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.26	9 (10%)
27	STE	b	625	-	15,15,19	0.86	0	15,15,19	1.13	2 (13%)
32	BCT	D	401	21	3,3,3	1.08	0	2,3,3	3.96	2 (100%)
27	STE	e	104	-	12,12,19	0.64	0	12,12,19	1.25	2 (16%)
25	BCR	C	515	-	41,41,41	1.32	4 (9%)	56,56,56	1.34	7 (12%)
25	BCR	k	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.15	3 (5%)
27	STE	M	102	-	14,14,19	0.76	0	14,14,19	0.98	1 (7%)
23	CLA	B	613	2	69,73,73	1.51	8 (11%)	82,113,113	1.12	6 (7%)
23	CLA	c	504	36	64,68,73	1.36	6 (9%)	76,107,113	1.27	9 (11%)
23	CLA	D	405	4	69,73,73	1.53	10 (14%)	82,113,113	1.21	8 (9%)
25	BCR	k	102	-	41,41,41	1.09	4 (9%)	56,56,56	1.15	4 (7%)
33	LHG	l	102	-	48,48,48	0.84	2 (4%)	51,54,54	1.24	4 (7%)
33	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.15	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	d	409	-	44,44,55	1.11	4 (9%)	52,52,63	1.33	7 (13%)
27	STE	E	102	-	11,11,19	1.00	1 (9%)	11,11,19	0.94	0
23	CLA	B	602	2	69,73,73	1.38	7 (10%)	82,113,113	1.21	7 (8%)
27	STE	m	101	-	11,11,19	0.80	0	11,11,19	0.98	1 (9%)
25	BCR	c	514	-	41,41,41	1.28	3 (7%)	56,56,56	1.29	6 (10%)
23	CLA	C	508	3	69,73,73	1.41	7 (10%)	82,113,113	1.39	11 (13%)
33	LHG	L	101	-	48,48,48	0.98	1 (2%)	51,54,54	1.29	8 (15%)
23	CLA	C	511	3	69,73,73	1.44	10 (14%)	82,113,113	1.26	9 (10%)
27	STE	b	624	-	19,19,19	0.67	0	19,19,19	1.14	0
23	CLA	b	614	2	69,73,73	1.28	10 (14%)	82,113,113	1.34	9 (10%)
29	SQD	l	101	-	52,54,54	1.55	10 (19%)	62,65,65	1.91	7 (11%)
27	STE	A	416	-	16,16,19	0.68	0	15,15,19	0.28	0
25	BCR	K	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
24	PHO	D	402	-	58,69,69	1.75	11 (18%)	55,99,99	1.43	6 (10%)
23	CLA	b	605	2	69,73,73	1.67	7 (10%)	82,113,113	1.39	7 (8%)
28	LMG	A	411	-	48,48,55	1.05	3 (6%)	56,56,63	1.35	6 (10%)
23	CLA	B	614	2	69,73,73	1.23	4 (5%)	82,113,113	1.29	10 (12%)
27	STE	C	527	-	7,7,19	0.65	0	6,6,19	0.41	0
23	CLA	C	506	3	69,73,73	1.56	7 (10%)	82,113,113	1.13	6 (7%)
28	LMG	C	524	-	48,48,55	1.03	4 (8%)	56,56,63	1.23	3 (5%)
23	CLA	c	511	3	69,73,73	1.27	7 (10%)	82,113,113	1.34	6 (7%)
23	CLA	c	512	3	69,73,73	1.24	7 (10%)	82,113,113	1.49	10 (12%)
25	BCR	a	409	-	41,41,41	1.13	4 (9%)	56,56,56	1.17	5 (8%)
23	CLA	A	407	1	58,62,73	1.61	5 (8%)	68,99,113	1.34	7 (10%)
24	PHO	A	406	-	58,69,69	1.89	10 (17%)	55,99,99	1.31	7 (12%)
27	STE	b	626	-	9,9,19	0.41	0	8,8,19	0.71	0
23	CLA	b	606	36	69,73,73	1.10	5 (7%)	82,113,113	1.26	7 (8%)
25	BCR	D	406	-	41,41,41	1.24	2 (4%)	56,56,56	1.18	5 (8%)
27	STE	A	410	-	8,8,19	0.41	0	7,7,19	0.72	0
27	STE	m	102	-	14,14,19	0.61	0	13,13,19	0.59	0
27	STE	C	525	-	11,11,19	0.67	0	11,11,19	1.44	3 (27%)
23	CLA	b	615	2	64,68,73	1.25	8 (12%)	76,107,113	1.38	9 (11%)
23	CLA	B	609	2	69,73,73	1.17	5 (7%)	82,113,113	1.27	6 (7%)
23	CLA	a	411	36	69,73,73	1.47	8 (11%)	82,113,113	1.28	7 (8%)
23	CLA	d	402	4	69,73,73	1.30	7 (10%)	82,113,113	1.41	12 (14%)
33	LHG	d	408	-	38,38,48	0.99	2 (5%)	41,44,54	1.14	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	D	404	4	69,73,73	1.09	3 (4%)	82,113,113	1.22	9 (10%)
27	STE	t	103	-	17,17,19	0.67	0	17,17,19	1.05	0
28	LMG	c	524	-	49,49,55	1.03	4 (8%)	57,57,63	1.31	6 (10%)
33	LHG	E	101	-	48,48,48	1.11	4 (8%)	51,54,54	1.14	2 (3%)
30	DGD	c	521	-	63,63,67	0.92	4 (6%)	77,77,81	1.48	11 (14%)
27	STE	a	416	-	9,9,19	0.74	0	8,8,19	0.40	0
27	STE	B	623	-	14,14,19	0.55	0	13,13,19	0.74	0
29	SQD	F	102	-	34,36,54	1.65	6 (17%)	42,45,65	3.00	8 (19%)
33	LHG	d	406	-	48,48,48	0.89	2 (4%)	51,54,54	1.38	7 (13%)
27	STE	t	102	-	13,13,19	0.71	0	13,13,19	1.04	1 (7%)
23	CLA	c	506	3	69,73,73	1.39	10 (14%)	82,113,113	1.23	7 (8%)
23	CLA	d	403	4	69,73,73	1.30	10 (14%)	82,113,113	1.06	6 (7%)
28	LMG	b	619	-	22,22,55	1.03	2 (9%)	23,23,63	1.04	1 (4%)
28	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.44	11 (18%)
23	CLA	B	608	2	69,73,73	1.04	5 (7%)	82,113,113	1.37	7 (8%)
25	BCR	c	515	-	41,41,41	1.38	3 (7%)	56,56,56	1.39	9 (16%)
23	CLA	a	408	1	69,73,73	1.37	9 (13%)	82,113,113	1.36	9 (10%)
27	STE	i	101	-	11,11,19	0.86	0	11,11,19	1.03	0
35	HEC	V	201	16	50,50,50	1.52	7 (14%)	68,82,82	1.28	8 (11%)
27	STE	B	622	-	11,11,19	0.90	0	11,11,19	0.96	0
30	DGD	C	523	-	63,63,67	0.95	4 (6%)	77,77,81	1.33	9 (11%)
23	CLA	C	512	3	69,73,73	1.34	12 (17%)	82,113,113	1.30	13 (15%)
23	CLA	B	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.37	12 (14%)
25	BCR	T	101	-	41,41,41	1.33	6 (14%)	56,56,56	1.43	8 (14%)
23	CLA	b	604	2	69,73,73	1.22	8 (11%)	82,113,113	1.39	13 (15%)
27	STE	E	104	-	19,19,19	0.82	1 (5%)	19,19,19	0.92	1 (5%)
23	CLA	C	504	36	63,67,73	1.25	9 (14%)	74,105,113	1.25	9 (12%)
23	CLA	B	611	2	69,73,73	1.40	7 (10%)	82,113,113	1.56	9 (10%)
23	CLA	c	502	3	69,73,73	1.07	6 (8%)	82,113,113	1.31	6 (7%)
23	CLA	B	615	2	69,73,73	1.29	9 (13%)	82,113,113	1.13	6 (7%)
25	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.28	8 (14%)
27	STE	T	102	-	15,15,19	0.53	0	14,14,19	0.55	0
23	CLA	c	509	3	69,73,73	1.17	7 (10%)	82,113,113	1.42	9 (10%)
23	CLA	C	509	3	69,73,73	1.27	9 (13%)	82,113,113	1.34	9 (10%)
28	LMG	c	518	-	29,29,55	1.15	2 (6%)	31,31,63	1.10	2 (6%)
23	CLA	C	513	3	69,73,73	1.40	9 (13%)	82,113,113	1.44	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	406	36	69,73,73	1.24	10 (14%)	82,113,113	1.53	10 (12%)
23	CLA	c	508	3	68,72,73	1.45	8 (11%)	80,111,113	1.43	10 (12%)
30	DGD	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	12 (15%)
27	STE	A	417	-	10,10,19	0.42	0	9,9,19	0.84	0
33	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.15	5 (9%)
23	CLA	b	608	2	69,73,73	1.32	6 (8%)	82,113,113	1.43	11 (13%)
27	STE	A	415	-	7,7,19	0.45	0	6,6,19	0.58	0
27	STE	C	526	-	15,15,19	0.60	0	14,14,19	0.47	0
28	LMG	c	523	-	48,48,55	1.04	2 (4%)	56,56,63	1.32	8 (14%)
35	HEC	v	201	16	50,50,50	1.64	5 (10%)	68,82,82	1.22	4 (5%)
27	STE	e	103	-	8,8,19	0.41	0	7,7,19	0.71	0
27	STE	j	101	-	11,11,19	0.81	0	11,11,19	0.94	0
27	STE	a	417	-	11,11,19	0.79	0	11,11,19	1.16	2 (18%)
23	CLA	c	503	3	69,73,73	1.13	6 (8%)	82,113,113	1.25	7 (8%)
34	HEM	F	101	6,5	50,50,50	1.42	8 (16%)	67,82,82	1.31	9 (13%)
23	CLA	b	612	2	69,73,73	1.23	9 (13%)	82,113,113	1.20	10 (12%)
23	CLA	C	505	3	69,73,73	1.23	7 (10%)	82,113,113	1.22	5 (6%)
28	LMG	B	620	-	45,45,55	1.04	2 (4%)	53,53,63	1.37	4 (7%)
28	LMG	D	408	-	50,50,55	1.07	3 (6%)	58,58,63	1.28	4 (6%)
28	LMG	c	522	-	46,46,55	1.21	5 (10%)	54,54,63	1.27	7 (12%)
23	CLA	b	603	2	69,73,73	1.20	6 (8%)	82,113,113	1.44	9 (10%)
23	CLA	B	607	36	69,73,73	1.21	8 (11%)	82,113,113	1.43	5 (6%)
27	STE	D	414	-	8,8,19	0.40	0	7,7,19	0.99	0
27	STE	d	410	-	16,16,19	0.93	0	16,16,19	0.81	0
27	STE	e	102	-	7,7,19	0.46	0	6,6,19	0.61	0
23	CLA	h	101	36	69,73,73	1.31	9 (13%)	82,113,113	1.53	10 (12%)
27	STE	D	413	-	19,19,19	0.71	0	19,19,19	1.30	2 (10%)
28	LMG	C	517	-	35,35,55	1.41	3 (8%)	43,43,63	1.72	8 (18%)
25	BCR	t	101	-	41,41,41	1.28	3 (7%)	56,56,56	1.30	6 (10%)
27	STE	C	516	-	13,13,19	0.77	0	13,13,19	0.87	0
30	DGD	c	520	-	63,63,67	1.32	11 (17%)	77,77,81	1.54	16 (20%)
23	CLA	B	606	2	69,73,73	1.46	10 (14%)	82,113,113	1.53	8 (9%)
27	STE	Z	101	-	16,16,19	0.52	0	15,15,19	0.50	0
25	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.11	3 (5%)
27	STE	b	627	-	10,10,19	0.41	0	9,9,19	0.68	0
32	BCT	a	404	21	3,3,3	1.16	0	2,3,3	3.44	2 (100%)
25	BCR	x	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.32	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	C	514	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
25	BCR	B	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	9 (16%)
29	SQD	A	412	-	50,52,54	1.57	8 (16%)	60,63,65	1.99	14 (23%)
23	CLA	B	605	2	69,73,73	1.12	6 (8%)	82,113,113	1.31	9 (10%)
29	SQD	f	102	-	39,41,54	1.71	9 (23%)	49,52,65	1.68	8 (16%)
33	LHG	D	411	-	46,46,48	1.03	3 (6%)	49,52,54	1.29	4 (8%)
27	STE	e	101	-	8,8,19	0.58	0	7,7,19	0.61	0
27	STE	H	103	-	17,17,19	0.59	0	16,16,19	0.66	0
23	CLA	b	609	36	69,73,73	1.24	8 (11%)	82,113,113	1.49	12 (14%)
23	CLA	c	513	3	69,73,73	1.43	11 (15%)	82,113,113	1.07	5 (6%)
25	BCR	b	616	-	41,41,41	1.18	4 (9%)	56,56,56	1.35	8 (14%)
27	STE	C	519	-	6,6,19	0.47	0	5,5,19	0.80	0
30	DGD	h	102	-	63,63,67	1.16	5 (7%)	77,77,81	1.45	13 (16%)
33	LHG	a	413	-	41,41,48	1.51	7 (17%)	44,47,54	1.35	4 (9%)
25	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	7 (12%)
27	STE	C	529	-	13,13,19	0.45	0	12,12,19	0.54	0
27	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.55	0
29	SQD	a	414	-	52,54,54	1.67	9 (17%)	62,65,65	1.67	7 (11%)
34	HEM	f	101	6,5	50,50,50	1.47	7 (14%)	67,82,82	1.45	7 (10%)
29	SQD	a	412	-	52,54,54	1.43	7 (13%)	62,65,65	2.08	18 (29%)
30	DGD	C	521	-	63,63,67	1.22	8 (12%)	77,77,81	1.51	12 (15%)
25	BCR	B	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.19	5 (8%)
30	DGD	C	522	-	63,63,67	1.48	10 (15%)	77,77,81	1.27	7 (9%)
23	CLA	b	602	2	69,73,73	1.18	7 (10%)	82,113,113	1.43	13 (15%)
28	LMG	a	415	-	55,55,55	1.45	8 (14%)	63,63,63	1.54	8 (12%)
29	SQD	A	413	-	52,54,54	1.66	9 (17%)	62,65,65	1.84	12 (19%)
23	CLA	B	604	2	69,73,73	1.21	5 (7%)	82,113,113	1.54	5 (6%)
23	CLA	b	611	2	69,73,73	1.51	9 (13%)	82,113,113	1.17	7 (8%)
27	STE	c	516	-	12,12,19	0.54	0	11,11,19	0.53	0
23	CLA	C	507	36	69,73,73	1.08	4 (5%)	82,113,113	1.42	11 (13%)
27	STE	B	621	-	16,16,19	0.71	0	16,16,19	0.97	0
23	CLA	C	510	3	69,73,73	1.25	11 (15%)	82,113,113	1.52	10 (12%)
23	CLA	B	601	36	69,73,73	1.43	7 (10%)	82,113,113	1.56	6 (7%)
28	LMG	b	621	-	51,51,55	1.01	4 (7%)	59,59,63	1.46	9 (15%)
28	LMG	b	623	-	55,55,55	1.02	2 (3%)	63,63,63	1.53	10 (15%)
27	STE	C	518	-	4,4,19	0.52	0	3,3,19	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	501	3	69,73,73	1.13	6 (8%)	82,113,113	1.46	7 (8%)
23	CLA	A	404	1	69,73,73	1.23	8 (11%)	82,113,113	1.12	4 (4%)
23	CLA	c	510	3	69,73,73	1.34	5 (7%)	82,113,113	1.41	6 (7%)
28	LMG	D	409	-	51,51,55	1.17	3 (5%)	59,59,63	1.35	5 (8%)
25	BCR	C	520	-	41,41,41	1.18	5 (12%)	56,56,56	1.15	5 (8%)
26	PL9	D	407	-	55,55,55	1.57	7 (12%)	68,69,69	1.59	16 (23%)
27	STE	j	102	-	15,15,19	0.58	0	14,14,19	0.55	0
27	STE	i	102	-	5,5,19	0.51	0	4,4,19	0.43	0
23	CLA	B	616	2	64,68,73	1.19	6 (9%)	76,107,113	1.41	6 (7%)
31	OEX	A	418	36,3,1	0,14,14	-	-	-	-	-
26	PL9	A	409	-	55,55,55	1.24	4 (7%)	68,69,69	1.62	13 (19%)
23	CLA	C	503	3	69,73,73	1.34	9 (13%)	82,113,113	1.42	9 (10%)
30	DGD	c	519	-	63,63,67	1.14	5 (7%)	77,77,81	1.45	11 (14%)
31	OEX	a	418	36,3,1	0,14,14	-	-	-	-	-
23	CLA	A	405	36	69,73,73	1.10	6 (8%)	82,113,113	1.16	8 (9%)
30	DGD	A	414	-	67,67,67	1.33	10 (14%)	81,81,81	1.54	15 (18%)
23	CLA	c	505	3	69,73,73	1.18	8 (11%)	82,113,113	1.14	4 (4%)
27	STE	I	102	-	16,16,19	0.86	0	16,16,19	0.90	1 (6%)
23	CLA	b	601	2	69,73,73	1.22	8 (11%)	82,113,113	1.47	10 (12%)
25	BCR	A	408	-	41,41,41	1.14	4 (9%)	56,56,56	1.37	7 (12%)
26	PL9	a	410	-	55,55,55	0.97	5 (9%)	68,69,69	1.59	12 (17%)
23	CLA	B	610	36	69,73,73	1.49	9 (13%)	82,113,113	1.37	7 (8%)
23	CLA	C	501	3	69,73,73	1.45	9 (13%)	82,113,113	1.38	8 (9%)
25	BCR	B	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	6 (10%)
24	PHO	a	407	-	58,69,69	1.89	11 (18%)	55,99,99	1.47	8 (14%)
27	STE	x	102	-	19,19,19	0.91	1 (5%)	19,19,19	0.85	2 (10%)
23	CLA	B	603	2	69,73,73	1.23	8 (11%)	82,113,113	1.51	11 (13%)
27	STE	J	101	-	11,11,19	0.61	0	11,11,19	1.48	2 (18%)
23	CLA	C	502	3	69,73,73	1.19	6 (8%)	82,113,113	1.34	6 (7%)
23	CLA	b	607	2	69,73,73	1.21	7 (10%)	82,113,113	1.23	8 (9%)
33	LHG	D	412	-	48,48,48	1.02	2 (4%)	51,54,54	1.33	6 (11%)
23	CLA	b	613	2	69,73,73	1.22	7 (10%)	82,113,113	1.55	10 (12%)
24	PHO	d	401	-	58,69,69	2.01	9 (15%)	55,99,99	1.59	11 (20%)
27	STE	E	103	-	11,11,19	0.49	0	10,10,19	0.62	0
27	STE	C	528	-	13,13,19	0.49	0	12,12,19	0.64	0
29	SQD	b	620	-	47,49,54	1.57	8 (17%)	57,60,65	2.22	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	STE	d	411	-	11,11,19	0.84	0	11,11,19	0.88	0
27	STE	b	622	-	19,19,19	0.78	1 (5%)	19,19,19	0.91	1 (5%)
27	STE	l	103	-	17,17,19	0.37	0	16,16,19	0.70	0
23	CLA	D	403	36	69,73,73	1.28	10 (14%)	82,113,113	1.23	3 (3%)
27	STE	c	517	-	17,17,19	0.59	0	16,16,19	0.55	0
27	STE	z	101	-	8,8,19	0.53	0	7,7,19	0.55	0
27	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.44	0
26	PL9	d	405	-	55,55,55	1.54	9 (16%)	68,69,69	1.57	12 (17%)
23	CLA	b	610	2	69,73,73	0.97	3 (4%)	82,113,113	1.33	10 (12%)
27	STE	d	412	-	9,9,19	0.51	0	8,8,19	0.60	0
25	BCR	b	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.16	8 (14%)
23	CLA	a	405	1	69,73,73	1.22	9 (13%)	82,113,113	1.26	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
23	CLA	c	507	36	-	7/39/115/115	-
27	STE	b	625	-	-	6/13/13/17	-
27	STE	e	104	-	-	5/10/10/17	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
25	BCR	k	101	-	-	10/29/63/63	0/2/2/2
27	STE	M	102	-	-	9/12/12/17	-
23	CLA	B	613	2	-	11/39/115/115	-
23	CLA	c	504	36	-	4/33/109/115	-
23	CLA	D	405	4	-	12/39/115/115	-
25	BCR	k	102	-	-	1/29/63/63	0/2/2/2
33	LHG	l	102	-	-	17/53/53/53	-
33	LHG	D	410	-	-	21/53/53/53	-
28	LMG	d	409	-	-	13/39/59/70	0/1/1/1
27	STE	E	102	-	-	5/9/9/17	-
23	CLA	B	602	2	-	8/39/115/115	-
27	STE	m	101	-	-	4/9/9/17	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
23	CLA	C	508	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	L	101	-	-	12/53/53/53	-
23	CLA	C	511	3	-	2/39/115/115	-
27	STE	b	624	-	-	7/17/17/17	-
23	CLA	b	614	2	-	5/39/115/115	-
29	SQD	l	101	-	-	23/49/69/69	0/1/1/1
27	STE	A	416	-	-	9/14/14/17	-
25	BCR	K	101	-	-	6/29/63/63	0/2/2/2
24	PHO	D	402	-	-	0/37/103/103	0/5/6/6
23	CLA	b	605	2	-	5/39/115/115	-
28	LMG	A	411	-	-	17/43/63/70	0/1/1/1
23	CLA	B	614	2	-	10/39/115/115	-
27	STE	C	527	-	-	4/5/5/17	-
23	CLA	C	506	3	-	8/39/115/115	-
28	LMG	C	524	-	-	10/43/63/70	0/1/1/1
23	CLA	c	511	3	-	7/39/115/115	-
23	CLA	c	512	3	-	16/39/115/115	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
23	CLA	A	407	1	-	2/26/102/115	-
24	PHO	A	406	-	-	0/37/103/103	0/5/6/6
27	STE	b	626	-	-	3/7/7/17	-
23	CLA	b	606	36	-	10/39/115/115	-
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
27	STE	A	410	-	-	4/6/6/17	-
27	STE	m	102	-	-	6/12/12/17	-
27	STE	C	525	-	-	4/9/9/17	-
23	CLA	b	615	2	-	9/33/109/115	-
23	CLA	B	609	2	-	3/39/115/115	-
23	CLA	a	411	36	-	2/39/115/115	-
23	CLA	d	402	4	-	7/39/115/115	-
33	LHG	d	408	-	-	11/43/43/53	-
23	CLA	D	404	4	-	2/39/115/115	-
27	STE	t	103	-	-	11/15/15/17	-
28	LMG	c	524	-	-	17/44/64/70	0/1/1/1
33	LHG	E	101	-	-	28/53/53/53	-
30	DGD	c	521	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	a	416	-	-	4/7/7/17	-
27	STE	B	623	-	-	7/12/12/17	-
29	SQD	F	102	-	-	12/28/48/69	0/1/1/1
33	LHG	d	406	-	-	18/53/53/53	-
27	STE	t	102	-	-	4/11/11/17	-
23	CLA	c	506	3	-	14/39/115/115	-
23	CLA	d	403	4	-	7/39/115/115	-
28	LMG	b	619	-	-	8/21/21/70	-
28	LMG	M	101	-	-	22/46/66/70	0/1/1/1
23	CLA	B	608	2	-	1/39/115/115	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
23	CLA	a	408	1	-	15/39/115/115	-
27	STE	i	101	-	-	6/9/9/17	-
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
27	STE	B	622	-	-	5/9/9/17	-
30	DGD	C	523	-	-	13/51/91/95	0/2/2/2
23	CLA	C	512	3	-	14/39/115/115	-
23	CLA	B	612	2	-	10/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	b	604	2	-	4/39/115/115	-
27	STE	E	104	-	-	13/17/17/17	-
23	CLA	C	504	36	-	5/32/108/115	-
23	CLA	B	611	2	-	6/39/115/115	-
23	CLA	c	502	3	-	2/39/115/115	-
23	CLA	B	615	2	-	10/39/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	STE	T	102	-	-	8/13/13/17	-
23	CLA	c	509	3	-	10/39/115/115	-
23	CLA	C	509	3	-	10/39/115/115	-
28	LMG	c	518	-	-	9/31/31/70	-
23	CLA	C	513	3	-	12/39/115/115	-
23	CLA	a	406	36	-	5/39/115/115	-
23	CLA	c	508	3	-	6/38/114/115	-
30	DGD	H	102	-	-	21/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	A	417	-	-	5/8/8/17	-
33	LHG	d	407	-	-	13/53/53/53	-
23	CLA	b	608	2	-	3/39/115/115	-
27	STE	A	415	-	-	4/5/5/17	-
27	STE	C	526	-	-	4/13/13/17	-
35	HEC	v	201	16	1/1/7/7	5/14/54/54	-
28	LMG	c	523	-	-	21/43/63/70	0/1/1/1
27	STE	e	103	-	-	4/6/6/17	-
27	STE	j	101	-	-	6/9/9/17	-
27	STE	a	417	-	-	4/9/9/17	-
23	CLA	c	503	3	-	8/39/115/115	-
34	HEM	F	101	6,5	-	2/14/54/54	-
23	CLA	b	612	2	-	4/39/115/115	-
23	CLA	C	505	3	-	10/39/115/115	-
28	LMG	B	620	-	-	13/40/60/70	0/1/1/1
28	LMG	D	408	-	-	18/45/65/70	0/1/1/1
28	LMG	c	522	-	-	17/41/61/70	0/1/1/1
23	CLA	b	603	2	-	11/39/115/115	-
23	CLA	B	607	36	-	3/39/115/115	-
27	STE	D	414	-	-	5/6/6/17	-
27	STE	d	410	-	-	4/14/14/17	-
27	STE	e	102	-	-	3/5/5/17	-
23	CLA	h	101	36	-	23/39/115/115	-
27	STE	D	413	-	-	5/17/17/17	-
28	LMG	C	517	-	-	17/30/50/70	0/1/1/1
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
27	STE	C	516	-	-	5/11/11/17	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
23	CLA	B	606	2	-	9/39/115/115	-
27	STE	Z	101	-	-	9/14/14/17	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	STE	b	627	-	-	6/8/8/17	-
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
25	BCR	C	514	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
29	SQD	A	412	-	-	19/47/67/69	0/1/1/1
23	CLA	B	605	2	-	6/39/115/115	-
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
33	LHG	D	411	-	-	13/51/51/53	-
27	STE	e	101	-	-	2/6/6/17	-
27	STE	H	103	-	-	8/15/15/17	-
23	CLA	b	609	36	-	6/39/115/115	-
23	CLA	c	513	3	-	18/39/115/115	-
25	BCR	b	616	-	-	4/29/63/63	0/2/2/2
27	STE	C	519	-	-	1/4/4/17	-
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
33	LHG	a	413	-	-	19/46/46/53	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
27	STE	C	529	-	-	6/11/11/17	-
27	STE	I	101	-	-	5/12/12/17	-
29	SQD	a	414	-	-	20/49/69/69	0/1/1/1
34	HEM	f	101	6,5	-	4/14/54/54	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
30	DGD	C	521	-	-	21/51/91/95	0/2/2/2
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
30	DGD	C	522	-	-	18/51/91/95	0/2/2/2
23	CLA	b	602	2	-	12/39/115/115	-
28	LMG	a	415	-	-	26/50/70/70	0/1/1/1
29	SQD	A	413	-	-	16/49/69/69	0/1/1/1
23	CLA	B	604	2	-	8/39/115/115	-
23	CLA	b	611	2	-	6/39/115/115	-
27	STE	c	516	-	-	3/10/10/17	-
23	CLA	C	507	36	-	7/39/115/115	-
27	STE	B	621	-	-	7/14/14/17	-
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	B	601	36	-	14/39/115/115	-
28	LMG	b	621	-	-	18/46/66/70	0/1/1/1
28	LMG	b	623	-	-	28/50/70/70	0/1/1/1
27	STE	C	518	-	-	1/2/2/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	501	3	-	4/39/115/115	-
23	CLA	A	404	1	-	3/39/115/115	-
23	CLA	c	510	3	-	10/39/115/115	-
28	LMG	D	409	-	-	16/46/66/70	0/1/1/1
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
26	PL9	D	407	-	-	4/53/73/73	0/1/1/1
27	STE	j	102	-	-	6/13/13/17	-
27	STE	i	102	-	-	3/3/3/17	-
23	CLA	B	616	2	-	5/33/109/115	-
26	PL9	A	409	-	-	16/53/73/73	0/1/1/1
23	CLA	C	503	3	-	2/39/115/115	-
30	DGD	c	519	-	-	26/51/91/95	0/2/2/2
23	CLA	A	405	36	-	1/39/115/115	-
30	DGD	A	414	-	-	22/55/95/95	0/2/2/2
23	CLA	c	505	3	-	10/39/115/115	-
27	STE	I	102	-	-	5/14/14/17	-
23	CLA	b	601	2	-	4/39/115/115	-
25	BCR	A	408	-	-	6/29/63/63	0/2/2/2
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
23	CLA	B	610	36	-	2/39/115/115	-
23	CLA	C	501	3	-	4/39/115/115	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
24	PHO	a	407	-	-	2/37/103/103	0/5/6/6
27	STE	x	102	-	-	4/17/17/17	-
23	CLA	B	603	2	-	3/39/115/115	-
27	STE	J	101	-	-	3/9/9/17	-
23	CLA	C	502	3	-	4/39/115/115	-
23	CLA	b	607	2	-	1/39/115/115	-
33	LHG	D	412	-	-	14/53/53/53	-
23	CLA	b	613	2	-	10/39/115/115	-
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
27	STE	E	103	-	-	1/9/9/17	-
27	STE	C	528	-	-	7/11/11/17	-
29	SQD	b	620	-	-	17/44/64/69	0/1/1/1
27	STE	d	411	-	-	1/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	b	622	-	-	8/17/17/17	-
27	STE	l	103	-	-	9/15/15/17	-
23	CLA	D	403	36	-	3/39/115/115	-
27	STE	c	517	-	-	4/15/15/17	-
27	STE	z	101	-	-	3/6/6/17	-
27	STE	M	103	-	-	1/7/7/17	-
26	PL9	d	405	-	-	9/53/73/73	0/1/1/1
23	CLA	b	610	2	-	4/39/115/115	-
27	STE	d	412	-	-	3/7/7/17	-
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
23	CLA	a	405	1	-	4/39/115/115	-

The worst 5 of 904 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	PHO	C1B-C2B	8.60	1.49	1.39
24	a	407	PHO	C1B-C2B	8.57	1.48	1.39
24	A	406	PHO	C1B-C2B	8.56	1.48	1.39
23	A	407	CLA	MG-ND	-8.47	1.89	2.05
23	B	613	CLA	MG-ND	-8.39	1.89	2.05

The worst 5 of 1200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	102	SQD	O6-C1-C2	15.38	131.64	108.27
23	B	601	CLA	C4A-NA-C1A	10.12	111.30	106.68
23	B	604	CLA	C4A-NA-C1A	9.43	110.98	106.68
23	B	606	CLA	C4A-NA-C1A	9.16	110.86	106.68
23	B	607	CLA	C4A-NA-C1A	9.12	110.84	106.68

All (2) chirality outliers are listed below:

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

5 of 1684 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

129 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	507	CLA	2	0
27	e	104	STE	3	0
25	C	515	BCR	1	0
25	k	101	BCR	1	0
23	B	613	CLA	2	0
23	c	504	CLA	1	0
33	l	102	LHG	1	0
33	D	410	LHG	3	0
28	d	409	LMG	1	0
23	B	602	CLA	2	0
25	c	514	BCR	6	0
23	C	508	CLA	4	0
23	C	511	CLA	2	0
27	b	624	STE	13	0
23	b	614	CLA	2	0
27	A	416	STE	8	0
25	K	101	BCR	3	0
24	D	402	PHO	1	0
23	b	605	CLA	1	0
28	A	411	LMG	2	0
23	C	506	CLA	2	0
23	c	511	CLA	2	0
23	c	512	CLA	2	0
25	a	409	BCR	3	0
24	A	406	PHO	3	0
23	b	606	CLA	1	0
25	D	406	BCR	6	0
23	b	615	CLA	1	0
23	a	411	CLA	1	0
23	D	404	CLA	1	0
28	c	524	LMG	1	0
33	E	101	LHG	4	0
29	F	102	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	406	LHG	7	0
23	c	506	CLA	1	0
23	d	403	CLA	3	0
28	b	619	LMG	10	0
25	c	515	BCR	1	0
27	i	101	STE	3	0
27	B	622	STE	1	0
23	C	512	CLA	2	0
23	B	612	CLA	3	0
25	T	101	BCR	4	0
23	b	604	CLA	4	0
27	E	104	STE	1	0
23	C	504	CLA	3	0
23	B	611	CLA	1	0
25	H	101	BCR	3	0
23	c	509	CLA	1	0
23	C	509	CLA	4	0
23	C	513	CLA	2	0
23	c	508	CLA	3	0
30	H	102	DGD	1	0
27	A	417	STE	9	0
27	A	415	STE	1	0
27	C	526	STE	2	0
28	c	523	LMG	1	0
35	v	201	HEC	3	0
23	c	503	CLA	2	0
34	F	101	HEM	2	0
23	b	612	CLA	5	0
23	C	505	CLA	1	0
28	B	620	LMG	1	0
28	D	408	LMG	5	0
28	c	522	LMG	1	0
23	b	603	CLA	1	0
27	D	414	STE	2	0
27	d	410	STE	2	0
23	h	101	CLA	2	0
28	C	517	LMG	3	0
25	t	101	BCR	4	0
30	c	520	DGD	3	0
23	B	606	CLA	1	0
25	d	404	BCR	2	0
27	b	627	STE	7	0

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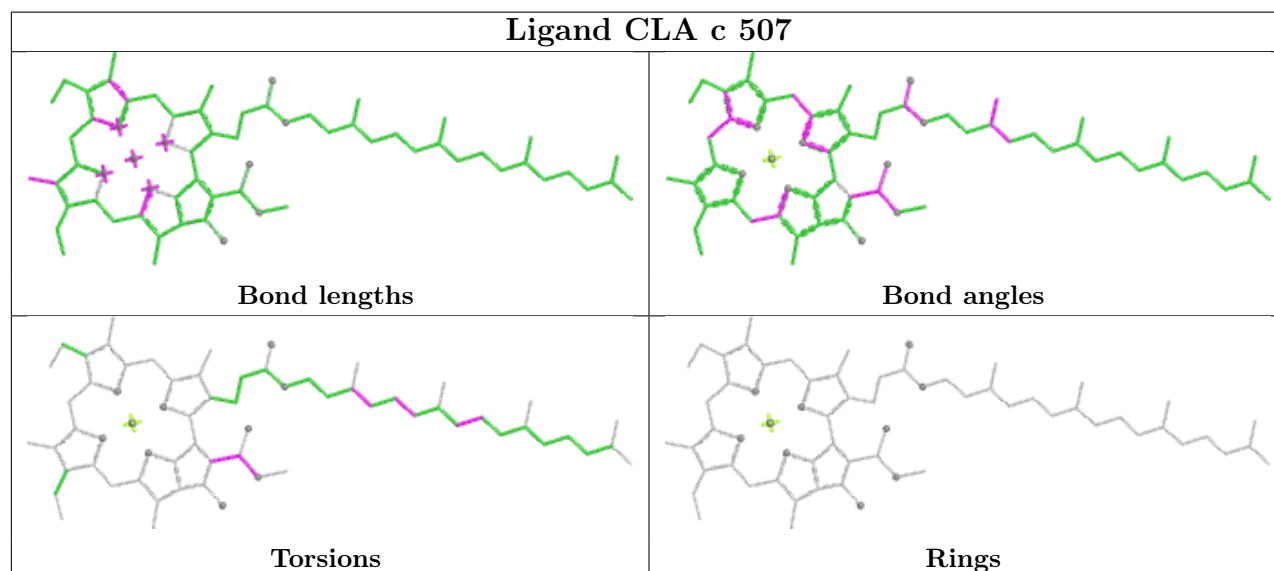
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	x	101	BCR	3	0
25	C	514	BCR	2	0
23	B	605	CLA	2	0
29	f	102	SQD	2	0
27	e	101	STE	4	0
23	b	609	CLA	1	0
23	c	513	CLA	6	0
25	b	616	BCR	1	0
33	a	413	LHG	1	0
25	b	618	BCR	1	0
27	I	101	STE	2	0
29	a	414	SQD	6	0
34	f	101	HEM	7	0
29	a	412	SQD	4	0
30	C	521	DGD	2	0
25	B	618	BCR	6	0
30	C	522	DGD	3	0
28	a	415	LMG	1	0
29	A	413	SQD	12	0
23	B	604	CLA	1	0
27	c	516	STE	1	0
23	C	507	CLA	3	0
23	C	510	CLA	1	0
23	B	601	CLA	2	0
28	b	621	LMG	2	0
28	b	623	LMG	2	0
23	c	501	CLA	2	0
23	A	404	CLA	3	0
23	c	510	CLA	1	0
25	C	520	BCR	1	0
27	j	102	STE	4	0
23	B	616	CLA	1	0
30	c	519	DGD	1	0
30	A	414	DGD	7	0
23	c	505	CLA	1	0
23	b	601	CLA	1	0
26	a	410	PL9	2	0
25	B	619	BCR	2	0
24	a	407	PHO	1	0
27	x	102	STE	1	0
27	J	101	STE	2	0
23	C	502	CLA	1	0

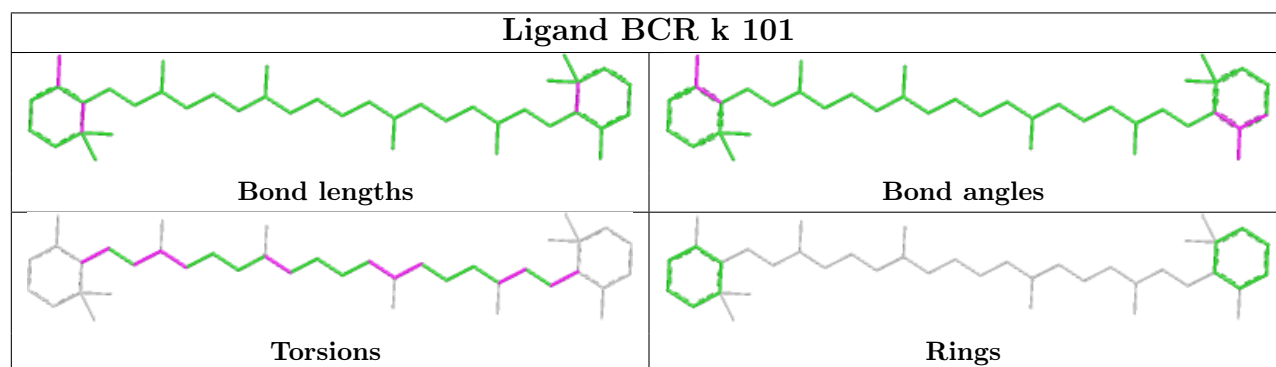
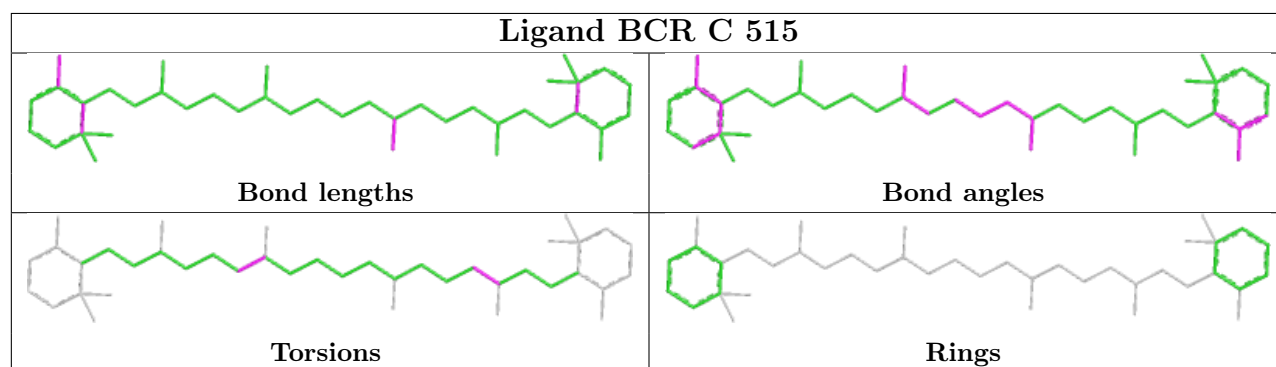
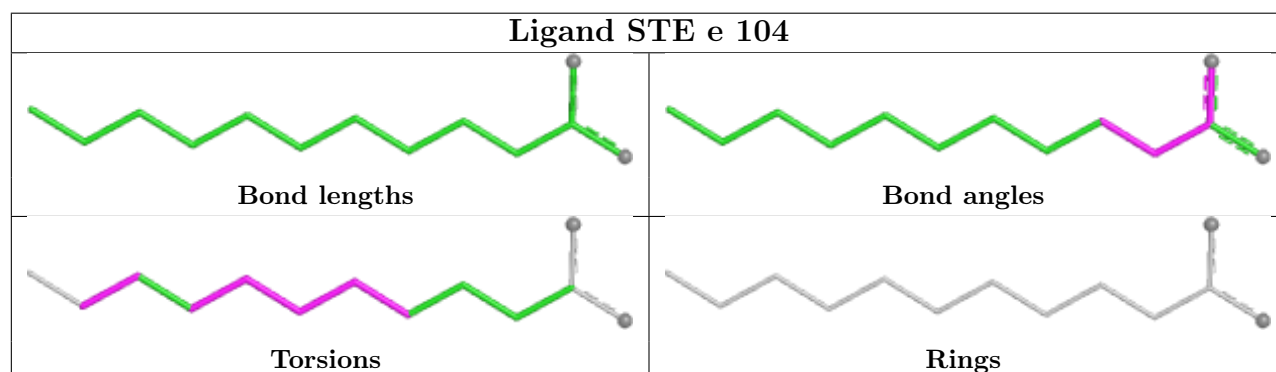
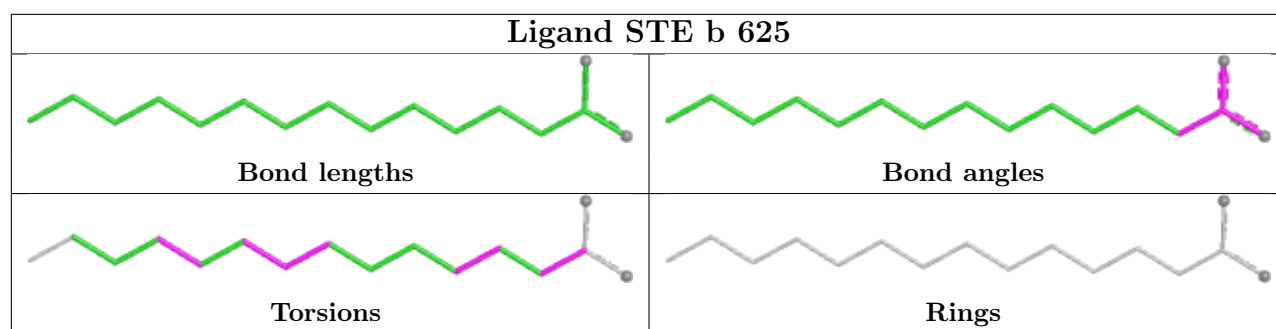
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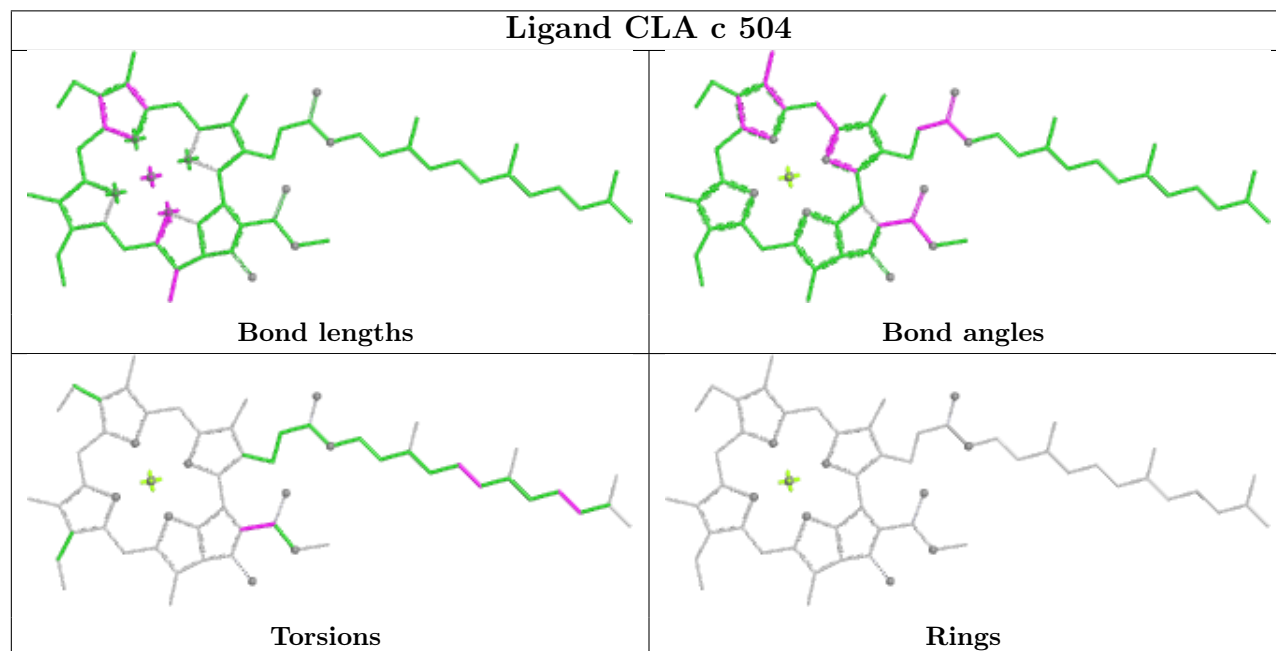
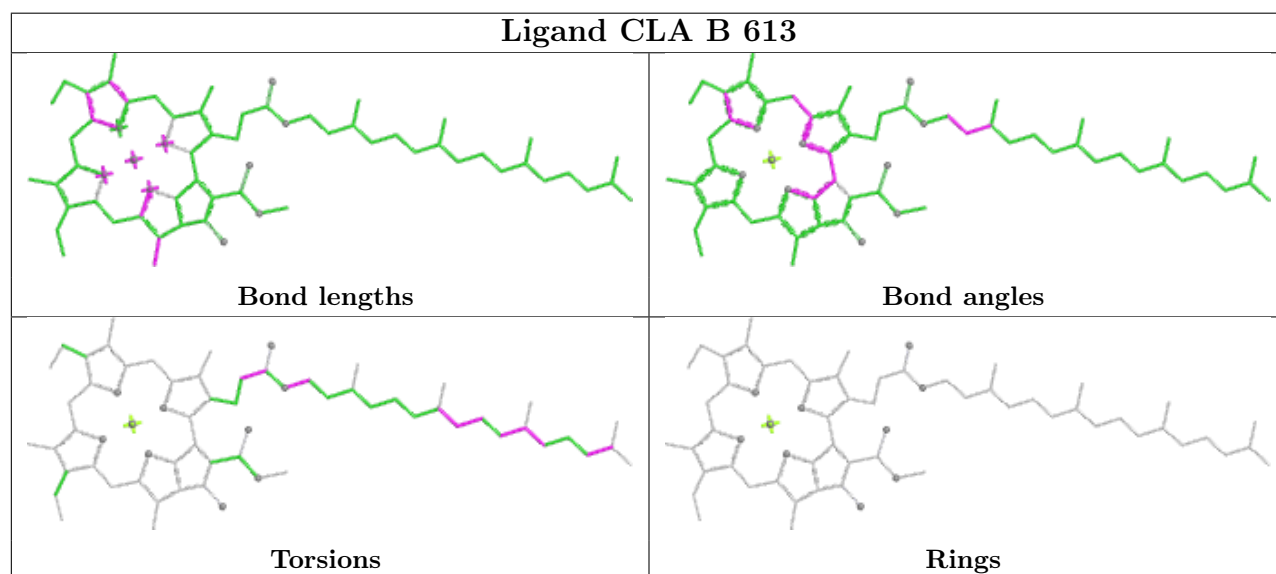
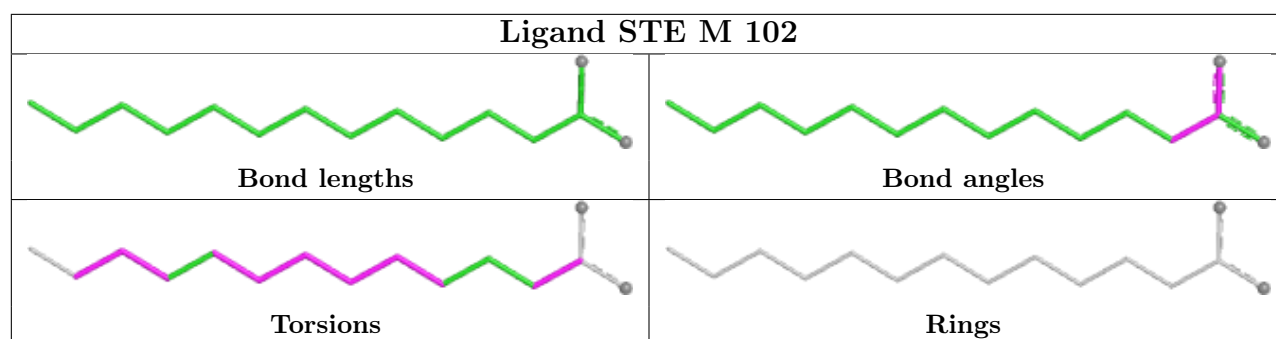
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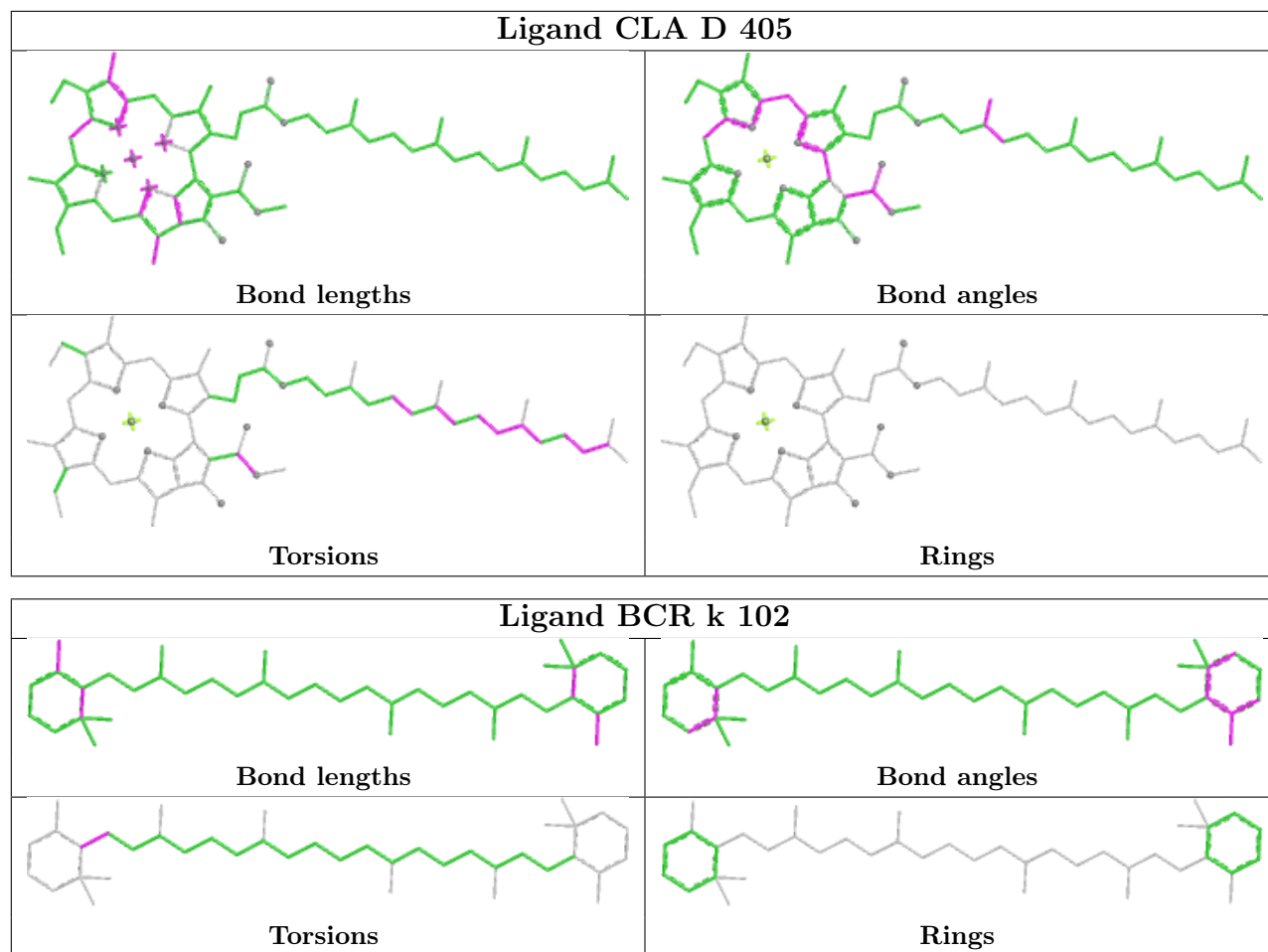
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	b	613	CLA	3	0
24	d	401	PHO	1	0
27	E	103	STE	5	0
27	C	528	STE	3	0
29	b	620	SQD	1	0
27	b	622	STE	1	0
27	l	103	STE	3	0
23	D	403	CLA	3	0
27	d	412	STE	2	0
25	b	617	BCR	4	0
23	a	405	CLA	1	0

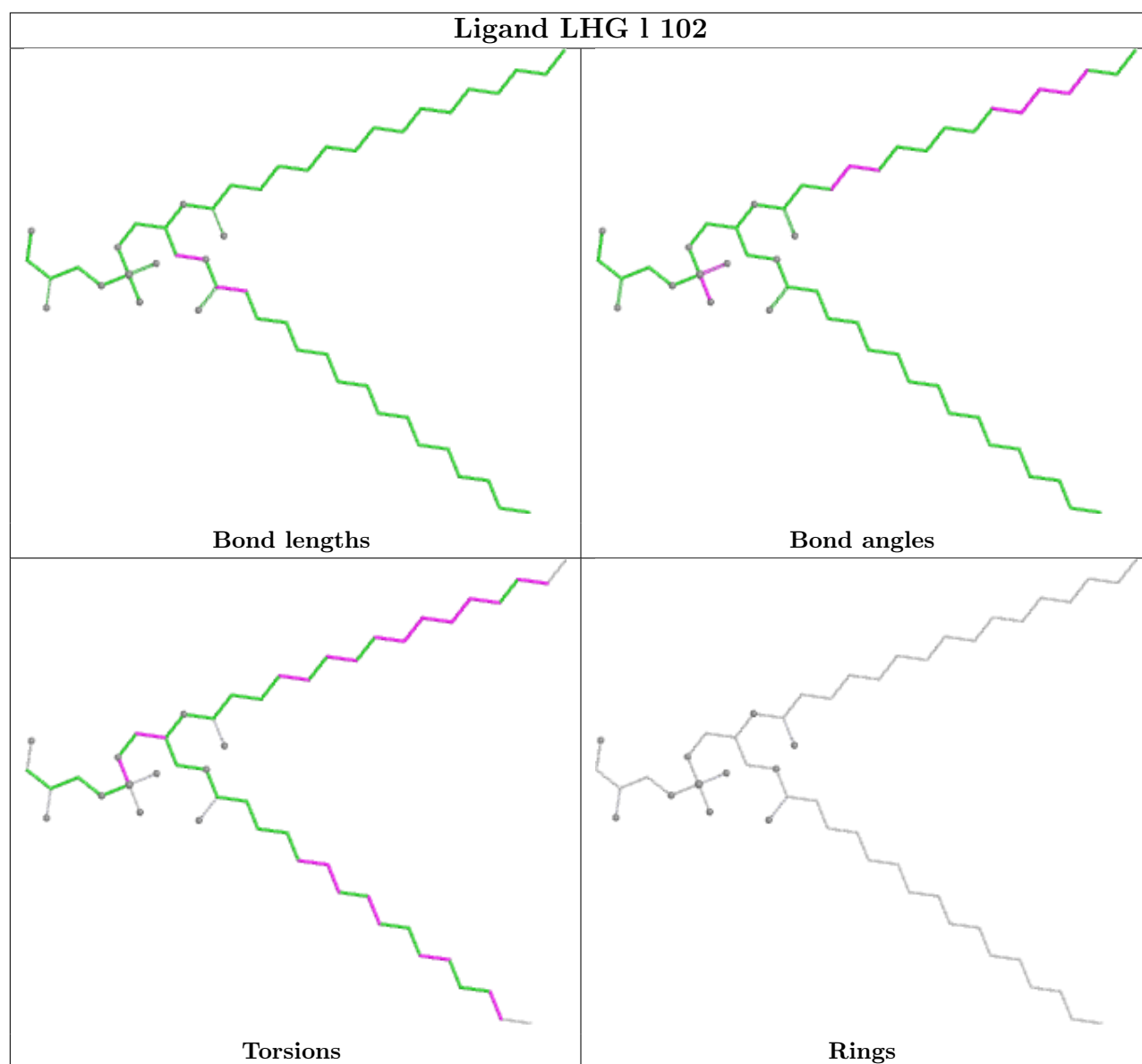
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

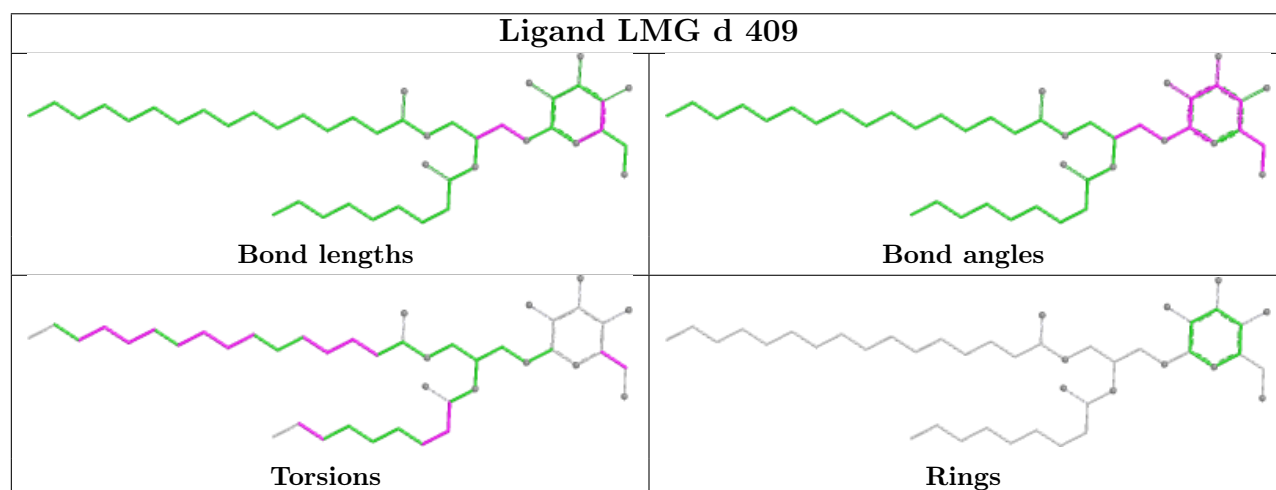
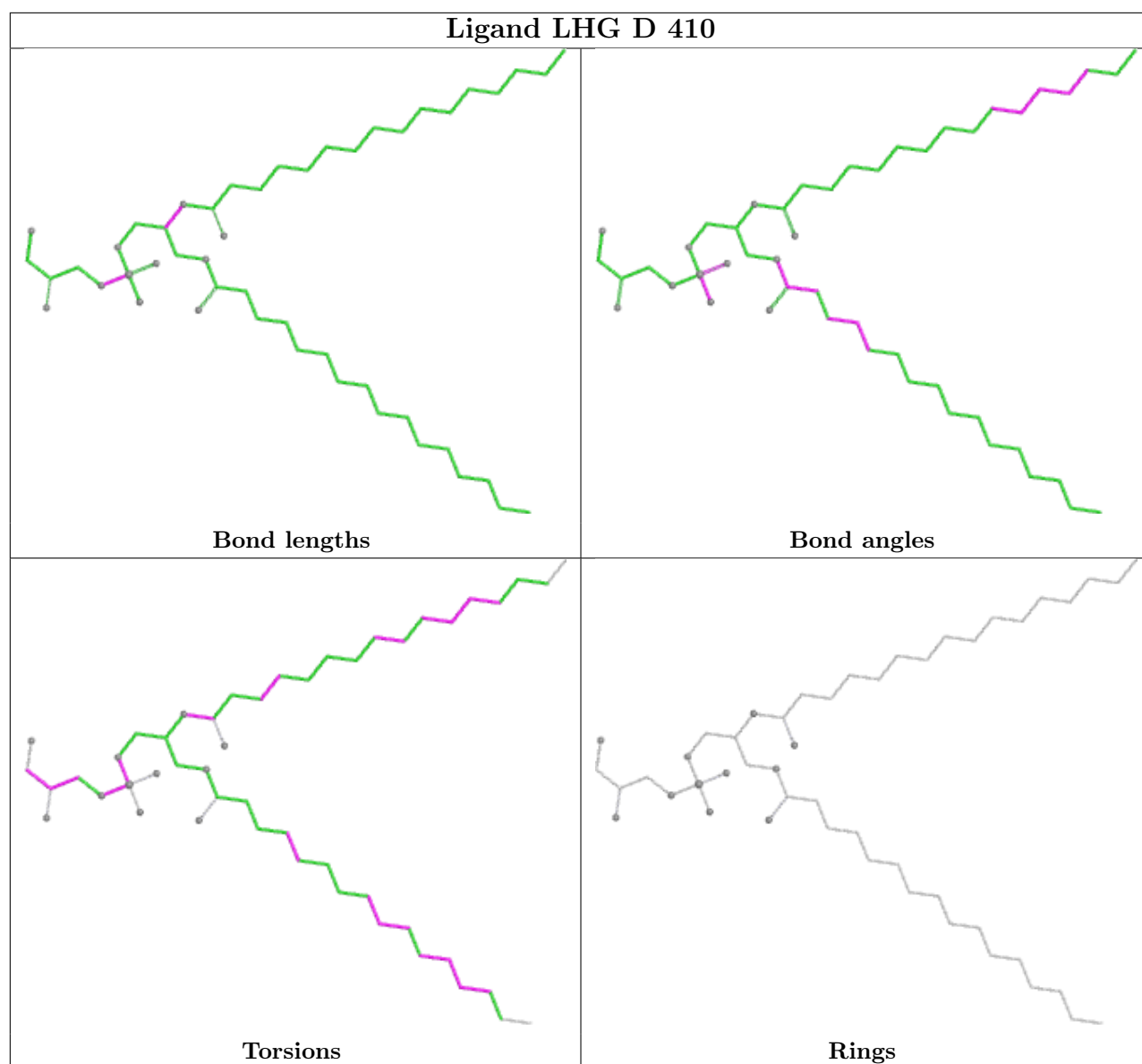


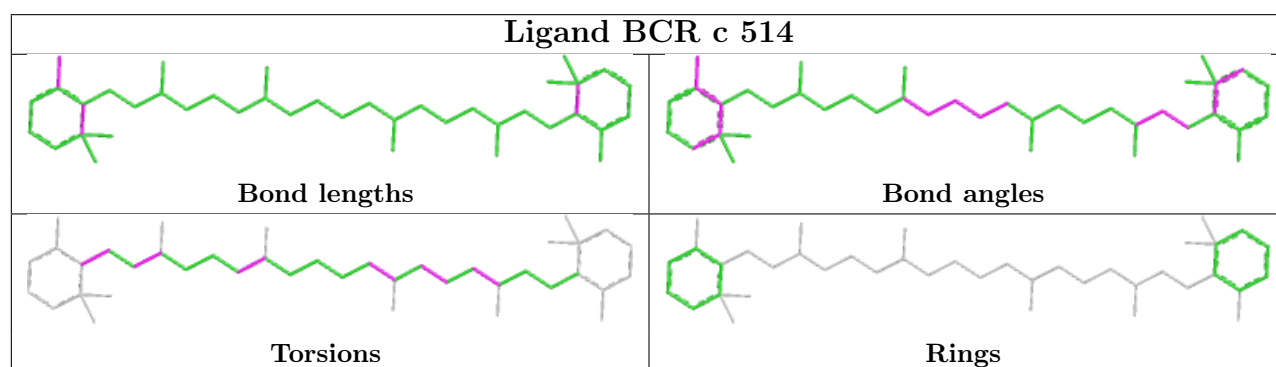
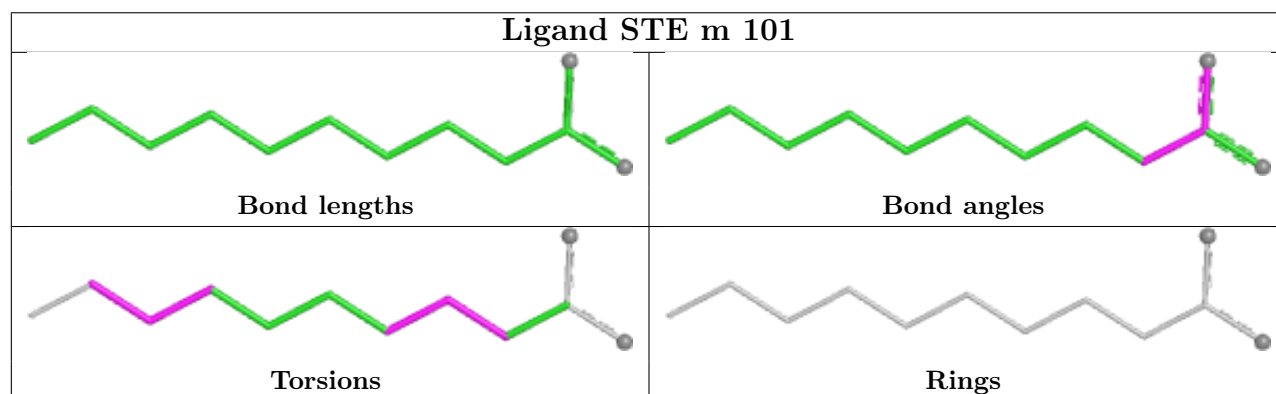
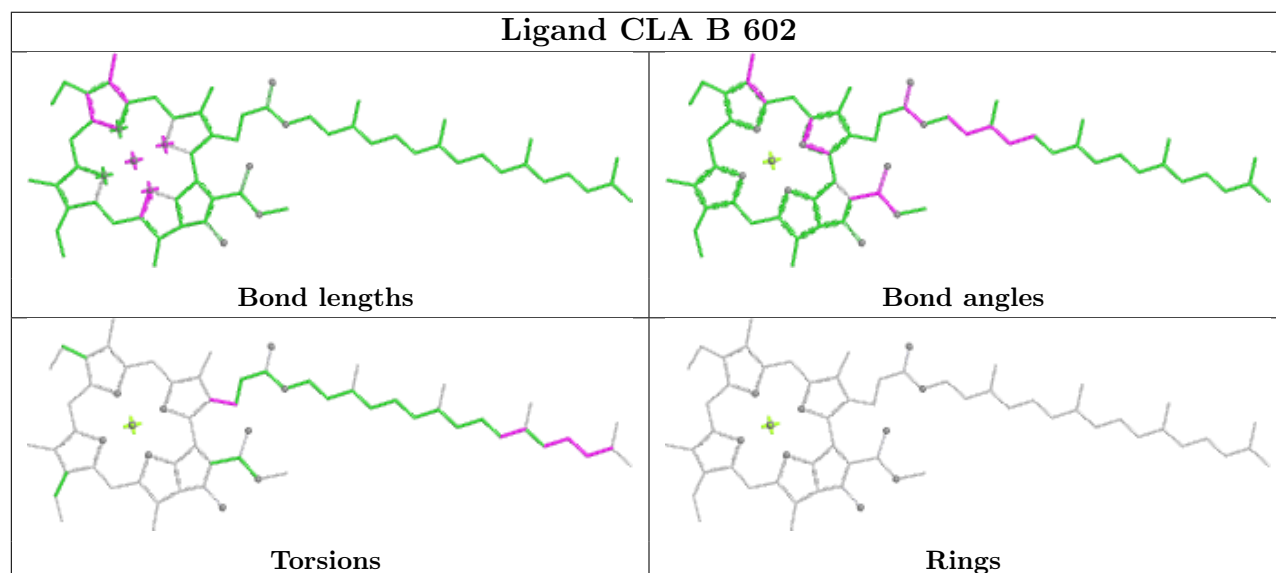
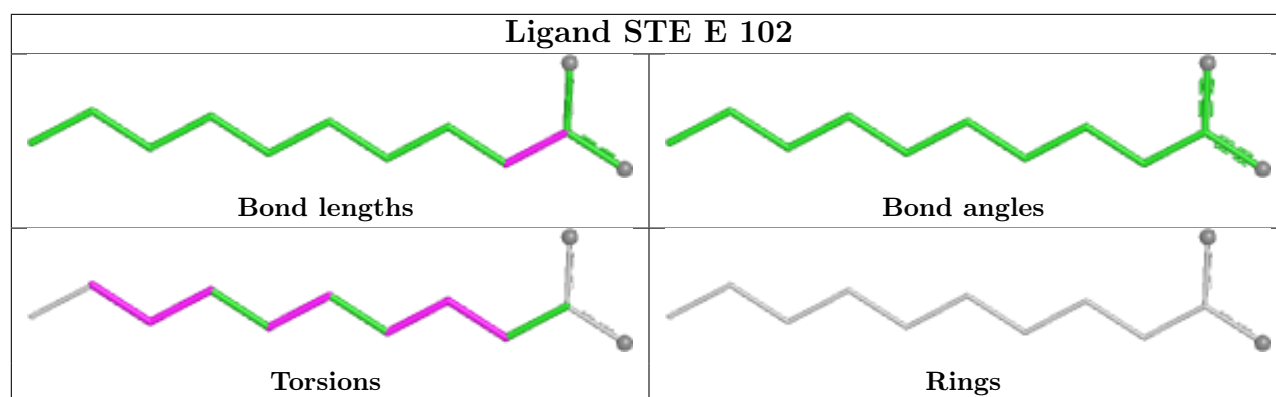


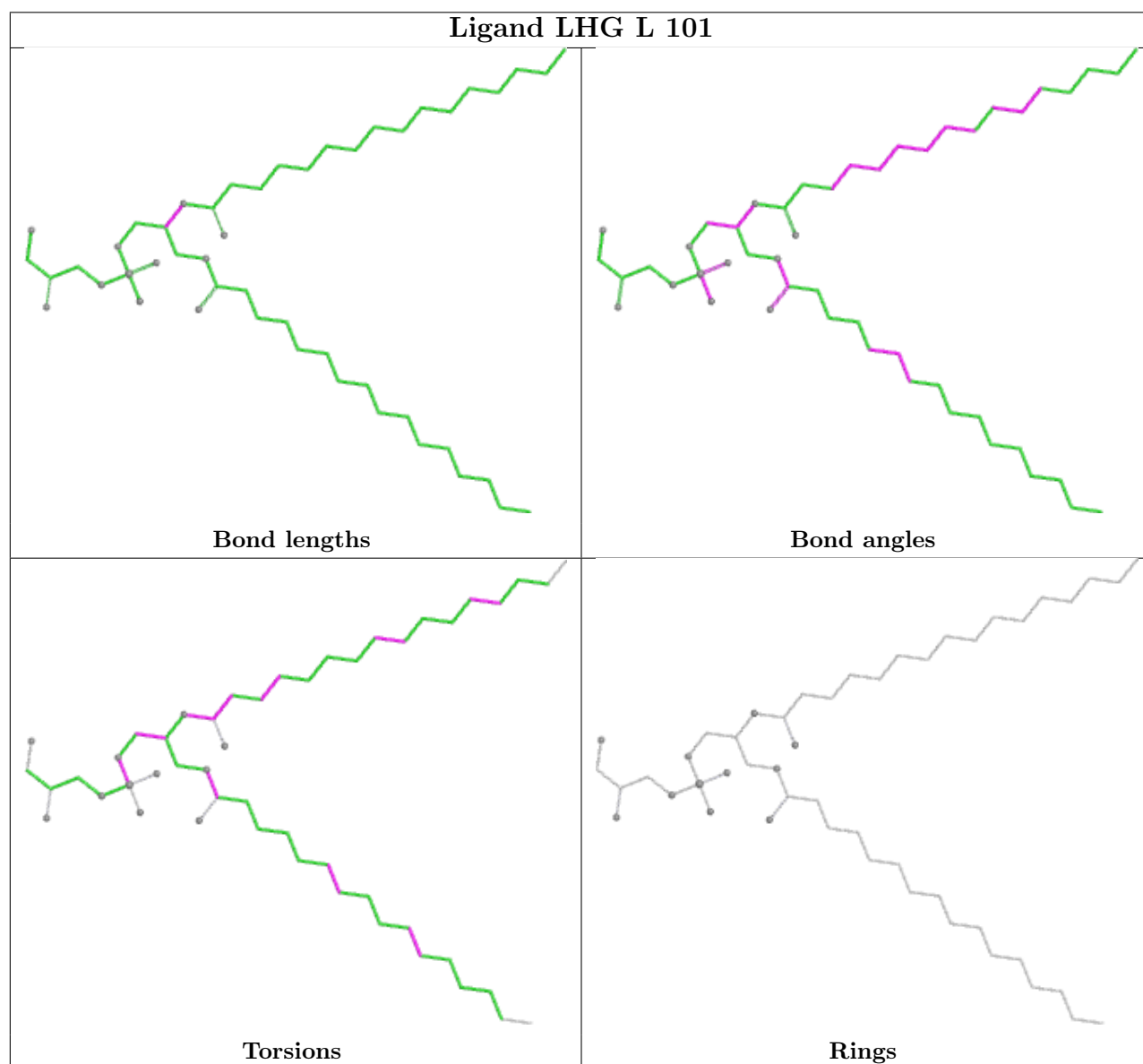
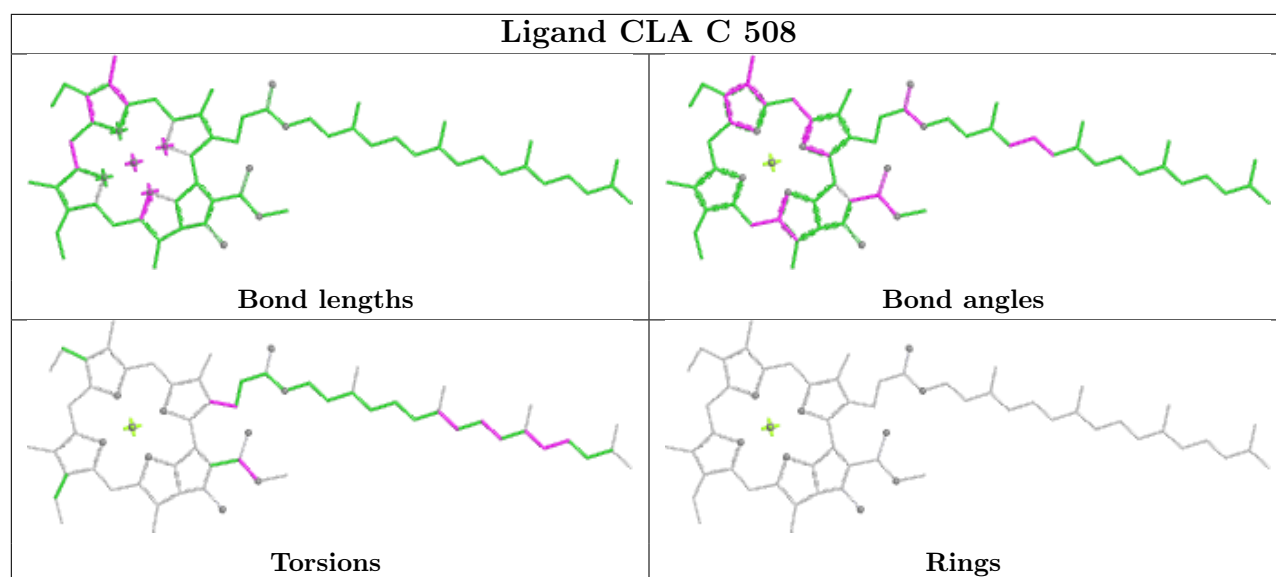


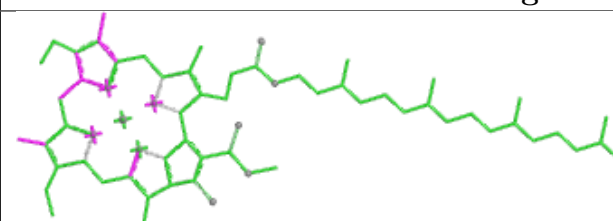
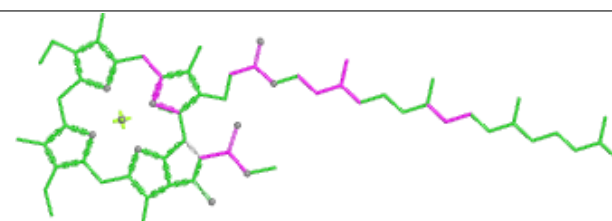
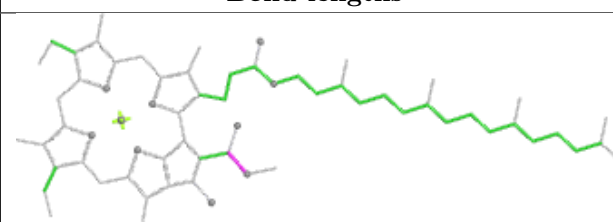
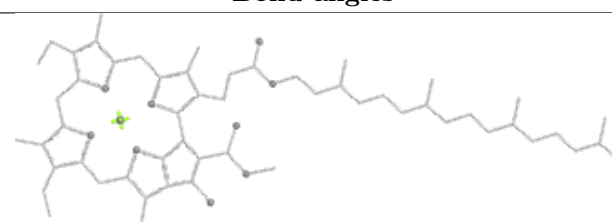


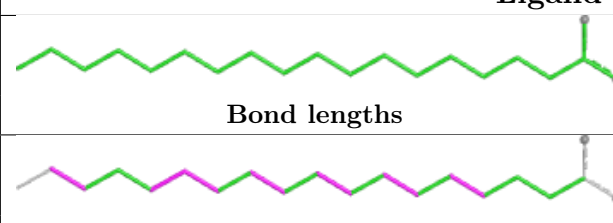
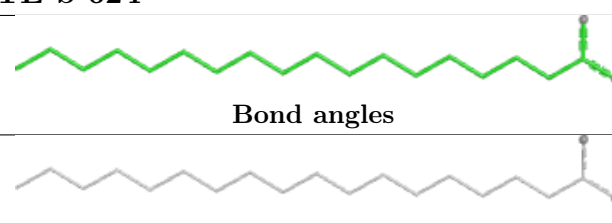
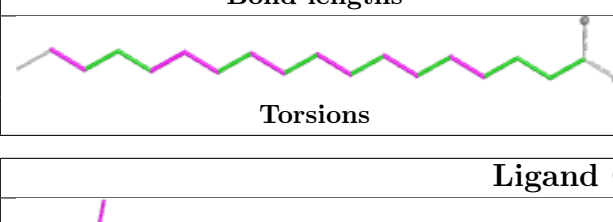


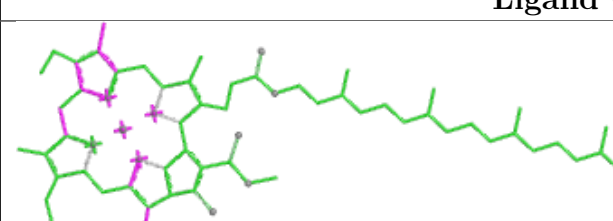
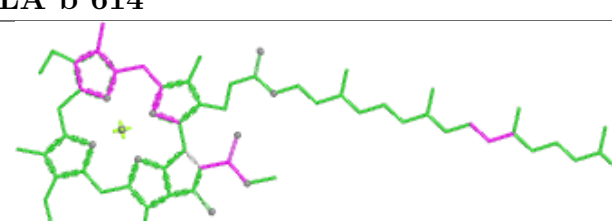
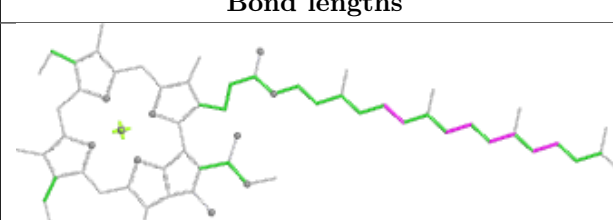
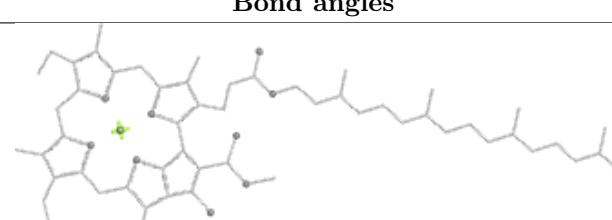


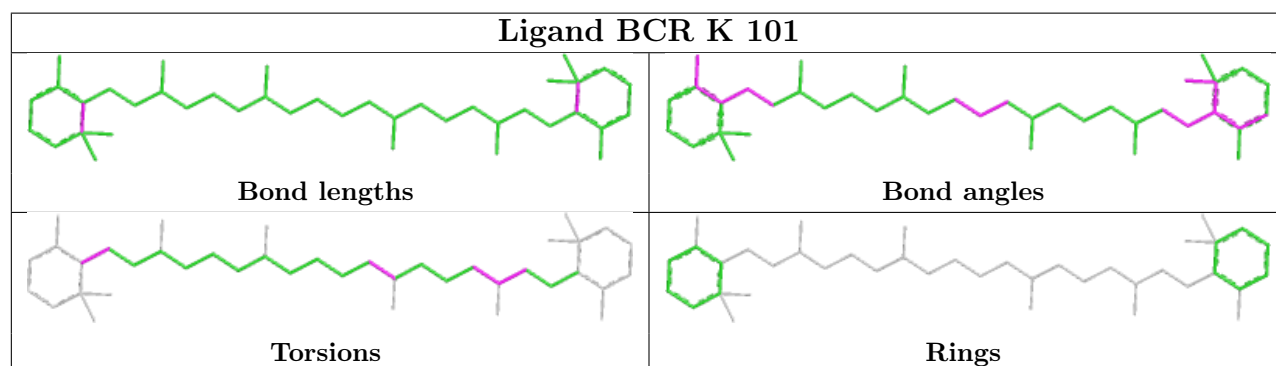
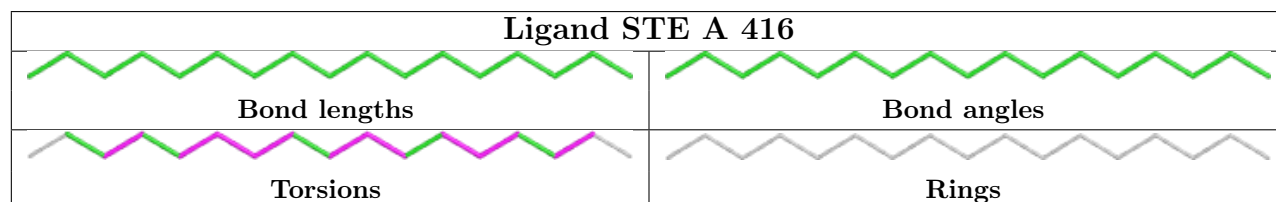
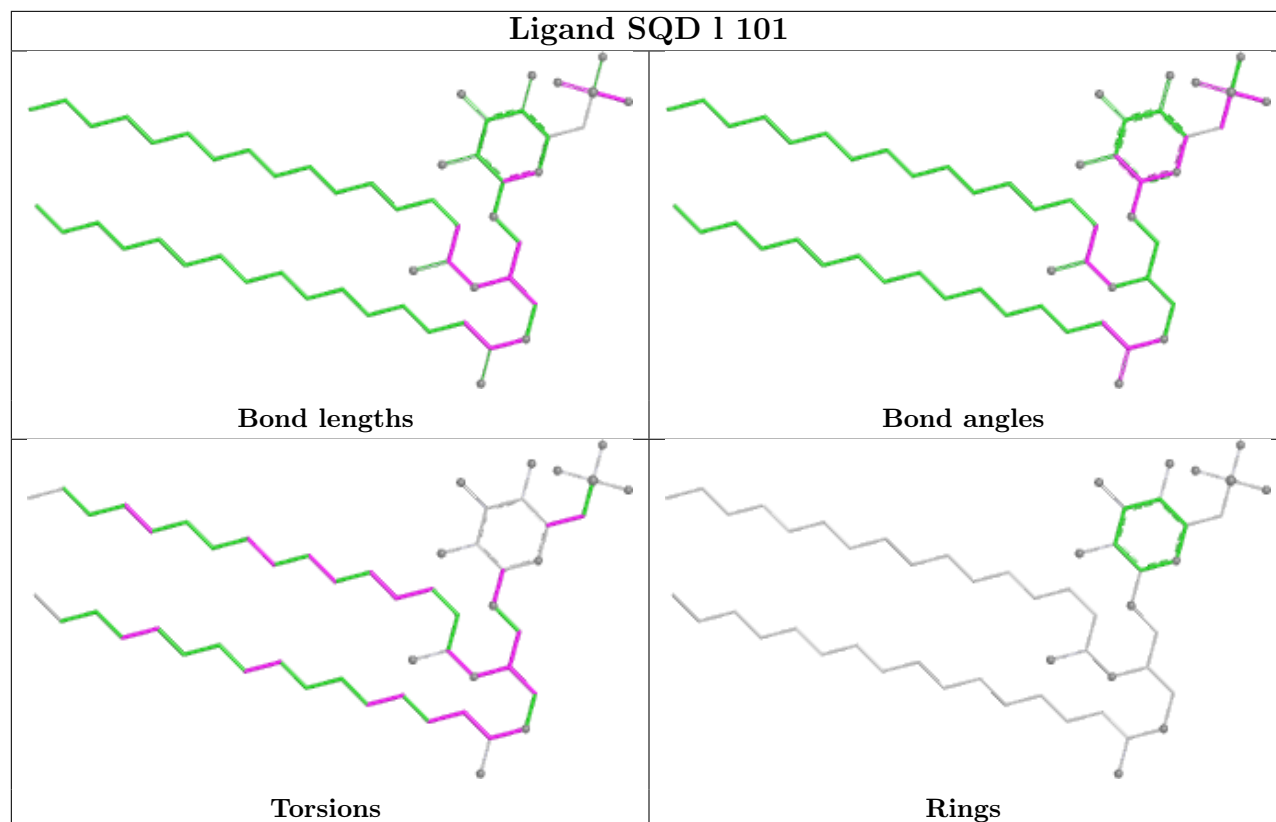


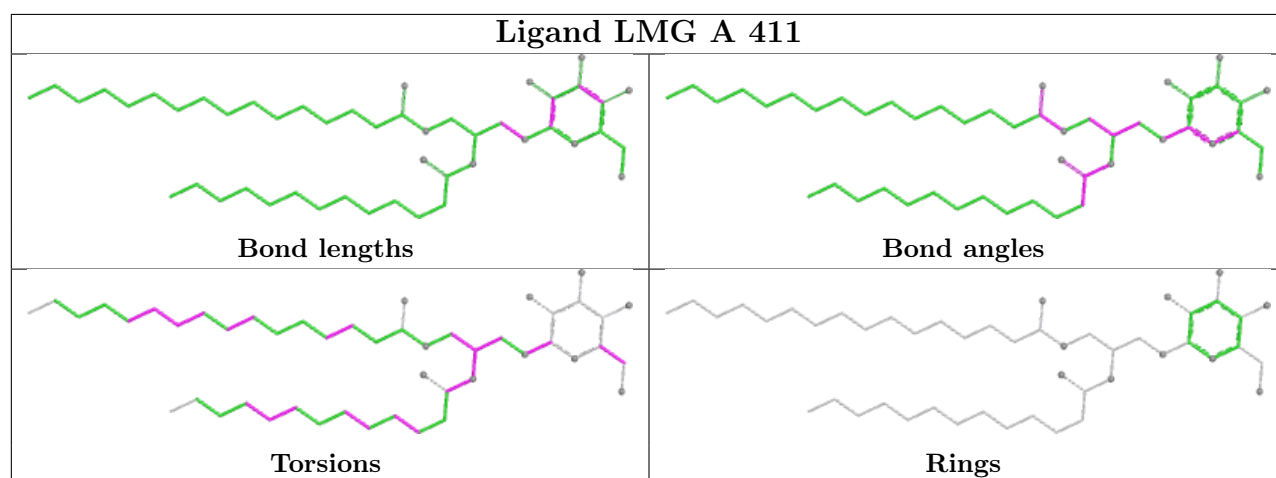
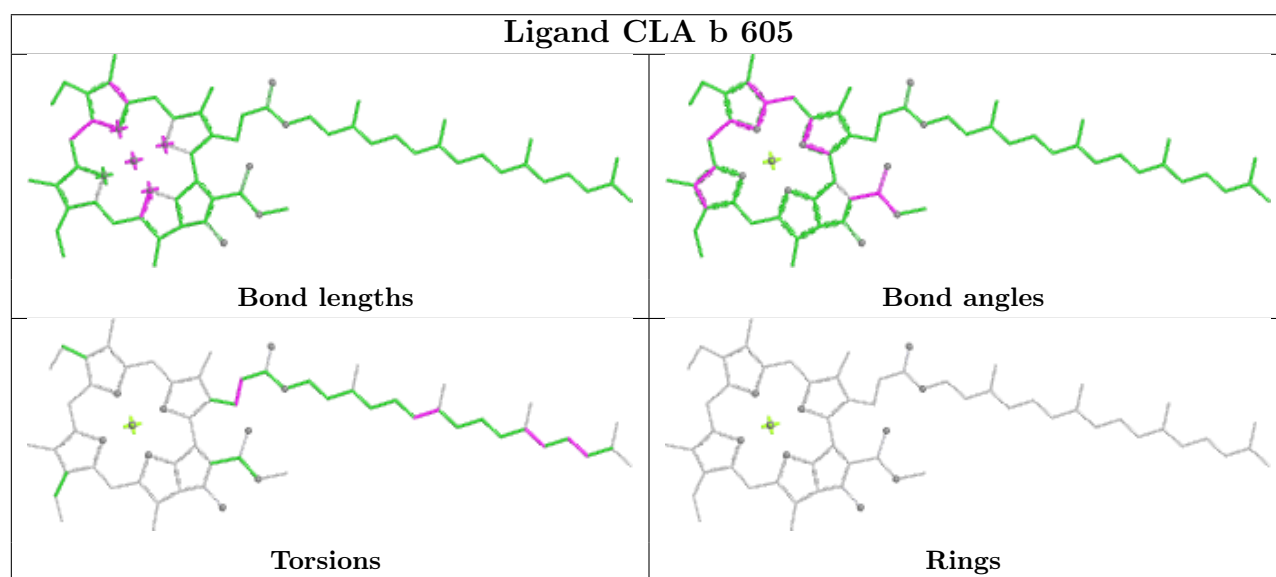
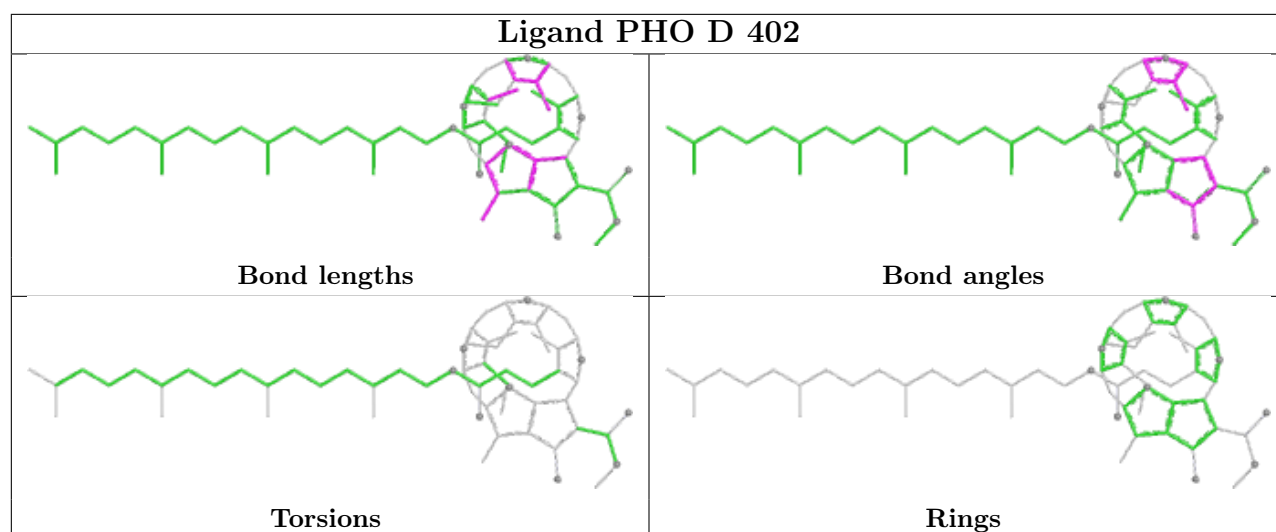


Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

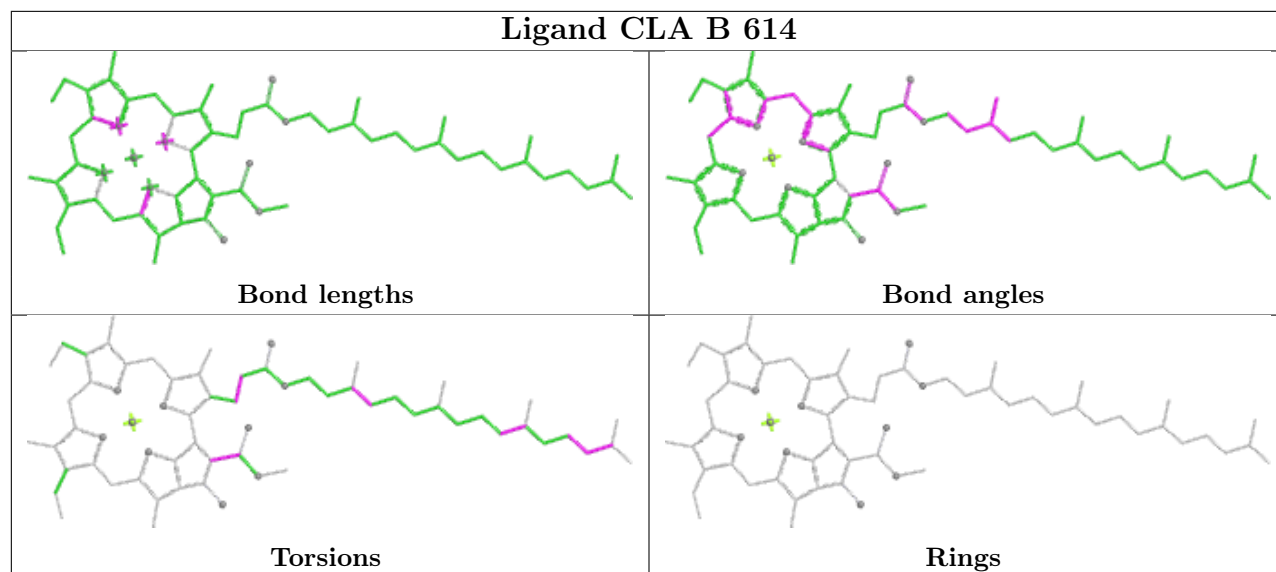
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

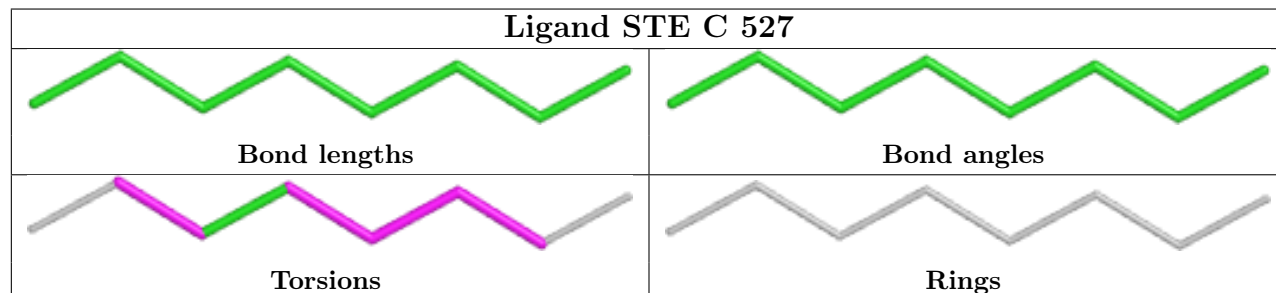




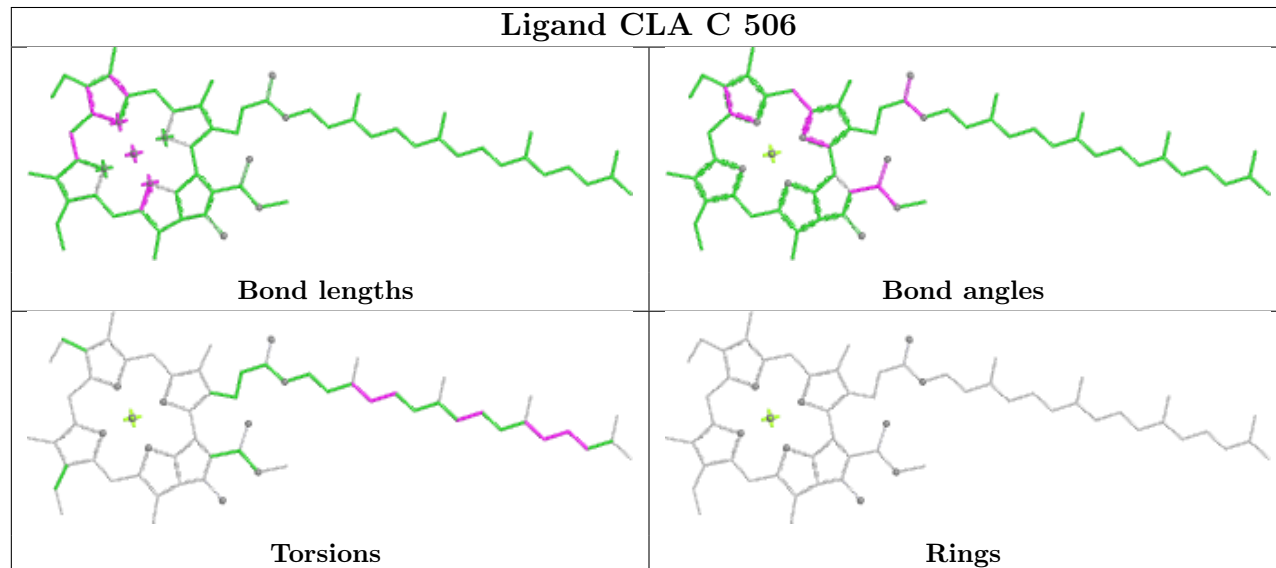
Ligand CLA B 614

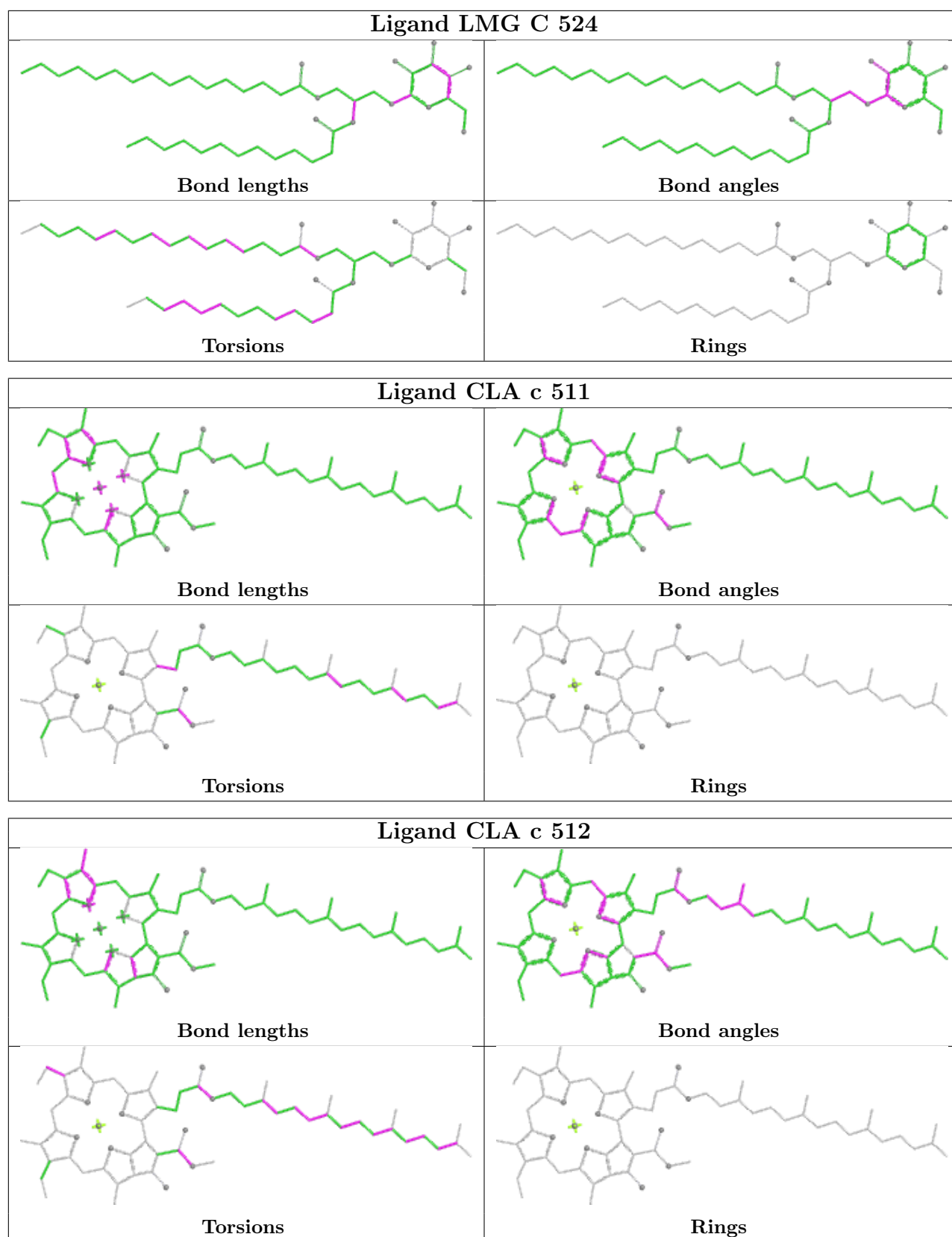


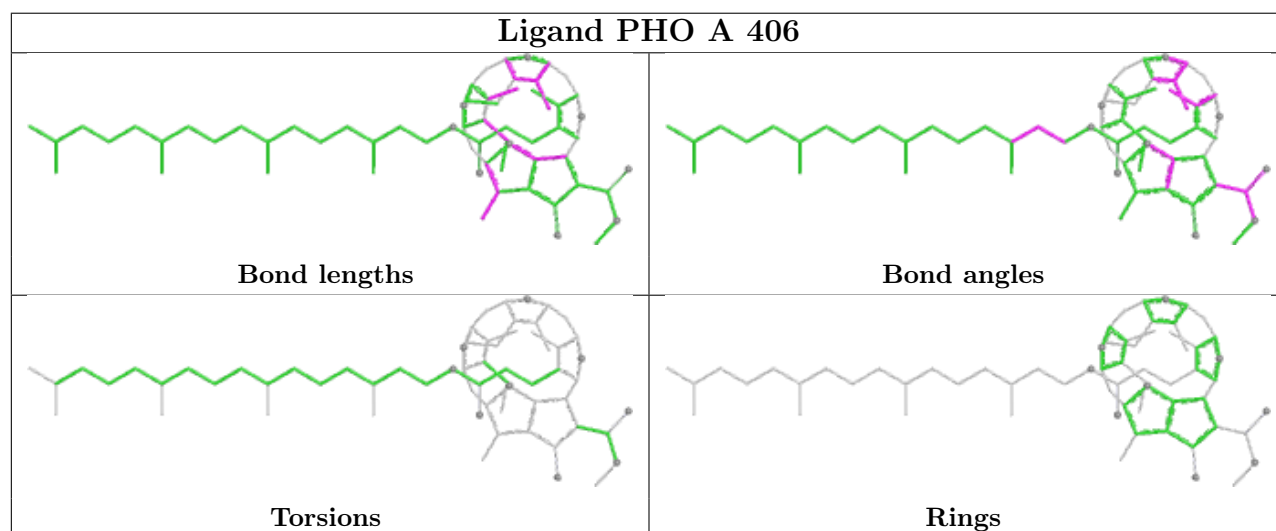
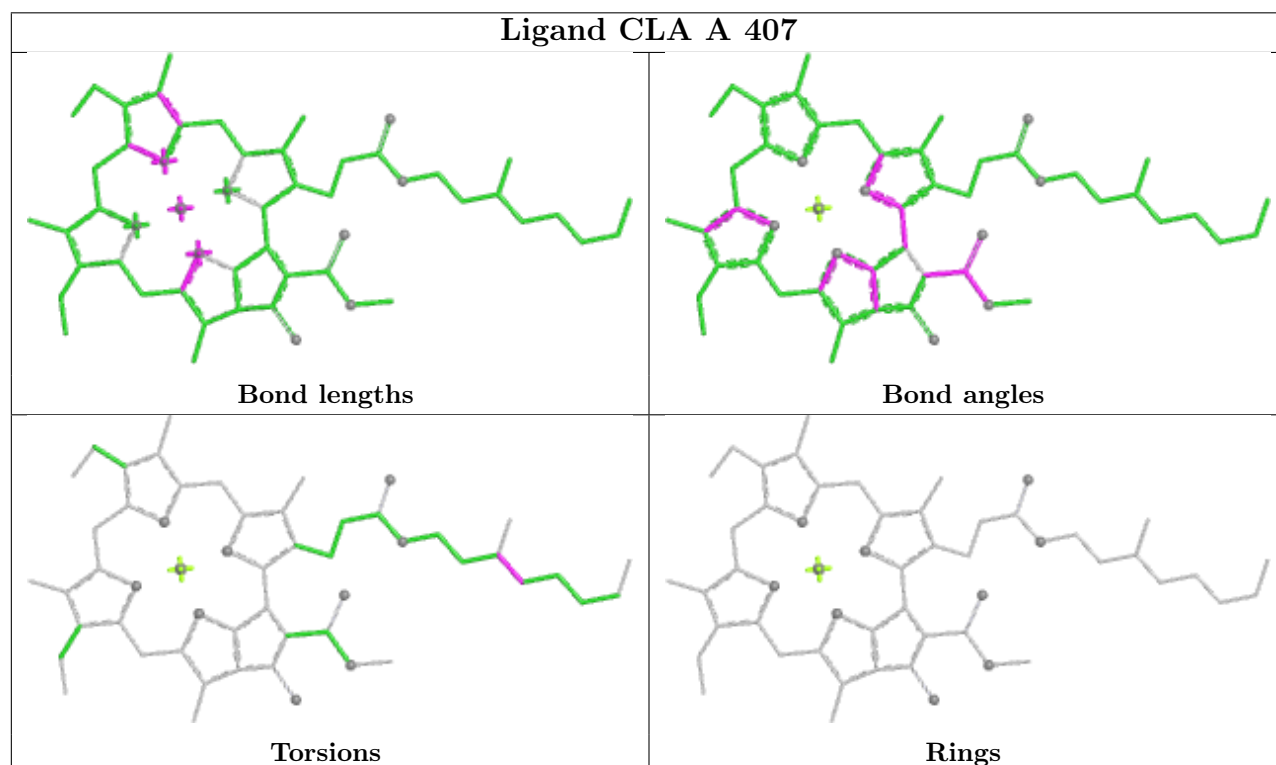
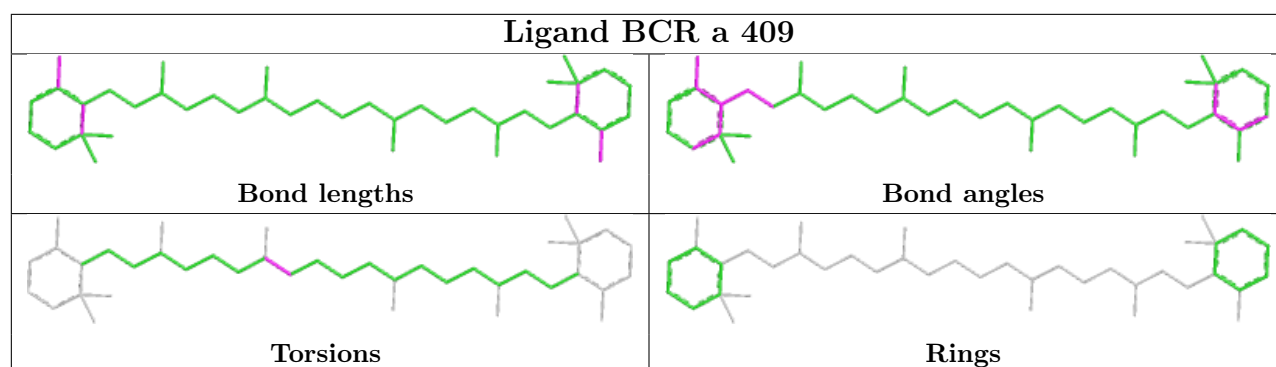
Ligand STE C 527

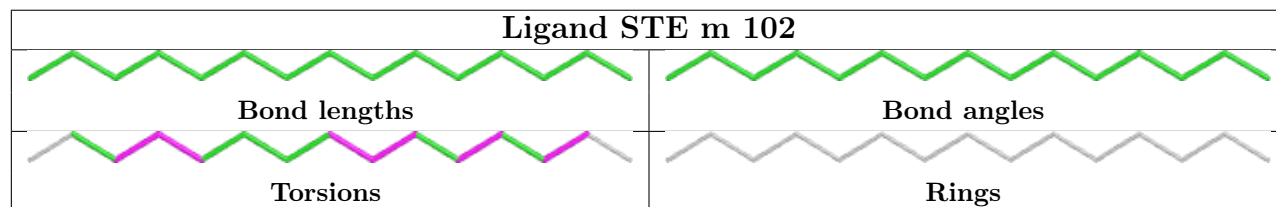
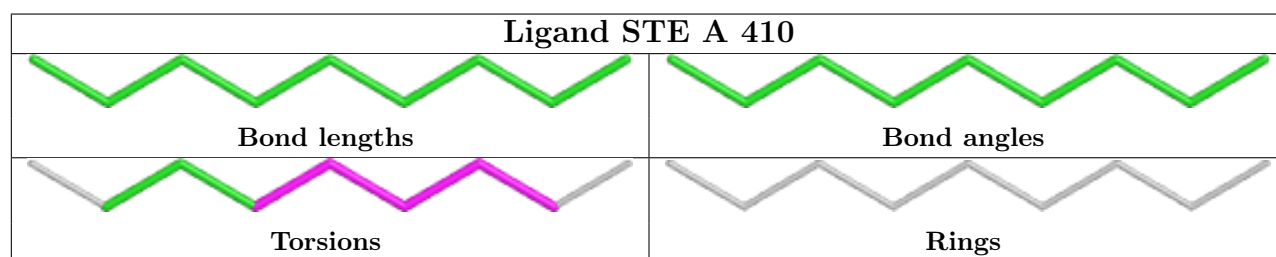
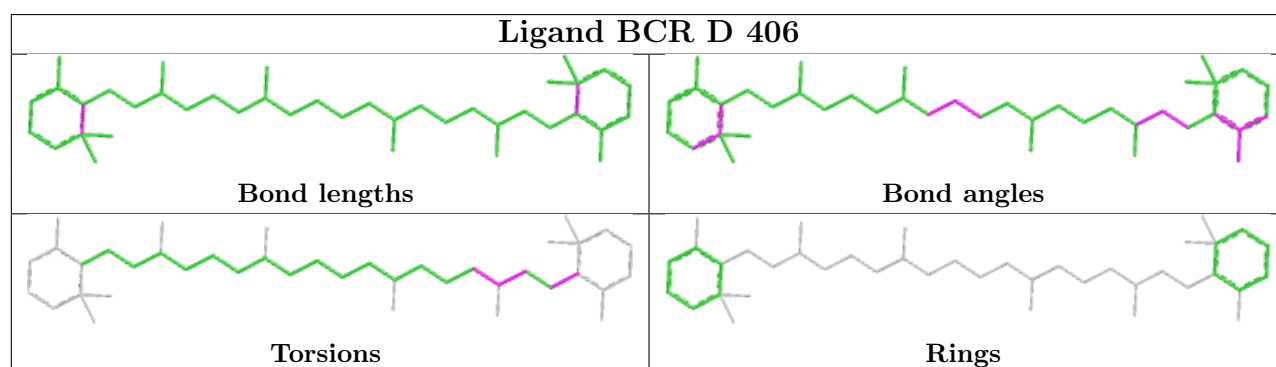
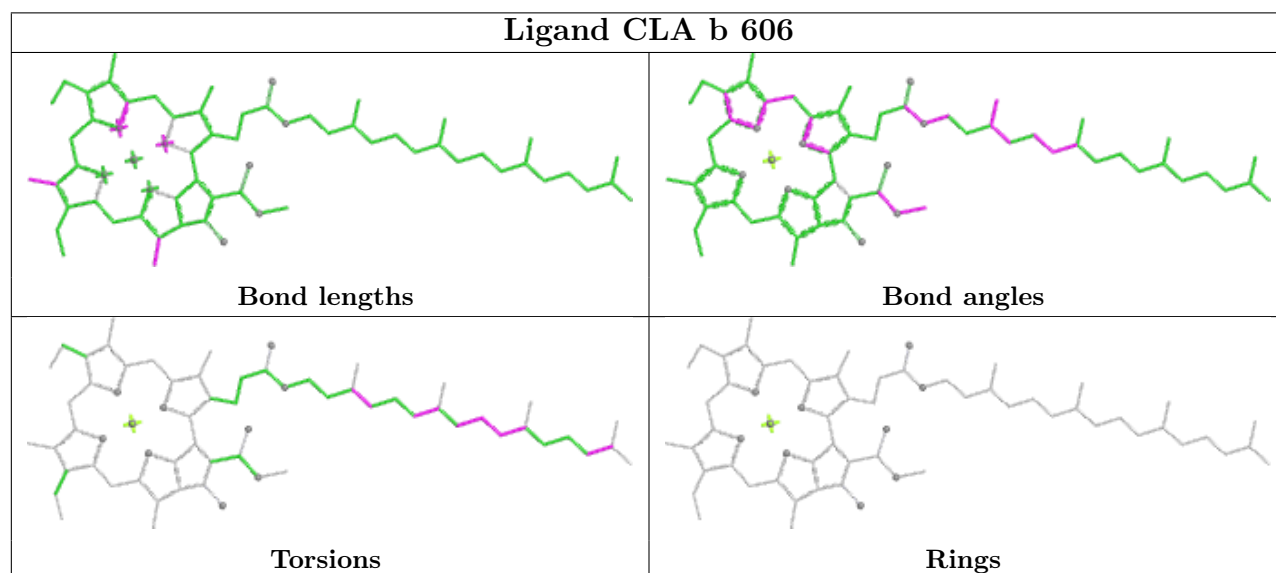
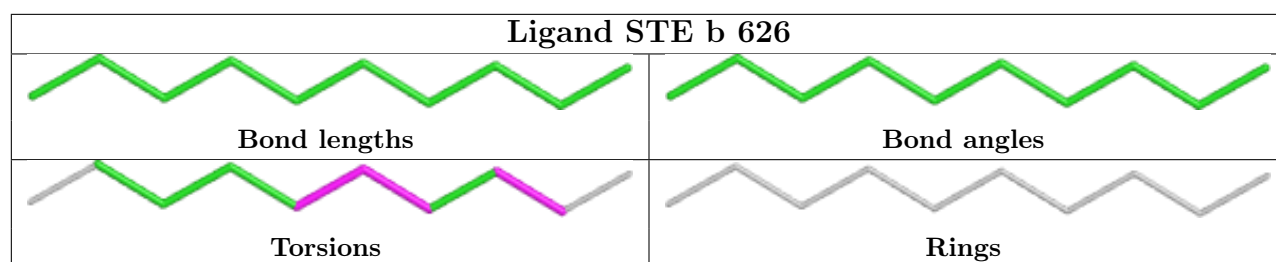


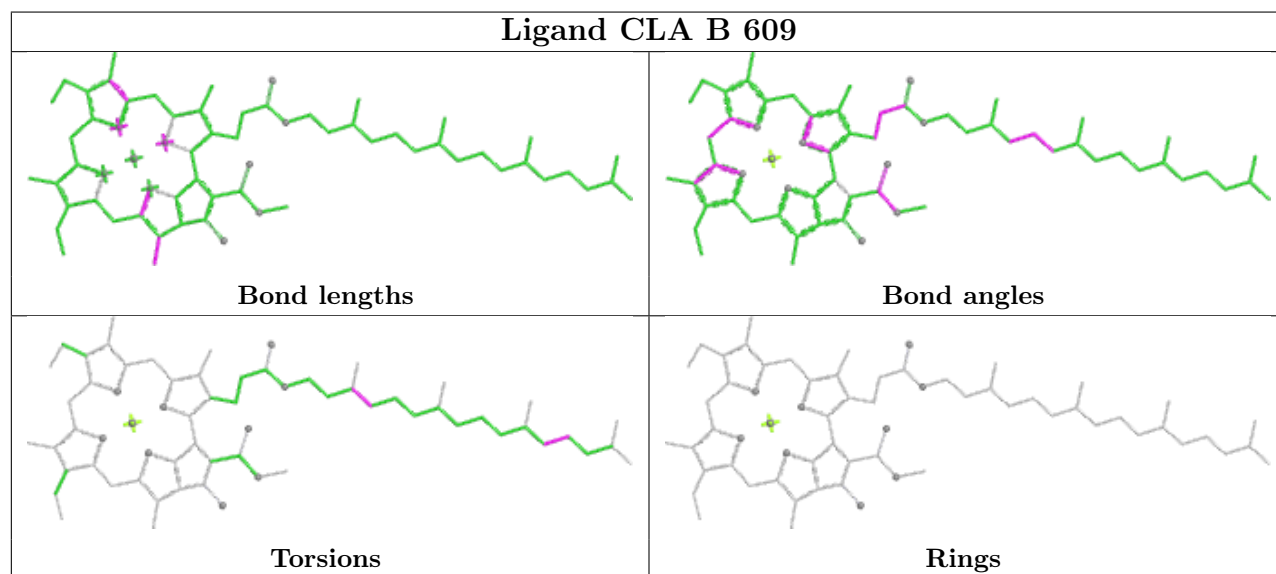
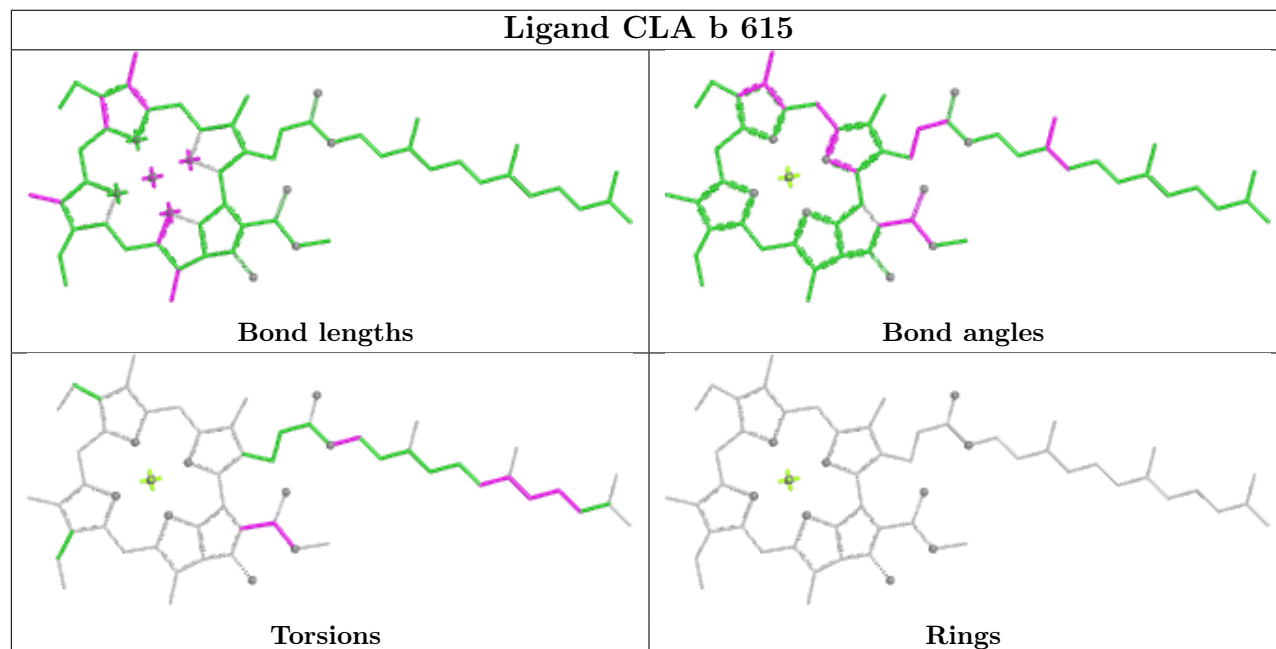
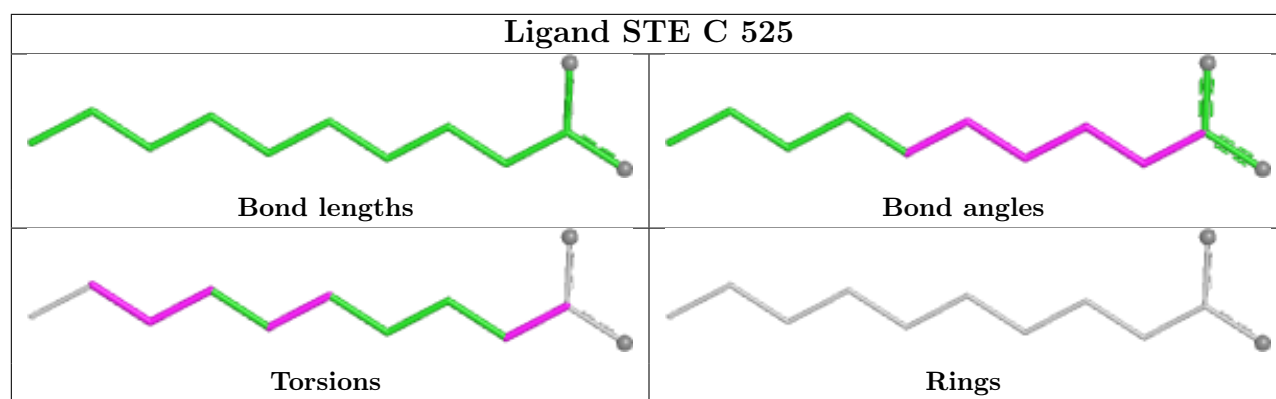
Ligand CLA C 506



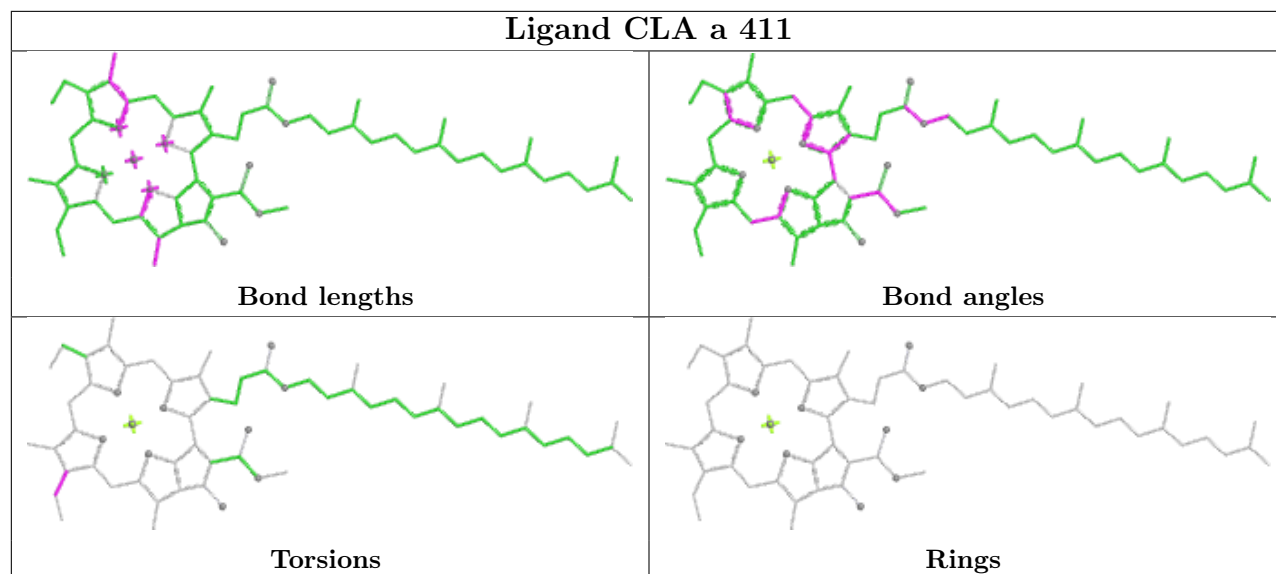




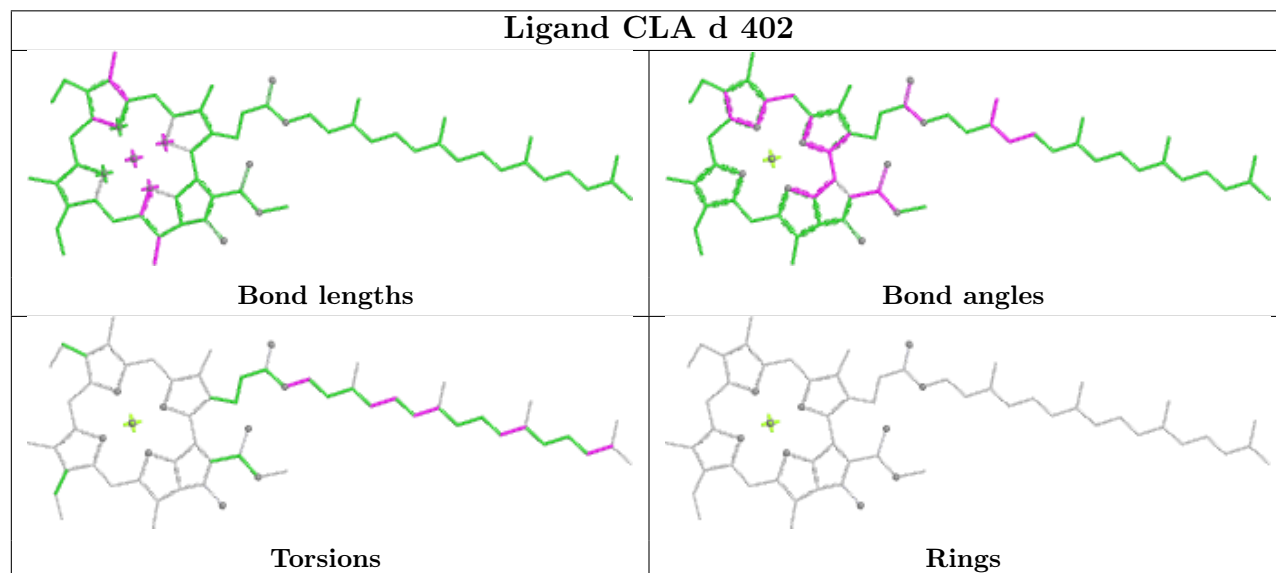


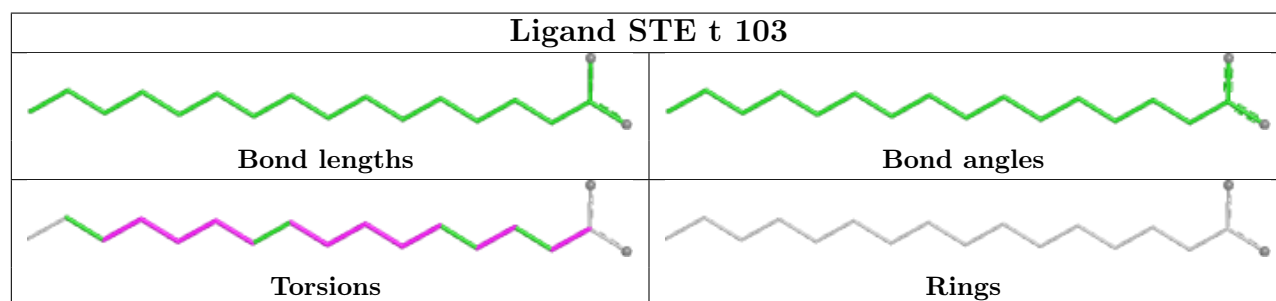
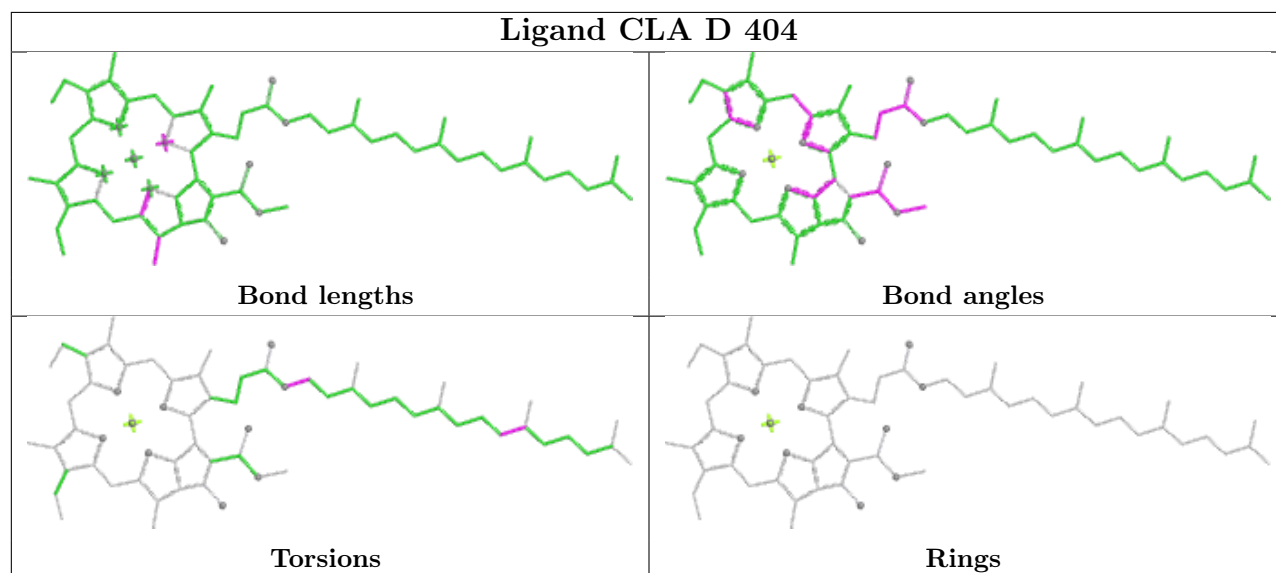
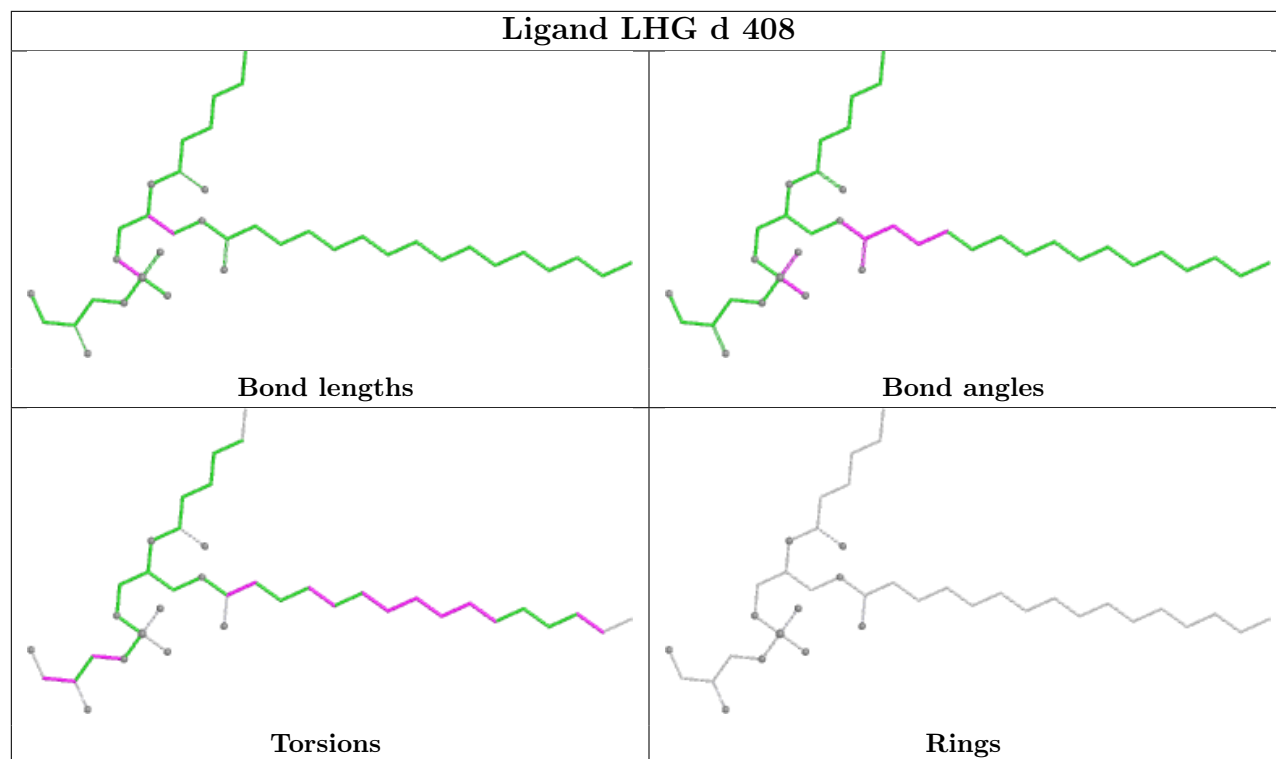


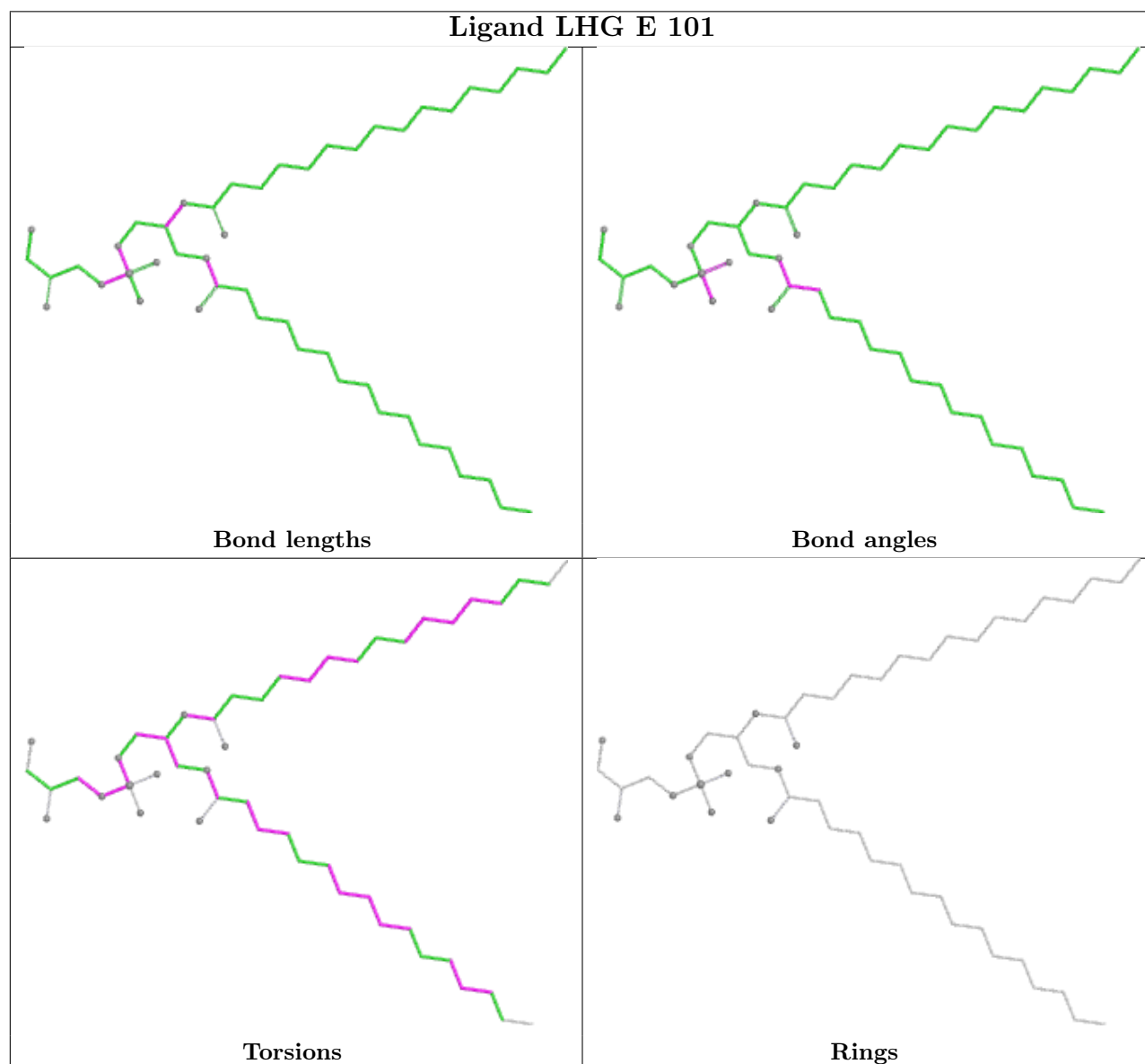
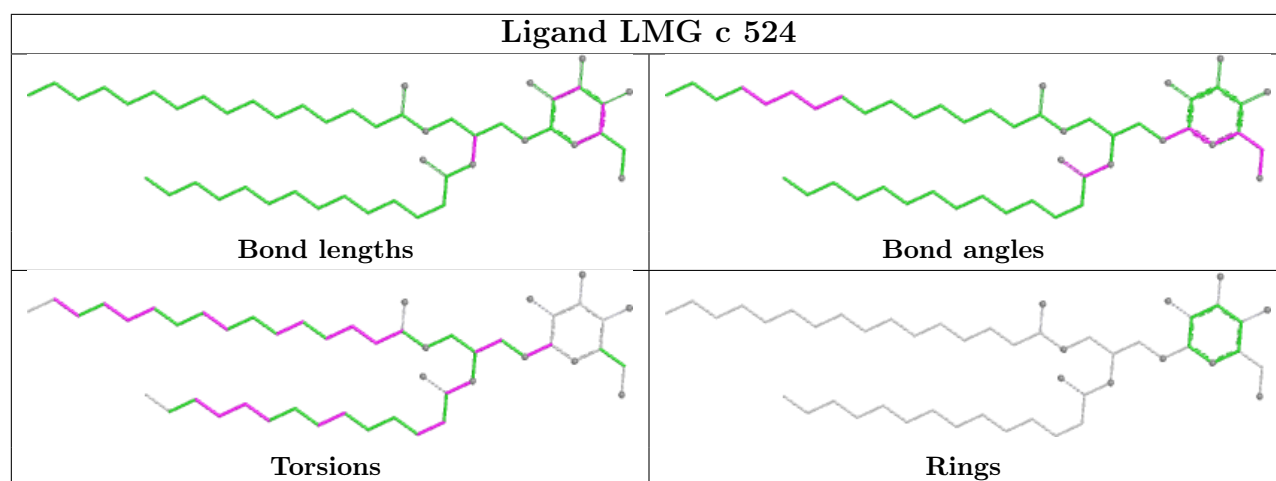
Ligand CLA a 411

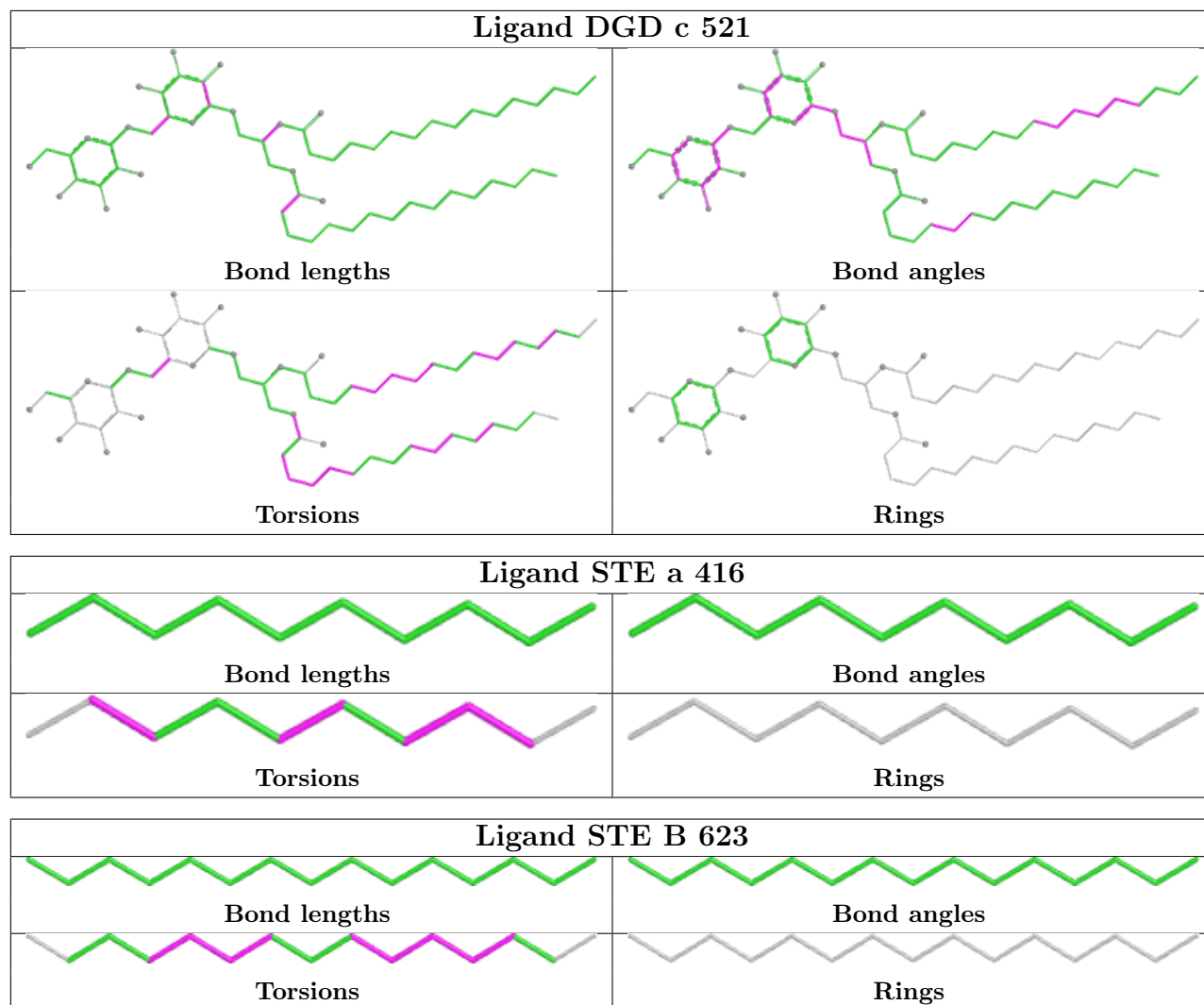


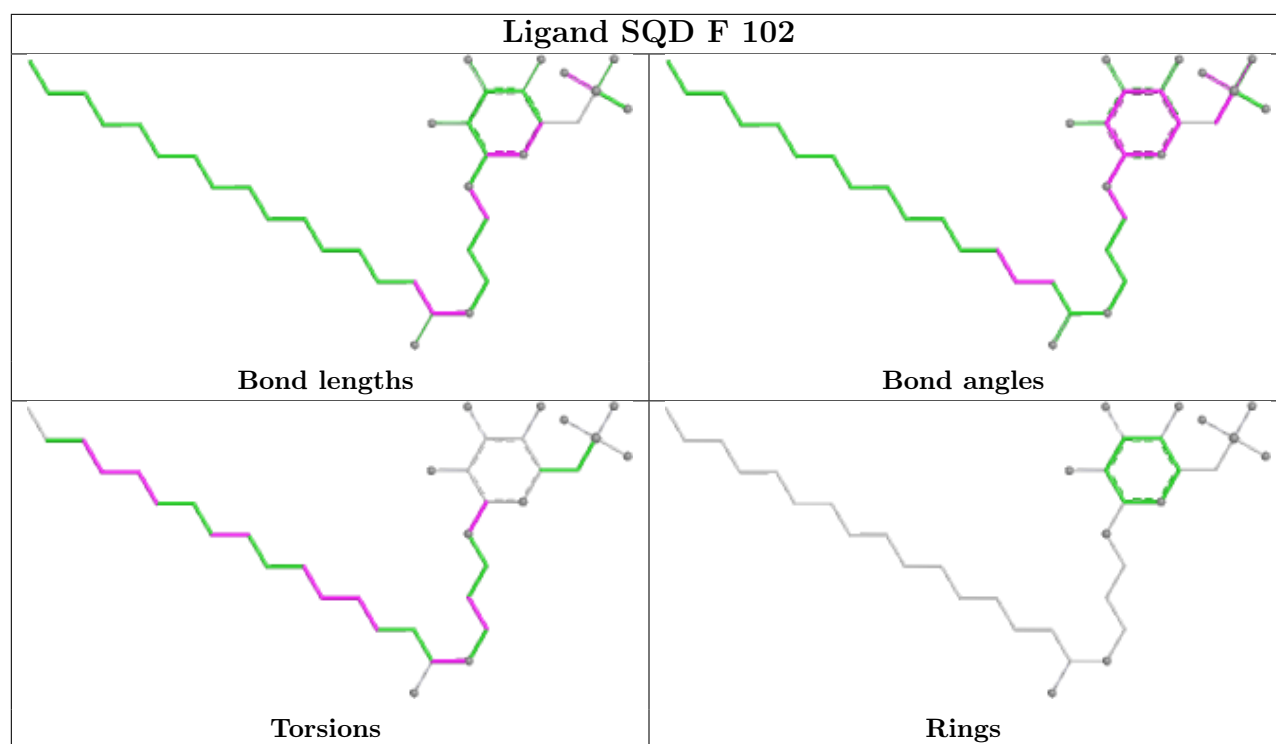
Ligand CLA d 402

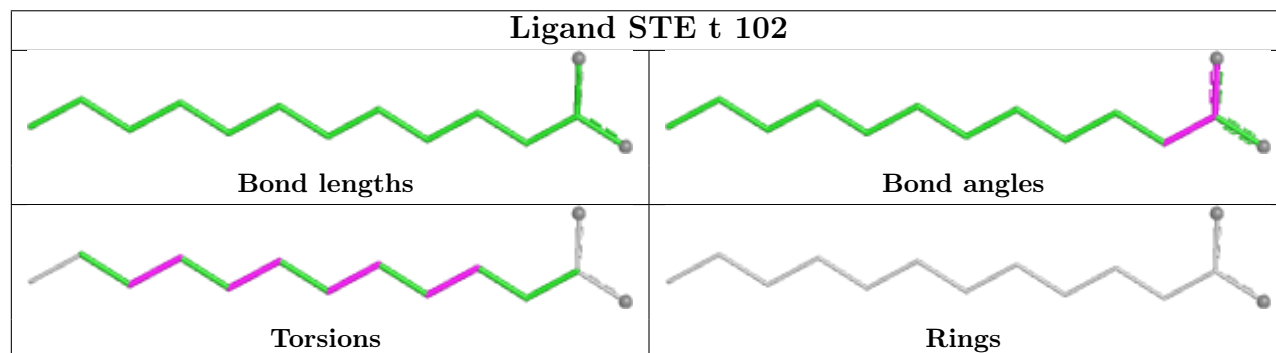
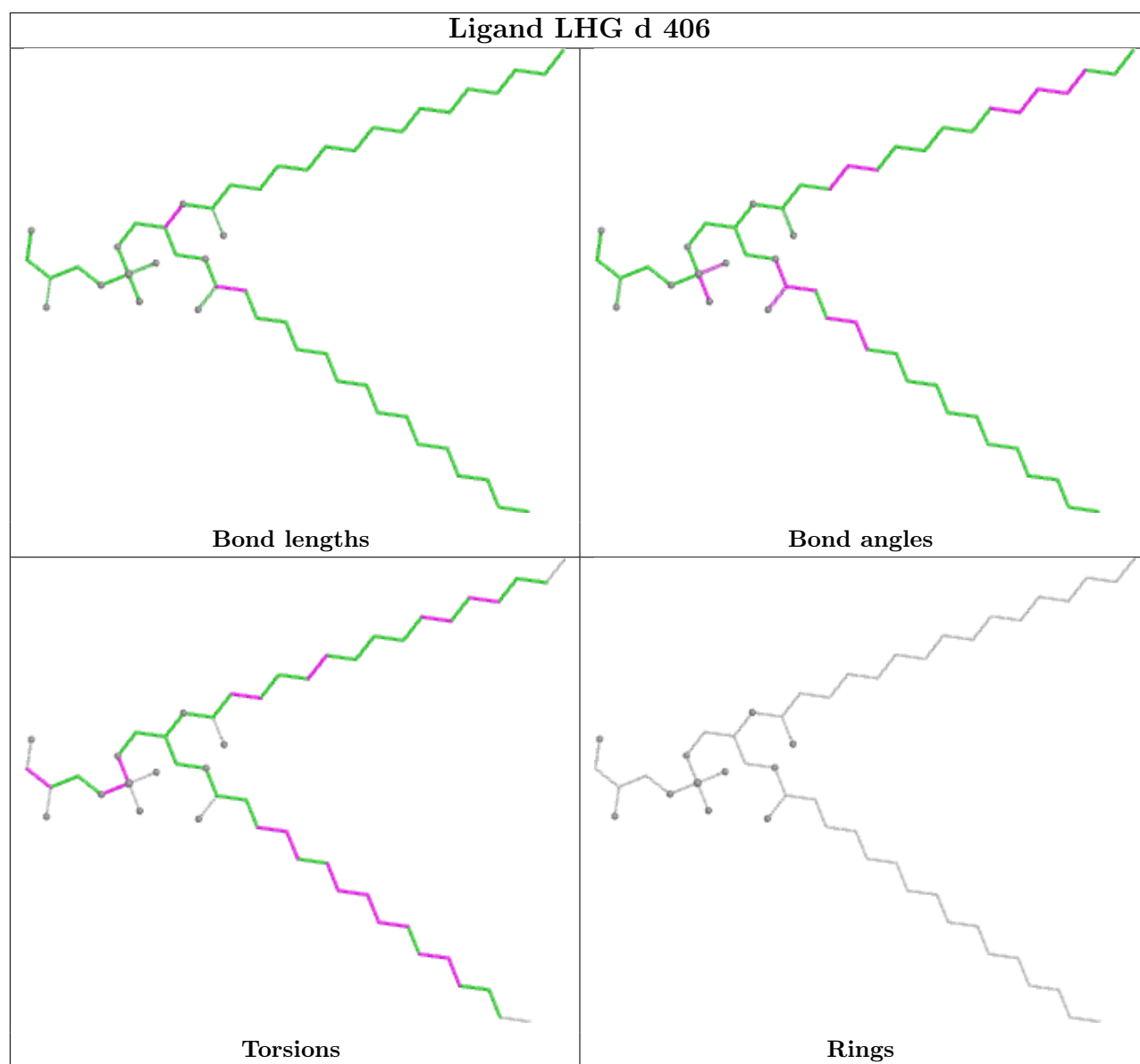


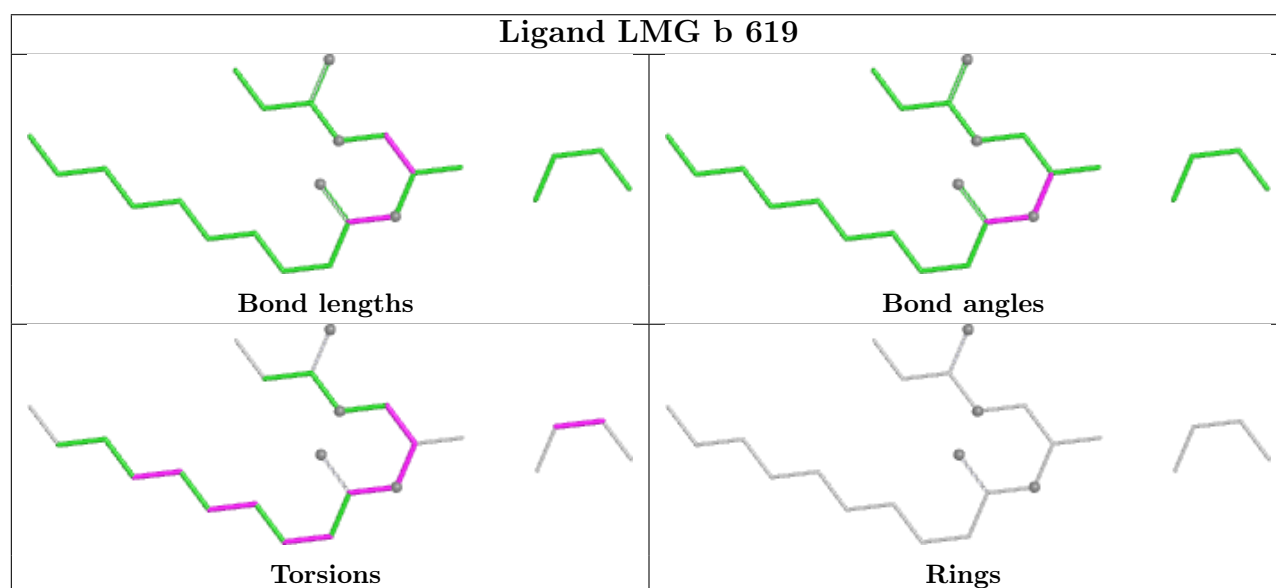
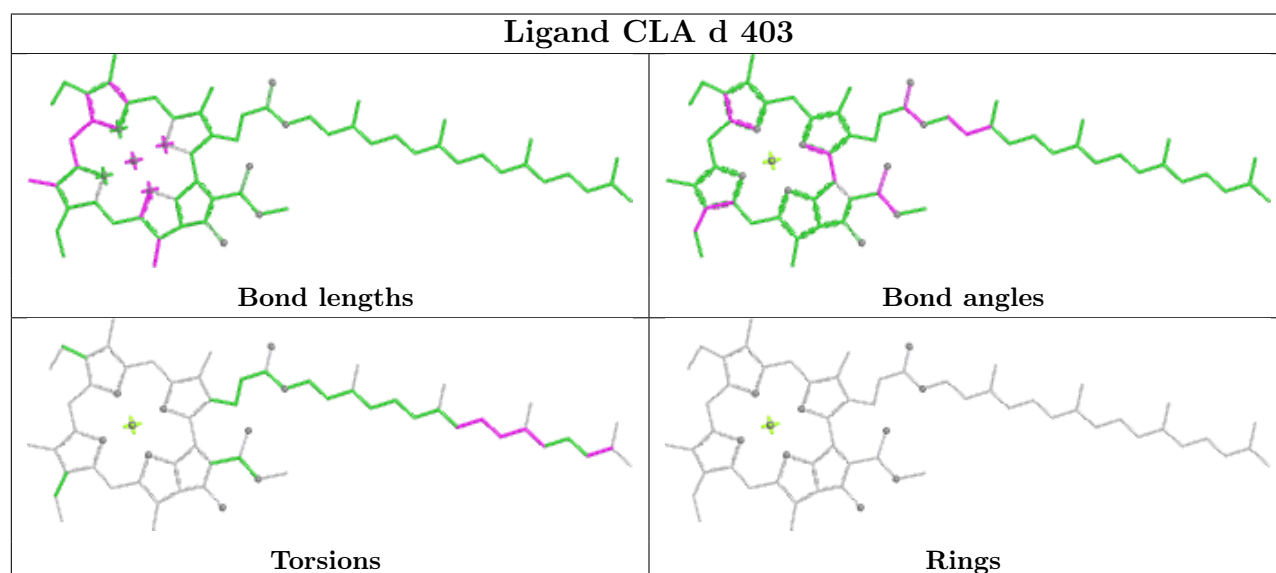
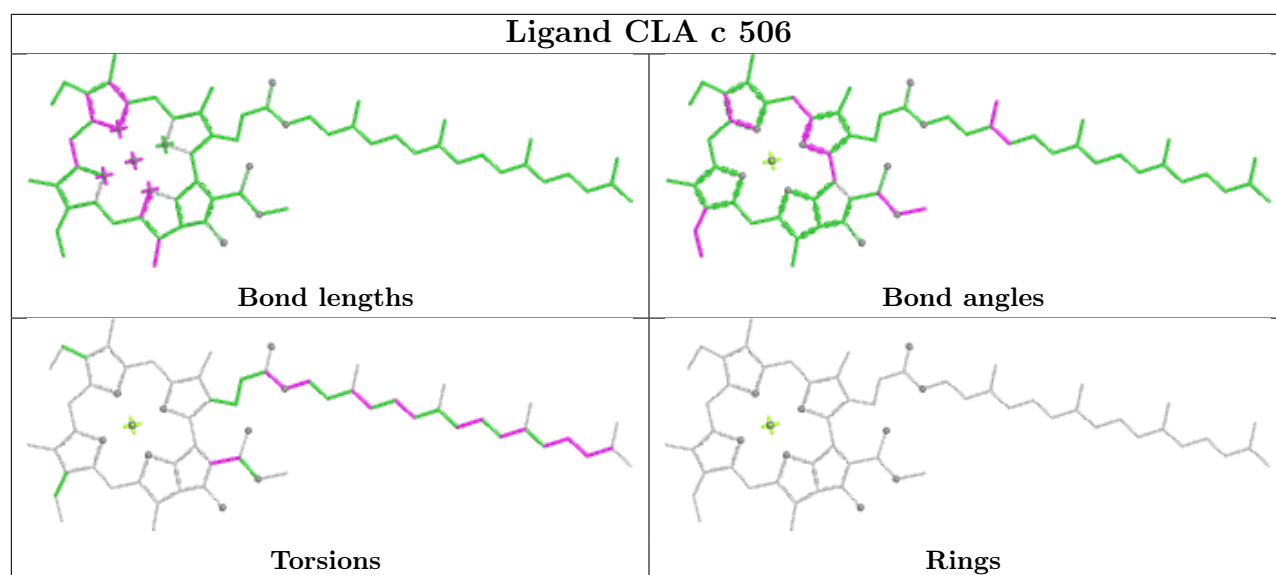


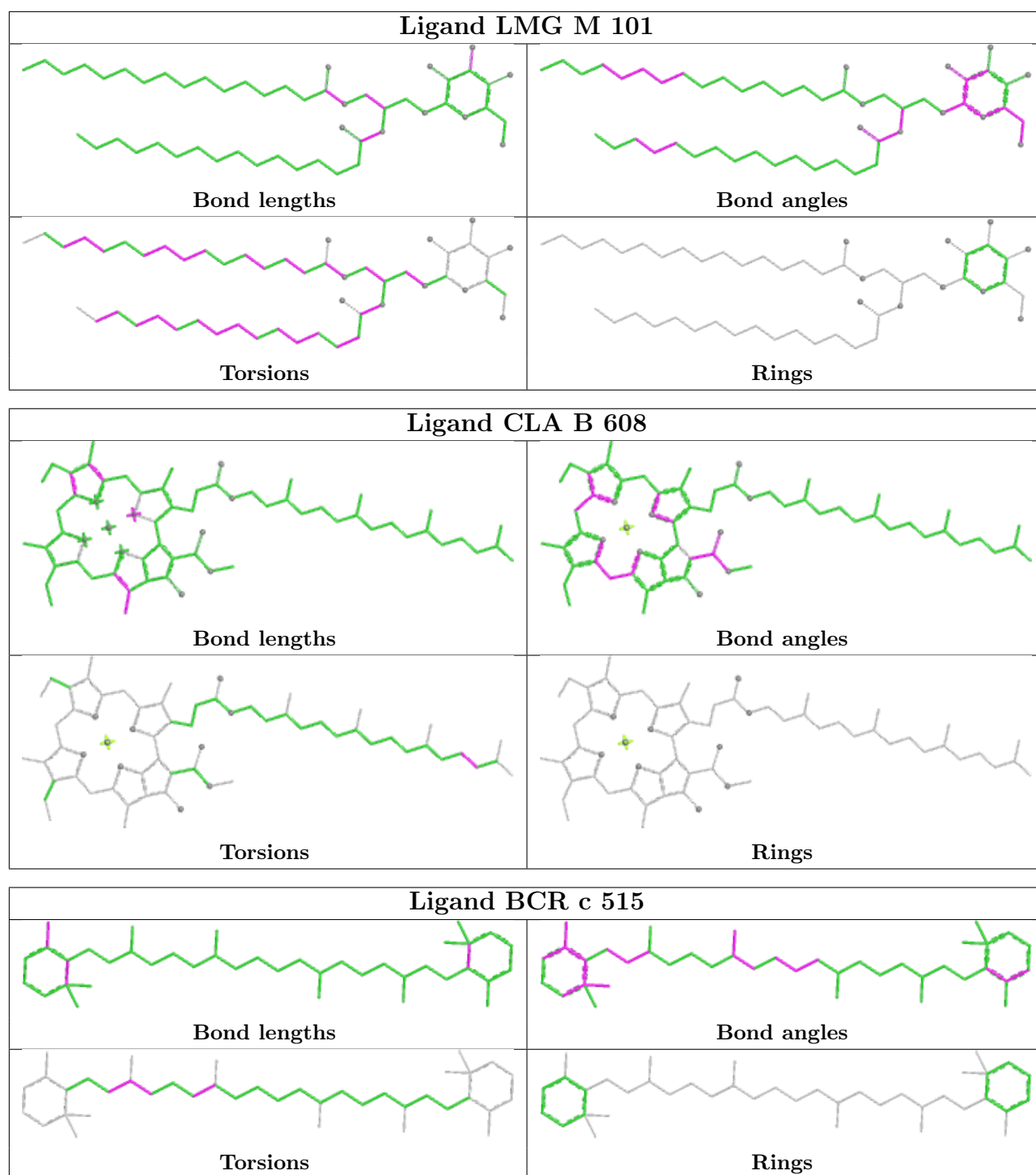


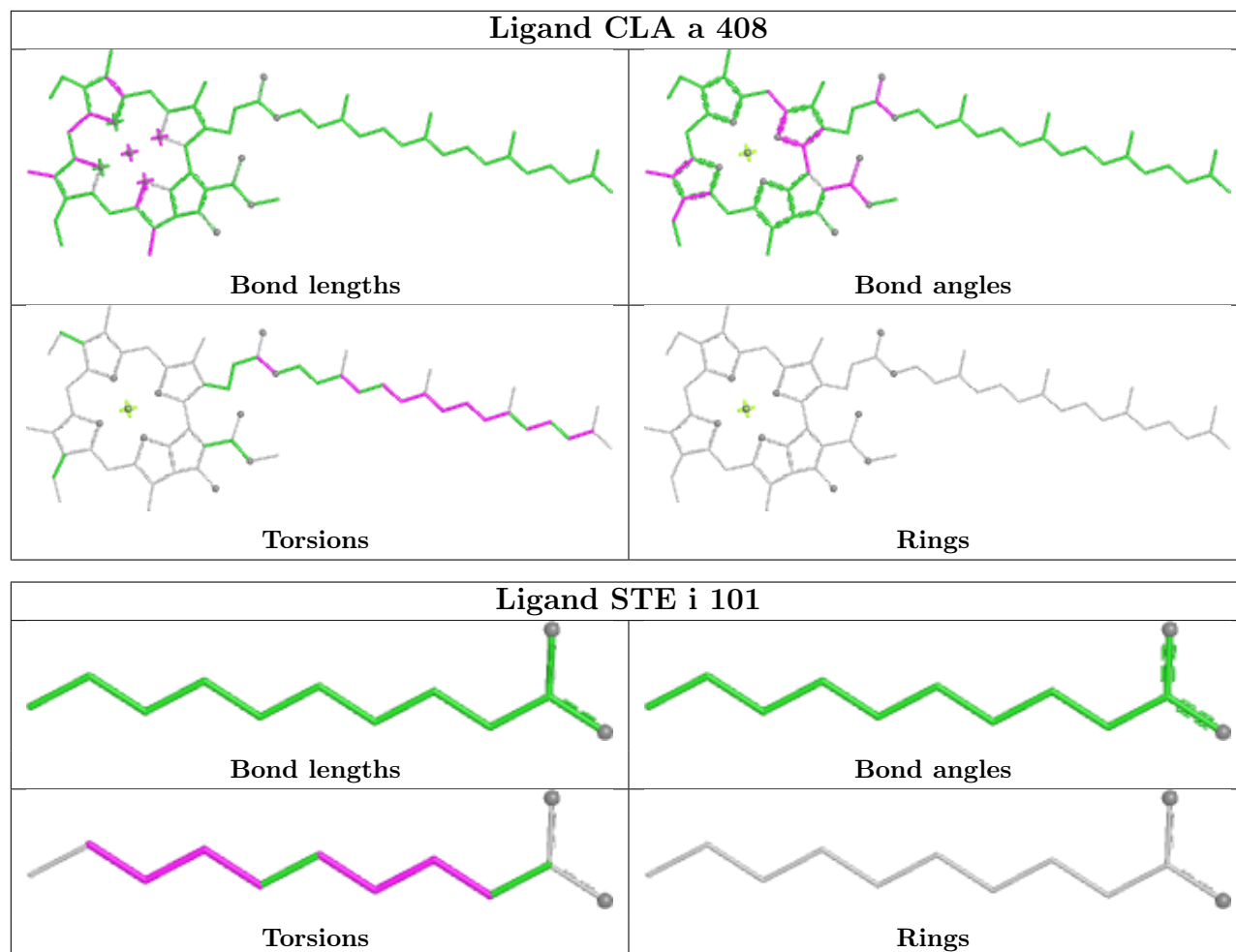




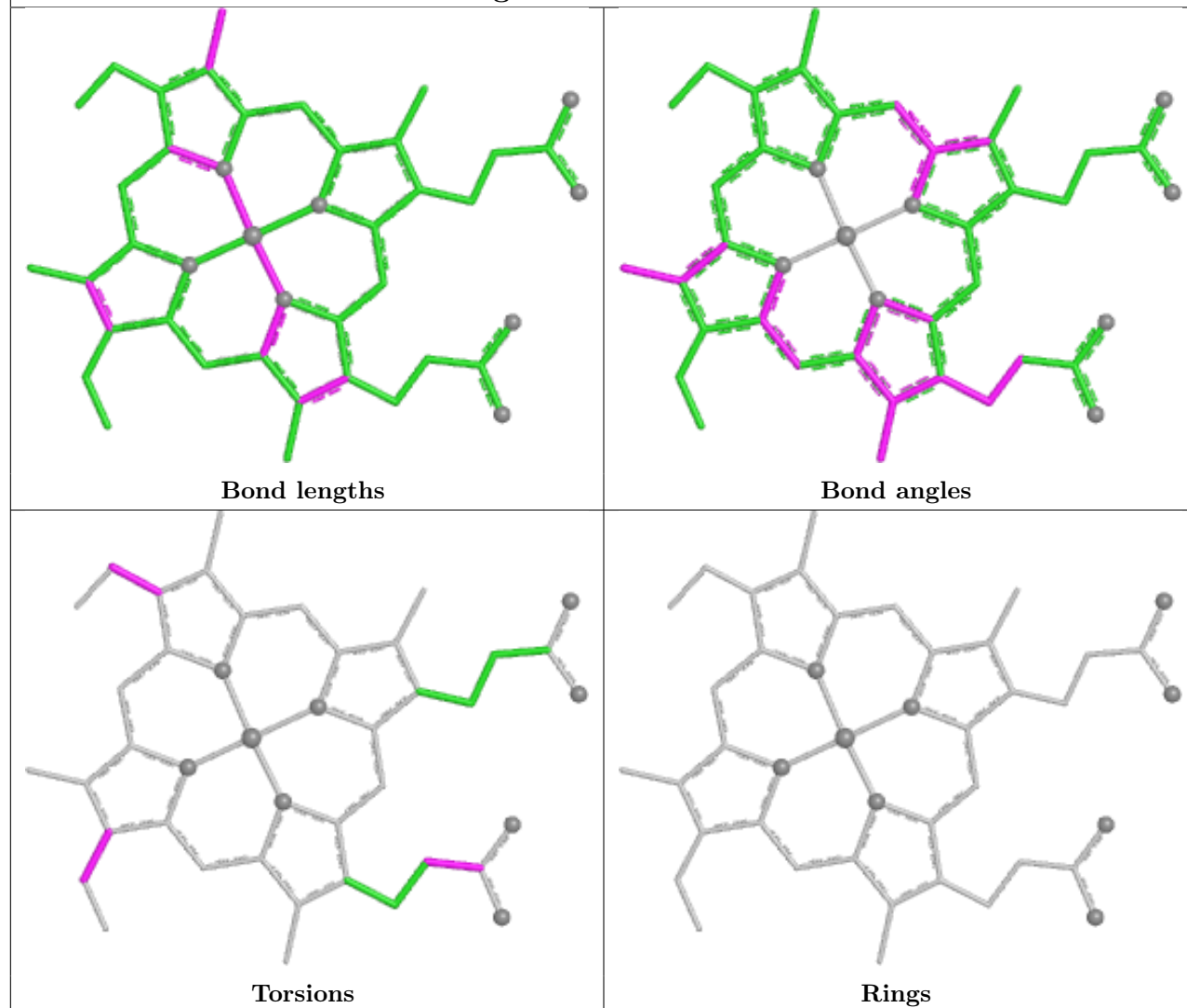




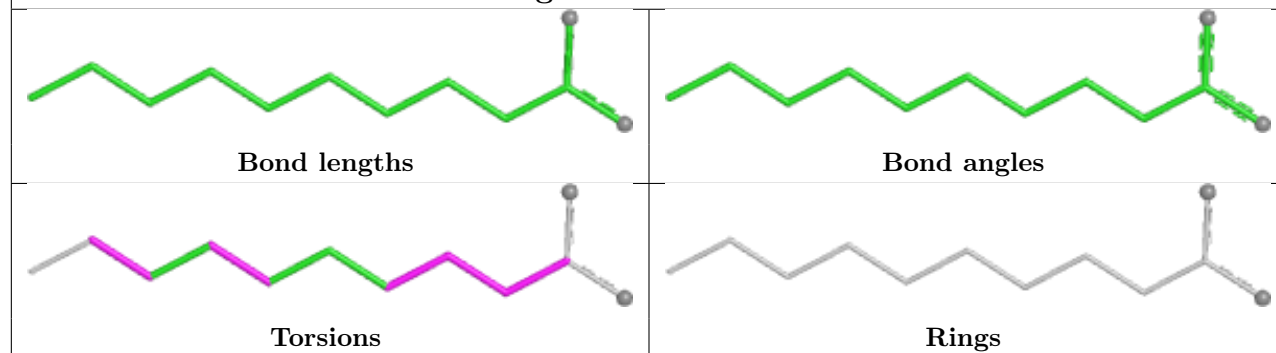


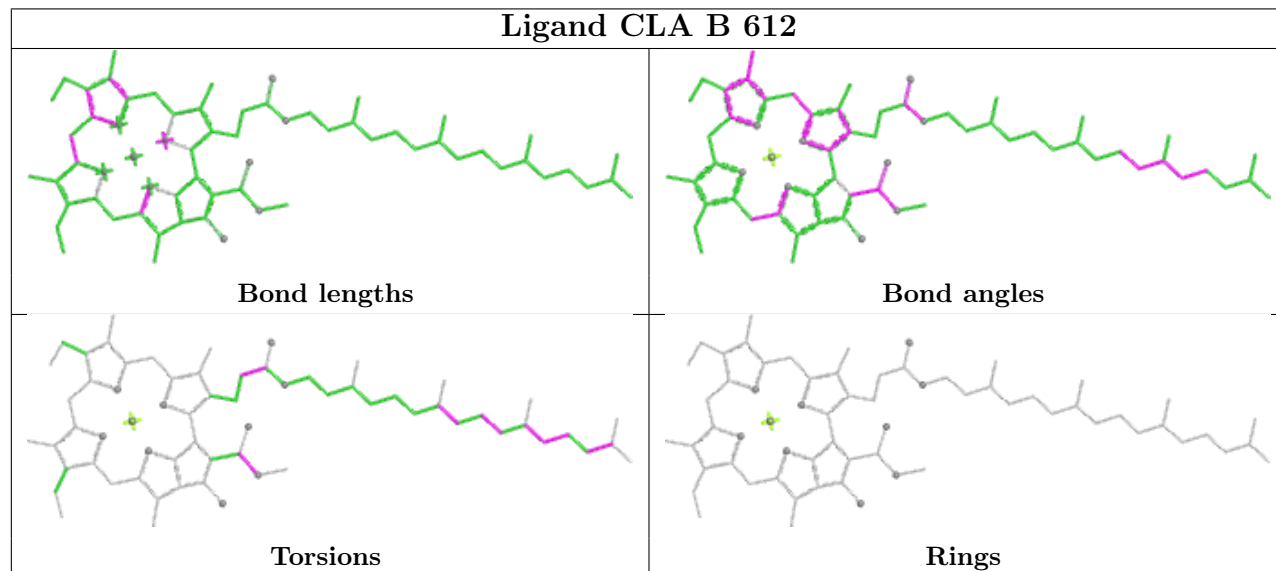
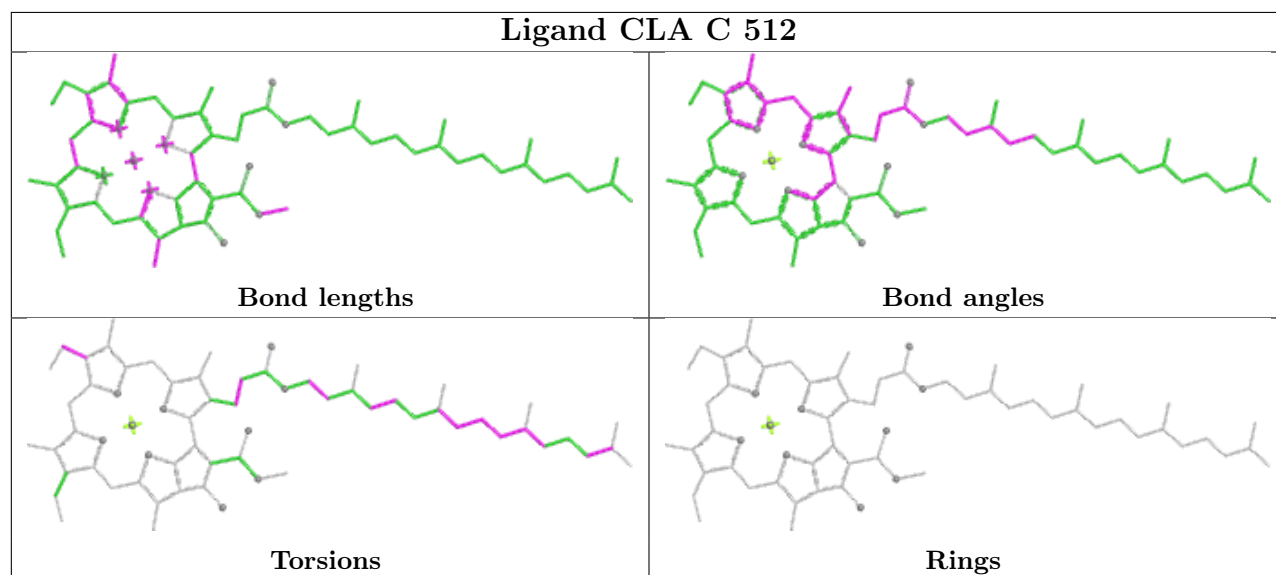
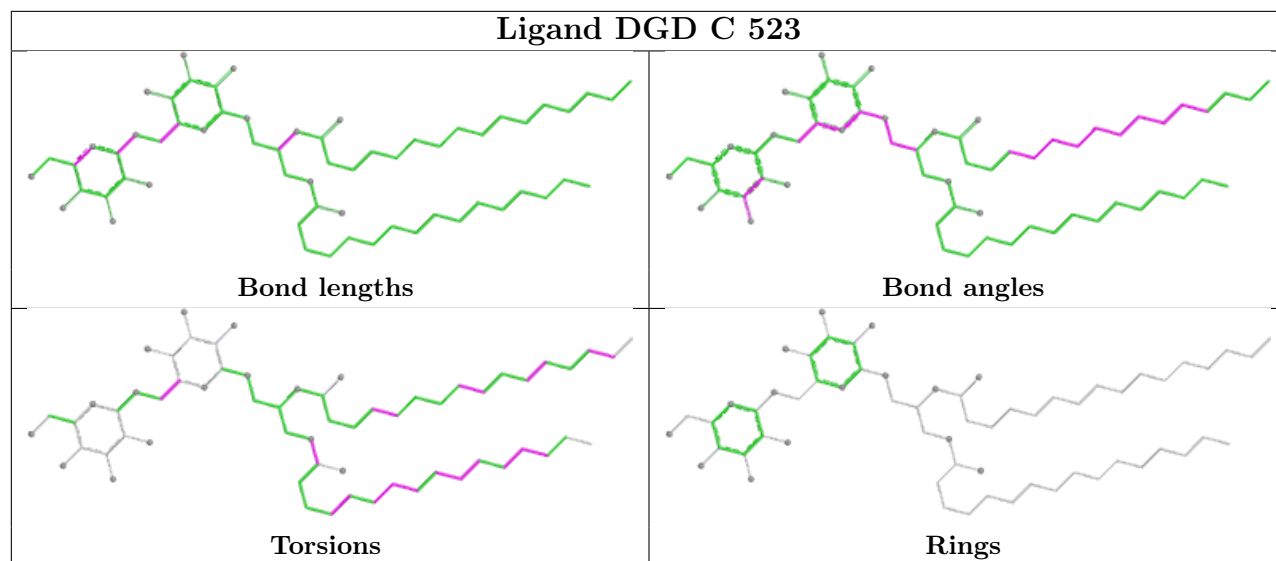


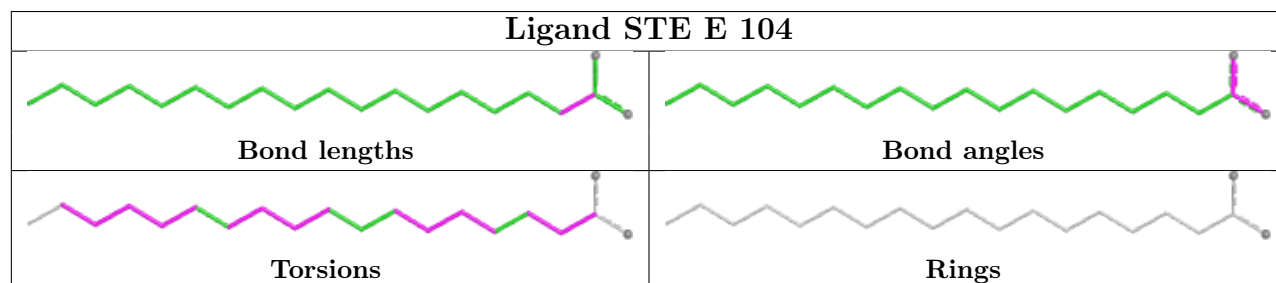
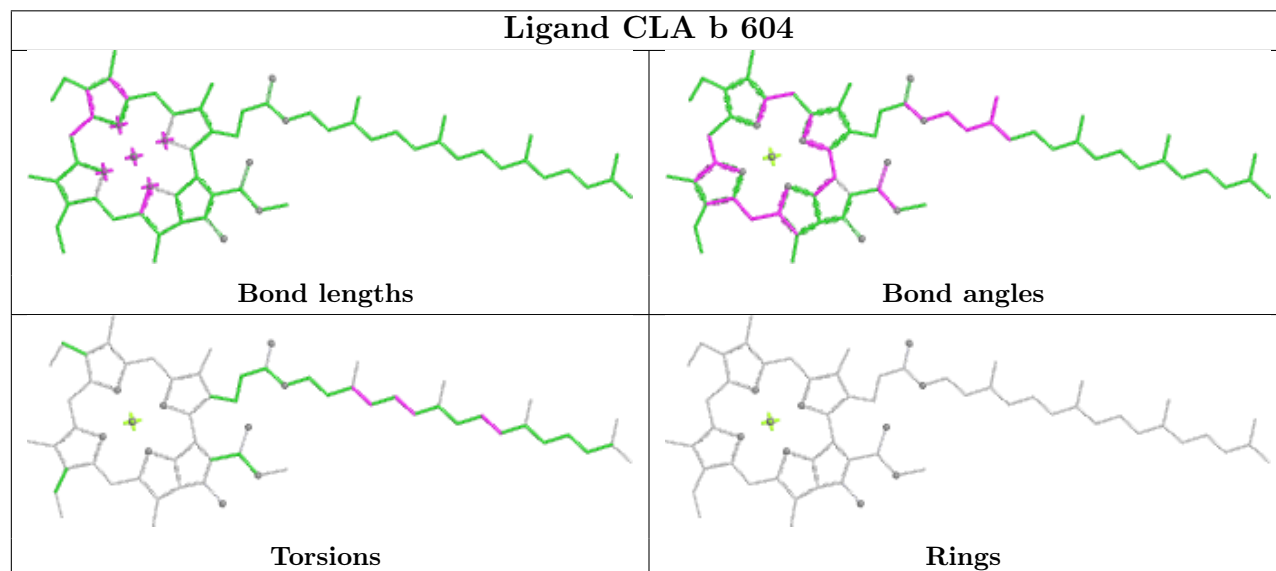
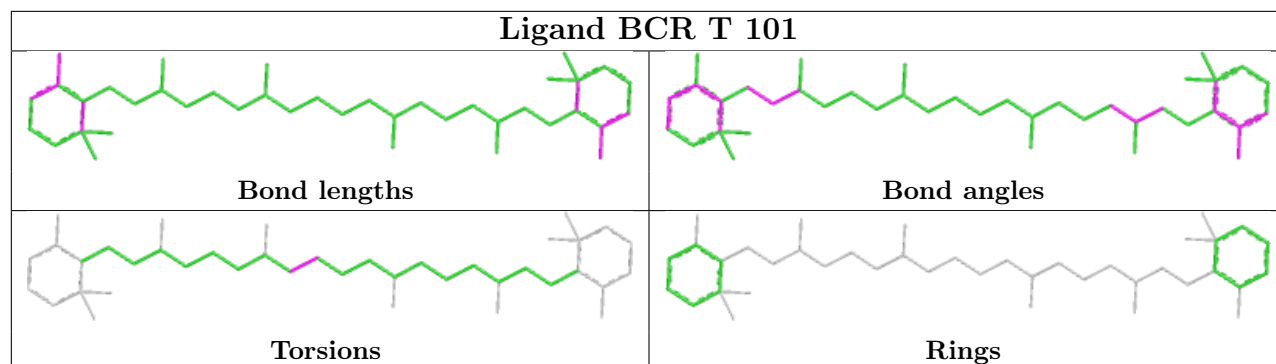
Ligand HEC V 201



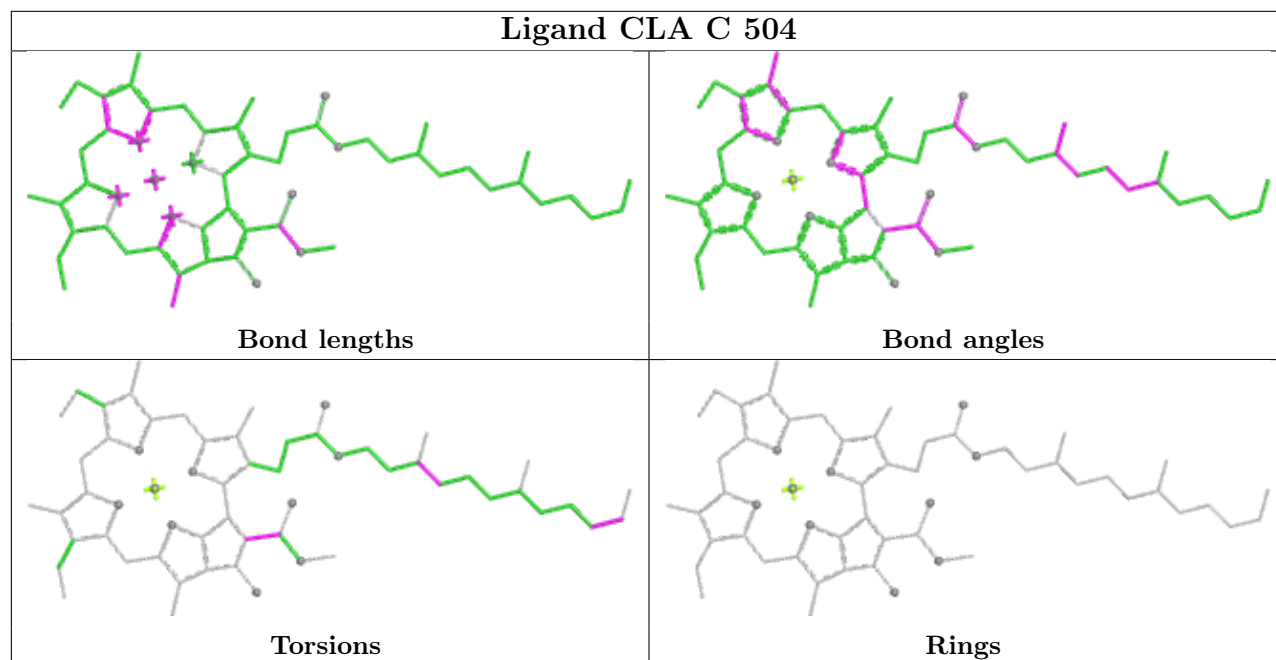
Ligand STE B 622



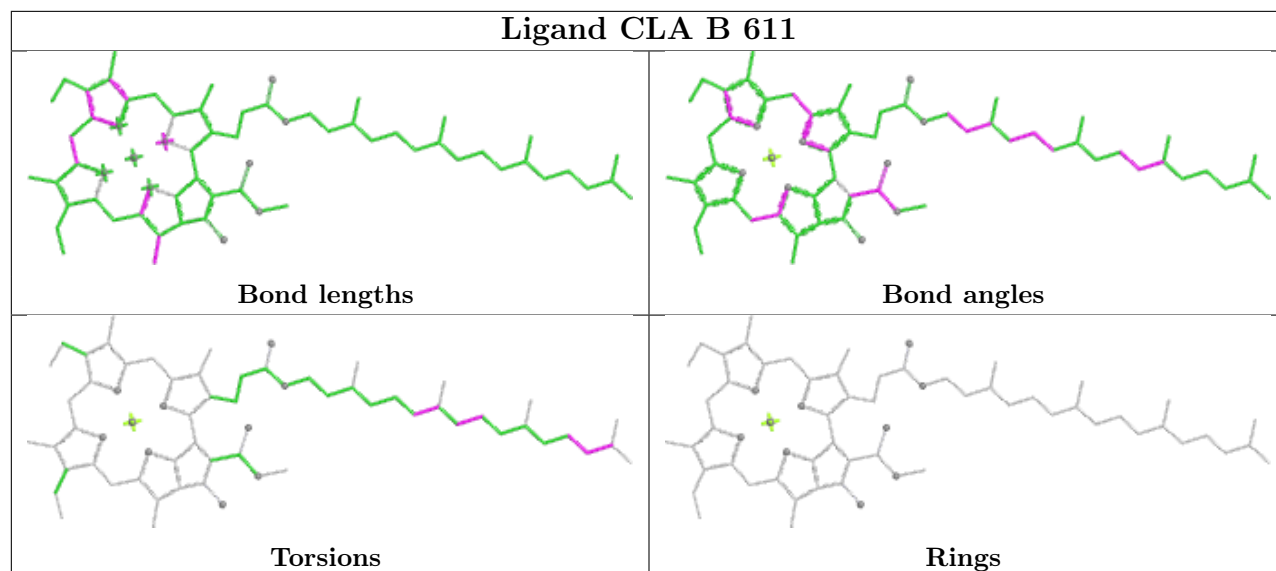


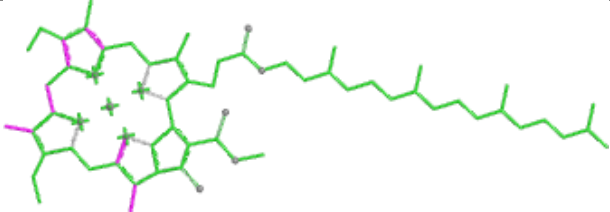
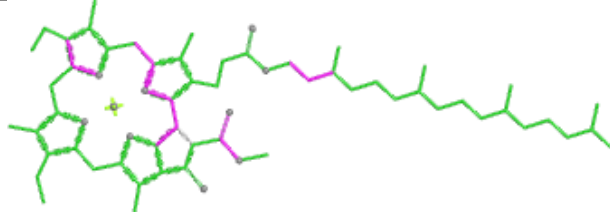
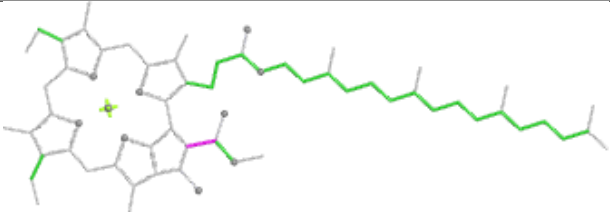
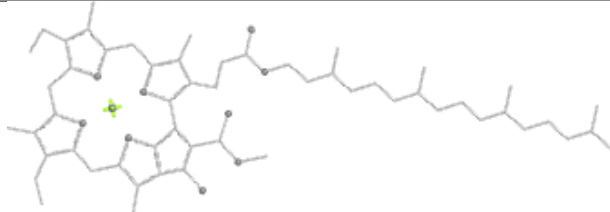
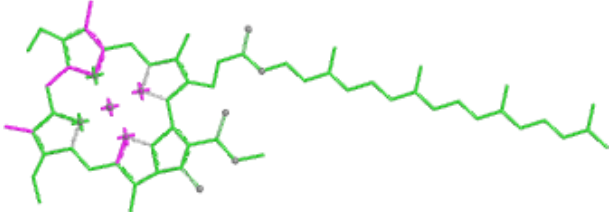
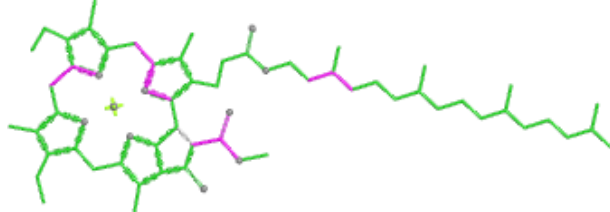
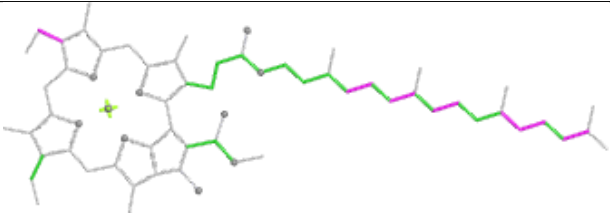
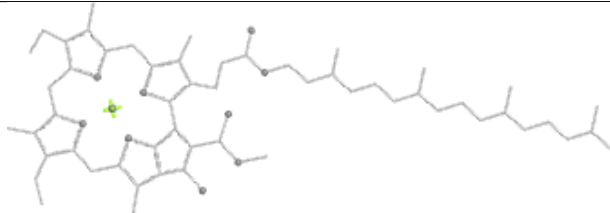
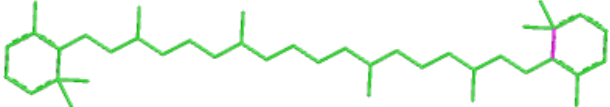
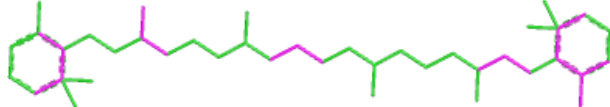
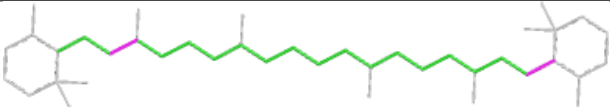
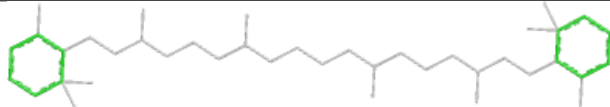


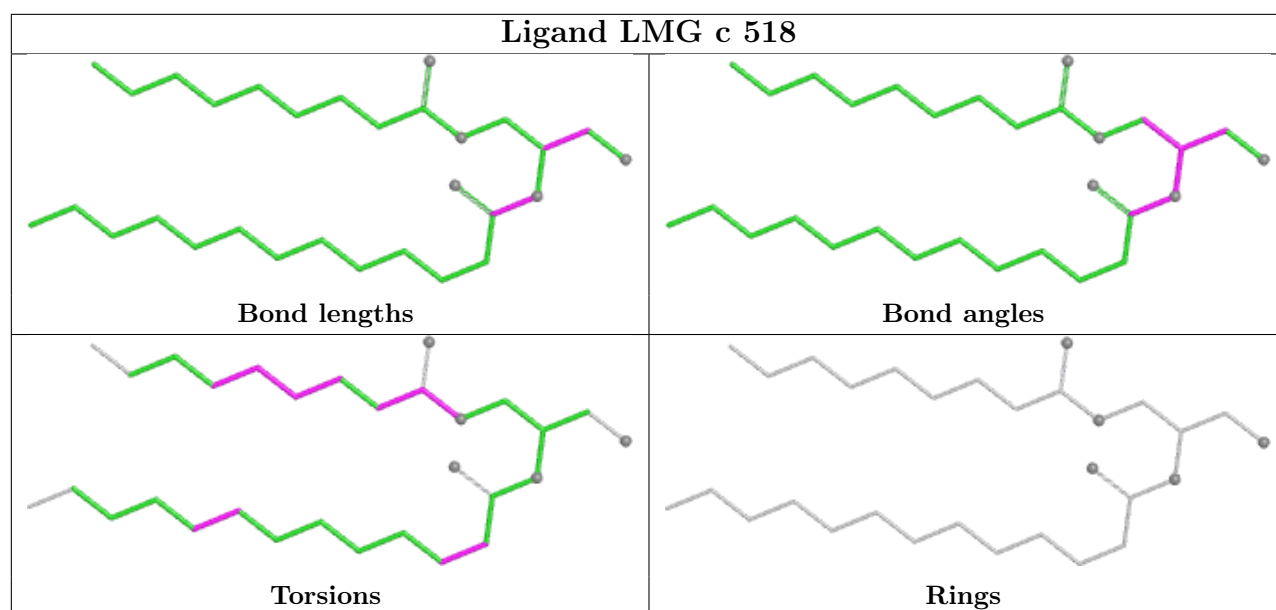
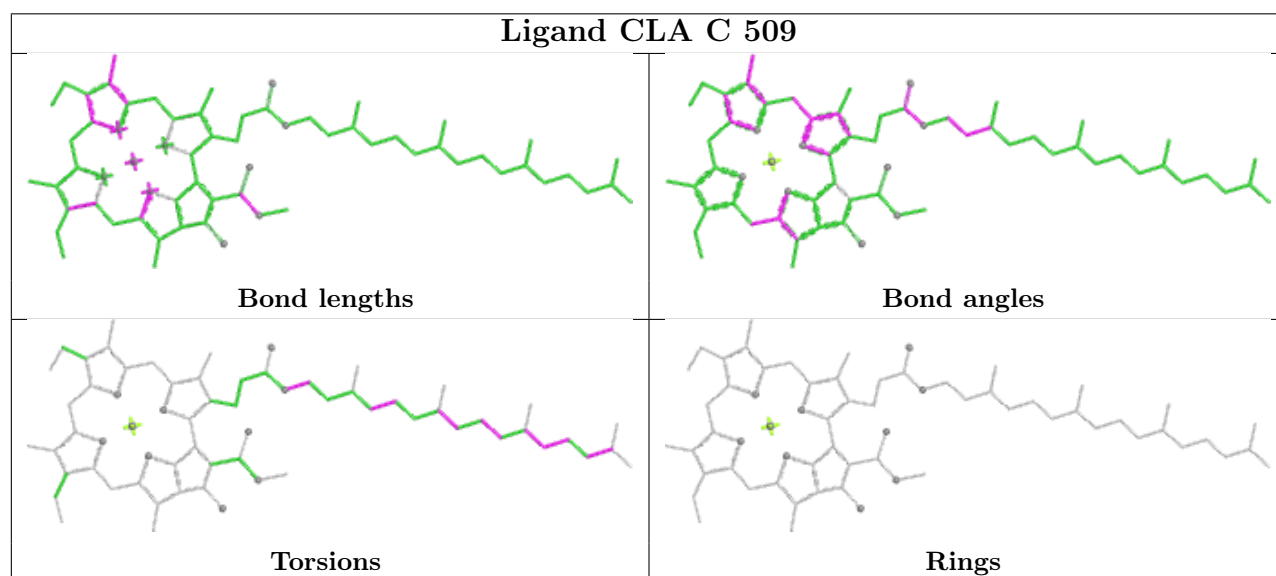
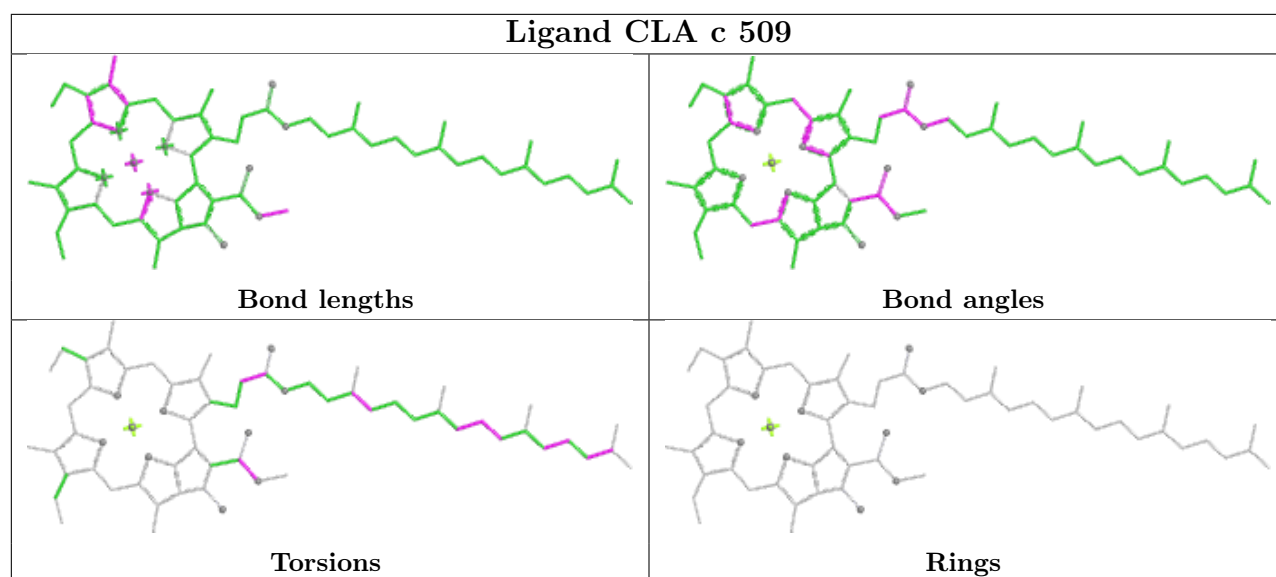
Ligand CLA C 504

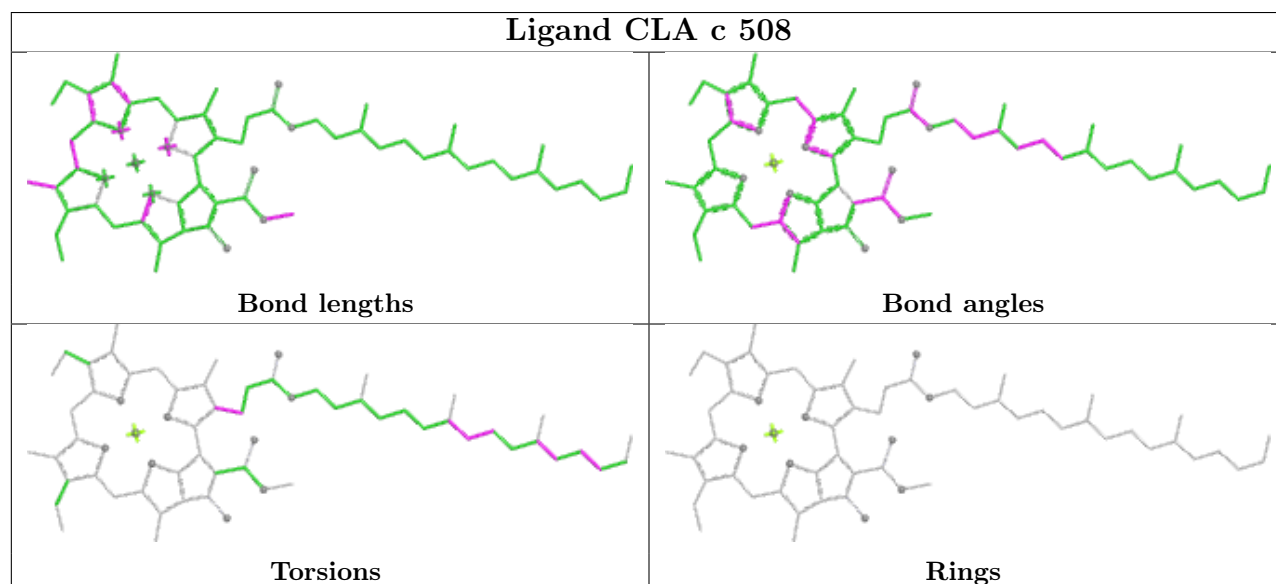
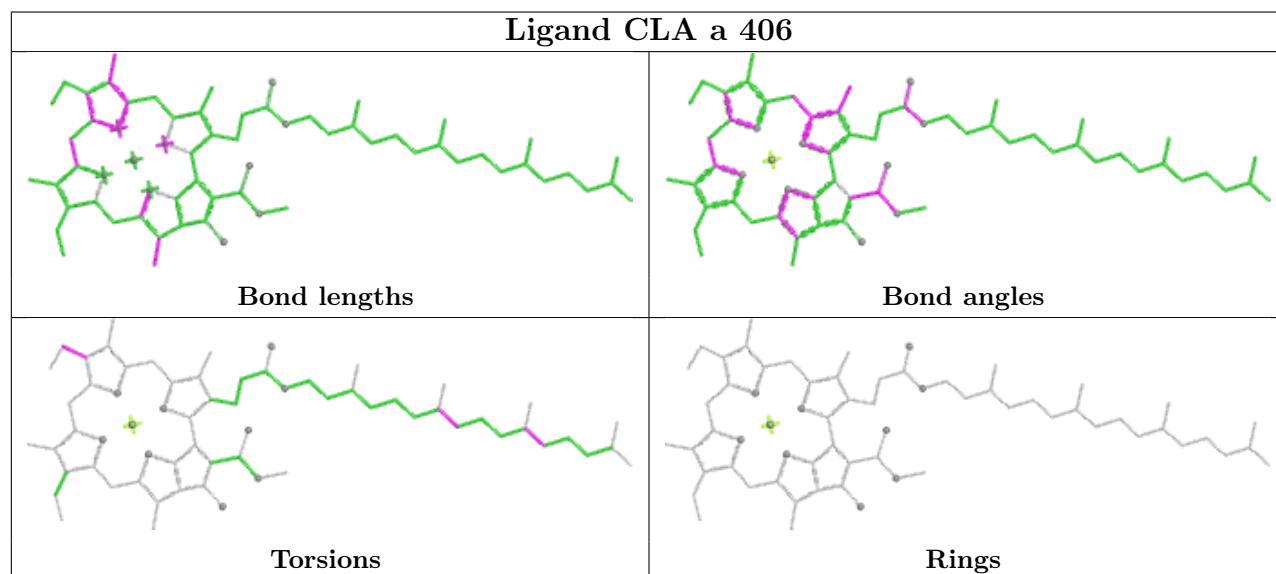
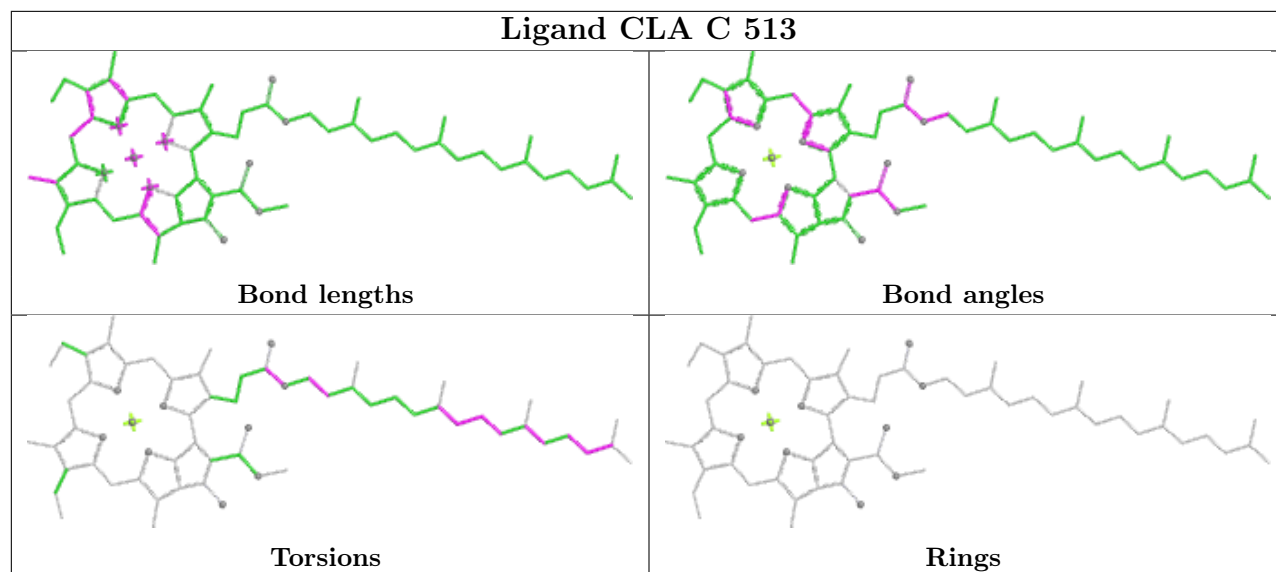


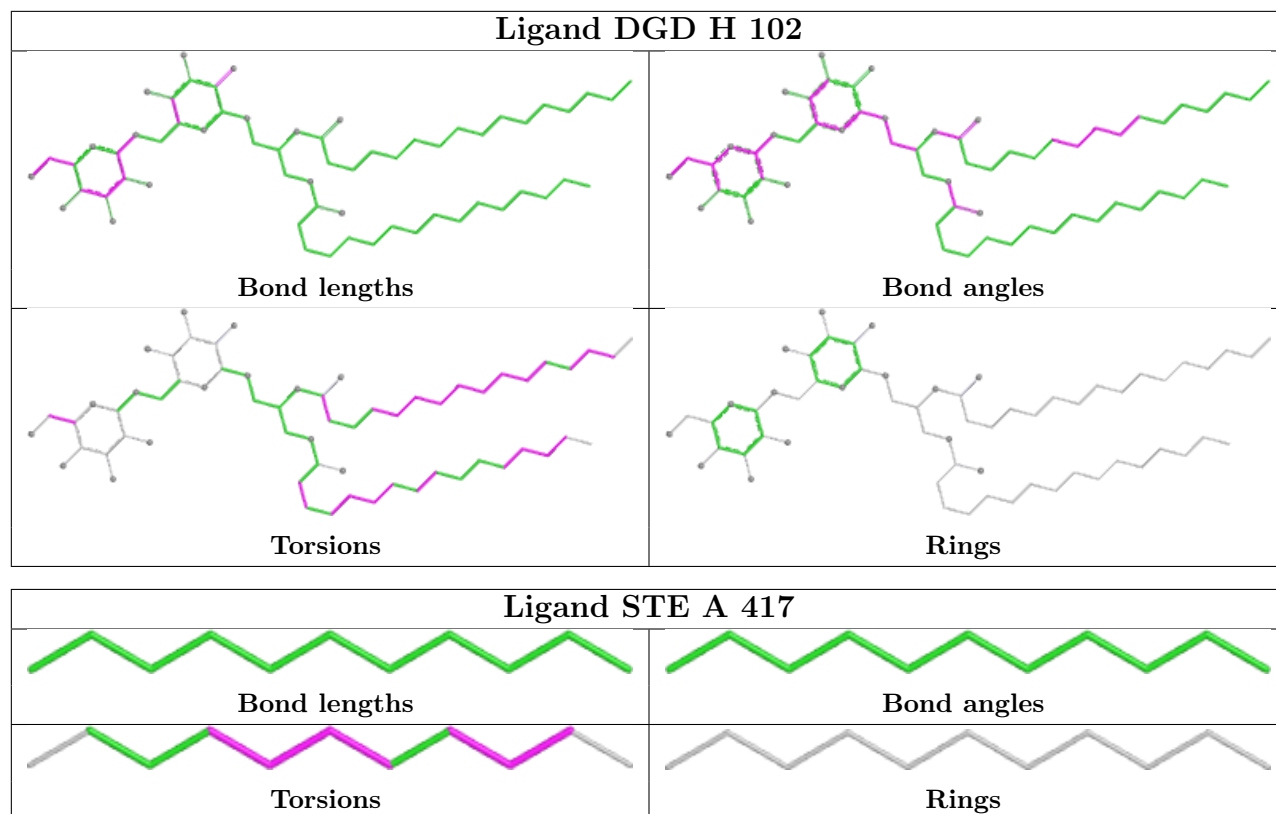
Ligand CLA B 611

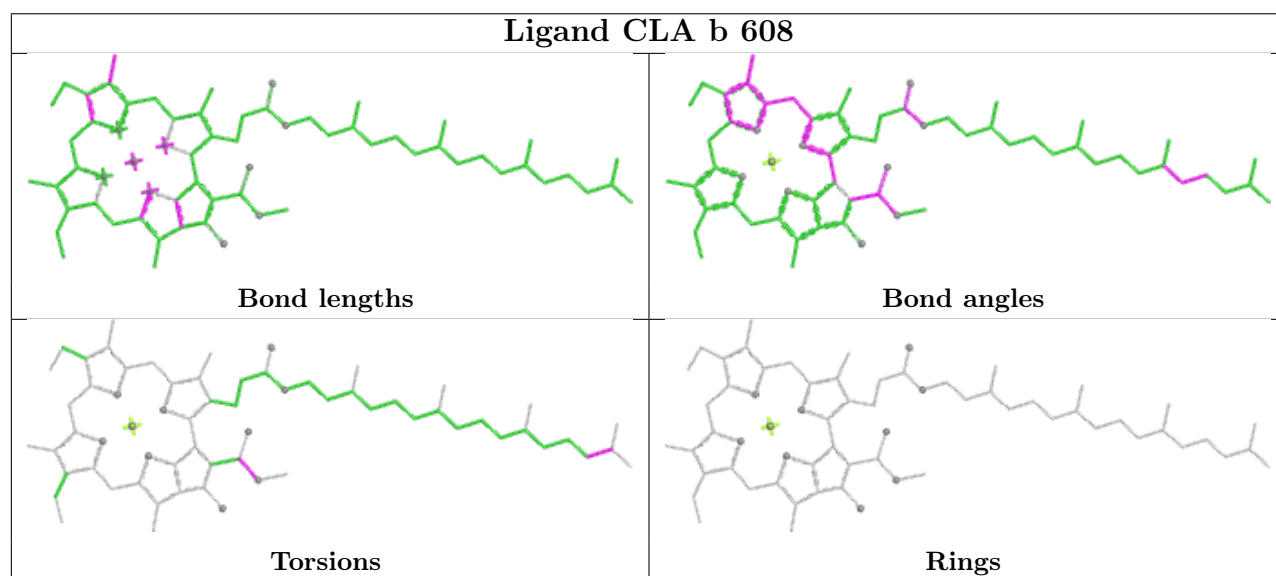
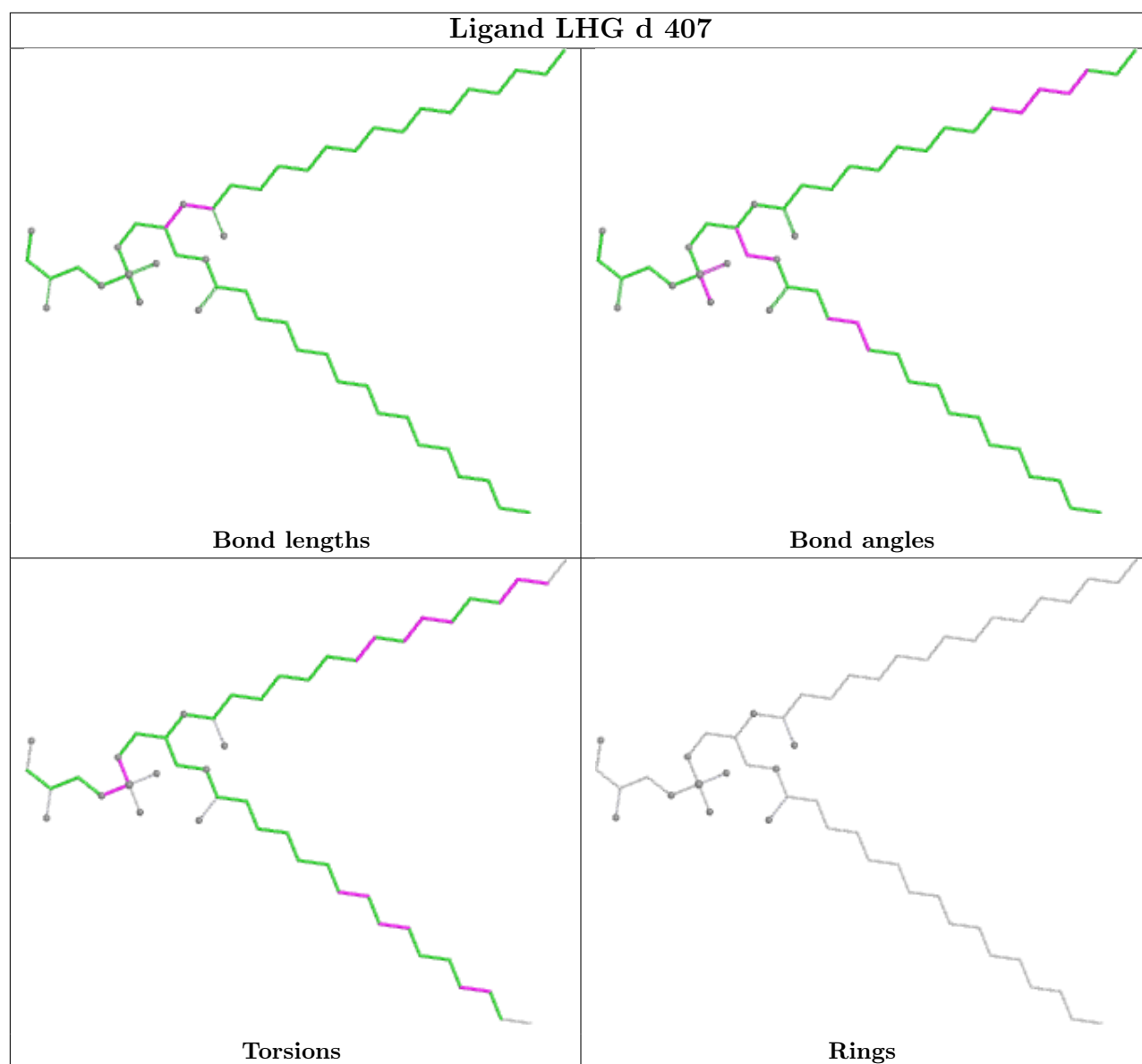


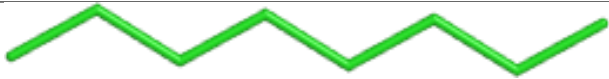
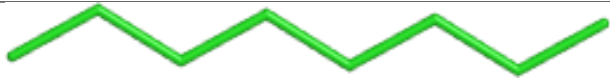
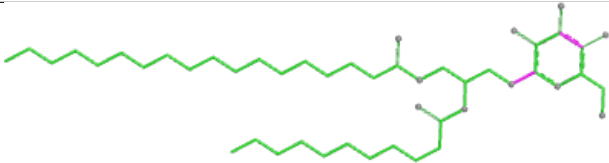
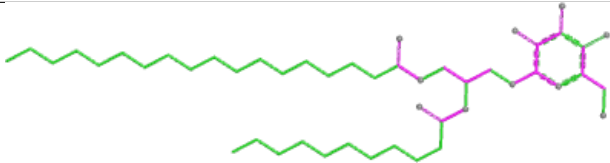
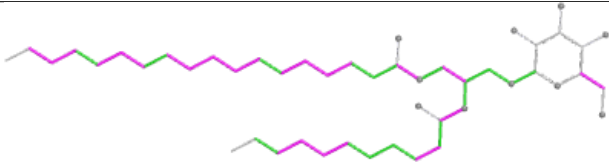
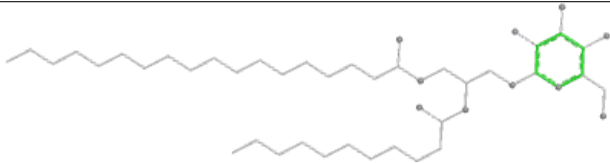
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



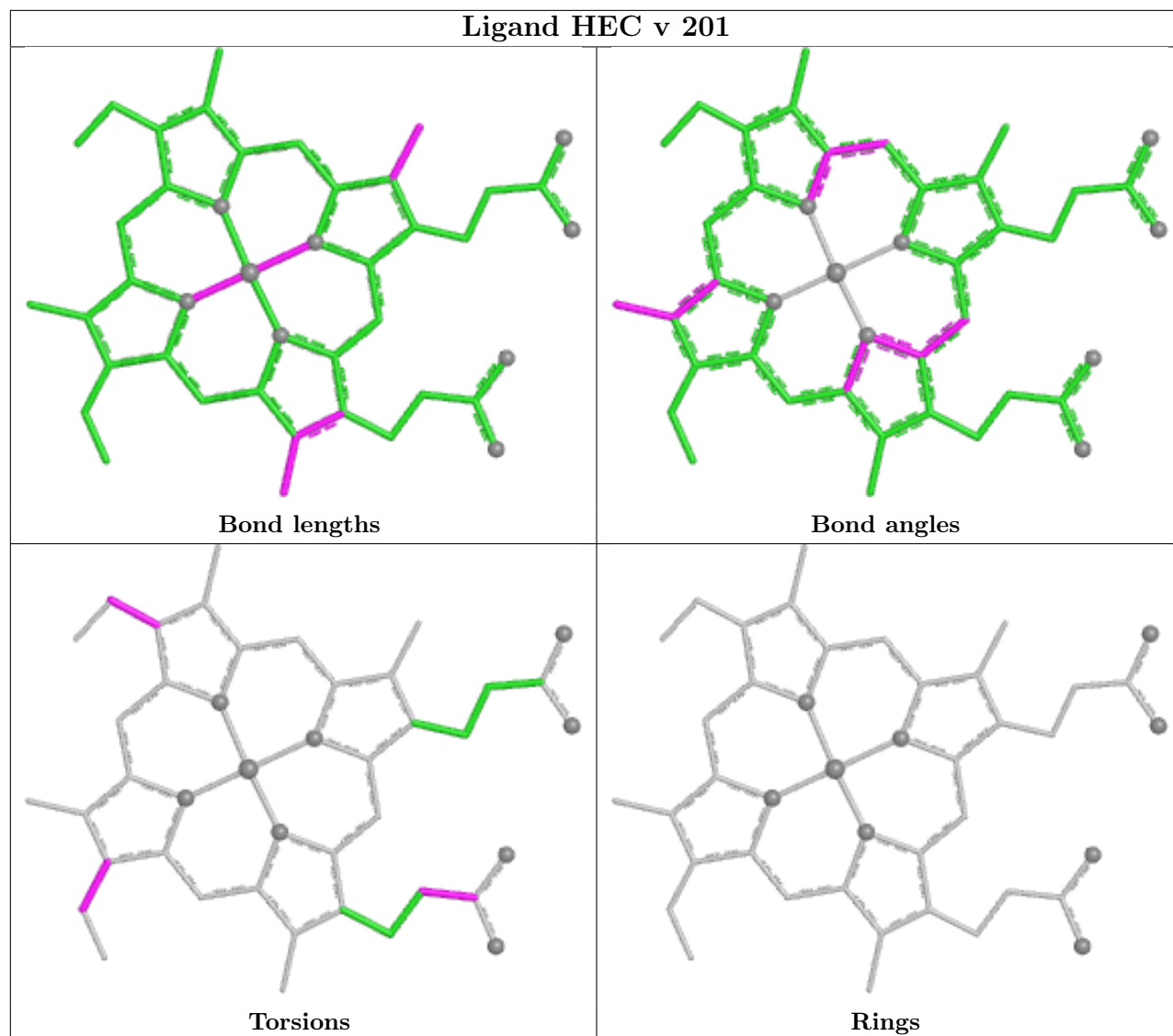




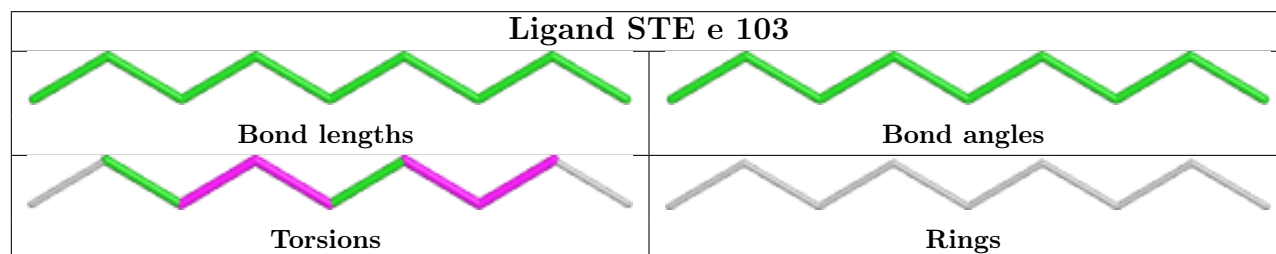


Ligand STE A 415	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 526	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

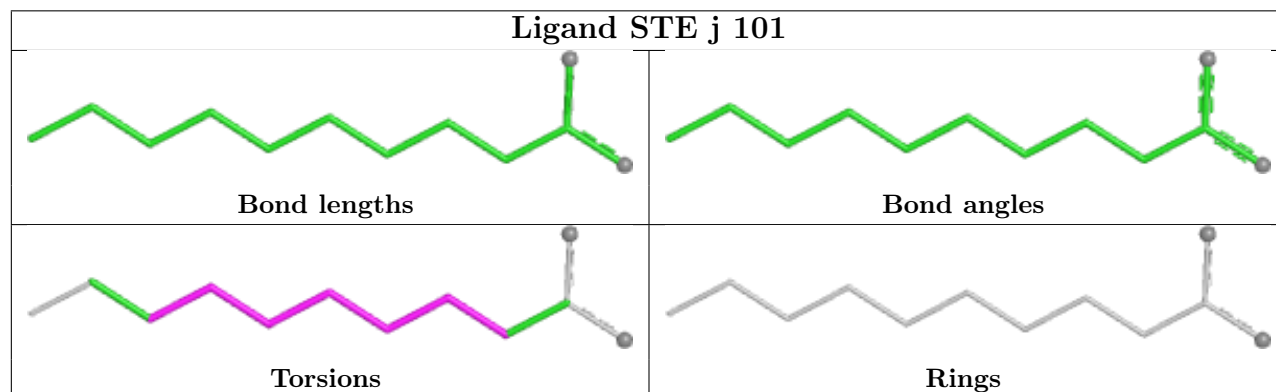
Ligand HEC v 201

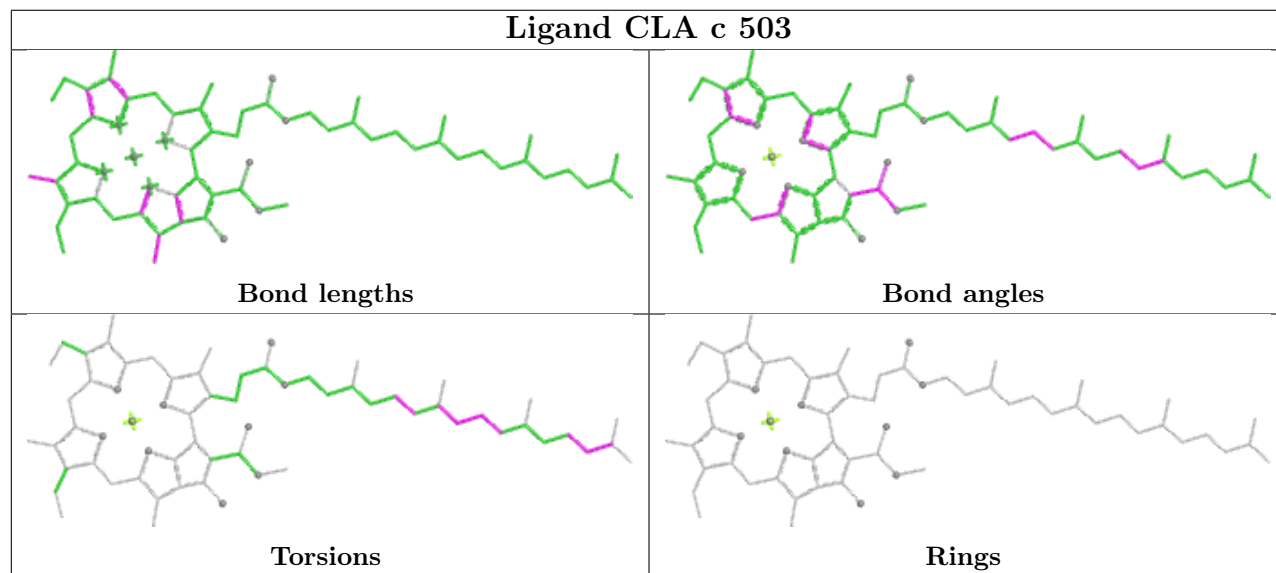
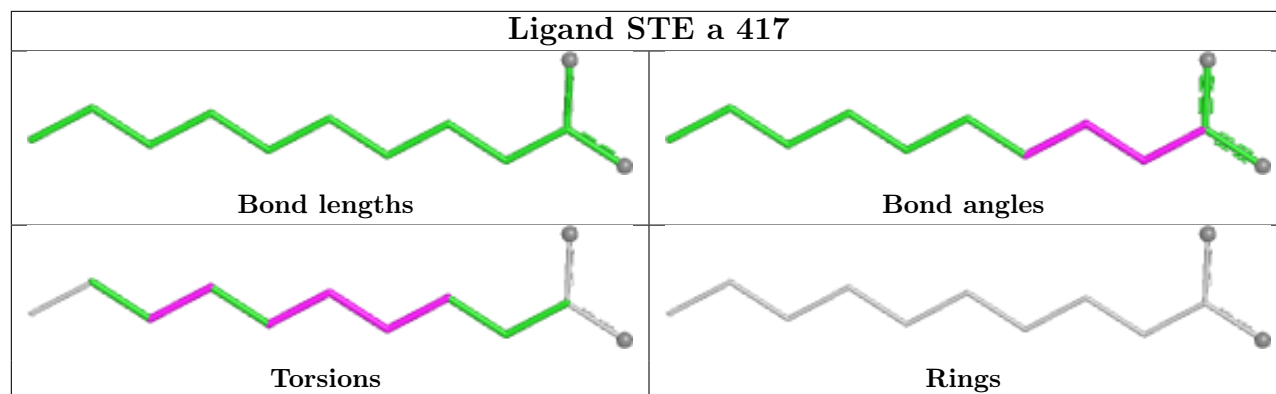


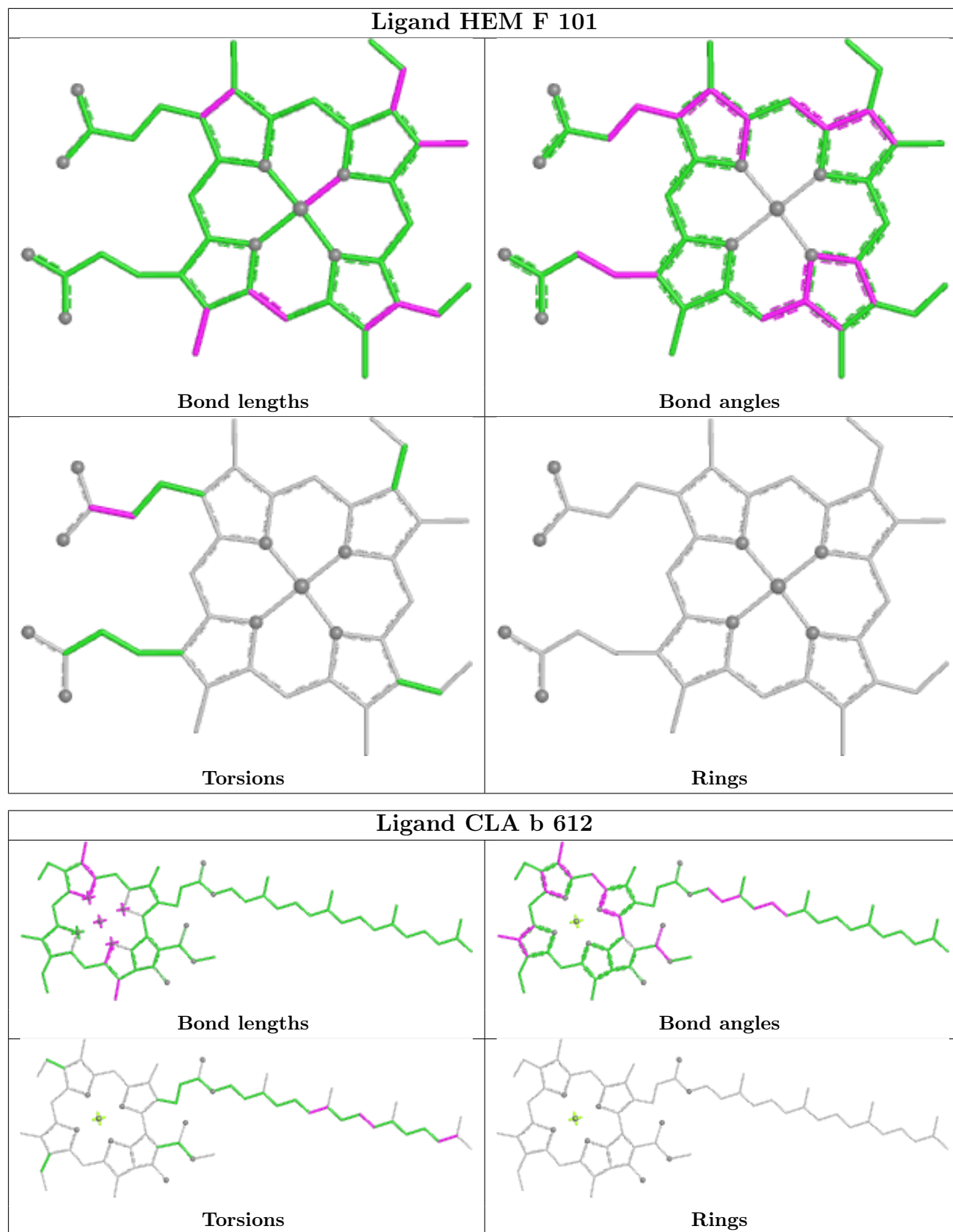
Ligand STE e 103

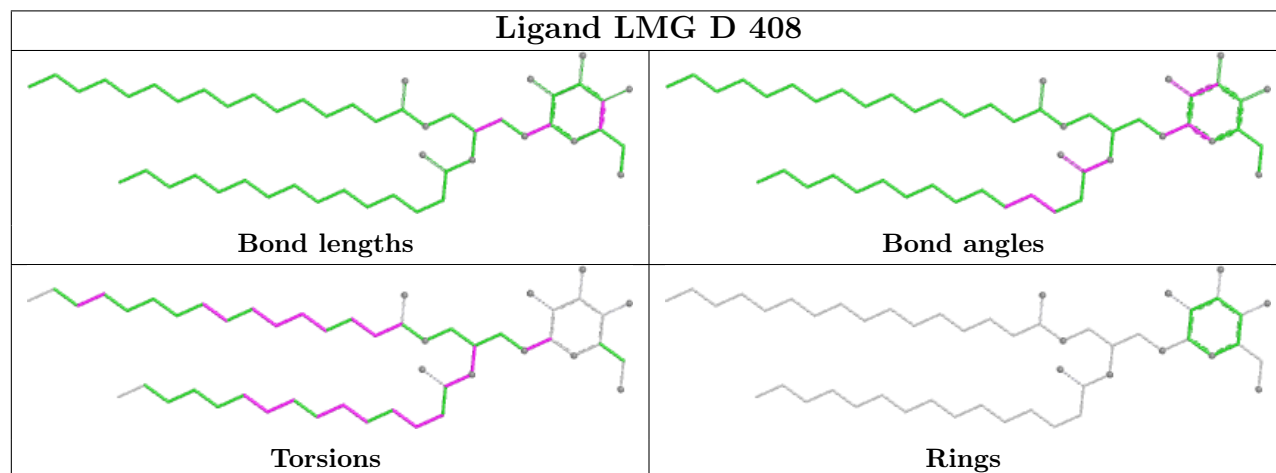
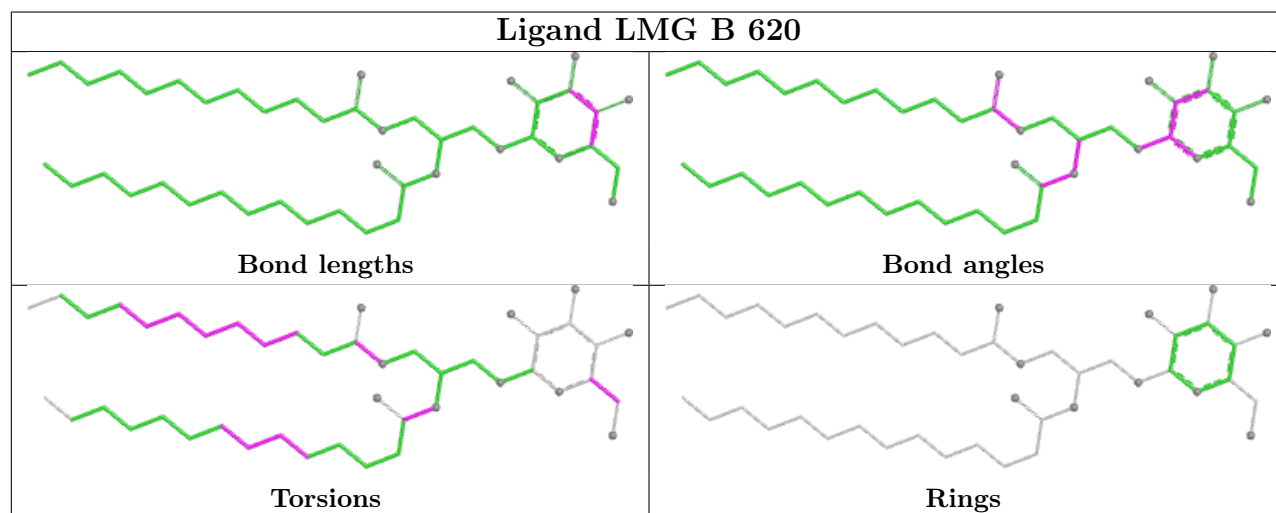
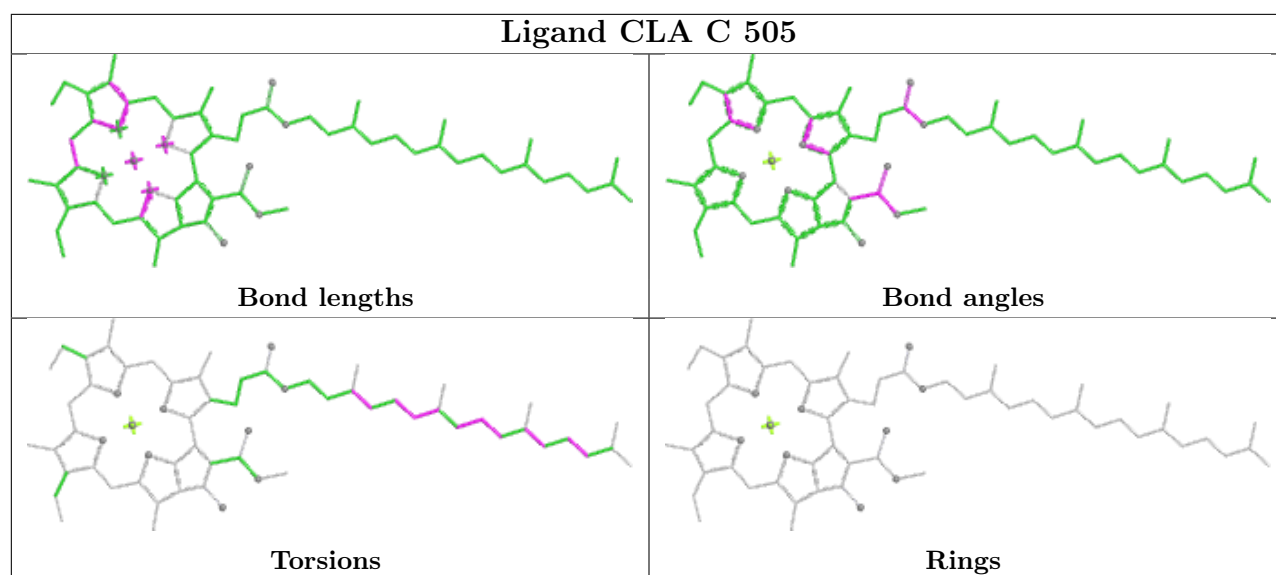


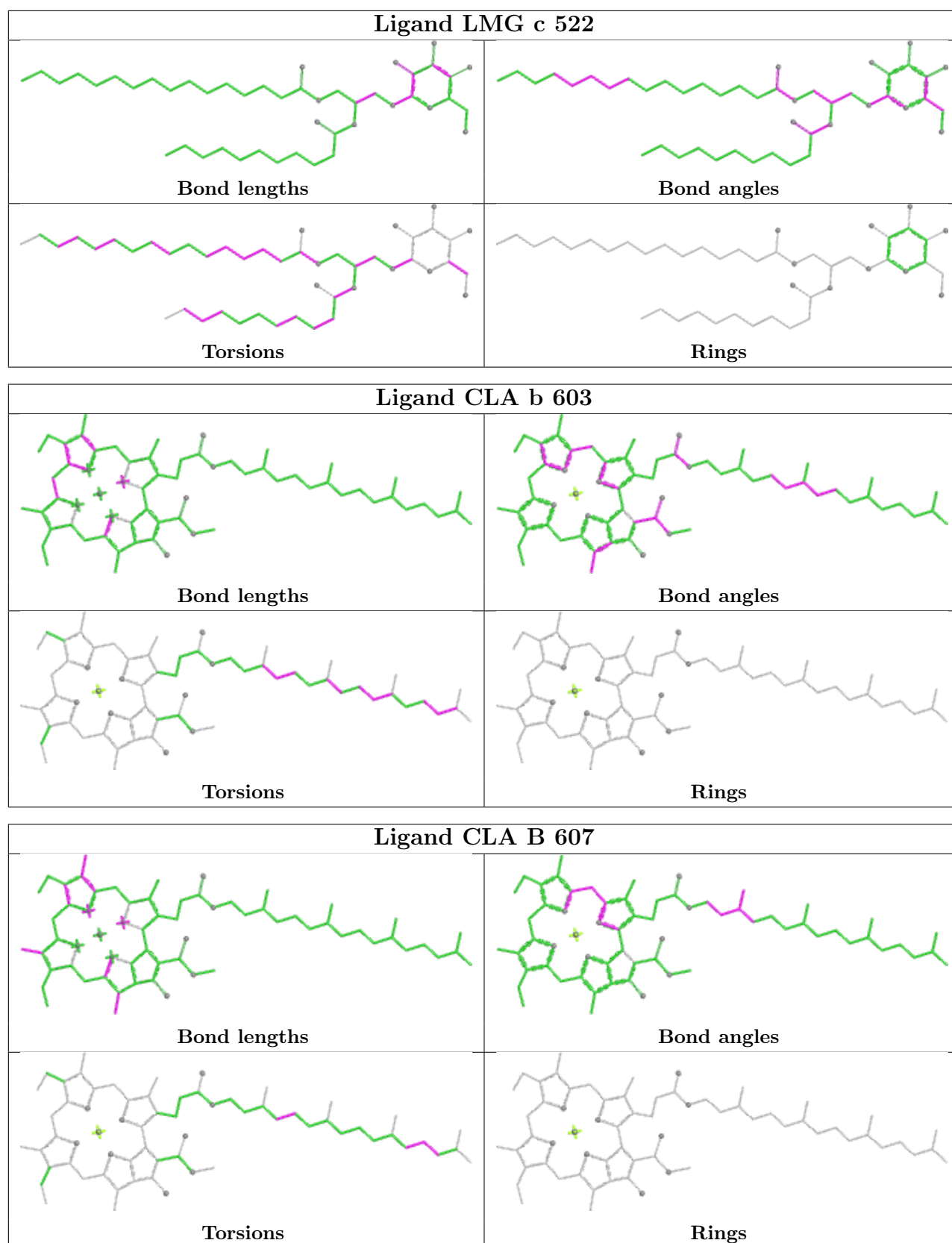
Ligand STE j 101

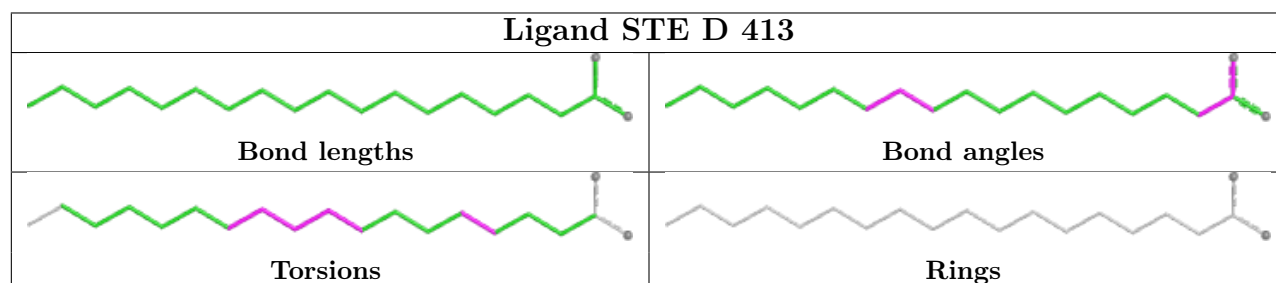
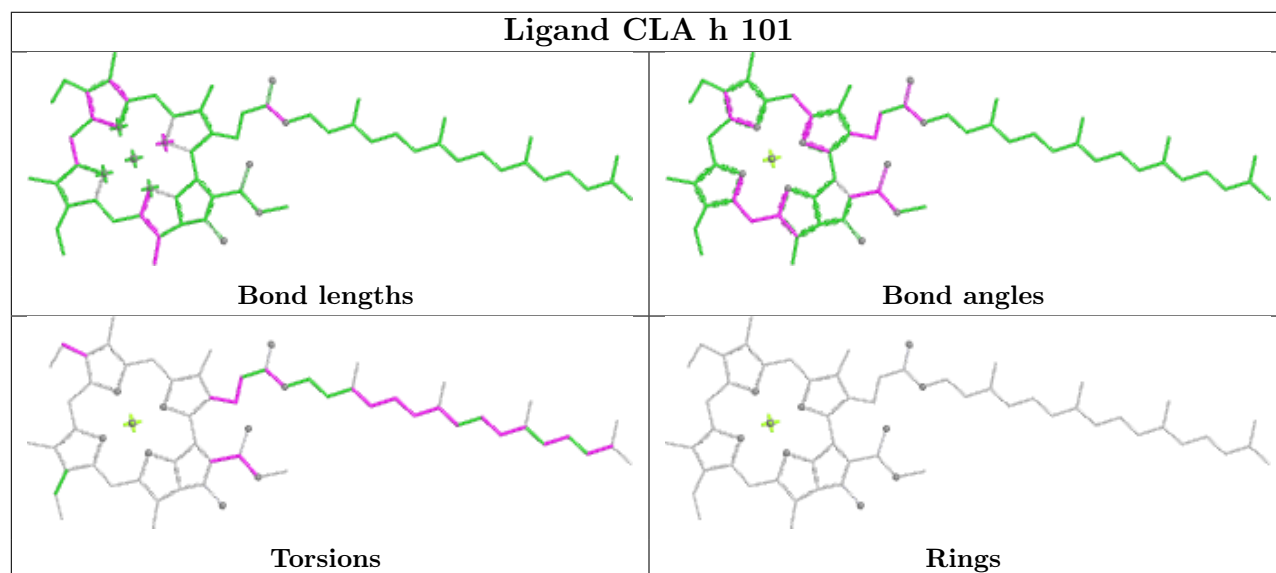
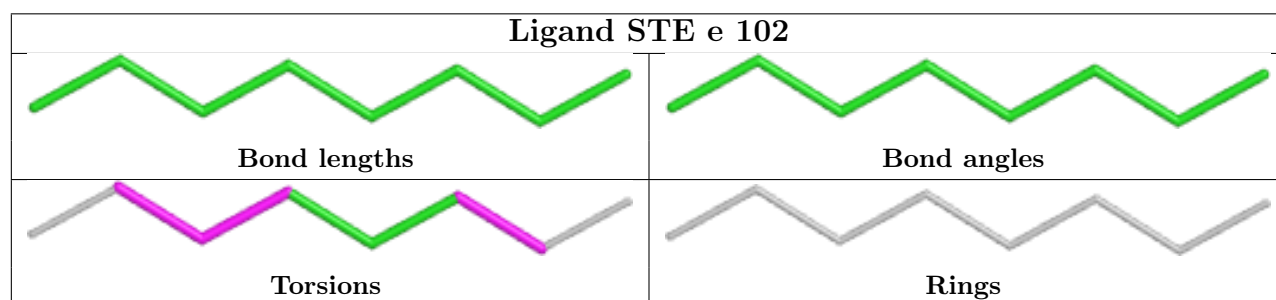
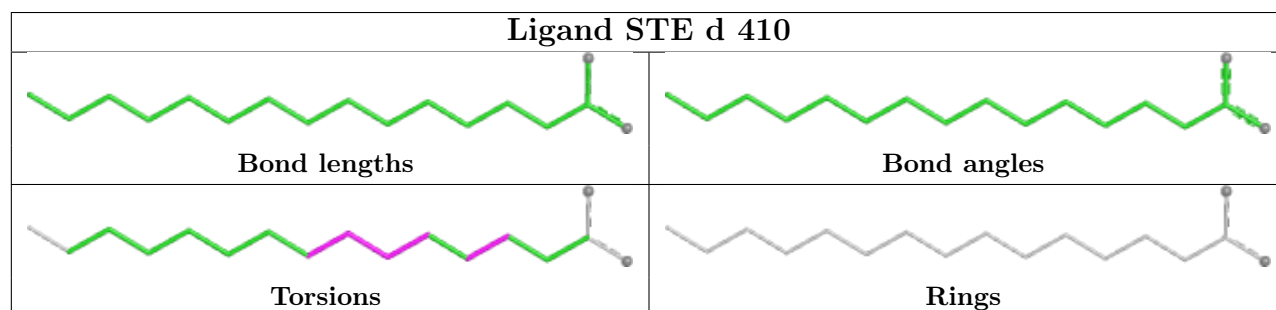
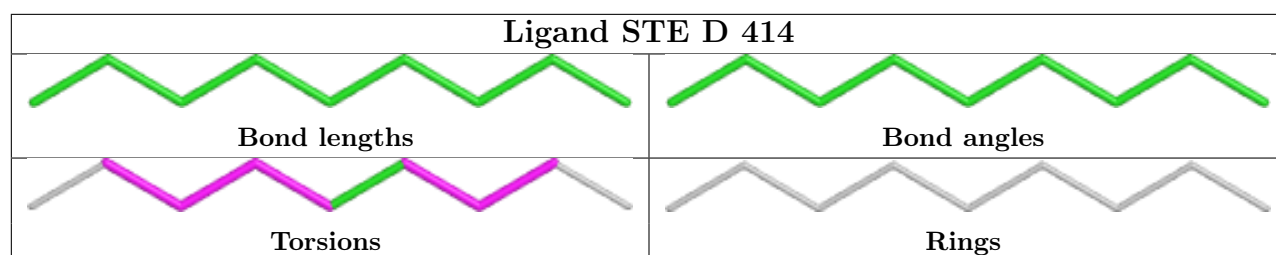


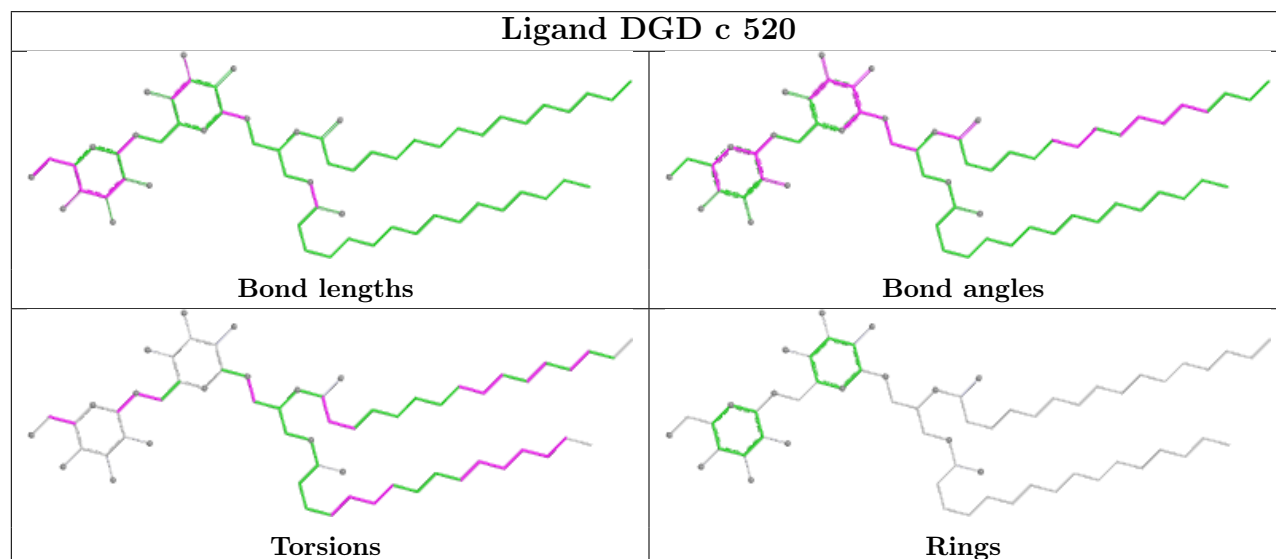
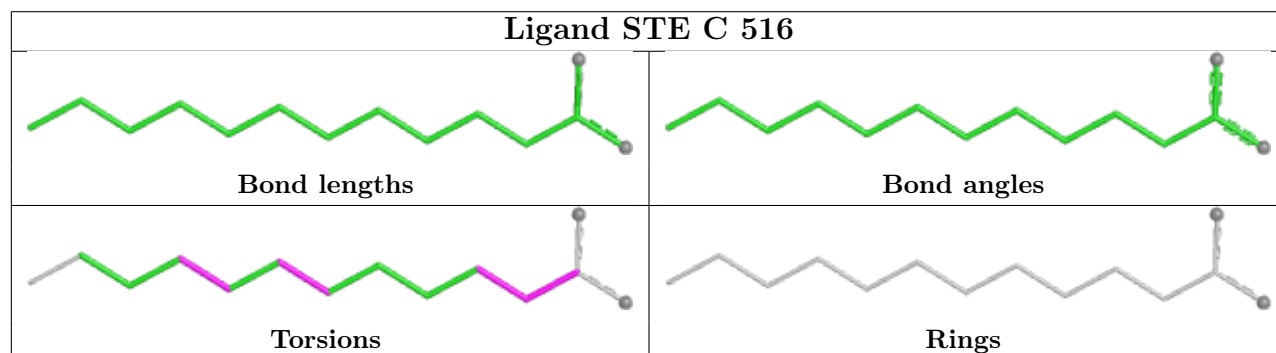
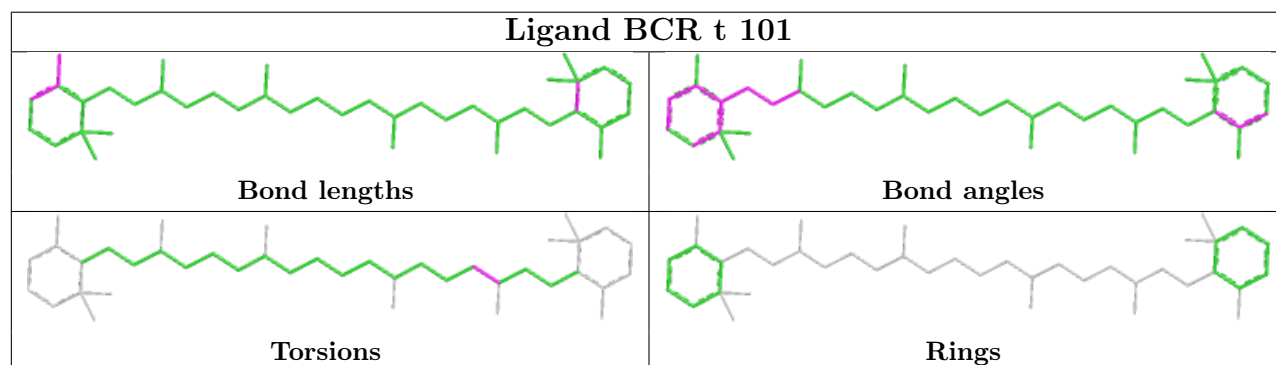
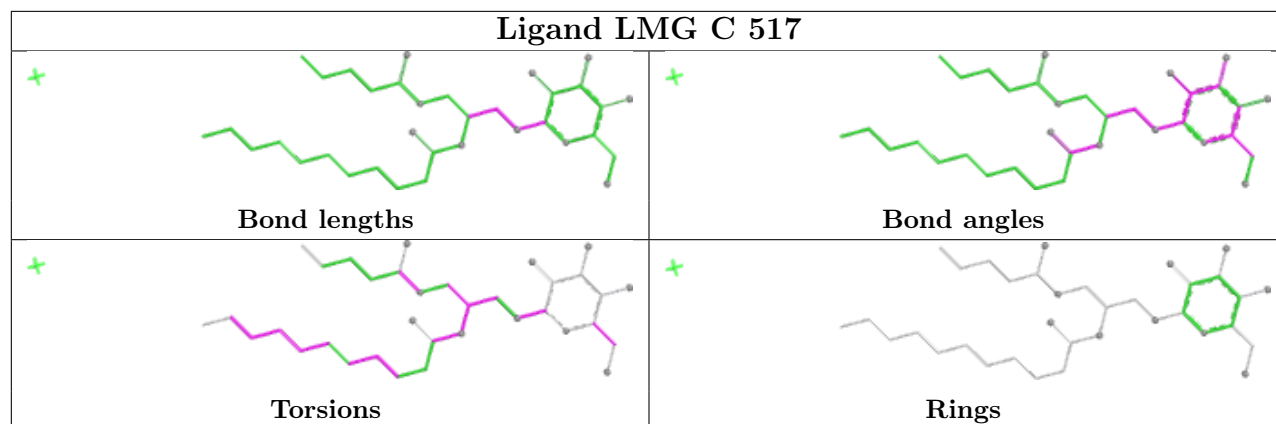


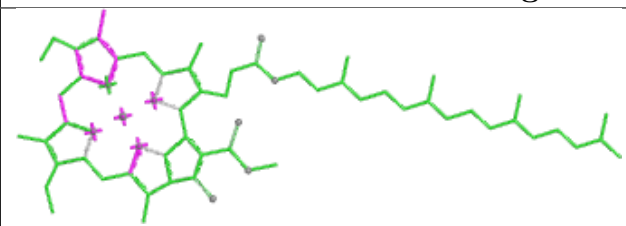
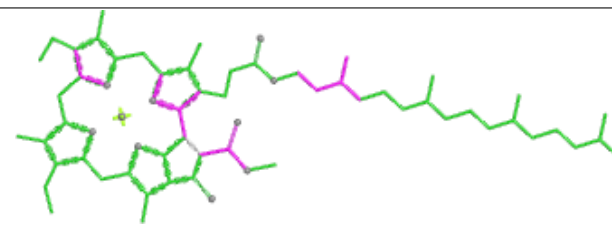
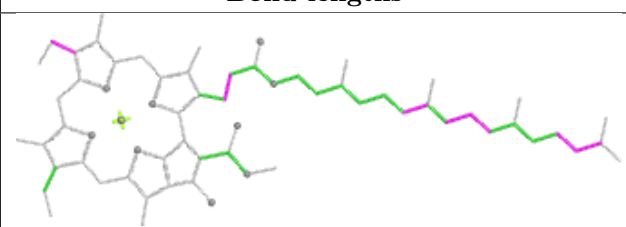
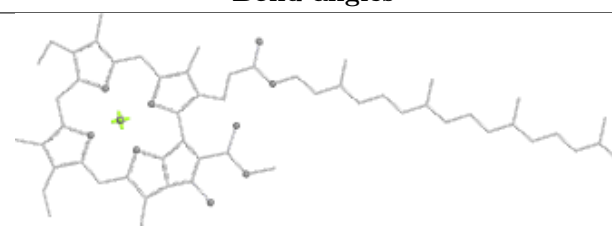


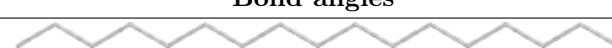


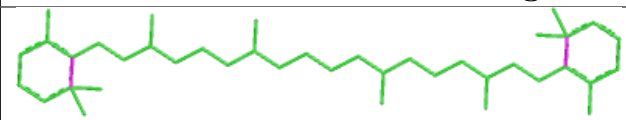
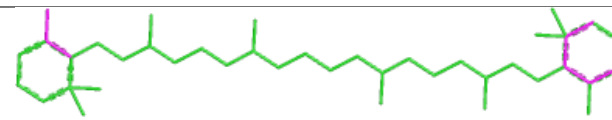
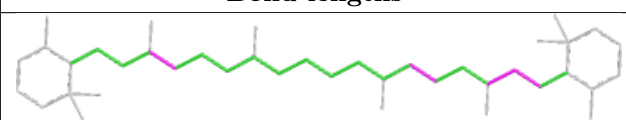
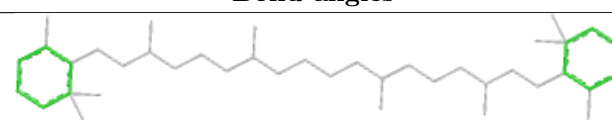


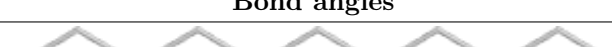


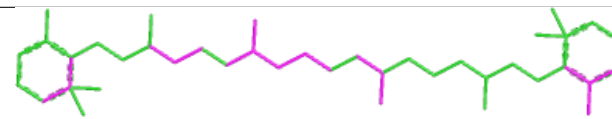
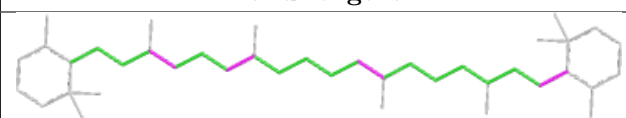
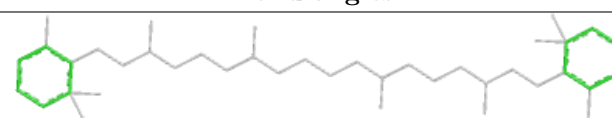


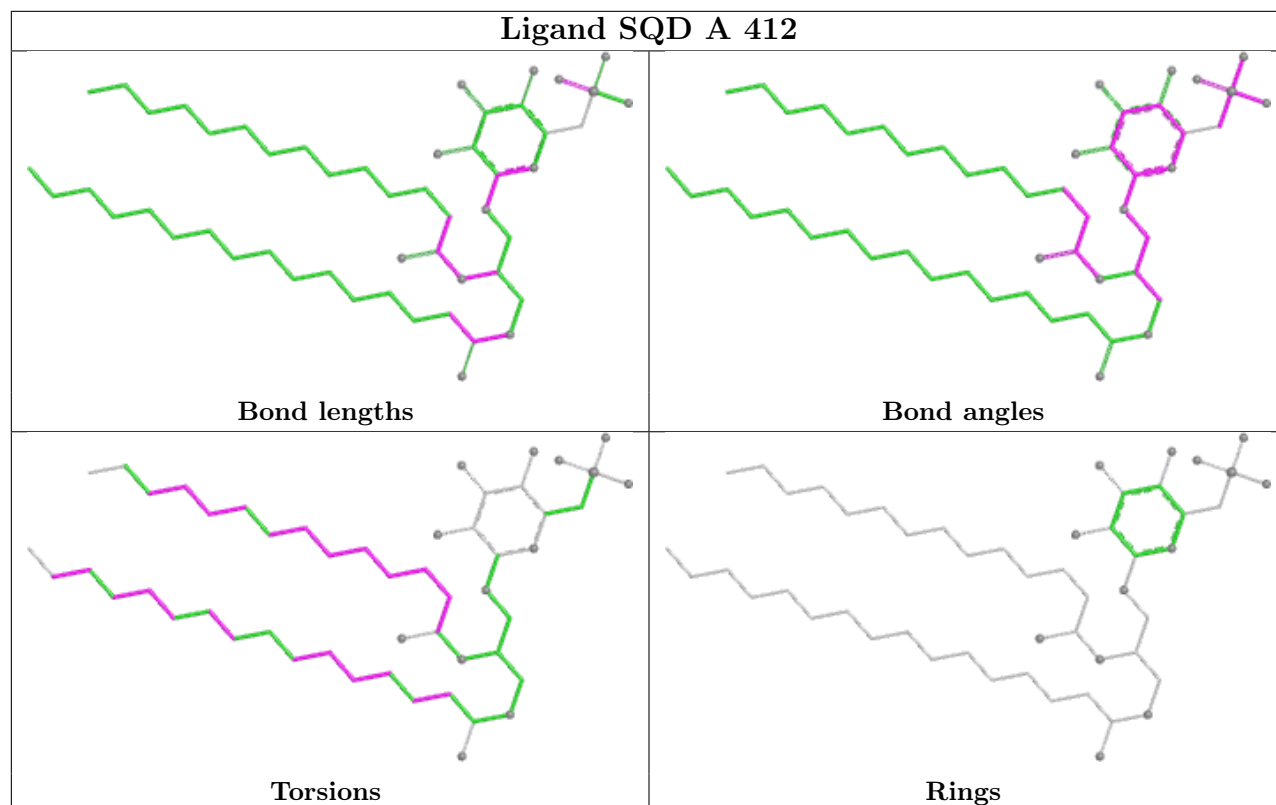
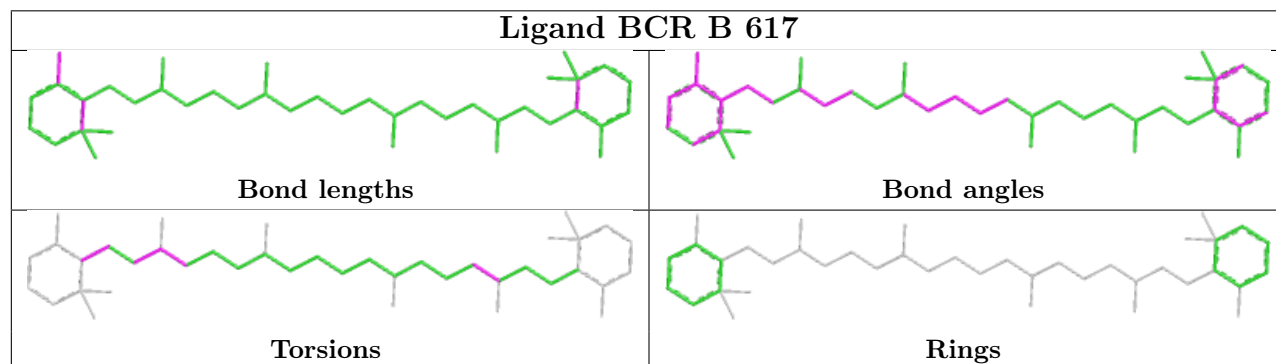
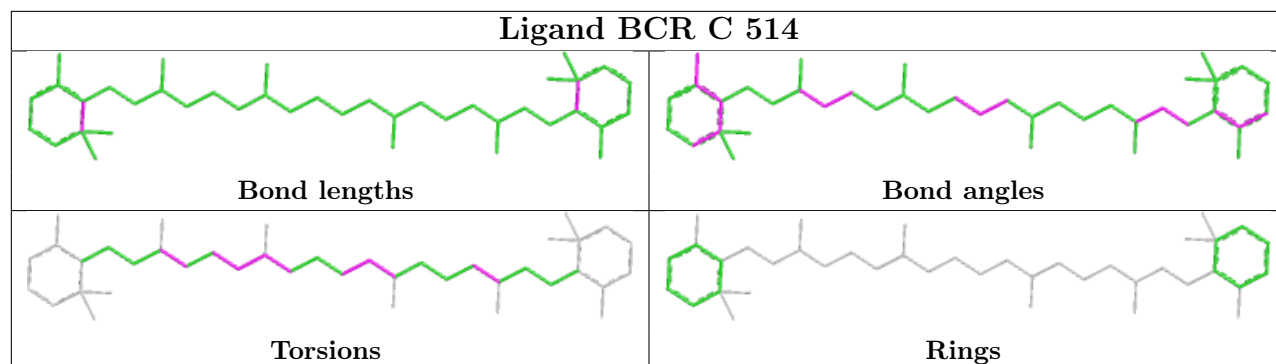
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

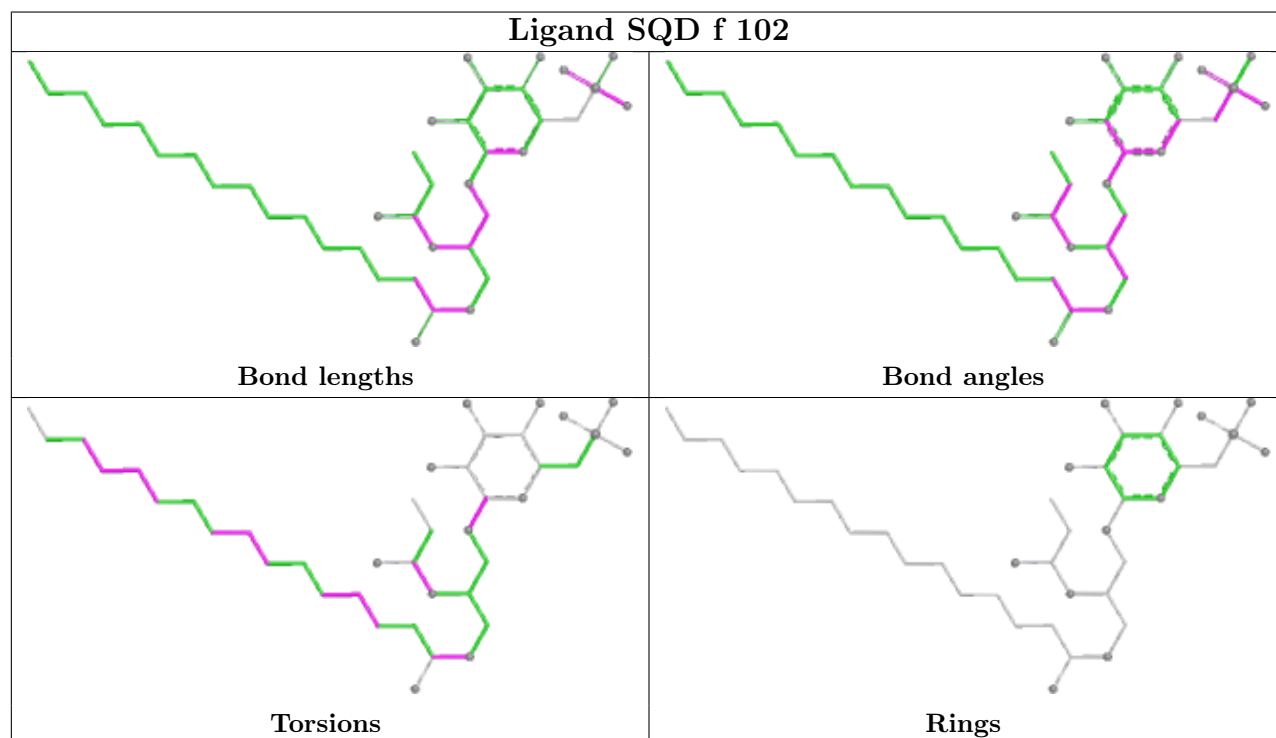
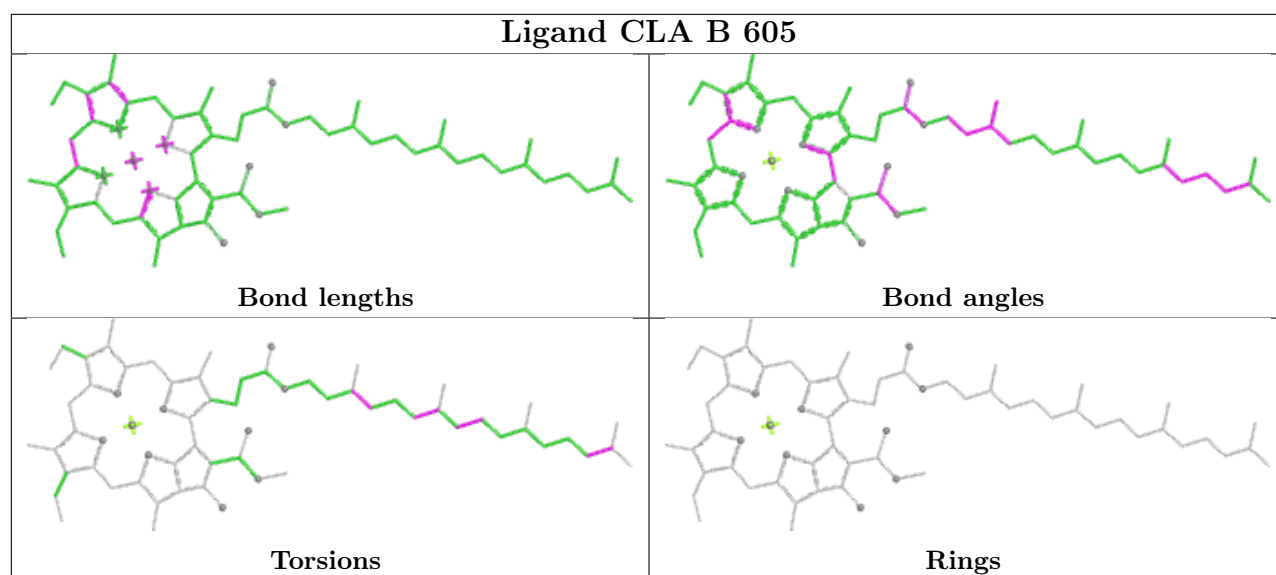
Ligand STE Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

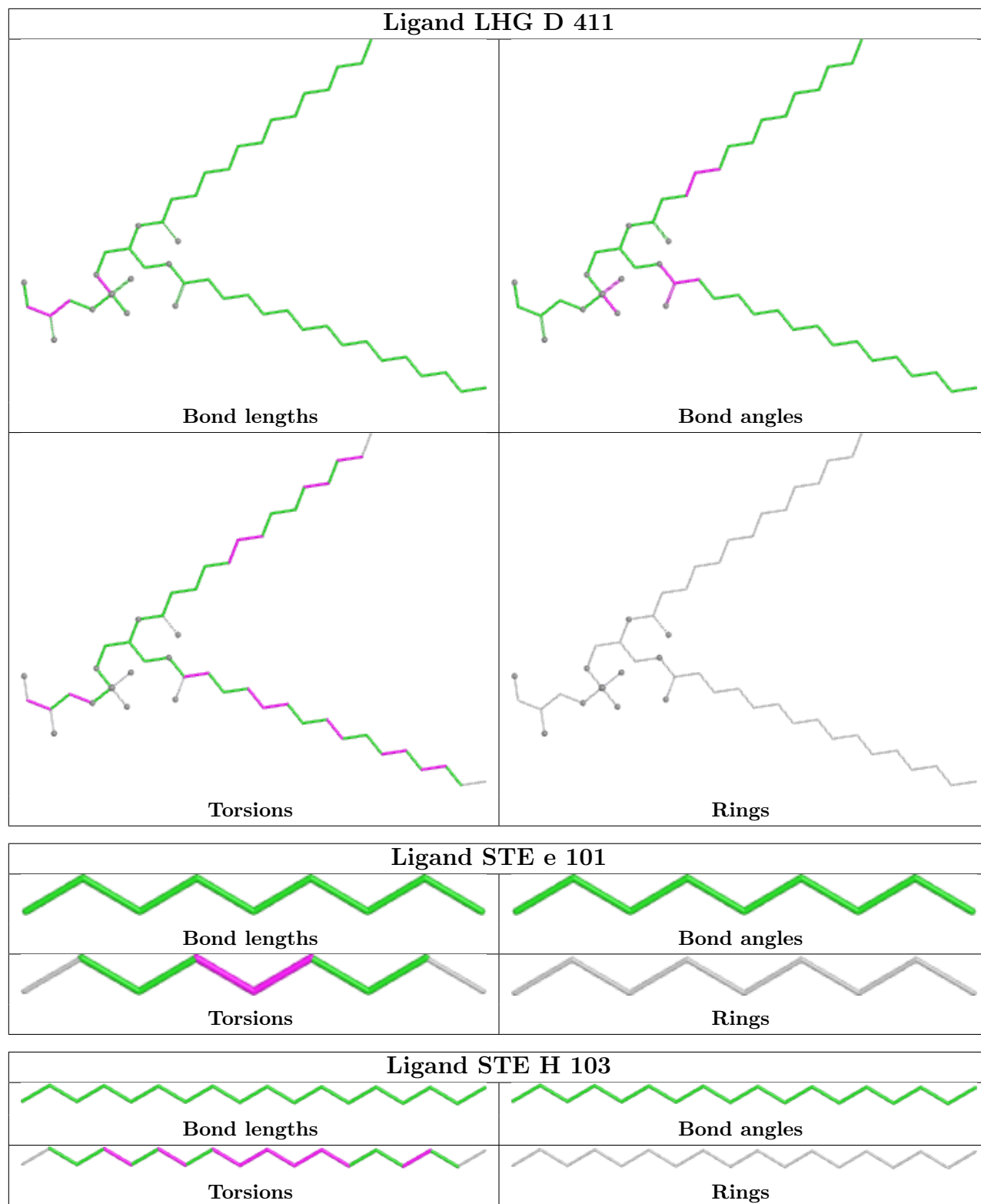
Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

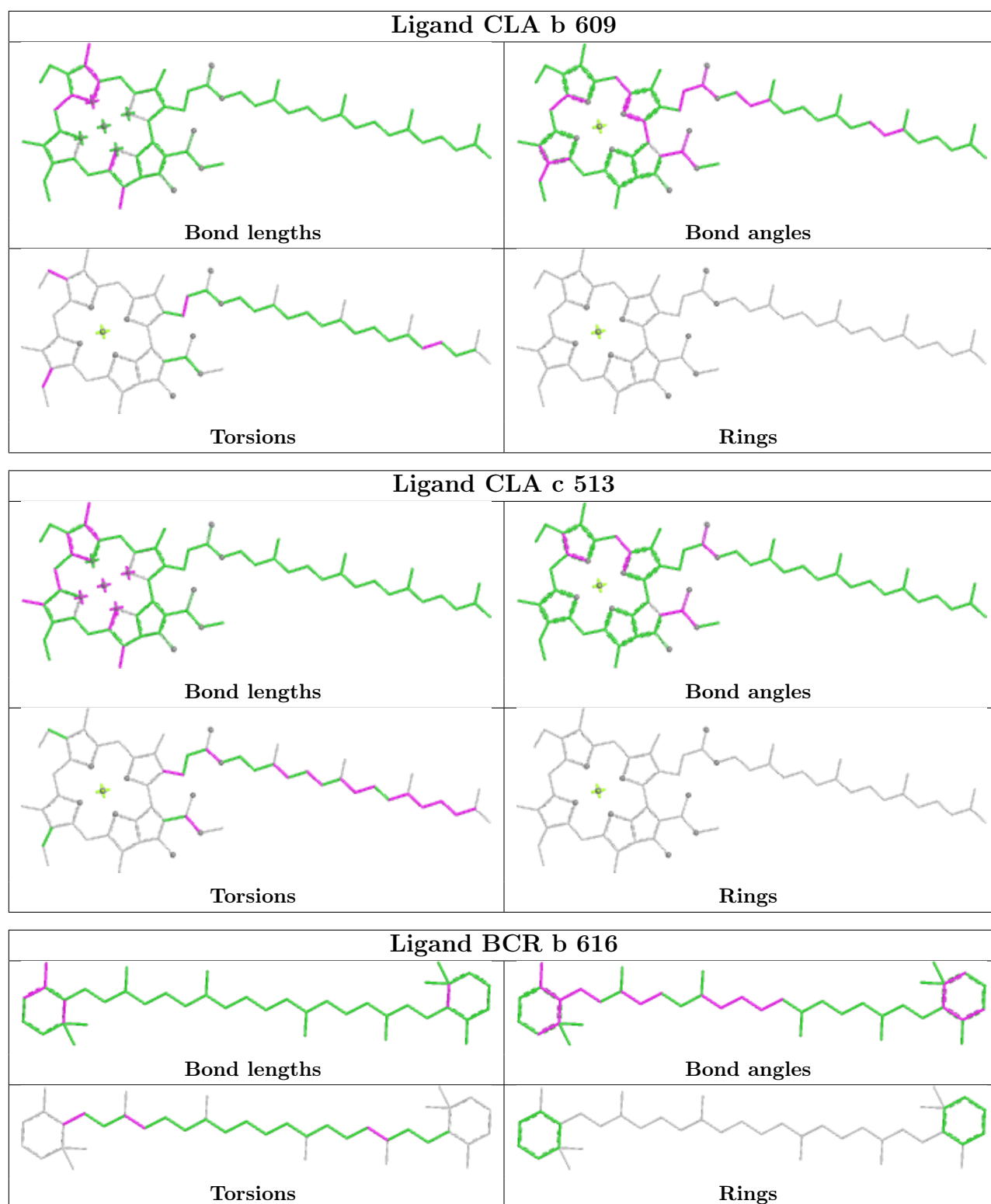
Ligand STE b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

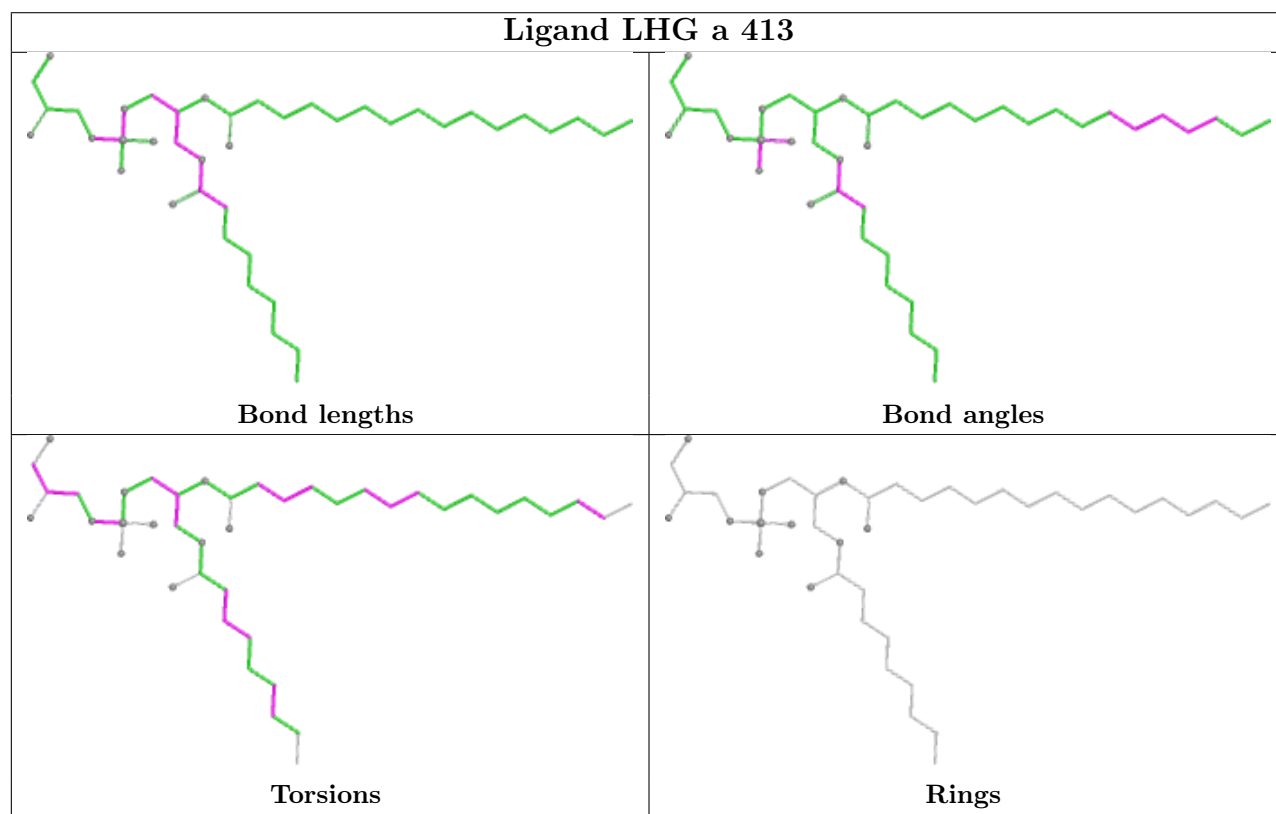
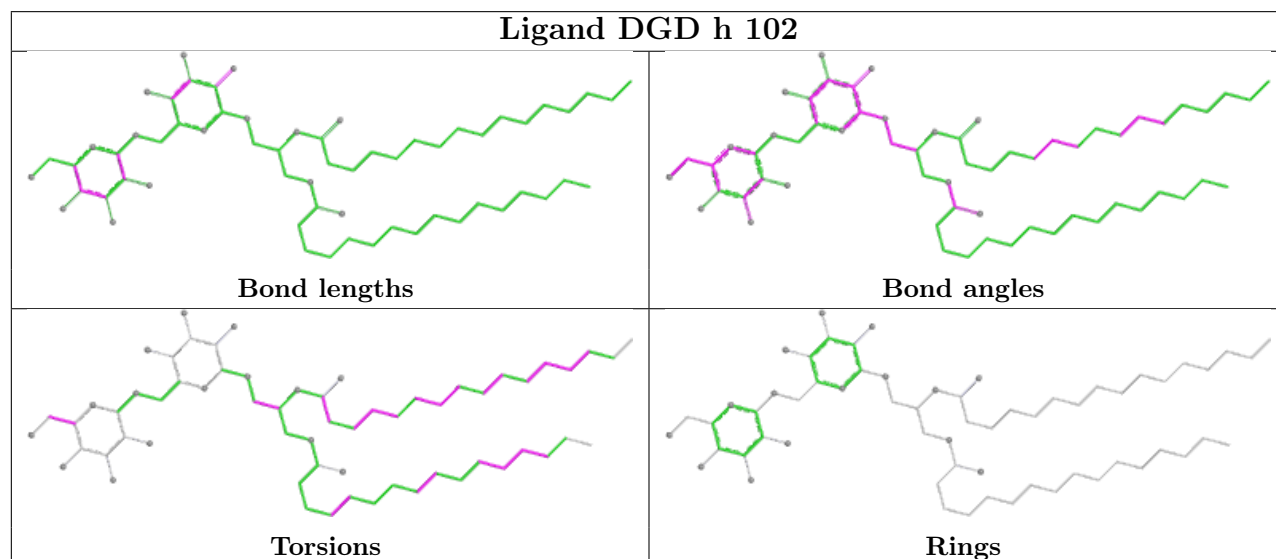
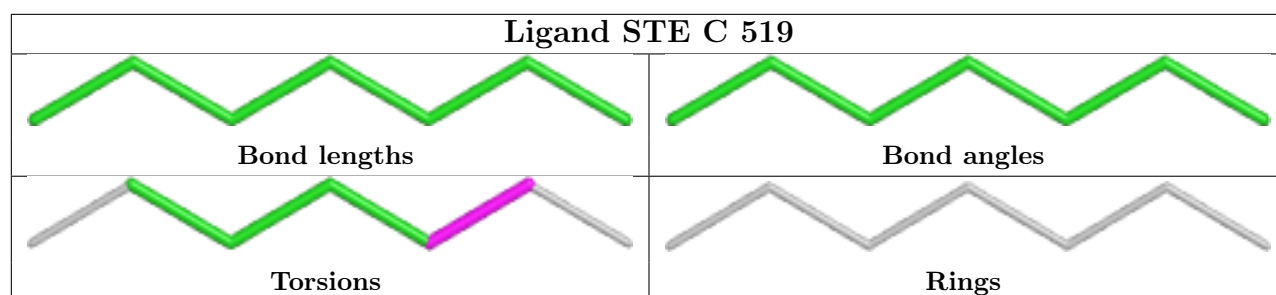
Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

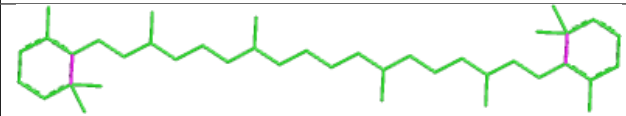
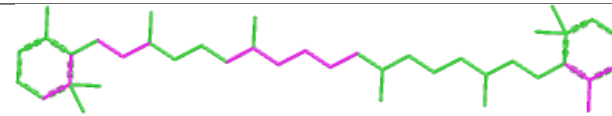
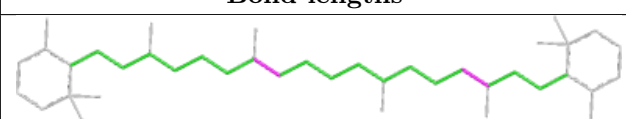
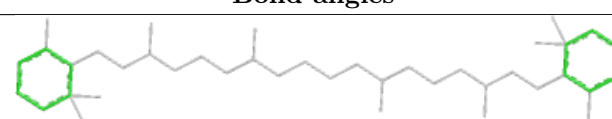


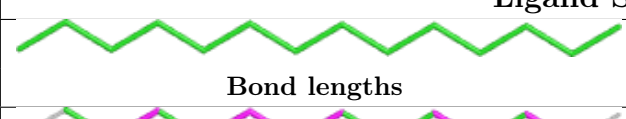
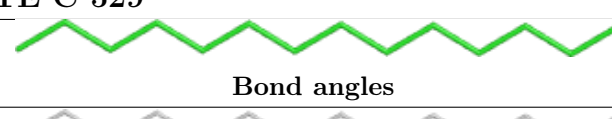


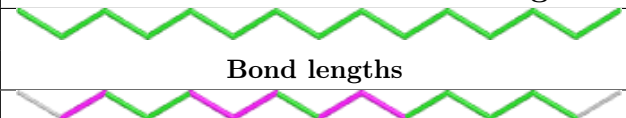
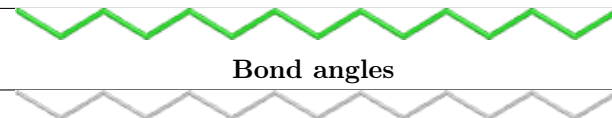
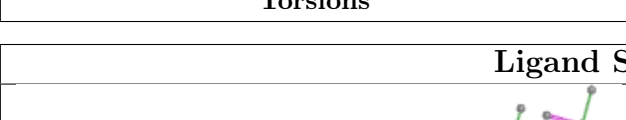


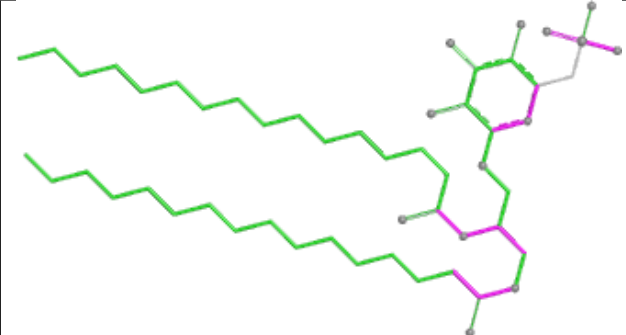
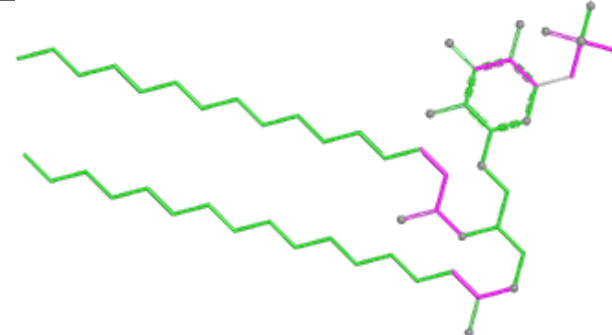
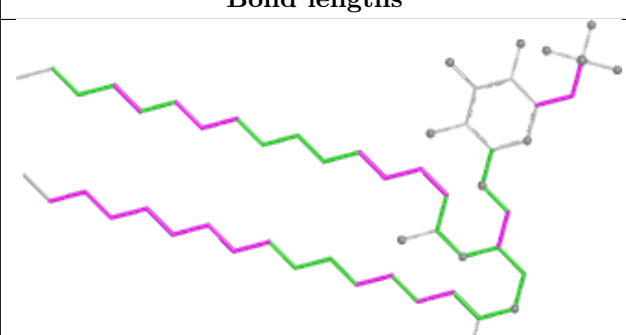
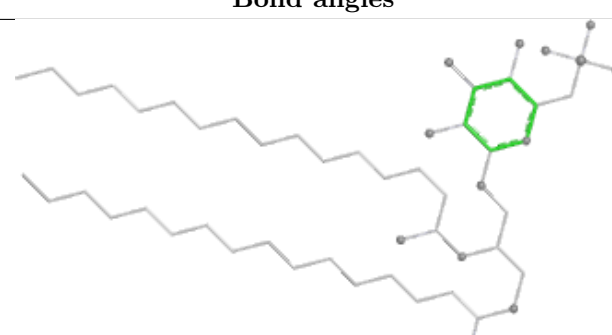




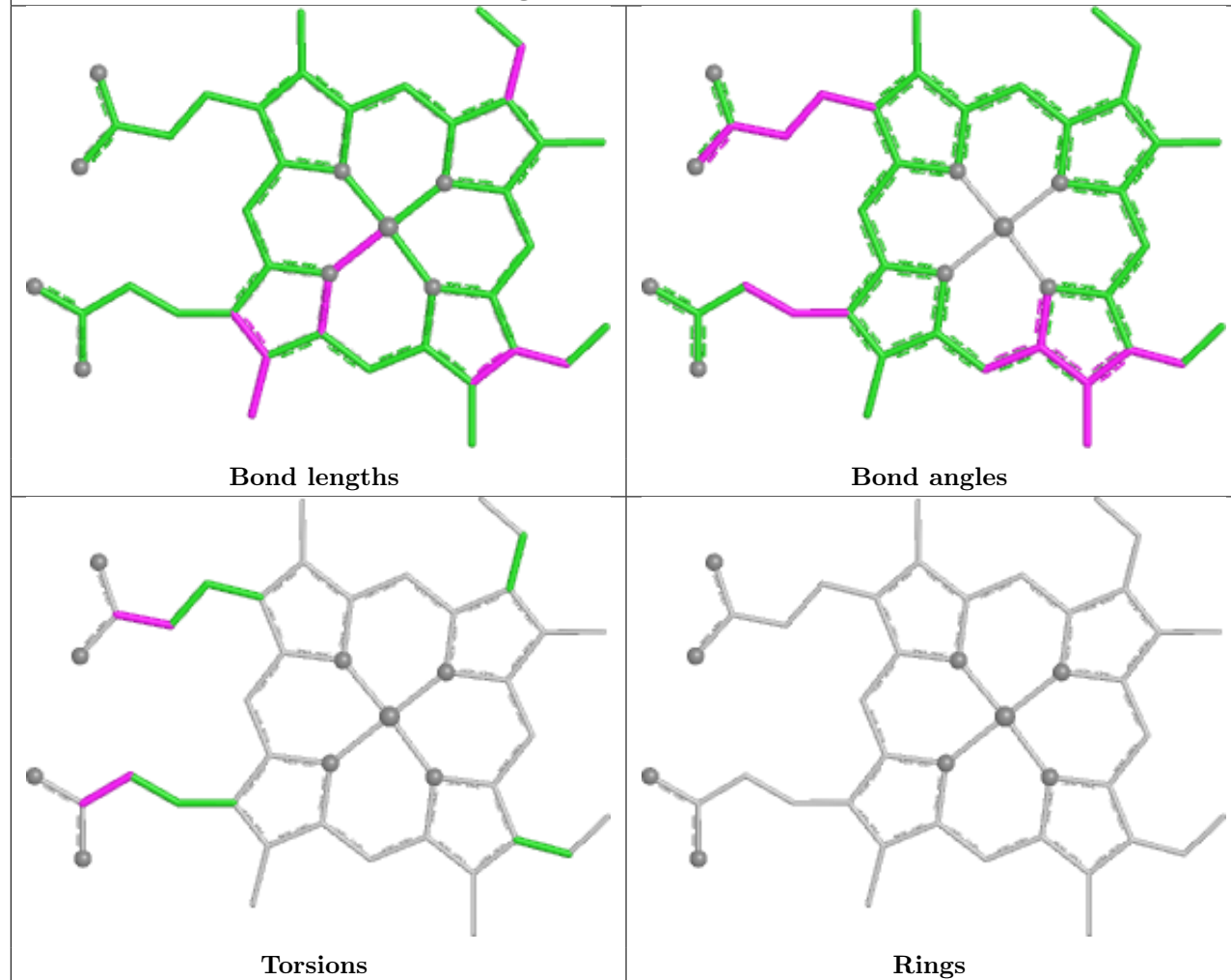
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

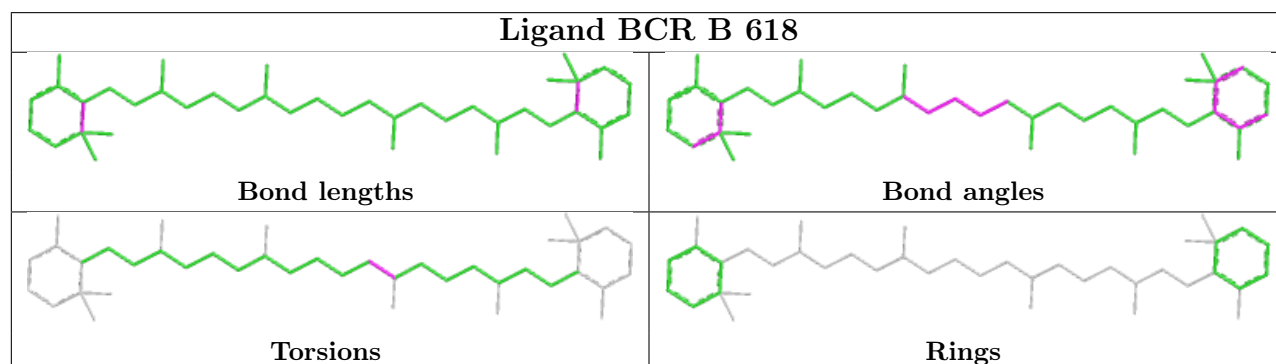
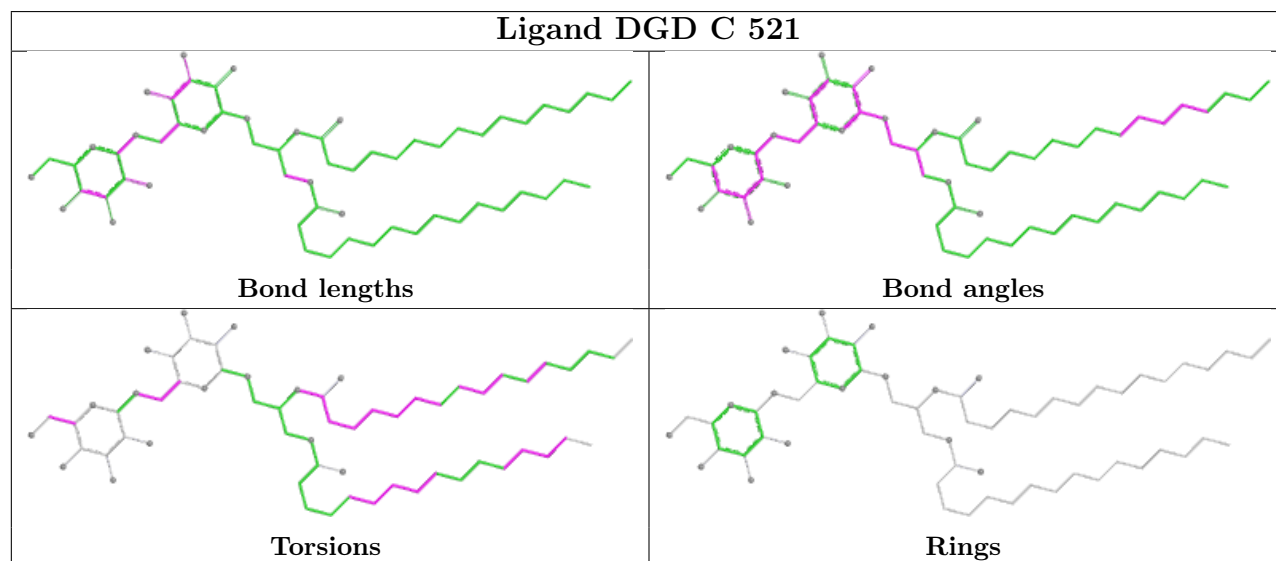
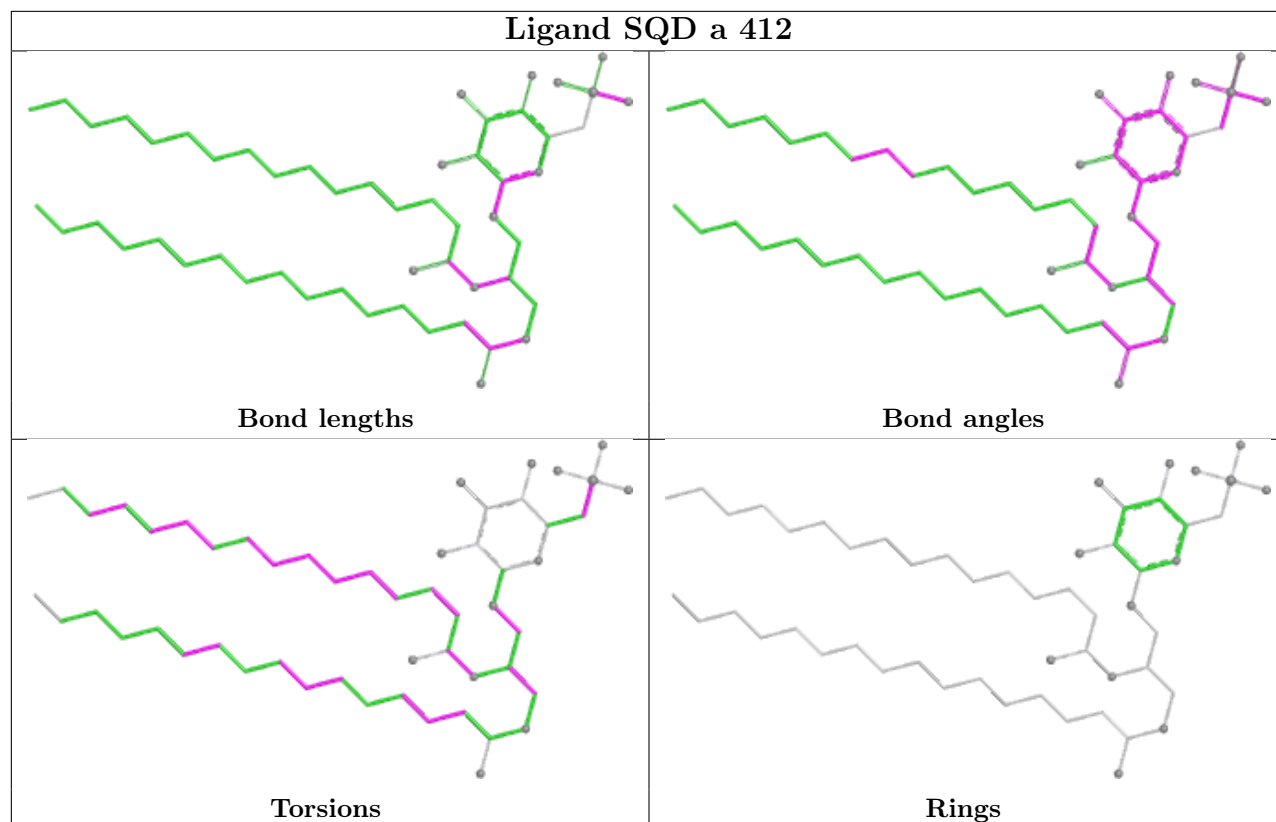
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Bond lengths	Bond angles
	
Torsions	Rings

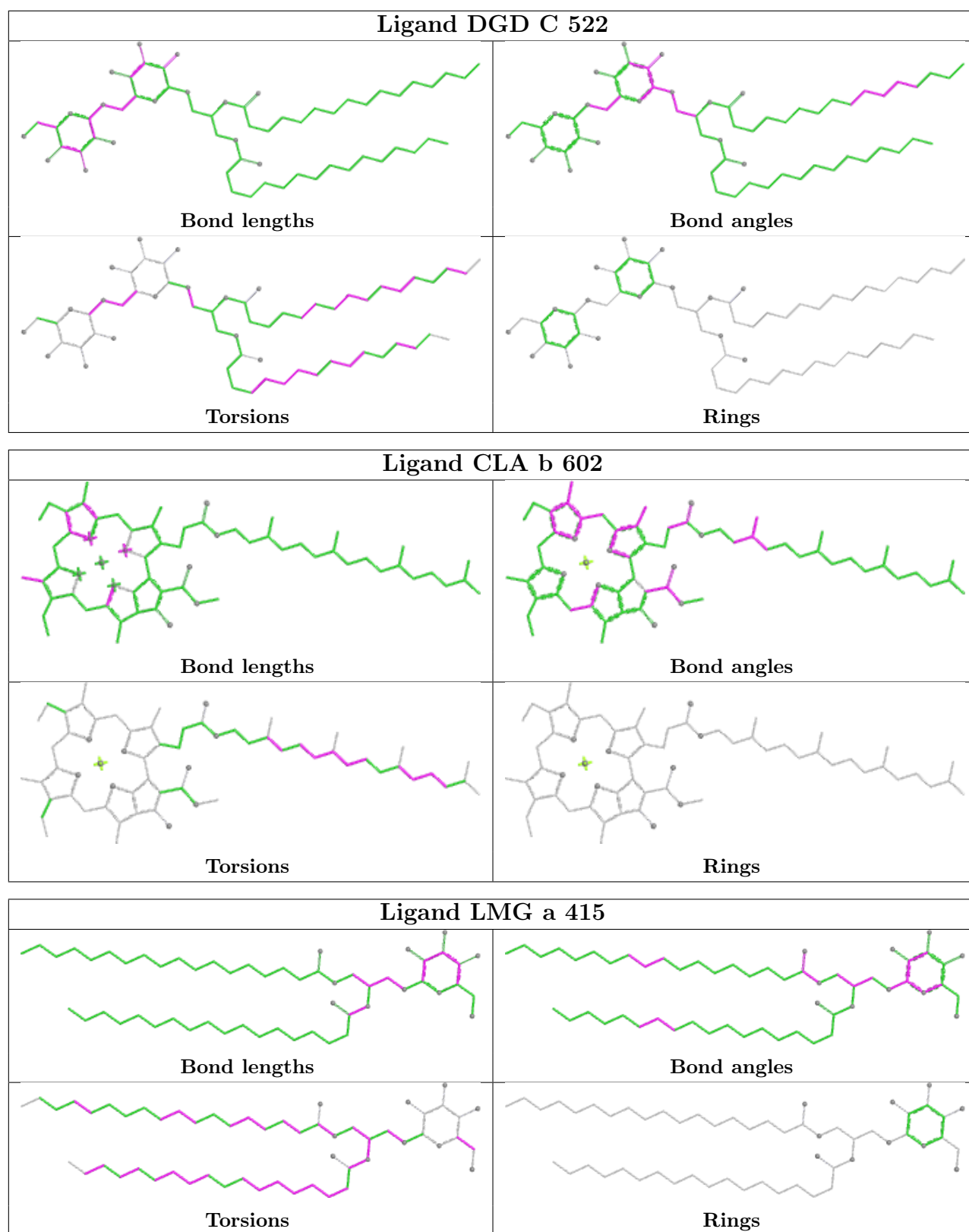
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

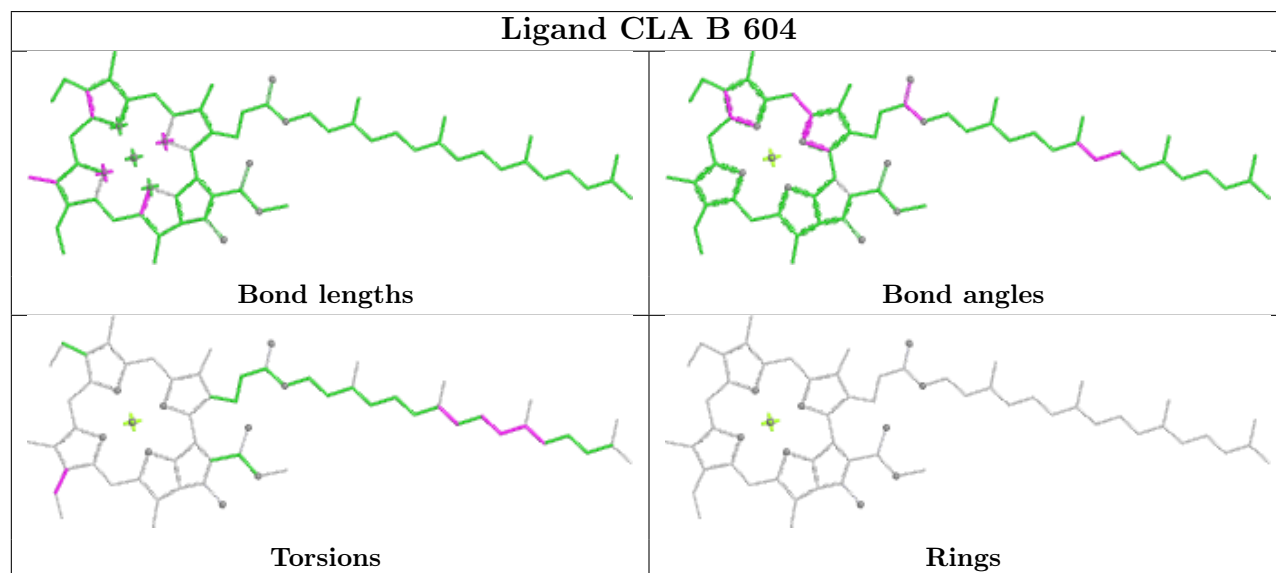
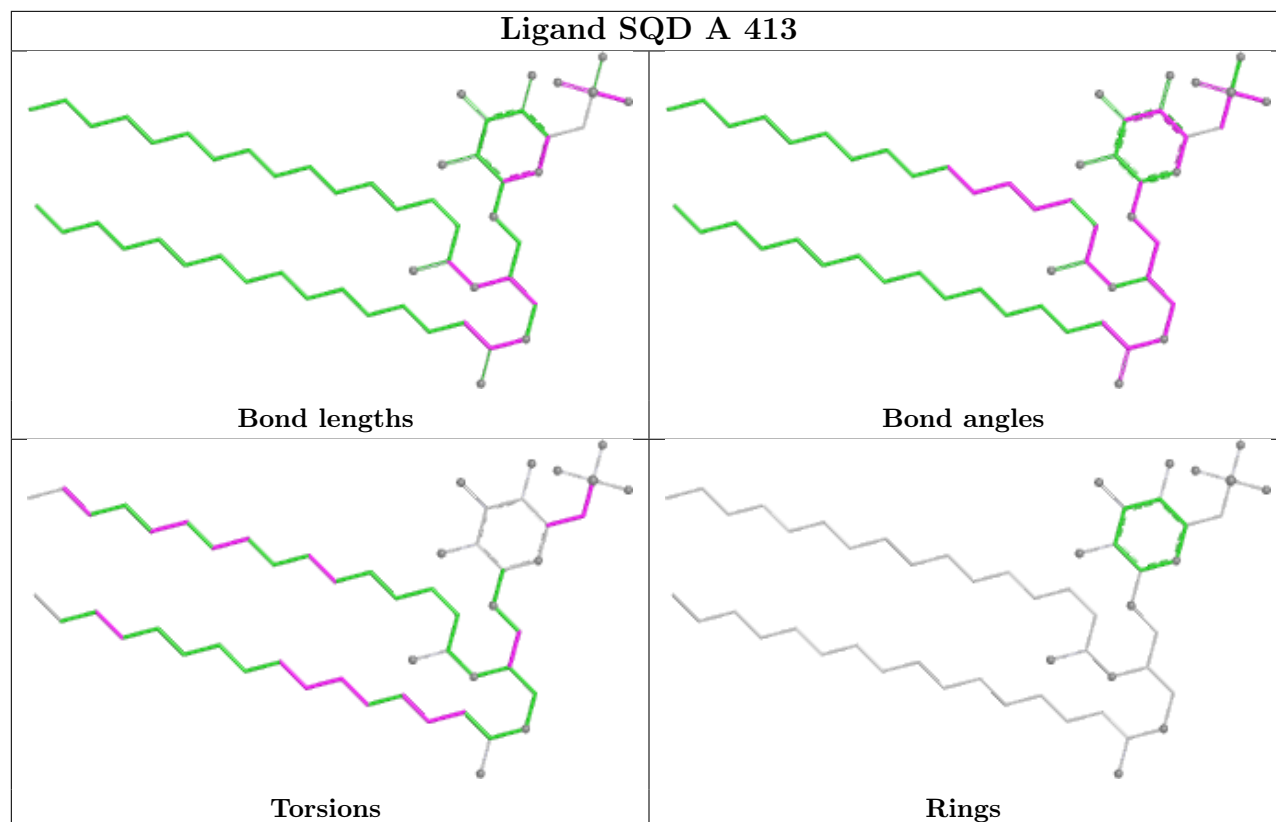
Ligand SQD a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

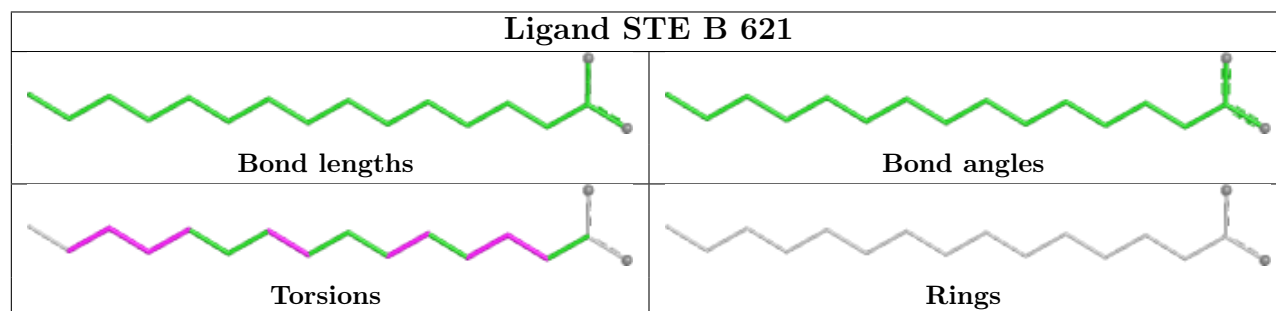
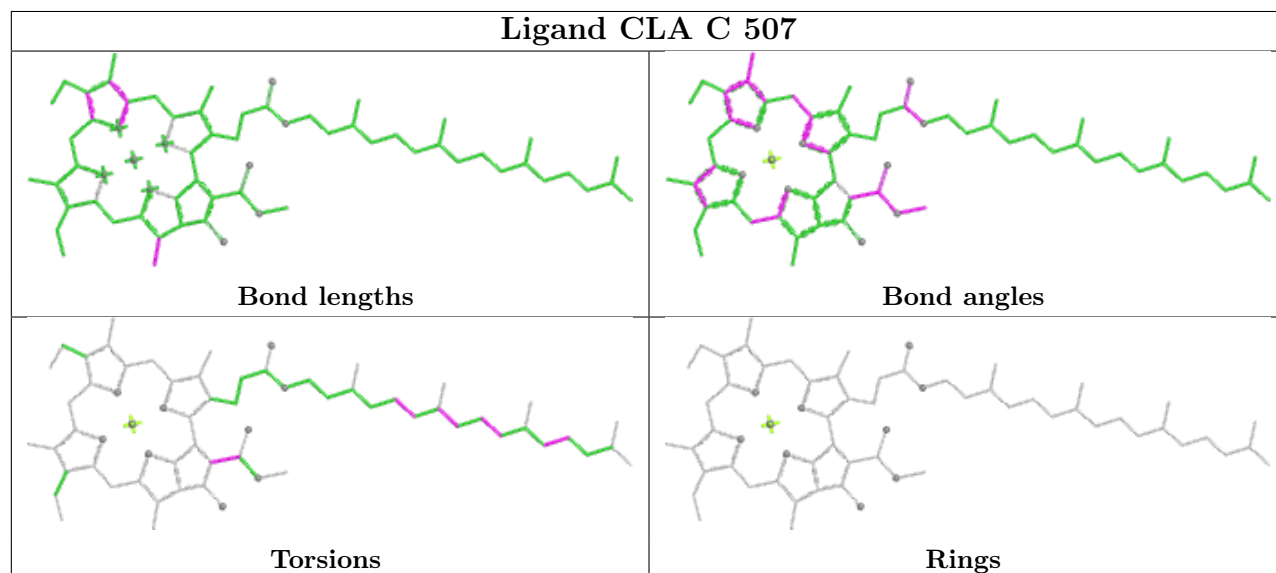
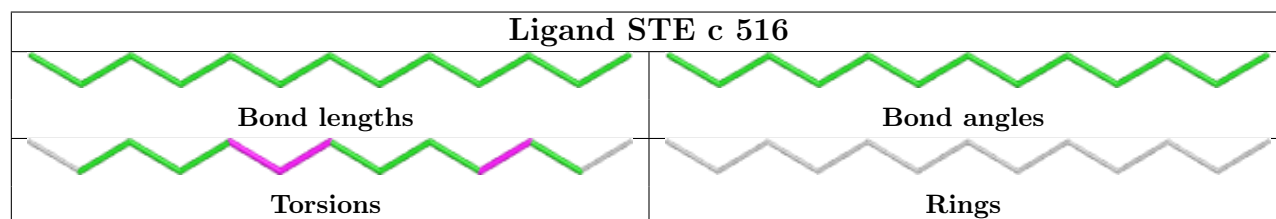
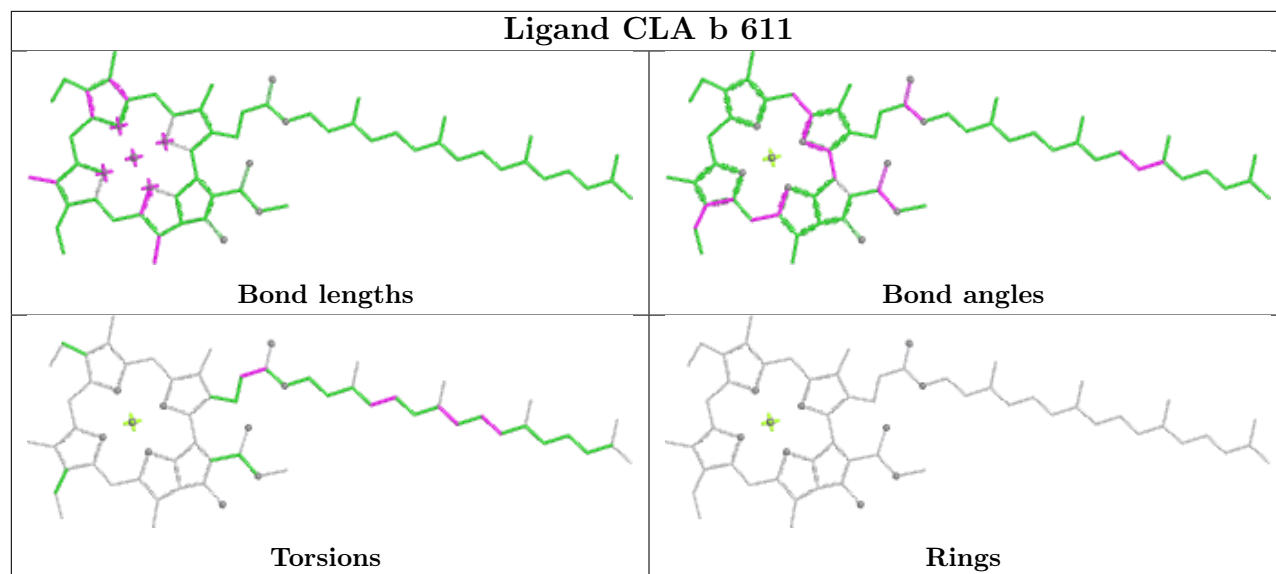
Ligand HEM f 101

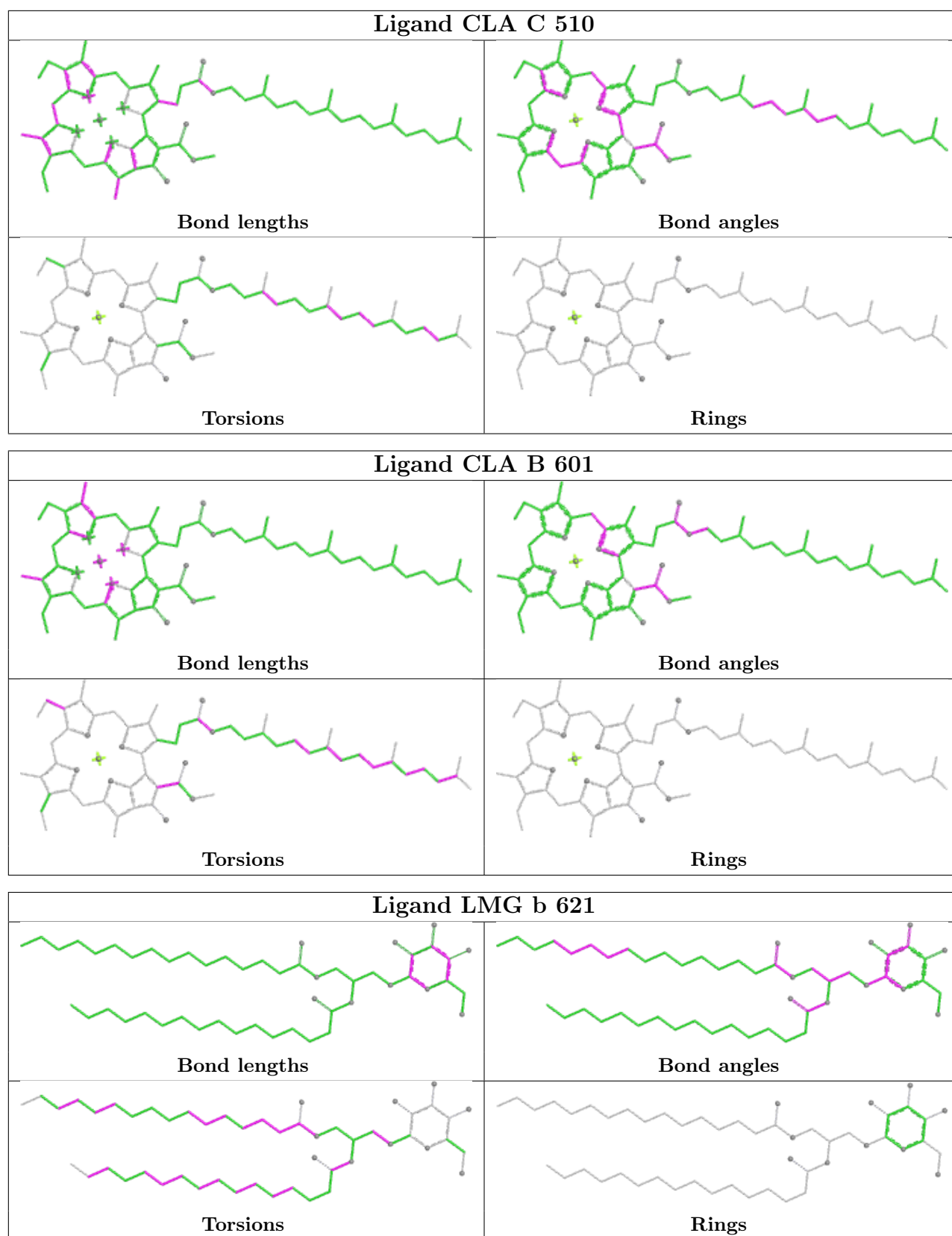


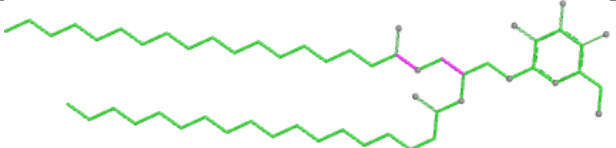
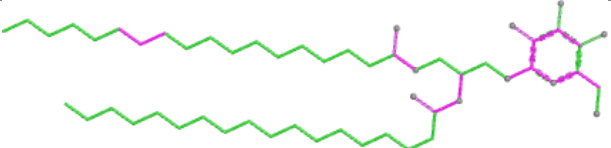
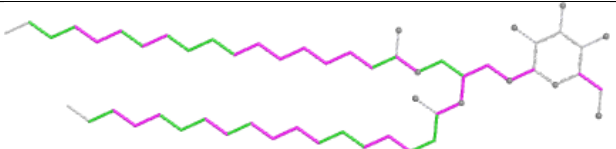
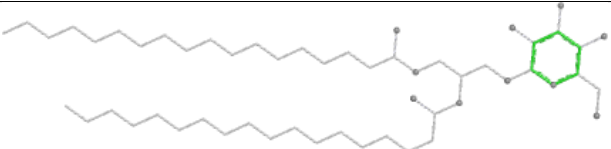


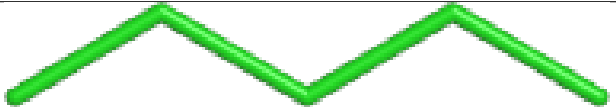
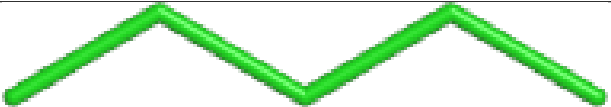


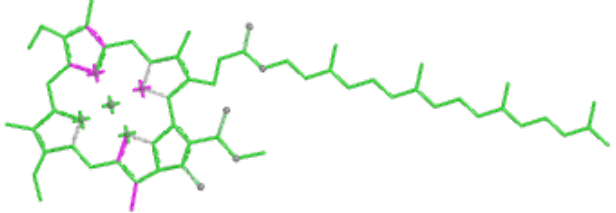
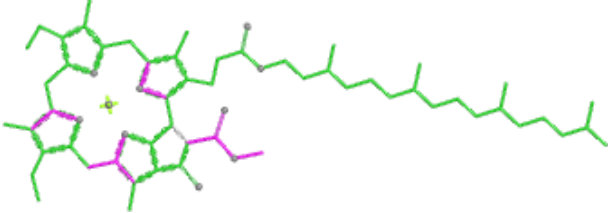
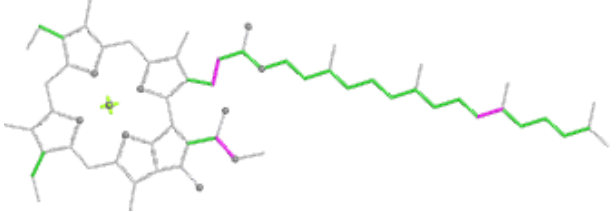
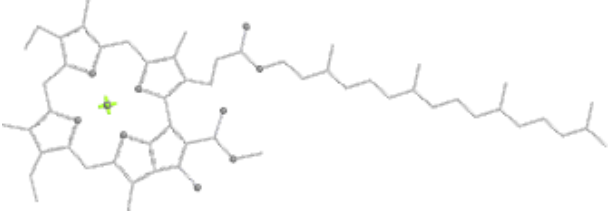


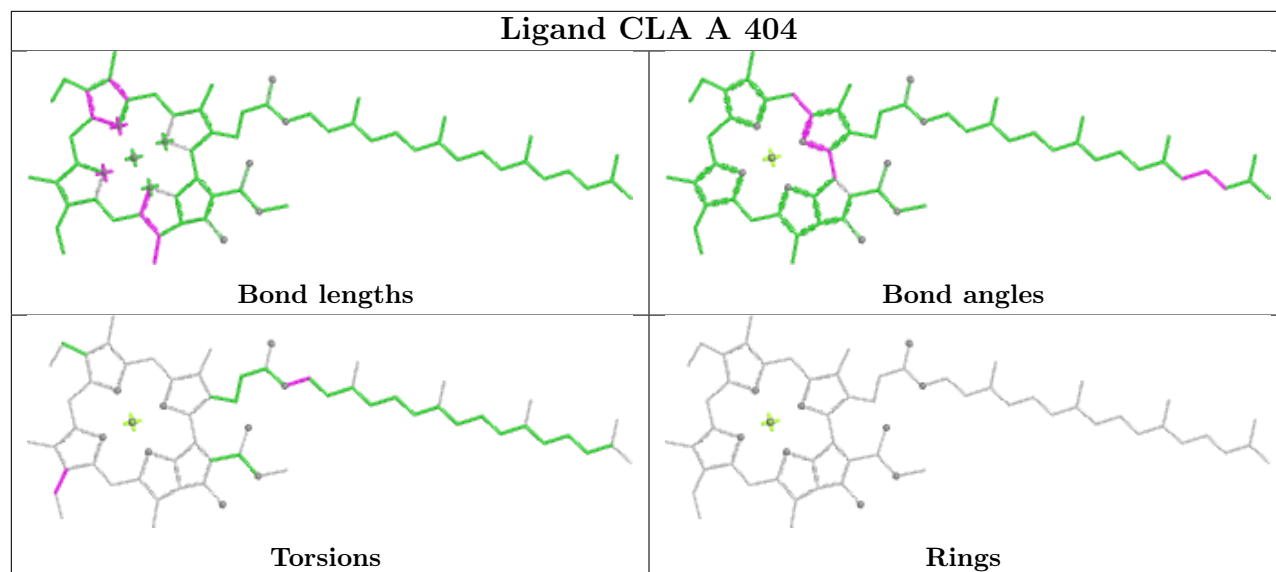
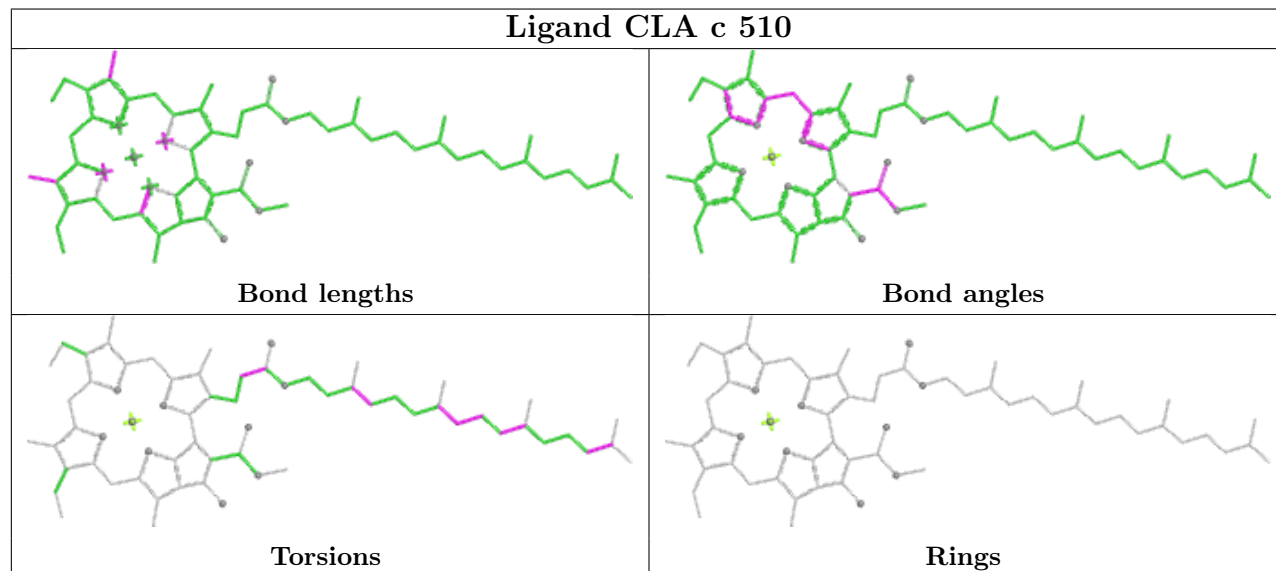
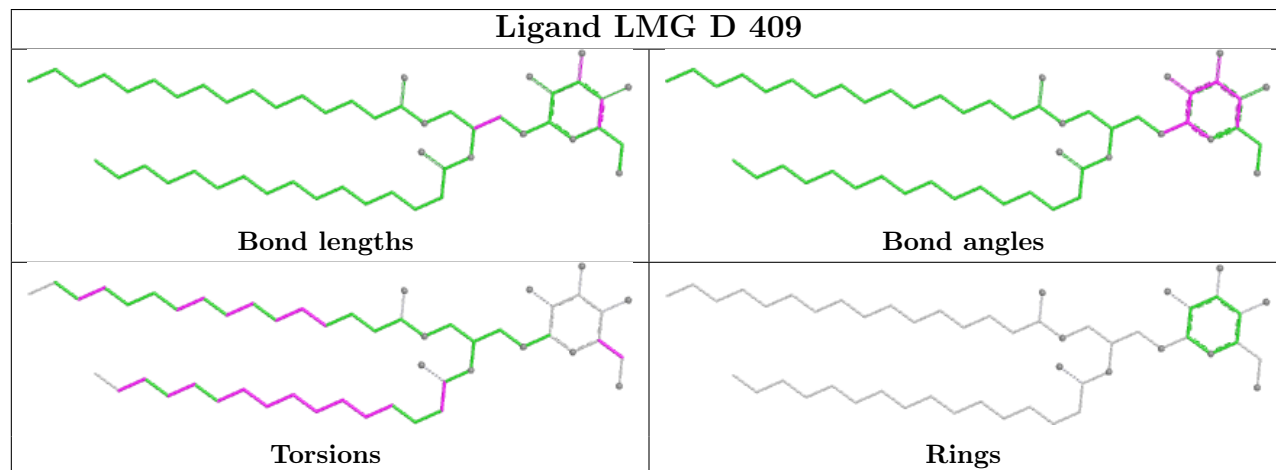


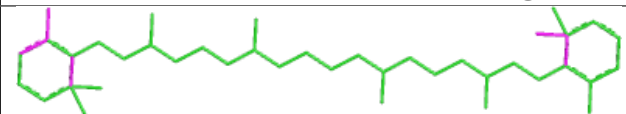
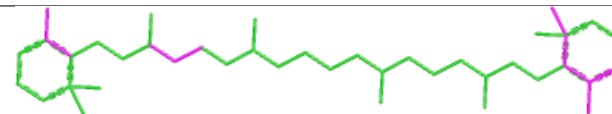
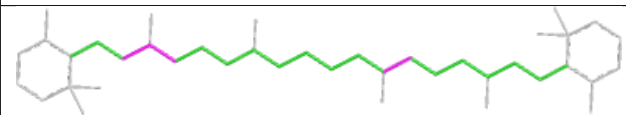
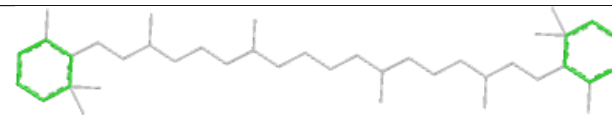


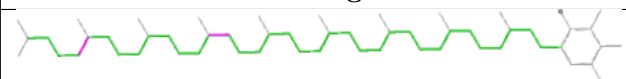
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

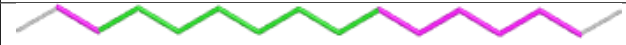
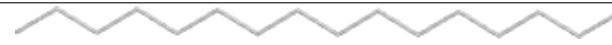
Ligand STE C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

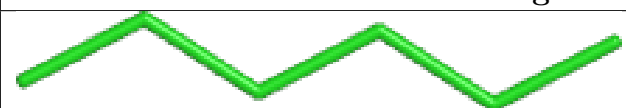
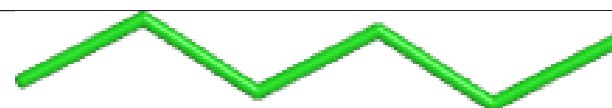
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

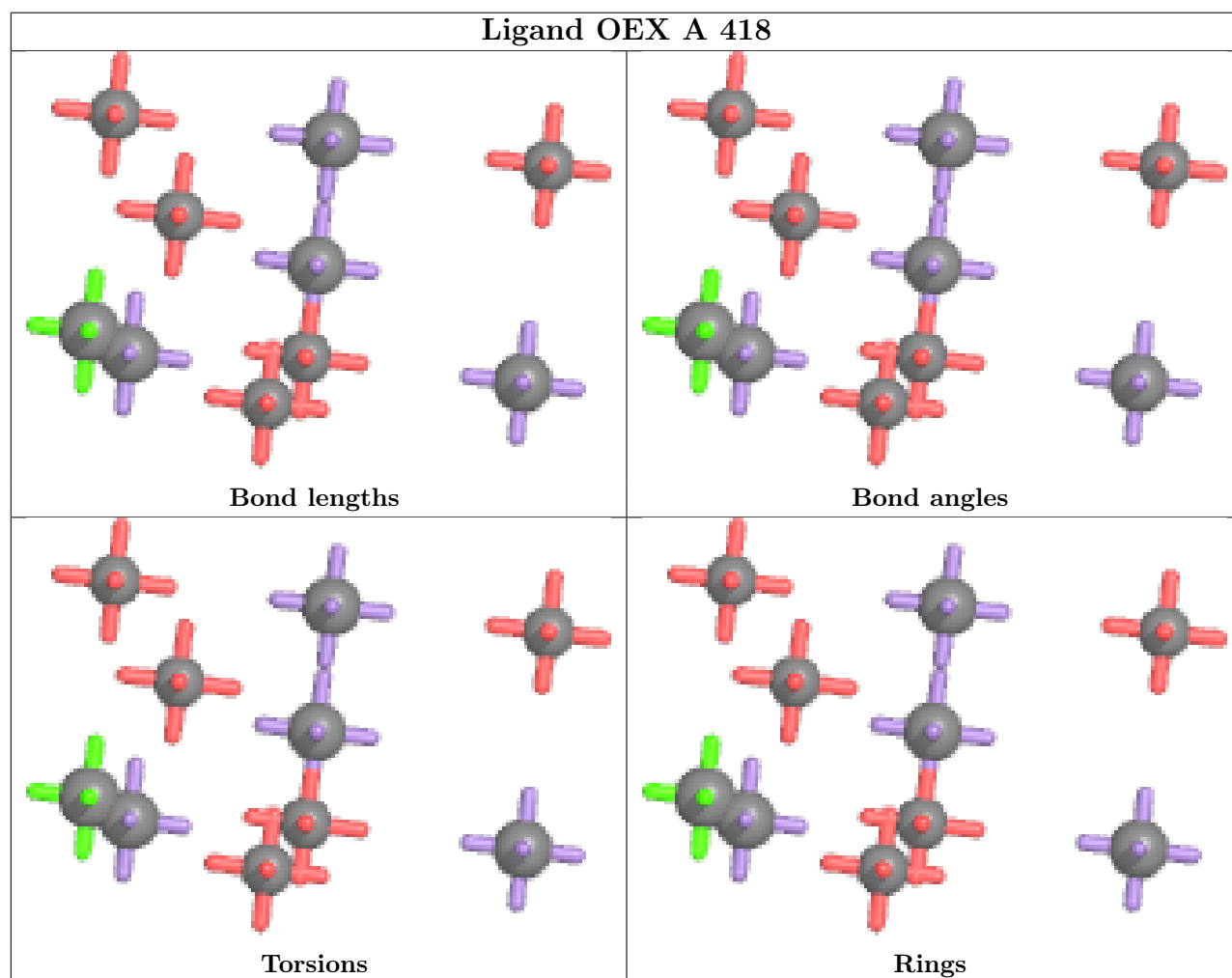
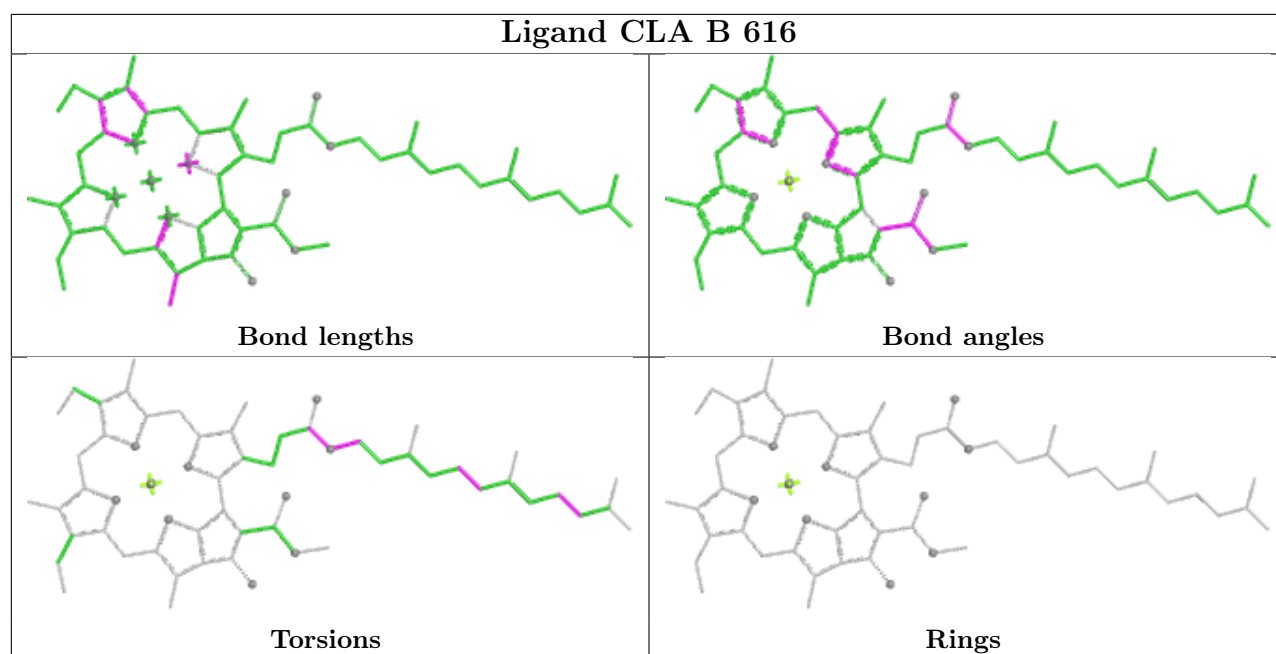
Ligand CLA A 404**Ligand CLA c 510****Ligand LMG D 409**

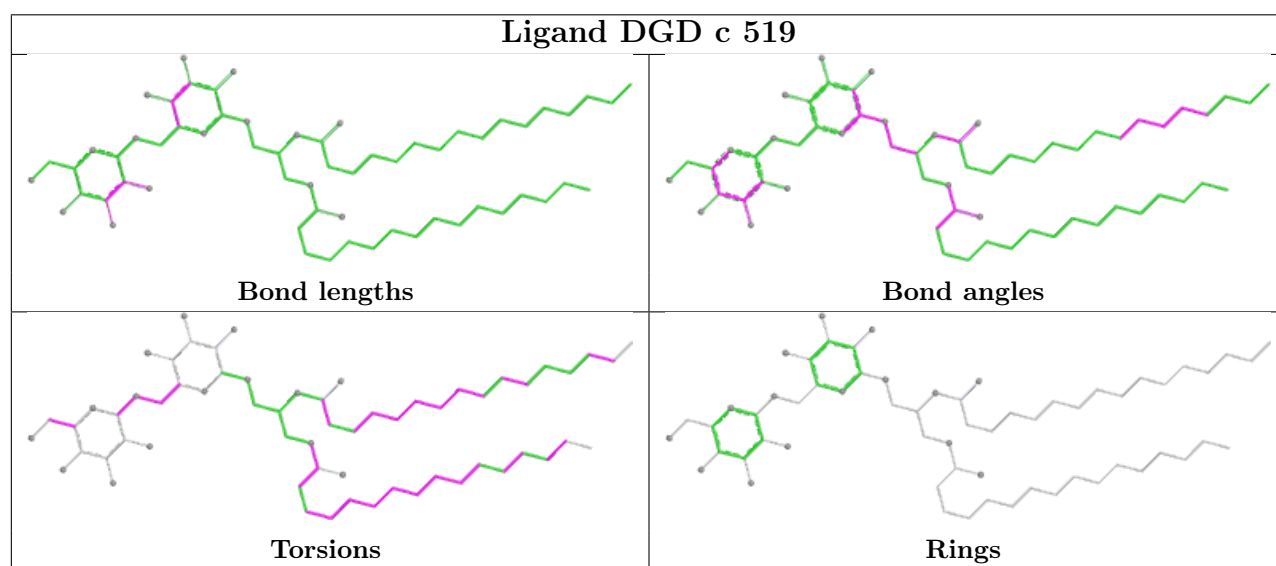
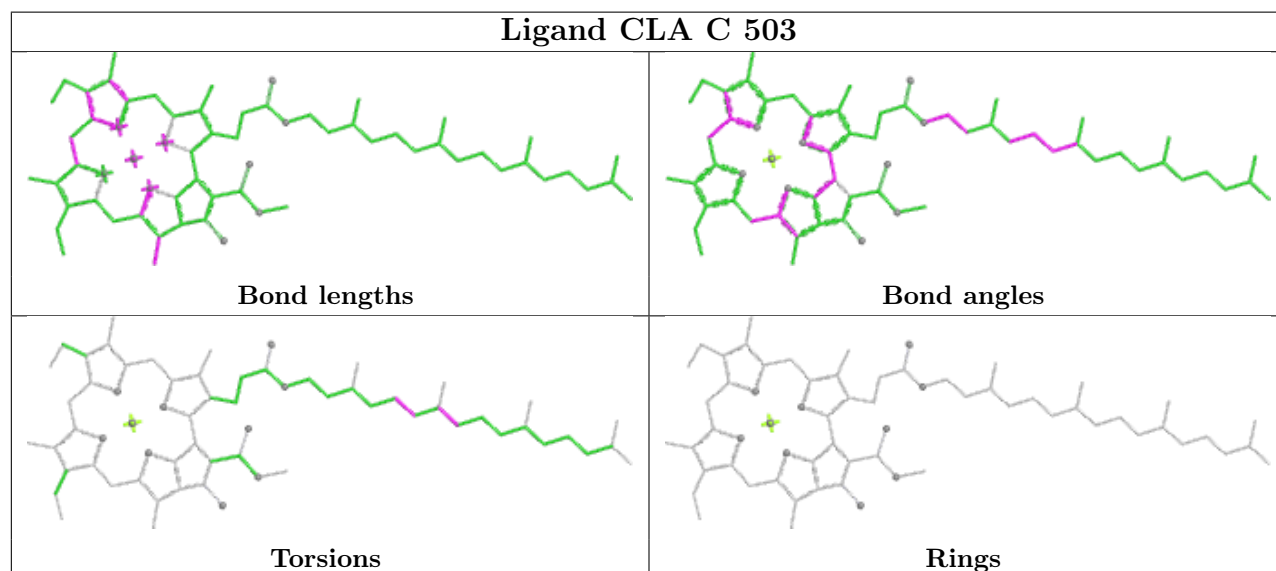
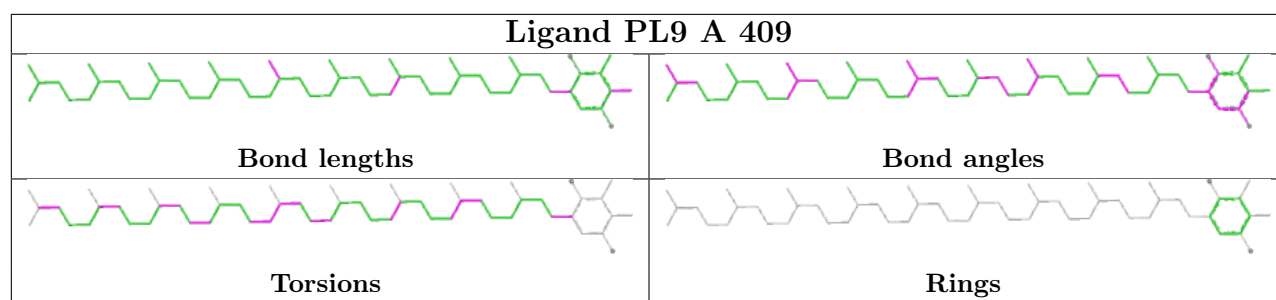
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Bond lengths	Bond angles
	
Torsions	Rings

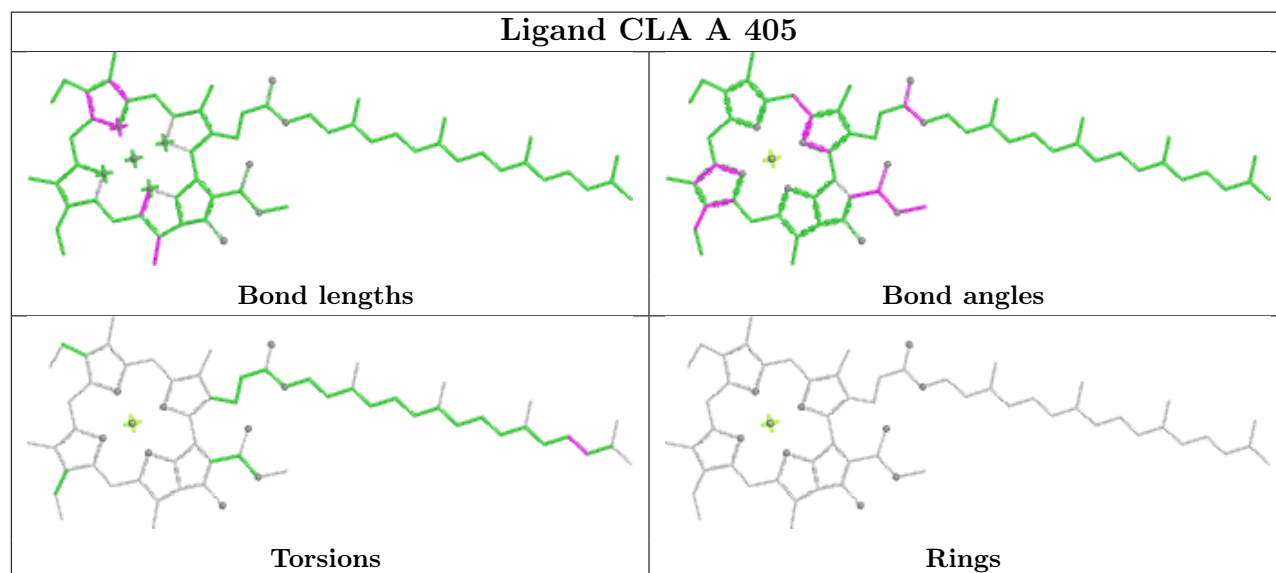
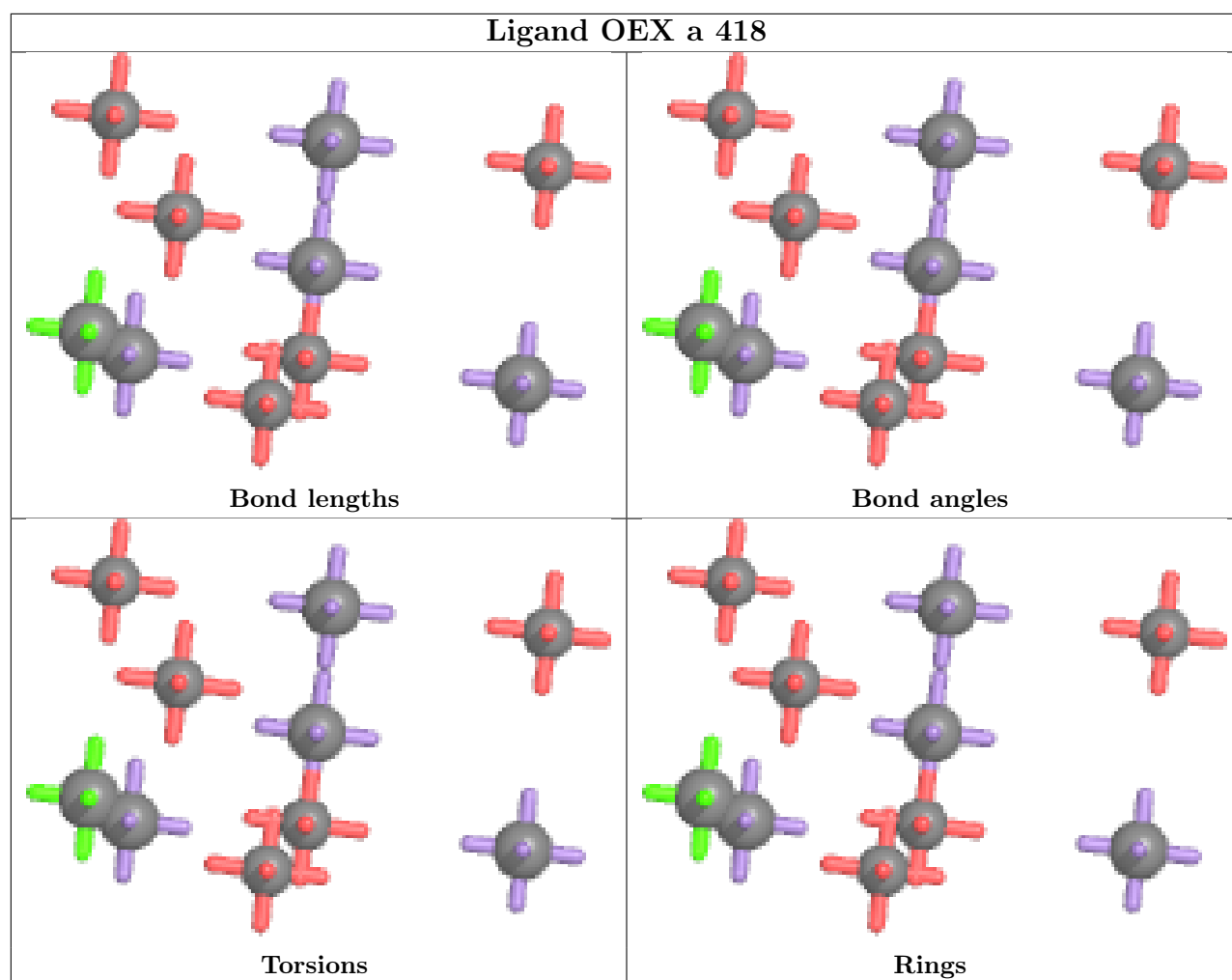
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

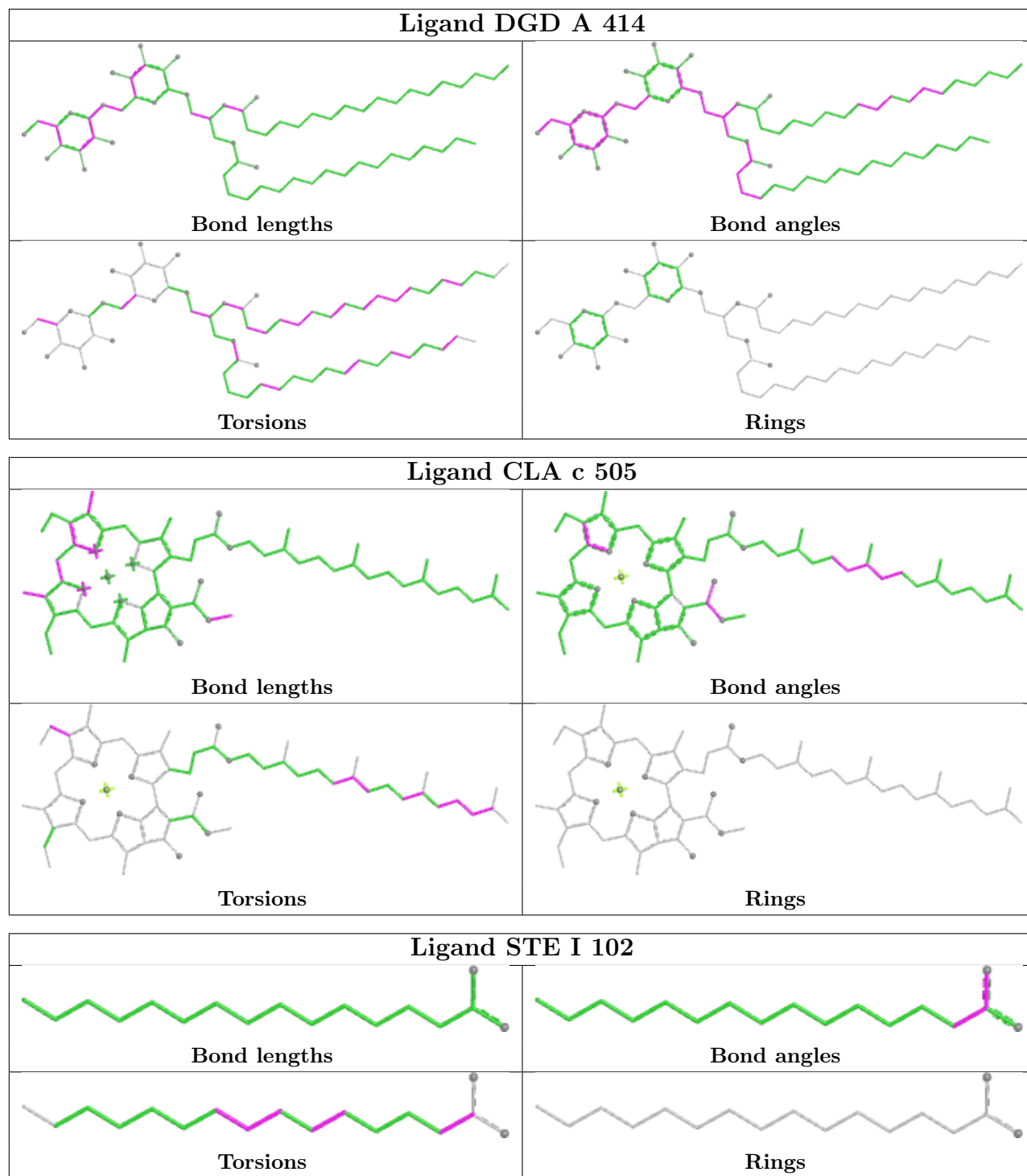
Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

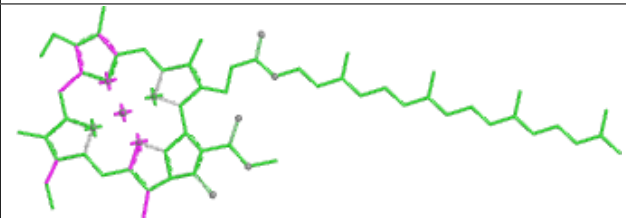
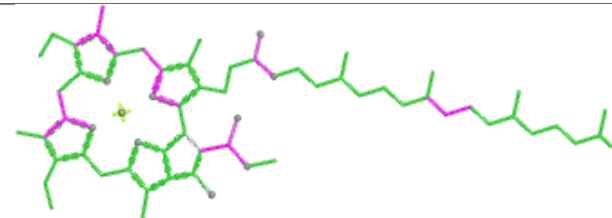
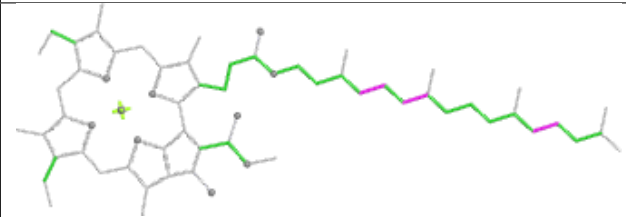
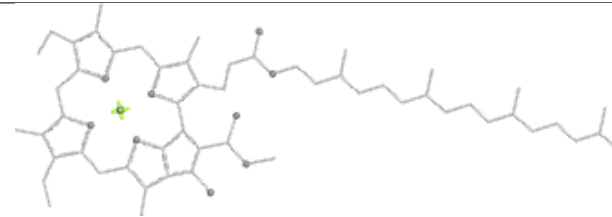
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Bond lengths	Bond angles
	
Torsions	Rings

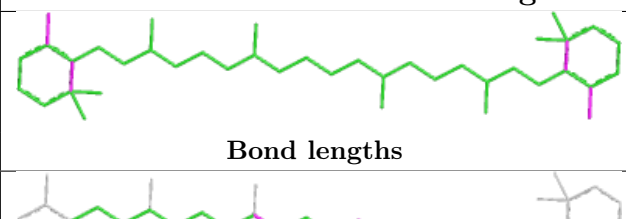
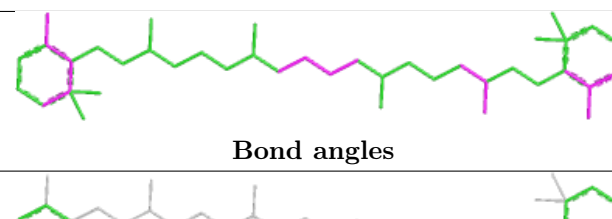
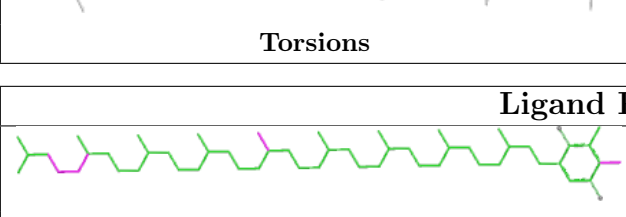
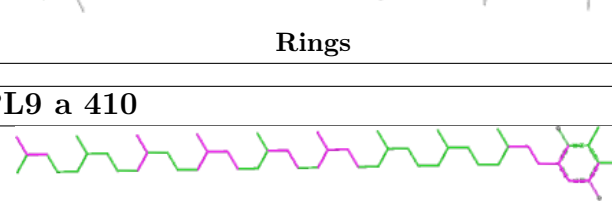


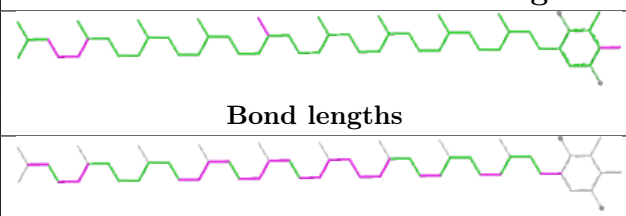
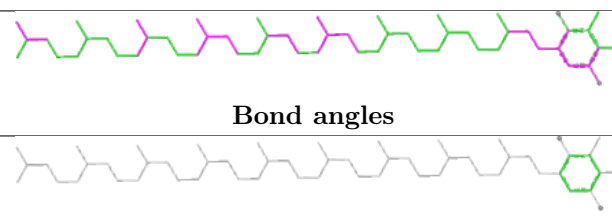


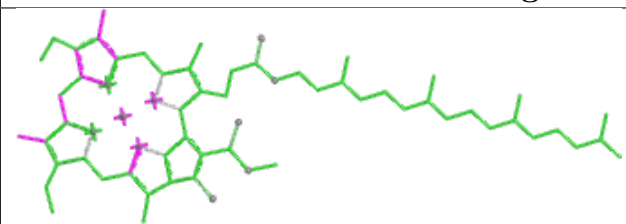
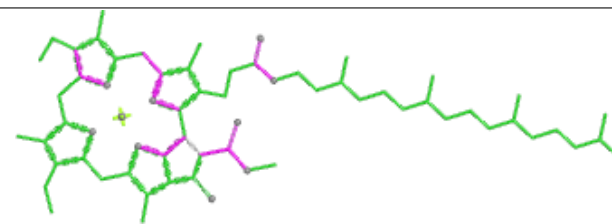
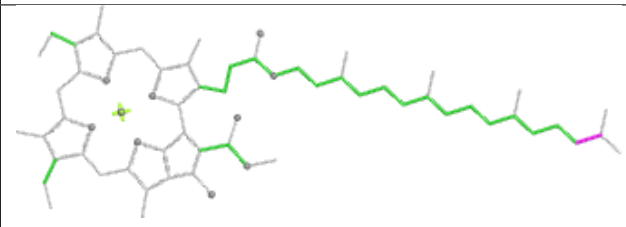
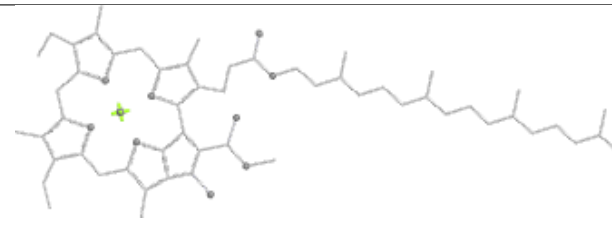
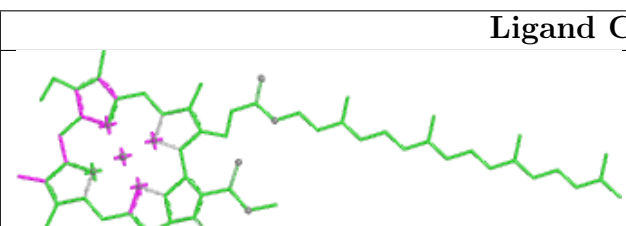
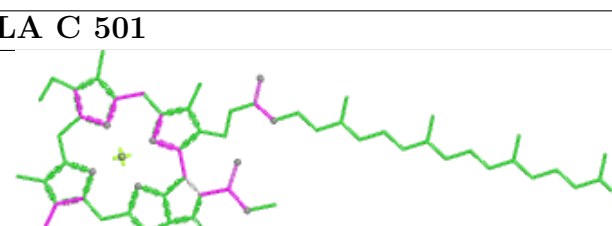
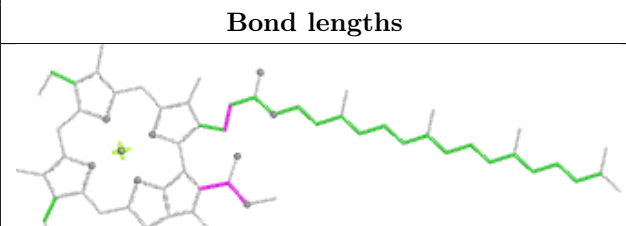
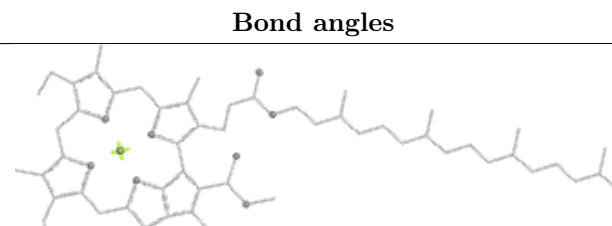
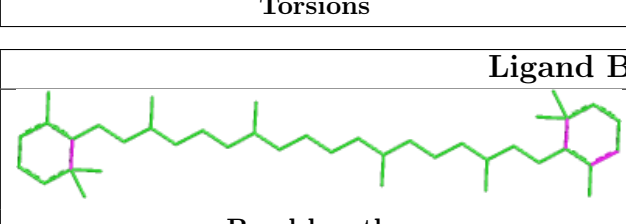
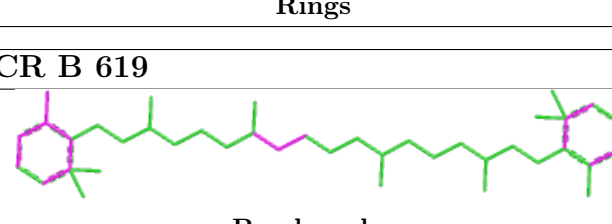
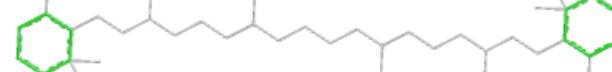


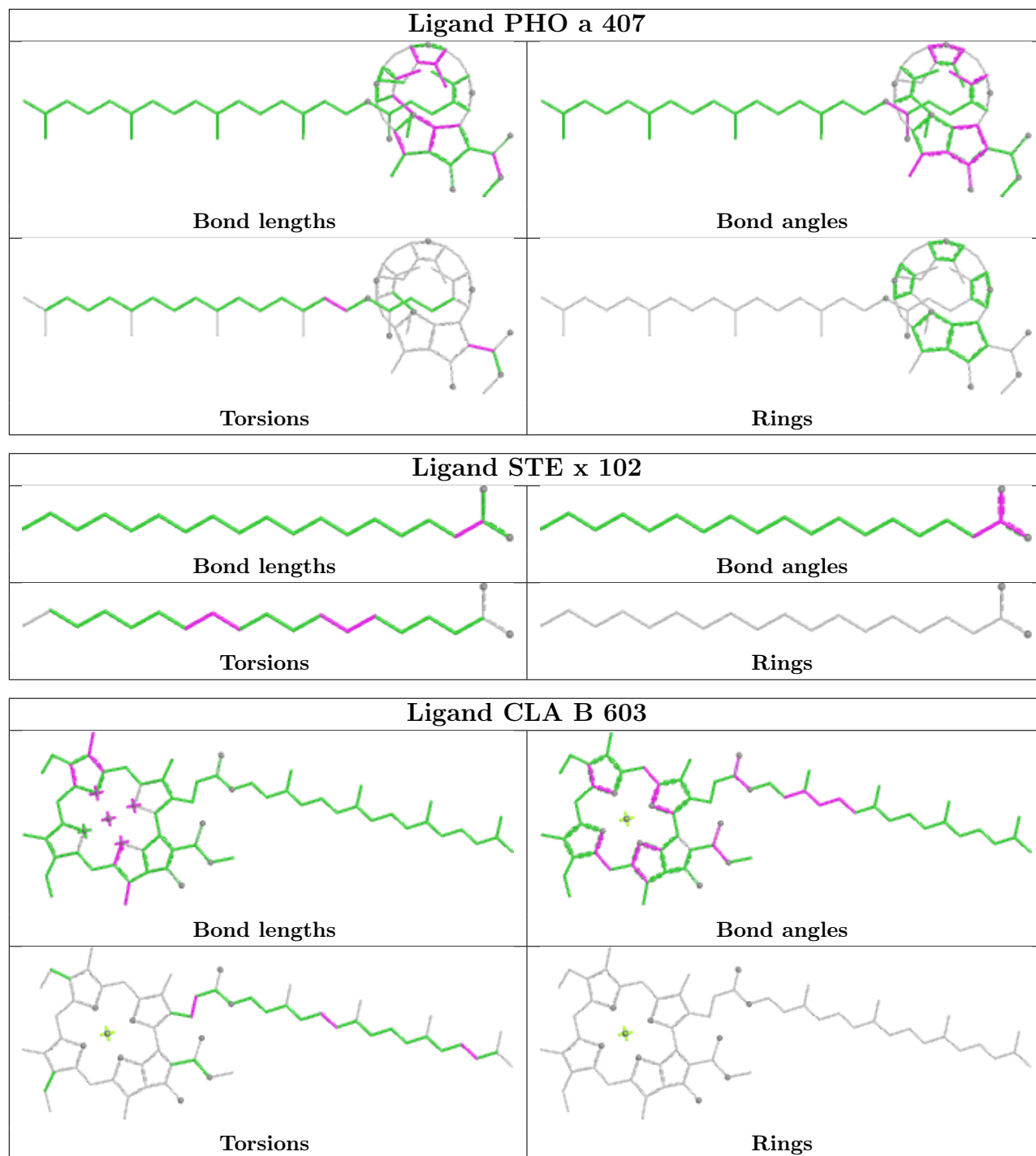


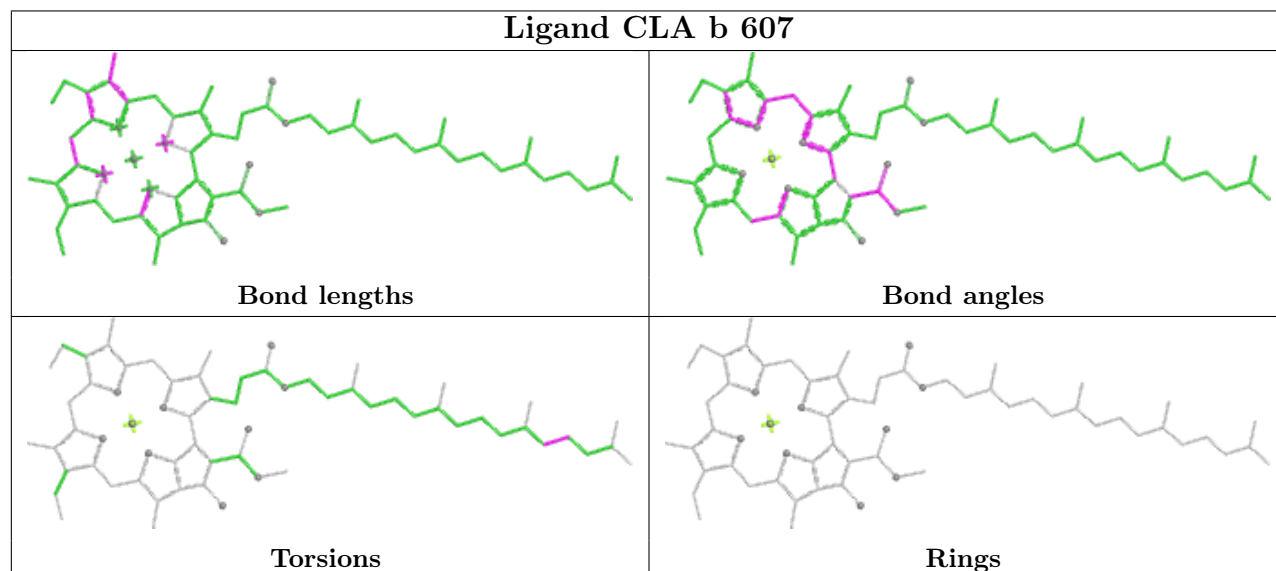
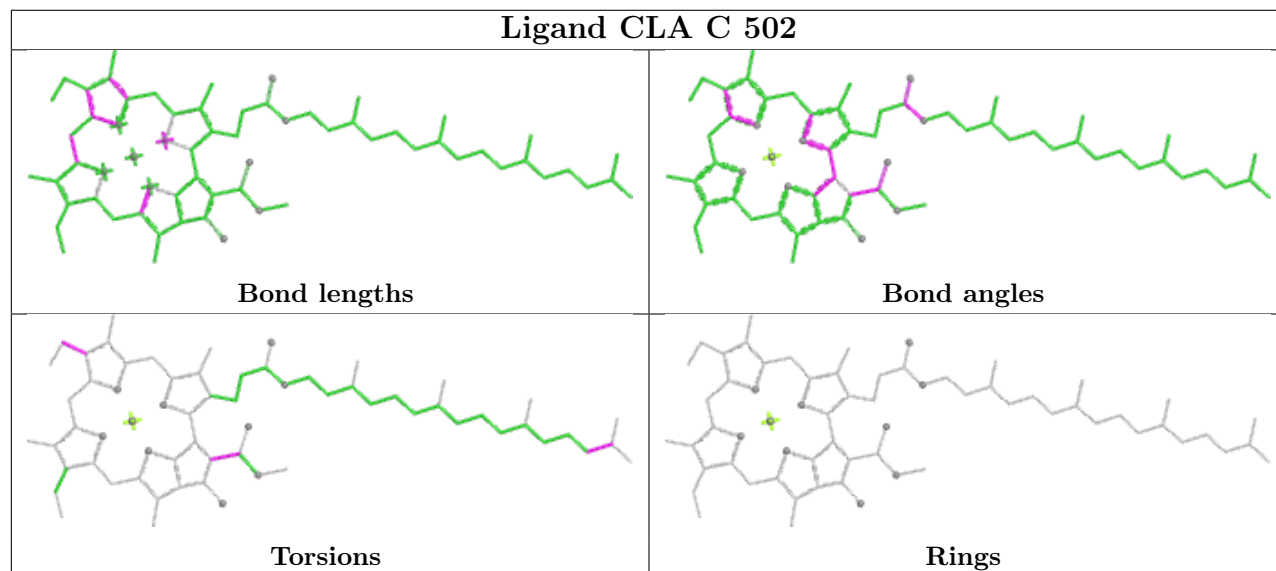
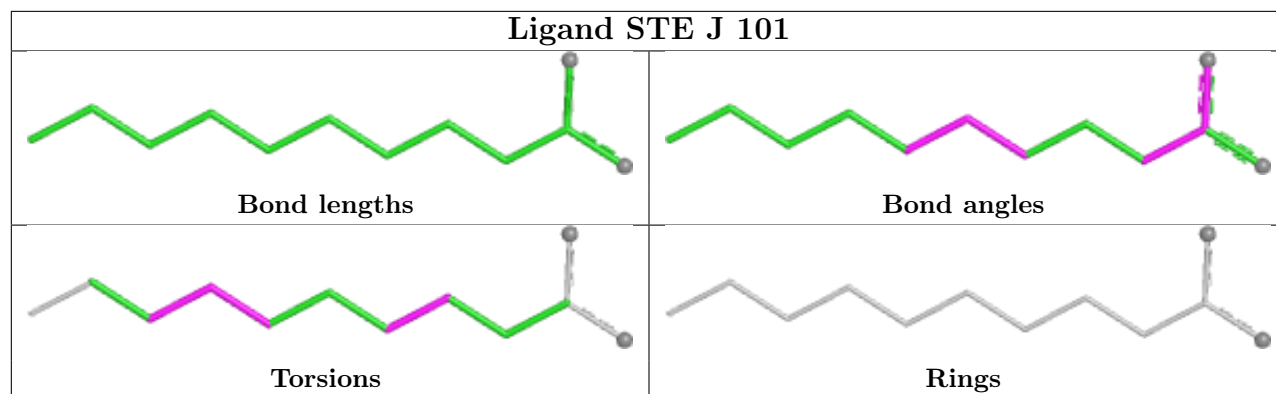
Ligand CLA b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

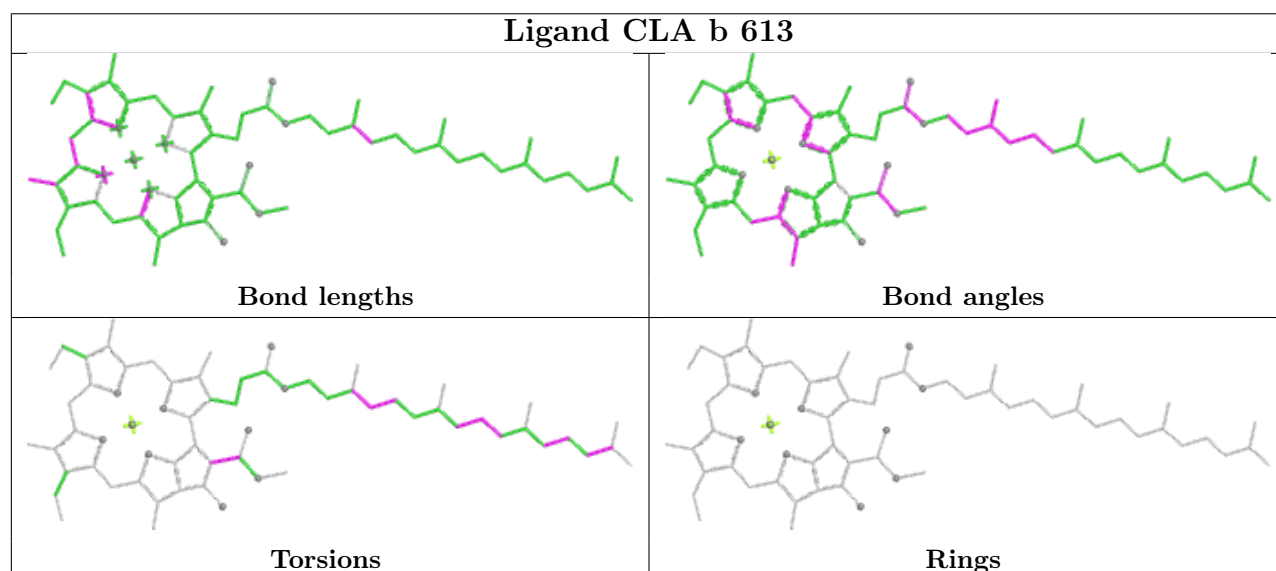
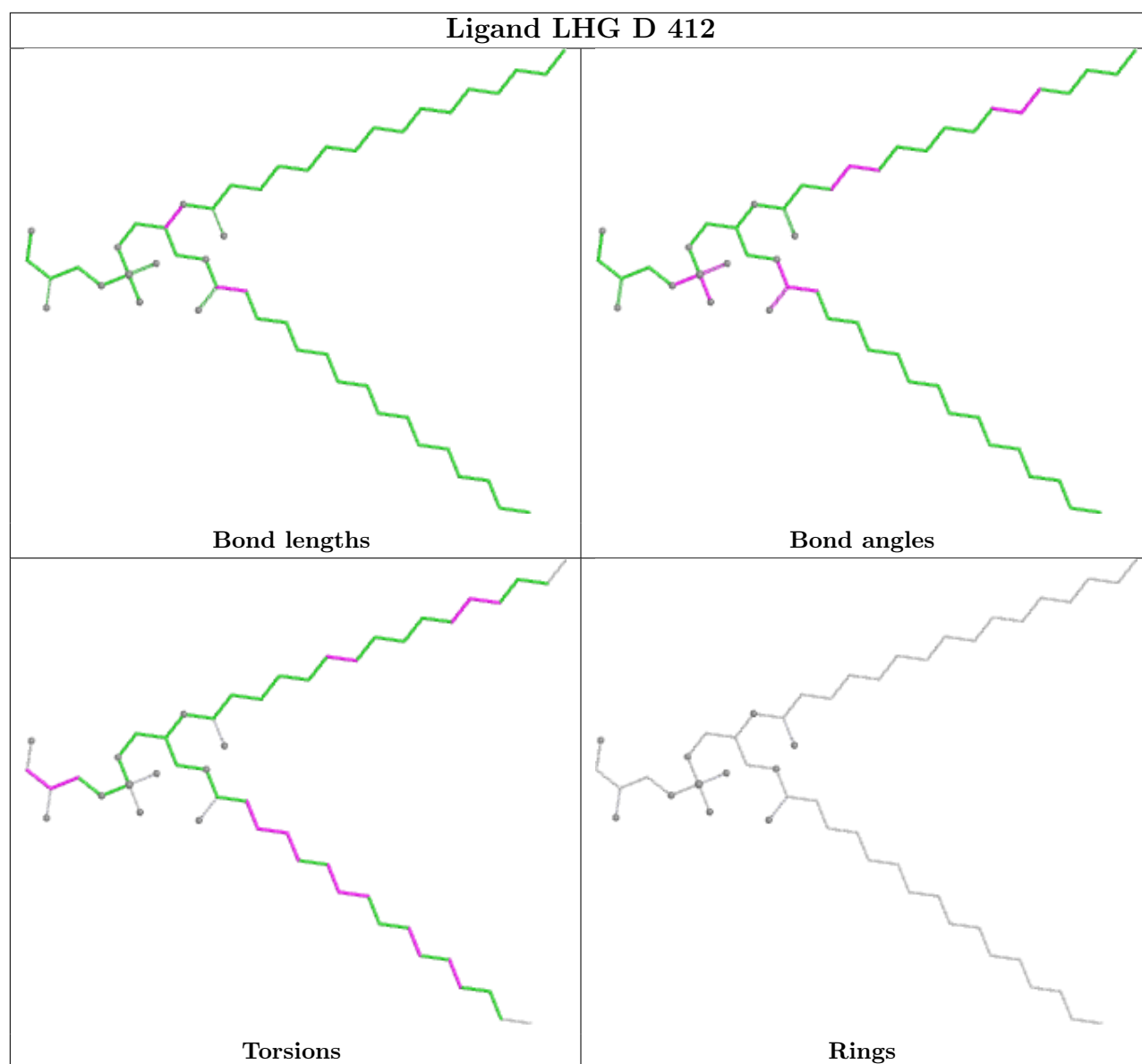
Ligand BCR A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

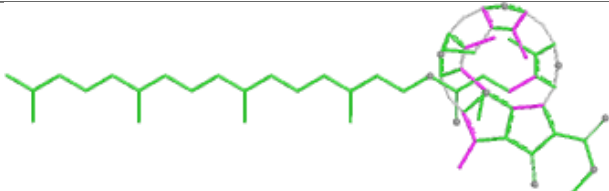
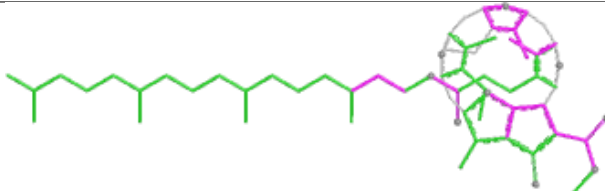
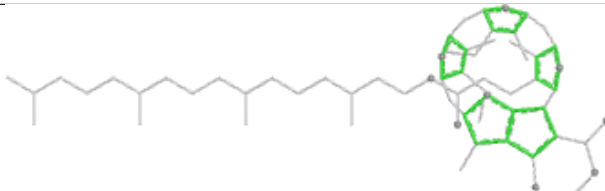
Ligand PL9 a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

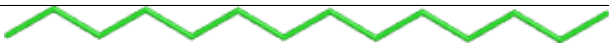


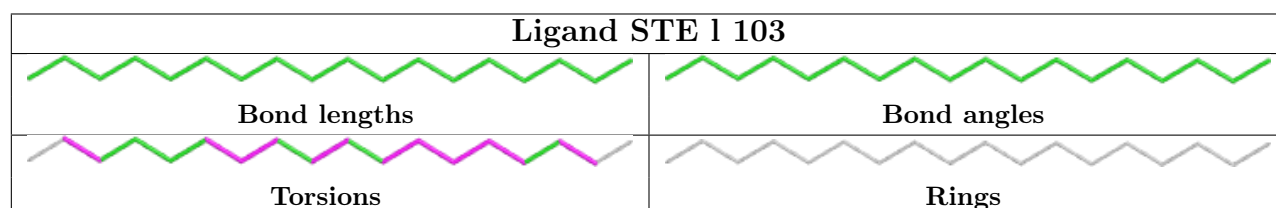
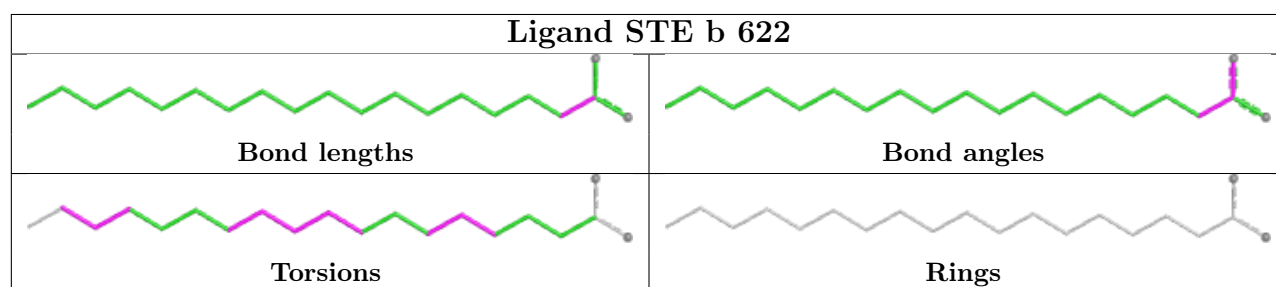
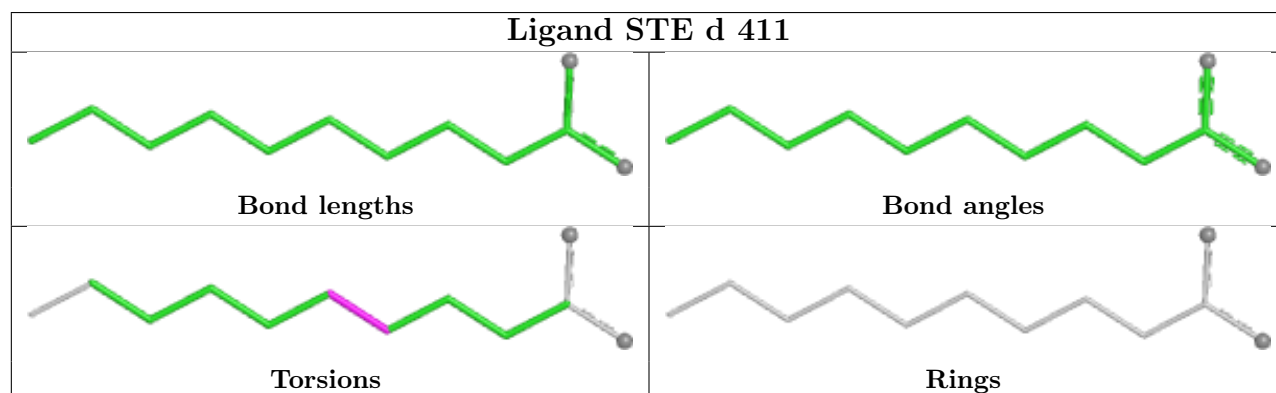
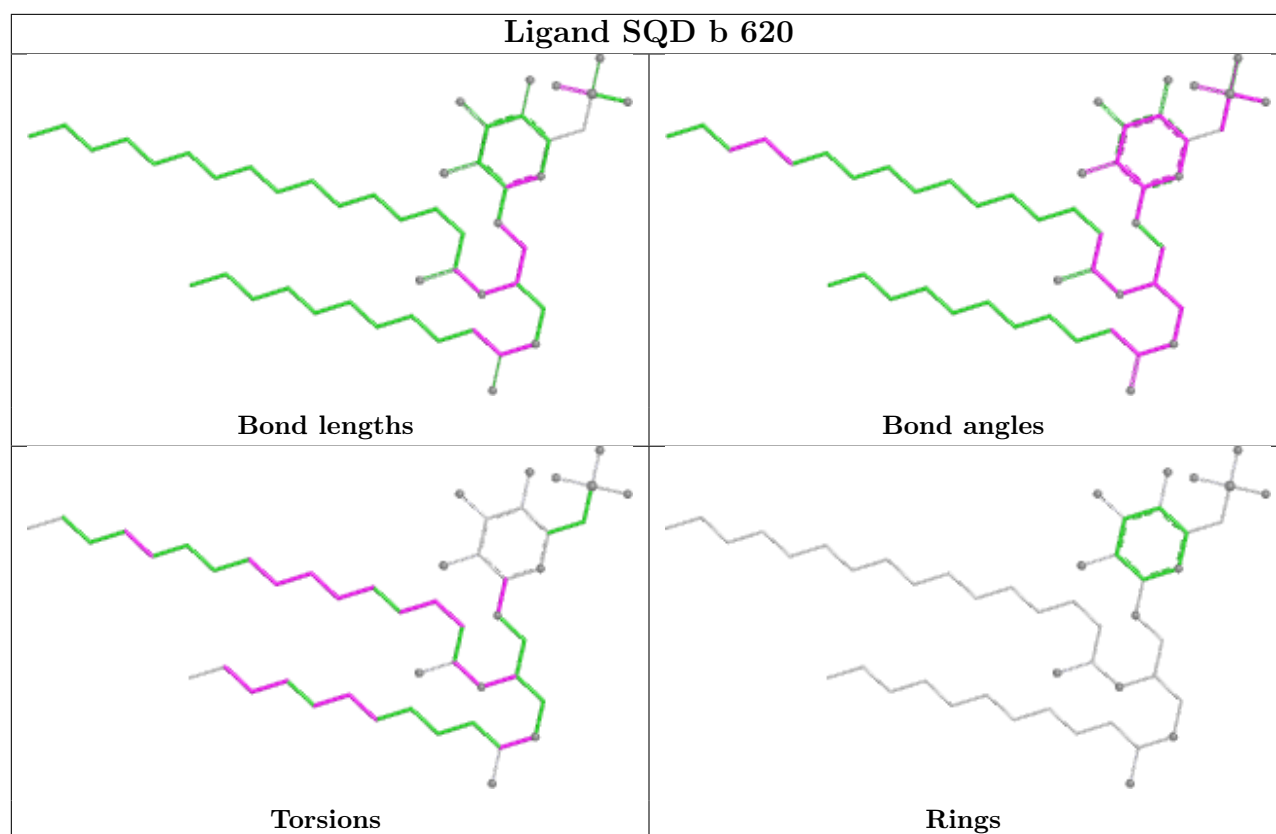


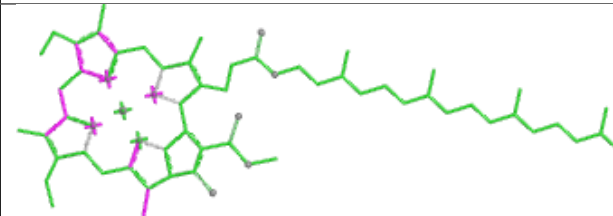
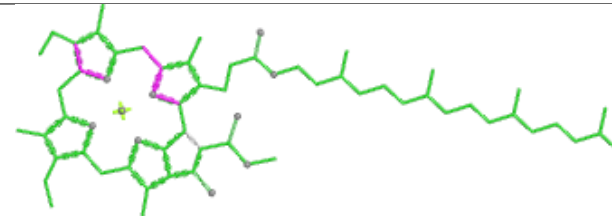
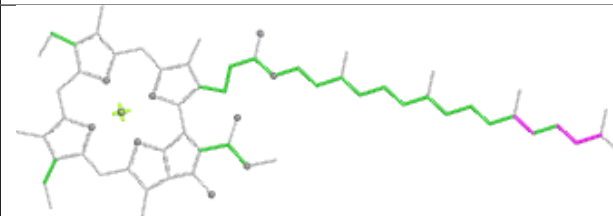
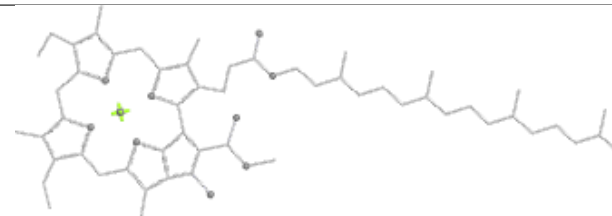


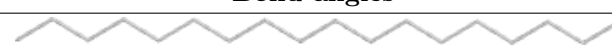
Ligand PHO d 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE E 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE C 528	
 Bond lengths	 Bond angles
 Torsions	 Rings

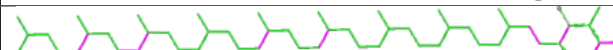
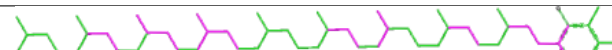


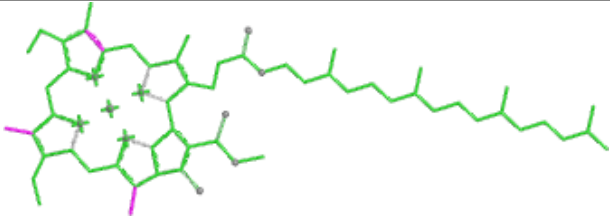
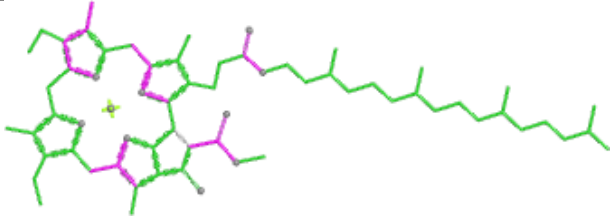
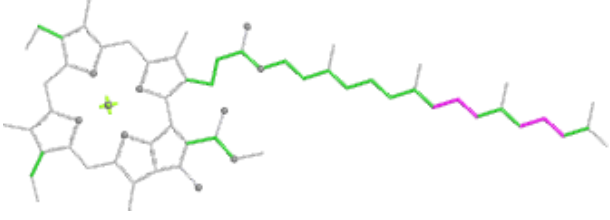
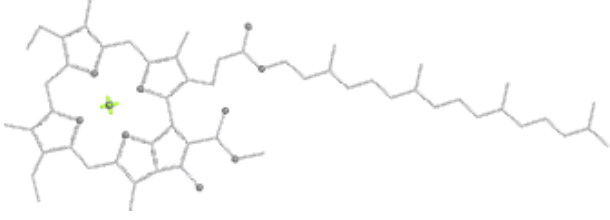
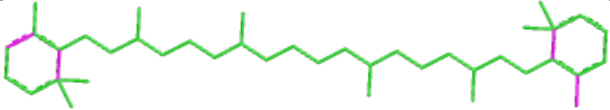
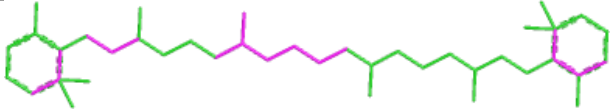
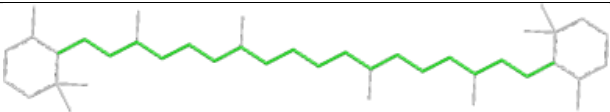
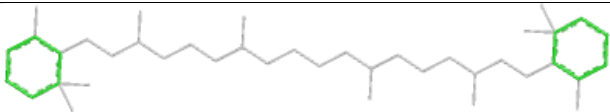
Ligand CLA D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

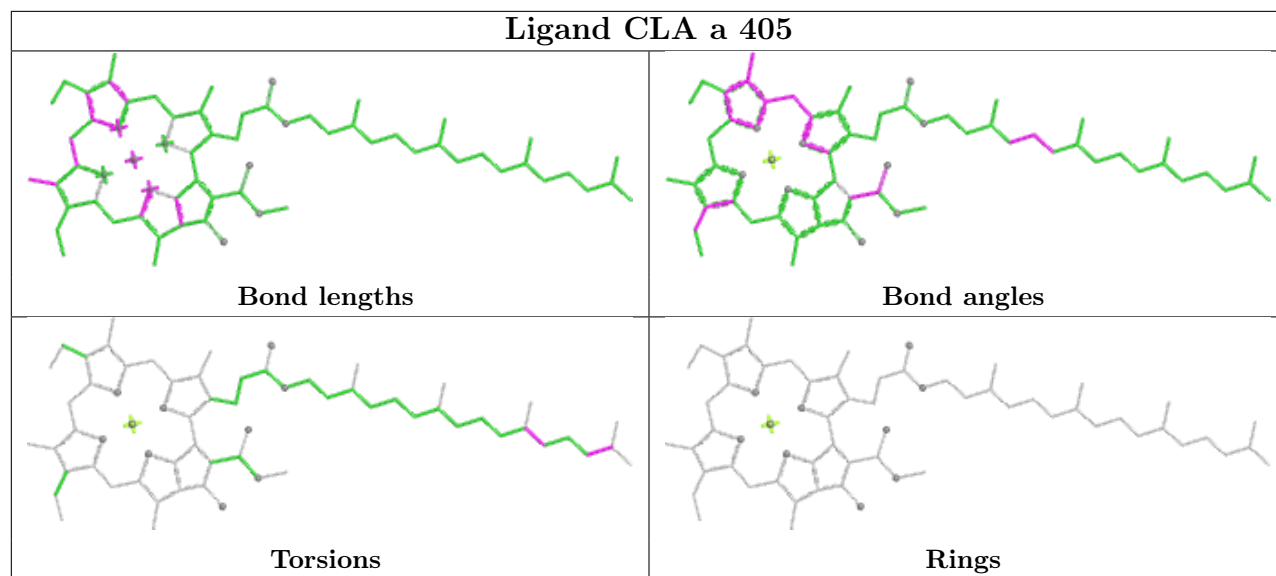
Ligand STE c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 610			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand STE d 412			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand BCR b 617			
			
Bond lengths			
		Bond angles	
			
Torsions			
		Rings	



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.61	0 100 100	21, 27, 48, 85	0
1	a	334/344 (97%)	-0.53	2 (0%) 85 87	20, 30, 57, 85	0
2	B	505/510 (99%)	-0.46	0 100 100	15, 32, 62, 99	4 (0%)
2	b	505/510 (99%)	-0.32	5 (0%) 79 82	25, 36, 73, 115	1 (0%)
3	C	442/461 (95%)	-0.45	0 100 100	15, 35, 53, 83	1 (0%)
3	c	451/461 (97%)	-0.34	2 (0%) 88 90	18, 39, 63, 99	2 (0%)
4	D	341/352 (96%)	-0.62	0 100 100	19, 29, 47, 85	0
4	d	341/352 (96%)	-0.47	0 100 100	23, 33, 57, 80	1 (0%)
5	E	82/84 (97%)	0.08	1 (1%) 76 79	28, 51, 69, 82	1 (1%)
5	e	82/84 (97%)	0.18	1 (1%) 76 79	37, 60, 78, 94	0
6	F	34/45 (75%)	-0.14	0 100 100	35, 42, 67, 90	0
6	f	34/45 (75%)	0.03	0 100 100	40, 50, 83, 102	0
7	H	65/66 (98%)	-0.25	3 (4%) 37 40	29, 41, 63, 83	0
7	h	63/66 (95%)	-0.03	3 (4%) 35 38	39, 50, 71, 78	0
8	I	35/38 (92%)	-0.44	0 100 100	28, 39, 71, 86	0
8	i	35/38 (92%)	-0.22	0 100 100	32, 40, 80, 86	0
9	J	36/40 (90%)	-0.15	0 100 100	32, 49, 75, 97	0
9	j	36/40 (90%)	-0.03	0 100 100	37, 52, 91, 94	0
10	K	37/46 (80%)	-0.14	0 100 100	40, 50, 76, 78	0
10	k	37/46 (80%)	-0.03	0 100 100	46, 56, 72, 78	0
11	L	37/37 (100%)	-0.57	0 100 100	22, 30, 68, 75	0
11	l	36/37 (97%)	-0.62	0 100 100	24, 30, 78, 83	0
12	M	32/36 (88%)	-0.42	0 100 100	27, 33, 58, 72	0
12	m	31/36 (86%)	-0.49	0 100 100	26, 34, 50, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.28	1 (0%) 88 90	23, 41, 86, 128	1 (0%)
13	o	244/272 (89%)	-0.32	1 (0%) 88 90	23, 40, 81, 130	0
14	T	29/32 (90%)	-0.54	2 (6%) 23 24	24, 30, 62, 80	0
14	t	29/32 (90%)	-0.45	2 (6%) 23 24	25, 30, 86, 96	0
15	U	97/134 (72%)	-0.22	0 100 100	28, 43, 69, 89	0
15	u	97/134 (72%)	-0.33	1 (1%) 79 82	27, 40, 56, 85	0
16	V	137/163 (84%)	-0.42	0 100 100	28, 39, 58, 77	0
16	v	137/163 (84%)	-0.18	0 100 100	31, 47, 70, 91	0
17	Y	27/46 (58%)	0.96	3 (11%) 10 11	53, 77, 91, 106	0
17	y	30/46 (65%)	0.55	0 100 100	60, 74, 95, 99	0
18	X	38/41 (92%)	-0.12	1 (2%) 57 61	37, 50, 79, 87	0
18	x	39/41 (95%)	0.10	1 (2%) 57 61	50, 60, 89, 100	0
19	Z	62/62 (100%)	0.67	4 (6%) 25 26	54, 70, 112, 124	0
19	z	62/62 (100%)	0.58	1 (1%) 70 74	54, 73, 107, 124	0
20	R	28/41 (68%)	0.70	1 (3%) 46 49	63, 74, 92, 102	0
20	r	28/41 (68%)	1.49	9 (32%) 1 1	77, 104, 114, 124	0
All	All	5293/5700 (92%)	-0.33	44 (0%) 82 85	15, 37, 75, 130	11 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	4.2
14	t	30	THR	4.1
3	c	23	ALA	3.5
7	H	41	PHE	3.5
13	o	58	ASN	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.96	0.07	37,48,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.96	0.09	39,50,77,85	0
14	FME	T	1	10/11	0.96	0.08	27,45,62,62	0
14	FME	t	1	10/11	0.96	0.07	23,40,71,71	0
8	FME	i	1	10/11	0.98	0.05	41,49,59,64	0
12	FME	m	1	10/11	0.98	0.05	31,44,69,83	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
27	STE	i	102	6/20	0.63	0.22	66,89,108,108	0
27	STE	i	101	12/20	0.68	0.18	58,75,94,95	0
27	STE	c	517	18/20	0.68	0.17	50,81,102,102	0
27	STE	C	527	8/20	0.69	0.24	38,55,61,70	0
27	STE	C	529	14/20	0.70	0.15	53,78,105,109	0
27	STE	I	102	17/20	0.73	0.15	56,72,86,87	0
27	STE	H	103	18/20	0.73	0.18	47,73,92,93	0
28	LMG	b	619	24/55	0.73	0.24	40,54,75,79	0
27	STE	A	417	11/20	0.74	0.21	45,56,73,77	0
27	STE	C	528	14/20	0.75	0.23	43,61,87,92	0
27	STE	j	102	16/20	0.76	0.20	42,60,69,70	0
27	STE	e	101	9/20	0.77	0.25	44,50,58,62	0
27	STE	B	623	15/20	0.77	0.20	38,62,88,89	0
27	STE	I	101	15/20	0.77	0.17	36,58,84,88	0
27	STE	E	102	12/20	0.77	0.18	50,74,88,91	0
27	STE	E	104	20/20	0.77	0.14	52,67,80,82	0
27	STE	d	411	12/20	0.78	0.13	46,73,99,104	0
27	STE	E	103	12/20	0.78	0.18	49,57,79,82	0
27	STE	A	416	17/20	0.78	0.15	51,74,94,96	0
28	LMG	D	408	50/55	0.79	0.15	35,67,111,123	0
33	LHG	a	413	42/49	0.79	0.15	61,86,110,123	0
27	STE	d	412	10/20	0.80	0.21	43,55,70,73	0
27	STE	a	417	12/20	0.80	0.14	47,66,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	STE	C	516	14/20	0.80	0.15	54,70,89,93	0
28	LMG	c	518	30/55	0.80	0.13	37,70,100,110	0
27	STE	a	416	10/20	0.80	0.14	43,64,70,70	0
27	STE	T	102	16/20	0.81	0.18	38,61,99,102	0
27	STE	b	626	10/20	0.81	0.14	46,58,66,69	0
27	STE	C	518	5/20	0.81	0.14	47,56,67,67	0
28	LMG	C	517	36/55	0.81	0.14	36,65,90,102	0
27	STE	c	516	13/20	0.82	0.13	47,75,84,88	0
27	STE	d	410	17/20	0.82	0.13	35,56,72,74	0
33	LHG	E	101	49/49	0.82	0.14	43,80,110,116	0
28	LMG	a	415	55/55	0.82	0.14	37,64,89,93	0
27	STE	m	102	15/20	0.83	0.15	41,58,87,92	0
27	STE	A	410	9/20	0.83	0.20	46,52,60,64	0
27	STE	B	622	12/20	0.84	0.13	49,66,81,85	0
27	STE	b	625	16/20	0.84	0.15	49,62,85,92	0
28	LMG	b	623	55/55	0.84	0.15	48,77,98,104	0
26	PL9	a	410	55/55	0.84	0.14	41,63,83,95	0
28	LMG	c	523	48/55	0.84	0.14	46,78,112,122	0
27	STE	Z	101	17/20	0.84	0.16	48,69,95,100	0
26	PL9	A	409	55/55	0.84	0.15	37,66,87,103	0
27	STE	C	519	7/20	0.85	0.17	45,47,51,52	0
27	STE	z	101	9/20	0.85	0.16	49,64,75,76	0
29	SQD	A	413	54/54	0.85	0.14	39,60,97,100	0
30	DGD	A	414	66/66	0.85	0.12	43,68,103,107	0
28	LMG	B	620	45/55	0.85	0.13	38,60,103,130	0
27	STE	C	526	16/20	0.85	0.12	36,56,73,74	0
29	SQD	a	414	54/54	0.86	0.14	36,53,87,104	0
27	STE	t	103	18/20	0.87	0.11	46,61,76,78	0
27	STE	b	624	20/20	0.87	0.14	36,54,73,77	0
27	STE	j	101	12/20	0.87	0.10	45,57,63,64	0
27	STE	e	104	13/20	0.87	0.17	61,66,79,81	0
23	CLA	h	101	65/65	0.87	0.12	39,64,95,103	0
28	LMG	C	524	48/55	0.88	0.12	35,69,87,101	0
27	STE	b	622	20/20	0.88	0.10	38,59,75,77	0
27	STE	e	102	8/20	0.88	0.22	48,58,60,67	0
27	STE	x	102	20/20	0.89	0.11	36,55,74,82	0
29	SQD	f	102	41/54	0.89	0.13	50,83,102,112	0
27	STE	C	525	12/20	0.89	0.11	37,50,60,60	0
27	STE	t	102	14/20	0.89	0.10	35,51,61,61	0
27	STE	m	101	12/20	0.89	0.12	44,57,75,75	0
28	LMG	c	522	46/55	0.90	0.11	40,67,84,89	0
27	STE	D	414	9/20	0.90	0.15	39,45,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	LMG	c	524	49/55	0.90	0.10	35,59,92,115	0
27	STE	e	103	9/20	0.90	0.16	46,49,56,57	0
27	STE	b	627	11/20	0.90	0.17	45,52,54,58	0
28	LMG	A	411	48/55	0.90	0.10	38,58,77,95	0
29	SQD	l	101	54/54	0.90	0.10	38,62,90,105	0
28	LMG	b	621	51/55	0.90	0.10	38,55,78,90	0
27	STE	J	101	12/20	0.90	0.11	48,62,68,73	0
27	STE	B	621	17/20	0.90	0.10	35,53,70,73	0
28	LMG	M	101	51/55	0.91	0.09	32,51,74,81	0
27	STE	M	103	10/20	0.91	0.11	32,47,57,65	0
32	BCT	a	404	4/4	0.91	0.11	30,30,45,54	0
29	SQD	b	620	49/54	0.91	0.09	38,58,89,103	0
25	BCR	C	514	40/40	0.91	0.11	41,56,69,74	0
27	STE	l	103	18/20	0.92	0.10	35,49,87,89	0
27	STE	M	102	15/20	0.92	0.10	38,47,60,75	0
25	BCR	K	101	40/40	0.92	0.09	33,51,69,76	0
25	BCR	d	404	40/40	0.92	0.09	32,48,86,93	0
25	BCR	k	101	40/40	0.92	0.08	40,56,69,72	0
23	CLA	c	513	65/65	0.93	0.09	41,66,99,112	0
23	CLA	B	601	65/65	0.93	0.09	30,63,91,105	0
27	STE	A	415	8/20	0.93	0.12	41,49,54,55	0
25	BCR	x	101	40/40	0.93	0.08	34,51,70,71	0
29	SQD	A	412	52/54	0.93	0.10	32,62,92,102	0
25	BCR	c	514	40/40	0.93	0.08	43,59,73,73	0
29	SQD	F	102	36/54	0.93	0.09	43,70,88,99	0
29	SQD	a	412	54/54	0.93	0.09	38,68,90,94	0
25	BCR	D	406	40/40	0.94	0.09	24,42,77,89	0
25	BCR	H	101	40/40	0.94	0.07	29,43,58,61	0
30	DGD	C	522	62/66	0.94	0.09	28,52,100,111	0
30	DGD	H	102	62/66	0.94	0.08	26,45,61,64	0
30	DGD	c	520	62/66	0.94	0.08	29,52,91,99	0
30	DGD	h	102	62/66	0.94	0.09	24,49,60,71	0
23	CLA	c	512	65/65	0.94	0.08	37,56,96,103	0
23	CLA	C	513	65/65	0.94	0.09	38,62,92,99	0
27	STE	D	413	20/20	0.94	0.08	30,47,73,81	0
33	LHG	d	406	49/49	0.94	0.10	33,52,73,84	0
23	CLA	C	510	65/65	0.95	0.07	25,40,61,63	0
25	BCR	k	102	40/40	0.95	0.08	35,49,64,69	0
25	BCR	C	515	40/40	0.95	0.07	24,38,49,58	0
25	BCR	C	520	40/40	0.95	0.09	30,48,65,70	0
23	CLA	C	512	65/65	0.95	0.08	34,52,95,108	0
23	CLA	C	503	65/65	0.95	0.06	25,39,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	A	408	40/40	0.95	0.06	21,34,45,48	0
25	BCR	b	616	40/40	0.95	0.06	26,38,49,52	0
28	LMG	d	409	44/55	0.95	0.09	29,51,86,99	0
32	BCT	D	401	4/4	0.95	0.11	26,28,34,40	0
25	BCR	b	618	40/40	0.95	0.06	26,42,59,63	0
25	BCR	B	618	40/40	0.95	0.07	21,37,53,54	0
28	LMG	D	409	51/55	0.95	0.10	24,54,83,89	0
25	BCR	B	619	40/40	0.95	0.07	20,39,59,65	0
25	BCR	T	101	40/40	0.96	0.06	22,36,49,50	0
25	BCR	a	409	40/40	0.96	0.05	20,33,44,45	0
23	CLA	c	506	65/65	0.96	0.08	28,45,91,97	0
25	BCR	b	617	40/40	0.96	0.06	24,37,54,55	0
23	CLA	c	508	64/65	0.96	0.08	26,41,95,111	0
23	CLA	c	509	65/65	0.96	0.07	27,43,67,72	0
25	BCR	c	515	40/40	0.96	0.07	28,42,57,65	0
23	CLA	c	511	65/65	0.96	0.07	35,49,69,71	0
23	CLA	C	509	65/65	0.96	0.07	22,41,62,69	0
23	CLA	C	502	65/65	0.96	0.06	23,37,56,61	0
25	BCR	t	101	40/40	0.96	0.06	22,36,53,53	0
23	CLA	d	403	65/65	0.96	0.08	26,46,89,98	0
23	CLA	C	511	65/65	0.96	0.07	28,46,65,71	0
24	PHO	a	407	64/64	0.96	0.06	17,28,39,40	0
26	PL9	d	405	55/55	0.96	0.06	20,33,45,50	0
24	PHO	d	401	64/64	0.96	0.06	24,35,48,48	0
23	CLA	B	606	65/65	0.96	0.07	21,32,69,72	0
25	BCR	B	617	40/40	0.96	0.06	23,34,54,56	0
30	DGD	C	523	62/66	0.96	0.08	25,48,79,87	0
23	CLA	C	505	65/65	0.96	0.08	21,36,71,85	0
23	CLA	b	601	65/65	0.96	0.07	24,40,60,66	0
30	DGD	c	521	62/66	0.96	0.08	24,53,88,94	0
23	CLA	b	605	65/65	0.96	0.07	21,36,74,84	0
23	CLA	b	608	65/65	0.96	0.07	24,42,62,67	0
23	CLA	b	609	65/65	0.96	0.07	23,36,48,51	0
33	LHG	D	411	47/49	0.96	0.09	23,48,78,94	0
33	LHG	D	412	49/49	0.96	0.09	27,44,73,79	0
23	CLA	b	614	65/65	0.96	0.07	24,38,61,64	0
23	CLA	b	615	60/65	0.96	0.08	25,38,95,99	0
23	CLA	c	503	65/65	0.96	0.06	29,42,52,60	0
33	LHG	d	408	39/49	0.96	0.08	30,43,74,86	0
33	LHG	l	102	49/49	0.96	0.07	25,43,59,71	0
23	CLA	c	510	65/65	0.97	0.06	26,45,63,67	0
23	CLA	C	506	65/65	0.97	0.07	20,38,96,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	507	65/65	0.97	0.06	21,37,63,67	0
23	CLA	C	508	65/65	0.97	0.07	23,38,101,106	0
23	CLA	d	402	65/65	0.97	0.06	17,31,63,66	0
23	CLA	A	404	65/65	0.97	0.06	12,26,48,57	0
23	CLA	B	607	65/65	0.97	0.07	16,31,62,64	0
24	PHO	A	406	64/64	0.97	0.05	21,31,41,48	0
24	PHO	D	402	64/64	0.97	0.05	16,26,35,39	0
23	CLA	B	608	65/65	0.97	0.05	18,34,52,61	0
23	CLA	B	609	65/65	0.97	0.06	23,34,58,62	0
23	CLA	B	610	65/65	0.97	0.06	19,30,42,46	0
23	CLA	D	403	65/65	0.97	0.05	16,26,50,58	0
23	CLA	D	404	65/65	0.97	0.06	16,27,57,62	0
23	CLA	D	405	65/65	0.97	0.07	21,40,105,116	0
23	CLA	a	405	65/65	0.97	0.06	16,28,49,59	0
23	CLA	a	406	65/65	0.97	0.07	22,35,95,100	0
23	CLA	a	408	65/65	0.97	0.07	18,34,79,90	0
23	CLA	a	411	65/65	0.97	0.06	17,27,49,53	0
23	CLA	B	611	65/65	0.97	0.05	17,29,51,54	0
23	CLA	b	602	65/65	0.97	0.06	21,33,69,82	0
23	CLA	b	603	65/65	0.97	0.07	17,32,81,98	0
23	CLA	b	604	65/65	0.97	0.06	19,32,51,55	0
23	CLA	B	612	65/65	0.97	0.06	18,29,47,51	0
23	CLA	b	606	65/65	0.97	0.07	17,34,67,70	0
23	CLA	b	607	65/65	0.97	0.07	22,40,58,68	0
23	CLA	B	614	65/65	0.97	0.08	19,32,82,94	0
23	CLA	B	615	65/65	0.97	0.06	22,34,62,70	0
23	CLA	b	610	65/65	0.97	0.05	20,30,53,58	0
30	DGD	C	521	62/66	0.97	0.07	18,43,81,98	0
23	CLA	b	611	65/65	0.97	0.06	18,33,49,64	0
23	CLA	b	612	65/65	0.97	0.07	16,31,72,80	0
23	CLA	b	613	65/65	0.97	0.06	22,36,74,85	0
30	DGD	c	519	62/66	0.97	0.07	18,42,79,86	0
23	CLA	B	616	60/65	0.97	0.08	20,34,98,116	0
23	CLA	C	501	65/65	0.97	0.06	19,33,49,58	0
26	PL9	D	407	55/55	0.97	0.05	18,31,46,50	0
23	CLA	c	501	65/65	0.97	0.06	26,36,50,57	0
23	CLA	c	502	65/65	0.97	0.06	26,39,59,63	0
33	LHG	D	410	49/49	0.97	0.06	18,41,53,62	0
23	CLA	B	602	65/65	0.97	0.06	20,33,56,62	0
23	CLA	c	504	60/65	0.97	0.07	27,44,81,84	0
23	CLA	c	505	65/65	0.97	0.07	24,38,69,81	0
33	LHG	L	101	49/49	0.97	0.06	22,42,59,69	0

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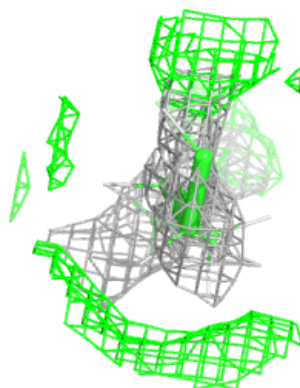
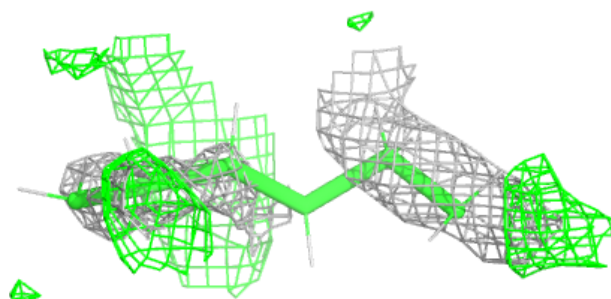
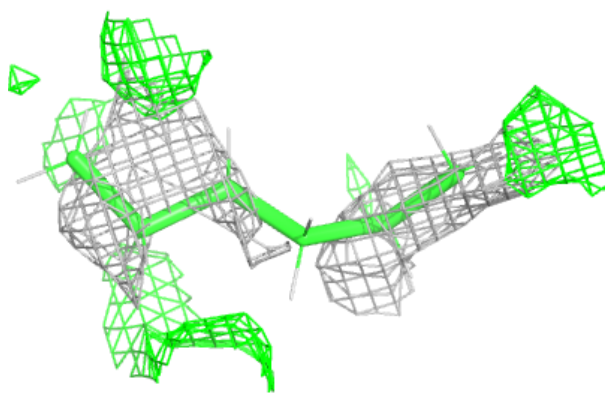
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	604	65/65	0.97	0.06	18,28,70,78	0
23	CLA	c	507	65/65	0.97	0.06	25,41,56,72	0
33	LHG	d	407	49/49	0.97	0.07	27,42,56,63	0
23	CLA	C	504	59/65	0.97	0.06	25,37,81,86	0
23	CLA	B	605	65/65	0.97	0.06	17,30,50,54	0
34	HEM	f	101	43/43	0.97	0.07	41,55,76,78	0
22	CL	A	403	1/1	0.98	0.04	24,24,24,24	0
23	CLA	A	405	65/65	0.98	0.07	18,31,97,104	0
23	CLA	B	603	65/65	0.98	0.06	19,30,61,69	0
23	CLA	A	407	54/65	0.98	0.05	16,30,63,69	0
34	HEM	F	101	43/43	0.98	0.07	28,45,59,61	0
23	CLA	B	613	65/65	0.98	0.06	18,30,69,75	0
35	HEC	v	201	43/43	0.98	0.05	23,33,40,43	0
22	CL	a	403	1/1	0.99	0.07	24,24,24,24	0
21	FE2	a	401	1/1	0.99	0.02	29,29,29,29	0
22	CL	A	402	1/1	0.99	0.03	25,25,25,25	0
21	FE2	A	401	1/1	0.99	0.01	23,23,23,23	0
31	OEX	A	418	10/10	0.99	0.04	22,23,26,27	0
31	OEX	a	418	10/10	0.99	0.03	22,23,27,30	0
35	HEC	V	201	43/43	0.99	0.05	21,29,38,42	0
22	CL	a	402	1/1	0.99	0.03	25,25,25,25	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.

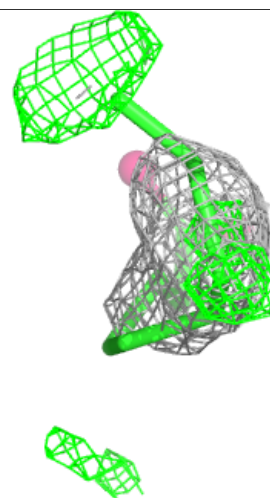
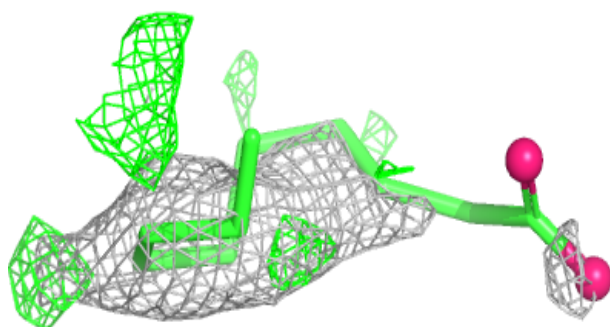
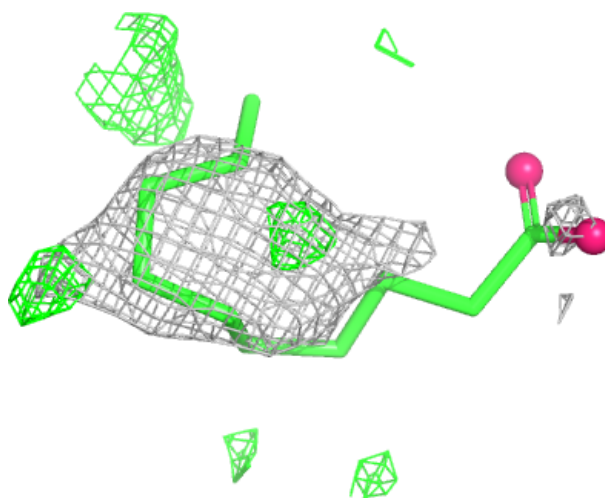
Electron density around STE i 102:

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



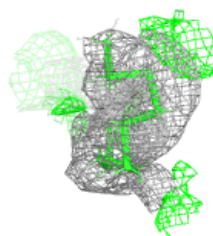
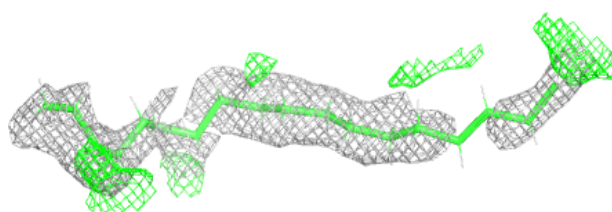
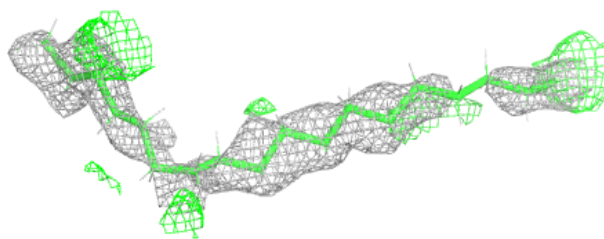
Electron density around STE i 101:

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

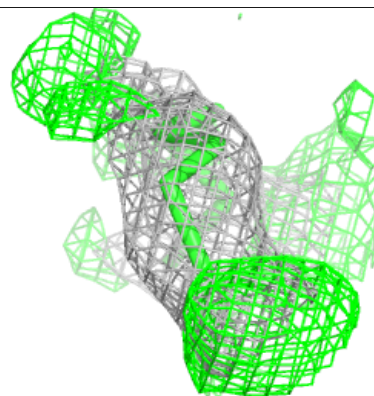
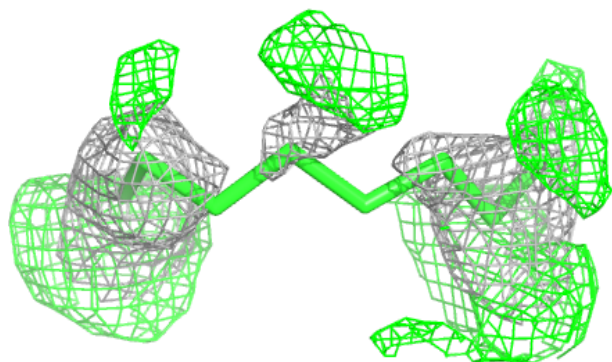
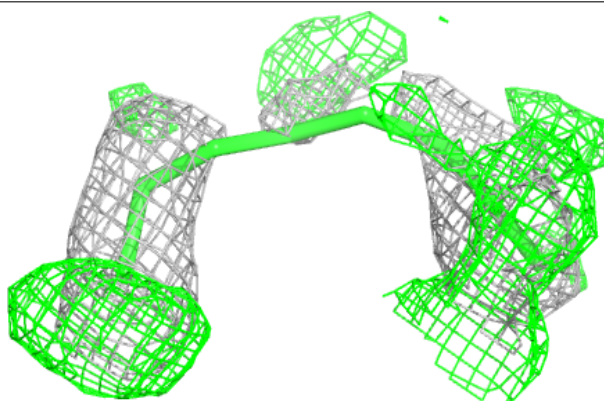


Electron density around STE c 517:

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

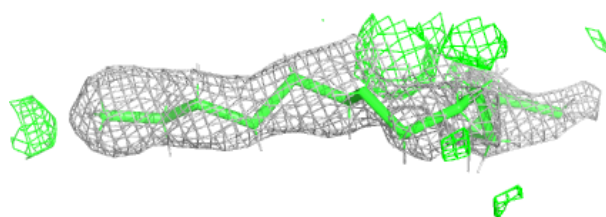
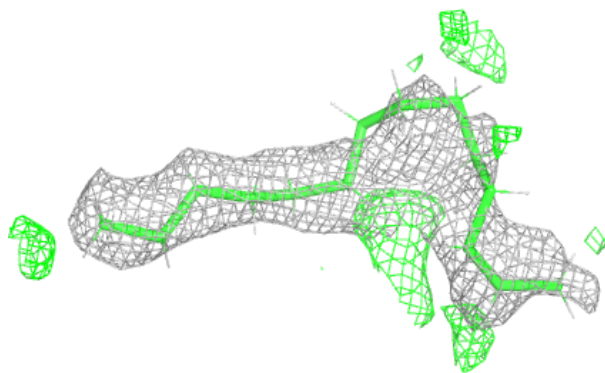
**Electron density around STE C 527:**

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

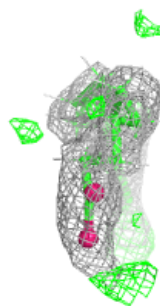
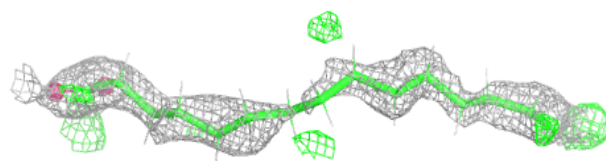
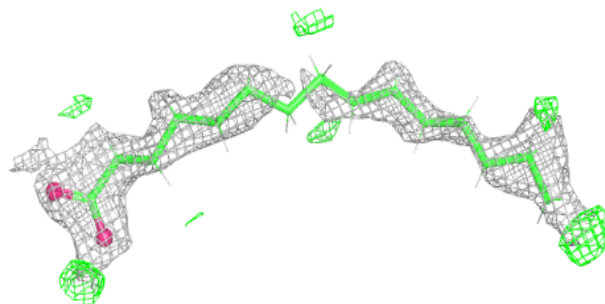


Electron density around STE C 529:

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

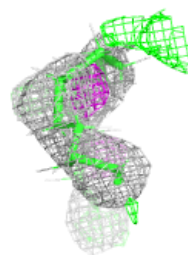
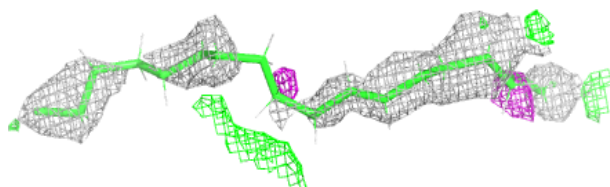
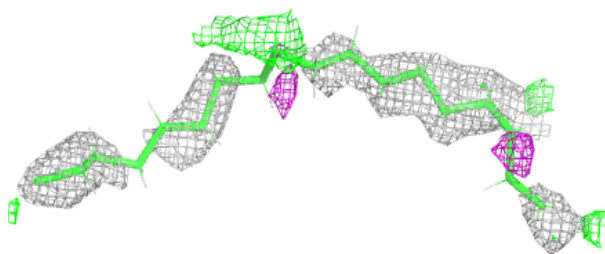
**Electron density around STE I 102:**

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

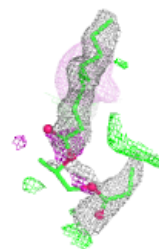
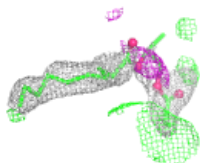
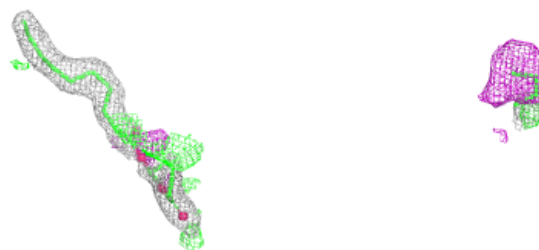


Electron density around STE H 103:

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

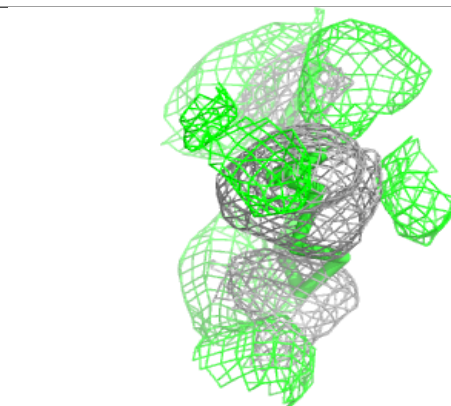
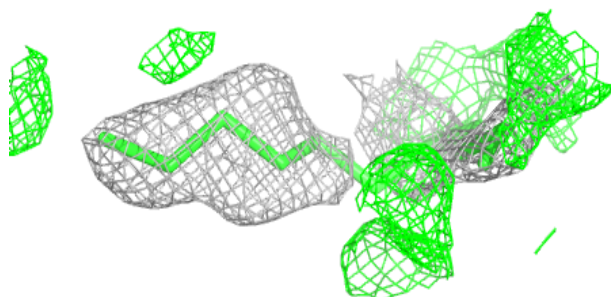
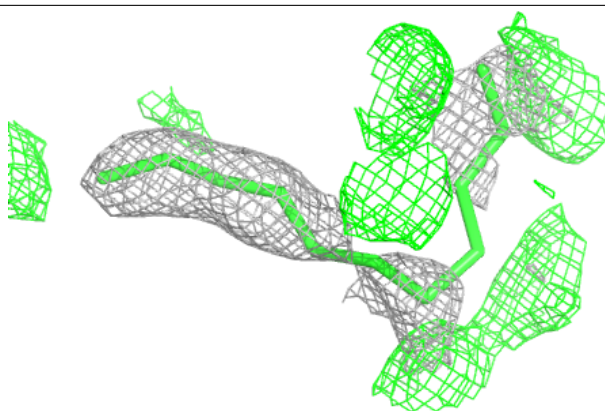
**Electron density around LMG b 619:**

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

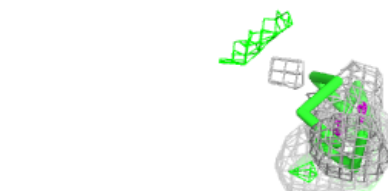
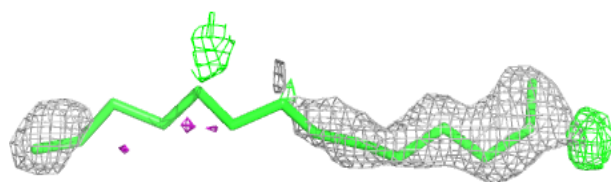
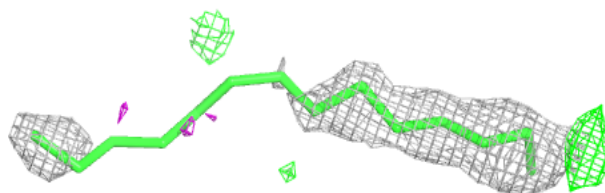


Electron density around STE A 417:

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

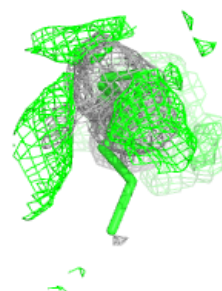
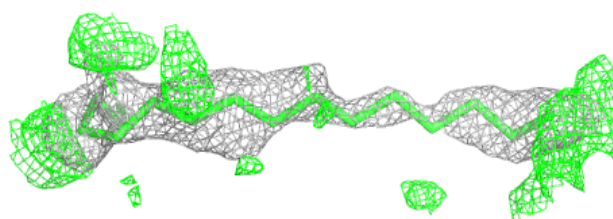
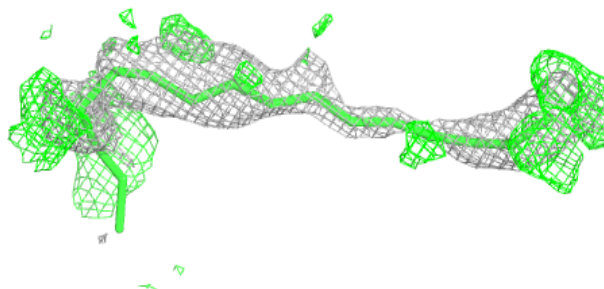
**Electron density around STE C 528:**

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and green (positive)

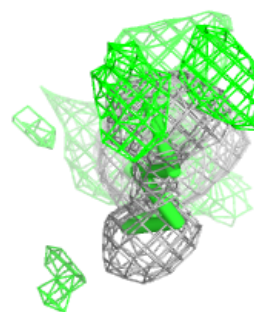
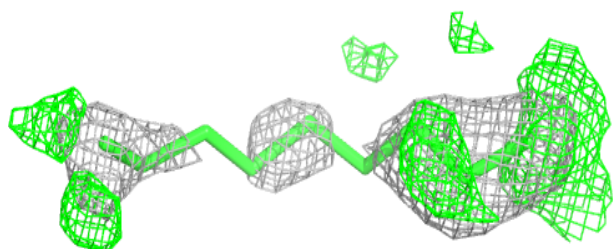
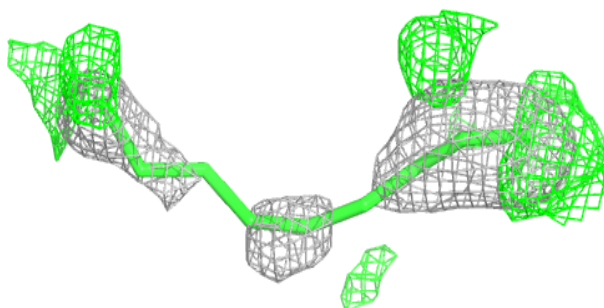


Electron density around STE j 102:

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

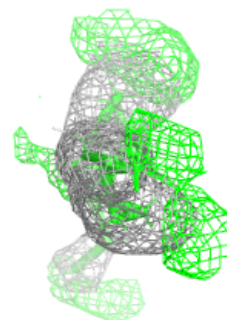
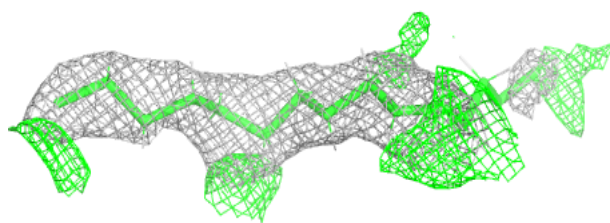
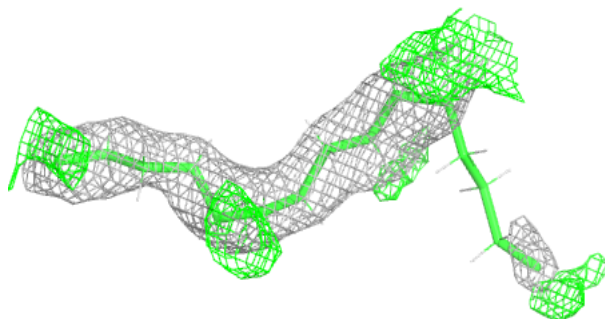
**Electron density around STE e 101:**

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and green (positive)

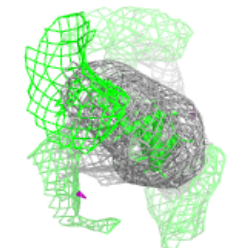
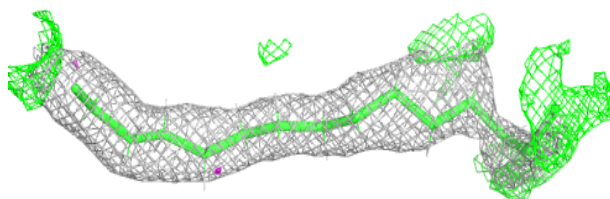
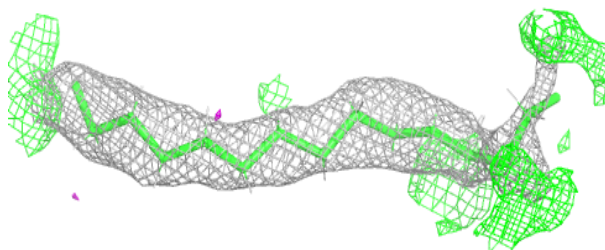


Electron density around STE B 623:

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and green (positive)

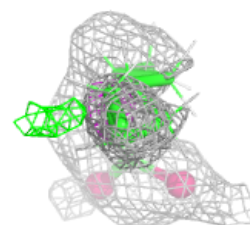
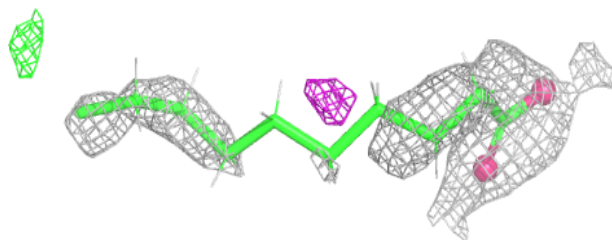
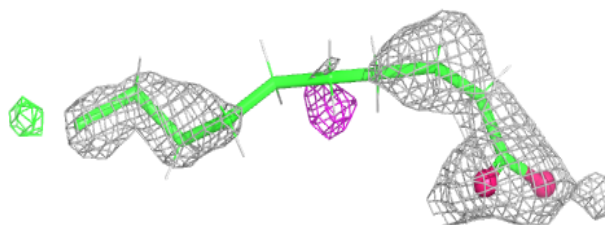
**Electron density around STE I 101:**

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

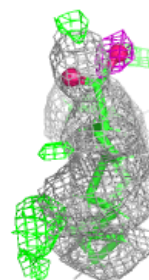
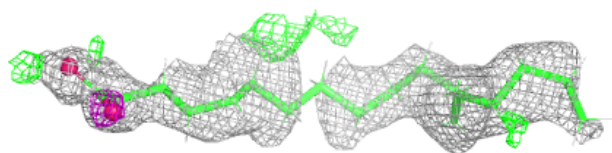
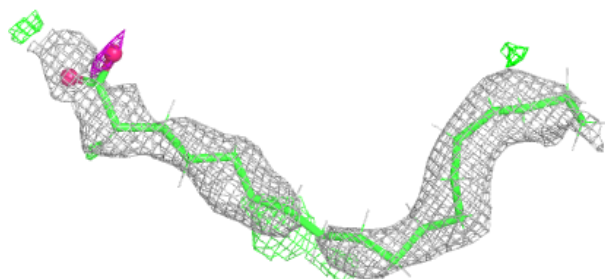


Electron density around STE E 102:

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and green (positive)

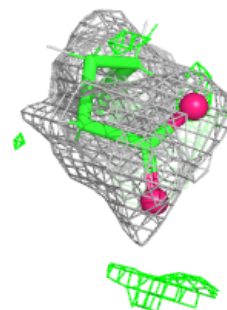
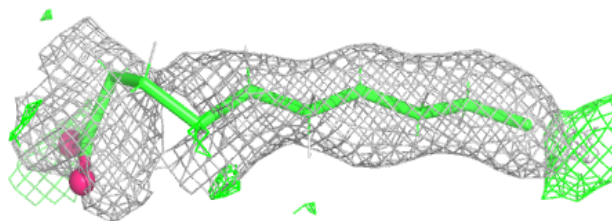
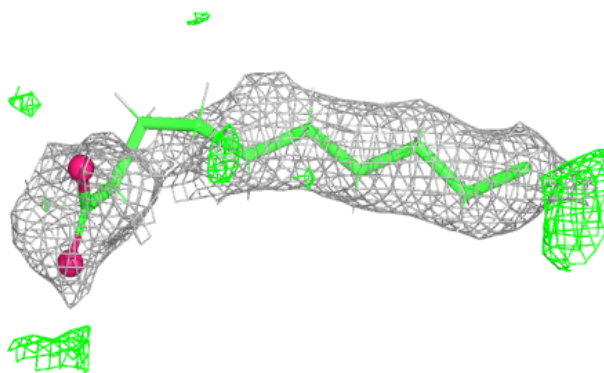
**Electron density around STE E 104:**

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and green (positive)

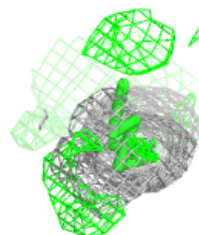
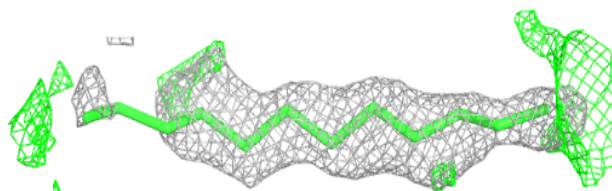
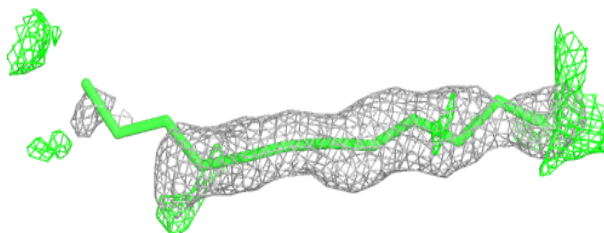


Electron density around STE d 411:

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

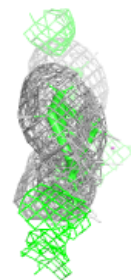
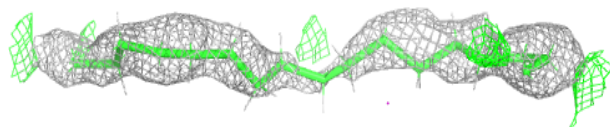
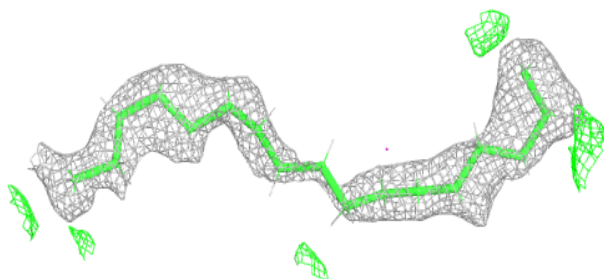
**Electron density around STE E 103:**

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

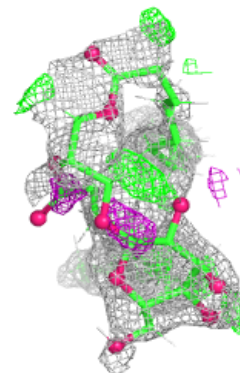
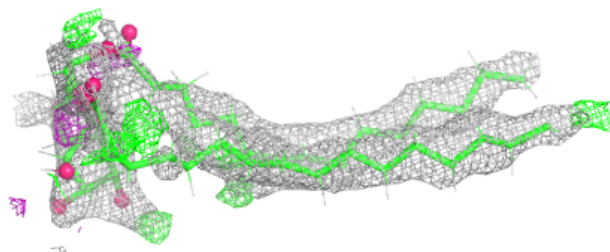
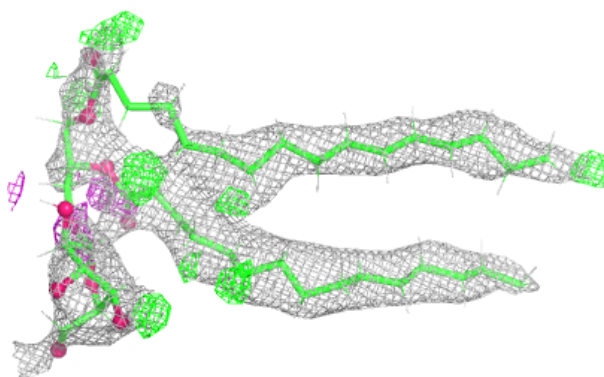


Electron density around STE A 416:

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

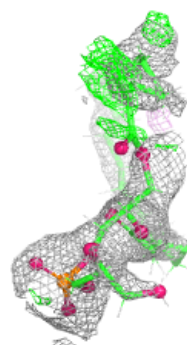
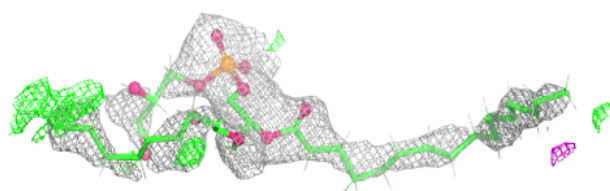
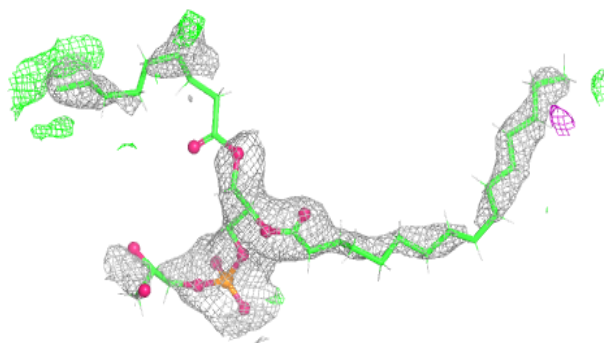
**Electron density around LMG D 408:**

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

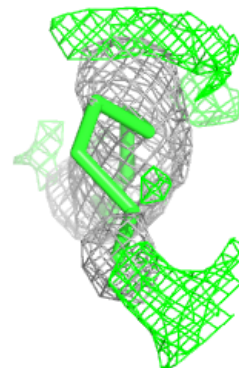
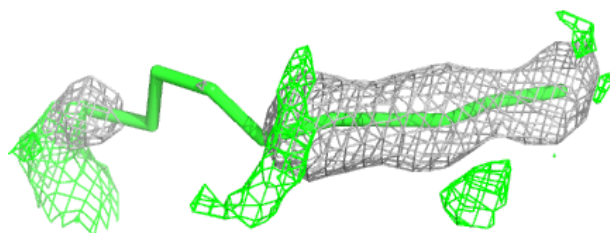
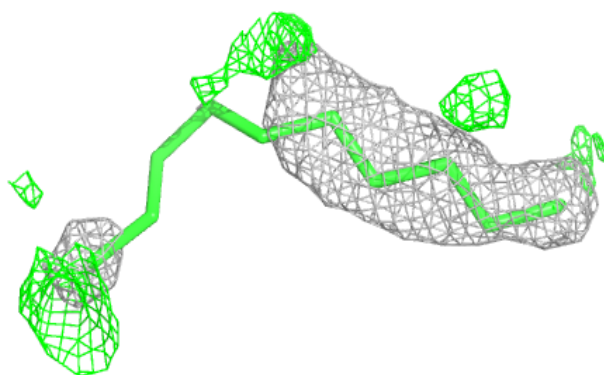


Electron density around LHG a 413:

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

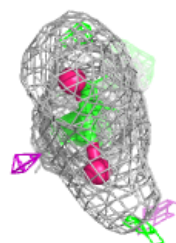
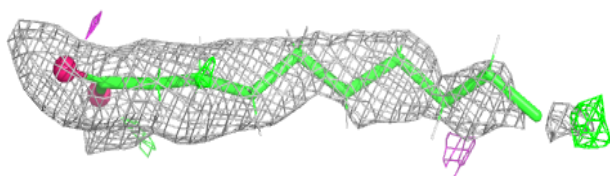
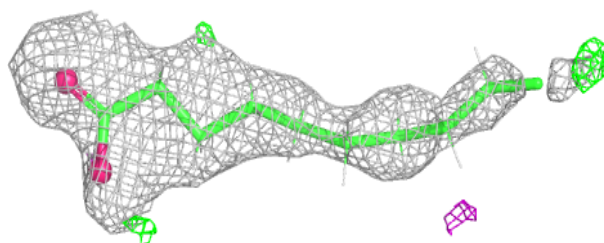
**Electron density around STE d 412:**

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

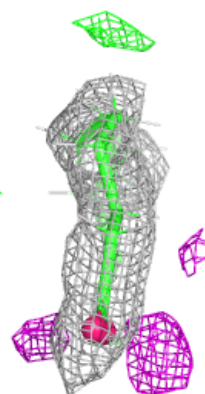
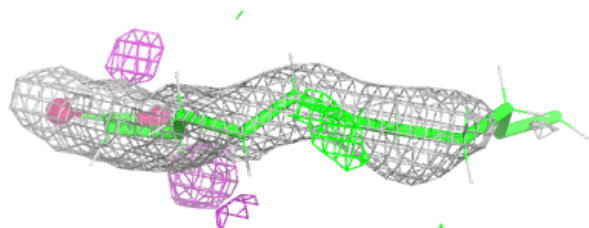
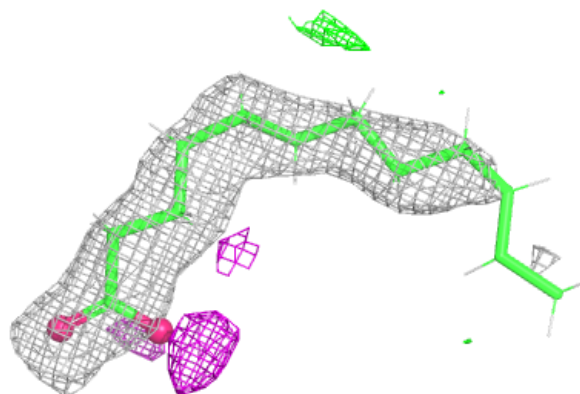


Electron density around STE a 417:

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

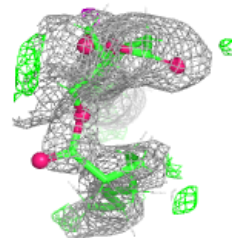
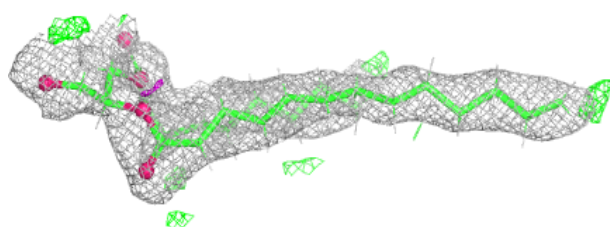
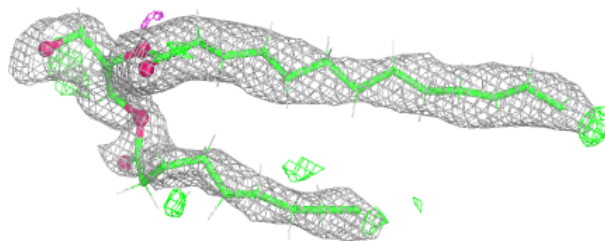
**Electron density around STE C 516:**

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

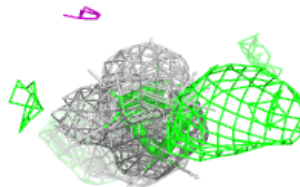
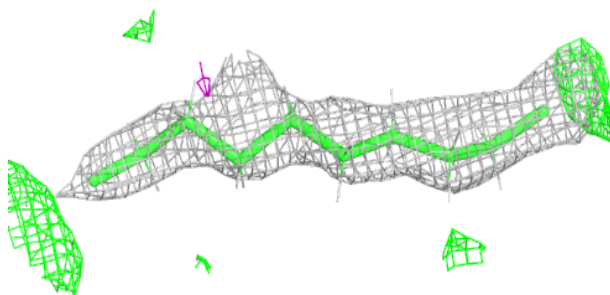
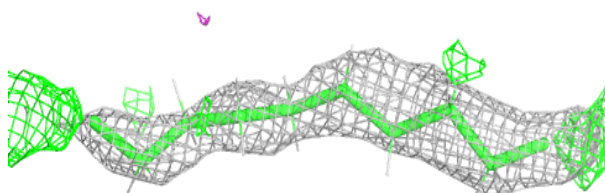


Electron density around LMG c 518:

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

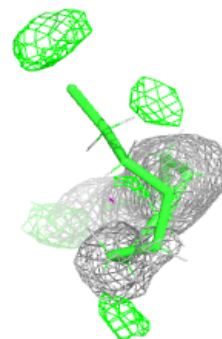
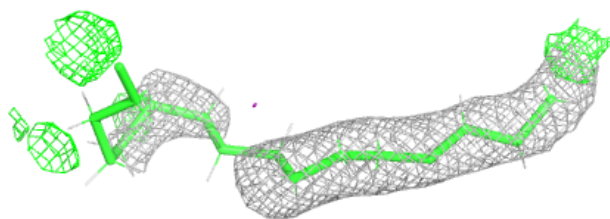
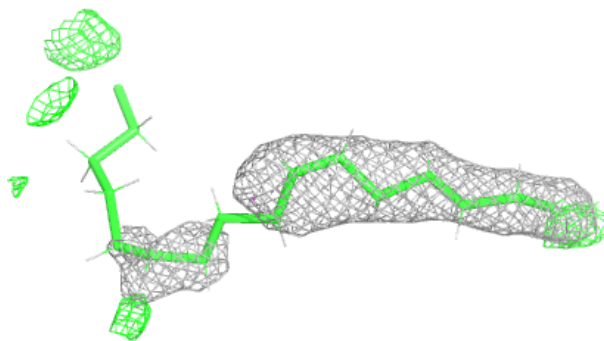
**Electron density around STE a 416:**

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

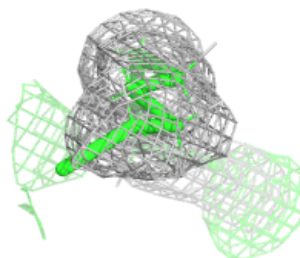
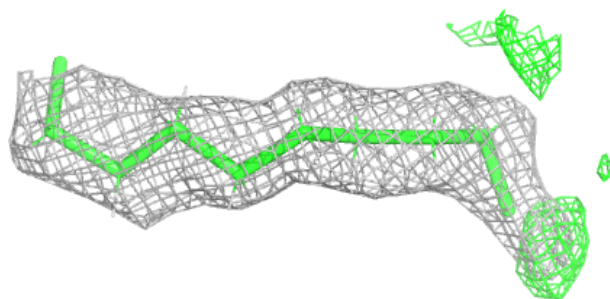
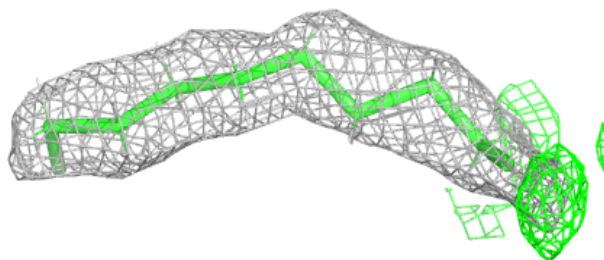


Electron density around STE T 102:

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

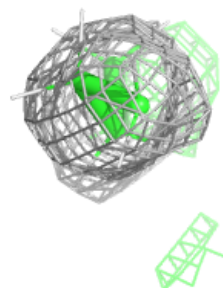
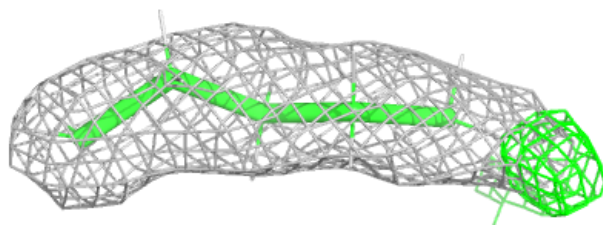
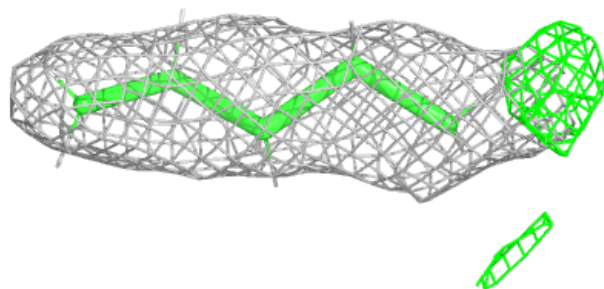
**Electron density around STE b 626:**

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



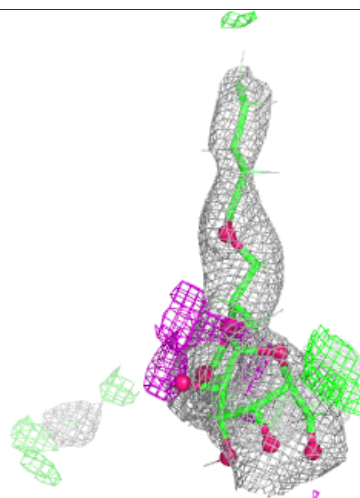
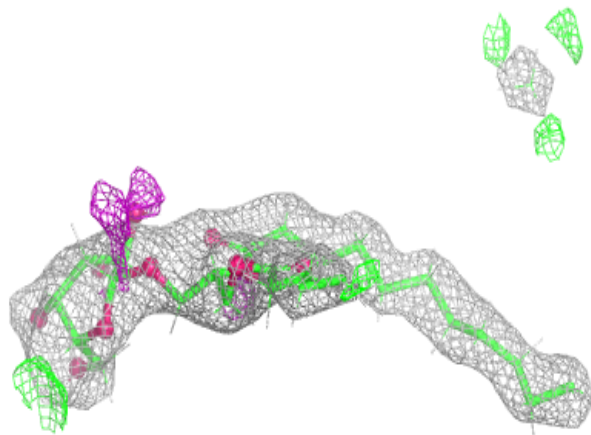
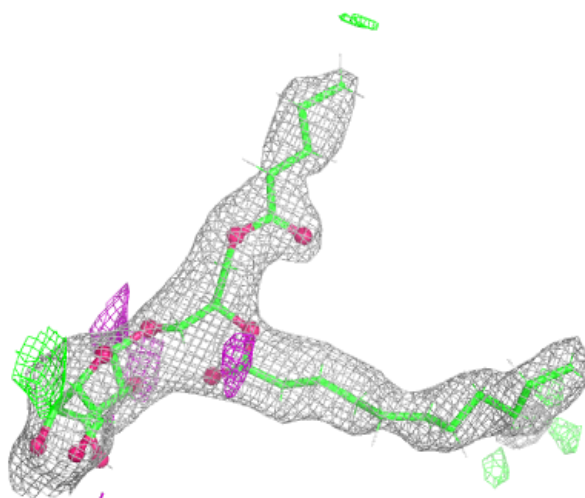
Electron density around STE C 518:

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



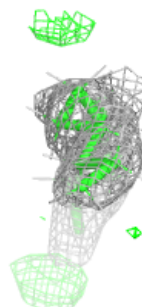
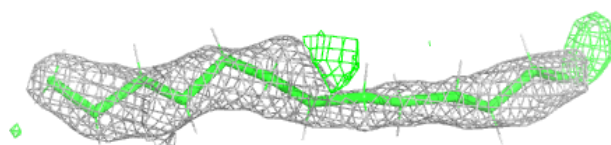
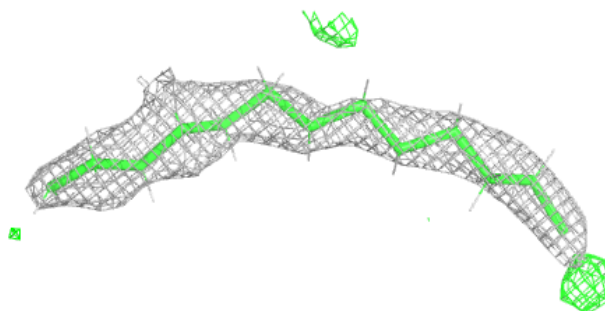
Electron density around LMG C 517:

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

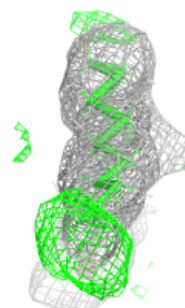
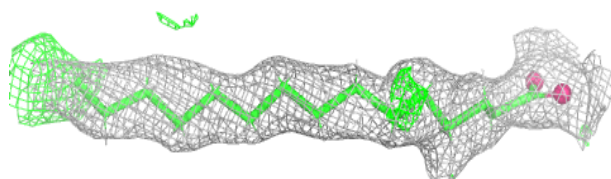
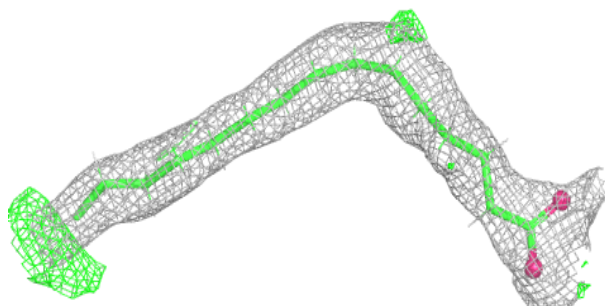


Electron density around STE c 516:

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

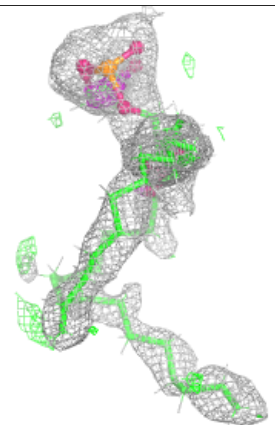
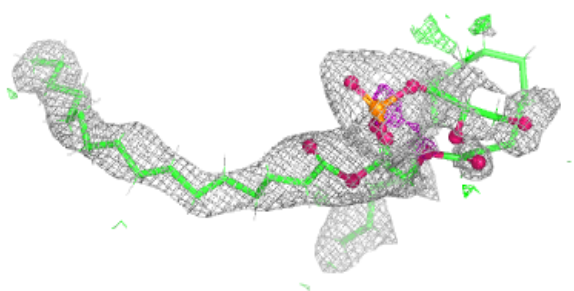
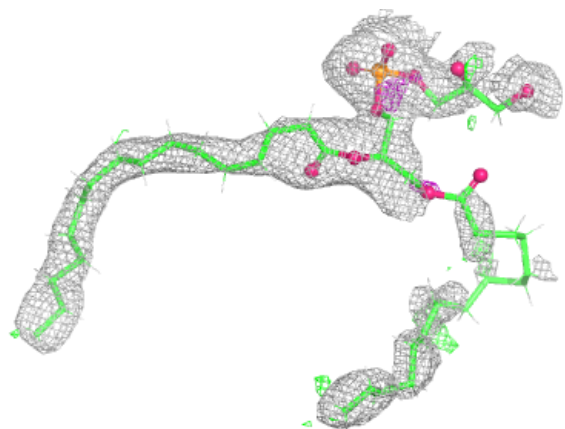
**Electron density around STE d 410:**

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



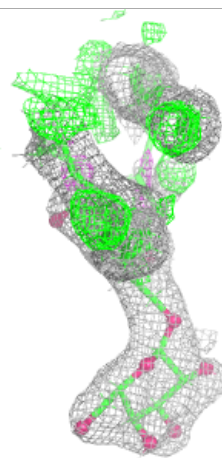
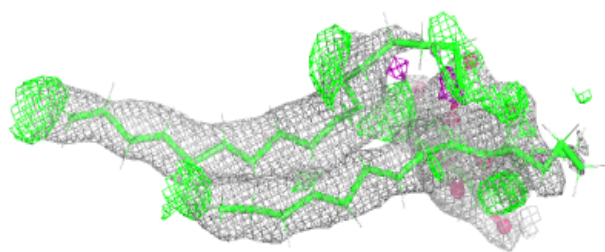
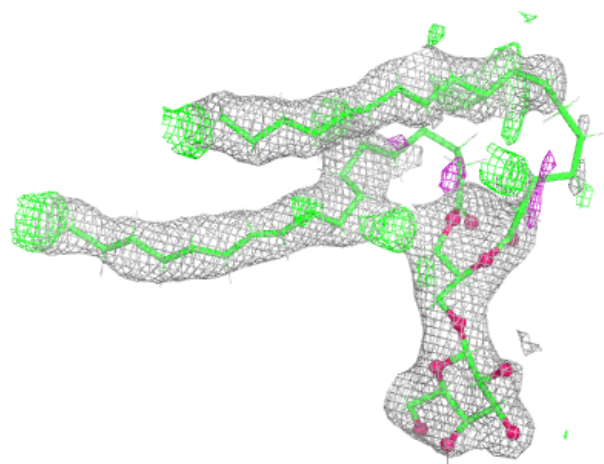
Electron density around LHG E 101:

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



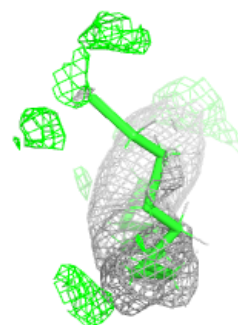
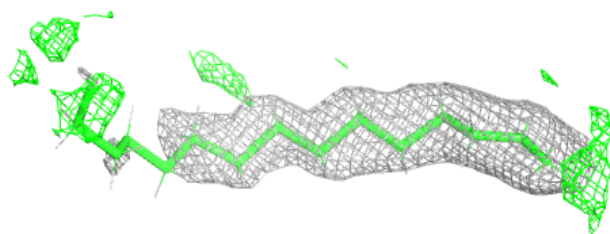
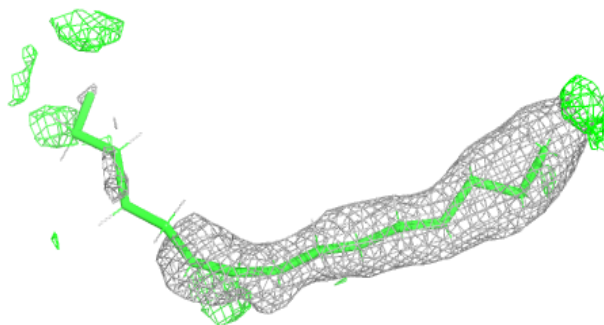
Electron density around LMG a 415:

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

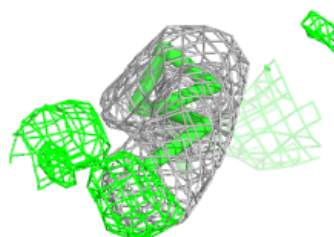
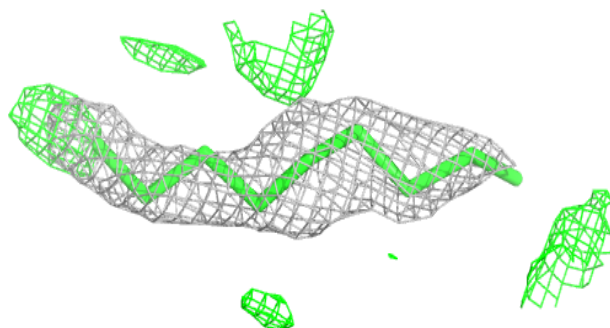
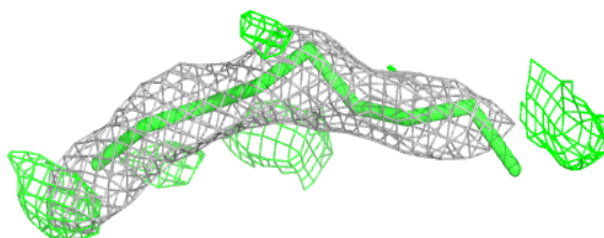


Electron density around STE m 102:

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

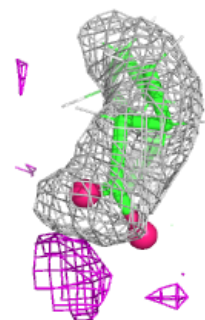
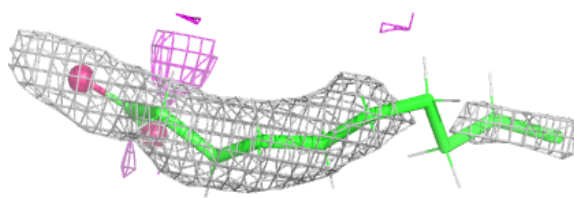
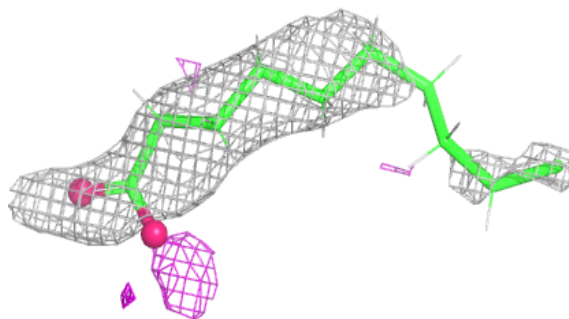
**Electron density around STE A 410:**

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

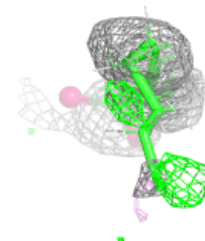
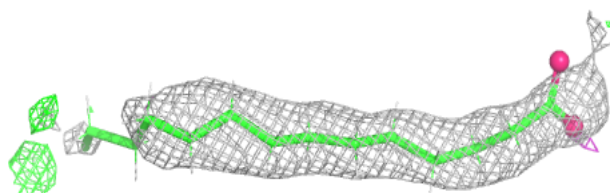
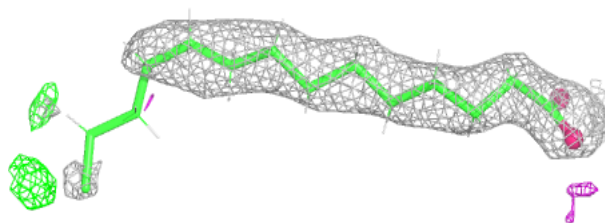


Electron density around STE B 622:

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

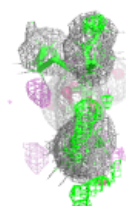
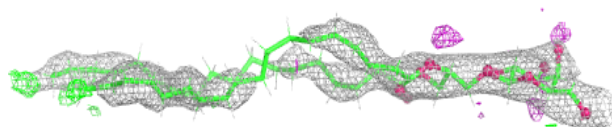
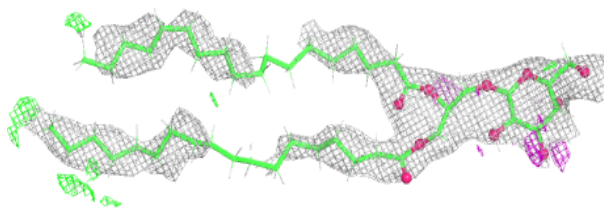
**Electron density around STE b 625:**

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

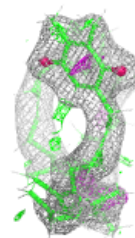
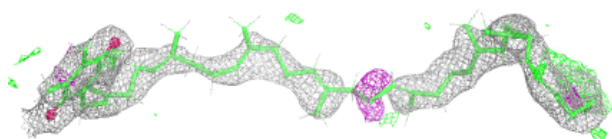
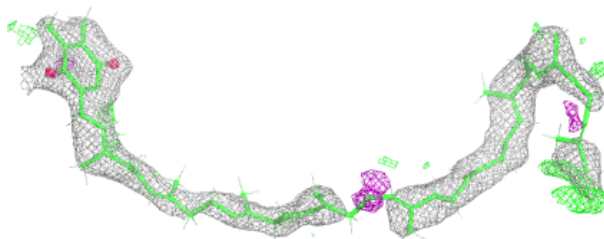


Electron density around LMG b 623:

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

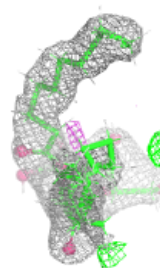
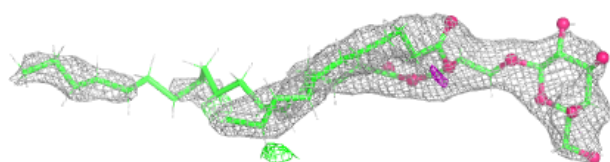
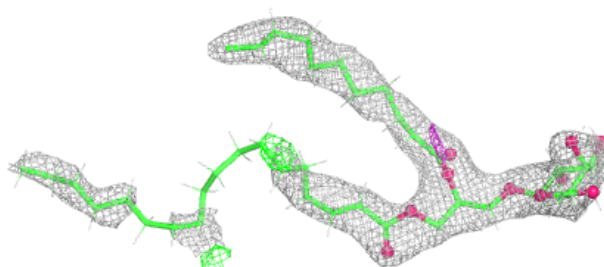
**Electron density around PL9 a 410:**

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

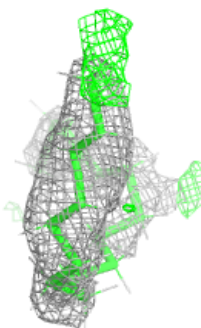
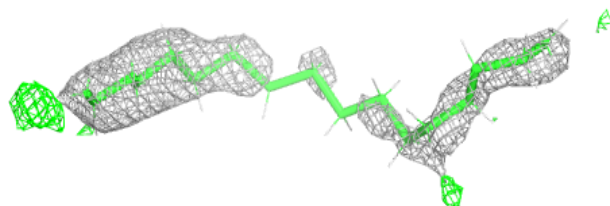
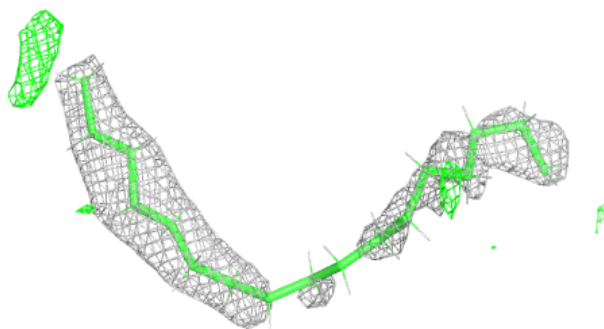


Electron density around LMG c 523:

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

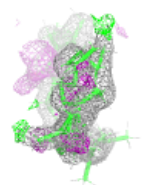
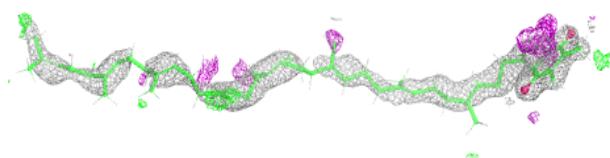
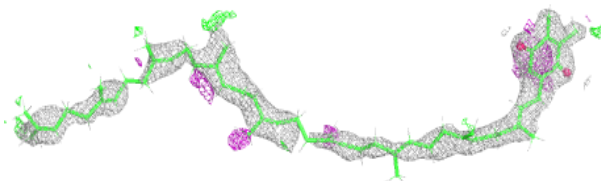
**Electron density around STE Z 101:**

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

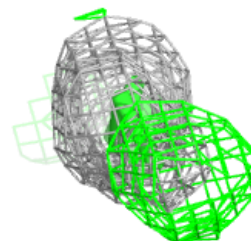
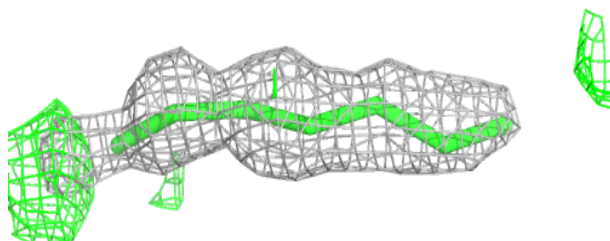
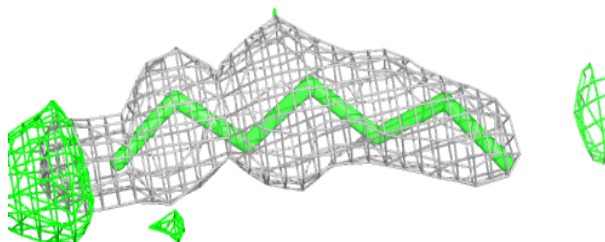


Electron density around PL9 A 409:

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

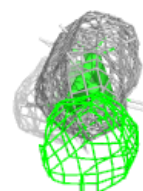
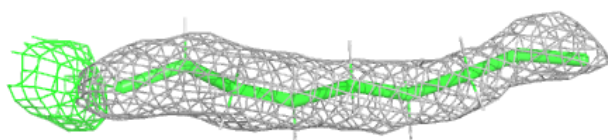
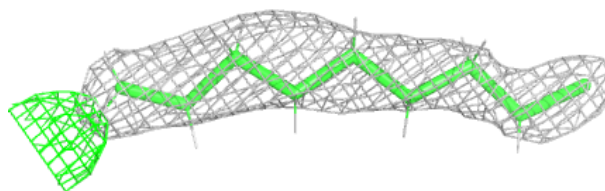
**Electron density around STE C 519:**

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

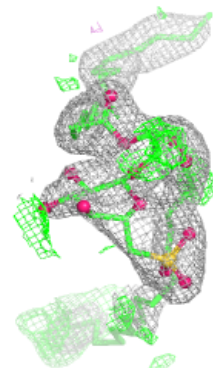
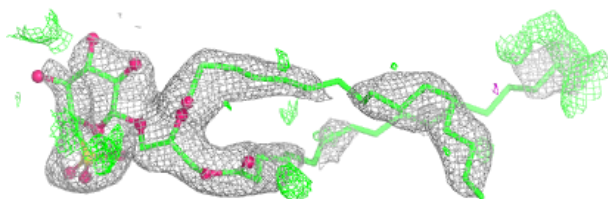
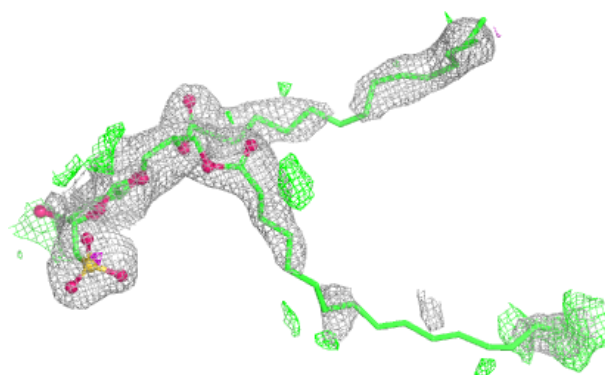


Electron density around STE z 101:

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

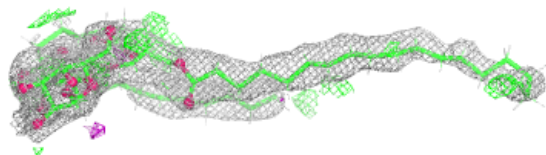
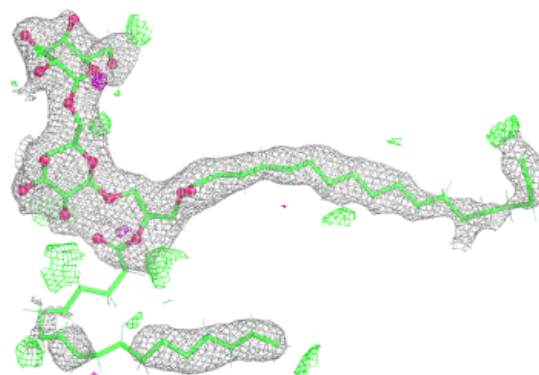
**Electron density around SQD A 413:**

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

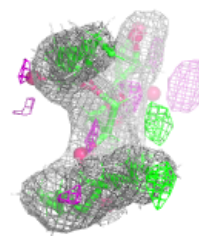
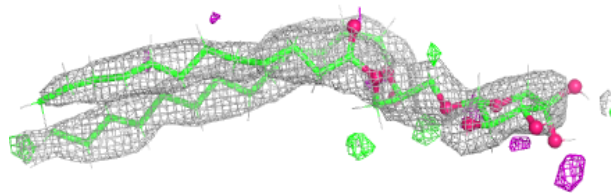
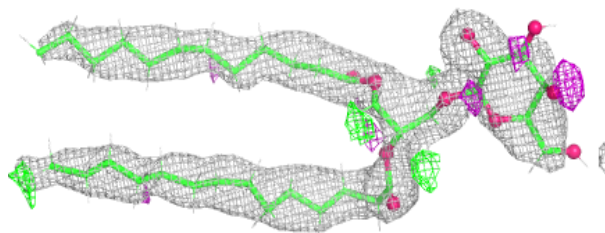


Electron density around DGD A 414:

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

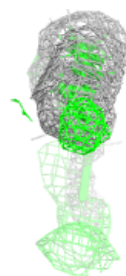
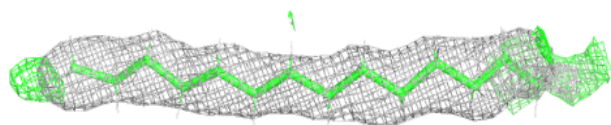
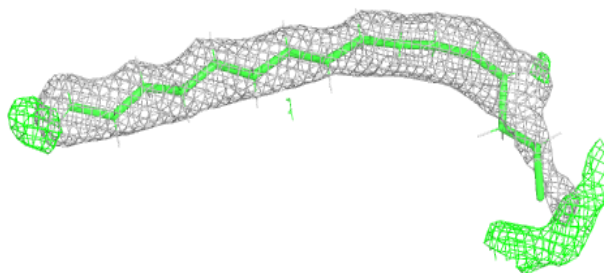
**Electron density around LMG B 620:**

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

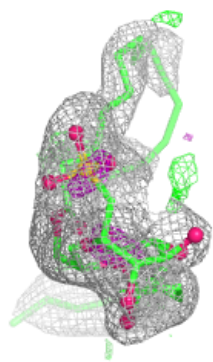
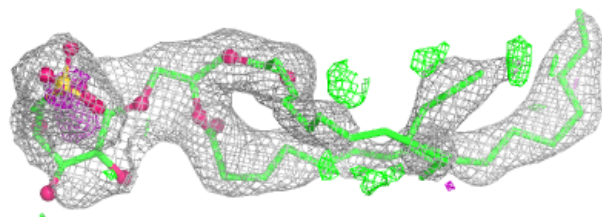
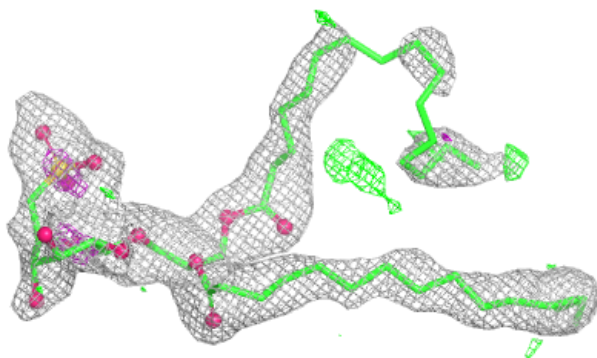


Electron density around STE C 526:

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

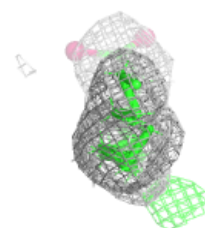
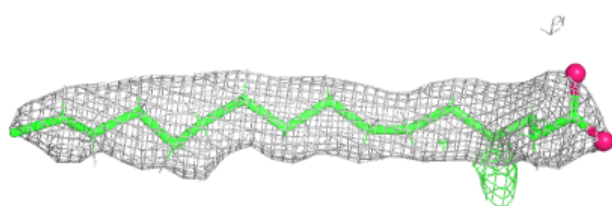
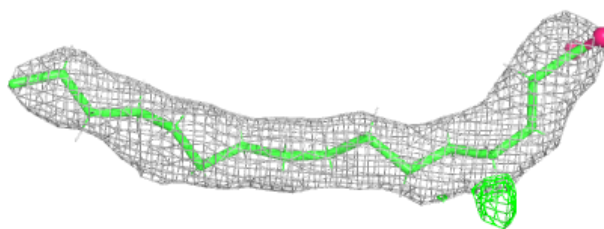
**Electron density around SQD a 414:**

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

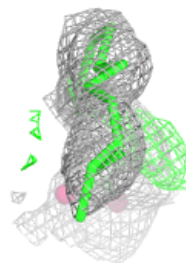
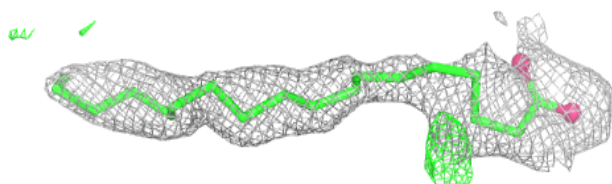
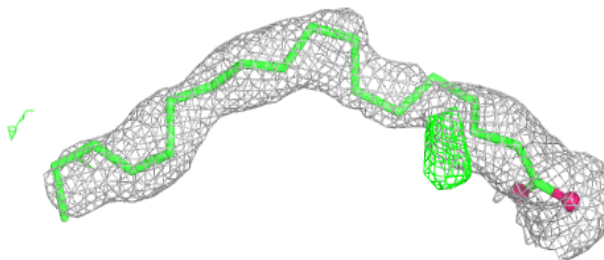


Electron density around STE t 103:

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

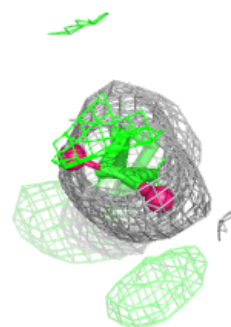
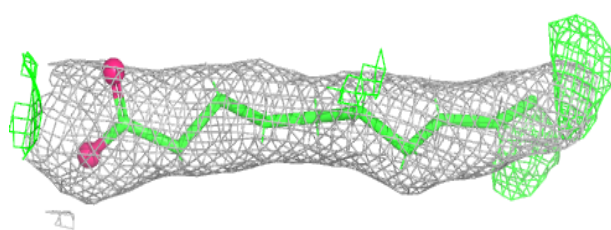
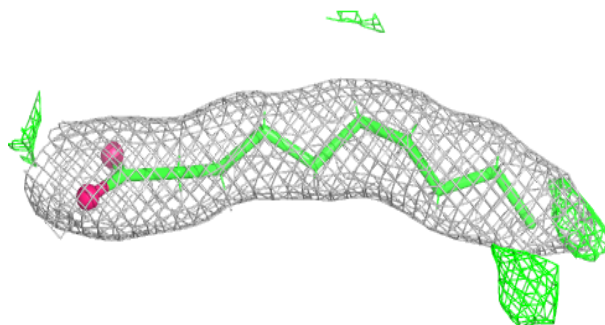
**Electron density around STE b 624:**

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

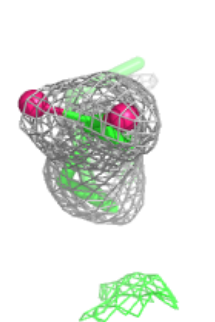
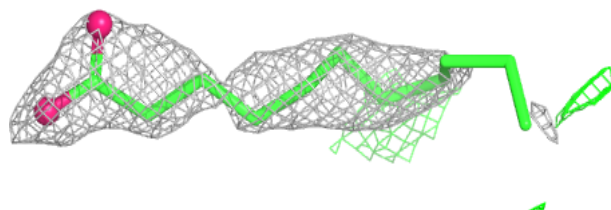
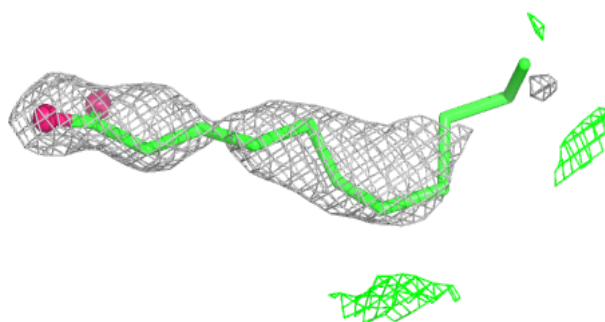


Electron density around STE j 101:

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

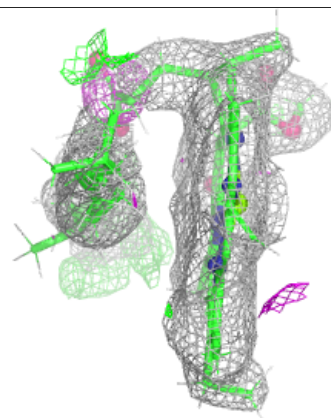
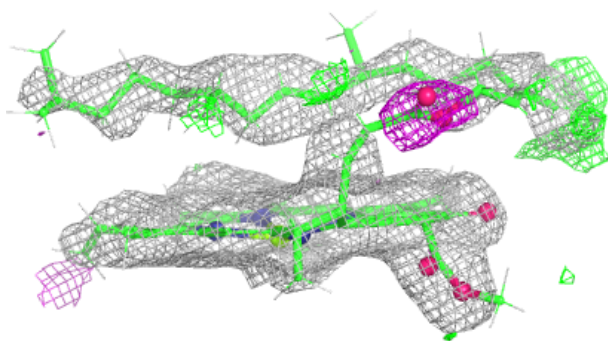
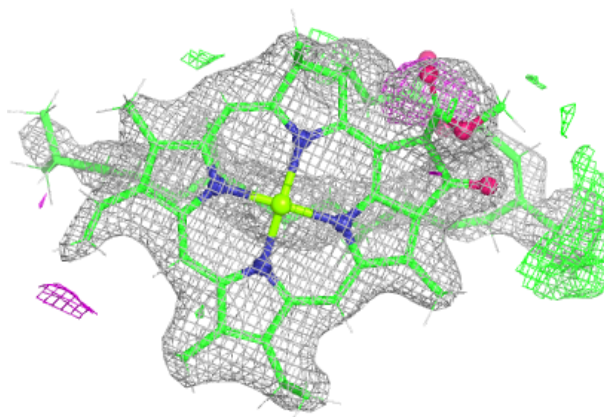
**Electron density around STE e 104:**

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



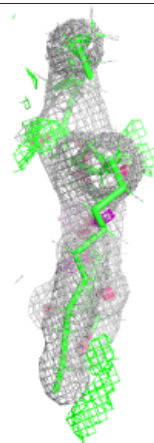
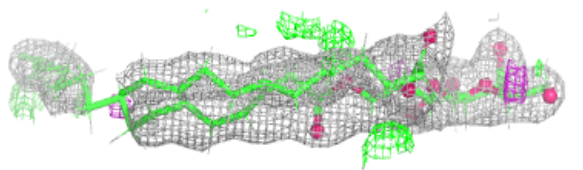
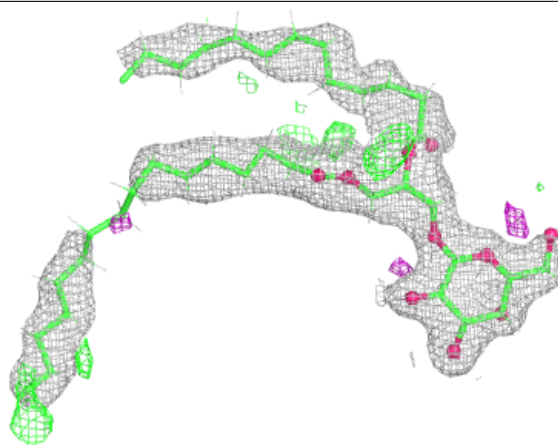
Electron density around CLA h 101:

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



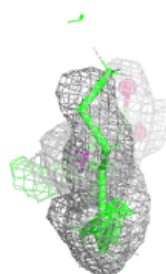
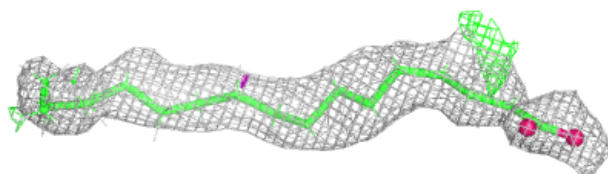
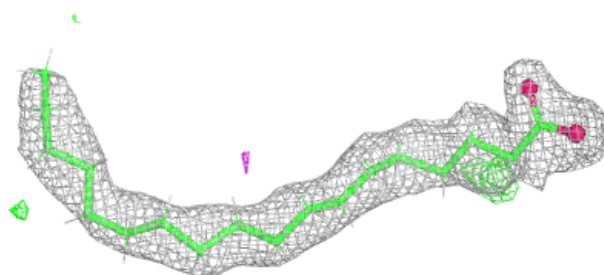
Electron density around LMG C 524:

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

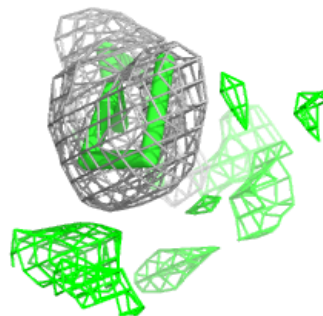
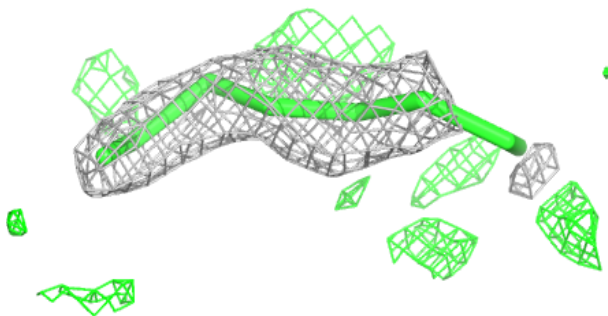
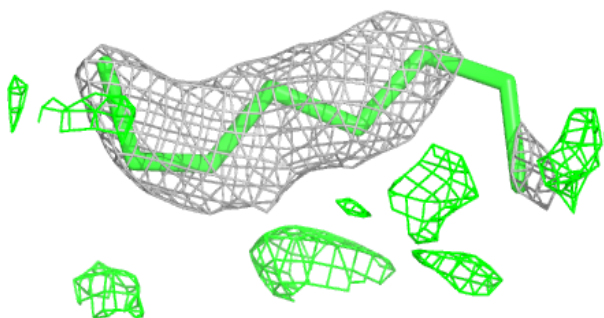


Electron density around STE b 622:

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

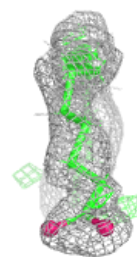
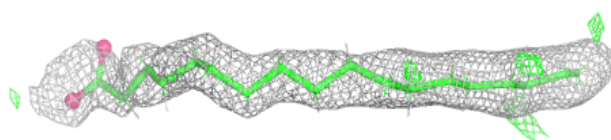
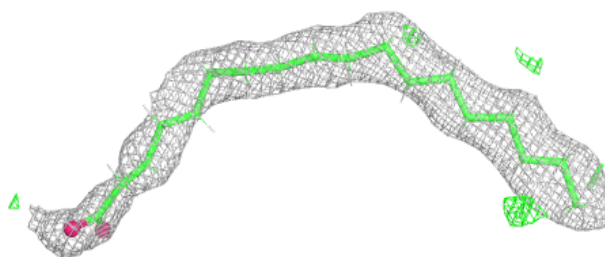
**Electron density around STE e 102:**

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

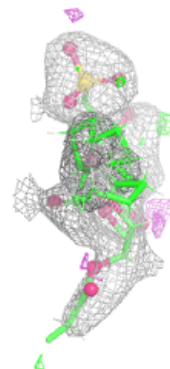
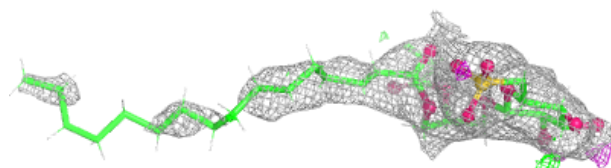
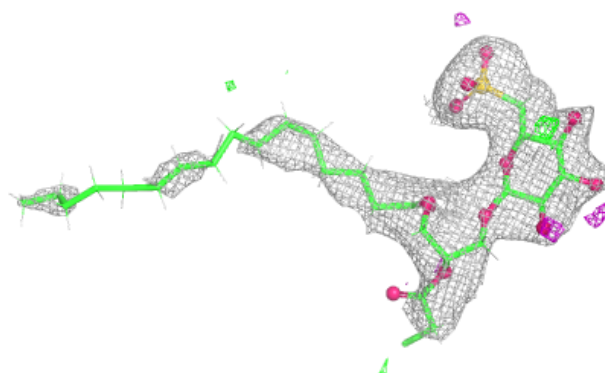


Electron density around STE x 102:

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

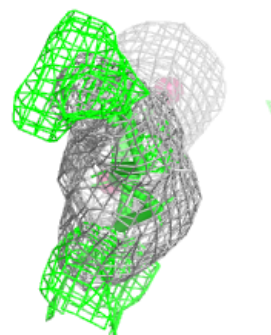
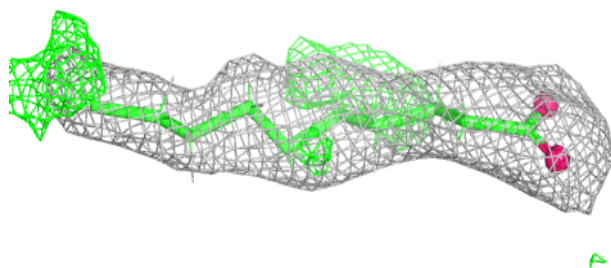
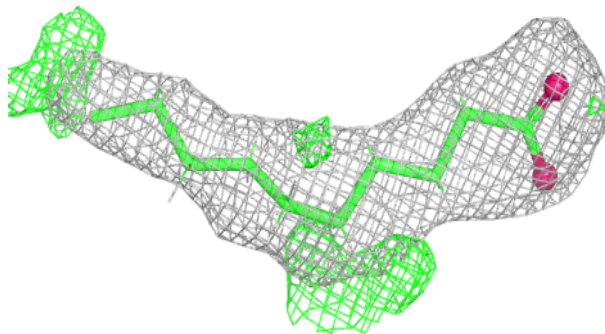
**Electron density around SQD f 102:**

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

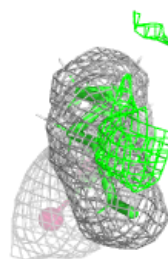
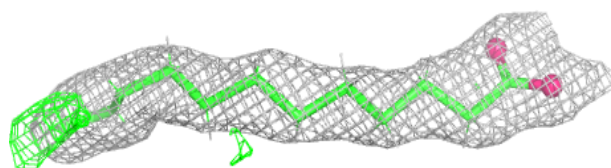
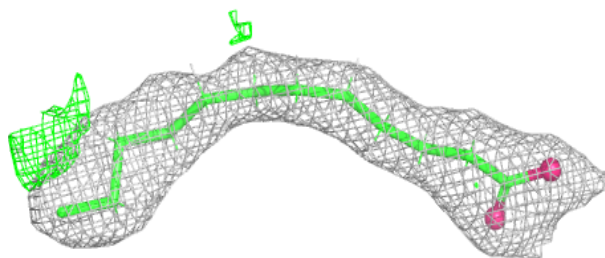


Electron density around STE C 525:

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

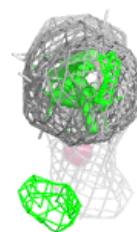
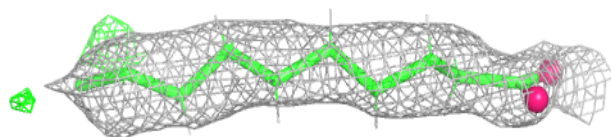
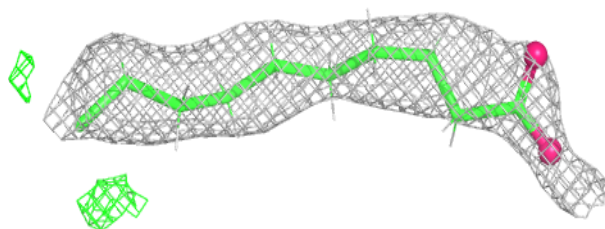
**Electron density around STE t 102:**

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

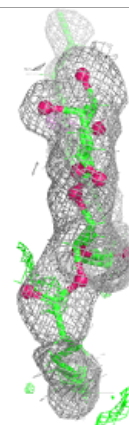
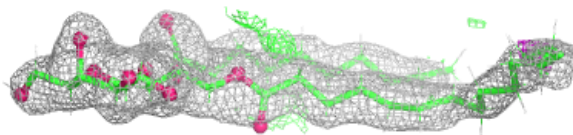
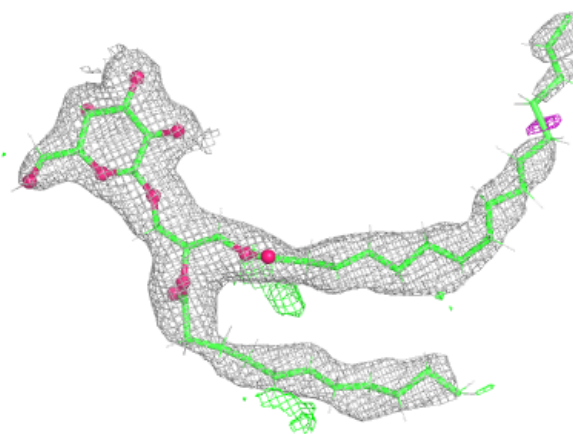


Electron density around STE m 101:

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

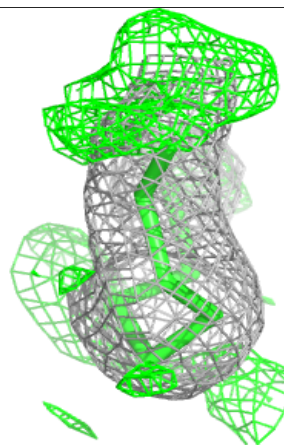
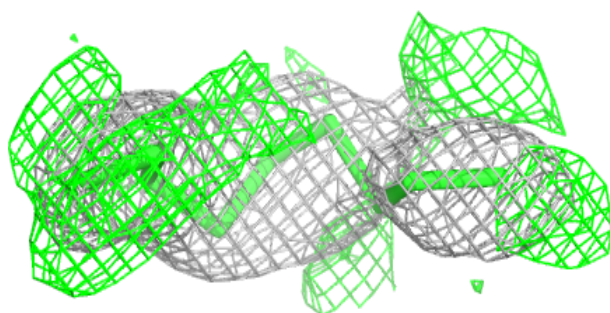
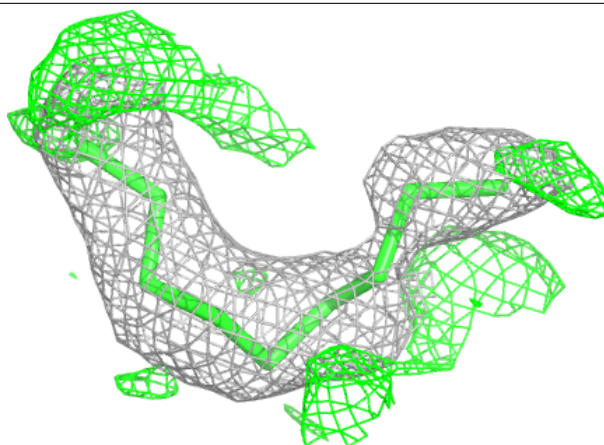
**Electron density around LMG c 522:**

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

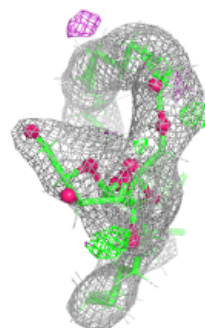
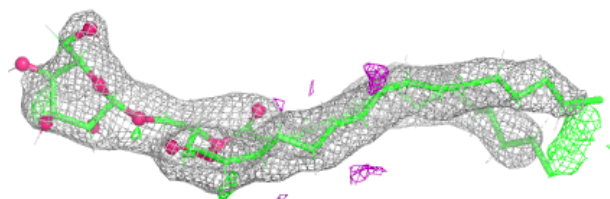
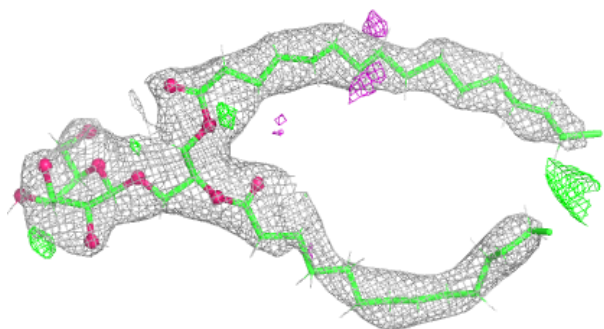


Electron density around STE D 414:

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

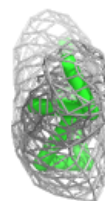
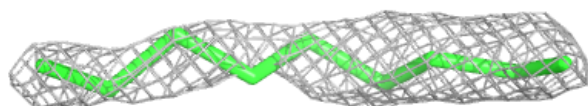
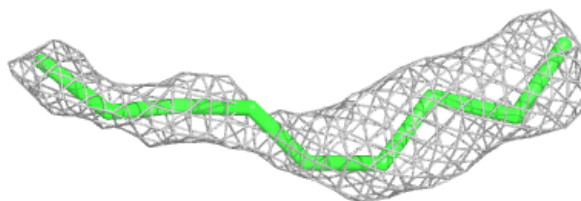
**Electron density around LMG c 524:**

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

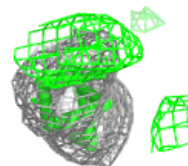
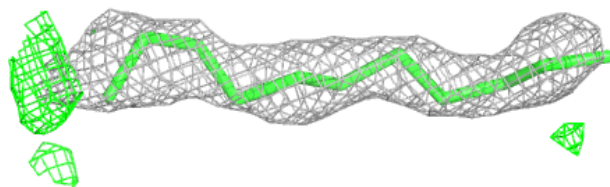
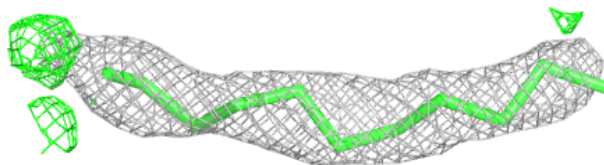


Electron density around STE e 103:

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

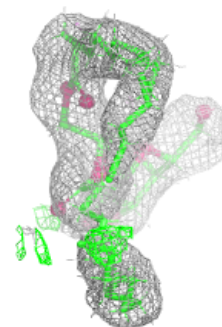
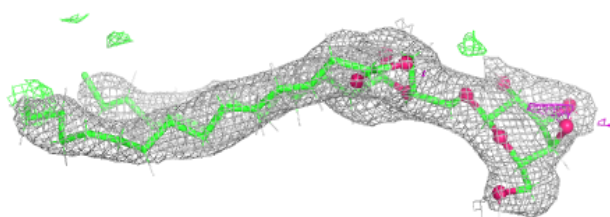
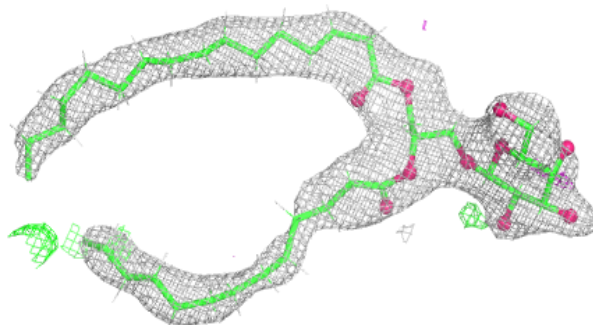
**Electron density around STE b 627:**

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

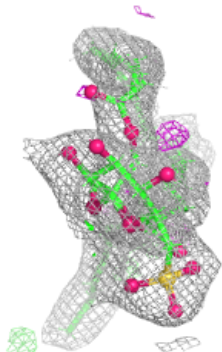
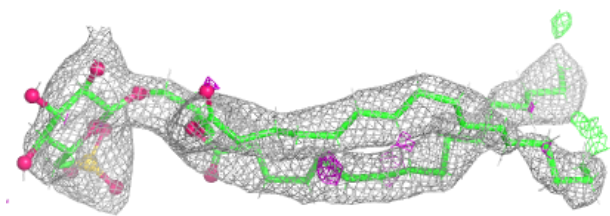
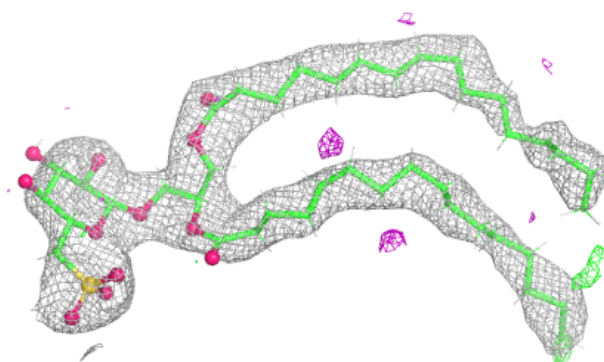


Electron density around LMG A 411:

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

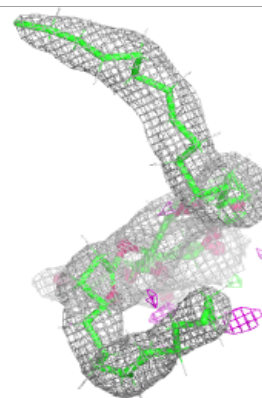
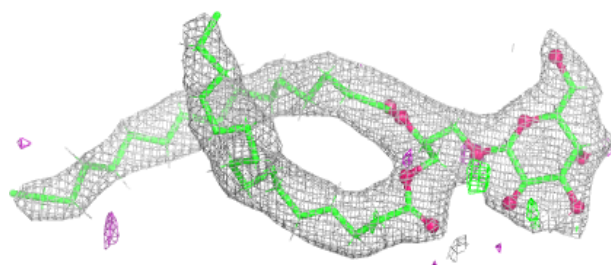
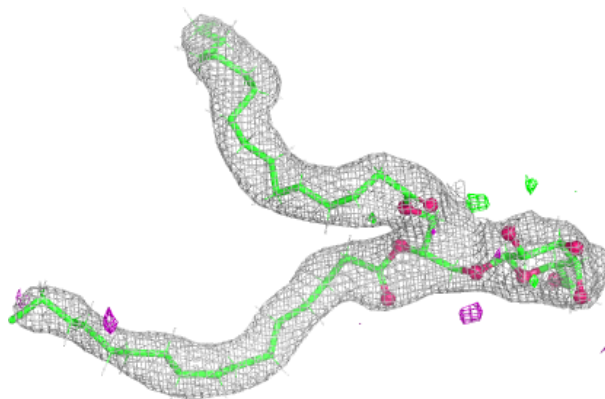
**Electron density around SQD 1 101:**

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

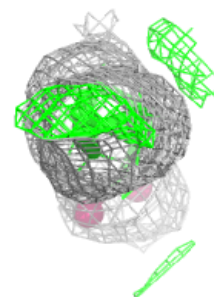
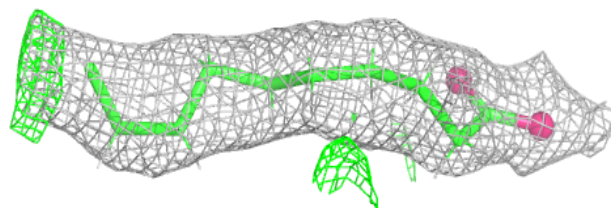


Electron density around LMG b 621:

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

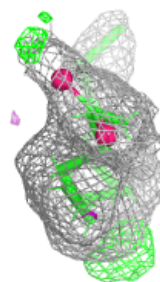
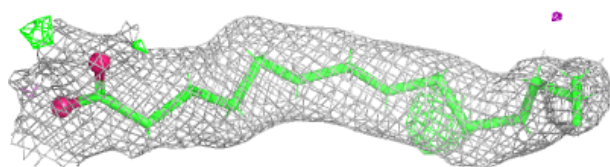
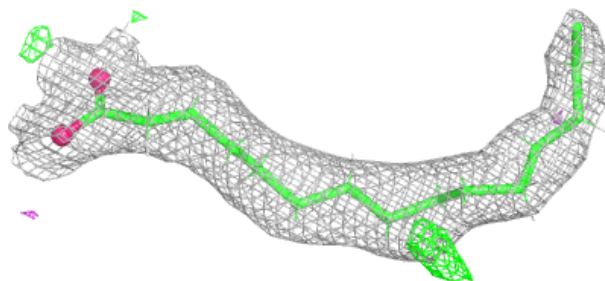
**Electron density around STE J 101:**

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

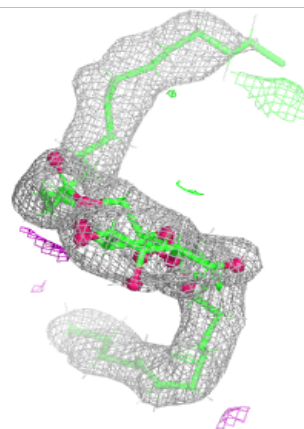
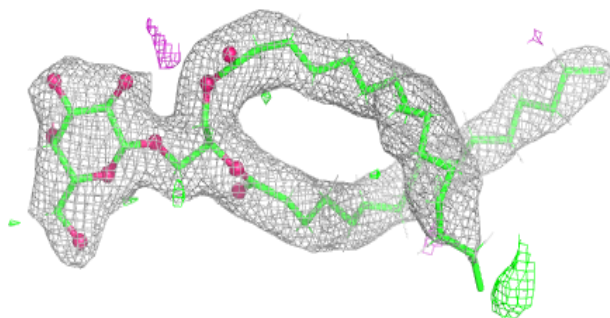
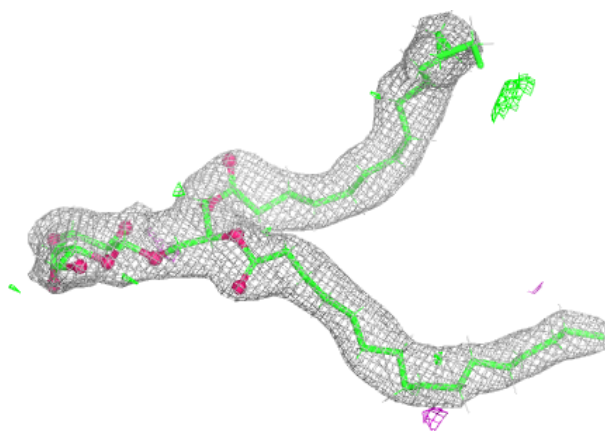


Electron density around STE B 621:

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

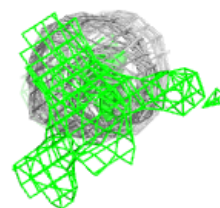
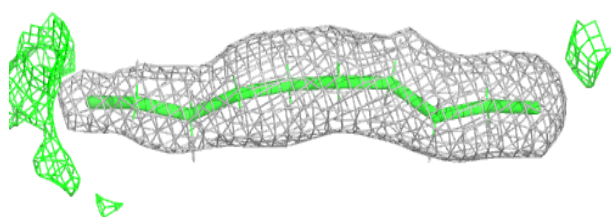
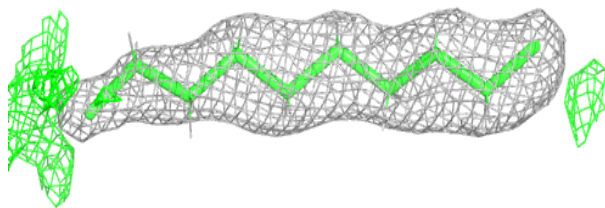
**Electron density around LMG M 101:**

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

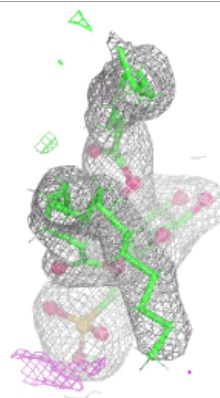
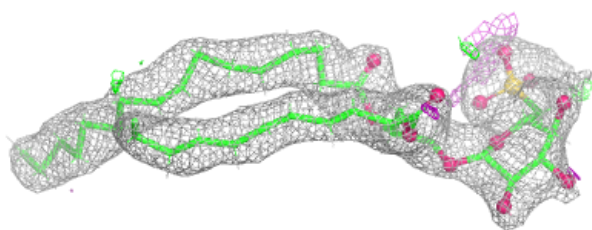
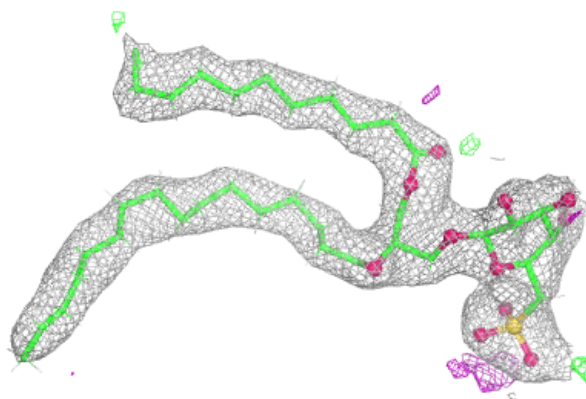


Electron density around STE M 103:

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

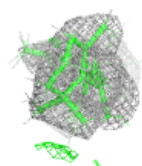
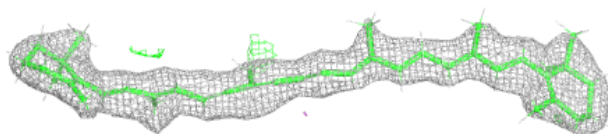
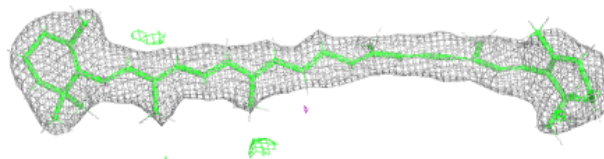
**Electron density around SQD b 620:**

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

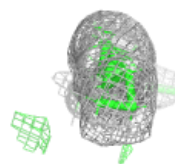
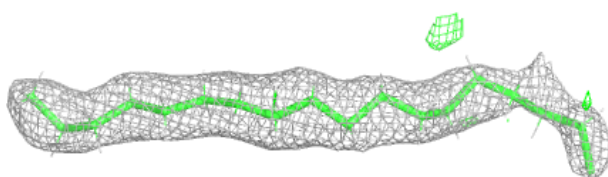
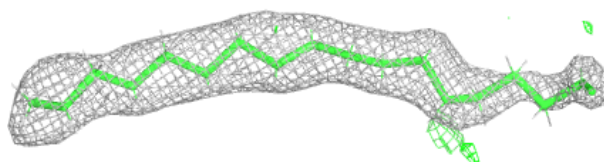


Electron density around BCR C 514:

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

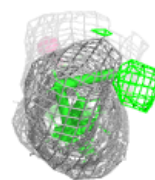
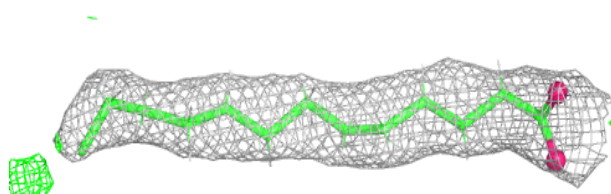
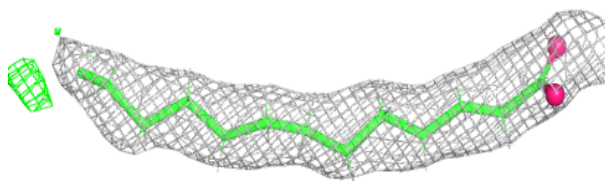
**Electron density around STE I 103:**

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

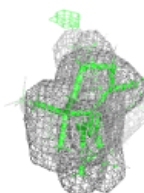
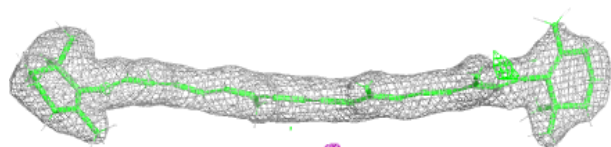
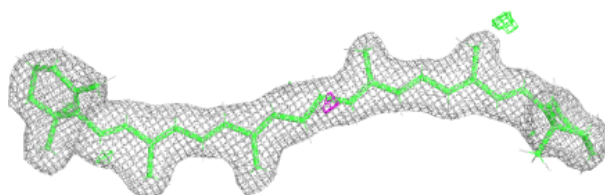


Electron density around STE M 102:

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

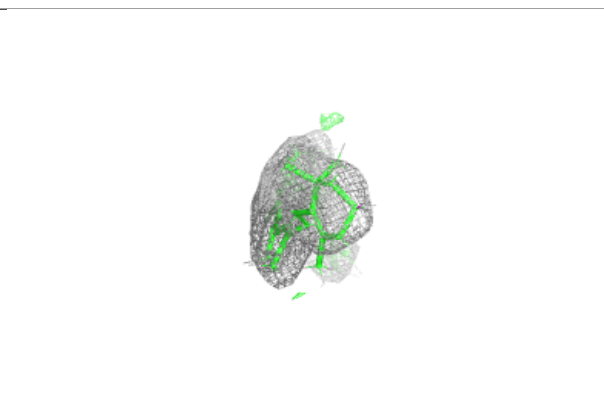
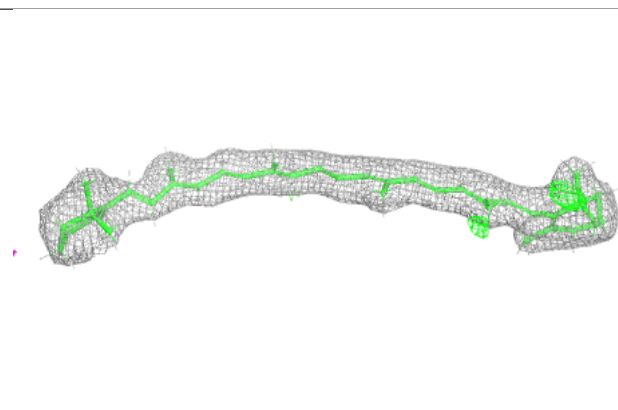
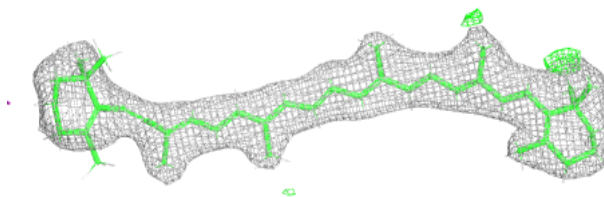
**Electron density around BCR K 101:**

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

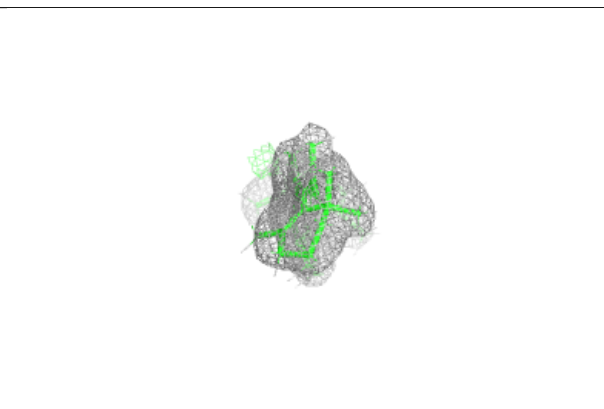
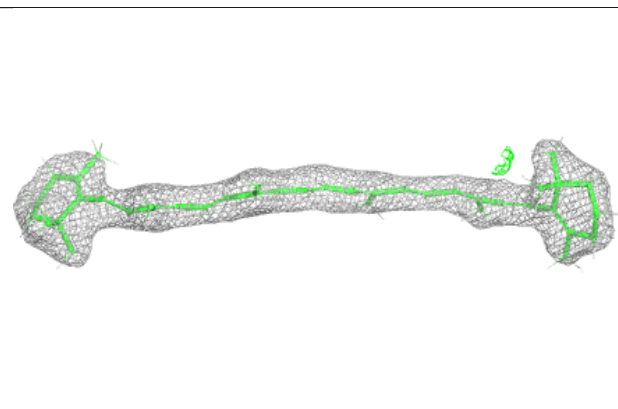
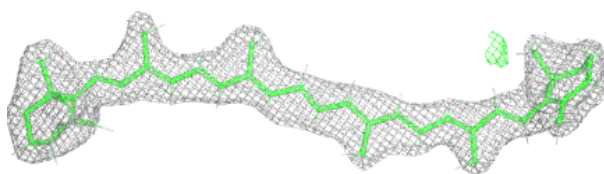


Electron density around BCR d 404:

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

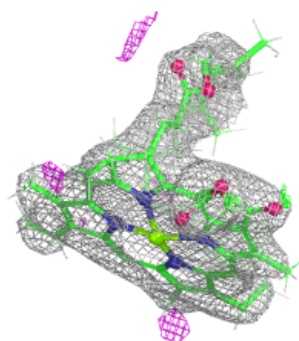
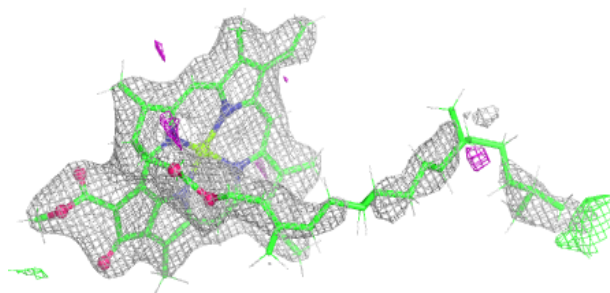
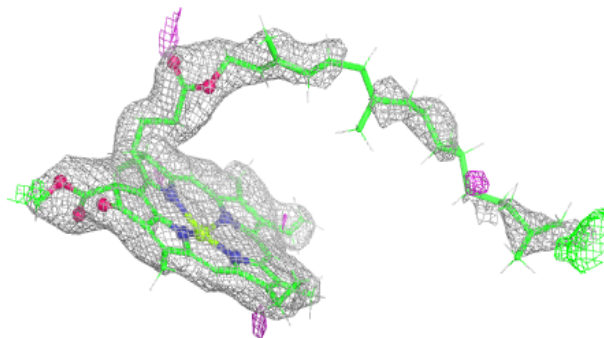
**Electron density around BCR k 101:**

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

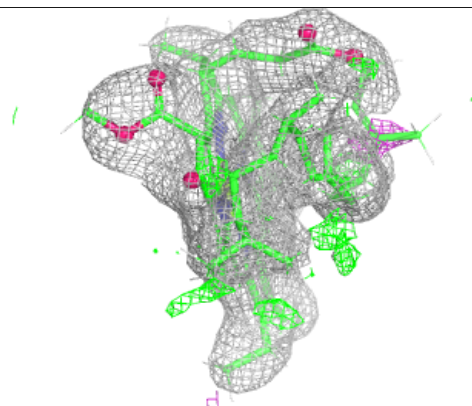
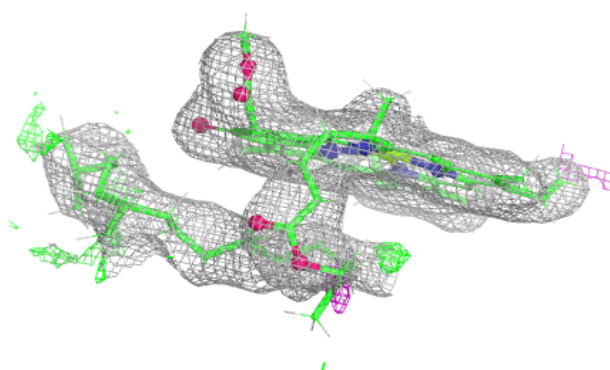
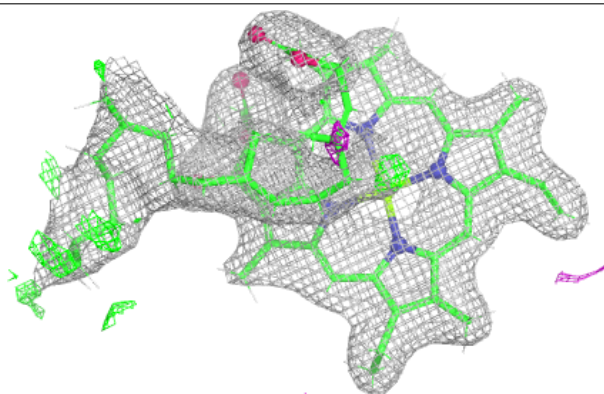


Electron density around CLA c 513:

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

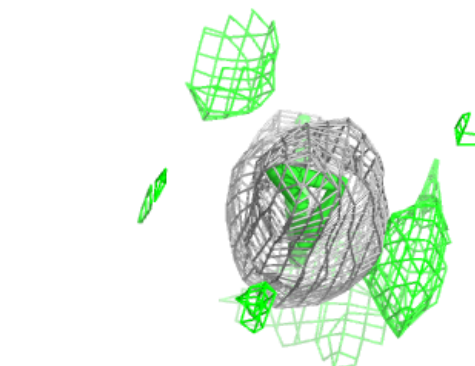
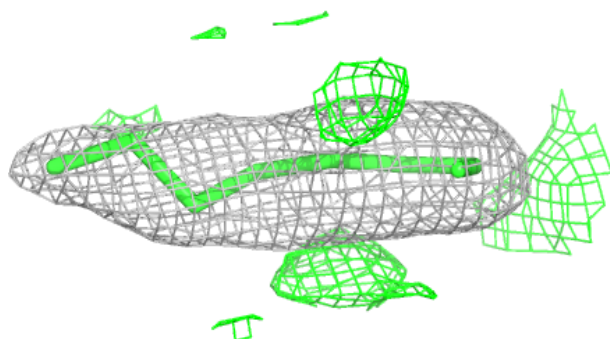
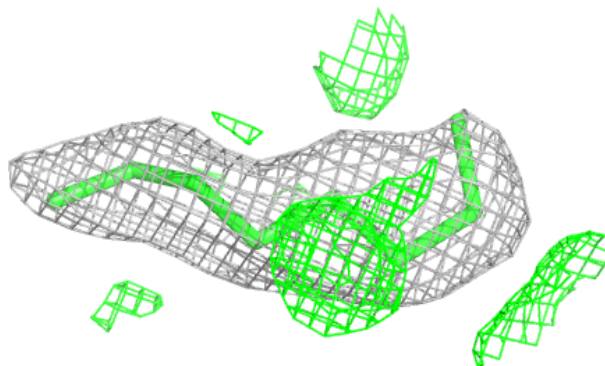
**Electron density around CLA B 601:**

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

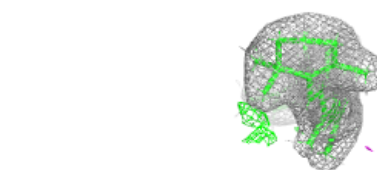
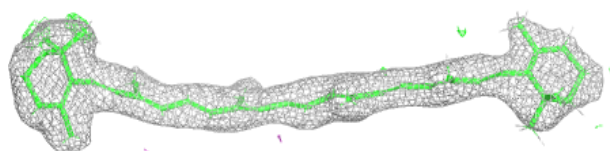
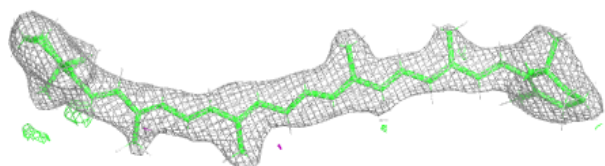


Electron density around STE A 415:

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

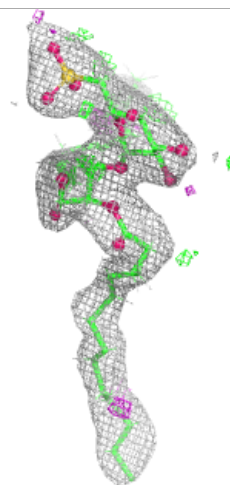
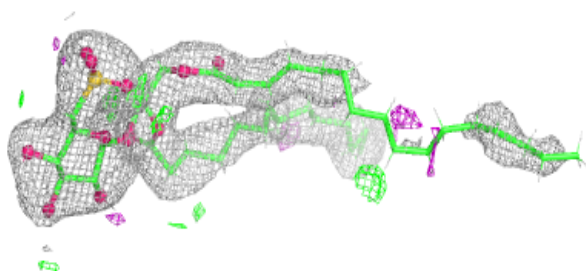
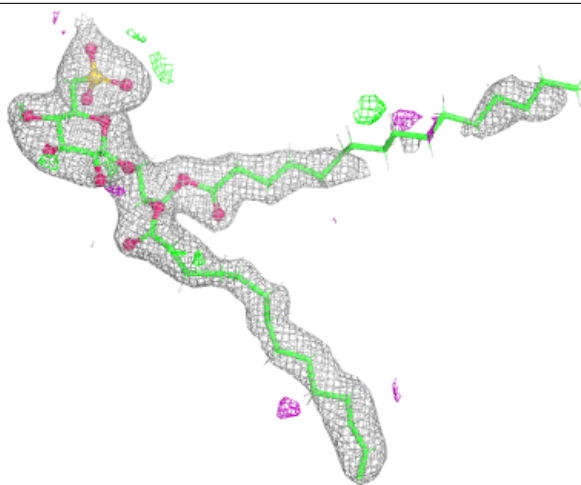
**Electron density around BCR x 101:**

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



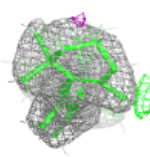
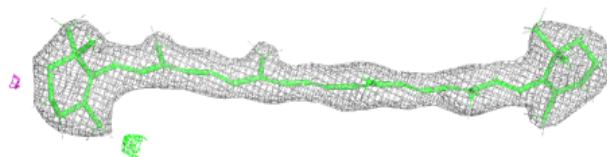
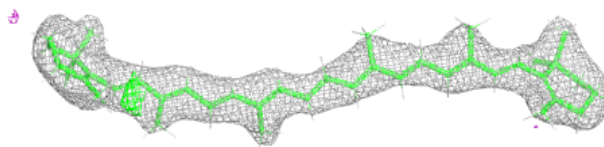
Electron density around SQD A 412:

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

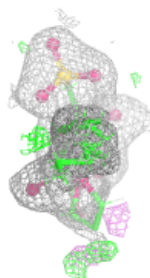
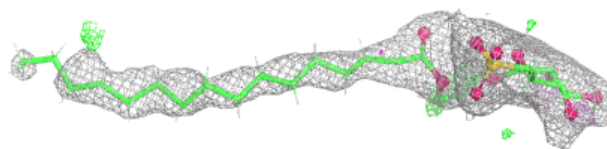
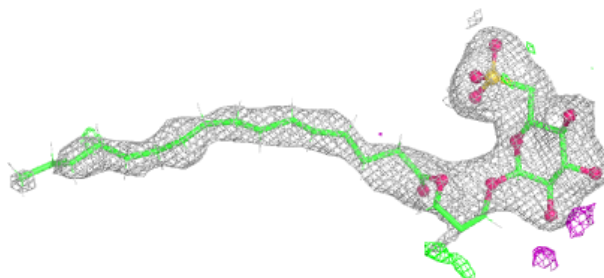


Electron density around BCR c 514:

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

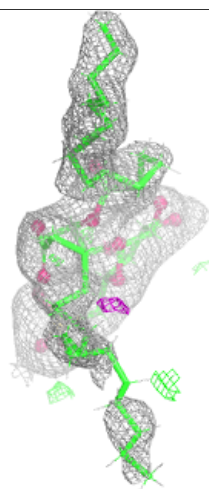
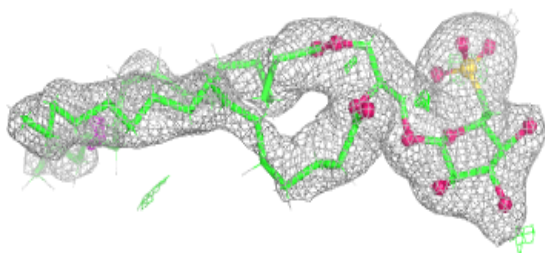
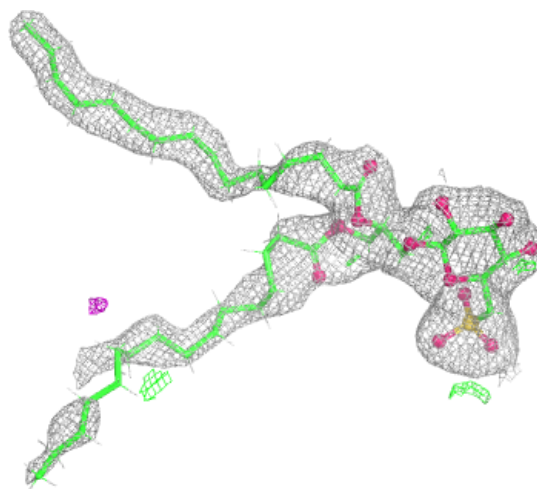
**Electron density around SQD F 102:**

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



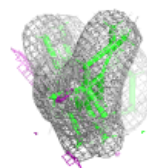
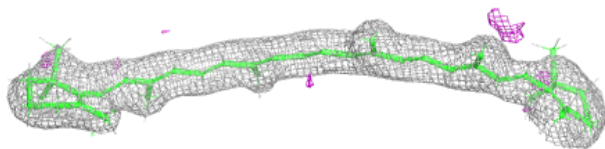
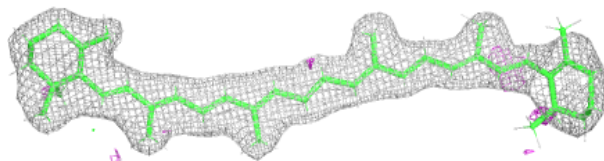
Electron density around SQD a 412:

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

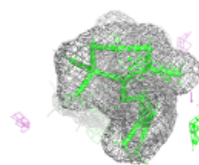
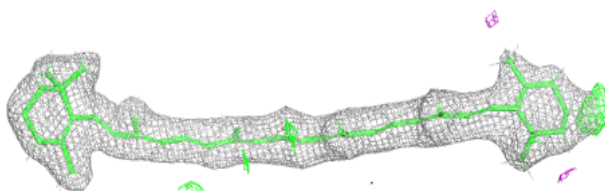
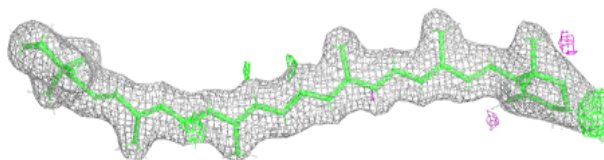


Electron density around BCR D 406:

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

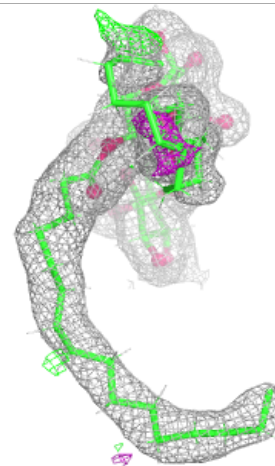
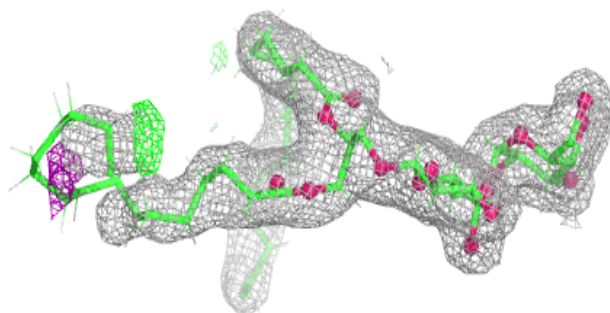
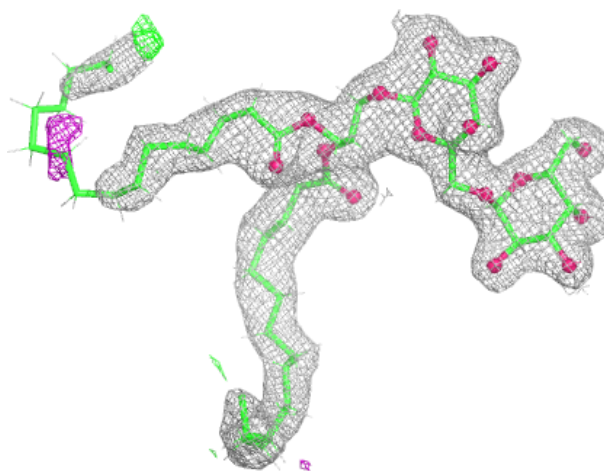
**Electron density around BCR H 101:**

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



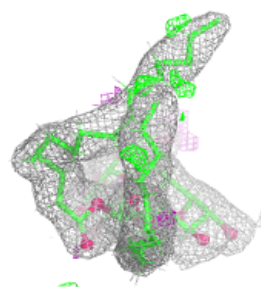
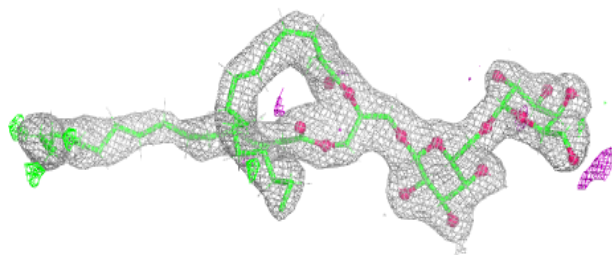
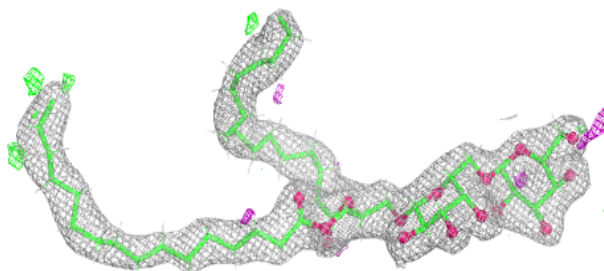
Electron density around DGD C 522:

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

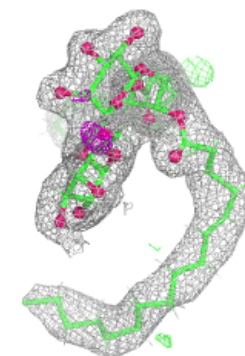
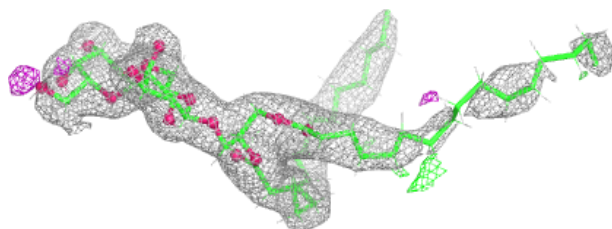


Electron density around DGD H 102:

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

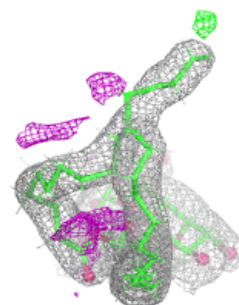
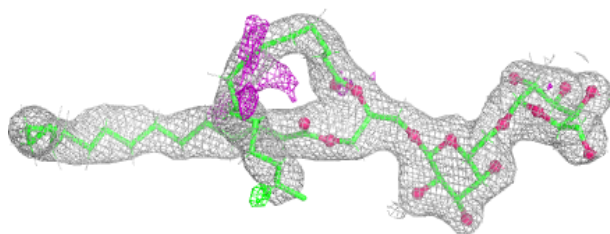
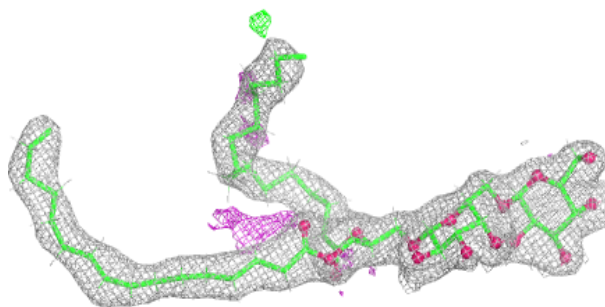
**Electron density around DGD c 520:**

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



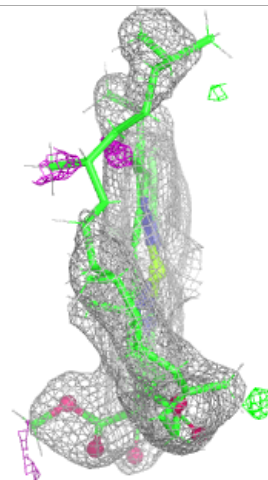
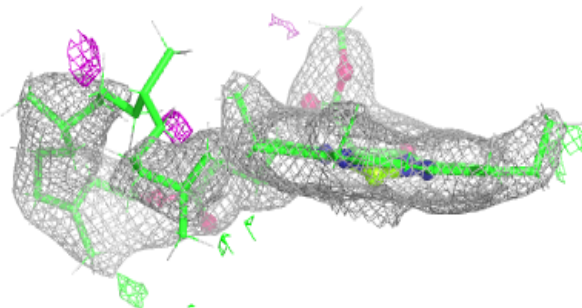
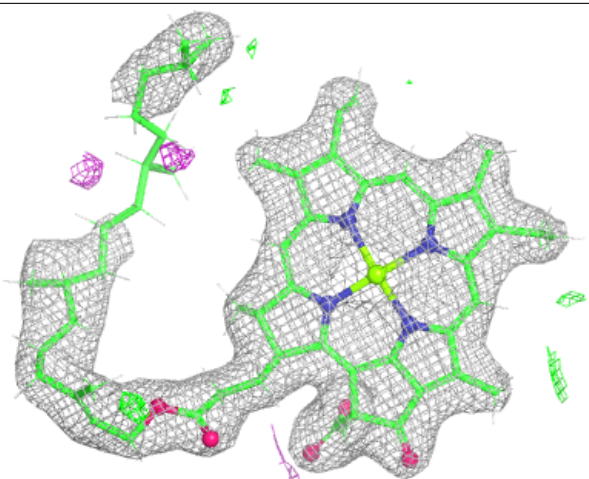
Electron density around DGD h 102:

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



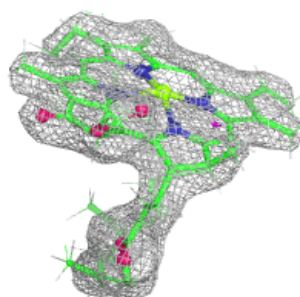
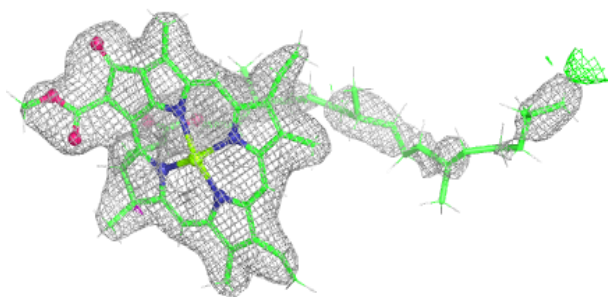
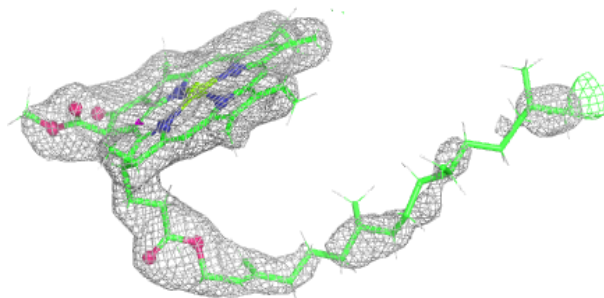
Electron density around CLA c 512:

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

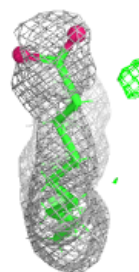
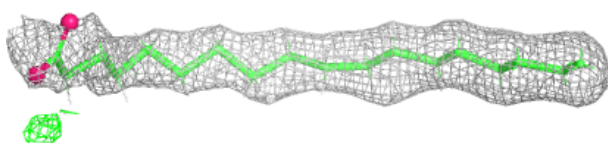
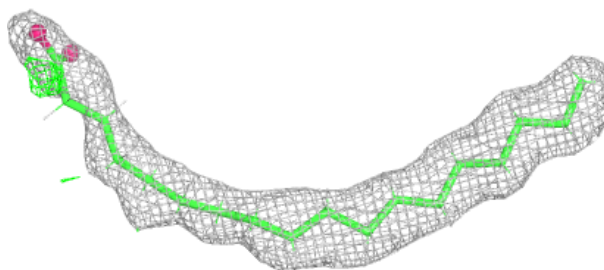


Electron density around CLA C 513:

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

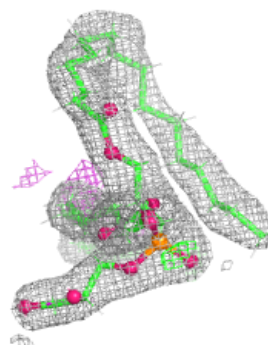
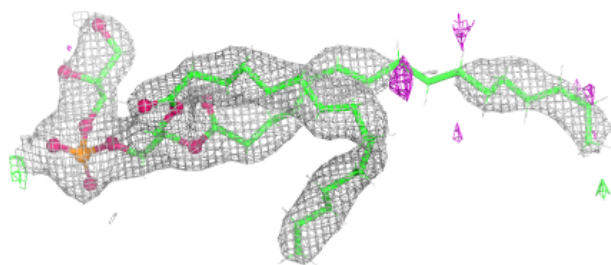
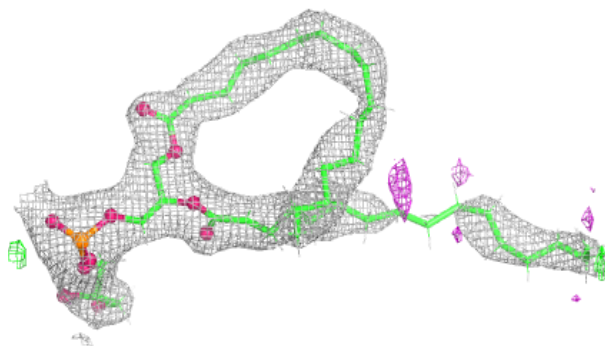
**Electron density around STE D 413:**

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



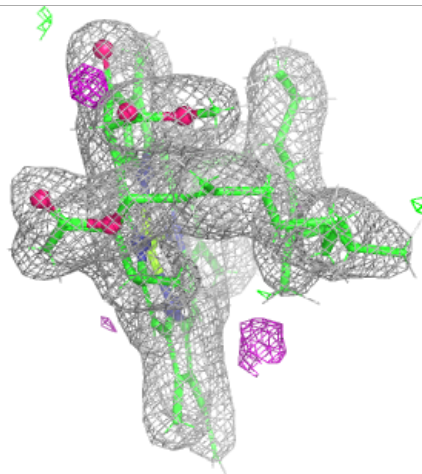
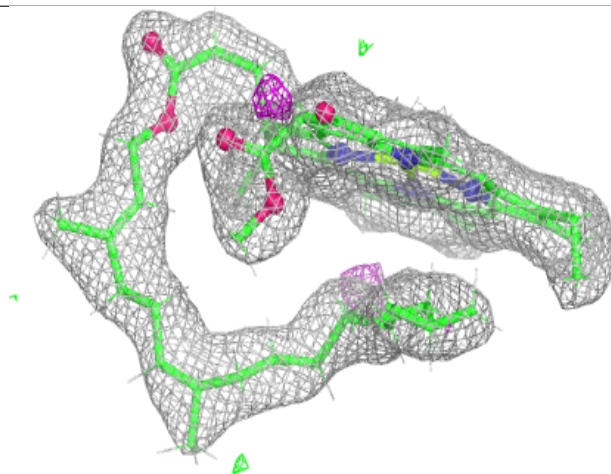
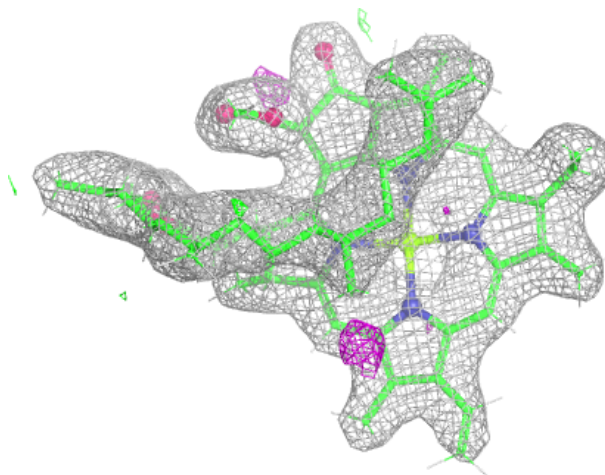
Electron density around LHG d 406:

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



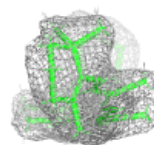
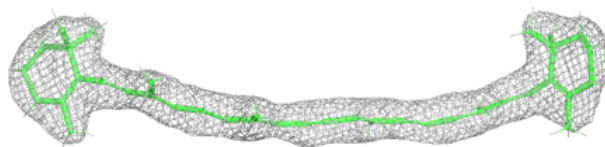
Electron density around CLA C 510:

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

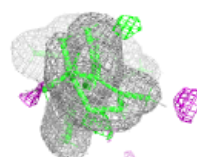
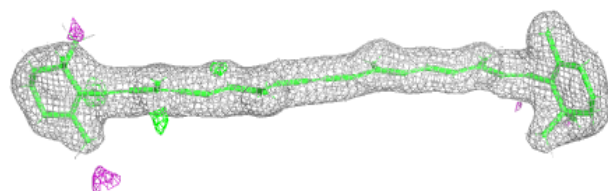
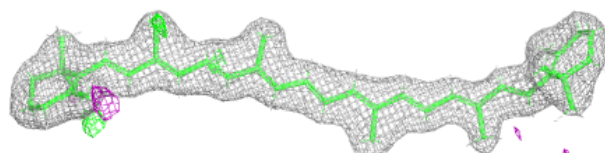


Electron density around BCR k 102:

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

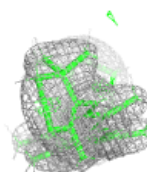
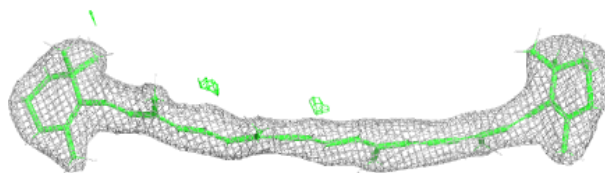
**Electron density around BCR C 515:**

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



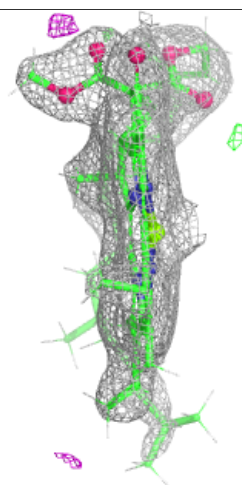
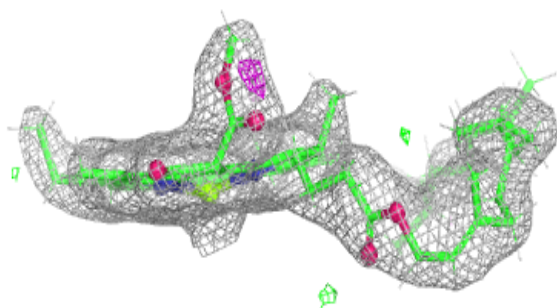
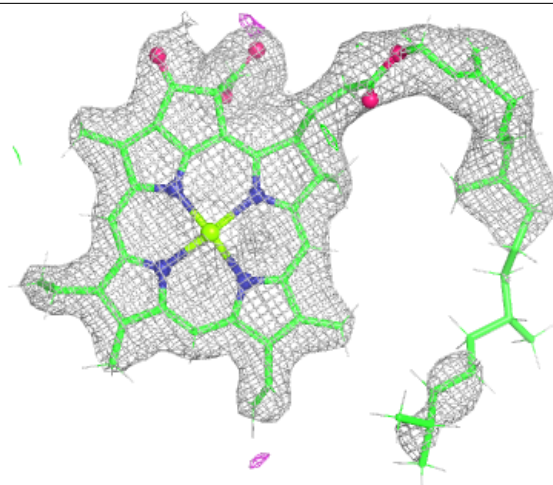
Electron density around BCR C 520:

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



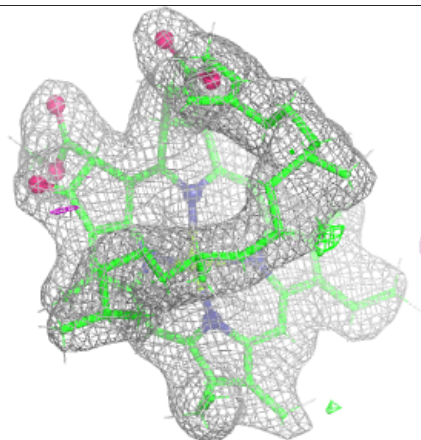
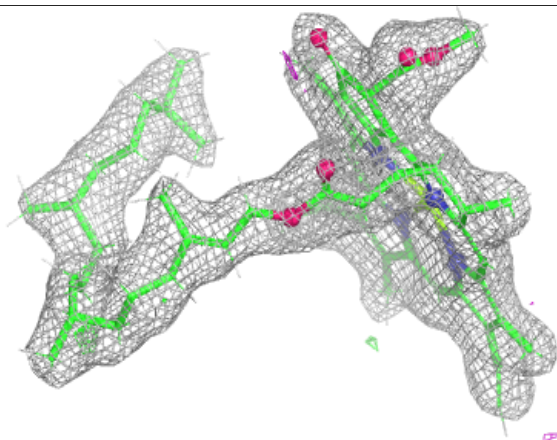
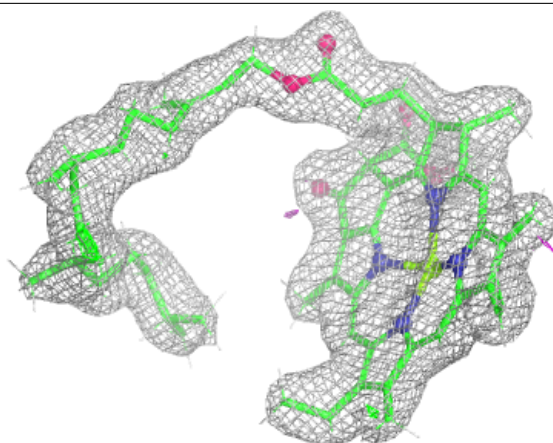
Electron density around CLA C 512:

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

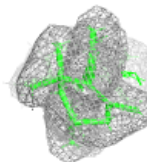
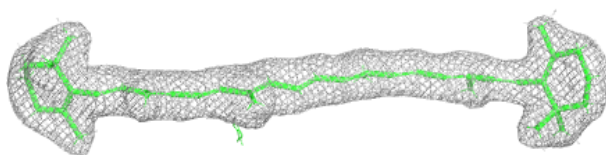
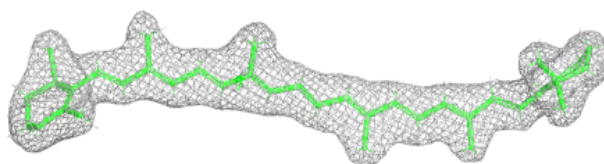


Electron density around CLA C 503:

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

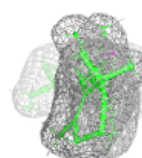
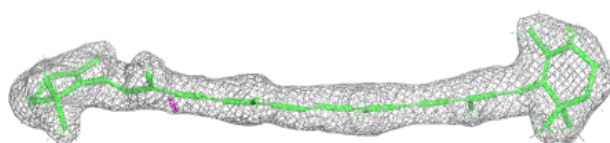
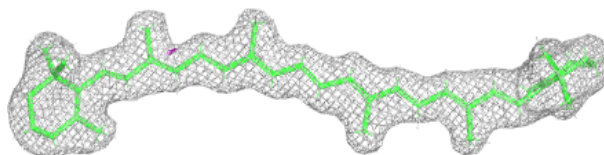
**Electron density around BCR A 408:**

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

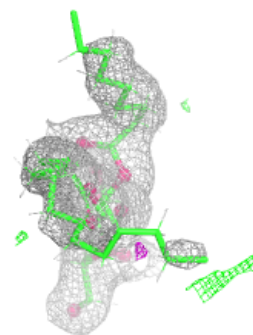
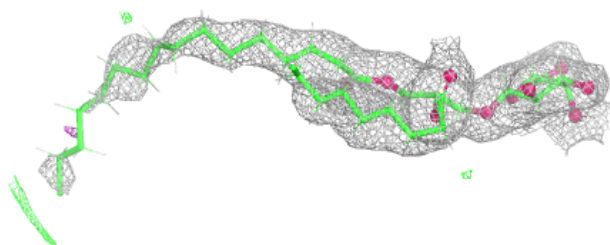


Electron density around BCR b 616:

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

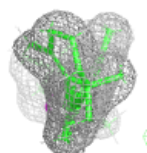
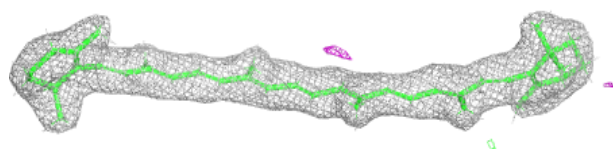
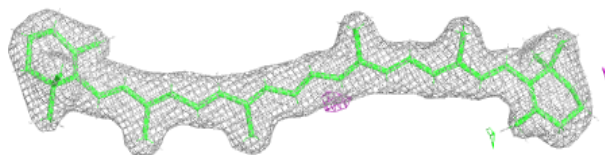
**Electron density around LMG d 409:**

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

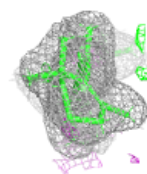
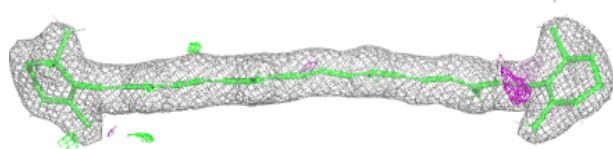
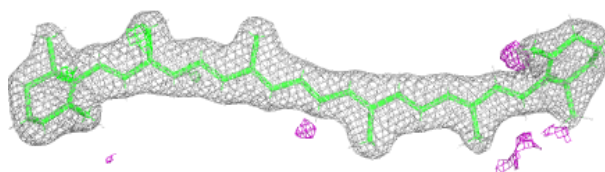


Electron density around BCR b 618:

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

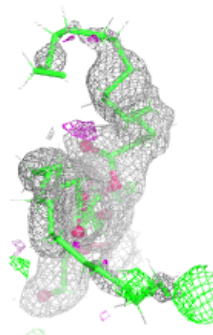
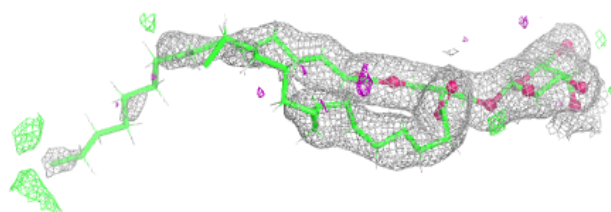
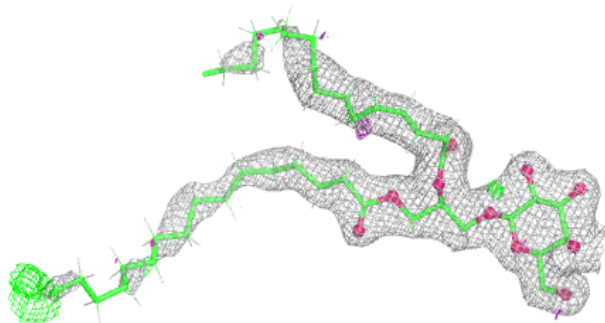
**Electron density around BCR B 618:**

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

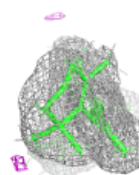
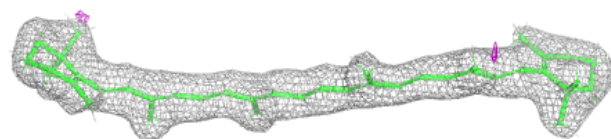
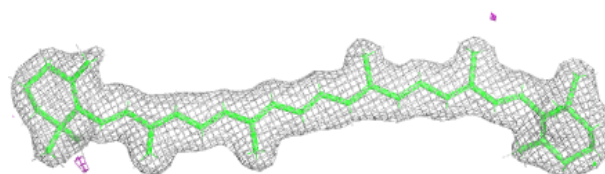


Electron density around LMG D 409:

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

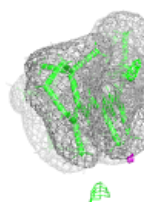
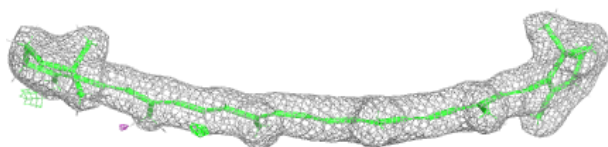
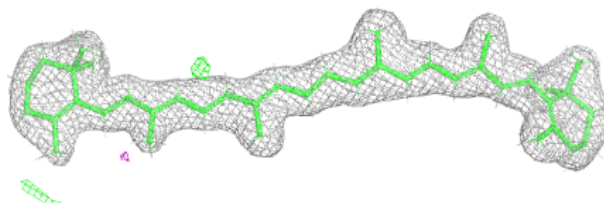
**Electron density around BCR B 619:**

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

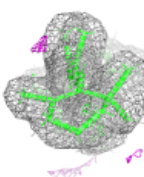
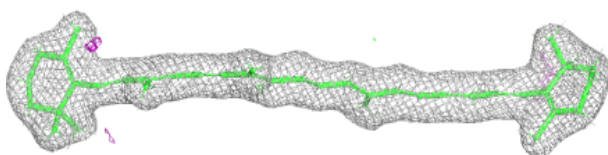
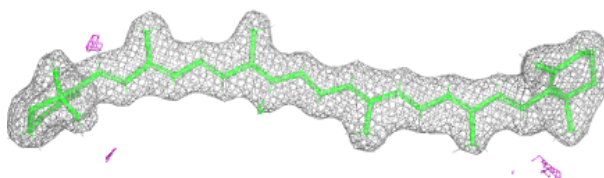


Electron density around BCR T 101:

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

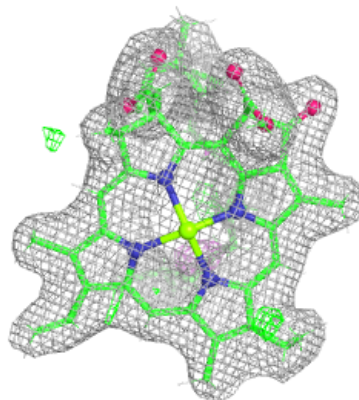
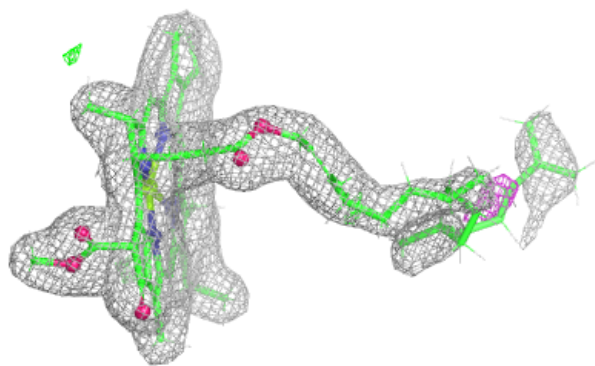
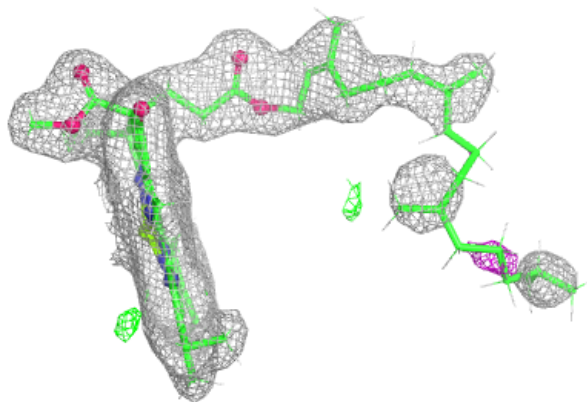
**Electron density around BCR a 409:**

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

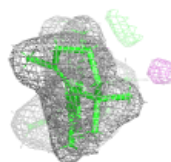
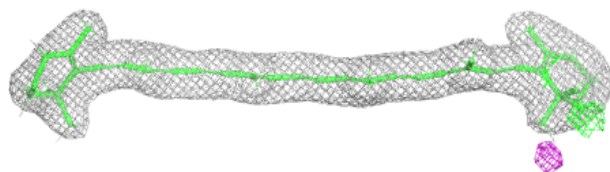
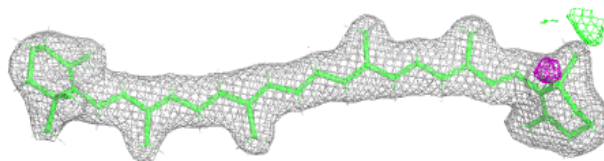


Electron density around CLA c 506:

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

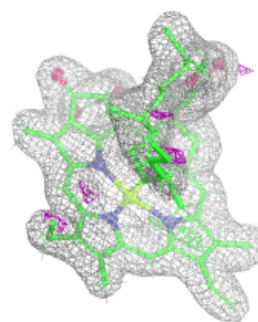
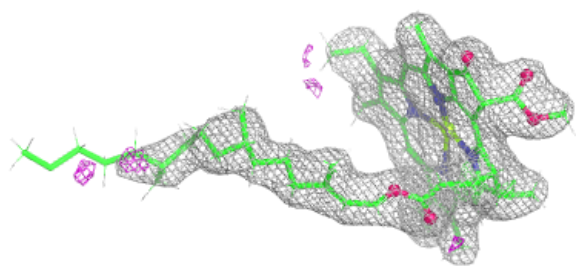
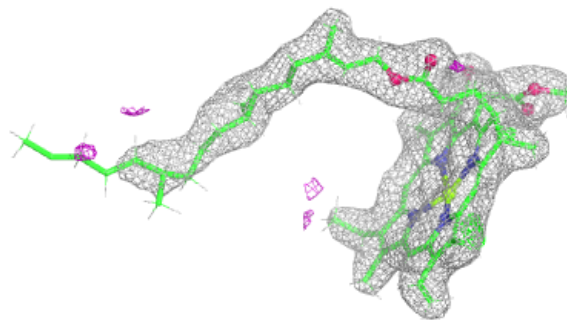
**Electron density around BCR b 617:**

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



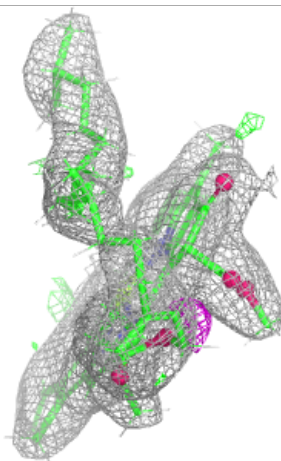
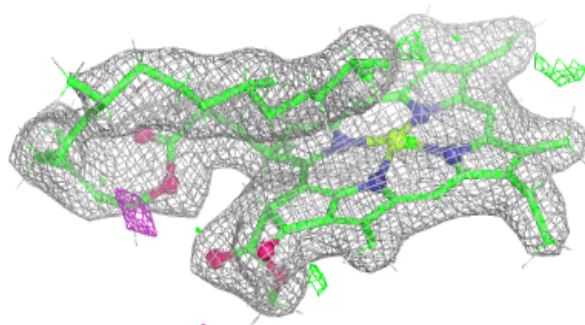
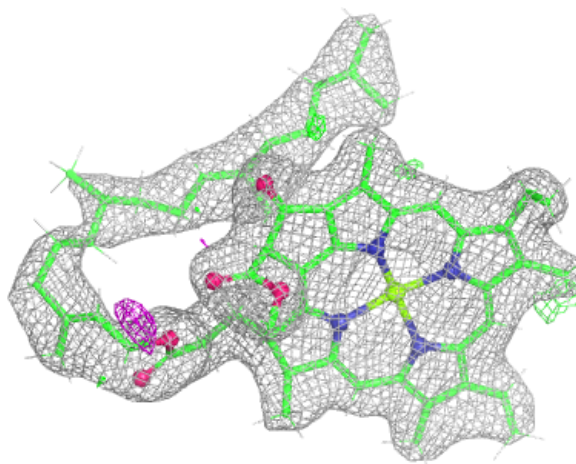
Electron density around CLA c 508:

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



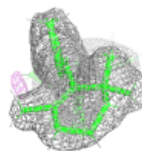
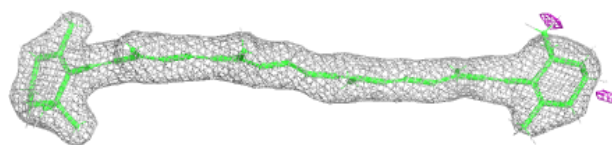
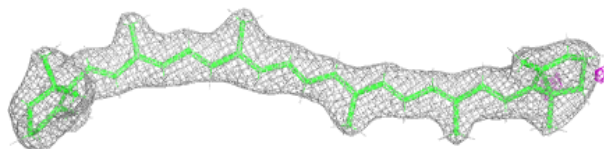
Electron density around CLA c 509:

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

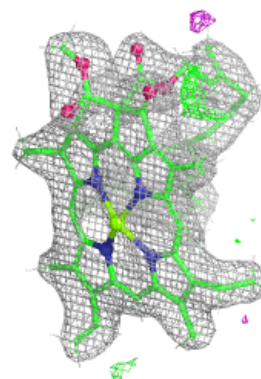
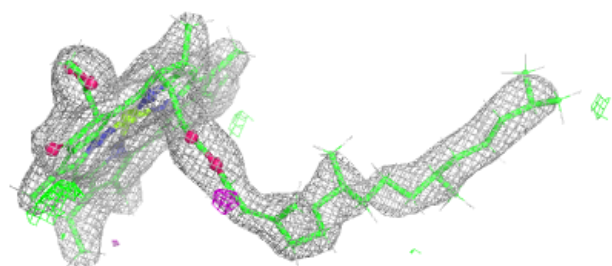
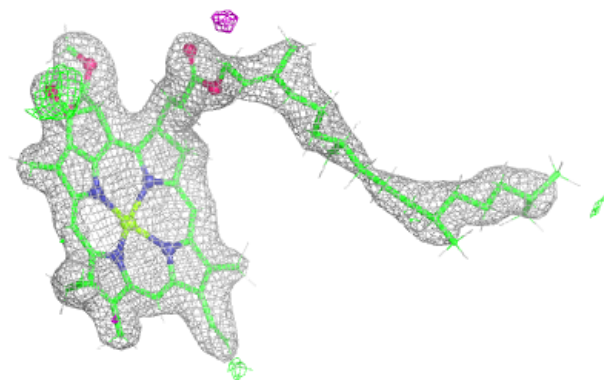


Electron density around BCR c 515:

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

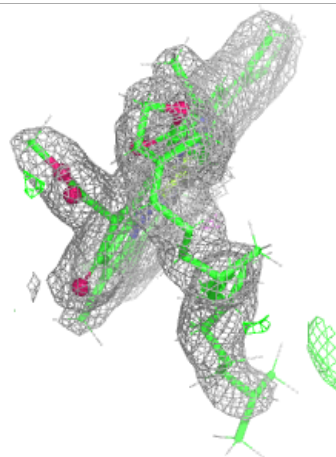
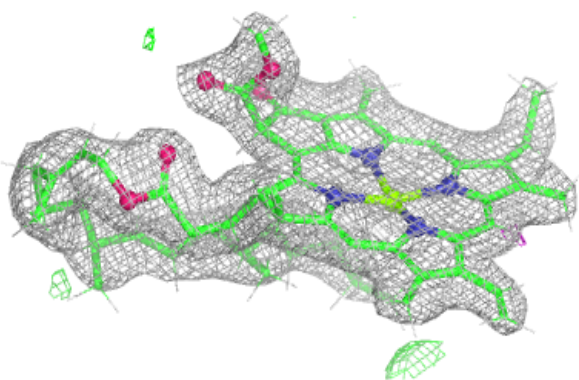
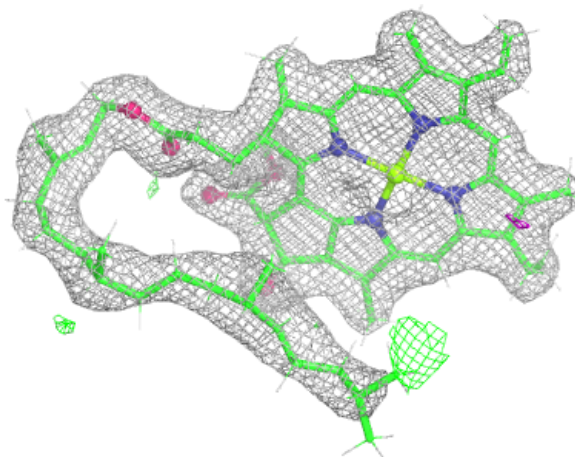
**Electron density around CLA c 511:**

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



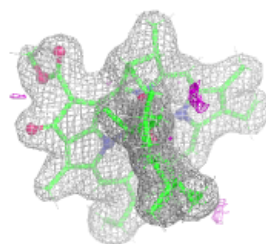
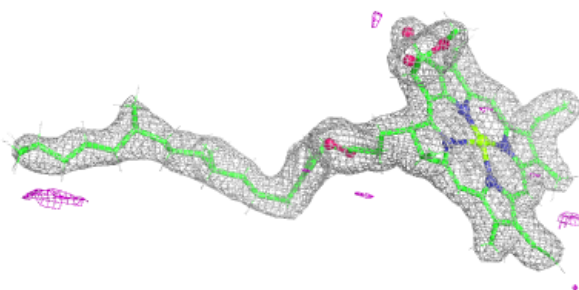
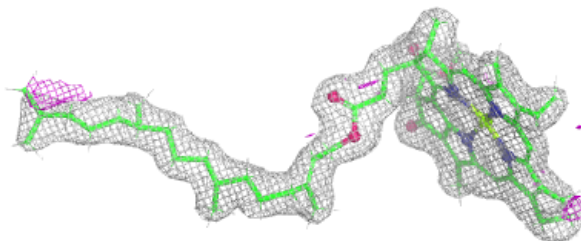
Electron density around CLA C 509:

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

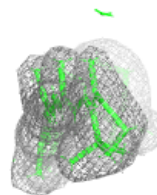
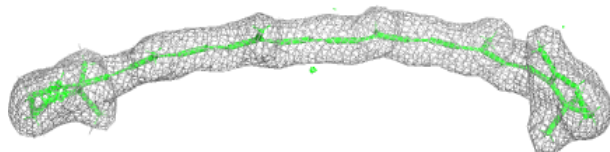
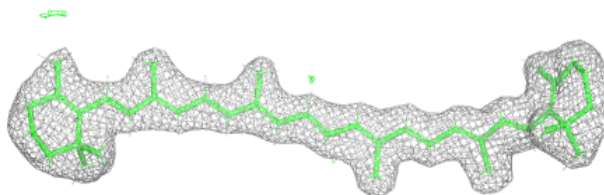


Electron density around CLA C 502:

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

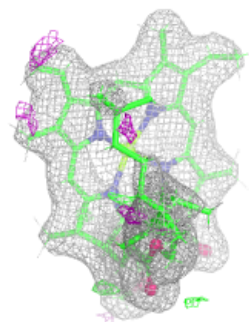
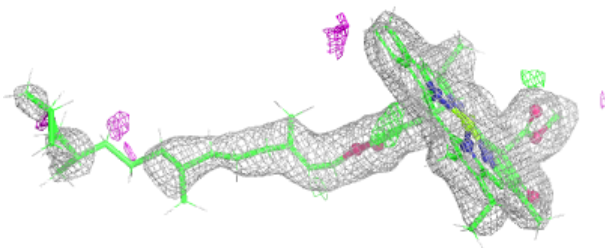
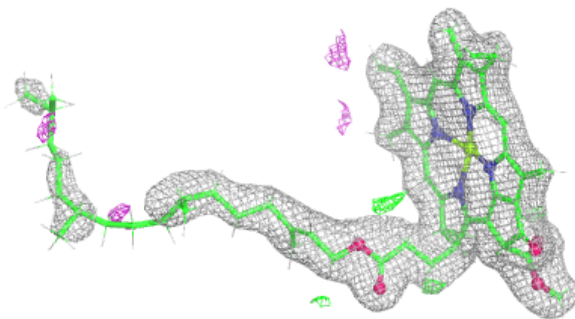
**Electron density around BCR t 101:**

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

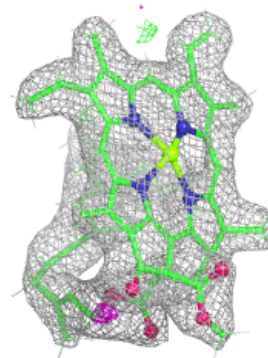
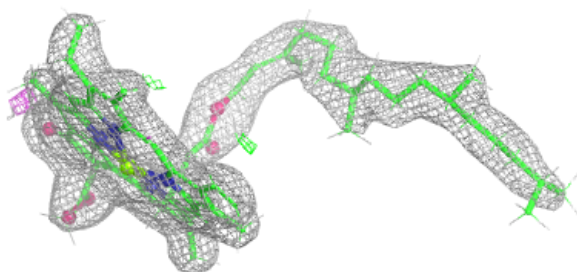
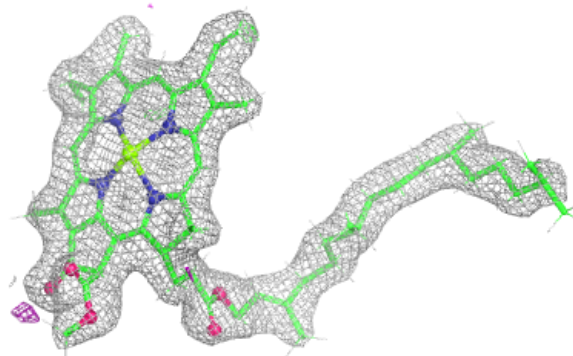


Electron density around CLA d 403:

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

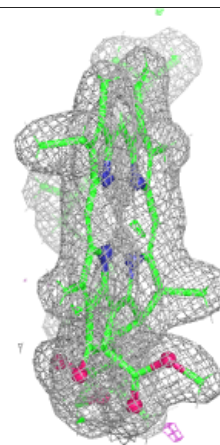
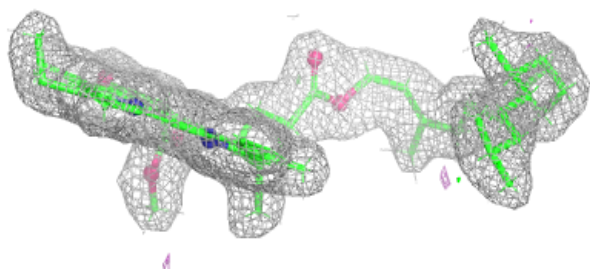
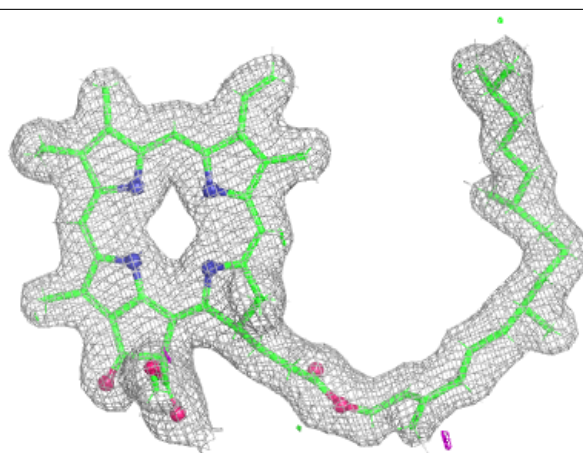
**Electron density around CLA C 511:**

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

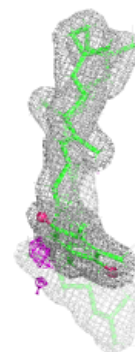
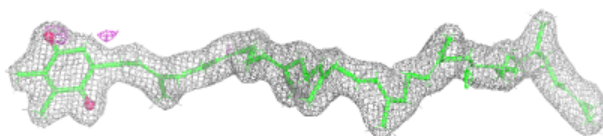
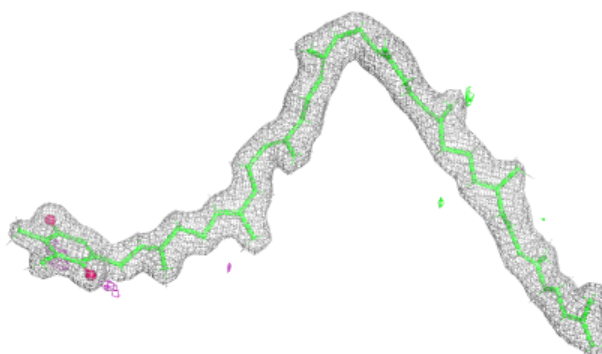


Electron density around PHO a 407:

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

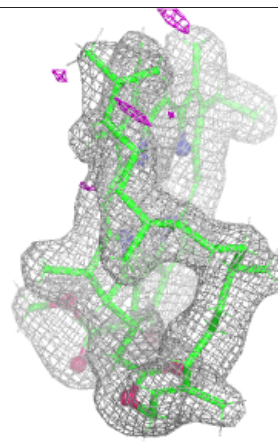
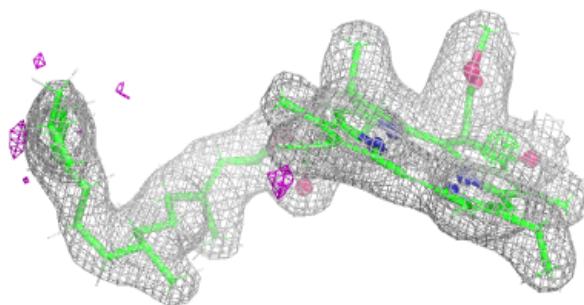
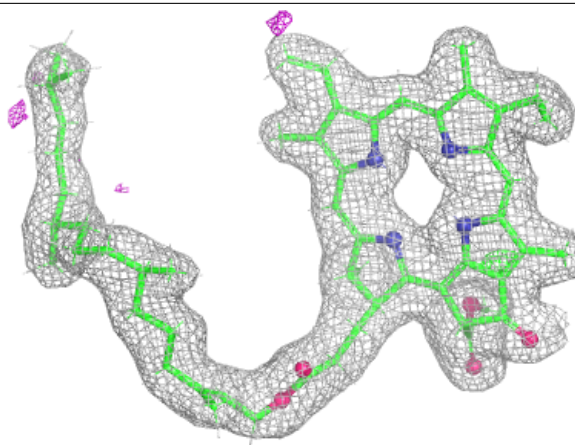
**Electron density around PL9 d 405:**

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



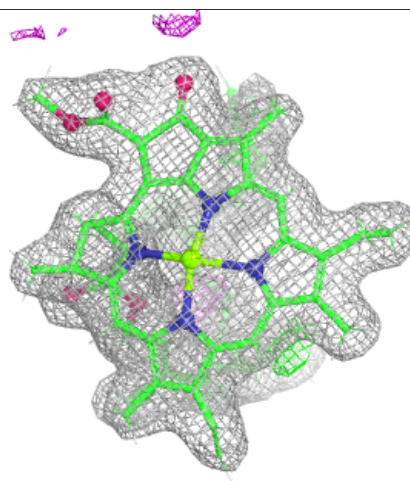
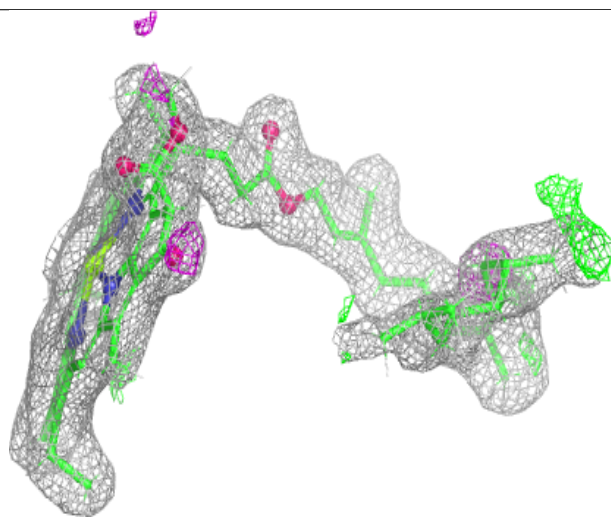
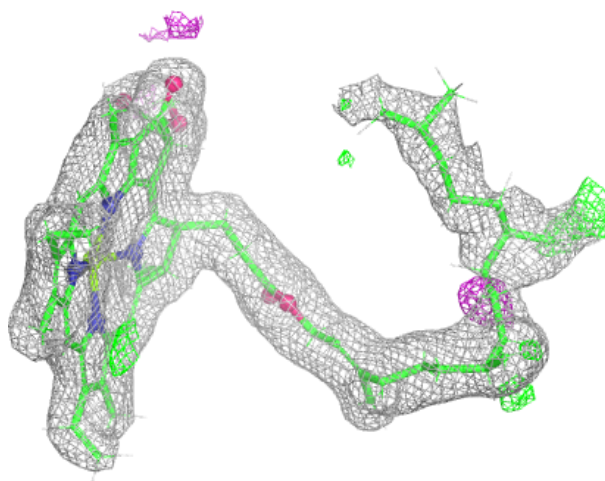
Electron density around PHO d 401:

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



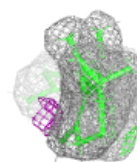
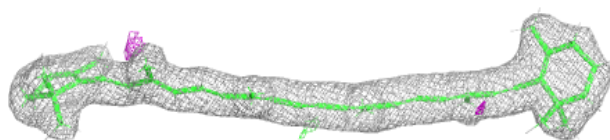
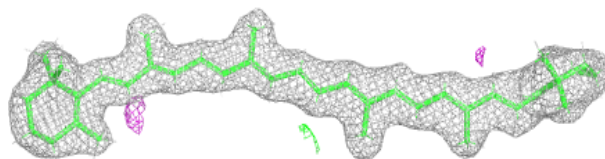
Electron density around CLA B 606:

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

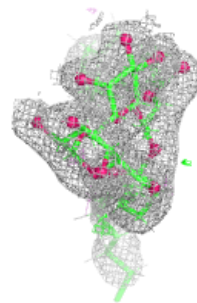
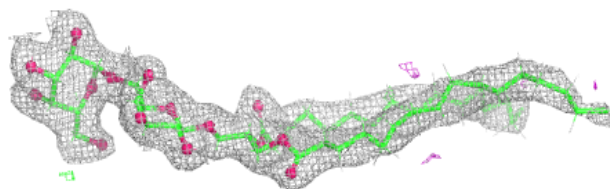
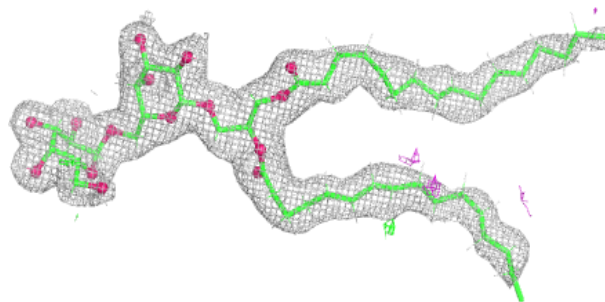


Electron density around BCR B 617:

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

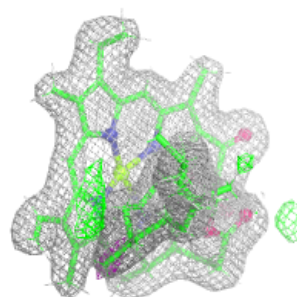
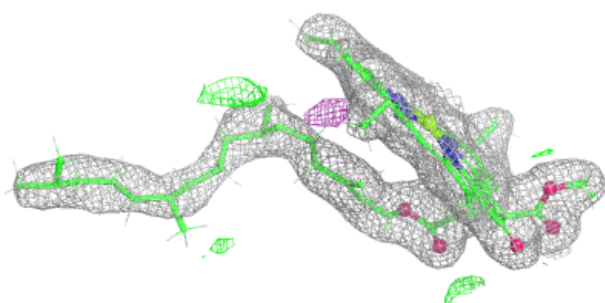
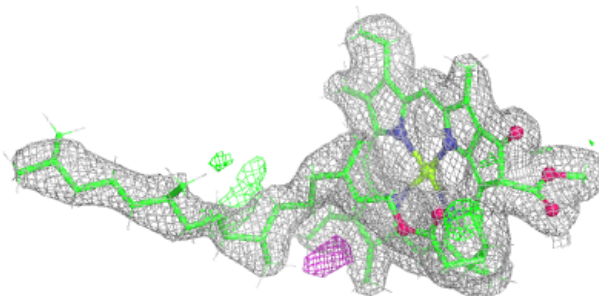
**Electron density around DGD C 523:**

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

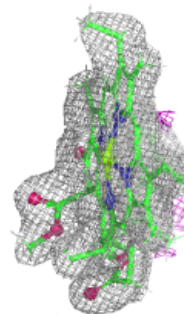
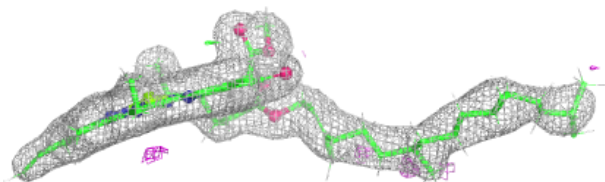
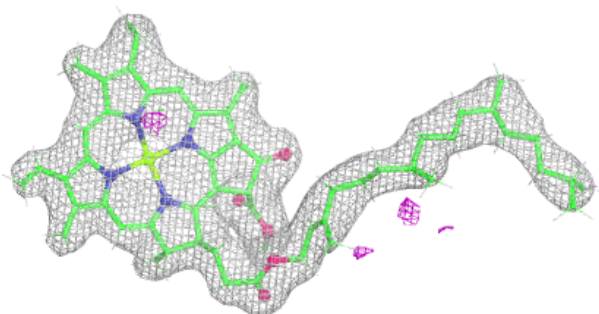


Electron density around CLA C 505:

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

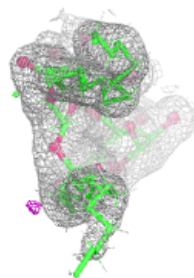
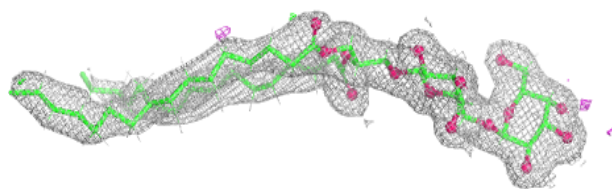
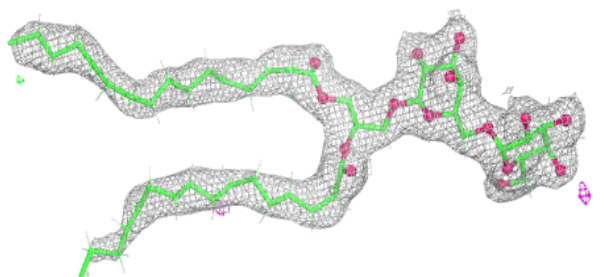
**Electron density around CLA b 601:**

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

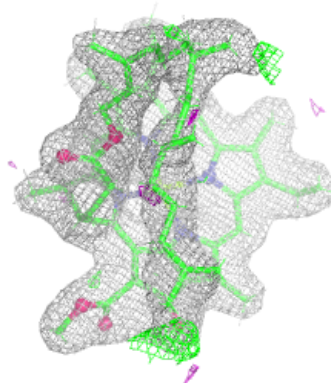
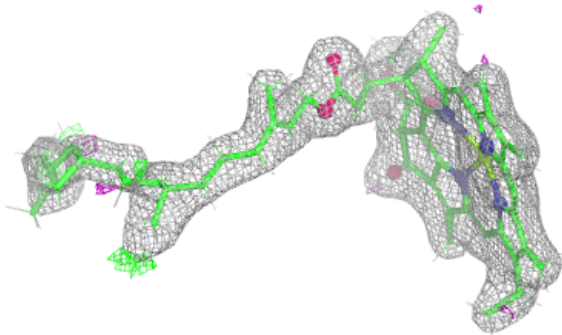
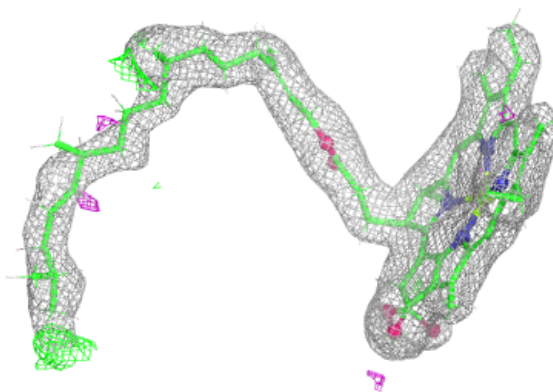


Electron density around DGD c 521:

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

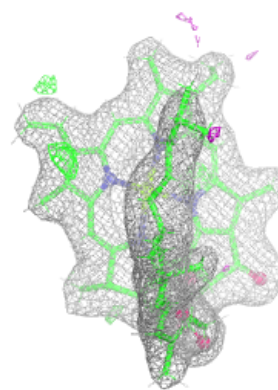
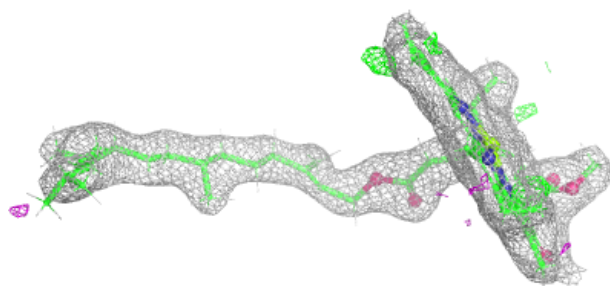
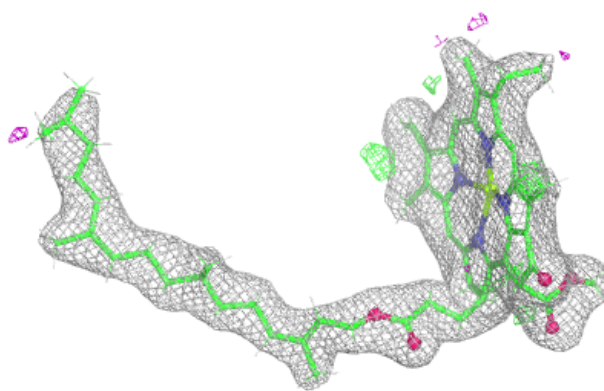
**Electron density around CLA b 605:**

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

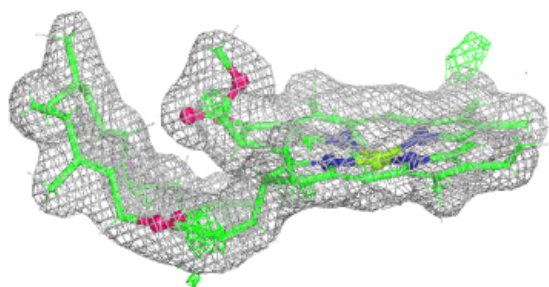
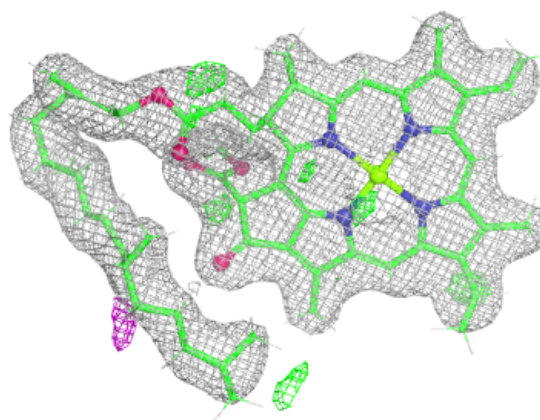


Electron density around CLA b 608:

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

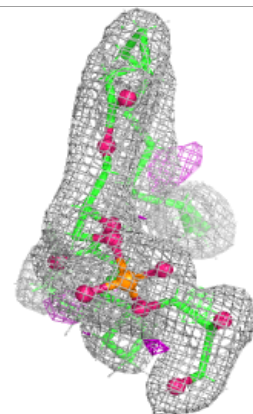
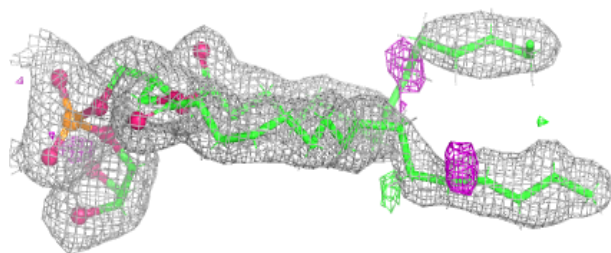
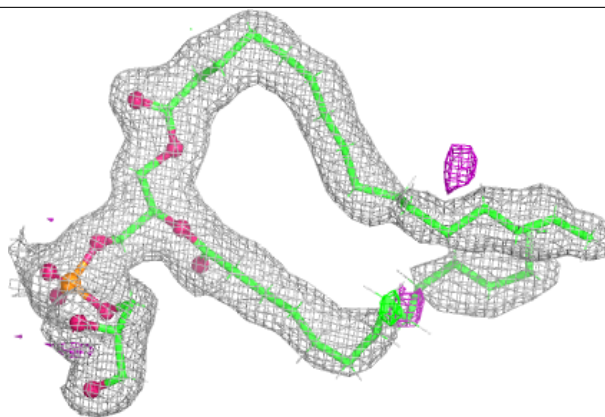
**Electron density around CLA b 609:**

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

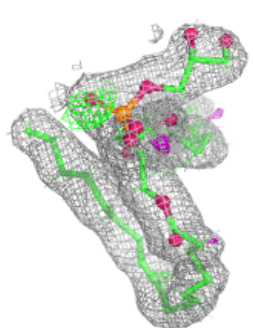
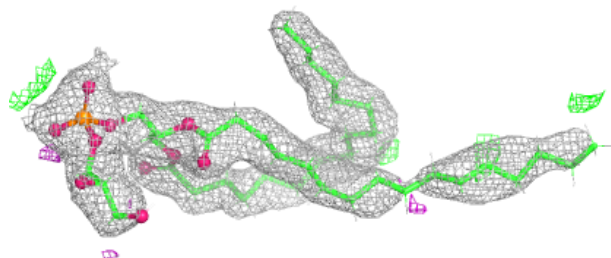
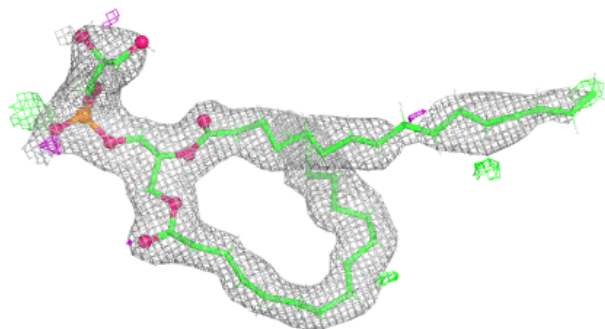


Electron density around LHG D 411:

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

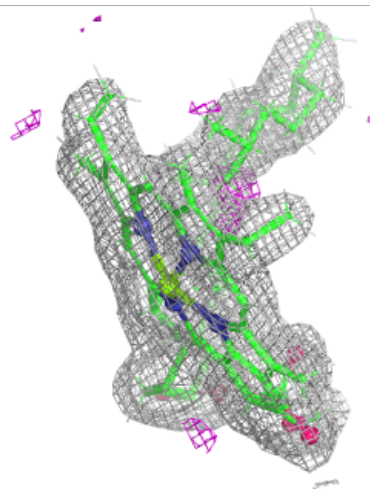
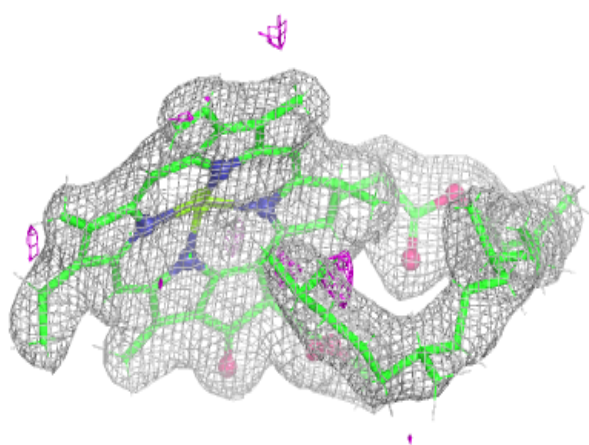
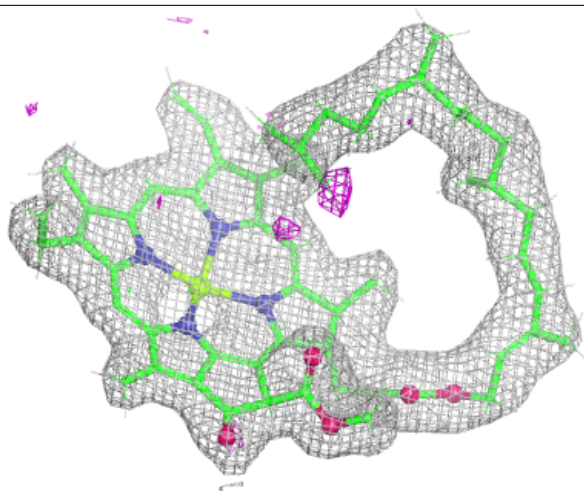
**Electron density around LHG D 412:**

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



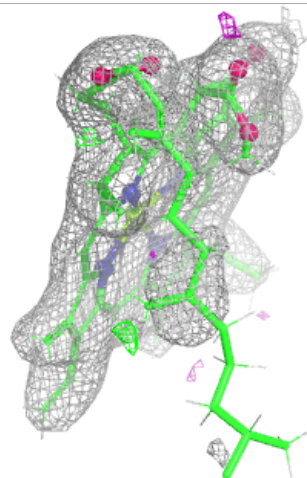
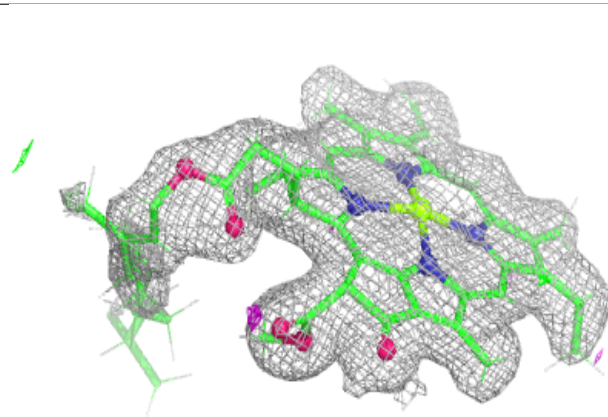
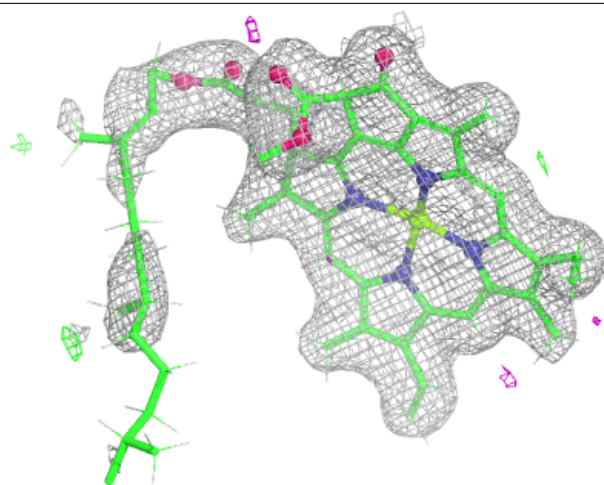
Electron density around CLA b 614:

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



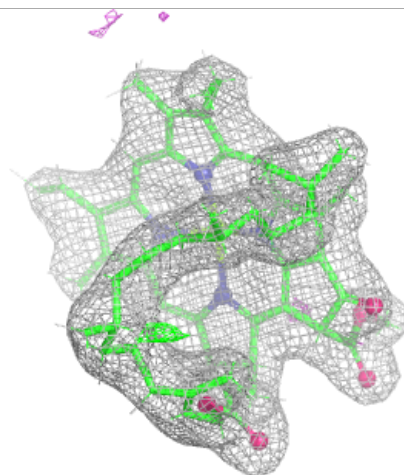
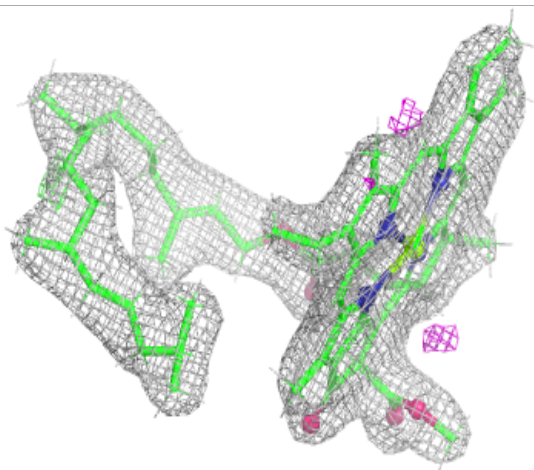
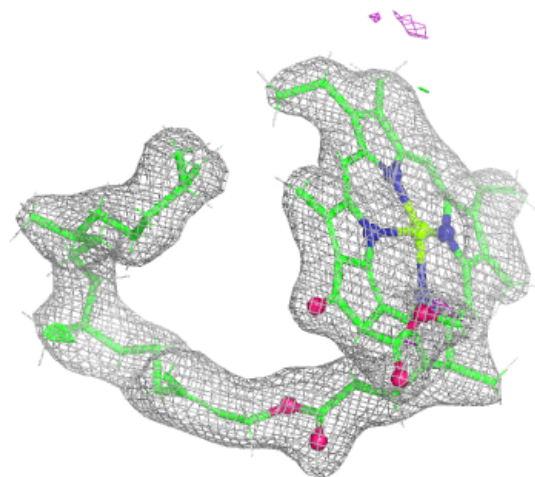
Electron density around CLA b 615:

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



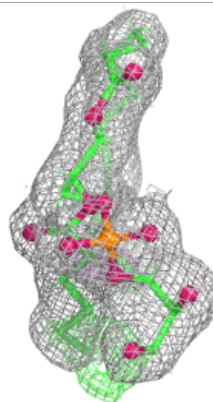
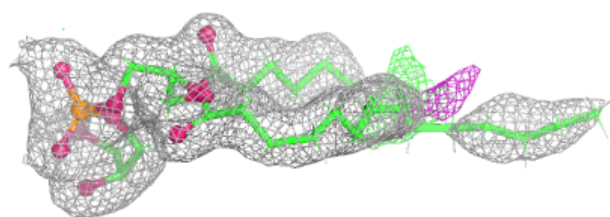
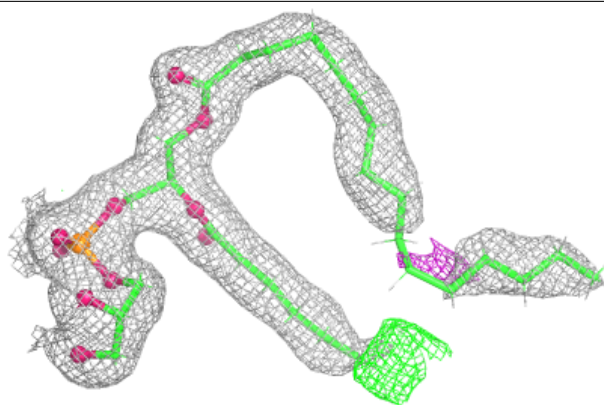
Electron density around CLA c 503:

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



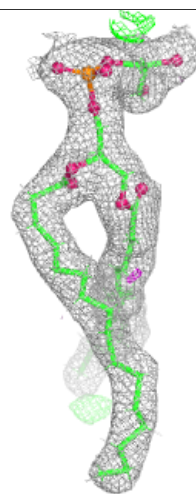
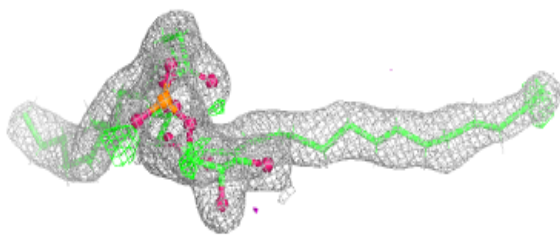
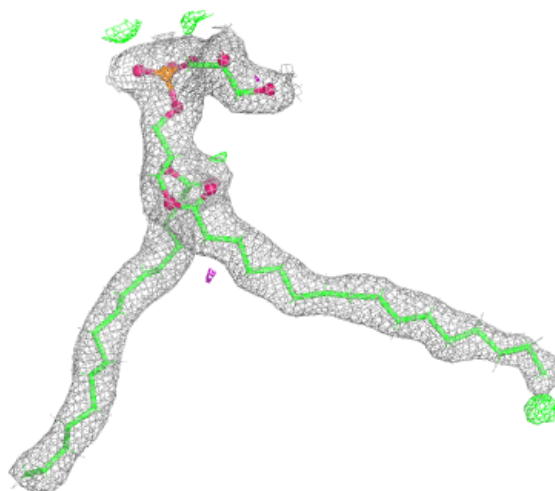
Electron density around LHG d 408:

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



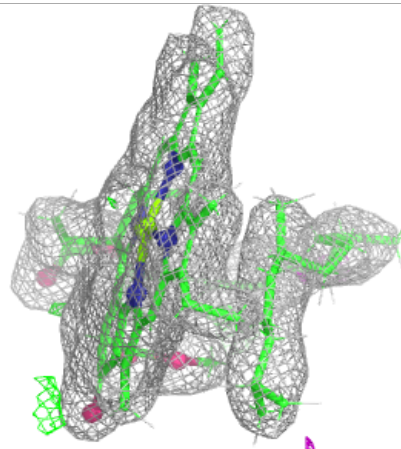
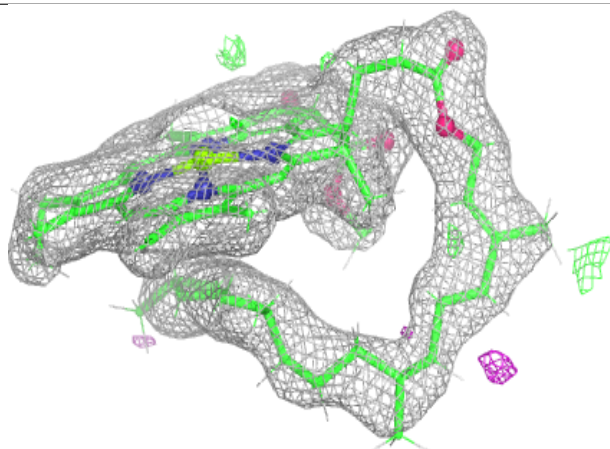
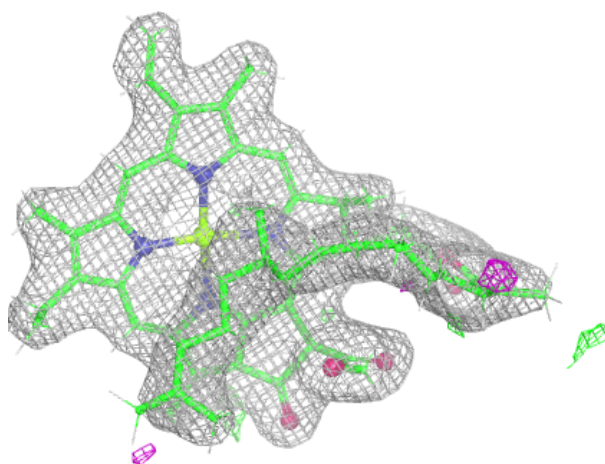
Electron density around LHG 1 102:

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



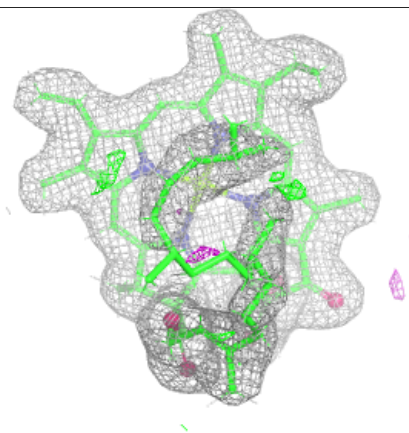
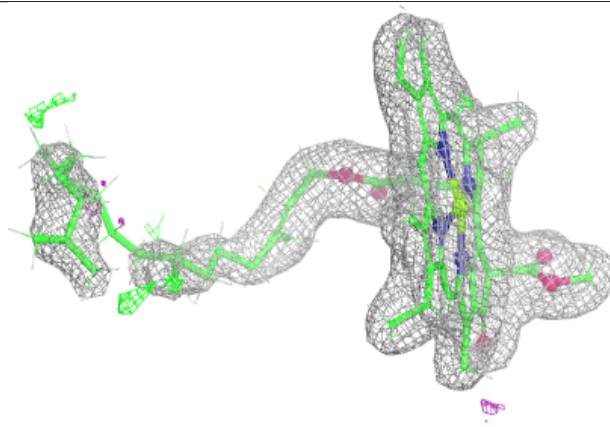
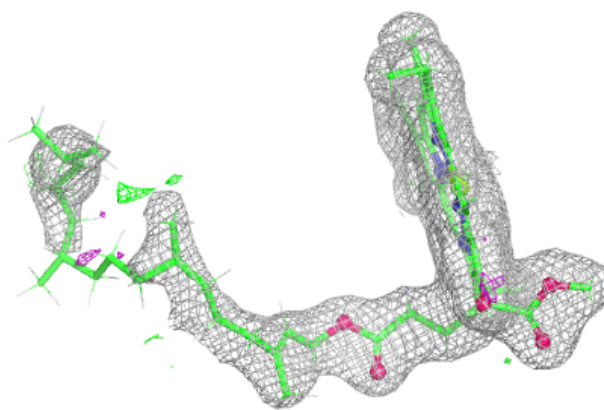
Electron density around CLA c 510:

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



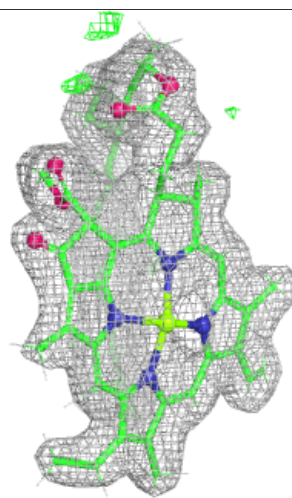
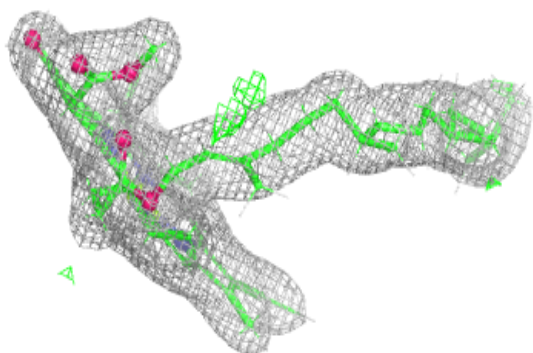
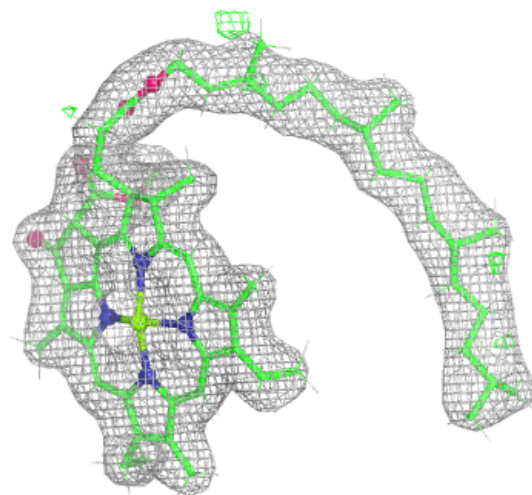
Electron density around CLA C 506:

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



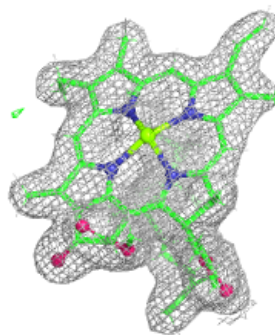
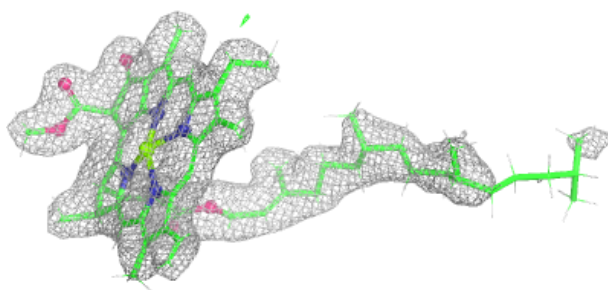
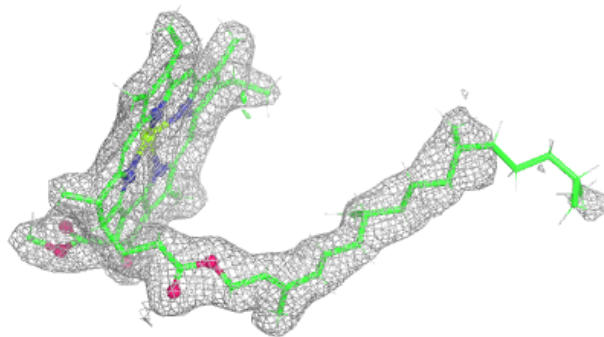
Electron density around CLA C 507:

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

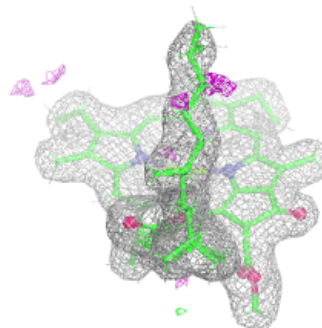
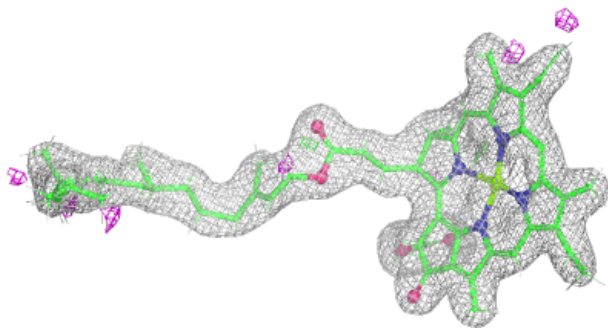
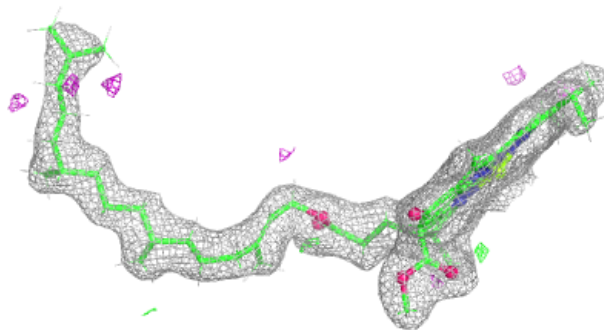


Electron density around CLA C 508:

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

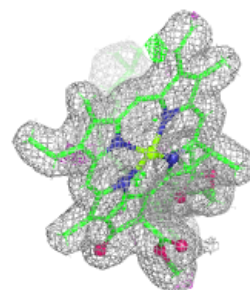
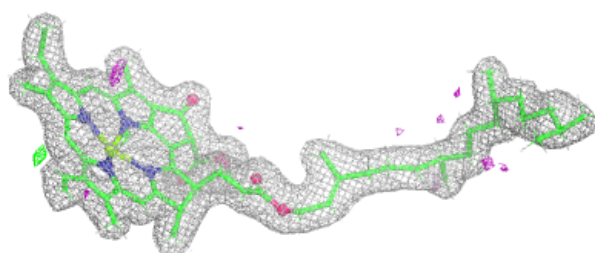
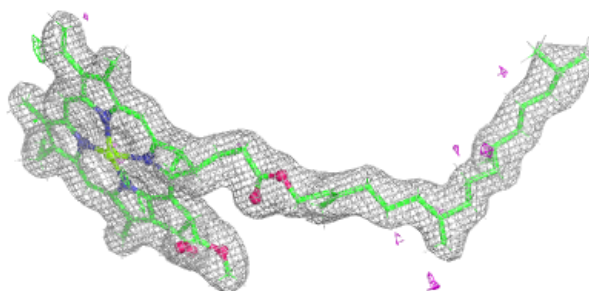
**Electron density around CLA d 402:**

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

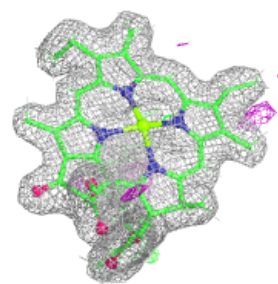
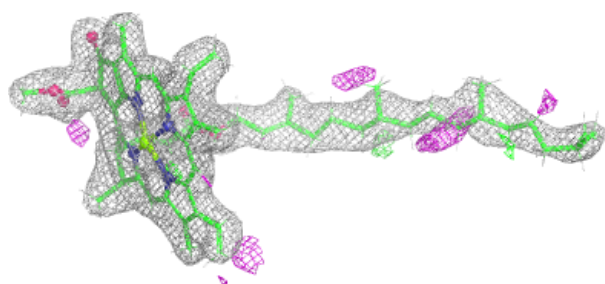
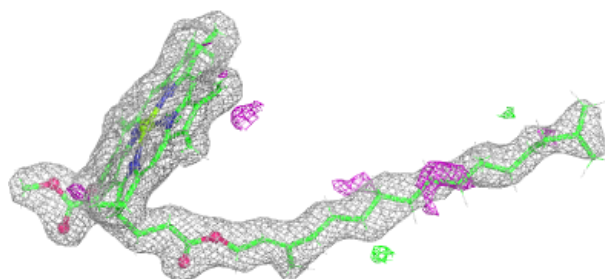


Electron density around CLA A 404:

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

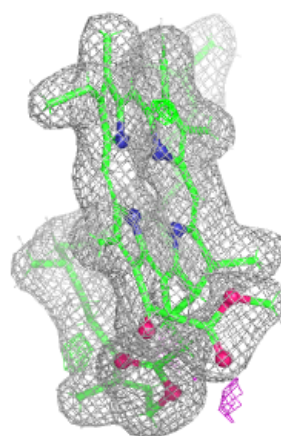
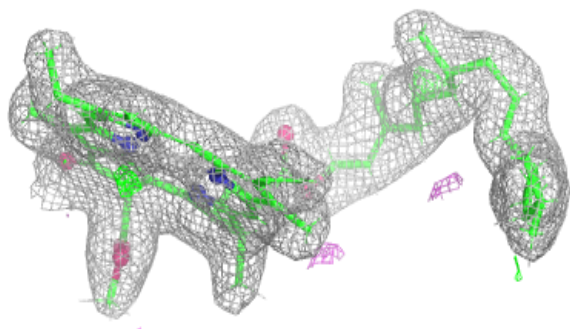
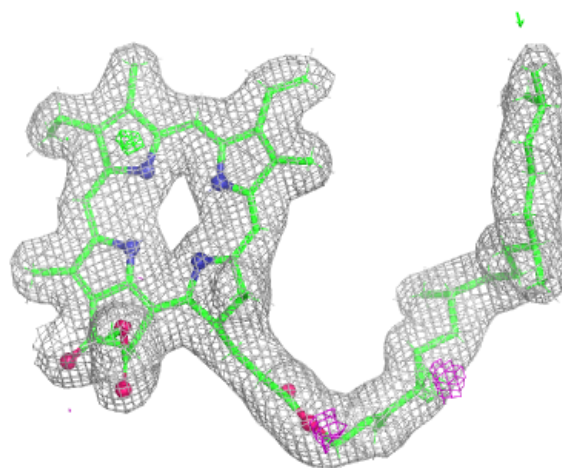
**Electron density around CLA B 607:**

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



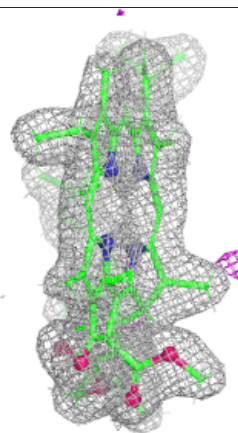
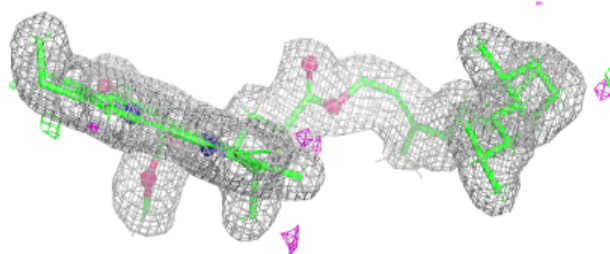
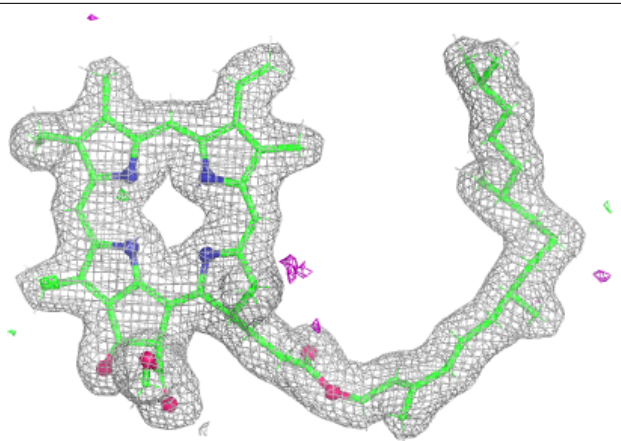
Electron density around PHO A 406:

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

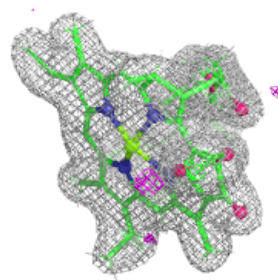
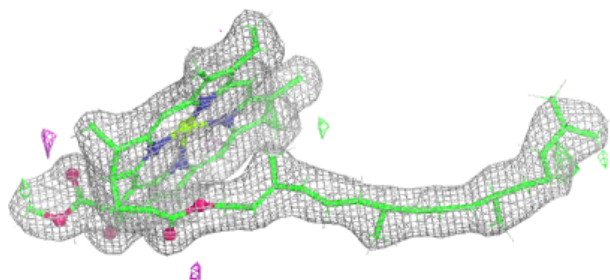
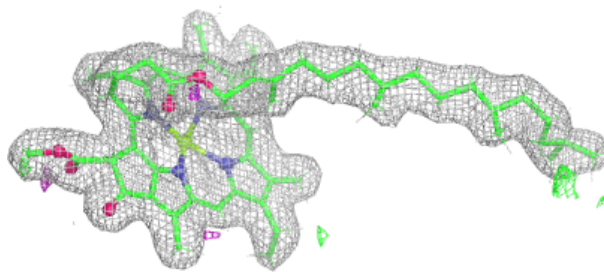


Electron density around PHO D 402:

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

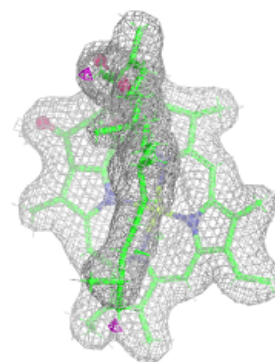
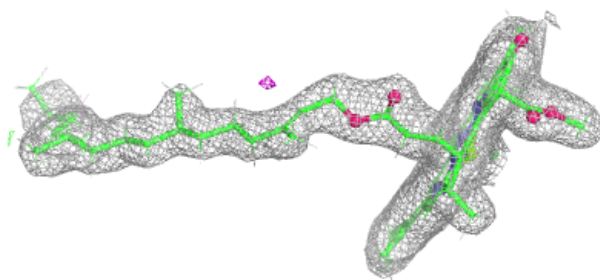
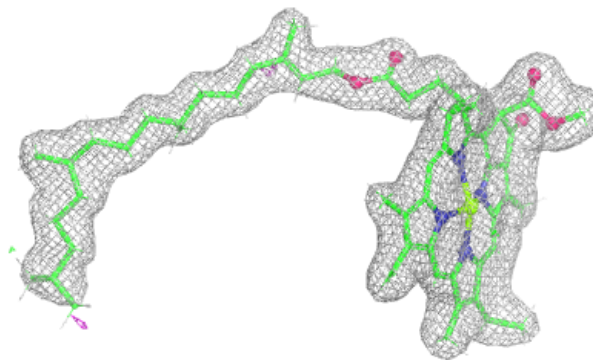
**Electron density around CLA B 608:**

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



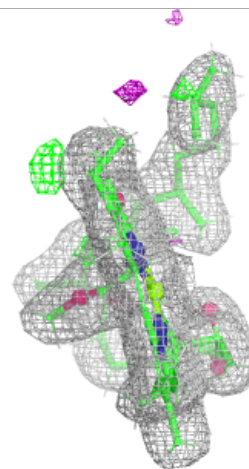
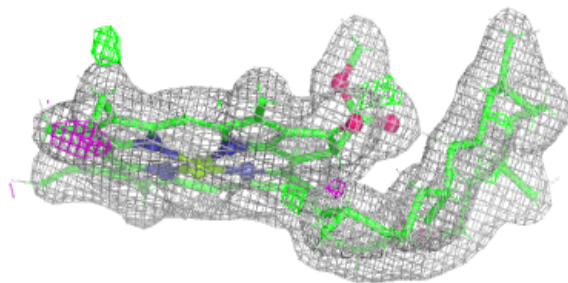
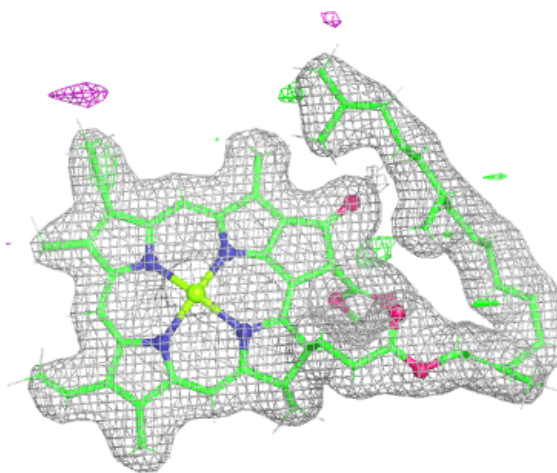
Electron density around CLA B 609:

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



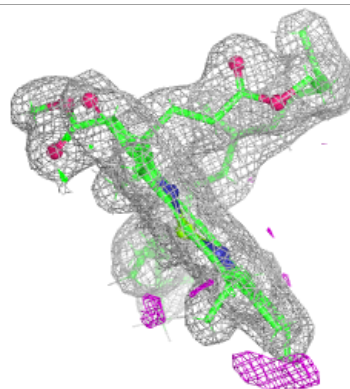
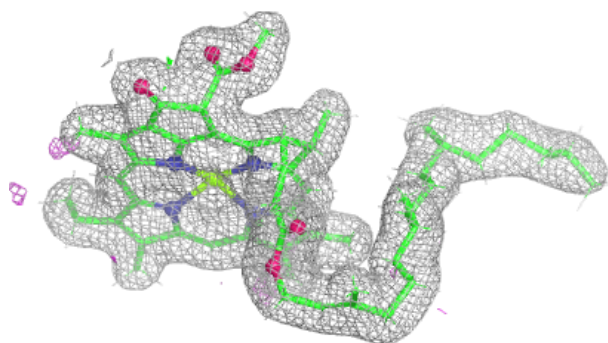
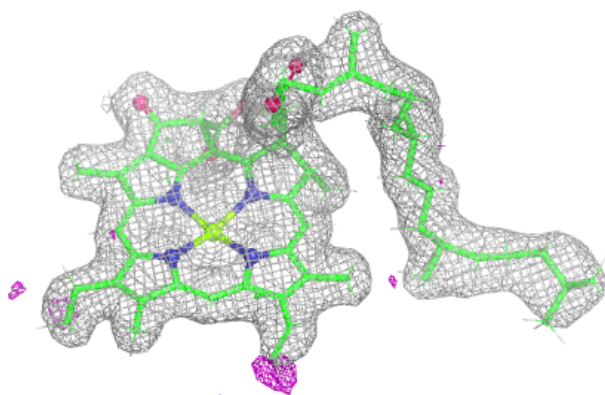
Electron density around CLA B 610:

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

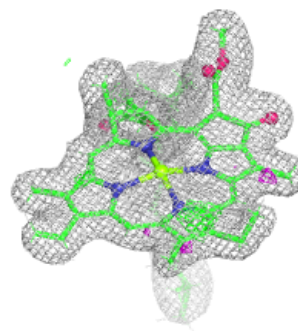
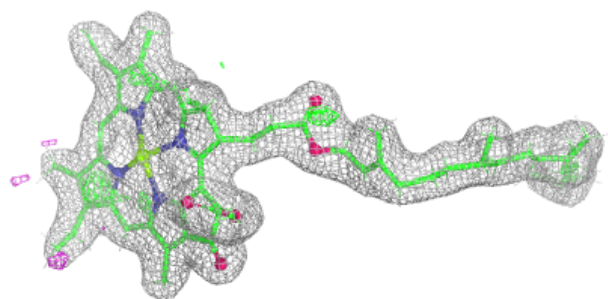
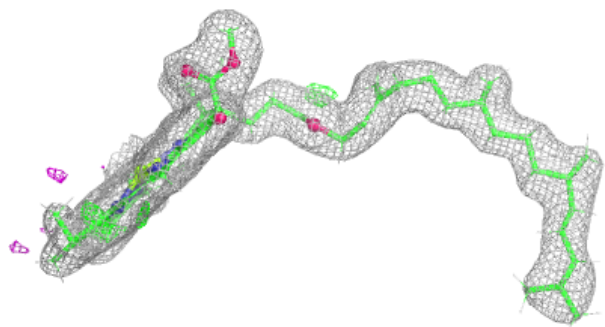


Electron density around CLA D 403:

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

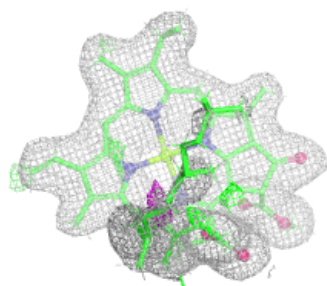
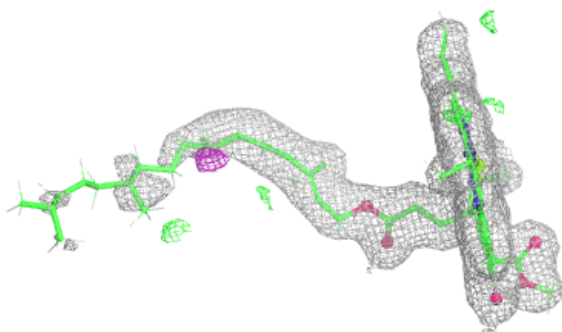
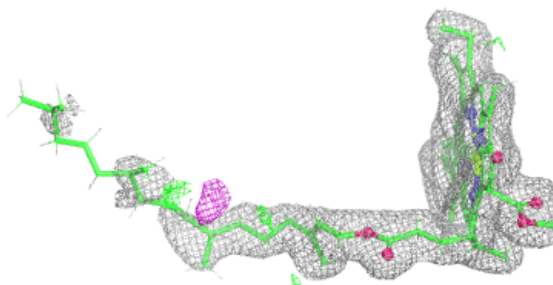
**Electron density around CLA D 404:**

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

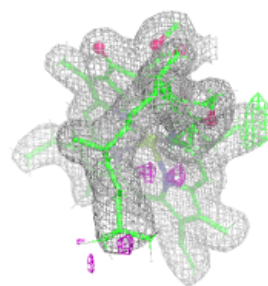
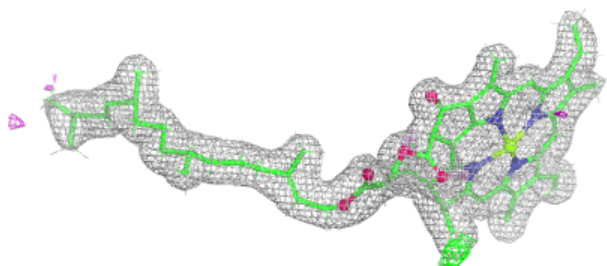
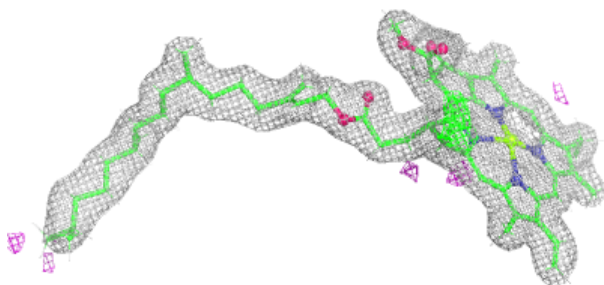


Electron density around CLA D 405:

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

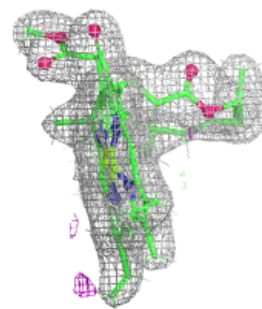
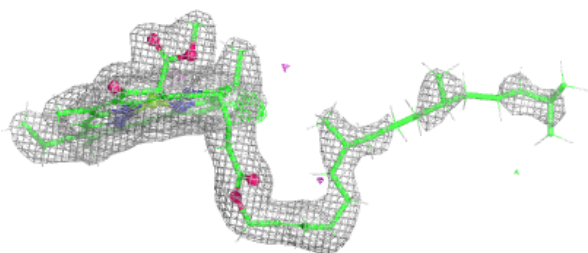
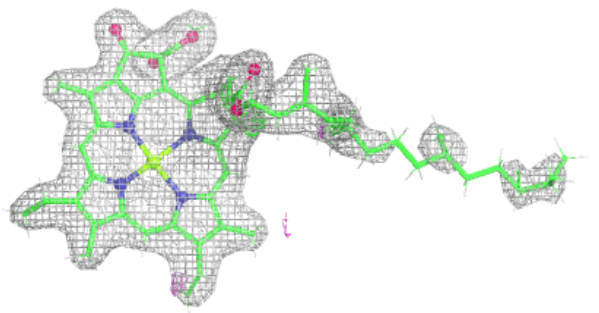
**Electron density around CLA a 405:**

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

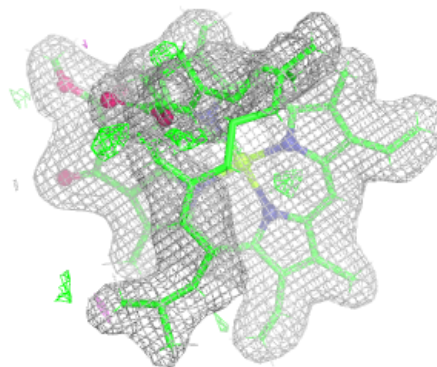
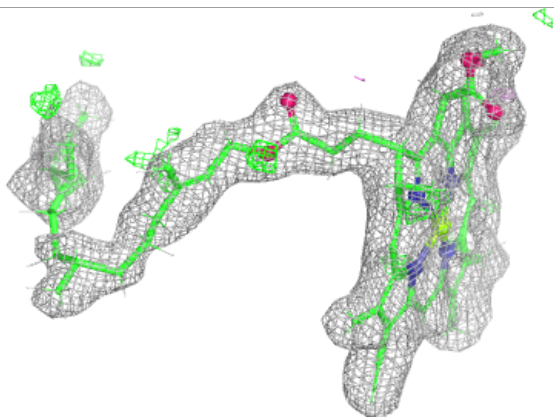
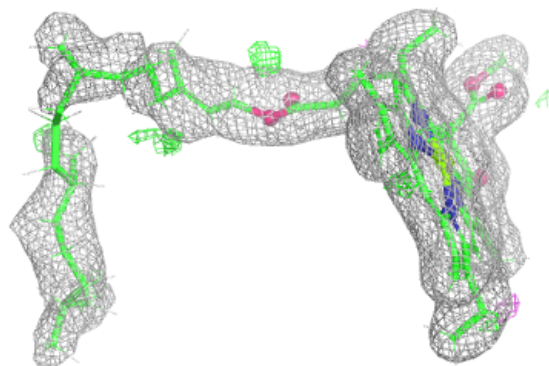


Electron density around CLA a 406:

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

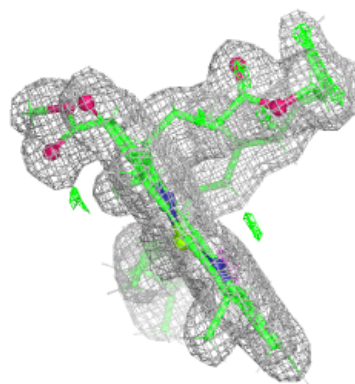
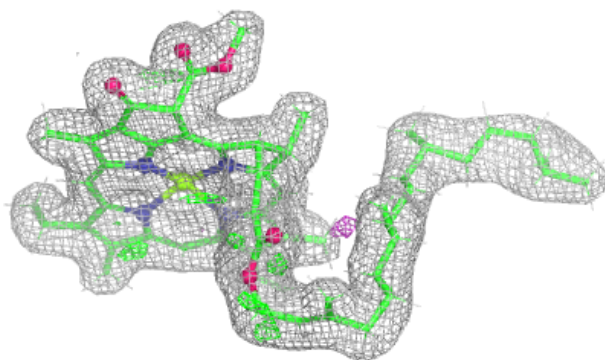
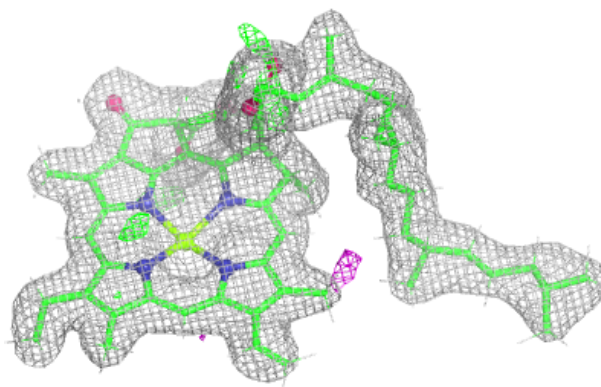
**Electron density around CLA a 408:**

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



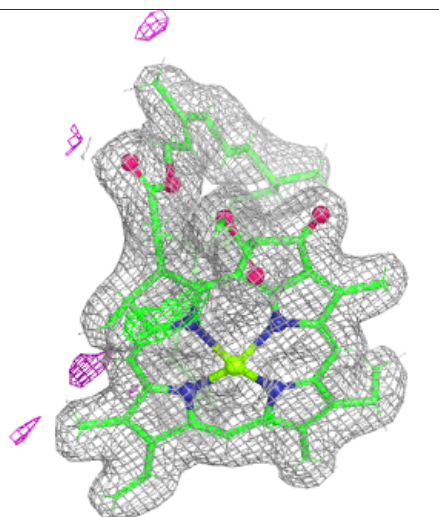
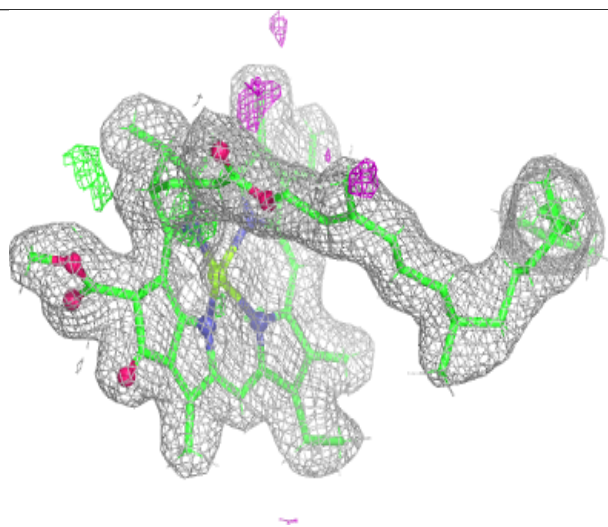
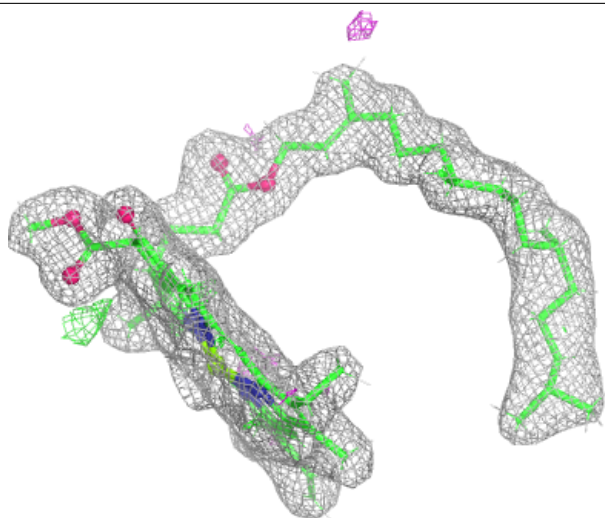
Electron density around CLA a 411:

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



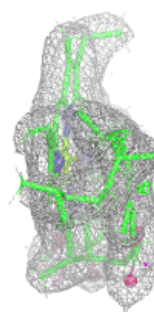
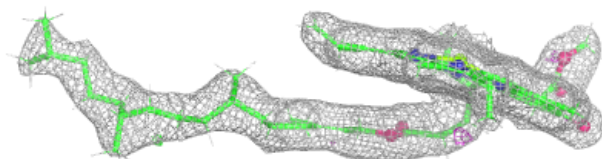
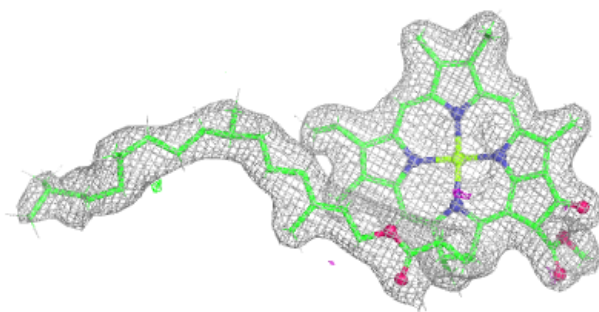
Electron density around CLA B 611:

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

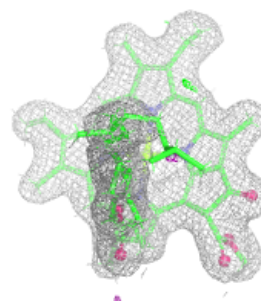
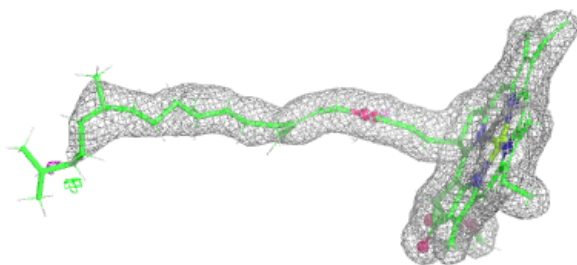
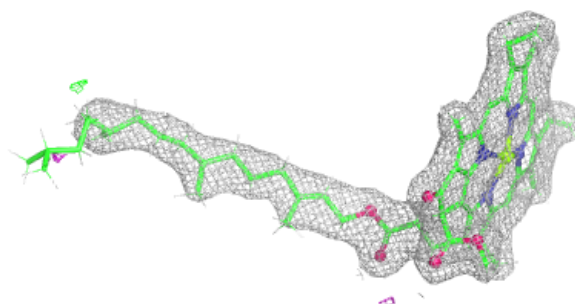


Electron density around CLA b 602:

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

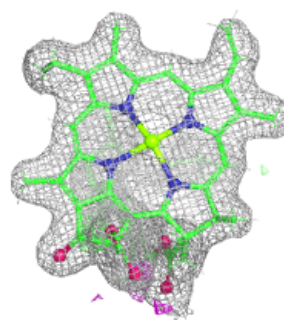
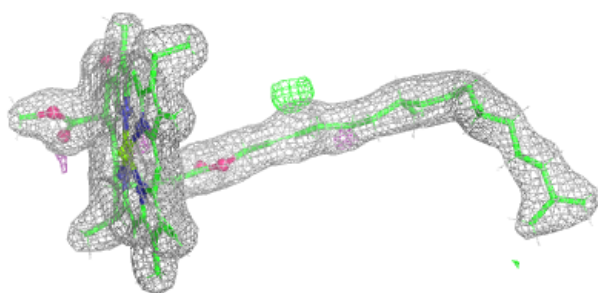
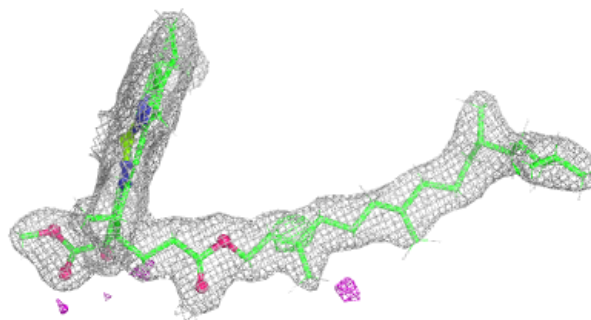
**Electron density around CLA b 603:**

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

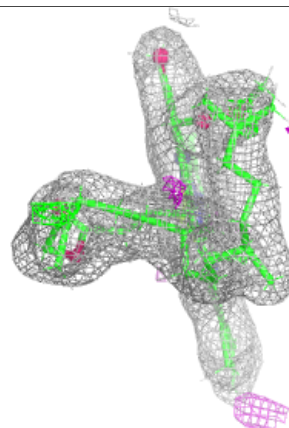
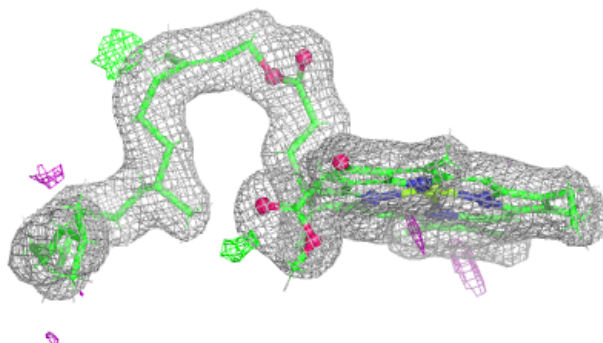
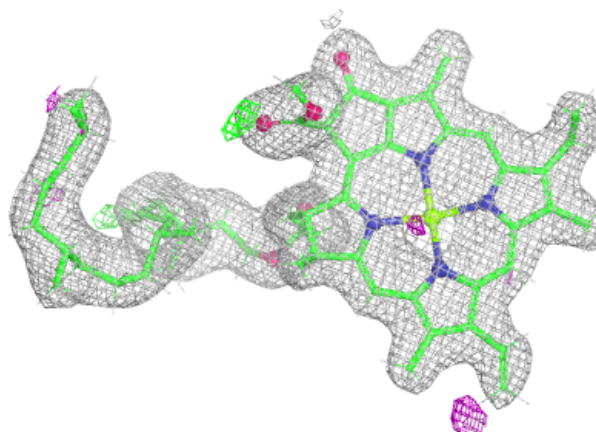


Electron density around CLA b 604:

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

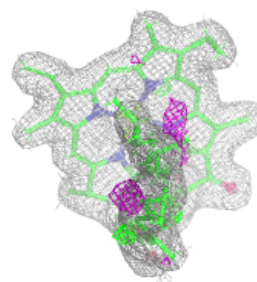
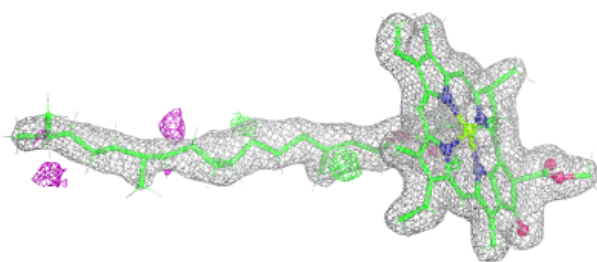
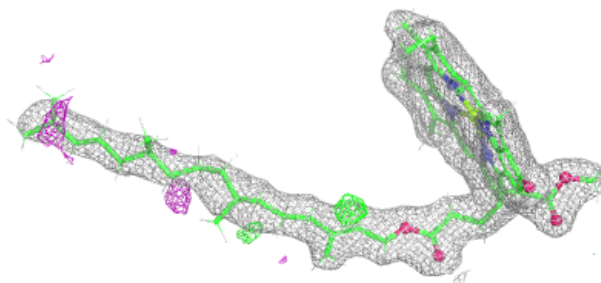
**Electron density around CLA B 612:**

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

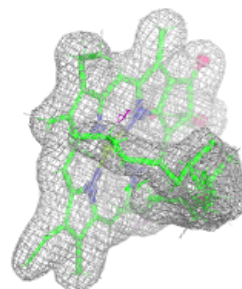
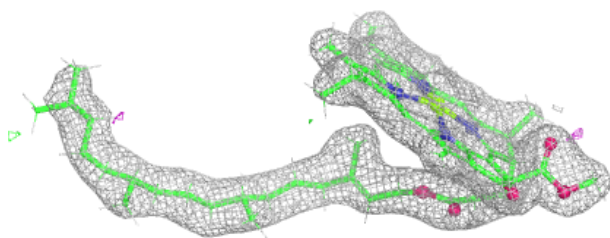
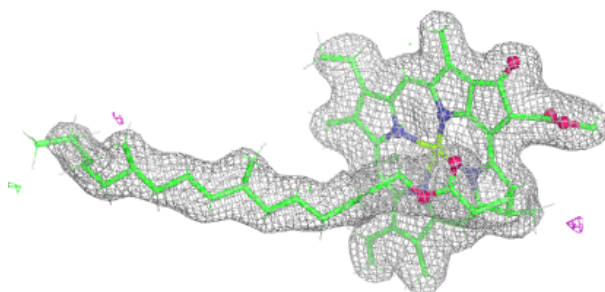


Electron density around CLA b 606:

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

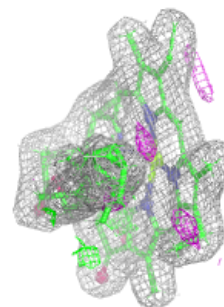
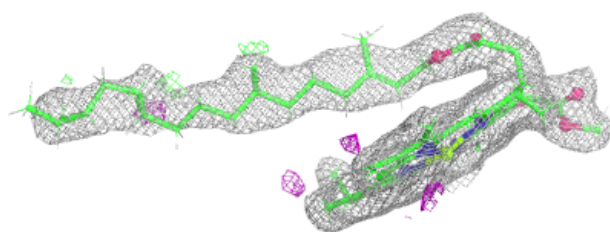
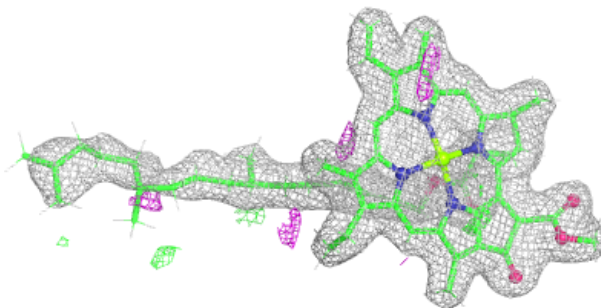
**Electron density around CLA b 607:**

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



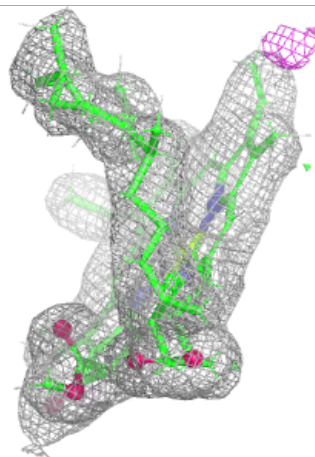
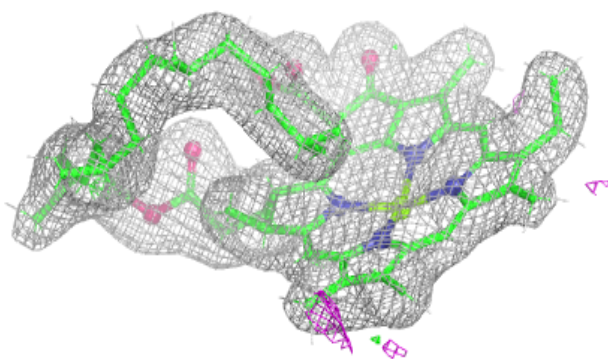
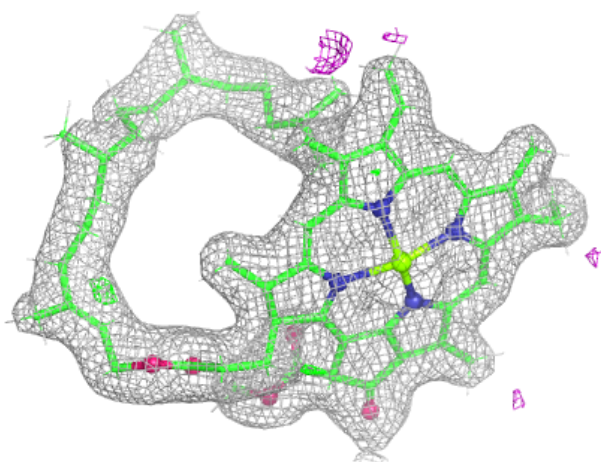
Electron density around CLA B 614:

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



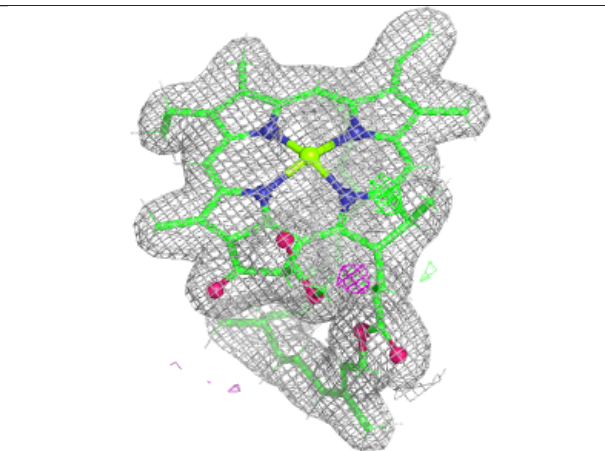
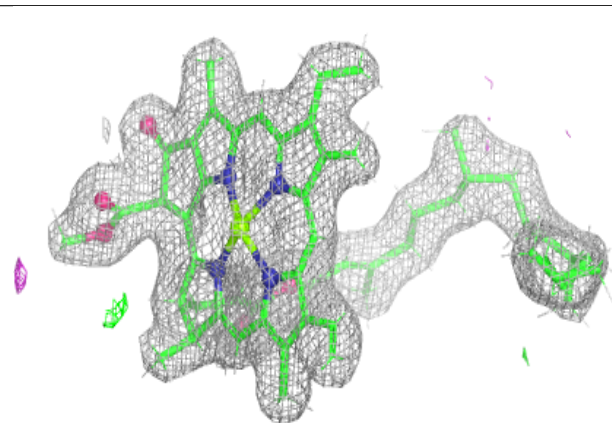
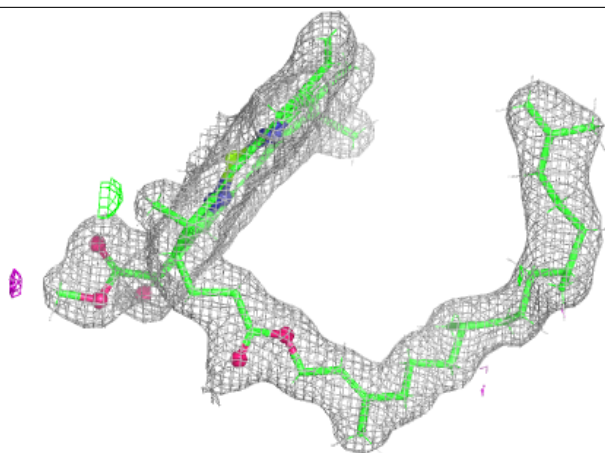
Electron density around CLA B 615:

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

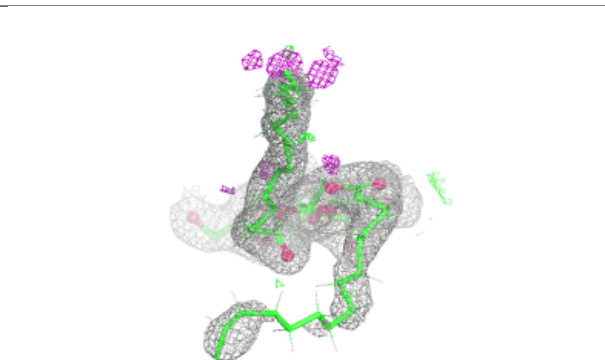
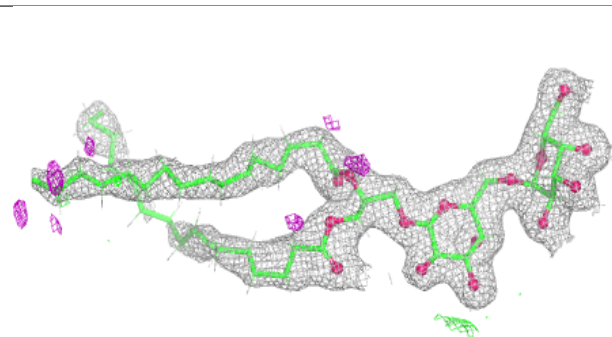
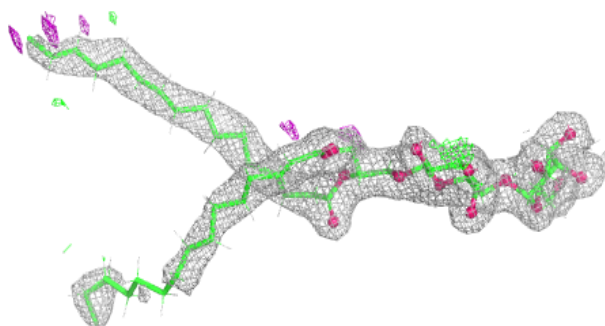


Electron density around CLA b 610:

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

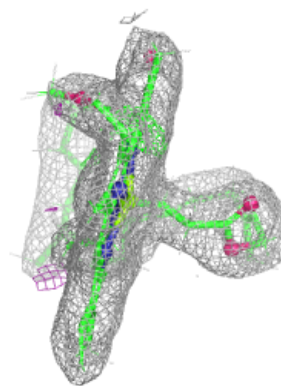
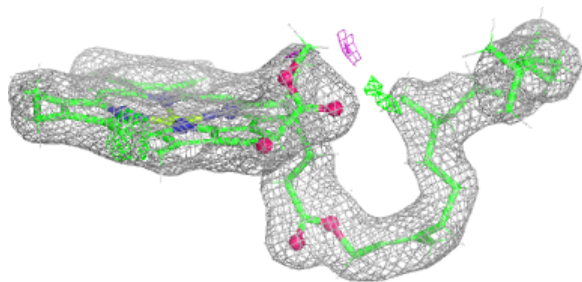
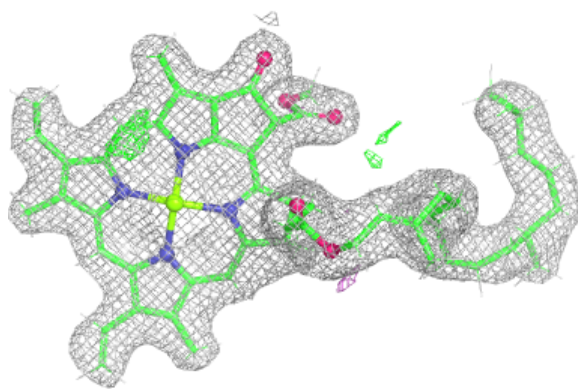
**Electron density around DGD C 521:**

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



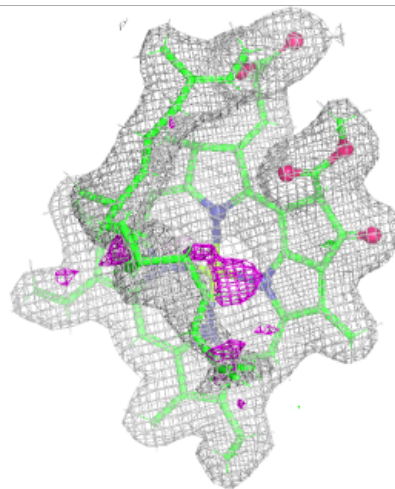
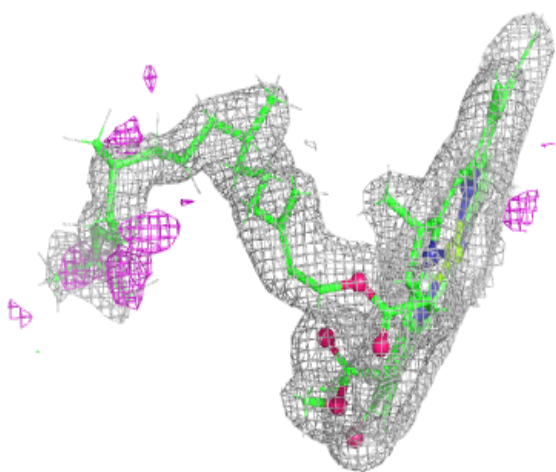
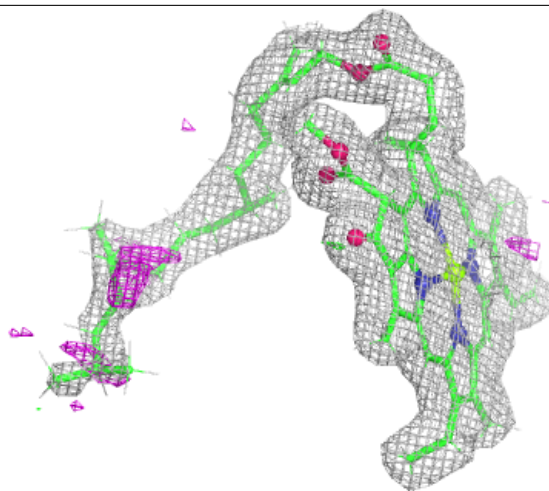
Electron density around CLA b 611:

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



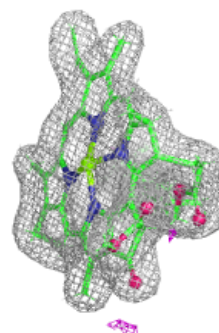
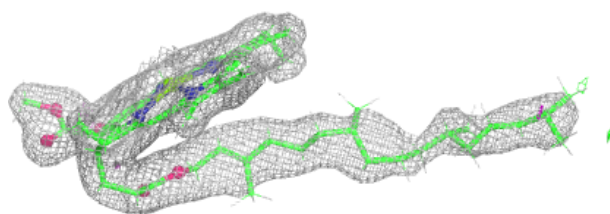
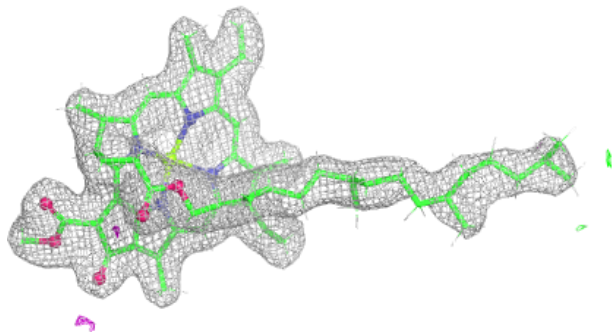
Electron density around CLA b 612:

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

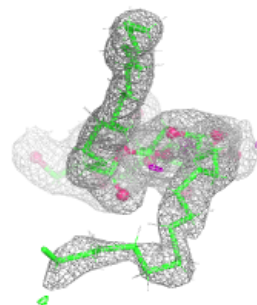
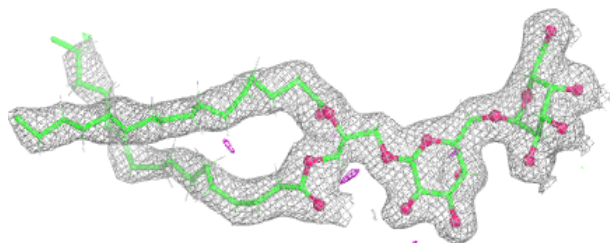
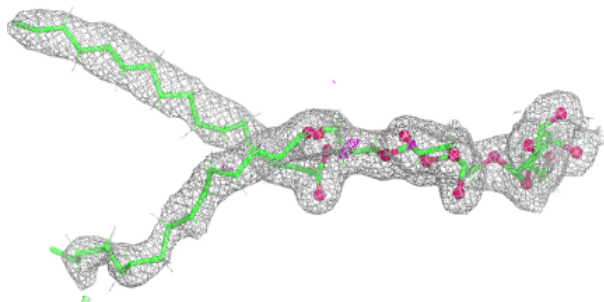


Electron density around CLA b 613:

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

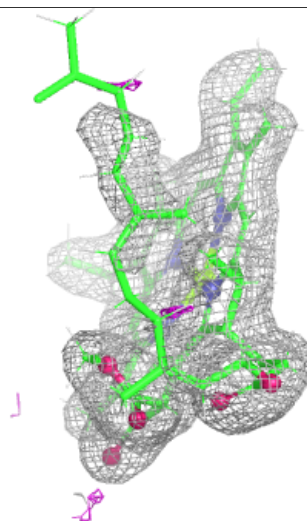
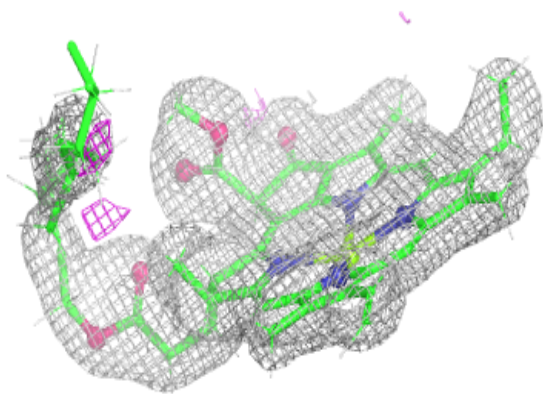
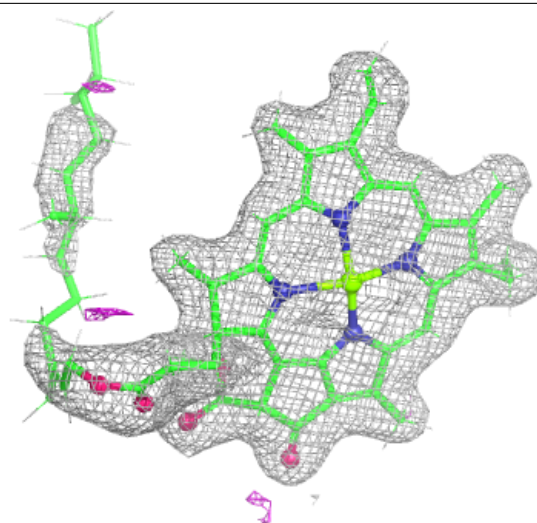
**Electron density around DGD c 519:**

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



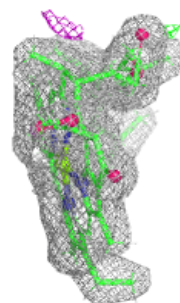
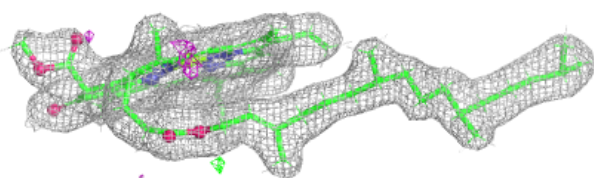
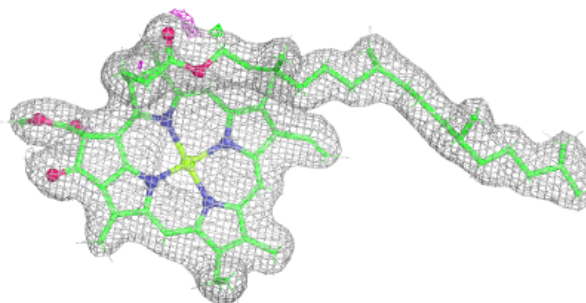
Electron density around CLA B 616:

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

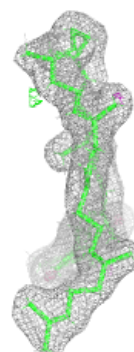
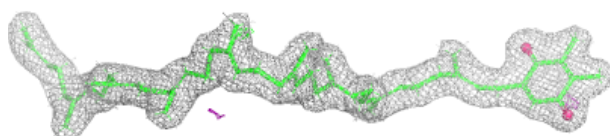
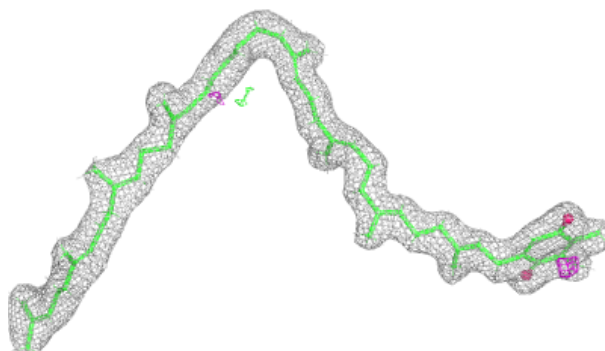


Electron density around CLA C 501:

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

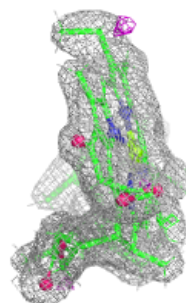
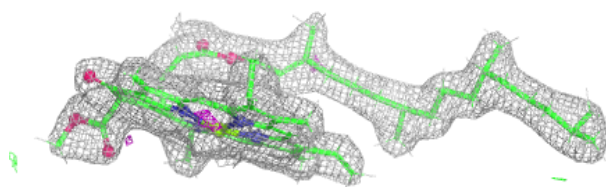
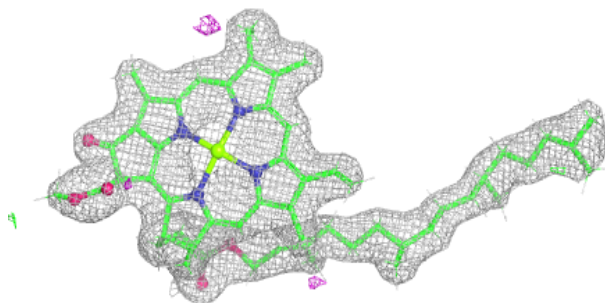
**Electron density around PL9 D 407:**

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

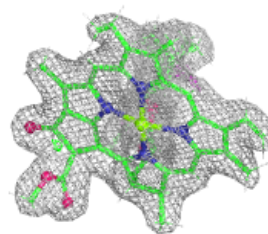
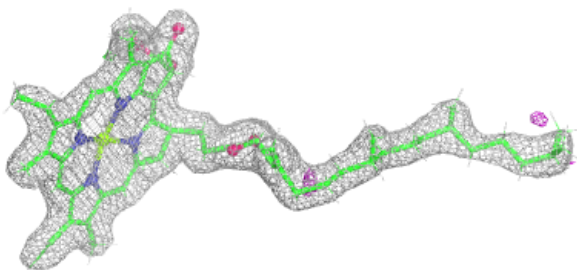
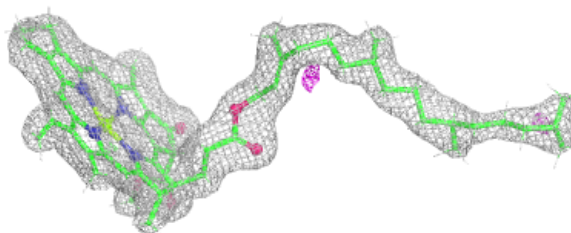


Electron density around CLA c 501:

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

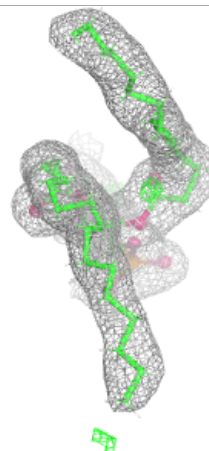
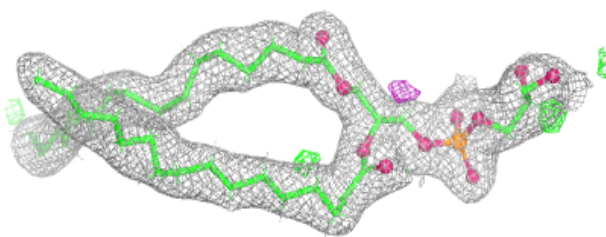
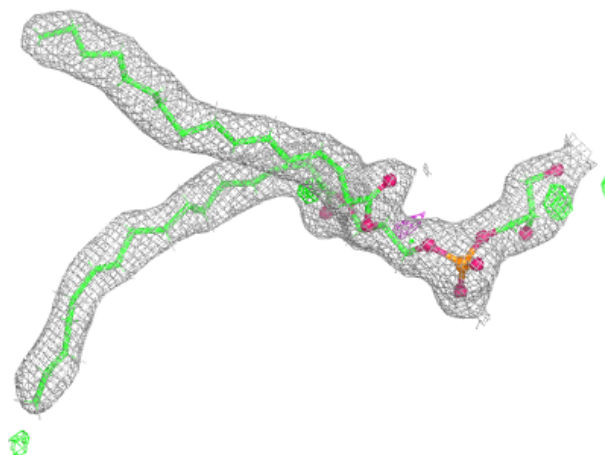
**Electron density around CLA c 502:**

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



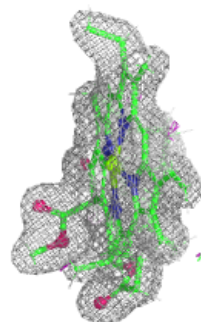
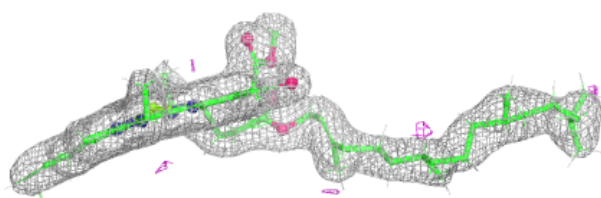
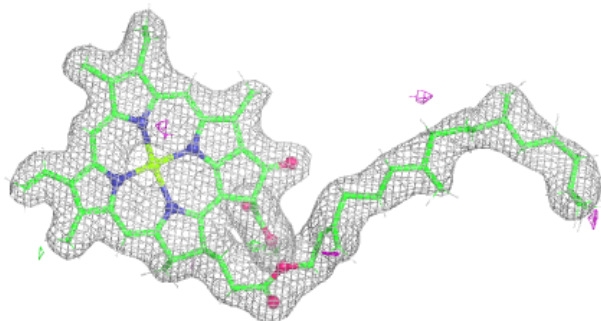
Electron density around LHG D 410:

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

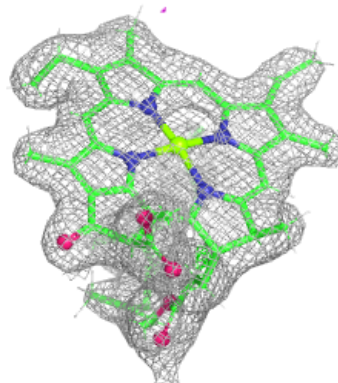
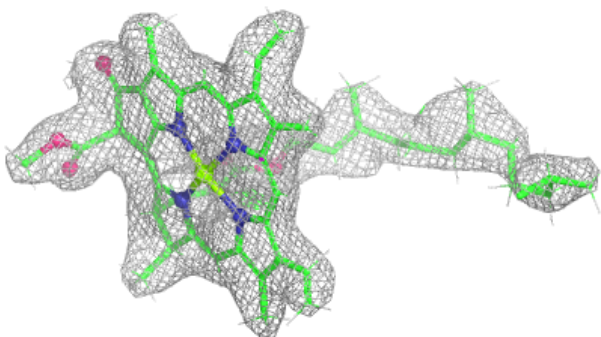
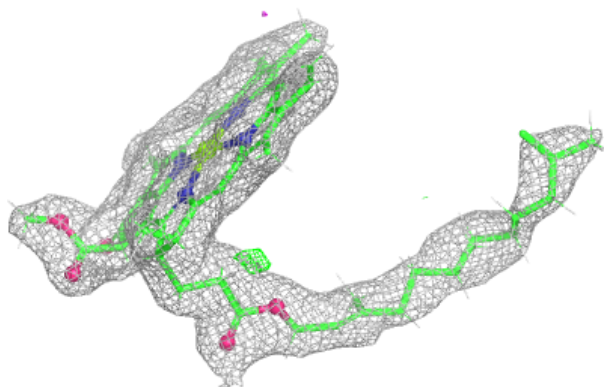


Electron density around CLA B 602:

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

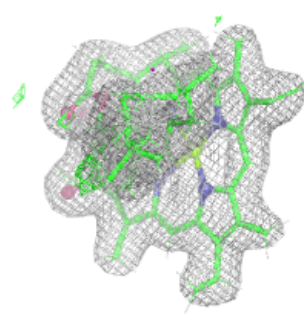
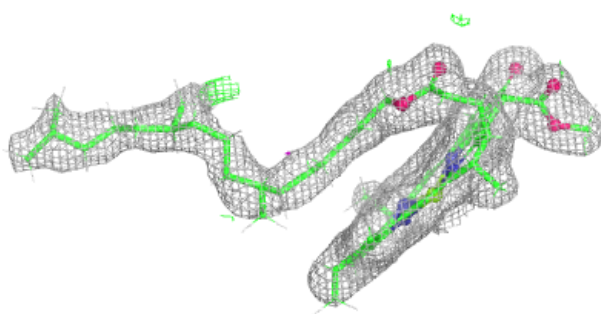
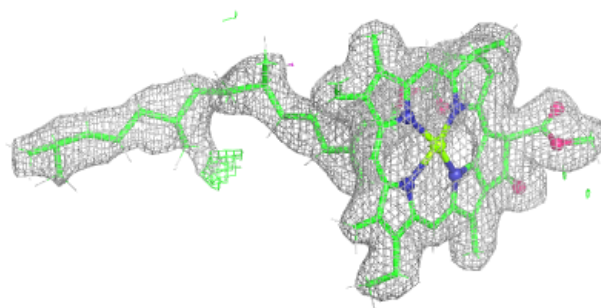
**Electron density around CLA c 504:**

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



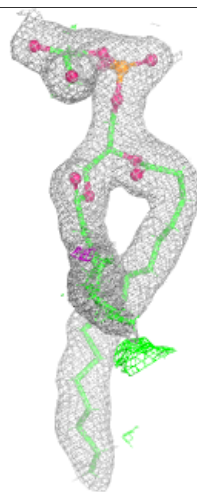
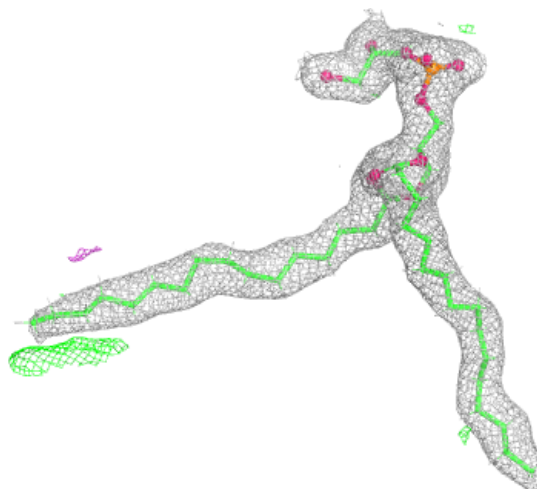
Electron density around CLA c 505:

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



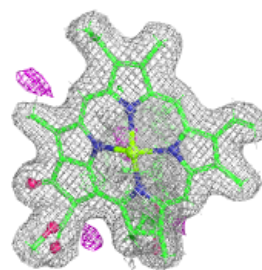
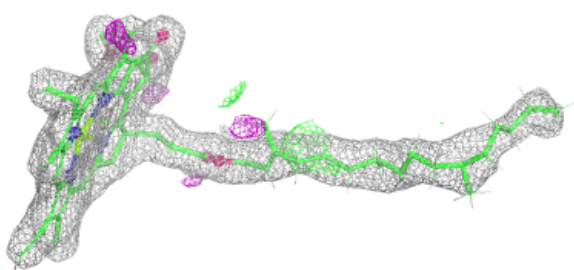
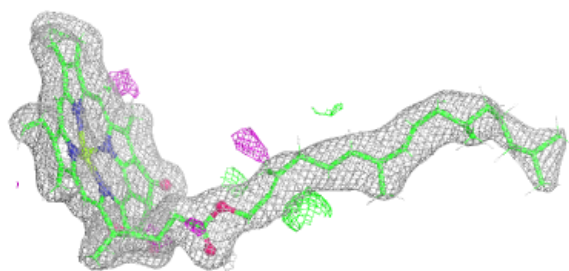
Electron density around LHG L 101:

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



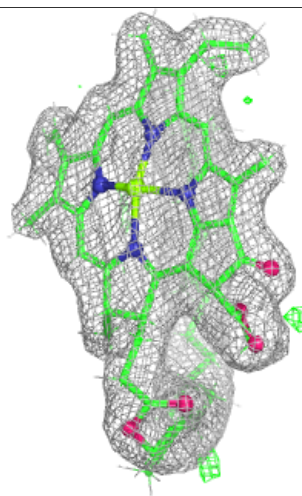
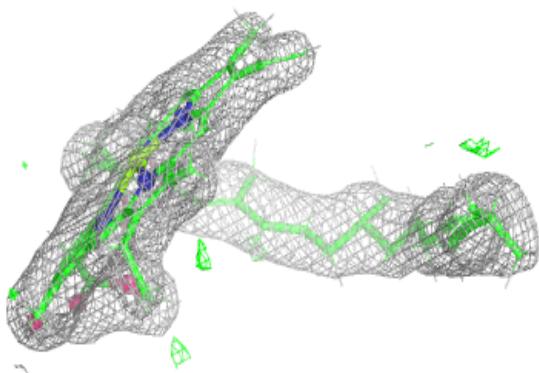
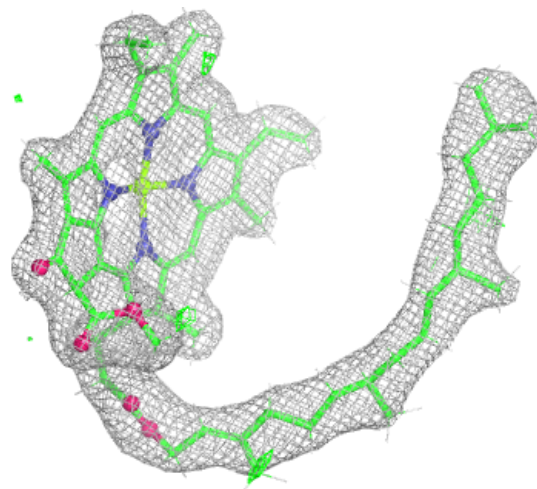
Electron density around CLA B 604:

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



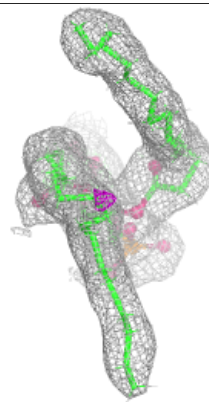
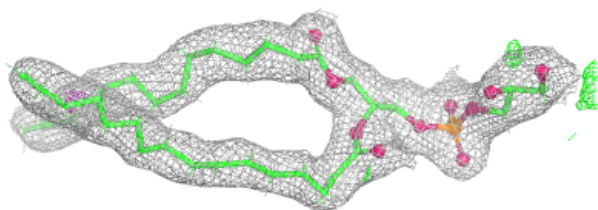
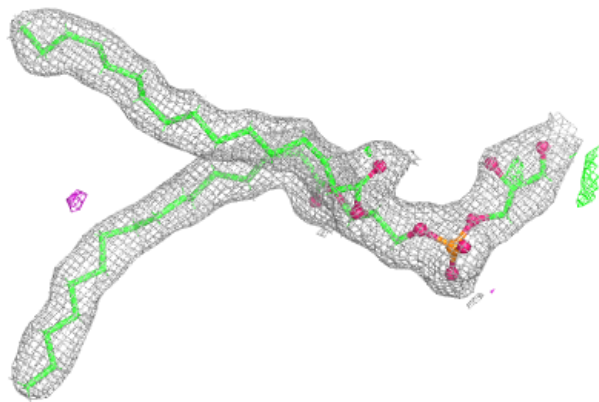
Electron density around CLA c 507:

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

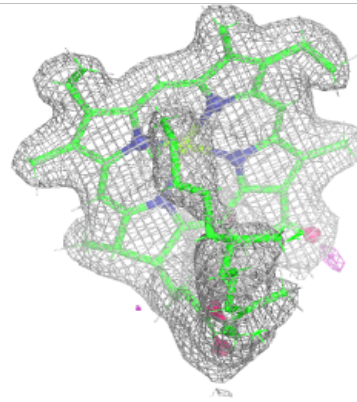
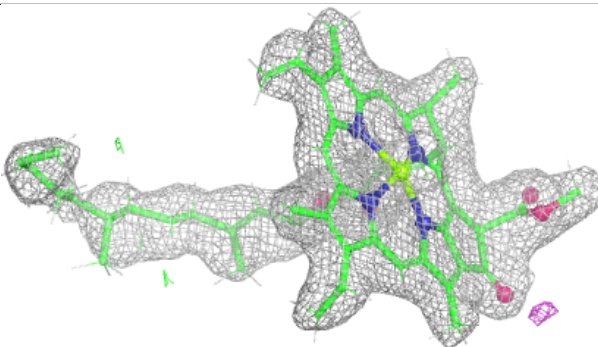
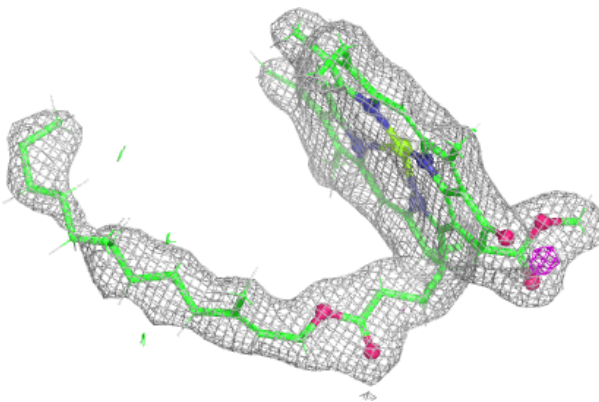


Electron density around LHG d 407:

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

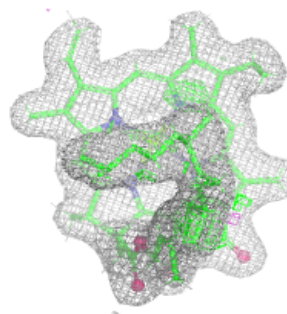
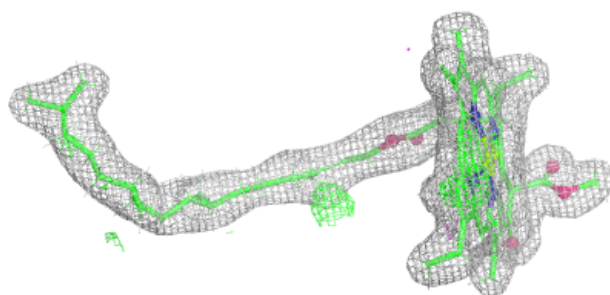
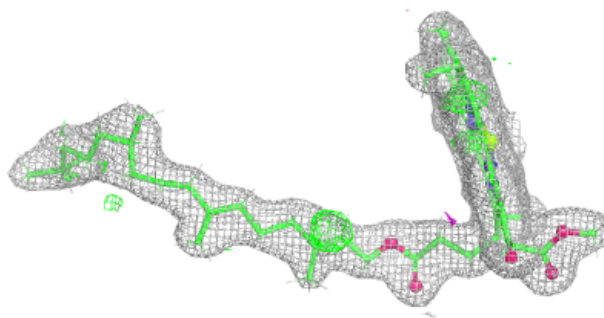
**Electron density around CLA C 504:**

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



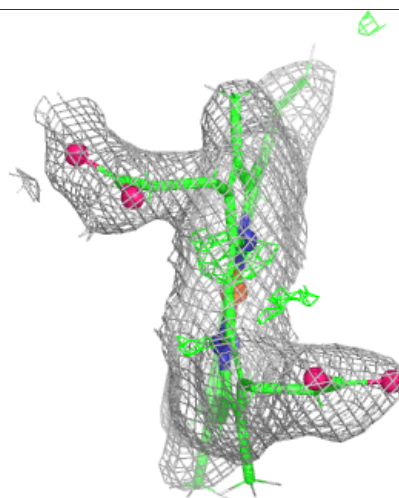
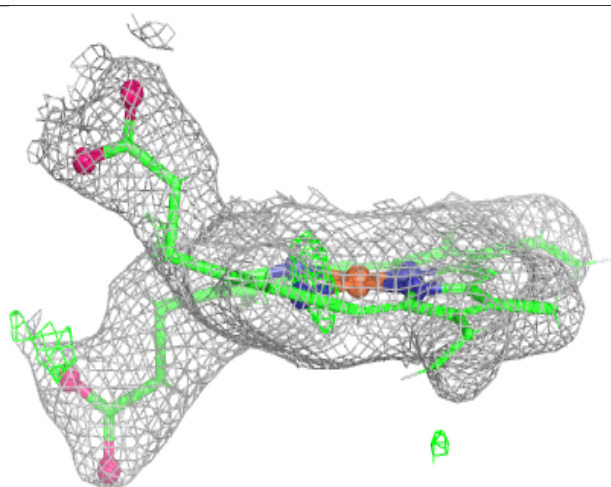
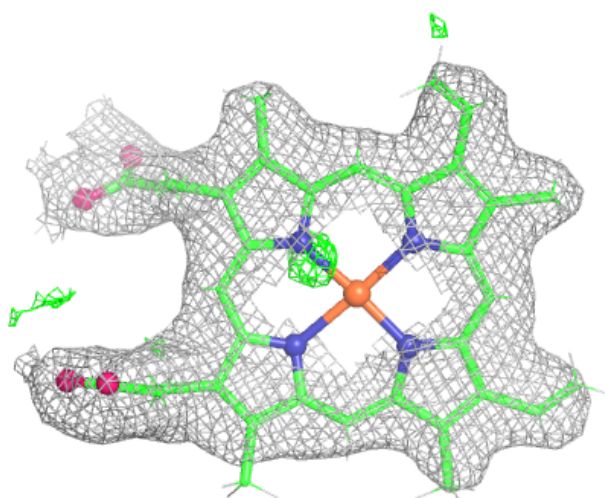
Electron density around CLA B 605:

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



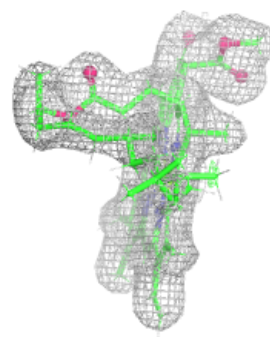
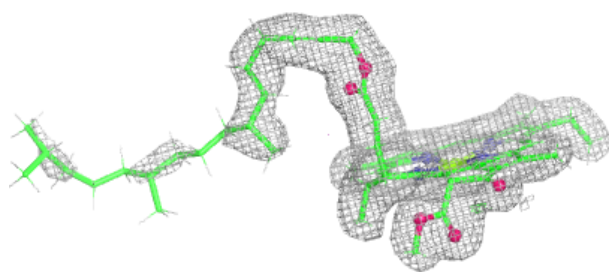
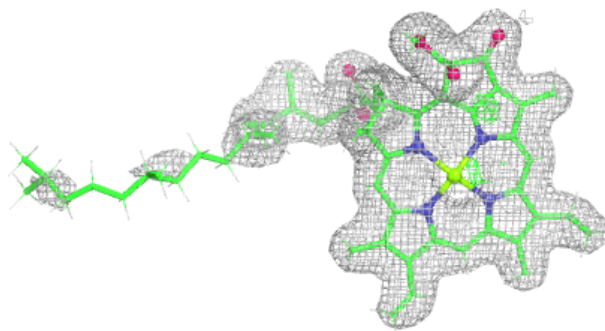
Electron density around HEM f 101:

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

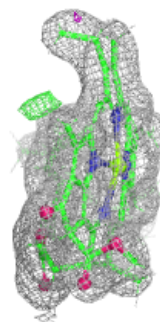
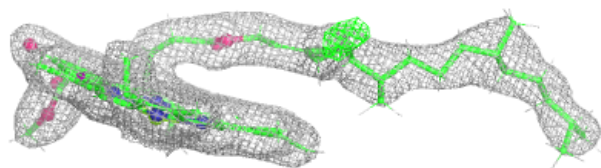
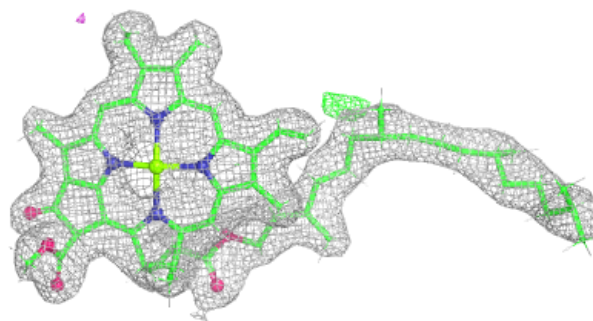


Electron density around CLA A 405:

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

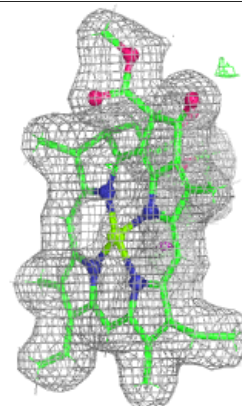
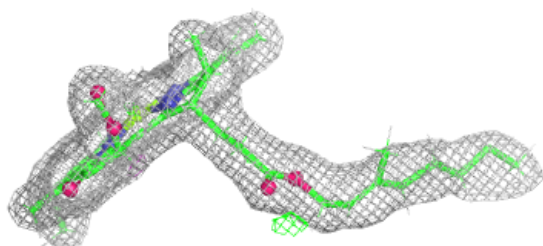
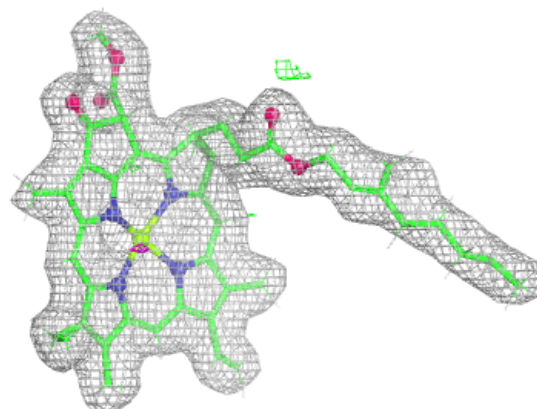
**Electron density around CLA B 603:**

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



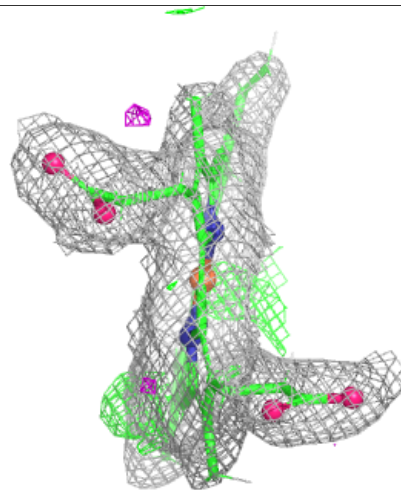
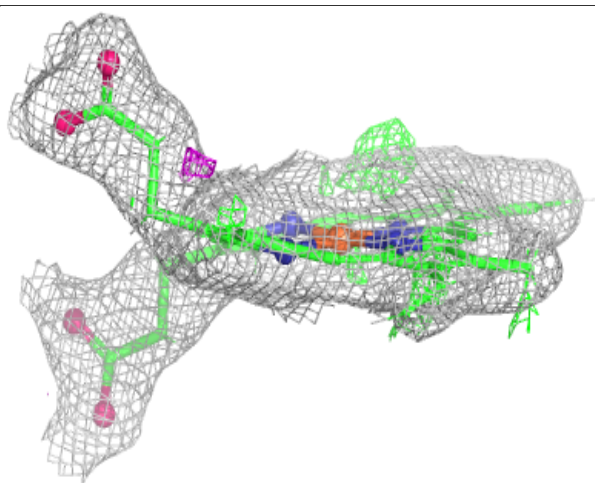
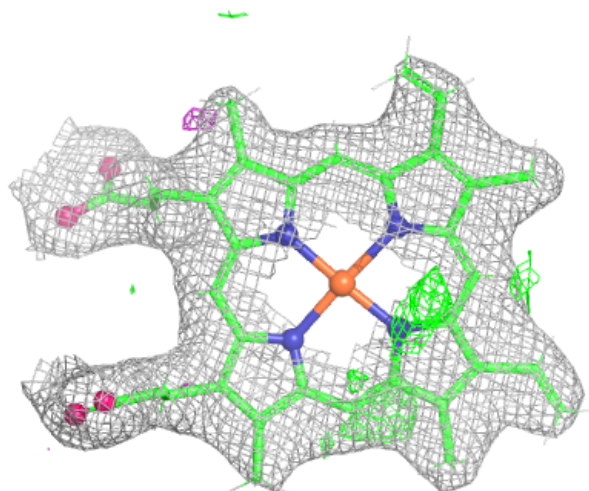
Electron density around CLA A 407:

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



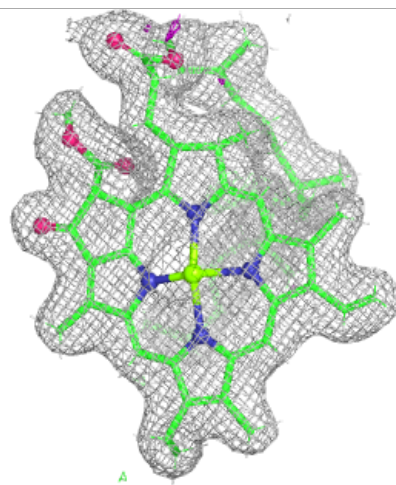
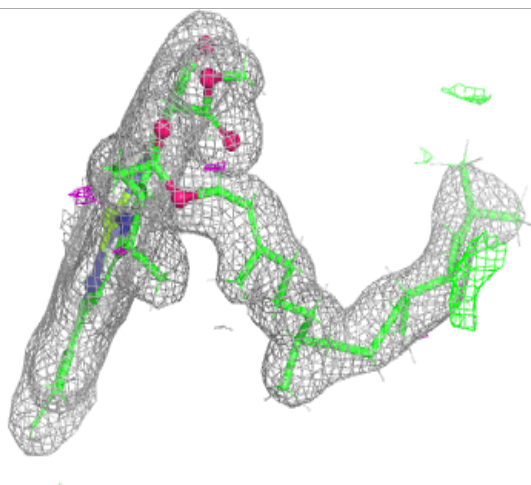
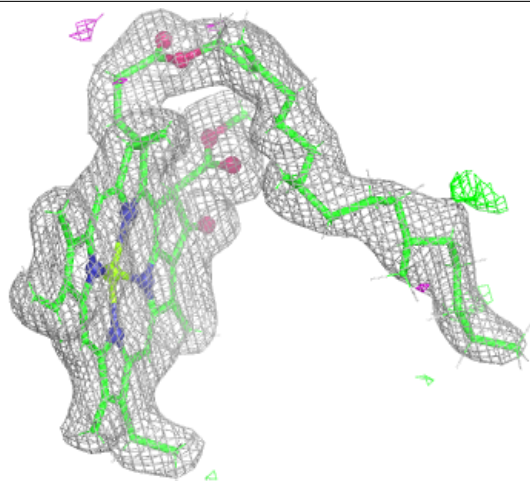
Electron density around HEM F 101:

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



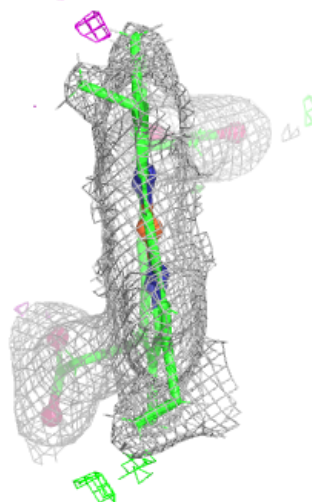
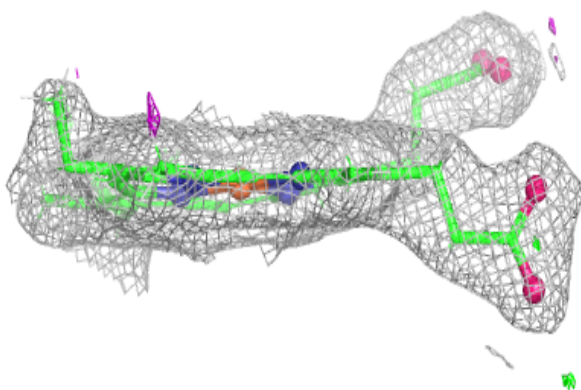
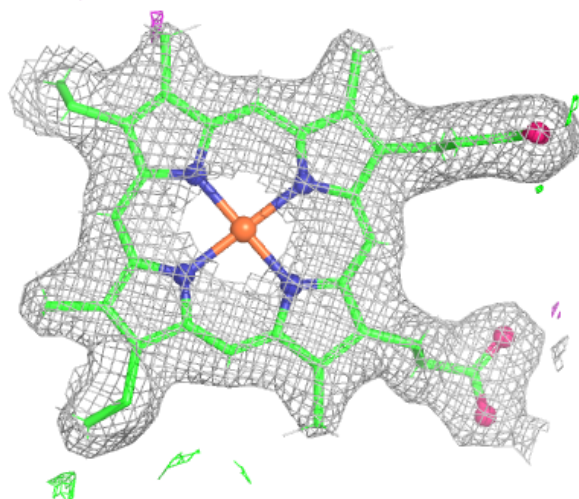
Electron density around CLA B 613:

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



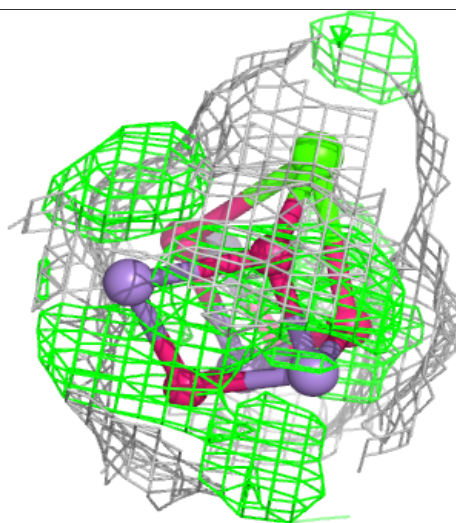
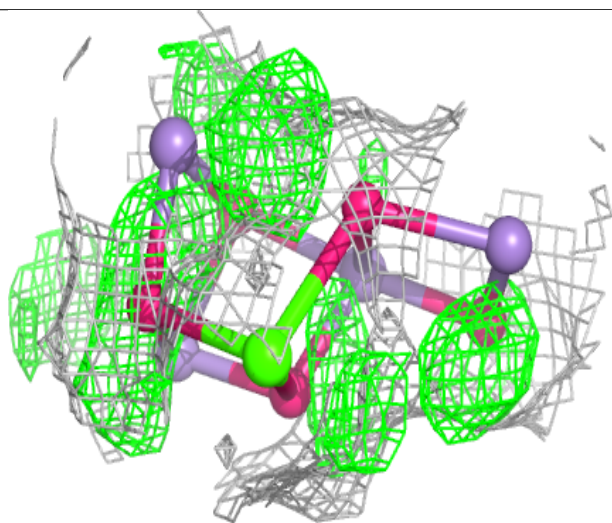
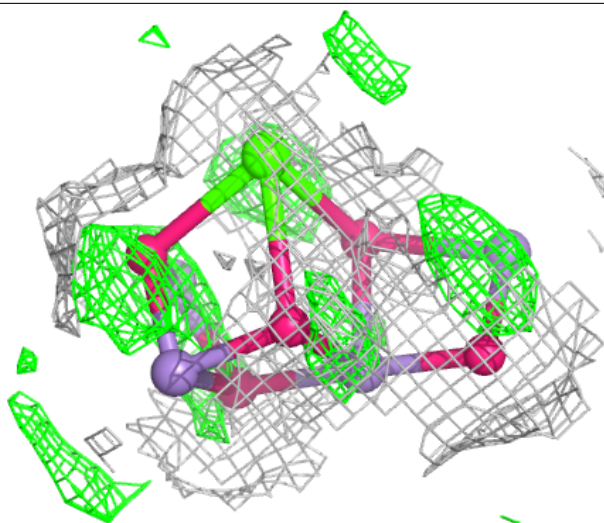
Electron density around HEC v 201:

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



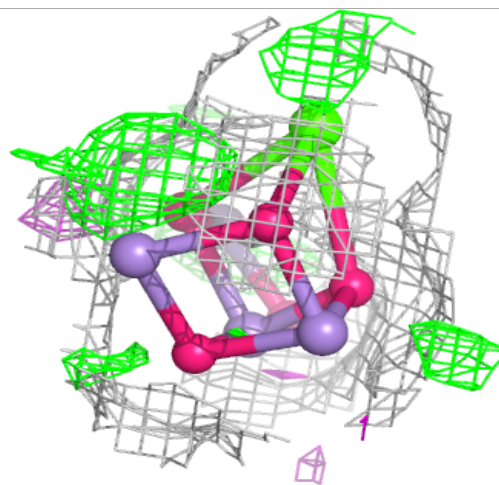
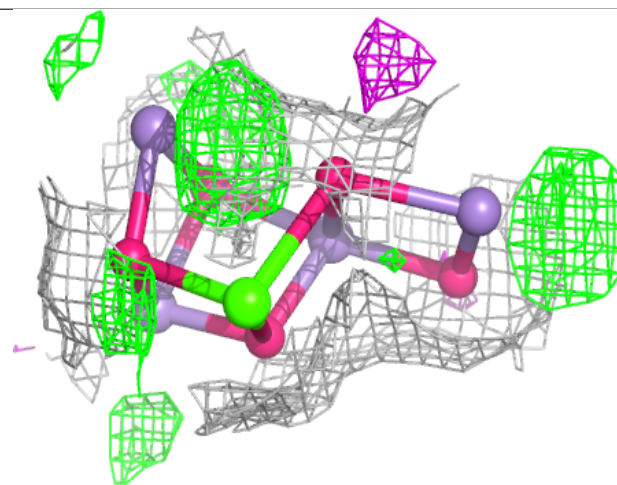
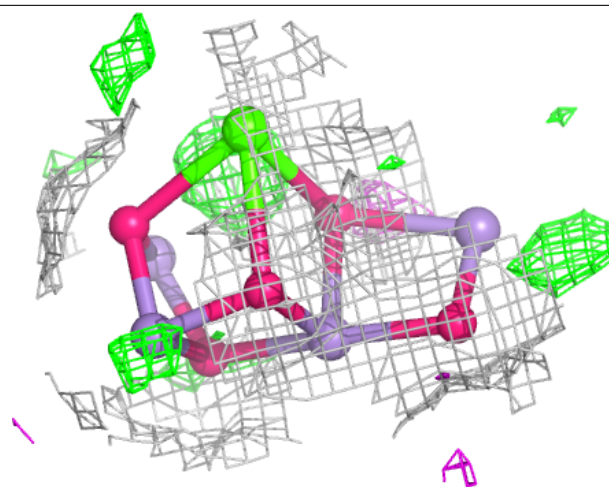
Electron density around OEX A 418:

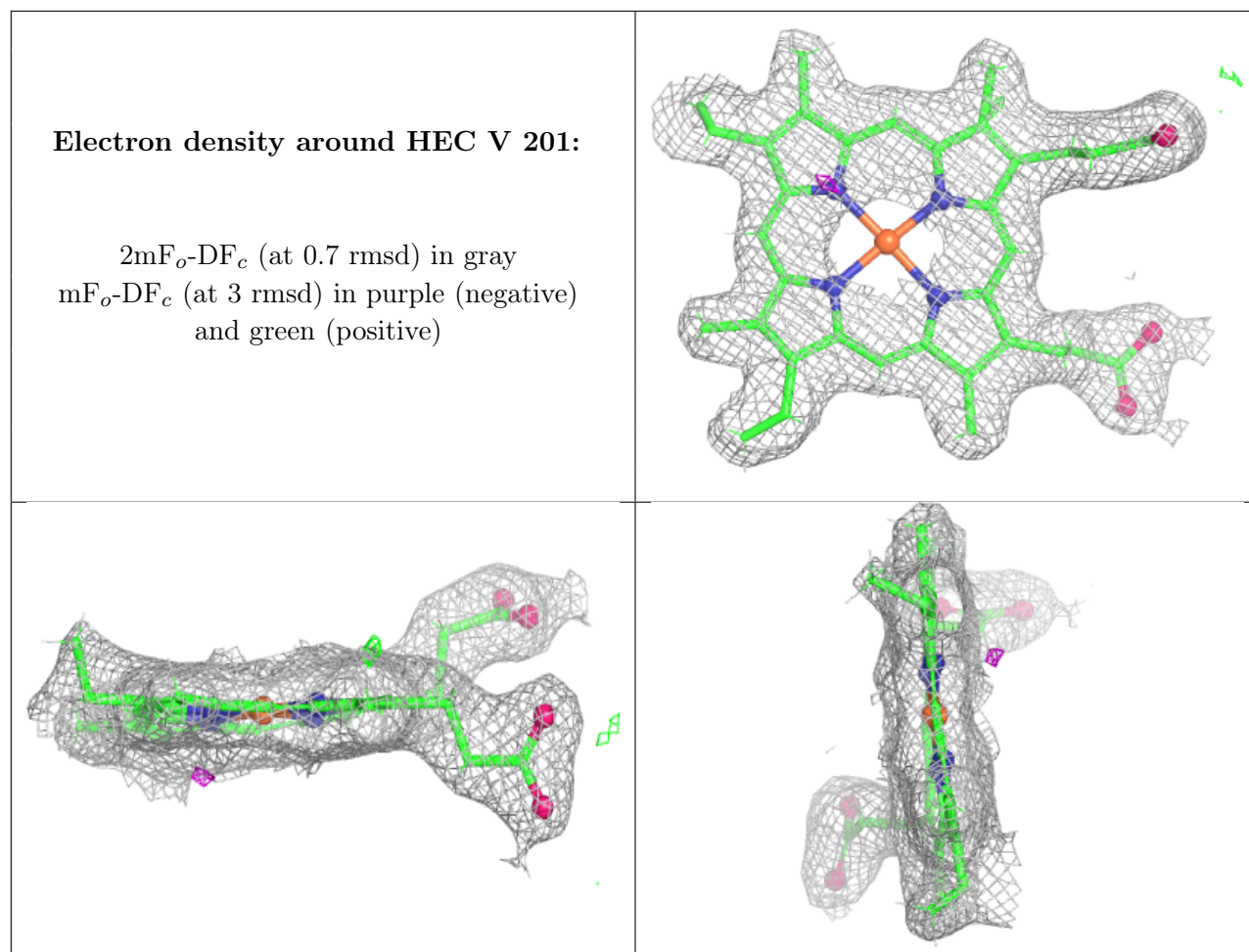
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 418:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.