



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:10 AM UTC

PDB ID : 6W1Q / pdb_00006w1q
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

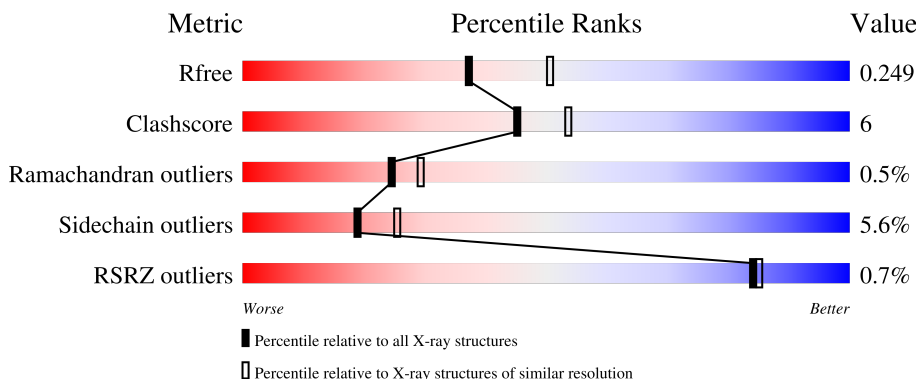
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	 87% 10% . .
1	a	344	 83% 14% . .

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

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Mol	Chain	Length	Quality of chain
2	B	506	
2	b	506	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	

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Mol	Chain	Length	Quality of chain
14	r	41	
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103197 atoms, of which 51556 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
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	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
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6767	2249	3341	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	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
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	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
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

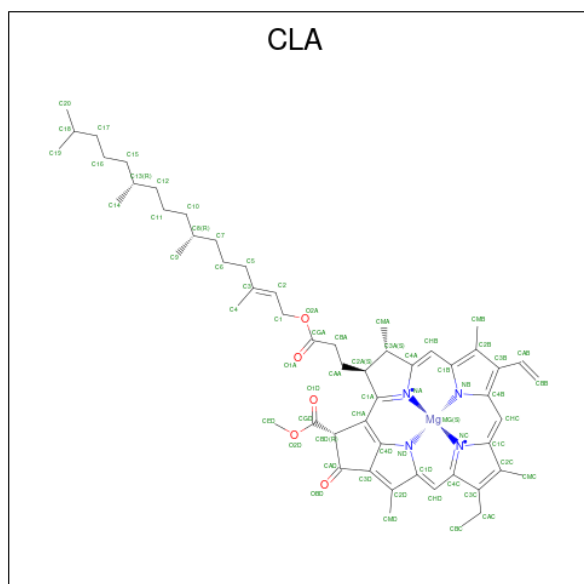
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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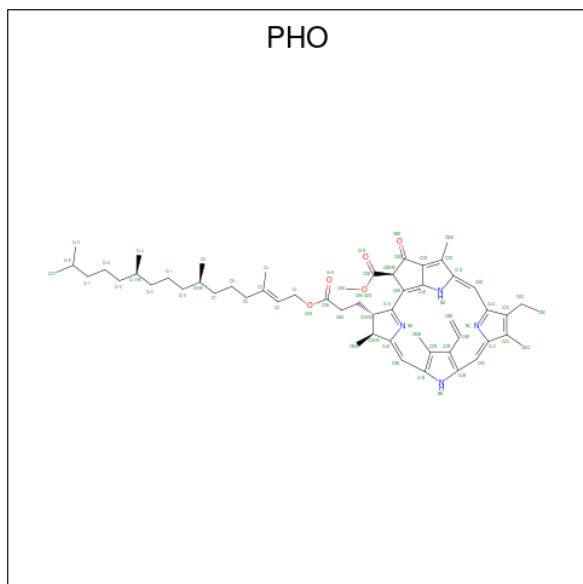
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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

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

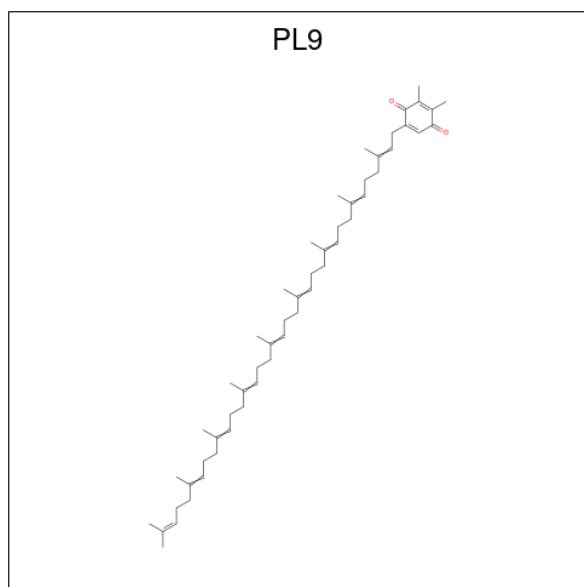


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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

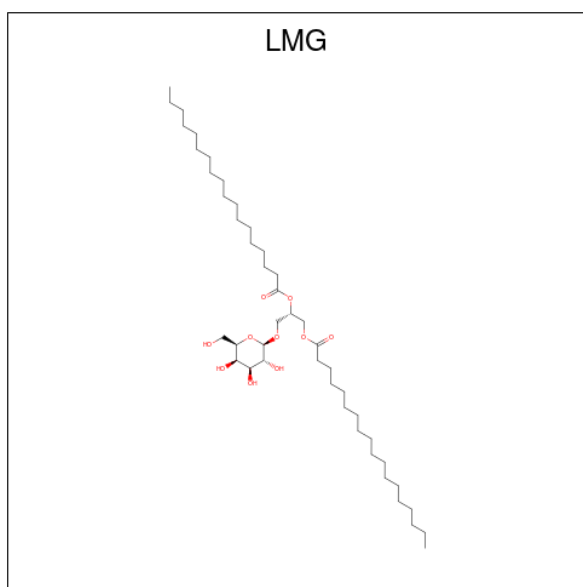
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



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

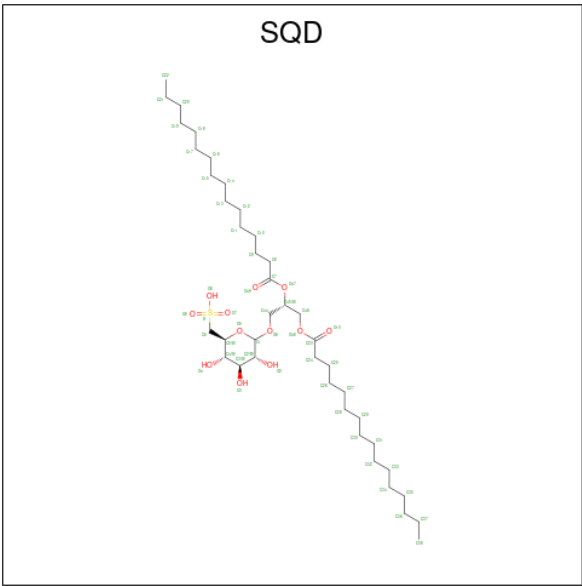
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			114	38	66	10		
26	B	1	Total	C	H	O	0	0
			68	24	40	4		
26	D	1	Total	C	H	O	0	0
			120	41	69	10		
26	D	1	Total	C	H	O	0	0
			78	27	45	6		
26	M	1	Total	C	H	O	0	0
			120	41	69	10		
26	Y	1	Total	C	H	O	0	0
			114	38	66	10		
26	a	1	Total	C	H	O	0	0
			140	45	85	10		
26	b	1	Total	C	H	O	0	0
			141	45	86	10		
26	c	1	Total	C	H	O	0	0
			79	27	42	10		
26	c	1	Total	C	H	O	0	0
			116	38	68	10		
26	c	1	Total	C	H	O	0	0
			117	39	68	10		
26	d	1	Total	C	H	O	0	0
			101	34	57	10		
26	m	1	Total	C	H	O	0	0
			122	41	71	10		

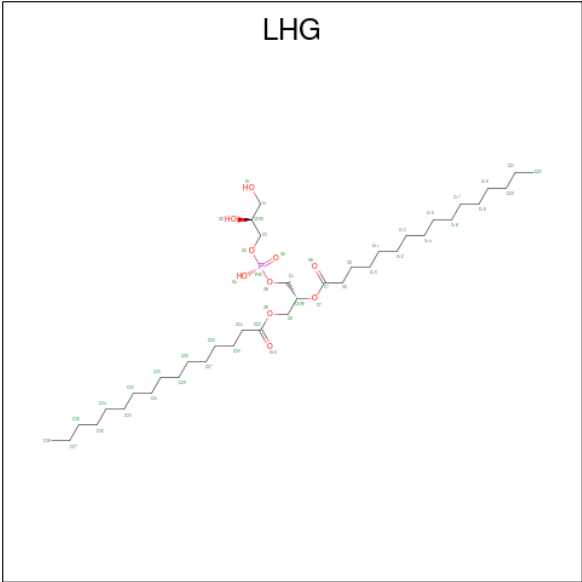
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



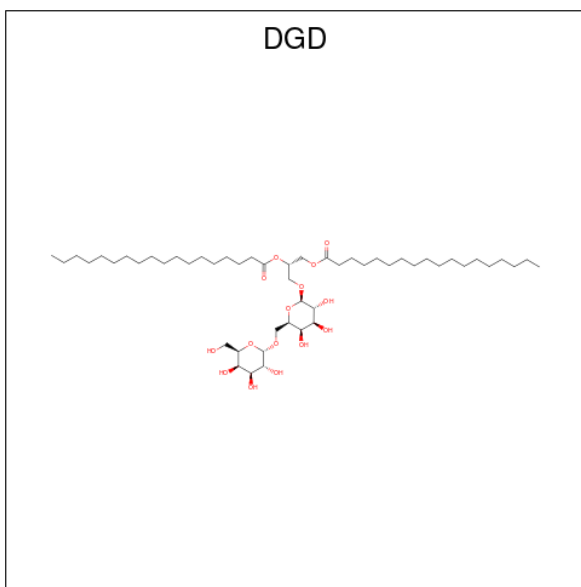
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			121	39	69	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

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



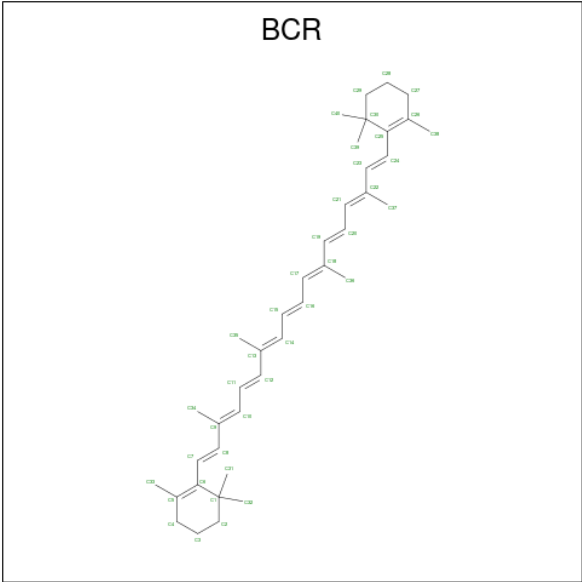
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	D	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	b	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			160	51	94	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			141	47	79	15		
29	H	1	Total	C	H	O	0	0
			139	47	77	15		
29	c	1	Total	C	H	O	0	0
			141	47	79	15		
29	c	1	Total	C	H	O	0	0
			140	47	78	15		
29	c	1	Total	C	H	O	0	0
			139	47	77	15		
29	h	1	Total	C	H	O	0	0
			141	47	79	15		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



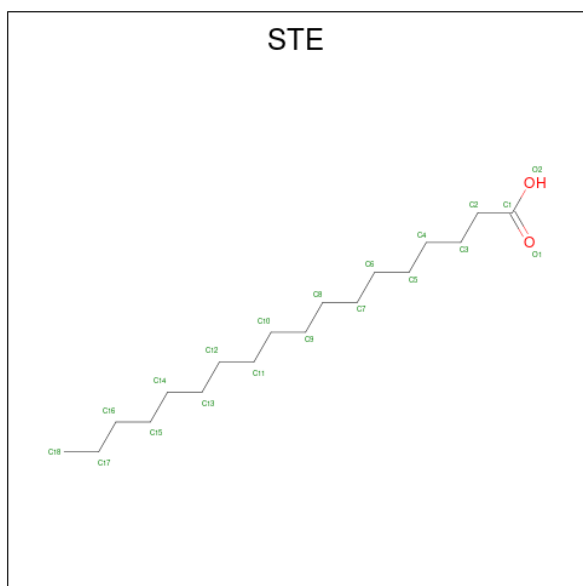
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	B	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	C	1	Total	C	H	0	0
			96	40	56		
30	D	1	Total	C	H	0	0
			96	40	56		
30	H	1	Total	C	H	0	0
			96	40	56		
30	I	1	Total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

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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			43	15	26	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		

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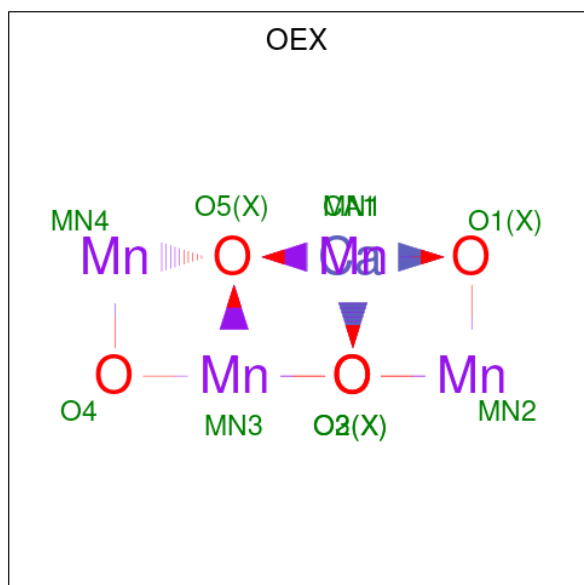
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C H 47 16 31	0	0
31	B	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	C	1	Total C H 47 16 31	0	0
31	C	1	Total C H O 28 10 16 2	0	0
31	H	1	Total C H 53 18 35	0	0
31	I	1	Total C H 41 15 26	0	0
31	J	1	Total C H O 28 10 16 2	0	0
31	L	1	Total C H O 28 10 16 2	0	0
31	M	1	Total C H O 37 13 22 2	0	0
31	M	1	Total C H 26 10 16	0	0
31	M	1	Total C H 53 18 35	0	0
31	R	1	Total C H O 28 10 16 2	0	0
31	X	1	Total C H O 55 18 35 2	0	0
31	Z	1	Total C H 20 8 12	0	0
31	a	1	Total C H O 28 10 16 2	0	0
31	a	1	Total C H 41 15 26	0	0
31	b	1	Total C H 47 16 31	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H O 40 14 24 2	0	0
31	b	1	Total C H 44 15 29	0	0

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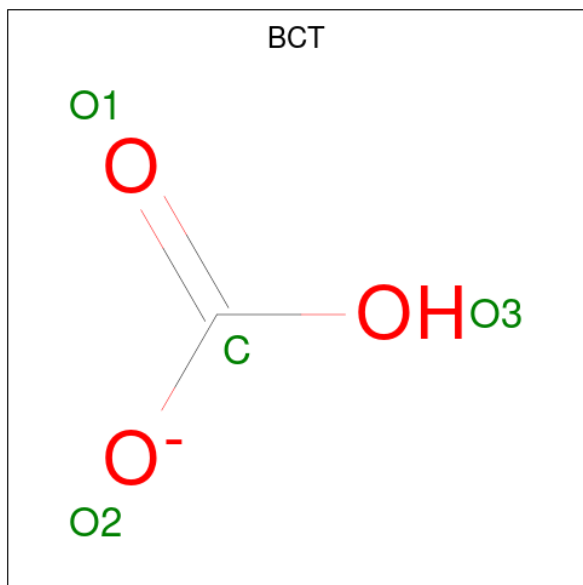
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	k	1	Total C H O 28 10 16 2	0	0
31	t	1	Total C H O 34 12 20 2	0	0
31	t	1	Total C H 26 10 16	0	0
31	x	1	Total C H O 55 18 35 2	0	0

- Molecule 32 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



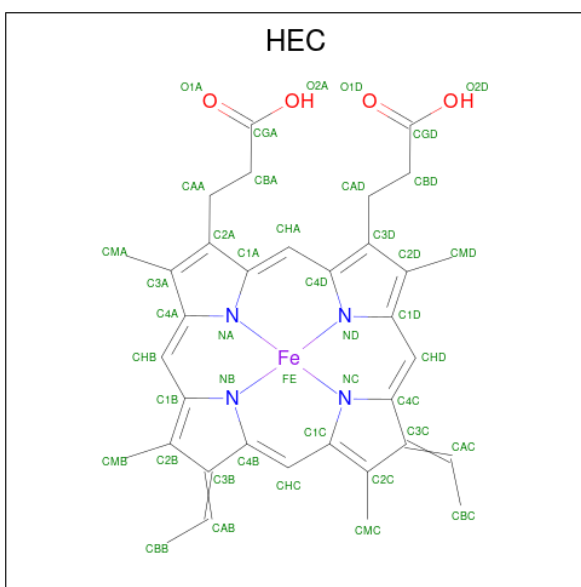
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	C	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
32	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



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

- Molecule 34 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	112	Total	O	0	0
			112	112		
36	B	142	Total	O	0	0
			142	142		
36	C	125	Total	O	0	0
			125	125		
36	D	96	Total	O	0	0
			96	96		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	E	22	Total O 22 22	0	0
36	F	6	Total O 6 6	0	0
36	H	16	Total O 16 16	0	0
36	I	10	Total O 10 10	0	0
36	J	14	Total O 14 14	0	0
36	K	3	Total O 3 3	0	0
36	L	10	Total O 10 10	0	0
36	M	9	Total O 9 9	0	0
36	O	60	Total O 60 60	0	0
36	R	11	Total O 11 11	0	0
36	T	8	Total O 8 8	0	0
36	U	28	Total O 28 28	0	0
36	V	49	Total O 49 49	0	0
36	X	10	Total O 10 10	0	0
36	Y	2	Total O 2 2	0	0
36	Z	7	Total O 7 7	0	0
36	a	96	Total O 96 96	0	0
36	b	116	Total O 116 116	0	0
36	c	108	Total O 108 108	0	0
36	d	87	Total O 87 87	0	0
36	e	11	Total O 11 11	0	0

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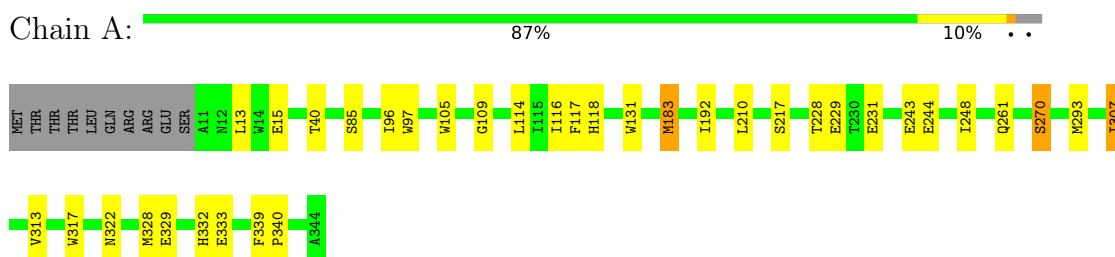
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	f	7	Total 7	O 7	0	0
36	h	17	Total 17	O 17	0	0
36	i	14	Total 14	O 14	0	0
36	j	8	Total 8	O 8	0	0
36	k	7	Total 7	O 7	0	0
36	l	11	Total 11	O 11	0	0
36	m	4	Total 4	O 4	0	0
36	o	67	Total 67	O 67	0	0
36	r	3	Total 3	O 3	0	0
36	t	8	Total 8	O 8	0	0
36	u	34	Total 34	O 34	0	0
36	v	30	Total 30	O 30	0	0
36	x	6	Total 6	O 6	0	0
36	y	12	Total 12	O 12	0	0
36	z	6	Total 6	O 6	0	0

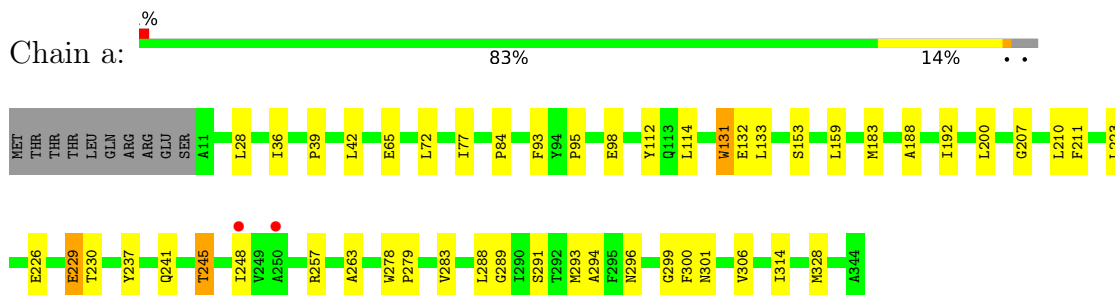
3 Residue-property plots [i](#)

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

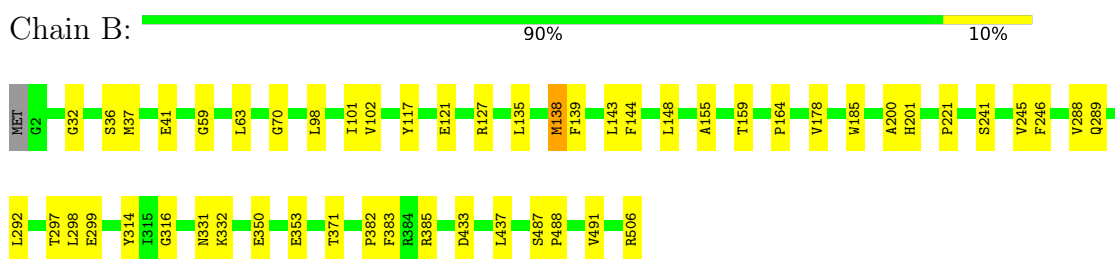
- Molecule 1: Photosystem II protein D1 1



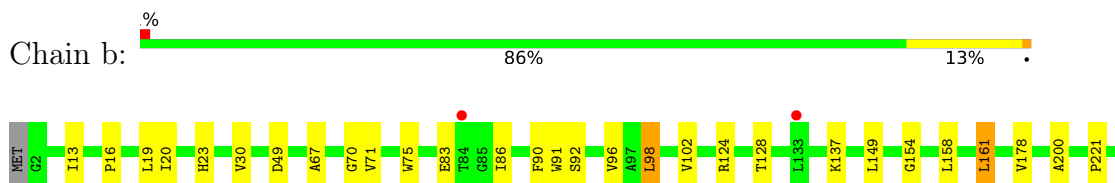
- Molecule 1: Photosystem II protein D1 1

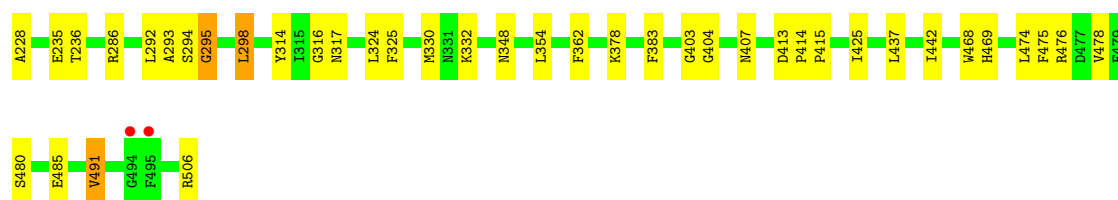


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





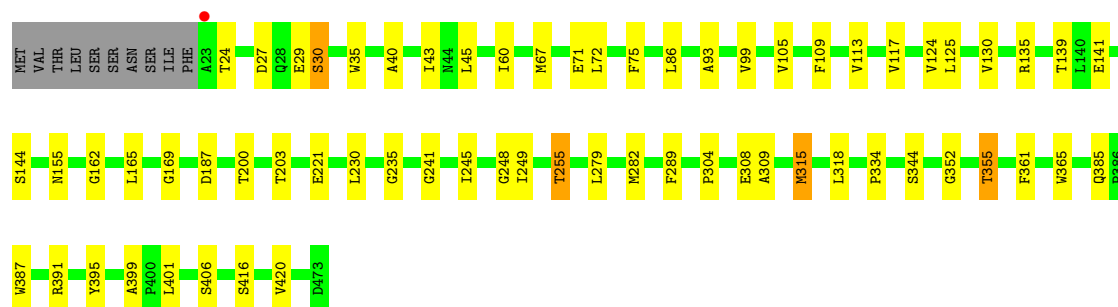
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12% ..



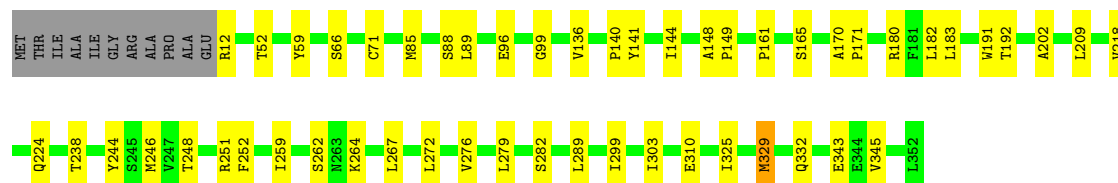
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 84% 13% ..



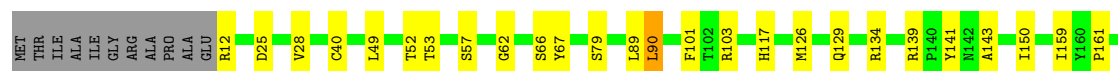
• Molecule 4: Photosystem II D2 protein

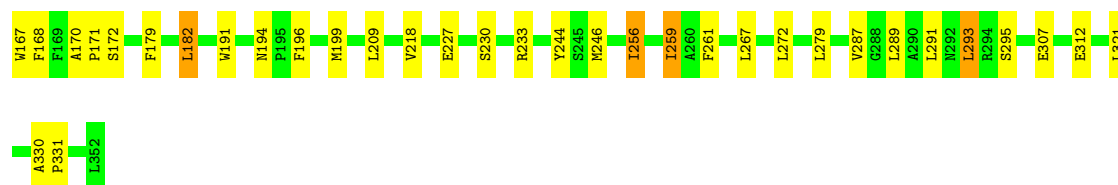
Chain D: 82% 14% .



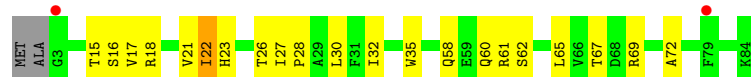
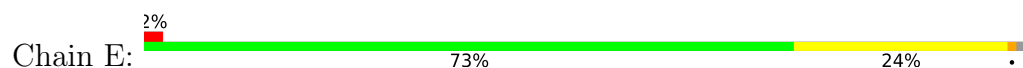
• Molecule 4: Photosystem II D2 protein

Chain d: 80% 16% ..





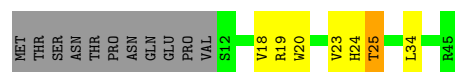
- Molecule 5: Cytochrome b559 subunit alpha



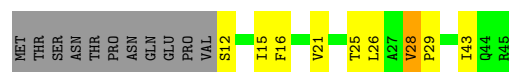
- Molecule 5: Cytochrome b559 subunit alpha



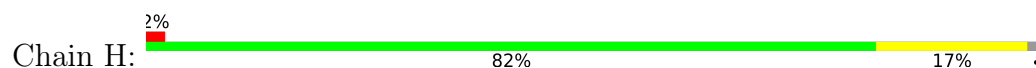
- Molecule 6: Cytochrome b559 subunit beta



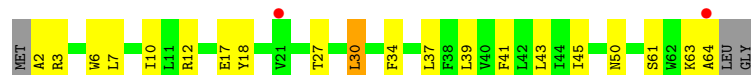
- Molecule 6: Cytochrome b559 subunit beta



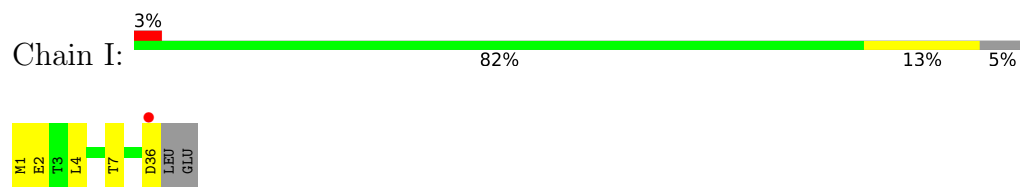
- Molecule 7: Photosystem II reaction center protein H



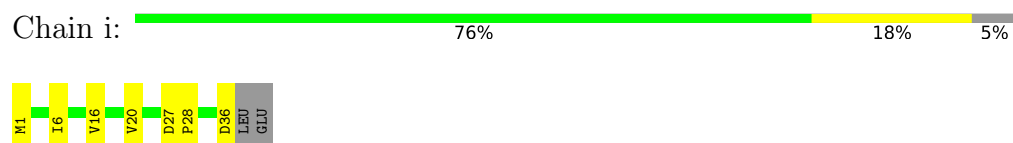
- Molecule 7: Photosystem II reaction center protein H



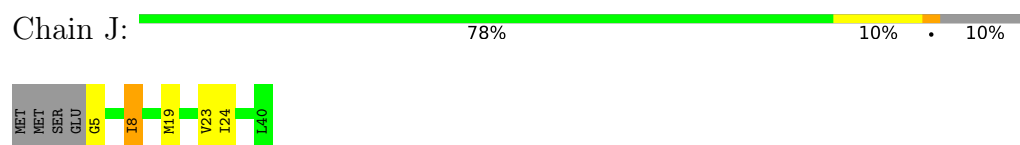
- Molecule 8: Photosystem II reaction center protein I



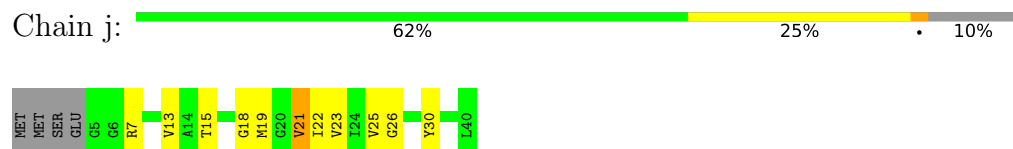
- Molecule 8: Photosystem II reaction center protein I



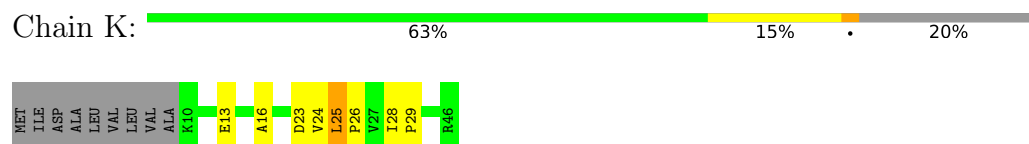
- Molecule 9: Photosystem II reaction center protein J



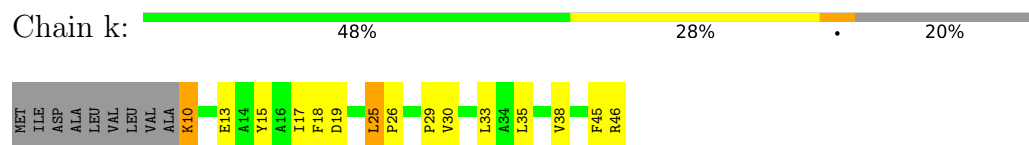
- Molecule 9: Photosystem II reaction center protein J



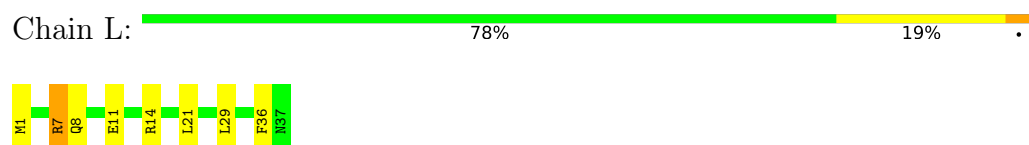
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

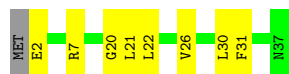


- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

Chain l:  76% 22% .



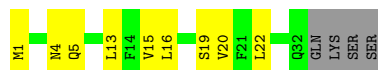
- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% . 8%



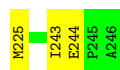
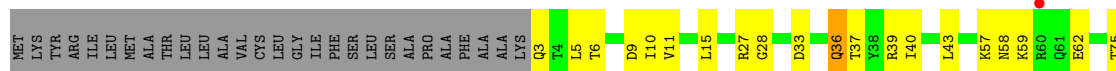
- Molecule 12: Photosystem II reaction center protein M

Chain m:  64% 25% 11%



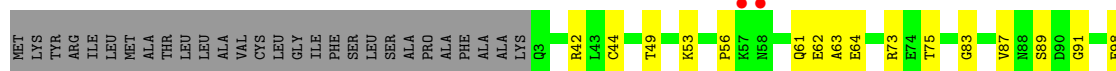
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  % 69% 19% . 10%



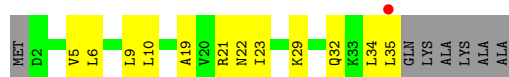
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  % 77% 13% 10%

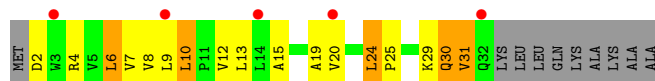


- Molecule 14: Photosystem II protein Y

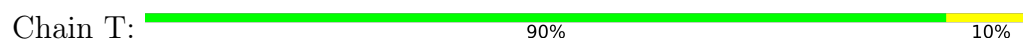
Chain R:  % 54% 29% 17%



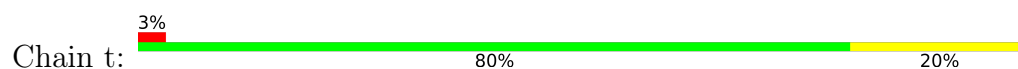
- Molecule 14: Photosystem II protein Y



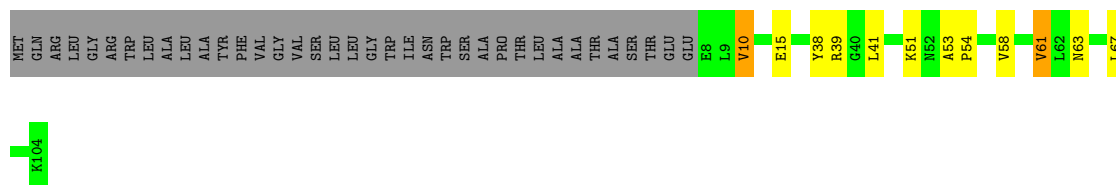
- Molecule 15: Photosystem II reaction center protein T



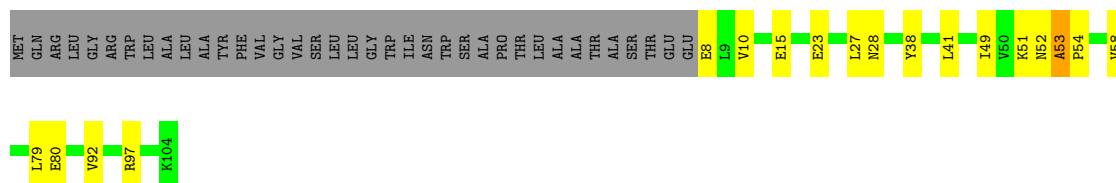
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein

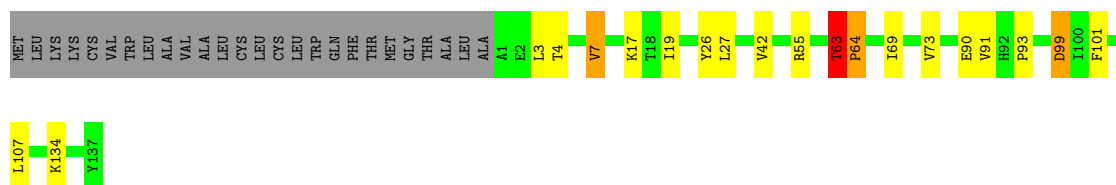


- Molecule 16: Photosystem II 12 kDa extrinsic protein

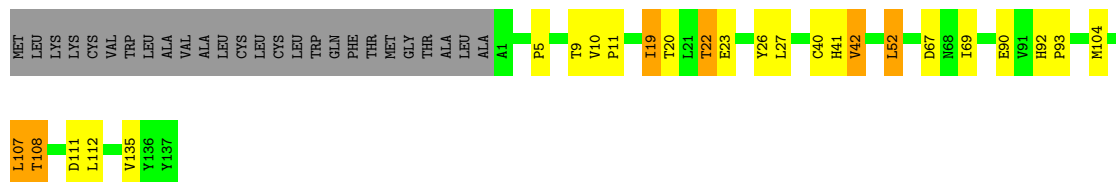


- Molecule 17: Cytochrome c-550

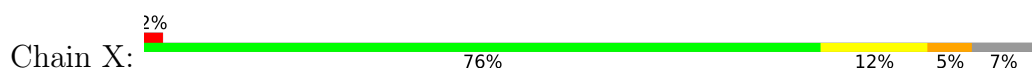




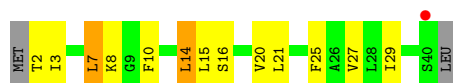
- Molecule 17: Cytochrome c-550



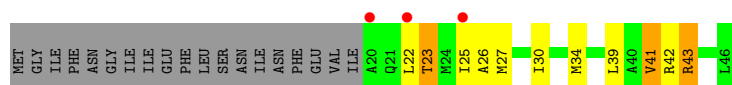
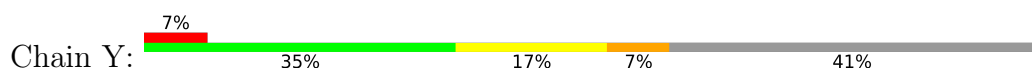
- Molecule 18: Photosystem II reaction center X protein



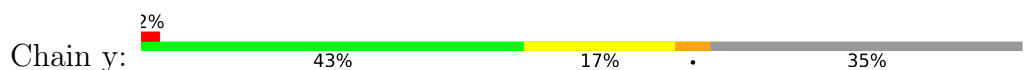
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Ycf12

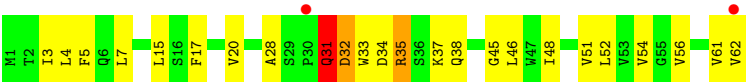


- Molecule 19: Photosystem II reaction center protein Ycf12

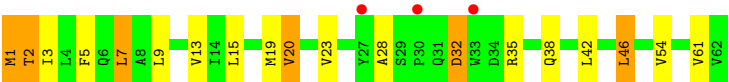


- Molecule 20: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.2 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.178 , 0.249 0.179 , 0.249	Depositor DCC
R_{free} test set	3275 reflections (0.52%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103197	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/2707	0.78	1/3692 (0.0%)
1	a	0.66	0/2704	0.76	1/3688 (0.0%)
2	B	0.64	0/4161	0.73	0/5669
2	b	0.61	0/4118	0.71	0/5611
3	C	0.62	0/3547	0.71	0/4830
3	c	0.59	0/3619	0.71	0/4926
4	D	0.68	0/2812	0.74	0/3832
4	d	0.65	0/2821	0.73	0/3844
5	E	0.56	0/688	0.65	0/940
5	e	0.52	0/683	0.62	0/932
6	F	0.52	0/284	0.65	0/387
6	f	0.51	0/284	0.67	0/387
7	H	0.67	0/523	0.73	0/713
7	h	0.53	0/511	0.67	0/697
8	I	0.62	0/293	0.76	0/396
8	i	0.62	0/293	0.69	0/396
9	J	0.54	0/263	0.72	0/356
9	j	0.51	0/263	0.71	0/356
10	K	0.51	0/303	0.64	0/416
10	k	0.46	0/303	0.61	0/416
11	L	0.68	0/311	0.71	0/422
11	l	0.69	0/303	0.68	0/412
12	M	0.66	0/249	0.69	0/341
12	m	0.69	0/244	0.79	0/334
13	O	0.62	0/1904	0.71	0/2585
13	o	0.66	0/1905	0.73	0/2583
14	R	0.48	0/277	0.64	0/380
14	r	0.37	0/246	0.51	0/339
15	T	0.70	0/257	0.81	0/349
15	t	0.67	0/255	0.68	0/346
16	U	0.58	0/785	0.69	0/1064
16	u	0.63	0/785	0.78	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.61	0/1085	0.74	1/1473 (0.1%)
17	v	0.56	0/1085	0.69	0/1473
18	X	0.55	0/284	0.66	0/384
18	x	0.49	0/289	0.64	0/391
19	Y	0.48	0/197	0.65	0/264
19	y	0.39	0/219	0.59	0/294
20	Z	0.43	0/490	0.60	0/669
20	z	0.40	0/488	0.54	0/666
All	All	0.62	0/42838	0.72	3/58317 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	MET	CA-CB-CG	5.13	124.36	114.10
1	a	131	TRP	CA-CB-CG	-5.05	104.00	113.60
17	V	63	THR	C-N-CD	-5.01	104.45	125.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2508	2519	20	0
1	a	2619	2499	2510	34	0
2	B	4005	3859	3867	30	0
2	b	3978	3822	3836	39	0
3	C	3426	3341	3343	37	0
3	c	3500	3413	3426	36	0
4	D	2717	2613	2621	39	0
4	d	2723	2619	2627	38	0
5	E	666	650	651	16	0
5	e	664	647	648	21	0
6	F	275	281	282	7	0
6	f	275	281	282	7	0
7	H	510	532	532	7	0
7	h	498	518	518	10	0
8	I	296	311	311	1	0
8	i	296	311	311	2	0
9	J	257	268	268	3	0
9	j	257	268	268	6	0
10	K	293	305	305	5	0
10	k	293	305	305	9	0
11	L	304	316	316	9	0
11	l	296	304	304	4	0
12	M	256	269	269	3	0
12	m	251	267	267	5	0
13	O	1870	1828	1830	35	0
13	o	1874	1844	1846	13	0
14	R	271	298	298	8	0
14	r	240	253	250	10	0
15	T	258	261	261	0	0
15	t	256	256	256	3	0
16	U	774	772	773	4	0
16	u	774	772	773	9	0
17	V	1064	1068	1073	11	0
17	v	1064	1068	1073	19	0
18	X	281	312	312	5	0
18	x	286	316	314	7	0
19	Y	196	217	217	9	0
19	y	218	241	241	8	0
20	Z	479	516	516	13	0
20	z	477	509	509	15	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	184	192	192	6	0
22	B	970	1067	1067	20	0
22	C	839	922	922	15	0
22	D	195	216	216	6	0
22	H	65	72	72	1	0
22	a	195	216	216	3	0
22	b	1035	1139	1139	22	0
22	c	839	919	919	14	0
22	d	195	216	216	2	0
23	A	64	74	74	0	0
23	D	64	74	74	3	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	4	0
25	D	55	80	80	2	0
25	a	55	80	80	1	0
25	d	55	80	80	1	0
26	A	48	66	66	0	0
26	B	28	40	40	0	0
26	D	84	114	117	1	0
26	M	51	69	72	1	0
26	Y	48	66	66	0	0
26	a	55	85	86	0	0
26	b	55	86	86	0	0
26	c	134	178	180	0	0
26	d	44	57	58	0	0
26	m	51	71	72	1	0
27	A	91	134	135	4	0
27	B	54	77	78	0	0
27	D	36	45	45	0	0
27	L	49	65	65	3	0
27	a	54	77	78	0	0
27	f	41	48	48	1	0
27	t	36	56	56	0	0
28	A	49	72	74	0	0
28	D	145	211	215	4	0
28	L	49	73	74	0	0
28	a	42	55	57	0	0
28	b	49	73	74	5	0
28	d	88	121	125	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	l	49	74	74	1	0
29	A	66	94	96	1	0
29	C	186	241	245	2	0
29	H	62	77	81	0	0
29	c	186	234	243	0	0
29	h	62	79	82	0	0
30	B	120	168	168	8	0
30	C	80	112	112	6	0
30	D	40	56	56	3	0
30	H	40	56	56	0	0
30	I	40	56	56	0	0
30	K	80	112	112	1	0
30	T	40	56	56	4	0
30	a	40	56	56	2	0
30	b	120	168	168	3	0
30	c	40	56	56	1	0
30	d	40	56	56	5	0
30	k	120	168	168	2	0
30	t	40	56	56	2	0
30	x	40	56	56	3	0
31	B	75	117	117	1	0
31	C	40	63	63	1	0
31	H	18	35	35	0	0
31	I	15	26	26	1	0
31	J	12	16	16	1	0
31	L	12	16	16	0	0
31	M	43	73	73	0	0
31	R	12	16	16	0	0
31	X	20	35	35	4	0
31	Z	8	12	12	0	0
31	a	27	42	42	0	0
31	b	131	232	232	4	0
31	c	20	35	35	1	0
31	d	17	26	26	0	0
31	j	12	16	16	1	0
31	k	12	16	16	0	0
31	t	24	36	36	1	0
31	x	20	35	35	0	0
32	C	10	0	0	0	0
32	a	10	0	0	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	F	43	32	32	5	0
34	V	43	30	31	1	0
34	f	43	32	32	5	0
34	v	43	30	30	4	0
35	V	1	0	0	0	0
36	A	112	0	0	2	0
36	B	142	0	0	1	0
36	C	125	0	0	1	0
36	D	96	0	0	2	0
36	E	22	0	0	0	0
36	F	6	0	0	0	0
36	H	16	0	0	1	0
36	I	10	0	0	0	0
36	J	14	0	0	1	0
36	K	3	0	0	1	0
36	L	10	0	0	4	0
36	M	9	0	0	1	0
36	O	60	0	0	5	0
36	R	11	0	0	2	0
36	T	8	0	0	0	0
36	U	28	0	0	0	0
36	V	49	0	0	2	0
36	X	10	0	0	2	0
36	Y	2	0	0	0	0
36	Z	7	0	0	0	0
36	a	96	0	0	1	0
36	b	116	0	0	1	0
36	c	108	0	0	3	0
36	d	87	0	0	0	0
36	e	11	0	0	0	0
36	f	7	0	0	1	0
36	h	17	0	0	1	0
36	i	14	0	0	0	0
36	j	8	0	0	0	0
36	k	7	0	0	1	0
36	l	11	0	0	0	0
36	m	4	0	0	1	0
36	o	67	0	0	0	0
36	r	3	0	0	1	0
36	t	8	0	0	1	0
36	u	34	0	0	2	0
36	v	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	x	6	0	0	0	0
36	y	12	0	0	2	0
36	z	6	0	0	0	0
All	All	51641	51556	51697	606	0

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

The worst 5 of 606 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:40:CYS:SG	34:v:201:HEC:CAC	2.03	1.44
18:x:3:ILE:HG23	18:x:7:LEU:HD23	1.56	0.88
1:a:229:GLU:OE1	36:a:501:HOH:O	1.97	0.82
9:J:5:GLY:N	36:J:201:HOH:O	2.12	0.82
31:X:101:STE:O1	36:X:201:HOH:O	1.99	0.81

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%)	324 (98%)	8 (2%)	0	100	100
1	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
2	B	508/506 (100%)	494 (97%)	14 (3%)	0	100	100
2	b	503/506 (99%)	484 (96%)	16 (3%)	3 (1%)	21	25
3	C	442/461 (96%)	423 (96%)	18 (4%)	1 (0%)	43	53
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	53
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	340/352 (97%)	327 (96%)	13 (4%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	10	10
5	e	80/84 (95%)	78 (98%)	1 (1%)	1 (1%)	9	9
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	28 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	2
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	3	2
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	227 (93%)	13 (5%)	3 (1%)	10	10
13	o	242/272 (89%)	224 (93%)	15 (6%)	3 (1%)	10	10
14	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
14	r	29/41 (71%)	25 (86%)	2 (7%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	89 (94%)	5 (5%)	1 (1%)	11	11
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	v	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	21
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	1
19	y	28/46 (61%)	20 (71%)	6 (21%)	2 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Z	60/62 (97%)	56 (93%)	2 (3%)	2 (3%)	3	1
20	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	3	1
All	All	5240/5688 (92%)	5024 (96%)	189 (4%)	27 (0%)	24	29

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	58	ASN
13	O	62	GLU
17	V	64	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	260 (96%)	10 (4%)	30	43
1	a	269/280 (96%)	258 (96%)	11 (4%)	27	38
2	B	408/404 (101%)	398 (98%)	10 (2%)	42	58
2	b	402/404 (100%)	386 (96%)	16 (4%)	28	40
3	C	346/362 (96%)	337 (97%)	9 (3%)	40	56
3	c	354/362 (98%)	338 (96%)	16 (4%)	24	35
4	D	276/283 (98%)	267 (97%)	9 (3%)	33	47
4	d	277/283 (98%)	259 (94%)	18 (6%)	15	20
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	18
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	25
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	44
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	17
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	15
7	h	53/55 (96%)	46 (87%)	7 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	4
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	21
9	J	24/28 (86%)	22 (92%)	2 (8%)	10	12
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	19
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	25
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	7
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	17
13	O	206/228 (90%)	193 (94%)	13 (6%)	16	21
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	32
14	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
14	r	23/33 (70%)	16 (70%)	7 (30%)	0	0
15	T	26/26 (100%)	24 (92%)	2 (8%)	12	14
15	t	25/26 (96%)	24 (96%)	1 (4%)	28	40
16	U	84/112 (75%)	78 (93%)	6 (7%)	13	17
16	u	84/112 (75%)	79 (94%)	5 (6%)	17	23
17	V	117/138 (85%)	111 (95%)	6 (5%)	21	29
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	23
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	8
18	x	31/34 (91%)	25 (81%)	6 (19%)	1	1
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	2
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	3
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	8
All	All	4328/4644 (93%)	4085 (94%)	243 (6%)	19	25

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	245	THR
16	u	80	GLU

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Mol	Chain	Res	Type
3	c	200	THR
16	u	23	GLU
19	y	23	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	378	ASN
13	o	219	GLN
7	h	59	ASN
13	o	124	ASN
13	O	88	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	1.29	1 (12%)	8,9,11	1.21	1 (12%)
15	FME	t	1	15	8,9,10	1.59	1 (12%)	8,9,11	1.12	0
15	FME	T	1	15	8,9,10	1.13	1 (12%)	8,9,11	0.89	0
8	FME	I	1	8	8,9,10	1.08	0	8,9,11	0.59	0
12	FME	m	1	12	8,9,10	0.93	0	8,9,11	1.56	2 (25%)
12	FME	M	1	12	8,9,10	1.20	1 (12%)	8,9,11	1.07	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	-	2/7/9/11	-
15	FME	t	1	15	-	4/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
8	FME	I	1	8	-	3/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.16	1.40	1.46
8	i	1	FME	CA-N	-2.82	1.42	1.46
12	M	1	FME	CA-N	-2.72	1.42	1.46
15	T	1	FME	CA-N	-2.21	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.85	127.20	122.82
12	m	1	FME	CB-CA-N	2.68	115.40	110.52
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
12	M	1	FME	CA-N-CN	-2.06	119.65	122.82

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	C	510	-	69,73,73	1.42	12 (17%)	82,113,113	1.67	9 (10%)
29	DGD	C	516	-	63,63,67	1.40	9 (14%)	77,77,81	1.38	11 (14%)
22	CLA	B	614	-	69,73,73	1.32	10 (14%)	82,113,113	1.42	10 (12%)
30	BCR	b	618	-	41,41,41	1.51	4 (9%)	56,56,56	1.33	10 (17%)
27	SQD	A	412	-	38,38,54	1.10	2 (5%)	40,40,65	1.41	5 (12%)
31	STE	I	102	-	14,14,19	0.71	0	13,13,19	0.41	0
22	CLA	a	405	-	69,73,73	1.45	8 (11%)	82,113,113	1.31	9 (10%)
26	LMG	M	101	-	51,51,55	1.10	4 (7%)	59,59,63	1.40	8 (13%)
22	CLA	d	405	-	69,73,73	1.68	12 (17%)	82,113,113	1.17	8 (9%)
29	DGD	A	413	-	67,67,67	1.41	10 (14%)	81,81,81	1.32	13 (16%)
31	STE	C	519	-	11,11,19	1.03	0	11,11,19	1.41	2 (18%)
22	CLA	C	512	-	69,73,73	1.28	8 (11%)	82,113,113	1.42	10 (12%)
22	CLA	C	504	36	63,67,73	1.34	8 (12%)	74,105,113	1.35	11 (14%)
22	CLA	b	613	-	69,73,73	1.52	9 (13%)	82,113,113	1.43	9 (10%)
22	CLA	b	607	36	69,73,73	1.35	12 (17%)	82,113,113	1.16	5 (6%)
30	BCR	H	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.25	6 (10%)
31	STE	M	102	-	14,14,19	0.92	0	14,14,19	1.01	1 (7%)
31	STE	R	101	-	11,11,19	0.76	0	11,11,19	1.09	1 (9%)
31	STE	Z	101	-	7,7,19	0.56	0	6,6,19	0.27	0
34	HEC	V	201	17	46,50,50	1.78	4 (8%)	58,82,82	1.93	11 (18%)
22	CLA	b	602	-	69,73,73	1.56	10 (14%)	82,113,113	1.52	12 (14%)
25	PL9	a	409	-	55,55,55	1.14	4 (7%)	68,69,69	1.52	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.29	1 (9%)
22	CLA	b	603	-	69,73,73	1.54	7 (10%)	82,113,113	1.76	15 (18%)
30	BCR	c	514	-	41,41,41	1.19	3 (7%)	56,56,56	1.61	12 (21%)
22	CLA	C	502	-	69,73,73	1.62	8 (11%)	82,113,113	1.38	10 (12%)
22	CLA	C	508	-	69,73,73	1.50	9 (13%)	82,113,113	1.36	14 (17%)
22	CLA	c	503	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	13 (15%)
22	CLA	c	504	36	64,68,73	1.27	9 (14%)	76,107,113	1.24	12 (15%)
22	CLA	c	511	3	69,73,73	1.52	8 (11%)	82,113,113	1.48	10 (12%)
30	BCR	C	515	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	8 (14%)
29	DGD	h	101	-	63,63,67	1.04	4 (6%)	77,77,81	1.46	14 (18%)
31	STE	L	103	-	11,11,19	0.77	0	11,11,19	1.70	2 (18%)
31	STE	a	413	-	14,14,19	0.49	0	13,13,19	0.66	0
22	CLA	B	606	36	69,73,73	1.40	10 (14%)	82,113,113	1.34	3 (3%)
22	CLA	B	611	-	69,73,73	1.30	10 (14%)	82,113,113	1.31	9 (10%)
26	LMG	c	518	-	37,37,55	1.43	8 (21%)	45,45,63	1.32	5 (11%)
31	STE	B	619	-	16,16,19	0.88	1 (6%)	16,16,19	0.90	0
28	LHG	D	413	-	48,48,48	1.05	3 (6%)	51,54,54	1.42	7 (13%)
28	LHG	a	411	-	41,41,48	1.18	5 (12%)	44,47,54	1.26	4 (9%)
26	LMG	a	414	-	55,55,55	1.53	9 (16%)	63,63,63	1.29	8 (12%)
26	LMG	A	409	-	48,48,55	1.17	5 (10%)	56,56,63	1.42	8 (14%)
25	PL9	d	407	-	55,55,55	1.60	11 (20%)	68,69,69	1.51	15 (22%)
29	DGD	c	516	-	63,63,67	1.09	7 (11%)	77,77,81	1.54	17 (22%)
28	LHG	d	409	-	38,38,48	1.08	4 (10%)	41,44,54	1.23	5 (12%)
30	BCR	b	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.38	9 (16%)
28	LHG	D	411	-	46,46,48	1.08	3 (6%)	49,52,54	1.24	5 (10%)
30	BCR	a	406	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	13 (23%)
22	CLA	B	610	-	69,73,73	1.50	11 (15%)	82,113,113	1.62	13 (15%)
31	STE	x	102	-	19,19,19	0.78	0	19,19,19	0.96	2 (10%)
22	CLA	a	402	-	69,73,73	1.32	9 (13%)	82,113,113	1.50	10 (12%)
31	STE	c	519	-	19,19,19	0.78	1 (5%)	19,19,19	0.84	0
22	CLA	B	609	36	69,73,73	1.36	10 (14%)	82,113,113	1.55	10 (12%)
22	CLA	c	505	-	69,73,73	1.11	6 (8%)	82,113,113	1.36	8 (9%)
22	CLA	c	512	-	69,73,73	1.59	13 (18%)	82,113,113	1.45	9 (10%)
22	CLA	B	613	-	69,73,73	1.20	5 (7%)	82,113,113	1.30	11 (13%)
22	CLA	B	605	-	69,73,73	1.74	9 (13%)	82,113,113	1.34	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	T	101	-	41,41,41	1.11	4 (9%)	56,56,56	1.29	5 (8%)
33	BCT	D	402	21	3,3,3	0.97	0	2,3,3	3.95	2 (100%)
22	CLA	c	513	-	69,73,73	1.28	9 (13%)	82,113,113	1.26	6 (7%)
29	DGD	c	517	-	63,63,67	1.22	9 (14%)	77,77,81	1.37	8 (10%)
22	CLA	b	608	-	69,73,73	1.09	8 (11%)	82,113,113	1.41	10 (12%)
30	BCR	K	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.35	9 (16%)
22	CLA	C	501	-	69,73,73	1.58	10 (14%)	82,113,113	1.55	10 (12%)
22	CLA	c	502	-	69,73,73	1.45	10 (14%)	82,113,113	1.36	13 (15%)
22	CLA	c	508	-	68,72,73	1.29	9 (13%)	80,111,113	1.32	10 (12%)
27	SQD	A	410	-	50,52,54	1.13	4 (8%)	60,63,65	2.02	17 (28%)
22	CLA	b	601	36	69,73,73	1.31	11 (15%)	82,113,113	1.48	10 (12%)
31	STE	b	629	-	19,19,19	0.78	1 (5%)	19,19,19	0.92	0
31	STE	a	412	-	11,11,19	0.84	0	11,11,19	0.95	0
28	LHG	L	102	-	48,48,48	0.91	2 (4%)	51,54,54	1.19	4 (7%)
28	LHG	b	623	-	48,48,48	0.96	2 (4%)	51,54,54	1.26	4 (7%)
30	BCR	B	616	-	41,41,41	1.10	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	C	511	3	69,73,73	1.42	11 (15%)	82,113,113	1.48	4 (4%)
26	LMG	Y	101	-	48,48,55	1.11	7 (14%)	56,56,63	1.26	6 (10%)
22	CLA	c	501	-	69,73,73	1.71	10 (14%)	82,113,113	1.55	8 (9%)
31	STE	H	104	-	17,17,19	0.48	0	16,16,19	0.64	0
22	CLA	B	612	-	69,73,73	1.93	10 (14%)	82,113,113	1.23	7 (8%)
31	STE	C	520	-	15,15,19	0.59	0	14,14,19	0.53	0
31	STE	b	627	-	9,9,19	0.61	0	8,8,19	0.46	0
22	CLA	B	601	-	69,73,73	1.51	10 (14%)	82,113,113	1.33	13 (15%)
22	CLA	b	614	-	69,73,73	1.61	12 (17%)	82,113,113	1.41	12 (14%)
26	LMG	c	520	-	48,48,55	1.07	3 (6%)	56,56,63	1.30	7 (12%)
30	BCR	C	514	-	41,41,41	1.28	2 (4%)	56,56,56	1.54	13 (23%)
31	STE	b	620	-	15,15,19	0.57	0	14,14,19	0.72	0
28	LHG	l	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.12	2 (3%)
30	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.42	9 (16%)
22	CLA	d	403	-	69,73,73	1.51	10 (14%)	82,113,113	1.32	7 (8%)
34	HEC	F	101	5,6	46,50,50	1.91	5 (10%)	58,82,82	1.67	8 (13%)
26	LMG	b	622	-	55,55,55	1.17	5 (9%)	63,63,63	1.46	5 (7%)
31	STE	d	411	-	16,16,19	0.80	0	16,16,19	0.98	1 (6%)
28	LHG	D	410	-	48,48,48	1.00	3 (6%)	51,54,54	1.24	5 (9%)
22	CLA	A	402	-	69,73,73	1.19	6 (8%)	82,113,113	1.51	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	506	-	69,73,73	1.66	7 (10%)	82,113,113	1.47	15 (18%)
31	STE	b	628	-	13,13,19	0.60	0	12,12,19	0.37	0
22	CLA	b	615	-	69,73,73	2.18	12 (17%)	82,113,113	1.39	9 (10%)
30	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
29	DGD	C	517	-	63,63,67	1.25	9 (14%)	77,77,81	1.39	10 (12%)
34	HEC	f	101	5,6	46,50,50	1.84	6 (13%)	58,82,82	2.21	7 (12%)
22	CLA	d	404	36	69,73,73	1.49	7 (10%)	82,113,113	1.66	14 (17%)
31	STE	b	621	-	19,19,19	0.75	0	19,19,19	0.95	1 (5%)
27	SQD	B	621	-	52,54,54	1.03	3 (5%)	62,65,65	1.89	15 (24%)
22	CLA	A	405	-	58,62,73	1.30	7 (12%)	68,99,113	1.53	10 (14%)
31	STE	b	625	-	14,14,19	0.40	0	13,13,19	0.92	0
22	CLA	C	506	-	69,73,73	1.66	12 (17%)	82,113,113	1.34	9 (10%)
22	CLA	H	101	36	69,73,73	1.55	8 (11%)	82,113,113	1.43	6 (7%)
22	CLA	b	616	-	64,68,73	1.19	7 (10%)	76,107,113	1.51	10 (13%)
22	CLA	B	602	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	14 (17%)
22	CLA	C	505	-	69,73,73	1.23	8 (11%)	82,113,113	1.28	9 (10%)
30	BCR	I	101	-	41,41,41	1.20	5 (12%)	56,56,56	1.58	12 (21%)
27	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.91	13 (26%)
30	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.53	11 (19%)
31	STE	k	104	-	11,11,19	0.94	0	11,11,19	0.87	0
22	CLA	C	513	-	69,73,73	1.22	10 (14%)	82,113,113	1.49	11 (13%)
22	CLA	B	603	-	69,73,73	1.32	9 (13%)	82,113,113	1.67	16 (19%)
23	PHO	d	401	-	58,69,69	2.27	11 (18%)	55,99,99	1.82	11 (20%)
27	SQD	t	102	-	35,35,54	1.22	3 (8%)	37,37,65	1.48	4 (10%)
27	SQD	L	101	-	47,49,54	1.00	2 (4%)	57,60,65	2.32	18 (31%)
31	STE	B	624	-	15,15,19	0.50	0	14,14,19	0.84	0
31	STE	B	622	-	11,11,19	0.79	0	11,11,19	1.39	1 (9%)
22	CLA	b	606	-	69,73,73	1.64	10 (14%)	82,113,113	1.48	10 (12%)
34	HEC	v	201	17	46,50,50	1.84	5 (10%)	58,82,82	2.13	11 (18%)
22	CLA	C	507	36	69,73,73	1.21	6 (8%)	82,113,113	1.41	6 (7%)
26	LMG	d	410	-	44,44,55	1.21	5 (11%)	52,52,63	1.26	6 (11%)
29	DGD	H	103	-	63,63,67	1.34	8 (12%)	77,77,81	1.58	13 (16%)
22	CLA	D	405	-	69,73,73	1.81	14 (20%)	82,113,113	1.12	5 (6%)
31	STE	t	103	-	13,13,19	0.91	0	13,13,19	1.09	2 (15%)
29	DGD	c	515	-	63,63,67	1.34	8 (12%)	77,77,81	1.44	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	403	36	69,73,73	1.31	10 (14%)	82,113,113	1.36	11 (13%)
22	CLA	c	507	36	69,73,73	1.85	11 (15%)	82,113,113	1.45	10 (12%)
22	CLA	A	403	36	69,73,73	1.45	10 (14%)	82,113,113	1.38	10 (12%)
28	LHG	A	411	-	48,48,48	1.03	3 (6%)	51,54,54	1.24	5 (9%)
22	CLA	D	404	36	69,73,73	1.47	10 (14%)	82,113,113	1.21	8 (9%)
31	STE	M	103	-	9,9,19	0.77	0	8,8,19	0.40	0
22	CLA	b	611	-	69,73,73	1.32	10 (14%)	82,113,113	1.47	15 (18%)
31	STE	j	101	-	11,11,19	1.03	1 (9%)	11,11,19	0.73	0
22	CLA	b	609	-	69,73,73	1.55	10 (14%)	82,113,113	1.42	11 (13%)
33	BCT	d	402	21	3,3,3	1.10	0	2,3,3	3.08	1 (50%)
22	CLA	b	605	-	69,73,73	1.23	12 (17%)	82,113,113	1.53	13 (15%)
26	LMG	B	620	-	26,26,55	1.44	5 (19%)	26,26,63	1.07	2 (7%)
31	STE	b	626	-	19,19,19	0.86	0	19,19,19	0.52	0
26	LMG	D	412	-	31,31,55	1.26	3 (9%)	33,33,63	1.13	2 (6%)
30	BCR	k	103	-	41,41,41	1.11	3 (7%)	56,56,56	1.33	5 (8%)
30	BCR	k	102	-	41,41,41	1.08	3 (7%)	56,56,56	1.18	4 (7%)
26	LMG	D	408	-	51,51,55	1.19	4 (7%)	59,59,63	1.35	6 (10%)
30	BCR	t	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.45	12 (21%)
27	SQD	D	409	-	34,36,54	1.08	2 (5%)	42,45,65	1.84	11 (26%)
27	SQD	a	410	-	52,54,54	1.04	3 (5%)	62,65,65	1.73	14 (22%)
29	DGD	C	518	-	63,63,67	1.12	6 (9%)	77,77,81	1.52	11 (14%)
31	STE	X	101	-	19,19,19	0.64	0	19,19,19	1.23	2 (10%)
22	CLA	D	403	-	69,73,73	1.31	6 (8%)	82,113,113	1.19	7 (8%)
22	CLA	B	604	-	69,73,73	1.00	5 (7%)	82,113,113	1.40	9 (10%)
32	OEX	a	415	3,1,36	0,15,15	-	-	-	-	-
22	CLA	b	610	36	69,73,73	1.81	9 (13%)	82,113,113	1.36	10 (12%)
22	CLA	B	615	-	64,68,73	1.55	10 (15%)	76,107,113	1.45	8 (10%)
22	CLA	c	510	-	69,73,73	1.10	7 (10%)	82,113,113	1.37	8 (9%)
22	CLA	B	608	-	69,73,73	1.21	7 (10%)	82,113,113	1.45	13 (15%)
23	PHO	A	404	-	58,69,69	1.76	10 (17%)	55,99,99	1.76	13 (23%)
30	BCR	x	101	-	41,41,41	1.05	3 (7%)	56,56,56	1.47	11 (19%)
31	STE	B	625	-	11,11,19	0.83	0	11,11,19	1.50	3 (27%)
31	STE	M	104	-	17,17,19	0.43	0	16,16,19	0.85	0
22	CLA	C	509	-	69,73,73	1.29	10 (14%)	82,113,113	1.30	10 (12%)
30	BCR	D	406	-	41,41,41	1.14	4 (9%)	56,56,56	1.33	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	604	-	69,73,73	1.26	7 (10%)	82,113,113	1.50	13 (15%)
28	LHG	d	408	-	48,48,48	0.80	2 (4%)	51,54,54	1.14	3 (5%)
30	BCR	k	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.44	11 (19%)
31	STE	b	624	-	15,15,19	0.88	0	15,15,19	0.90	0
30	BCR	B	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.61	11 (19%)
22	CLA	c	509	-	69,73,73	1.35	8 (11%)	82,113,113	1.48	11 (13%)
25	PL9	A	408	-	55,55,55	1.54	5 (9%)	68,69,69	1.50	12 (17%)
31	STE	C	521	-	11,11,19	0.68	0	11,11,19	1.43	2 (18%)
25	PL9	D	407	-	55,55,55	1.62	12 (21%)	68,69,69	1.64	15 (22%)
22	CLA	C	503	-	69,73,73	1.43	12 (17%)	82,113,113	1.73	12 (14%)
26	LMG	c	521	-	49,49,55	1.12	6 (12%)	57,57,63	1.34	8 (14%)
22	CLA	B	607	-	69,73,73	1.48	9 (13%)	82,113,113	1.13	8 (9%)
31	STE	B	623	-	17,17,19	0.77	0	17,17,19	0.94	0
22	CLA	b	612	-	69,73,73	1.32	9 (13%)	82,113,113	1.46	10 (12%)
32	OEX	C	522	3,1,36	0,15,15	-	-	-	-	-
23	PHO	a	404	-	58,69,69	1.92	10 (17%)	55,99,99	1.71	11 (20%)
31	STE	t	104	-	9,9,19	0.60	0	8,8,19	0.37	0
23	PHO	D	401	-	58,69,69	2.03	9 (15%)	55,99,99	1.58	10 (18%)
30	BCR	B	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.43	11 (19%)
26	LMG	m	101	-	51,51,55	1.26	4 (7%)	59,59,63	1.50	8 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	510	-	1/1/20/20	12/39/115/115	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
22	CLA	B	614	-	1/1/20/20	9/39/115/115	-
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
27	SQD	A	412	-	-	19/39/39/69	-
31	STE	I	102	-	-	5/12/12/17	-
22	CLA	a	405	-	1/1/20/20	7/39/115/115	-
26	LMG	M	101	-	-	17/46/66/70	0/1/1/1
22	CLA	d	405	-	1/1/20/20	7/39/115/115	-
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	C	519	-	-	5/9/9/17	-
22	CLA	C	512	-	1/1/20/20	11/39/115/115	-
22	CLA	C	504	36	1/1/18/20	6/32/108/115	-
22	CLA	b	613	-	1/1/20/20	10/39/115/115	-
22	CLA	b	607	36	1/1/20/20	15/39/115/115	-
30	BCR	H	102	-	-	10/29/63/63	0/2/2/2
31	STE	M	102	-	-	6/12/12/17	-
31	STE	R	101	-	-	4/9/9/17	-
31	STE	Z	101	-	-	4/5/5/17	-
34	HEC	V	201	17	-	6/14/54/54	-
22	CLA	b	602	-	1/1/20/20	12/39/115/115	-
25	PL9	a	409	-	-	26/53/73/73	0/1/1/1
31	STE	J	101	-	-	5/9/9/17	-
22	CLA	b	603	-	1/1/20/20	10/39/115/115	-
30	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	C	502	-	1/1/20/20	9/39/115/115	-
22	CLA	c	504	36	1/1/19/20	4/33/109/115	-
22	CLA	c	511	3	1/1/20/20	9/39/115/115	-
22	CLA	C	508	-	-	10/39/115/115	-
22	CLA	c	503	-	-	9/39/115/115	-
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
29	DGD	h	101	-	-	16/51/91/95	0/2/2/2
31	STE	L	103	-	-	5/9/9/17	-
31	STE	a	413	-	-	9/12/12/17	-
22	CLA	B	606	36	1/1/20/20	17/39/115/115	-
22	CLA	B	611	-	1/1/20/20	6/39/115/115	-
26	LMG	c	518	-	-	11/31/51/70	0/1/1/1
31	STE	B	619	-	-	6/14/14/17	-
28	LHG	D	413	-	-	20/53/53/53	-
28	LHG	a	411	-	-	25/46/46/53	-
26	LMG	a	414	-	-	31/50/70/70	0/1/1/1
26	LMG	A	409	-	-	16/43/63/70	0/1/1/1
25	PL9	d	407	-	-	18/53/73/73	0/1/1/1
29	DGD	c	516	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	409	-	-	13/43/43/53	-
30	BCR	b	617	-	-	9/29/63/63	0/2/2/2
28	LHG	D	411	-	-	21/51/51/53	-
30	BCR	a	406	-	-	2/29/63/63	0/2/2/2
22	CLA	B	610	-	-	6/39/115/115	-
31	STE	x	102	-	-	11/17/17/17	-
22	CLA	a	402	-	-	1/39/115/115	-
31	STE	c	519	-	-	7/17/17/17	-
22	CLA	B	609	36	1/1/20/20	7/39/115/115	-
22	CLA	c	505	-	1/1/20/20	13/39/115/115	-
22	CLA	c	512	-	1/1/20/20	20/39/115/115	-
22	CLA	B	613	-	1/1/20/20	15/39/115/115	-
22	CLA	B	605	-	1/1/20/20	12/39/115/115	-
30	BCR	T	101	-	-	12/29/63/63	0/2/2/2
22	CLA	c	513	-	1/1/20/20	9/39/115/115	-
29	DGD	c	517	-	-	14/51/91/95	0/2/2/2
22	CLA	b	608	-	1/1/20/20	6/39/115/115	-
30	BCR	K	102	-	-	11/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	5/39/115/115	-
22	CLA	c	502	-	1/1/20/20	12/39/115/115	-
22	CLA	c	508	-	-	12/38/114/115	-
27	SQD	A	410	-	-	23/47/67/69	0/1/1/1
22	CLA	b	601	36	1/1/20/20	23/39/115/115	-
31	STE	b	629	-	-	6/17/17/17	-
31	STE	a	412	-	-	4/9/9/17	-
28	LHG	L	102	-	-	23/53/53/53	-
28	LHG	b	623	-	-	26/53/53/53	-
30	BCR	B	616	-	-	7/29/63/63	0/2/2/2
22	CLA	C	511	3	1/1/20/20	7/39/115/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
22	CLA	c	501	-	1/1/20/20	5/39/115/115	-
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	B	612	-	1/1/20/20	10/39/115/115	-
31	STE	C	520	-	-	4/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	b	627	-	-	5/7/7/17	-
22	CLA	b	614	-	1/1/20/20	17/39/115/115	-
22	CLA	B	601	-	-	7/39/115/115	-
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
30	BCR	C	514	-	-	8/29/63/63	0/2/2/2
31	STE	b	620	-	-	6/13/13/17	-
28	LHG	l	101	-	-	17/53/53/53	-
30	BCR	d	406	-	-	7/29/63/63	0/2/2/2
22	CLA	d	403	-	1/1/20/20	10/39/115/115	-
34	HEC	F	101	5,6	-	5/14/54/54	-
26	LMG	b	622	-	-	27/50/70/70	0/1/1/1
31	STE	d	411	-	-	9/14/14/17	-
28	LHG	D	410	-	-	22/53/53/53	-
22	CLA	A	402	-	1/1/20/20	3/39/115/115	-
22	CLA	c	506	-	1/1/20/20	12/39/115/115	-
31	STE	b	628	-	-	7/11/11/17	-
22	CLA	b	615	-	1/1/20/20	13/39/115/115	-
30	BCR	b	619	-	-	3/29/63/63	0/2/2/2
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
34	HEC	f	101	5,6	-	6/14/54/54	-
22	CLA	d	404	36	1/1/20/20	1/39/115/115	-
31	STE	b	621	-	-	10/17/17/17	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
22	CLA	A	405	-	1/1/17/20	3/26/102/115	-
31	STE	b	625	-	-	7/12/12/17	-
22	CLA	C	506	-	1/1/20/20	21/39/115/115	-
22	CLA	H	101	36	1/1/20/20	18/39/115/115	-
22	CLA	b	616	-	1/1/19/20	5/33/109/115	-
22	CLA	B	602	-	1/1/20/20	11/39/115/115	-
22	CLA	C	505	-	1/1/20/20	7/39/115/115	-
30	BCR	I	101	-	-	7/29/63/63	0/2/2/2
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
30	BCR	K	101	-	-	12/29/63/63	0/2/2/2
31	STE	k	104	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	513	-	1/1/20/20	7/39/115/115	-
22	CLA	B	603	-	1/1/20/20	13/39/115/115	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
27	SQD	t	102	-	-	12/37/37/69	-
27	SQD	L	101	-	-	26/44/64/69	0/1/1/1
31	STE	B	624	-	-	7/13/13/17	-
31	STE	B	622	-	-	5/9/9/17	-
22	CLA	b	606	-	1/1/20/20	8/39/115/115	-
34	HEC	v	201	17	-	6/14/54/54	-
22	CLA	C	507	36	1/1/20/20	6/39/115/115	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
22	CLA	D	405	-	-	13/39/115/115	-
31	STE	t	103	-	-	5/11/11/17	-
29	DGD	c	515	-	-	22/51/91/95	0/2/2/2
22	CLA	c	507	36	1/1/20/20	12/39/115/115	-
22	CLA	a	403	36	-	10/39/115/115	-
22	CLA	A	403	36	-	8/39/115/115	-
28	LHG	A	411	-	-	23/53/53/53	-
22	CLA	D	404	36	1/1/20/20	7/39/115/115	-
31	STE	M	103	-	-	2/7/7/17	-
22	CLA	b	611	-	-	7/39/115/115	-
31	STE	j	101	-	-	2/9/9/17	-
22	CLA	b	609	-	1/1/20/20	9/39/115/115	-
22	CLA	b	605	-	1/1/20/20	13/39/115/115	-
26	LMG	B	620	-	-	8/22/22/70	-
31	STE	b	626	-	-	9/17/17/17	-
26	LMG	D	412	-	-	19/33/33/70	-
30	BCR	k	103	-	-	6/29/63/63	0/2/2/2
30	BCR	k	102	-	-	15/29/63/63	0/2/2/2
26	LMG	D	408	-	-	17/46/66/70	0/1/1/1
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
27	SQD	D	409	-	-	14/28/48/69	0/1/1/1
27	SQD	a	410	-	-	22/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
31	STE	X	101	-	-	10/17/17/17	-
22	CLA	D	403	-	1/1/20/20	6/39/115/115	-
22	CLA	B	604	-	1/1/20/20	11/39/115/115	-
22	CLA	b	610	36	1/1/20/20	7/39/115/115	-
22	CLA	B	615	-	1/1/19/20	7/33/109/115	-
22	CLA	c	510	-	1/1/20/20	12/39/115/115	-
22	CLA	B	608	-	-	6/39/115/115	-
23	PHO	A	404	-	-	6/37/103/103	0/5/6/6
30	BCR	x	101	-	-	7/29/63/63	0/2/2/2
31	STE	B	625	-	-	4/9/9/17	-
31	STE	M	104	-	-	9/15/15/17	-
22	CLA	C	509	-	1/1/20/20	16/39/115/115	-
30	BCR	D	406	-	-	8/29/63/63	0/2/2/2
22	CLA	b	604	-	1/1/20/20	12/39/115/115	-
28	LHG	d	408	-	-	21/53/53/53	-
30	BCR	k	101	-	-	10/29/63/63	0/2/2/2
31	STE	b	624	-	-	10/13/13/17	-
30	BCR	B	618	-	-	9/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	6/39/115/115	-
25	PL9	A	408	-	-	21/53/73/73	0/1/1/1
31	STE	C	521	-	-	2/9/9/17	-
25	PL9	D	407	-	-	14/53/73/73	0/1/1/1
22	CLA	C	503	-	1/1/20/20	4/39/115/115	-
26	LMG	c	521	-	-	24/44/64/70	0/1/1/1
22	CLA	B	607	-	1/1/20/20	8/39/115/115	-
31	STE	B	623	-	-	11/15/15/17	-
22	CLA	b	612	-	1/1/20/20	6/39/115/115	-
23	PHO	a	404	-	-	1/37/103/103	0/5/6/6
31	STE	t	104	-	-	3/7/7/17	-
23	PHO	D	401	-	-	4/37/103/103	0/5/6/6
30	BCR	B	617	-	-	10/29/63/63	0/2/2/2
26	LMG	m	101	-	-	18/46/66/70	0/1/1/1

The worst 5 of 990 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-ND	-12.14	1.81	2.05
22	b	610	CLA	MG-NB	-10.90	1.84	2.05
22	b	615	CLA	MG-ND	-10.89	1.84	2.05
23	d	401	PHO	C1B-C2B	9.91	1.50	1.39
22	B	605	CLA	MG-NA	9.19	2.28	2.06

The worst 5 of 1402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O6-C1-C2	10.62	124.41	108.27
22	C	510	CLA	C4A-NA-C1A	10.25	111.35	106.68
34	f	101	HEC	CBC-CAC-C3C	-10.03	107.38	127.43
22	C	503	CLA	C4A-NA-C1A	9.78	111.14	106.68
34	V	201	HEC	CBB-CAB-C3B	-9.16	109.13	127.43

5 of 59 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND

5 of 1966 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	605	CLA	C11-C10-C8-C9
22	C	501	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

102 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	510	CLA	1	0
30	b	618	BCR	1	0
27	A	412	SQD	1	0
31	I	102	STE	1	0
26	M	101	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	413	DGD	1	0
22	C	512	CLA	2	0
22	C	504	CLA	1	0
22	b	613	CLA	3	0
22	b	607	CLA	3	0
34	V	201	HEC	1	0
22	b	602	CLA	1	0
25	a	409	PL9	1	0
31	J	101	STE	1	0
22	b	603	CLA	1	0
30	c	514	BCR	1	0
22	C	508	CLA	4	0
22	c	503	CLA	2	0
22	c	504	CLA	1	0
22	c	511	CLA	2	0
22	B	606	CLA	1	0
28	D	413	LHG	1	0
25	d	407	PL9	1	0
28	d	409	LHG	1	0
30	b	617	BCR	1	0
28	D	411	LHG	3	0
30	a	406	BCR	2	0
22	B	610	CLA	1	0
22	a	402	CLA	3	0
31	c	519	STE	1	0
22	B	609	CLA	1	0
22	B	613	CLA	3	0
22	B	605	CLA	2	0
30	T	101	BCR	4	0
22	c	513	CLA	1	0
30	K	102	BCR	1	0
22	C	501	CLA	3	0
22	c	502	CLA	1	0
22	c	508	CLA	2	0
27	A	410	SQD	3	0
22	b	601	CLA	3	0
31	b	629	STE	1	0
28	b	623	LHG	5	0
22	C	511	CLA	1	0
22	c	501	CLA	2	0
22	B	612	CLA	1	0
31	C	520	STE	1	0

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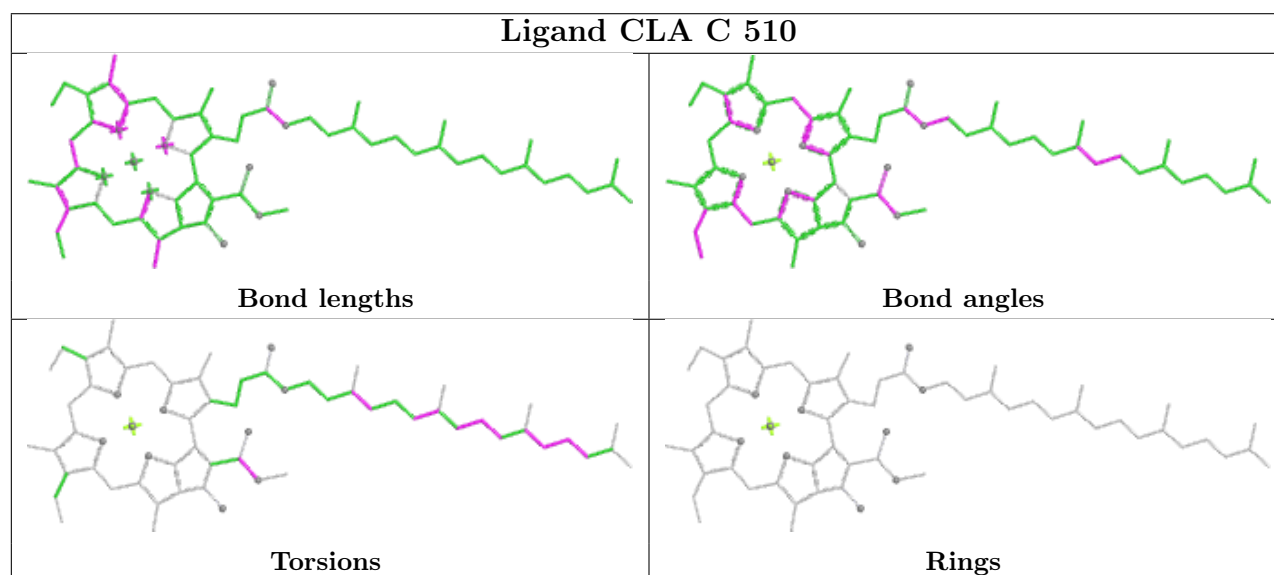
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	b	614	CLA	2	0
30	C	514	BCR	6	0
28	l	101	LHG	1	0
30	d	406	BCR	5	0
34	F	101	HEC	5	0
22	A	402	CLA	2	0
31	b	628	STE	2	0
22	b	615	CLA	2	0
30	b	619	BCR	1	0
29	C	517	DGD	2	0
34	f	101	HEC	5	0
22	d	404	CLA	2	0
31	b	621	STE	2	0
22	H	101	CLA	1	0
27	f	102	SQD	1	0
22	C	513	CLA	4	0
22	B	603	CLA	4	0
23	d	401	PHO	1	0
27	L	101	SQD	3	0
22	b	606	CLA	3	0
34	v	201	HEC	4	0
22	C	507	CLA	1	0
31	t	103	STE	1	0
22	c	507	CLA	3	0
22	A	403	CLA	4	0
31	j	101	STE	1	0
22	b	609	CLA	1	0
22	b	605	CLA	8	0
30	k	103	BCR	1	0
30	k	102	BCR	1	0
26	D	408	LMG	1	0
30	t	101	BCR	2	0
31	X	101	STE	4	0
22	D	403	CLA	6	0
22	B	604	CLA	3	0
22	b	610	CLA	1	0
22	B	615	CLA	1	0
22	c	510	CLA	1	0
22	B	608	CLA	3	0
30	x	101	BCR	3	0
30	D	406	BCR	3	0

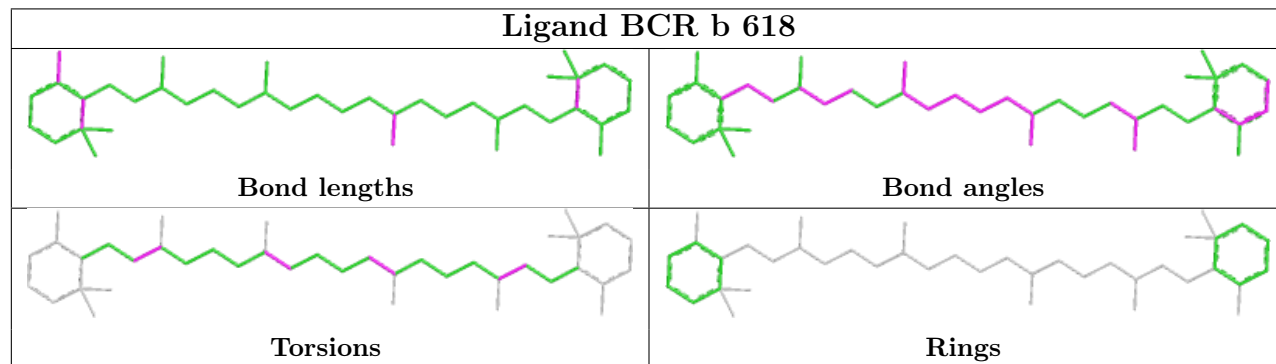
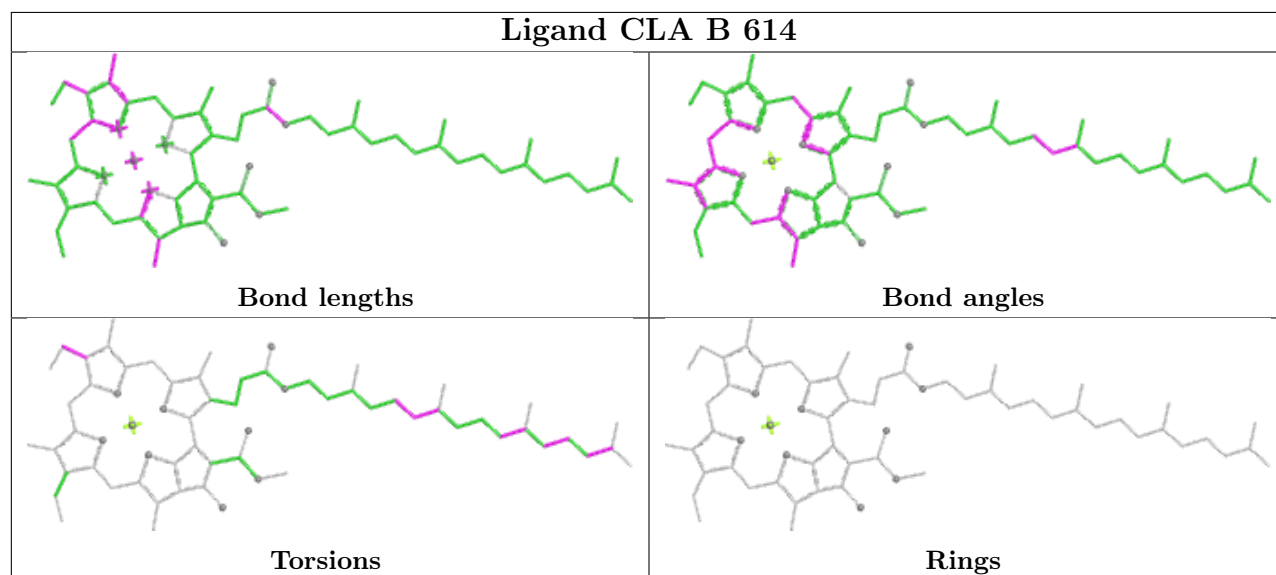
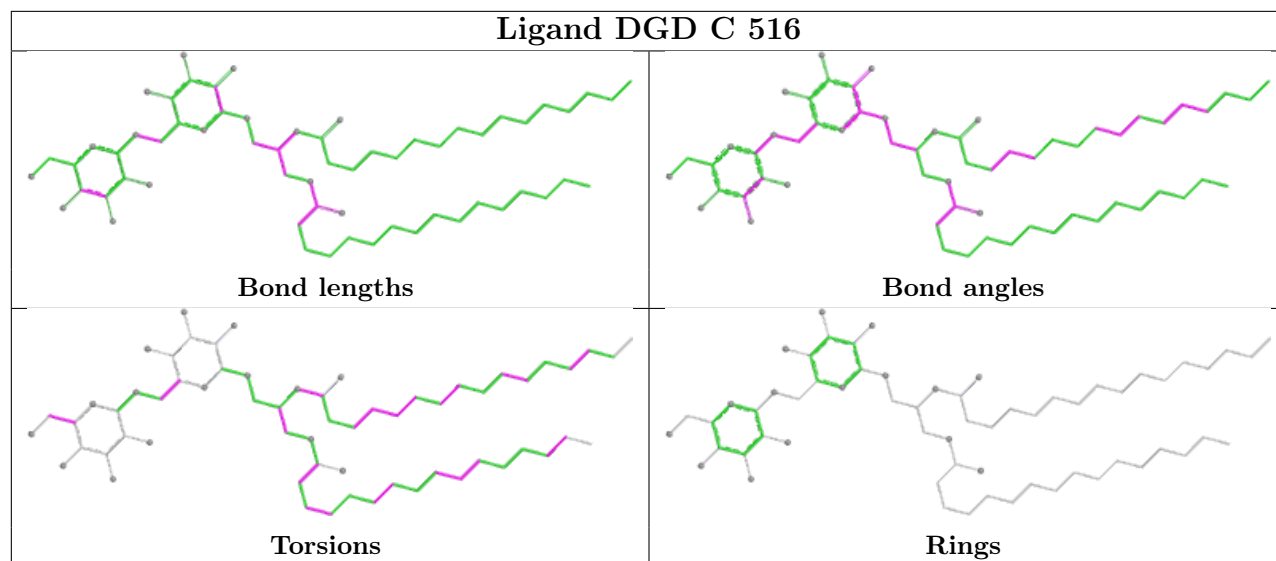
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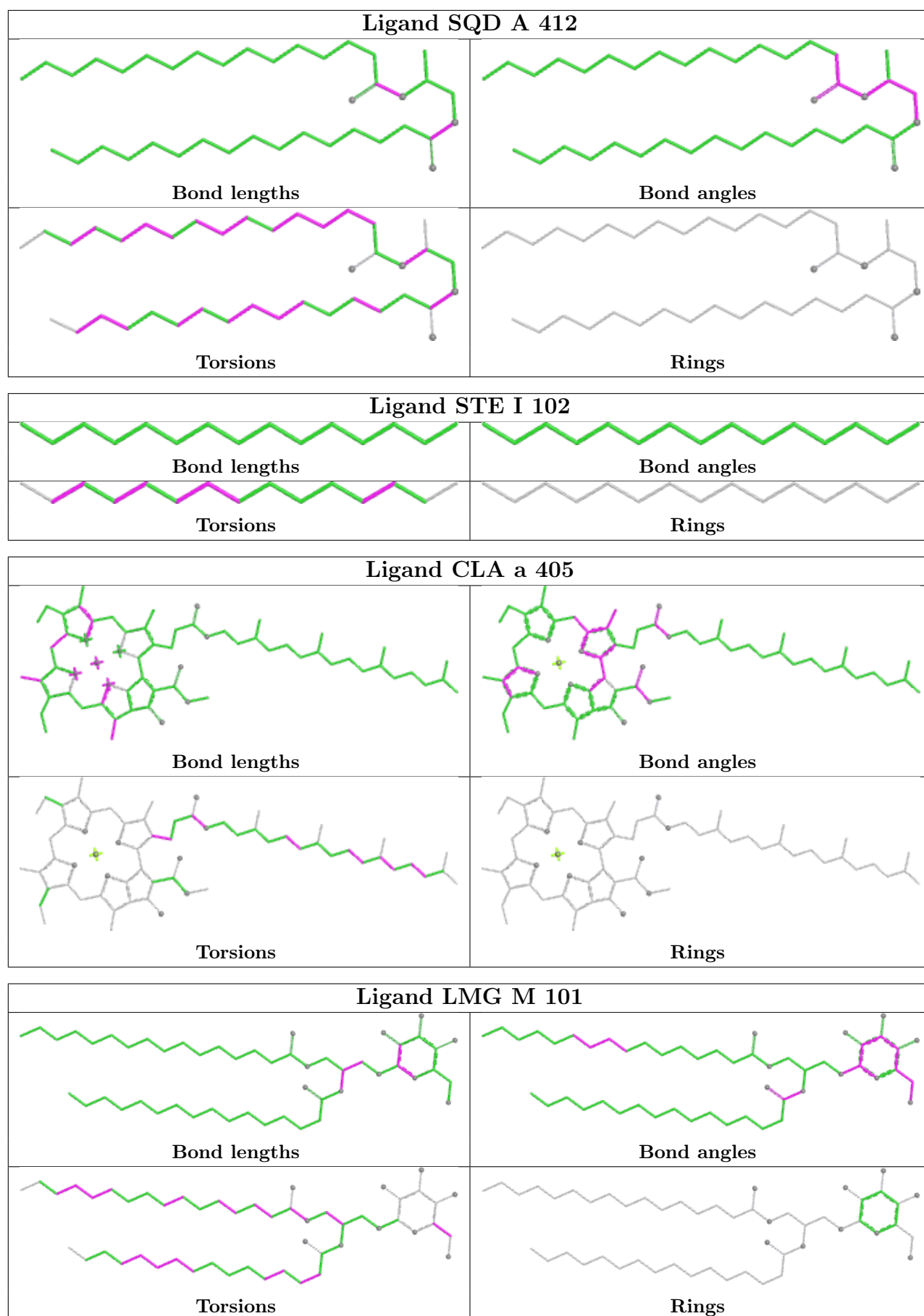
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	408	LHG	3	0
30	k	101	BCR	1	0
30	B	618	BCR	2	0
22	c	509	CLA	2	0
25	A	408	PL9	4	0
25	D	407	PL9	2	0
22	B	607	CLA	2	0
31	B	623	STE	1	0
22	b	612	CLA	1	0
23	a	404	PHO	1	0
23	D	401	PHO	3	0
30	B	617	BCR	6	0
26	m	101	LMG	1	0

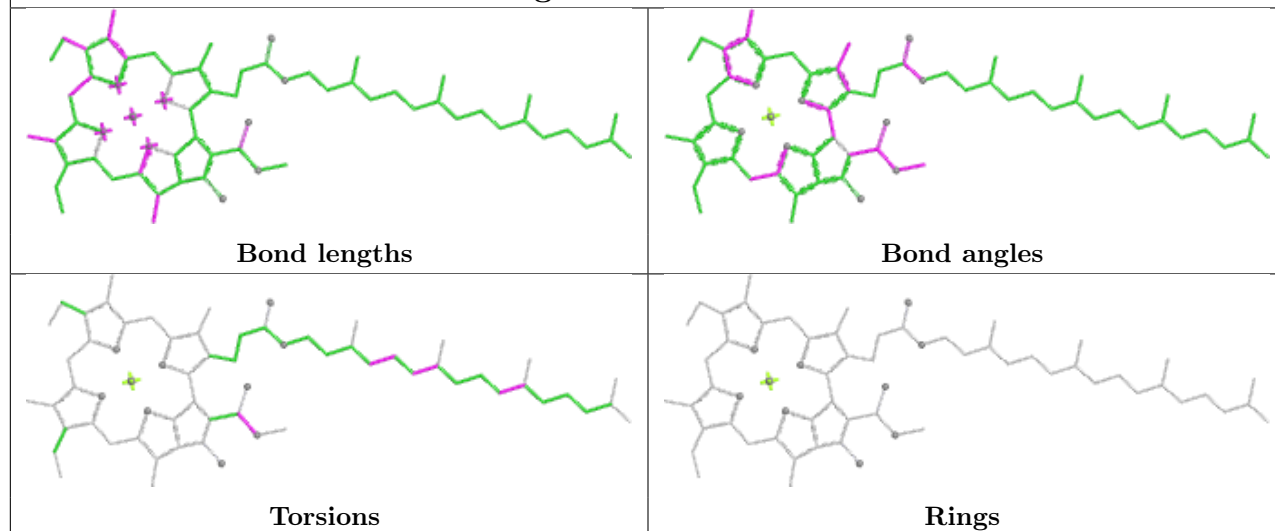
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



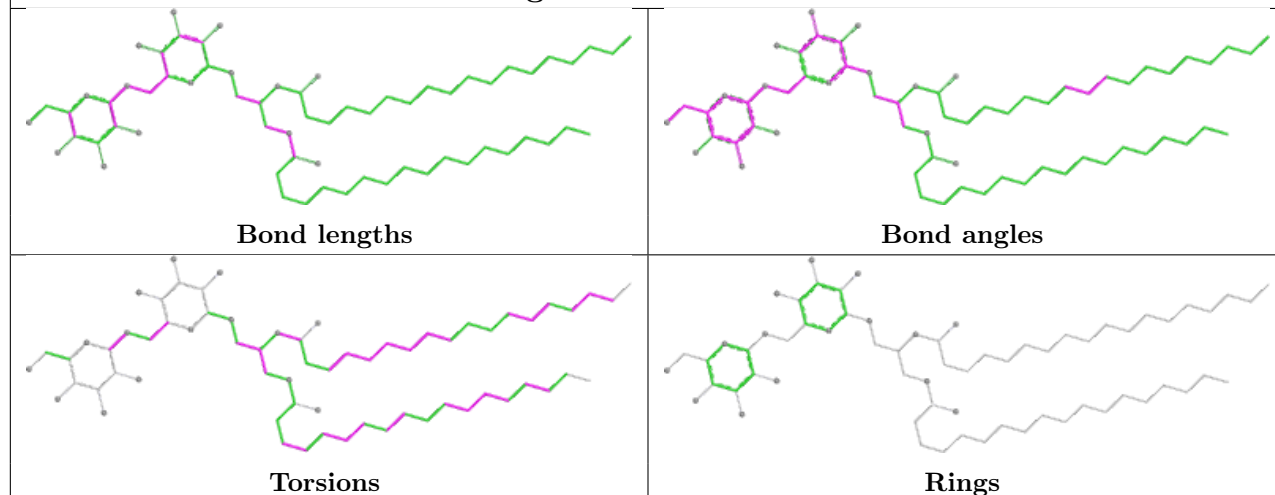




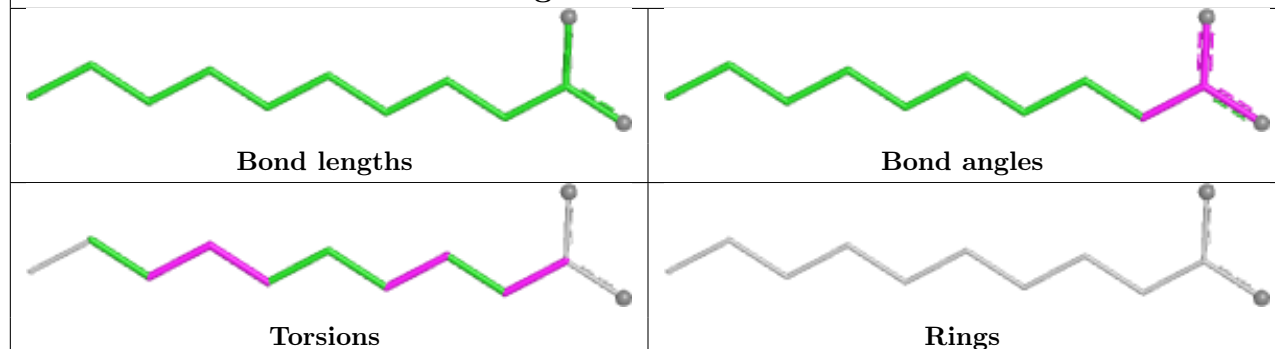
Ligand CLA d 405

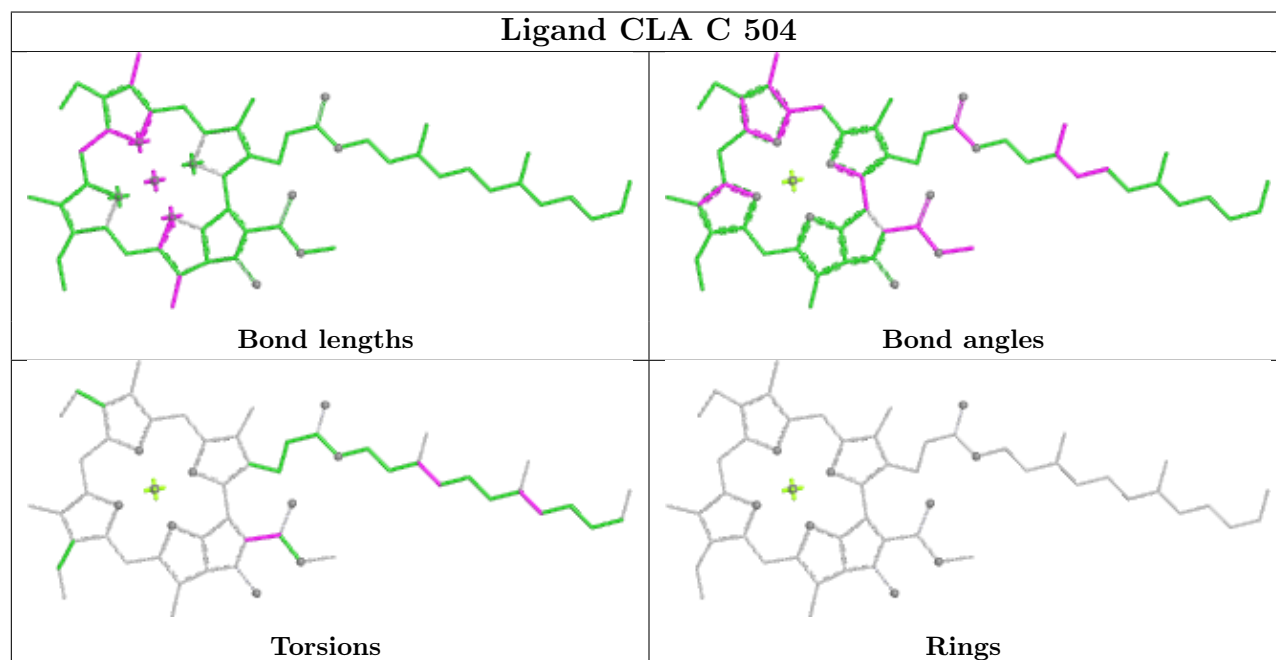
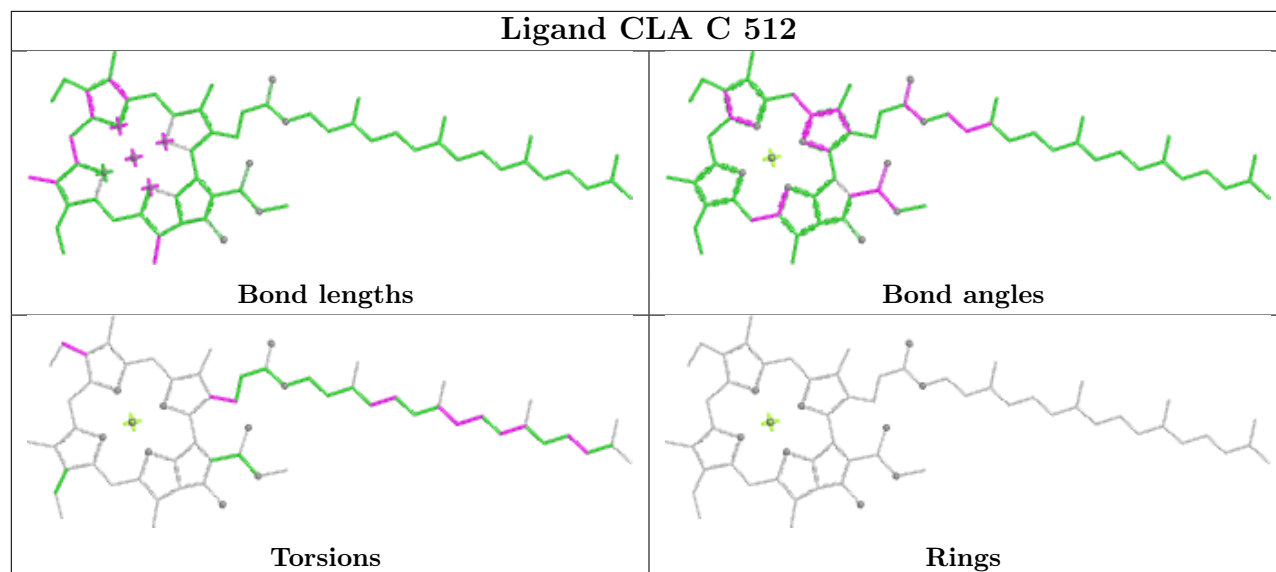


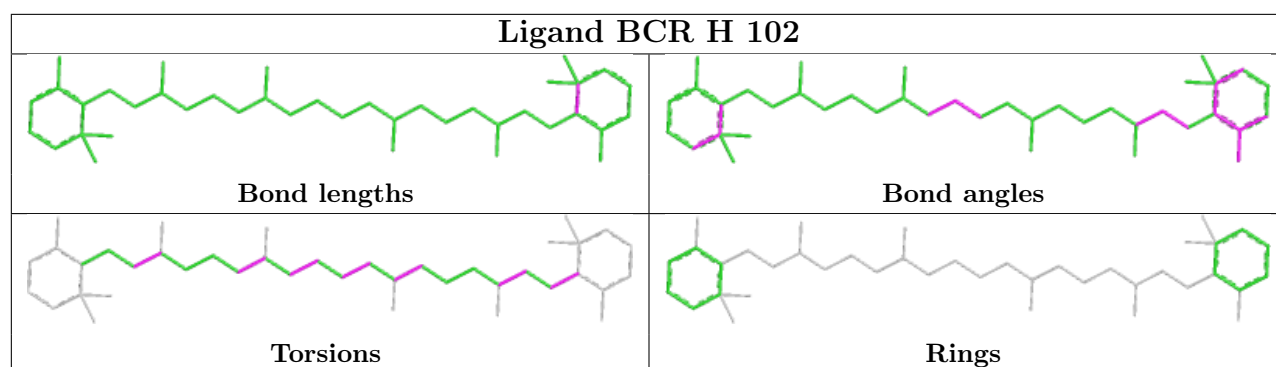
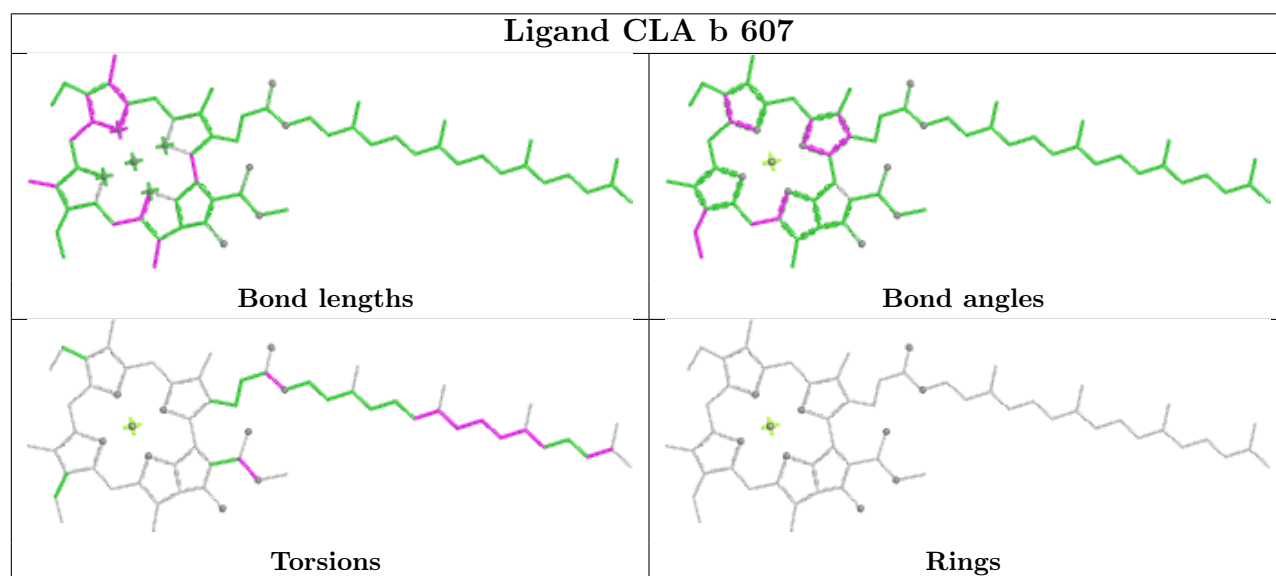
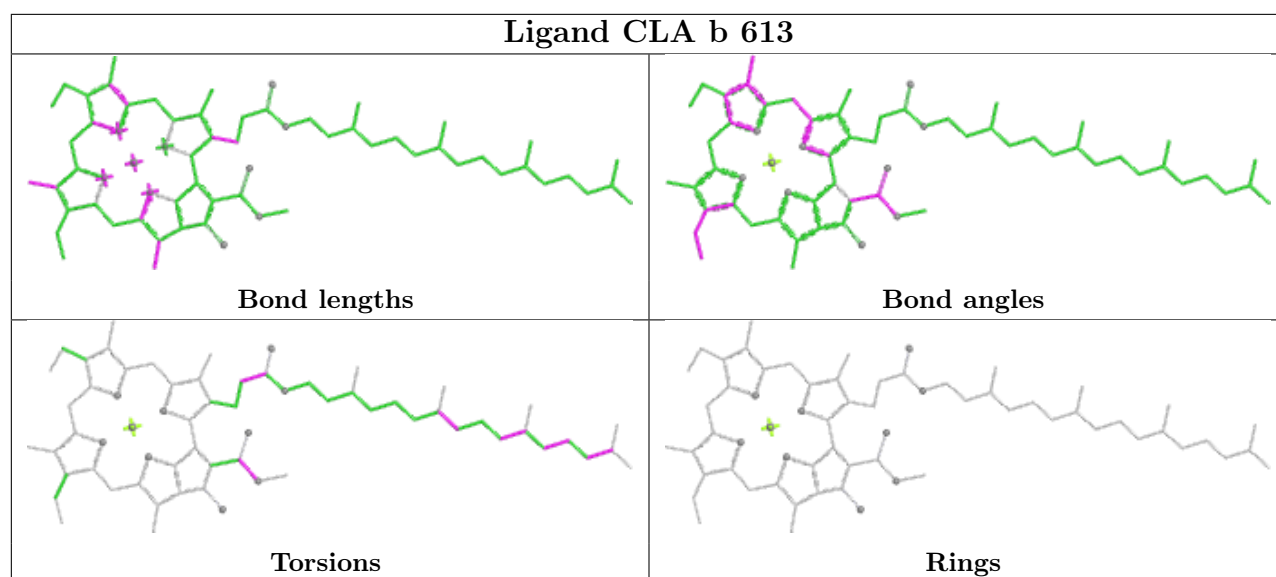
Ligand DGD A 413

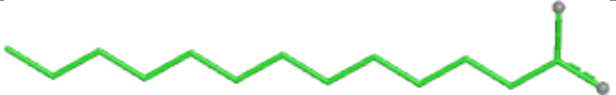
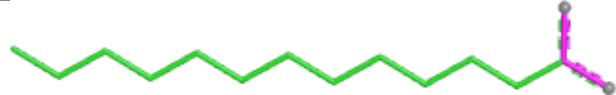
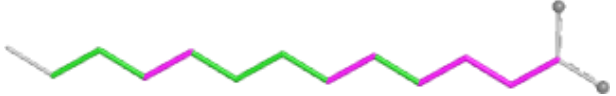
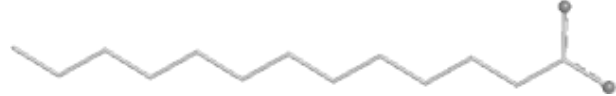


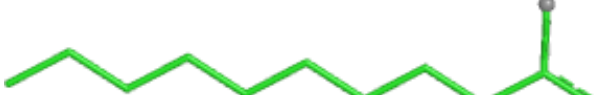
Ligand STE C 519





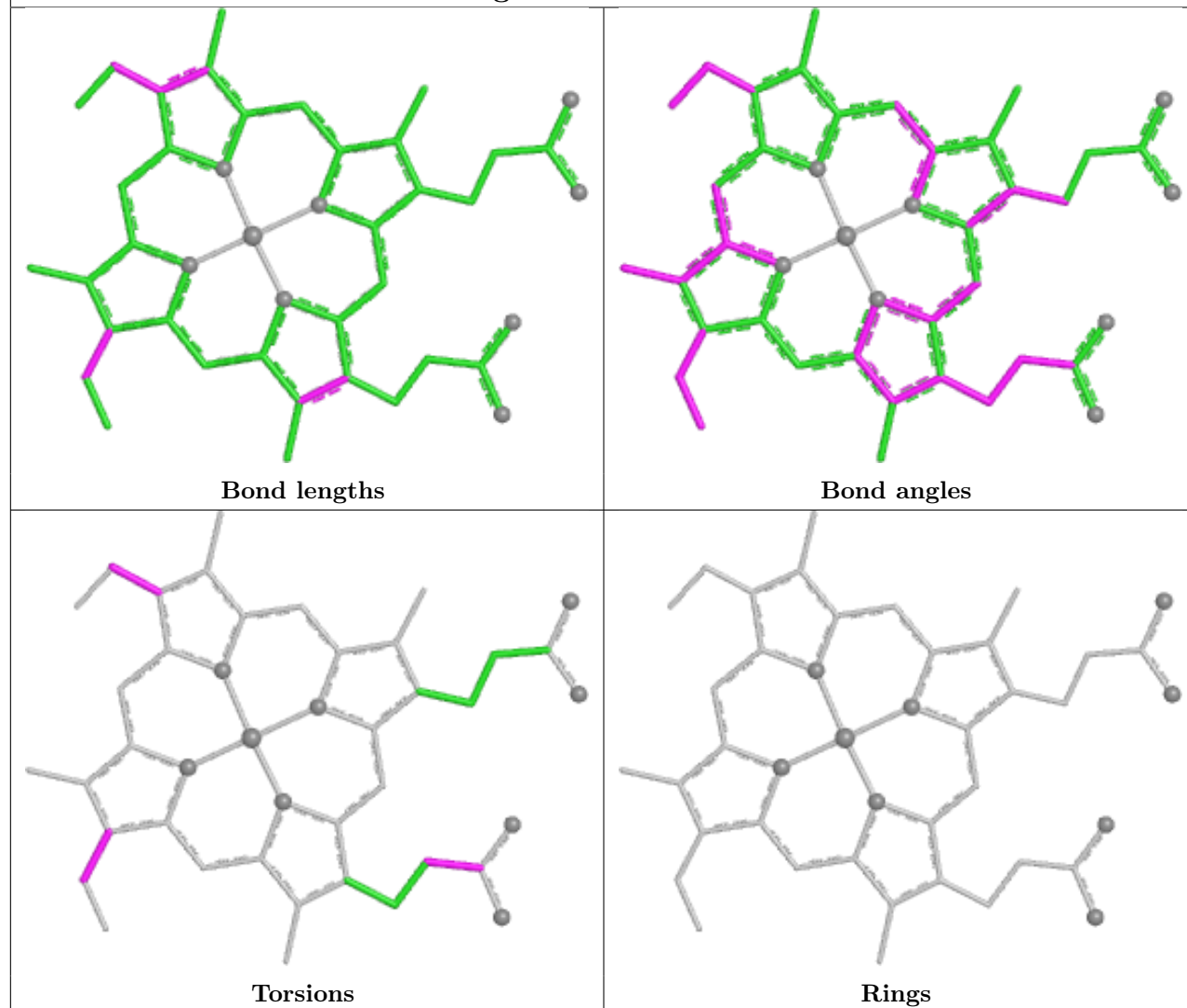


Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

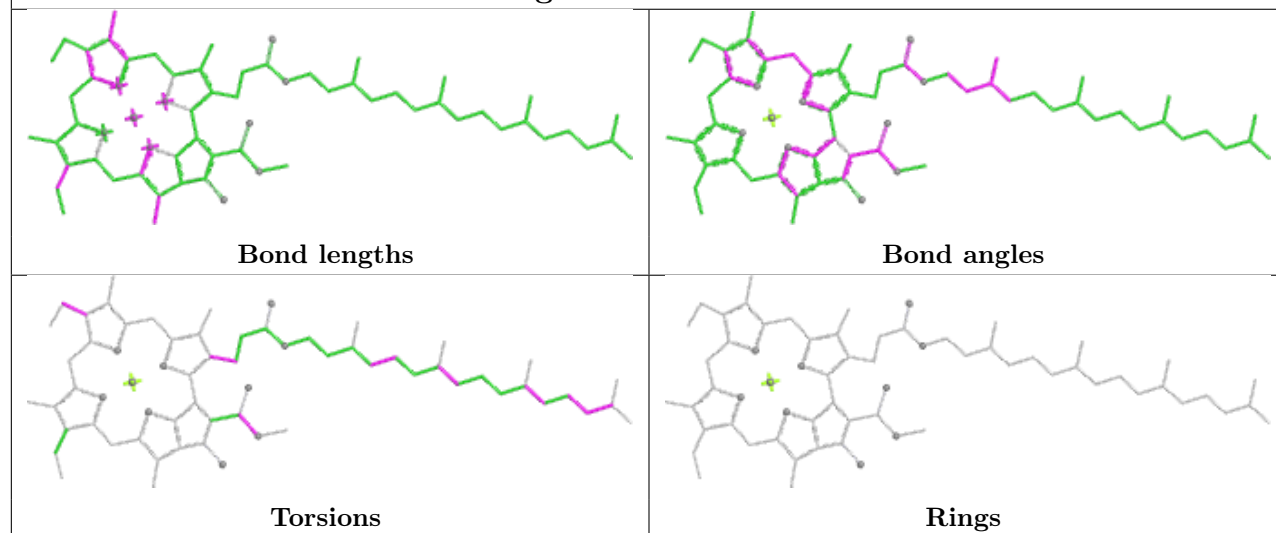
Ligand STE R 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

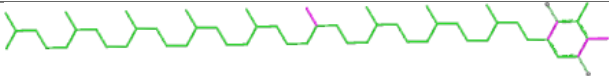
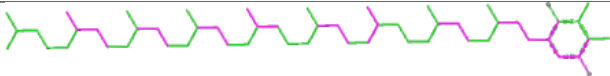
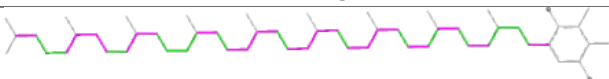
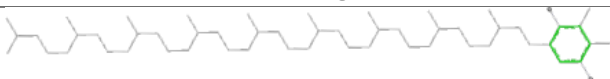
Ligand STE Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

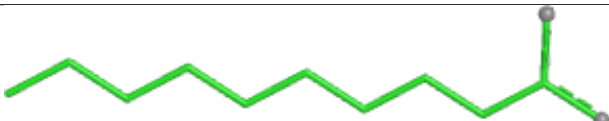
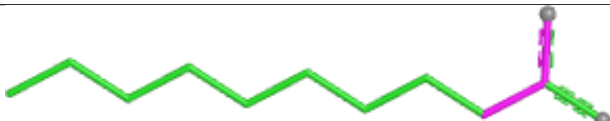
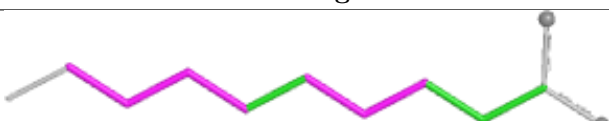
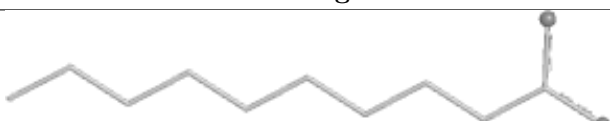
Ligand HEC V 201

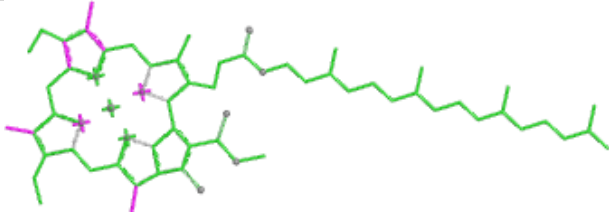
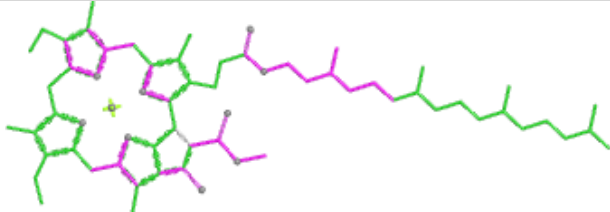
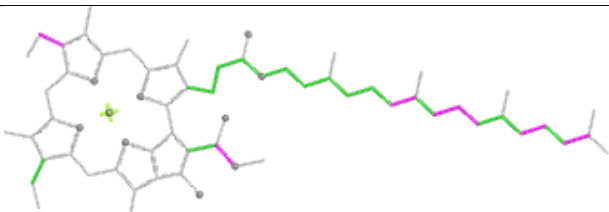
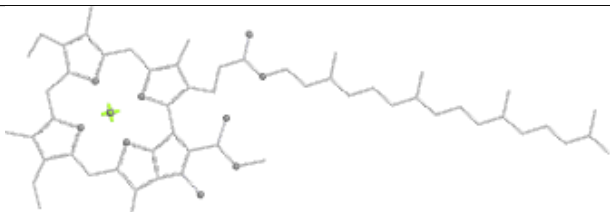


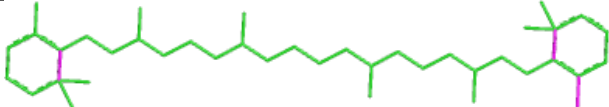
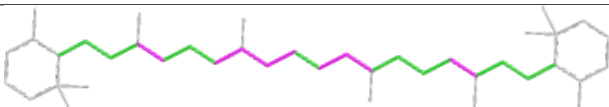
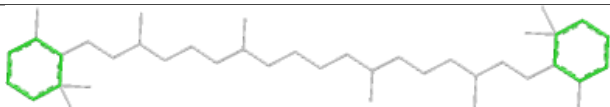
Ligand CLA b 602

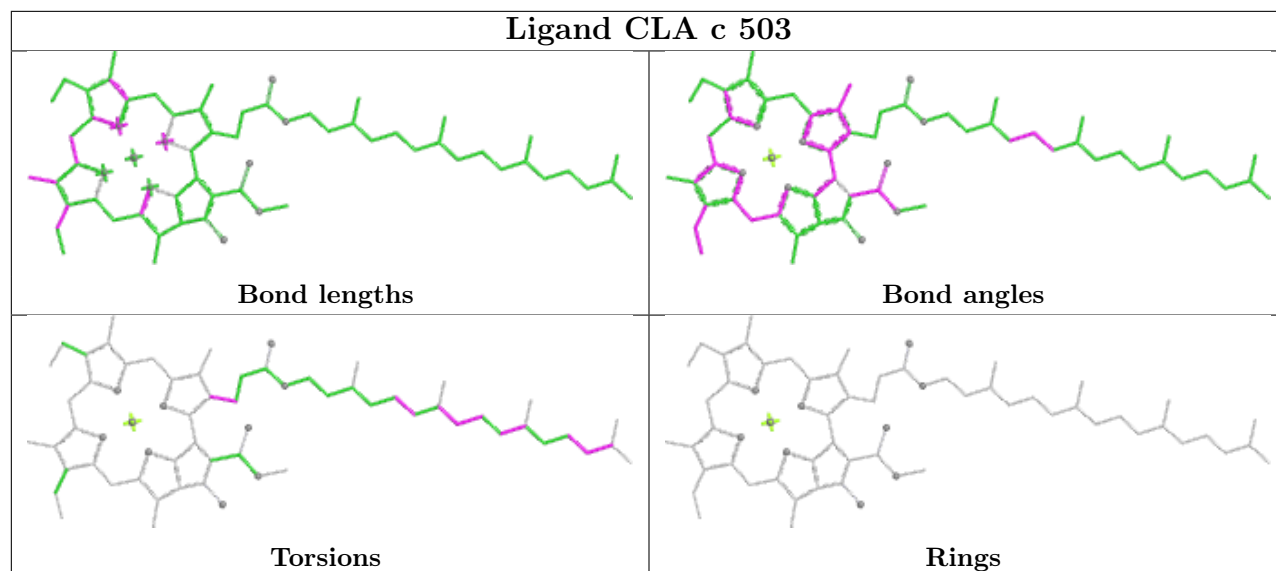
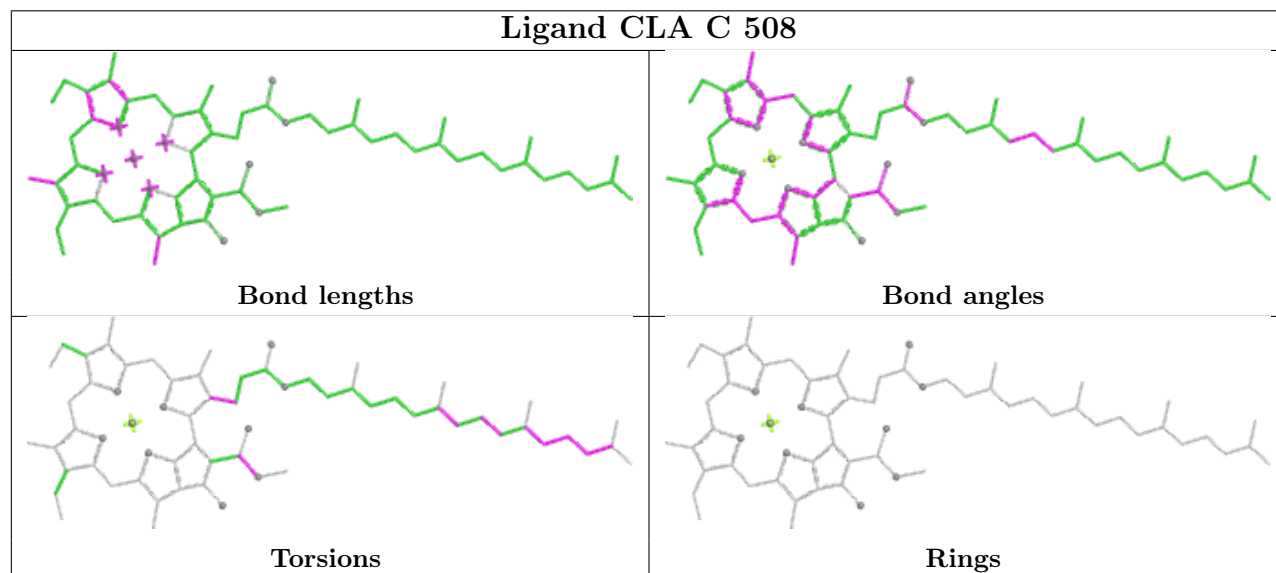
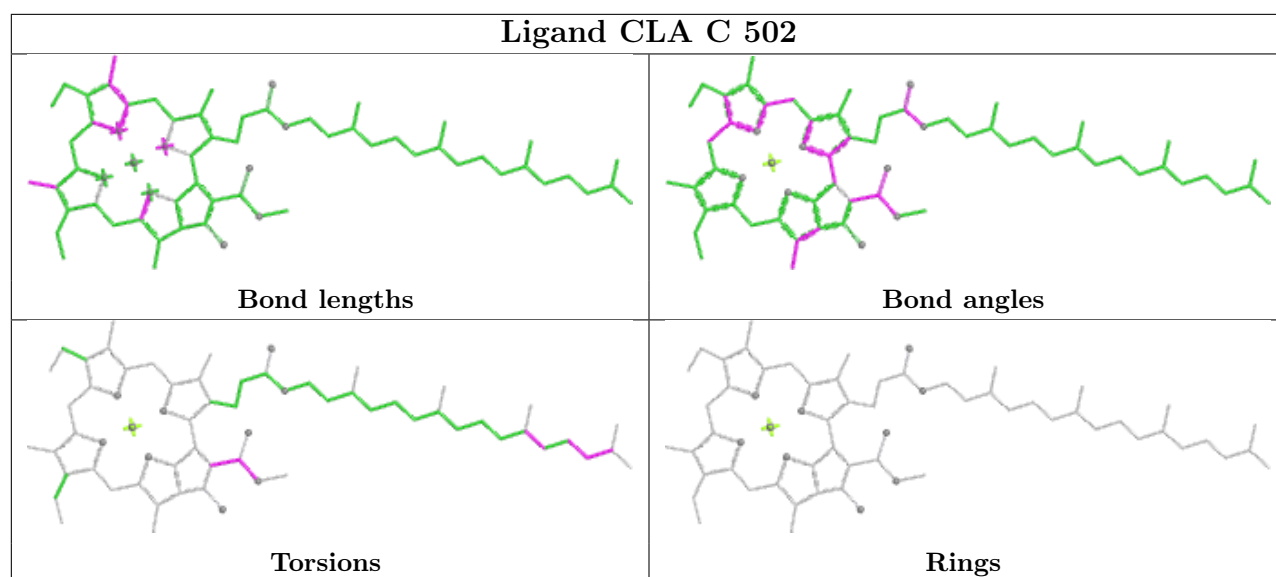


Ligand PL9 a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

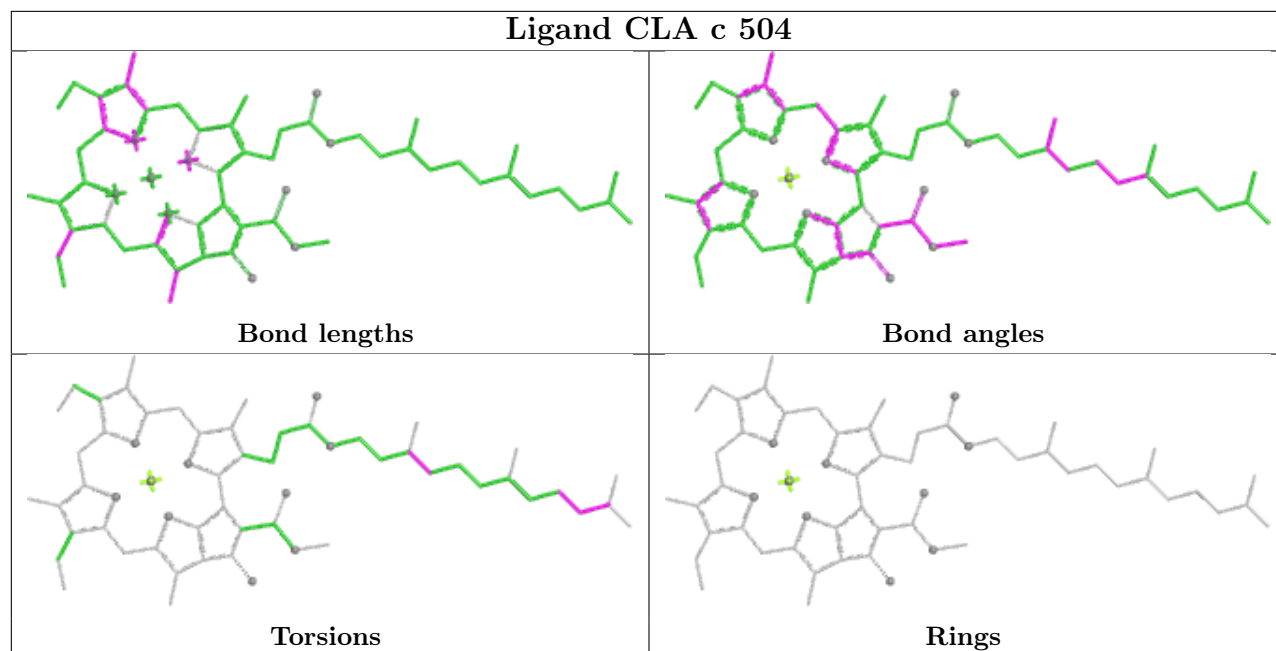
Ligand STE J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

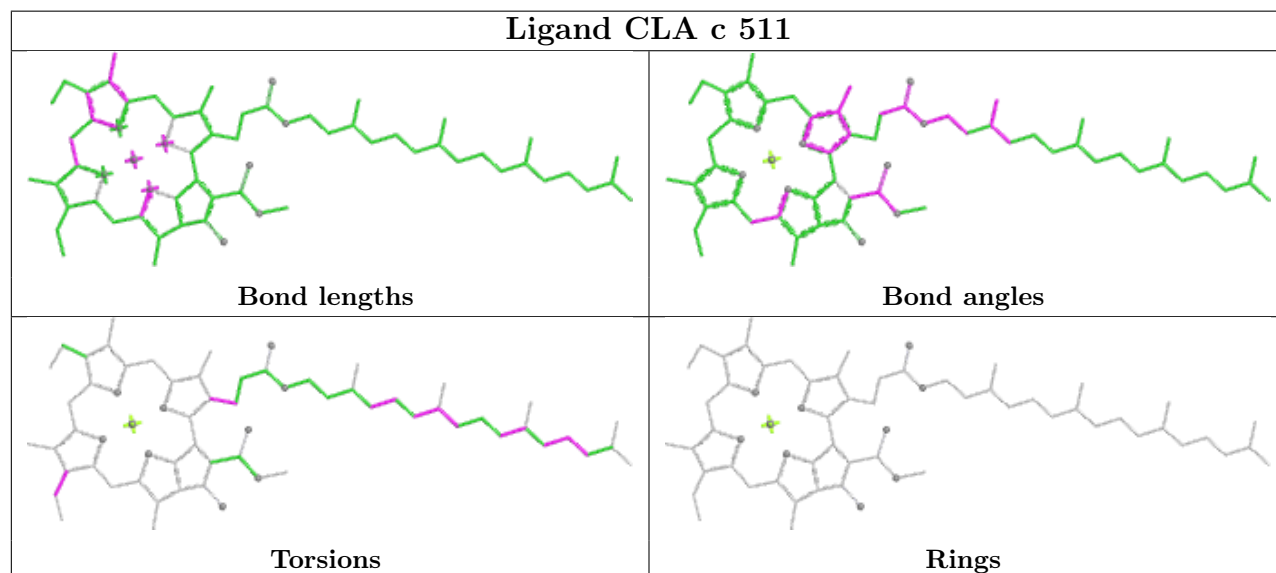
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings



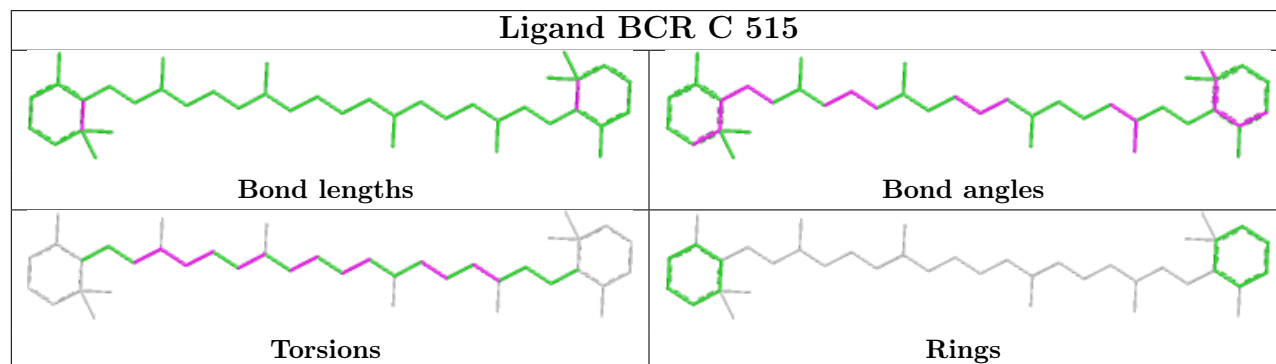
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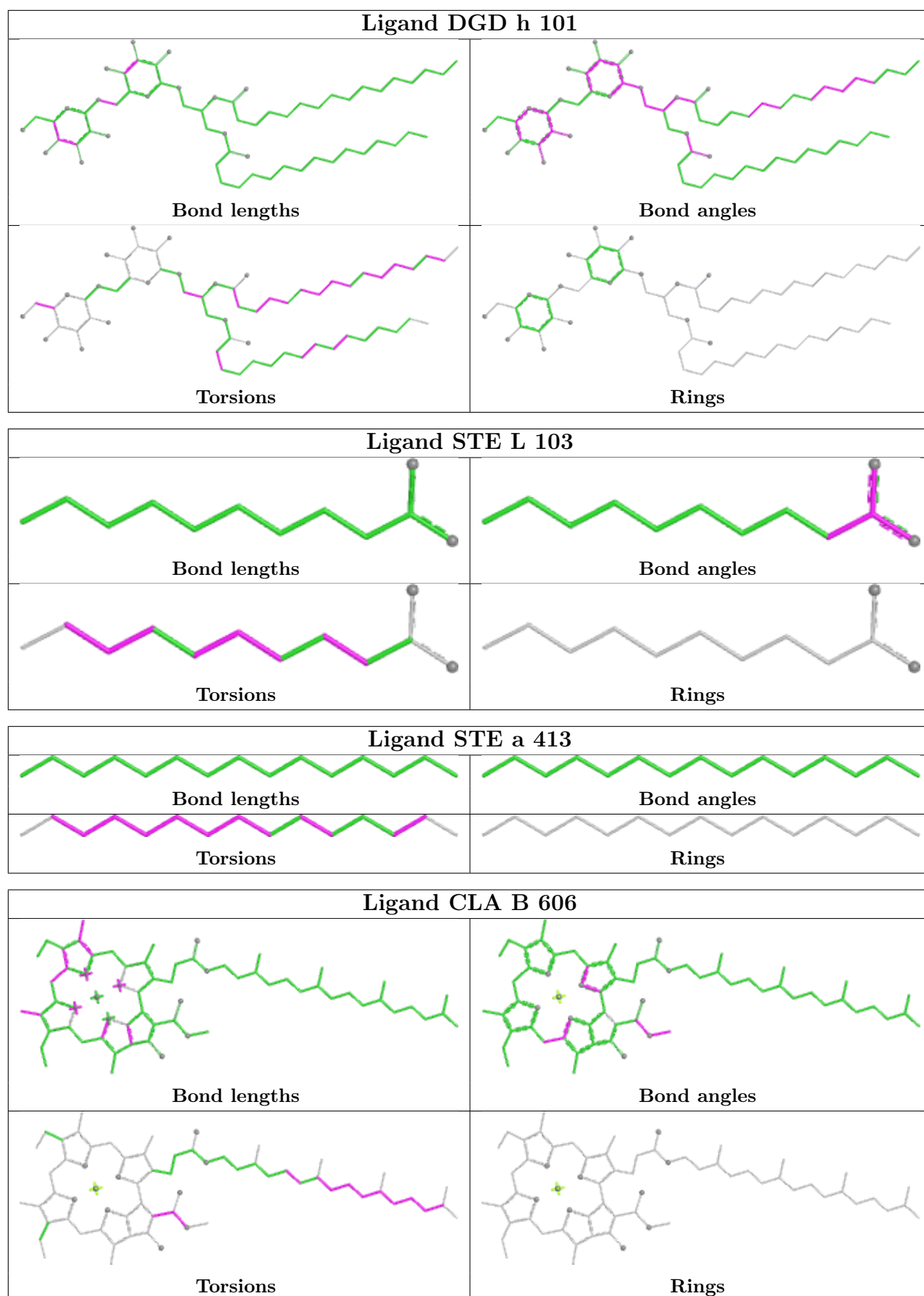


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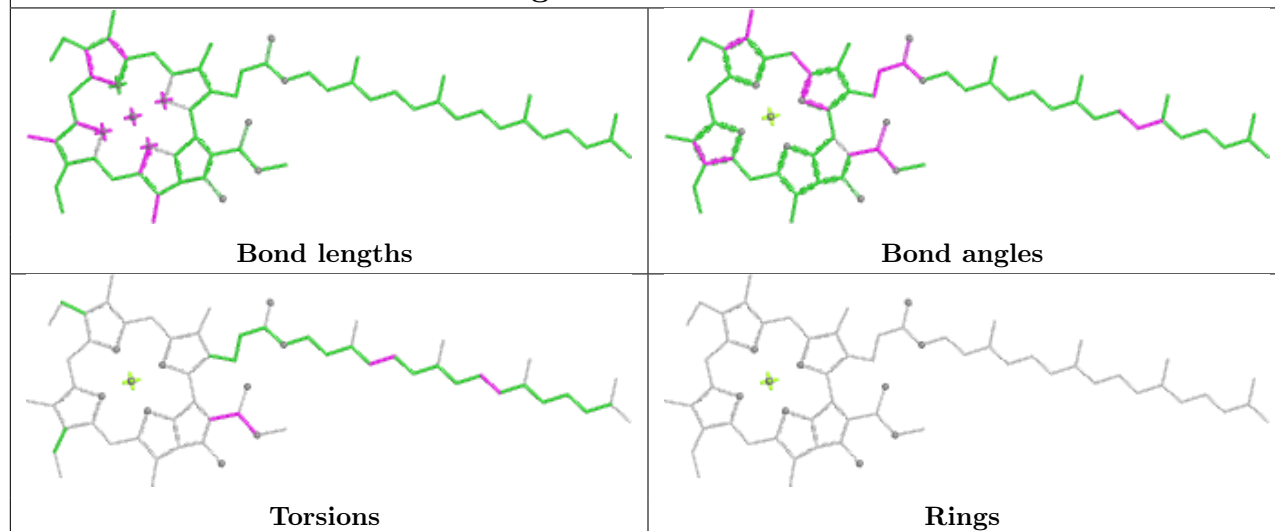


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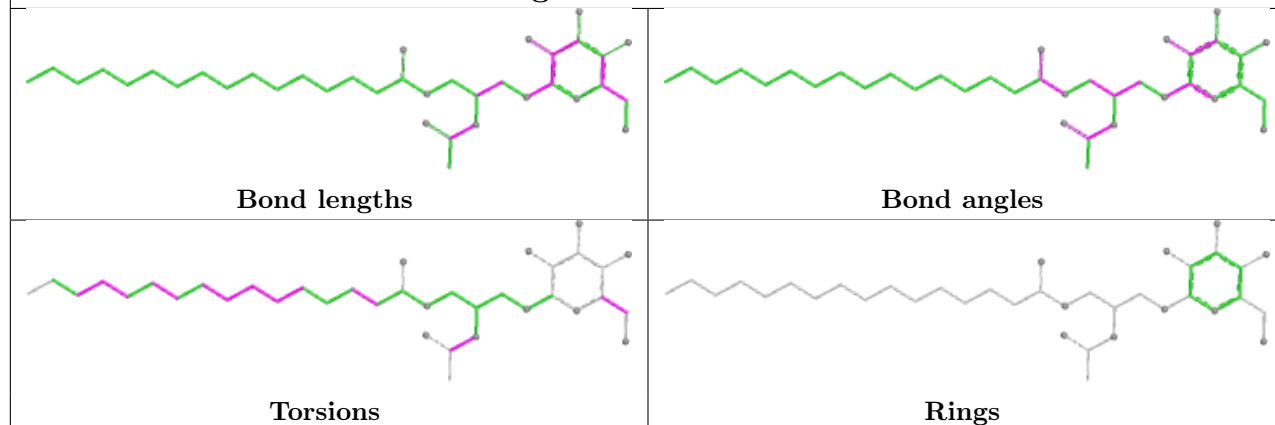




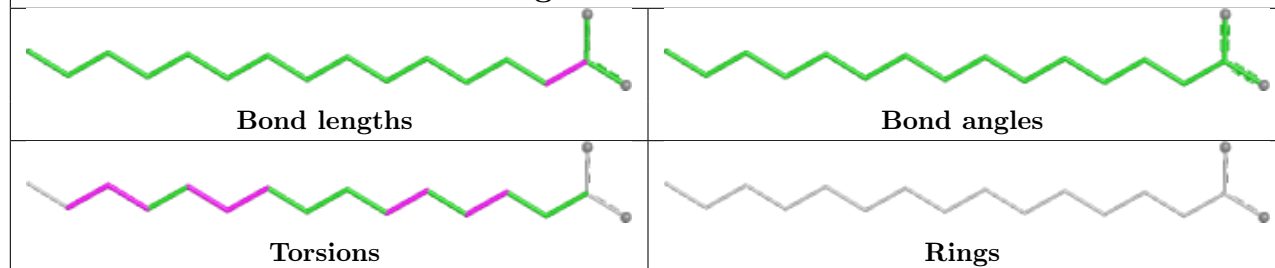
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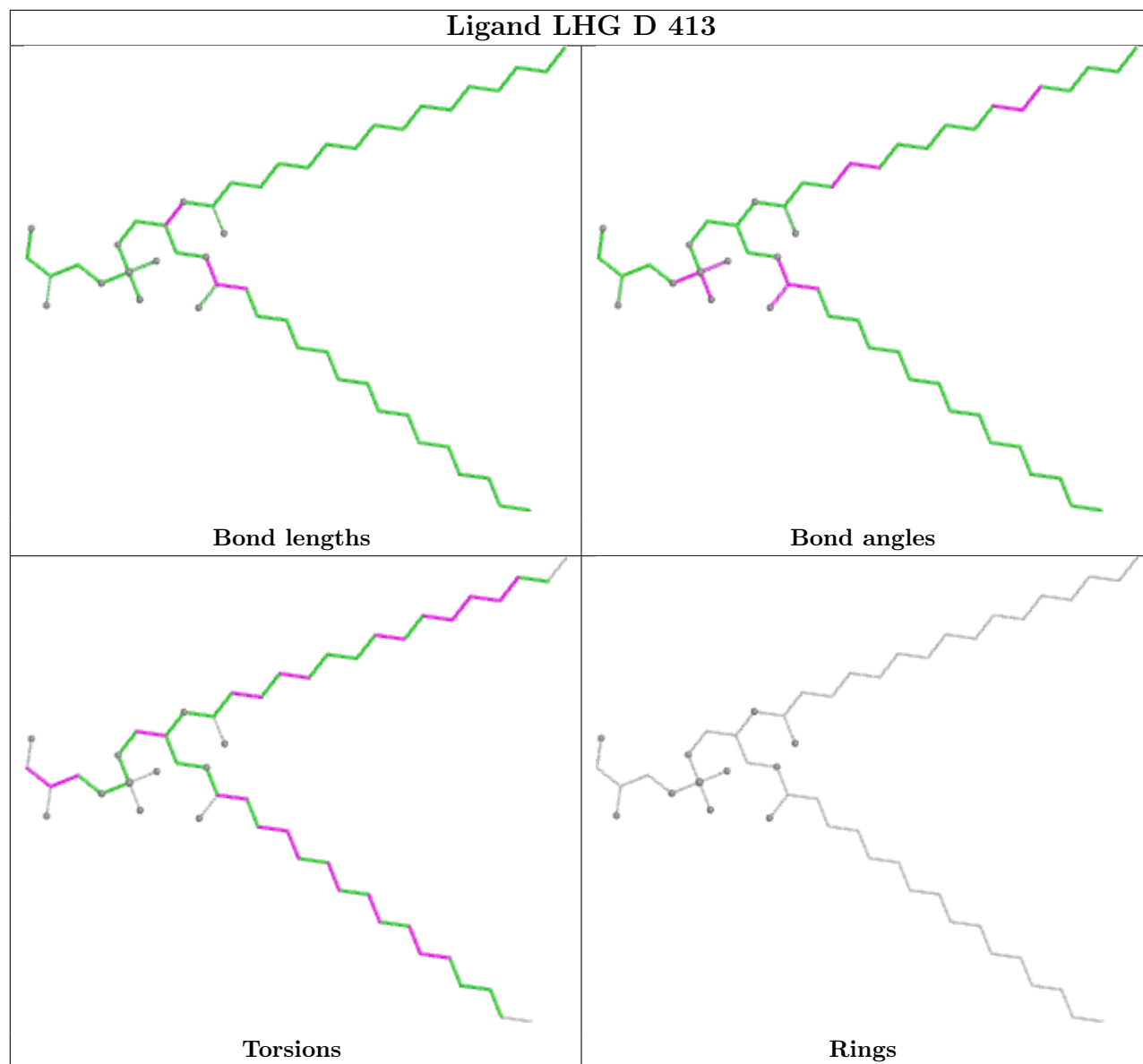


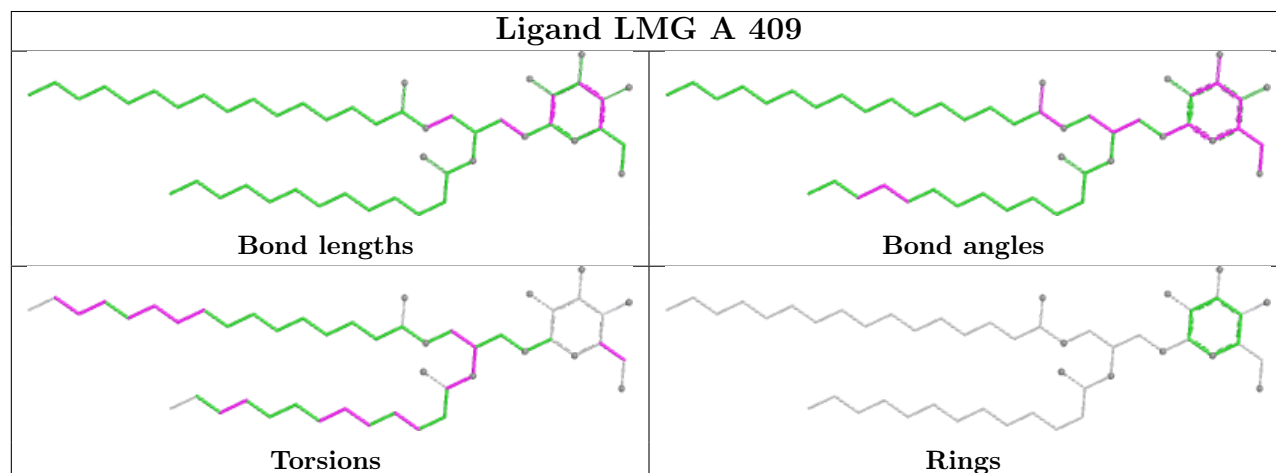
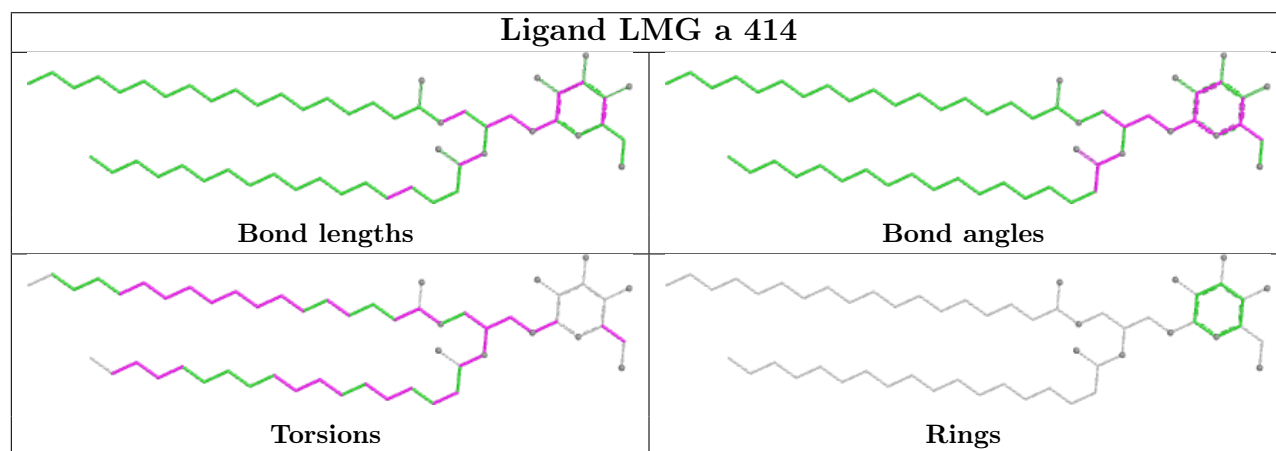
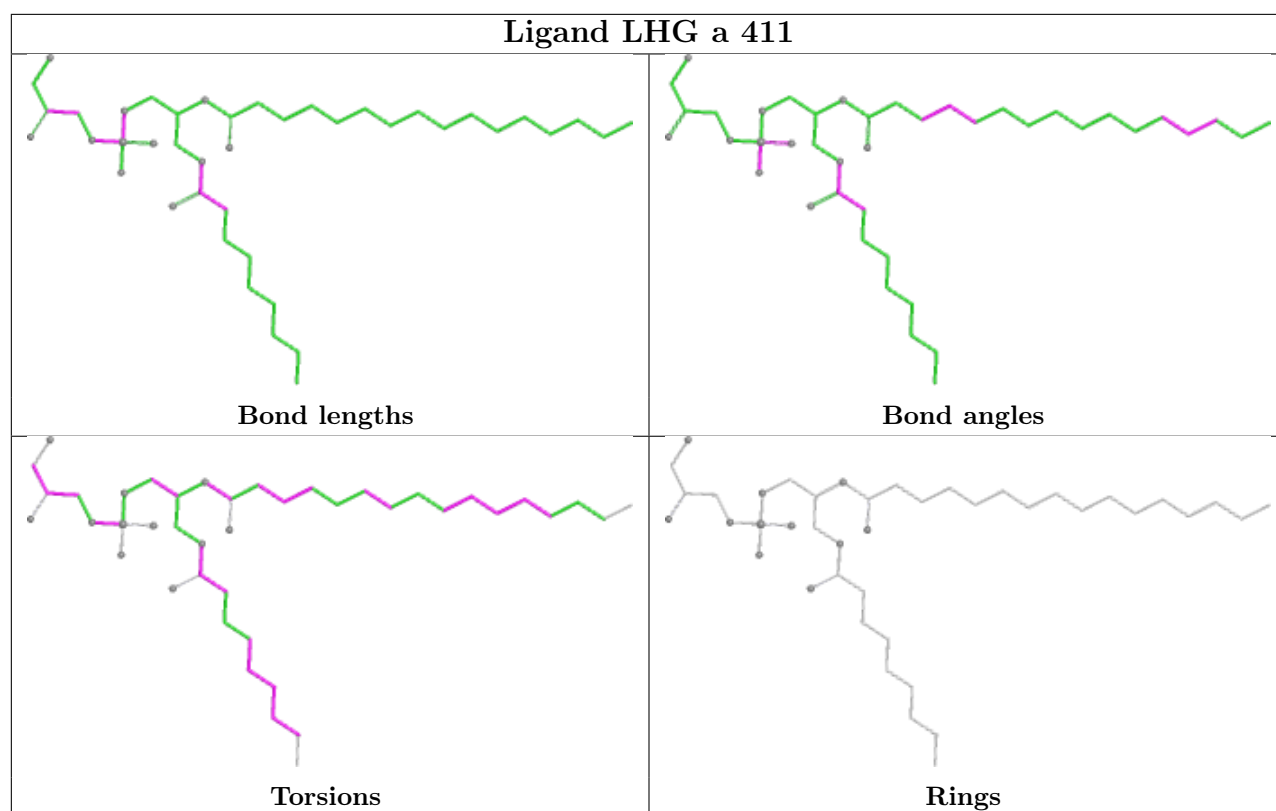
Ligand LMG c 518

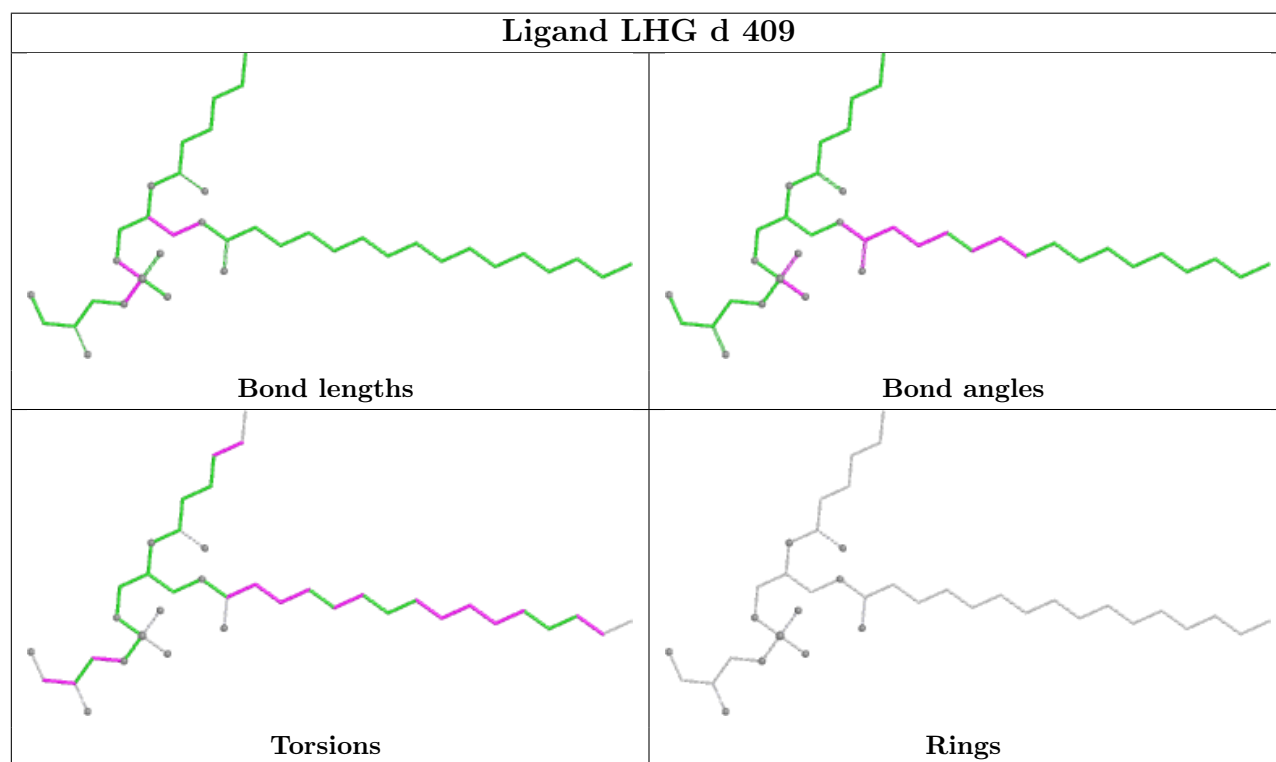
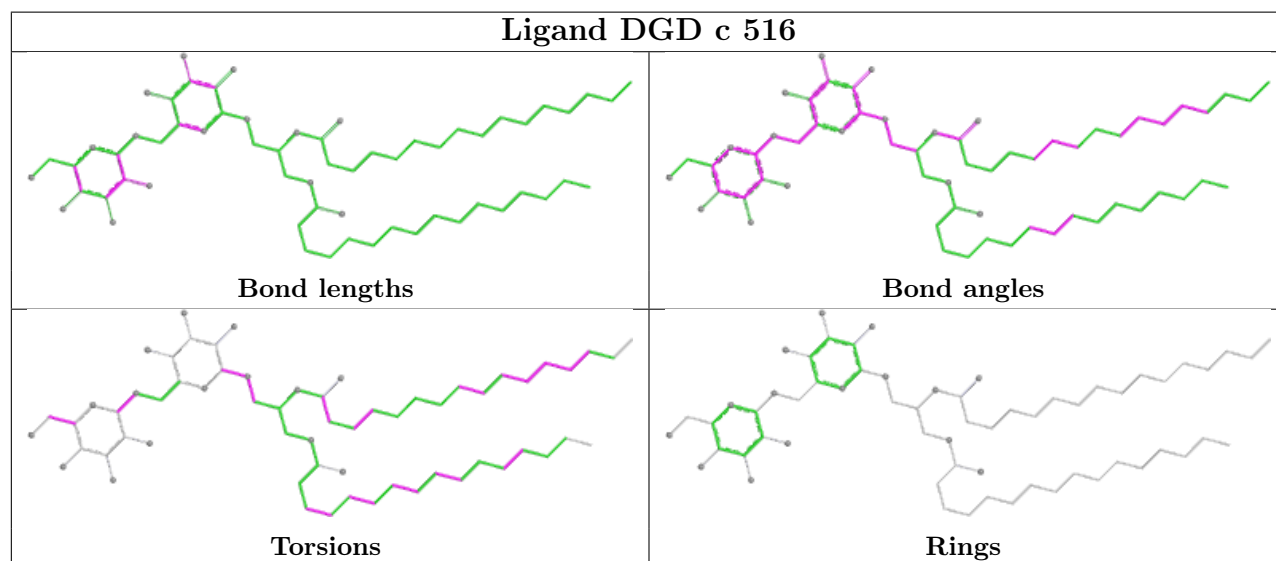
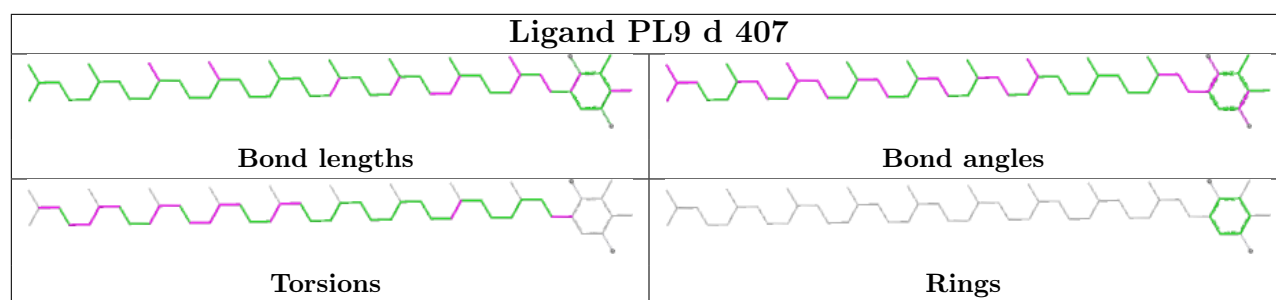


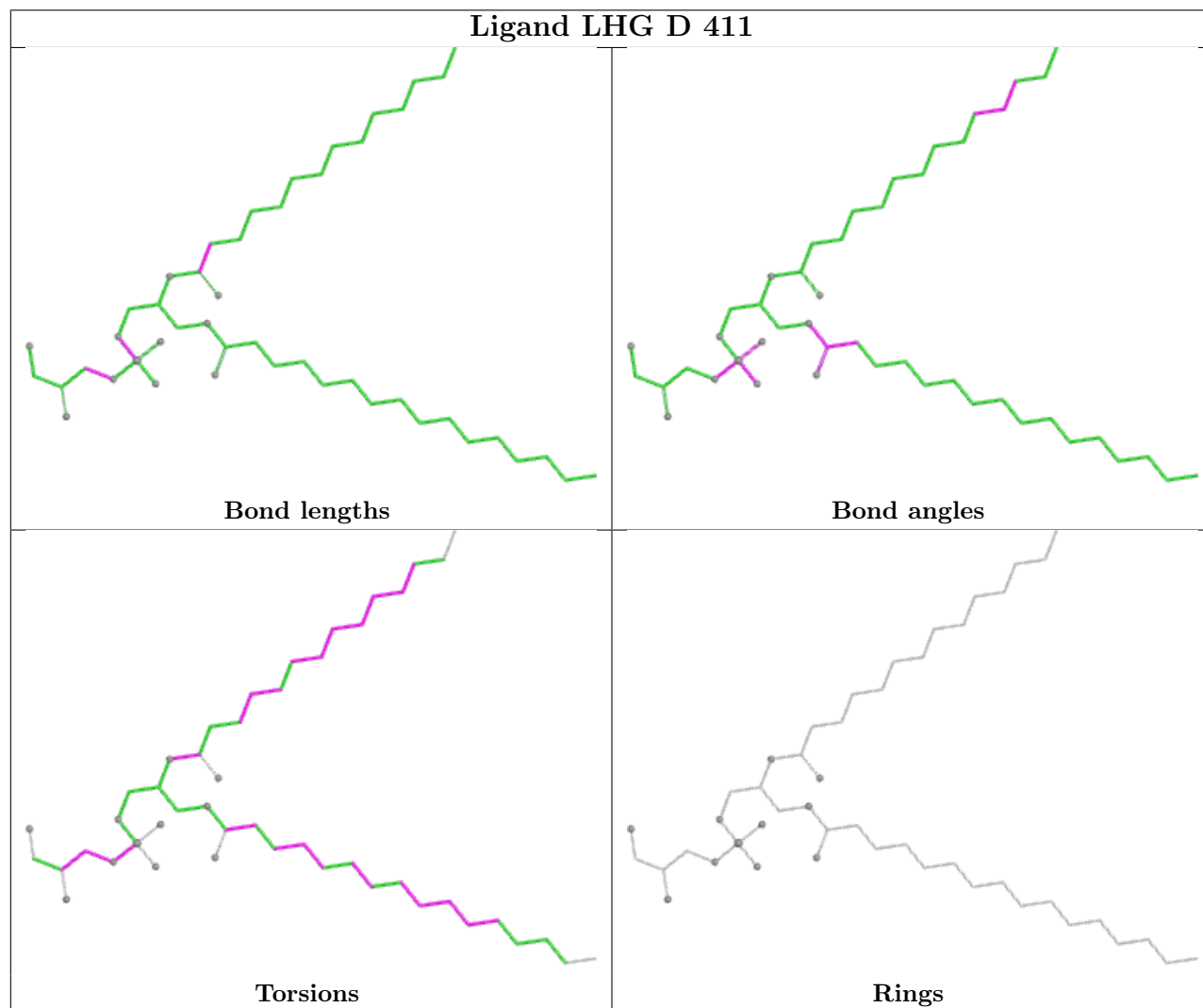
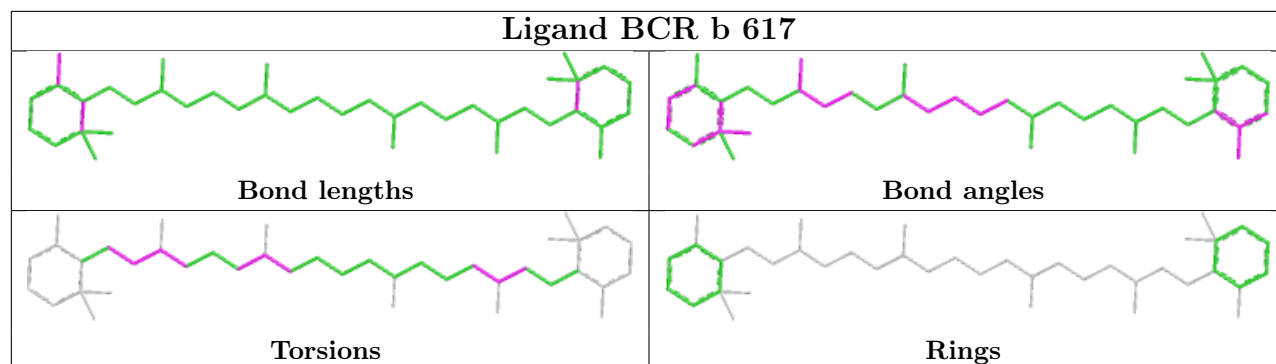
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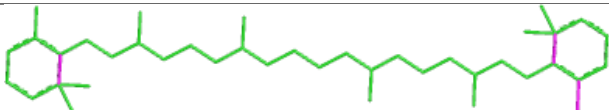
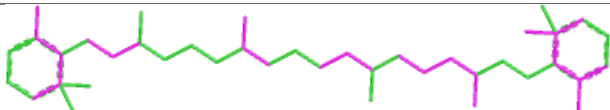
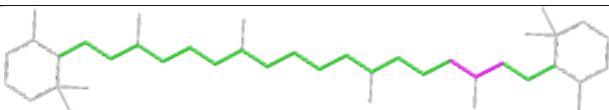
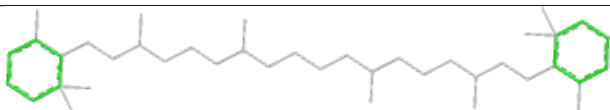


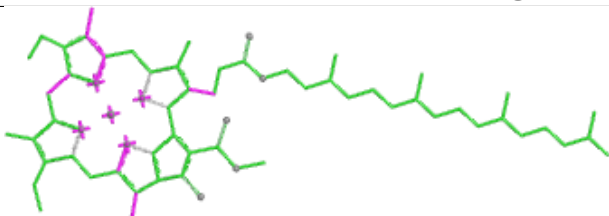
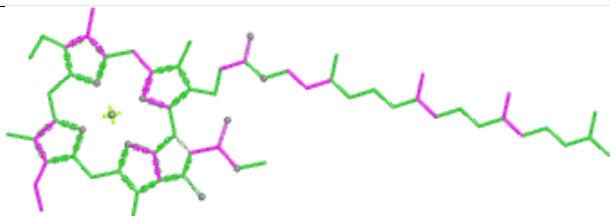
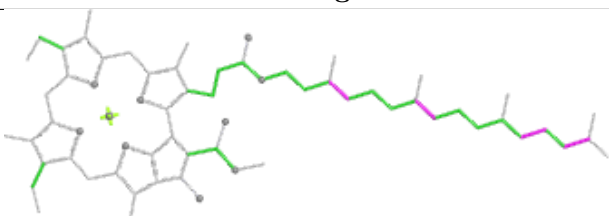
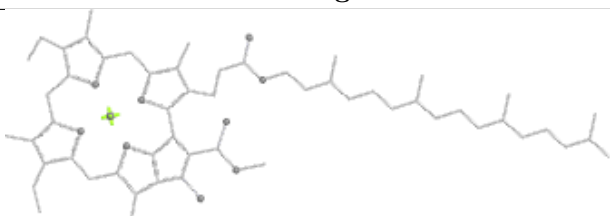


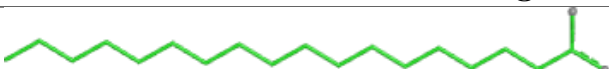
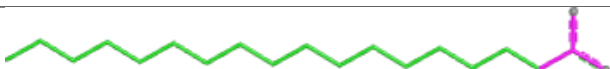




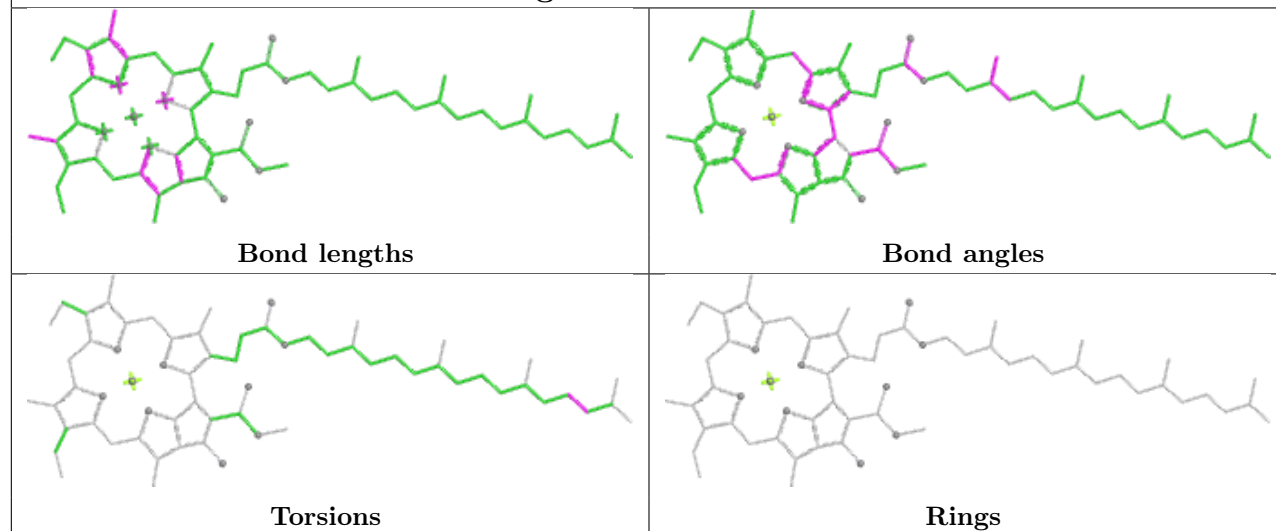


Ligand BCR a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

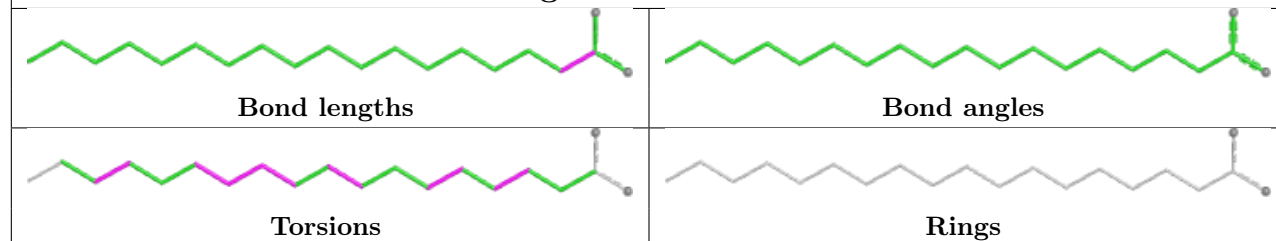
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE x 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

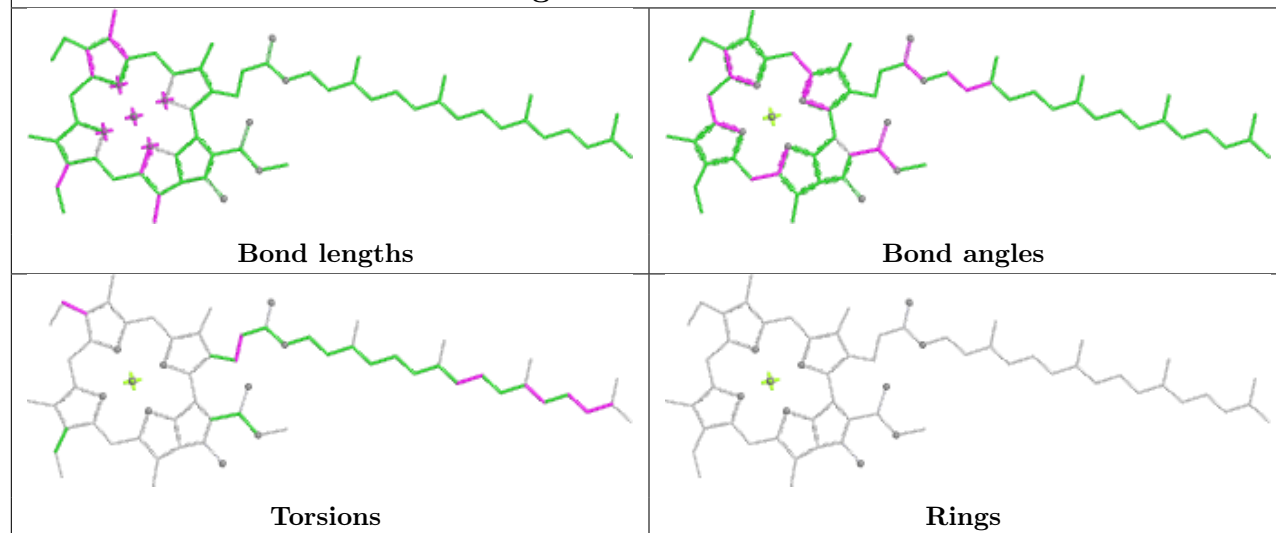
Ligand CLA a 402

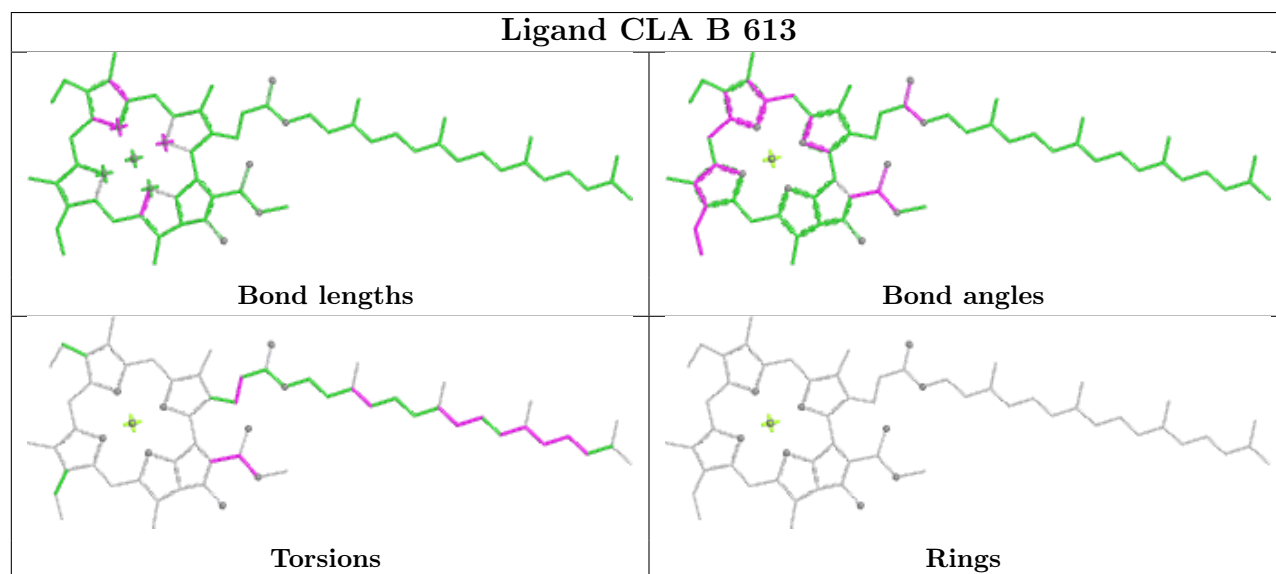
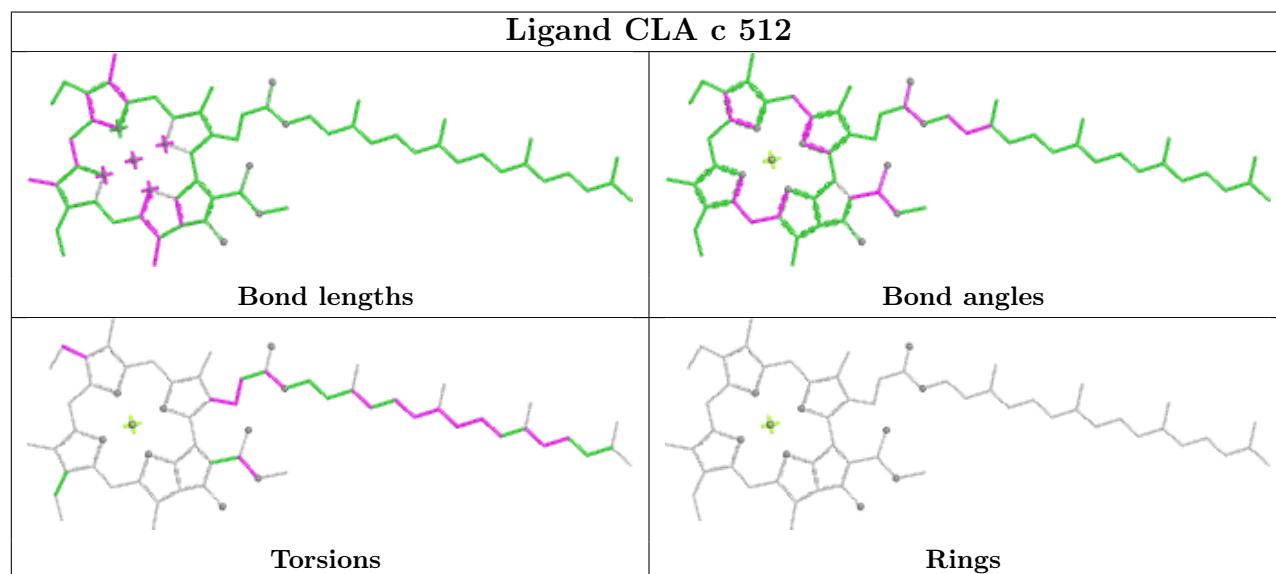
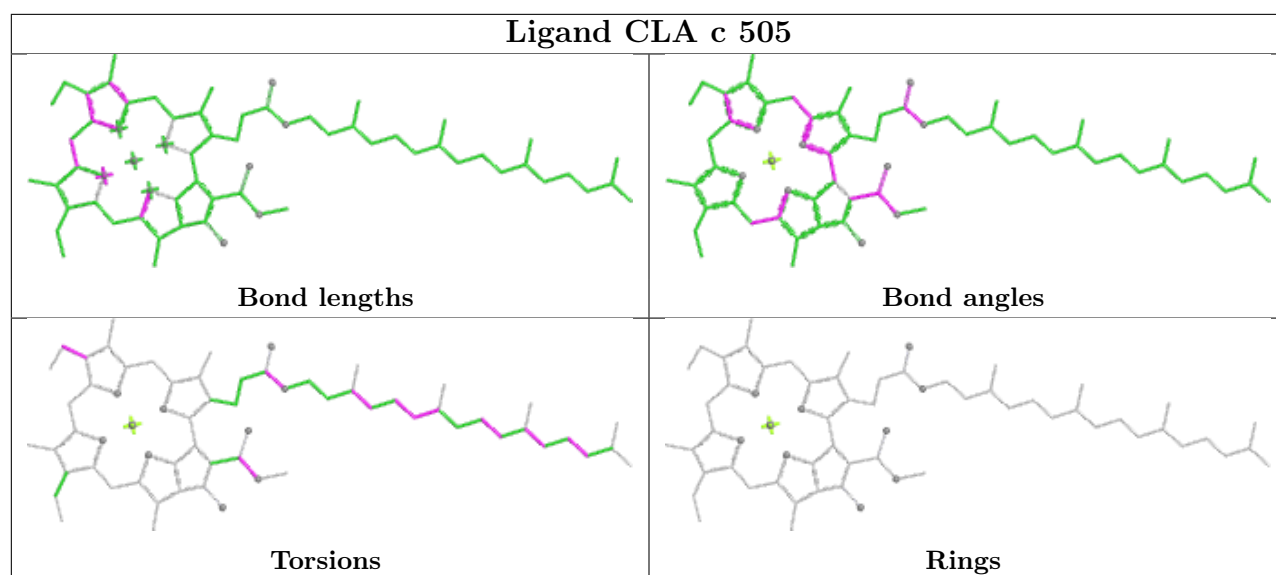


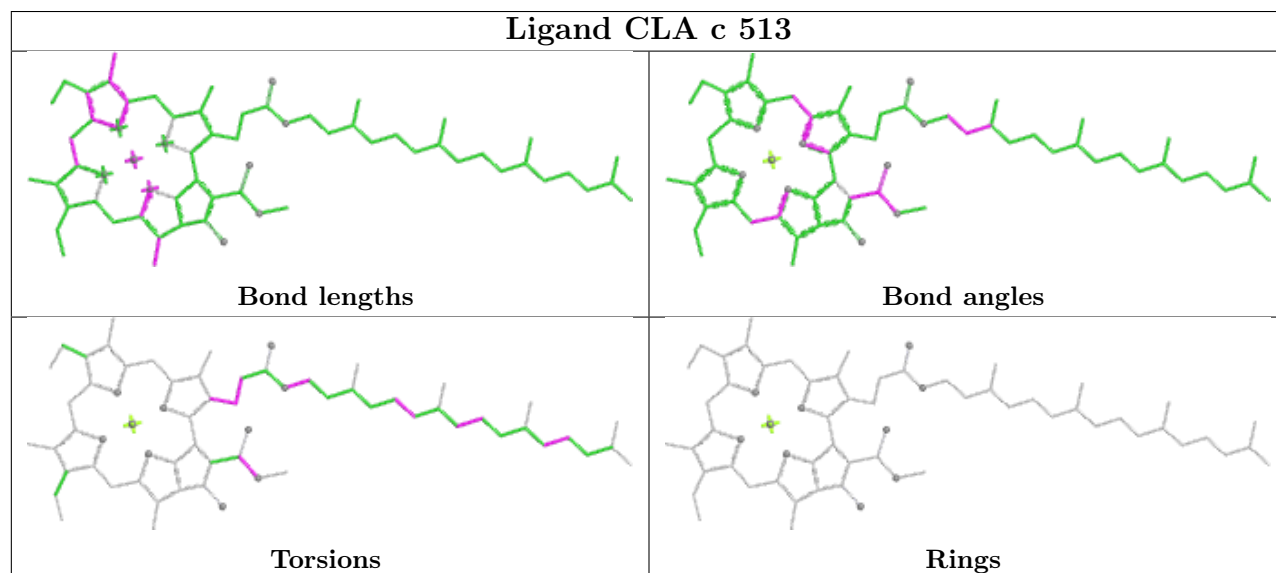
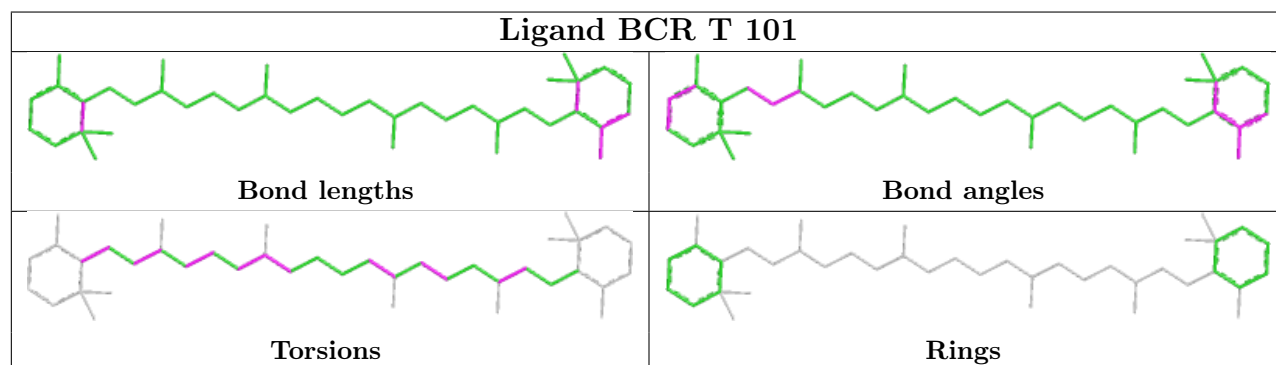
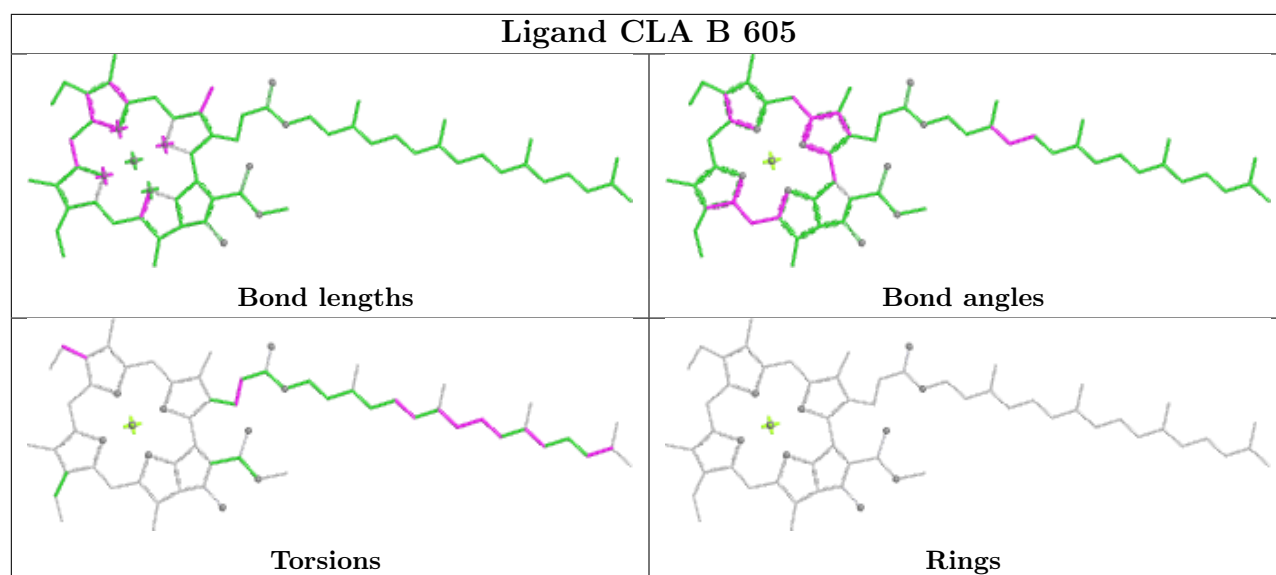
Ligand STE c 519

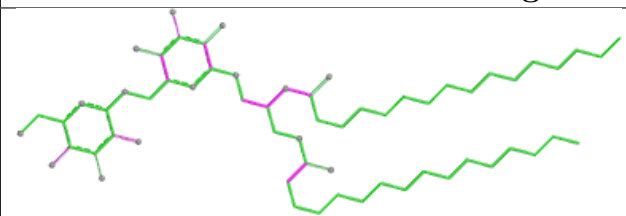
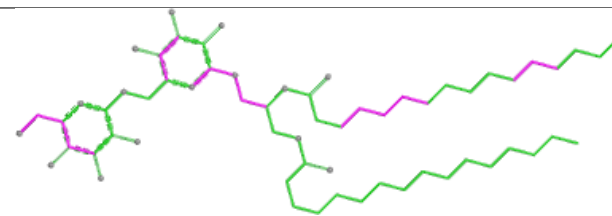
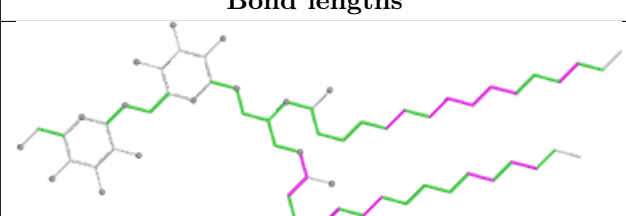
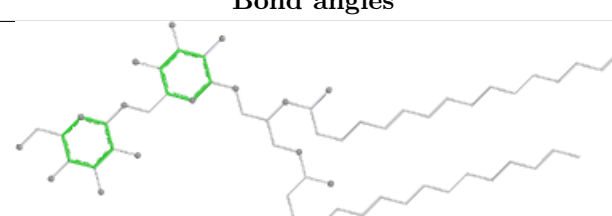


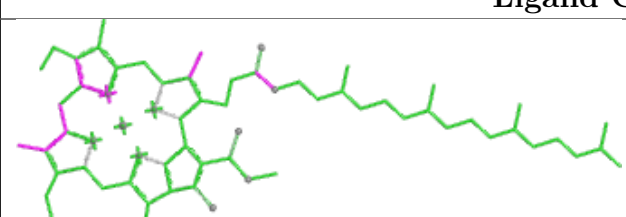
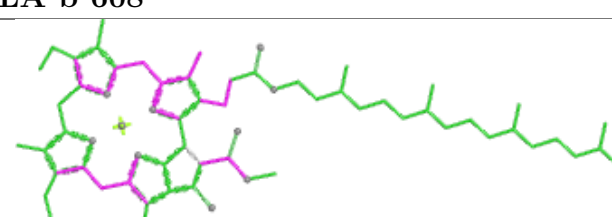
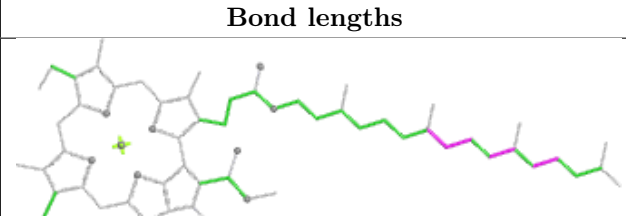
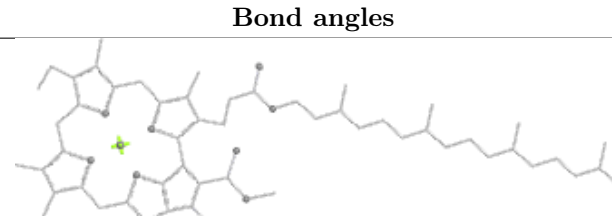
Ligand CLA B 609

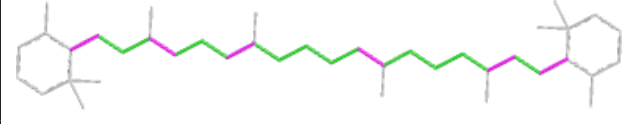
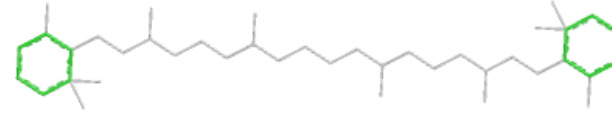


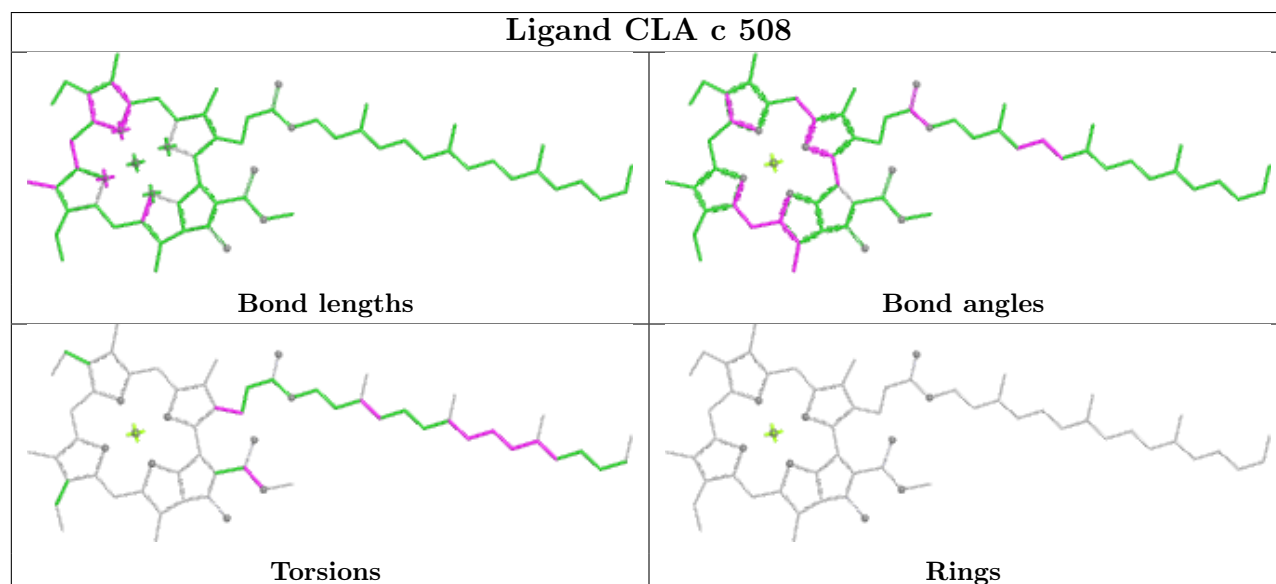
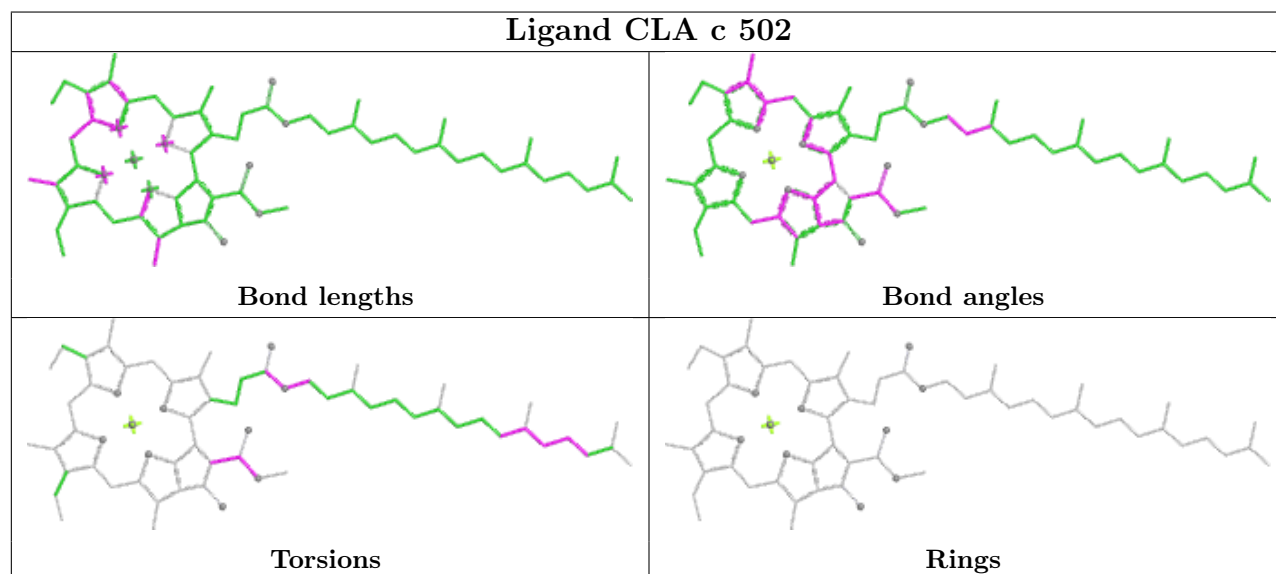
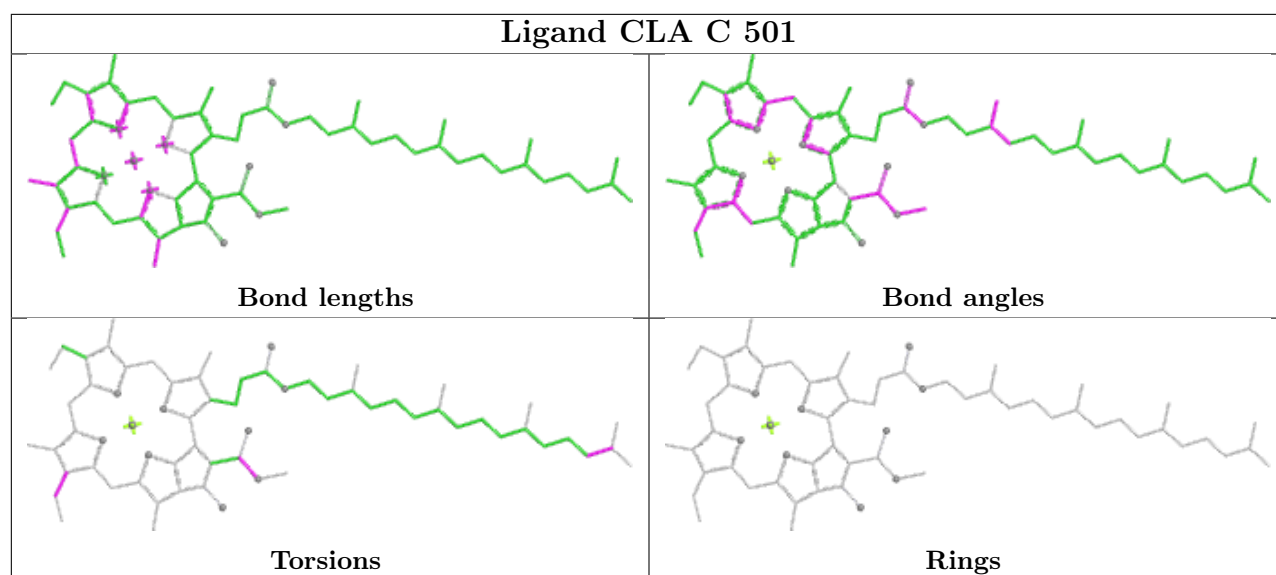


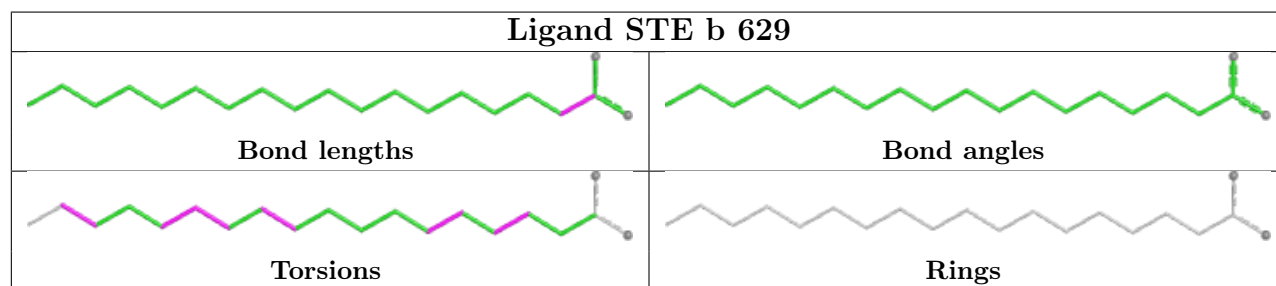
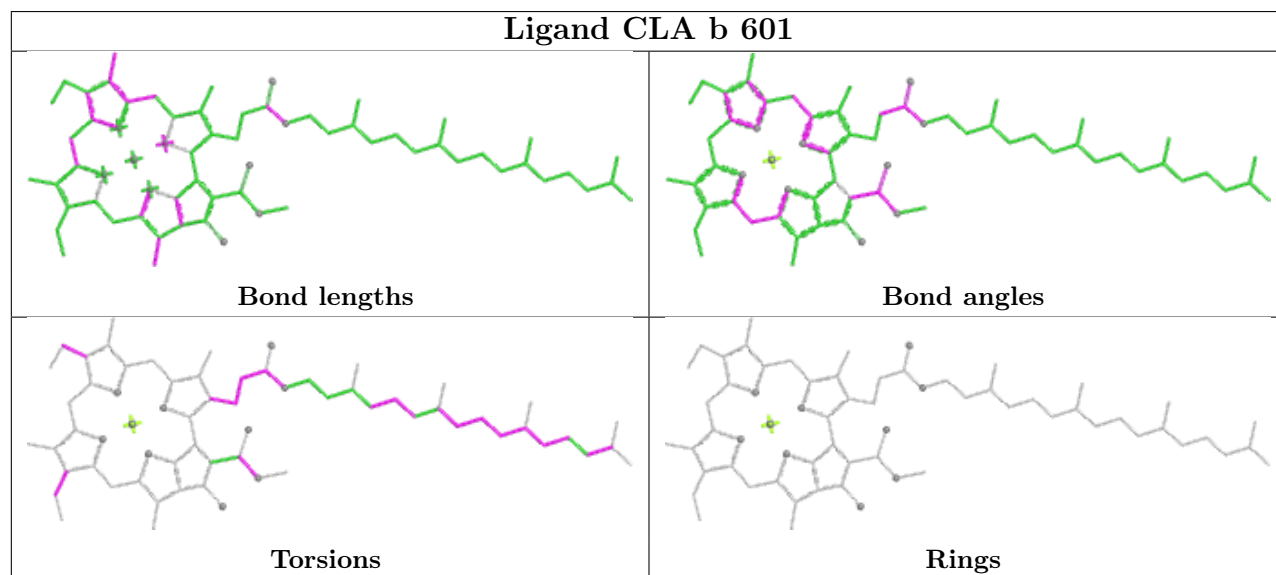
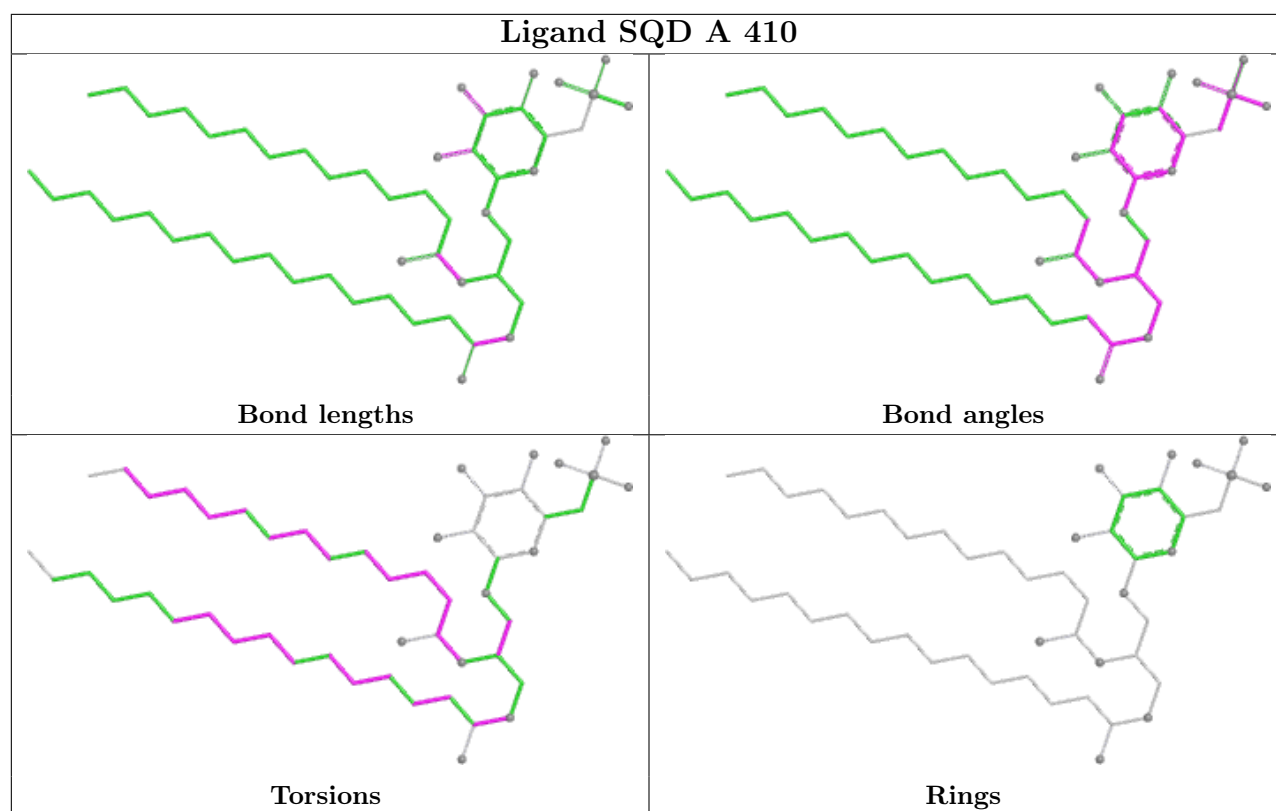


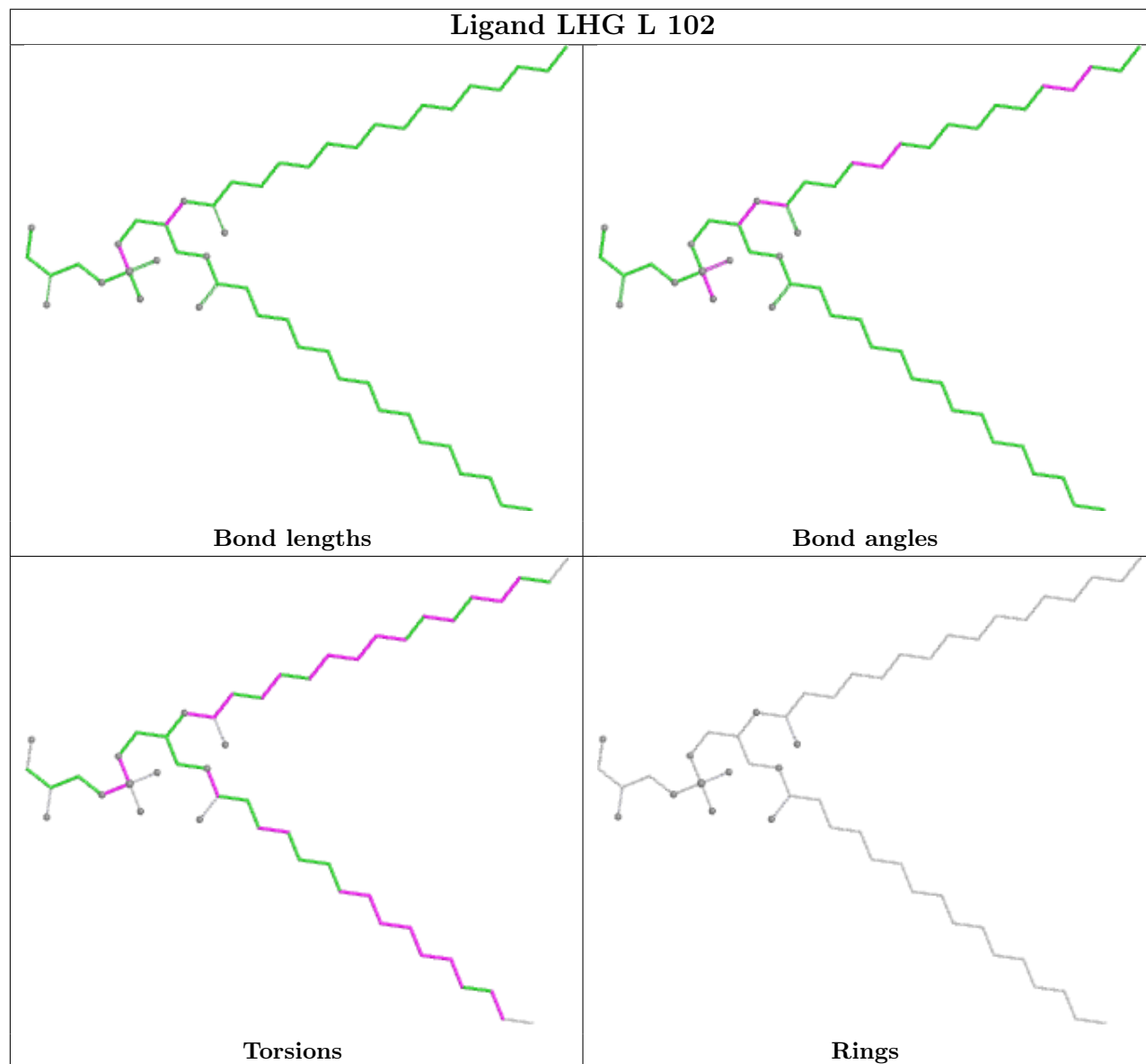
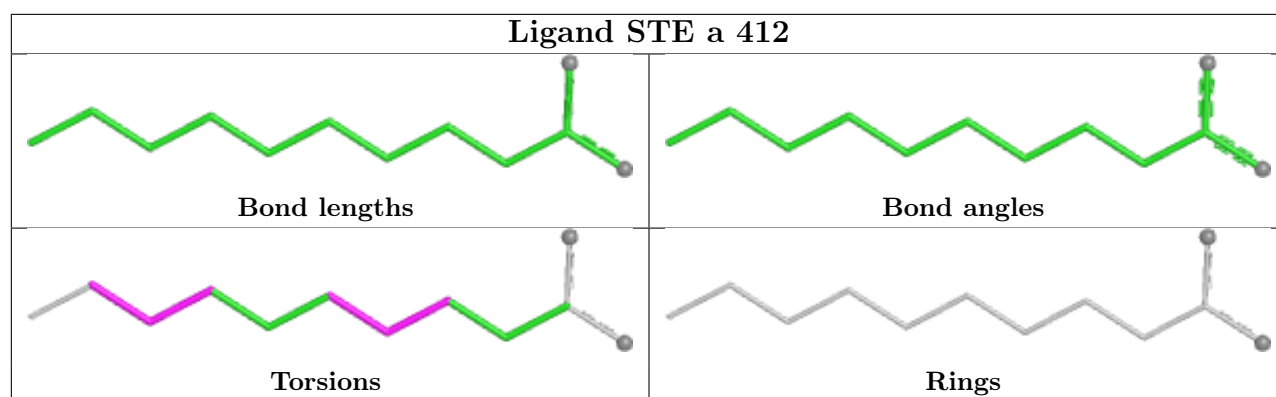
Ligand DGD c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

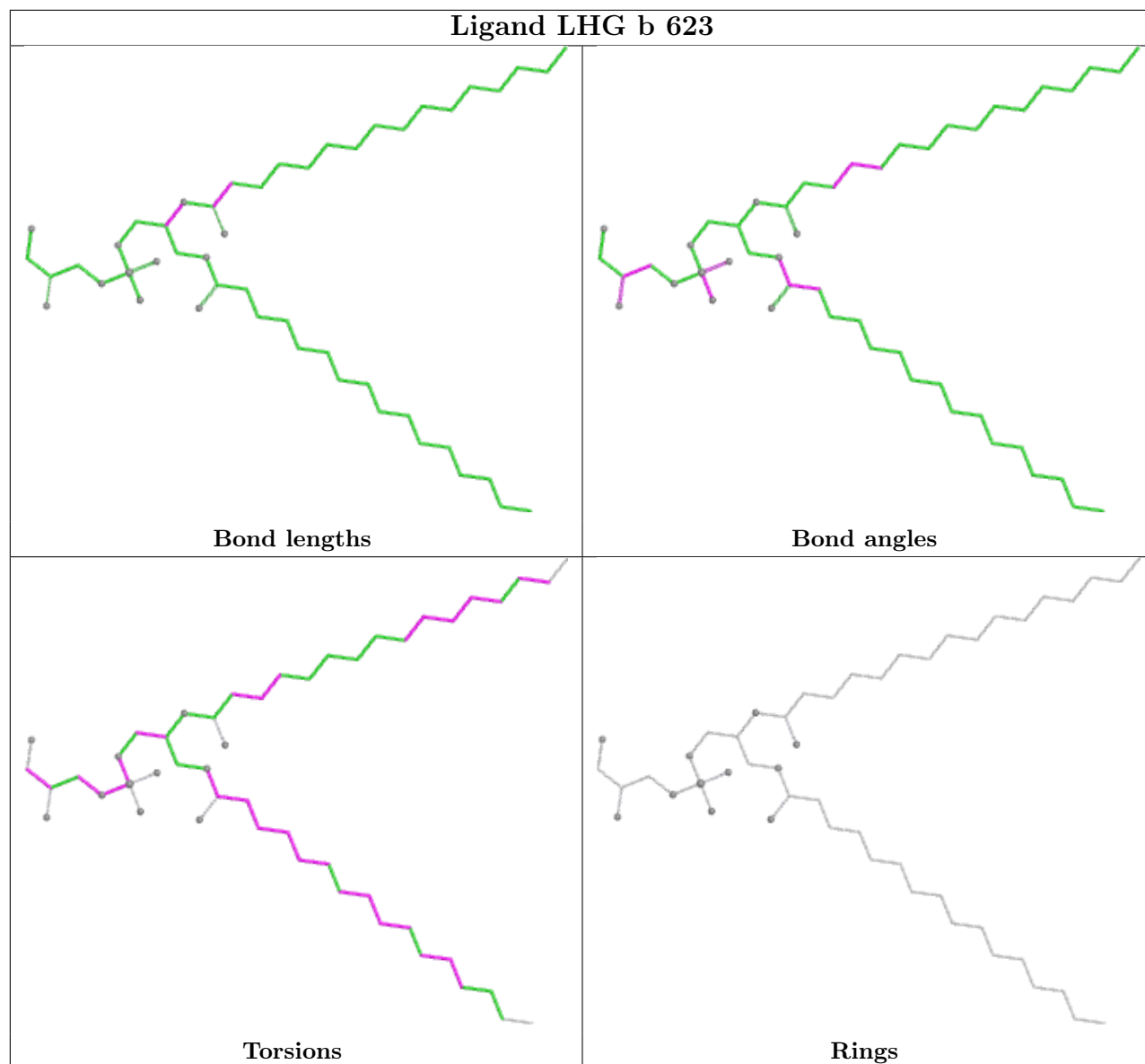
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



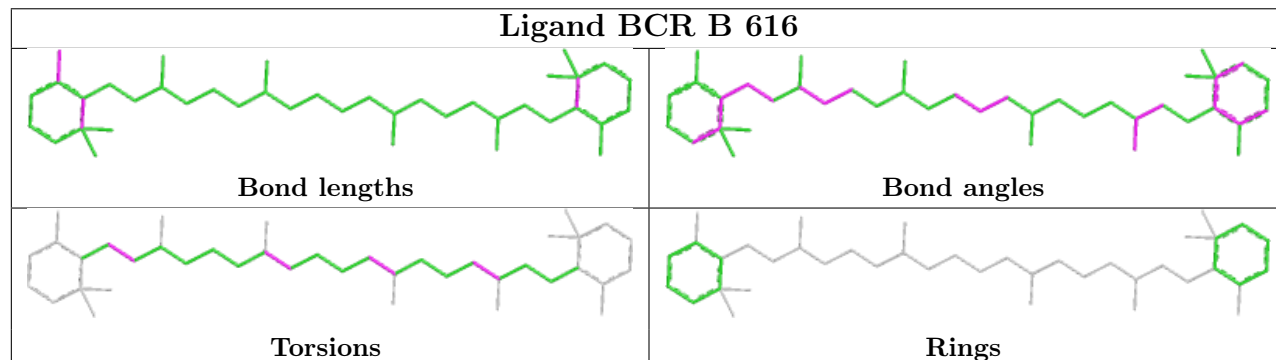




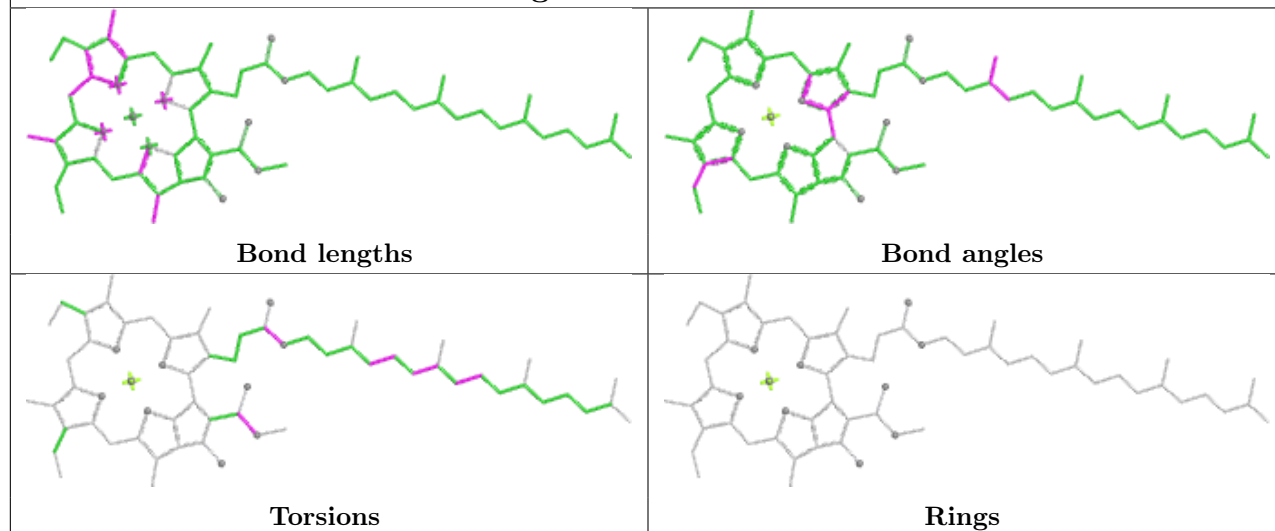
Ligand LHG b 623



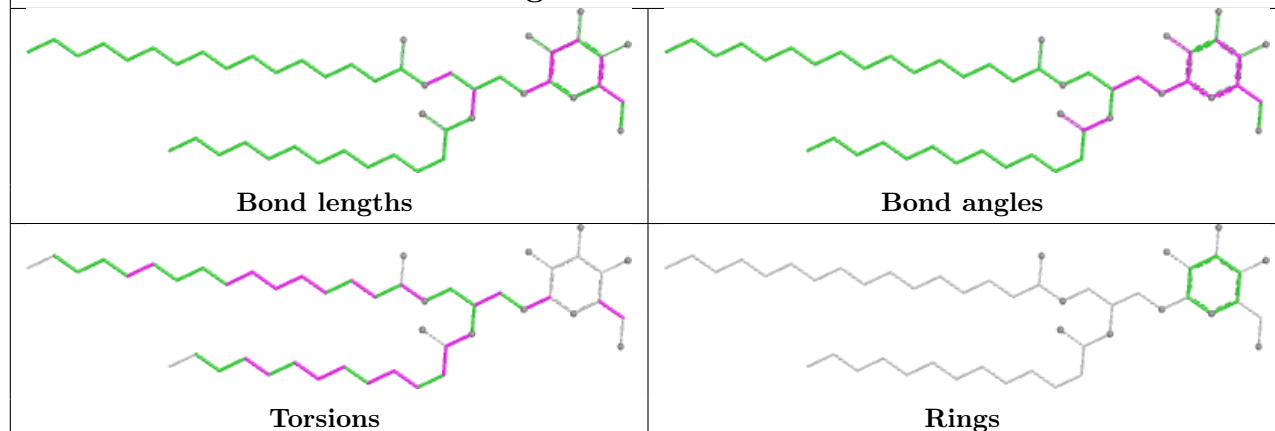
Ligand BCR B 616



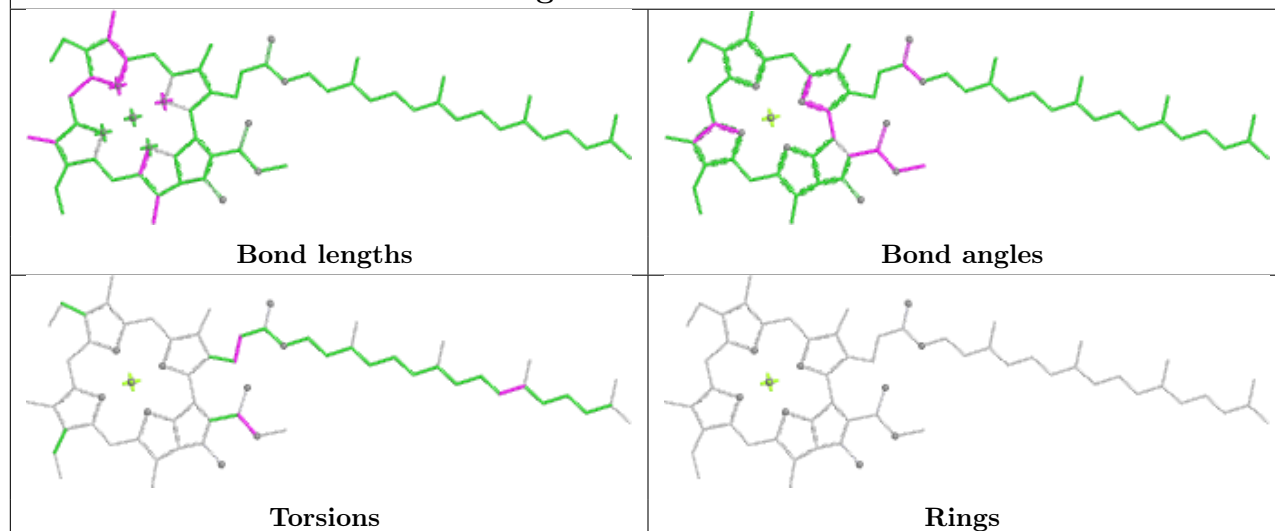
Ligand CLA C 511

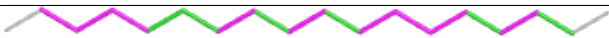
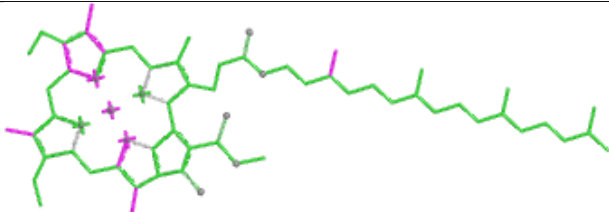
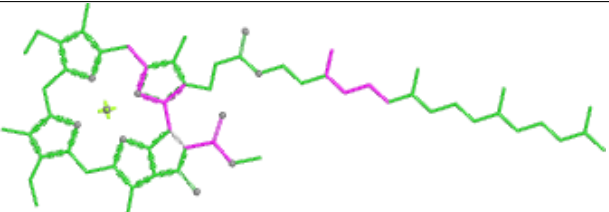
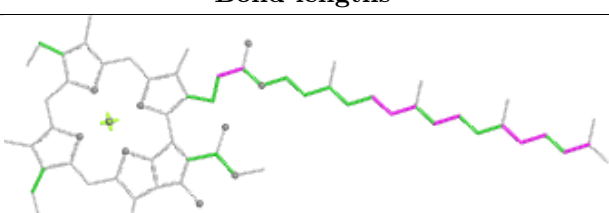
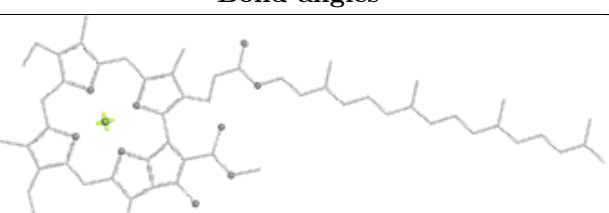
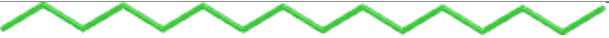
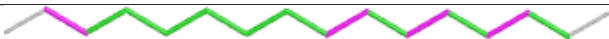
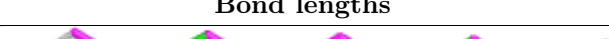
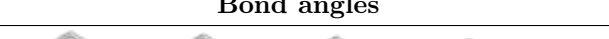


Ligand LMG Y 101

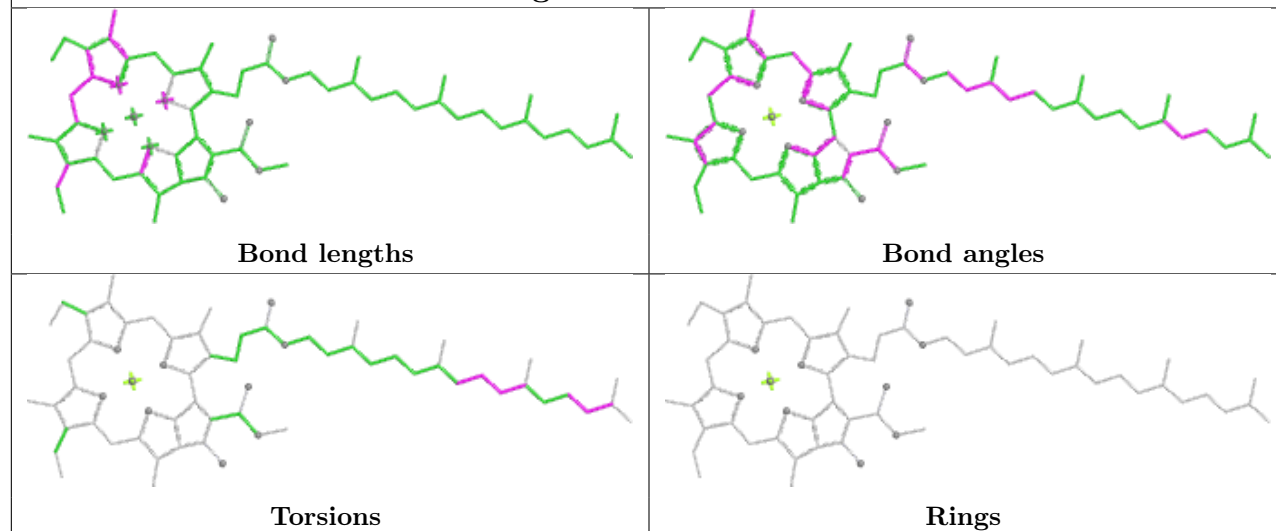


Ligand CLA c 501

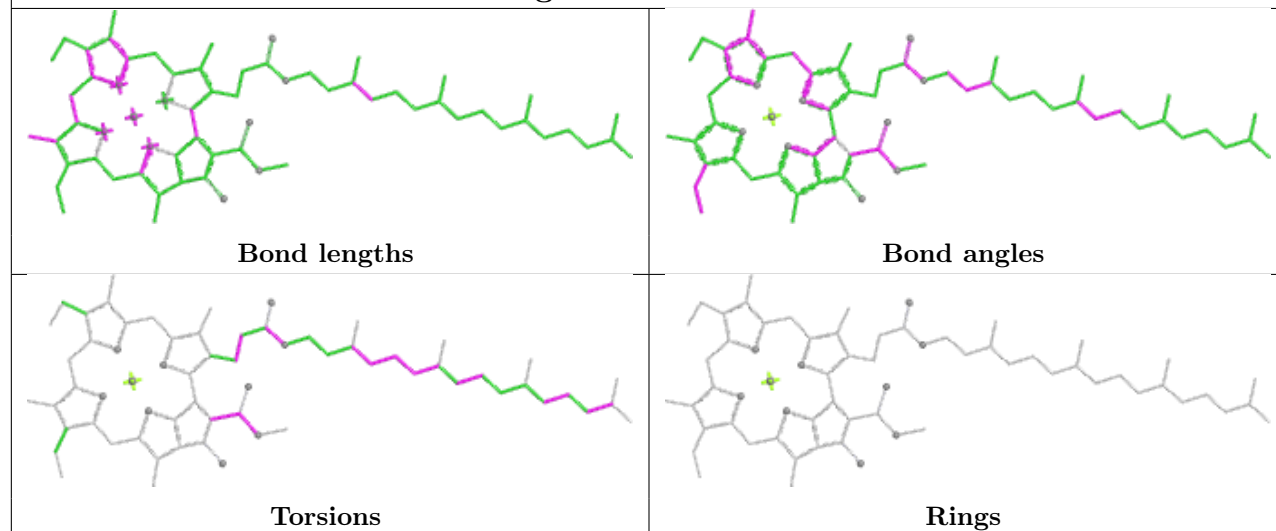


Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE b 627	
 Bond lengths	 Bond angles
 Torsions	 Rings

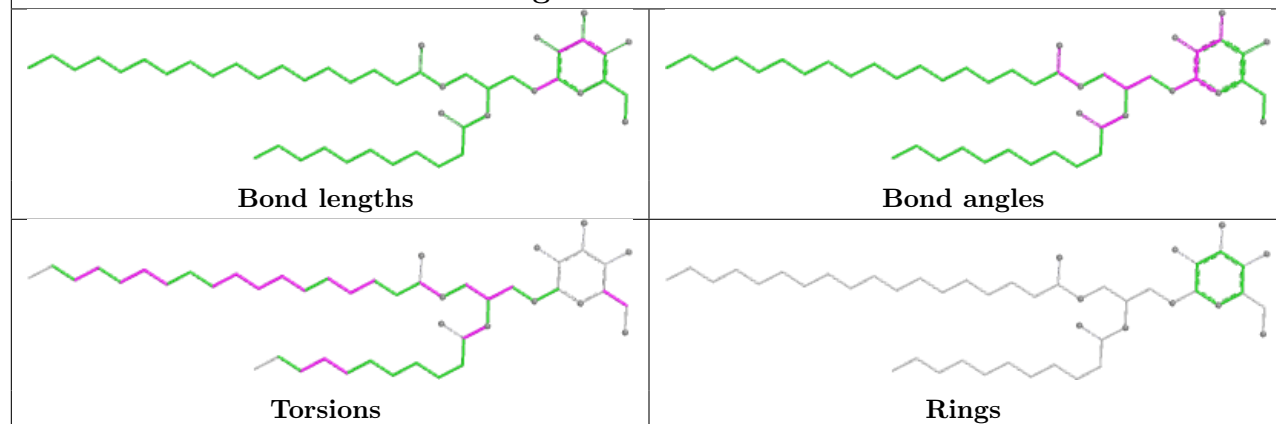
Ligand CLA B 601

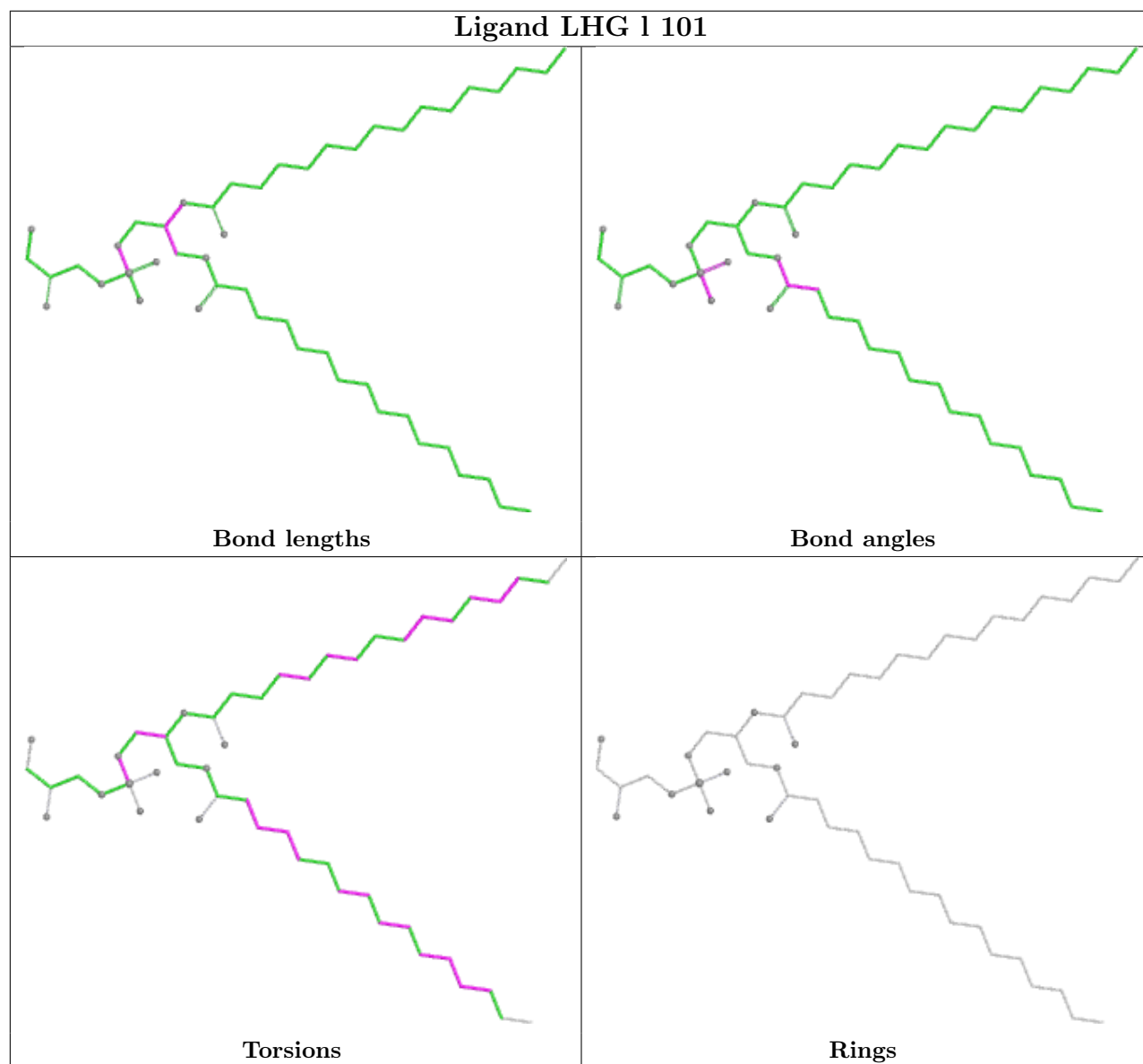
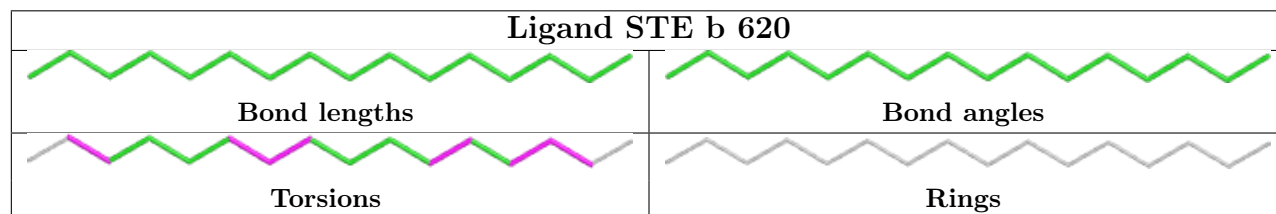
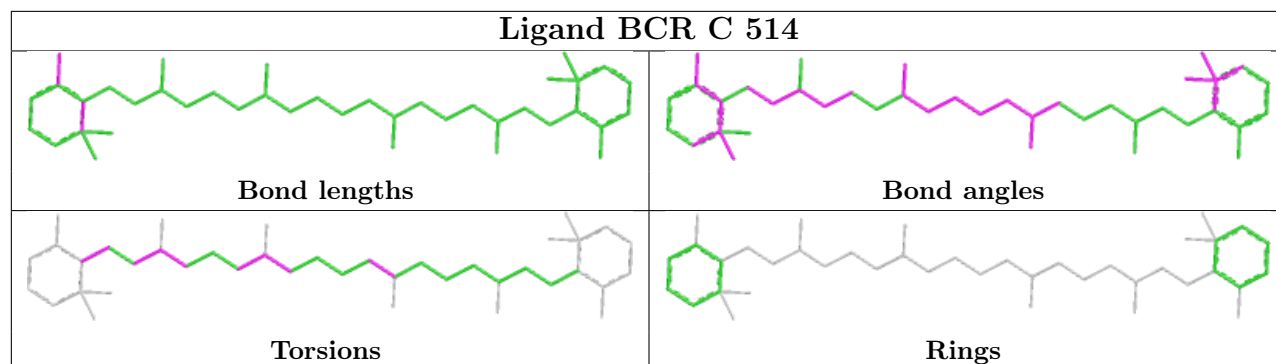


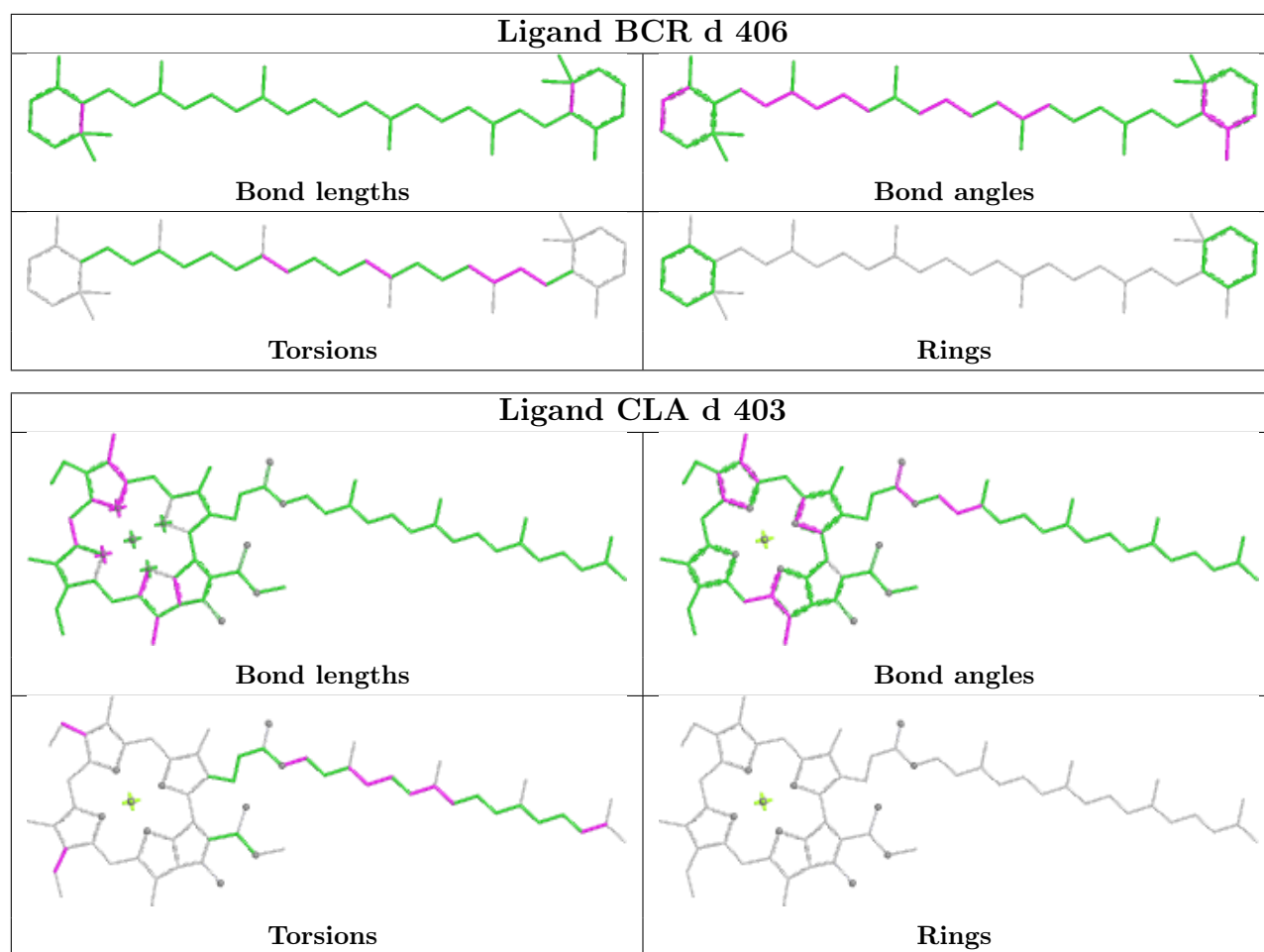
Ligand CLA b 614



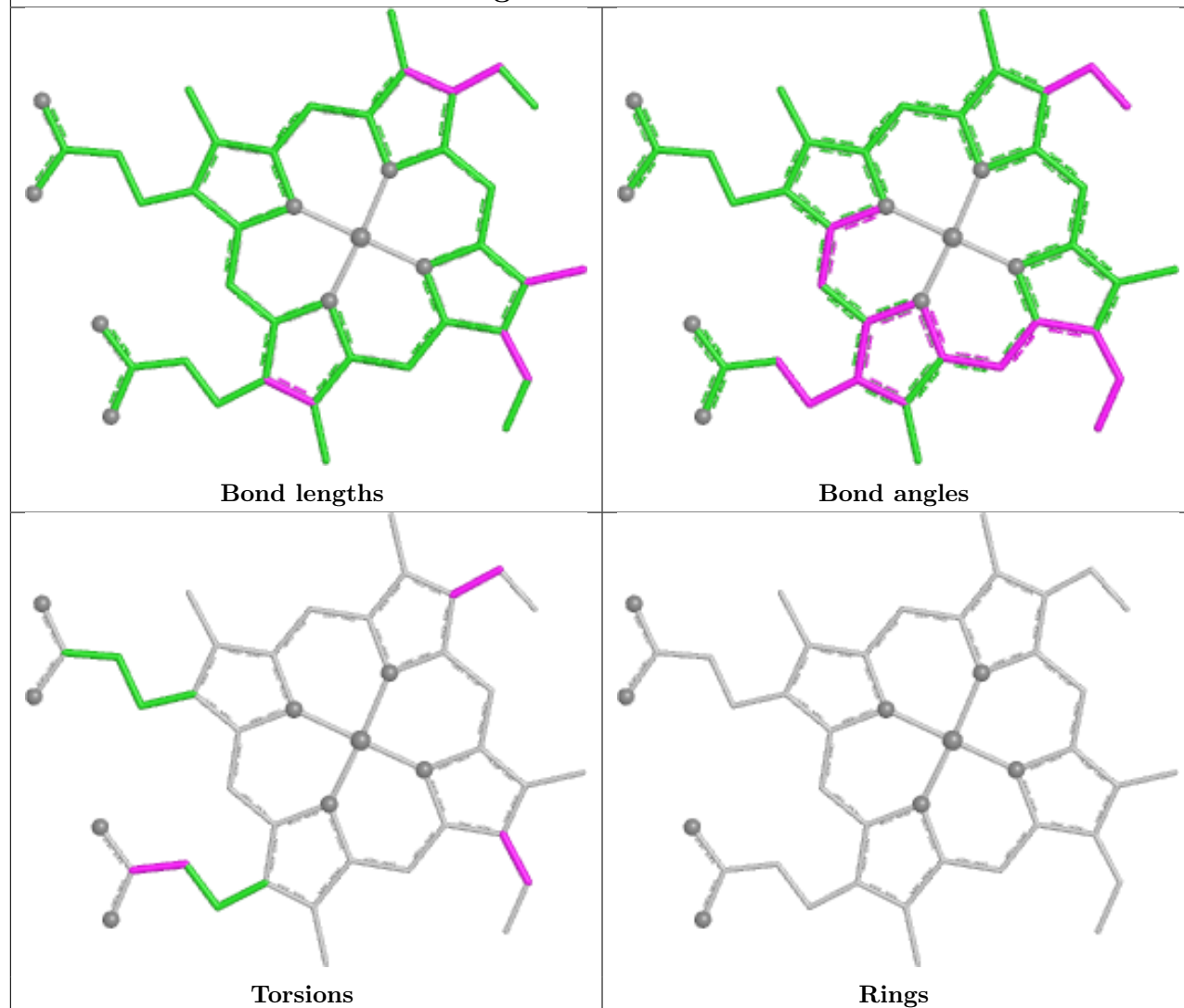
Ligand LMG c 520



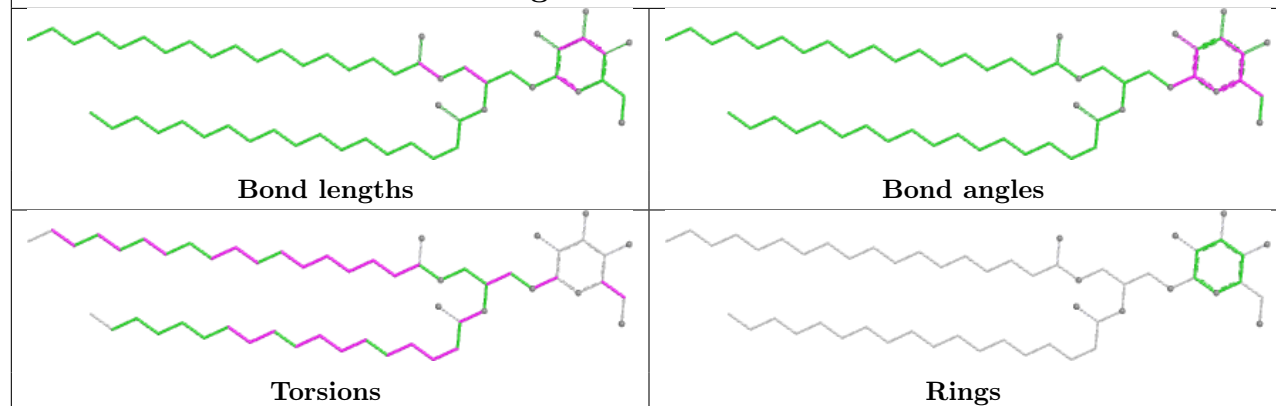


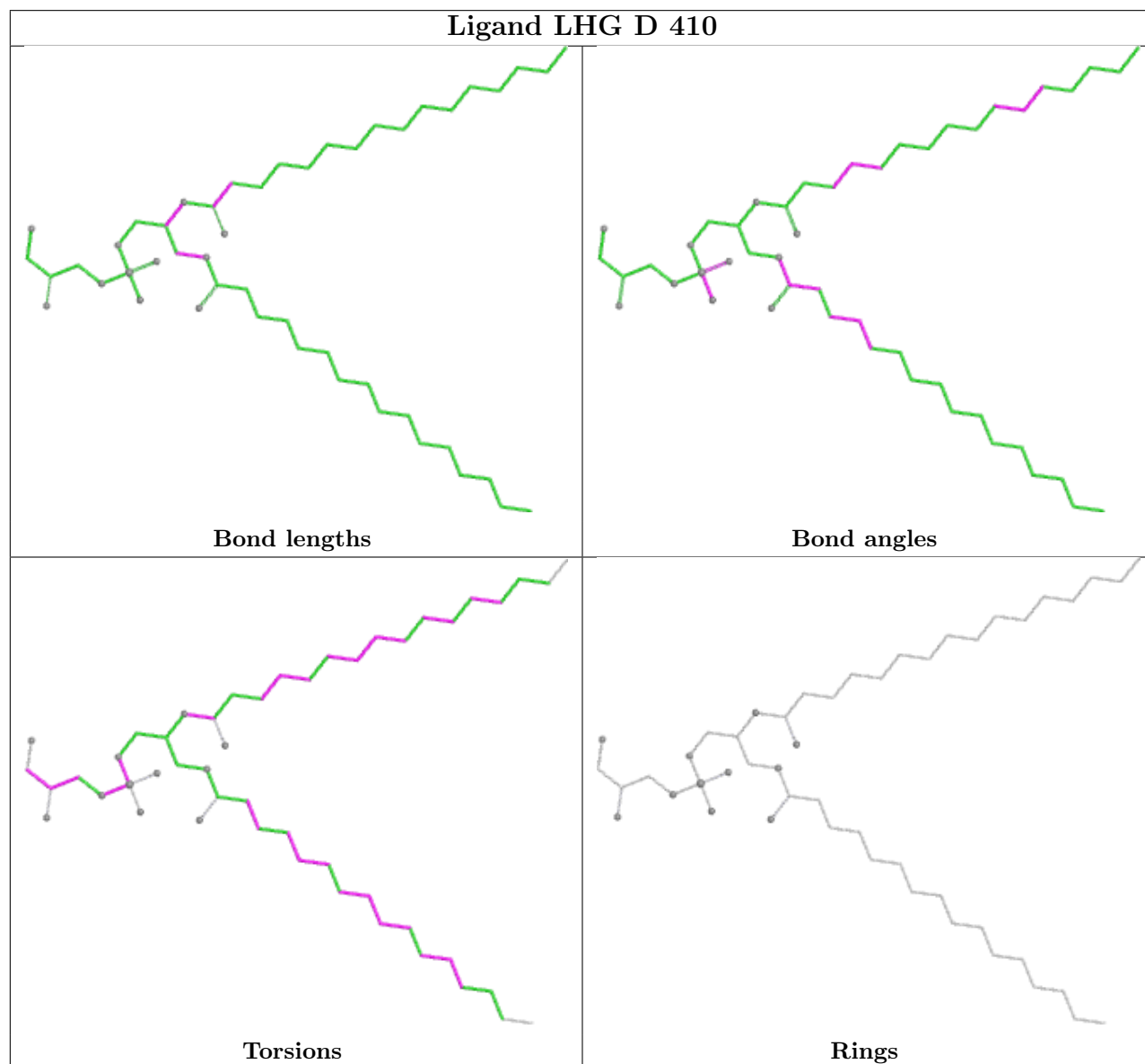
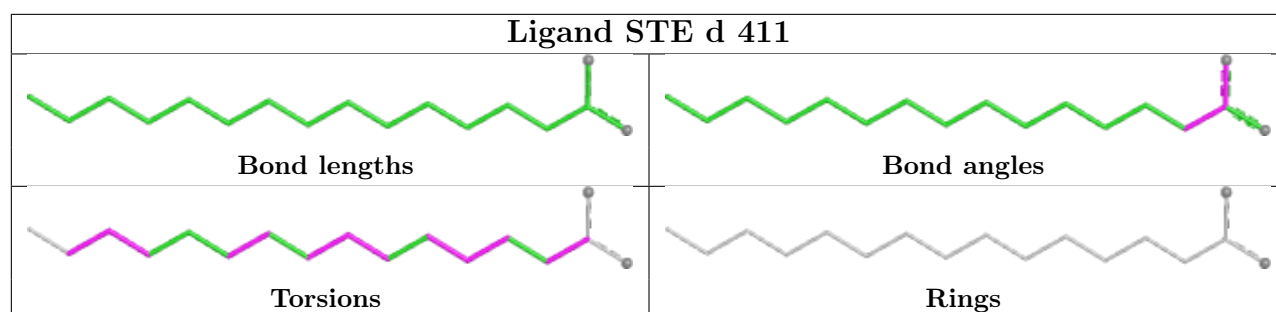


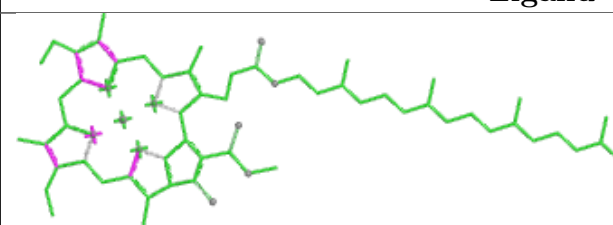
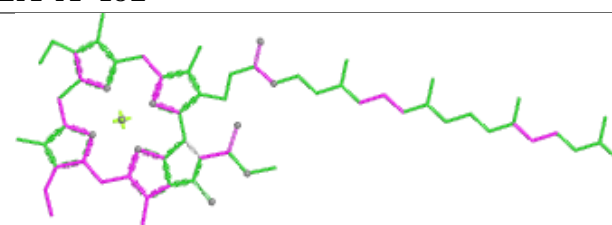
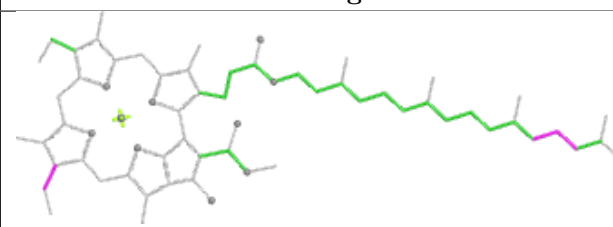
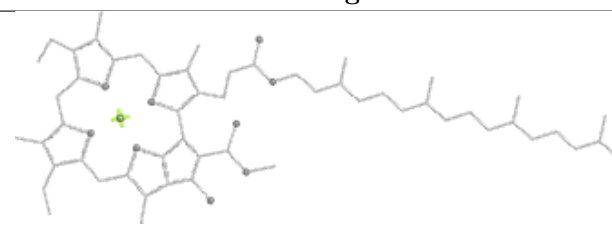
Ligand HEC F 101

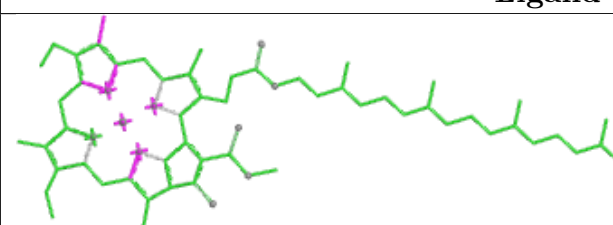
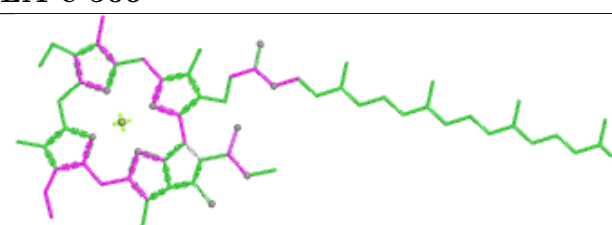
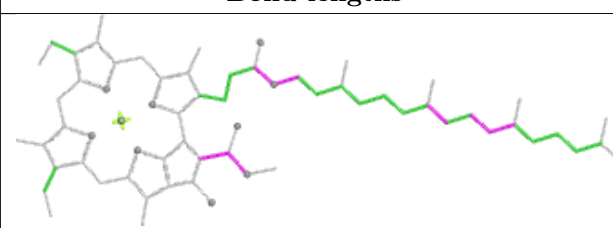
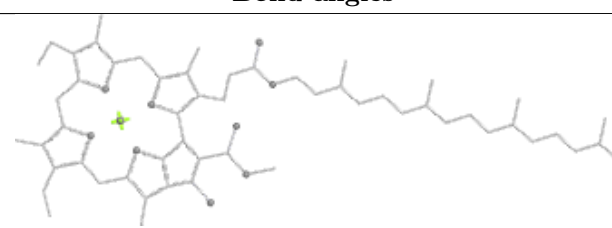


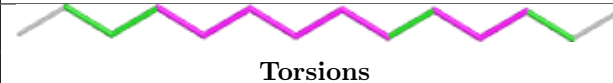
Ligand LMG b 622

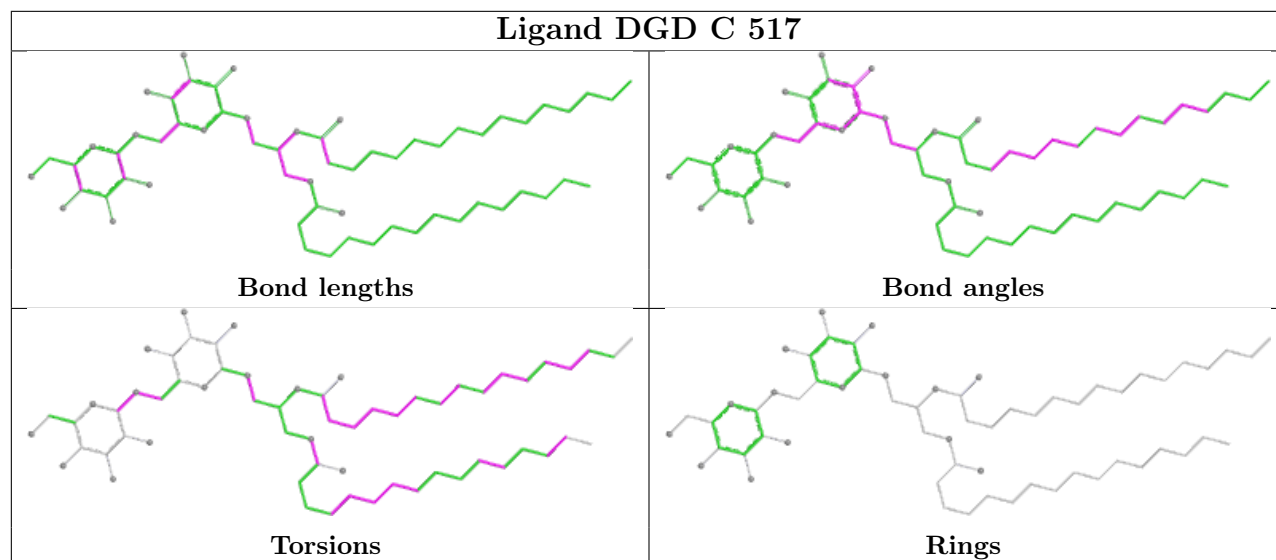
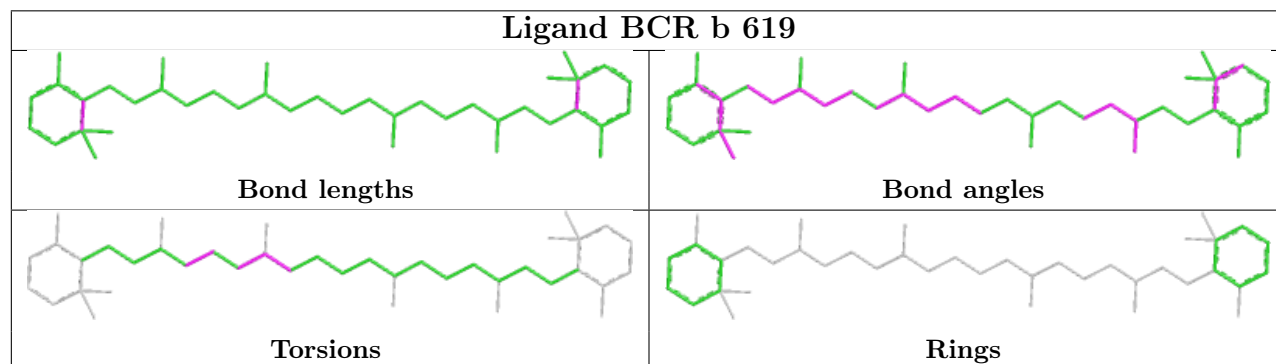
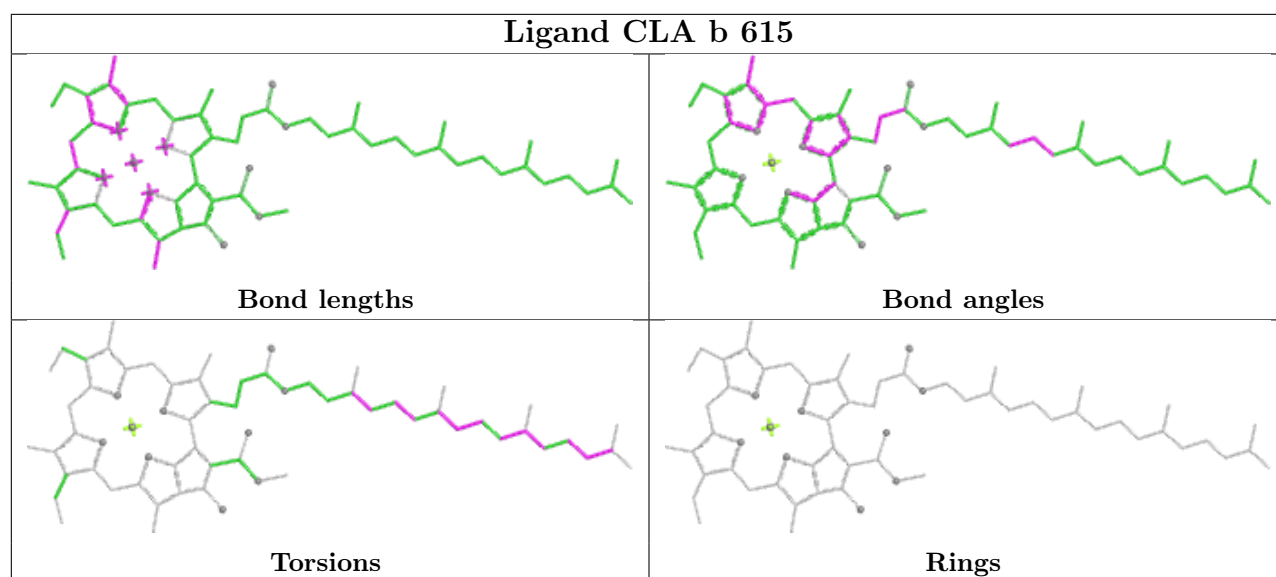




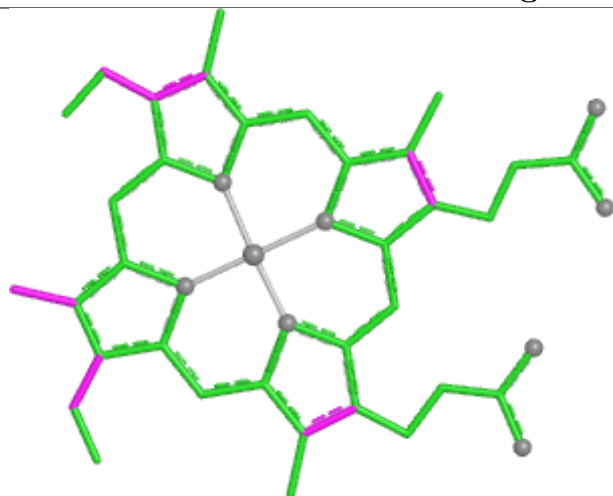
Ligand CLA A 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

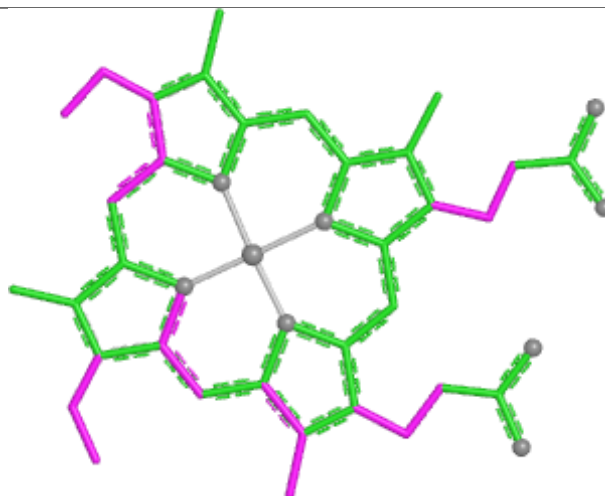
Ligand STE b 628	
	
Bond lengths	Bond angles
	
Torsions	Rings



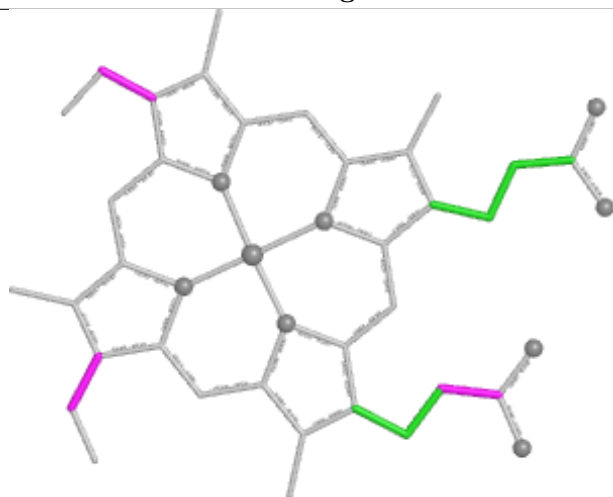
Ligand HEC f 101



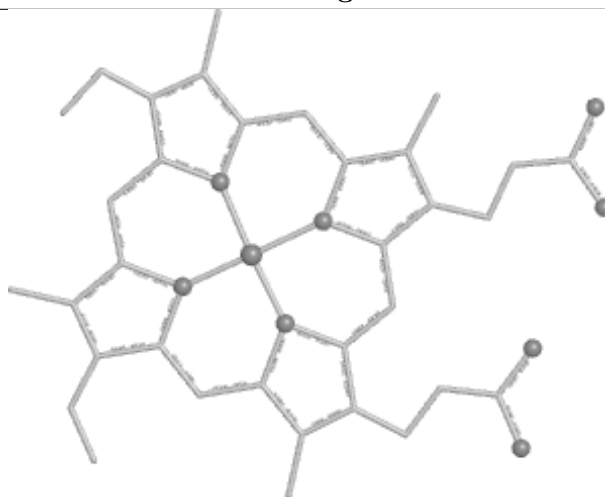
Bond lengths



Bond angles

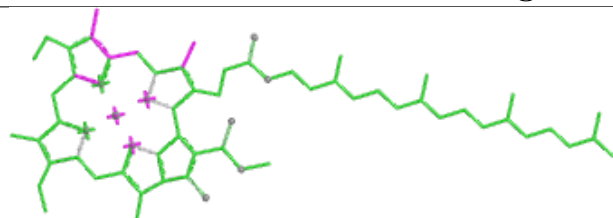


Torsions

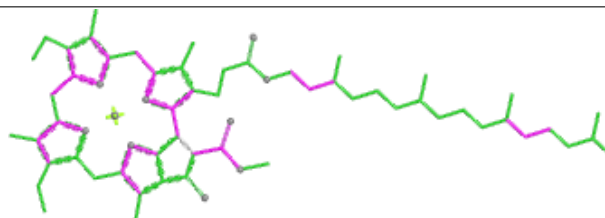


Rings

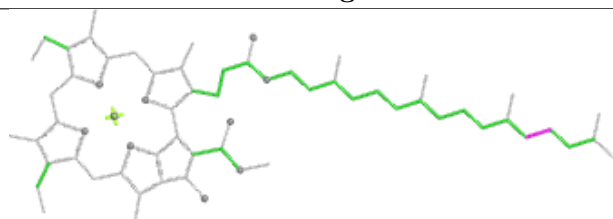
Ligand CLA d 404



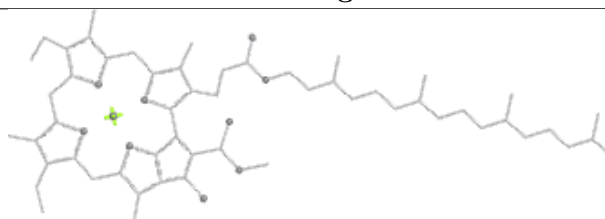
Bond lengths



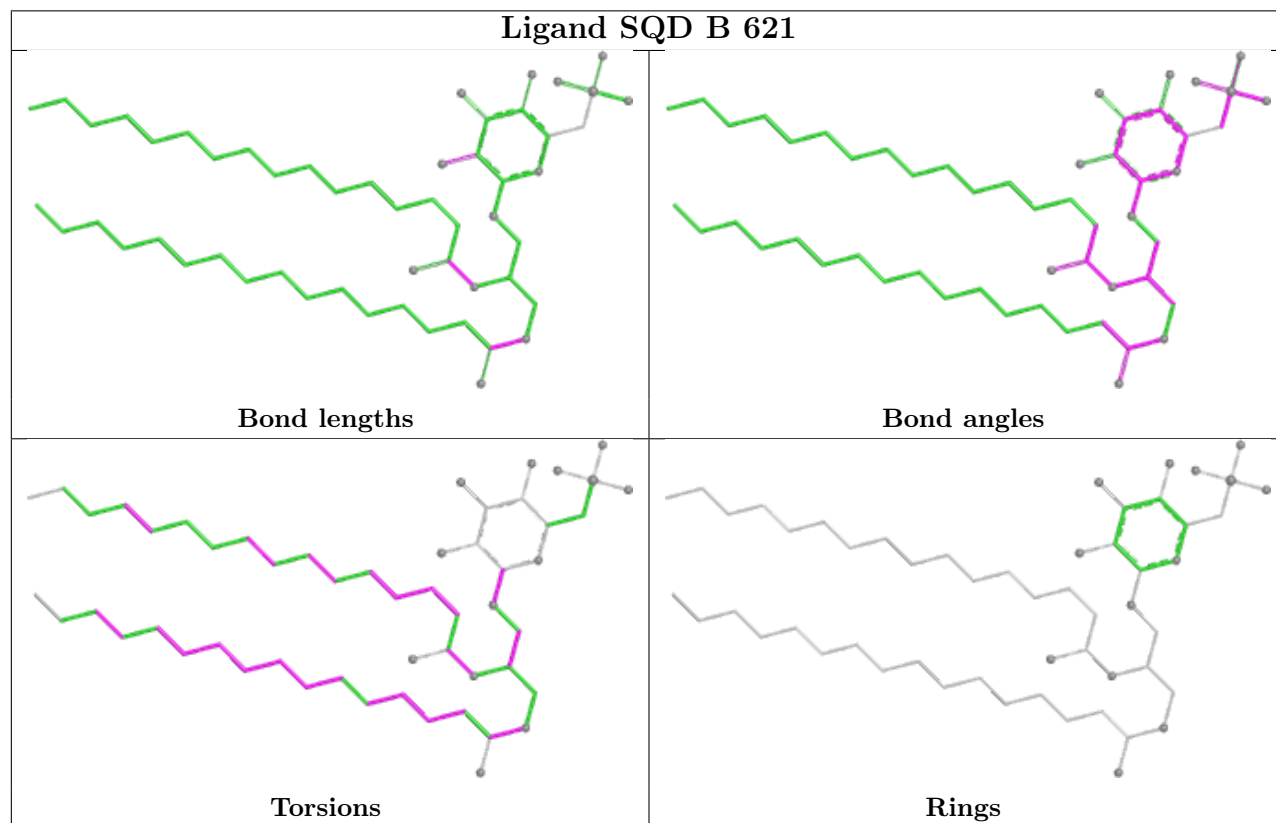
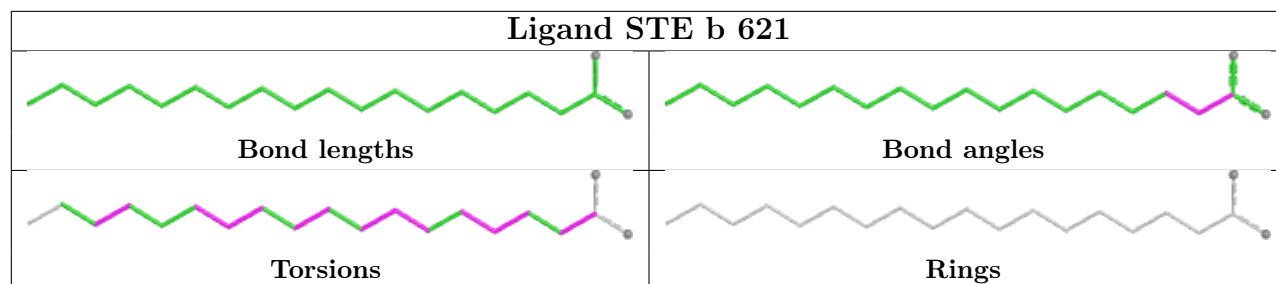
Bond angles

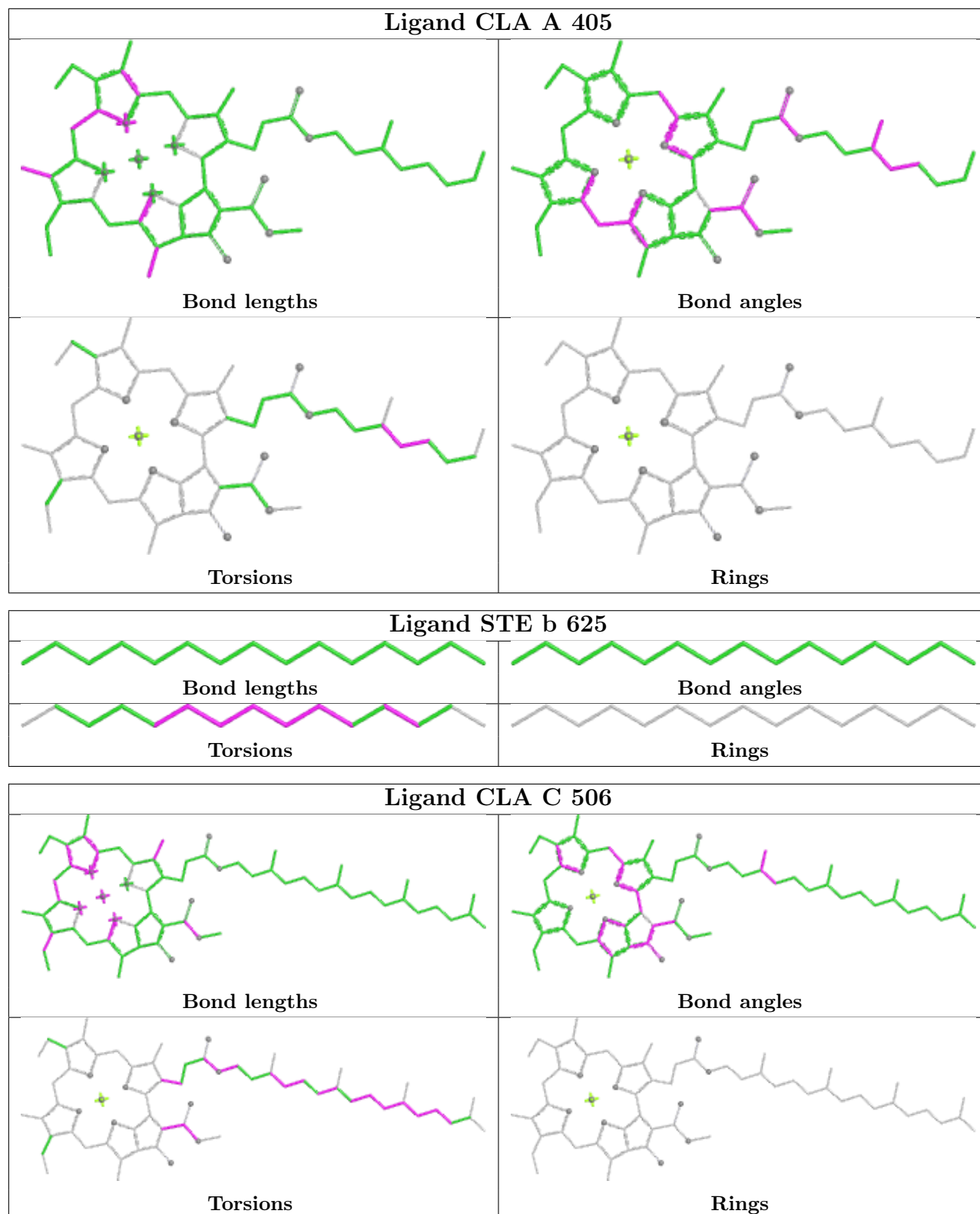


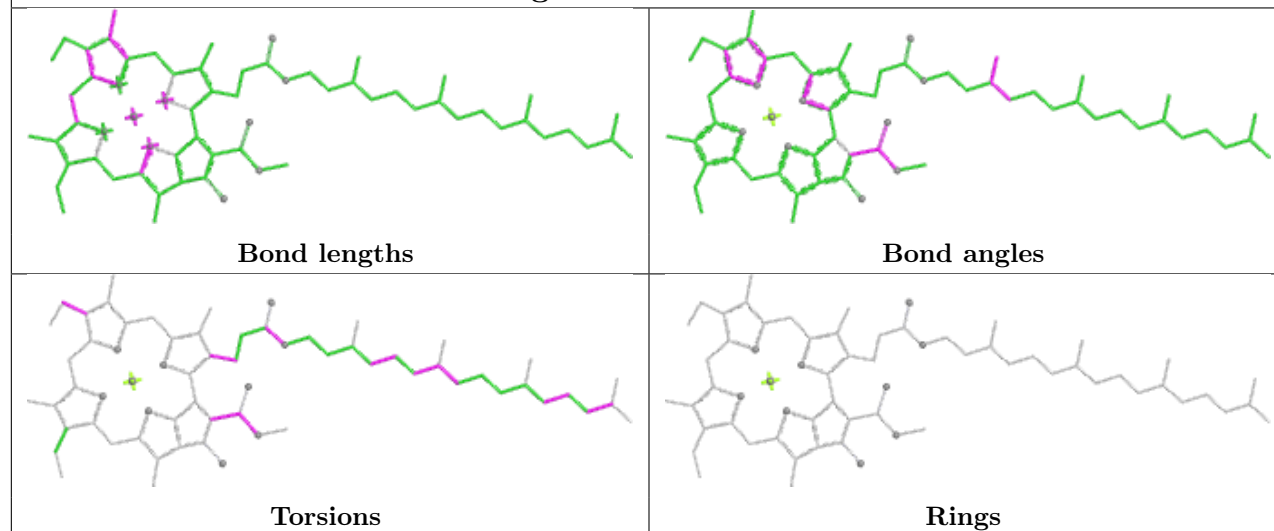
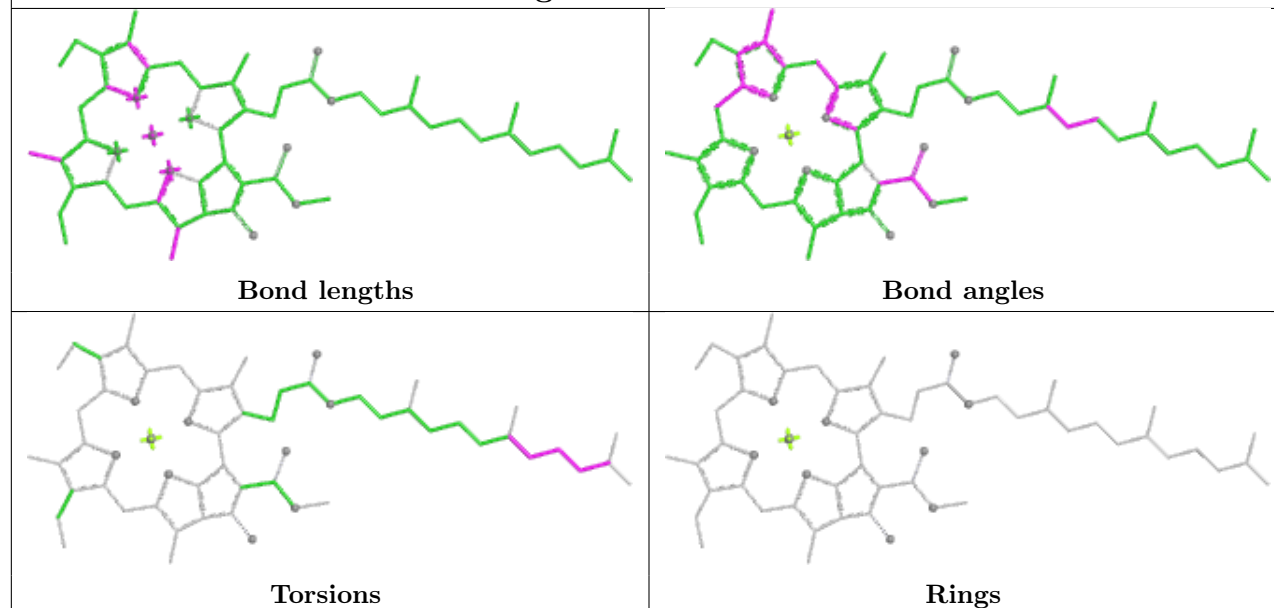
Torsions

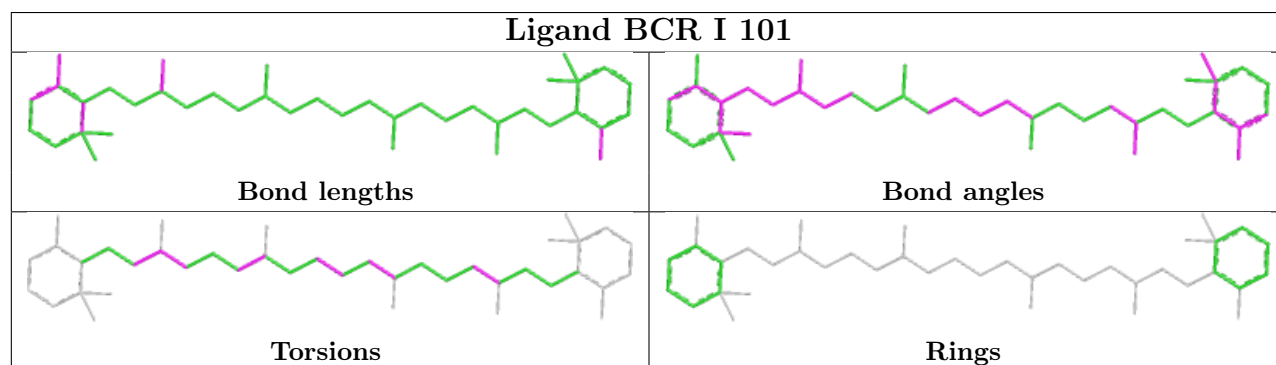
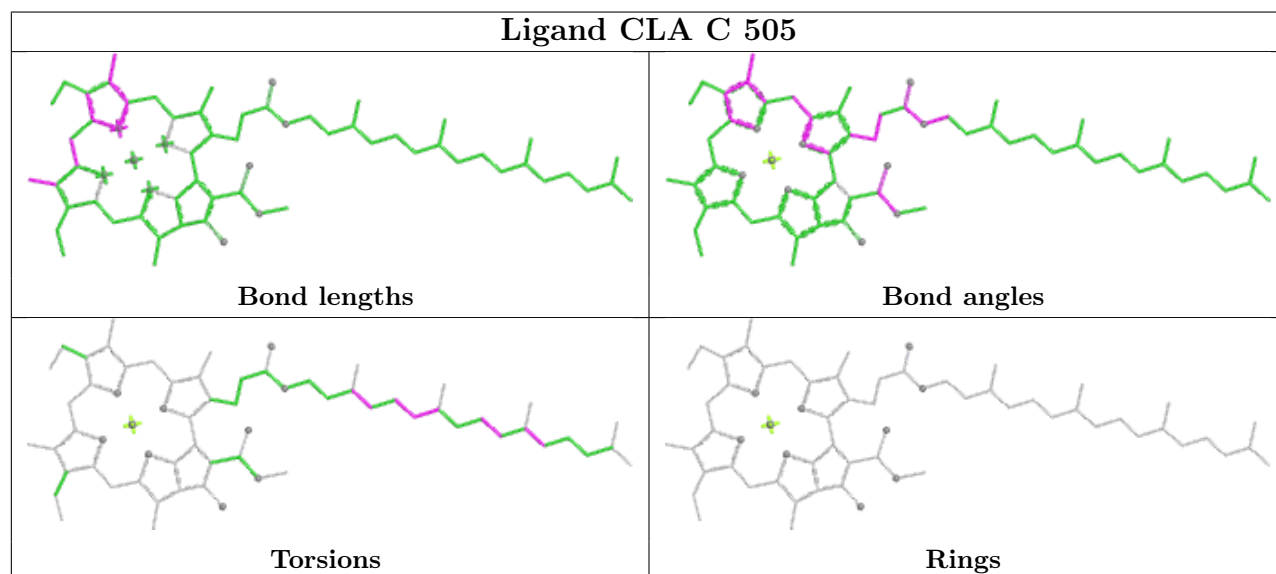
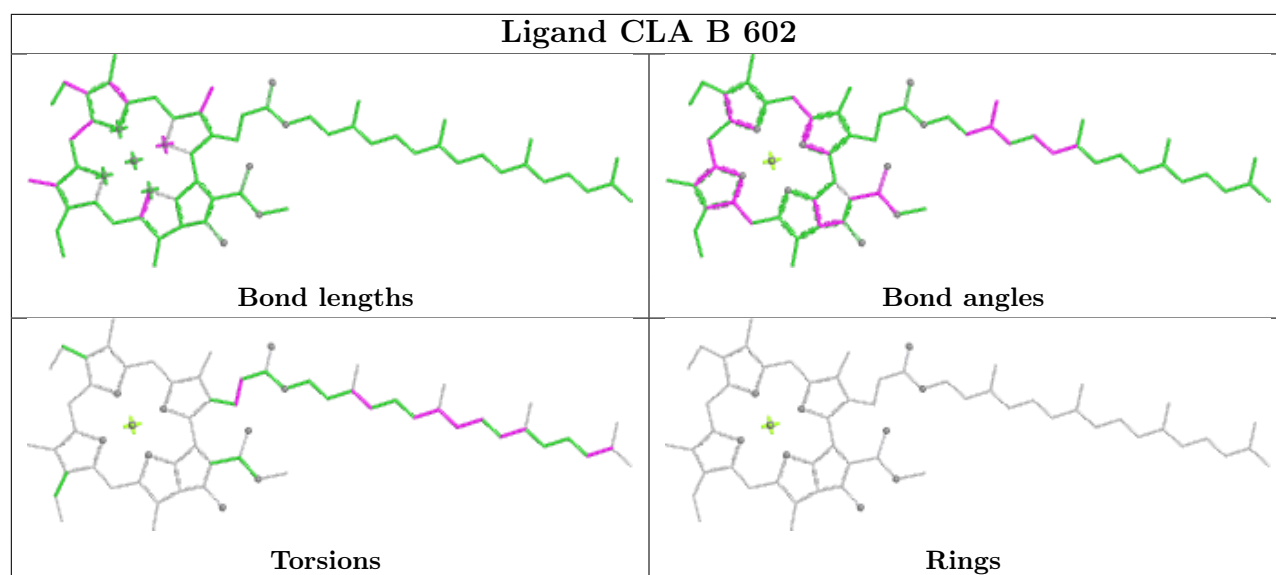


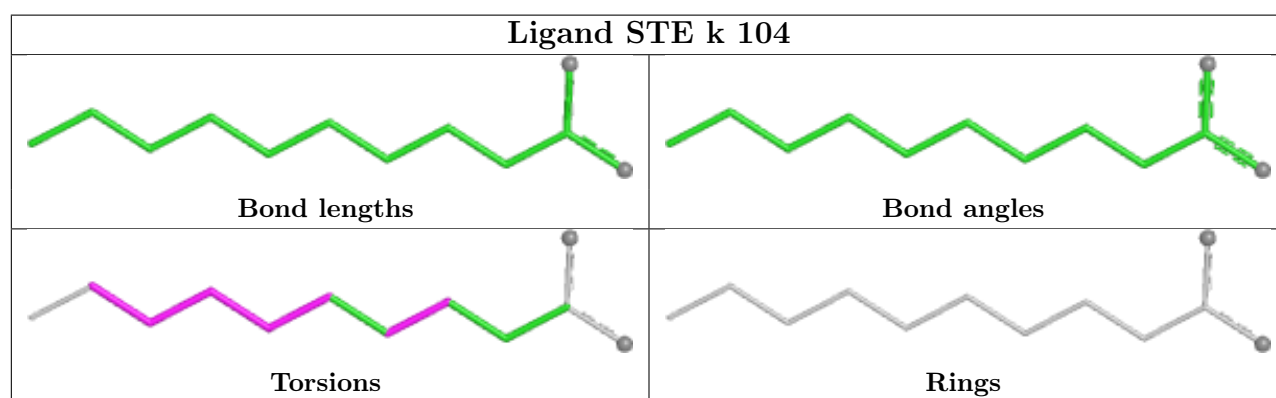
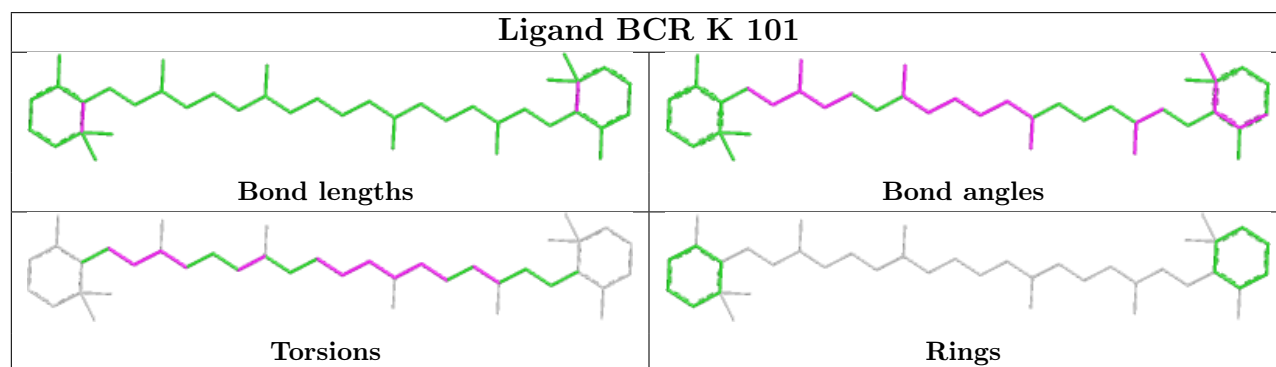
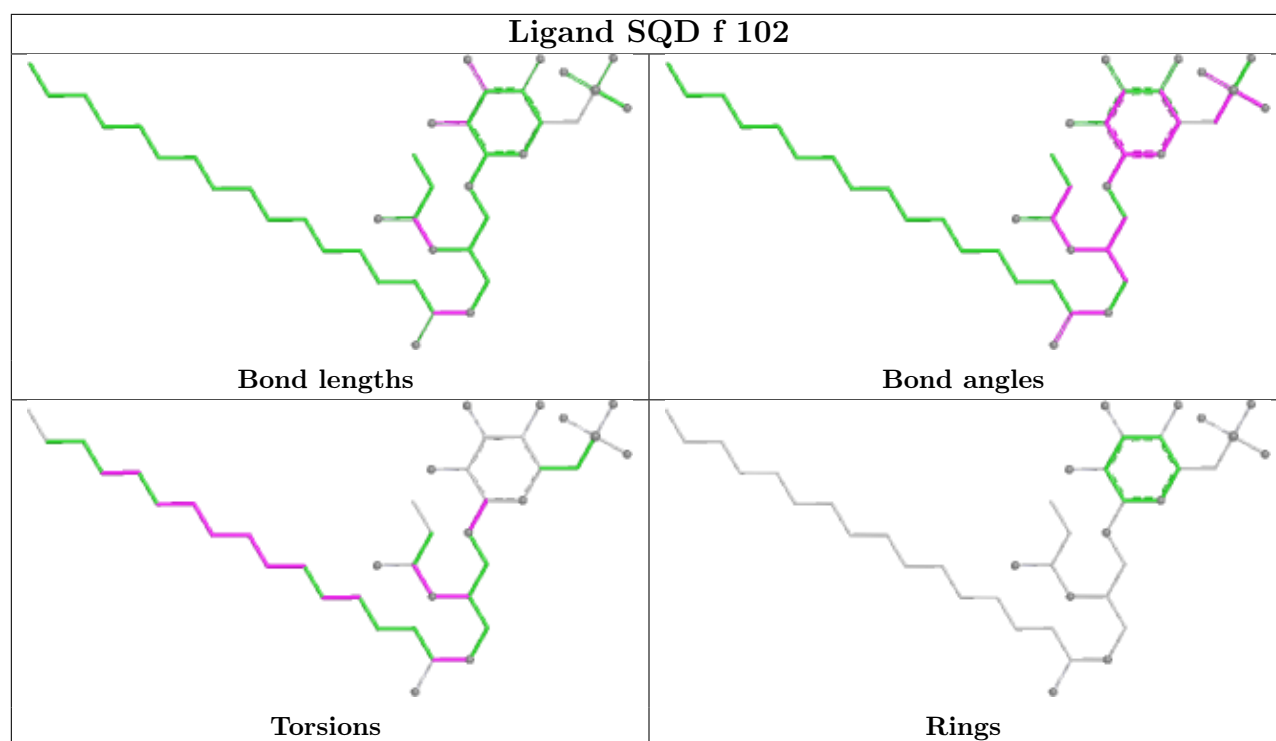
Rings



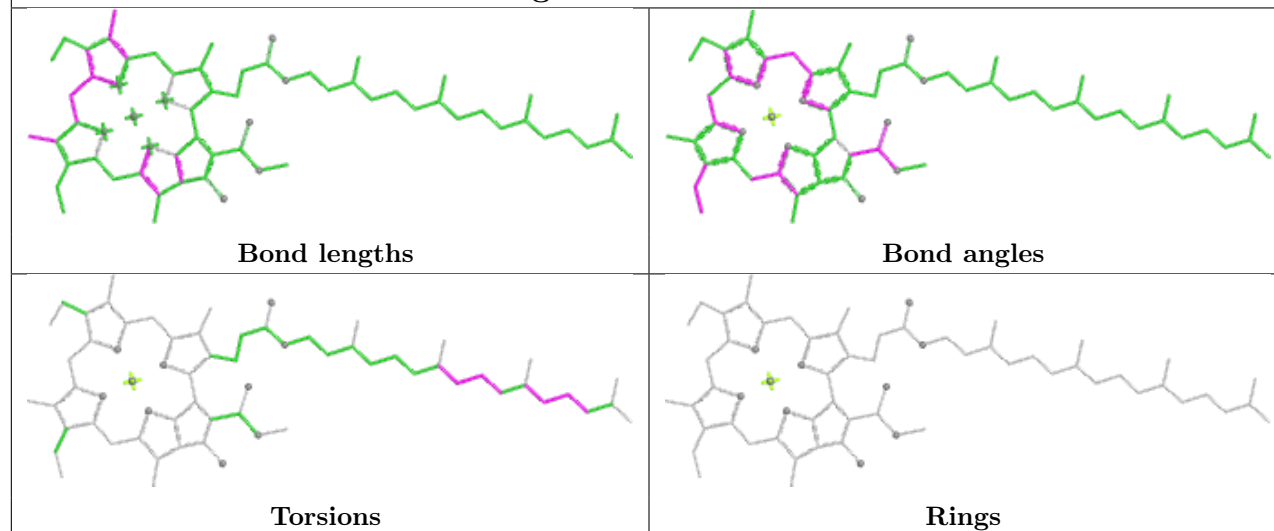


Ligand CLA H 101**Ligand CLA b 616**

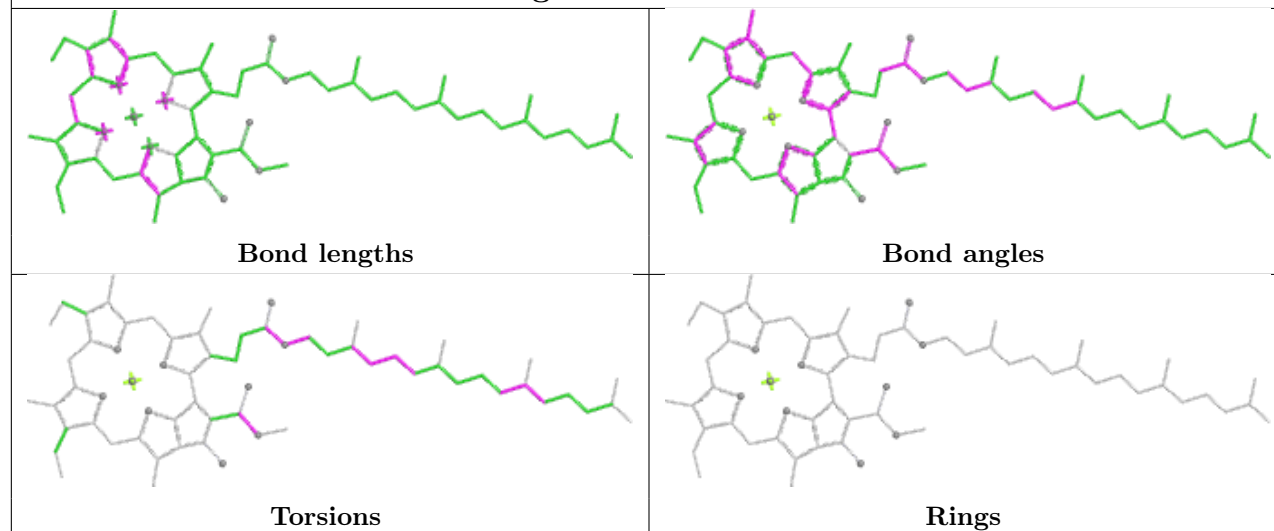




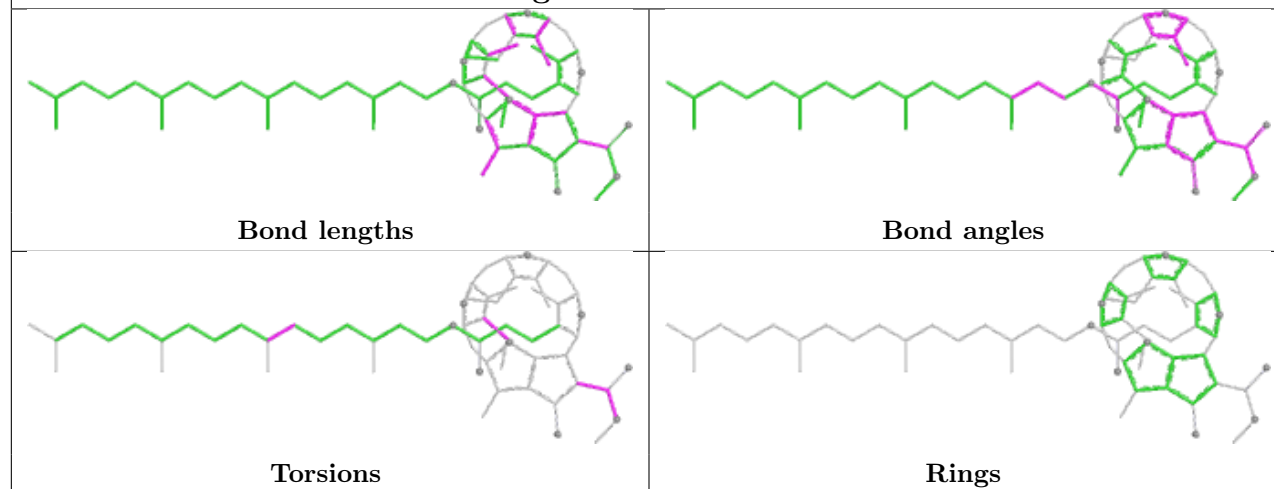
Ligand CLA C 513

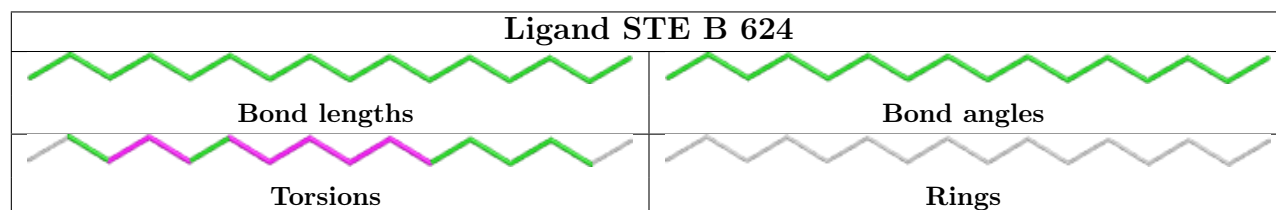
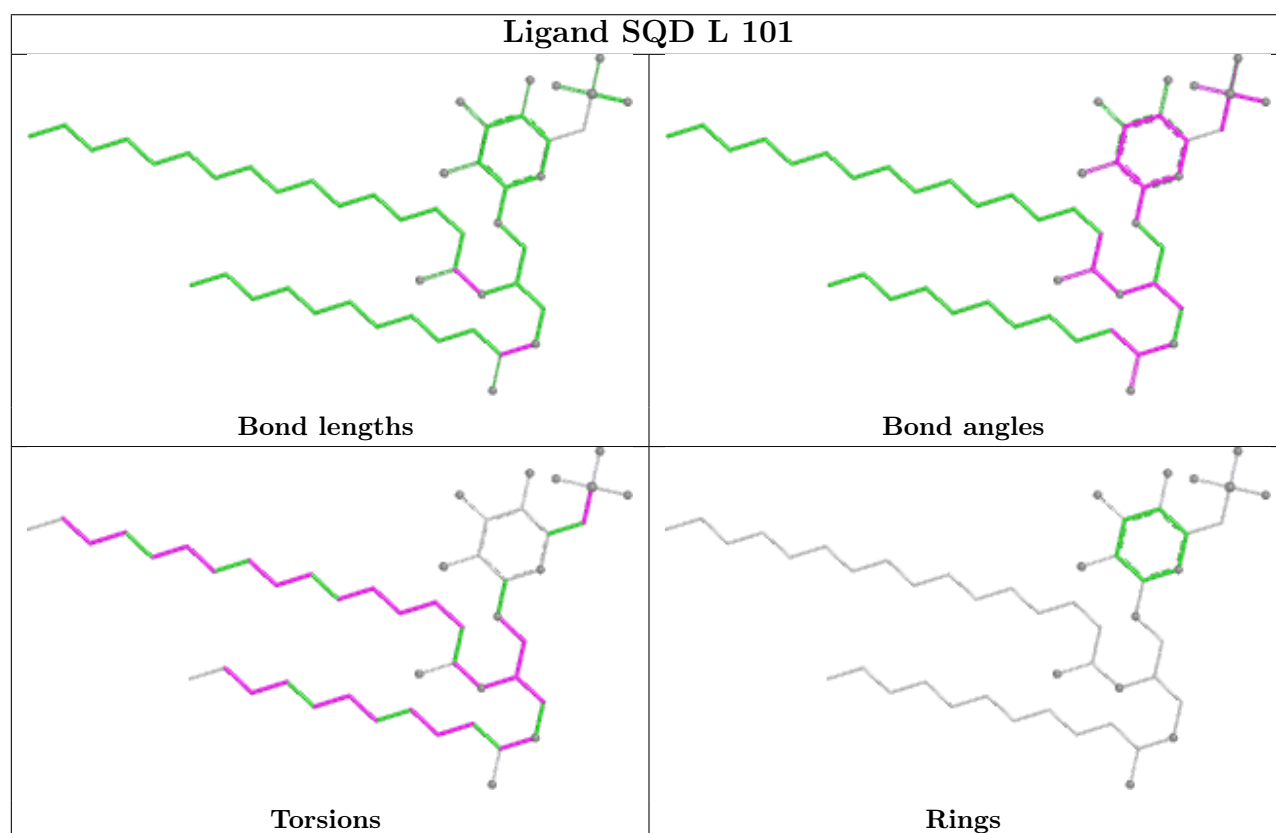
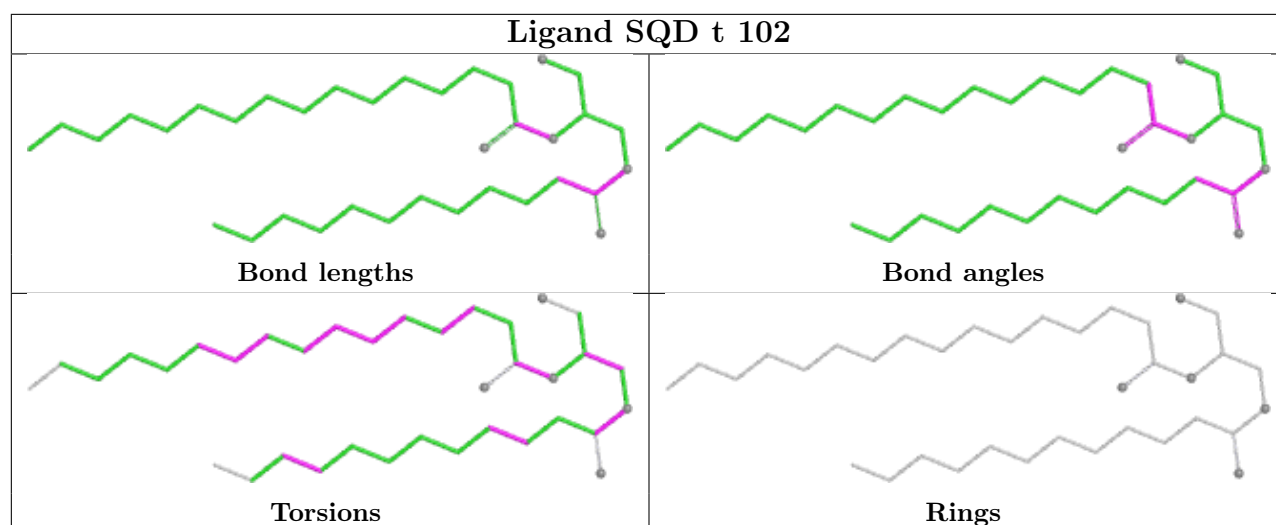


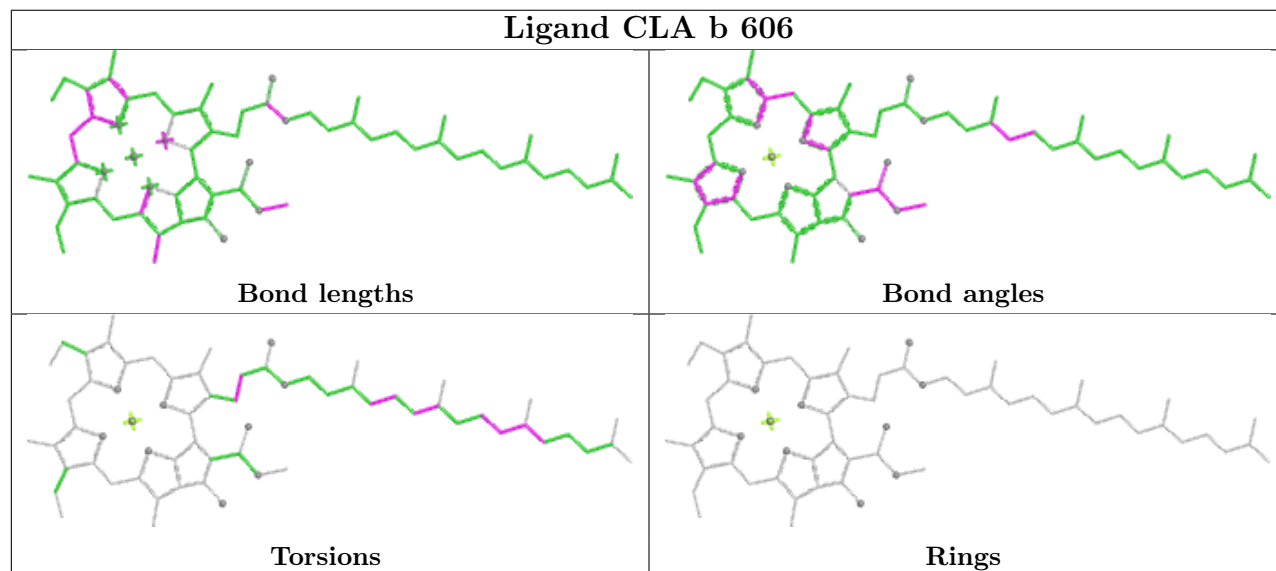
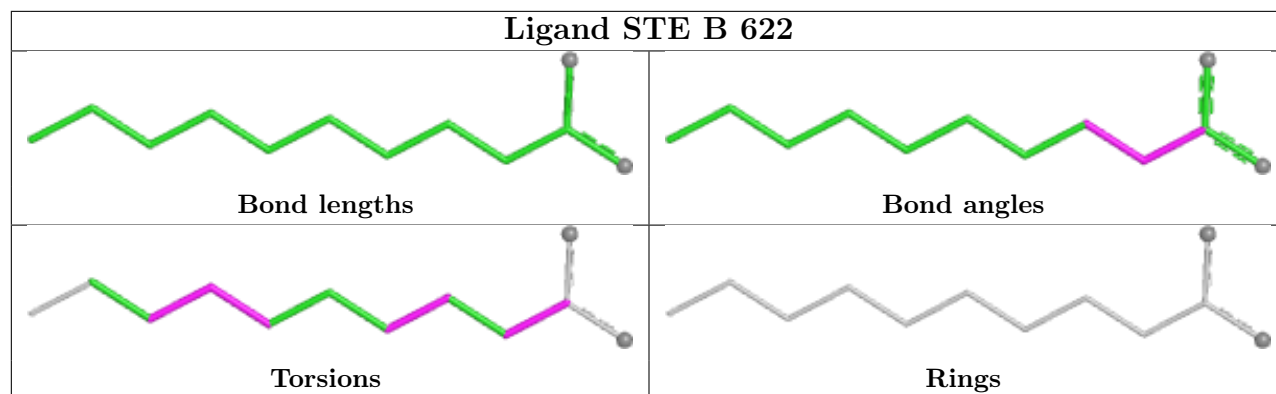
Ligand CLA B 603



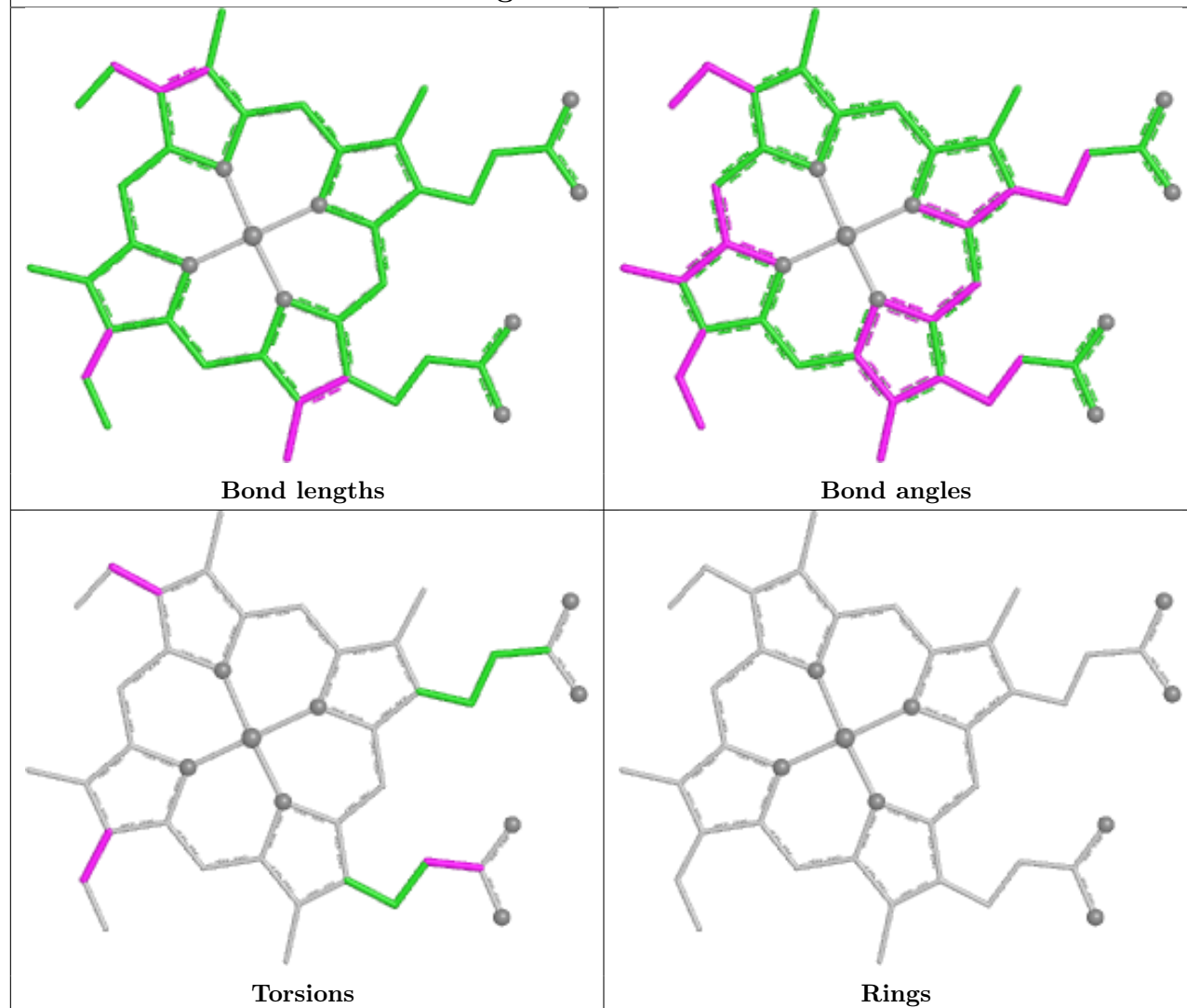
Ligand PHO d 401



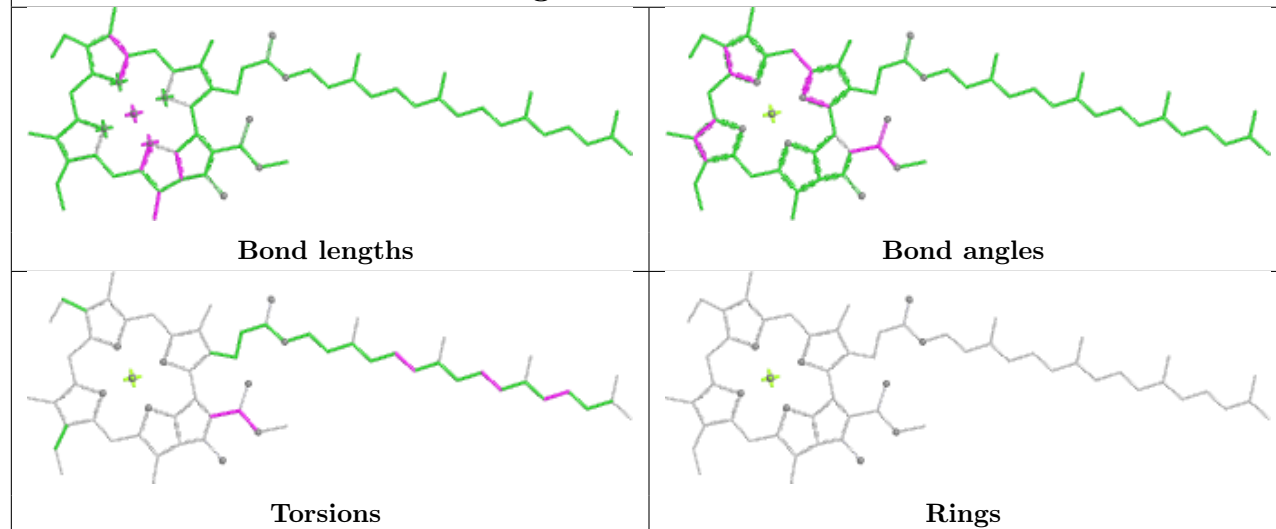


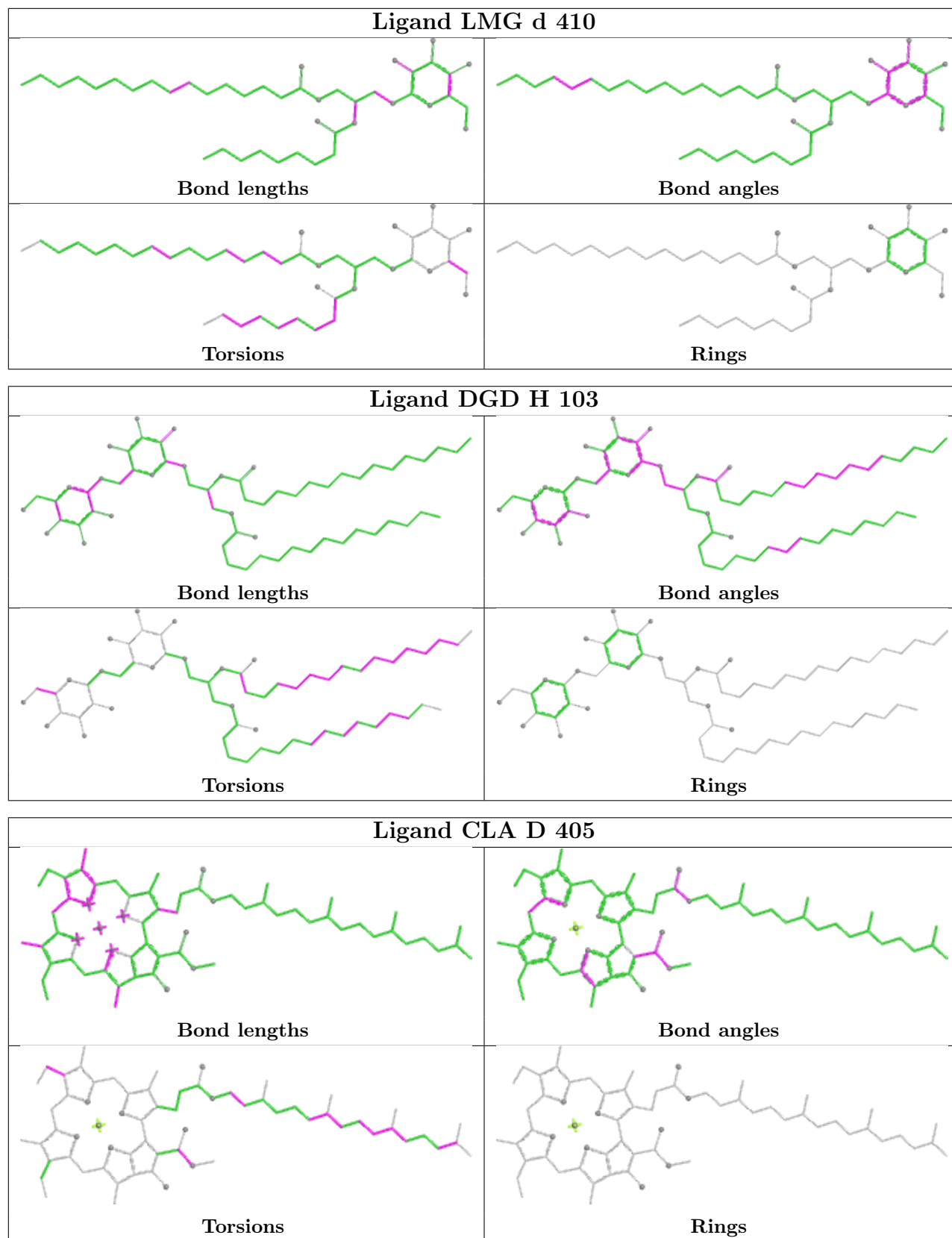


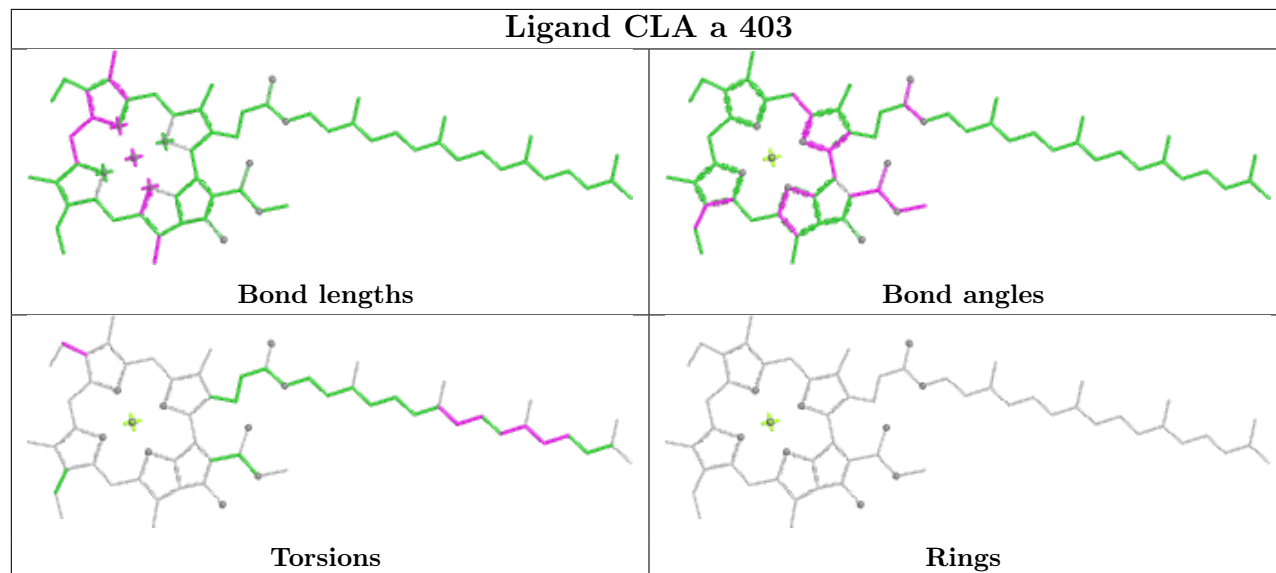
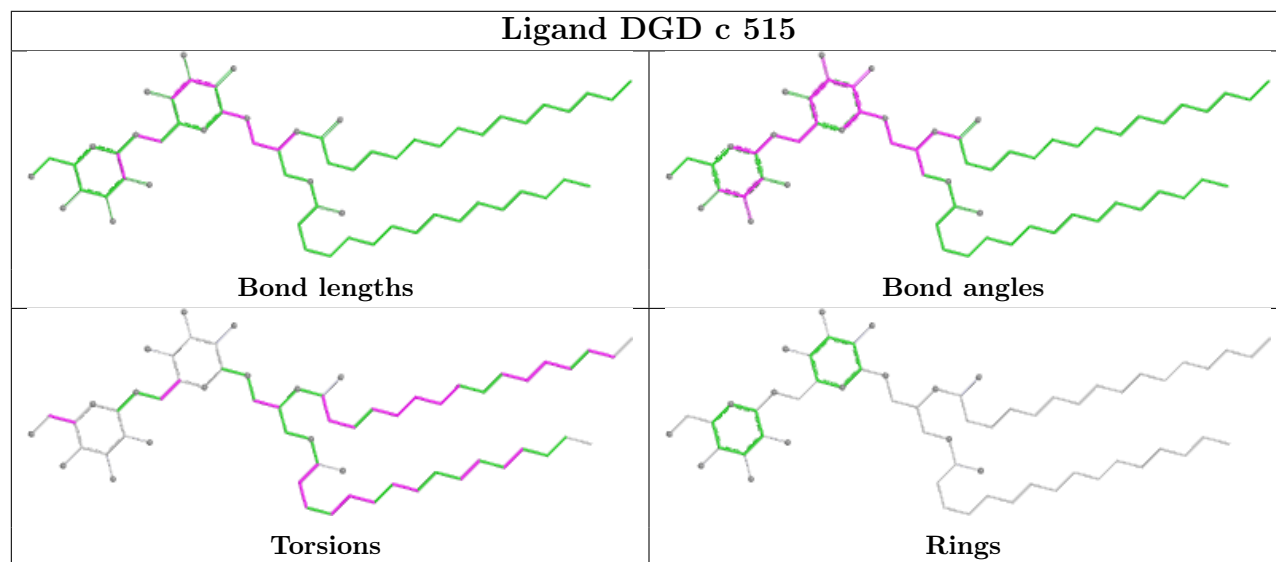
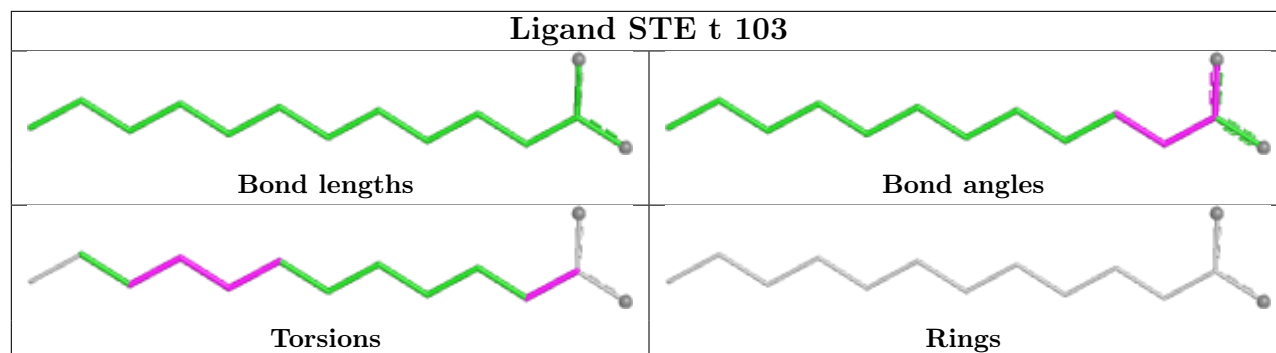
Ligand HEC v 201

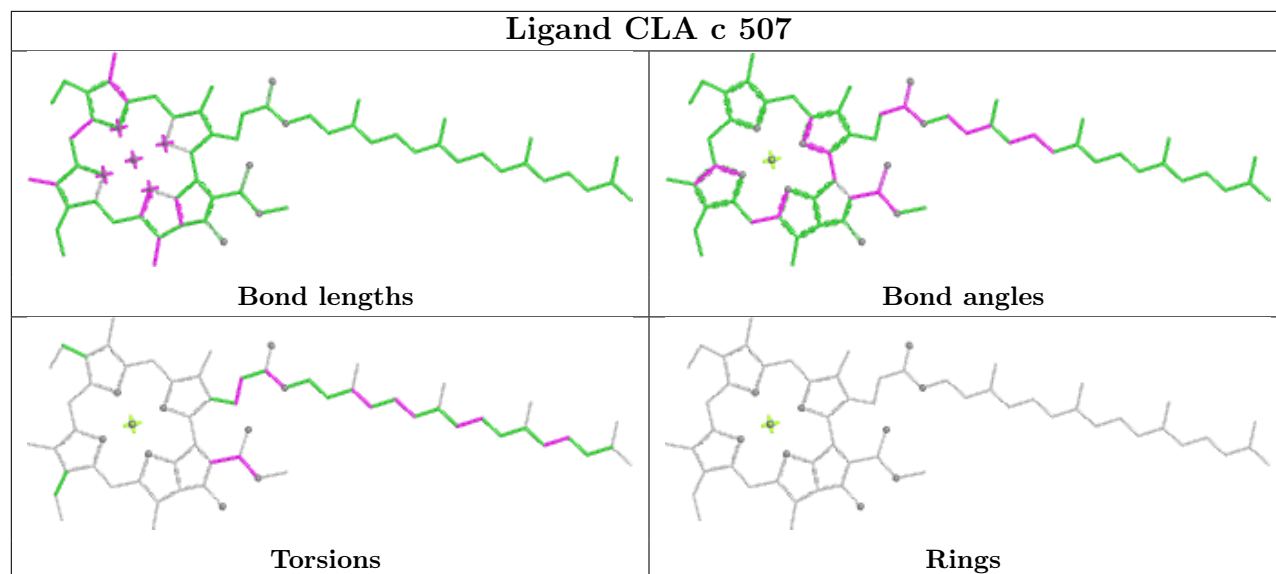
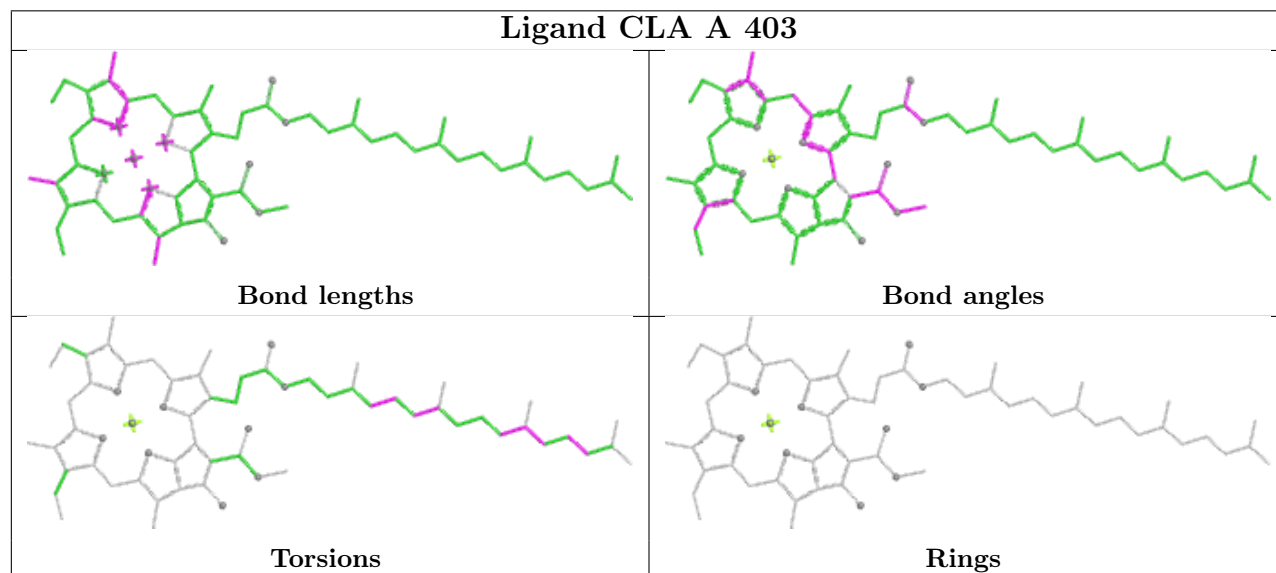


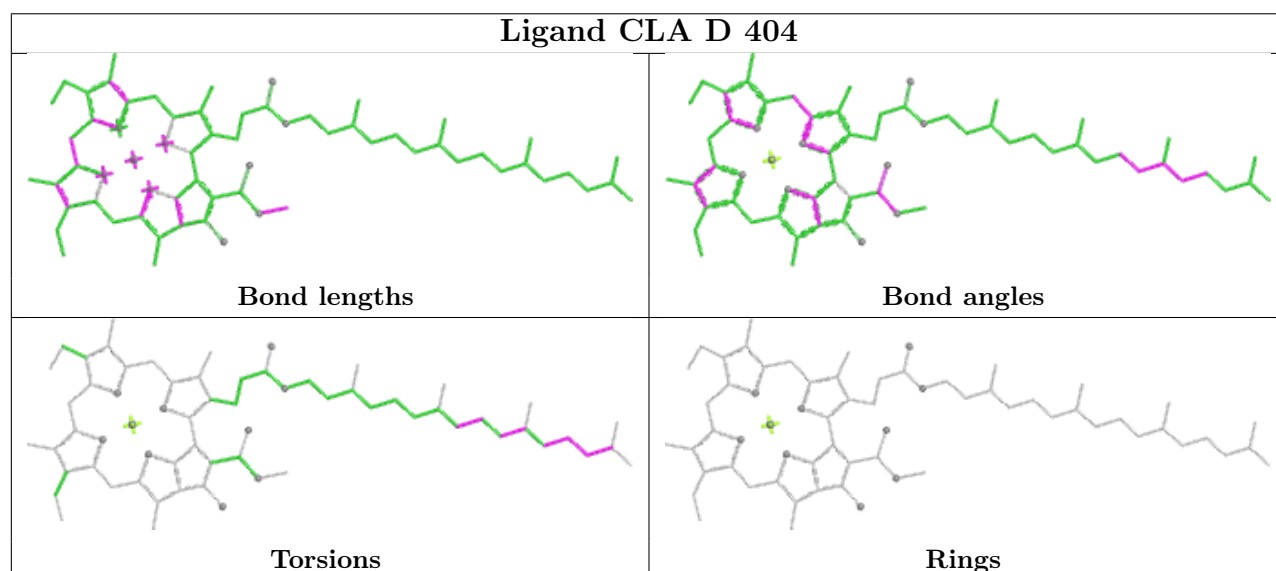
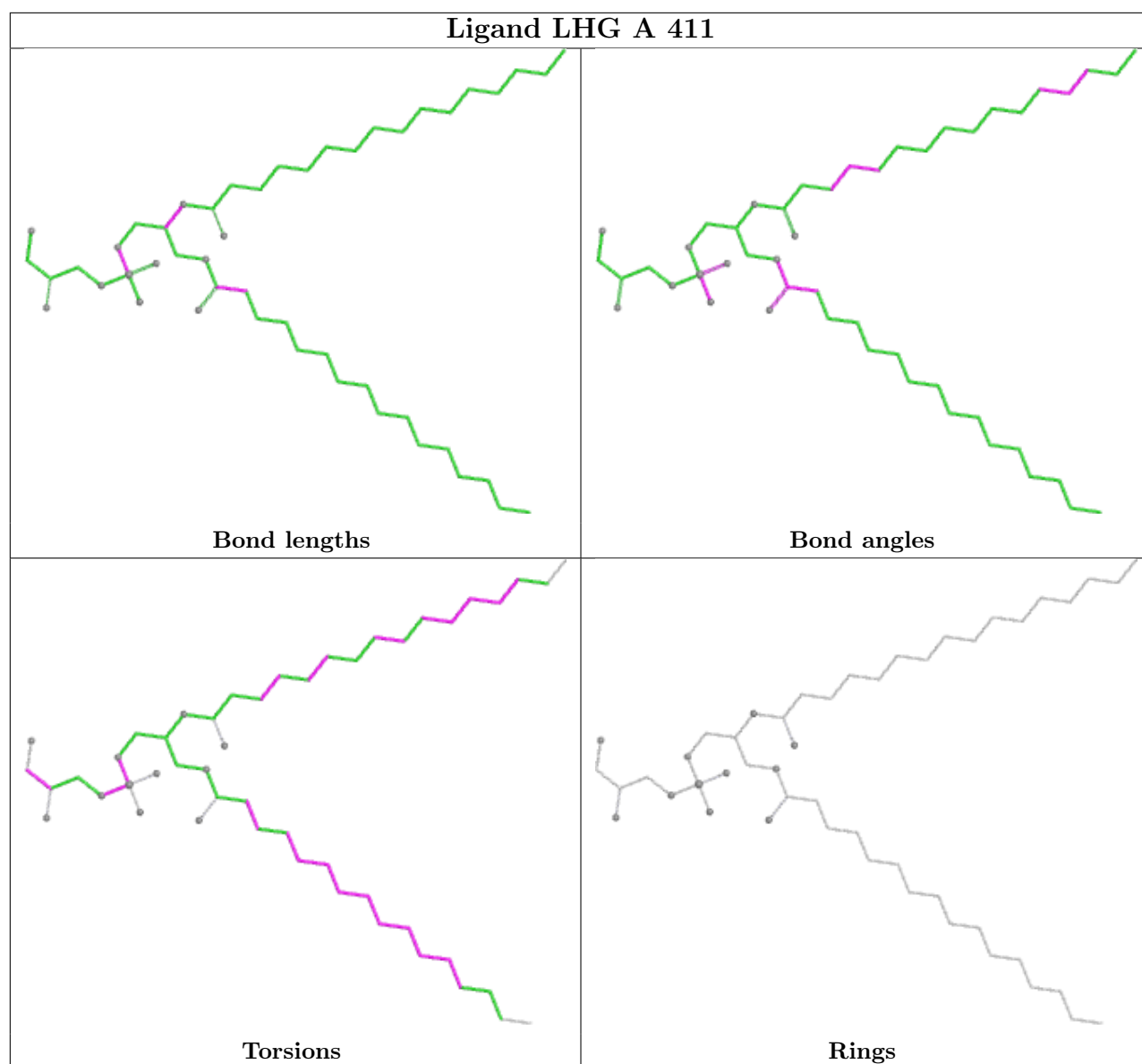
Ligand CLA C 507

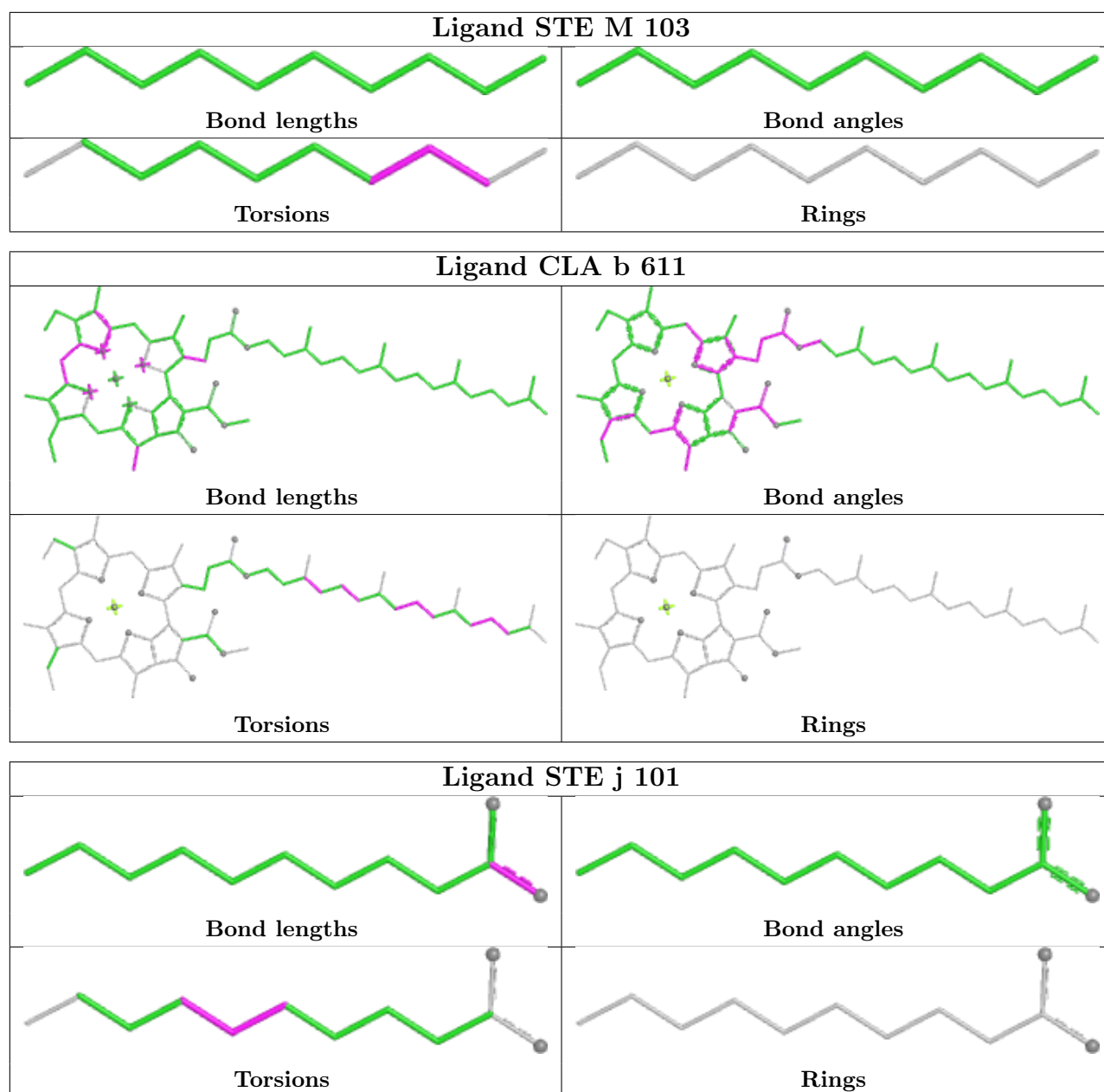


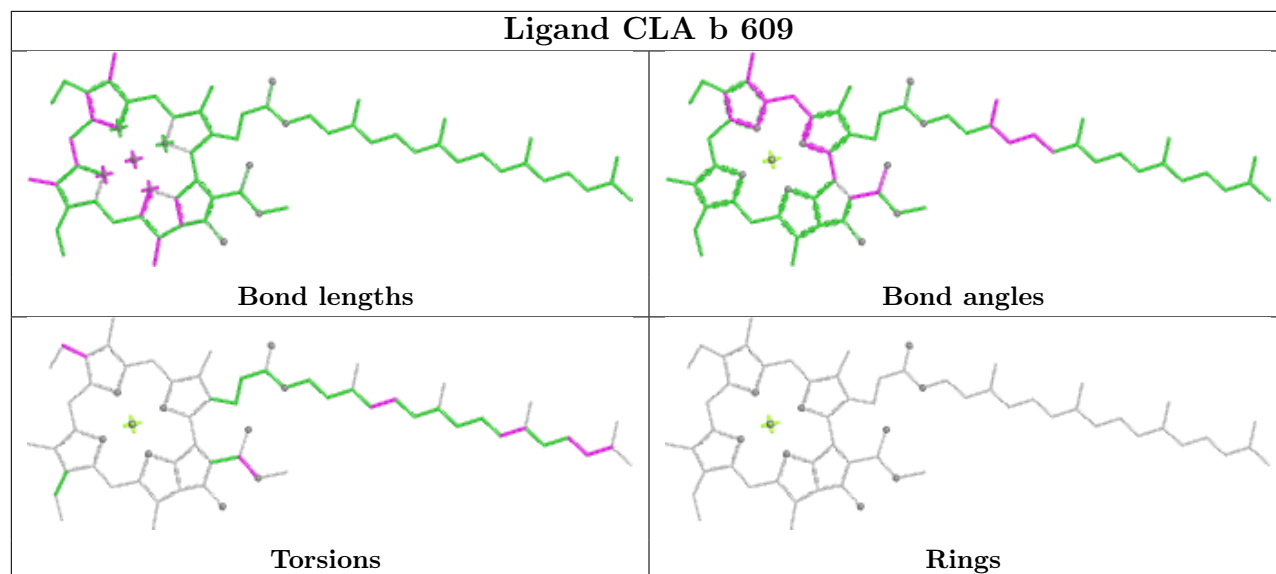
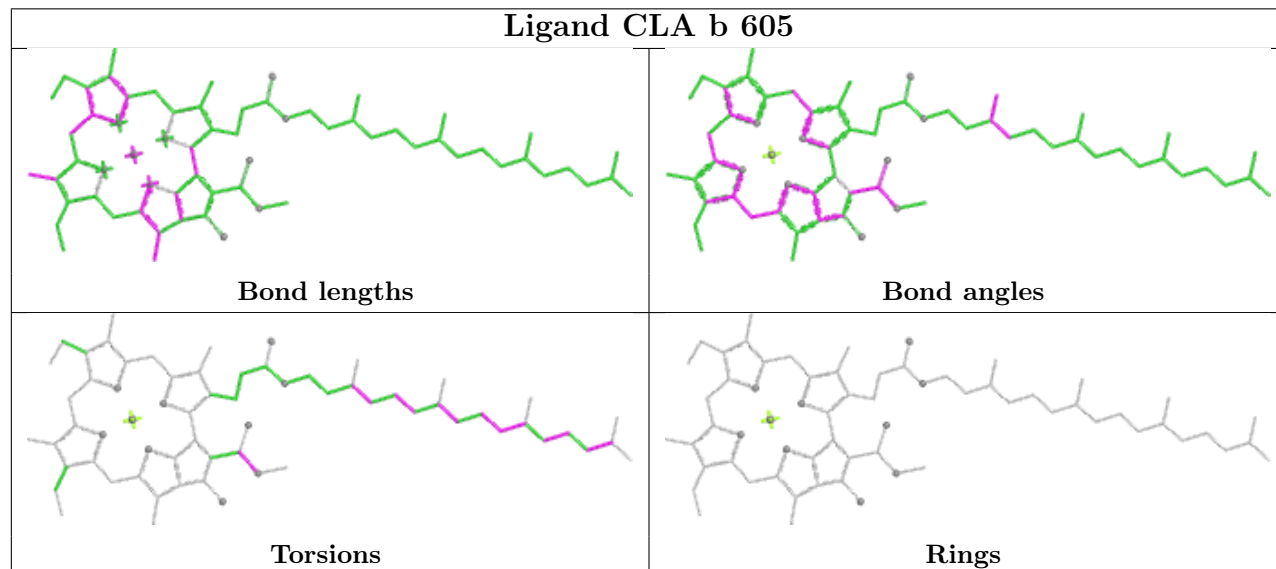


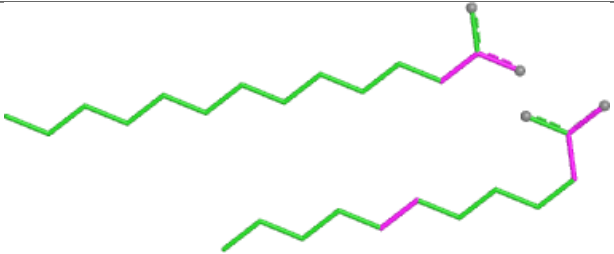
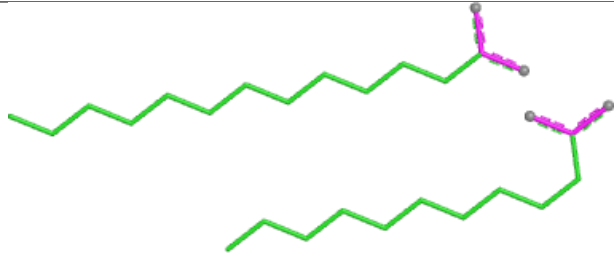
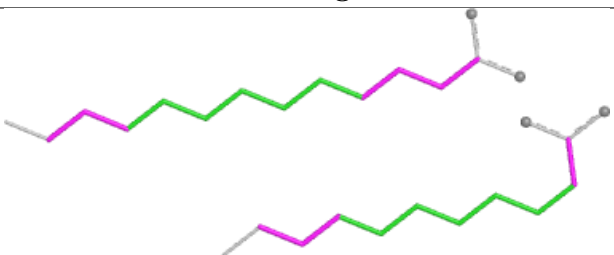
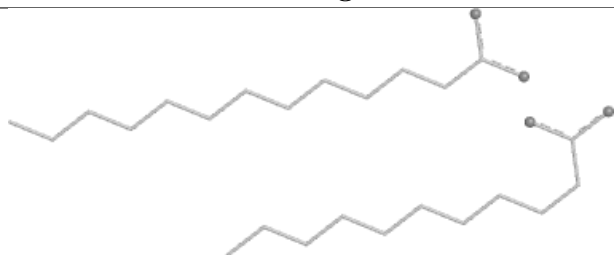


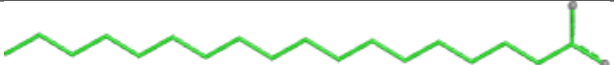
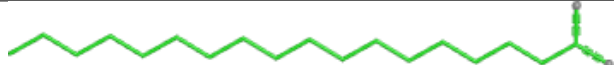
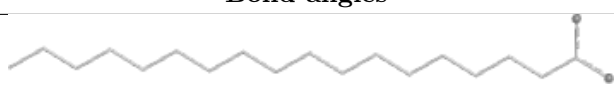
Ligand CLA c 507**Ligand CLA A 403**

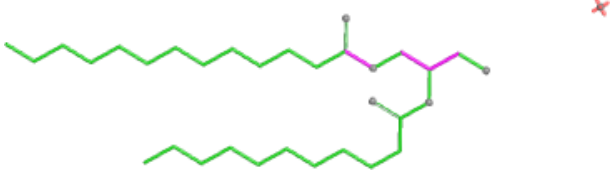
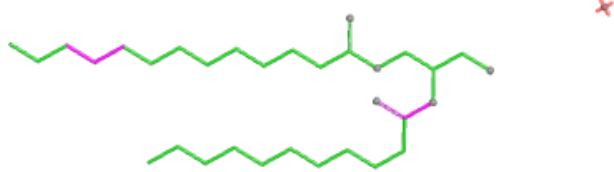
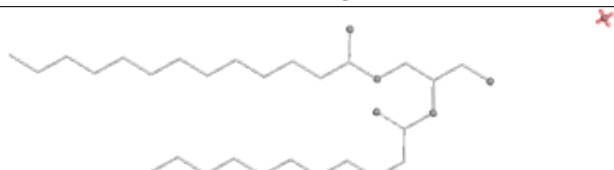


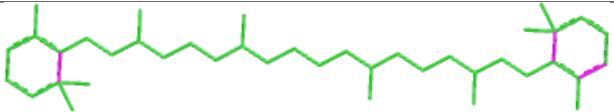
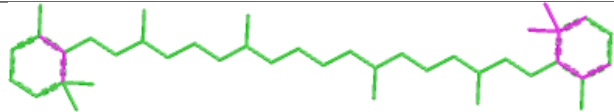
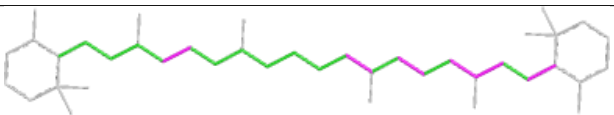
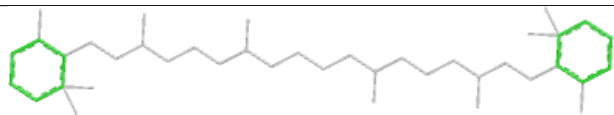


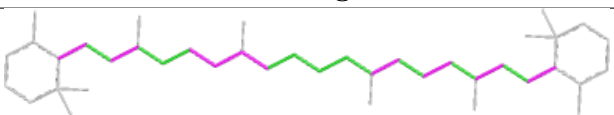
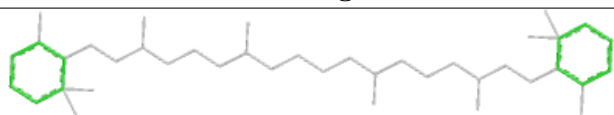
Ligand CLA b 609**Ligand CLA b 605**

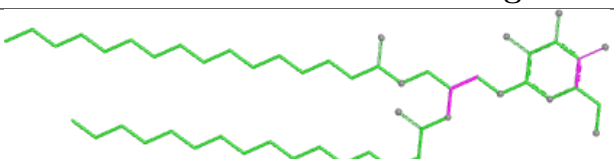
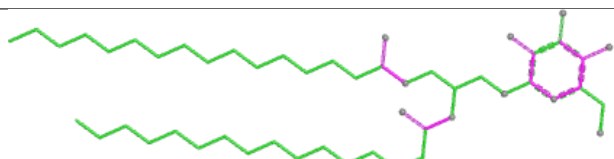
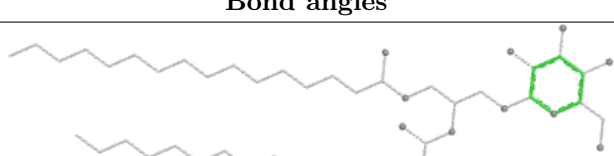
Ligand LMG B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

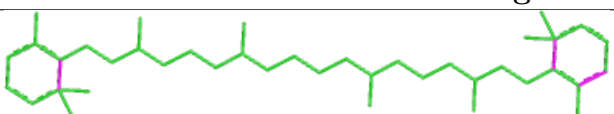
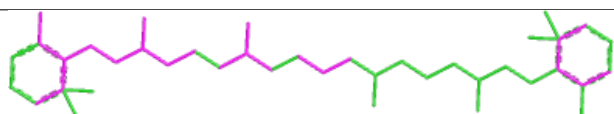
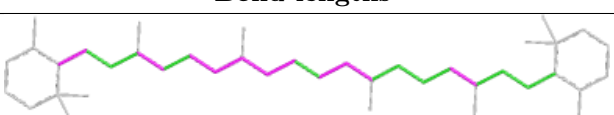
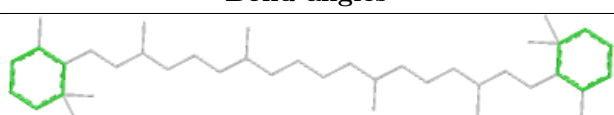
Ligand STE b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

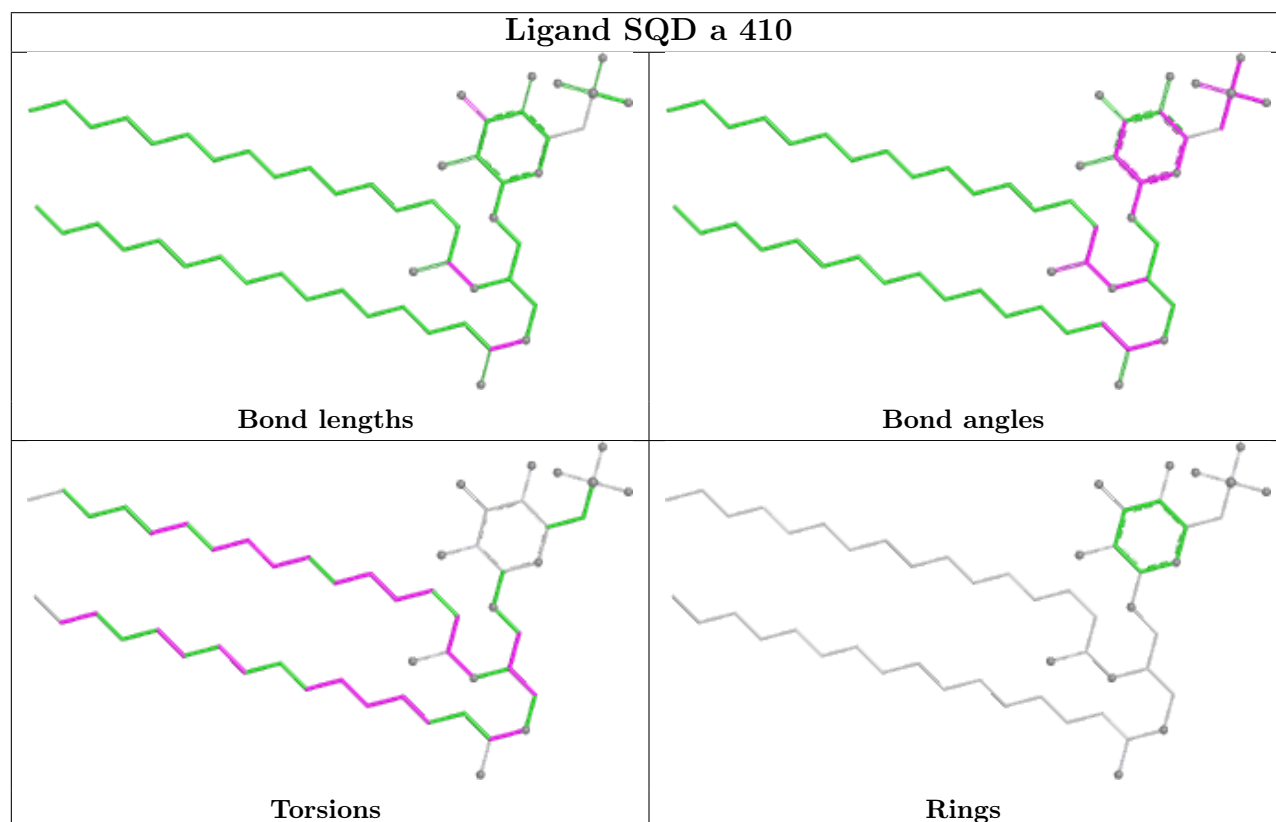
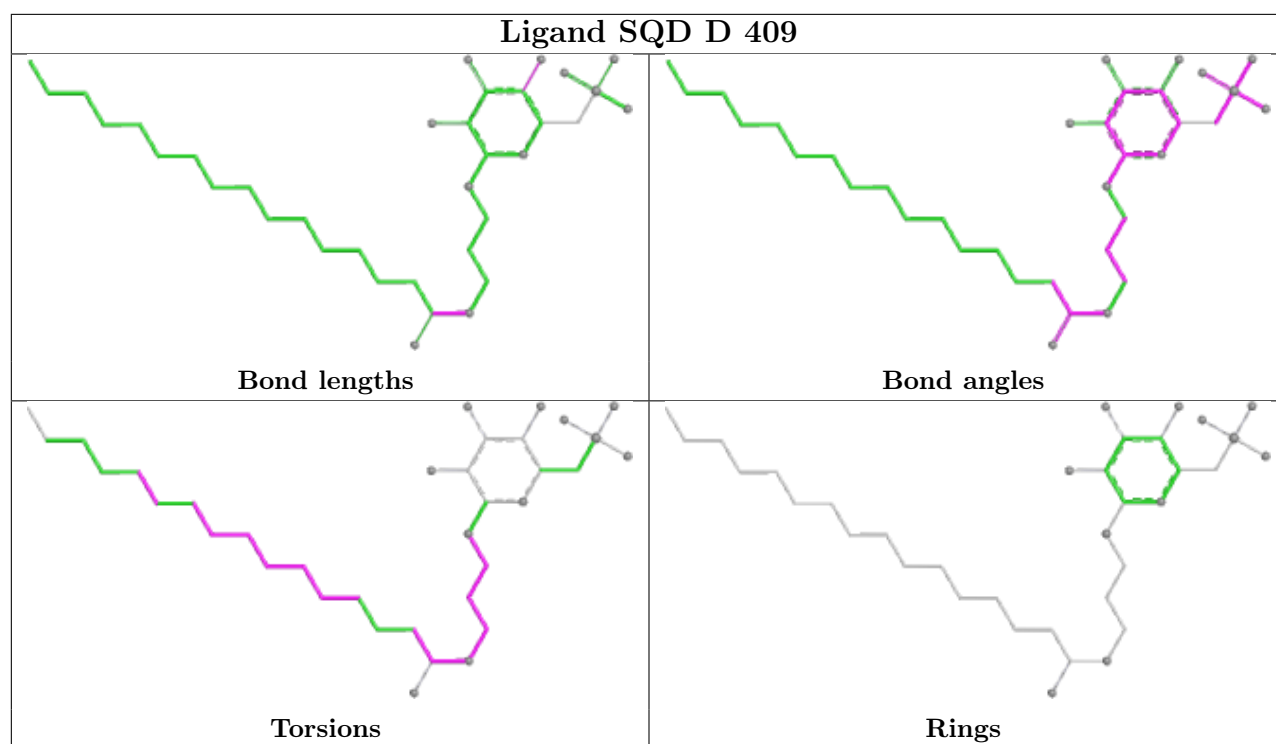
Ligand LMG D 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

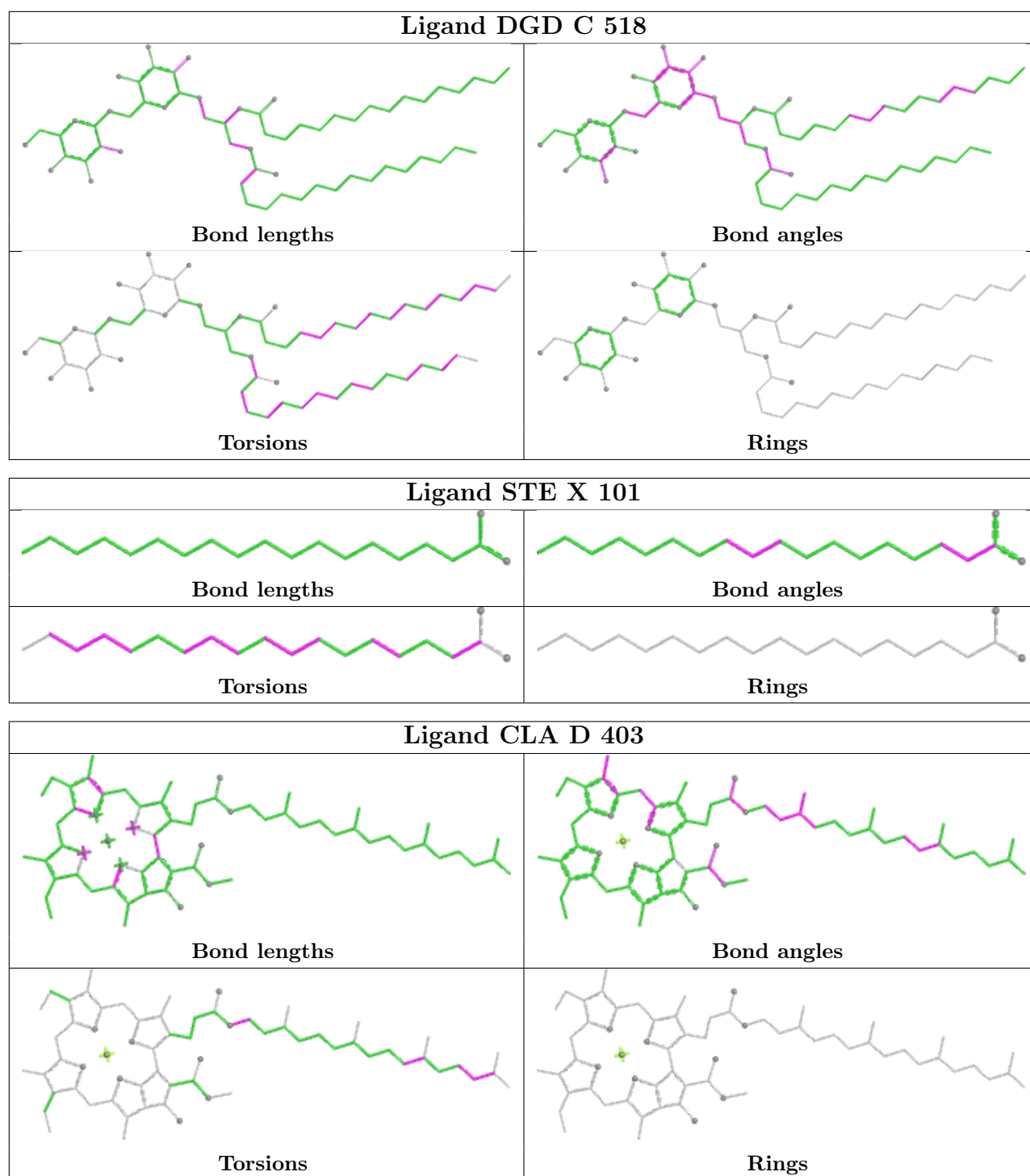
Ligand BCR k 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

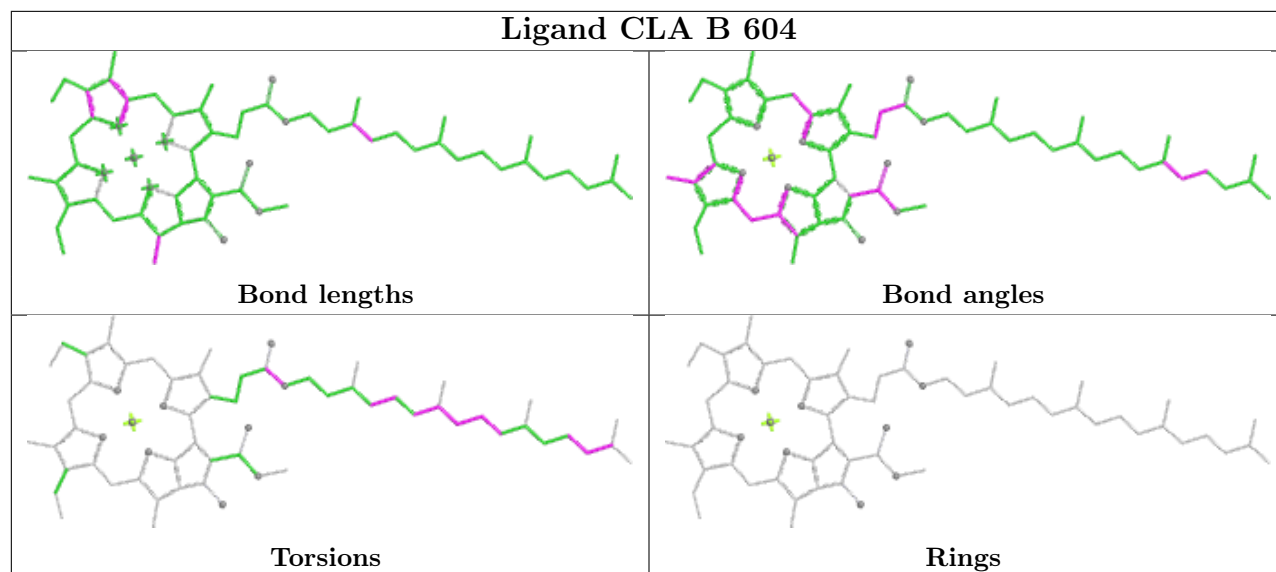
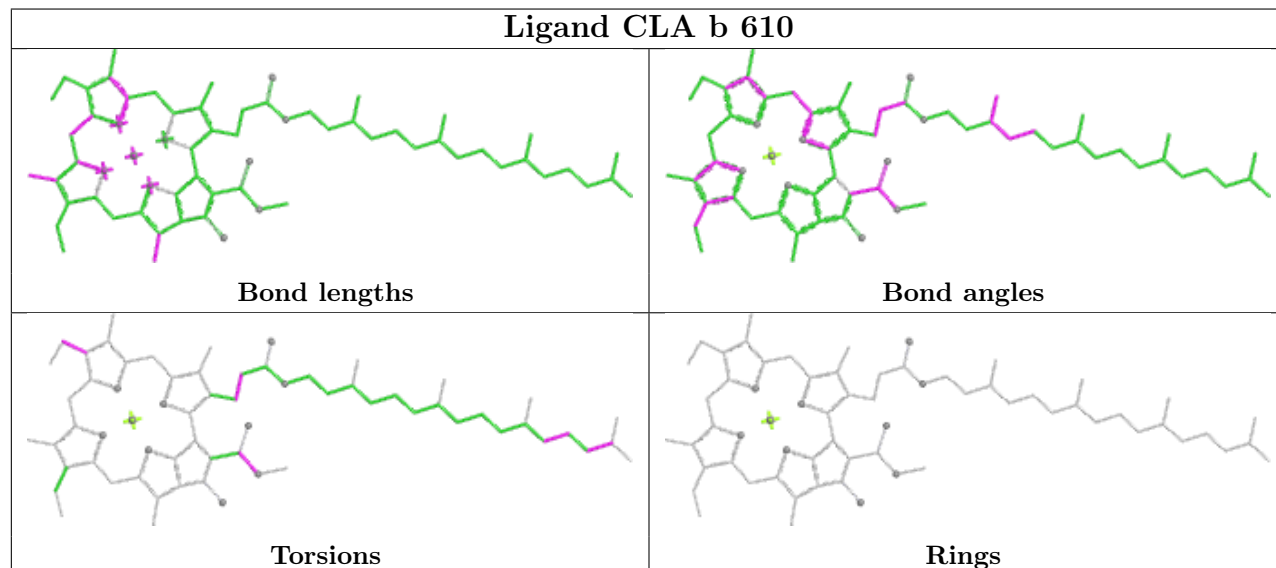
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Bond lengths	Bond angles
	
Torsions	Rings

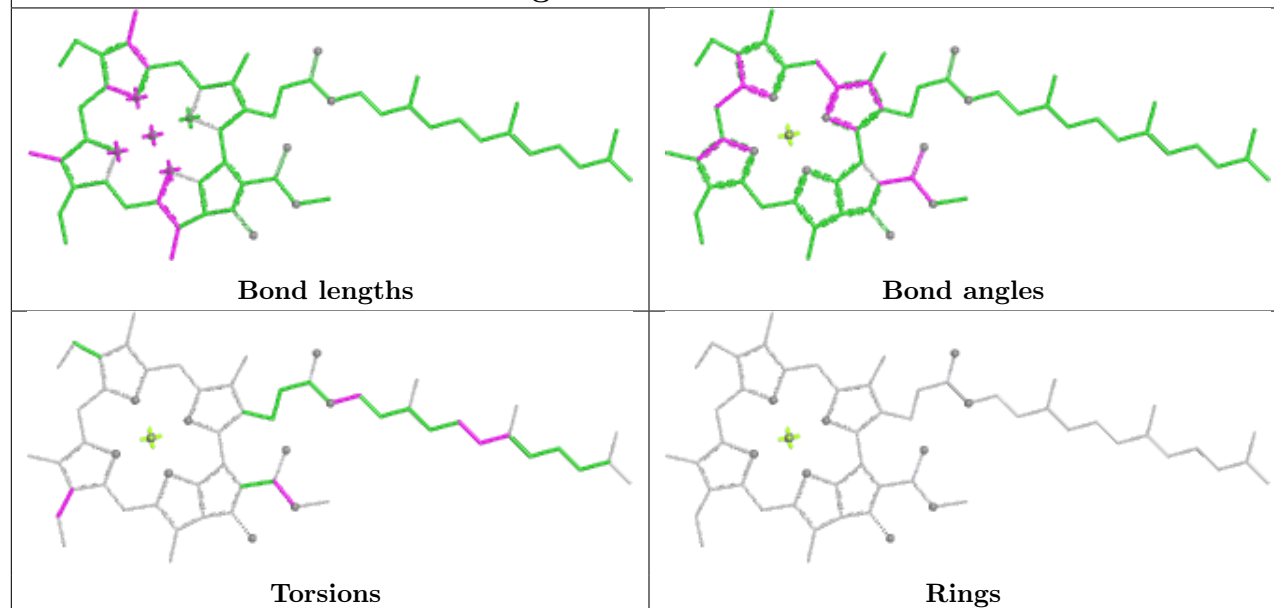
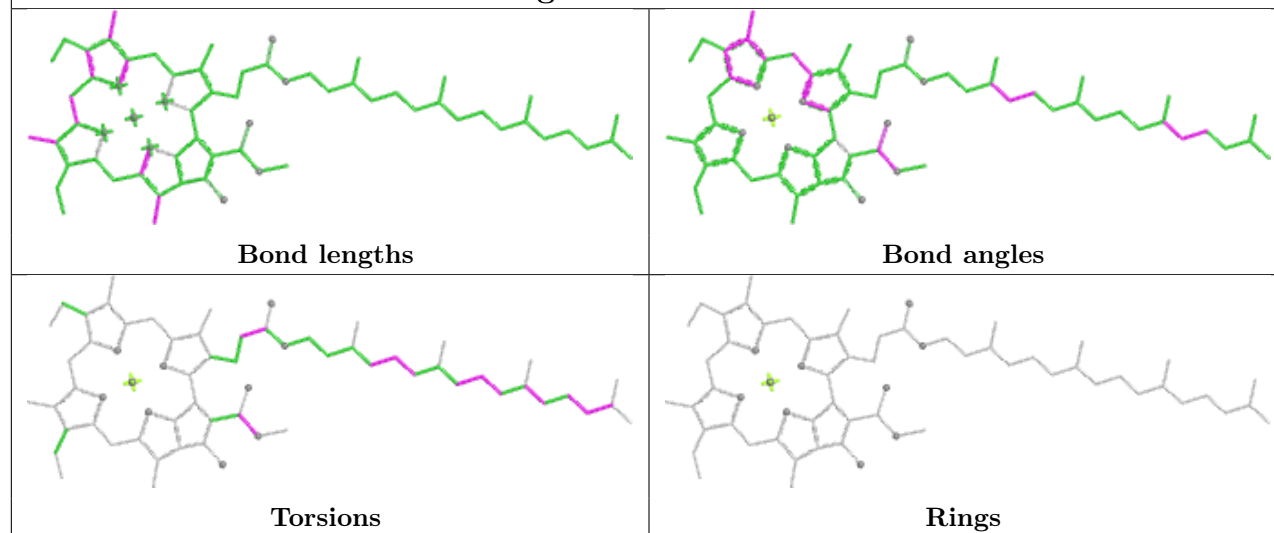
Ligand LMG D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

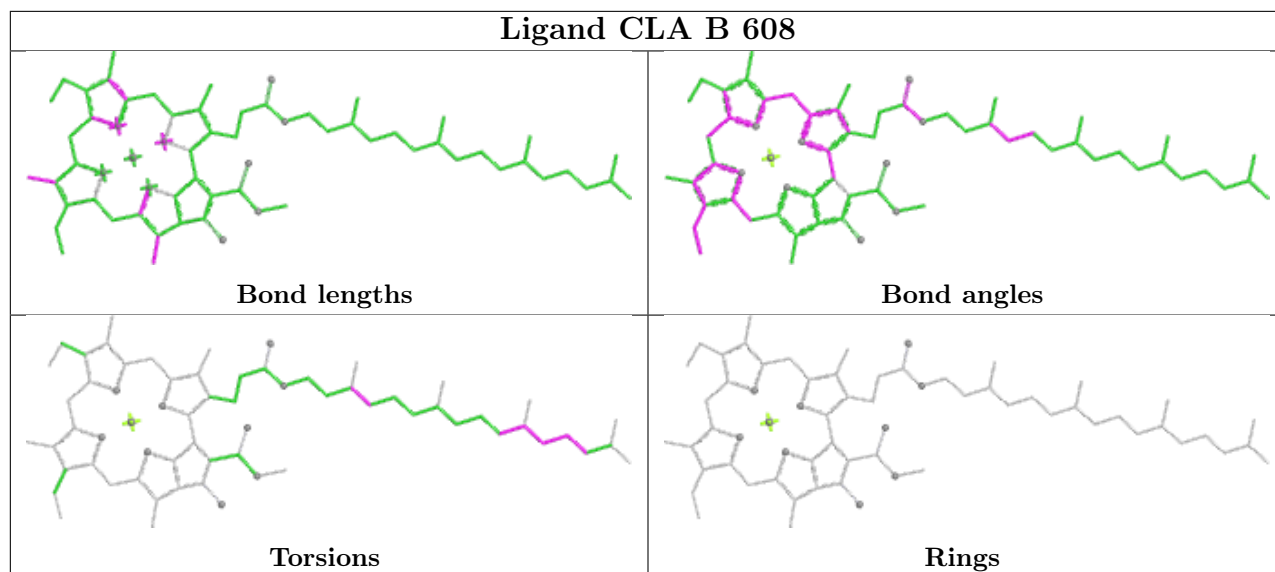




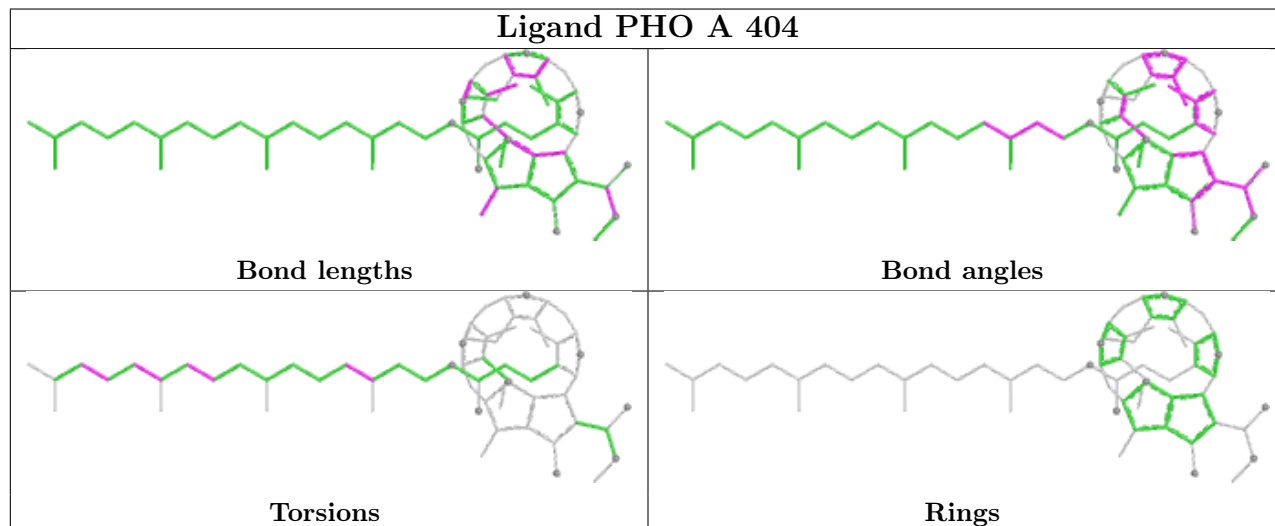
Ligand CLA B 604**Ligand CLA b 610**

Ligand CLA B 615**Ligand CLA c 510**

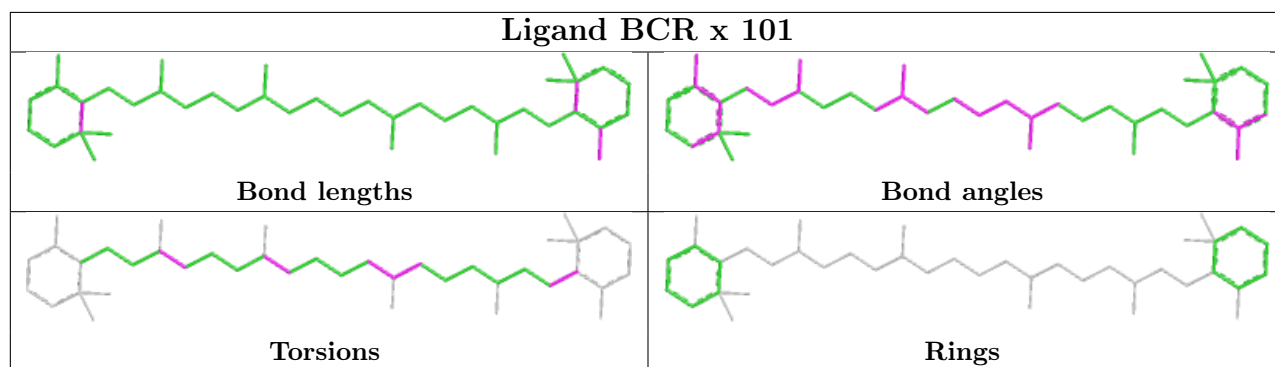
Ligand CLA B 608

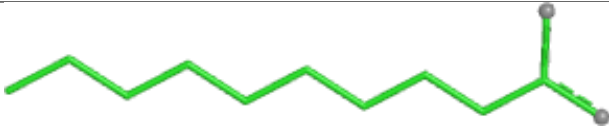
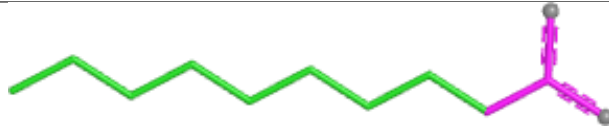
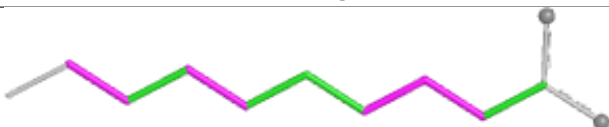
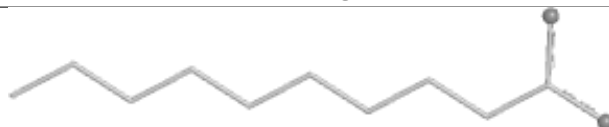
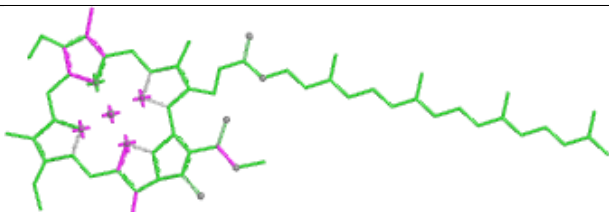
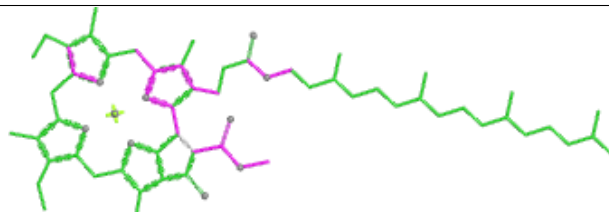
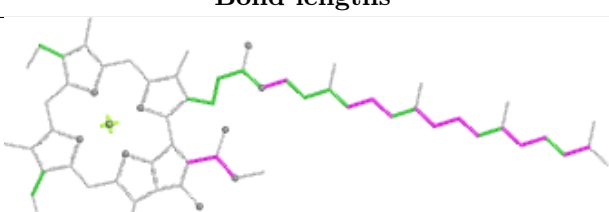
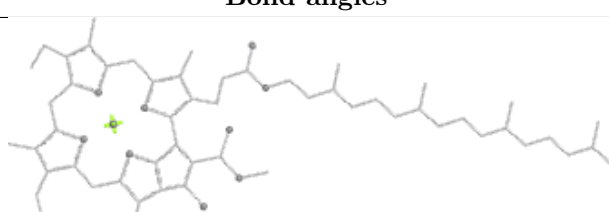
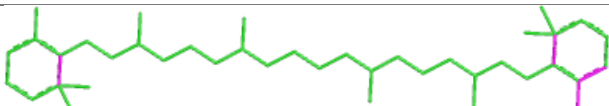
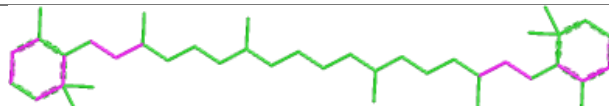
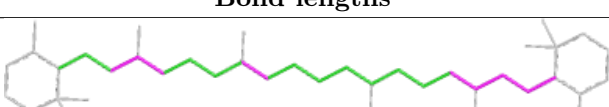
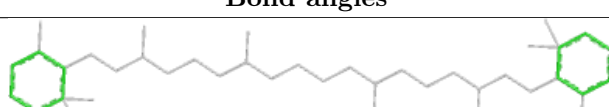


Ligand PHO A 404

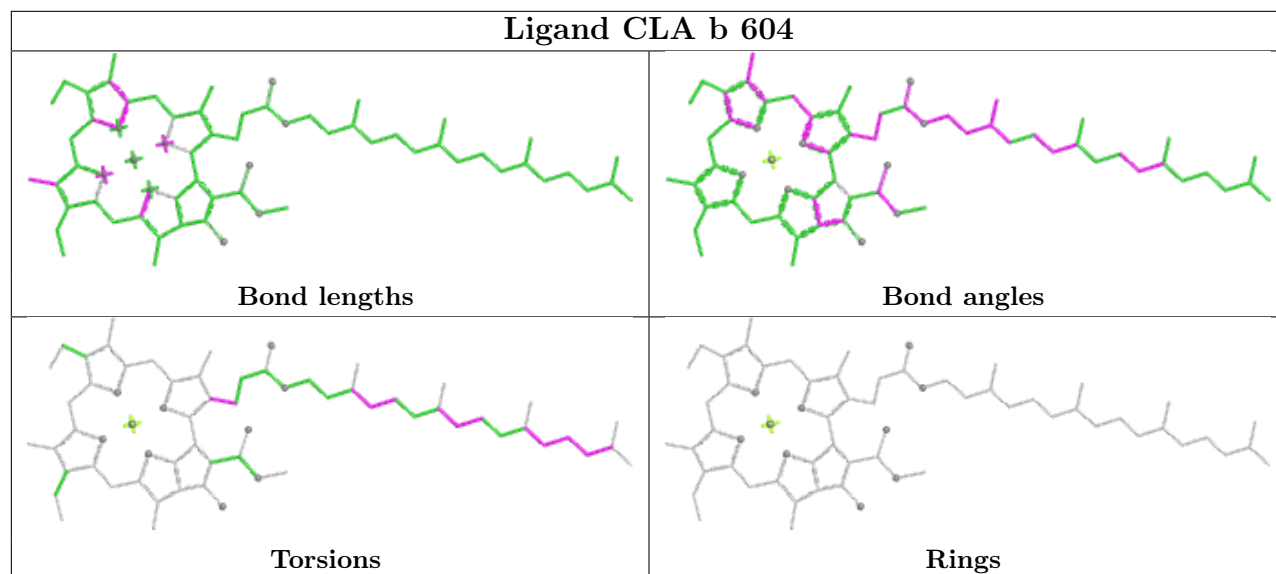


Ligand BCR x 101

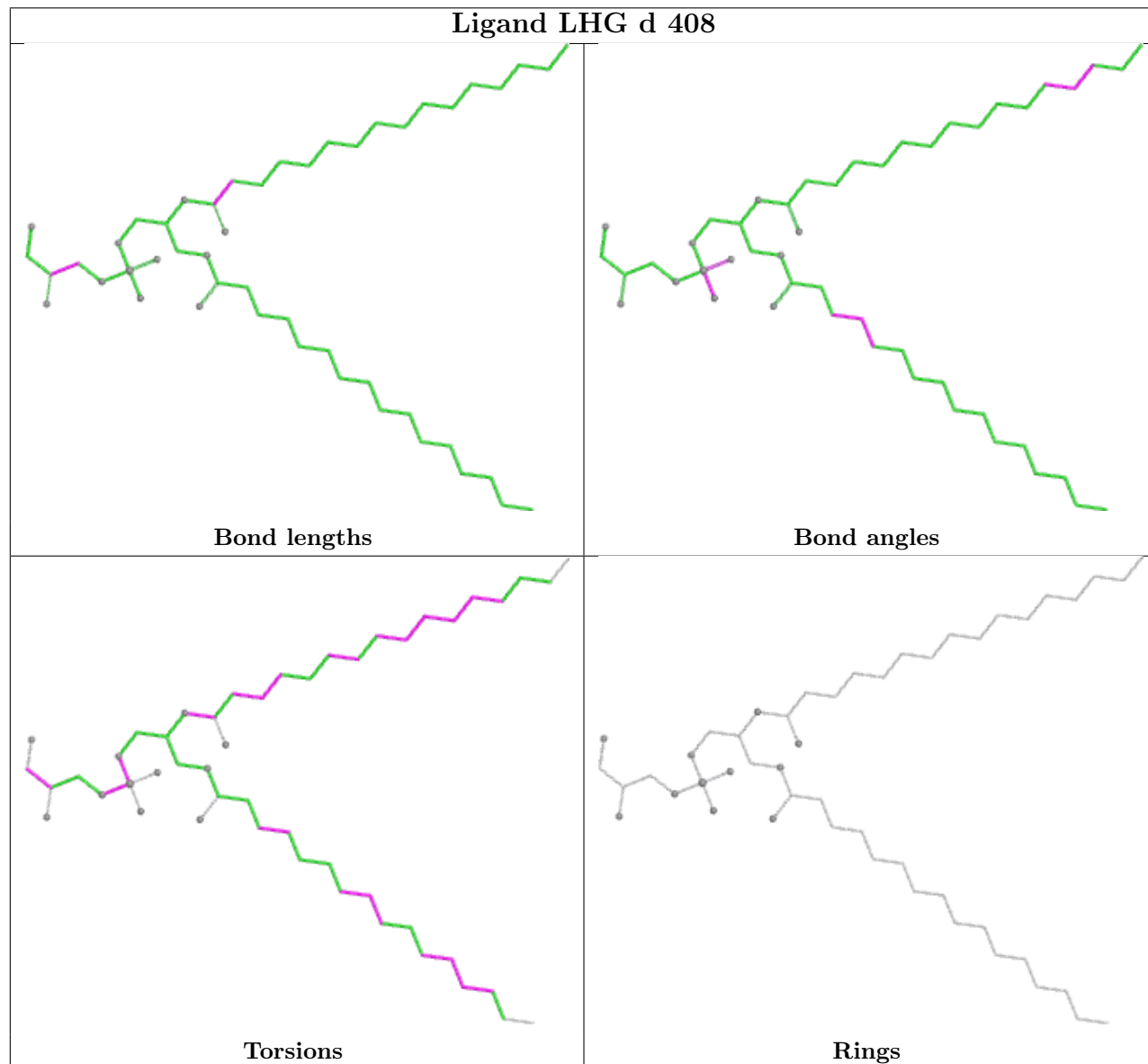


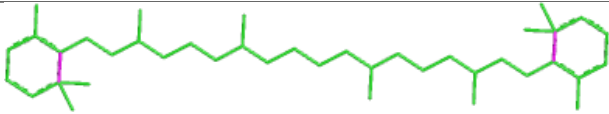
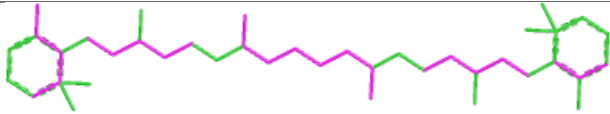
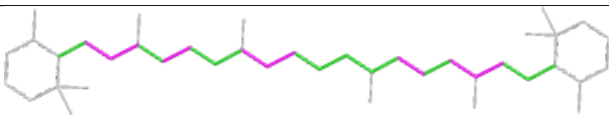
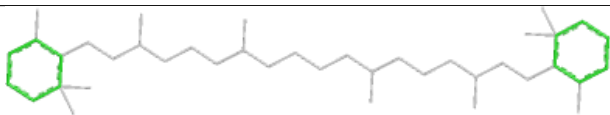
Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand STE M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

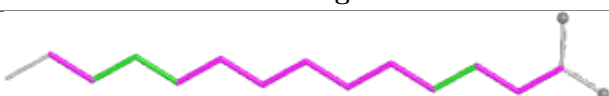
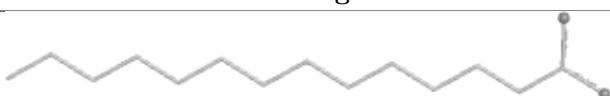
Ligand CLA b 604

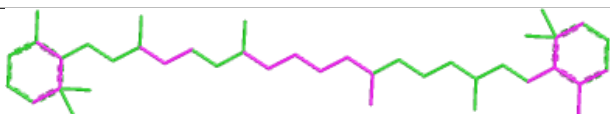
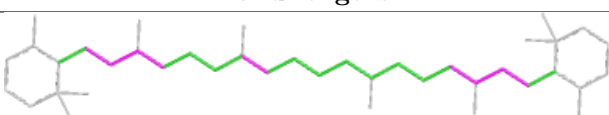
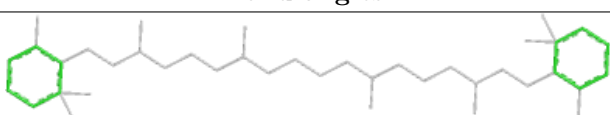


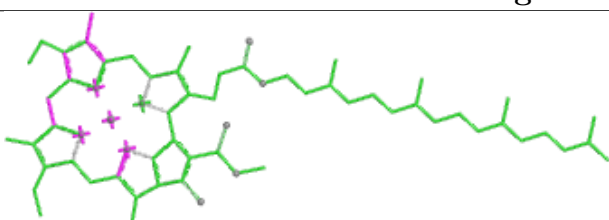
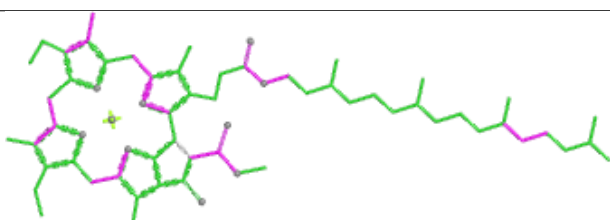
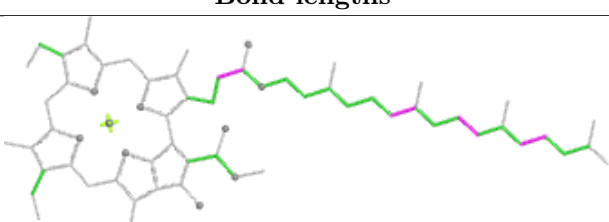
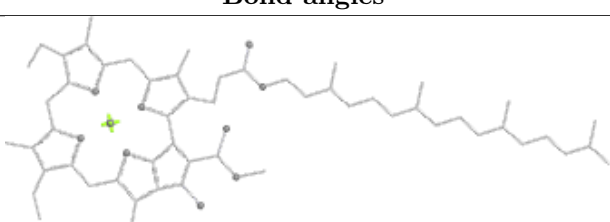
Ligand LHG d 408

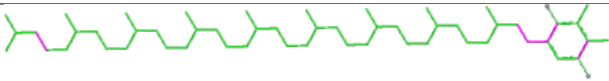
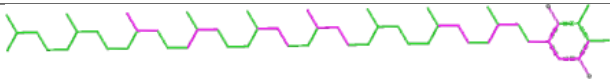
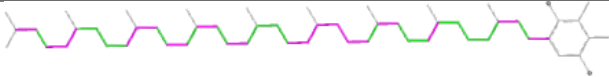
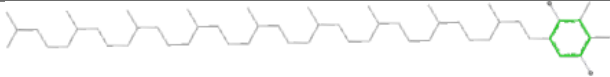


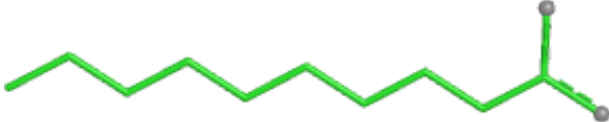
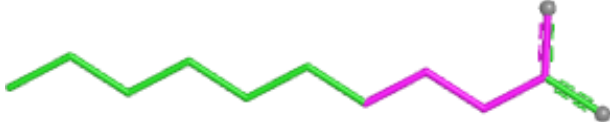
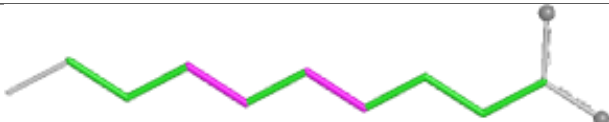
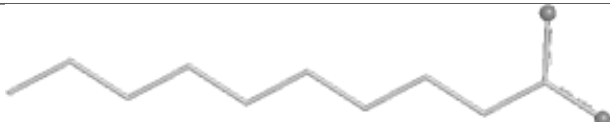
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

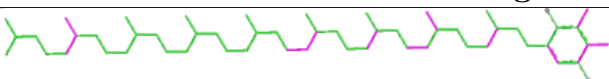
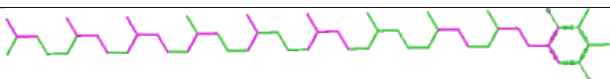
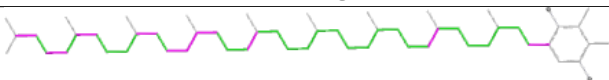
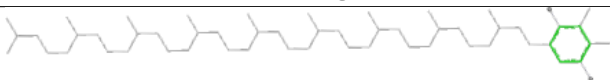
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

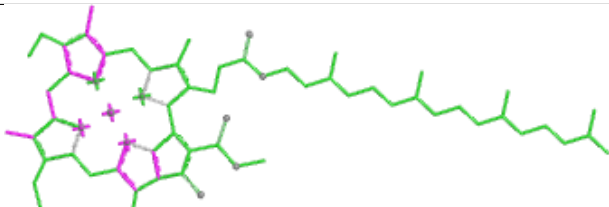
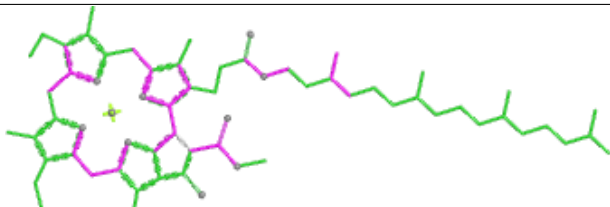
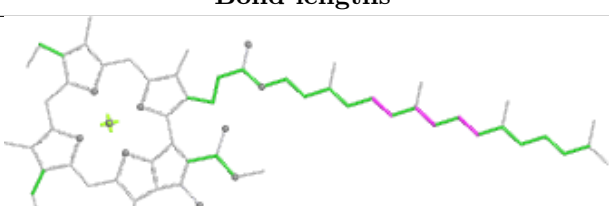
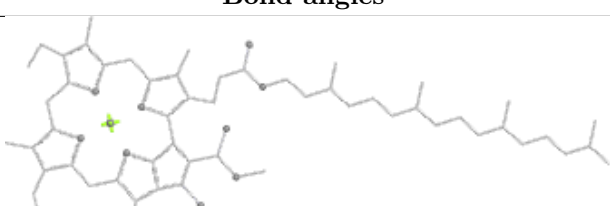
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

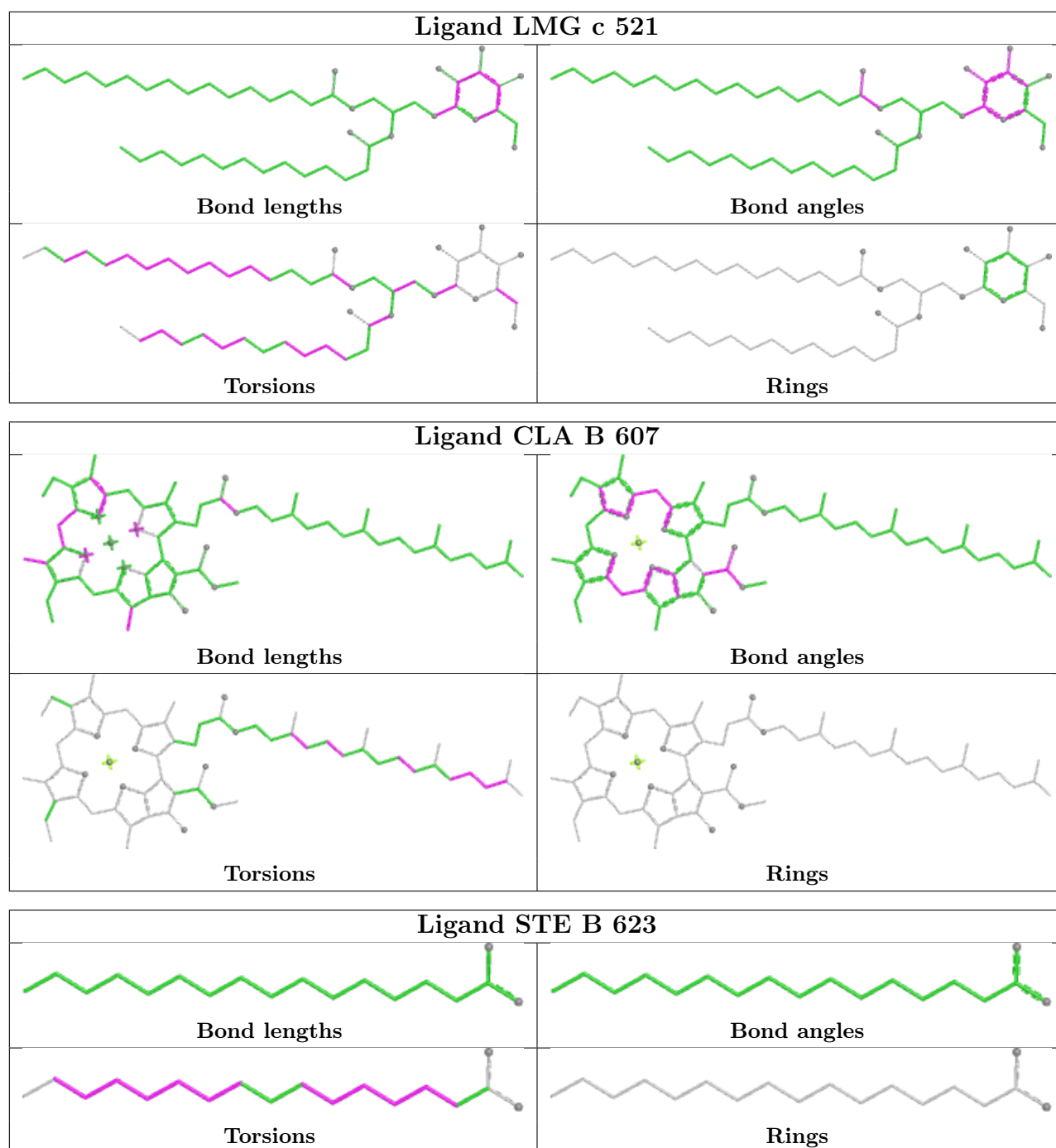
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

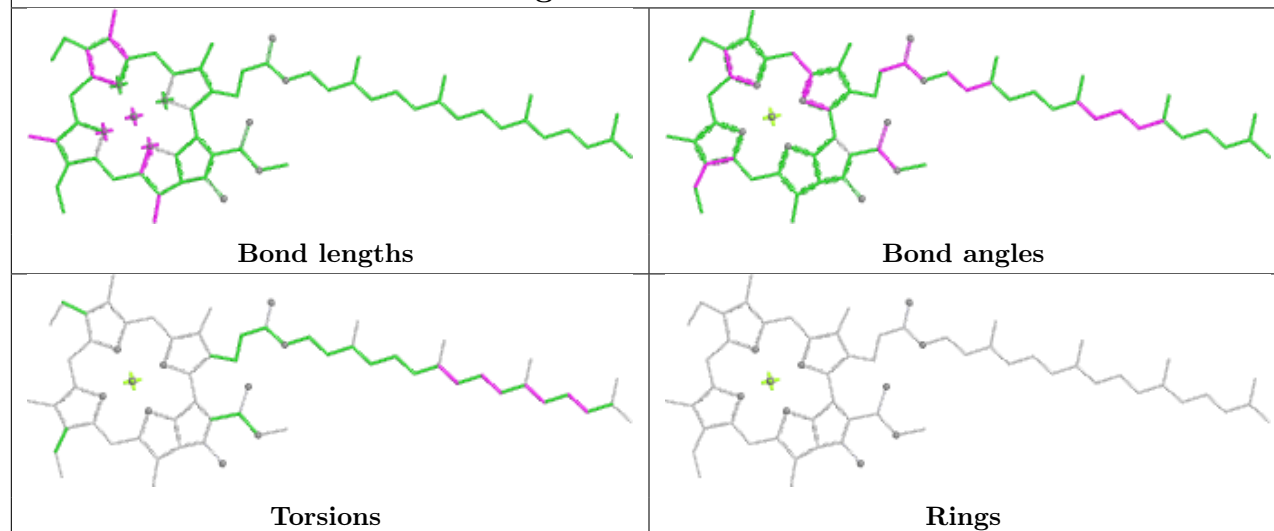
Ligand STE C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

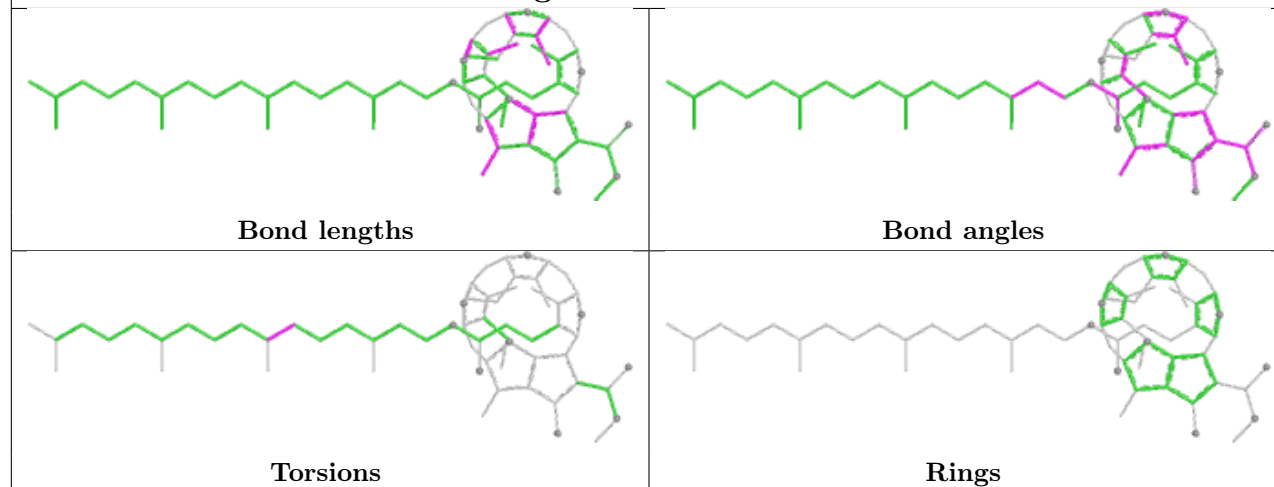
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings



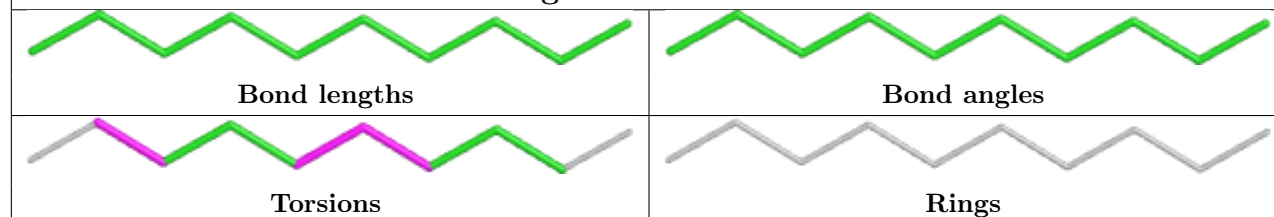
Ligand CLA b 612

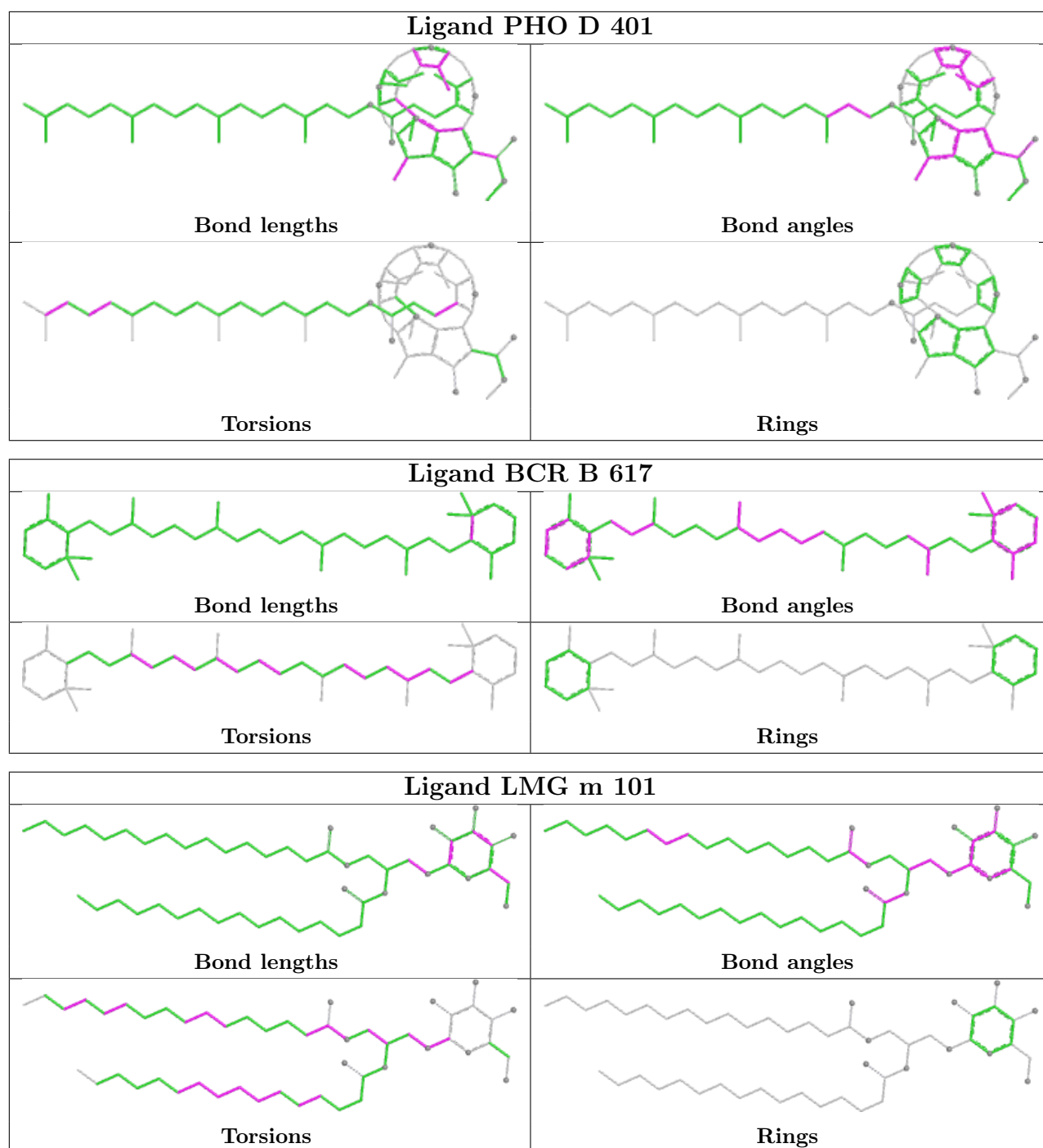


Ligand PHO a 404



Ligand STE t 104





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

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%)	-0.56	0 100 100	28, 38, 58, 91	0
1	a	334/344 (97%)	-0.46	2 (0%) 85 86	29, 40, 69, 87	0
2	B	505/506 (99%)	-0.43	0 100 100	22, 42, 74, 101	4 (0%)
2	b	505/506 (99%)	-0.31	4 (0%) 82 84	31, 46, 83, 115	0
3	C	442/461 (95%)	-0.37	0 100 100	22, 46, 64, 94	1 (0%)
3	c	451/461 (97%)	-0.29	1 (0%) 91 91	25, 50, 75, 112	2 (0%)
4	D	341/352 (96%)	-0.53	0 100 100	29, 40, 59, 95	0
4	d	341/352 (96%)	-0.39	0 100 100	29, 43, 68, 94	1 (0%)
5	E	82/84 (97%)	0.03	2 (2%) 59 61	34, 62, 81, 88	1 (1%)
5	e	82/84 (97%)	0.18	1 (1%) 76 78	47, 73, 91, 100	0
6	F	34/45 (75%)	-0.30	0 100 100	44, 54, 74, 88	0
6	f	34/45 (75%)	-0.15	0 100 100	51, 60, 88, 106	0
7	H	65/66 (98%)	-0.26	1 (1%) 72 73	40, 51, 72, 78	0
7	h	63/66 (95%)	0.04	2 (3%) 50 52	48, 63, 74, 87	0
8	I	35/38 (92%)	-0.32	1 (2%) 53 55	39, 49, 80, 95	0
8	i	35/38 (92%)	-0.18	0 100 100	38, 50, 85, 94	0
9	J	36/40 (90%)	-0.13	0 100 100	44, 60, 85, 100	0
9	j	36/40 (90%)	0.04	0 100 100	49, 64, 100, 119	0
10	K	37/46 (80%)	-0.19	0 100 100	49, 63, 80, 86	0
10	k	37/46 (80%)	0.06	0 100 100	60, 68, 85, 92	0
11	L	37/37 (100%)	-0.64	0 100 100	33, 39, 73, 83	0
11	l	36/37 (97%)	-0.57	0 100 100	32, 41, 86, 93	0
12	M	32/36 (88%)	-0.43	0 100 100	37, 45, 73, 84	0
12	m	31/36 (86%)	-0.48	0 100 100	37, 44, 61, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.23	2 (0%) 82 84	30, 52, 96, 138	1 (0%)
13	o	244/272 (89%)	-0.27	2 (0%) 82 84	31, 50, 90, 145	0
14	R	34/41 (82%)	0.61	1 (2%) 53 55	70, 83, 103, 108	0
14	r	31/41 (75%)	1.23	5 (16%) 4 5	88, 109, 130, 145	0
15	T	29/30 (96%)	-0.57	0 100 100	32, 40, 75, 96	0
15	t	29/30 (96%)	-0.39	1 (3%) 48 50	35, 41, 92, 97	0
16	U	97/134 (72%)	-0.20	0 100 100	36, 54, 81, 106	0
16	u	97/134 (72%)	-0.31	0 100 100	39, 52, 68, 83	0
17	V	137/163 (84%)	-0.42	0 100 100	34, 50, 65, 87	0
17	v	137/163 (84%)	-0.20	0 100 100	40, 58, 84, 91	0
18	X	38/41 (92%)	-0.11	1 (2%) 57 59	51, 62, 87, 98	0
18	x	39/41 (95%)	0.06	1 (2%) 57 59	58, 69, 98, 118	0
19	Y	27/46 (58%)	0.78	3 (11%) 10 11	64, 87, 104, 113	0
19	y	30/46 (65%)	0.54	1 (3%) 49 51	73, 87, 100, 117	0
20	Z	62/62 (100%)	0.48	2 (3%) 50 52	63, 79, 130, 143	0
20	z	62/62 (100%)	0.54	3 (4%) 35 36	70, 87, 124, 133	0
All	All	5302/5688 (93%)	-0.29	36 (0%) 84 85	22, 48, 87, 145	10 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.6
15	t	30	THR	4.5
20	z	33	TRP	3.9
18	x	40	SER	3.4
14	R	35	LEU	3.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.93	0.10	46,62,75,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.95	0.09	44,61,78,87	0
12	FME	m	1	10/11	0.95	0.09	46,57,89,91	0
15	FME	T	1	10/11	0.95	0.09	30,62,79,79	0
15	FME	t	1	10/11	0.96	0.07	33,54,70,73	0
8	FME	i	1	10/11	0.97	0.07	45,59,72,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	STE	b	629	20/20	0.76	0.18	40,71,89,93	0
31	STE	b	628	14/20	0.78	0.19	57,77,110,110	0
31	STE	b	627	10/20	0.79	0.16	45,58,65,68	0
31	STE	B	624	16/20	0.79	0.17	43,71,87,89	0
31	STE	a	412	12/20	0.79	0.15	46,79,97,98	0
31	STE	k	104	12/20	0.79	0.13	56,73,85,89	0
31	STE	I	102	15/20	0.80	0.16	40,58,82,84	0
28	LHG	a	411	42/49	0.80	0.15	66,95,118,141	0
31	STE	H	104	18/20	0.81	0.15	49,76,90,93	0
31	STE	B	623	18/20	0.82	0.14	54,72,94,94	0
31	STE	b	625	15/20	0.82	0.16	52,68,93,94	0
28	LHG	A	411	49/49	0.82	0.14	50,86,108,119	0
26	LMG	c	520	48/55	0.83	0.14	35,83,112,118	0
31	STE	b	626	20/20	0.83	0.15	43,74,97,100	0
31	STE	c	519	20/20	0.83	0.12	43,66,97,102	0
26	LMG	b	622	55/55	0.83	0.15	48,80,110,117	0
31	STE	b	620	16/20	0.84	0.14	42,55,83,100	0
26	LMG	a	414	55/55	0.85	0.13	40,67,93,105	0
27	SQD	A	412	39/54	0.85	0.14	47,69,107,111	0
22	CLA	b	601	65/65	0.85	0.12	51,74,102,106	0
31	STE	B	625	12/20	0.85	0.14	47,69,89,93	0
31	STE	b	624	16/20	0.85	0.14	53,74,88,95	0
31	STE	C	519	12/20	0.85	0.13	41,55,68,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	STE	t	104	10/20	0.85	0.15	45,59,73,73	0
31	STE	C	520	16/20	0.86	0.14	43,63,75,79	0
25	PL9	A	408	55/55	0.86	0.14	34,70,94,98	0
31	STE	b	621	20/20	0.86	0.12	44,63,85,87	0
26	LMG	c	518	37/55	0.86	0.12	49,72,93,98	0
31	STE	J	101	12/20	0.86	0.13	51,71,80,81	0
31	STE	M	103	10/20	0.86	0.14	35,56,69,69	0
25	PL9	a	409	55/55	0.87	0.14	42,77,102,105	0
31	STE	R	101	12/20	0.87	0.14	59,80,103,104	0
22	CLA	H	101	65/65	0.87	0.11	36,70,99,108	0
31	STE	j	101	12/20	0.87	0.11	50,63,72,76	0
31	STE	a	413	15/20	0.87	0.16	35,65,81,92	0
31	STE	L	103	12/20	0.87	0.15	49,66,79,86	0
29	DGD	A	413	66/66	0.88	0.10	41,65,89,95	0
31	STE	B	619	17/20	0.88	0.12	37,58,76,80	0
31	STE	B	622	12/20	0.88	0.11	36,57,72,72	0
26	LMG	D	412	33/55	0.88	0.13	36,63,101,106	0
31	STE	d	411	17/20	0.88	0.12	49,65,73,79	0
27	SQD	t	102	36/54	0.88	0.13	31,69,96,103	0
26	LMG	Y	101	48/55	0.88	0.11	54,76,95,104	0
26	LMG	B	620	28/55	0.88	0.13	35,52,67,71	0
31	STE	x	102	20/20	0.88	0.12	51,68,91,94	0
27	SQD	f	102	41/54	0.89	0.13	61,87,110,127	0
26	LMG	A	409	48/55	0.89	0.10	36,63,86,104	0
31	STE	M	104	18/20	0.89	0.11	38,53,75,86	0
27	SQD	L	101	49/54	0.89	0.11	40,66,106,121	0
26	LMG	c	521	49/55	0.90	0.11	32,66,98,113	0
31	STE	t	103	14/20	0.90	0.10	41,59,67,71	0
26	LMG	M	101	51/55	0.90	0.10	37,56,84,88	0
27	SQD	B	621	54/54	0.90	0.10	40,67,93,104	0
26	LMG	m	101	51/55	0.91	0.10	40,61,86,96	0
31	STE	C	521	12/20	0.91	0.11	37,48,59,64	0
26	LMG	d	410	44/55	0.91	0.10	41,61,90,108	0
31	STE	Z	101	8/20	0.91	0.12	38,65,78,78	0
30	BCR	k	101	40/40	0.91	0.11	48,67,82,91	0
30	BCR	x	101	40/40	0.91	0.09	40,59,76,81	0
27	SQD	a	410	54/54	0.91	0.11	44,70,104,112	0
22	CLA	c	512	65/65	0.92	0.10	44,62,97,112	0
22	CLA	c	513	65/65	0.92	0.10	44,80,112,121	0
22	CLA	C	513	65/65	0.92	0.10	43,65,107,118	0
30	BCR	C	514	40/40	0.92	0.10	30,47,58,76	0
30	BCR	K	101	40/40	0.92	0.10	45,63,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	BCR	K	102	40/40	0.92	0.09	37,57,74,74	0
30	BCR	d	406	40/40	0.92	0.09	30,58,103,111	0
27	SQD	D	409	36/54	0.92	0.11	50,78,97,114	0
31	STE	X	101	20/20	0.92	0.10	40,60,81,91	0
30	BCR	H	102	40/40	0.93	0.08	35,51,67,75	0
27	SQD	A	410	52/54	0.93	0.10	39,68,101,103	0
29	DGD	C	517	62/66	0.93	0.09	30,57,112,139	0
30	BCR	b	619	40/40	0.93	0.08	24,55,73,87	0
29	DGD	H	103	62/66	0.93	0.09	34,51,67,75	0
29	DGD	c	516	62/66	0.93	0.08	36,61,97,110	0
30	BCR	k	102	40/40	0.93	0.09	46,67,84,86	0
31	STE	M	102	15/20	0.93	0.09	37,54,63,69	0
30	BCR	k	103	40/40	0.93	0.11	45,63,78,85	0
29	DGD	c	517	62/66	0.93	0.10	36,64,94,109	0
29	DGD	h	101	62/66	0.93	0.09	35,53,70,78	0
30	BCR	B	617	40/40	0.93	0.08	29,44,57,64	0
30	BCR	B	618	40/40	0.93	0.09	24,48,68,80	0
26	LMG	D	408	51/55	0.93	0.11	34,66,92,114	0
30	BCR	D	406	40/40	0.93	0.09	35,50,88,108	0
22	CLA	c	511	65/65	0.94	0.10	41,62,80,90	0
30	BCR	c	514	40/40	0.94	0.09	35,51,69,74	0
22	CLA	C	512	65/65	0.94	0.09	40,61,96,105	0
22	CLA	C	510	65/65	0.94	0.08	30,50,68,81	0
30	BCR	C	515	40/40	0.94	0.10	42,60,73,75	0
22	CLA	c	506	65/65	0.94	0.09	34,56,106,111	0
28	LHG	b	623	49/49	0.94	0.10	38,58,85,104	0
30	BCR	I	101	40/40	0.94	0.07	22,40,52,54	0
28	LHG	d	409	39/49	0.94	0.09	37,55,73,83	0
30	BCR	B	616	40/40	0.94	0.08	30,46,69,72	0
30	BCR	T	101	40/40	0.94	0.07	30,46,61,66	0
30	BCR	a	406	40/40	0.94	0.07	24,38,59,64	0
30	BCR	b	617	40/40	0.94	0.08	34,48,64,67	0
30	BCR	b	618	40/40	0.94	0.07	29,44,61,68	0
22	CLA	a	405	65/65	0.95	0.08	20,44,90,104	0
22	CLA	C	503	65/65	0.95	0.07	31,49,59,63	0
22	CLA	b	606	65/65	0.95	0.08	29,47,83,90	0
22	CLA	b	609	65/65	0.95	0.08	31,54,74,77	0
22	CLA	b	612	65/65	0.95	0.07	27,40,54,58	0
22	CLA	b	615	65/65	0.95	0.08	27,47,67,74	0
22	CLA	b	616	60/65	0.95	0.09	31,48,93,99	0
22	CLA	c	502	65/65	0.95	0.07	30,49,69,76	0
22	CLA	c	503	65/65	0.95	0.08	34,50,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	C	506	65/65	0.95	0.08	28,50,90,108	0
22	CLA	c	508	64/65	0.95	0.08	36,56,98,124	0
22	CLA	c	509	65/65	0.95	0.09	32,54,74,84	0
22	CLA	C	508	65/65	0.95	0.08	29,48,112,124	0
22	CLA	C	509	65/65	0.95	0.08	31,51,68,77	0
22	CLA	B	605	65/65	0.95	0.08	29,45,82,98	0
22	CLA	d	405	65/65	0.95	0.08	32,56,101,116	0
23	PHO	D	401	64/64	0.95	0.06	26,39,51,54	0
23	PHO	d	401	64/64	0.95	0.07	25,43,55,67	0
22	CLA	C	511	65/65	0.95	0.09	34,59,80,85	0
28	LHG	D	410	49/49	0.95	0.08	31,47,58,65	0
28	LHG	D	411	47/49	0.95	0.10	27,54,84,95	0
25	PL9	D	407	55/55	0.95	0.07	26,39,57,63	0
22	CLA	B	614	65/65	0.95	0.08	26,42,69,86	0
30	BCR	t	101	40/40	0.95	0.06	28,44,55,63	0
25	PL9	d	407	55/55	0.95	0.07	25,40,54,60	0
22	CLA	B	615	60/65	0.95	0.09	23,43,96,105	0
29	DGD	C	516	62/66	0.95	0.10	28,48,85,107	0
22	CLA	C	502	65/65	0.95	0.07	29,48,70,79	0
29	DGD	C	518	62/66	0.95	0.08	33,57,77,94	0
22	CLA	a	403	65/65	0.95	0.09	29,47,106,117	0
33	BCT	d	402	4/4	0.95	0.08	35,40,52,62	0
22	CLA	d	404	65/65	0.96	0.07	22,37,47,53	0
28	LHG	D	413	49/49	0.96	0.08	32,48,80,93	0
22	CLA	C	504	59/65	0.96	0.08	30,49,95,100	0
23	PHO	A	404	64/64	0.96	0.06	15,35,45,47	0
28	LHG	d	408	49/49	0.96	0.08	28,48,60,65	0
22	CLA	C	505	65/65	0.96	0.08	27,47,75,82	0
28	LHG	l	101	49/49	0.96	0.08	34,50,65,71	0
23	PHO	a	404	64/64	0.96	0.06	24,37,46,47	0
22	CLA	b	602	65/65	0.96	0.08	31,48,68,71	0
22	CLA	b	603	65/65	0.96	0.07	26,43,82,91	0
22	CLA	b	604	65/65	0.96	0.08	24,45,87,105	0
22	CLA	b	605	65/65	0.96	0.07	24,39,59,63	0
29	DGD	c	515	62/66	0.96	0.08	31,49,85,92	0
22	CLA	B	609	65/65	0.96	0.07	25,39,49,58	0
22	CLA	b	608	65/65	0.96	0.07	30,48,73,79	0
22	CLA	C	507	65/65	0.96	0.07	25,46,67,73	0
22	CLA	b	610	65/65	0.96	0.07	28,43,58,69	0
22	CLA	b	611	65/65	0.96	0.07	25,41,55,66	0
22	CLA	B	610	65/65	0.96	0.06	19,38,54,62	0
22	CLA	b	613	65/65	0.96	0.08	21,41,83,97	0

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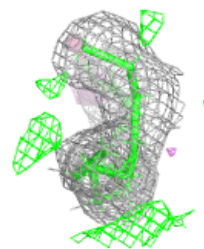
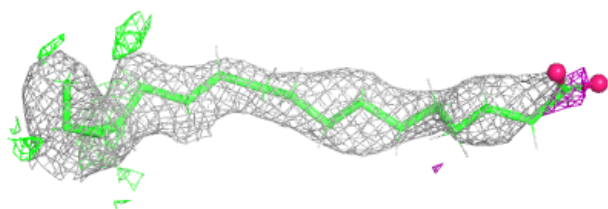
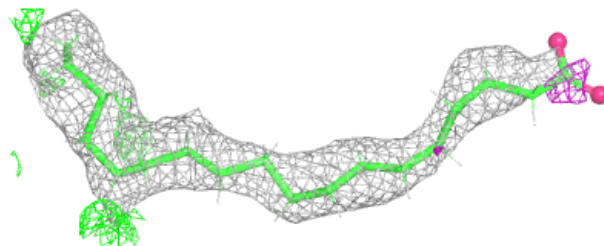
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	614	65/65	0.96	0.07	26,43,87,93	0
22	CLA	B	611	65/65	0.96	0.07	22,37,50,60	0
22	CLA	B	612	65/65	0.96	0.07	21,40,75,84	0
22	CLA	c	501	65/65	0.96	0.07	30,50,65,68	0
22	CLA	B	613	65/65	0.96	0.08	26,45,87,104	0
22	CLA	B	603	65/65	0.96	0.07	25,40,97,105	0
22	CLA	c	504	60/65	0.96	0.07	36,51,85,99	0
22	CLA	c	505	65/65	0.96	0.08	30,47,73,77	0
22	CLA	B	604	65/65	0.96	0.07	21,38,53,63	0
22	CLA	c	507	65/65	0.96	0.07	31,50,65,78	0
22	CLA	D	403	65/65	0.96	0.06	22,36,53,65	0
22	CLA	D	404	65/65	0.96	0.07	22,35,57,66	0
22	CLA	c	510	65/65	0.96	0.07	36,51,66,92	0
22	CLA	A	402	65/65	0.96	0.06	19,33,52,62	0
22	CLA	a	402	65/65	0.96	0.07	24,36,51,59	0
22	CLA	B	608	65/65	0.96	0.07	27,43,60,65	0
22	CLA	d	403	65/65	0.96	0.08	25,41,70,83	0
34	HEC	f	101	43/43	0.96	0.09	44,62,87,99	0
22	CLA	B	601	65/65	0.97	0.07	26,42,63,67	0
22	CLA	b	607	65/65	0.97	0.07	26,42,86,96	0
22	CLA	B	606	65/65	0.97	0.07	18,39,81,92	0
22	CLA	B	607	65/65	0.97	0.06	27,43,71,75	0
22	CLA	B	602	65/65	0.97	0.07	23,38,67,75	0
22	CLA	A	403	65/65	0.97	0.09	23,42,94,109	0
28	LHG	L	102	49/49	0.97	0.07	30,47,67,80	0
22	CLA	C	501	65/65	0.97	0.06	25,43,59,65	0
33	BCT	D	402	4/4	0.97	0.08	28,35,46,55	0
22	CLA	D	405	65/65	0.97	0.08	26,50,132,139	0
34	HEC	F	101	43/43	0.97	0.07	37,54,73,76	0
22	CLA	A	405	54/65	0.97	0.06	22,36,72,78	0
35	NA	V	202	1/1	0.97	0.10	61,61,61,61	0
24	CL	A	407	1/1	0.98	0.04	39,39,39,39	0
34	HEC	v	201	43/43	0.98	0.07	31,42,53,61	0
34	HEC	V	201	43/43	0.98	0.06	25,39,48,49	0
24	CL	a	407	1/1	0.99	0.03	34,34,34,34	0
24	CL	a	408	1/1	0.99	0.07	35,35,35,35	0
24	CL	A	406	1/1	0.99	0.04	35,35,35,35	0
32	OEX	C	522	10/10	0.99	0.03	26,33,37,38	0
32	OEX	a	415	10/10	0.99	0.03	26,34,36,40	0
21	FE2	A	401	1/1	0.99	0.03	32,32,32,32	0
21	FE2	a	401	1/1	1.00	0.02	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

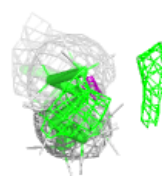
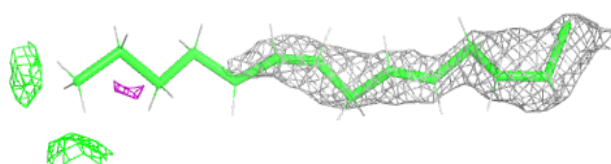
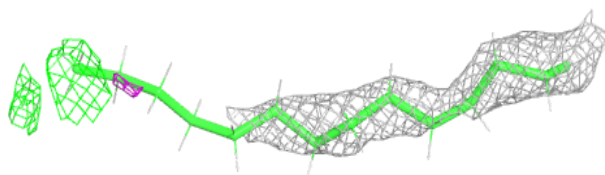
Electron density around STE b 629:

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

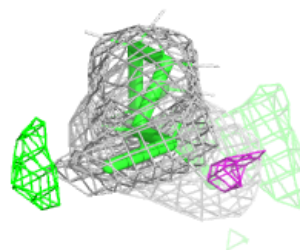
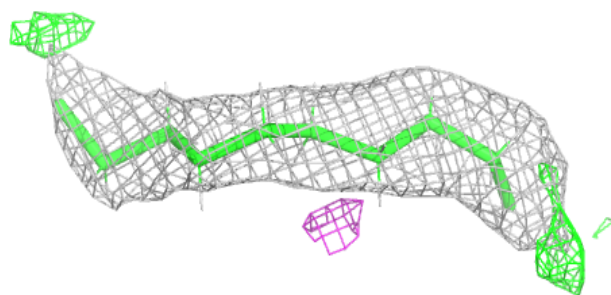
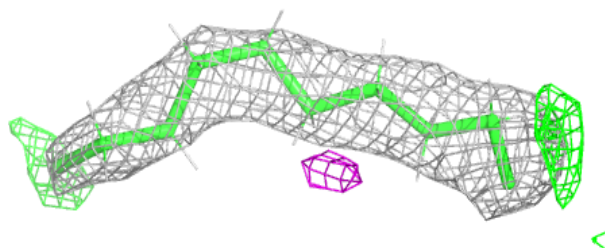


Electron density around STE b 628:

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

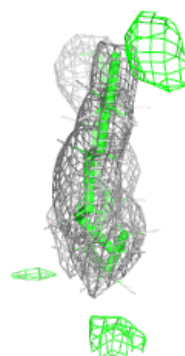
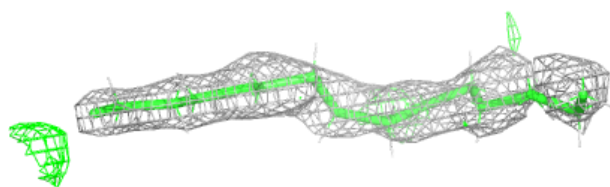
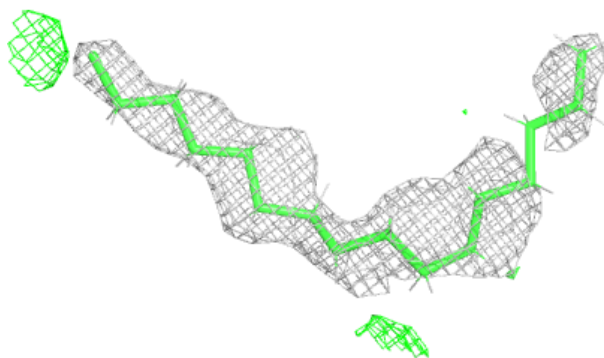
**Electron density around STE b 627:**

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

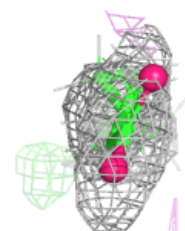
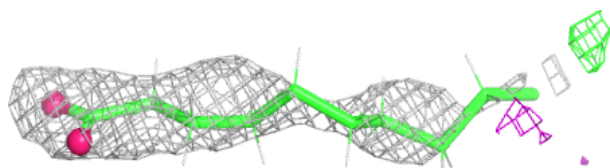
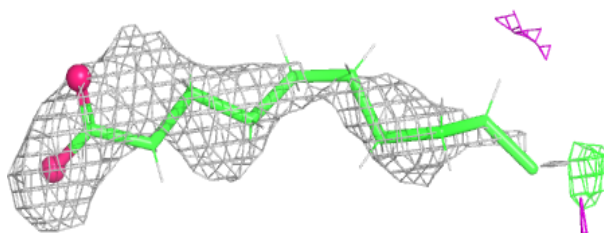


Electron density around STE B 624:

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

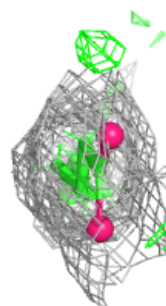
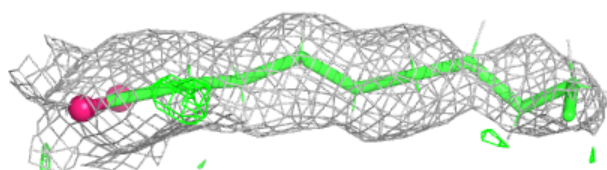
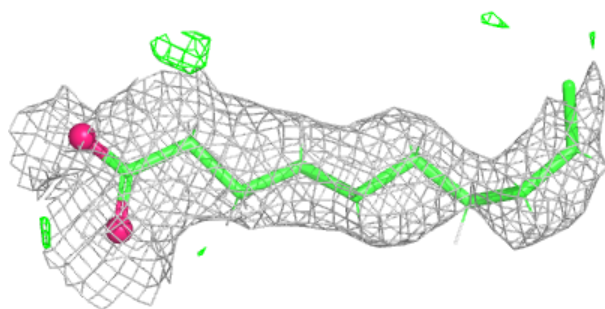
**Electron density around STE a 412:**

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

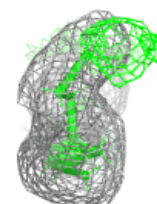
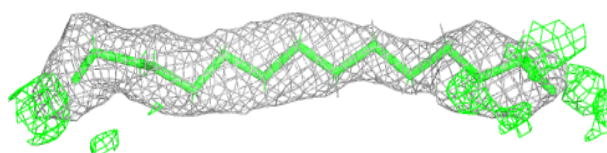
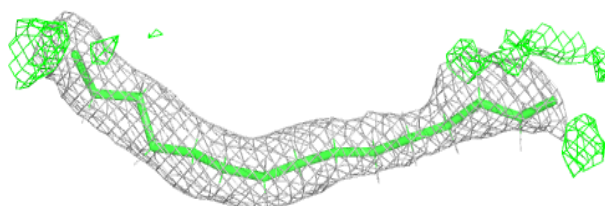


Electron density around STE k 104:

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

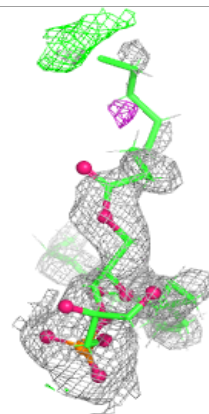
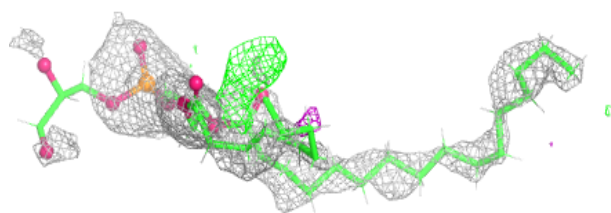
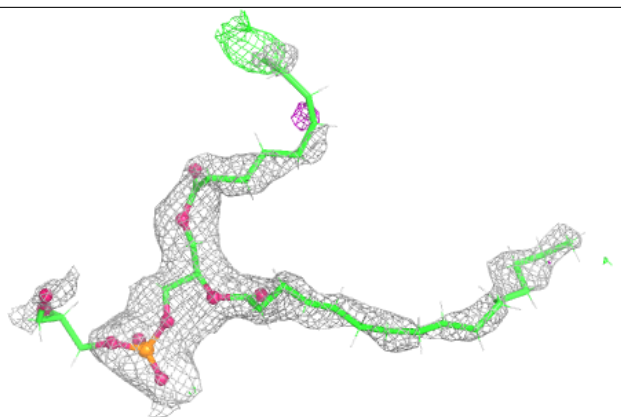
**Electron density around STE I 102:**

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

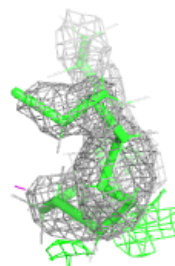
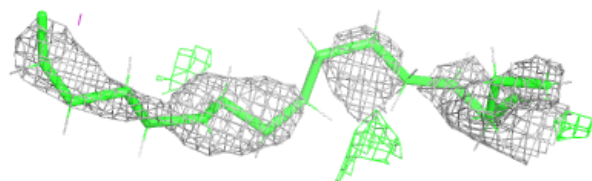
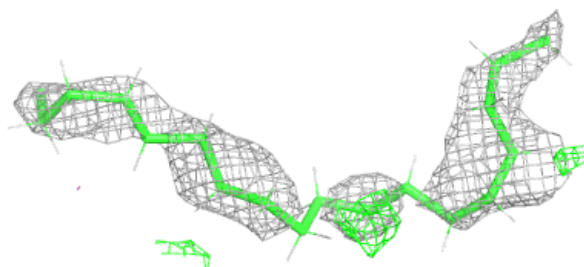


Electron density around LHG a 411:

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

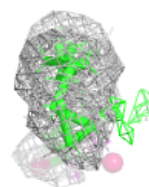
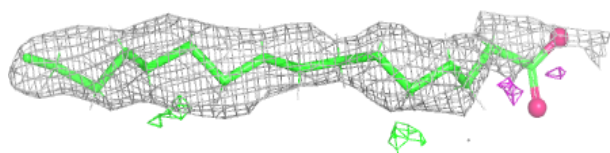
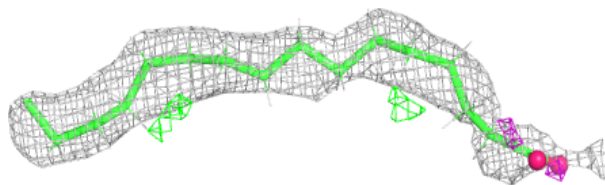
**Electron density around STE H 104:**

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

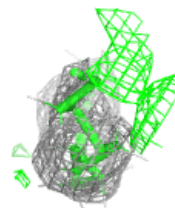
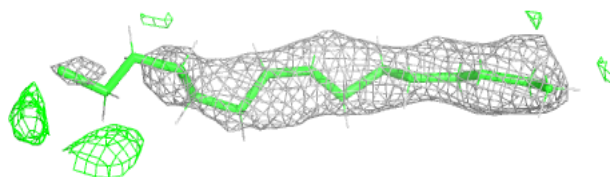
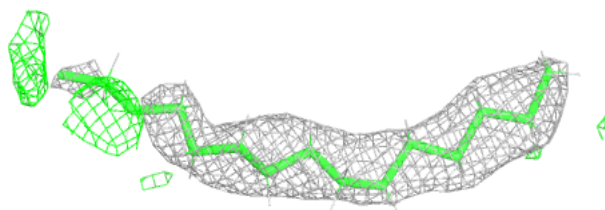


Electron density around STE B 623:

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

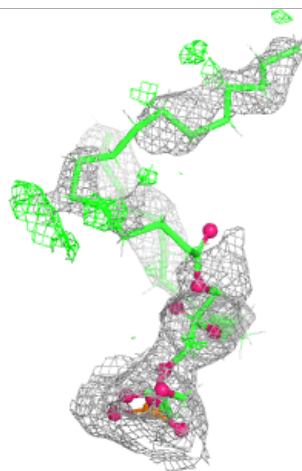
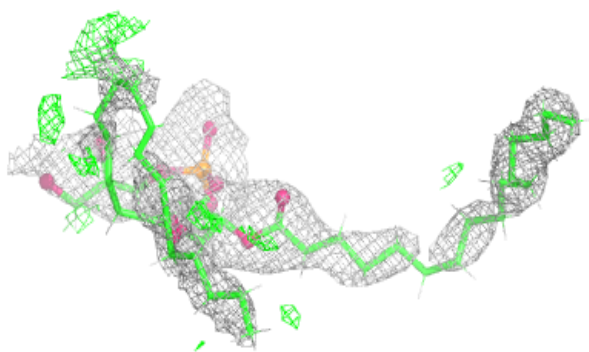
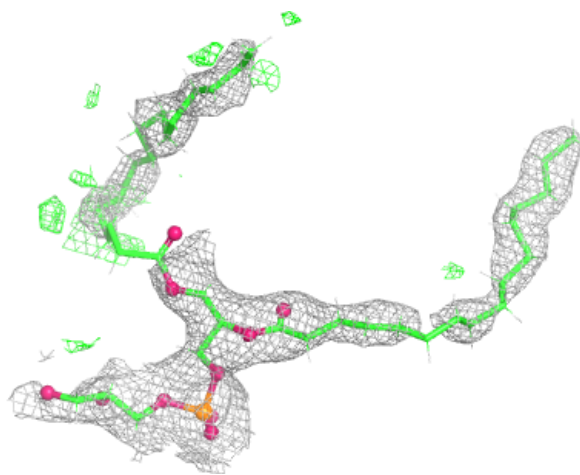
**Electron density around STE b 625:**

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



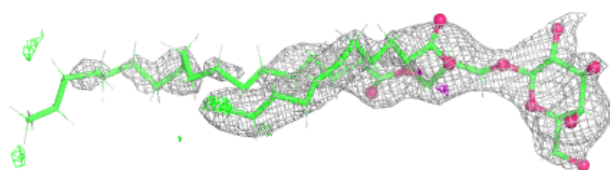
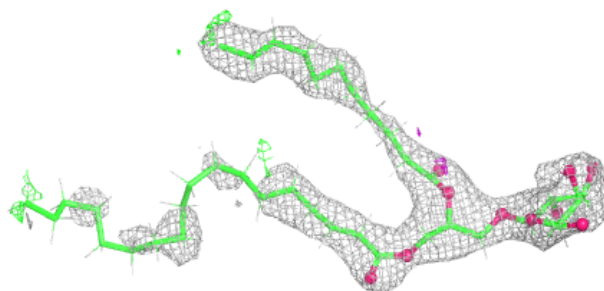
Electron density around LHG A 411:

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

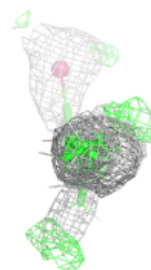
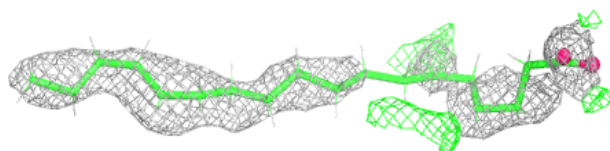
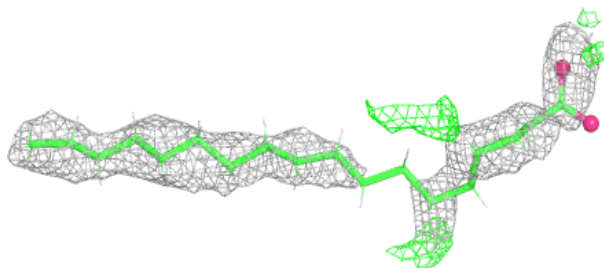


Electron density around LMG c 520:

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

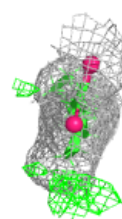
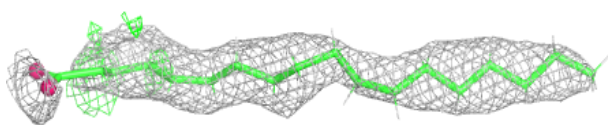
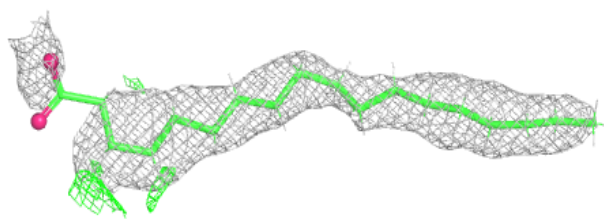
**Electron density around STE b 626:**

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

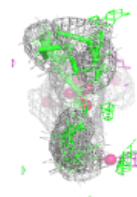
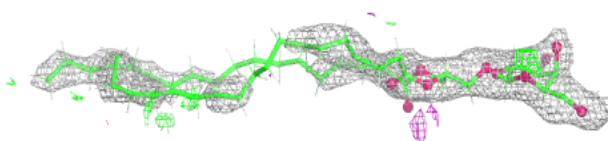
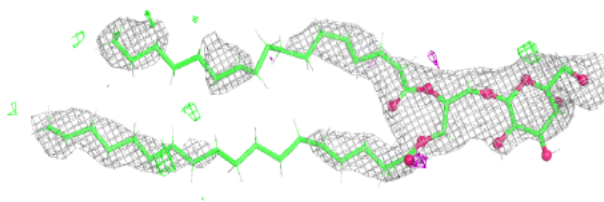


Electron density around STE c 519:

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

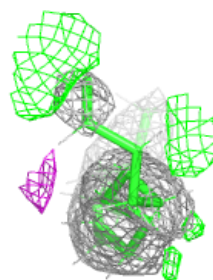
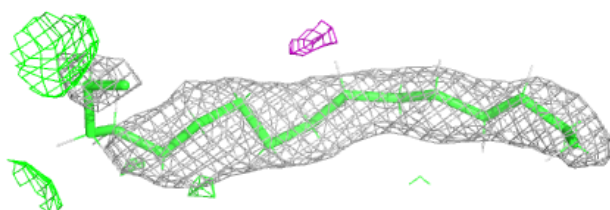
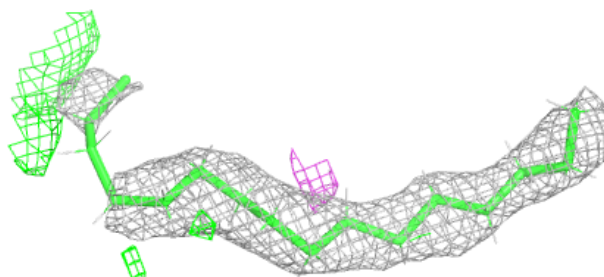
**Electron density around LMG b 622:**

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

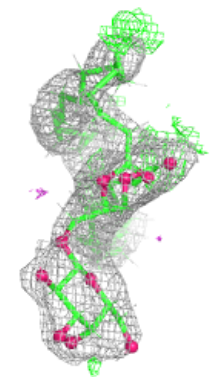
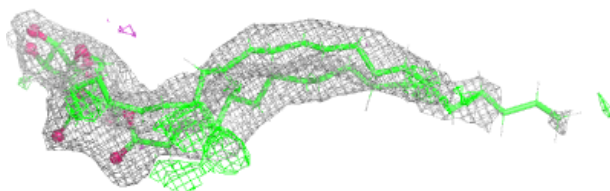
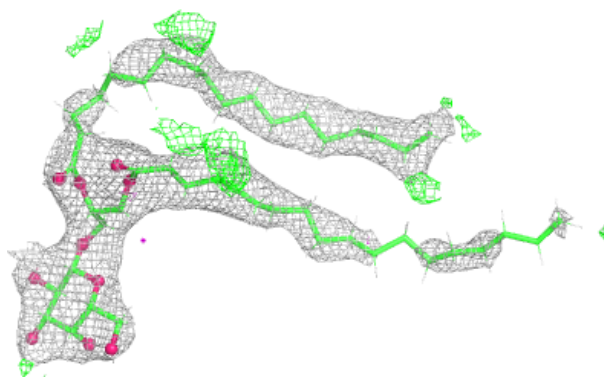


Electron density around STE b 620:

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

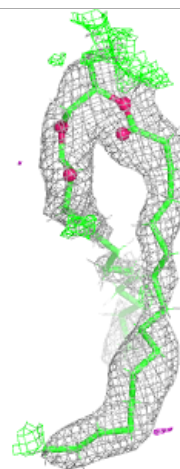
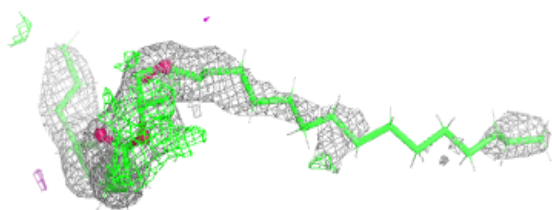
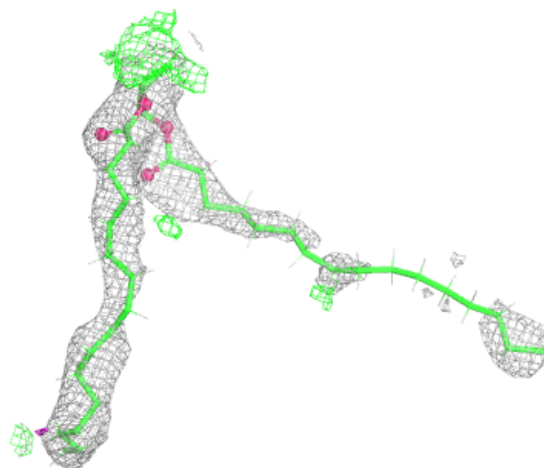
**Electron density around LMG a 414:**

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



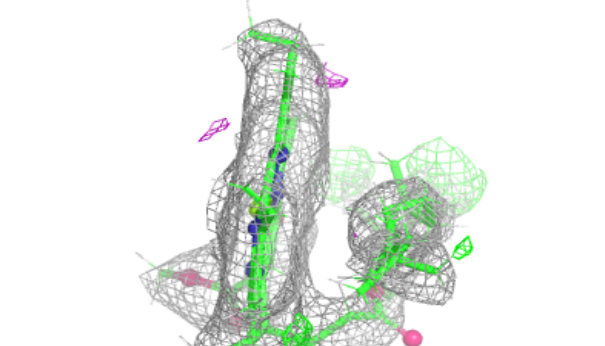
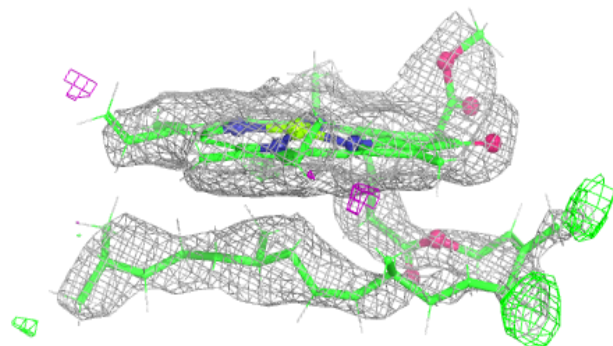
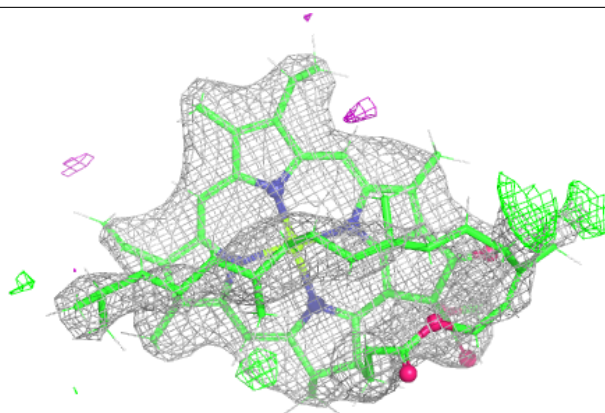
Electron density around SQD A 412:

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

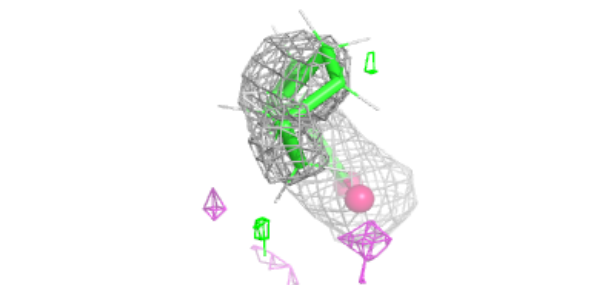
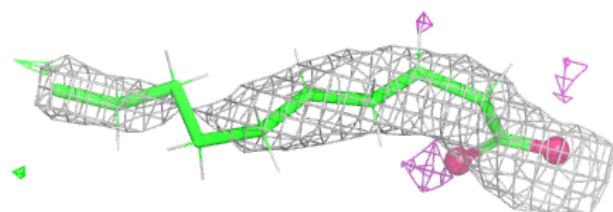
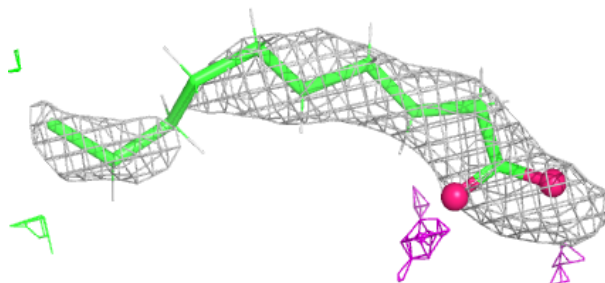


Electron density around CLA b 601:

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and green (positive)

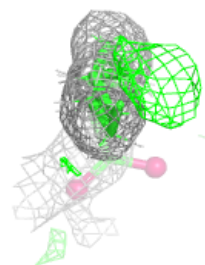
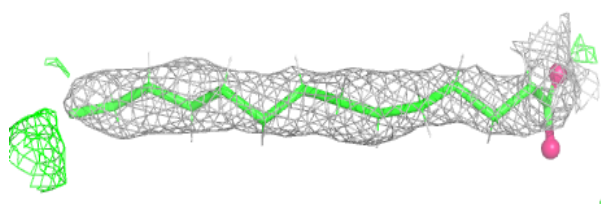
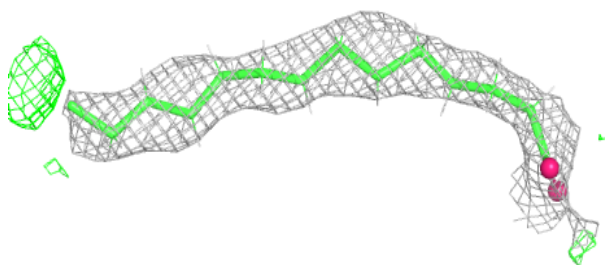
**Electron density around STE B 625:**

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

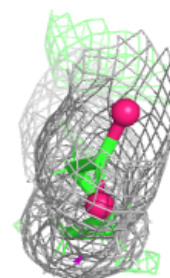
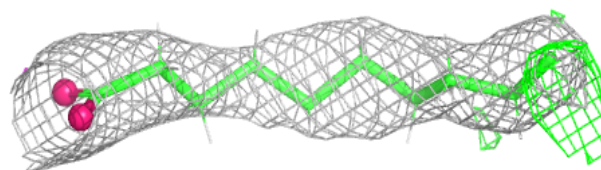
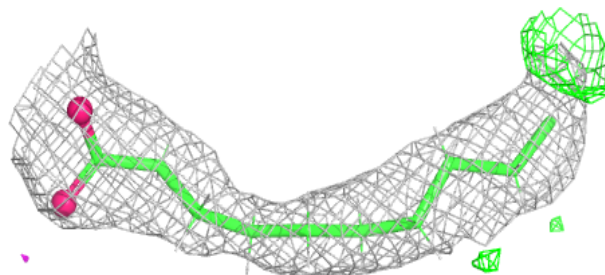


Electron density around STE b 624:

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

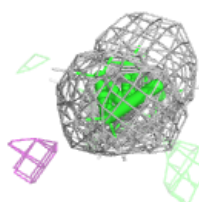
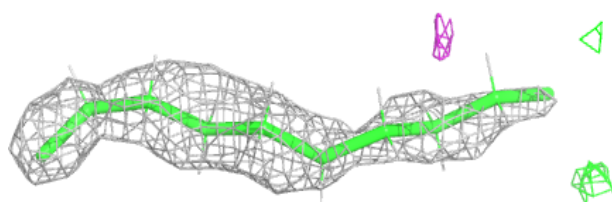
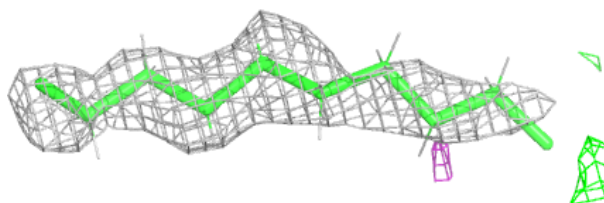
**Electron density around STE C 519:**

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

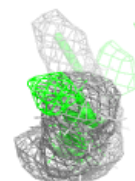
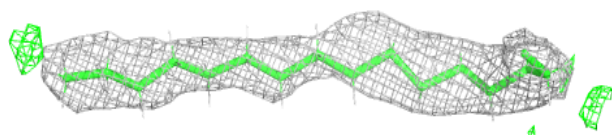
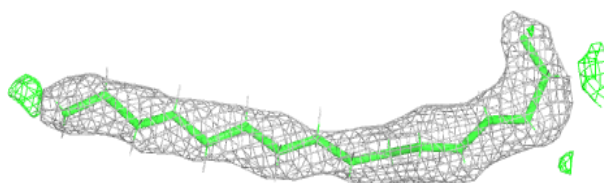


Electron density around STE t 104:

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

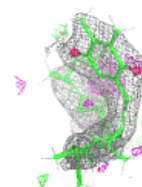
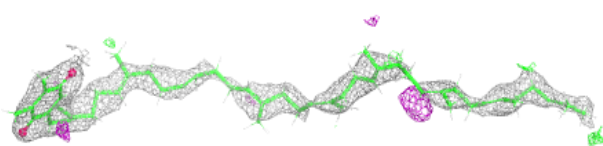
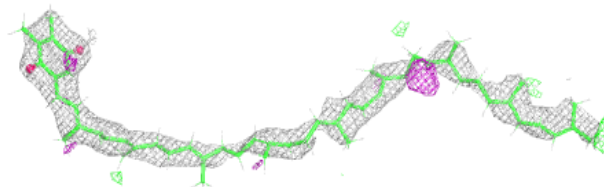
**Electron density around STE C 520:**

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

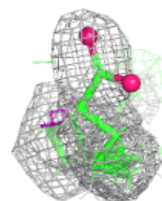
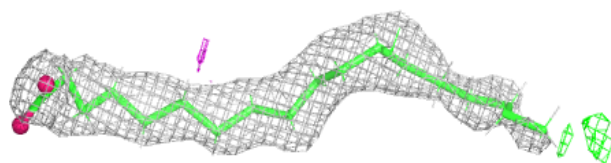
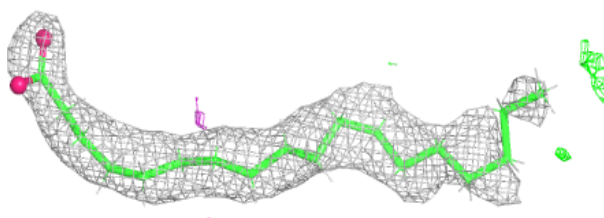


Electron density around PL9 A 408:

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

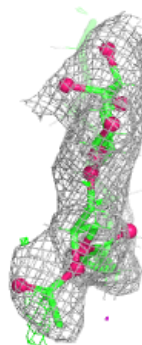
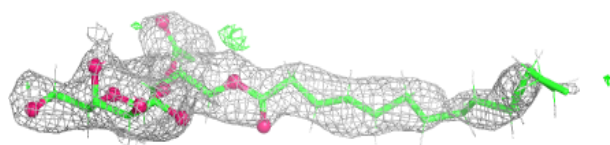
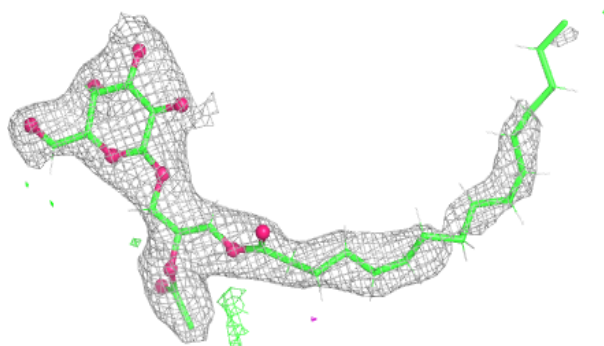
**Electron density around STE b 621:**

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

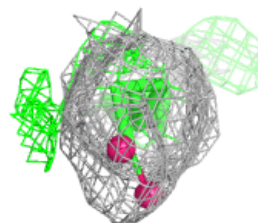
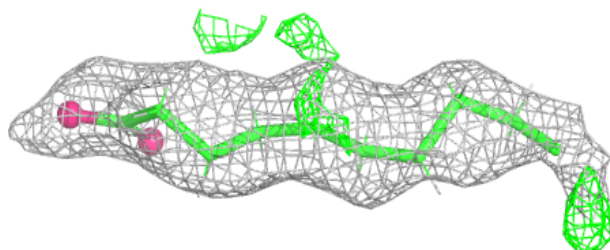
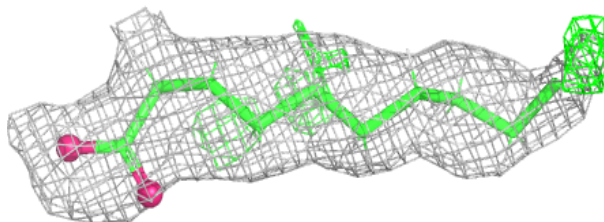


Electron density around LMG c 518:

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

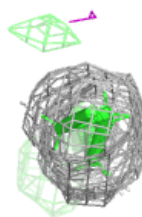
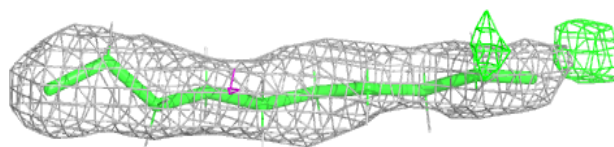
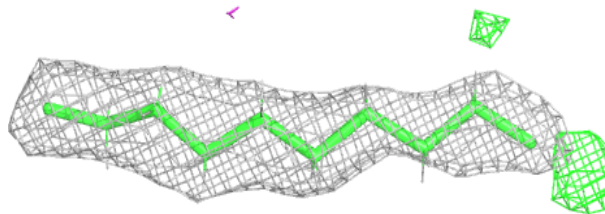
**Electron density around STE J 101:**

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

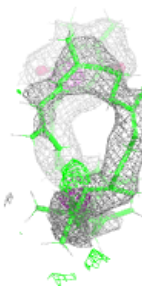
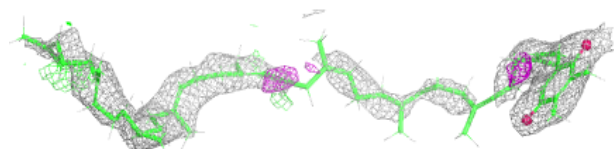
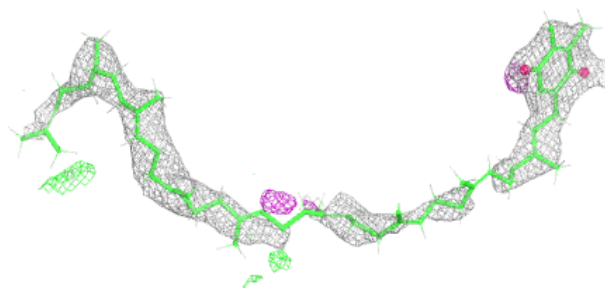


Electron density around STE M 103:

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

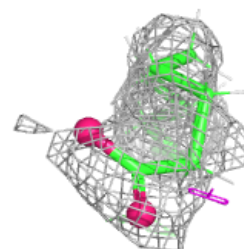
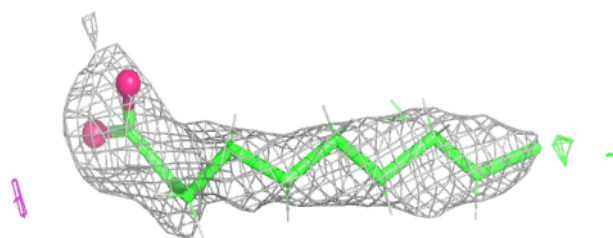
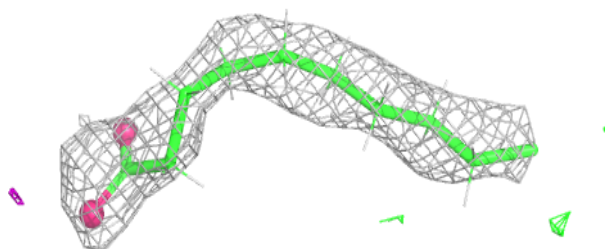
**Electron density around PL9 a 409:**

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

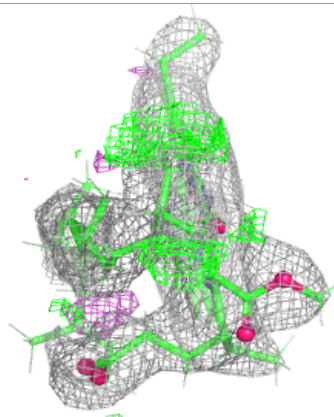
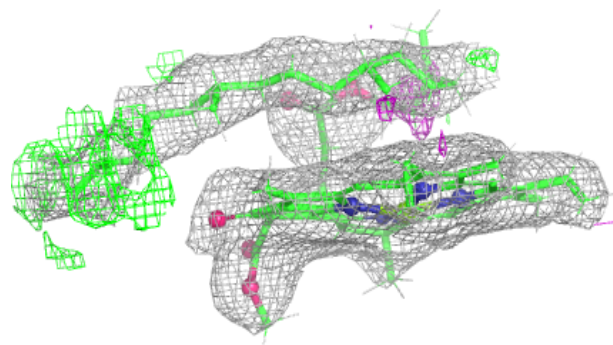
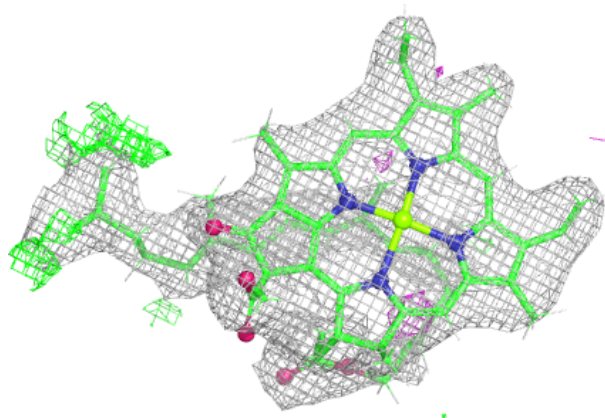


Electron density around STE R 101:

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

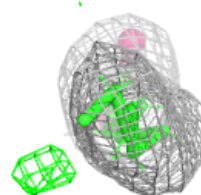
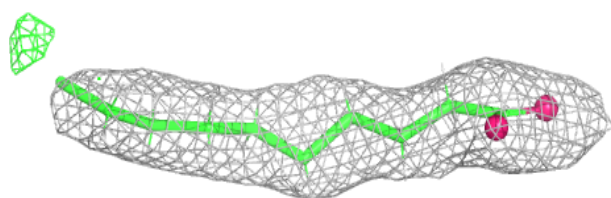
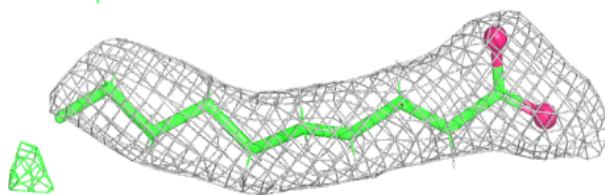
**Electron density around CLA H 101:**

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

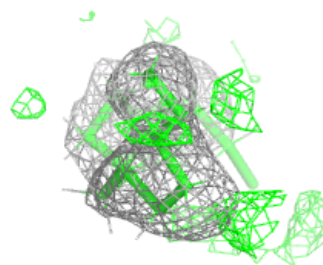
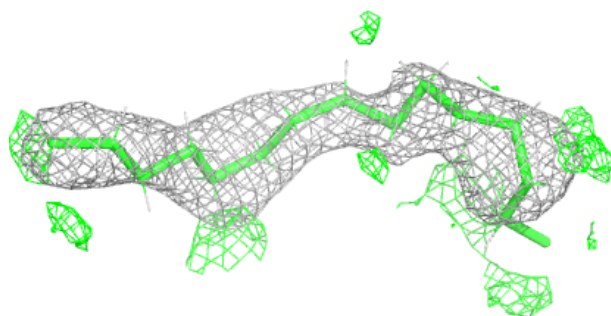
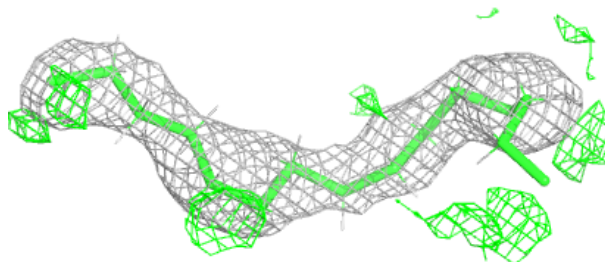


Electron density around STE j 101:

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

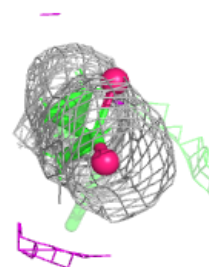
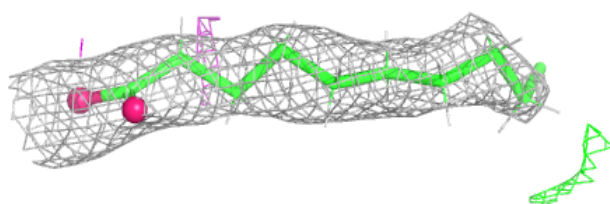
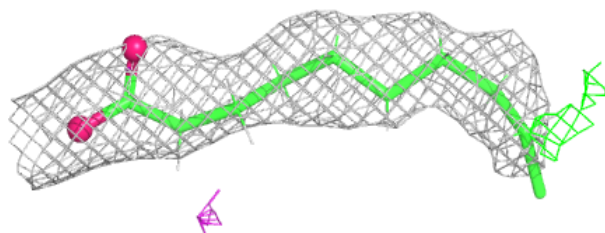
**Electron density around STE a 413:**

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

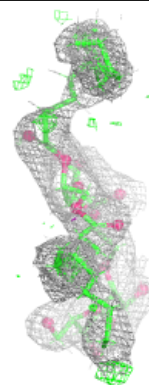
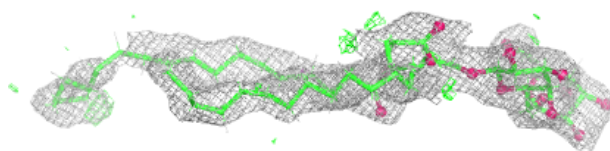
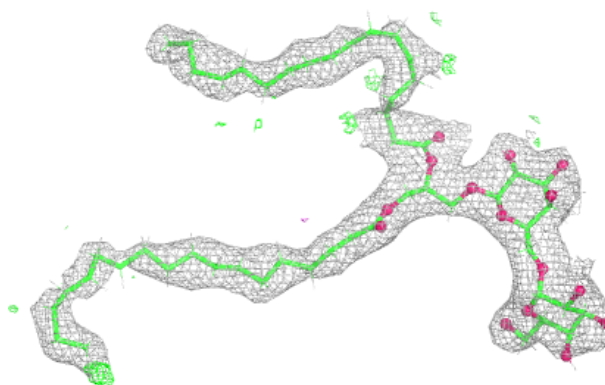


Electron density around STE L 103:

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

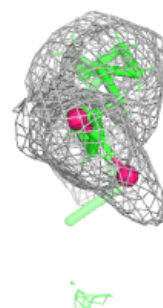
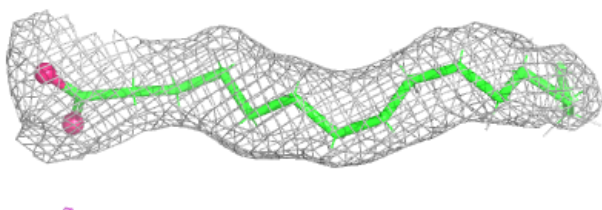
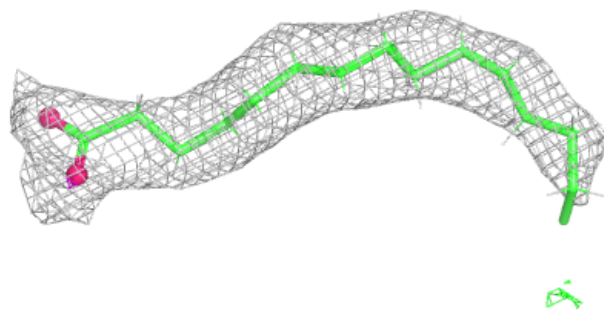
**Electron density around DGD A 413:**

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

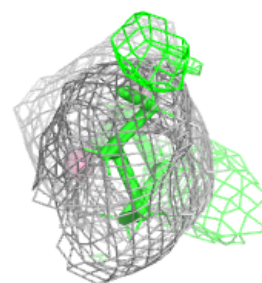
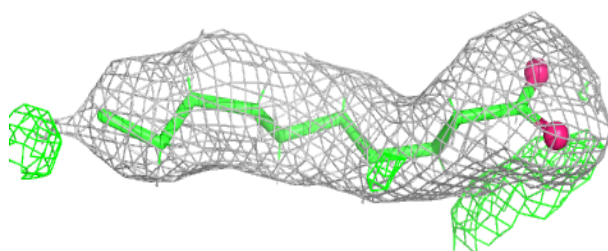
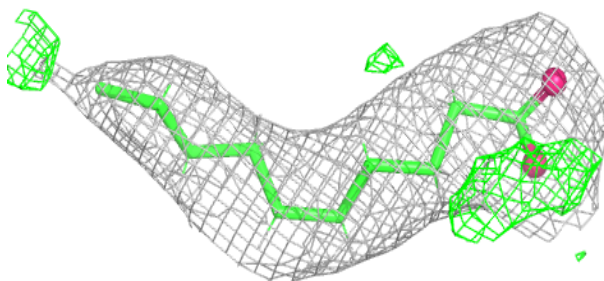


Electron density around STE B 619:

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

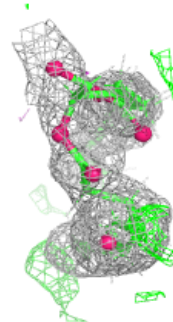
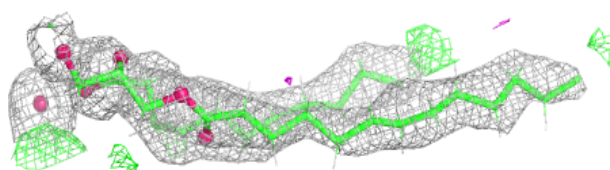
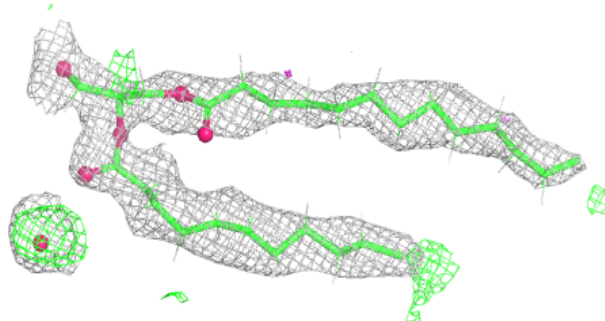
**Electron density around STE B 622:**

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

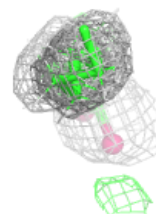
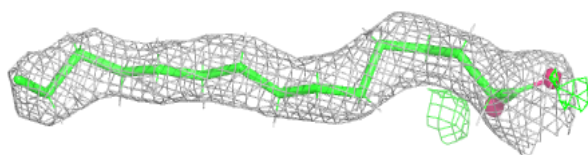
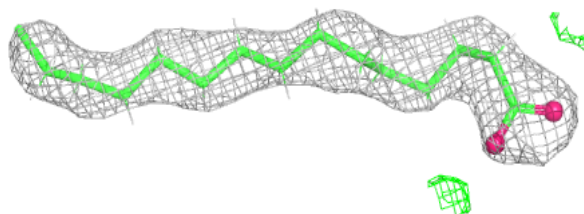


Electron density around LMG D 412:

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

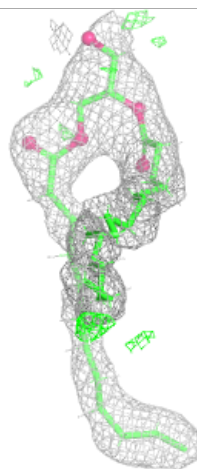
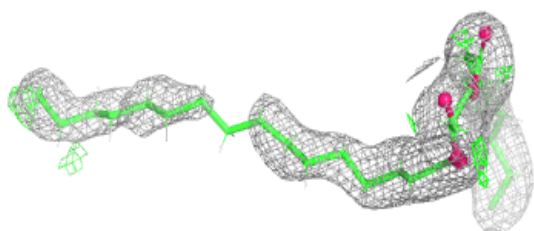
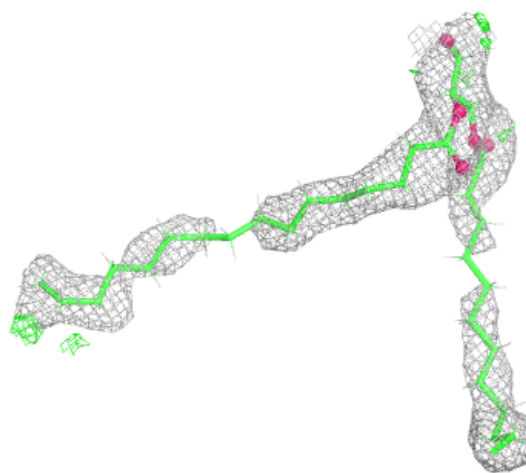
**Electron density around STE d 411:**

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



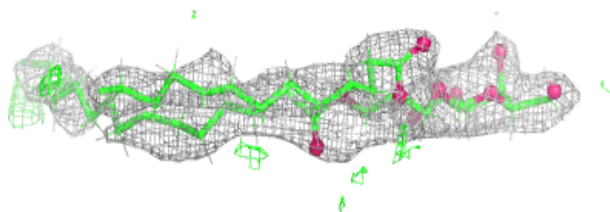
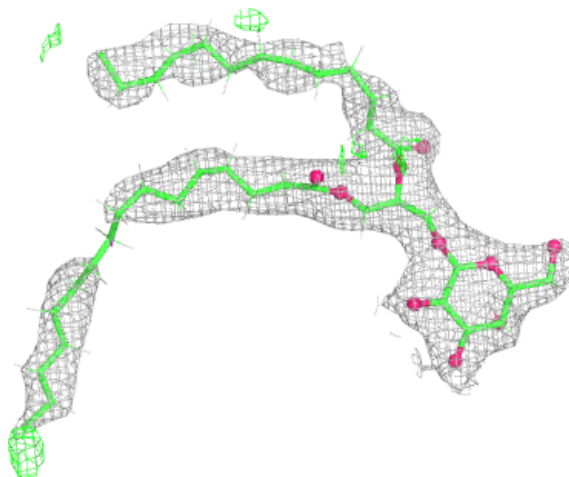
Electron density around SQD t 102:

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



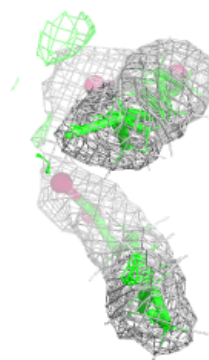
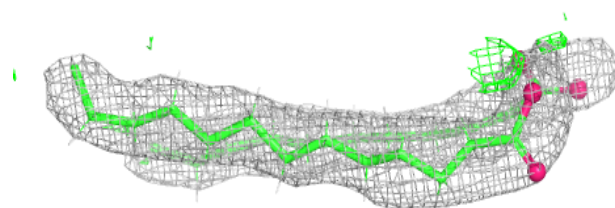
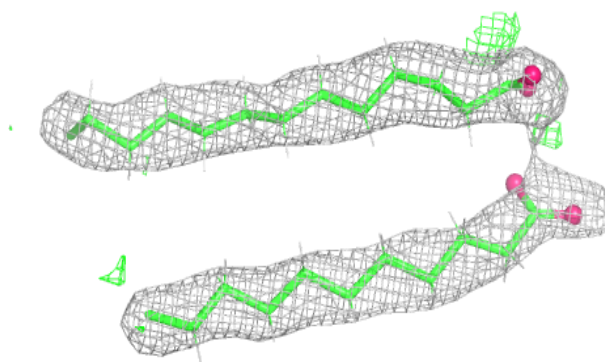
Electron density around LMG Y 101:

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

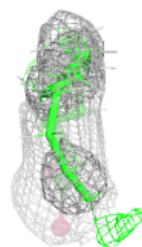
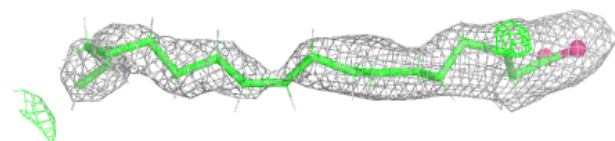
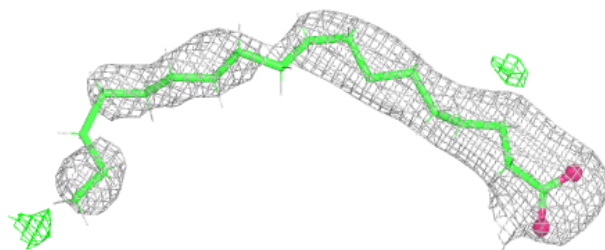


Electron density around LMG B 620:

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

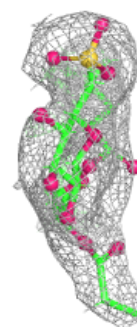
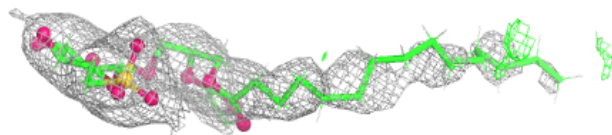
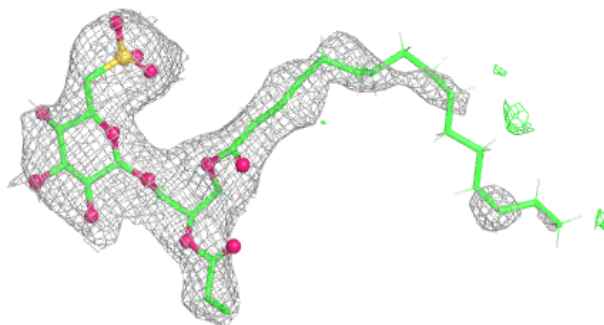
**Electron density around STE x 102:**

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

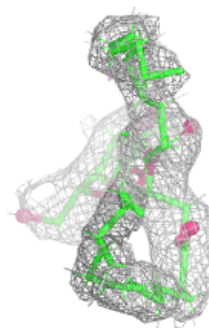
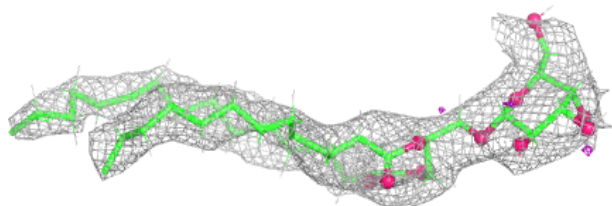
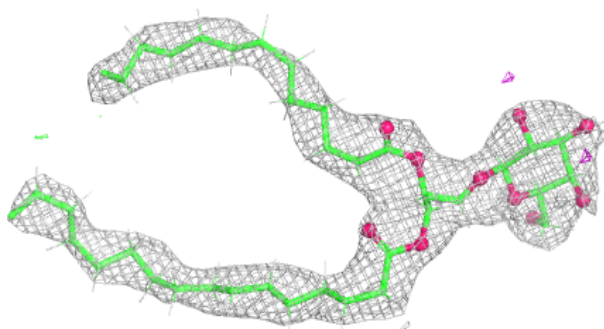


Electron density around SQD f 102:

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

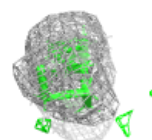
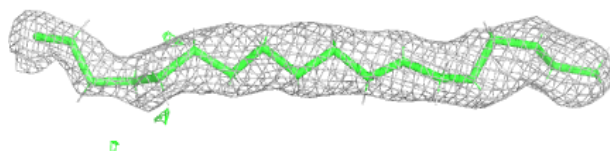
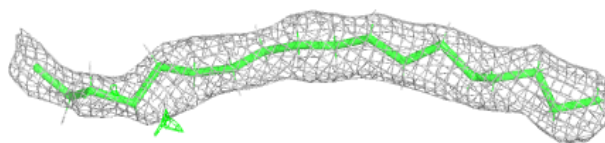
**Electron density around LMG A 409:**

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

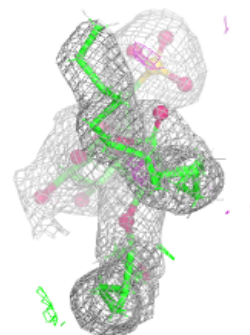
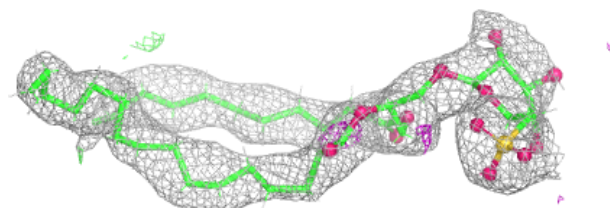
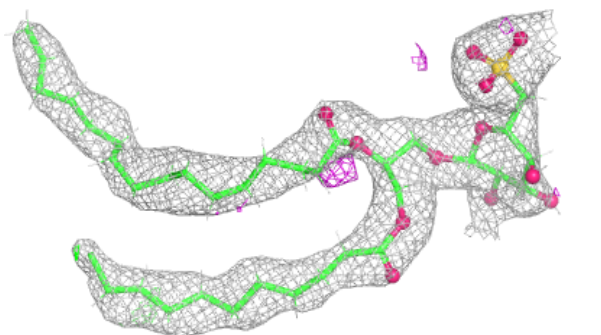


Electron density around STE M 104:

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

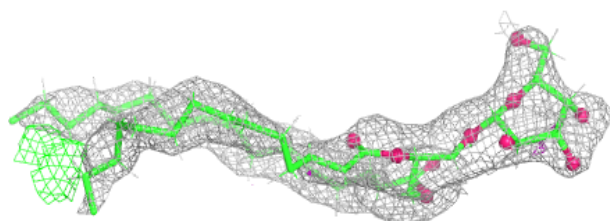
**Electron density around SQD L 101:**

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

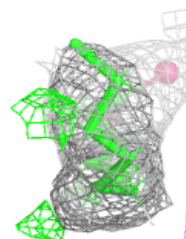
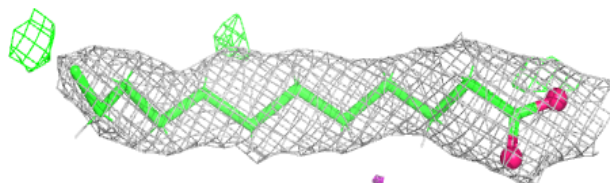
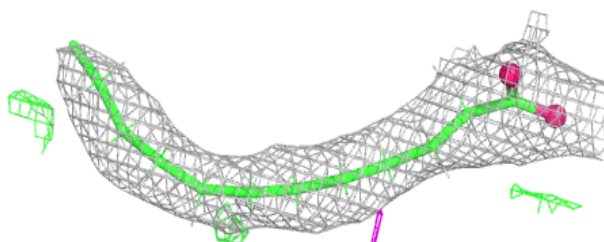


Electron density around LMG c 521:

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

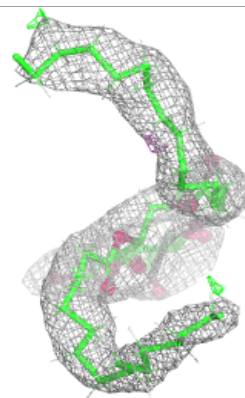
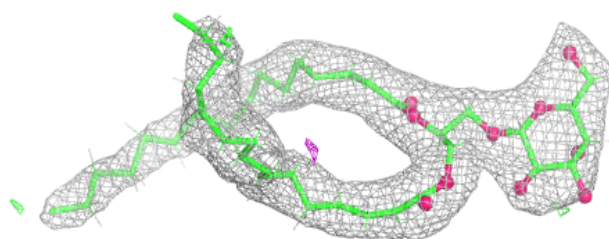
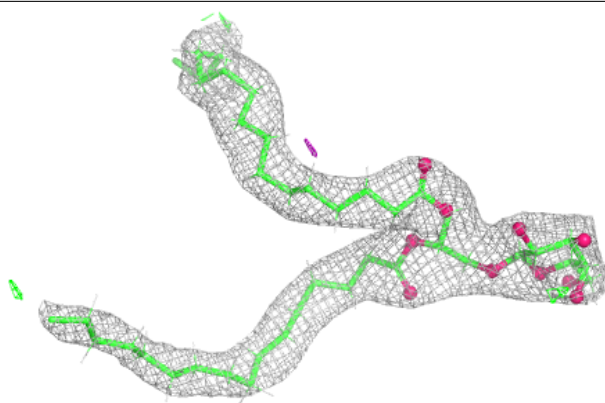
**Electron density around STE t 103:**

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

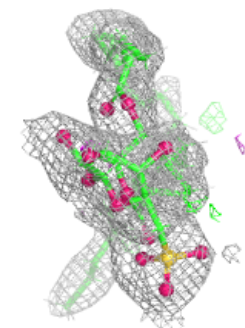
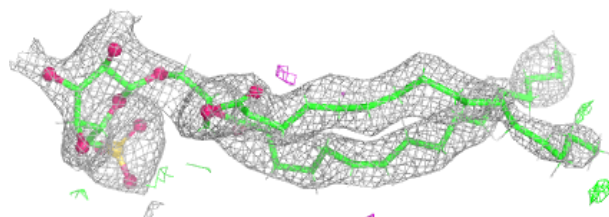
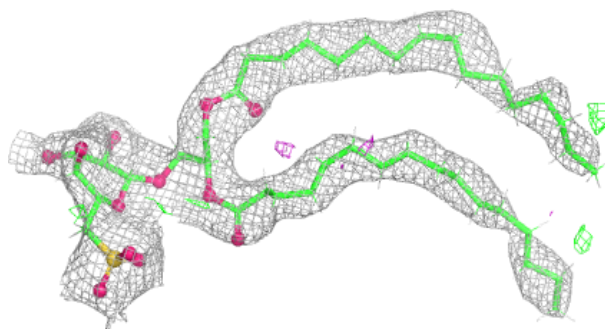


Electron density around LMG M 101:

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

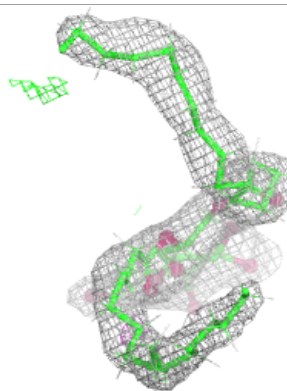
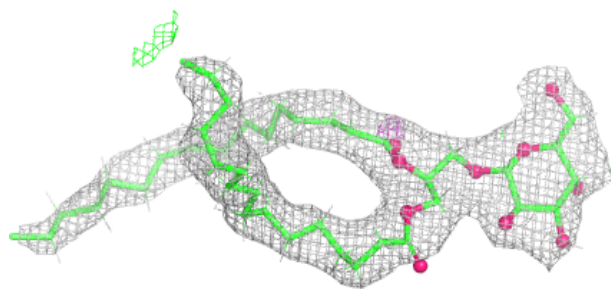
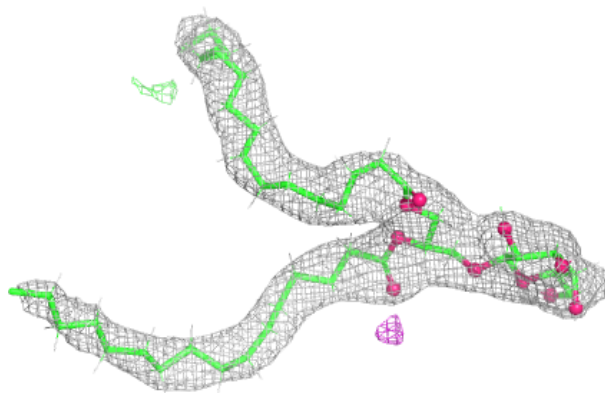
**Electron density around SQD B 621:**

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

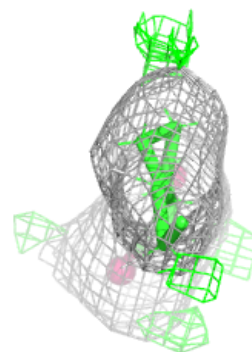
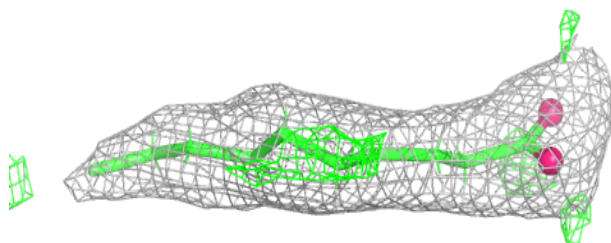
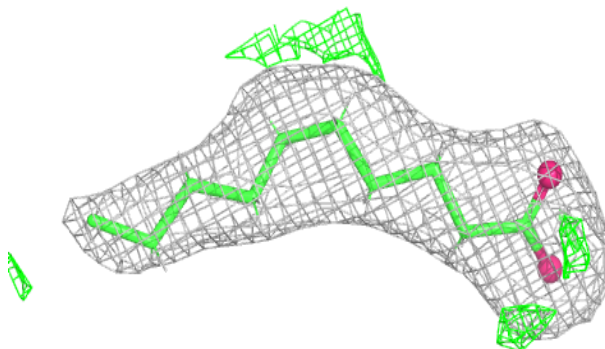


Electron density around LMG m 101:

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

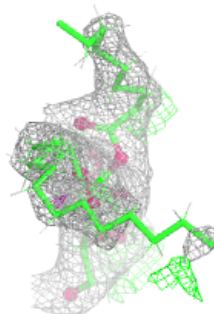
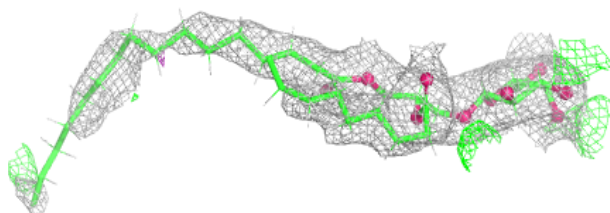
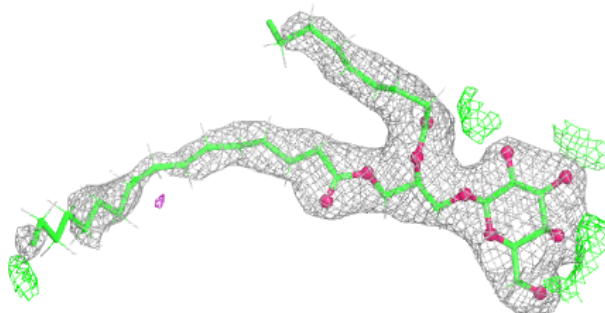
**Electron density around STE C 521:**

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

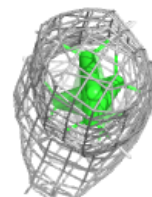
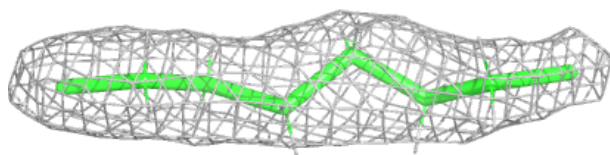
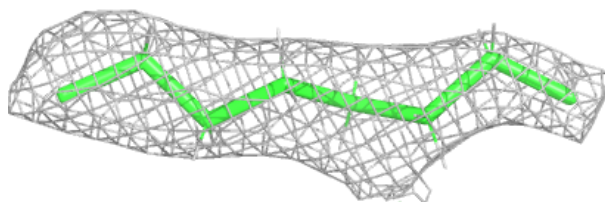


Electron density around LMG d 410:

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

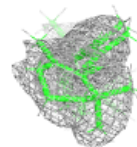
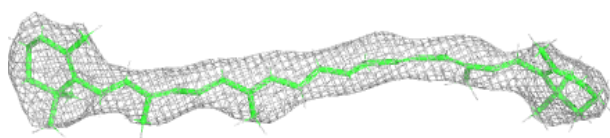
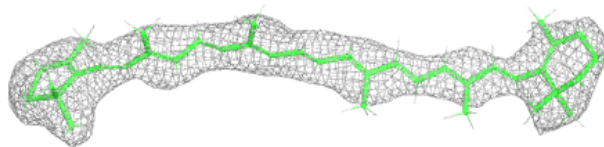
**Electron density around STE Z 101:**

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

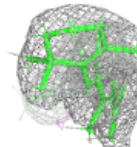
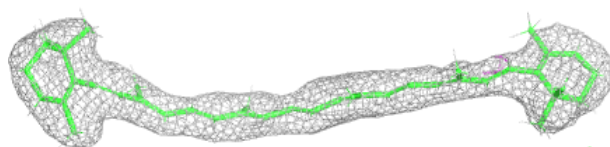
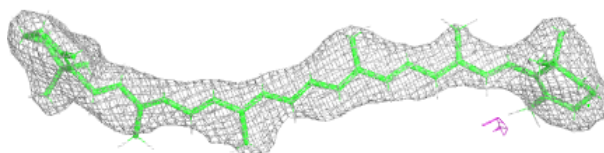


Electron density around BCR k 101:

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

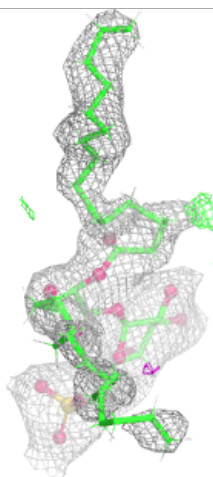
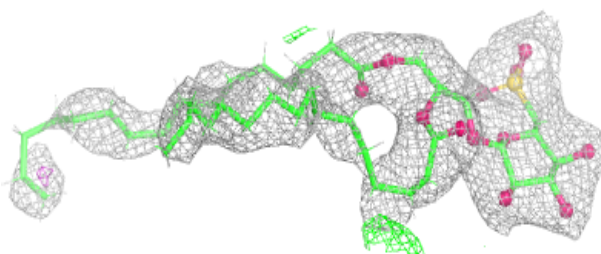
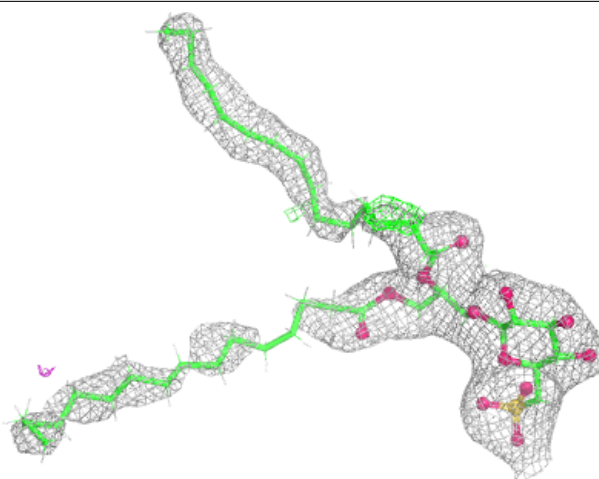
**Electron density around BCR x 101:**

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



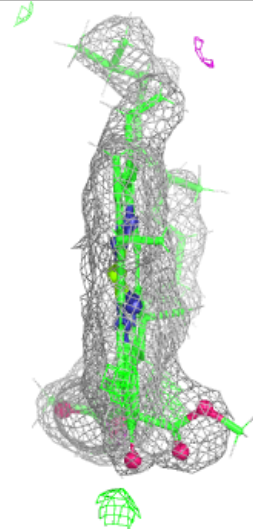
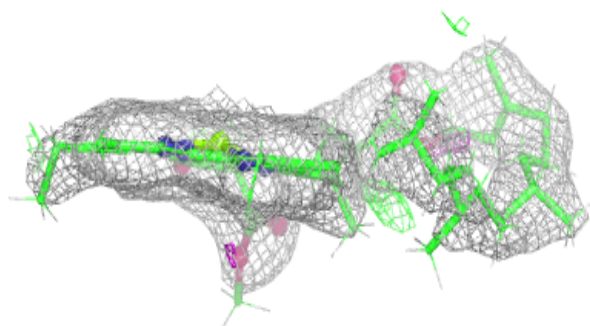
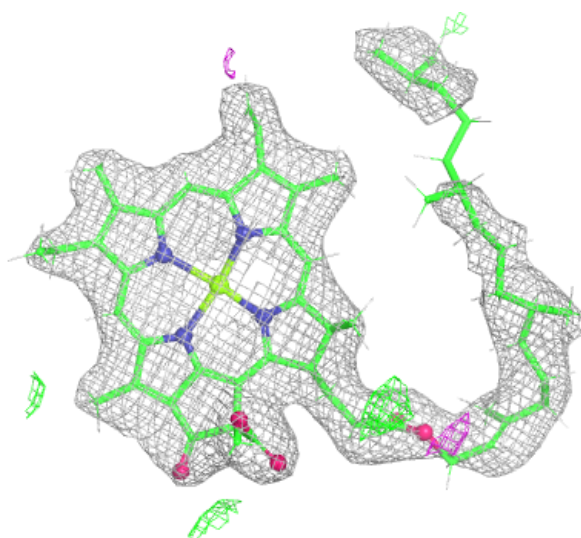
Electron density around SQD a 410:

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



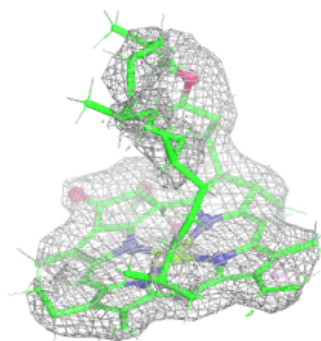
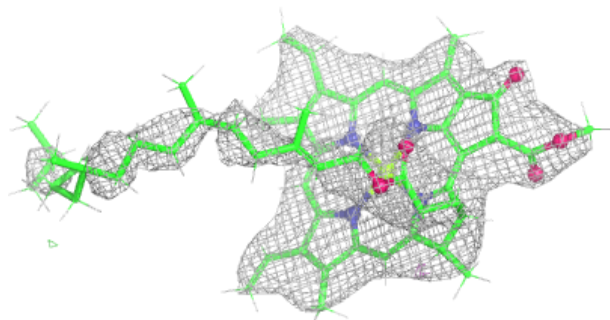
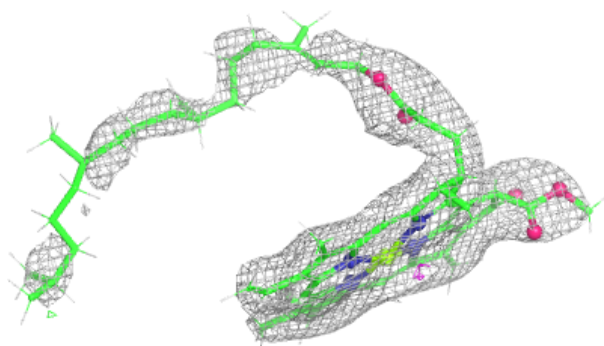
Electron density around CLA c 512:

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

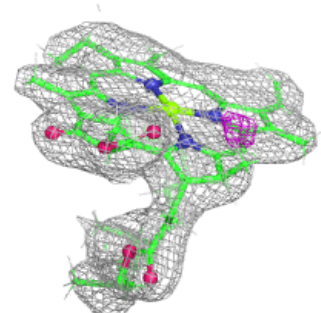
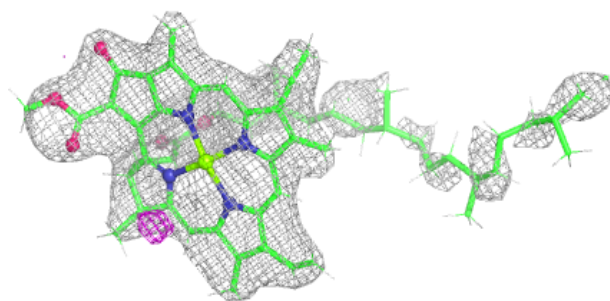
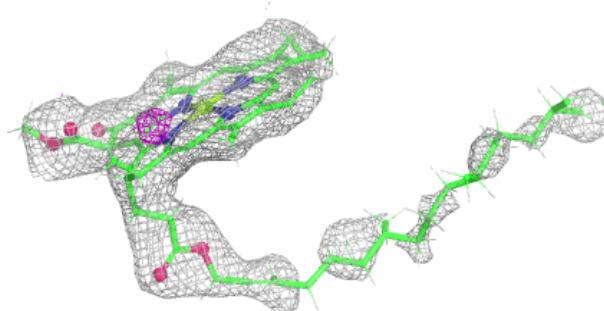


Electron density around CLA c 513:

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

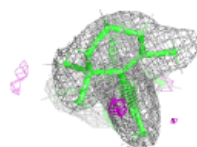
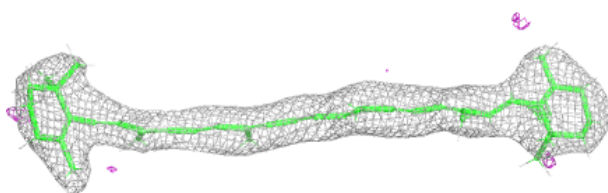
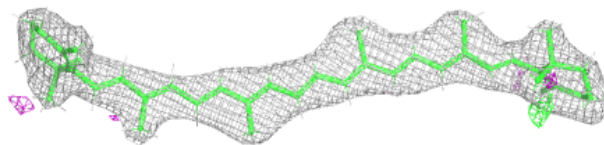
**Electron density around CLA C 513:**

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

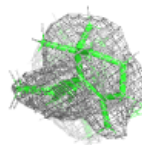
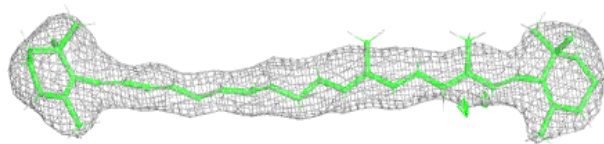


Electron density around BCR C 514:

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

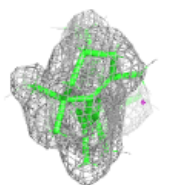
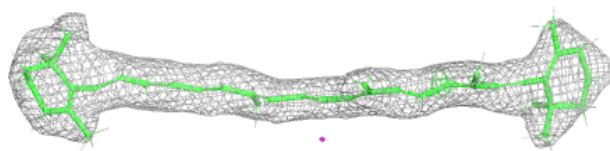
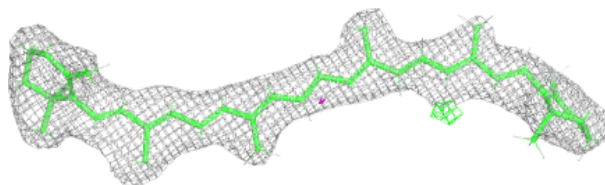
**Electron density around BCR K 101:**

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

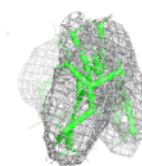
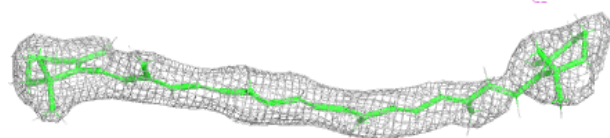
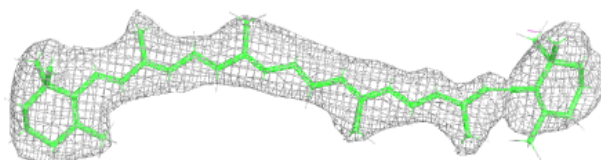


Electron density around BCR K 102:

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

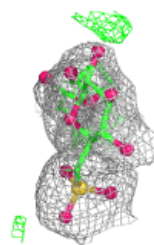
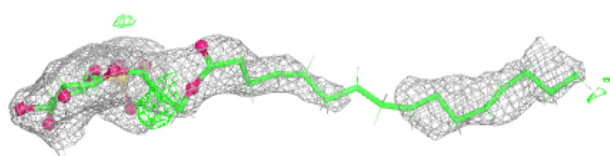
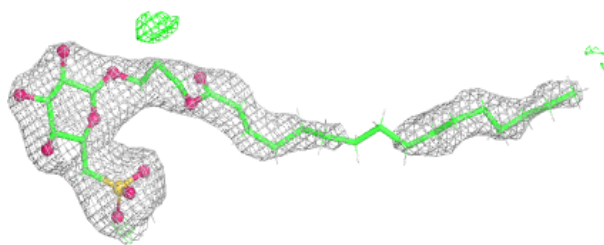
**Electron density around BCR d 406:**

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

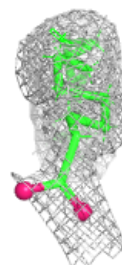
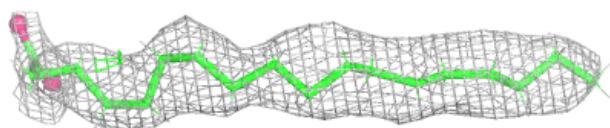
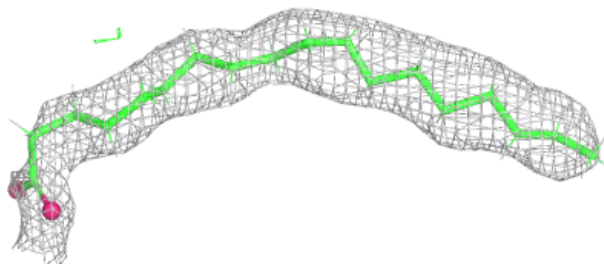


Electron density around SQD D 409:

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

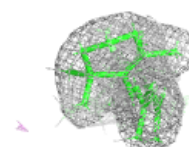
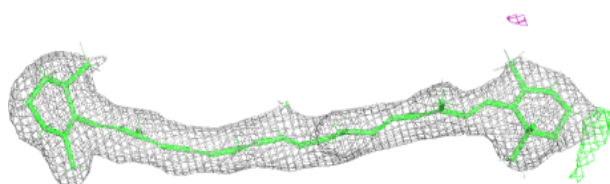
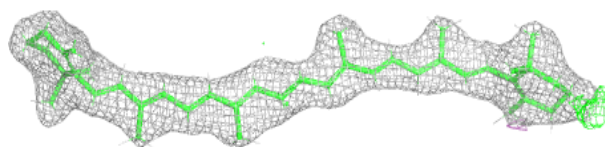
**Electron density around STE X 101:**

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

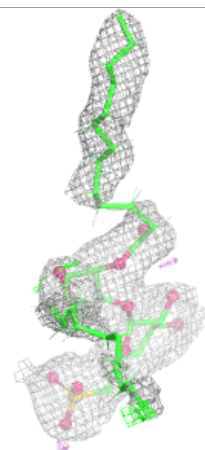
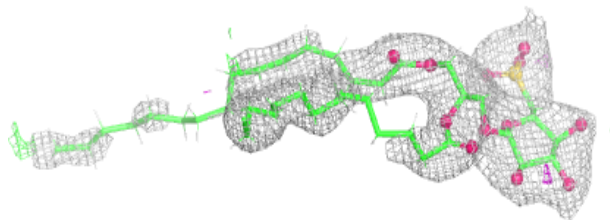
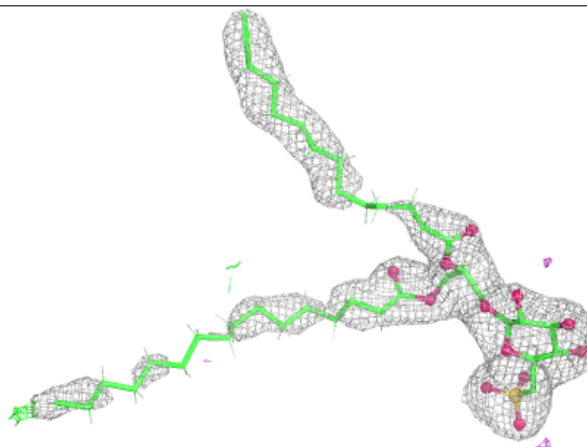


Electron density around BCR H 102:

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

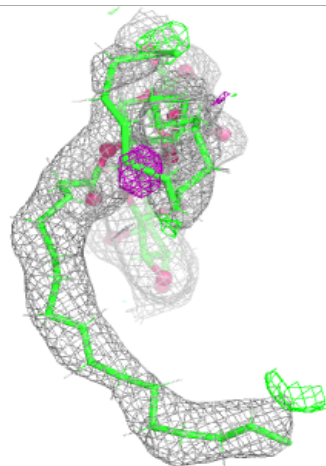
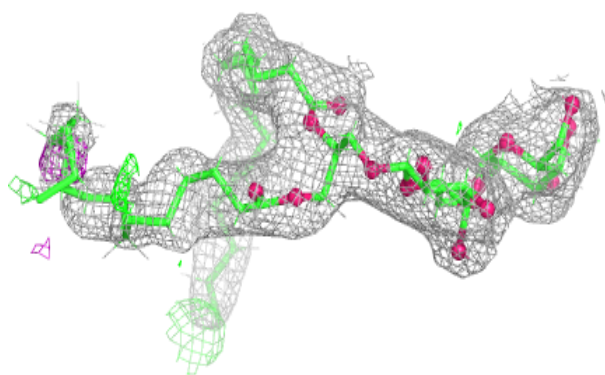
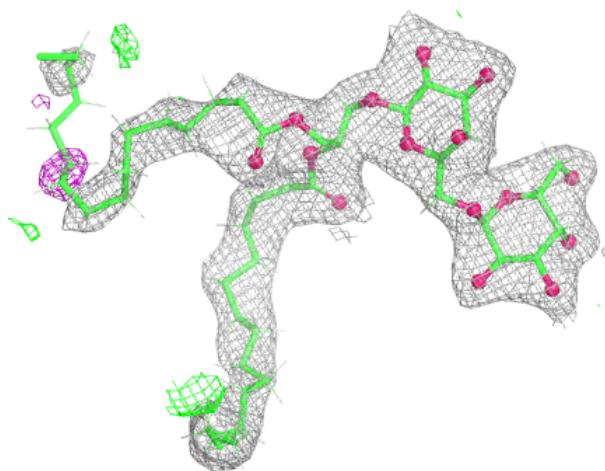
**Electron density around SQD A 410:**

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



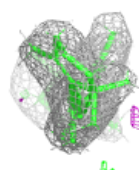
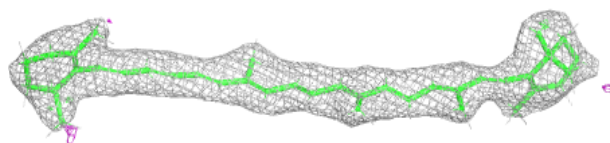
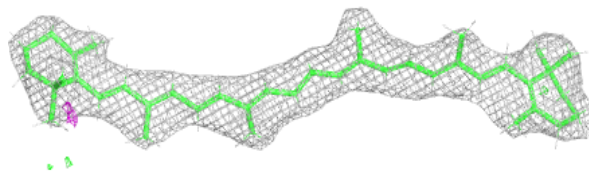
Electron density around DGD C 517:

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

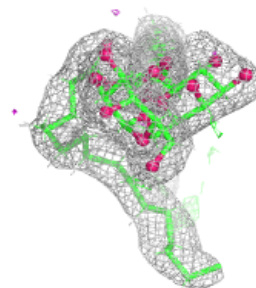
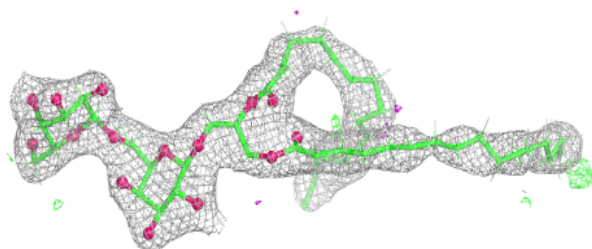
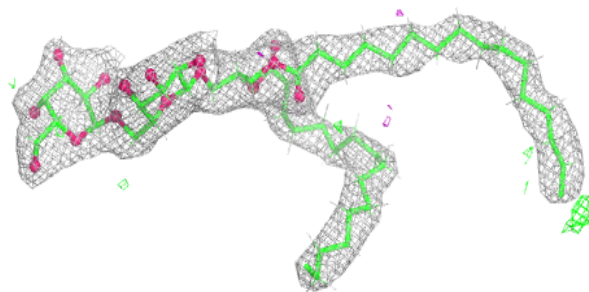


Electron density around BCR b 619:

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

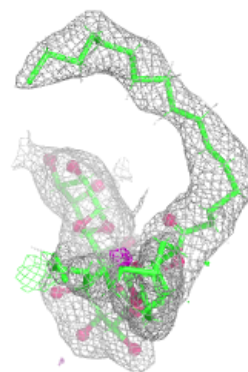
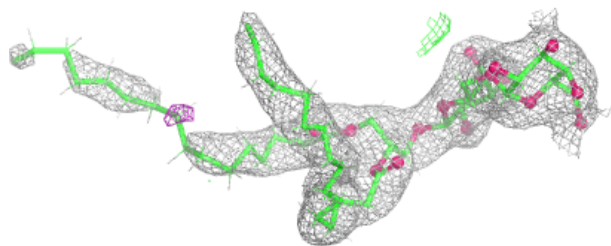
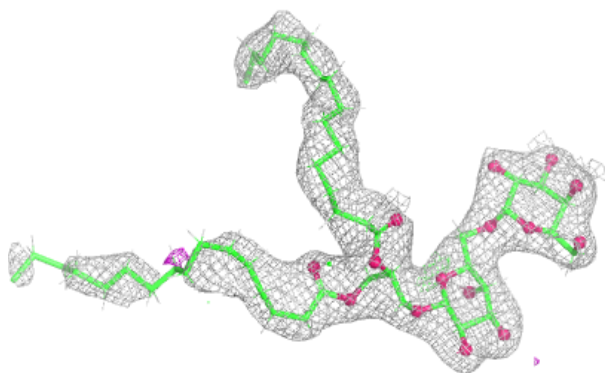
**Electron density around DGD H 103:**

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

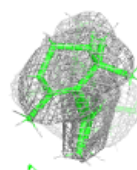
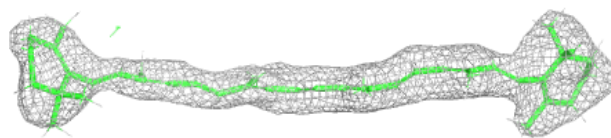
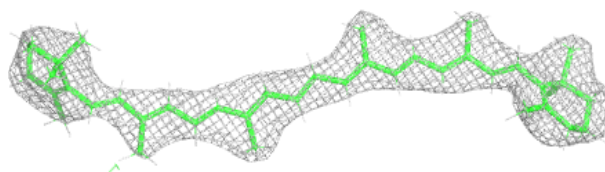


Electron density around DGD c 516:

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

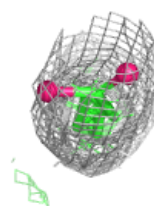
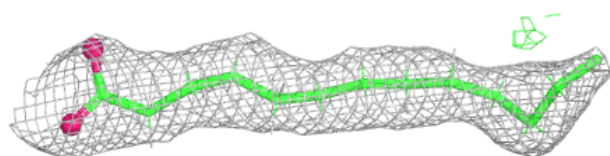
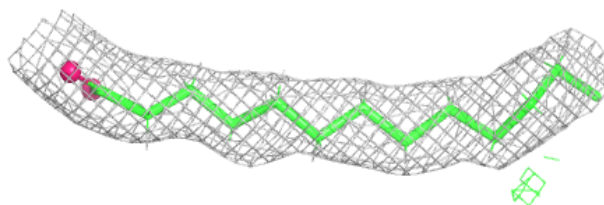
**Electron density around BCR k 102:**

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

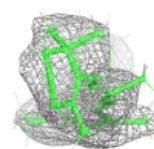
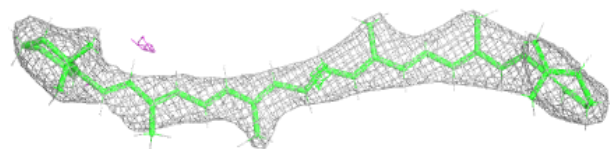
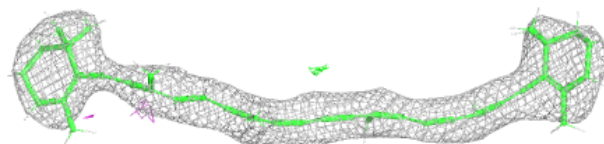


Electron density around STE M 102:

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

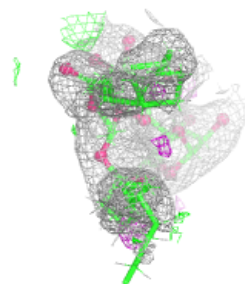
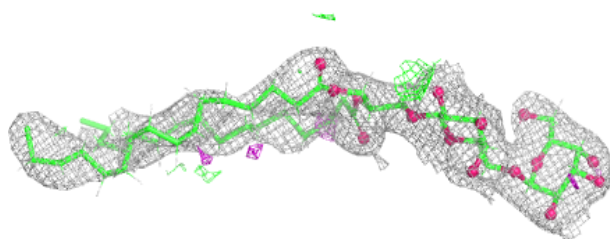
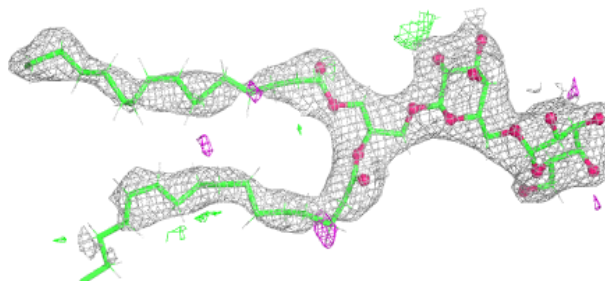
**Electron density around BCR k 103:**

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

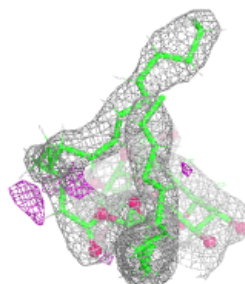
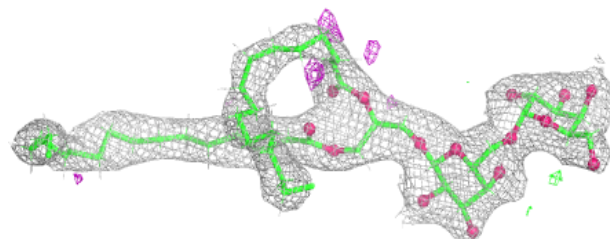
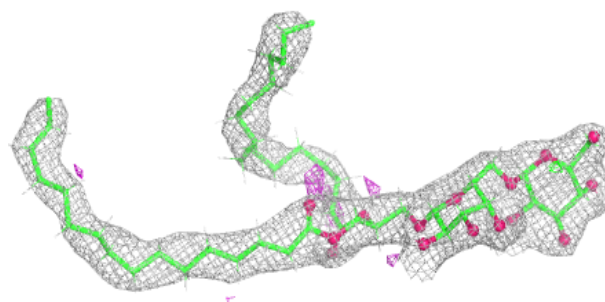


Electron density around DGD c 517:

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

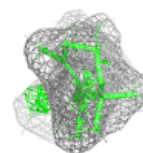
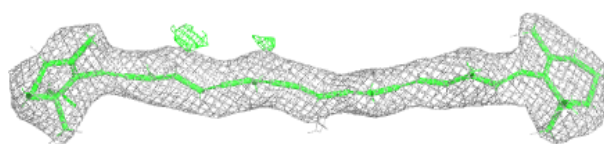
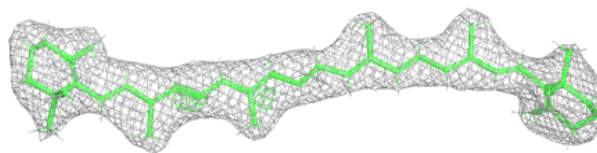
**Electron density around DGD h 101:**

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

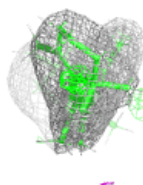
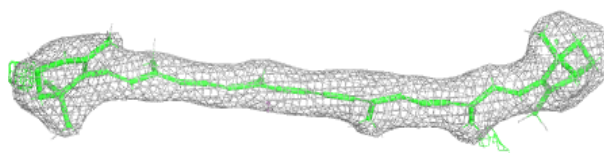
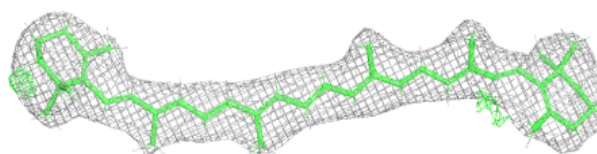


Electron density around BCR B 617:

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

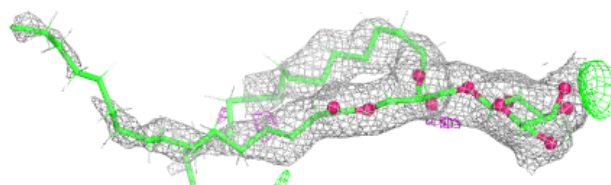
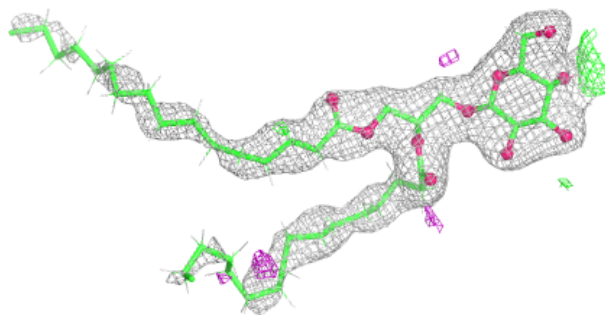
**Electron density around BCR B 618:**

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

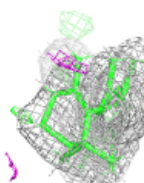
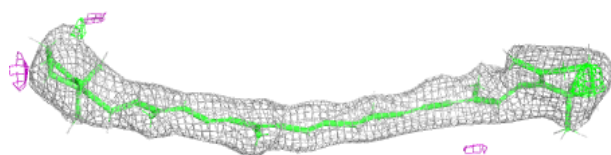
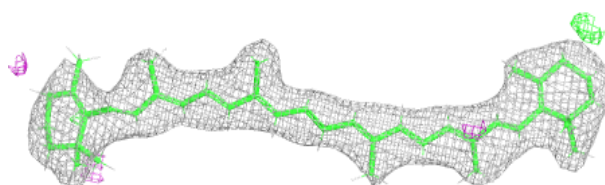


Electron density around LMG D 408:

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

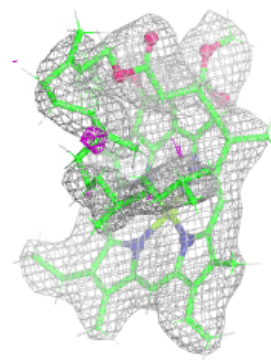
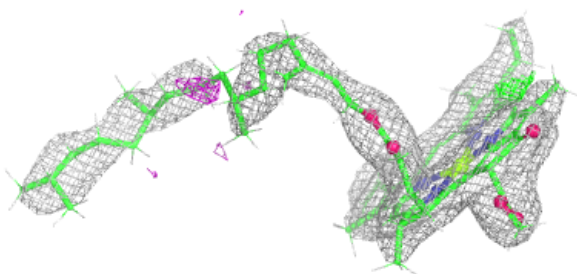
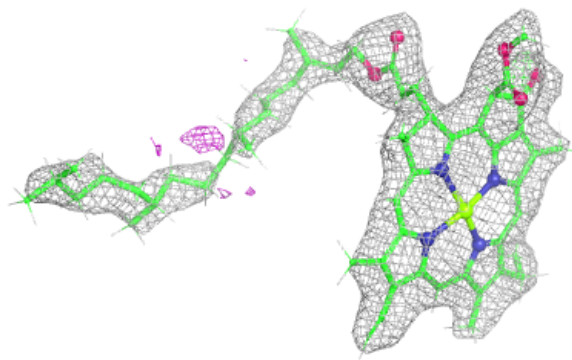
**Electron density around BCR D 406:**

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

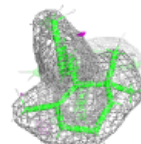
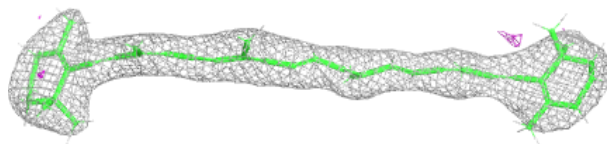
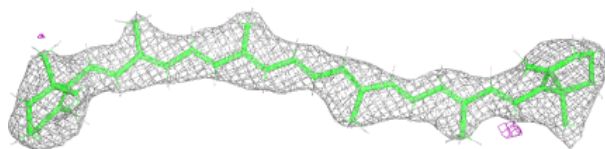


Electron density around CLA c 511:

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

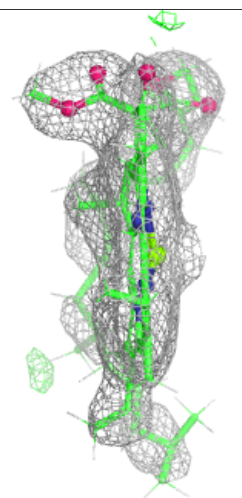
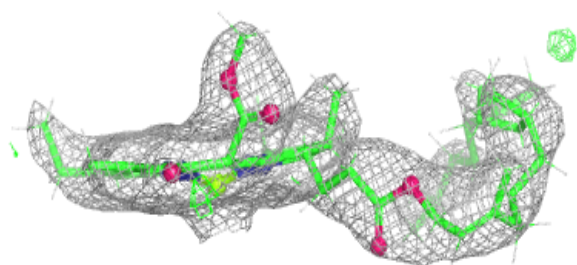
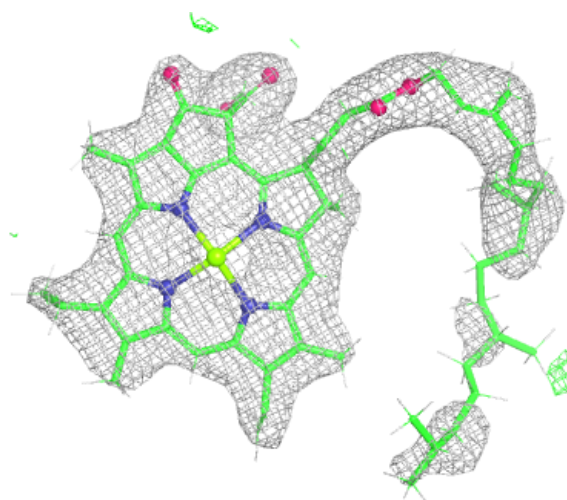
**Electron density around BCR c 514:**

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



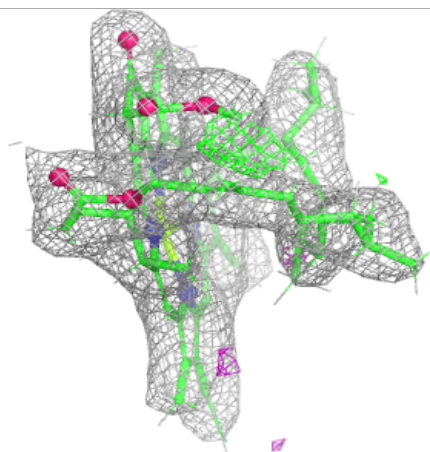
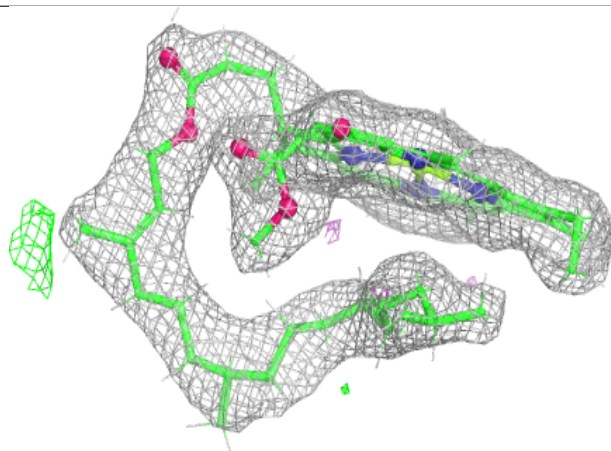
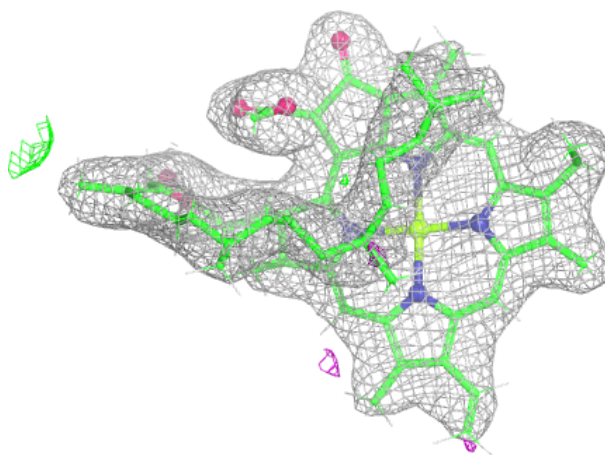
Electron density around CLA C 512:

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



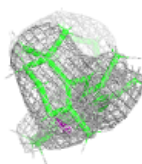
Electron density around CLA C 510:

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

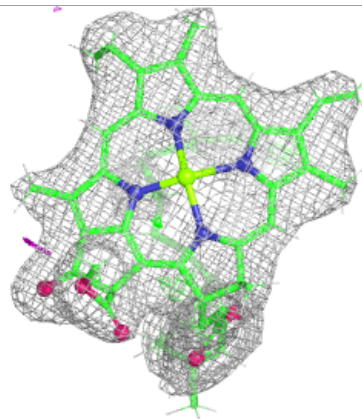
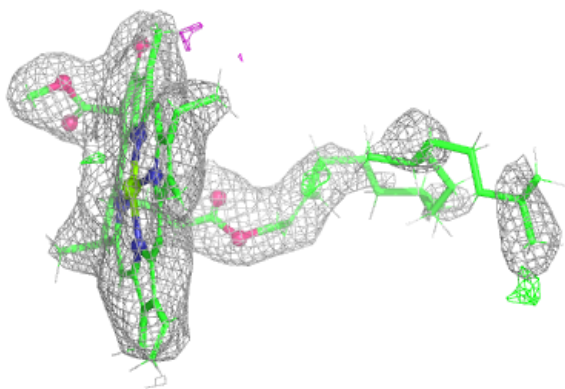
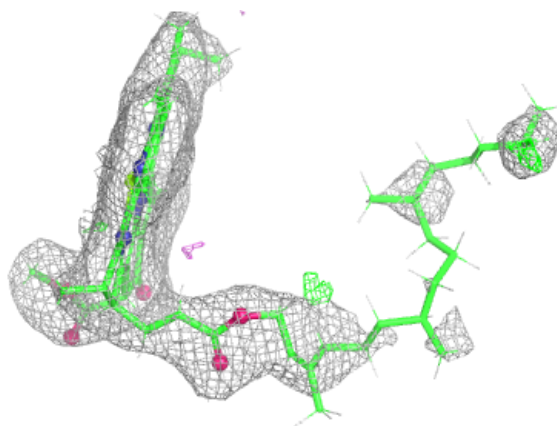


Electron density around BCR C 515:

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

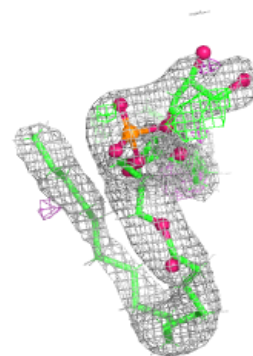
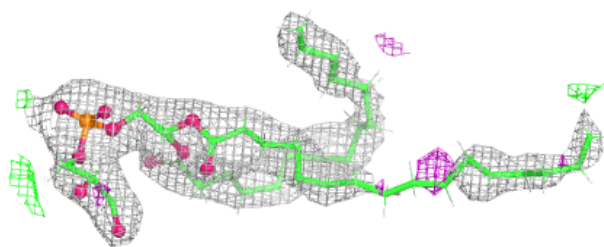
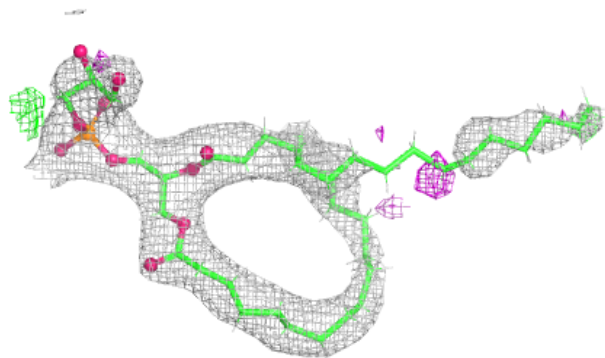
**Electron density around CLA c 506:**

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

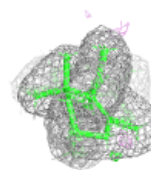
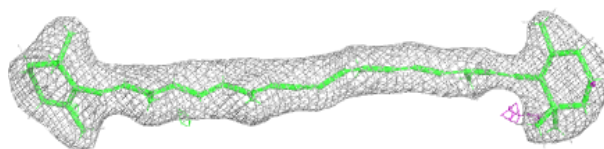
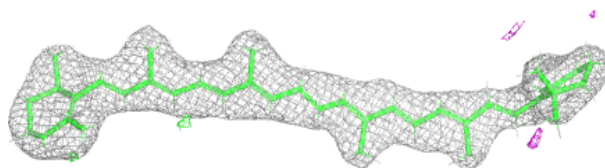


Electron density around LHG b 623:

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

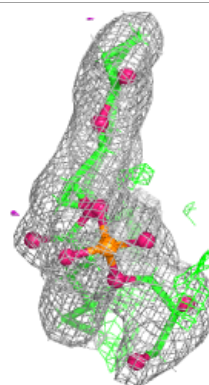
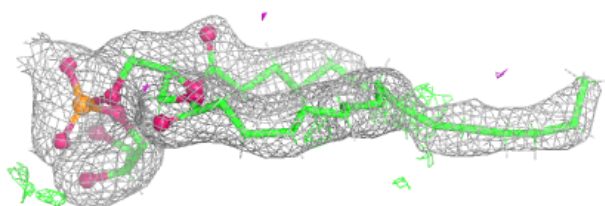
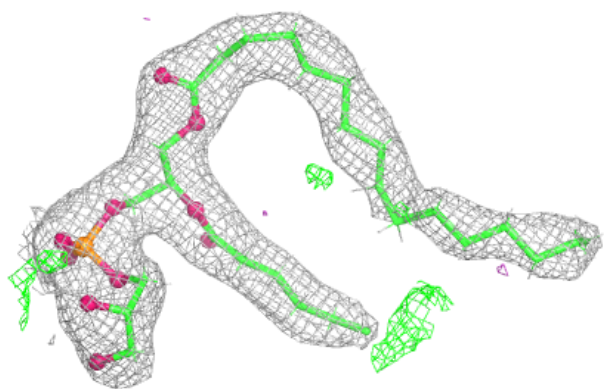
**Electron density around BCR I 101:**

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

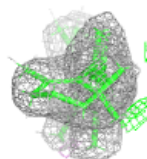
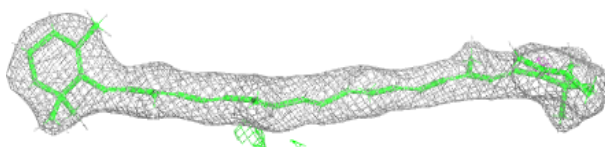
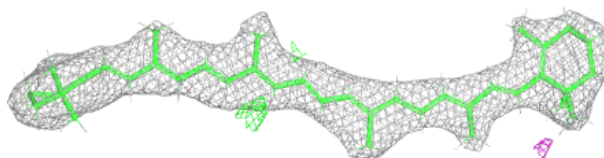


Electron density around LHG d 409:

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

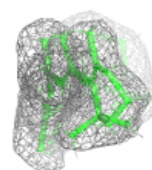
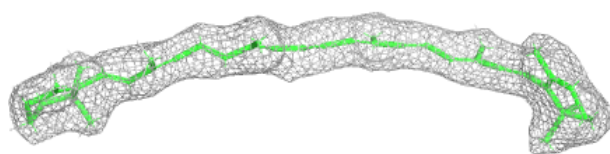
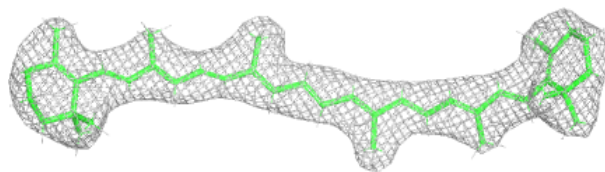
**Electron density around BCR B 616:**

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

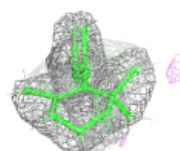
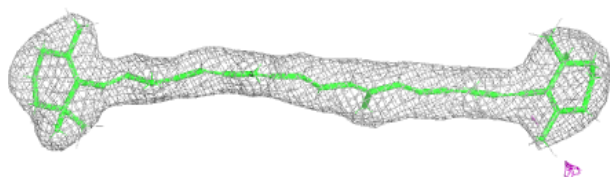
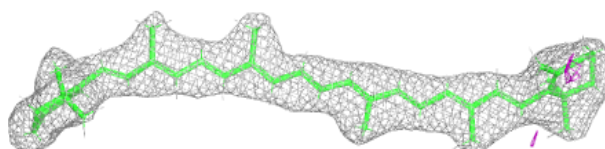


Electron density around BCR T 101:

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

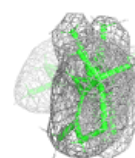
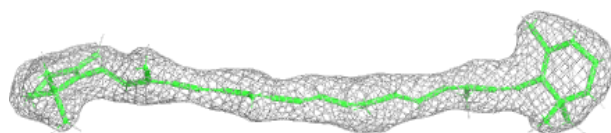
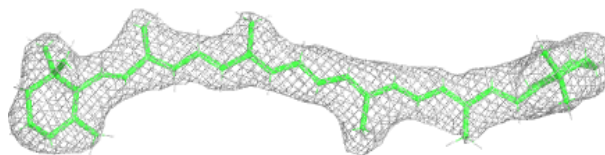
**Electron density around BCR a 406:**

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

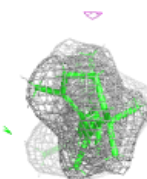
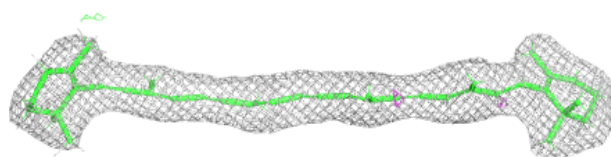
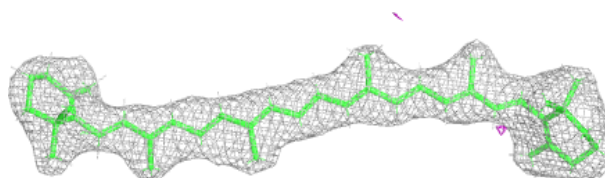


Electron density around BCR b 617:

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

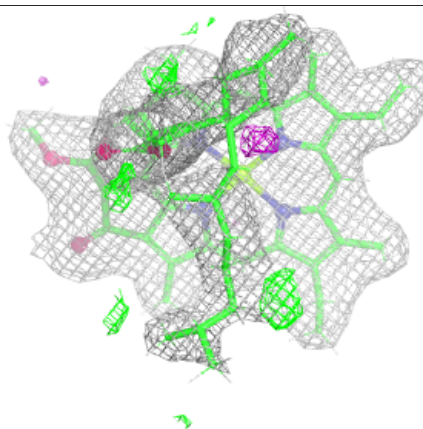
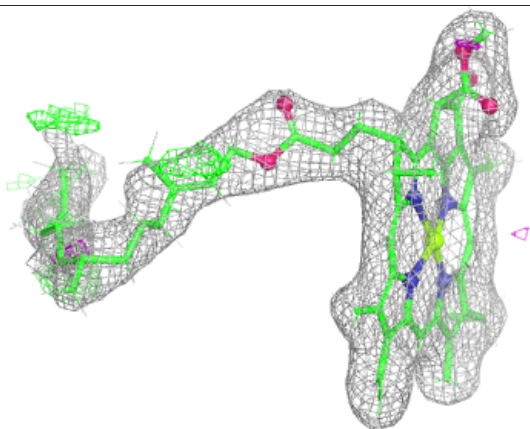
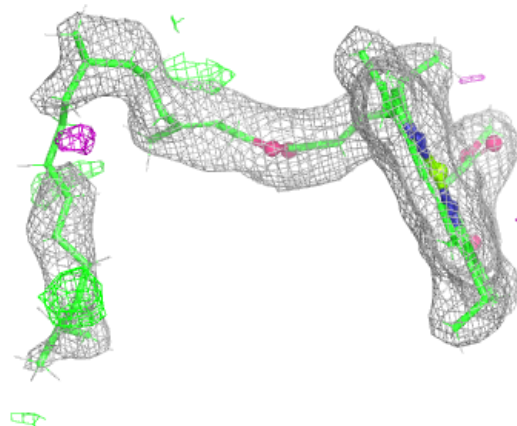
**Electron density around BCR b 618:**

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



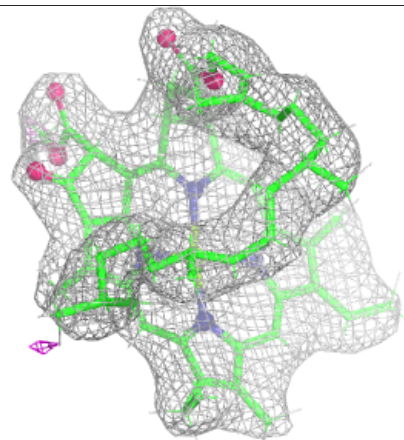
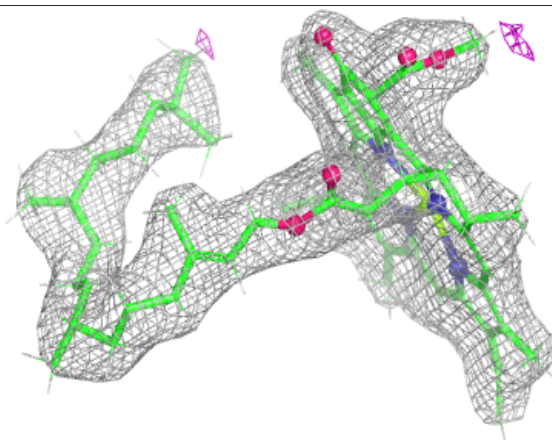
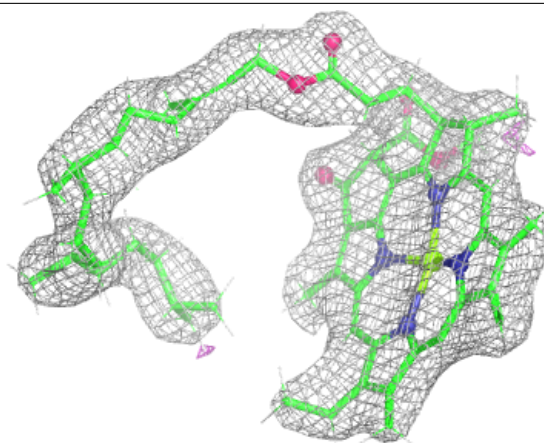
Electron density around CLA a 405:

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



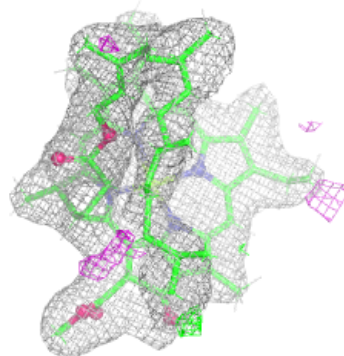
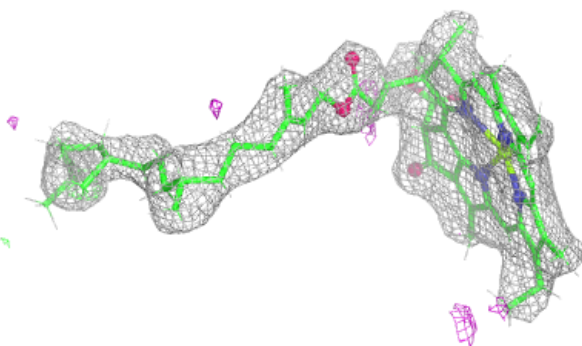
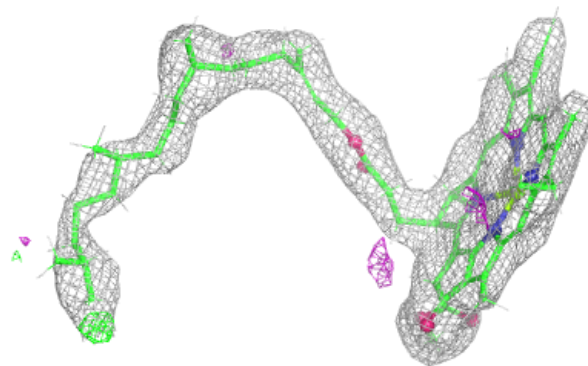
Electron density around CLA C 503:

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

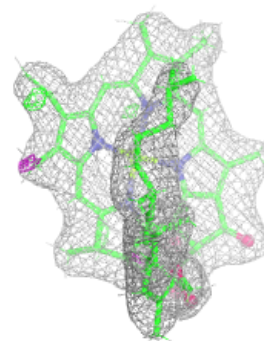
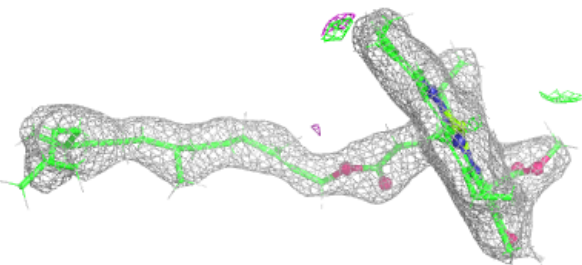
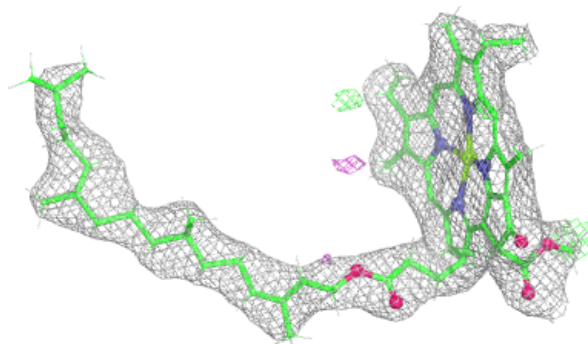


Electron density around CLA b 606:

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

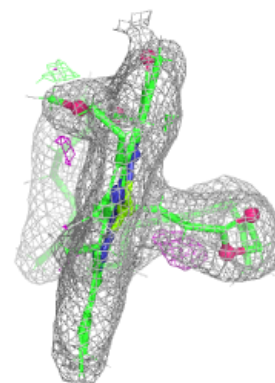
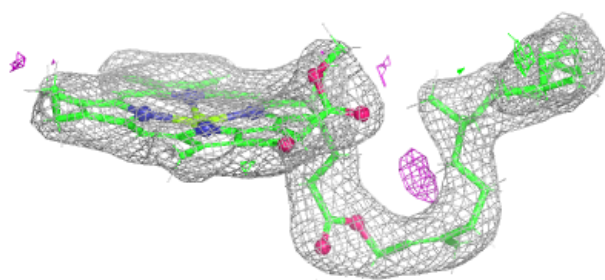
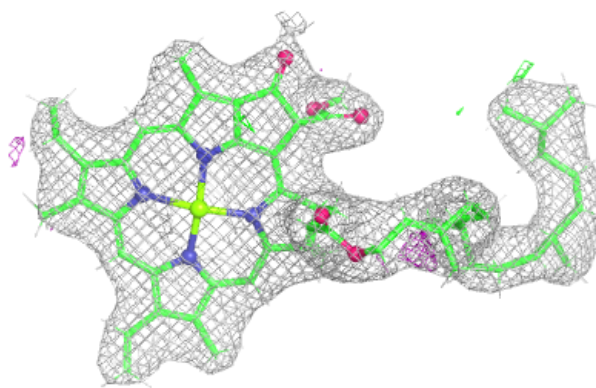
**Electron density around CLA b 609:**

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



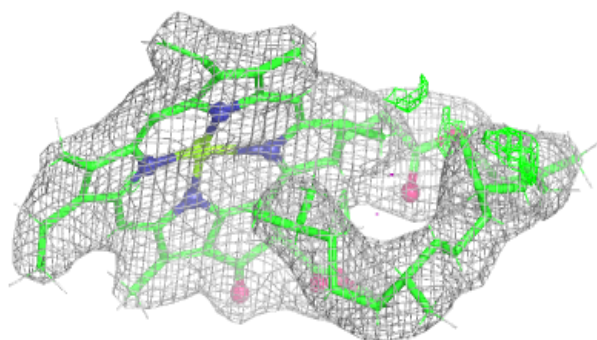
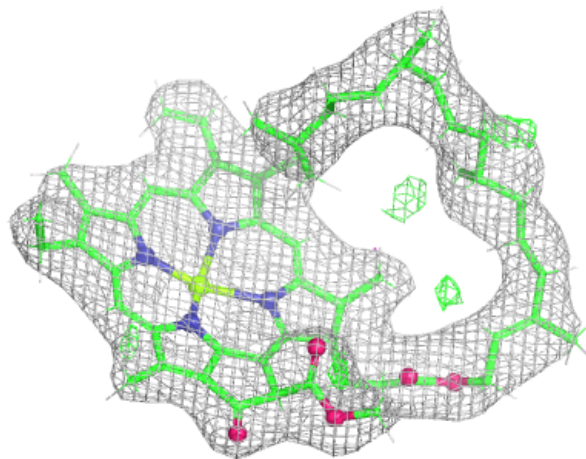
Electron density around CLA b 612:

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



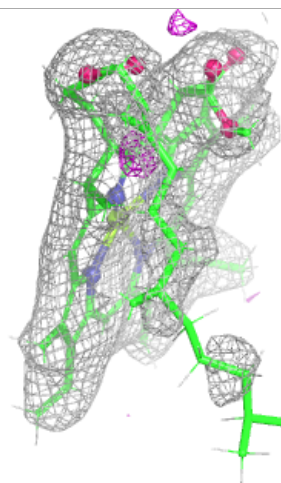
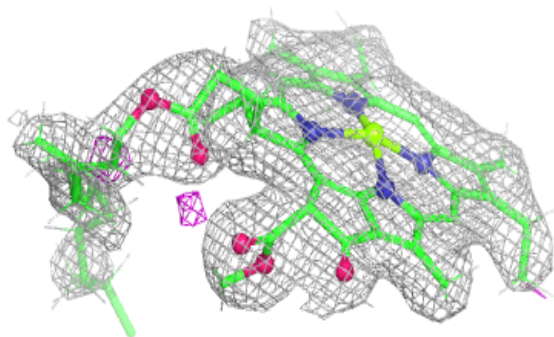
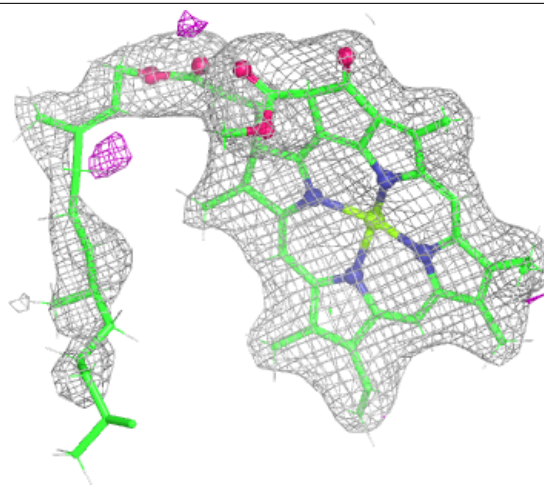
Electron density around CLA b 615:

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



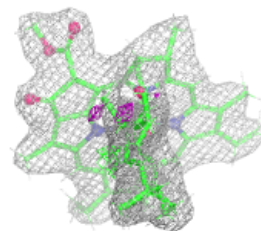
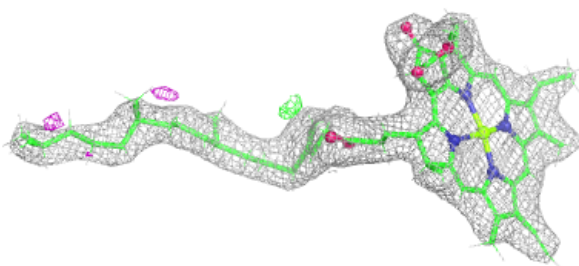
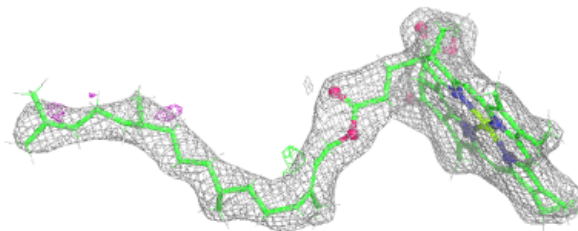
Electron density around CLA b 616:

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



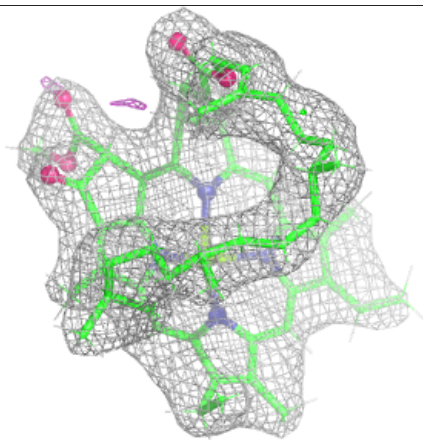
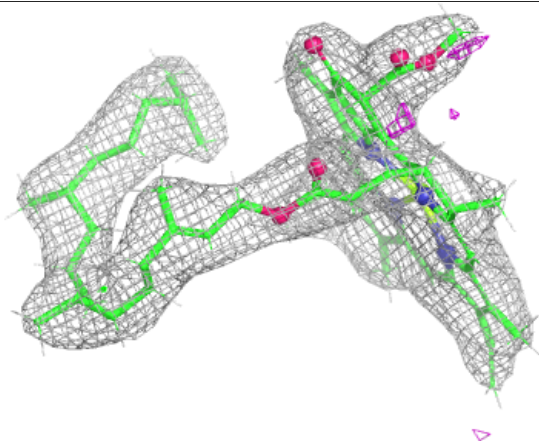
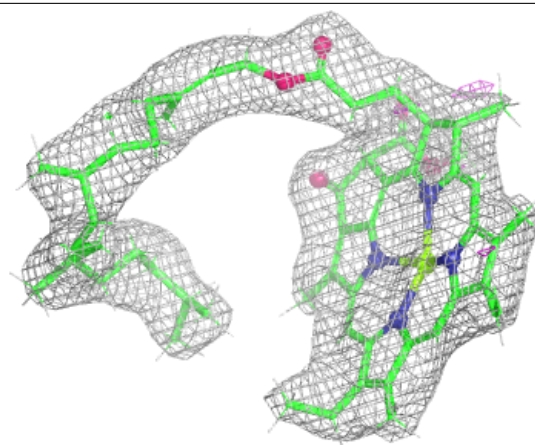
Electron density around CLA c 502:

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



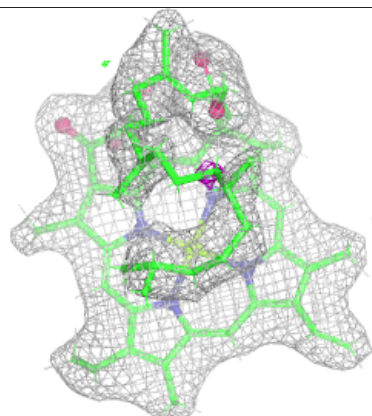
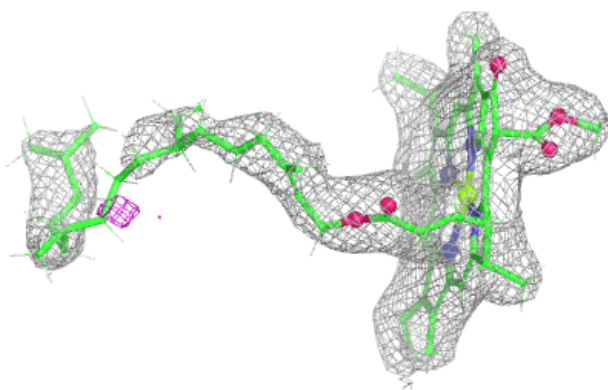
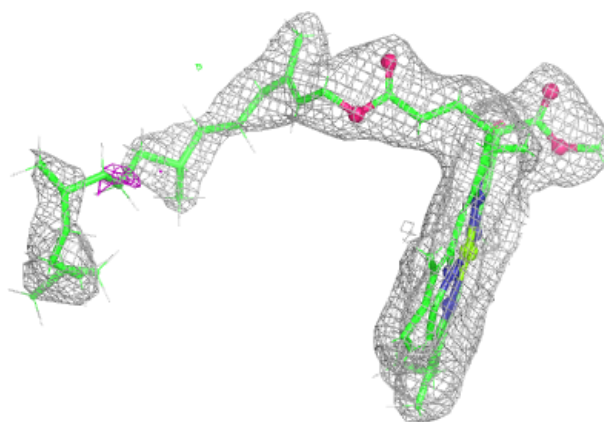
Electron density around CLA c 503:

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

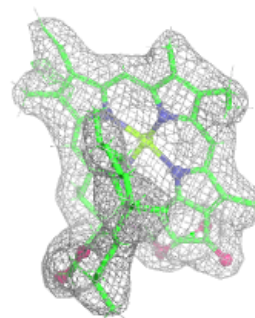
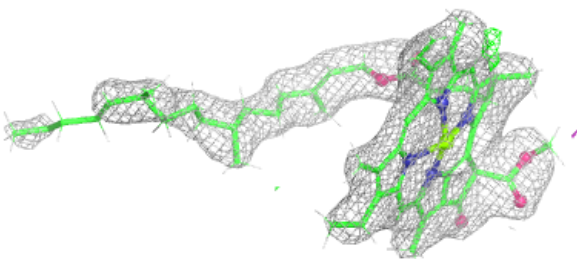
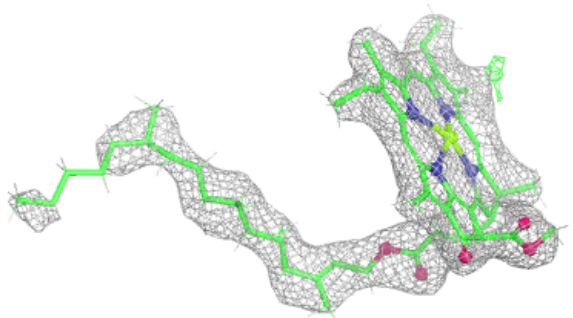


Electron density around CLA C 506:

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

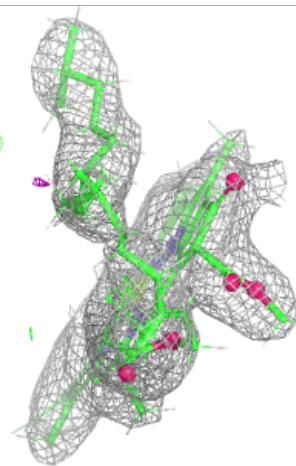
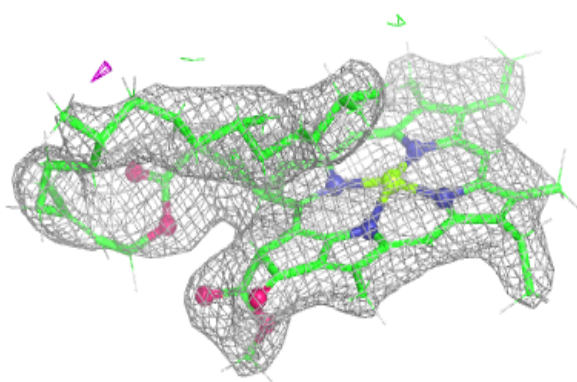
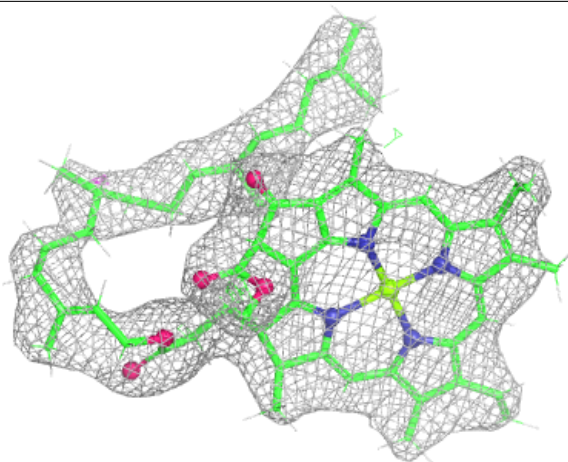
**Electron density around CLA c 508:**

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



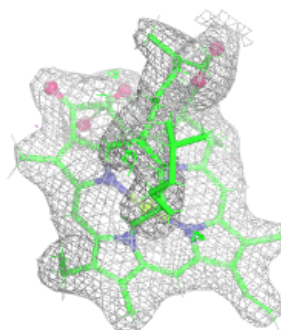
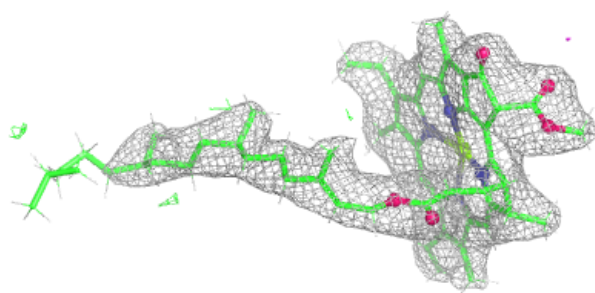
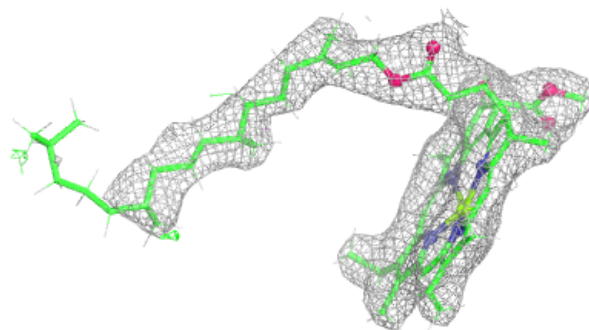
Electron density around CLA c 509:

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



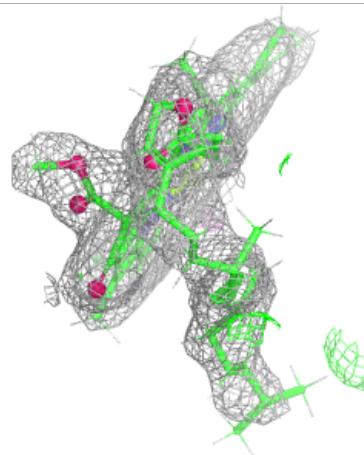
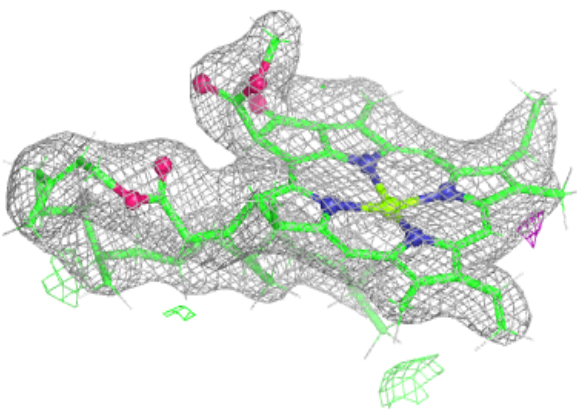
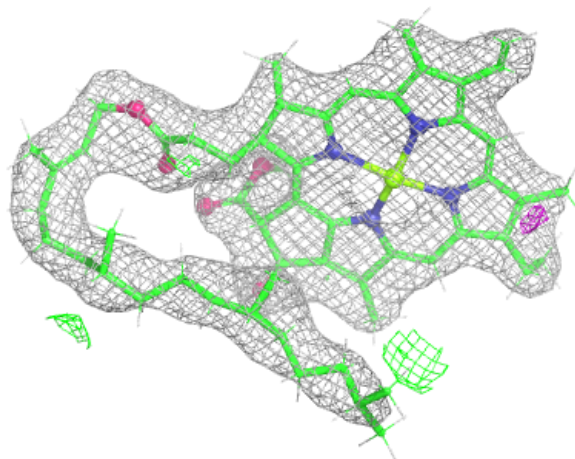
Electron density around CLA C 508:

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



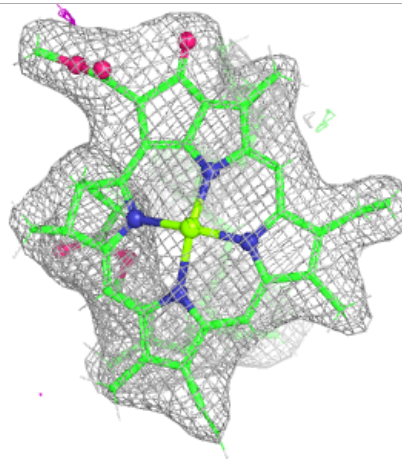
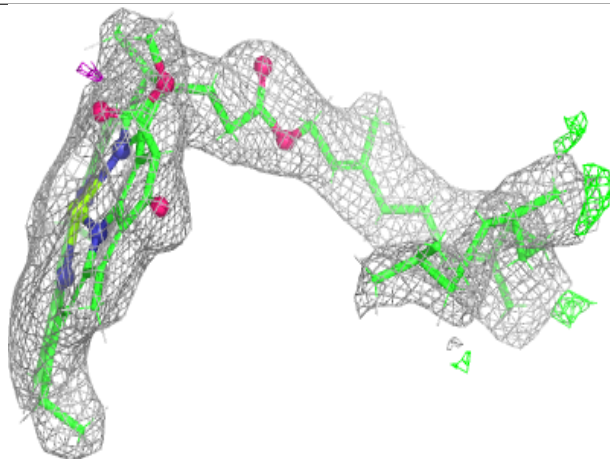
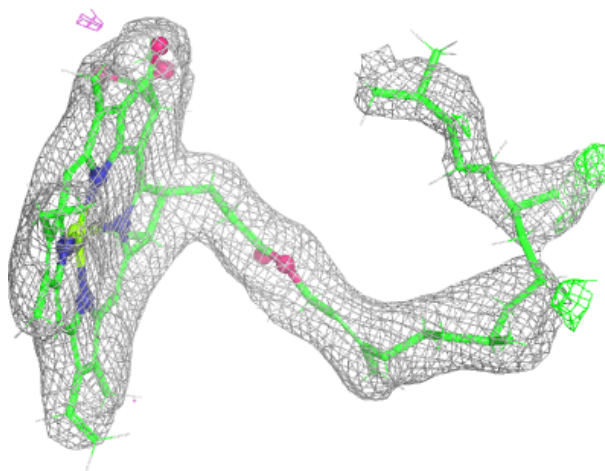
Electron density around CLA C 509:

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



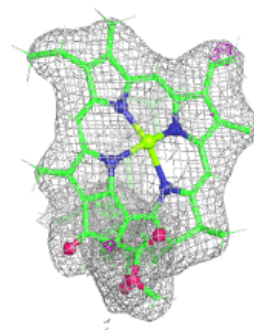
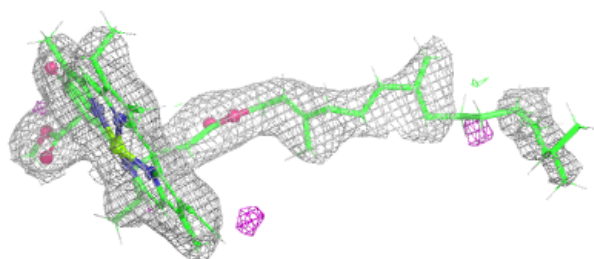
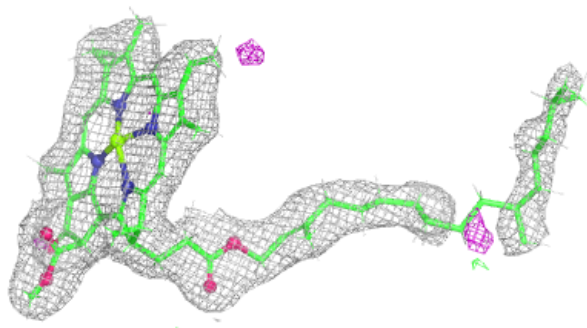
Electron density around CLA B 605:

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



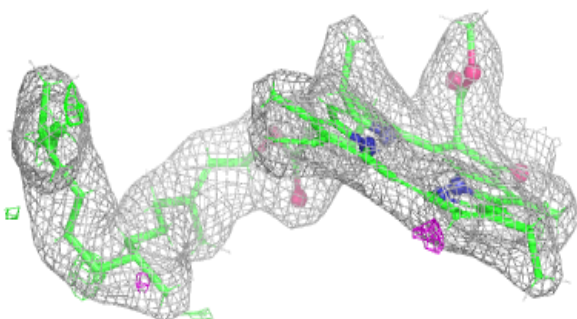
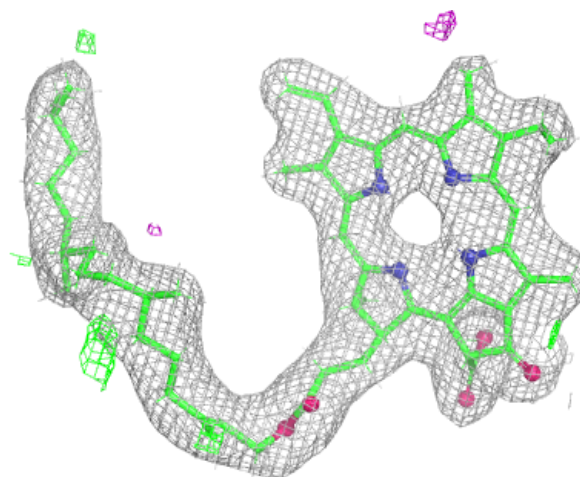
Electron density around CLA d 405:

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



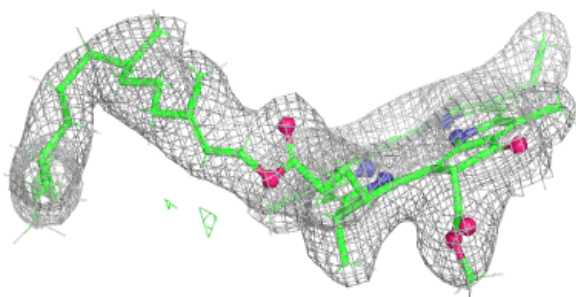
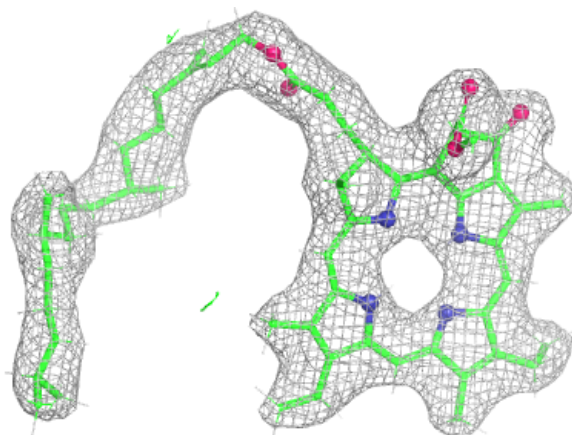
Electron density around PHO D 401:

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



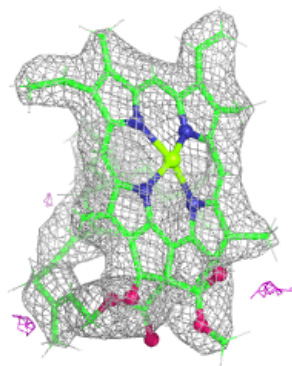
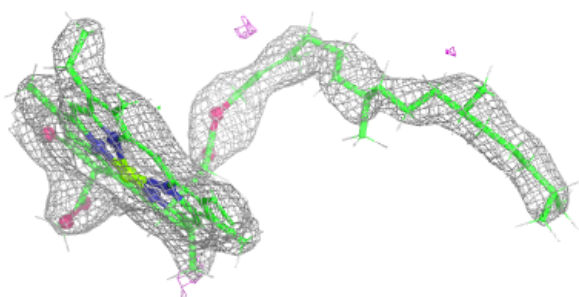
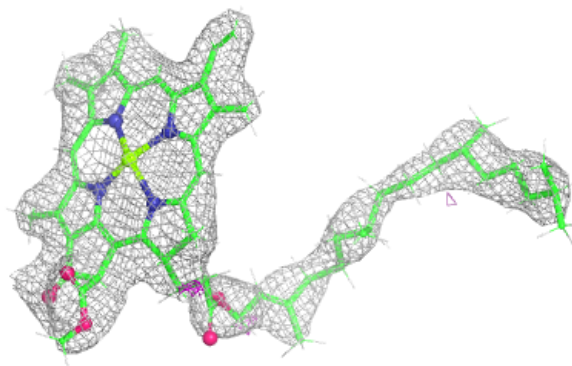
Electron density around PHO d 401:

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

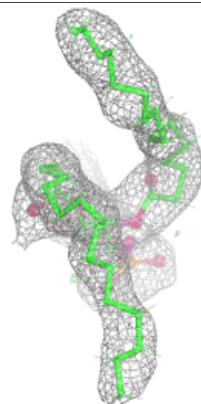
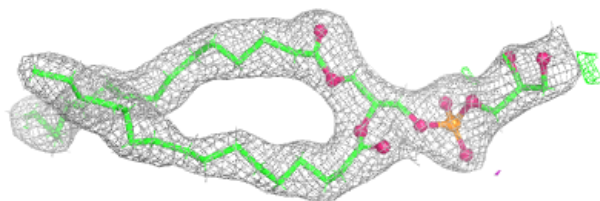
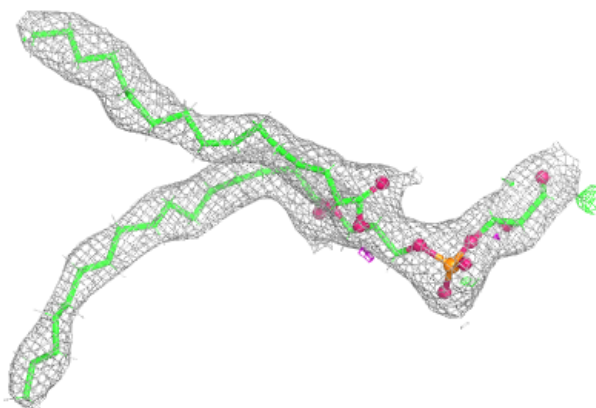


Electron density around CLA C 511:

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

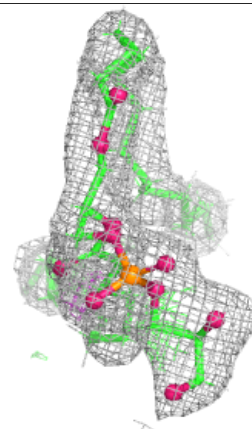
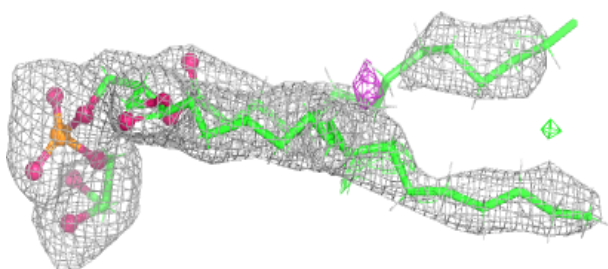
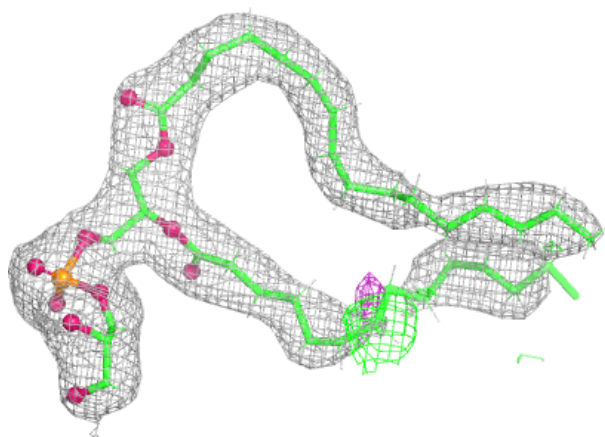
**Electron density around LHG D 410:**

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

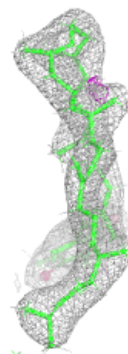
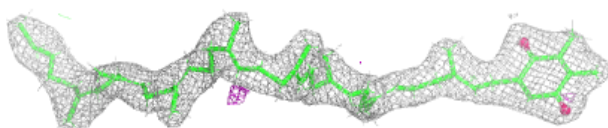
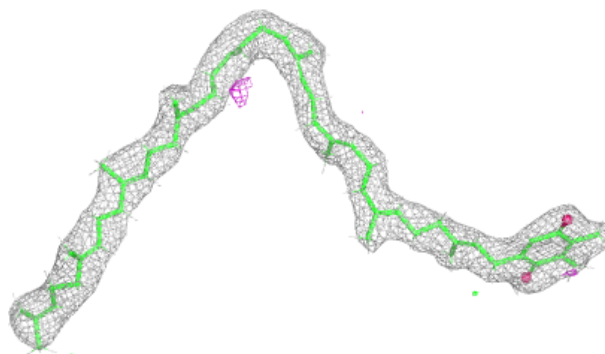


Electron density around LHG D 411:

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

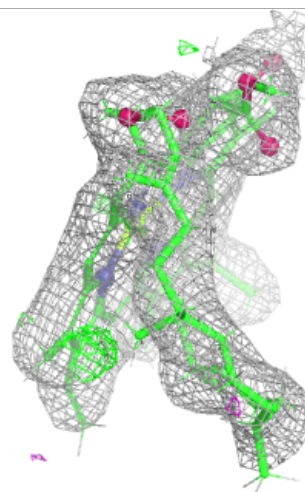
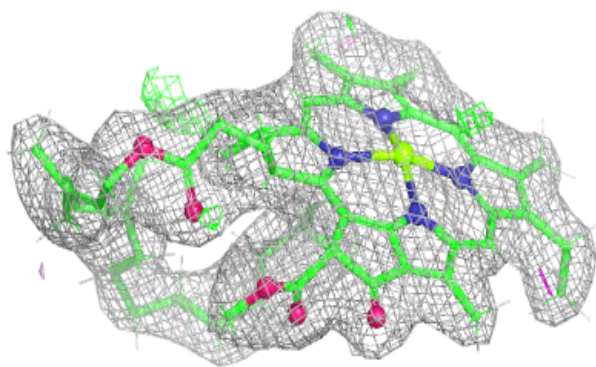
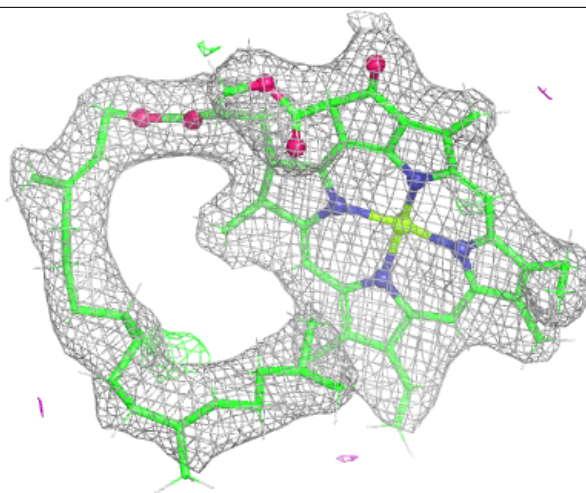
**Electron density around PL9 D 407:**

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



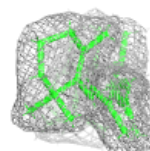
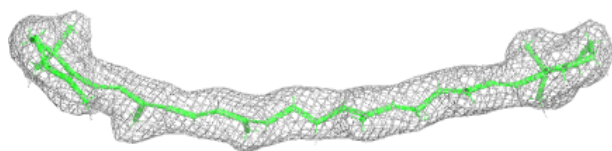
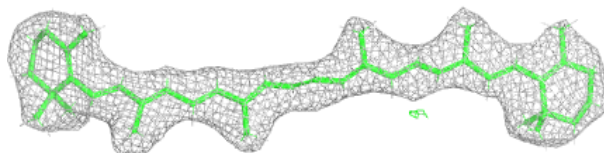
Electron density around CLA B 614:

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

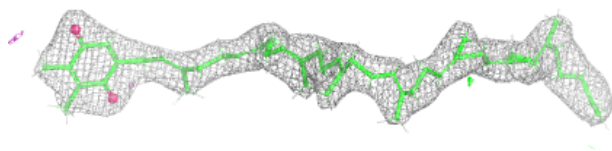
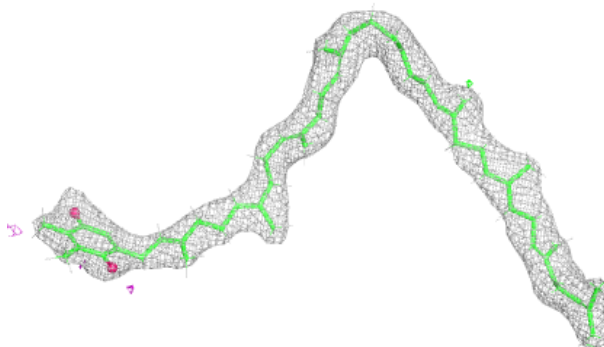


Electron density around BCR t 101:

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

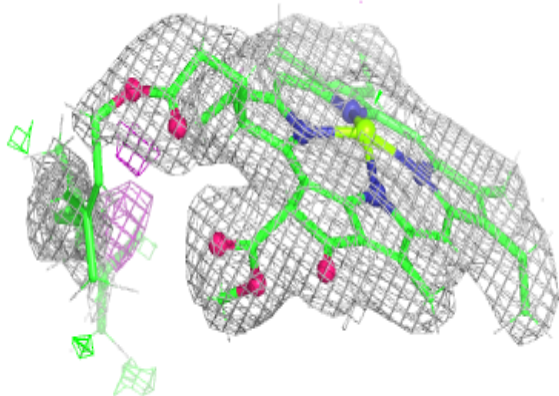
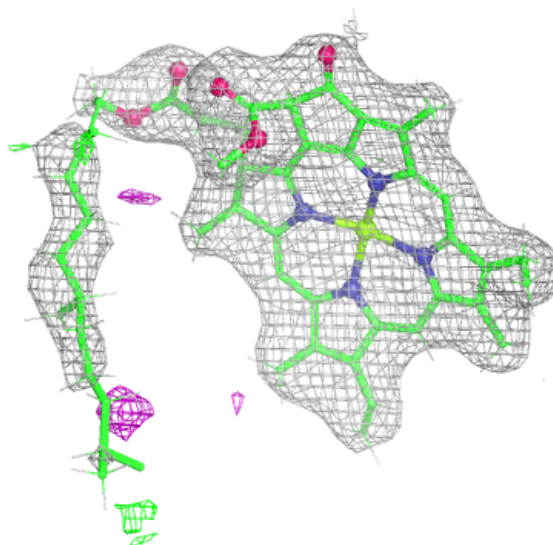
**Electron density around PL9 d 407:**

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



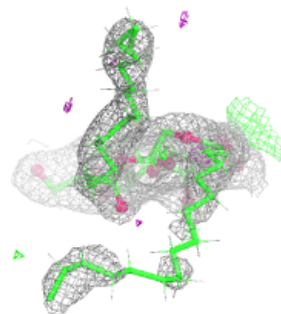
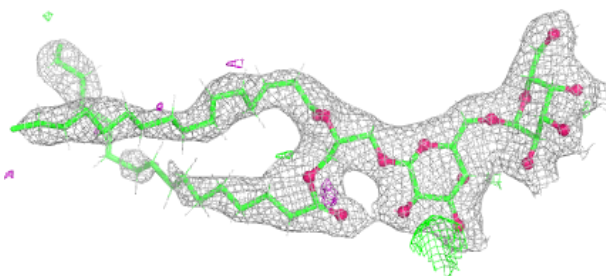
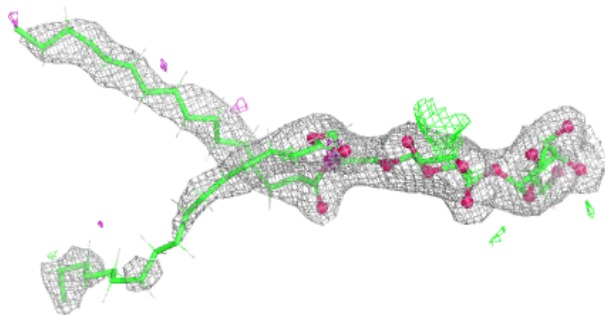
Electron density around CLA B 615:

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

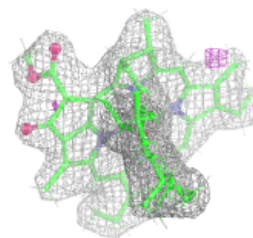
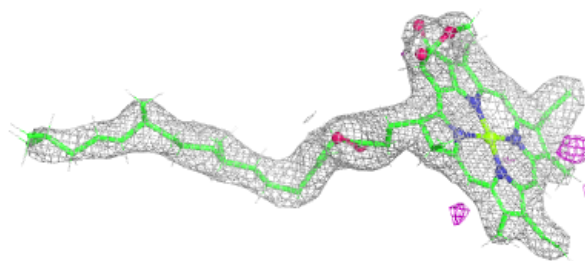
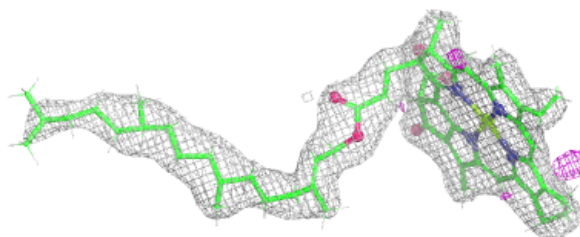


Electron density around DGD C 516:

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

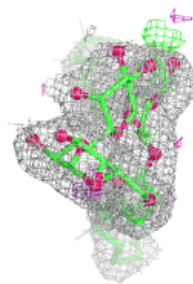
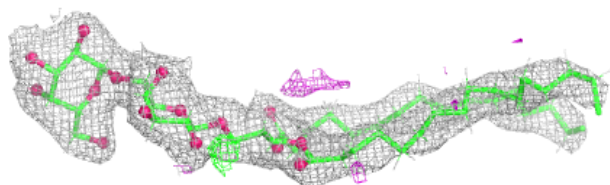
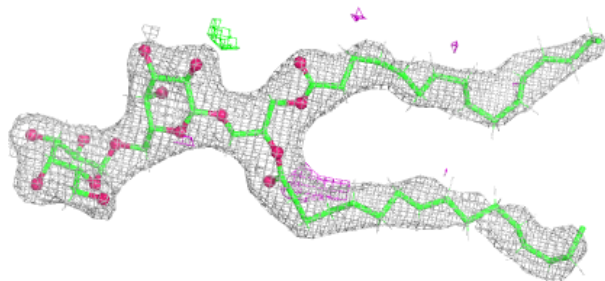
**Electron density around CLA C 502:**

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

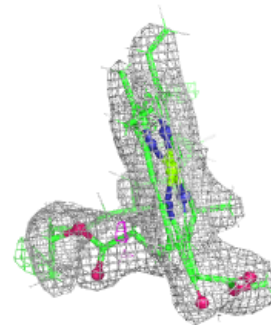
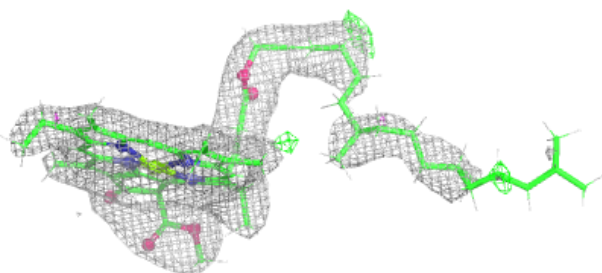
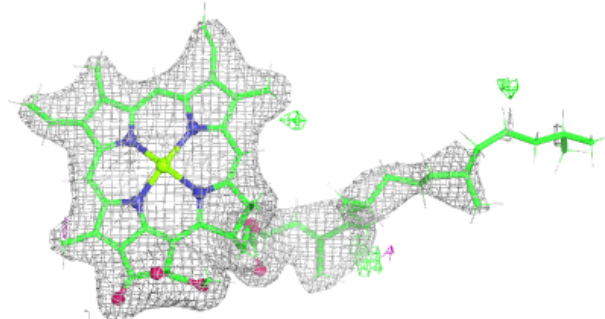


Electron density around DGD C 518:

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

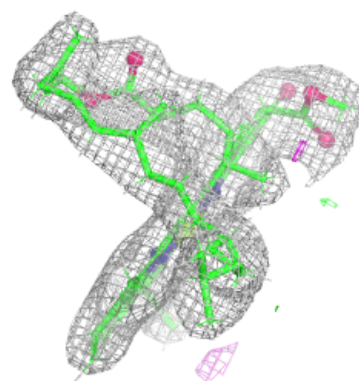
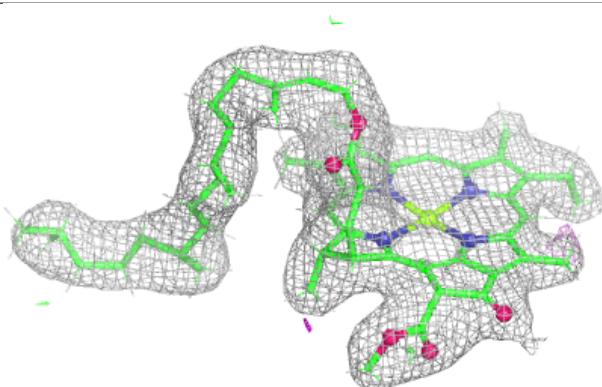
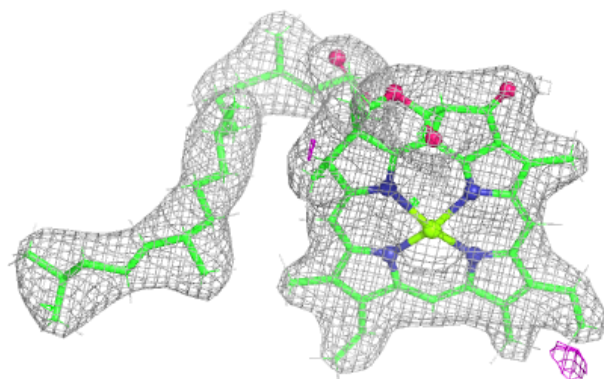
**Electron density around CLA a 403:**

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

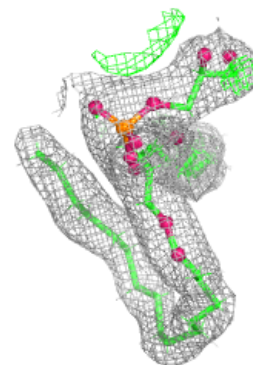
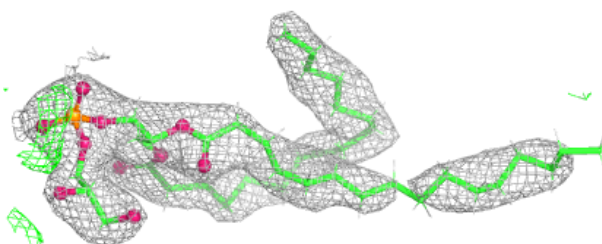
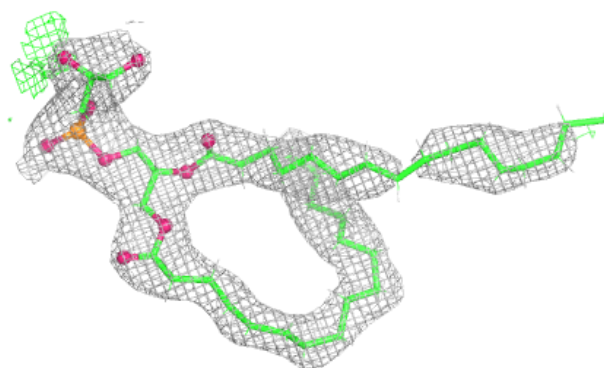


Electron density around CLA d 404:

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

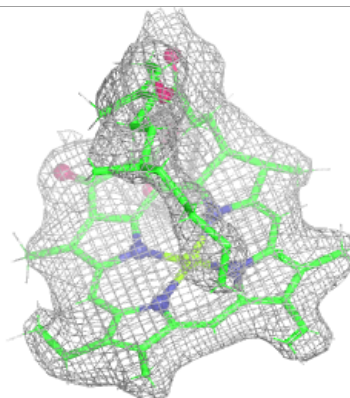
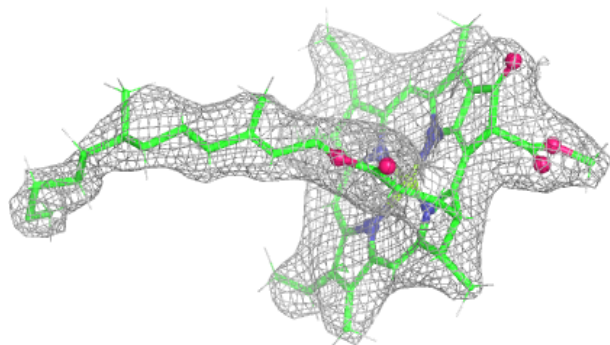
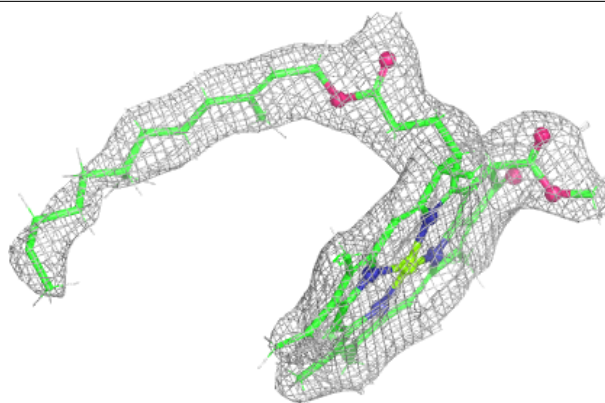
**Electron density around LHG D 413:**

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

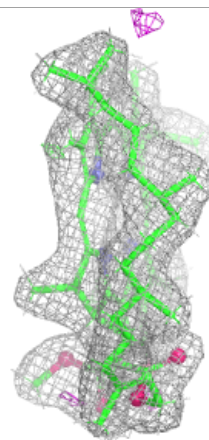
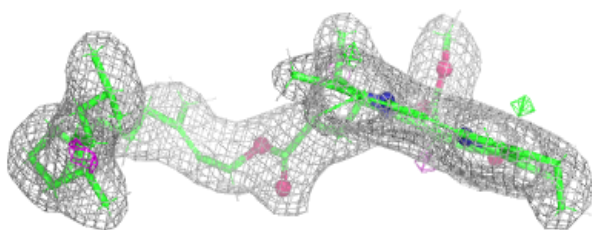
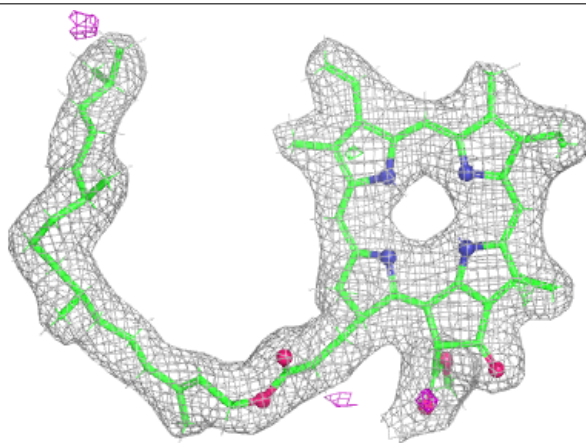


Electron density around CLA C 504:

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

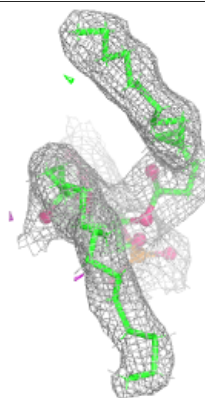
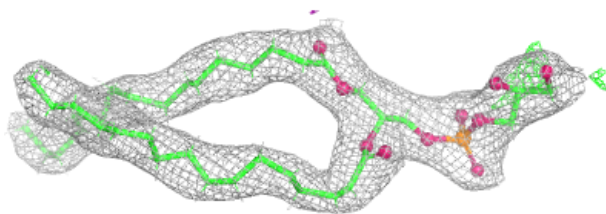
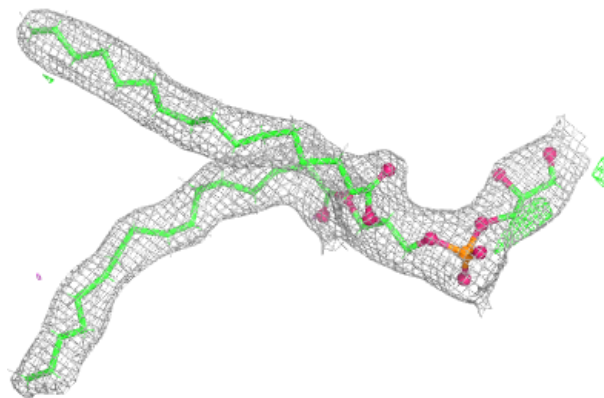
**Electron density around PHO A 404:**

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

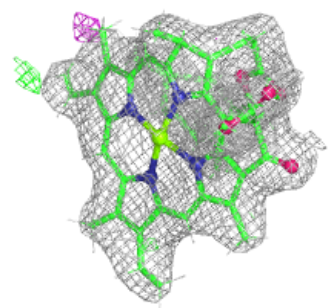
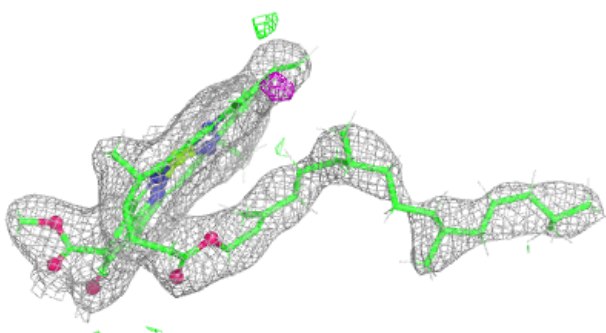
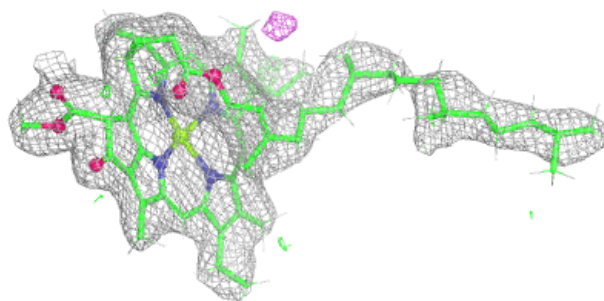


Electron density around LHG d 408:

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

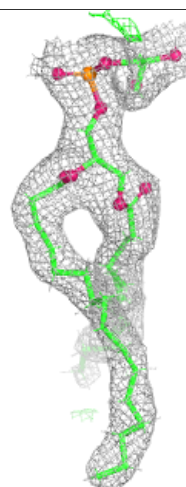
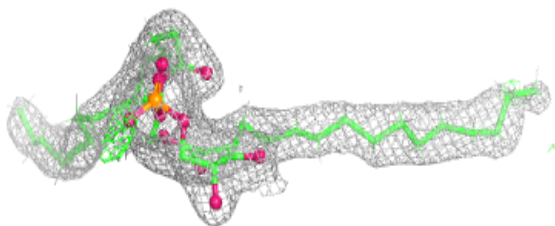
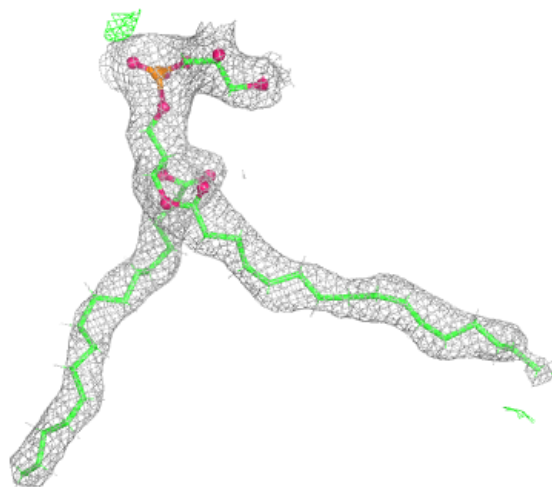
**Electron density around CLA C 505:**

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



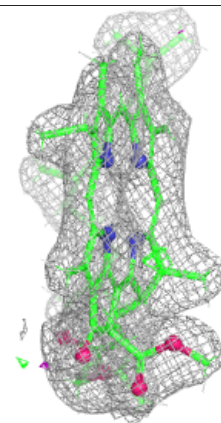
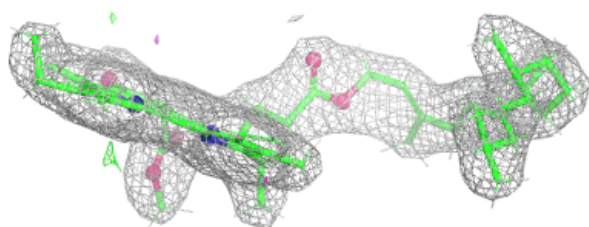
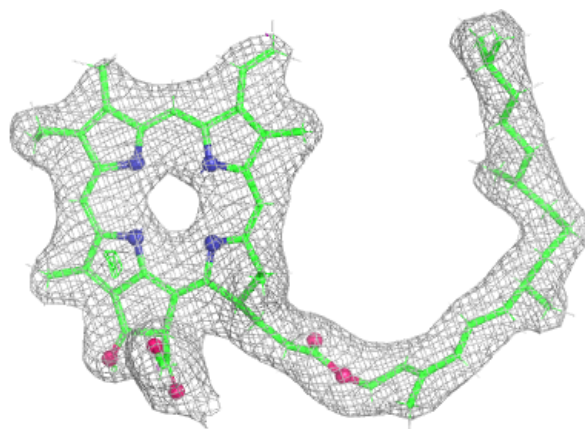
Electron density around LHG 1 101:

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

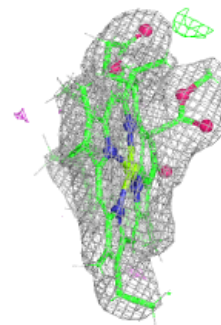
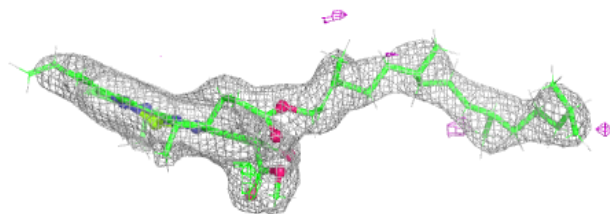
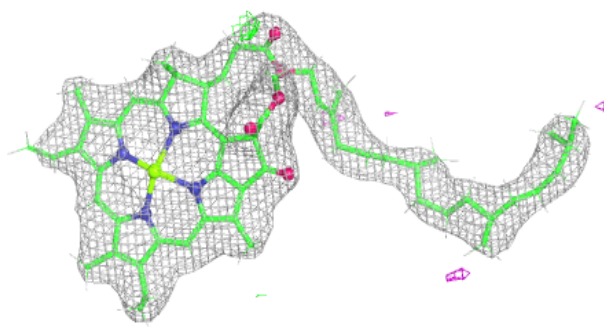


Electron density around PHO a 404:

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

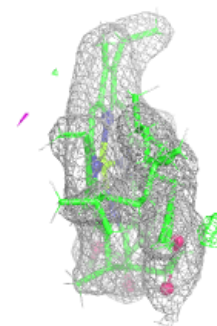
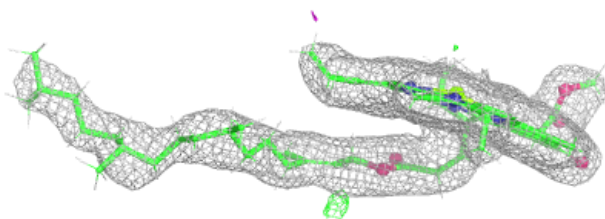
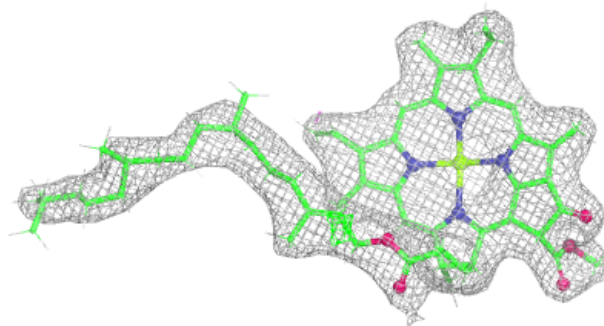
**Electron density around CLA b 602:**

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

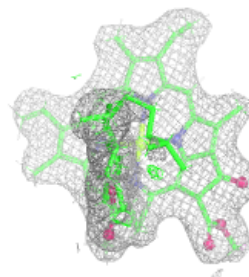
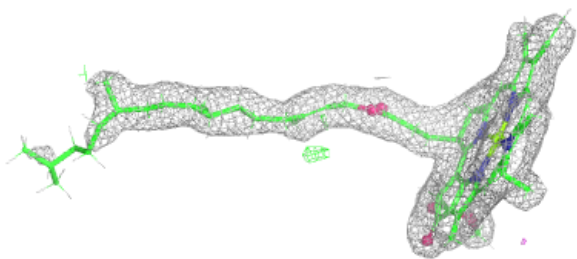
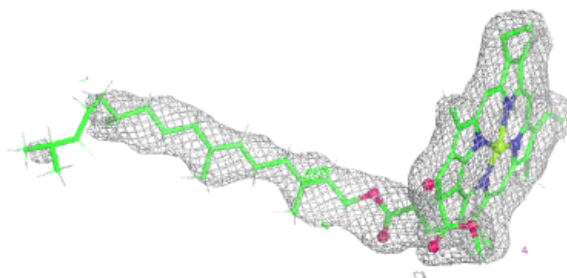


Electron density around CLA b 603:

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

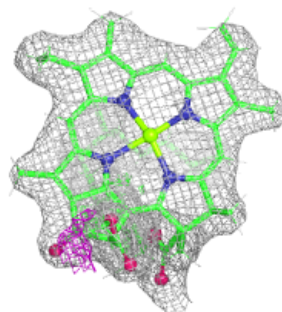
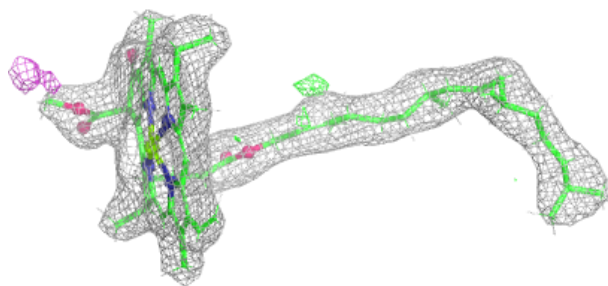
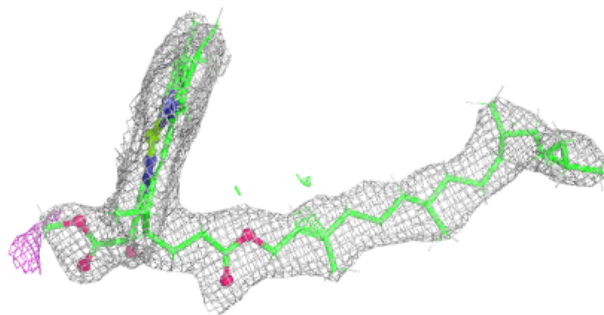
**Electron density around CLA b 604:**

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

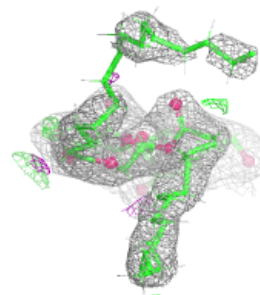
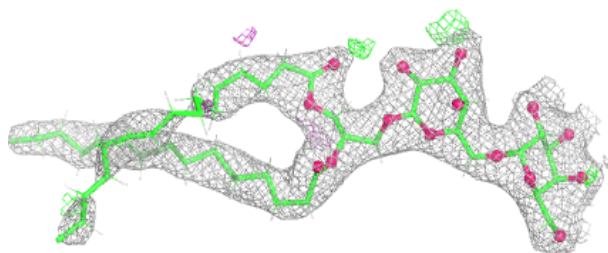
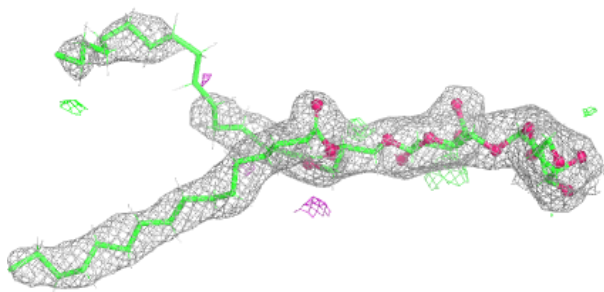


Electron density around CLA b 605:

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

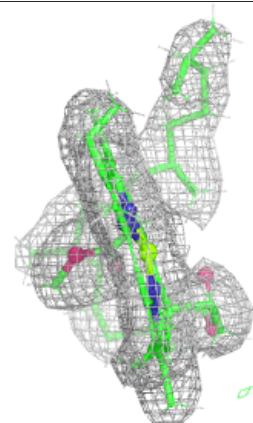
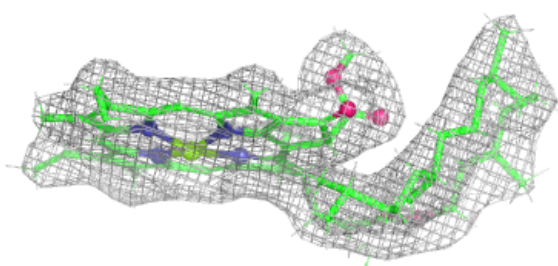
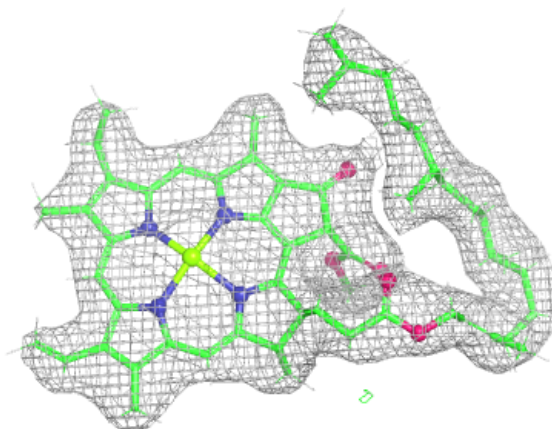
**Electron density around DGD c 515:**

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

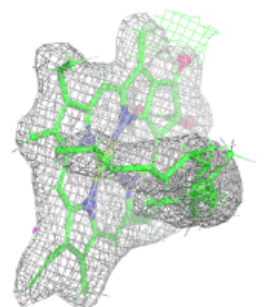
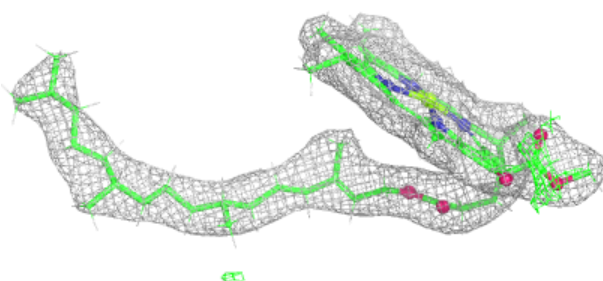
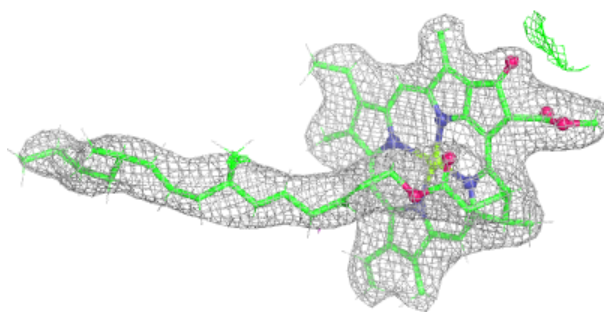


Electron density around CLA B 609:

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

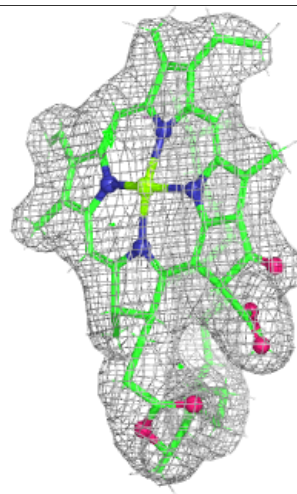
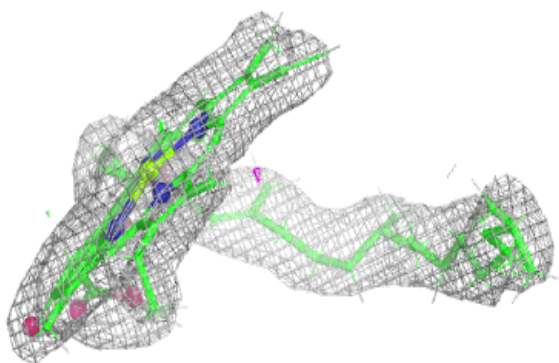
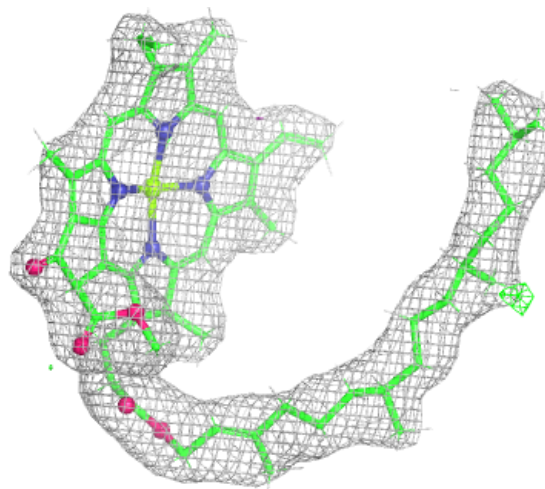
**Electron density around CLA b 608:**

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



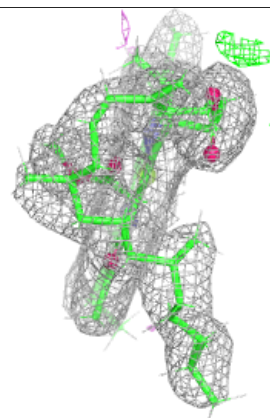
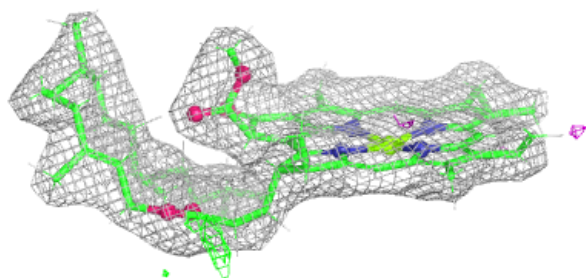
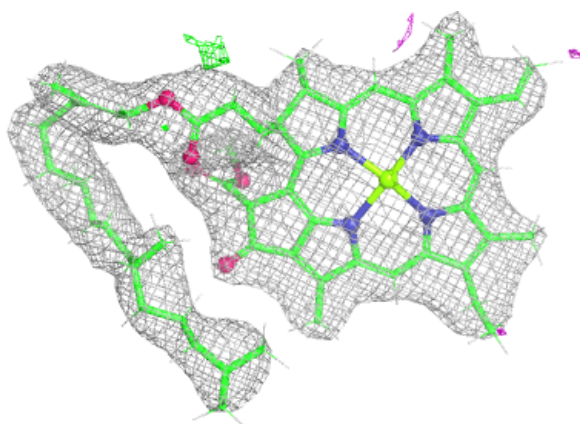
Electron density around CLA C 507:

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



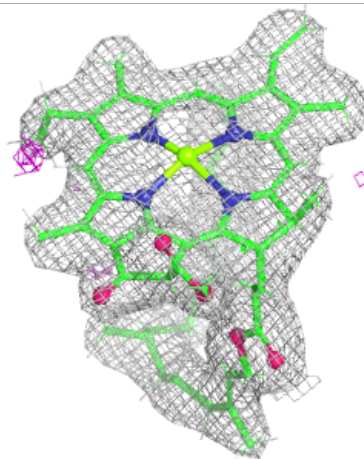
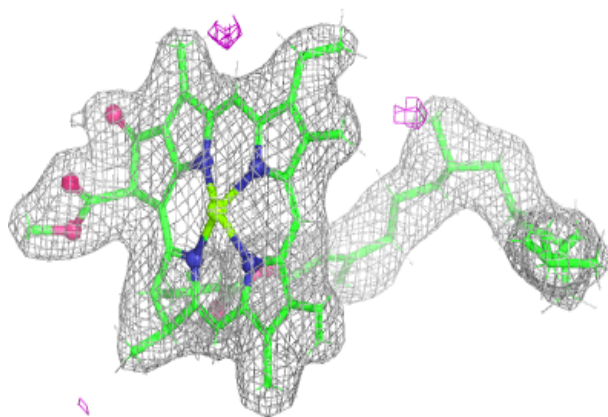
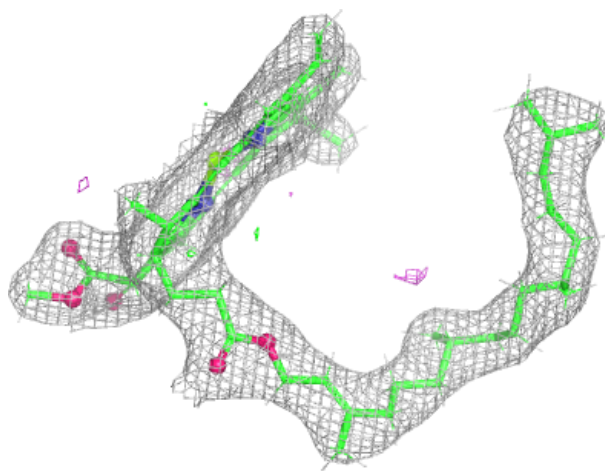
Electron density around CLA b 610:

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



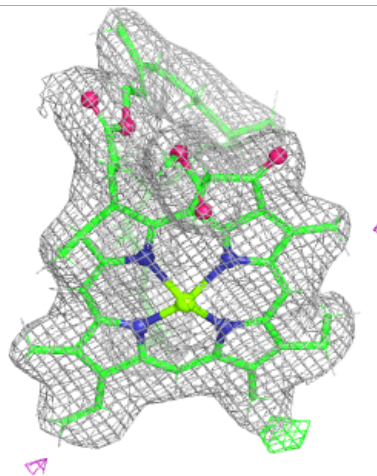
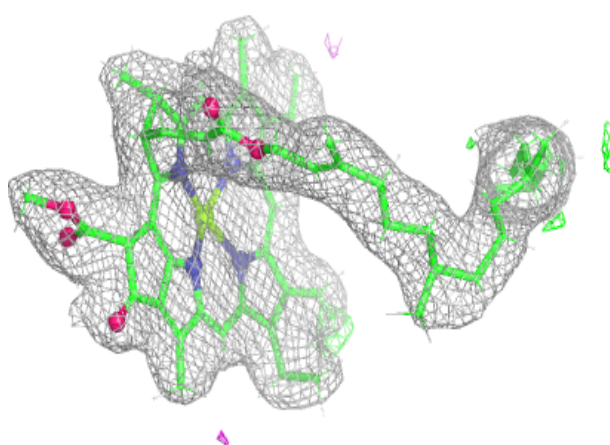
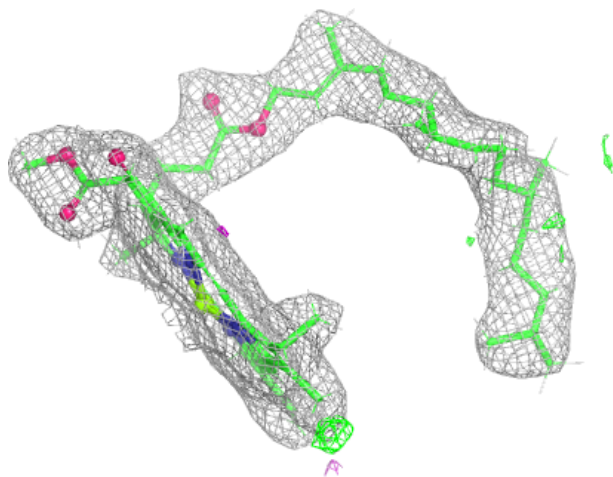
Electron density around CLA b 611:

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



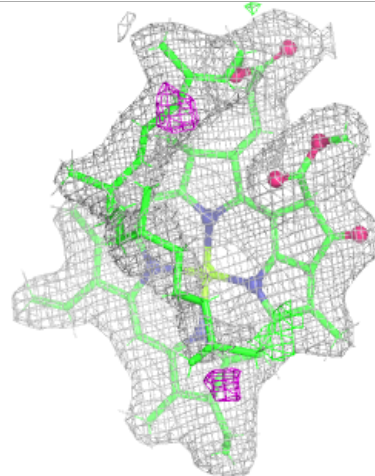
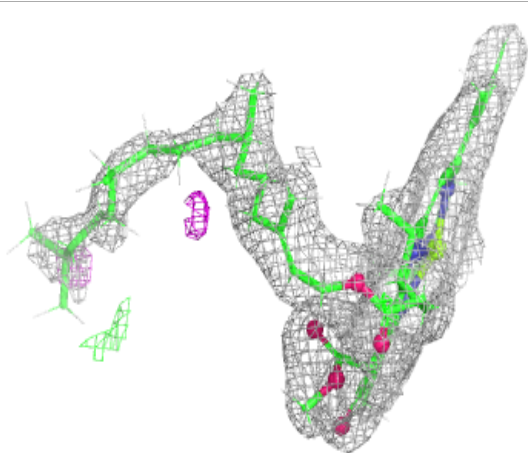
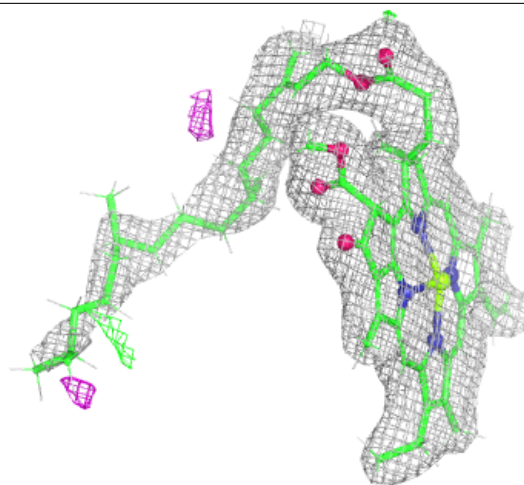
Electron density around CLA B 610:

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



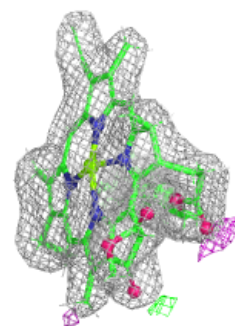
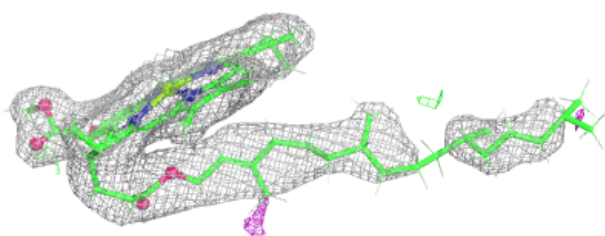
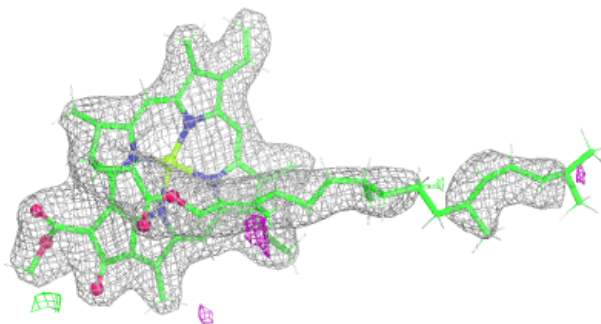
Electron density around CLA b 613:

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

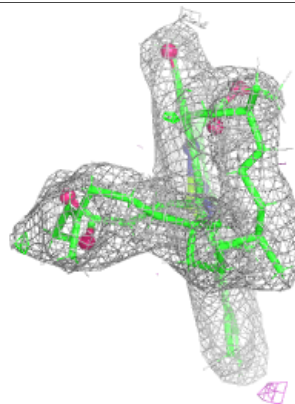
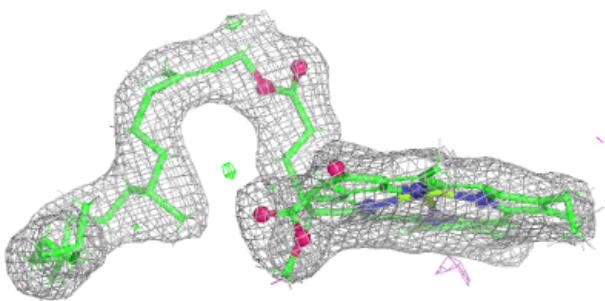
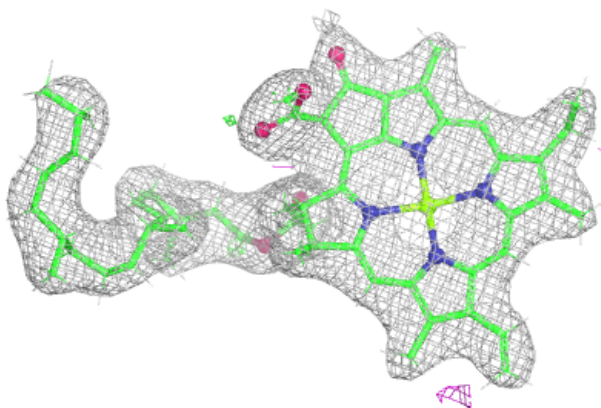


Electron density around CLA b 614:

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

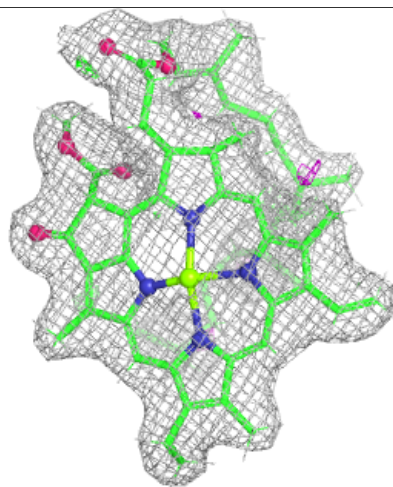
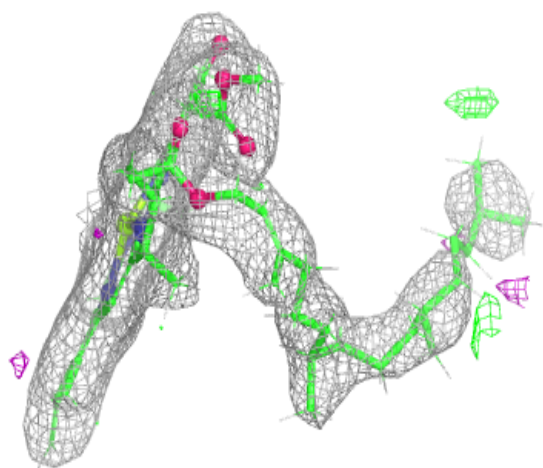
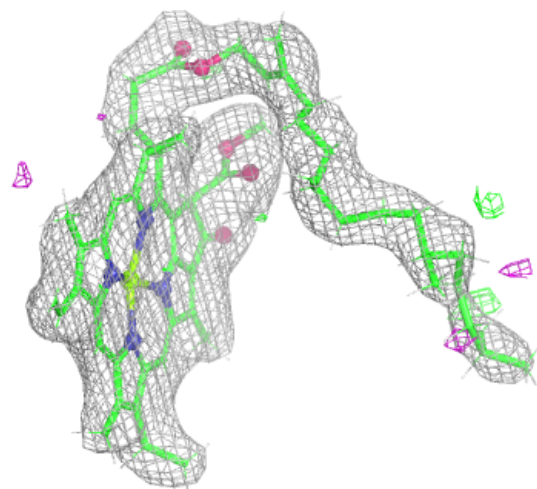
**Electron density around CLA B 611:**

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



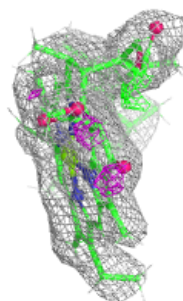
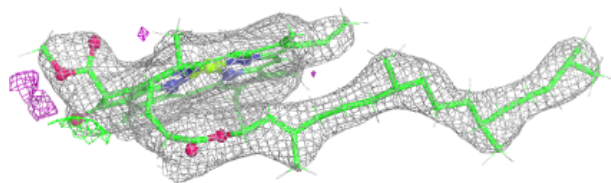
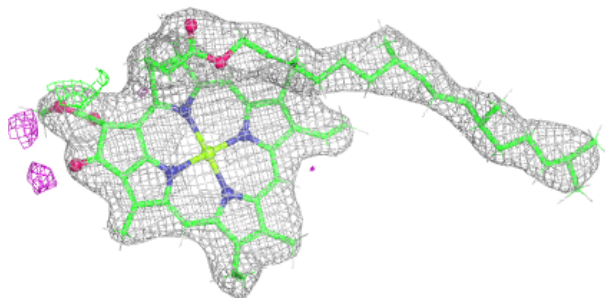
Electron density around CLA B 612:

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

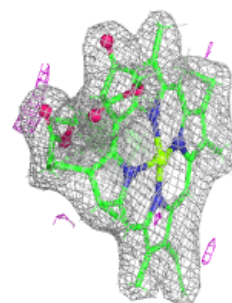
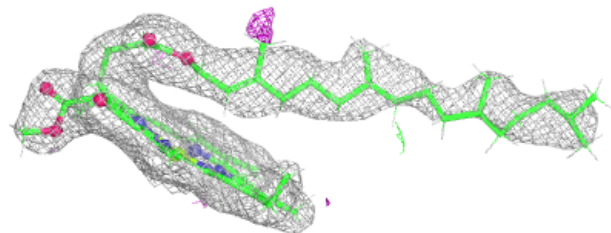
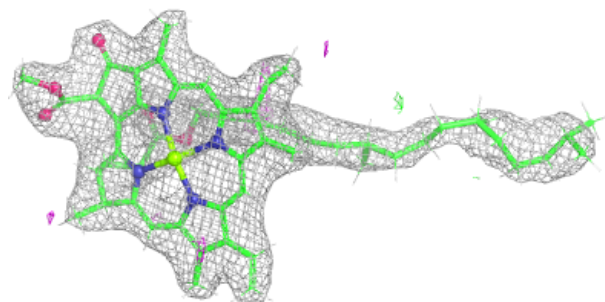


Electron density around CLA c 501:

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

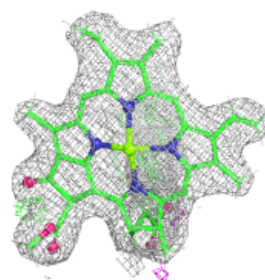
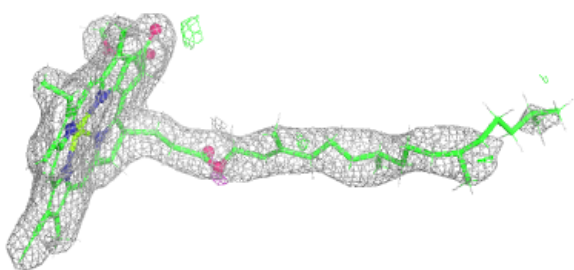
**Electron density around CLA B 613:**

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

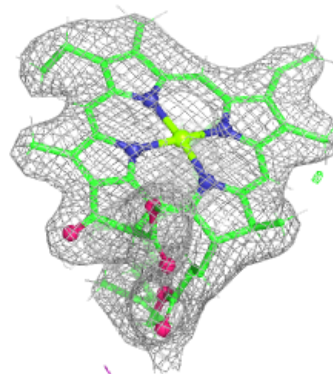
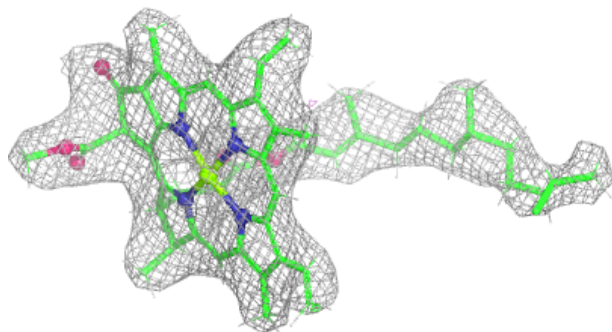
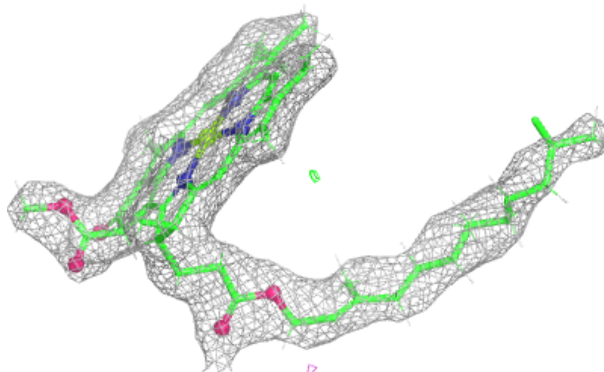


Electron density around CLA B 603:

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

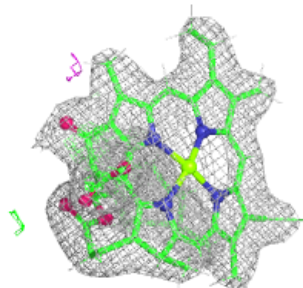
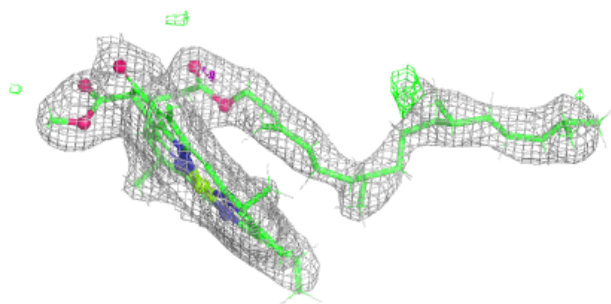
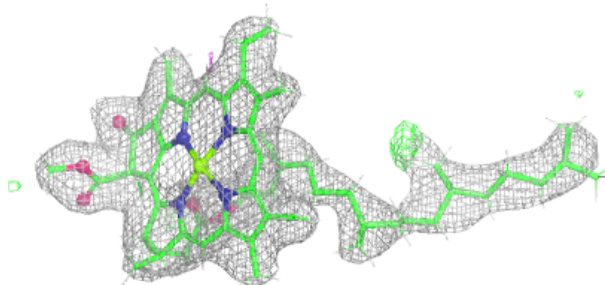
**Electron density around CLA c 504:**

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

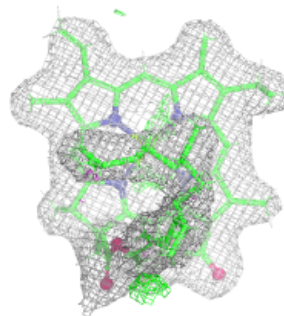
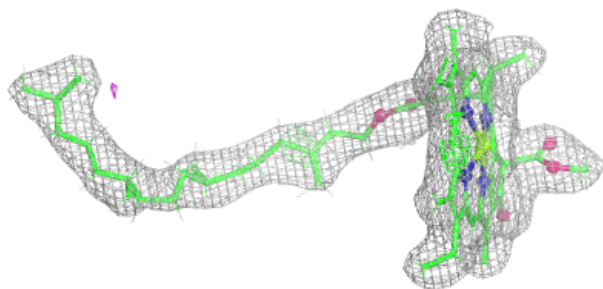
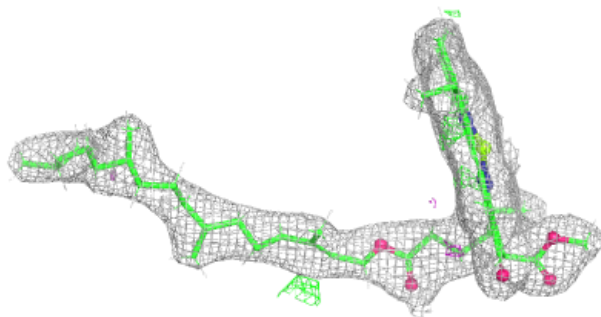


Electron density around CLA c 505:

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

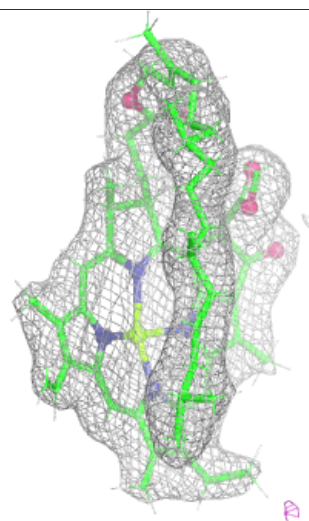
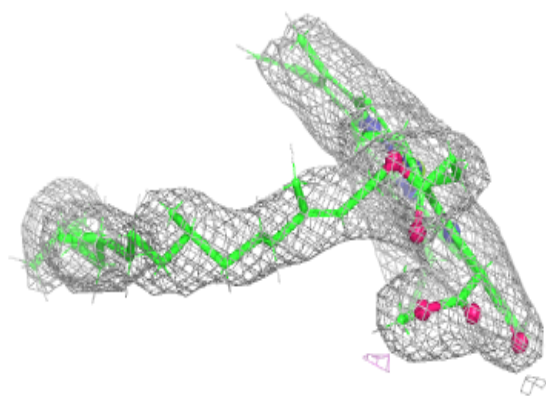
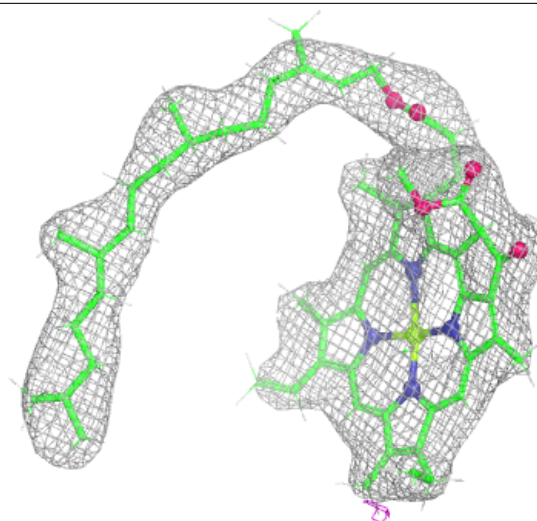
**Electron density around CLA B 604:**

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



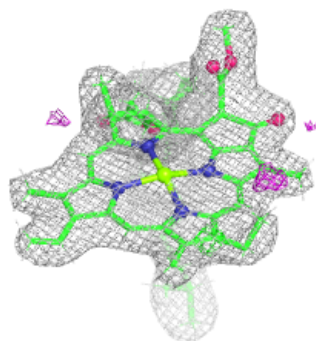
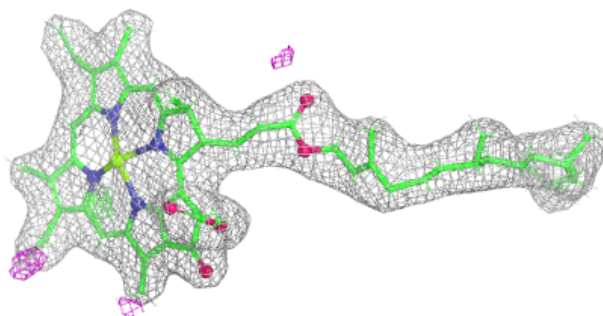
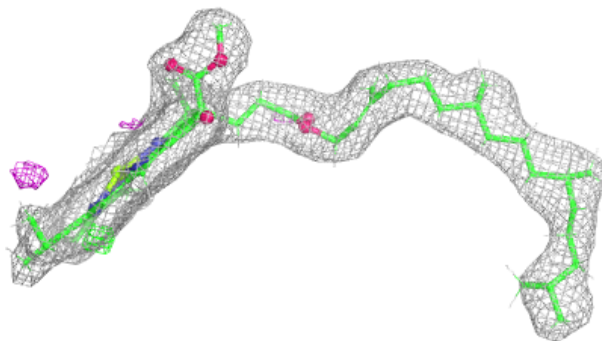
Electron density around CLA c 507:

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

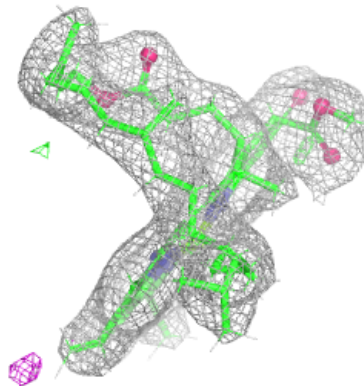
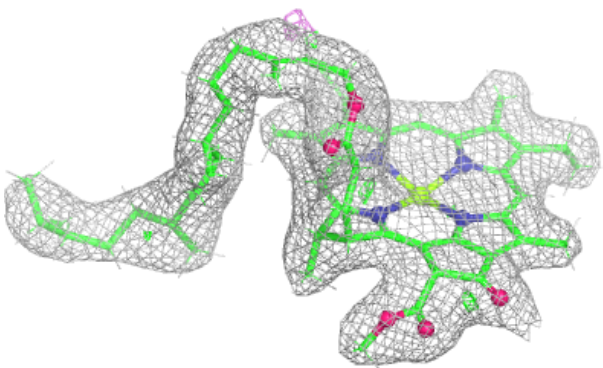
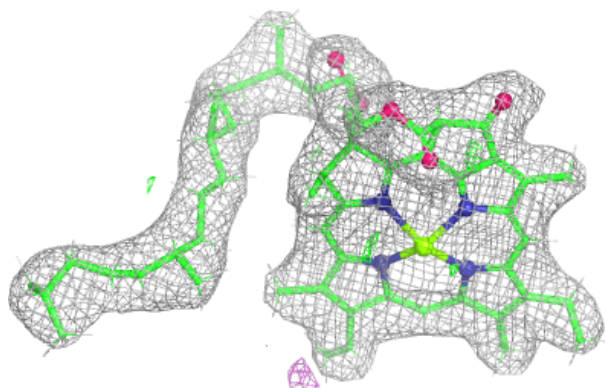


Electron density around CLA D 403:

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

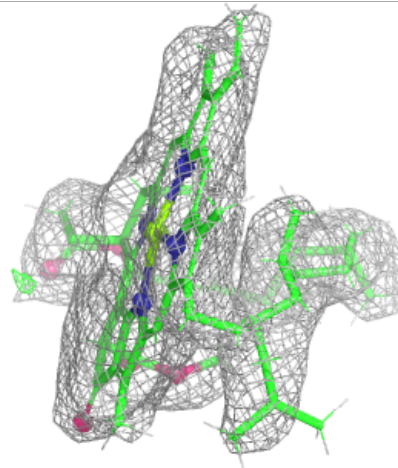
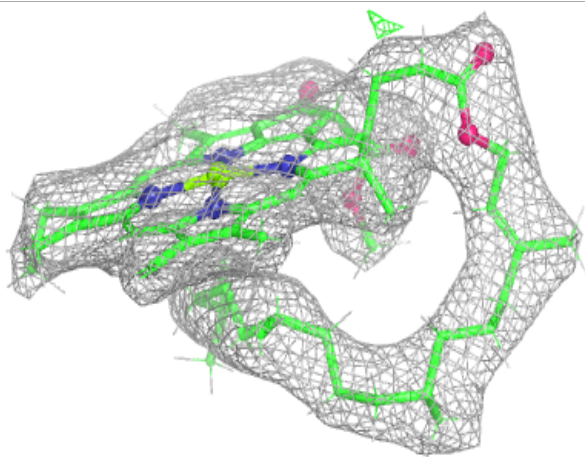
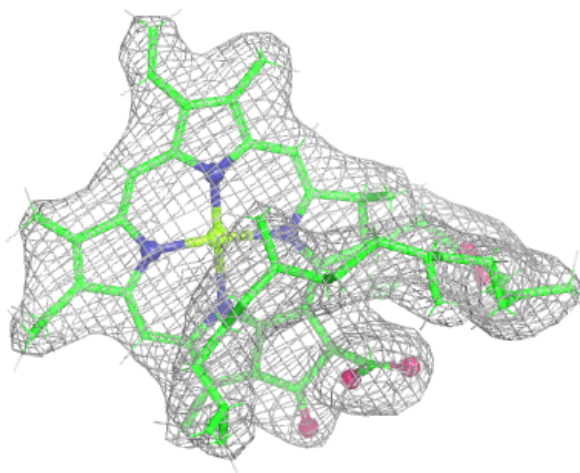
**Electron density around CLA D 404:**

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



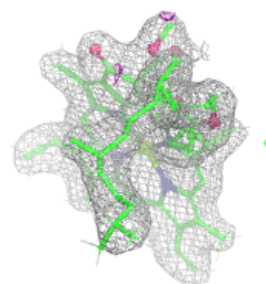
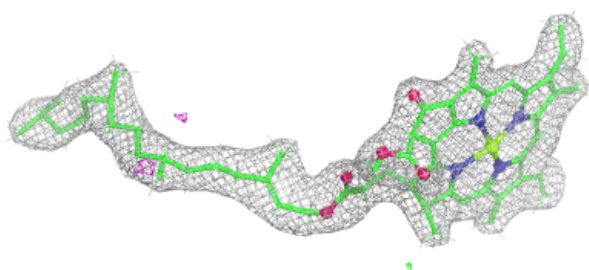
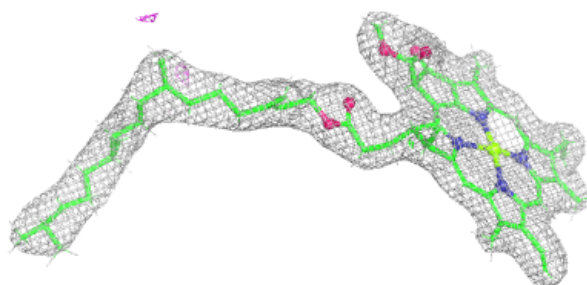
Electron density around CLA c 510:

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

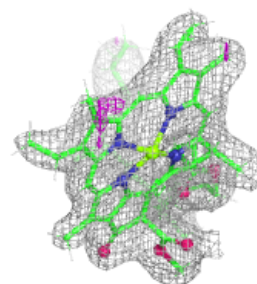
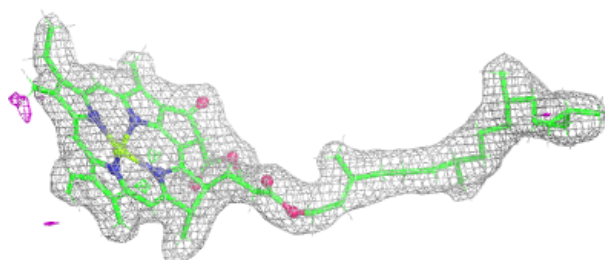
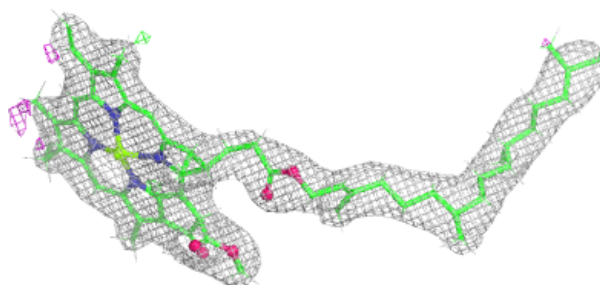


Electron density around CLA A 402:

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

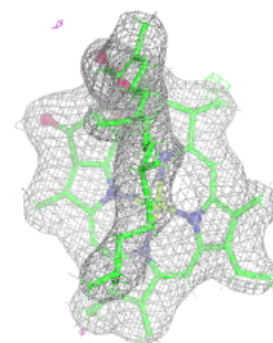
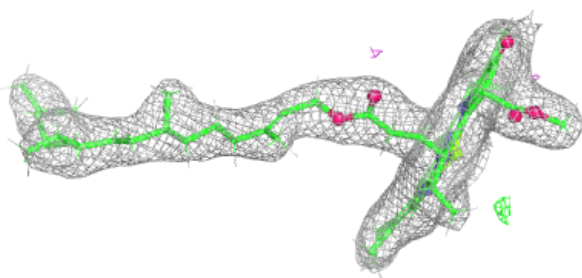
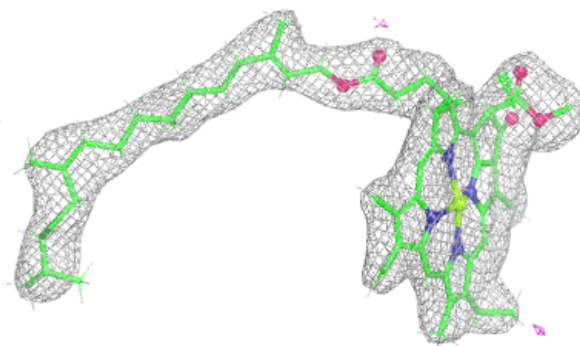
**Electron density around CLA a 402:**

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

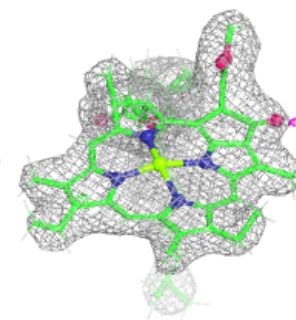
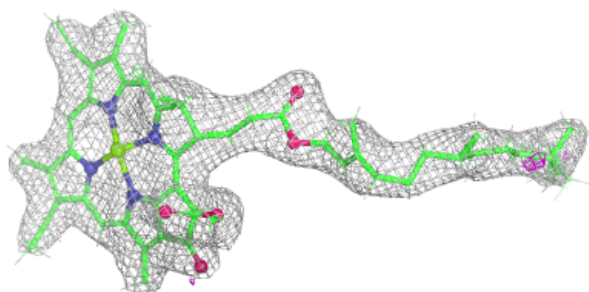
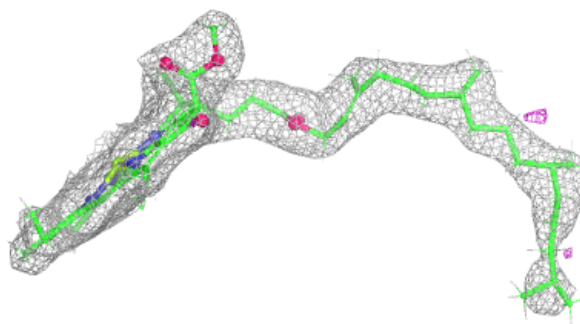


Electron density around CLA B 608:

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

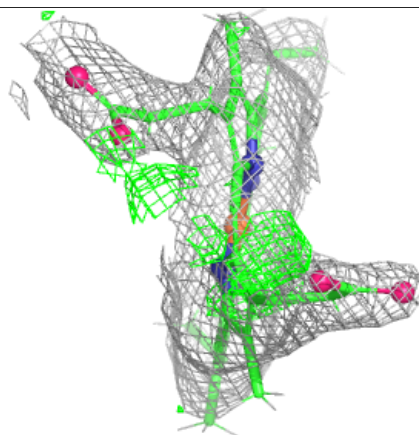
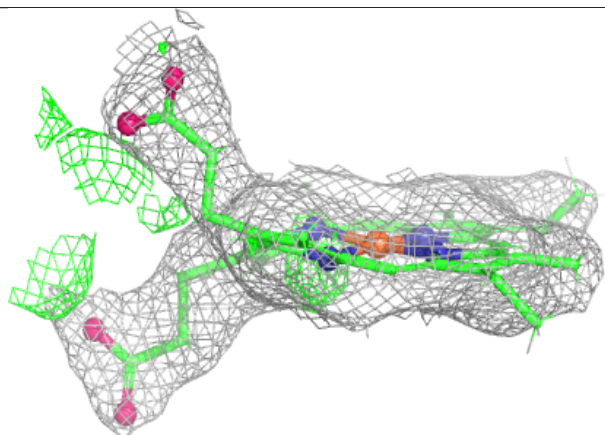
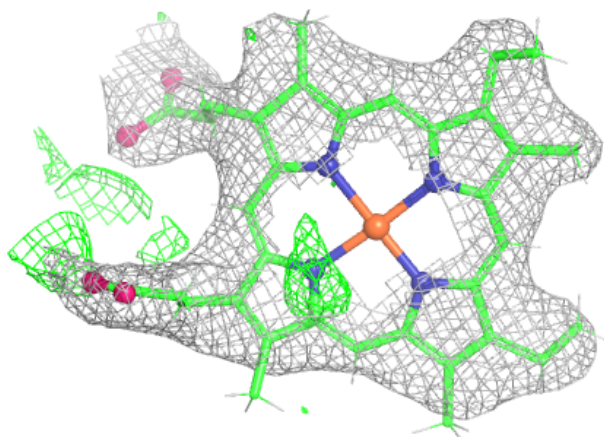
**Electron density around CLA d 403:**

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

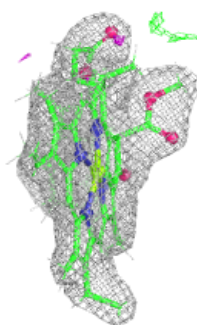
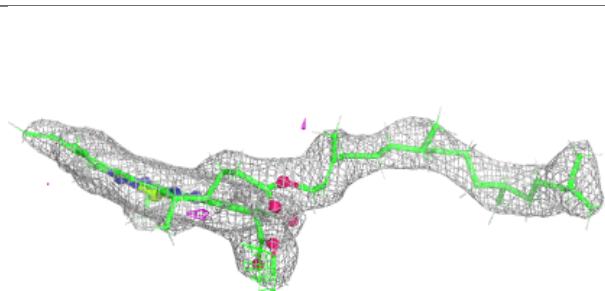
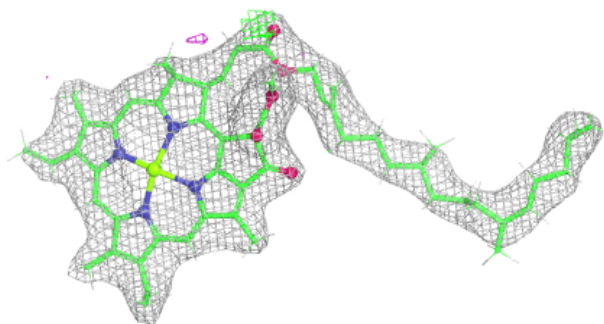


Electron density around HEC f 101:

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

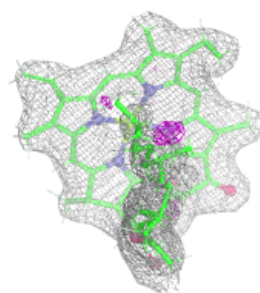
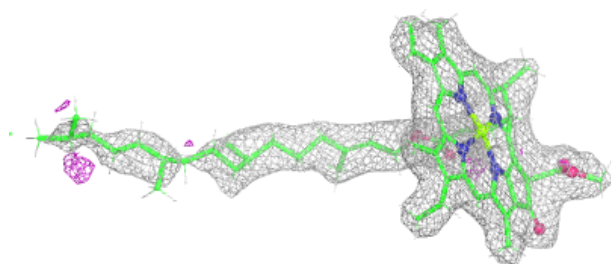
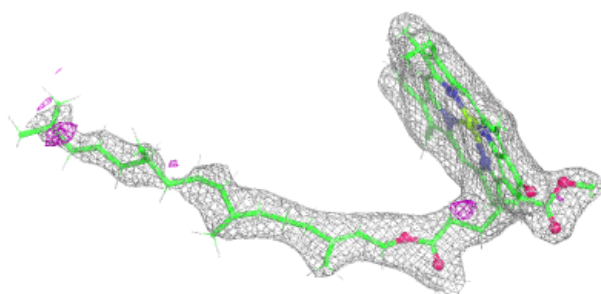
**Electron density around CLA B 601:**

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

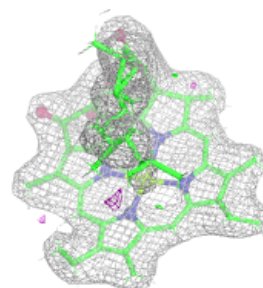
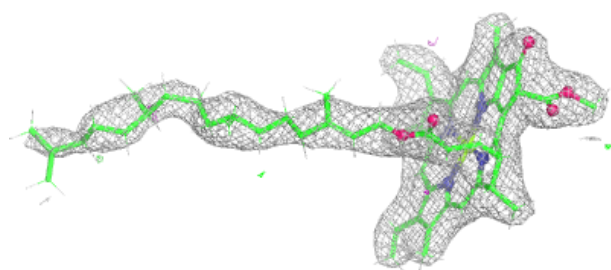
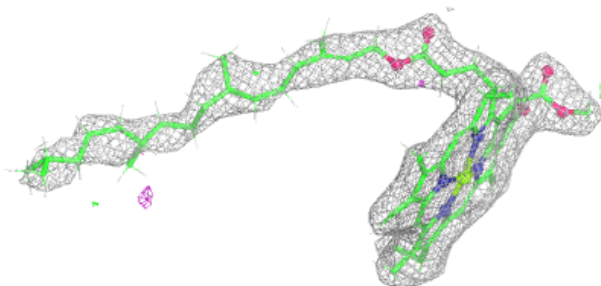


Electron density around CLA b 607:

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

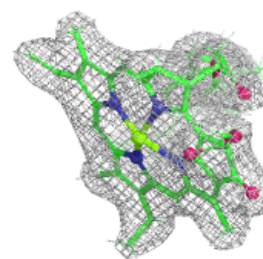
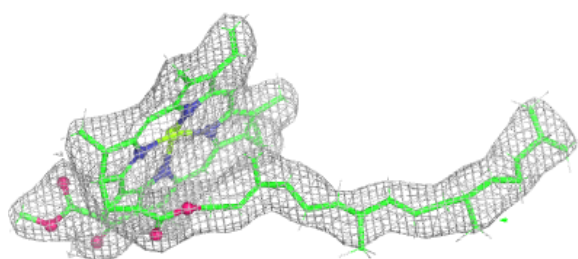
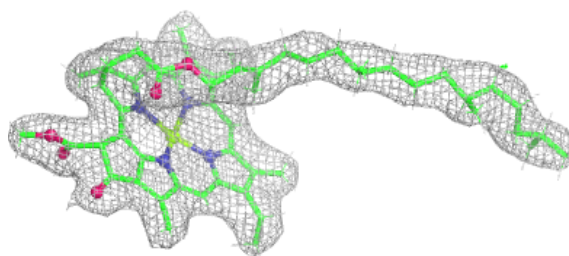
**Electron density around CLA B 606:**

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

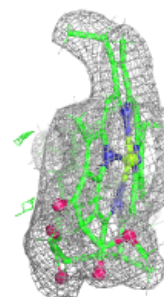
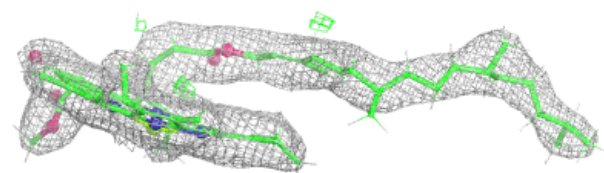
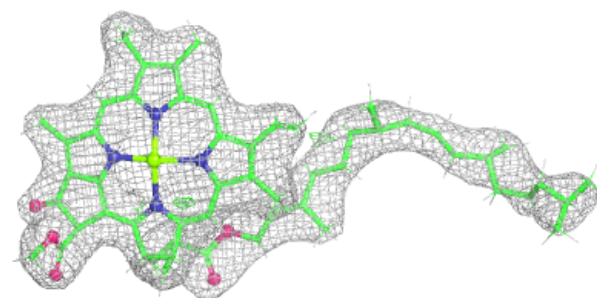


Electron density around CLA B 607:

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

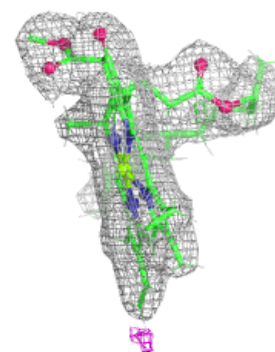
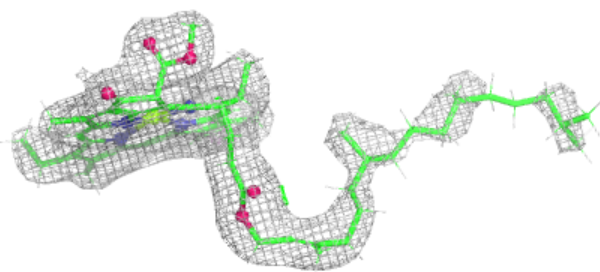
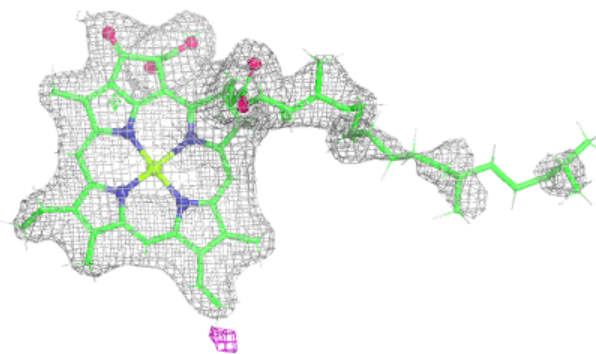
**Electron density around CLA B 602:**

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



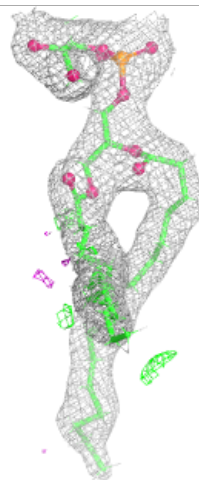
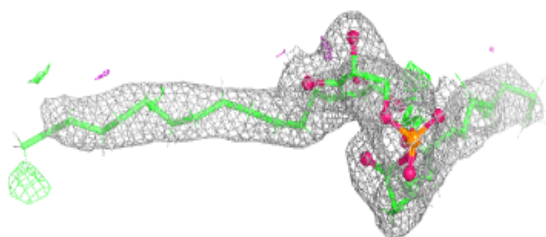
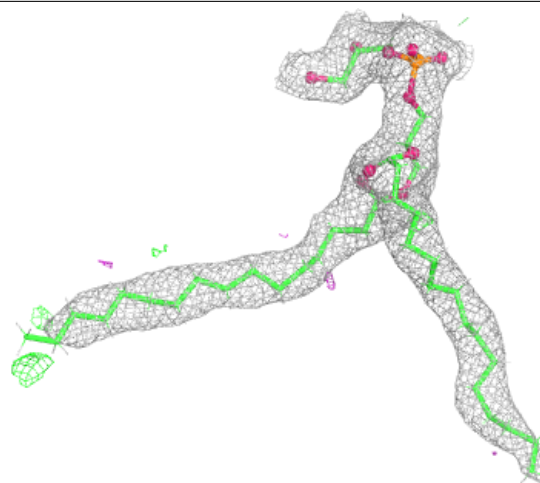
Electron density around CLA A 403:

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



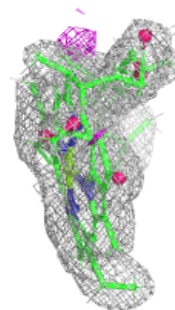
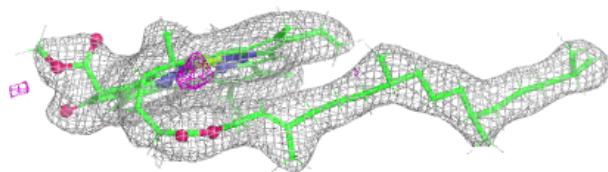
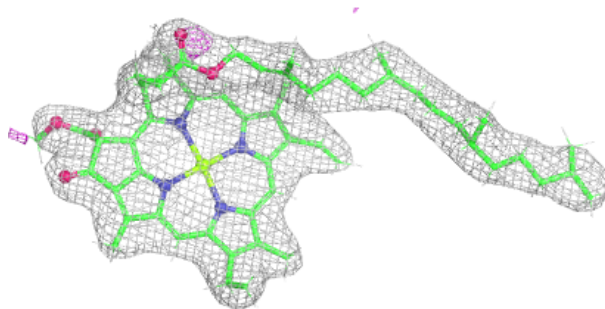
Electron density around LHG L 102:

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

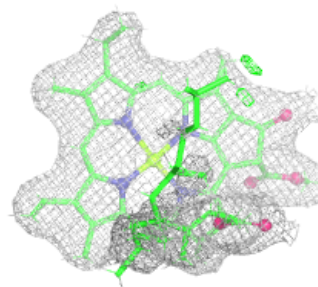
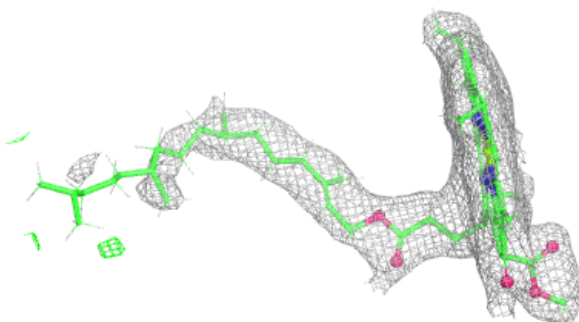
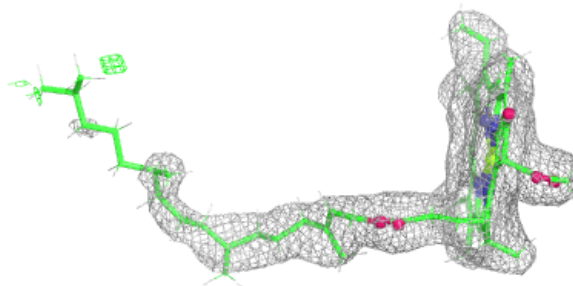


Electron density around CLA C 501:

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

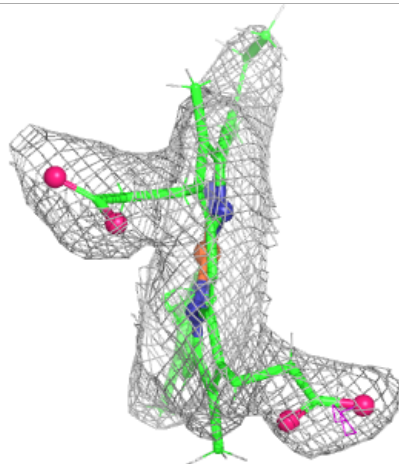
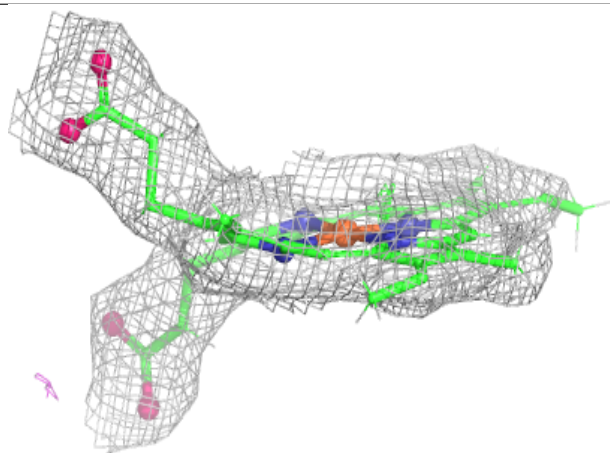
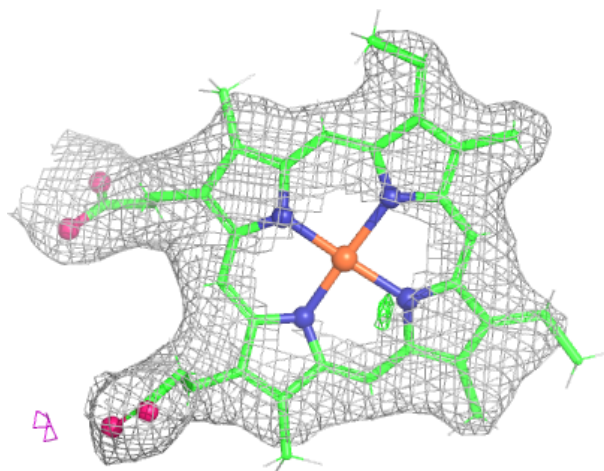
**Electron density around CLA D 405:**

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



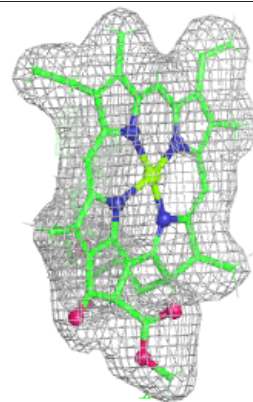
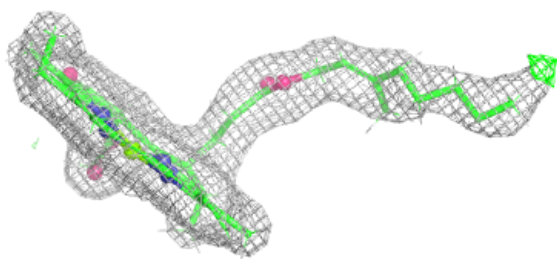
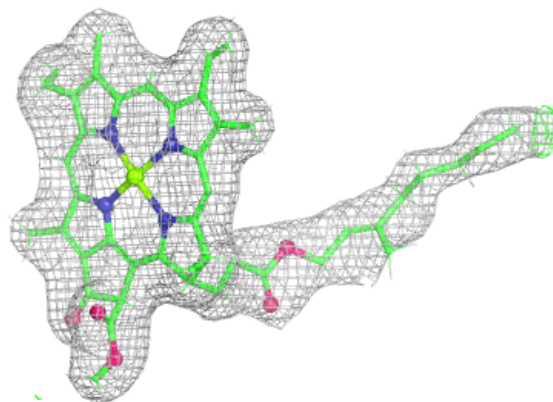
Electron density around HEC F 101:

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



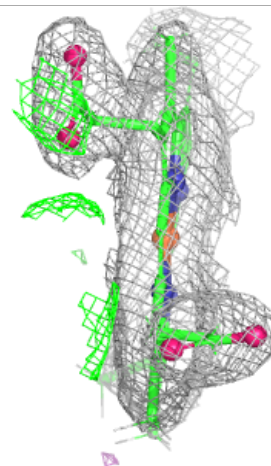
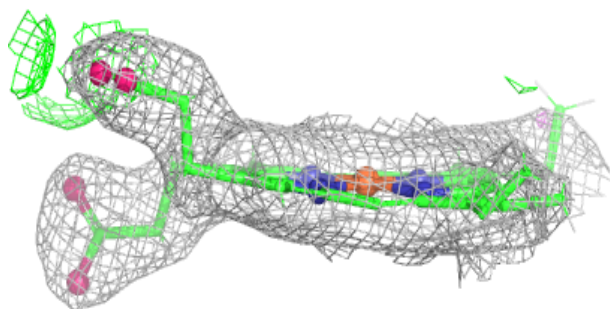
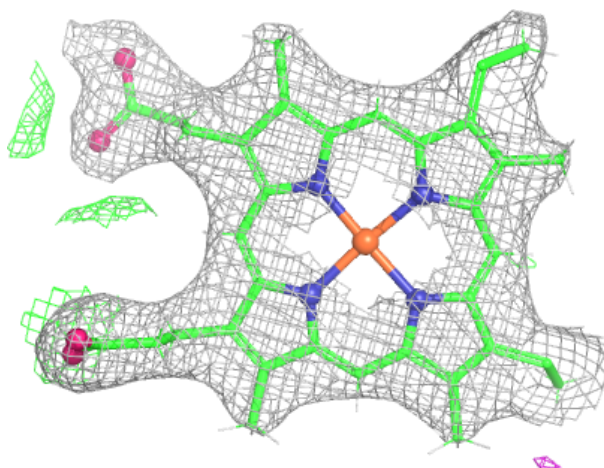
Electron density around CLA A 405:

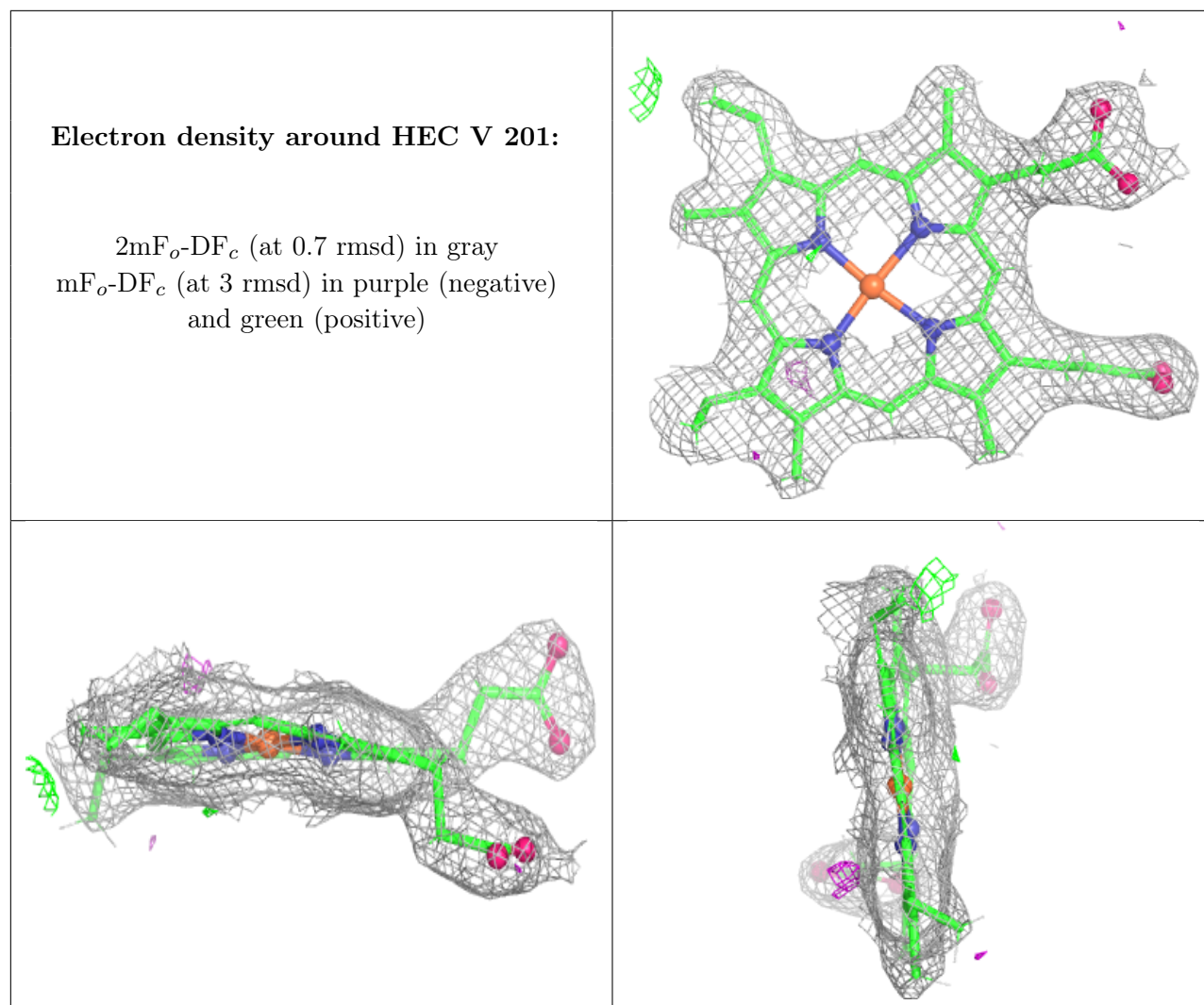
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 201:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.