



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 02:24 PM EDT

PDB ID : 9Z6A / pdb_00009z6a
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3 rich) at 1.93 Angstrom obtained from conventional data at 9.5 keV
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Minnetian, N.M.; Zhang, M.
Deposited on : 2025-11-14
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

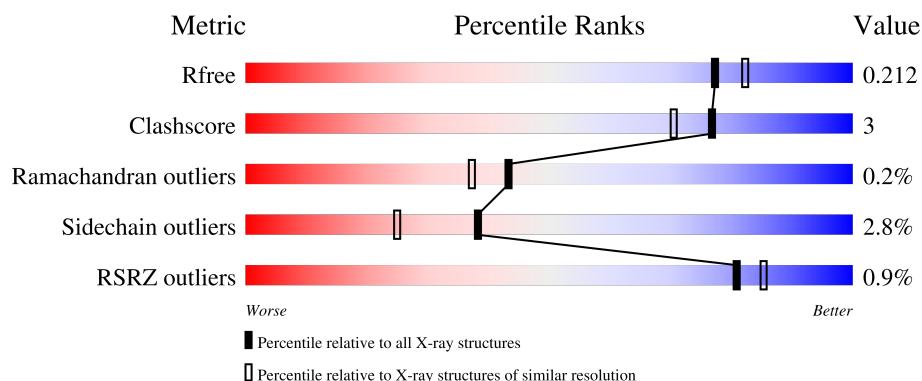
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



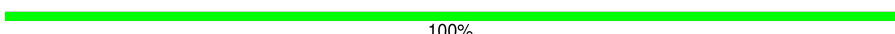
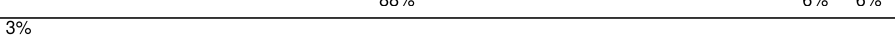
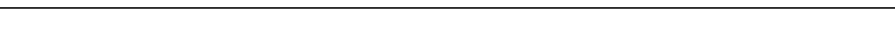
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	92% 6% .
1	a	344	89% 7% ..
2	B	510	95% . ..
2	b	510	% 95% 5% .

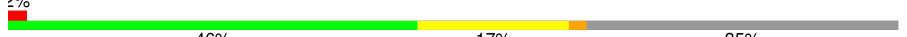
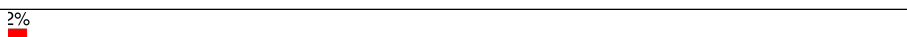
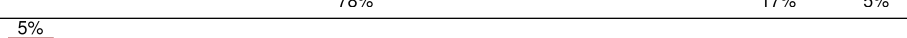
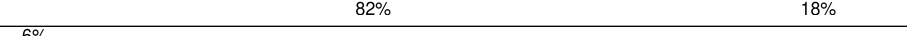
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

Continued on next page...

Continued from previous page...

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

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

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 107900 atoms, of which 53180 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	72	0
			6074	2055	2922	520	558	19			
1	a	334	Total	C	H	N	O	S	0	72	0
			6062	2052	2913	520	558	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	7	0
			7903	2637	3887	670	696	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7826	2614	3842	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	14	0
			6925	2302	3416	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7070	2343	3487	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	11	0
			5509	1859	2704	456	478	12			
4	d	341	Total	C	H	N	O	S	0	12	0
			5521	1863	2710	456	480	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1033	335	528	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1007	327	514	80	83			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	conflict	UNP Q8DJ43
h	41	CYS	PHE	conflict	UNP Q8DJ43

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
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
			523	171	267	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

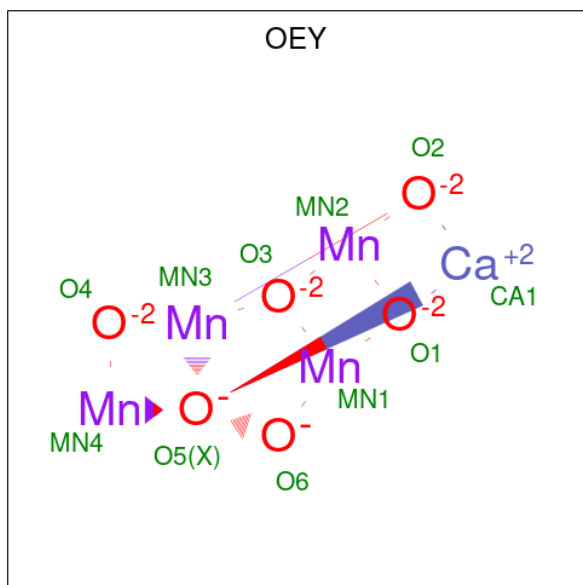
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

Continued on next page...

Continued from previous page...

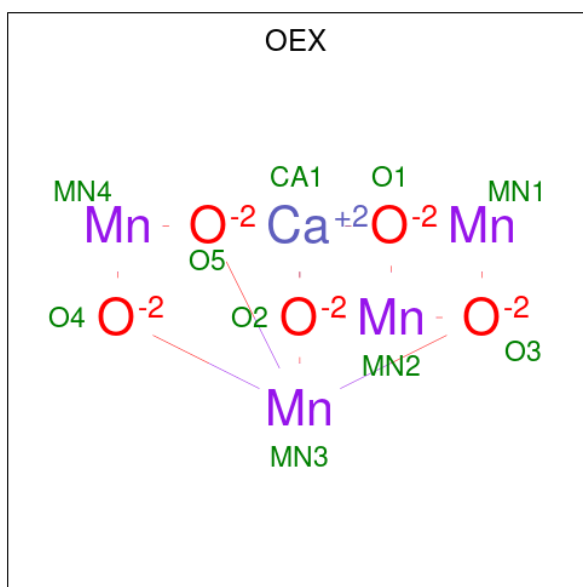
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

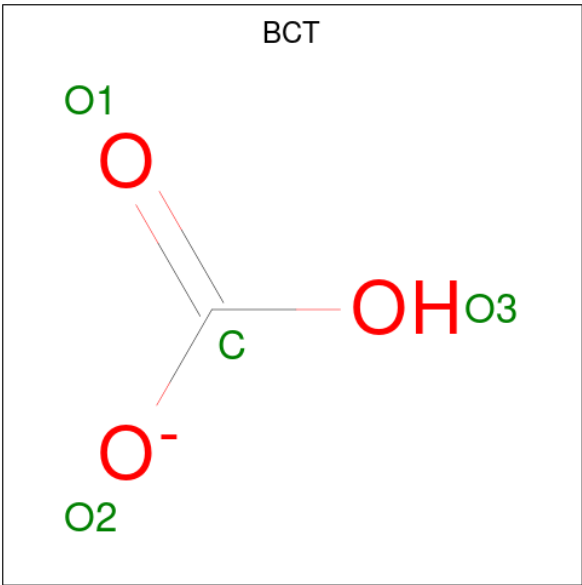
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

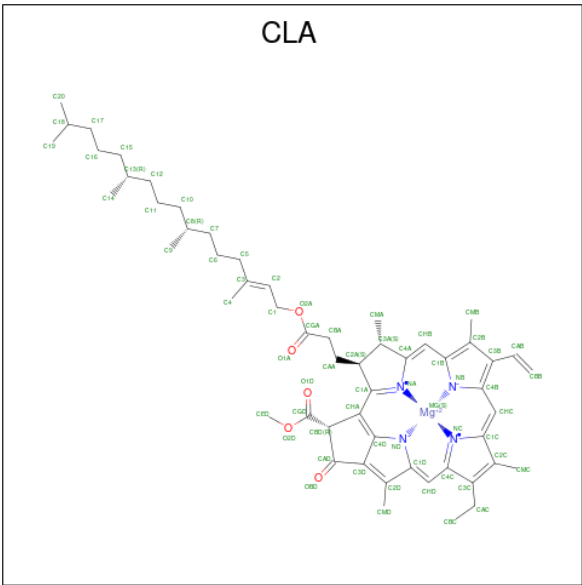
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

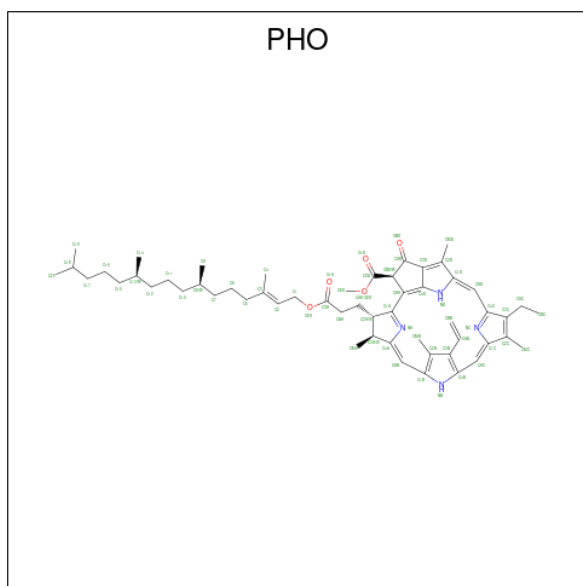
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
26	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
26	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
26	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
26	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
26	b	1	Total 137	C 55	H 72	Mg 1	N 4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

Continued on next page...

Continued from previous page...

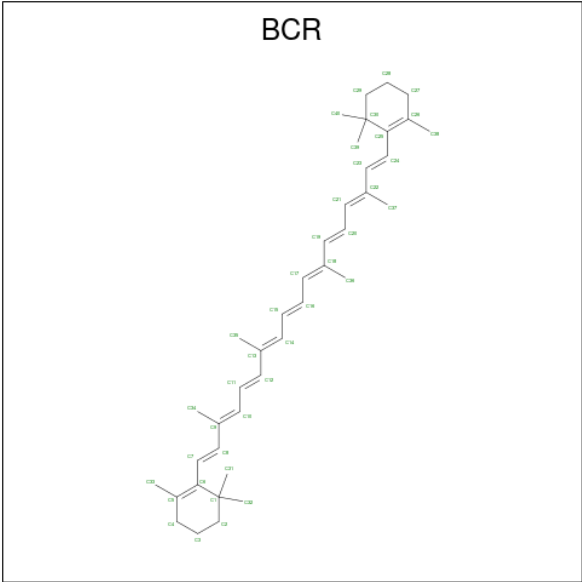
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
26	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



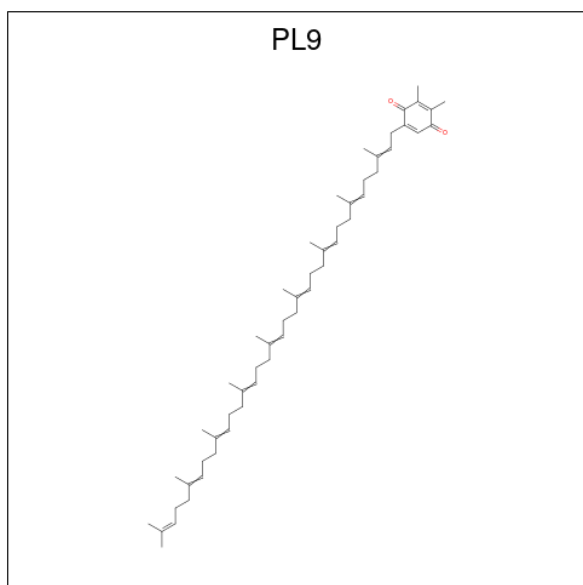
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	B	1	Total	C	H	0	0
			96	40	56		
28	C	1	Total	C	H	0	0
			96	40	56		
28	C	1	Total	C	H	0	0
			96	40	56		
28	D	1	Total	C	H	0	0
			96	40	56		
28	H	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



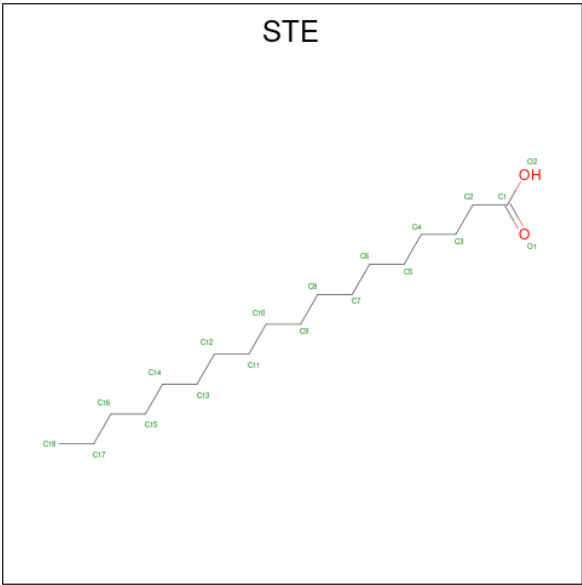
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			135	53	80	2		
29	D	1	Total	C	H	O	0	0
			135	53	80	2		

Continued on next page...

Continued from previous page...

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

- Molecule 30 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H		0	0
			23	9	14			
30	A	1	Total	C	H		0	0
			23	8	15			
30	A	1	Total	C	H		0	0
			50	17	33			
30	A	1	Total	C	H		0	0
			32	11	21			
30	B	1	Total	C	H	O	0	0
			43	15	26	2		
30	B	1	Total	C	H	O	0	0
			34	12	20	2		
30	B	1	Total	C	H	O	0	0
			46	16	28	2		
30	B	1	Total	C	H	O	0	0
			28	10	16	2		
30	B	1	Total	C	H		0	0
			41	15	26			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C H O 34 12 20 2	0	0
30	C	1	Total C H 11 5 6	0	0
30	C	1	Total C H 17 7 10	0	0
30	C	1	Total C H 26 10 16	0	0
30	C	1	Total C H O 28 10 16 2	0	0
30	C	1	Total C H 47 16 31	0	0
30	C	1	Total C H 41 14 27	0	0
30	D	1	Total C H O 55 18 35 2	0	0
30	E	1	Total C H O 28 10 16 2	0	0
30	E	1	Total C H 35 12 23	0	0
30	E	1	Total C H O 55 18 35 2	0	0
30	H	1	Total C H 53 18 35	0	0
30	H	1	Total C H 26 9 17	0	0
30	I	1	Total C H O 43 15 26 2	0	0
30	I	1	Total C H O 37 13 22 2	0	0
30	J	1	Total C H O 28 10 16 2	0	0
30	K	1	Total C H 41 14 27	0	0
30	M	1	Total C H O 37 13 22 2	0	0
30	M	1	Total C H 26 10 16	0	0
30	T	1	Total C H 47 16 31	0	0
30	T	1	Total C H 44 15 29	0	0

Continued on next page...

Continued from previous page...

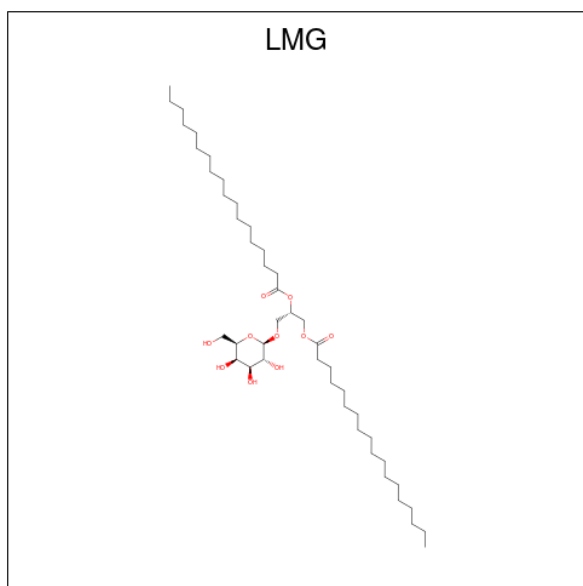
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Z	1	Total C H 50 17 33	0	0
30	a	1	Total C H O 28 10 16 2	0	0
30	b	1	Total C H O 55 18 35 2	0	0
30	b	1	Total C H O 40 14 24 2	0	0
30	b	1	Total C H 26 10 16	0	0
30	b	1	Total C H 32 11 21	0	0
30	c	1	Total C H 53 18 35	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	d	1	Total C H O 55 18 35 2	0	0
30	e	1	Total C H 26 9 17	0	0
30	e	1	Total C H 23 8 15	0	0
30	e	1	Total C H 26 9 17	0	0
30	e	1	Total C H O 31 11 18 2	0	0
30	h	1	Total C H 29 10 19	0	0
30	i	1	Total C H O 28 10 16 2	0	0
30	i	1	Total C H 14 6 8	0	0
30	j	1	Total C H O 28 10 16 2	0	0
30	j	1	Total C H 47 16 31	0	0
30	k	1	Total C H O 34 12 20 2	0	0
30	m	1	Total C H O 28 10 16 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	H	0	0
			53	18	35		
30	t	1	Total	C	H	0	0
			26	10	16		
30	z	1	Total	C	H	0	0
			35	13	22		
30	z	1	Total	C	H	0	0
			23	9	14		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



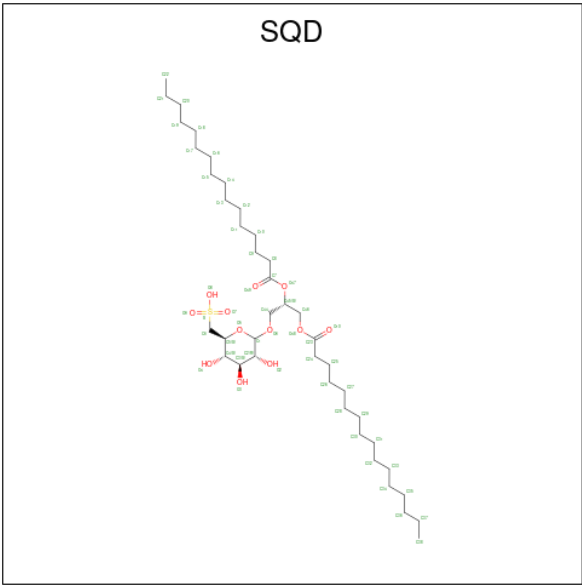
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			114	38	66	10		
31	B	1	Total	C	H	O	0	0
			105	35	60	10		
31	C	1	Total	C	H	O	0	0
			76	26	40	10		
31	C	1	Total	C	H	O	0	0
			114	38	66	10		
31	D	1	Total	C	H	O	0	0
			120	40	70	10		
31	D	1	Total	C	H	O	0	0
			123	41	72	10		
31	M	1	Total	C	H	O	0	0
			123	41	72	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	a	1	Total	C	H	O	0	0
			141	45	86	10		
31	a	1	Total	C	H	O	0	0
			117	39	68	10		
31	b	1	Total	C	H	O	0	0
			141	45	86	10		
31	c	1	Total	C	H	O	0	0
			71	25	41	5		
31	c	1	Total	C	H	O	0	0
			108	36	62	10		
31	c	1	Total	C	H	O	0	0
			117	38	69	10		
31	d	1	Total	C	H	O	0	0
			102	34	58	10		
31	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



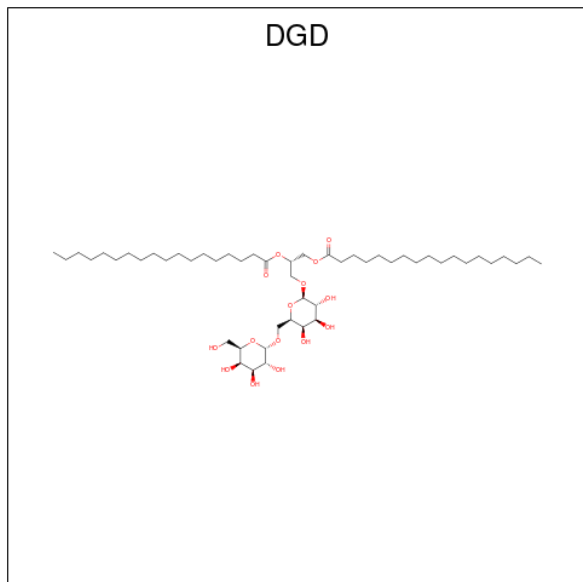
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	A	1	Total 95	C 30	H 52	O 12	S 1	0	0
32	B	1	Total 131	C 41	H 77	O 12	S 1	0	0
32	D	1	Total 122	C 39	H 70	O 12	S 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



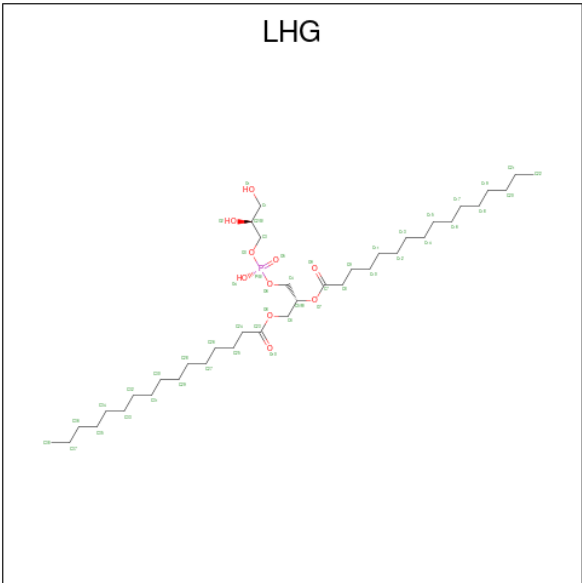
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	A	1	Total	C	H	O		0	0
			150	51	84	15			
33	C	1	Total	C	H	O		0	0
			132	47	70	15			
33	C	1	Total	C	H	O		0	0
			132	47	70	15			
33	C	1	Total	C	H	O		0	0
			132	47	70	15			
33	H	1	Total	C	H	O		0	0
			132	47	70	15			
33	c	1	Total	C	H	O		0	0
			132	47	70	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	c	1	Total	C	H	O	0	0
			132	47	70	15		
33	c	1	Total	C	H	O	0	0
			132	47	70	15		
33	h	1	Total	C	H	O	0	0
			132	47	70	15		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



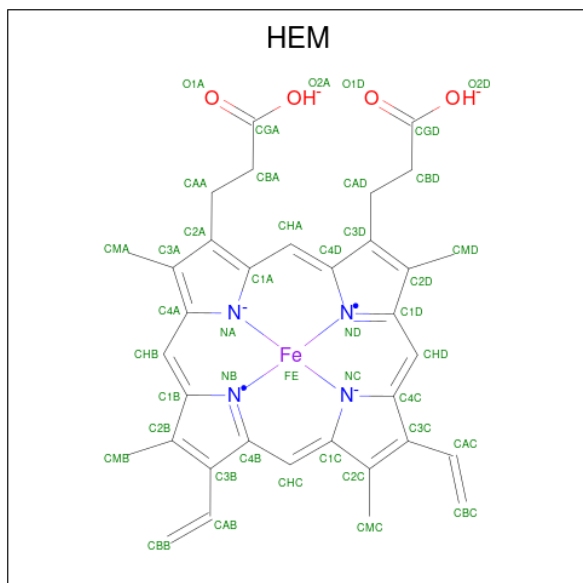
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
34	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
34	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		

Continued on next page...

Continued from previous page...

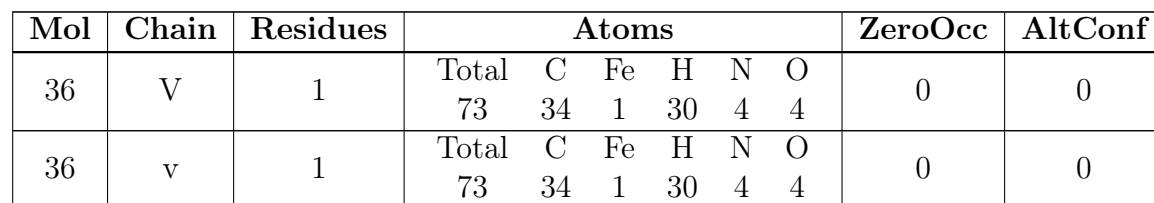
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	e	1	Total 99	C 31	H 57	O 10	P 1	0	0
34	l	1	Total 123	C 38	H 74	O 10	P 1	0	0

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



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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 37 | A | 178 | Total O
182 182 | 0 | 4 |
| 37 | B | 319 | Total O
319 319 | 0 | 0 |
| 37 | C | 254 | Total O
254 254 | 0 | 0 |
| 37 | D | 159 | Total O
159 159 | 0 | 0 |
| 37 | E | 42 | Total O
42 42 | 0 | 0 |
| 37 | F | 20 | Total O
20 20 | 0 | 0 |
| 37 | H | 41 | Total O
41 41 | 0 | 0 |
| 37 | I | 17 | Total O
17 17 | 0 | 0 |
| 37 | J | 11 | Total O
11 11 | 0 | 0 |
| 37 | K | 4 | Total O
4 4 | 0 | 0 |



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	11	Total 11	O 11	0	0
37	M	13	Total 13	O 13	0	0
37	O	149	Total 149	O 149	0	0
37	T	13	Total 13	O 13	0	0
37	U	67	Total 67	O 67	0	0
37	V	96	Total 96	O 96	0	0
37	Y	9	Total 9	O 9	0	0
37	X	14	Total 14	O 14	0	0
37	Z	8	Total 8	O 8	0	0
37	R	1	Total 1	O 1	0	0
37	a	144	Total 148	O 148	0	4
37	b	280	Total 280	O 280	0	0
37	c	228	Total 228	O 228	0	0
37	d	171	Total 171	O 171	0	0
37	e	25	Total 25	O 25	0	0
37	f	14	Total 14	O 14	0	0
37	h	33	Total 33	O 33	0	0
37	i	12	Total 12	O 12	0	0
37	j	8	Total 8	O 8	0	0
37	k	11	Total 11	O 11	0	0
37	l	14	Total 14	O 14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	17	Total 17	O 17	0	0
37	o	159	Total 159	O 159	0	0
37	t	16	Total 16	O 16	0	0
37	u	89	Total 89	O 89	0	0
37	v	77	Total 77	O 77	0	0
37	y	6	Total 6	O 6	0	0
37	x	11	Total 11	O 11	0	0
37	z	8	Total 8	O 8	0	0
37	r	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

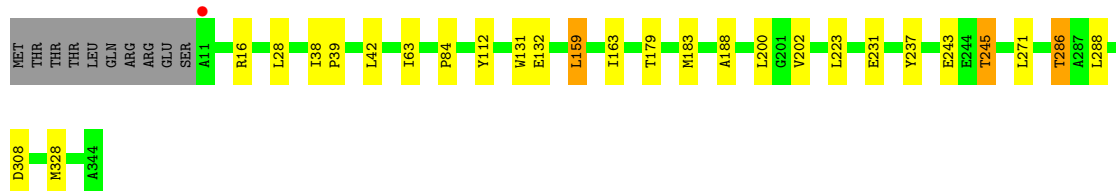
- Molecule 1: Photosystem II protein D1 1

Chain A: 

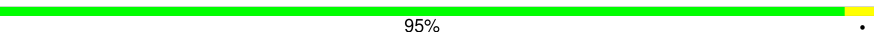


- Molecule 1: Photosystem II protein D1 1

Chain a: 

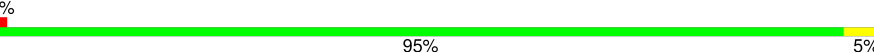


- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 



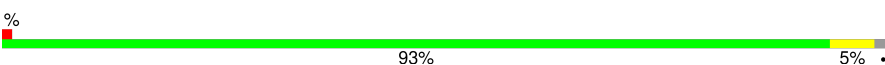
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 



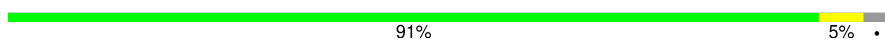
D473

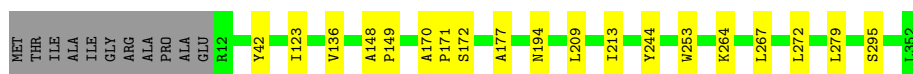
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  93% 5%



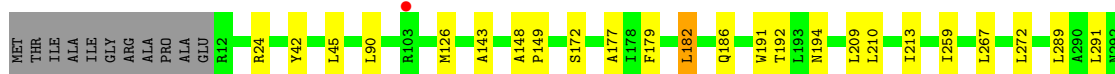
- Molecule 4: Photosystem II D2 protein

Chain D:  91% 5%



- Molecule 4: Photosystem II D2 protein

Chain d:  89% 8%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  87% 11%



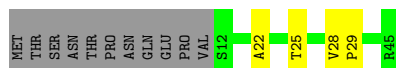
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  89% 8%



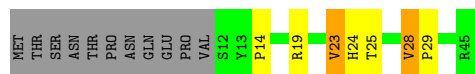
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  67% 9% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  60% 11% 24%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 8%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 85% 6% 5% 5%

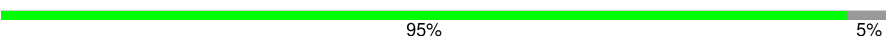


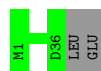
- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 5% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  95% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  85% 5% 10%



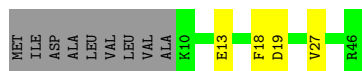
- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 80% 10% 10%



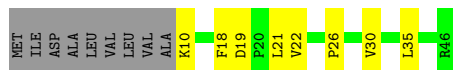
- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%

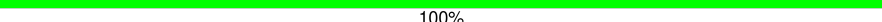


- Molecule 10: Photosystem II reaction center protein K

Chain k:  63% 17% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 11% •



- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 78% 11% • 8%



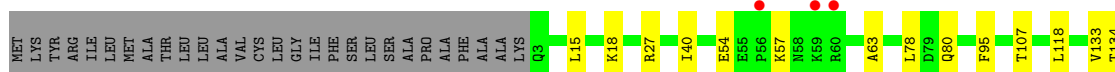
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%



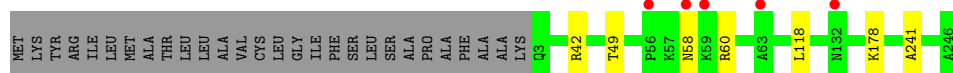
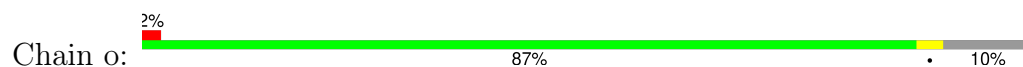
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  83% 7% 10%

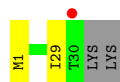
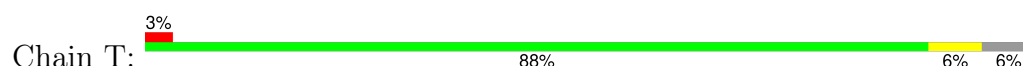




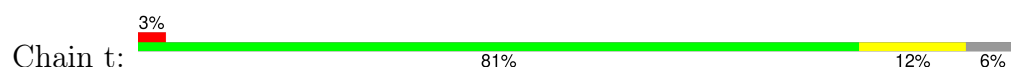
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



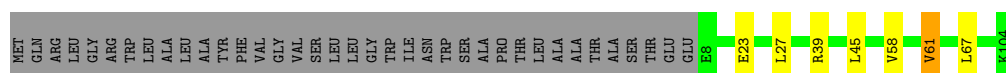
- Molecule 14: Photosystem II reaction center protein T



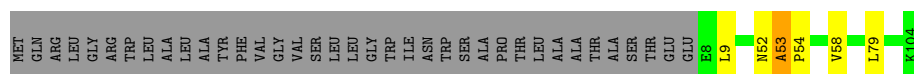
- Molecule 14: Photosystem II reaction center protein T



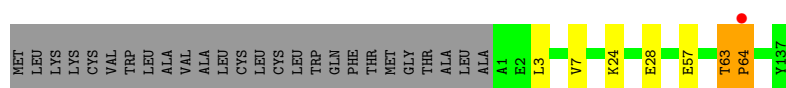
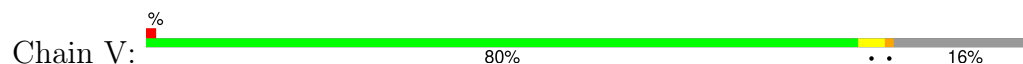
- Molecule 15: Photosystem II 12 kDa extrinsic protein



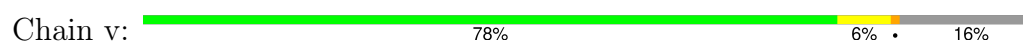
- Molecule 15: Photosystem II 12 kDa extrinsic protein

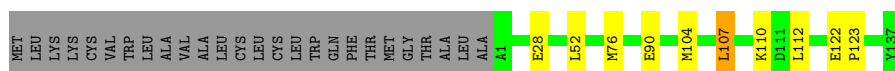


- Molecule 16: Cytochrome c-550

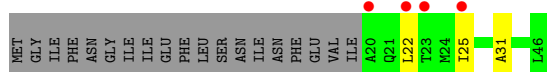


- Molecule 16: Cytochrome c-550

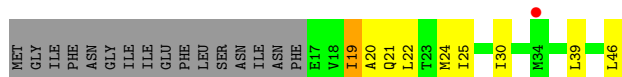




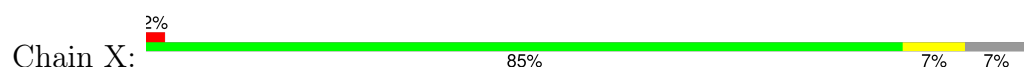
- Molecule 17: Photosystem II reaction center protein Ycf12



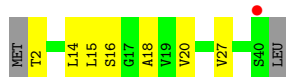
- Molecule 17: Photosystem II reaction center protein Ycf12



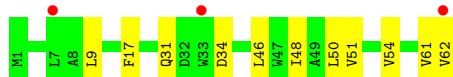
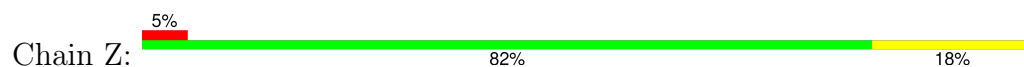
- Molecule 18: Photosystem II reaction center X protein



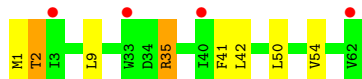
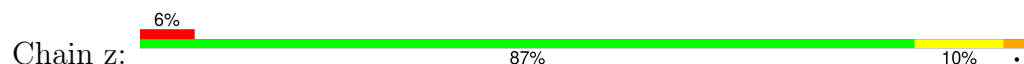
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



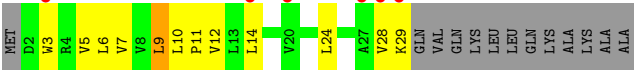
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.53Å 222.82Å 308.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.83 – 1.93 33.83 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.83-1.93) 86.0 (33.83-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 1.94Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.175 , 0.212 0.175 , 0.212	Depositor DCC
R_{free} test set	5354 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	107900	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/3275	0.43	0/4462
1	a	0.20	0/3272	0.44	0/4458
2	B	0.20	0/4179	0.42	0/5693
2	b	0.20	0/4127	0.41	0/5623
3	C	0.20	0/3647	0.41	0/4965
3	c	0.18	0/3719	0.39	0/5061
4	D	0.22	0/2910	0.44	0/3962
4	d	0.19	0/2919	0.43	0/3974
5	E	0.18	0/688	0.37	0/940
5	e	0.16	0/683	0.36	0/932
6	F	0.19	0/284	0.37	0/387
6	f	0.17	0/284	0.41	0/387
7	H	0.19	0/517	0.40	0/705
7	h	0.17	0/505	0.38	0/689
8	I	0.18	0/293	0.40	0/396
8	i	0.19	0/293	0.34	0/396
9	J	0.16	0/263	0.34	0/356
9	j	0.15	0/263	0.35	0/356
10	K	0.16	0/303	0.35	0/416
10	k	0.15	0/303	0.36	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.20	0/303	0.41	0/412
12	M	0.20	0/249	0.43	0/341
12	m	0.21	0/244	0.42	0/334
13	O	0.21	0/1904	0.44	0/2585
13	o	0.20	0/1905	0.42	0/2583
14	T	0.20	0/257	0.45	0/349
14	t	0.21	0/255	0.45	0/346
15	U	0.19	0/785	0.39	0/1064
15	u	0.19	0/785	0.41	0/1064
16	V	0.20	0/1085	0.43	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.18	0/1085	0.36	0/1473
17	Y	0.17	0/197	0.31	0/264
17	y	0.15	0/219	0.36	0/294
18	X	0.16	0/284	0.32	0/384
18	x	0.15	0/289	0.30	0/391
19	Z	0.13	0/490	0.32	0/669
19	z	0.13	0/488	0.31	0/666
20	R	0.12	0/227	0.29	0/313
20	r	0.12	0/227	0.32	0/313
All	All	0.19	0/44316	0.41	0/60314

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3152	2922	2992	13	0
1	a	3149	2913	2983	17	0
2	B	4016	3887	3871	11	0
2	b	3984	3842	3842	19	0
3	C	3509	3416	3409	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	3487	3492	9	0
4	D	2805	2704	2692	14	0
4	d	2811	2710	2698	17	0
5	E	666	651	651	6	0
5	e	664	648	648	5	0
6	F	275	282	282	6	0
6	f	275	282	282	5	0
7	H	505	528	528	3	0
7	h	493	514	514	4	0
8	I	296	311	311	0	0
8	i	296	311	311	0	0
9	J	257	268	268	0	0
9	j	257	268	268	1	0
10	K	293	305	305	3	0
10	k	293	305	305	6	0
11	L	304	316	316	0	0
11	l	296	304	304	0	0
12	M	256	267	269	2	0
12	m	251	267	267	2	0
13	O	1870	1830	1830	11	0
13	o	1874	1846	1846	1	0
14	T	258	261	261	0	0
14	t	256	256	256	3	0
15	U	774	773	773	3	0
15	u	774	773	773	4	0
16	V	1064	1071	1073	4	0
16	v	1064	1071	1073	4	0
17	Y	196	217	217	3	0
17	y	218	241	241	8	0
18	X	281	312	312	4	0
18	x	286	316	314	4	0
19	Z	479	516	516	6	0
19	z	477	509	509	5	0
20	R	221	238	238	1	0
20	r	221	238	238	5	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	4	1	1	0	0
25	a	4	1	1	0	0
26	A	249	264	264	7	0
26	B	1035	1139	1139	18	0
26	C	839	922	922	11	0
26	D	130	144	144	0	0
26	a	260	288	288	4	0
26	b	1035	1139	1139	14	0
26	c	839	919	919	7	0
26	d	130	144	144	6	0
27	A	64	74	74	1	0
27	D	64	74	74	2	0
27	a	64	74	74	0	0
27	d	64	74	74	0	0
28	A	40	56	56	1	0
28	B	120	168	168	4	0
28	C	80	112	112	1	0
28	D	40	56	56	1	0
28	H	40	56	56	2	0
28	K	40	56	56	0	0
28	T	40	56	56	3	0
28	Z	40	56	56	2	0
28	a	40	56	56	2	0
28	b	120	168	168	3	0
28	c	80	112	112	0	0
28	d	40	56	56	0	0
28	k	80	112	112	4	0
28	t	40	56	56	5	0
28	x	40	56	56	3	0
29	A	55	80	80	2	0
29	D	55	80	80	0	0
29	a	55	80	80	3	0
29	d	55	80	80	0	0
30	A	45	83	83	1	0
30	B	76	116	116	0	0
30	C	78	126	126	2	0
30	D	20	35	35	3	0
30	E	44	74	74	1	0
30	H	27	52	52	3	0
30	I	32	48	48	2	0
30	J	12	16	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	14	27	27	1	0
30	M	25	38	38	0	0
30	T	31	60	60	0	0
30	Z	17	33	33	1	0
30	a	12	16	16	0	0
30	b	57	96	96	1	0
30	c	18	35	35	1	0
30	d	60	105	105	1	0
30	e	39	67	67	0	0
30	h	10	19	19	0	0
30	i	18	24	24	0	0
30	j	28	47	47	0	0
30	k	14	20	20	0	0
30	m	30	51	51	0	0
30	t	10	16	16	0	0
30	z	22	36	36	0	0
31	A	48	66	66	0	0
31	B	45	60	60	1	0
31	C	84	106	106	2	0
31	D	101	142	142	0	0
31	M	51	72	72	1	0
31	a	104	154	154	1	0
31	b	55	86	86	0	0
31	c	124	172	172	1	0
31	d	44	58	58	0	0
31	m	51	72	72	0	0
32	A	43	52	53	0	0
32	B	54	77	78	2	0
32	D	52	70	71	1	0
32	F	36	45	46	2	0
32	a	108	154	156	0	0
32	b	49	64	65	2	0
32	f	41	48	49	1	0
33	A	66	84	96	4	0
33	C	186	210	246	5	0
33	H	62	70	82	1	0
33	c	186	210	246	0	0
33	h	62	70	82	0	0
34	B	49	74	74	3	0
34	D	145	215	215	3	0
34	E	49	74	74	0	0
34	d	137	199	199	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	42	57	57	1	0
34	l	49	74	74	0	0
35	F	43	30	30	4	0
35	f	43	30	30	4	0
36	V	43	30	30	0	0
36	v	43	30	30	1	0
37	A	182	0	0	2	0
37	B	319	0	0	4	0
37	C	254	0	0	4	0
37	D	159	0	0	2	0
37	E	42	0	0	3	0
37	F	20	0	0	3	0
37	H	41	0	0	1	0
37	I	17	0	0	1	0
37	J	11	0	0	1	0
37	K	4	0	0	0	0
37	L	11	0	0	0	0
37	M	13	0	0	0	0
37	O	149	0	0	2	0
37	R	1	0	0	0	0
37	T	13	0	0	0	0
37	U	67	0	0	0	0
37	V	96	0	0	1	0
37	X	14	0	0	1	0
37	Y	9	0	0	1	0
37	Z	8	0	0	0	0
37	a	148	0	0	2	0
37	b	280	0	0	12	0
37	c	228	0	0	1	0
37	d	171	0	0	2	0
37	e	25	0	0	0	0
37	f	14	0	0	1	0
37	h	33	0	0	0	0
37	i	12	0	0	1	0
37	j	8	0	0	0	0
37	k	11	0	0	2	0
37	l	14	0	0	0	0
37	m	17	0	0	0	0
37	o	159	0	0	0	0
37	r	1	0	0	0	0
37	t	16	0	0	3	0
37	u	89	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	v	77	0	0	0	0
37	x	11	0	0	0	0
37	y	6	0	0	2	0
37	z	8	0	0	0	0
All	All	54720	53180	53398	305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 305 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)
28:t:101:BCR:H363	37:t:201:HOH:O	1.70	0.91
28:t:101:BCR:HC8	28:t:101:BCR:H311	1.58	0.85
2:B:96:VAL:HG13	37:B:715:HOH:O	1.78	0.82
3:C:87:ILE:HD11	37:C:731:HOH:O	1.79	0.82
26:B:601:CLA:H41	30:H:103:STE:H183	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/344 (117%)	398 (99%)	5 (1%)	0	100	100
1	a	403/344 (117%)	397 (98%)	6 (2%)	0	100	100
2	B	510/510 (100%)	502 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	495 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	445 (98%)	8 (2%)	1 (0%)	43	37
3	c	463/461 (100%)	451 (97%)	11 (2%)	1 (0%)	43	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	349/352 (99%)	340 (97%)	9 (3%)	0	100	100
4	d	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	2 (3%)	1 (2%)	7	1
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	0
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	10 (4%)	1 (0%)	30	22
13	o	242/272 (89%)	233 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	4
16	V	135/163 (83%)	132 (98%)	2 (2%)	1 (1%)	18	9
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	1
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
All	All	5420/5700 (95%)	5299 (98%)	113 (2%)	8 (0%)	43	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	c	416	SER
19	z	2	THR
3	C	416	SER
15	u	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/280 (118%)	326 (99%)	3 (1%)	70	67
1	a	328/280 (117%)	316 (96%)	12 (4%)	30	16
2	B	410/407 (101%)	404 (98%)	6 (2%)	57	49
2	b	403/407 (99%)	399 (99%)	4 (1%)	68	64
3	C	356/362 (98%)	351 (99%)	5 (1%)	59	52
3	c	364/362 (101%)	351 (96%)	13 (4%)	31	17
4	D	286/283 (101%)	286 (100%)	0	100	100
4	d	287/283 (101%)	281 (98%)	6 (2%)	47	37
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	13
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	13
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	6
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	21
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	13
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	2
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	4
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	0
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	1
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	17
13	O	206/228 (90%)	202 (98%)	4 (2%)	50	40
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	31
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	15
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	14
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	5
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	57
16	V	117/138 (85%)	114 (97%)	3 (3%)	40	28
16	v	117/138 (85%)	112 (96%)	5 (4%)	26	13
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	1
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	20
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	4
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	3
19	z	51/52 (98%)	48 (94%)	3 (6%)	18	6
20	R	22/33 (67%)	20 (91%)	2 (9%)	9	1
20	r	22/33 (67%)	16 (73%)	6 (27%)	0	0
All	All	4482/4654 (96%)	4358 (97%)	124 (3%)	38	25

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	v	110	LYS
3	c	354[B]	GLU
16	v	107	LEU
20	r	3	TRP

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

Mol	Chain	Res	Type
16	v	118	HIS
18	x	33	GLN
19	z	38	GLN
2	b	338	GLN
1	a	19	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.38	0	8,9,11	0.82	0
12	FME	M	1	12	8,9,10	0.39	0	8,9,11	0.89	0
14	FME	T	1	14	8,9,10	0.43	0	8,9,11	1.44	2 (25%)
14	FME	t	1	14	8,9,10	0.42	0	8,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.35	0	8,9,11	0.94	1 (12%)
8	FME	i	1	8	8,9,10	0.38	0	8,9,11	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	2.53	126.72	122.82
14	T	1	FME	CG-CB-CA	2.29	119.86	112.87
8	I	1	FME	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
12	m	1	FME	O-C-CA-CB
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-CA-CB-CG
14	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 213 ligands modelled in this entry, 6 are monoatomic - leaving 207 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	$\# Z > 2$
26	CLA	C	511	3	69,73,73	1.29	8 (11%)	82,113,113	1.25	5 (6%)
26	CLA	C	504	37	63,67,73	1.26	7 (11%)	74,105,113	1.24	8 (10%)
30	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.12	0
28	BCR	D	404	-	41,41,41	0.44	0	56,56,56	0.87	1 (1%)
31	LMG	C	517	-	35,35,55	0.55	0	43,43,63	1.22	5 (11%)
30	STE	b	624	-	9,9,19	0.35	0	8,8,19	0.73	0
26	CLA	a	613	37	69,73,73	1.22	8 (11%)	82,113,113	1.12	6 (7%)
26	CLA	B	602	2	69,73,73	1.20	8 (11%)	82,113,113	1.11	7 (8%)
30	STE	e	103	-	7,7,19	0.38	0	6,6,19	0.57	0
26	CLA	D	402	4	69,73,73	1.15	6 (8%)	82,113,113	1.21	6 (7%)
26	CLA	C	507	37	69,73,73	1.24	6 (8%)	82,113,113	1.28	7 (8%)
26	CLA	b	604	2	69,73,73	1.23	7 (10%)	82,113,113	1.38	11 (13%)
30	STE	C	527	-	13,13,19	0.35	0	12,12,19	0.73	0
28	BCR	c	515	-	41,41,41	0.41	0	56,56,56	0.70	1 (1%)
33	DGD	C	522	-	63,63,67	0.57	0	77,77,81	0.74	1 (1%)
26	CLA	C	505	3	69,73,73	1.21	7 (10%)	82,113,113	1.26	9 (10%)
26	CLA	C	501	3	69,73,73	1.35	8 (11%)	82,113,113	1.22	5 (6%)
30	STE	z	701	-	12,12,19	0.39	0	11,11,19	0.67	0
26	CLA	b	605	2	69,73,73	1.22	7 (10%)	82,113,113	1.28	8 (9%)
30	STE	i	102	-	5,5,19	0.37	0	4,4,19	0.53	0
26	CLA	c	502	3	69,73,73	1.16	7 (10%)	82,113,113	1.15	4 (4%)
30	STE	A	619	-	16,16,19	0.32	0	15,15,19	0.79	0
31	LMG	M	101	-	51,51,55	0.58	0	59,59,63	0.80	2 (3%)
36	HEC	V	201	16	50,50,50	1.64	4 (8%)	68,82,82	1.31	9 (13%)
26	CLA	a	610	1	69,73,73	1.25	7 (10%)	82,113,113	1.20	6 (7%)
34	LHG	d	409	-	38,38,48	0.60	0	41,44,54	0.61	1 (2%)
26	CLA	C	513	3	69,73,73	1.26	8 (11%)	82,113,113	1.20	7 (8%)
34	LHG	d	407	-	48,48,48	0.52	0	51,54,54	0.59	1 (1%)
30	STE	m	102	-	11,11,19	0.74	0	11,11,19	1.09	1 (9%)
30	STE	h	102	-	9,9,19	0.36	0	8,8,19	0.66	0
31	LMG	d	411	-	44,44,55	0.52	0	52,52,63	0.63	0
33	DGD	H	102	-	63,63,67	0.58	0	77,77,81	0.85	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	T	101	-	41,41,41	0.50	0	56,56,56	0.87	0
26	CLA	b	610	37	69,73,73	1.23	7 (10%)	82,113,113	1.16	7 (8%)
33	DGD	c	520	-	63,63,67	0.54	0	77,77,81	0.74	1 (1%)
26	CLA	c	512	3	69,73,73	1.13	7 (10%)	82,113,113	1.30	6 (7%)
26	CLA	C	508	3	69,73,73	1.27	7 (10%)	82,113,113	1.27	6 (7%)
21	OXY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
30	STE	C	520	-	9,9,19	0.40	0	8,8,19	0.61	0
28	BCR	A	611	-	41,41,41	0.39	0	56,56,56	0.57	0
30	STE	I	101	-	16,16,19	0.63	0	16,16,19	1.03	0
26	CLA	D	403	4	69,73,73	1.20	8 (11%)	82,113,113	1.20	6 (7%)
31	LMG	B	620	-	45,45,55	0.51	0	53,53,63	0.71	2 (3%)
32	SQD	b	620	-	47,49,54	1.62	7 (14%)	57,60,65	1.64	10 (17%)
28	BCR	C	515	-	41,41,41	0.39	0	56,56,56	0.61	0
26	CLA	B	605	2	69,73,73	1.22	7 (10%)	82,113,113	1.27	9 (10%)
26	CLA	b	608	2	69,73,73	1.15	6 (8%)	82,113,113	1.27	6 (7%)
32	SQD	f	102	-	39,41,54	1.66	7 (17%)	49,52,65	1.65	10 (20%)
33	DGD	C	523	-	63,63,67	0.59	1 (1%)	77,77,81	0.69	0
26	CLA	c	506	3	69,73,73	1.24	6 (8%)	82,113,113	1.16	5 (6%)
33	DGD	A	617	-	67,67,67	0.54	0	81,81,81	0.85	4 (4%)
26	CLA	d	403	4	69,73,73	1.34	9 (13%)	82,113,113	1.07	6 (7%)
34	LHG	D	409	-	46,46,48	0.55	0	49,52,54	0.50	0
27	PHO	A	609	-	58,69,69	2.04	11 (18%)	55,99,99	1.70	7 (12%)
30	STE	C	526	-	15,15,19	0.34	0	14,14,19	0.79	0
30	STE	m	103	-	17,17,19	0.33	0	16,16,19	0.84	0
27	PHO	d	401	-	58,69,69	2.16	10 (17%)	55,99,99	1.69	10 (18%)
26	CLA	A	610	1	58,62,73	1.20	5 (8%)	68,99,113	1.32	7 (10%)
28	BCR	t	101	-	41,41,41	0.51	0	56,56,56	0.75	1 (1%)
30	STE	E	104	-	19,19,19	0.61	0	19,19,19	1.10	2 (10%)
30	STE	T	102	-	15,15,19	0.36	0	14,14,19	0.70	0
30	STE	d	410	-	19,19,19	0.60	0	19,19,19	0.94	0
30	STE	I	102	-	14,14,19	0.70	0	14,14,19	1.02	0
25	BCT	A	606	23	3,3,3	0.83	0	2,3,3	2.20	1 (50%)
34	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.67	0
28	BCR	b	618	-	41,41,41	0.44	0	56,56,56	0.75	1 (1%)
30	STE	A	620	-	10,10,19	0.35	0	9,9,19	0.74	0
26	CLA	B	604	2	69,73,73	1.42	8 (11%)	82,113,113	1.36	10 (12%)
30	STE	b	623	-	15,15,19	0.62	0	15,15,19	1.18	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	512	3	69,73,73	1.24	8 (11%)	82,113,113	1.24	8 (9%)
30	STE	b	625	-	10,10,19	0.31	0	9,9,19	0.82	0
30	STE	C	519	-	6,6,19	0.36	0	5,5,19	0.68	0
30	STE	C	516	-	13,13,19	0.73	0	13,13,19	1.02	1 (7%)
30	STE	B	621	-	16,16,19	0.61	0	16,16,19	1.17	0
28	BCR	a	611	-	41,41,41	0.42	0	56,56,56	0.67	0
35	HEM	F	101	6,5	50,50,50	1.41	6 (12%)	67,82,82	1.13	4 (5%)
31	LMG	D	406	-	50,50,55	0.51	0	58,58,63	1.14	5 (8%)
26	CLA	b	615	2	69,73,73	1.31	9 (13%)	82,113,113	1.25	4 (4%)
26	CLA	c	505	3	69,73,73	1.16	6 (8%)	82,113,113	1.23	5 (6%)
26	CLA	B	616	2	64,68,73	1.44	7 (10%)	76,107,113	1.25	6 (7%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-		
26	CLA	C	503	3	69,73,73	1.36	7 (10%)	82,113,113	1.34	7 (8%)
30	STE	e	101	-	8,8,19	0.37	0	7,7,19	0.63	0
30	STE	A	613	-	8,8,19	0.35	0	7,7,19	0.63	0
26	CLA	a	608	37	69,73,73	1.30	8 (11%)	82,113,113	1.14	6 (7%)
22	OEX	a	602[A]	3,37,1	0,14,14	-	-	-		
26	CLA	B	613	2	69,73,73	1.22	8 (11%)	82,113,113	1.25	5 (6%)
30	STE	B	625	-	17,17,19	0.62	0	17,17,19	1.05	0
26	CLA	B	610	37	69,73,73	1.21	6 (8%)	82,113,113	1.26	7 (8%)
26	CLA	C	502	3	69,73,73	1.31	8 (11%)	82,113,113	1.28	6 (7%)
27	PHO	a	609	-	58,69,69	2.07	12 (20%)	55,99,99	1.67	7 (12%)
28	BCR	Z	101	-	41,41,41	0.41	0	56,56,56	0.84	2 (3%)
26	CLA	b	601	37	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
26	CLA	b	613	2	69,73,73	1.19	7 (10%)	82,113,113	1.20	6 (7%)
32	SQD	a	615	-	52,54,54	1.59	8 (15%)	62,65,65	1.38	7 (11%)
33	DGD	C	521	-	63,63,67	0.62	1 (1%)	77,77,81	0.86	3 (3%)
26	CLA	B	609	2	69,73,73	1.25	5 (7%)	82,113,113	1.20	7 (8%)
30	STE	H	103	-	17,17,19	0.38	0	16,16,19	0.74	0
26	CLA	C	506	3	69,73,73	1.20	6 (8%)	82,113,113	1.10	5 (6%)
29	PL9	A	612	-	55,55,55	0.80	1 (1%)	68,69,69	1.40	8 (11%)
30	STE	k	103	-	13,13,19	0.67	0	13,13,19	1.09	0
25	BCT	a	606	23	3,3,3	0.85	0	2,3,3	1.82	1 (50%)
30	STE	e	104	-	8,8,19	0.36	0	7,7,19	0.63	0
28	BCR	C	514	-	41,41,41	0.36	0	56,56,56	0.59	0
30	STE	B	626	-	11,11,19	0.74	0	11,11,19	1.15	0
26	CLA	c	508	3	68,72,73	1.19	6 (8%)	80,111,113	1.20	7 (8%)
31	LMG	A	615	-	48,48,55	0.50	0	56,56,63	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HEM	f	101	6,5	50,50,50	1.47	8 (16%)	67,82,82	1.33	8 (11%)
26	CLA	b	616	2	64,68,73	1.18	6 (9%)	76,107,113	1.40	7 (9%)
30	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.06	0
26	CLA	b	611	2	69,73,73	1.19	7 (10%)	82,113,113	1.29	7 (8%)
31	LMG	a	617	-	49,49,55	0.57	1 (2%)	57,57,63	0.82	2 (3%)
30	STE	M	102	-	14,14,19	0.69	0	14,14,19	1.06	0
26	CLA	B	608	2	69,73,73	1.19	7 (10%)	82,113,113	1.30	7 (8%)
30	STE	B	627	-	14,14,19	0.34	0	13,13,19	0.77	0
30	STE	M	103	-	9,9,19	0.31	0	8,8,19	0.83	0
26	CLA	B	612	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
30	STE	E	103	-	11,11,19	0.34	0	10,10,19	0.77	0
30	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.05	0
31	LMG	a	616	-	55,55,55	0.51	0	63,63,63	0.83	4 (6%)
31	LMG	c	522	-	48,48,55	0.53	0	56,56,63	0.80	1 (1%)
26	CLA	A	608	37	69,73,73	1.25	6 (8%)	82,113,113	1.11	4 (4%)
26	CLA	c	510	3	69,73,73	1.25	8 (11%)	82,113,113	1.20	5 (6%)
28	BCR	d	404	-	41,41,41	0.41	0	56,56,56	1.27	4 (7%)
31	LMG	c	521	-	46,46,55	0.51	0	54,54,63	0.63	0
22	OEX	A	602[A]	3,37,1	0,14,14	-	-	-	-	-
34	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.63	0
28	BCR	B	619	-	41,41,41	0.39	0	56,56,56	0.71	0
28	BCR	c	514	-	41,41,41	0.38	0	56,56,56	0.53	0
29	PL9	D	405	-	55,55,55	1.09	4 (7%)	68,69,69	1.45	13 (19%)
26	CLA	B	615	2	69,73,73	1.33	8 (11%)	82,113,113	1.33	5 (6%)
32	SQD	F	102	-	34,36,54	1.49	5 (14%)	42,45,65	1.80	12 (28%)
28	BCR	b	617	-	41,41,41	0.46	0	56,56,56	0.79	1 (1%)
32	SQD	D	410	-	50,52,54	1.59	6 (12%)	60,63,65	1.76	11 (18%)
28	BCR	K	101	-	41,41,41	0.40	0	56,56,56	0.80	1 (1%)
28	BCR	k	102	-	41,41,41	0.43	0	56,56,56	0.73	1 (1%)
30	STE	z	702	-	8,8,19	0.39	0	7,7,19	0.61	0
27	PHO	D	401	-	58,69,69	2.06	11 (18%)	55,99,99	1.55	10 (18%)
31	LMG	C	524	-	48,48,55	0.50	0	56,56,63	0.63	0
34	LHG	E	101	-	48,48,48	0.53	0	51,54,54	0.54	0
26	CLA	c	509	3	69,73,73	1.25	8 (11%)	82,113,113	1.28	6 (7%)
30	STE	C	525	-	11,11,19	0.75	0	11,11,19	1.19	1 (9%)
26	CLA	b	602	2	69,73,73	1.26	9 (13%)	82,113,113	1.22	6 (7%)
30	STE	K	102	-	13,13,19	0.35	0	12,12,19	0.72	0
30	STE	T	103	-	14,14,19	0.34	0	13,13,19	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	STE	D	412	-	19,19,19	0.60	0	19,19,19	1.03	1 (5%)
29	PL9	d	405	-	55,55,55	0.99	4 (7%)	68,69,69	1.64	13 (19%)
26	CLA	c	504	37	64,68,73	1.27	8 (12%)	76,107,113	1.26	5 (6%)
26	CLA	c	513	3	69,73,73	1.13	7 (10%)	82,113,113	1.15	6 (7%)
30	STE	b	621	-	19,19,19	0.57	0	19,19,19	1.04	0
30	STE	e	105	-	12,12,19	0.67	0	12,12,19	1.25	2 (16%)
28	BCR	B	617	-	41,41,41	0.42	0	56,56,56	0.69	0
30	STE	a	618	-	11,11,19	0.75	0	11,11,19	1.00	0
33	DGD	h	101	-	63,63,67	0.57	0	77,77,81	0.83	5 (6%)
36	HEC	v	201	16	50,50,50	1.67	3 (6%)	68,82,82	1.19	5 (7%)
28	BCR	k	101	-	41,41,41	0.44	0	56,56,56	0.76	0
30	STE	t	102	-	9,9,19	0.42	0	8,8,19	0.63	0
32	SQD	a	614	-	52,54,54	1.59	7 (13%)	62,65,65	1.80	10 (16%)
26	CLA	B	603	2	69,73,73	1.23	7 (10%)	82,113,113	1.27	6 (7%)
26	CLA	b	614	2	69,73,73	1.19	6 (8%)	82,113,113	1.24	6 (7%)
26	CLA	B	611	2	69,73,73	1.18	6 (8%)	82,113,113	1.35	8 (9%)
28	BCR	H	101	-	41,41,41	0.43	0	56,56,56	0.82	1 (1%)
26	CLA	c	503	3	69,73,73	1.34	7 (10%)	82,113,113	1.32	6 (7%)
30	STE	Z	102	-	16,16,19	0.35	0	15,15,19	0.75	0
30	STE	d	406	-	19,19,19	0.61	0	19,19,19	1.00	1 (5%)
28	BCR	x	101	-	41,41,41	0.47	0	56,56,56	0.76	1 (1%)
30	STE	j	102	-	15,15,19	0.35	0	14,14,19	0.77	0
26	CLA	c	501	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	5 (6%)
26	CLA	B	606	2	69,73,73	1.41	8 (11%)	82,113,113	1.34	6 (7%)
26	CLA	b	609	2	69,73,73	1.25	5 (7%)	82,113,113	1.25	8 (9%)
31	LMG	b	622	-	55,55,55	0.51	0	63,63,63	0.91	2 (3%)
26	CLA	A	614	37	69,73,73	1.21	9 (13%)	82,113,113	1.25	5 (6%)
33	DGD	c	519	-	63,63,67	0.57	1 (1%)	77,77,81	0.80	2 (2%)
26	CLA	b	607	37	69,73,73	1.30	6 (8%)	82,113,113	1.17	4 (4%)
34	LHG	B	622	-	48,48,48	0.52	0	51,54,54	0.74	1 (1%)
26	CLA	b	606	2	69,73,73	1.36	7 (10%)	82,113,113	1.34	6 (7%)
34	LHG	e	102	-	41,41,48	0.56	0	44,47,54	0.57	0
31	LMG	m	101	-	51,51,55	0.50	0	59,59,63	0.68	1 (1%)
26	CLA	b	612	2	69,73,73	1.14	8 (11%)	82,113,113	1.15	9 (10%)
32	SQD	A	616	-	41,43,54	1.77	8 (19%)	51,54,65	1.42	6 (11%)
28	BCR	B	618	-	41,41,41	0.45	0	56,56,56	0.66	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	509	3	69,73,73	1.18	8 (11%)	82,113,113	1.18	6 (7%)
26	CLA	B	607	37	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
32	SQD	B	623	-	52,54,54	1.55	7 (13%)	62,65,65	1.62	11 (17%)
26	CLA	c	507	37	69,73,73	1.16	7 (10%)	82,113,113	1.25	5 (6%)
30	STE	A	618	-	7,7,19	0.33	0	6,6,19	0.71	0
26	CLA	B	601	37	69,73,73	1.28	8 (11%)	82,113,113	1.31	6 (7%)
30	STE	H	104	-	8,8,19	0.32	0	7,7,19	0.76	0
26	CLA	C	510	3	69,73,73	1.21	7 (10%)	82,113,113	1.22	5 (6%)
26	CLA	b	603	2	69,73,73	1.23	8 (11%)	82,113,113	1.28	7 (8%)
33	DGD	c	518	-	63,63,67	0.55	0	77,77,81	0.80	2 (2%)
34	LHG	D	411	-	48,48,48	0.55	0	51,54,54	0.70	0
31	LMG	D	407	-	51,51,55	0.50	0	59,59,63	0.78	2 (3%)
26	CLA	a	607	1	69,73,73	1.24	7 (10%)	82,113,113	1.24	8 (9%)
29	PL9	a	612	-	55,55,55	0.80	2 (3%)	68,69,69	1.50	10 (14%)
30	STE	C	518	-	4,4,19	0.37	0	3,3,19	0.51	0
26	CLA	d	402	4	69,73,73	1.16	6 (8%)	82,113,113	1.16	7 (8%)
30	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.09	1 (9%)
26	CLA	c	511	3	69,73,73	1.46	6 (8%)	82,113,113	1.22	5 (6%)
26	CLA	B	614	2	69,73,73	1.23	8 (11%)	82,113,113	1.22	6 (7%)
28	BCR	b	619	-	41,41,41	0.44	0	56,56,56	0.78	1 (1%)
31	LMG	c	517	-	29,29,55	0.46	0	31,31,63	0.58	0
34	LHG	D	408	-	48,48,48	0.55	0	51,54,54	0.57	1 (1%)
30	STE	d	412	-	19,19,19	0.60	0	19,19,19	0.98	0
26	CLA	A	607	1	69,73,73	1.34	7 (10%)	82,113,113	1.15	5 (6%)
30	STE	c	516	-	17,17,19	0.36	0	16,16,19	0.75	0
30	STE	B	624	-	13,13,19	0.64	0	13,13,19	1.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	511	3	-	3/39/115/115	-
26	CLA	C	504	37	-	8/32/108/115	-
30	STE	E	102	-	-	3/9/9/17	-
28	BCR	D	404	-	-	0/29/63/63	0/2/2/2
31	LMG	C	517	-	-	14/30/50/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	b	624	-	-	5/7/7/17	-
26	CLA	a	613	37	-	4/39/115/115	-
26	CLA	B	602	2	-	5/39/115/115	-
30	STE	e	103	-	-	2/5/5/17	-
26	CLA	D	402	4	-	2/39/115/115	-
26	CLA	C	507	37	-	7/39/115/115	-
26	CLA	b	604	2	-	6/39/115/115	-
30	STE	C	527	-	-	6/11/11/17	-
28	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	DGD	C	522	-	-	19/51/91/95	0/2/2/2
26	CLA	C	505	3	-	9/39/115/115	-
26	CLA	C	501	3	-	6/39/115/115	-
30	STE	z	701	-	-	4/10/10/17	-
26	CLA	b	605	2	-	5/39/115/115	-
30	STE	i	102	-	-	1/3/3/17	-
26	CLA	c	502	3	-	6/39/115/115	-
30	STE	A	619	-	-	1/14/14/17	-
31	LMG	M	101	-	-	21/46/66/70	0/1/1/1
36	HEC	V	201	16	1/1/7/7	5/14/54/54	-
26	CLA	a	610	1	-	10/39/115/115	-
34	LHG	d	409	-	-	10/43/43/53	-
26	CLA	C	513	3	-	10/39/115/115	-
34	LHG	d	407	-	-	17/53/53/53	-
30	STE	m	102	-	-	6/9/9/17	-
30	STE	h	102	-	-	3/7/7/17	-
31	LMG	d	411	-	-	10/39/59/70	0/1/1/1
33	DGD	H	102	-	-	18/51/91/95	0/2/2/2
28	BCR	T	101	-	-	4/29/63/63	0/2/2/2
26	CLA	b	610	37	-	6/39/115/115	-
33	DGD	c	520	-	-	18/51/91/95	0/2/2/2
26	CLA	c	512	3	-	10/39/115/115	-
26	CLA	C	508	3	-	4/39/115/115	-
30	STE	C	520	-	-	5/7/7/17	-
28	BCR	A	611	-	-	0/29/63/63	0/2/2/2
30	STE	I	101	-	-	7/14/14/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	D	403	4	-	9/39/115/115	-
31	LMG	B	620	-	-	23/40/60/70	0/1/1/1
32	SQD	b	620	-	-	15/44/64/69	0/1/1/1
28	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	CLA	B	605	2	-	7/39/115/115	-
26	CLA	b	608	2	-	1/39/115/115	-
32	SQD	f	102	-	-	14/36/56/69	0/1/1/1
33	DGD	C	523	-	-	13/51/91/95	0/2/2/2
26	CLA	c	506	3	-	10/39/115/115	-
33	DGD	A	617	-	-	19/55/95/95	0/2/2/2
26	CLA	d	403	4	-	4/39/115/115	-
34	LHG	D	409	-	-	8/51/51/53	-
27	PHO	A	609	-	-	3/37/103/103	0/5/6/6
30	STE	C	526	-	-	4/13/13/17	-
30	STE	m	103	-	-	4/15/15/17	-
27	PHO	d	401	-	-	5/37/103/103	0/5/6/6
26	CLA	A	610	1	-	1/26/102/115	-
28	BCR	t	101	-	-	3/29/63/63	0/2/2/2
30	STE	E	104	-	-	8/17/17/17	-
30	STE	T	102	-	-	11/13/13/17	-
30	STE	d	410	-	-	5/17/17/17	-
30	STE	I	102	-	-	6/12/12/17	-
34	LHG	d	408	-	-	14/53/53/53	-
28	BCR	b	618	-	-	0/29/63/63	0/2/2/2
30	STE	A	620	-	-	6/8/8/17	-
26	CLA	B	604	2	-	10/39/115/115	-
30	STE	b	623	-	-	2/13/13/17	-
26	CLA	C	512	3	-	10/39/115/115	-
30	STE	b	625	-	-	3/8/8/17	-
30	STE	C	519	-	-	2/4/4/17	-
30	STE	C	516	-	-	4/11/11/17	-
30	STE	B	621	-	-	6/14/14/17	-
28	BCR	a	611	-	-	0/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	3/14/54/54	-
31	LMG	D	406	-	-	24/45/65/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	615	2	-	6/39/115/115	-
26	CLA	c	505	3	-	7/39/115/115	-
26	CLA	B	616	2	-	7/33/109/115	-
26	CLA	C	503	3	-	3/39/115/115	-
30	STE	e	101	-	-	2/6/6/17	-
30	STE	A	613	-	-	3/6/6/17	-
26	CLA	a	608	37	-	5/39/115/115	-
26	CLA	B	613	2	-	12/39/115/115	-
30	STE	B	625	-	-	10/15/15/17	-
26	CLA	B	610	37	-	2/39/115/115	-
26	CLA	C	502	3	-	4/39/115/115	-
27	PHO	a	609	-	-	1/37/103/103	0/5/6/6
28	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
26	CLA	b	601	37	-	11/39/115/115	-
26	CLA	b	613	2	-	4/39/115/115	-
32	SQD	a	615	-	-	18/49/69/69	0/1/1/1
33	DGD	C	521	-	-	20/51/91/95	0/2/2/2
26	CLA	B	609	2	-	4/39/115/115	-
30	STE	H	103	-	-	7/15/15/17	-
26	CLA	C	506	3	-	10/39/115/115	-
29	PL9	A	612	-	-	16/53/73/73	0/1/1/1
30	STE	k	103	-	-	5/11/11/17	-
30	STE	e	104	-	-	3/6/6/17	-
28	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	STE	B	626	-	-	4/9/9/17	-
26	CLA	c	508	3	-	8/38/114/115	-
31	LMG	A	615	-	-	15/43/63/70	0/1/1/1
35	HEM	f	101	6,5	-	2/14/54/54	-
26	CLA	b	616	2	-	5/33/109/115	-
30	STE	J	101	-	-	3/9/9/17	-
26	CLA	b	611	2	-	4/39/115/115	-
31	LMG	a	617	-	-	17/44/64/70	0/1/1/1
30	STE	M	102	-	-	8/12/12/17	-
26	CLA	B	608	2	-	4/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	B	627	-	-	4/12/12/17	-
30	STE	M	103	-	-	4/7/7/17	-
26	CLA	B	612	2	-	8/39/115/115	-
30	STE	E	103	-	-	2/9/9/17	-
30	STE	i	101	-	-	6/9/9/17	-
31	LMG	a	616	-	-	24/50/70/70	0/1/1/1
31	LMG	c	522	-	-	18/43/63/70	0/1/1/1
26	CLA	A	608	37	-	2/39/115/115	-
26	CLA	c	510	3	-	4/39/115/115	-
28	BCR	d	404	-	-	2/29/63/63	0/2/2/2
31	LMG	c	521	-	-	17/41/61/70	0/1/1/1
34	LHG	l	101	-	-	12/53/53/53	-
28	BCR	B	619	-	-	1/29/63/63	0/2/2/2
28	BCR	c	514	-	-	1/29/63/63	0/2/2/2
29	PL9	D	405	-	-	5/53/73/73	0/1/1/1
26	CLA	B	615	2	-	13/39/115/115	-
32	SQD	F	102	-	-	11/28/48/69	0/1/1/1
28	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	SQD	D	410	-	-	16/47/67/69	0/1/1/1
28	BCR	K	101	-	-	3/29/63/63	0/2/2/2
28	BCR	k	102	-	-	3/29/63/63	0/2/2/2
30	STE	z	702	-	-	2/6/6/17	-
27	PHO	D	401	-	-	1/37/103/103	0/5/6/6
31	LMG	C	524	-	-	10/43/63/70	0/1/1/1
34	LHG	E	101	-	-	14/53/53/53	-
26	CLA	c	509	3	-	9/39/115/115	-
30	STE	C	525	-	-	3/9/9/17	-
26	CLA	b	602	2	-	7/39/115/115	-
30	STE	K	102	-	-	6/11/11/17	-
30	STE	T	103	-	-	7/12/12/17	-
30	STE	D	412	-	-	6/17/17/17	-
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
26	CLA	c	504	37	-	8/33/109/115	-
26	CLA	c	513	3	-	12/39/115/115	-
30	STE	b	621	-	-	7/17/17/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	e	105	-	-	4/10/10/17	-
28	BCR	B	617	-	-	4/29/63/63	0/2/2/2
30	STE	a	618	-	-	6/9/9/17	-
33	DGD	h	101	-	-	12/51/91/95	0/2/2/2
36	HEC	v	201	16	1/1/7/7	4/14/54/54	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
30	STE	t	102	-	-	1/7/7/17	-
32	SQD	a	614	-	-	27/49/69/69	0/1/1/1
26	CLA	B	603	2	-	5/39/115/115	-
26	CLA	b	614	2	-	12/39/115/115	-
26	CLA	B	611	2	-	4/39/115/115	-
28	BCR	H	101	-	-	1/29/63/63	0/2/2/2
26	CLA	c	503	3	-	8/39/115/115	-
30	STE	Z	102	-	-	7/14/14/17	-
30	STE	d	406	-	-	9/17/17/17	-
28	BCR	x	101	-	-	1/29/63/63	0/2/2/2
30	STE	j	102	-	-	5/13/13/17	-
26	CLA	c	501	3	-	1/39/115/115	-
26	CLA	B	606	2	-	7/39/115/115	-
26	CLA	b	609	2	-	4/39/115/115	-
31	LMG	b	622	-	-	21/50/70/70	0/1/1/1
26	CLA	A	614	37	-	4/39/115/115	-
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
26	CLA	b	607	37	-	5/39/115/115	-
34	LHG	B	622	-	-	15/53/53/53	-
26	CLA	b	606	2	-	9/39/115/115	-
34	LHG	e	102	-	-	21/46/46/53	-
31	LMG	m	101	-	-	15/46/66/70	0/1/1/1
26	CLA	b	612	2	-	4/39/115/115	-
32	SQD	A	616	-	-	14/38/58/69	0/1/1/1
28	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	CLA	C	509	3	-	9/39/115/115	-
26	CLA	B	607	37	-	6/39/115/115	-
32	SQD	B	623	-	-	21/49/69/69	0/1/1/1
26	CLA	c	507	37	-	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	STE	A	618	-	-	2/5/5/17	-
26	CLA	B	601	37	-	22/39/115/115	-
30	STE	H	104	-	-	2/6/6/17	-
26	CLA	C	510	3	-	7/39/115/115	-
26	CLA	b	603	2	-	14/39/115/115	-
33	DGD	c	518	-	-	17/51/91/95	0/2/2/2
34	LHG	D	411	-	-	14/53/53/53	-
31	LMG	D	407	-	-	10/46/66/70	0/1/1/1
26	CLA	a	607	1	-	4/39/115/115	-
29	PL9	a	612	-	-	22/53/73/73	0/1/1/1
30	STE	C	518	-	-	1/2/2/17	-
26	CLA	d	402	4	-	6/39/115/115	-
30	STE	j	101	-	-	5/9/9/17	-
26	CLA	c	511	3	-	7/39/115/115	-
26	CLA	B	614	2	-	13/39/115/115	-
28	BCR	b	619	-	-	0/29/63/63	0/2/2/2
31	LMG	c	517	-	-	6/31/31/70	-
34	LHG	D	408	-	-	13/53/53/53	-
30	STE	d	412	-	-	9/17/17/17	-
26	CLA	A	607	1	-	4/39/115/115	-
30	STE	c	516	-	-	9/15/15/17	-
30	STE	B	624	-	-	4/11/11/17	-

The worst 5 of 634 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	PHO	C1B-C2B	9.66	1.50	1.39
27	a	609	PHO	C1B-C2B	9.01	1.49	1.39
27	D	401	PHO	C1B-C2B	9.00	1.49	1.39
27	d	401	PHO	C3B-C4B	8.75	1.50	1.41
27	A	609	PHO	C1B-C2B	8.62	1.49	1.39

The worst 5 of 702 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	609	PHO	C4D-CHA-CBD	-8.56	104.35	108.45
26	B	615	CLA	C4A-NA-C1A	8.21	110.42	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	609	PHO	C4D-CHA-CBD	-7.90	104.66	108.45
26	b	606	CLA	C4A-NA-C1A	7.50	110.10	106.68
26	b	601	CLA	C4A-NA-C1A	7.41	110.06	106.68

All (2) chirality outliers are listed below:

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

5 of 1520 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	C1A-C2A-CAA-CBA
26	B	601	CLA	CBA-CGA-O2A-C1
26	B	601	CLA	O1A-CGA-O2A-C1
26	B	614	CLA	CAD-CBD-CGD-O1D
26	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

100 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	511	CLA	1	0
28	D	404	BCR	1	0
31	C	517	LMG	1	0
26	B	602	CLA	2	0
26	b	604	CLA	2	0
30	C	527	STE	1	0
33	C	522	DGD	4	0
26	C	505	CLA	2	0
26	c	502	CLA	1	0
31	M	101	LMG	1	0
26	C	513	CLA	1	0
34	d	407	LHG	4	0
33	H	102	DGD	1	0
28	T	101	BCR	3	0
26	b	610	CLA	1	0
26	C	508	CLA	2	0
21	A	601[B]	OEY	1	0
28	A	611	BCR	1	0
31	B	620	LMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	620	SQD	2	0
28	C	515	BCR	1	0
26	B	605	CLA	1	0
26	b	608	CLA	1	0
32	f	102	SQD	1	0
33	C	523	DGD	1	0
33	A	617	DGD	4	0
26	d	403	CLA	4	0
27	A	609	PHO	1	0
28	t	101	BCR	5	0
30	E	104	STE	1	0
30	I	102	STE	2	0
28	b	618	BCR	2	0
26	B	604	CLA	1	0
30	b	623	STE	1	0
26	C	512	CLA	2	0
30	C	519	STE	1	0
28	a	611	BCR	2	0
35	F	101	HEM	4	0
26	b	615	CLA	1	0
26	c	505	CLA	1	0
21	a	601[B]	OEY	1	0
26	a	608	CLA	1	0
26	B	613	CLA	1	0
26	B	610	CLA	2	0
26	C	502	CLA	1	0
28	Z	101	BCR	2	0
26	b	601	CLA	1	0
26	b	613	CLA	5	0
30	H	103	STE	3	0
26	C	506	CLA	1	0
29	A	612	PL9	2	0
35	f	101	HEM	4	0
26	b	616	CLA	1	0
26	B	612	CLA	2	0
31	a	616	LMG	1	0
31	c	522	LMG	1	0
26	A	608	CLA	2	0
26	B	615	CLA	1	0
32	F	102	SQD	2	0
32	D	410	SQD	1	0
28	k	102	BCR	1	0

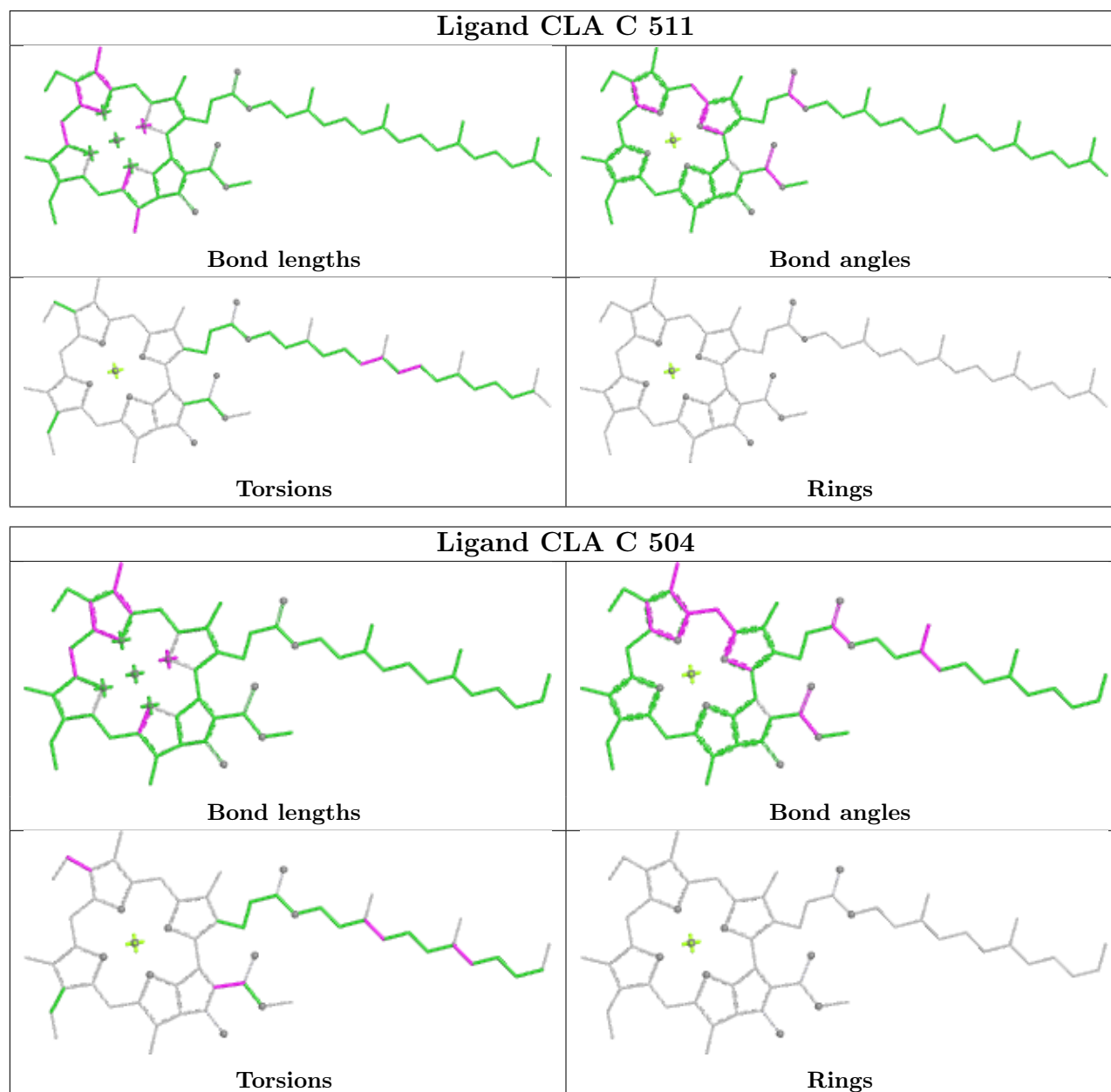
Continued on next page...

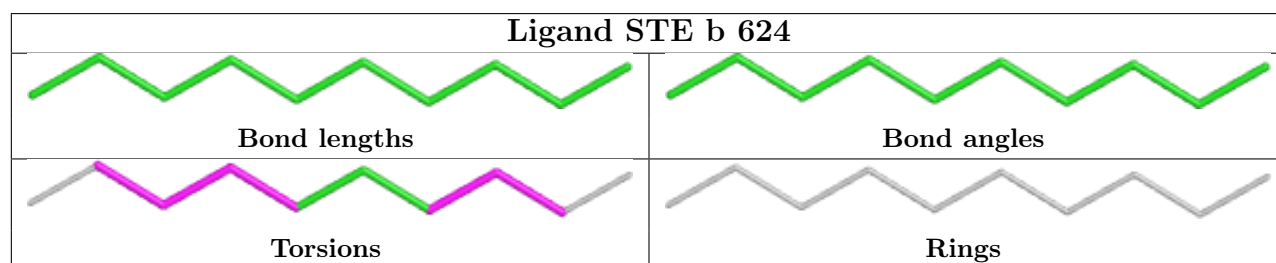
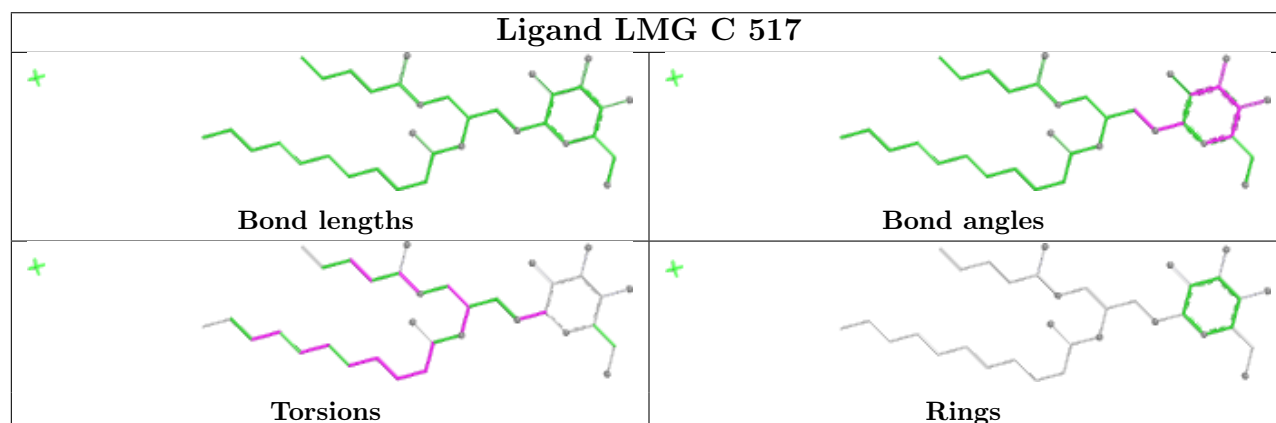
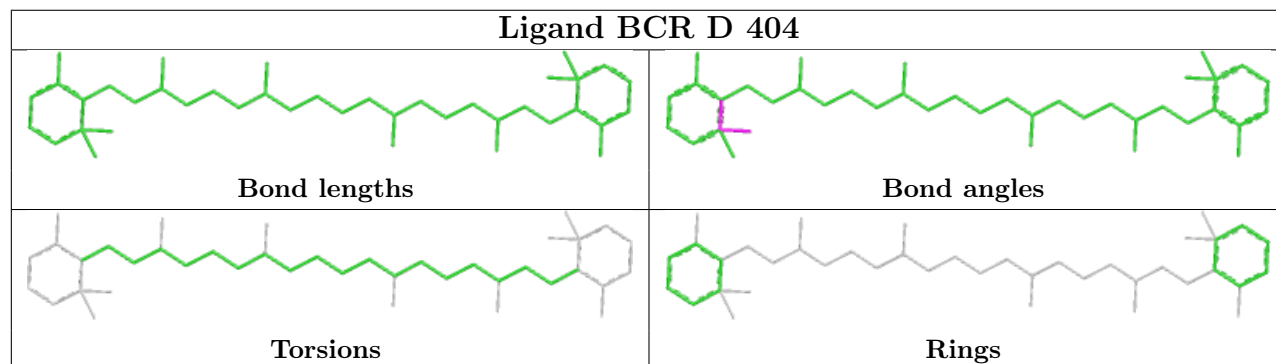
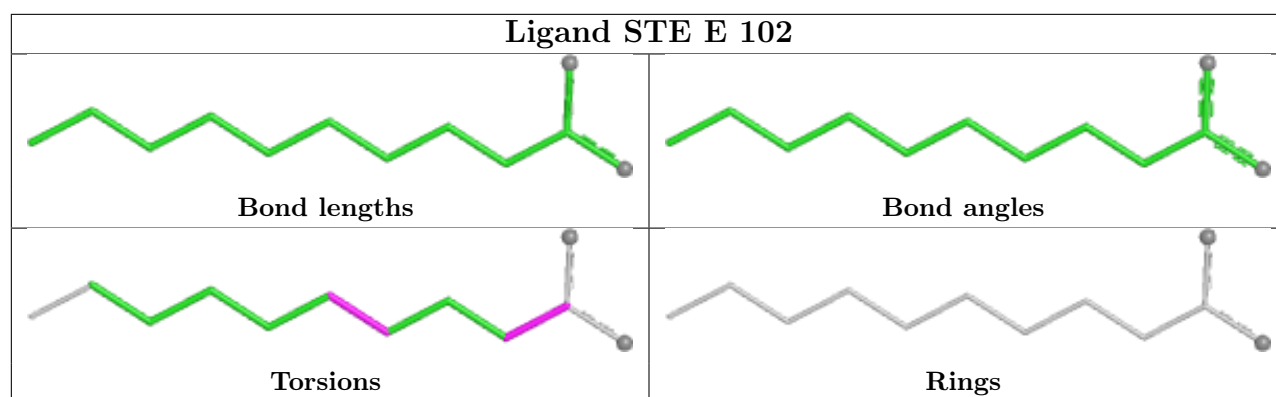
Continued from previous page...

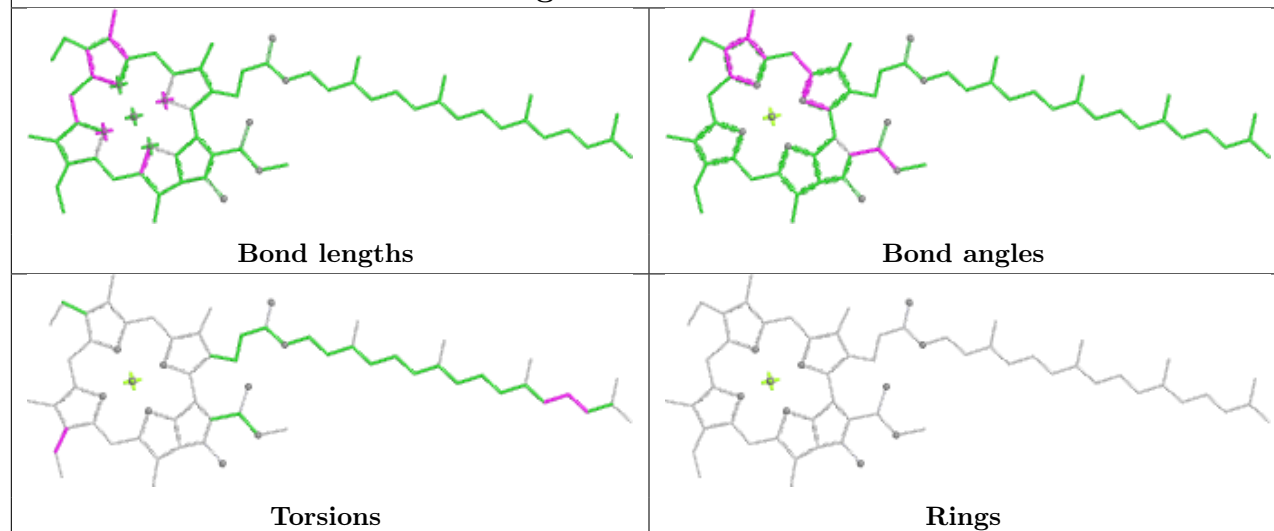
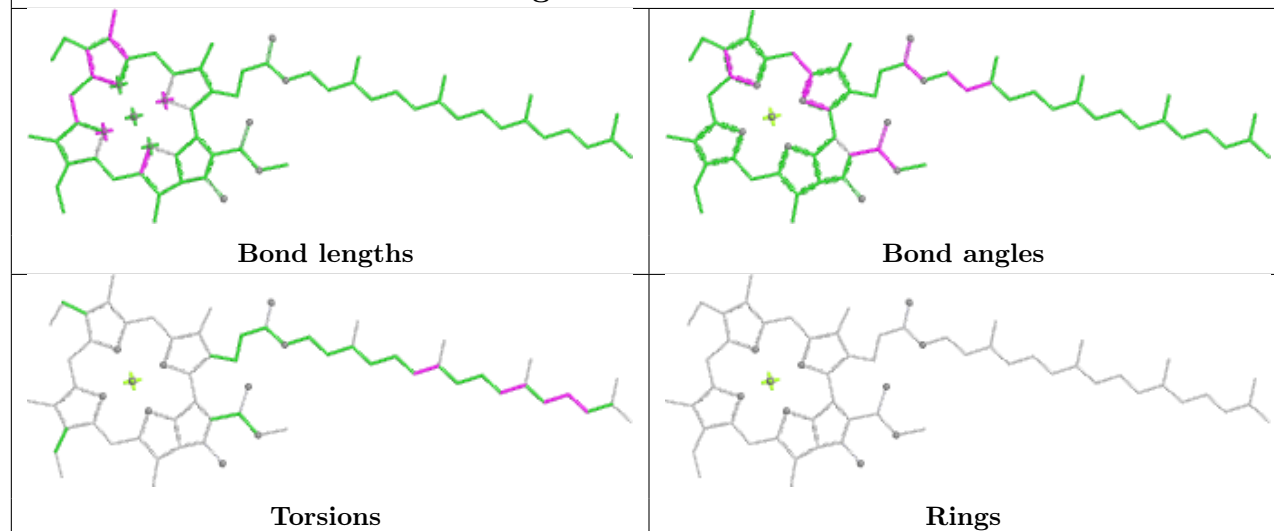
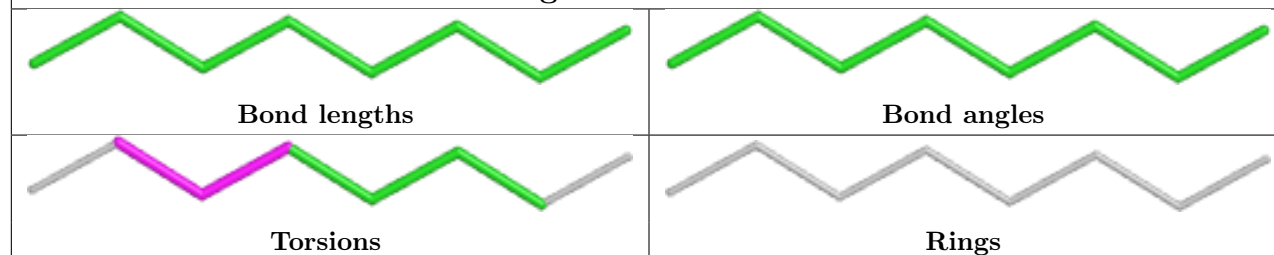
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	401	PHO	2	0
31	C	524	LMG	1	0
26	c	509	CLA	1	0
26	b	602	CLA	1	0
30	K	102	STE	1	0
30	D	412	STE	3	0
26	c	513	CLA	1	0
28	B	617	BCR	1	0
36	v	201	HEC	1	0
28	k	101	BCR	4	0
26	B	603	CLA	1	0
26	B	611	CLA	1	0
28	H	101	BCR	2	0
30	Z	102	STE	1	0
30	d	406	STE	1	0
28	x	101	BCR	3	0
26	c	501	CLA	2	0
26	B	606	CLA	2	0
26	b	609	CLA	1	0
34	B	622	LHG	3	0
26	b	606	CLA	1	0
34	e	102	LHG	1	0
26	b	612	CLA	1	0
28	B	618	BCR	3	0
26	C	509	CLA	2	0
32	B	623	SQD	2	0
26	c	507	CLA	1	0
30	A	618	STE	1	0
26	B	601	CLA	4	0
34	D	411	LHG	1	0
26	a	607	CLA	3	0
29	a	612	PL9	3	0
26	d	402	CLA	2	0
26	c	511	CLA	1	0
26	B	614	CLA	1	0
28	b	619	BCR	1	0
34	D	408	LHG	2	0
26	A	607	CLA	5	0
30	c	516	STE	1	0

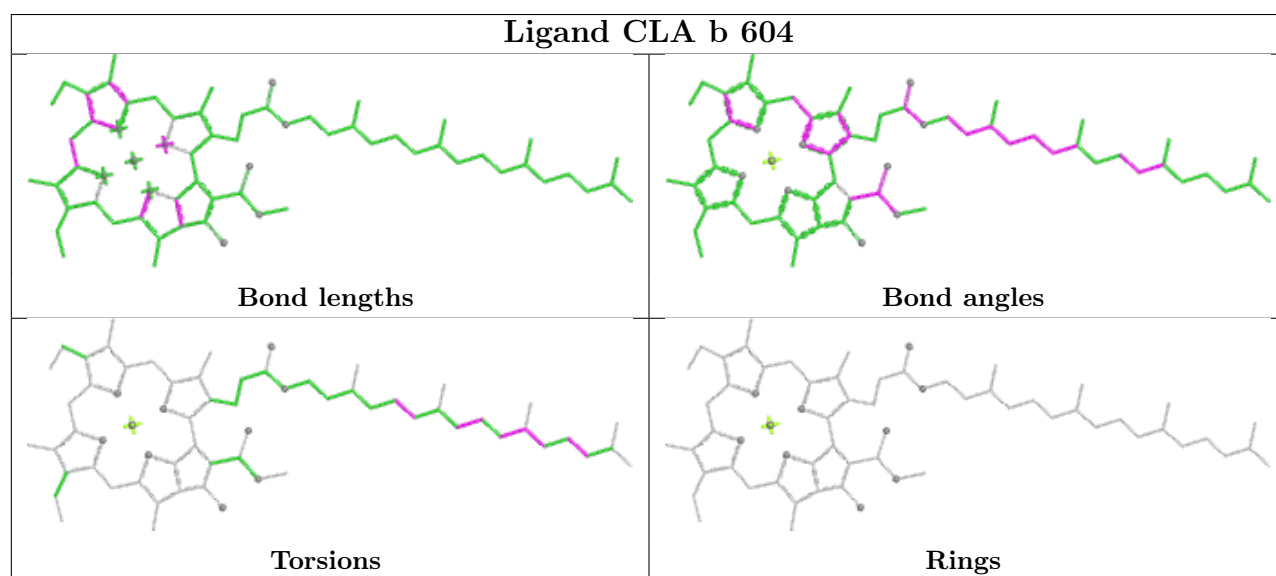
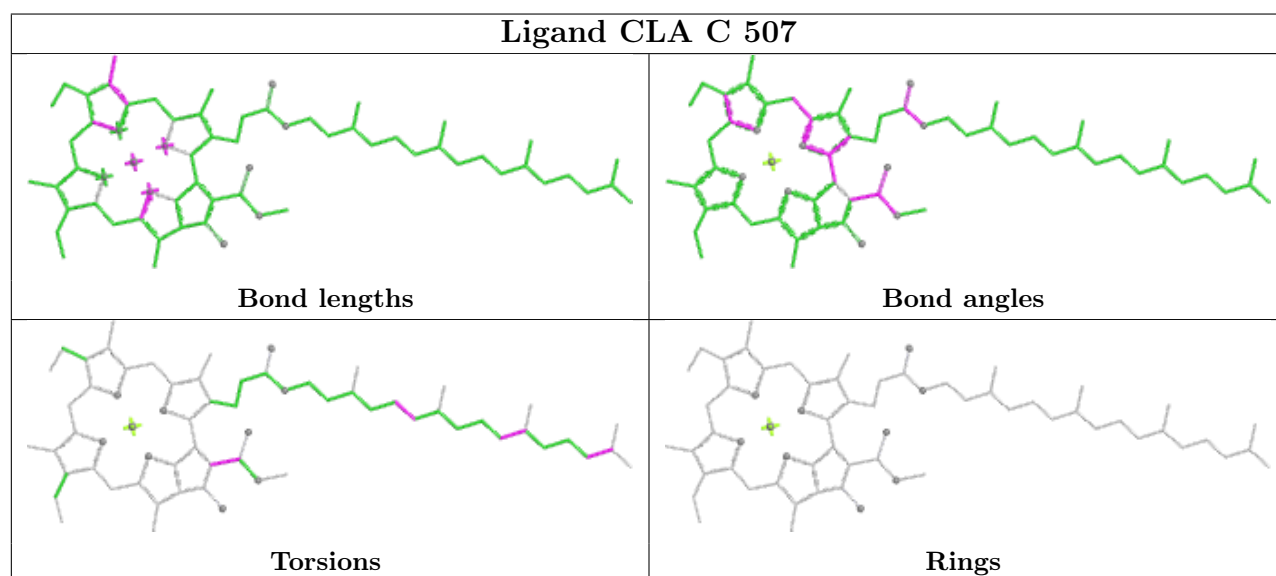
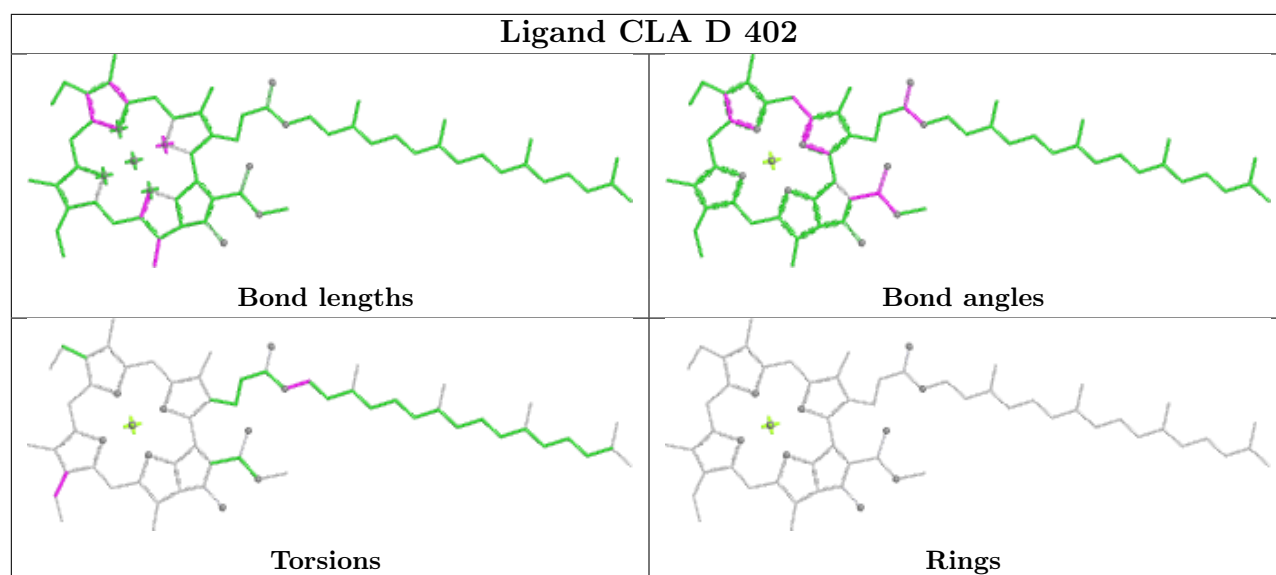
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

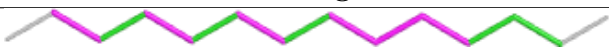
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

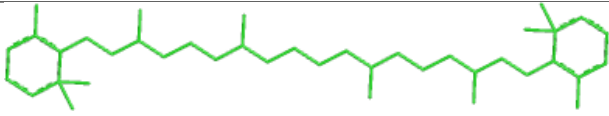
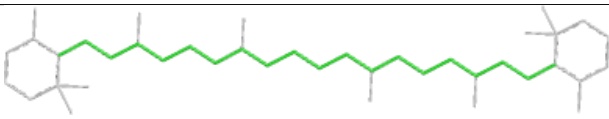
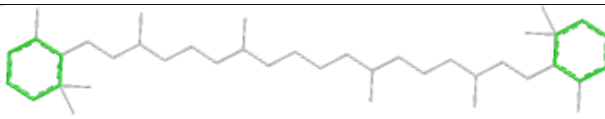


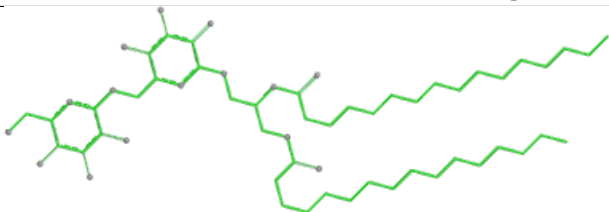
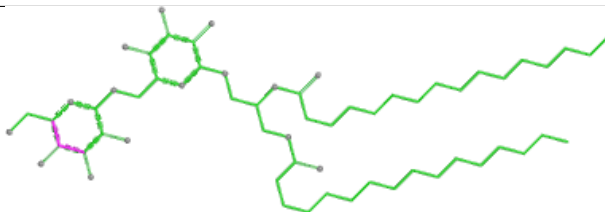
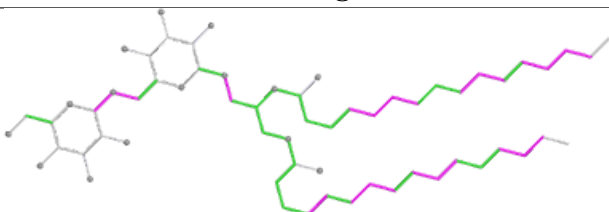
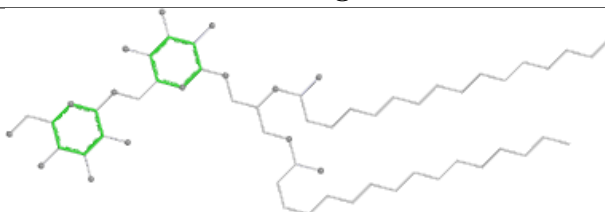


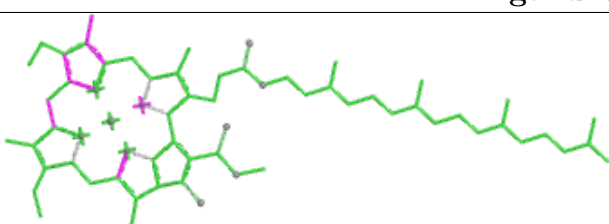
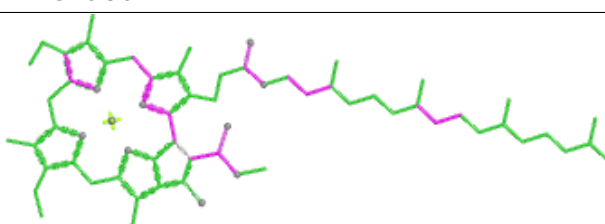
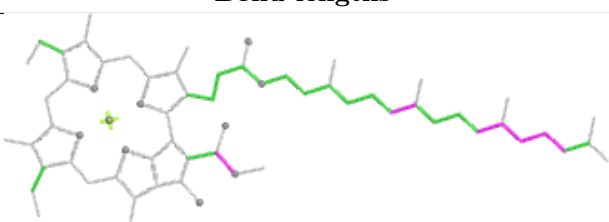
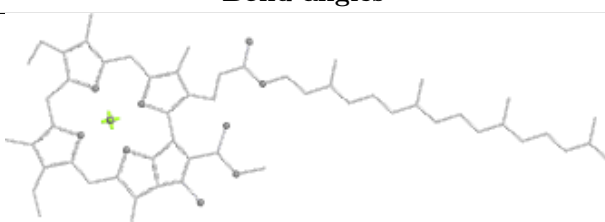
Ligand CLA a 613**Ligand CLA B 602****Ligand STE e 103**

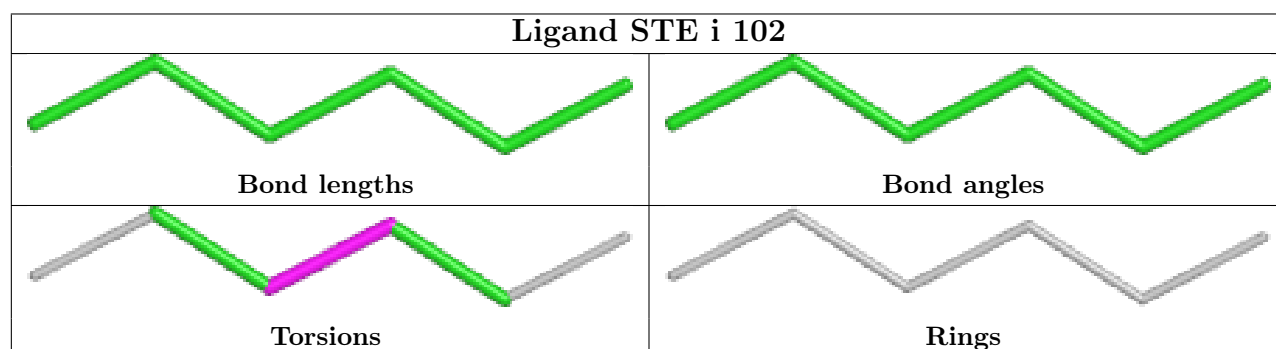
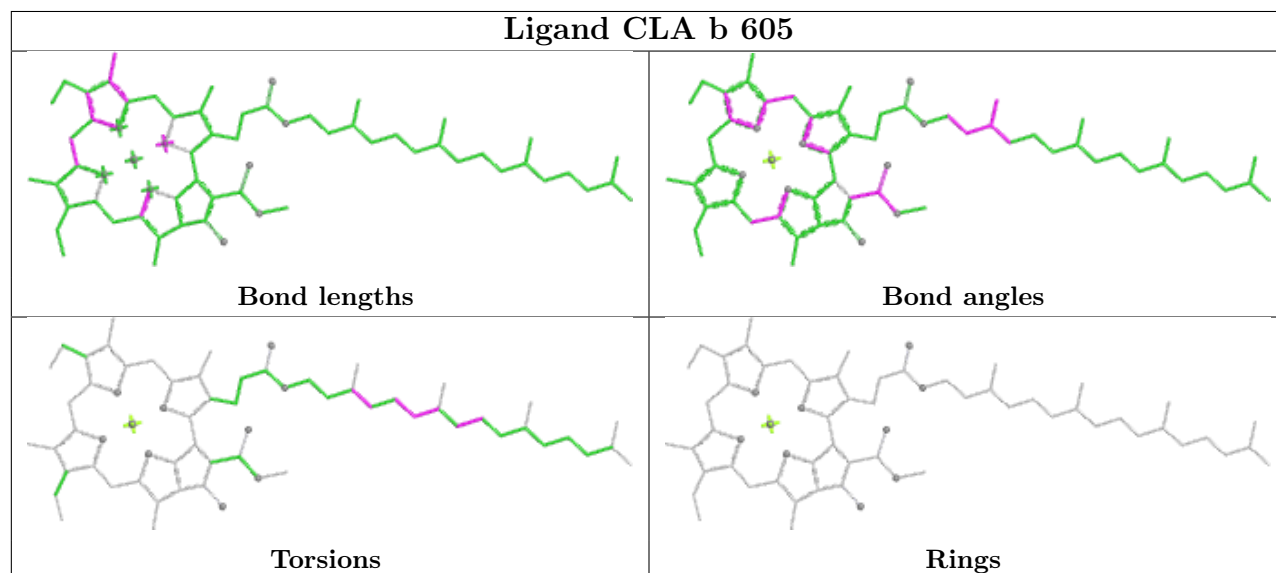
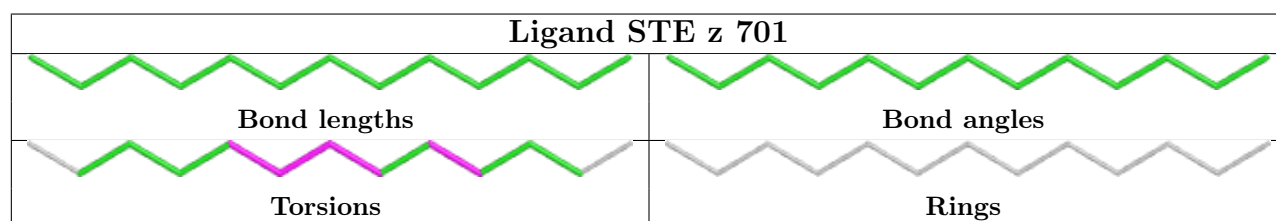
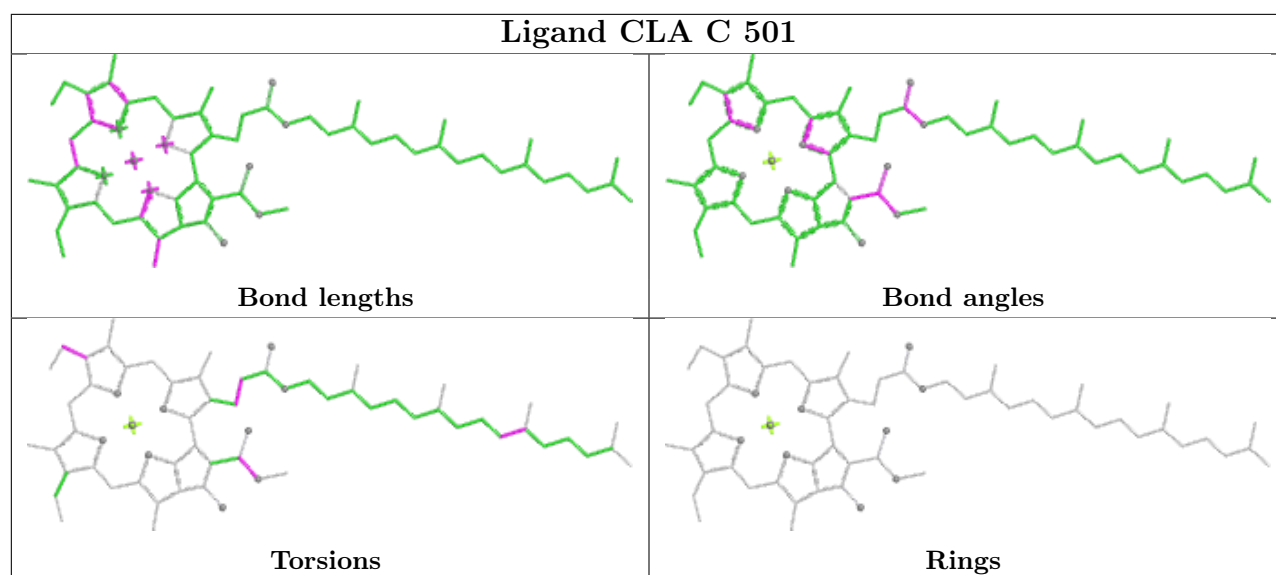


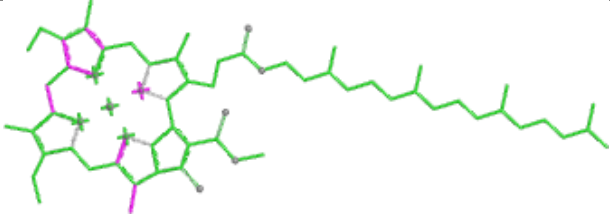
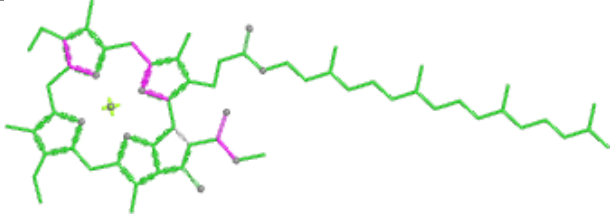
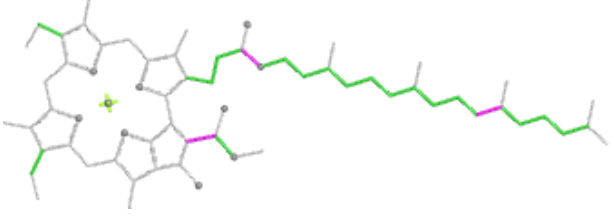
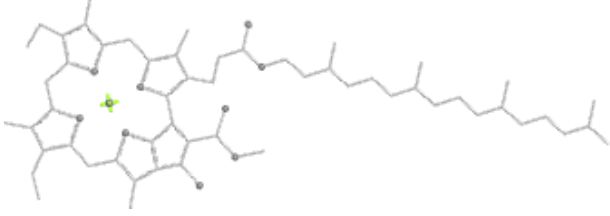
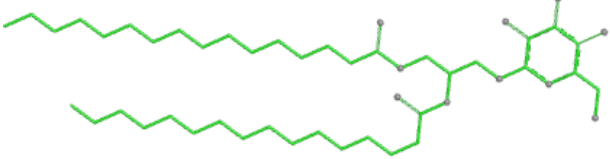
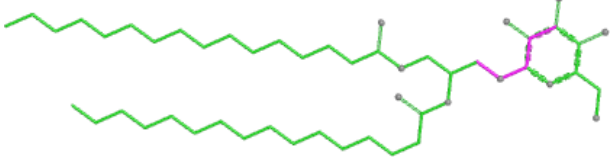
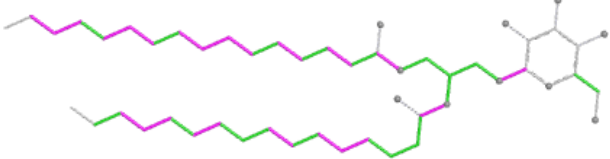
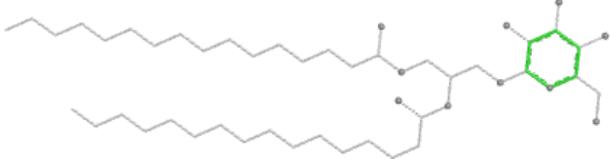
Ligand STE C 527	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

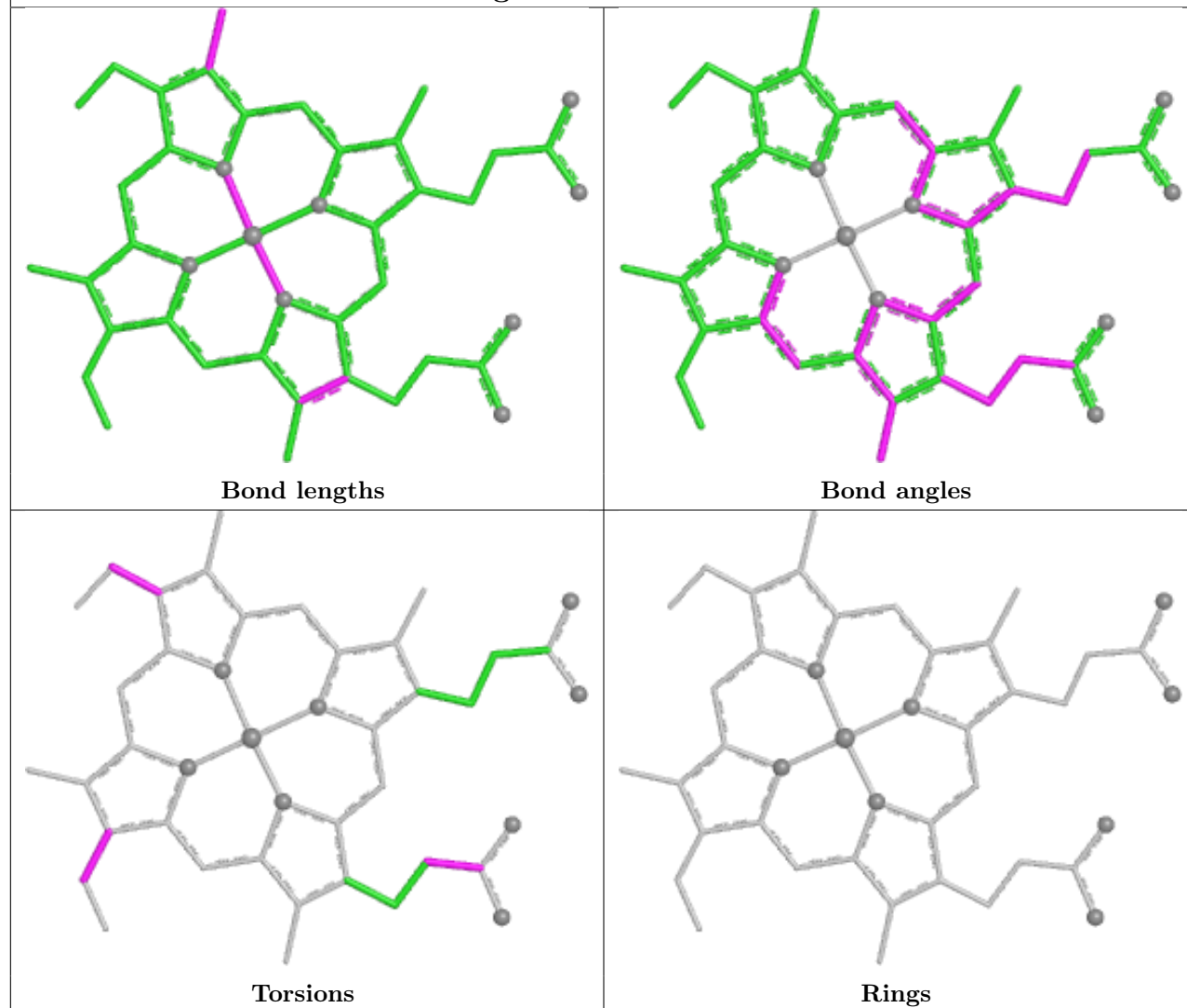
Ligand DGD C 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

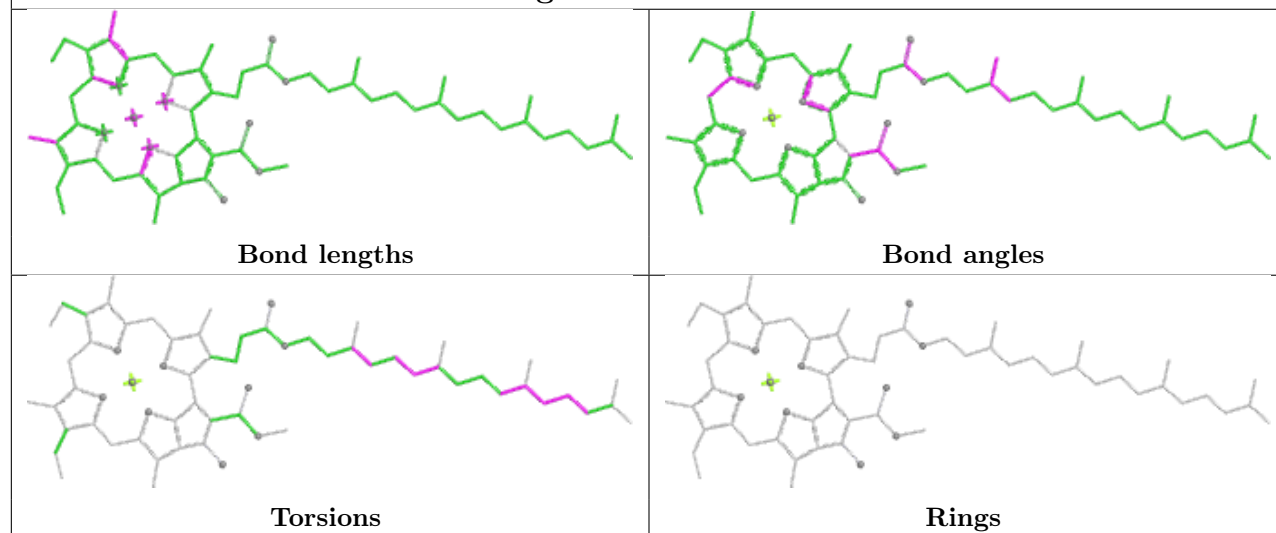


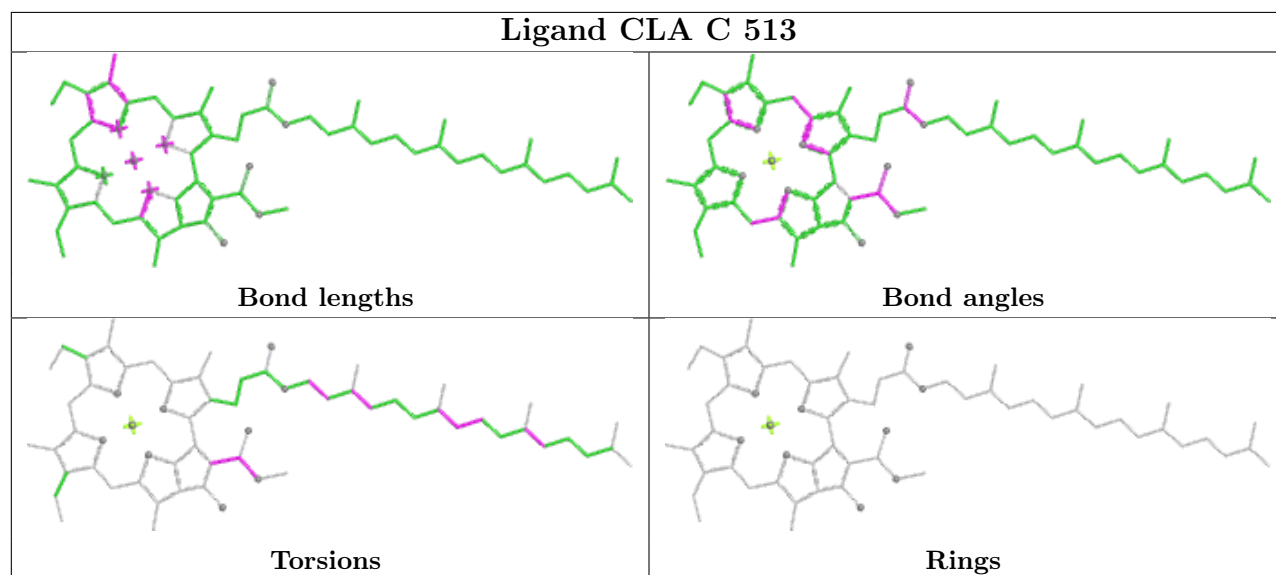
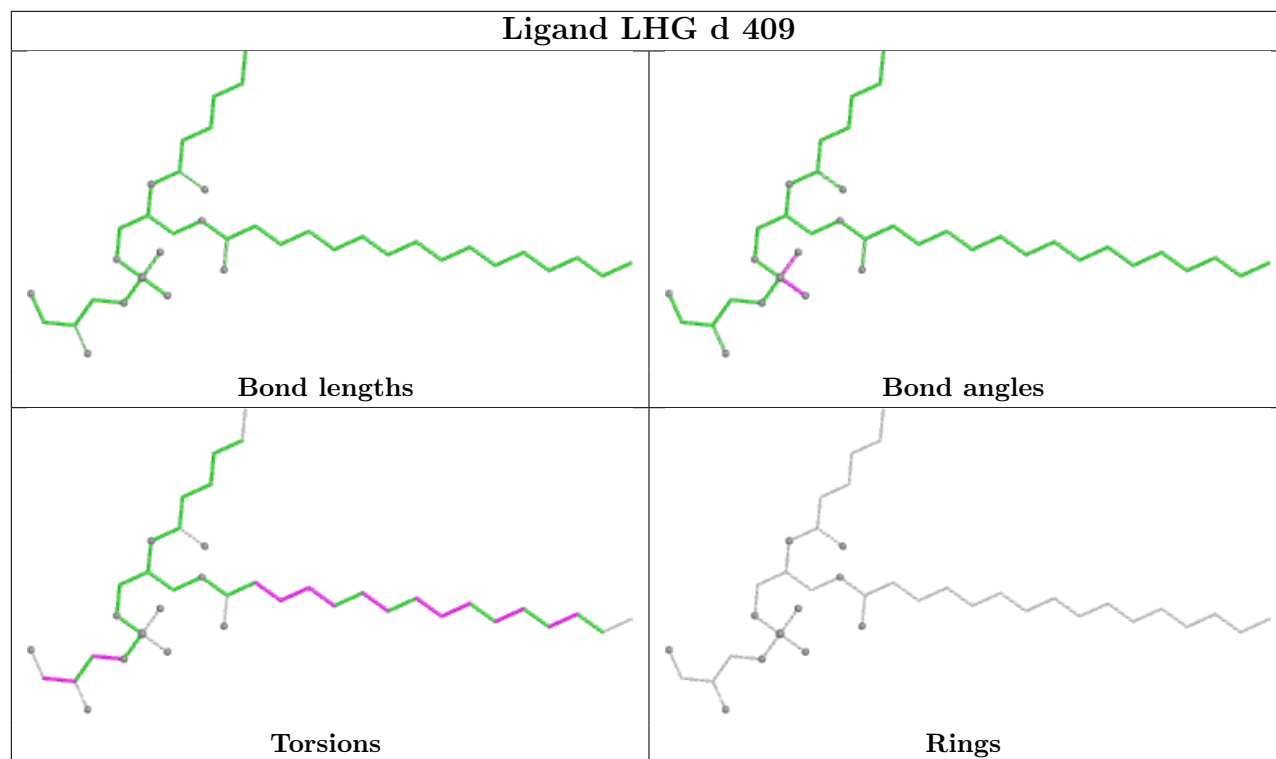
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE A 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

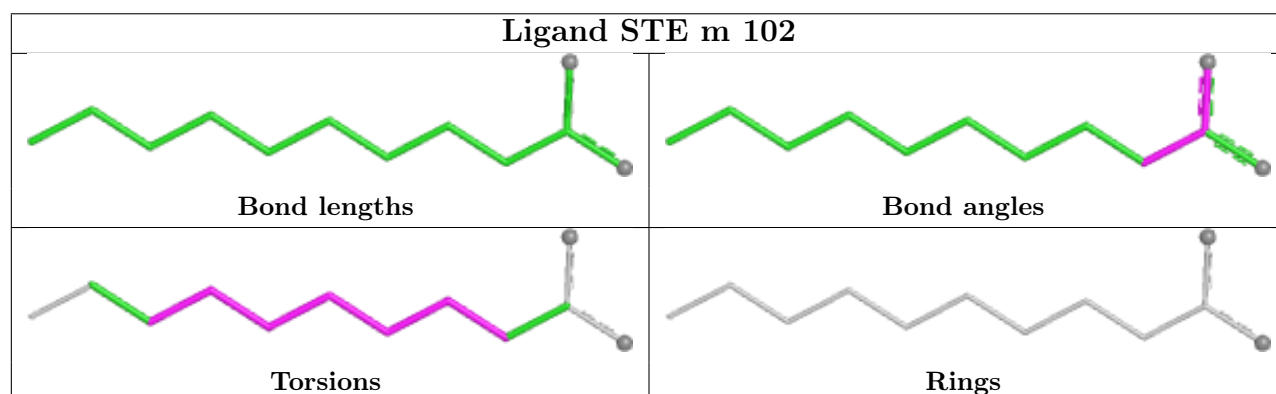
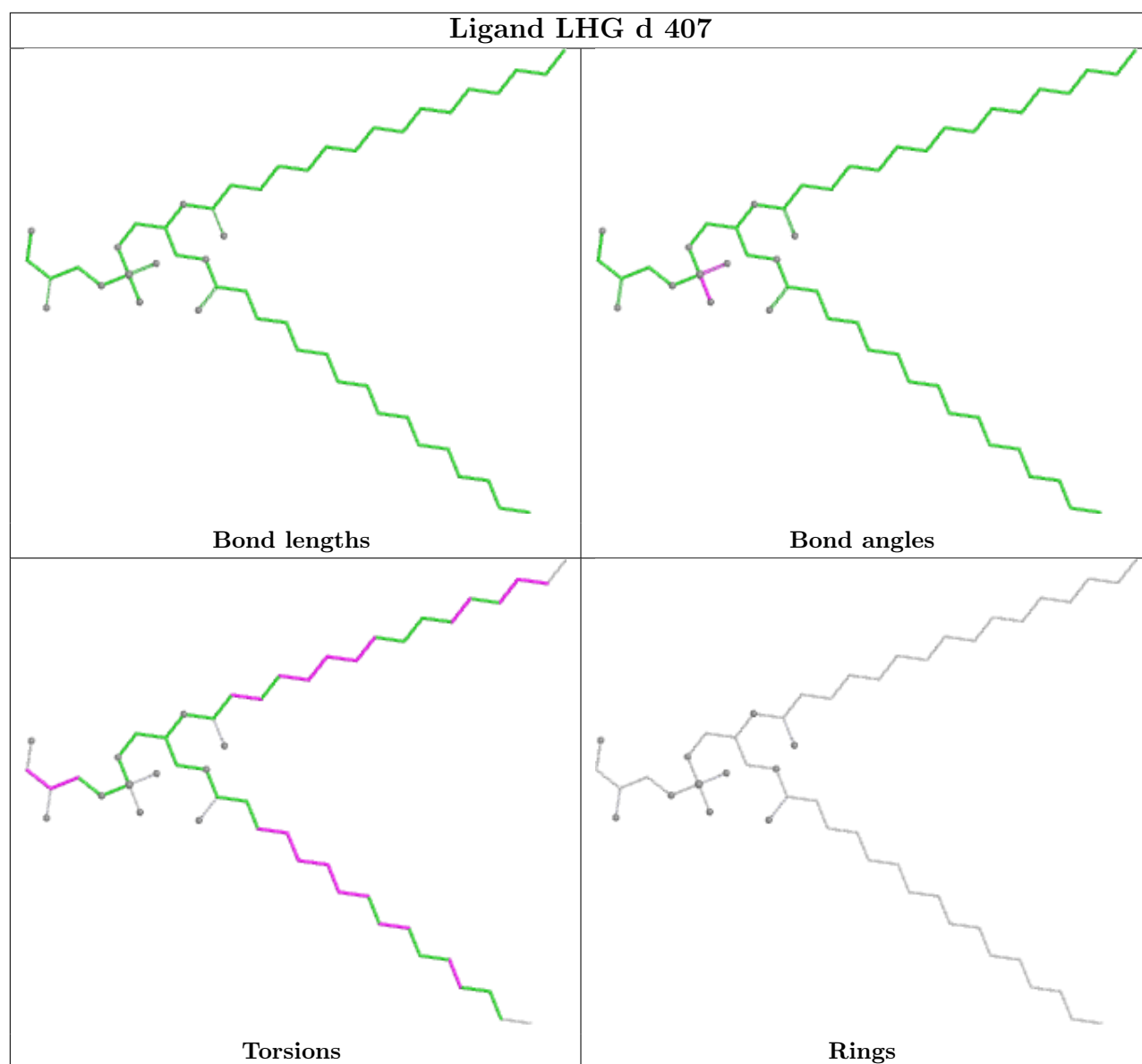
Ligand HEC V 201

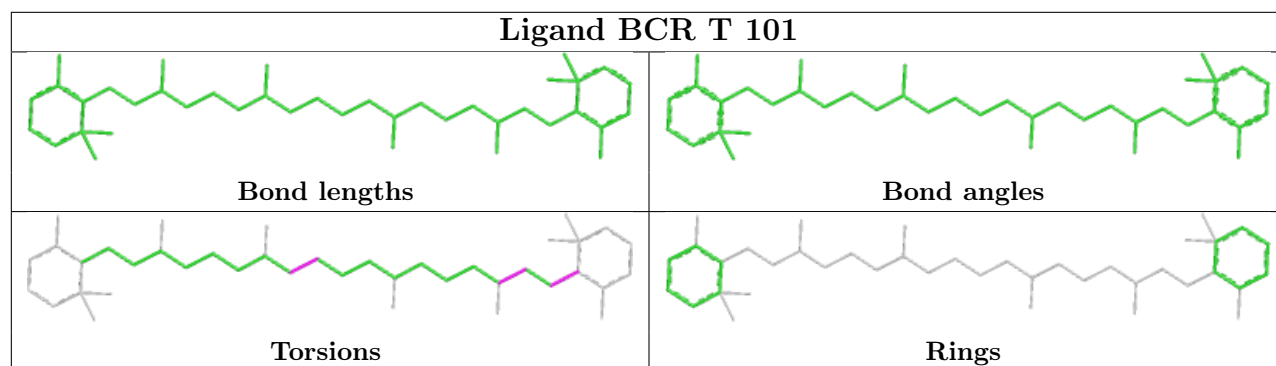
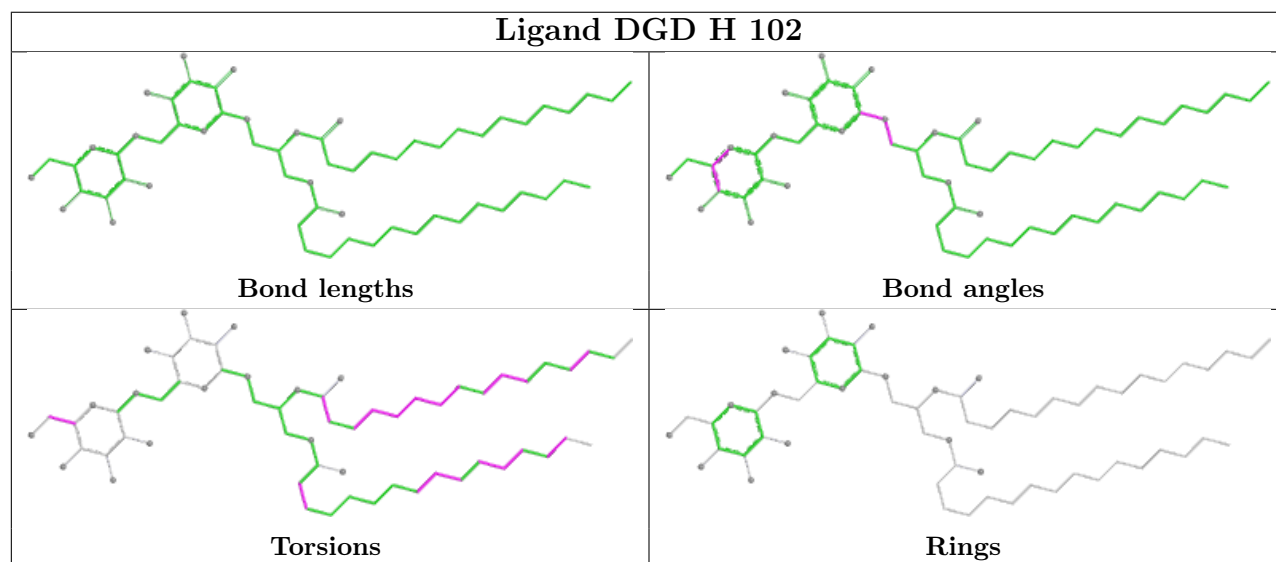
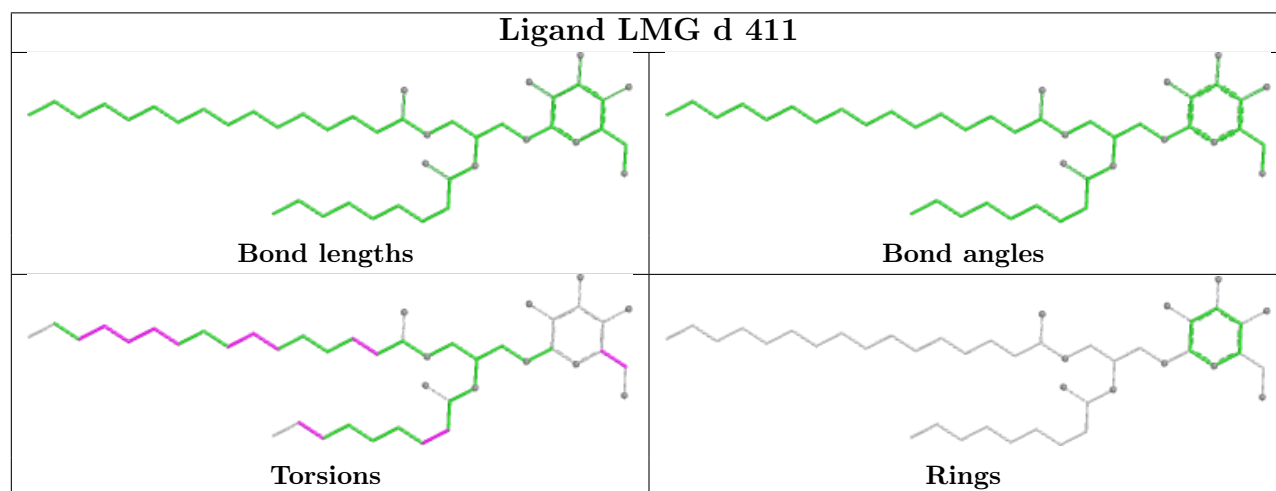
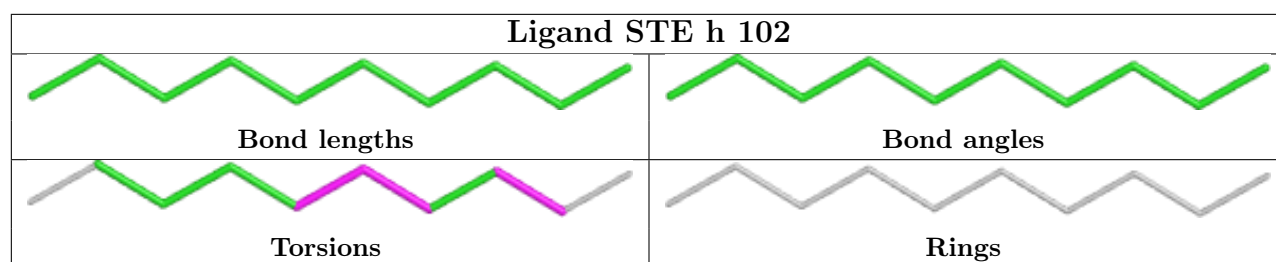


Ligand CLA a 610

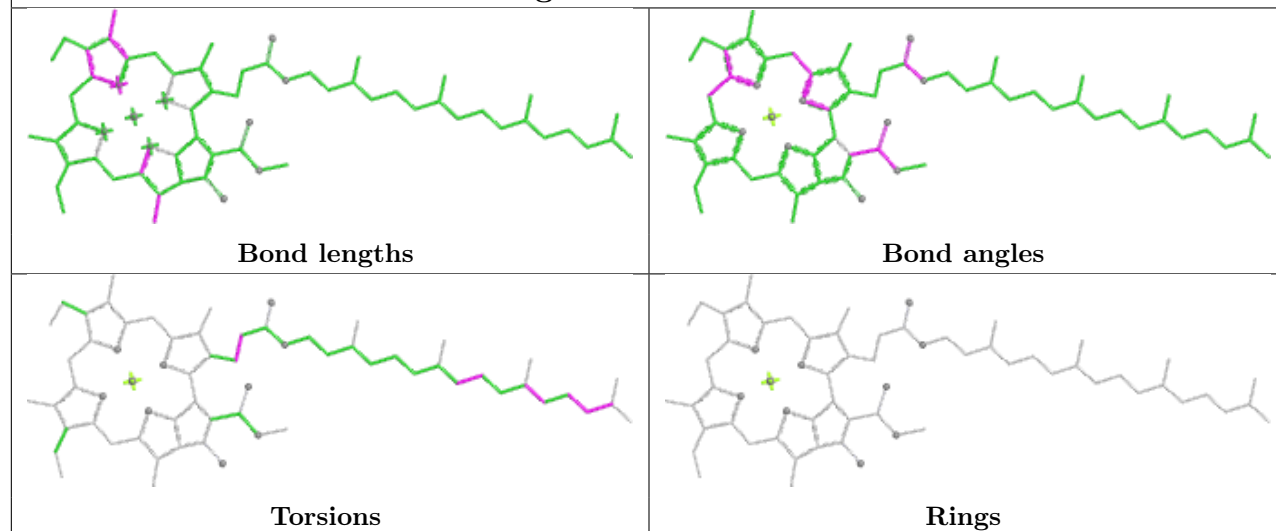




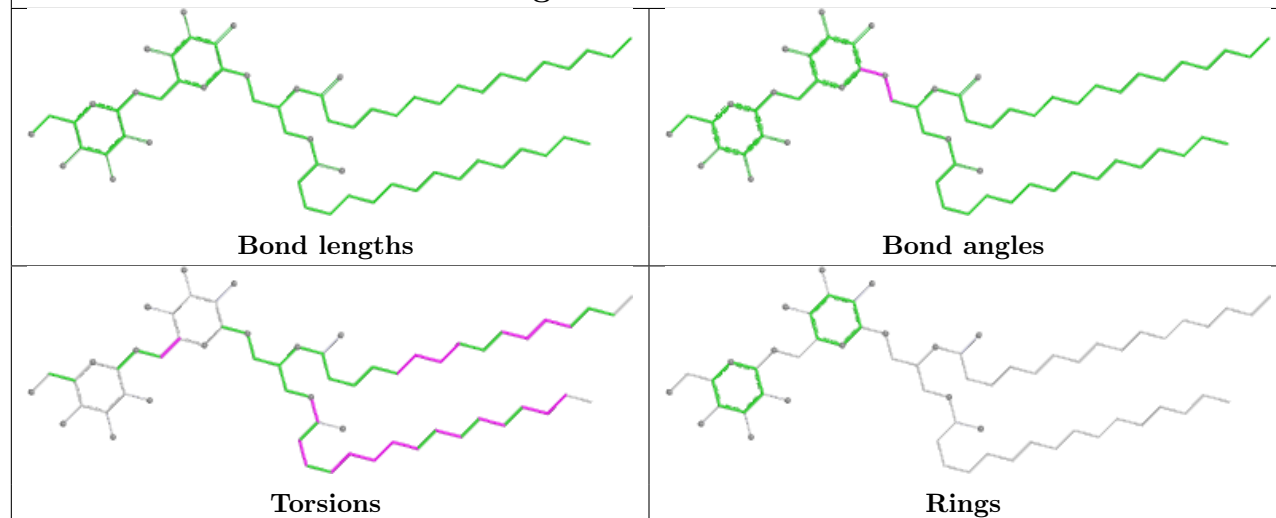




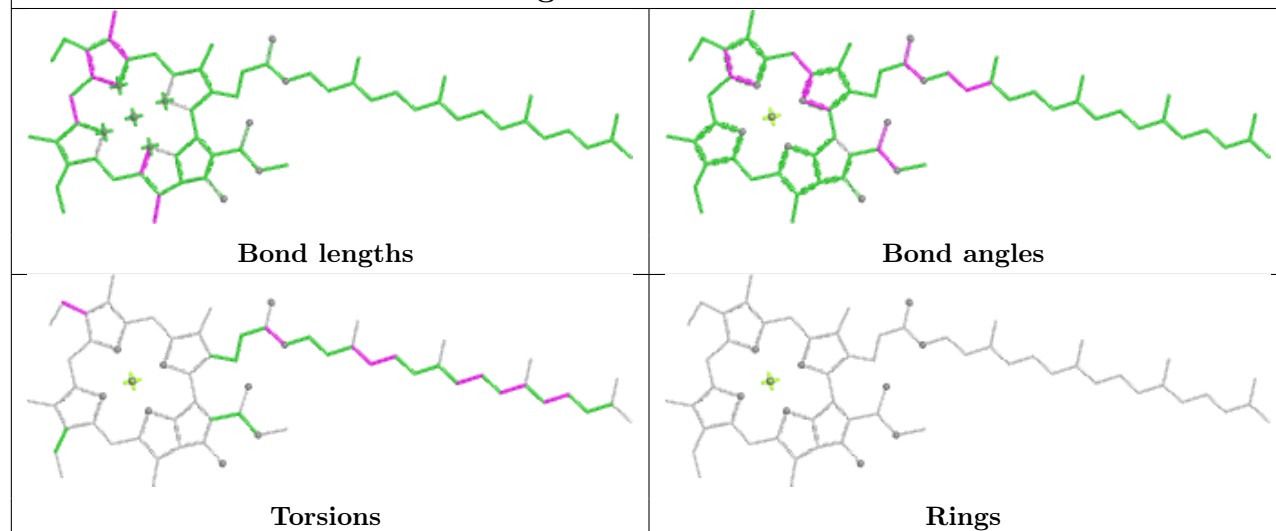
Ligand CLA b 610

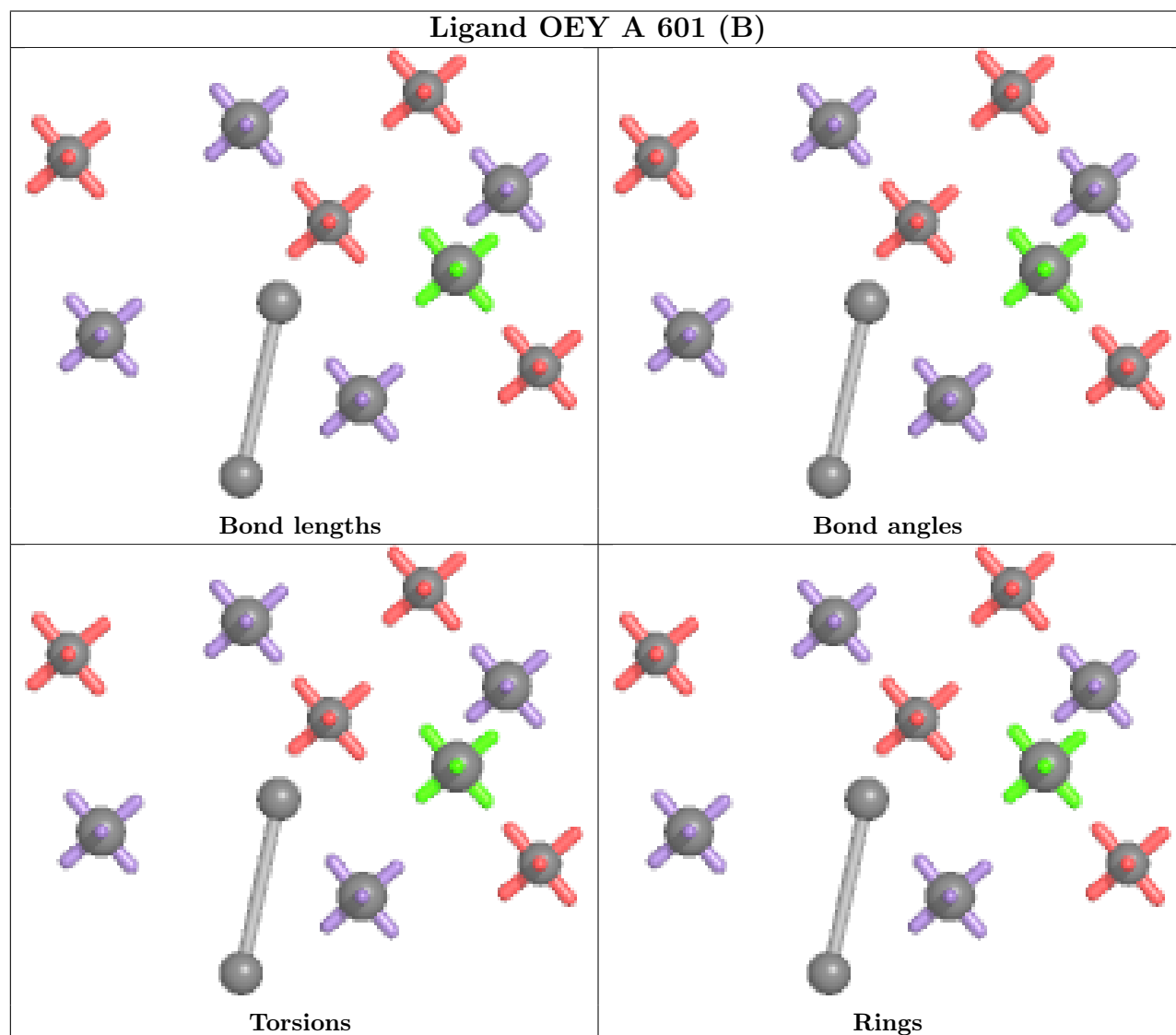
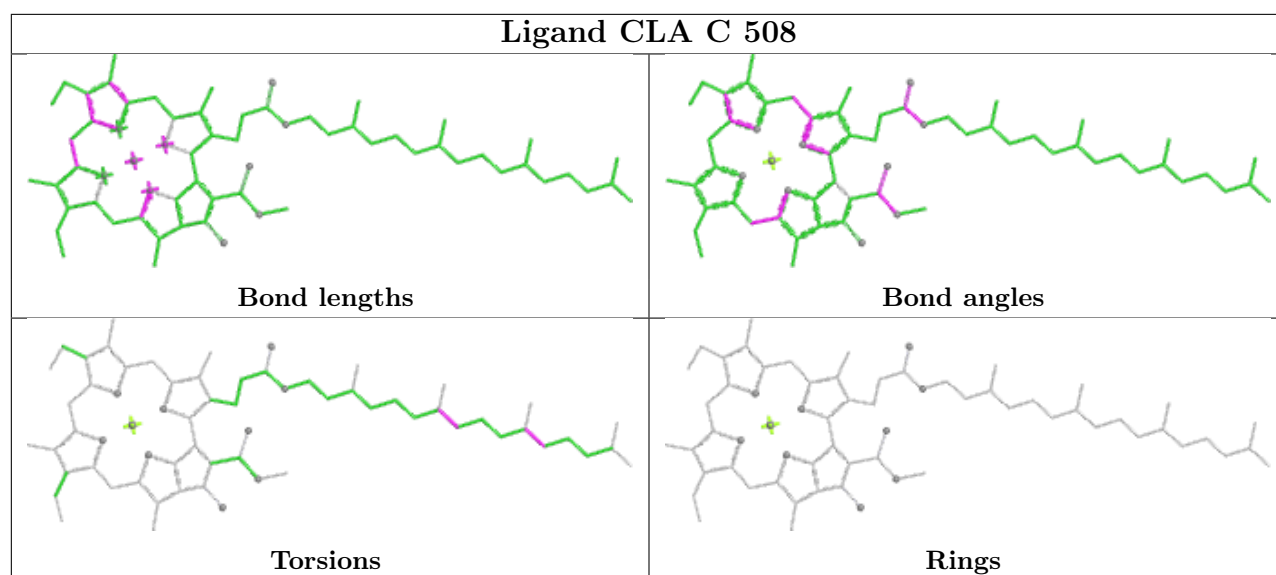


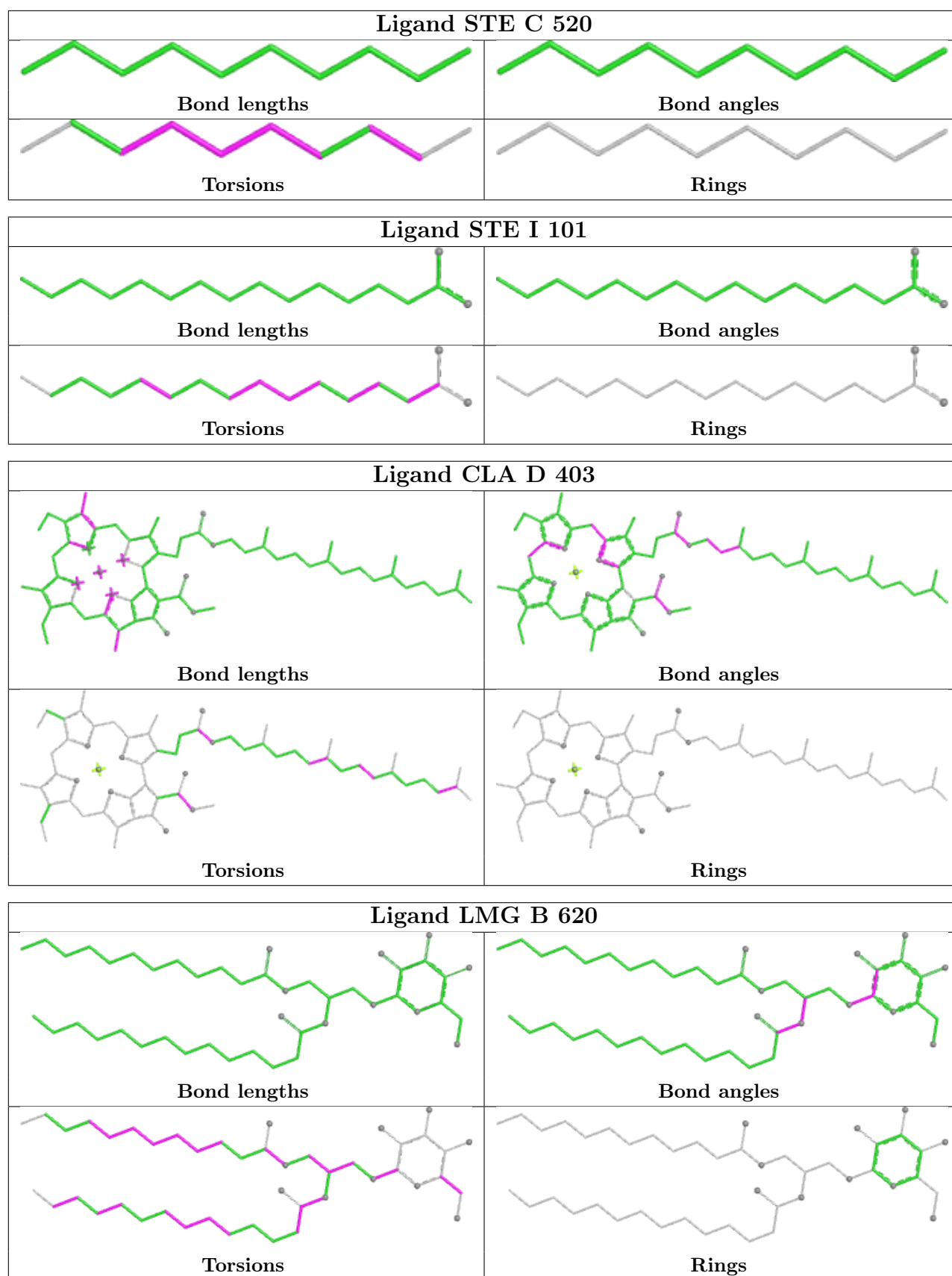
Ligand DGD c 520

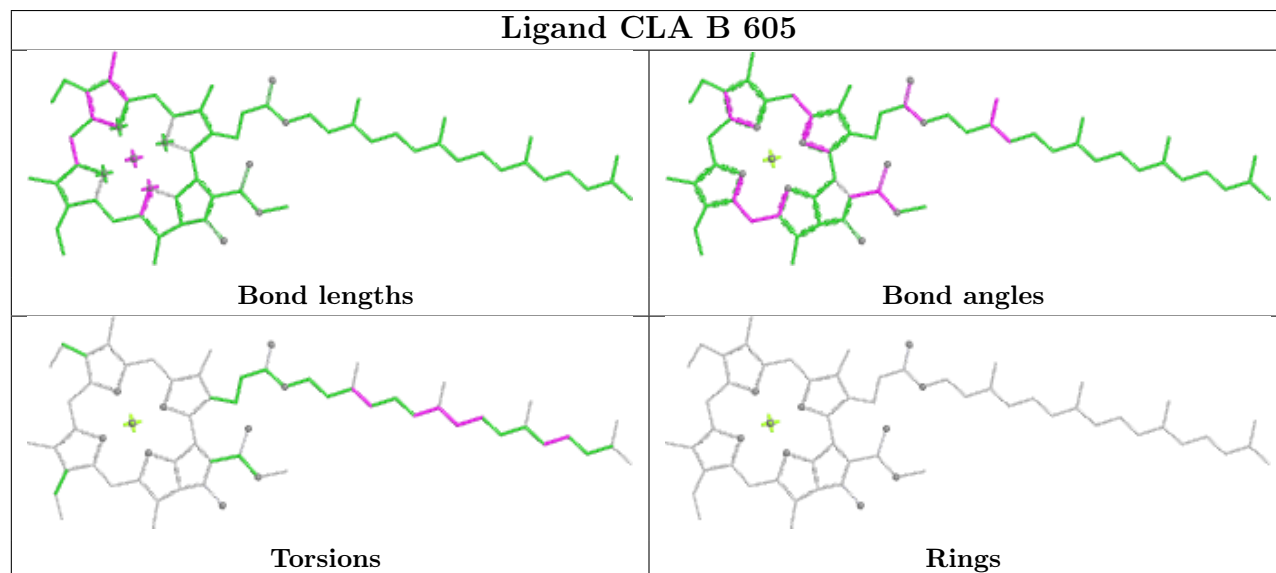
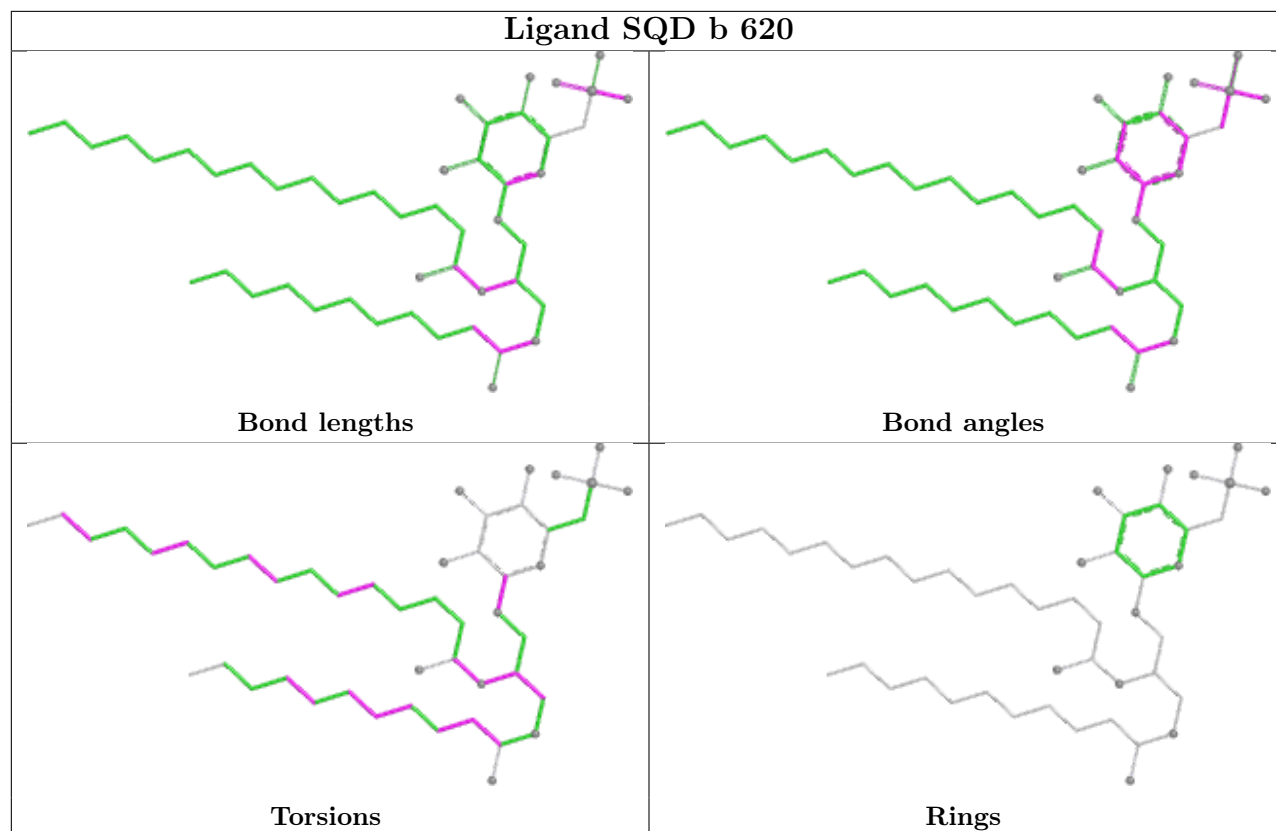


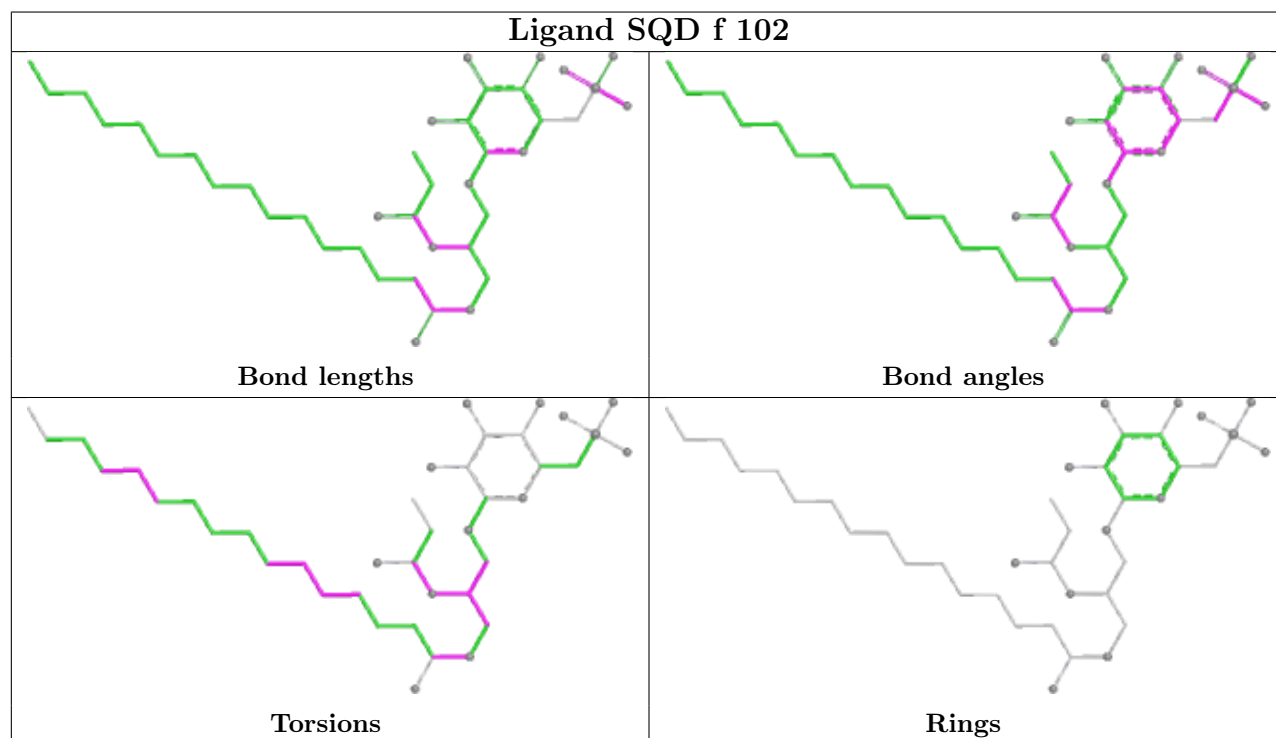
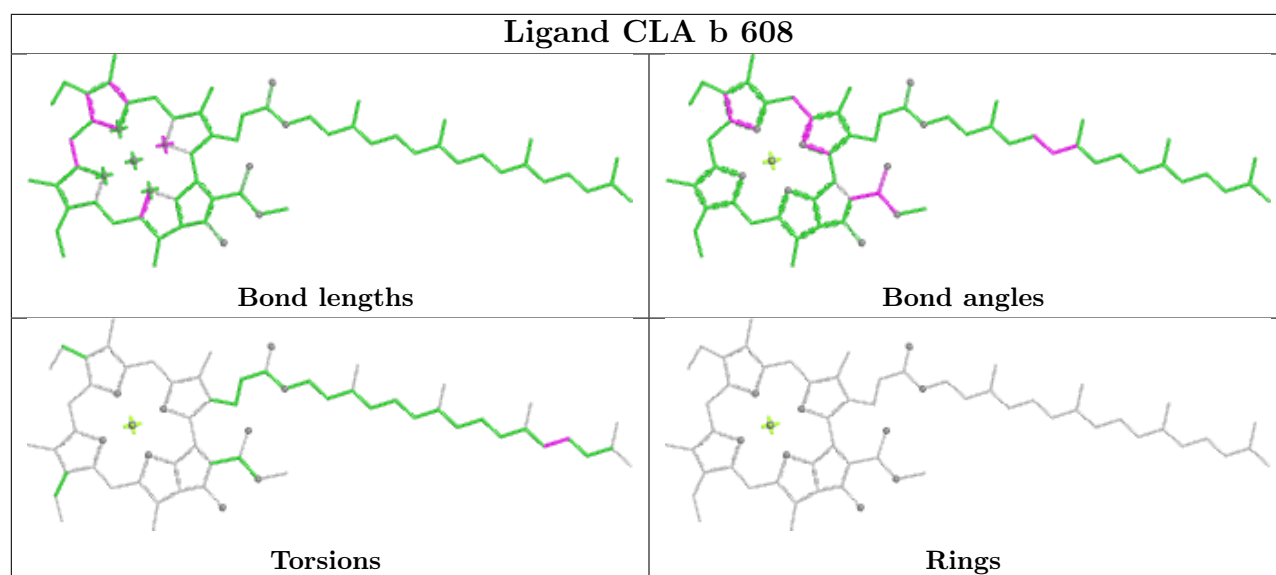
Ligand CLA c 512

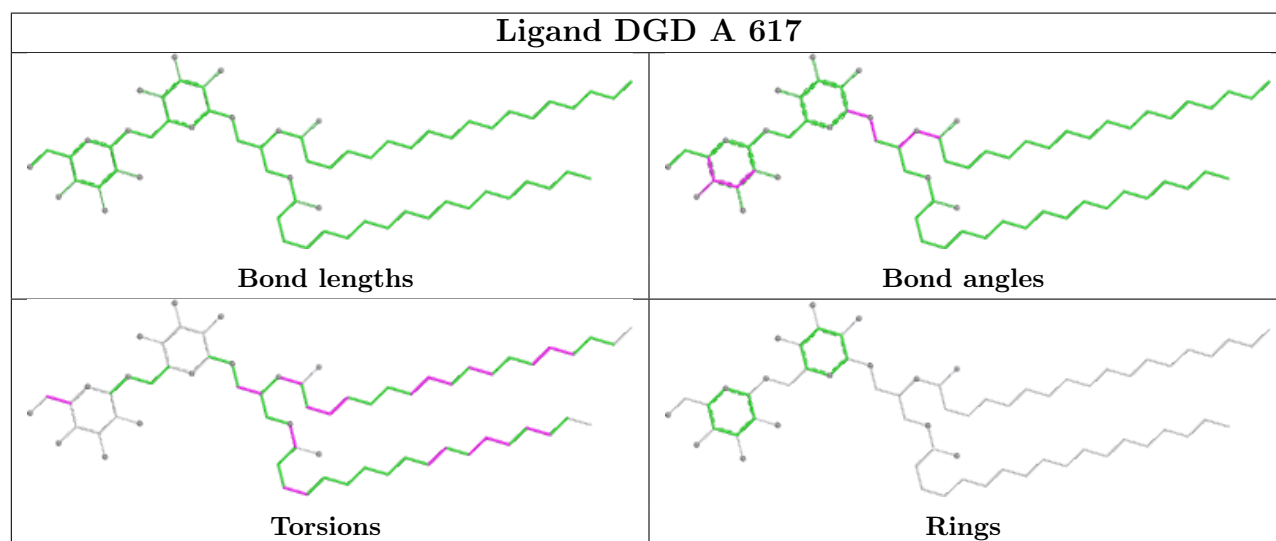
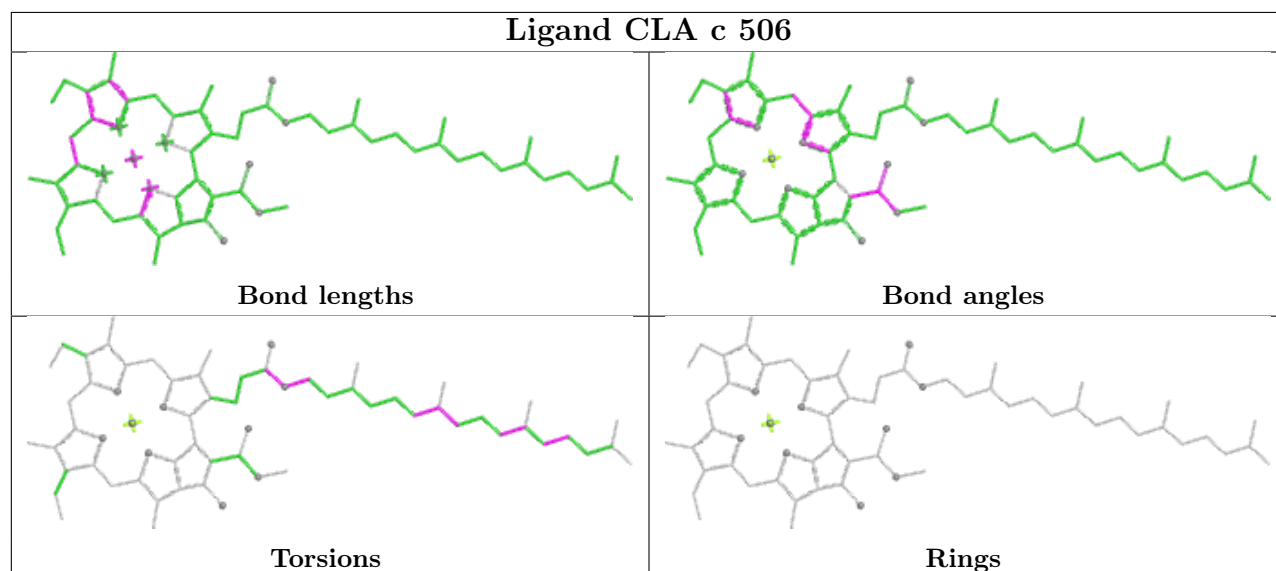
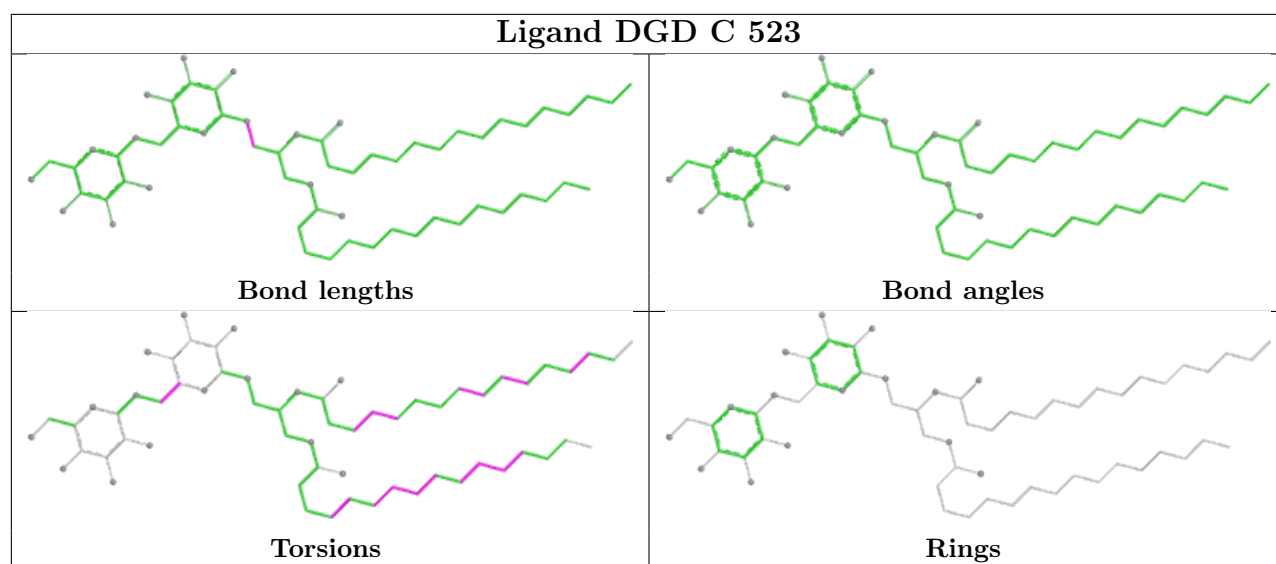




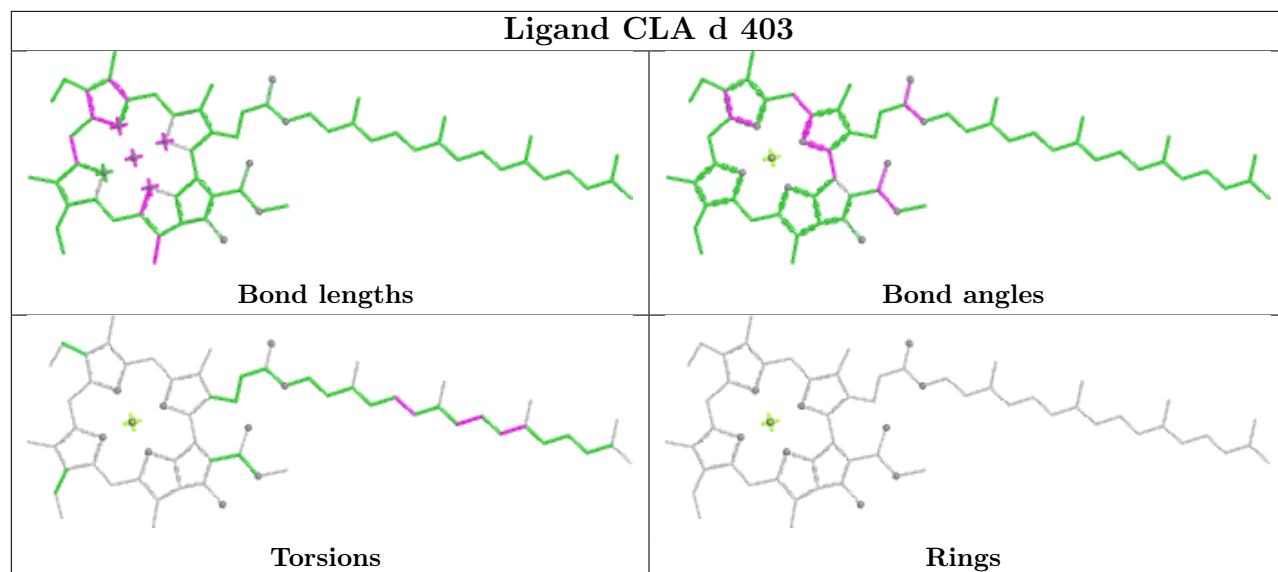




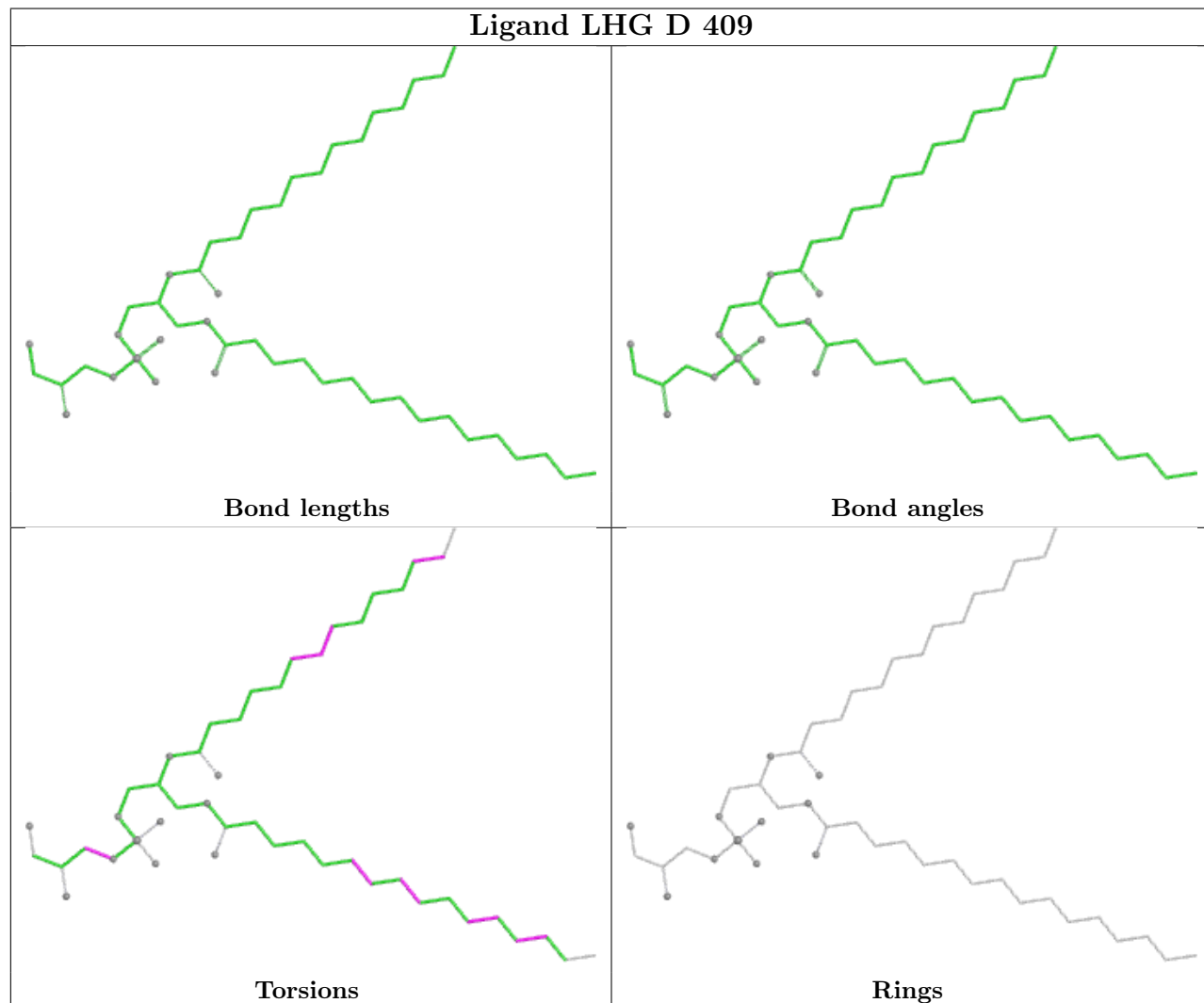


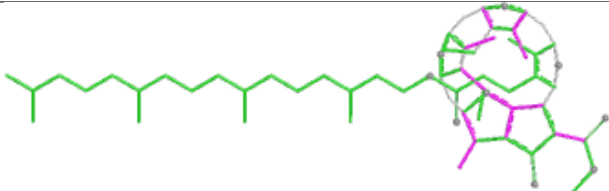
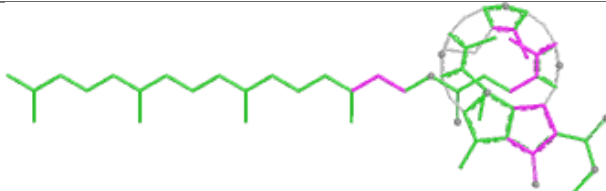
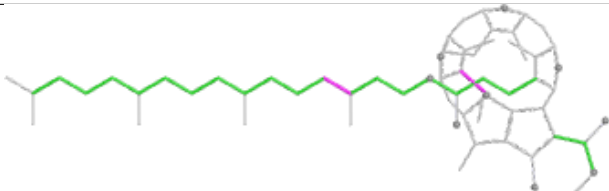
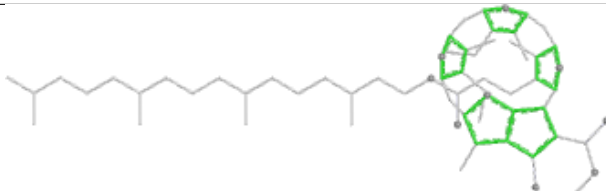


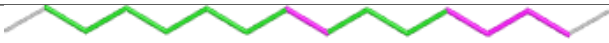
Ligand CLA d 403



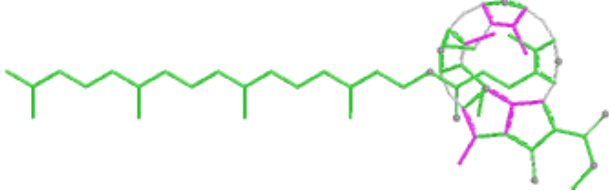
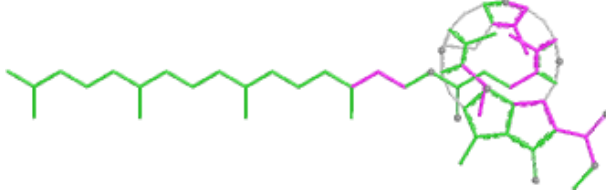
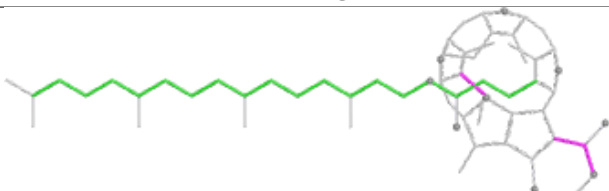
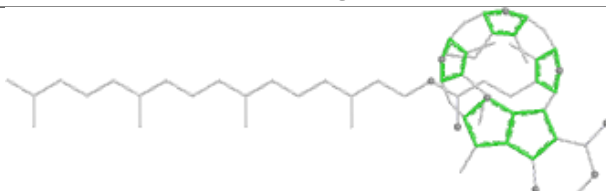
Ligand LHG D 409

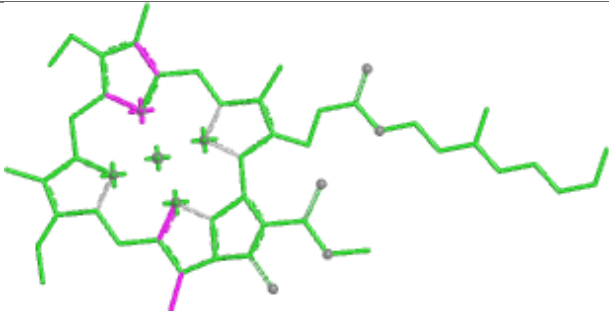
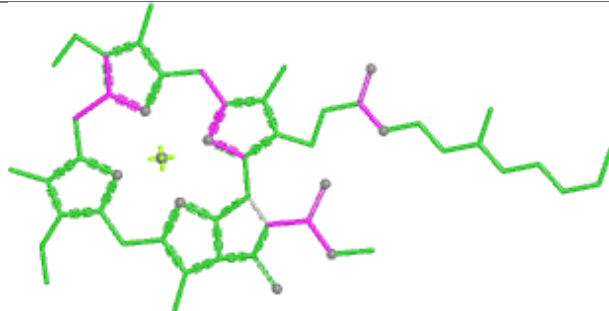
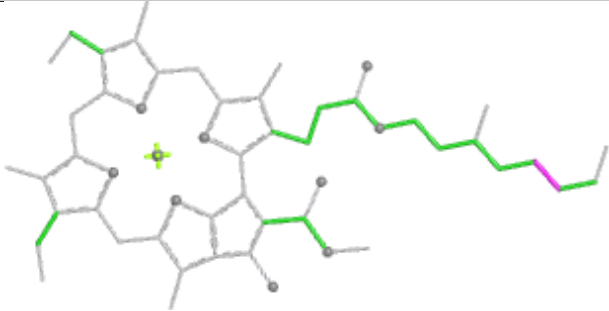
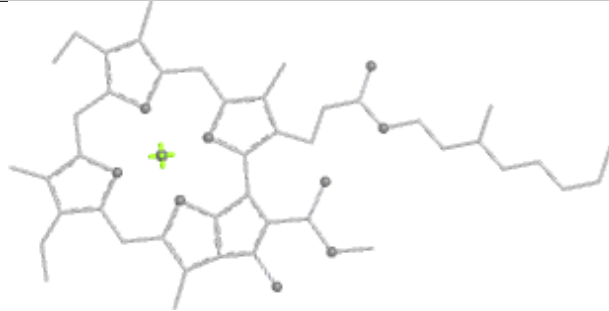
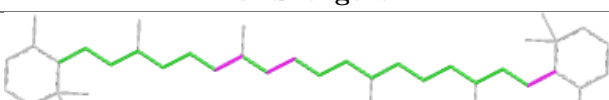
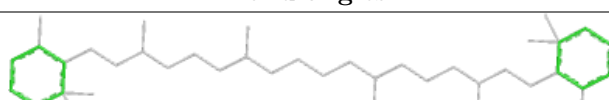
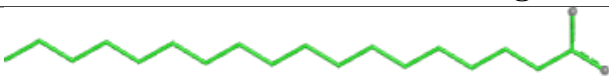
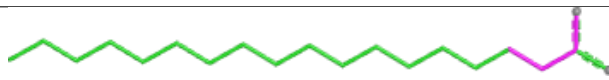
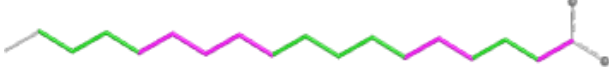
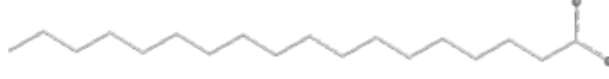
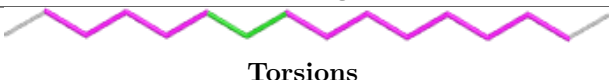


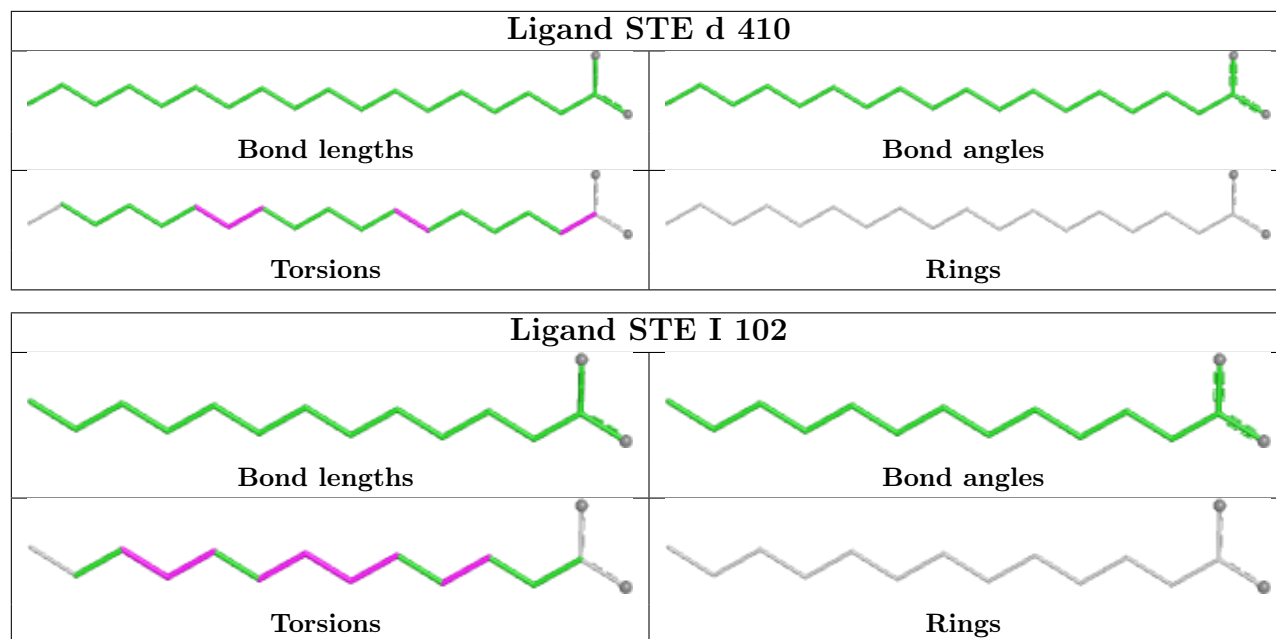
Ligand PHO A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE C 526	
 Bond lengths	 Bond angles
 Torsions	 Rings

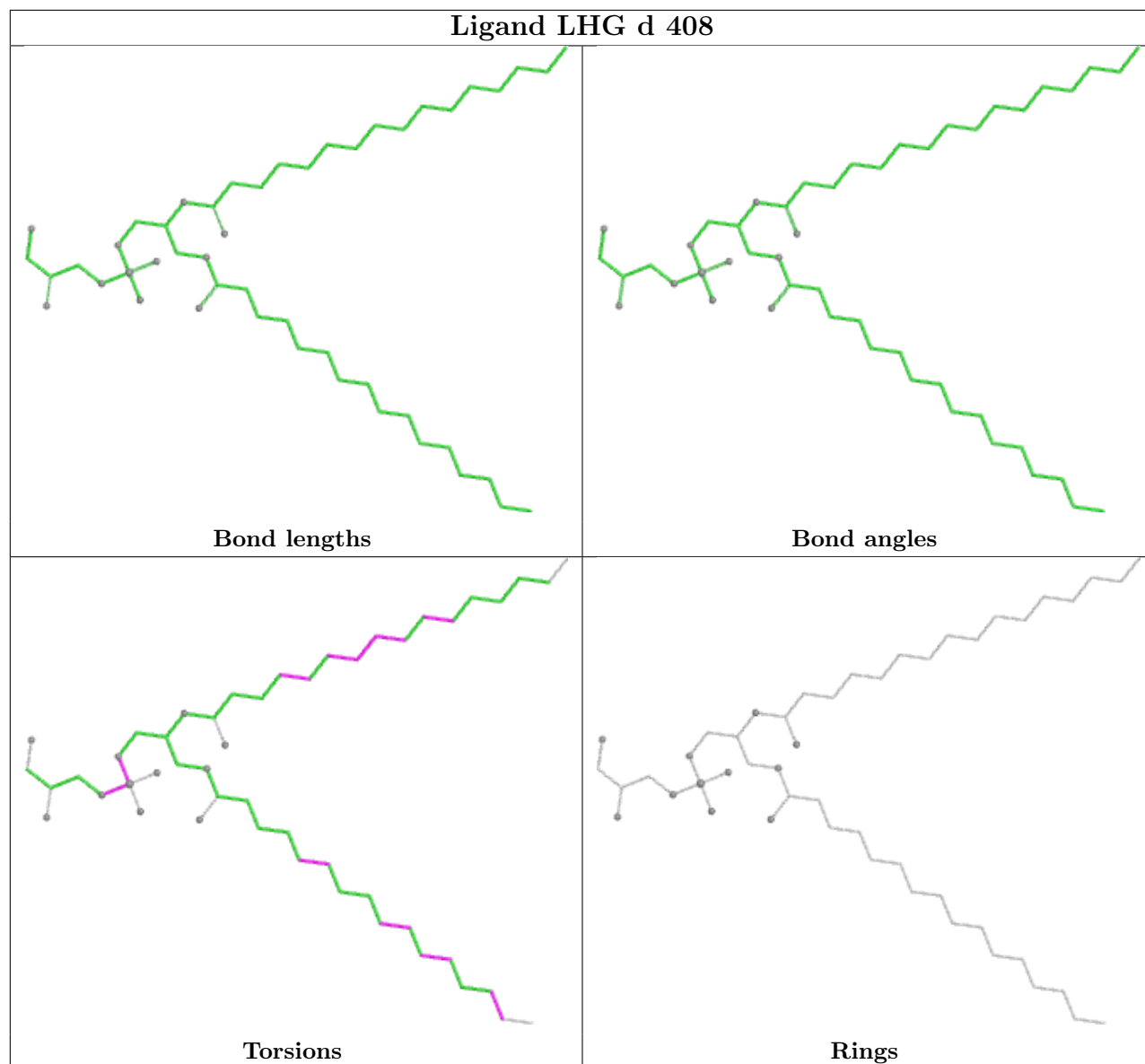
Ligand STE m 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO d 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

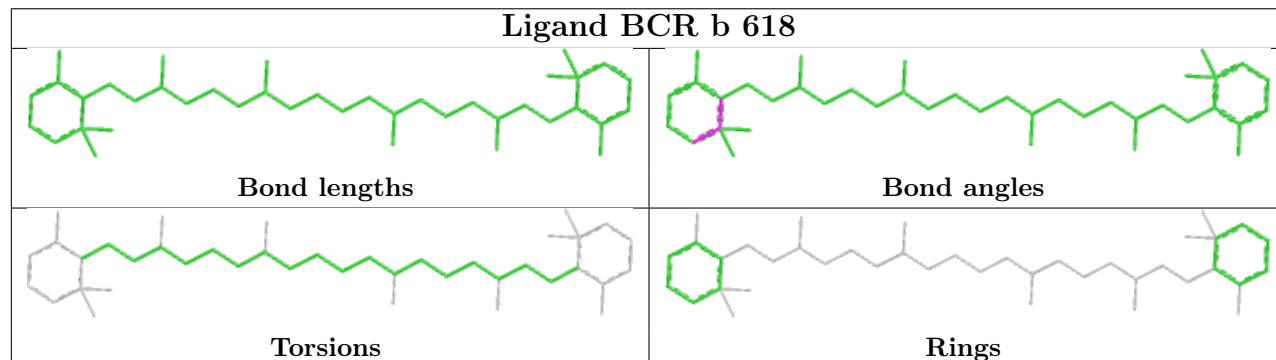
Ligand CLA A 610			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand BCR t 101			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand STE E 104			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand STE T 102			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

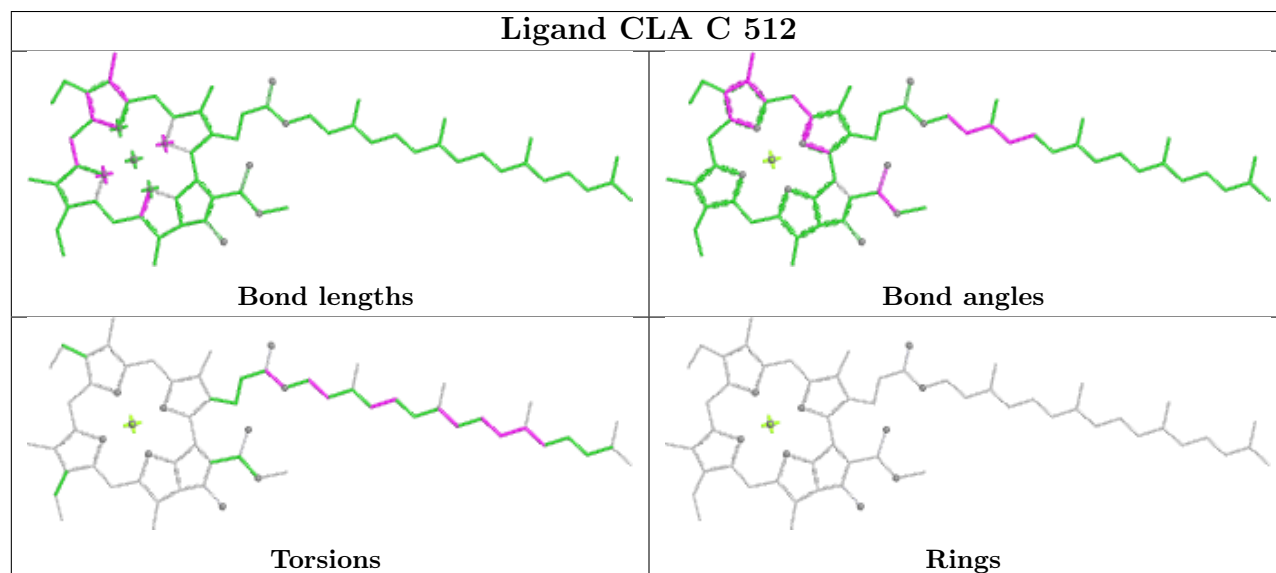
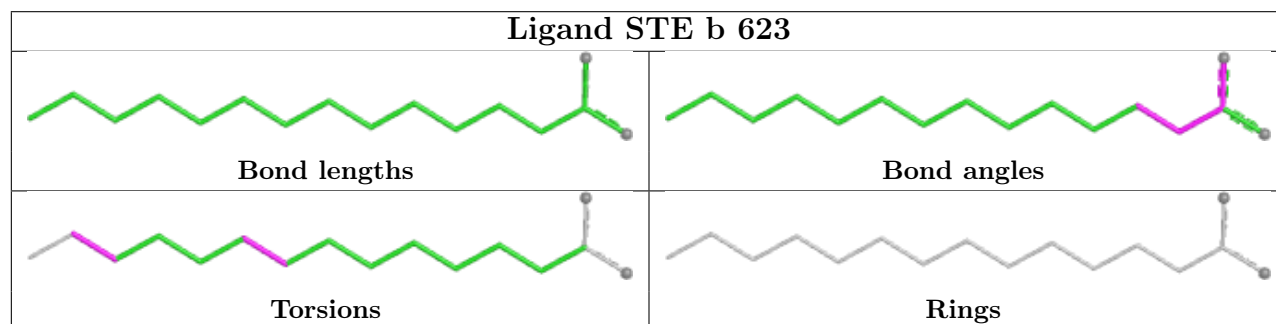
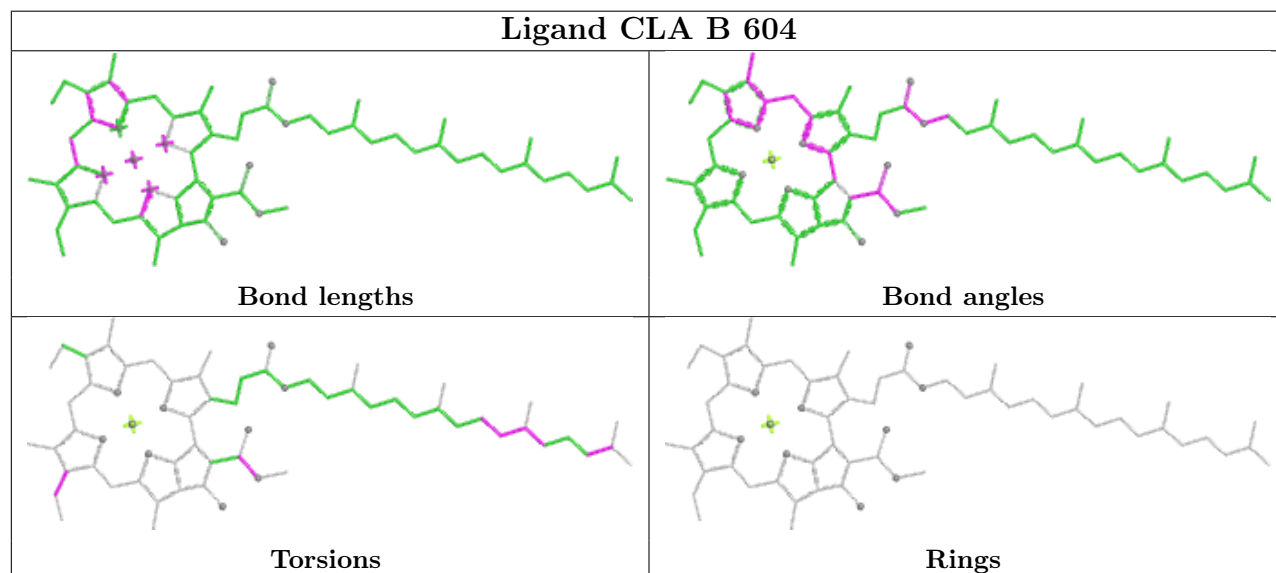
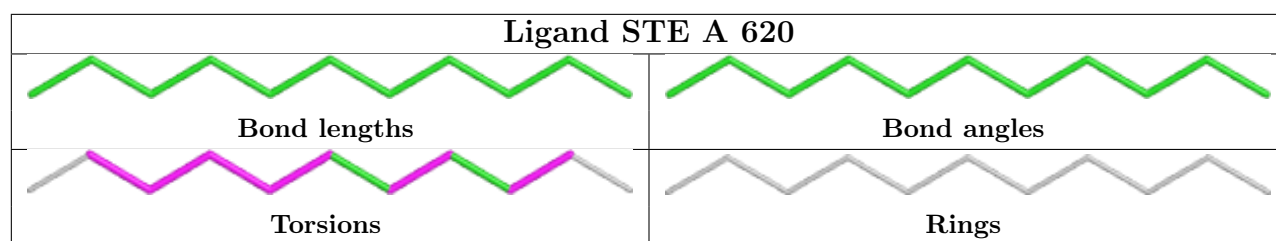


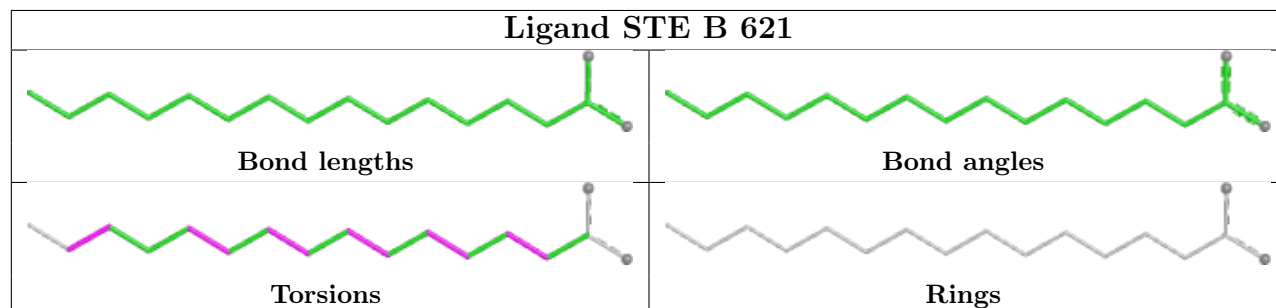
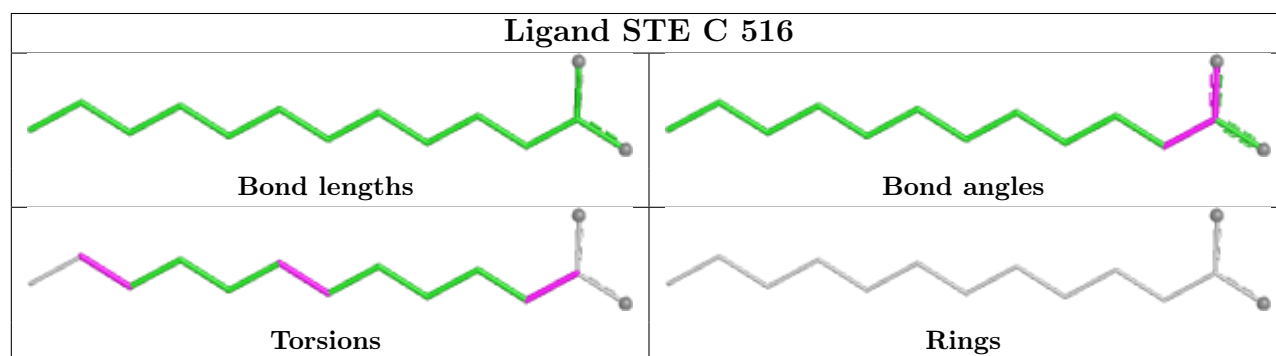
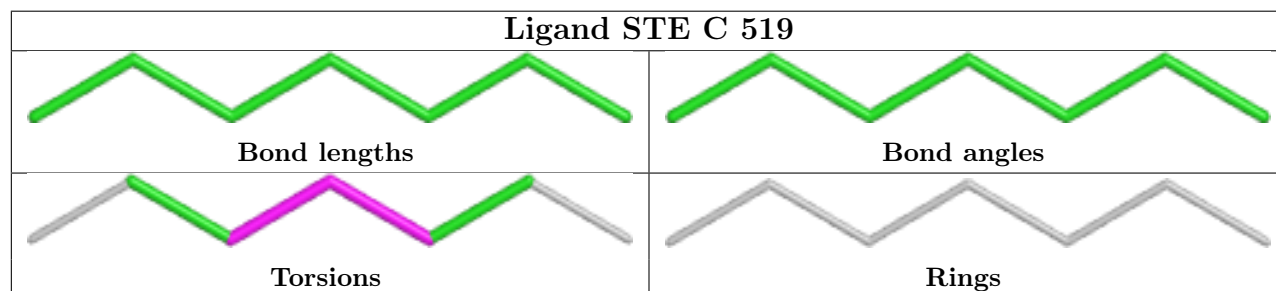
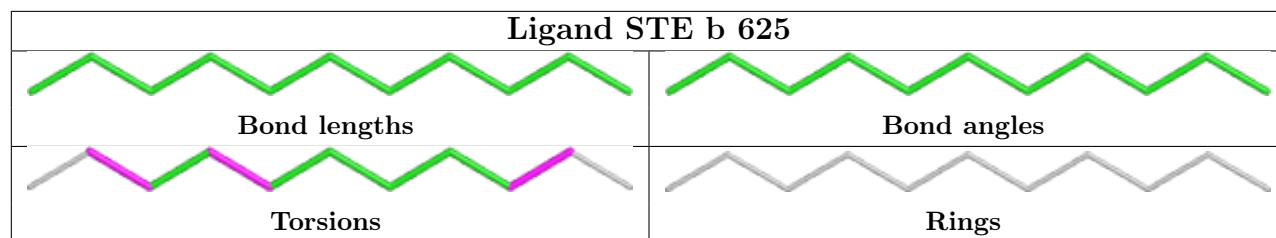
Ligand LHG d 408

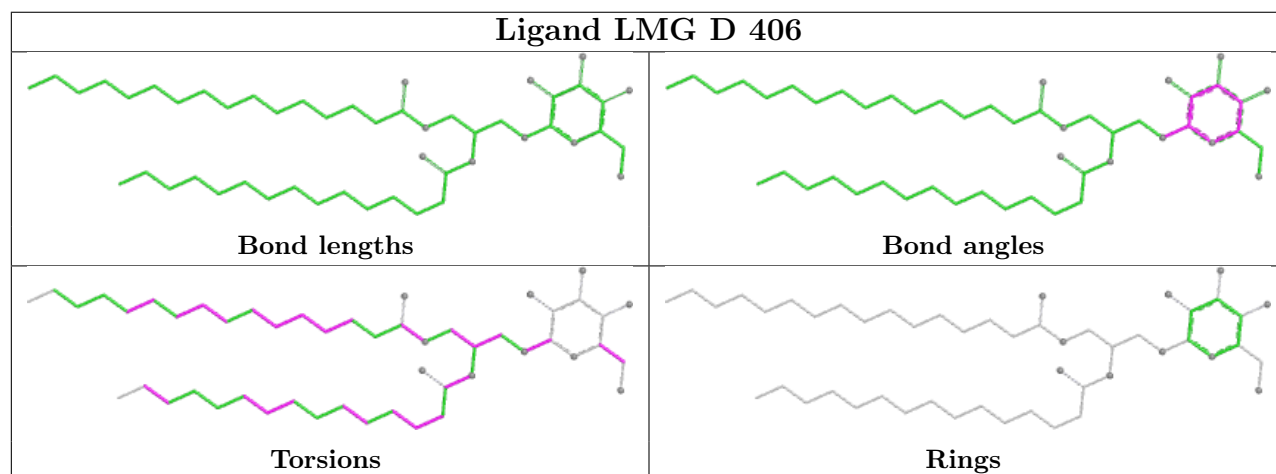
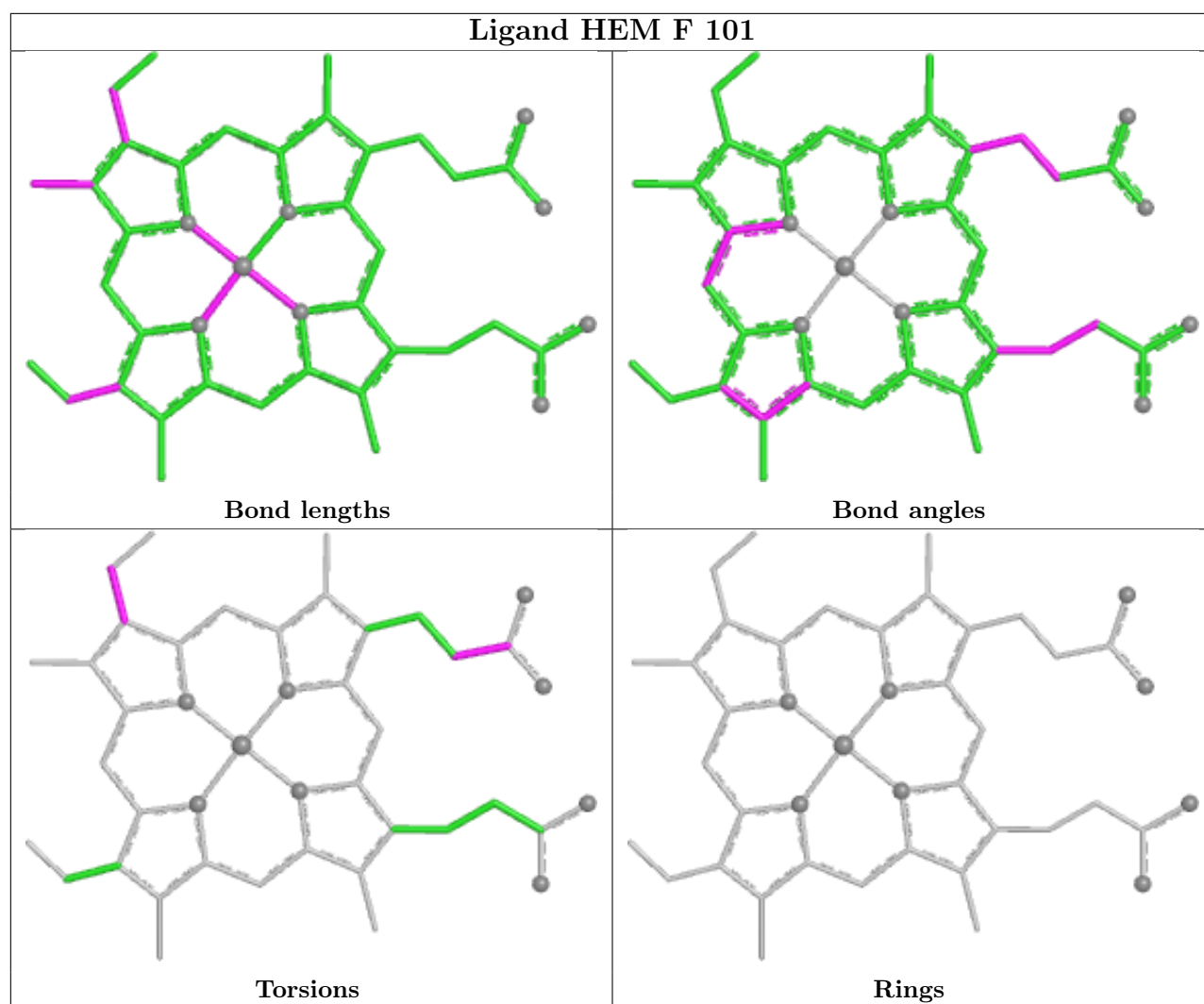


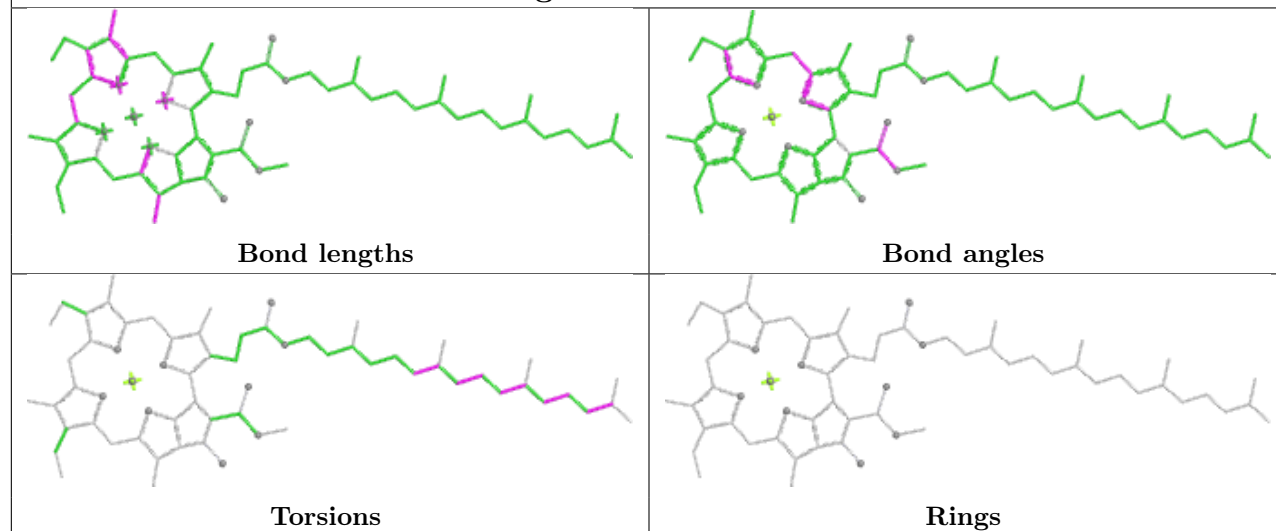
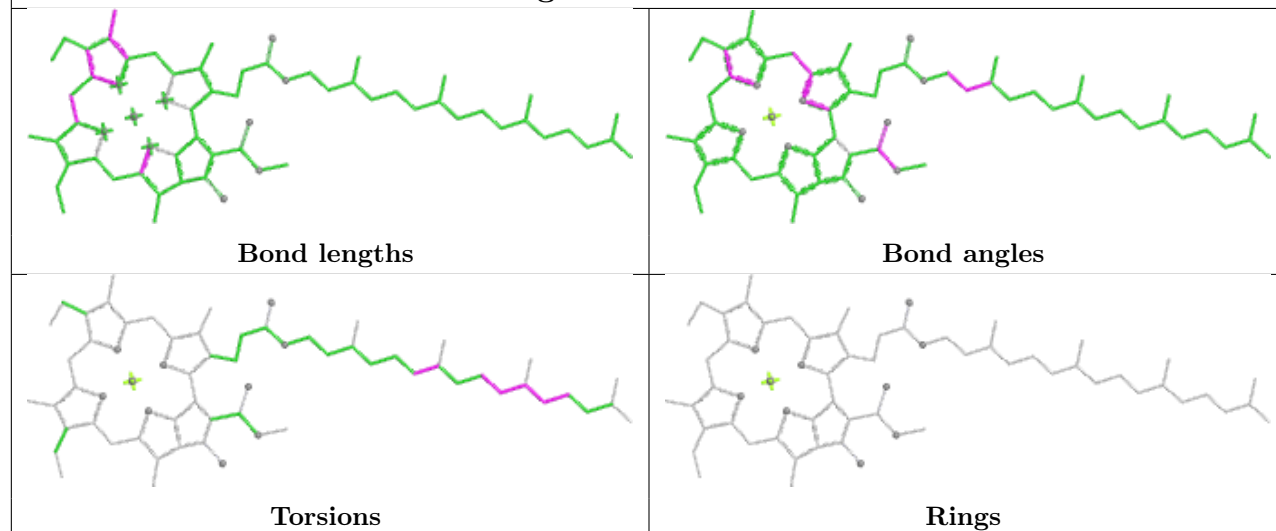
Ligand BCR b 618



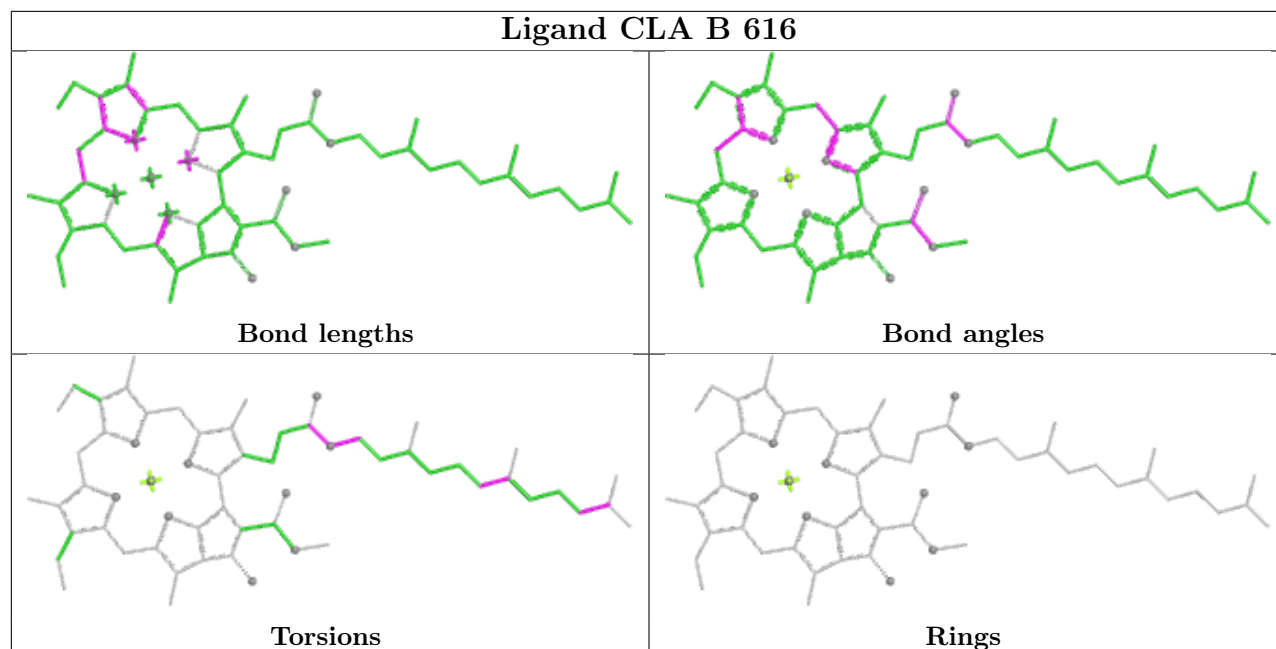




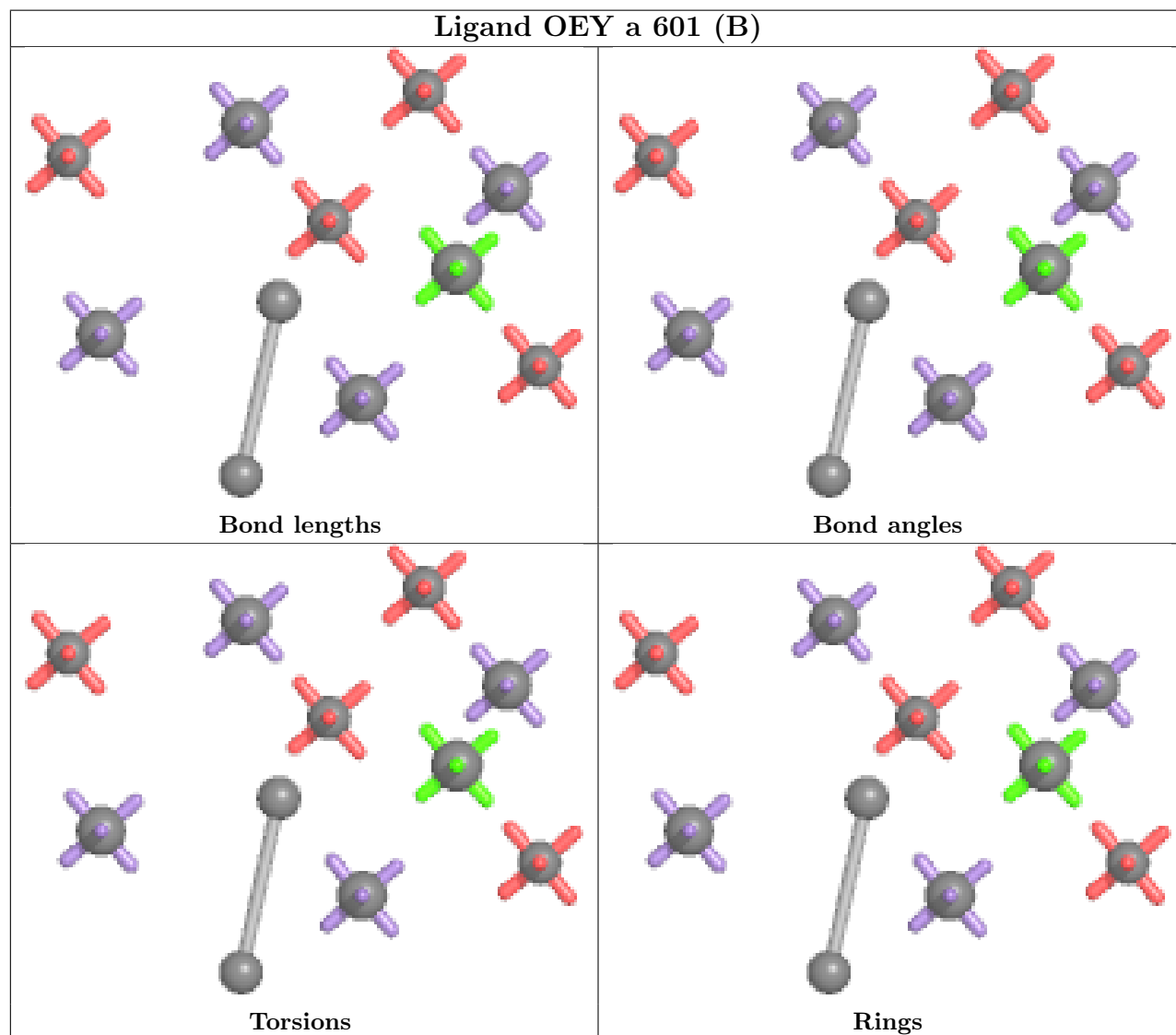


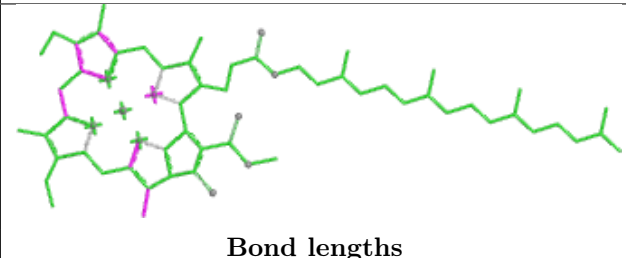
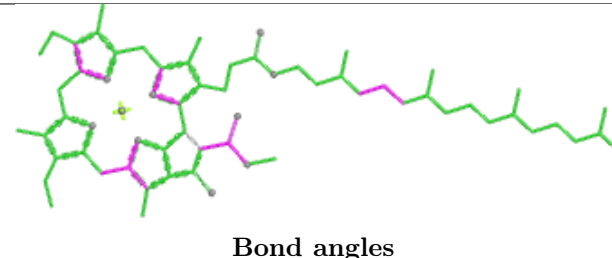
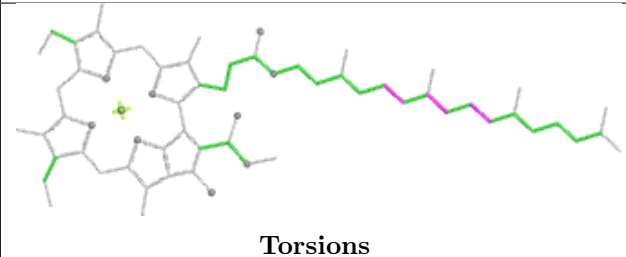
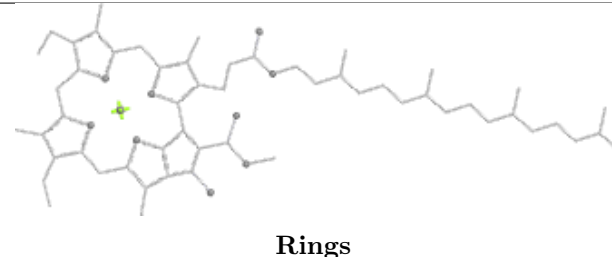
Ligand CLA b 615**Ligand CLA c 505**

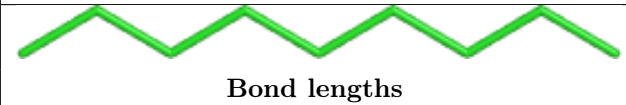
Ligand CLA B 616



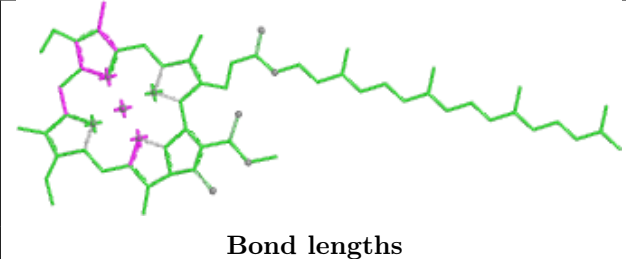
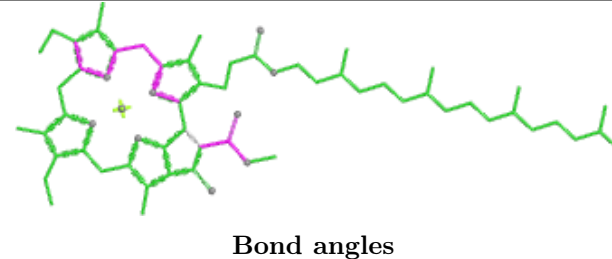
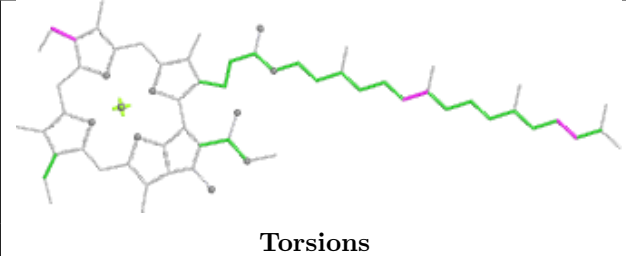
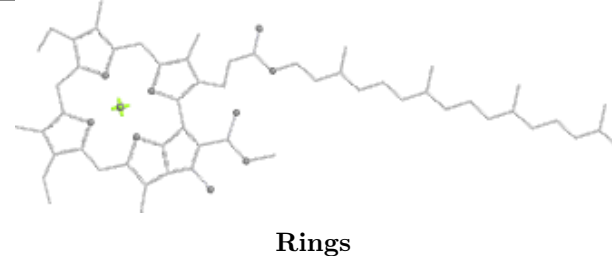
Ligand OEY a 601 (B)



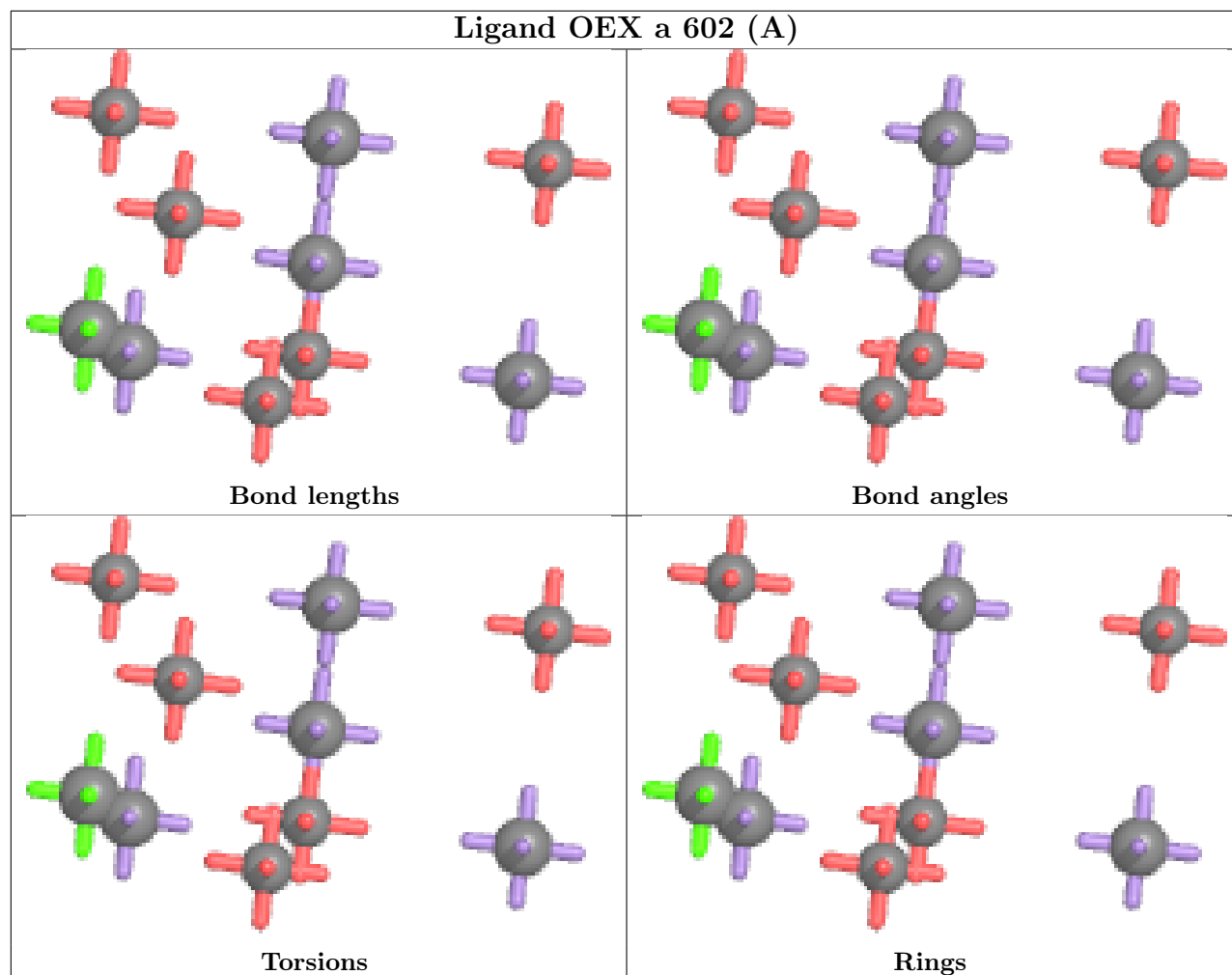
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE e 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

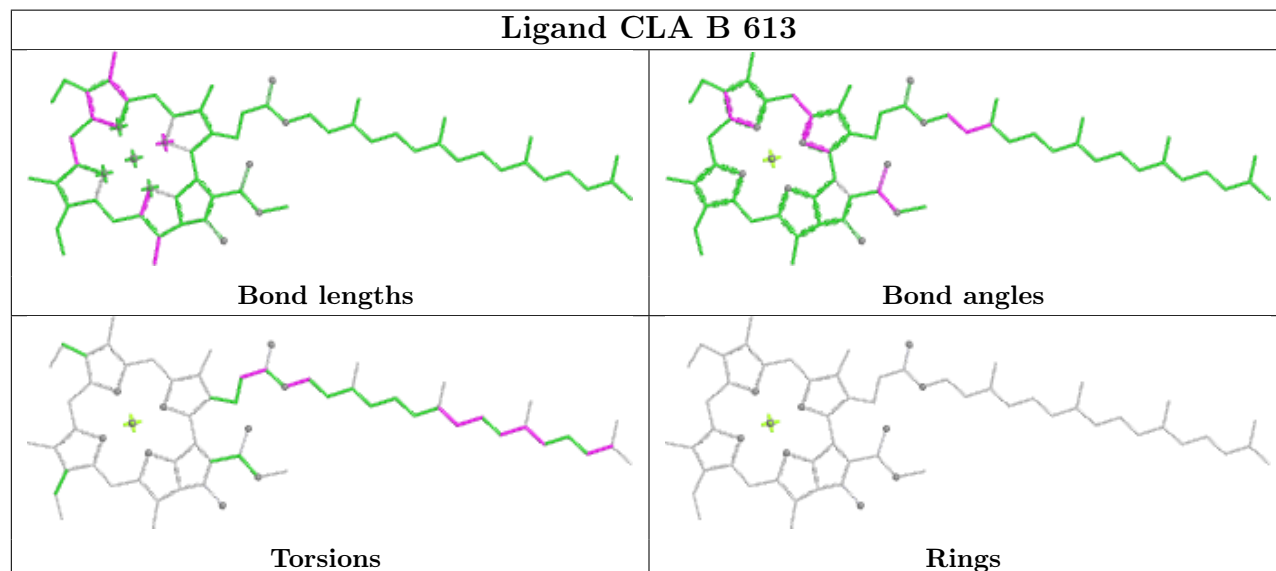
Ligand STE A 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

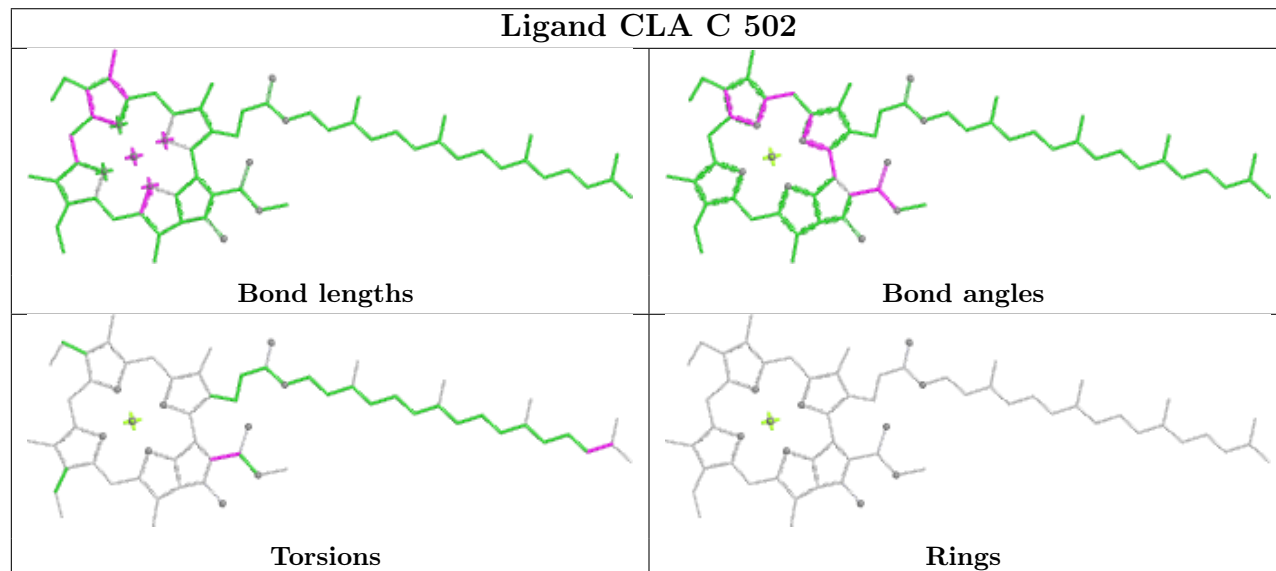
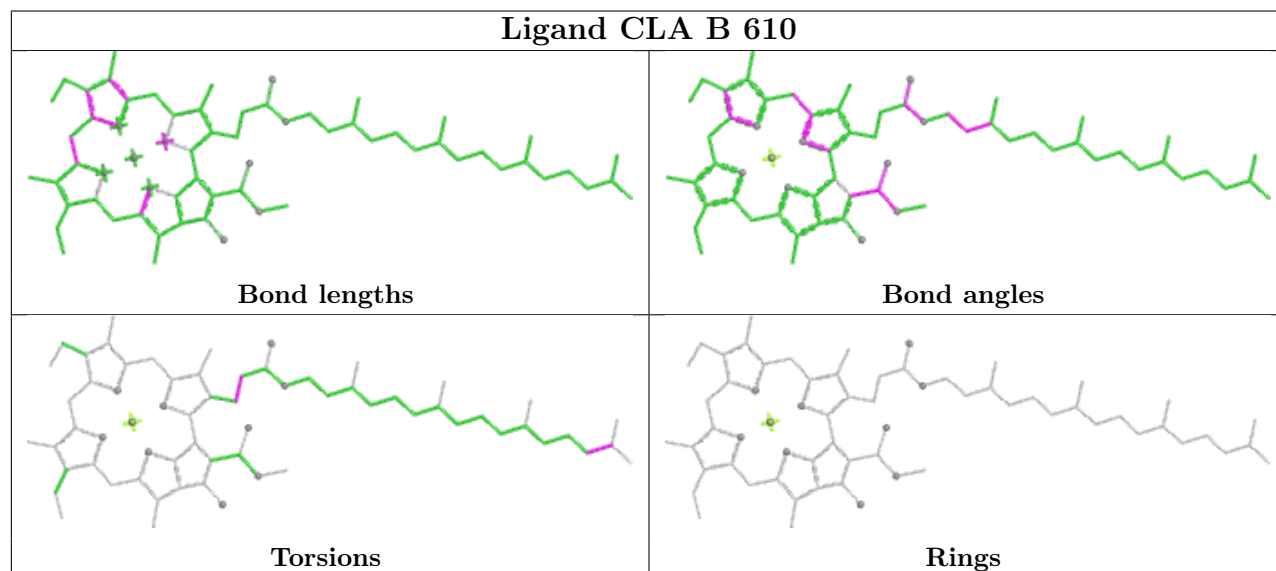
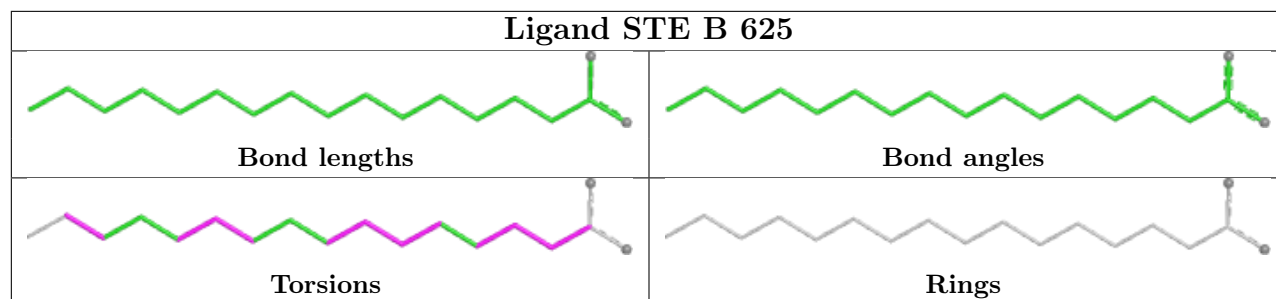
Ligand CLA a 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

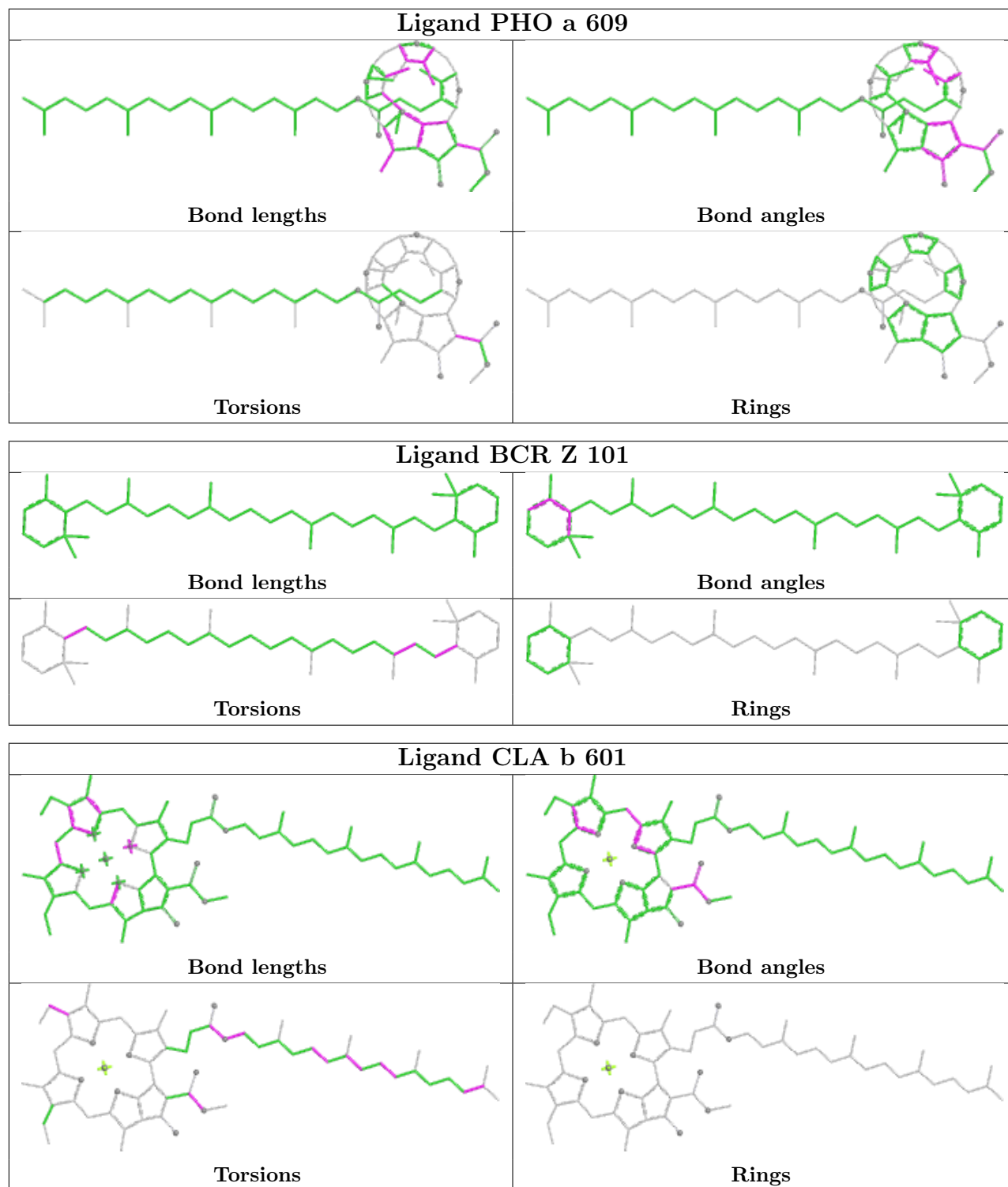
Ligand OEX a 602 (A)

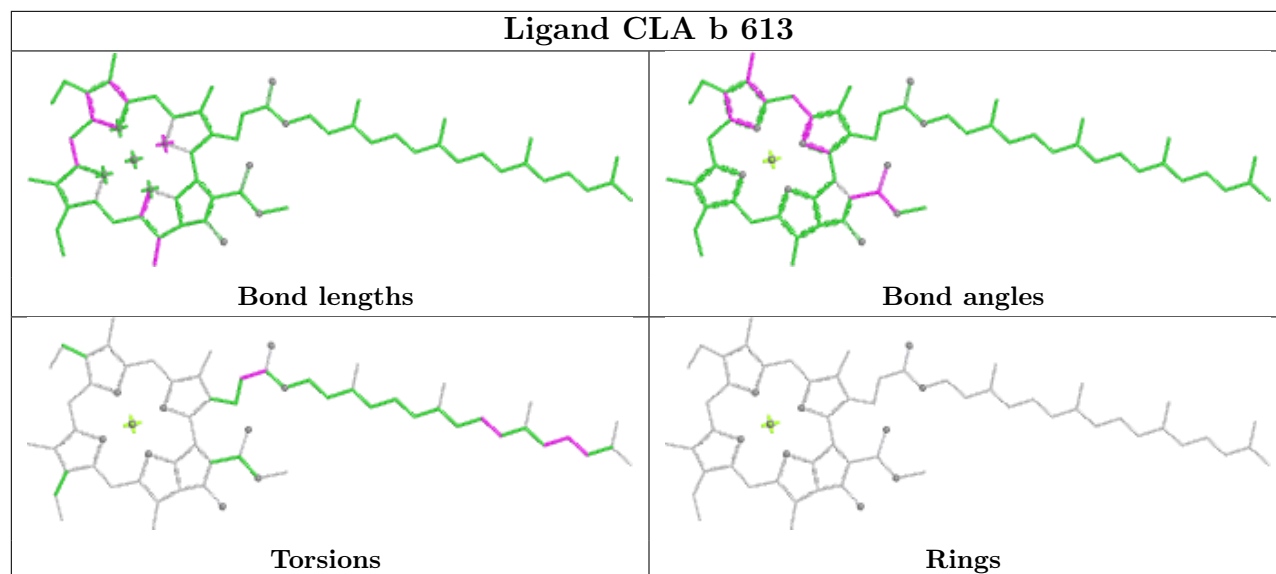
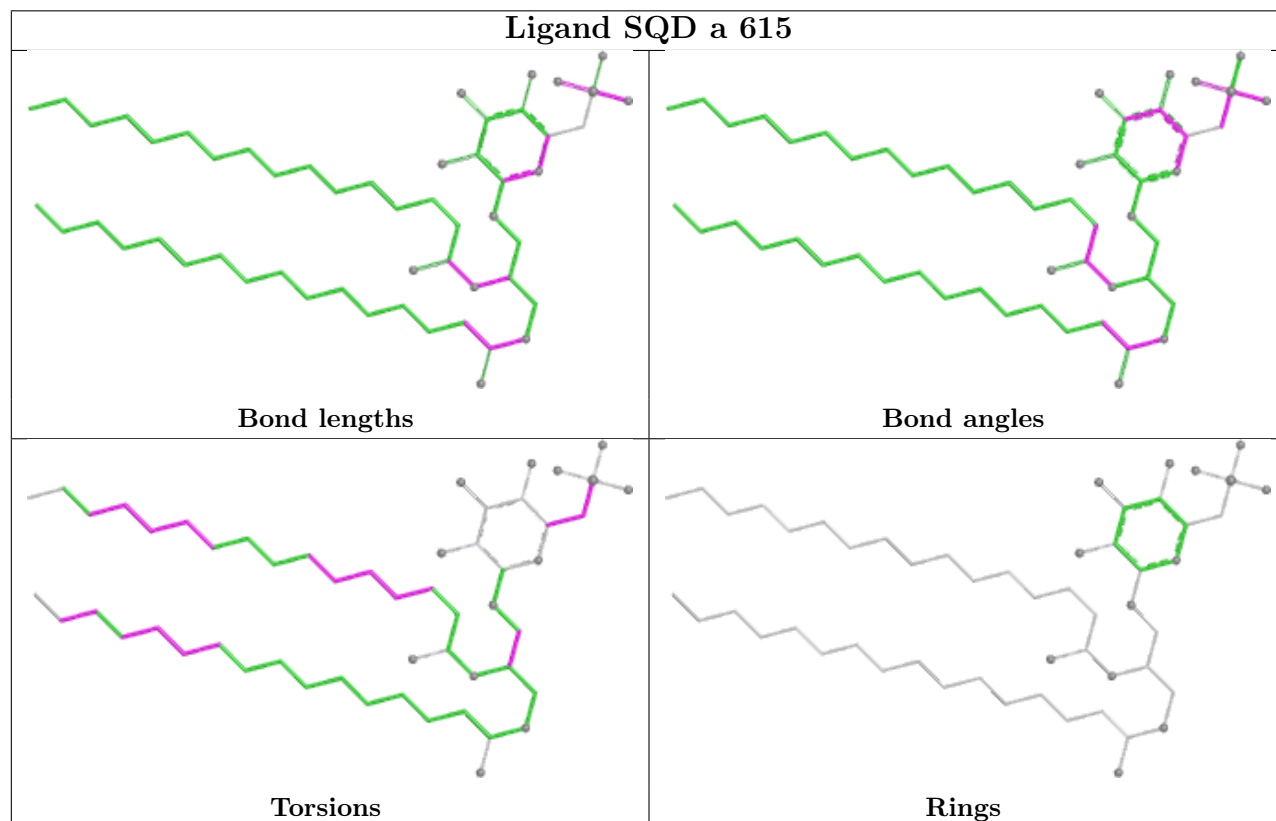


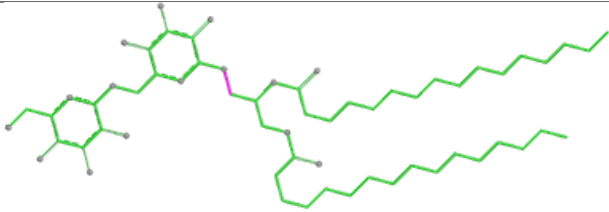
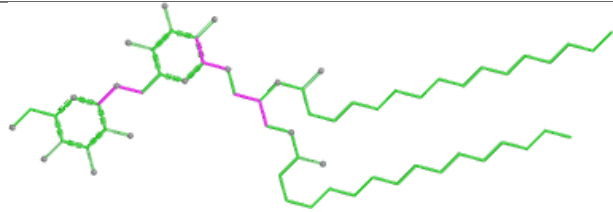
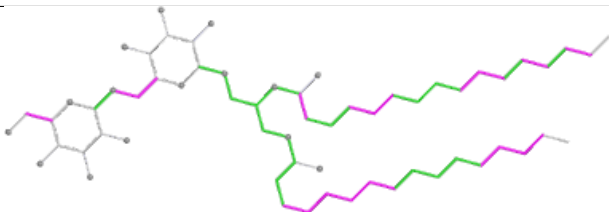
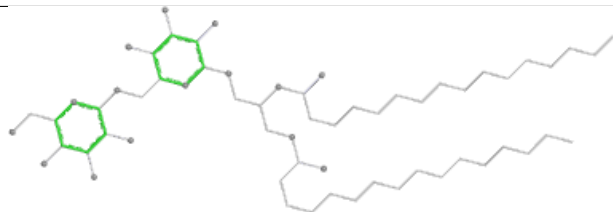
Ligand CLA B 613

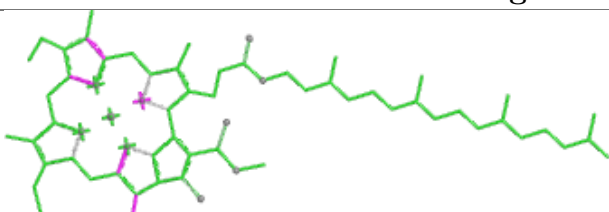
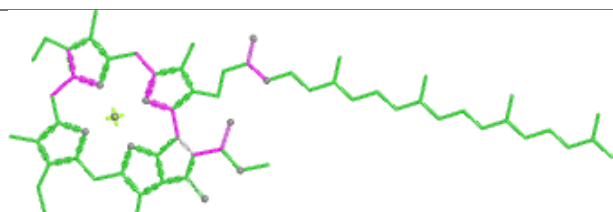
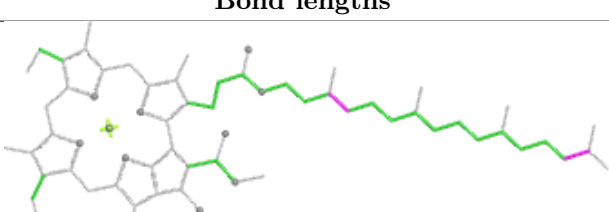
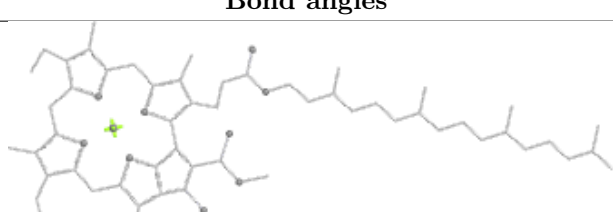




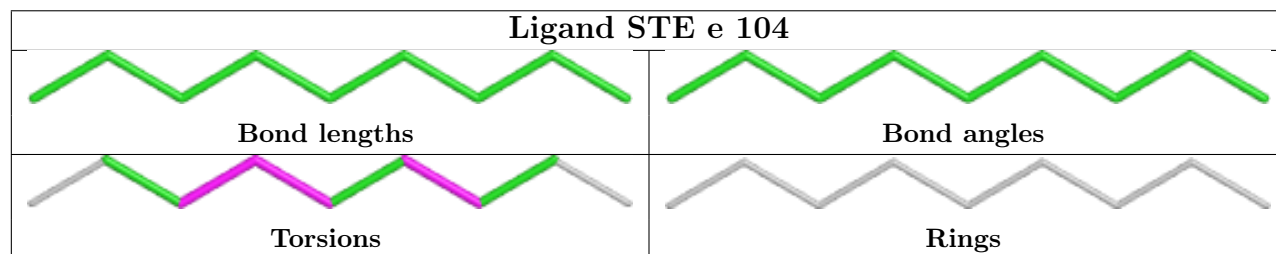
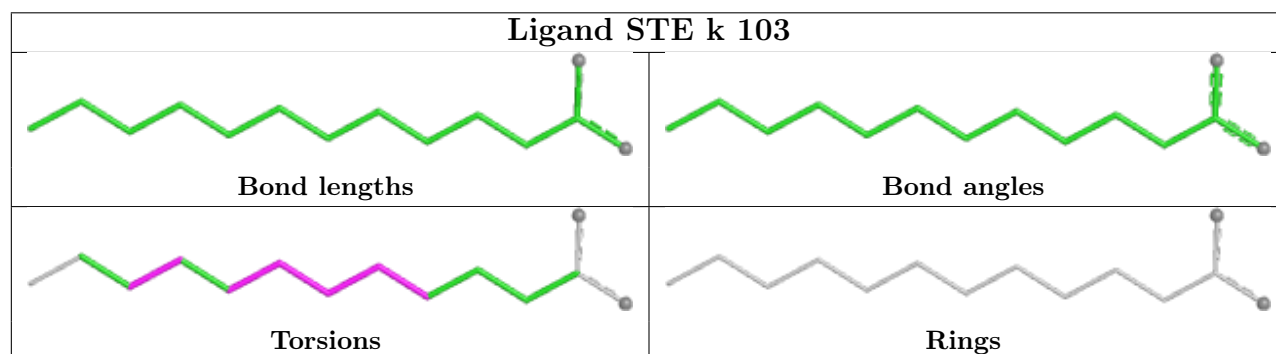
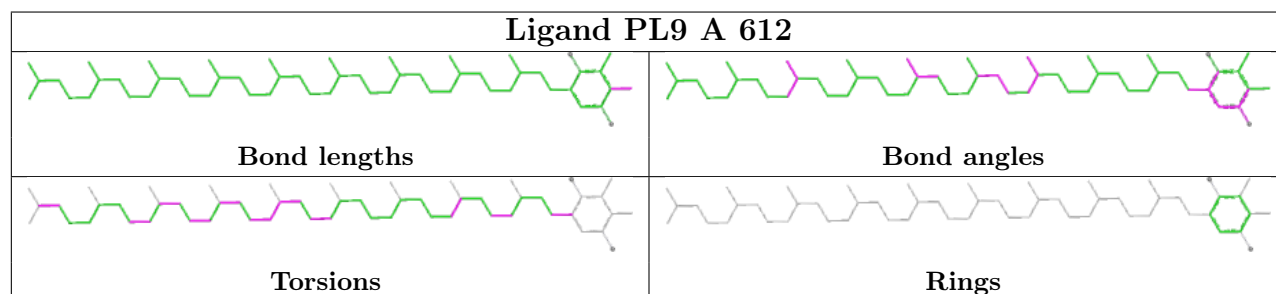
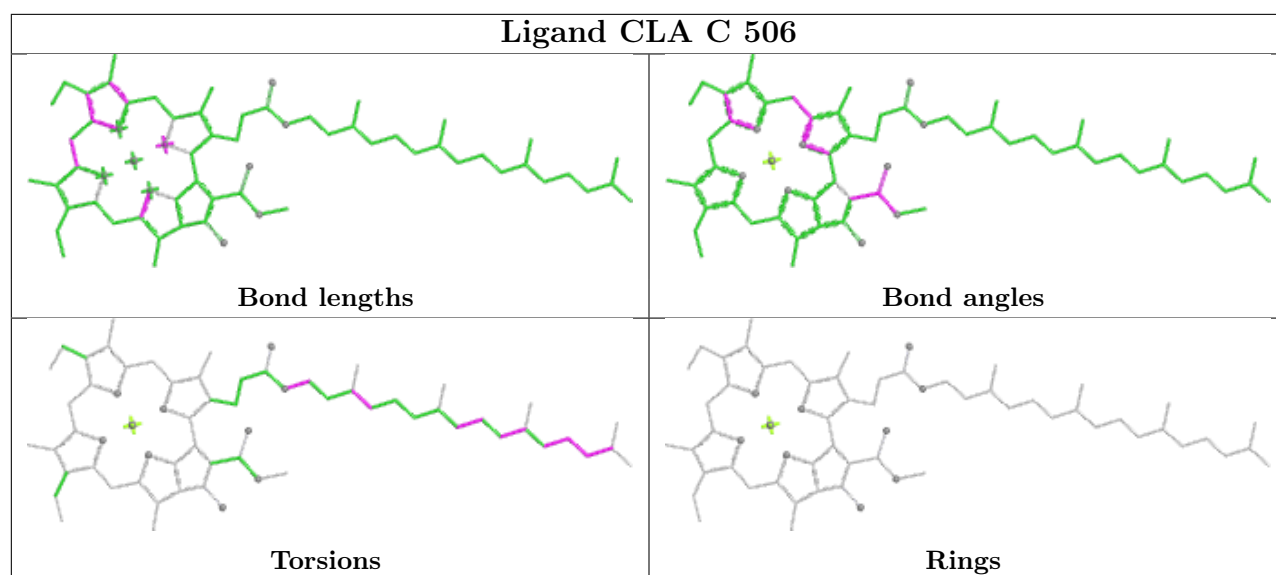


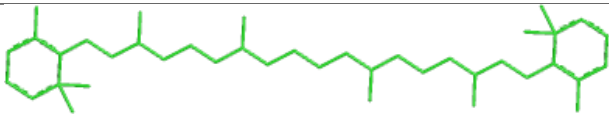
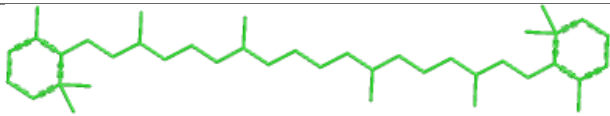
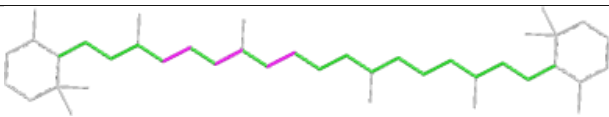
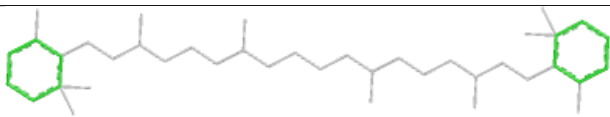
Ligand CLA b 613**Ligand SQD a 615**

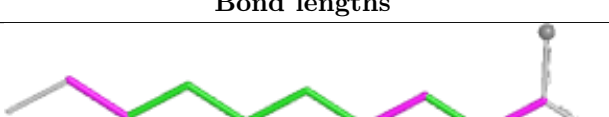
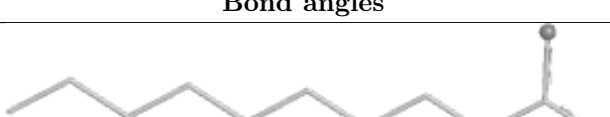
Ligand DGD C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

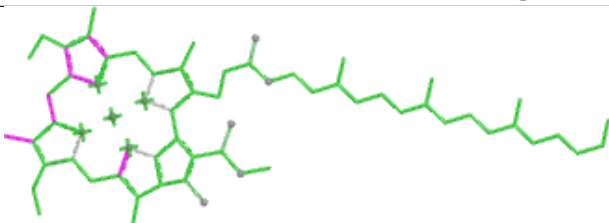
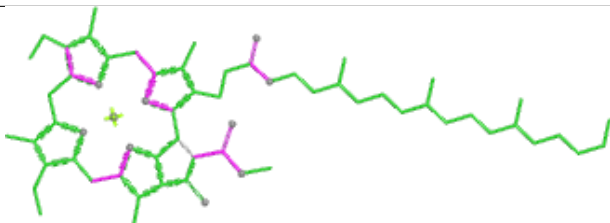
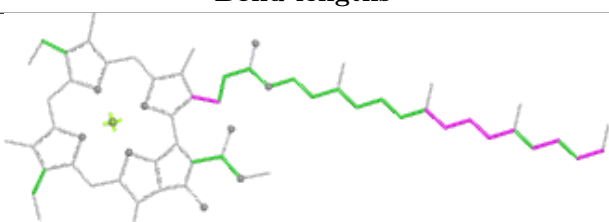
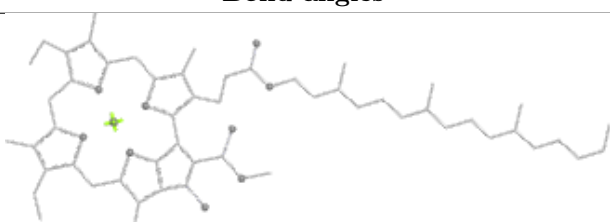
Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

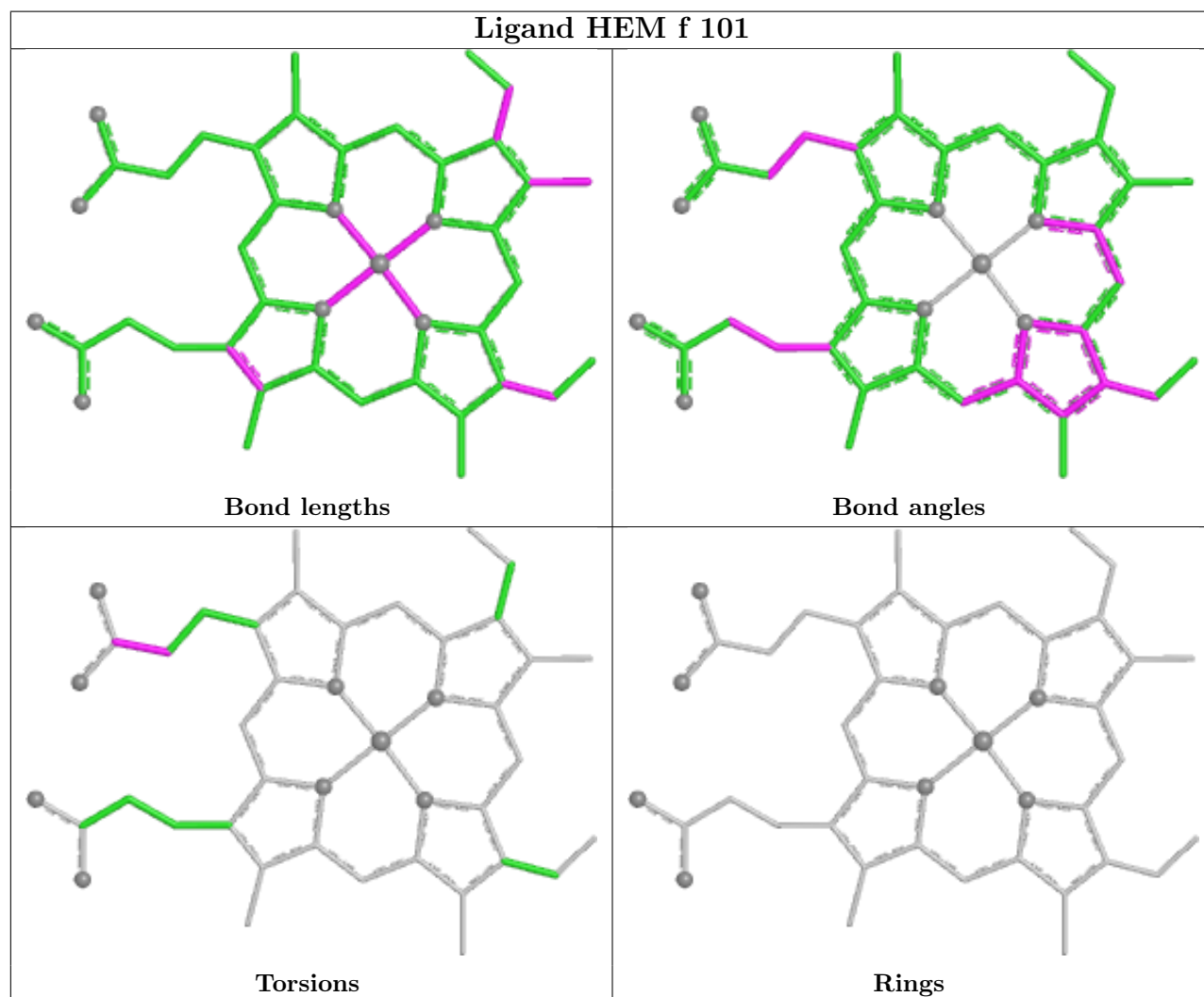
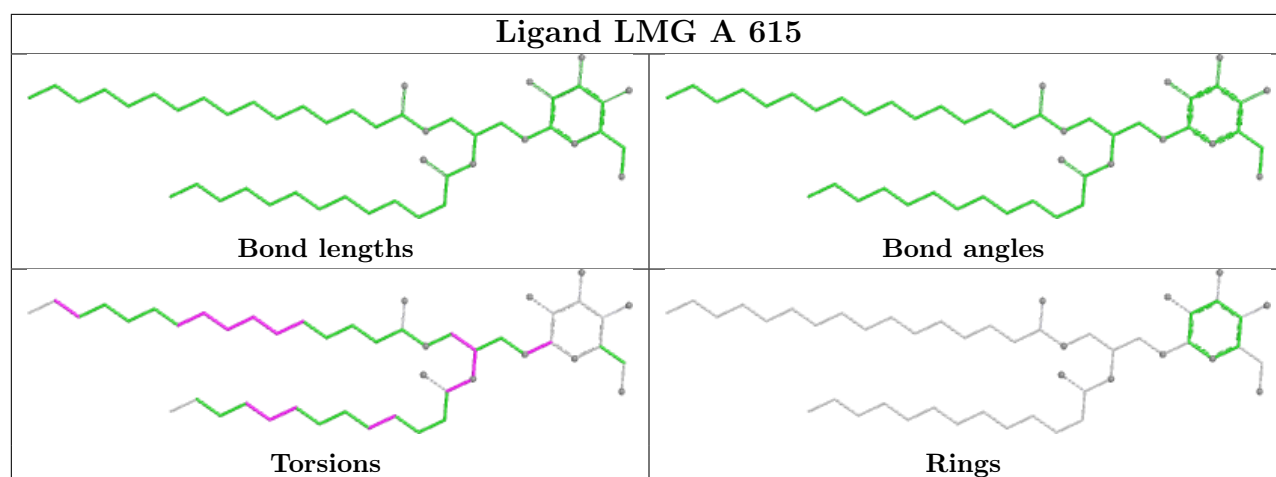
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



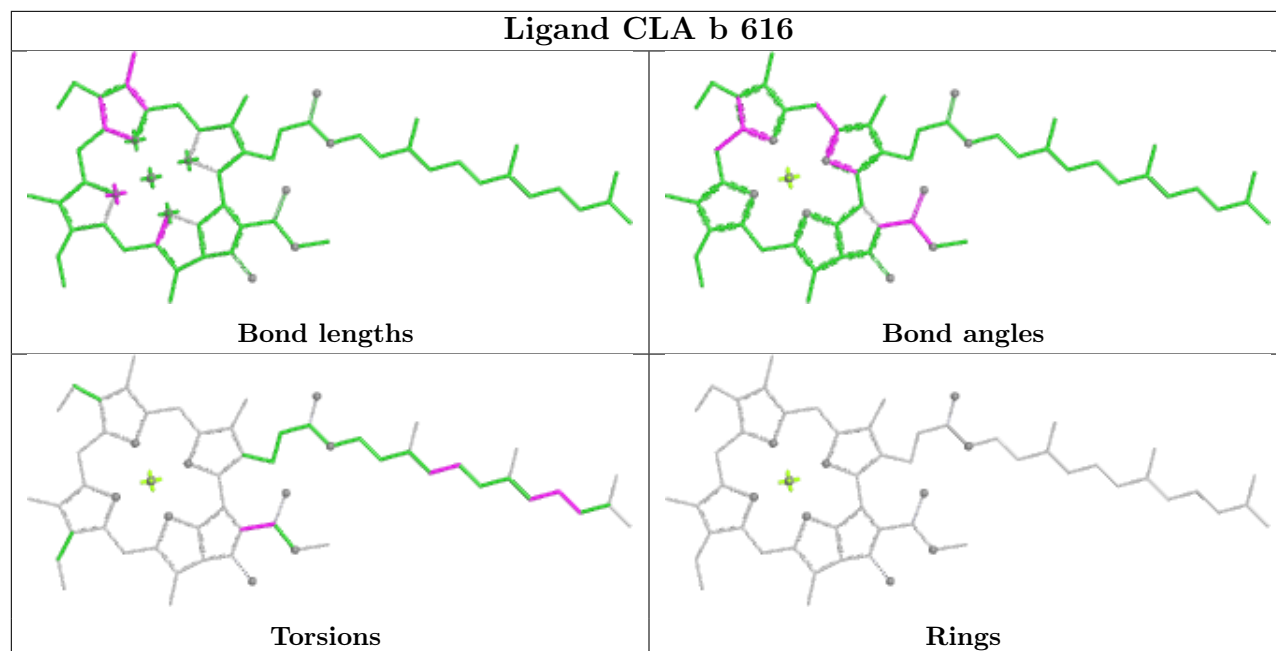
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

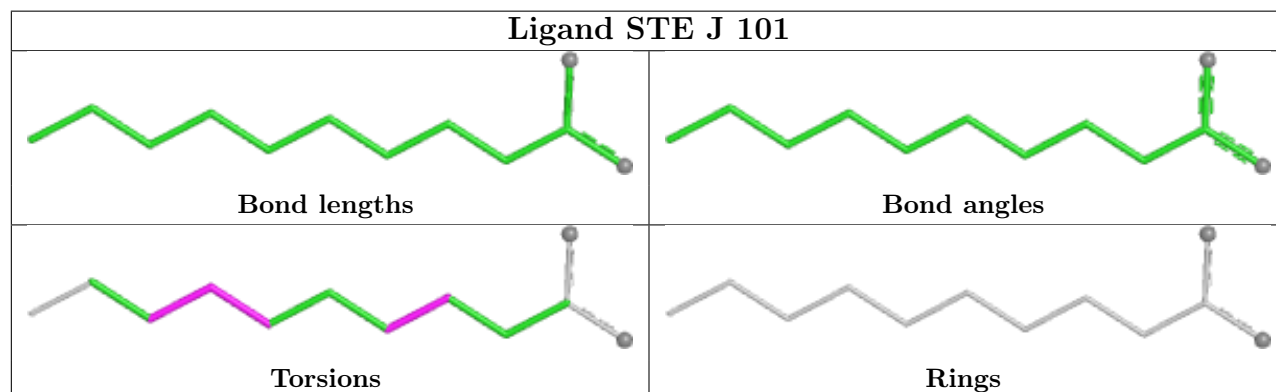
Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings



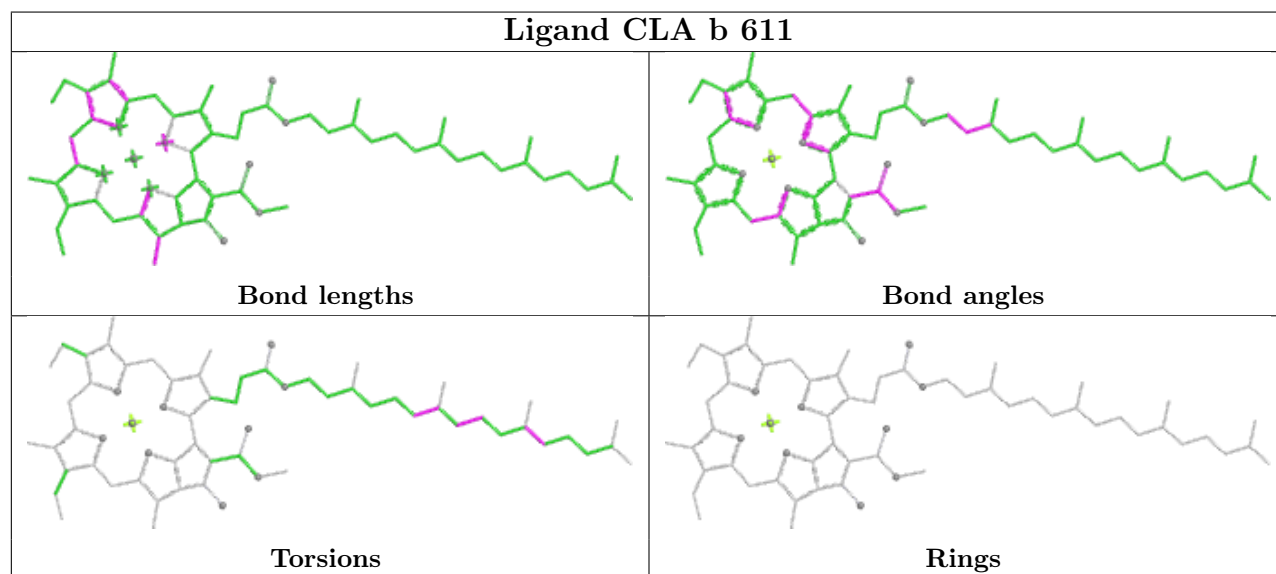
Ligand CLA b 616

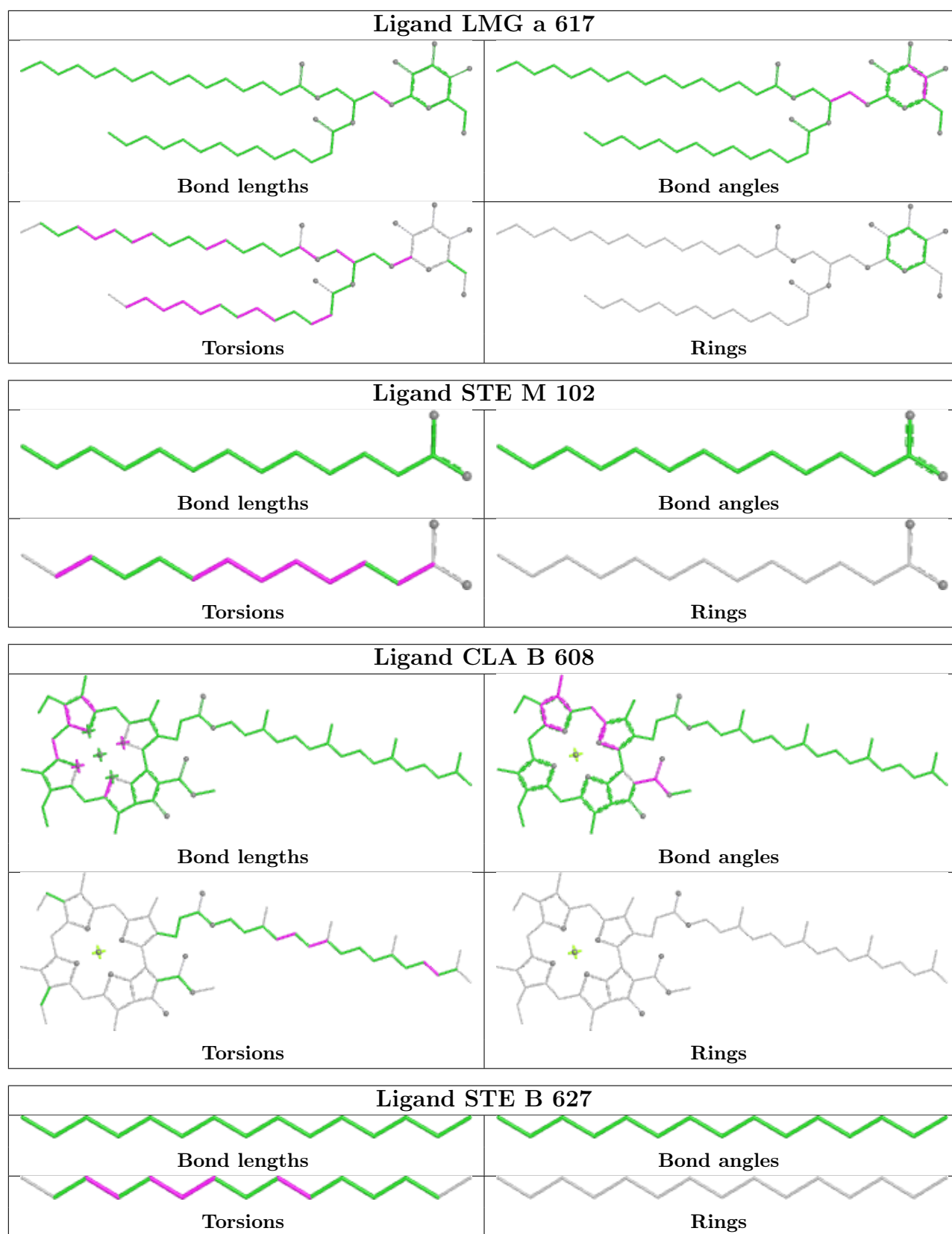


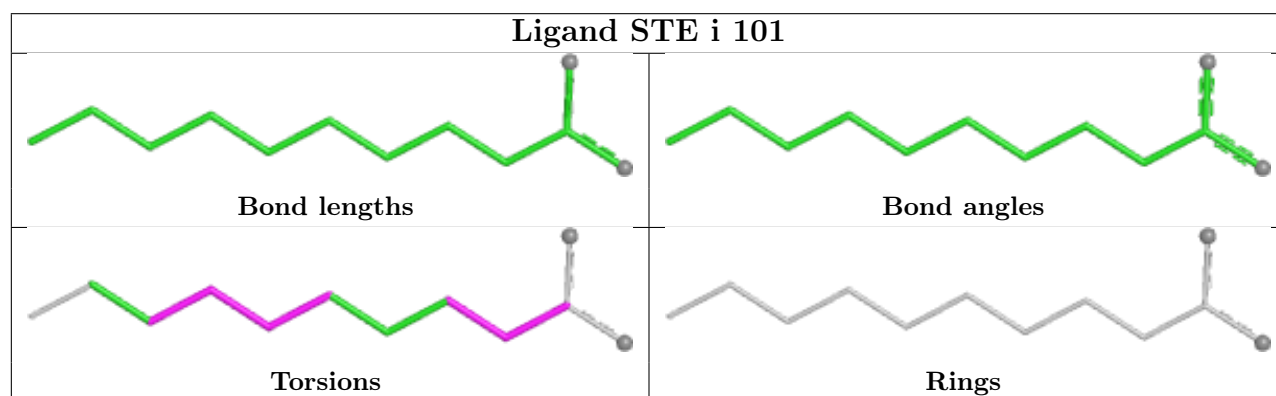
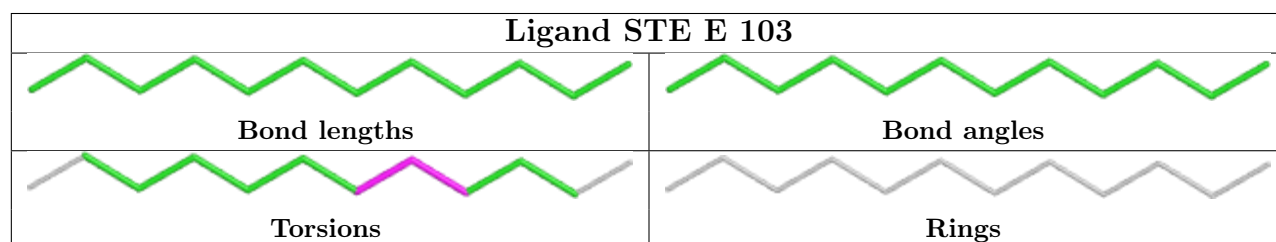
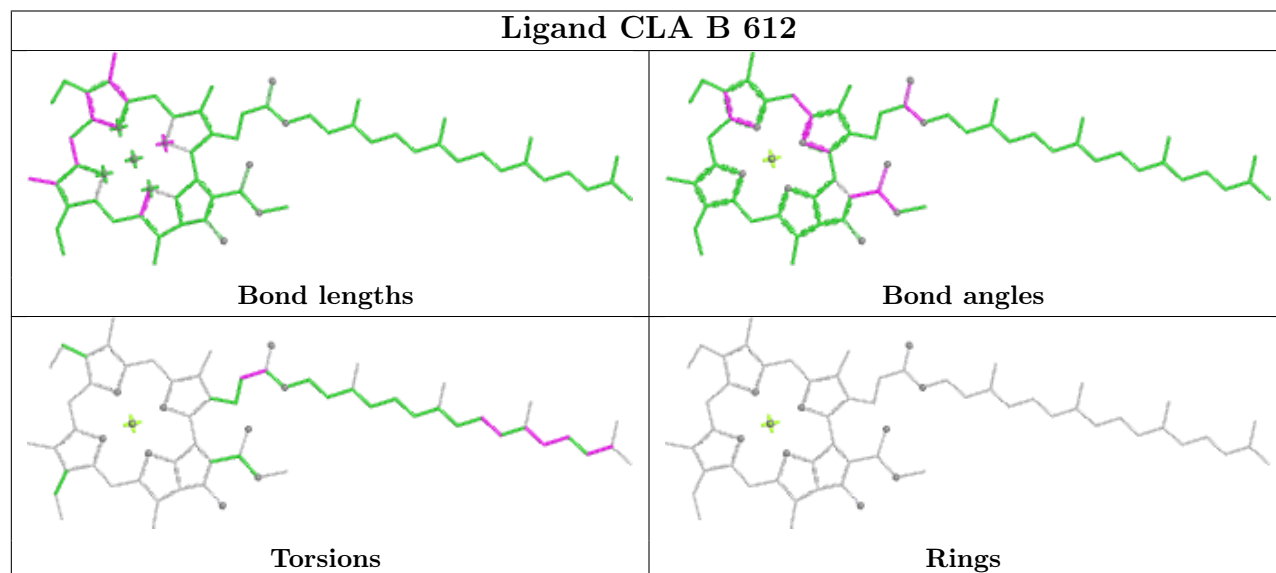
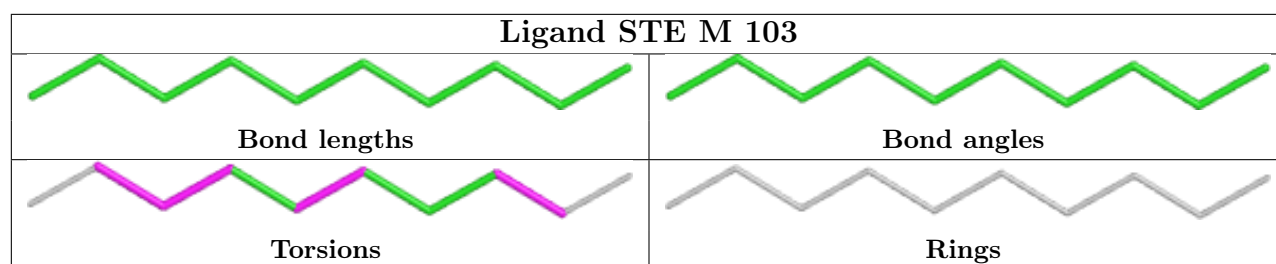
Ligand STE J 101

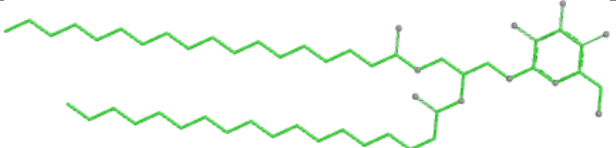
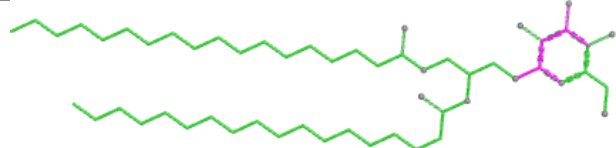
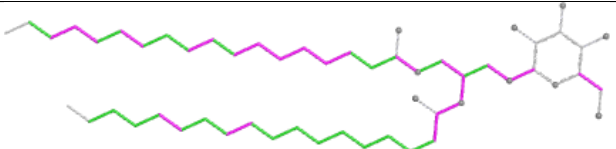
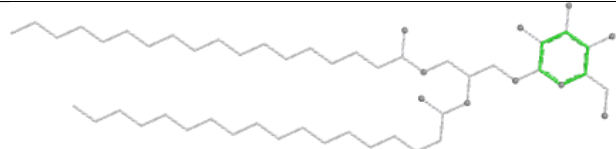


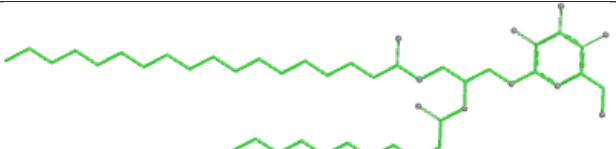
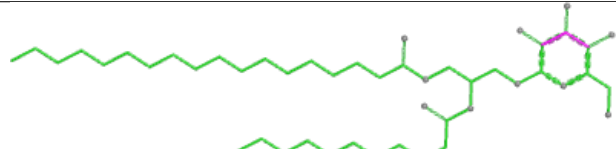
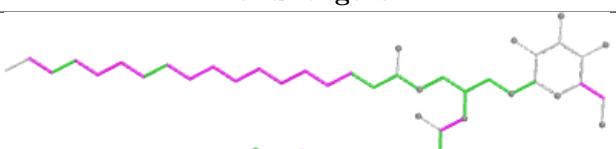
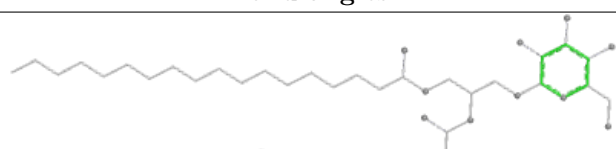
Ligand CLA b 611

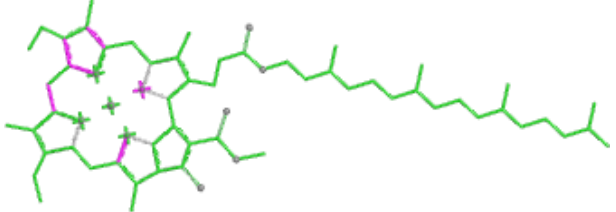
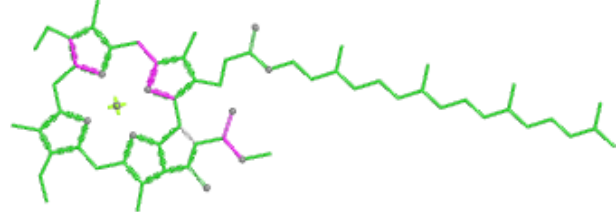
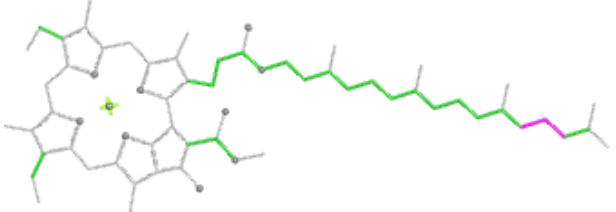
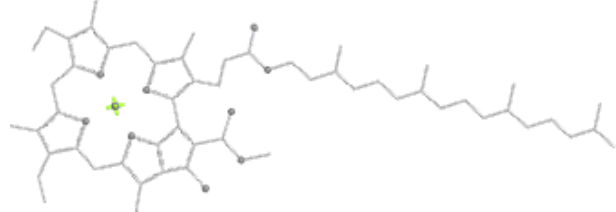


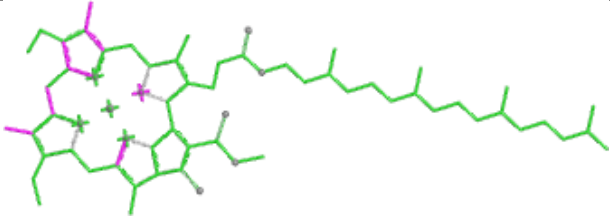
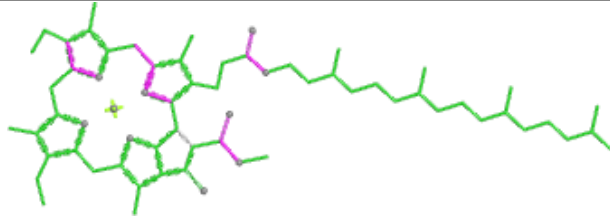
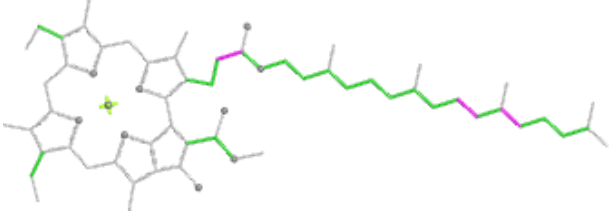
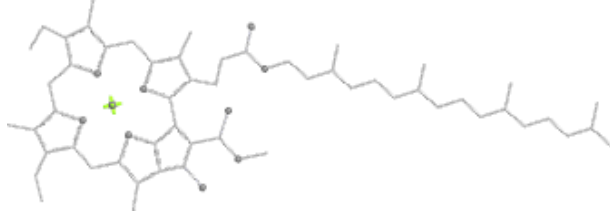
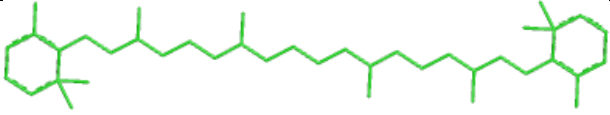
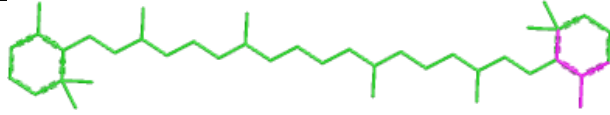
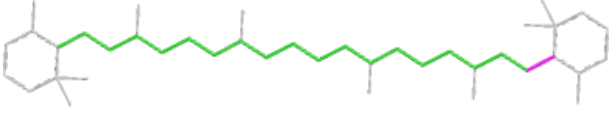
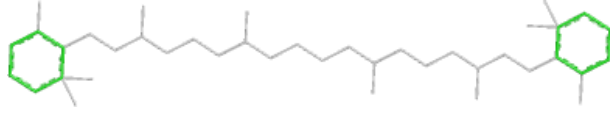
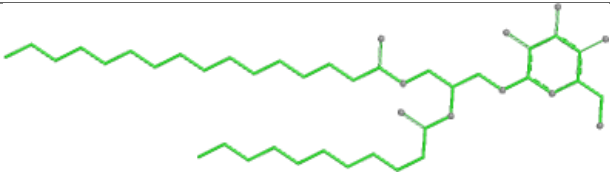
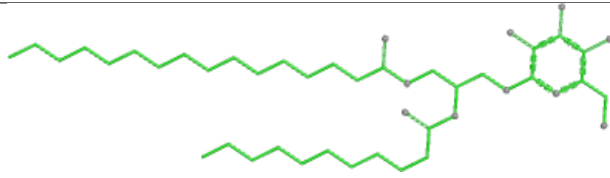
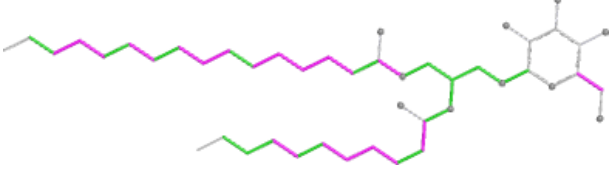
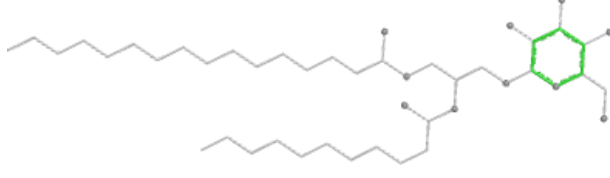




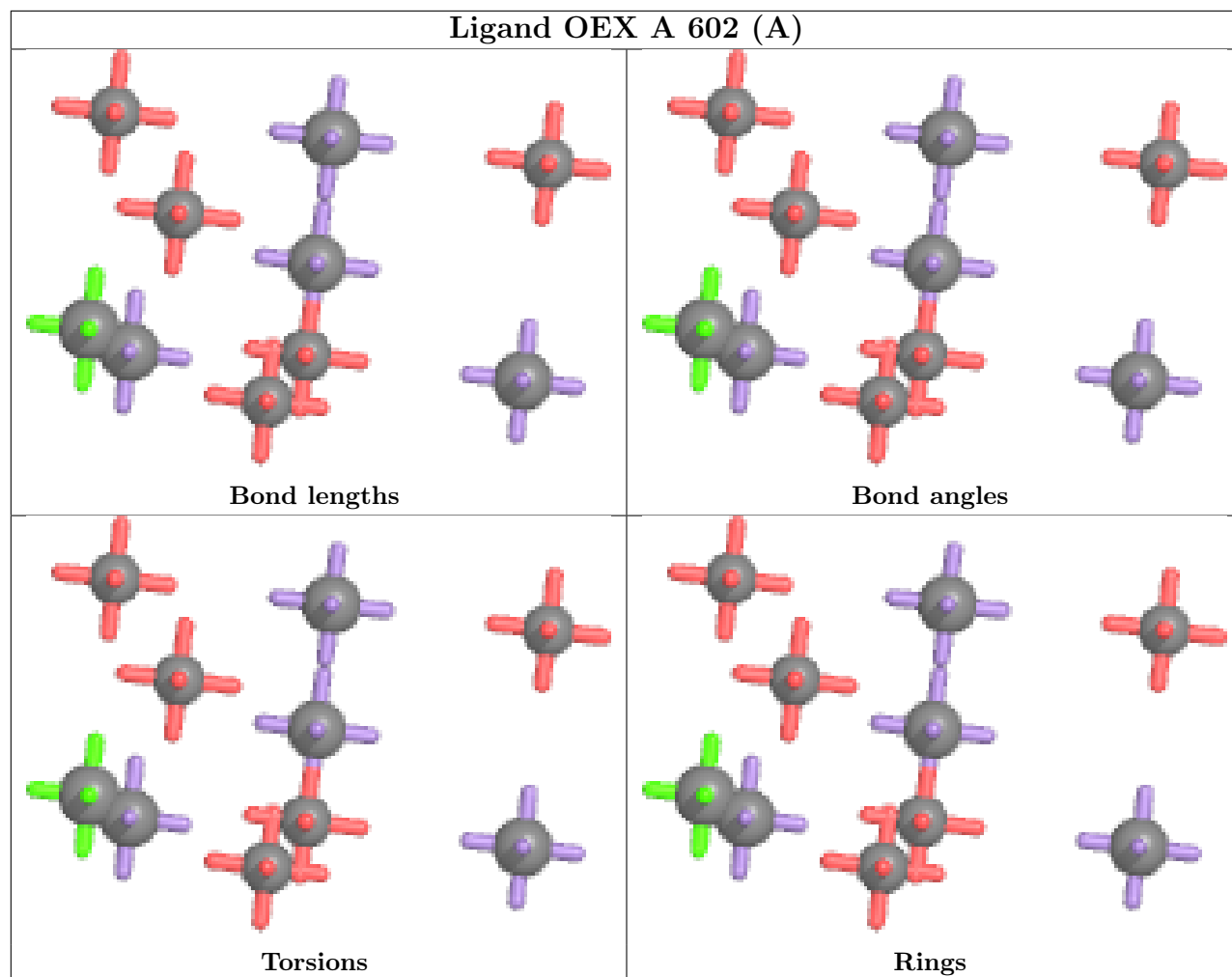
Ligand LMG a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

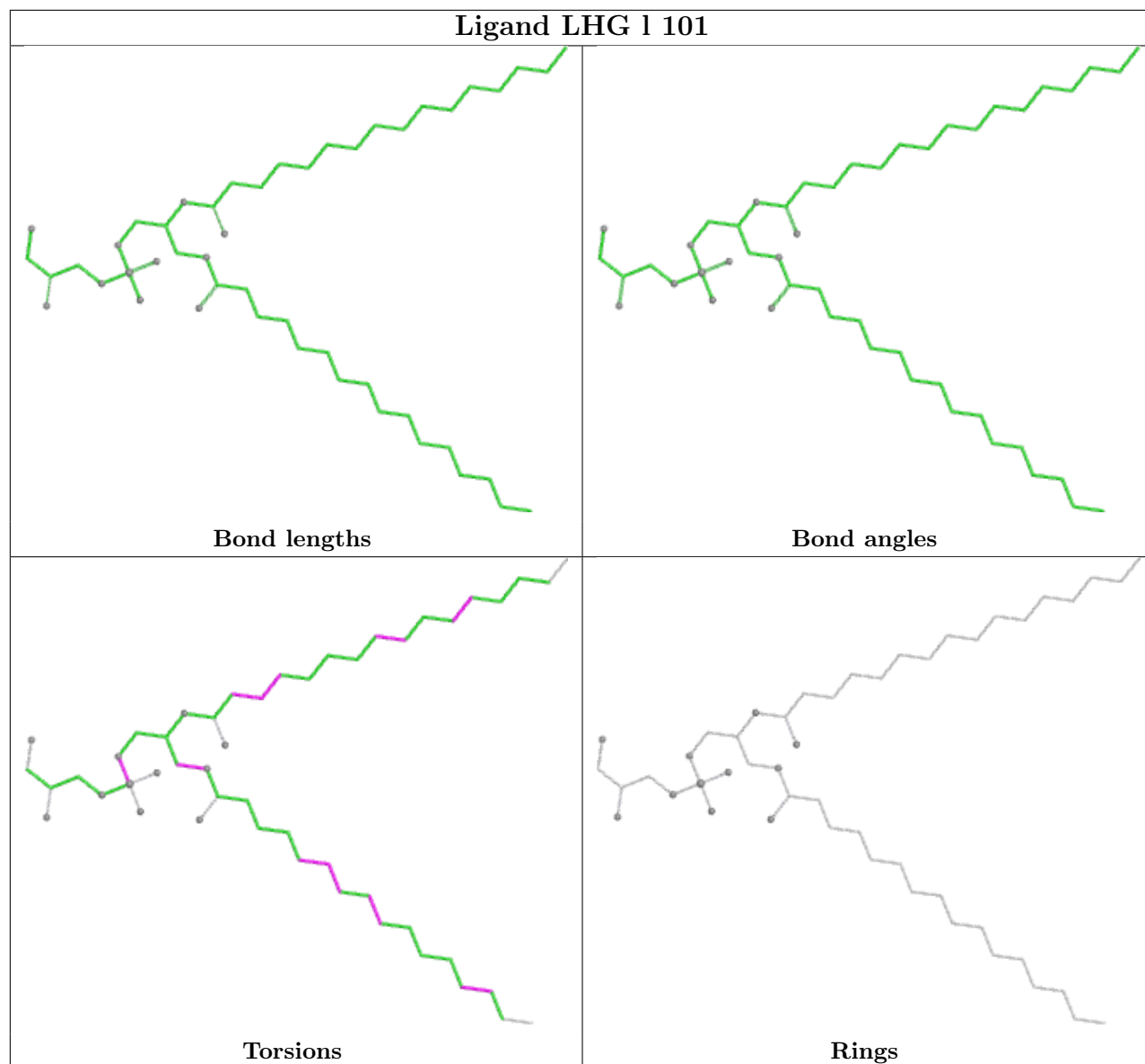
Ligand CLA A 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 510	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

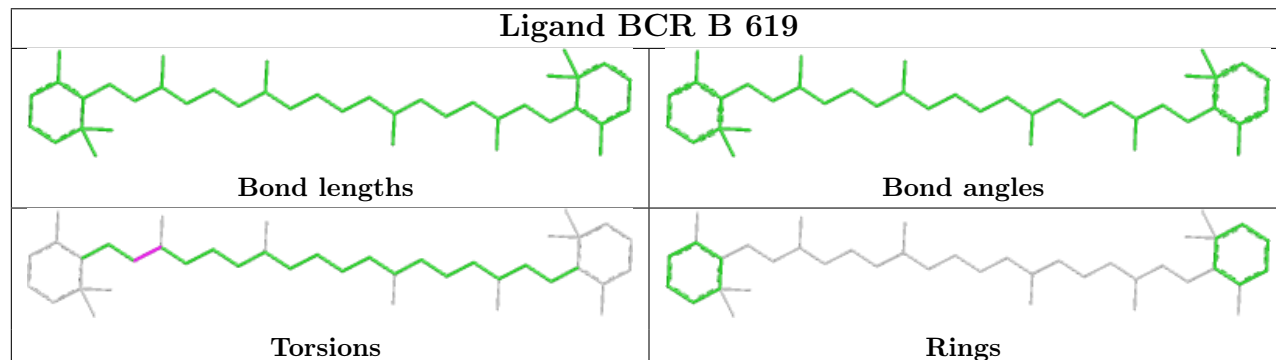
Ligand OEX A 602 (A)

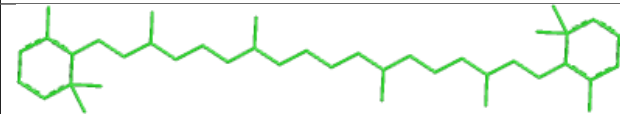
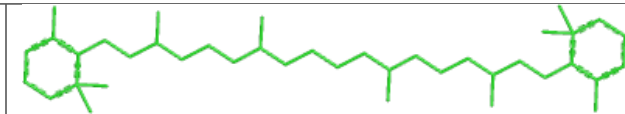
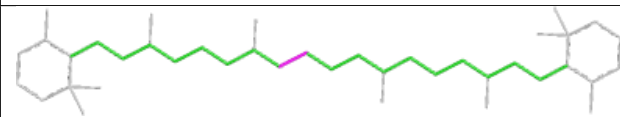
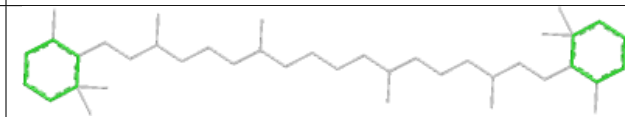


Ligand LHG 1 101

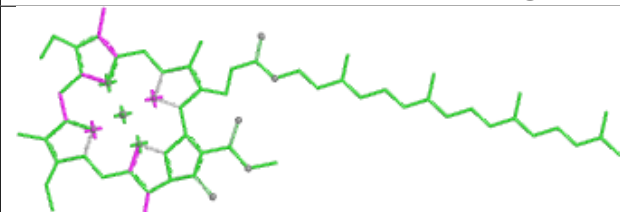
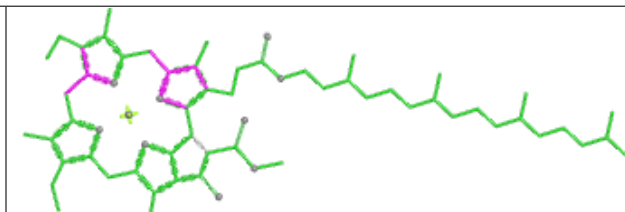
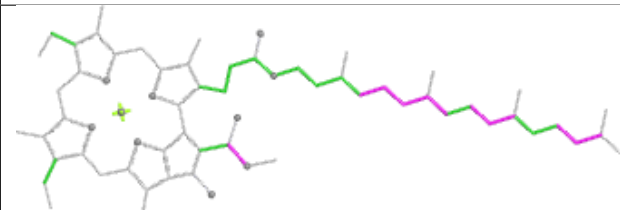
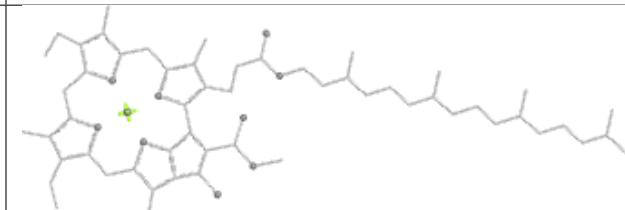


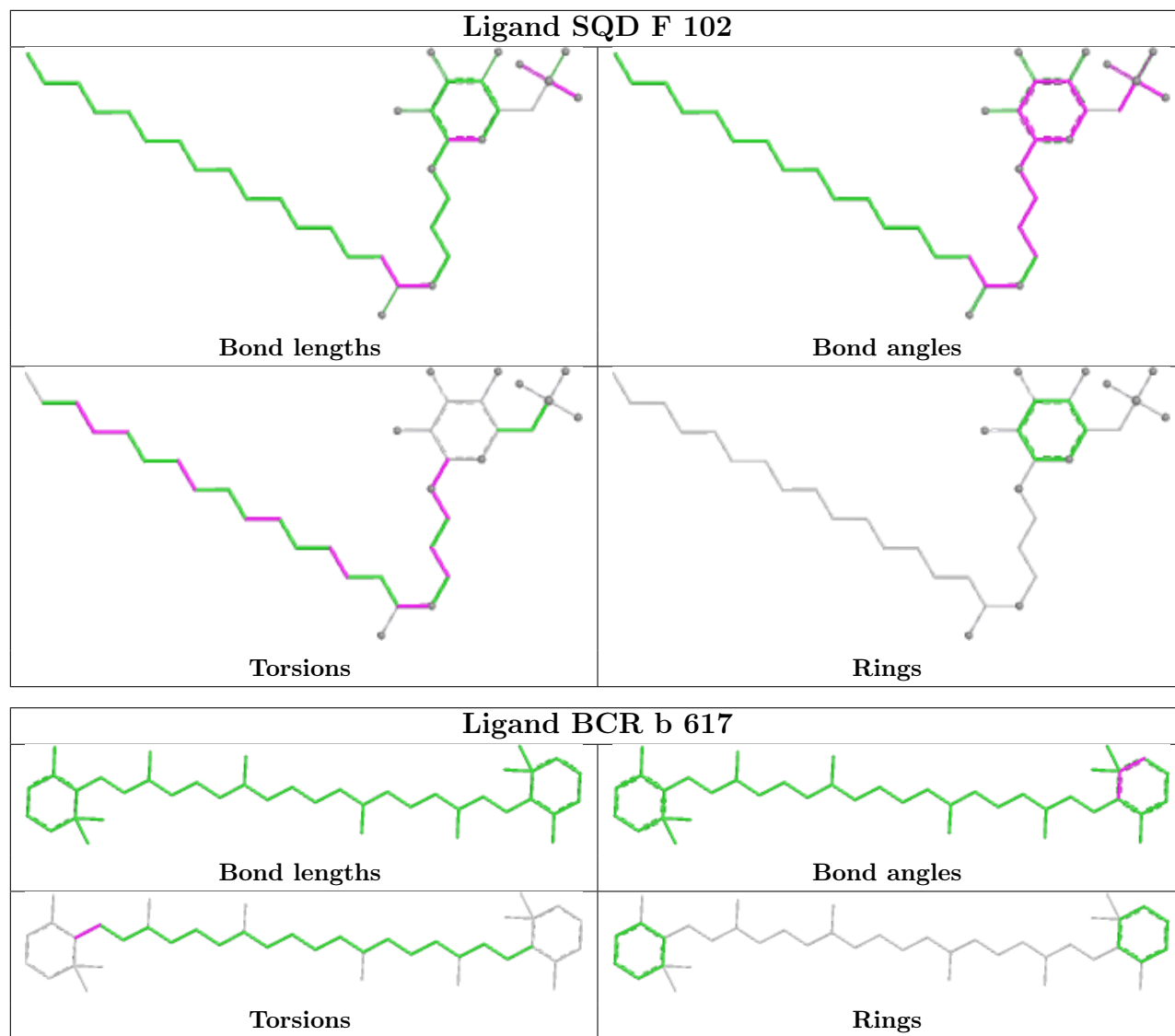
Ligand BCR B 619

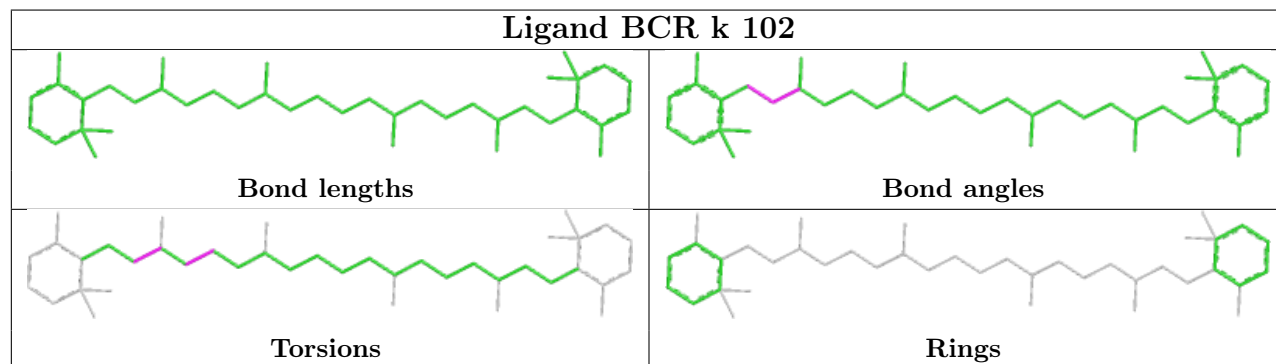
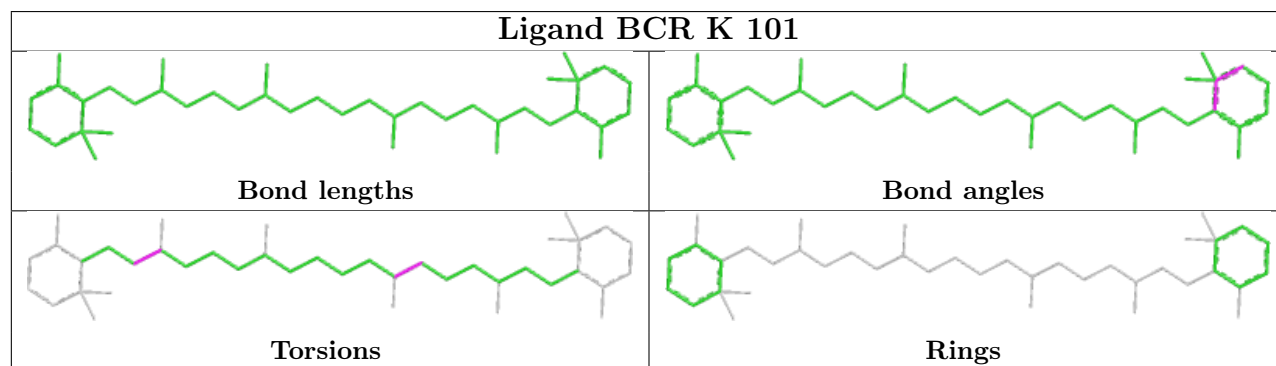
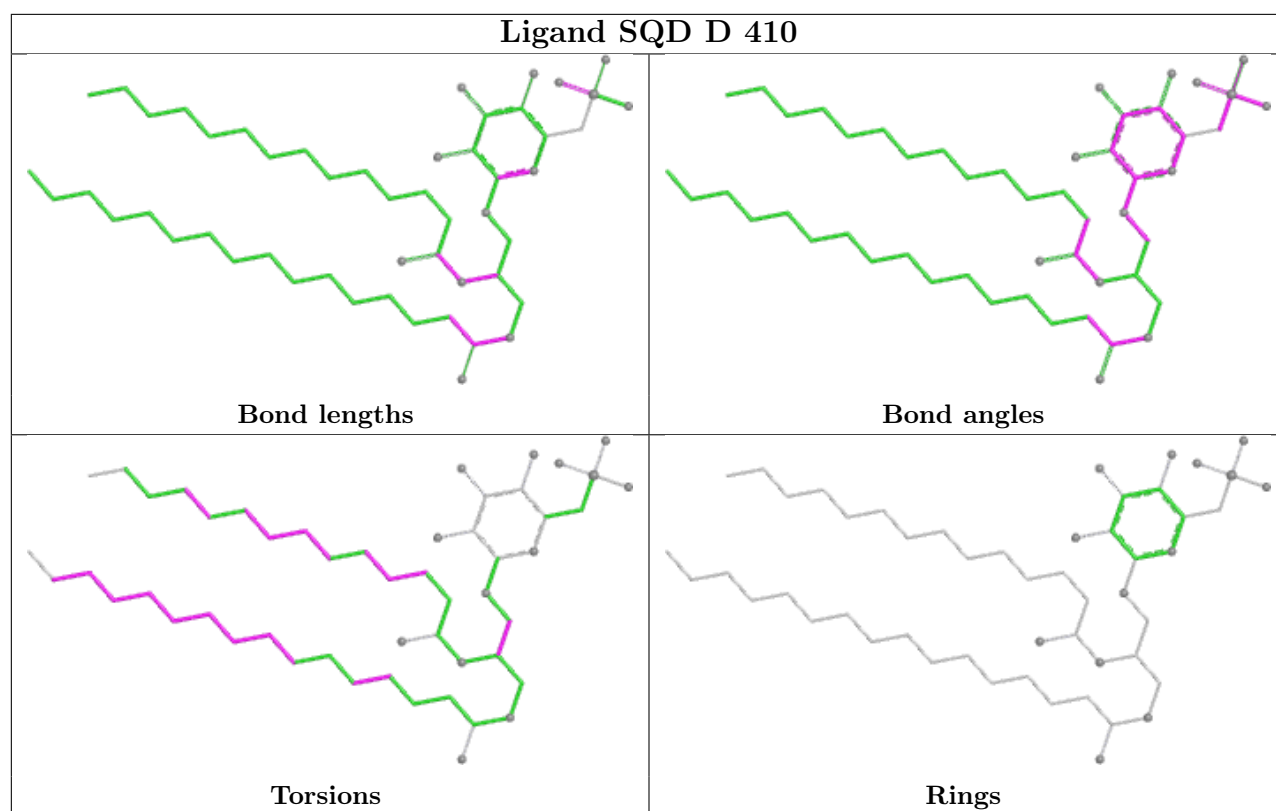


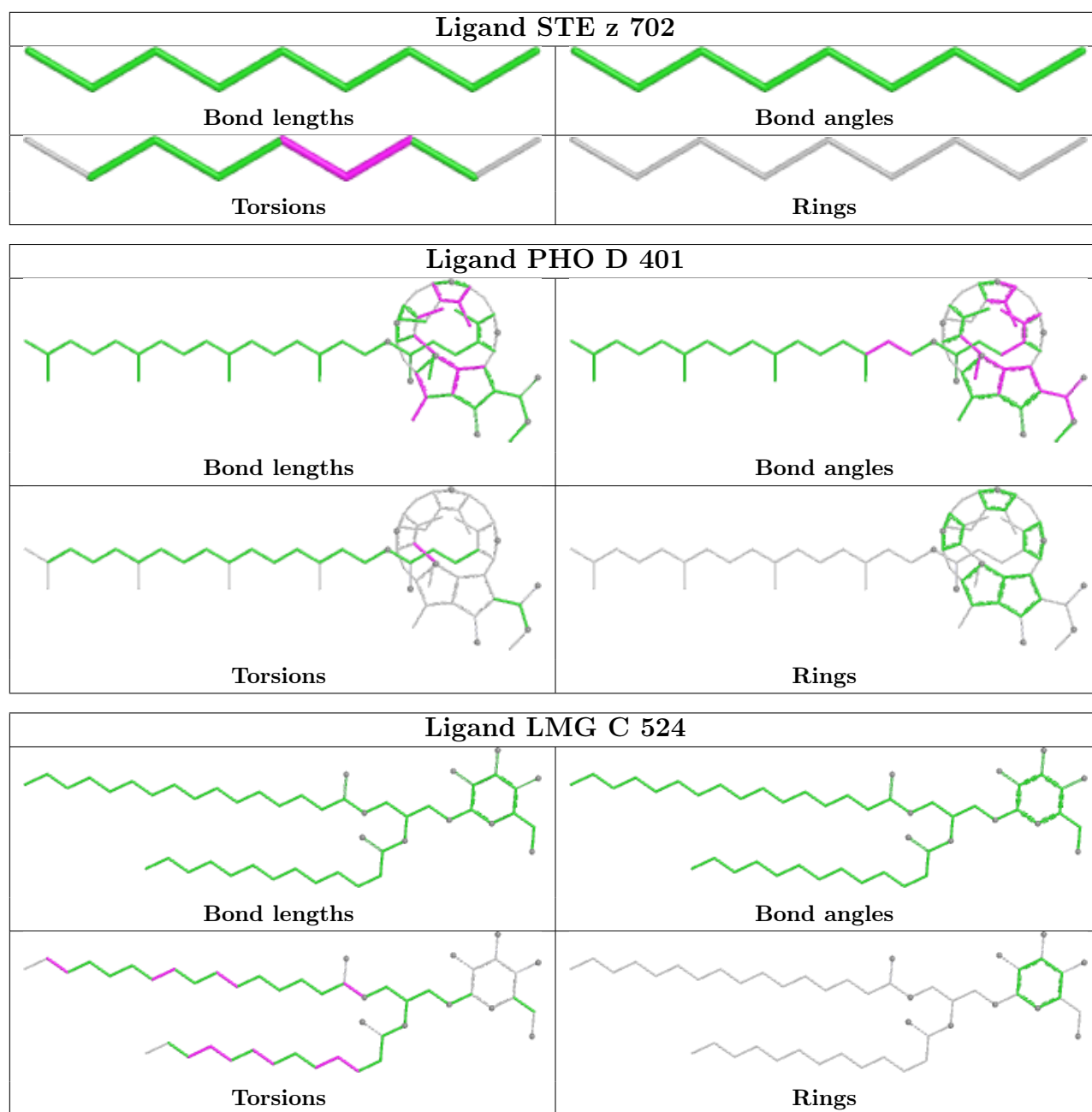
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

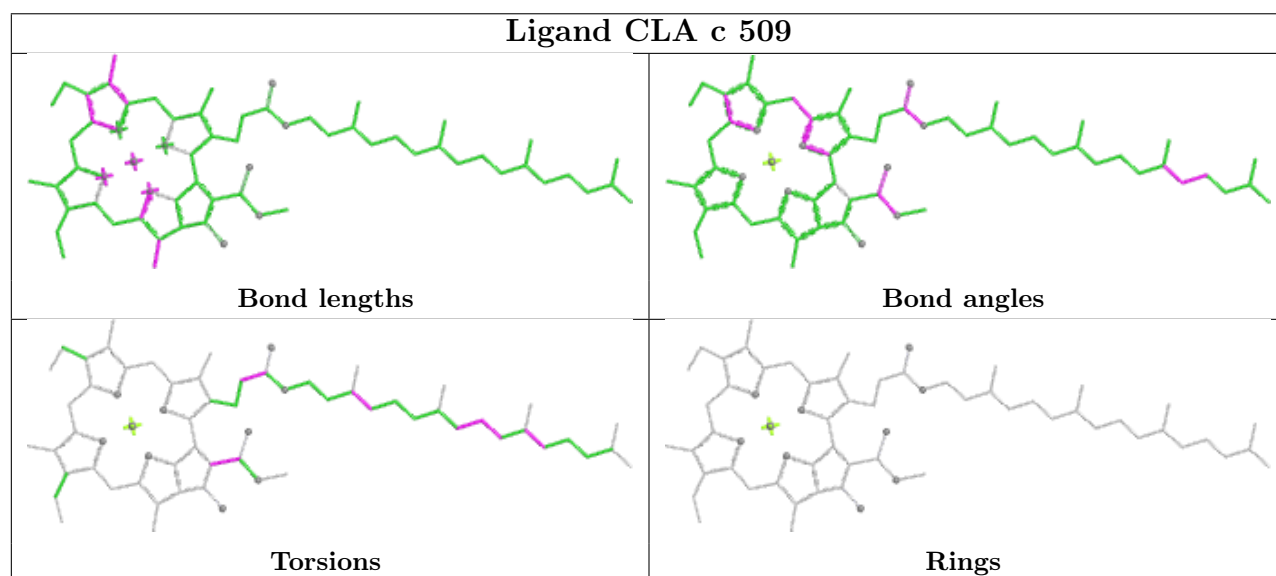
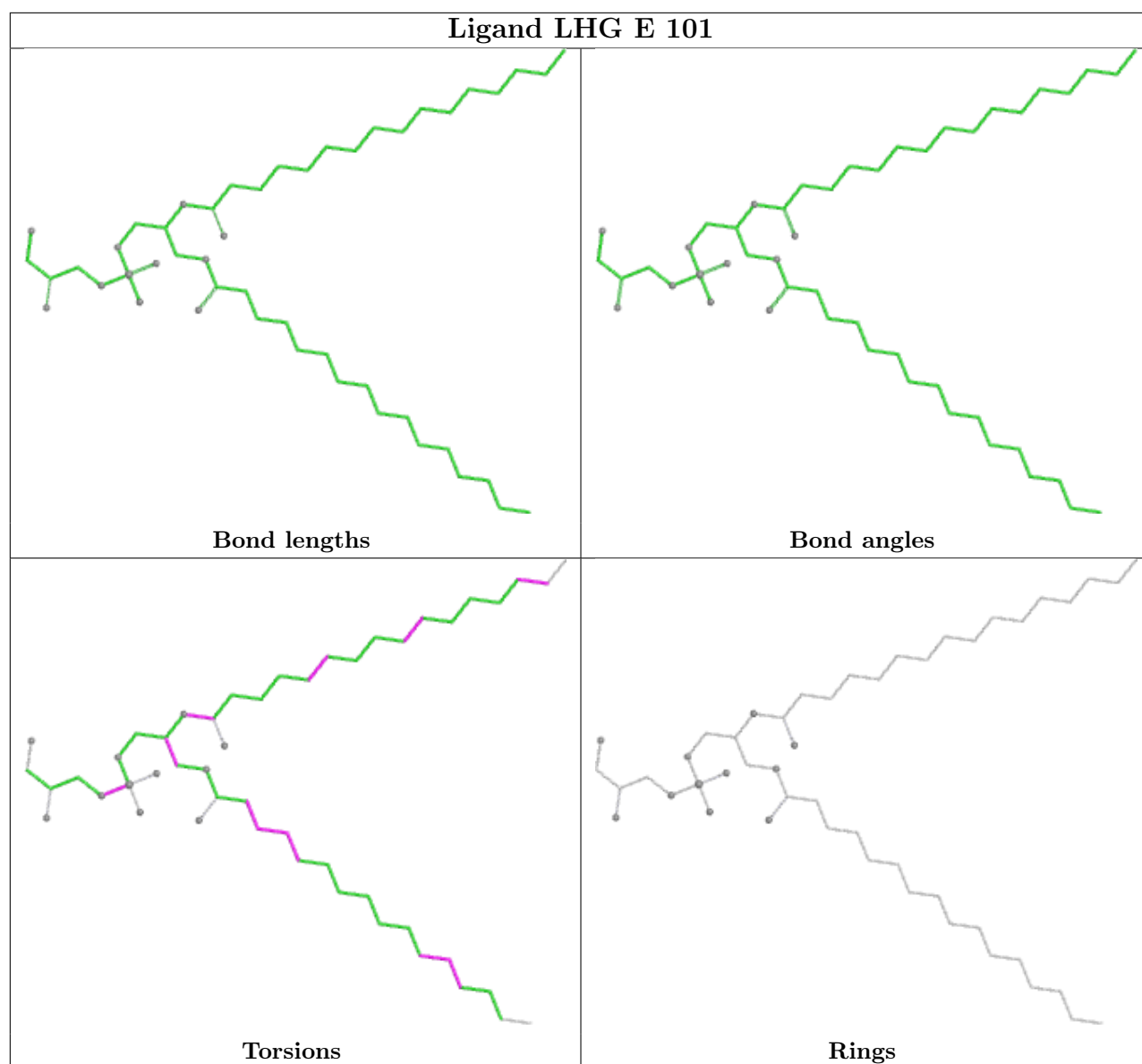
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

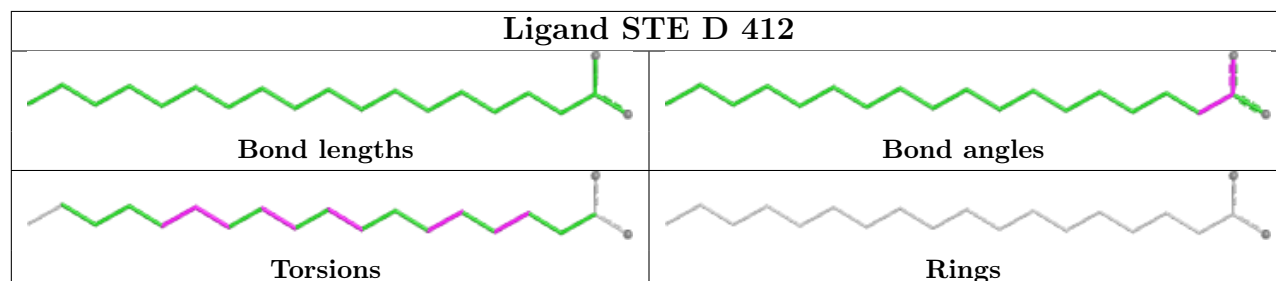
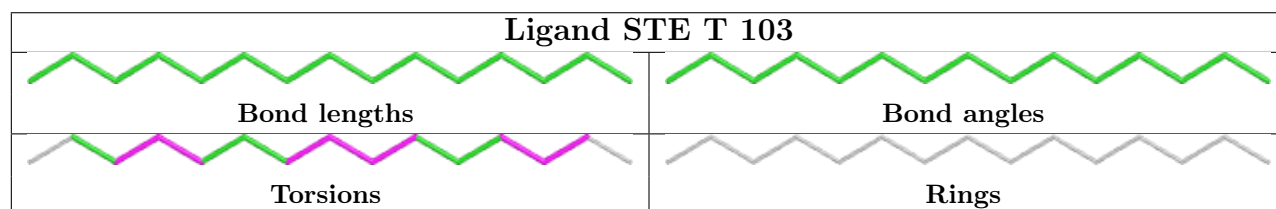
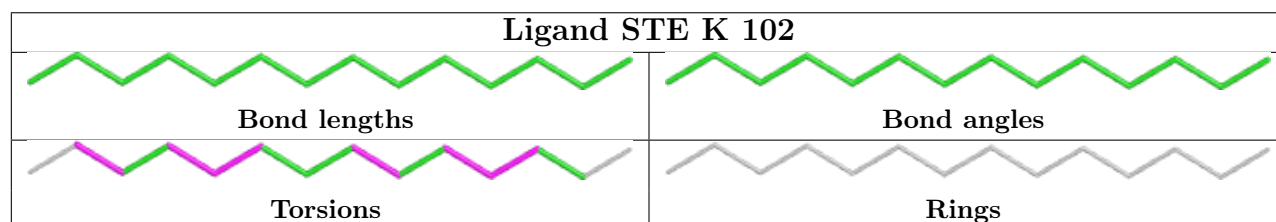
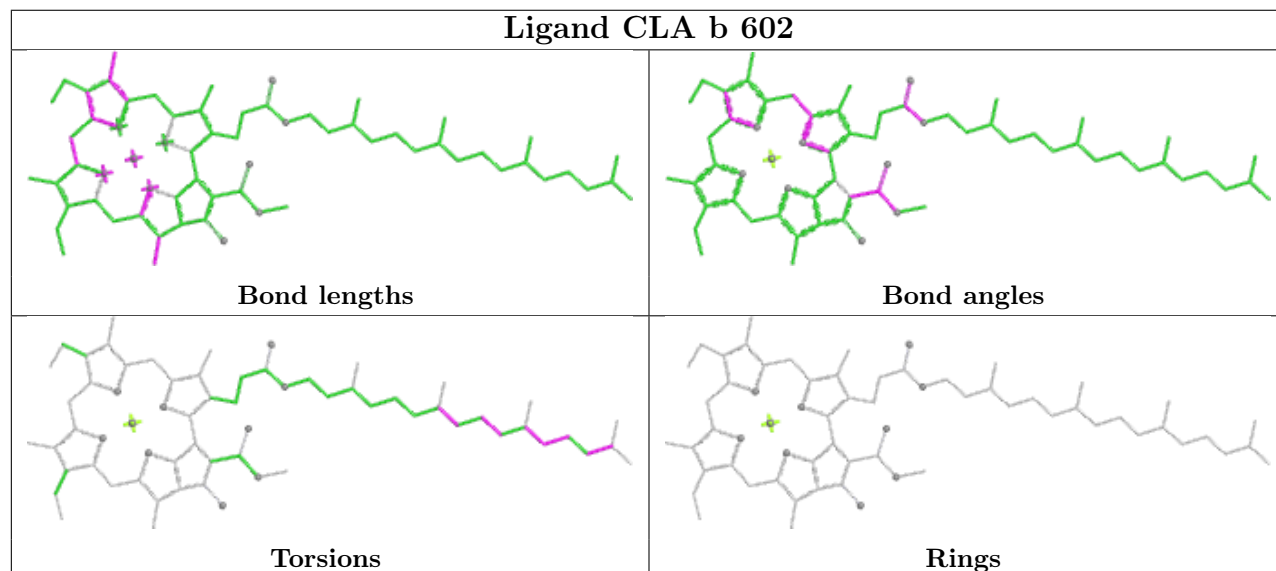
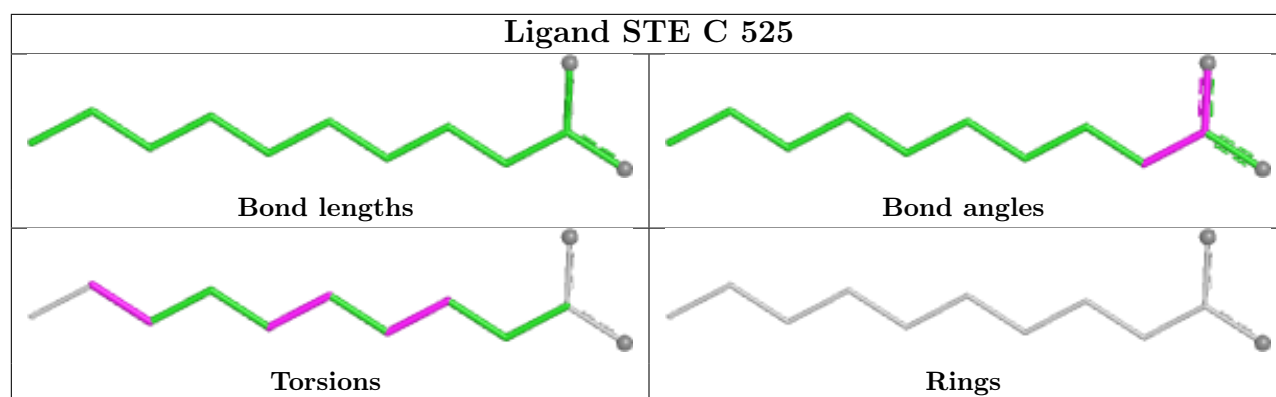
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

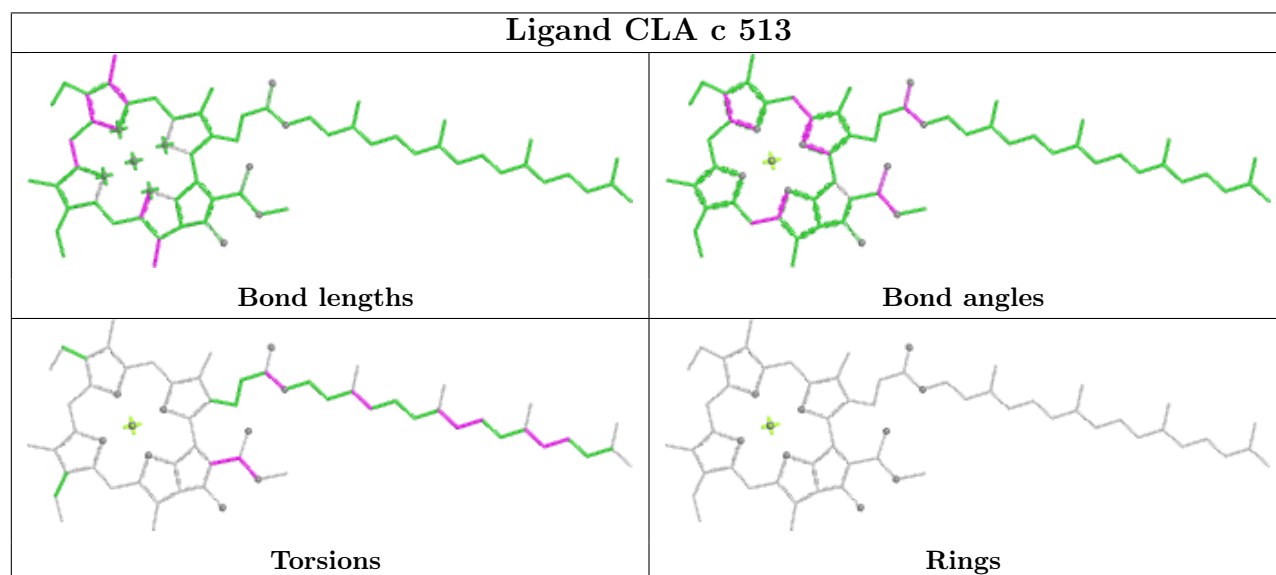
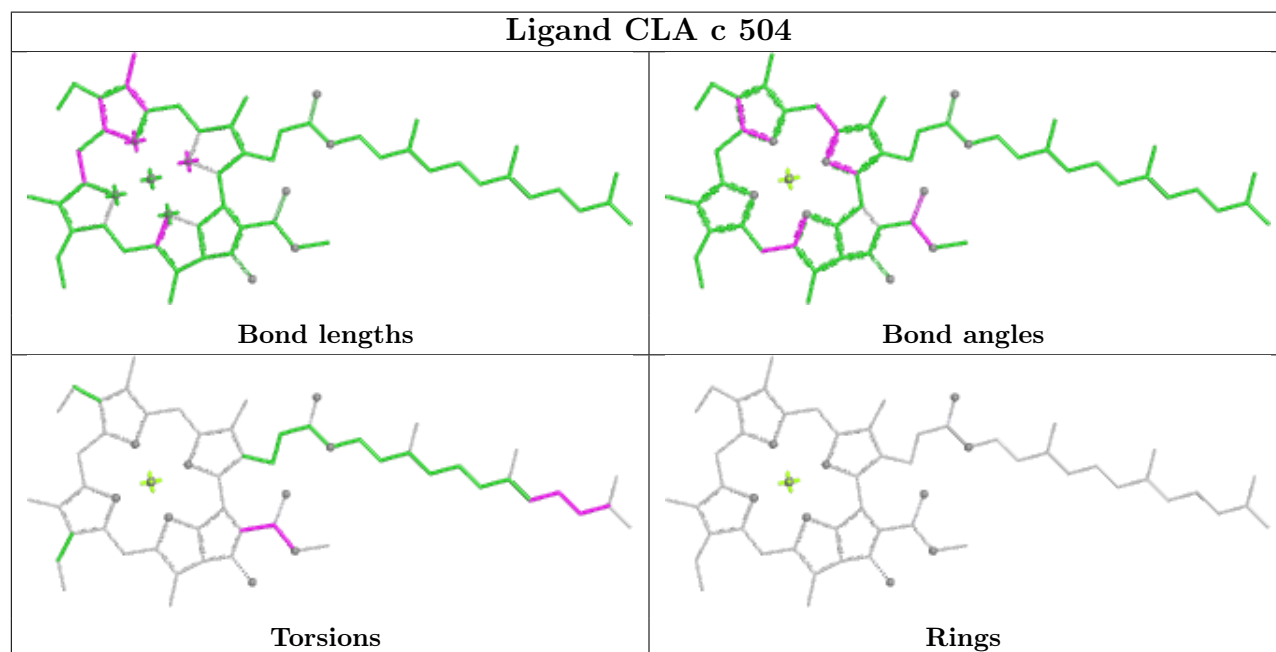
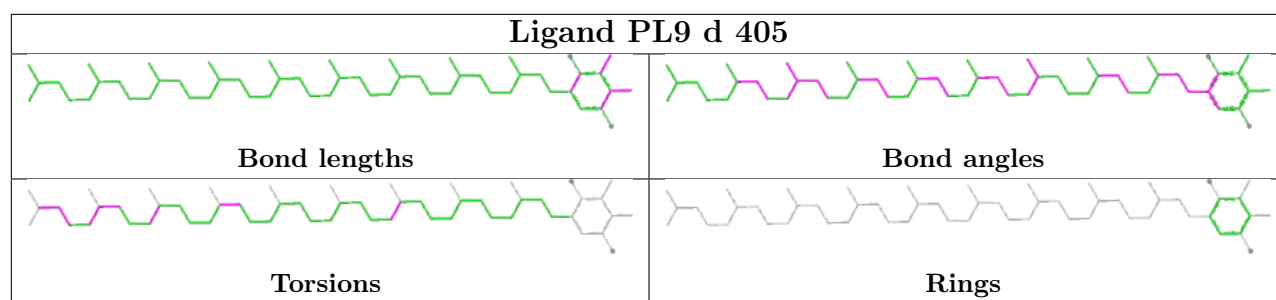


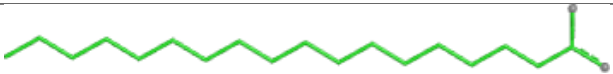
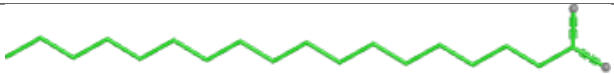


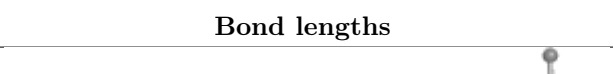
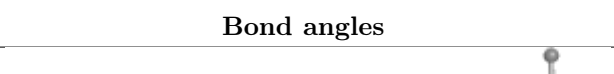


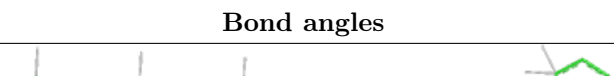




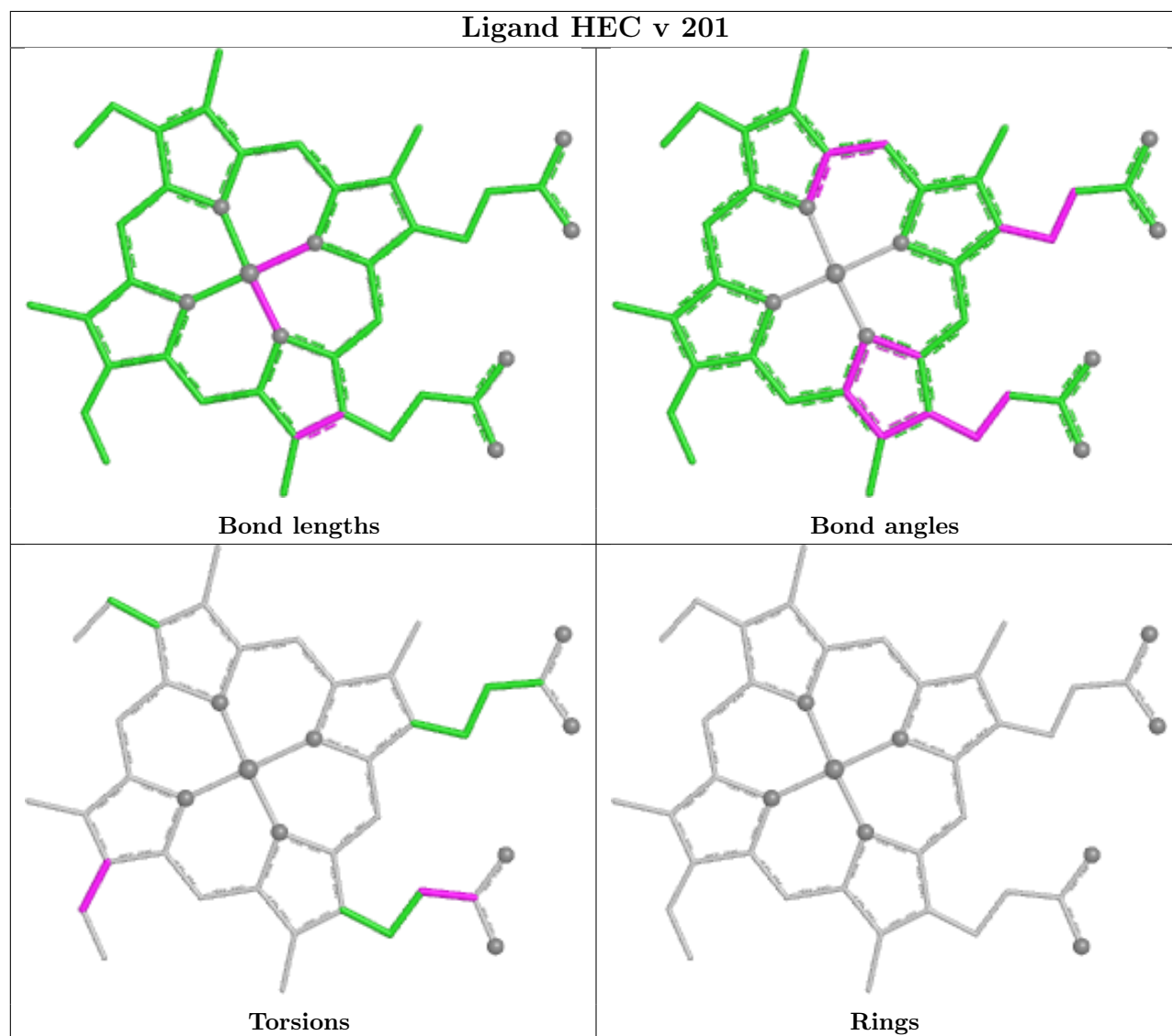
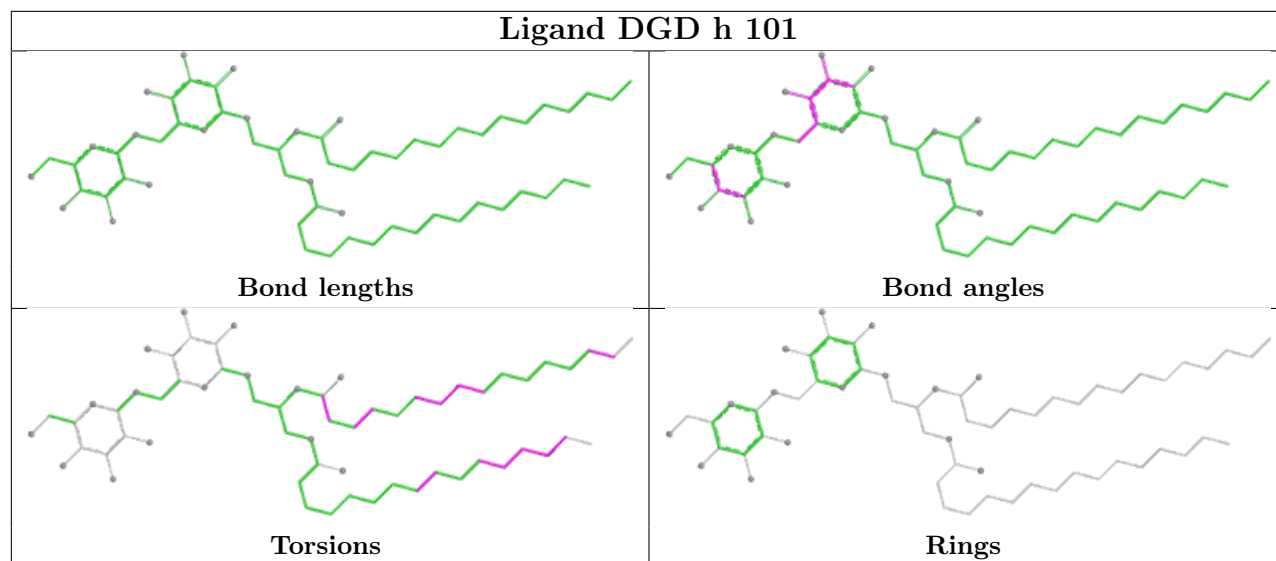


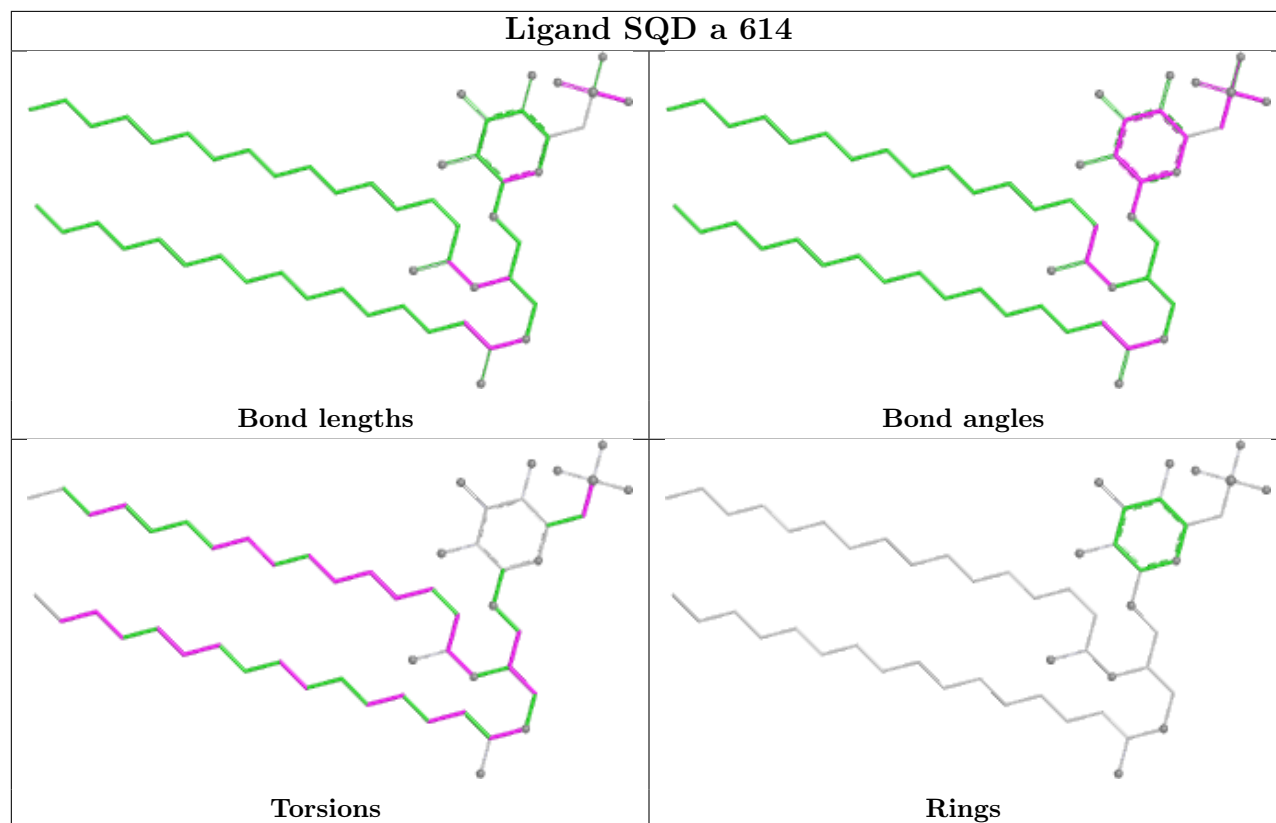
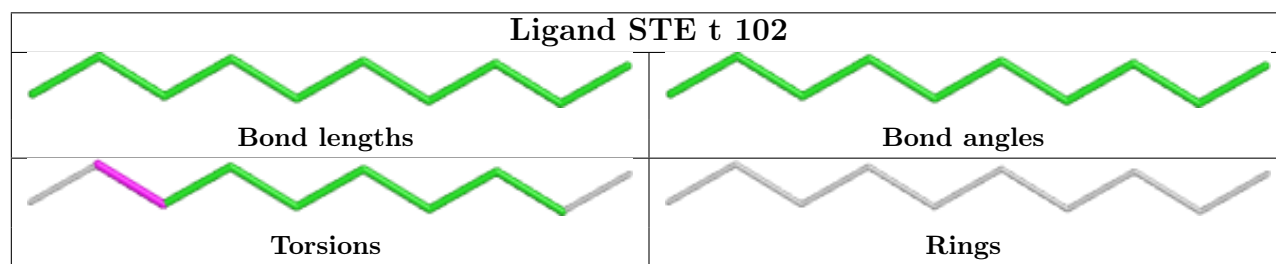
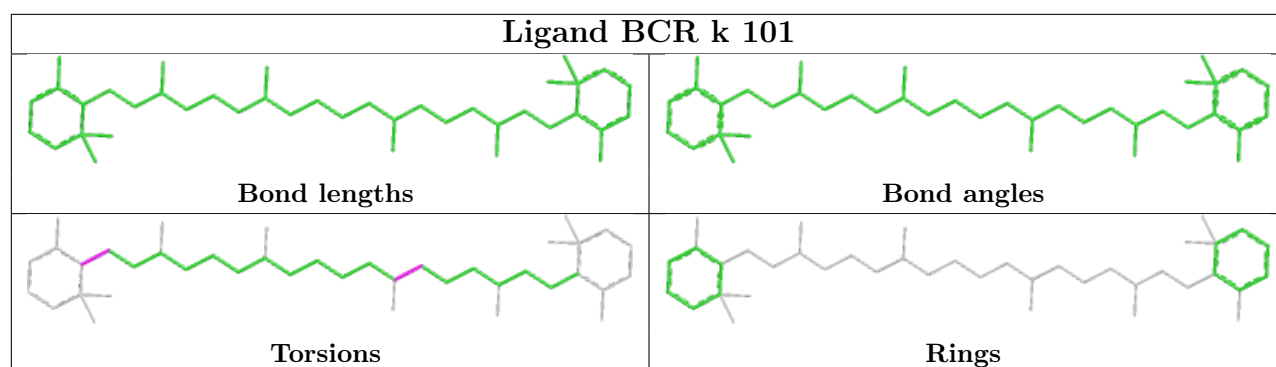
Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

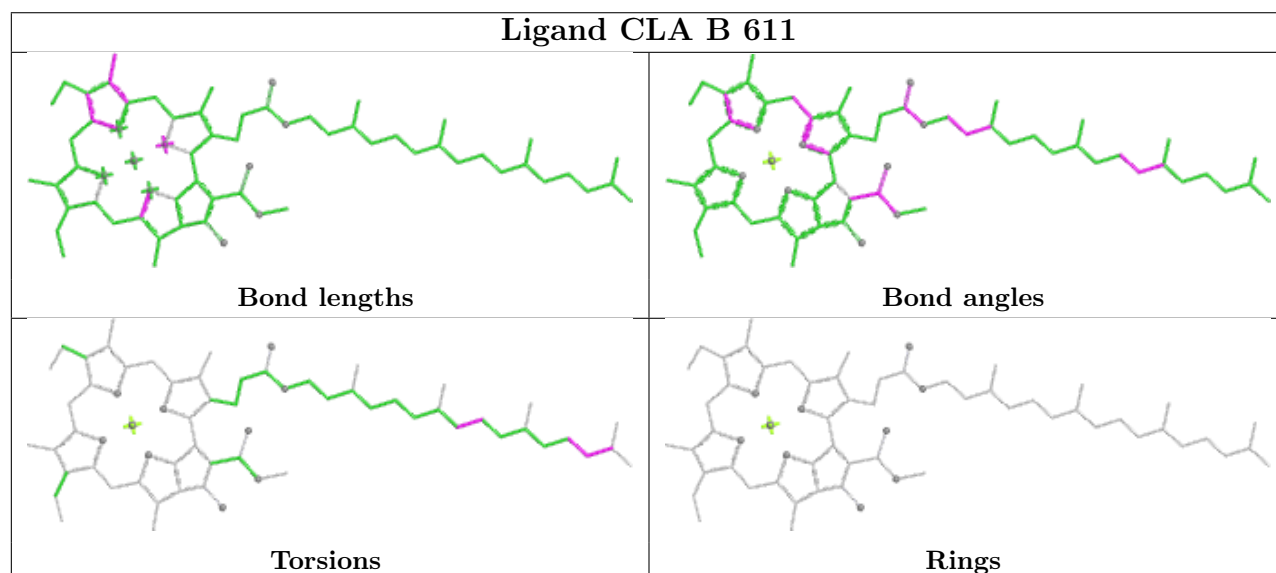
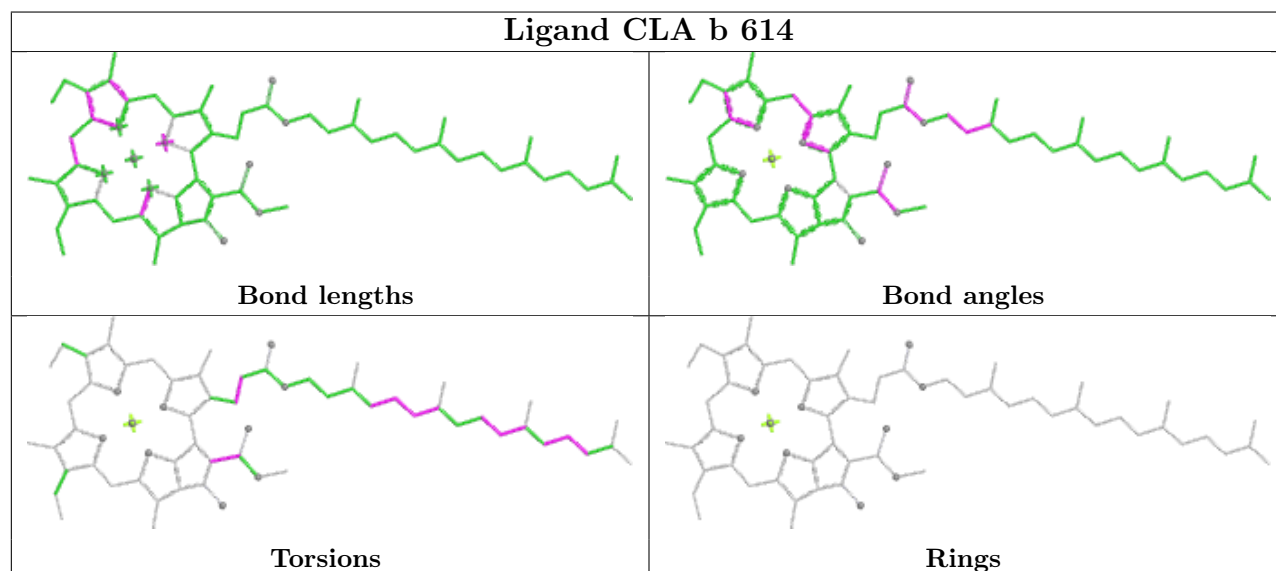
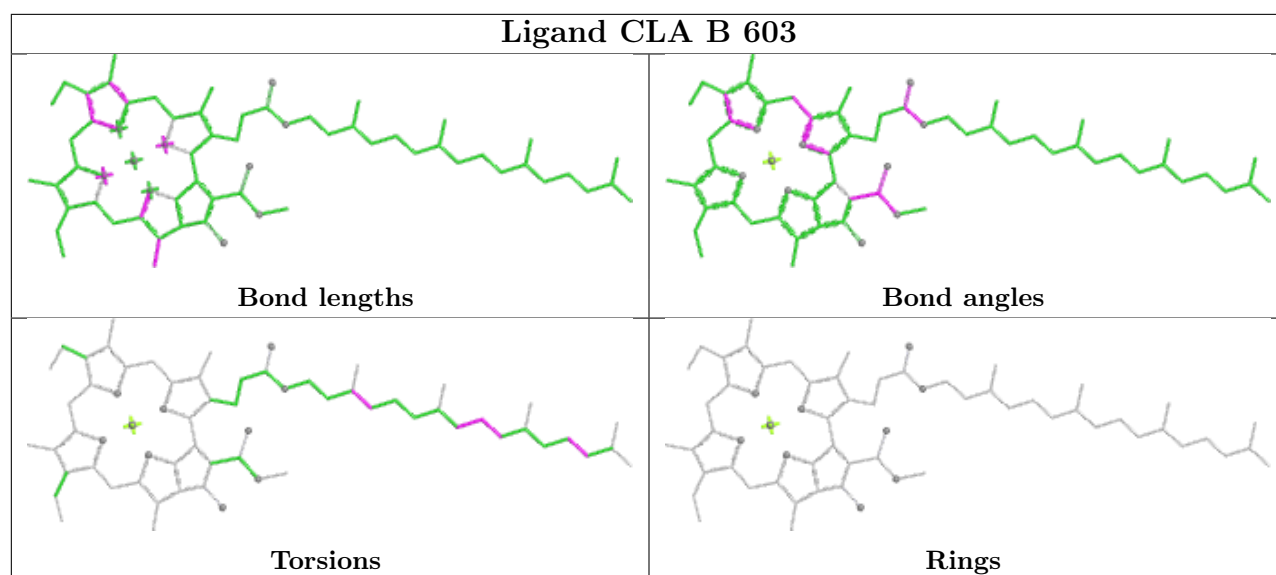
Ligand STE e 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

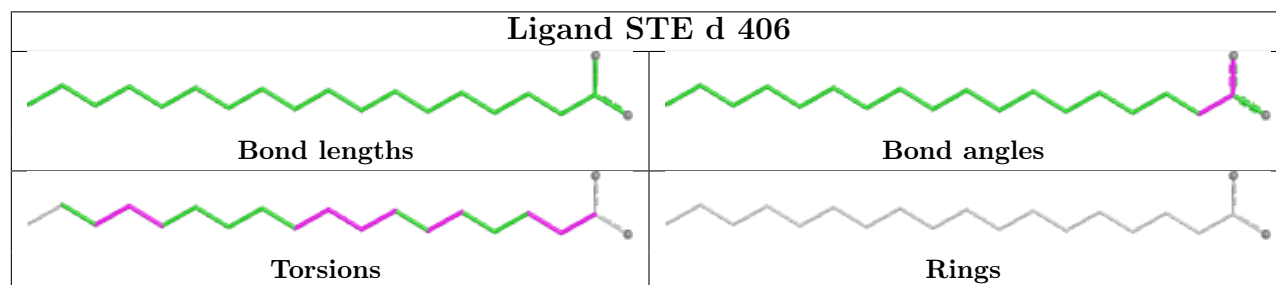
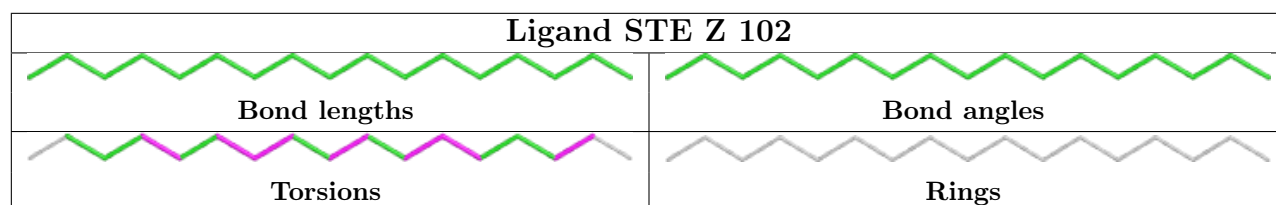
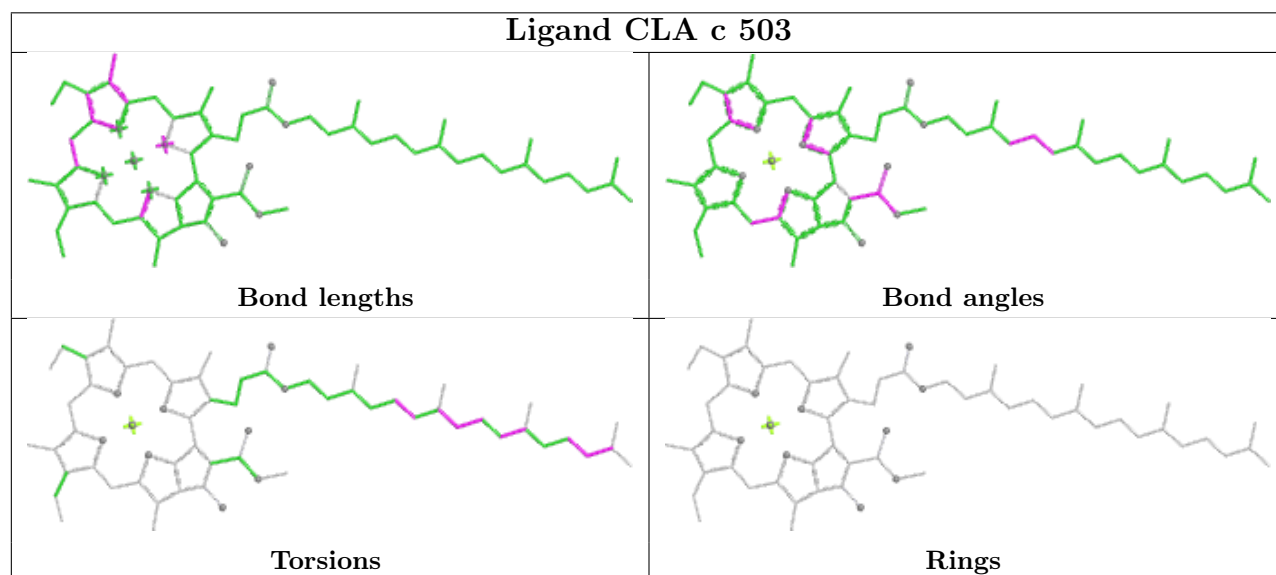
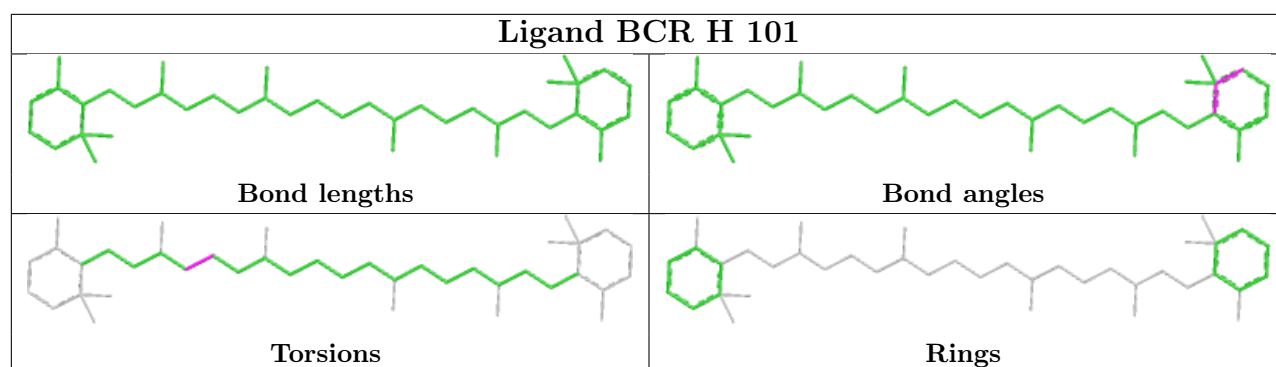
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

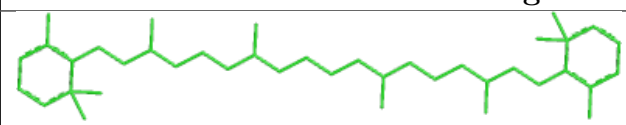
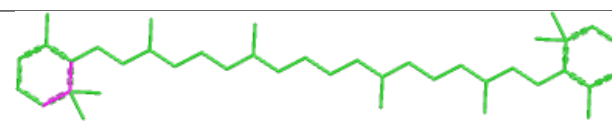
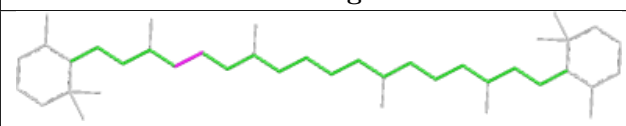
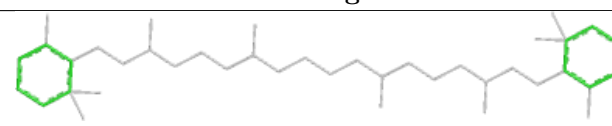
Ligand STE a 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

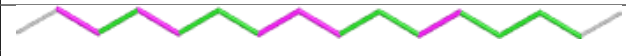


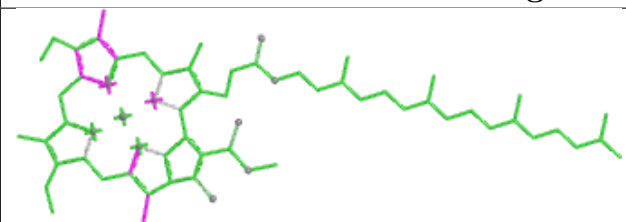
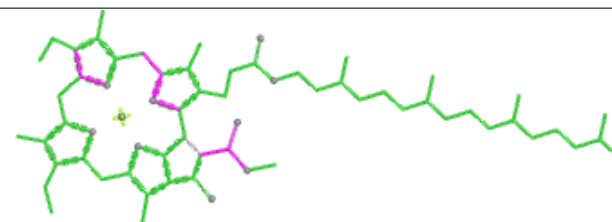
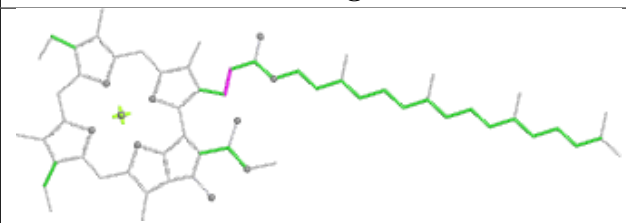
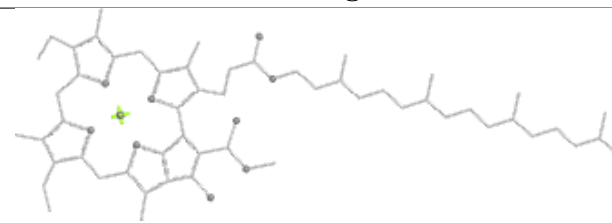


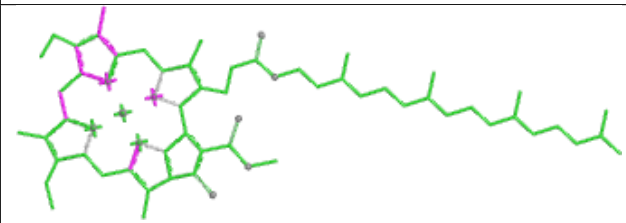
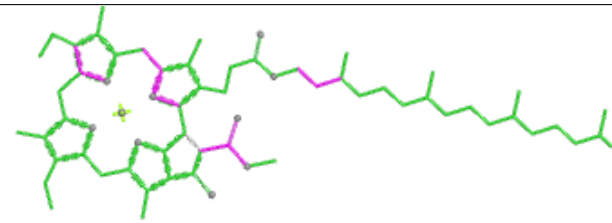
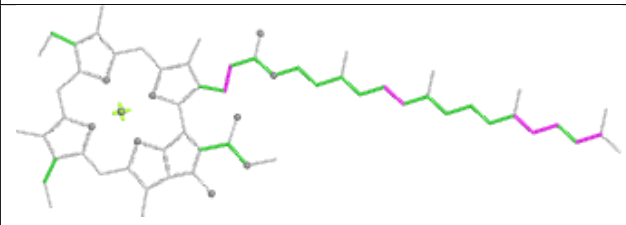
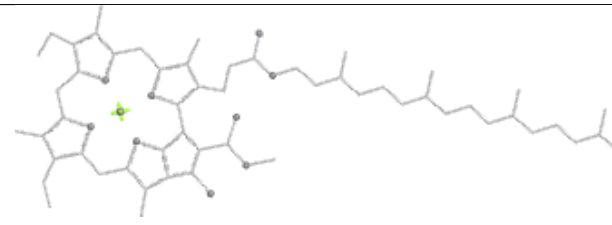


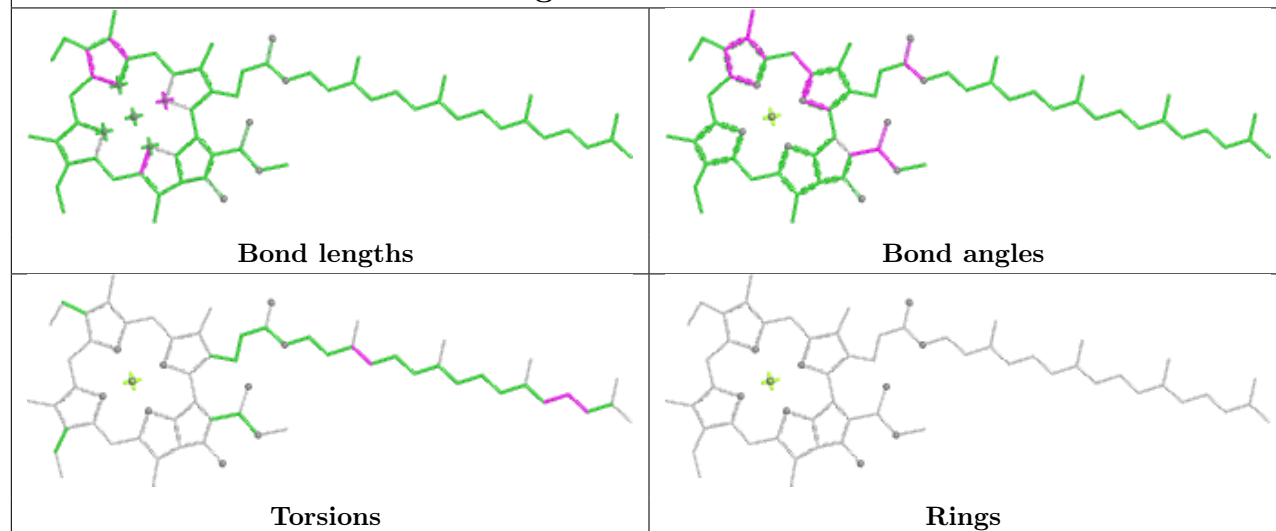
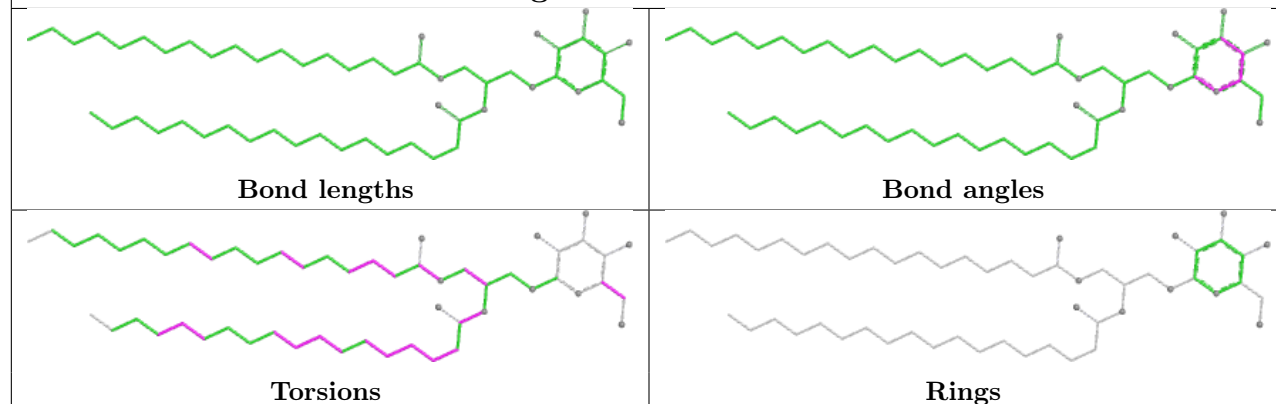
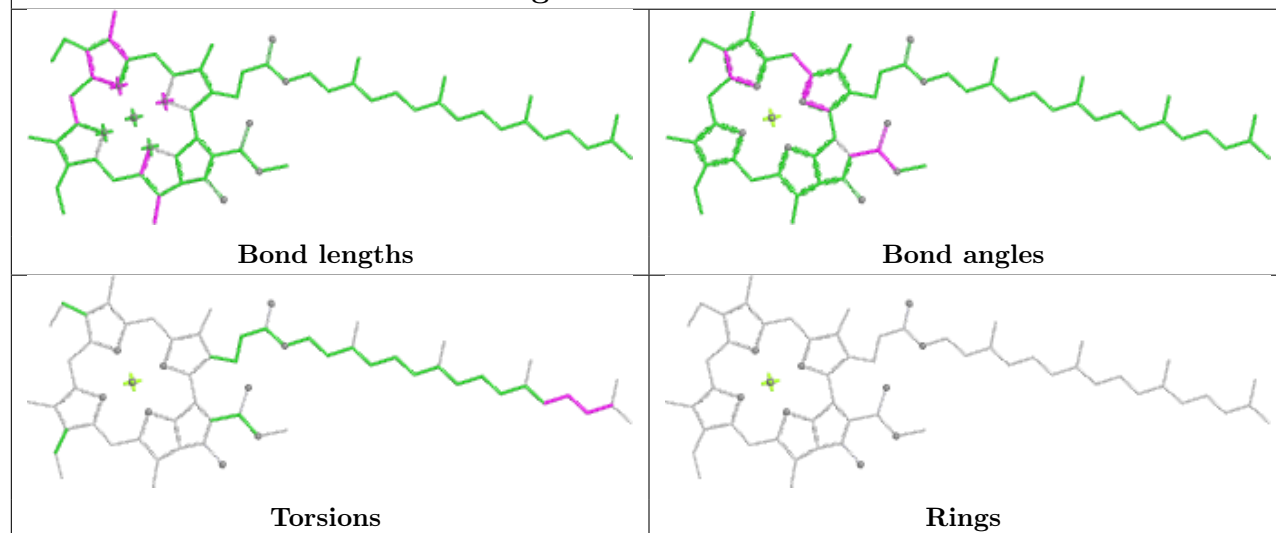


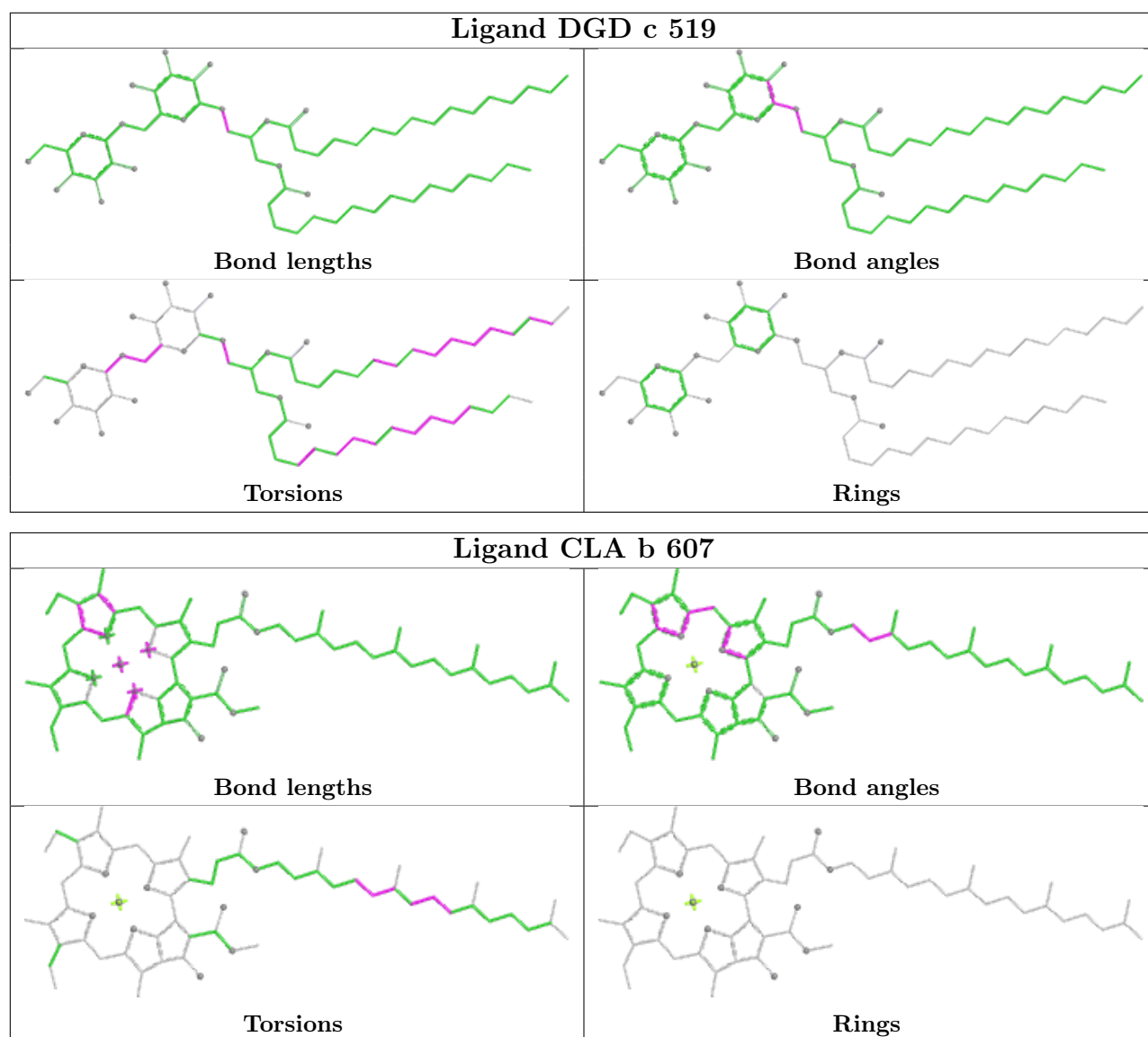
Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

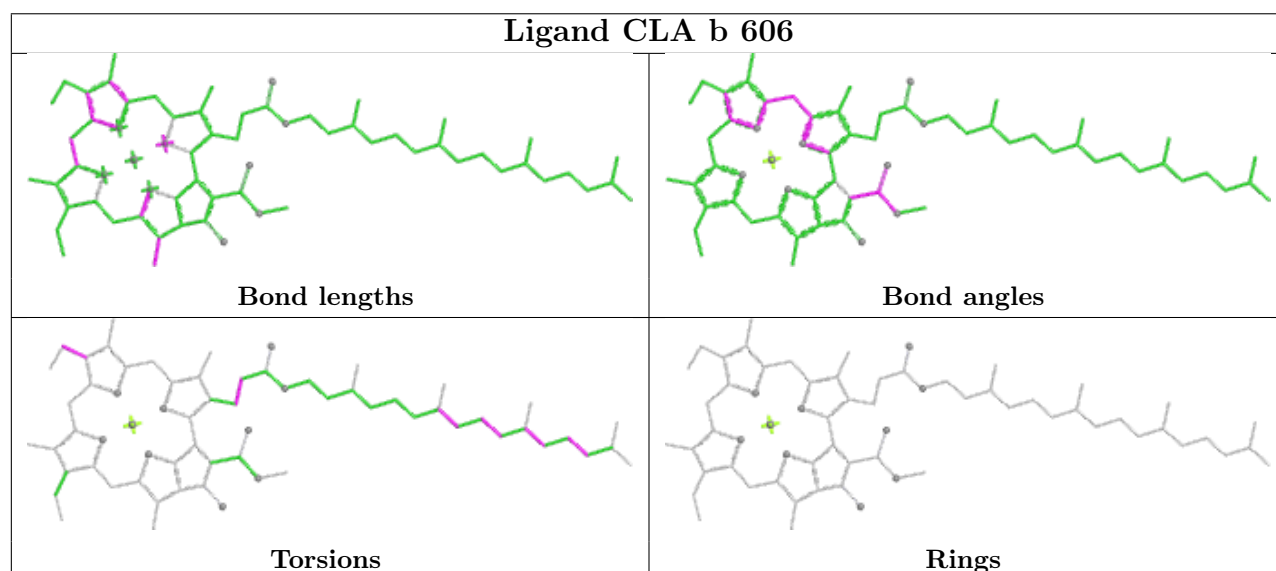
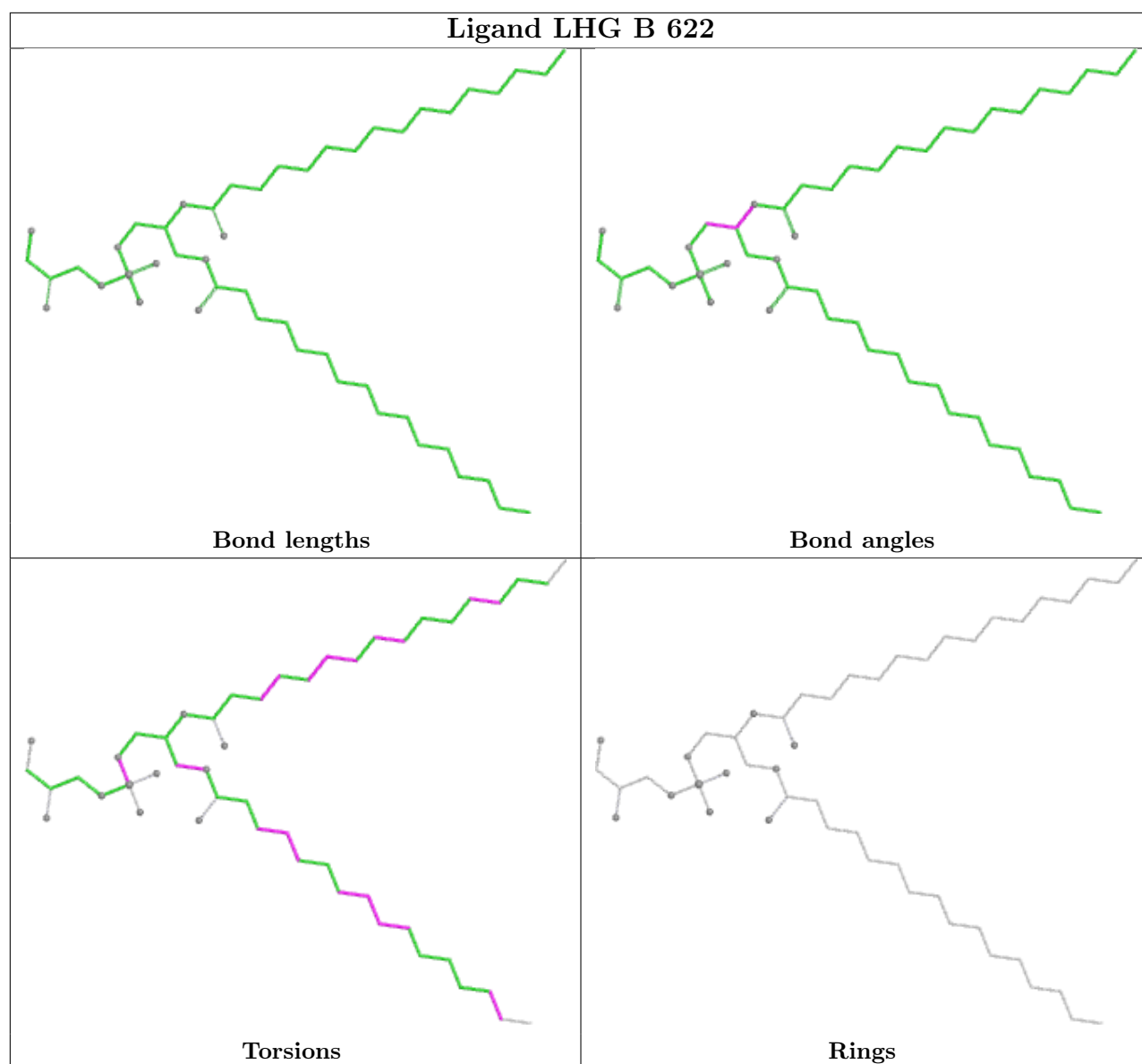
Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

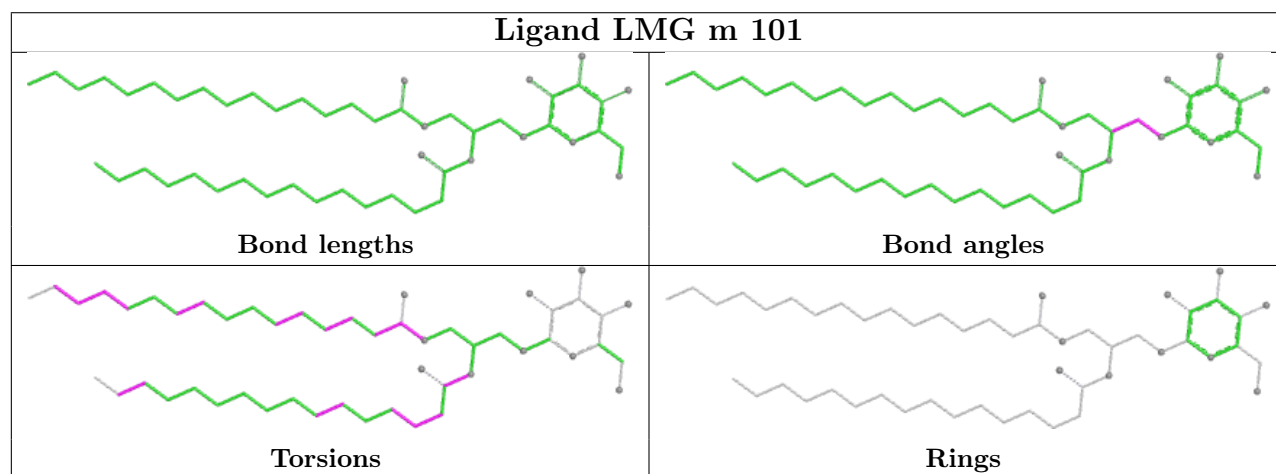
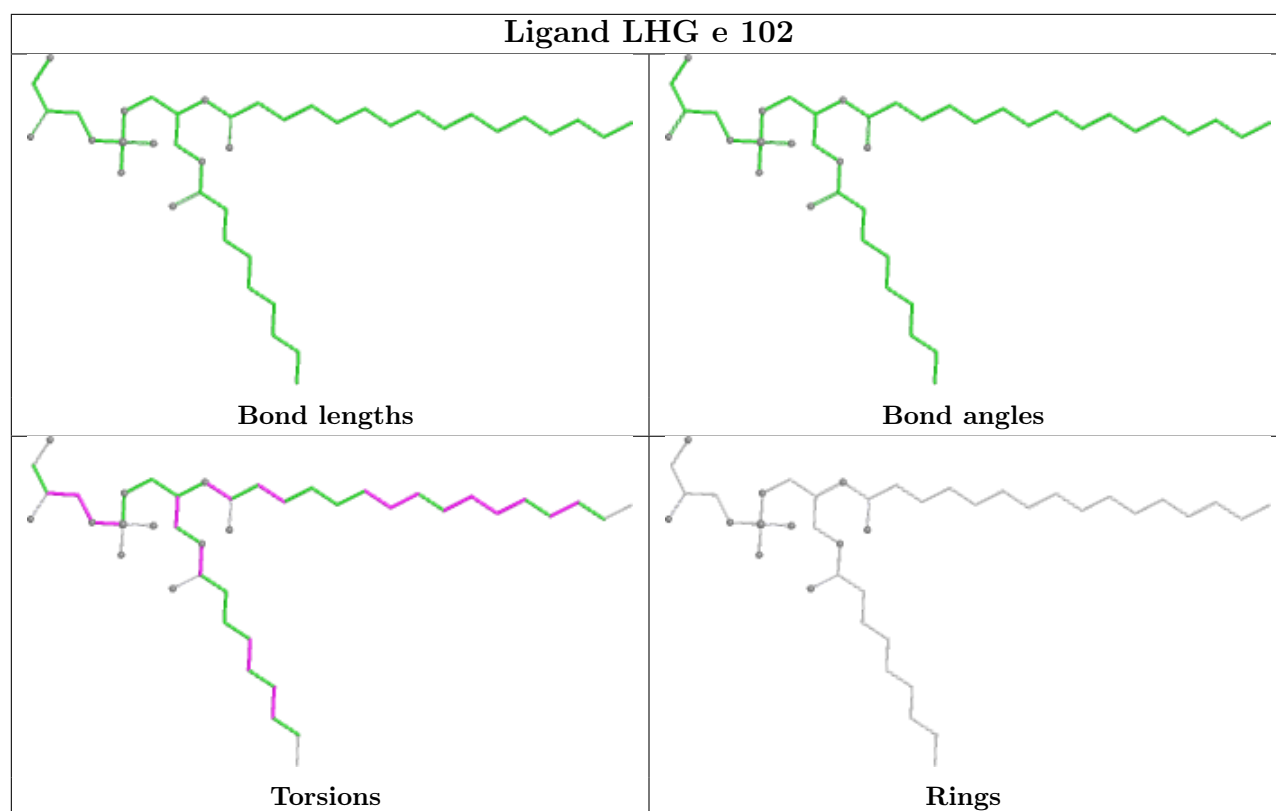
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

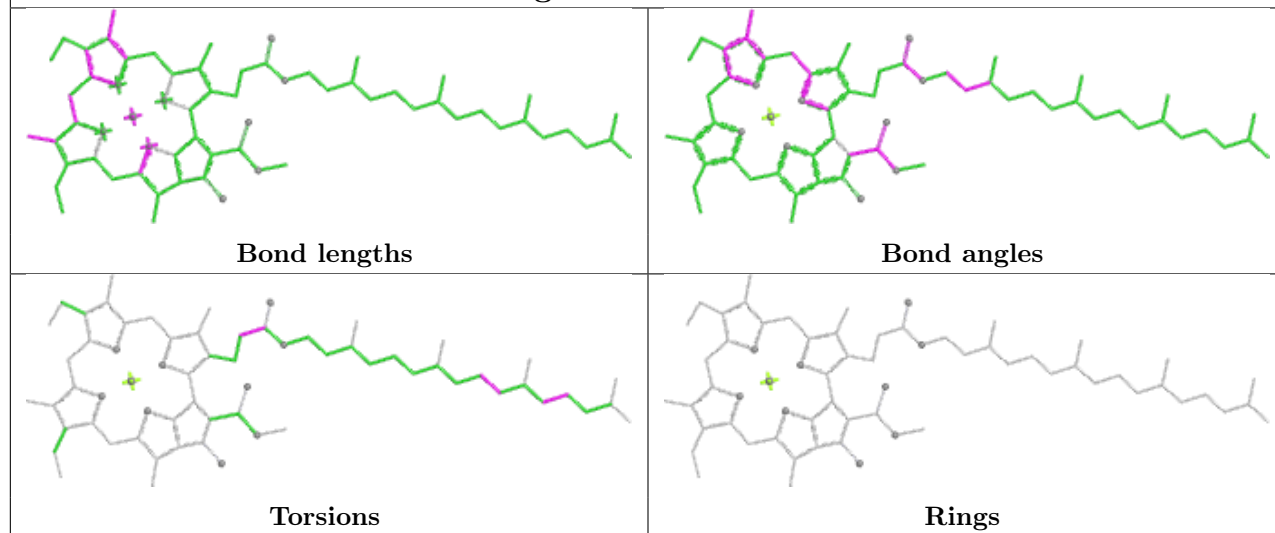
Ligand CLA b 609**Ligand LMG b 622****Ligand CLA A 614**



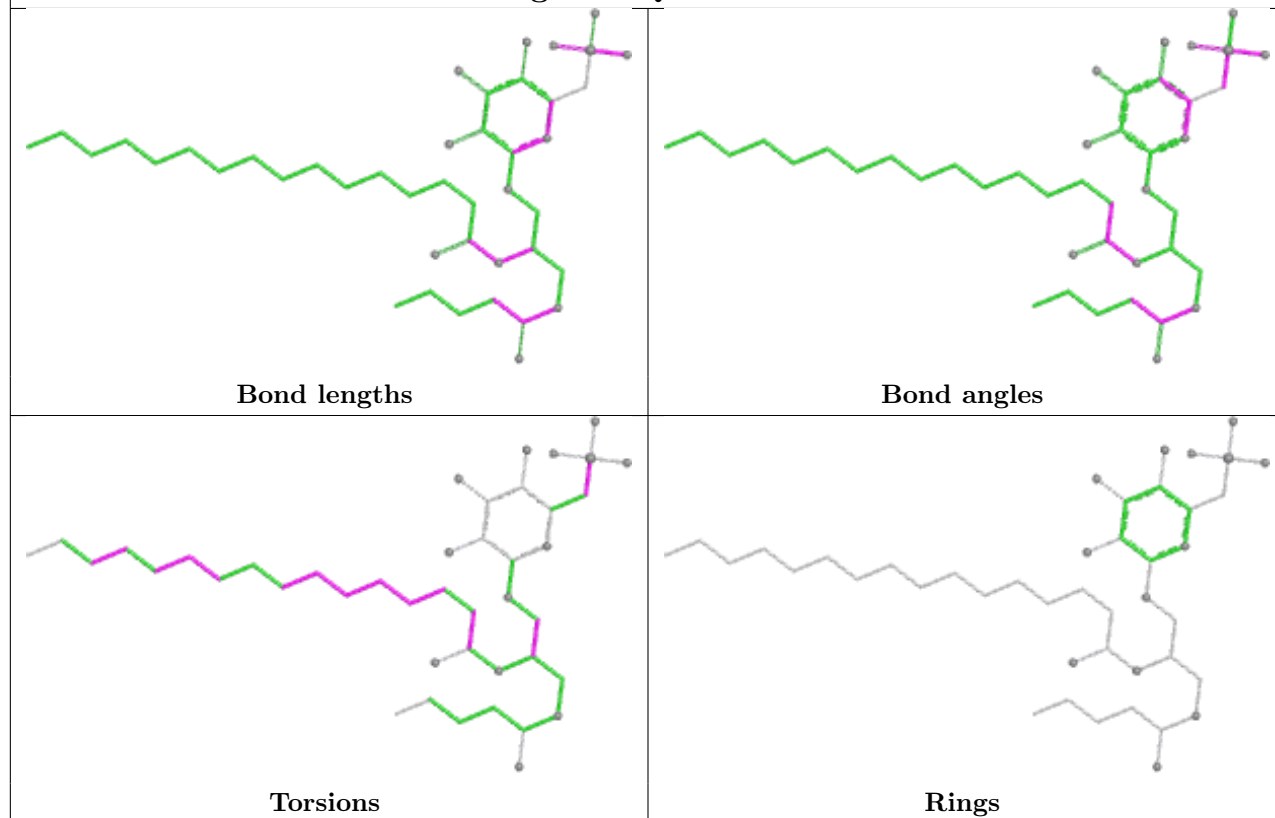


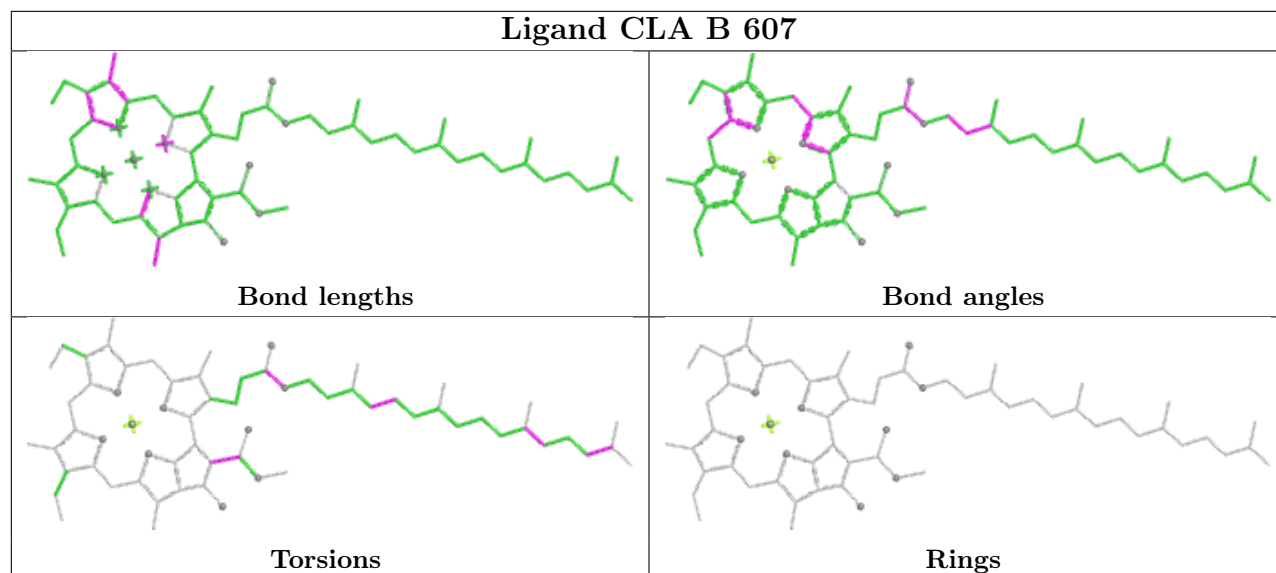
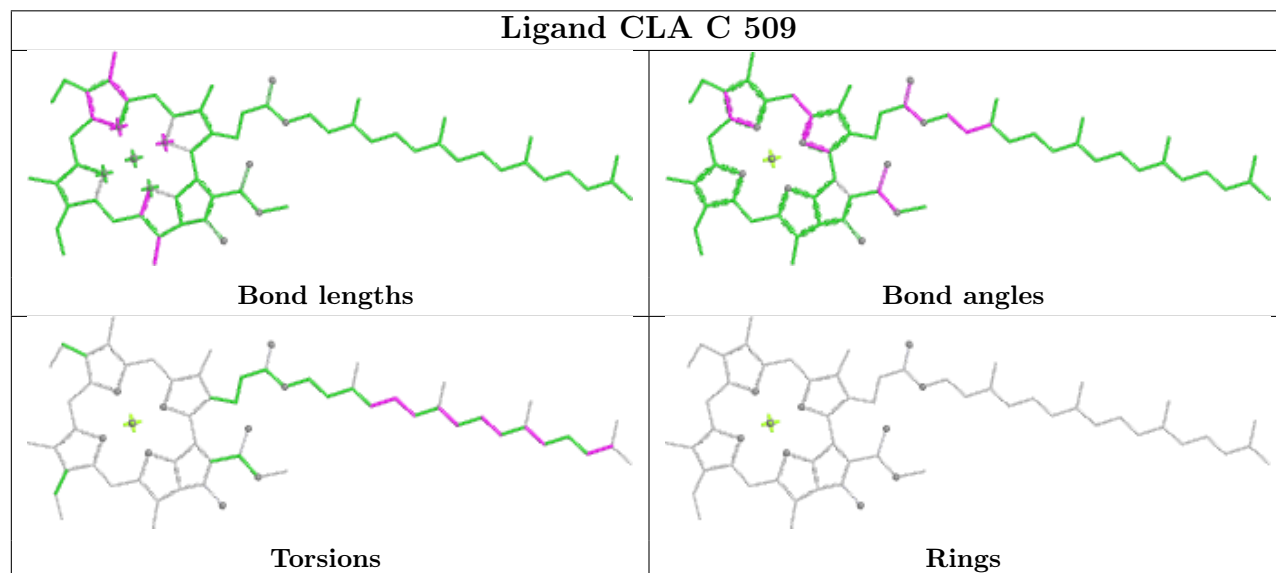
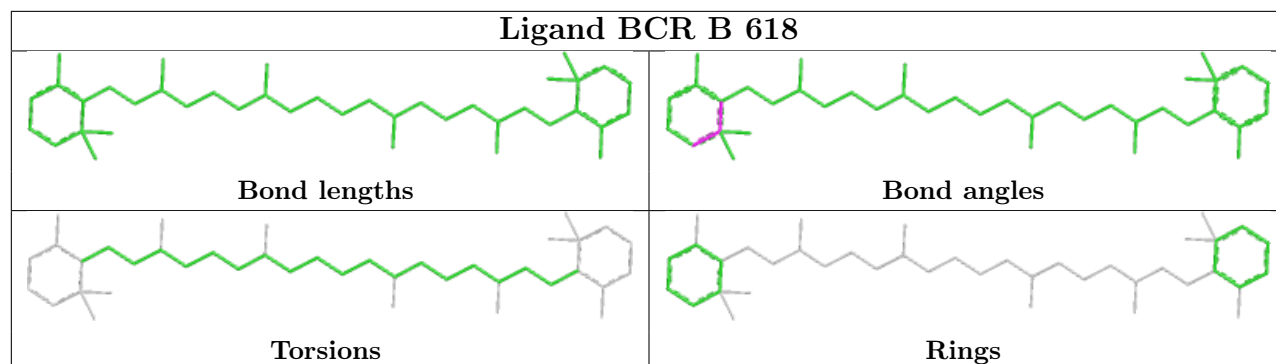


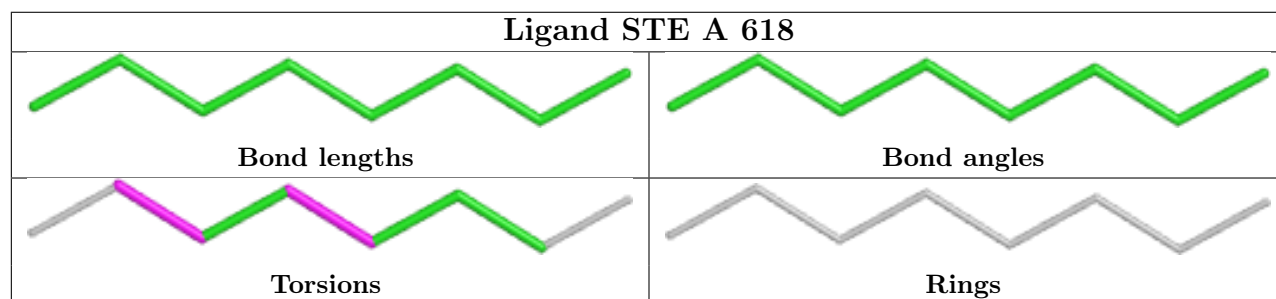
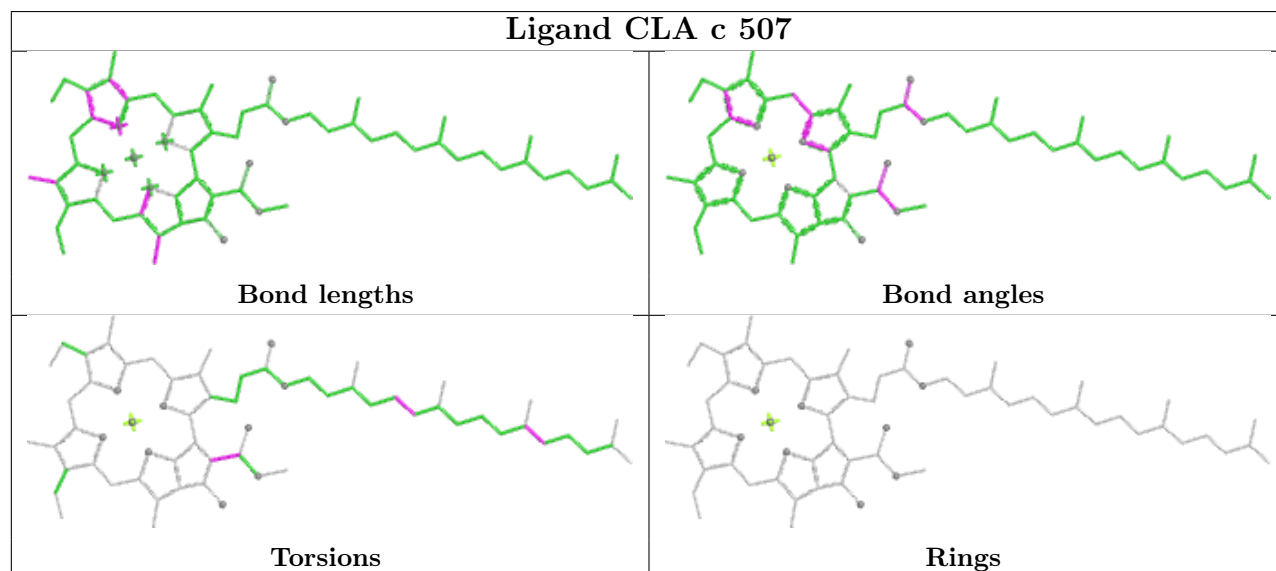
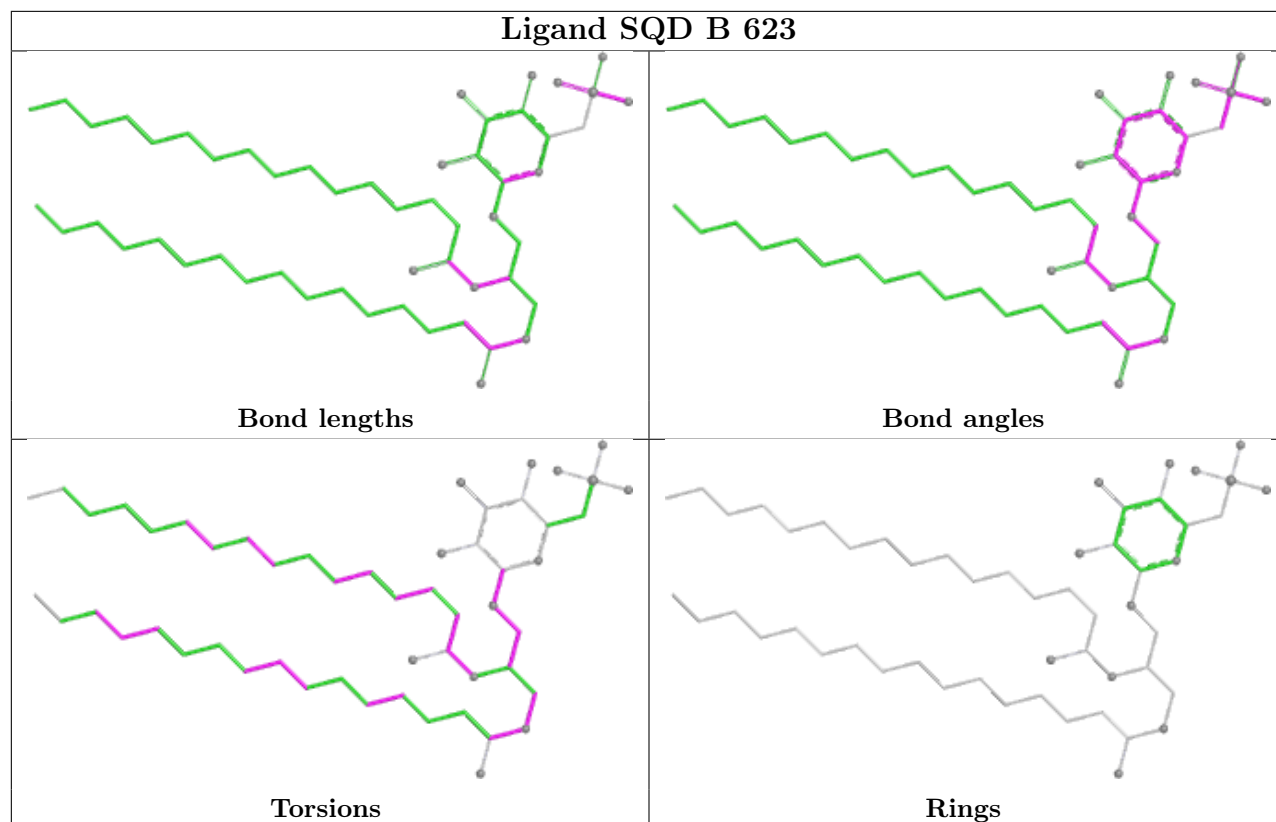
Ligand CLA b 612



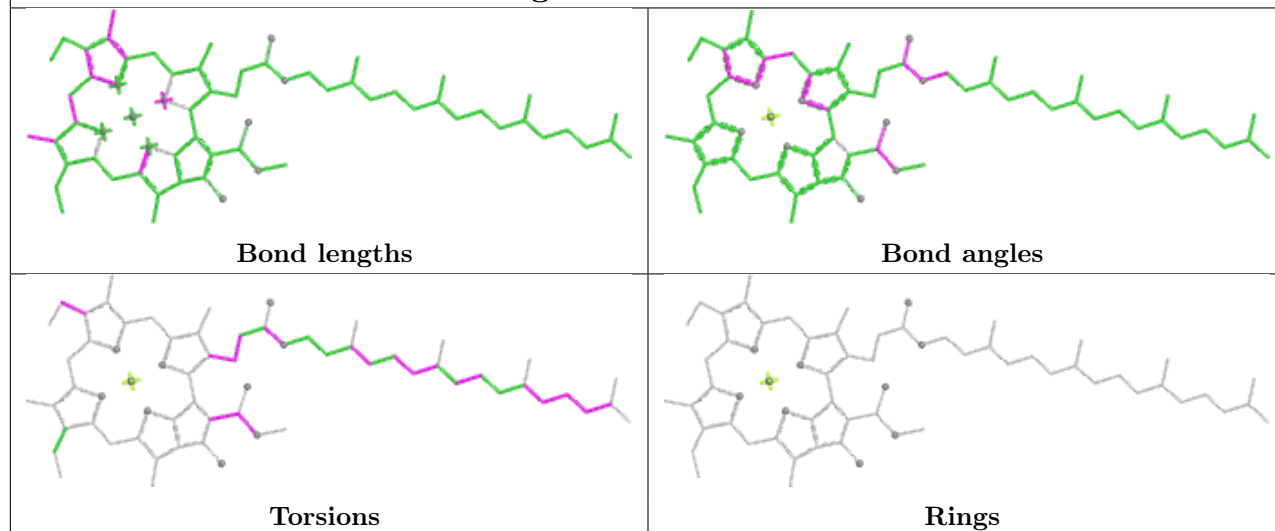
Ligand SQD A 616



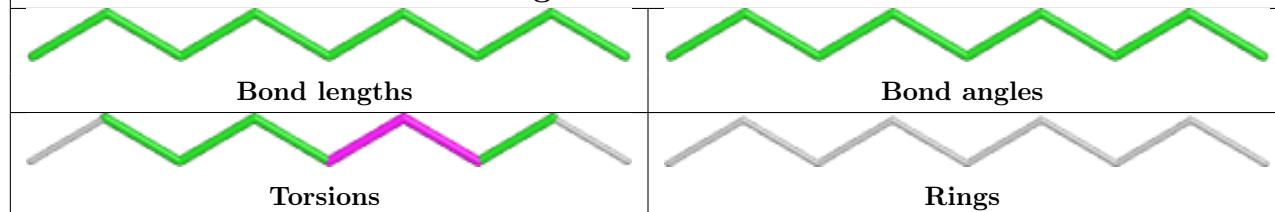




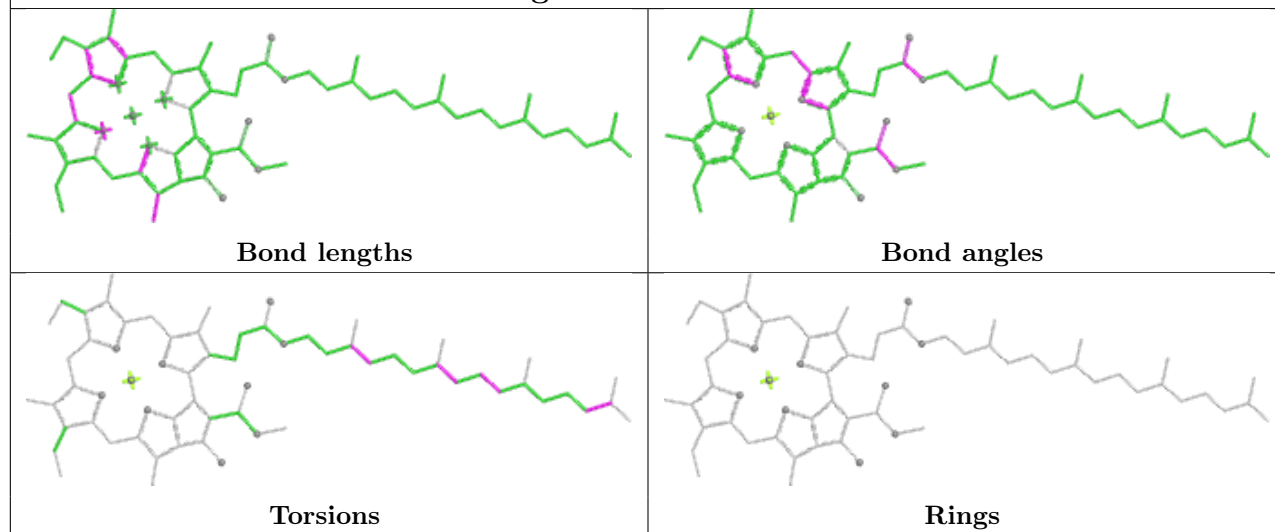
Ligand CLA B 601

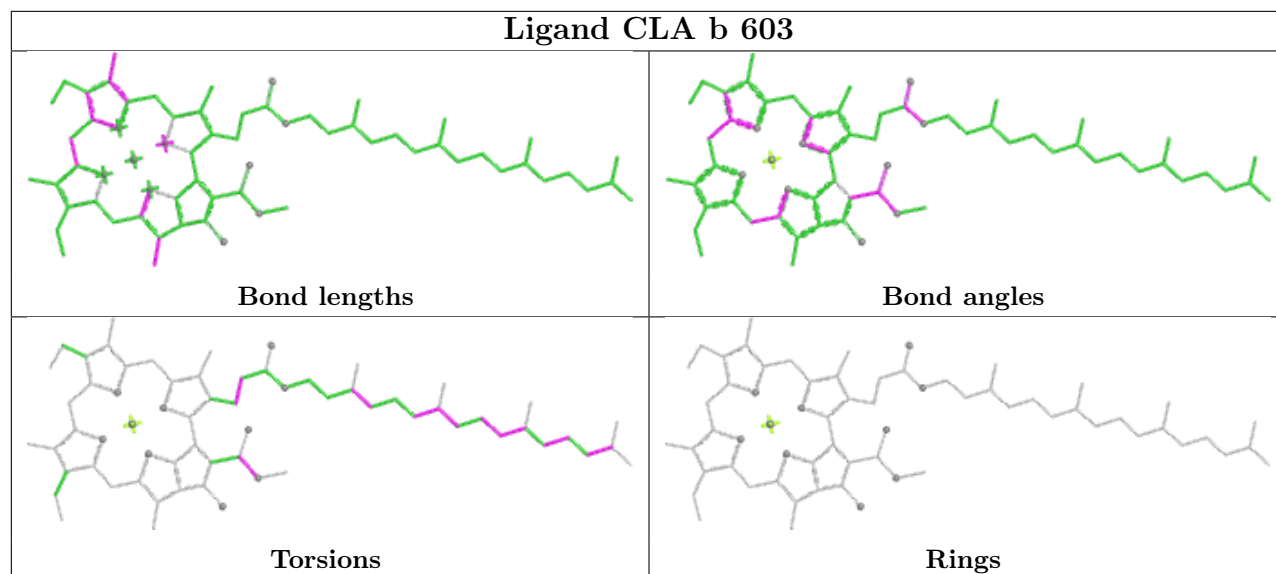
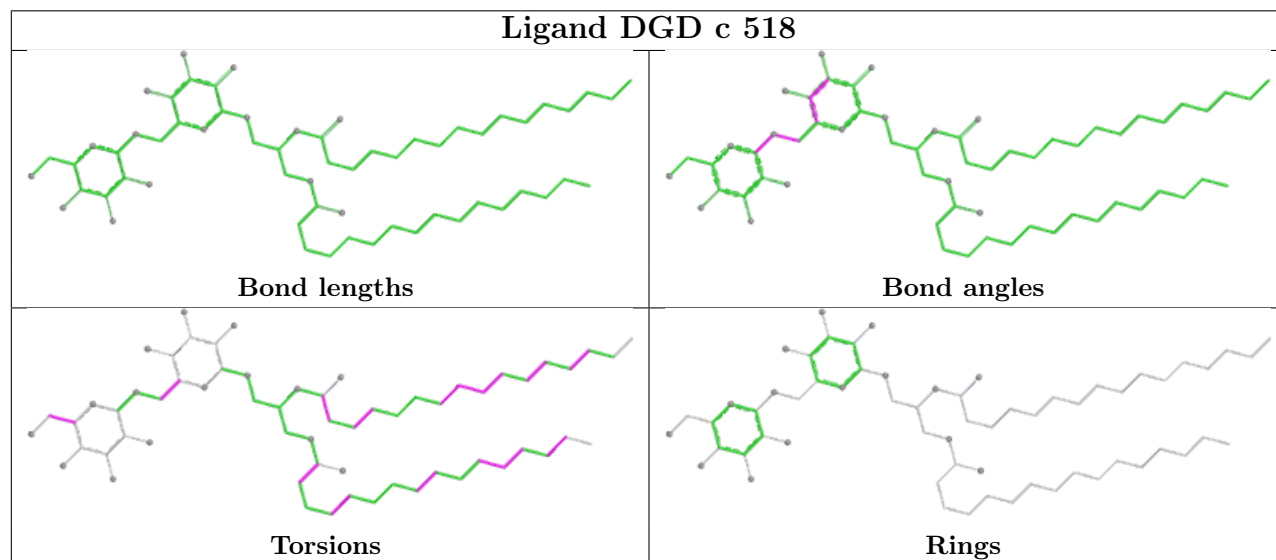


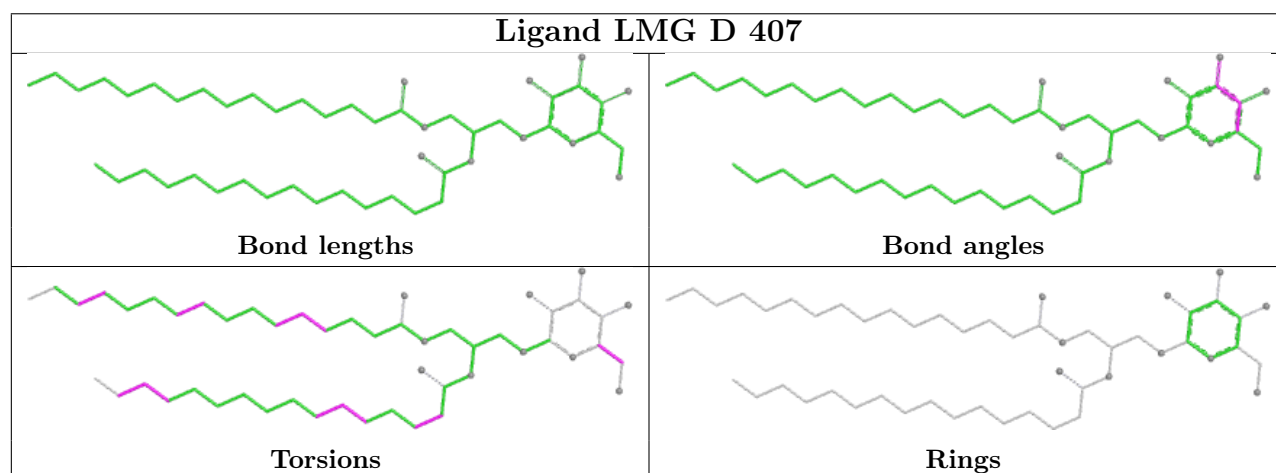
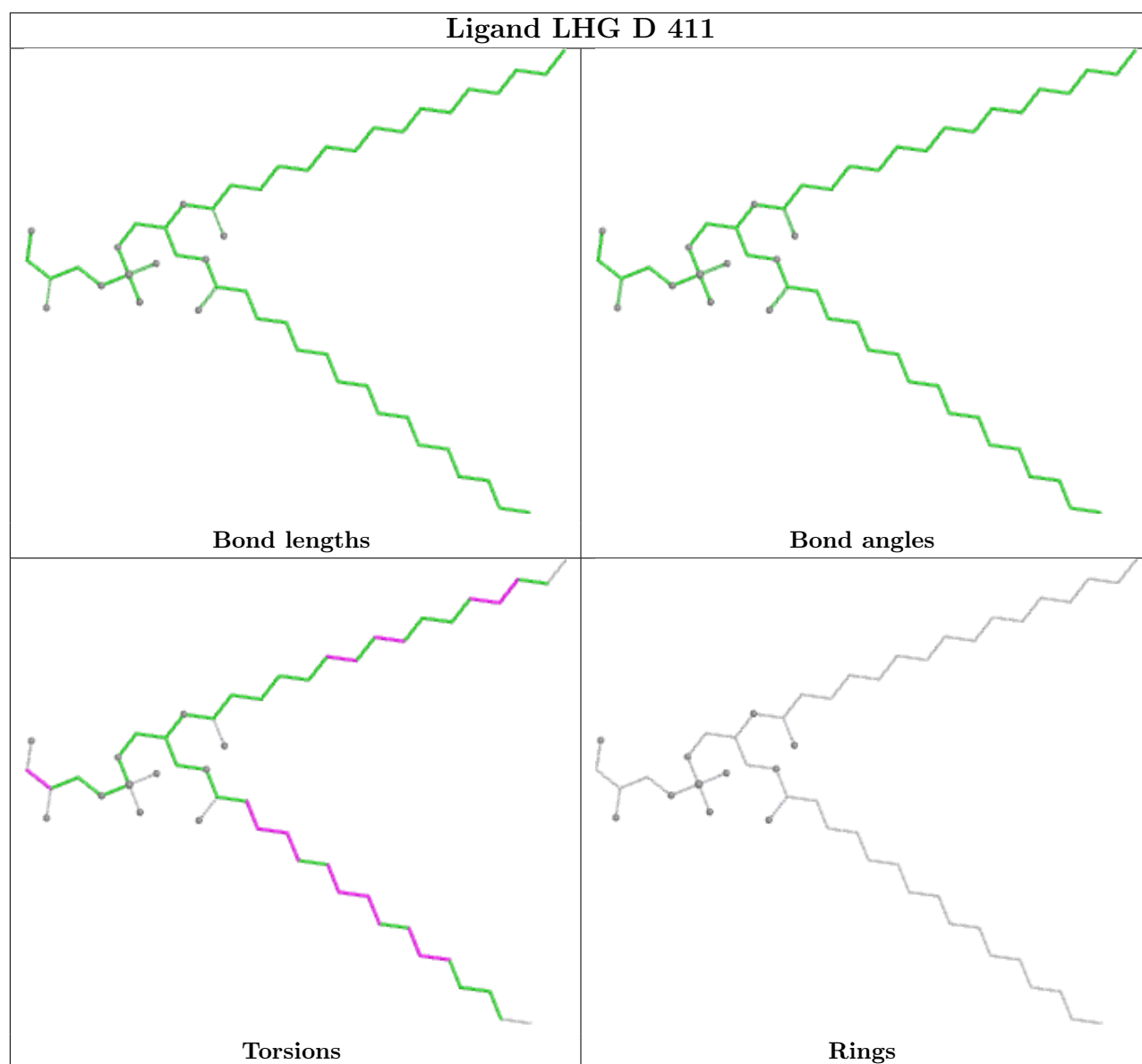
Ligand STE H 104

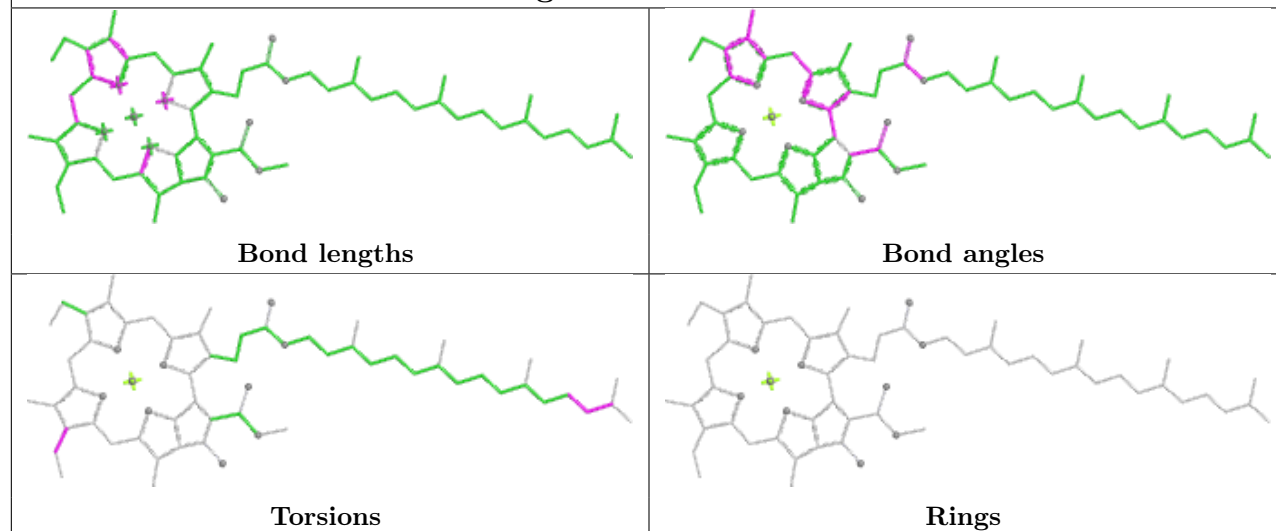
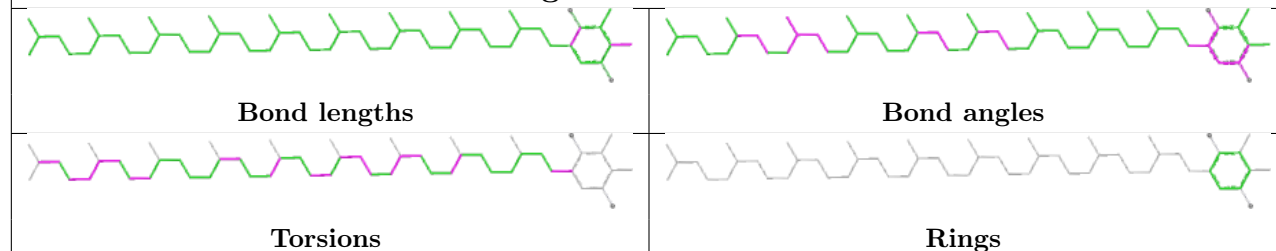
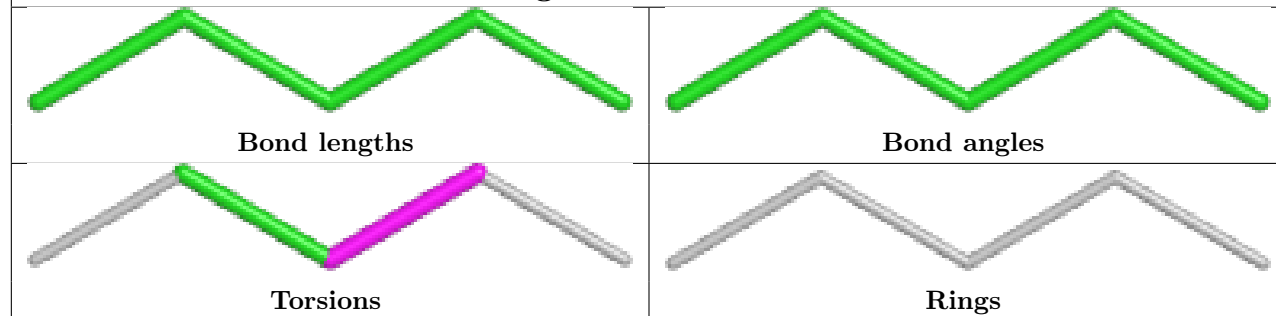


Ligand CLA C 510

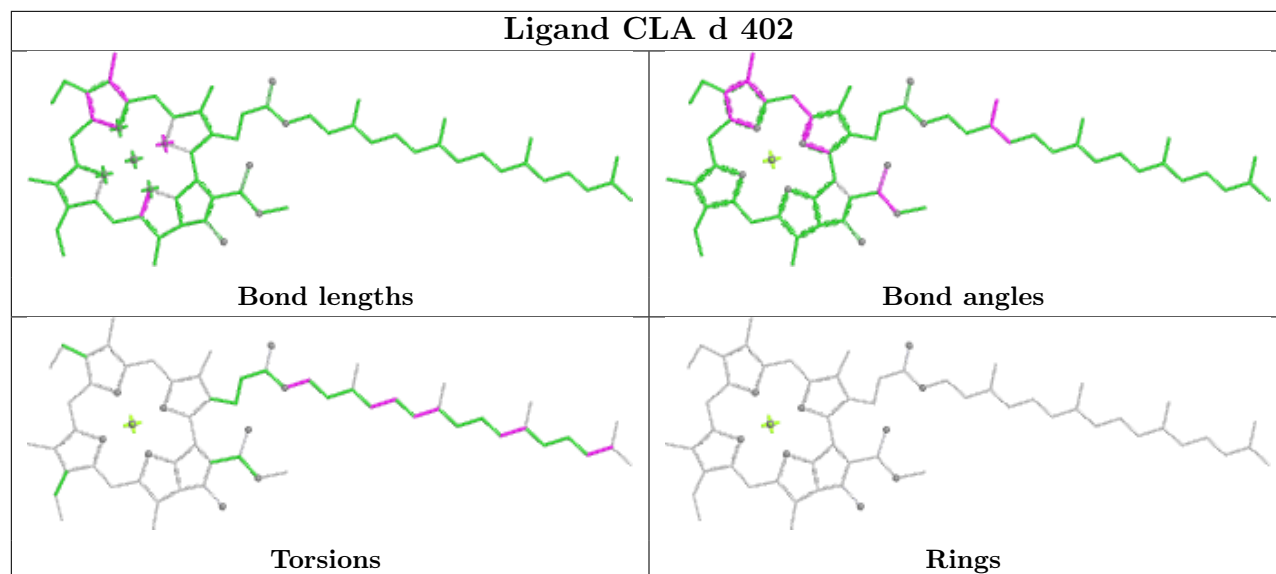


Ligand CLA b 603**Ligand DGD c 518**

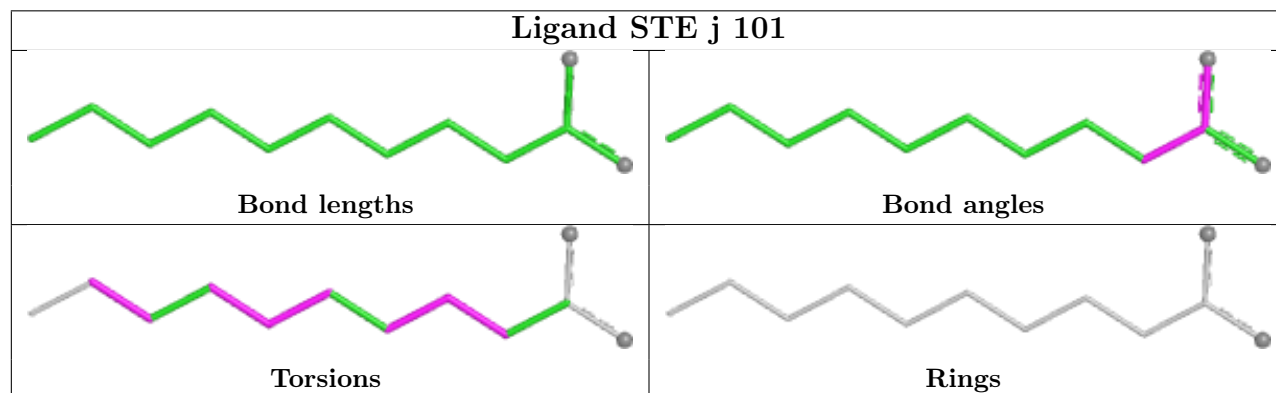


Ligand CLA a 607**Ligand PL9 a 612****Ligand STE C 518**

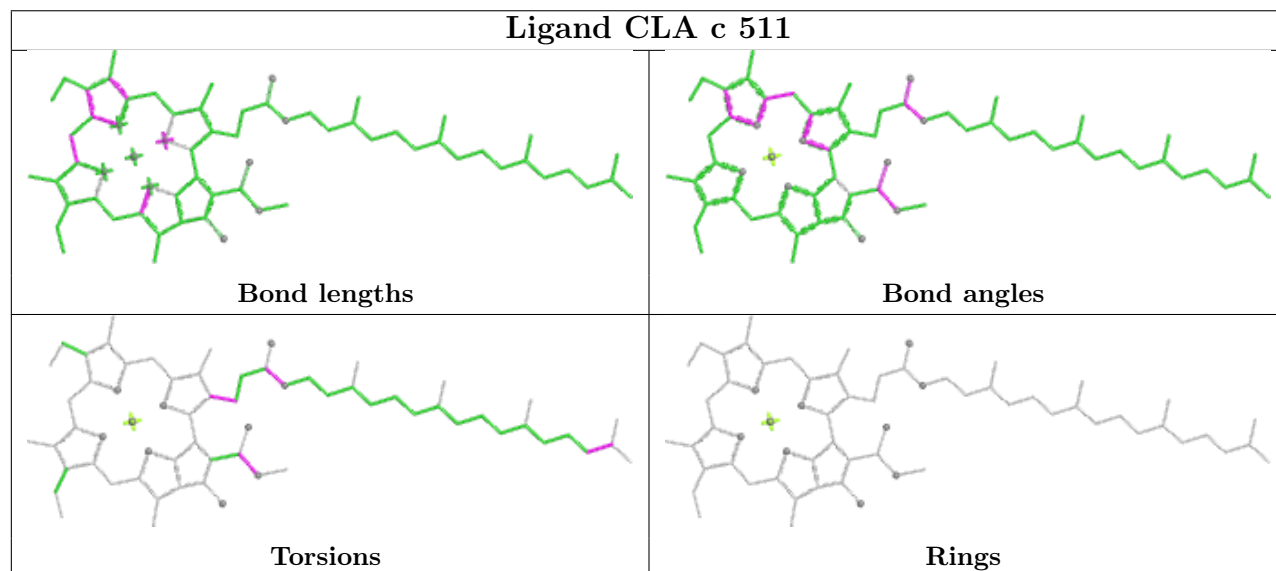
Ligand CLA d 402



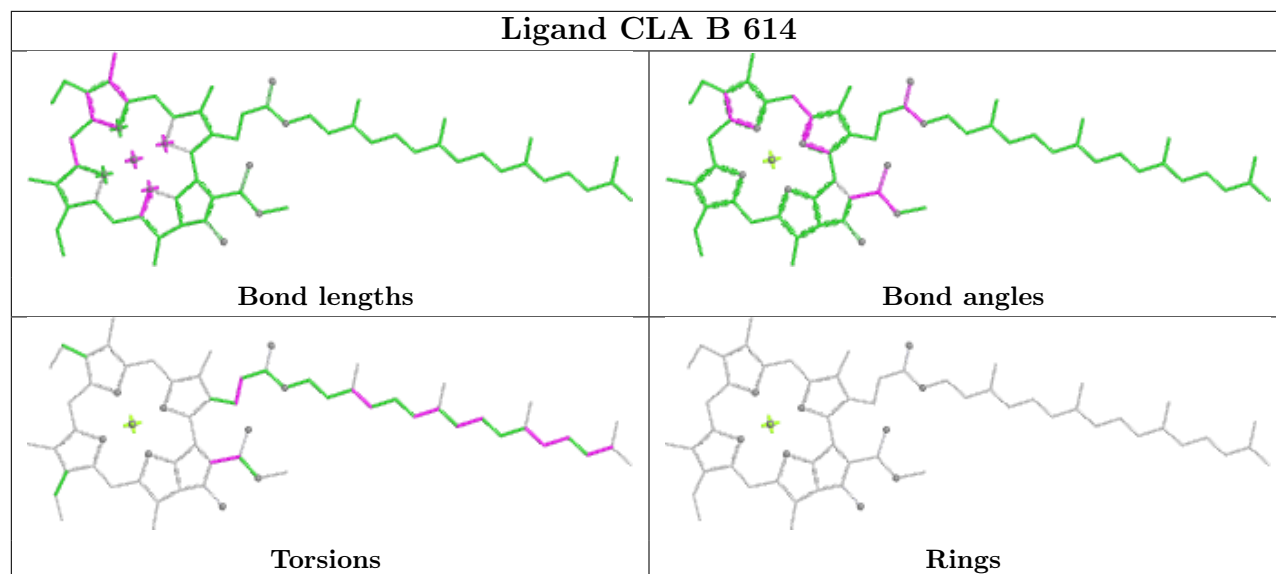
Ligand STE j 101



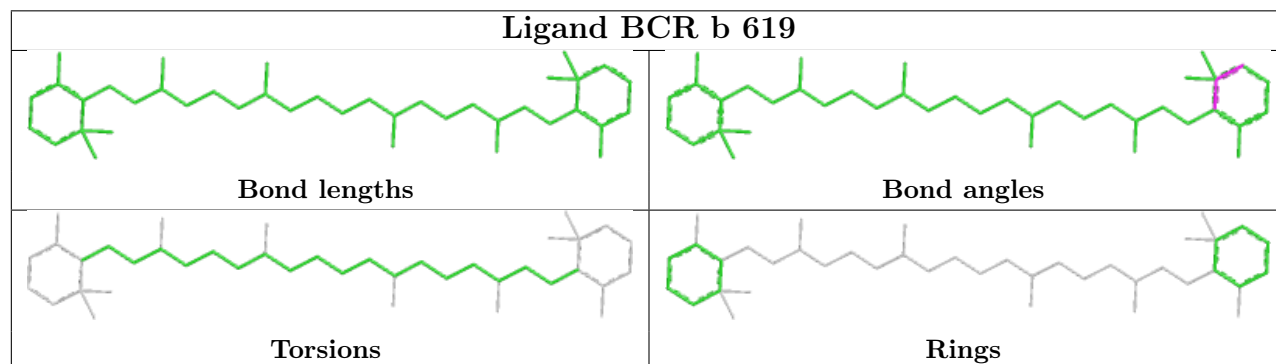
Ligand CLA c 511



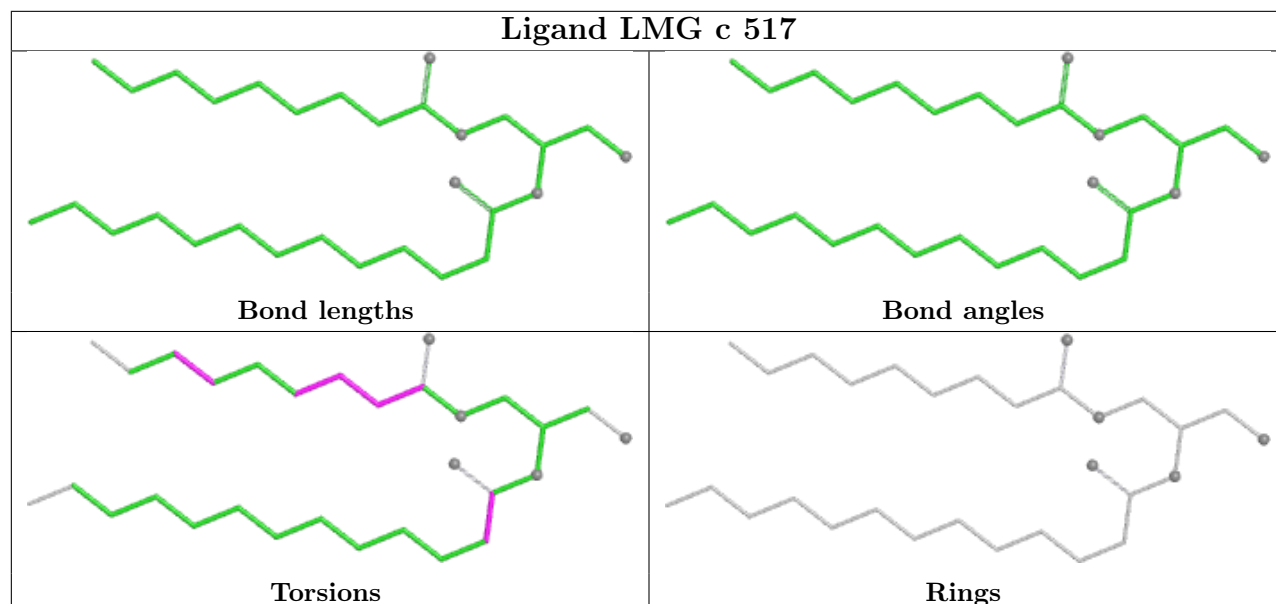
Ligand CLA B 614

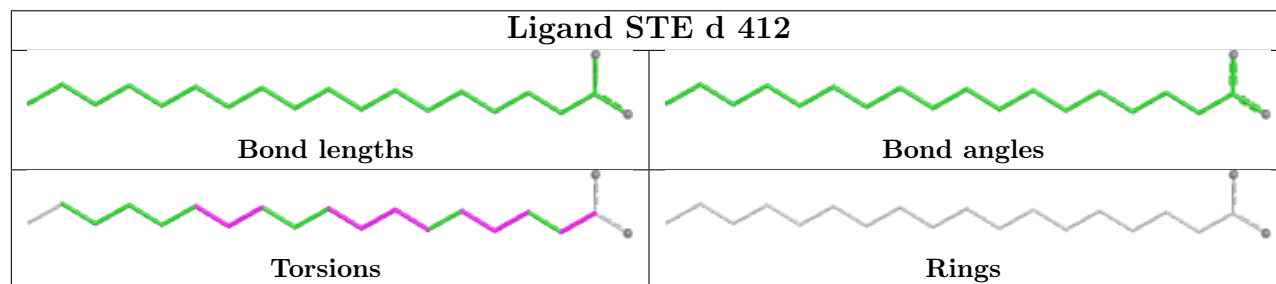
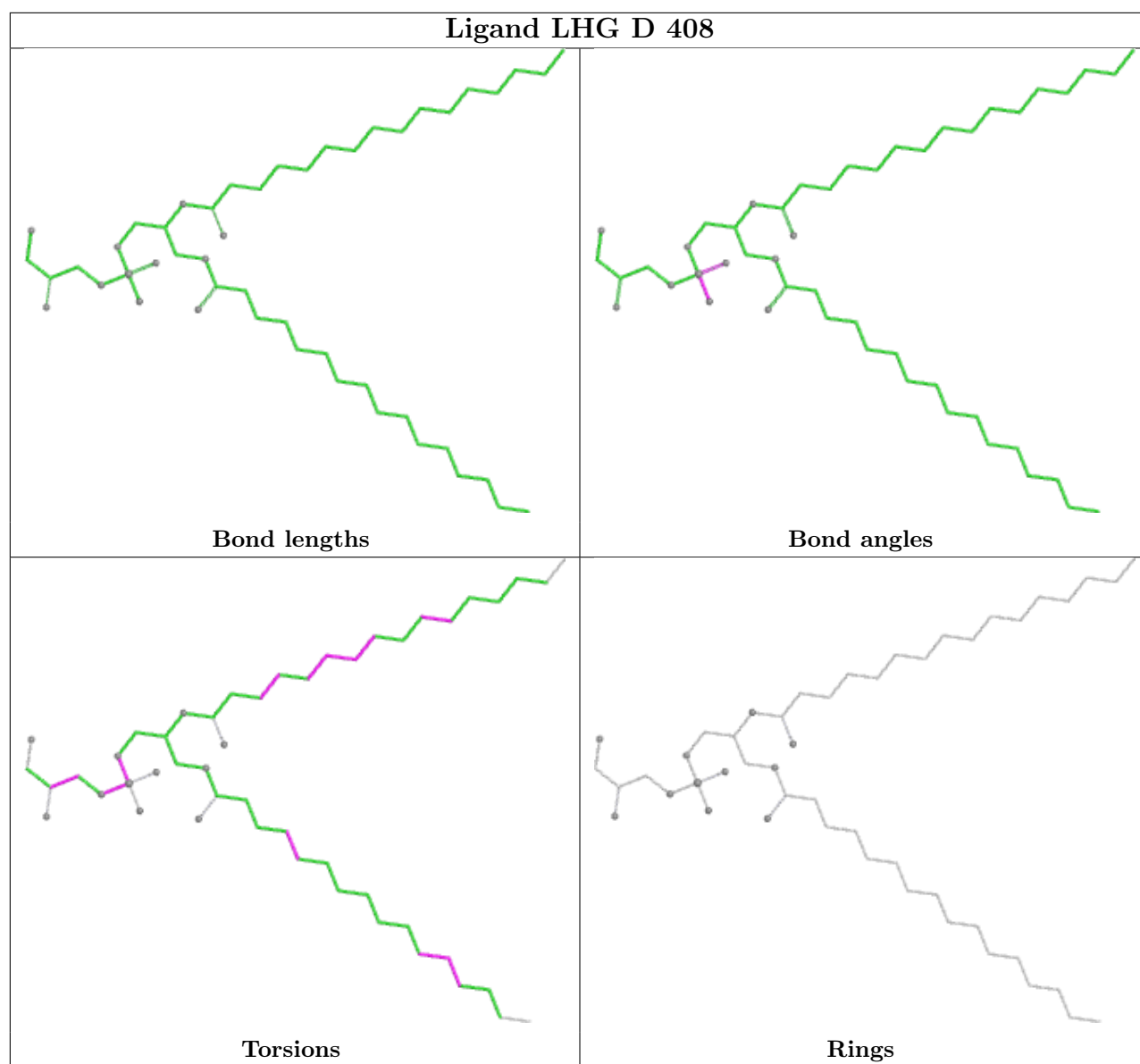


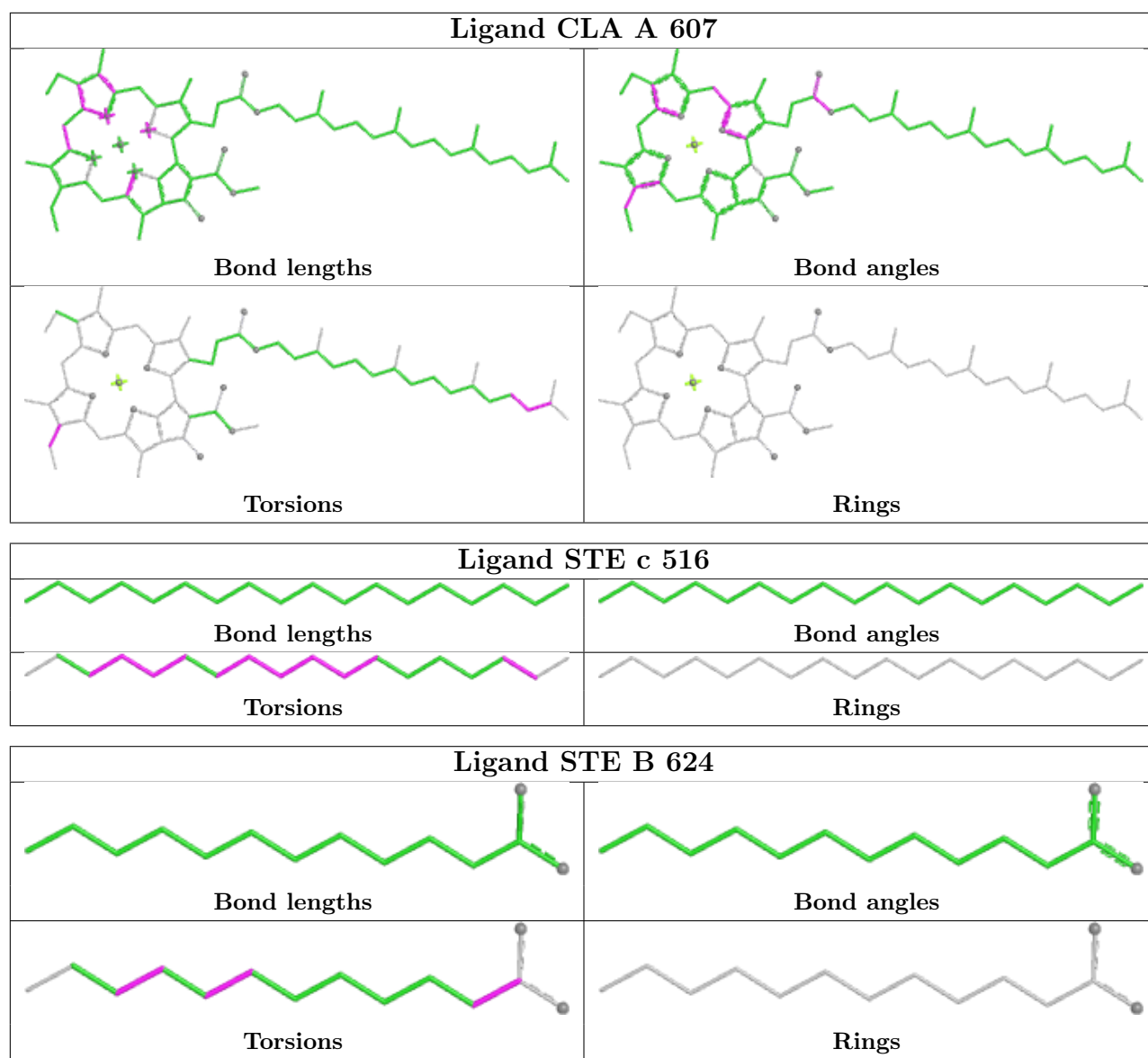
Ligand BCR b 619



Ligand LMG c 517







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%)	-0.57	0 100 100	13, 30, 53, 84	69 (20%)
1	a	334/344 (97%)	-0.48	1 (0%) 90 93	13, 33, 58, 82	69 (20%)
2	B	505/510 (99%)	-0.43	2 (0%) 88 92	18, 35, 63, 100	5 (0%)
2	b	505/510 (99%)	-0.27	4 (0%) 82 87	28, 40, 73, 113	1 (0%)
3	C	442/461 (95%)	-0.39	0 100 100	14, 39, 56, 87	11 (2%)
3	c	451/461 (97%)	-0.25	3 (0%) 84 88	14, 43, 64, 101	12 (2%)
4	D	341/352 (96%)	-0.62	0 100 100	14, 33, 50, 85	10 (2%)
4	d	341/352 (96%)	-0.42	1 (0%) 90 93	14, 37, 60, 81	11 (3%)
5	E	82/84 (97%)	0.23	2 (2%) 59 67	31, 52, 72, 86	1 (1%)
5	e	82/84 (97%)	0.33	2 (2%) 59 67	40, 62, 78, 94	0
6	F	34/45 (75%)	-0.07	0 100 100	38, 46, 64, 88	0
6	f	34/45 (75%)	0.08	0 100 100	44, 52, 79, 96	0
7	H	65/66 (98%)	-0.25	0 100 100	32, 42, 66, 76	0
7	h	63/66 (95%)	0.05	1 (1%) 70 77	39, 51, 67, 74	0
8	I	35/38 (92%)	-0.38	0 100 100	34, 42, 75, 88	0
8	i	35/38 (92%)	-0.27	0 100 100	35, 45, 81, 92	0
9	J	36/40 (90%)	-0.01	0 100 100	38, 53, 77, 102	0
9	j	36/40 (90%)	0.17	1 (2%) 55 62	42, 58, 95, 97	0
10	K	37/46 (80%)	0.04	0 100 100	45, 55, 76, 82	0
10	k	37/46 (80%)	0.21	0 100 100	48, 58, 75, 87	0
11	L	37/37 (100%)	-0.47	0 100 100	27, 33, 67, 75	0
11	l	36/37 (97%)	-0.58	0 100 100	29, 35, 73, 84	0
12	M	32/36 (88%)	-0.26	1 (3%) 51 57	30, 36, 61, 78	0
12	m	31/36 (86%)	-0.36	0 100 100	31, 37, 54, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.15	3 (1%) 76 81	27, 45, 87, 137	1 (0%)
13	o	244/272 (89%)	-0.11	5 (2%) 65 72	26, 45, 86, 136	0
14	T	29/32 (90%)	-0.46	1 (3%) 48 54	28, 35, 65, 85	0
14	t	29/32 (90%)	-0.39	1 (3%) 48 54	30, 35, 78, 83	0
15	U	97/134 (72%)	-0.17	0 100 100	33, 46, 76, 103	0
15	u	97/134 (72%)	-0.26	0 100 100	34, 44, 60, 92	0
16	V	137/163 (84%)	-0.31	1 (0%) 84 88	30, 43, 61, 77	0
16	v	137/163 (84%)	-0.12	0 100 100	34, 50, 73, 88	0
17	Y	27/46 (58%)	1.10	4 (14%) 5 6	57, 79, 104, 107	0
17	y	30/46 (65%)	0.74	1 (3%) 49 55	65, 75, 93, 110	0
18	X	38/41 (92%)	0.04	1 (2%) 57 64	40, 52, 76, 86	0
18	x	39/41 (95%)	0.21	1 (2%) 57 64	47, 60, 82, 102	0
19	Z	62/62 (100%)	0.74	3 (4%) 35 40	56, 72, 119, 127	0
19	z	62/62 (100%)	0.82	4 (6%) 25 28	59, 75, 115, 132	0
20	R	28/41 (68%)	0.61	1 (3%) 46 52	60, 71, 85, 98	0
20	r	28/41 (68%)	1.09	6 (21%) 2 2	68, 86, 100, 110	0
All	All	5293/5700 (92%)	-0.26	50 (0%) 81 85	13, 41, 77, 137	190 (3%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.7
19	z	33	TRP	4.0
2	b	495	PHE	3.9
17	Y	25	ILE	3.7
3	c	24	THR	3.6

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
14	FME	T	1	10/11	0.94	0.08	29,46,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.94	0.08	32,47,68,68	0
8	FME	I	1	10/11	0.96	0.07	40,50,59,63	0
12	FME	M	1	10/11	0.96	0.09	42,50,70,80	0
12	FME	m	1	10/11	0.97	0.07	36,47,75,82	0
8	FME	i	1	10/11	0.97	0.07	39,47,59,62	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
30	STE	C	520	10/20	0.57	0.20	46,73,90,91	0
30	STE	i	101	12/20	0.62	0.14	66,91,107,110	0
30	STE	K	102	14/20	0.66	0.16	60,75,96,98	0
30	STE	C	527	14/20	0.67	0.17	58,84,120,123	0
30	STE	A	620	11/20	0.68	0.18	51,70,96,98	0
30	STE	H	103	18/20	0.70	0.18	48,75,90,90	0
30	STE	e	101	9/20	0.71	0.22	56,81,97,97	0
30	STE	i	102	6/20	0.71	0.22	49,75,83,83	0
30	STE	j	102	16/20	0.71	0.17	56,80,100,102	0
30	STE	e	103	8/20	0.73	0.19	53,66,79,86	0
30	STE	I	101	17/20	0.74	0.15	53,71,83,86	0
30	STE	E	104	20/20	0.74	0.15	52,73,91,93	0
30	STE	a	618	12/20	0.74	0.14	49,72,82,93	0
30	STE	E	103	12/20	0.74	0.15	57,76,107,107	0
30	STE	h	102	10/20	0.75	0.17	59,76,89,91	0
30	STE	C	518	5/20	0.76	0.17	48,61,73,73	0
30	STE	A	619	17/20	0.76	0.14	55,77,95,97	0
30	STE	C	516	14/20	0.76	0.16	52,70,81,86	0
30	STE	t	102	10/20	0.76	0.17	44,65,76,77	0
30	STE	c	516	18/20	0.77	0.16	62,85,102,105	0
30	STE	Z	102	17/20	0.77	0.18	50,80,102,103	0
31	LMG	D	406	50/55	0.77	0.16	42,66,117,137	0
31	LMG	c	517	30/55	0.77	0.14	40,79,117,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	PL9	a	612	55/55	0.78	0.16	45,70,89,96	0
34	LHG	e	102	42/49	0.78	0.15	53,86,122,141	0
31	LMG	b	622	55/55	0.79	0.16	53,74,100,104	0
31	LMG	C	517	36/55	0.79	0.15	42,60,84,94	0
31	LMG	a	616	55/55	0.79	0.14	38,64,87,99	0
30	STE	e	104	9/20	0.80	0.17	60,75,91,92	0
33	DGD	A	617	66/66	0.80	0.14	48,68,97,105	0
29	PL9	A	612	55/55	0.80	0.16	39,69,86,90	0
30	STE	k	103	14/20	0.81	0.12	59,74,87,88	0
31	LMG	c	522	48/55	0.81	0.14	50,78,99,110	0
30	STE	e	105	13/20	0.82	0.16	67,85,93,100	0
34	LHG	E	101	49/49	0.82	0.14	48,77,111,120	0
30	STE	z	701	13/20	0.82	0.14	59,75,85,87	0
30	STE	z	702	9/20	0.83	0.20	55,71,79,84	0
30	STE	d	410	20/20	0.83	0.12	51,68,89,90	0
30	STE	B	627	15/20	0.83	0.18	35,64,74,86	0
30	STE	B	626	12/20	0.83	0.14	43,65,79,81	0
30	STE	C	526	16/20	0.83	0.12	40,56,68,72	0
30	STE	C	519	7/20	0.84	0.13	50,64,74,74	0
30	STE	A	613	9/20	0.84	0.16	49,71,82,83	0
30	STE	b	624	10/20	0.85	0.12	40,58,78,86	0
30	STE	T	103	15/20	0.85	0.15	46,62,92,94	0
30	STE	E	102	12/20	0.85	0.14	53,74,88,89	0
30	STE	T	102	16/20	0.85	0.17	38,54,107,111	0
30	STE	C	525	12/20	0.86	0.13	34,47,58,59	0
31	LMG	B	620	45/55	0.86	0.13	37,59,107,132	0
32	SQD	a	615	54/54	0.86	0.12	43,67,104,119	0
30	STE	b	625	11/20	0.87	0.13	54,67,71,75	0
31	LMG	A	615	48/55	0.87	0.12	40,60,81,90	0
30	STE	I	102	15/20	0.87	0.12	42,56,77,81	0
32	SQD	A	616	43/54	0.87	0.11	41,61,101,108	0
30	STE	A	618	8/20	0.88	0.12	50,61,74,74	0
30	STE	B	625	18/20	0.88	0.11	44,58,83,88	0
30	STE	j	101	12/20	0.88	0.11	49,59,71,71	0
31	LMG	c	521	46/55	0.88	0.11	41,68,82,83	0
30	STE	b	623	16/20	0.88	0.13	49,63,78,79	0
30	STE	H	104	9/20	0.89	0.12	51,64,74,76	0
32	SQD	B	623	54/54	0.89	0.10	38,60,90,96	0
30	STE	b	621	20/20	0.89	0.09	36,57,76,77	0
32	SQD	b	620	49/54	0.89	0.10	42,58,84,95	0
32	SQD	f	102	41/54	0.89	0.12	52,78,95,97	0
30	STE	J	101	12/20	0.89	0.11	45,58,68,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMG	C	524	48/55	0.89	0.12	44,73,97,104	0
30	STE	B	624	14/20	0.89	0.10	38,53,61,65	0
30	STE	B	621	17/20	0.90	0.10	37,54,67,67	0
31	LMG	a	617	49/55	0.90	0.10	37,61,86,100	0
31	LMG	m	101	51/55	0.90	0.10	37,53,72,81	0
30	STE	d	412	20/20	0.90	0.10	39,55,71,72	0
31	LMG	M	101	51/55	0.90	0.10	31,53,73,79	0
32	SQD	a	614	54/54	0.90	0.11	43,67,94,96	0
26	CLA	b	601	65/65	0.91	0.10	42,65,91,113	0
30	STE	D	412	20/20	0.91	0.10	34,50,65,73	0
30	STE	d	406	20/20	0.91	0.09	40,55,72,74	0
30	STE	m	102	12/20	0.91	0.11	46,59,77,77	0
30	STE	m	103	18/20	0.91	0.10	37,50,77,81	0
28	BCR	c	514	40/40	0.92	0.10	51,64,73,77	0
32	SQD	D	410	52/54	0.92	0.10	31,63,98,105	0
26	CLA	c	513	65/65	0.92	0.11	46,70,103,111	0
28	BCR	d	404	40/40	0.93	0.08	36,52,85,86	0
28	BCR	k	101	40/40	0.93	0.09	45,59,70,73	0
32	SQD	F	102	36/54	0.93	0.10	43,70,88,92	0
30	STE	M	102	15/20	0.93	0.09	39,51,59,71	0
30	STE	M	103	10/20	0.93	0.09	40,50,57,62	0
26	CLA	c	512	65/65	0.93	0.09	42,60,93,99	0
26	CLA	C	513	65/65	0.93	0.09	43,66,99,107	0
28	BCR	C	514	40/40	0.93	0.09	43,58,68,70	0
33	DGD	C	522	62/66	0.93	0.09	33,50,94,108	0
28	BCR	Z	101	40/40	0.93	0.08	38,55,73,75	0
26	CLA	B	601	65/65	0.93	0.10	27,54,87,92	0
26	CLA	c	503	65/65	0.94	0.07	33,46,55,63	0
28	BCR	b	618	40/40	0.94	0.07	28,41,55,61	0
28	BCR	B	618	40/40	0.94	0.07	26,40,52,54	0
28	BCR	c	515	40/40	0.94	0.09	30,45,60,68	0
26	CLA	C	503	65/65	0.94	0.07	32,43,52,55	0
28	BCR	H	101	40/40	0.94	0.07	29,42,56,59	0
31	LMG	D	407	51/55	0.94	0.10	30,58,94,98	0
33	DGD	H	102	62/66	0.94	0.08	28,42,55,59	0
33	DGD	c	519	62/66	0.94	0.08	34,50,90,94	0
33	DGD	h	101	62/66	0.94	0.08	31,48,59,61	0
34	LHG	D	411	49/49	0.94	0.10	30,46,70,79	0
28	BCR	k	102	40/40	0.94	0.09	44,56,66,80	0
34	LHG	d	407	49/49	0.94	0.09	32,52,78,83	0
28	BCR	x	101	40/40	0.94	0.07	37,49,62,65	0
28	BCR	T	101	40/40	0.95	0.06	26,40,54,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	b	616	60/65	0.95	0.08	29,46,91,94	0
28	BCR	b	617	40/40	0.95	0.06	30,42,51,53	0
26	CLA	C	510	65/65	0.95	0.07	32,46,67,77	0
28	BCR	b	619	40/40	0.95	0.07	30,48,64,66	0
26	CLA	c	508	64/65	0.95	0.08	34,45,101,124	0
26	CLA	c	509	65/65	0.95	0.09	33,49,66,69	0
26	CLA	c	511	65/65	0.95	0.08	40,55,71,73	0
26	CLA	C	511	65/65	0.95	0.08	36,51,67,69	0
26	CLA	C	512	65/65	0.95	0.09	37,55,90,100	0
28	BCR	t	101	40/40	0.95	0.06	30,41,52,56	0
27	PHO	d	401	64/64	0.95	0.07	29,38,47,52	0
28	BCR	A	611	40/40	0.95	0.06	27,38,45,46	0
33	DGD	C	523	62/66	0.95	0.08	29,46,80,96	0
26	CLA	C	506	65/65	0.95	0.08	27,42,89,107	0
28	BCR	B	619	40/40	0.95	0.07	27,42,58,66	0
33	DGD	c	520	62/66	0.95	0.08	30,50,73,95	0
26	CLA	C	509	65/65	0.95	0.08	29,45,65,68	0
34	LHG	D	409	47/49	0.95	0.09	29,48,82,98	0
28	BCR	C	515	40/40	0.95	0.07	27,40,54,61	0
28	BCR	D	404	40/40	0.95	0.08	30,46,92,105	0
26	CLA	b	606	65/65	0.95	0.07	29,40,73,81	0
34	LHG	d	409	39/49	0.95	0.09	33,46,74,83	0
28	BCR	K	101	40/40	0.95	0.08	40,52,66,71	0
27	PHO	A	609	64/64	0.96	0.06	20,30,39,44	0
27	PHO	D	401	64/64	0.96	0.06	23,33,43,46	0
27	PHO	a	609	64/64	0.96	0.06	22,33,39,43	0
26	CLA	b	602	65/65	0.96	0.07	27,41,60,66	0
26	CLA	B	610	65/65	0.96	0.07	23,34,44,47	0
28	BCR	B	617	40/40	0.96	0.06	27,40,52,56	0
26	CLA	b	608	65/65	0.96	0.06	27,42,62,63	0
26	CLA	b	609	65/65	0.96	0.07	30,44,61,71	0
31	LMG	d	411	44/55	0.96	0.08	34,53,82,93	0
26	CLA	b	610	65/65	0.96	0.08	27,39,53,56	0
26	CLA	b	611	65/65	0.96	0.07	25,35,53,56	0
26	CLA	b	614	65/65	0.96	0.07	26,41,78,84	0
26	CLA	b	615	65/65	0.96	0.07	27,40,65,75	0
26	CLA	C	502	65/65	0.96	0.06	29,42,57,68	0
26	CLA	c	501	65/65	0.96	0.07	29,41,53,62	0
26	CLA	c	502	65/65	0.96	0.06	30,43,64,69	0
28	BCR	a	611	40/40	0.96	0.06	26,36,46,50	0
25	BCT	a	606	4/4	0.96	0.07	36,39,46,56	0
26	CLA	c	504	60/65	0.96	0.07	30,45,82,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	DGD	C	521	62/66	0.96	0.08	26,42,75,90	0
26	CLA	c	505	65/65	0.96	0.07	31,42,69,72	0
26	CLA	c	506	65/65	0.96	0.09	32,49,105,112	0
26	CLA	c	507	65/65	0.96	0.07	31,45,58,63	0
33	DGD	c	518	62/66	0.96	0.08	24,40,76,80	0
26	CLA	C	504	59/65	0.96	0.07	29,41,94,100	0
26	CLA	C	505	65/65	0.96	0.08	28,39,68,74	0
26	CLA	c	510	65/65	0.96	0.07	32,47,64,75	0
26	CLA	a	608	65/65	0.96	0.08	27,39,100,110	0
26	CLA	a	610	65/65	0.96	0.08	21,37,90,100	0
26	CLA	B	606	65/65	0.96	0.07	23,36,72,82	0
29	PL9	D	405	55/55	0.96	0.06	22,34,45,46	0
26	CLA	d	403	65/65	0.96	0.08	31,49,89,100	0
29	PL9	d	405	55/55	0.96	0.06	24,36,46,53	0
34	LHG	l	101	49/49	0.96	0.08	32,47,61,75	0
26	CLA	B	612	65/65	0.97	0.06	22,33,46,55	0
26	CLA	B	613	65/65	0.97	0.06	22,32,75,85	0
26	CLA	b	603	65/65	0.97	0.06	25,37,66,70	0
26	CLA	b	604	65/65	0.97	0.07	25,35,79,99	0
26	CLA	b	605	65/65	0.97	0.06	25,37,52,57	0
26	CLA	B	614	65/65	0.97	0.08	23,38,80,89	0
26	CLA	b	607	65/65	0.97	0.08	22,38,75,86	0
26	CLA	B	615	65/65	0.97	0.07	24,38,67,74	0
26	CLA	B	616	60/65	0.97	0.08	26,40,92,106	0
26	CLA	C	501	65/65	0.97	0.06	25,37,49,55	0
26	CLA	A	610	54/65	0.97	0.06	22,35,67,71	0
26	CLA	b	612	65/65	0.97	0.07	23,38,50,60	0
26	CLA	b	613	65/65	0.97	0.07	20,35,80,89	0
26	CLA	A	614	65/65	0.97	0.06	21,29,52,69	0
25	BCT	A	606	4/4	0.97	0.08	25,30,35,42	0
26	CLA	B	602	65/65	0.97	0.06	25,34,59,65	0
26	CLA	B	603	65/65	0.97	0.06	22,32,58,58	0
26	CLA	C	507	65/65	0.97	0.06	26,42,56,61	0
26	CLA	C	508	65/65	0.97	0.07	29,42,121,129	0
26	CLA	B	604	65/65	0.97	0.07	21,32,77,83	0
26	CLA	B	605	65/65	0.97	0.06	22,33,49,53	0
26	CLA	A	607	65/65	0.97	0.06	19,29,49,59	0
26	CLA	B	607	65/65	0.97	0.06	21,35,64,75	0
26	CLA	B	608	65/65	0.97	0.06	21,35,52,64	0
34	LHG	B	622	49/49	0.97	0.07	28,43,56,68	0
34	LHG	D	408	49/49	0.97	0.06	27,41,50,58	0
26	CLA	D	402	65/65	0.97	0.06	20,31,57,62	0

Continued on next page...

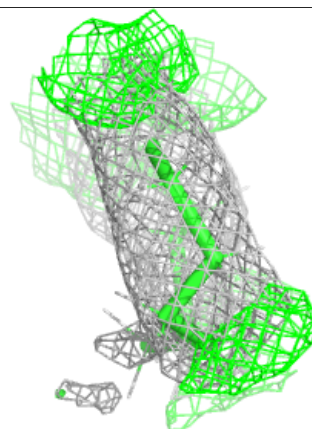
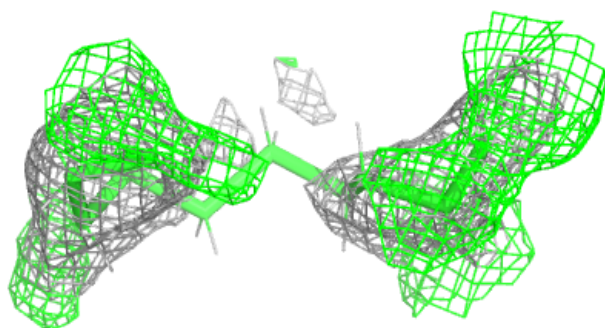
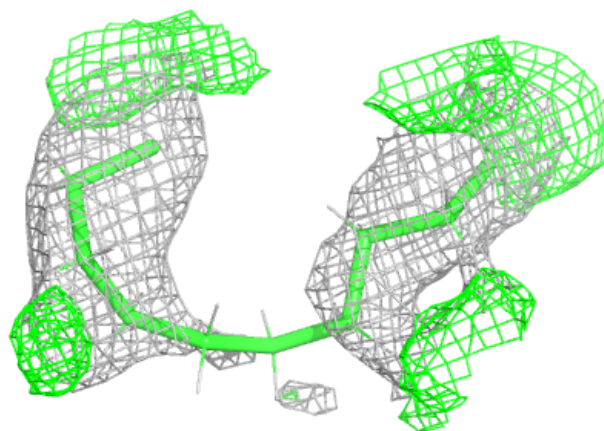
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	CLA	D	403	65/65	0.97	0.07	25,40,119,132	0
26	CLA	a	607	65/65	0.97	0.06	20,31,49,61	0
26	CLA	B	609	65/65	0.97	0.06	25,37,56,64	0
34	LHG	d	408	49/49	0.97	0.07	26,44,58,69	0
26	CLA	A	608	65/65	0.97	0.09	24,35,102,111	0
26	CLA	d	402	65/65	0.97	0.06	23,33,61,69	0
26	CLA	a	613	65/65	0.97	0.06	22,31,49,54	0
35	HEM	F	101	43/43	0.97	0.07	35,46,61,68	0
35	HEM	f	101	43/43	0.97	0.08	44,56,71,73	0
26	CLA	B	611	65/65	0.98	0.05	20,32,51,55	0
24	CL	A	605	1/1	0.99	0.07	26,26,26,26	0
24	CL	a	604	1/1	0.99	0.04	26,26,26,26	0
21	OEY	A	601[B]	11/11	0.99	0.03	22,26,29,30	11
22	OEX	A	602[A]	10/10	0.99	0.03	26,27,30,30	10
22	OEX	a	602[A]	10/10	0.99	0.02	25,27,31,31	10
23	FE2	a	603	1/1	0.99	0.02	35,35,35,35	0
24	CL	A	604	1/1	0.99	0.02	27,27,27,27	0
36	HEC	V	201	43/43	0.99	0.05	26,33,41,42	0
36	HEC	v	201	43/43	0.99	0.05	29,38,47,47	0
24	CL	a	605	1/1	1.00	0.06	29,29,29,29	0
21	OEY	a	601[B]	11/11	1.00	0.02	23,27,30,30	11
23	FE2	A	603	1/1	1.00	0.01	28,28,28,28	0

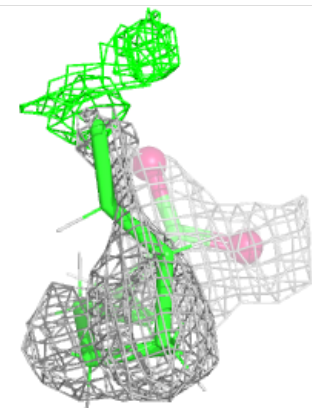
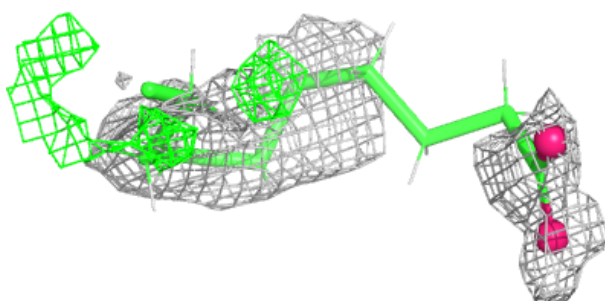
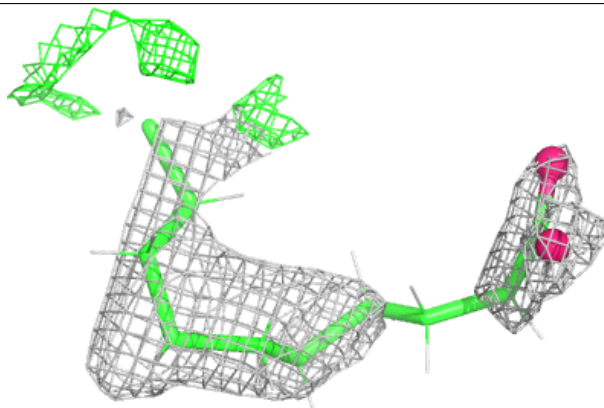
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

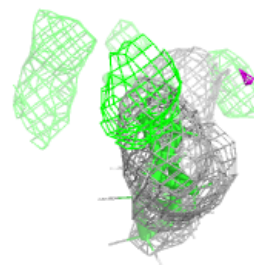
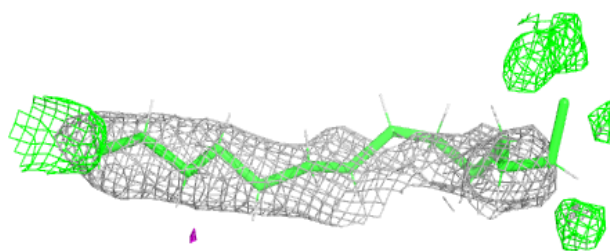
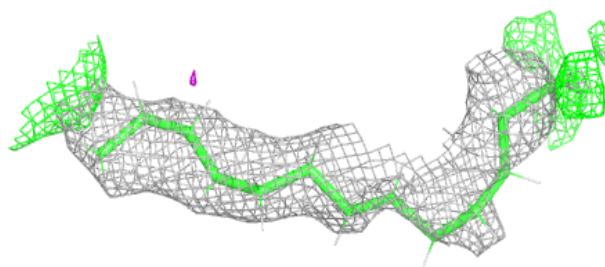
**Electron density around STE i 101:**

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

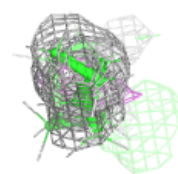
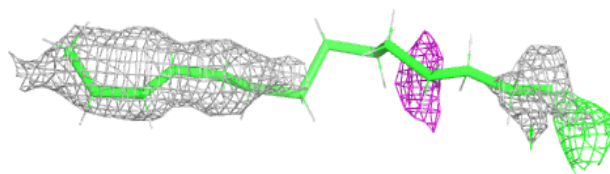
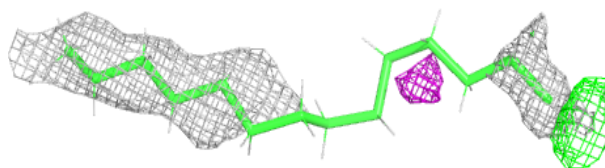


Electron density around STE K 102:

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

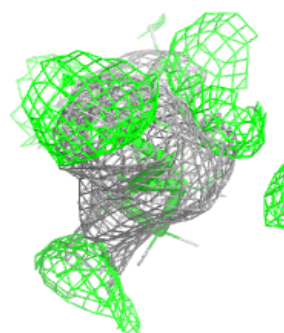
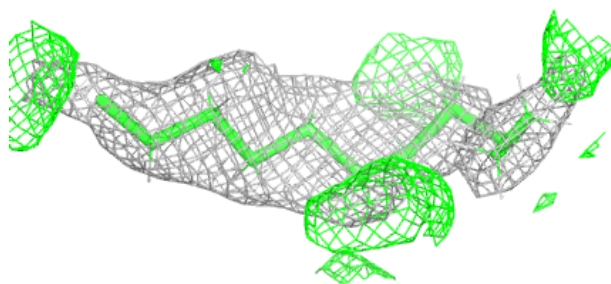
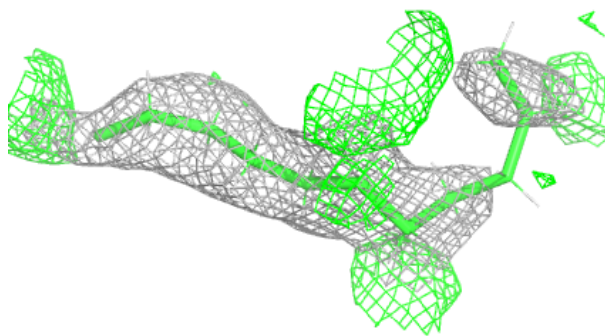
**Electron density around STE C 527:**

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

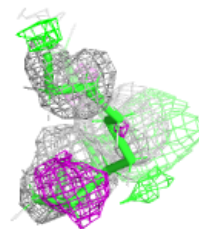
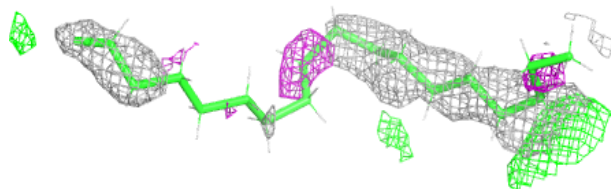
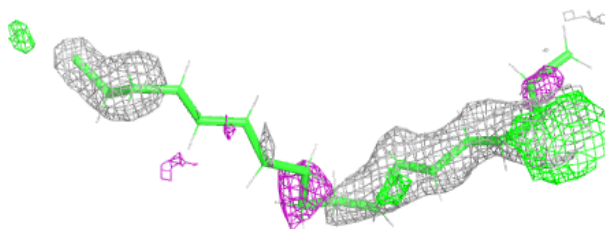


Electron density around STE A 620:

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

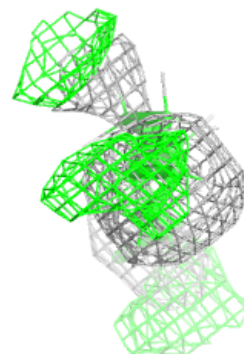
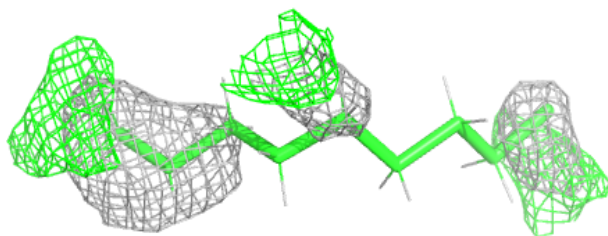
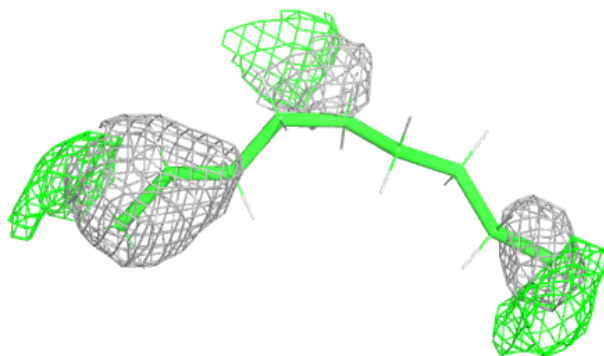
**Electron density around STE H 103:**

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

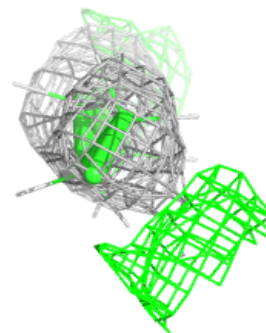
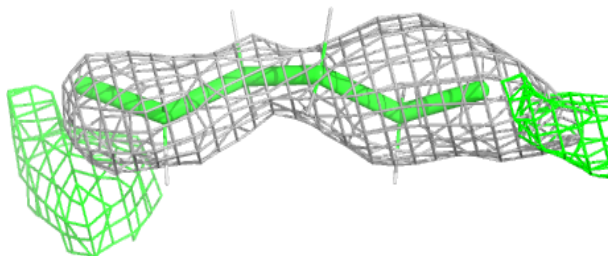
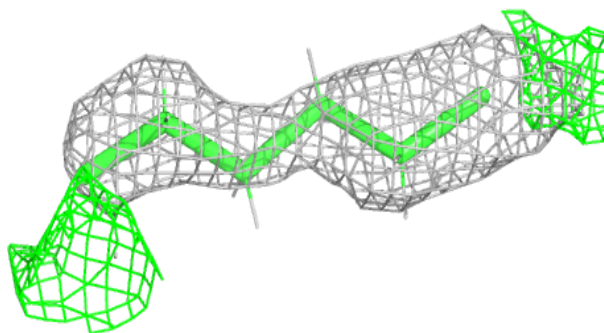


Electron density around STE e 101:

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

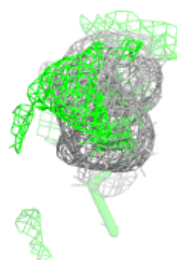
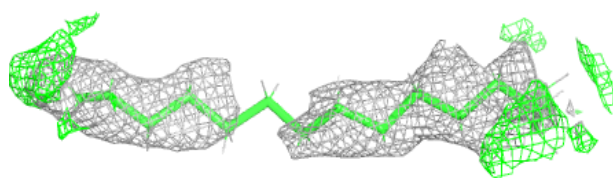
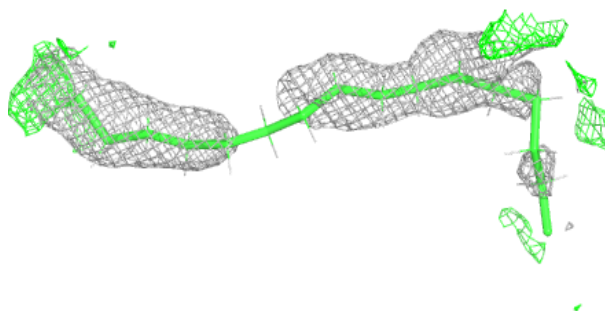
**Electron density around STE i 102:**

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

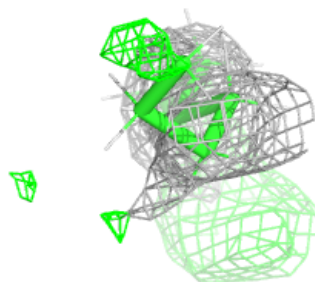
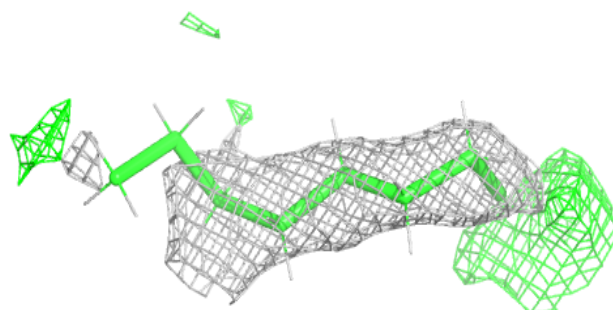
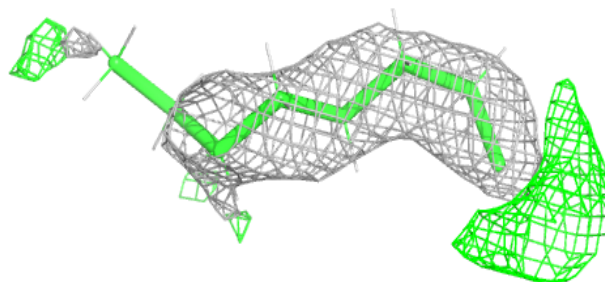


Electron density around STE j 102:

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

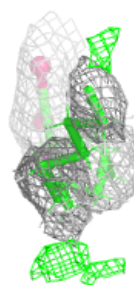
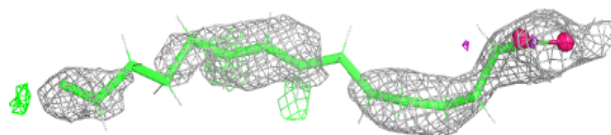
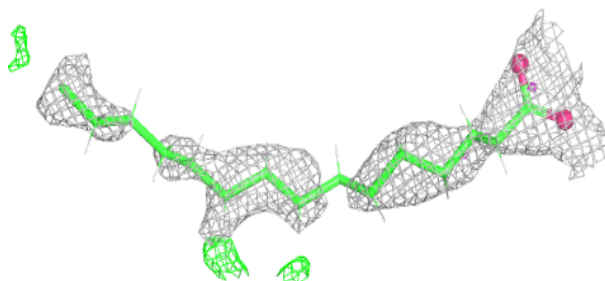
**Electron density around STE e 103:**

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

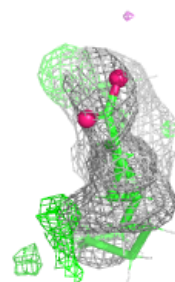
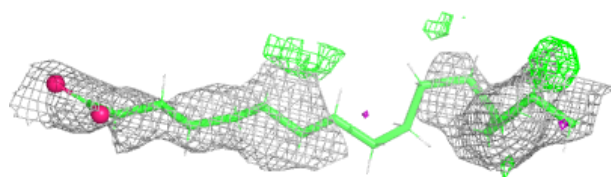
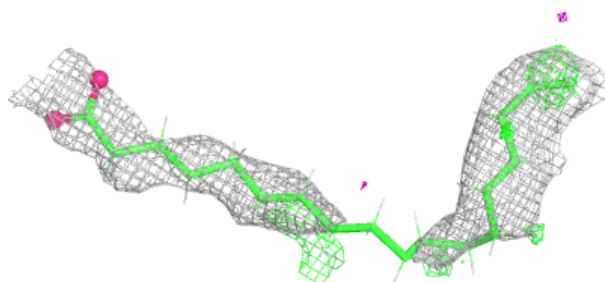


Electron density around STE I 101:

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

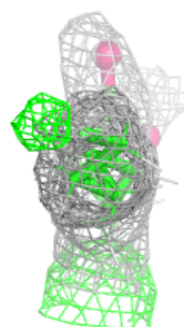
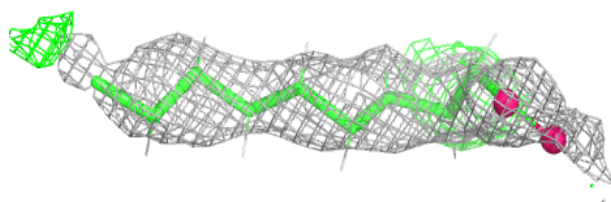
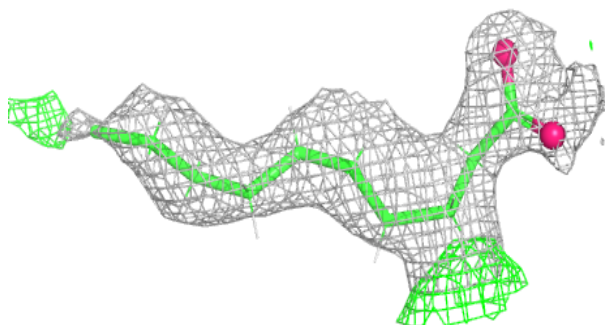
**Electron density around STE E 104:**

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

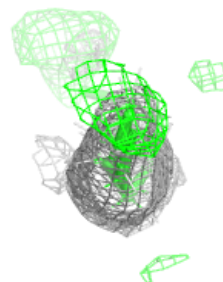
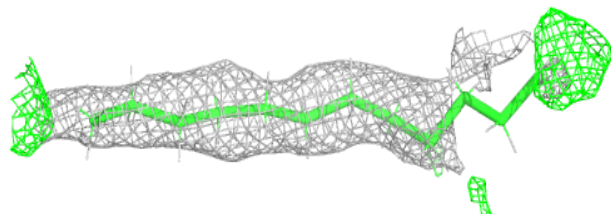
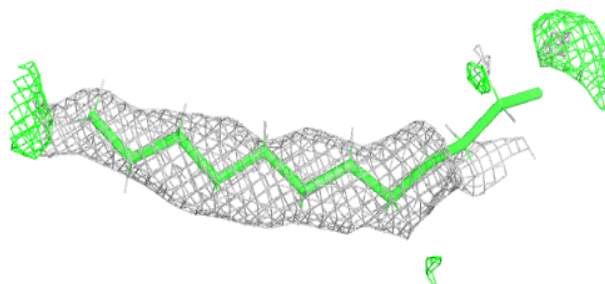


Electron density around STE a 618:

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

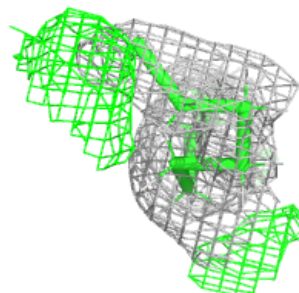
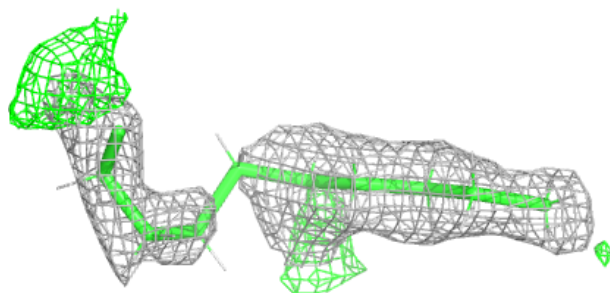
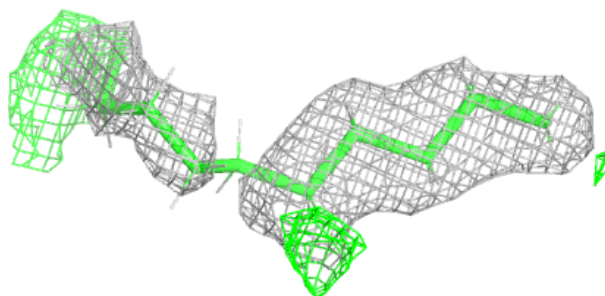
**Electron density around STE E 103:**

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

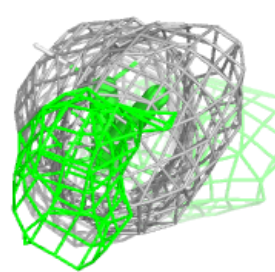
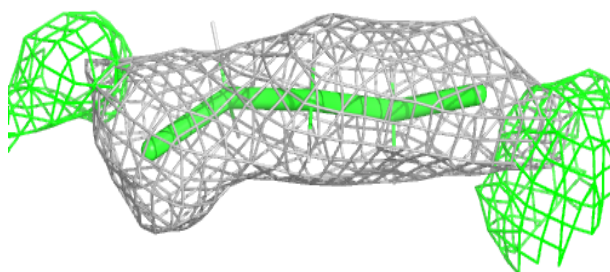
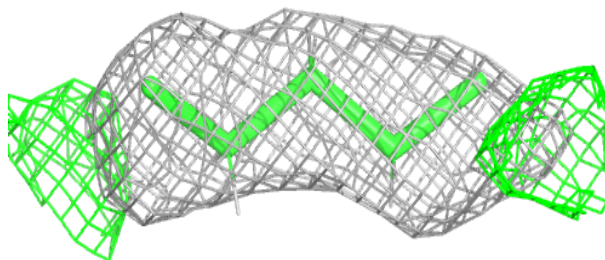


Electron density around STE h 102:

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

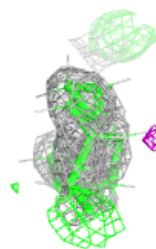
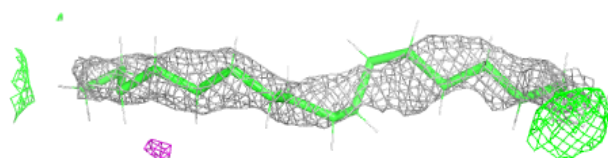
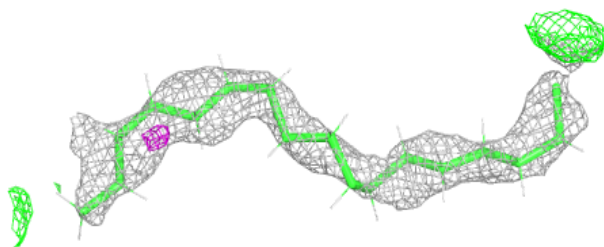
**Electron density around STE C 518:**

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

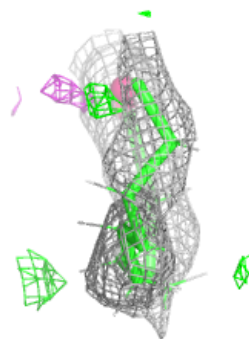
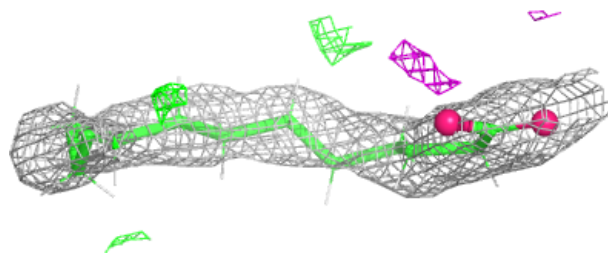
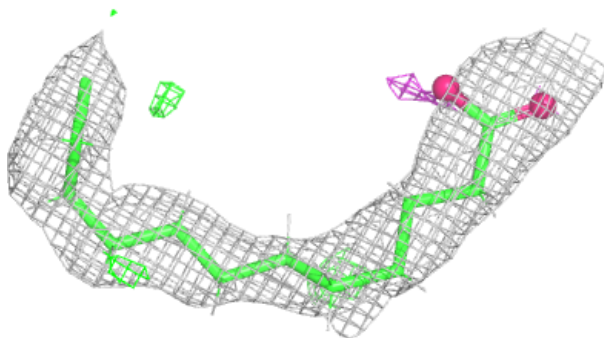


Electron density around STE A 619:

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

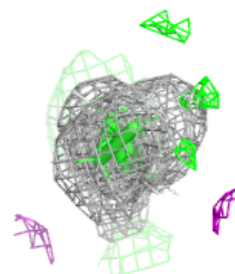
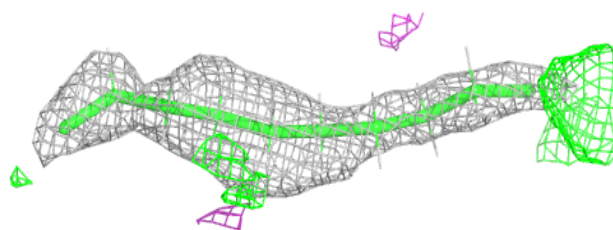
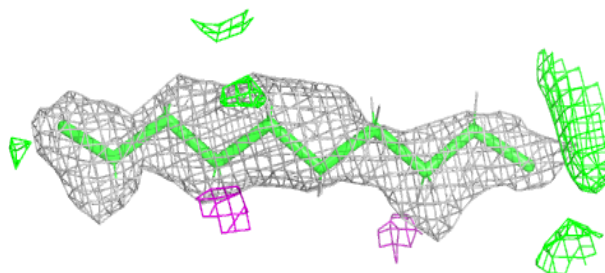
**Electron density around STE C 516:**

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

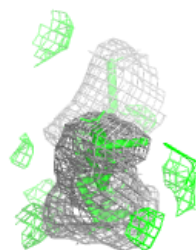
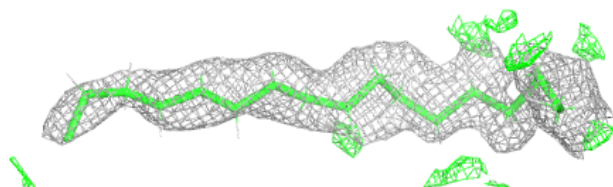
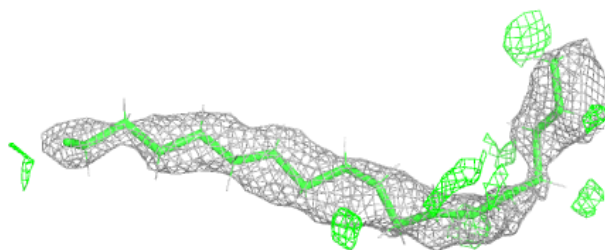


Electron density around STE t 102:

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

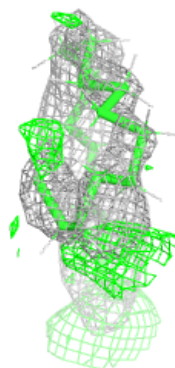
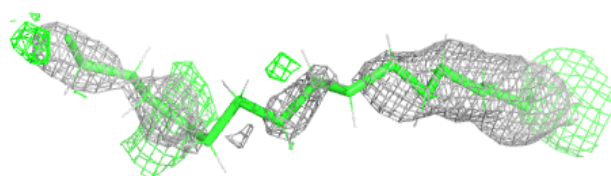
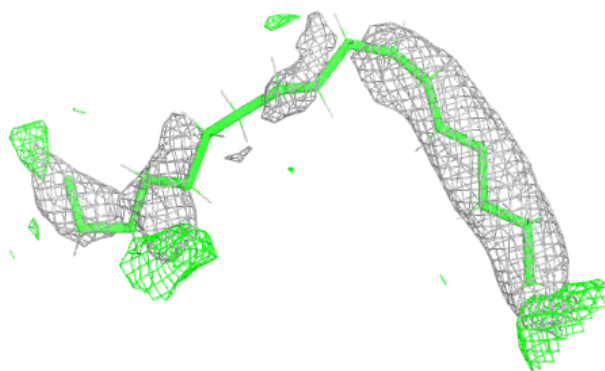
**Electron density around STE c 516:**

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

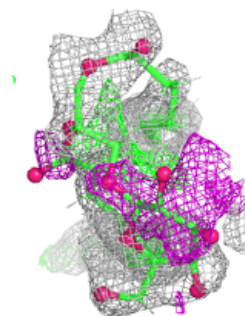
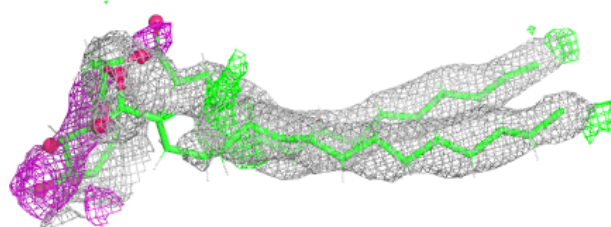
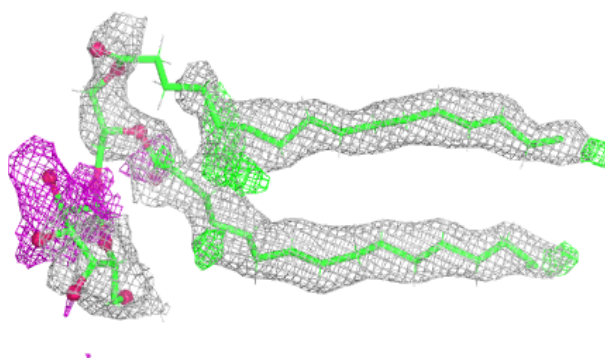


Electron density around STE Z 102:

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

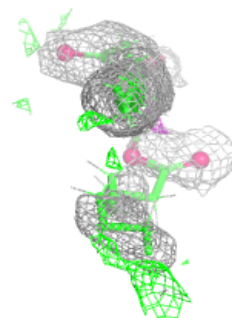
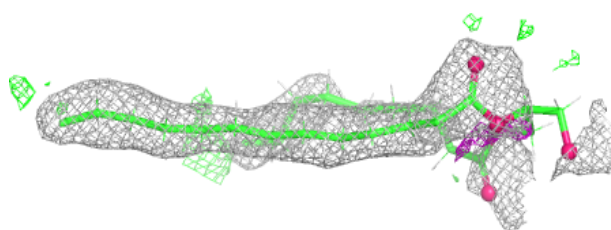
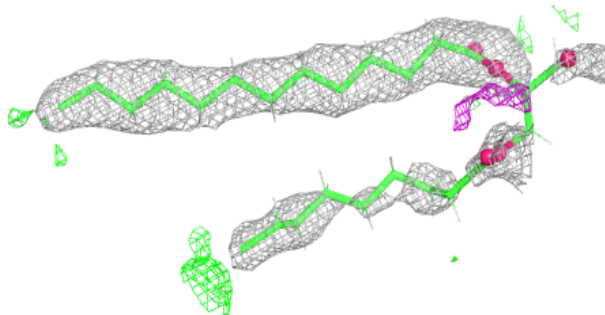
**Electron density around LMG D 406:**

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

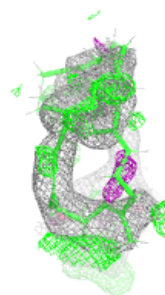
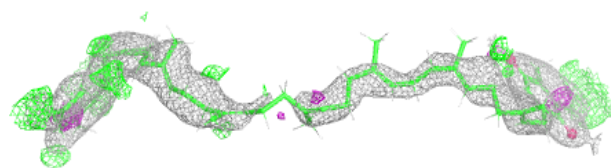
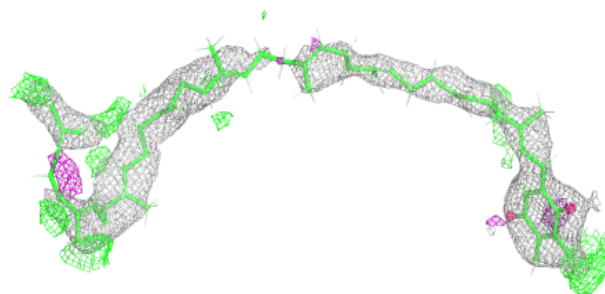


Electron density around LMG c 517:

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

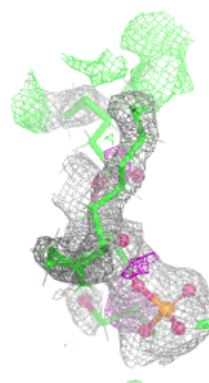
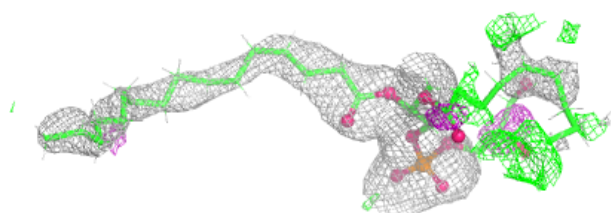
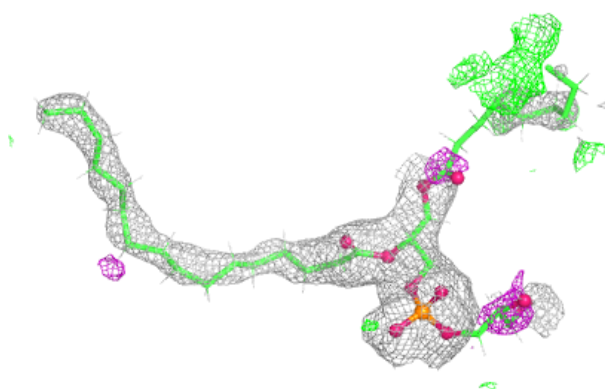
**Electron density around PL9 a 612:**

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

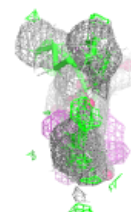
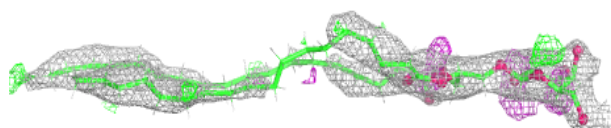
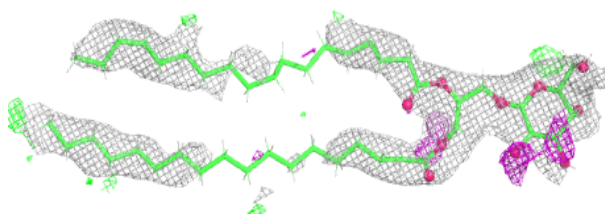


Electron density around LHG e 102:

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

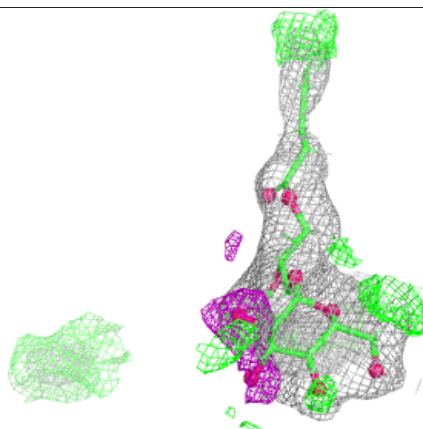
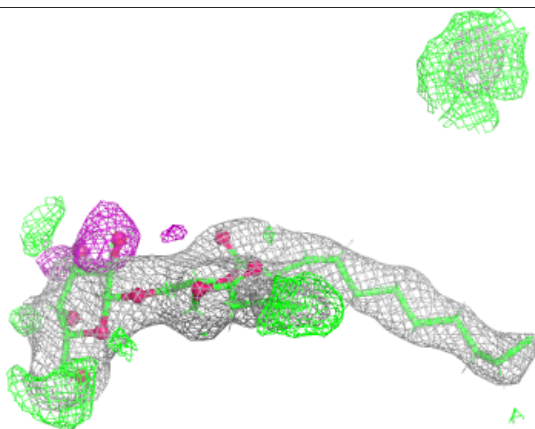
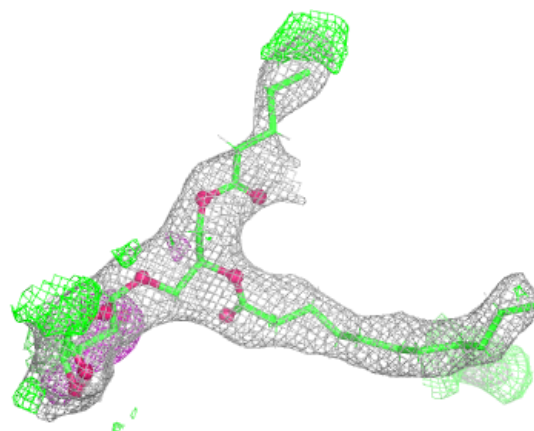
**Electron density around LMG b 622:**

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



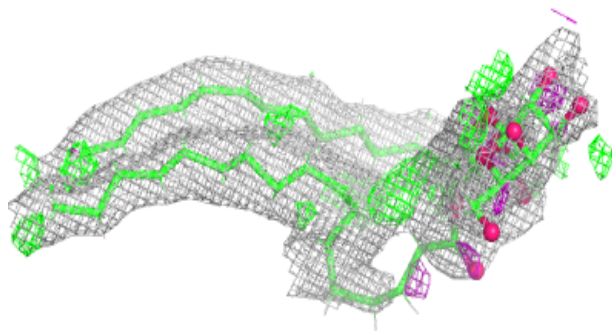
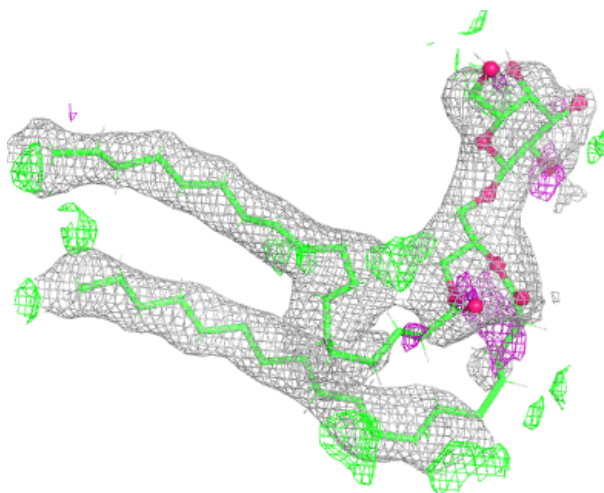
Electron density around LMG C 517:

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



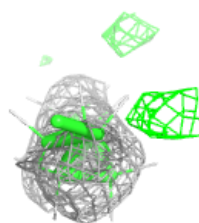
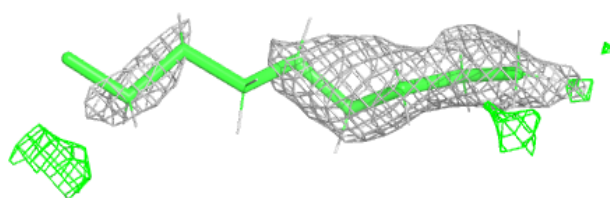
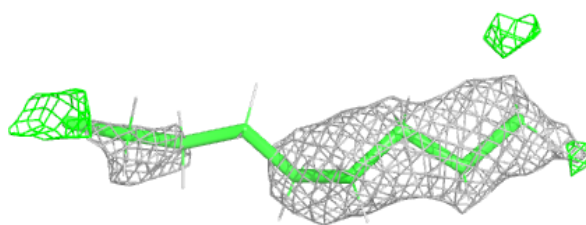
Electron density around LMG a 616:

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

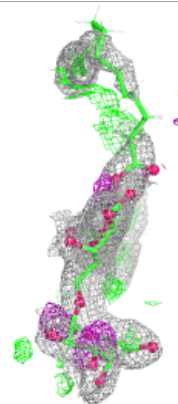
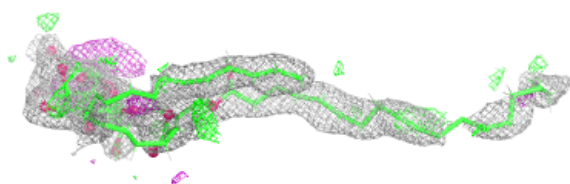
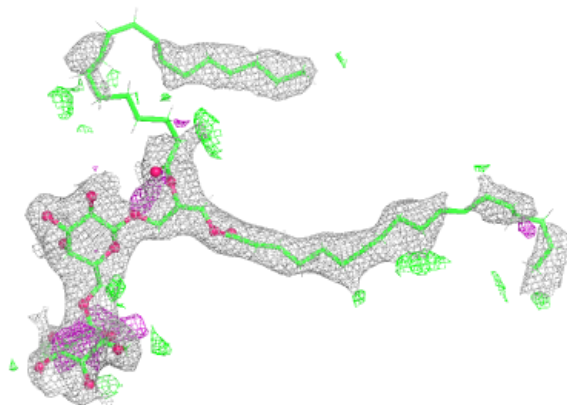


Electron density around STE e 104:

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

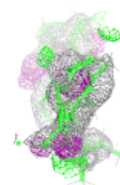
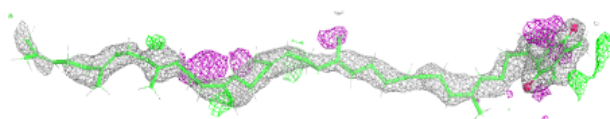
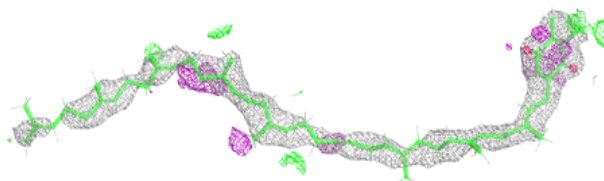
**Electron density around DGD A 617:**

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

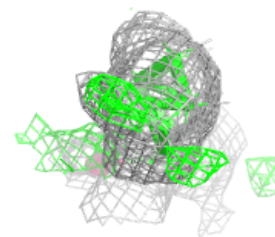
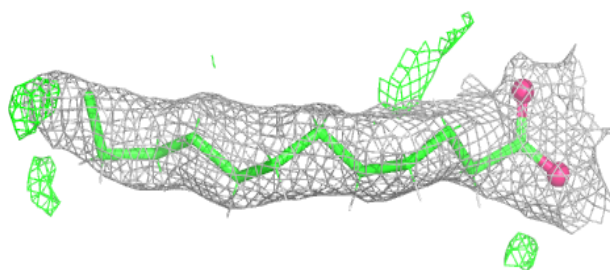
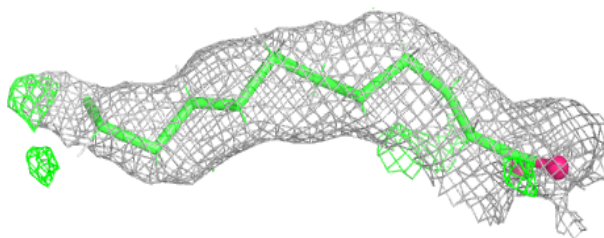


Electron density around PL9 A 612:

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

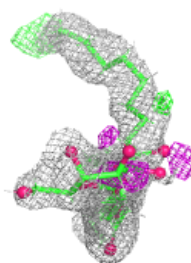
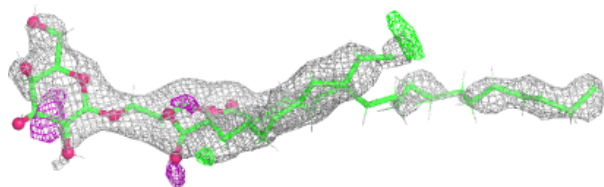
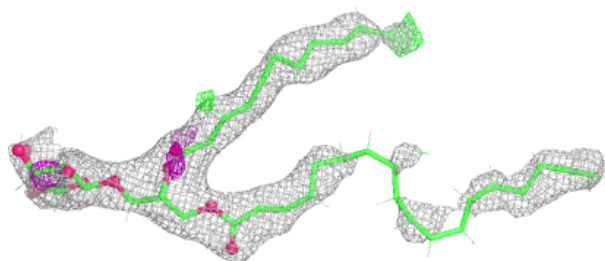
**Electron density around STE k 103:**

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

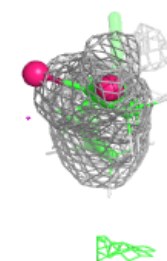
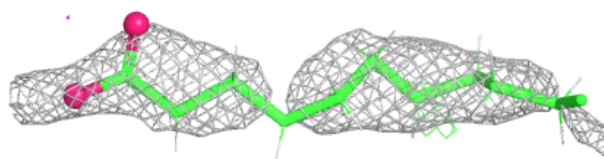
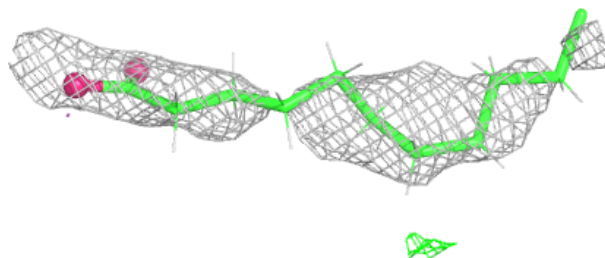


Electron density around LMG c 522:

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

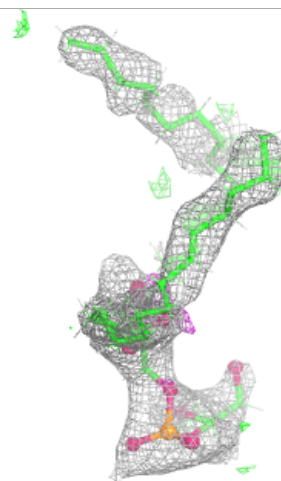
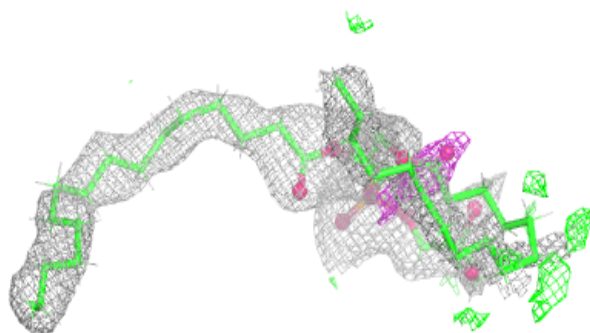
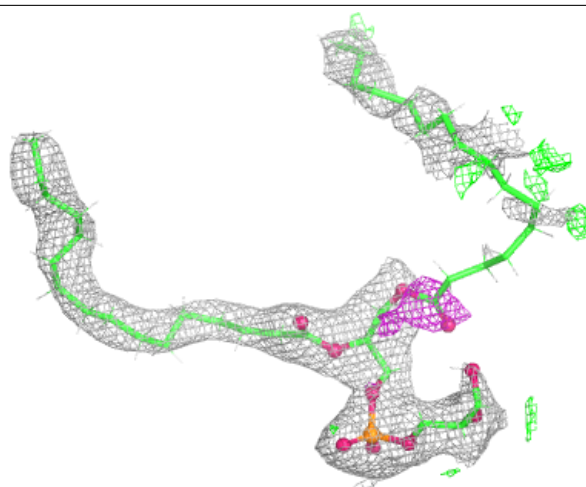
**Electron density around STE e 105:**

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



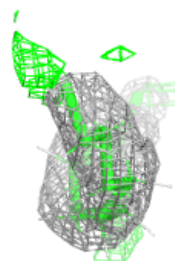
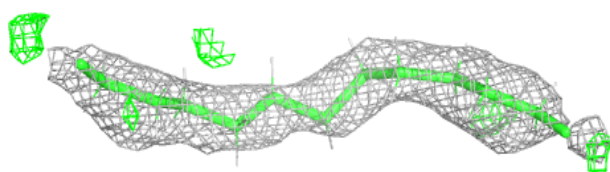
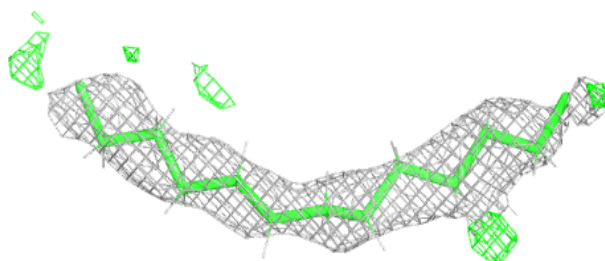
Electron density around LHG E 101:

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

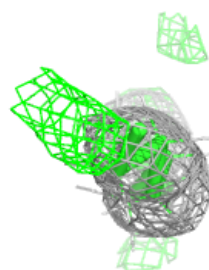
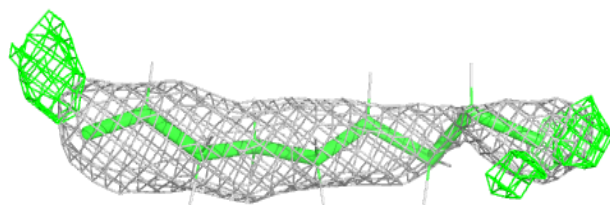
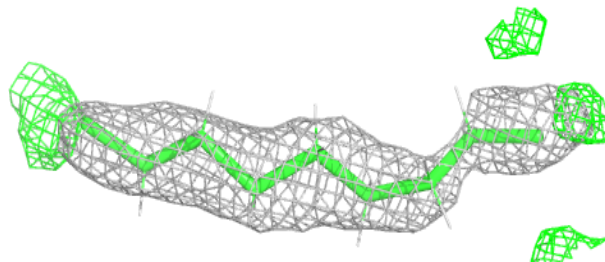


Electron density around STE z 701:

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

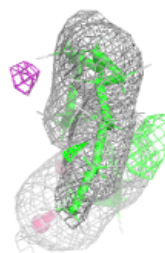
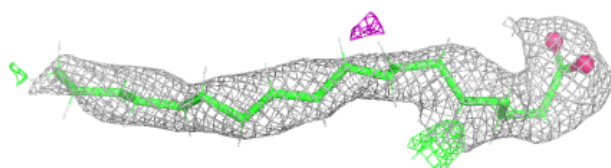
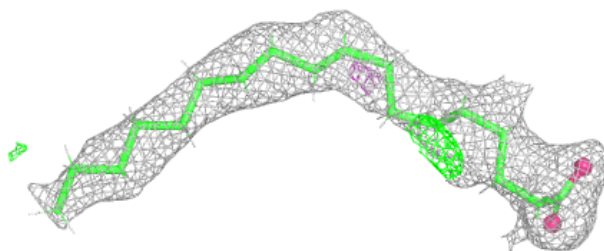
**Electron density around STE z 702:**

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

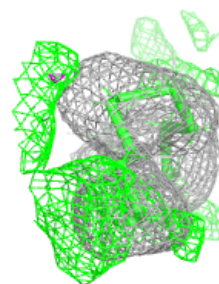
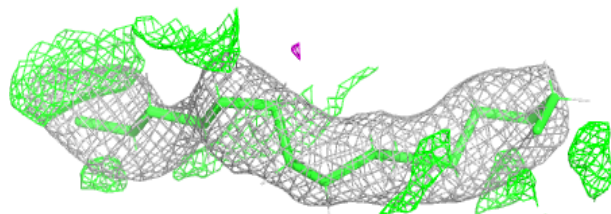
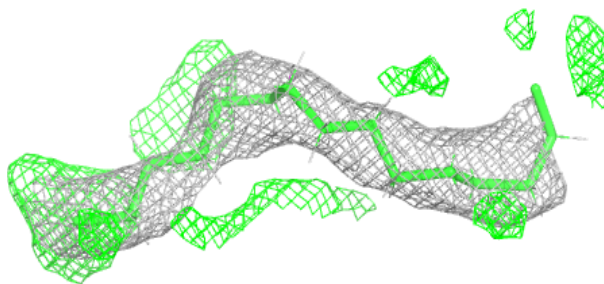


Electron density around STE d 410:

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

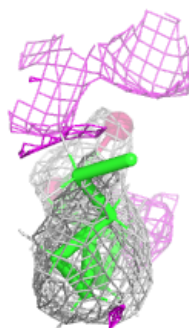
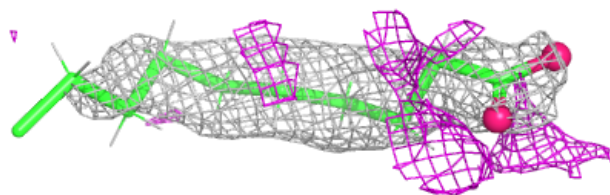
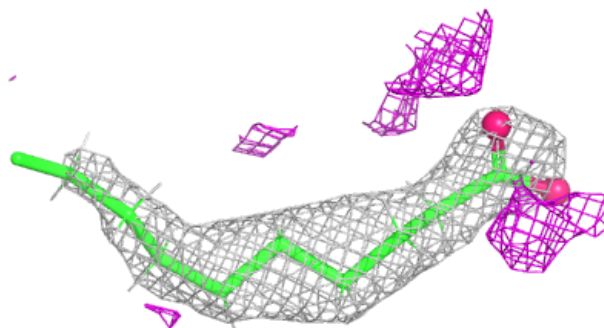
**Electron density around STE B 627:**

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

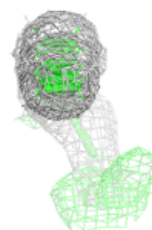
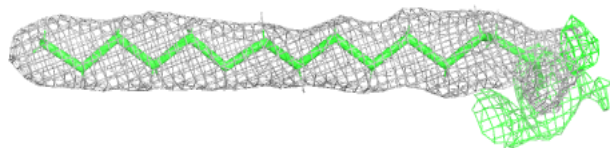
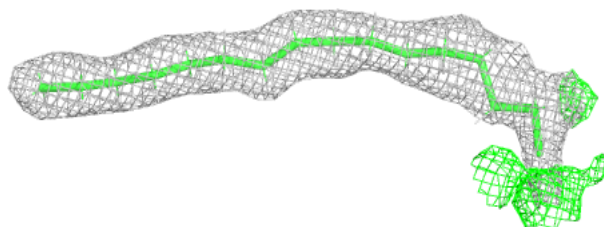


Electron density around STE B 626:

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

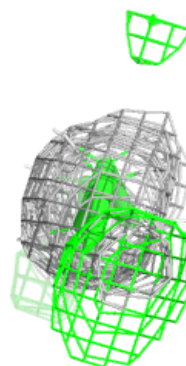
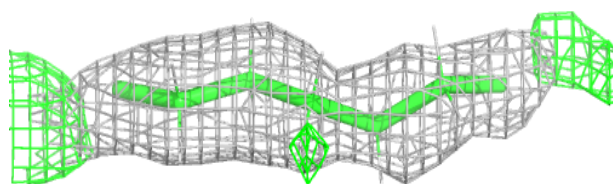
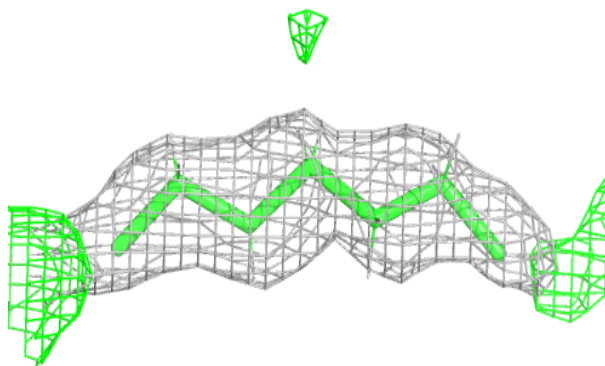
**Electron density around STE C 526:**

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

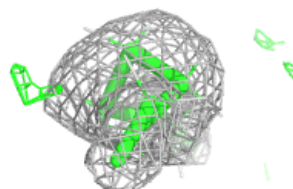
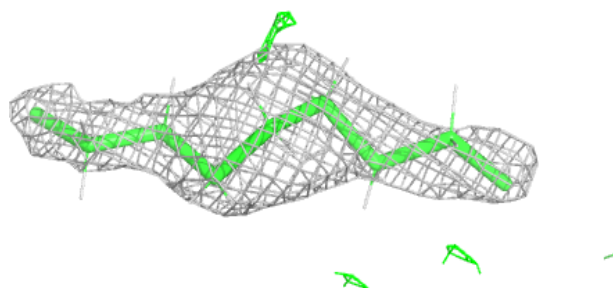
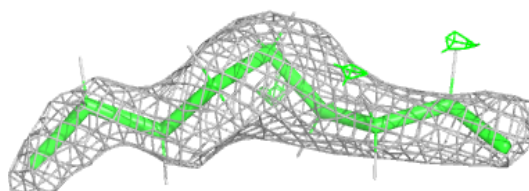


Electron density around STE C 519:

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

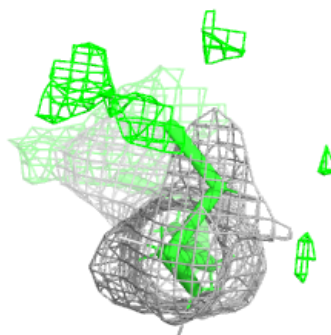
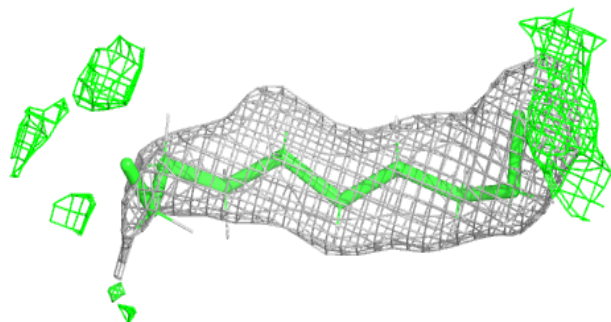
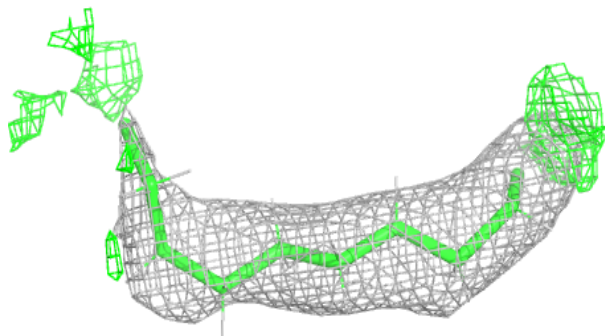
**Electron density around STE A 613:**

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

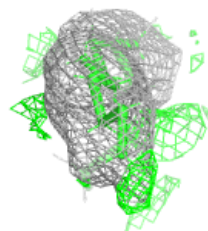
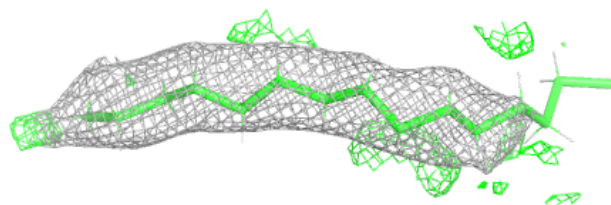
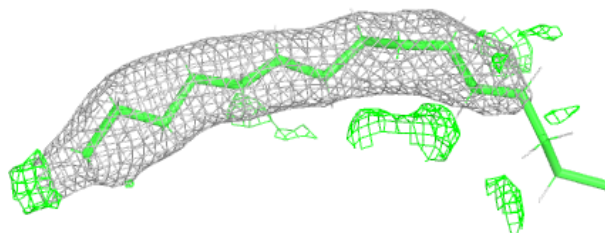


Electron density around STE b 624:

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

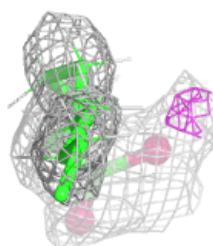
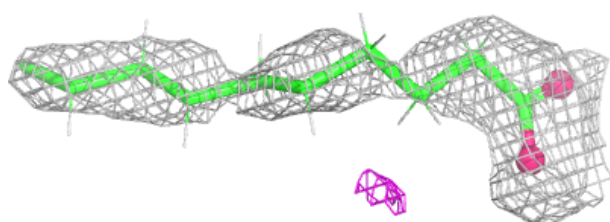
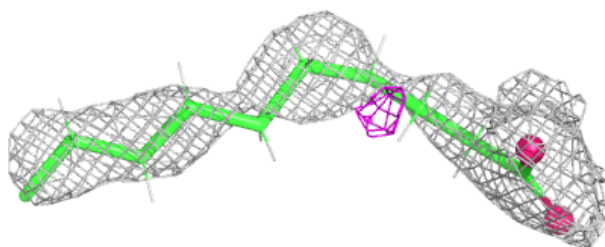
**Electron density around STE T 103:**

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

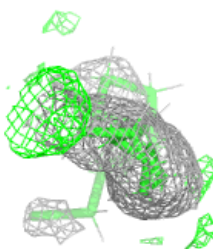
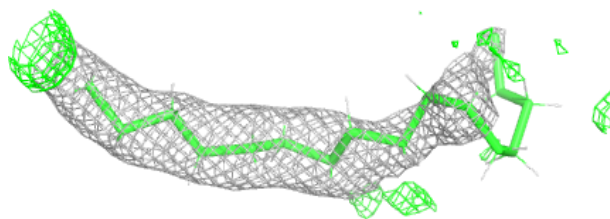
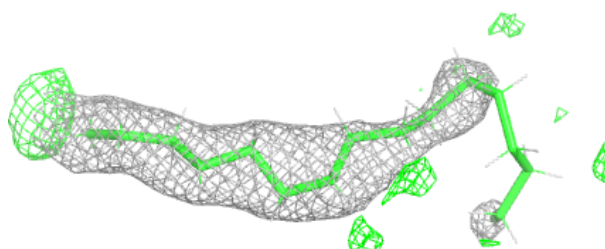


Electron density around STE E 102:

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

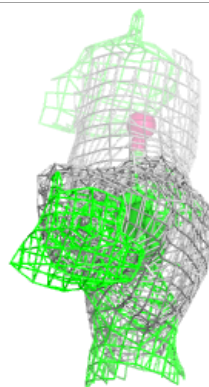
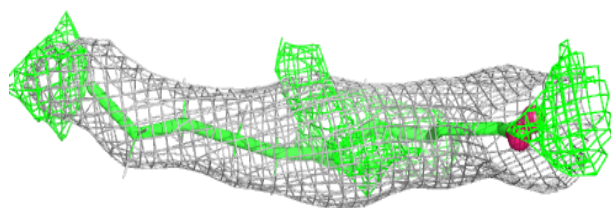
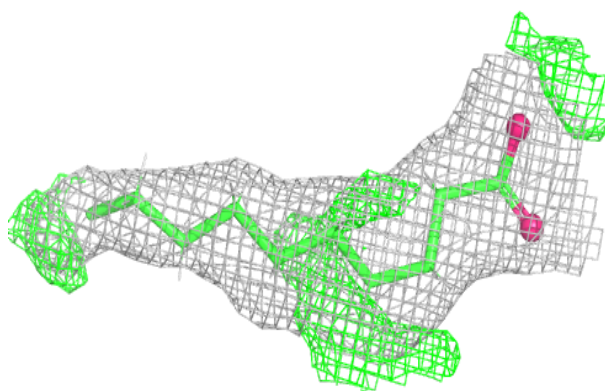
**Electron density around STE T 102:**

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

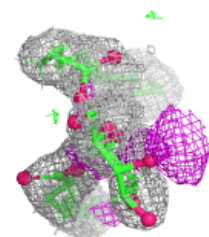
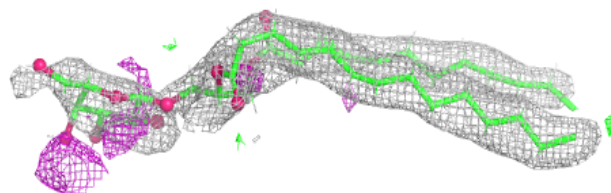
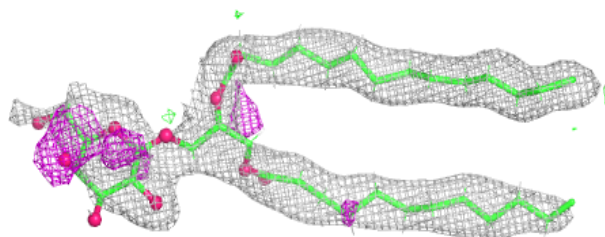


Electron density around STE C 525:

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

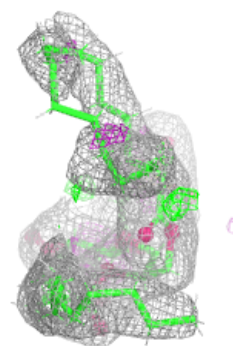
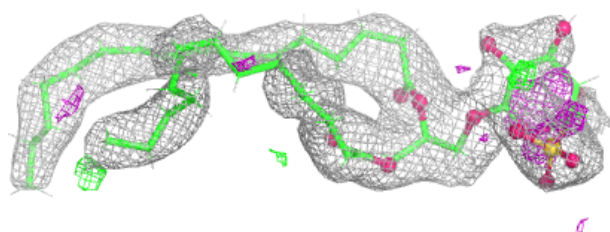
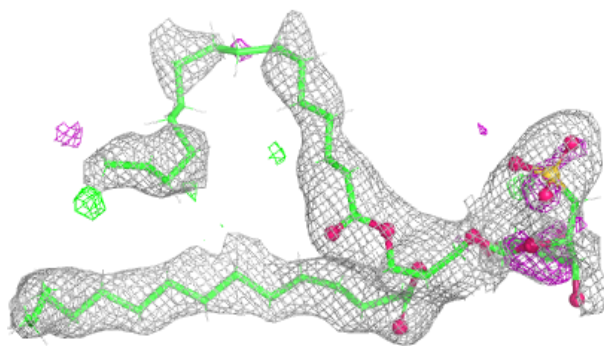
**Electron density around LMG B 620:**

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

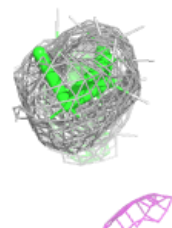
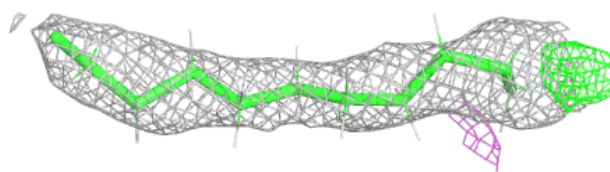
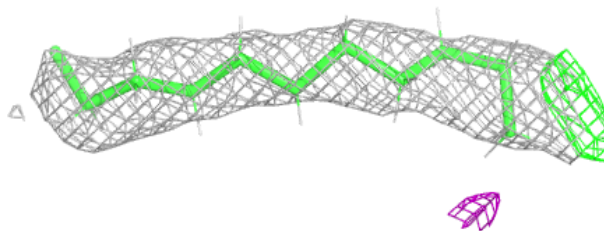


Electron density around SQD a 615:

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

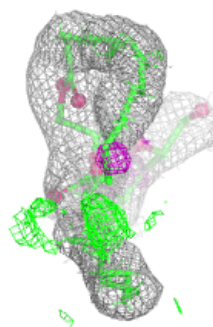
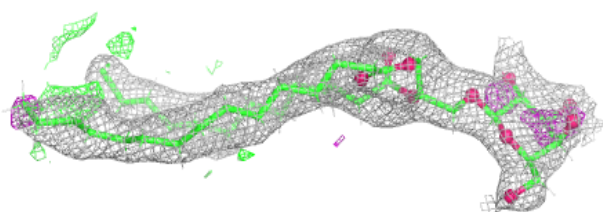
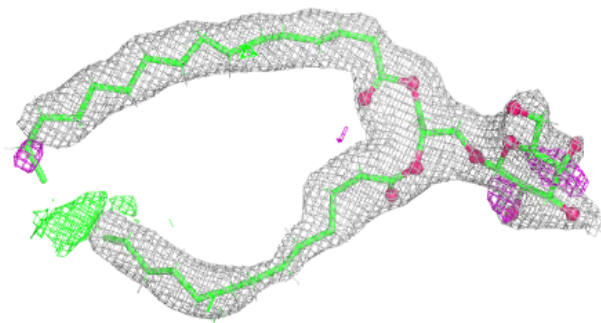
**Electron density around STE b 625:**

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

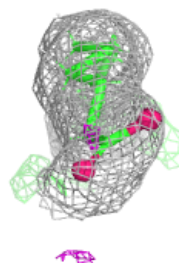
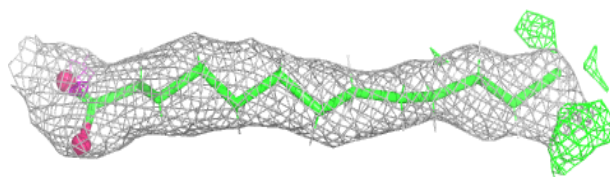
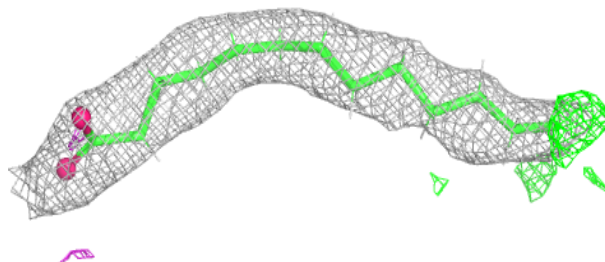


Electron density around LMG A 615:

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

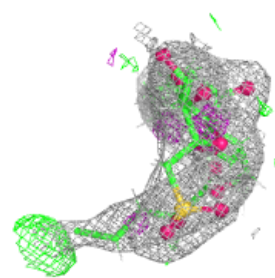
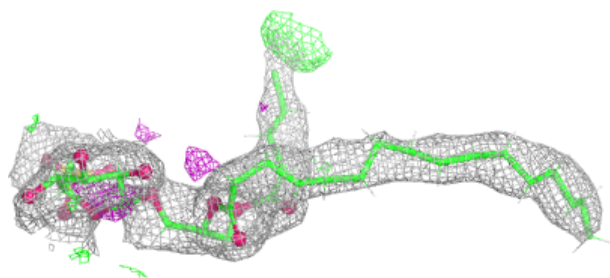
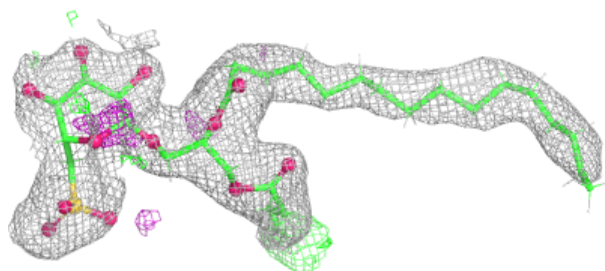
**Electron density around STE I 102:**

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

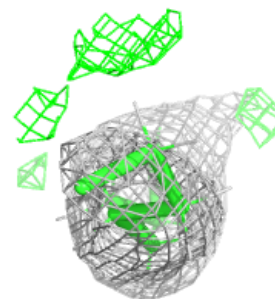
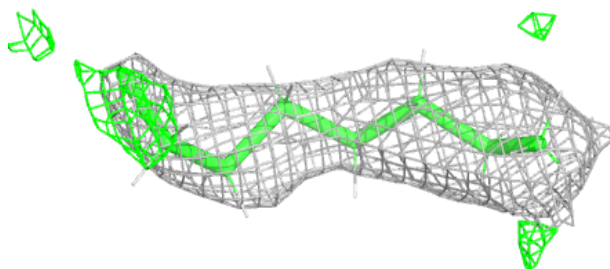
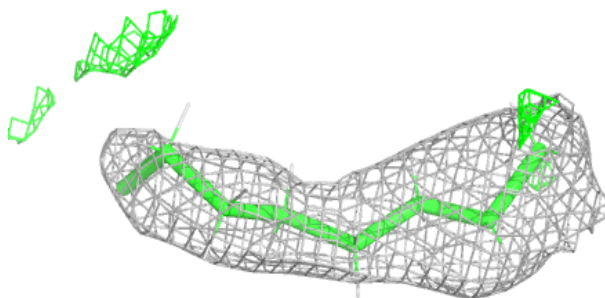


Electron density around SQD A 616:

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

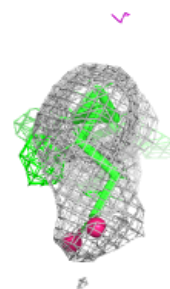
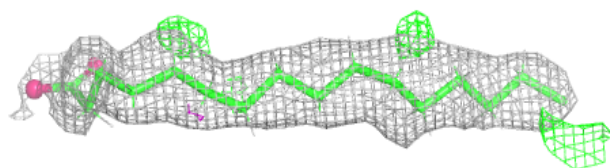
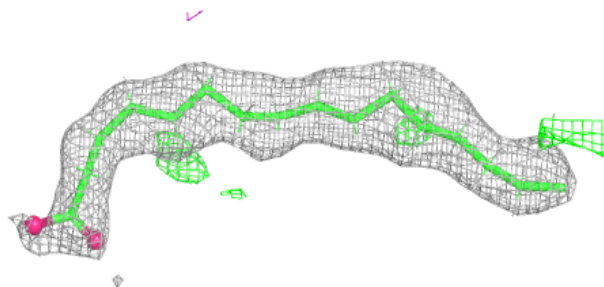
**Electron density around STE A 618:**

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

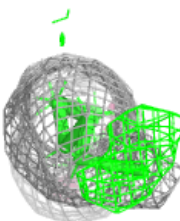
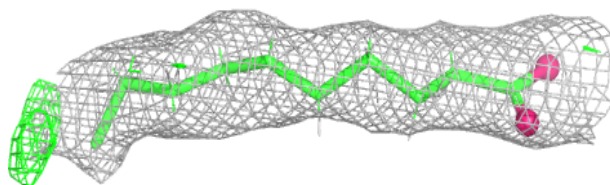
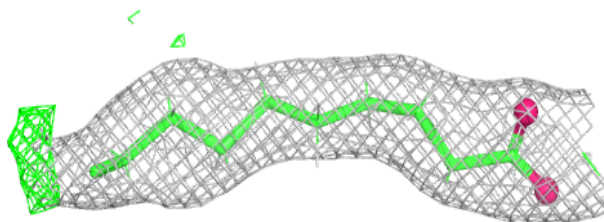


Electron density around STE B 625:

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

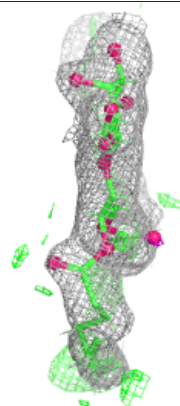
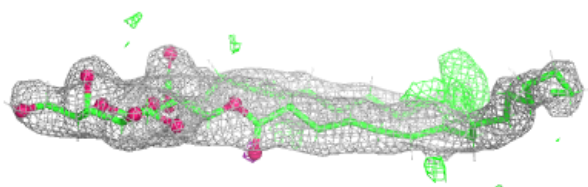
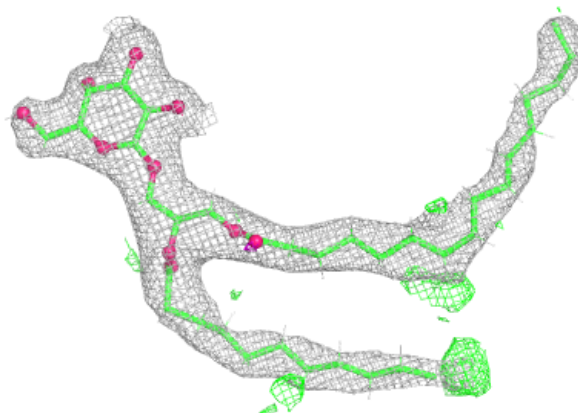
**Electron density around STE j 101:**

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

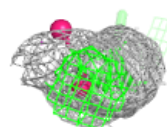
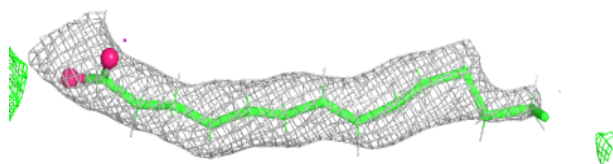
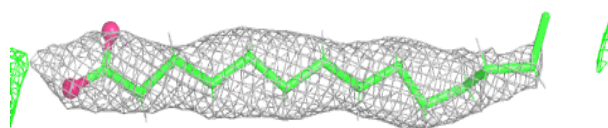


Electron density around LMG c 521:

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

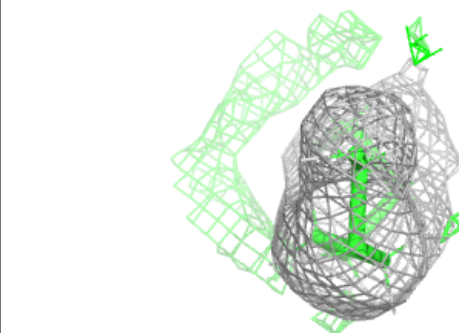
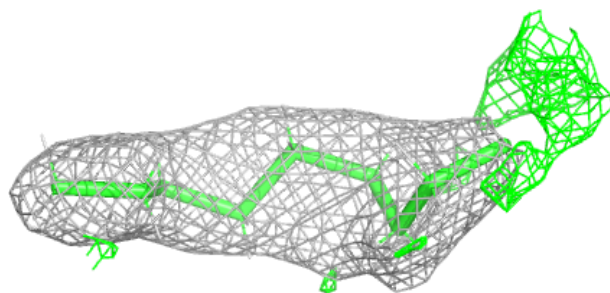
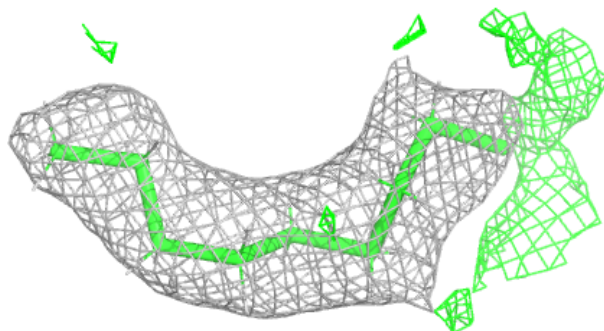
**Electron density around STE b 623:**

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

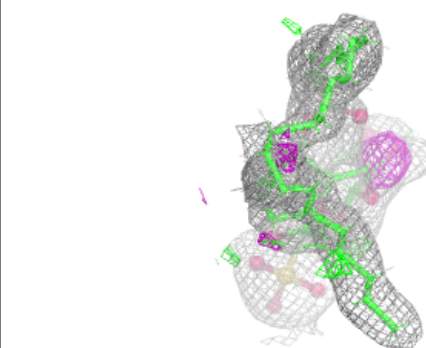
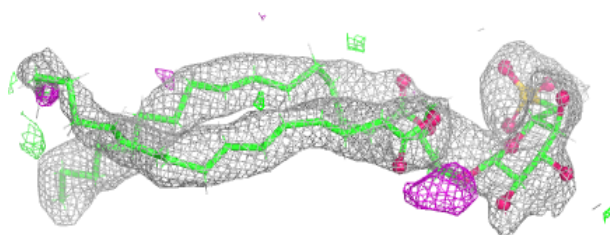
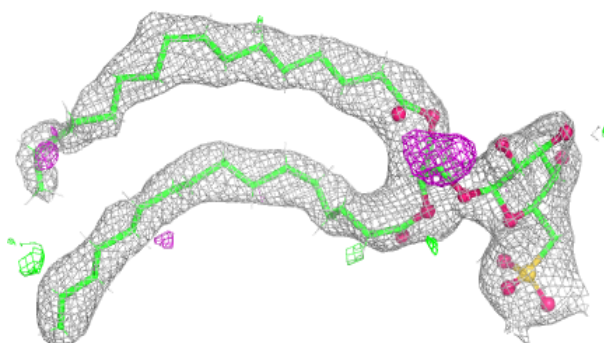


Electron density around STE H 104:

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

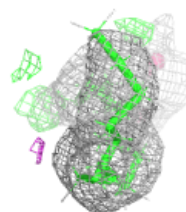
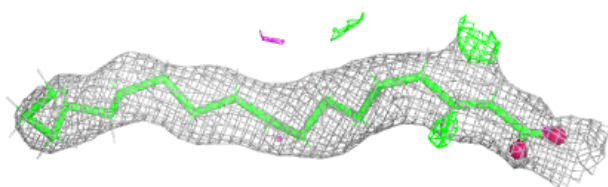
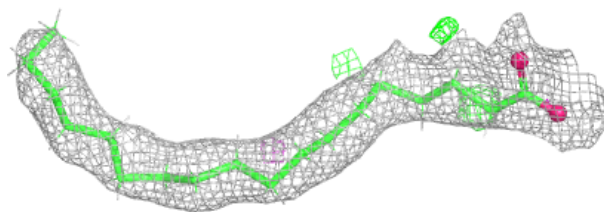
**Electron density around SQD B 623:**

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

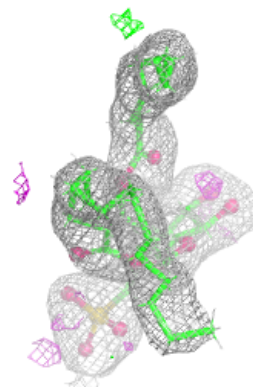
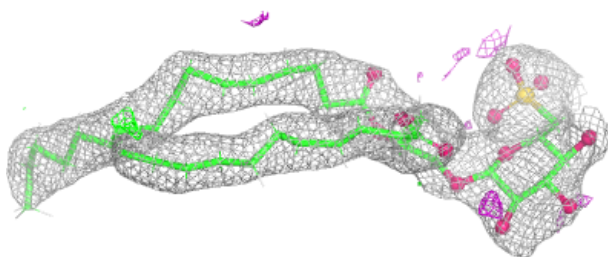
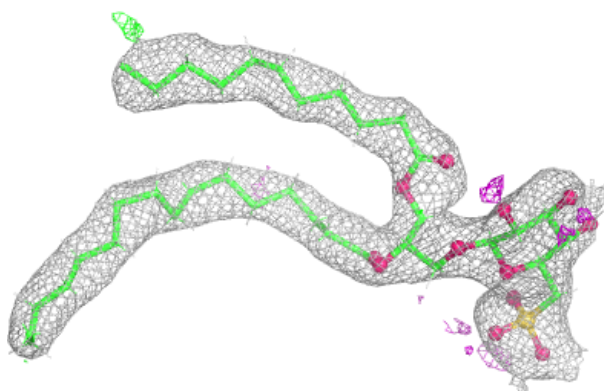


Electron density around STE b 621:

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

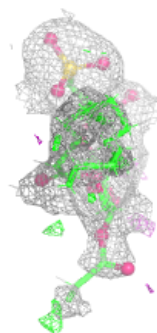
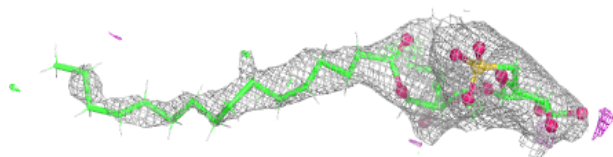
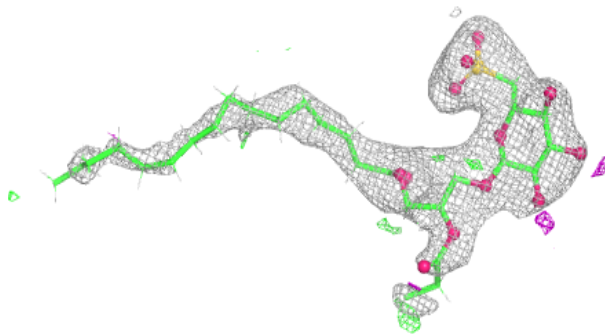
**Electron density around SQD b 620:**

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

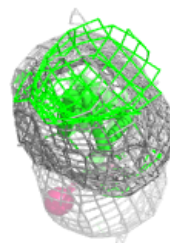
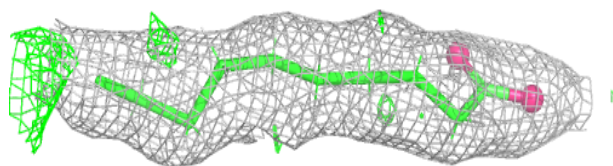
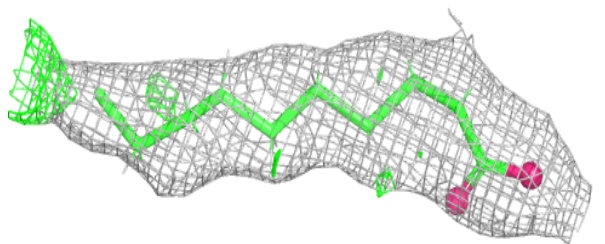


Electron density around SQD f 102:

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

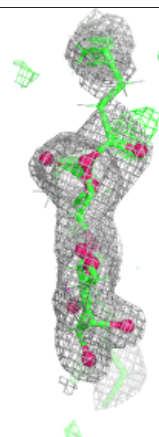
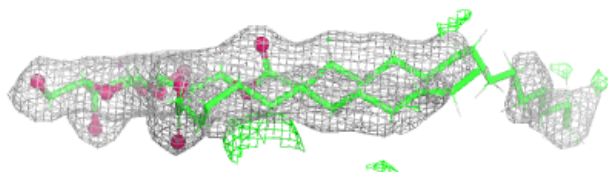
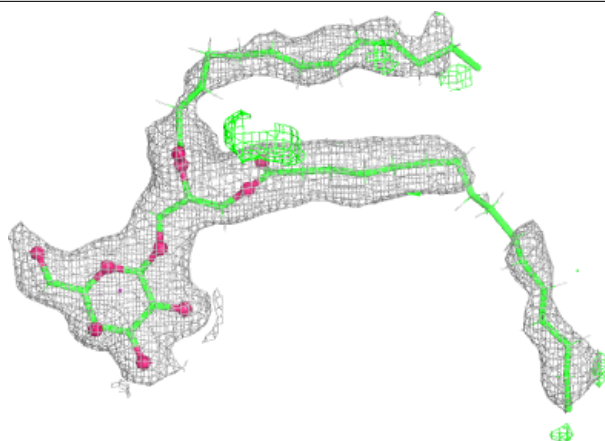
**Electron density around STE J 101:**

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

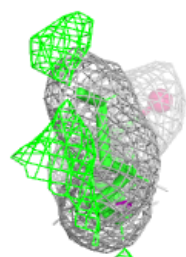
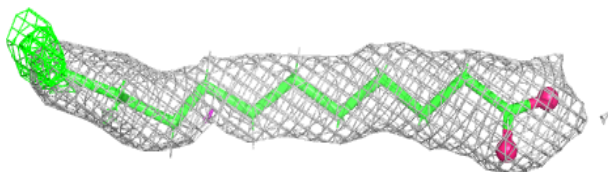
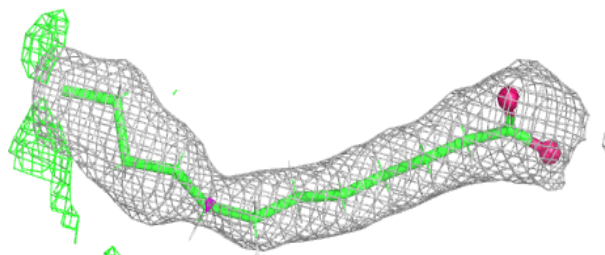


Electron density around LMG C 524:

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

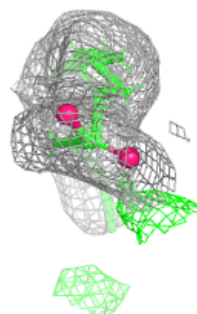
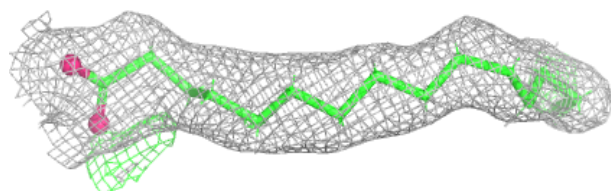
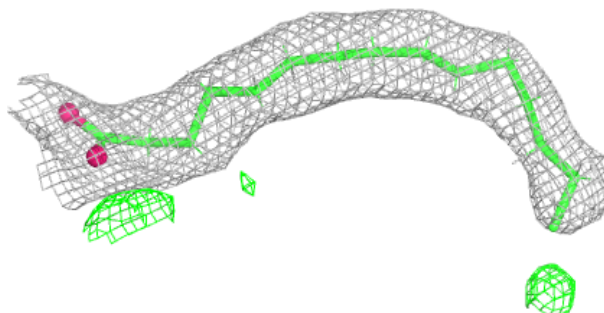
**Electron density around STE B 624:**

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

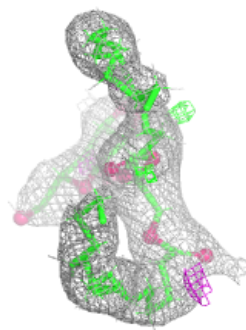
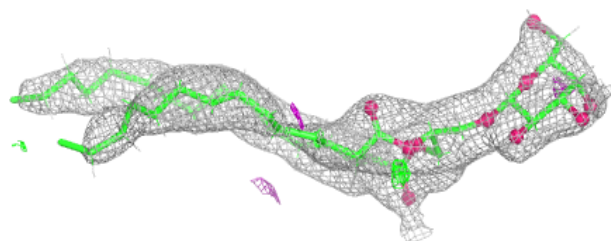
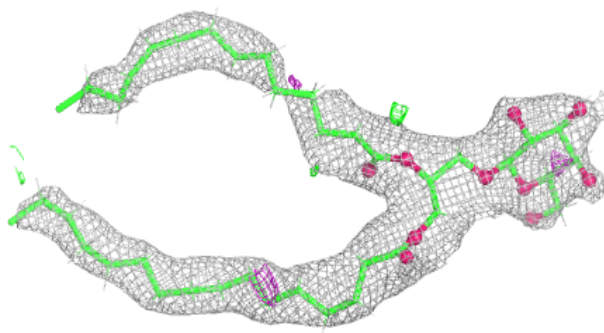


Electron density around STE B 621:

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

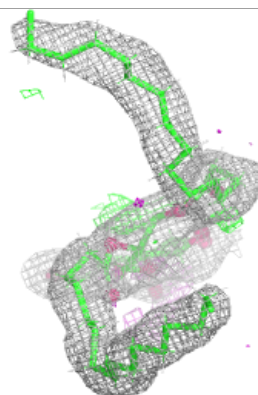
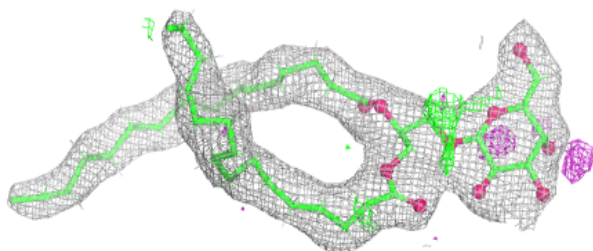
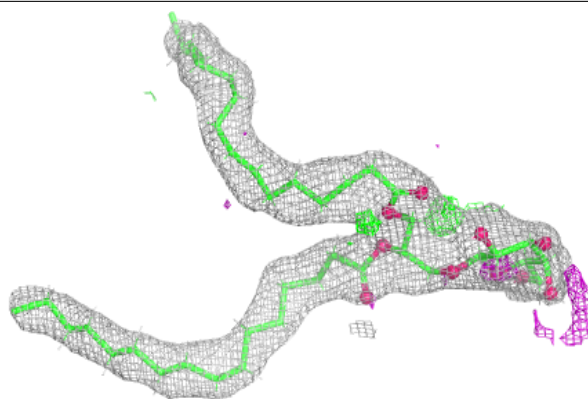
**Electron density around LMG a 617:**

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

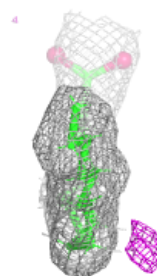
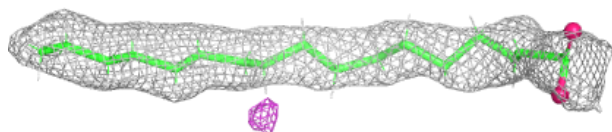
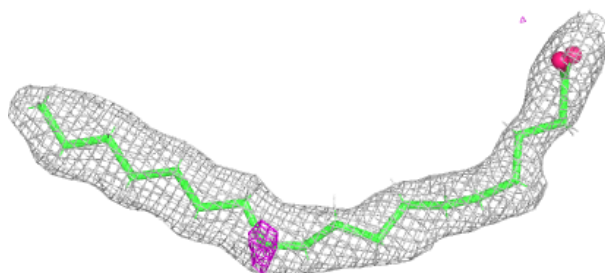


Electron density around LMG m 101:

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

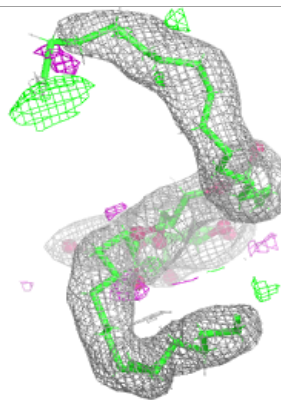
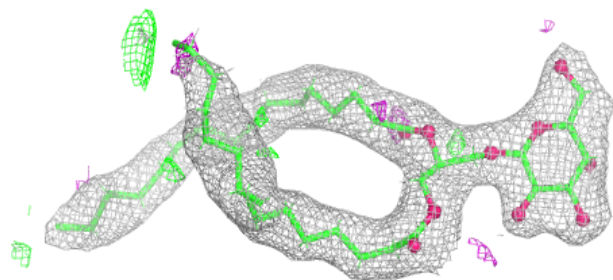
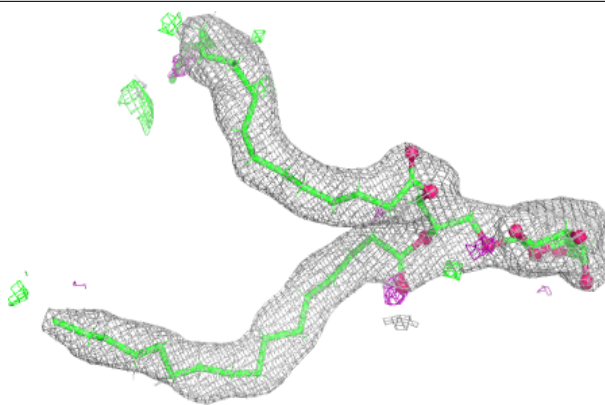
**Electron density around STE d 412:**

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



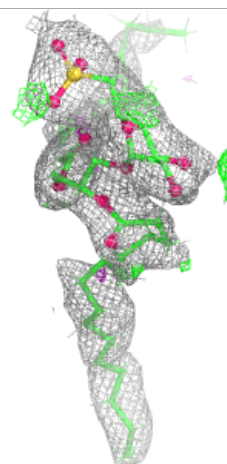
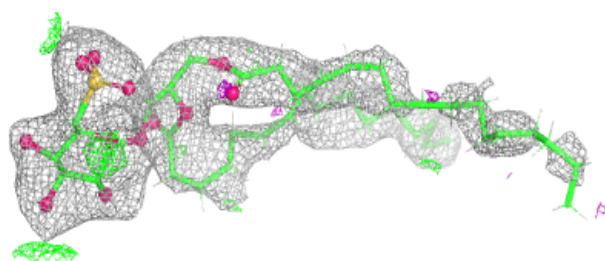
Electron density around LMG M 101:

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



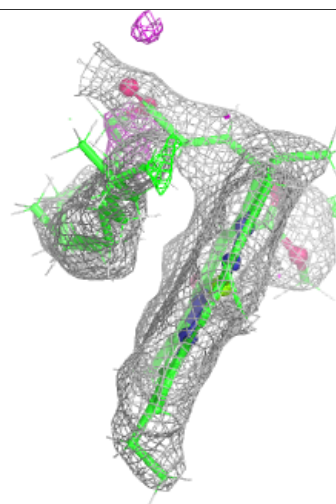
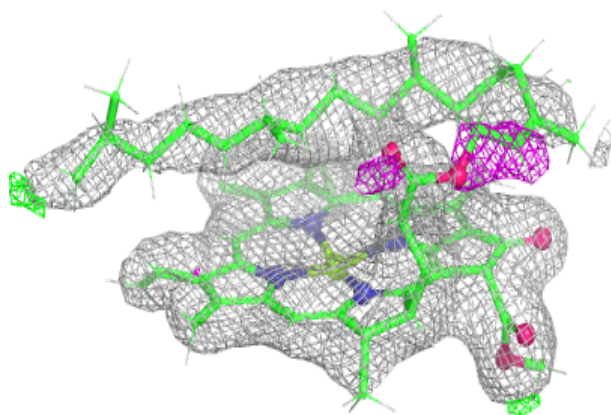
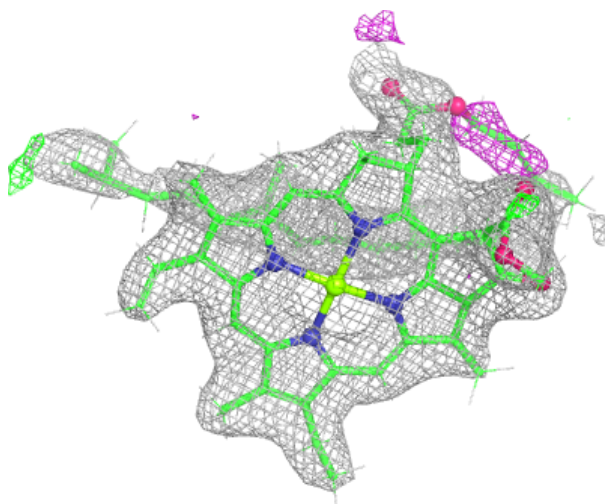
Electron density around SQD a 614:

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



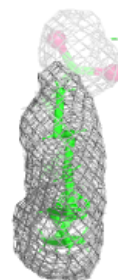
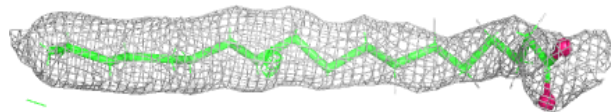
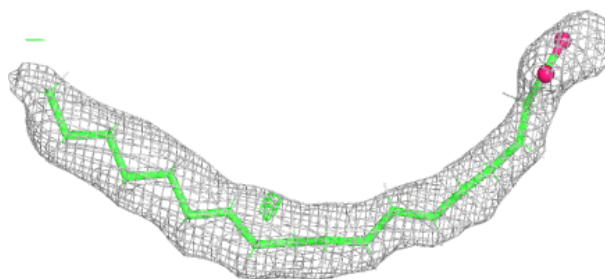
Electron density around CLA b 601:

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

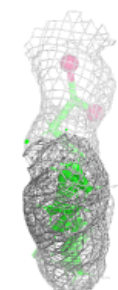
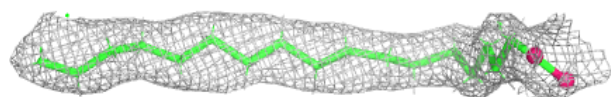
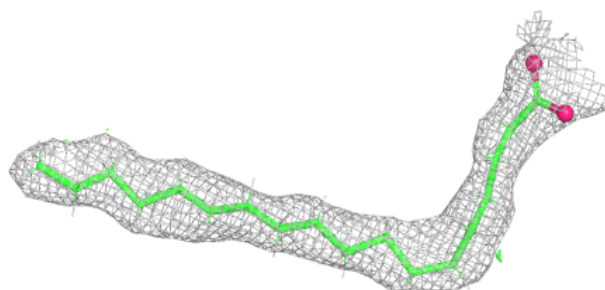


Electron density around STE D 412:

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

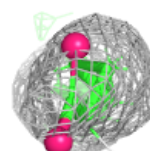
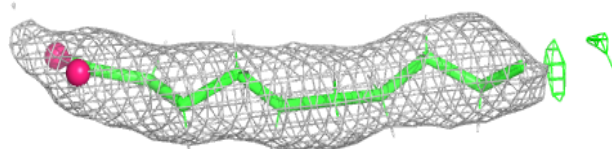
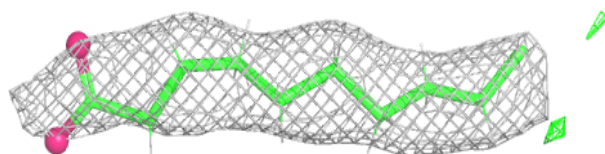
**Electron density around STE d 406:**

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

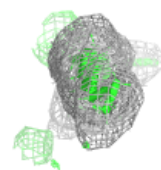
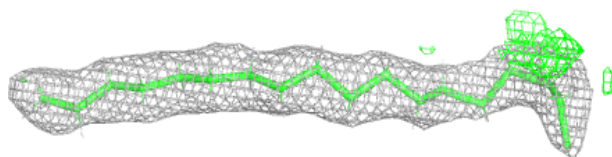
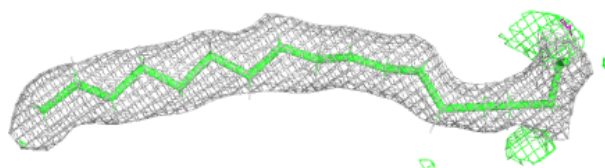


Electron density around STE m 102:

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

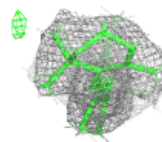
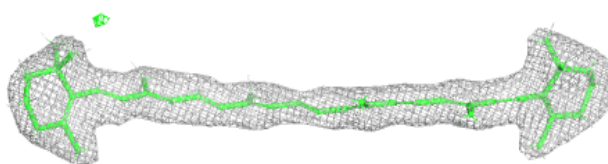
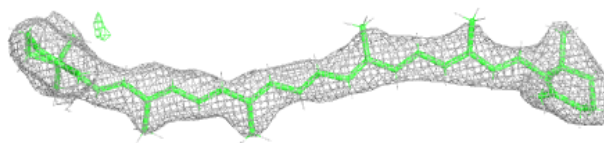
**Electron density around STE m 103:**

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



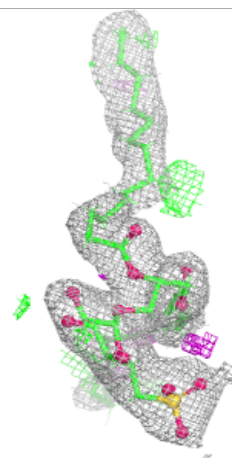
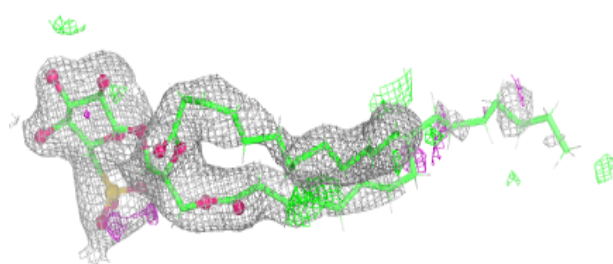
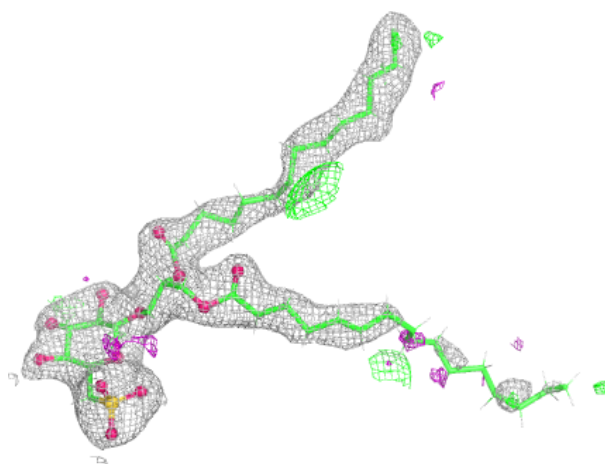
Electron density around BCR c 514:

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



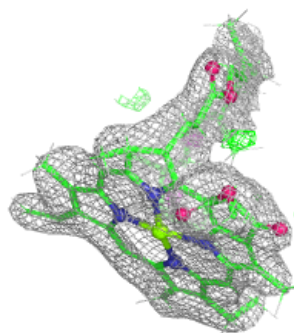
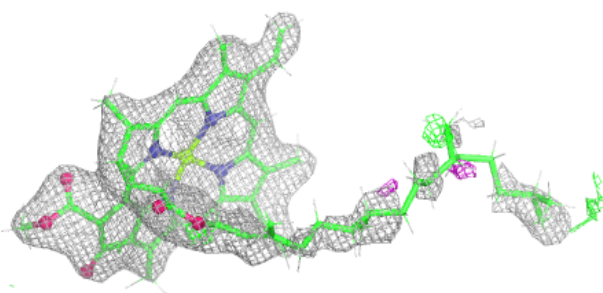
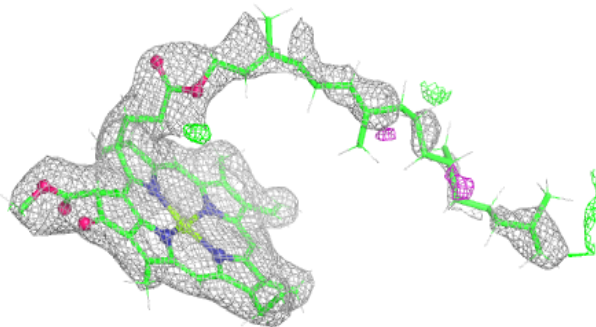
Electron density around SQD D 410:

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

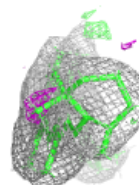
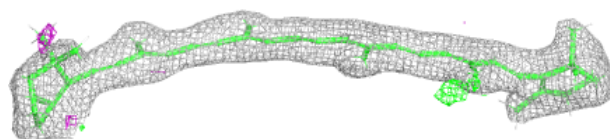
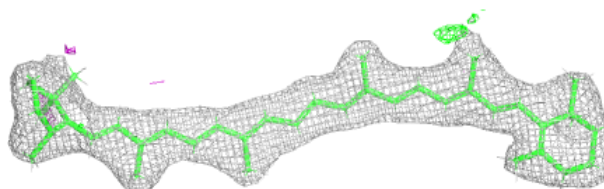


Electron density around CLA c 513:

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

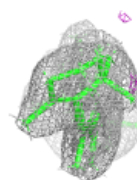
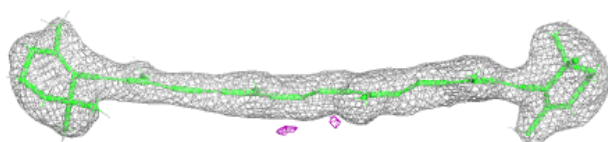
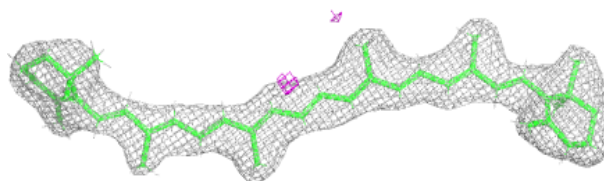
**Electron density around BCR d 404:**

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

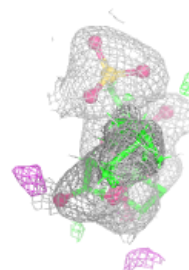
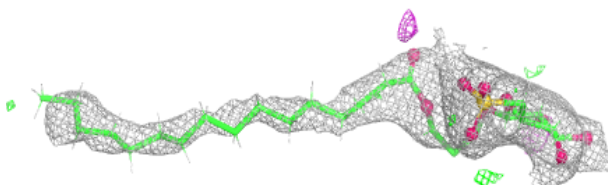
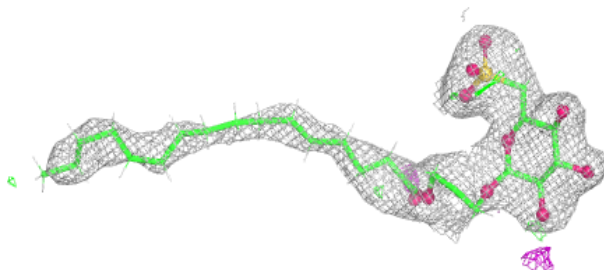


Electron density around BCR k 101:

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

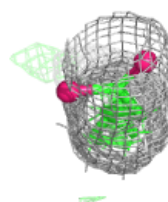
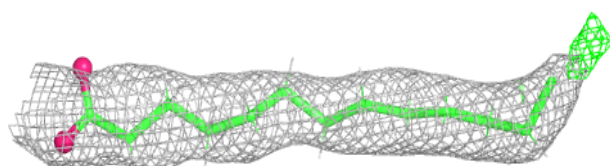
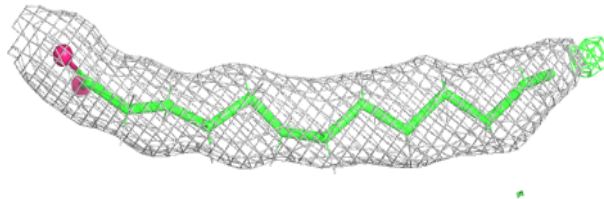
**Electron density around SQD F 102:**

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

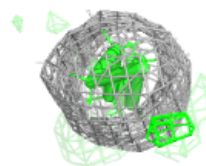
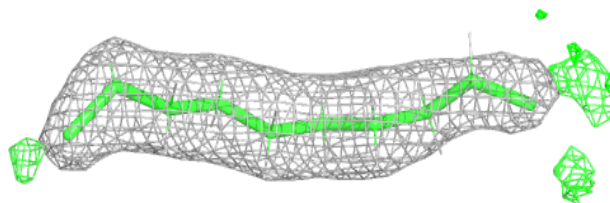
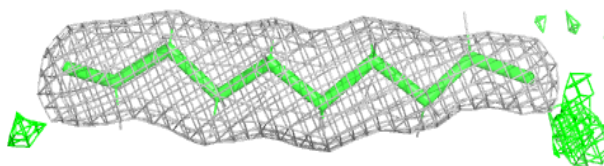


Electron density around STE M 102:

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

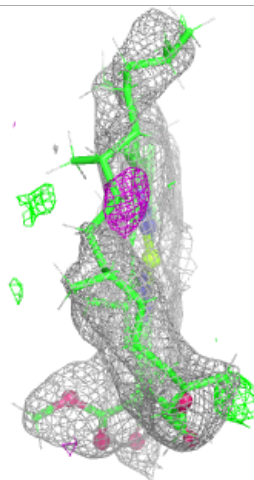
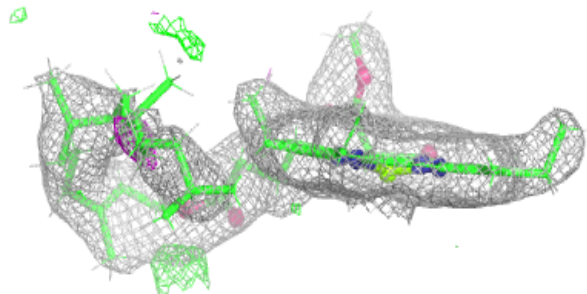
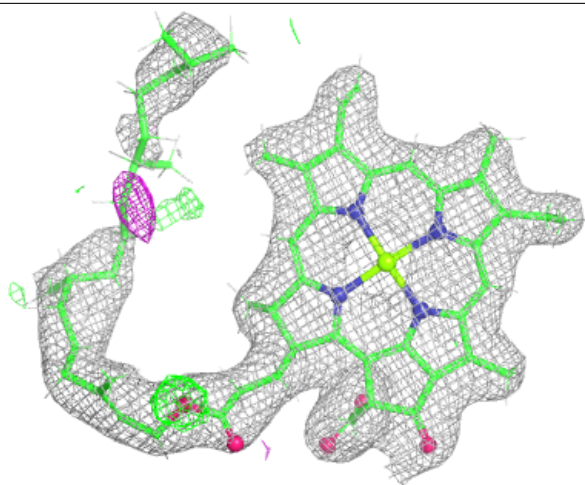
**Electron density around STE M 103:**

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



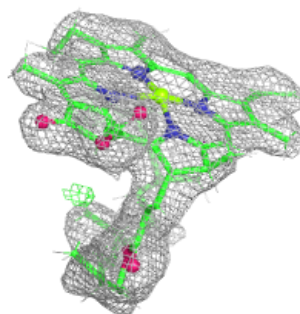
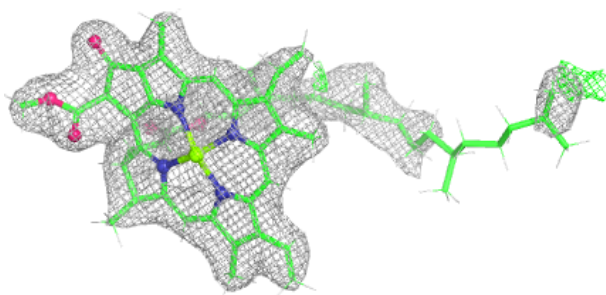
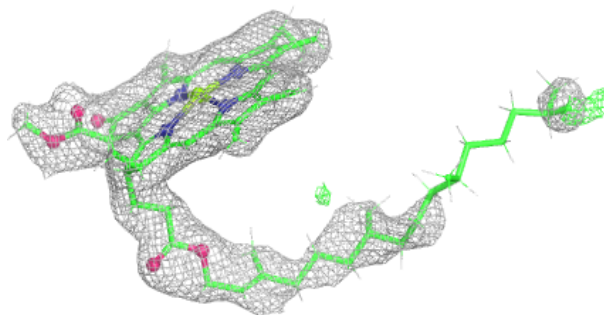
Electron density around CLA c 512:

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

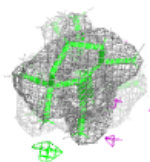
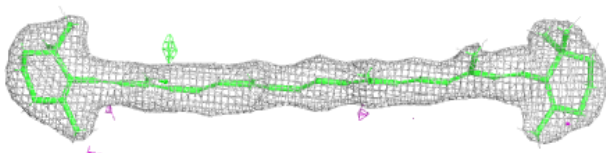


Electron density around CLA C 513:

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

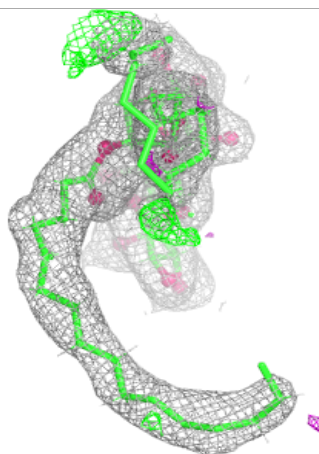
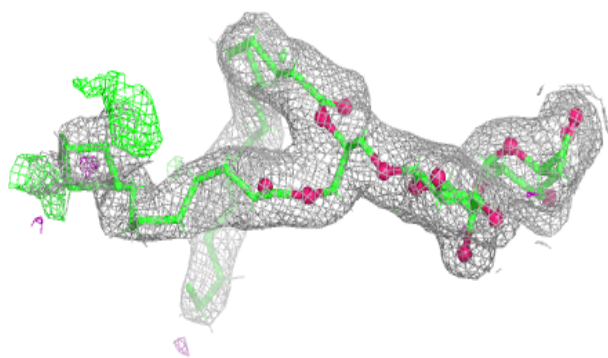
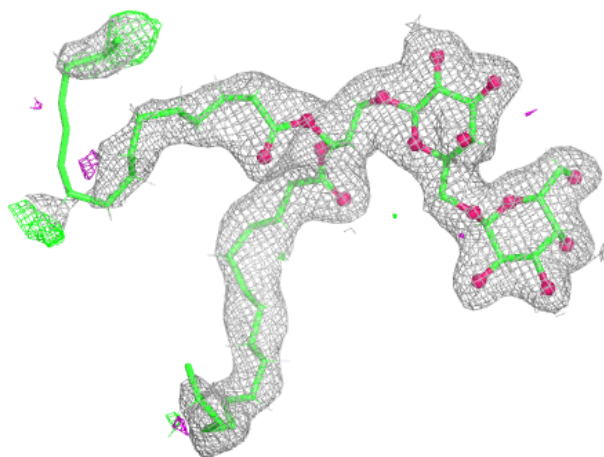
**Electron density around BCR C 514:**

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



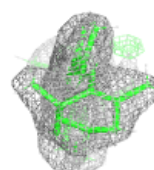
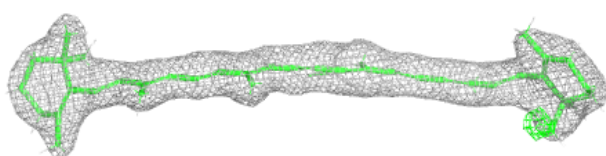
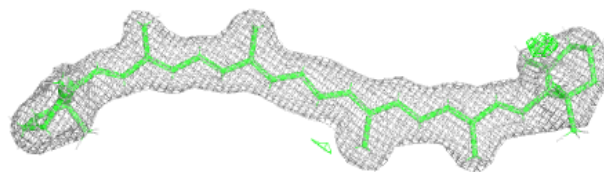
Electron density around DGD C 522:

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

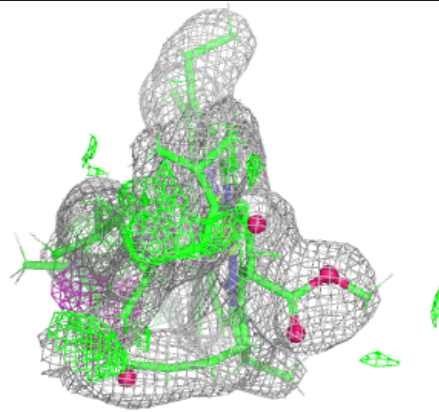
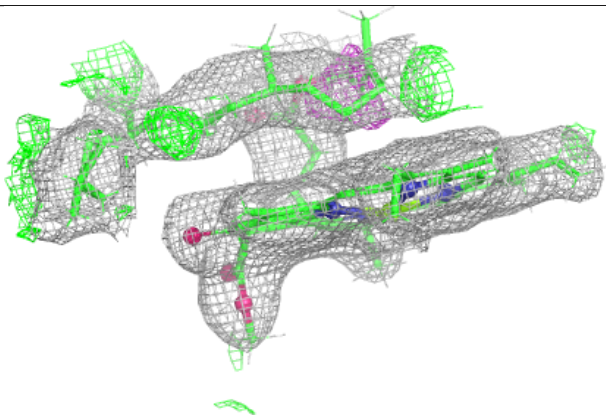
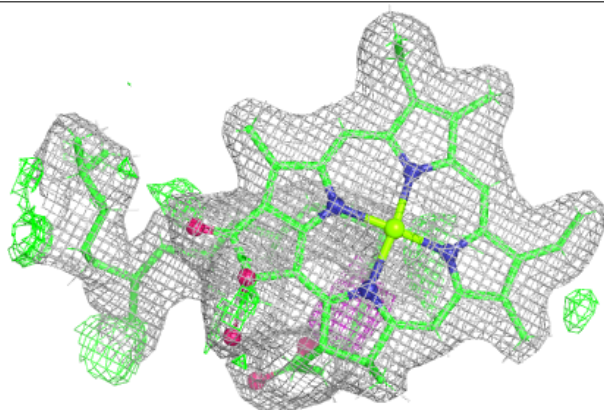


Electron density around BCR Z 101:

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

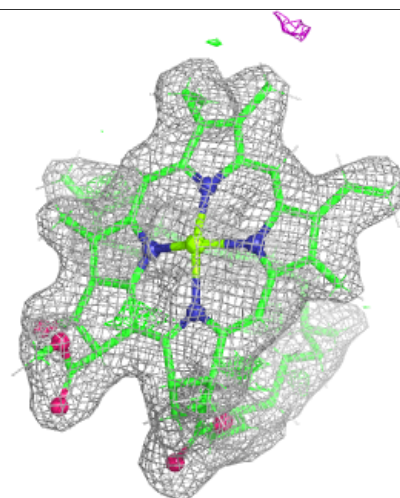
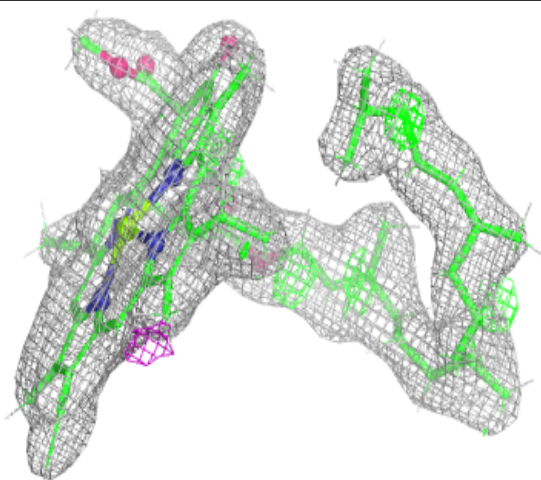
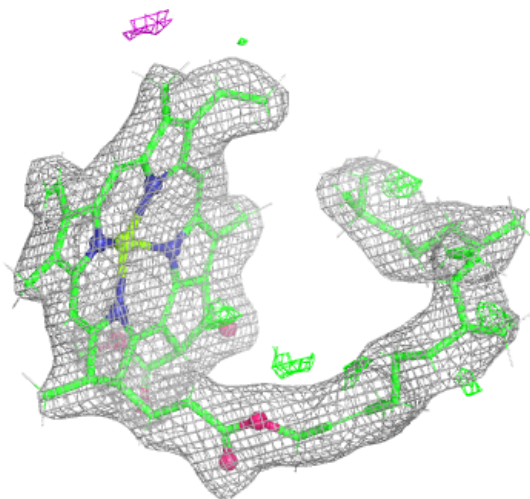
**Electron density around CLA B 601:**

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



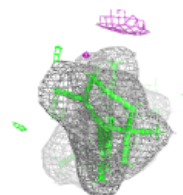
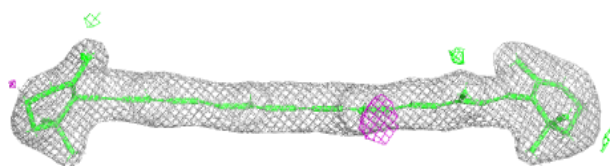
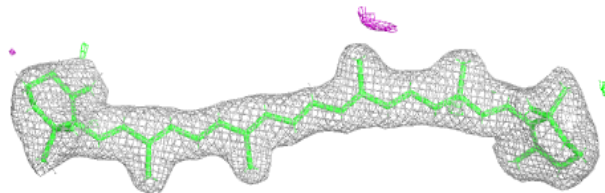
Electron density around CLA c 503:

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

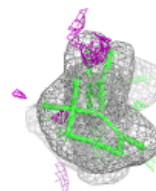
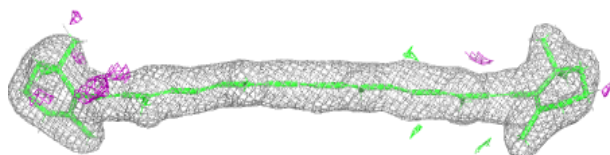
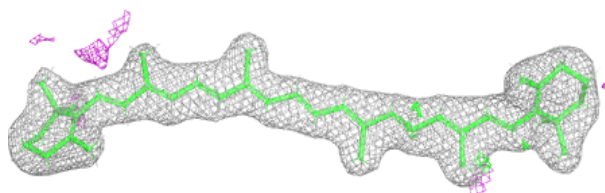


Electron density around BCR b 618:

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

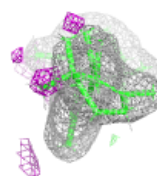
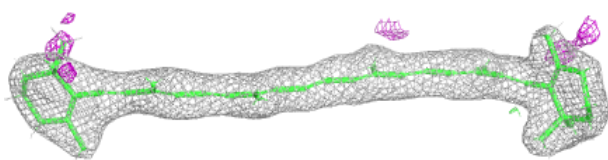
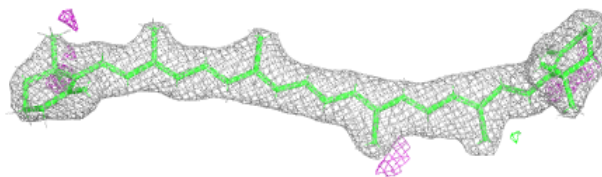
**Electron density around BCR B 618:**

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

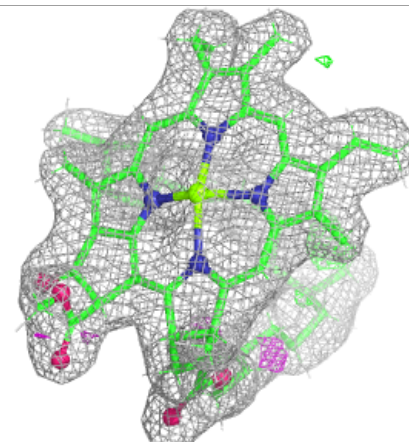
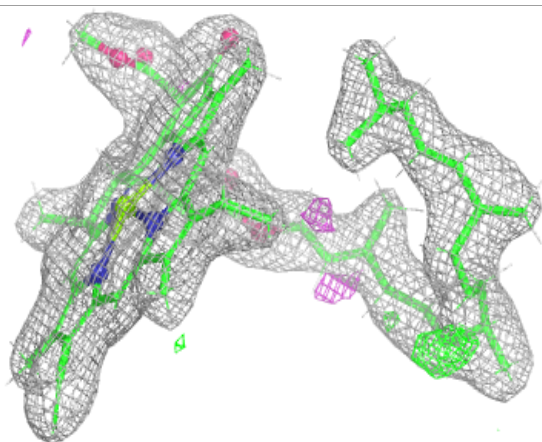
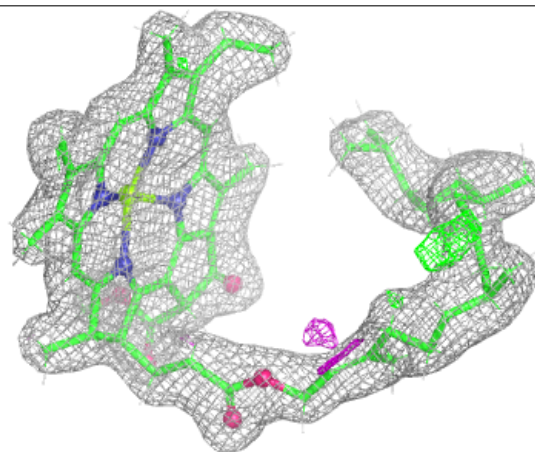


Electron density around BCR c 515:

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

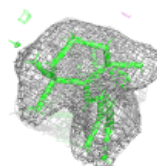
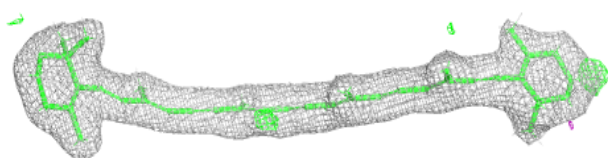
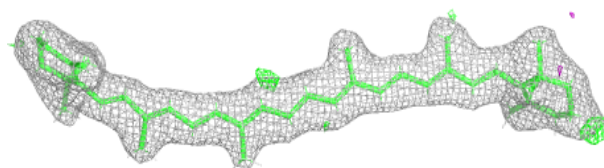
**Electron density around CLA C 503:**

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

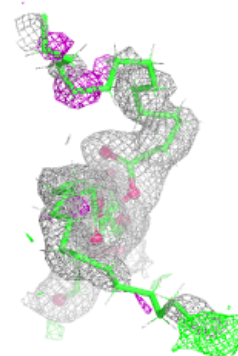
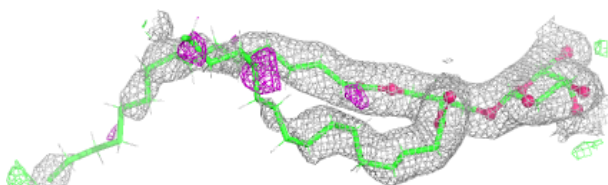
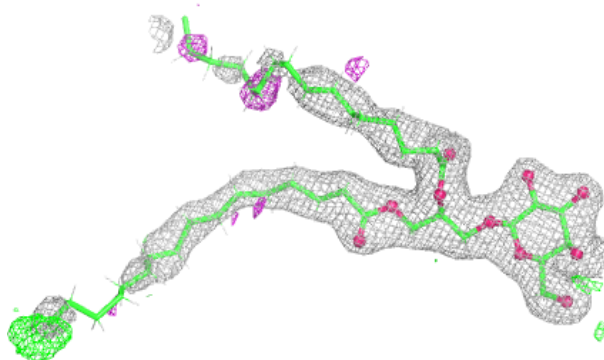


Electron density around BCR H 101:

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

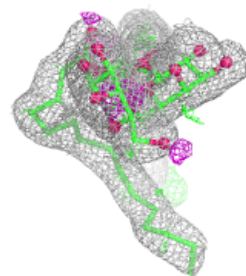
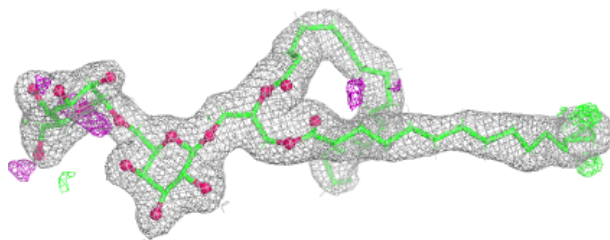
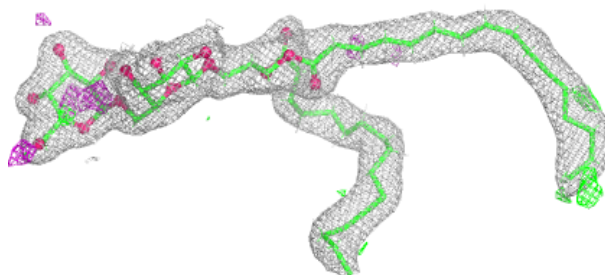
**Electron density around LMG D 407:**

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

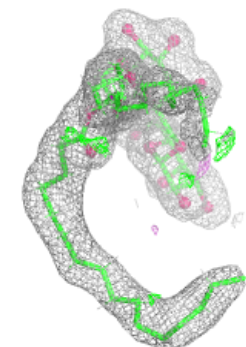
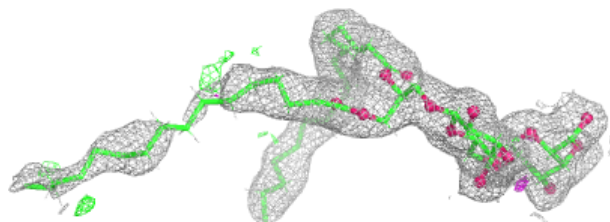
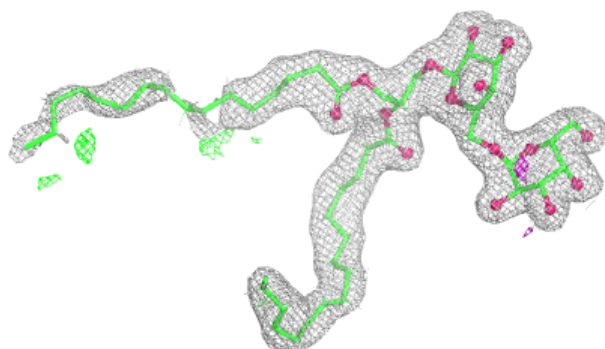


Electron density around DGD H 102:

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

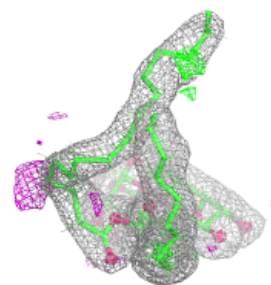
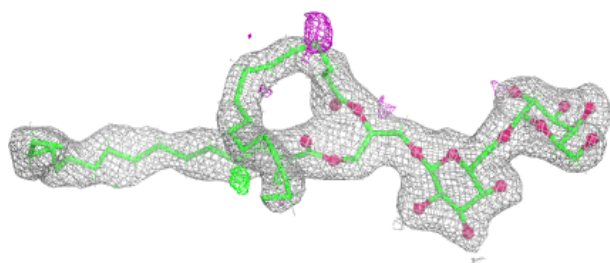
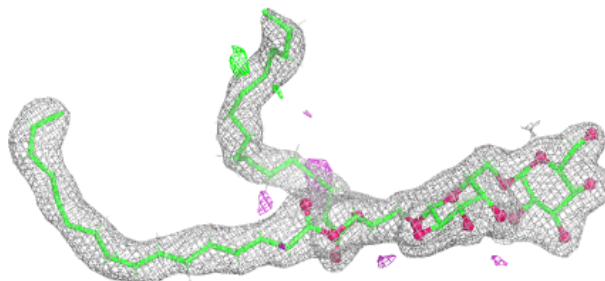
**Electron density around DGD c 519:**

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

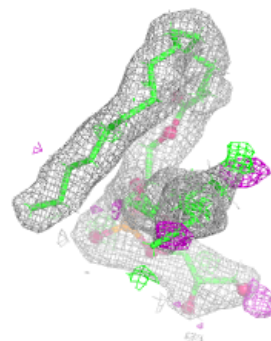
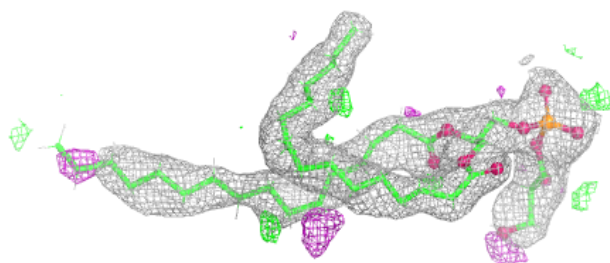
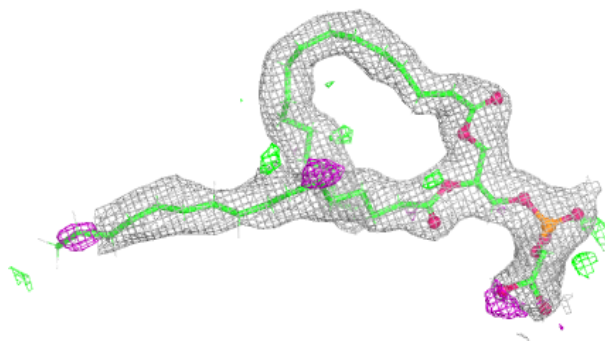


Electron density around DGD h 101:

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

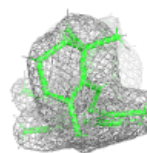
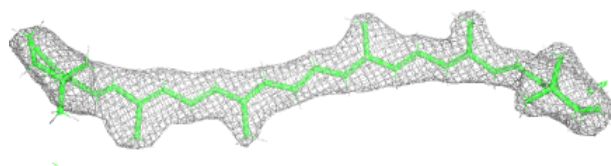
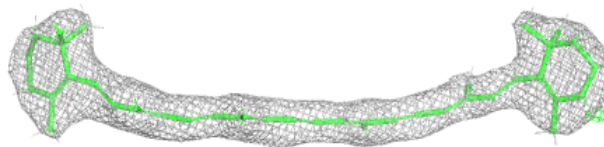
**Electron density around LHG D 411:**

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

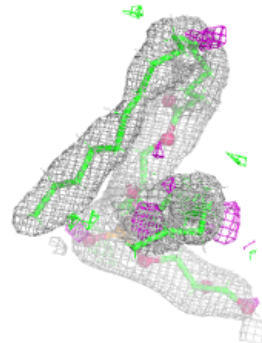
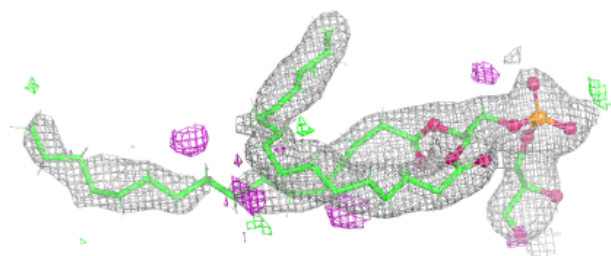
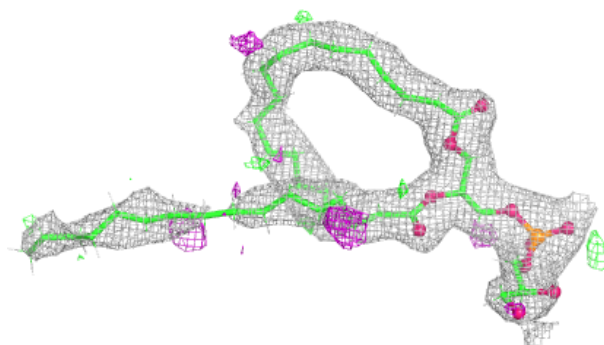


Electron density around BCR k 102:

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

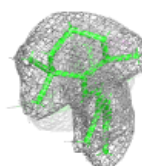
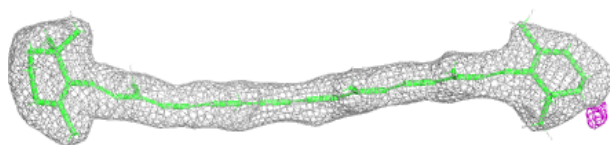
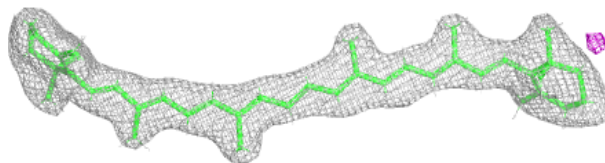
**Electron density around LHG d 407:**

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

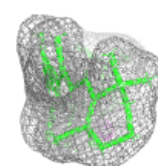
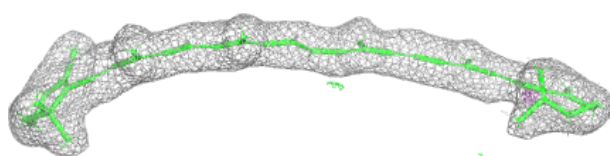
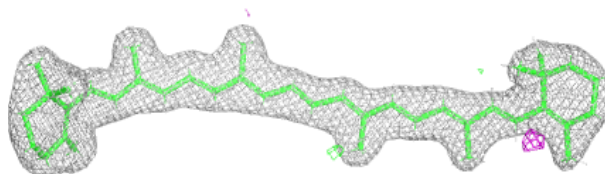


Electron density around BCR x 101:

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

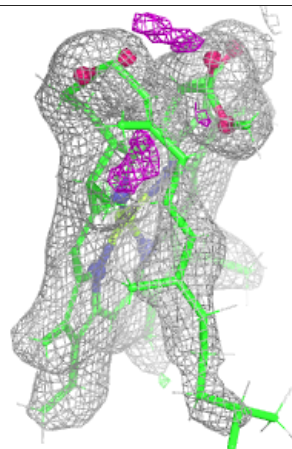
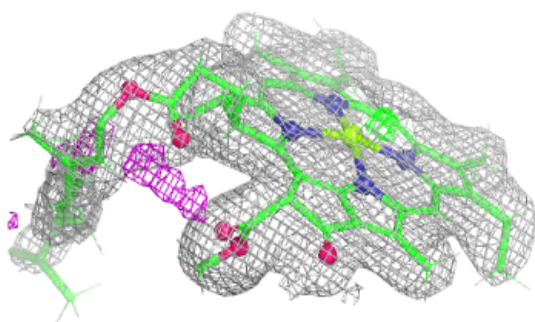
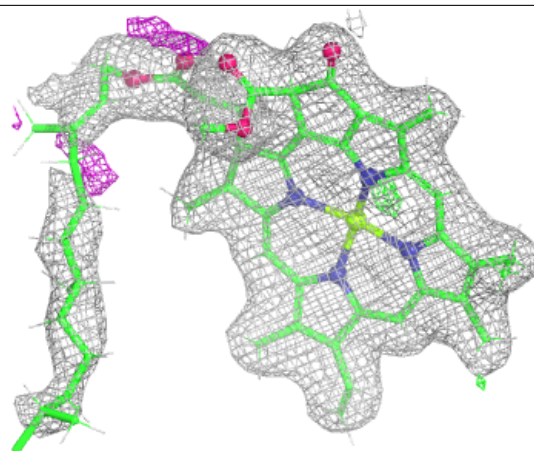
**Electron density around BCR T 101:**

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

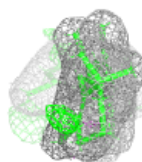
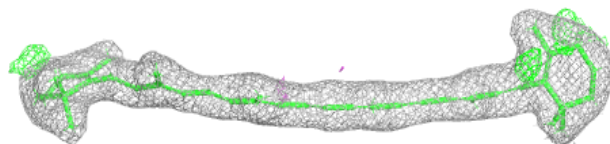
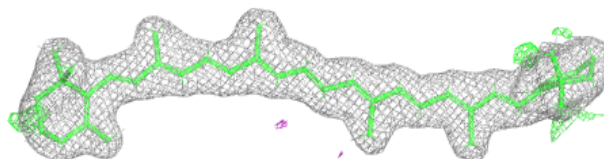


Electron density around CLA b 616:

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

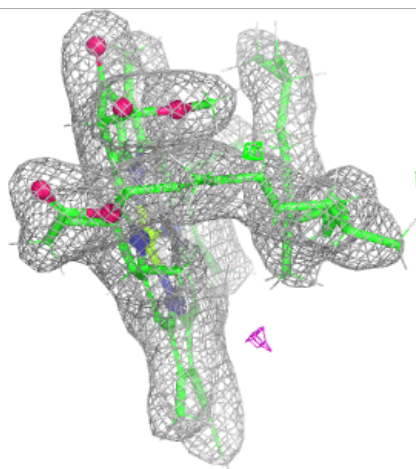
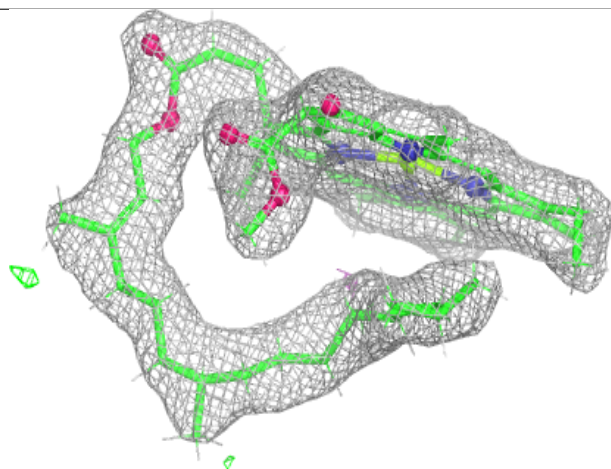
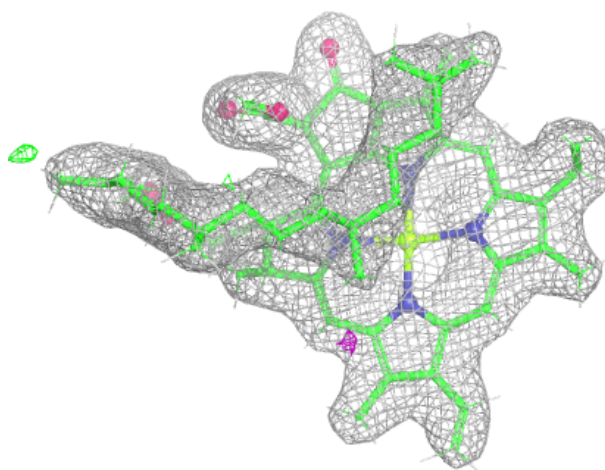
**Electron density around BCR b 617:**

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



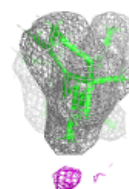
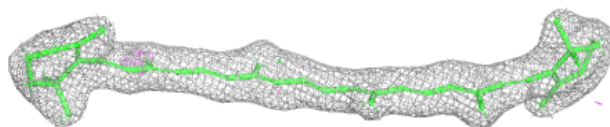
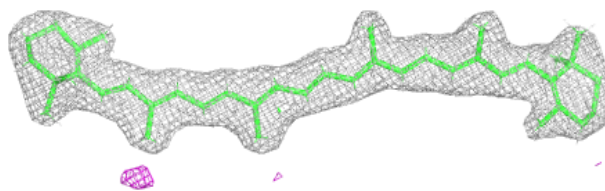
Electron density around CLA C 510:

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

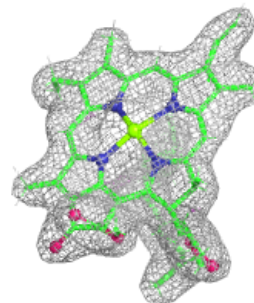
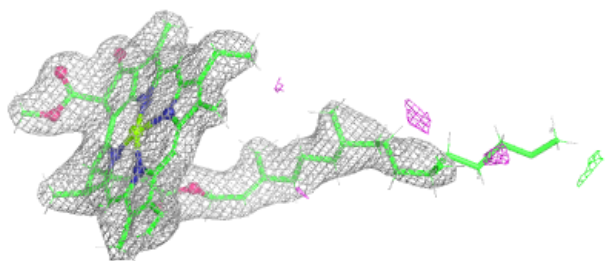
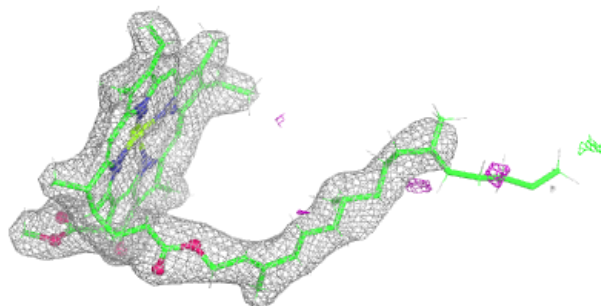


Electron density around BCR b 619:

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

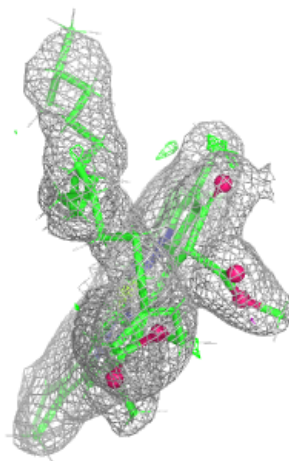
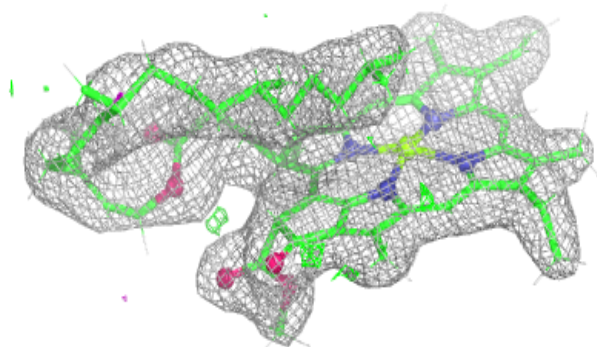
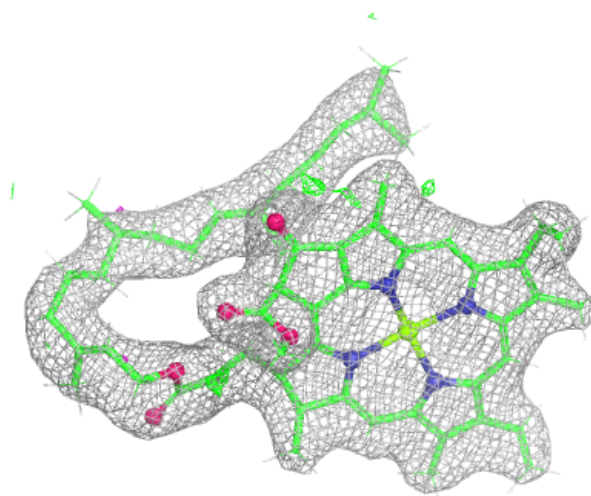
**Electron density around CLA c 508:**

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



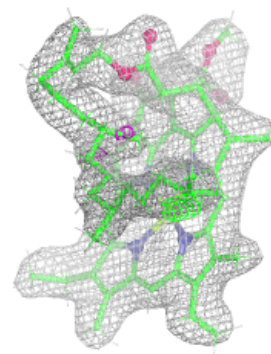
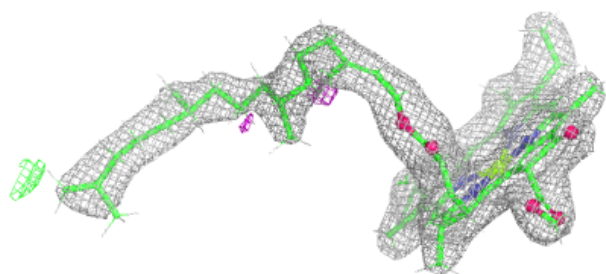
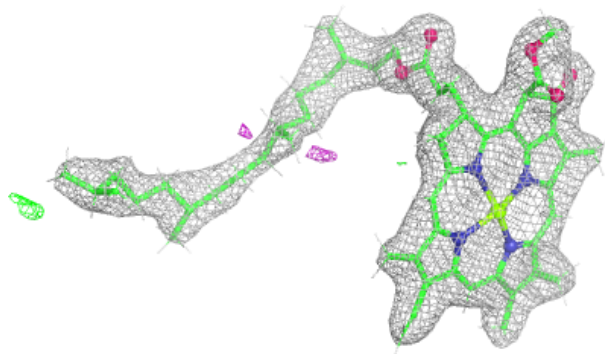
Electron density around CLA c 509:

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

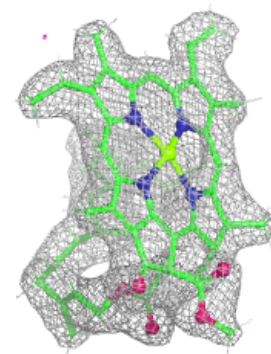
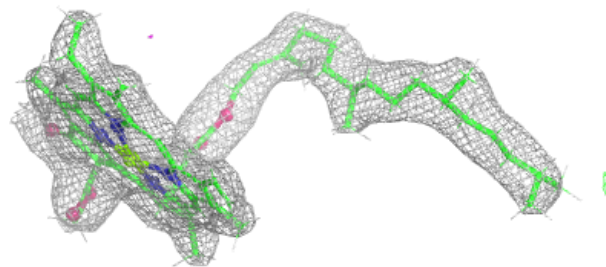
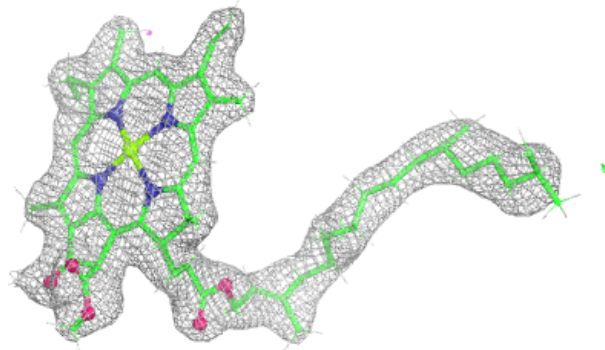


Electron density around CLA c 511:

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

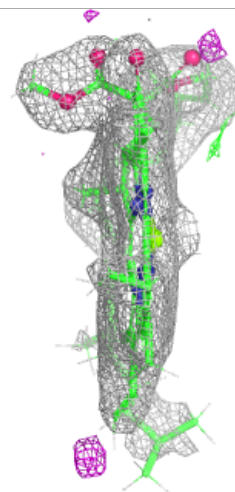
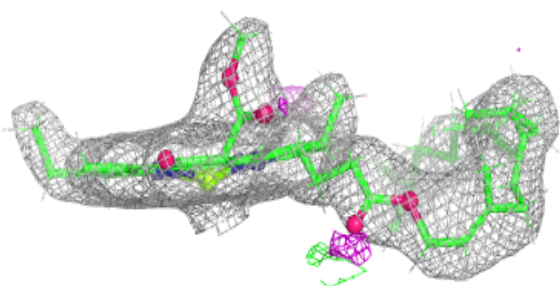
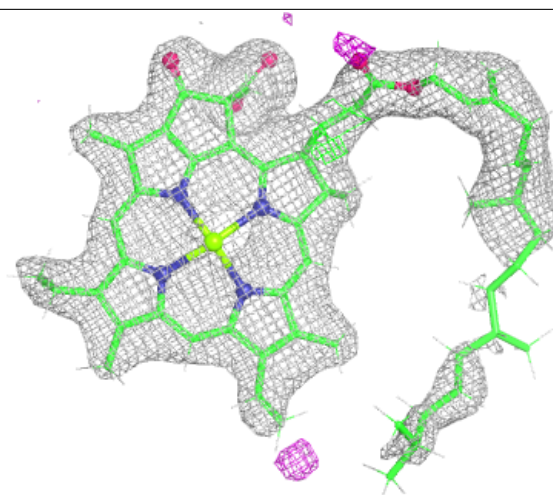
**Electron density around CLA C 511:**

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



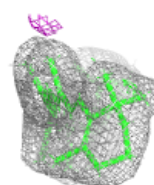
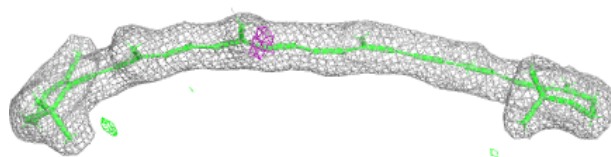
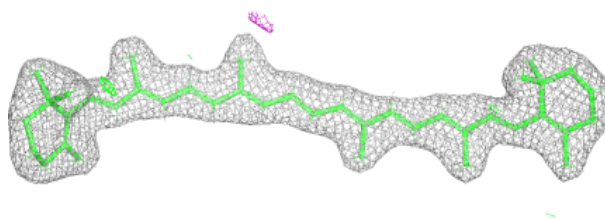
Electron density around CLA C 512:

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

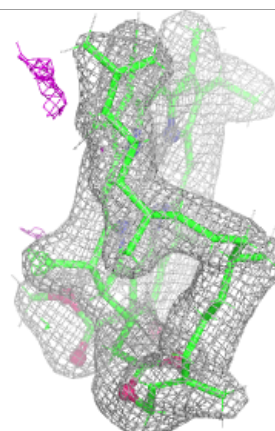
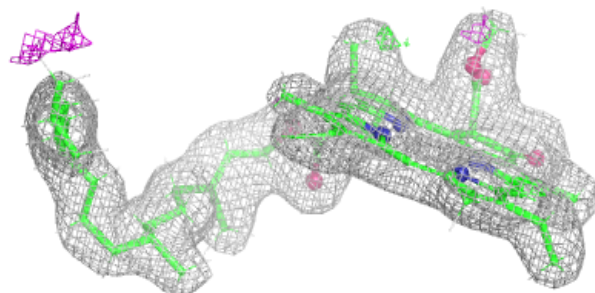
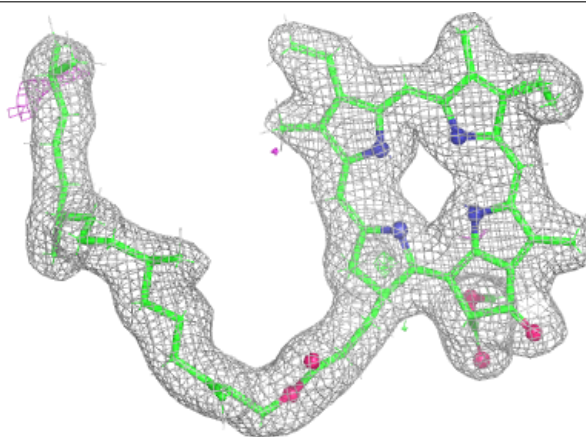


Electron density around BCR t 101:

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

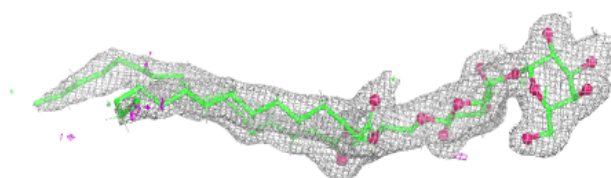
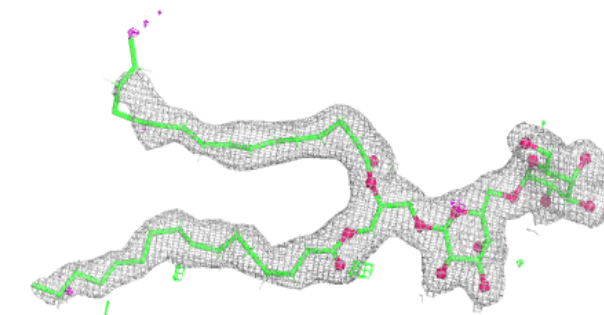
**Electron density around PHO d 401:**

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

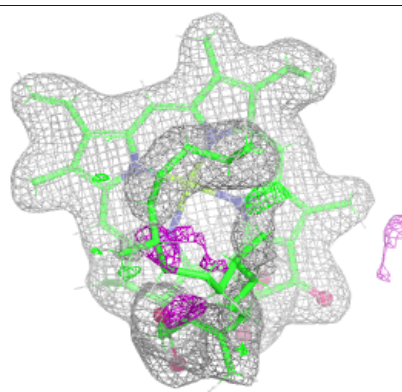
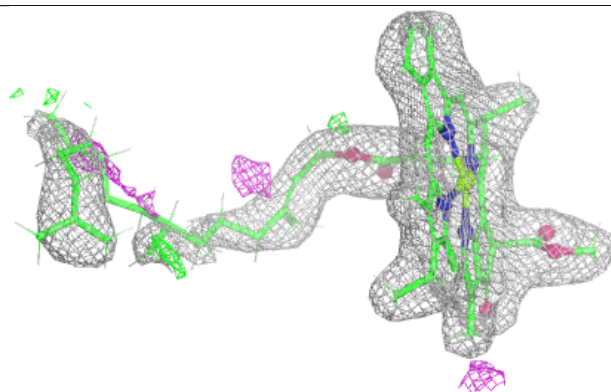
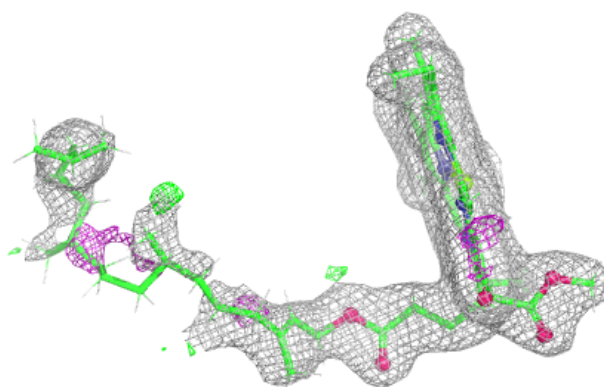


Electron density around DGD C 523:

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

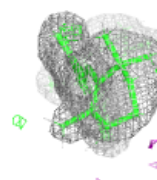
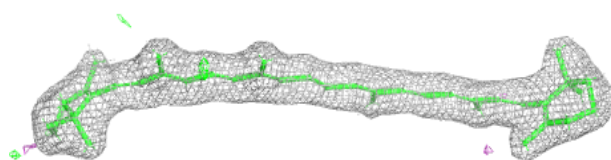
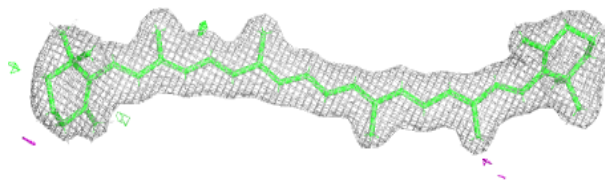
**Electron density around CLA C 506:**

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

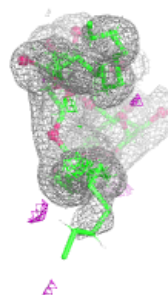
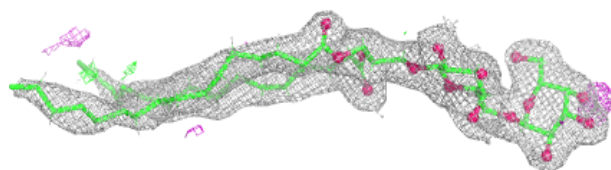
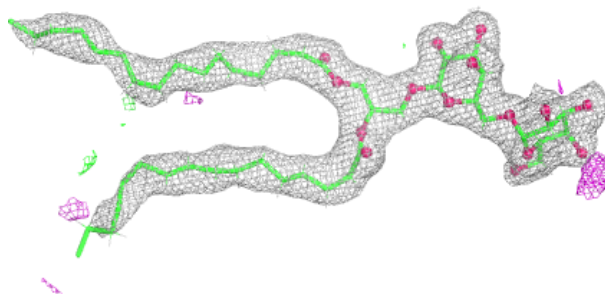


Electron density around BCR B 619:

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

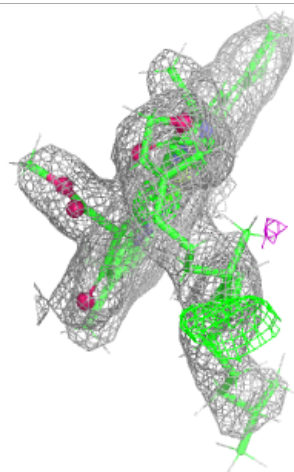
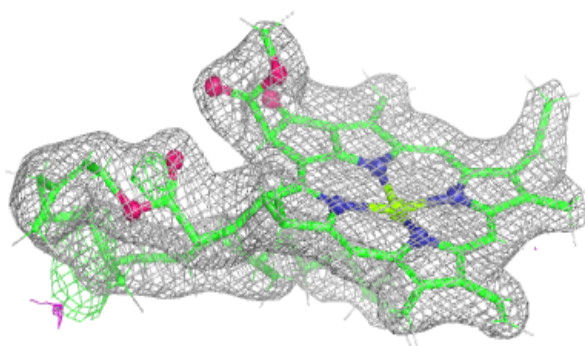
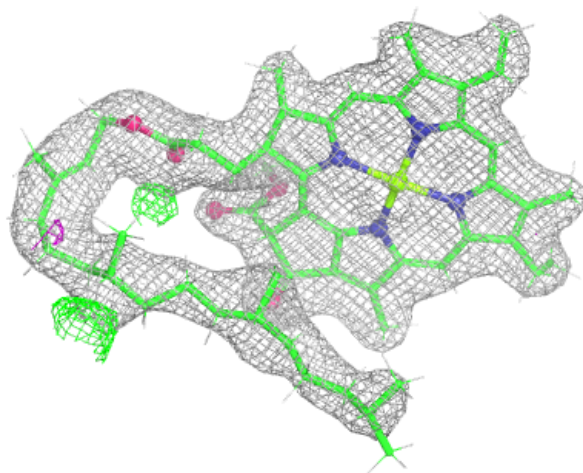
**Electron density around DGD c 520:**

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



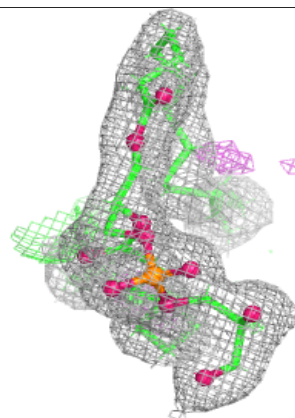
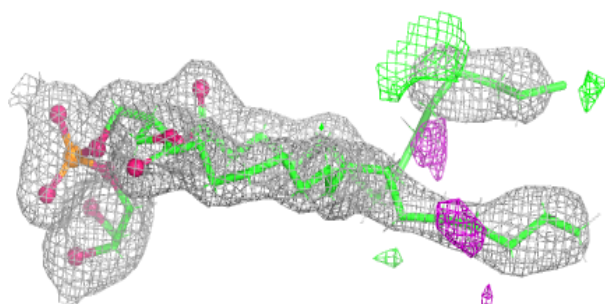
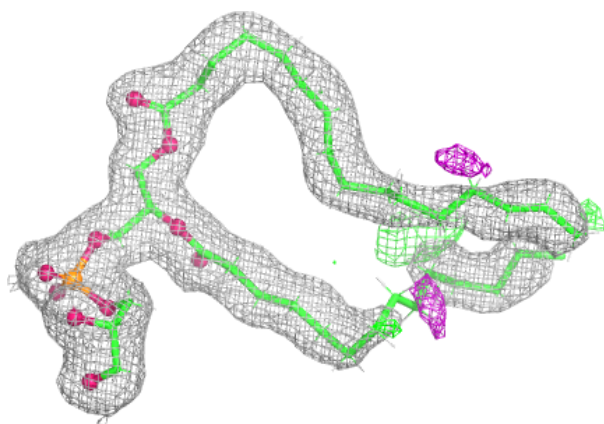
Electron density around CLA C 509:

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

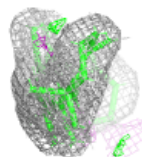
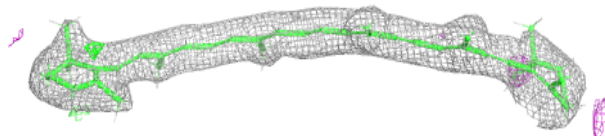
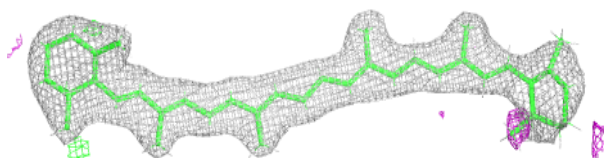


Electron density around LHG D 409:

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

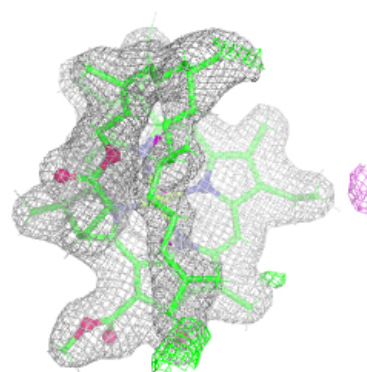
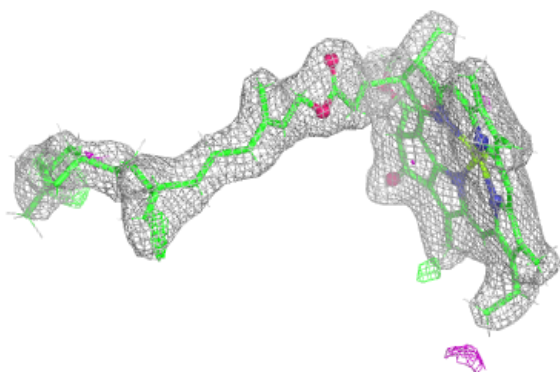
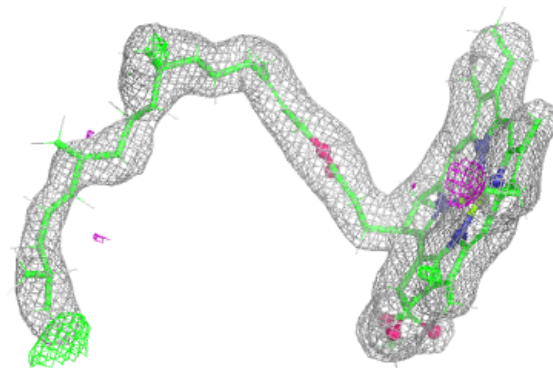
**Electron density around BCR D 404:**

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

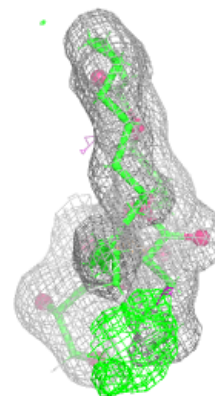
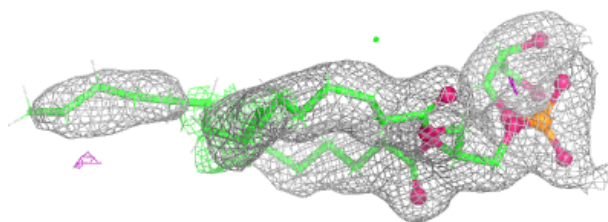
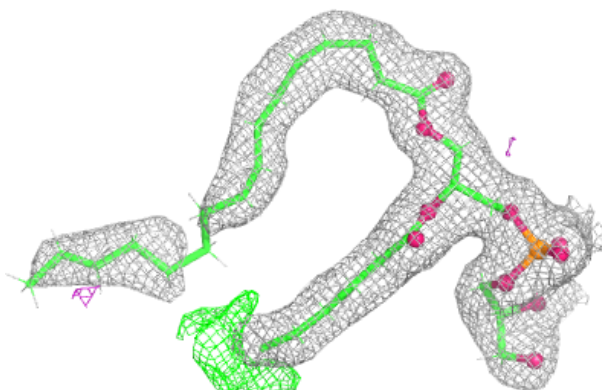


Electron density around CLA b 606:

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

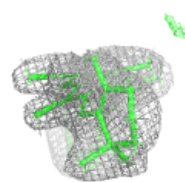
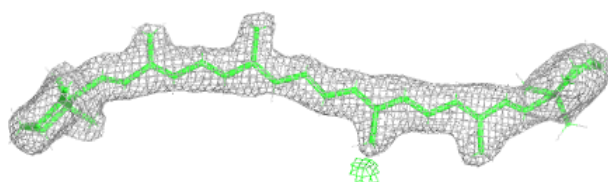
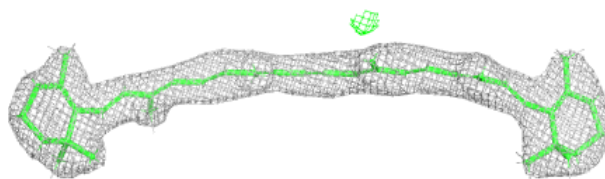
**Electron density around LHG d 409:**

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

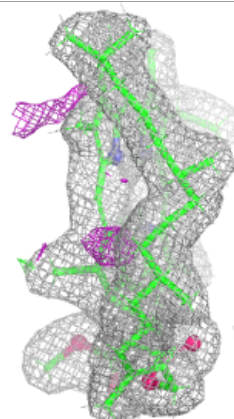
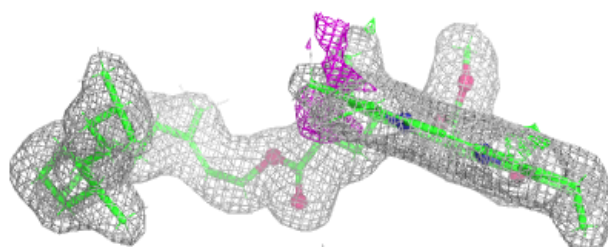
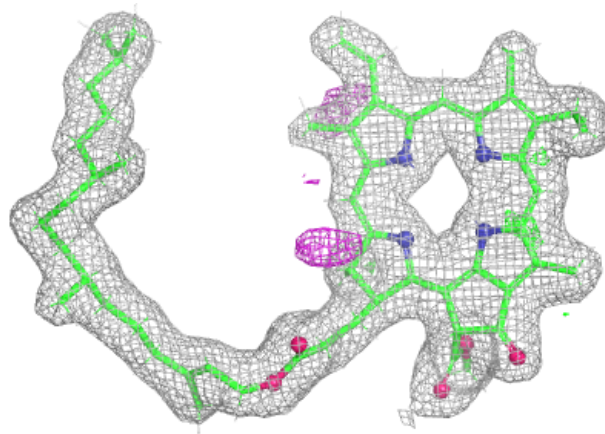


Electron density around BCR K 101:

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

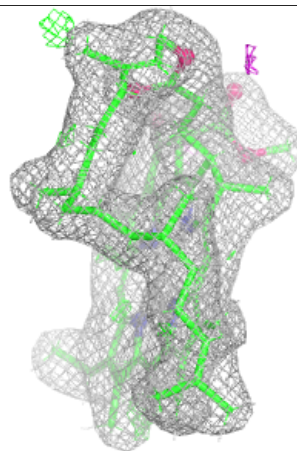
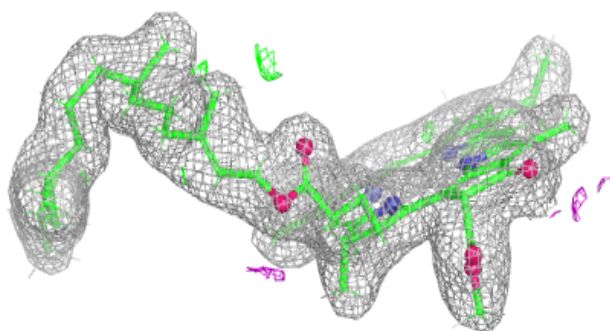
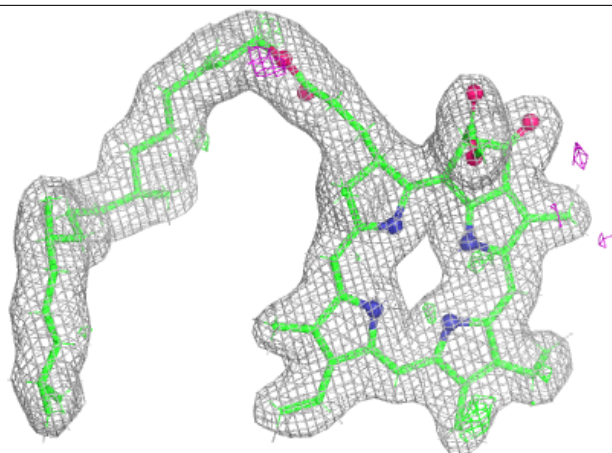
**Electron density around PHO A 609:**

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



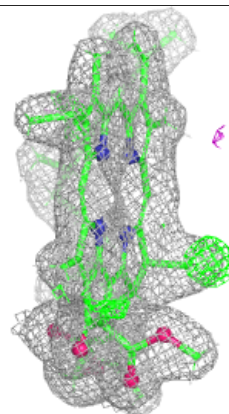
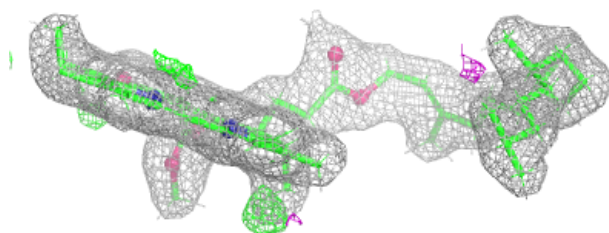
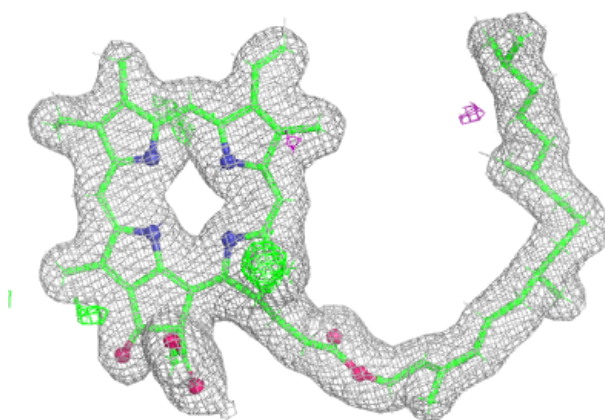
Electron density around PHO D 401:

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

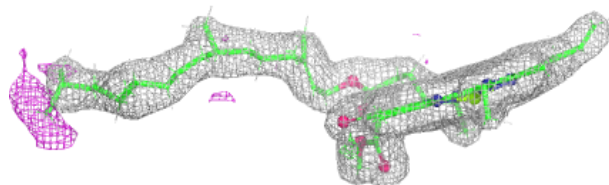
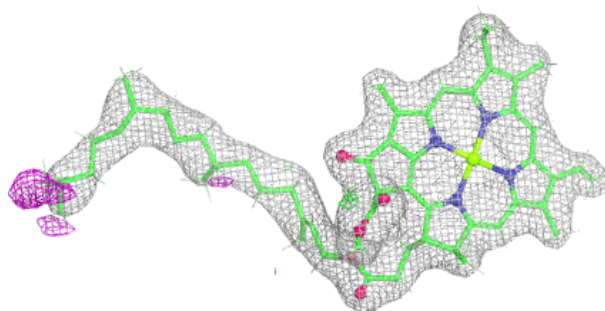


Electron density around PHO a 609:

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

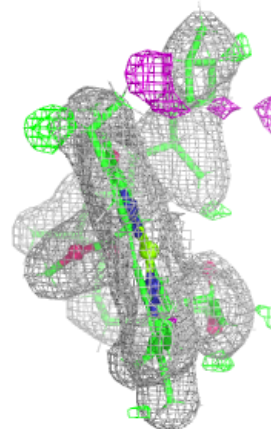
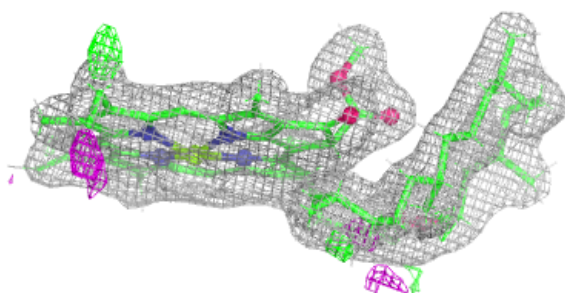
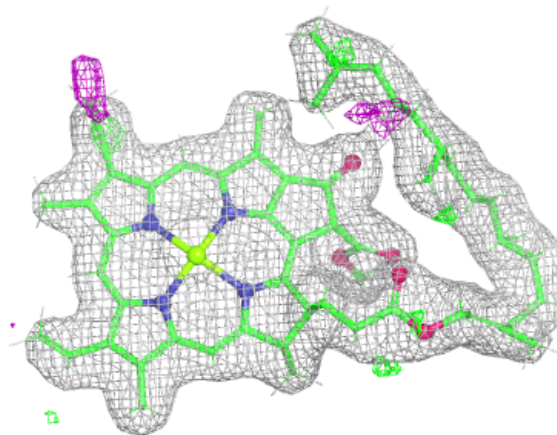
**Electron density around CLA b 602:**

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

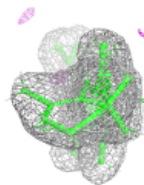
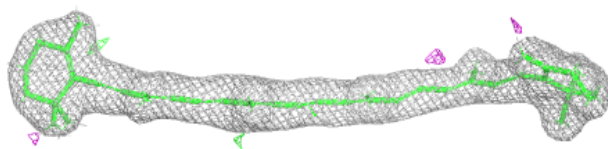
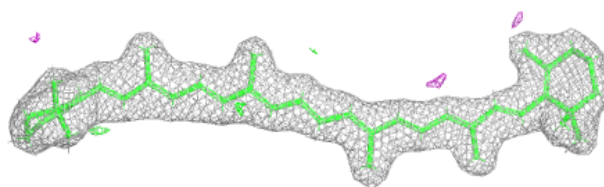


Electron density around CLA B 610:

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

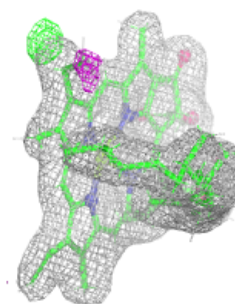
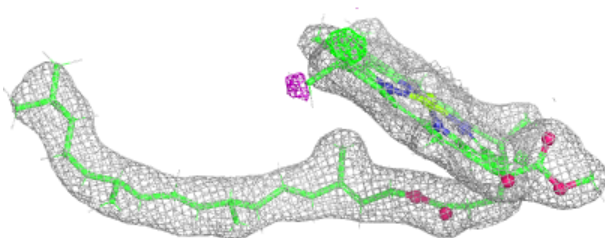
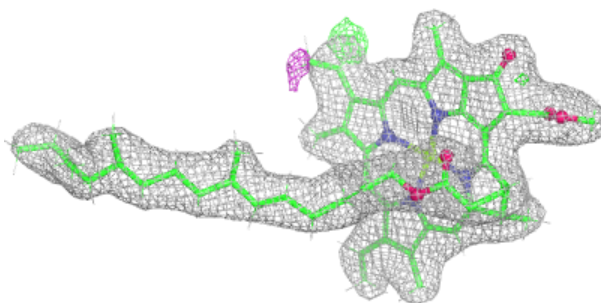
**Electron density around BCR B 617:**

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

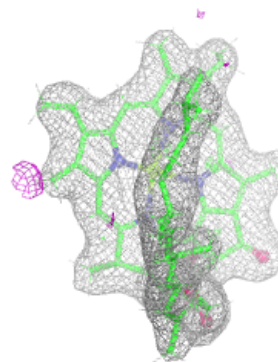
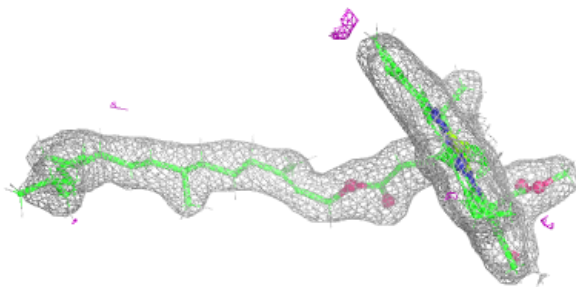
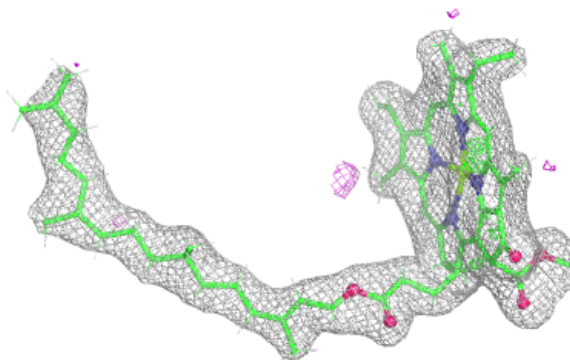


Electron density around CLA b 608:

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

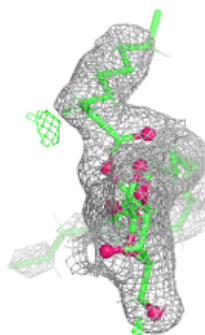
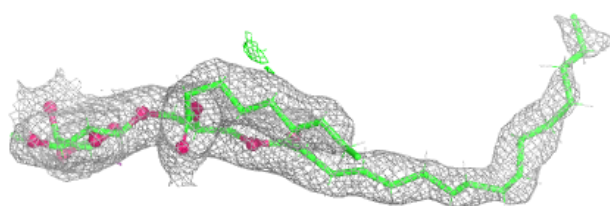
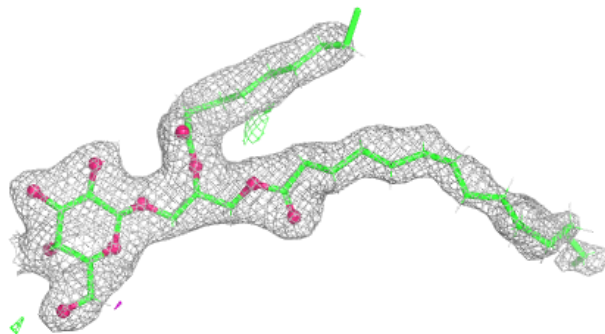
**Electron density around CLA b 609:**

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

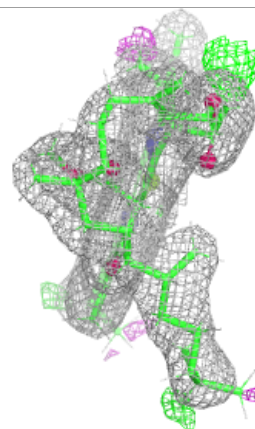
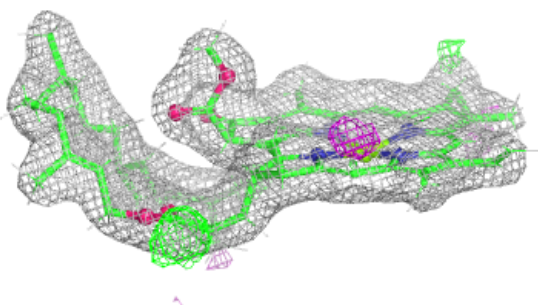
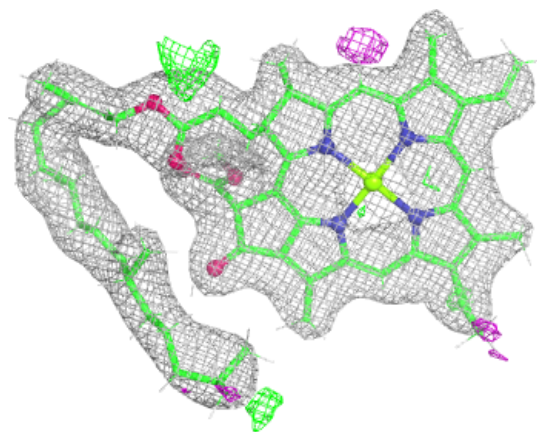


Electron density around LMG d 411:

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

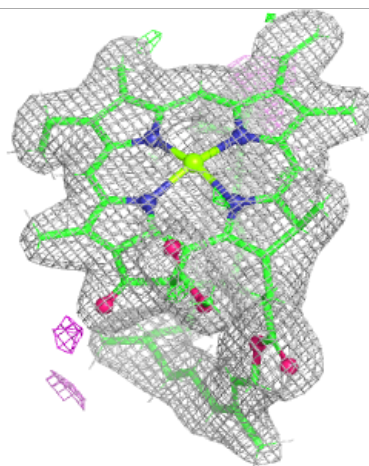
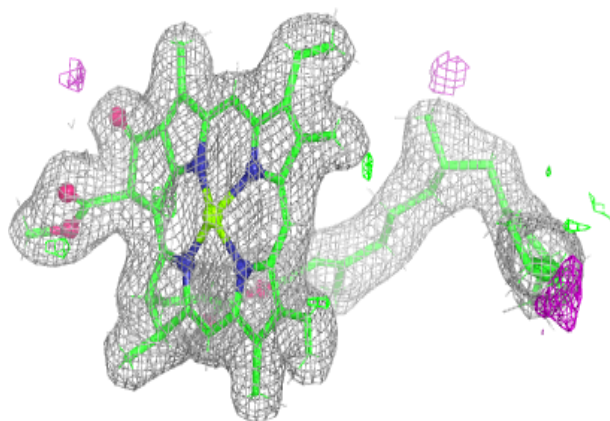
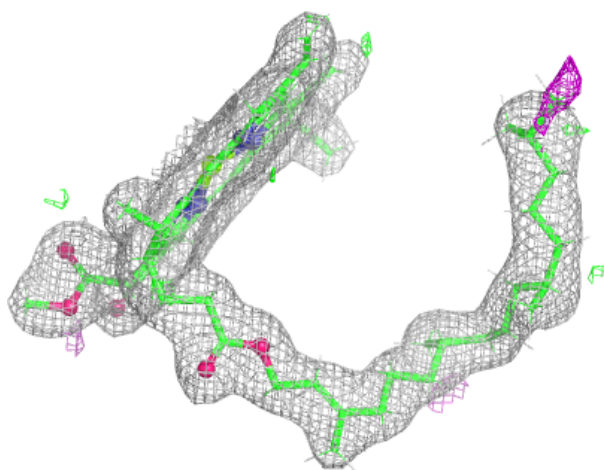
**Electron density around CLA b 610:**

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



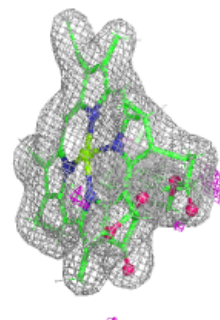
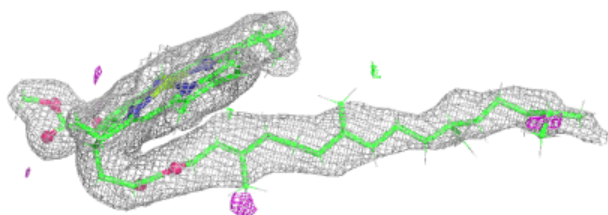
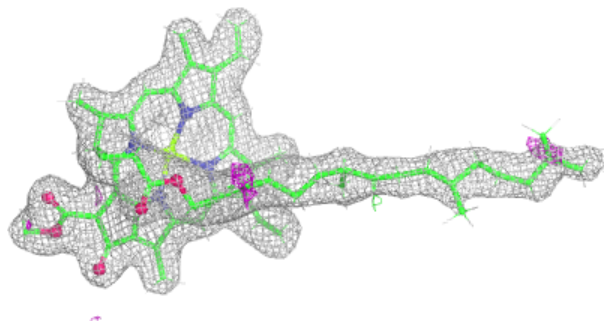
Electron density around CLA b 611:

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



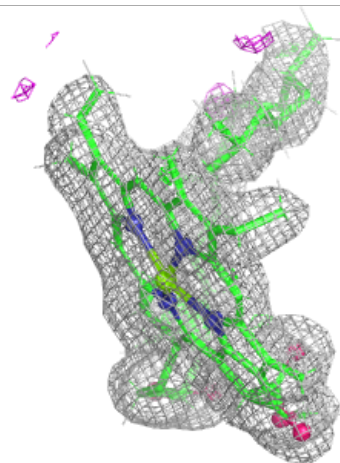
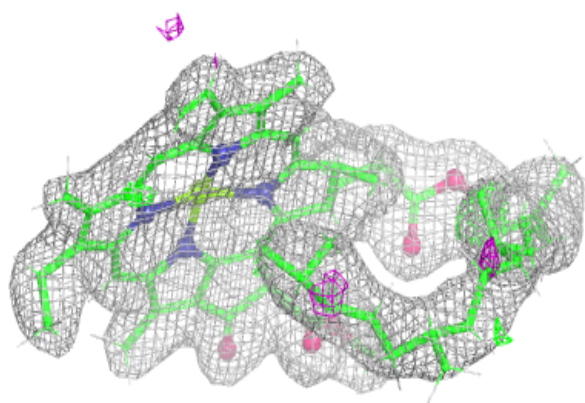
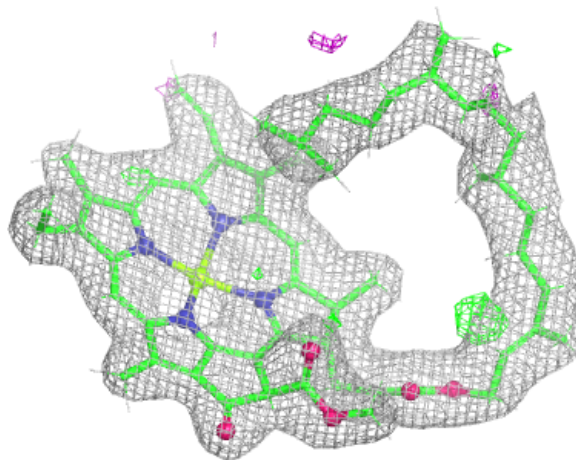
Electron density around CLA b 614:

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



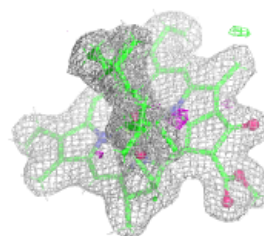
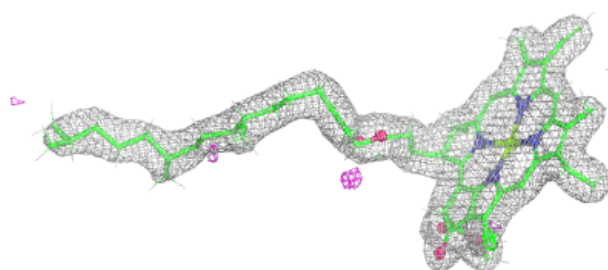
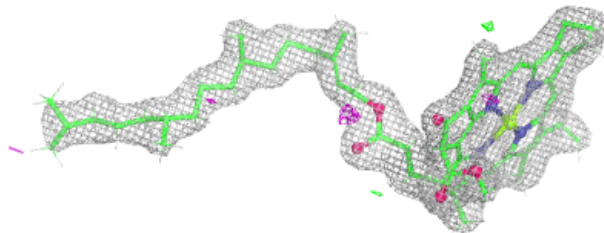
Electron density around CLA b 615:

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

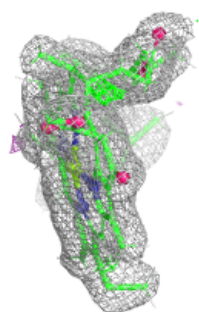
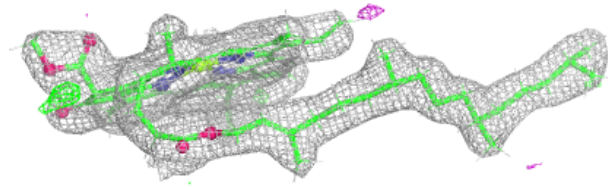
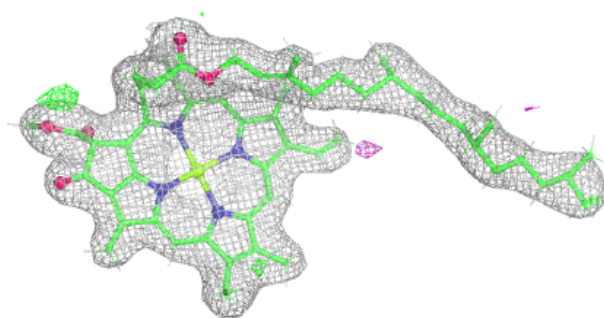


Electron density around CLA C 502:

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

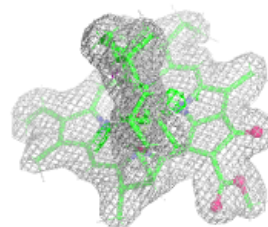
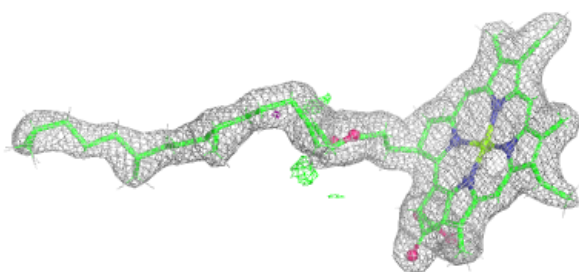
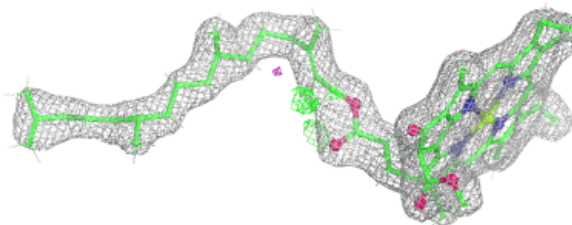
**Electron density around CLA c 501:**

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

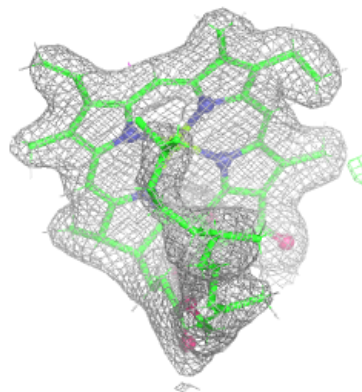
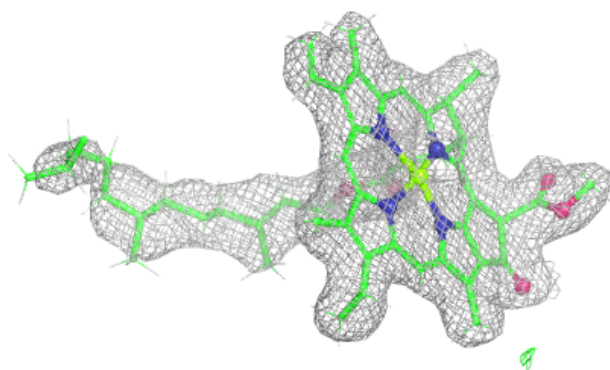
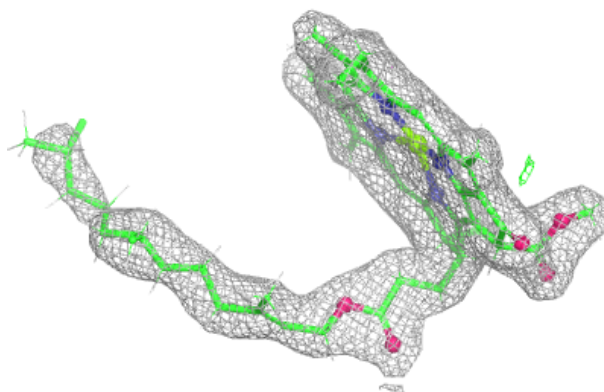


Electron density around CLA c 502:

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

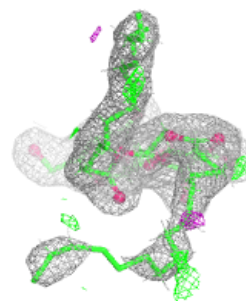
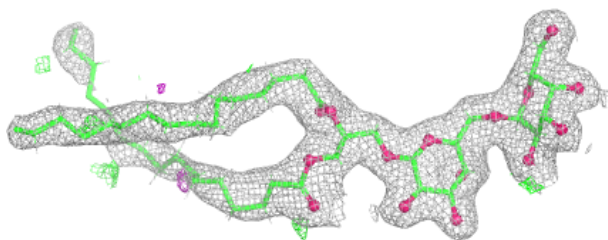
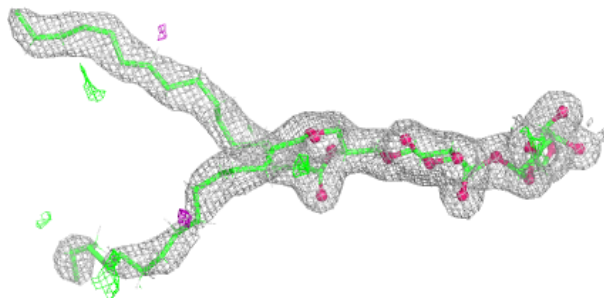
**Electron density around CLA c 504:**

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

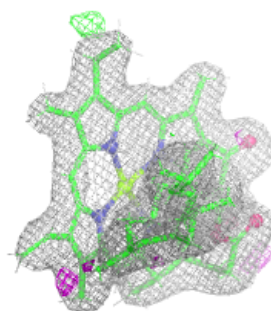
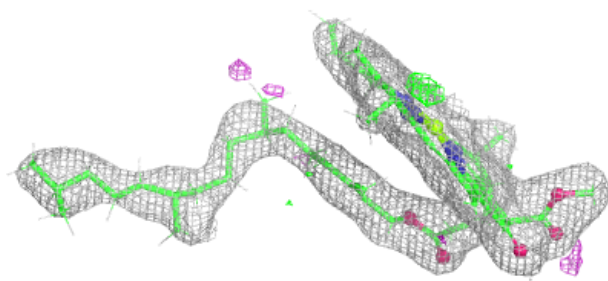
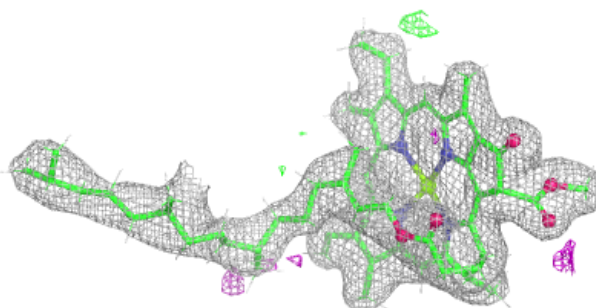


Electron density around DGD C 521:

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

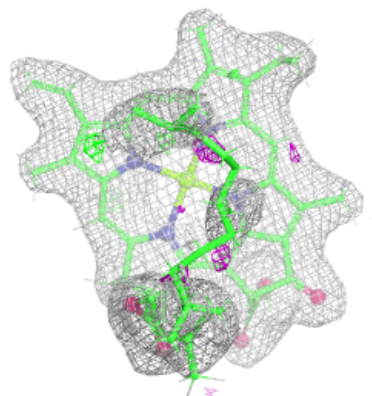
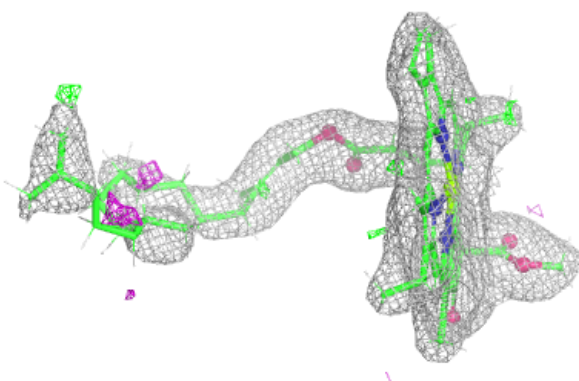
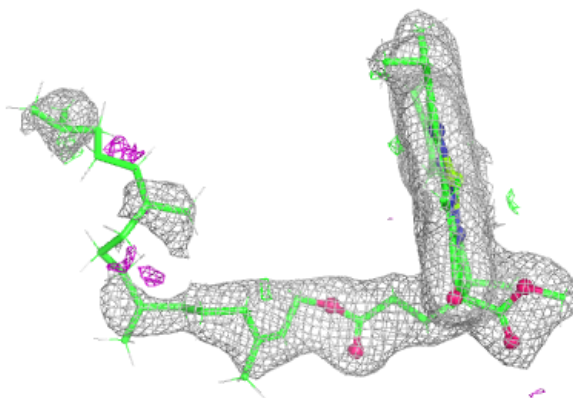
**Electron density around CLA c 505:**

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



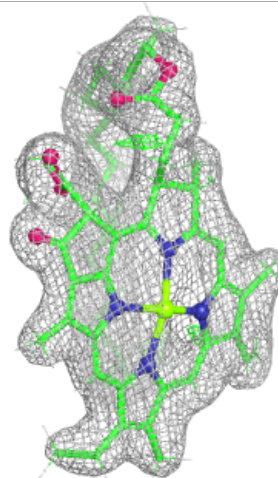
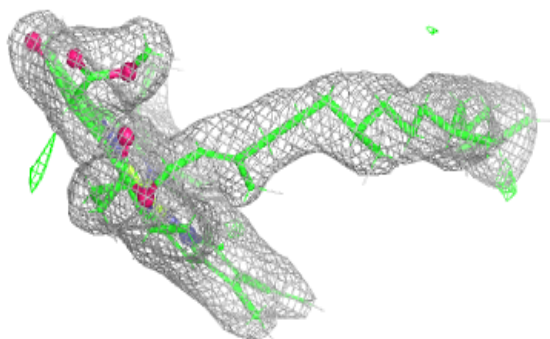
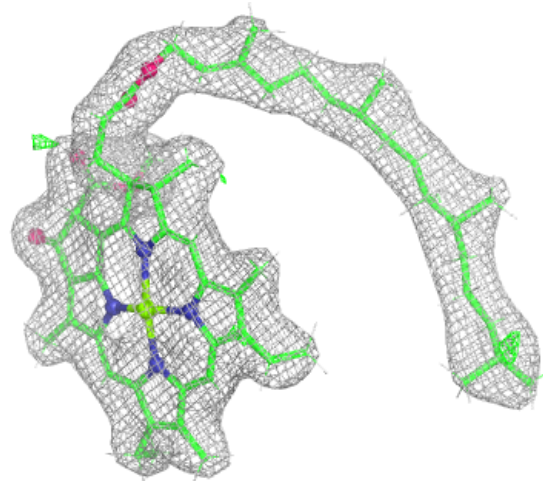
Electron density around CLA c 506:

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



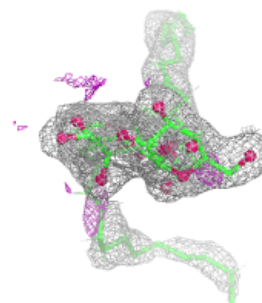
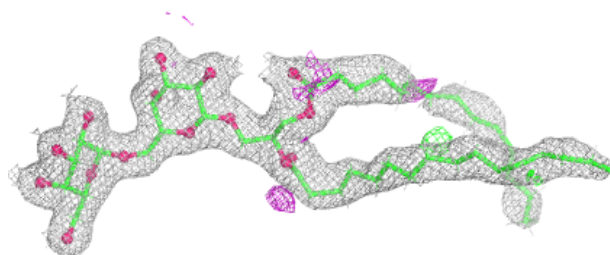
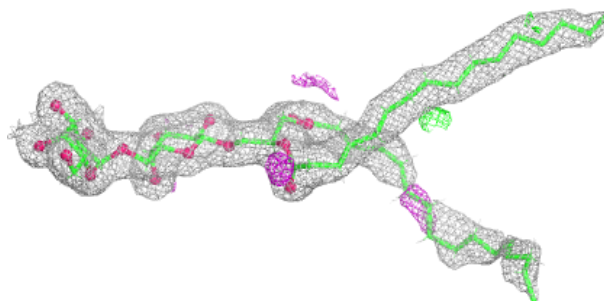
Electron density around CLA c 507:

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

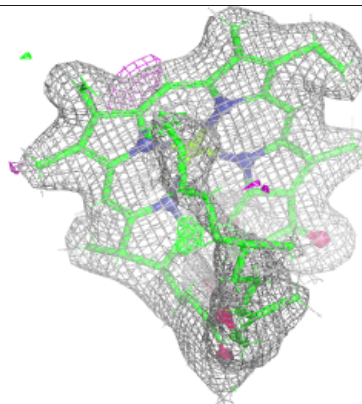
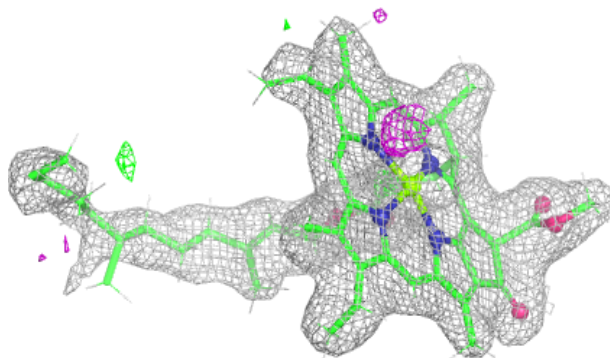
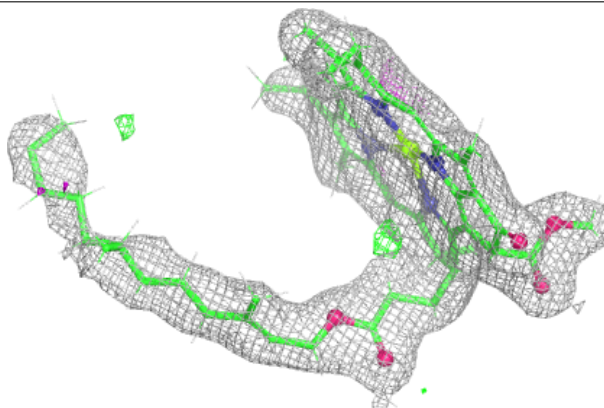


Electron density around DGD c 518:

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

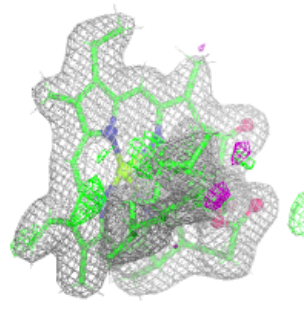
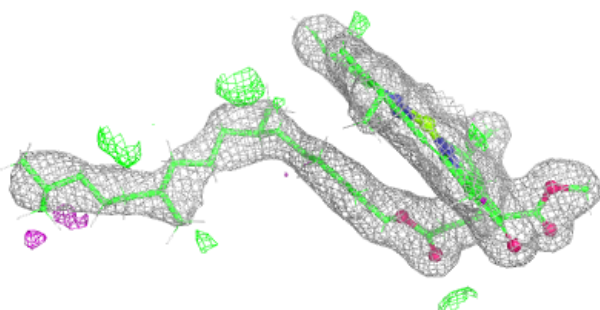
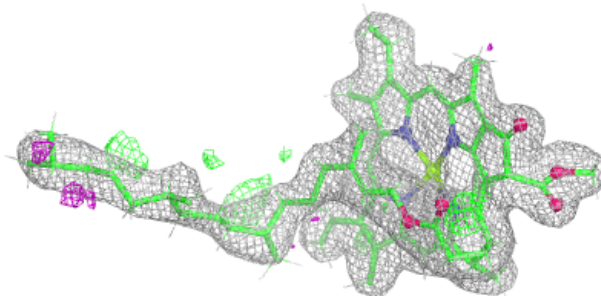
**Electron density around CLA C 504:**

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

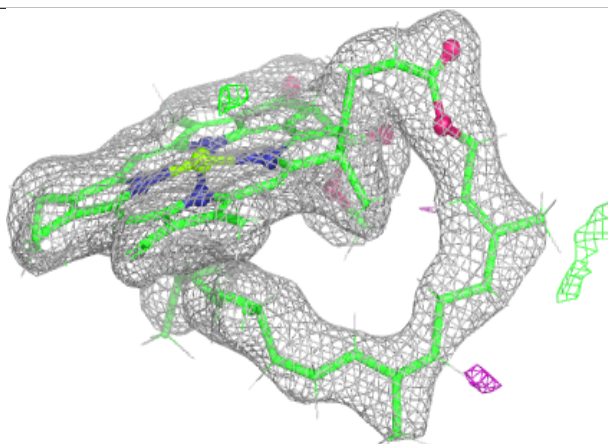
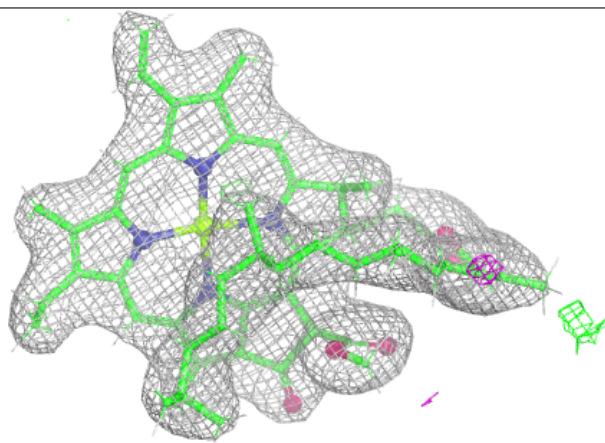


Electron density around CLA C 505:

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

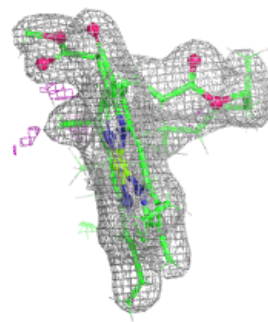
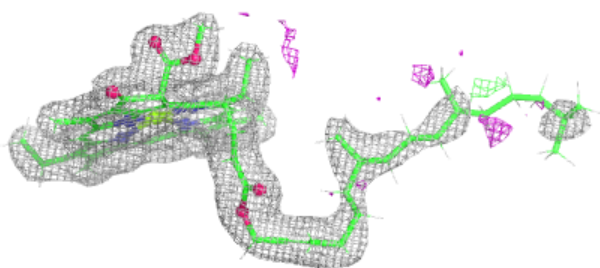
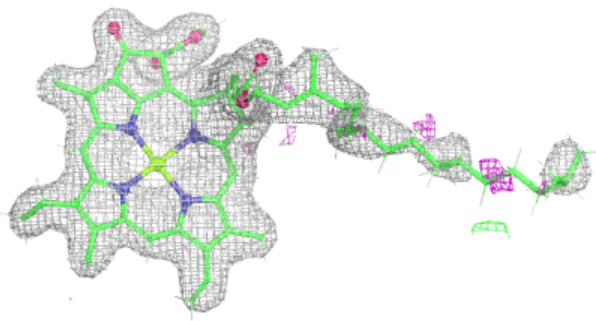
**Electron density around CLA c 510:**

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

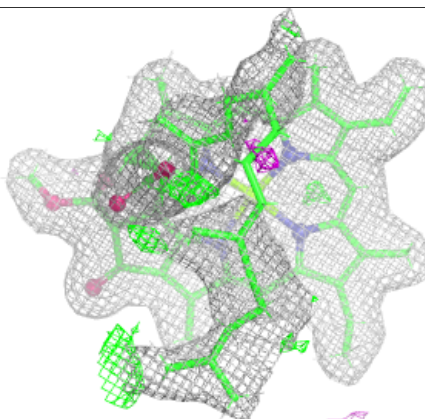
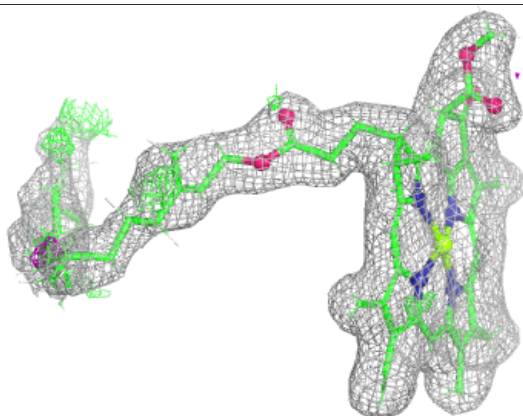
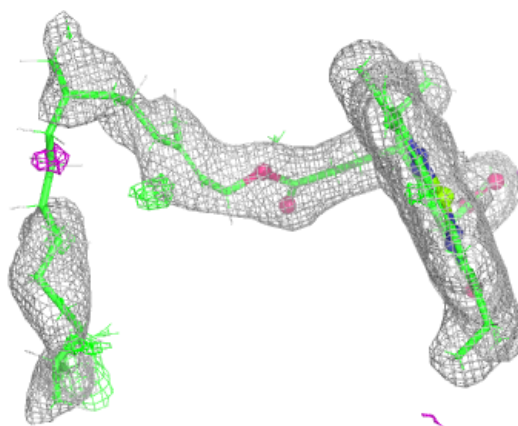


Electron density around CLA a 608:

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

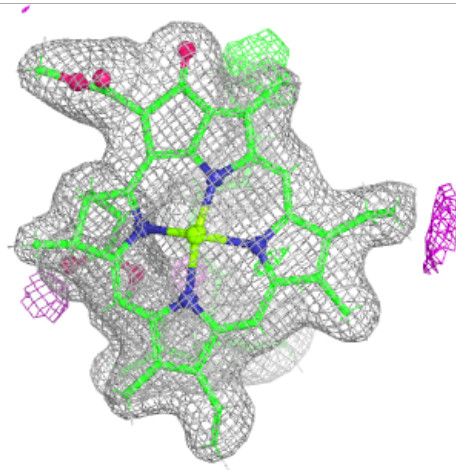
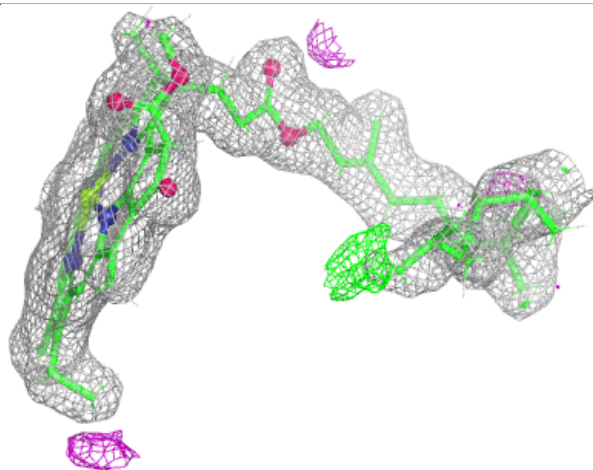
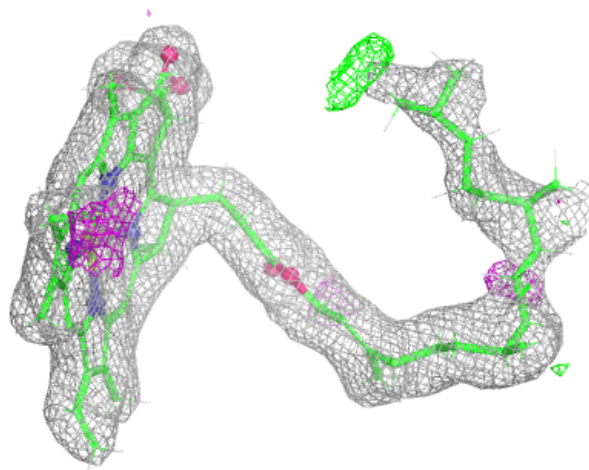
**Electron density around CLA a 610:**

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



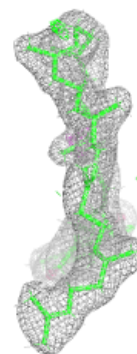
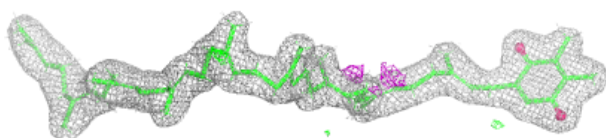
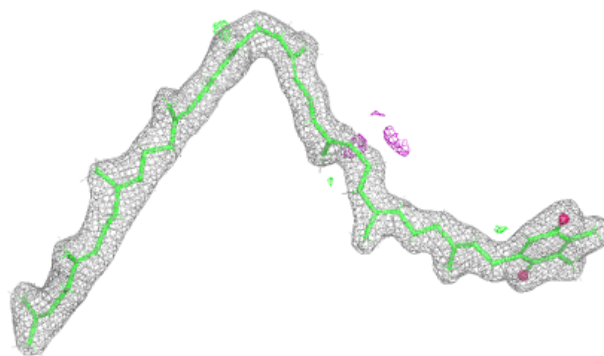
Electron density around CLA B 606:

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

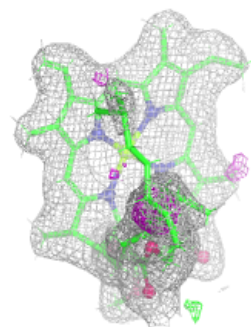
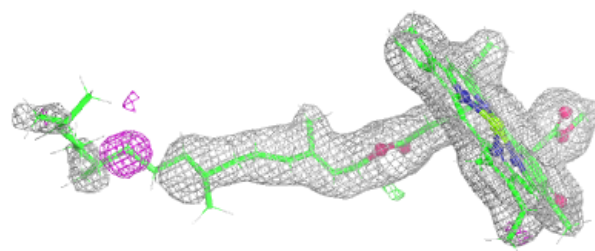
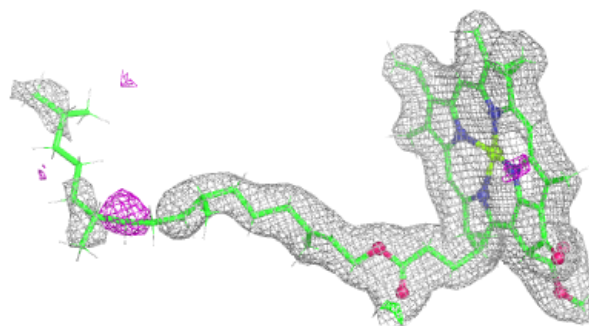


Electron density around PL9 D 405:

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

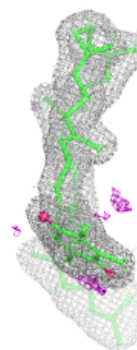
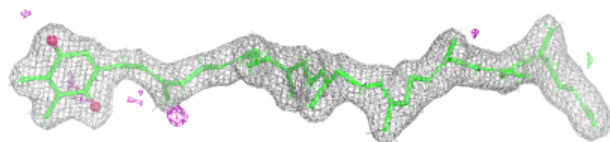
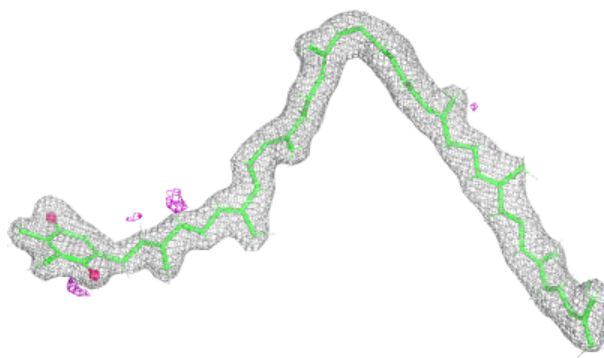
**Electron density around CLA d 403:**

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



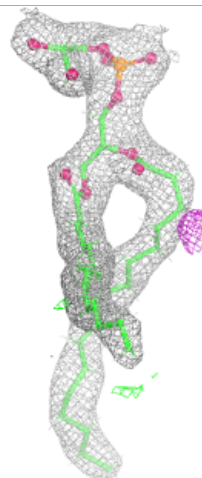
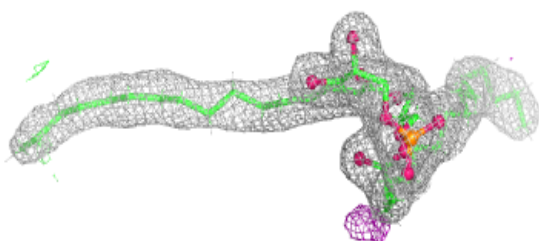
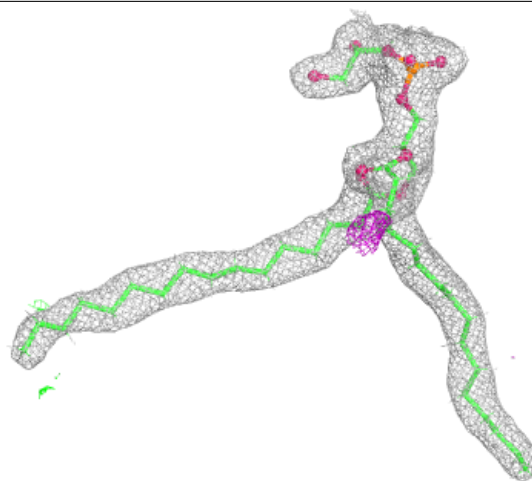
Electron density around PL9 d 405:

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



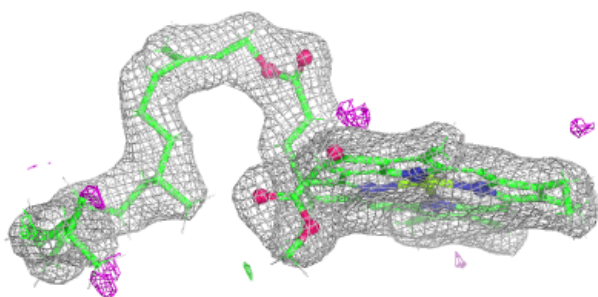
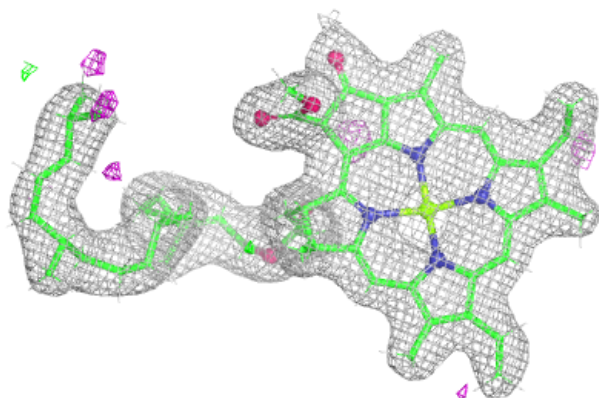
Electron density around LHG 1 101:

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



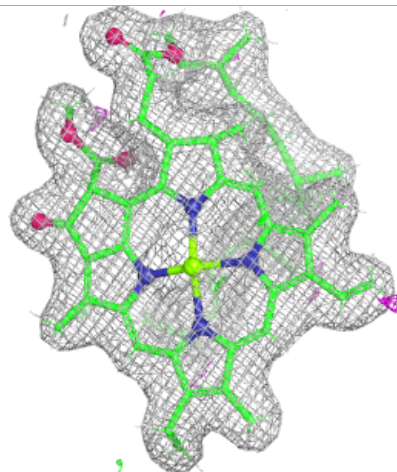
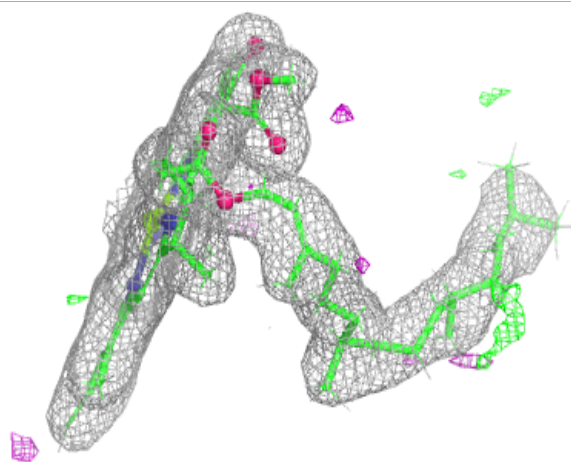
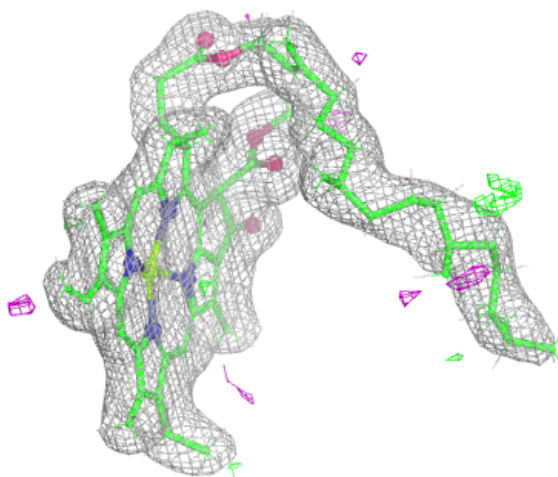
Electron density around CLA B 612:

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



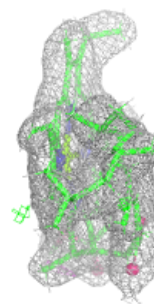
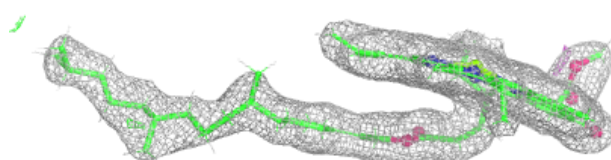
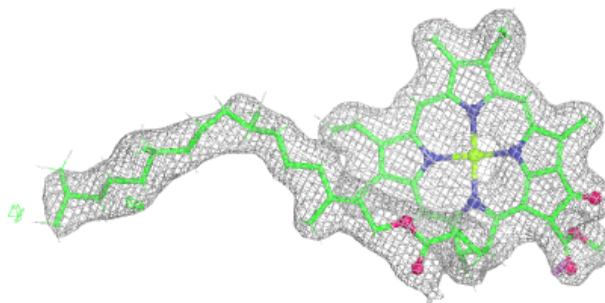
Electron density around CLA B 613:

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

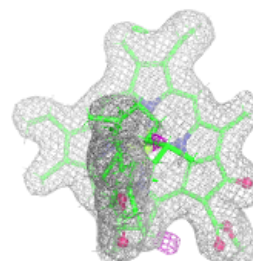
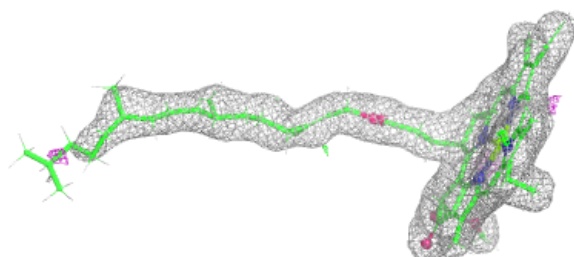
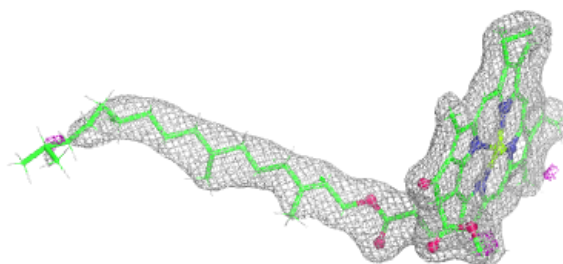


Electron density around CLA b 603:

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

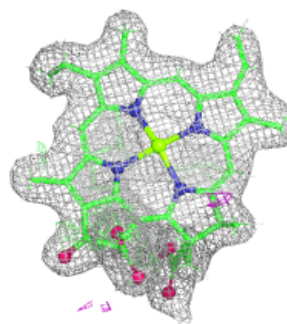
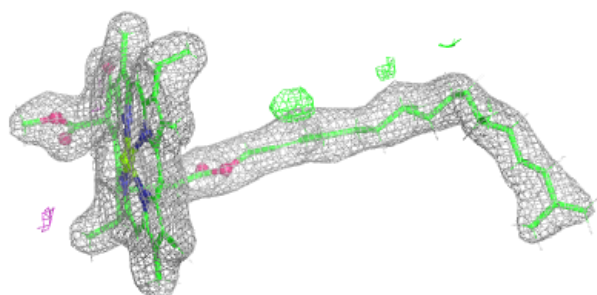
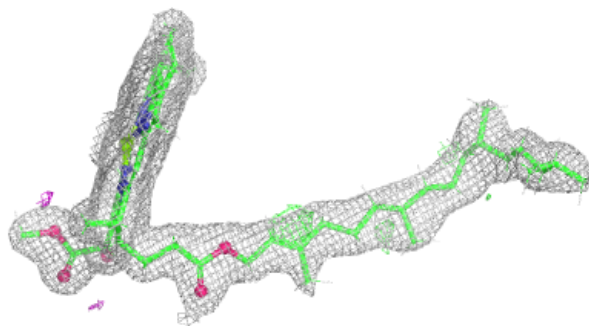
**Electron density around CLA b 604:**

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

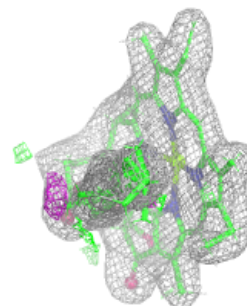
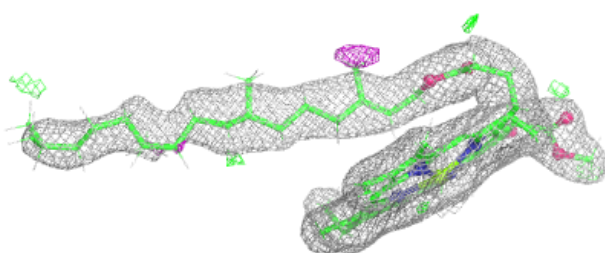
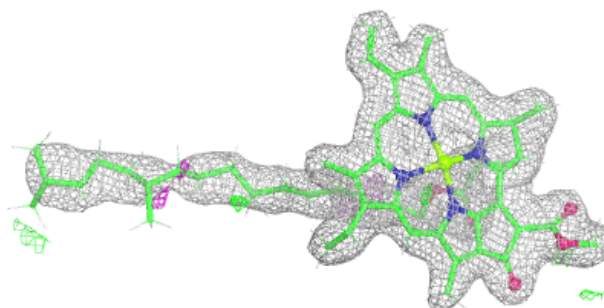


Electron density around CLA b 605:

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

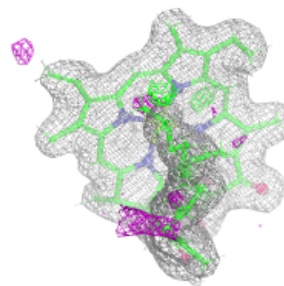
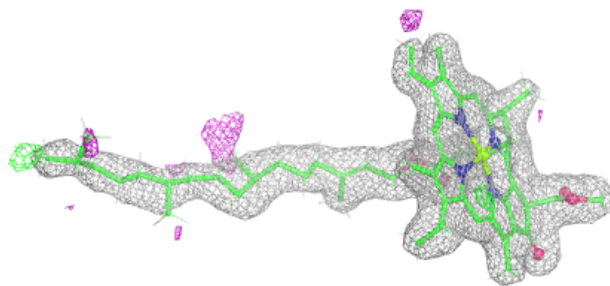
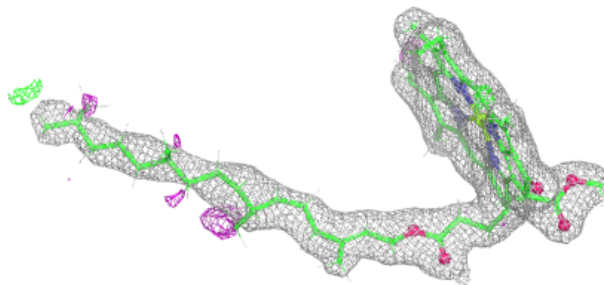
**Electron density around CLA B 614:**

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



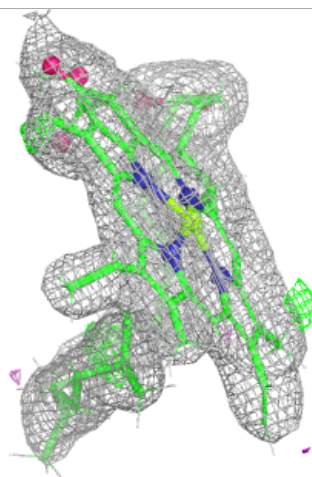
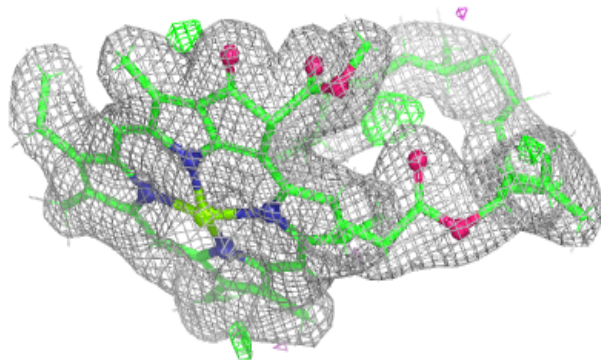
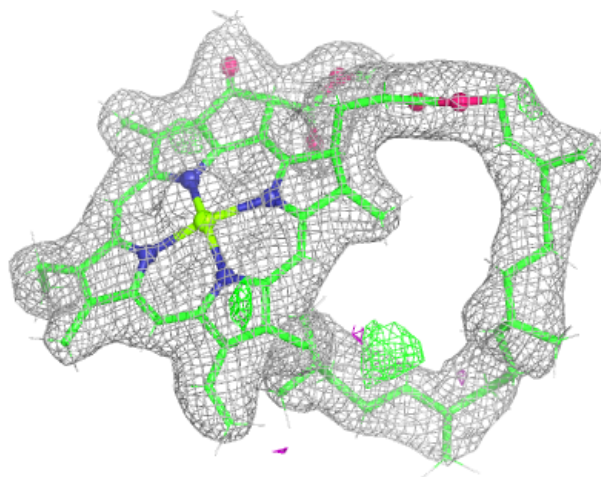
Electron density around CLA b 607:

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



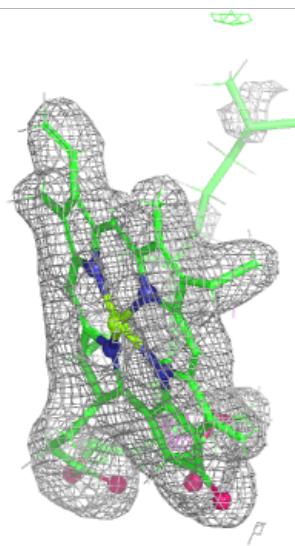
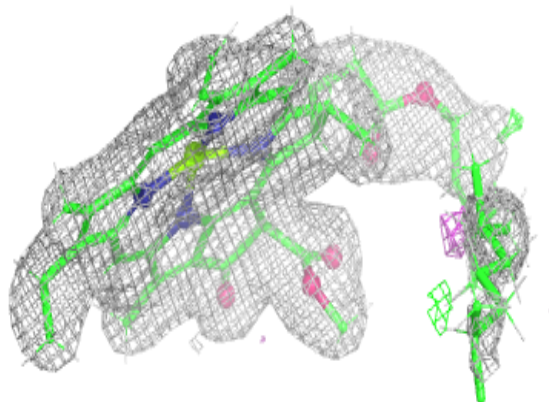
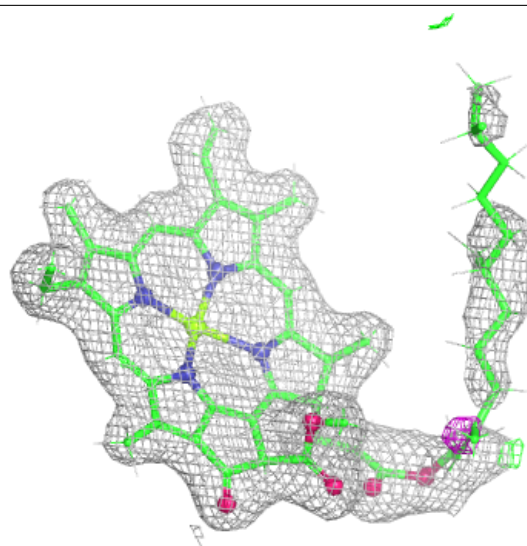
Electron density around CLA B 615:

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



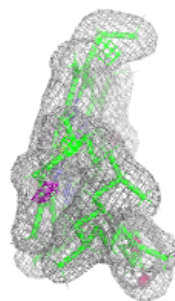
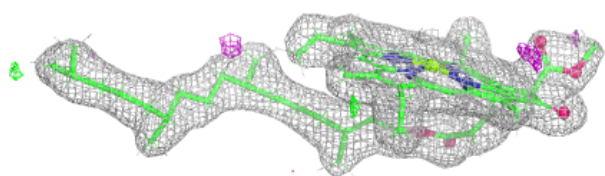
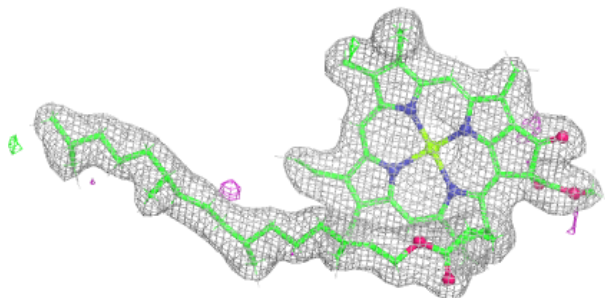
Electron density around CLA B 616:

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

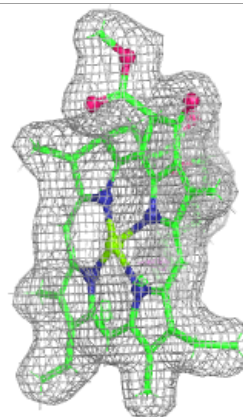
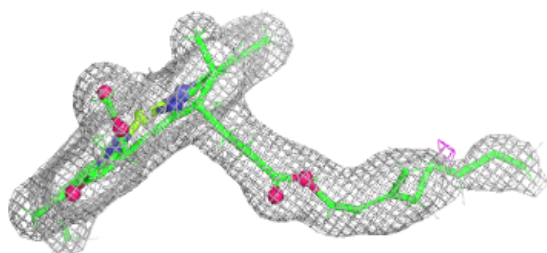
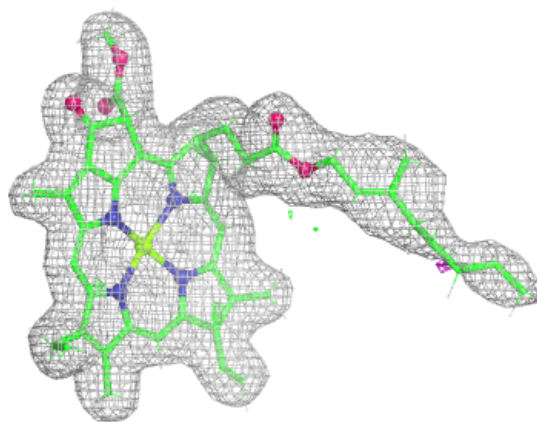


Electron density around CLA C 501:

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

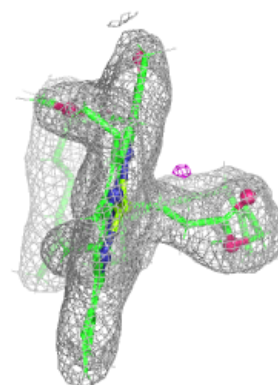
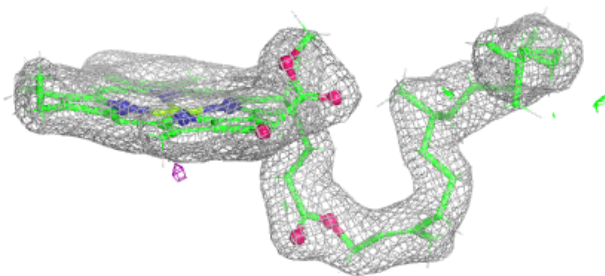
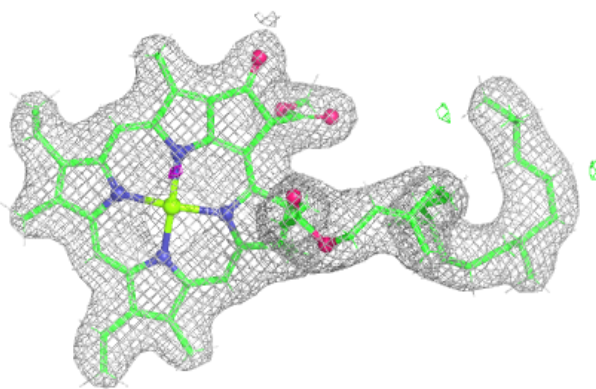
**Electron density around CLA A 610:**

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



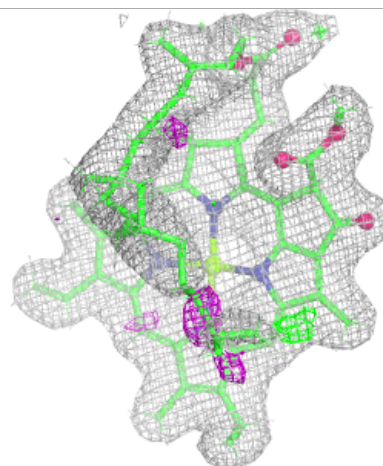
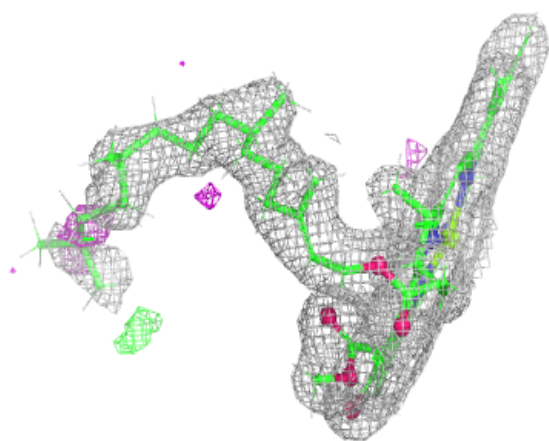
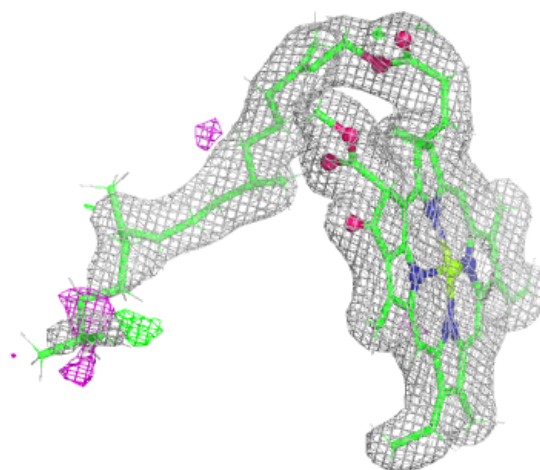
Electron density around CLA b 612:

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



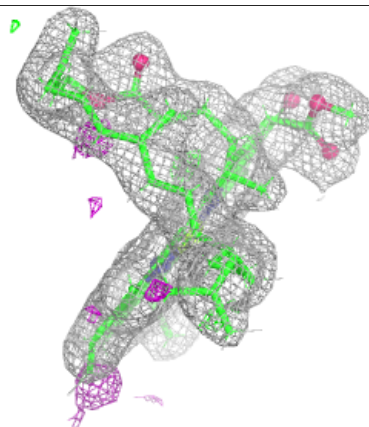
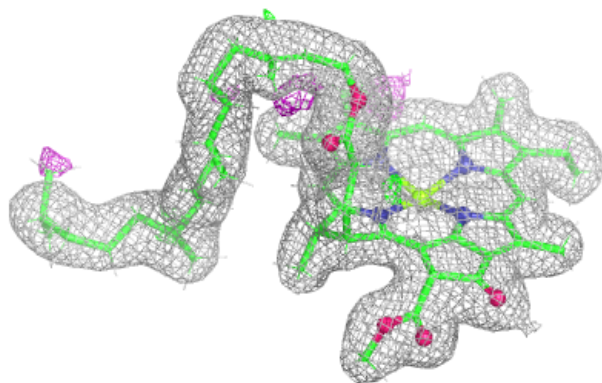
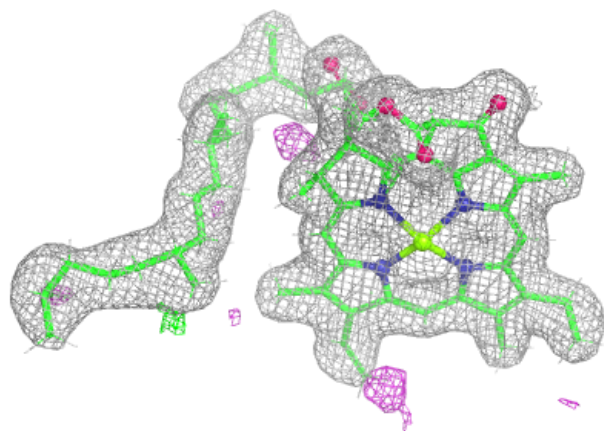
Electron density around CLA b 613:

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

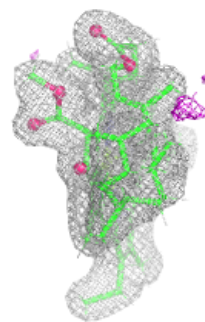
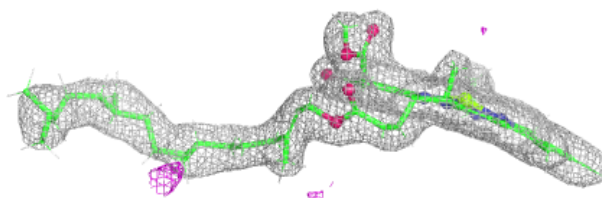
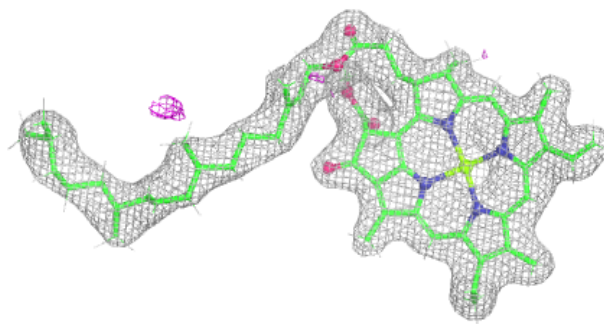


Electron density around CLA A 614:

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

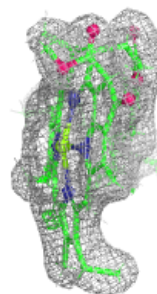
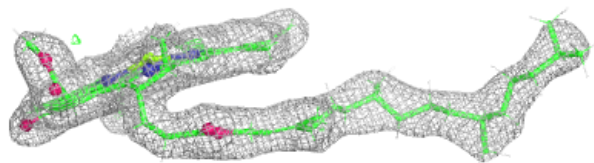
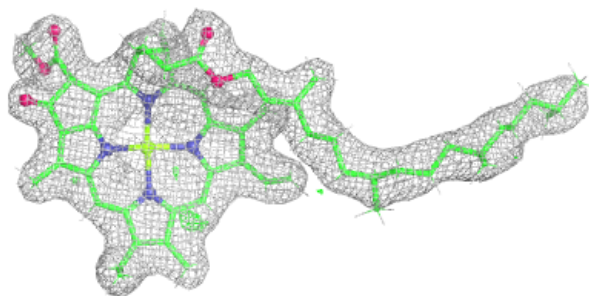
**Electron density around CLA B 602:**

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



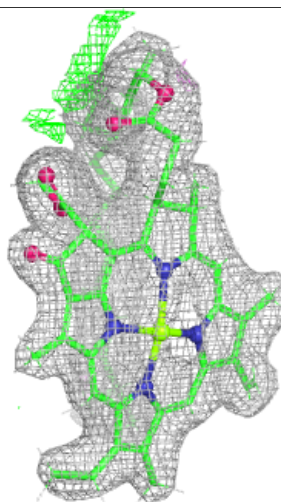
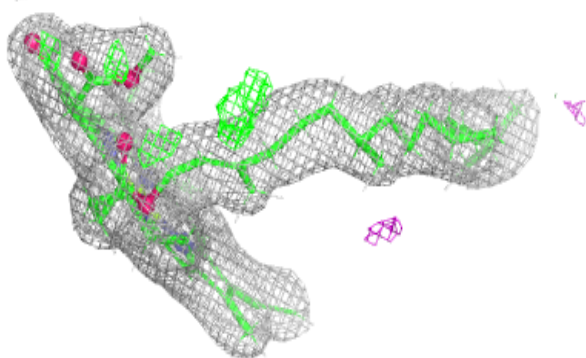
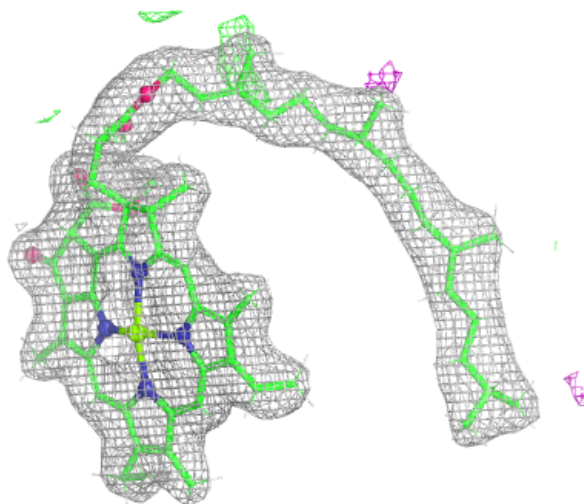
Electron density around CLA B 603:

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



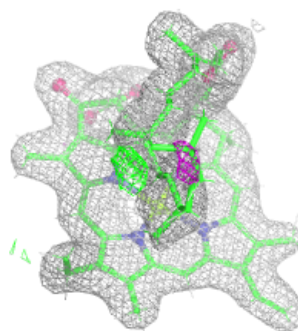
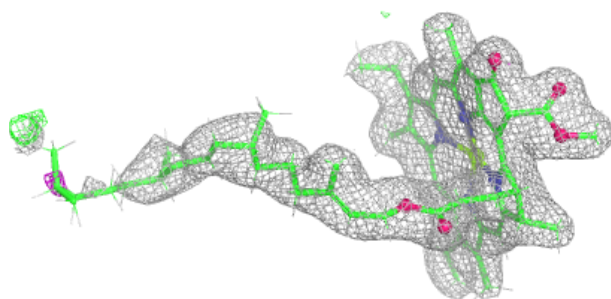
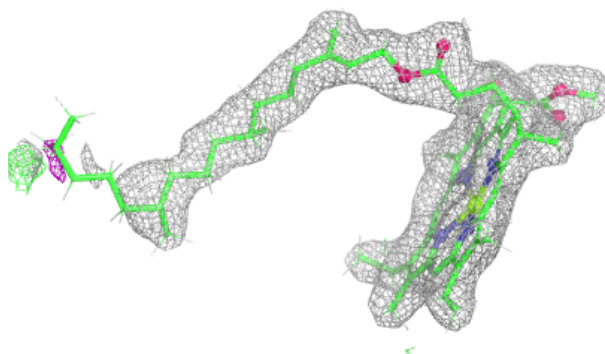
Electron density around CLA C 507:

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

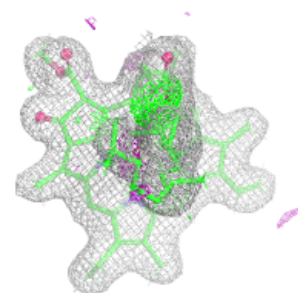
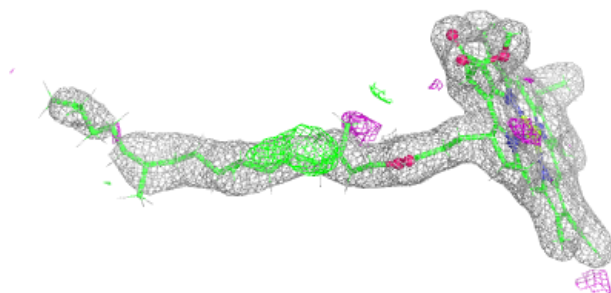
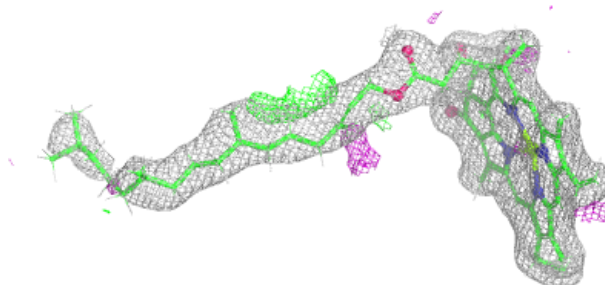


Electron density around CLA C 508:

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

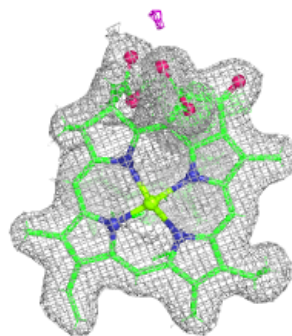
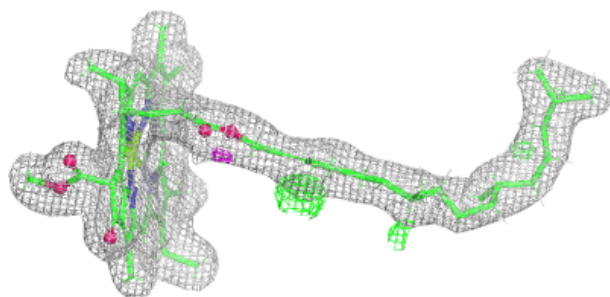
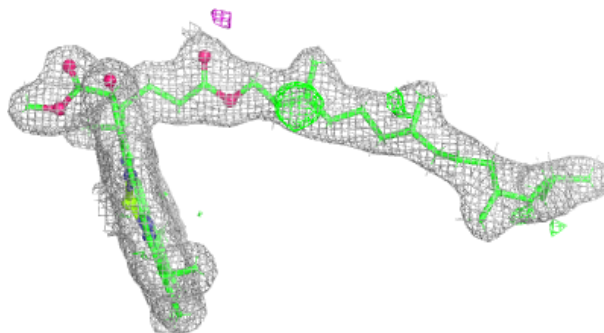
**Electron density around CLA B 604:**

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

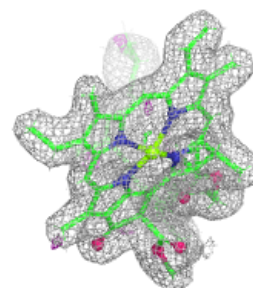
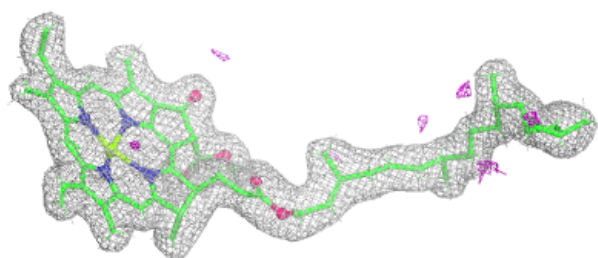
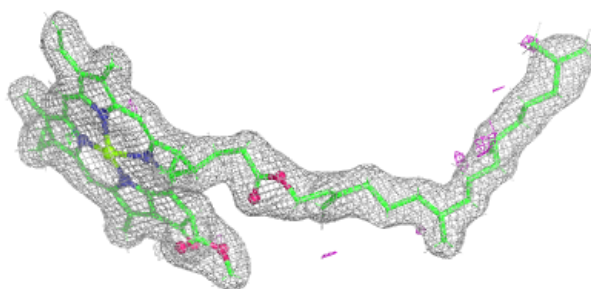


Electron density around CLA B 605:

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

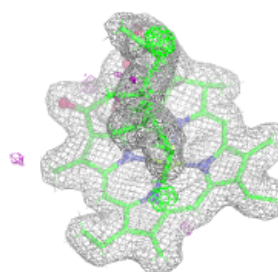
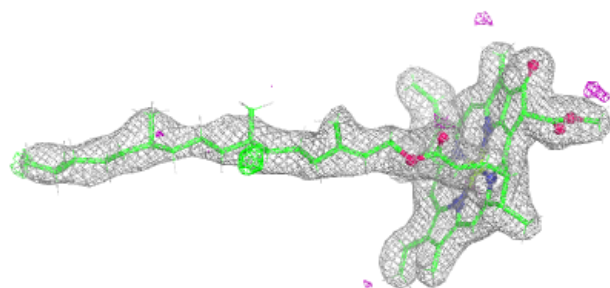
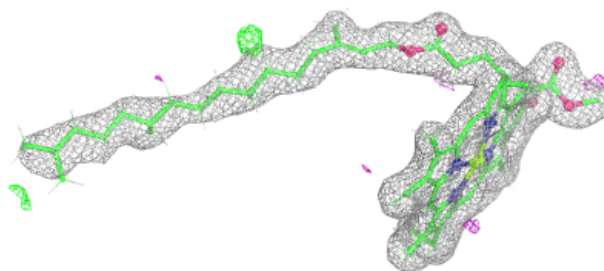
**Electron density around CLA A 607:**

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

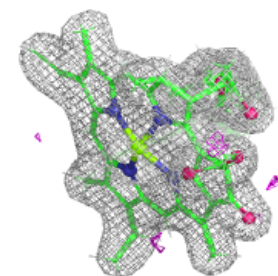
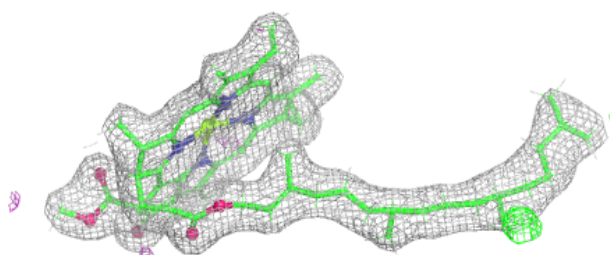
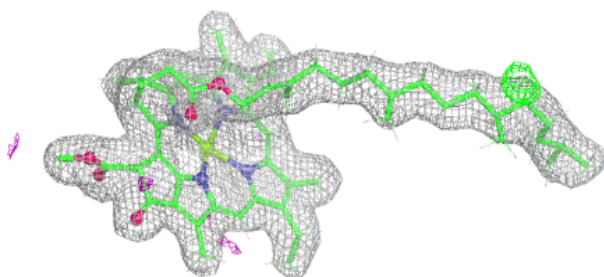


Electron density around CLA B 607:

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

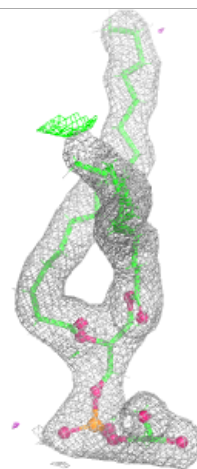
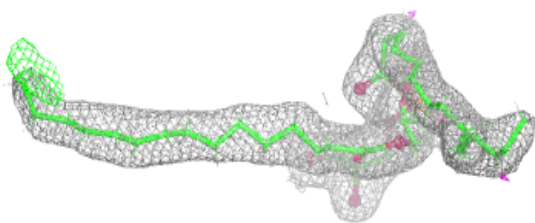
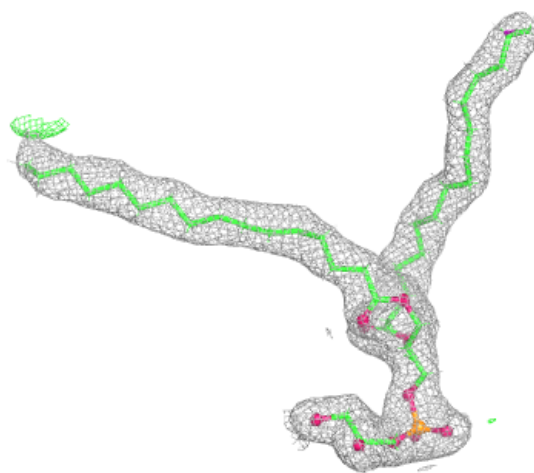
**Electron density around CLA B 608:**

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



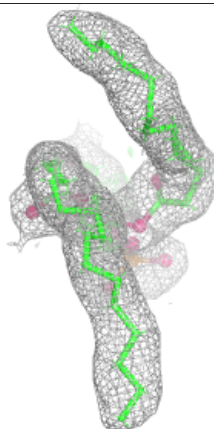
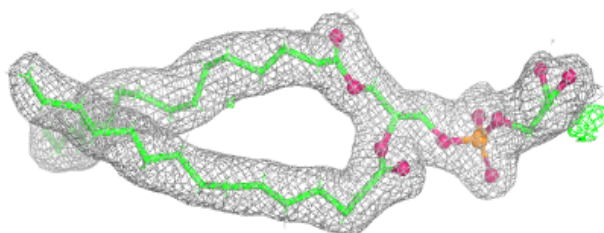
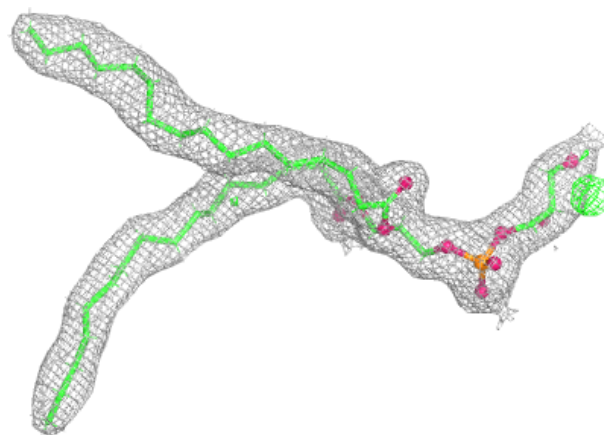
Electron density around LHG B 622:

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



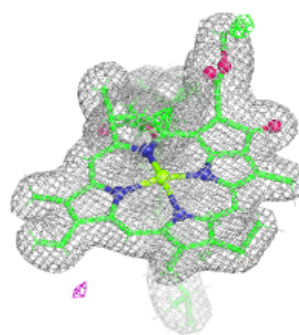
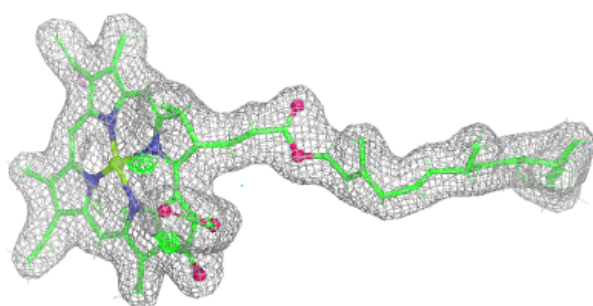
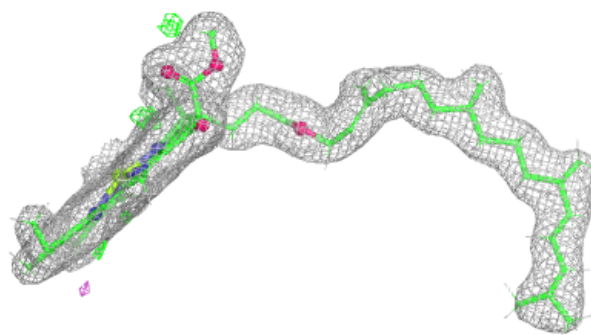
Electron density around LHG D 408:

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

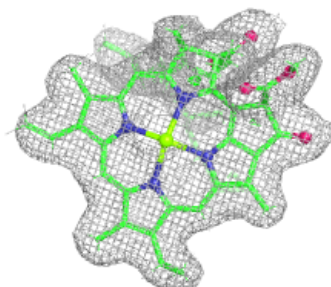
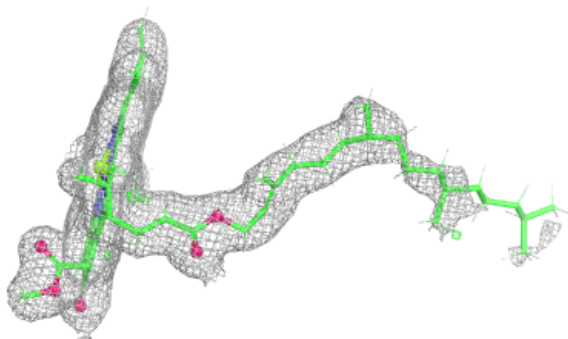
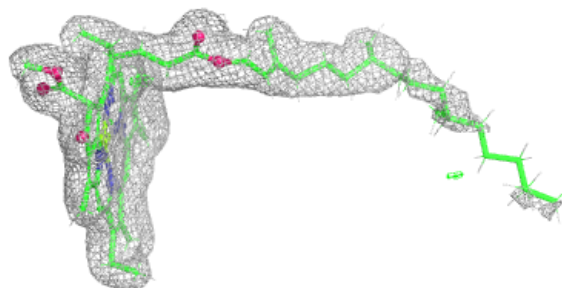


Electron density around CLA D 402:

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

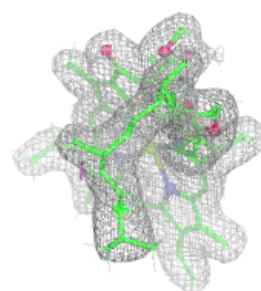
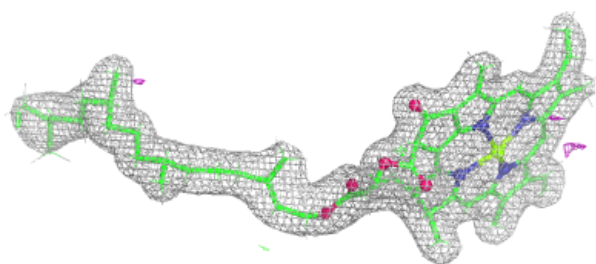
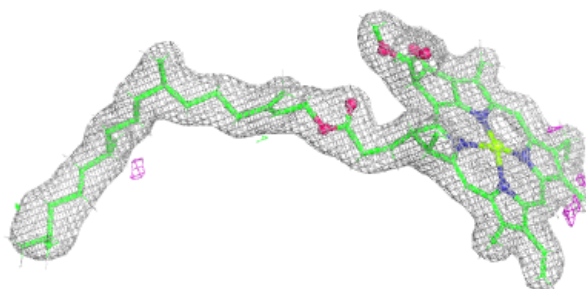
**Electron density around CLA D 403:**

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

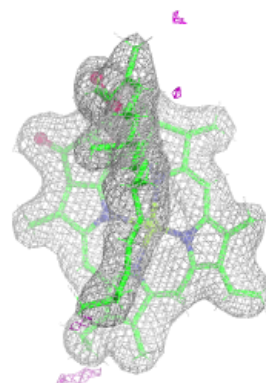
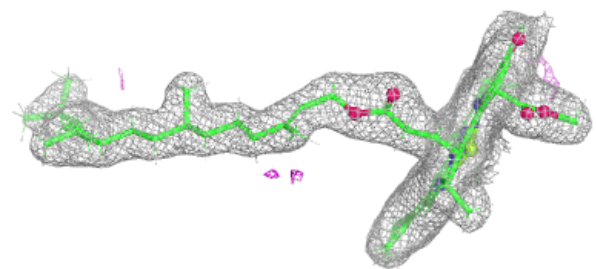
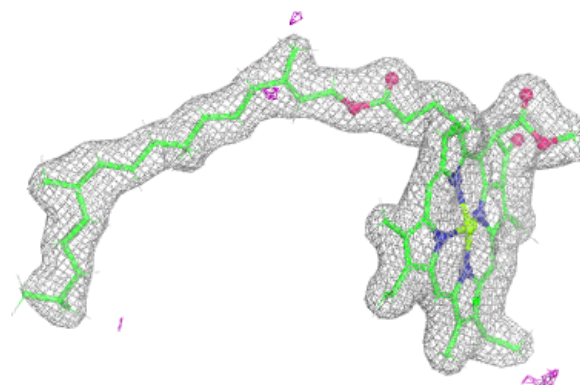


Electron density around CLA a 607:

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

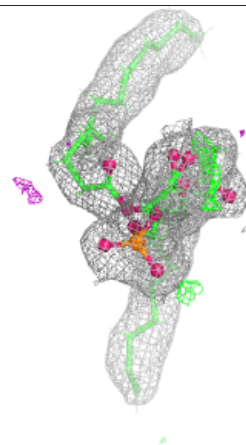
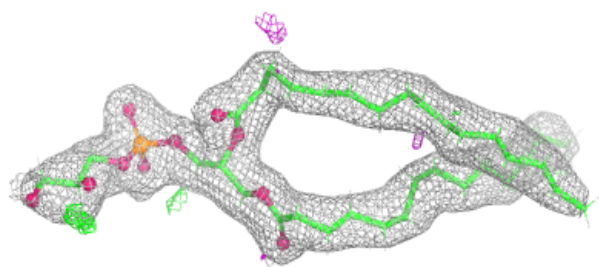
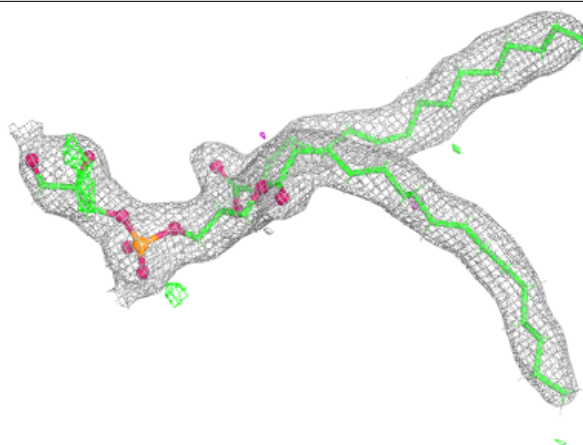
**Electron density around CLA B 609:**

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

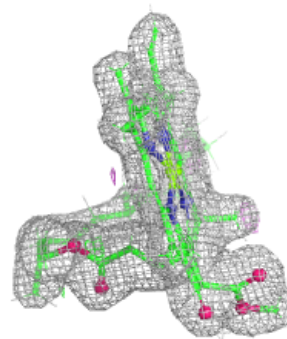
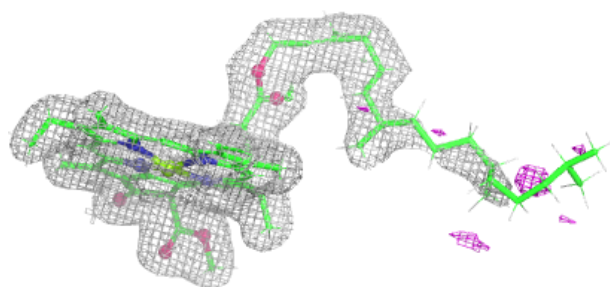
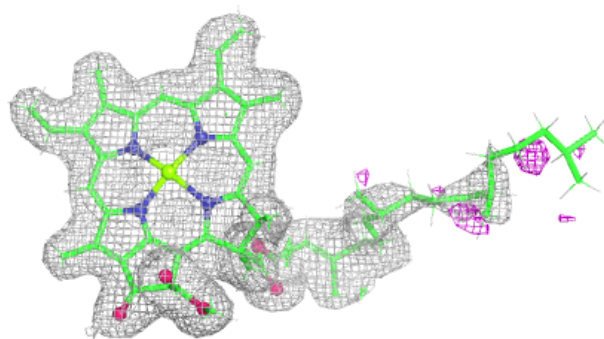


Electron density around LHG d 408:

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

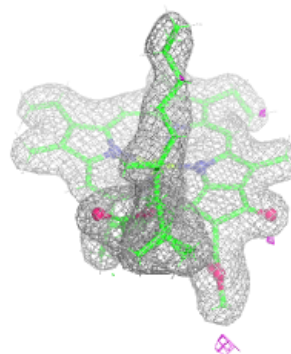
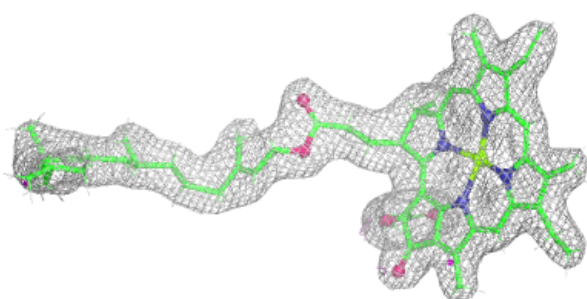
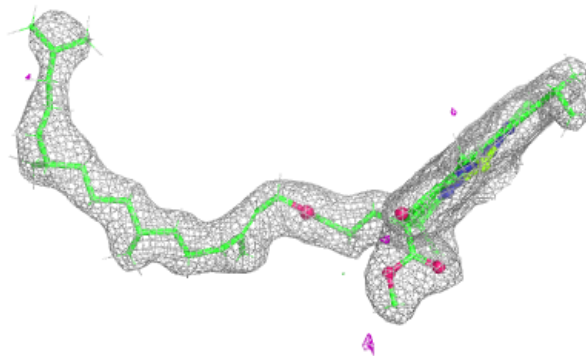
**Electron density around CLA A 608:**

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

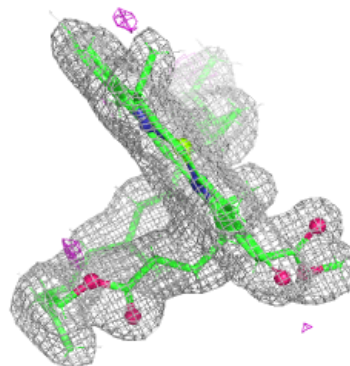
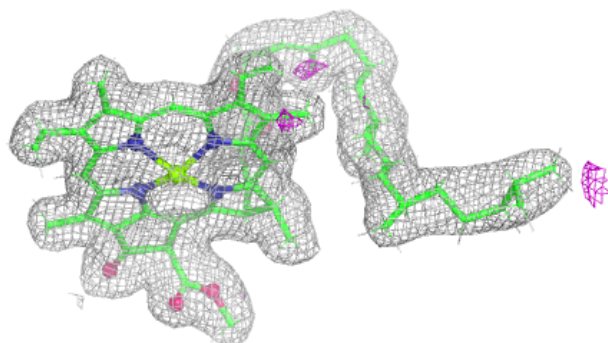
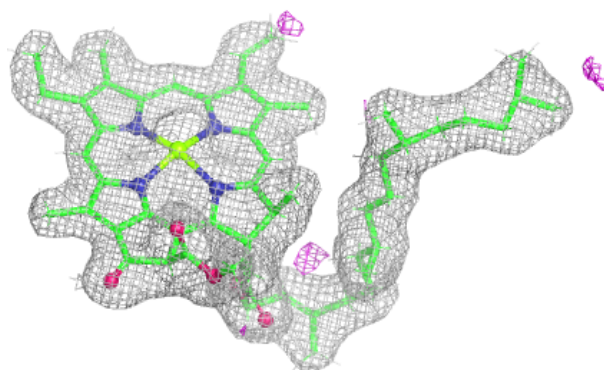


Electron density around CLA d 402:

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

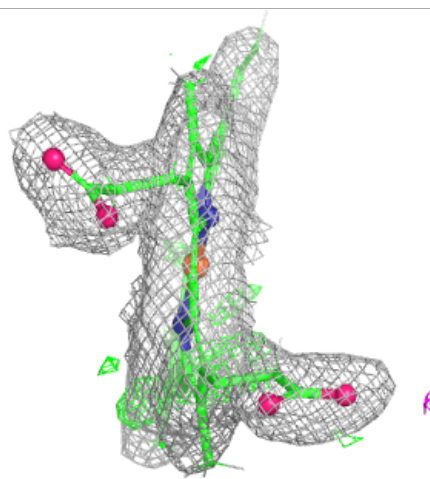
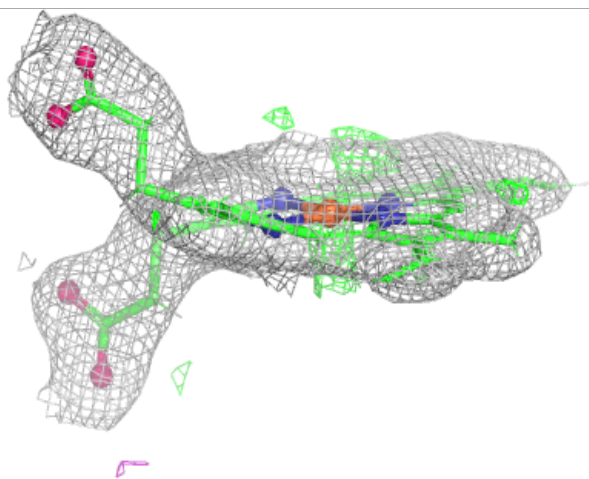
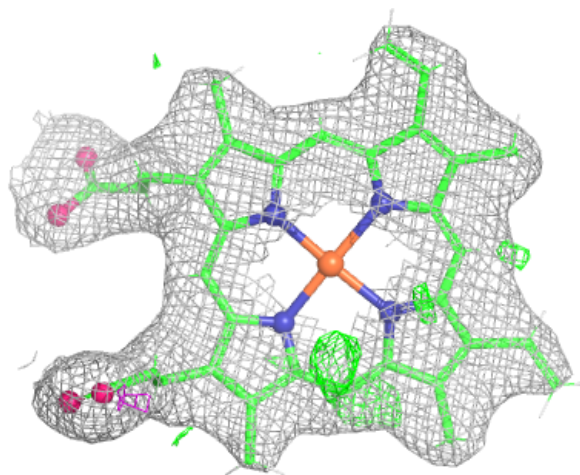
**Electron density around CLA a 613:**

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



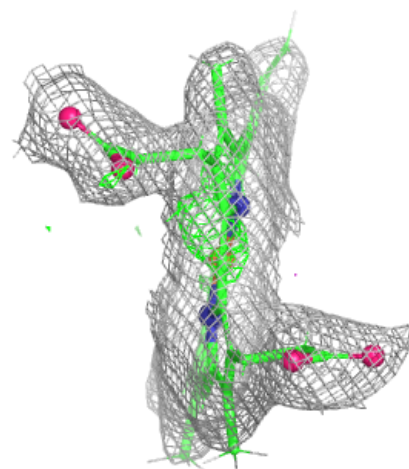
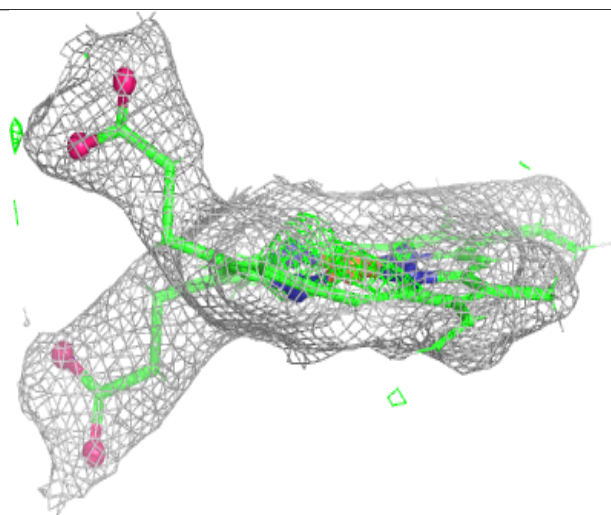
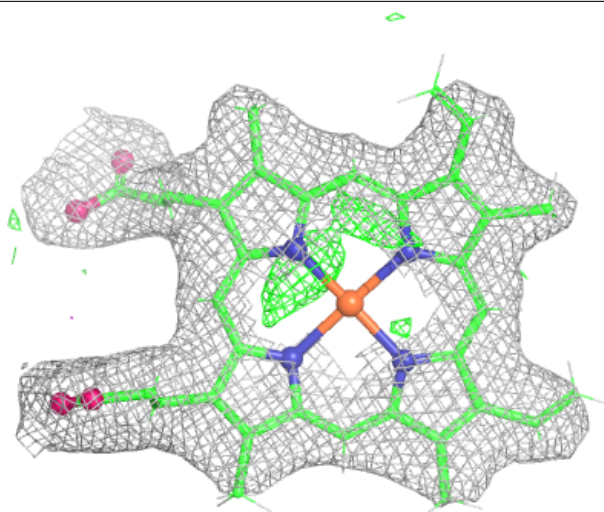
Electron density around HEM F 101:

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



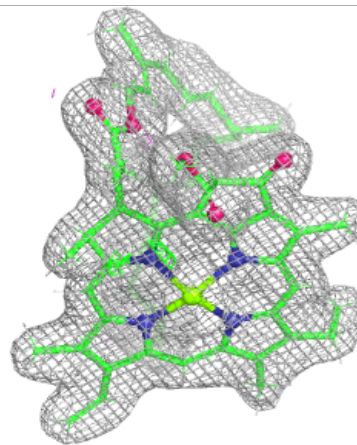
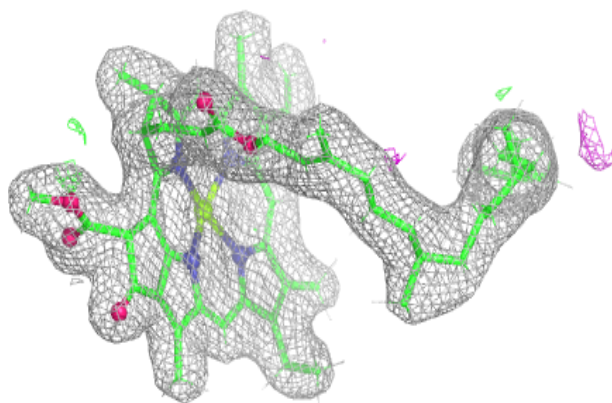
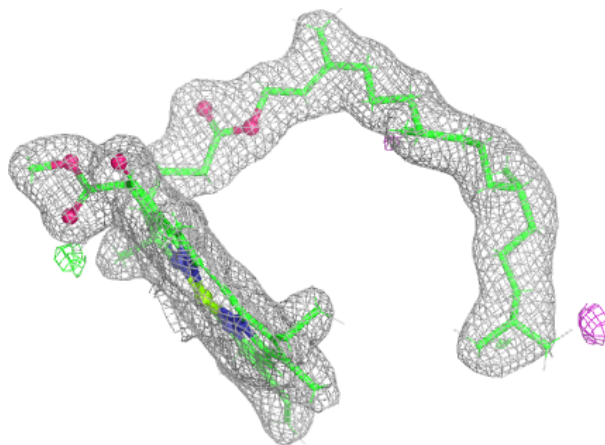
Electron density around HEM f 101:

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



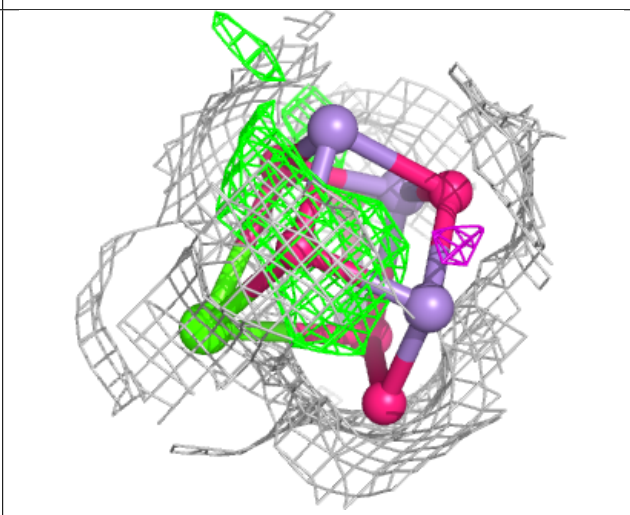
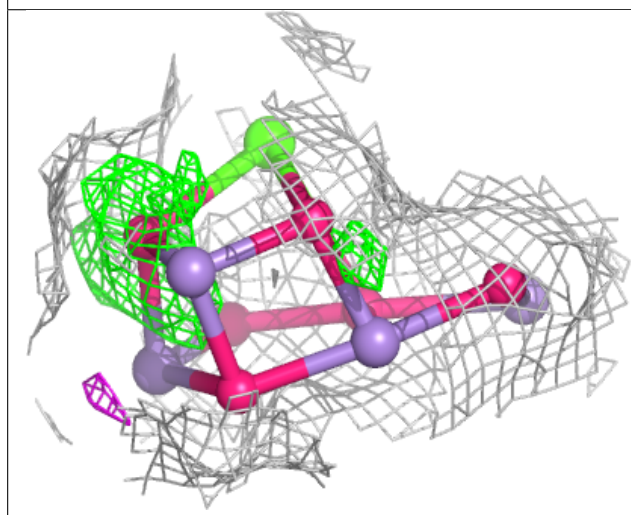
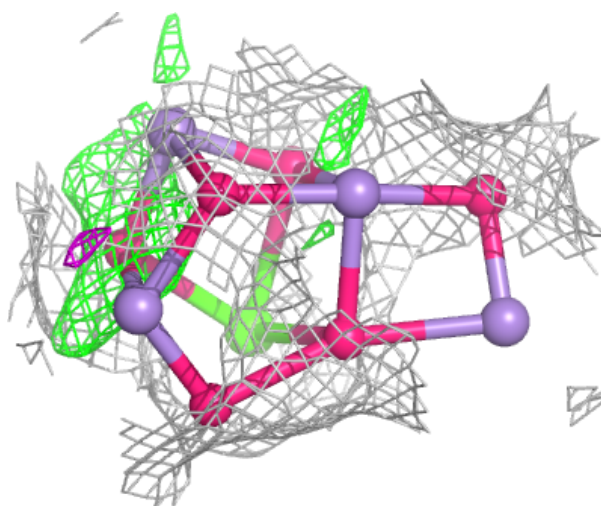
Electron density around CLA B 611:

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



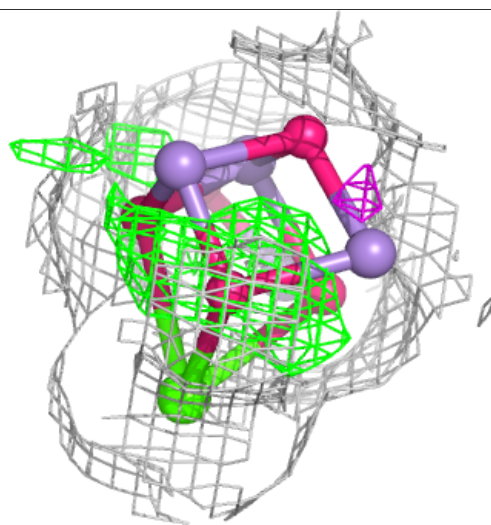
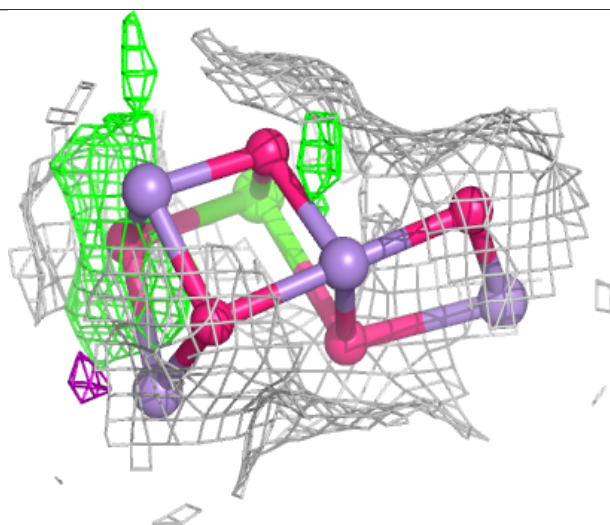
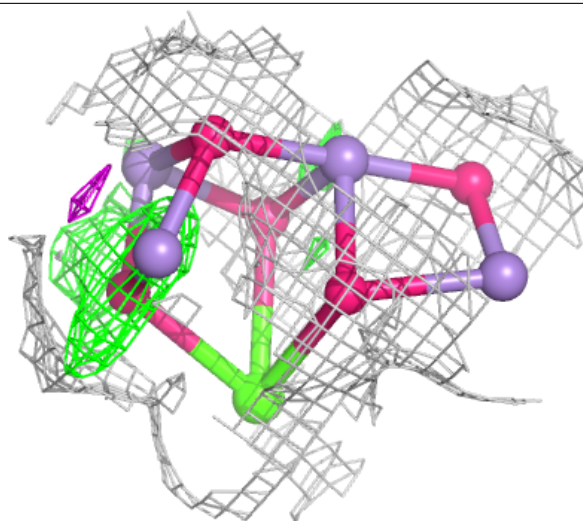
Electron density around OEY A 601 (B):

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



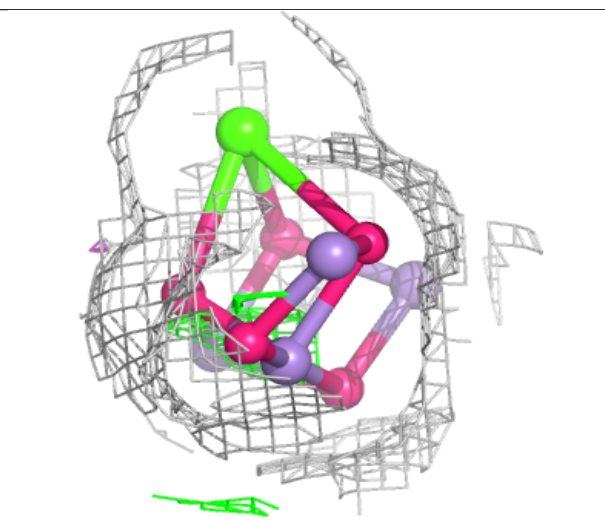
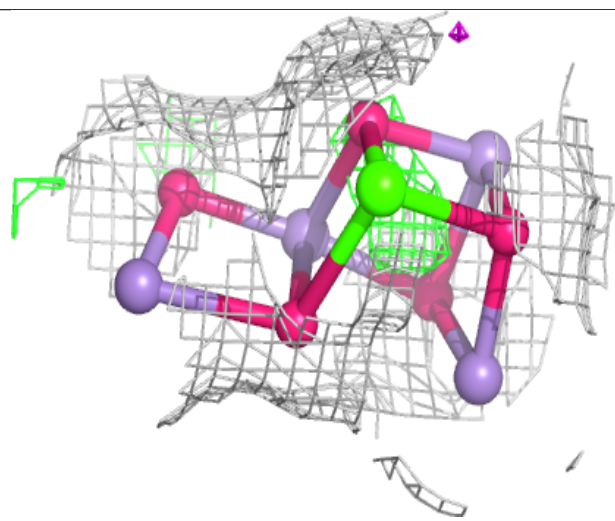
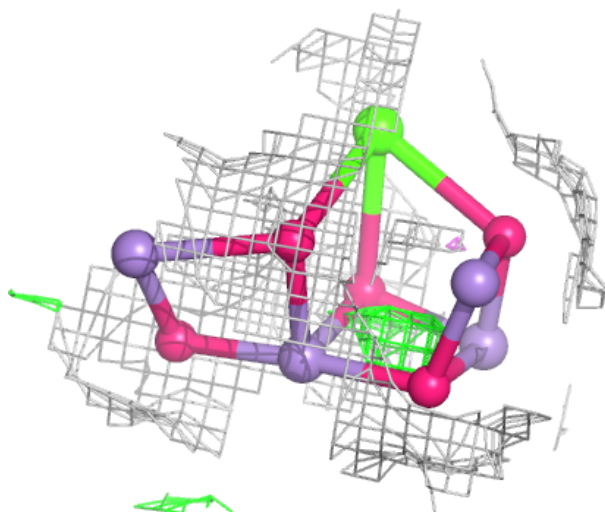
Electron density around OEX A 602 (A):

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



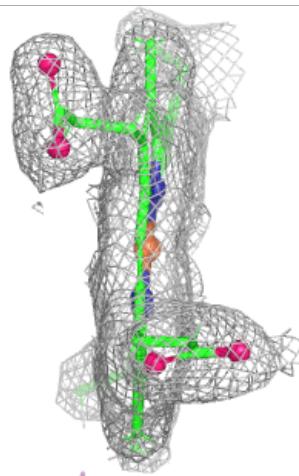
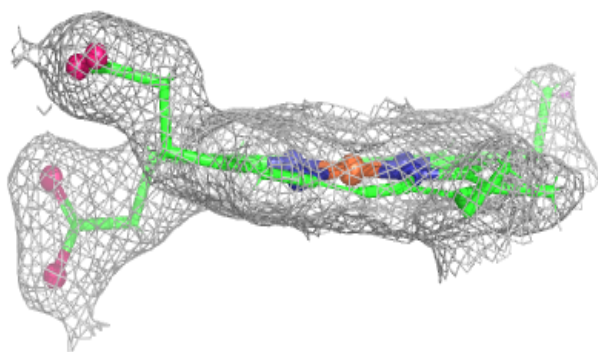
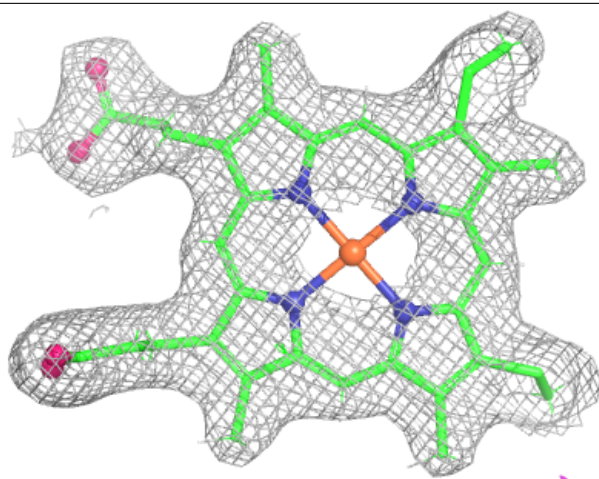
Electron density around OEX a 602 (A):

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



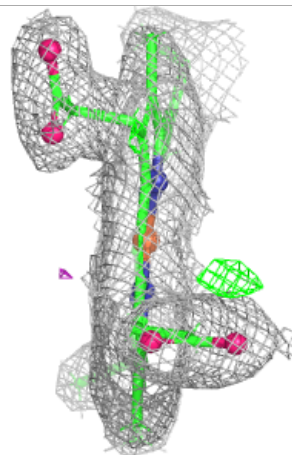
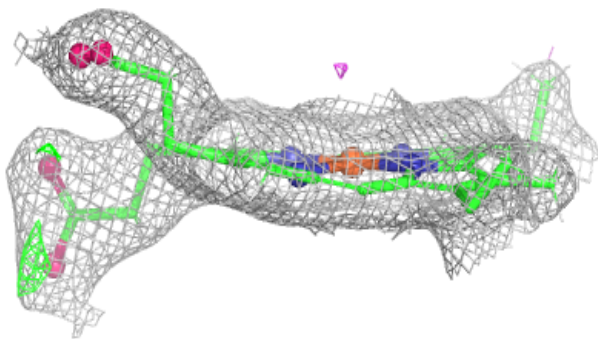
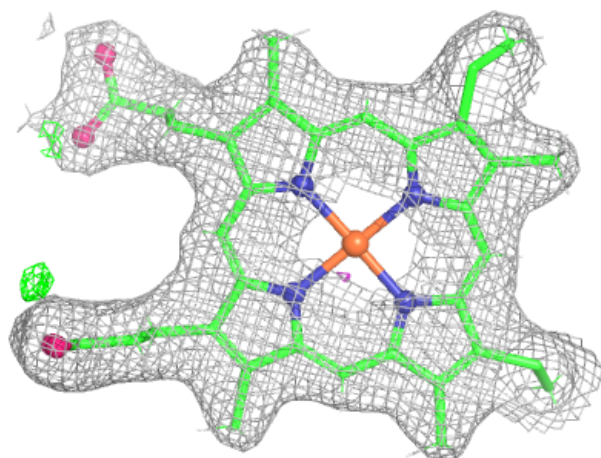
Electron density around HEC V 201:

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



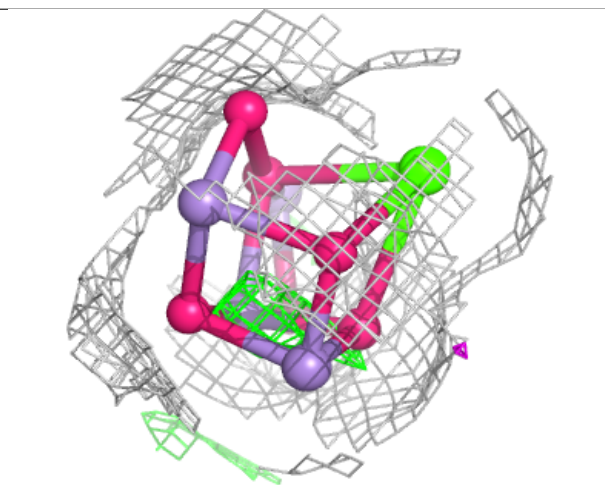
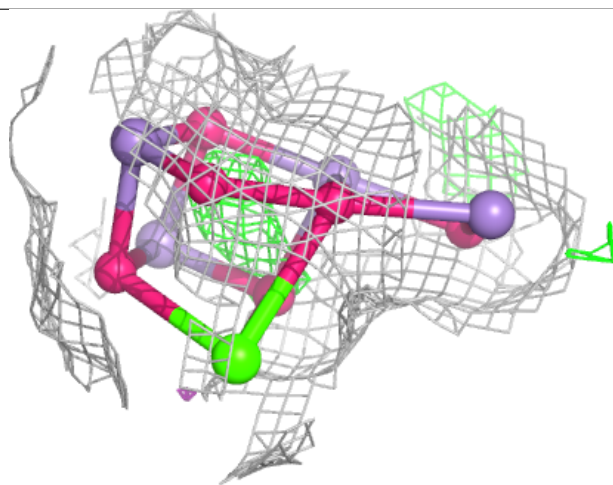
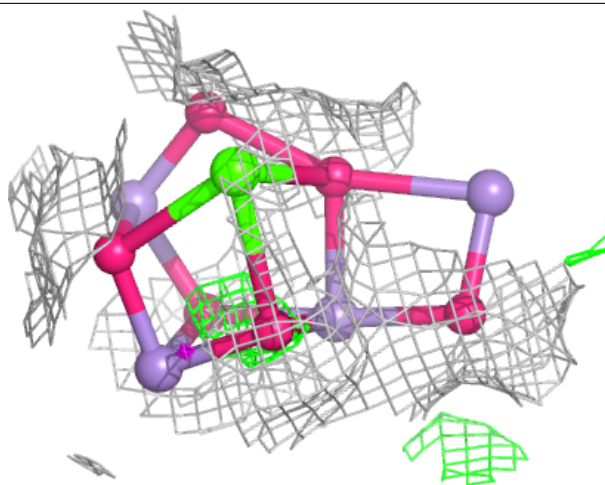
Electron density around HEC v 201:

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



Electron density around OEY a 601 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.