



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 12:15 PM EDT

PDB ID : 6W1V / pdb_00006w1v
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

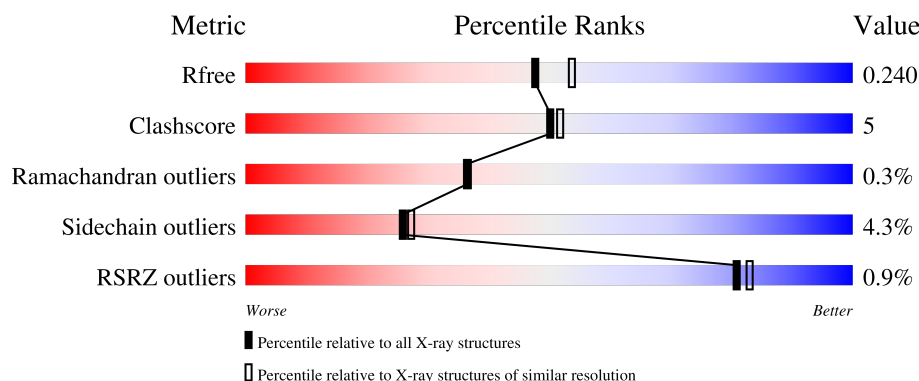
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



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

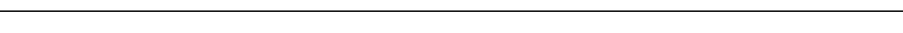
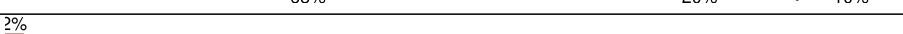
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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

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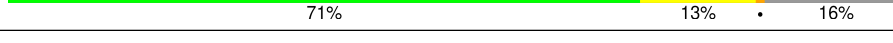
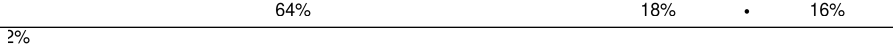
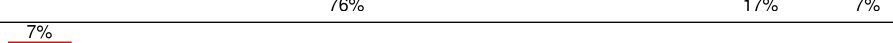
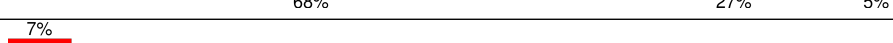
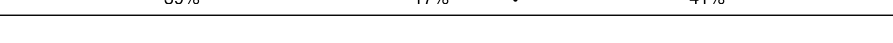
CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	HEC	E	103	X	-	-	-
35	HEC	V	201	X	-	-	-
35	HEC	e	101	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 106211 atoms, of which 52744 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	66	0
			6084	2030	2971	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6072	2027	2962	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			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	14	0
			6928	2302	3419	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7073	2343	3490	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5360	1809	2629	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5372	1813	2635	446	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	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
			490	162	250	42	36			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

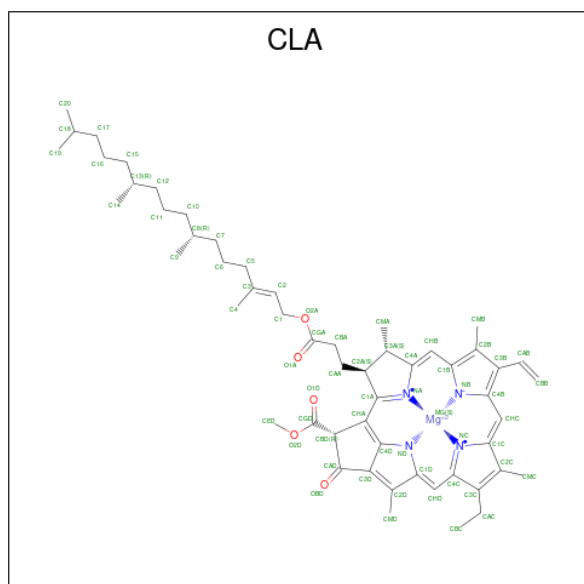
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

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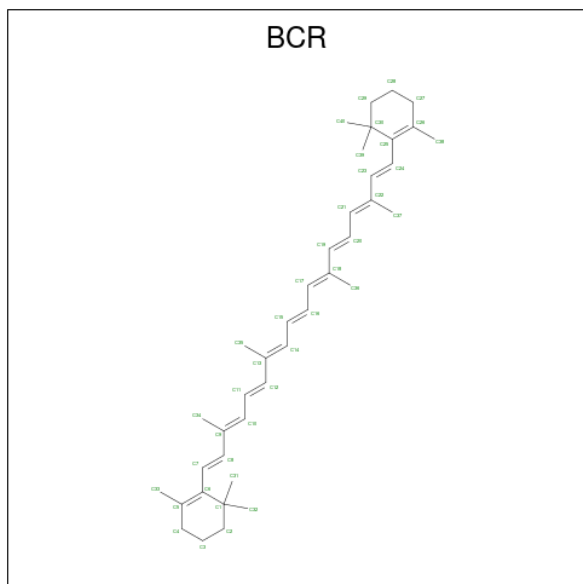
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

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



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

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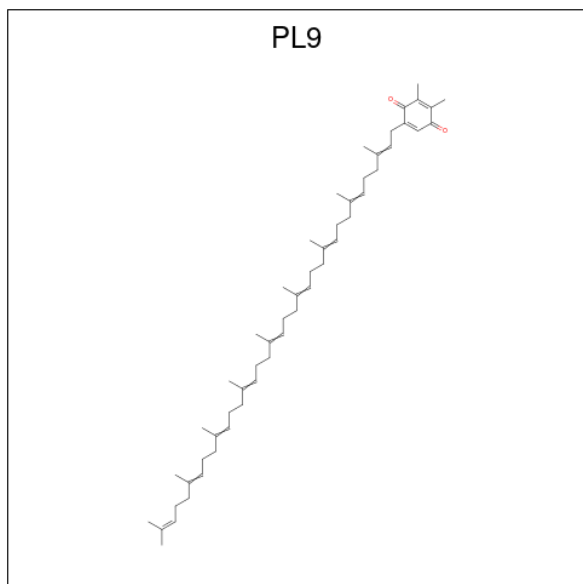
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	H	0	0
			96	40	56		
23	D	1	Total	C	H	0	0
			96	40	56		
23	H	1	Total	C	H	0	0
			96	40	56		
23	K	1	Total	C	H	0	0
			96	40	56		
23	T	1	Total	C	H	0	0
			96	40	56		
23	Y	1	Total	C	H	0	0
			96	40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

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

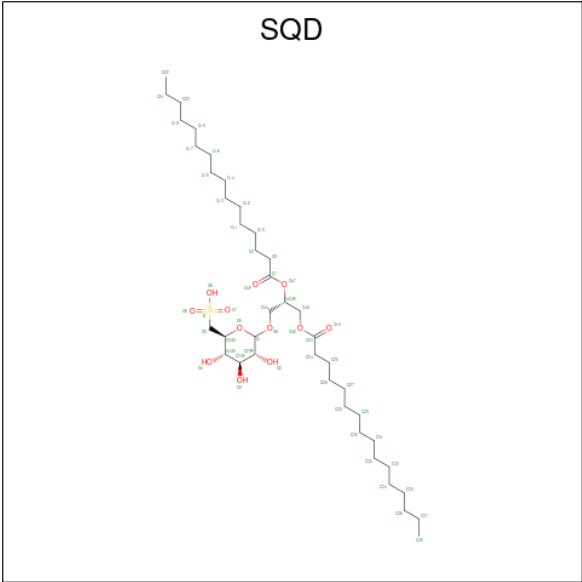
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

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



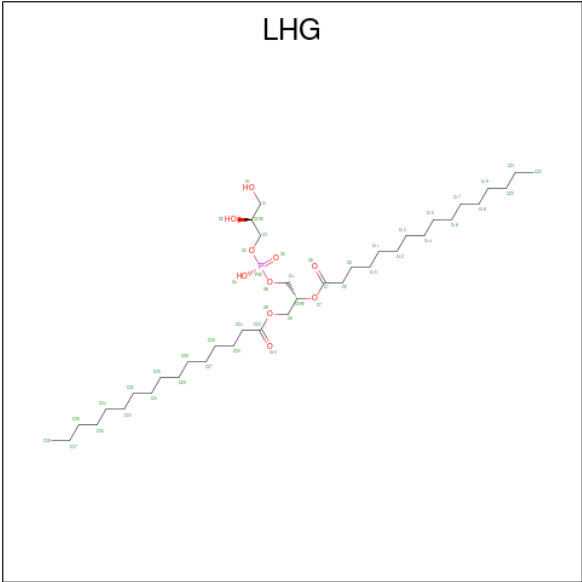
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			135	53	80	2		
25	D	1	Total	C	H	O	0	0
			135	53	80	2		
25	a	1	Total	C	H	O	0	0
			135	53	80	2		
25	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



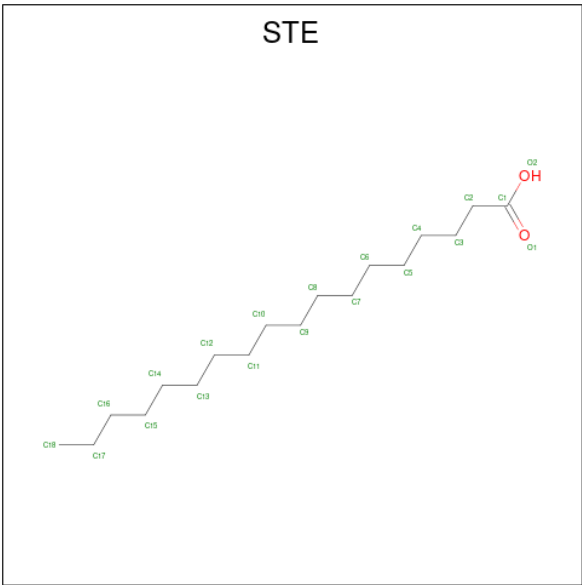
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
26	A	1	Total	C	H	O		0	0
			104	35	65	4			
26	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
26	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
26	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
26	a	1	Total	C	H	O		0	0
			92	31	56	5			
26	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
26	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H 47 16 31	0	0
28	A	1	Total C H 11 5 6	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 43 15 26 2	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 46 16 28 2	0	0
28	B	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	C	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H 17 7 10	0	0
28	H	1	Total C H 53 18 35	0	0
28	H	1	Total C H 20 8 12	0	0

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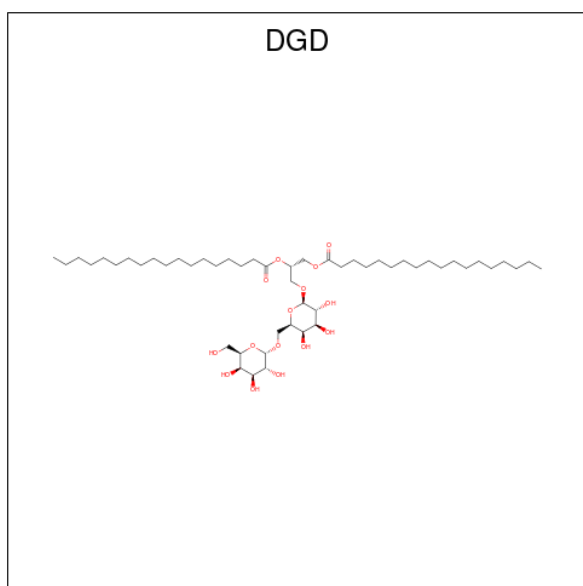
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	I	1	Total C H 41 15 26	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	T	1	Total C H 44 15 29	0	0
28	X	1	Total C H O 55 18 35 2	0	0
28	Z	1	Total C H 20 8 12	0	0
28	a	1	Total C H 26 10 16	0	0
28	a	1	Total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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	x	1	Total	C	H	O	0	0
			55	18	35	2		

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



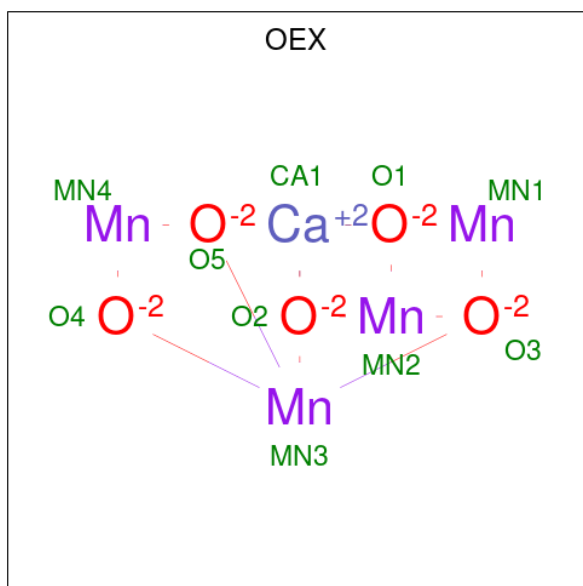
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			142	47	80	15		

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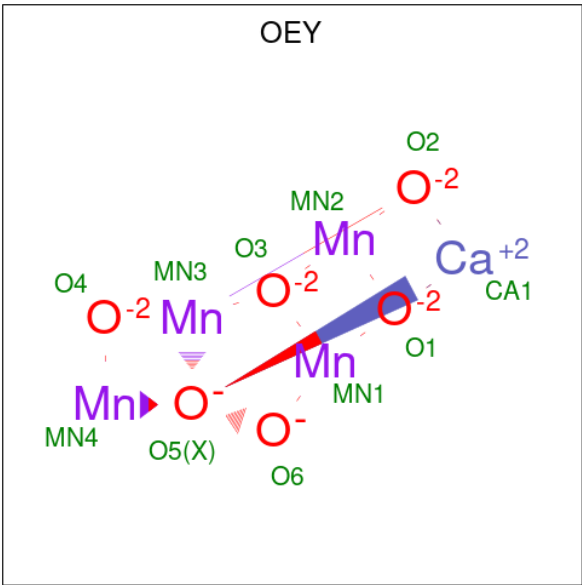
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	h	1	Total	C	H	O	0	0
			142	47	80	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



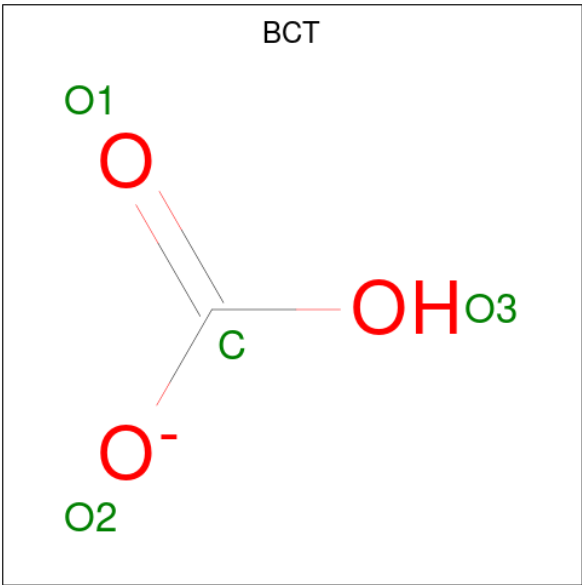
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



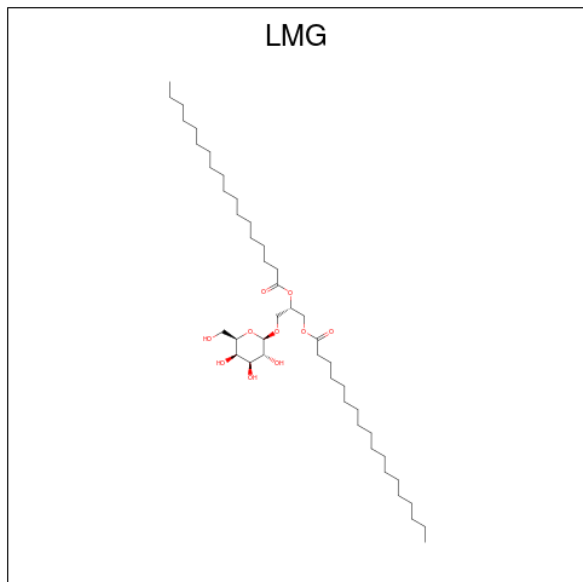
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
31	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



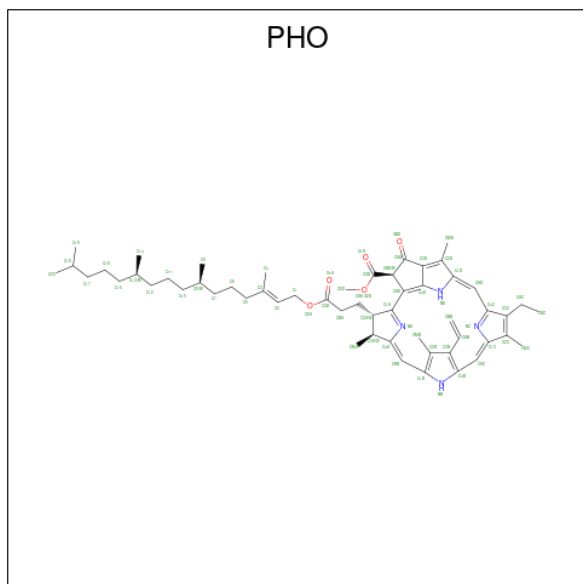
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			68	24	40	4		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			123	41	72	10		
33	D	1	Total	C	H	O	0	0
			77	27	45	5		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	a	1	Total	C	H	O	0	0
			141	45	86	10		
33	b	1	Total	C	H	O	0	0
			123	41	72	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		

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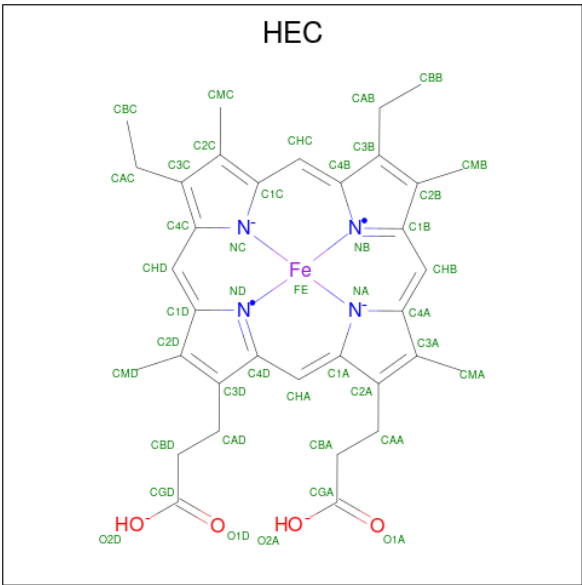
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	145	Total	O	0	8
			145	145		
36	B	233	Total	O	0	0
			233	233		
36	C	168	Total	O	0	0
			168	168		
36	D	115	Total	O	0	0
			115	115		
36	E	37	Total	O	0	0
			37	37		
36	F	6	Total	O	0	0
			6	6		
36	H	35	Total	O	0	0
			35	35		
36	I	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	15	Total 15	O 15	0	0
36	K	3	Total 3	O 3	0	0
36	L	9	Total 9	O 9	0	0
36	M	8	Total 8	O 8	0	0
36	O	106	Total 106	O 106	0	0
36	R	3	Total 3	O 3	0	0
36	T	9	Total 9	O 9	0	0
36	U	53	Total 53	O 53	0	0
36	V	63	Total 63	O 63	0	0
36	X	17	Total 17	O 17	0	0
36	Y	3	Total 3	O 3	0	0
36	a	130	Total 130	O 130	0	8
36	b	193	Total 193	O 193	0	0
36	c	169	Total 169	O 169	0	0
36	d	106	Total 106	O 106	0	0
36	e	23	Total 23	O 23	0	0
36	f	4	Total 4	O 4	0	0
36	h	22	Total 22	O 22	0	0
36	i	17	Total 17	O 17	0	0
36	j	7	Total 7	O 7	0	0
36	k	4	Total 4	O 4	0	0

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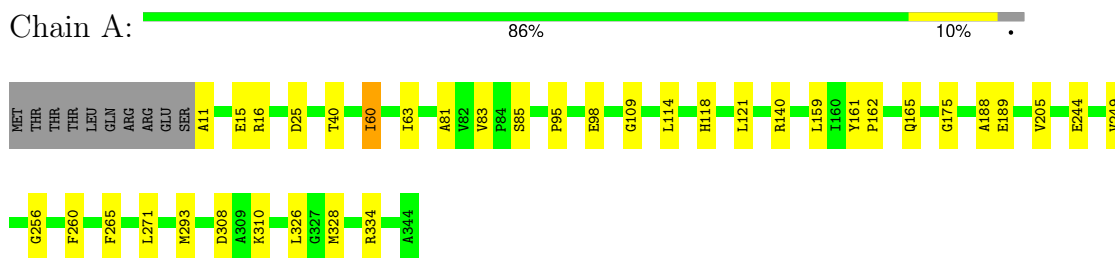
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	l	12	Total 12	O 12	0	0
36	m	5	Total 5	O 5	0	0
36	o	97	Total 97	O 97	0	0
36	r	8	Total 8	O 8	0	0
36	t	7	Total 7	O 7	0	0
36	u	63	Total 63	O 63	0	0
36	v	64	Total 64	O 64	0	0
36	x	7	Total 7	O 7	0	0
36	y	8	Total 8	O 8	0	0
36	z	8	Total 8	O 8	0	0

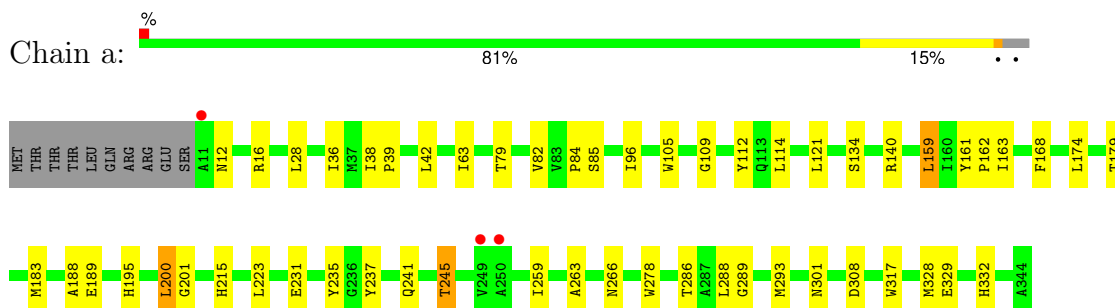
3 Residue-property plots [i](#)

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.

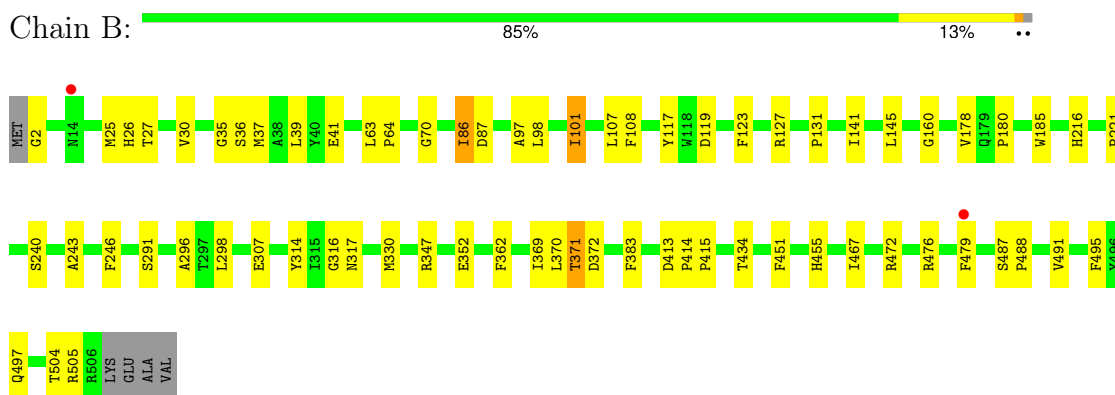
- Molecule 1: Photosystem II protein D1 1



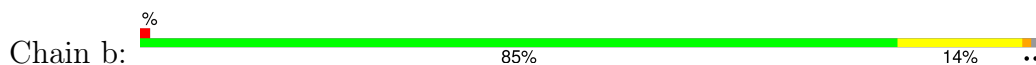
- Molecule 1: Photosystem II protein D1 1

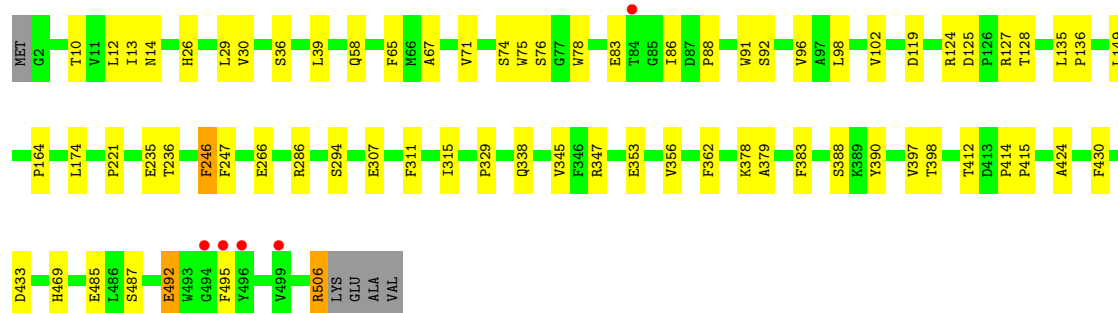


- Molecule 2: Photosystem II CP47 reaction center protein



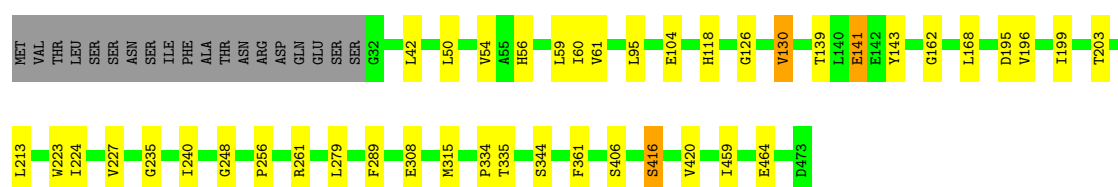
- Molecule 2: Photosystem II CP47 reaction center protein





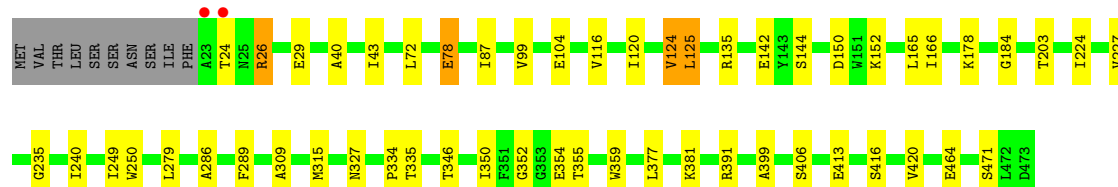
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 9% . .



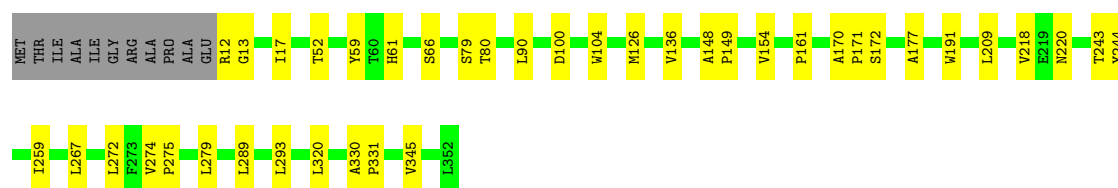
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 11% . .



• Molecule 4: Photosystem II D2 protein

Chain D: 86% 11% .



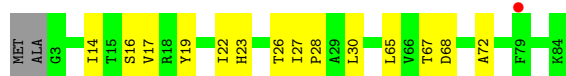
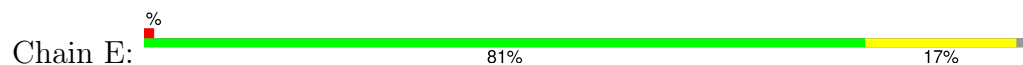
• Molecule 4: Photosystem II D2 protein

Chain d: 84% 13% .





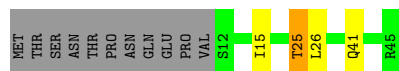
- Molecule 5: Cytochrome b559 subunit alpha



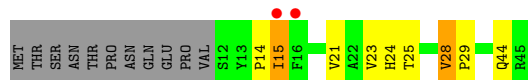
- Molecule 5: Cytochrome b559 subunit alpha



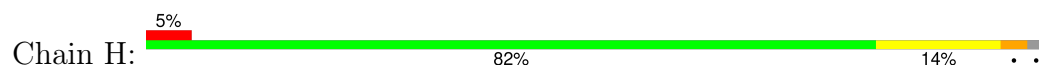
- Molecule 6: Cytochrome b559 subunit beta



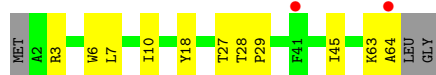
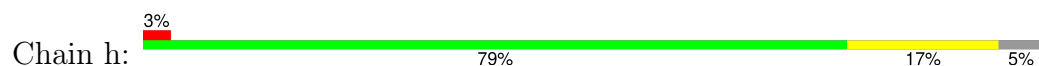
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  87% 8% 5%



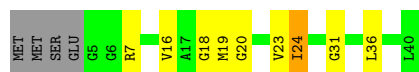
- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



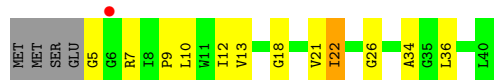
- Molecule 9: Photosystem II reaction center protein J

Chain J:  68% 20% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 60% 28% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  54% 20% 7% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  52% 28% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  89% 11%



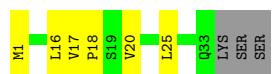
- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 16% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



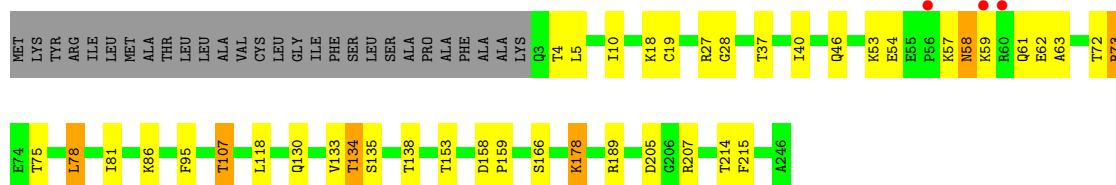
- Molecule 12: Photosystem II reaction center protein M

Chain m:  67% 19% . 11%



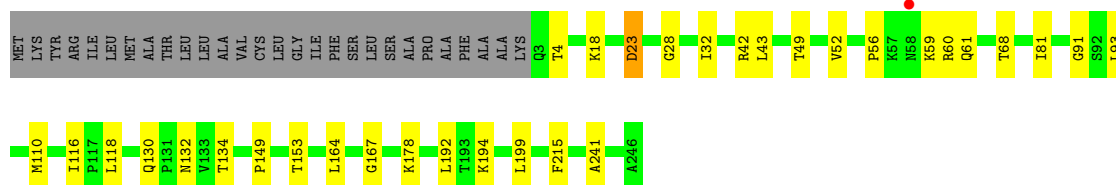
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  % 74% 13% . 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  78% 12% 10%

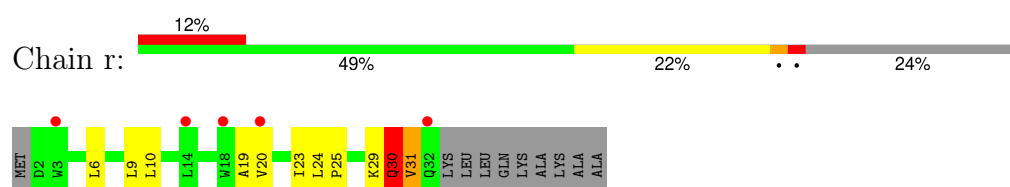


- Molecule 14: Photosystem II protein Y

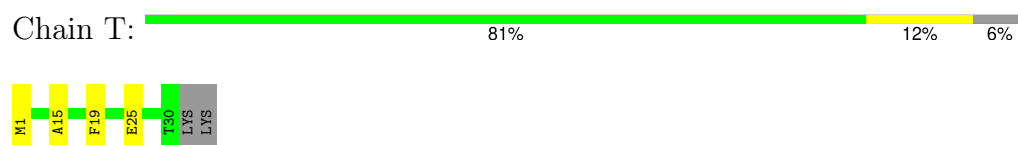
Chain R:  7% 59% 20% 5% 17%



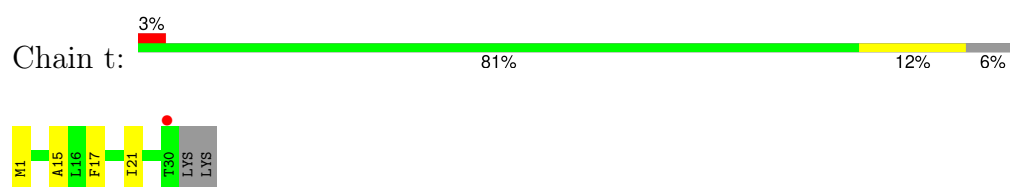
- Molecule 14: Photosystem II protein Y



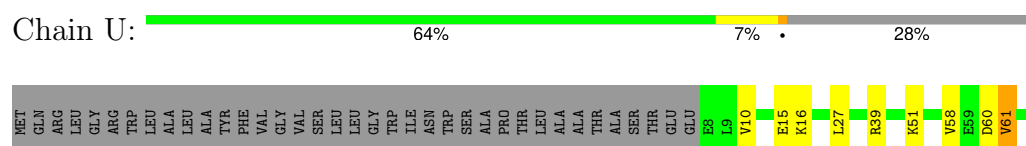
- Molecule 15: Photosystem II reaction center protein T



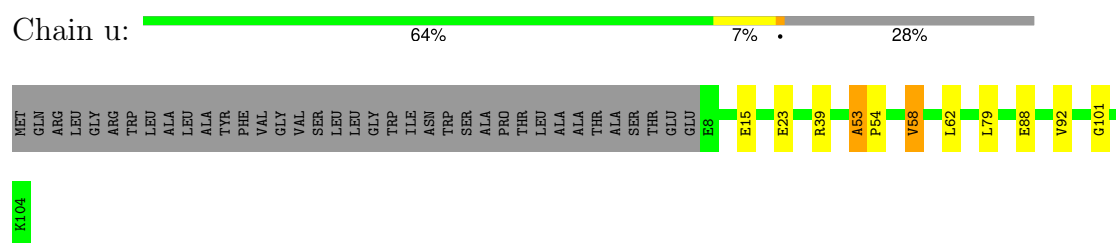
- Molecule 15: Photosystem II reaction center protein T



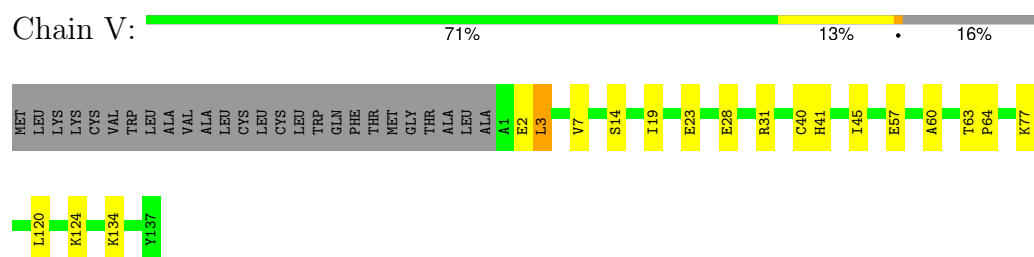
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein

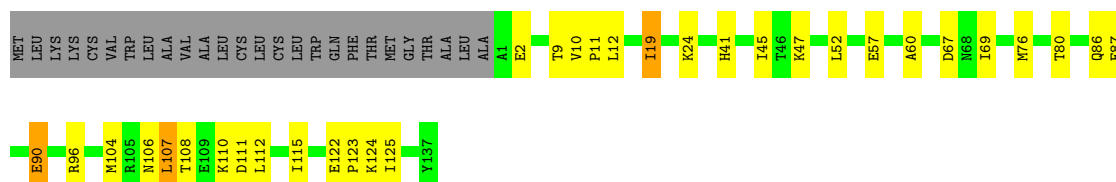


- Molecule 17: Cytochrome c-550

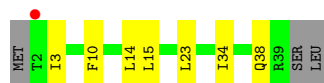
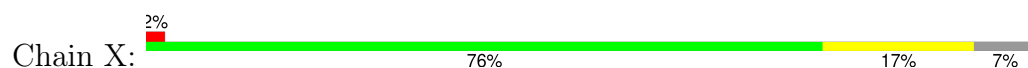


- Molecule 17: Cytochrome c-550





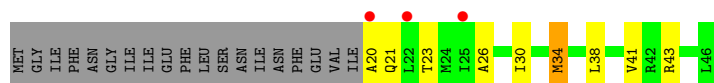
- Molecule 18: Photosystem II reaction center X protein



- 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	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.65-2.09) 84.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.240	Depositor DCC
R_{free} test set	4165 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.3	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	106211	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: OEY, HEC, LMG, FME, CL, OEX, DGD, PL9, PHO, FE2, SQD, STE, CLA, BCR, BCT, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/3227	0.65	0/4397
1	a	0.54	0/3224	0.64	0/4393
2	B	0.60	0/4161	0.69	0/5669
2	b	0.60	0/4118	0.66	0/5611
3	C	0.59	0/3647	0.67	0/4965
3	c	0.54	0/3719	0.66	0/5061
4	D	0.64	0/2825	0.70	0/3847
4	d	0.62	0/2834	0.70	0/3859
5	E	0.47	0/688	0.59	0/940
5	e	0.42	0/683	0.55	0/932
6	F	0.50	0/284	0.56	0/387
6	f	0.46	0/284	0.63	0/387
7	H	0.61	0/523	0.68	0/713
7	h	0.51	0/511	0.62	0/697
8	I	0.57	0/293	0.66	0/396
8	i	0.59	0/293	0.60	0/396
9	J	0.47	0/263	0.62	0/356
9	j	0.47	0/263	0.51	0/356
10	K	0.48	0/303	0.59	0/416
10	k	0.42	0/303	0.57	0/416
11	L	0.64	0/311	0.71	0/422
11	l	0.65	0/303	0.71	0/412
12	M	0.64	0/249	0.78	0/341
12	m	0.63	0/244	0.70	0/334
13	O	0.57	0/1904	0.67	0/2585
13	o	0.59	0/1905	0.68	0/2583
14	R	0.39	0/277	0.72	0/380
14	r	0.36	0/246	0.63	2/339 (0.6%)
15	T	0.63	0/257	0.77	0/349
15	t	0.62	0/255	0.64	0/346
16	U	0.51	0/785	0.65	0/1064
16	u	0.57	0/785	0.71	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.59	0/1085	0.72	0/1473
17	v	0.54	0/1085	0.64	0/1473
18	X	0.44	0/284	0.56	0/384
18	x	0.38	0/289	0.52	0/391
19	Y	0.43	0/197	0.56	0/264
19	y	0.34	0/219	0.51	0/294
20	Z	0.40	0/490	0.58	0/669
20	z	0.32	0/488	0.48	0/666
All	All	0.57	0/44104	0.66	2/60027 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	r	30	GLN	CA-C-N	5.57	131.72	121.70
14	r	30	GLN	C-N-CA	5.57	131.72	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	2971	2963	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3110	2962	2954	33	0
2	B	4005	3859	3867	40	0
2	b	3978	3822	3836	44	0
3	C	3509	3419	3409	25	0
3	c	3583	3490	3492	34	0
4	D	2731	2629	2637	30	0
4	d	2737	2635	2643	36	0
5	E	666	650	651	8	0
5	e	664	647	648	17	0
6	F	275	281	282	4	0
6	f	275	281	282	5	0
7	H	510	532	532	6	0
7	h	498	518	518	5	0
8	I	296	311	311	0	0
8	i	296	311	311	1	0
9	J	257	268	268	10	0
9	j	257	268	268	9	0
10	K	293	305	305	8	0
10	k	293	305	305	6	0
11	L	304	316	316	4	0
11	l	296	304	304	2	0
12	M	256	269	269	4	0
12	m	251	267	267	5	0
13	O	1870	1828	1830	27	0
13	o	1874	1844	1846	14	0
14	R	271	298	298	5	0
14	r	240	250	250	9	0
15	T	258	261	261	1	0
15	t	256	256	256	3	0
16	U	774	772	773	7	0
16	u	774	772	773	8	0
17	V	1064	1068	1073	19	0
17	v	1064	1068	1073	22	0
18	X	281	312	312	2	0
18	x	286	316	314	8	0
19	Y	196	217	217	4	0
19	y	218	241	241	6	0
20	Z	479	516	516	8	0
20	z	477	509	509	9	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	970	1067	1067	10	0
22	C	839	922	922	14	0
22	D	195	216	216	2	0
22	H	65	72	72	2	0
22	a	260	288	288	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	8	0
22	d	130	144	144	1	0
23	A	40	56	56	1	0
23	B	120	168	168	8	0
23	C	80	112	112	2	0
23	D	40	56	56	2	0
23	H	40	56	56	4	0
23	K	40	56	56	1	0
23	T	40	56	56	1	0
23	Y	40	56	56	3	0
23	a	40	56	56	2	0
23	b	120	168	168	3	0
23	c	80	112	112	3	0
23	d	40	56	56	2	0
23	h	40	56	56	1	0
23	k	80	112	112	2	0
23	t	40	56	56	3	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	3	0
25	D	55	80	80	2	0
25	a	55	80	80	4	0
25	d	55	80	80	0	0
26	A	91	136	135	0	0
26	B	54	78	78	0	0
26	D	36	46	46	0	0
26	a	90	133	133	0	0
26	b	49	65	65	1	0
26	f	41	48	48	0	0
27	A	49	74	74	0	0
27	B	49	74	74	1	0
27	D	96	141	141	1	0
27	L	49	74	74	0	0
27	a	91	131	131	1	0
27	d	88	125	125	5	0
27	l	49	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	21	37	37	0	0
28	B	75	117	117	1	0
28	C	40	63	63	0	0
28	E	19	26	26	1	0
28	H	26	47	47	0	0
28	I	15	26	26	1	0
28	J	12	16	16	0	0
28	M	25	38	38	0	0
28	T	15	29	29	0	0
28	X	20	35	35	0	0
28	Z	8	12	12	0	0
28	a	37	58	58	1	0
28	b	86	145	145	5	0
28	c	32	51	51	0	0
28	d	17	26	26	0	0
28	h	14	27	27	1	0
28	j	12	16	16	1	0
28	l	18	35	35	0	0
28	m	12	16	16	0	0
28	t	14	20	20	0	0
28	x	20	35	35	2	0
29	A	66	96	96	2	0
29	C	186	245	245	1	0
29	H	62	81	81	0	0
29	c	186	243	243	1	0
29	h	62	80	81	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	11	0	0	2	0
31	a	11	0	0	1	0
32	A	4	1	1	0	0
32	a	4	1	1	0	0
33	B	28	40	40	0	0
33	C	96	132	132	0	0
33	D	83	117	117	1	0
33	M	51	72	72	0	0
33	a	55	86	86	4	0
33	b	106	158	158	2	0
33	c	134	181	181	1	0
33	d	44	58	58	0	0
34	D	128	148	148	1	0
34	a	64	74	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	d	64	74	74	1	0
35	E	43	32	32	3	0
35	V	43	30	31	6	0
35	e	43	32	32	6	0
35	v	43	30	30	0	0
36	A	145	0	0	4	0
36	B	233	0	0	3	1
36	C	168	0	0	0	1
36	D	115	0	0	0	0
36	E	37	0	0	0	0
36	F	6	0	0	0	0
36	H	35	0	0	1	0
36	I	20	0	0	0	0
36	J	15	0	0	5	0
36	K	3	0	0	2	0
36	L	9	0	0	0	0
36	M	8	0	0	0	0
36	O	106	0	0	7	0
36	R	3	0	0	0	0
36	T	9	0	0	0	0
36	U	53	0	0	3	0
36	V	63	0	0	4	0
36	X	17	0	0	0	0
36	Y	3	0	0	0	0
36	a	130	0	0	2	0
36	b	193	0	0	6	0
36	c	169	0	0	8	0
36	d	106	0	0	1	0
36	e	23	0	0	1	0
36	f	4	0	0	1	0
36	h	22	0	0	0	0
36	i	17	0	0	0	0
36	j	7	0	0	3	0
36	k	4	0	0	1	0
36	l	12	0	0	0	0
36	m	5	0	0	2	0
36	o	97	0	0	2	0
36	r	8	0	0	1	0
36	t	7	0	0	0	0
36	u	63	0	0	2	0
36	v	64	0	0	3	0
36	x	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	8	0	0	0	0
36	z	8	0	0	0	0
All	All	53467	52744	52777	549	1

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

The worst 5 of 549 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:40:CYS:SG	35:V:201:HEC:CAC	2.03	1.44
3:c:327[A]:ASN:ND2	36:c:601:HOH:O	1.99	0.95
13:O:27:ARG:NH1	36:O:302:HOH:O	1.99	0.94
9:J:19:MET:N	36:J:201:HOH:O	1.94	0.92
17:V:40:CYS:SG	35:V:201:HEC:HAC	2.09	0.91

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:1026:HOH:O	36:C:763:HOH:O[1_455]	2.09	0.11

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	397/344 (115%)	387 (98%)	10 (2%)	0	100	100
1	a	397/344 (115%)	387 (98%)	9 (2%)	1 (0%)	36	36
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	11 (2%)	1 (0%)	43	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	43	44
3	c	463/461 (100%)	447 (96%)	15 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	4
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	11 (4%)	4 (2%)	7	4
13	o	242/272 (89%)	228 (94%)	12 (5%)	2 (1%)	16	12
14	R	32/41 (78%)	27 (84%)	5 (16%)	0	100	100
14	r	29/41 (71%)	27 (93%)	1 (3%)	1 (3%)	3	1
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7	3
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	3
All	All	5396/5700 (95%)	5212 (97%)	166 (3%)	18 (0%)	36	36

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	59	LYS
17	V	64	PRO
14	r	31	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	320 (99%)	4 (1%)	63	72
1	a	323/280 (115%)	310 (96%)	13 (4%)	28	29
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	53
2	b	402/407 (99%)	385 (96%)	17 (4%)	26	28
3	C	356/362 (98%)	348 (98%)	8 (2%)	45	53
3	c	364/362 (101%)	344 (94%)	20 (6%)	19	18
4	D	277/283 (98%)	273 (99%)	4 (1%)	59	67
4	d	278/283 (98%)	271 (98%)	7 (2%)	42	48
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	18
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	28
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	4
7	H	54/55 (98%)	51 (94%)	3 (6%)	19	18
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	17
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	14
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	28
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	34
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	194 (94%)	12 (6%)	18	16
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
14	r	23/33 (70%)	19 (83%)	4 (17%)	2	1
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	32
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	34
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	34
17	V	117/138 (85%)	113 (97%)	4 (3%)	32	35
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	27
18	X	31/34 (91%)	27 (87%)	4 (13%)	4	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	38
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	25
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	1
All	All	4458/4654 (96%)	4269 (96%)	189 (4%)	26	28

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	125	LEU
9	j	7	ARG
3	c	240	ILE
4	d	291	LEU
11	l	2	GLU

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

Mol	Chain	Res	Type
12	m	5	GLN
13	o	61	GLN
17	v	118	HIS
14	R	22	ASN
13	O	155	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
15	FME	T	1	15	8,9,10	1.12	1 (12%)	8,9,11	1.19	1 (12%)
8	FME	I	1	8	8,9,10	1.04	1 (12%)	8,9,11	0.95	0
15	FME	t	1	15	8,9,10	1.45	1 (12%)	8,9,11	0.98	1 (12%)
12	FME	M	1	12	8,9,10	1.14	1 (12%)	8,9,11	0.96	0
12	FME	m	1	12	8,9,10	1.20	1 (12%)	8,9,11	1.45	1 (12%)
8	FME	i	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.90	3 (37%)

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
15	FME	T	1	15	-	4/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.01	1.42	1.46
12	m	1	FME	CA-N	-2.77	1.42	1.46
8	i	1	FME	CA-N	-2.47	1.43	1.46
12	M	1	FME	CA-N	-2.39	1.43	1.46
8	I	1	FME	CA-N	-2.37	1.43	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-3.44	117.53	122.82
8	i	1	FME	C-CA-N	2.47	114.27	109.50
8	i	1	FME	O1-CN-N	-2.31	119.35	125.32
15	t	1	FME	CB-CA-N	2.29	114.69	110.52
12	m	1	FME	CA-N-CN	-2.22	119.40	122.82

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 194 ligands modelled in this entry, 6 are monoatomic - leaving 188 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	c	505	36	64,68,73	1.32	10 (15%)	76,107,113	1.42	10 (13%)
33	LMG	c	522	-	48,48,55	1.22	4 (8%)	56,56,63	1.25	8 (14%)
22	CLA	d	401	4	69,73,73	1.16	7 (10%)	82,113,113	1.23	8 (9%)
22	CLA	b	716	2	64,68,73	1.35	11 (17%)	76,107,113	1.42	10 (13%)
22	CLA	c	509	3	68,72,73	1.37	11 (16%)	80,111,113	1.55	12 (15%)
28	STE	b	727	-	19,19,19	0.51	0	19,19,19	1.21	2 (10%)
35	HEC	e	101	5,6	50,50,50	1.78	6 (12%)	68,82,82	1.56	11 (16%)
22	CLA	c	504	3	69,73,73	1.41	8 (11%)	82,113,113	1.59	9 (10%)
23	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
22	CLA	b	709	2	69,73,73	1.27	7 (10%)	82,113,113	1.35	10 (12%)
29	DGD	c	518	-	63,63,67	1.24	9 (14%)	77,77,81	1.43	11 (14%)
28	STE	a	416	-	9,9,19	0.61	0	8,8,19	0.32	0
22	CLA	C	506	3	69,73,73	1.16	6 (8%)	82,113,113	1.25	7 (8%)
23	BCR	B	717	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	5 (8%)
27	LHG	a	414	-	41,41,48	0.80	1 (2%)	44,47,54	1.26	3 (6%)
22	CLA	A	402	1	69,73,73	1.29	8 (11%)	82,113,113	1.23	9 (10%)
22	CLA	a	403	1	69,73,73	1.37	10 (14%)	82,113,113	1.43	14 (17%)
22	CLA	b	701	36	69,73,73	1.35	9 (13%)	82,113,113	1.53	5 (6%)
28	STE	J	101	-	11,11,19	0.61	0	11,11,19	1.52	2 (18%)
29	DGD	C	519	-	63,63,67	0.96	5 (7%)	77,77,81	1.42	12 (15%)
27	LHG	D	411	-	46,46,48	1.24	5 (10%)	49,52,54	1.26	5 (10%)
25	PL9	a	411	-	55,55,55	0.88	1 (1%)	68,69,69	1.62	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	B	724	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
22	CLA	D	403	4	69,73,73	1.52	12 (17%)	82,113,113	1.50	11 (13%)
26	SQD	A	412	-	38,38,54	1.06	3 (7%)	40,40,65	1.12	3 (7%)
22	CLA	c	513	3	69,73,73	1.36	11 (15%)	82,113,113	1.35	10 (12%)
23	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.30	6 (10%)
28	STE	a	418	-	14,14,19	0.47	0	13,13,19	0.71	0
28	STE	m	101	-	11,11,19	0.82	0	11,11,19	1.40	2 (18%)
27	LHG	B	722	-	48,48,48	1.10	3 (6%)	51,54,54	1.37	5 (9%)
28	STE	b	724	-	15,15,19	0.79	0	15,15,19	0.97	1 (6%)
28	STE	C	522	-	15,15,19	0.47	0	14,14,19	0.81	0
22	CLA	c	506	3	69,73,73	1.11	7 (10%)	82,113,113	1.32	9 (10%)
23	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
28	STE	C	521	-	11,11,19	0.89	0	11,11,19	1.38	3 (27%)
34	PHO	d	405	-	58,69,69	2.08	10 (17%)	55,99,99	1.56	8 (14%)
22	CLA	C	504	3	69,73,73	1.62	8 (11%)	82,113,113	1.64	17 (20%)
27	LHG	d	406	-	48,48,48	0.79	0	51,54,54	1.12	4 (7%)
35	HEC	E	103	5,6	50,50,50	1.66	6 (12%)	68,82,82	1.48	11 (16%)
22	CLA	D	402	36	69,73,73	1.41	10 (14%)	82,113,113	1.21	6 (7%)
27	LHG	L	101	-	48,48,48	0.85	2 (4%)	51,54,54	1.26	4 (7%)
22	CLA	A	404	1	58,62,73	1.49	6 (10%)	68,99,113	1.49	13 (19%)
23	BCR	b	718	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	6 (10%)
22	CLA	c	502	3	69,73,73	1.19	7 (10%)	82,113,113	1.42	7 (8%)
28	STE	B	720	-	16,16,19	0.64	0	16,16,19	1.35	2 (12%)
22	CLA	B	716	2	64,68,73	1.27	5 (7%)	76,107,113	1.59	13 (17%)
22	CLA	H	102	36	69,73,73	1.75	13 (18%)	82,113,113	1.54	12 (14%)
28	STE	E	102	-	6,6,19	0.42	0	5,5,19	0.57	0
28	STE	c	521	-	19,19,19	0.70	0	19,19,19	1.00	2 (10%)
29	DGD	c	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.35	10 (12%)
22	CLA	b	711	2	69,73,73	1.27	6 (8%)	82,113,113	1.47	10 (12%)
32	BCT	a	410	21	3,3,3	1.16	0	2,3,3	3.26	2 (100%)
22	CLA	b	710	36	69,73,73	1.42	10 (14%)	82,113,113	1.27	9 (10%)
23	BCR	B	718	-	41,41,41	1.15	4 (9%)	56,56,56	1.43	7 (12%)
33	LMG	b	723	-	55,55,55	1.11	5 (9%)	63,63,63	1.46	11 (17%)
23	BCR	b	719	-	41,41,41	1.10	2 (4%)	56,56,56	1.41	8 (14%)
22	CLA	B	708	2	69,73,73	1.26	9 (13%)	82,113,113	1.71	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	C	523	-	11,11,19	0.86	0	11,11,19	1.02	1 (9%)
22	CLA	B	703	2	69,73,73	1.39	9 (13%)	82,113,113	1.36	7 (8%)
23	BCR	C	501	-	41,41,41	1.08	3 (7%)	56,56,56	1.17	3 (5%)
32	BCT	A	417	21	3,3,3	1.06	0	2,3,3	3.87	2 (100%)
23	BCR	B	719	-	41,41,41	1.13	3 (7%)	56,56,56	1.50	8 (14%)
22	CLA	b	706	2	69,73,73	1.44	6 (8%)	82,113,113	1.54	12 (14%)
34	PHO	D	406	-	58,69,69	1.74	8 (13%)	55,99,99	1.58	15 (27%)
28	STE	b	722	-	19,19,19	0.64	0	19,19,19	0.89	0
22	CLA	c	511	3	69,73,73	1.17	7 (10%)	82,113,113	1.46	11 (13%)
23	BCR	a	407	-	41,41,41	1.10	4 (9%)	56,56,56	1.44	13 (23%)
29	DGD	A	413	-	67,67,67	1.22	9 (13%)	81,81,81	1.54	15 (18%)
33	LMG	c	523	-	49,49,55	1.00	2 (4%)	57,57,63	1.31	6 (10%)
28	STE	H	104	-	17,17,19	0.53	0	16,16,19	0.58	0
23	BCR	d	403	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	8 (14%)
22	CLA	B	707	36	69,73,73	1.58	11 (15%)	82,113,113	1.43	4 (4%)
22	CLA	b	702	2	69,73,73	1.23	9 (13%)	82,113,113	1.43	13 (15%)
28	STE	I	101	-	14,14,19	0.66	0	13,13,19	0.36	0
28	STE	A	414	-	4,4,19	0.52	0	3,3,19	0.34	0
23	BCR	D	404	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	7 (12%)
34	PHO	a	405	-	58,69,69	2.03	11 (18%)	55,99,99	1.56	10 (18%)
30	OEX	A	415[A]	1,36,3	0,14,14	-	-	-	-	-
33	LMG	c	520	-	37,37,55	1.22	5 (13%)	45,45,63	1.30	4 (8%)
25	PL9	A	408	-	55,55,55	1.11	4 (7%)	68,69,69	1.56	14 (20%)
29	DGD	h	702	-	63,63,67	1.22	7 (11%)	77,77,81	1.57	17 (22%)
22	CLA	B	705	2	69,73,73	1.31	7 (10%)	82,113,113	1.42	13 (15%)
22	CLA	b	707	36	69,73,73	1.54	7 (10%)	82,113,113	1.30	10 (12%)
23	BCR	Y	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.17	4 (7%)
33	LMG	M	101	-	51,51,55	1.01	3 (5%)	59,59,63	1.42	8 (13%)
22	CLA	b	712	2	69,73,73	1.31	8 (11%)	82,113,113	1.28	7 (8%)
33	LMG	b	721	-	51,51,55	0.97	4 (7%)	59,59,63	1.45	7 (11%)
22	CLA	B	709	2	69,73,73	1.27	9 (13%)	82,113,113	1.16	6 (7%)
22	CLA	B	706	2	69,73,73	1.18	9 (13%)	82,113,113	1.62	12 (14%)
22	CLA	C	505	36	63,67,73	1.25	7 (11%)	74,105,113	1.25	8 (10%)
33	LMG	d	408	-	44,44,55	1.14	6 (13%)	52,52,63	1.45	8 (15%)
22	CLA	C	508	36	69,73,73	1.30	9 (13%)	82,113,113	1.48	9 (10%)
27	LHG	a	412	-	48,48,48	0.88	1 (2%)	51,54,54	1.39	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	409	-	50,52,54	1.02	4 (8%)	60,63,65	2.02	16 (26%)
29	DGD	H	103	-	63,63,67	1.35	10 (15%)	77,77,81	1.47	11 (14%)
22	CLA	A	403	36	69,73,73	1.25	7 (10%)	82,113,113	1.28	10 (12%)
23	BCR	A	405	-	41,41,41	1.14	3 (7%)	56,56,56	1.40	8 (14%)
28	STE	d	409	-	16,16,19	0.74	0	16,16,19	1.34	2 (12%)
23	BCR	c	516	-	41,41,41	1.25	3 (7%)	56,56,56	1.43	9 (16%)
28	STE	T	702	-	14,14,19	0.51	0	13,13,19	0.58	0
22	CLA	a	406	1	69,73,73	1.43	9 (13%)	82,113,113	1.21	6 (7%)
22	CLA	B	710	36	69,73,73	1.25	10 (14%)	82,113,113	1.42	8 (9%)
22	CLA	c	503	3	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
28	STE	A	411	-	15,15,19	0.52	0	14,14,19	0.70	0
22	CLA	B	712	2	69,73,73	1.10	4 (5%)	82,113,113	1.45	12 (14%)
26	SQD	a	415	-	35,35,54	1.13	2 (5%)	37,37,65	1.35	4 (10%)
22	CLA	B	702	2	69,73,73	1.40	10 (14%)	82,113,113	1.37	12 (14%)
22	CLA	C	503	3	69,73,73	1.35	10 (14%)	82,113,113	1.35	10 (12%)
22	CLA	C	509	3	69,73,73	1.40	8 (11%)	82,113,113	1.44	9 (10%)
22	CLA	a	401	36	69,73,73	1.38	6 (8%)	82,113,113	1.60	13 (15%)
28	STE	B	725	-	17,17,19	0.75	0	17,17,19	0.85	0
28	STE	E	101	-	11,11,19	0.95	0	11,11,19	0.84	0
25	PL9	d	404	-	55,55,55	1.49	8 (14%)	68,69,69	1.74	14 (20%)
23	BCR	k	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
23	BCR	t	701	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	5 (8%)
22	CLA	c	508	36	69,73,73	1.16	6 (8%)	82,113,113	1.30	10 (12%)
22	CLA	C	512	3	69,73,73	1.39	11 (15%)	82,113,113	1.19	6 (7%)
22	CLA	D	401	4	69,73,73	1.40	9 (13%)	82,113,113	1.15	6 (7%)
28	STE	t	702	-	13,13,19	0.63	0	13,13,19	1.24	2 (15%)
22	CLA	C	502	3	69,73,73	1.24	9 (13%)	82,113,113	1.36	9 (10%)
22	CLA	b	715	2	69,73,73	1.37	9 (13%)	82,113,113	1.39	12 (14%)
22	CLA	c	507	3	69,73,73	1.32	11 (15%)	82,113,113	1.34	8 (9%)
29	DGD	c	519	-	63,63,67	1.29	9 (14%)	77,77,81	1.40	13 (16%)
28	STE	Z	101	-	7,7,19	0.43	0	6,6,19	0.52	0
33	LMG	B	721	-	26,26,55	0.77	0	26,26,63	1.33	2 (7%)
26	SQD	D	409	-	34,36,54	0.96	2 (5%)	42,45,65	1.95	12 (28%)
27	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.14	5 (9%)
22	CLA	c	510	3	69,73,73	1.30	7 (10%)	82,113,113	1.62	9 (10%)
27	LHG	d	407	-	38,38,48	0.89	3 (7%)	41,44,54	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	D	410	-	48,48,48	0.95	3 (6%)	51,54,54	1.23	4 (7%)
33	LMG	a	419	-	55,55,55	1.31	7 (12%)	63,63,63	1.33	5 (7%)
22	CLA	c	512	3	69,73,73	1.44	8 (11%)	82,113,113	1.58	8 (9%)
28	STE	M	102	-	14,14,19	0.70	0	14,14,19	1.08	0
22	CLA	b	713	2	69,73,73	1.42	10 (14%)	82,113,113	1.58	13 (15%)
28	STE	X	101	-	19,19,19	0.55	0	19,19,19	1.28	1 (5%)
31	OEY	A	416[B]	1,36,3	0,16,16	-	-	-		
26	SQD	B	723	-	52,54,54	0.96	2 (3%)	62,65,65	1.67	11 (17%)
28	STE	j	101	-	11,11,19	0.81	0	11,11,19	1.52	2 (18%)
28	STE	h	703	-	13,13,19	0.43	0	12,12,19	0.72	0
22	CLA	b	705	2	69,73,73	1.48	8 (11%)	82,113,113	1.46	12 (14%)
28	STE	B	726	-	15,15,19	0.50	0	14,14,19	0.66	0
35	HEC	V	201	17	50,50,50	1.54	5 (10%)	68,82,82	1.44	12 (17%)
35	HEC	v	201	17	50,50,50	1.73	6 (12%)	68,82,82	1.36	9 (13%)
23	BCR	b	717	-	41,41,41	1.20	4 (9%)	56,56,56	1.51	11 (19%)
28	STE	H	105	-	7,7,19	0.44	0	6,6,19	0.60	0
30	OEX	a	420[A]	1,36,3	0,14,14	-	-	-		
28	STE	B	701	-	11,11,19	0.99	0	11,11,19	1.03	1 (9%)
25	PL9	D	405	-	55,55,55	1.41	6 (10%)	68,69,69	1.77	15 (22%)
33	LMG	D	412	-	31,31,55	1.20	3 (9%)	33,33,63	1.09	2 (6%)
28	STE	c	501	-	11,11,19	0.78	0	11,11,19	1.10	1 (9%)
29	DGD	C	518	-	63,63,67	1.36	6 (9%)	77,77,81	1.47	12 (15%)
34	PHO	D	407	-	58,69,69	1.99	11 (18%)	55,99,99	1.71	11 (20%)
28	STE	a	417	-	11,11,19	0.89	1 (9%)	11,11,19	1.01	0
33	LMG	C	516	-	48,48,55	0.97	4 (8%)	56,56,63	1.36	6 (10%)
22	CLA	c	514	3	69,73,73	1.12	7 (10%)	82,113,113	1.28	7 (8%)
22	CLA	C	510	3	69,73,73	1.51	13 (18%)	82,113,113	1.36	8 (9%)
22	CLA	C	514	3	69,73,73	1.42	10 (14%)	82,113,113	1.52	10 (12%)
22	CLA	B	704	2	69,73,73	1.31	7 (10%)	82,113,113	1.71	13 (15%)
22	CLA	B	711	2	69,73,73	1.32	9 (13%)	82,113,113	1.36	10 (12%)
22	CLA	a	404	36	69,73,73	1.35	9 (13%)	82,113,113	1.37	12 (14%)
28	STE	b	726	-	9,9,19	0.56	0	8,8,19	0.44	0
22	CLA	b	704	2	69,73,73	1.20	9 (13%)	82,113,113	1.68	12 (14%)
22	CLA	b	703	2	69,73,73	1.39	8 (11%)	82,113,113	1.47	14 (17%)
33	LMG	D	408	-	51,51,55	1.00	4 (7%)	59,59,63	1.27	6 (10%)
28	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	x	101	-	19,19,19	0.80	0	19,19,19	0.75	1 (5%)
22	CLA	C	507	3	69,73,73	1.18	7 (10%)	82,113,113	1.26	10 (12%)
22	CLA	C	511	3	69,73,73	1.27	9 (13%)	82,113,113	1.23	7 (8%)
27	LHG	A	410	-	48,48,48	0.81	2 (4%)	51,54,54	1.23	4 (7%)
31	OEY	a	421[B]	1,36,3	0,16,16	-	-	-	-	-
23	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.45	10 (17%)
22	CLA	B	714	2	69,73,73	1.10	4 (5%)	82,113,113	1.19	6 (7%)
22	CLA	C	513	3	69,73,73	1.80	12 (17%)	82,113,113	1.43	12 (14%)
23	BCR	C	515	-	41,41,41	1.29	4 (9%)	56,56,56	1.33	7 (12%)
29	DGD	C	517	-	63,63,67	1.09	5 (7%)	77,77,81	1.30	9 (11%)
28	STE	b	725	-	19,19,19	0.79	0	19,19,19	0.97	1 (5%)
26	SQD	f	101	-	39,41,54	1.14	5 (12%)	49,52,65	1.71	12 (24%)
26	SQD	a	413	-	52,54,54	0.99	6 (11%)	62,65,65	1.84	12 (19%)
33	LMG	C	520	-	48,48,55	1.01	3 (6%)	56,56,63	1.35	8 (14%)
22	CLA	b	708	2	69,73,73	1.27	10 (14%)	82,113,113	1.51	11 (13%)
22	CLA	B	715	2	69,73,73	1.60	9 (13%)	82,113,113	1.49	11 (13%)
22	CLA	d	402	4	69,73,73	1.51	8 (11%)	82,113,113	1.17	10 (12%)
23	BCR	h	701	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
22	CLA	B	713	2	69,73,73	1.24	5 (7%)	82,113,113	1.43	12 (14%)
26	SQD	b	720	-	47,49,54	0.99	2 (4%)	57,60,65	2.11	14 (24%)
22	CLA	b	714	2	69,73,73	1.24	9 (13%)	82,113,113	1.26	7 (8%)
28	STE	l	102	-	17,17,19	0.49	0	16,16,19	0.69	0
23	BCR	T	701	-	41,41,41	1.09	4 (9%)	56,56,56	1.36	7 (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
22	CLA	c	505	36	-	7/33/109/115	-
33	LMG	c	522	-	-	25/43/63/70	0/1/1/1
22	CLA	d	401	4	-	10/39/115/115	-
35	HEC	e	101	5,6	1/1/7/7	5/14/54/54	-
22	CLA	b	716	2	-	11/33/109/115	-
22	CLA	c	509	3	-	5/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	b	727	-	-	9/17/17/17	-
22	CLA	c	504	3	-	8/39/115/115	-
23	BCR	c	515	-	-	11/29/63/63	0/2/2/2
22	CLA	b	709	2	-	9/39/115/115	-
29	DGD	c	518	-	-	26/51/91/95	0/2/2/2
28	STE	a	416	-	-	4/7/7/17	-
22	CLA	C	506	3	-	13/39/115/115	-
23	BCR	B	717	-	-	8/29/63/63	0/2/2/2
27	LHG	a	414	-	-	20/46/46/53	-
22	CLA	A	402	1	-	6/39/115/115	-
22	CLA	a	403	1	-	7/39/115/115	-
22	CLA	b	701	36	-	11/39/115/115	-
28	STE	J	101	-	-	4/9/9/17	-
29	DGD	C	519	-	-	15/51/91/95	0/2/2/2
27	LHG	D	411	-	-	21/51/51/53	-
25	PL9	a	411	-	-	20/53/73/73	0/1/1/1
28	STE	B	724	-	-	4/9/9/17	-
22	CLA	D	403	4	-	7/39/115/115	-
26	SQD	A	412	-	-	15/39/39/69	-
22	CLA	c	513	3	-	21/39/115/115	-
23	BCR	H	101	-	-	5/29/63/63	0/2/2/2
28	STE	a	418	-	-	4/12/12/17	-
28	STE	m	101	-	-	2/9/9/17	-
27	LHG	B	722	-	-	17/53/53/53	-
28	STE	b	724	-	-	12/13/13/17	-
28	STE	C	522	-	-	3/13/13/17	-
22	CLA	c	506	3	-	11/39/115/115	-
23	BCR	k	101	-	-	13/29/63/63	0/2/2/2
28	STE	C	521	-	-	2/9/9/17	-
34	PHO	d	405	-	-	5/37/103/103	0/5/6/6
22	CLA	C	504	3	-	7/39/115/115	-
35	HEC	E	103	5,6	1/1/7/7	6/14/54/54	-
27	LHG	d	406	-	-	14/53/53/53	-
22	CLA	D	402	36	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	L	101	-	-	20/53/53/53	-
22	CLA	A	404	1	-	4/26/102/115	-
23	BCR	b	718	-	-	2/29/63/63	0/2/2/2
22	CLA	c	502	3	-	3/39/115/115	-
28	STE	B	720	-	-	9/14/14/17	-
22	CLA	B	716	2	-	10/33/109/115	-
22	CLA	H	102	36	-	13/39/115/115	-
28	STE	E	102	-	-	1/4/4/17	-
28	STE	c	521	-	-	7/17/17/17	-
29	DGD	c	517	-	-	22/51/91/95	0/2/2/2
22	CLA	b	711	2	-	7/39/115/115	-
22	CLA	b	710	36	-	4/39/115/115	-
23	BCR	B	718	-	-	7/29/63/63	0/2/2/2
33	LMG	b	723	-	-	21/50/70/70	0/1/1/1
23	BCR	b	719	-	-	5/29/63/63	0/2/2/2
22	CLA	B	708	2	-	3/39/115/115	-
28	STE	C	523	-	-	6/9/9/17	-
22	CLA	B	703	2	-	11/39/115/115	-
23	BCR	C	501	-	-	12/29/63/63	0/2/2/2
23	BCR	B	719	-	-	1/29/63/63	0/2/2/2
22	CLA	b	706	2	-	8/39/115/115	-
34	PHO	D	406	-	-	4/37/103/103	0/5/6/6
28	STE	b	722	-	-	10/17/17/17	-
22	CLA	c	511	3	-	9/39/115/115	-
23	BCR	a	407	-	-	3/29/63/63	0/2/2/2
29	DGD	A	413	-	-	27/55/95/95	0/2/2/2
33	LMG	c	523	-	-	21/44/64/70	0/1/1/1
28	STE	H	104	-	-	6/15/15/17	-
23	BCR	d	403	-	-	10/29/63/63	0/2/2/2
22	CLA	B	707	36	-	5/39/115/115	-
22	CLA	b	702	2	-	8/39/115/115	-
28	STE	I	101	-	-	4/12/12/17	-
28	STE	A	414	-	-	1/2/2/17	-
23	BCR	D	404	-	-	10/29/63/63	0/2/2/2
34	PHO	a	405	-	-	5/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	520	-	-	12/31/51/70	0/1/1/1
25	PL9	A	408	-	-	22/53/73/73	0/1/1/1
29	DGD	h	702	-	-	14/51/91/95	0/2/2/2
22	CLA	B	705	2	-	8/39/115/115	-
22	CLA	b	707	36	-	15/39/115/115	-
23	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
33	LMG	M	101	-	-	24/46/66/70	0/1/1/1
22	CLA	b	712	2	-	5/39/115/115	-
33	LMG	b	721	-	-	15/46/66/70	0/1/1/1
22	CLA	B	709	2	-	3/39/115/115	-
22	CLA	B	706	2	-	6/39/115/115	-
22	CLA	C	505	36	-	4/32/108/115	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
22	CLA	C	508	36	-	9/39/115/115	-
27	LHG	a	412	-	-	25/53/53/53	-
26	SQD	A	409	-	-	21/47/67/69	0/1/1/1
29	DGD	H	103	-	-	18/51/91/95	0/2/2/2
22	CLA	A	403	36	-	10/39/115/115	-
23	BCR	A	405	-	-	5/29/63/63	0/2/2/2
28	STE	d	409	-	-	6/14/14/17	-
23	BCR	c	516	-	-	3/29/63/63	0/2/2/2
28	STE	T	702	-	-	8/12/12/17	-
22	CLA	a	406	1	-	10/39/115/115	-
22	CLA	B	710	36	-	6/39/115/115	-
22	CLA	c	503	3	-	5/39/115/115	-
28	STE	A	411	-	-	7/13/13/17	-
22	CLA	B	712	2	-	8/39/115/115	-
26	SQD	a	415	-	-	18/37/37/69	-
22	CLA	B	702	2	-	8/39/115/115	-
22	CLA	C	503	3	-	10/39/115/115	-
22	CLA	C	509	3	-	5/39/115/115	-
22	CLA	a	401	36	-	5/39/115/115	-
28	STE	B	725	-	-	6/15/15/17	-
28	STE	E	101	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	d	404	-	-	18/53/73/73	0/1/1/1
23	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	BCR	t	701	-	-	9/29/63/63	0/2/2/2
22	CLA	c	508	36	-	3/39/115/115	-
22	CLA	C	512	3	-	6/39/115/115	-
22	CLA	D	401	4	-	5/39/115/115	-
28	STE	t	702	-	-	4/11/11/17	-
22	CLA	C	502	3	-	4/39/115/115	-
22	CLA	b	715	2	-	10/39/115/115	-
22	CLA	c	507	3	-	15/39/115/115	-
29	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	STE	Z	101	-	-	3/5/5/17	-
33	LMG	B	721	-	-	12/22/22/70	-
26	SQD	D	409	-	-	6/28/48/69	0/1/1/1
27	LHG	l	101	-	-	23/53/53/53	-
22	CLA	c	510	3	-	10/39/115/115	-
27	LHG	d	407	-	-	11/43/43/53	-
27	LHG	D	410	-	-	17/53/53/53	-
33	LMG	a	419	-	-	23/50/70/70	0/1/1/1
22	CLA	c	512	3	-	12/39/115/115	-
28	STE	M	102	-	-	5/12/12/17	-
22	CLA	b	713	2	-	5/39/115/115	-
28	STE	X	101	-	-	9/17/17/17	-
26	SQD	B	723	-	-	28/49/69/69	0/1/1/1
28	STE	j	101	-	-	2/9/9/17	-
28	STE	h	703	-	-	6/11/11/17	-
22	CLA	b	705	2	-	13/39/115/115	-
35	HEC	v	201	17	1/1/7/7	4/14/54/54	-
35	HEC	V	201	17	1/1/7/7	5/14/54/54	-
28	STE	B	726	-	-	5/13/13/17	-
23	BCR	b	717	-	-	8/29/63/63	0/2/2/2
28	STE	H	105	-	-	3/5/5/17	-
28	STE	B	701	-	-	4/9/9/17	-
25	PL9	D	405	-	-	13/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	D	412	-	-	14/33/33/70	-
28	STE	c	501	-	-	4/9/9/17	-
29	DGD	C	518	-	-	14/51/91/95	0/2/2/2
34	PHO	D	407	-	-	2/37/103/103	0/5/6/6
28	STE	a	417	-	-	4/9/9/17	-
33	LMG	C	516	-	-	18/43/63/70	0/1/1/1
22	CLA	c	514	3	-	7/39/115/115	-
22	CLA	C	510	3	-	13/39/115/115	-
22	CLA	C	514	3	-	15/39/115/115	-
22	CLA	B	704	2	-	10/39/115/115	-
22	CLA	B	711	2	-	7/39/115/115	-
22	CLA	a	404	36	-	1/39/115/115	-
28	STE	b	726	-	-	4/7/7/17	-
22	CLA	b	704	2	-	8/39/115/115	-
22	CLA	b	703	2	-	8/39/115/115	-
33	LMG	D	408	-	-	13/46/66/70	0/1/1/1
28	STE	M	103	-	-	4/7/7/17	-
28	STE	x	101	-	-	11/17/17/17	-
22	CLA	C	507	3	-	8/39/115/115	-
22	CLA	C	511	3	-	9/39/115/115	-
27	LHG	A	410	-	-	28/53/53/53	-
23	BCR	K	101	-	-	7/29/63/63	0/2/2/2
22	CLA	B	714	2	-	10/39/115/115	-
22	CLA	C	513	3	-	14/39/115/115	-
23	BCR	C	515	-	-	6/29/63/63	0/2/2/2
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
28	STE	b	725	-	-	8/17/17/17	-
26	SQD	f	101	-	-	14/36/56/69	0/1/1/1
26	SQD	a	413	-	-	22/49/69/69	0/1/1/1
33	LMG	C	520	-	-	20/43/63/70	0/1/1/1
22	CLA	b	708	2	-	9/39/115/115	-
22	CLA	B	715	2	-	7/39/115/115	-
22	CLA	d	402	4	-	7/39/115/115	-
23	BCR	h	701	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	713	2	-	14/39/115/115	-
26	SQD	b	720	-	-	21/44/64/69	0/1/1/1
22	CLA	b	714	2	-	13/39/115/115	-
28	STE	l	102	-	-	5/15/15/17	-
23	BCR	T	701	-	-	4/29/63/63	0/2/2/2

The worst 5 of 903 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	405	PHO	C1B-C2B	10.00	1.50	1.39
34	a	405	PHO	C1B-C2B	8.63	1.49	1.39
22	C	504	CLA	MG-NA	8.03	2.25	2.06
34	D	407	PHO	C1B-C2B	7.98	1.48	1.39
34	D	407	PHO	C3B-C4B	7.67	1.49	1.41

The worst 5 of 1327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	704	CLA	C4A-NA-C1A	9.71	111.11	106.68
22	c	510	CLA	C4A-NA-C1A	9.37	110.95	106.68
22	b	701	CLA	C4A-NA-C1A	9.34	110.94	106.68
22	c	512	CLA	C4A-NA-C1A	9.27	110.91	106.68
22	B	707	CLA	C4A-NA-C1A	8.99	110.78	106.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	E	103	HEC	NA
35	V	201	HEC	NA
35	e	101	HEC	NA
35	v	201	HEC	NA

5 of 1784 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	705	CLA	C11-C12-C13-C14
22	B	714	CLA	CAD-CBD-CGD-O1D
22	B	714	CLA	CAD-CBD-CGD-O2D
22	B	714	CLA	C4-C3-C5-C6
22	C	503	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

100 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	716	CLA	1	0
28	b	727	STE	2	0
35	e	101	HEC	6	0
22	c	504	CLA	1	0
23	c	515	BCR	2	0
22	b	709	CLA	1	0
22	C	506	CLA	2	0
22	A	402	CLA	1	0
25	a	411	PL9	4	0
28	B	724	STE	1	0
22	D	403	CLA	1	0
22	c	513	CLA	1	0
23	H	101	BCR	4	0
27	B	722	LHG	1	0
22	c	506	CLA	1	0
34	d	405	PHO	1	0
22	C	504	CLA	1	0
27	d	406	LHG	5	0
35	E	103	HEC	3	0
22	D	402	CLA	1	0
23	b	718	BCR	2	0
22	c	502	CLA	1	0
22	B	716	CLA	1	0
22	H	102	CLA	2	0
28	E	102	STE	1	0
23	B	718	BCR	4	0
33	b	723	LMG	1	0
23	b	719	BCR	1	0
22	B	703	CLA	1	0
23	C	501	BCR	1	0
23	B	719	BCR	4	0
22	b	706	CLA	6	0
34	D	406	PHO	1	0
28	b	722	STE	2	0
22	c	511	CLA	1	0
23	a	407	BCR	2	0
29	A	413	DGD	2	0
33	c	523	LMG	1	0
23	d	403	BCR	2	0
22	B	707	CLA	1	0

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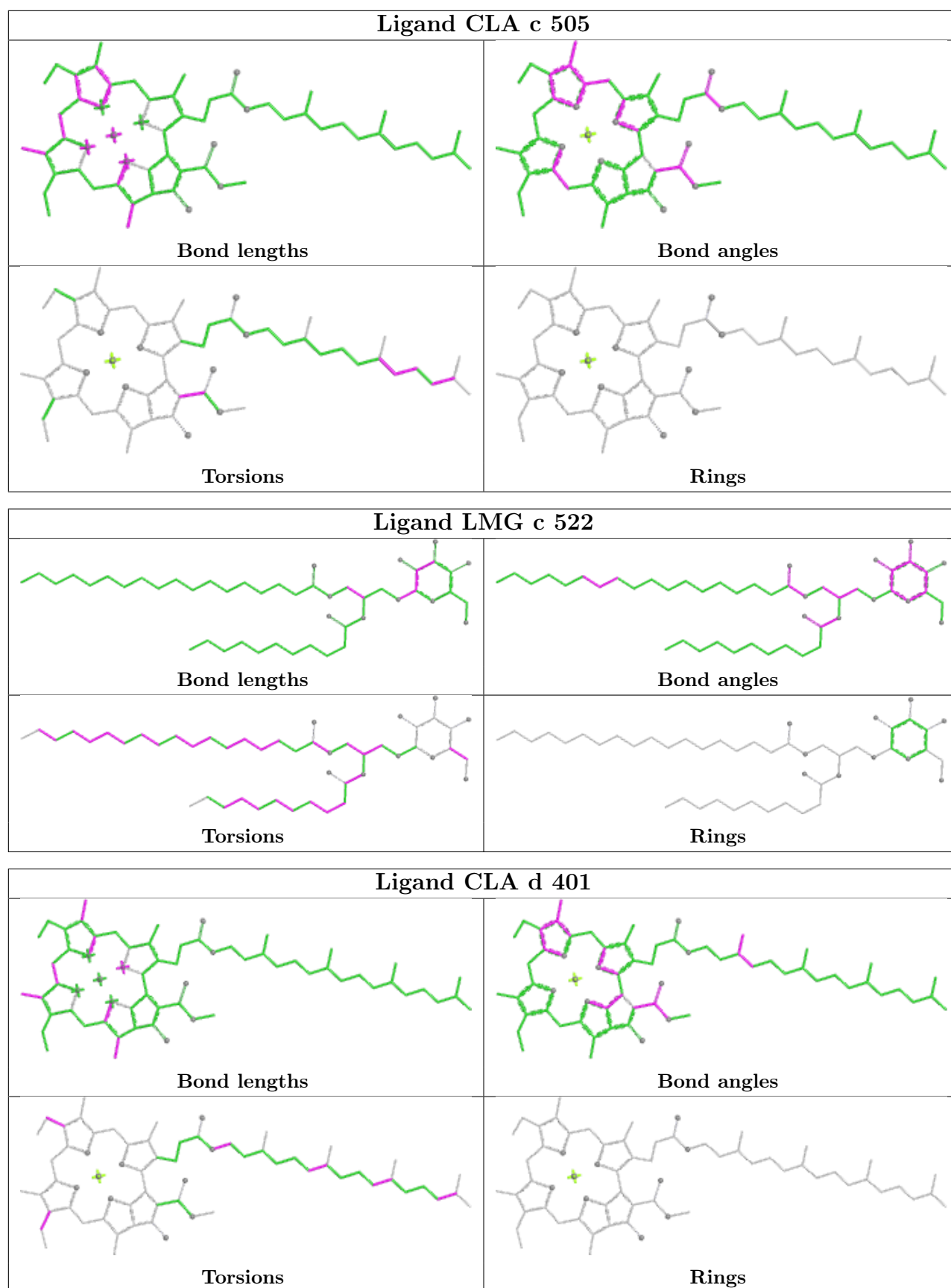
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	702	CLA	2	0
28	I	101	STE	1	0
23	D	404	BCR	2	0
25	A	408	PL9	3	0
22	B	705	CLA	3	0
23	Y	101	BCR	3	0
22	b	712	CLA	1	0
33	b	721	LMG	1	0
22	B	709	CLA	2	0
22	B	706	CLA	1	0
27	a	412	LHG	1	0
23	A	405	BCR	1	0
23	c	516	BCR	1	0
22	a	406	CLA	1	0
22	c	503	CLA	3	0
22	C	503	CLA	1	0
22	C	509	CLA	1	0
22	a	401	CLA	1	0
23	k	102	BCR	2	0
23	t	701	BCR	3	0
22	c	508	CLA	1	0
22	C	512	CLA	1	0
22	C	502	CLA	2	0
22	b	715	CLA	1	0
22	c	507	CLA	1	0
29	c	519	DGD	1	0
27	l	101	LHG	1	0
27	D	410	LHG	1	0
33	a	419	LMG	4	0
31	A	416[B]	OEY	2	0
28	j	101	STE	1	0
28	h	703	STE	1	0
22	b	705	CLA	1	0
35	V	201	HEC	6	0
25	D	405	PL9	2	0
29	C	518	DGD	1	0
28	a	417	STE	1	0
22	C	510	CLA	2	0
22	C	514	CLA	1	0
22	B	704	CLA	2	0
22	B	711	CLA	1	0
22	b	704	CLA	2	0

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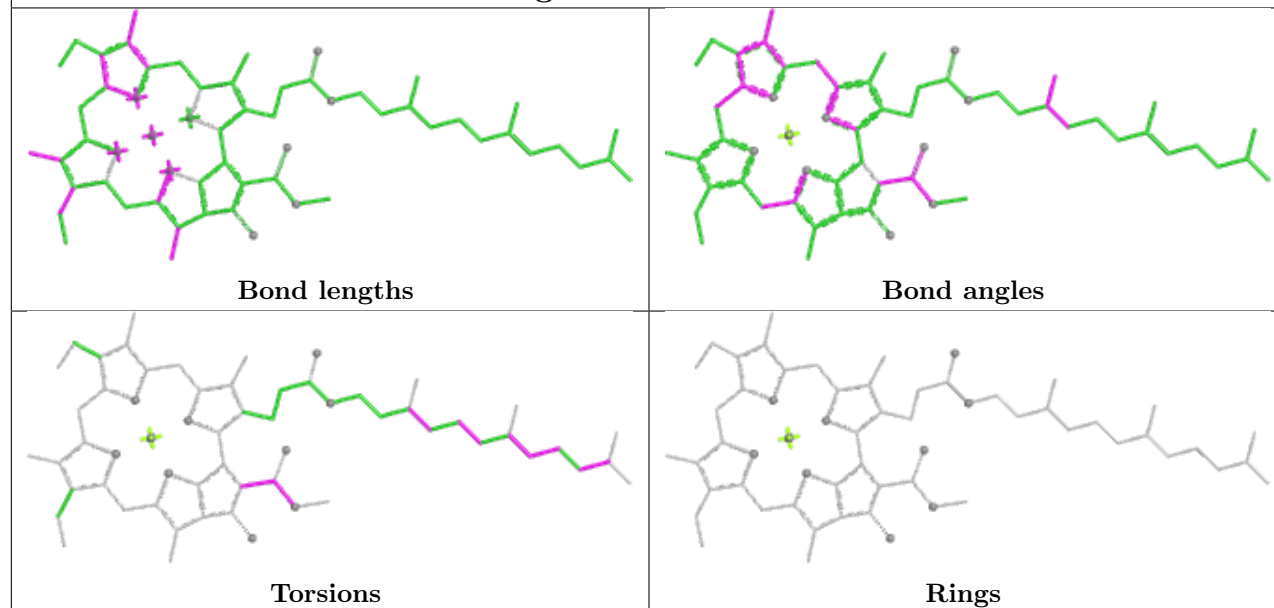
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	703	CLA	1	0
33	D	408	LMG	1	0
28	x	101	STE	2	0
22	C	507	CLA	1	0
22	C	511	CLA	1	0
31	a	421[B]	OEY	1	0
23	K	101	BCR	1	0
22	B	714	CLA	1	0
22	C	513	CLA	3	0
23	C	515	BCR	1	0
28	b	725	STE	1	0
22	b	708	CLA	1	0
22	B	715	CLA	1	0
22	d	402	CLA	1	0
23	h	701	BCR	1	0
22	B	713	CLA	1	0
26	b	720	SQD	1	0
23	T	701	BCR	1	0

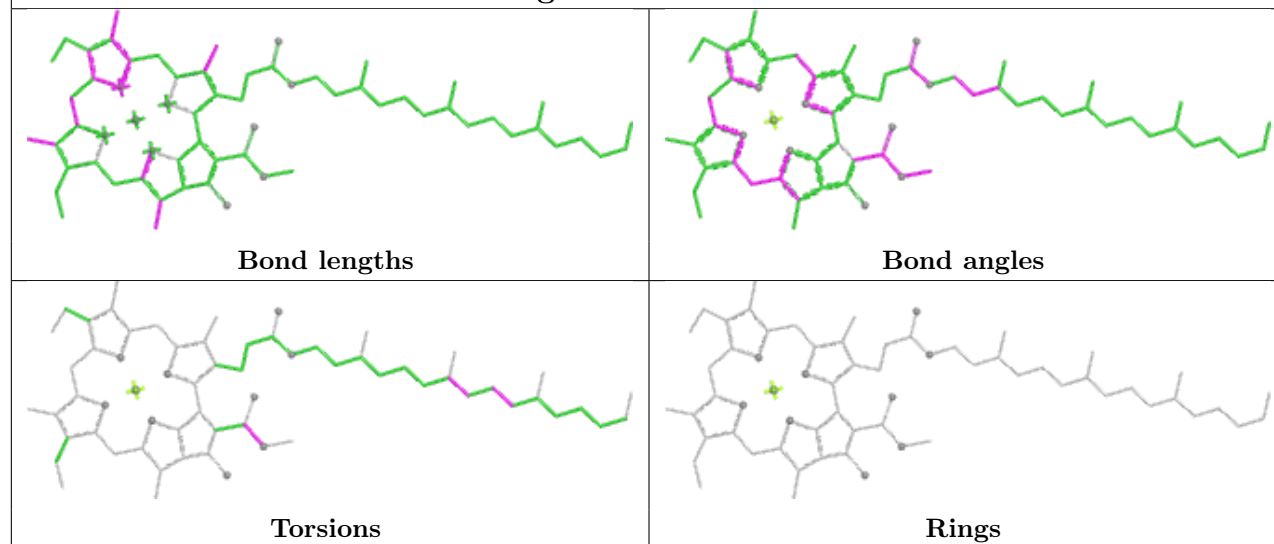
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



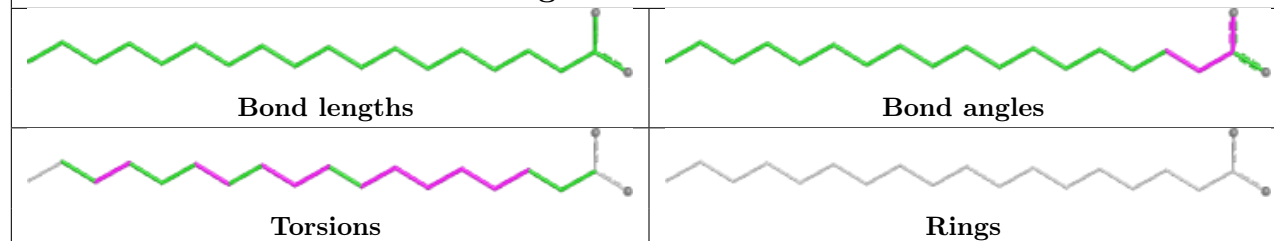
Ligand CLA b 716



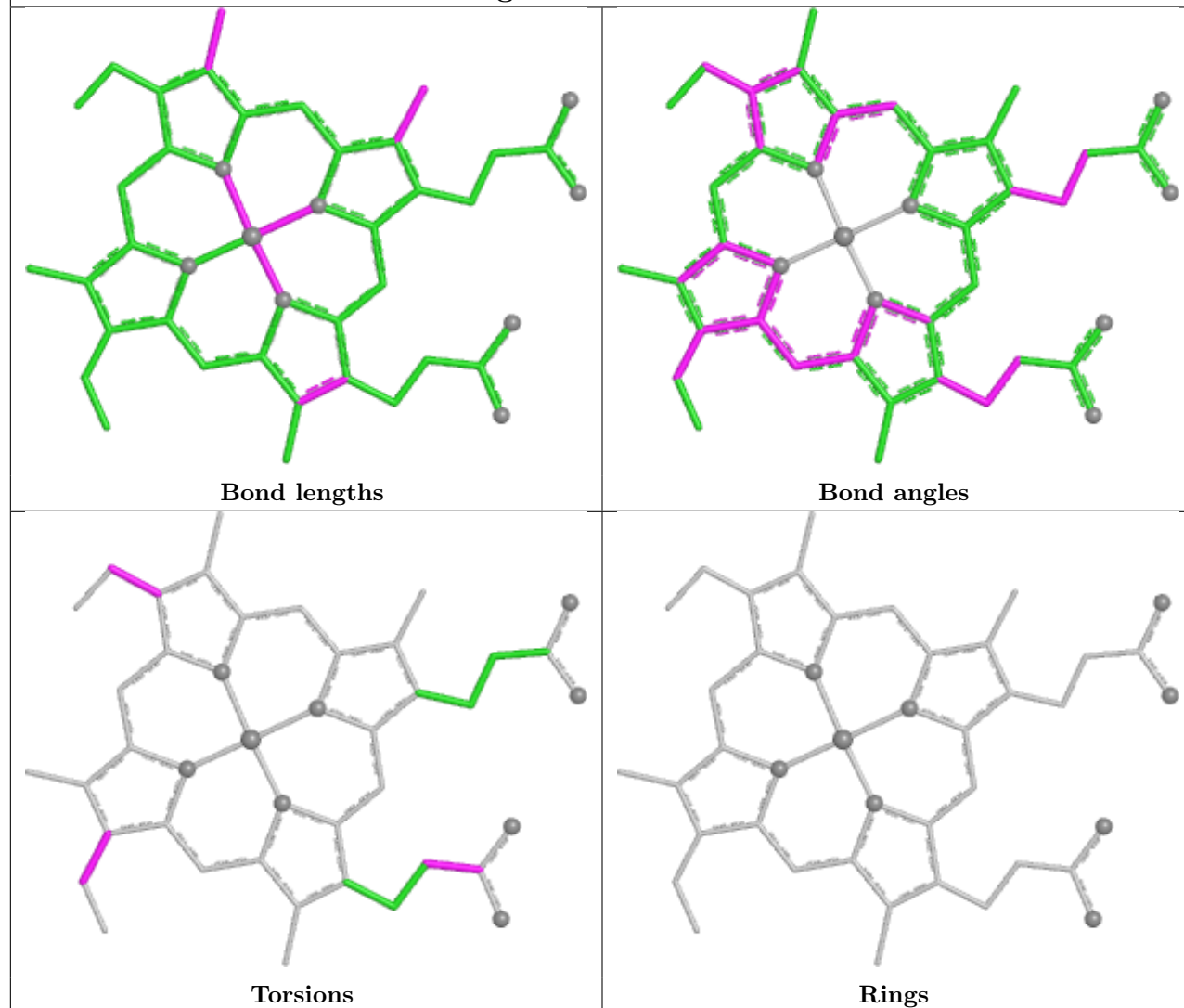
Ligand CLA c 509



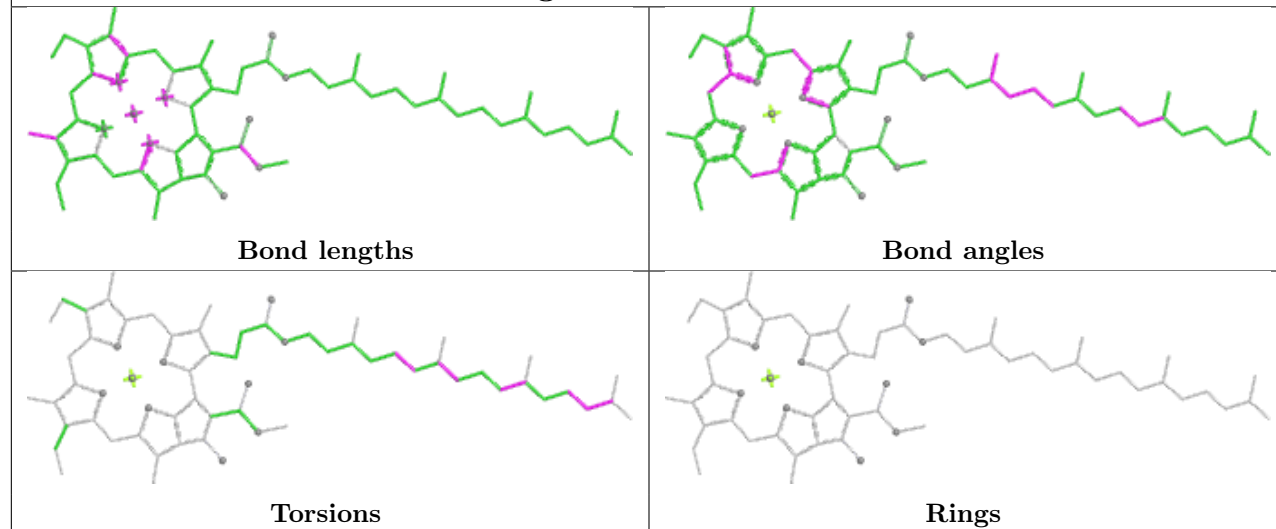
Ligand STE b 727

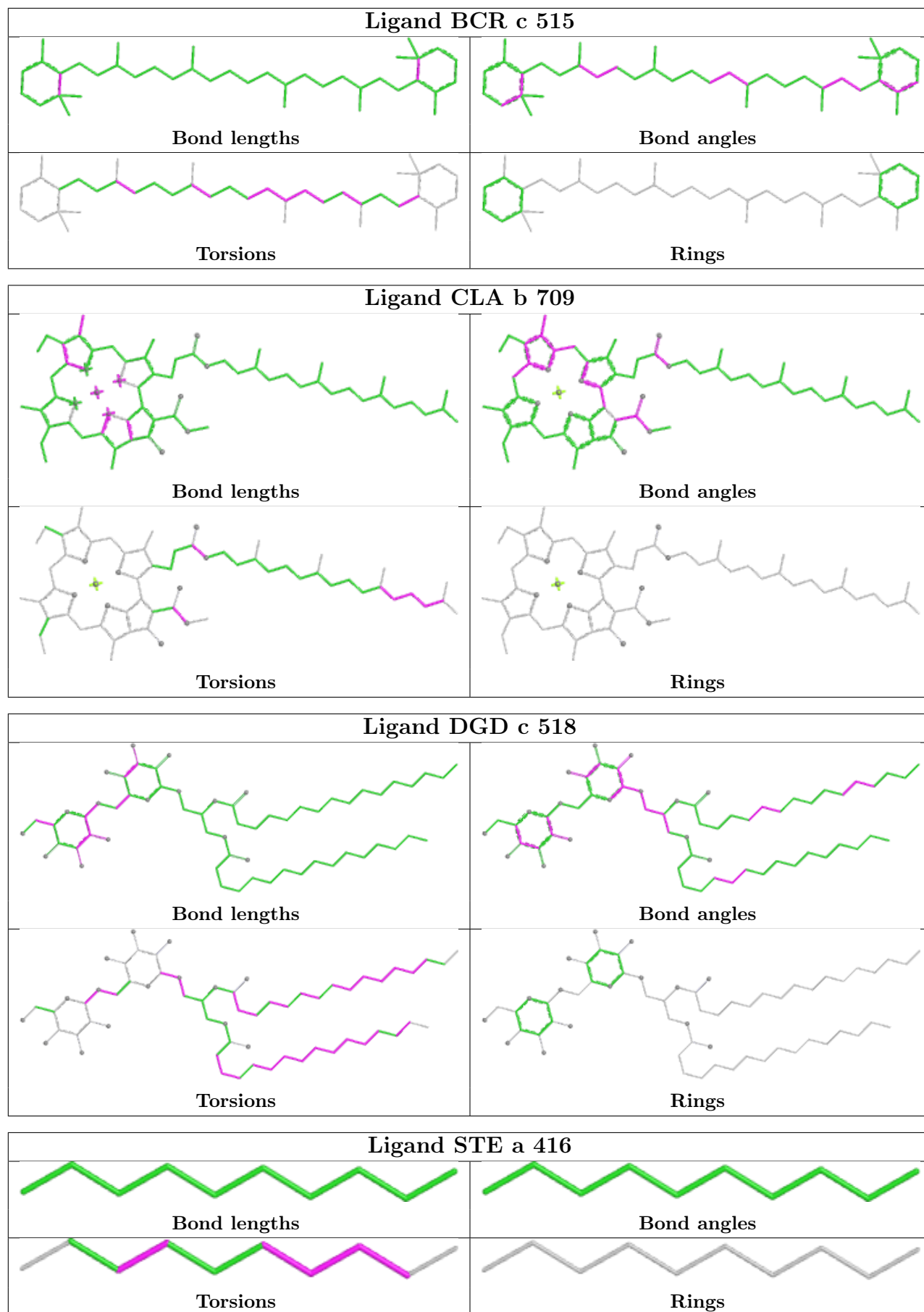


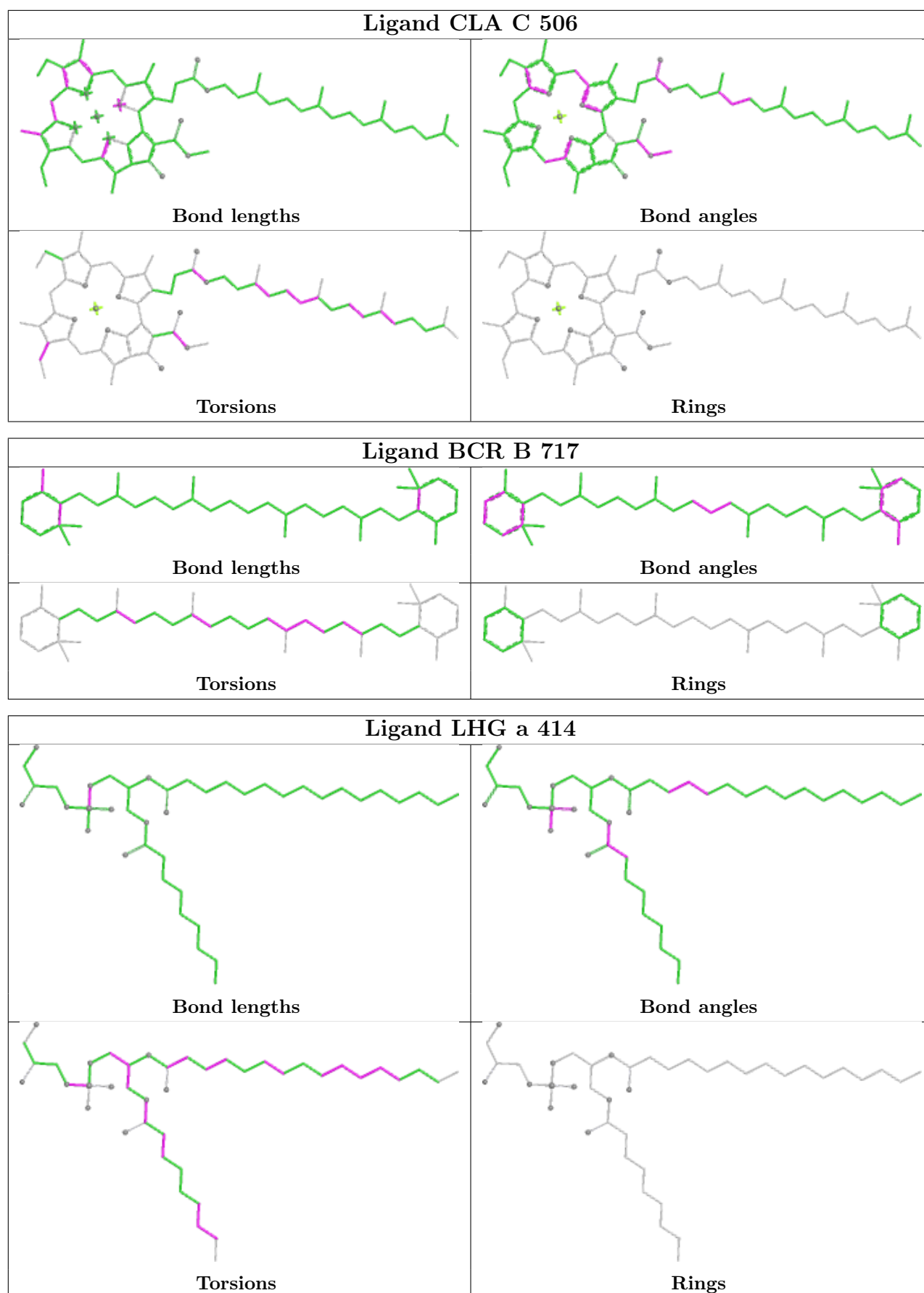
Ligand HEC e 101

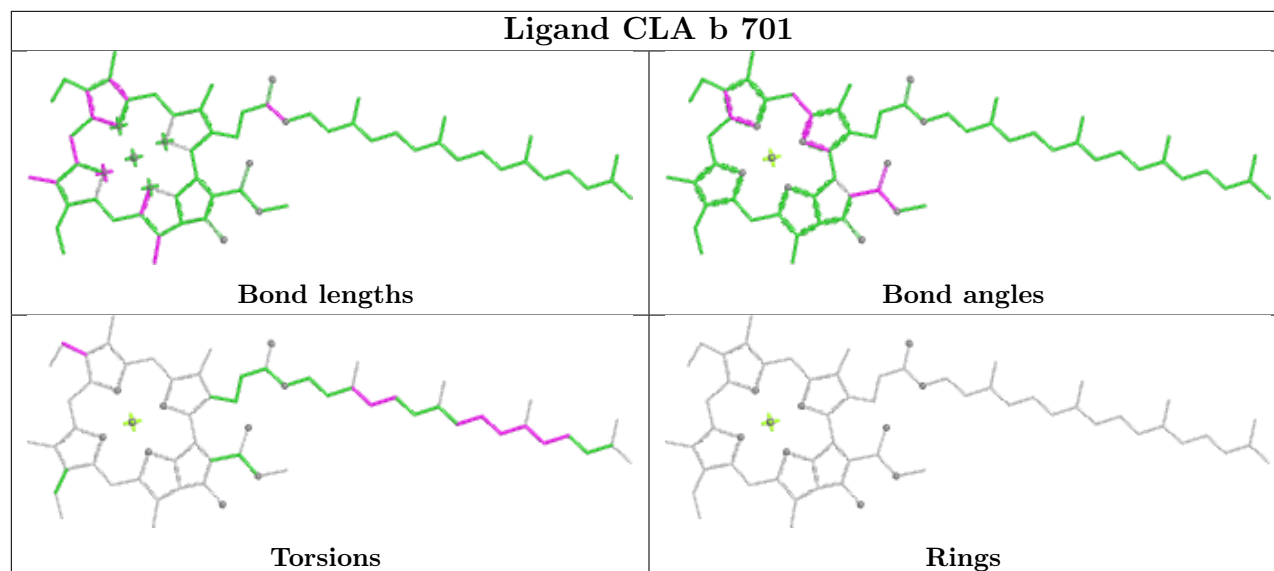
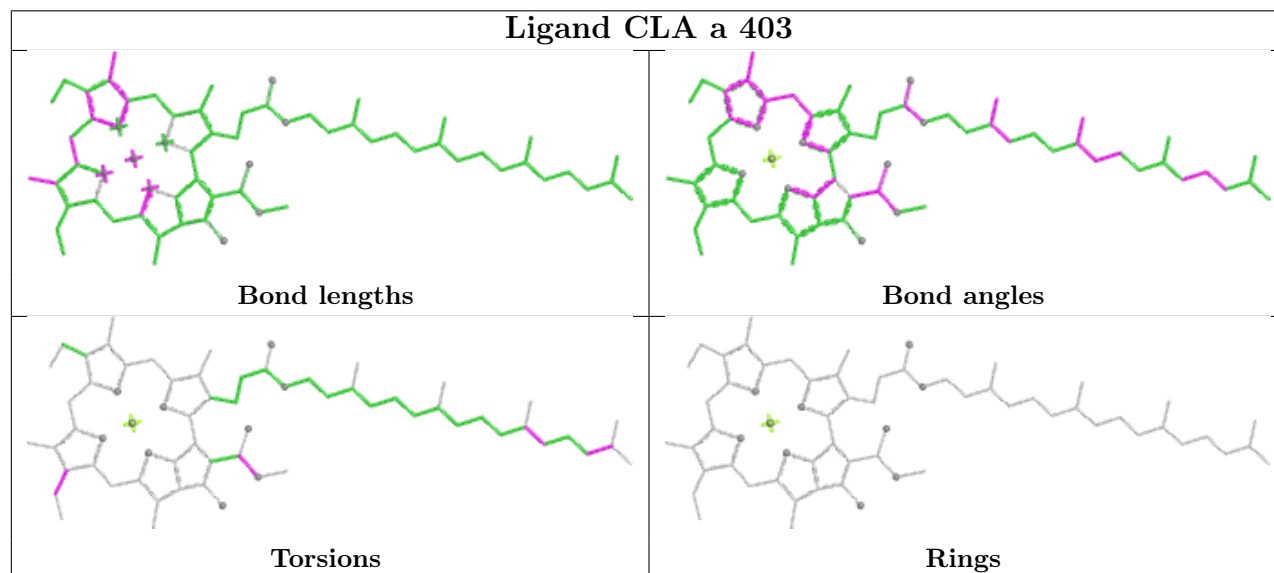
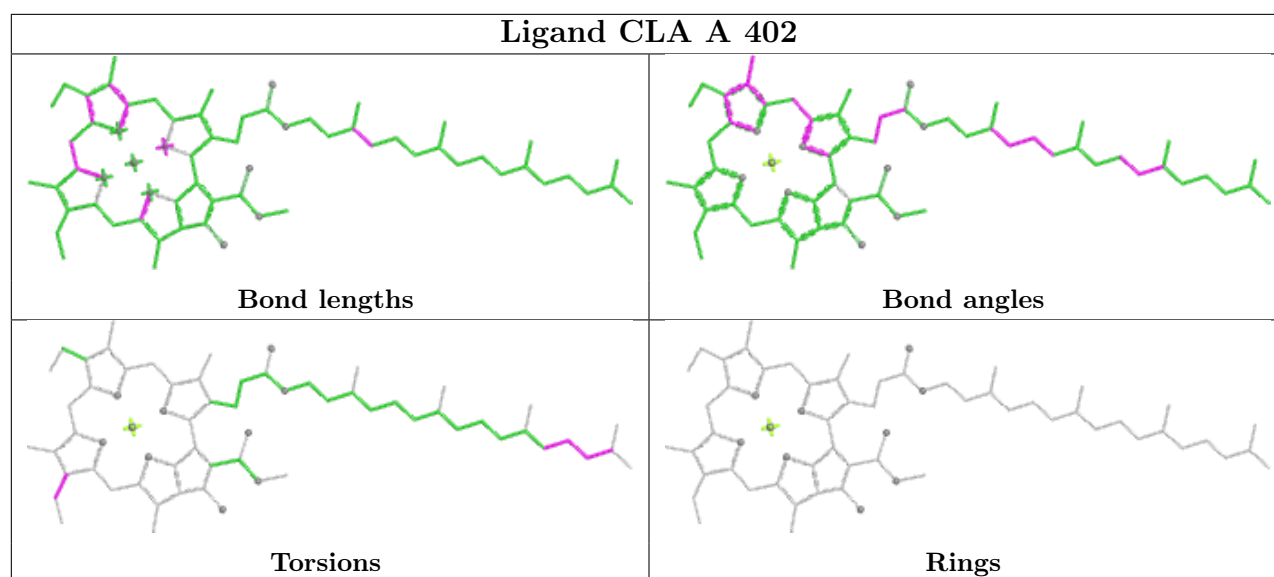


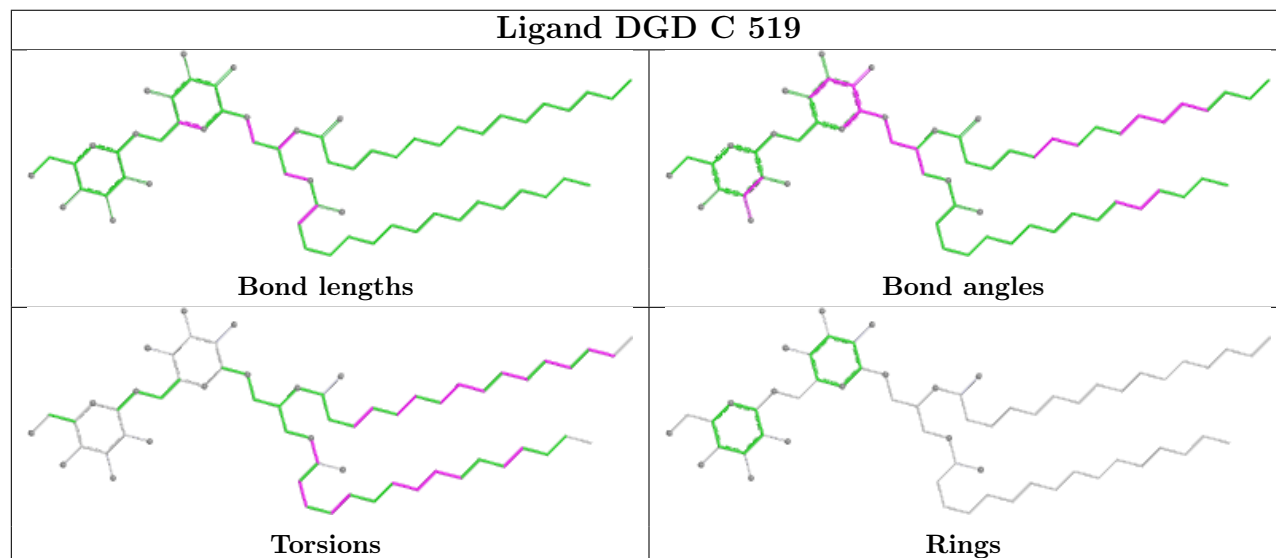
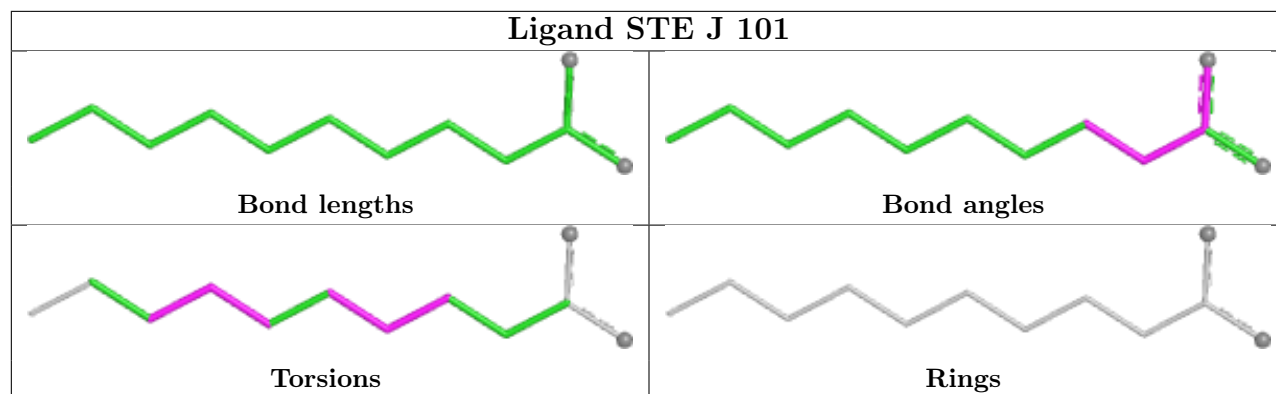
Ligand CLA c 504

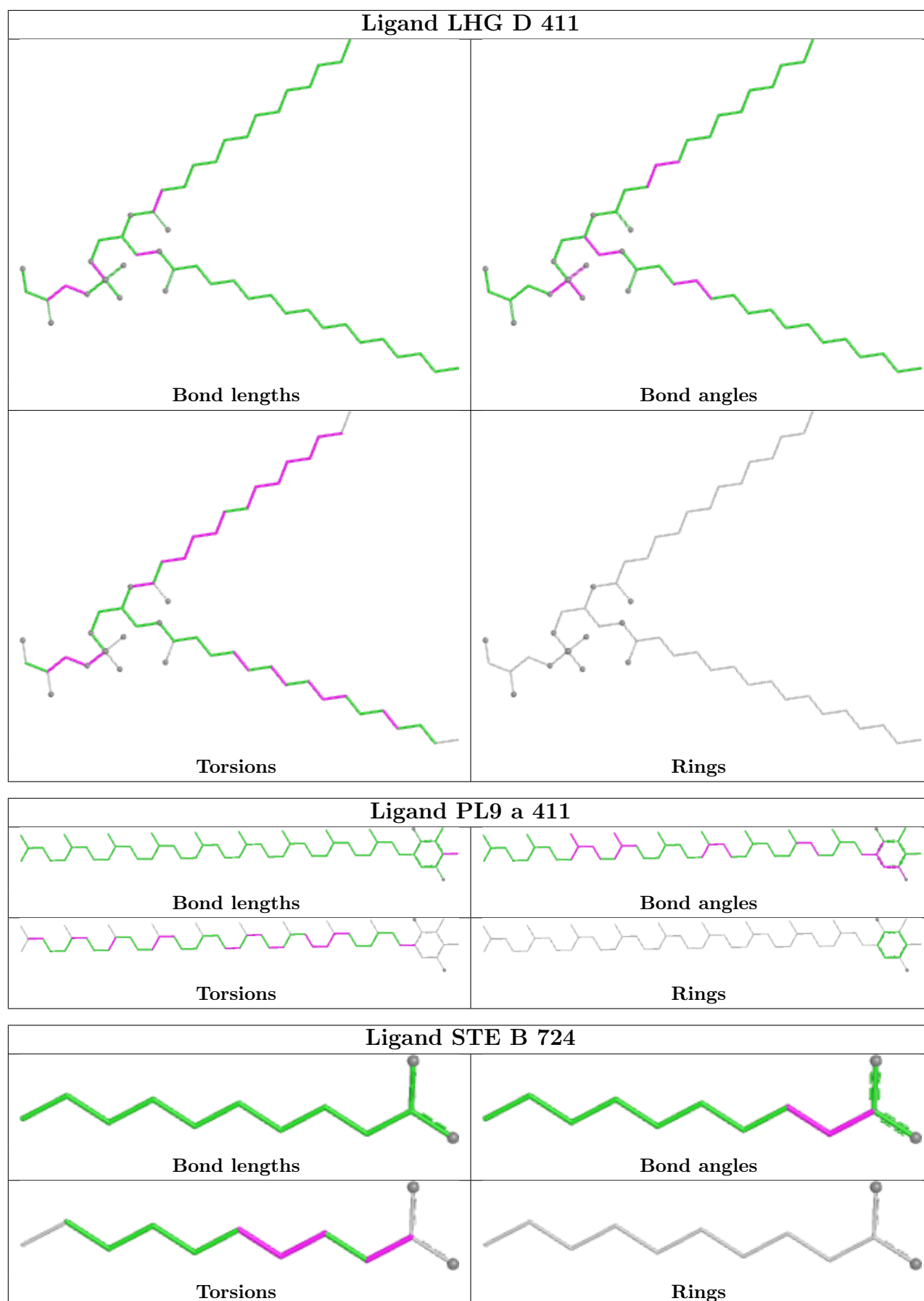


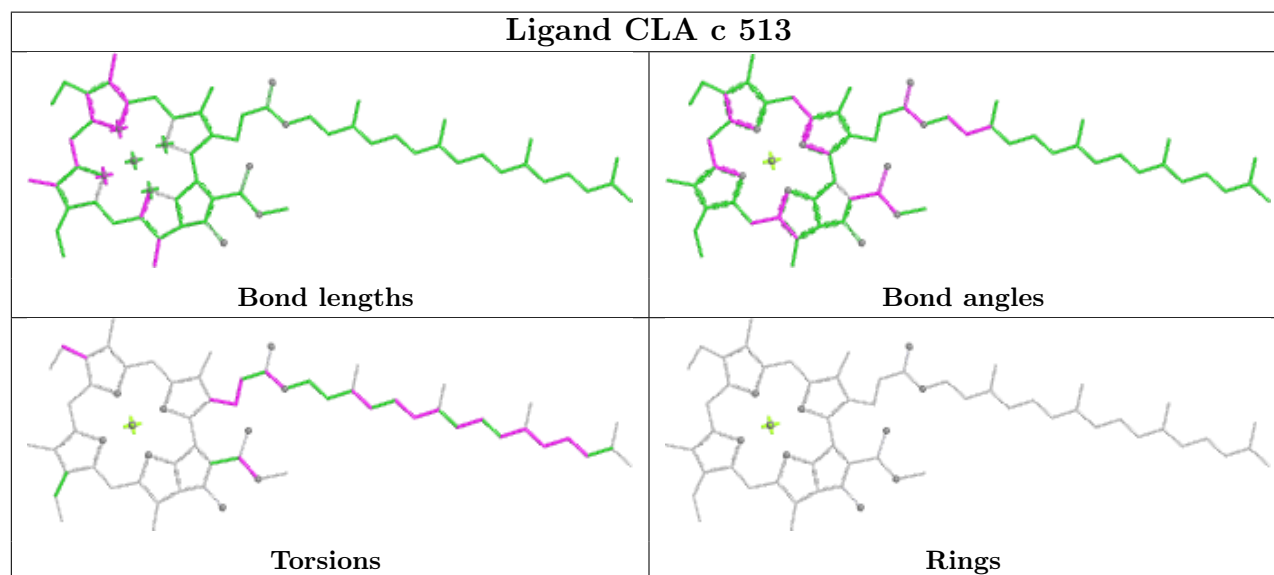
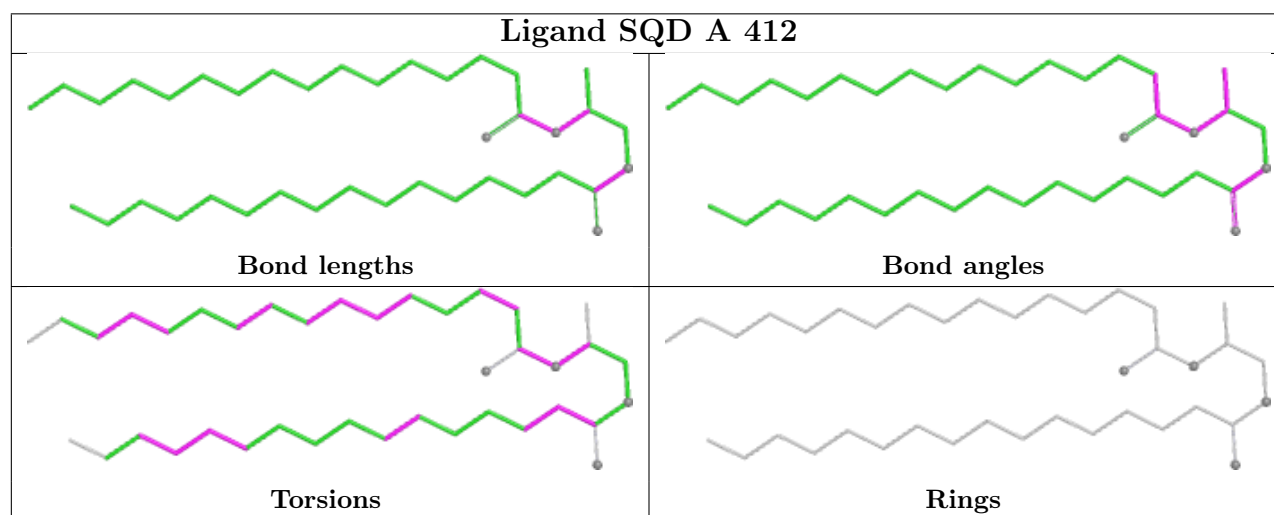
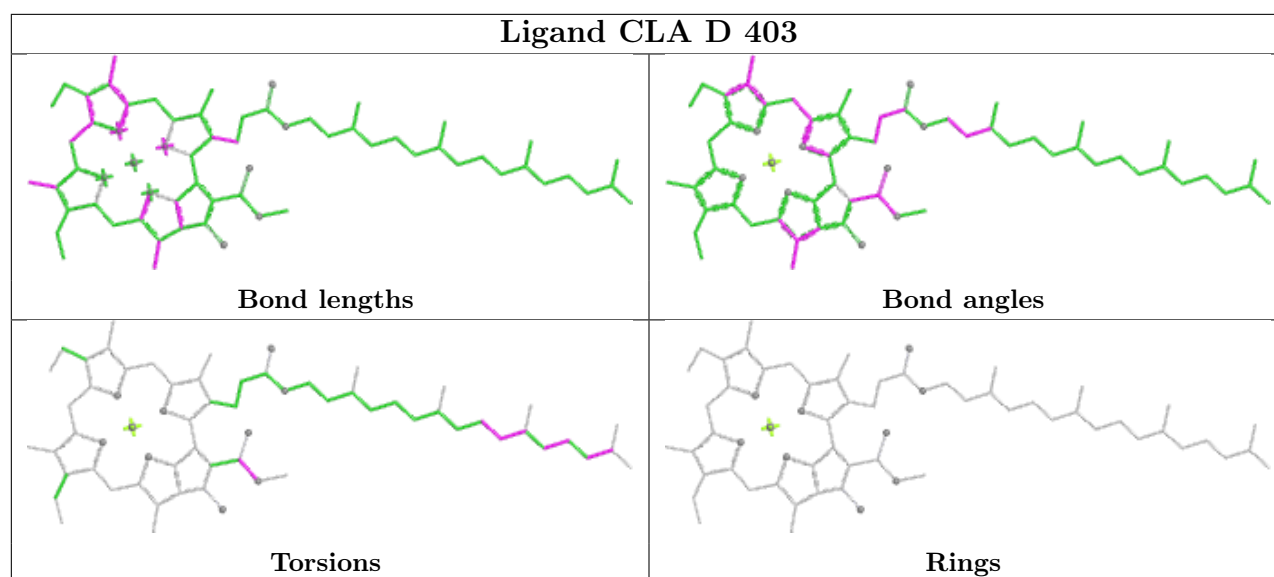


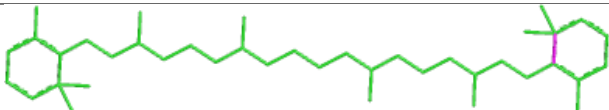
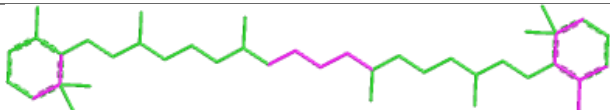
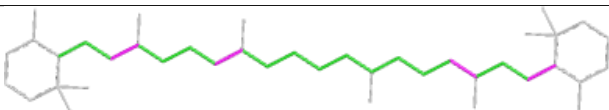
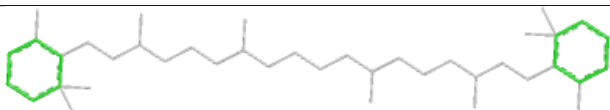




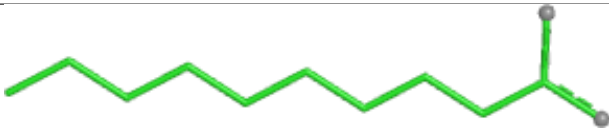
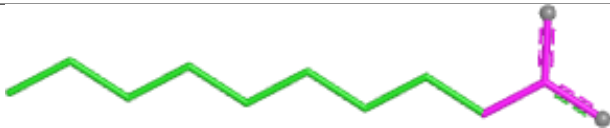
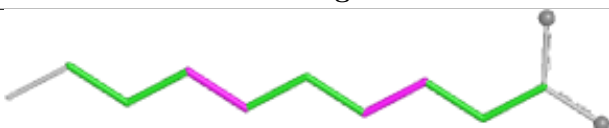
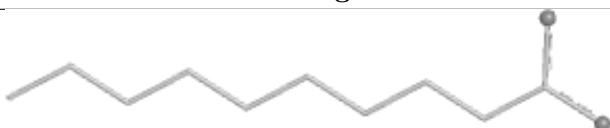


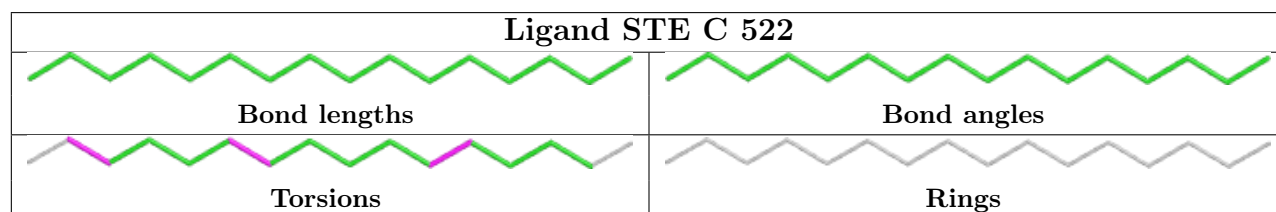
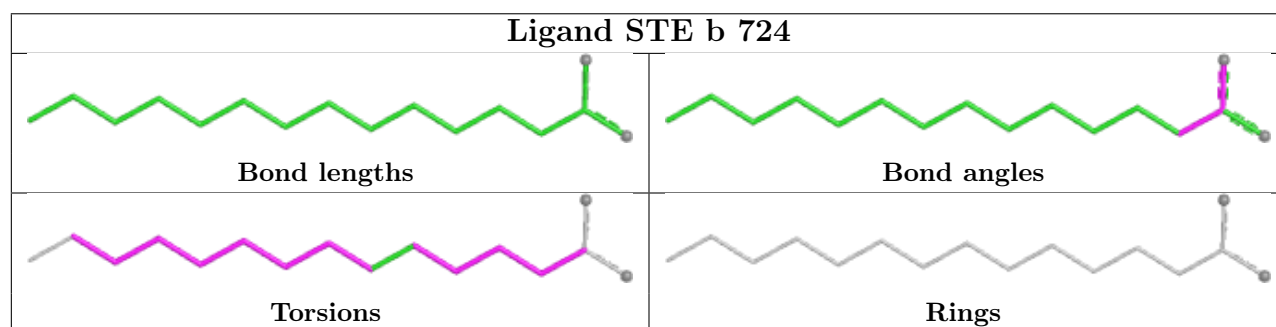
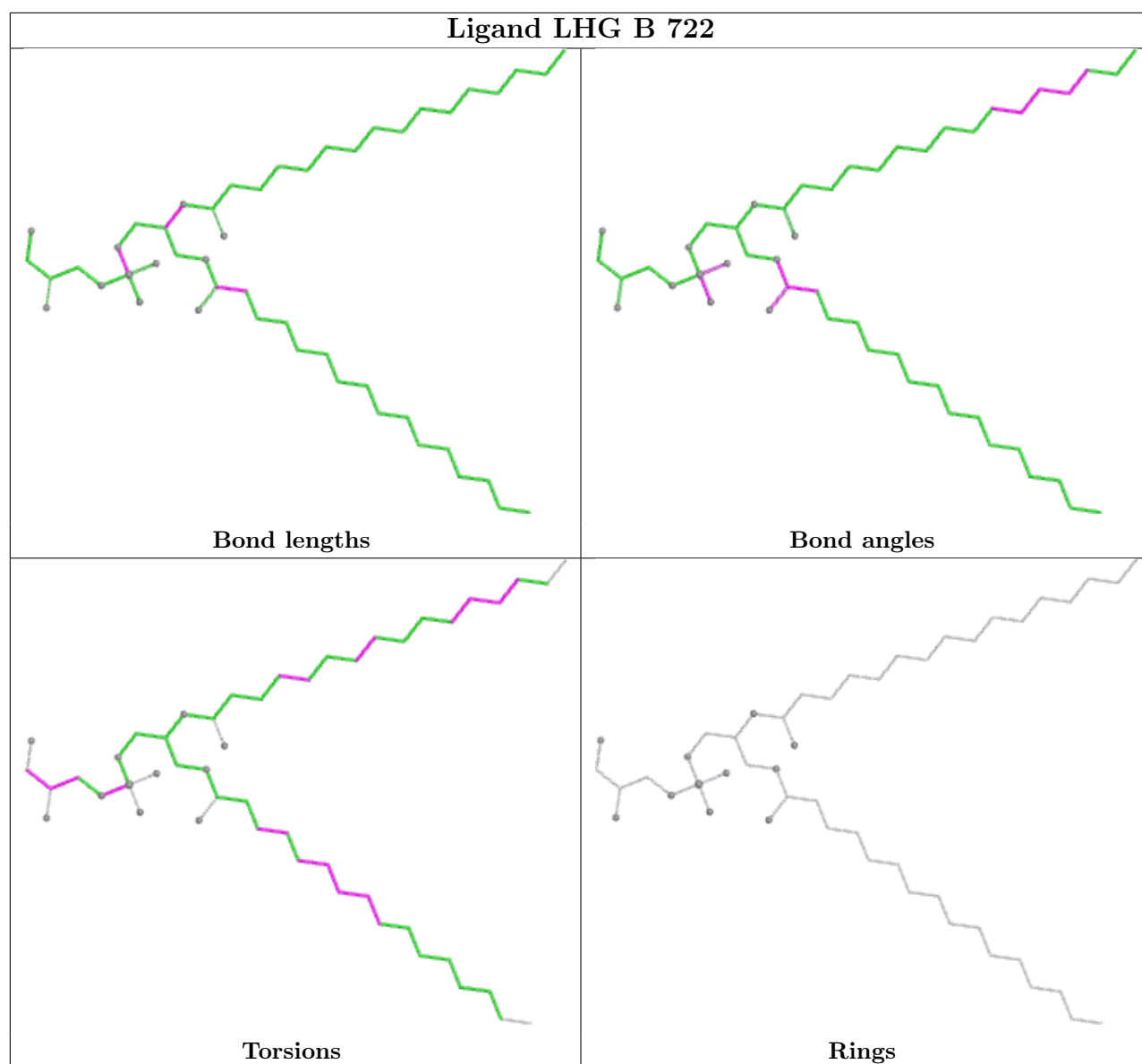


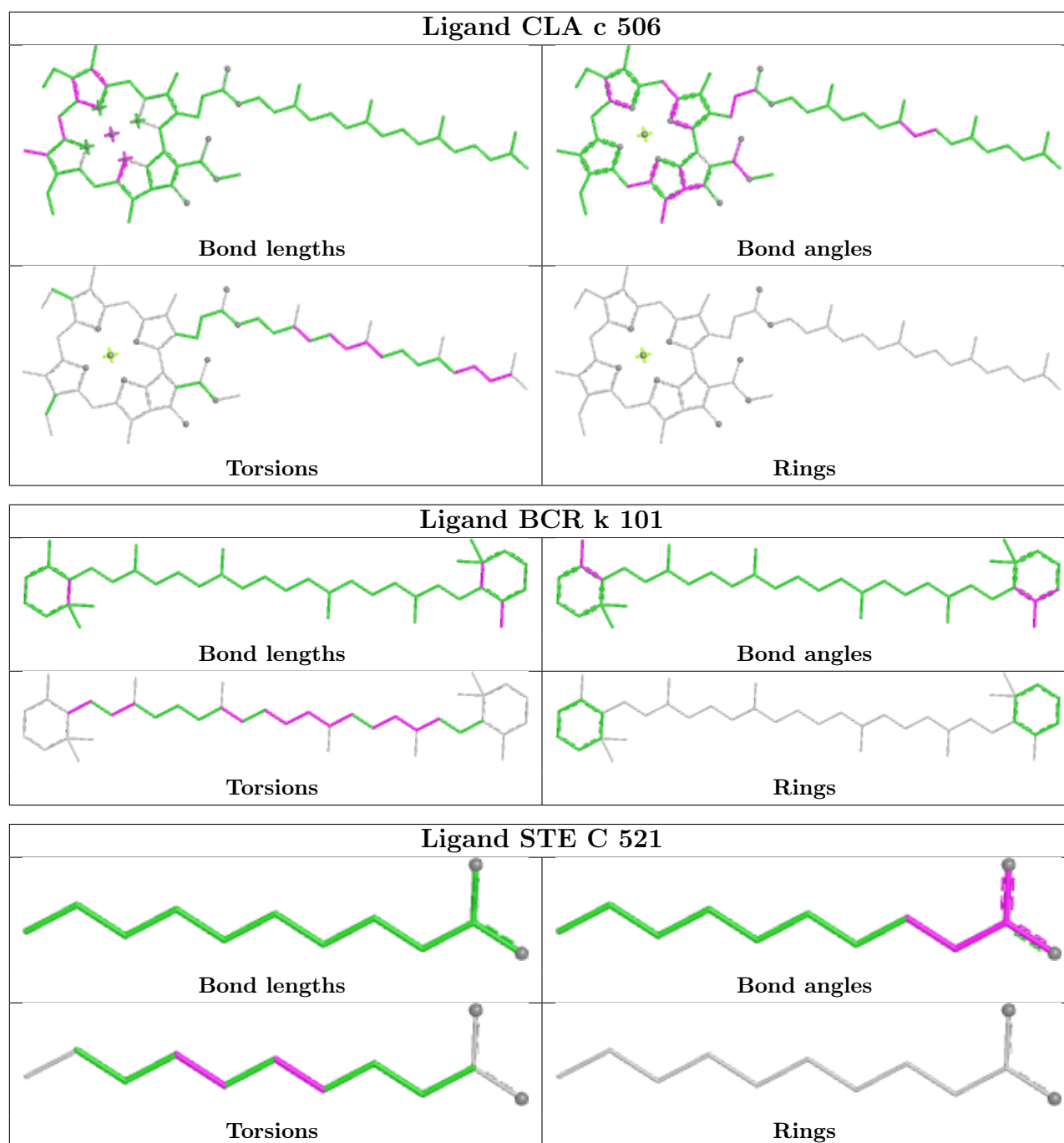


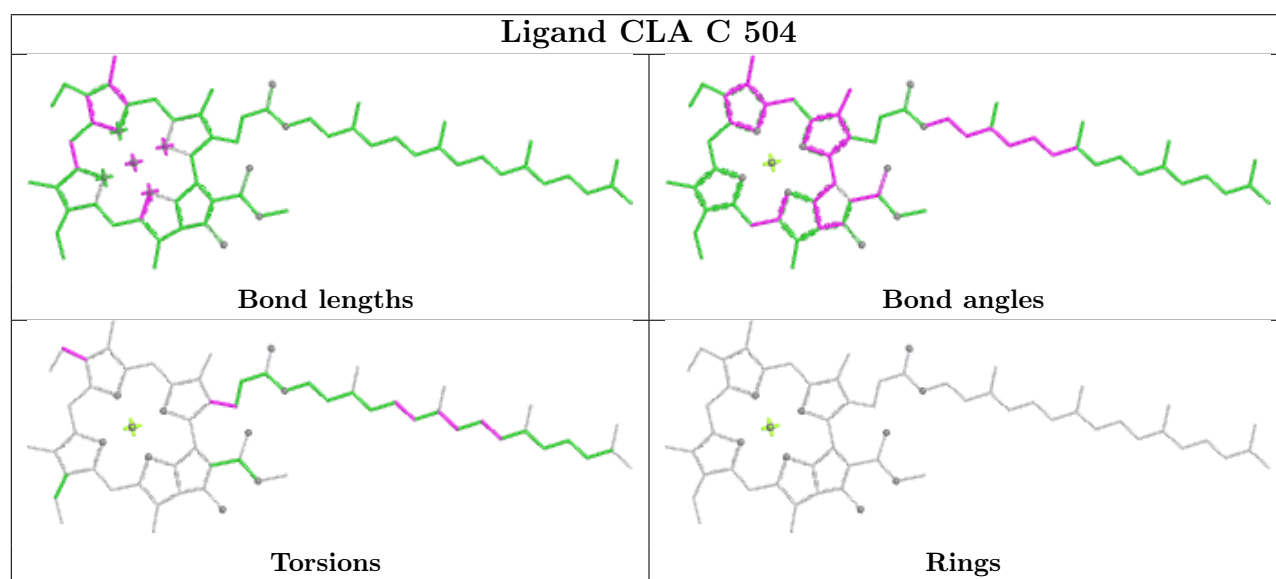
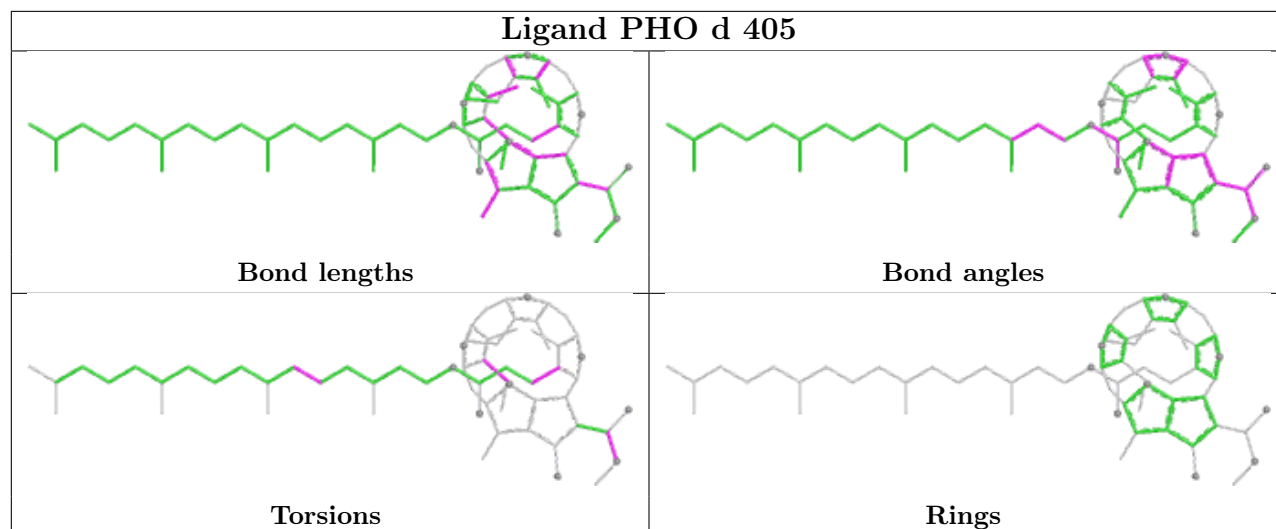
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

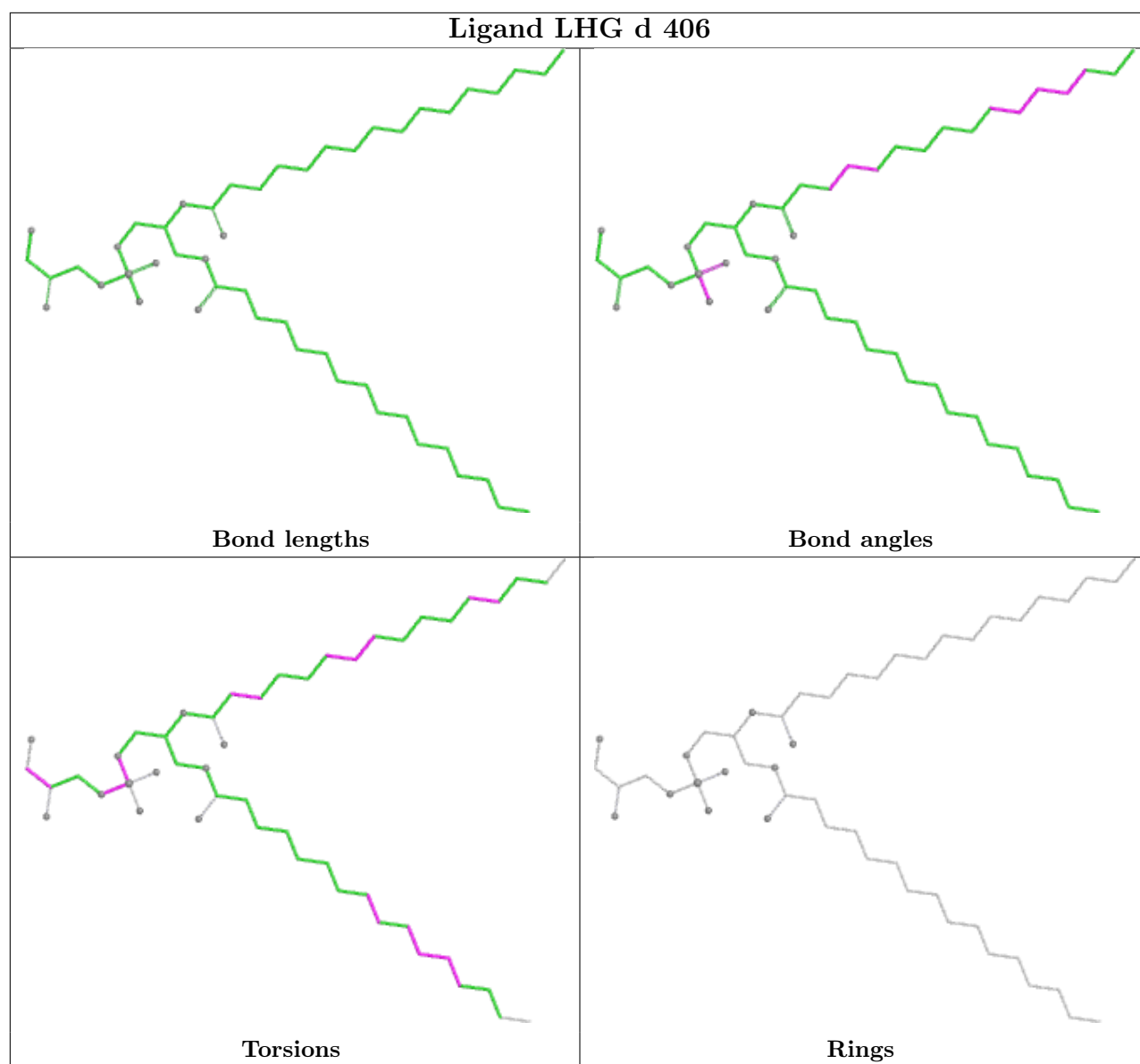
Ligand STE a 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

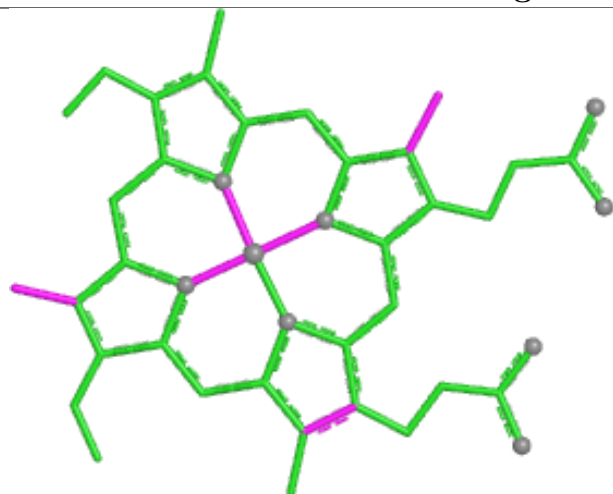




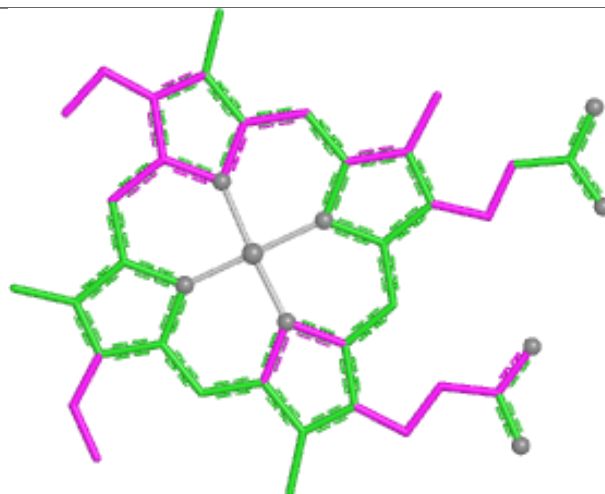




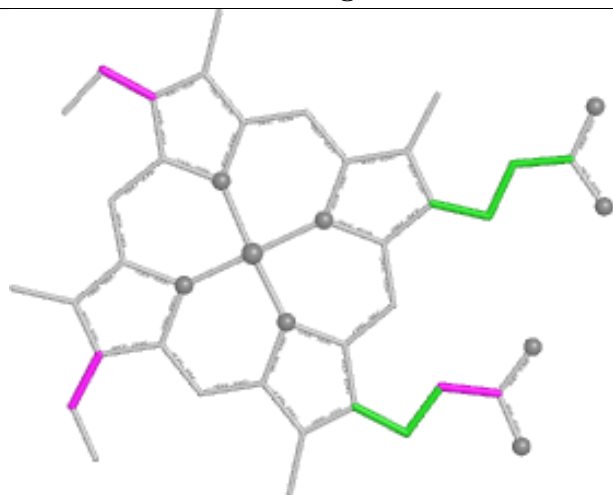
Ligand HEC E 103



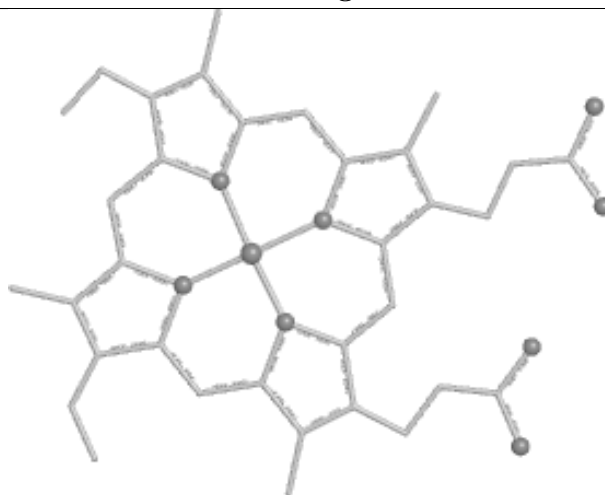
Bond lengths



Bond angles

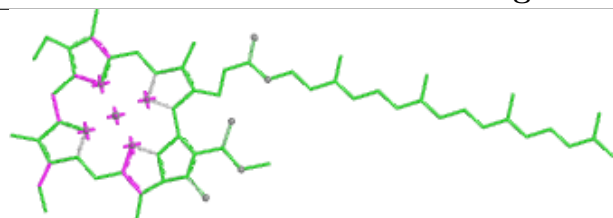


Torsions

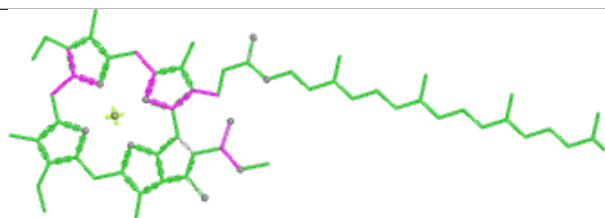


Rings

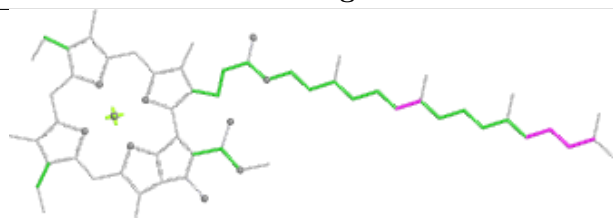
Ligand CLA D 402



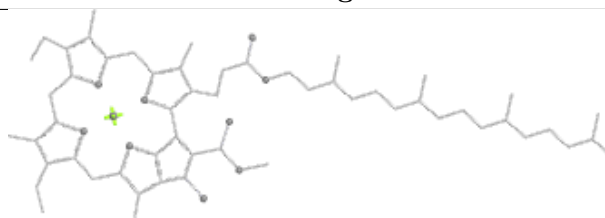
Bond lengths



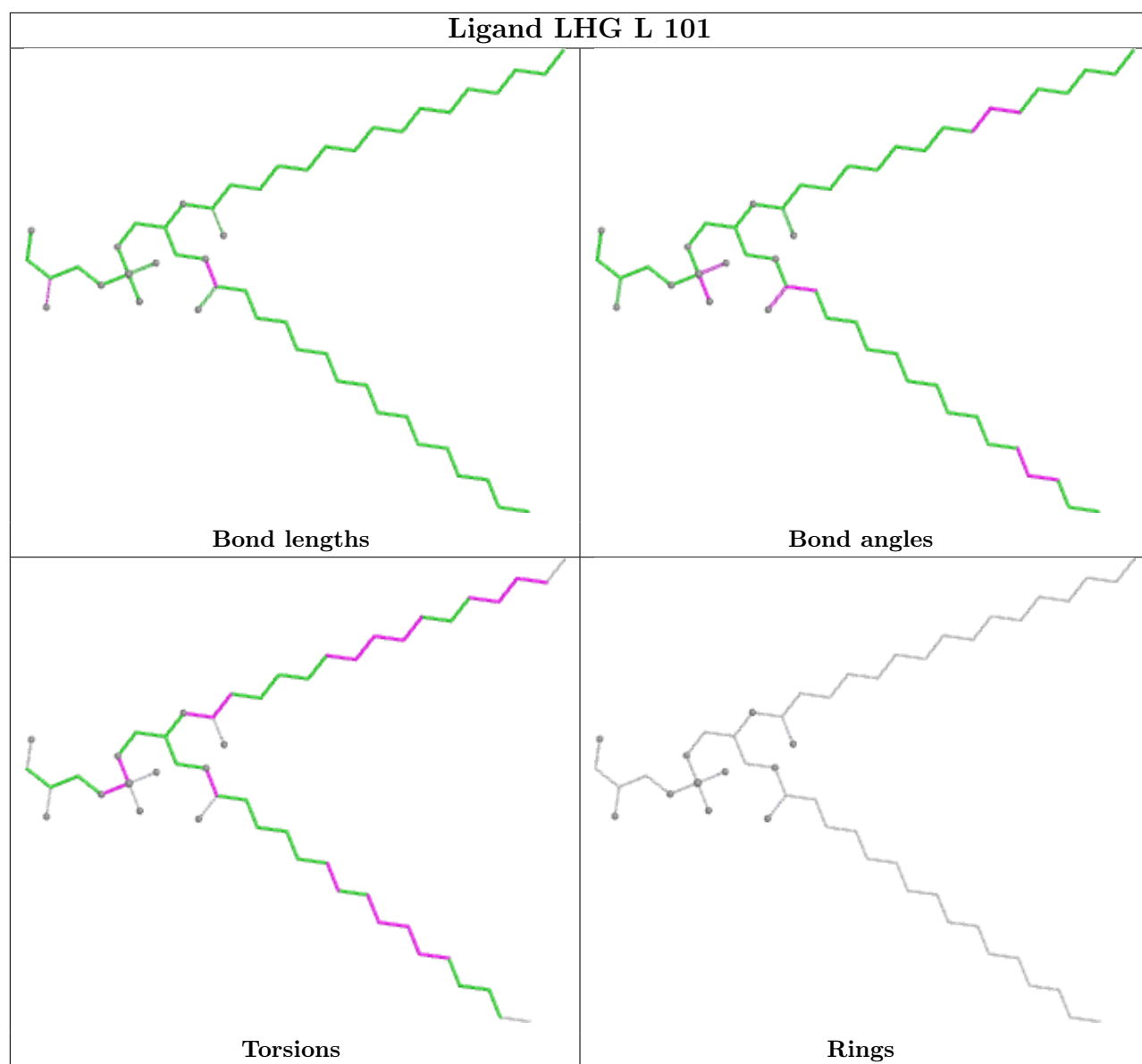
Bond angles

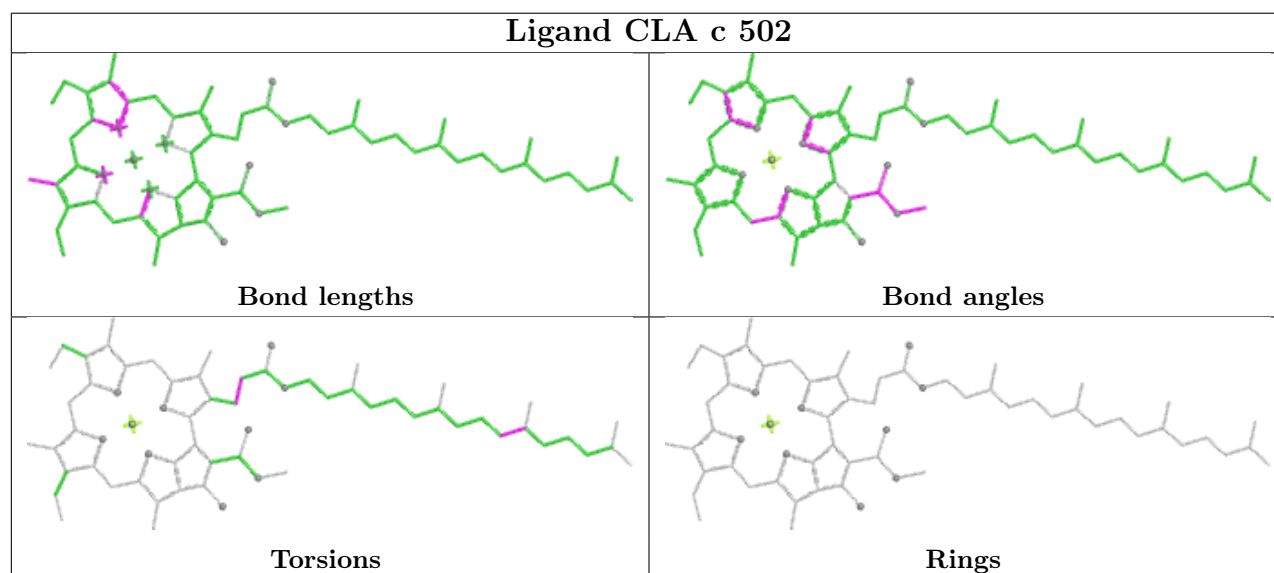
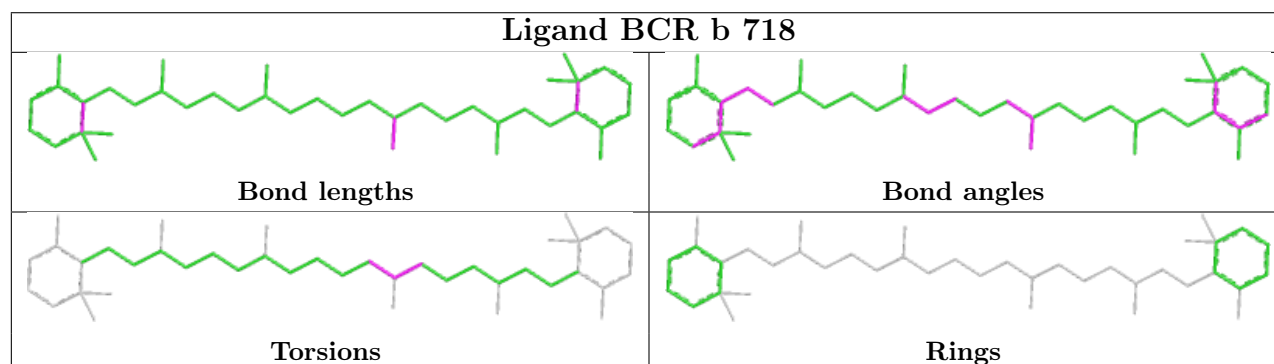
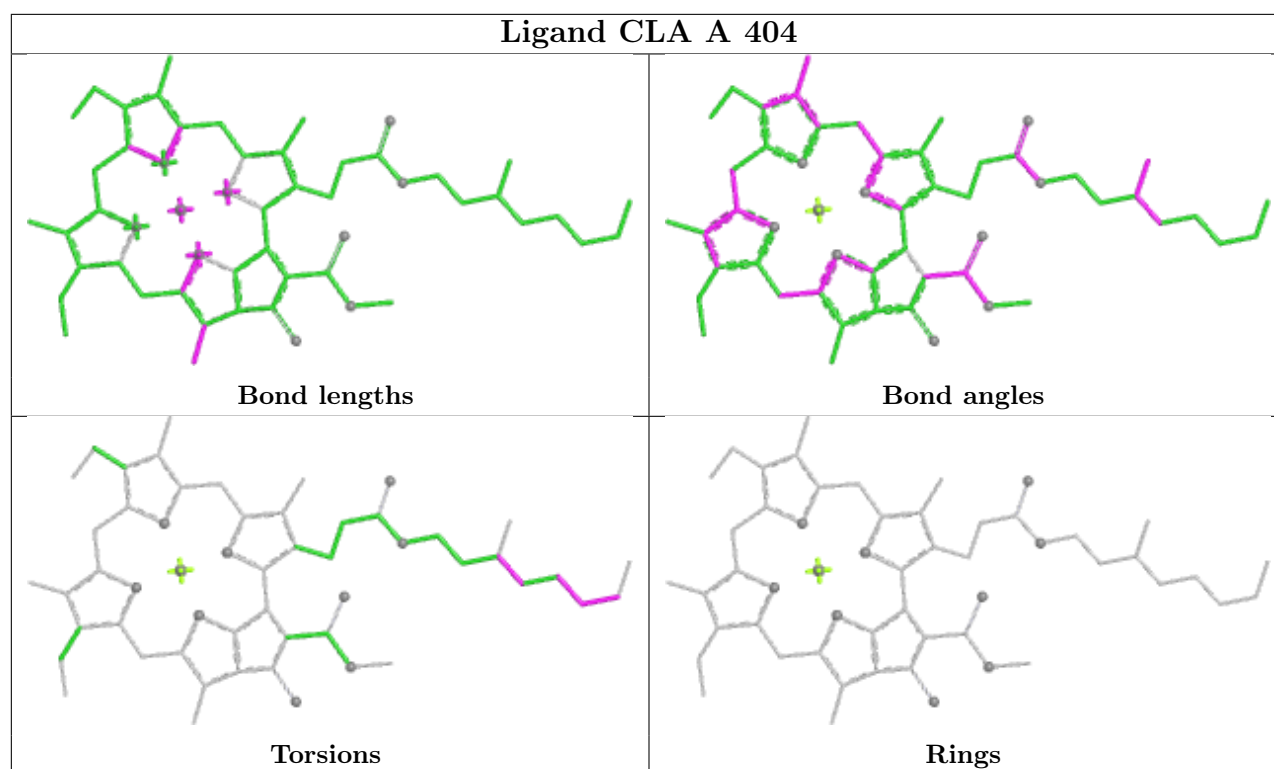


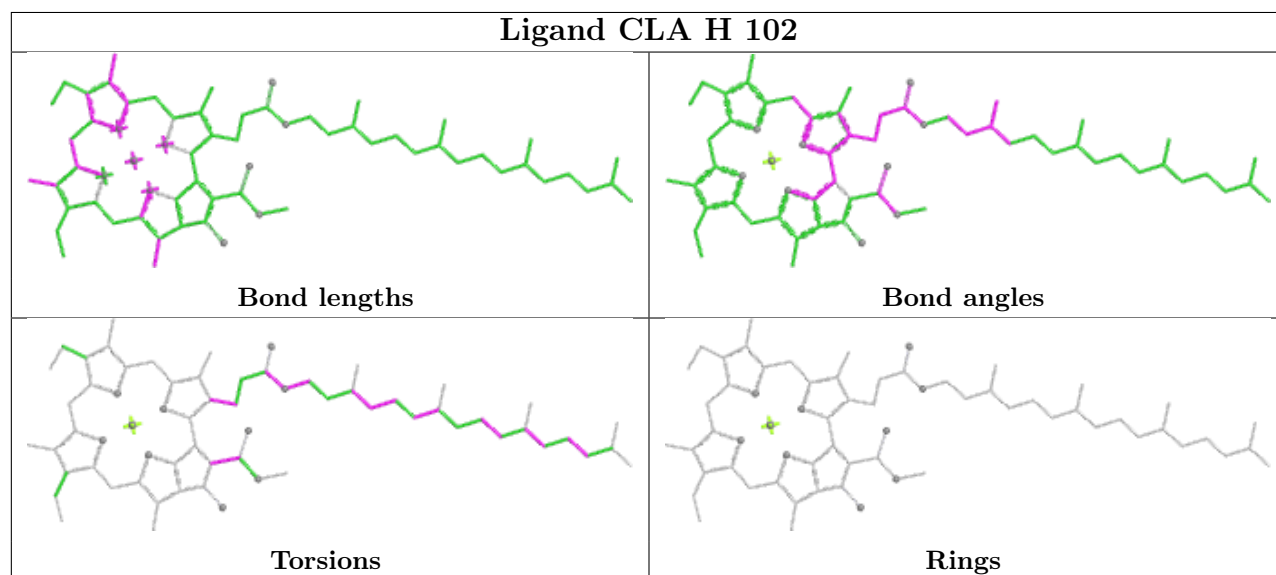
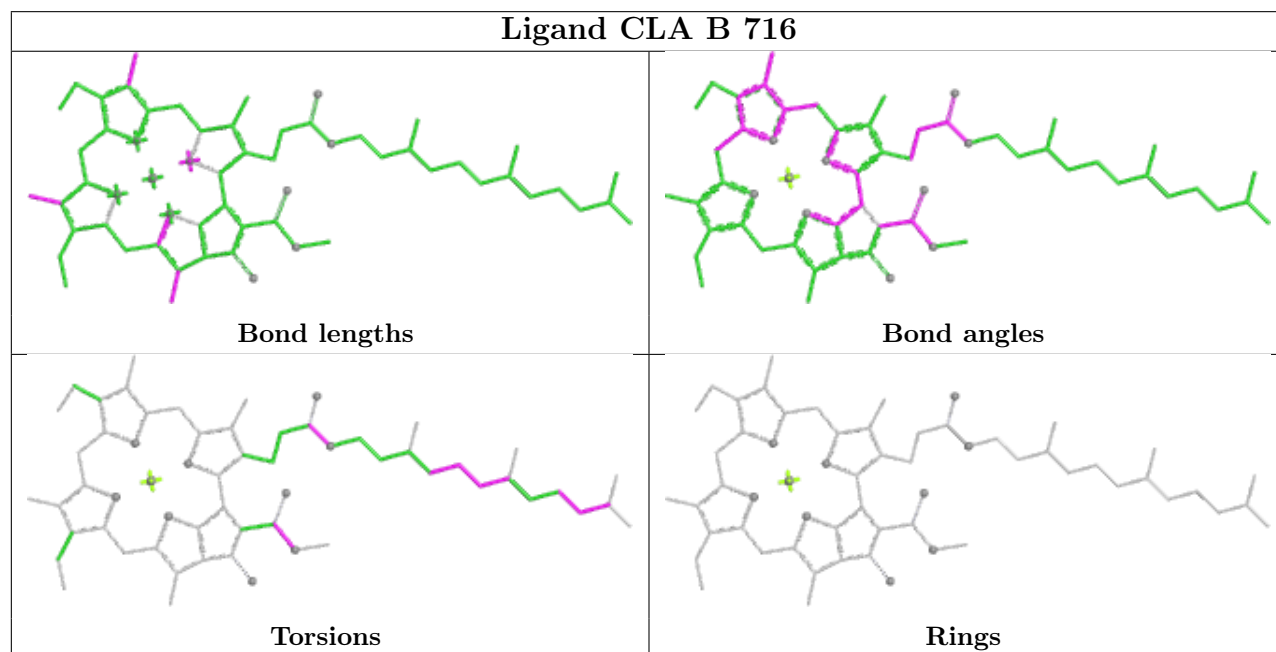
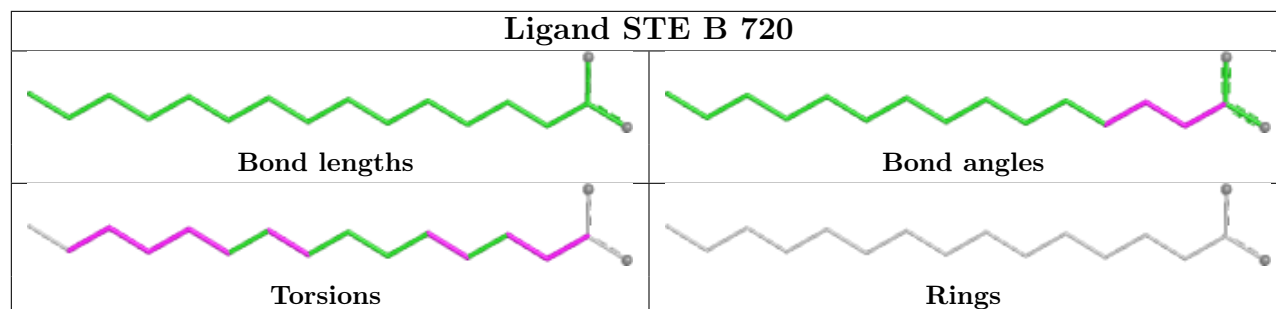
Torsions

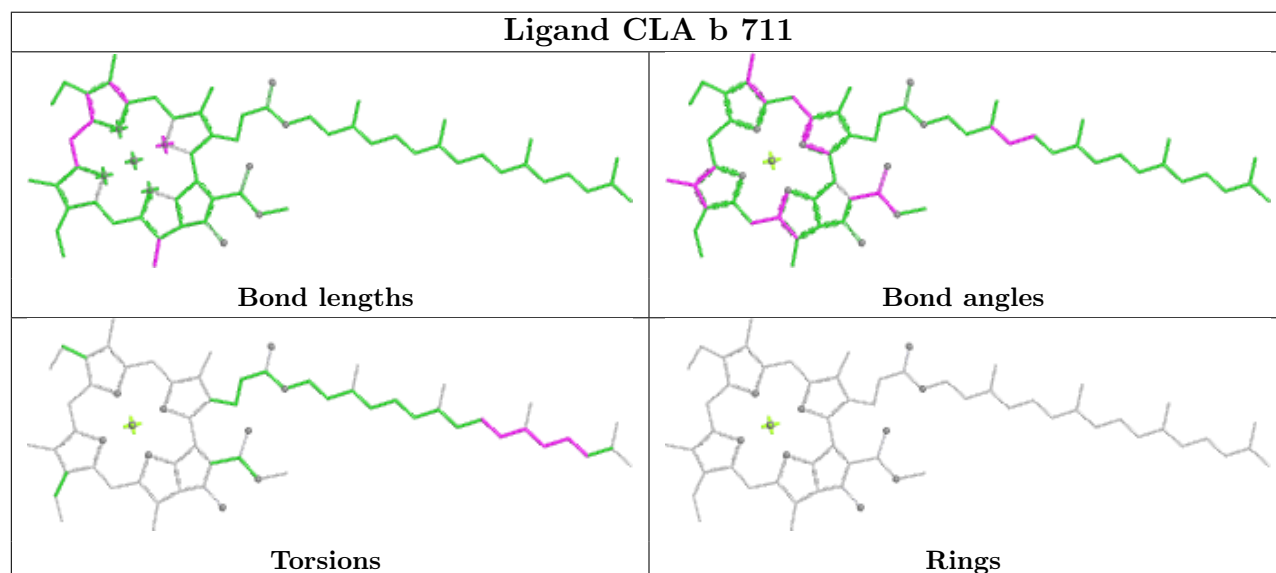
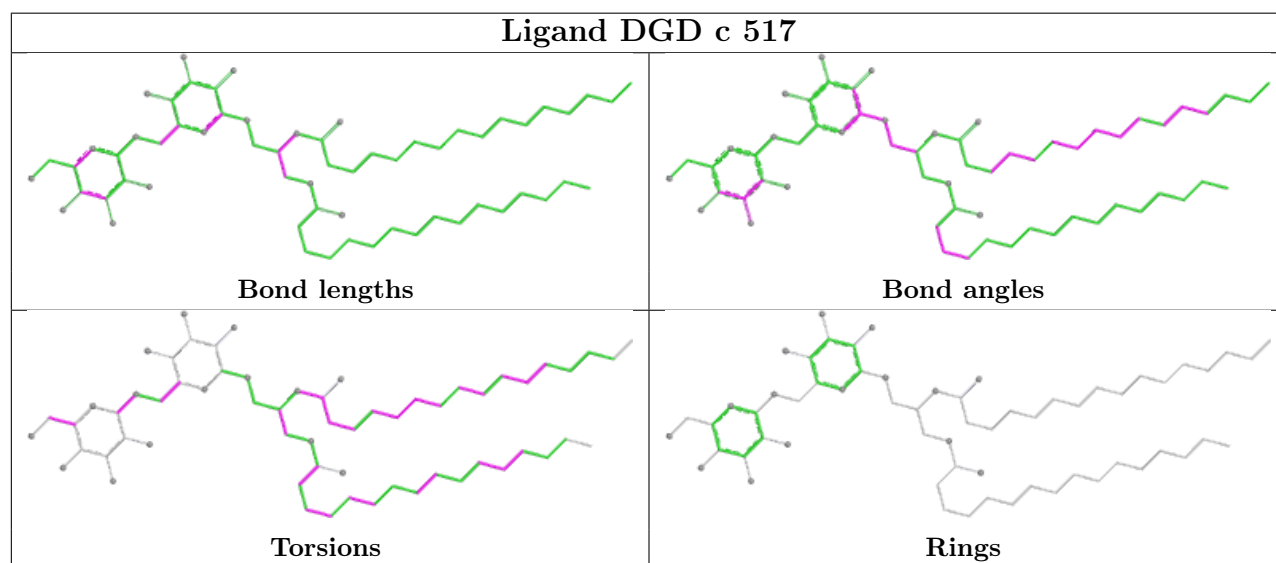
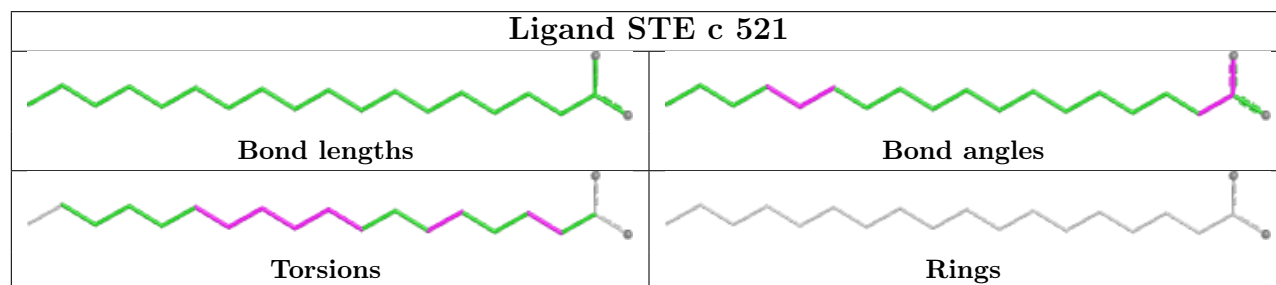
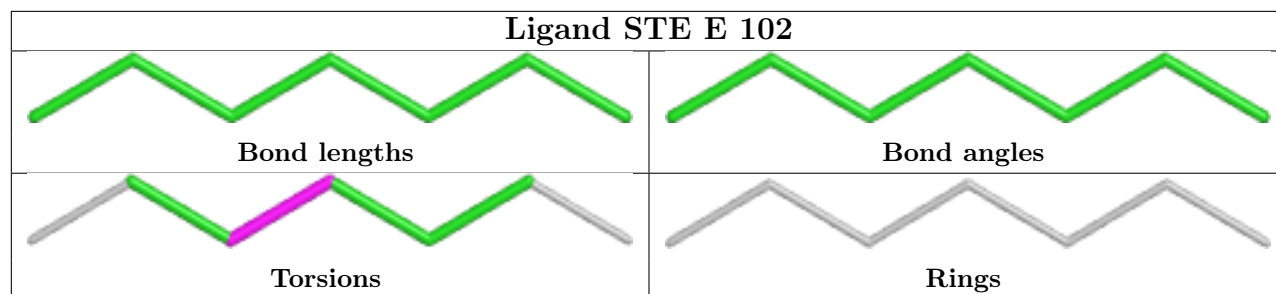


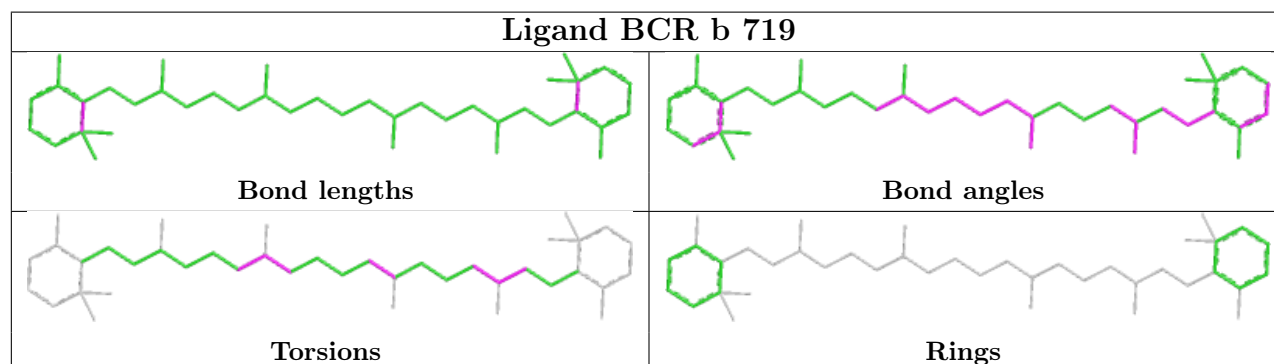
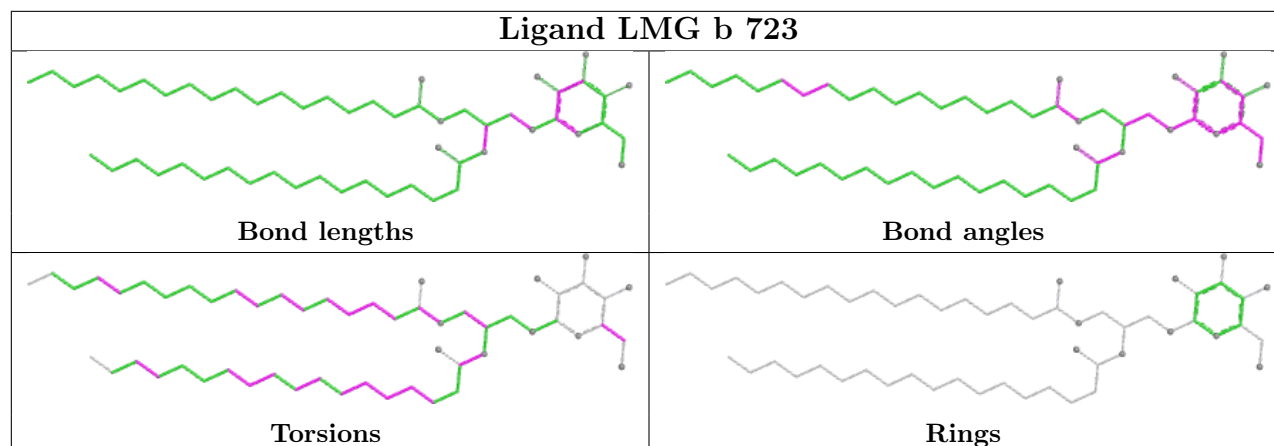
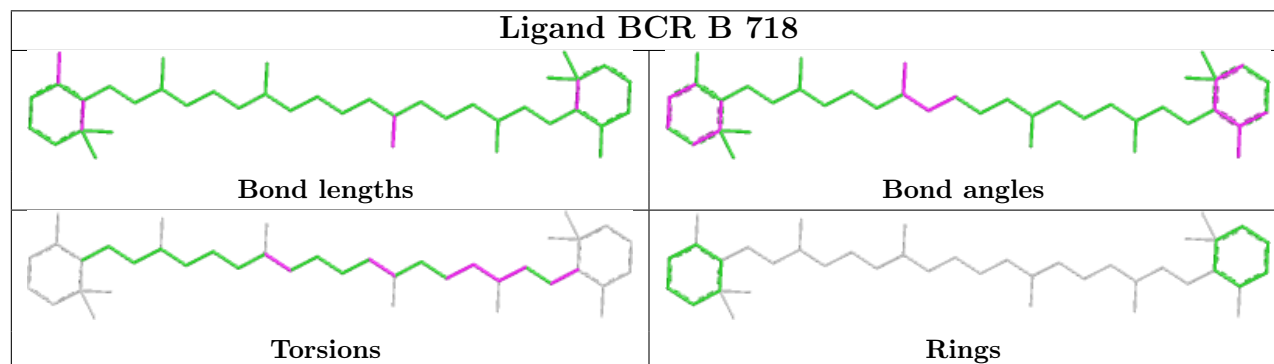
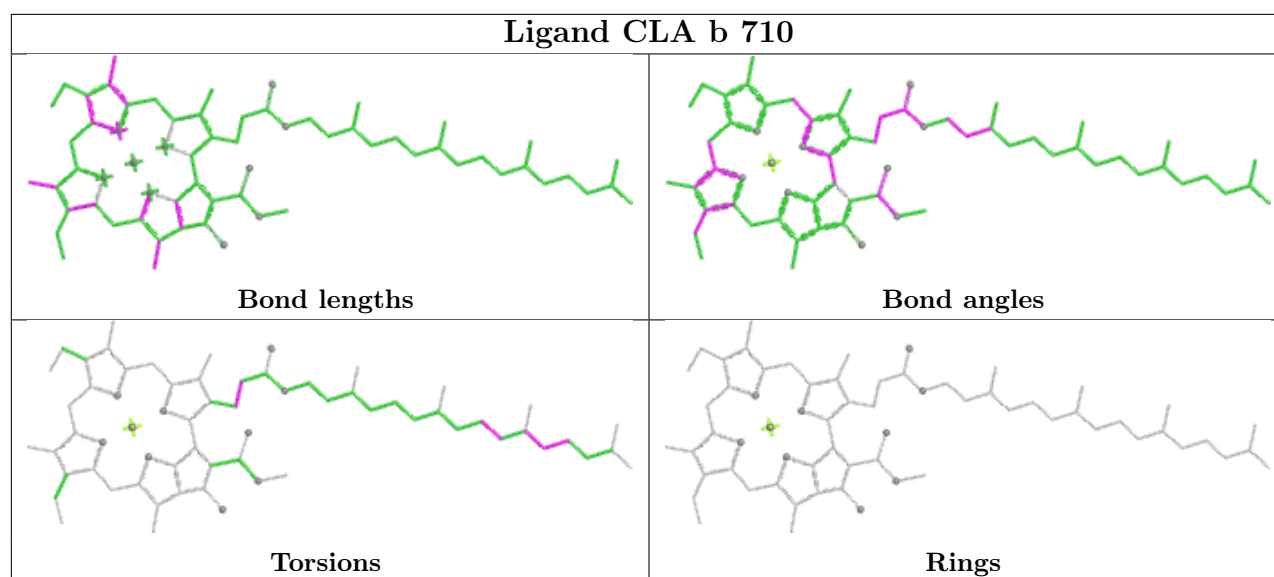
Rings



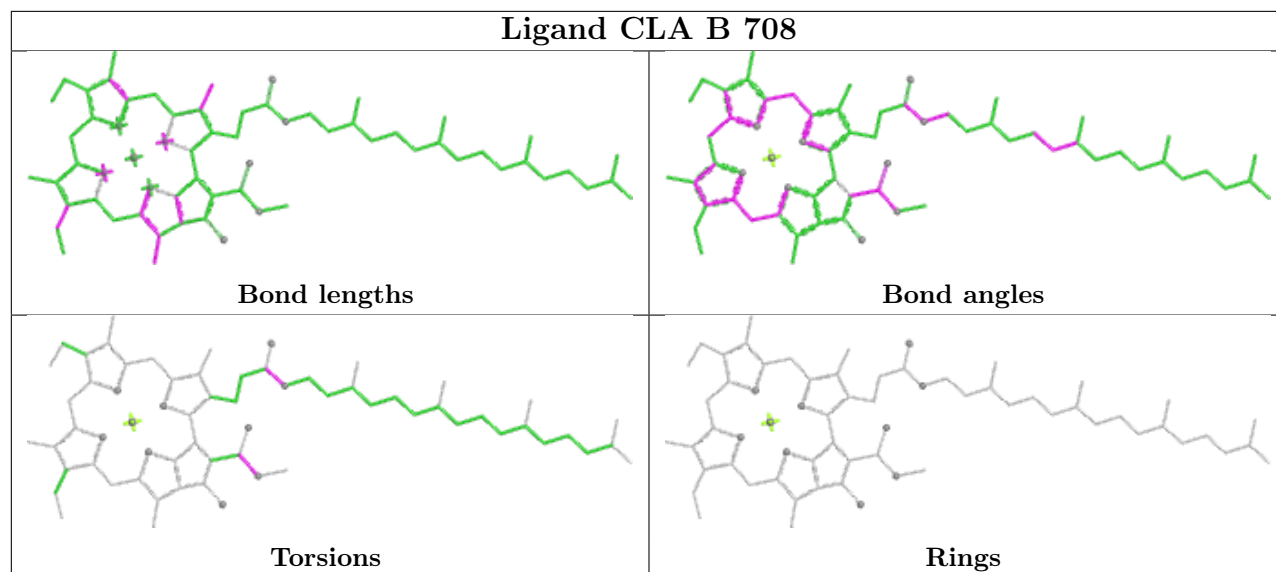




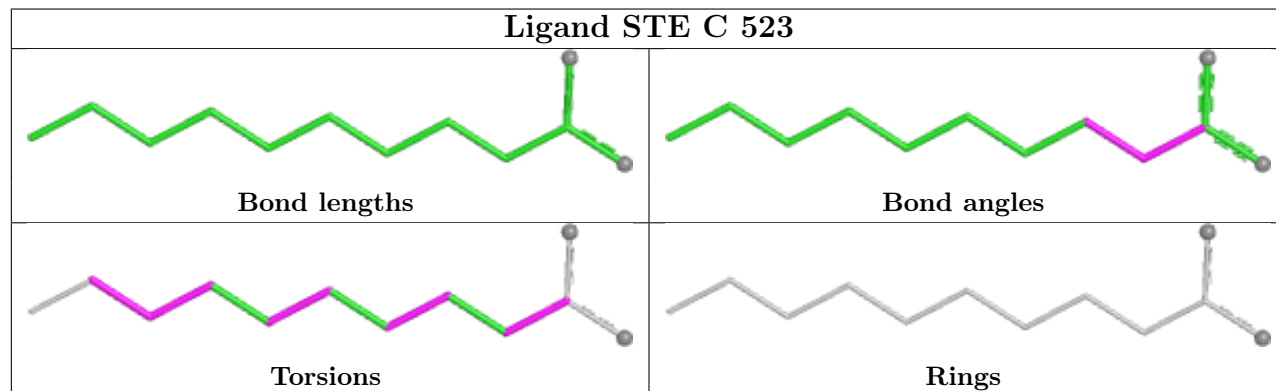




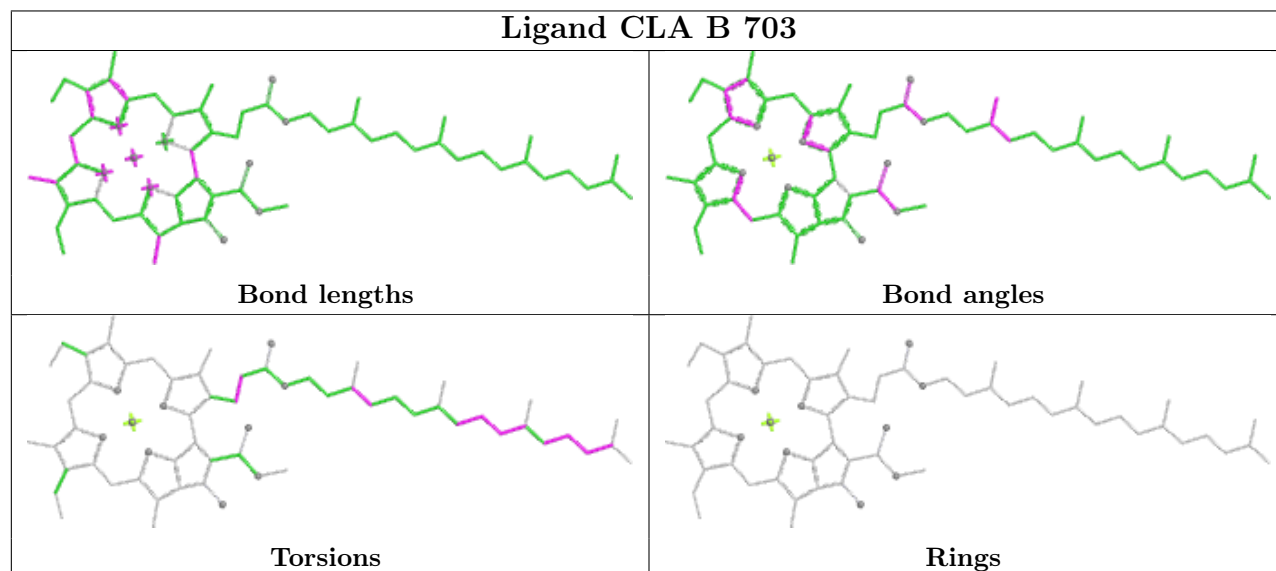
Ligand CLA B 708

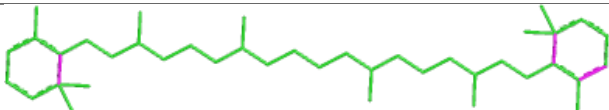
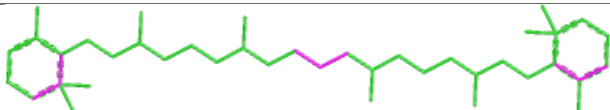
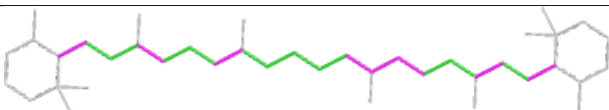
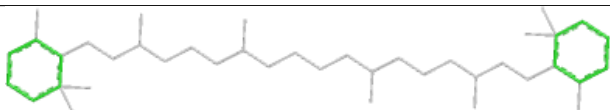


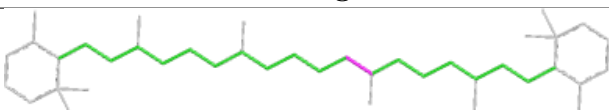
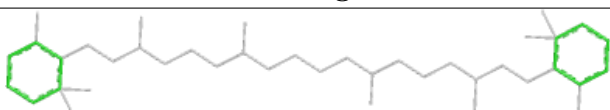
Ligand STE C 523

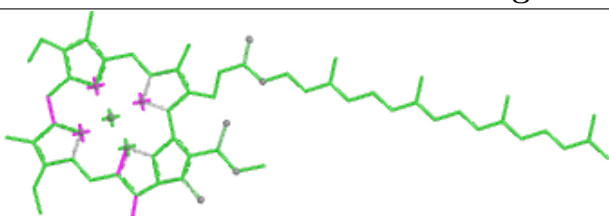
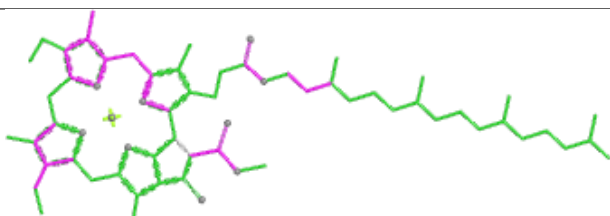
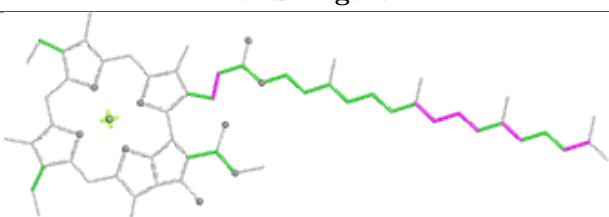
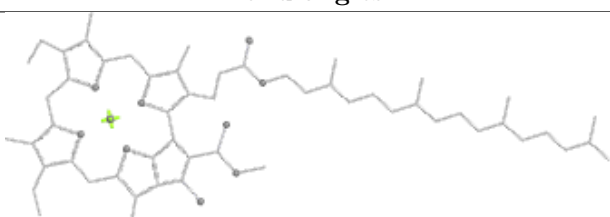


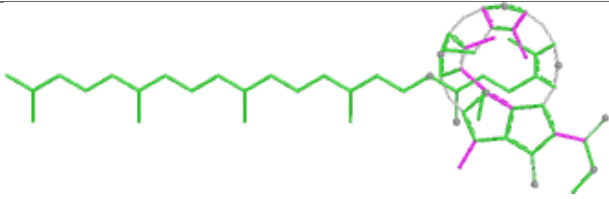
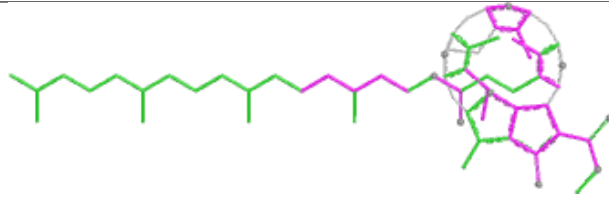
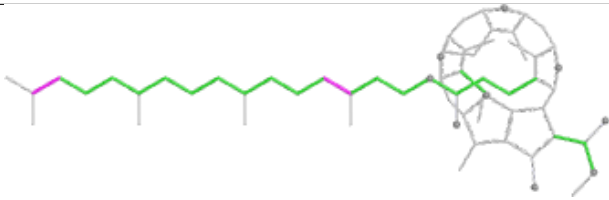
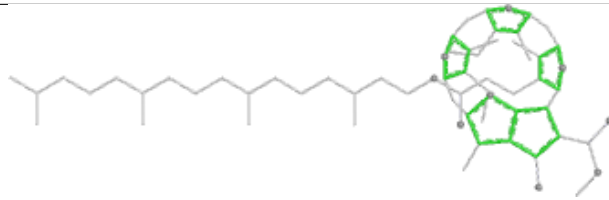
Ligand CLA B 703

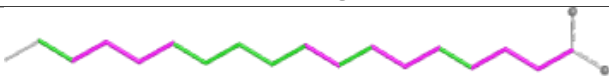
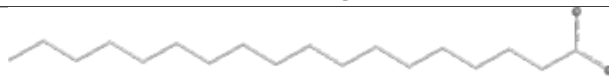


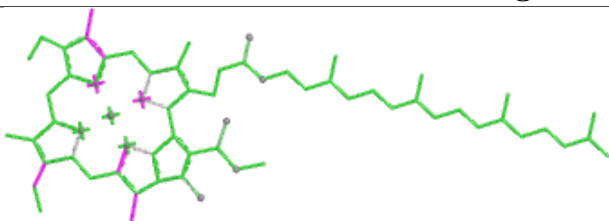
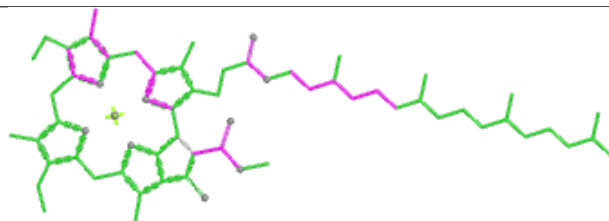
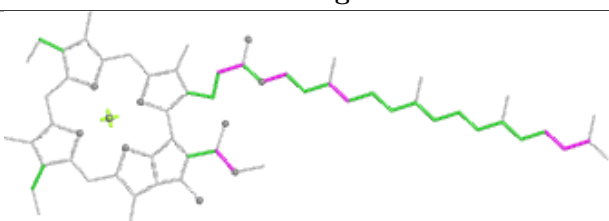
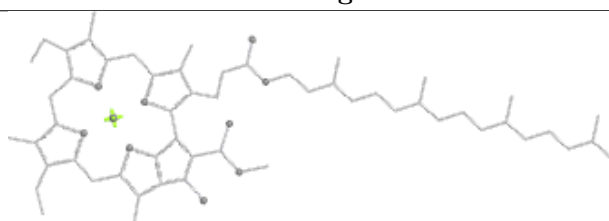
Ligand BCR C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

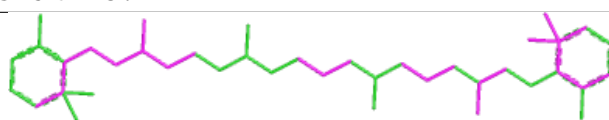
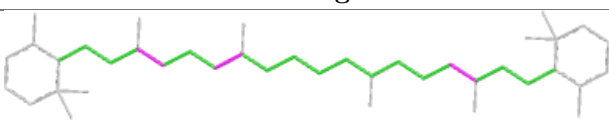
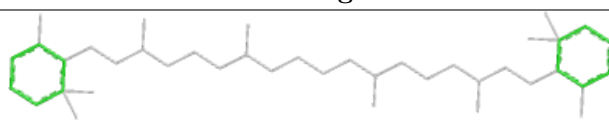
Ligand BCR B 719	
	
Bond lengths	Bond angles
	
Torsions	Rings

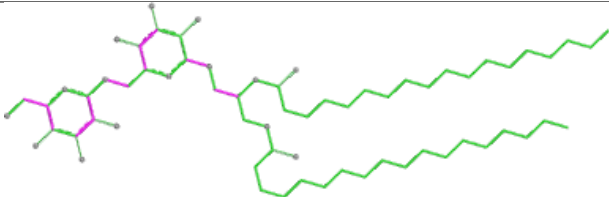
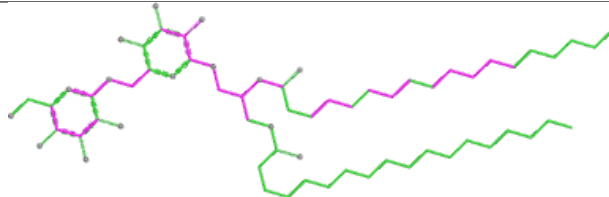
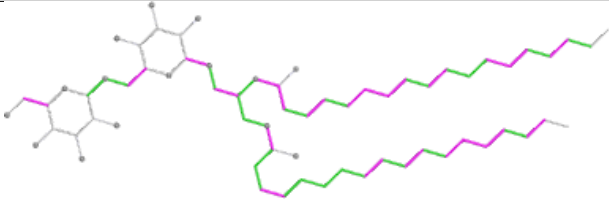
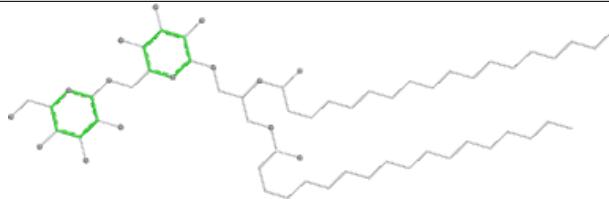
Ligand CLA b 706	
	
Bond lengths	Bond angles
	
Torsions	Rings

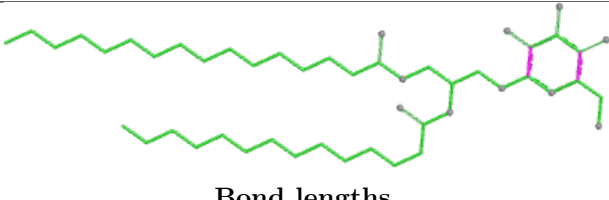
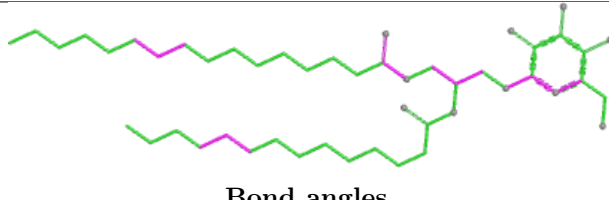
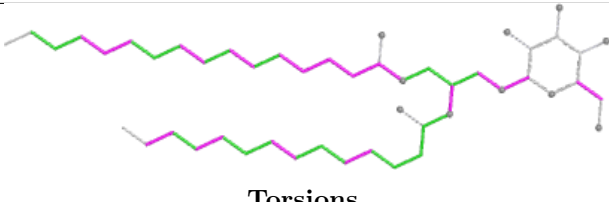
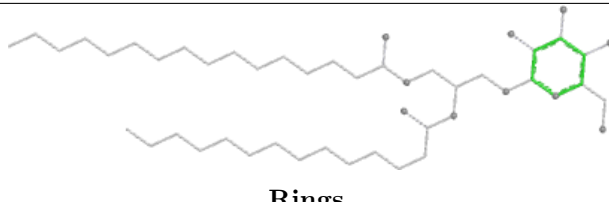
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Bond lengths	Bond angles
	
Torsions	Rings

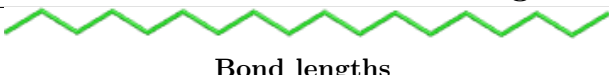
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Bond lengths	Bond angles
	
Torsions	Rings

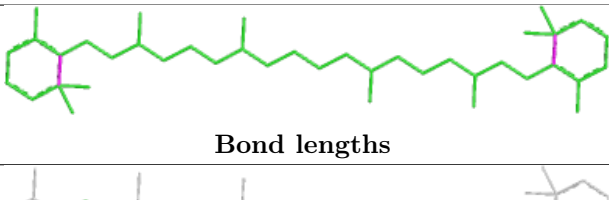
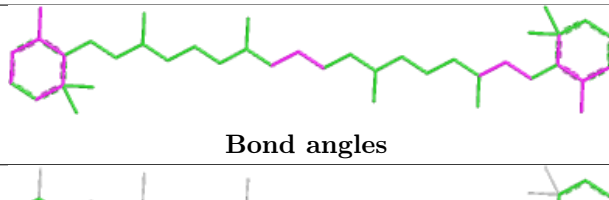
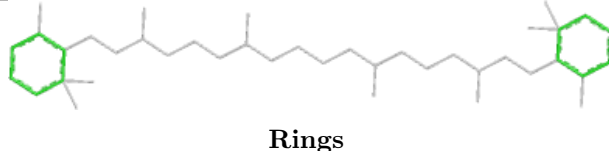
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

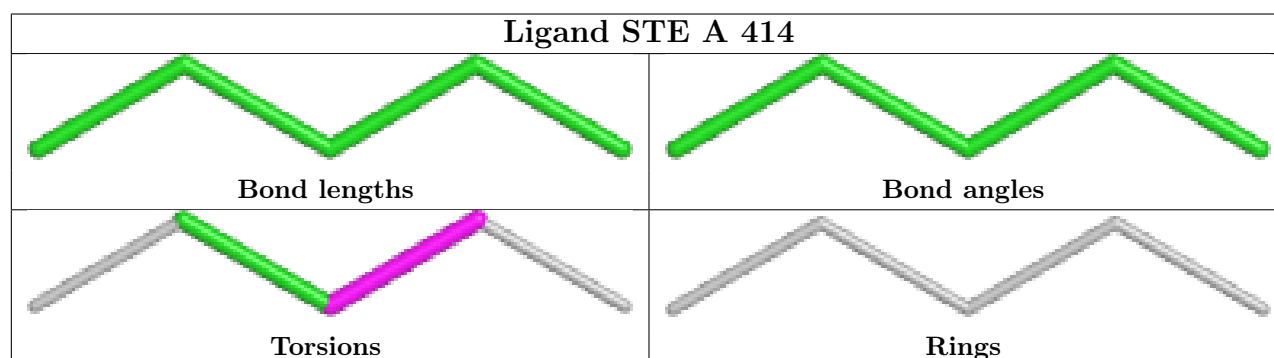
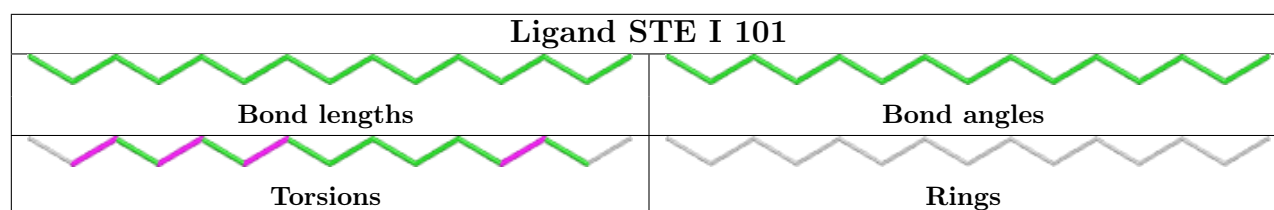
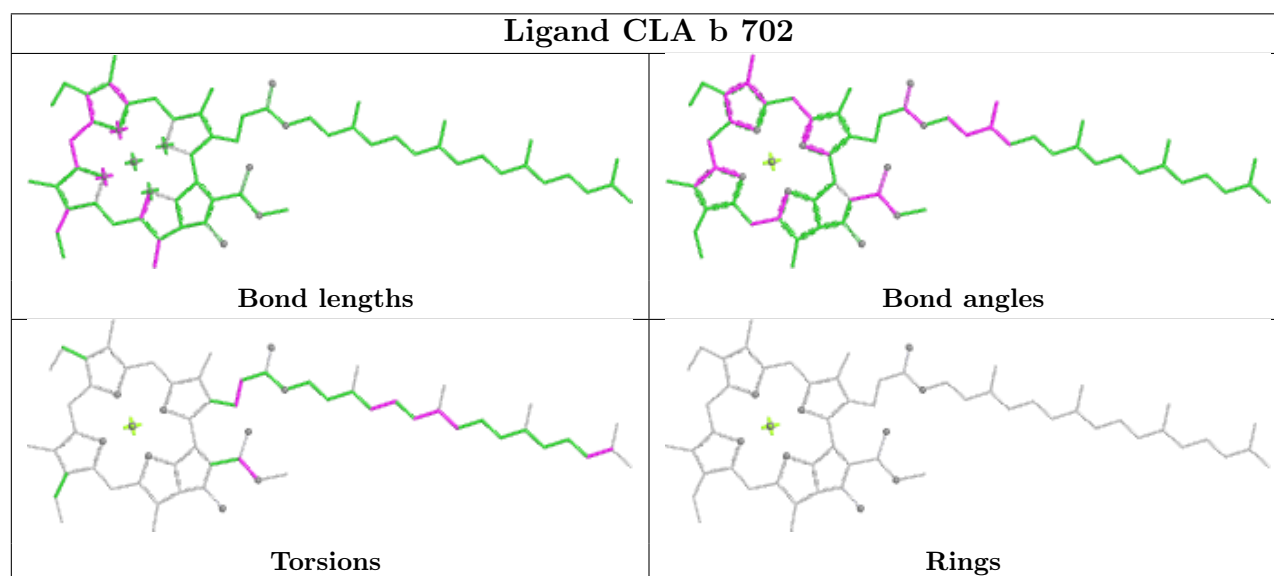
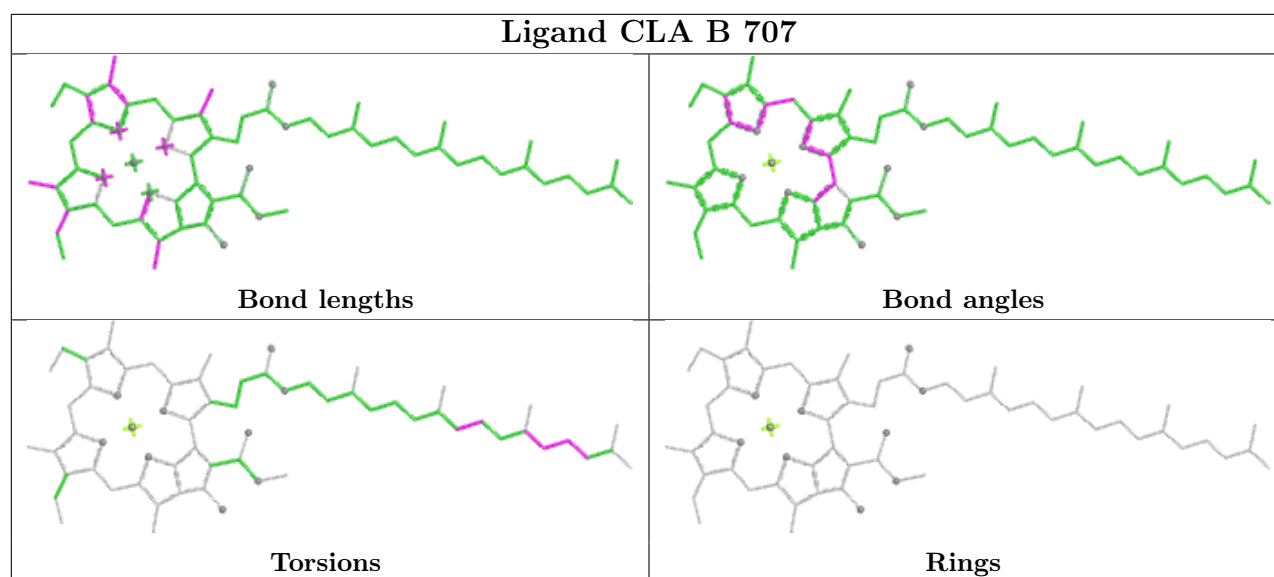
Ligand BCR a 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

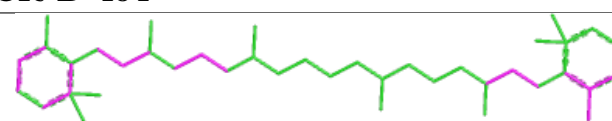
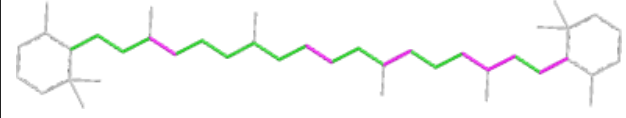
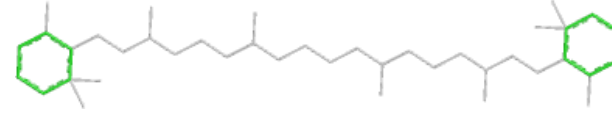
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Bond lengths	Bond angles
	
Torsions	Rings

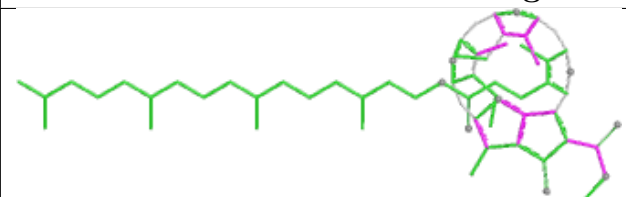
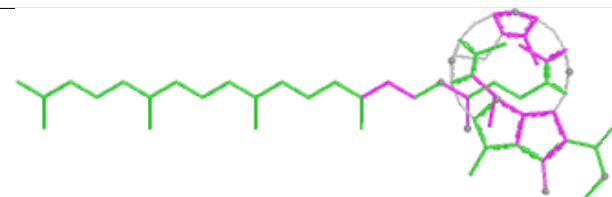
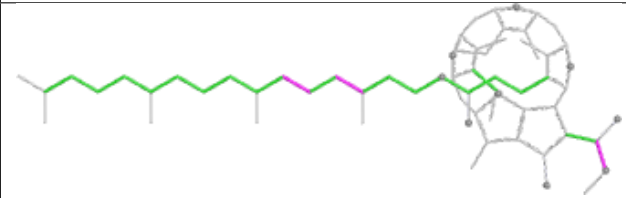
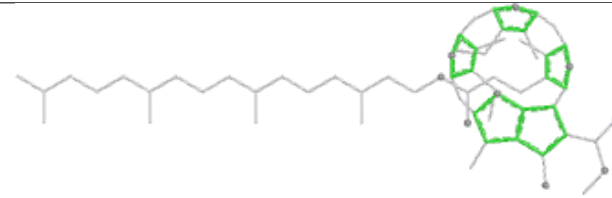
Ligand LMG c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

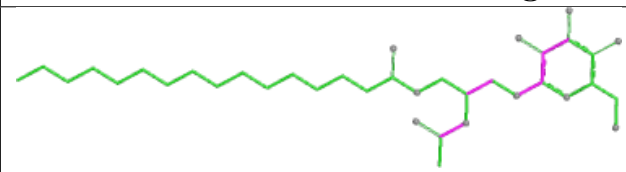
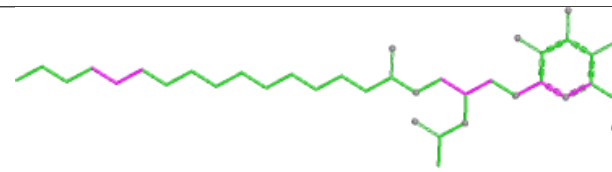
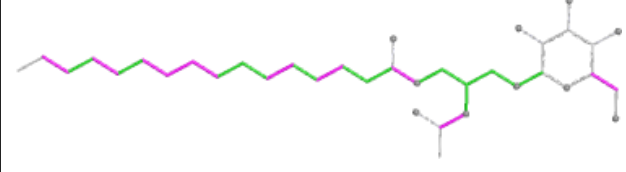
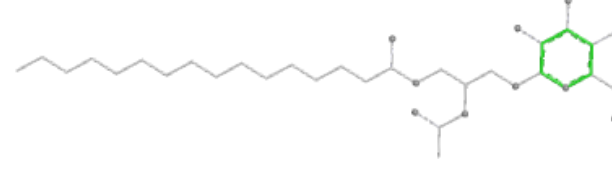
Ligand STE H 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

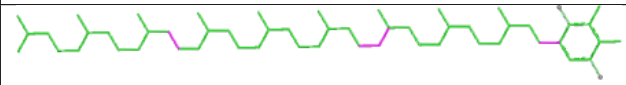
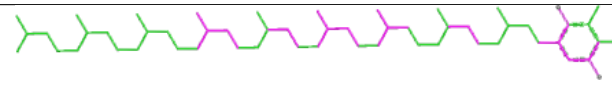
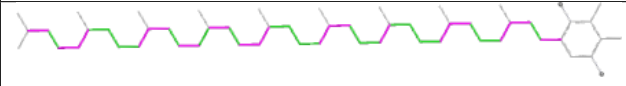
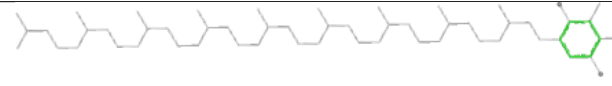
Ligand BCR d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

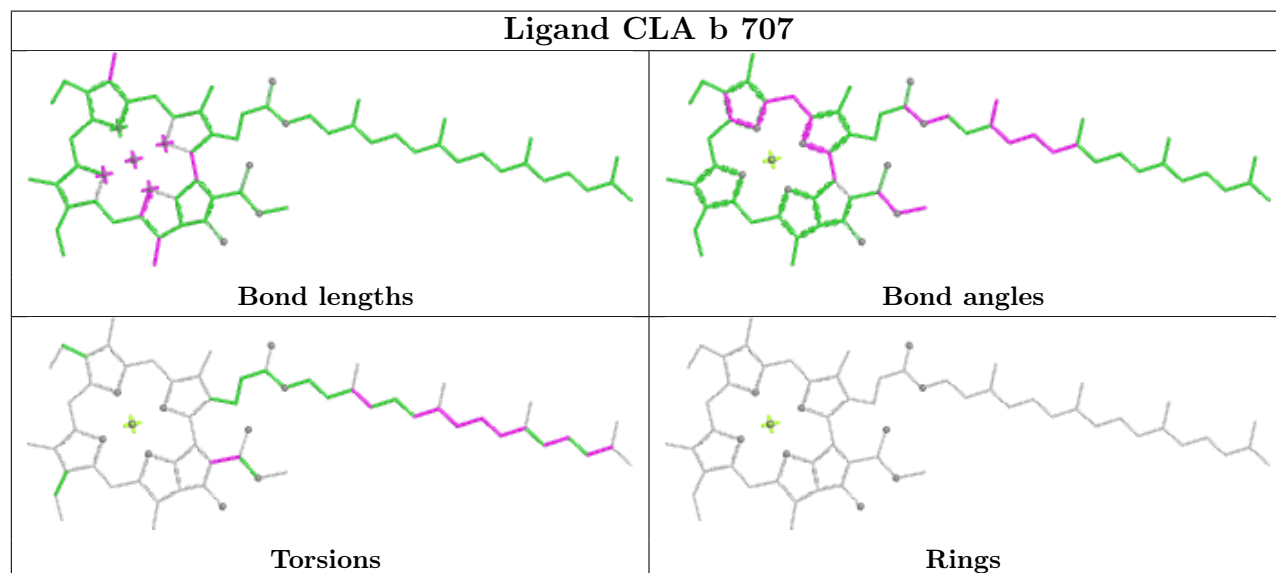
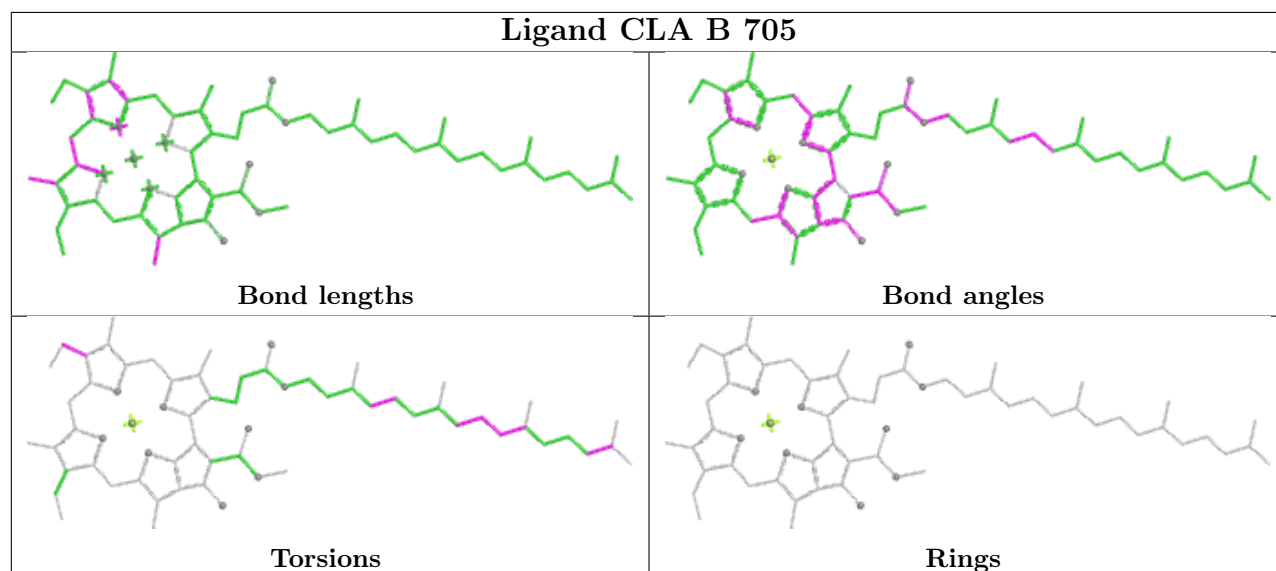
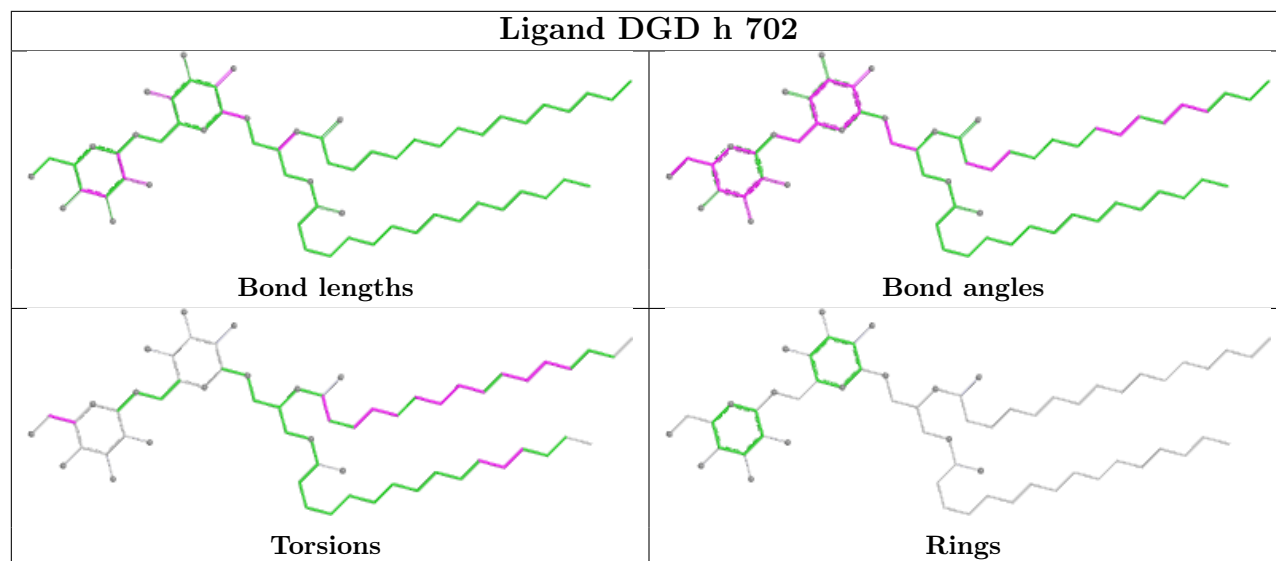


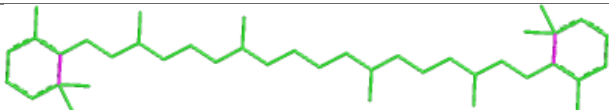
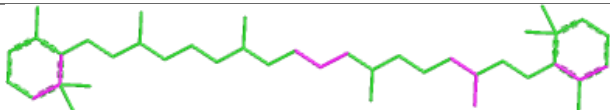
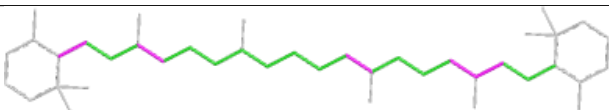
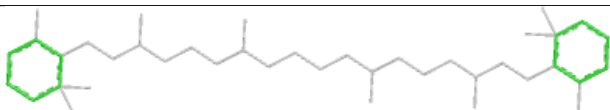
Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

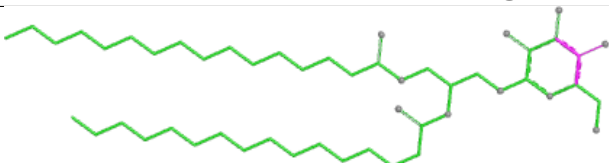
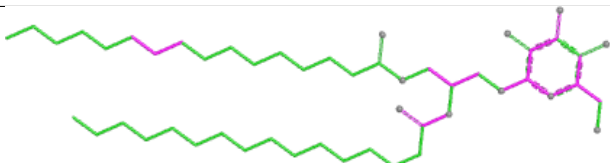
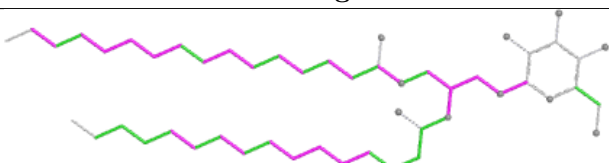
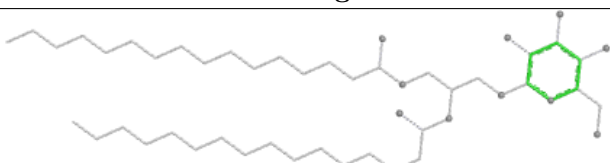
Ligand PHO a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

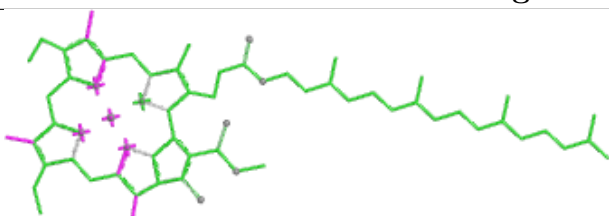
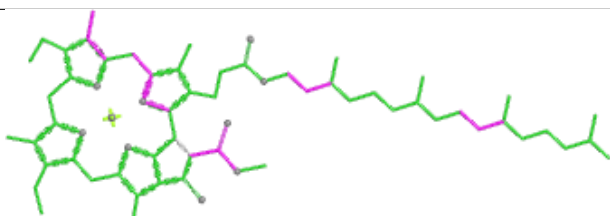
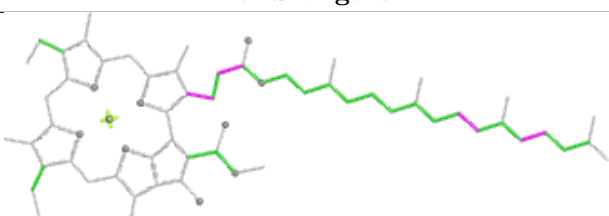
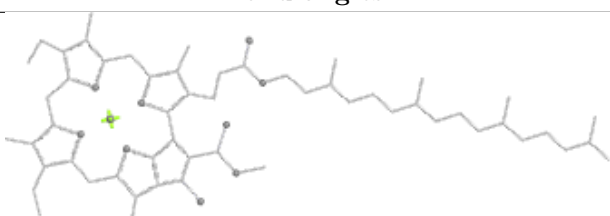
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Bond lengths	Bond angles
	
Torsions	Rings

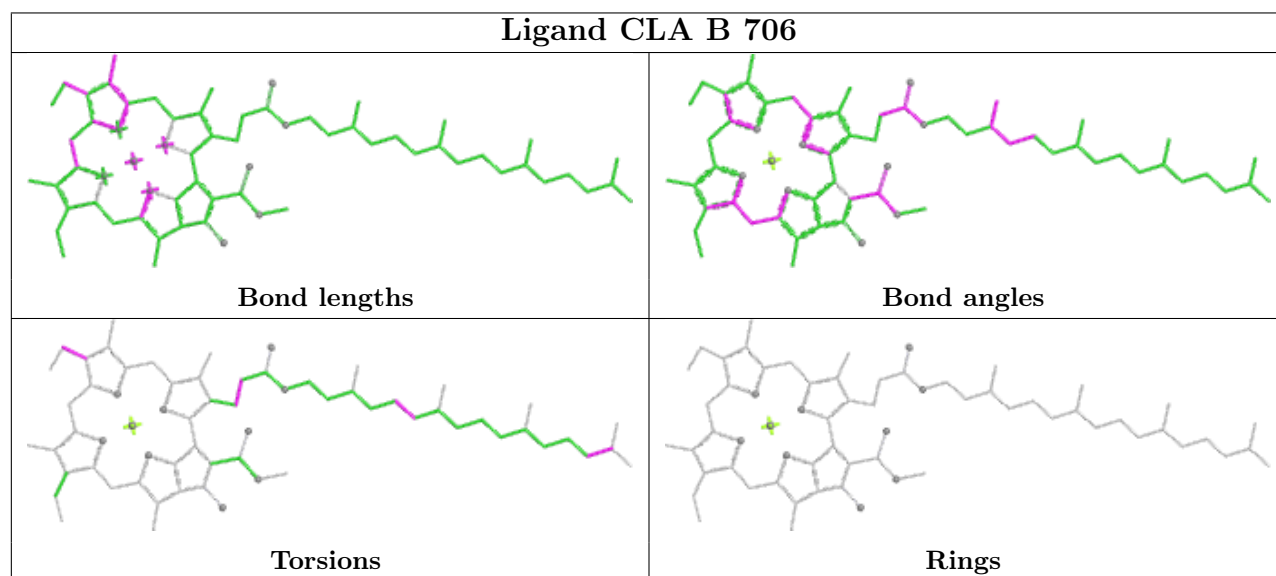
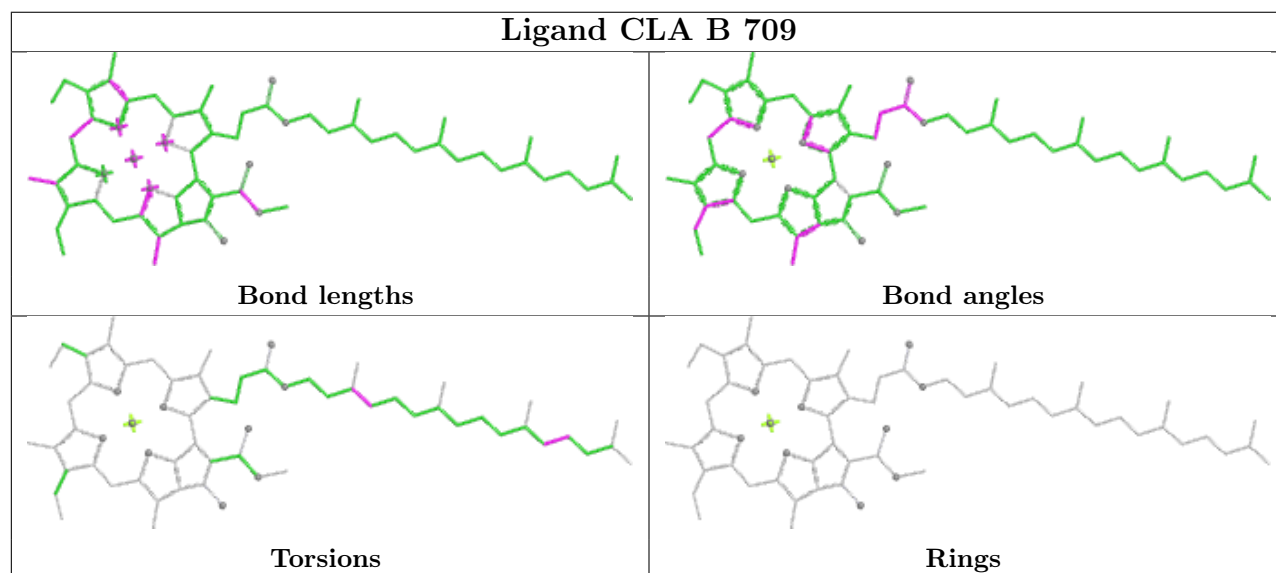
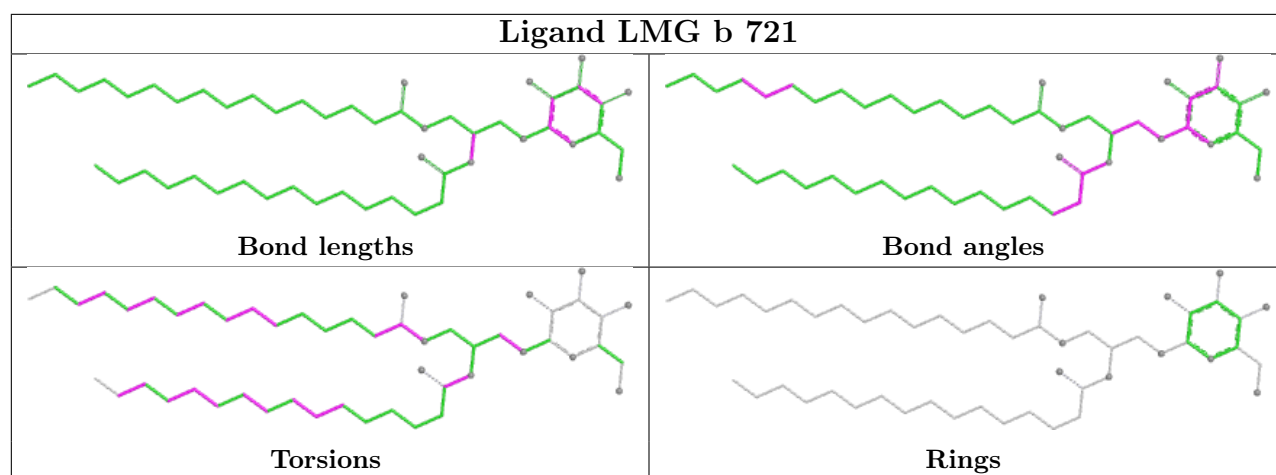
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Bond lengths	Bond angles
	
Torsions	Rings

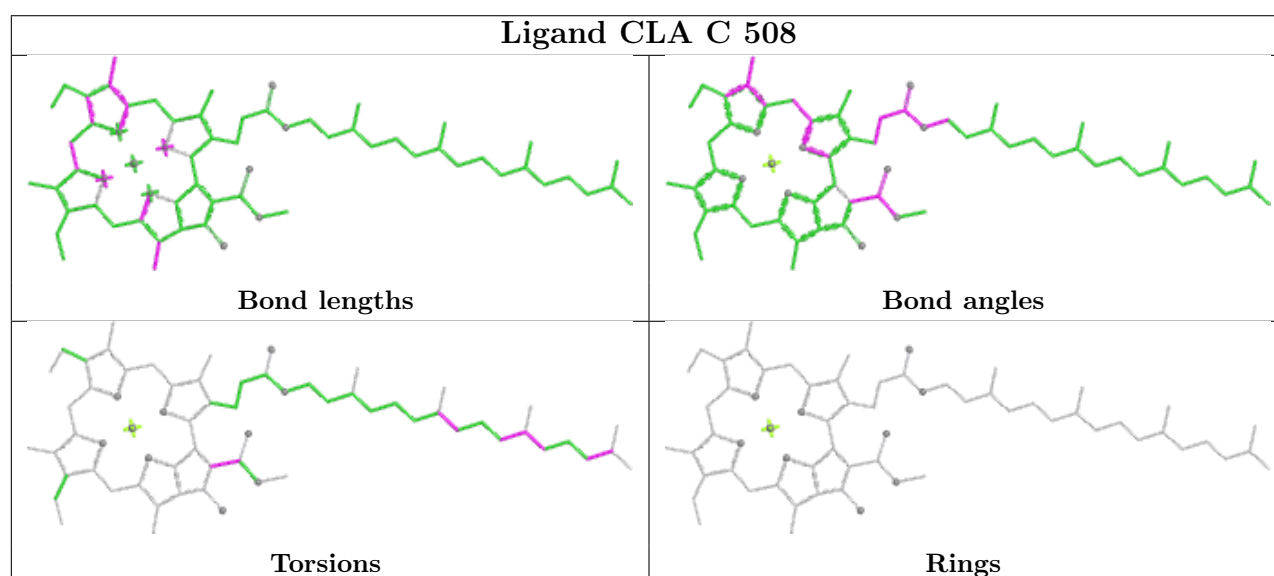
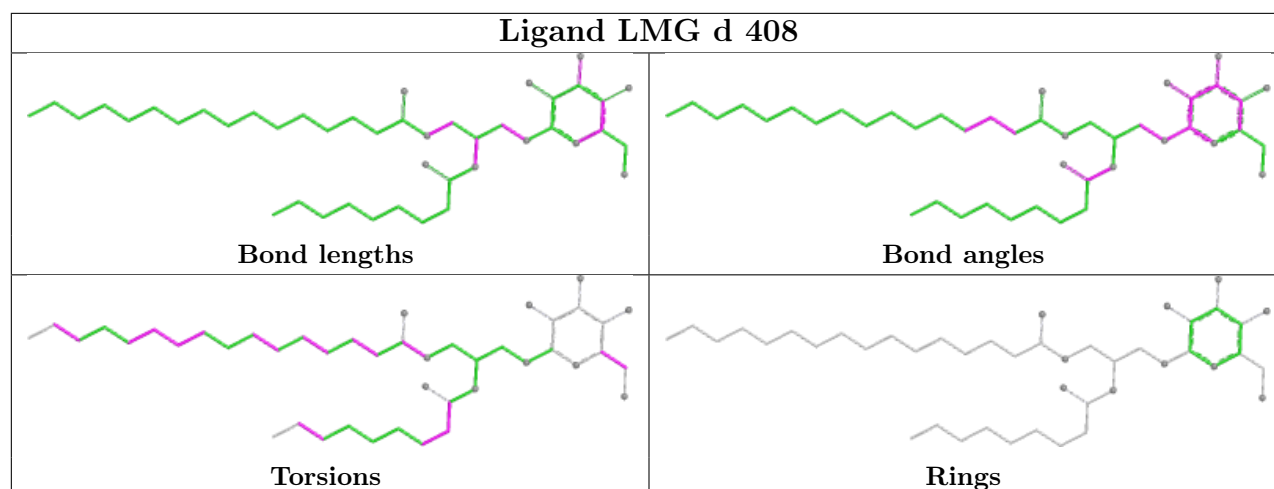
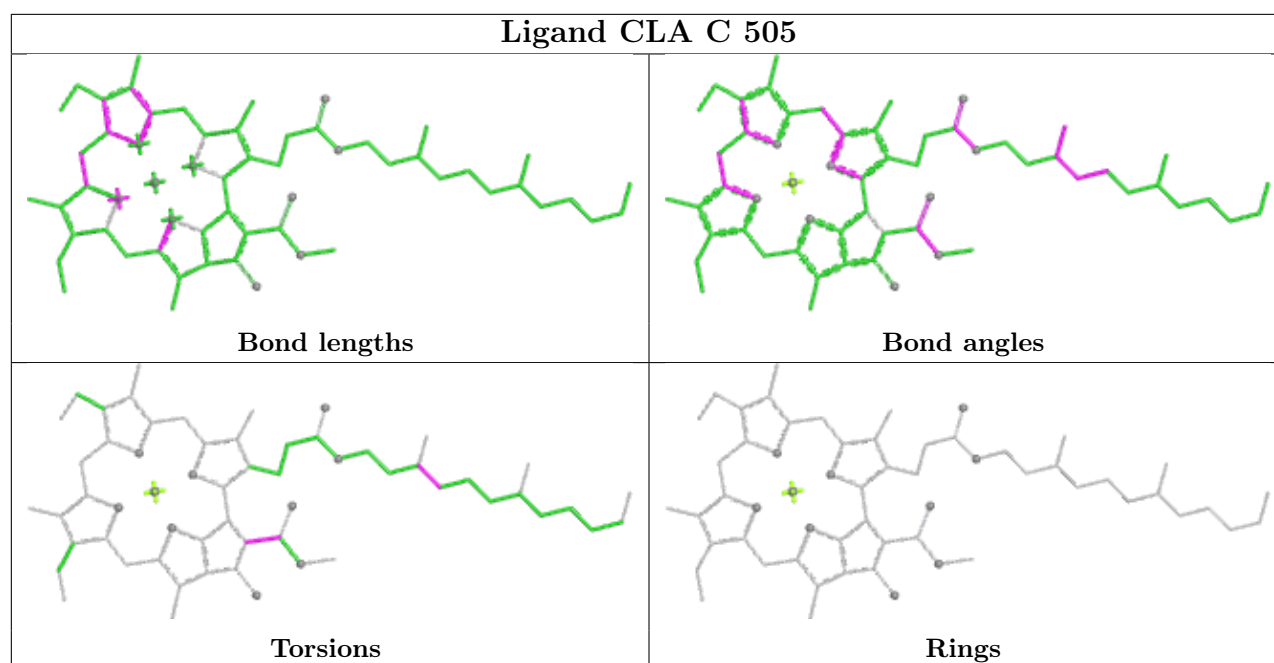


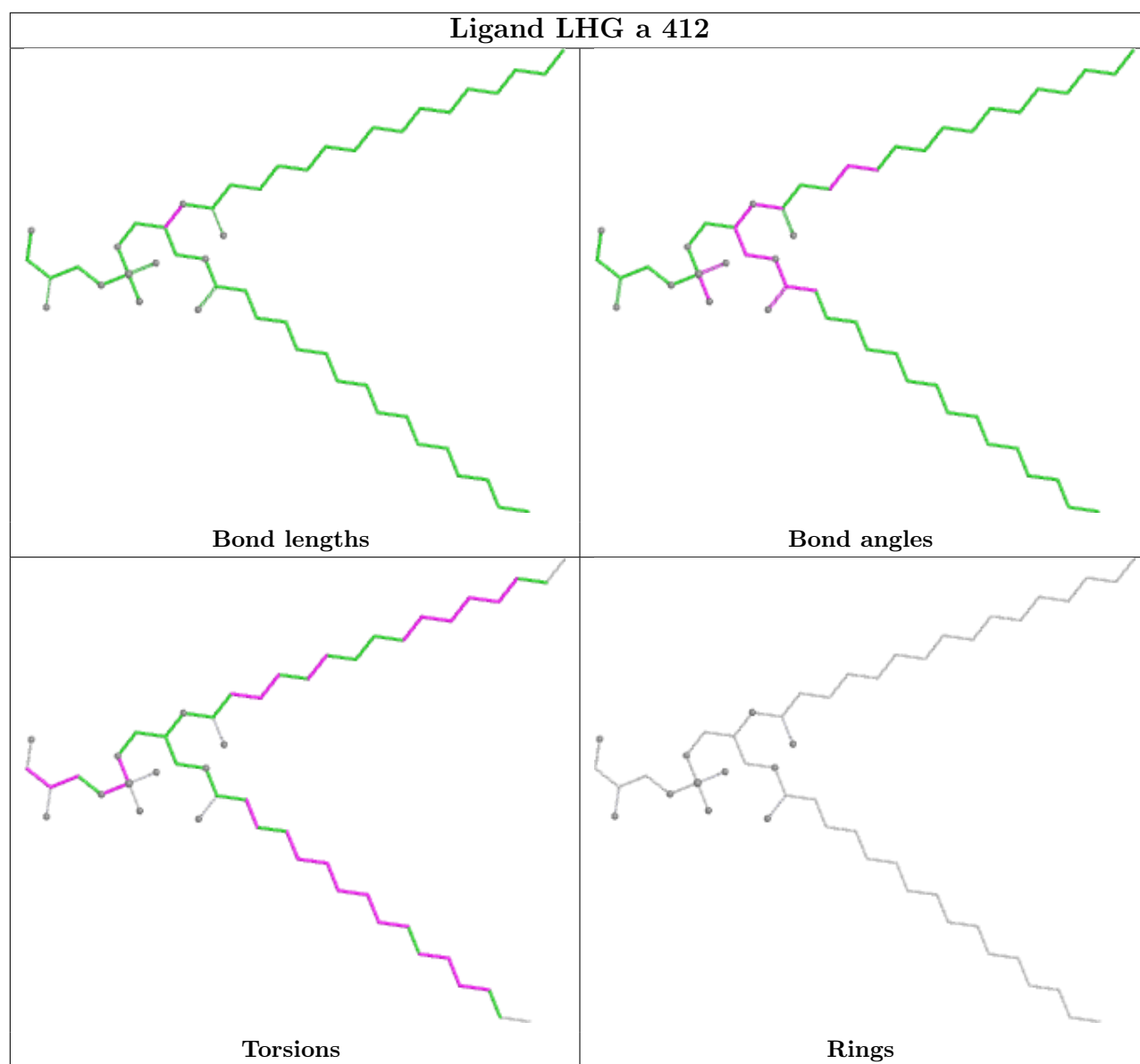
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

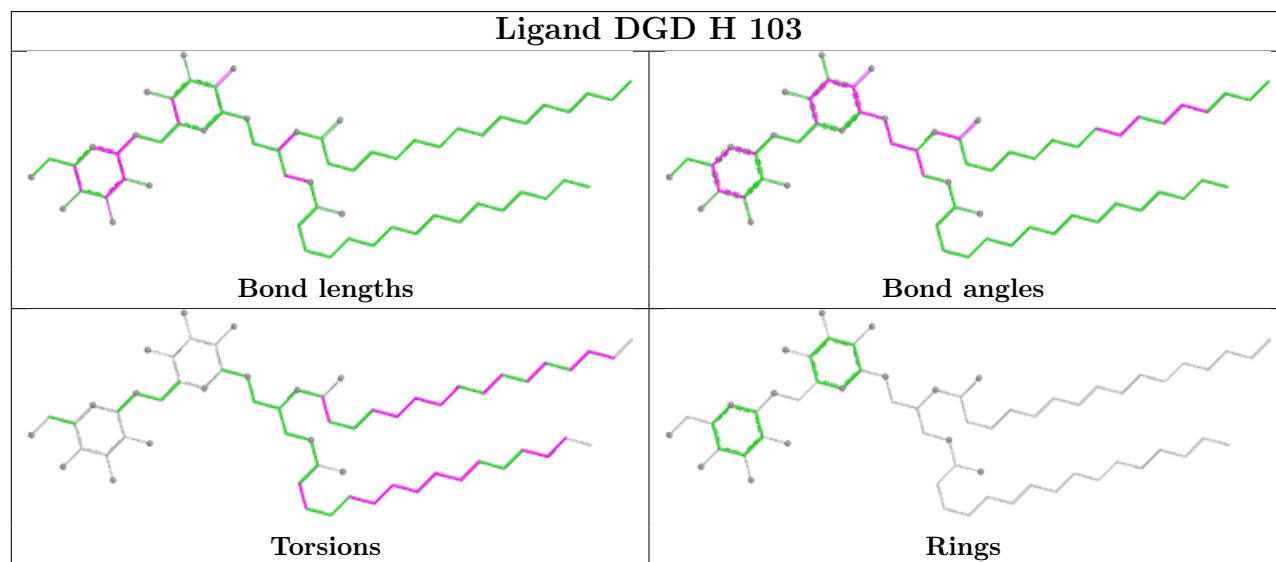
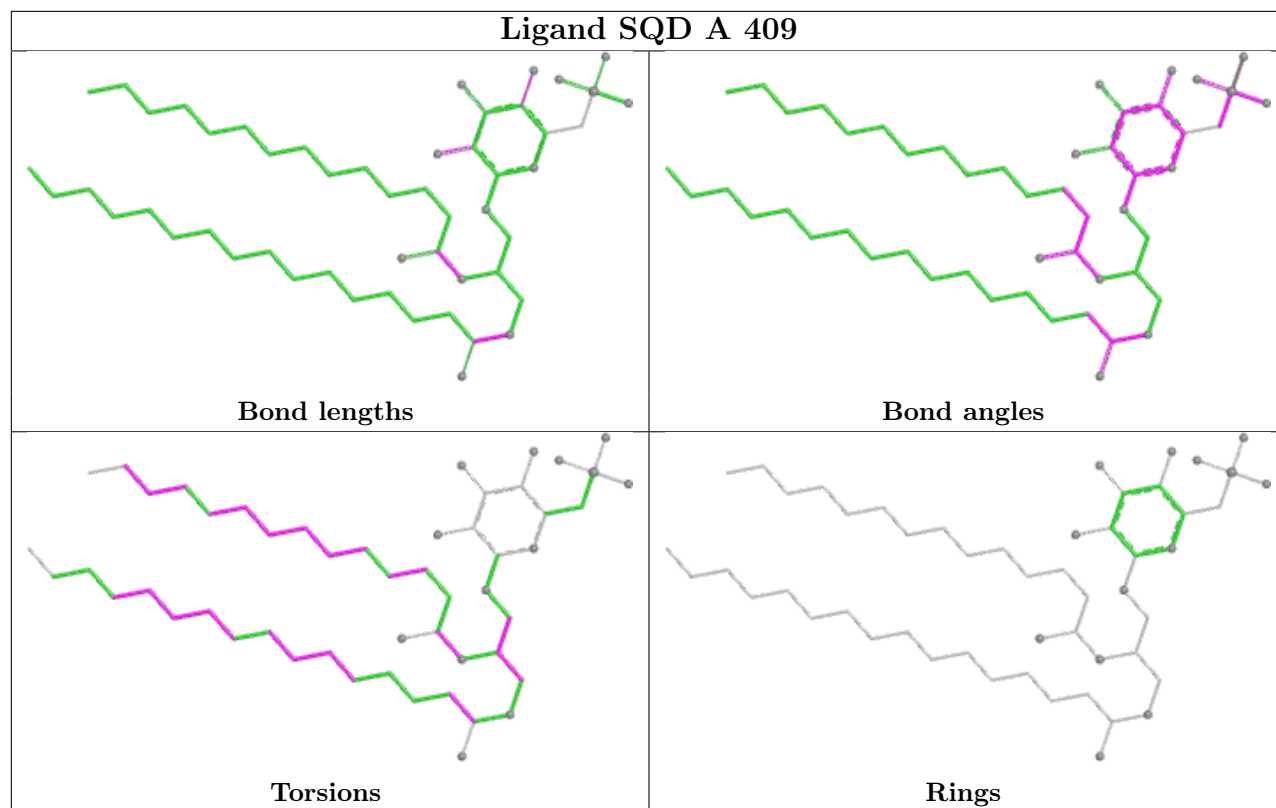
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Bond lengths	Bond angles
	
Torsions	Rings

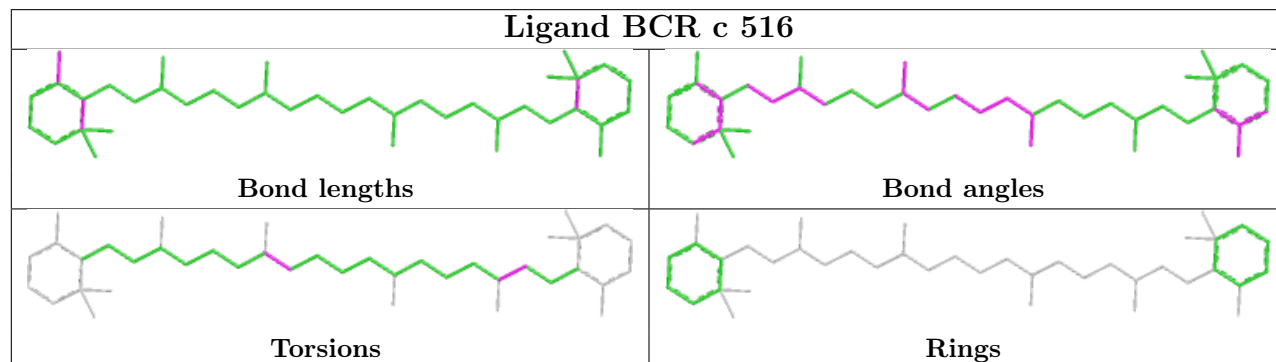
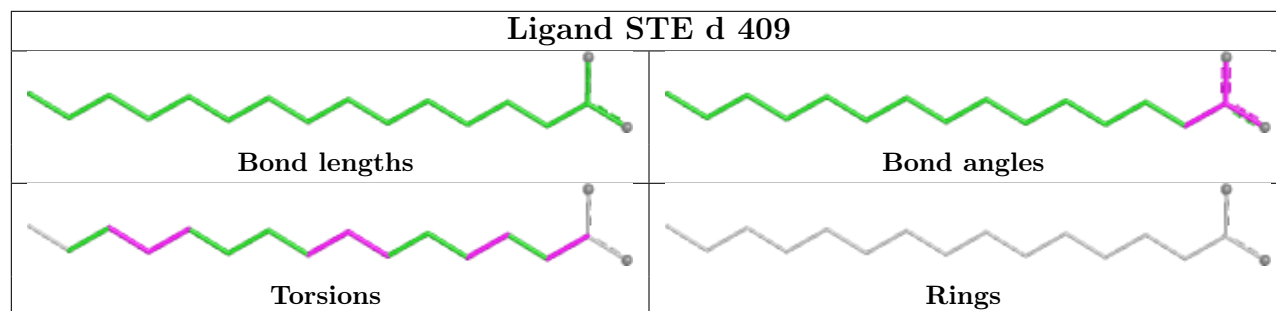
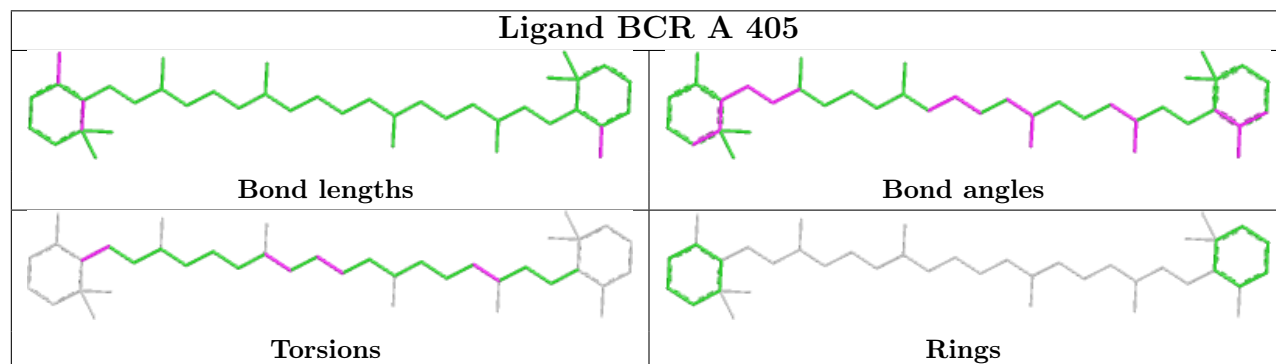
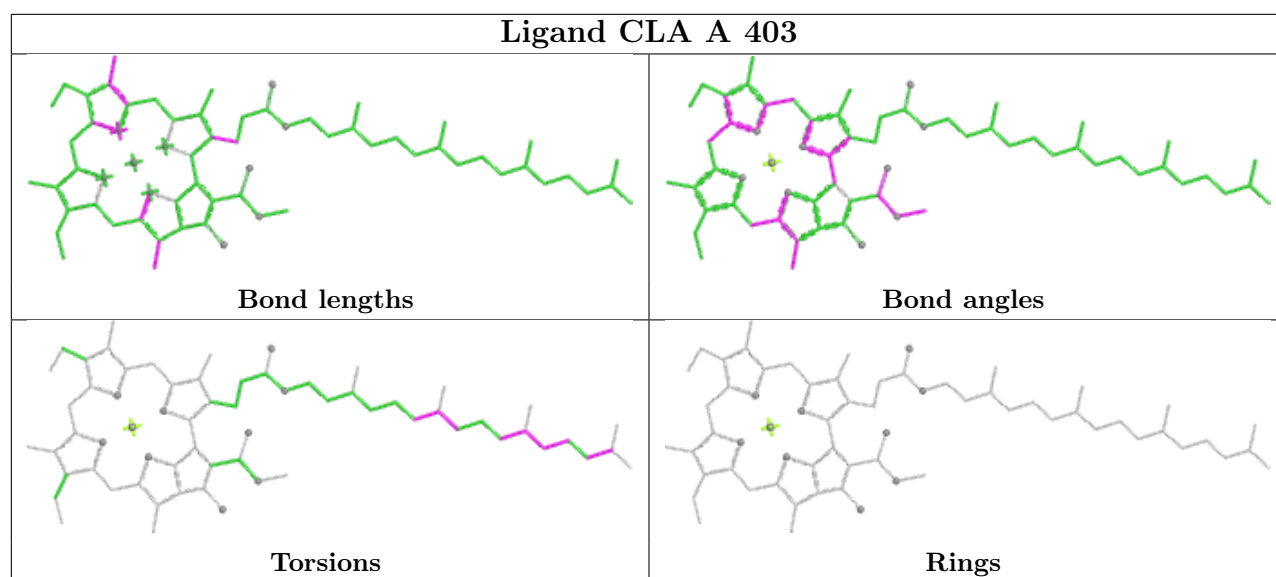
Ligand CLA b 712	
	
Bond lengths	Bond angles
	
Torsions	Rings

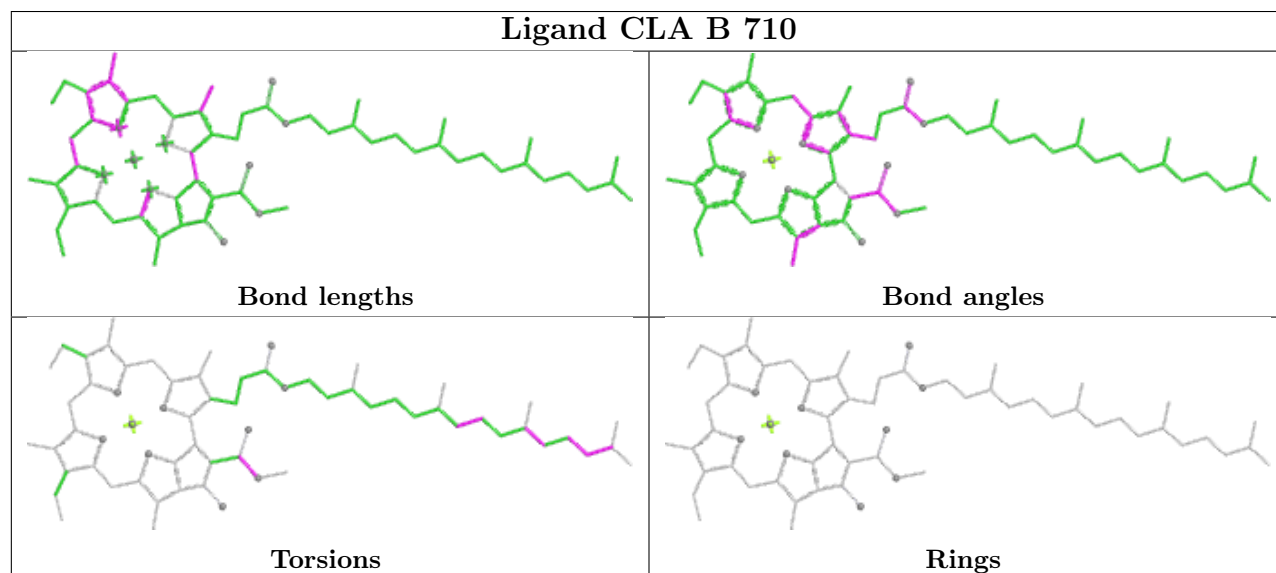
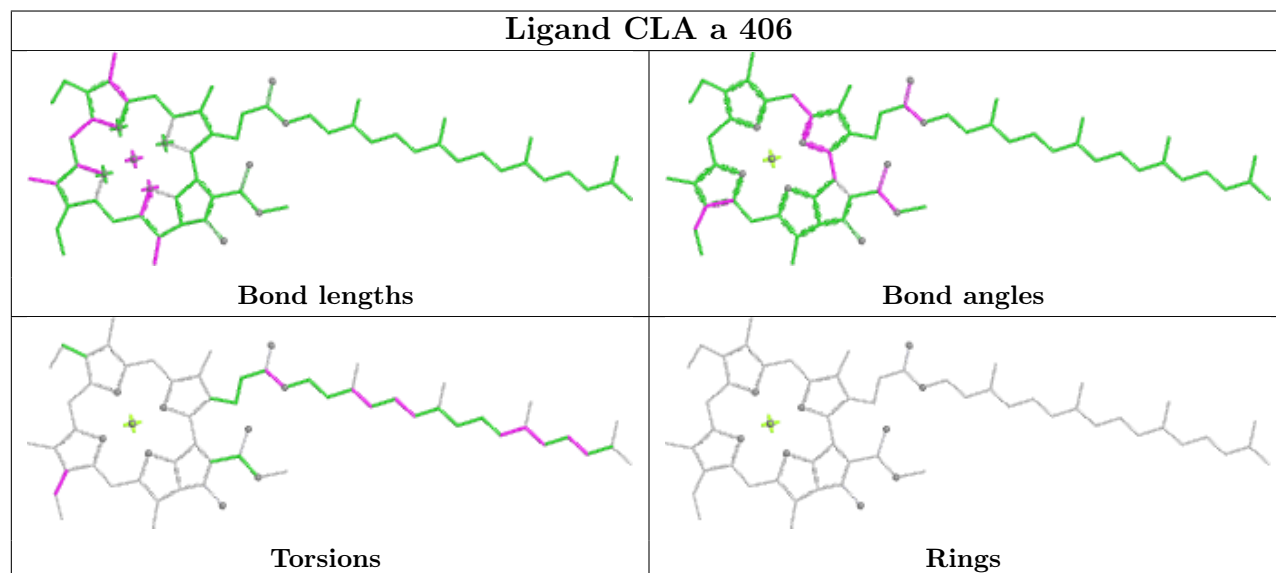
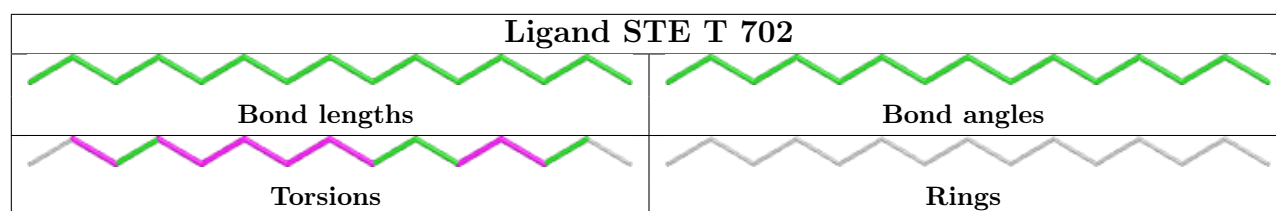


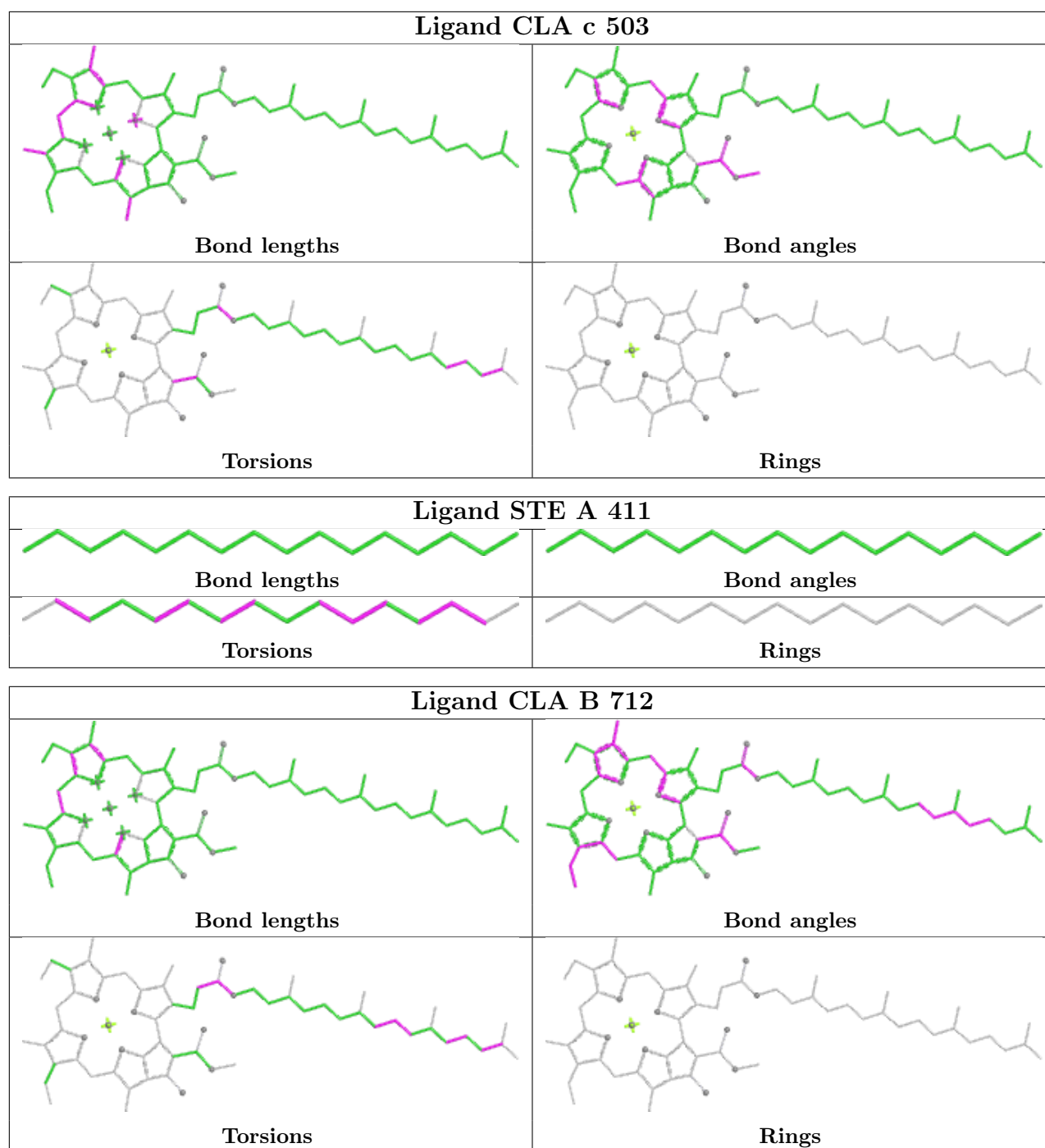


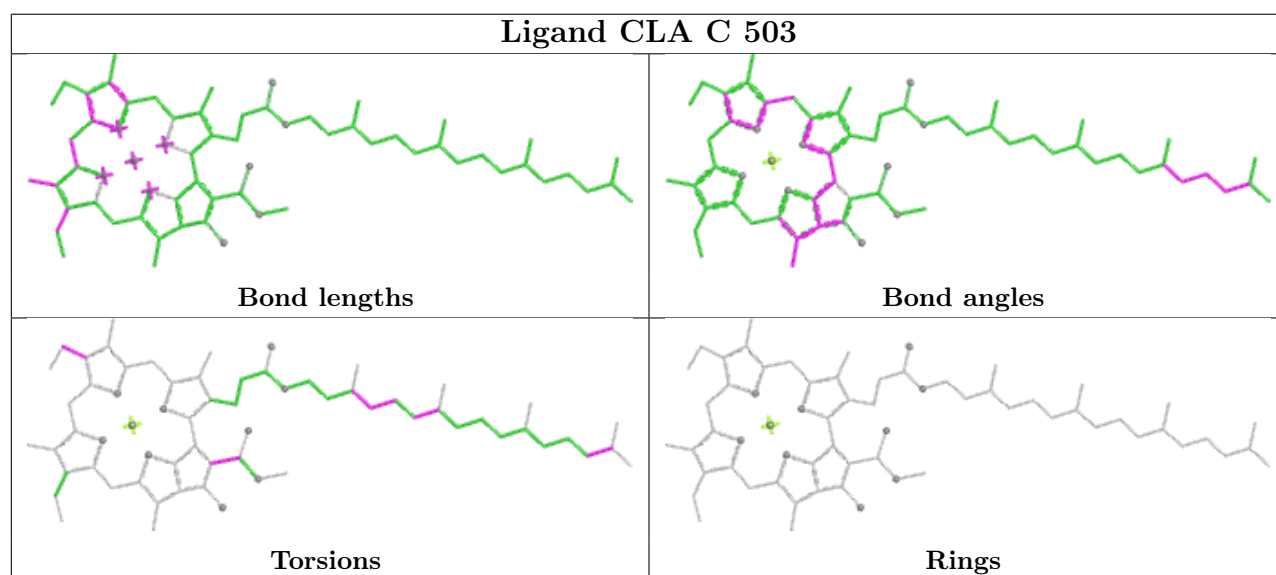
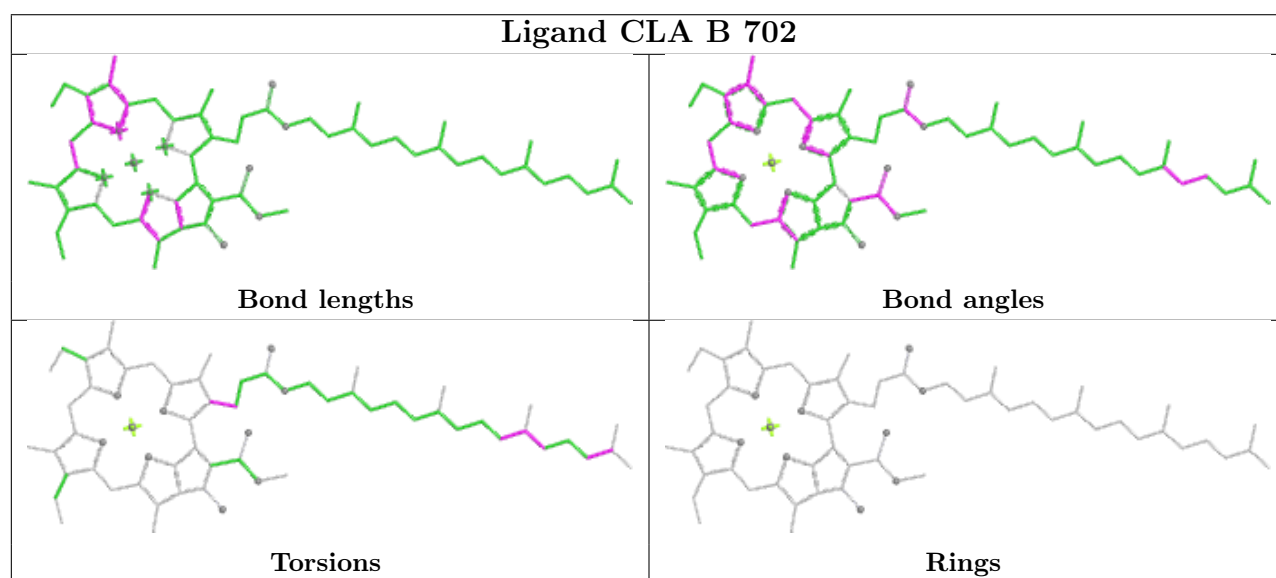
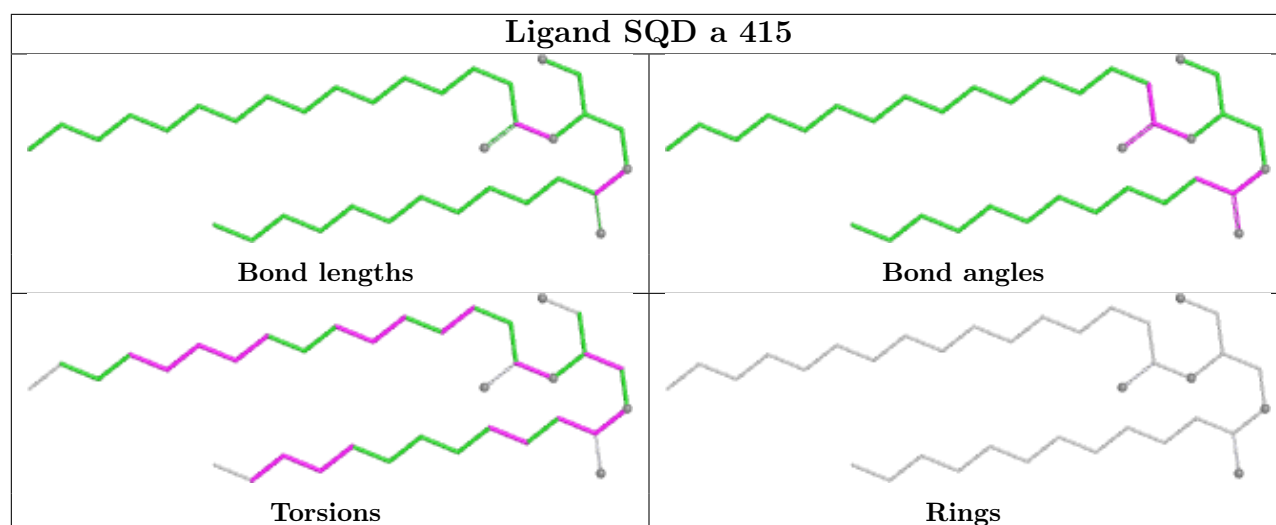


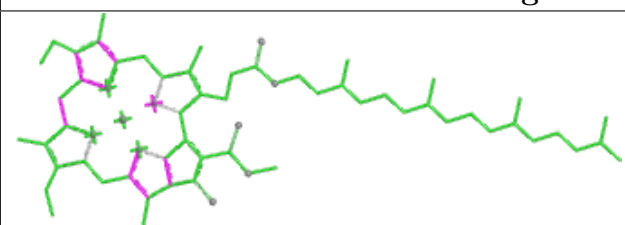
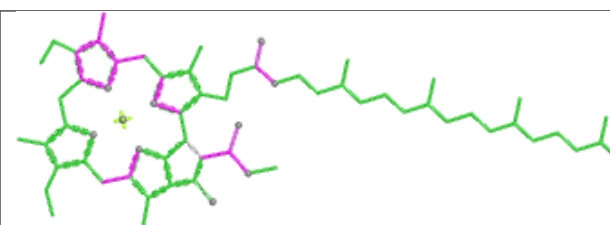
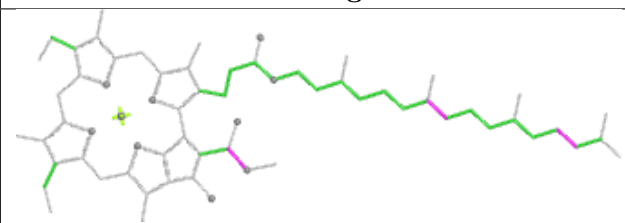
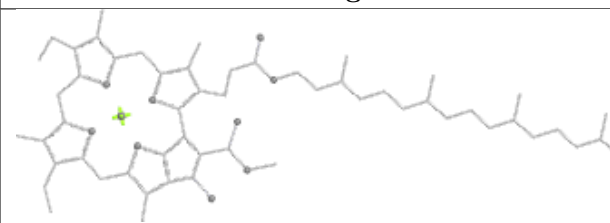


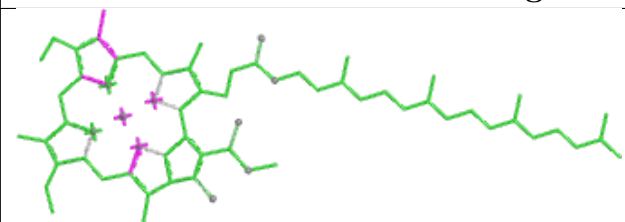
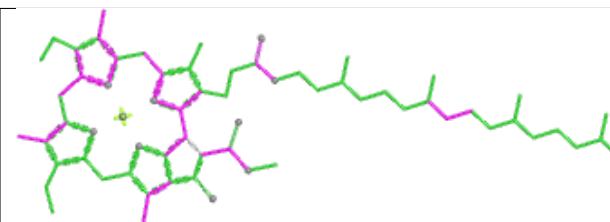
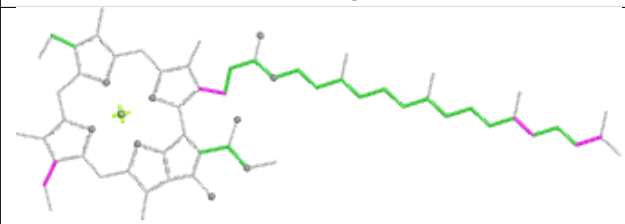
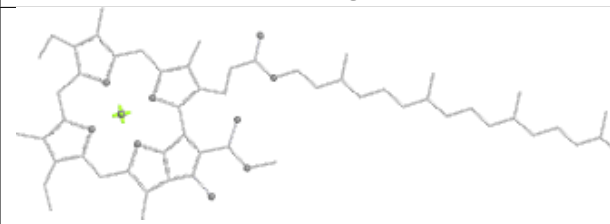


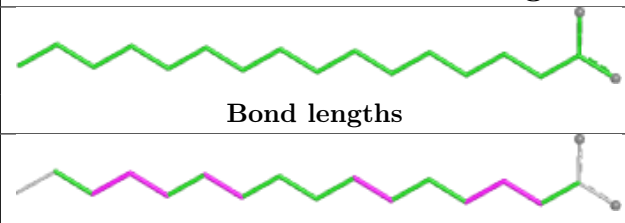
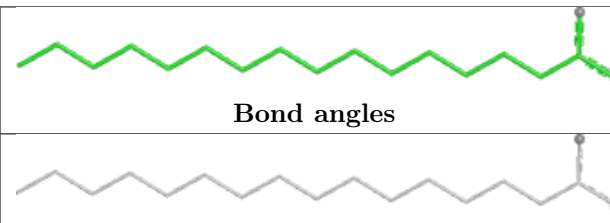
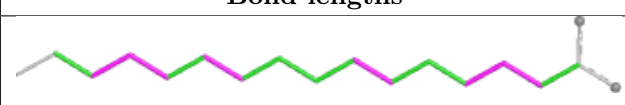
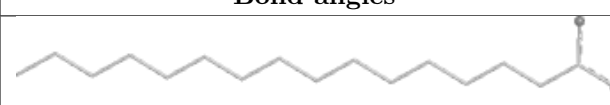


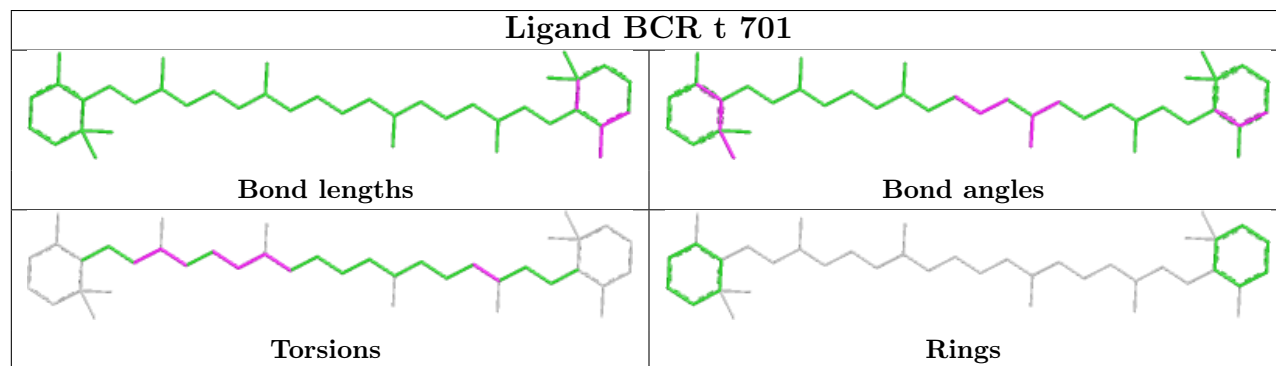
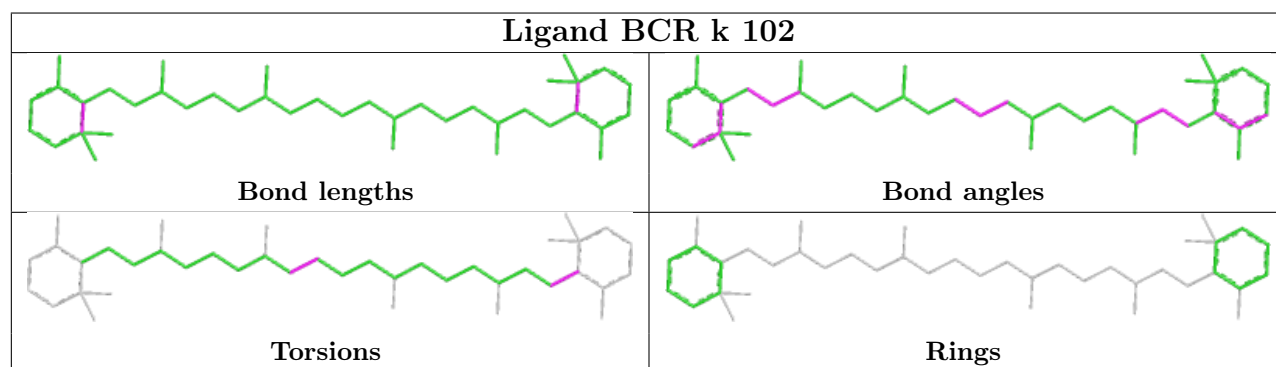
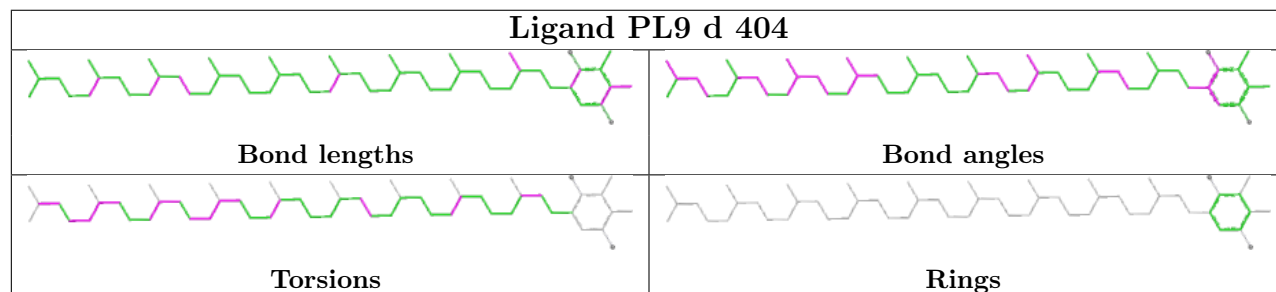
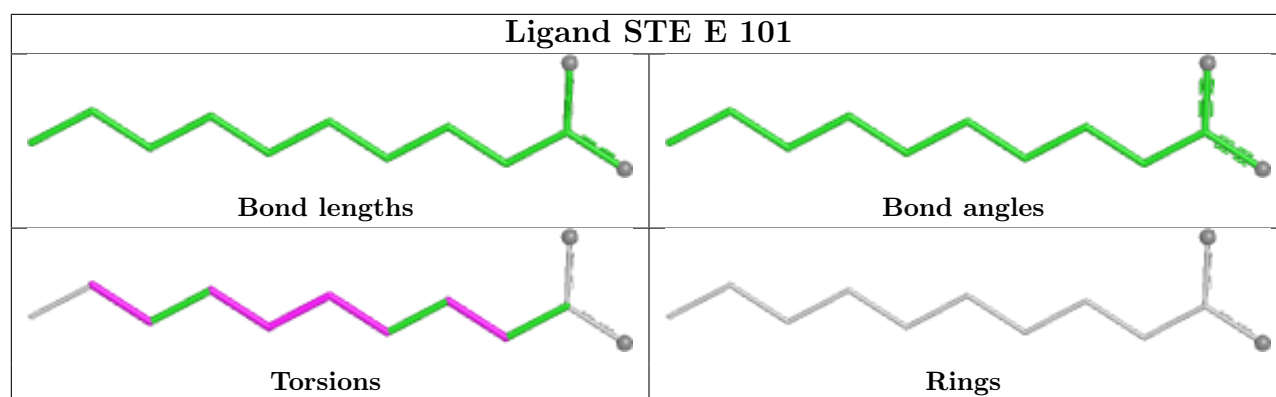




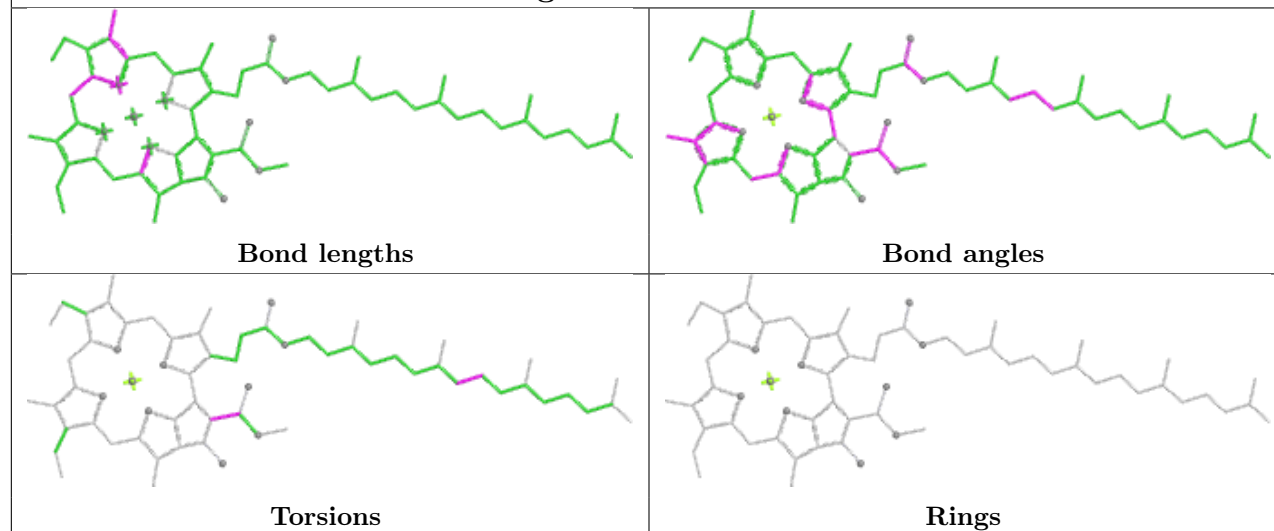
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

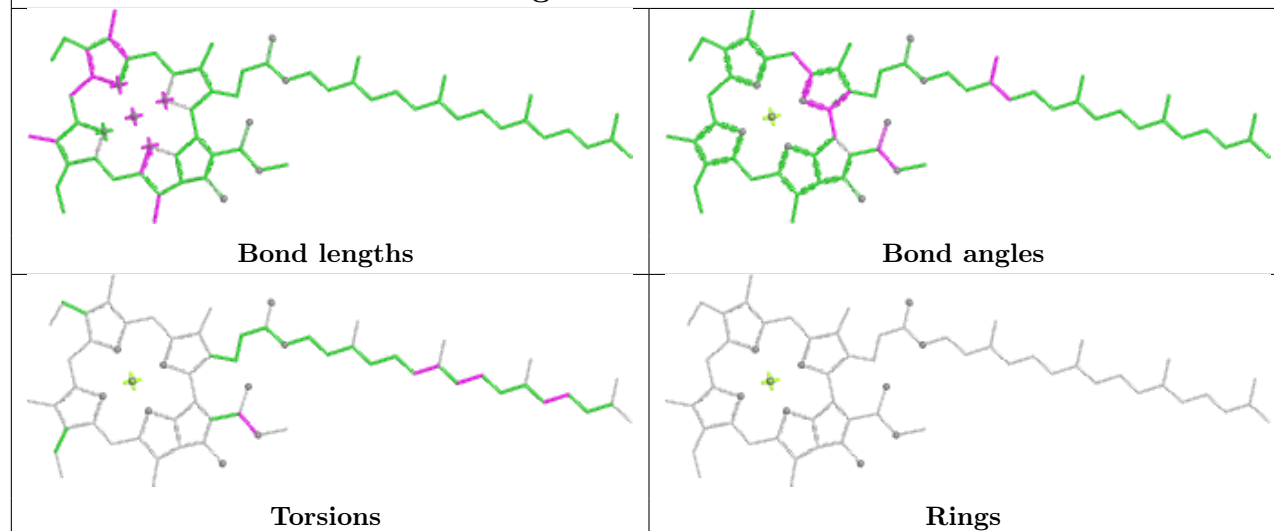
Ligand STE B 725	
	
Bond lengths	Bond angles
	
Torsions	Rings



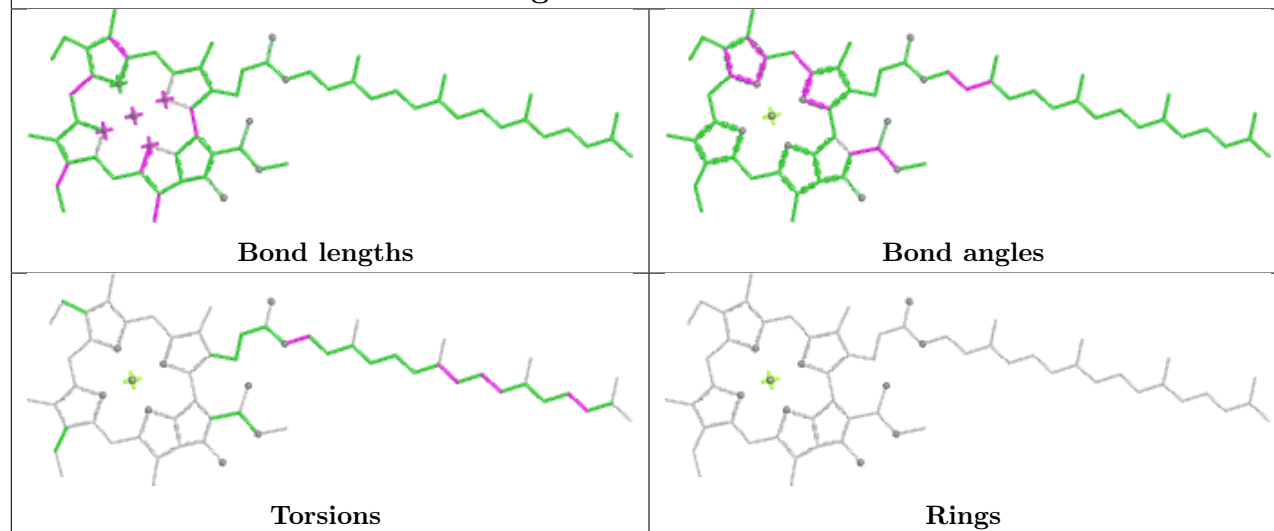
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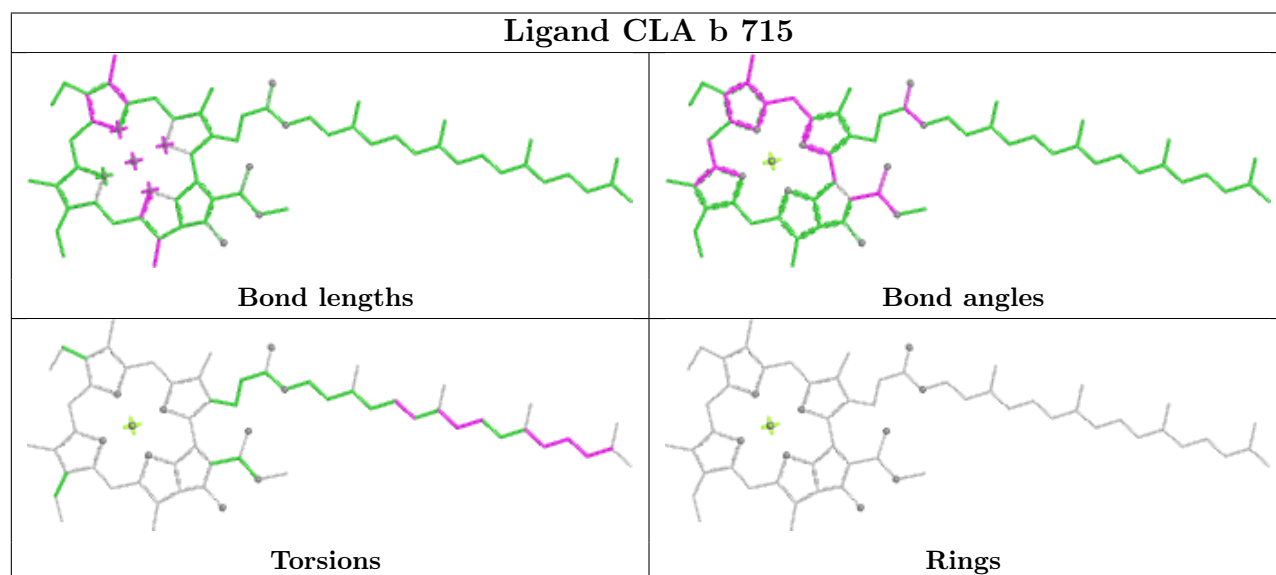
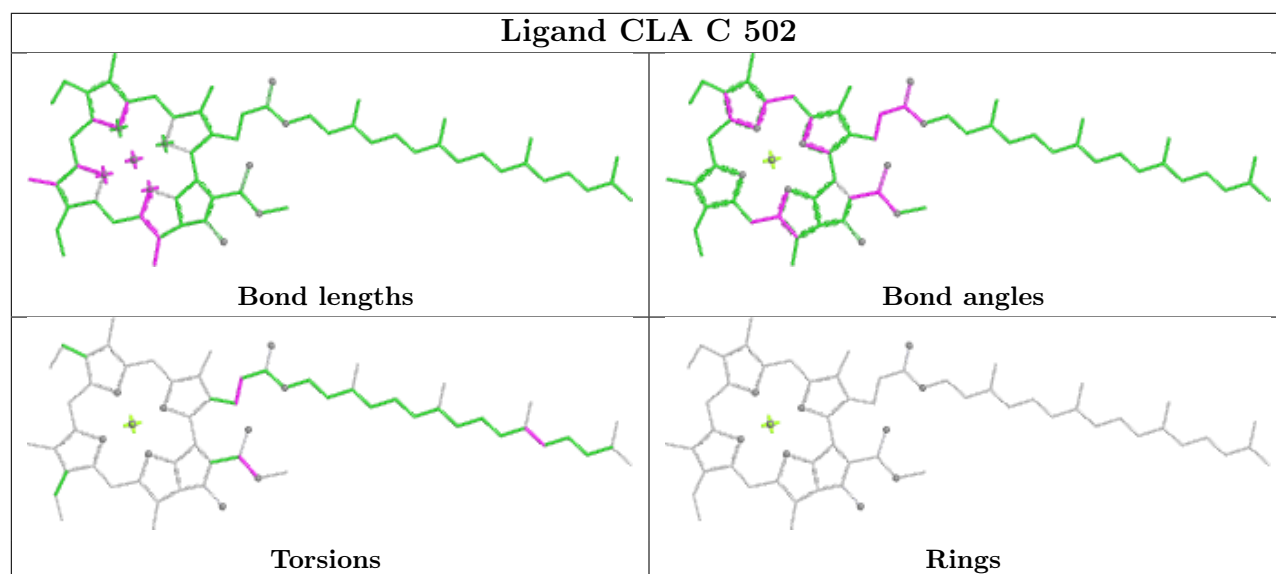
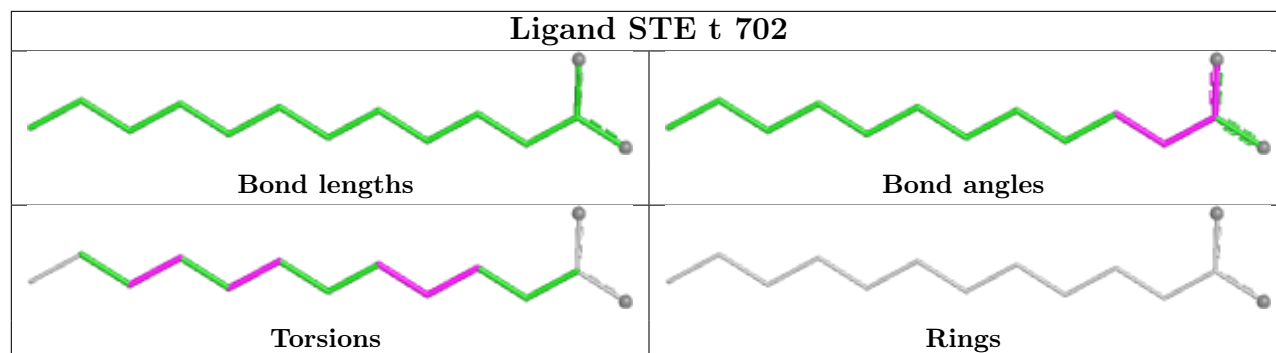


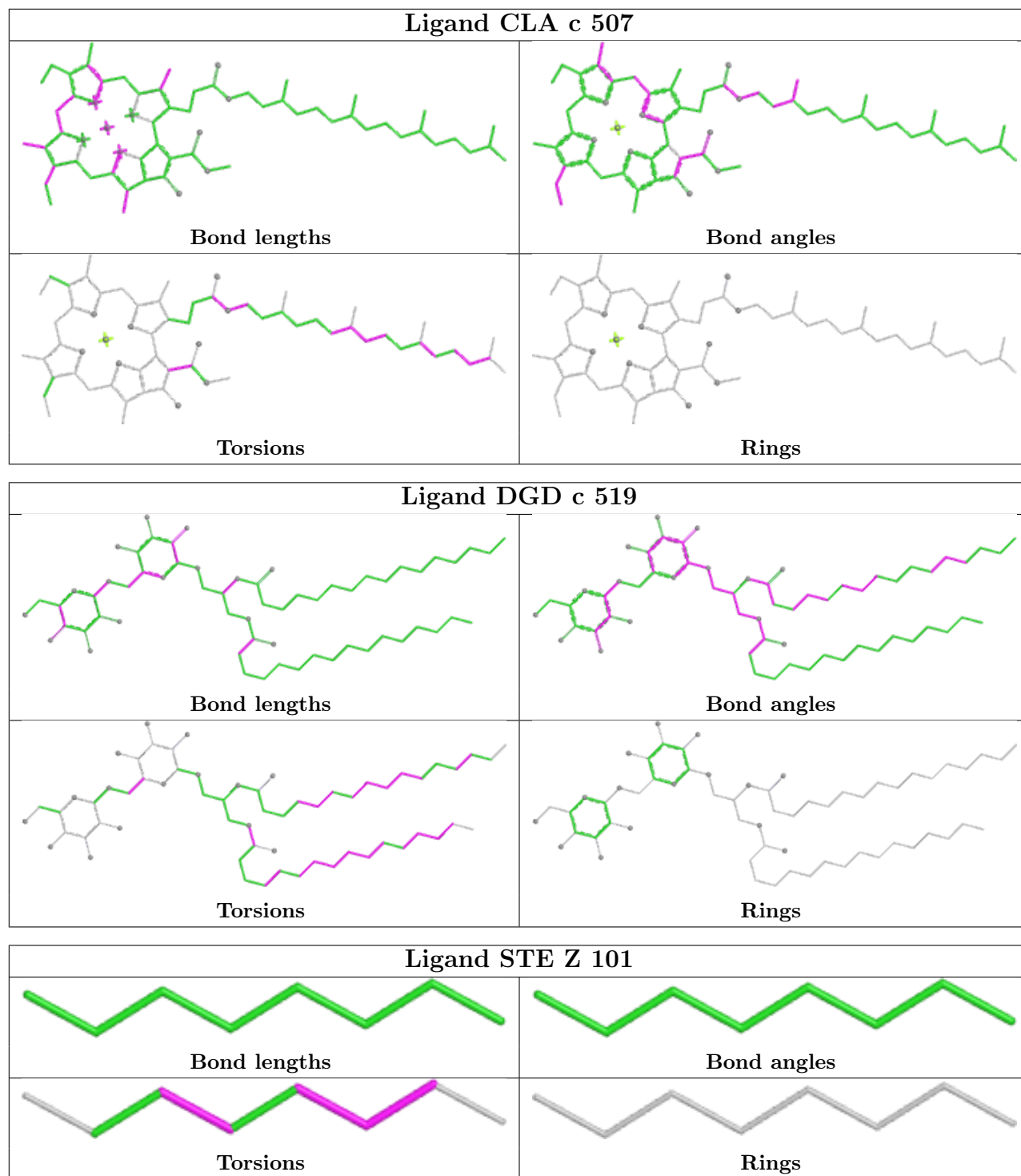
Ligand CLA C 512

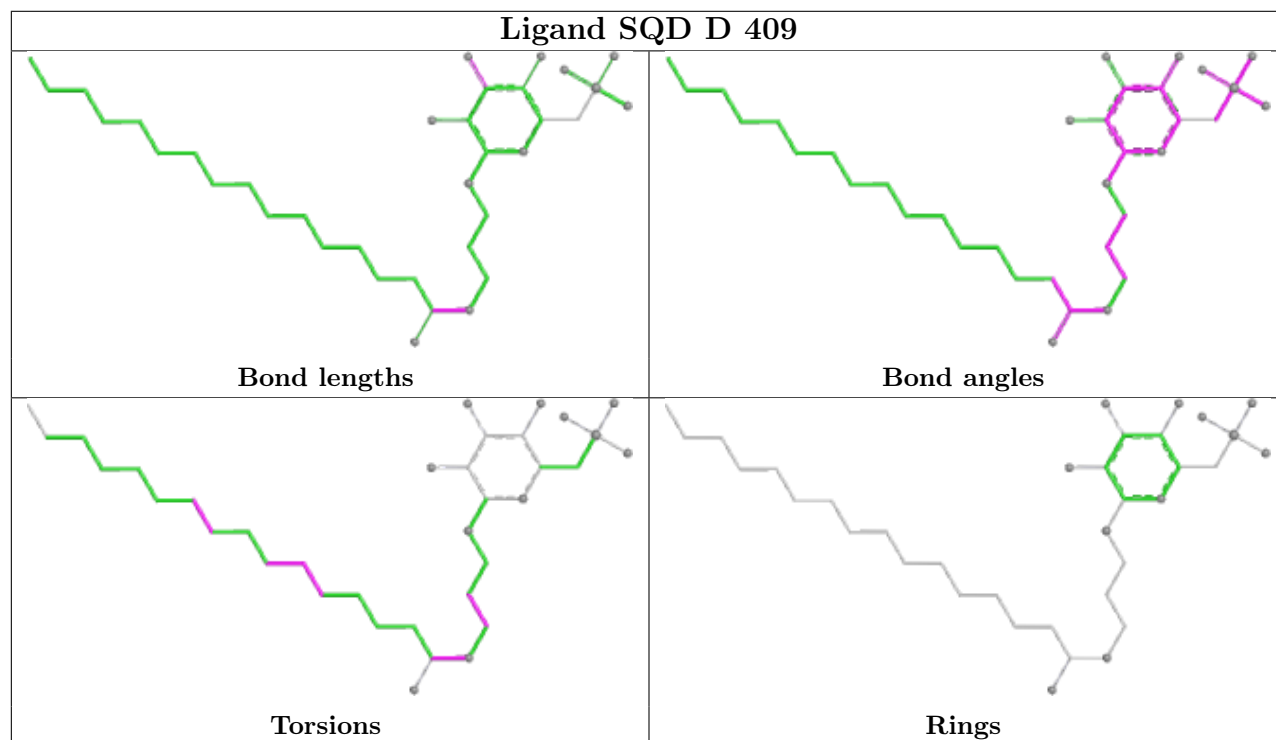
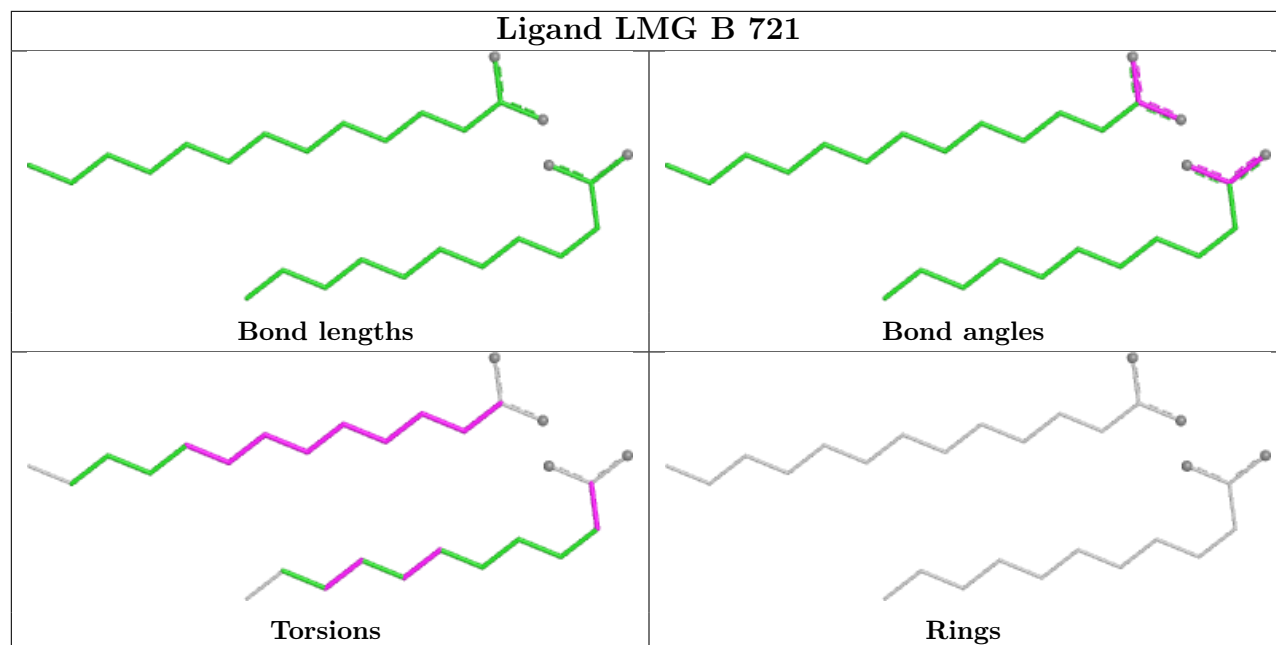


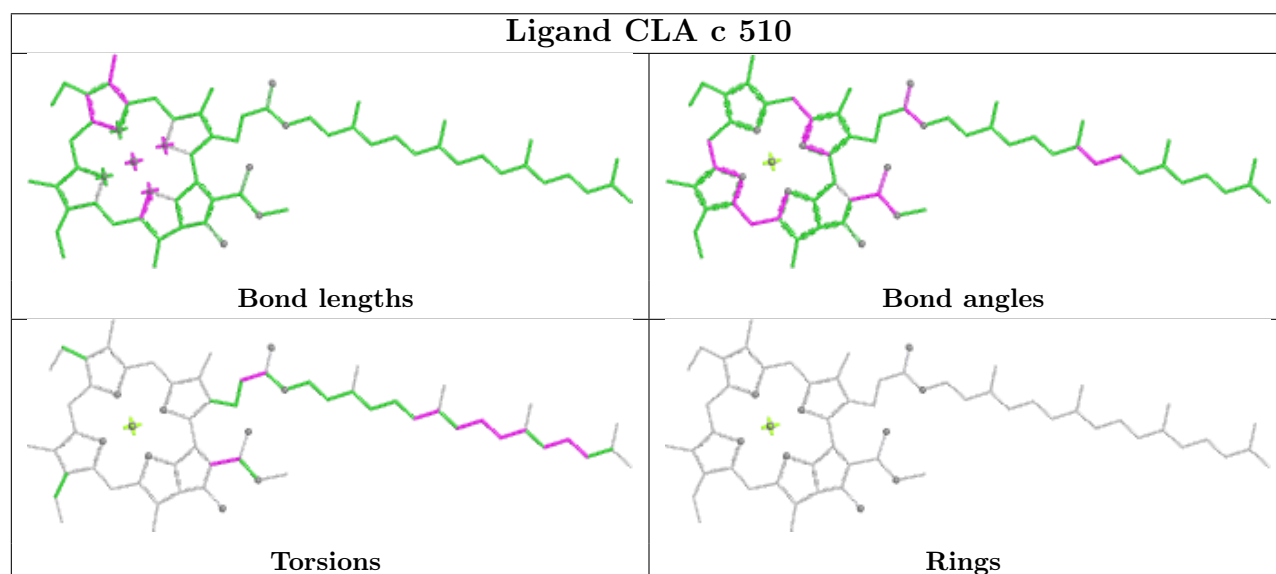
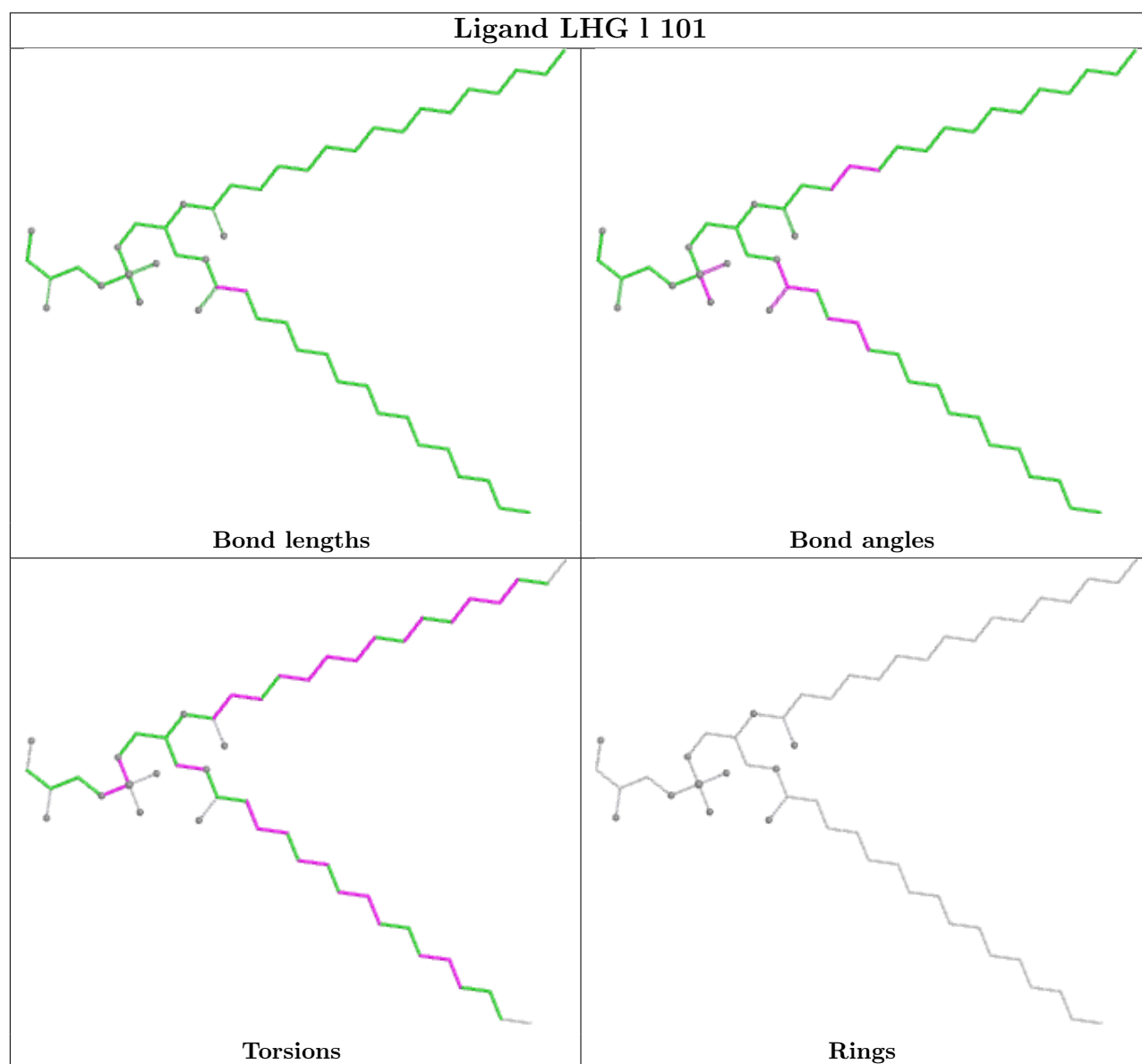
Ligand CLA D 401

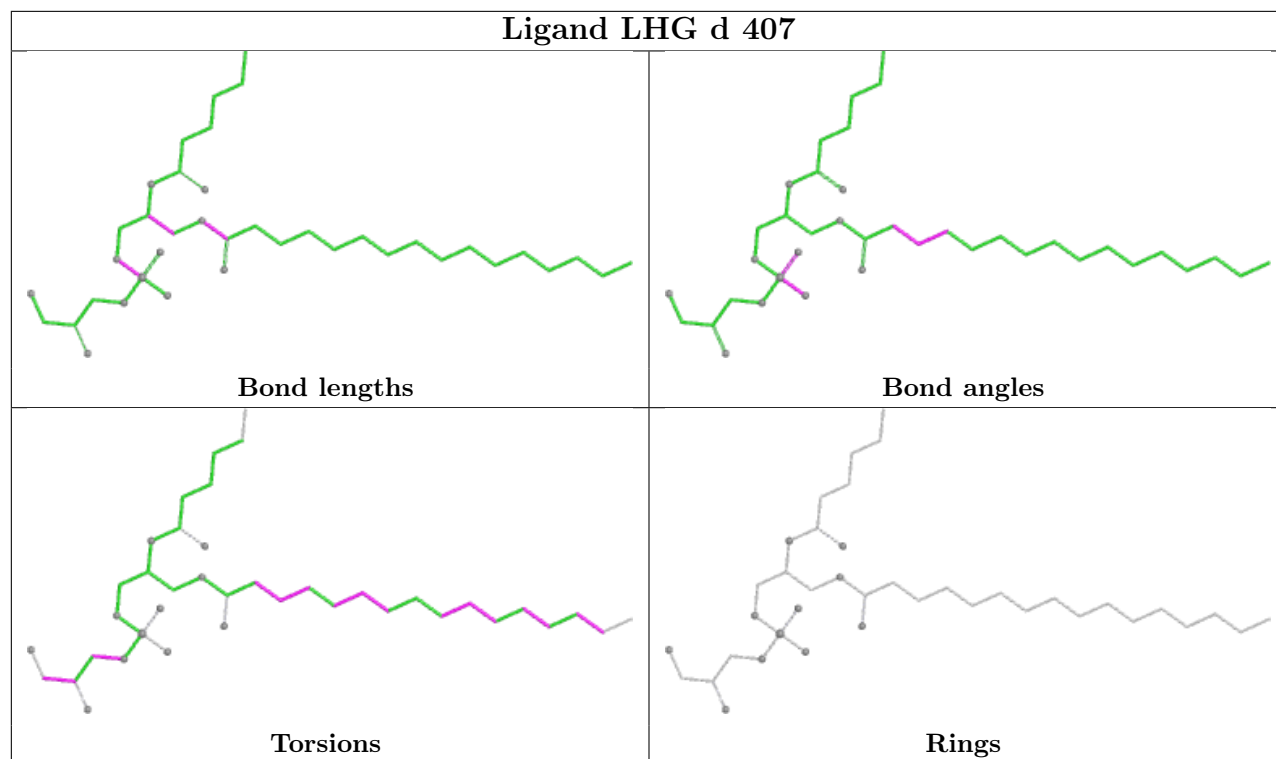


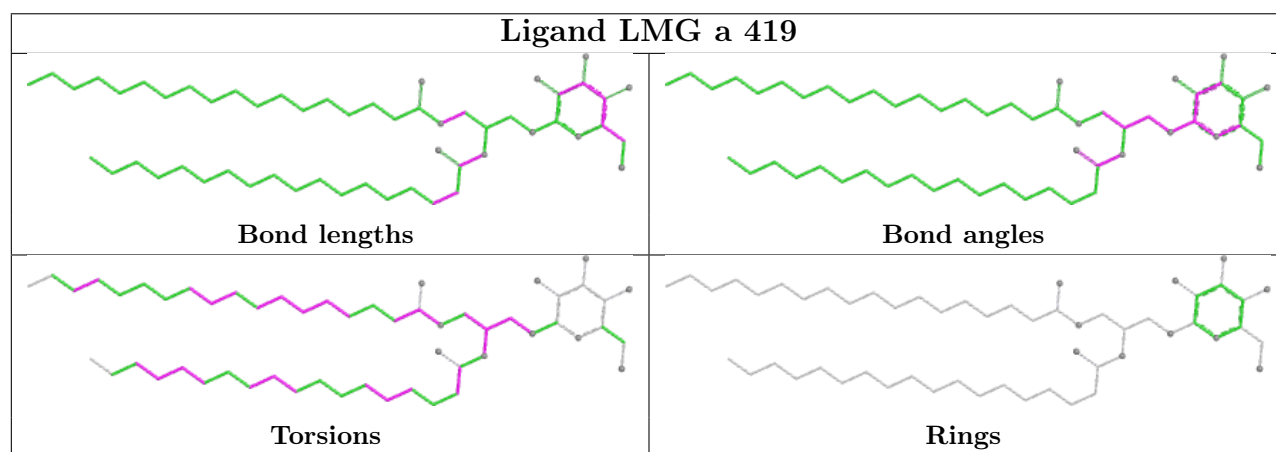
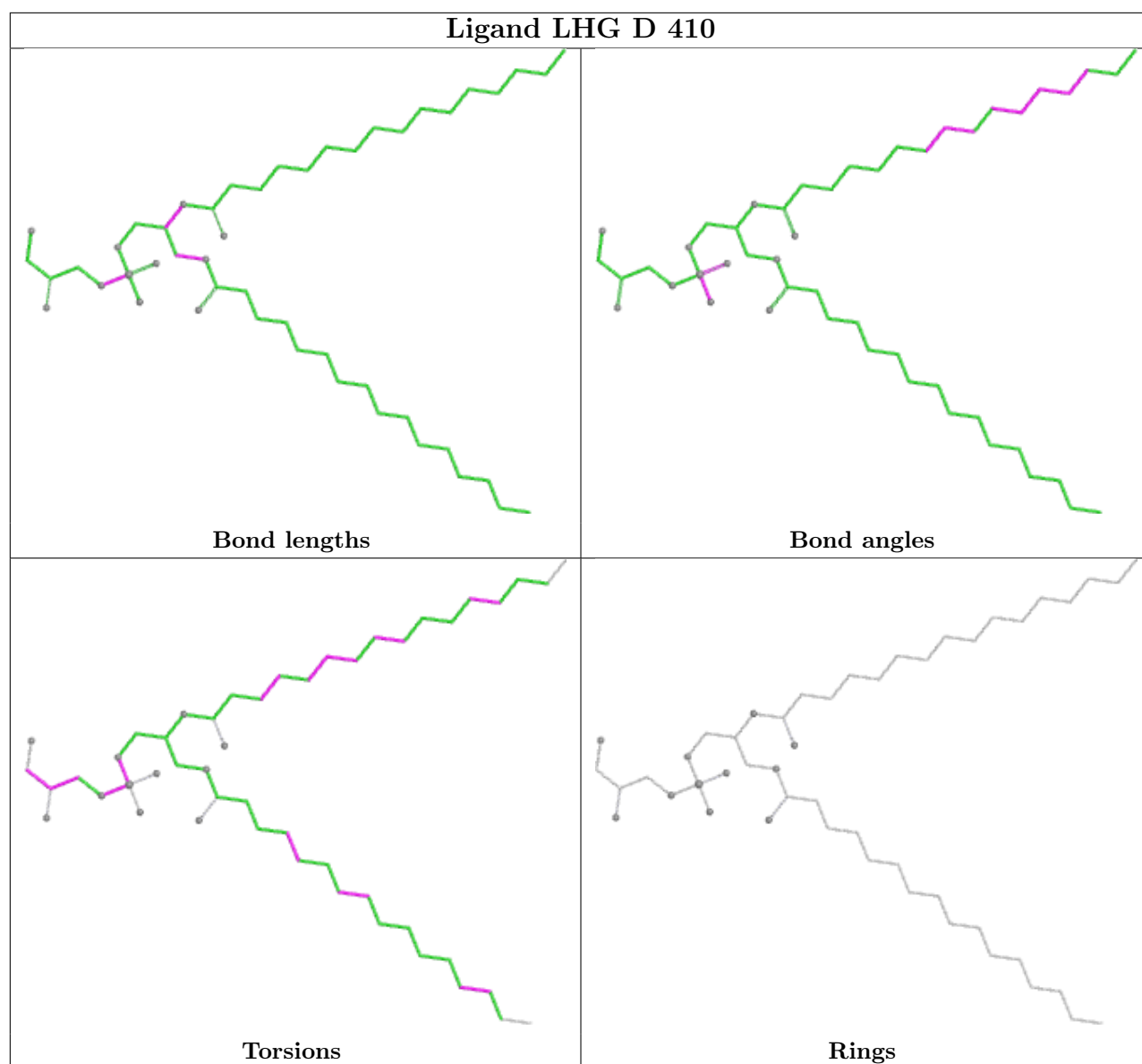




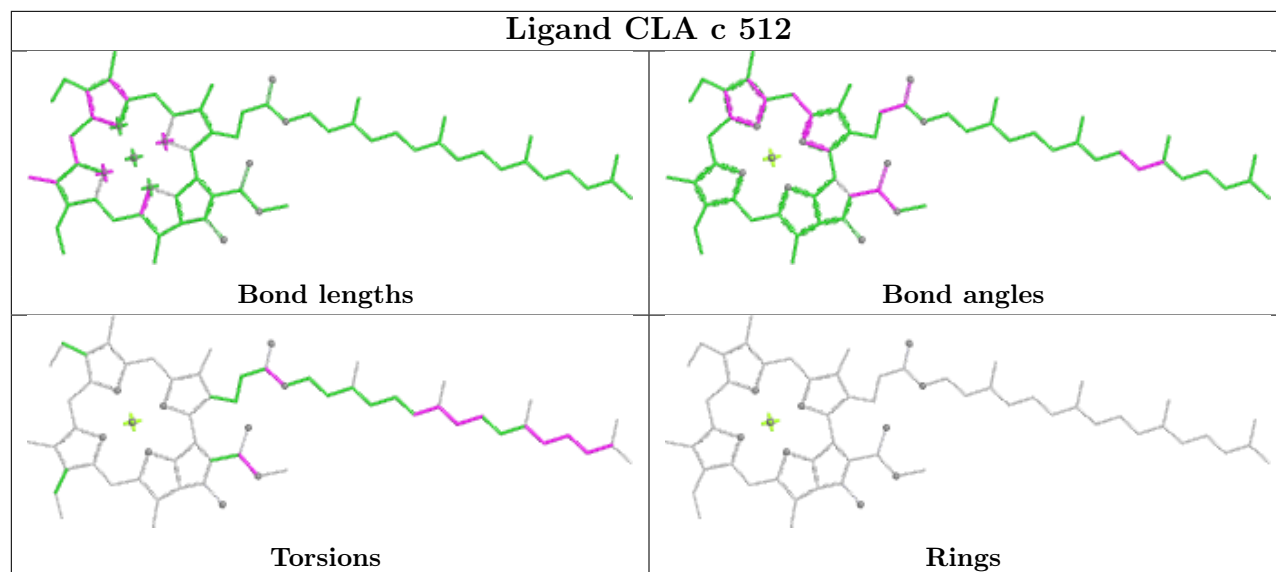




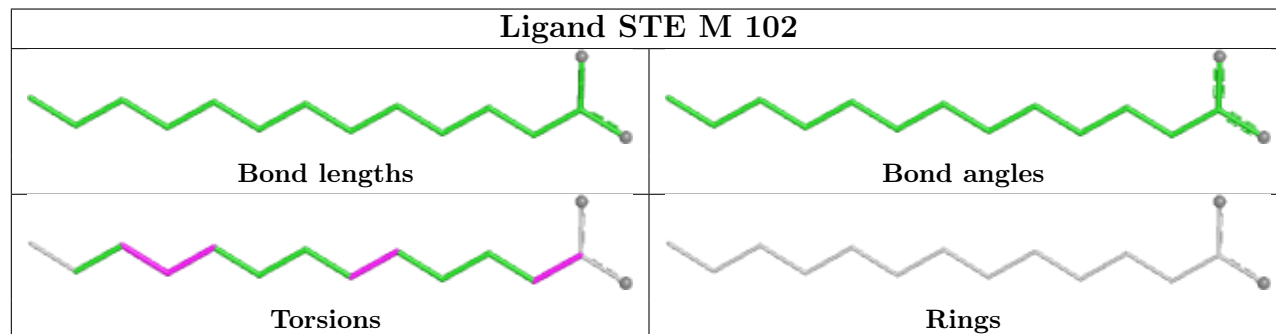




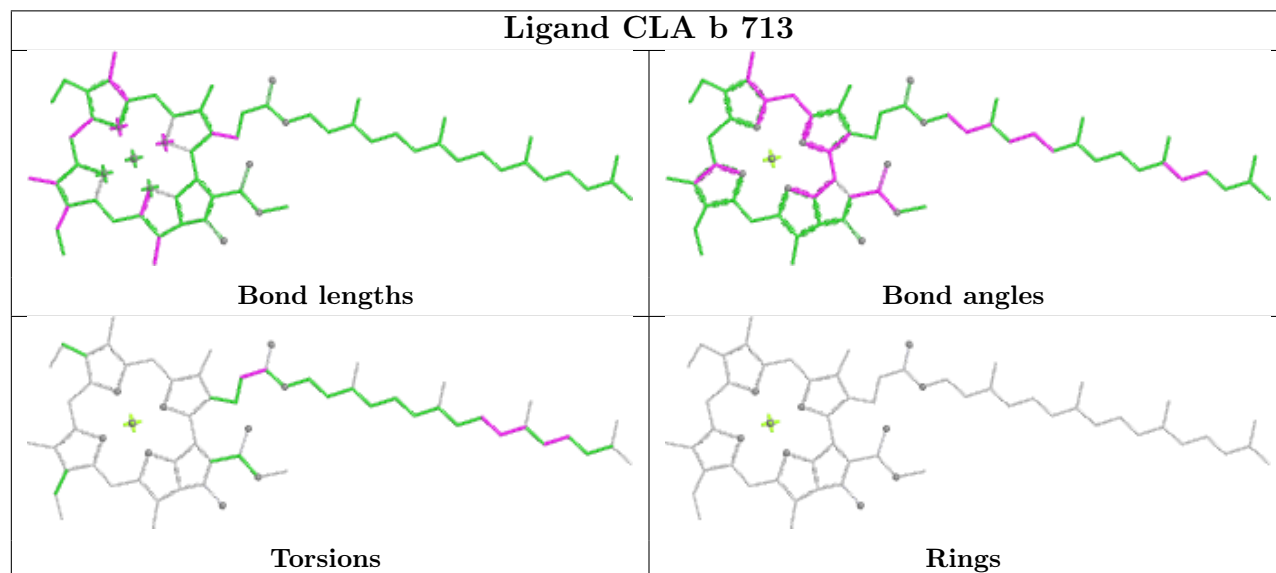
Ligand CLA c 512



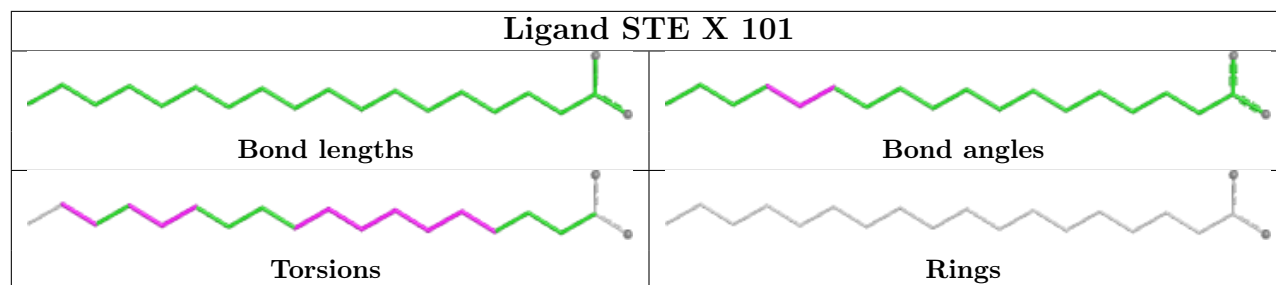
Ligand STE M 102

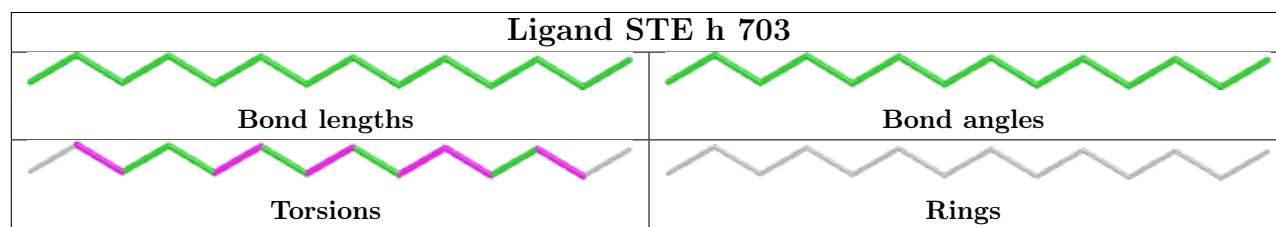
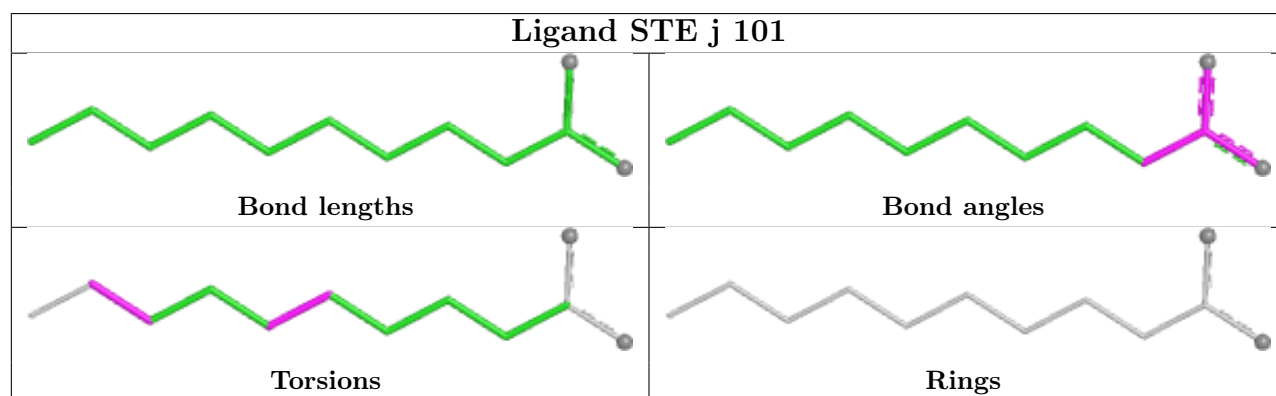
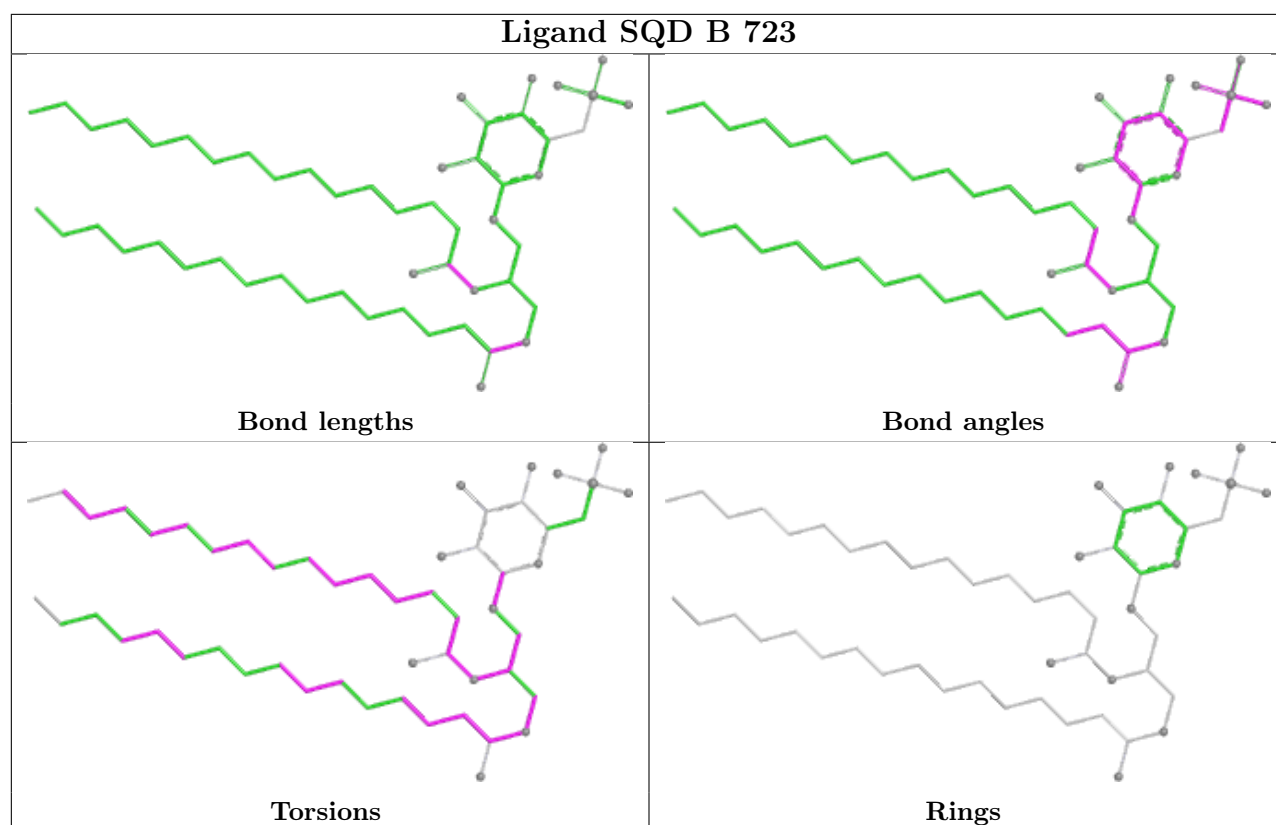


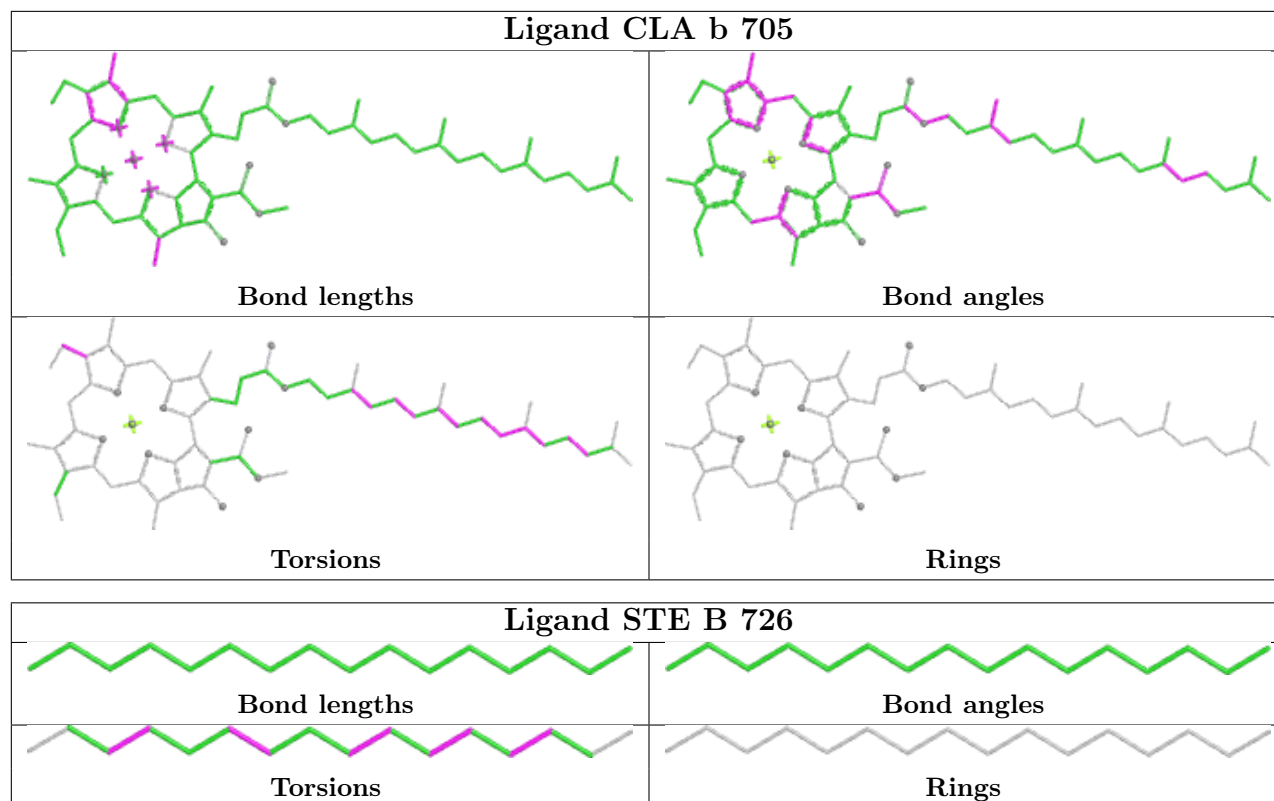
Ligand CLA b 713



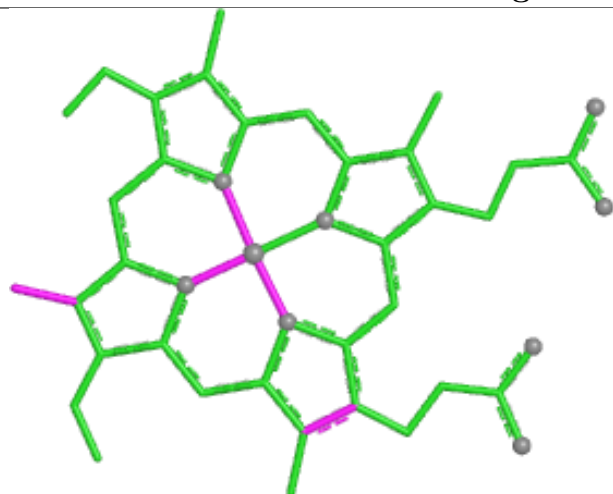
Ligand STE X 101



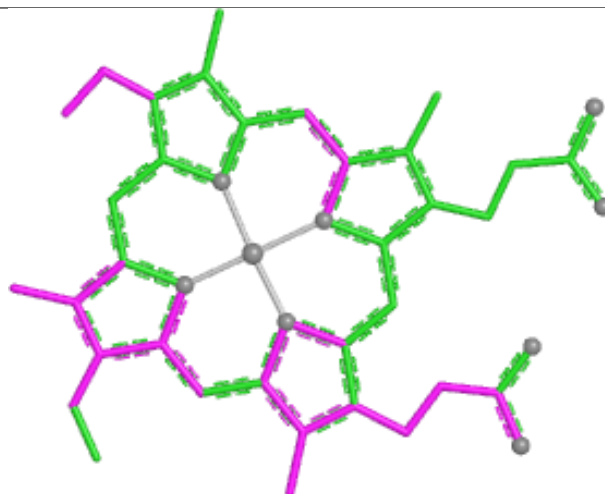




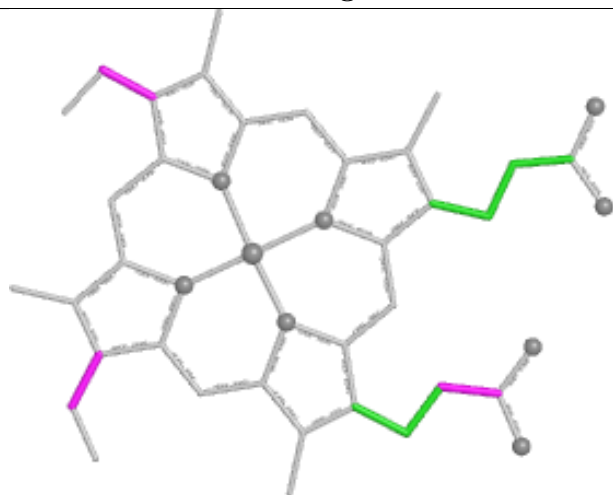
Ligand HEC V 201



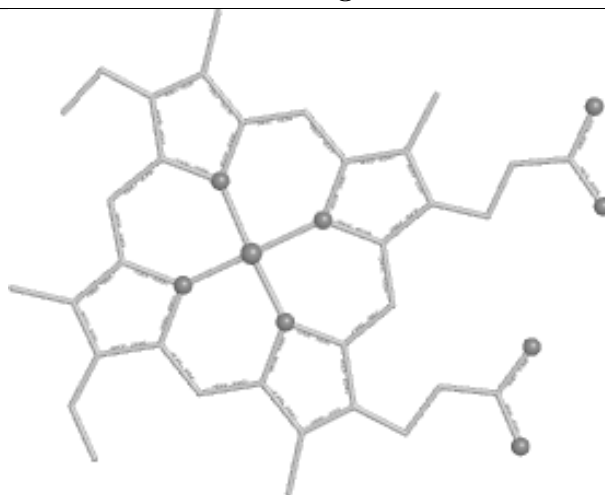
Bond lengths



Bond angles

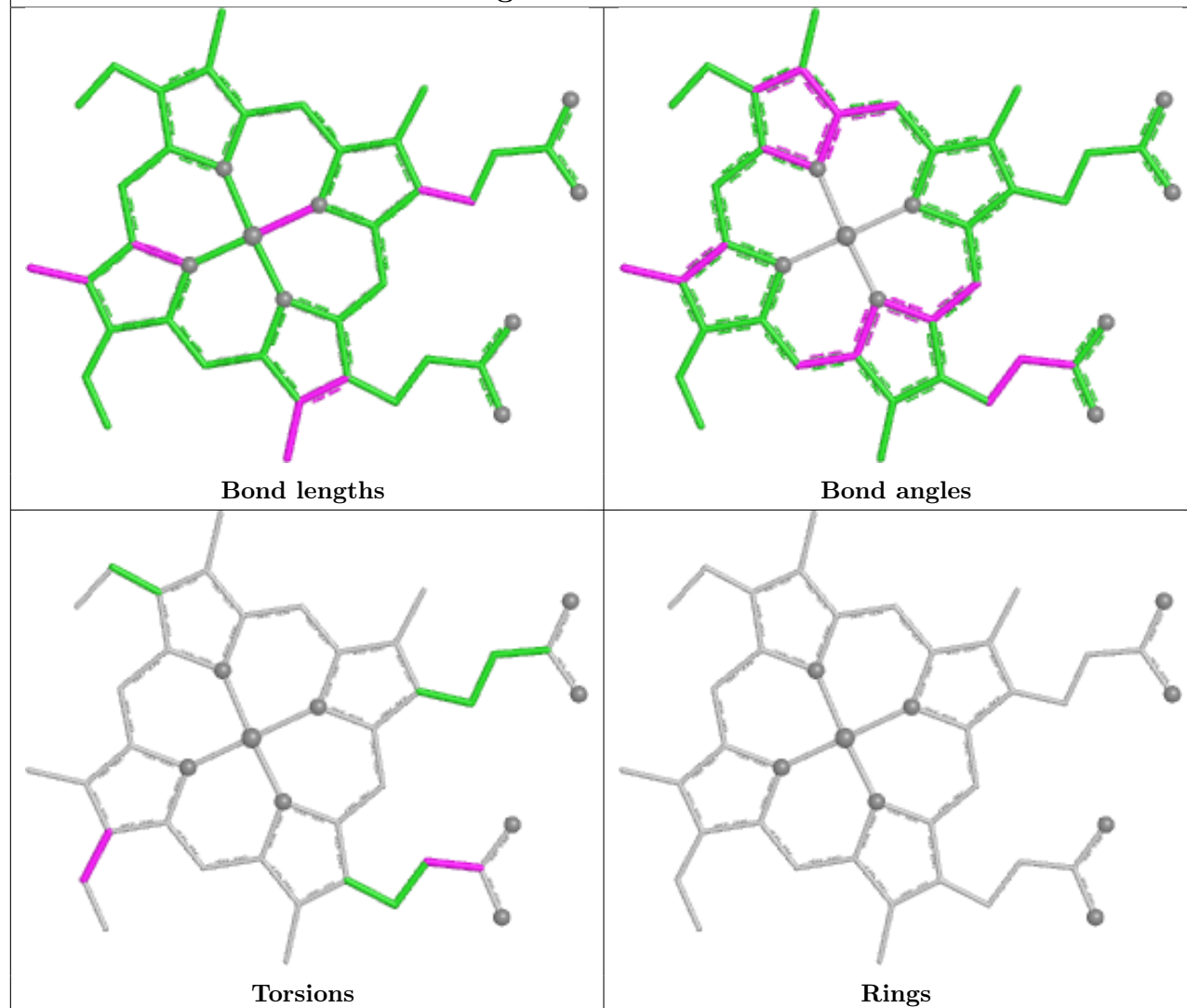


Torsions

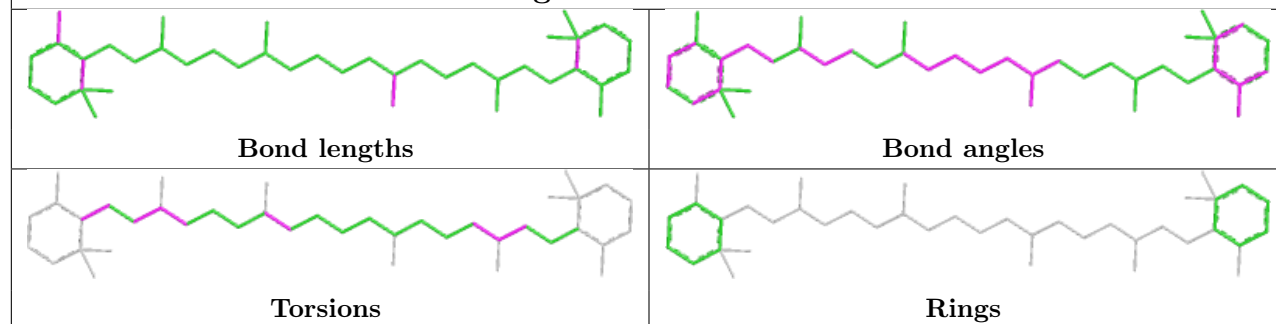


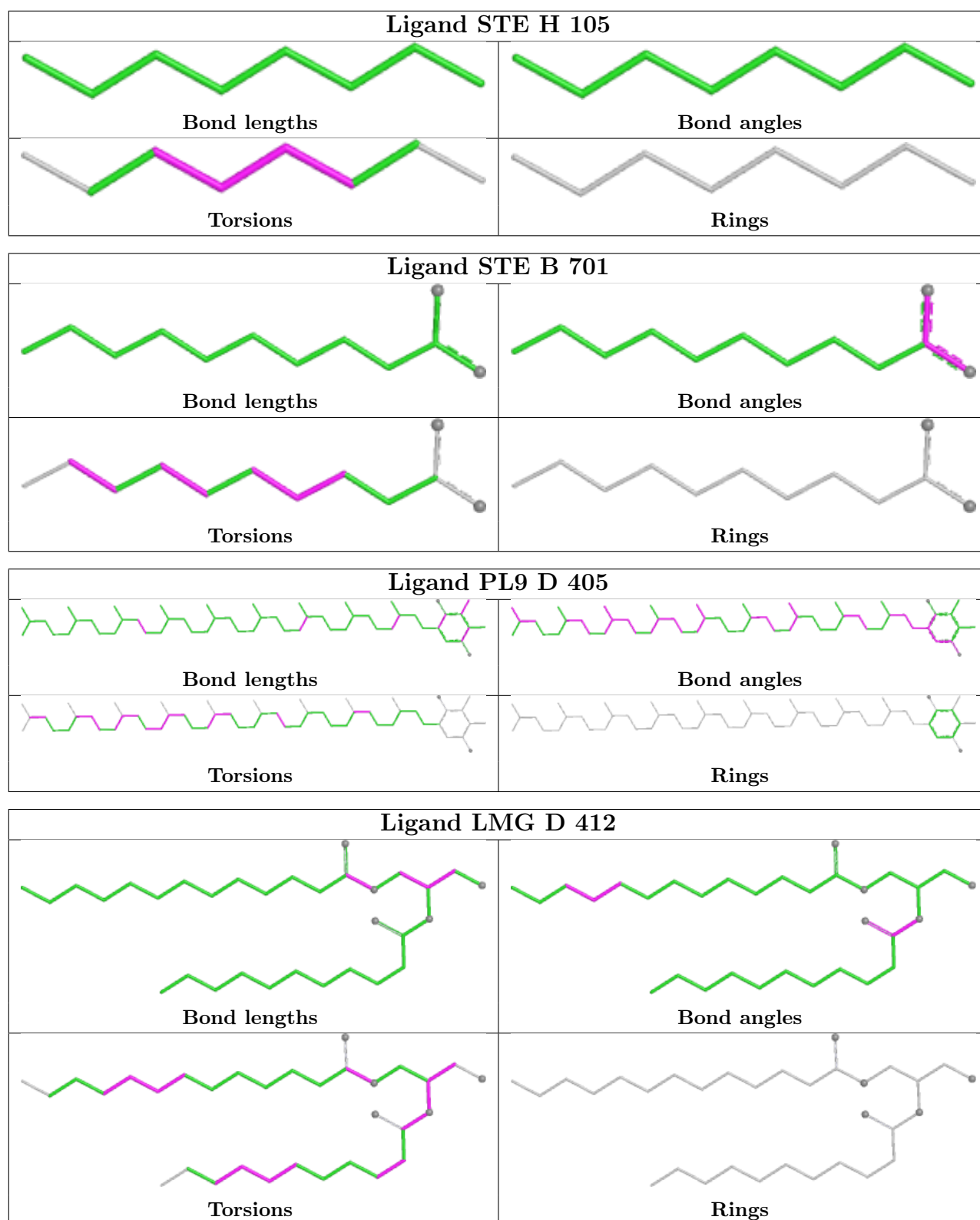
Rings

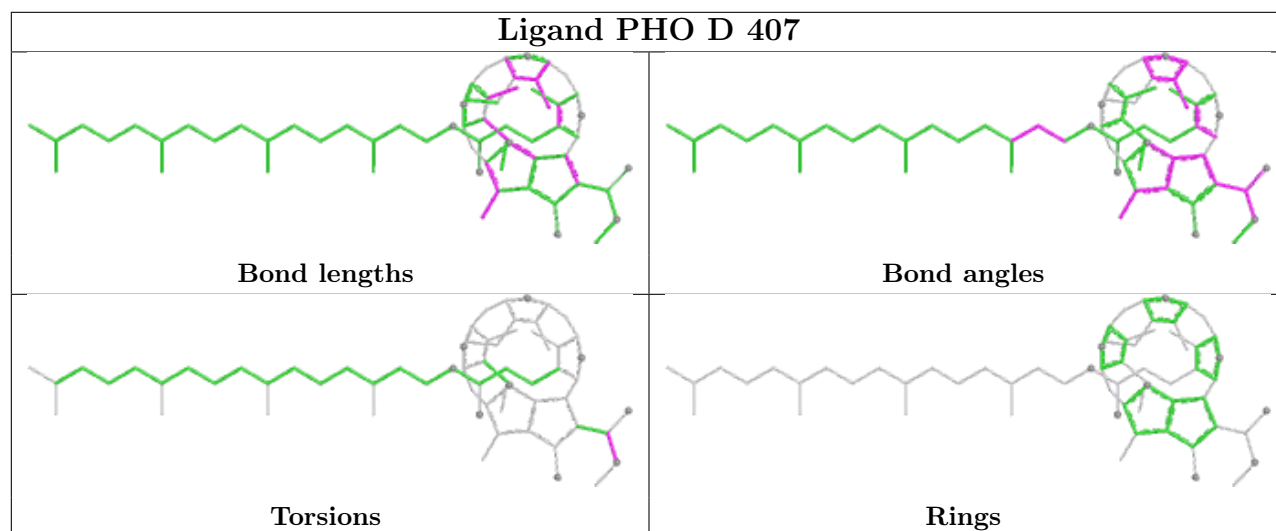
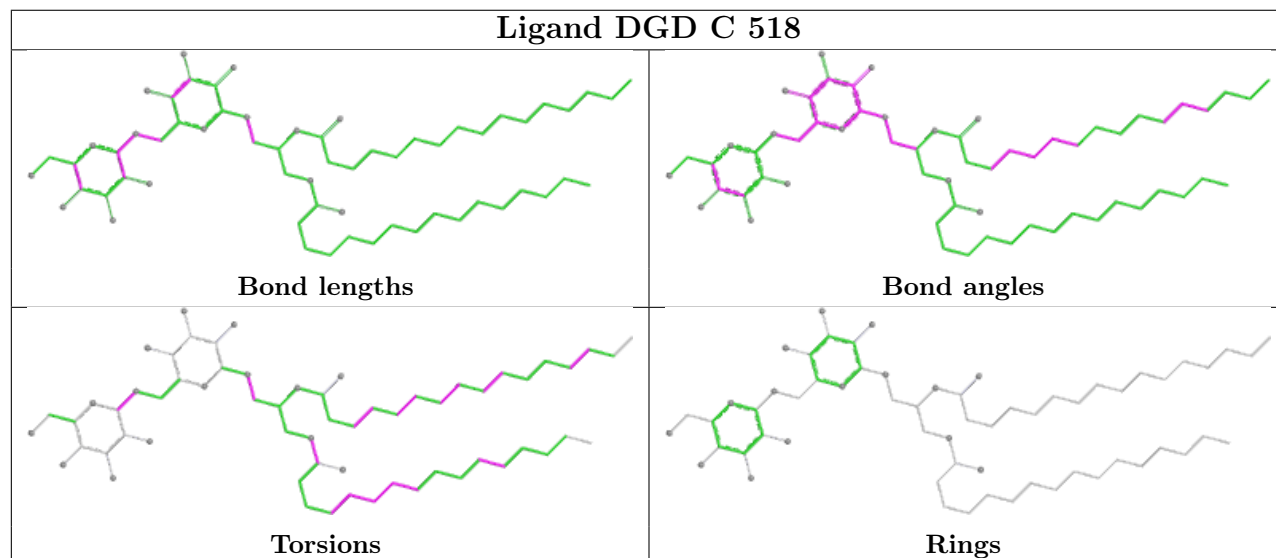
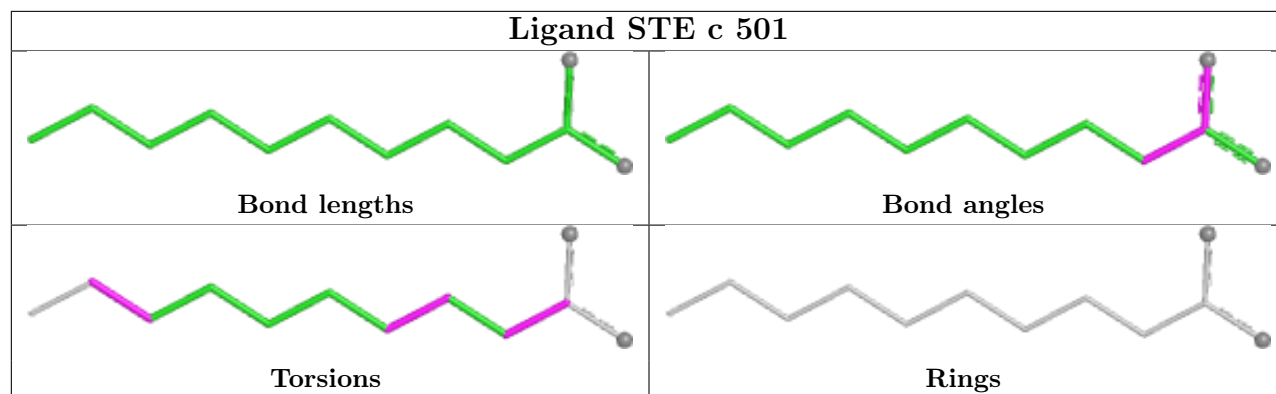
Ligand HEC v 201

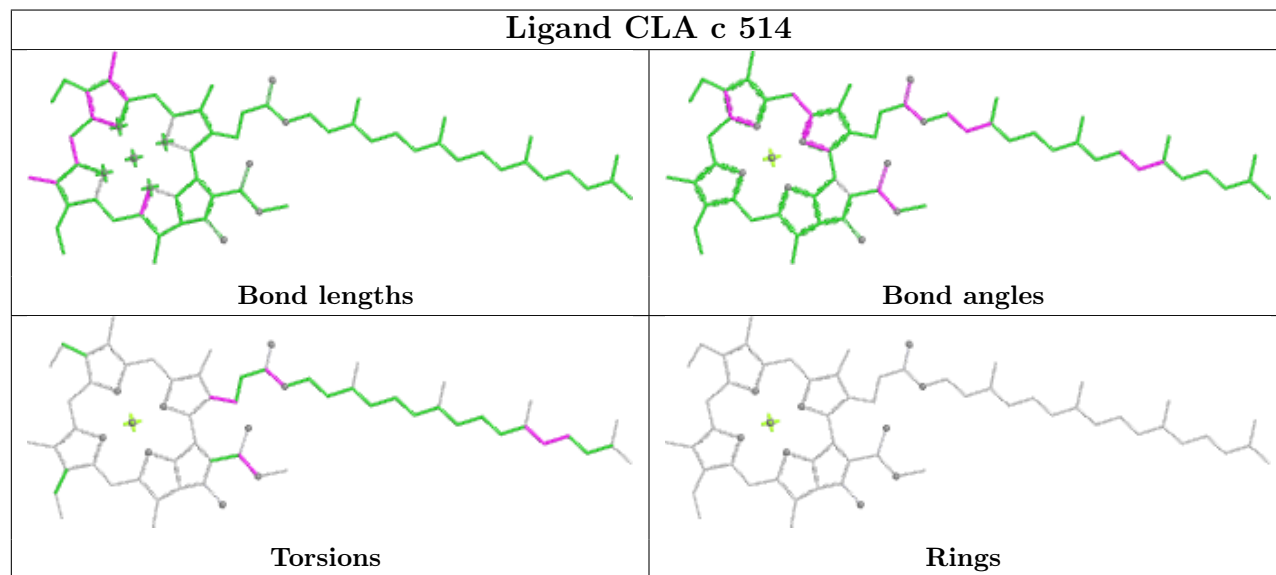
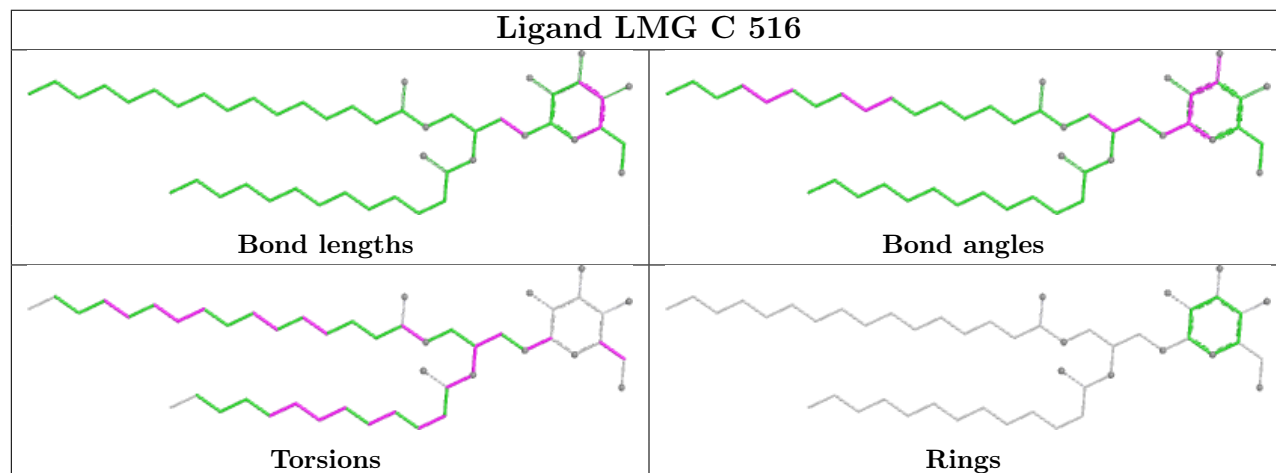
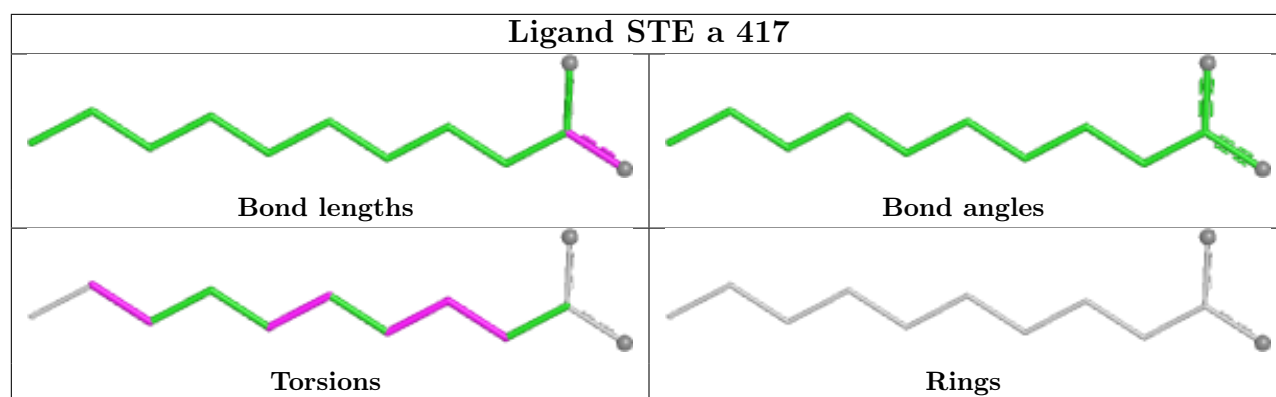


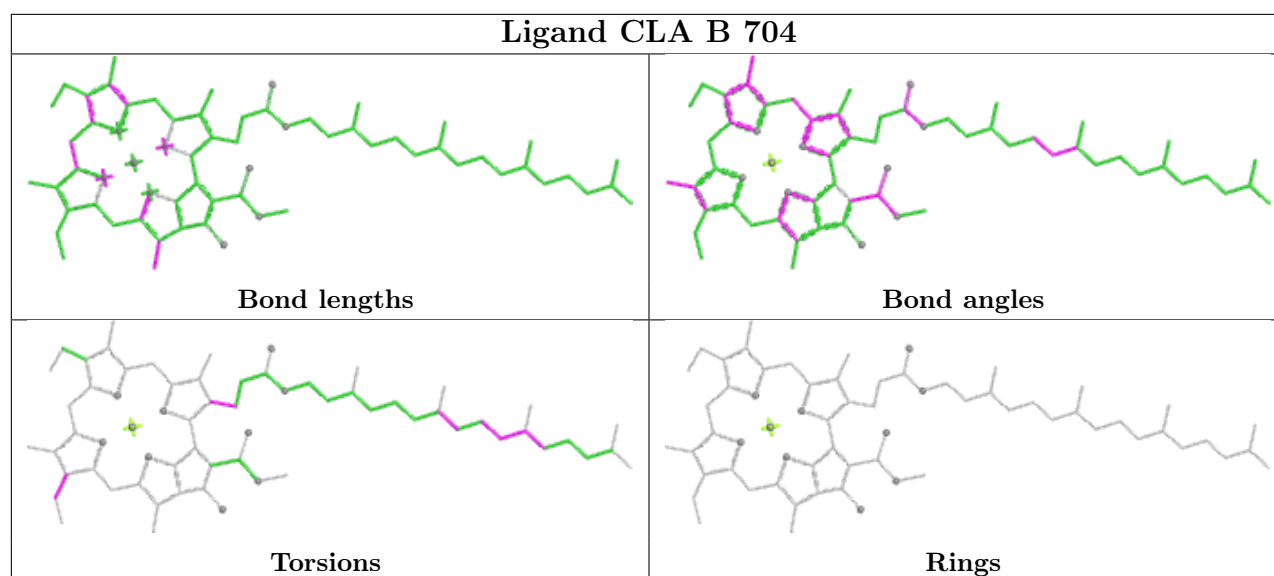
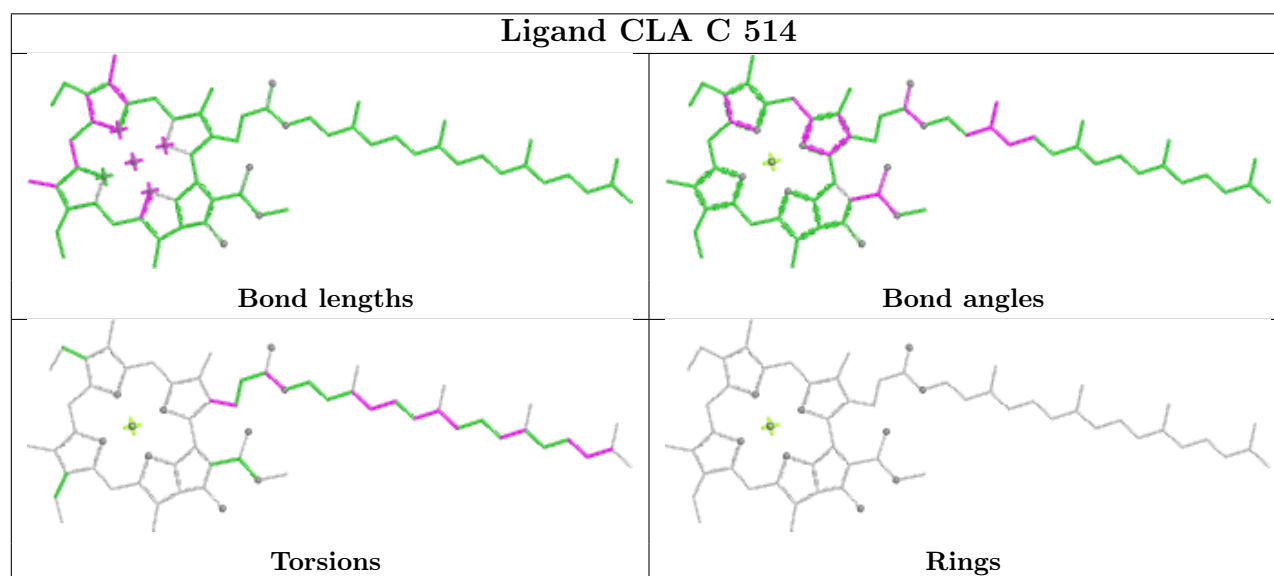
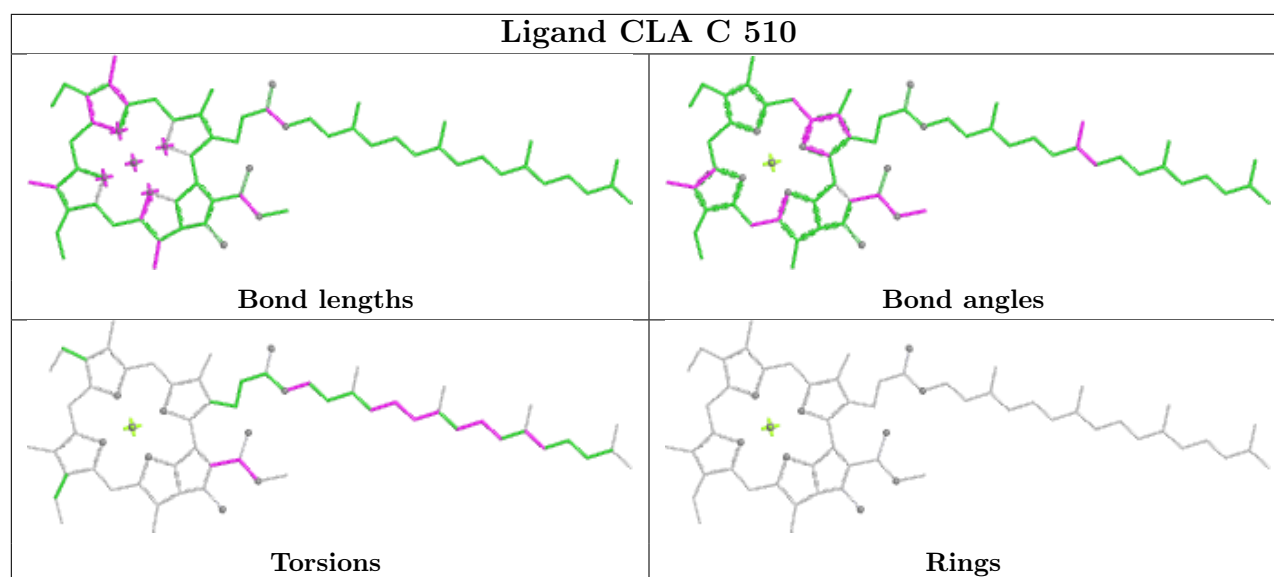
Ligand BCR b 717

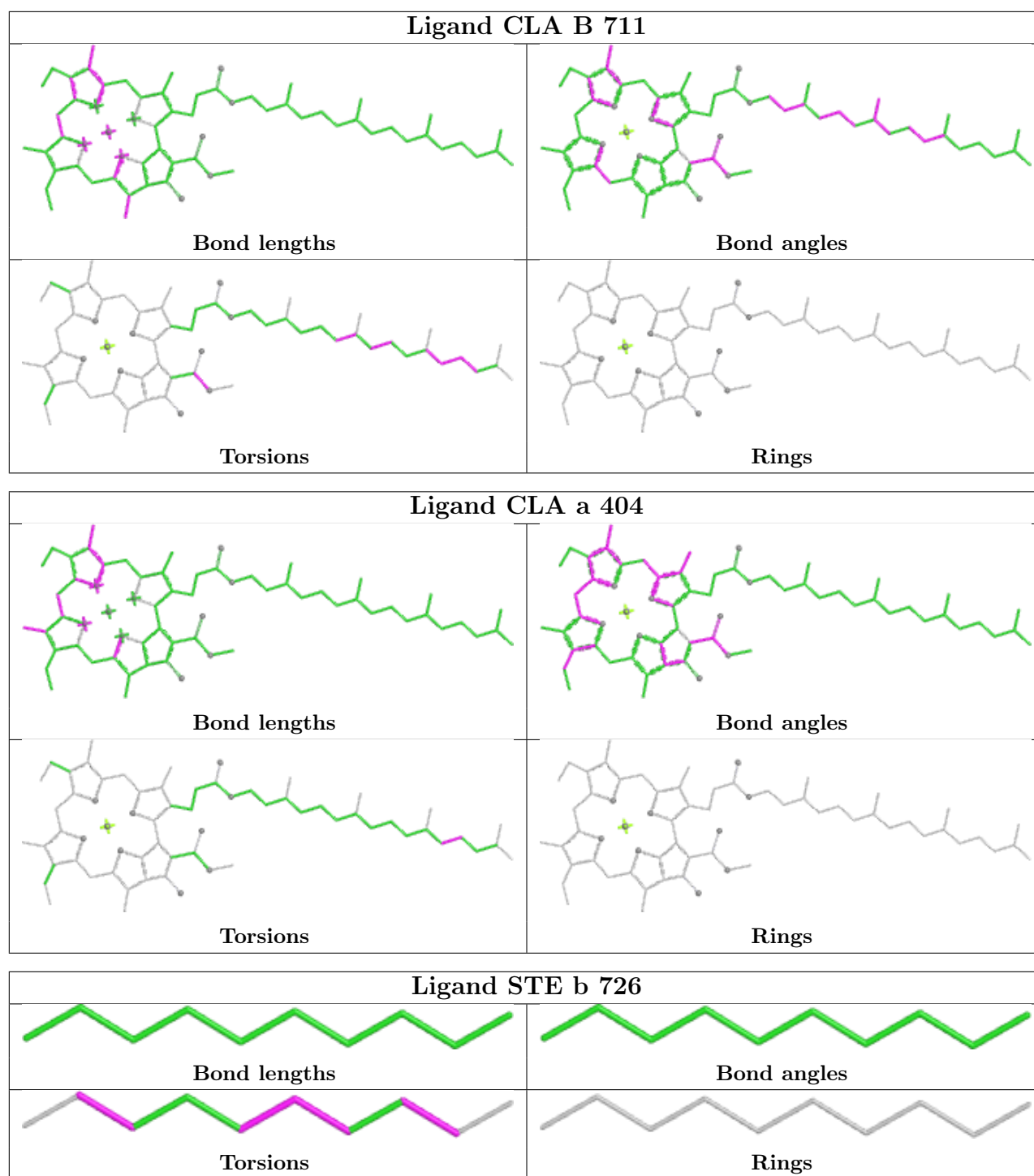


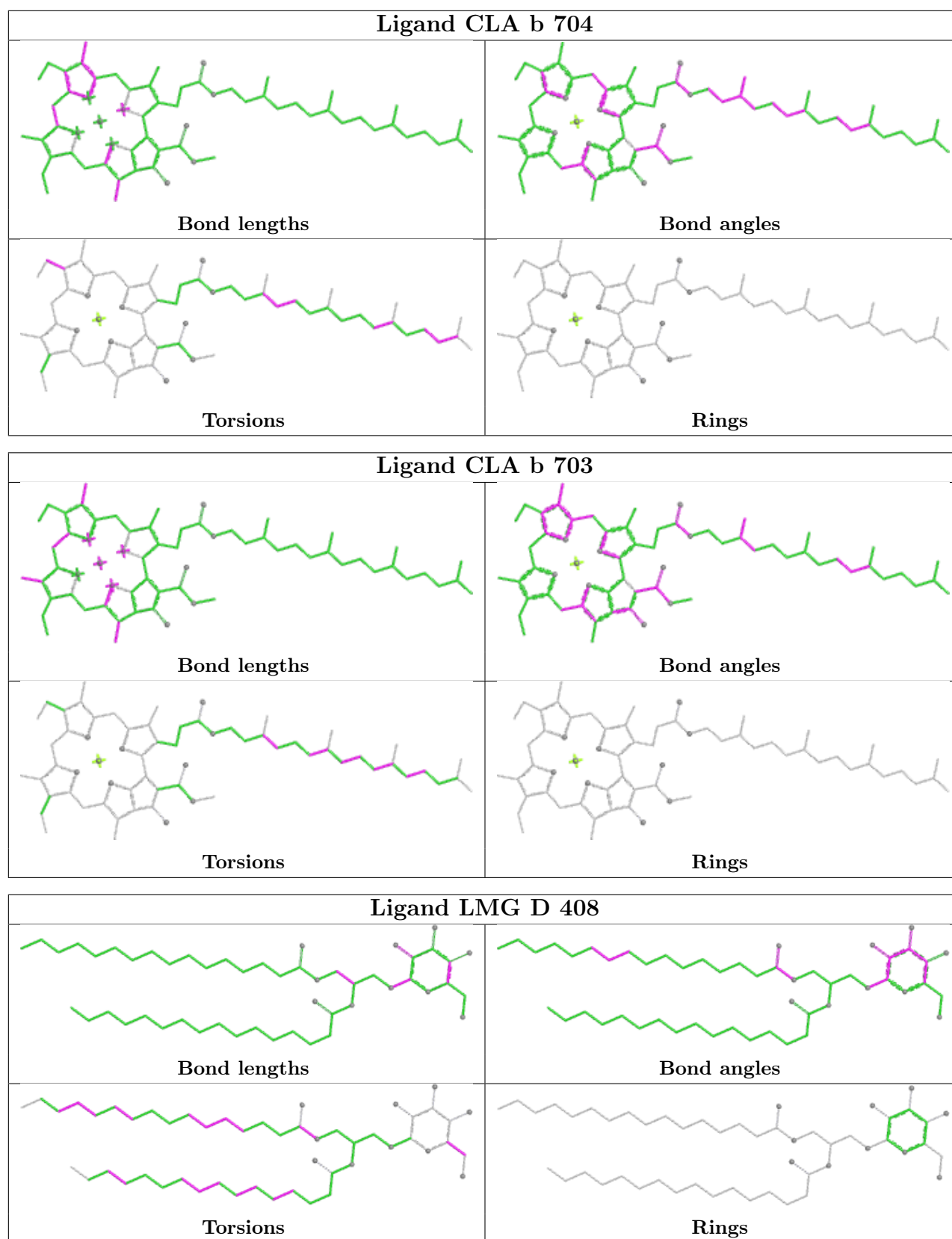


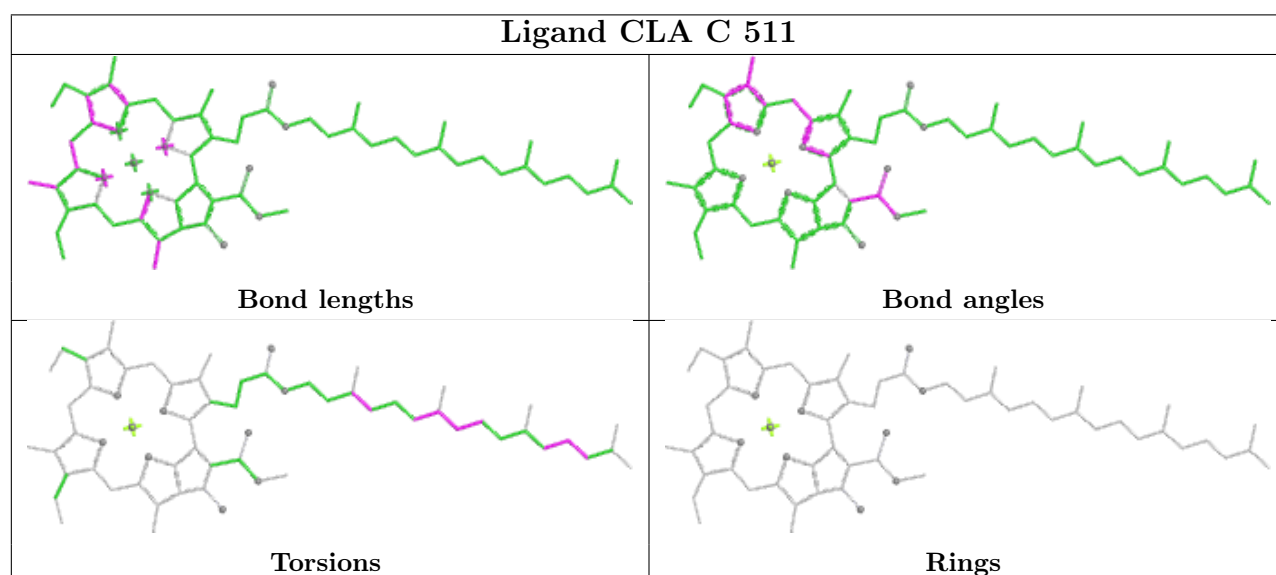
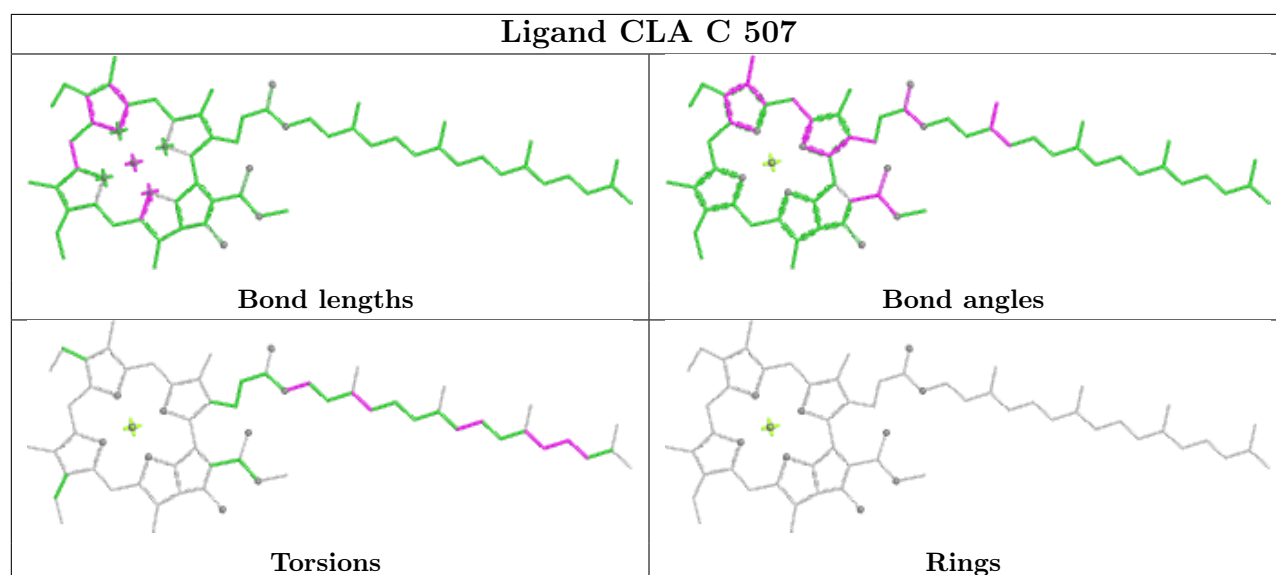
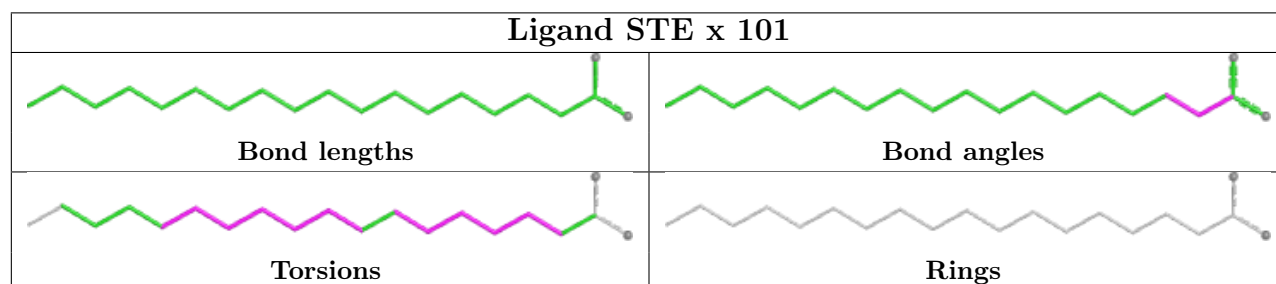
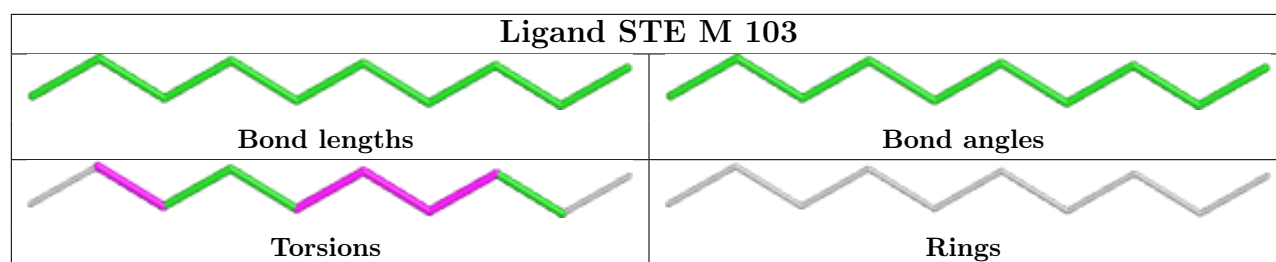


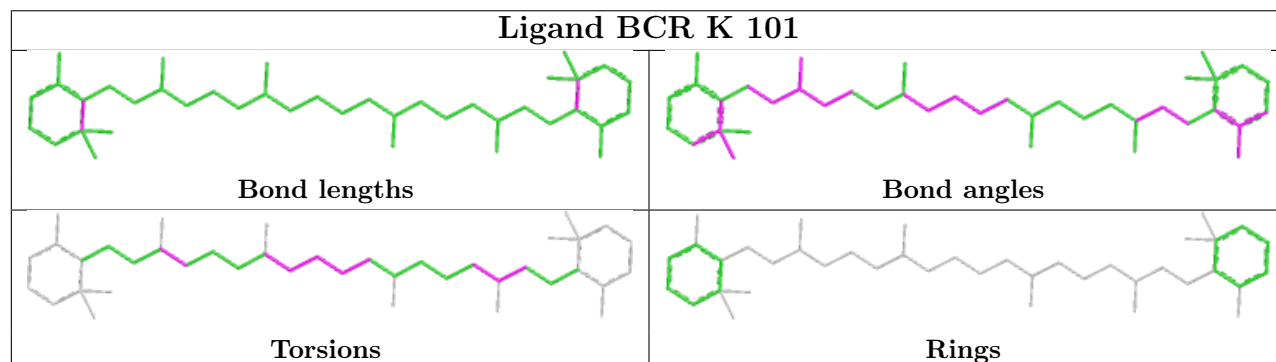
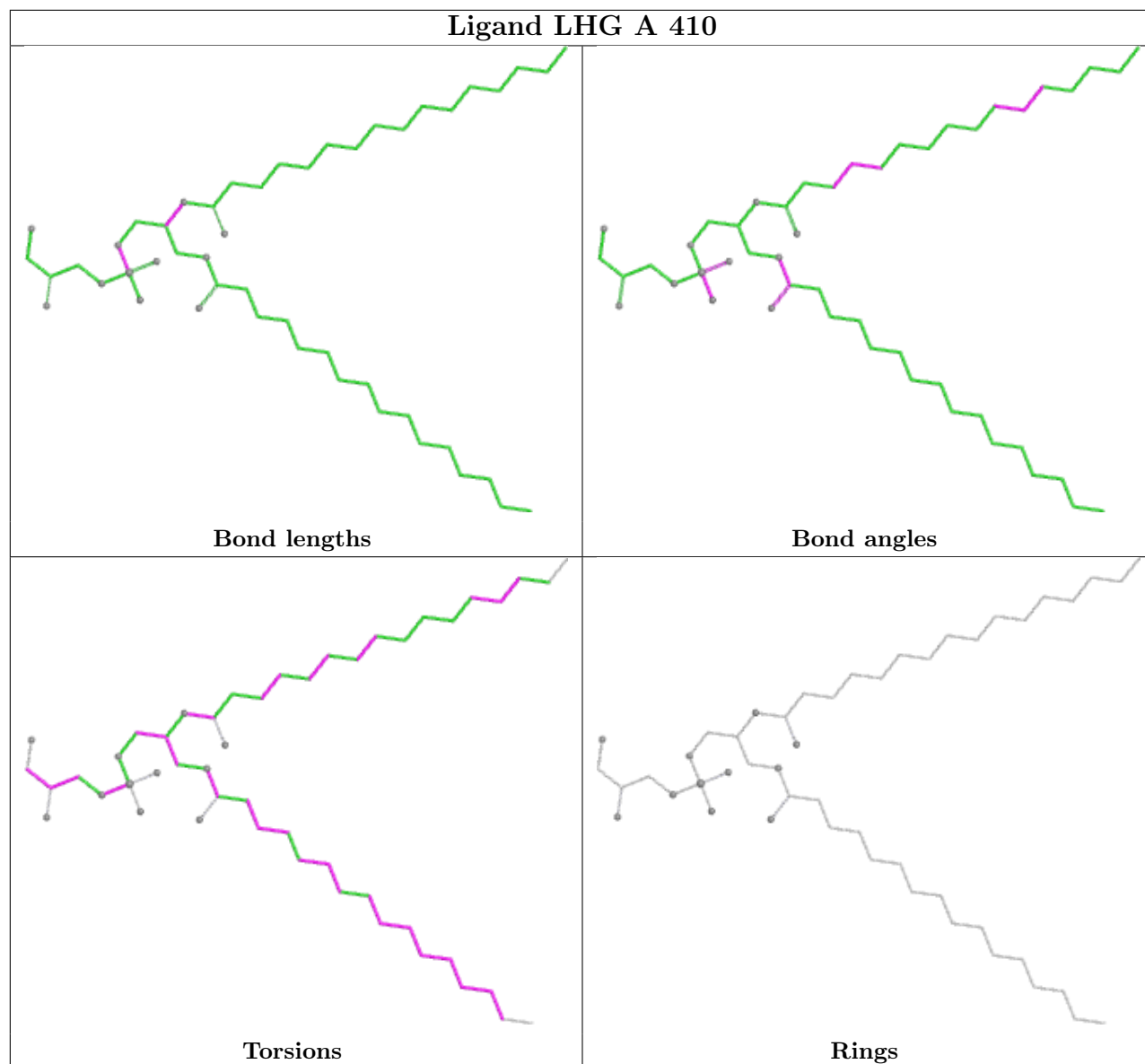


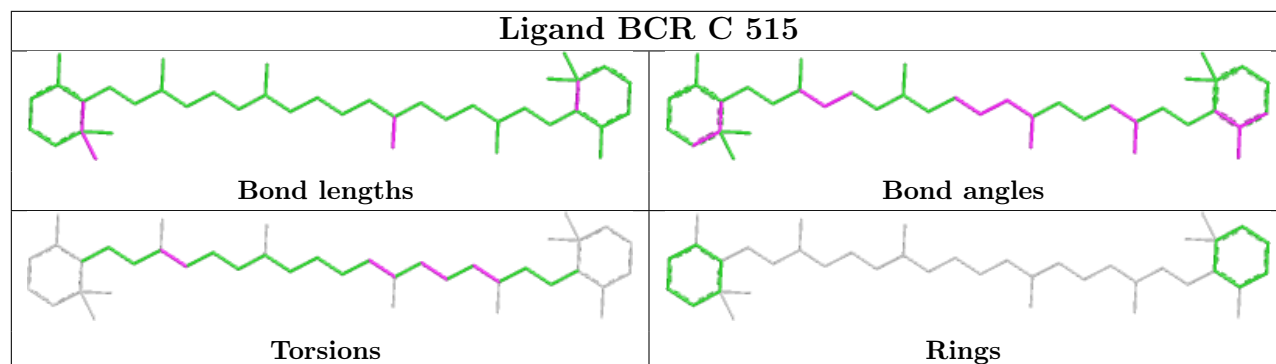
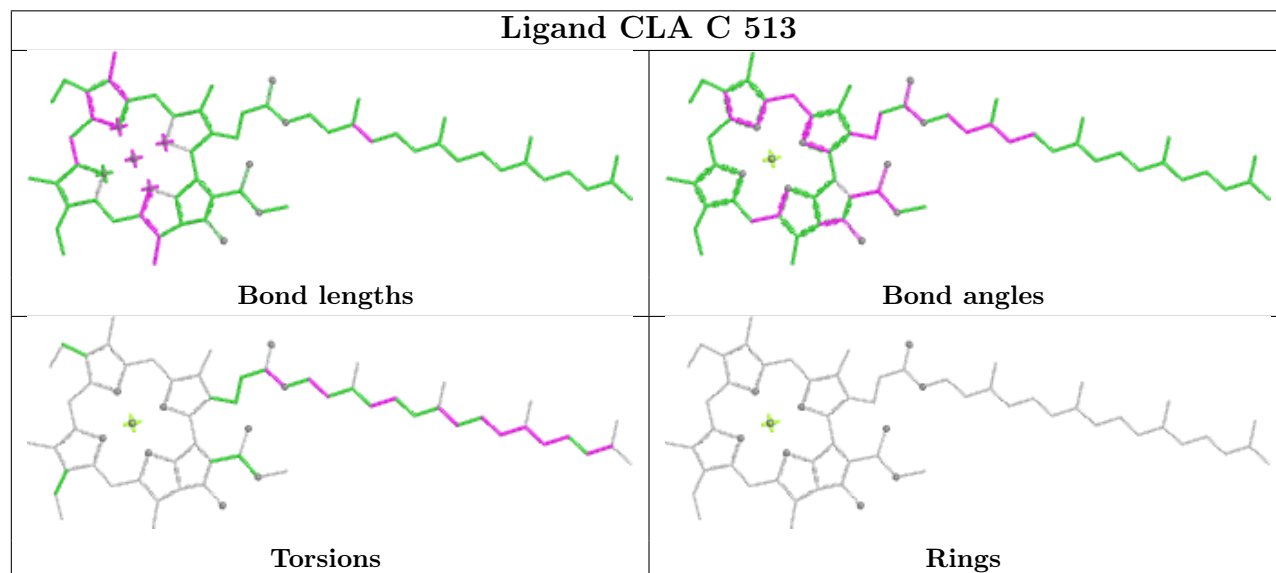
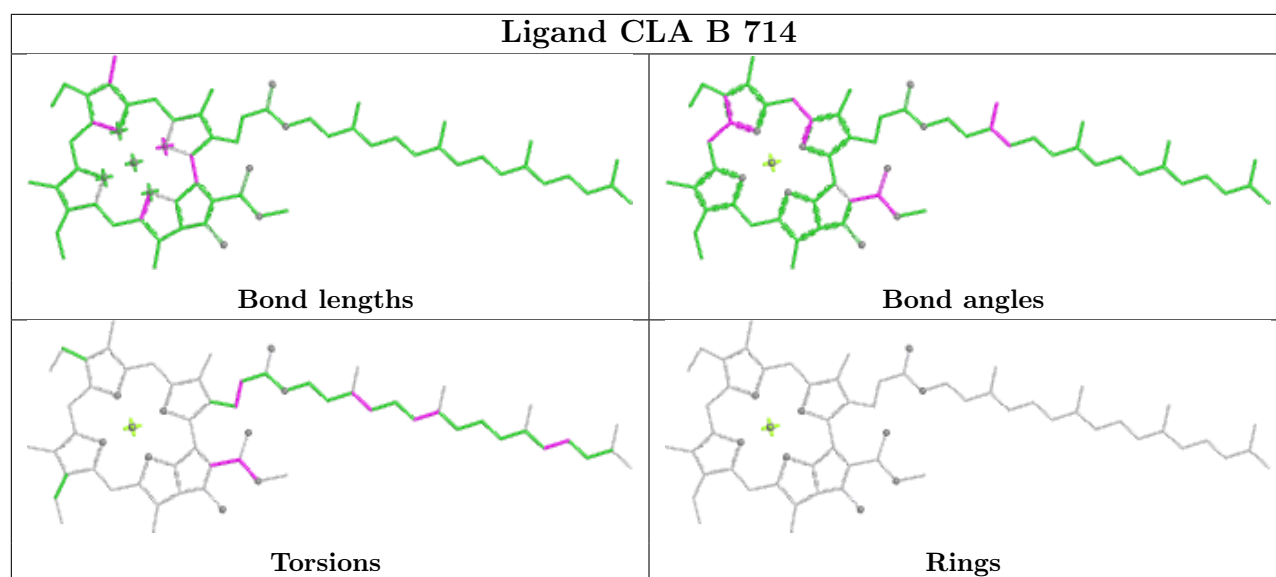


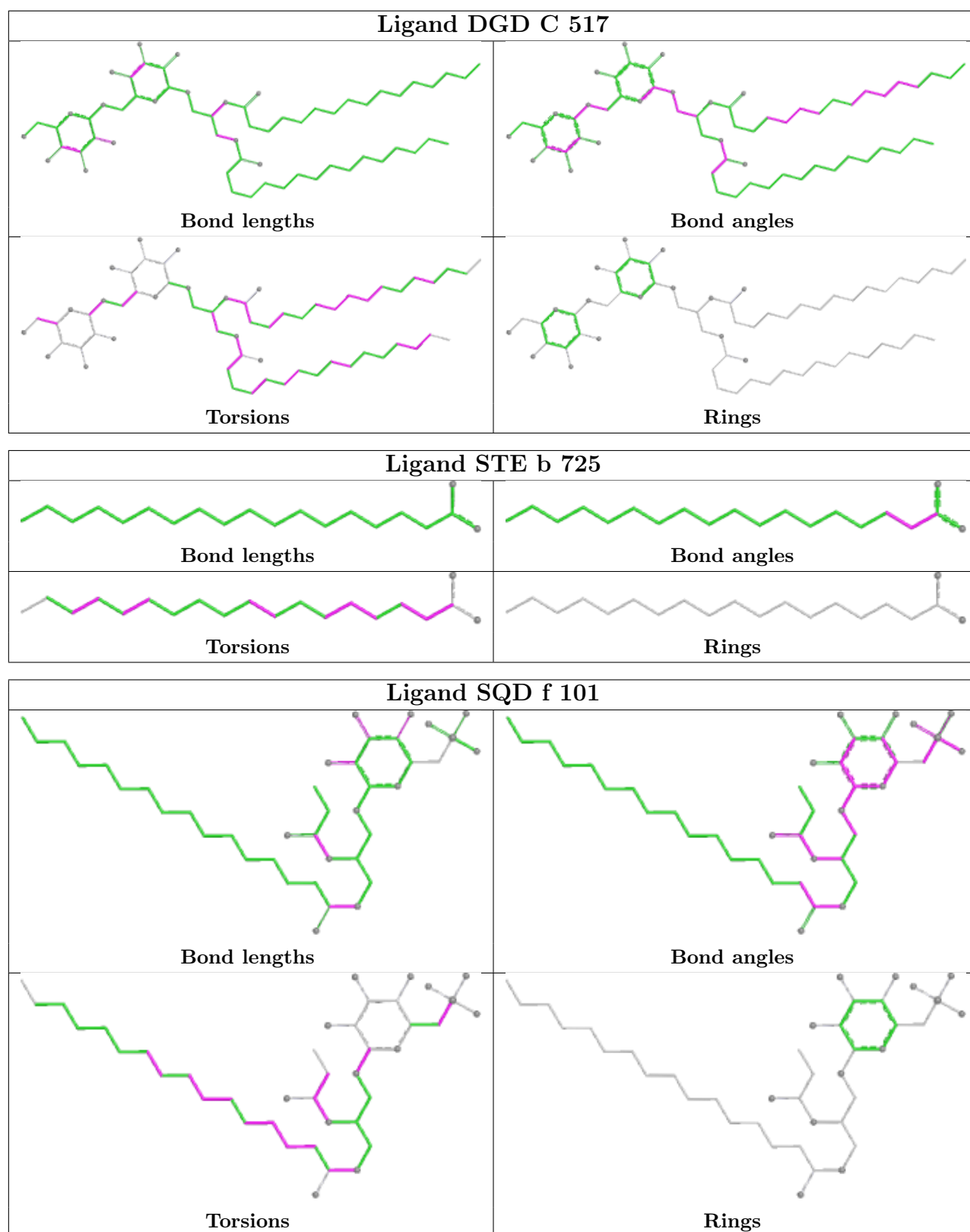


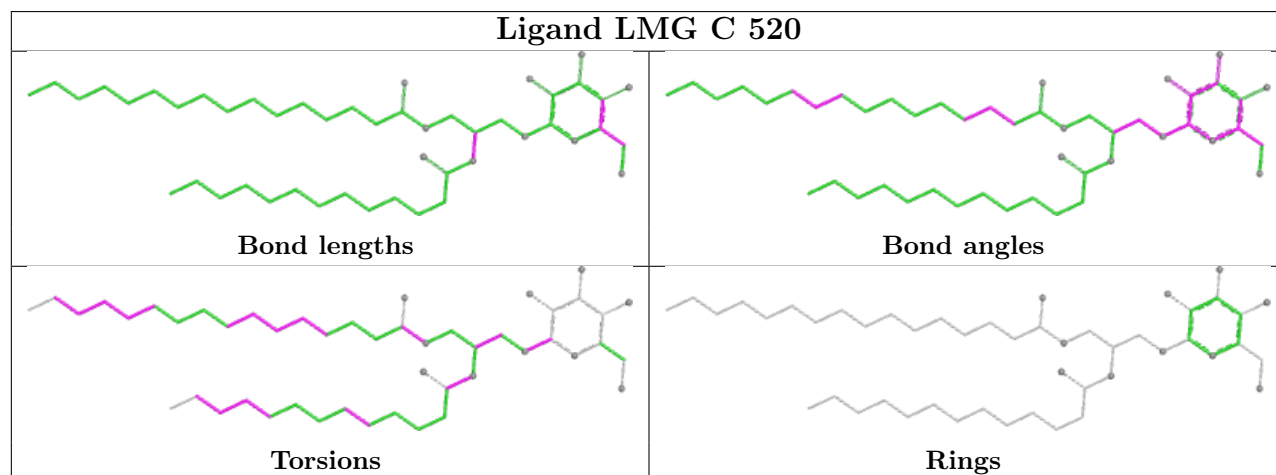
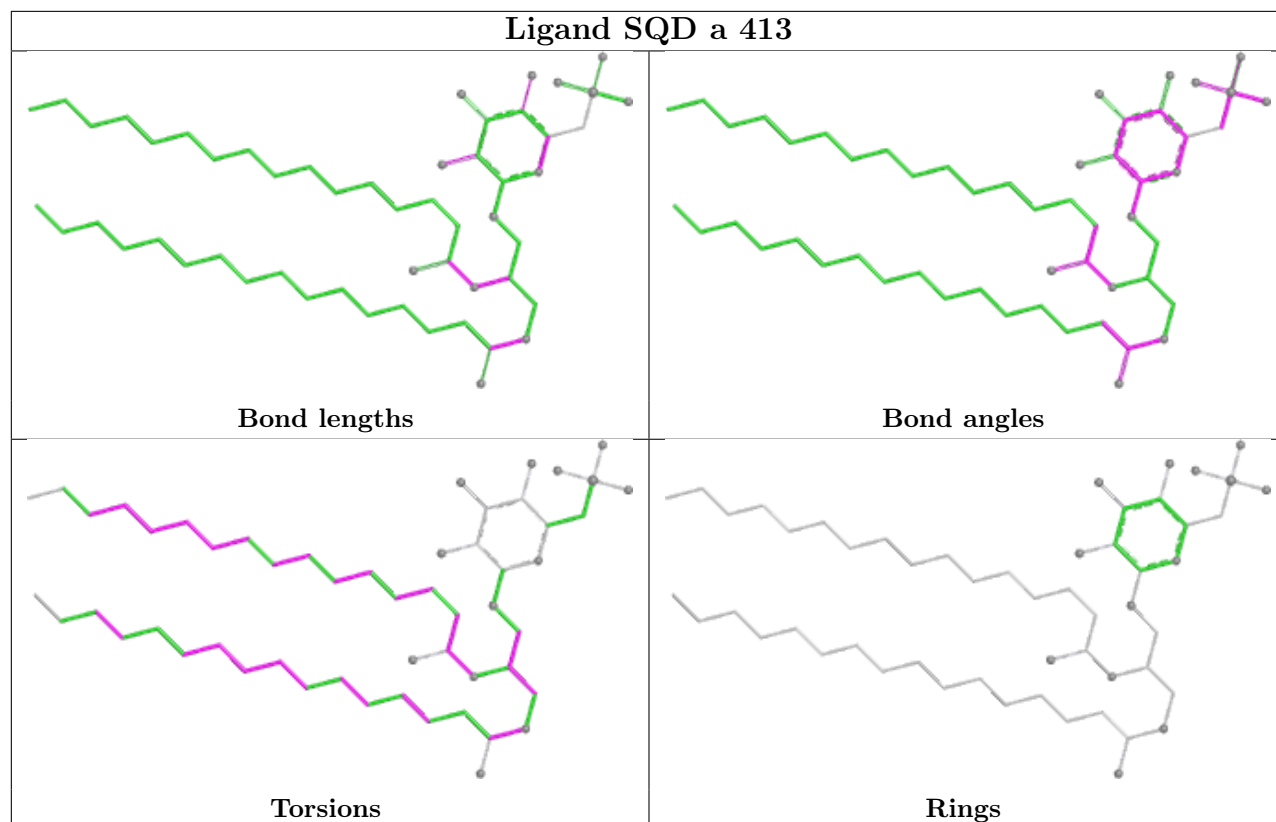




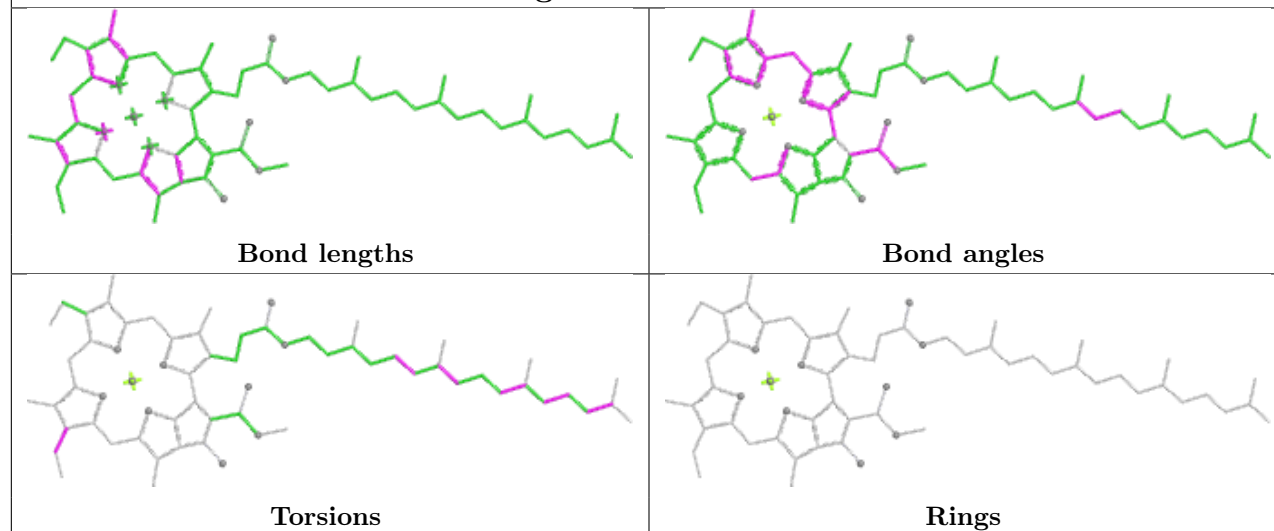




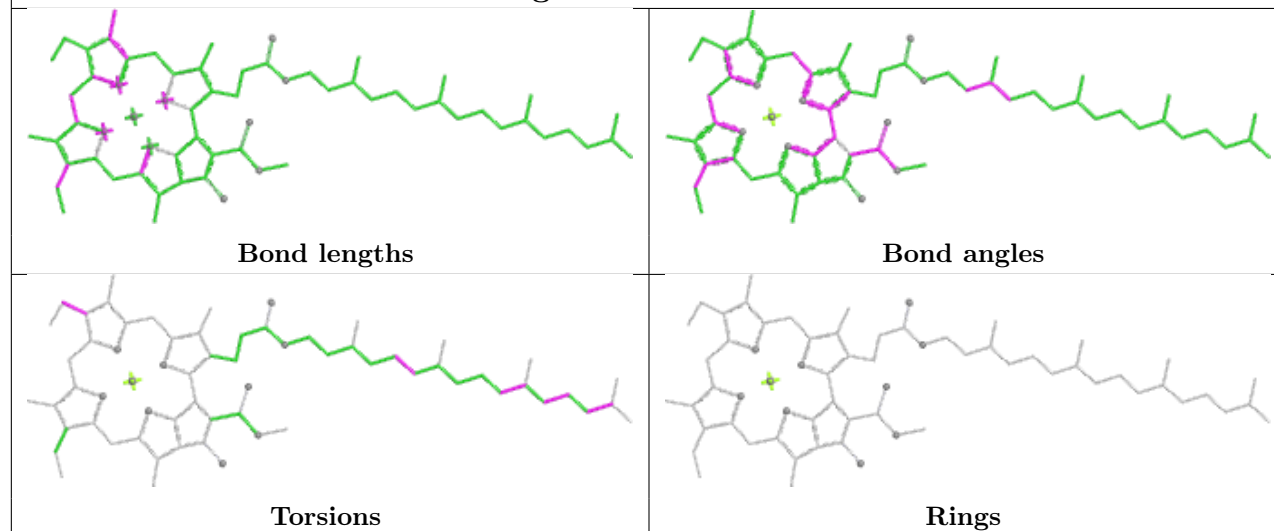




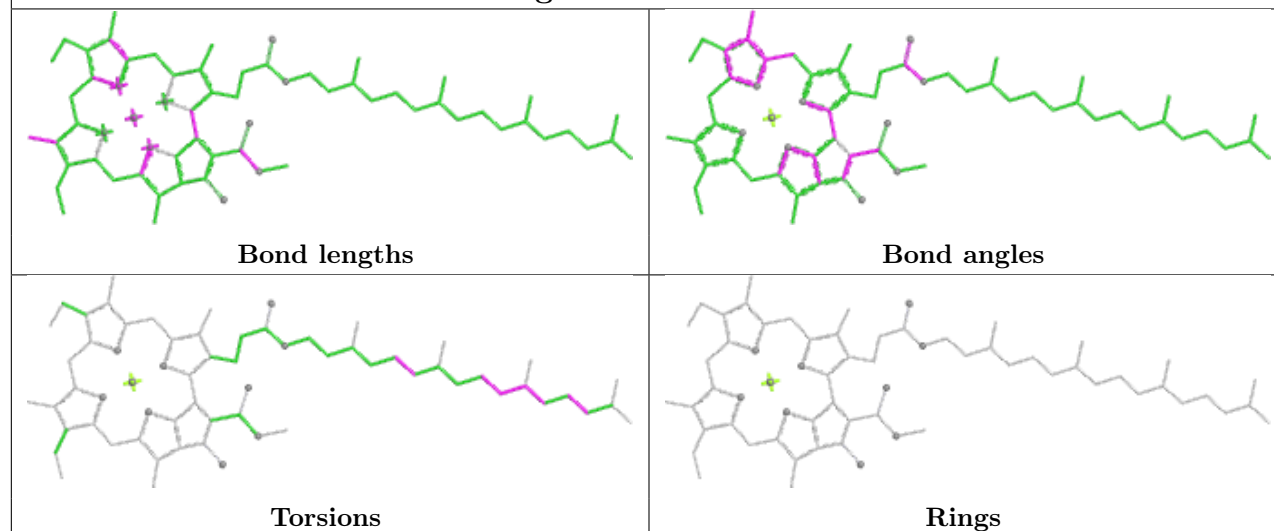
Ligand CLA b 708



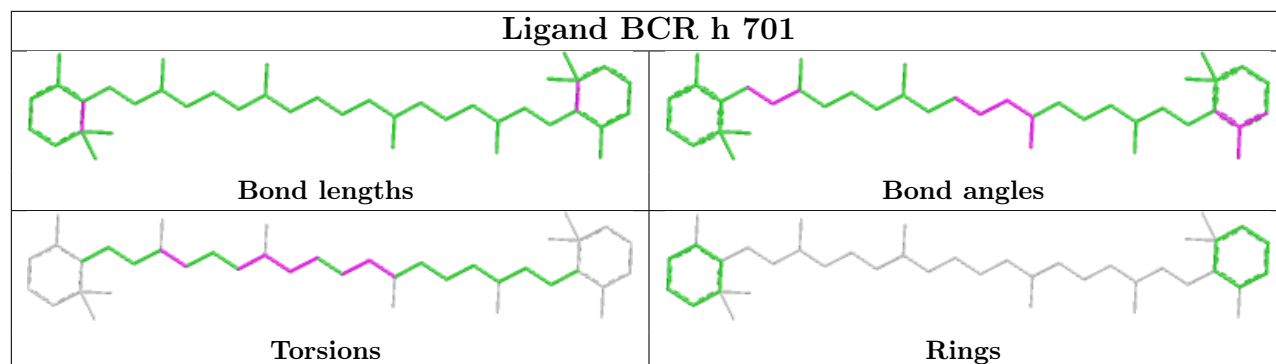
Ligand CLA B 715



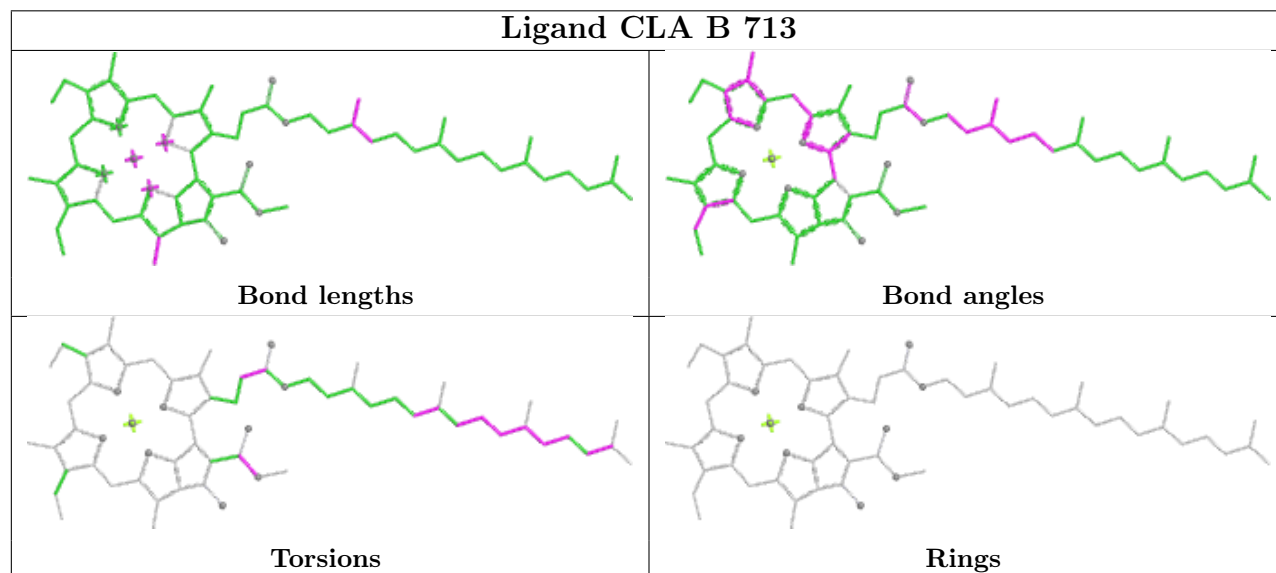
Ligand CLA d 402



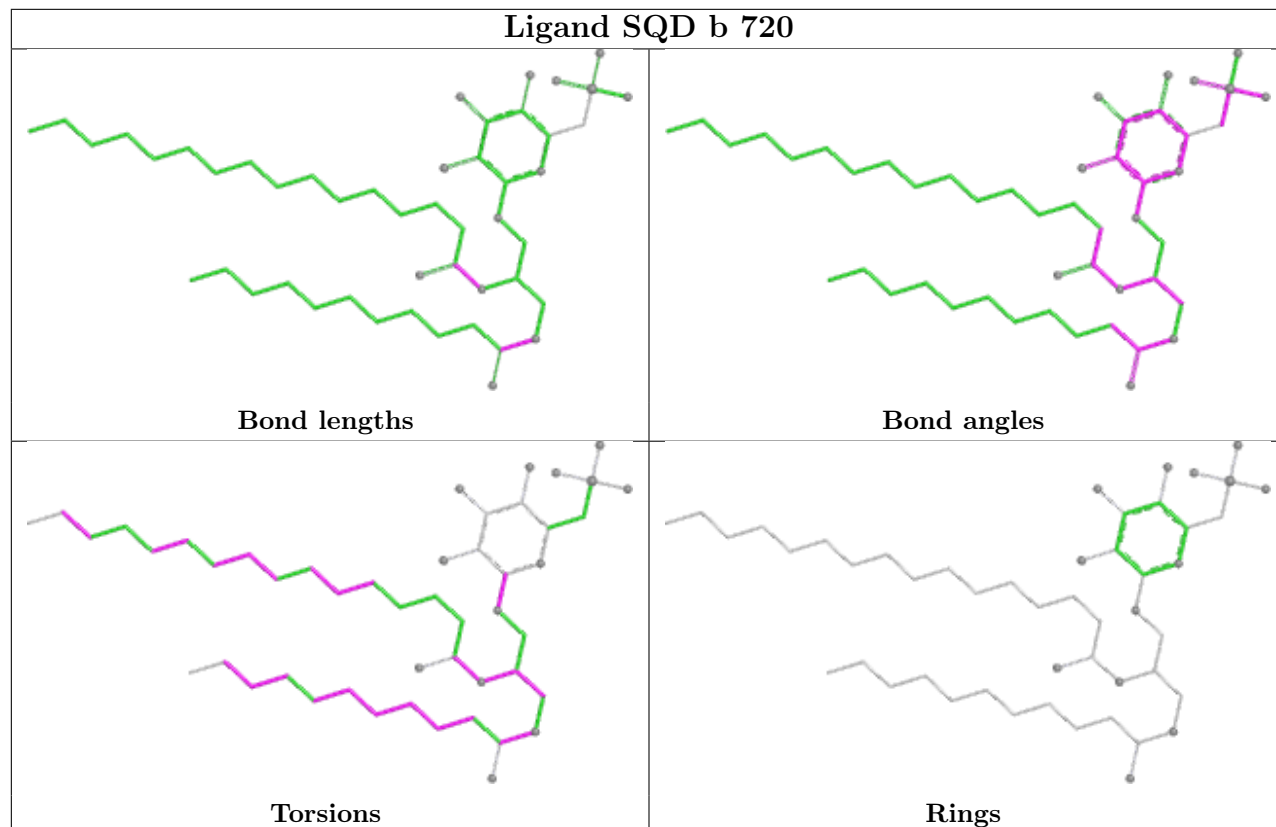
Ligand BCR h 701

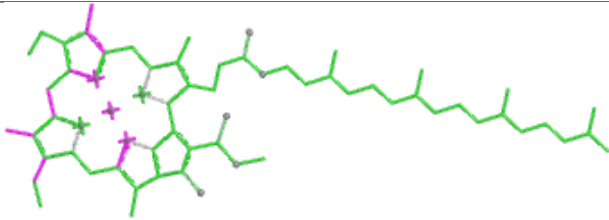
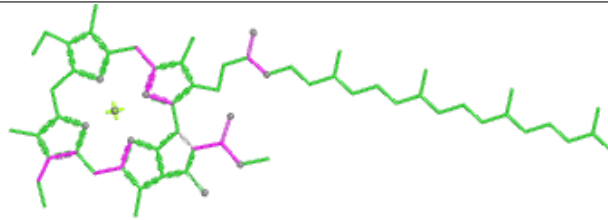
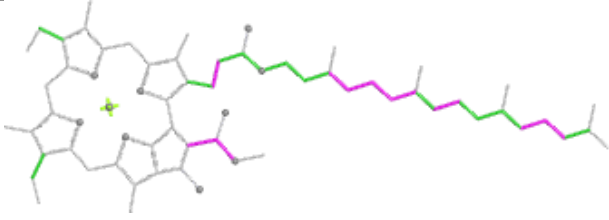
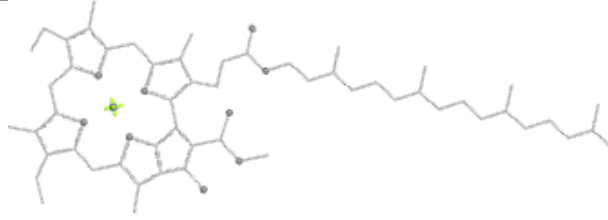
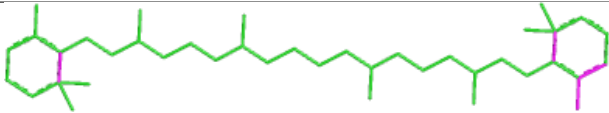
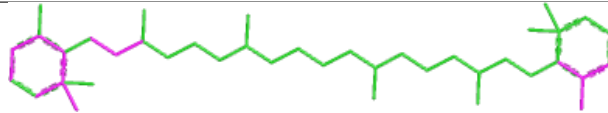
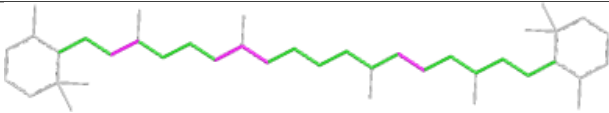
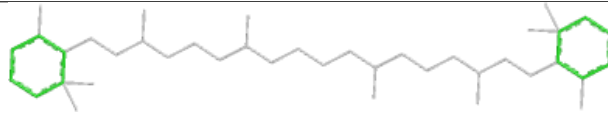


Ligand CLA B 713



Ligand SQD b 720



Ligand CLA b 714	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR T 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.41	0 100 100	12, 31, 56, 88	64 (19%)
1	a	334/344 (97%)	-0.32	3 (0%) 81 83	14, 33, 63, 91	64 (19%)
2	B	505/510 (99%)	-0.41	2 (0%) 88 90	18, 36, 67, 100	4 (0%)
2	b	505/510 (99%)	-0.29	5 (0%) 79 81	26, 40, 79, 117	0
3	C	442/461 (95%)	-0.34	0 100 100	15, 40, 57, 90	11 (2%)
3	c	451/461 (97%)	-0.24	2 (0%) 88 90	15, 43, 69, 101	12 (2%)
4	D	341/352 (96%)	-0.53	0 100 100	16, 34, 52, 88	2 (0%)
4	d	341/352 (96%)	-0.37	2 (0%) 85 87	16, 37, 65, 83	3 (0%)
5	E	82/84 (97%)	0.27	1 (1%) 76 78	35, 57, 76, 88	1 (1%)
5	e	82/84 (97%)	0.27	1 (1%) 76 78	41, 64, 85, 87	0
6	F	34/45 (75%)	-0.08	0 100 100	42, 49, 73, 90	0
6	f	34/45 (75%)	0.19	2 (5%) 28 30	44, 54, 86, 99	0
7	H	65/66 (98%)	-0.18	3 (4%) 37 39	36, 45, 64, 75	0
7	h	63/66 (95%)	0.09	2 (3%) 50 53	43, 55, 68, 81	0
8	I	35/38 (92%)	-0.35	0 100 100	35, 42, 77, 88	0
8	i	35/38 (92%)	-0.17	0 100 100	34, 45, 78, 85	0
9	J	36/40 (90%)	-0.11	0 100 100	35, 54, 83, 100	0
9	j	36/40 (90%)	0.20	1 (2%) 55 57	44, 56, 89, 104	0
10	K	37/46 (80%)	0.09	0 100 100	48, 58, 79, 87	0
10	k	37/46 (80%)	0.21	0 100 100	53, 61, 76, 86	0
11	L	37/37 (100%)	-0.54	0 100 100	28, 35, 70, 75	0
11	l	36/37 (97%)	-0.56	0 100 100	25, 34, 80, 95	0
12	M	32/36 (88%)	-0.47	0 100 100	28, 38, 61, 76	0
12	m	31/36 (86%)	-0.51	0 100 100	27, 38, 54, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.19	3 (1%) 76 78	26, 45, 85, 139	1 (0%)
13	o	244/272 (89%)	-0.23	1 (0%) 88 90	27, 44, 86, 128	0
14	R	34/41 (82%)	1.10	3 (8%) 15 16	68, 86, 101, 114	0
14	r	31/41 (75%)	1.45	5 (16%) 4 5	85, 108, 125, 139	0
15	T	29/32 (90%)	-0.56	0 100 100	29, 34, 69, 80	0
15	t	29/32 (90%)	-0.40	1 (3%) 48 50	29, 36, 85, 92	0
16	U	97/134 (72%)	-0.17	0 100 100	33, 48, 76, 94	0
16	u	97/134 (72%)	-0.24	0 100 100	33, 44, 63, 82	0
17	V	137/163 (84%)	-0.34	0 100 100	32, 43, 59, 85	0
17	v	137/163 (84%)	-0.15	0 100 100	31, 51, 75, 89	0
18	X	38/41 (92%)	-0.02	1 (2%) 57 60	46, 57, 82, 88	0
18	x	39/41 (95%)	0.23	3 (7%) 19 21	54, 66, 96, 113	0
19	Y	27/46 (58%)	0.95	3 (11%) 10 10	58, 82, 96, 105	0
19	y	30/46 (65%)	0.64	0 100 100	66, 79, 94, 105	0
20	Z	62/62 (100%)	0.70	2 (3%) 50 53	58, 73, 117, 131	0
20	z	62/62 (100%)	0.70	4 (6%) 25 26	58, 77, 117, 129	0
All	All	5302/5700 (93%)	-0.23	50 (0%) 81 83	12, 42, 81, 139	162 (3%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	R	35	LEU	4.2
13	o	58	ASN	3.9
14	r	32	GLN	3.8
13	O	60	ARG	3.7
15	t	30	THR	3.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.93	0.09	39,52,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	FME	t	1	10/11	0.94	0.08	29,46,71,71	0
15	FME	T	1	10/11	0.95	0.08	27,47,63,64	0
12	FME	M	1	10/11	0.95	0.08	41,50,66,80	0
8	FME	i	1	10/11	0.96	0.09	38,48,60,62	0
12	FME	m	1	10/11	0.96	0.07	34,48,69,82	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
28	STE	b	726	10/20	0.75	0.16	43,56,67,75	0
28	STE	I	101	15/20	0.77	0.17	40,55,81,86	0
28	STE	H	104	18/20	0.77	0.17	43,76,86,92	0
28	STE	b	725	20/20	0.81	0.14	45,63,80,83	0
33	LMG	c	522	48/55	0.81	0.14	35,77,108,113	0
28	STE	a	416	10/20	0.82	0.14	30,64,69,73	0
28	STE	B	726	16/20	0.82	0.14	43,64,79,86	0
25	PL9	A	408	55/55	0.82	0.16	44,70,86,96	0
28	STE	b	727	20/20	0.82	0.14	43,67,93,95	0
28	STE	c	501	12/20	0.82	0.11	55,68,85,93	0
33	LMG	b	723	55/55	0.82	0.15	45,73,94,109	0
27	LHG	A	410	49/49	0.82	0.13	45,80,104,115	0
28	STE	A	414	5/20	0.83	0.22	41,57,71,71	0
27	LHG	a	414	42/49	0.83	0.14	45,87,109,127	0
28	STE	E	101	12/20	0.83	0.16	56,79,85,90	0
28	STE	h	703	14/20	0.84	0.16	43,66,89,90	0
28	STE	a	417	12/20	0.84	0.12	51,64,76,77	0
28	STE	a	418	15/20	0.84	0.16	36,61,76,79	0
28	STE	C	522	16/20	0.85	0.12	38,53,66,67	0
25	PL9	a	411	55/55	0.85	0.15	42,69,93,98	0
28	STE	E	102	7/20	0.85	0.15	49,62,76,76	0
28	STE	A	411	16/20	0.85	0.14	34,47,74,75	0
28	STE	x	101	20/20	0.85	0.12	45,62,75,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	DGD	A	413	66/66	0.85	0.11	42,64,79,94	0
33	LMG	a	419	55/55	0.85	0.14	35,62,103,143	0
28	STE	b	724	16/20	0.85	0.14	52,66,82,85	0
28	STE	H	105	8/20	0.85	0.15	47,58,69,69	0
28	STE	C	523	12/20	0.86	0.13	33,46,58,69	0
26	SQD	A	412	39/54	0.86	0.13	38,64,94,99	0
28	STE	c	521	20/20	0.86	0.11	39,57,79,84	0
26	SQD	a	415	36/54	0.86	0.12	25,59,84,92	0
33	LMG	c	520	37/55	0.86	0.12	44,70,84,92	0
28	STE	m	101	12/20	0.86	0.12	42,57,70,79	0
28	STE	J	101	12/20	0.87	0.12	48,67,71,71	0
28	STE	B	720	17/20	0.87	0.11	30,50,62,73	0
33	LMG	D	412	32/55	0.87	0.12	37,57,80,84	0
22	CLA	b	701	65/65	0.87	0.11	48,68,91,96	0
28	STE	C	521	12/20	0.87	0.10	34,52,63,66	0
26	SQD	f	101	41/54	0.87	0.13	55,88,106,108	0
26	SQD	B	723	54/54	0.87	0.10	37,60,94,106	0
33	LMG	C	520	48/55	0.88	0.12	43,70,88,94	0
28	STE	l	102	18/20	0.88	0.12	37,50,81,85	0
28	STE	B	724	12/20	0.88	0.10	40,51,66,66	0
28	STE	B	725	18/20	0.88	0.11	37,54,75,81	0
28	STE	j	101	12/20	0.88	0.11	41,57,67,69	0
33	LMG	C	516	48/55	0.88	0.10	38,59,78,100	0
28	STE	t	702	14/20	0.89	0.10	34,53,65,67	0
26	SQD	D	409	36/54	0.89	0.12	48,76,93,99	0
28	STE	B	701	12/20	0.89	0.13	46,61,86,87	0
28	STE	b	722	20/20	0.89	0.10	35,54,74,77	0
28	STE	d	409	17/20	0.89	0.11	42,55,64,68	0
26	SQD	b	720	49/54	0.90	0.09	37,59,91,109	0
22	CLA	C	514	65/65	0.90	0.10	40,65,98,108	0
33	LMG	b	721	51/55	0.90	0.10	34,52,76,93	0
33	LMG	B	721	28/55	0.90	0.11	33,50,62,68	0
23	BCR	c	515	40/40	0.90	0.10	45,61,76,80	0
23	BCR	h	701	40/40	0.90	0.11	37,56,75,86	0
28	STE	Z	101	8/20	0.91	0.14	39,57,68,68	0
23	BCR	d	403	40/40	0.91	0.10	36,54,93,108	0
33	LMG	M	101	51/55	0.91	0.09	30,48,73,79	0
23	BCR	K	101	40/40	0.91	0.11	42,57,71,79	0
26	SQD	a	413	54/54	0.91	0.10	41,64,90,97	0
23	BCR	k	101	40/40	0.91	0.10	36,63,79,87	0
28	STE	T	702	15/20	0.91	0.11	39,54,81,81	0
28	STE	X	101	20/20	0.91	0.10	33,49,69,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	c	523	49/55	0.91	0.10	34,57,82,100	0
22	CLA	c	513	65/65	0.92	0.10	40,59,95,110	0
23	BCR	Y	101	40/40	0.92	0.09	40,54,75,77	0
29	DGD	h	702	62/66	0.92	0.09	32,48,61,73	0
23	BCR	H	101	40/40	0.92	0.09	34,48,61,78	0
28	STE	M	102	15/20	0.92	0.10	34,51,65,75	0
28	STE	M	103	10/20	0.92	0.09	34,47,51,58	0
23	BCR	k	102	40/40	0.92	0.10	40,54,68,71	0
22	CLA	c	514	65/65	0.93	0.10	43,71,109,112	0
33	LMG	D	408	51/55	0.93	0.10	34,55,84,90	0
23	BCR	B	718	40/40	0.93	0.07	22,39,53,54	0
23	BCR	B	719	40/40	0.93	0.07	22,42,58,64	0
29	DGD	C	518	62/66	0.93	0.09	35,52,99,119	0
29	DGD	H	103	62/66	0.93	0.08	28,46,60,64	0
29	DGD	c	518	62/66	0.93	0.09	32,53,87,94	0
23	BCR	C	501	40/40	0.93	0.10	38,56,70,74	0
23	BCR	D	404	40/40	0.93	0.09	26,42,91,98	0
22	CLA	H	102	65/65	0.93	0.09	30,60,95,107	0
22	CLA	C	511	65/65	0.94	0.08	32,48,65,80	0
27	LHG	d	407	39/49	0.94	0.08	33,49,68,71	0
22	CLA	C	513	65/65	0.94	0.10	35,56,93,98	0
32	BCT	a	410	4/4	0.94	0.09	30,32,44,53	0
26	SQD	A	409	52/54	0.94	0.09	27,61,89,95	0
23	BCR	b	717	40/40	0.94	0.07	27,41,52,56	0
23	BCR	b	719	40/40	0.94	0.07	33,48,65,76	0
22	CLA	c	509	64/65	0.94	0.09	31,47,87,108	0
23	BCR	c	516	40/40	0.94	0.09	30,43,58,70	0
22	CLA	c	510	65/65	0.94	0.09	33,48,63,69	0
23	BCR	C	515	40/40	0.94	0.07	25,39,51,59	0
22	CLA	c	512	65/65	0.94	0.09	38,55,71,74	0
22	CLA	C	504	65/65	0.94	0.07	30,45,56,58	0
27	LHG	B	722	49/49	0.94	0.09	29,46,70,77	0
27	LHG	a	412	49/49	0.94	0.10	30,48,76,83	0
29	DGD	C	519	62/66	0.94	0.08	32,49,69,84	0
33	LMG	d	408	44/55	0.94	0.09	34,53,82,87	0
22	CLA	C	509	65/65	0.95	0.08	27,44,105,117	0
22	CLA	C	510	65/65	0.95	0.08	27,45,63,74	0
22	CLA	B	709	65/65	0.95	0.07	23,38,52,56	0
23	BCR	t	701	40/40	0.95	0.06	22,38,54,56	0
22	CLA	d	402	65/65	0.95	0.09	28,49,81,95	0
25	PL9	D	405	55/55	0.95	0.06	23,33,48,54	0
23	BCR	A	405	40/40	0.95	0.06	24,36,47,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PL9	d	404	55/55	0.95	0.06	21,34,43,47	0
29	DGD	C	517	62/66	0.95	0.09	23,42,75,85	0
23	BCR	B	717	40/40	0.95	0.07	24,41,58,62	0
22	CLA	b	702	65/65	0.95	0.08	28,42,63,66	0
22	CLA	b	706	65/65	0.95	0.08	23,39,75,80	0
22	CLA	b	709	65/65	0.95	0.07	27,47,68,80	0
29	DGD	c	519	62/66	0.95	0.08	28,55,83,95	0
22	CLA	b	714	65/65	0.95	0.07	22,40,73,86	0
22	CLA	b	715	65/65	0.95	0.08	27,42,60,65	0
22	CLA	b	716	60/65	0.95	0.09	29,46,92,95	0
22	CLA	c	503	65/65	0.95	0.07	27,45,68,75	0
23	BCR	T	701	40/40	0.95	0.07	28,41,57,60	0
22	CLA	c	504	65/65	0.95	0.07	23,44,56,64	0
27	LHG	D	411	47/49	0.95	0.09	24,49,85,96	0
23	BCR	a	407	40/40	0.95	0.06	23,34,50,54	0
22	CLA	c	507	65/65	0.95	0.09	30,48,97,104	0
23	BCR	b	718	40/40	0.95	0.06	27,39,52,55	0
27	LHG	l	101	49/49	0.95	0.07	31,44,53,61	0
22	CLA	c	508	65/65	0.95	0.07	26,43,60,64	0
22	CLA	C	512	65/65	0.95	0.08	30,52,67,74	0
22	CLA	C	507	65/65	0.95	0.09	26,44,83,94	0
22	CLA	c	511	65/65	0.95	0.07	34,49,63,75	0
34	PHO	a	405	64/64	0.95	0.06	18,32,41,46	0
34	PHO	d	405	64/64	0.95	0.06	28,39,48,63	0
27	LHG	L	101	49/49	0.96	0.07	31,41,55,65	0
22	CLA	b	705	65/65	0.96	0.06	19,35,49,61	0
22	CLA	B	715	65/65	0.96	0.07	24,36,67,75	0
27	LHG	d	406	49/49	0.96	0.07	26,45,56,62	0
22	CLA	b	707	65/65	0.96	0.08	19,36,68,75	0
22	CLA	b	708	65/65	0.96	0.07	28,44,64,66	0
22	CLA	C	503	65/65	0.96	0.06	30,44,57,62	0
22	CLA	b	710	65/65	0.96	0.07	24,38,49,61	0
22	CLA	b	712	65/65	0.96	0.07	23,36,47,52	0
22	CLA	b	713	65/65	0.96	0.07	18,36,67,82	0
22	CLA	A	403	65/65	0.96	0.09	21,35,88,102	0
22	CLA	C	505	59/65	0.96	0.07	28,43,75,85	0
22	CLA	C	506	65/65	0.96	0.08	23,41,69,80	0
22	CLA	c	502	65/65	0.96	0.07	27,41,52,56	0
22	CLA	B	702	65/65	0.96	0.06	25,36,56,64	0
29	DGD	c	517	62/66	0.96	0.08	24,42,78,87	0
22	CLA	C	508	65/65	0.96	0.07	25,42,57,63	0
22	CLA	c	505	60/65	0.96	0.07	34,47,77,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	506	65/65	0.96	0.08	25,41,69,76	0
32	BCT	A	417	4/4	0.96	0.07	25,31,36,43	0
22	CLA	B	704	65/65	0.96	0.07	20,32,76,78	0
22	CLA	B	705	65/65	0.96	0.06	15,31,45,52	0
22	CLA	B	706	65/65	0.96	0.07	24,37,81,90	0
22	CLA	A	402	65/65	0.96	0.06	15,29,44,57	0
22	CLA	B	710	65/65	0.96	0.07	17,33,45,48	0
22	CLA	B	711	65/65	0.96	0.06	18,30,50,56	0
22	CLA	D	402	65/65	0.96	0.06	15,27,51,56	0
22	CLA	B	712	65/65	0.96	0.07	20,31,45,54	0
22	CLA	a	401	65/65	0.96	0.06	21,32,41,47	0
22	CLA	a	403	65/65	0.96	0.06	19,31,42,58	0
22	CLA	a	404	65/65	0.96	0.09	27,42,102,112	0
22	CLA	a	406	65/65	0.96	0.07	18,38,76,81	0
22	CLA	B	713	65/65	0.96	0.07	19,32,72,74	0
22	CLA	B	714	65/65	0.96	0.08	19,37,78,96	0
34	PHO	D	406	64/64	0.96	0.06	16,28,37,42	0
34	PHO	D	407	64/64	0.96	0.06	23,32,44,51	0
27	LHG	D	410	49/49	0.96	0.07	21,40,54,65	0
22	CLA	b	704	65/65	0.96	0.08	21,37,84,97	0
35	HEC	e	101	43/43	0.96	0.09	42,59,80,88	0
22	CLA	C	502	65/65	0.97	0.06	22,36,50,61	0
22	CLA	B	707	65/65	0.97	0.07	17,35,65,75	0
22	CLA	B	708	65/65	0.97	0.06	19,36,54,59	0
22	CLA	D	401	65/65	0.97	0.06	14,29,57,68	0
22	CLA	B	703	65/65	0.97	0.06	20,33,57,65	0
22	CLA	D	403	65/65	0.97	0.08	24,42,107,122	0
22	CLA	b	711	65/65	0.97	0.06	22,34,59,64	0
22	CLA	d	401	65/65	0.97	0.06	20,36,54,62	0
22	CLA	b	703	65/65	0.97	0.07	24,37,68,78	0
35	HEC	E	103	43/43	0.97	0.09	34,51,70,74	0
22	CLA	B	716	60/65	0.97	0.09	23,39,87,103	0
24	CL	A	406	1/1	0.98	0.04	29,29,29,29	0
22	CLA	A	404	54/65	0.98	0.05	17,31,61,68	0
35	HEC	V	201	43/43	0.98	0.06	17,33,43,50	0
30	OEX	A	415[A]	10/10	0.98	0.04	32,35,38,40	10
35	HEC	v	201	43/43	0.98	0.06	26,37,51,52	0
30	OEX	a	420[A]	10/10	0.99	0.03	29,35,39,39	10
31	OEY	A	416[B]	11/11	0.99	0.03	14,24,29,31	11
24	CL	a	408	1/1	0.99	0.04	28,28,28,28	0
24	CL	a	409	1/1	0.99	0.07	28,28,28,28	0
24	CL	A	407	1/1	0.99	0.06	27,27,27,27	0

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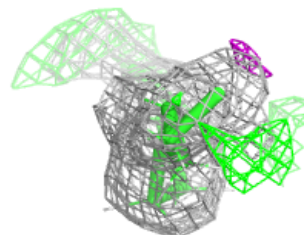
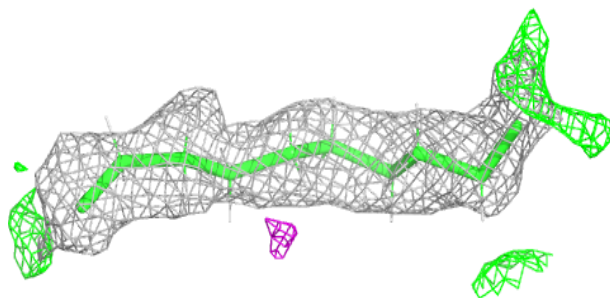
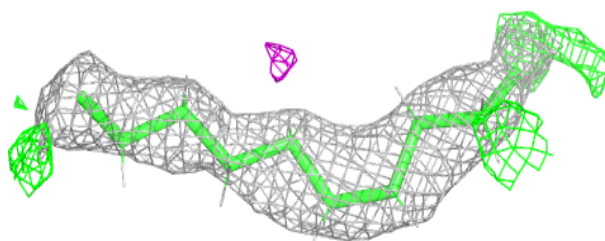
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	OEY	a	421[B]	11/11	1.00	0.02	19,25,29,33	11
21	FE2	A	401	1/1	1.00	0.01	29,29,29,29	0
21	FE2	a	402	1/1	1.00	0.02	33,33,33,33	0

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.

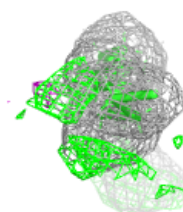
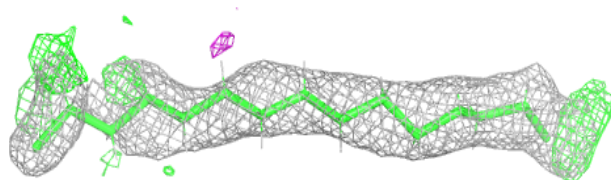
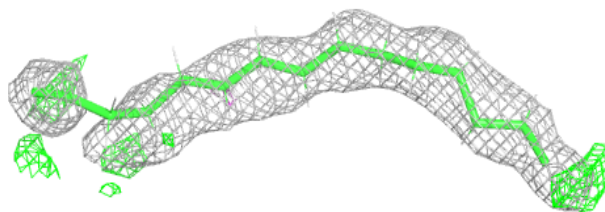
Electron density around STE b 726:

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

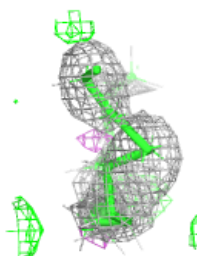
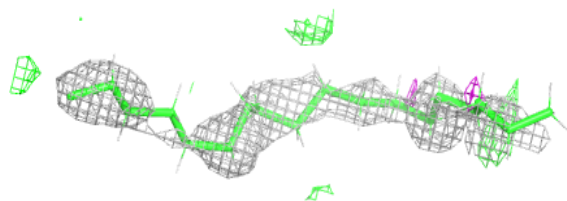
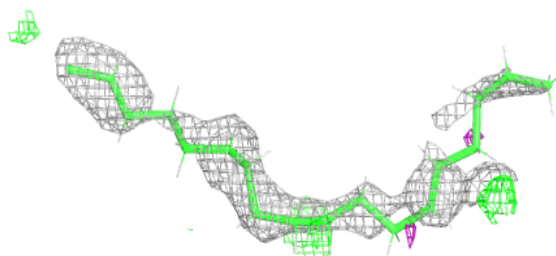


Electron density around STE I 101:

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

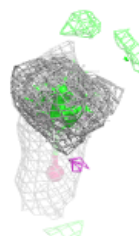
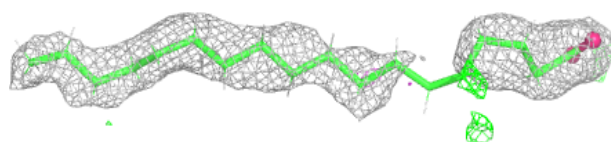
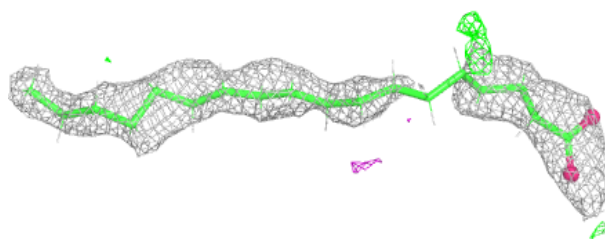
**Electron density around STE H 104:**

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

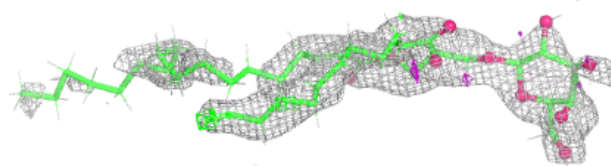
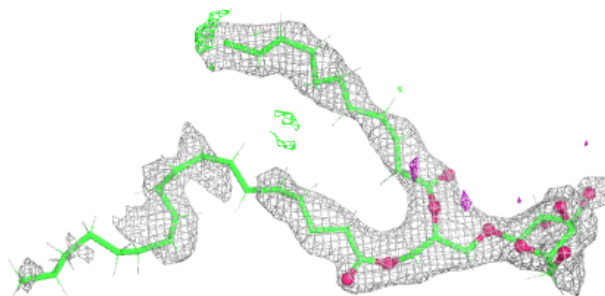


Electron density around STE b 725:

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

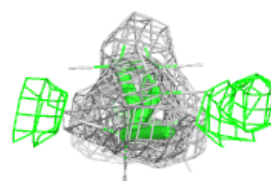
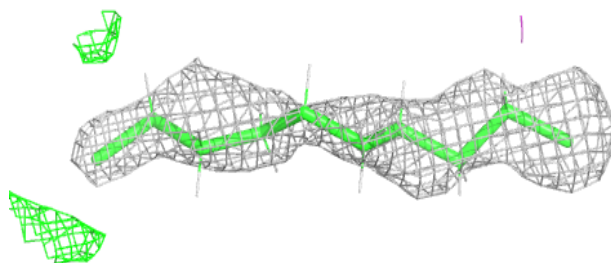
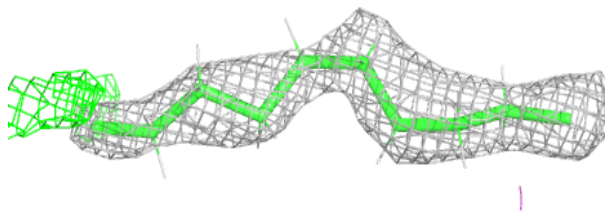
**Electron density around LMG c 522:**

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

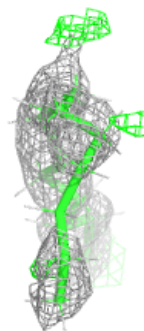
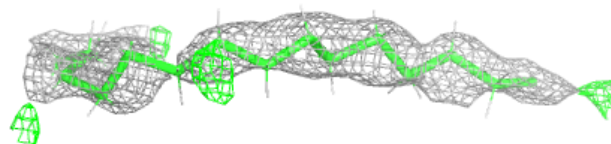
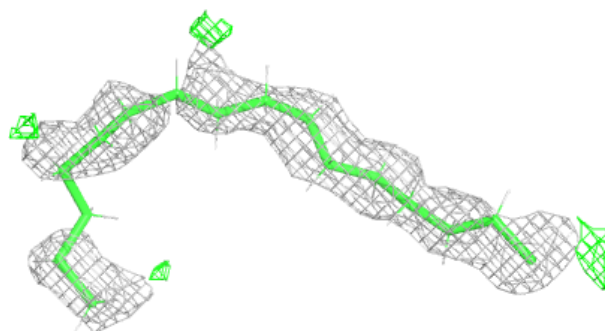


Electron density around STE a 416:

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

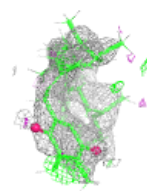
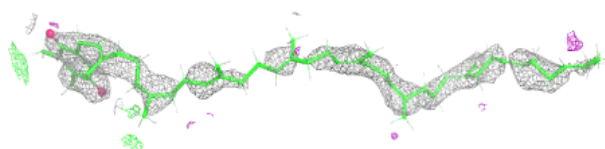
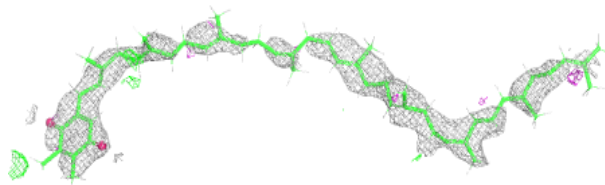
**Electron density around STE B 726:**

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

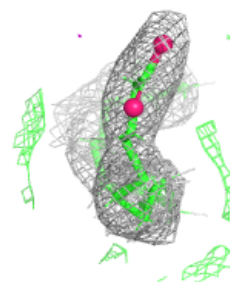
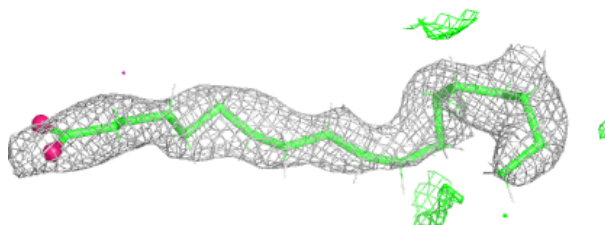
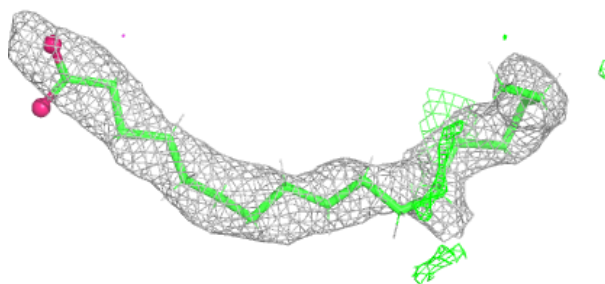


Electron density around PL9 A 408:

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

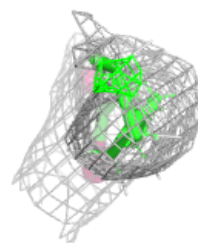
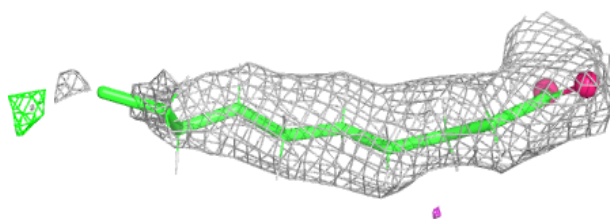
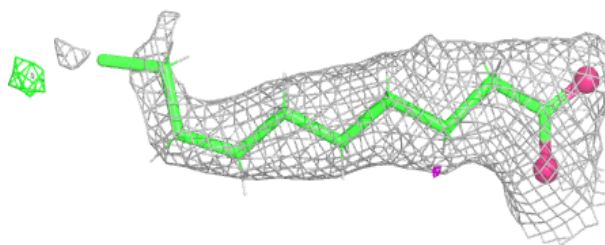
**Electron density around STE b 727:**

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

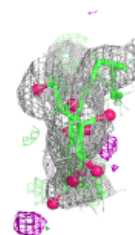
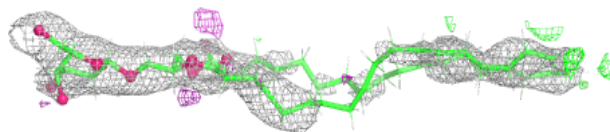
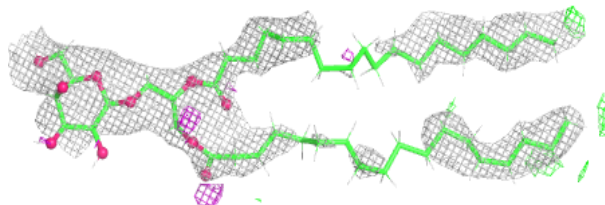


Electron density around STE c 501:

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

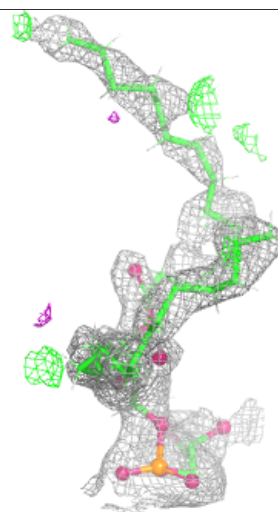
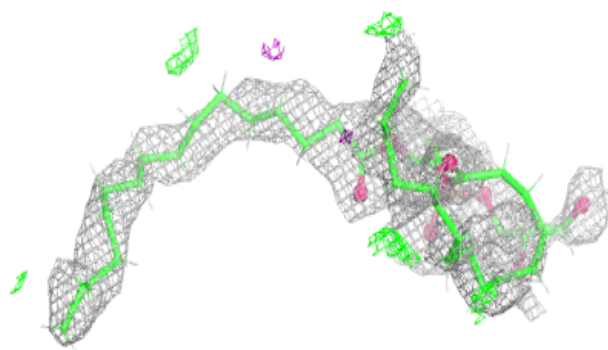
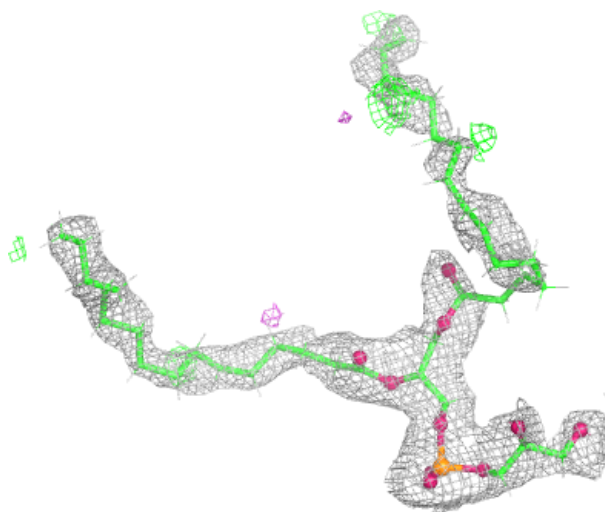
**Electron density around LMG b 723:**

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



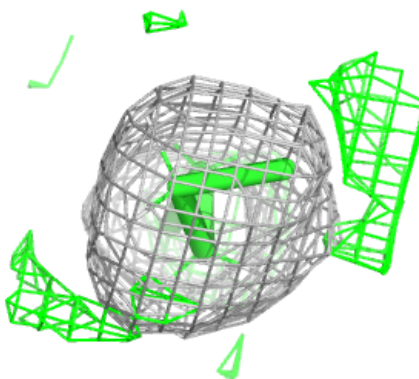
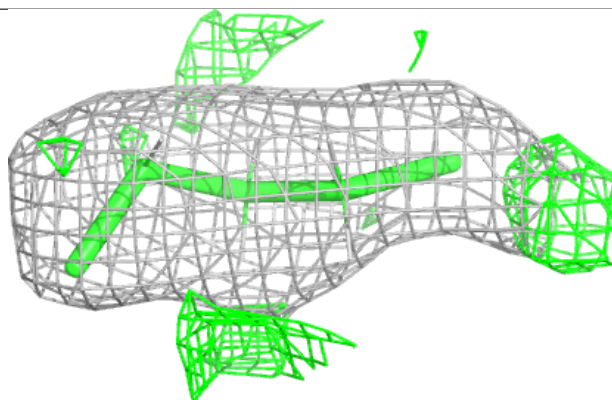
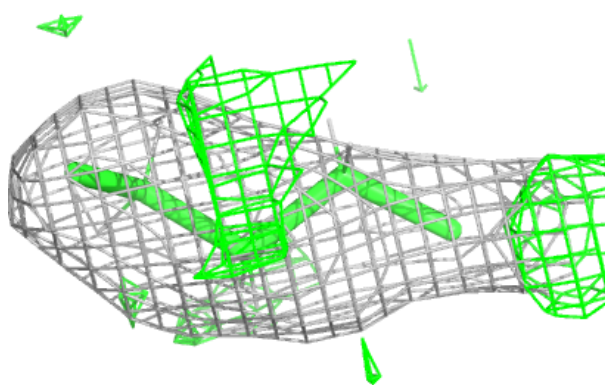
Electron density around LHG A 410:

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

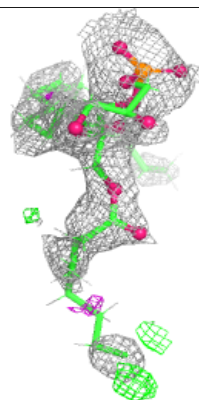
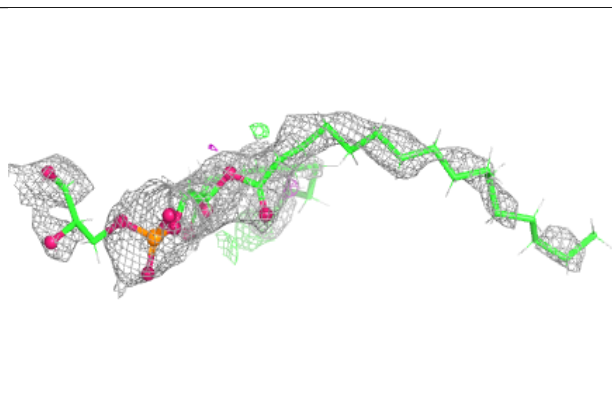
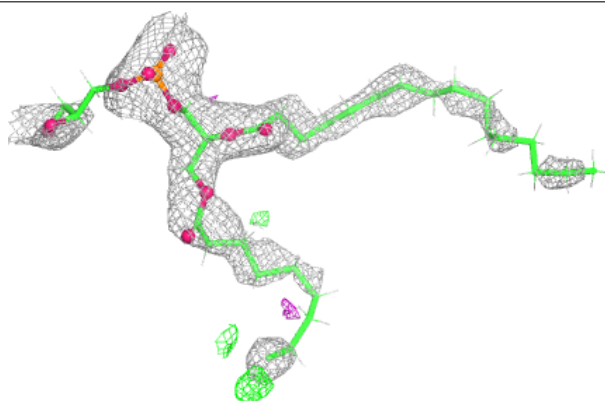


Electron density around STE A 414:

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

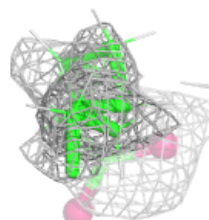
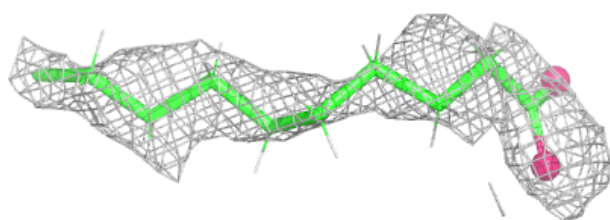
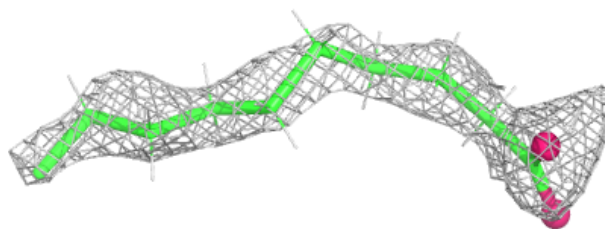
**Electron density around LHG a 414:**

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

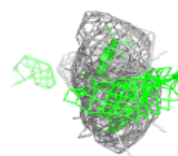
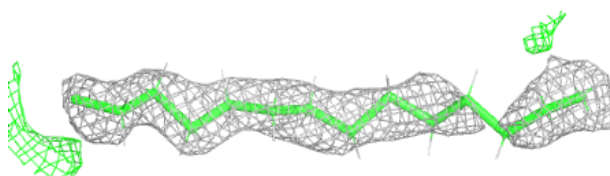
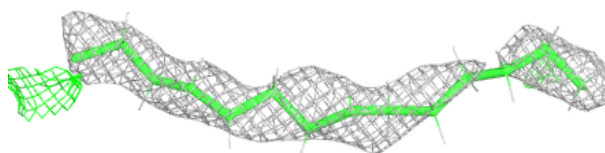


Electron density around STE E 101:

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

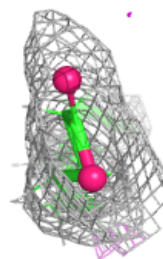
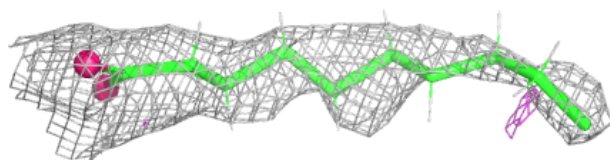
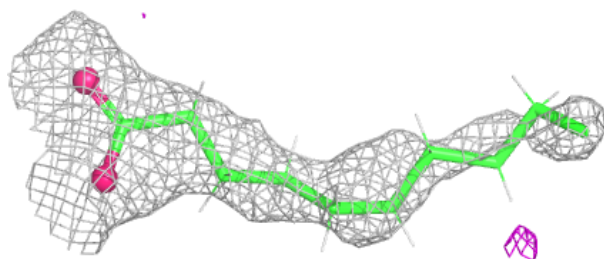
**Electron density around STE h 703:**

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

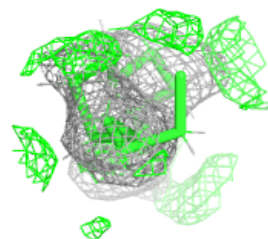
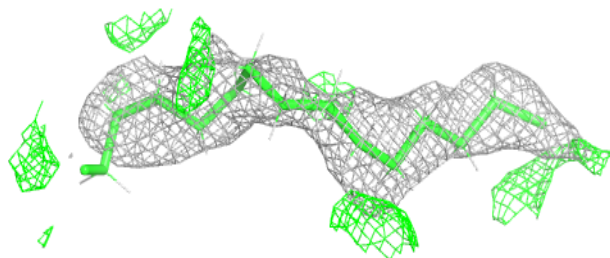
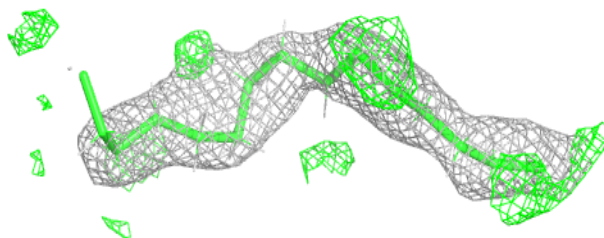


Electron density around STE a 417:

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

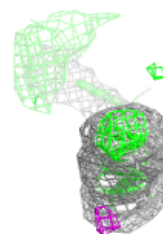
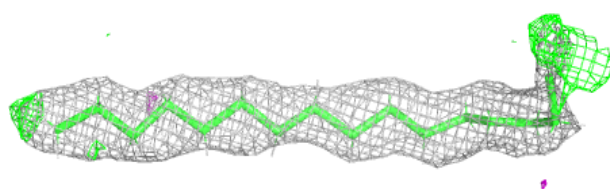
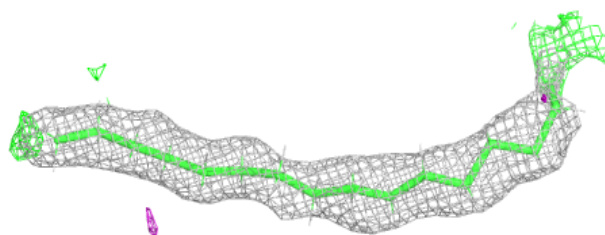
**Electron density around STE a 418:**

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

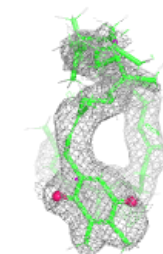
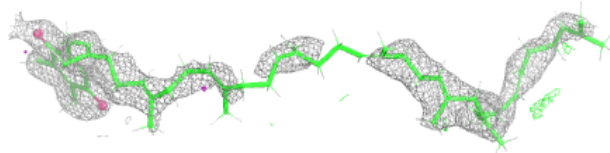
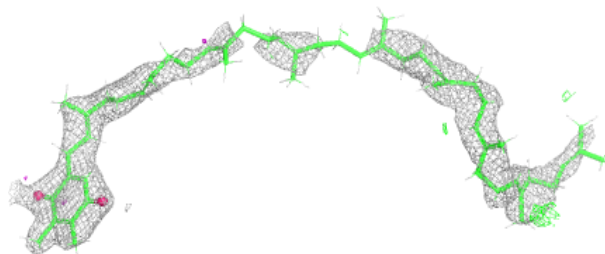


Electron density around STE C 522:

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

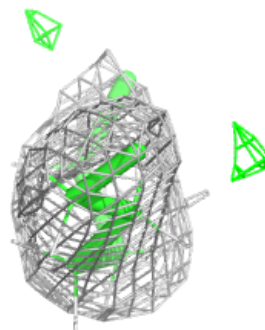
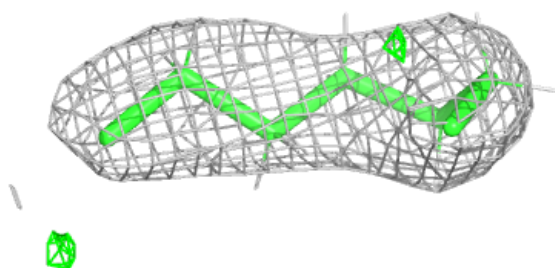
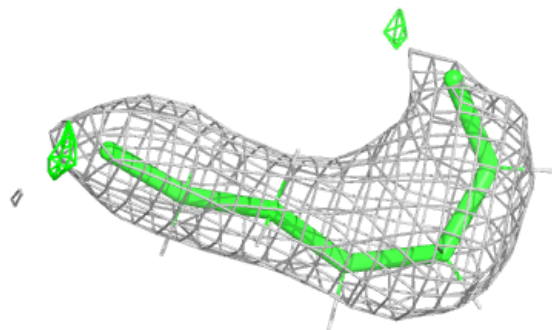
**Electron density around PL9 a 411:**

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

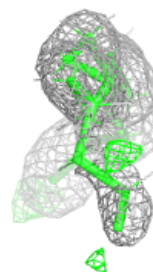
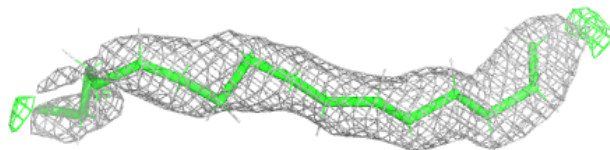
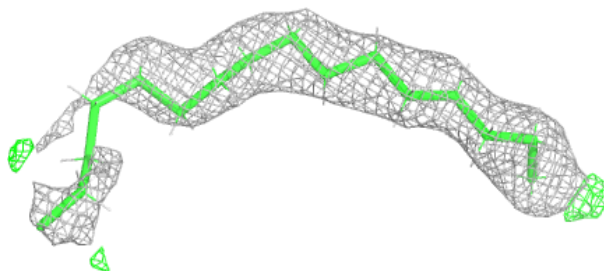


Electron density around STE E 102:

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

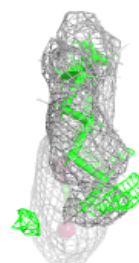
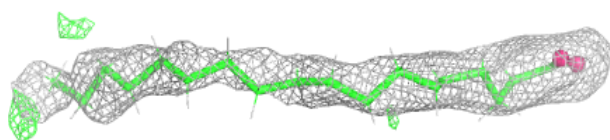
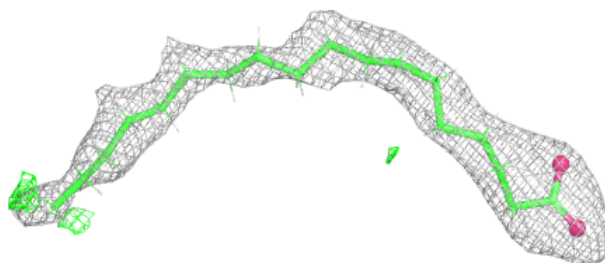
**Electron density around STE A 411:**

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

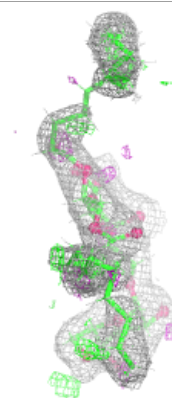
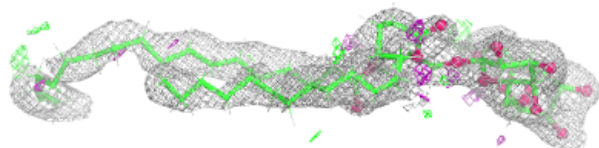
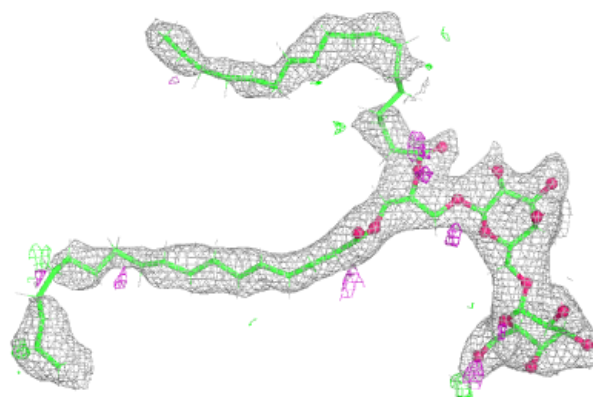


Electron density around STE x 101:

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

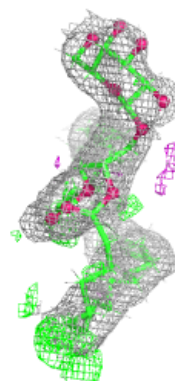
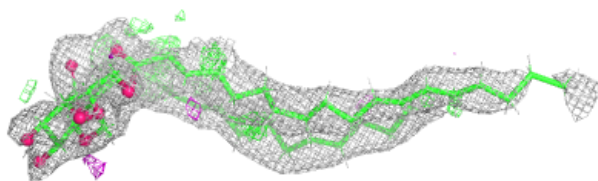
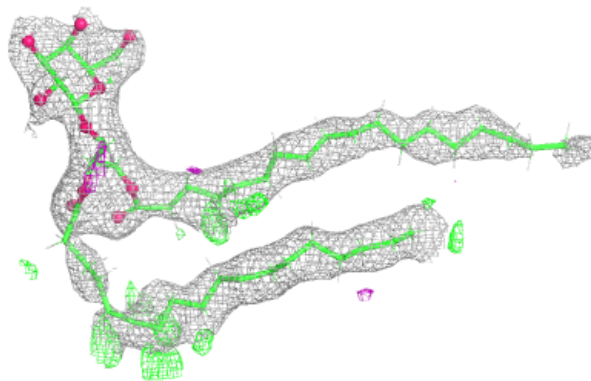
**Electron density around DGD A 413:**

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

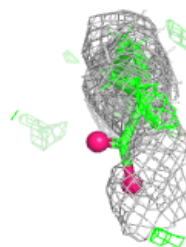
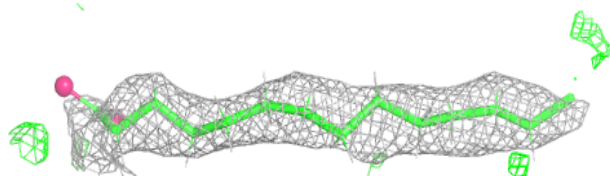
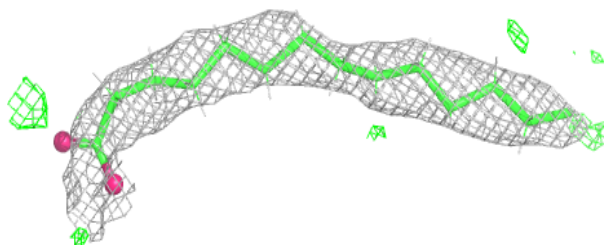


Electron density around LMG a 419:

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

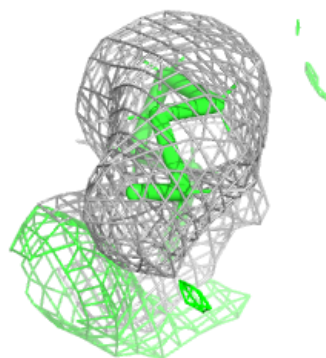
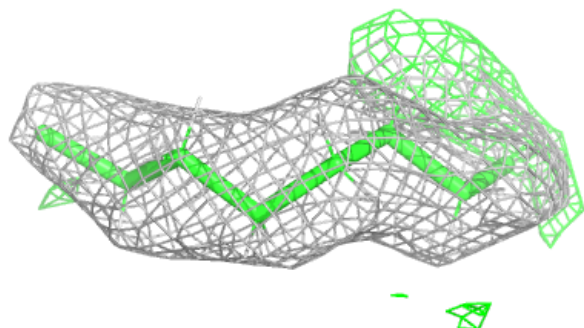
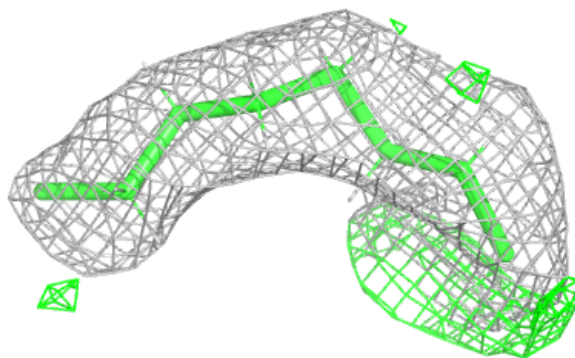
**Electron density around STE b 724:**

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

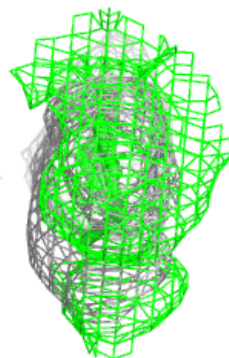
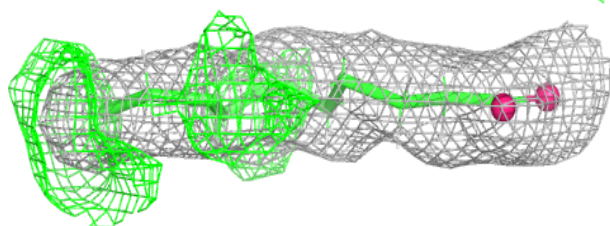
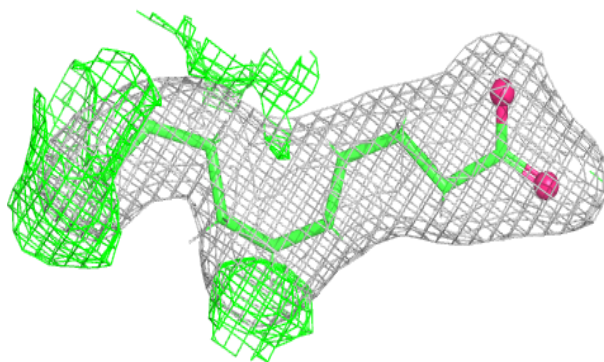


Electron density around STE H 105:

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

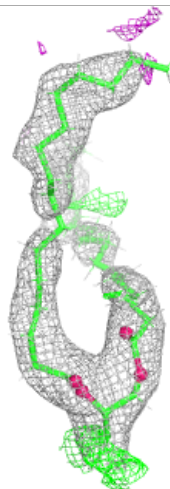
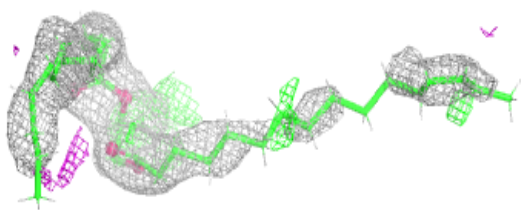
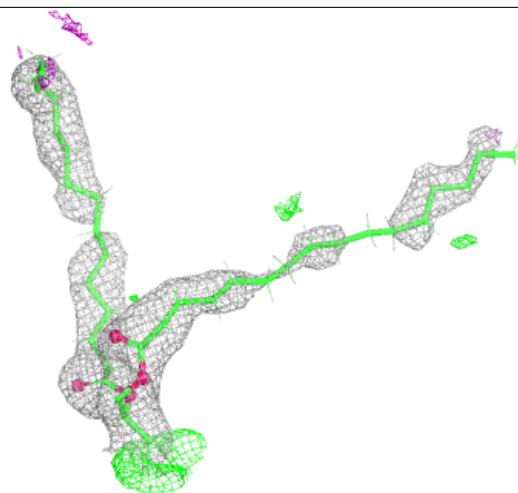
**Electron density around STE C 523:**

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



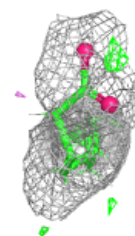
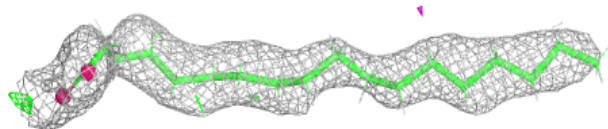
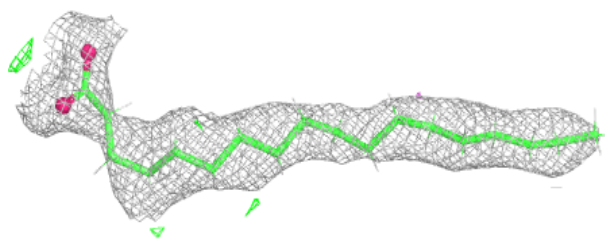
Electron density around SQD A 412:

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



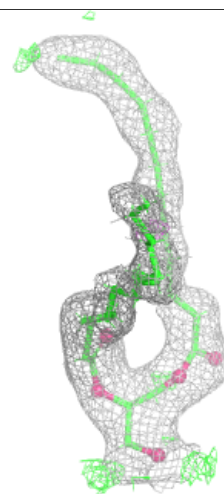
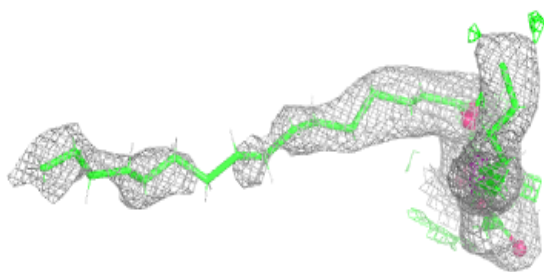
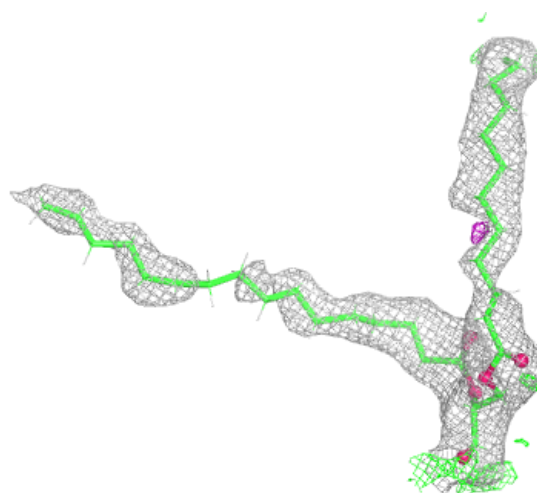
Electron density around STE c 521:

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



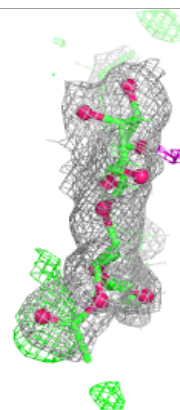
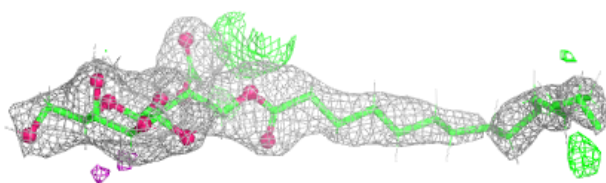
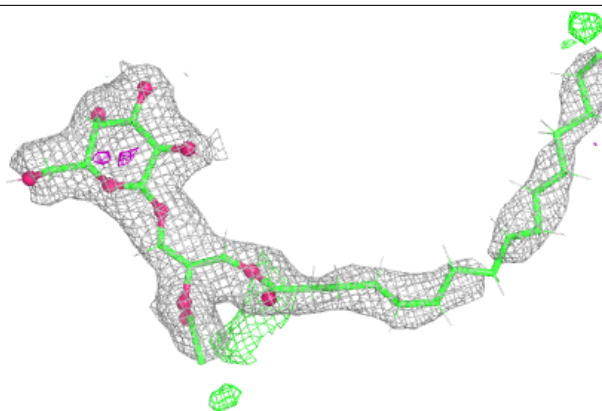
Electron density around SQD a 415:

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

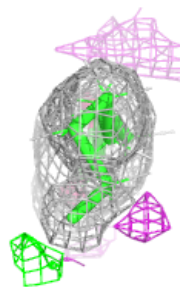
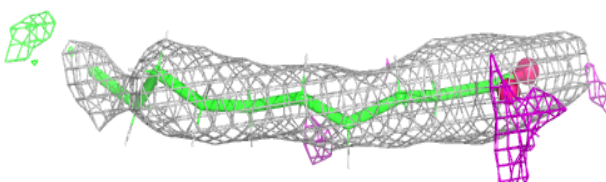
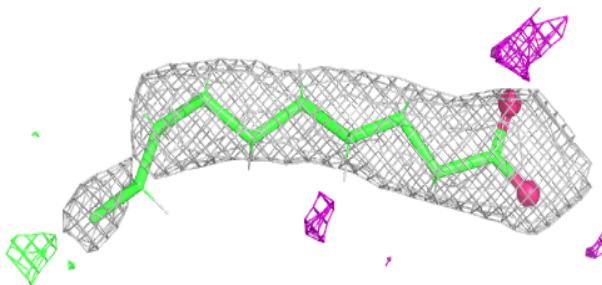


Electron density around LMG c 520:

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

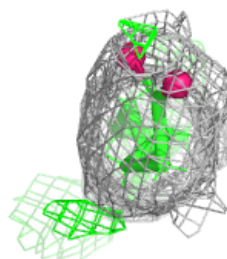
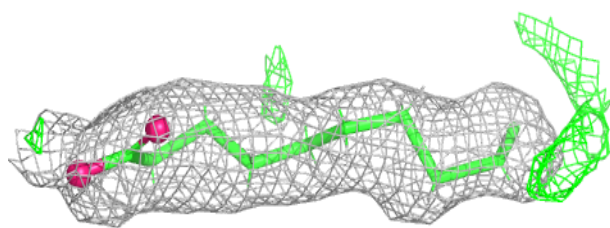
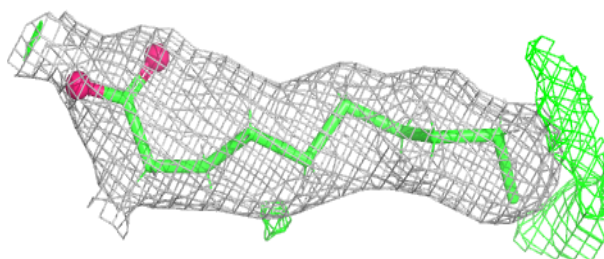
**Electron density around STE m 101:**

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

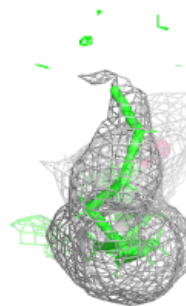
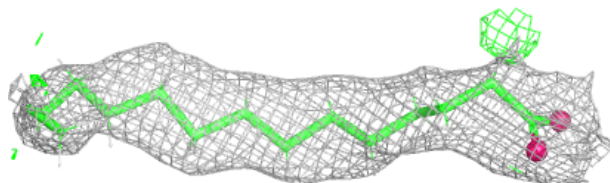
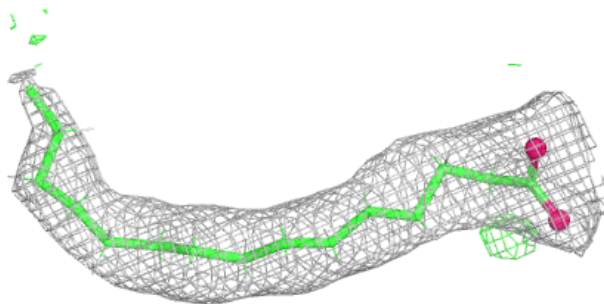


Electron density around STE J 101:

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

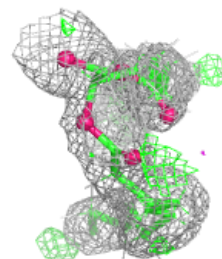
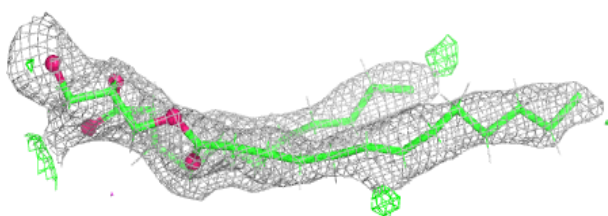
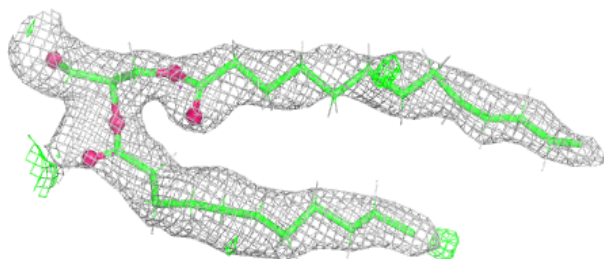
**Electron density around STE B 720:**

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

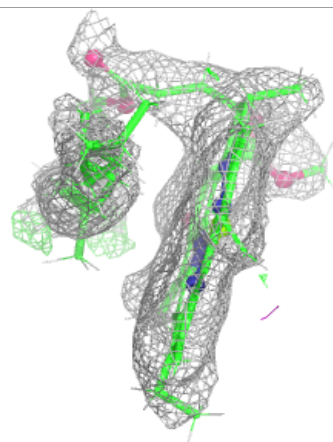
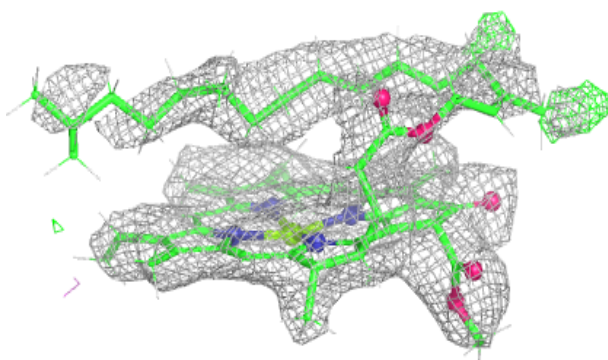
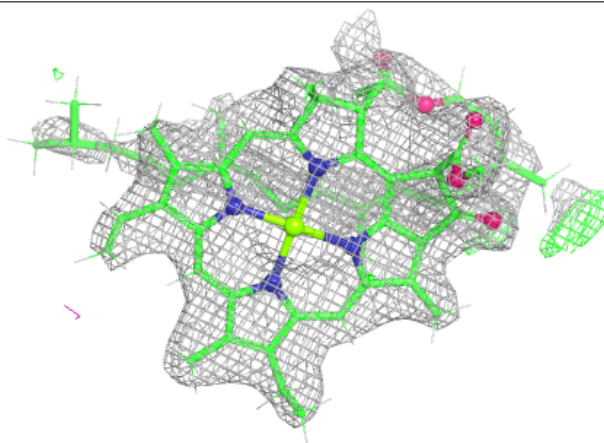


Electron density around LMG D 412:

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

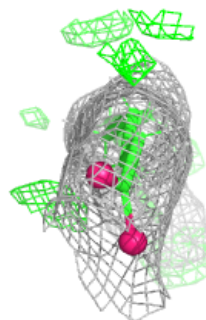
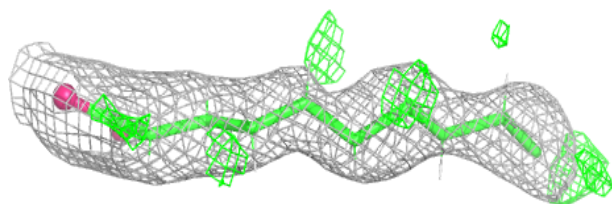
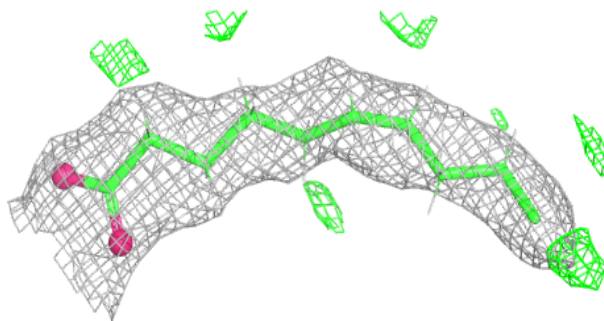
**Electron density around CLA b 701:**

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

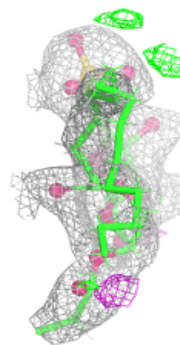
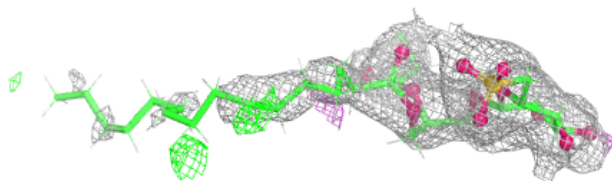
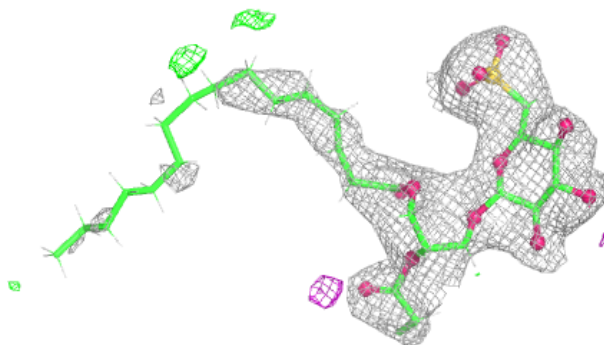


Electron density around STE C 521:

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

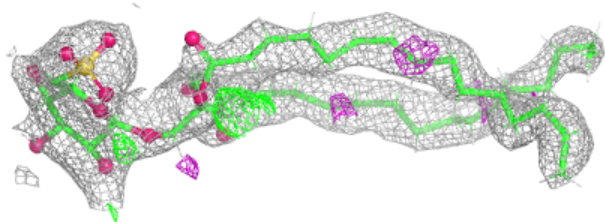
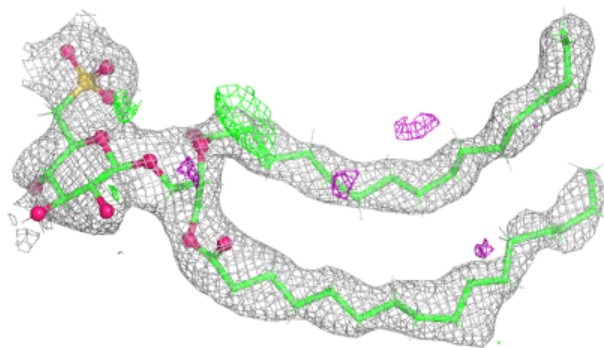
**Electron density around SQD f 101:**

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

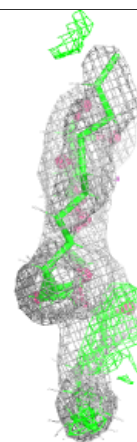
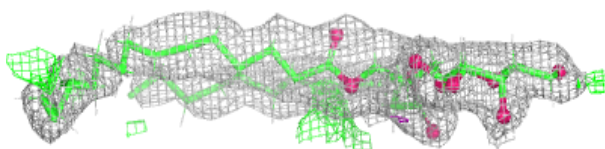
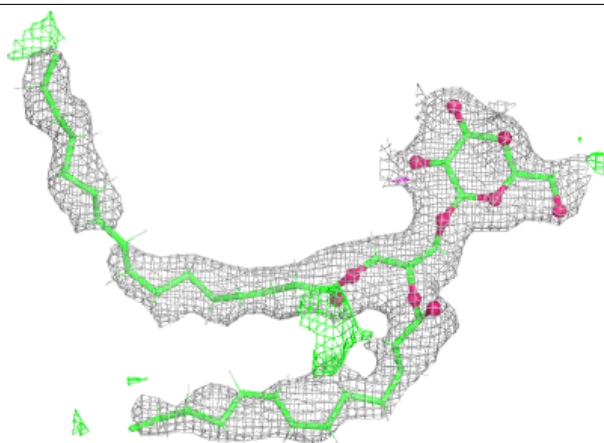


Electron density around SQD B 723:

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

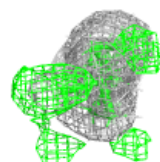
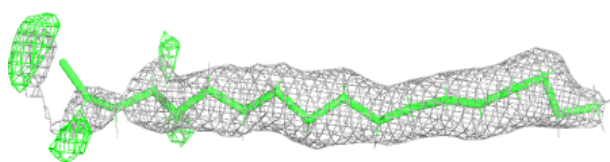
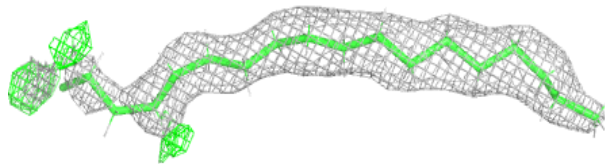
**Electron density around LMG C 520:**

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

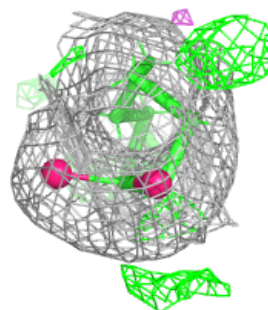
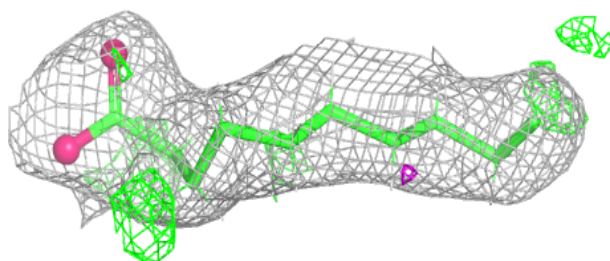
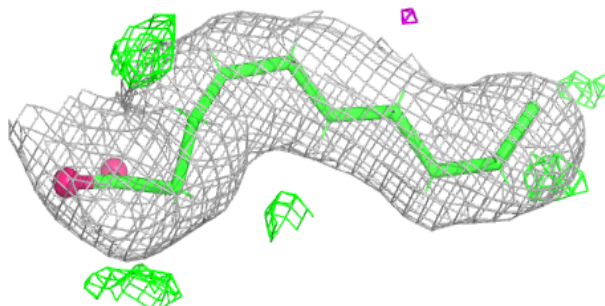


Electron density around STE I 102:

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

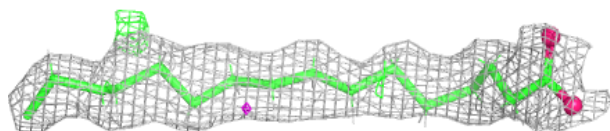
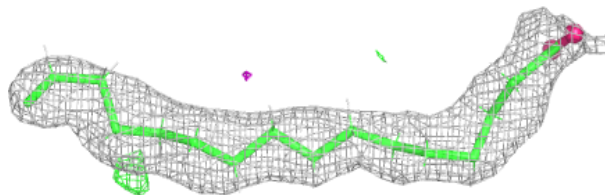
**Electron density around STE B 724:**

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

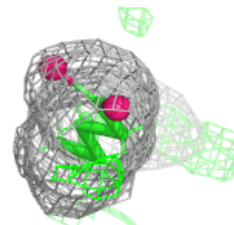
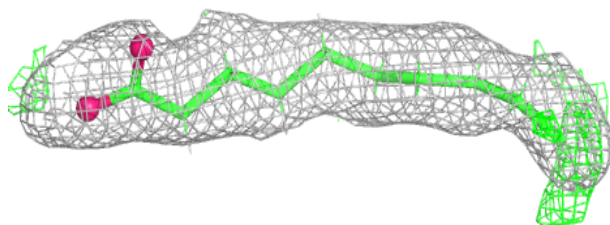
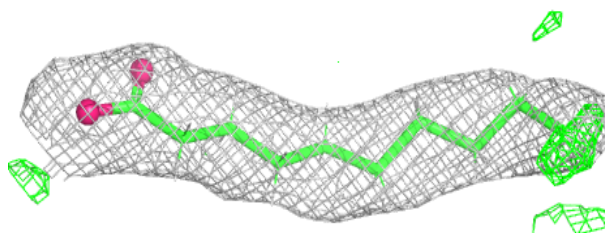


Electron density around STE B 725:

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

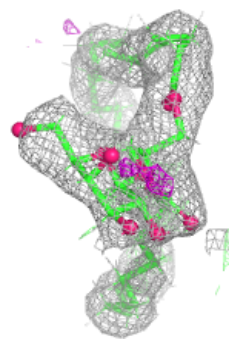
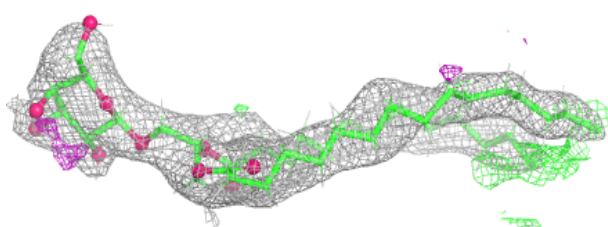
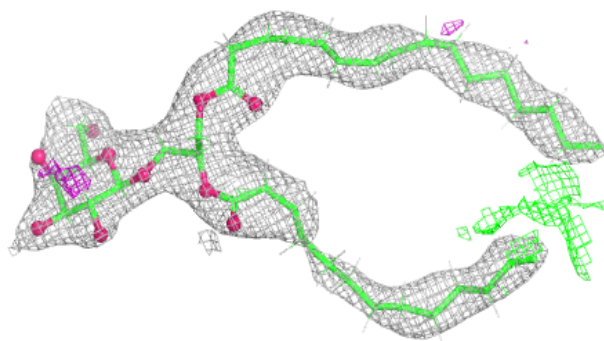
**Electron density around STE j 101:**

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

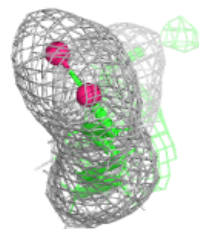
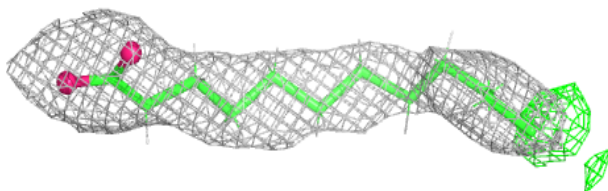
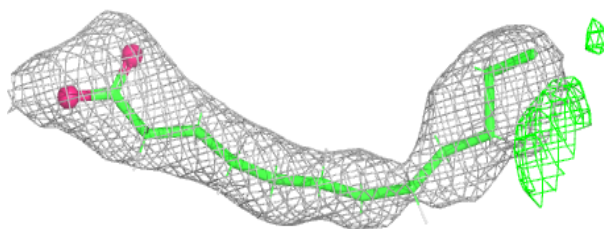


Electron density around LMG C 516:

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

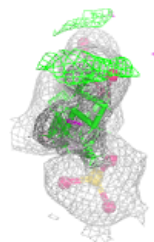
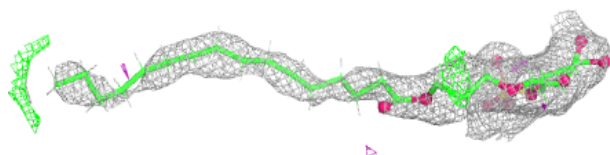
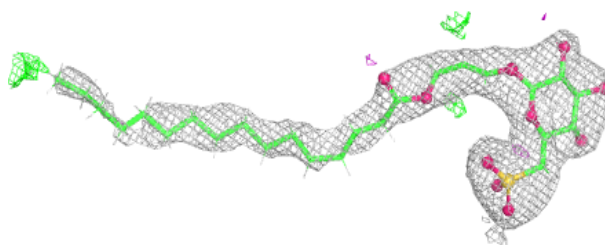
**Electron density around STE t 702:**

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

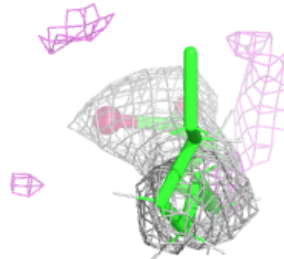
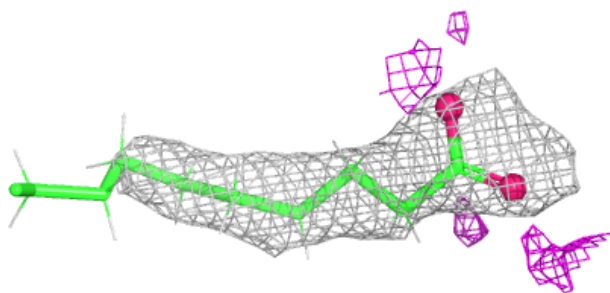
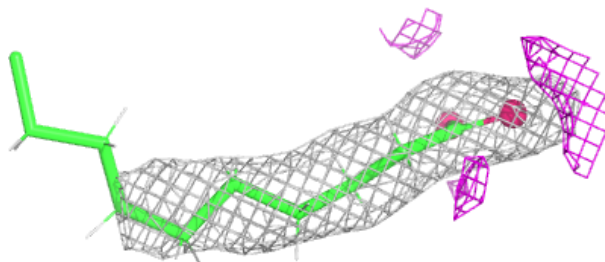


Electron density around SQD D 409:

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

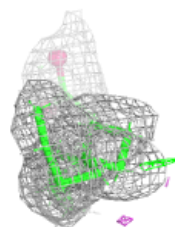
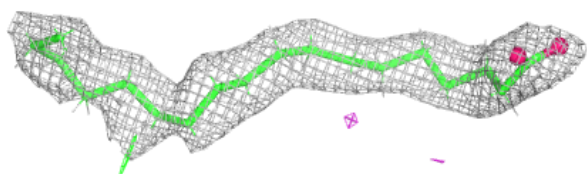
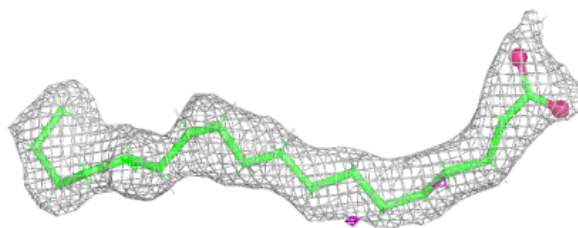
**Electron density around STE B 701:**

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

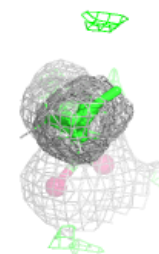
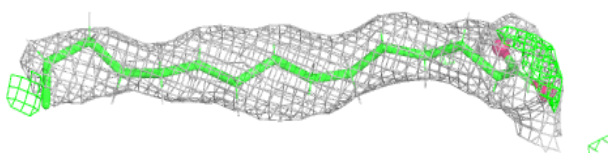
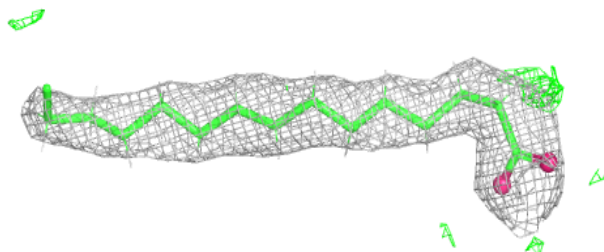


Electron density around STE b 722:

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

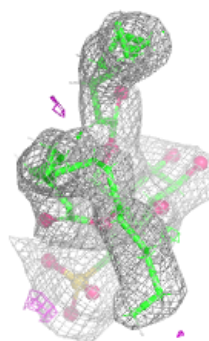
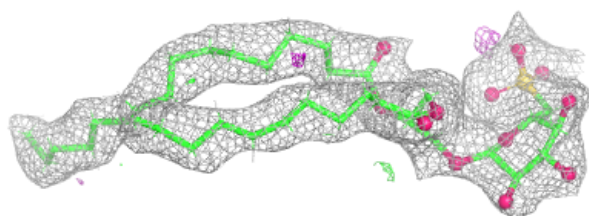
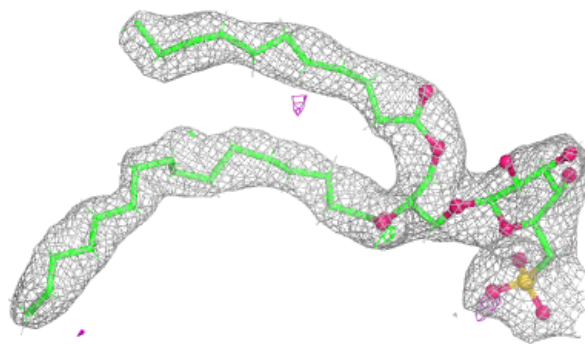
**Electron density around STE d 409:**

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

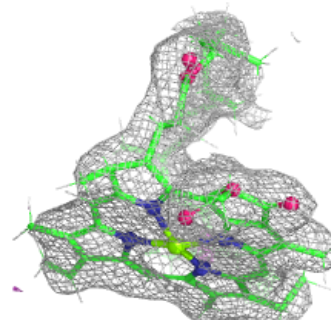
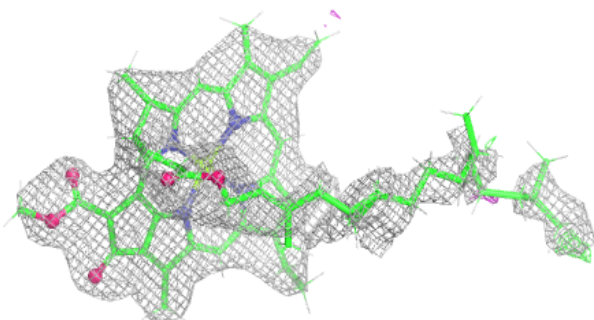
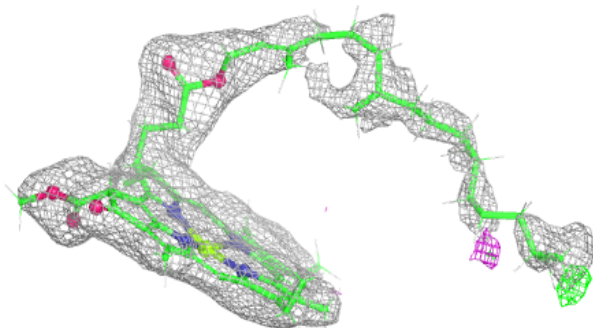


Electron density around SQD b 720:

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

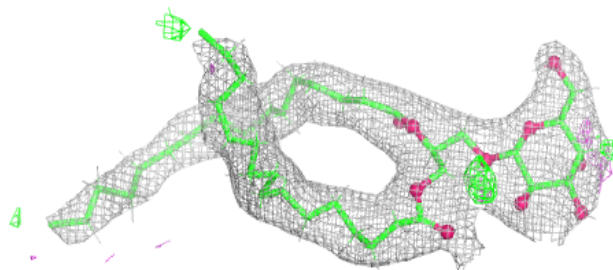
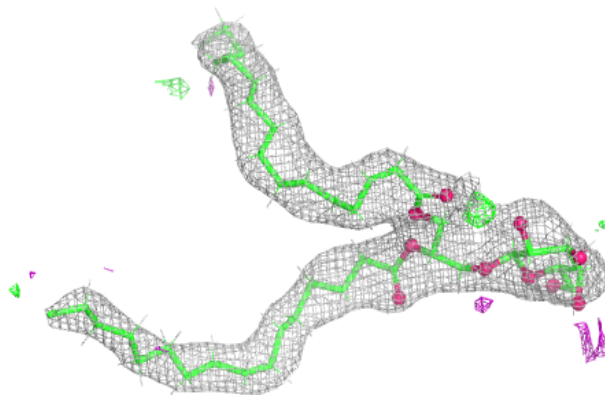
**Electron density around CLA C 514:**

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

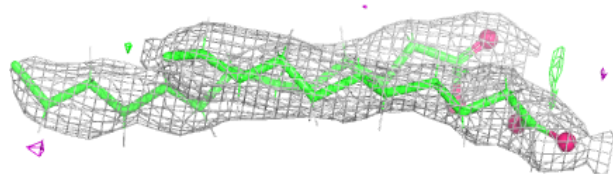
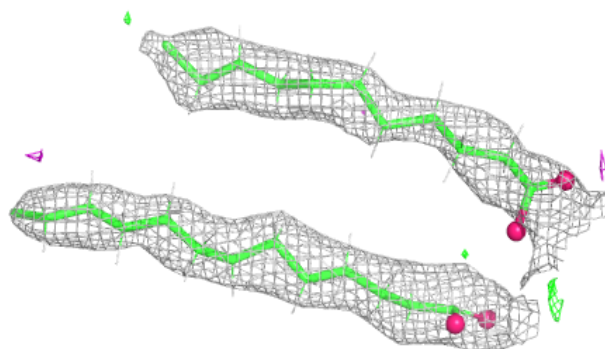


Electron density around LMG b 721:

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

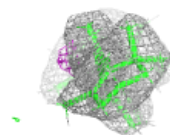
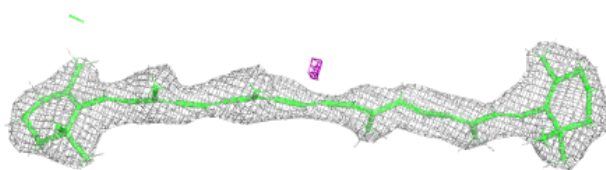
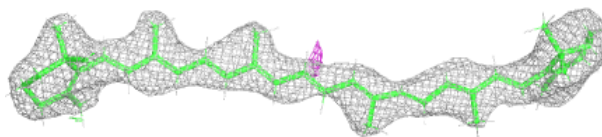
**Electron density around LMG B 721:**

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

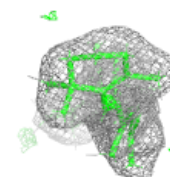
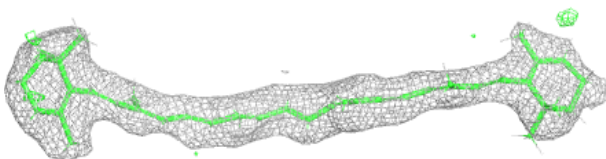
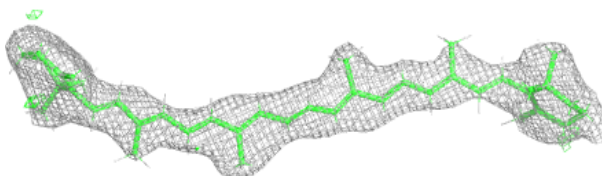


Electron density around BCR c 515:

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

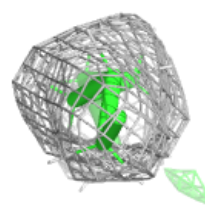
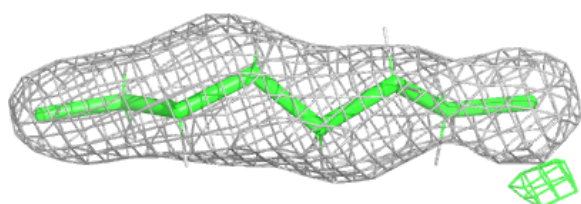
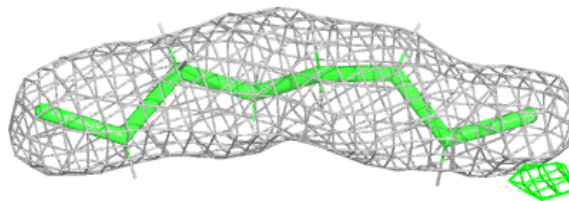
**Electron density around BCR h 701:**

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

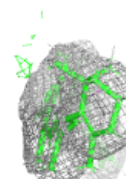
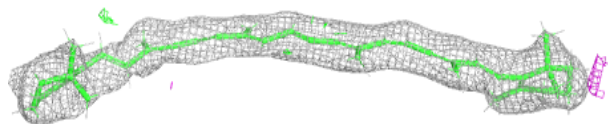


Electron density around STE Z 101:

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

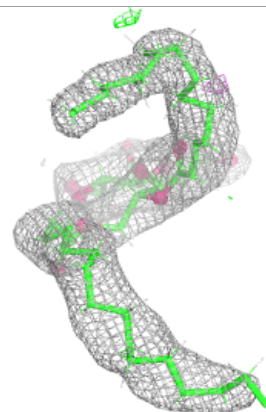
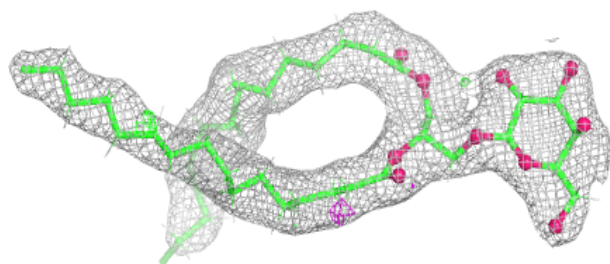
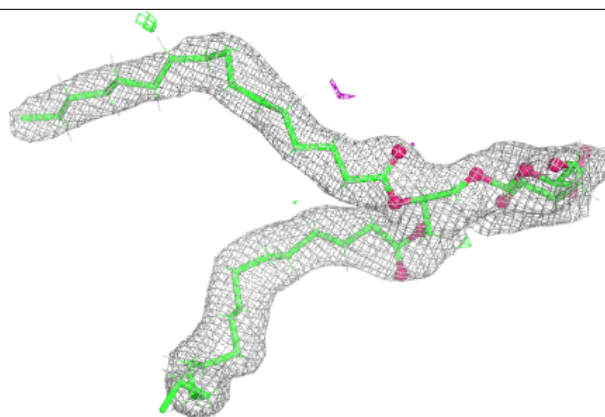
**Electron density around BCR d 403:**

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

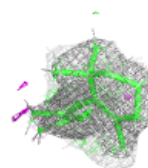
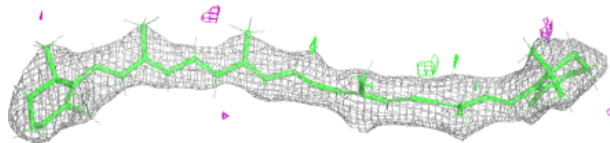
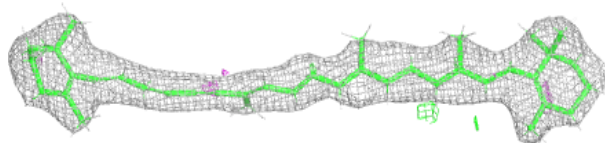


Electron density around LMG M 101:

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

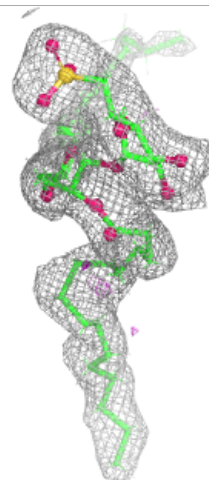
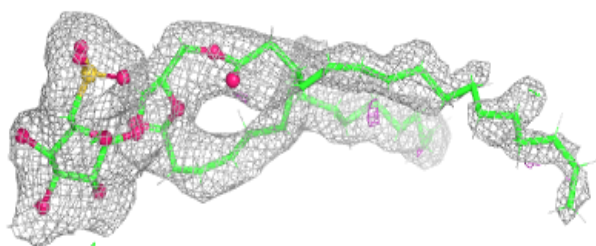
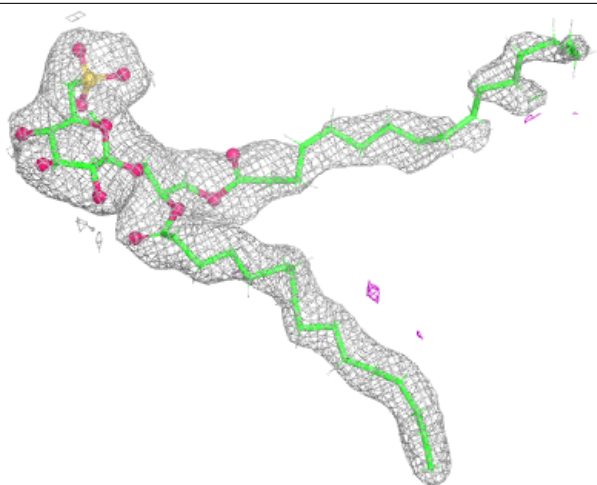
**Electron density around BCR K 101:**

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



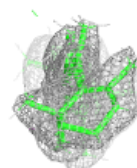
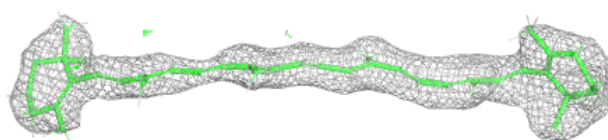
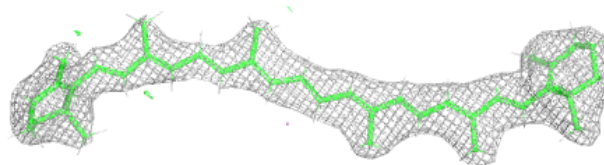
Electron density around SQD a 413:

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

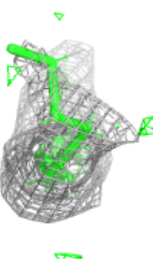
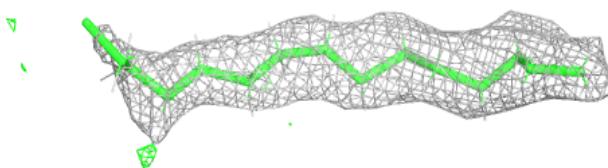
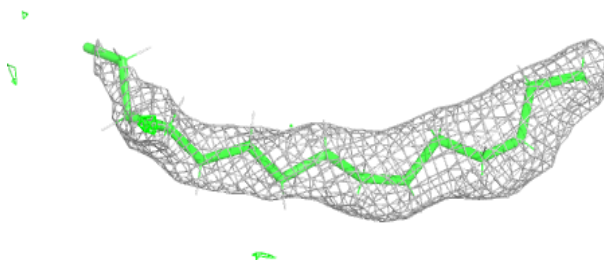


Electron density around BCR k 101:

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

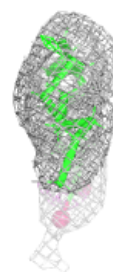
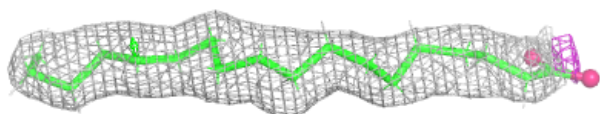
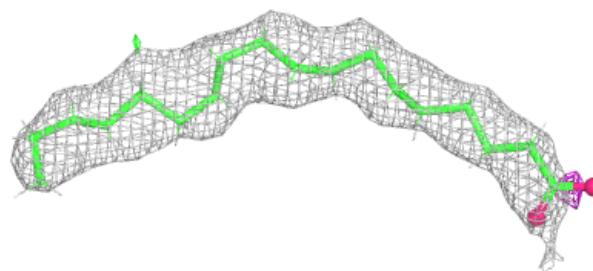
**Electron density around STE T 702:**

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

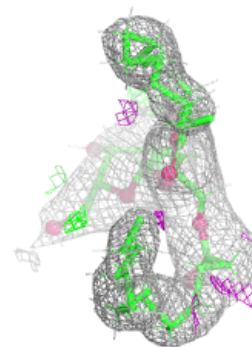
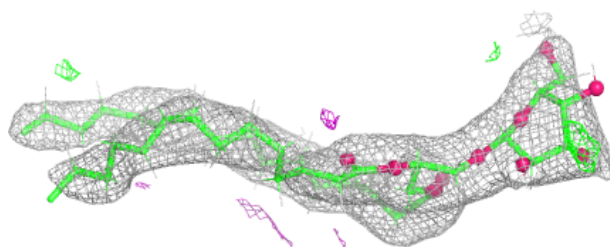
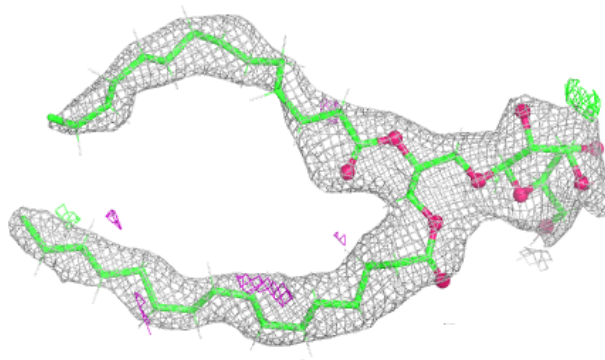


Electron density around STE X 101:

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

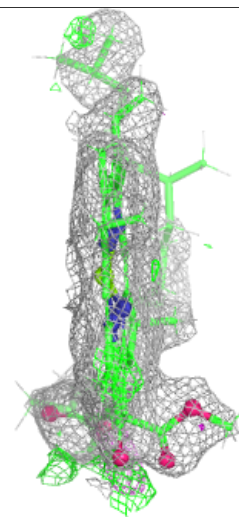
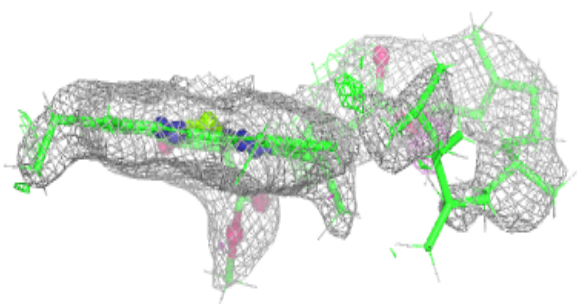
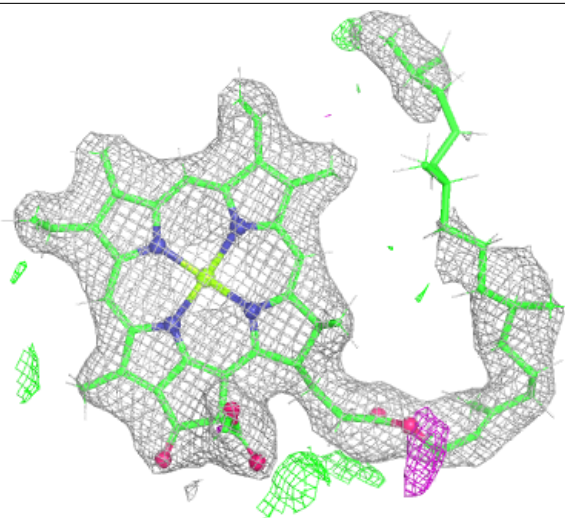
**Electron density around LMG c 523:**

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



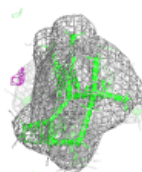
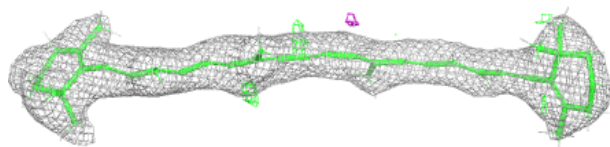
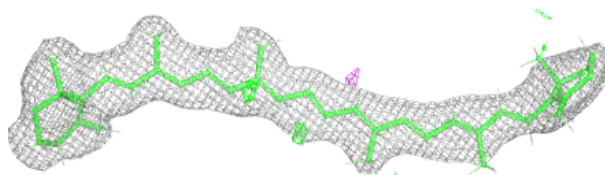
Electron density around CLA c 513:

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

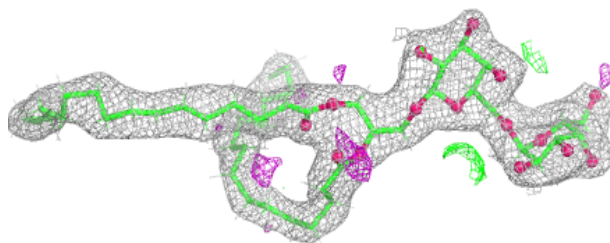
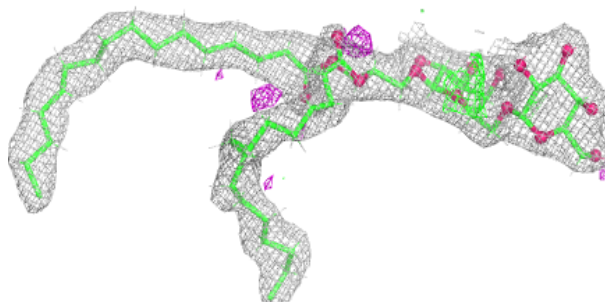


Electron density around BCR Y 101:

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

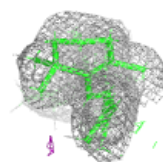
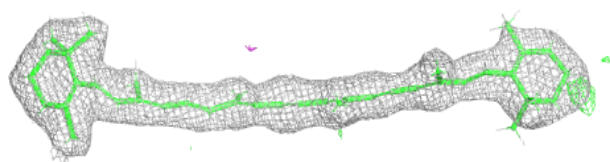
**Electron density around DGD h 702:**

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

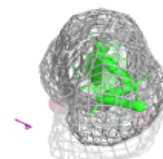
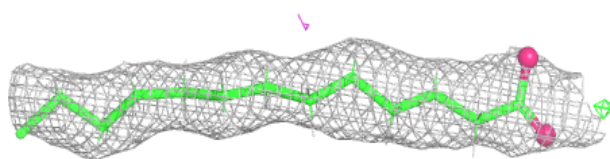
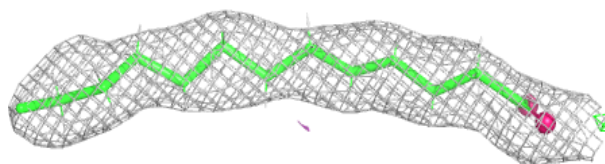


Electron density around BCR H 101:

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

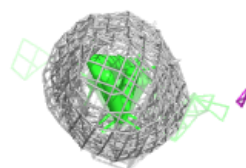
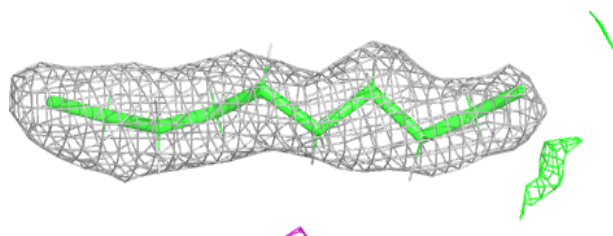
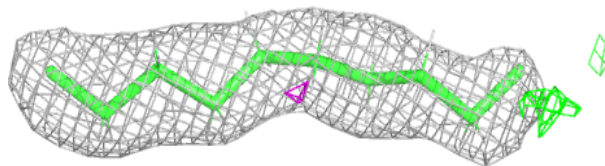
**Electron density around STE M 102:**

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

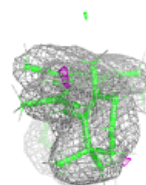
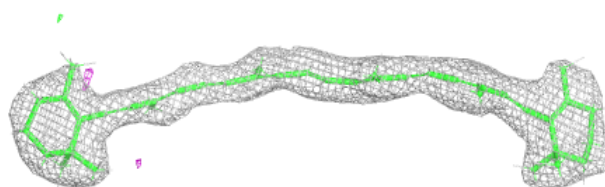


Electron density around STE M 103:

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

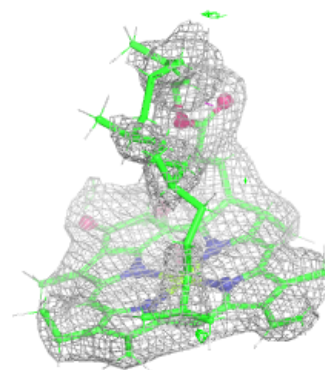
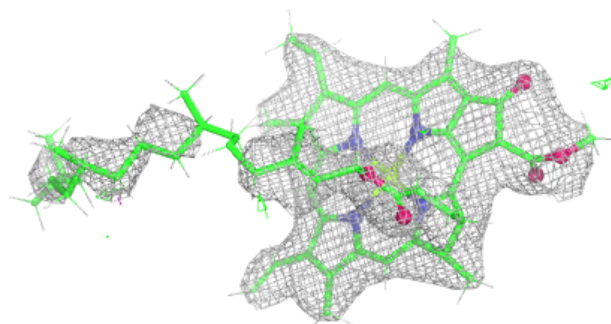
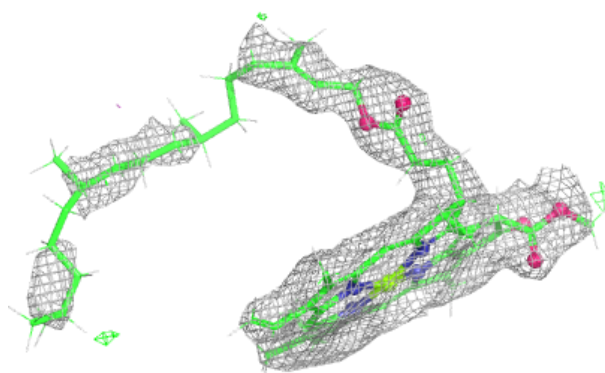
**Electron density around BCR k 102:**

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

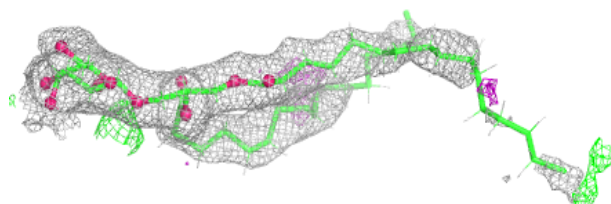


Electron density around CLA c 514:

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

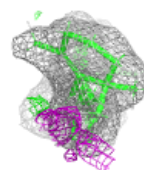
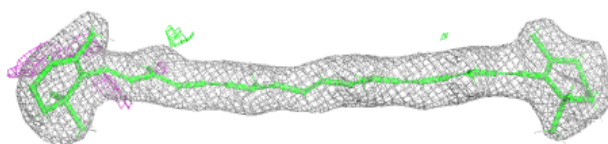
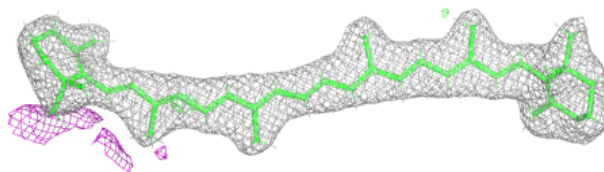
**Electron density around LMG D 408:**

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

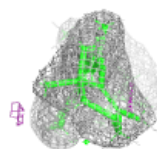
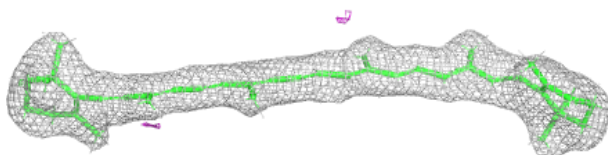
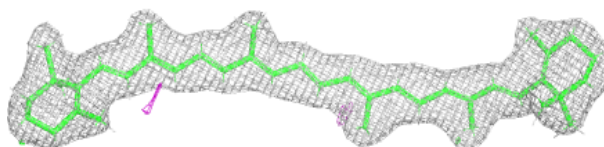


Electron density around BCR B 718:

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

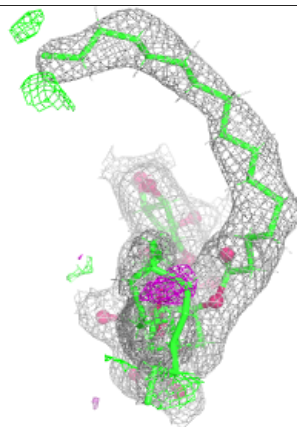
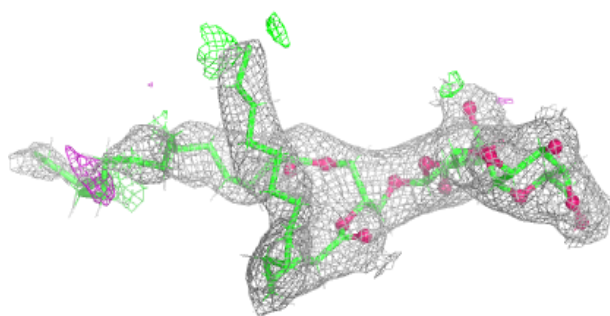
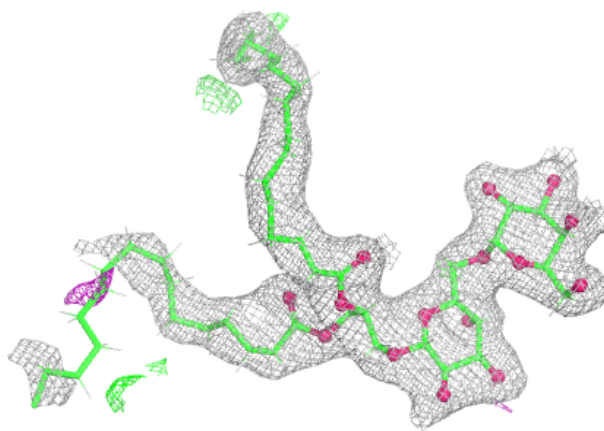
**Electron density around BCR B 719:**

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

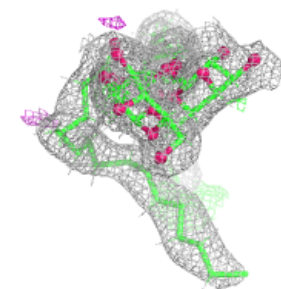
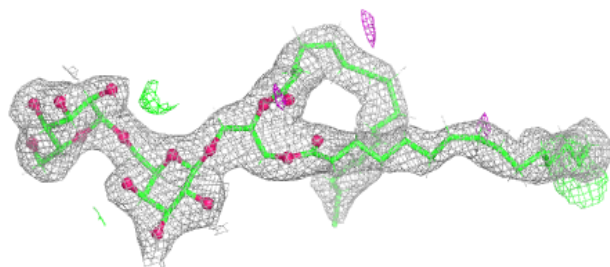
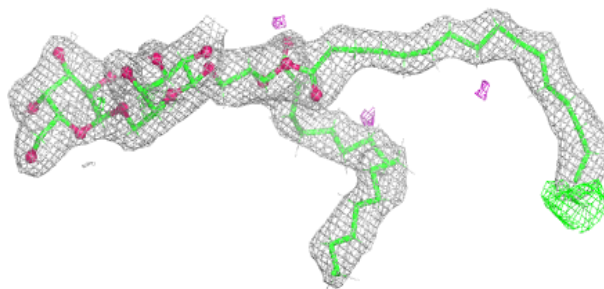


Electron density around DGD C 518:

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

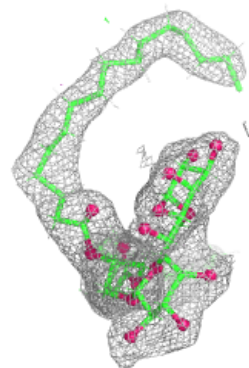
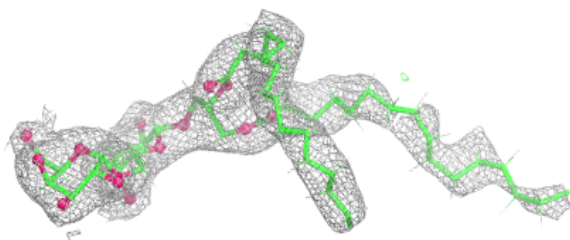
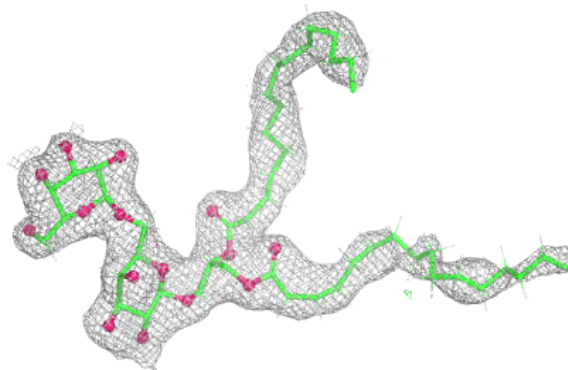
**Electron density around DGD H 103:**

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

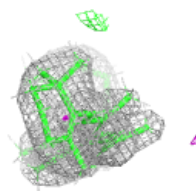
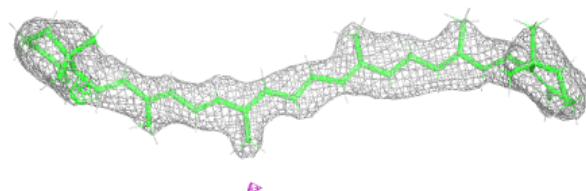
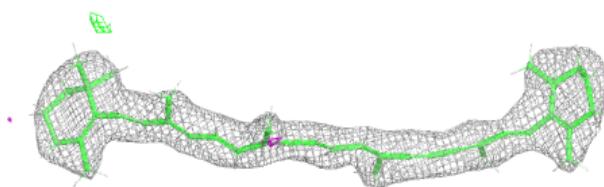


Electron density around DGD c 518:

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

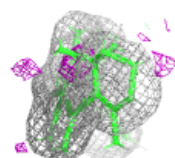
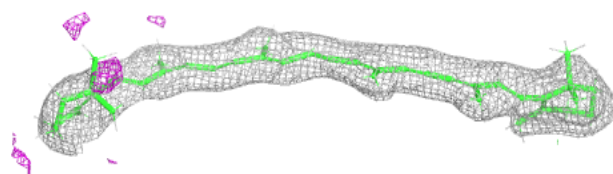
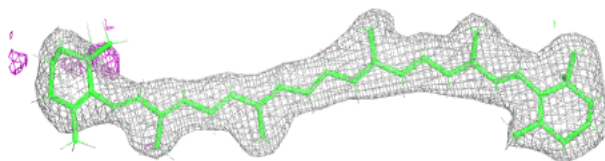
**Electron density around BCR C 501:**

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



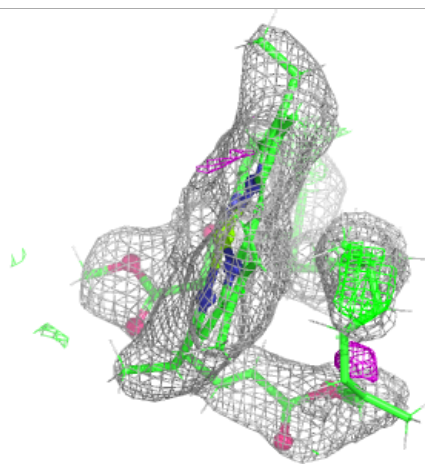
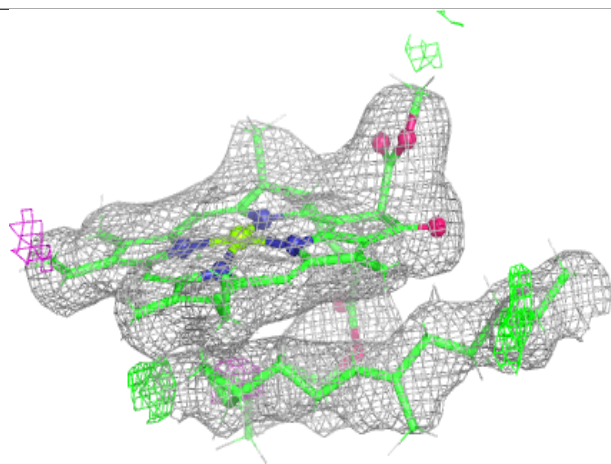
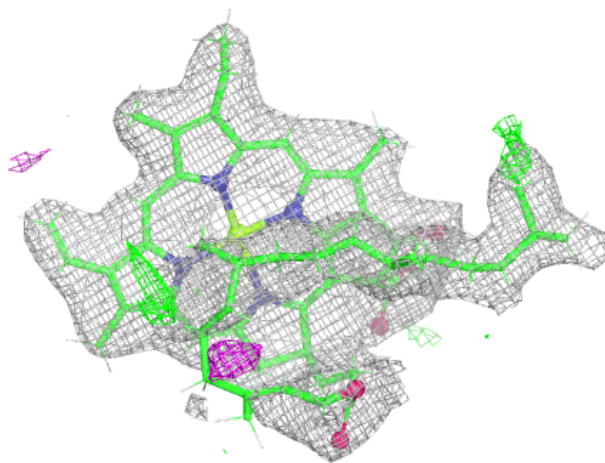
Electron density around BCR D 404:

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



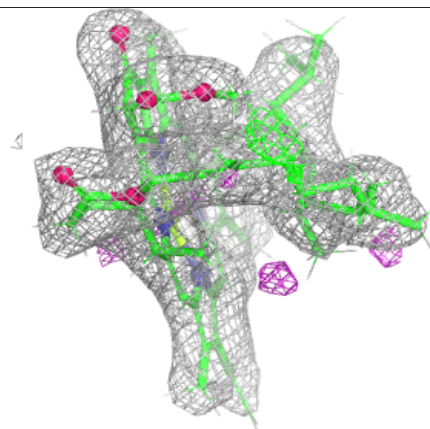
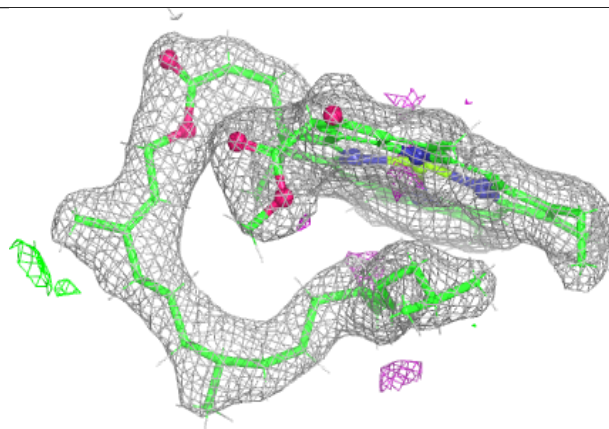
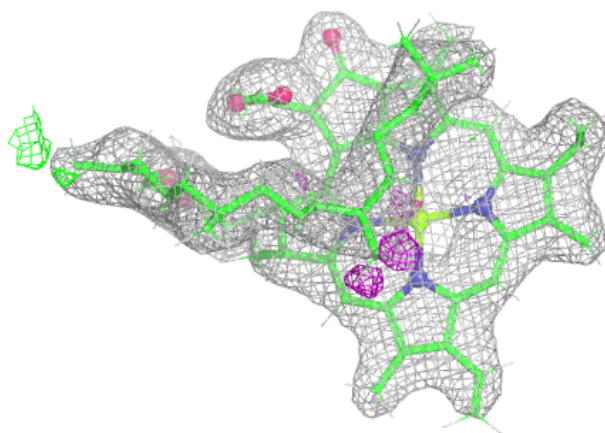
Electron density around CLA H 102:

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



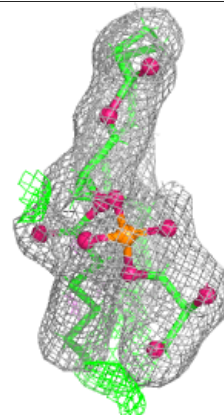
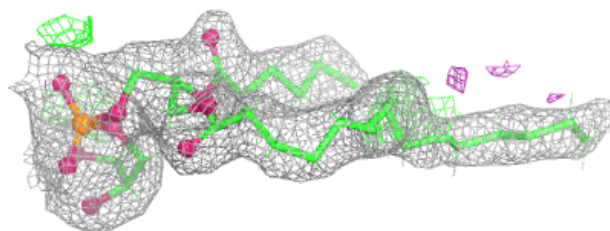
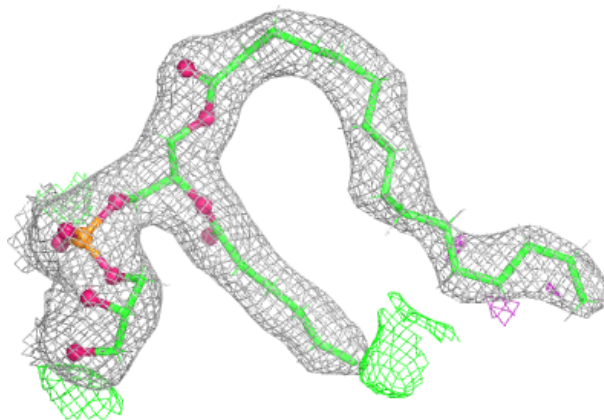
Electron density around CLA C 511:

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



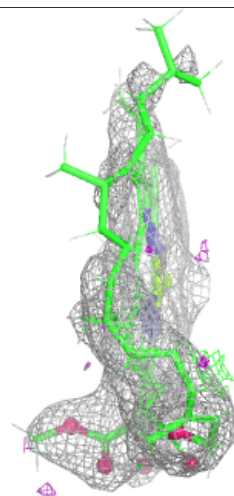
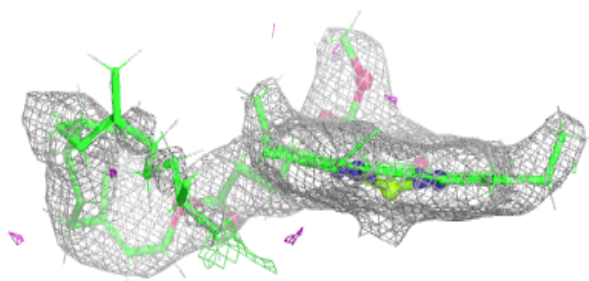
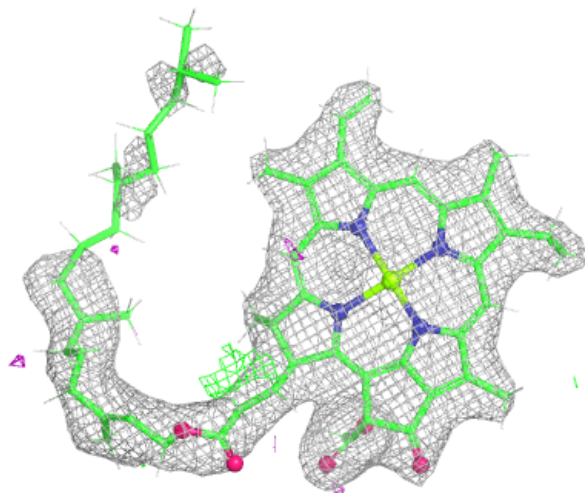
Electron density around LHG d 407:

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



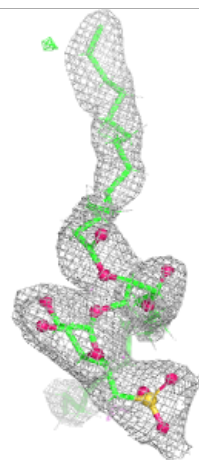
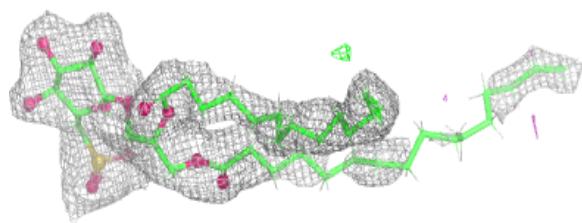
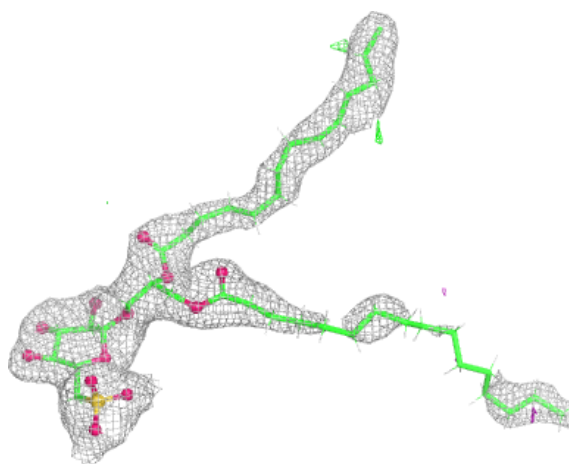
Electron density around CLA C 513:

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



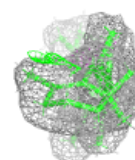
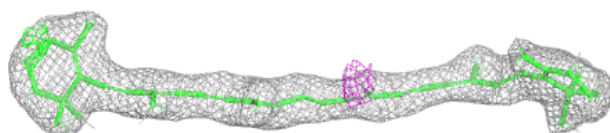
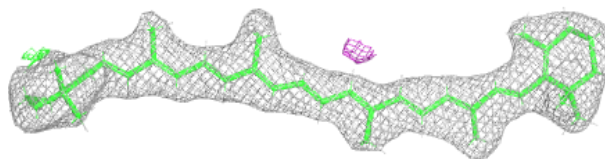
Electron density around SQD A 409:

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

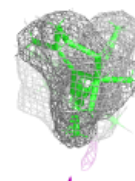
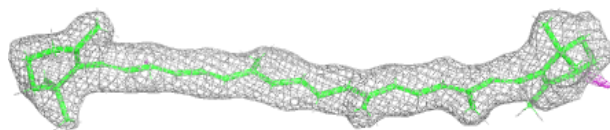
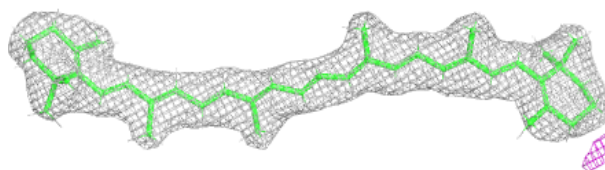


Electron density around BCR b 717:

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

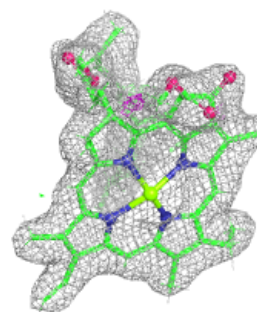
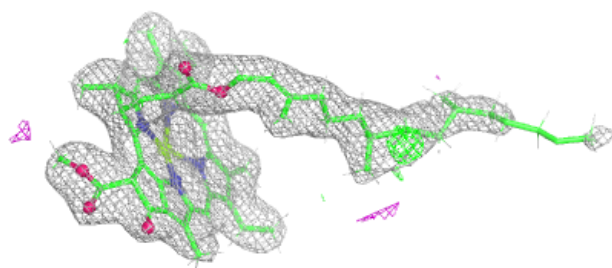
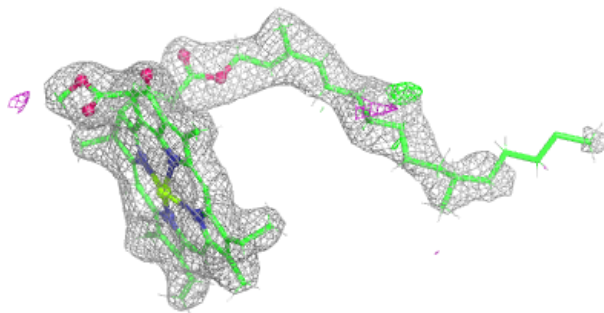
**Electron density around BCR b 719:**

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

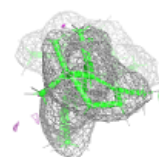
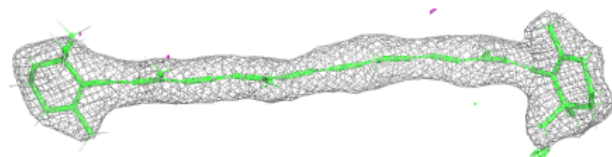
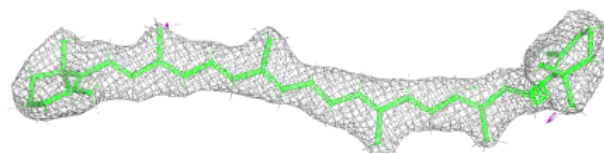


Electron density around CLA c 509:

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

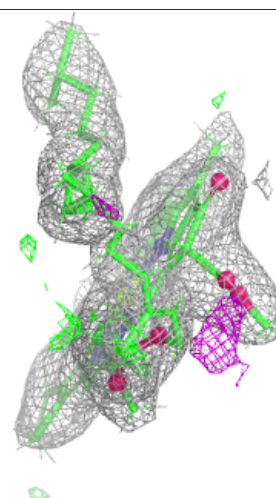
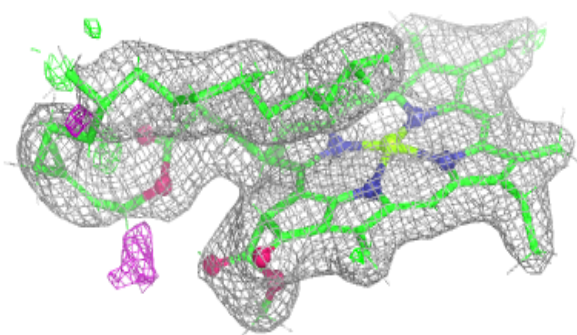
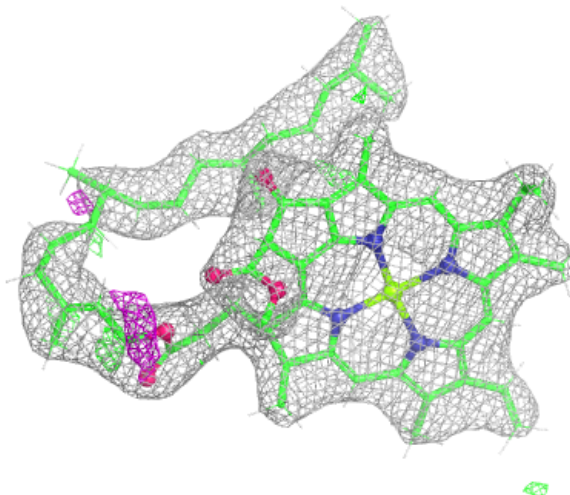
**Electron density around BCR c 516:**

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



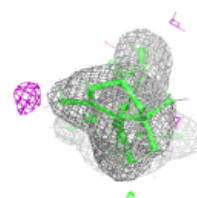
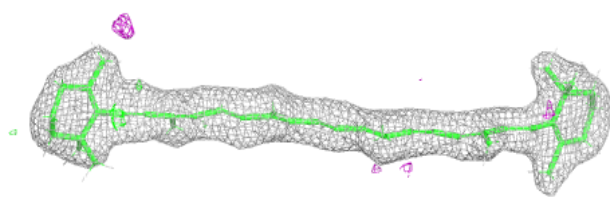
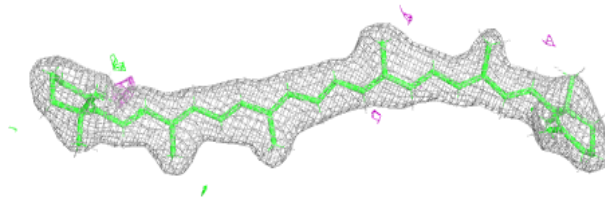
Electron density around CLA c 510:

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

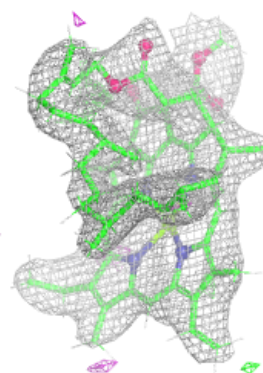
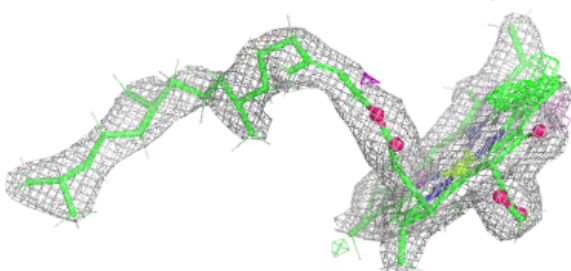
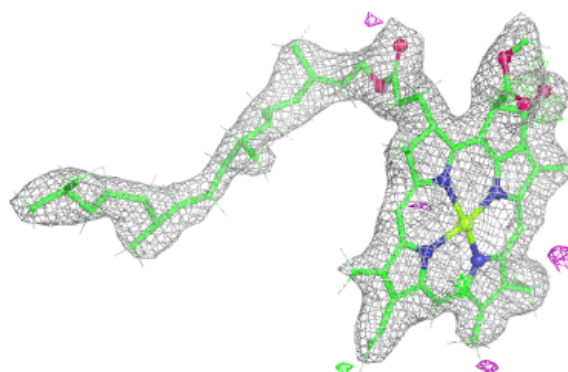


Electron density around BCR C 515:

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

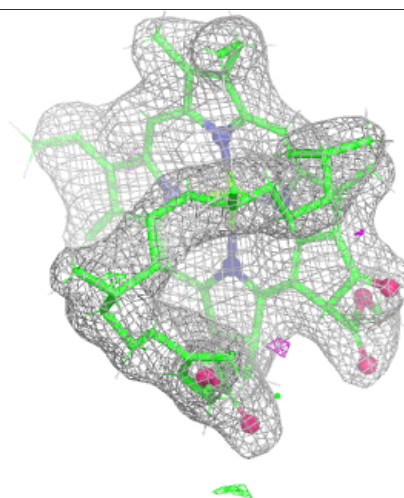
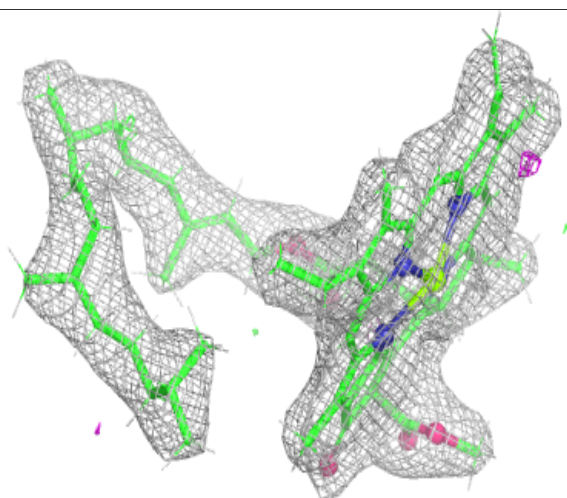
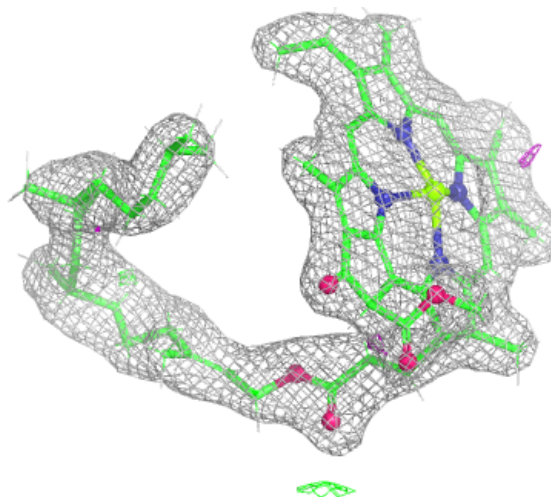
**Electron density around CLA c 512:**

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



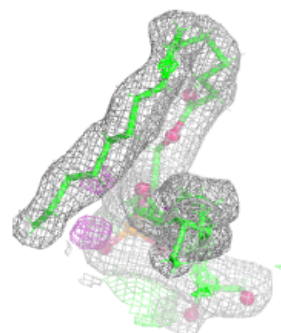
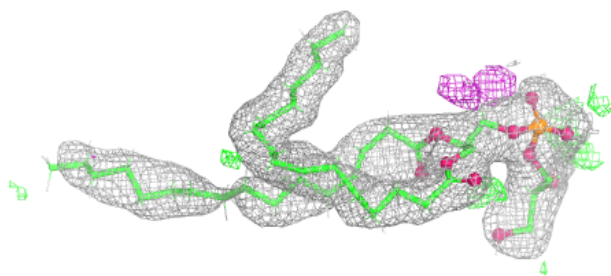
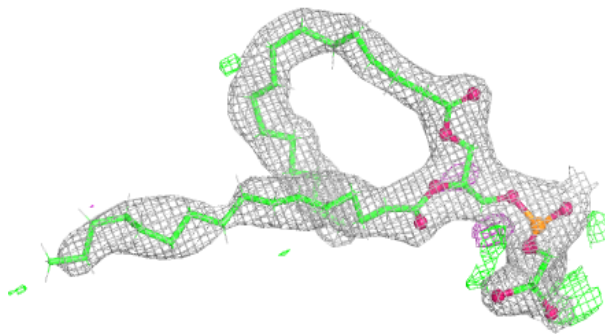
Electron density around CLA C 504:

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

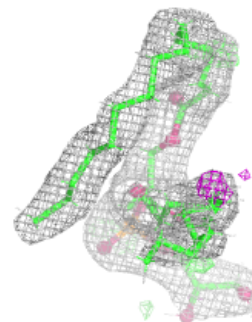
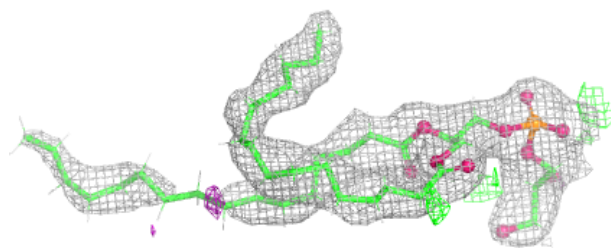
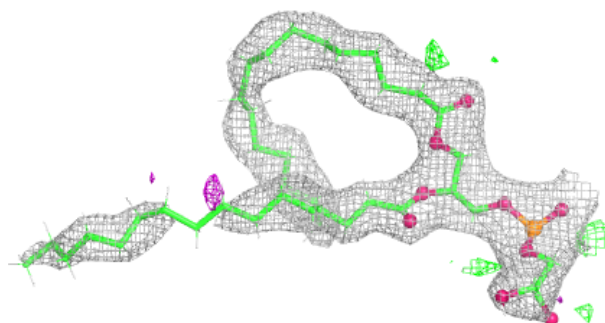


Electron density around LHG B 722:

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

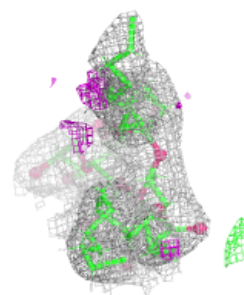
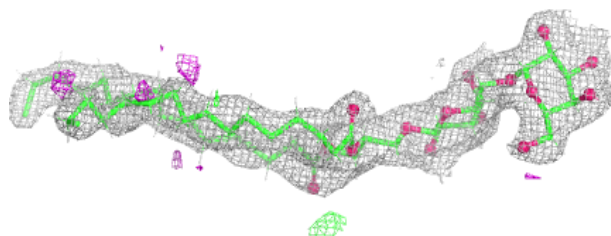
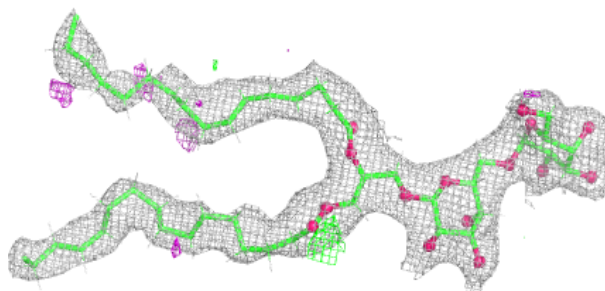
**Electron density around LHG a 412:**

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

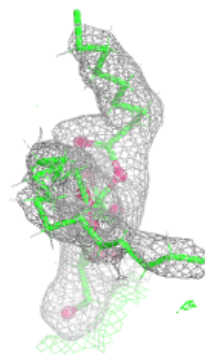
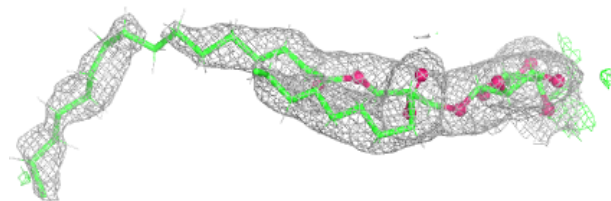
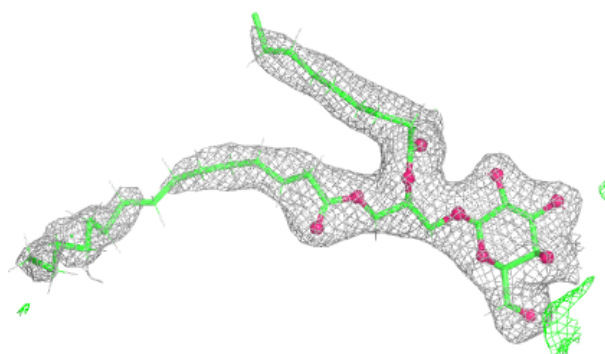


Electron density around DGD C 519:

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

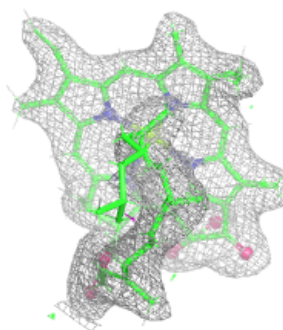
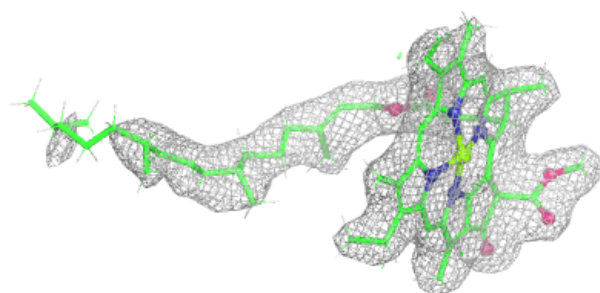
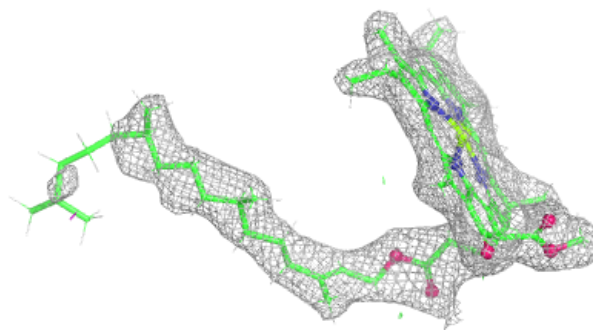
**Electron density around LMG d 408:**

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



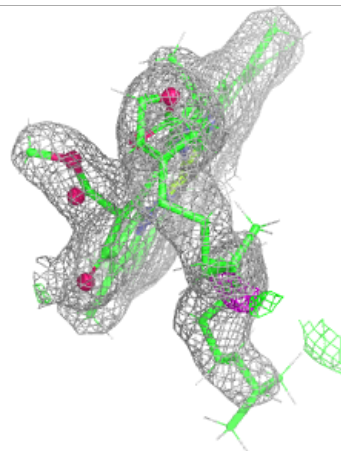
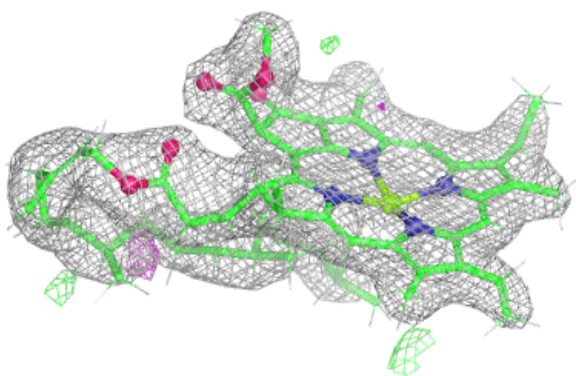
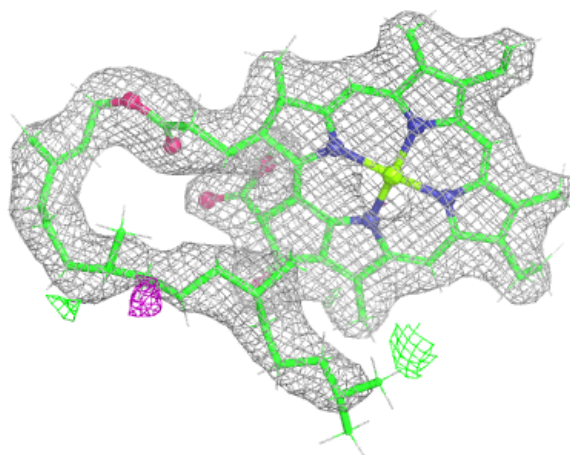
Electron density around CLA C 509:

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



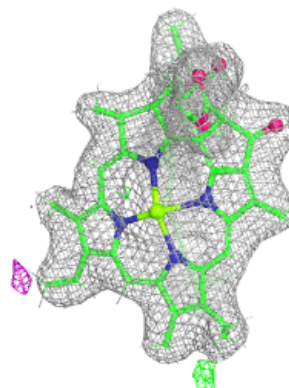
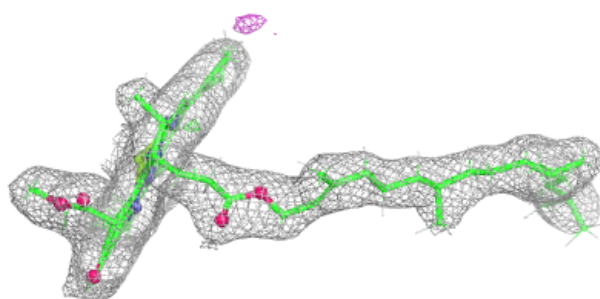
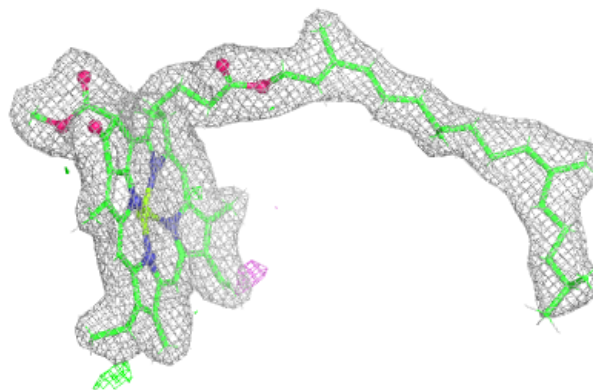
Electron density around CLA C 510:

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

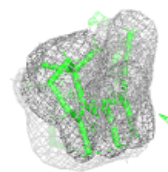
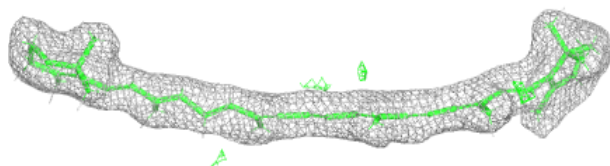
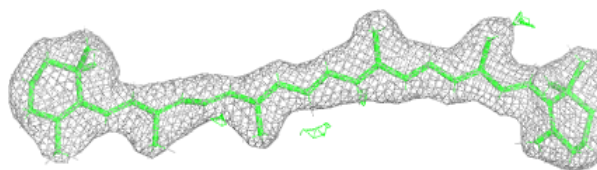


Electron density around CLA B 709:

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

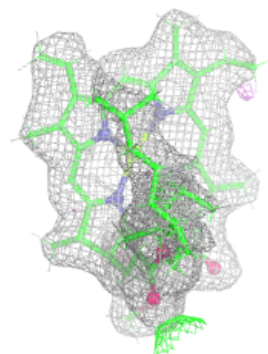
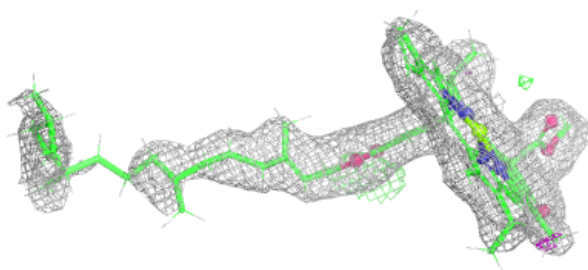
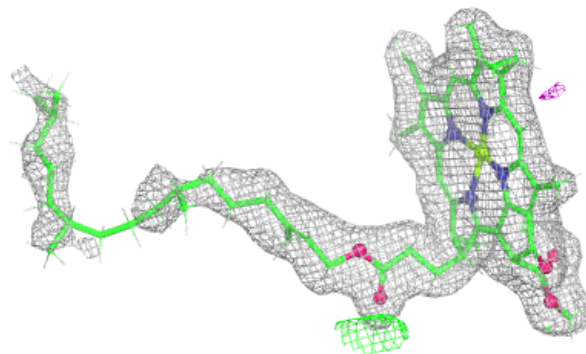
**Electron density around BCR t 701:**

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

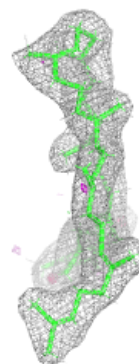
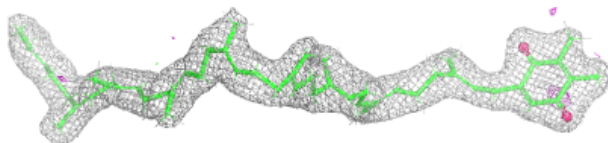
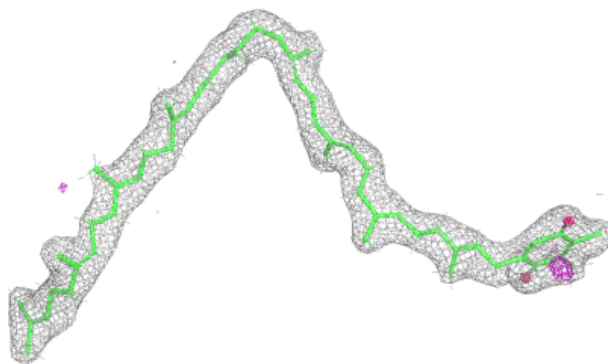


Electron density around CLA d 402:

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

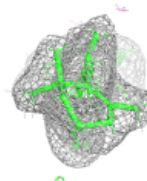
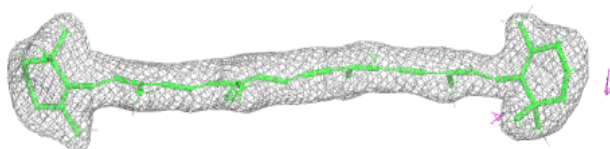
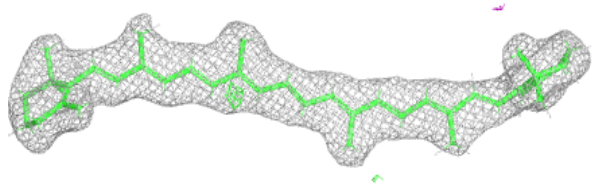
**Electron density around PL9 D 405:**

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

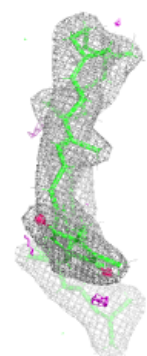
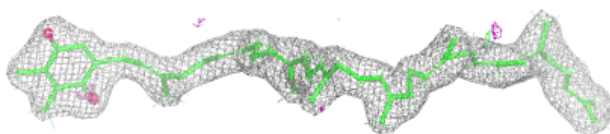
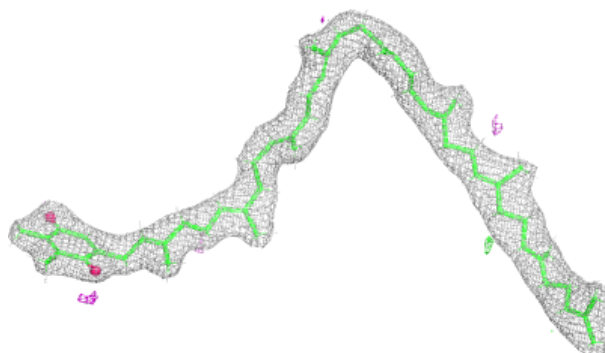


Electron density around BCR A 405:

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

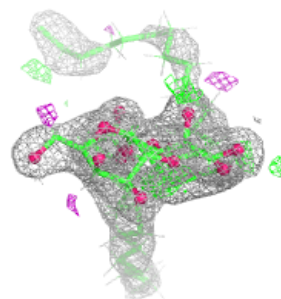
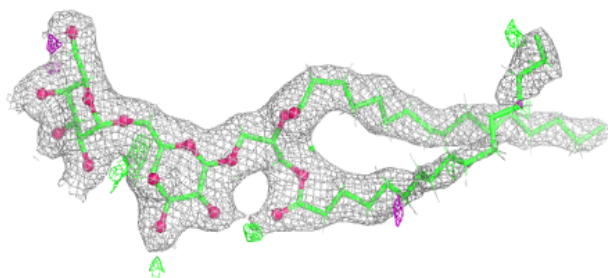
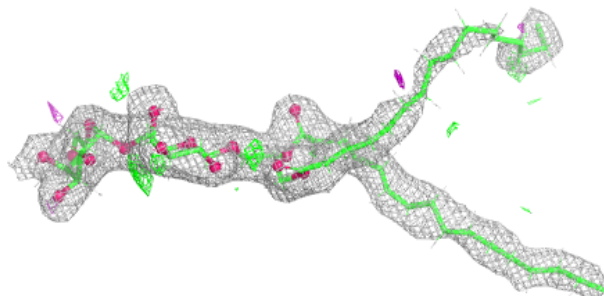
**Electron density around PL9 d 404:**

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

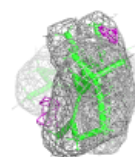
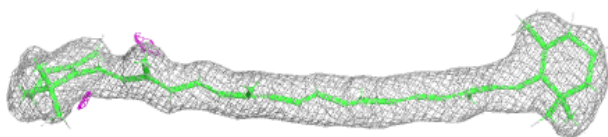
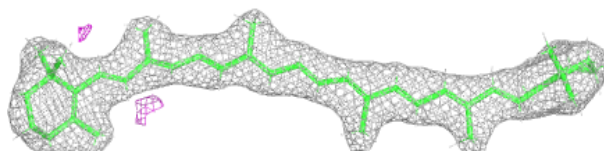


Electron density around DGD C 517:

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

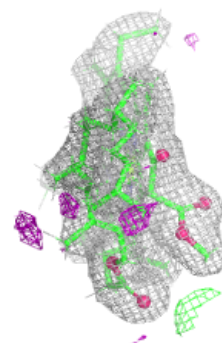
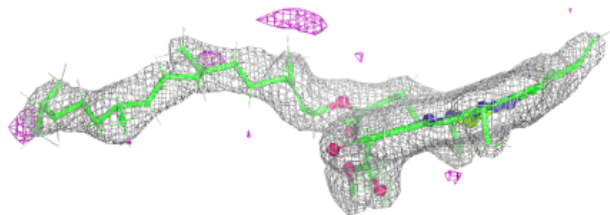
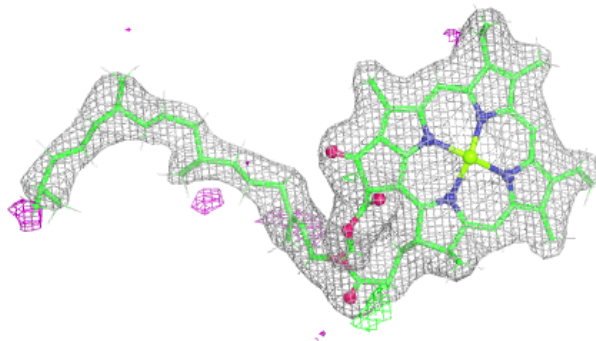
**Electron density around BCR B 717:**

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

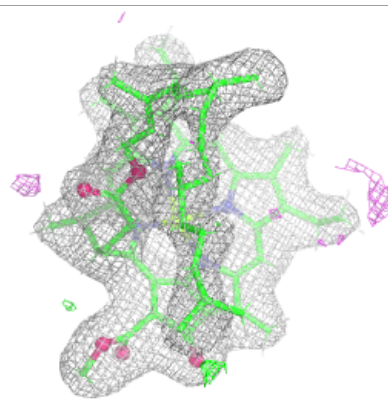
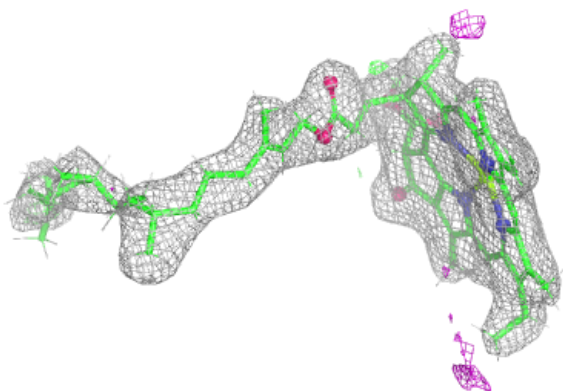
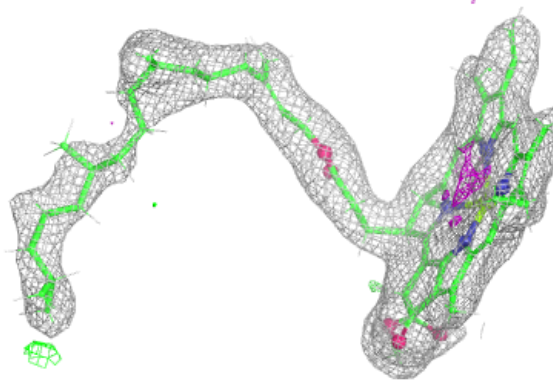


Electron density around CLA b 702:

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

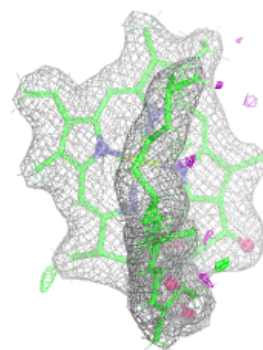
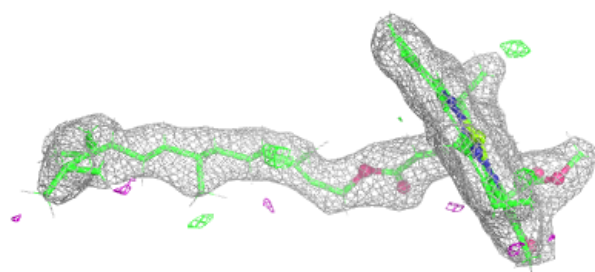
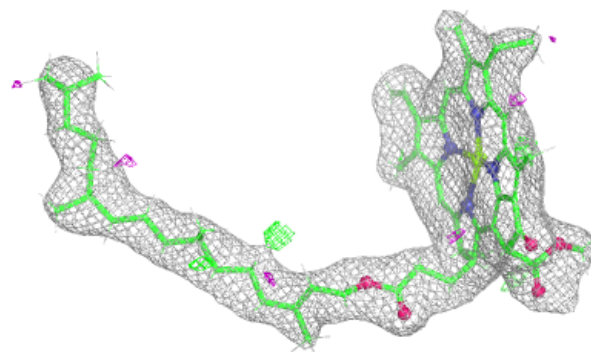
**Electron density around CLA b 706:**

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

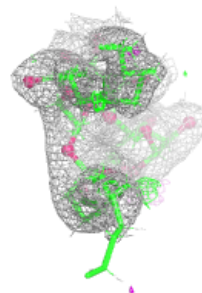
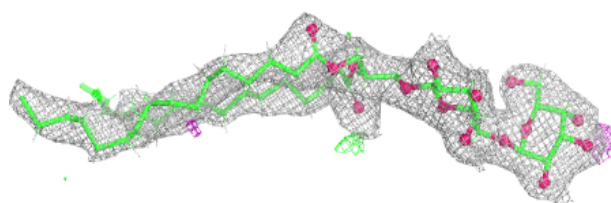
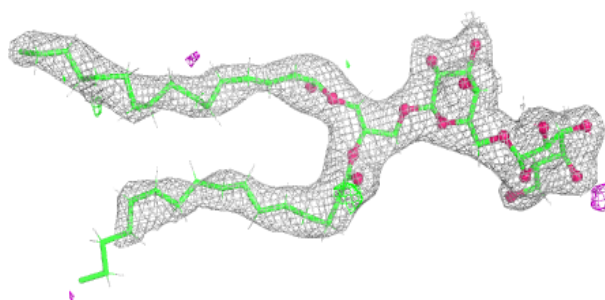


Electron density around CLA b 709:

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

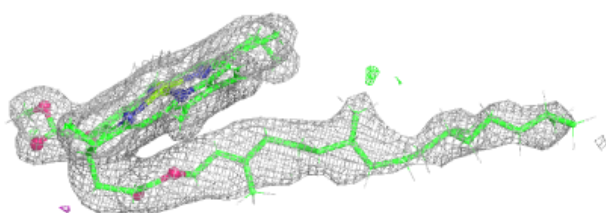
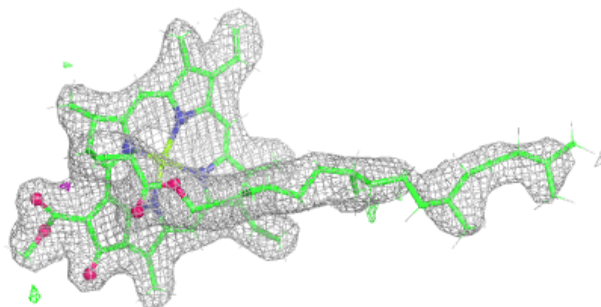
**Electron density around DGD c 519:**

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



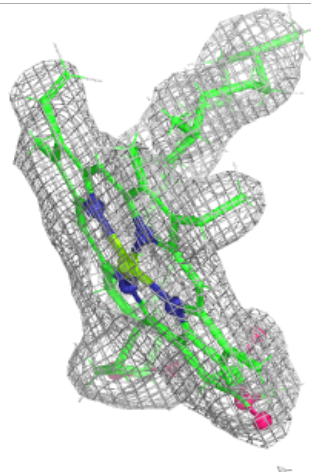
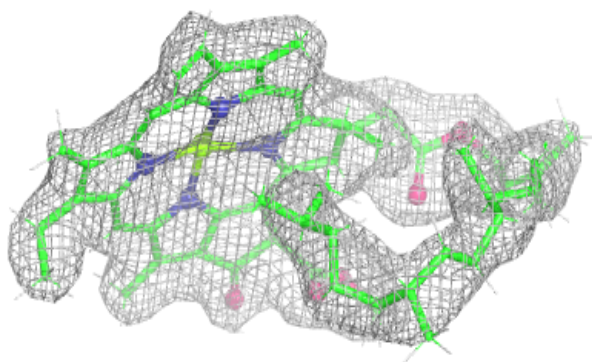
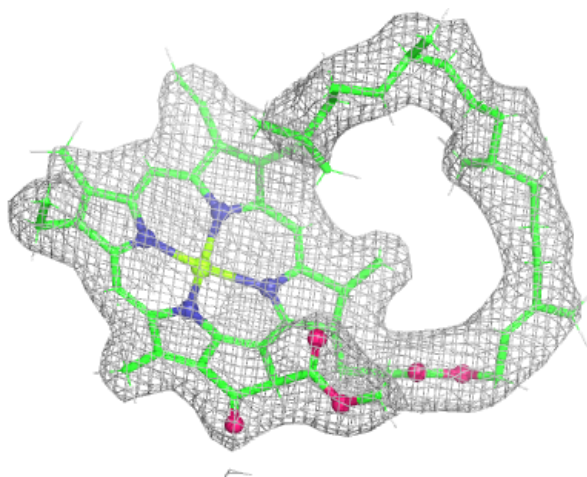
Electron density around CLA b 714:

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



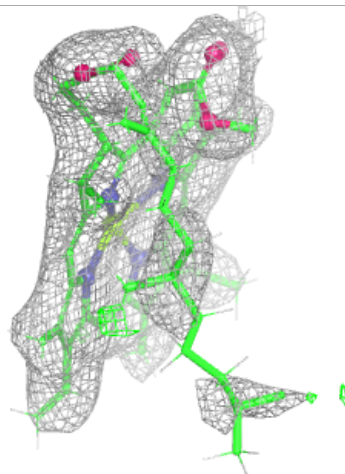
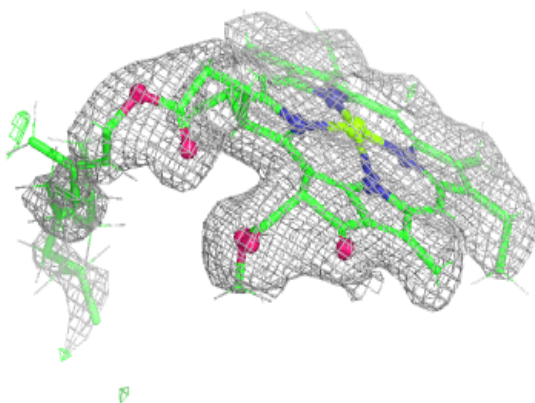
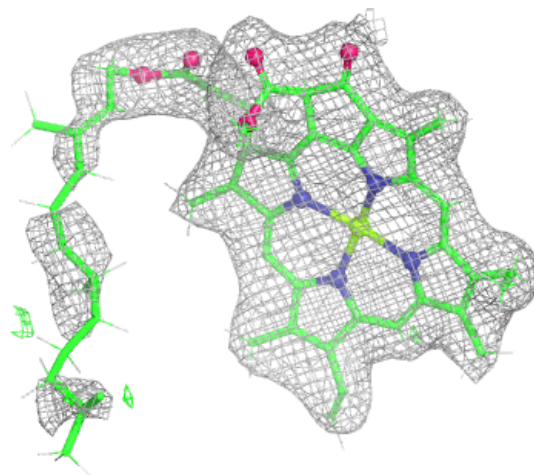
Electron density around CLA b 715:

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



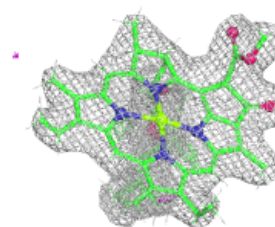
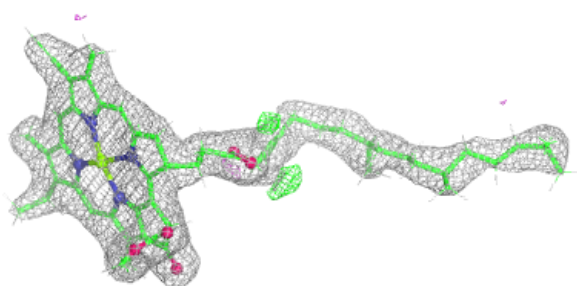
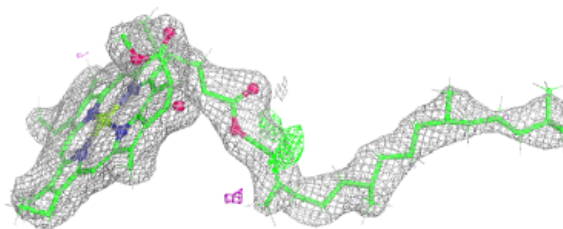
Electron density around CLA b 716:

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

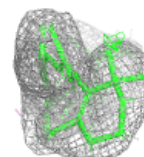
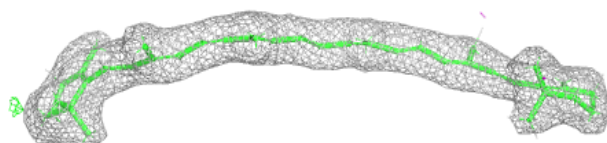
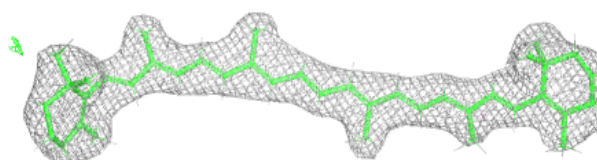


Electron density around CLA c 503:

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

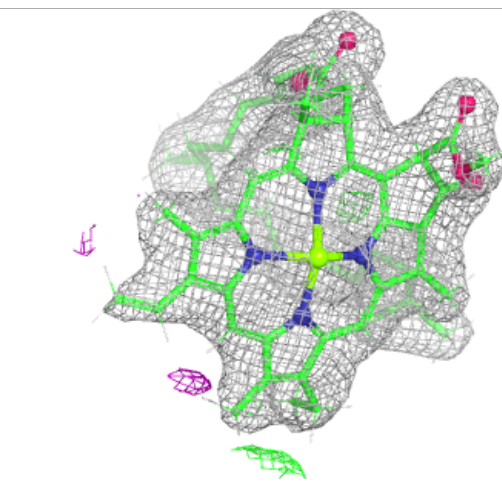
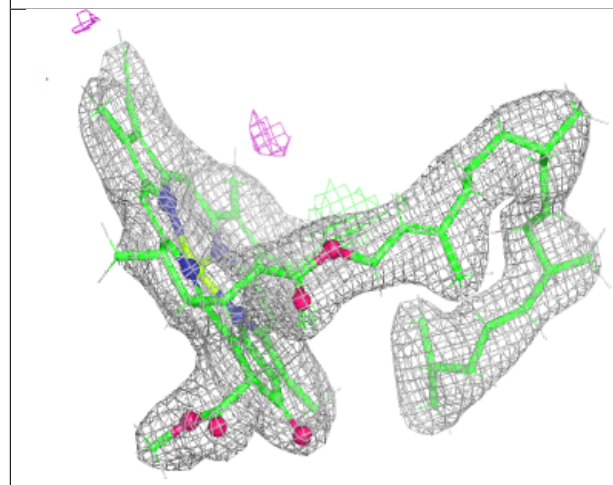
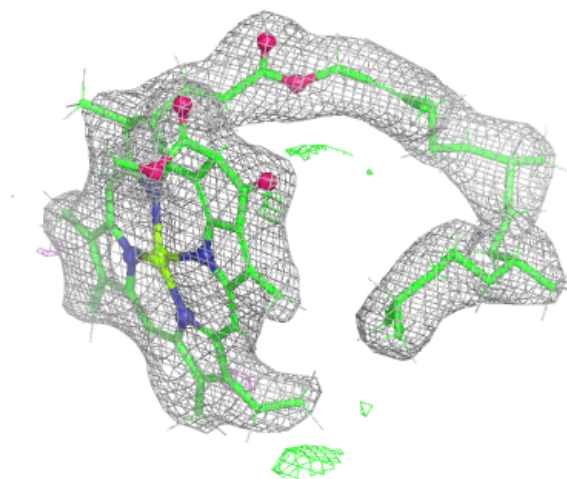
**Electron density around BCR T 701:**

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



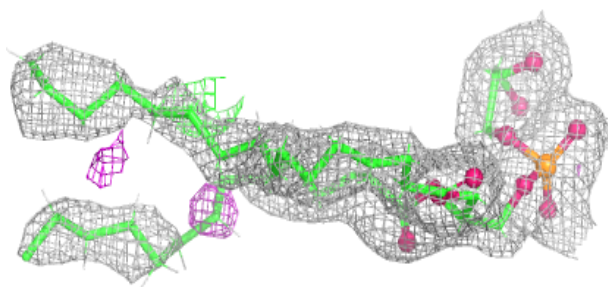
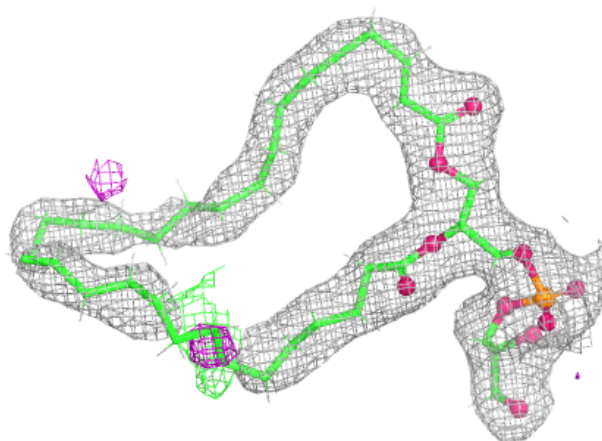
Electron density around CLA c 504:

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

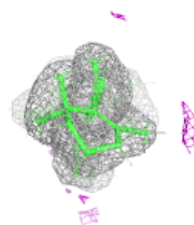
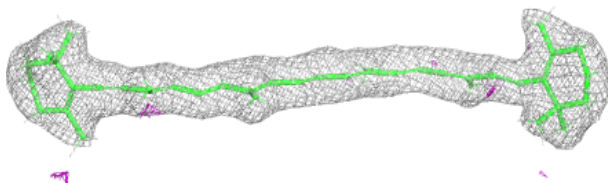
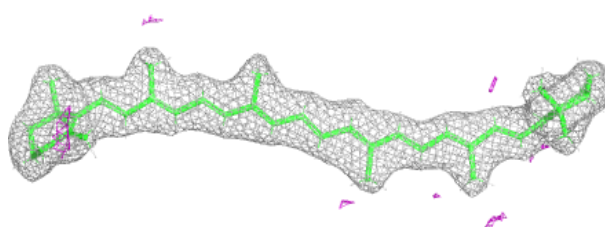


Electron density around LHG D 411:

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

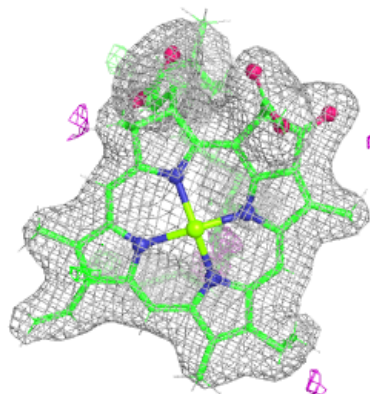
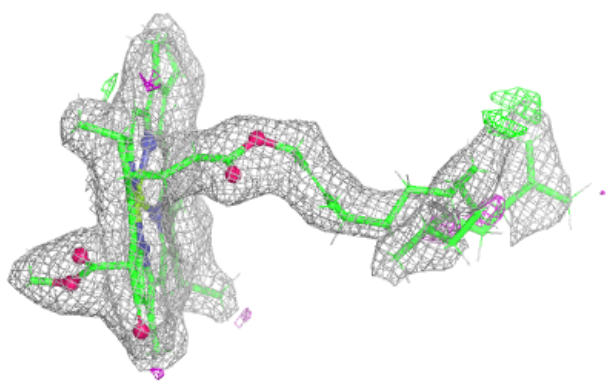
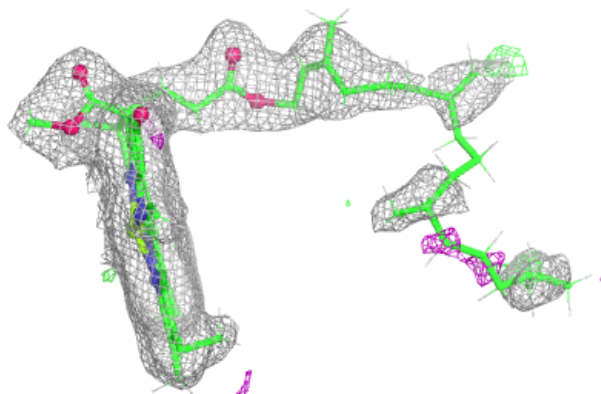
**Electron density around BCR a 407:**

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

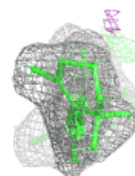
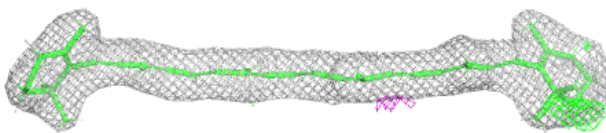
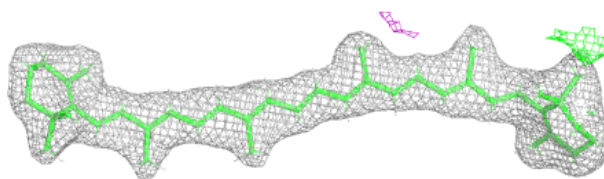


Electron density around CLA c 507:

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

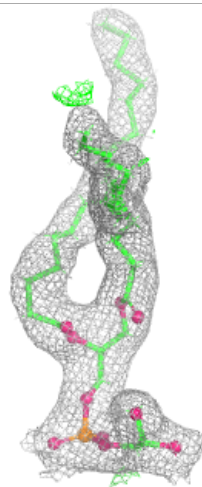
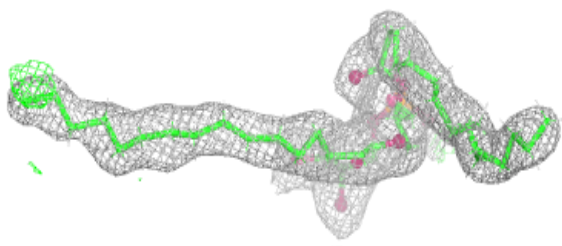
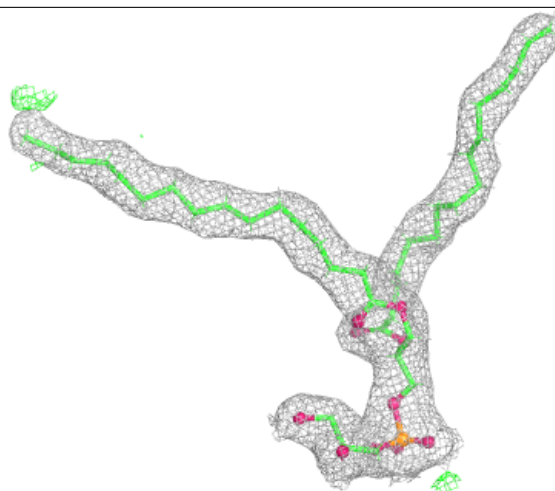
**Electron density around BCR b 718:**

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



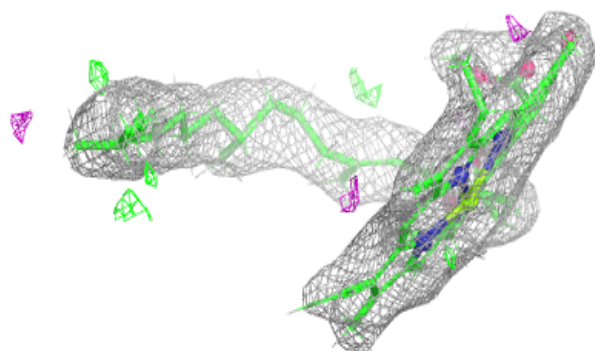
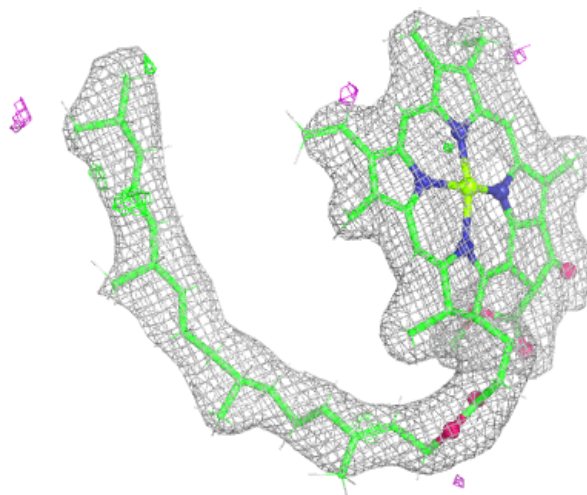
Electron density around LHG 1 101:

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



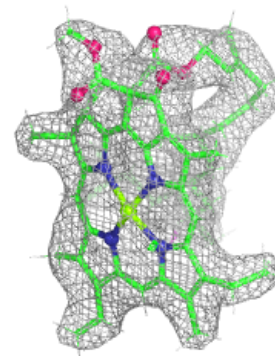
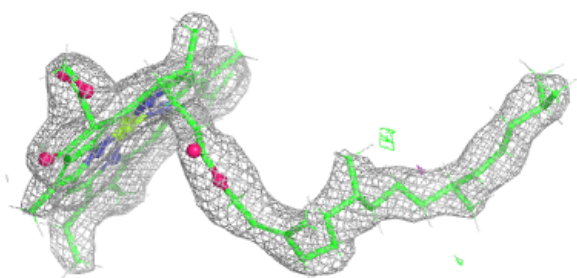
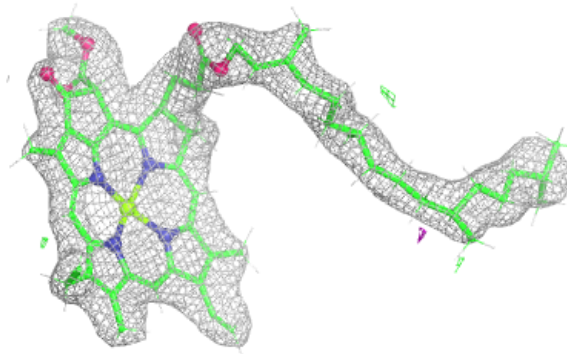
Electron density around CLA c 508:

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



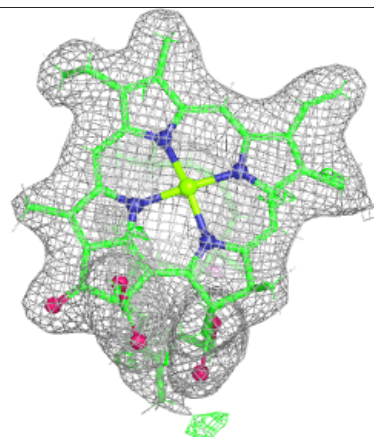
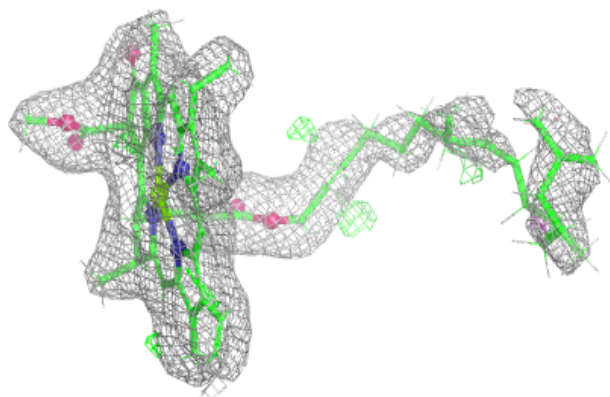
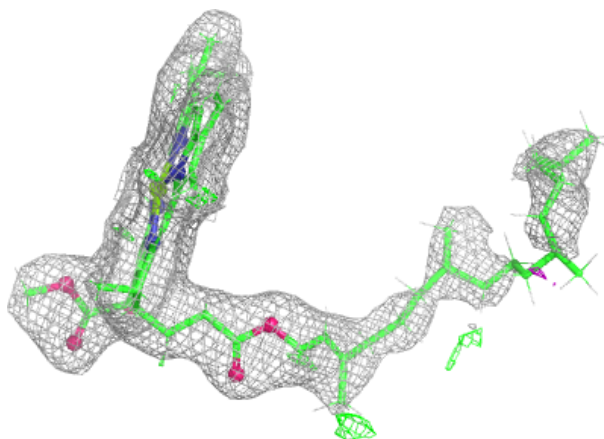
Electron density around CLA C 512:

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



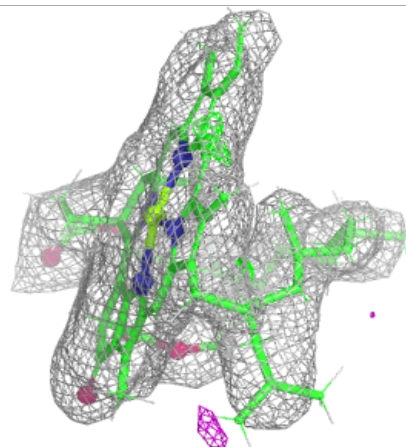
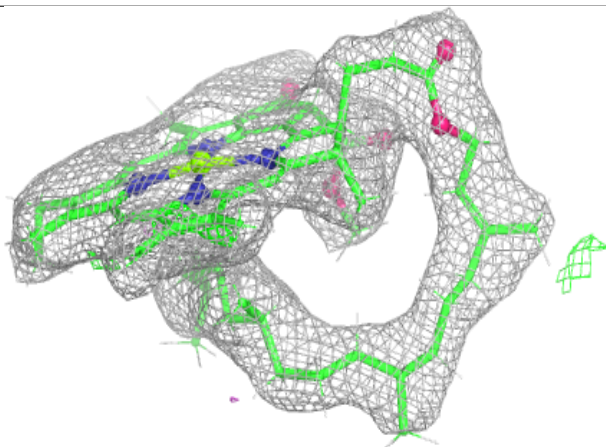
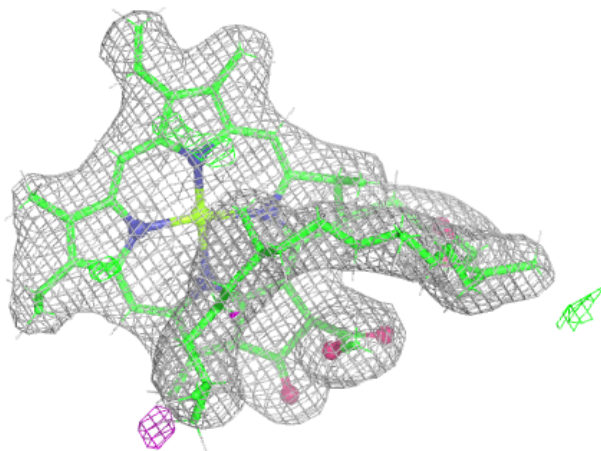
Electron density around CLA C 507:

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



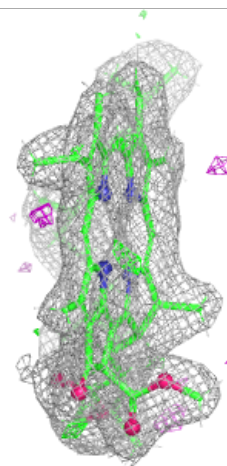
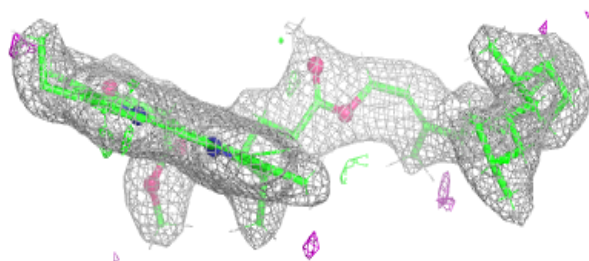
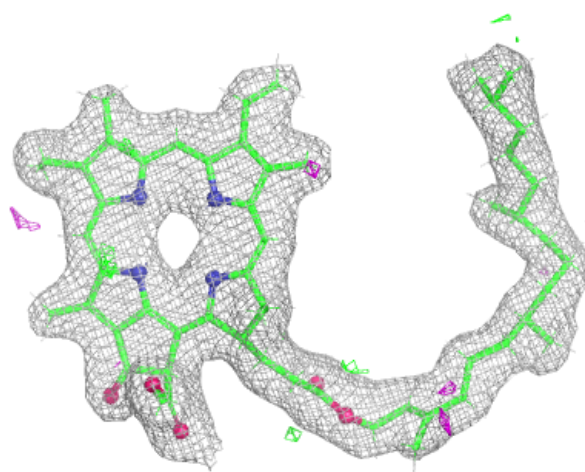
Electron density around CLA c 511:

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



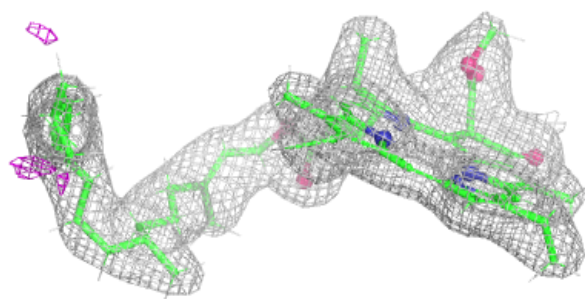
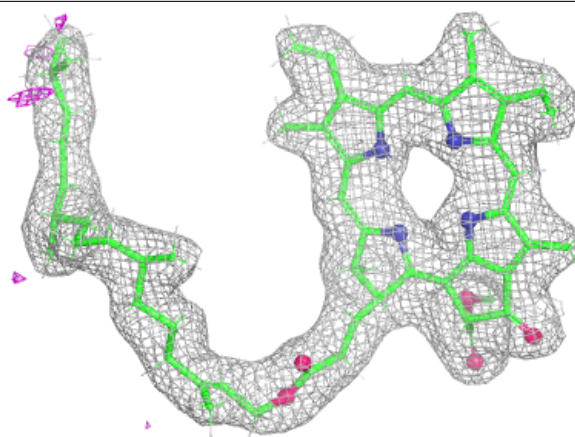
Electron density around PHO a 405:

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



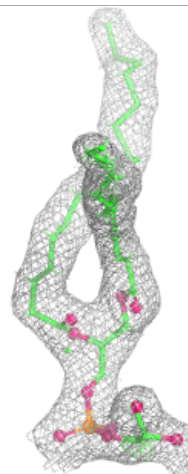
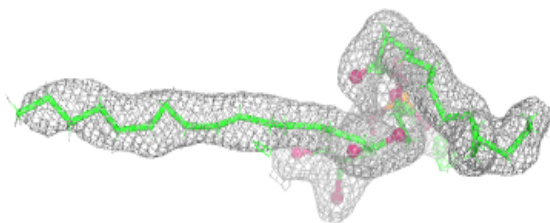
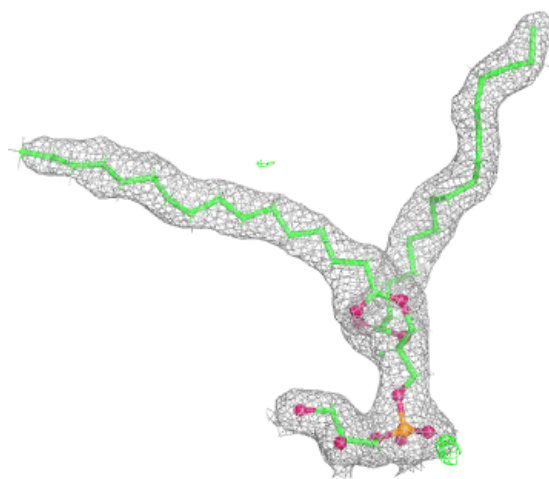
Electron density around PHO d 405:

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



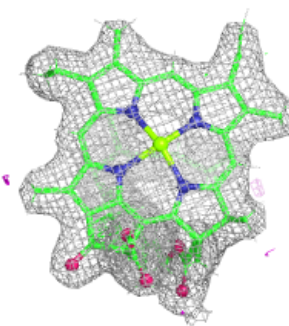
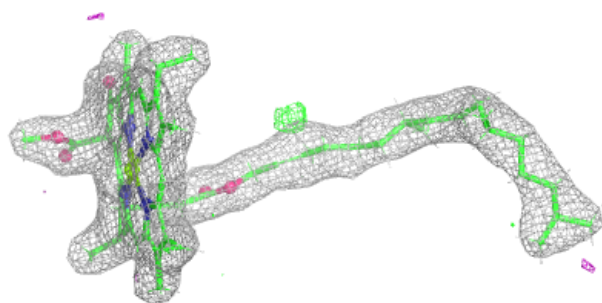
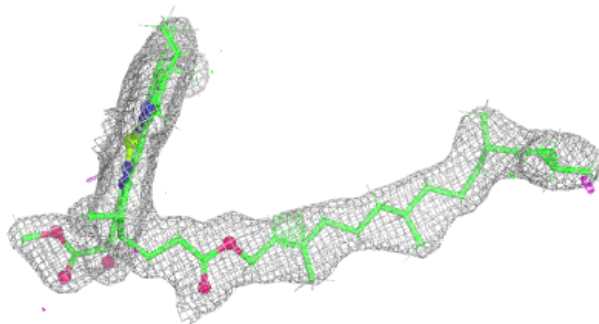
Electron density around LHG L 101:

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



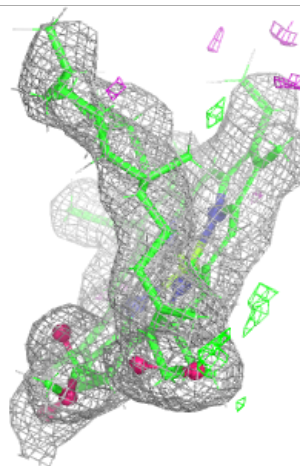
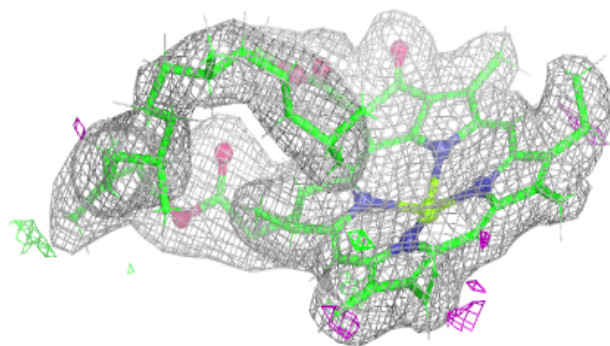
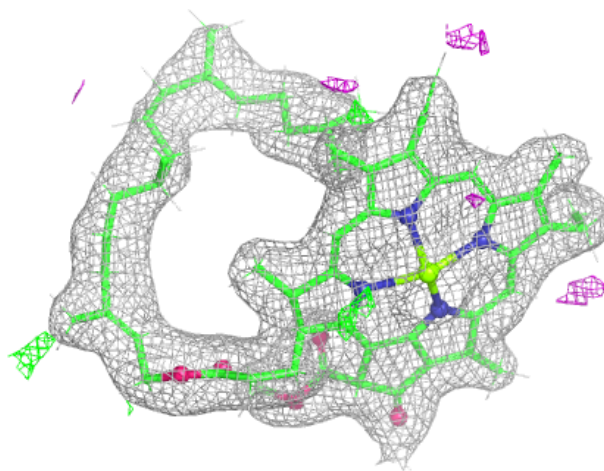
Electron density around CLA b 705:

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



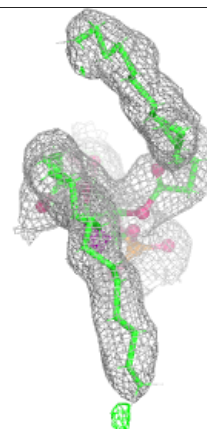
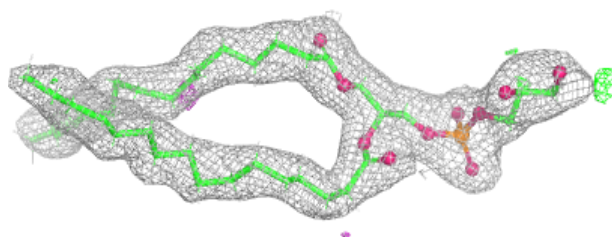
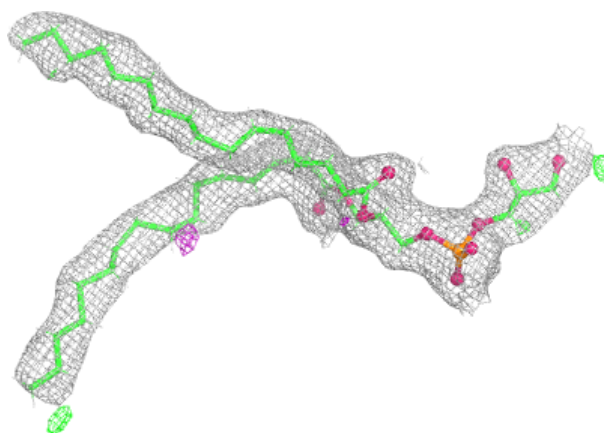
Electron density around CLA B 715:

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

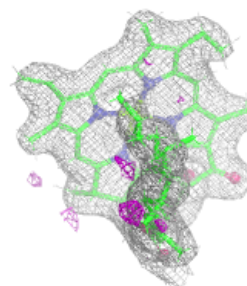
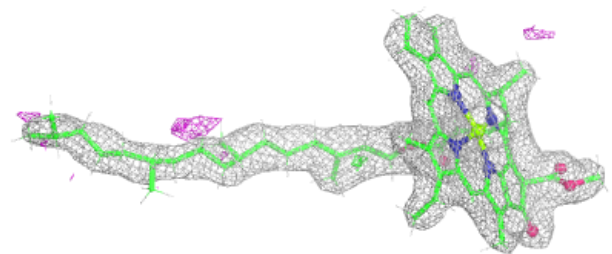
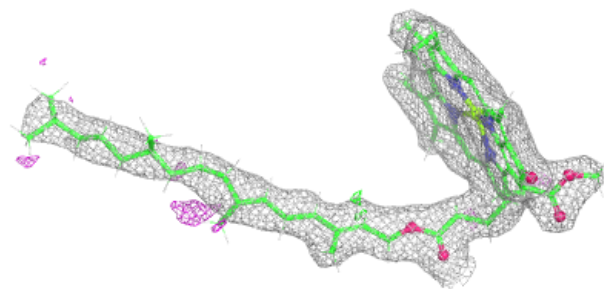


Electron density around LHG d 406:

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

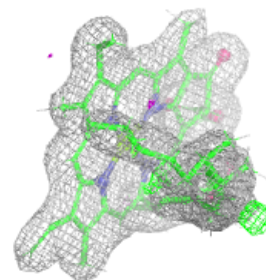
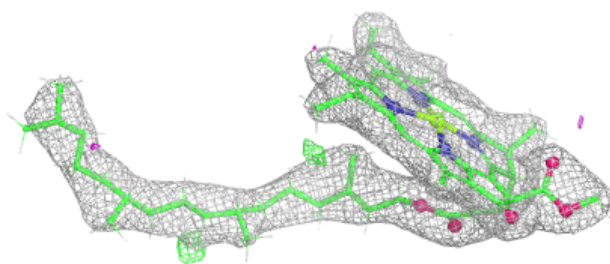
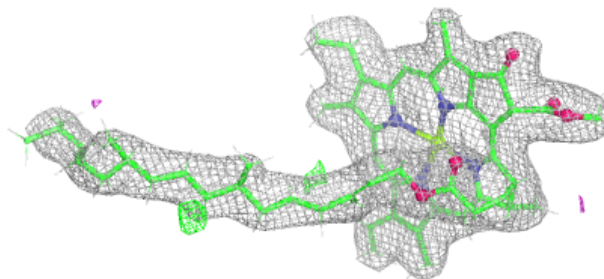
**Electron density around CLA b 707:**

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

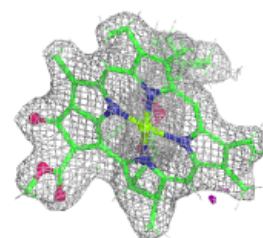
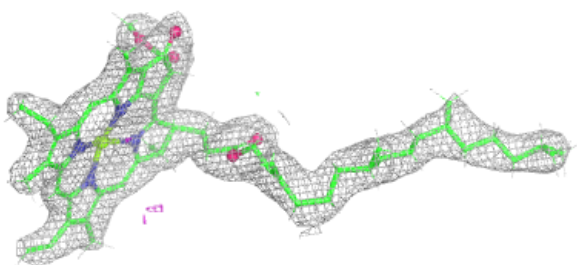
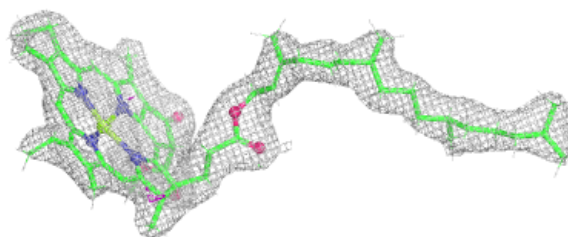


Electron density around CLA b 708:

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

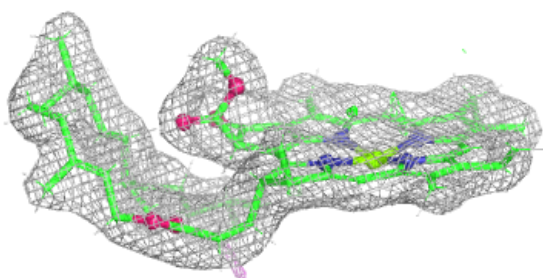
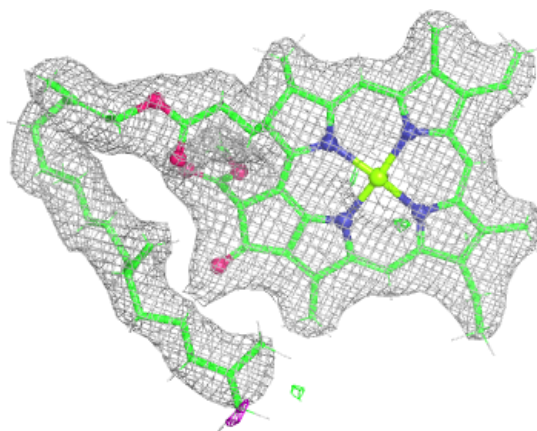
**Electron density around CLA C 503:**

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

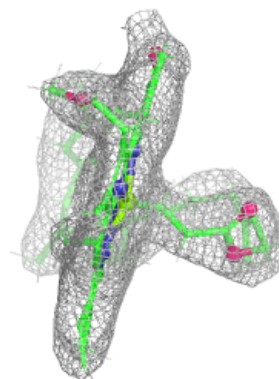
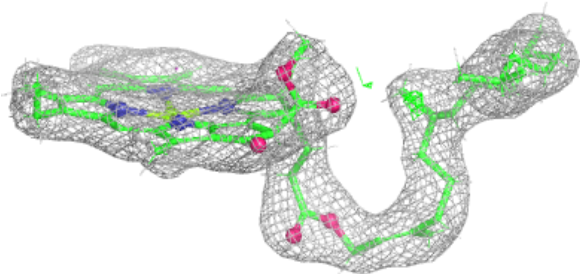
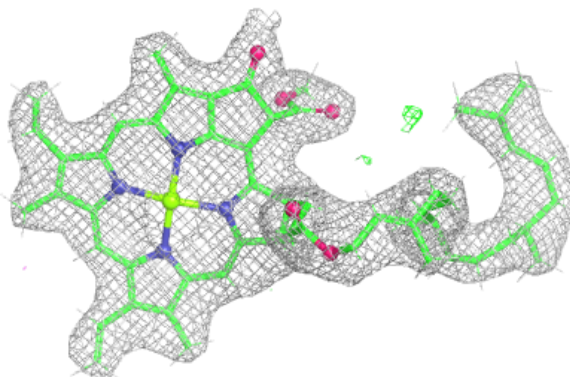


Electron density around CLA b 710:

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

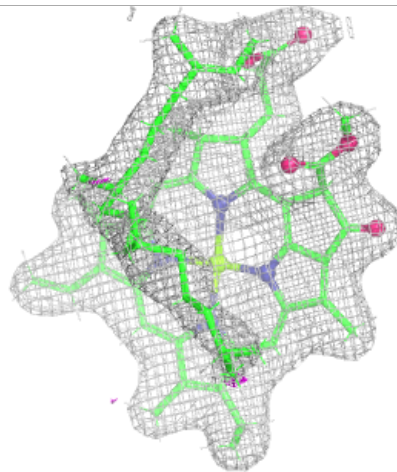
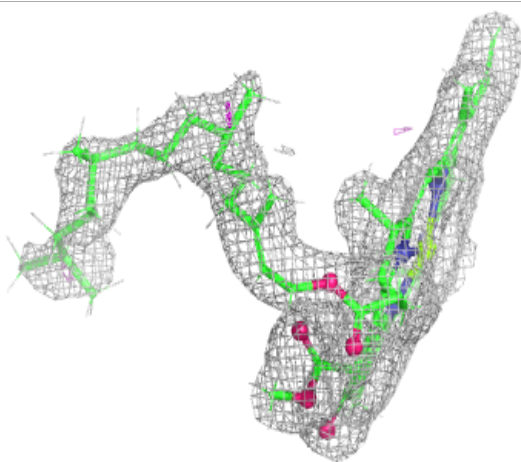
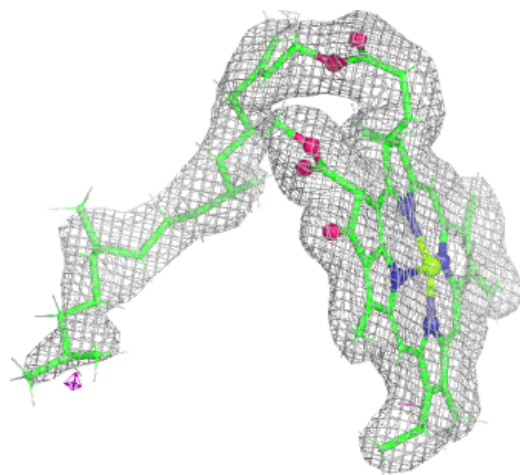
**Electron density around CLA b 712:**

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



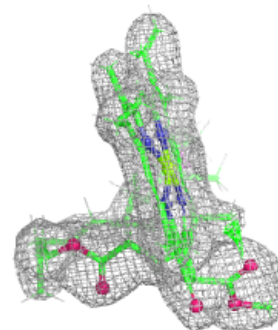
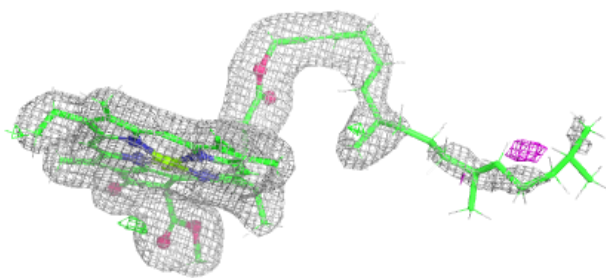
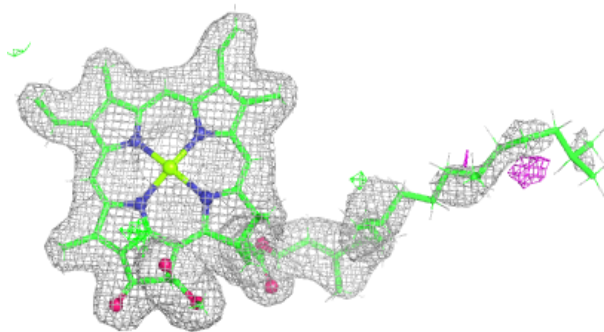
Electron density around CLA b 713:

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

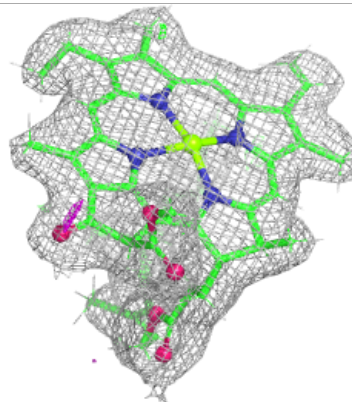
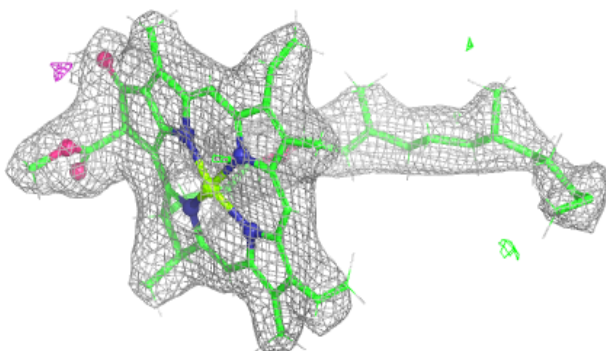
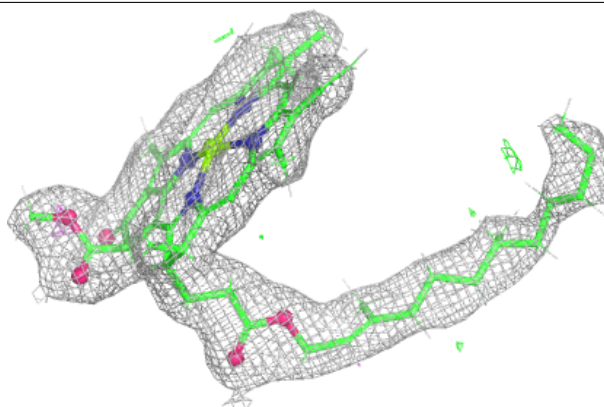


Electron density around CLA A 403:

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

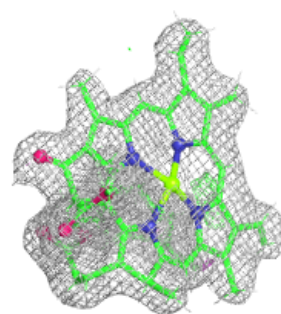
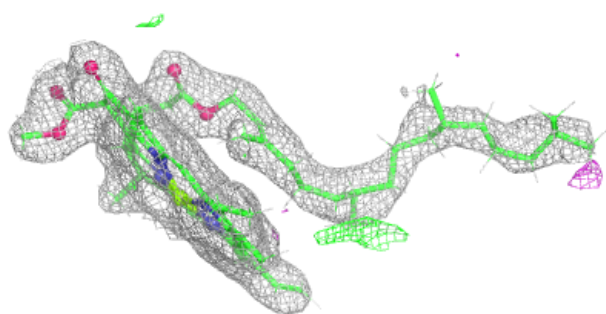
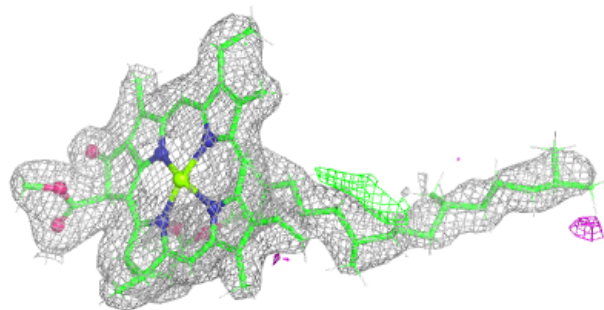
**Electron density around CLA C 505:**

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

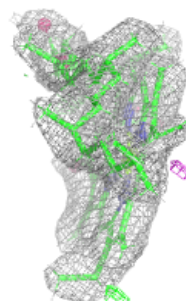
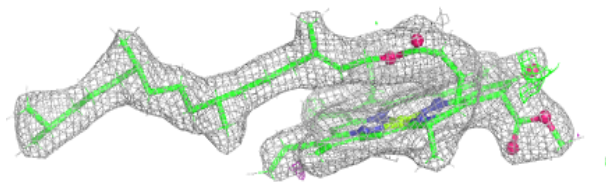
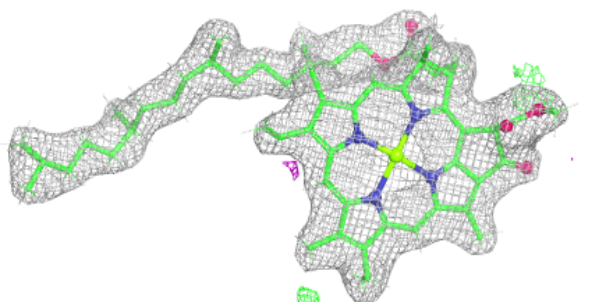


Electron density around CLA C 506:

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

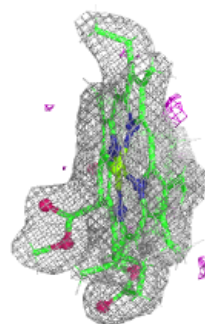
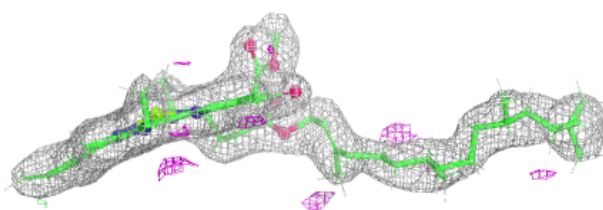
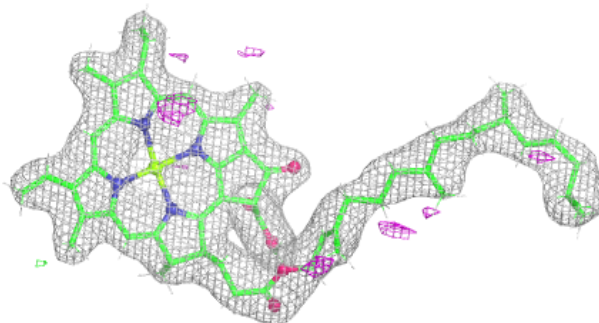
**Electron density around CLA c 502:**

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

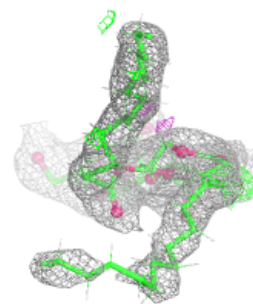
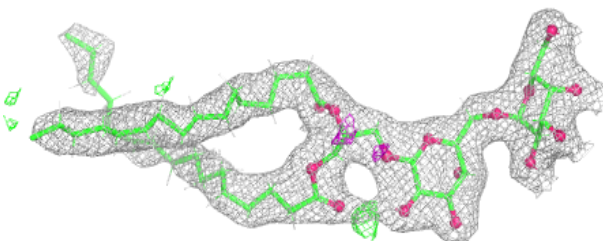
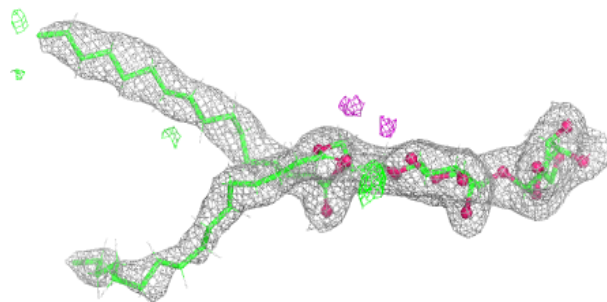


Electron density around CLA B 702:

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

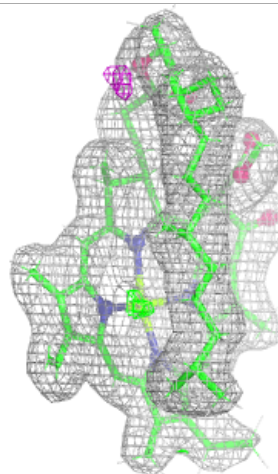
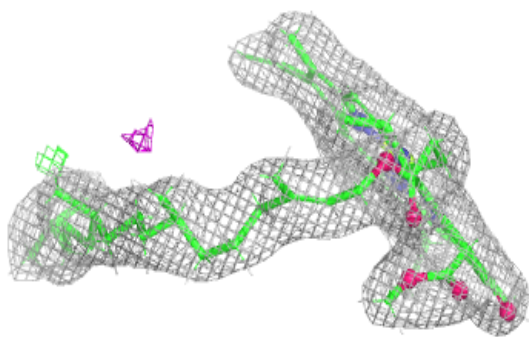
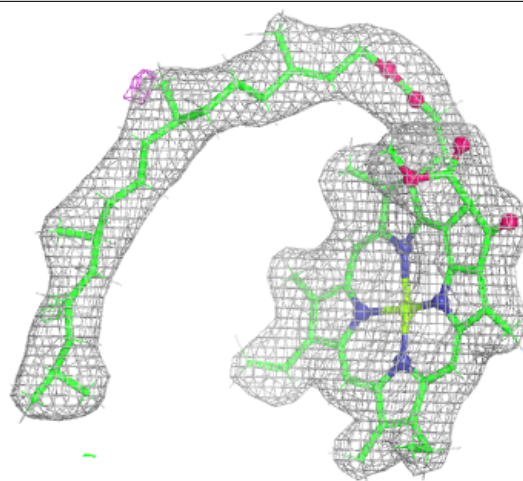
**Electron density around DGD c 517:**

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



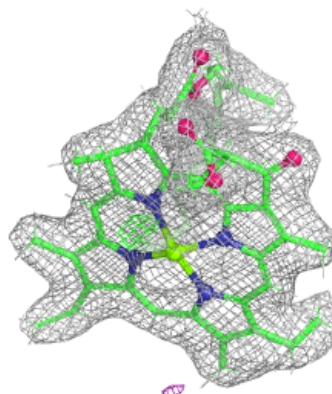
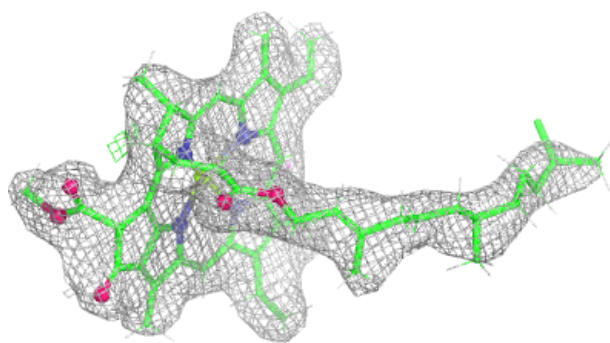
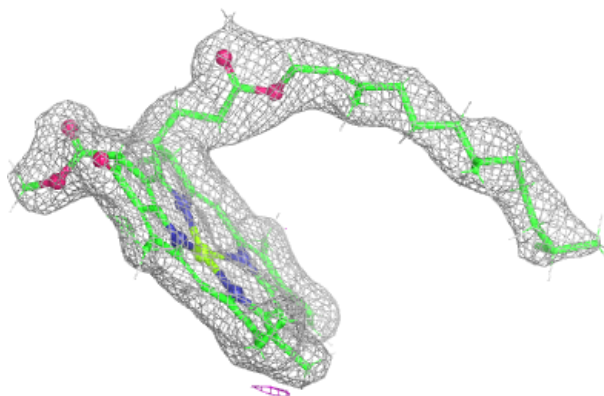
Electron density around CLA C 508:

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

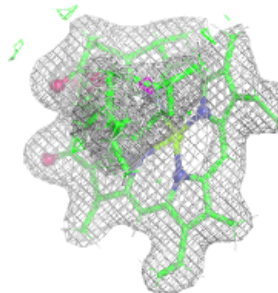
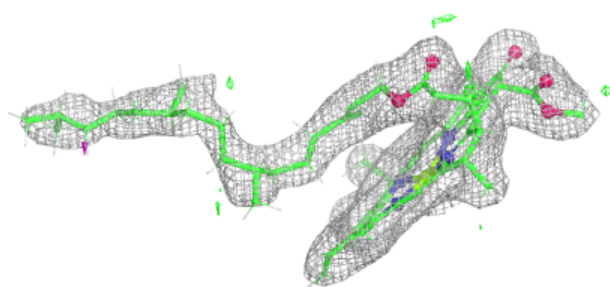
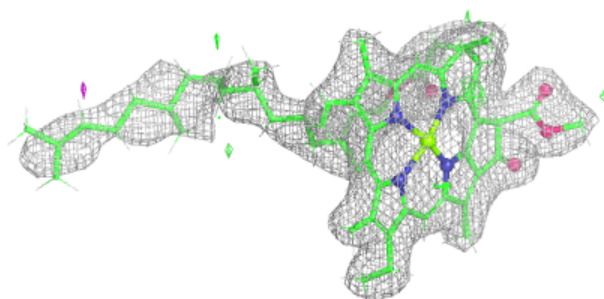


Electron density around CLA c 505:

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

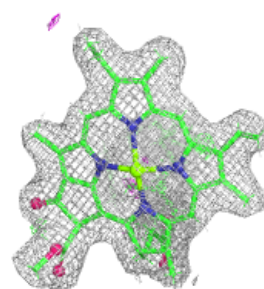
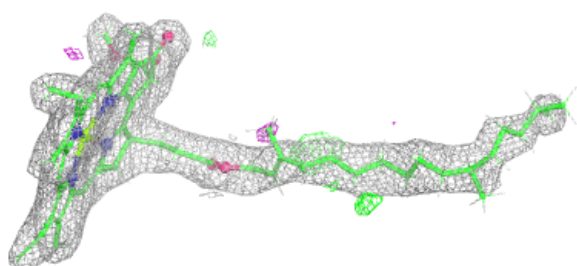
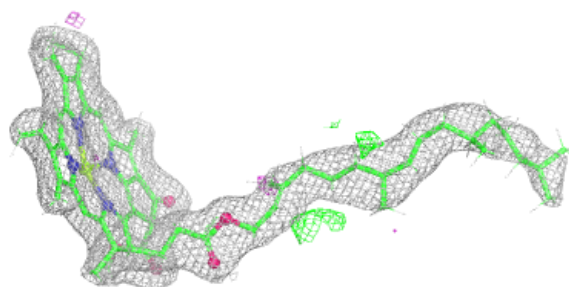
**Electron density around CLA c 506:**

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

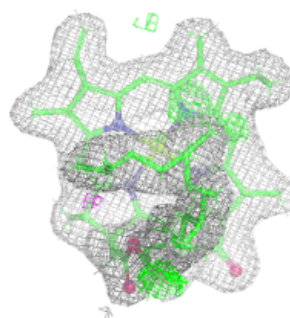
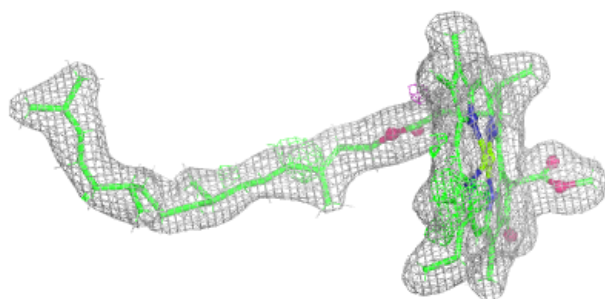
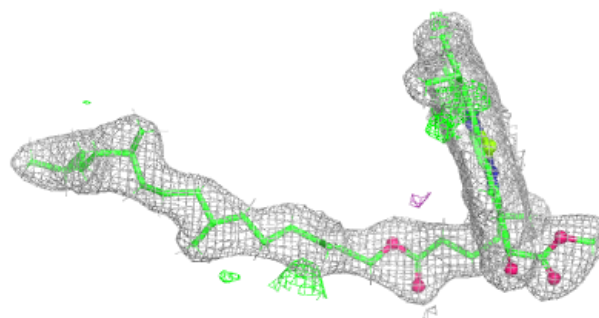


Electron density around CLA B 704:

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

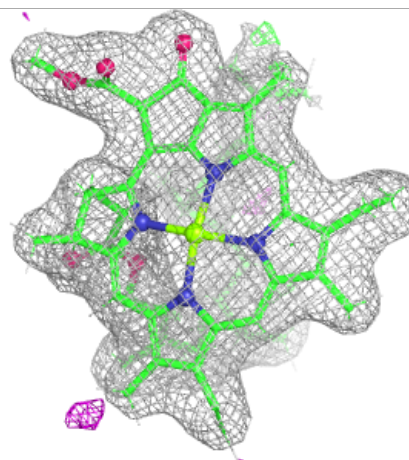
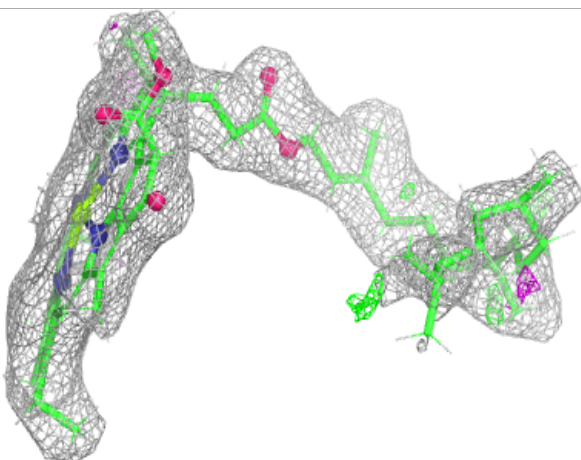
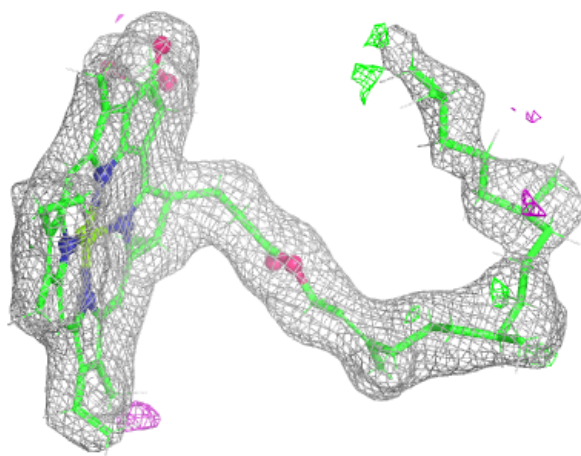
**Electron density around CLA B 705:**

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



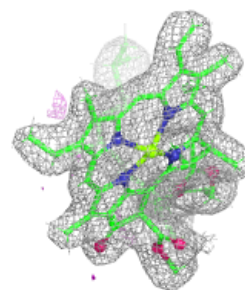
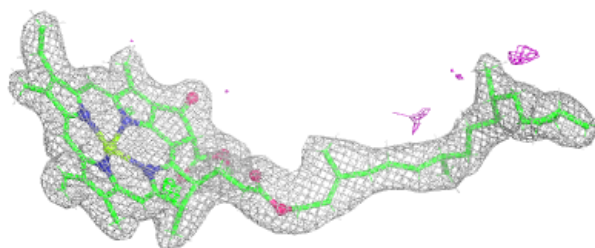
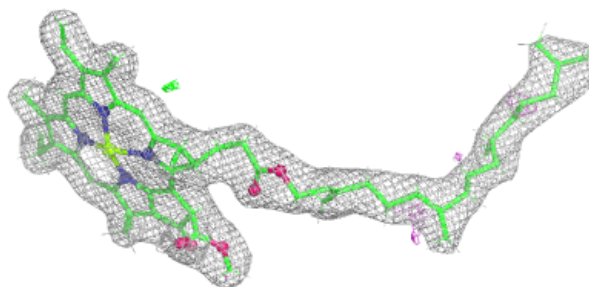
Electron density around CLA B 706:

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



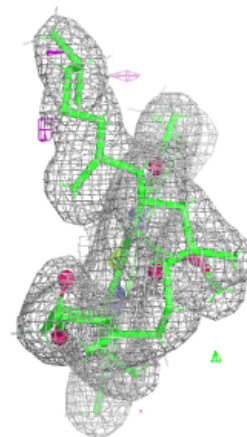
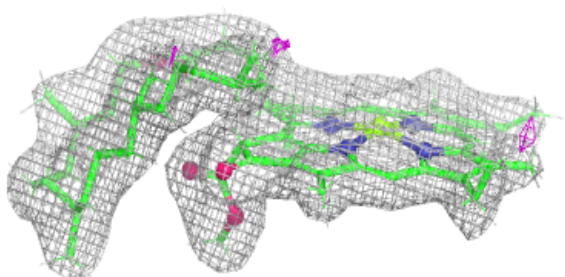
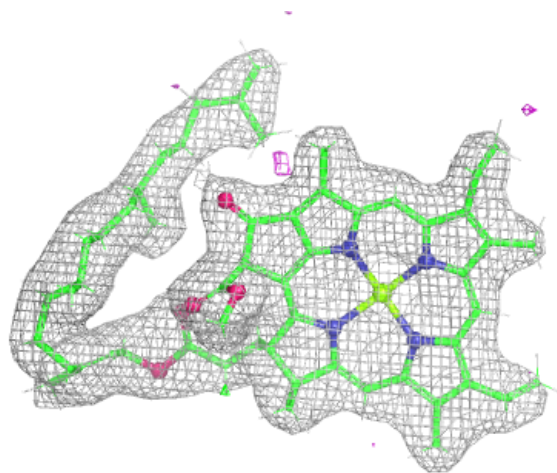
Electron density around CLA A 402:

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



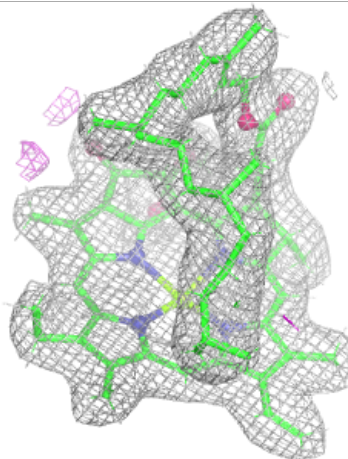
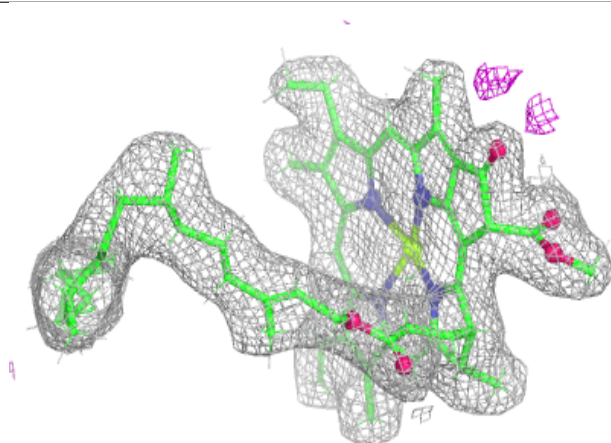
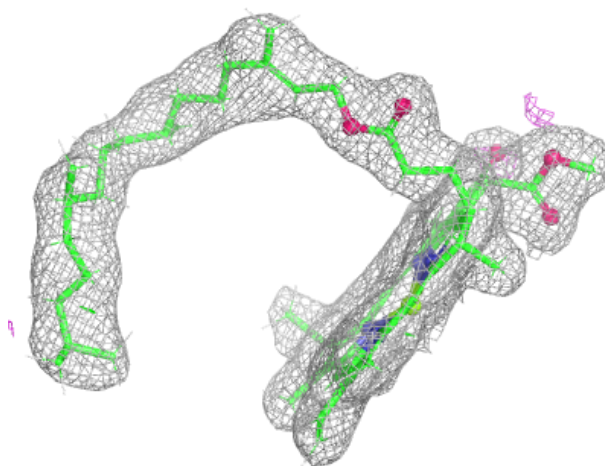
Electron density around CLA B 710:

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



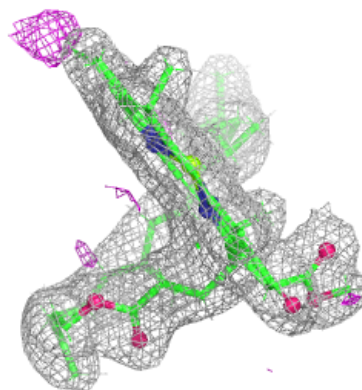
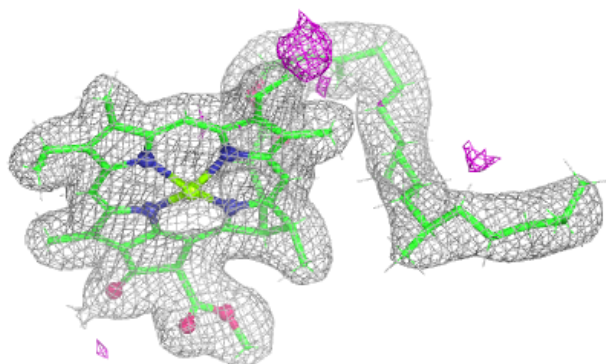
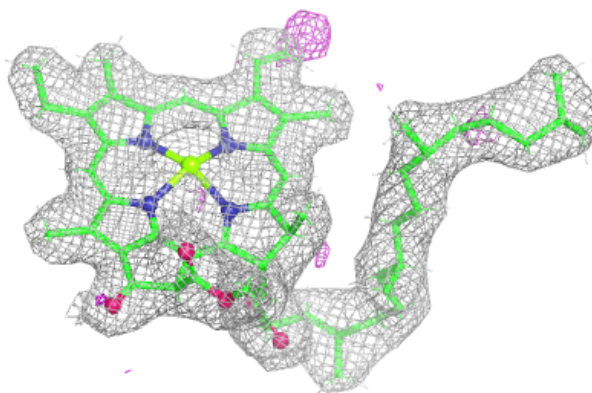
Electron density around CLA B 711:

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

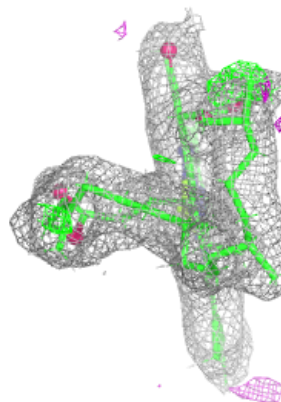
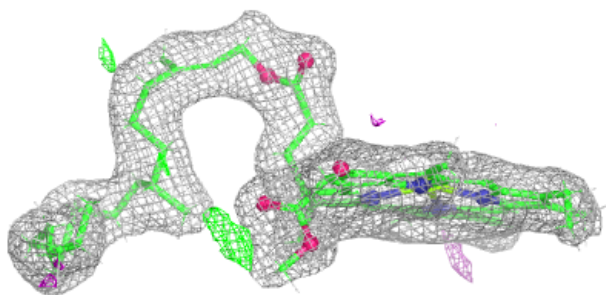
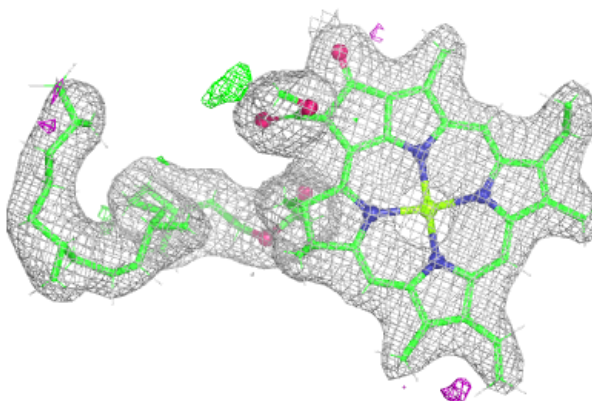


Electron density around CLA D 402:

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

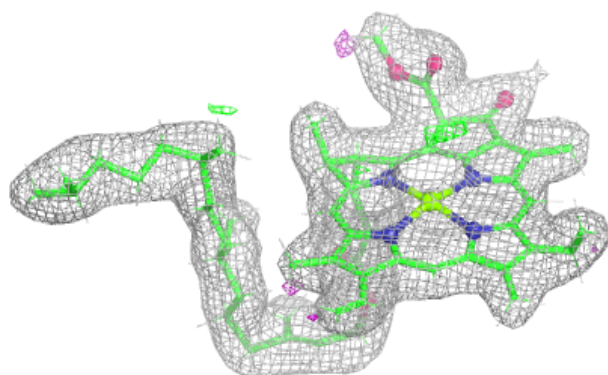
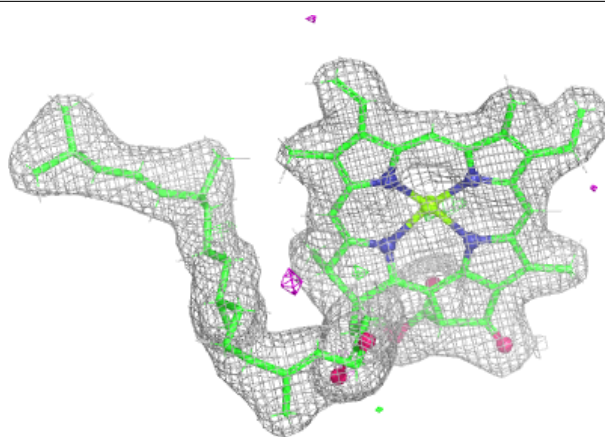
**Electron density around CLA B 712:**

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

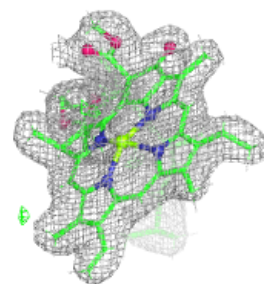
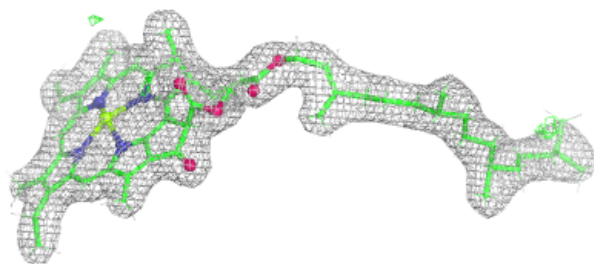
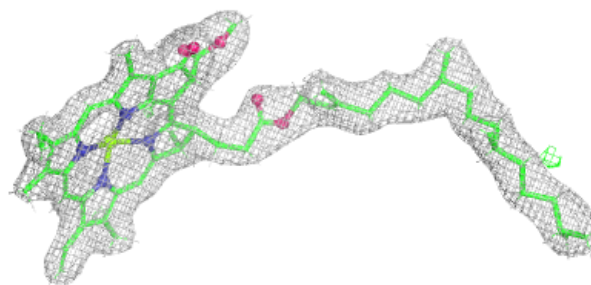


Electron density around CLA a 401:

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

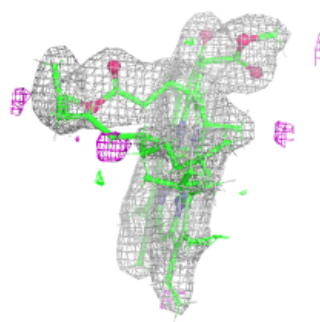
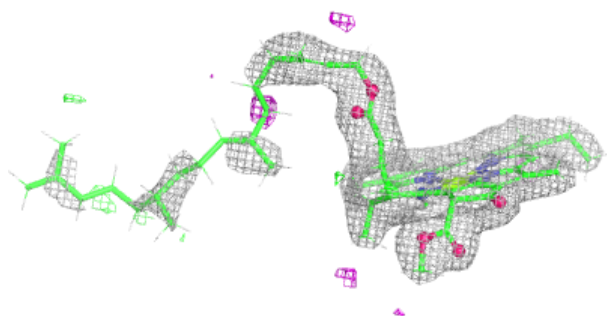
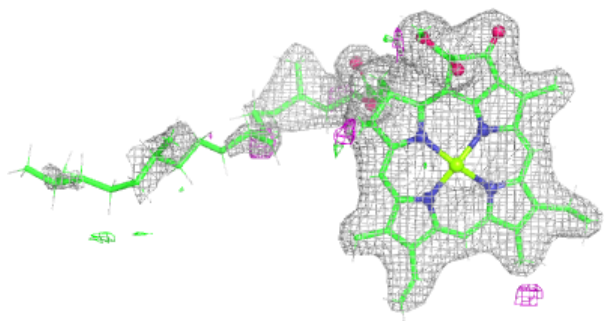
**Electron density around CLA a 403:**

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

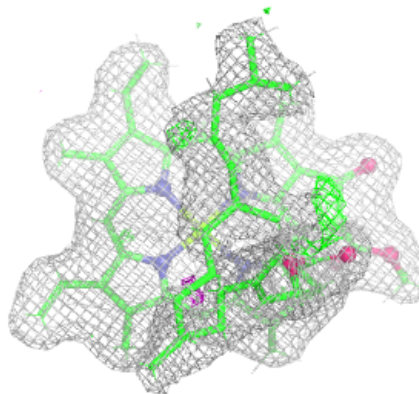
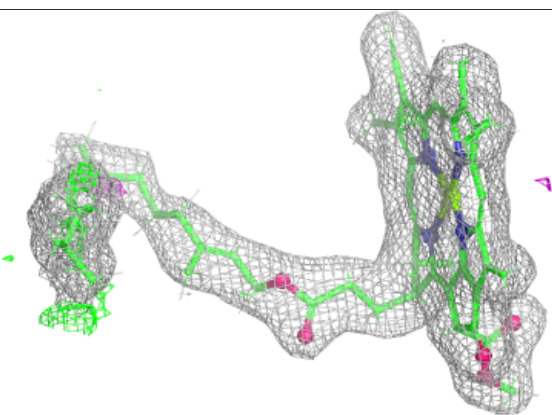
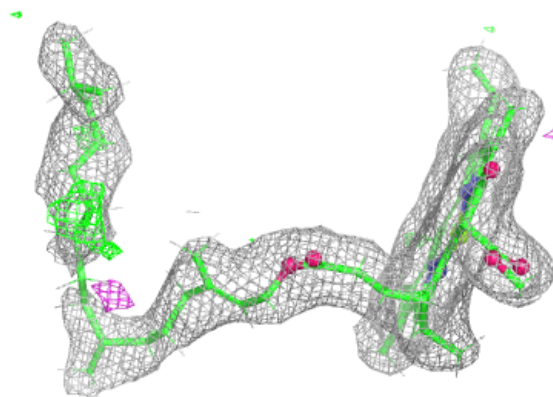


Electron density around CLA a 404:

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

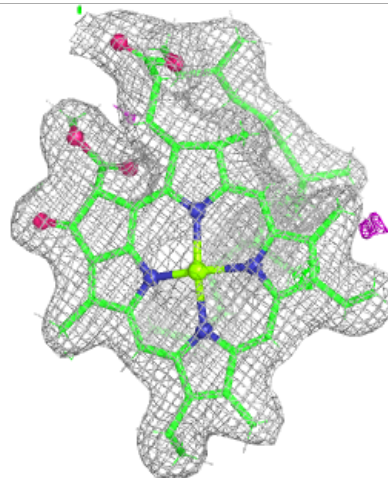
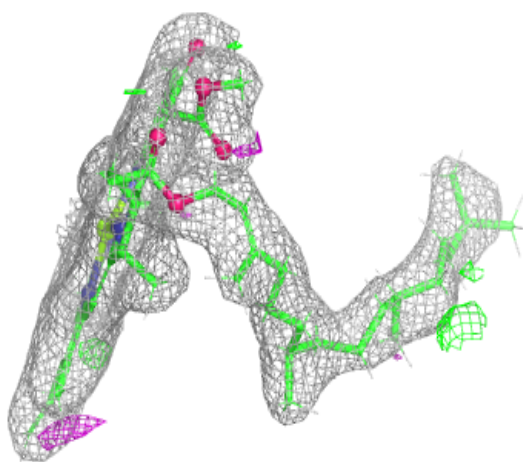
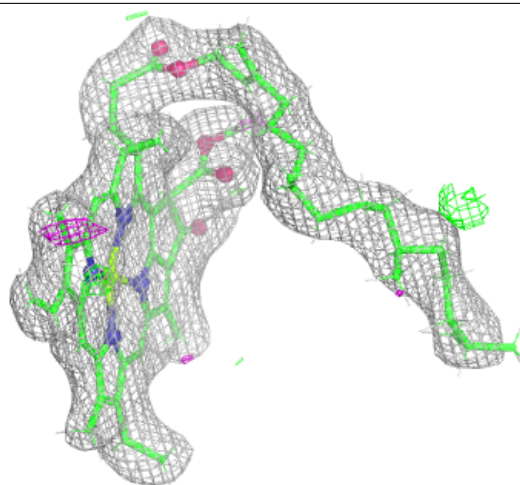
**Electron density around CLA a 406:**

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



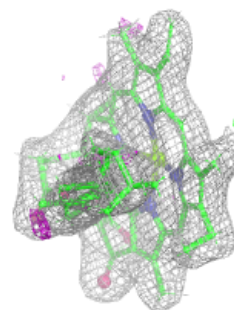
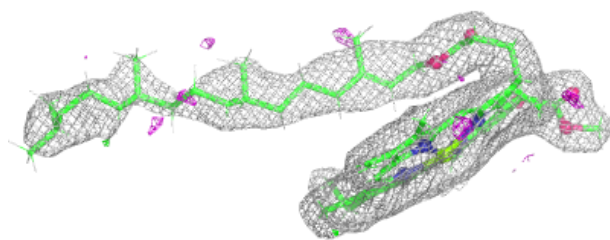
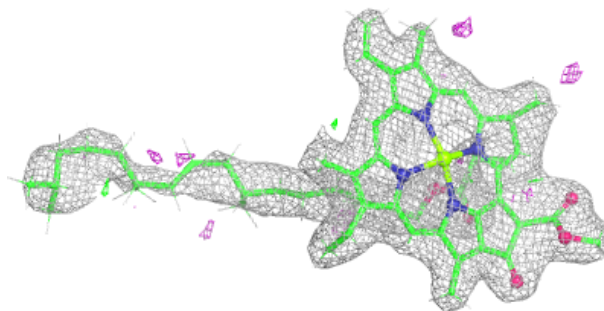
Electron density around CLA B 713:

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



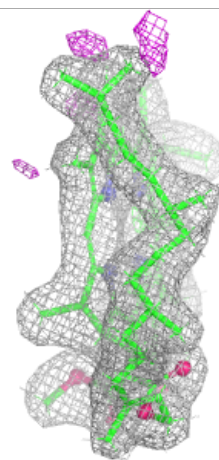
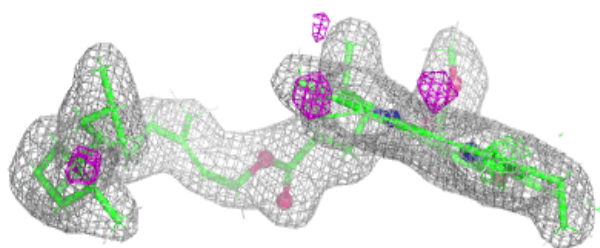
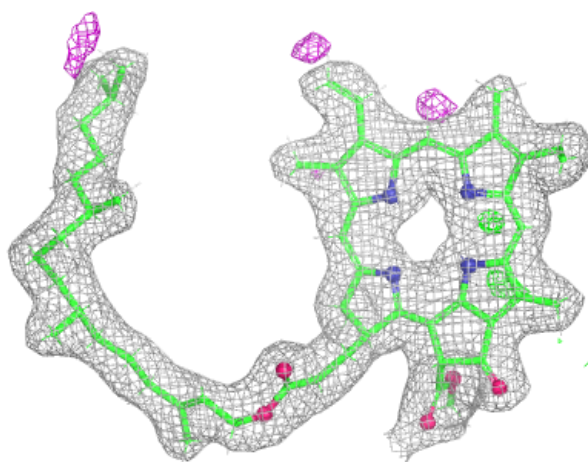
Electron density around CLA B 714:

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



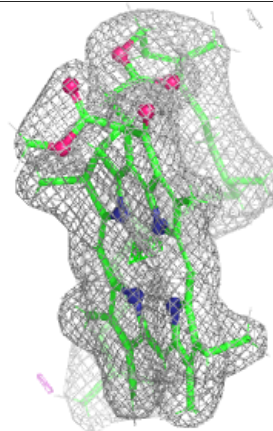
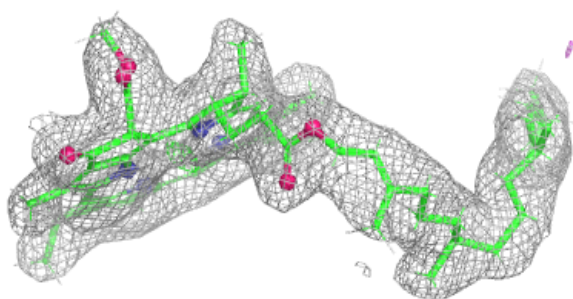
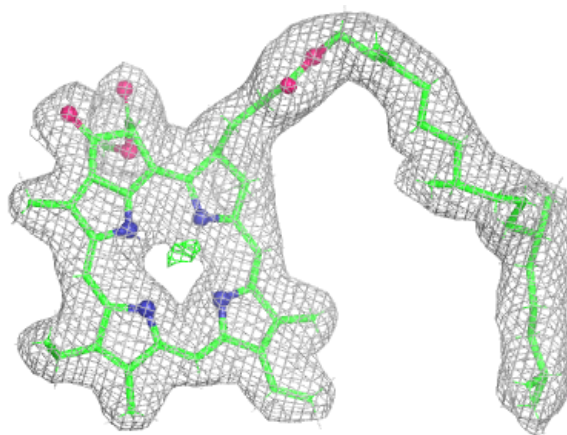
Electron density around PHO D 406:

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



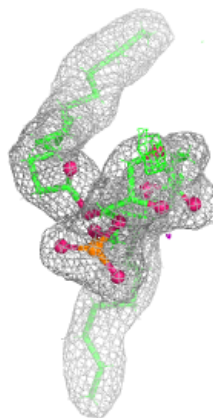
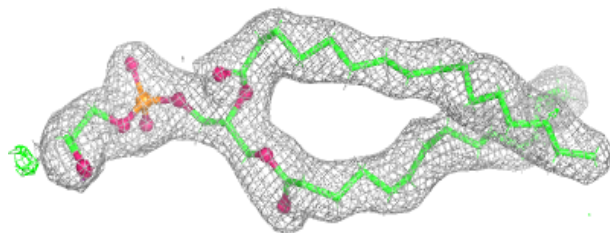
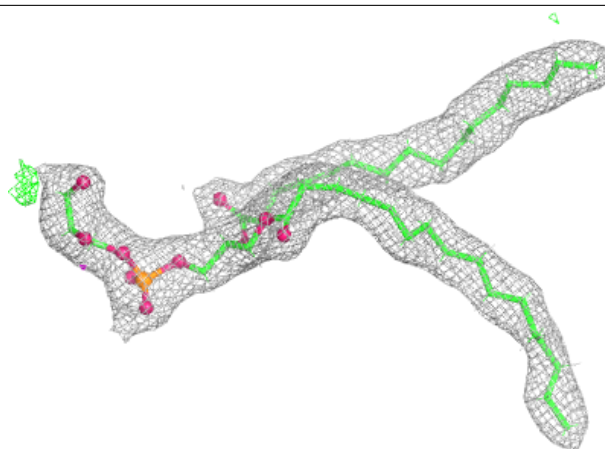
Electron density around PHO D 407:

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



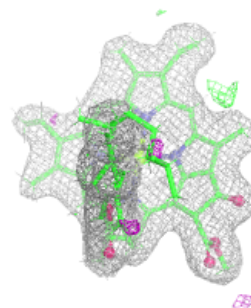
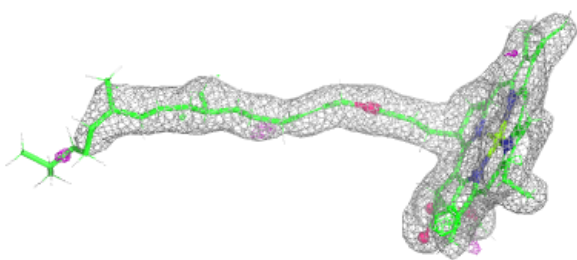
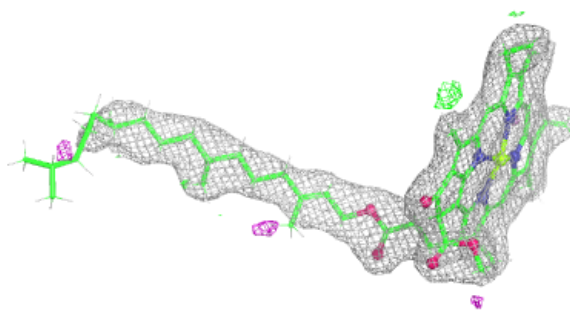
Electron density around LHG D 410:

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



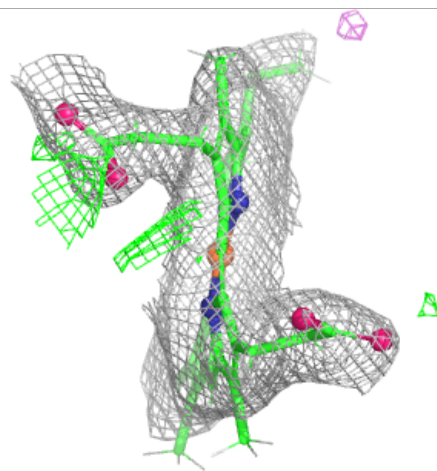
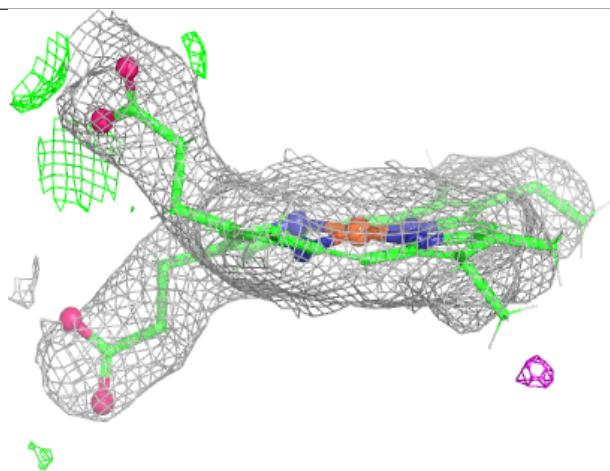
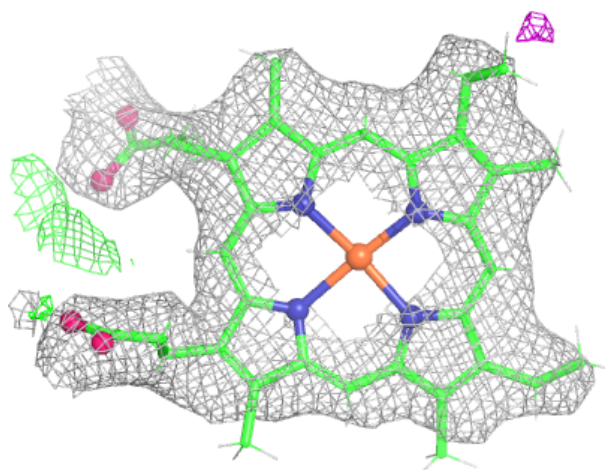
Electron density around CLA b 704:

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



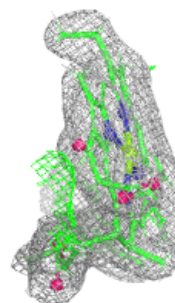
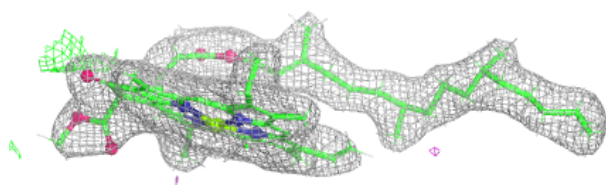
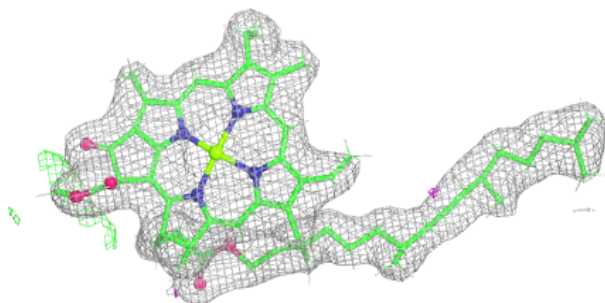
Electron density around HEC e 101:

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

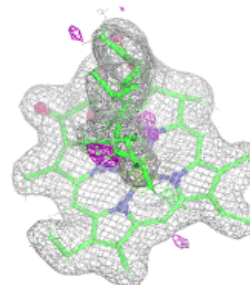
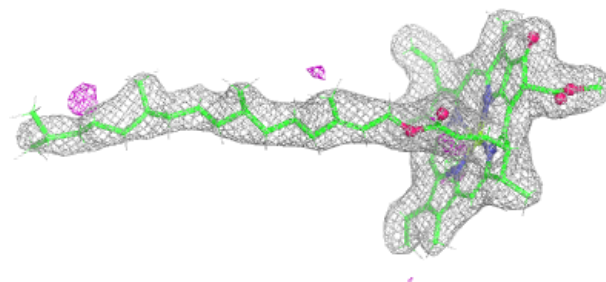
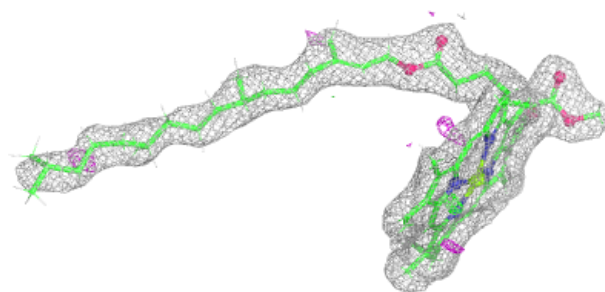


Electron density around CLA C 502:

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

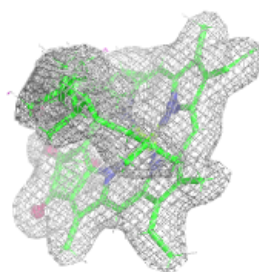
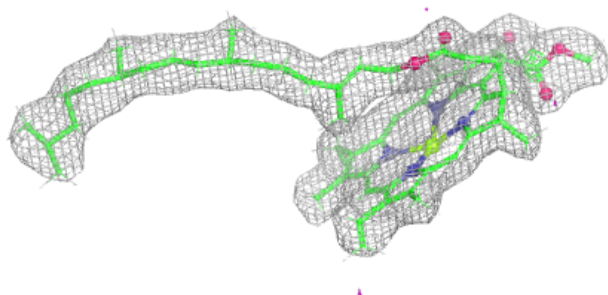
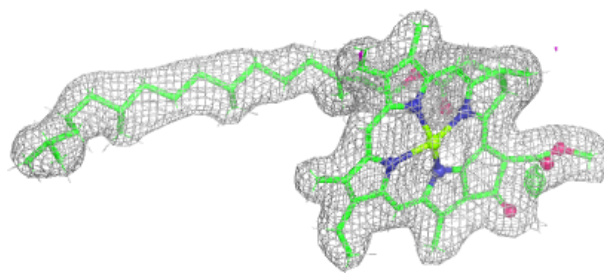
**Electron density around CLA B 707:**

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

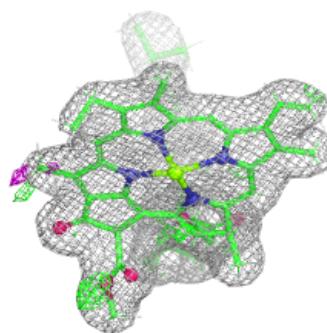
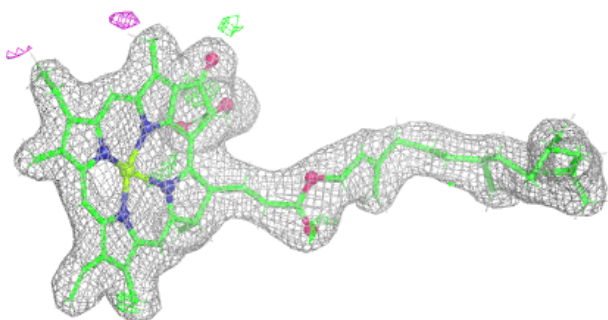
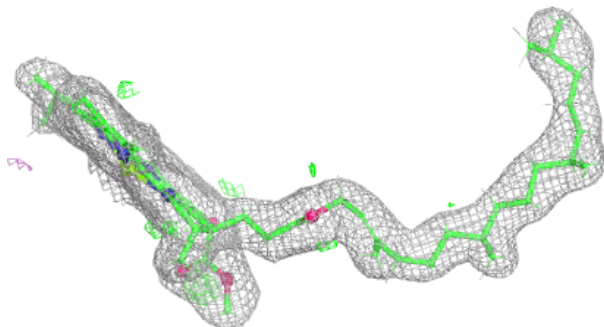


Electron density around CLA B 708:

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

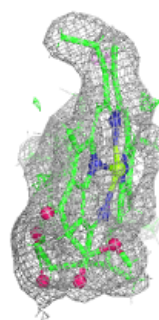
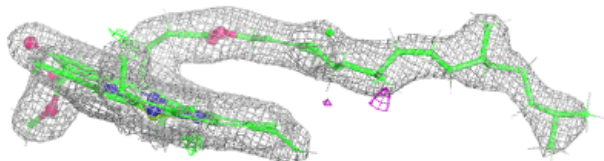
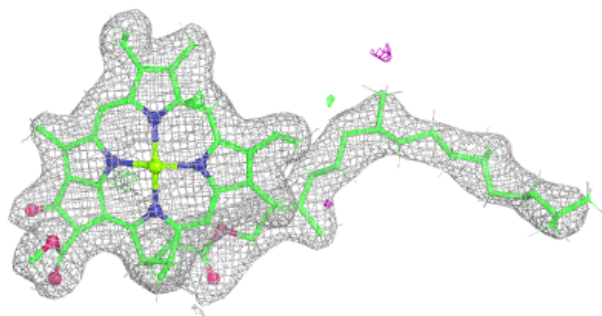
**Electron density around CLA D 401:**

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

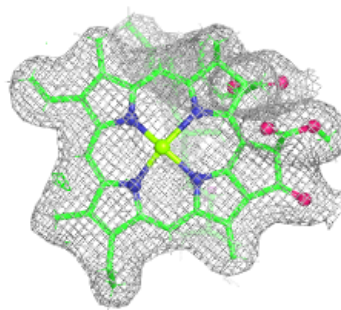
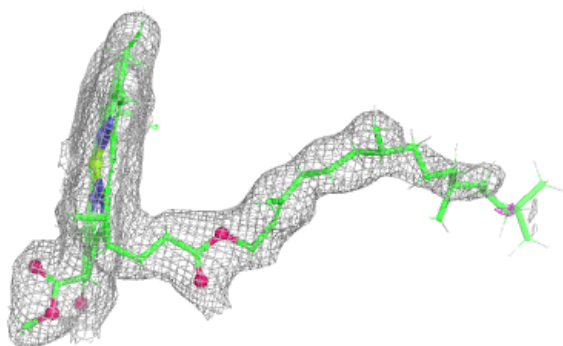
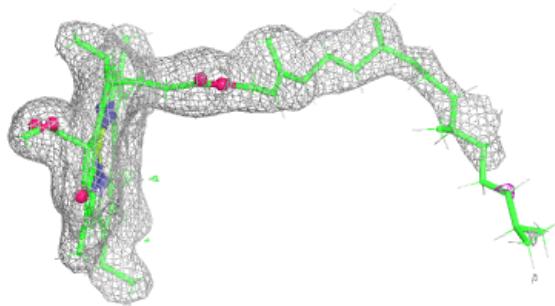


Electron density around CLA B 703:

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

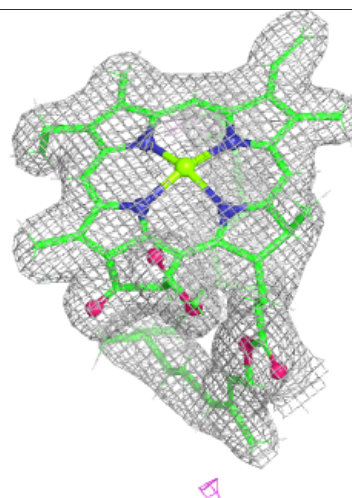
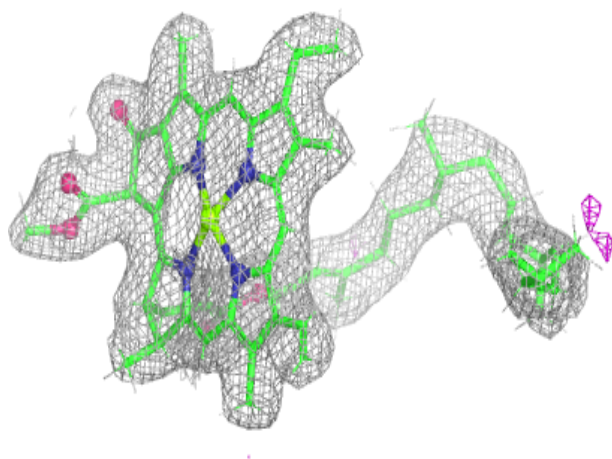
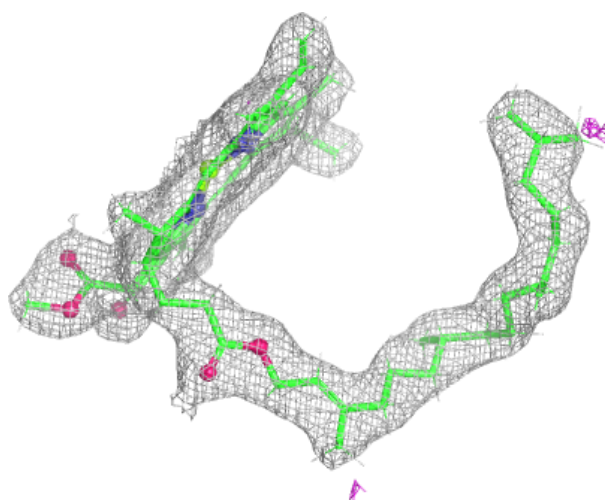
**Electron density around CLA D 403:**

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



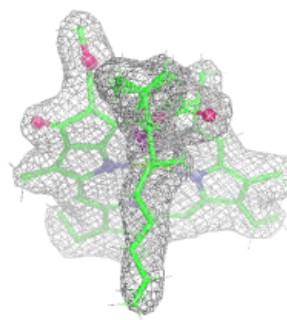
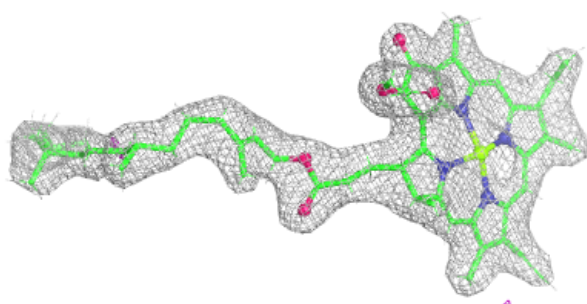
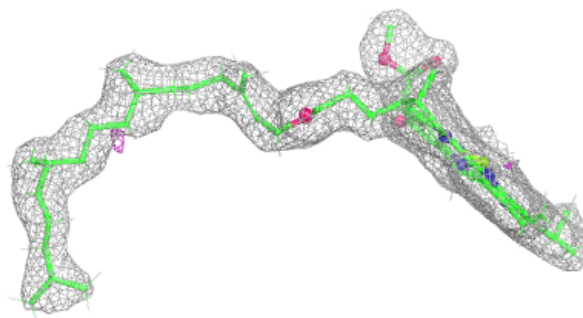
Electron density around CLA b 711:

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

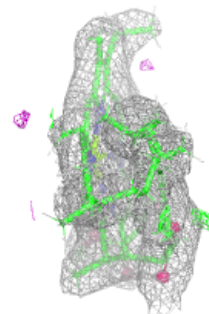
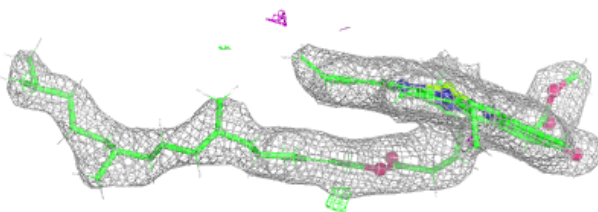
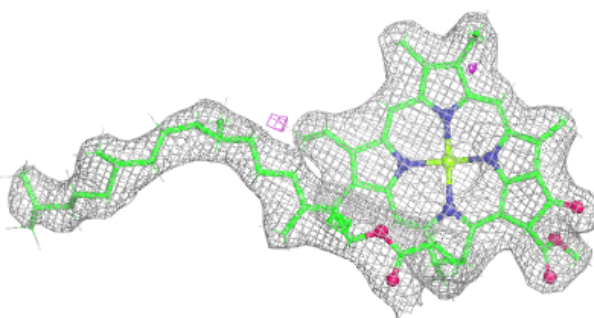


Electron density around CLA d 401:

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

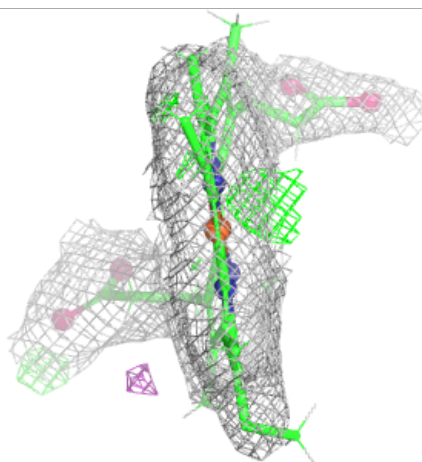
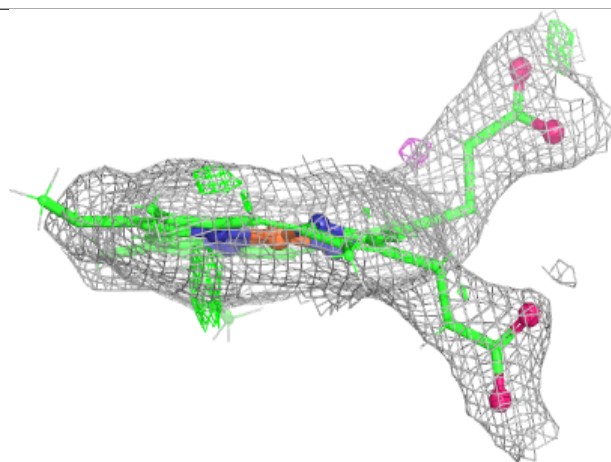
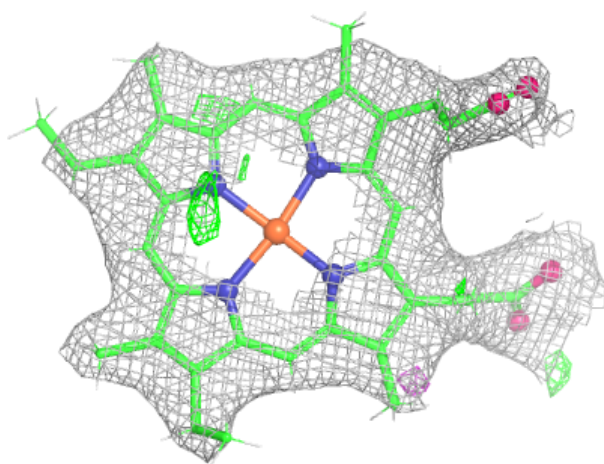
**Electron density around CLA b 703:**

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



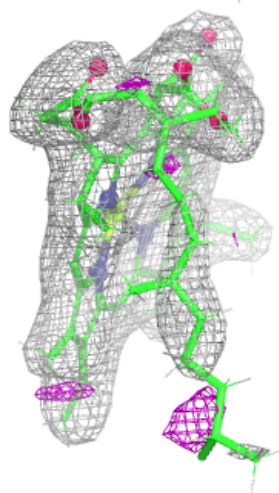
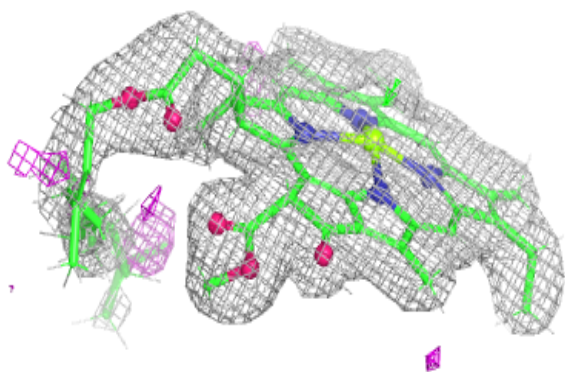
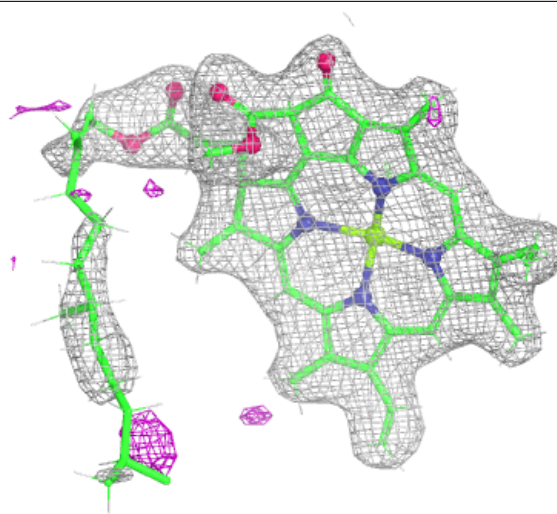
Electron density around HEC E 103:

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



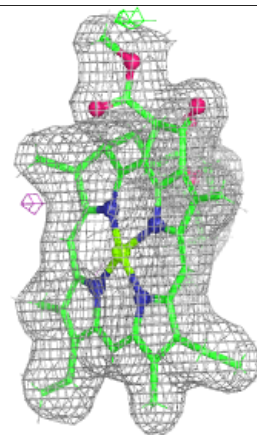
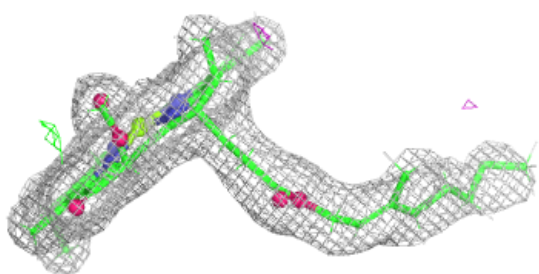
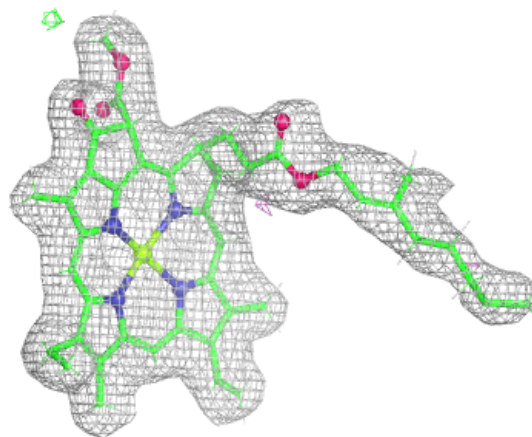
Electron density around CLA B 716:

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



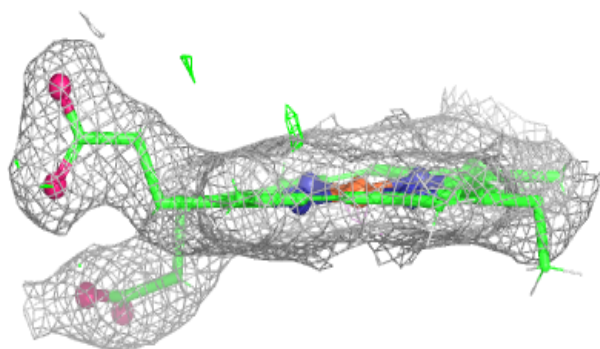
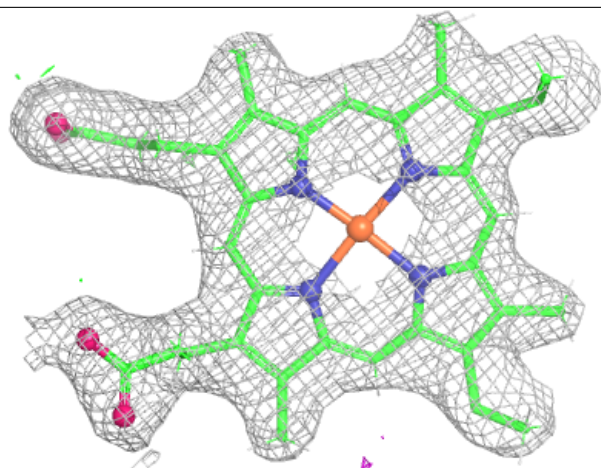
Electron density around CLA A 404:

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



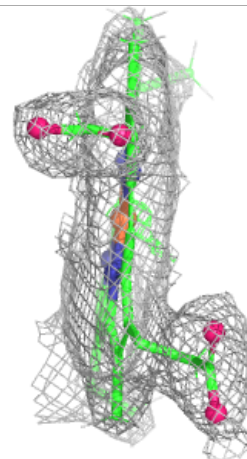
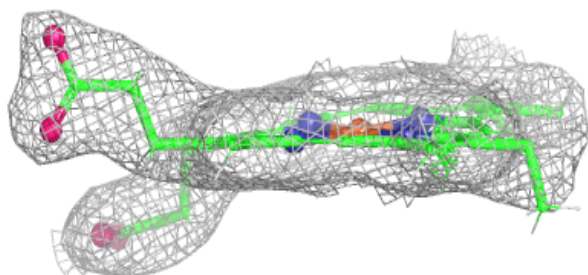
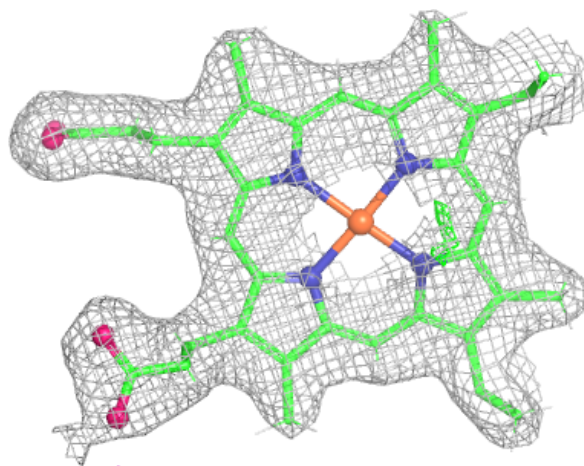
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.