



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 02:26 PM EDT

PDB ID : 9Z68 / pdb_00009z68
Title : RT XFEL structure of the dark-stable state of Photosystem II (0F, S1 rich) at 1.97 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 : 1.97 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:

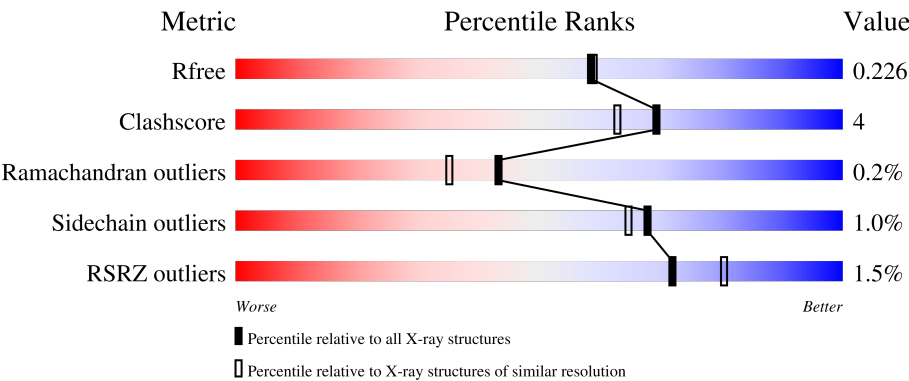
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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.



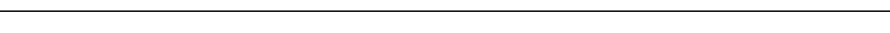
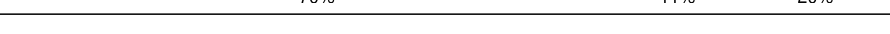
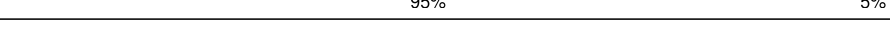
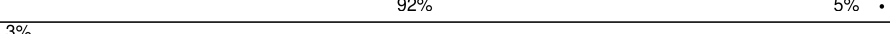
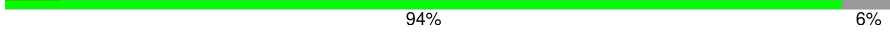
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	% 90%7%.
2	B	510	% 91%8%.
2	b	510	2% 94%5%.

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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	

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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
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 104120 atoms, of which 52077 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5091	1717	2469	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5081	1714	2462	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	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	2	0
			6773	2249	3347	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6918	2290	3418	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5337	1800	2620	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5349	1804	2626	444	463	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			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.

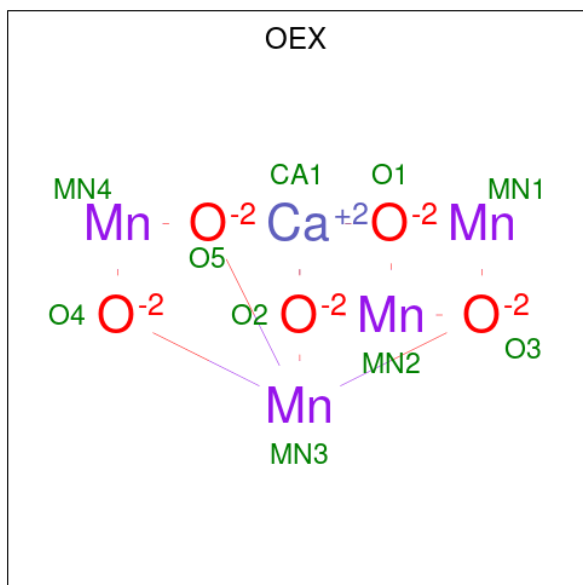
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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



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

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

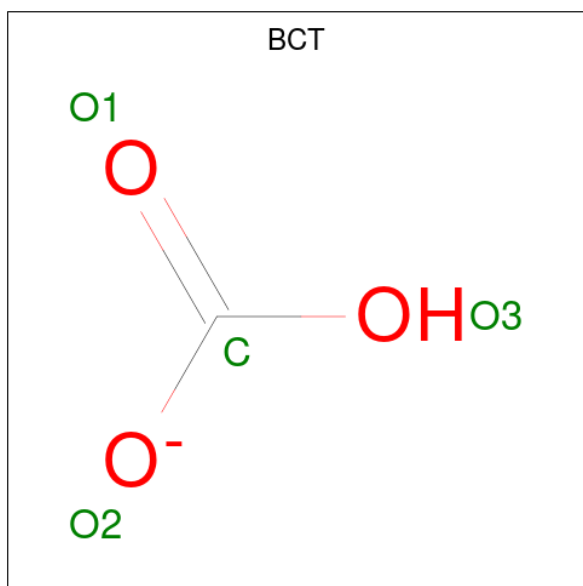
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
25	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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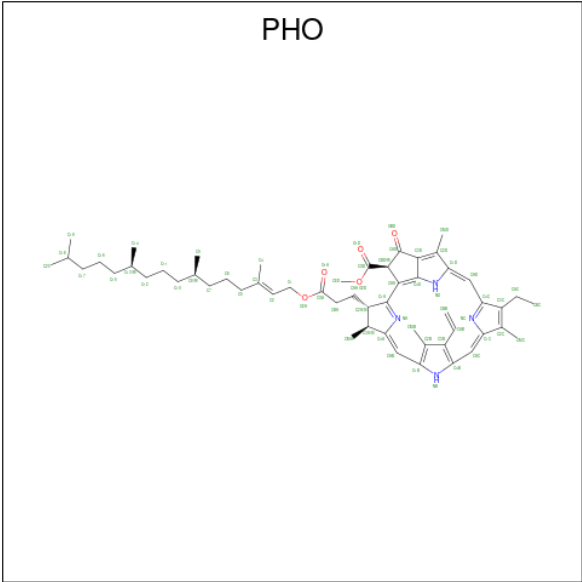
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
25	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
25	b	1	Total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

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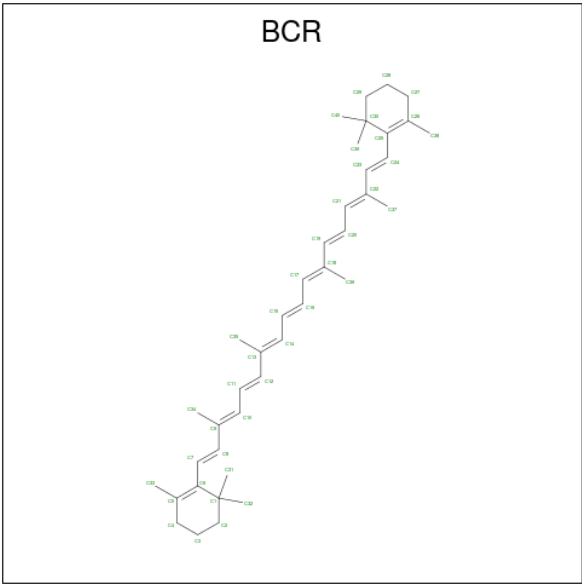
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
25	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
25	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
25	c	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
25	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
25	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
25	c	1	Total 137	C 55	H 72	Mg 1	N 4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

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



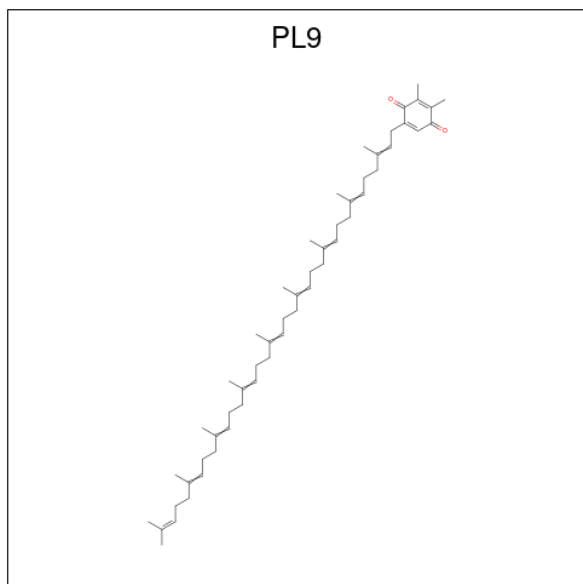
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
26	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
26	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
26	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



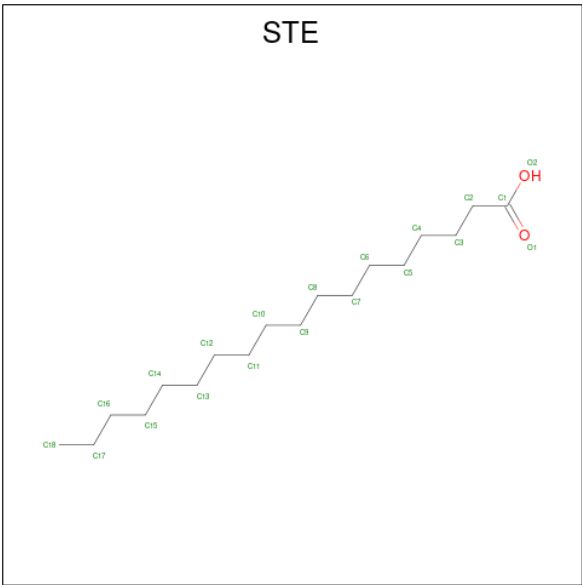
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	H	0	0
			96	40	56		
27	B	1	Total	C	H	0	0
			96	40	56		
27	B	1	Total	C	H	0	0
			96	40	56		
27	B	1	Total	C	H	0	0
			96	40	56		
27	C	1	Total	C	H	0	0
			96	40	56		
27	D	1	Total	C	H	0	0
			96	40	56		
27	H	1	Total	C	H	0	0
			96	40	56		
27	K	1	Total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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H		0	0
			23	9	14			
29	A	1	Total	C	H		0	0
			50	17	33			
29	A	1	Total	C	H		0	0
			32	11	21			
29	B	1	Total	C	H	O	0	0
			43	15	26	2		
29	B	1	Total	C	H	O	0	0
			46	16	28	2		
29	B	1	Total	C	H	O	0	0
			28	10	16	2		
29	B	1	Total	C	H		0	0
			41	15	26			
29	C	1	Total	C	H	O	0	0
			34	12	20	2		
29	C	1	Total	C	H		0	0
			11	5	6			
29	C	1	Total	C	H		0	0
			17	7	10			
29	C	1	Total	C	H		0	0
			26	10	16			
29	C	1	Total	C	H	O	0	0
			28	10	16	2		
29	C	1	Total	C	H		0	0
			47	16	31			
29	C	1	Total	C	H		0	0
			41	14	27			

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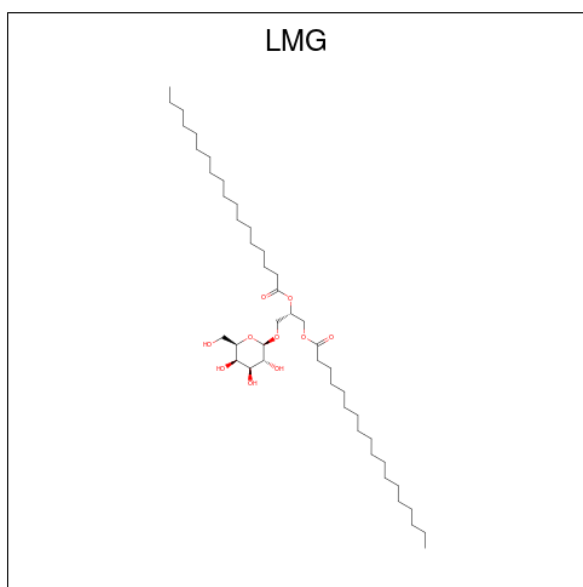
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total C H 26 9 17	0	0
29	E	1	Total C H O 28 10 16 2	0	0
29	E	1	Total C H 35 12 23	0	0
29	E	1	Total C H O 55 18 35 2	0	0
29	H	1	Total C H 53 18 35	0	0
29	I	1	Total C H O 43 15 26 2	0	0
29	I	1	Total C H O 37 13 22 2	0	0
29	J	1	Total C H O 28 10 16 2	0	0
29	K	1	Total C H 41 14 27	0	0
29	M	1	Total C H O 37 13 22 2	0	0
29	M	1	Total C H 26 10 16	0	0
29	M	1	Total C H 44 15 29	0	0
29	T	1	Total C H 47 16 31	0	0
29	X	1	Total C H O 55 18 35 2	0	0
29	Z	1	Total C H 50 17 33	0	0
29	a	1	Total C H O 28 10 16 2	0	0
29	b	1	Total C H O 55 18 35 2	0	0
29	b	1	Total C H O 40 14 24 2	0	0
29	b	1	Total C H 26 10 16	0	0
29	b	1	Total C H 23 8 15	0	0
29	c	1	Total C H 35 13 22	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C H 53 18 35	0	0
29	d	1	Total C H O 55 18 35 2	0	0
29	d	1	Total C H O 55 18 35 2	0	0
29	d	1	Total C H O 34 12 20 2	0	0
29	e	1	Total C H 26 9 17	0	0
29	e	1	Total C H 26 9 17	0	0
29	e	1	Total C H O 31 11 18 2	0	0
29	f	1	Total C H 23 8 15	0	0
29	h	1	Total C H 29 10 19	0	0
29	h	1	Total C H 32 11 21	0	0
29	i	1	Total C H O 28 10 16 2	0	0
29	i	1	Total C H 14 6 8	0	0
29	j	1	Total C H O 28 10 16 2	0	0
29	j	1	Total C H 47 16 31	0	0
29	l	1	Total C H 53 18 35	0	0
29	m	1	Total C H O 28 10 16 2	0	0
29	t	1	Total C H O 34 12 20 2	0	0
29	t	1	Total C H 26 10 16	0	0
29	x	1	Total C H O 55 18 35 2	0	0
29	z	1	Total C H 23 9 14	0	0

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



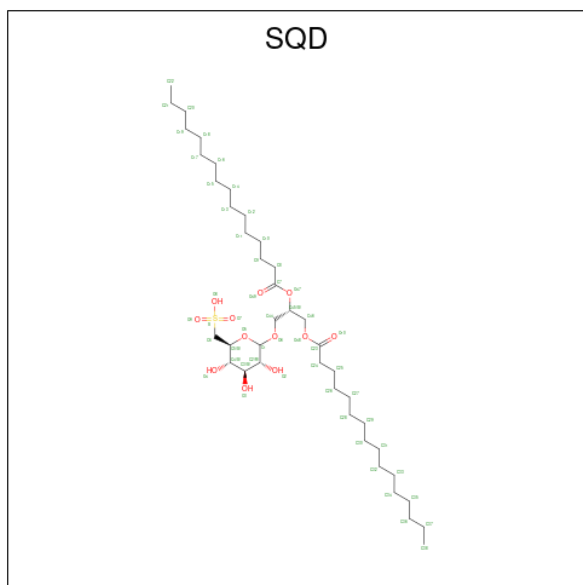
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			114	38	66	10		
30	B	1	Total	C	H	O	0	0
			105	35	60	10		
30	B	1	Total	C	H	O	0	0
			123	41	72	10		
30	C	1	Total	C	H	O	0	0
			76	26	40	10		
30	C	1	Total	C	H	O	0	0
			114	38	66	10		
30	D	1	Total	C	H	O	0	0
			120	40	70	10		
30	D	1	Total	C	H	O	0	0
			123	41	72	10		
30	a	1	Total	C	H	O	0	0
			141	45	86	10		
30	a	1	Total	C	H	O	0	0
			117	39	68	10		
30	b	1	Total	C	H	O	0	0
			123	41	72	10		
30	b	1	Total	C	H	O	0	0
			141	45	86	10		
30	c	1	Total	C	H	O	0	0
			71	25	41	5		
30	c	1	Total	C	H	O	0	0
			108	36	62	10		
30	c	1	Total	C	H	O	0	0
			117	38	69	10		

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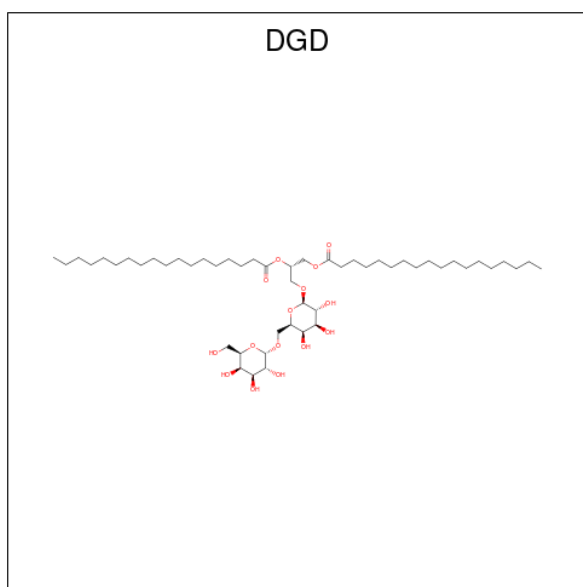
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



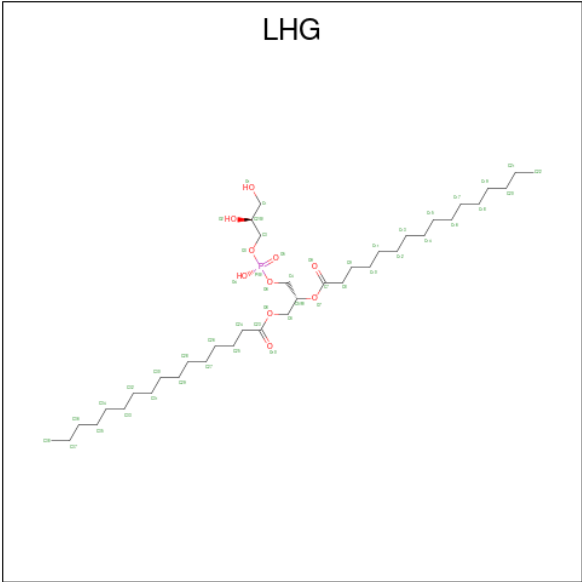
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
31	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
31	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
31	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
31	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
31	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
31	b	1	Total	C	H	O	S	0	0
			113	36	64	12	1		
31	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



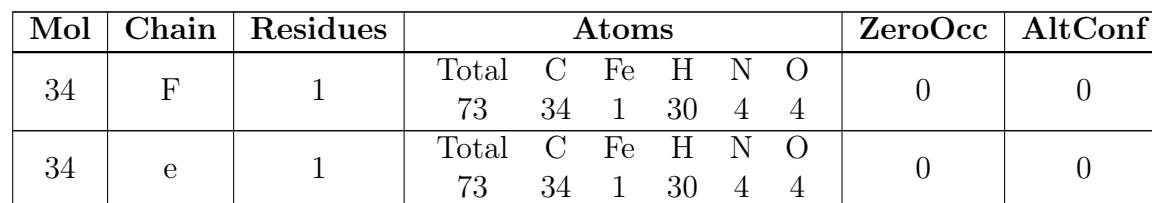
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	H	O	0	0
			162	51	96	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	H	1	Total	C	H	O	0	0
			143	47	81	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total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

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



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

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



- # HEC
-
- The diagram illustrates the chemical structure of the HEC (Hexaethylcyclen) ligand complexed with an iron(II) ion. The ligand is a macrocyclic polyamine with six nitrogen atoms (N⁺), each substituted with an ethyl group (CH₂CH₃). The iron ion (Fe²⁺) is coordinated by the six nitrogen atoms in an octahedral geometry. The structure is labeled with various atoms: N⁺ (nitrogen), Fe (iron), C (carbon), H (hydrogen), and O (oxygen). The ligand is shown in a 3D perspective, with the iron ion at the center of the macrocycle.

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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	125	Total O 125 125	0	0
36	B	175	Total O 175 175	0	0
36	C	139	Total O 139 139	0	0
36	D	102	Total O 102 102	0	0
36	E	16	Total O 16 16	0	0
36	F	7	Total O 7 7	0	0
36	H	25	Total O 25 25	0	0
36	I	11	Total O 11 11	0	0
36	J	11	Total O 11 11	0	0
36	K	1	Total O 1 1	0	0
36	L	7	Total O 7 7	0	0
36	M	6	Total O 6 6	0	0
36	O	78	Total O 78 78	0	0
36	T	6	Total O 6 6	0	0
36	U	33	Total O 33 33	0	0
36	V	49	Total O 49 49	0	0
36	X	11	Total O 11 11	0	0
36	Z	1	Total O 1 1	0	0
36	R	2	Total O 2 2	0	0
36	a	107	Total O 107 107	0	0
36	b	150	Total O 150 150	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	c	130	Total 130	O 130	0	0
36	d	96	Total 96	O 96	0	0
36	e	9	Total 9	O 9	0	0
36	f	1	Total 1	O 1	0	0
36	h	10	Total 10	O 10	0	0
36	i	4	Total 4	O 4	0	0
36	j	4	Total 4	O 4	0	0
36	k	2	Total 2	O 2	0	0
36	l	10	Total 10	O 10	0	0
36	m	4	Total 4	O 4	0	0
36	o	75	Total 75	O 75	0	0
36	t	7	Total 7	O 7	0	0
36	u	48	Total 48	O 48	0	0
36	v	33	Total 33	O 33	0	0
36	x	5	Total 5	O 5	0	0
36	z	4	Total 4	O 4	0	0
36	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.

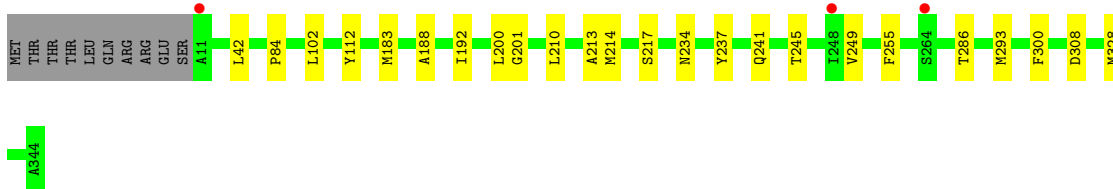
- Molecule 1: Photosystem II protein D1 1

Chain A: 

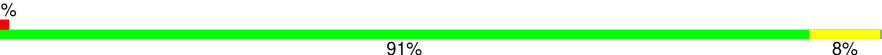


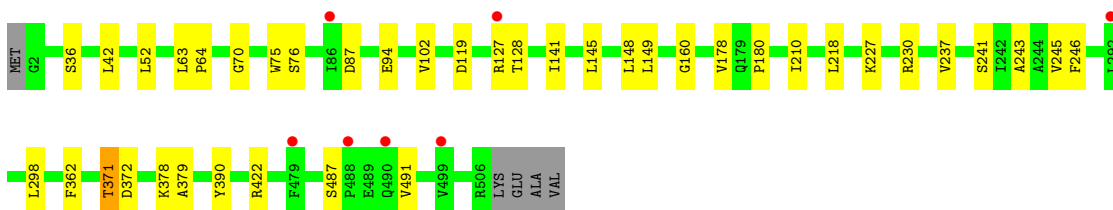
- Molecule 1: Photosystem II protein D1 1

Chain a: 

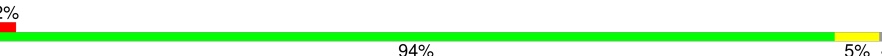


- Molecule 2: Photosystem II CP47 reaction center protein

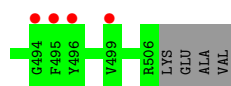
Chain B: 



- Molecule 2: Photosystem II CP47 reaction center protein

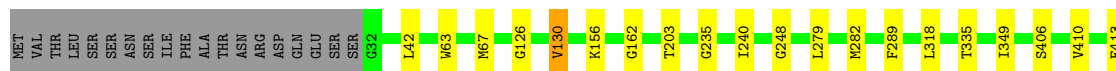
Chain b: 





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91%



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 92%



• Molecule 4: Photosystem II D2 protein

Chain D: 89%



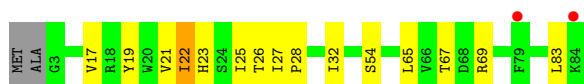
• Molecule 4: Photosystem II D2 protein

Chain d: 89%

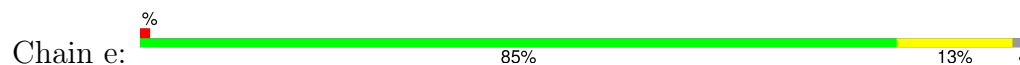


• Molecule 5: Cytochrome b559 subunit alpha

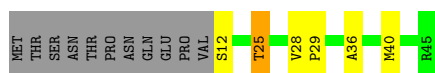
Chain E: 80%



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



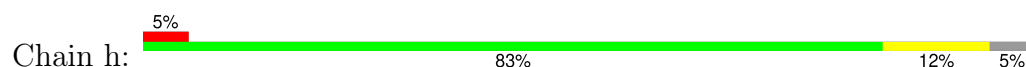
- Molecule 6: Cytochrome b559 subunit beta



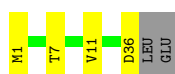
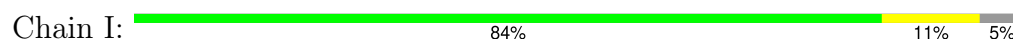
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

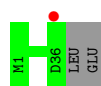


- Molecule 8: Photosystem II reaction center protein I

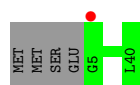
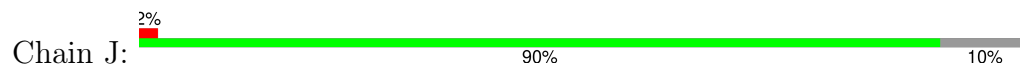


- Molecule 8: Photosystem II reaction center protein I





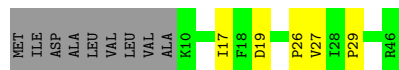
- Molecule 9: Photosystem II reaction center protein J



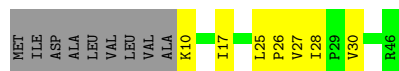
- Molecule 9: Photosystem II reaction center protein J



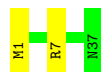
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



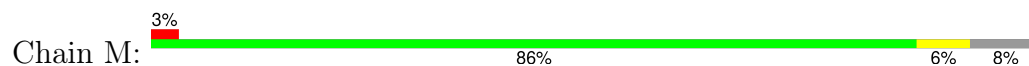
- Molecule 11: Photosystem II reaction center protein L

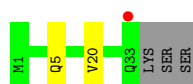


- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 8% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 10%



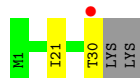
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 84% 5% 10%



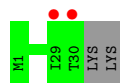
- Molecule 14: Photosystem II reaction center protein T

Chain T: 88% 3% 6%



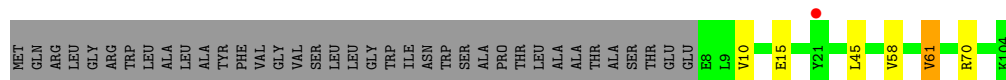
- Molecule 14: Photosystem II reaction center protein T

Chain t: 94% 6% 6%

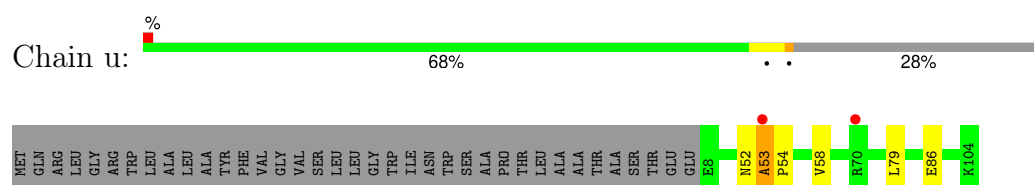


- Molecule 15: Photosystem II 12 kDa extrinsic protein

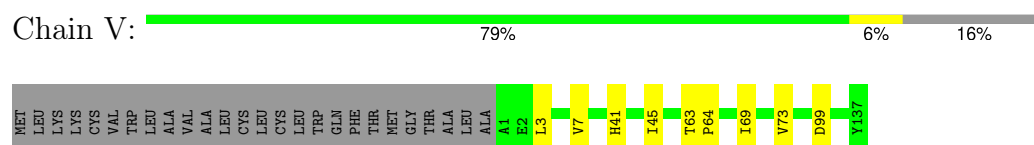
Chain U: 68% 28%



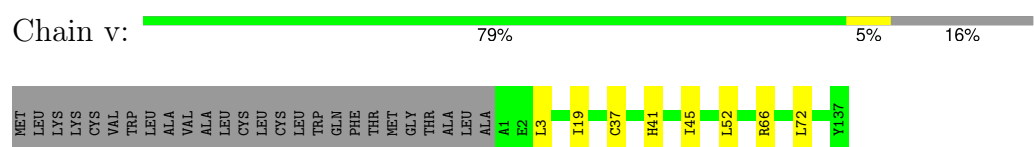
- Molecule 15: Photosystem II 12 kDa extrinsic protein



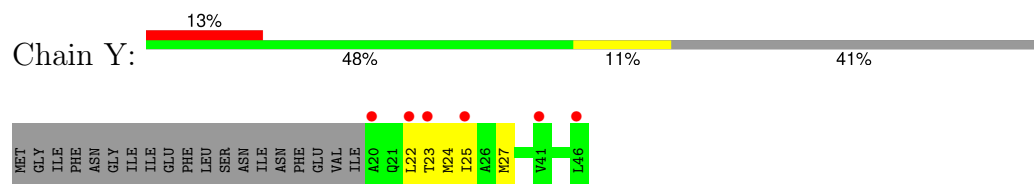
- Molecule 16: Cytochrome c-550



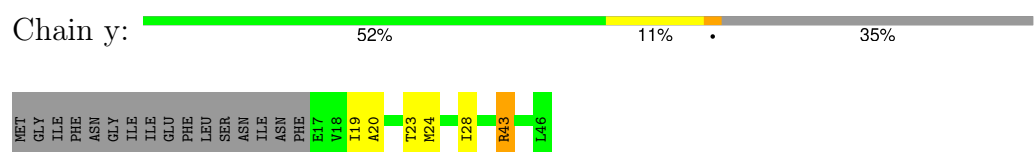
- Molecule 16: Cytochrome c-550



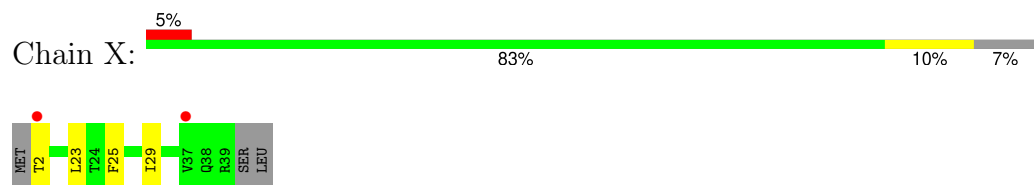
- Molecule 17: Photosystem II reaction center protein Ycf12



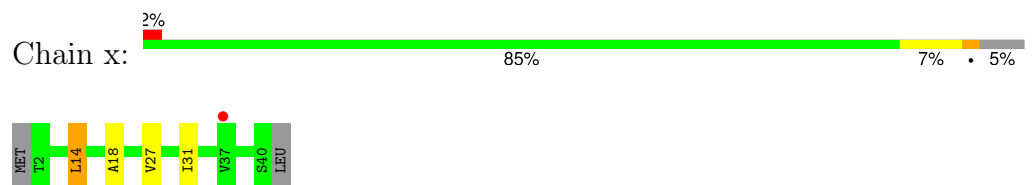
- Molecule 17: Photosystem II reaction center protein Ycf12



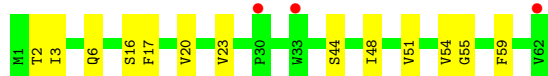
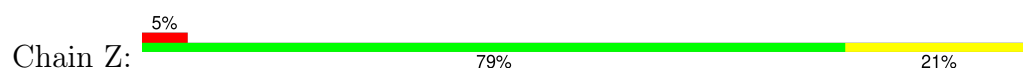
- Molecule 18: Photosystem II reaction center X protein



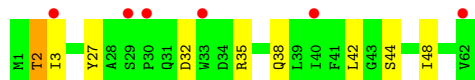
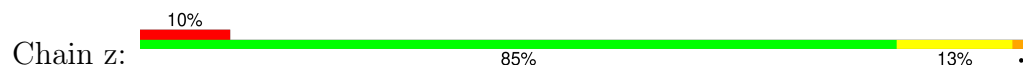
- Molecule 18: Photosystem II reaction center X protein



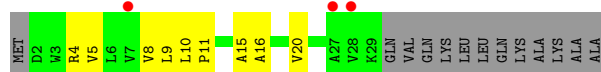
- Molecule 19: Photosystem II reaction center protein Z



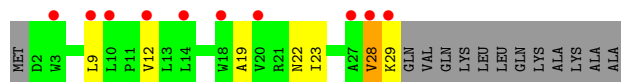
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.48Å 222.57Å 308.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.14 – 1.97 35.14 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.14-1.97) 85.9 (35.14-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.38 (at 1.97Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.188 , 0.226 0.188 , 0.226	Depositor DCC
R_{free} test set	5026 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	104120	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, BCT, DGD, PL9, CL, BCR, LMG, CLA, STE, FE2, OEX, LHG, PHO, HEC, HEM, 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	0.51	0/2707	0.60	0/3692
1	a	0.48	0/2704	0.58	0/3688
2	B	0.45	0/4179	0.56	0/5693
2	b	0.42	0/4127	0.53	0/5623
3	C	0.44	0/3547	0.54	0/4830
3	c	0.39	0/3619	0.53	0/4926
4	D	0.48	0/2812	0.58	0/3832
4	d	0.44	0/2821	0.55	0/3844
5	E	0.34	0/688	0.49	0/940
5	e	0.30	0/683	0.46	0/932
6	F	0.34	0/284	0.47	0/387
6	f	0.32	0/284	0.56	0/387
7	H	0.42	0/517	0.51	0/705
7	h	0.34	0/505	0.50	0/689
8	I	0.42	0/293	0.49	0/396
8	i	0.45	0/293	0.48	0/396
9	J	0.36	0/263	0.46	0/356
9	j	0.29	0/263	0.46	0/356
10	K	0.33	0/303	0.46	0/416
10	k	0.32	0/303	0.43	0/416
11	L	0.48	0/311	0.53	0/422
11	l	0.45	0/303	0.50	0/412
12	M	0.46	0/249	0.58	0/341
12	m	0.45	0/244	0.58	0/334
13	O	0.42	0/1904	0.59	0/2585
13	o	0.42	0/1905	0.59	0/2583
14	T	0.45	0/257	0.57	0/349
14	t	0.41	0/255	0.50	0/346
15	U	0.39	0/785	0.54	0/1064
15	u	0.43	0/785	0.58	0/1064
16	V	0.43	0/1085	0.58	0/1473
16	v	0.37	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.31	0/197	0.41	0/264
17	y	0.24	0/219	0.43	0/294
18	X	0.33	0/284	0.46	0/384
18	x	0.28	0/289	0.40	0/391
19	Z	0.38	1/490 (0.2%)	0.43	0/669
19	z	0.24	0/488	0.44	0/666
20	R	0.26	0/227	0.41	0/313
20	r	0.23	0/227	0.32	0/313
All	All	0.43	1/42784 (0.0%)	0.54	0/58244

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
2	B	0	1
13	o	0	1
15	u	0	1
16	V	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	23	VAL	CA-CB	-6.18	1.51	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	422	ARG	Sidechain
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain
15	u	52	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2469	2519	13	0
1	a	2619	2462	2510	20	0
2	B	4016	3887	3871	31	0
2	b	3984	3842	3842	21	0
3	C	3426	3347	3343	14	0
3	c	3500	3418	3426	17	0
4	D	2717	2620	2621	23	0
4	d	2723	2626	2627	20	0
5	E	666	651	651	12	0
5	e	664	648	648	11	0
6	F	275	282	282	3	0
6	f	275	282	282	5	0
7	H	505	528	528	5	0
7	h	493	514	514	5	0
8	I	296	311	311	1	0
8	i	296	311	311	0	0
9	J	257	268	268	0	0
9	j	257	268	268	5	0
10	K	293	305	305	4	0
10	k	293	305	305	5	0
11	L	304	316	316	3	0
11	l	296	304	304	1	0
12	M	256	267	269	3	0
12	m	251	267	267	3	0
13	O	1870	1830	1830	6	0
13	o	1874	1846	1846	6	0
14	T	258	261	261	1	0
14	t	256	256	256	0	0
15	U	774	773	773	3	0
15	u	774	773	773	5	0
16	V	1064	1071	1073	3	0
16	v	1064	1071	1073	5	0
17	Y	196	217	217	4	0
17	y	218	241	241	4	0
18	X	281	312	312	3	0
18	x	286	316	314	3	0
19	Z	479	516	516	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	477	509	509	5	0
20	R	221	238	238	5	0
20	r	221	238	238	4	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	1	1	0	0
24	a	4	1	1	0	0
25	A	249	264	264	4	0
25	B	1035	1139	1139	12	0
25	C	839	922	922	11	0
25	D	130	144	144	3	0
25	a	260	288	288	4	0
25	b	1035	1139	1139	18	0
25	c	839	919	919	15	0
25	d	130	144	144	4	0
26	A	64	74	74	1	0
26	D	64	74	74	0	0
26	a	64	74	74	0	0
26	d	64	74	74	3	0
27	A	40	56	56	0	0
27	B	120	168	168	4	0
27	C	40	56	56	1	0
27	D	40	56	56	4	0
27	H	40	56	56	2	0
27	K	80	112	112	5	0
27	T	40	56	56	4	0
27	Y	40	56	56	2	0
27	a	40	56	56	1	0
27	b	120	168	168	5	0
27	c	80	112	112	3	0
27	d	40	56	56	3	0
27	h	40	56	56	5	0
27	k	80	112	112	2	0
27	t	40	56	56	3	0
28	A	55	80	80	7	0
28	D	55	80	80	0	0
28	a	55	80	80	4	0
28	d	55	80	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	37	68	68	3	0
29	B	62	96	96	1	0
29	C	78	126	126	3	0
29	D	9	17	17	0	0
29	E	44	74	74	1	0
29	H	18	35	35	0	0
29	I	32	48	48	0	0
29	J	12	16	16	0	0
29	K	14	27	27	0	0
29	M	40	67	67	1	0
29	T	16	31	31	0	0
29	X	20	35	35	1	0
29	Z	17	33	33	0	0
29	a	12	16	16	0	0
29	b	54	90	90	1	0
29	c	31	57	57	0	0
29	d	54	90	90	1	0
29	e	31	52	52	0	0
29	f	8	15	15	0	0
29	h	21	40	40	1	0
29	i	18	24	24	0	0
29	j	28	47	47	0	0
29	l	18	35	35	0	0
29	m	12	16	16	0	0
29	t	24	36	36	0	0
29	x	20	35	35	0	0
29	z	9	14	14	0	0
30	A	48	66	66	0	0
30	B	96	132	132	9	0
30	C	84	106	106	1	0
30	D	101	142	142	3	0
30	a	104	154	154	6	0
30	b	106	158	158	3	0
30	c	124	172	172	1	0
30	d	44	58	58	1	0
31	A	95	122	124	0	0
31	B	54	77	78	1	0
31	D	36	45	46	1	0
31	a	108	154	156	1	0
31	b	49	64	65	2	0
31	f	41	48	49	1	0
32	A	66	96	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	186	246	246	3	0
32	H	62	81	82	0	0
32	c	186	246	246	1	0
32	h	62	82	82	0	0
33	B	49	74	74	1	0
33	D	96	141	141	1	0
33	E	49	74	74	3	0
33	L	49	74	74	3	0
33	a	42	57	57	0	0
33	d	137	199	199	5	0
33	l	49	74	74	0	0
34	F	43	30	30	3	0
34	e	43	30	30	3	0
35	V	43	30	30	0	0
35	v	43	30	30	1	0
36	A	125	0	0	1	0
36	B	175	0	0	1	0
36	C	139	0	0	1	0
36	D	102	0	0	0	0
36	E	16	0	0	0	0
36	F	7	0	0	0	0
36	H	25	0	0	0	0
36	I	11	0	0	0	0
36	J	11	0	0	0	0
36	K	1	0	0	0	0
36	L	7	0	0	0	0
36	M	6	0	0	0	0
36	O	78	0	0	0	0
36	R	2	0	0	0	0
36	T	6	0	0	0	0
36	U	33	0	0	0	0
36	V	49	0	0	0	0
36	X	11	0	0	0	0
36	Z	1	0	0	0	0
36	a	107	0	0	0	0
36	b	150	0	0	1	0
36	c	130	0	0	1	0
36	d	96	0	0	1	0
36	e	9	0	0	0	0
36	f	1	0	0	0	0
36	h	10	0	0	0	0
36	i	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	j	4	0	0	0	0
36	k	2	0	0	1	0
36	l	10	0	0	0	0
36	m	4	0	0	0	0
36	o	75	0	0	1	0
36	r	1	0	0	0	0
36	t	7	0	0	0	0
36	u	48	0	0	0	0
36	v	33	0	0	0	0
36	x	5	0	0	0	0
36	z	4	0	0	0	0
All	All	52043	52077	52178	364	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 4.

The worst 5 of 364 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)
13:o:189:ARG:NH1	36:o:301:HOH:O	2.02	0.91
3:C:156:LYS:NZ	36:C:601:HOH:O	2.05	0.89
27:H:101:BCR:HC8	27:H:101:BCR:H331	1.54	0.88
27:Y:101:BCR:H322	19:Z:17:PHE:CE1	2.20	0.77
34:F:101:HEM:HBC2	34:F:101:HEM:HHO	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/344 (96%)	328 (99%)	3 (1%)	1 (0%)	36 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	332/344 (96%)	326 (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	442/461 (96%)	433 (98%)	8 (2%)	1 (0%)	43	35
3	c	451/461 (98%)	442 (98%)	8 (2%)	1 (0%)	43	35
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	340/352 (97%)	334 (98%)	6 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	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%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	10 (4%)	1 (0%)	30	20
13	o	242/272 (89%)	231 (96%)	9 (4%)	2 (1%)	16	7
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	4
16	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	18	9
16	v	135/163 (83%)	128 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	0
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
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%)	22 (85%)	3 (12%)	1 (4%)	2	0
All	All	5234/5700 (92%)	5093 (97%)	130 (2%)	11 (0%)	43	35

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
13	o	58	ASN
15	u	53	ALA
19	z	2	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	82
1	a	269/280 (96%)	267 (99%)	2 (1%)	76	73
2	B	410/407 (101%)	406 (99%)	4 (1%)	68	65
2	b	403/407 (99%)	400 (99%)	3 (1%)	76	73
3	C	346/362 (96%)	342 (99%)	4 (1%)	63	58
3	c	354/362 (98%)	352 (99%)	2 (1%)	78	76
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	277/283 (98%)	275 (99%)	2 (1%)	76	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	29
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	26 (93%)	2 (7%)	13	5
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	20
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	44
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	26
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	3
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	23
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	28
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	203 (98%)	3 (2%)	57	52
13	o	207/228 (91%)	203 (98%)	4 (2%)	50	44
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	19
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	35
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	48
16	v	117/138 (85%)	116 (99%)	1 (1%)	70	67
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	22 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	24
19	Z	52/52 (100%)	52 (100%)	0	100	100
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	r	22/33 (67%)	21 (96%)	1 (4%)	24	13
All	All	4324/4654 (93%)	4280 (99%)	44 (1%)	68	65

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	124	VAL
9	j	21	VAL
3	c	240	ILE
6	f	23	VAL
13	o	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
7	h	59	ASN
12	m	32	GLN
13	o	155	ASN
19	Z	6	GLN
15	U	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.58	0	8,9,11	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	T	1	14	8,9,10	0.70	0	8,9,11	0.90	0
12	FME	m	1	12	8,9,10	0.39	0	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	0.56	0	8,9,11	1.01	0
8	FME	I	1	8	8,9,10	0.47	0	8,9,11	1.12	1 (12%)
12	FME	M	1	12	8,9,10	0.57	0	8,9,11	0.87	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
8	FME	i	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CG-CB-CA	2.04	119.11	112.87

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O-C-CA-CB
8	I	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG

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 211 ligands modelled in this entry, 6 are monoatomic - leaving 205 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	DGD	C	520	-	63,63,67	0.75	1 (1%)	77,77,81	1.06	6 (7%)
29	STE	b	626	-	7,7,19	0.36	0	6,6,19	0.77	0
29	STE	M	103	-	14,14,19	0.36	0	13,13,19	0.90	0
29	STE	A	619	-	10,10,19	0.42	0	9,9,19	0.65	0
29	STE	x	101	-	19,19,19	0.67	0	19,19,19	0.87	0
33	LHG	D	409	-	48,48,48	0.64	1 (2%)	51,54,54	0.88	1 (1%)
27	BCR	K	101	-	41,41,41	0.32	0	56,56,56	0.69	0
29	STE	C	526	-	13,13,19	0.43	0	12,12,19	0.71	0
33	LHG	D	410	-	46,46,48	0.60	0	49,52,54	0.64	1 (2%)
29	STE	M	101	-	14,14,19	0.70	0	14,14,19	1.09	1 (7%)
31	SQD	A	616	-	41,43,54	1.78	8 (19%)	51,54,65	1.51	6 (11%)
29	STE	b	622	-	19,19,19	0.63	0	19,19,19	1.05	0
25	CLA	b	614	2	69,73,73	1.36	6 (8%)	82,113,113	1.38	9 (10%)
29	STE	t	103	-	9,9,19	0.53	0	8,8,19	0.42	0
27	BCR	H	101	-	41,41,41	0.58	0	56,56,56	1.07	3 (5%)
32	DGD	c	521	-	63,63,67	0.55	0	77,77,81	0.98	4 (5%)
30	LMG	a	616	-	55,55,55	0.56	0	63,63,63	1.42	9 (14%)
30	LMG	d	411	-	44,44,55	0.59	0	52,52,63	0.75	2 (3%)
28	PL9	a	611	-	55,55,55	1.14	2 (3%)	68,69,69	1.53	11 (16%)
25	CLA	C	510	3	69,73,73	1.22	10 (14%)	82,113,113	1.38	5 (6%)
29	STE	E	102	-	11,11,19	0.79	0	11,11,19	1.11	1 (9%)
28	PL9	A	611	-	55,55,55	1.14	4 (7%)	68,69,69	1.57	8 (11%)
27	BCR	b	618	-	41,41,41	0.52	0	56,56,56	0.89	1 (1%)
25	CLA	C	504	36	63,67,73	1.27	8 (12%)	74,105,113	1.44	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	610	36	69,73,73	1.32	7 (10%)	82,113,113	1.30	9 (10%)
25	CLA	a	612	36	69,73,73	1.41	6 (8%)	82,113,113	1.24	4 (4%)
25	CLA	b	610	36	69,73,73	1.35	10 (14%)	82,113,113	1.25	8 (9%)
25	CLA	b	604	2	69,73,73	1.15	8 (11%)	82,113,113	1.50	14 (17%)
25	CLA	A	606	1	69,73,73	1.26	6 (8%)	82,113,113	1.32	6 (7%)
26	PHO	A	608	-	58,69,69	1.98	9 (15%)	55,99,99	1.85	10 (18%)
29	STE	D	411	-	8,8,19	0.44	0	7,7,19	0.63	0
33	LHG	a	614	-	41,41,48	0.62	0	44,47,54	0.65	1 (2%)
27	BCR	D	404	-	41,41,41	0.48	0	56,56,56	1.06	5 (8%)
29	STE	b	624	-	15,15,19	0.77	0	15,15,19	1.26	3 (20%)
31	SQD	A	615	-	50,52,54	1.57	7 (14%)	60,63,65	2.07	12 (20%)
25	CLA	B	612	2	69,73,73	1.16	6 (8%)	82,113,113	1.41	8 (9%)
33	LHG	d	409	-	38,38,48	0.59	0	41,44,54	0.69	0
25	CLA	b	612	2	69,73,73	1.29	10 (14%)	82,113,113	1.32	11 (13%)
32	DGD	h	102	-	63,63,67	0.57	0	77,77,81	1.01	6 (7%)
25	CLA	c	503	3	69,73,73	1.25	10 (14%)	82,113,113	1.31	8 (9%)
25	CLA	B	607	36	69,73,73	1.28	6 (8%)	82,113,113	1.38	9 (10%)
25	CLA	C	512	3	69,73,73	1.37	11 (15%)	82,113,113	1.36	8 (9%)
25	CLA	B	602	2	69,73,73	1.27	9 (13%)	82,113,113	1.19	6 (7%)
29	STE	e	104	-	12,12,19	0.69	0	12,12,19	1.19	2 (16%)
30	LMG	B	621	-	51,51,55	0.39	0	59,59,63	1.16	3 (5%)
30	LMG	b	621	-	51,51,55	0.48	0	59,59,63	0.88	2 (3%)
33	LHG	B	623	-	48,48,48	0.55	1 (2%)	51,54,54	0.84	2 (3%)
25	CLA	d	402	4	69,73,73	1.20	9 (13%)	82,113,113	1.25	4 (4%)
25	CLA	A	607	36	69,73,73	1.22	7 (10%)	82,113,113	1.34	8 (9%)
25	CLA	c	506	3	69,73,73	1.13	6 (8%)	82,113,113	1.38	8 (9%)
29	STE	A	618	-	16,16,19	0.52	0	15,15,19	0.49	0
25	CLA	c	513	3	69,73,73	1.19	7 (10%)	82,113,113	1.18	5 (6%)
27	BCR	c	515	-	41,41,41	0.45	0	56,56,56	0.76	0
29	STE	C	525	-	15,15,19	0.39	0	14,14,19	0.73	0
25	CLA	b	608	2	69,73,73	1.19	8 (11%)	82,113,113	1.39	8 (9%)
25	CLA	c	505	3	69,73,73	1.27	11 (15%)	82,113,113	1.49	9 (10%)
25	CLA	b	605	2	69,73,73	1.33	8 (11%)	82,113,113	1.42	13 (15%)
25	CLA	C	507	36	69,73,73	1.20	8 (11%)	82,113,113	1.60	10 (12%)
25	CLA	C	501	3	69,73,73	1.49	8 (11%)	82,113,113	1.54	7 (8%)
29	STE	B	627	-	14,14,19	0.52	0	13,13,19	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PHO	D	401	-	58,69,69	1.90	11 (18%)	55,99,99	1.84	10 (18%)
29	STE	e	103	-	8,8,19	0.40	0	7,7,19	0.65	0
27	BCR	b	617	-	41,41,41	0.44	0	56,56,56	0.86	4 (7%)
29	STE	C	515	-	13,13,19	0.84	0	13,13,19	0.84	0
29	STE	B	626	-	11,11,19	0.74	0	11,11,19	1.15	1 (9%)
24	BCT	A	605	22	3,3,3	0.74	0	2,3,3	2.87	1 (50%)
30	LMG	C	523	-	48,48,55	0.48	0	56,56,63	0.63	0
27	BCR	a	610	-	41,41,41	0.45	0	56,56,56	0.84	2 (3%)
25	CLA	a	609	1	69,73,73	1.44	9 (13%)	82,113,113	1.26	10 (12%)
29	STE	b	625	-	9,9,19	0.41	0	8,8,19	0.68	0
29	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.03	1 (9%)
25	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.37	9 (10%)
25	CLA	c	504	36	64,68,73	1.16	8 (12%)	76,107,113	1.34	10 (13%)
25	CLA	b	603	2	69,73,73	1.25	7 (10%)	82,113,113	1.45	9 (10%)
33	LHG	d	407	-	48,48,48	0.57	0	51,54,54	0.63	0
25	CLA	A	613	36	69,73,73	1.42	9 (13%)	82,113,113	1.42	6 (7%)
27	BCR	h	101	-	41,41,41	0.39	0	56,56,56	0.97	3 (5%)
27	BCR	b	619	-	41,41,41	0.41	0	56,56,56	1.07	3 (5%)
24	BCT	a	605	22	3,3,3	0.76	0	2,3,3	2.37	1 (50%)
25	CLA	B	614	2	69,73,73	1.15	6 (8%)	82,113,113	1.30	9 (10%)
27	BCR	d	404	-	41,41,41	0.51	0	56,56,56	1.04	3 (5%)
31	SQD	a	615	-	52,54,54	1.65	8 (15%)	62,65,65	1.41	7 (11%)
27	BCR	k	102	-	41,41,41	0.40	0	56,56,56	0.85	1 (1%)
25	CLA	D	402	4	69,73,73	1.14	8 (11%)	82,113,113	1.40	7 (8%)
25	CLA	c	511	3	69,73,73	1.57	9 (13%)	82,113,113	1.36	8 (9%)
27	BCR	k	101	-	41,41,41	0.42	0	56,56,56	0.75	1 (1%)
29	STE	C	517	-	4,4,19	0.42	0	3,3,19	0.41	0
29	STE	C	518	-	6,6,19	0.47	0	5,5,19	0.48	0
29	STE	C	524	-	11,11,19	0.83	1 (9%)	11,11,19	1.38	1 (9%)
31	SQD	a	613	-	52,54,54	1.54	7 (13%)	62,65,65	1.84	12 (19%)
25	CLA	d	403	4	69,73,73	1.51	9 (13%)	82,113,113	1.11	6 (7%)
34	HEM	F	101	5,6	50,50,50	1.46	7 (14%)	67,82,82	1.32	11 (16%)
25	CLA	C	511	3	69,73,73	1.41	9 (13%)	82,113,113	1.43	6 (7%)
28	PL9	d	405	-	55,55,55	1.31	4 (7%)	68,69,69	1.67	15 (22%)
29	STE	E	104	-	19,19,19	0.72	0	19,19,19	0.97	1 (5%)
34	HEM	e	102	5,6	50,50,50	1.52	8 (16%)	67,82,82	1.36	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	c	518	-	29,29,55	0.42	0	31,31,63	0.72	1 (3%)
25	CLA	b	607	36	69,73,73	1.33	7 (10%)	82,113,113	1.27	7 (8%)
27	BCR	B	618	-	41,41,41	0.50	0	56,56,56	1.05	3 (5%)
27	BCR	K	102	-	41,41,41	0.43	0	56,56,56	1.09	3 (5%)
30	LMG	A	614	-	48,48,55	0.48	0	56,56,63	0.87	2 (3%)
29	STE	M	102	-	9,9,19	0.36	0	8,8,19	0.89	0
29	STE	E	103	-	11,11,19	0.43	0	10,10,19	0.60	0
29	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.10	1 (9%)
32	DGD	C	522	-	63,63,67	0.60	1 (1%)	77,77,81	0.81	1 (1%)
32	DGD	c	519	-	63,63,67	0.73	3 (4%)	77,77,81	0.81	2 (2%)
29	STE	d	410	-	19,19,19	0.68	0	19,19,19	0.85	0
25	CLA	c	510	3	69,73,73	1.21	8 (11%)	82,113,113	1.22	7 (8%)
25	CLA	c	507	36	69,73,73	1.25	6 (8%)	82,113,113	1.34	8 (9%)
33	LHG	d	408	-	48,48,48	0.59	0	51,54,54	0.75	1 (1%)
25	CLA	A	609	1	58,62,73	1.38	8 (13%)	68,99,113	1.26	6 (8%)
25	CLA	B	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	7 (8%)
21	OEX	a	601	36,1,3	0,14,14	-	-	-	-	-
25	CLA	C	502	3	69,73,73	1.20	7 (10%)	82,113,113	1.33	5 (6%)
26	PHO	d	401	-	58,69,69	2.14	9 (15%)	55,99,99	1.78	10 (18%)
25	CLA	C	503	3	69,73,73	1.40	7 (10%)	82,113,113	1.52	9 (10%)
25	CLA	C	509	3	69,73,73	1.16	10 (14%)	82,113,113	1.30	7 (8%)
29	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.21	0
32	DGD	C	521	-	63,63,67	0.63	1 (1%)	77,77,81	0.76	0
25	CLA	b	602	2	69,73,73	1.22	9 (13%)	82,113,113	1.31	6 (7%)
25	CLA	a	607	36	69,73,73	1.20	10 (14%)	82,113,113	1.31	6 (7%)
29	STE	e	101	-	8,8,19	0.45	0	7,7,19	0.53	0
29	STE	A	612	-	8,8,19	0.45	0	7,7,19	0.57	0
32	DGD	A	617	-	67,67,67	0.56	0	81,81,81	0.99	4 (4%)
33	LHG	E	101	-	48,48,48	0.60	0	51,54,54	0.58	0
27	BCR	B	617	-	41,41,41	0.44	0	56,56,56	0.77	1 (1%)
25	CLA	c	501	3	69,73,73	1.22	9 (13%)	82,113,113	1.39	6 (7%)
29	STE	m	101	-	11,11,19	0.77	0	11,11,19	1.41	2 (18%)
30	LMG	a	617	-	49,49,55	0.54	1 (2%)	57,57,63	0.73	0
31	SQD	b	620	-	47,49,54	1.65	11 (23%)	57,60,65	2.00	14 (24%)
21	OEX	A	601	36,1,3	0,14,14	-	-	-	-	-
29	STE	d	412	-	13,13,19	0.72	0	13,13,19	1.14	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	611	2	69,73,73	1.31	8 (11%)	82,113,113	1.35	9 (10%)
35	HEC	V	201	16	50,50,50	1.71	4 (8%)	68,82,82	1.41	10 (14%)
25	CLA	B	611	2	69,73,73	1.12	5 (7%)	82,113,113	1.56	10 (12%)
25	CLA	B	613	2	69,73,73	1.18	5 (7%)	82,113,113	1.30	7 (8%)
25	CLA	b	613	2	69,73,73	1.26	12 (17%)	82,113,113	1.33	8 (9%)
25	CLA	b	615	2	69,73,73	1.26	7 (10%)	82,113,113	1.22	9 (10%)
27	BCR	t	101	-	41,41,41	0.50	0	56,56,56	1.27	8 (14%)
29	STE	B	622	-	16,16,19	0.69	0	16,16,19	1.06	0
30	LMG	b	623	-	55,55,55	0.47	0	63,63,63	1.20	8 (12%)
25	CLA	C	513	3	69,73,73	1.51	8 (11%)	82,113,113	1.31	8 (9%)
29	STE	c	517	-	17,17,19	0.46	0	16,16,19	0.62	0
31	SQD	D	408	-	34,36,54	1.53	4 (11%)	42,45,65	2.15	11 (26%)
25	CLA	B	609	2	69,73,73	1.36	5 (7%)	82,113,113	1.32	6 (7%)
27	BCR	B	619	-	41,41,41	0.35	0	56,56,56	1.10	4 (7%)
29	STE	K	103	-	13,13,19	0.40	0	12,12,19	0.72	0
25	CLA	B	616	2	64,68,73	1.44	5 (7%)	76,107,113	1.45	10 (13%)
30	LMG	D	406	-	50,50,55	0.49	0	58,58,63	1.19	4 (6%)
25	CLA	B	601	36	69,73,73	1.47	8 (11%)	82,113,113	1.56	9 (10%)
27	BCR	T	101	-	41,41,41	0.49	0	56,56,56	1.11	2 (3%)
32	DGD	c	520	-	63,63,67	0.59	0	77,77,81	0.89	2 (2%)
29	STE	h	104	-	10,10,19	0.38	0	9,9,19	0.66	0
29	STE	z	101	-	8,8,19	0.47	0	7,7,19	0.53	0
30	LMG	D	407	-	51,51,55	0.55	0	59,59,63	0.90	3 (5%)
35	HEC	v	201	16	50,50,50	1.55	4 (8%)	68,82,82	1.27	7 (10%)
28	PL9	D	405	-	55,55,55	1.38	6 (10%)	68,69,69	1.43	8 (11%)
25	CLA	B	606	2	69,73,73	1.42	7 (10%)	82,113,113	1.42	10 (12%)
25	CLA	B	608	2	69,73,73	1.16	4 (5%)	82,113,113	1.25	7 (8%)
29	STE	a	618	-	11,11,19	0.83	0	11,11,19	0.89	0
29	STE	j	102	-	15,15,19	0.46	0	14,14,19	0.62	0
30	LMG	B	620	-	45,45,55	0.49	0	53,53,63	1.18	5 (9%)
30	LMG	C	516	-	35,35,55	0.48	0	43,43,63	1.51	8 (18%)
25	CLA	B	603	2	69,73,73	1.16	5 (7%)	82,113,113	1.37	11 (13%)
29	STE	d	406	-	19,19,19	0.76	0	19,19,19	0.93	1 (5%)
29	STE	I	102	-	14,14,19	0.80	0	14,14,19	0.95	1 (7%)
25	CLA	b	616	2	64,68,73	1.24	6 (9%)	76,107,113	1.47	13 (17%)
33	LHG	l	101	-	48,48,48	0.48	0	51,54,54	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	601	36	69,73,73	1.28	8 (11%)	82,113,113	1.41	5 (6%)
29	STE	I	101	-	16,16,19	0.73	0	16,16,19	1.02	1 (6%)
29	STE	i	101	-	11,11,19	0.78	0	11,11,19	1.05	0
29	STE	i	102	-	5,5,19	0.41	0	4,4,19	0.53	0
29	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.55	0
29	STE	X	101	-	19,19,19	0.71	0	19,19,19	1.08	0
29	STE	c	516	-	12,12,19	0.46	0	11,11,19	0.63	0
25	CLA	c	509	3	69,73,73	1.20	7 (10%)	82,113,113	1.44	7 (8%)
31	SQD	B	624	-	52,54,54	1.57	7 (13%)	62,65,65	1.87	10 (16%)
25	CLA	D	403	4	69,73,73	1.32	9 (13%)	82,113,113	1.20	5 (6%)
32	DGD	H	102	-	63,63,67	0.59	0	77,77,81	0.88	3 (3%)
25	CLA	b	606	2	69,73,73	1.41	7 (10%)	82,113,113	1.60	5 (6%)
25	CLA	B	604	2	69,73,73	1.31	9 (13%)	82,113,113	1.58	9 (10%)
29	STE	Z	101	-	16,16,19	0.49	0	15,15,19	0.54	0
31	SQD	f	101	-	39,41,54	1.67	7 (17%)	49,52,65	1.89	11 (22%)
29	STE	l	102	-	17,17,19	0.45	0	16,16,19	0.64	0
25	CLA	C	506	3	69,73,73	1.28	6 (8%)	82,113,113	1.25	6 (7%)
29	STE	C	519	-	9,9,19	0.55	0	8,8,19	0.45	0
25	CLA	B	615	2	69,73,73	1.39	7 (10%)	82,113,113	1.26	5 (6%)
30	LMG	c	522	-	46,46,55	0.53	0	54,54,63	0.75	0
33	LHG	L	101	-	48,48,48	0.57	0	51,54,54	0.75	2 (3%)
25	CLA	a	606	1	69,73,73	1.27	10 (14%)	82,113,113	1.34	9 (10%)
26	PHO	a	608	-	58,69,69	1.97	12 (20%)	55,99,99	1.73	12 (21%)
25	CLA	b	609	2	69,73,73	1.08	4 (5%)	82,113,113	1.33	6 (7%)
25	CLA	c	508	3	68,72,73	1.22	9 (13%)	80,111,113	1.20	8 (10%)
29	STE	B	625	-	17,17,19	0.69	0	17,17,19	1.07	1 (5%)
30	LMG	c	523	-	48,48,55	0.50	0	56,56,63	0.78	1 (1%)
25	CLA	c	512	3	69,73,73	1.24	7 (10%)	82,113,113	1.37	10 (12%)
29	STE	h	103	-	9,9,19	0.44	0	8,8,19	0.60	0
27	BCR	Y	101	-	41,41,41	0.49	0	56,56,56	0.92	0
29	STE	T	102	-	15,15,19	0.40	0	14,14,19	0.88	0
27	BCR	A	610	-	41,41,41	0.37	0	56,56,56	0.93	2 (3%)
25	CLA	c	502	3	69,73,73	1.38	7 (10%)	82,113,113	1.33	7 (8%)
27	BCR	C	514	-	41,41,41	0.41	0	56,56,56	1.06	4 (7%)
25	CLA	C	508	3	69,73,73	1.37	9 (13%)	82,113,113	1.42	8 (9%)
29	STE	f	102	-	7,7,19	0.41	0	6,6,19	0.59	0
27	BCR	c	514	-	41,41,41	0.36	0	56,56,56	0.57	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
32	DGD	C	520	-	-	19/51/91/95	0/2/2/2
29	STE	b	626	-	-	4/5/5/17	-
29	STE	M	103	-	-	8/12/12/17	-
29	STE	A	619	-	-	4/8/8/17	-
29	STE	x	101	-	-	10/17/17/17	-
33	LHG	D	409	-	-	12/53/53/53	-
27	BCR	K	101	-	-	5/29/63/63	0/2/2/2
29	STE	C	526	-	-	3/11/11/17	-
33	LHG	D	410	-	-	12/51/51/53	-
29	STE	M	101	-	-	9/12/12/17	-
31	SQD	A	616	-	-	11/38/58/69	0/1/1/1
29	STE	b	622	-	-	9/17/17/17	-
25	CLA	b	614	2	-	10/39/115/115	-
29	STE	t	103	-	-	4/7/7/17	-
27	BCR	H	101	-	-	4/29/63/63	0/2/2/2
32	DGD	c	521	-	-	14/51/91/95	0/2/2/2
30	LMG	a	616	-	-	25/50/70/70	0/1/1/1
30	LMG	d	411	-	-	10/39/59/70	0/1/1/1
28	PL9	a	611	-	-	21/53/73/73	0/1/1/1
25	CLA	C	510	3	-	5/39/115/115	-
29	STE	E	102	-	-	2/9/9/17	-
28	PL9	A	611	-	-	17/53/73/73	0/1/1/1
27	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	CLA	C	504	36	-	5/32/108/115	-
25	CLA	B	610	36	-	5/39/115/115	-
25	CLA	a	612	36	-	4/39/115/115	-
25	CLA	b	610	36	-	8/39/115/115	-
25	CLA	b	604	2	-	7/39/115/115	-
25	CLA	A	606	1	-	4/39/115/115	-
26	PHO	A	608	-	-	4/37/103/103	0/5/6/6
29	STE	D	411	-	-	3/6/6/17	-
33	LHG	a	614	-	-	20/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	D	404	-	-	2/29/63/63	0/2/2/2
29	STE	b	624	-	-	6/13/13/17	-
31	SQD	A	615	-	-	19/47/67/69	0/1/1/1
25	CLA	B	612	2	-	10/39/115/115	-
33	LHG	d	409	-	-	10/43/43/53	-
25	CLA	b	612	2	-	7/39/115/115	-
32	DGD	h	102	-	-	20/51/91/95	0/2/2/2
25	CLA	c	503	3	-	8/39/115/115	-
25	CLA	B	607	36	-	5/39/115/115	-
25	CLA	C	512	3	-	10/39/115/115	-
25	CLA	B	602	2	-	3/39/115/115	-
29	STE	e	104	-	-	4/10/10/17	-
30	LMG	B	621	-	-	20/46/66/70	0/1/1/1
30	LMG	b	621	-	-	14/46/66/70	0/1/1/1
33	LHG	B	623	-	-	17/53/53/53	-
25	CLA	d	402	4	-	4/39/115/115	-
25	CLA	A	607	36	-	7/39/115/115	-
25	CLA	c	506	3	-	12/39/115/115	-
29	STE	A	618	-	-	9/14/14/17	-
25	CLA	c	513	3	-	14/39/115/115	-
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
29	STE	C	525	-	-	6/13/13/17	-
25	CLA	b	608	2	-	2/39/115/115	-
25	CLA	c	505	3	-	8/39/115/115	-
25	CLA	b	605	2	-	3/39/115/115	-
25	CLA	C	507	36	-	7/39/115/115	-
25	CLA	C	501	3	-	1/39/115/115	-
29	STE	B	627	-	-	9/12/12/17	-
26	PHO	D	401	-	-	0/37/103/103	0/5/6/6
29	STE	e	103	-	-	4/6/6/17	-
27	BCR	b	617	-	-	2/29/63/63	0/2/2/2
29	STE	C	515	-	-	7/11/11/17	-
29	STE	B	626	-	-	2/9/9/17	-
30	LMG	C	523	-	-	16/43/63/70	0/1/1/1
33	LHG	L	101	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	a	610	-	-	0/29/63/63	0/2/2/2
25	CLA	a	609	1	-	12/39/115/115	-
29	STE	b	625	-	-	5/7/7/17	-
29	STE	j	101	-	-	4/9/9/17	-
25	CLA	C	505	3	-	5/39/115/115	-
25	CLA	c	504	36	-	6/33/109/115	-
25	CLA	b	603	2	-	9/39/115/115	-
33	LHG	d	407	-	-	12/53/53/53	-
25	CLA	A	613	36	-	1/39/115/115	-
27	BCR	h	101	-	-	1/29/63/63	0/2/2/2
27	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	BCR	d	404	-	-	3/29/63/63	0/2/2/2
25	CLA	B	614	2	-	9/39/115/115	-
31	SQD	a	615	-	-	23/49/69/69	0/1/1/1
27	BCR	k	102	-	-	5/29/63/63	0/2/2/2
25	CLA	D	402	4	-	4/39/115/115	-
25	CLA	c	511	3	-	5/39/115/115	-
27	BCR	k	101	-	-	7/29/63/63	0/2/2/2
29	STE	C	517	-	-	0/2/2/17	-
29	STE	C	518	-	-	3/4/4/17	-
29	STE	C	524	-	-	3/9/9/17	-
31	SQD	a	613	-	-	25/49/69/69	0/1/1/1
25	CLA	d	403	4	-	4/39/115/115	-
34	HEM	F	101	5,6	-	3/14/54/54	-
25	CLA	C	511	3	-	2/39/115/115	-
28	PL9	d	405	-	-	9/53/73/73	0/1/1/1
29	STE	E	104	-	-	11/17/17/17	-
34	HEM	e	102	5,6	-	4/14/54/54	-
30	LMG	c	518	-	-	8/31/31/70	-
25	CLA	b	607	36	-	13/39/115/115	-
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	K	102	-	-	5/29/63/63	0/2/2/2
30	LMG	A	614	-	-	15/43/63/70	0/1/1/1
29	STE	M	102	-	-	4/7/7/17	-
29	STE	E	103	-	-	6/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	STE	J	101	-	-	7/9/9/17	-
32	DGD	C	522	-	-	10/51/91/95	0/2/2/2
32	DGD	c	519	-	-	19/51/91/95	0/2/2/2
29	STE	d	410	-	-	7/17/17/17	-
25	CLA	c	510	3	-	5/39/115/115	-
25	CLA	c	507	36	-	6/39/115/115	-
33	LHG	d	408	-	-	14/53/53/53	-
25	CLA	A	609	1	-	2/26/102/115	-
25	CLA	B	605	2	-	11/39/115/115	-
25	CLA	C	502	3	-	13/39/115/115	-
26	PHO	d	401	-	-	5/37/103/103	0/5/6/6
25	CLA	C	503	3	-	1/39/115/115	-
25	CLA	C	509	3	-	12/39/115/115	-
29	STE	t	102	-	-	6/11/11/17	-
32	DGD	C	521	-	-	19/51/91/95	0/2/2/2
25	CLA	b	602	2	-	7/39/115/115	-
25	CLA	a	607	36	-	6/39/115/115	-
29	STE	e	101	-	-	3/6/6/17	-
29	STE	A	612	-	-	2/6/6/17	-
32	DGD	A	617	-	-	26/55/95/95	0/2/2/2
33	LHG	E	101	-	-	25/53/53/53	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	c	501	3	-	5/39/115/115	-
29	STE	m	101	-	-	3/9/9/17	-
30	LMG	a	617	-	-	20/44/64/70	0/1/1/1
31	SQD	b	620	-	-	19/44/64/69	0/1/1/1
29	STE	d	412	-	-	7/11/11/17	-
25	CLA	b	611	2	-	8/39/115/115	-
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
25	CLA	B	611	2	-	5/39/115/115	-
25	CLA	B	613	2	-	9/39/115/115	-
25	CLA	b	613	2	-	9/39/115/115	-
25	CLA	b	615	2	-	10/39/115/115	-
27	BCR	t	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	STE	B	622	-	-	7/14/14/17	-
30	LMG	b	623	-	-	25/50/70/70	0/1/1/1
25	CLA	C	513	3	-	9/39/115/115	-
29	STE	c	517	-	-	6/15/15/17	-
31	SQD	D	408	-	-	16/28/48/69	0/1/1/1
25	CLA	B	609	2	-	4/39/115/115	-
27	BCR	B	619	-	-	3/29/63/63	0/2/2/2
29	STE	K	103	-	-	5/11/11/17	-
25	CLA	B	616	2	-	10/33/109/115	-
30	LMG	D	406	-	-	18/45/65/70	0/1/1/1
25	CLA	B	601	36	-	14/39/115/115	-
27	BCR	T	101	-	-	4/29/63/63	0/2/2/2
32	DGD	c	520	-	-	18/51/91/95	0/2/2/2
29	STE	h	104	-	-	1/8/8/17	-
29	STE	z	101	-	-	2/6/6/17	-
30	LMG	D	407	-	-	15/46/66/70	0/1/1/1
35	HEC	v	201	16	1/1/7/7	6/14/54/54	-
28	PL9	D	405	-	-	7/53/73/73	0/1/1/1
25	CLA	B	606	2	-	11/39/115/115	-
25	CLA	B	608	2	-	2/39/115/115	-
29	STE	a	618	-	-	3/9/9/17	-
29	STE	j	102	-	-	6/13/13/17	-
30	LMG	B	620	-	-	14/40/60/70	0/1/1/1
30	LMG	C	516	-	-	14/30/50/70	0/1/1/1
25	CLA	B	603	2	-	10/39/115/115	-
29	STE	d	406	-	-	12/17/17/17	-
29	STE	I	102	-	-	4/12/12/17	-
25	CLA	b	616	2	-	12/33/109/115	-
33	LHG	l	101	-	-	22/53/53/53	-
25	CLA	b	601	36	-	10/39/115/115	-
29	STE	I	101	-	-	7/14/14/17	-
29	STE	i	101	-	-	5/9/9/17	-
29	STE	i	102	-	-	0/3/3/17	-
29	STE	H	103	-	-	8/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	STE	X	101	-	-	5/17/17/17	-
29	STE	c	516	-	-	7/10/10/17	-
25	CLA	c	509	3	-	12/39/115/115	-
31	SQD	B	624	-	-	21/49/69/69	0/1/1/1
25	CLA	D	403	4	-	7/39/115/115	-
32	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	CLA	b	606	2	-	10/39/115/115	-
25	CLA	B	604	2	-	5/39/115/115	-
29	STE	Z	101	-	-	8/14/14/17	-
31	SQD	f	101	-	-	13/36/56/69	0/1/1/1
29	STE	l	102	-	-	10/15/15/17	-
25	CLA	C	506	3	-	8/39/115/115	-
29	STE	C	519	-	-	5/7/7/17	-
25	CLA	B	615	2	-	12/39/115/115	-
30	LMG	c	522	-	-	16/41/61/70	0/1/1/1
25	CLA	a	606	1	-	3/39/115/115	-
26	PHO	a	608	-	-	0/37/103/103	0/5/6/6
25	CLA	b	609	2	-	6/39/115/115	-
25	CLA	c	508	3	-	5/38/114/115	-
29	STE	B	625	-	-	10/15/15/17	-
30	LMG	c	523	-	-	19/43/63/70	0/1/1/1
25	CLA	c	512	3	-	15/39/115/115	-
29	STE	h	103	-	-	1/7/7/17	-
27	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
29	STE	T	102	-	-	6/13/13/17	-
27	BCR	A	610	-	-	1/29/63/63	0/2/2/2
25	CLA	c	502	3	-	4/39/115/115	-
27	BCR	C	514	-	-	1/29/63/63	0/2/2/2
25	CLA	C	508	3	-	6/39/115/115	-
29	STE	f	102	-	-	5/5/5/17	-
27	BCR	c	514	-	-	4/29/63/63	0/2/2/2

The worst 5 of 687 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C1B-C2B	9.42	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C3B-C4B	9.04	1.50	1.41
26	a	608	PHO	C1B-C2B	8.77	1.49	1.39
26	A	608	PHO	C3B-C4B	8.39	1.50	1.41
25	B	606	CLA	MG-NA	7.96	2.25	2.06

The worst 5 of 912 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	606	CLA	C4A-NA-C1A	10.35	111.40	106.68
25	B	601	CLA	C4A-NA-C1A	10.01	111.25	106.68
25	B	604	CLA	C4A-NA-C1A	9.34	110.94	106.68
25	C	507	CLA	C4A-NA-C1A	8.98	110.77	106.68
25	C	511	CLA	C4A-NA-C1A	8.95	110.76	106.68

All (2) chirality outliers are listed below:

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

5 of 1655 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	O1A-CGA-O2A-C1
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

112 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	520	DGD	2	0
29	M	103	STE	1	0
29	A	619	STE	3	0
33	D	409	LHG	1	0
27	K	101	BCR	5	0
29	C	526	STE	1	0
29	b	622	STE	1	0
25	b	614	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	H	101	BCR	2	0
32	c	521	DGD	1	0
30	a	616	LMG	5	0
30	d	411	LMG	1	0
28	a	611	PL9	4	0
28	A	611	PL9	7	0
27	b	618	BCR	3	0
25	C	504	CLA	1	0
25	B	610	CLA	2	0
25	a	612	CLA	2	0
25	b	610	CLA	2	0
25	A	606	CLA	1	0
26	A	608	PHO	1	0
27	D	404	BCR	4	0
25	B	612	CLA	2	0
33	d	409	LHG	1	0
25	c	503	CLA	1	0
25	B	607	CLA	1	0
25	C	512	CLA	1	0
25	B	602	CLA	1	0
30	B	621	LMG	3	0
30	b	621	LMG	1	0
33	B	623	LHG	1	0
25	d	402	CLA	2	0
25	A	607	CLA	1	0
29	A	618	STE	2	0
25	c	513	CLA	4	0
29	C	525	STE	1	0
25	c	505	CLA	2	0
25	b	605	CLA	4	0
25	C	507	CLA	2	0
25	C	501	CLA	1	0
27	b	617	BCR	2	0
29	B	626	STE	1	0
27	a	610	BCR	1	0
33	d	407	LHG	4	0
25	A	613	CLA	2	0
27	h	101	BCR	5	0
27	d	404	BCR	3	0
31	a	615	SQD	1	0
27	k	102	BCR	1	0
25	D	402	CLA	2	0

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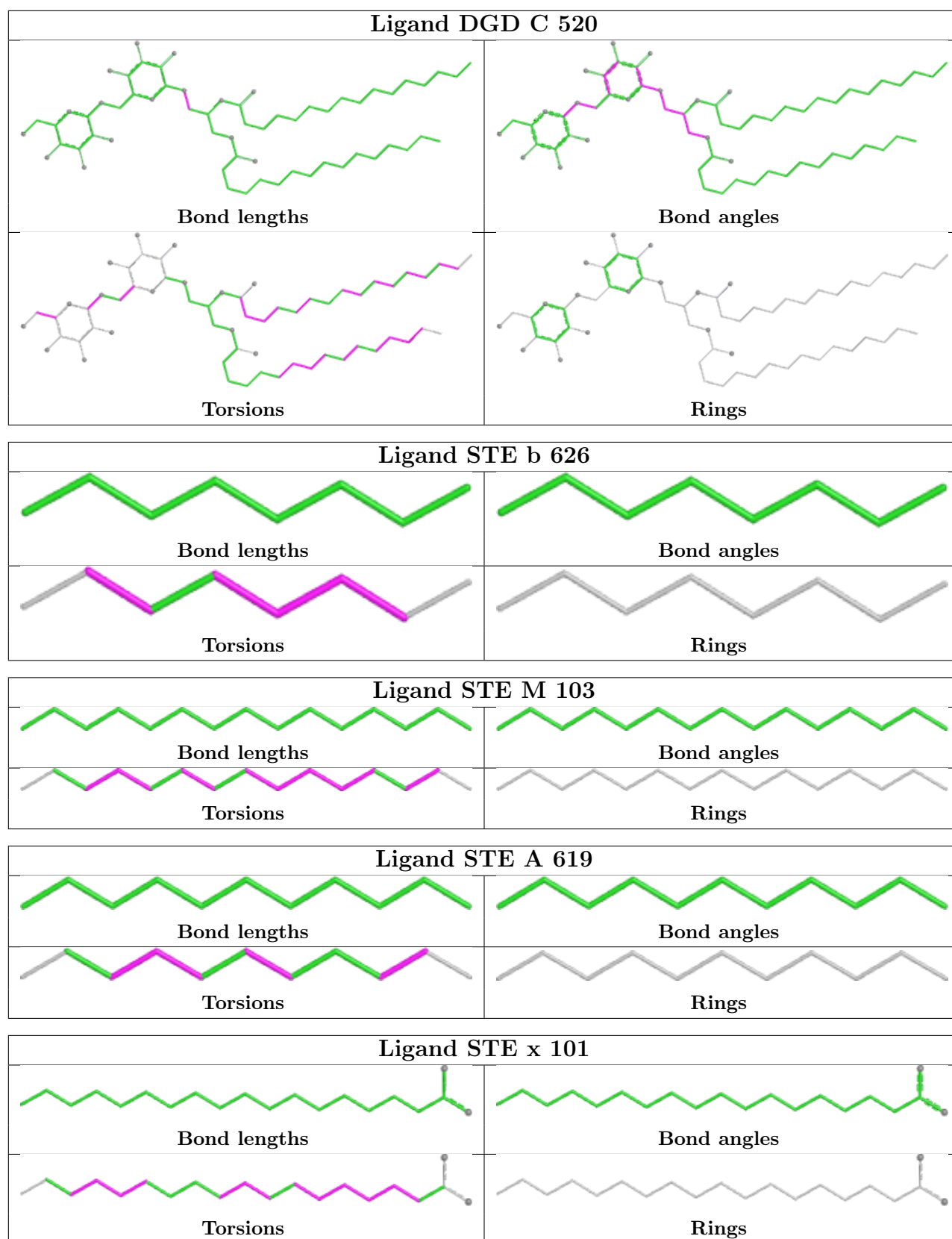
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	511	CLA	1	0
27	k	101	BCR	1	0
29	C	518	STE	1	0
25	d	403	CLA	2	0
34	F	101	HEM	3	0
25	C	511	CLA	1	0
29	E	104	STE	1	0
34	e	102	HEM	3	0
25	b	607	CLA	1	0
27	B	618	BCR	3	0
29	d	410	STE	1	0
25	c	510	CLA	2	0
25	c	507	CLA	1	0
25	B	605	CLA	1	0
25	C	502	CLA	1	0
26	d	401	PHO	3	0
25	C	509	CLA	1	0
32	C	521	DGD	1	0
25	b	602	CLA	1	0
25	a	607	CLA	1	0
32	A	617	DGD	1	0
33	E	101	LHG	3	0
27	B	617	BCR	1	0
25	c	501	CLA	1	0
30	a	617	LMG	1	0
31	b	620	SQD	2	0
25	B	611	CLA	1	0
25	b	613	CLA	3	0
25	b	615	CLA	1	0
27	t	101	BCR	3	0
30	b	623	LMG	2	0
25	C	513	CLA	3	0
31	D	408	SQD	1	0
25	B	616	CLA	1	0
30	D	406	LMG	2	0
25	B	601	CLA	1	0
27	T	101	BCR	4	0
29	h	104	STE	1	0
30	D	407	LMG	1	0
35	v	201	HEC	1	0
25	B	606	CLA	1	0
30	B	620	LMG	6	0

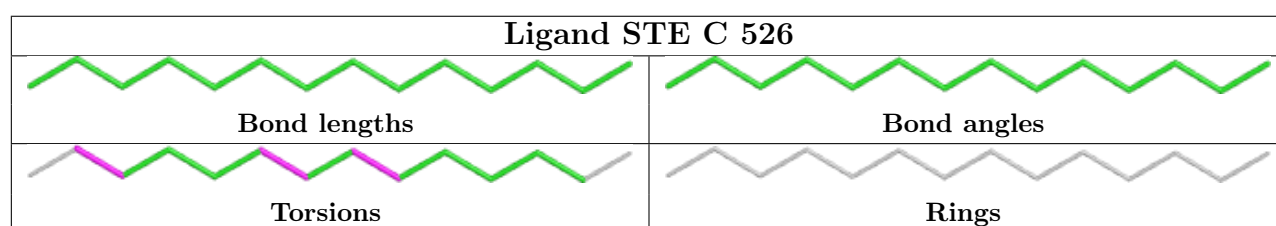
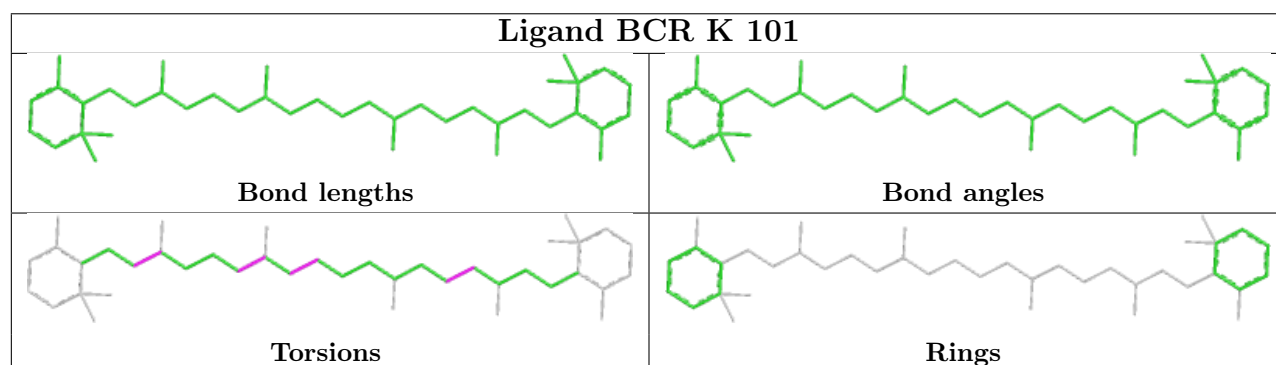
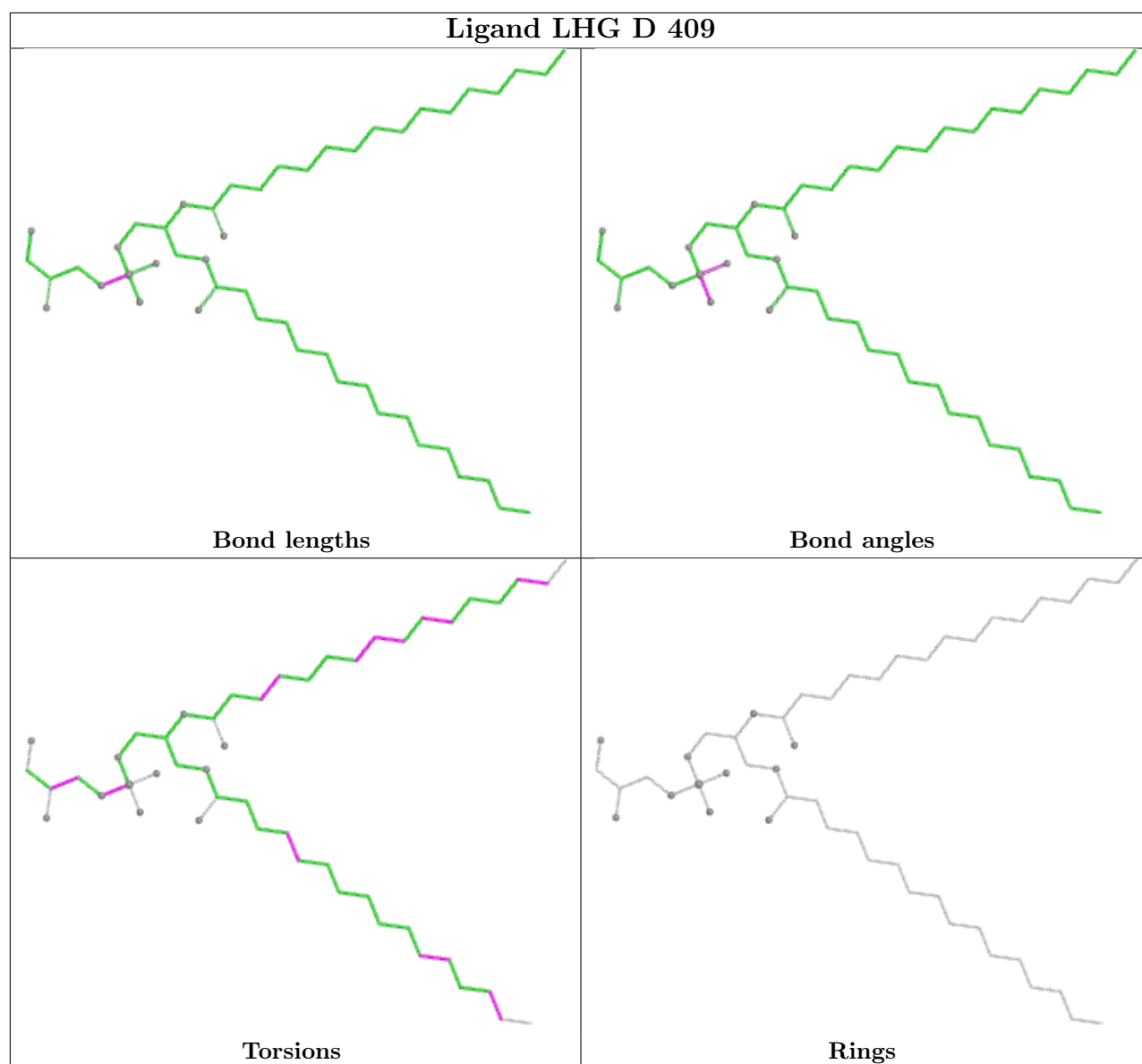
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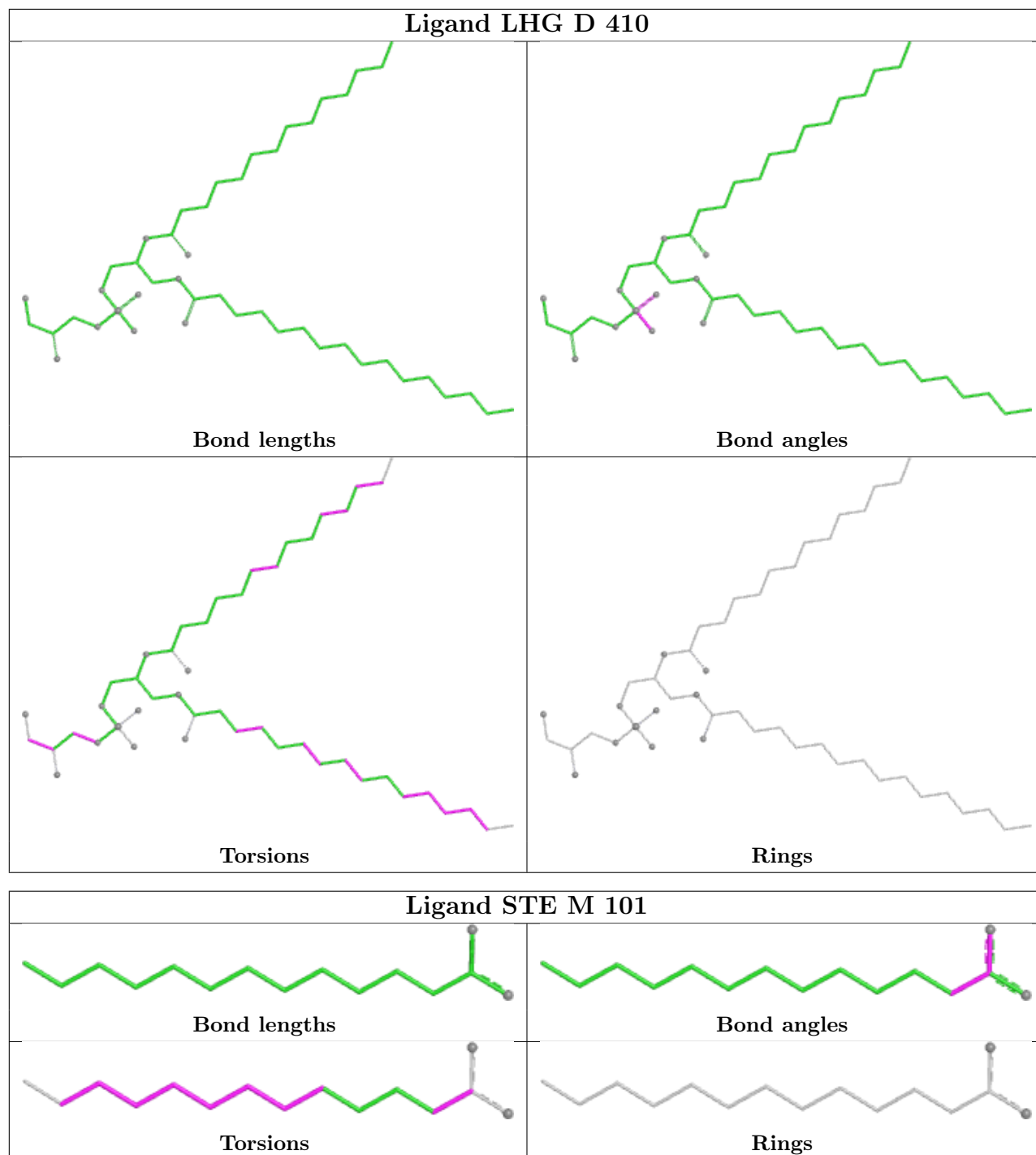
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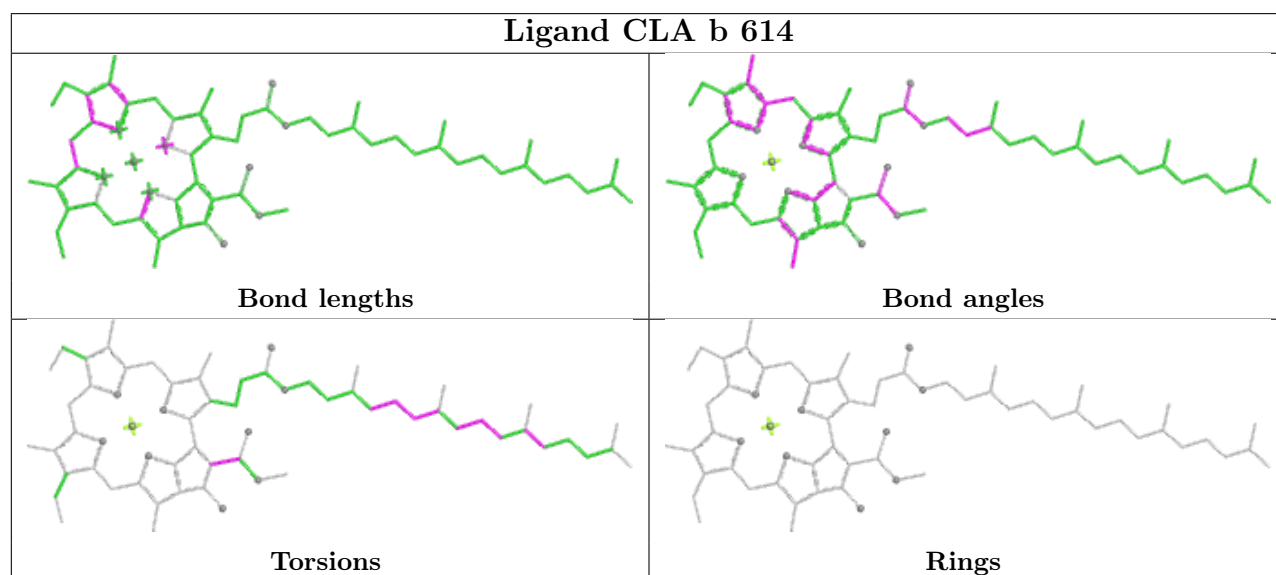
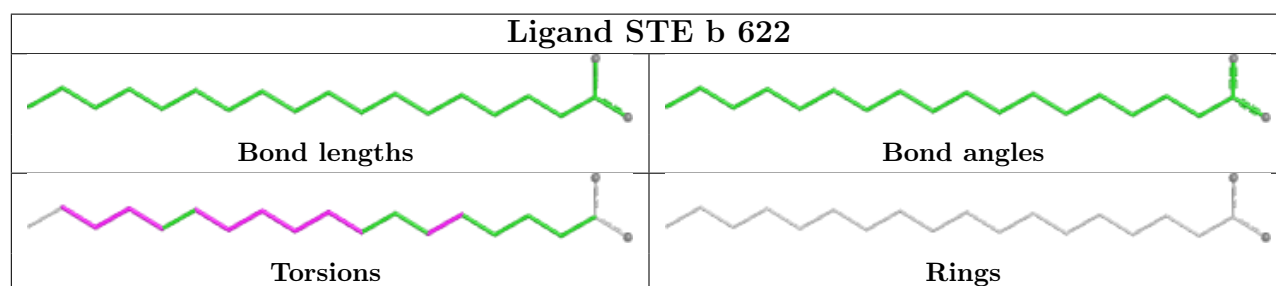
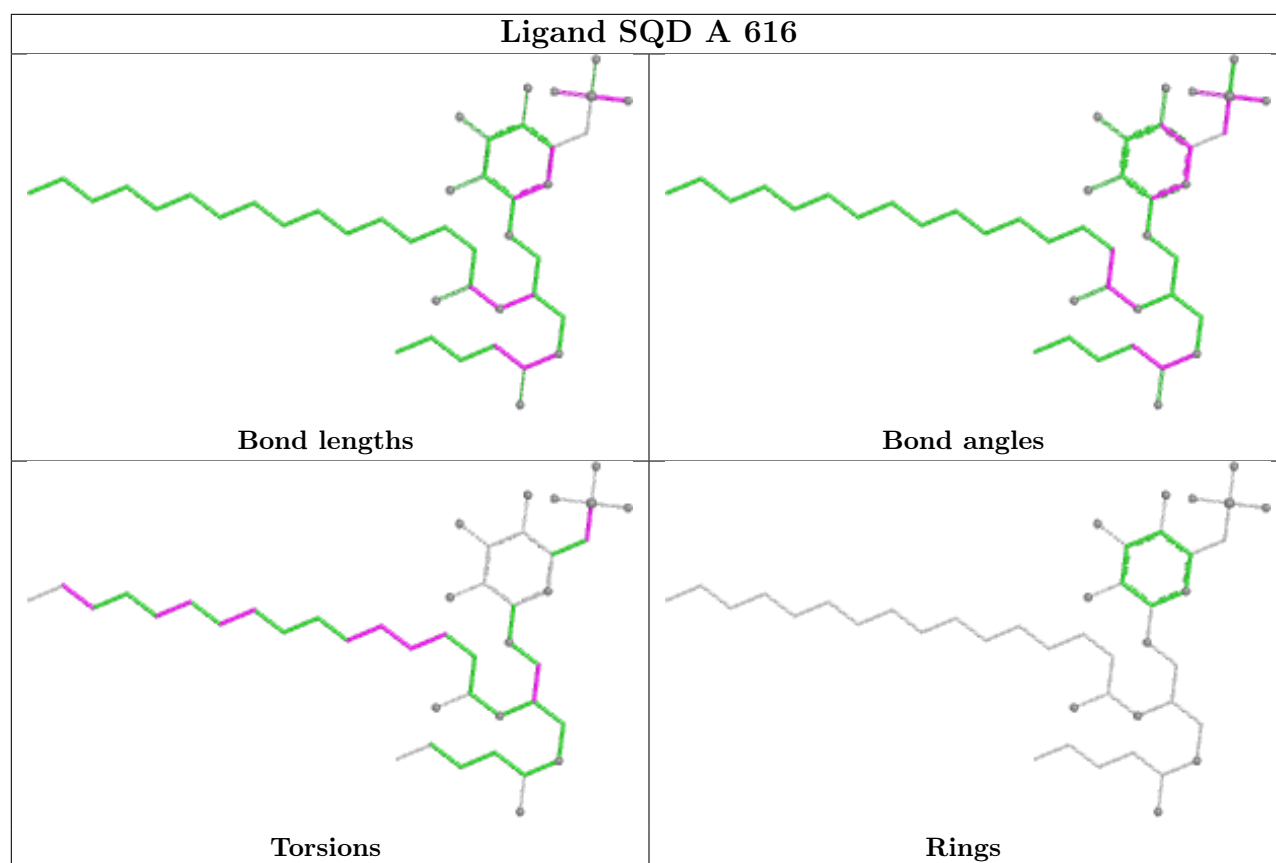
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	516	LMG	1	0
25	b	616	CLA	2	0
25	b	601	CLA	2	0
29	X	101	STE	1	0
25	c	509	CLA	2	0
31	B	624	SQD	1	0
25	D	403	CLA	1	0
25	B	604	CLA	1	0
31	f	101	SQD	1	0
25	C	506	CLA	1	0
25	B	615	CLA	2	0
33	L	101	LHG	3	0
25	a	606	CLA	1	0
30	c	523	LMG	1	0
25	c	512	CLA	2	0
27	Y	101	BCR	2	0
25	c	502	CLA	1	0
27	C	514	BCR	1	0
25	C	508	CLA	2	0
27	c	514	BCR	3	0

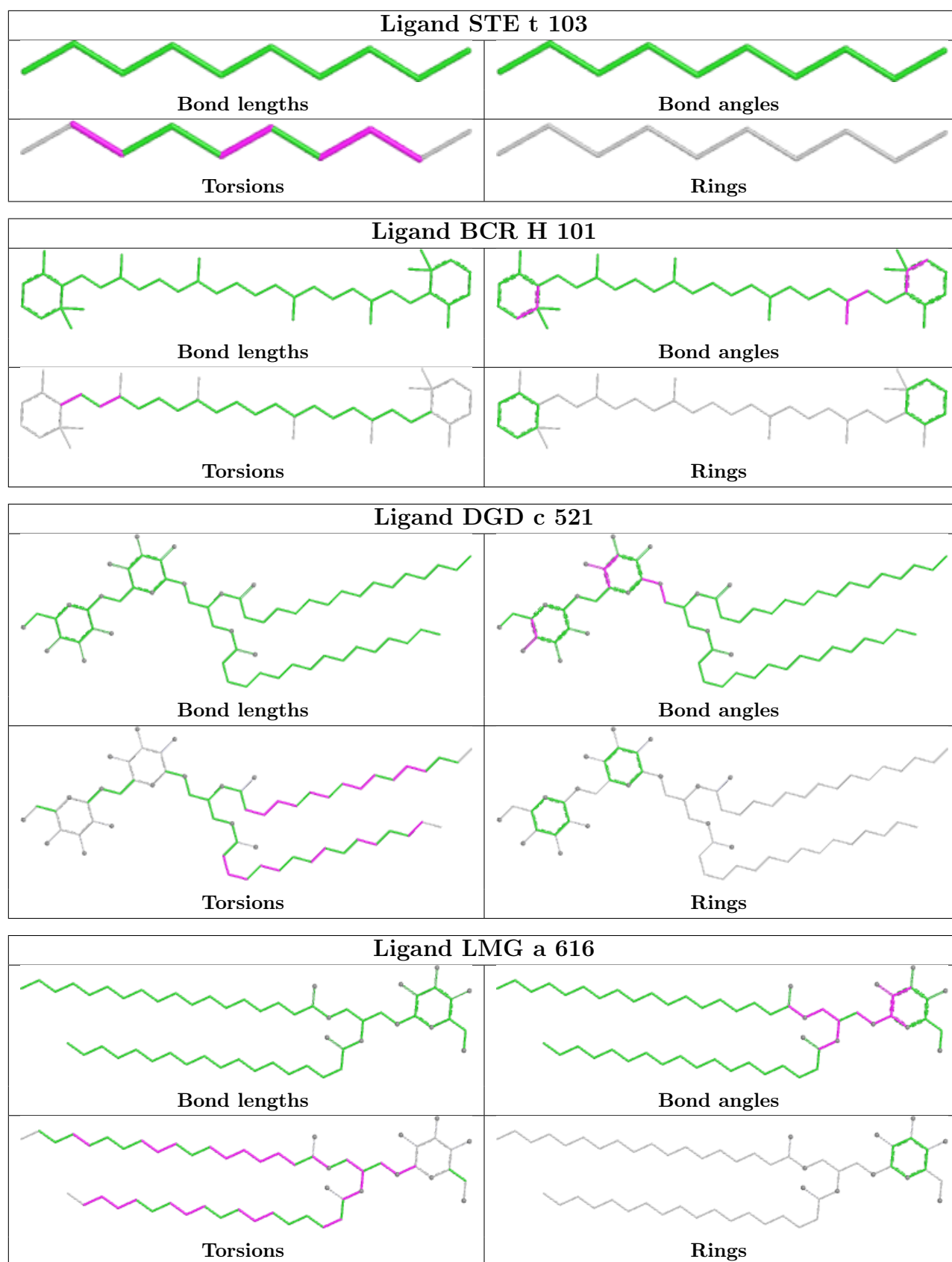
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

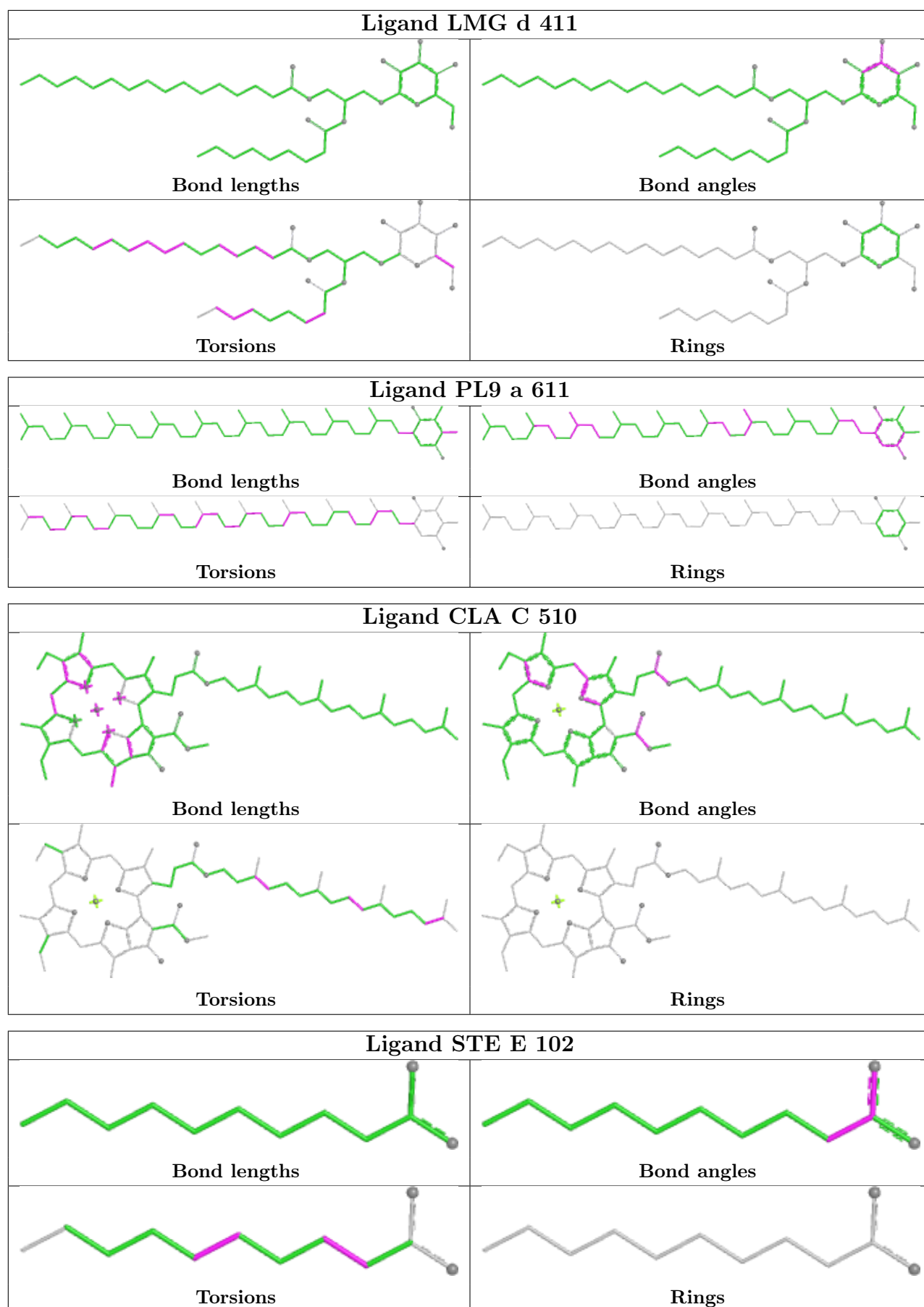


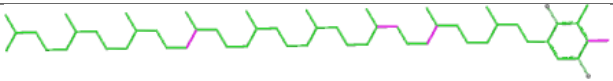
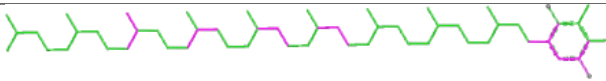
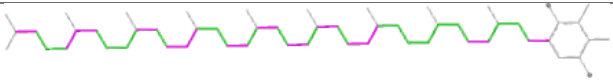
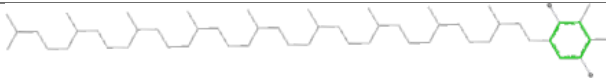


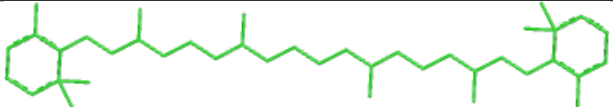
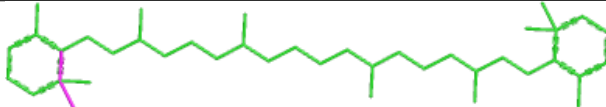
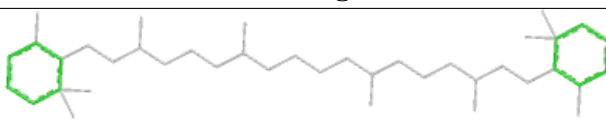


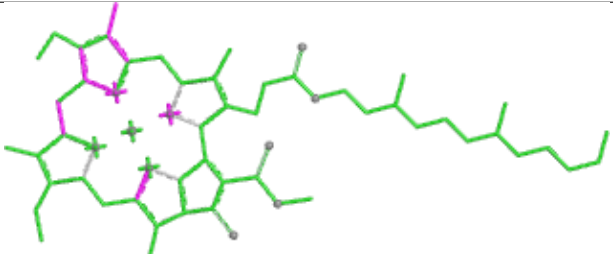
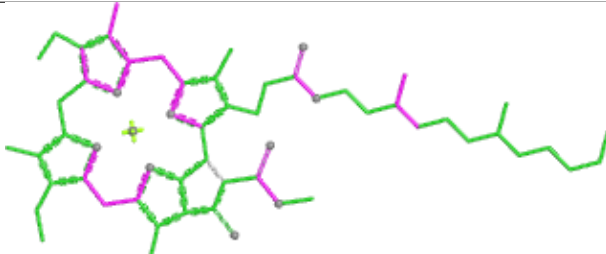
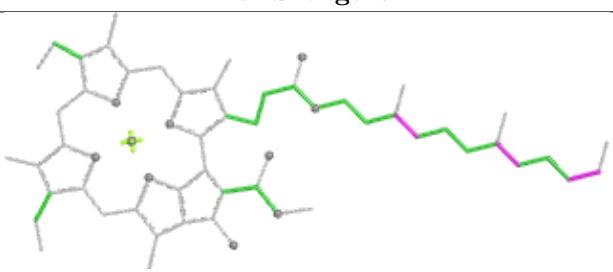
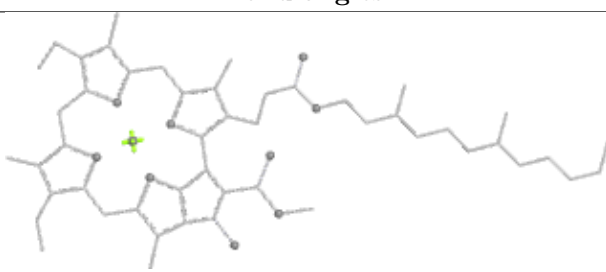




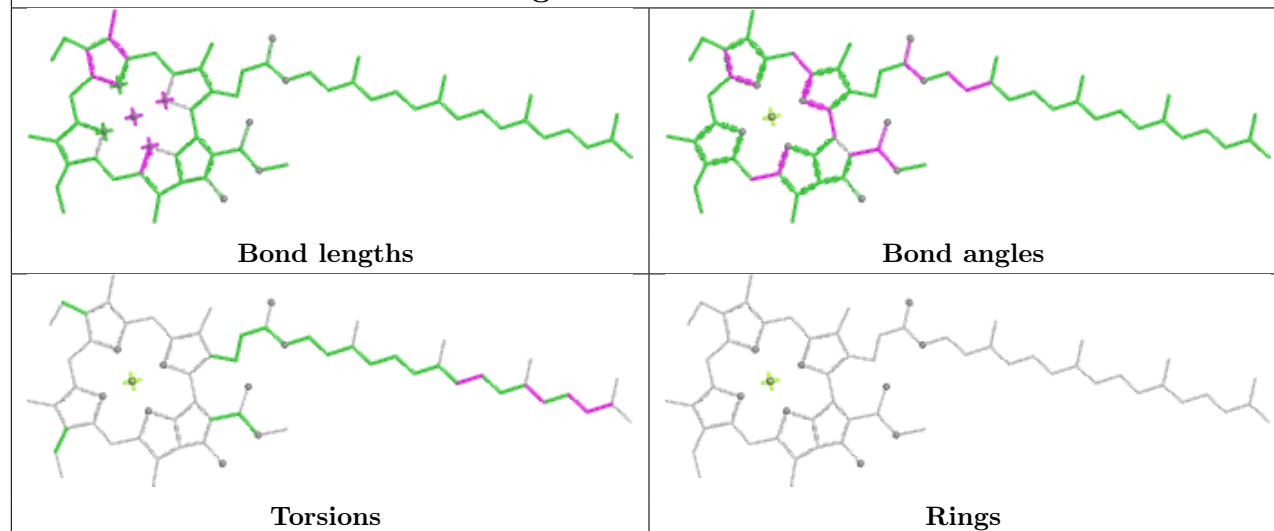


Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

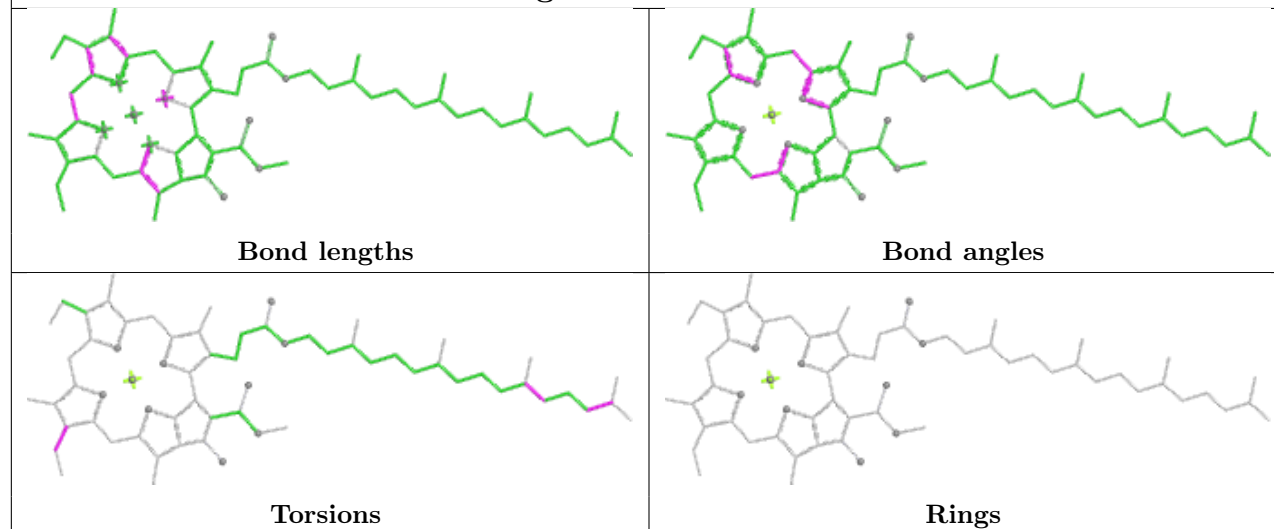
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

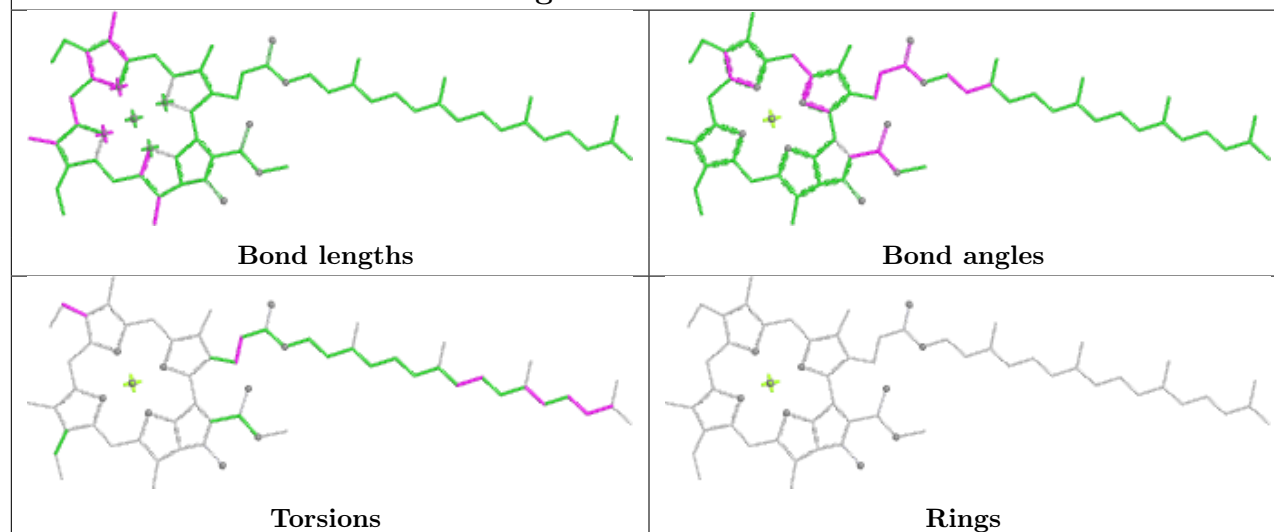
Ligand CLA B 610

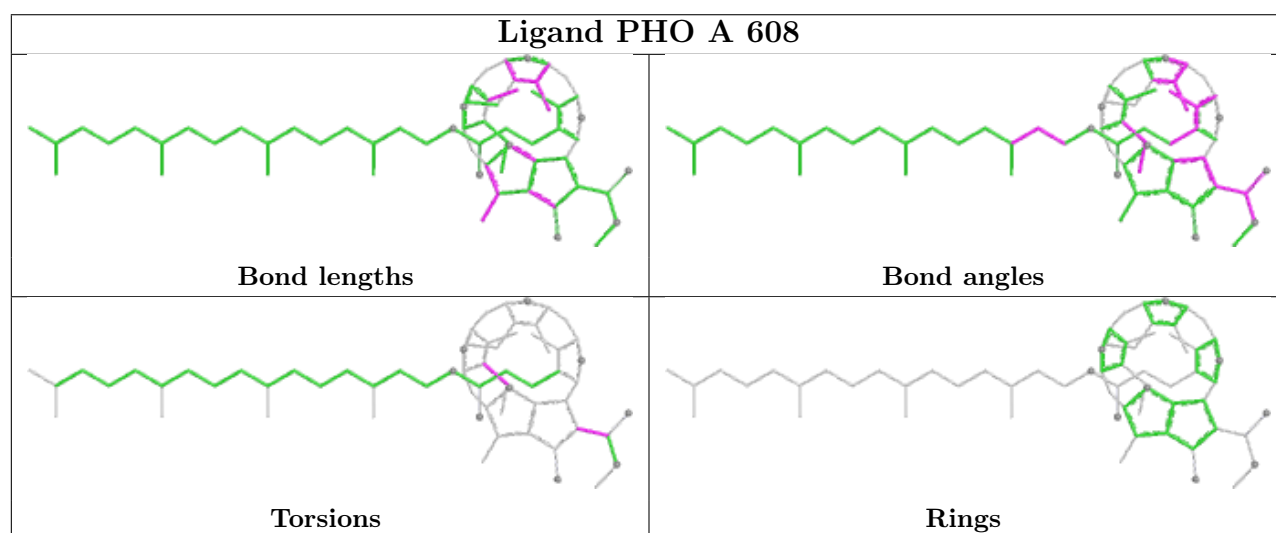
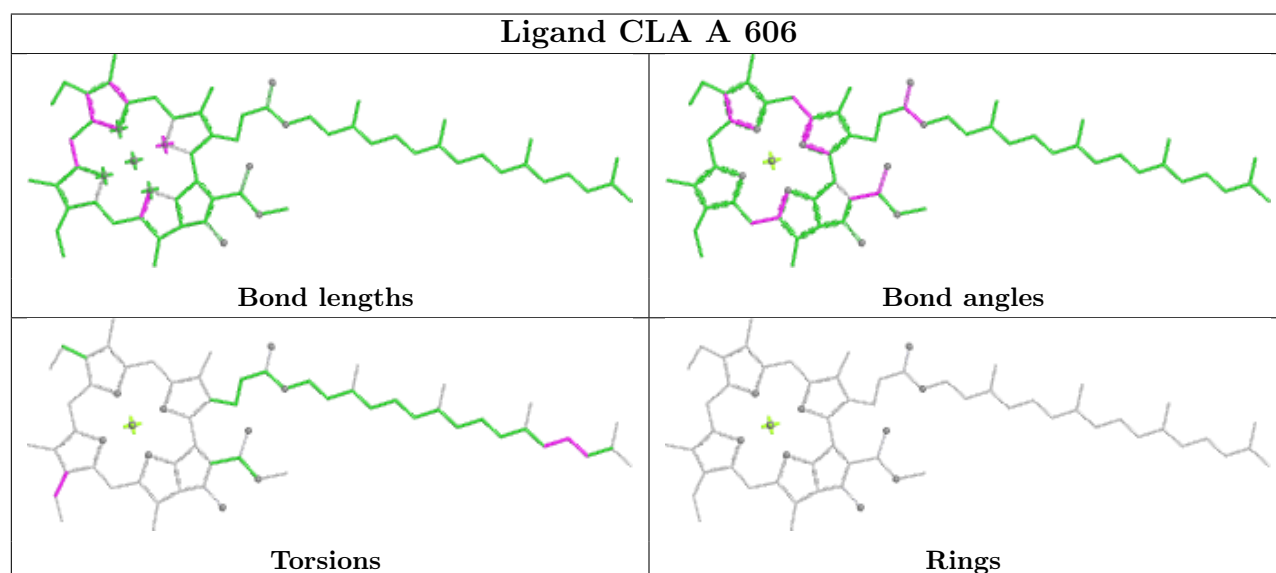
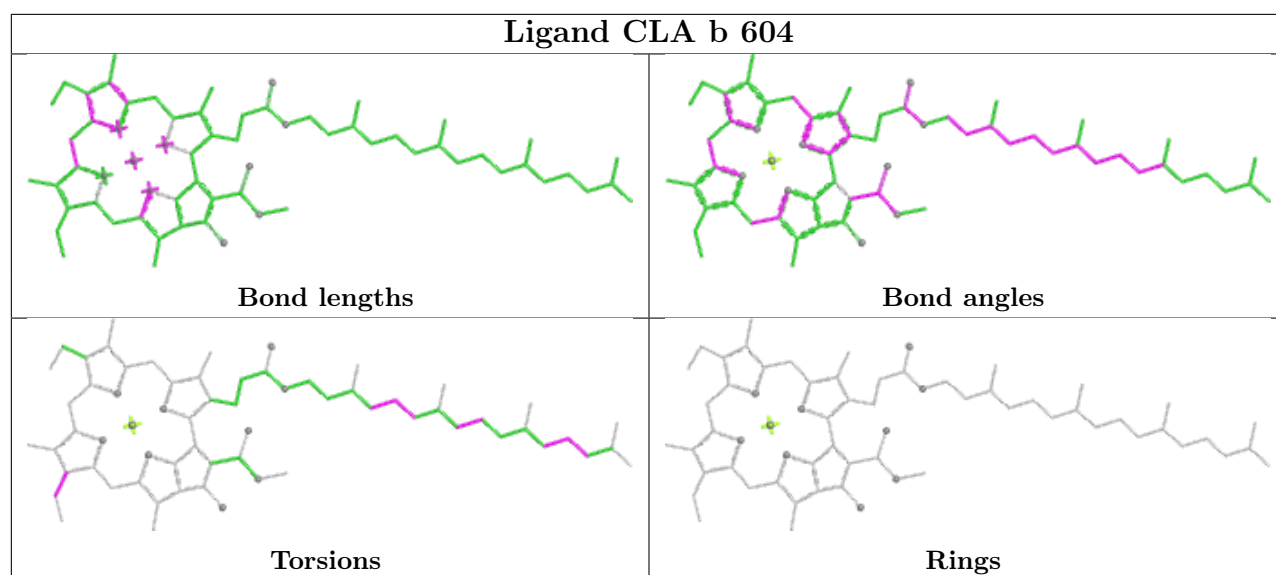


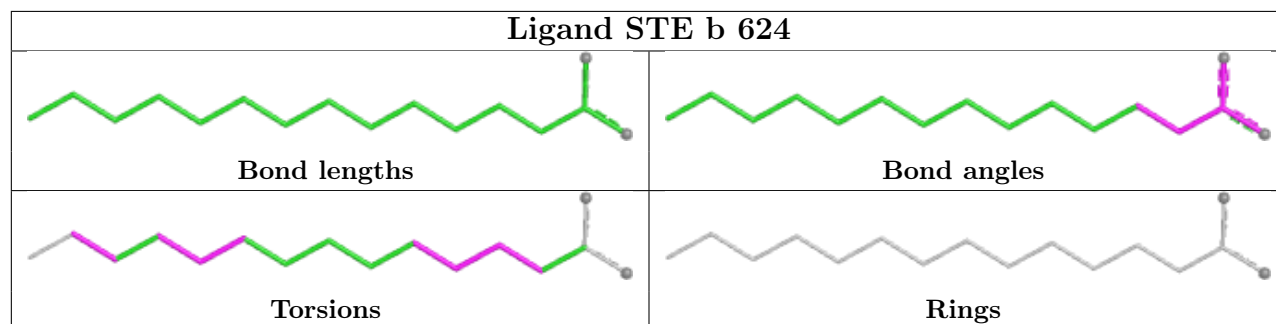
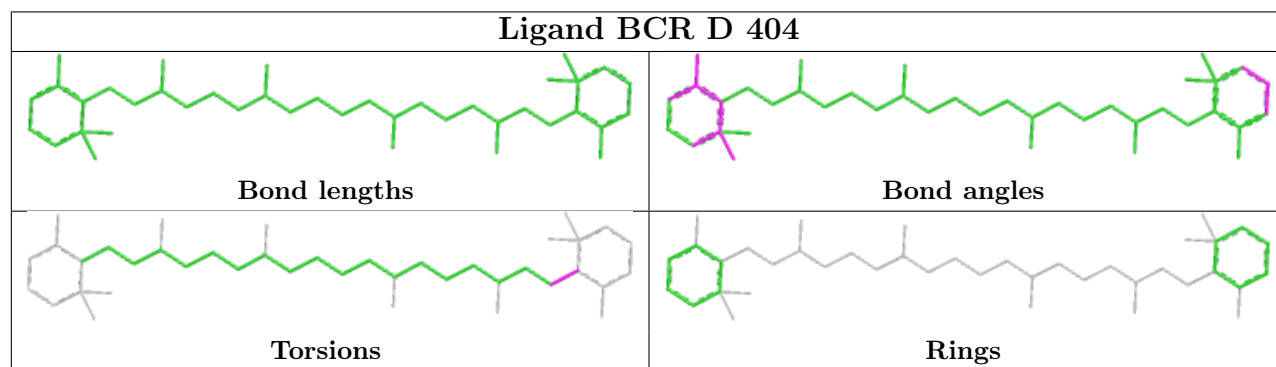
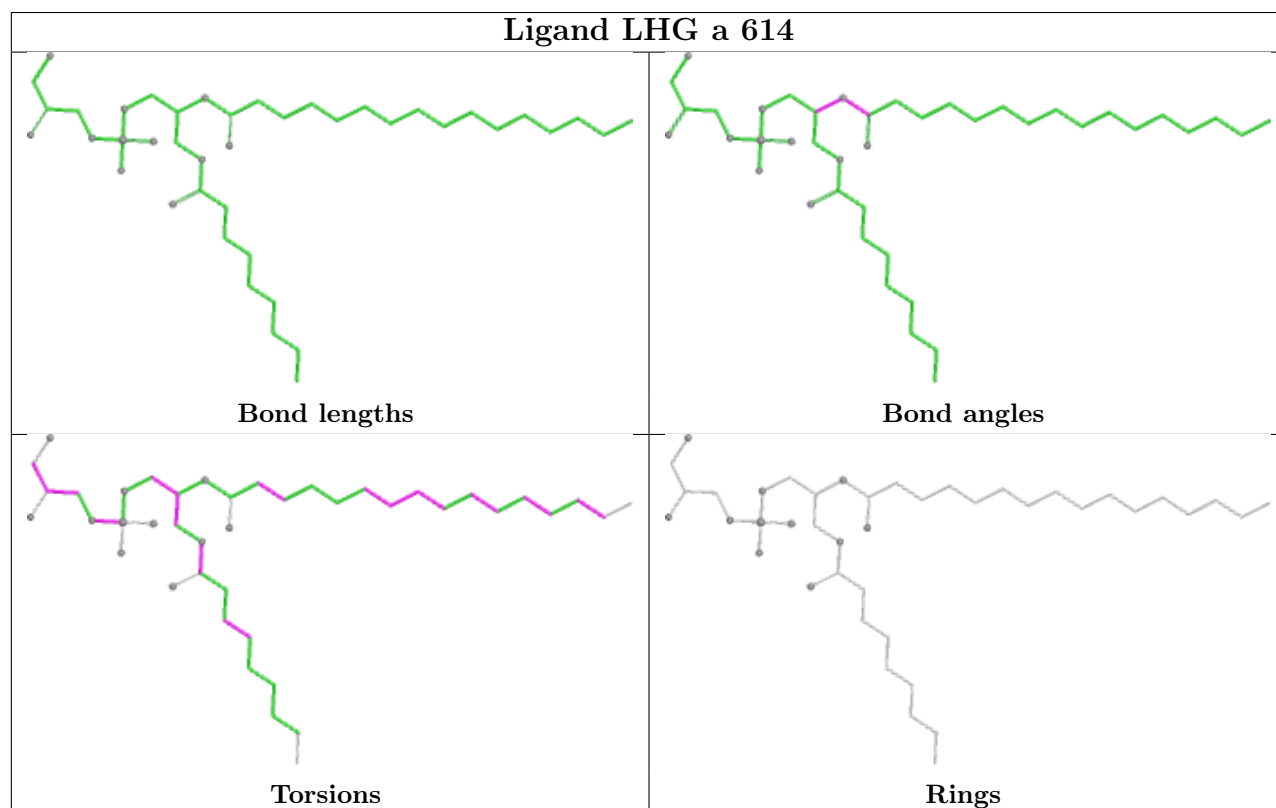
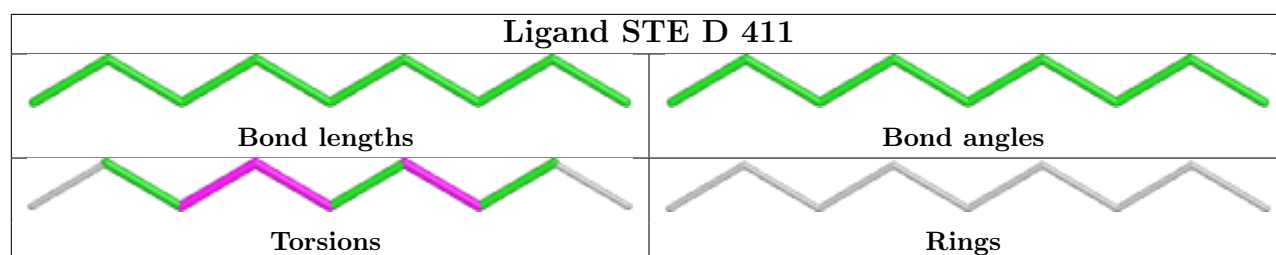
Ligand CLA a 612

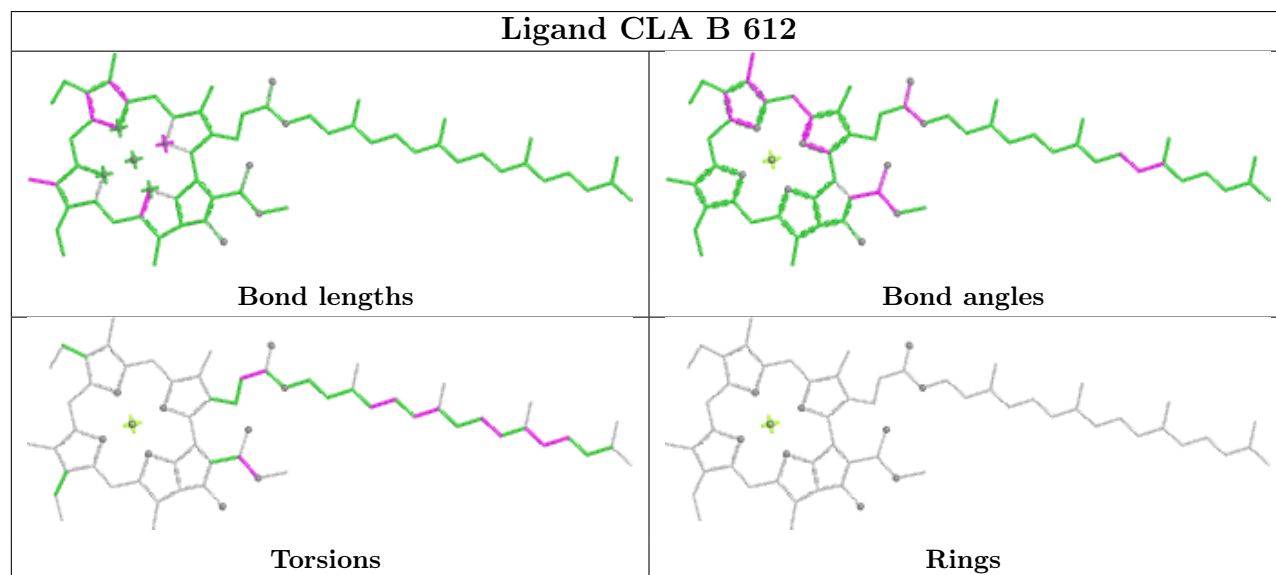
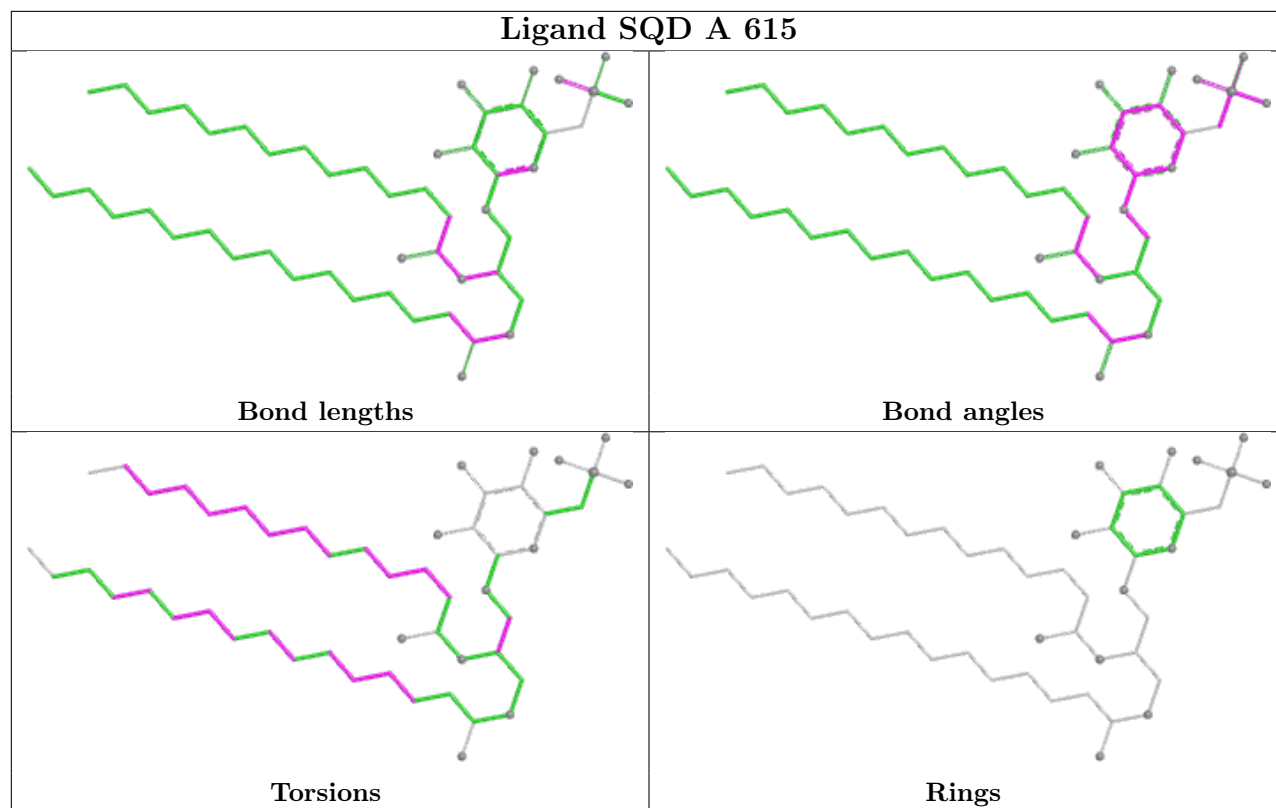


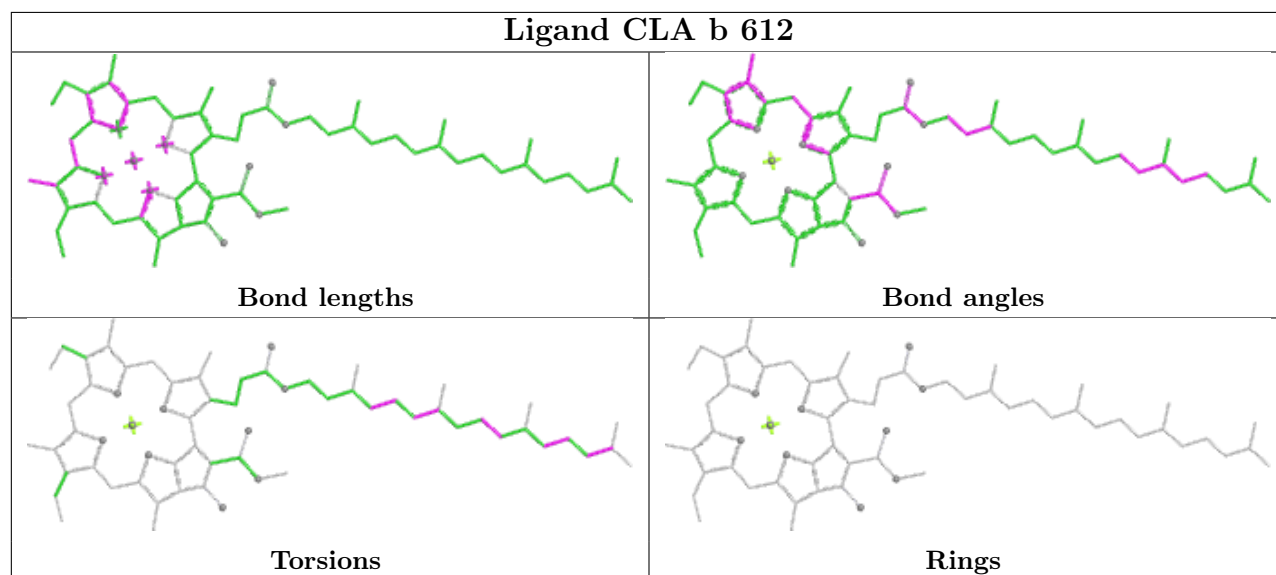
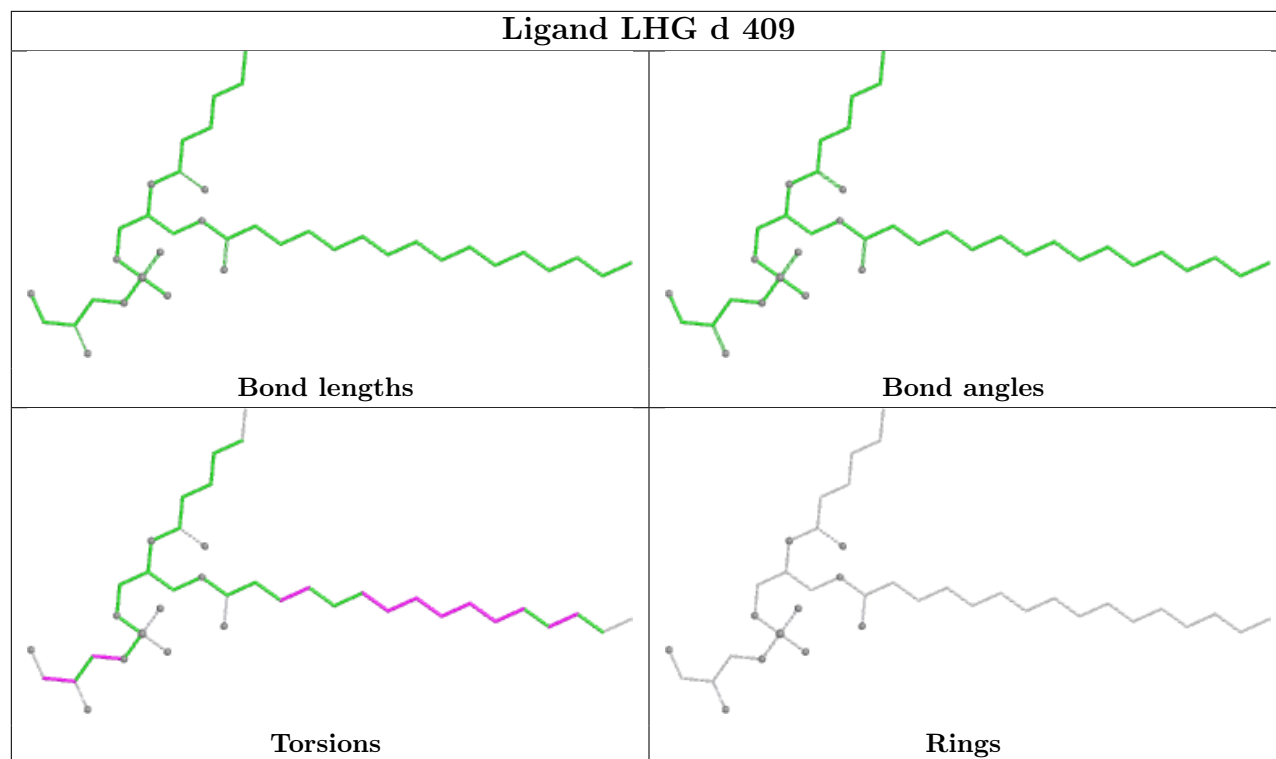
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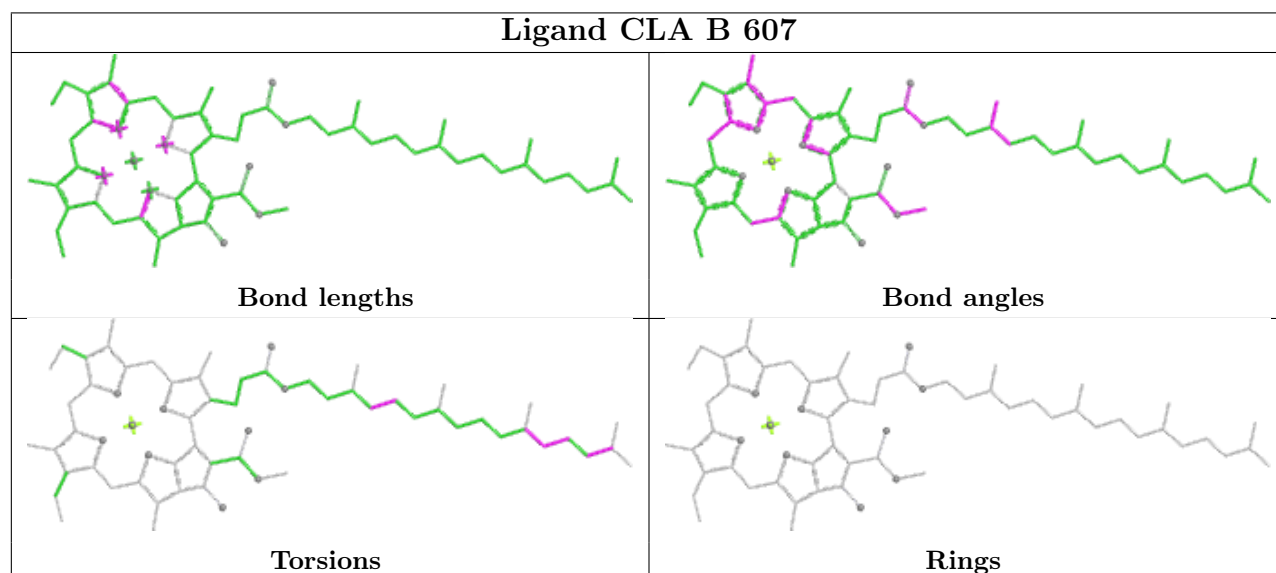
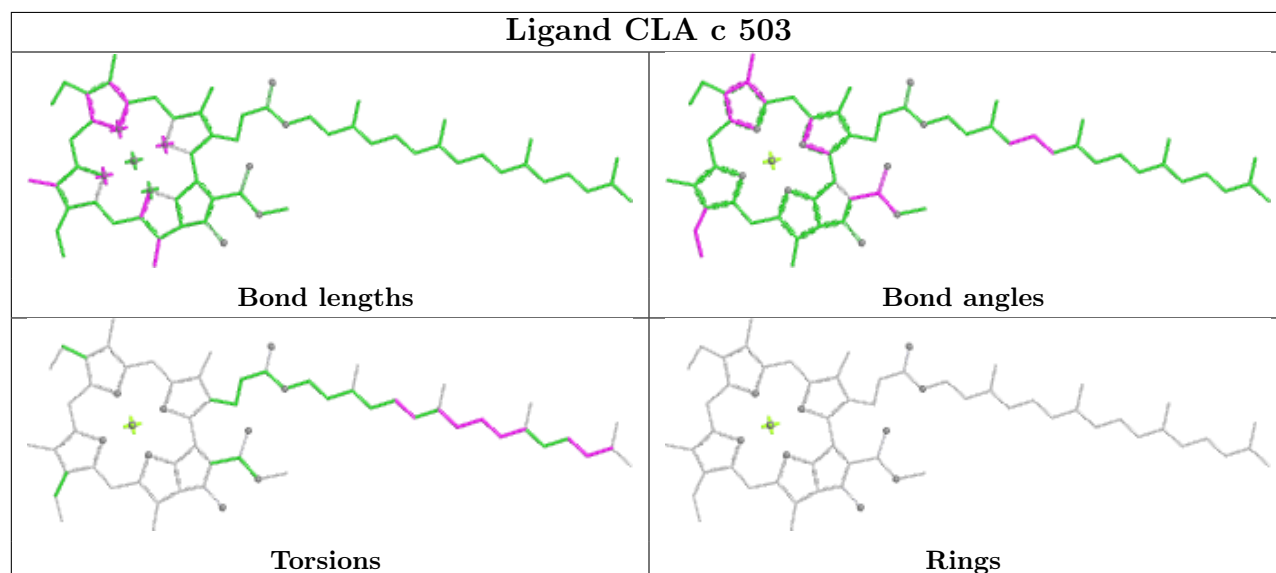
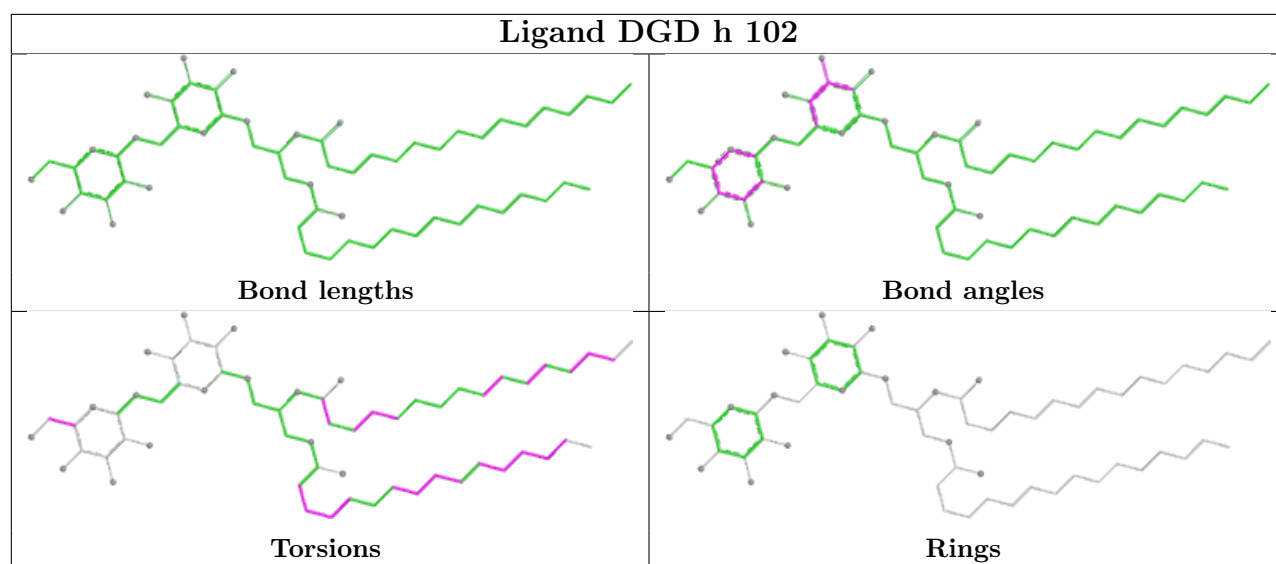


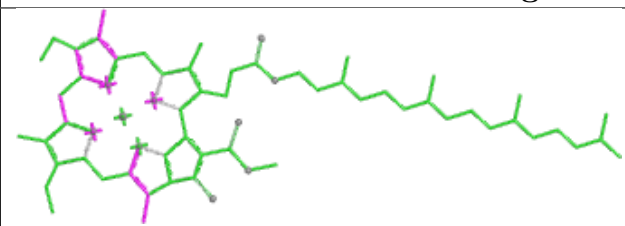
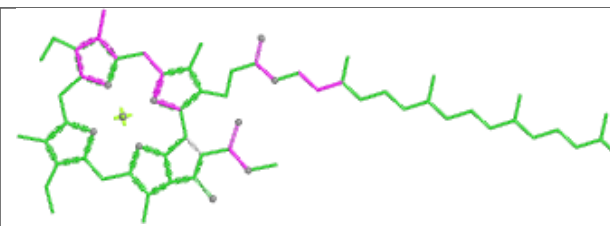
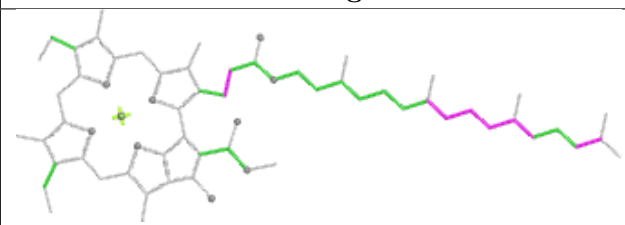
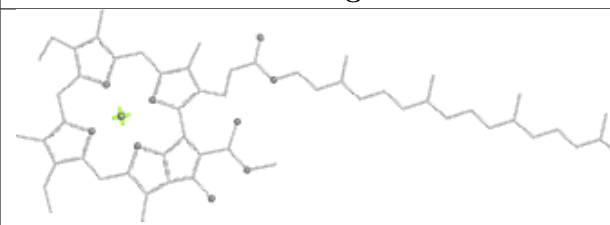


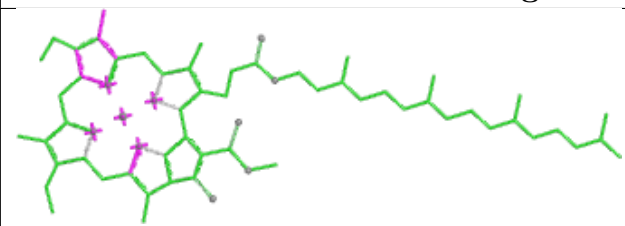
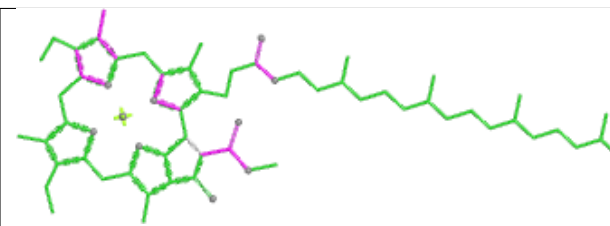
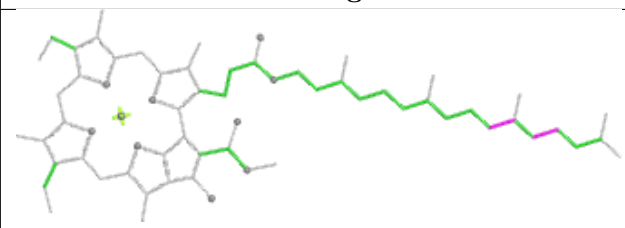
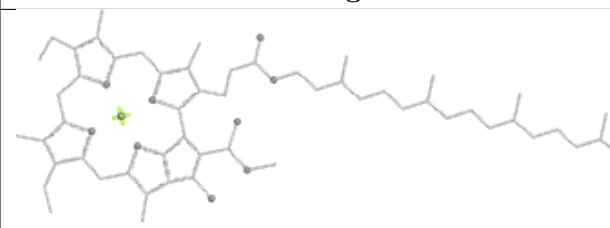


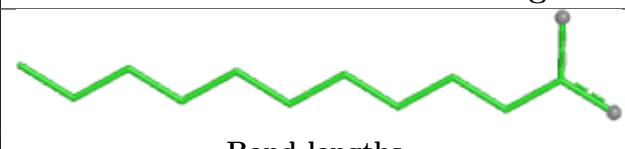
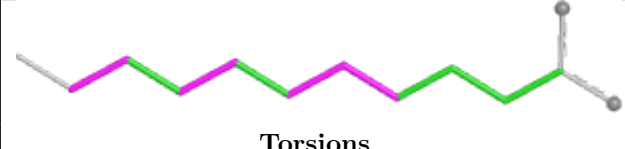
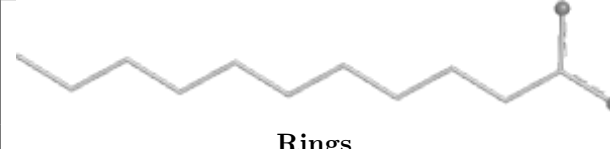


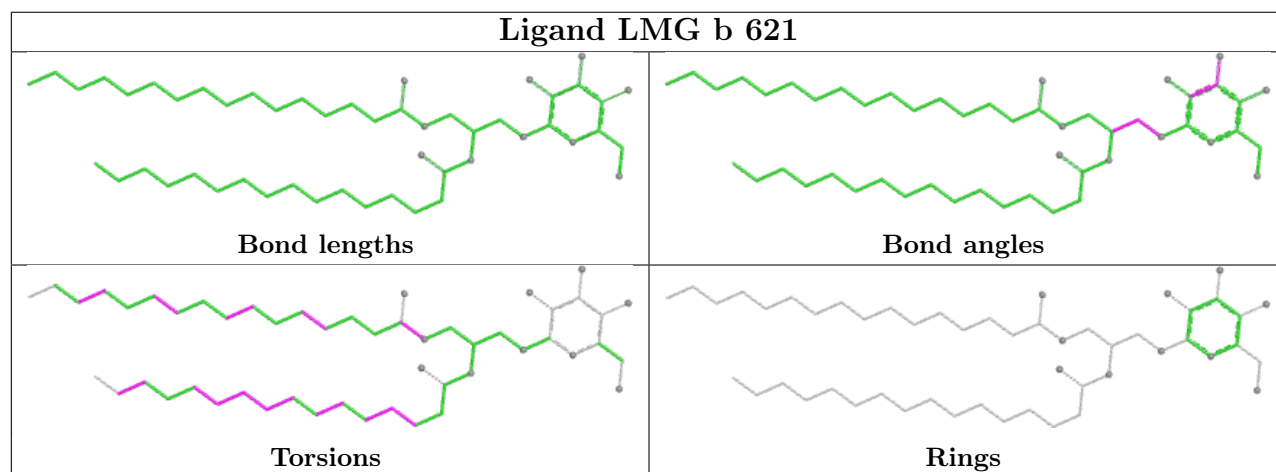
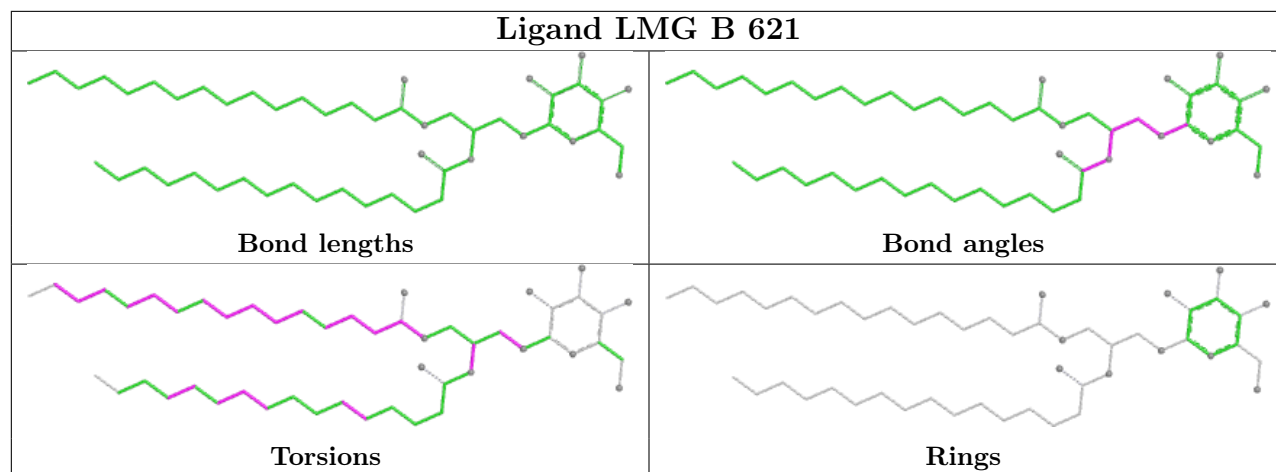


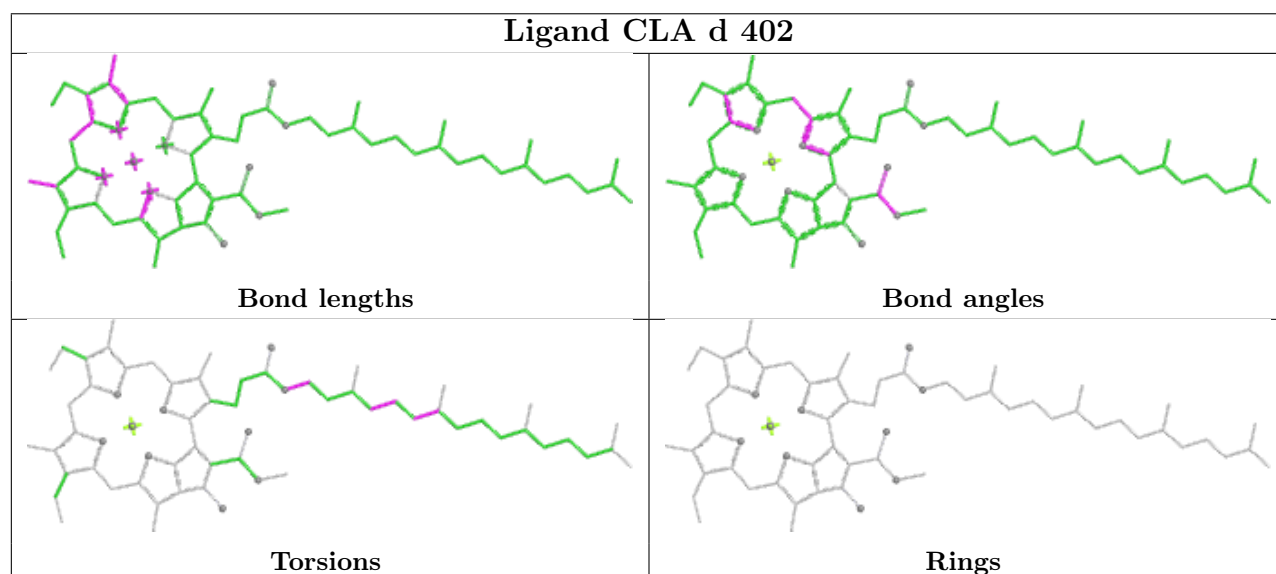
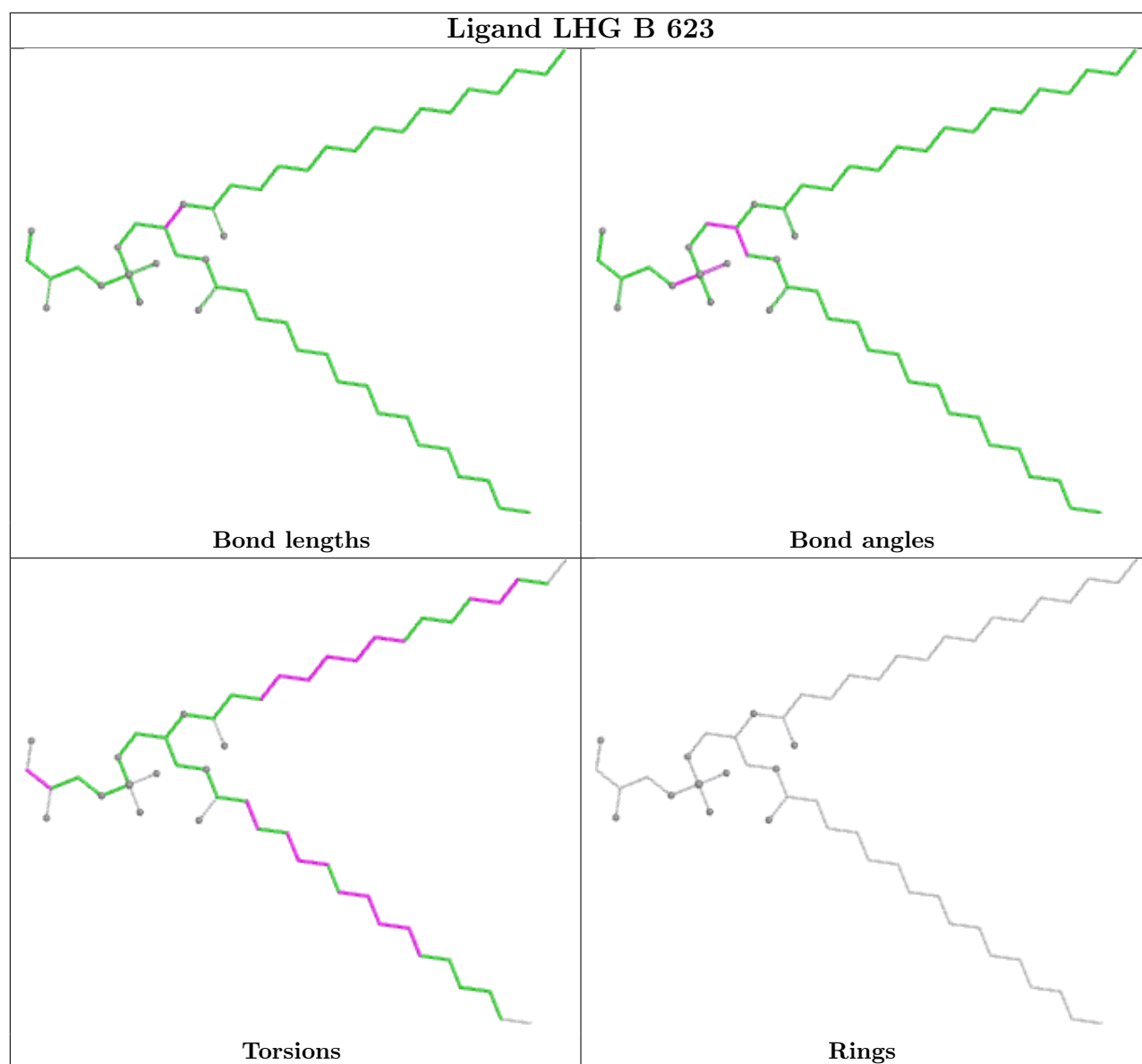


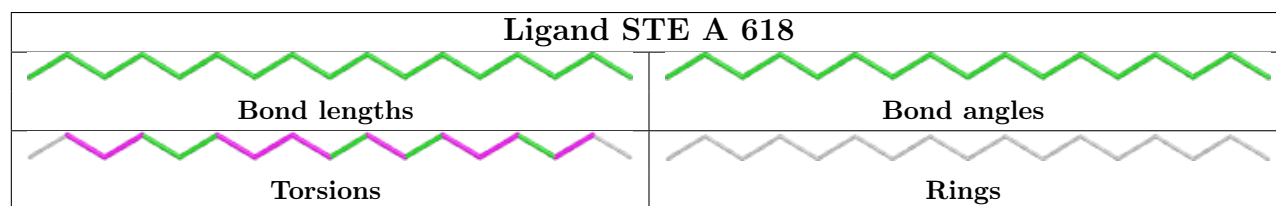
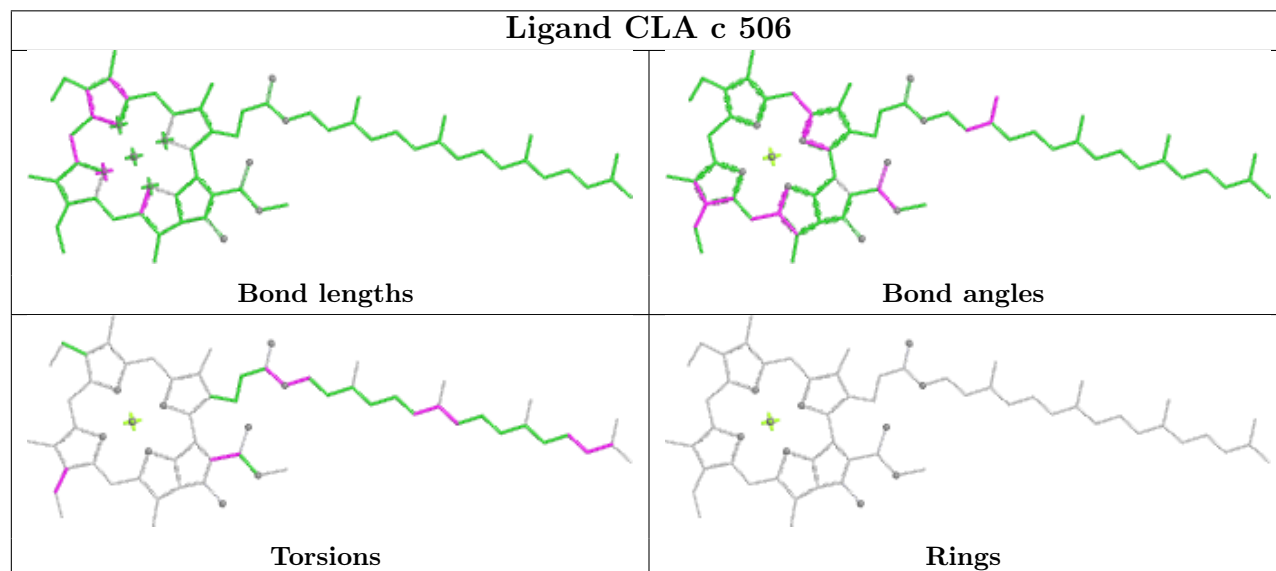
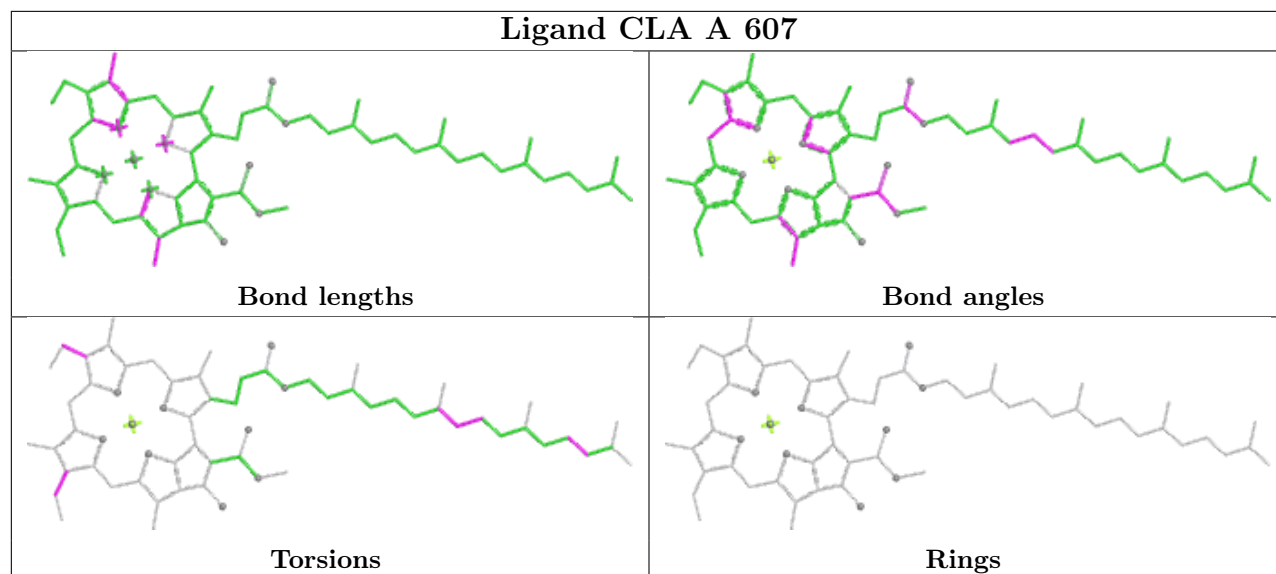
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

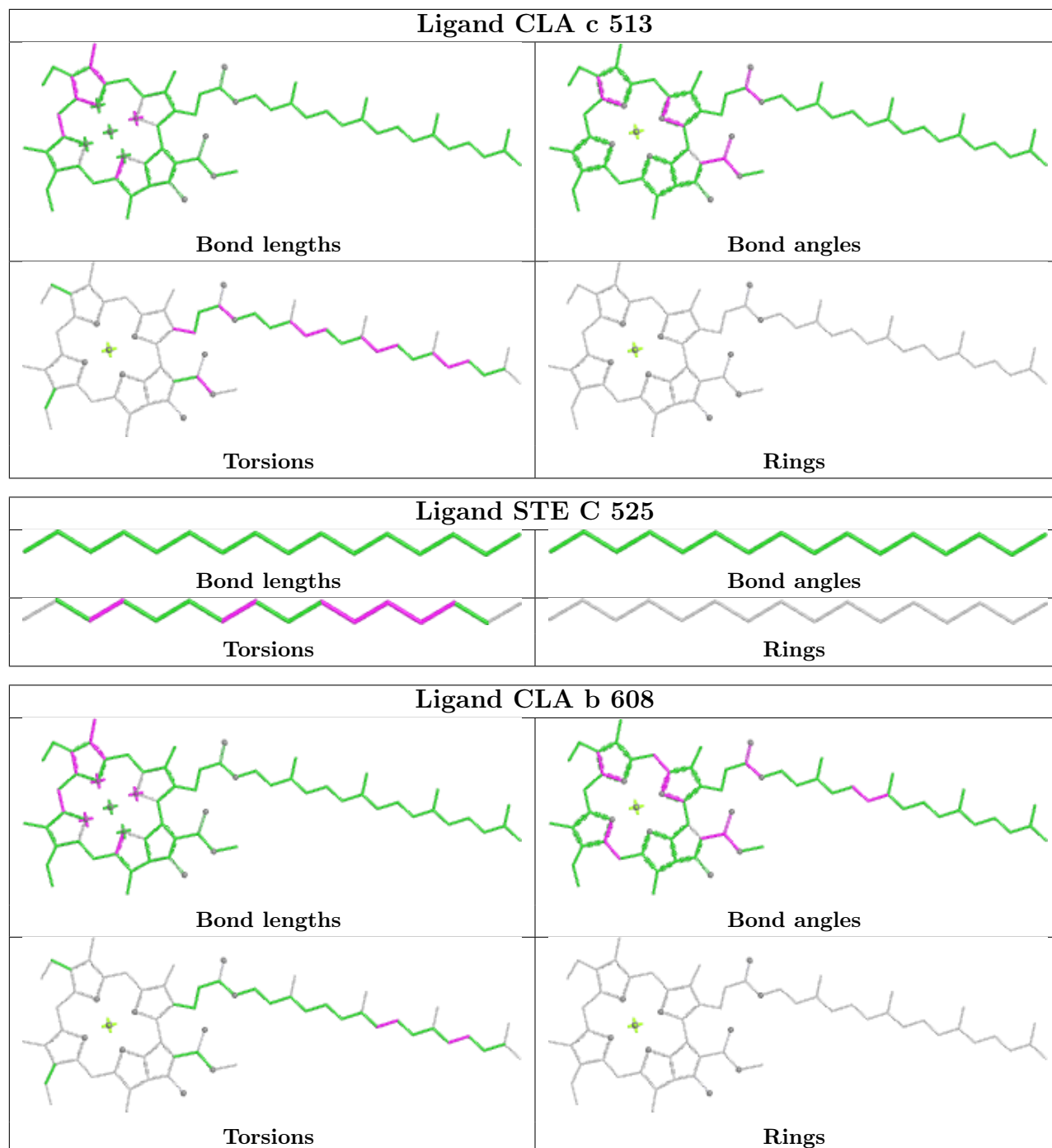
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE e 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

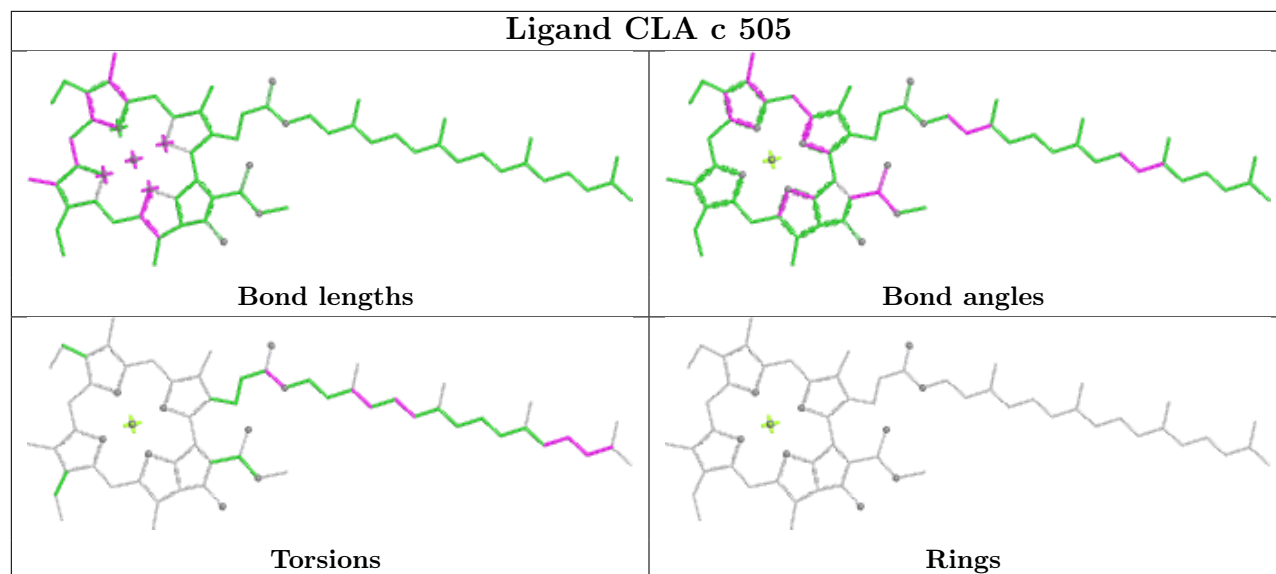




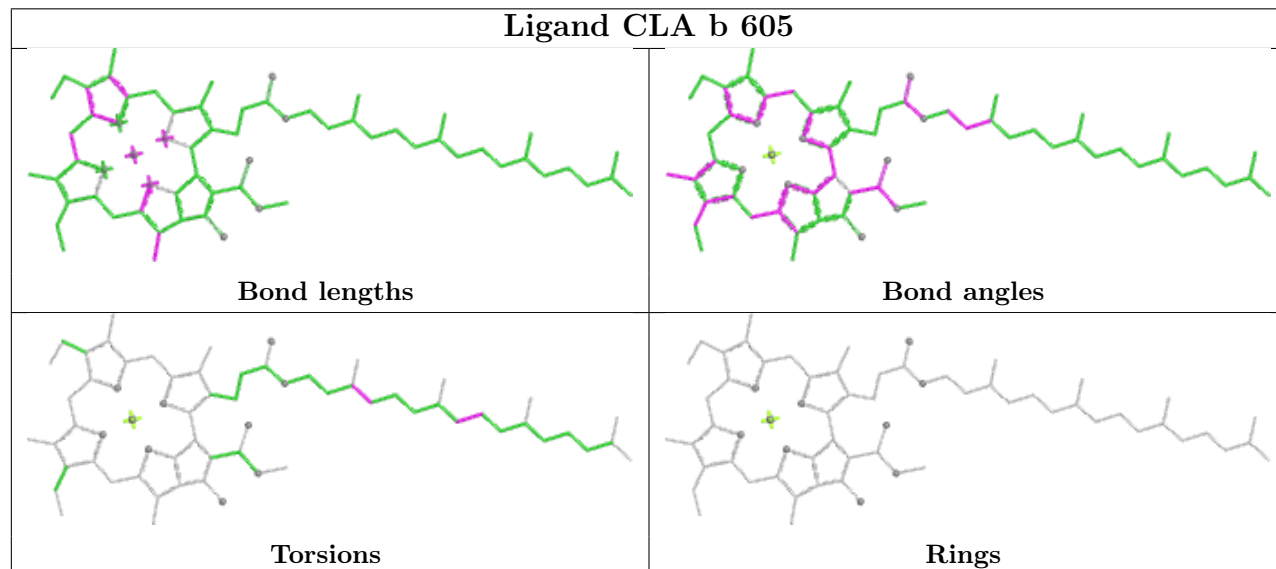




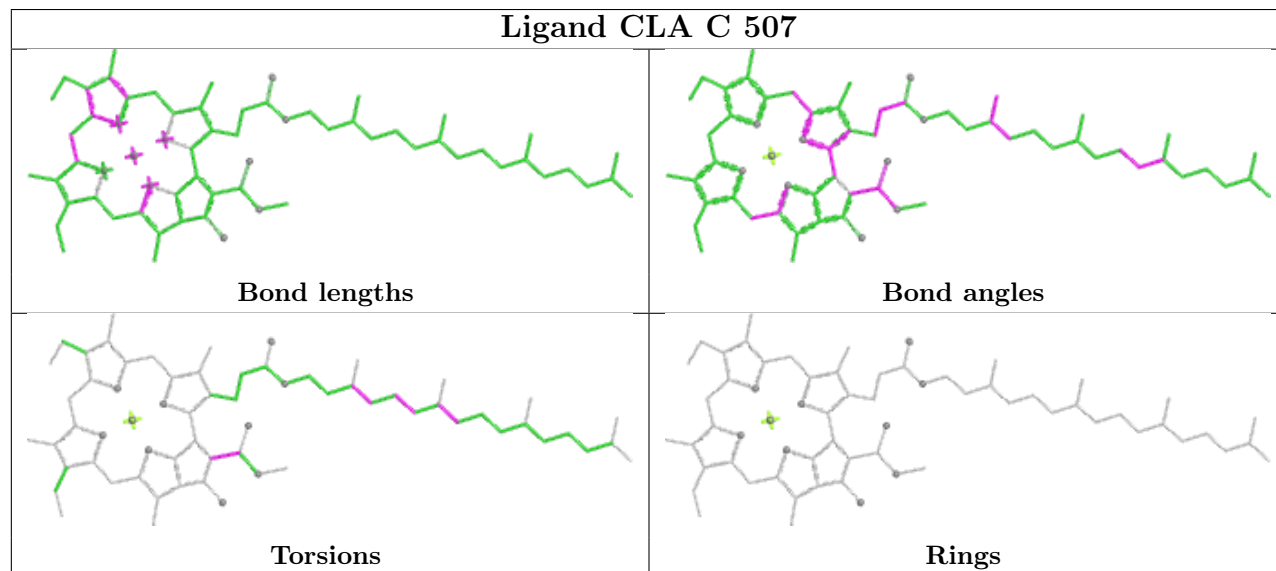
Ligand CLA c 505

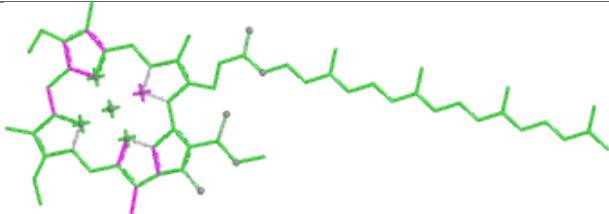
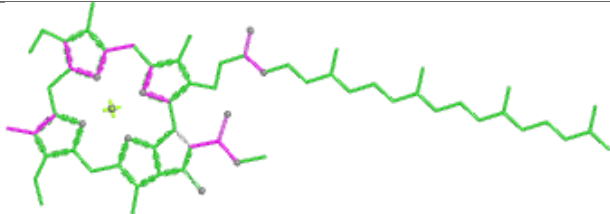
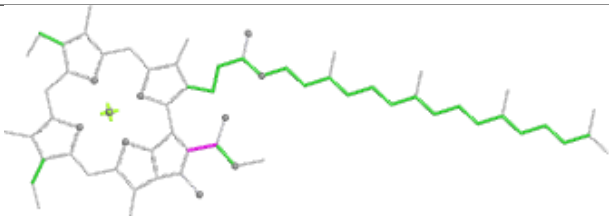
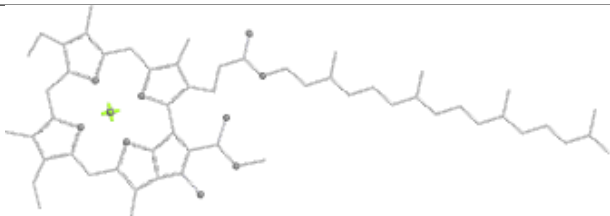


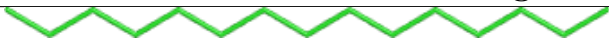
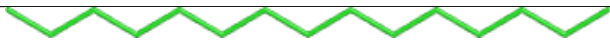
Ligand CLA b 605

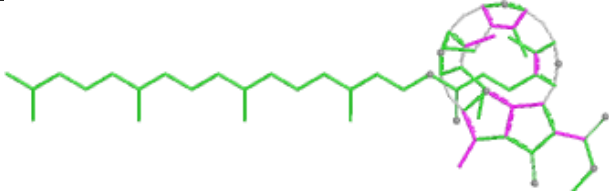
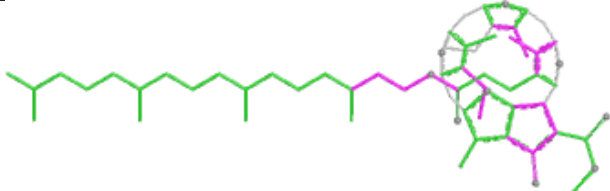
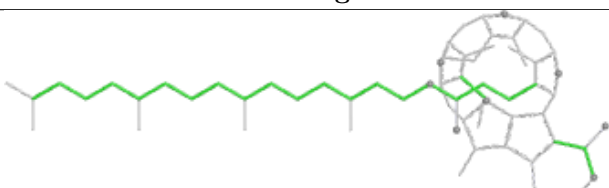
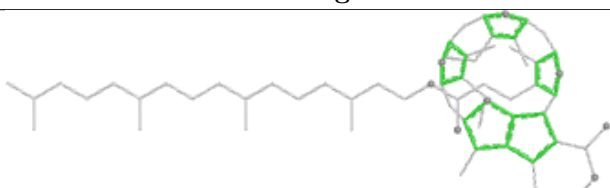


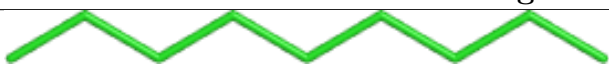
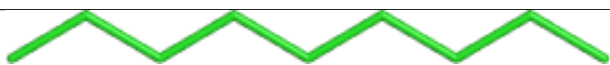
Ligand CLA C 507

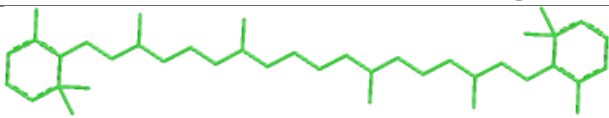
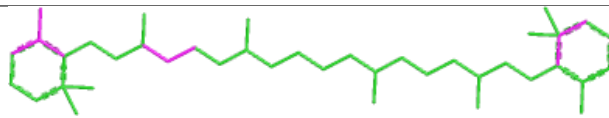
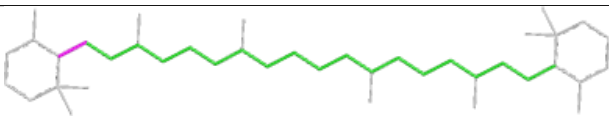
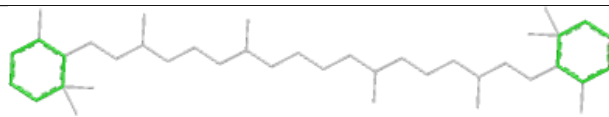


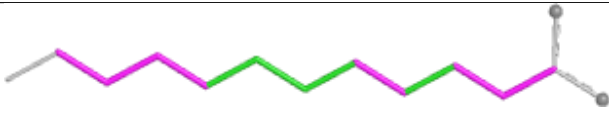
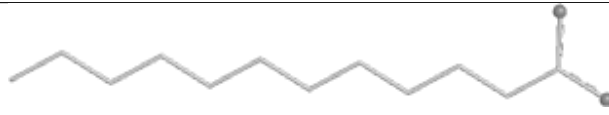
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

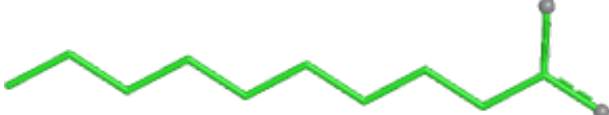
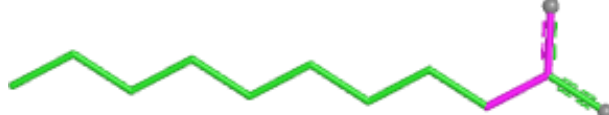
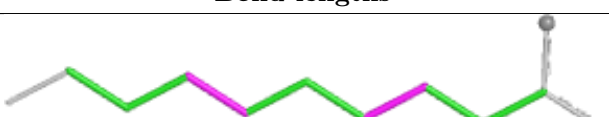
Ligand STE B 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

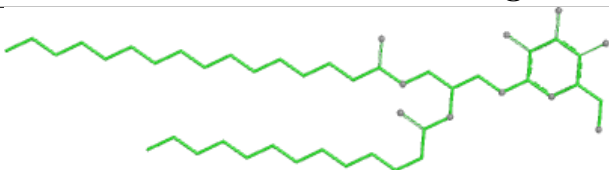
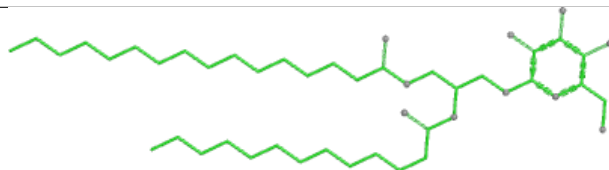
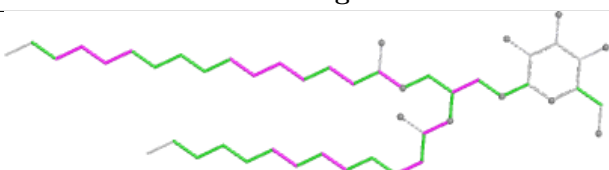
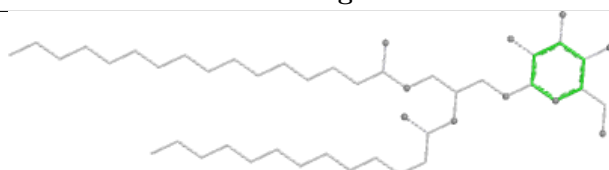
Ligand PHO D 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

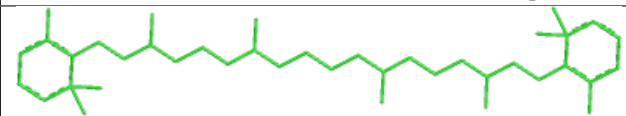
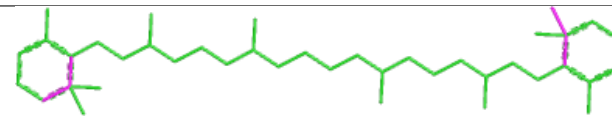
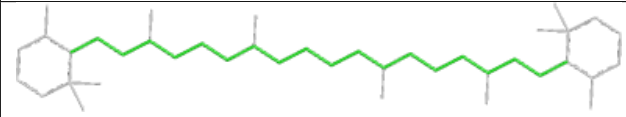
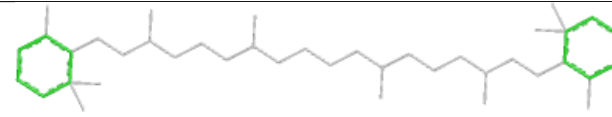
Ligand STE e 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

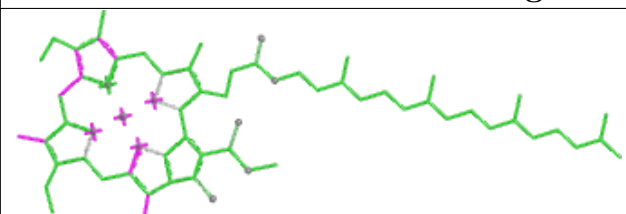
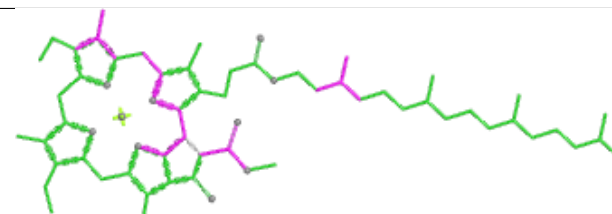
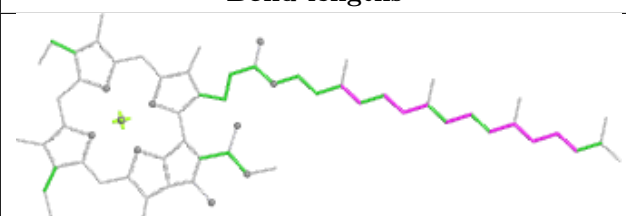
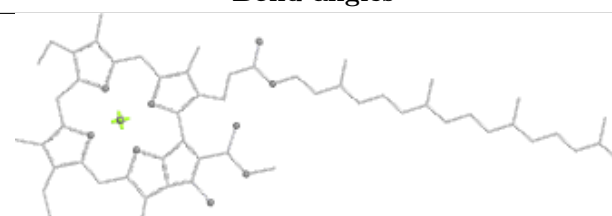
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

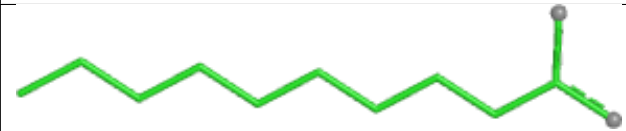
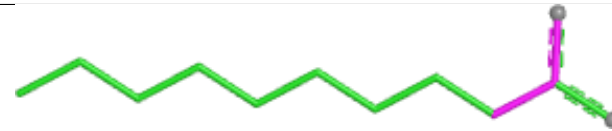
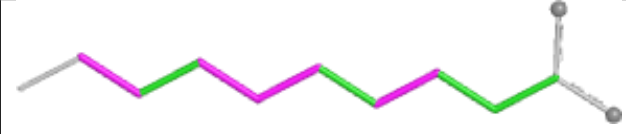
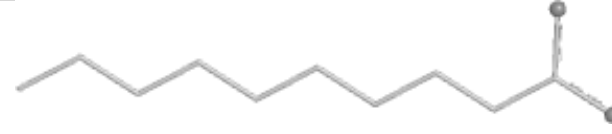
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Bond lengths	Bond angles
	
Torsions	Rings

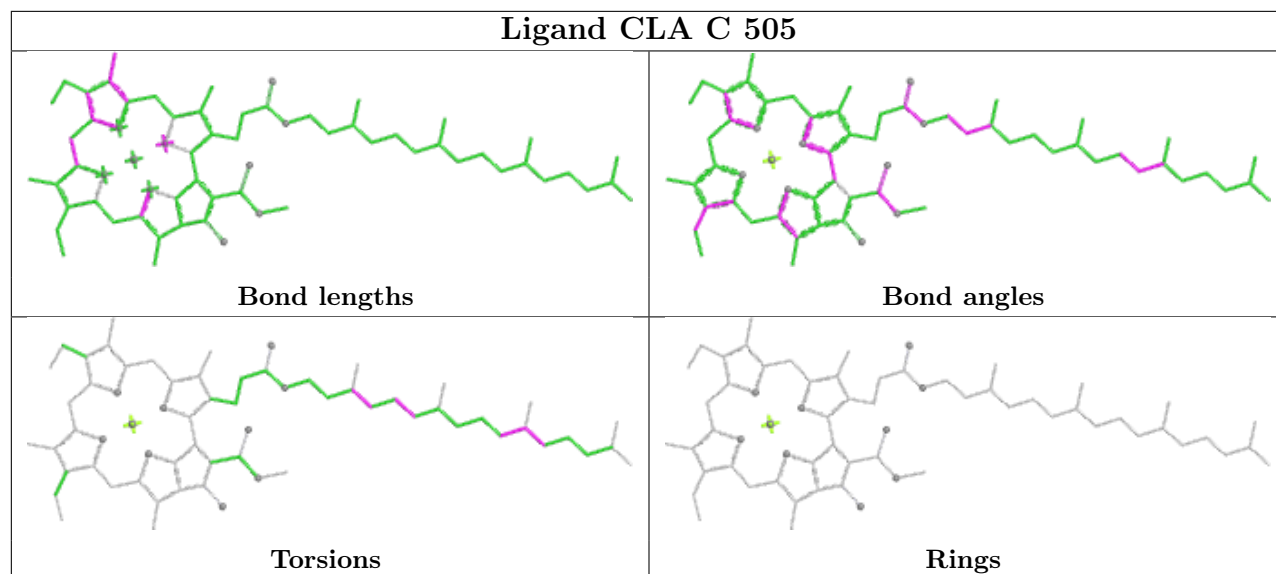
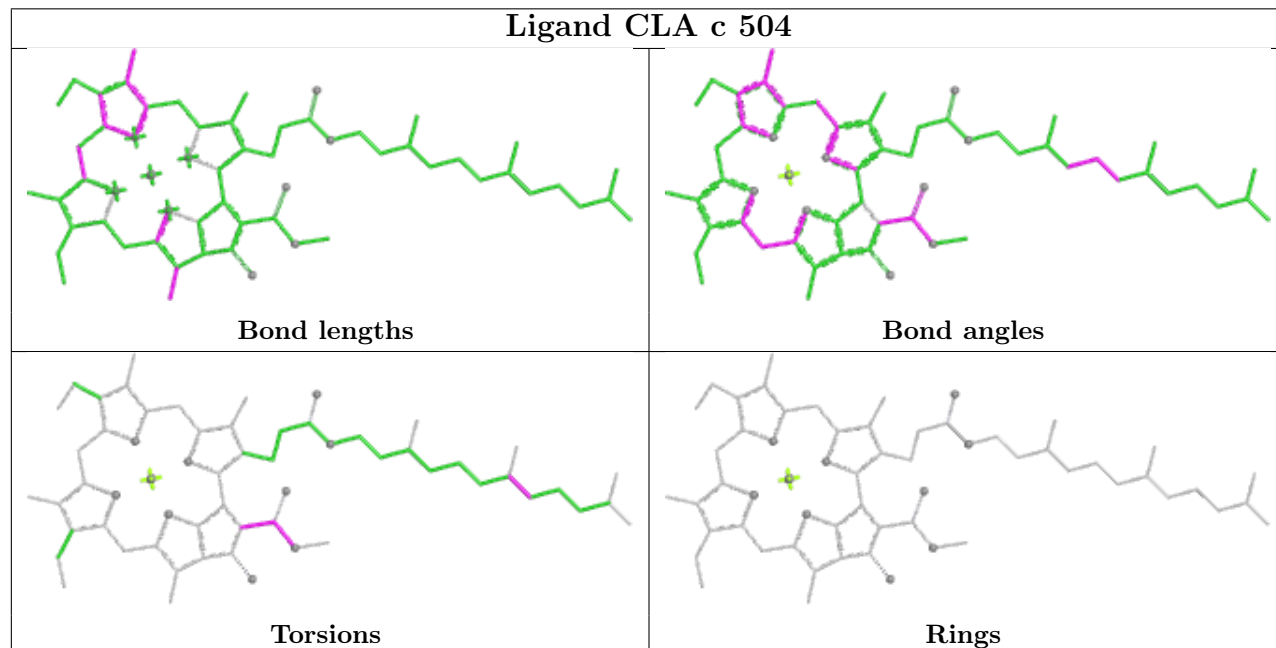
Ligand LMG C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

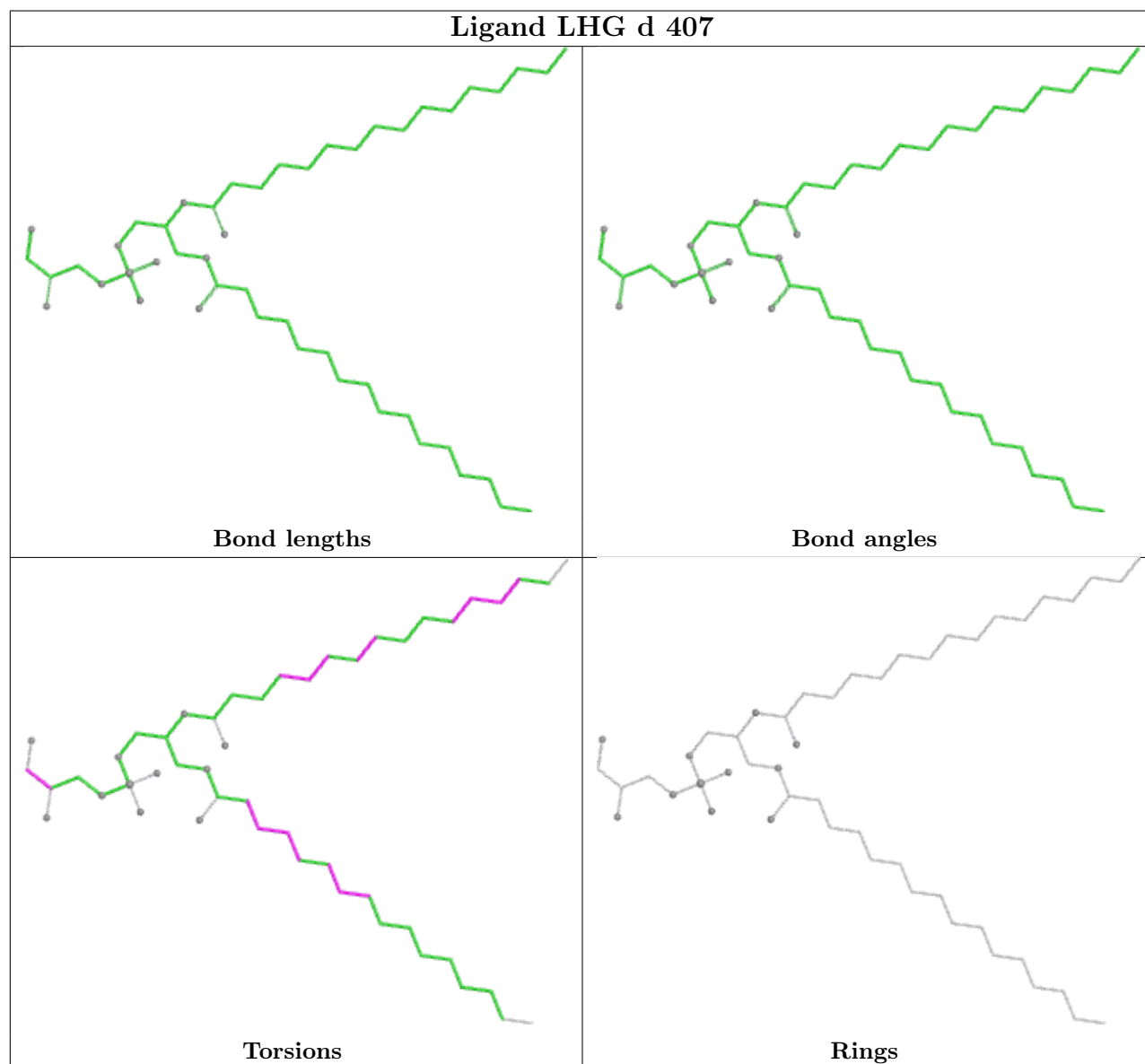
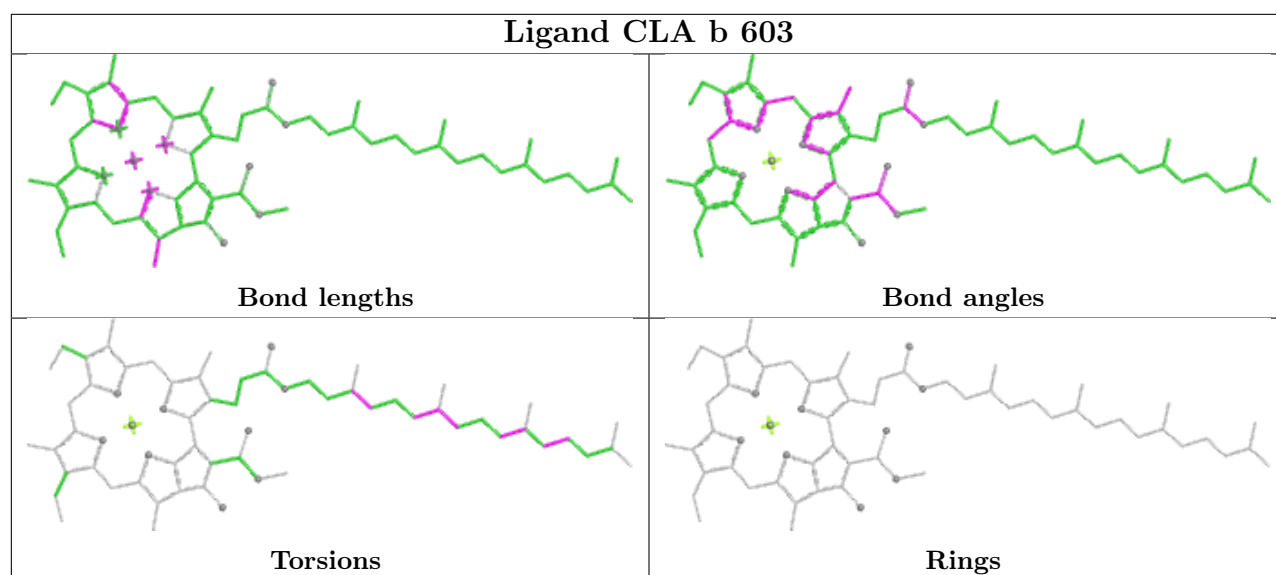
Ligand BCR a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

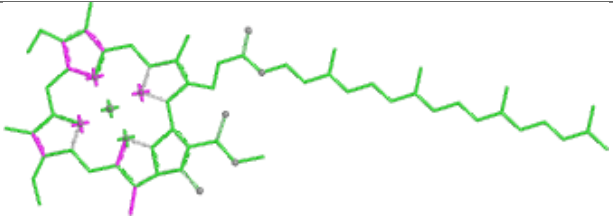
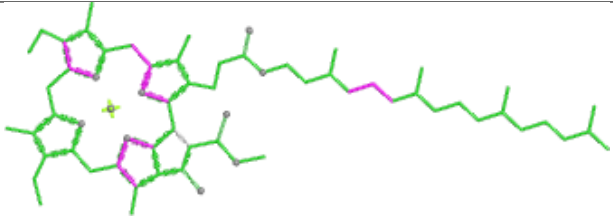
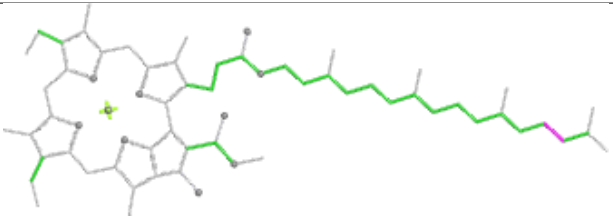
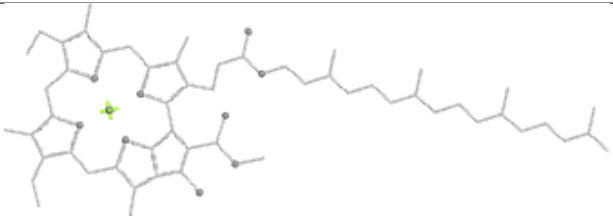
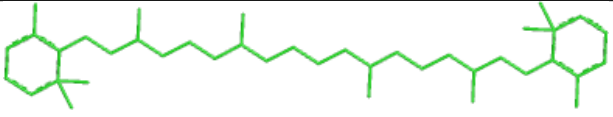
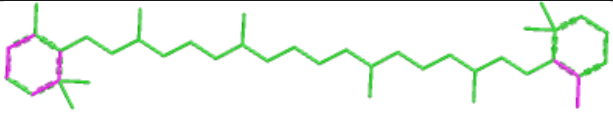
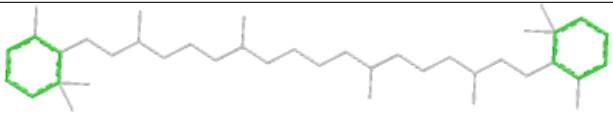
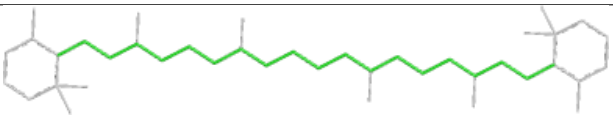
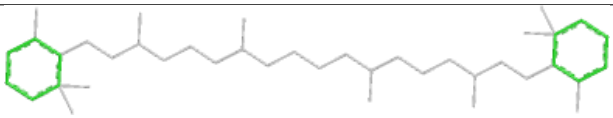
Ligand CLA a 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

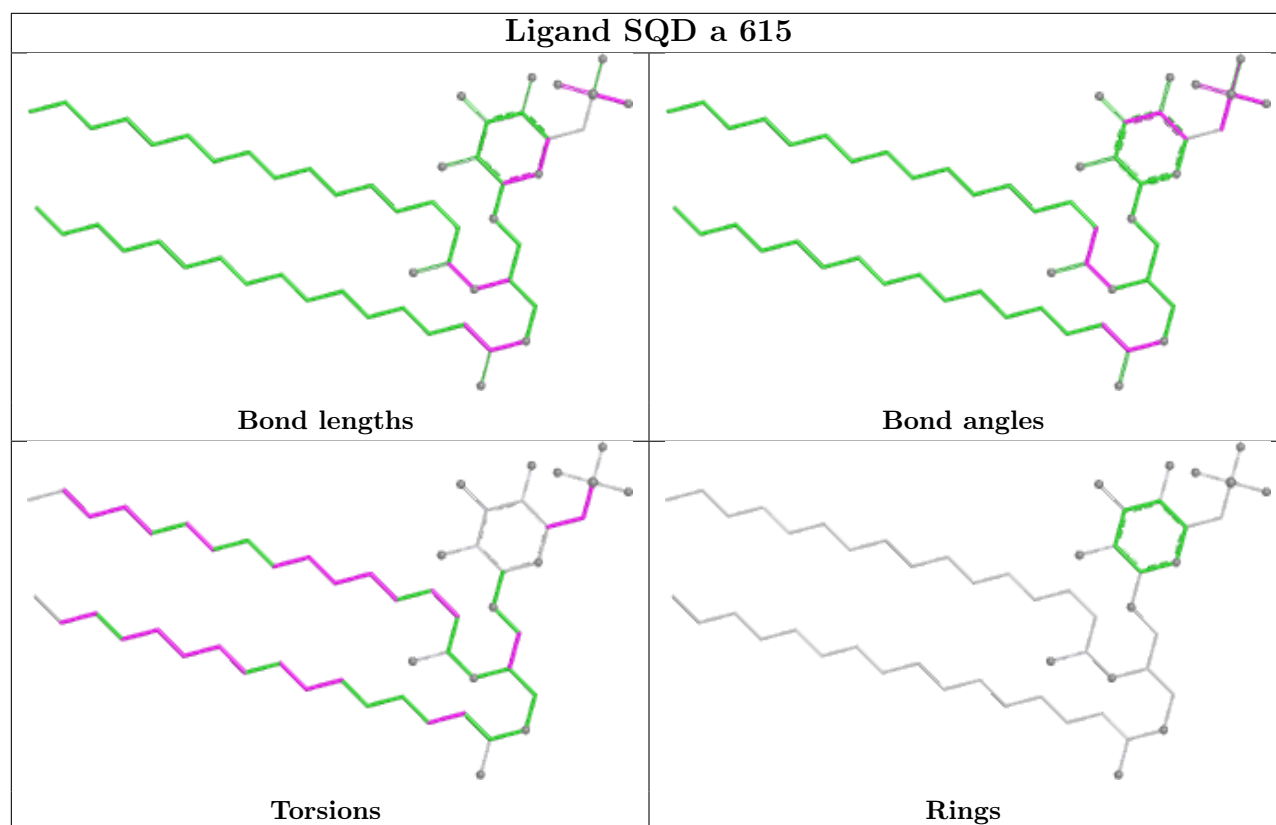
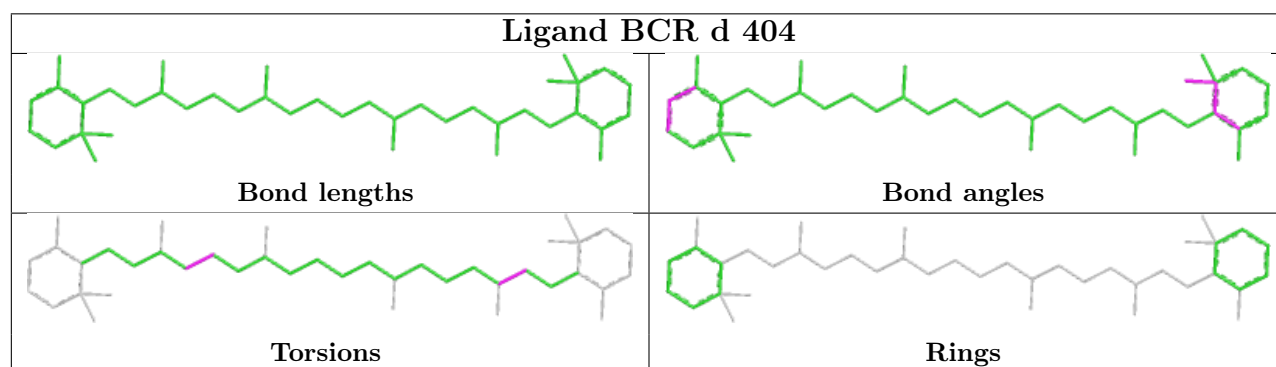
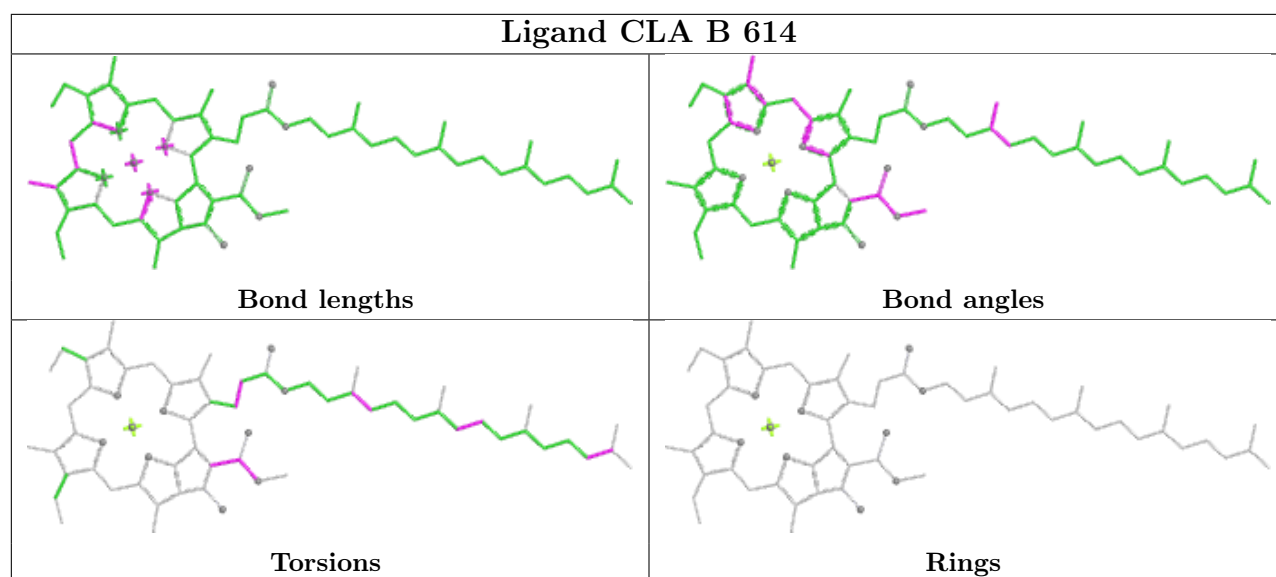
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Bond lengths	Bond angles
	
Torsions	Rings

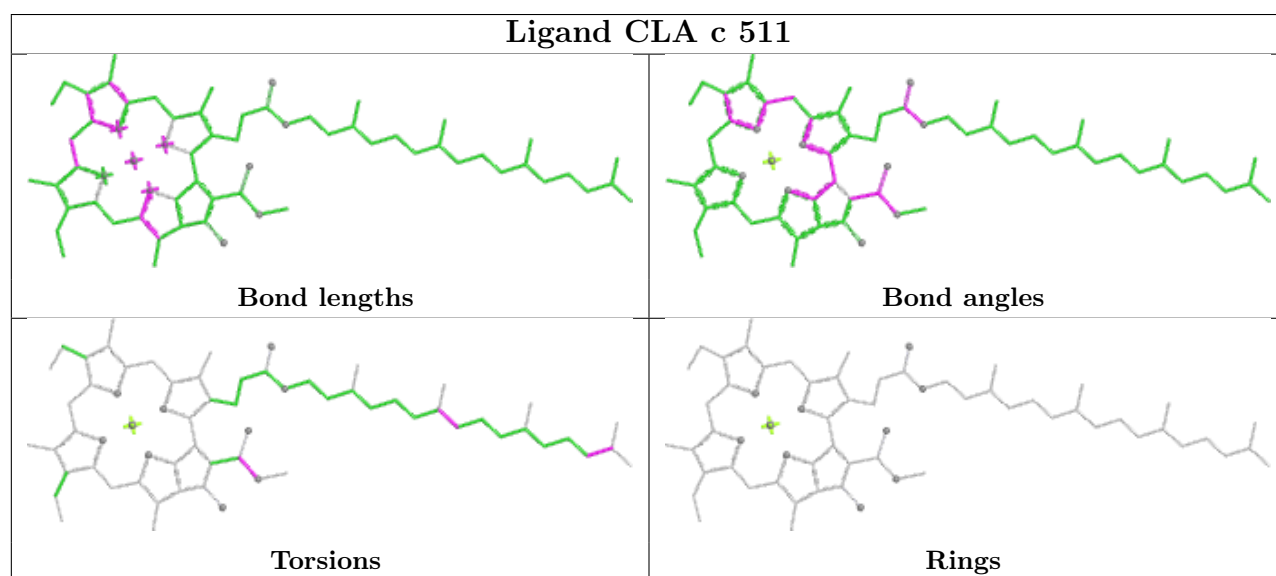
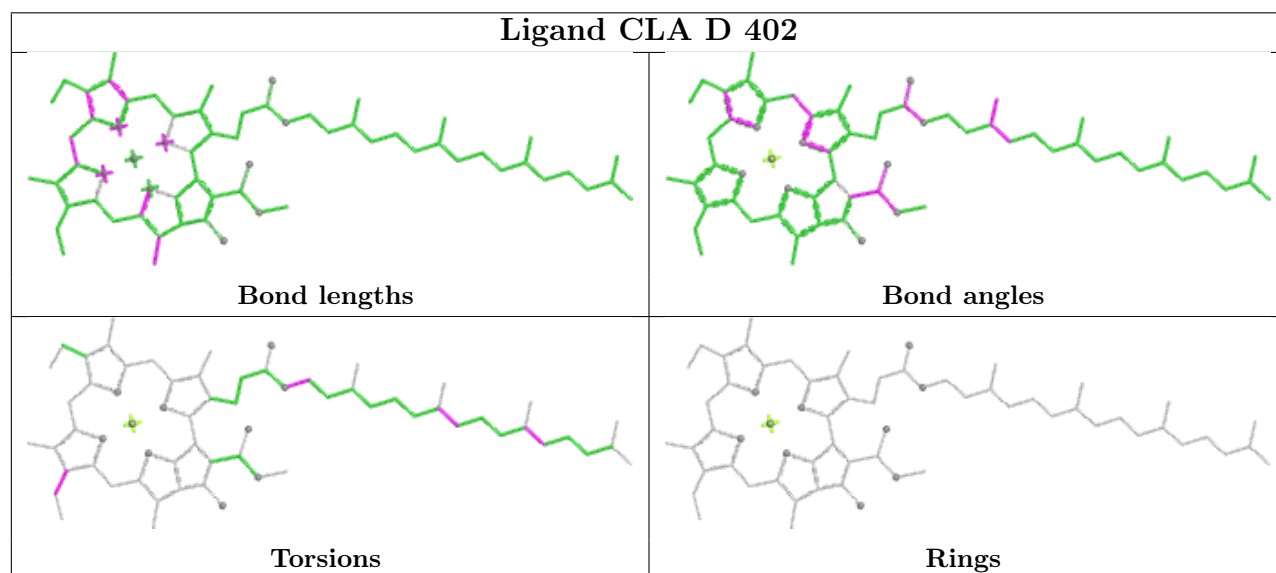
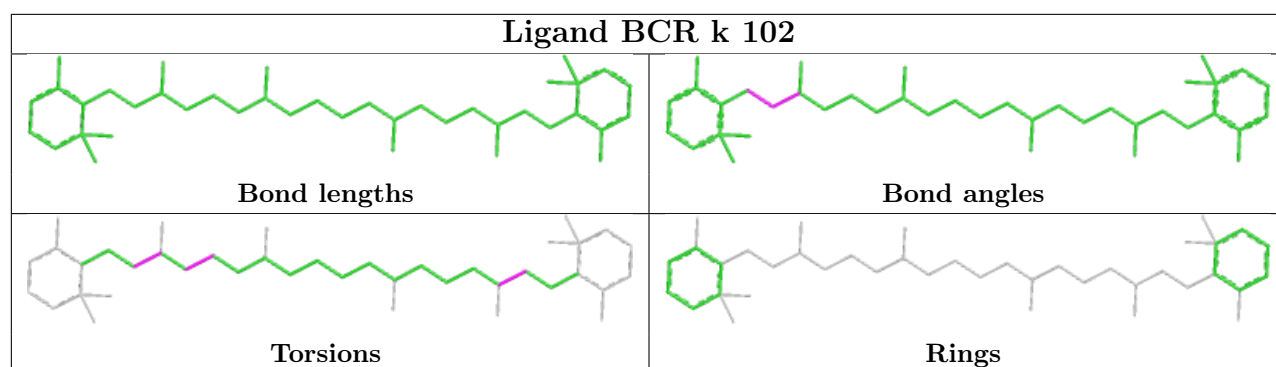
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

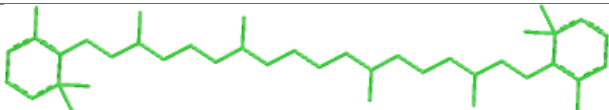
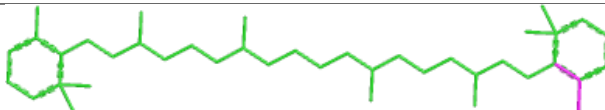
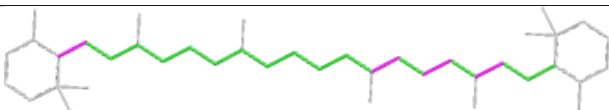
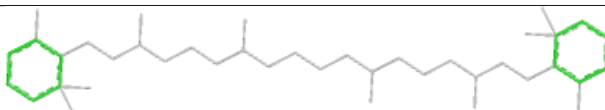
Ligand CLA C 505**Ligand CLA c 504**

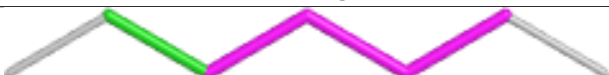


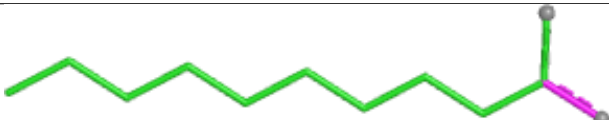
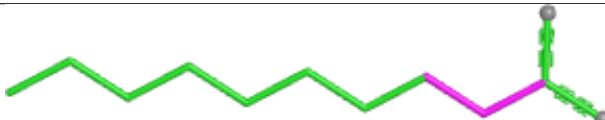
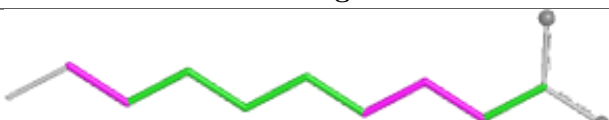
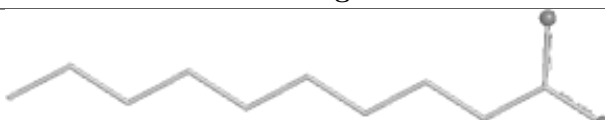
Ligand CLA A 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

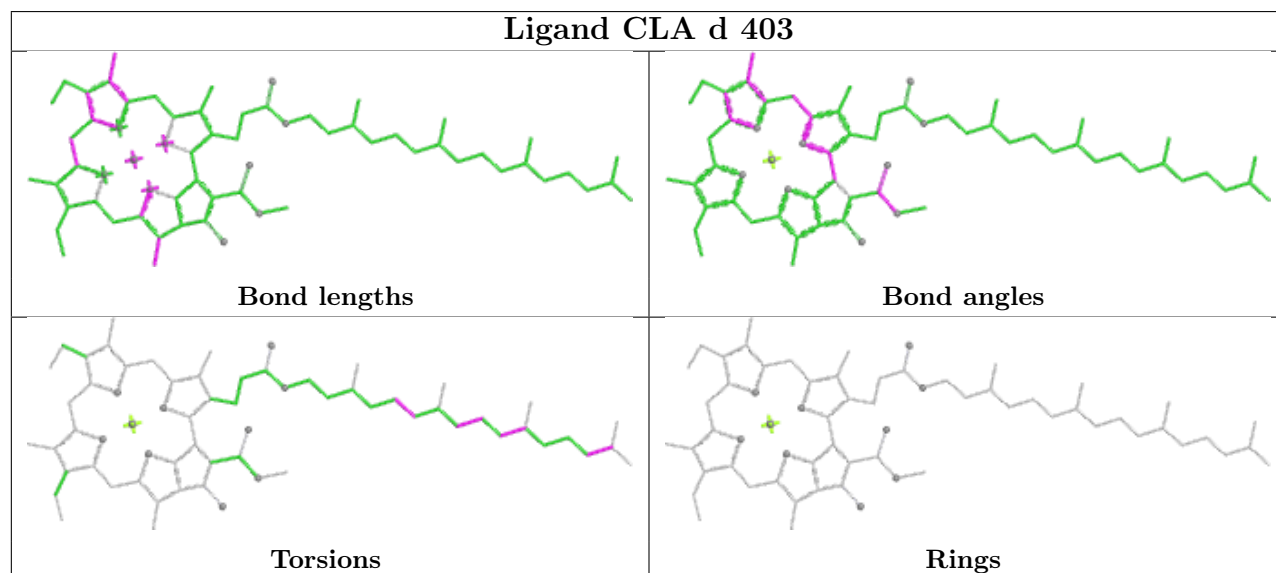
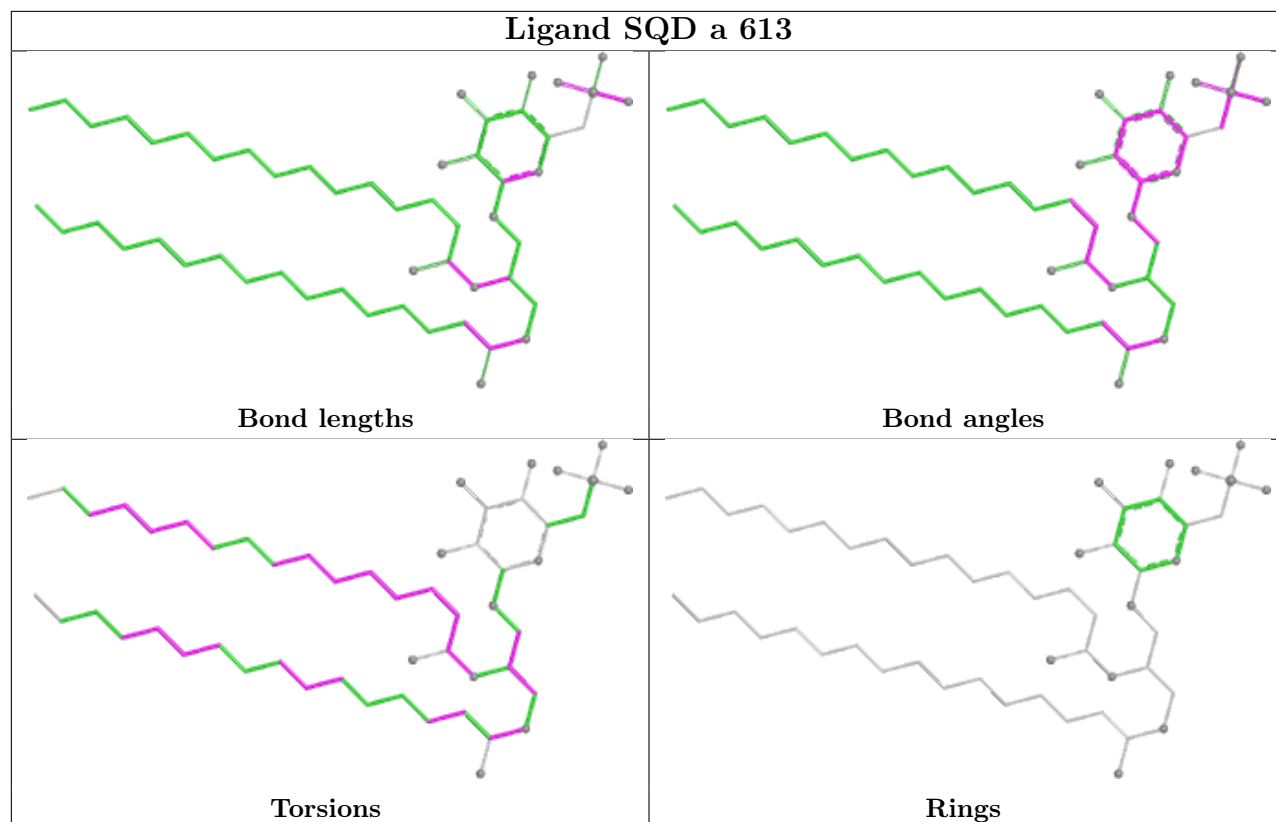


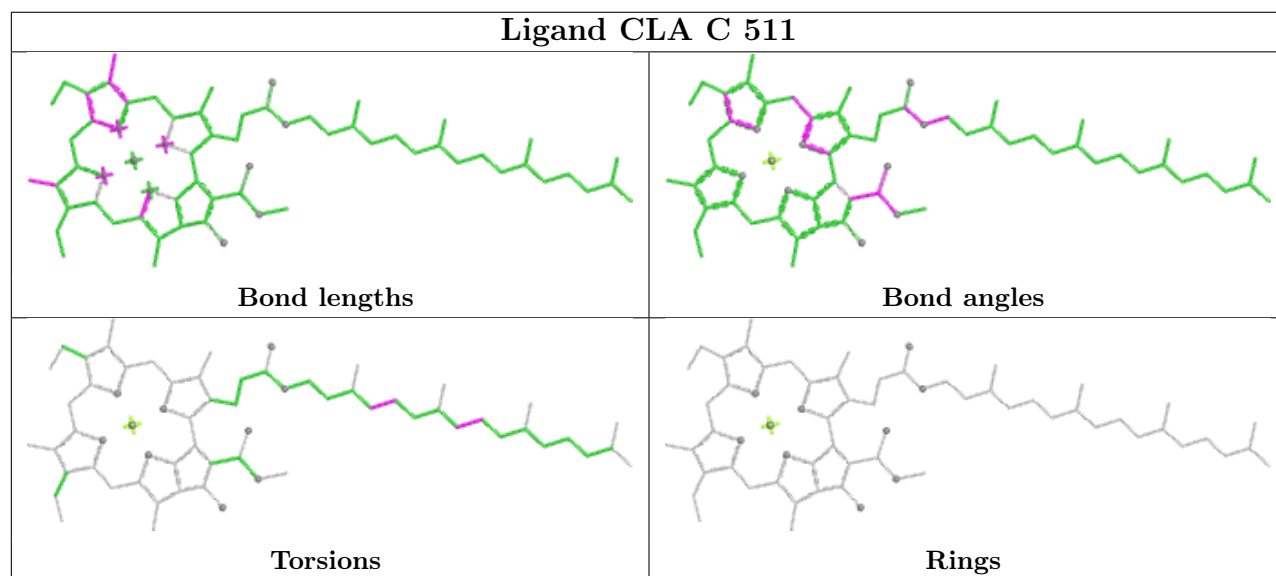
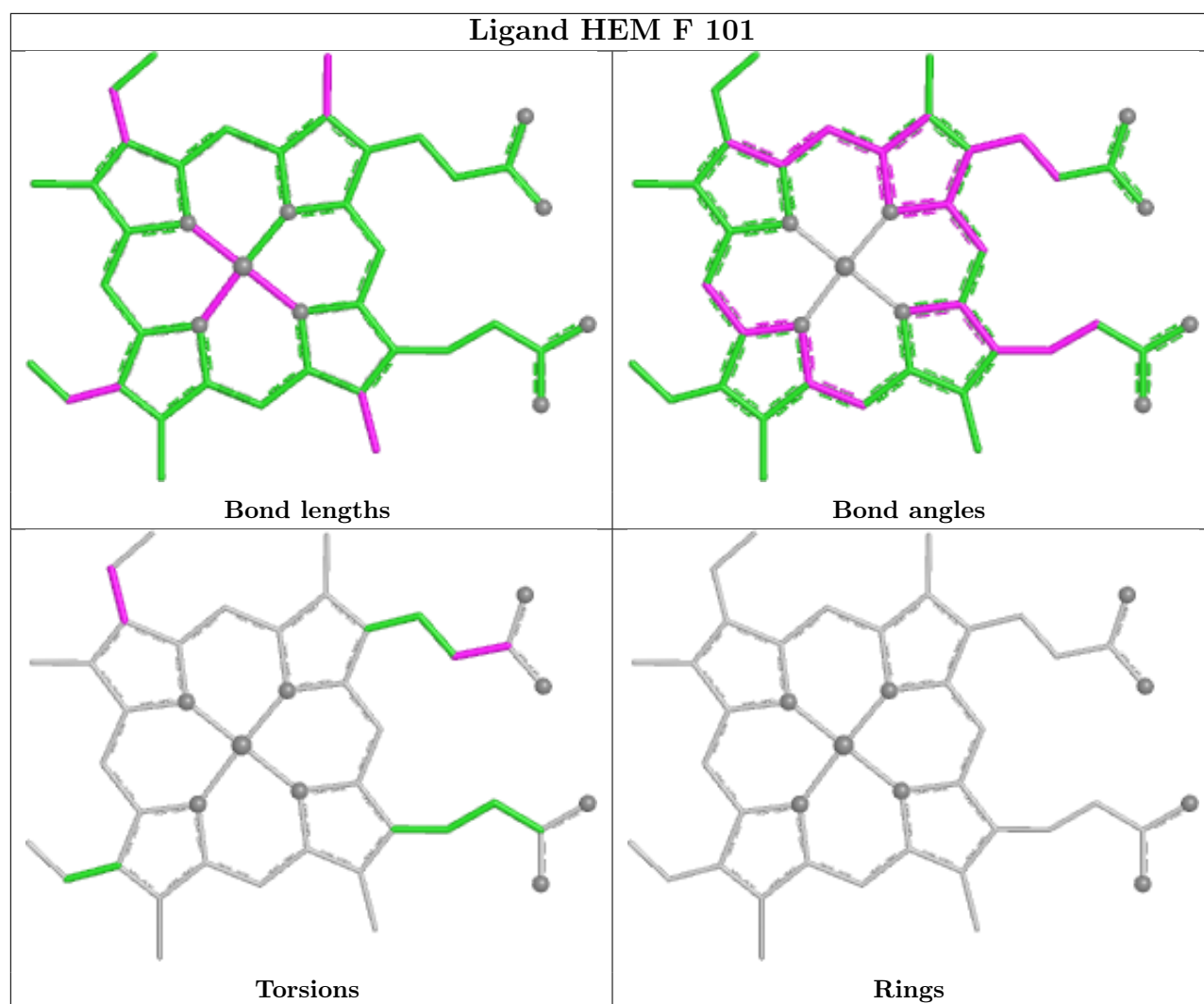


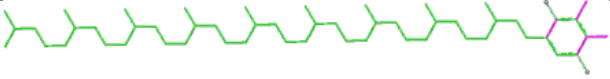
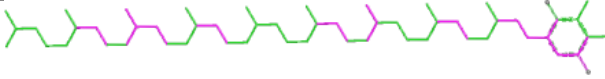
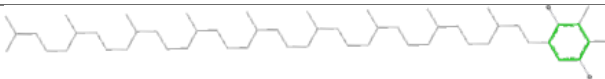
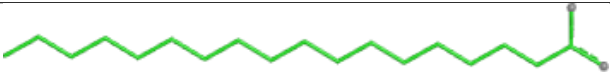
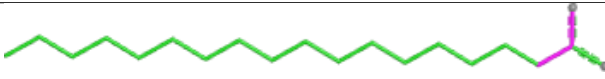
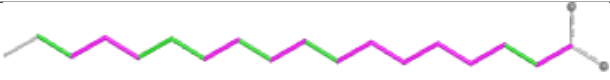
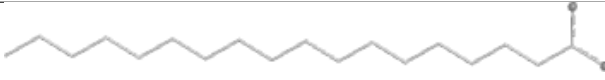
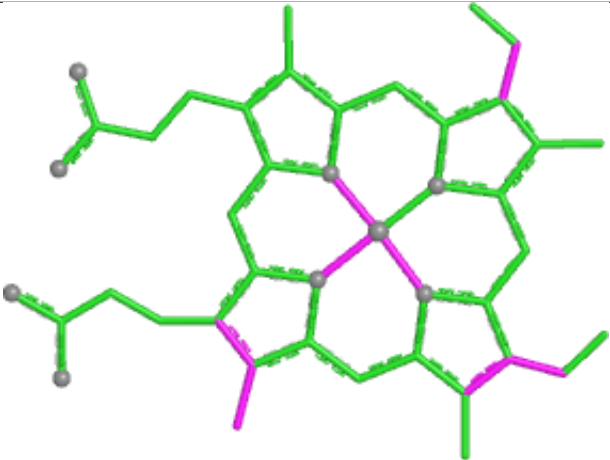
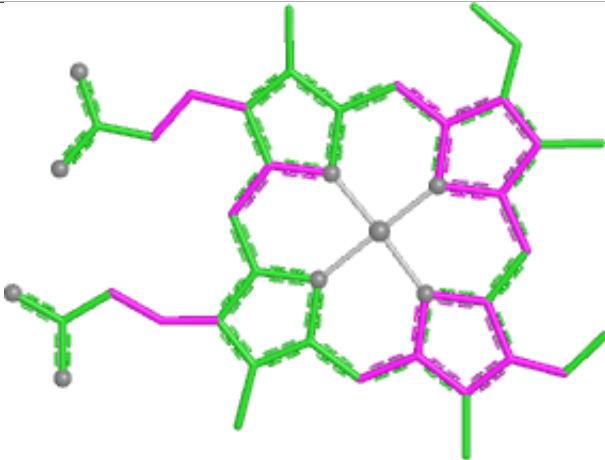
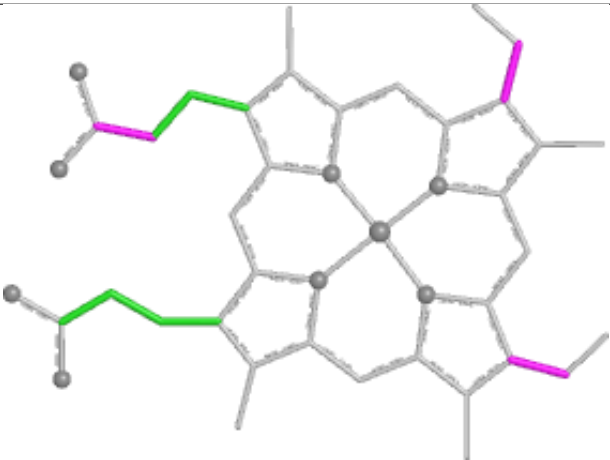
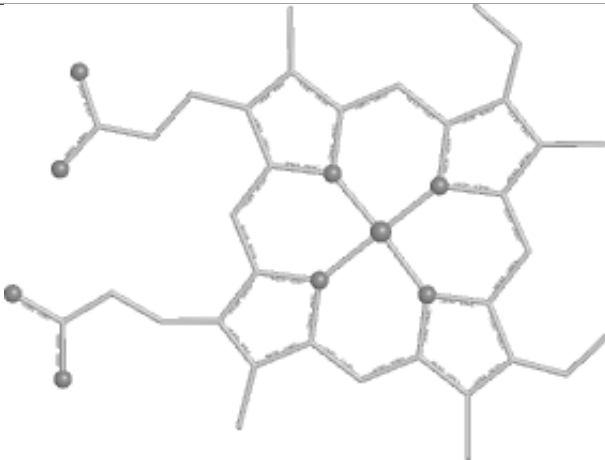
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

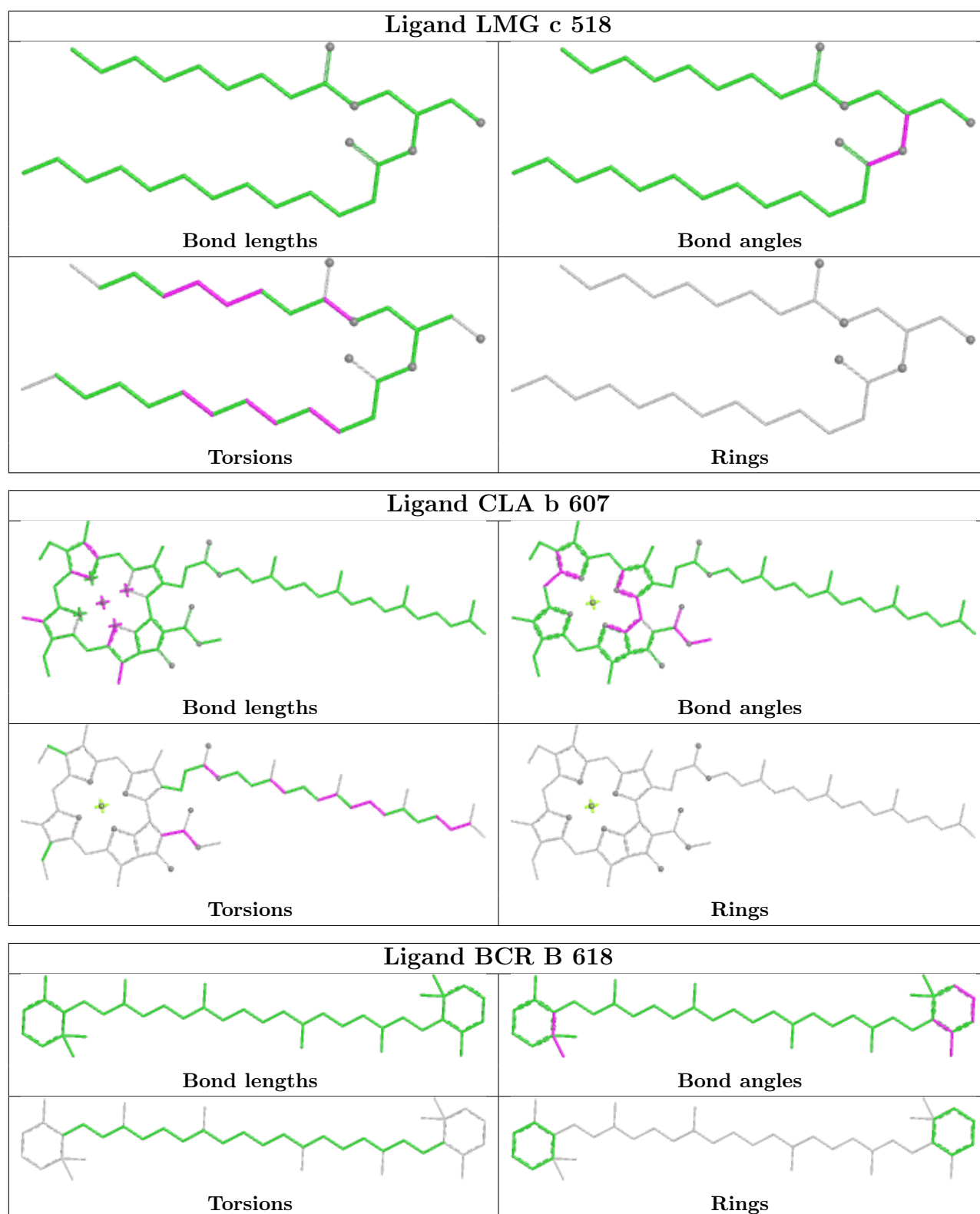
Ligand STE C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

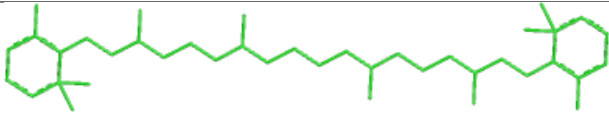
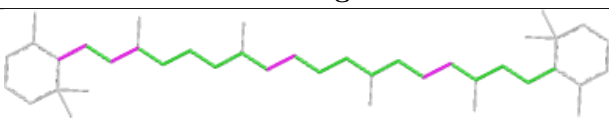
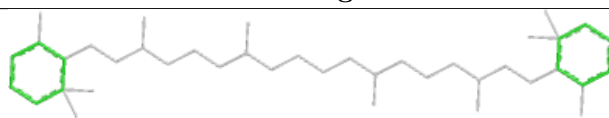
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Bond lengths	Bond angles
	
Torsions	Rings

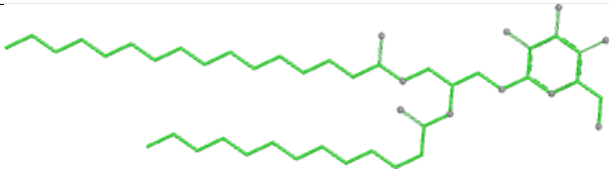
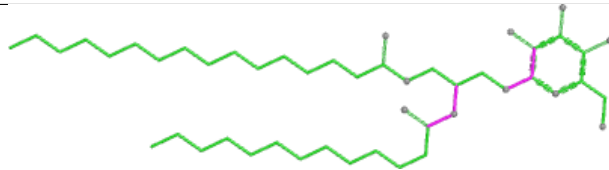
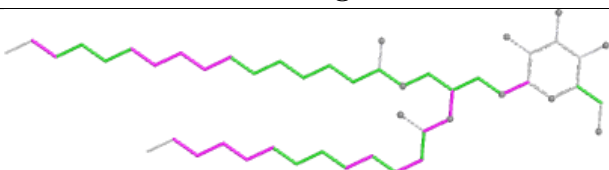
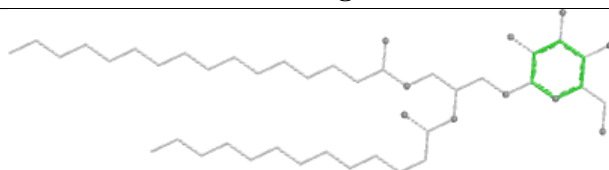


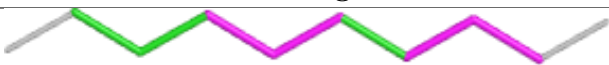


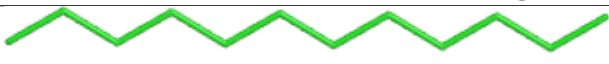
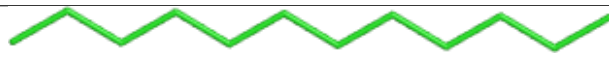
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE E 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand HEM e 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

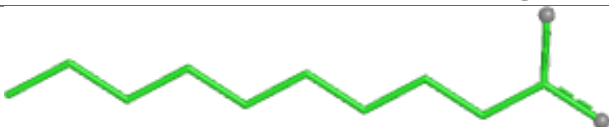
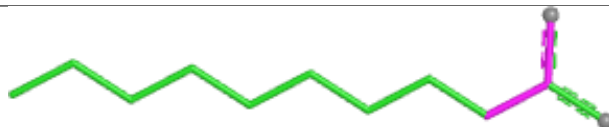
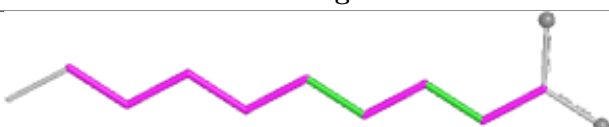
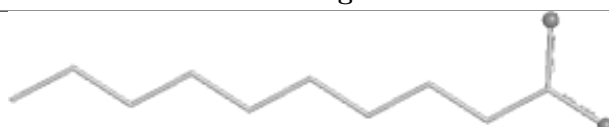


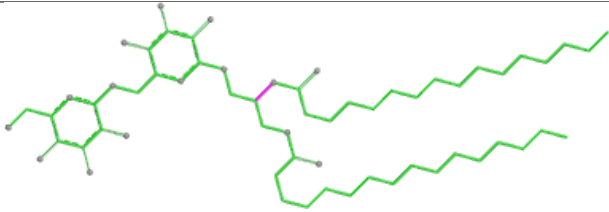
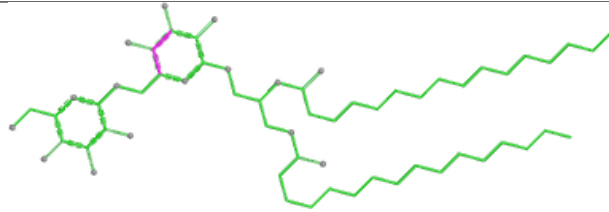
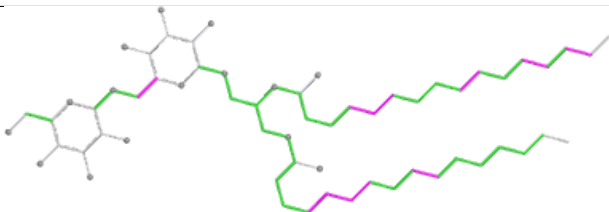
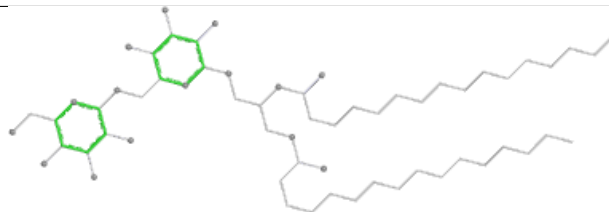
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

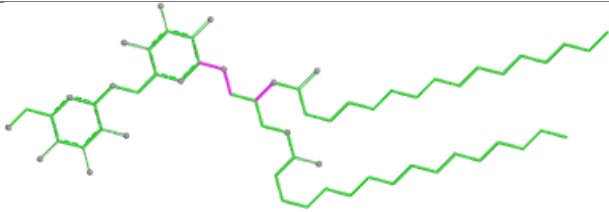
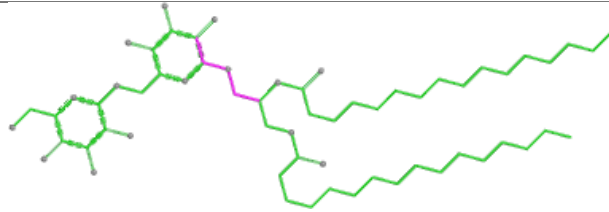
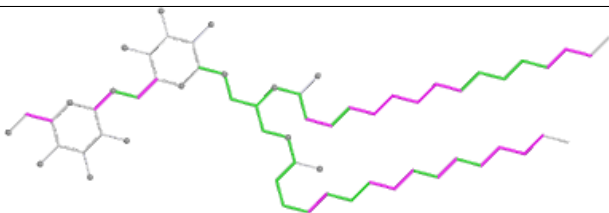
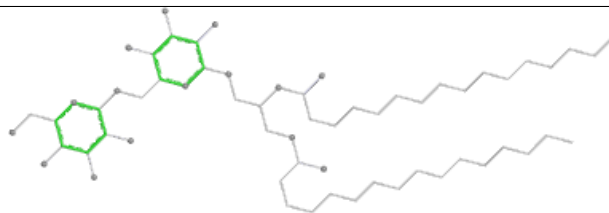
Ligand LMG A 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

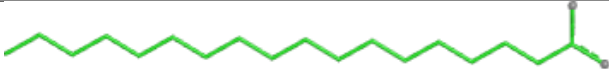
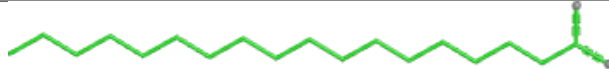
Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

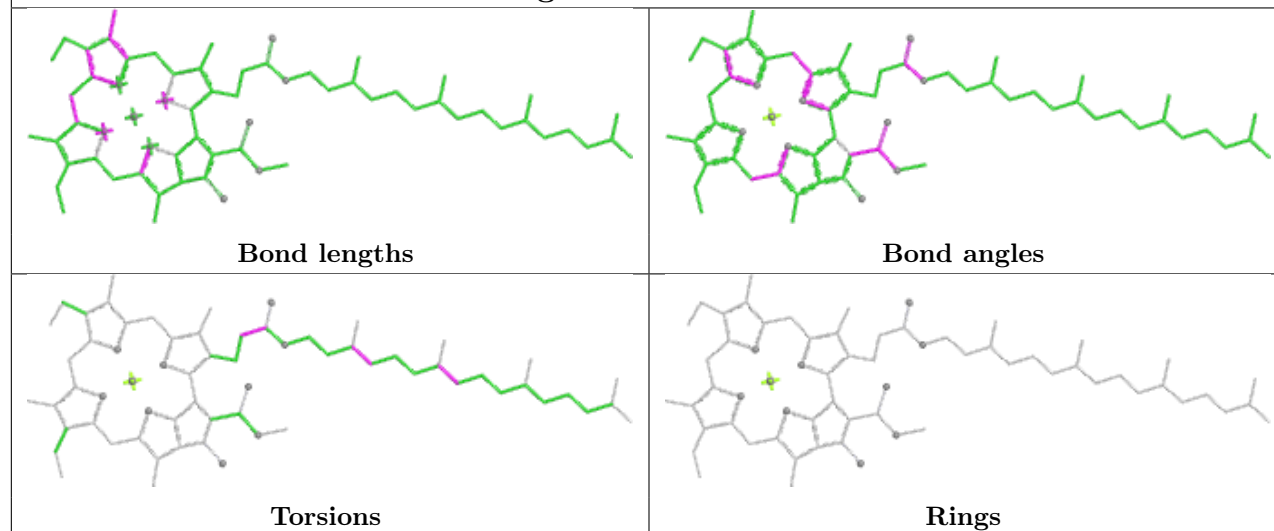
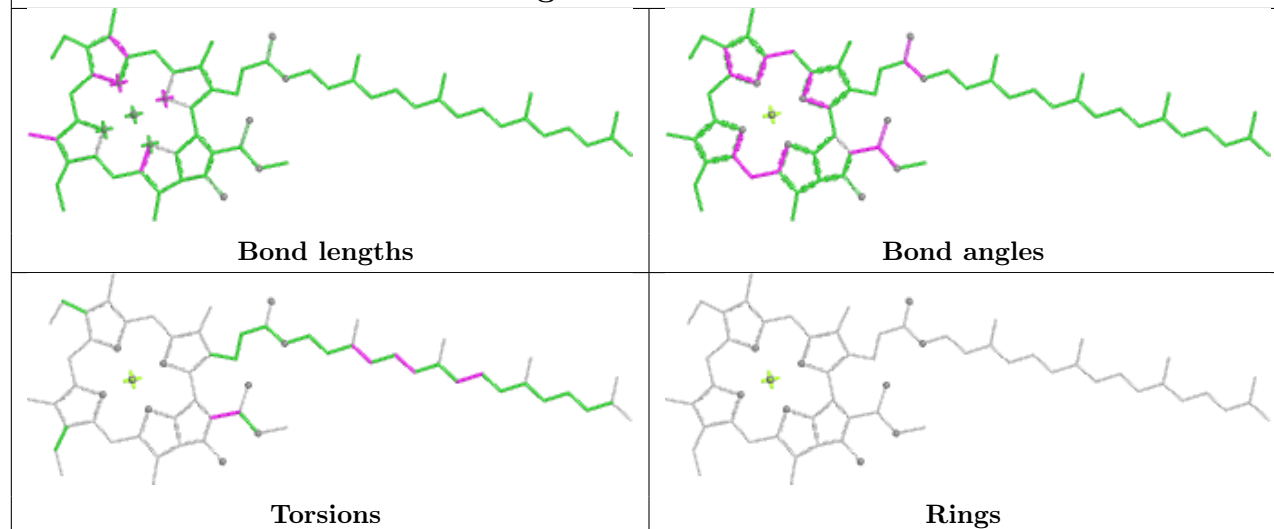
Ligand STE E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

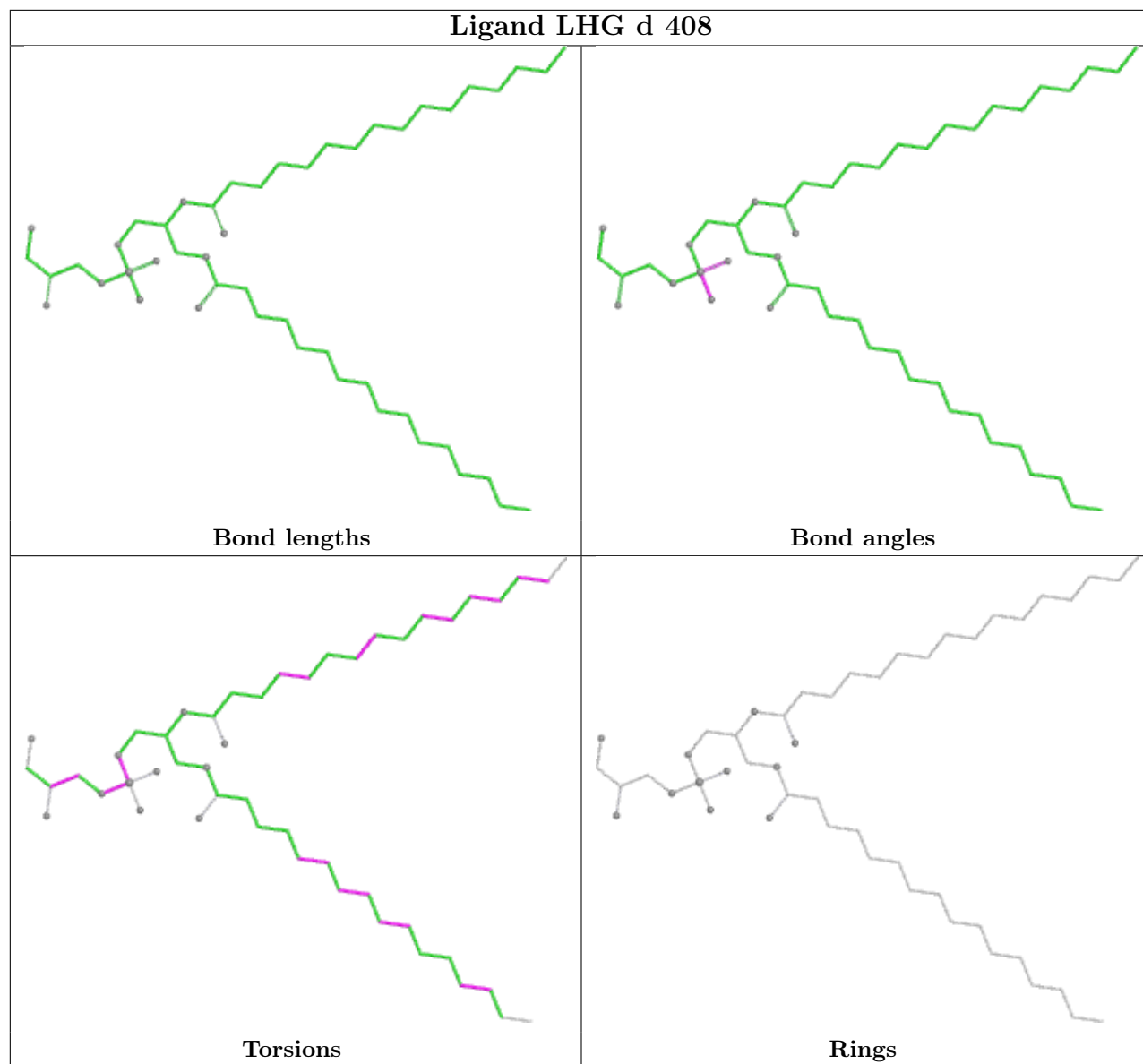
Ligand STE J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

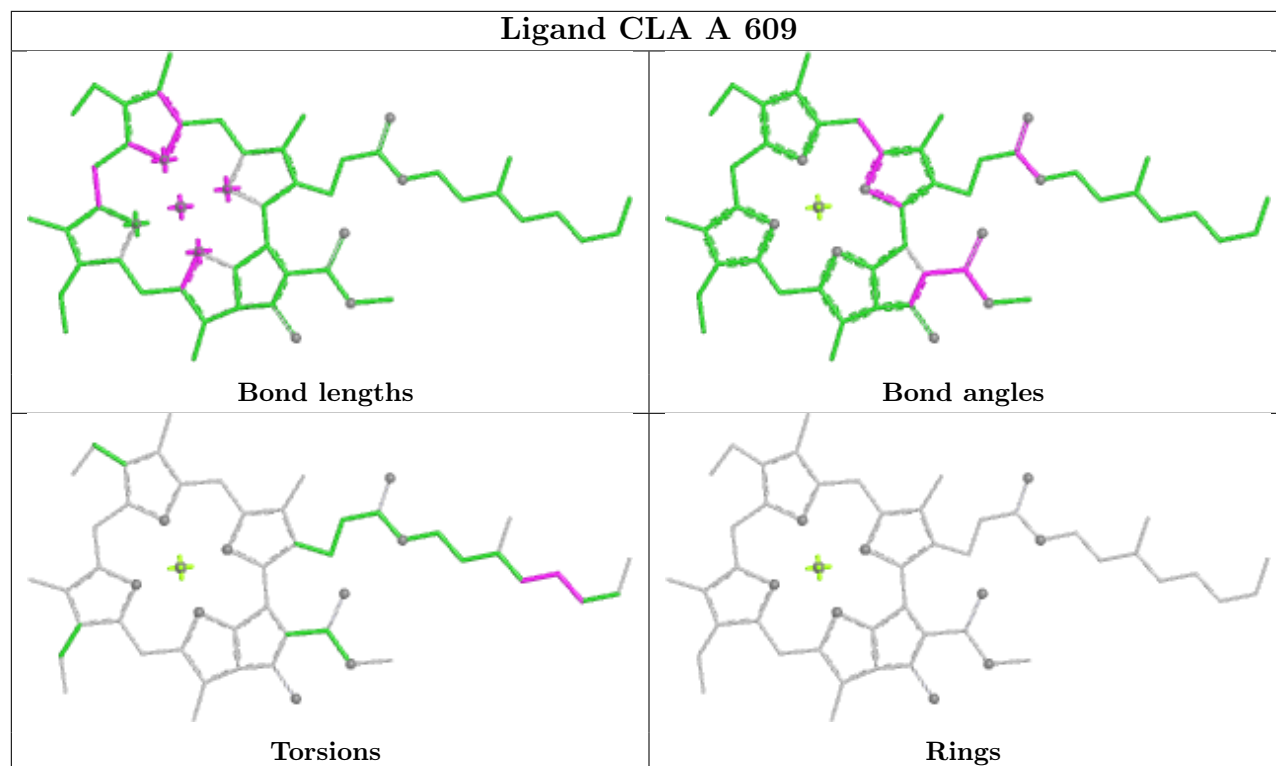
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

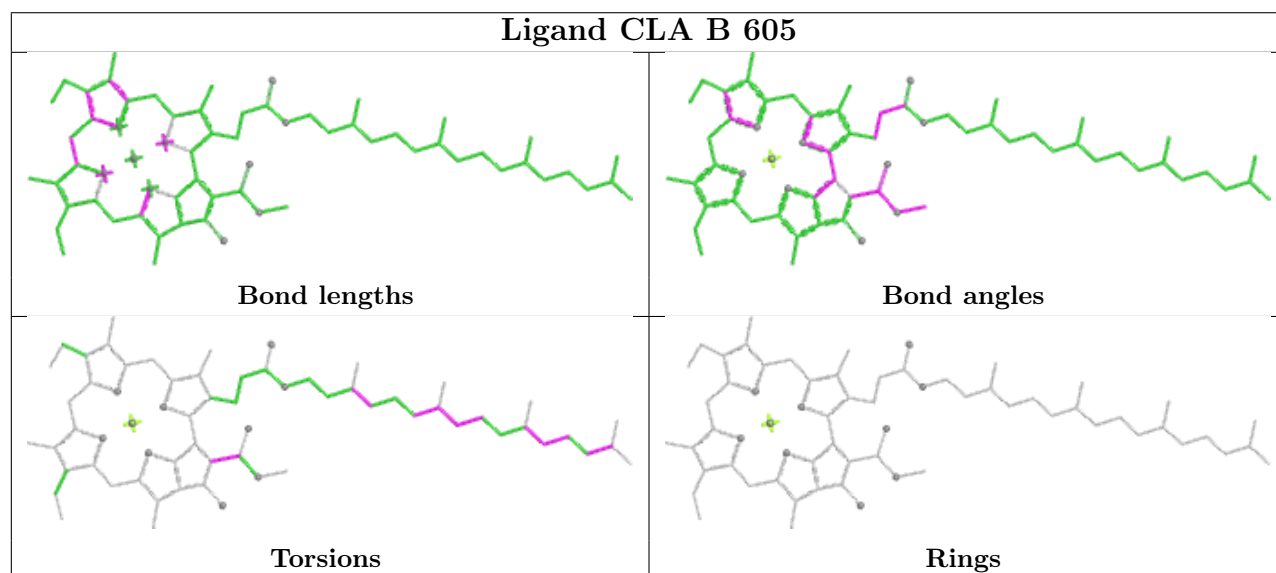
Ligand CLA c 510**Ligand CLA c 507**

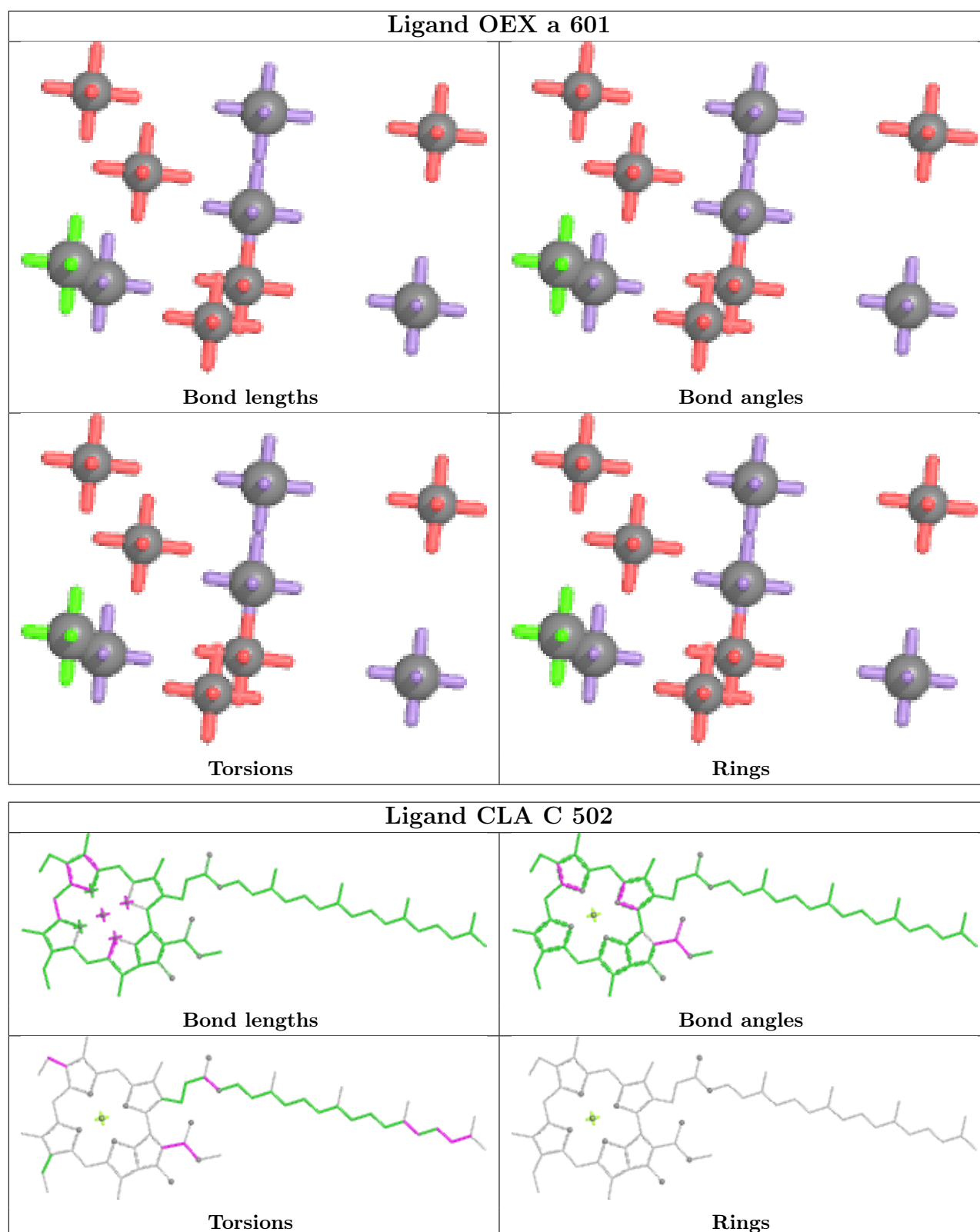


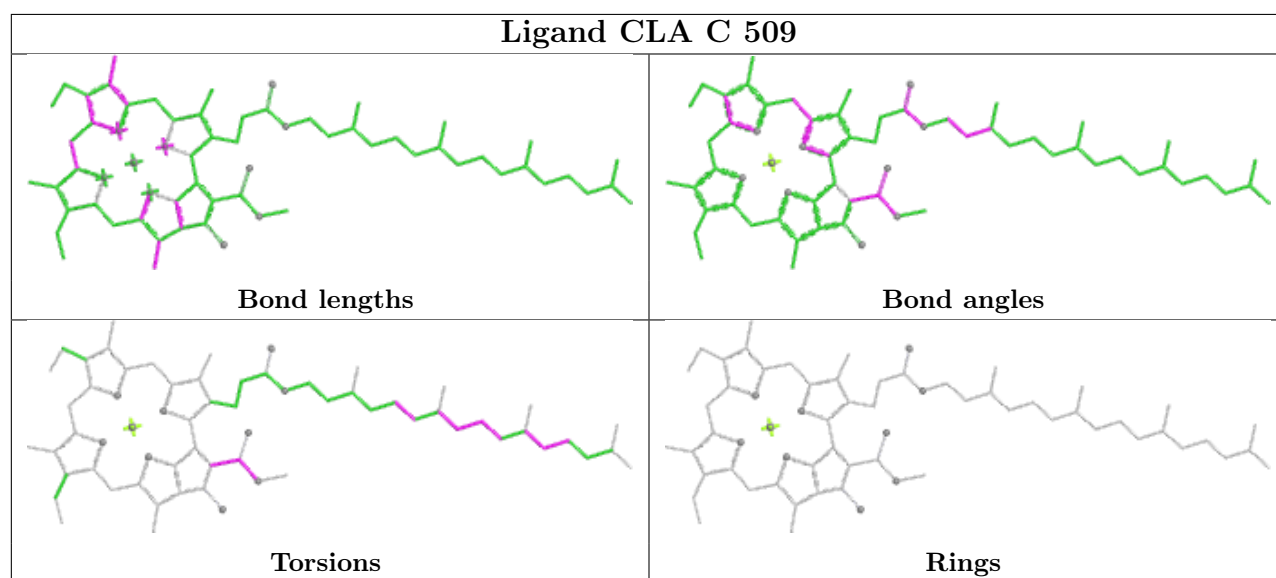
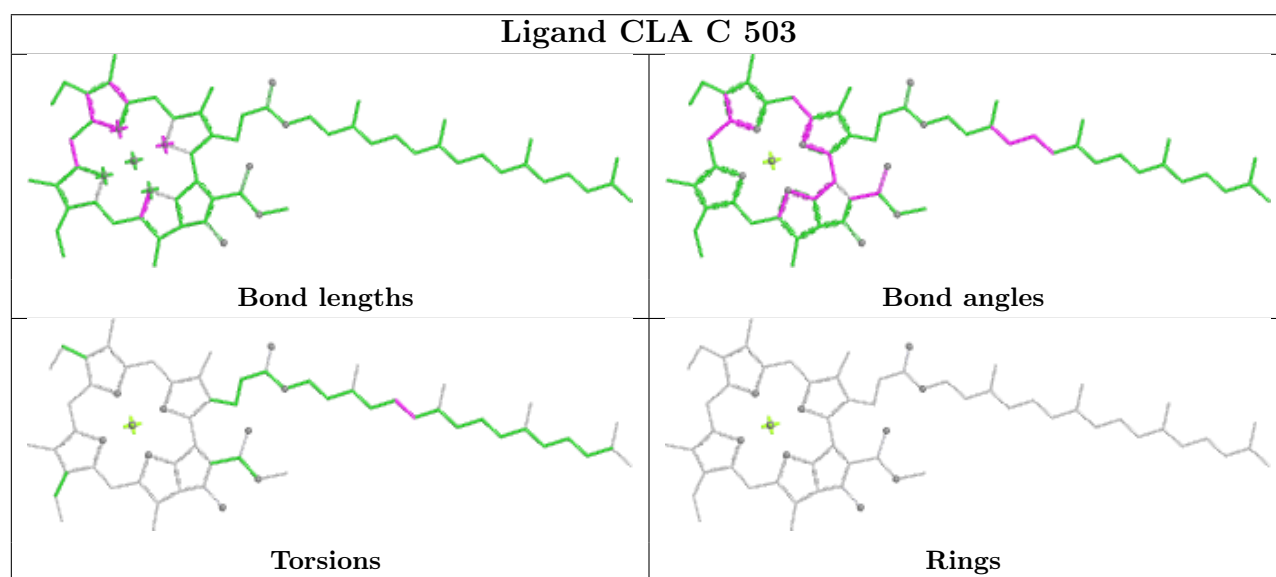
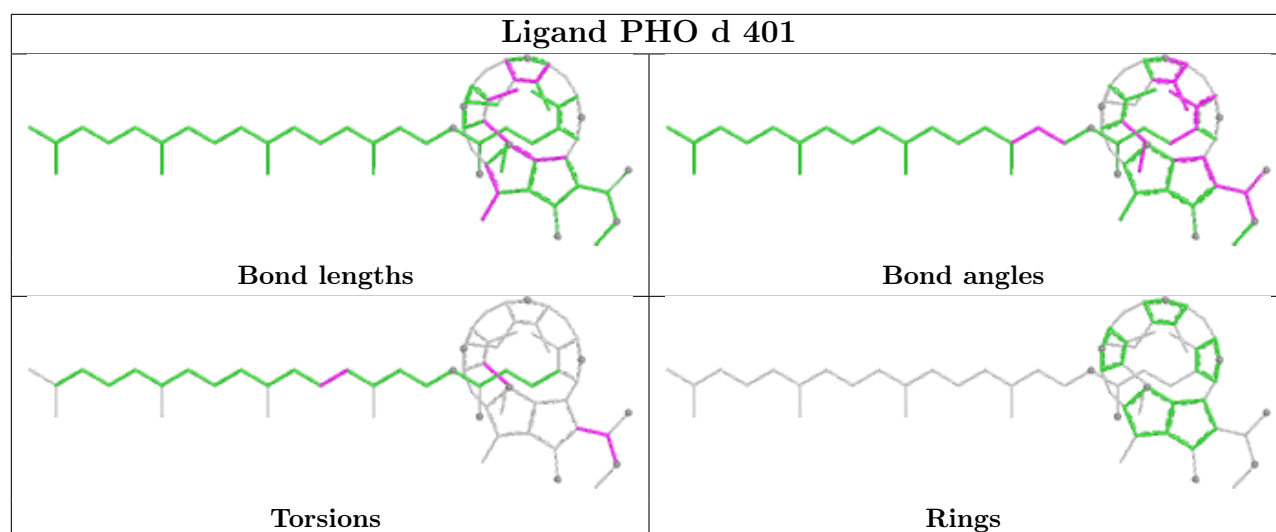
Ligand CLA A 609

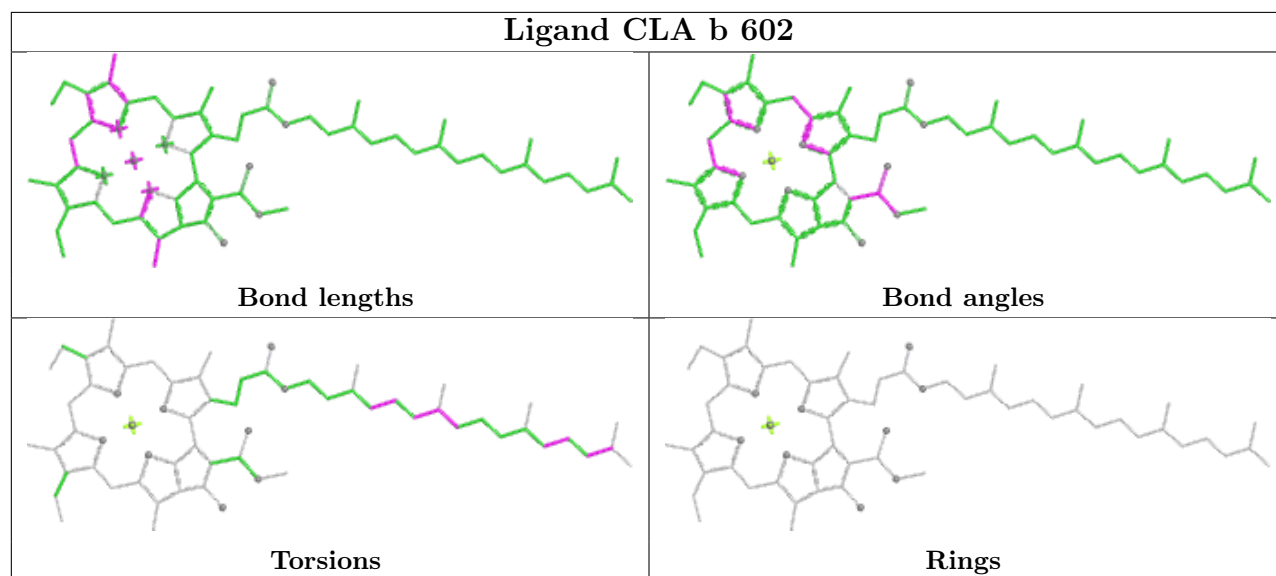
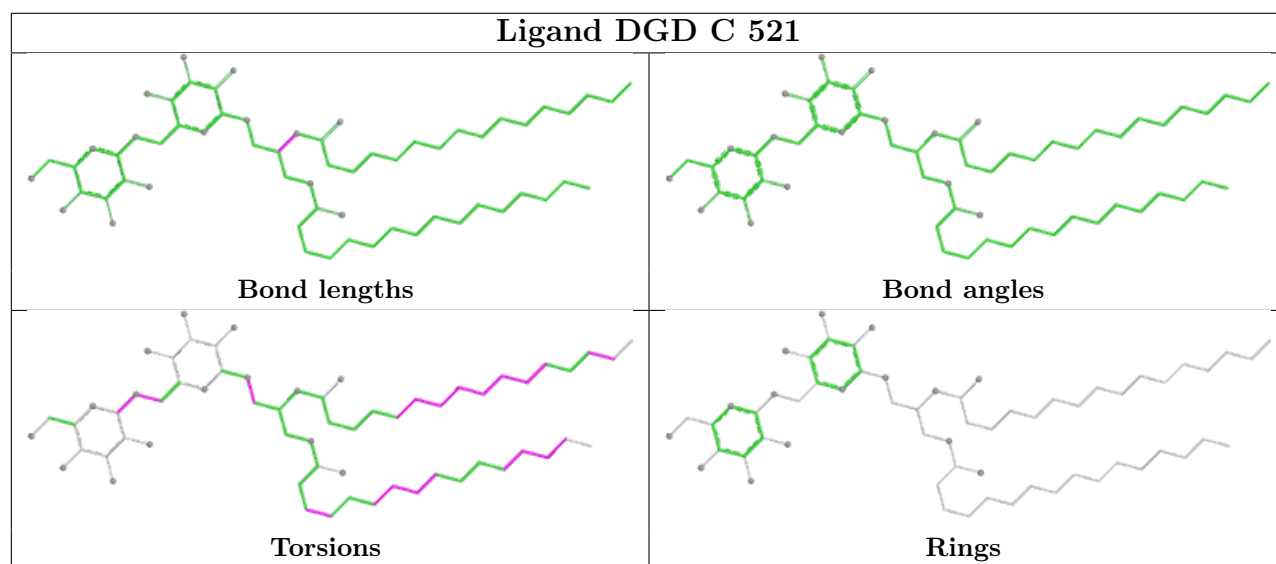
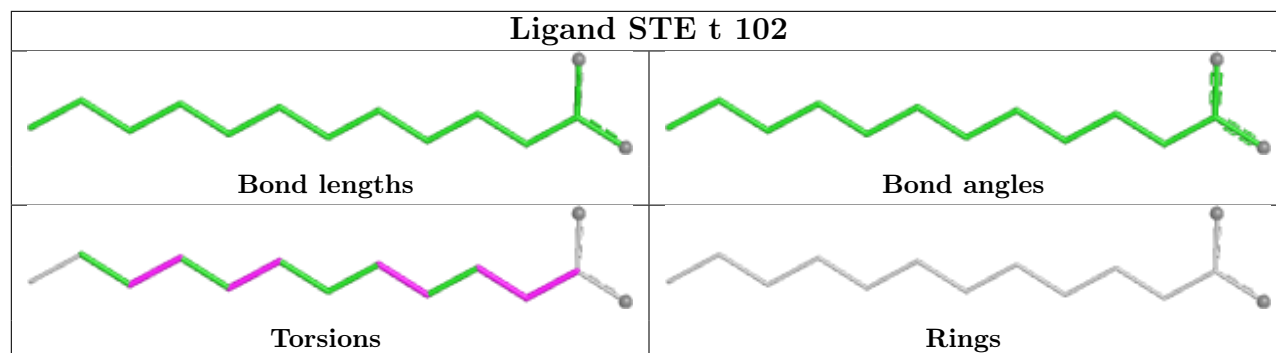


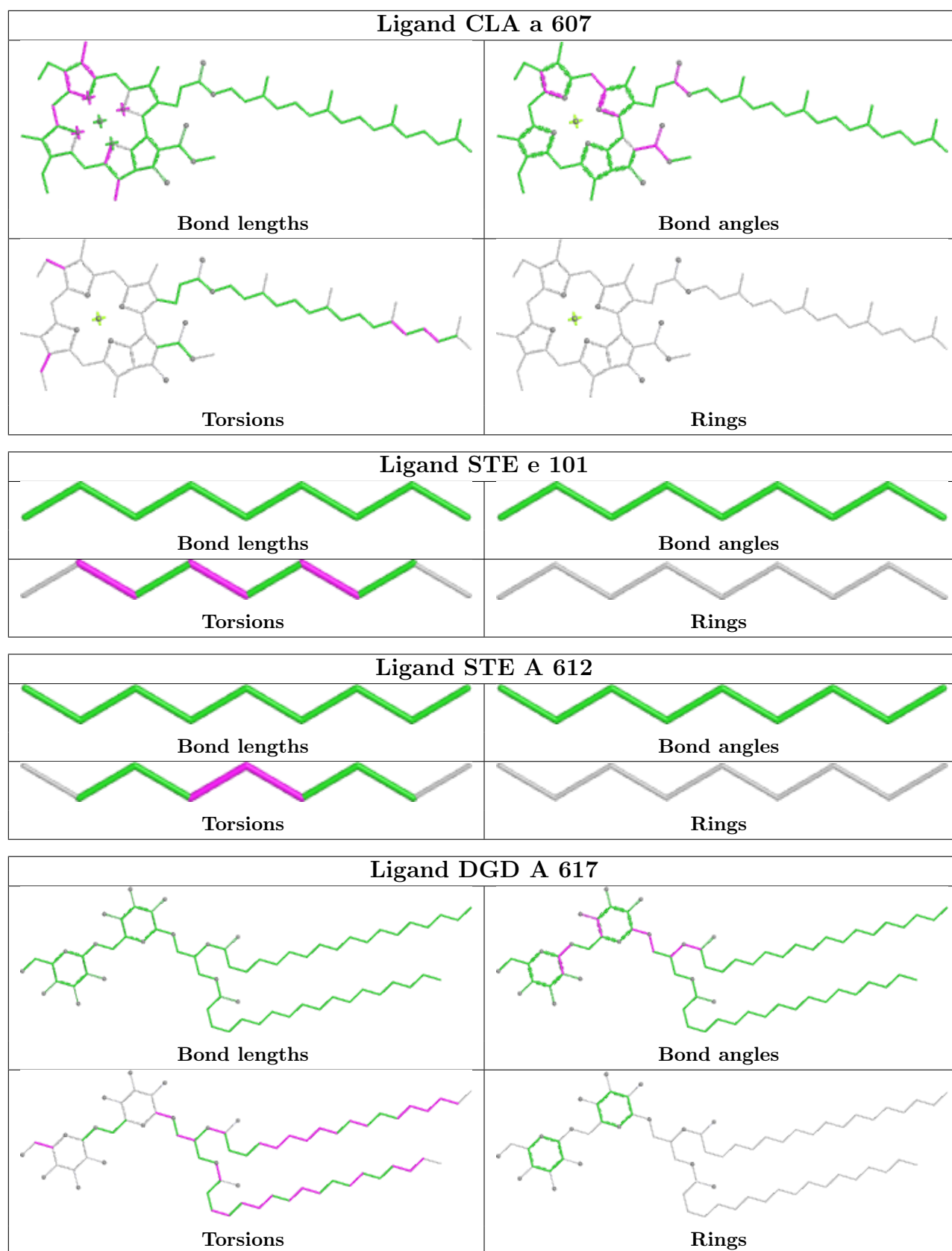
Ligand CLA B 605

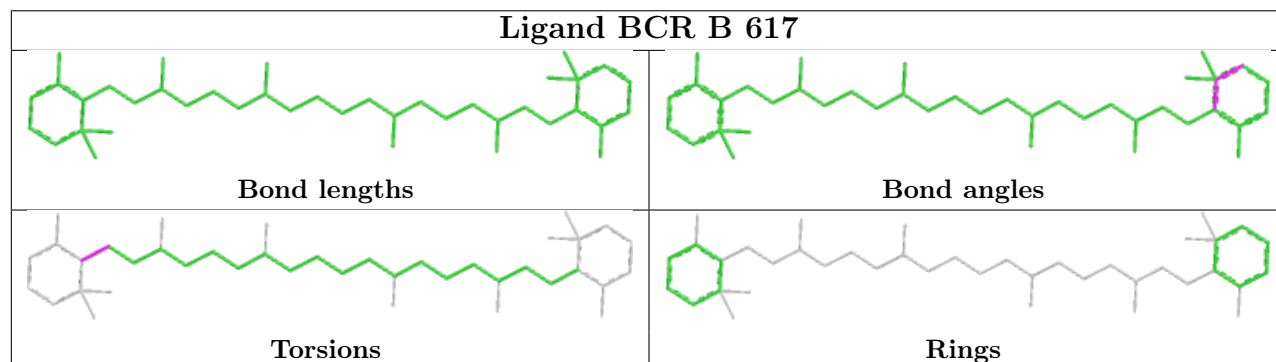
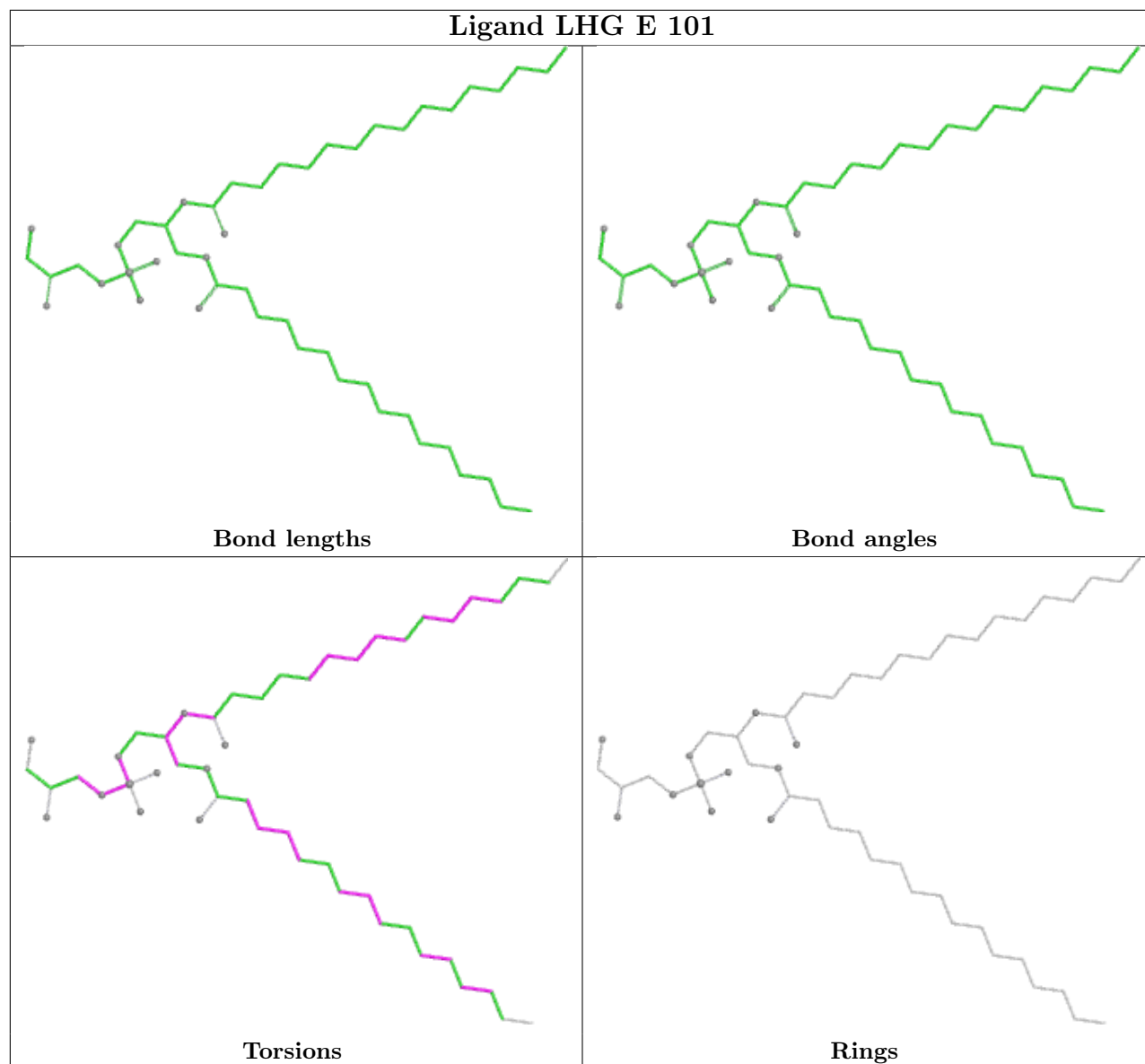


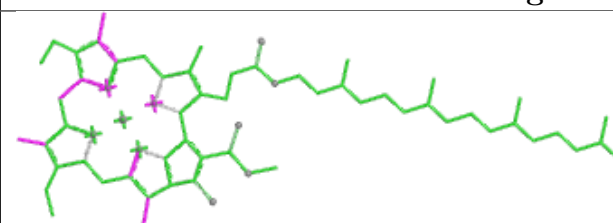
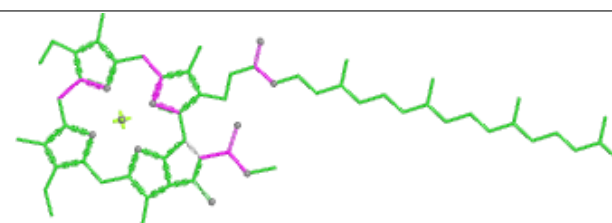
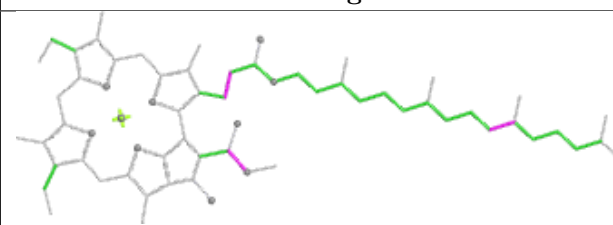
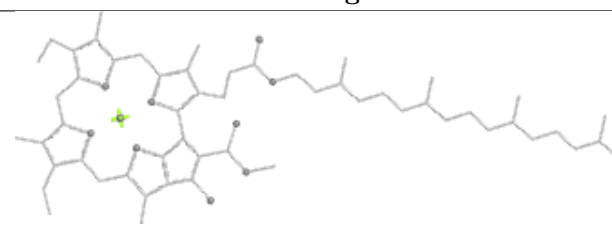


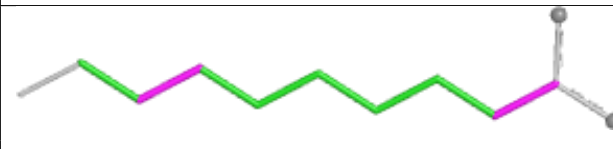
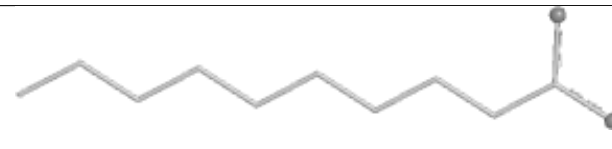


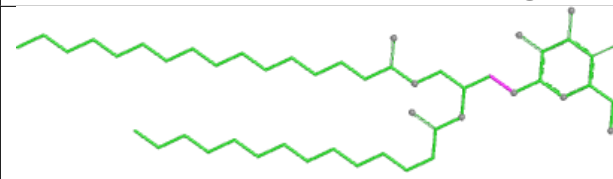
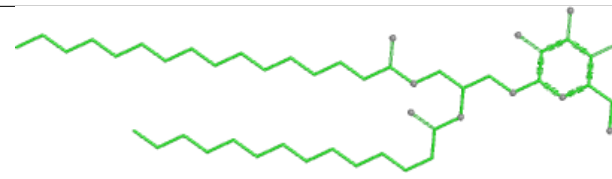
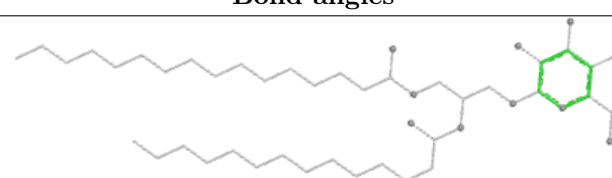


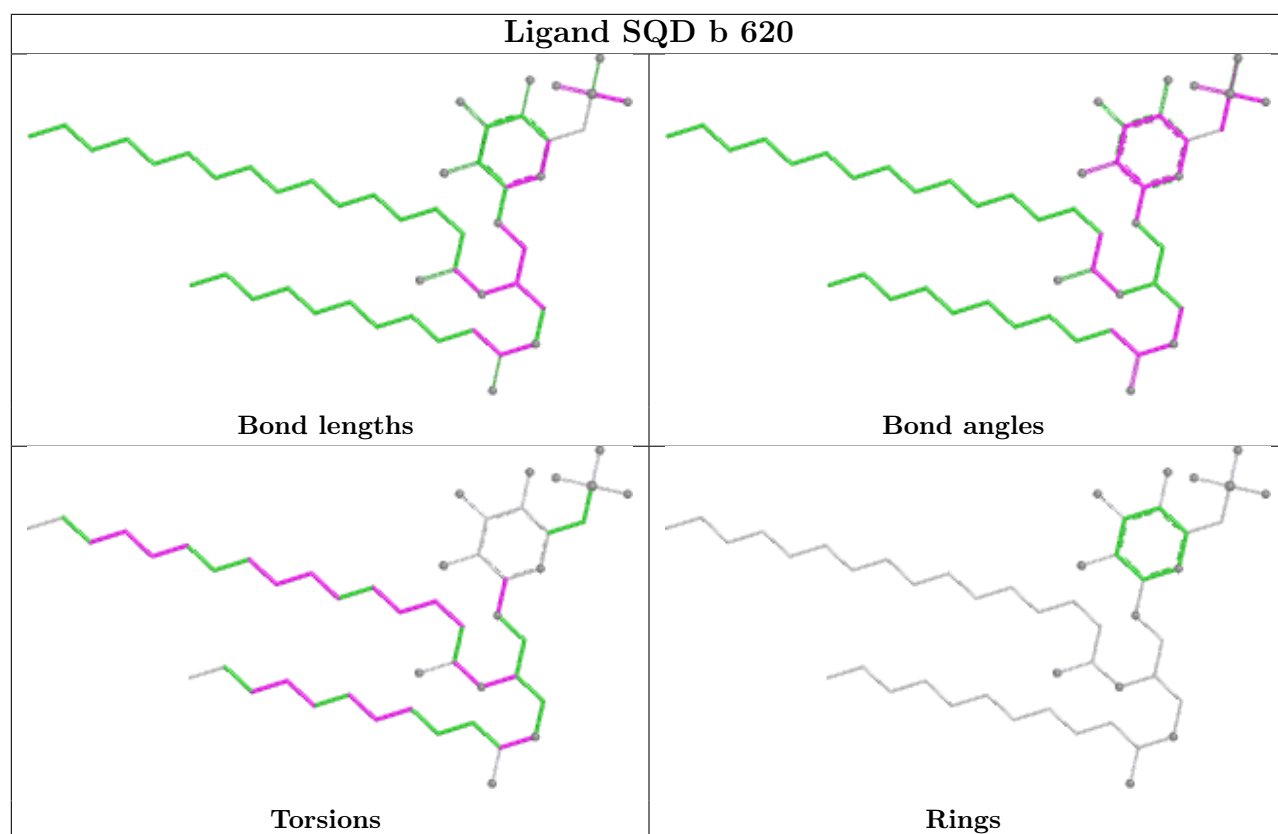


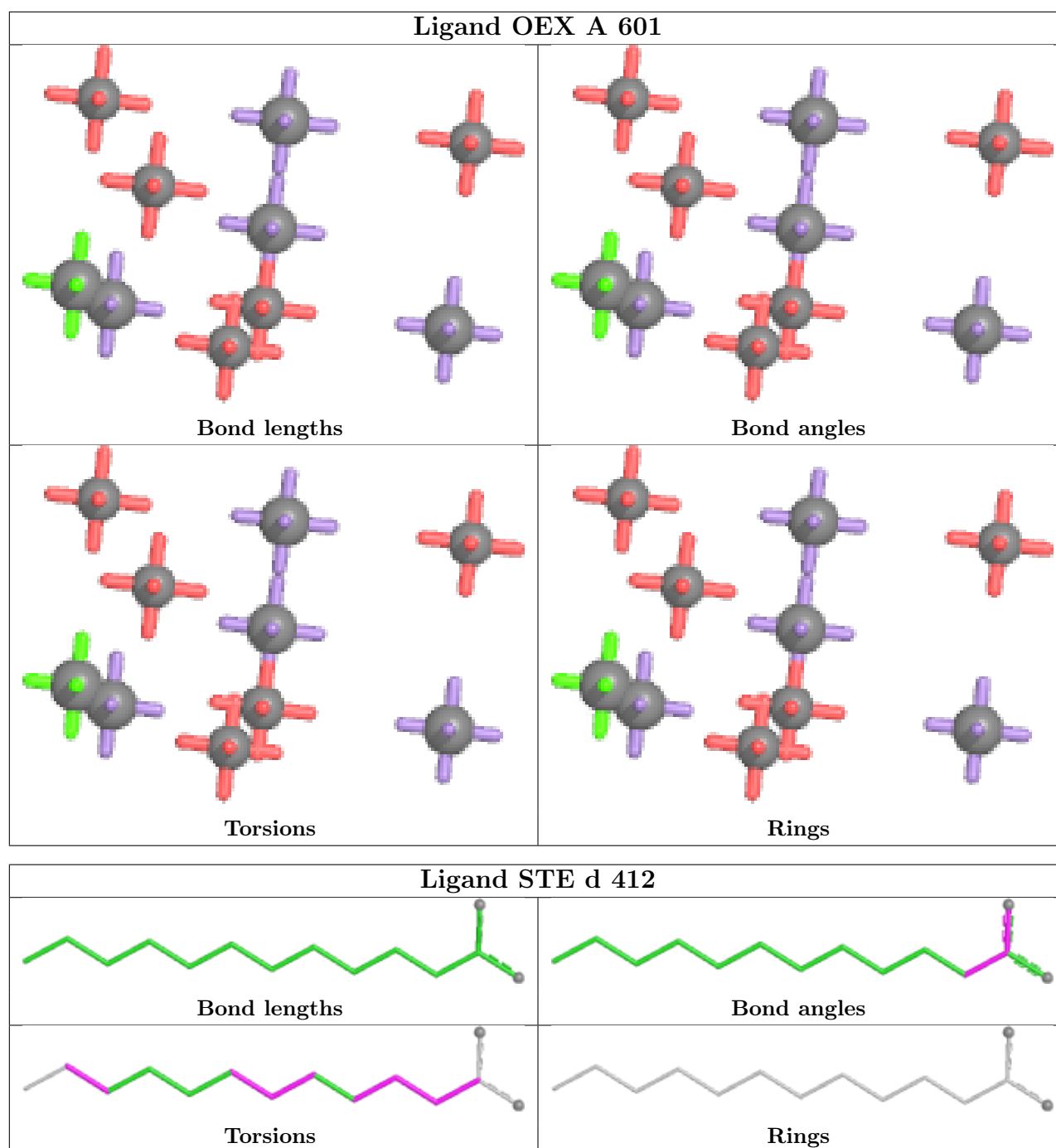


Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

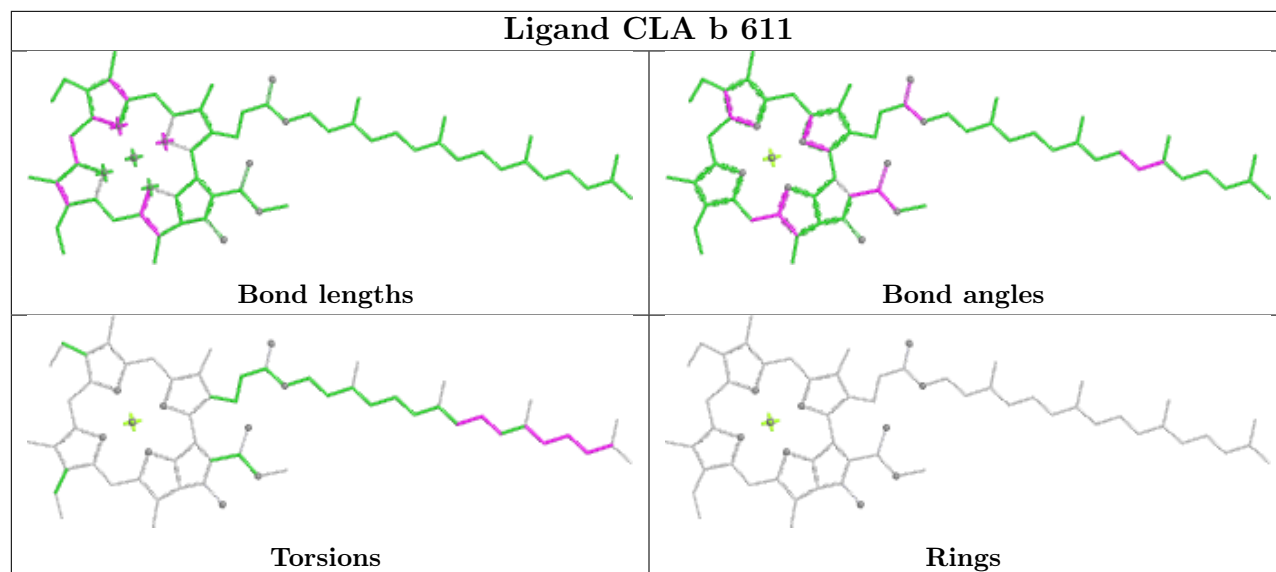
Ligand STE m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG a 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

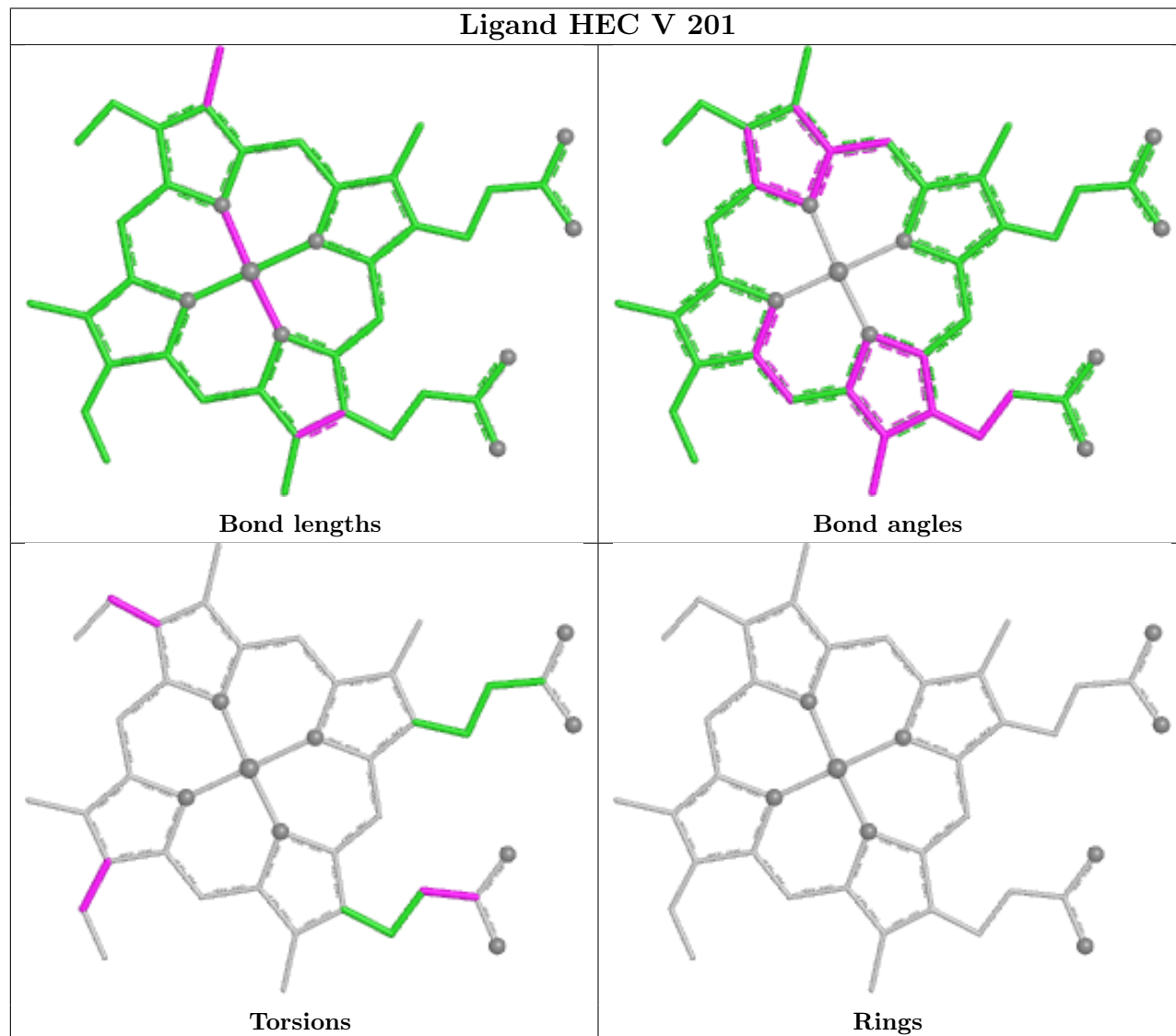


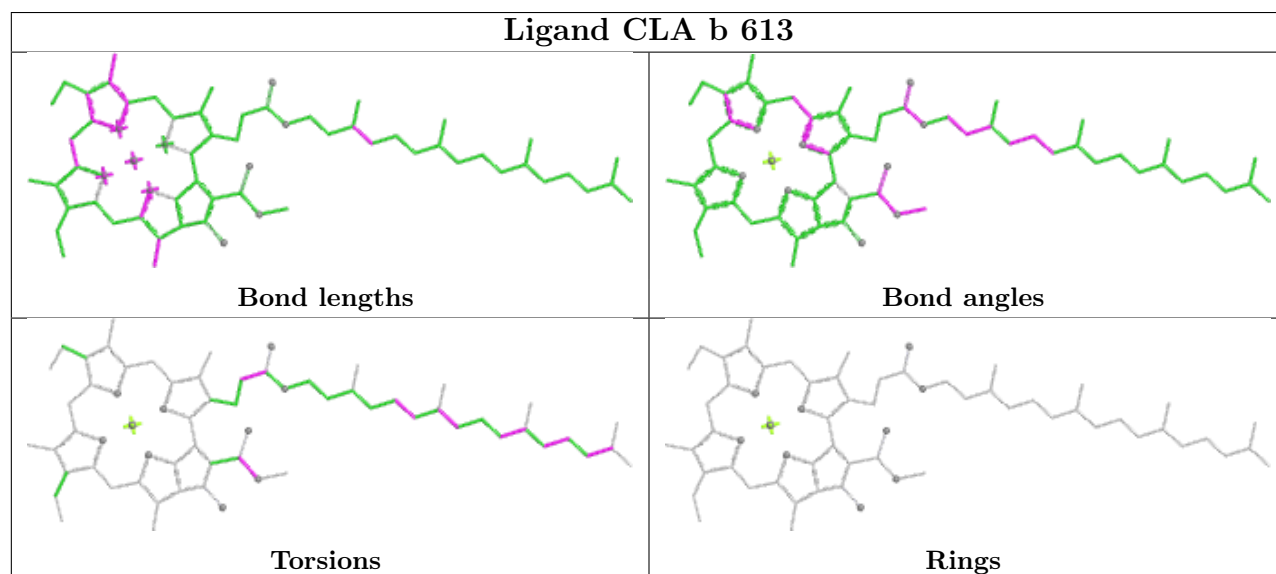
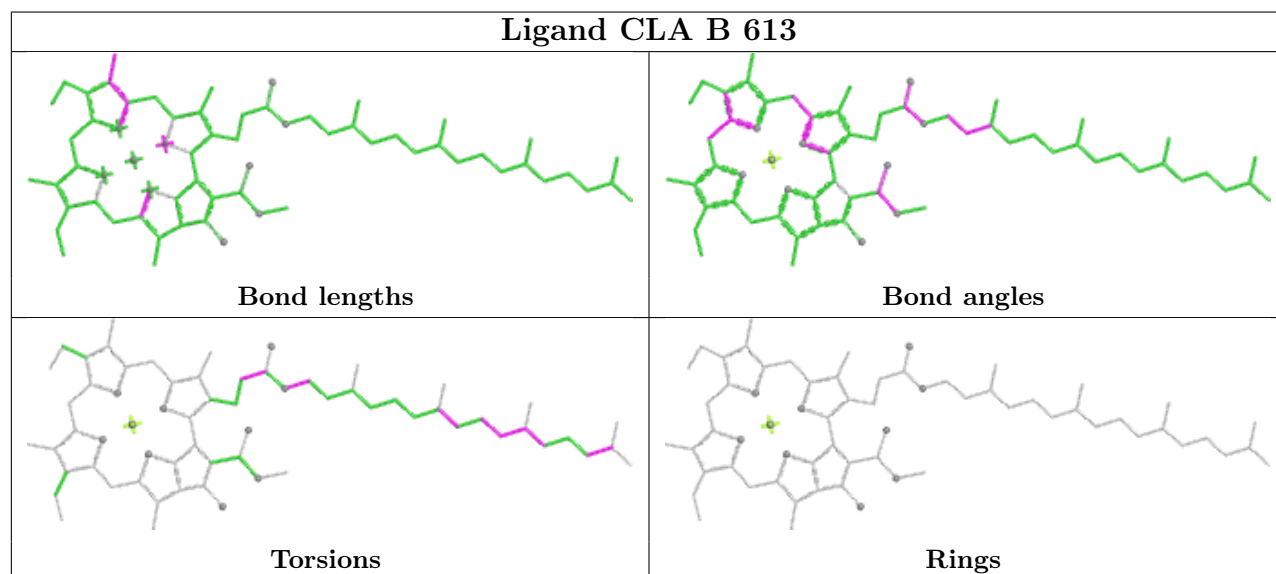
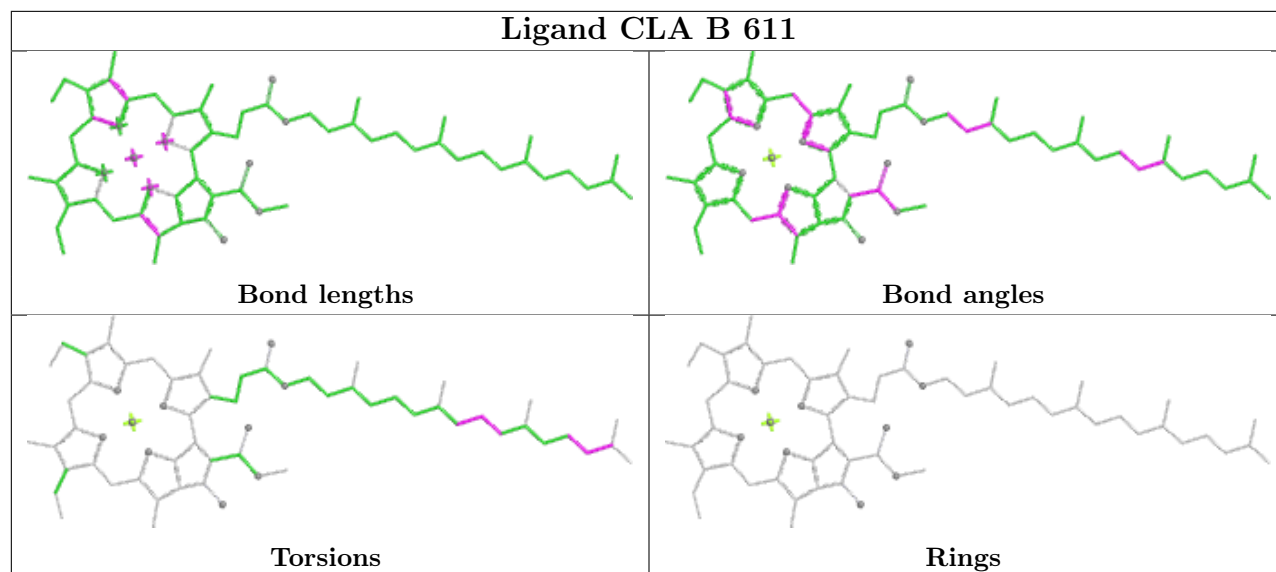


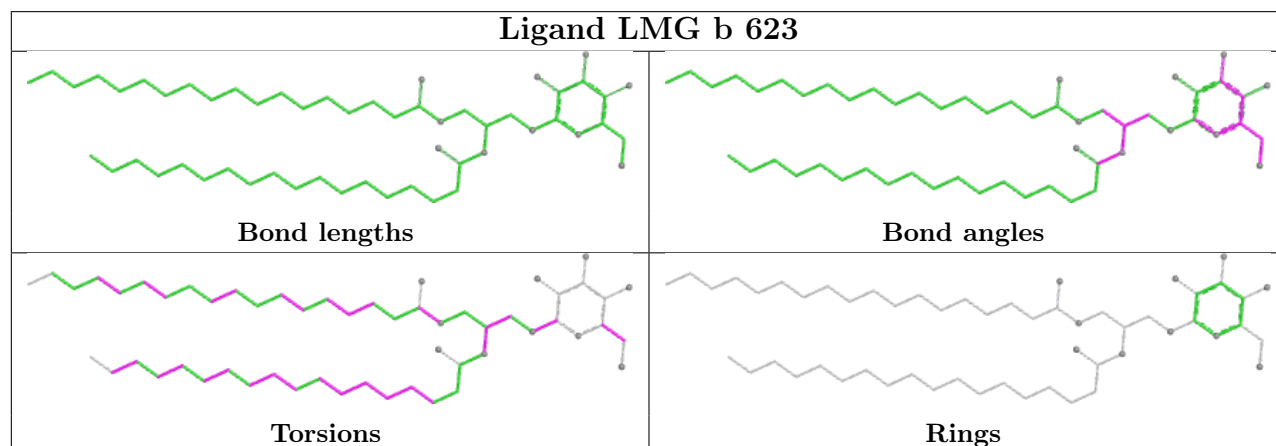
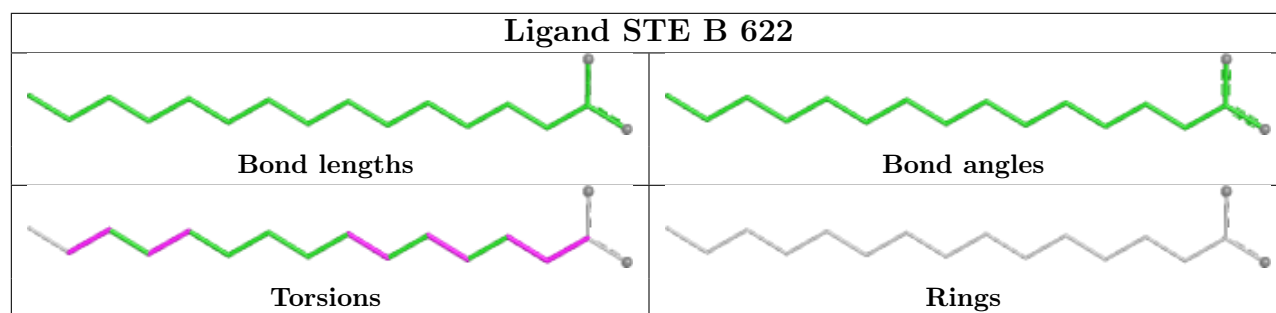
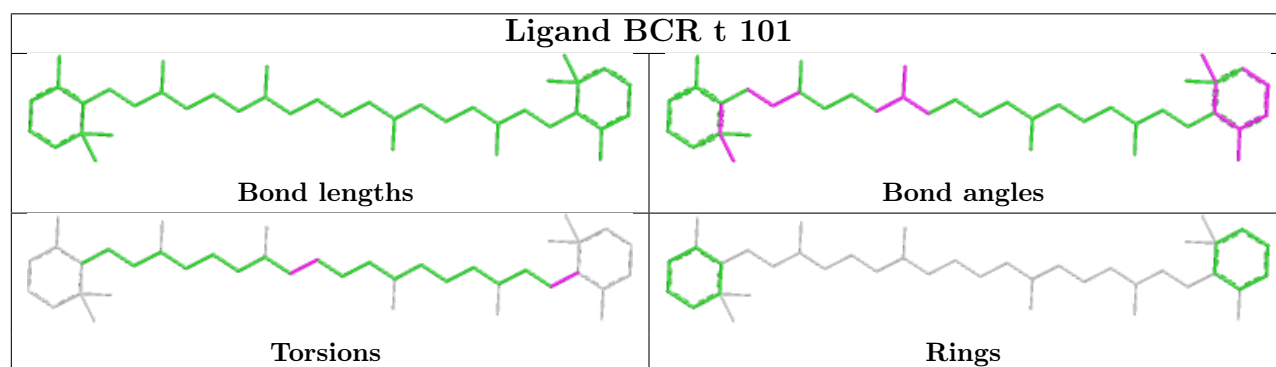
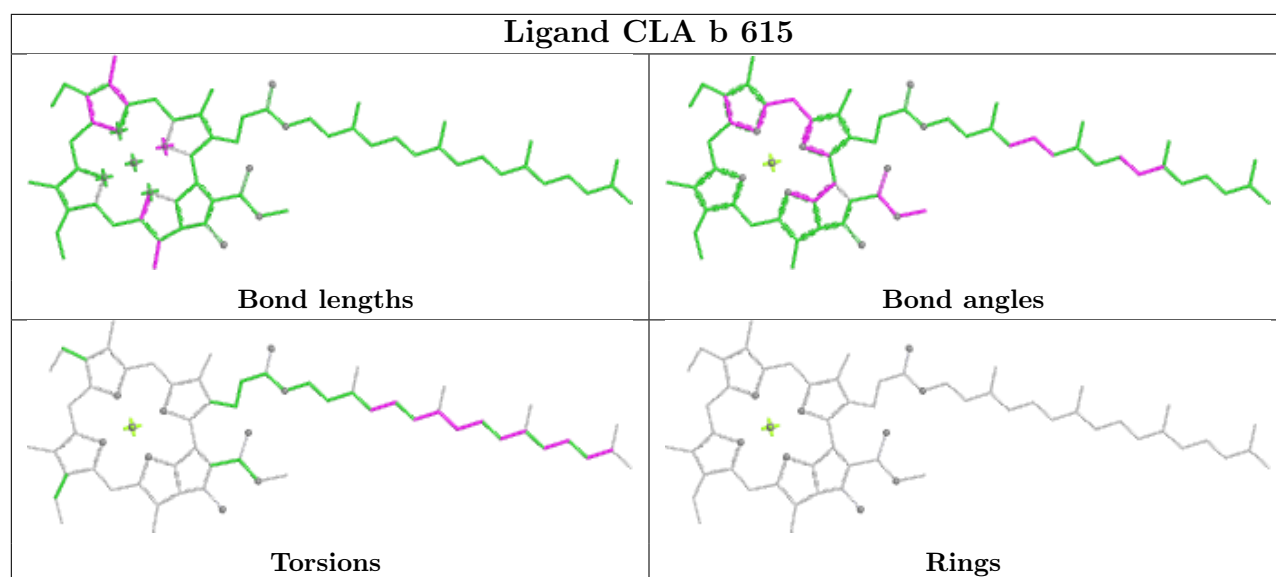
Ligand CLA b 611

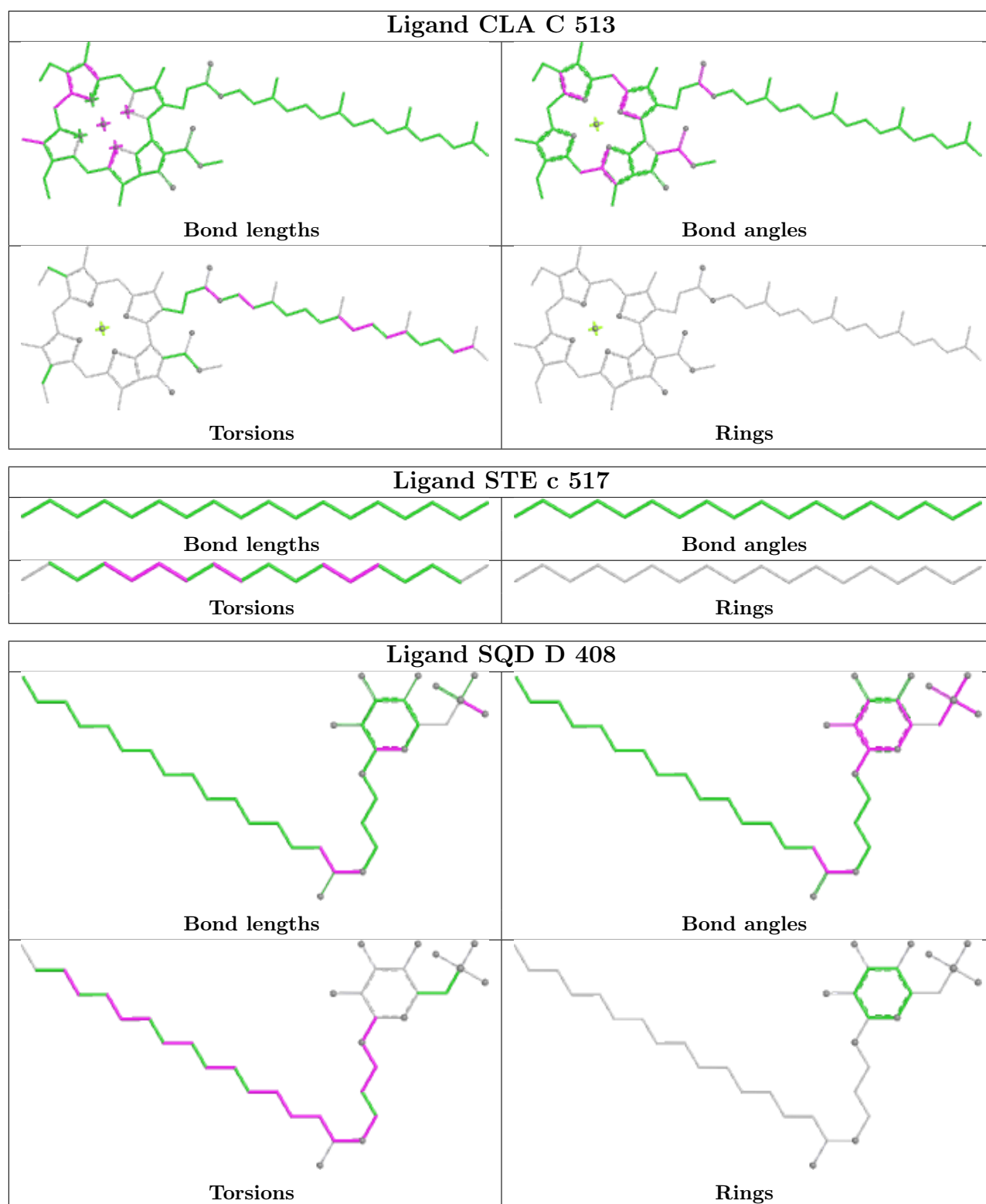


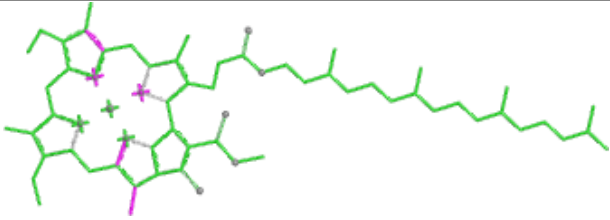
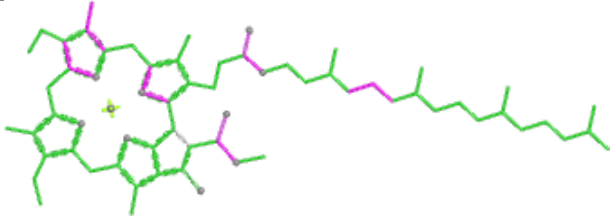
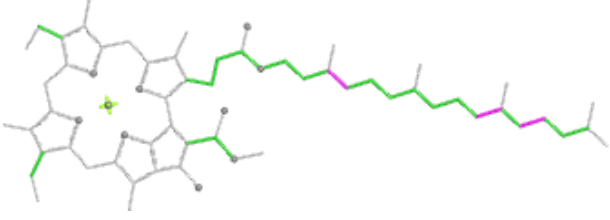
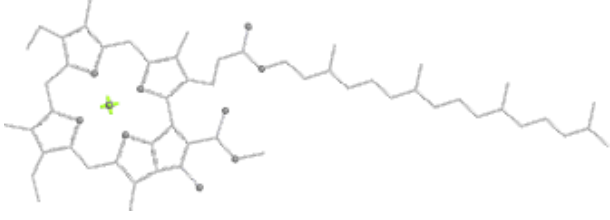
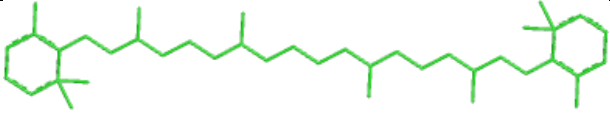
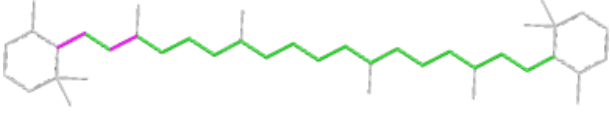
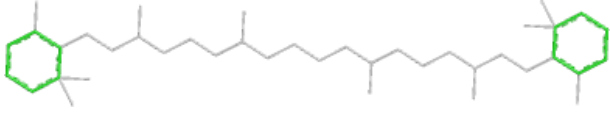
Ligand HEC V 201

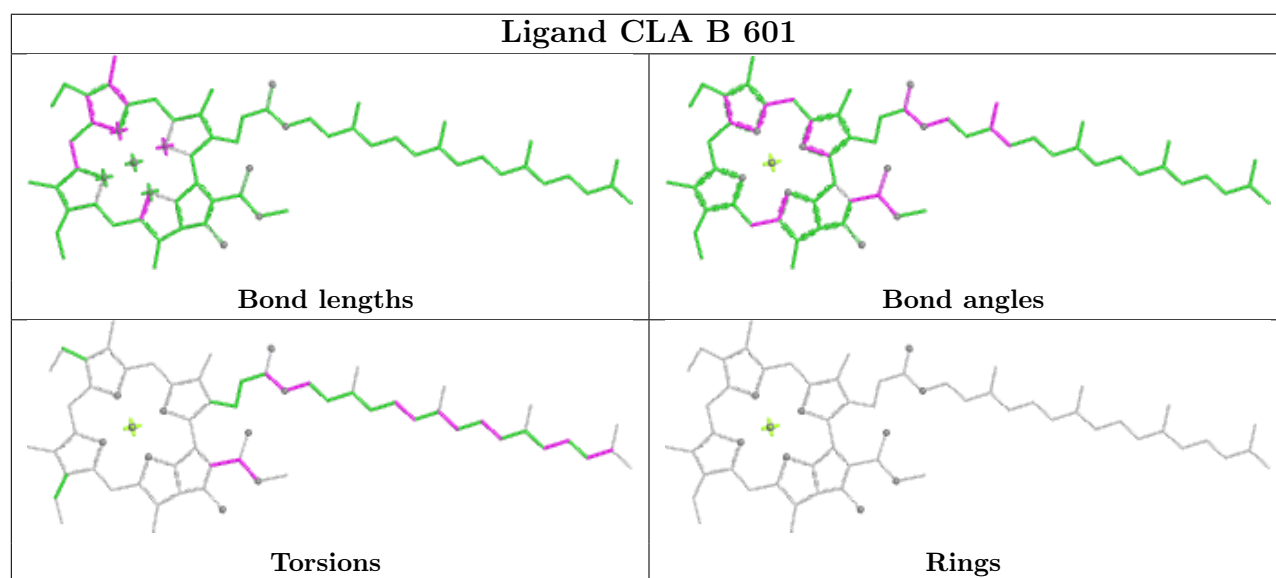
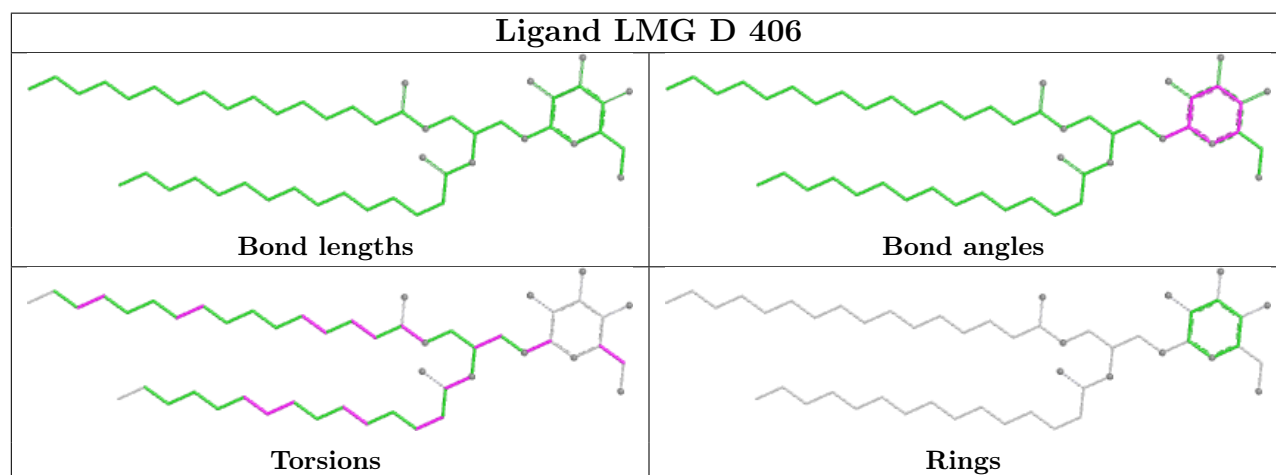
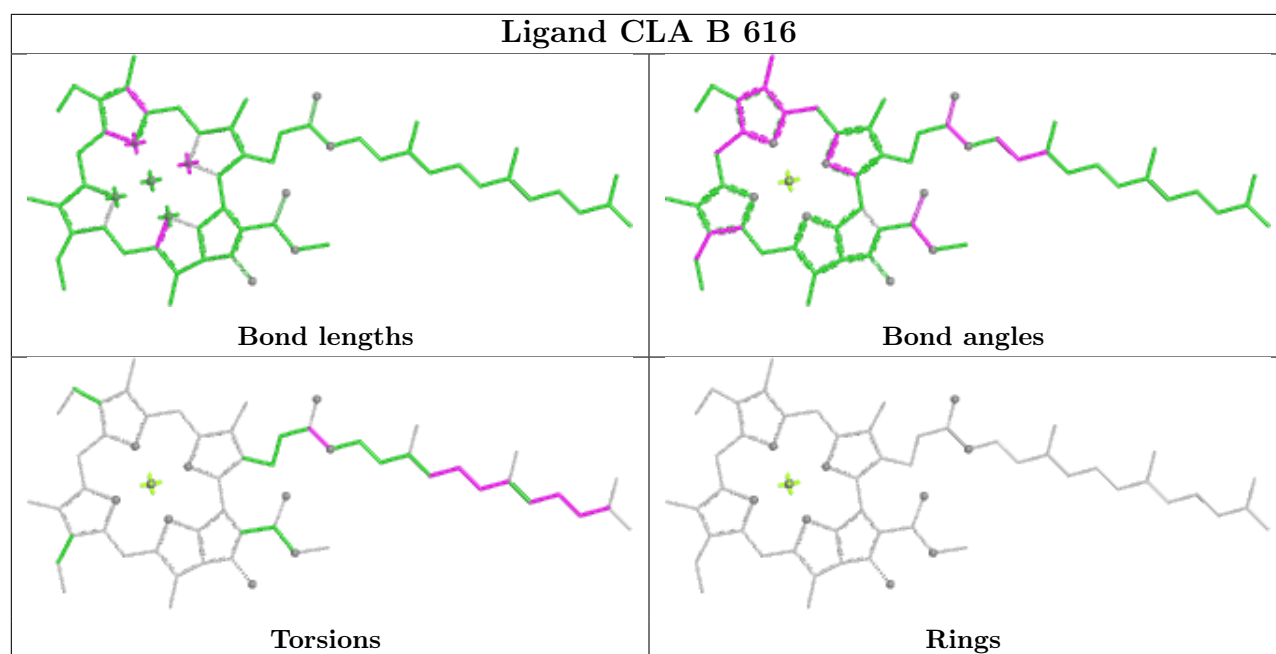


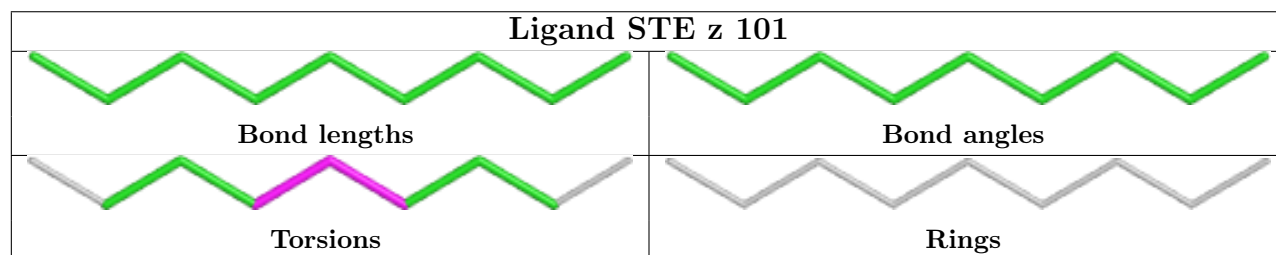
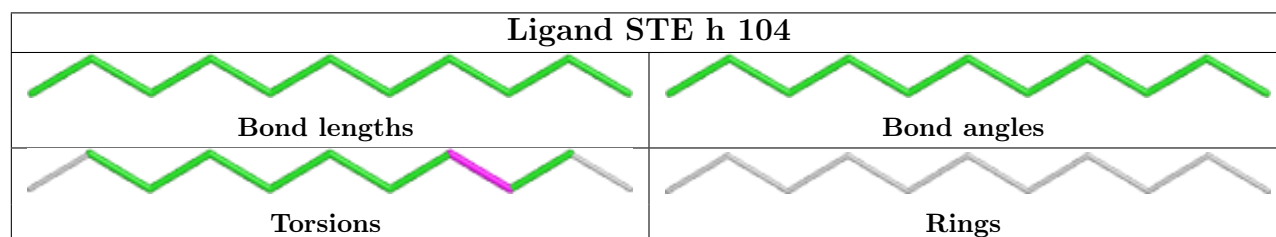
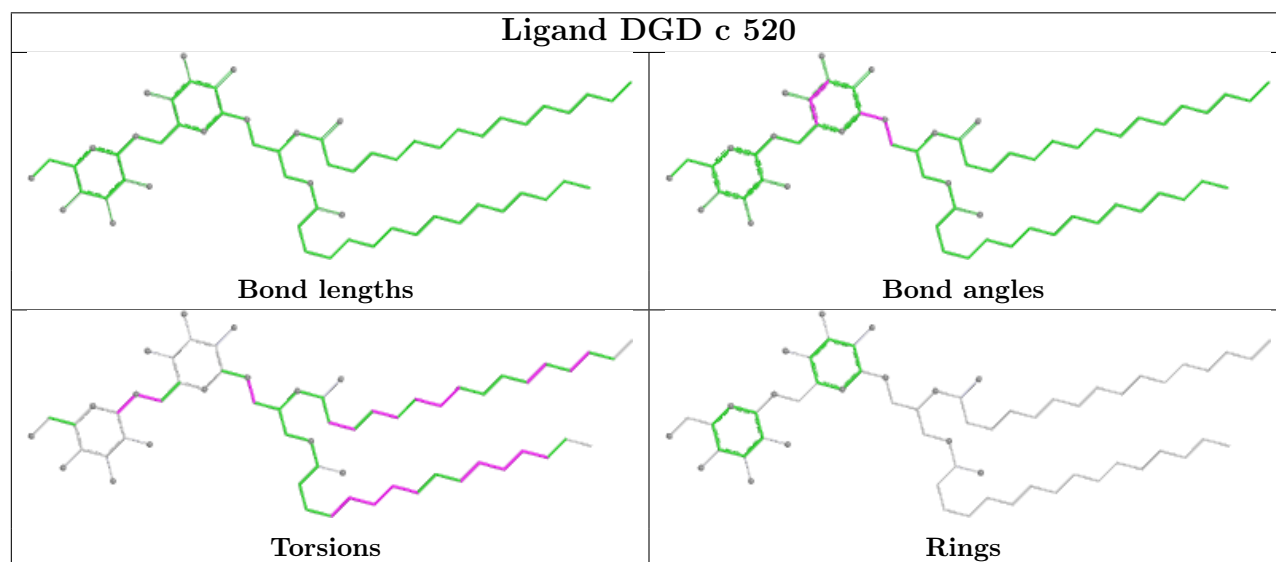
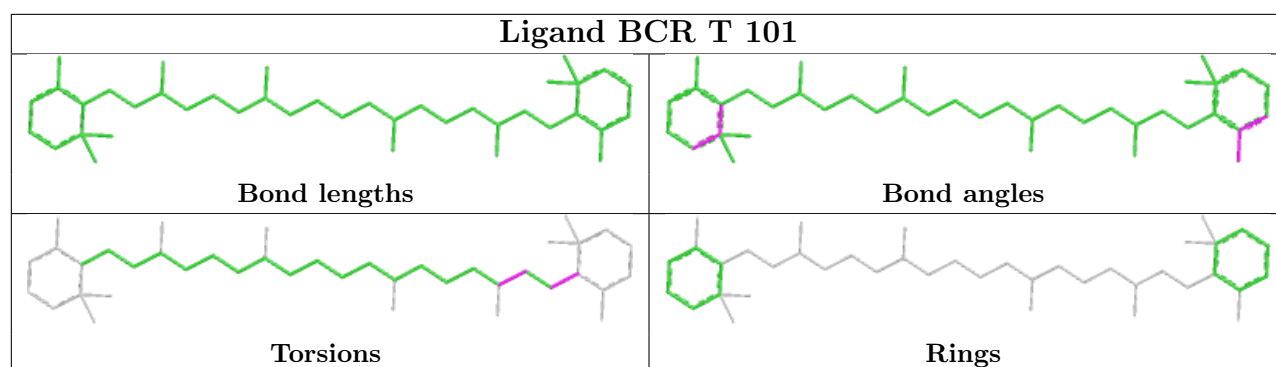


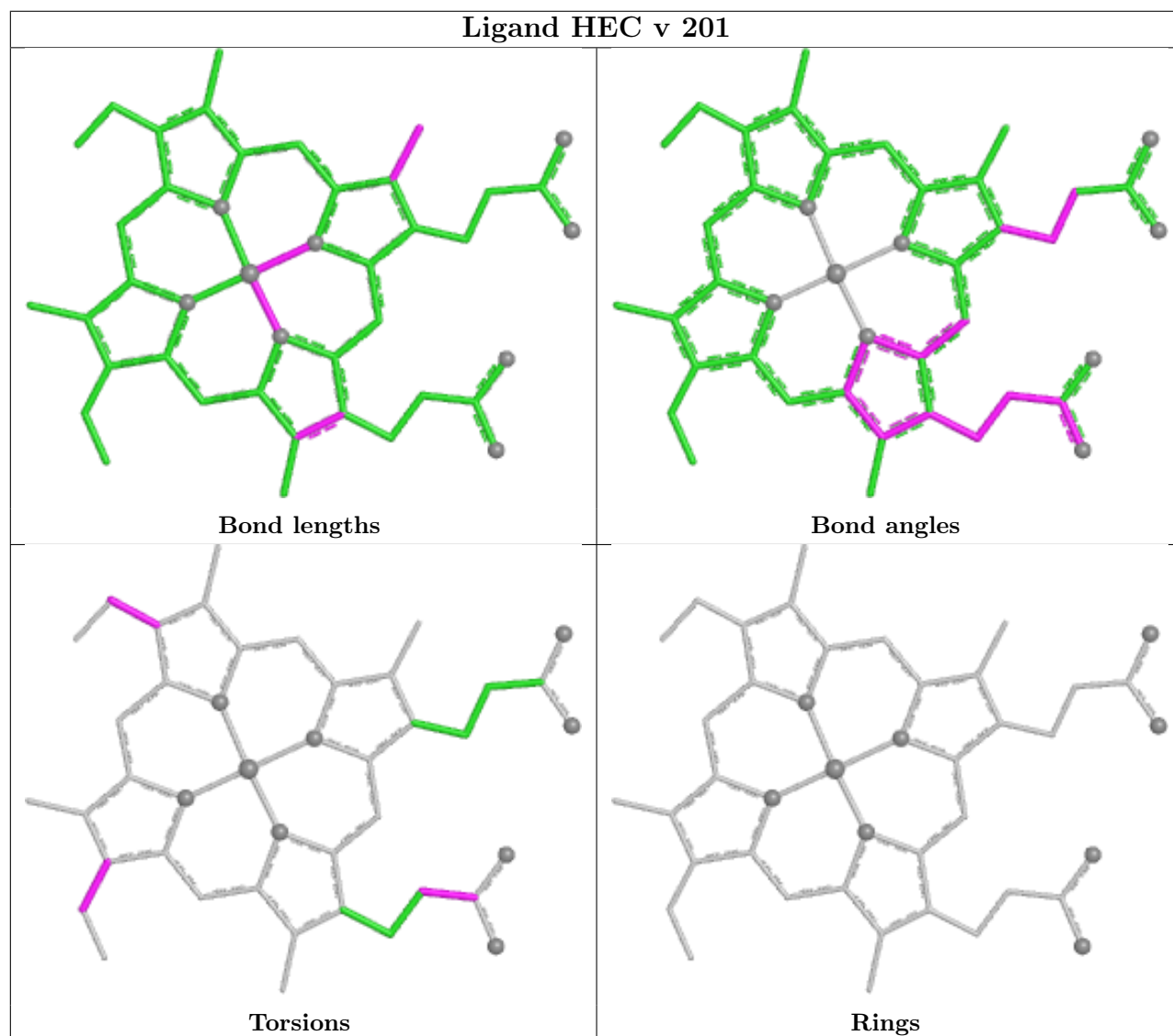
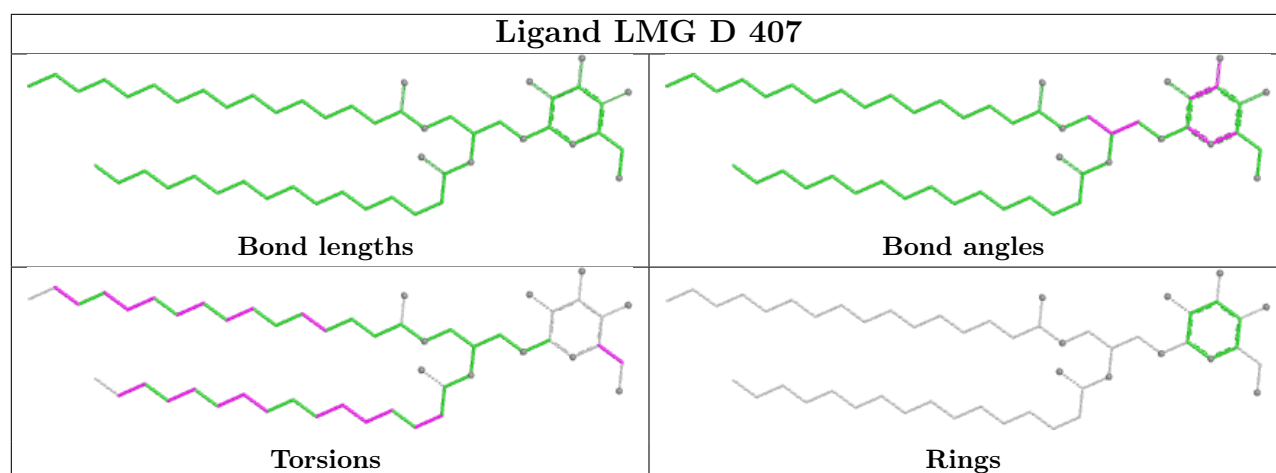


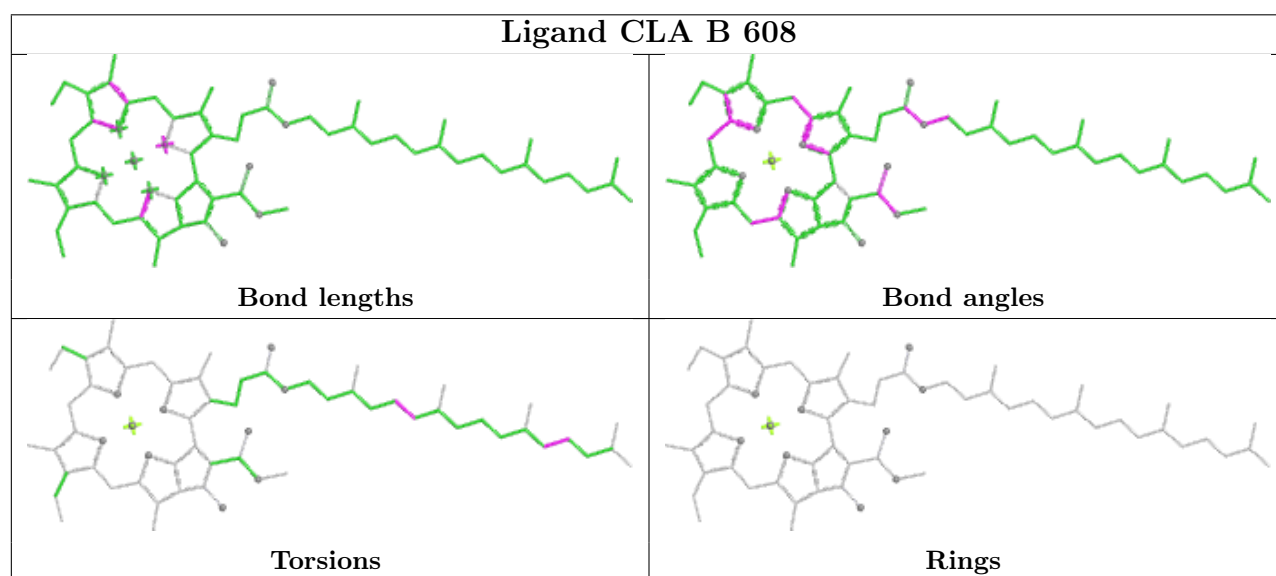
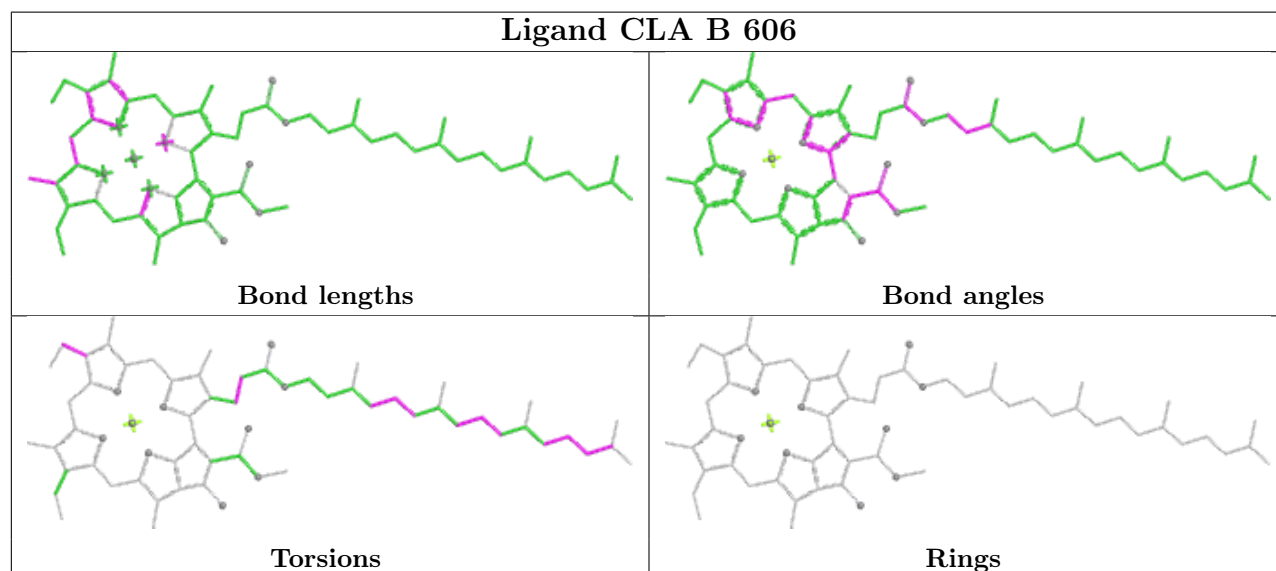
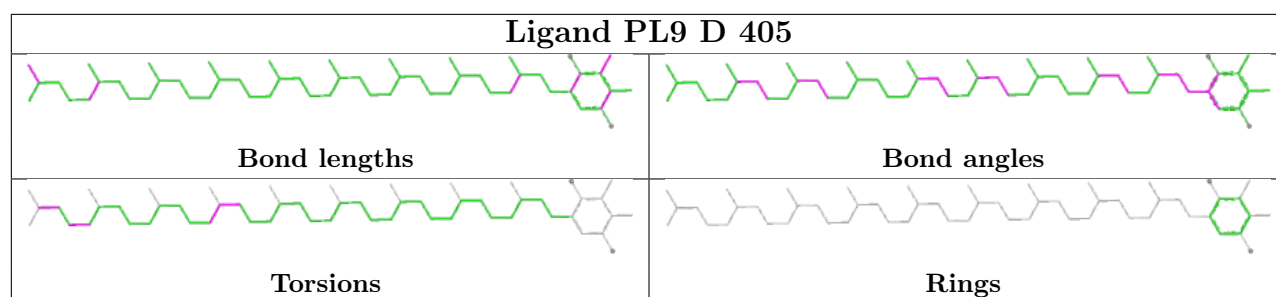


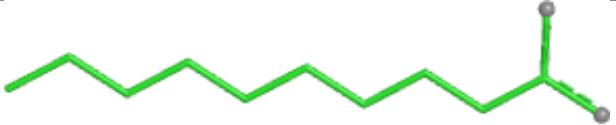
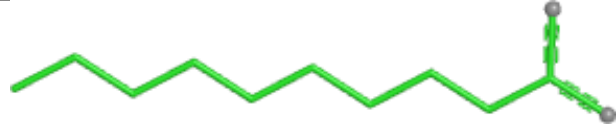
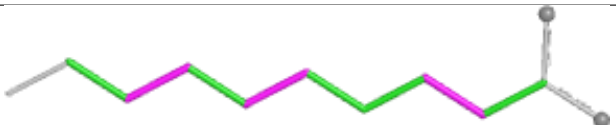
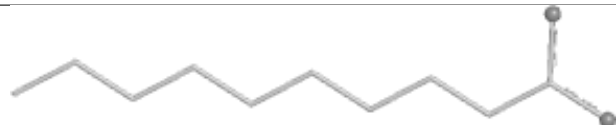
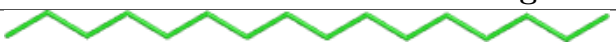
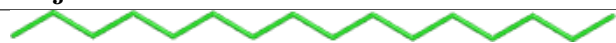
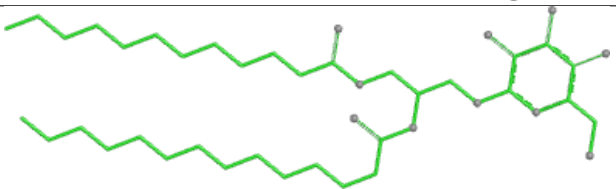
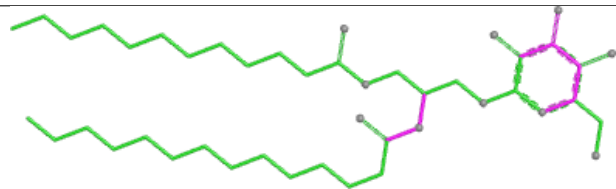
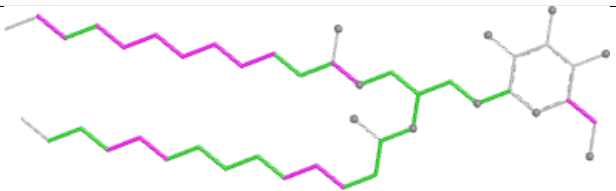
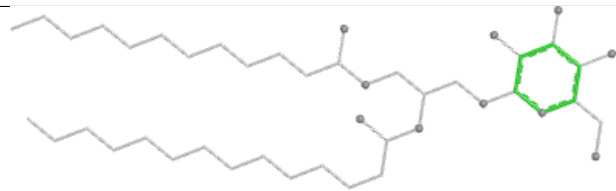
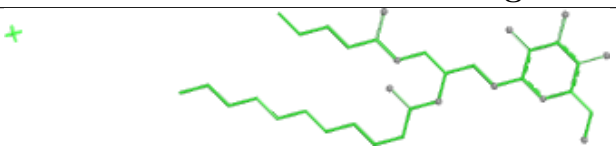
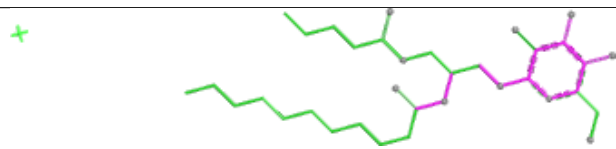
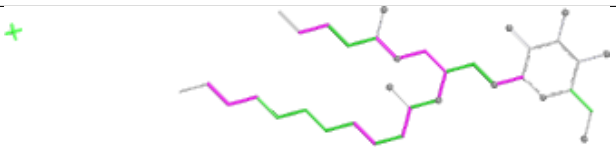
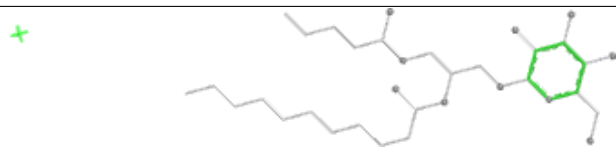
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

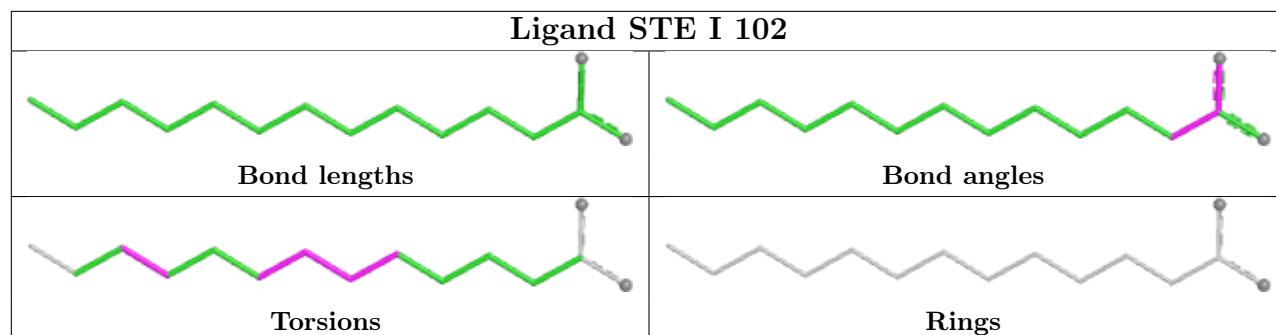
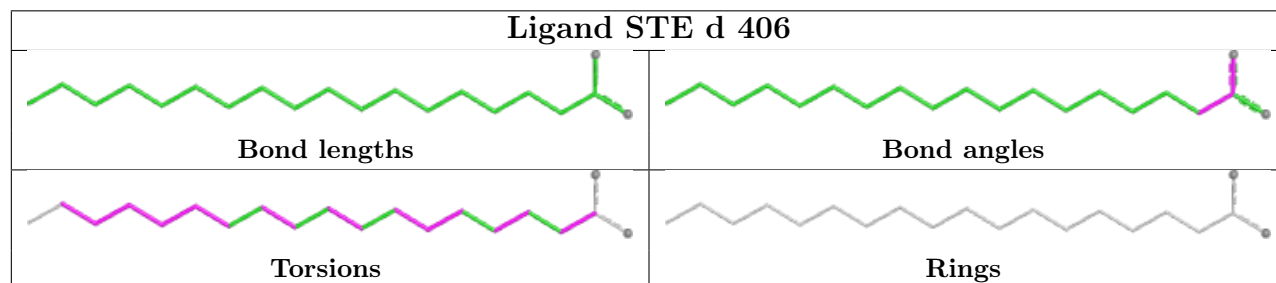
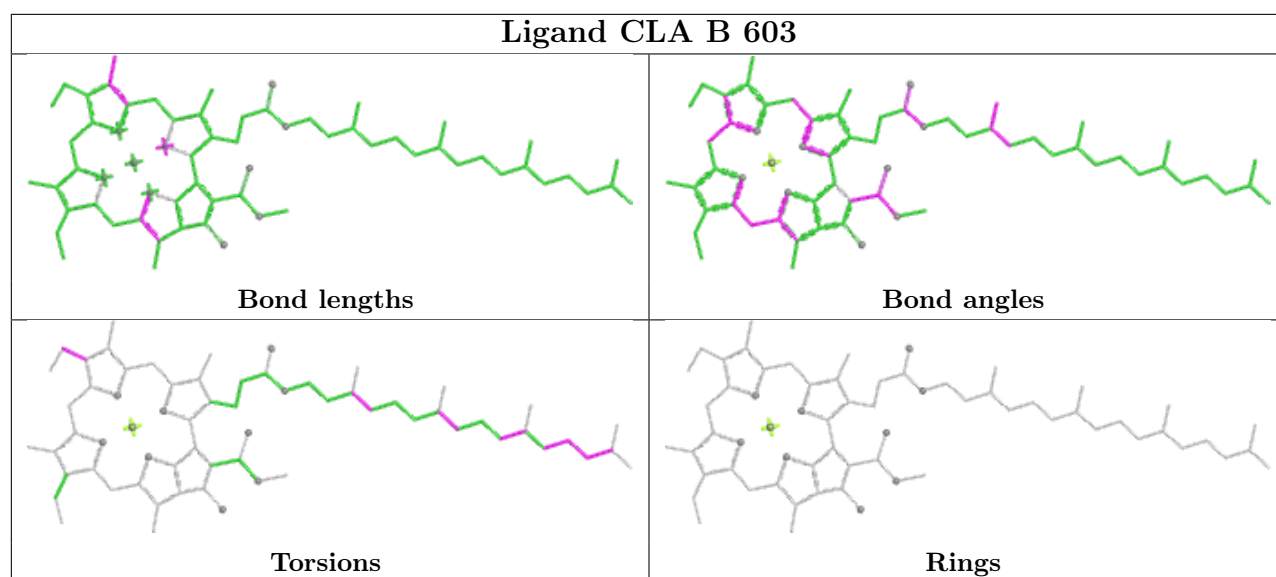


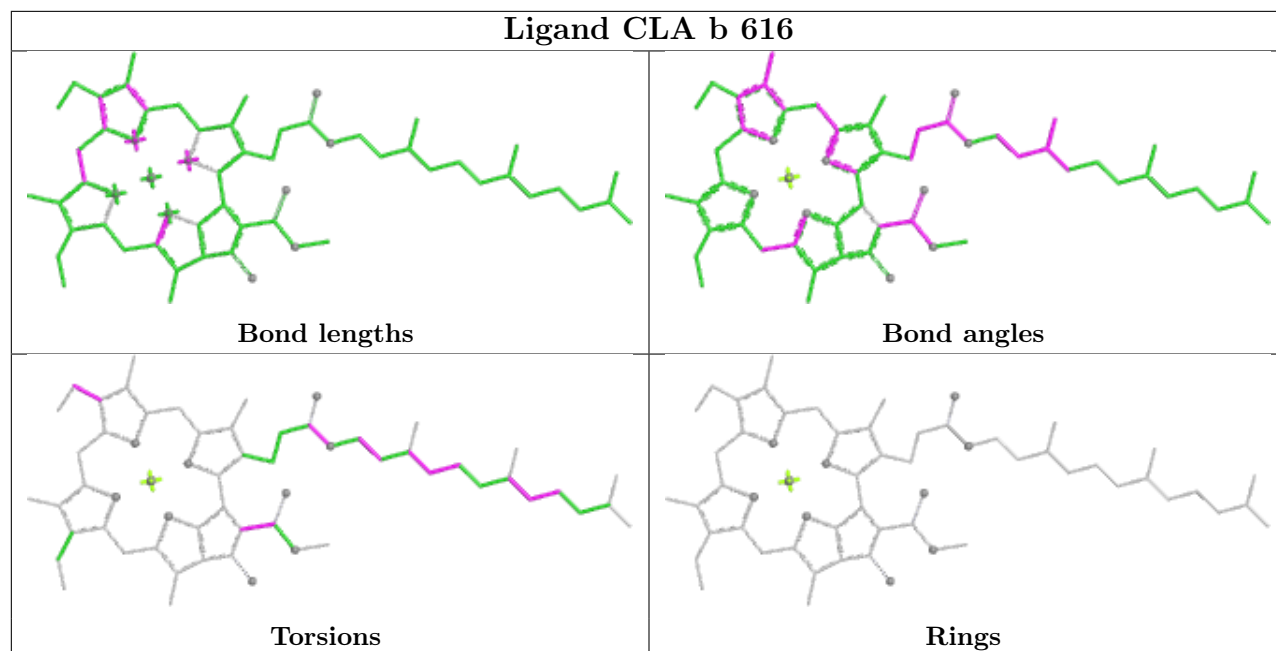


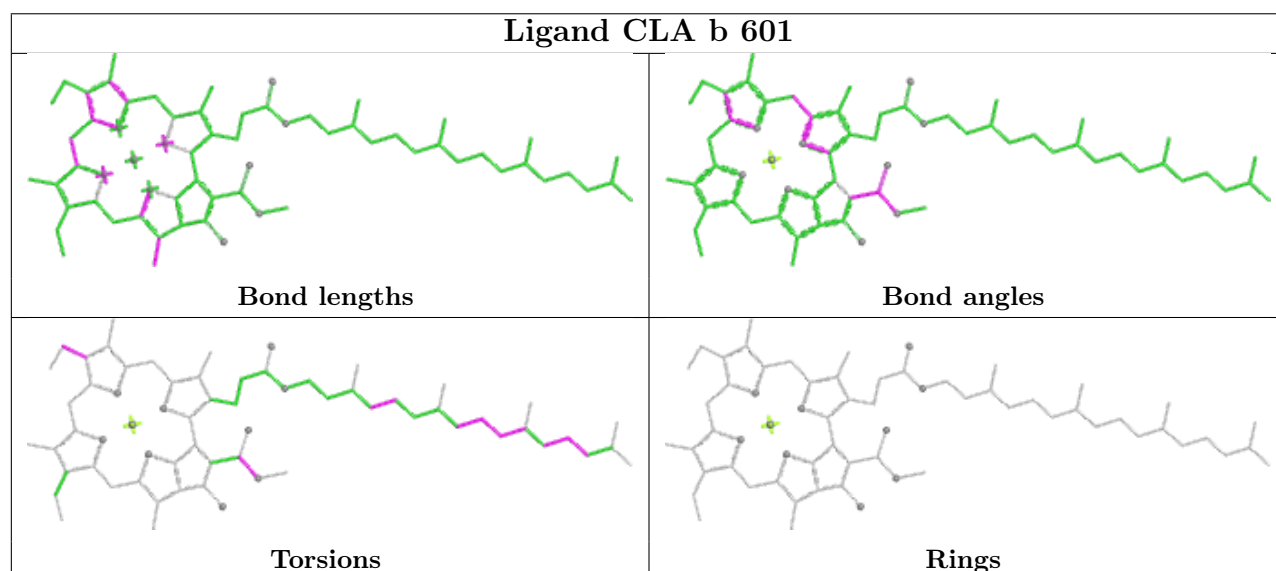
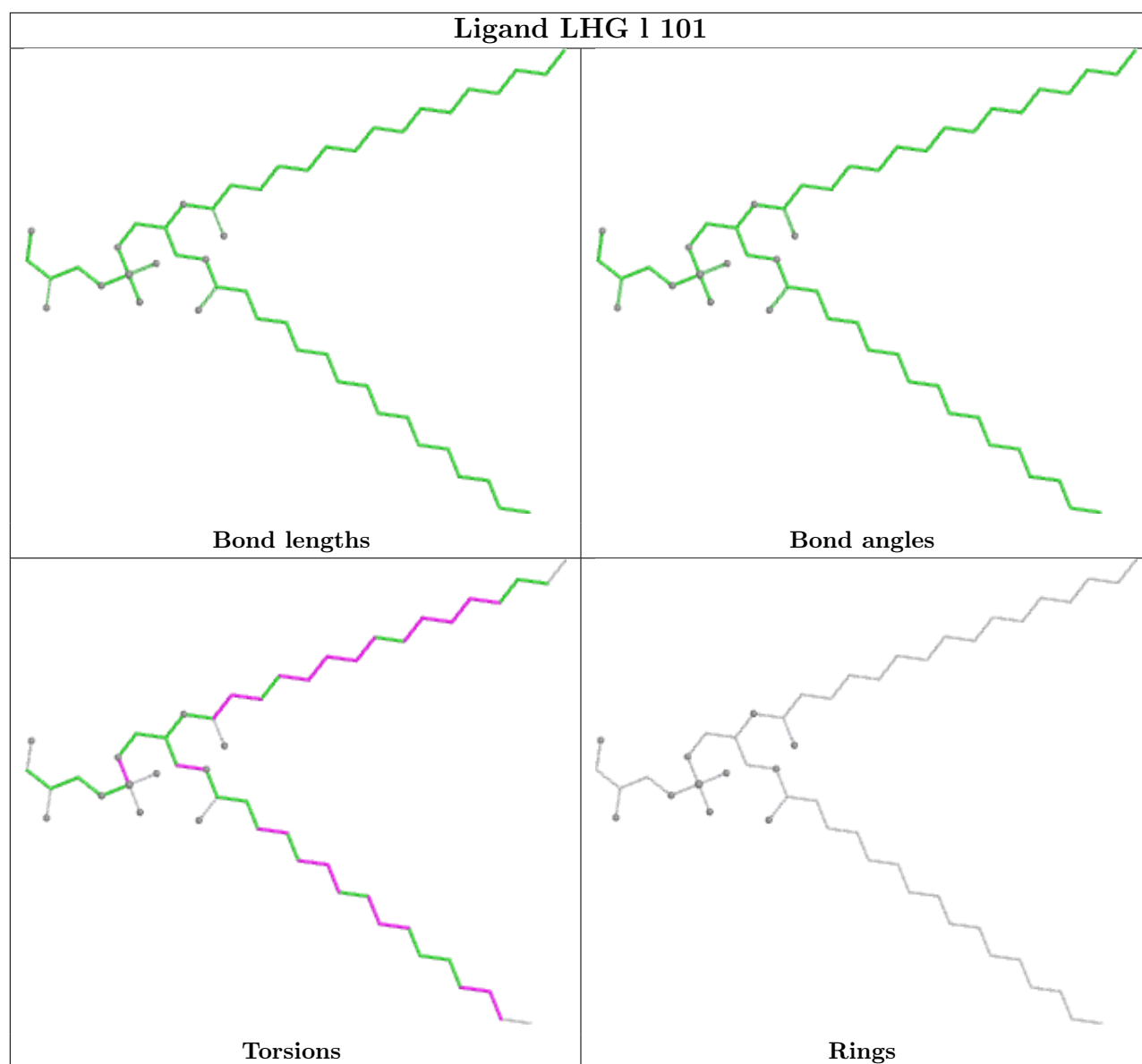


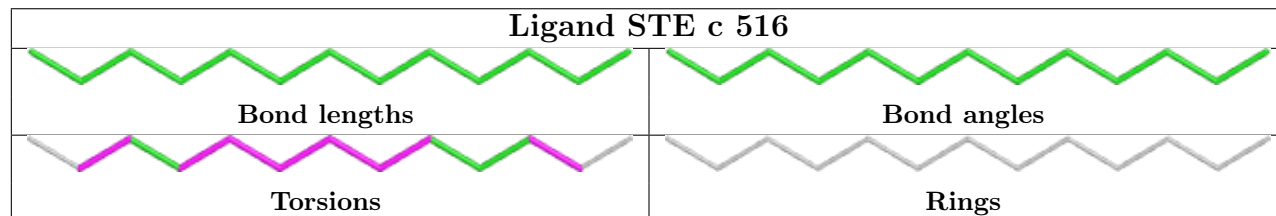
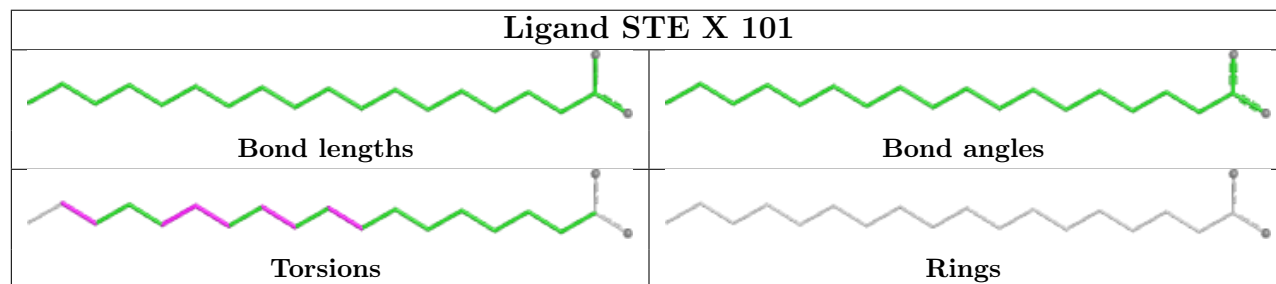
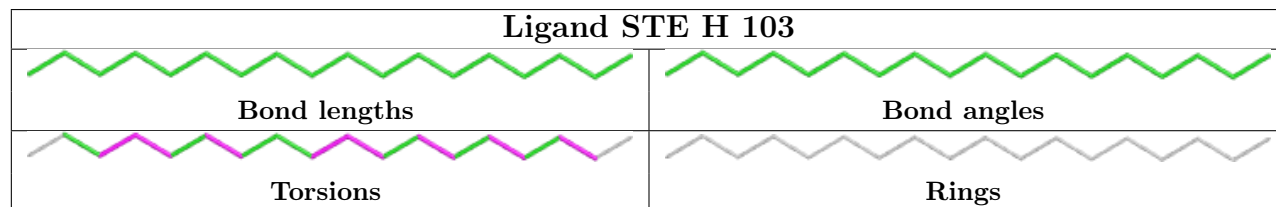
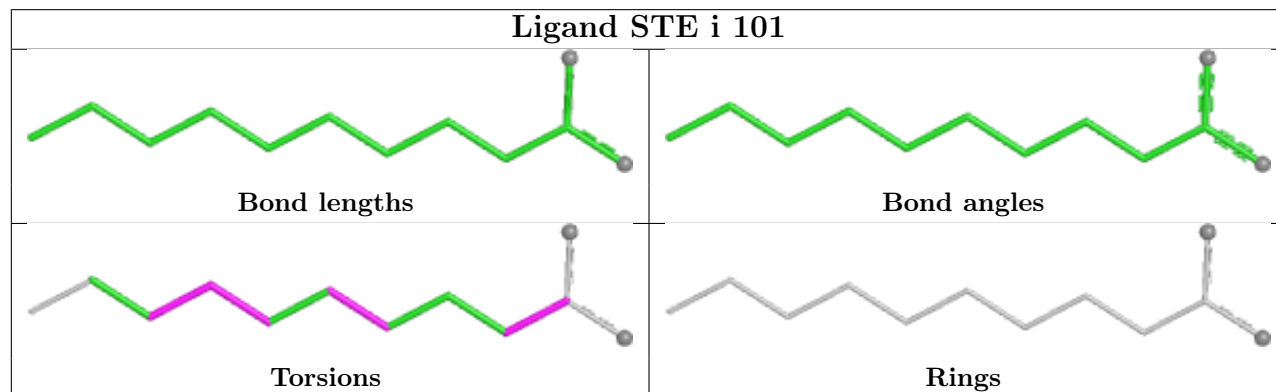
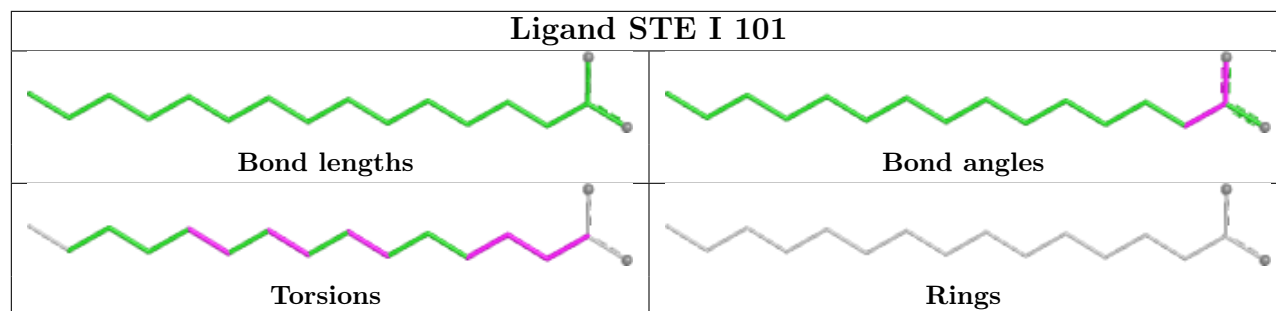


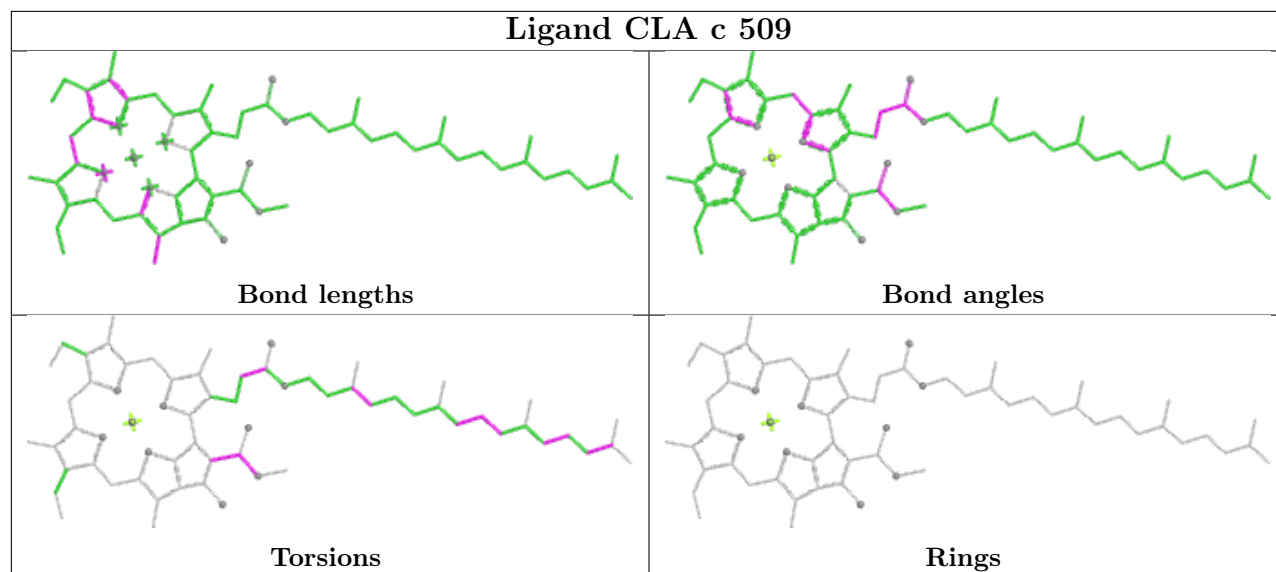
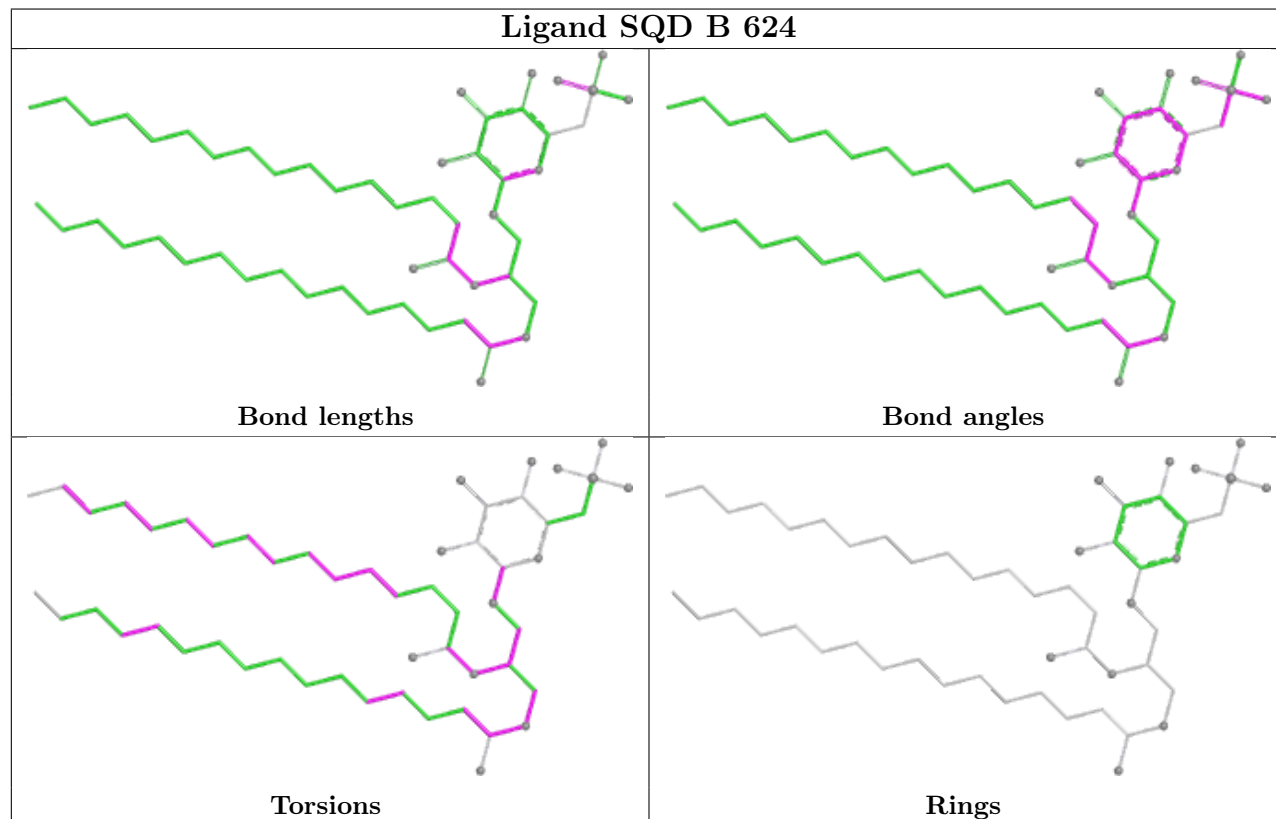
Ligand STE a 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE j 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

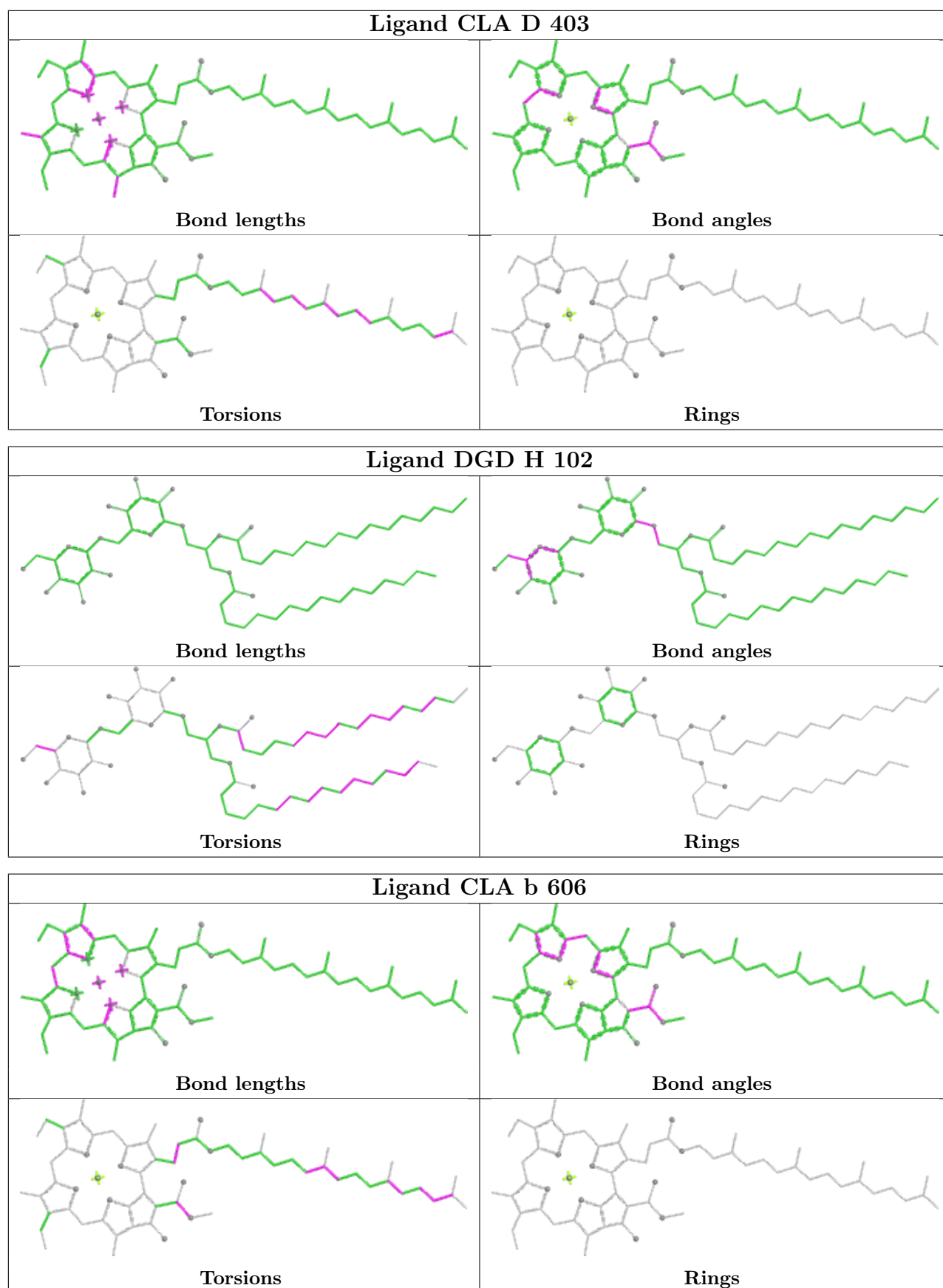


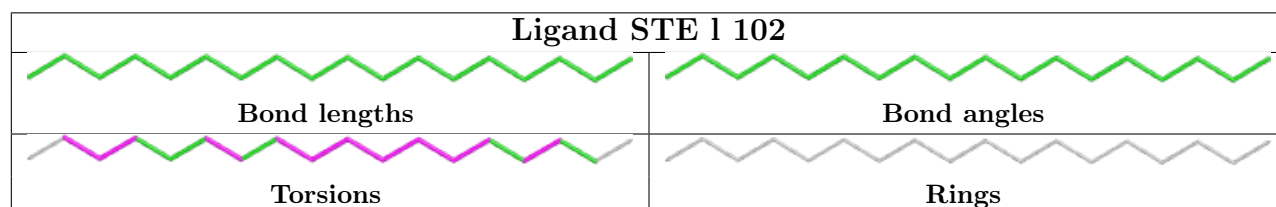
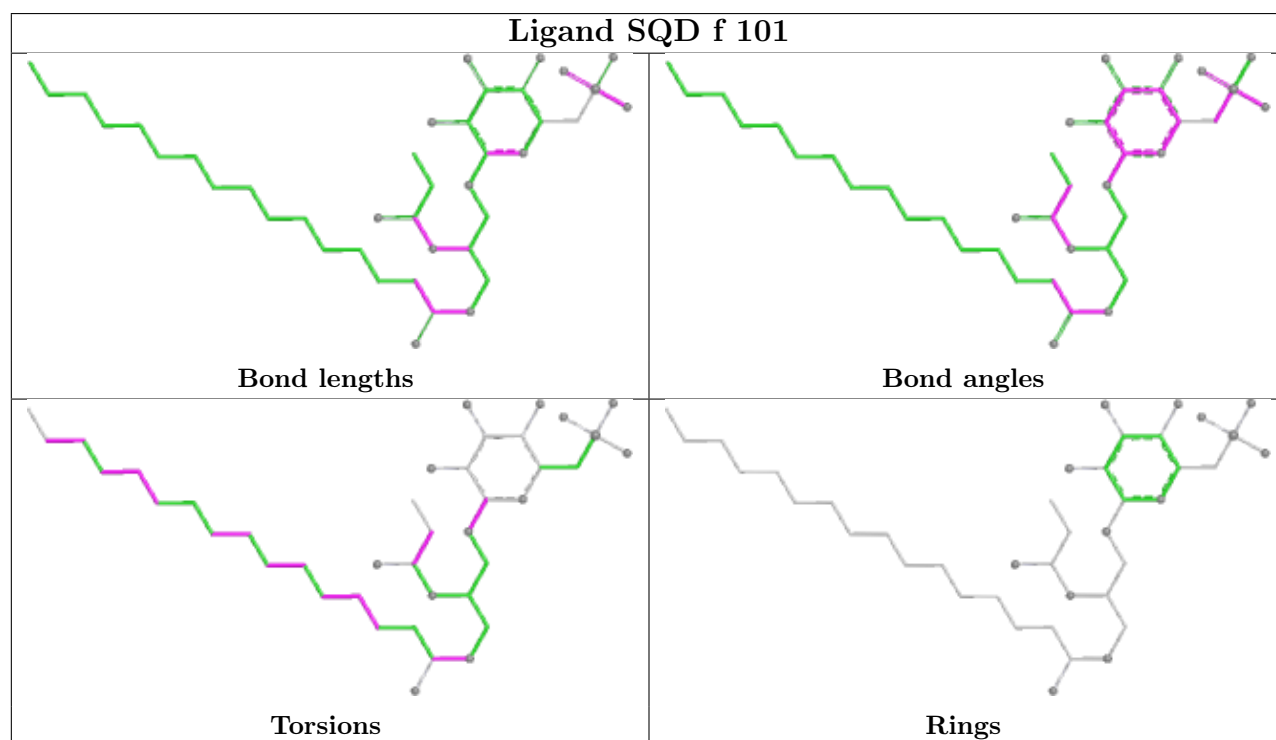
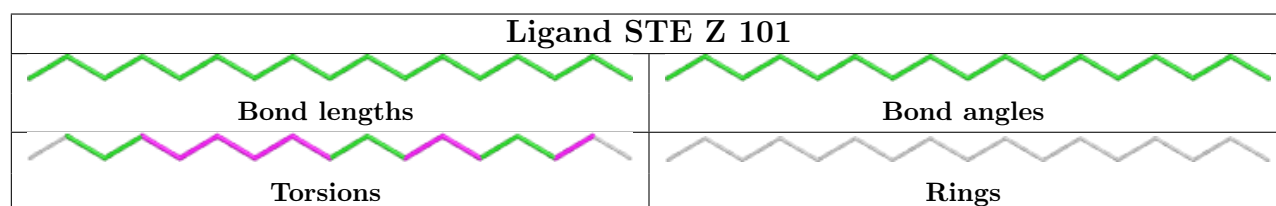
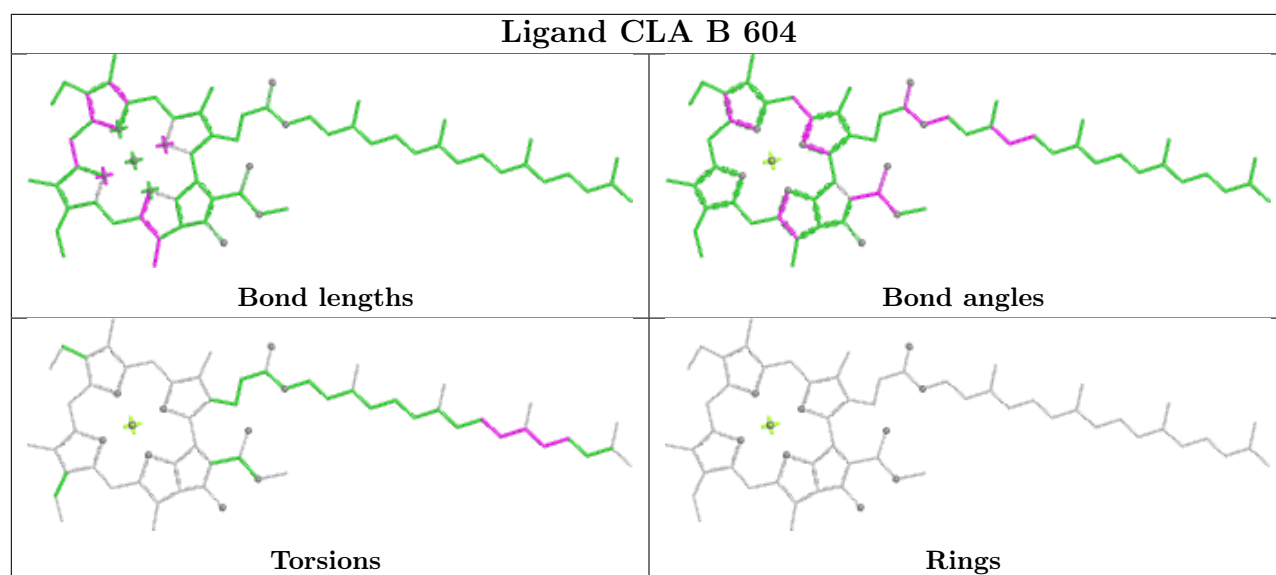


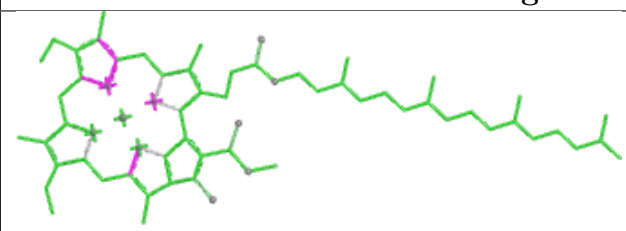
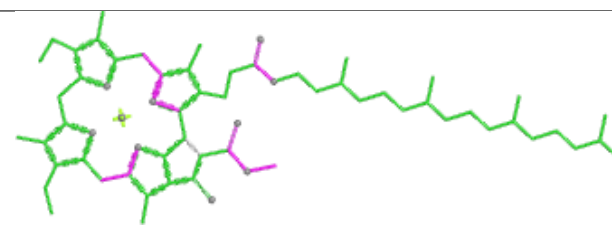
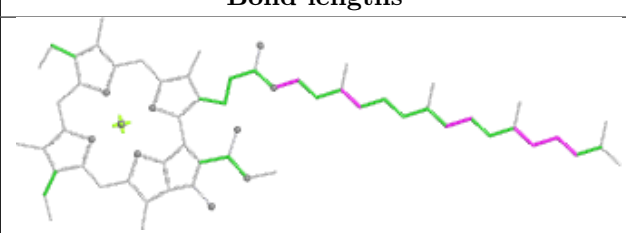
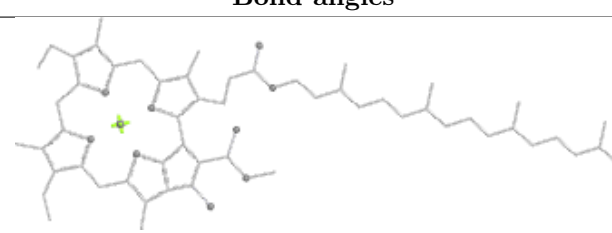




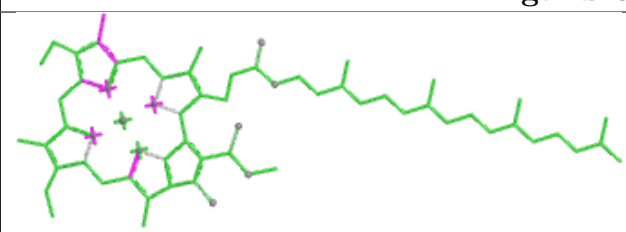
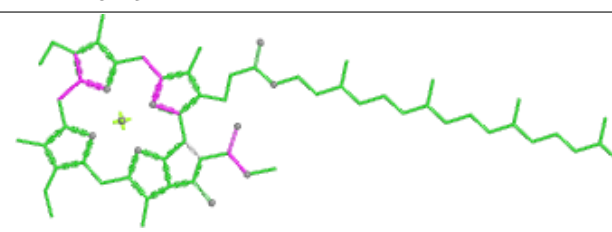
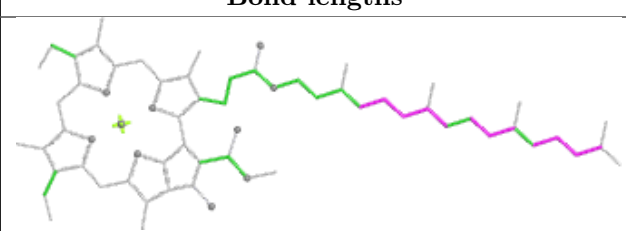
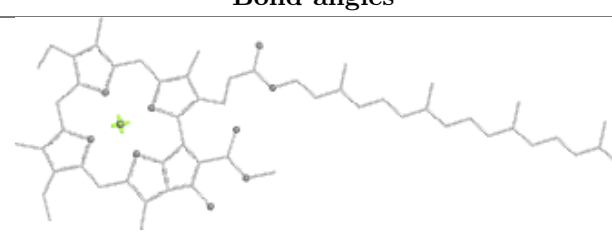
Ligand CLA c 509**Ligand SQD B 624**

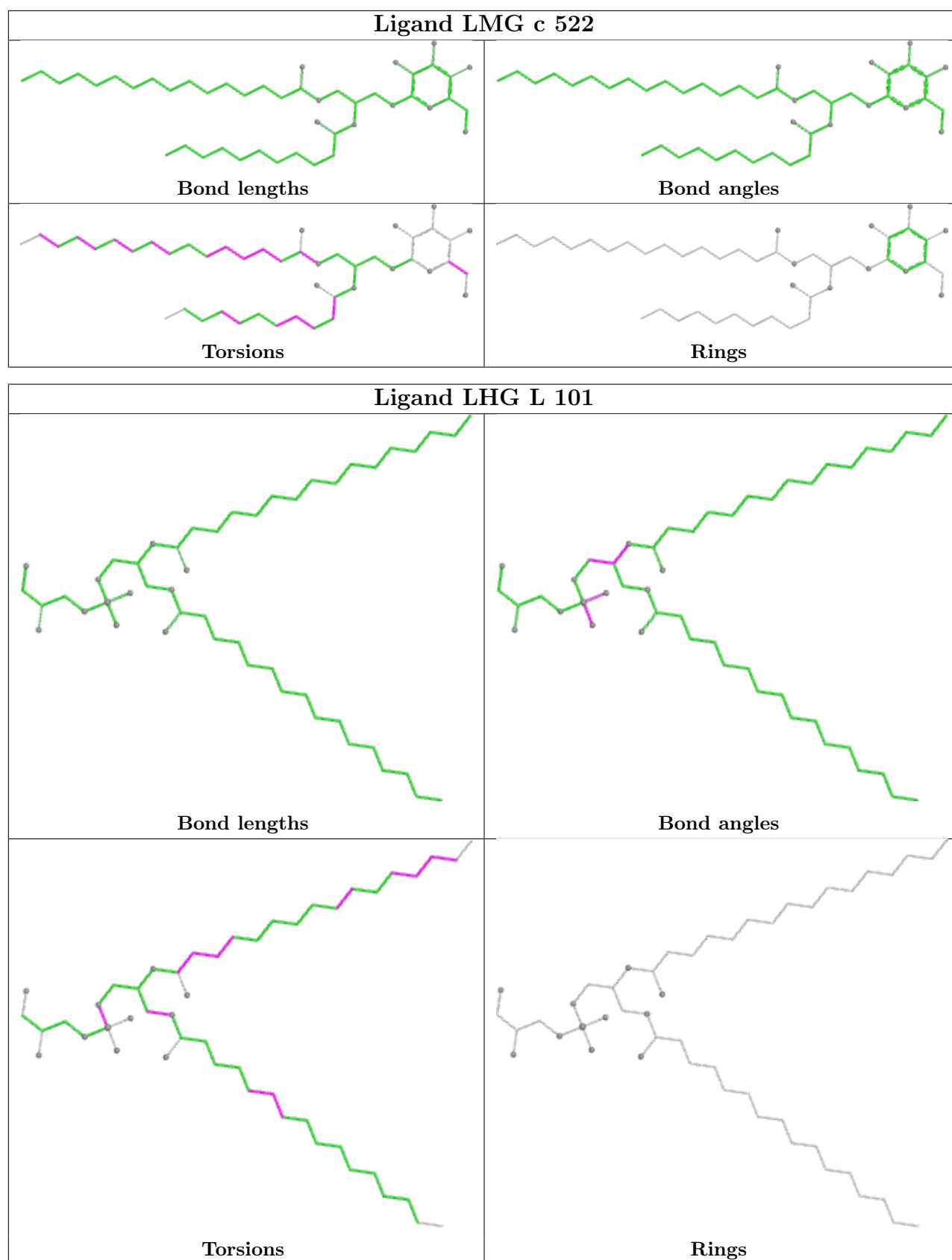


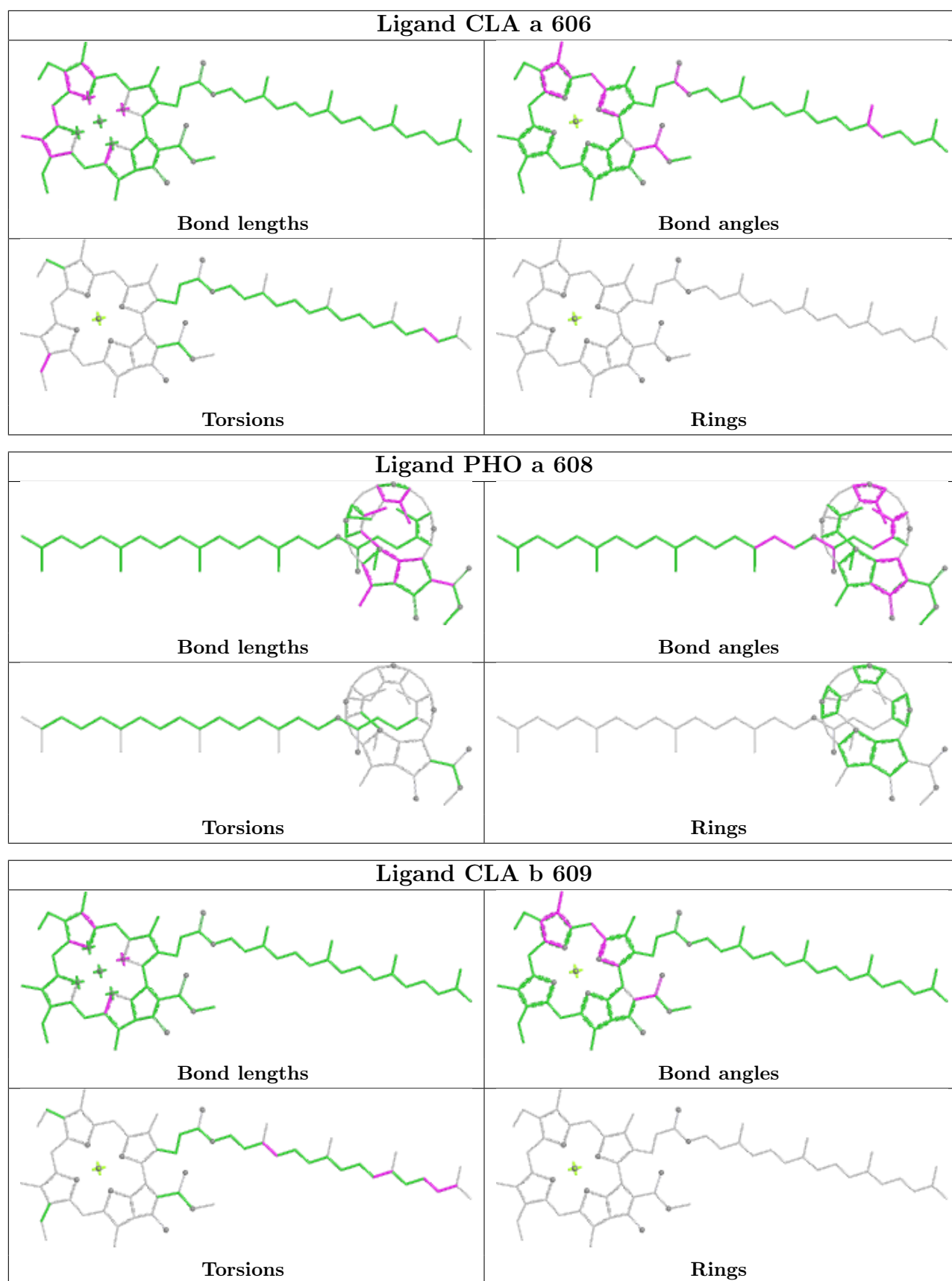


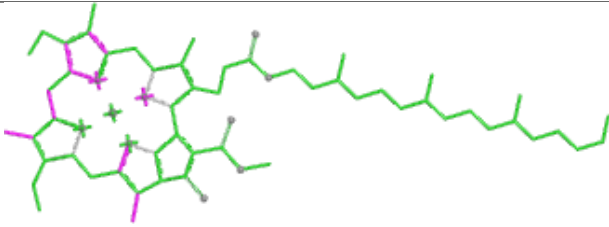
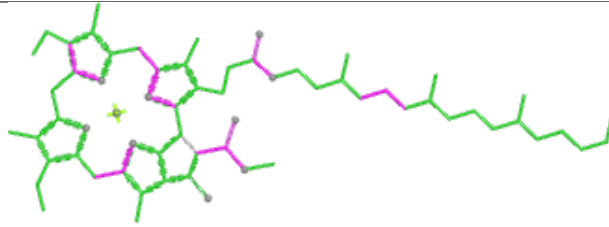
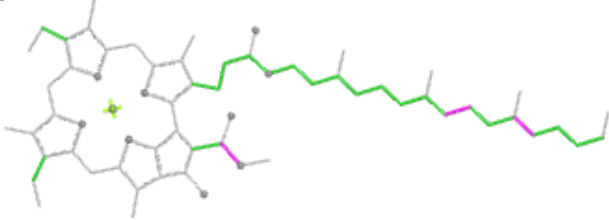
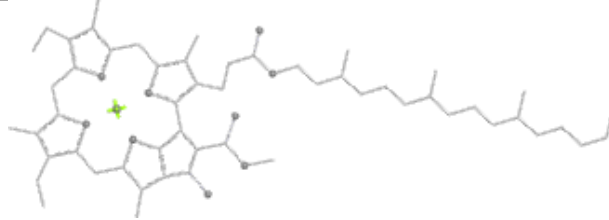
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

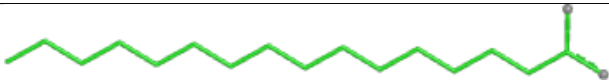
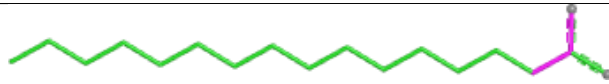
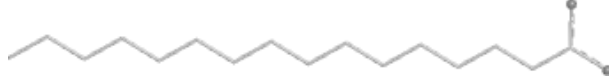
Ligand STE C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

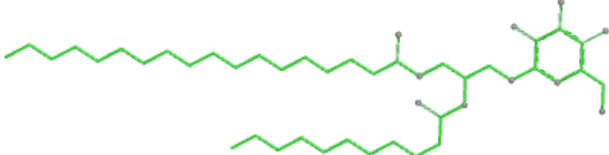
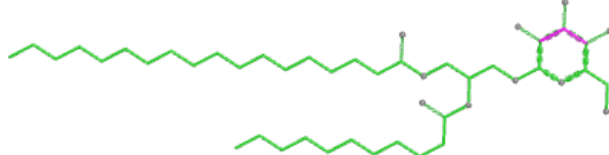
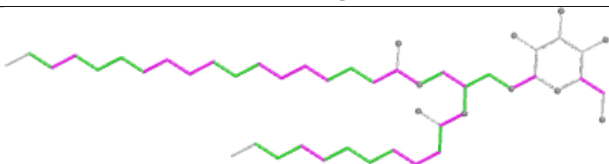
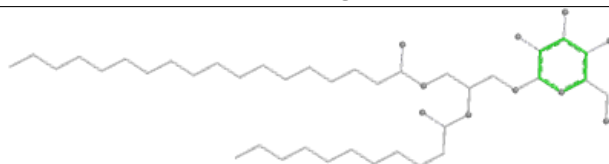
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

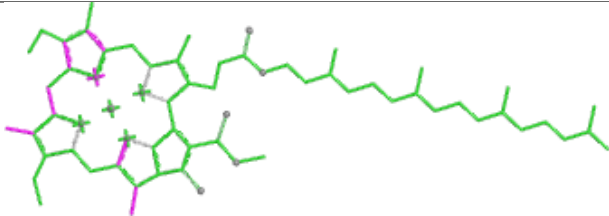
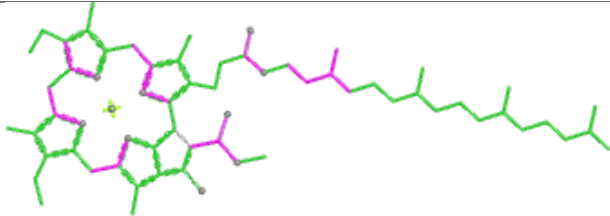
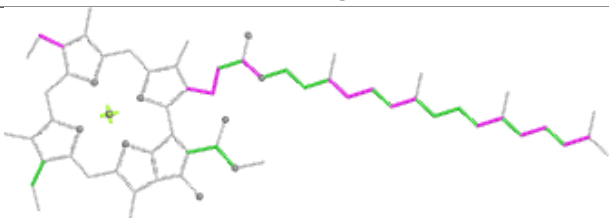
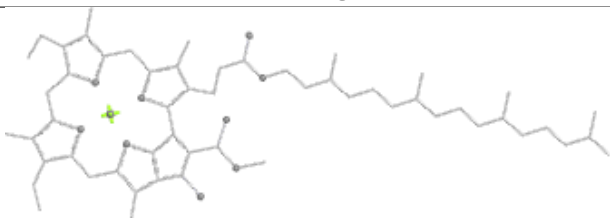




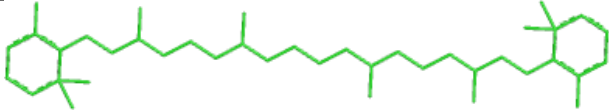
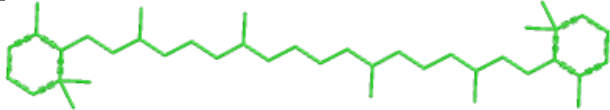
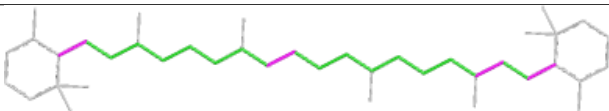
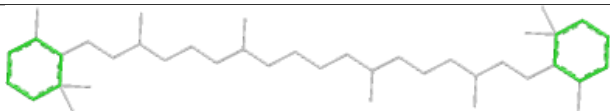
Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

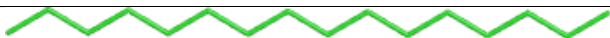
Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

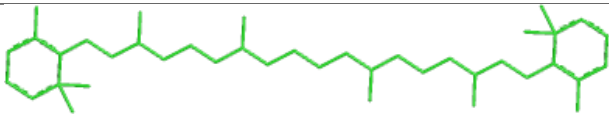
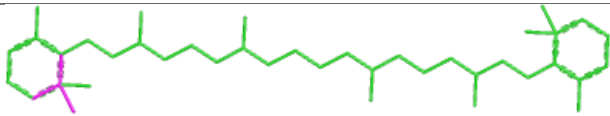
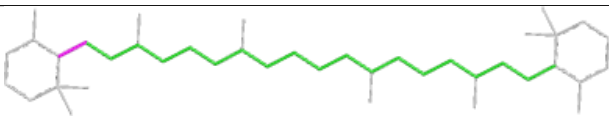
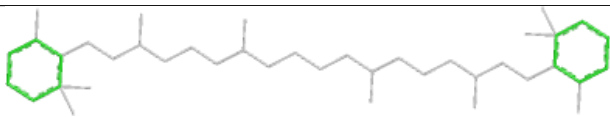
Ligand LMG c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

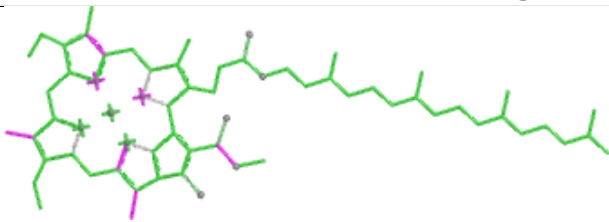
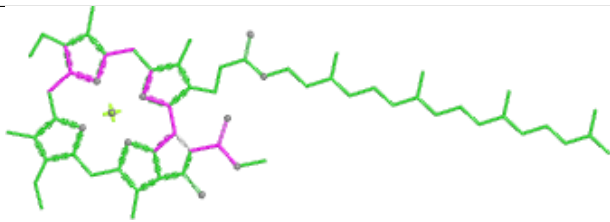
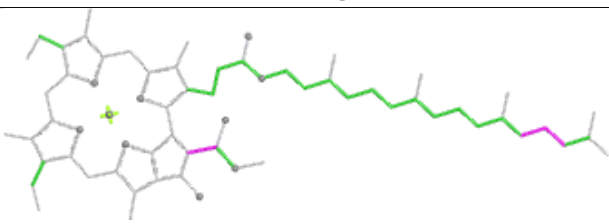
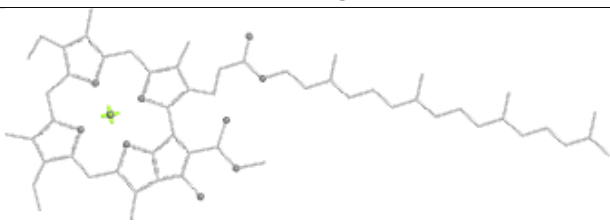
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

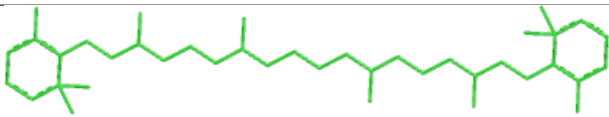
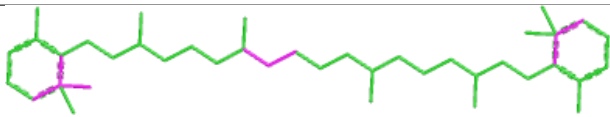
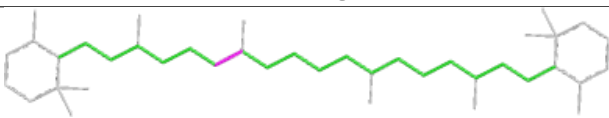
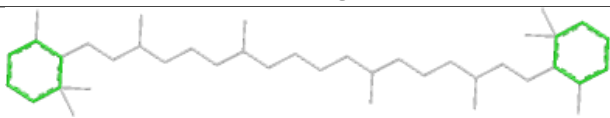
Ligand STE h 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

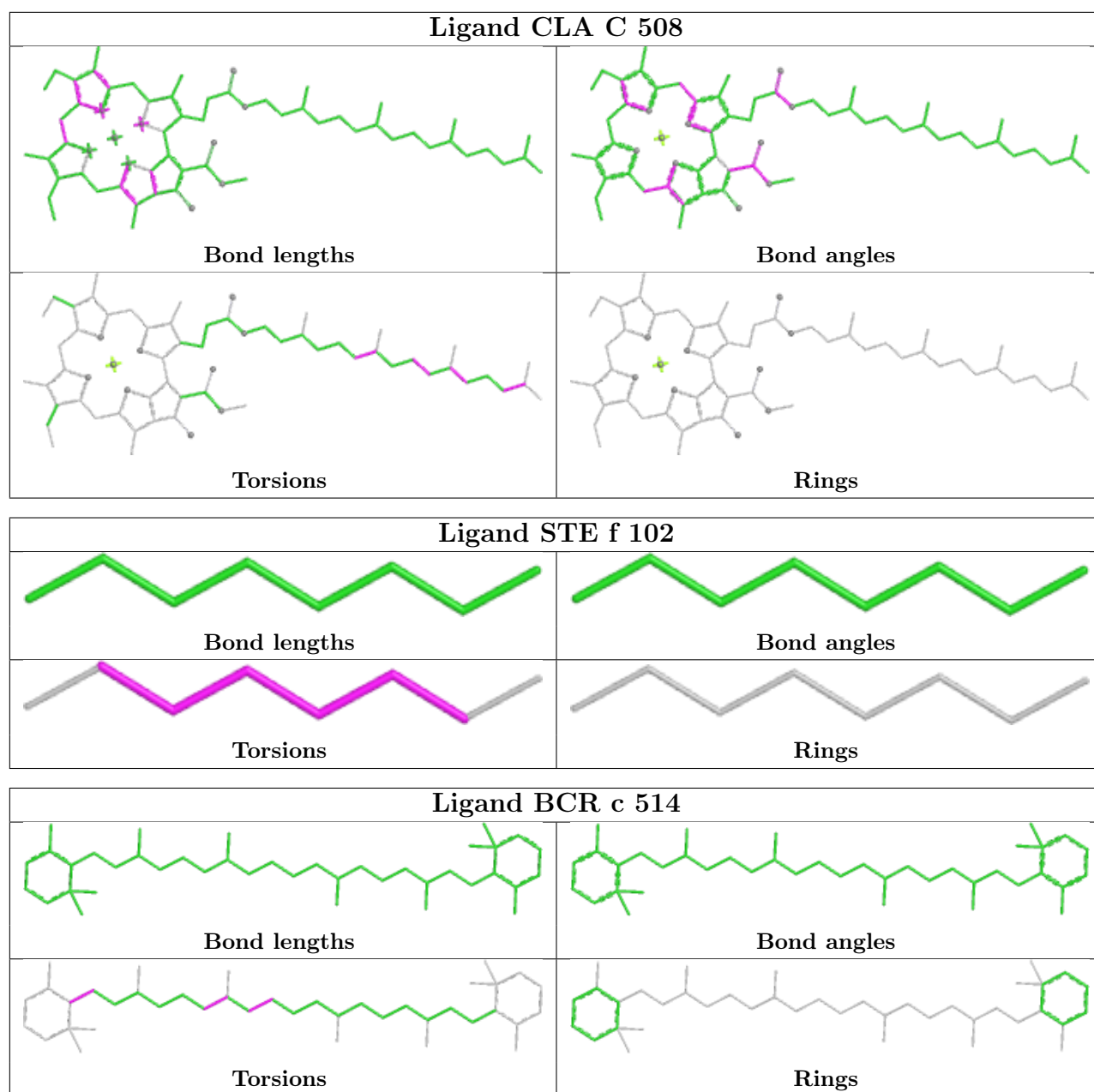
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.38	1 (0%) 90 93	27, 32, 56, 82	0
1	a	334/344 (97%)	-0.30	3 (0%) 81 86	28, 35, 65, 83	0
2	B	505/510 (99%)	-0.22	7 (1%) 73 81	20, 37, 66, 104	5 (0%)
2	b	505/510 (99%)	-0.06	8 (1%) 70 79	30, 41, 76, 116	1 (0%)
3	C	442/461 (95%)	-0.16	0 100 100	19, 41, 58, 86	1 (0%)
3	c	451/461 (97%)	-0.02	4 (0%) 81 86	22, 46, 67, 98	2 (0%)
4	D	341/352 (96%)	-0.38	1 (0%) 90 93	27, 35, 54, 86	0
4	d	341/352 (96%)	-0.19	2 (0%) 85 90	29, 40, 67, 84	1 (0%)
5	E	82/84 (97%)	0.48	2 (2%) 59 69	34, 59, 74, 83	1 (1%)
5	e	82/84 (97%)	0.67	1 (1%) 76 83	46, 68, 88, 94	0
6	F	34/45 (75%)	0.15	0 100 100	42, 50, 70, 86	0
6	f	34/45 (75%)	0.41	0 100 100	49, 60, 86, 95	0
7	H	65/66 (98%)	0.04	2 (3%) 51 61	39, 47, 62, 76	0
7	h	63/66 (95%)	0.49	3 (4%) 35 45	48, 58, 69, 76	0
8	I	35/38 (92%)	-0.21	0 100 100	37, 43, 69, 77	0
8	i	35/38 (92%)	0.01	1 (2%) 53 63	38, 45, 77, 91	0
9	J	36/40 (90%)	0.39	1 (2%) 55 65	42, 58, 81, 106	0
9	j	36/40 (90%)	0.40	0 100 100	46, 63, 90, 99	0
10	K	37/46 (80%)	0.27	0 100 100	50, 60, 78, 80	0
10	k	37/46 (80%)	0.41	0 100 100	57, 64, 79, 87	0
11	L	37/37 (100%)	-0.34	0 100 100	29, 34, 63, 68	0
11	l	36/37 (97%)	-0.34	0 100 100	31, 36, 72, 81	0
12	M	32/36 (88%)	-0.18	1 (3%) 51 61	33, 38, 59, 75	0
12	m	31/36 (86%)	-0.23	0 100 100	33, 39, 52, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.04	4 (1%) 70 79	27, 46, 84, 130	1 (0%)
13	o	244/272 (89%)	0.00	4 (1%) 70 79	29, 45, 81, 130	0
14	T	29/32 (90%)	-0.31	1 (3%) 48 58	31, 35, 61, 79	0
14	t	29/32 (90%)	-0.12	2 (6%) 23 30	31, 37, 75, 87	0
15	U	97/134 (72%)	0.01	1 (1%) 79 86	36, 47, 74, 91	0
15	u	97/134 (72%)	-0.05	2 (2%) 63 72	34, 45, 57, 83	0
16	V	137/163 (84%)	-0.15	0 100 100	33, 44, 57, 70	0
16	v	137/163 (84%)	0.15	0 100 100	39, 54, 73, 83	0
17	Y	27/46 (58%)	1.49	6 (22%) 2 2	60, 79, 103, 106	0
17	y	30/46 (65%)	0.85	0 100 100	70, 81, 92, 103	0
18	X	38/41 (92%)	0.33	2 (5%) 32 41	47, 59, 81, 88	0
18	x	39/41 (95%)	0.38	1 (2%) 57 67	58, 69, 88, 102	0
19	Z	62/62 (100%)	0.85	3 (4%) 35 45	62, 76, 122, 126	0
19	z	62/62 (100%)	1.09	6 (9%) 13 19	68, 84, 115, 132	0
20	R	28/41 (68%)	1.07	3 (10%) 11 15	69, 79, 90, 98	0
20	r	28/41 (68%)	1.89	10 (35%) 1 1	83, 105, 124, 139	0
All	All	5293/5700 (92%)	-0.04	82 (1%) 72 80	19, 43, 80, 139	12 (0%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	24	THR	4.9
20	r	28	VAL	4.7
19	z	33	TRP	4.7
20	r	29	LYS	4.4
1	A	265	PHE	4.4

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
12	FME	M	1	10/11	0.93	0.10	39,47,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.93	0.09	32,46,62,62	0
14	FME	t	1	10/11	0.94	0.08	31,43,64,64	0
8	FME	i	1	10/11	0.96	0.08	40,48,61,62	0
12	FME	m	1	10/11	0.97	0.06	36,44,61,64	0
8	FME	I	1	10/11	0.97	0.06	40,49,62,64	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
29	STE	C	517	5/20	0.58	0.28	52,60,72,72	0
29	STE	C	519	10/20	0.58	0.19	52,69,83,90	0
29	STE	A	618	17/20	0.63	0.16	54,69,86,87	0
29	STE	H	103	18/20	0.63	0.21	56,76,85,90	0
29	STE	C	526	14/20	0.64	0.20	61,81,104,110	0
29	STE	A	619	11/20	0.64	0.18	49,75,94,95	0
29	STE	j	102	16/20	0.66	0.20	65,83,104,106	0
29	STE	c	517	18/20	0.69	0.19	58,84,99,99	0
29	STE	i	101	12/20	0.70	0.12	66,85,100,107	0
29	STE	h	103	10/20	0.70	0.20	65,83,91,91	0
29	STE	B	627	15/20	0.71	0.22	43,63,78,82	0
29	STE	I	101	17/20	0.71	0.16	58,73,86,88	0
29	STE	E	104	20/20	0.71	0.14	50,70,84,84	0
29	STE	D	411	9/20	0.72	0.17	53,68,76,78	0
29	STE	C	515	14/20	0.72	0.18	51,70,78,81	0
29	STE	K	103	14/20	0.73	0.14	55,70,85,90	0
28	PL9	A	611	55/55	0.73	0.19	47,69,90,93	0
29	STE	e	101	9/20	0.73	0.22	63,82,95,97	0
30	LMG	D	406	50/55	0.73	0.15	46,69,110,117	0
33	LHG	a	614	42/49	0.73	0.17	54,89,110,121	0
28	PL9	a	611	55/55	0.74	0.19	49,73,91,93	0
29	STE	b	624	16/20	0.75	0.19	57,70,92,93	0
29	STE	a	618	12/20	0.76	0.12	52,70,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	LMG	c	518	30/55	0.76	0.17	46,81,105,108	0
30	LMG	c	523	48/55	0.76	0.15	49,76,93,106	0
33	LHG	E	101	49/49	0.76	0.15	51,83,108,119	0
30	LMG	C	516	36/55	0.76	0.15	47,64,79,82	0
30	LMG	b	623	55/55	0.77	0.17	54,74,94,104	0
29	STE	f	102	8/20	0.77	0.21	60,74,82,84	0
29	STE	t	103	10/20	0.77	0.16	45,60,72,74	0
29	STE	E	103	12/20	0.77	0.17	67,84,109,110	0
29	STE	Z	101	17/20	0.77	0.20	53,78,97,99	0
30	LMG	a	616	55/55	0.78	0.14	41,60,81,89	0
29	STE	E	102	12/20	0.78	0.18	62,81,97,98	0
29	STE	d	410	20/20	0.78	0.14	56,73,90,95	0
29	STE	d	412	14/20	0.79	0.14	62,75,87,89	0
29	STE	B	626	12/20	0.79	0.15	51,65,78,78	0
29	STE	C	518	7/20	0.79	0.18	53,71,77,77	0
29	STE	c	516	13/20	0.80	0.17	65,78,84,85	0
29	STE	e	103	9/20	0.80	0.18	62,79,88,88	0
29	STE	T	102	16/20	0.80	0.17	40,53,94,96	0
32	DGD	A	617	66/66	0.81	0.13	49,64,92,97	0
29	STE	d	406	20/20	0.81	0.14	49,61,77,77	0
29	STE	z	101	9/20	0.81	0.22	53,78,83,84	0
30	LMG	B	620	45/55	0.82	0.14	38,60,99,115	0
29	STE	j	101	12/20	0.82	0.13	53,64,72,73	0
29	STE	J	101	12/20	0.82	0.13	52,63,68,70	0
29	STE	A	612	9/20	0.82	0.15	56,70,82,83	0
29	STE	i	102	6/20	0.82	0.16	51,66,80,80	0
29	STE	b	625	10/20	0.83	0.14	49,62,72,74	0
29	STE	e	104	13/20	0.83	0.16	72,92,102,105	0
31	SQD	a	615	54/54	0.84	0.13	41,62,100,110	0
29	STE	C	524	12/20	0.84	0.14	41,51,60,61	0
31	SQD	f	101	41/54	0.85	0.14	63,87,99,106	0
29	STE	h	104	11/20	0.86	0.16	61,76,79,81	0
31	SQD	A	616	43/54	0.86	0.11	42,59,92,104	0
30	LMG	C	523	48/55	0.86	0.13	48,74,91,94	0
25	CLA	b	601	65/65	0.86	0.12	50,71,93,106	0
29	STE	x	101	20/20	0.86	0.12	45,61,79,80	0
29	STE	b	626	8/20	0.86	0.13	45,64,69,70	0
29	STE	I	102	15/20	0.86	0.13	45,56,74,75	0
29	STE	M	101	15/20	0.87	0.12	38,49,61,62	0
29	STE	B	625	18/20	0.87	0.11	41,55,71,78	0
31	SQD	B	624	54/54	0.87	0.10	40,57,78,85	0
30	LMG	c	522	46/55	0.87	0.13	48,74,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	STE	X	101	20/20	0.88	0.11	39,53,68,76	0
25	CLA	B	601	65/65	0.88	0.11	40,64,90,94	0
29	STE	M	102	10/20	0.88	0.14	47,57,60,64	0
29	STE	M	103	15/20	0.88	0.13	41,57,86,88	0
29	STE	C	525	16/20	0.88	0.11	43,56,60,64	0
30	LMG	b	621	51/55	0.89	0.10	37,51,66,77	0
30	LMG	B	621	51/55	0.89	0.10	33,52,69,73	0
29	STE	B	622	17/20	0.89	0.10	38,51,65,66	0
29	STE	b	622	20/20	0.89	0.10	39,55,67,67	0
30	LMG	A	614	48/55	0.89	0.11	38,59,72,80	0
27	BCR	K	101	40/40	0.89	0.12	52,64,73,77	0
24	BCT	A	605	4/4	0.90	0.13	31,35,38,46	0
31	SQD	D	408	36/54	0.90	0.12	51,76,91,95	0
31	SQD	a	613	54/54	0.90	0.11	39,69,92,97	0
27	BCR	d	404	40/40	0.90	0.11	40,55,85,89	0
31	SQD	b	620	49/54	0.90	0.09	41,60,79,87	0
27	BCR	h	101	40/40	0.90	0.10	42,59,75,76	0
29	STE	m	101	12/20	0.90	0.10	47,57,62,67	0
29	STE	t	102	14/20	0.90	0.10	42,52,57,63	0
30	LMG	a	617	49/55	0.90	0.10	40,59,77,85	0
27	BCR	k	101	40/40	0.91	0.10	52,66,77,78	0
27	BCR	H	101	40/40	0.91	0.09	36,49,64,65	0
25	CLA	C	513	65/65	0.91	0.10	49,68,97,101	0
29	STE	l	102	18/20	0.91	0.12	36,49,76,77	0
27	BCR	Y	101	40/40	0.91	0.10	46,58,70,74	0
27	BCR	c	514	40/40	0.91	0.12	57,70,78,79	0
32	DGD	H	102	62/66	0.91	0.09	33,47,61,62	0
32	DGD	h	102	62/66	0.91	0.10	38,52,63,66	0
25	CLA	c	512	65/65	0.91	0.10	49,64,93,99	0
25	CLA	c	513	65/65	0.91	0.11	51,73,100,105	0
27	BCR	C	514	40/40	0.92	0.10	30,42,55,57	0
32	DGD	C	521	62/66	0.92	0.10	36,53,99,109	0
27	BCR	c	515	40/40	0.92	0.10	36,47,60,61	0
33	LHG	d	409	39/49	0.92	0.10	36,51,74,80	0
27	BCR	K	102	40/40	0.93	0.10	45,57,70,73	0
27	BCR	B	617	40/40	0.93	0.08	33,41,50,53	0
27	BCR	b	619	40/40	0.93	0.09	35,48,62,68	0
27	BCR	B	618	40/40	0.93	0.07	28,38,49,50	0
25	CLA	c	503	65/65	0.93	0.08	38,48,57,62	0
27	BCR	D	404	40/40	0.93	0.11	37,47,91,96	0
30	LMG	d	411	44/55	0.93	0.10	42,60,87,96	0
32	DGD	c	520	62/66	0.93	0.09	41,56,90,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	SQD	A	615	52/54	0.93	0.09	33,62,85,96	0
24	BCT	a	605	4/4	0.93	0.11	37,39,47,57	0
30	LMG	D	407	51/55	0.93	0.11	35,60,82,85	0
33	LHG	d	407	49/49	0.93	0.10	37,51,70,73	0
25	CLA	C	512	65/65	0.93	0.09	44,59,92,99	0
26	PHO	d	401	64/64	0.94	0.07	32,42,50,58	0
27	BCR	A	610	40/40	0.94	0.07	31,39,49,51	0
27	BCR	b	618	40/40	0.94	0.07	28,40,52,55	0
25	CLA	b	616	60/65	0.94	0.09	34,47,94,97	0
32	DGD	C	522	62/66	0.94	0.09	33,49,79,93	0
25	CLA	C	511	65/65	0.94	0.09	41,54,68,70	0
27	BCR	B	619	40/40	0.94	0.08	31,45,58,64	0
25	CLA	c	506	65/65	0.94	0.10	37,50,90,94	0
33	LHG	B	623	49/49	0.94	0.09	32,44,62,70	0
25	CLA	c	509	65/65	0.94	0.09	39,51,67,70	0
25	CLA	C	510	65/65	0.94	0.07	38,48,67,71	0
27	BCR	k	102	40/40	0.94	0.10	49,60,75,82	0
25	CLA	b	606	65/65	0.94	0.08	32,42,71,74	0
25	CLA	c	504	60/65	0.95	0.08	36,49,81,84	0
25	CLA	c	505	65/65	0.95	0.08	34,44,68,78	0
25	CLA	C	506	65/65	0.95	0.10	33,47,84,89	0
25	CLA	c	507	65/65	0.95	0.08	36,47,58,61	0
25	CLA	c	508	64/65	0.95	0.09	37,51,98,106	0
27	BCR	t	101	40/40	0.95	0.06	30,40,56,57	0
25	CLA	C	508	65/65	0.95	0.08	34,46,106,111	0
28	PL9	D	405	55/55	0.95	0.06	26,34,44,46	0
25	CLA	c	510	65/65	0.95	0.07	38,52,66,75	0
28	PL9	d	405	55/55	0.95	0.06	29,37,45,45	0
25	CLA	c	511	65/65	0.95	0.09	46,59,77,79	0
25	CLA	C	509	65/65	0.95	0.08	33,48,63,68	0
25	CLA	B	603	65/65	0.95	0.07	26,34,63,65	0
25	CLA	d	403	65/65	0.95	0.10	35,52,91,98	0
26	PHO	A	608	64/64	0.95	0.06	27,36,45,50	0
26	PHO	a	608	64/64	0.95	0.07	27,34,38,43	0
25	CLA	B	604	65/65	0.95	0.08	25,33,67,71	0
25	CLA	B	606	65/65	0.95	0.08	28,37,70,76	0
25	CLA	B	609	65/65	0.95	0.08	29,41,62,65	0
25	CLA	a	607	65/65	0.95	0.09	31,44,98,100	0
25	CLA	C	501	65/65	0.95	0.07	30,39,51,56	0
25	CLA	b	602	65/65	0.95	0.09	33,46,64,66	0
25	CLA	C	502	65/65	0.95	0.07	33,44,59,59	0
25	CLA	b	609	65/65	0.95	0.08	36,49,69,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	610	65/65	0.95	0.08	31,41,50,51	0
25	CLA	b	612	65/65	0.95	0.07	28,36,47,49	0
27	BCR	T	101	40/40	0.95	0.07	31,40,53,54	0
32	DGD	c	521	62/66	0.95	0.08	36,57,81,89	0
25	CLA	b	614	65/65	0.95	0.08	29,40,76,79	0
27	BCR	a	610	40/40	0.95	0.07	27,37,47,48	0
33	LHG	D	410	47/49	0.95	0.09	33,53,82,86	0
27	BCR	b	617	40/40	0.95	0.06	33,42,50,51	0
25	CLA	C	503	65/65	0.95	0.07	37,45,53,61	0
25	CLA	c	502	65/65	0.95	0.08	36,47,67,71	0
33	LHG	d	408	49/49	0.95	0.08	32,43,53,59	0
25	CLA	C	504	59/65	0.95	0.09	35,46,89,94	0
25	CLA	D	403	65/65	0.96	0.09	31,45,121,130	0
25	CLA	a	606	65/65	0.96	0.06	25,33,45,54	0
25	CLA	B	616	60/65	0.96	0.08	28,41,92,100	0
25	CLA	a	609	65/65	0.96	0.09	26,38,77,85	0
25	CLA	a	612	65/65	0.96	0.06	25,32,45,49	0
25	CLA	A	607	65/65	0.96	0.10	26,38,102,112	0
25	CLA	B	605	65/65	0.96	0.07	25,35,44,46	0
25	CLA	b	603	65/65	0.96	0.07	30,40,71,77	0
25	CLA	B	602	65/65	0.96	0.07	30,39,61,64	0
26	PHO	D	401	64/64	0.96	0.06	24,31,36,39	0
25	CLA	b	607	65/65	0.96	0.08	26,37,68,71	0
25	CLA	b	608	65/65	0.96	0.07	34,45,66,67	0
25	CLA	B	607	65/65	0.96	0.07	25,35,59,63	0
32	DGD	C	520	62/66	0.96	0.08	27,42,77,83	0
25	CLA	C	505	65/65	0.96	0.08	29,40,69,74	0
25	CLA	b	611	65/65	0.96	0.07	28,37,52,53	0
25	CLA	A	613	65/65	0.96	0.06	24,32,49,55	0
32	DGD	c	519	62/66	0.96	0.08	28,43,80,84	0
25	CLA	b	613	65/65	0.96	0.08	27,35,75,79	0
25	CLA	C	507	65/65	0.96	0.07	31,42,61,68	0
25	CLA	b	615	65/65	0.96	0.07	31,43,62,67	0
25	CLA	B	610	65/65	0.96	0.06	27,34,41,44	0
25	CLA	c	501	65/65	0.96	0.07	34,44,54,56	0
25	CLA	B	611	65/65	0.96	0.06	25,32,48,52	0
33	LHG	L	101	49/49	0.96	0.07	31,42,55,66	0
25	CLA	B	612	65/65	0.96	0.06	24,33,46,49	0
25	CLA	B	613	65/65	0.96	0.07	24,32,65,71	0
25	CLA	B	614	65/65	0.96	0.08	28,39,80,88	0
25	CLA	B	615	65/65	0.96	0.07	27,38,58,61	0
33	LHG	l	101	49/49	0.96	0.07	34,47,59,72	0

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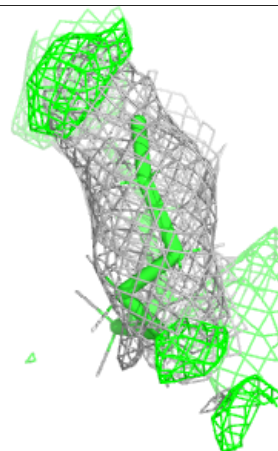
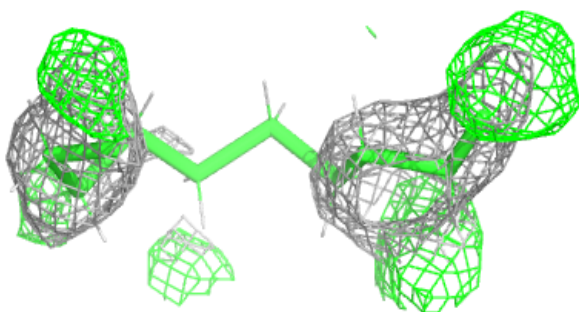
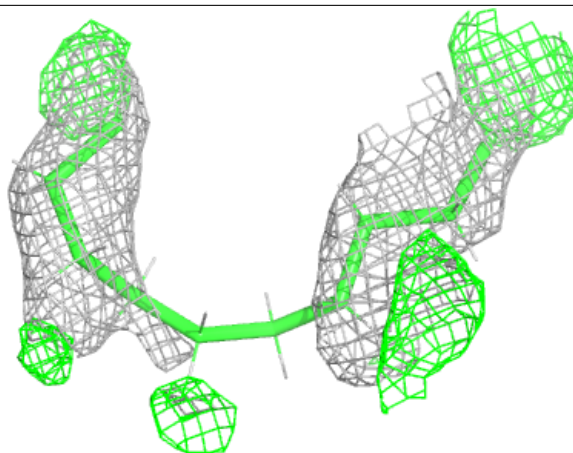
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HEM	F	101	43/43	0.96	0.09	46,53,66,68	0
25	CLA	D	402	65/65	0.97	0.06	23,32,56,58	0
25	CLA	B	608	65/65	0.97	0.06	28,38,56,61	0
25	CLA	A	606	65/65	0.97	0.06	24,30,46,52	0
25	CLA	b	604	65/65	0.97	0.07	28,38,69,79	0
33	LHG	D	409	49/49	0.97	0.06	29,41,50,53	0
25	CLA	d	402	65/65	0.97	0.06	27,34,66,67	0
25	CLA	b	605	65/65	0.97	0.06	28,37,48,50	0
34	HEM	e	102	43/43	0.97	0.09	56,66,83,84	0
23	CL	a	603	1/1	0.98	0.04	28,28,28,28	0
25	CLA	A	609	54/65	0.98	0.06	24,33,63,64	0
35	HEC	V	201	43/43	0.98	0.05	29,34,40,41	0
35	HEC	v	201	43/43	0.98	0.06	33,38,48,49	0
21	OEX	A	601	10/10	0.99	0.04	27,29,30,30	0
23	CL	a	604	1/1	0.99	0.09	28,28,28,28	0
22	FE2	a	602	1/1	0.99	0.02	35,35,35,35	0
23	CL	A	603	1/1	0.99	0.03	28,28,28,28	0
23	CL	A	604	1/1	0.99	0.04	28,28,28,28	0
21	OEX	a	601	10/10	1.00	0.02	26,28,30,32	0
22	FE2	A	602	1/1	1.00	0.02	30,30,30,30	0

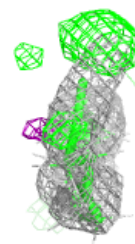
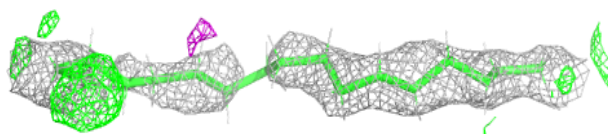
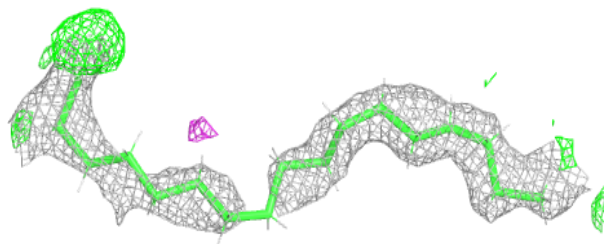
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE C 519:

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

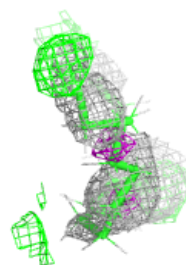
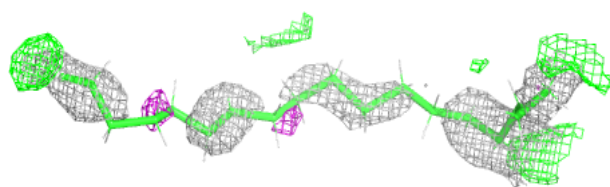
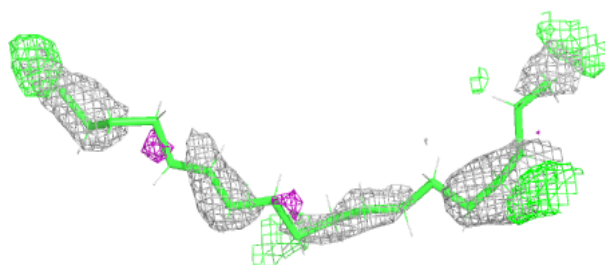
**Electron density around STE A 618:**

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

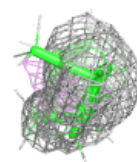
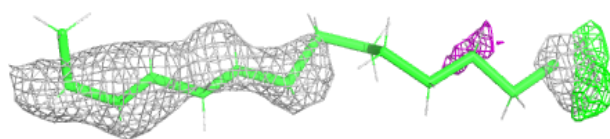
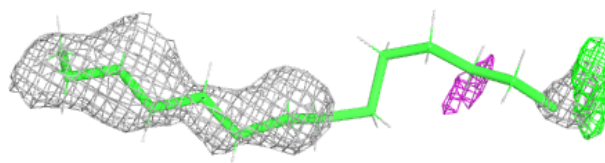


Electron density around STE H 103:

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

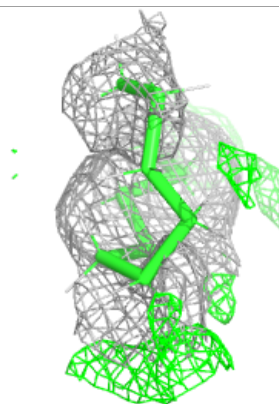
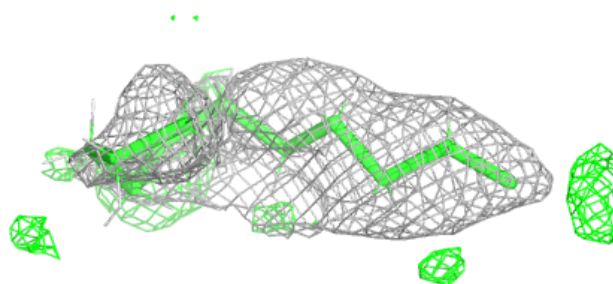
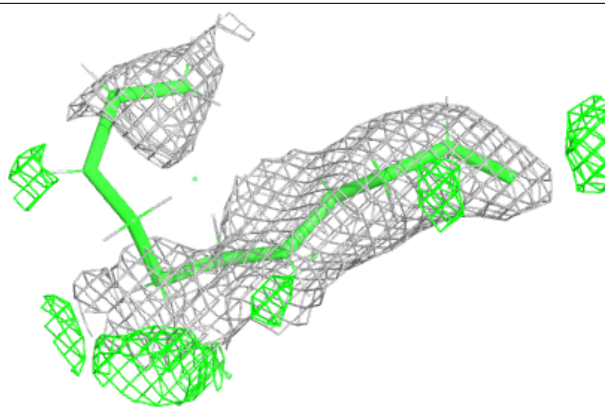
**Electron density around STE C 526:**

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

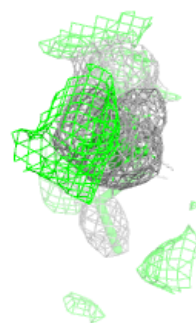
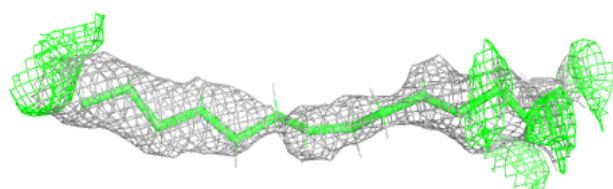
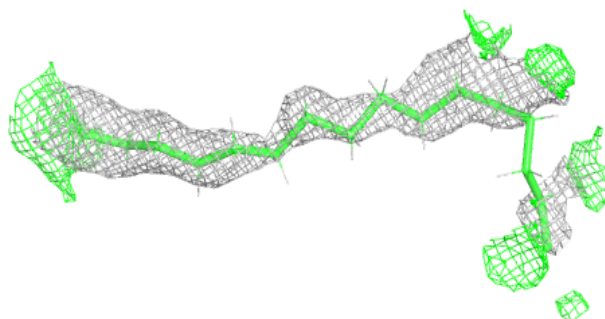


Electron density around STE A 619:

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

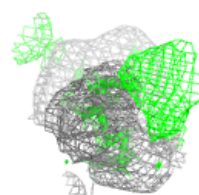
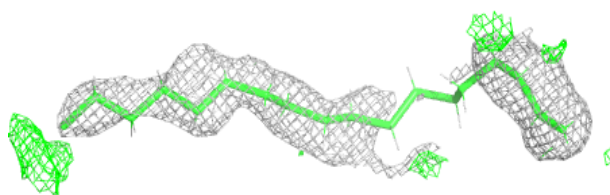
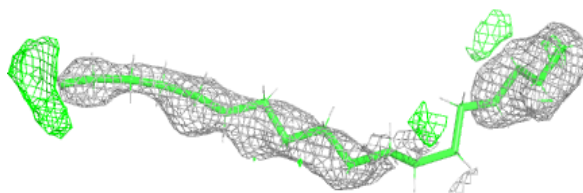
**Electron density around STE j 102:**

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

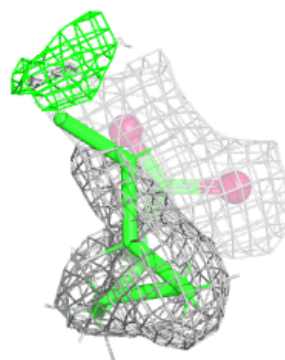
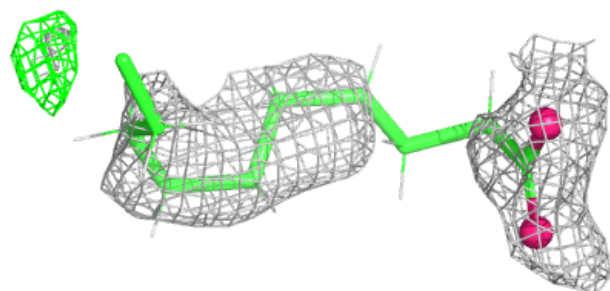
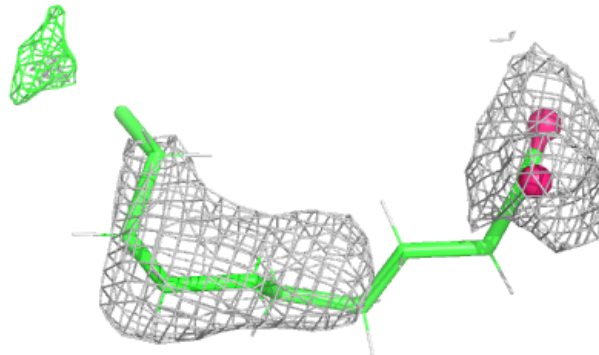


Electron density around STE c 517:

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

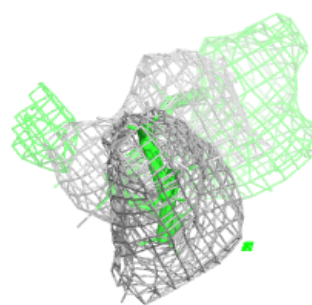
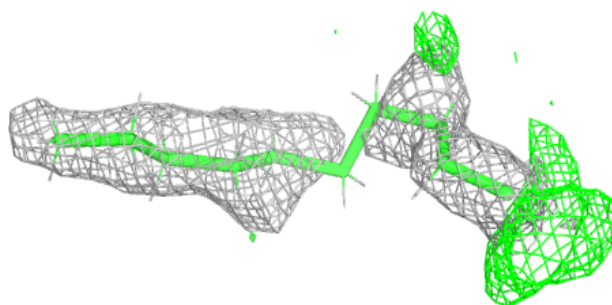
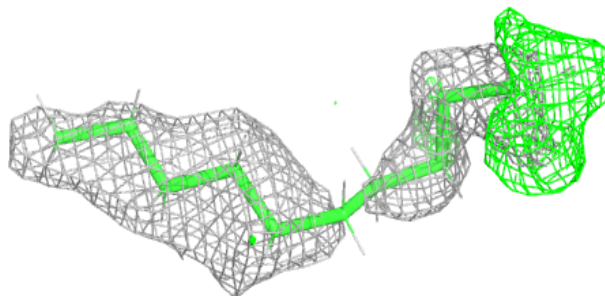
**Electron density around STE i 101:**

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

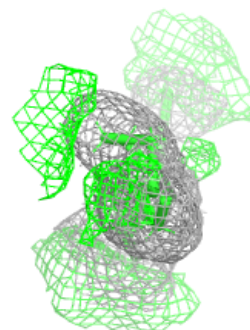
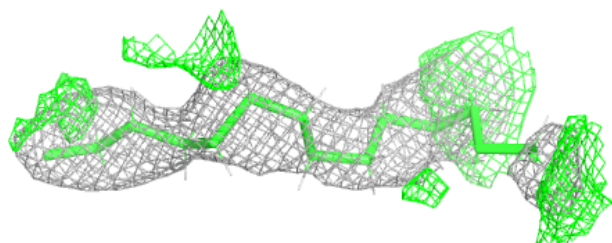
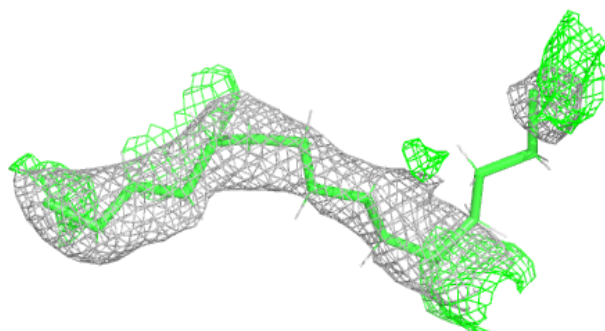


Electron density around STE h 103:

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and green (positive)

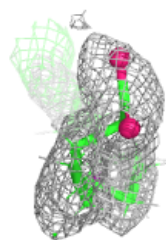
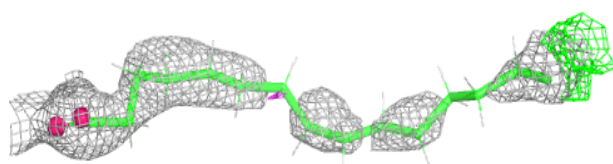
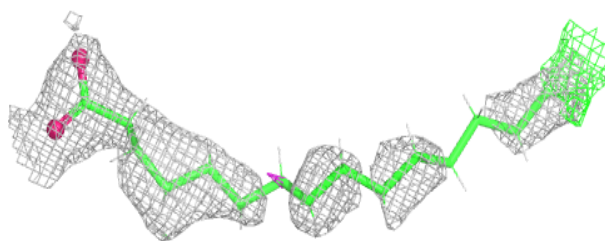
**Electron density around STE B 627:**

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and green (positive)

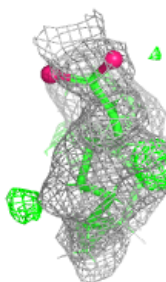
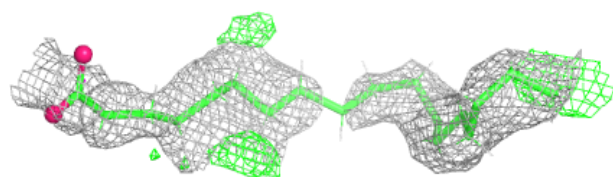
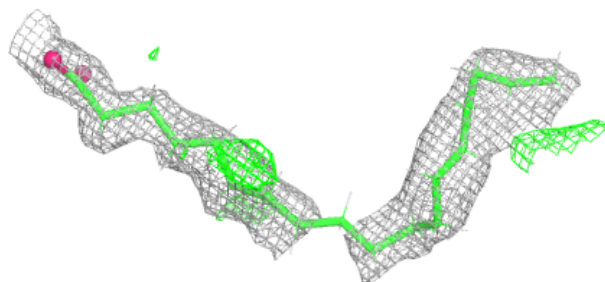


Electron density around STE I 101:

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

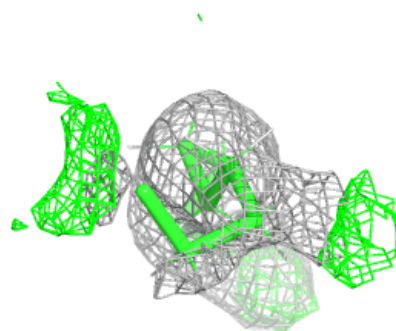
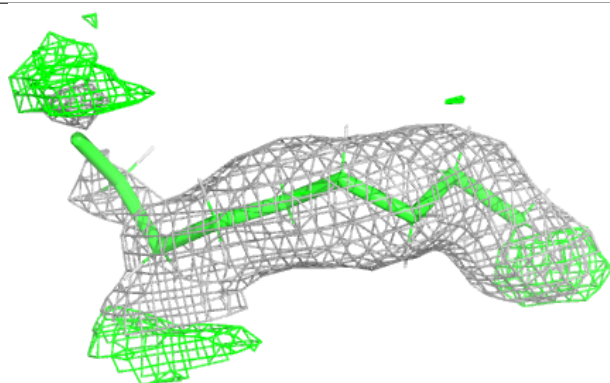
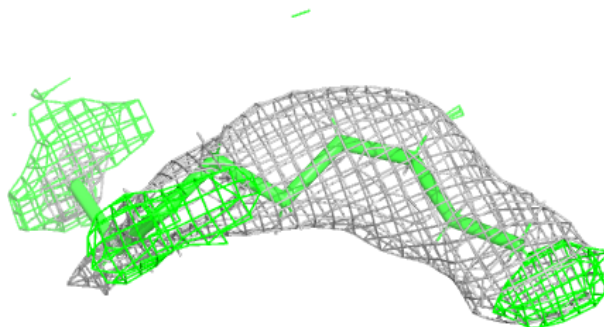
**Electron density around STE E 104:**

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

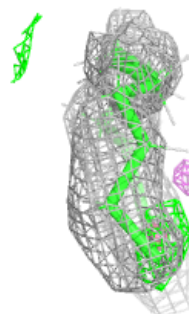
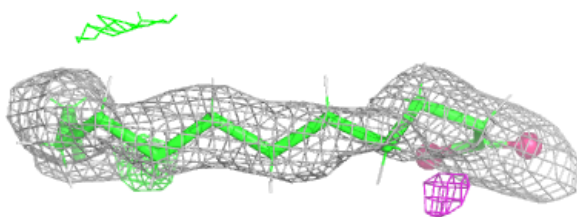
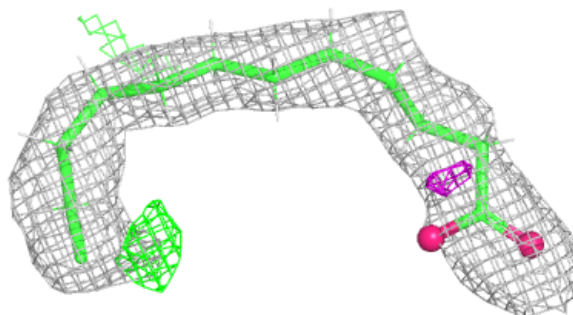


Electron density around STE D 411:

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

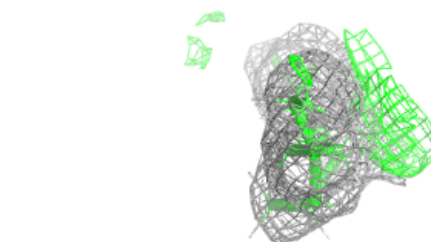
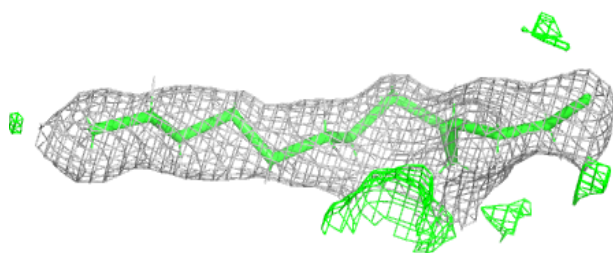
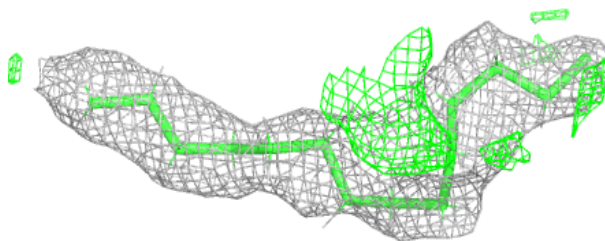
**Electron density around STE C 515:**

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

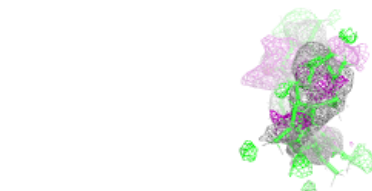
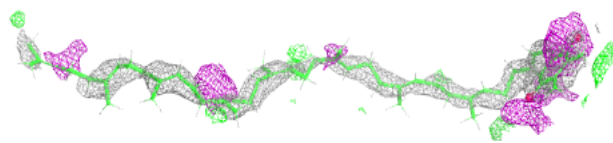
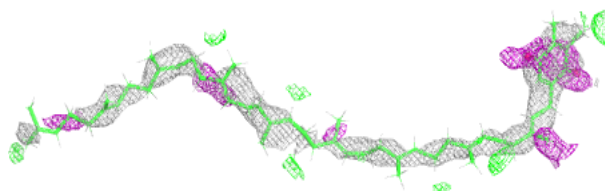


Electron density around STE K 103:

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

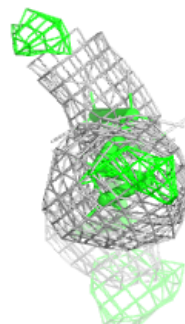
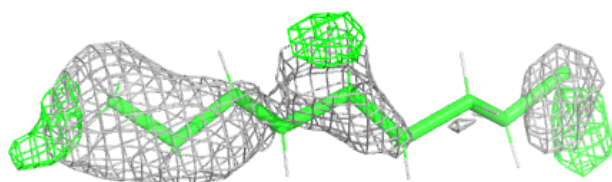
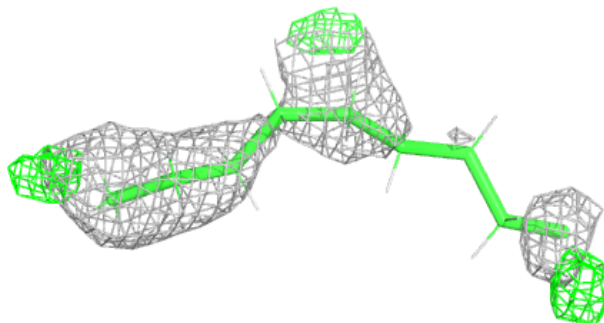
**Electron density around PL9 A 611:**

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

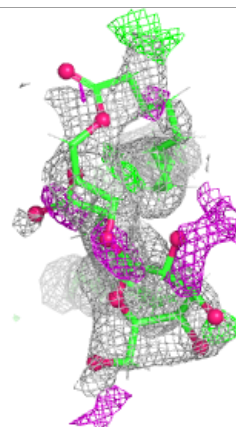
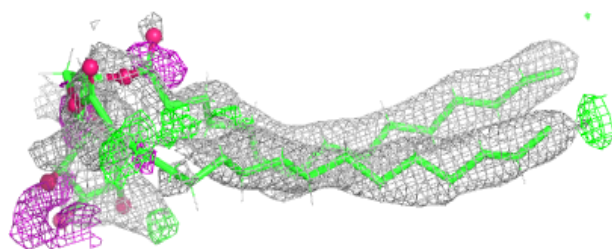
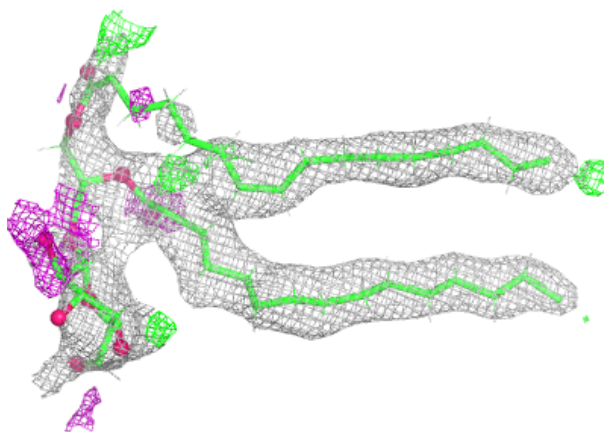


Electron density around STE e 101:

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

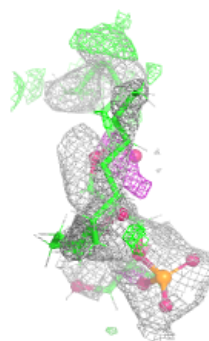
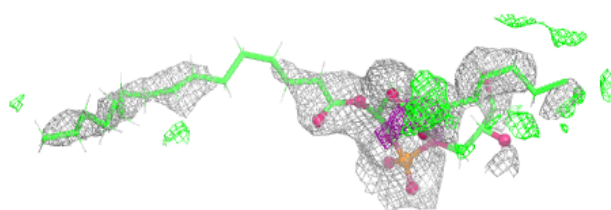
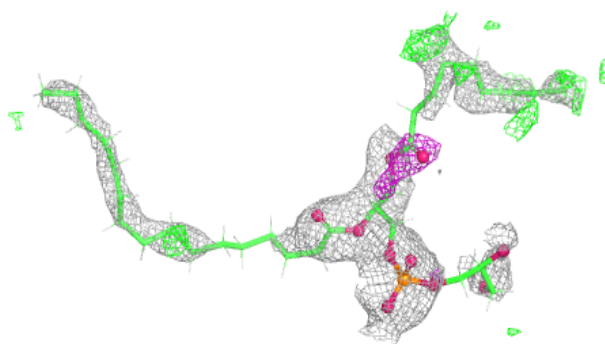
**Electron density around LMG D 406:**

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

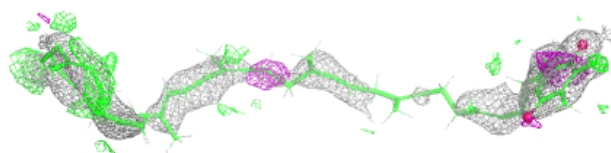
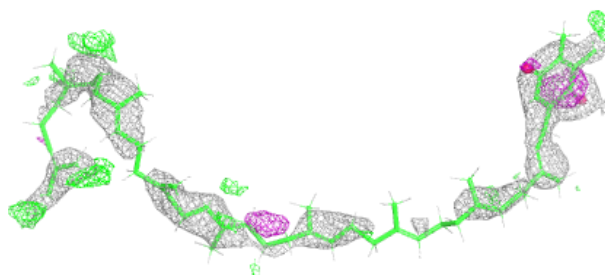


Electron density around LHG a 614:

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

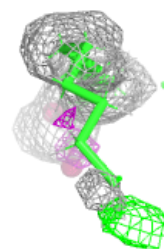
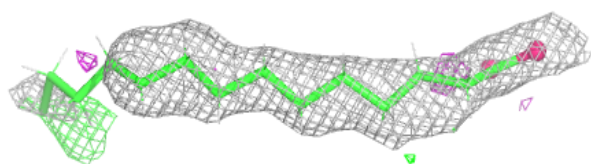
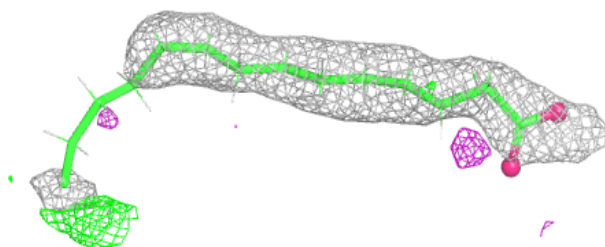
**Electron density around PL9 a 611:**

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

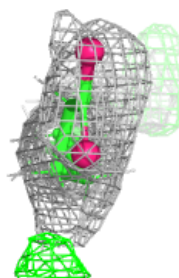
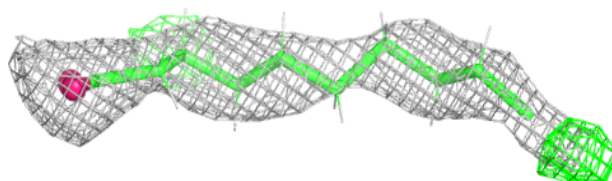
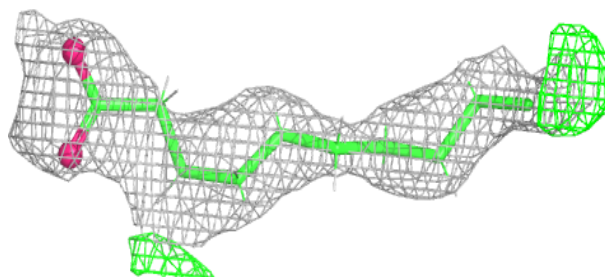


Electron density around STE b 624:

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

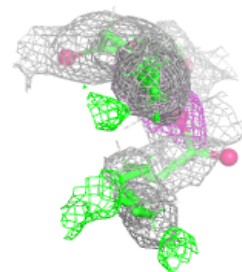
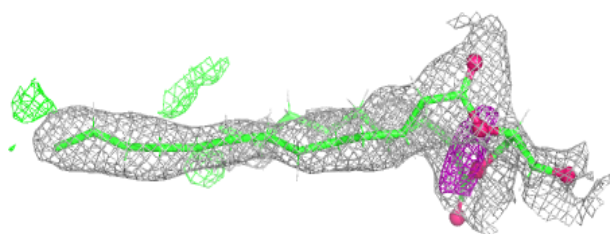
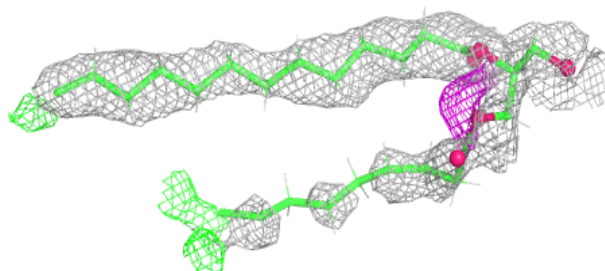
**Electron density around STE a 618:**

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

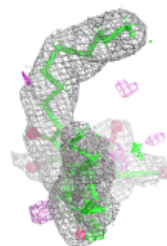
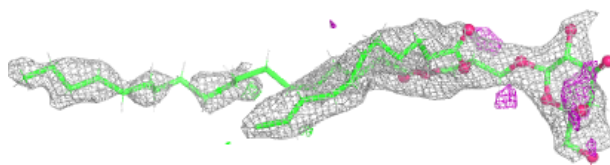
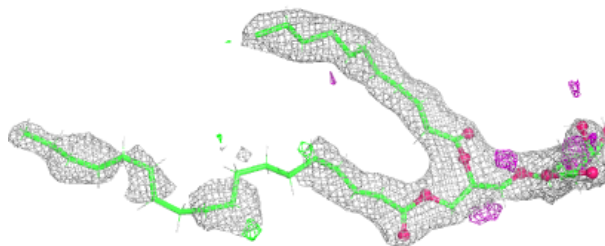


Electron density around LMG c 518:

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

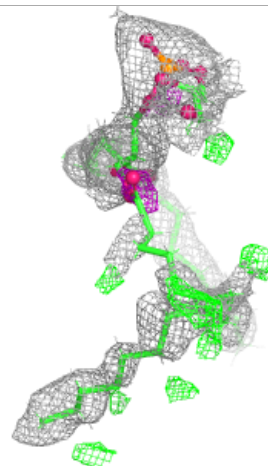
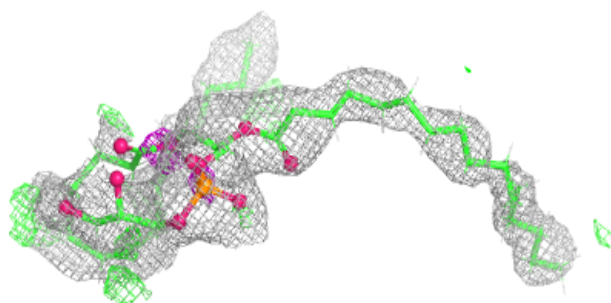
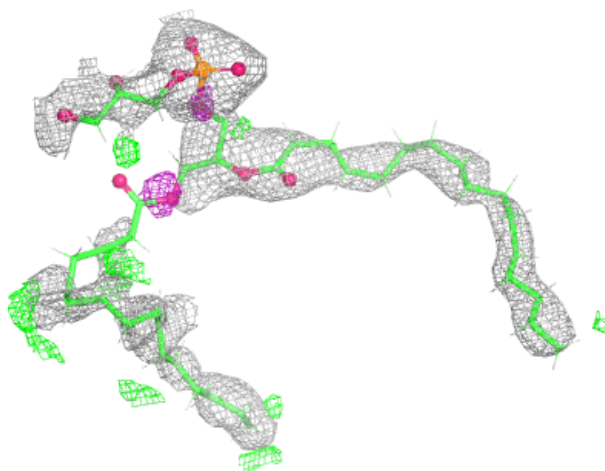
**Electron density around LMG c 523:**

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



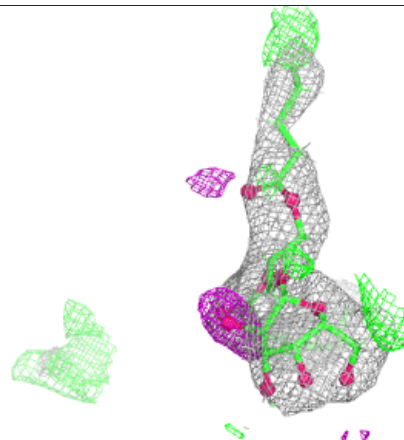
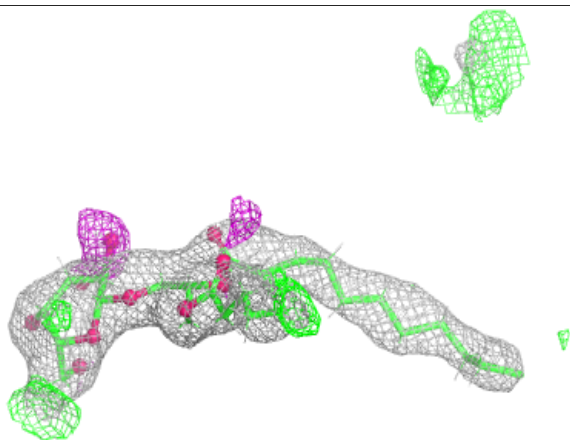
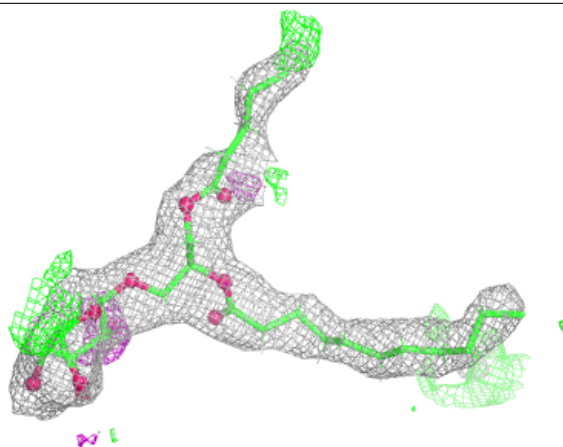
Electron density around LHG E 101:

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

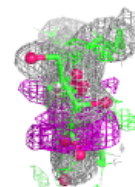
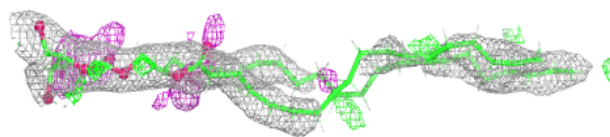
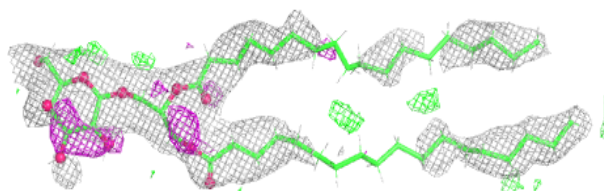


Electron density around LMG C 516:

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

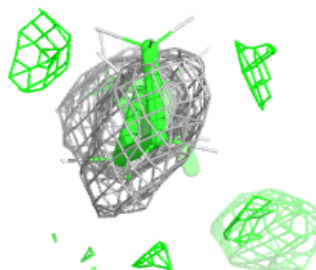
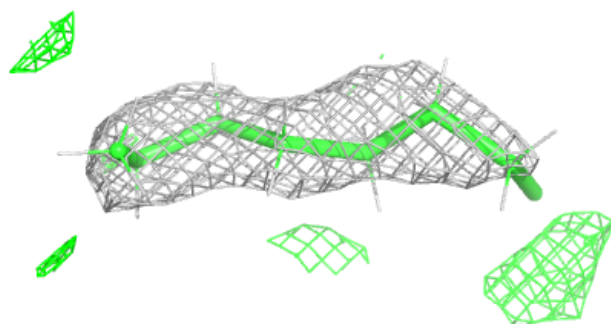
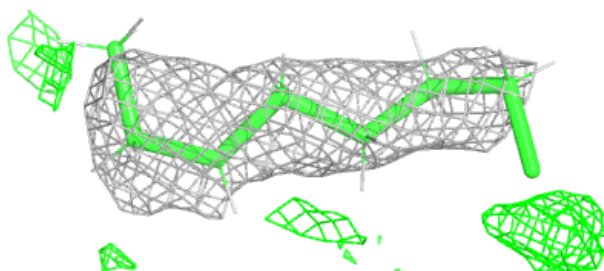
**Electron density around LMG b 623:**

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

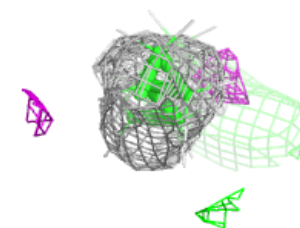
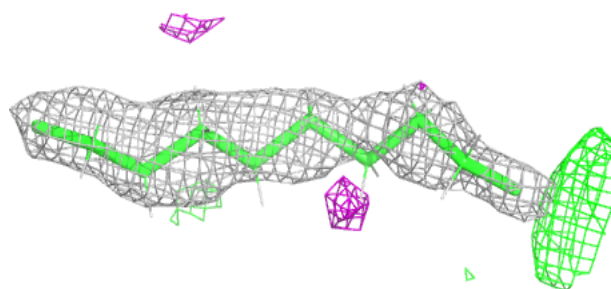
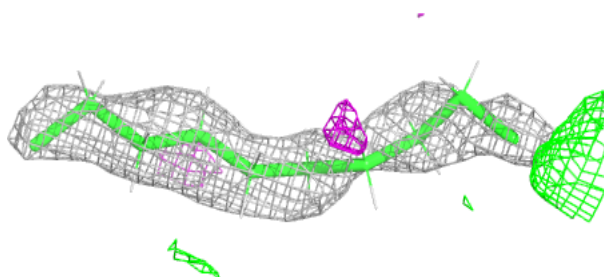


Electron density around STE f 102:

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

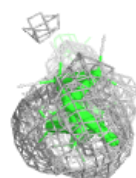
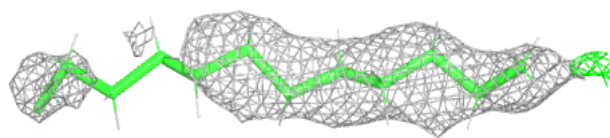
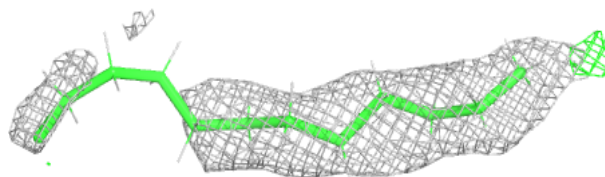
**Electron density around STE t 103:**

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

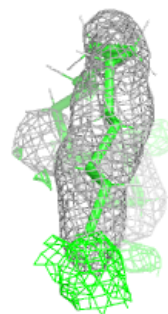
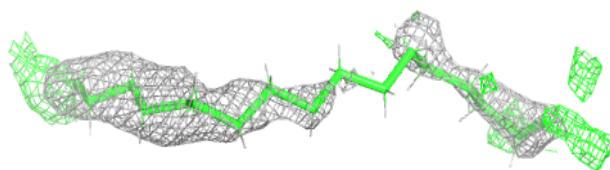
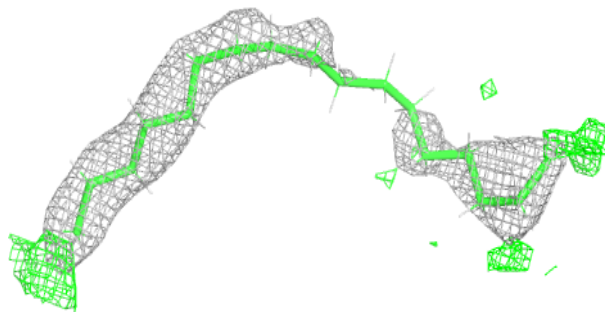


Electron density around STE E 103:

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

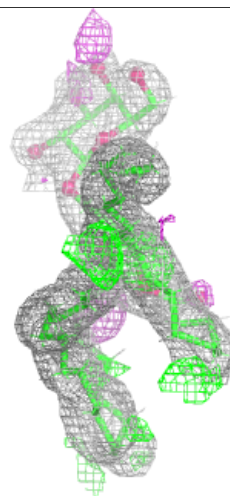
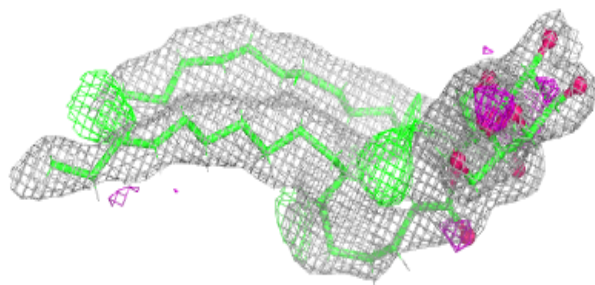
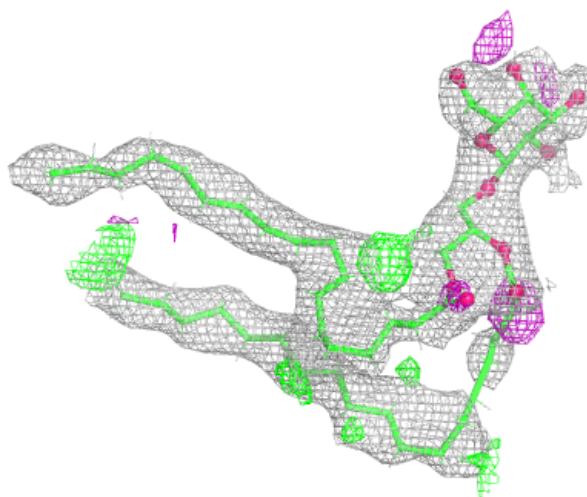
**Electron density around STE Z 101:**

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



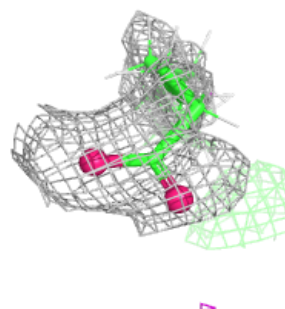
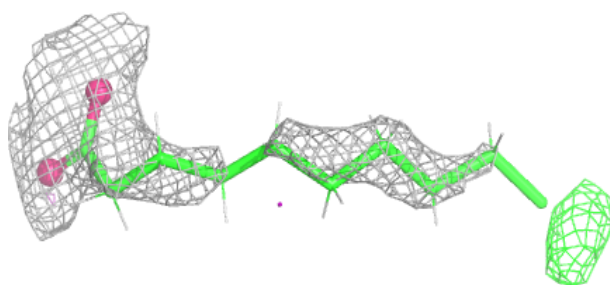
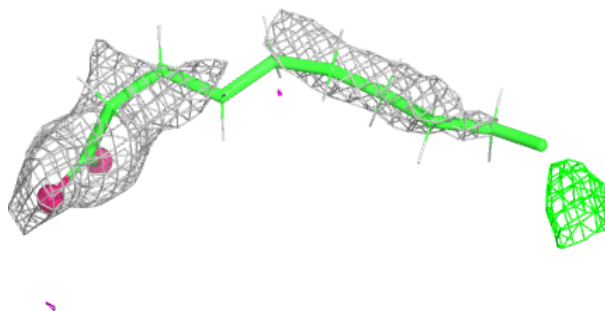
Electron density around LMG a 616:

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

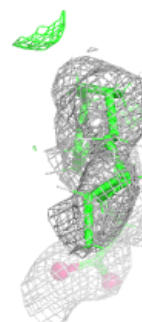
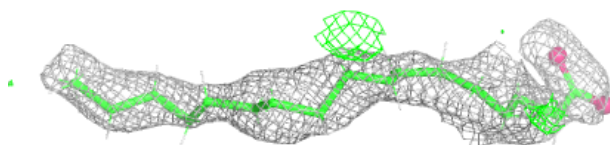
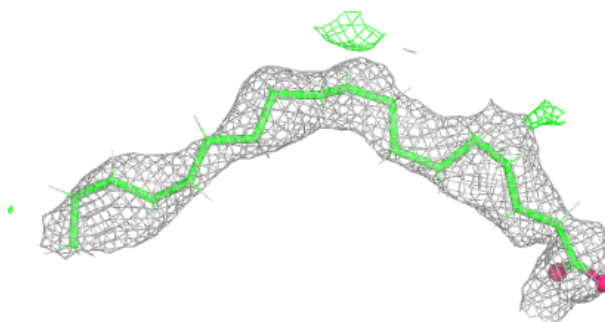


Electron density around STE E 102:

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

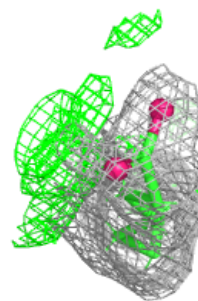
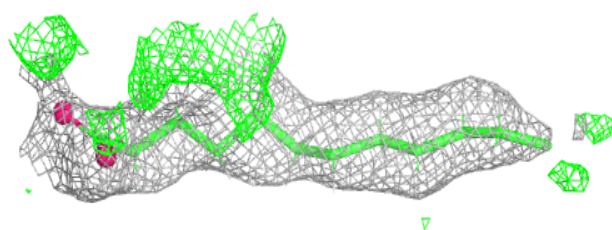
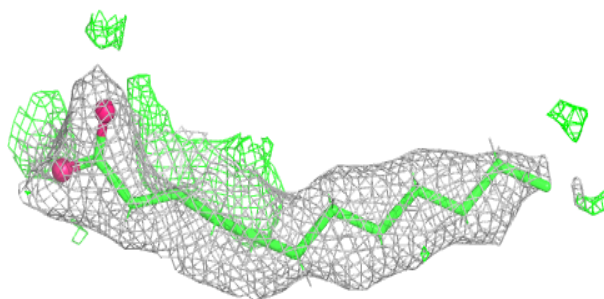
**Electron density around STE d 410:**

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

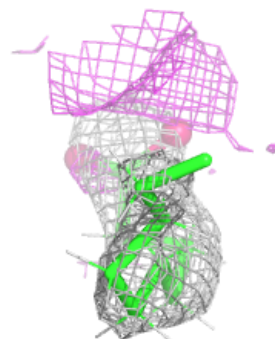
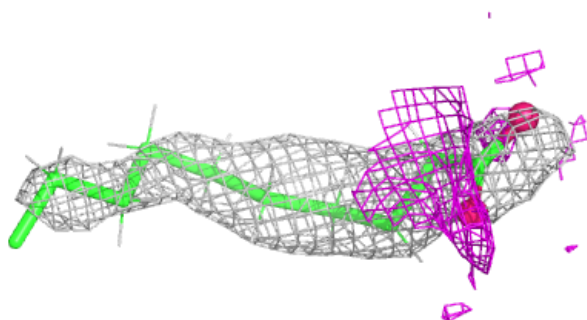
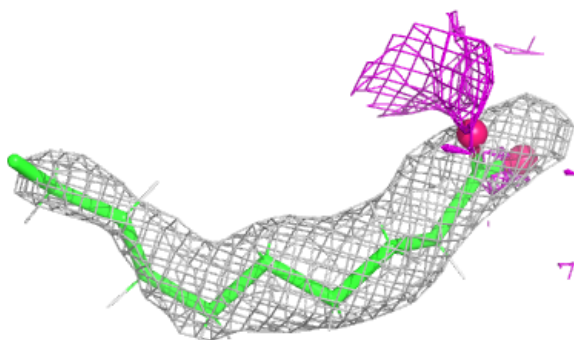


Electron density around STE d 412:

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

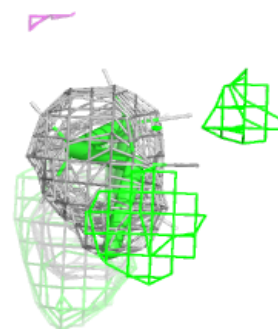
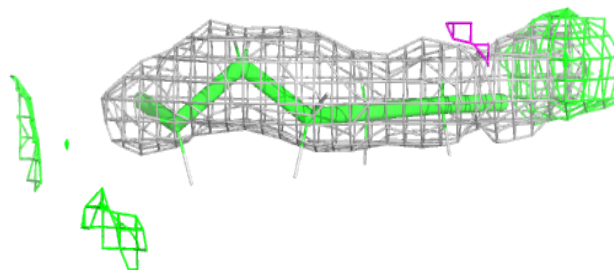
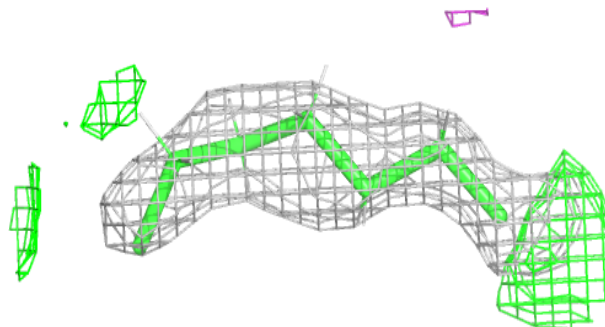
**Electron density around STE B 626:**

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

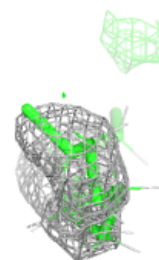
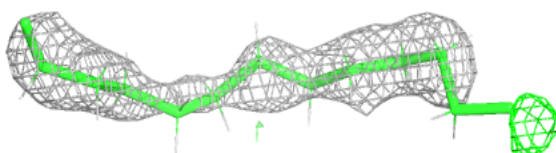
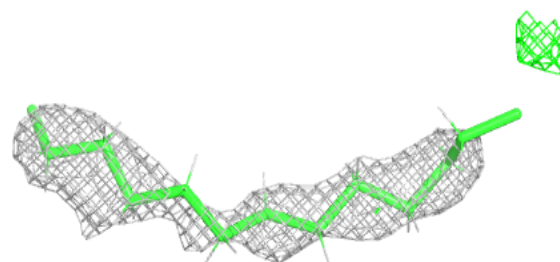


Electron density around STE C 518:

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

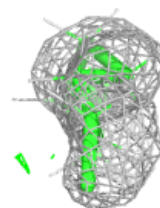
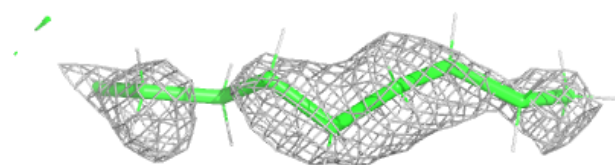
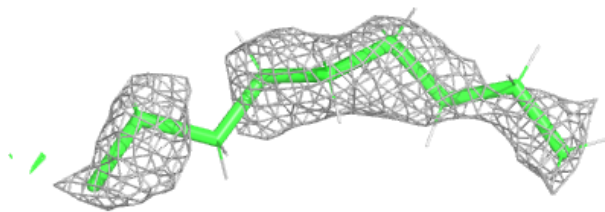
**Electron density around STE c 516:**

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

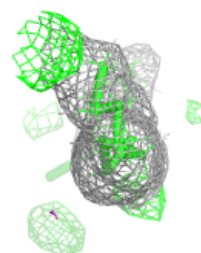
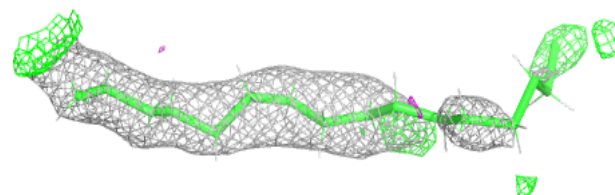
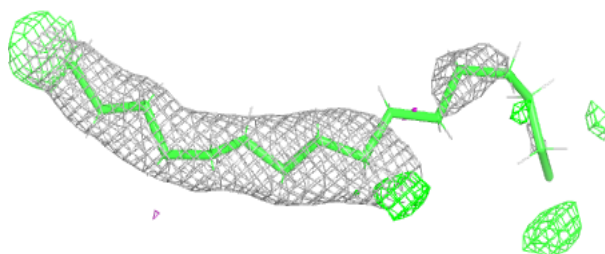


Electron density around STE e 103:

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

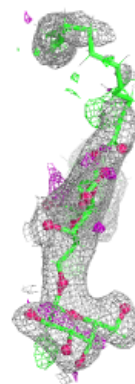
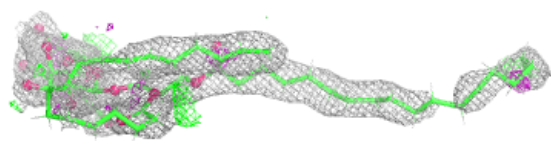
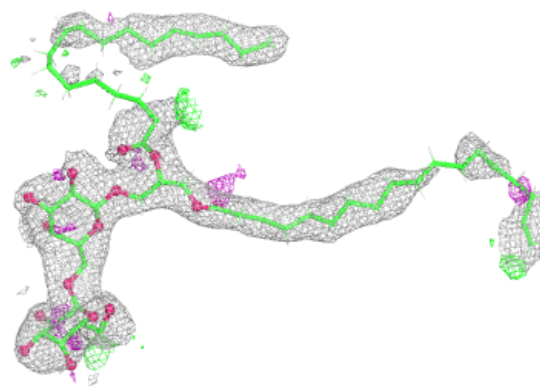
**Electron density around STE T 102:**

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

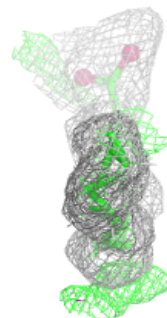
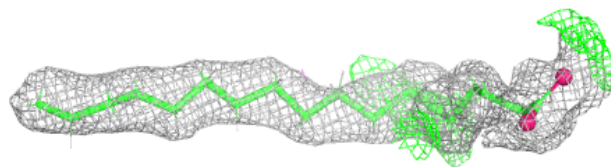
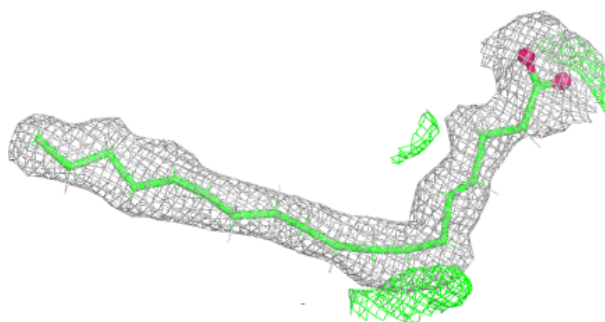


Electron density around DGD A 617:

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

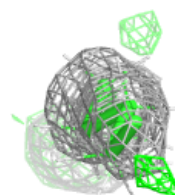
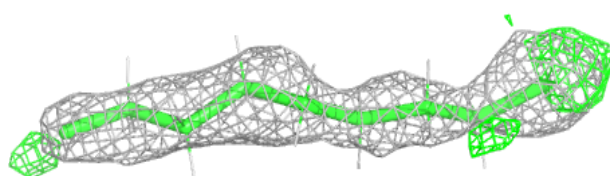
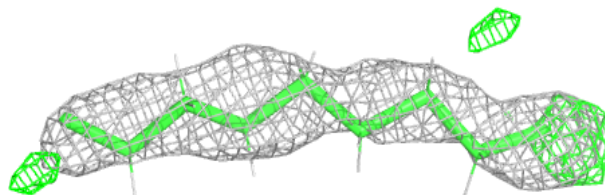
**Electron density around STE d 406:**

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

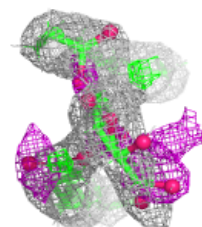
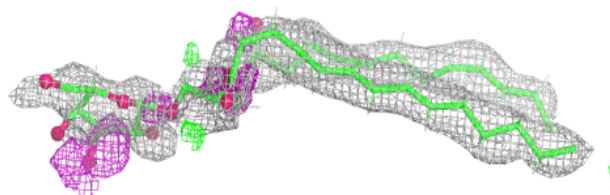
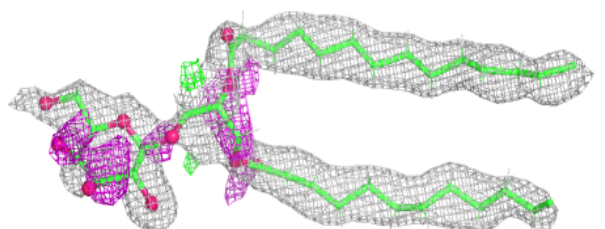


Electron density around STE z 101:

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

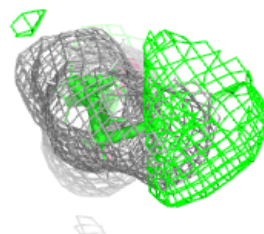
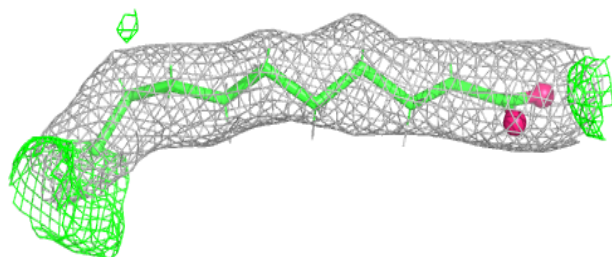
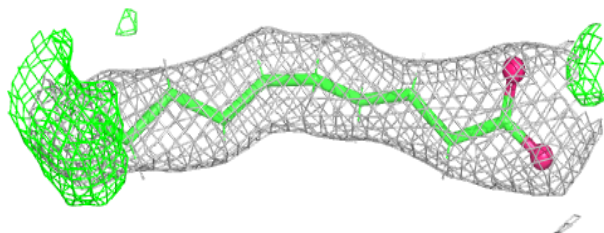
**Electron density around LMG B 620:**

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

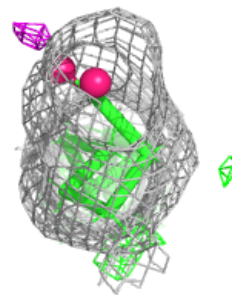
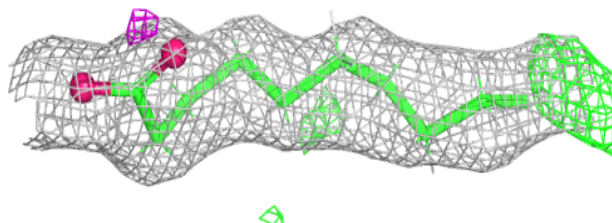
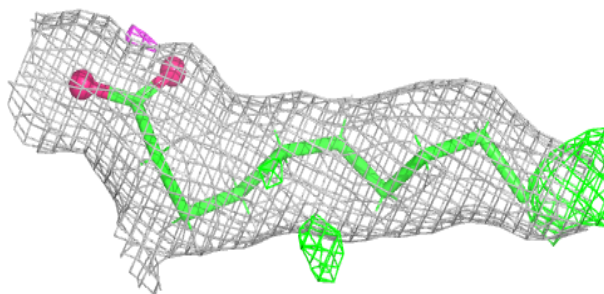


Electron density around STE j 101:

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

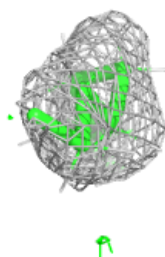
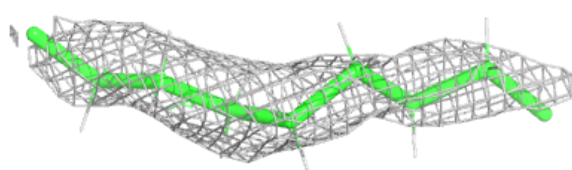
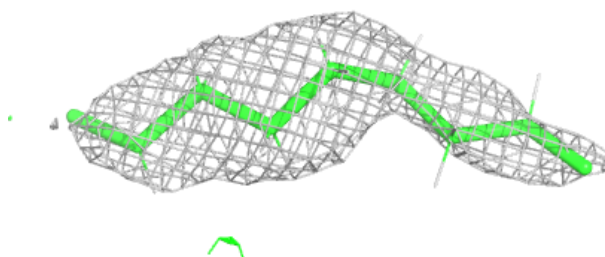
**Electron density around STE J 101:**

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

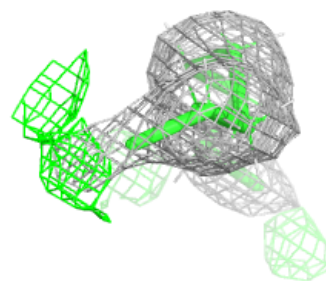
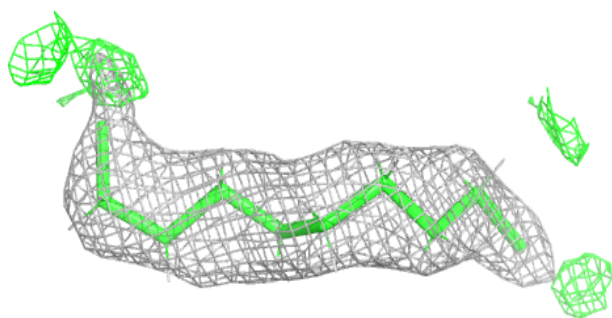
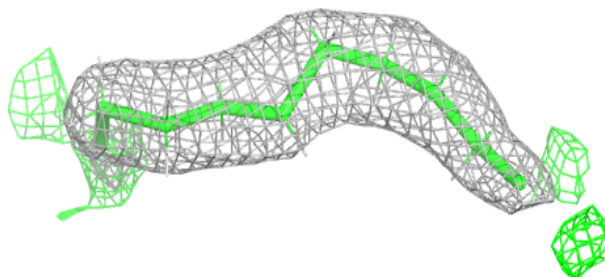


Electron density around STE A 612:

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

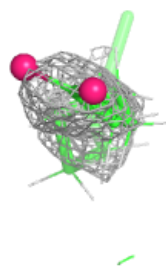
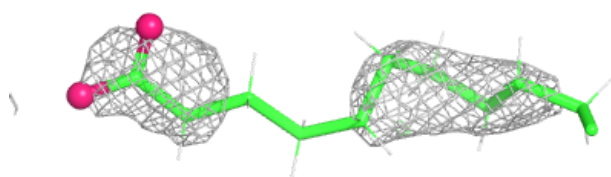
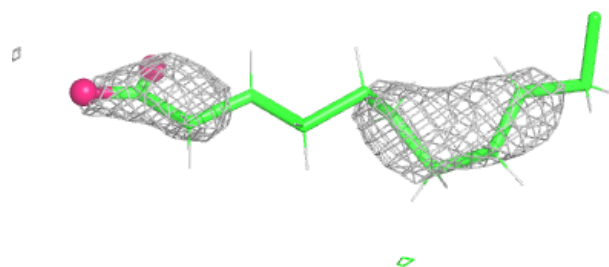
**Electron density around STE b 625:**

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

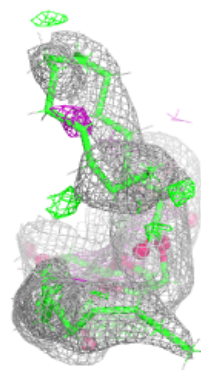
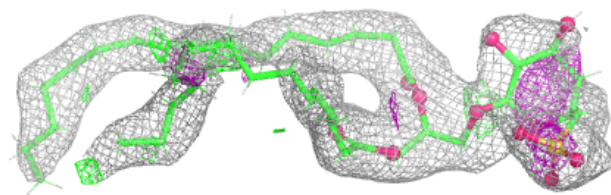
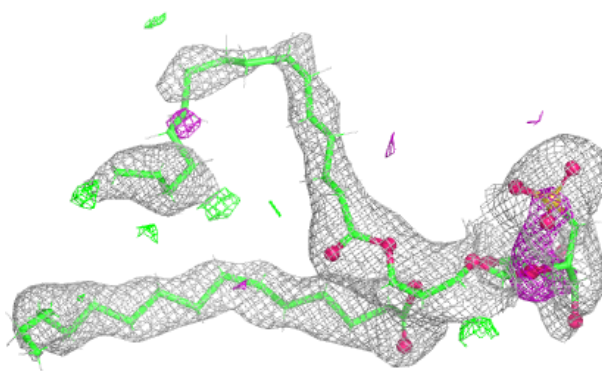


Electron density around STE e 104:

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

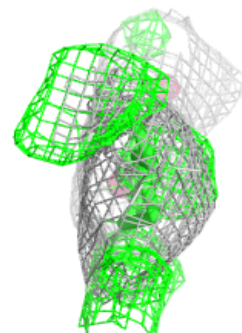
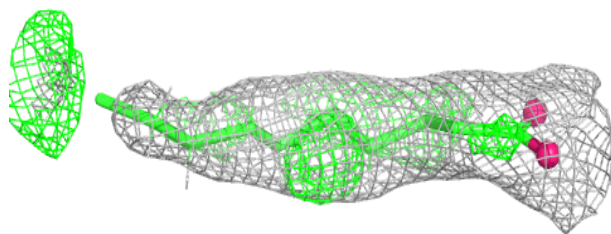
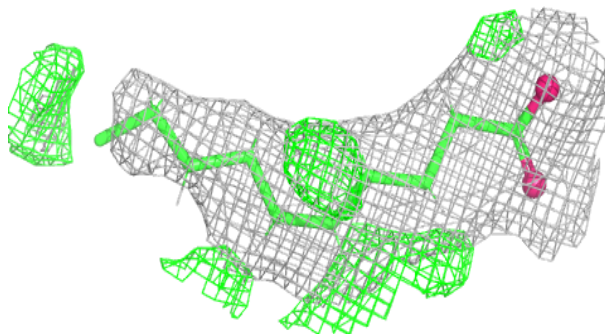
**Electron density around SQD a 615:**

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

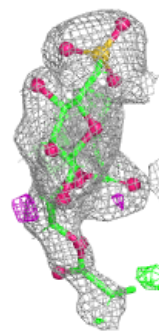
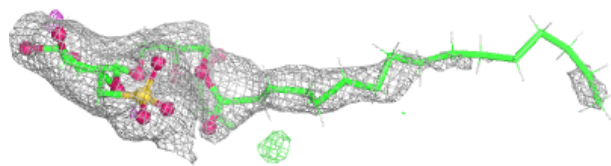
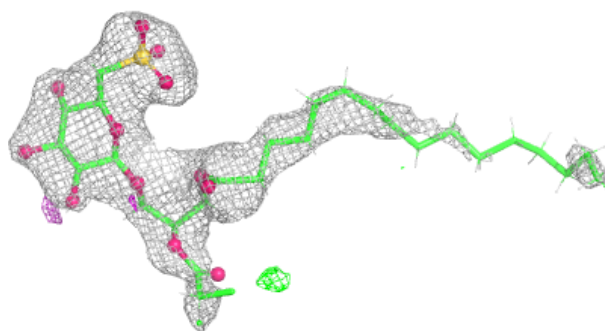


Electron density around STE C 524:

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

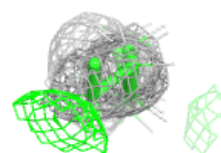
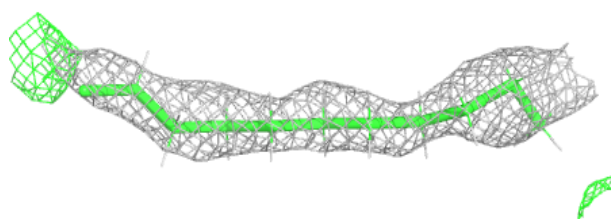
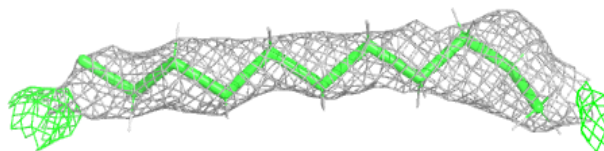
**Electron density around SQD f 101:**

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

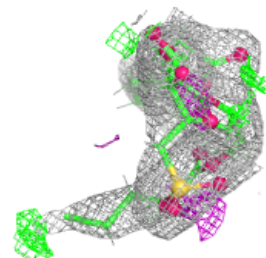
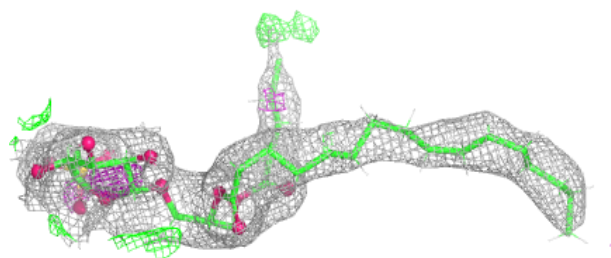
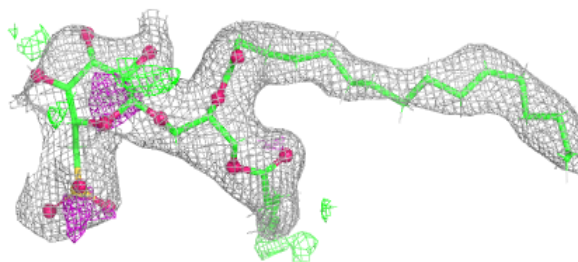


Electron density around STE h 104:

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

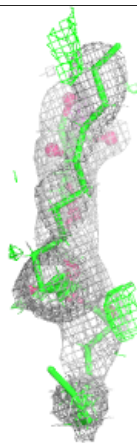
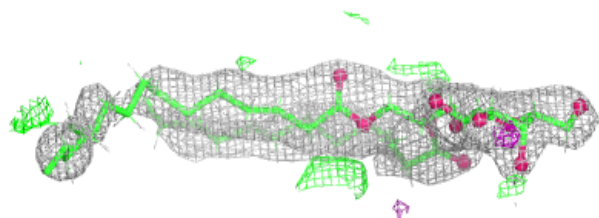
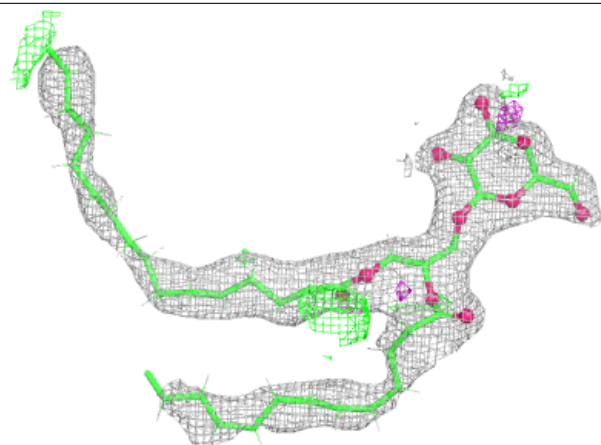
**Electron density around SQD A 616:**

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

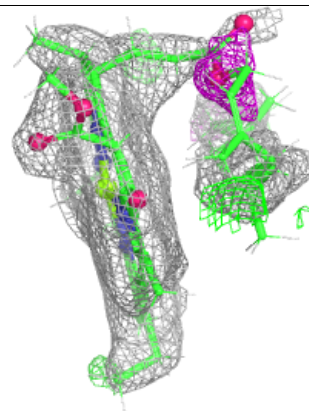
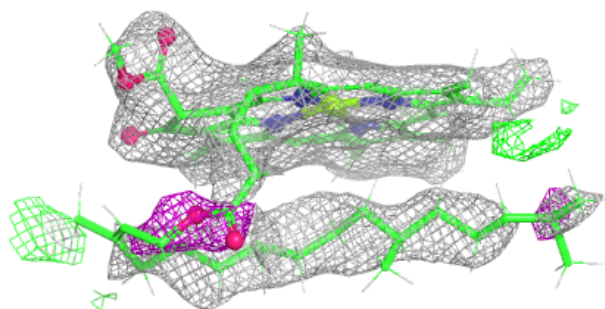
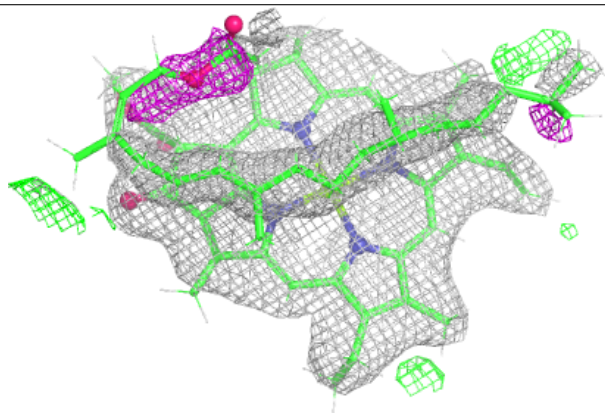


Electron density around LMG C 523:

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

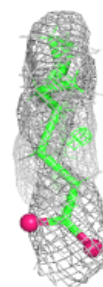
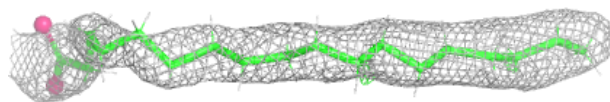
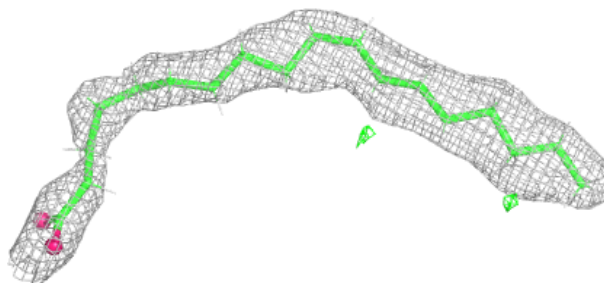
**Electron density around CLA b 601:**

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

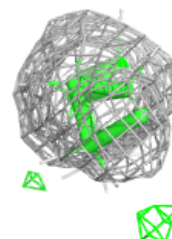
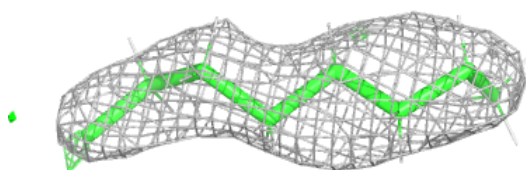
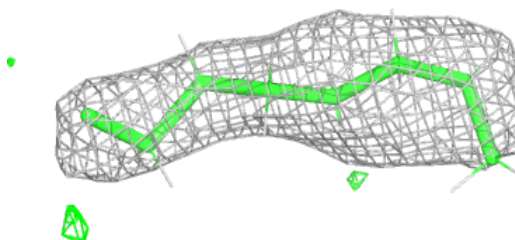


Electron density around STE x 101:

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

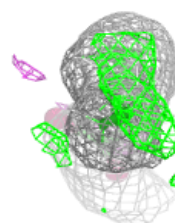
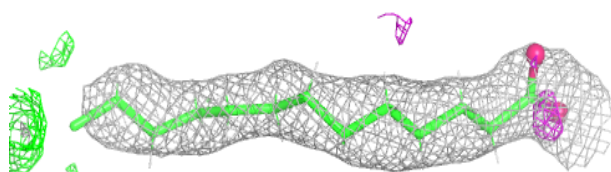
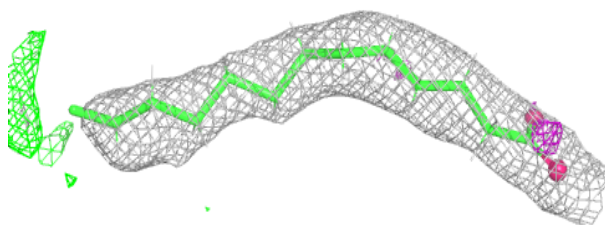
**Electron density around STE b 626:**

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

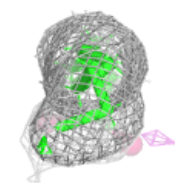
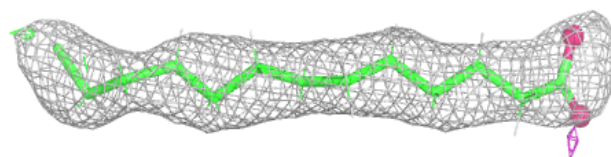
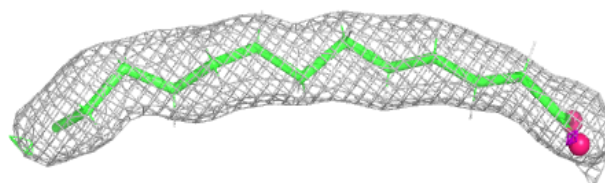


Electron density around STE I 102:

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

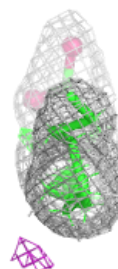
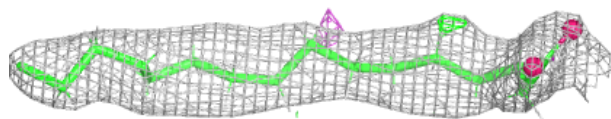
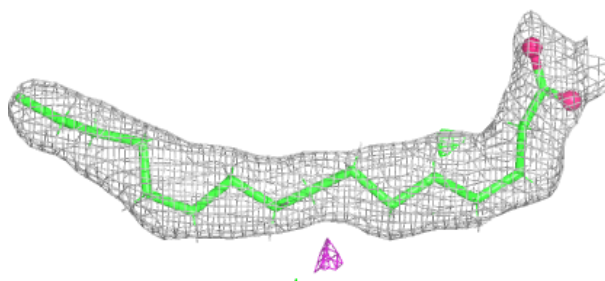
**Electron density around STE M 101:**

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

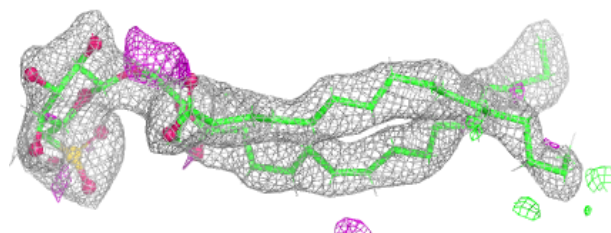
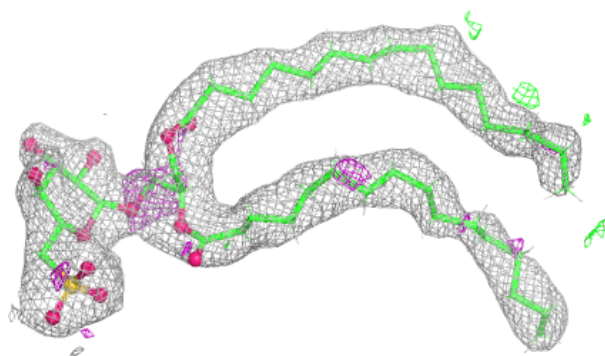


Electron density around STE B 625:

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

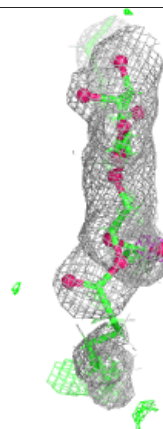
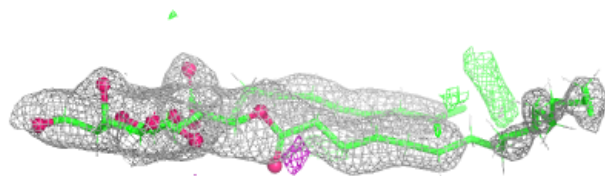
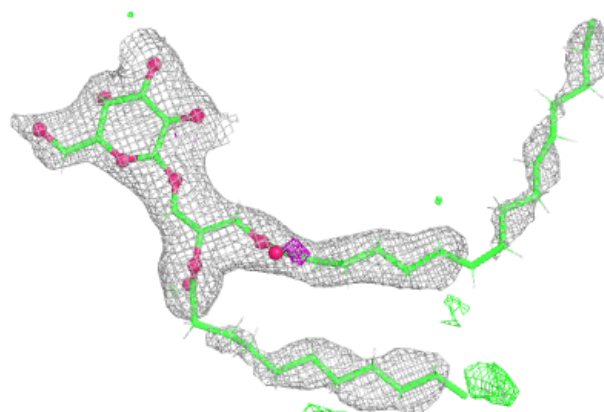
**Electron density around SQD B 624:**

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

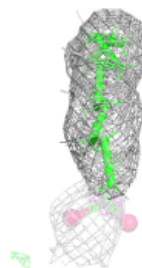
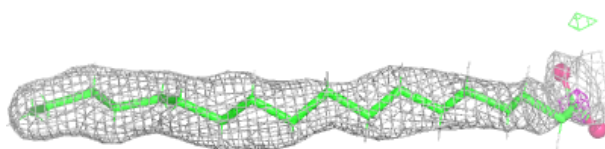
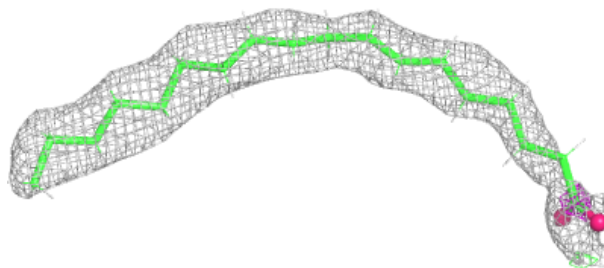


Electron density around LMG c 522:

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

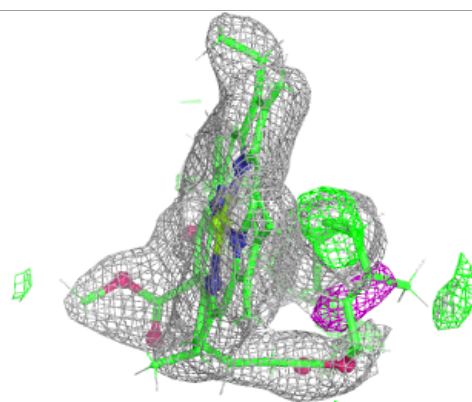
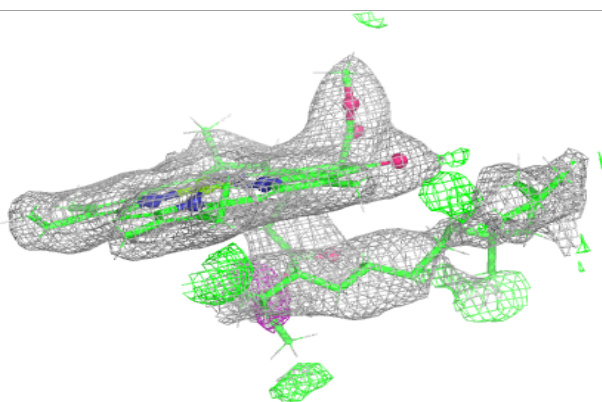
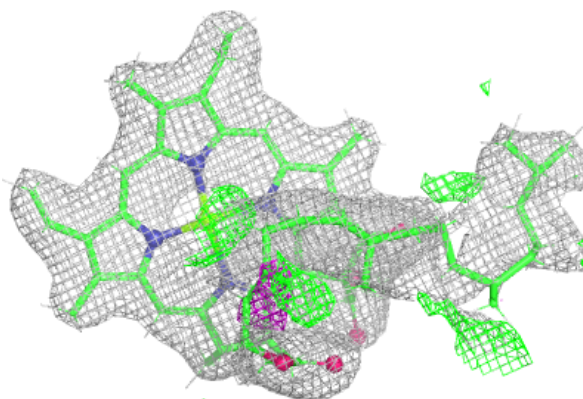
**Electron density around STE X 101:**

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

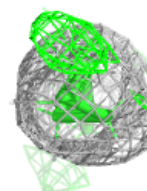
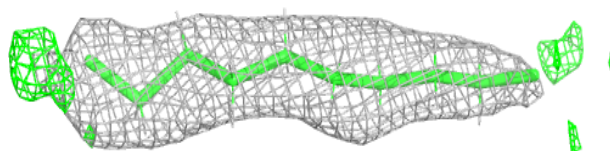
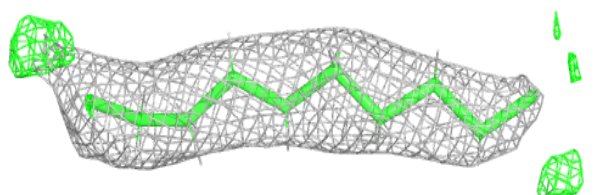


Electron density around CLA B 601:

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

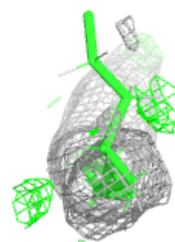
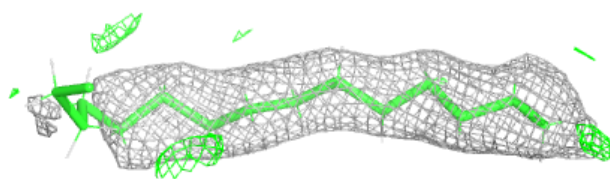
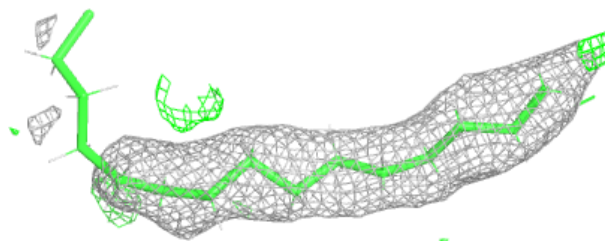
**Electron density around STE M 102:**

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

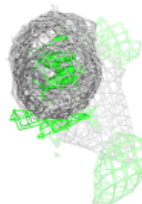
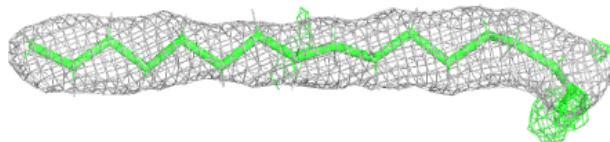
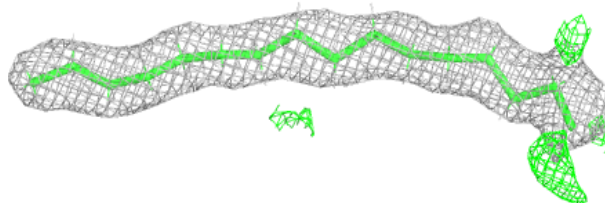


Electron density around STE M 103:

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

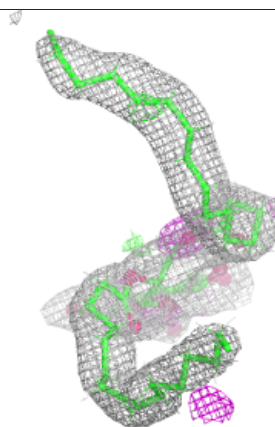
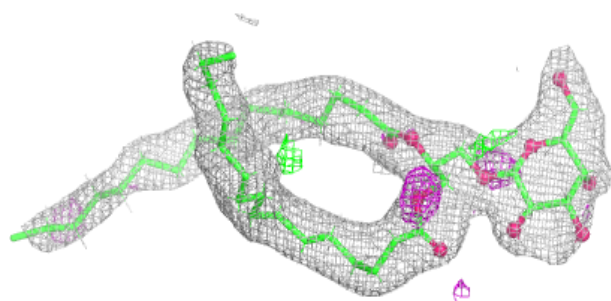
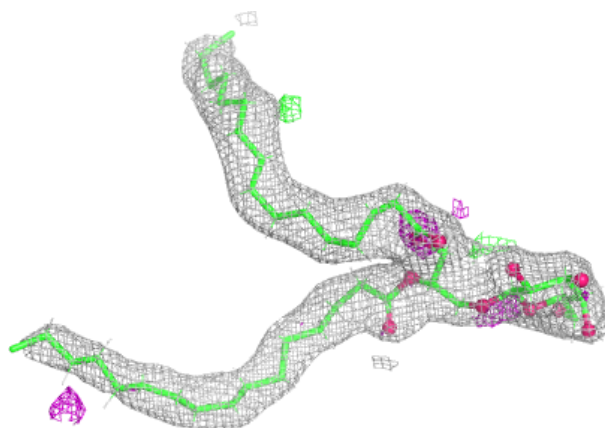
**Electron density around STE C 525:**

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

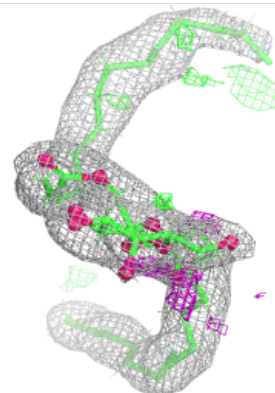
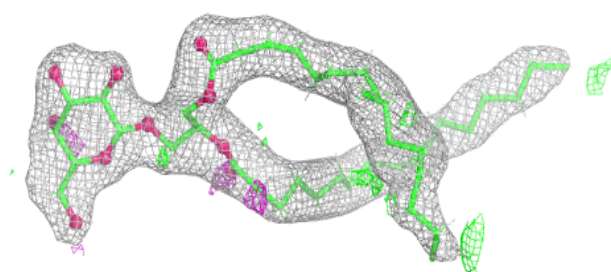
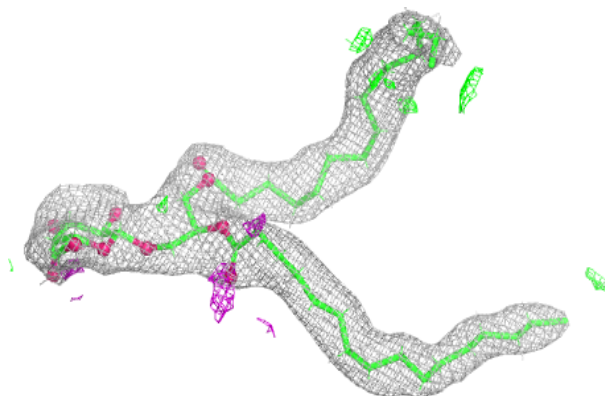


Electron density around LMG b 621:

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

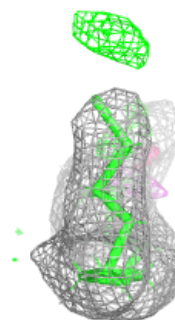
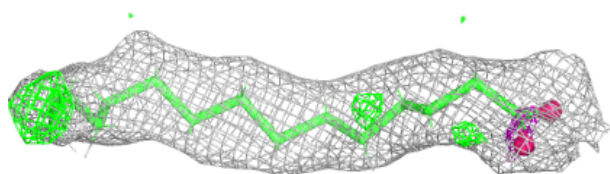
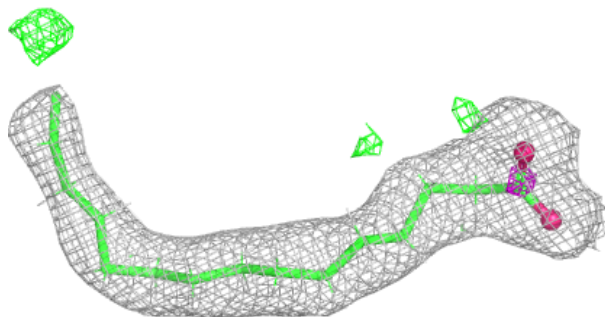
**Electron density around LMG B 621:**

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

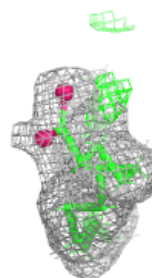
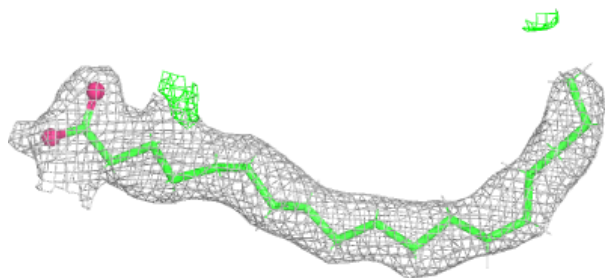


Electron density around STE B 622:

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

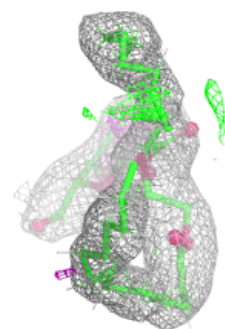
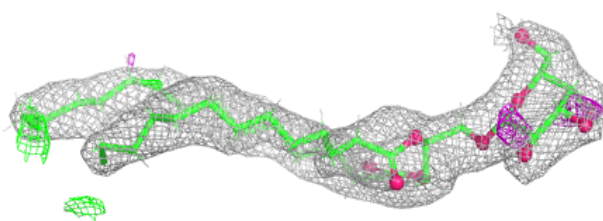
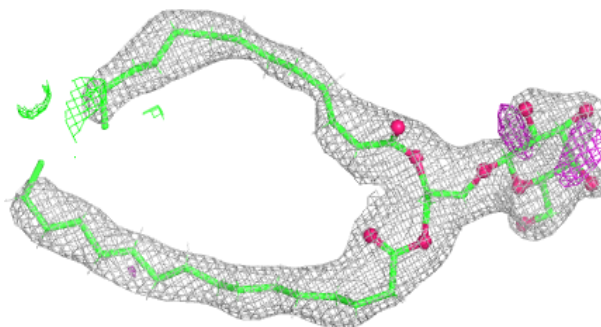
**Electron density around STE b 622:**

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

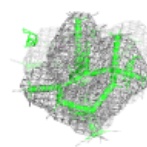
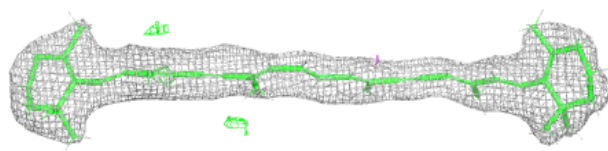
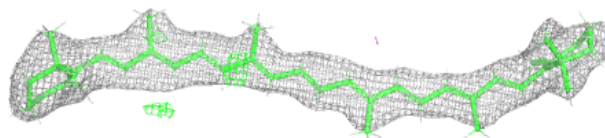


Electron density around LMG A 614:

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

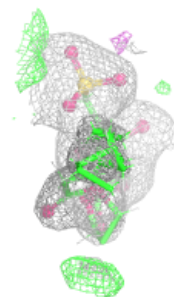
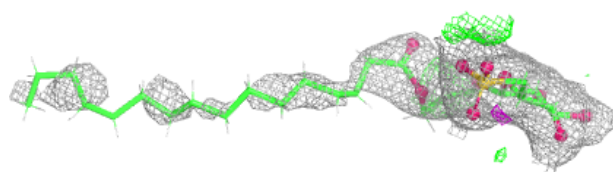
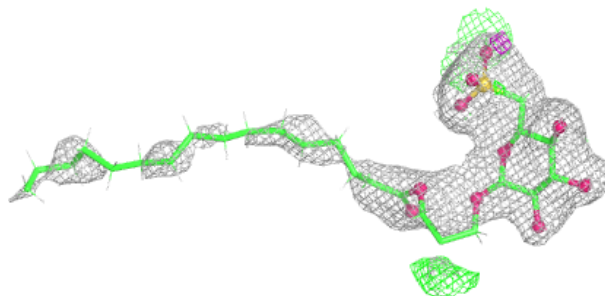
**Electron density around BCR K 101:**

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



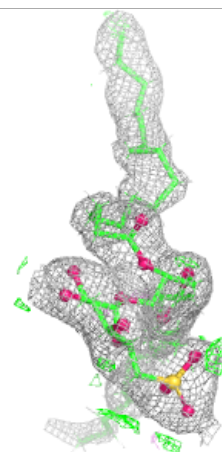
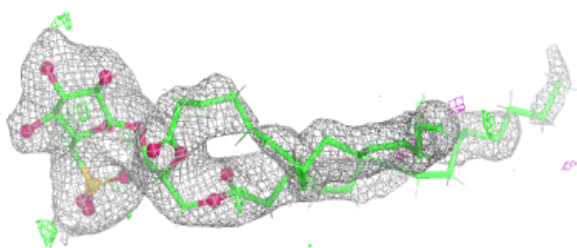
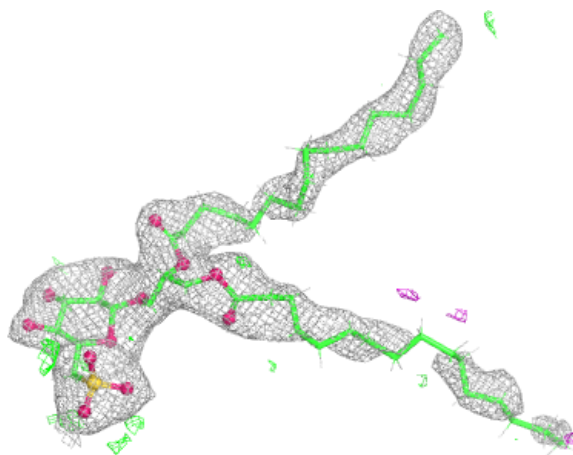
Electron density around SQD D 408:

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



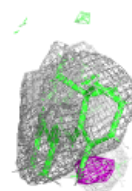
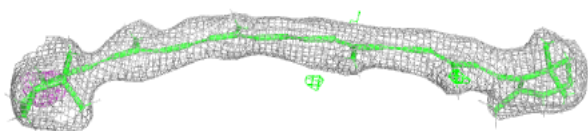
Electron density around SQD a 613:

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

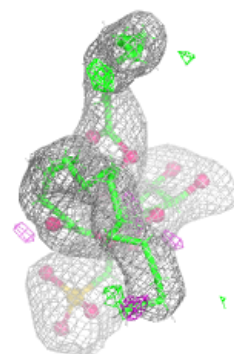
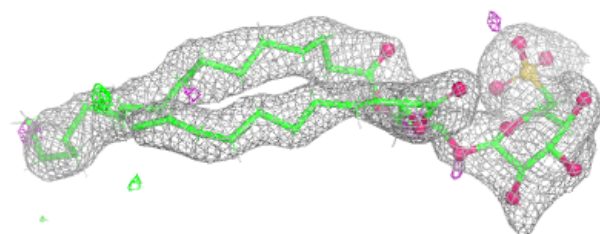
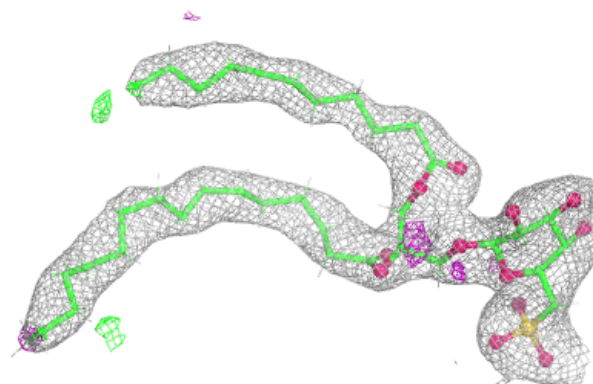


Electron density around BCR d 404:

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

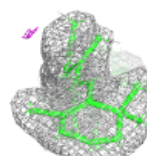
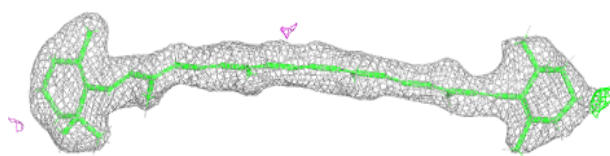
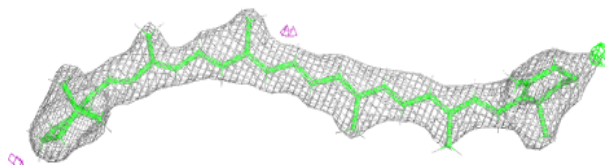
**Electron density around SQD b 620:**

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

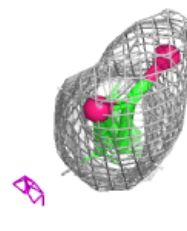
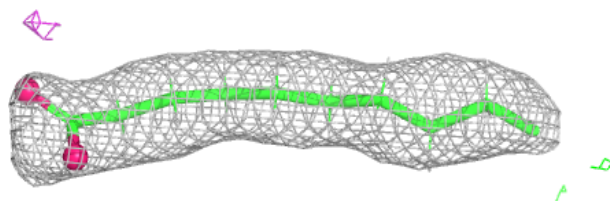
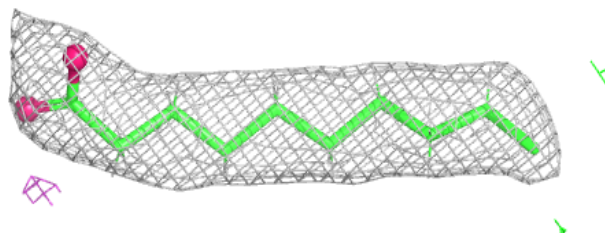


Electron density around BCR h 101:

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

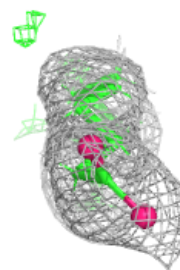
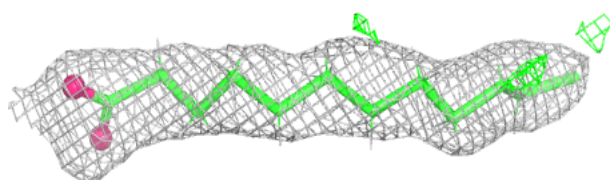
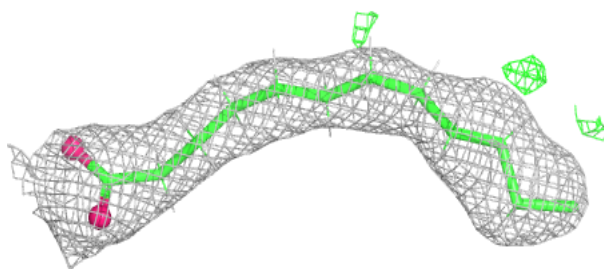
**Electron density around STE m 101:**

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

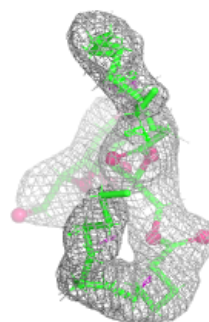
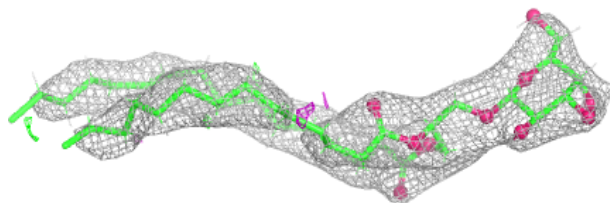
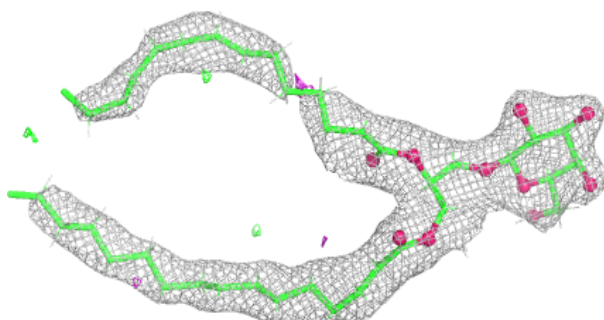


Electron density around STE t 102:

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

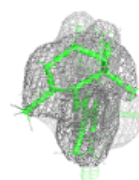
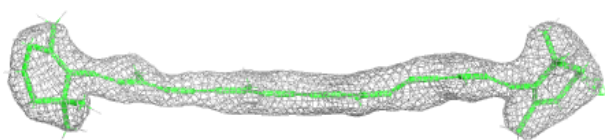
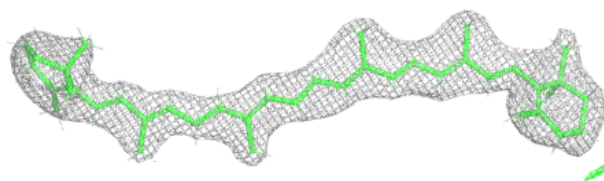
**Electron density around LMG a 617:**

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

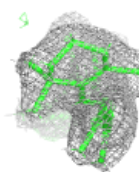
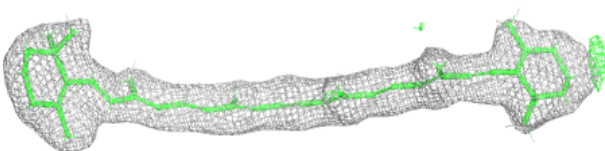
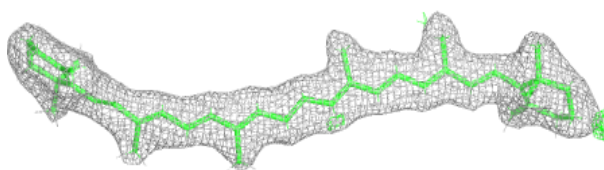


Electron density around BCR k 101:

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

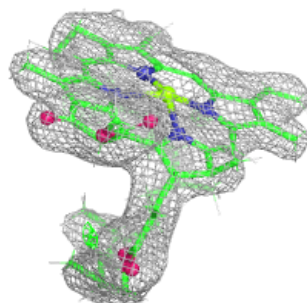
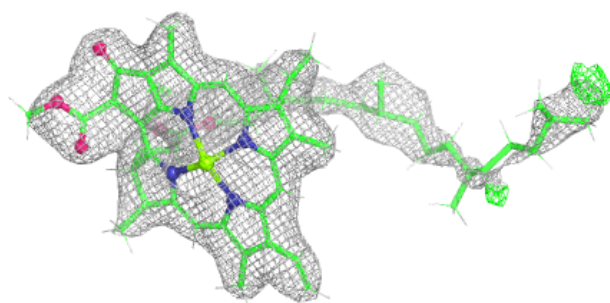
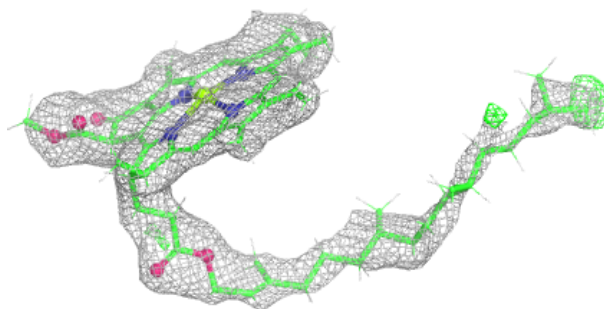
**Electron density around BCR H 101:**

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

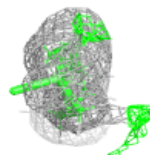
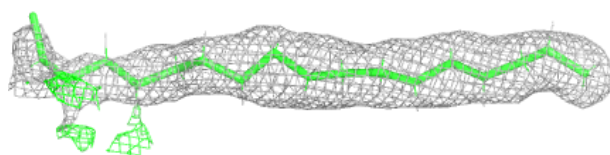
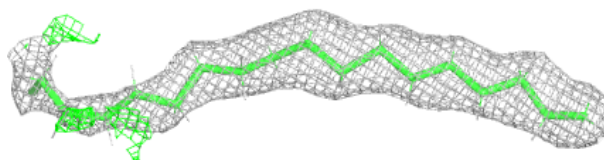


Electron density around CLA C 513:

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

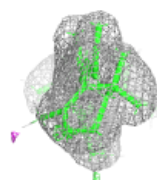
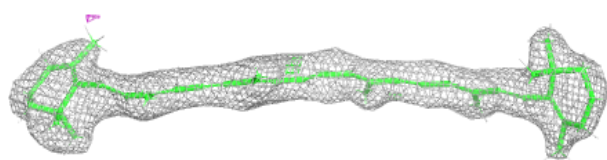
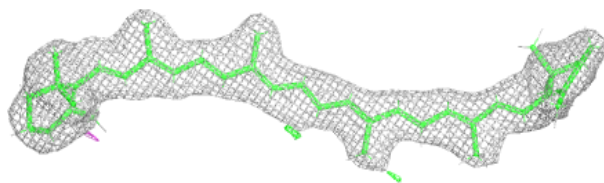
**Electron density around STE I 102:**

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

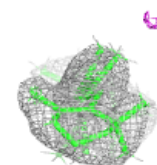
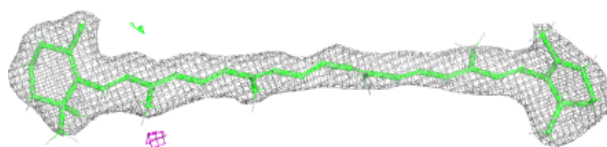
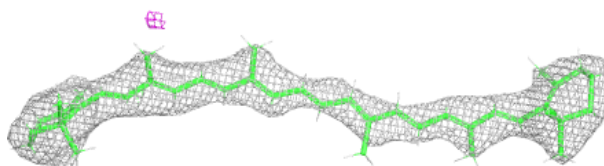


Electron density around BCR Y 101:

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

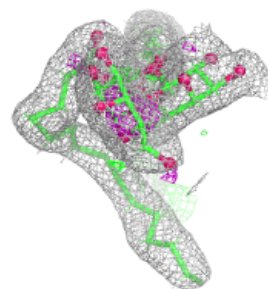
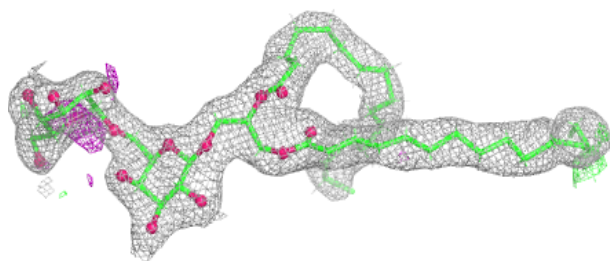
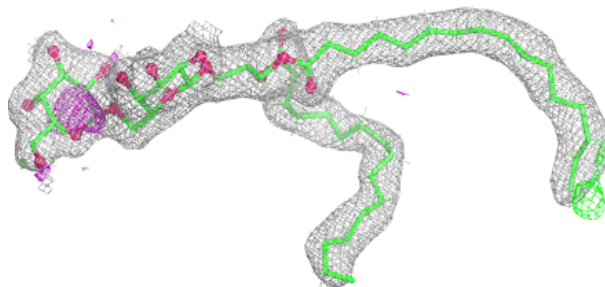
**Electron density around BCR c 514:**

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

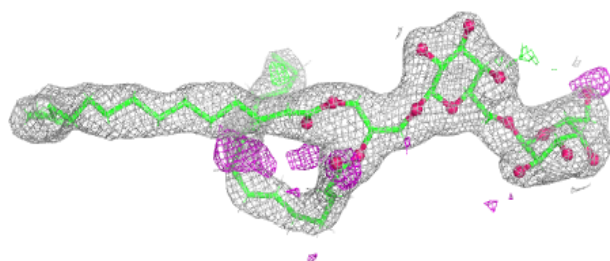
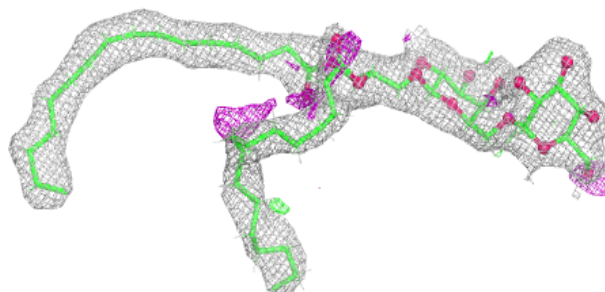


Electron density around DGD H 102:

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

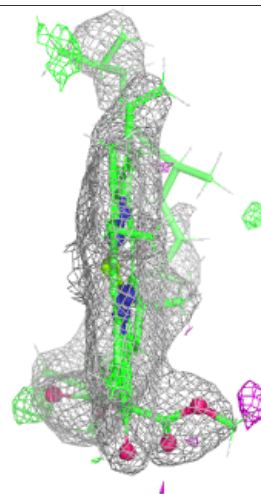
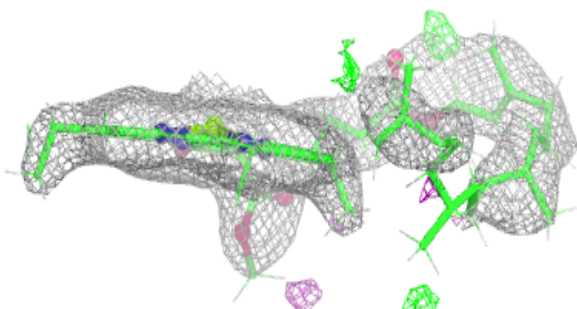
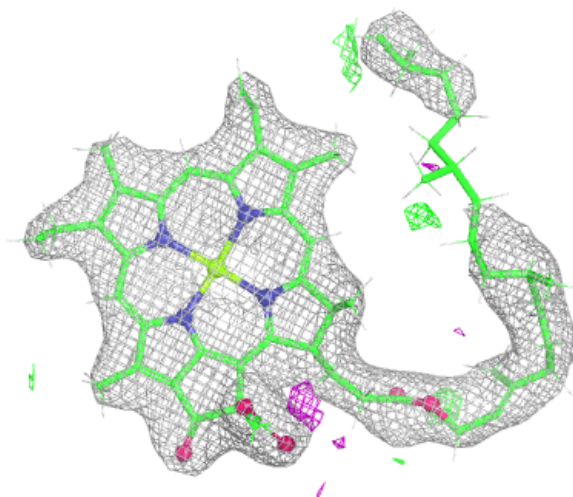
**Electron density around DGD h 102:**

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



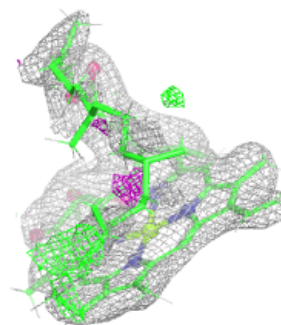
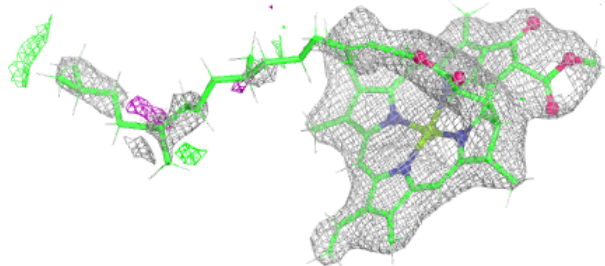
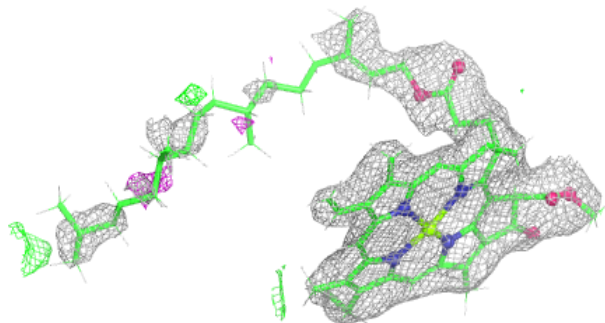
Electron density around CLA c 512:

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

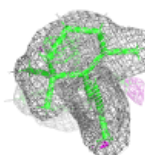
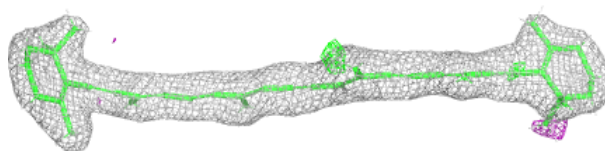
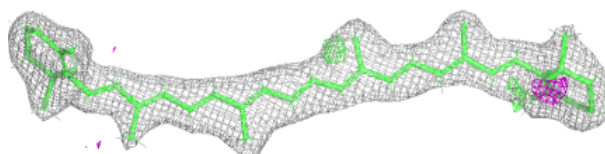


Electron density around CLA c 513:

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

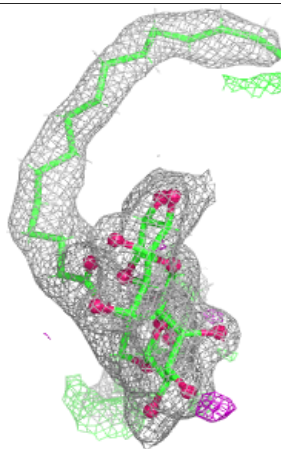
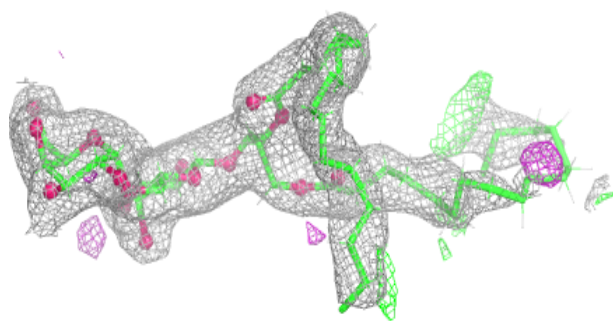
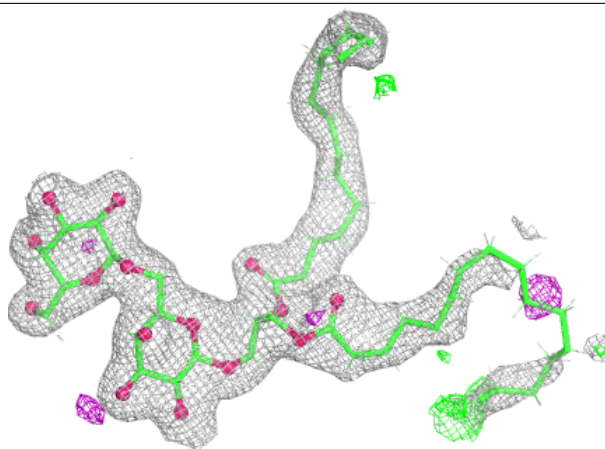
**Electron density around BCR C 514:**

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



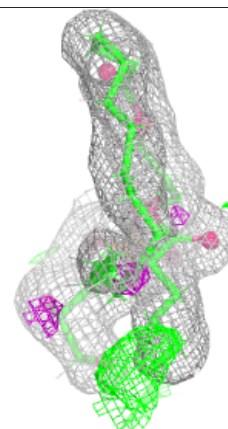
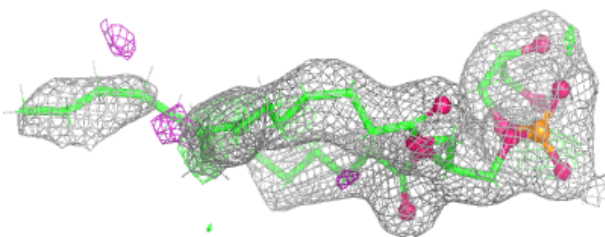
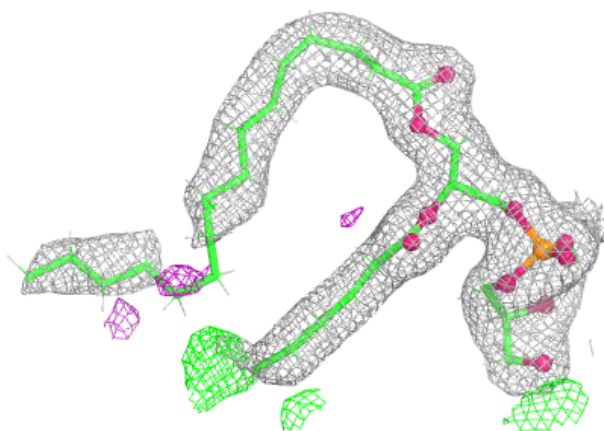
Electron density around DGD C 521:

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

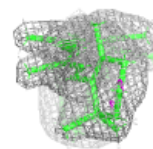
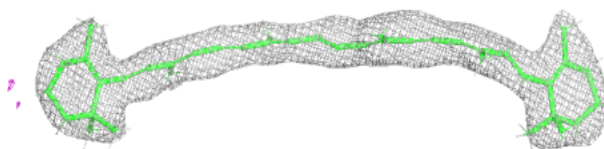


Electron density around LHG d 409:

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

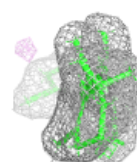
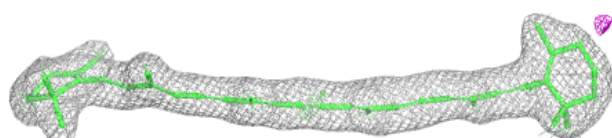
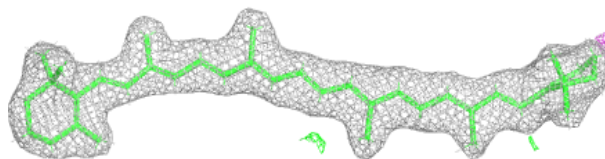
**Electron density around BCR K 102:**

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

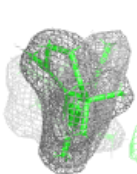
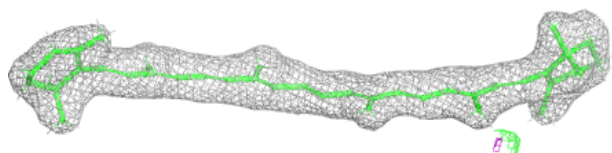
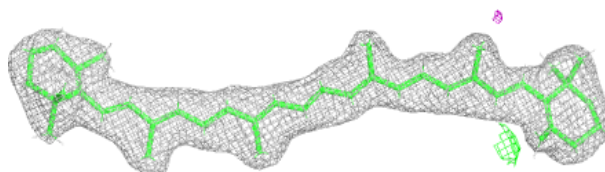


Electron density around BCR B 617:

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

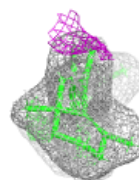
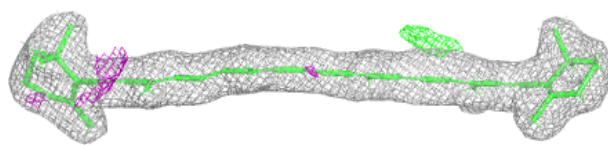
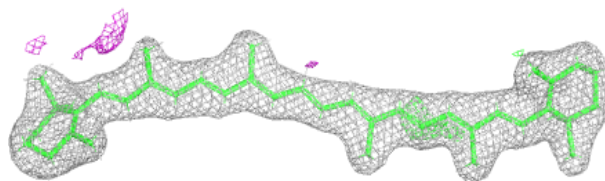
**Electron density around BCR b 619:**

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

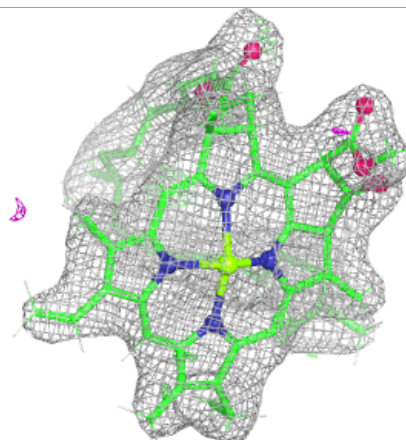
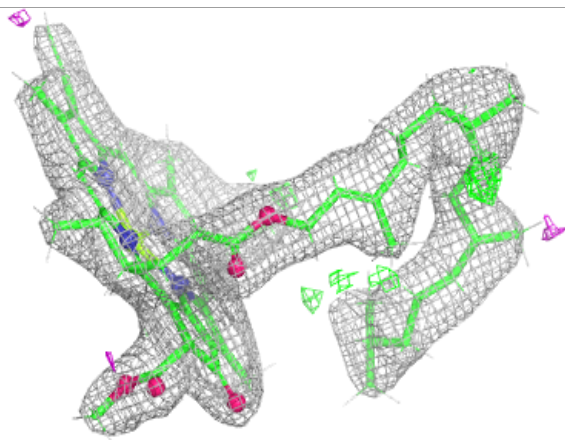
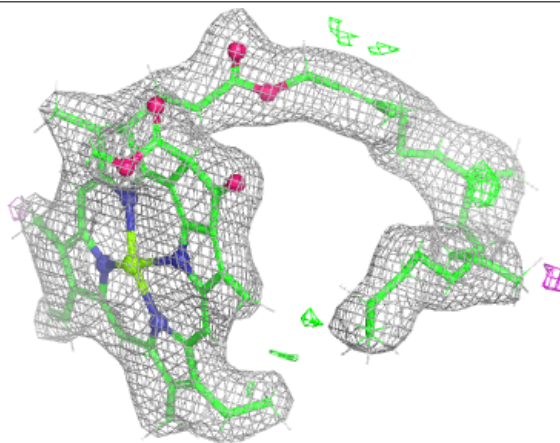


Electron density around BCR B 618:

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

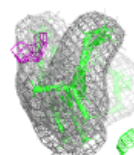
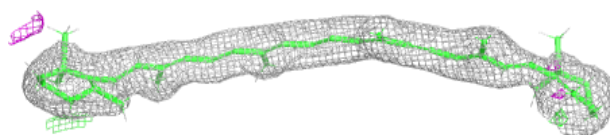
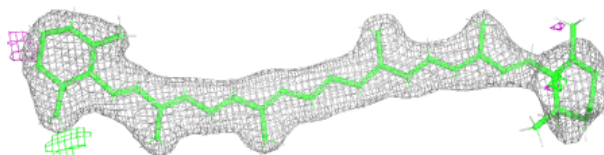
**Electron density around CLA c 503:**

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

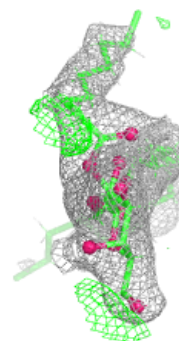
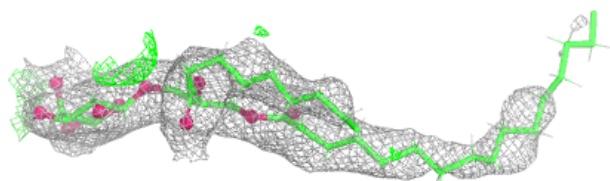
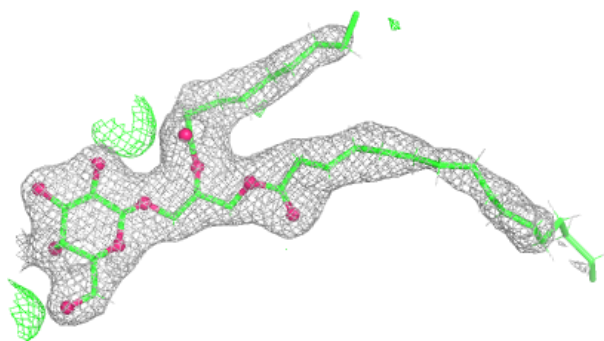


Electron density around BCR D 404:

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

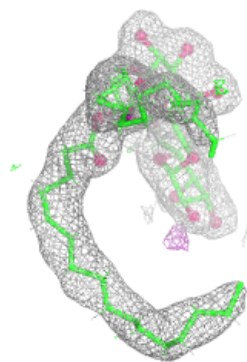
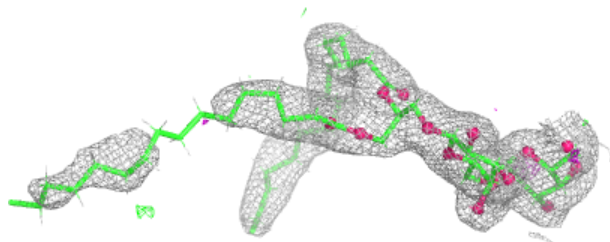
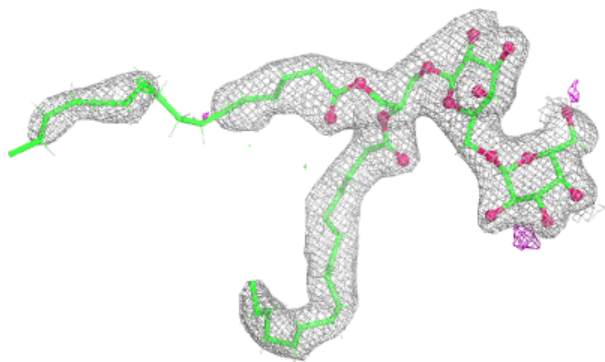
**Electron density around LMG d 411:**

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



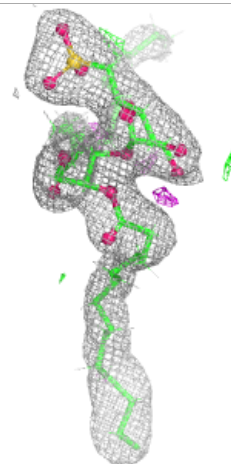
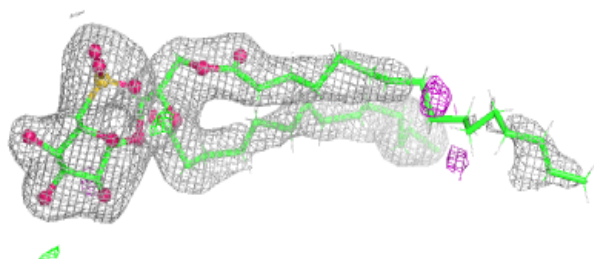
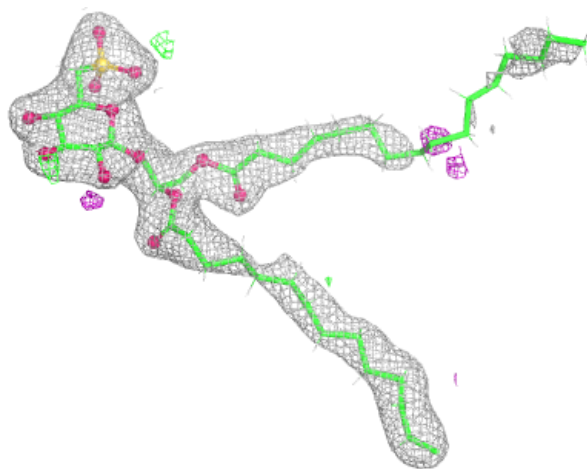
Electron density around DGD c 520:

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



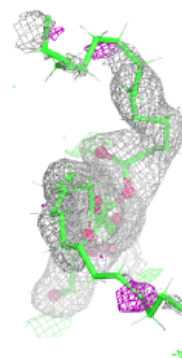
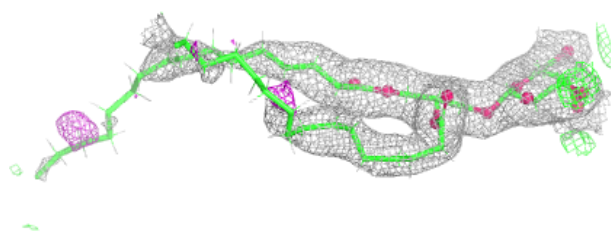
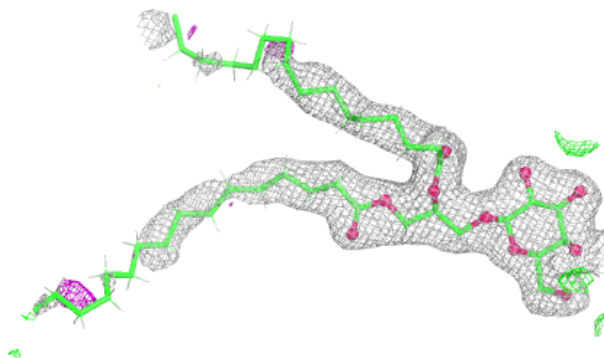
Electron density around SQD A 615:

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

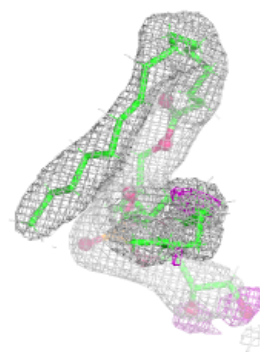
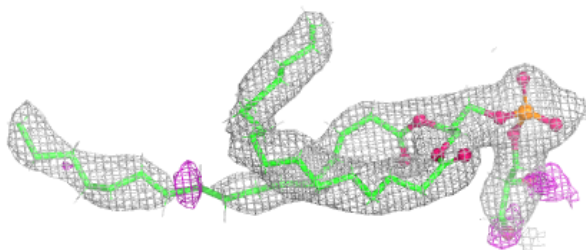
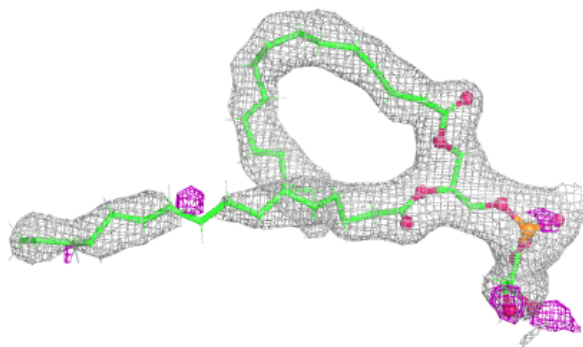


Electron density around LMG D 407:

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

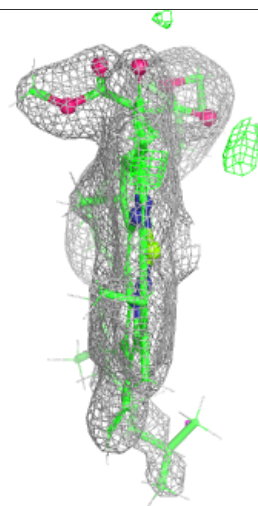
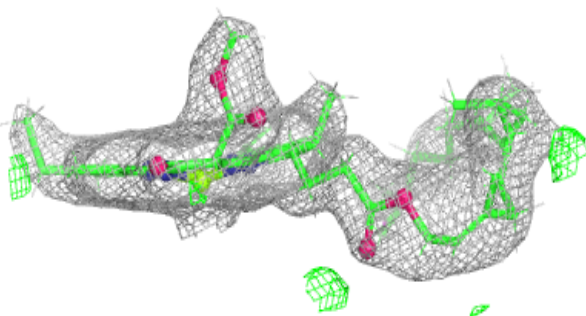
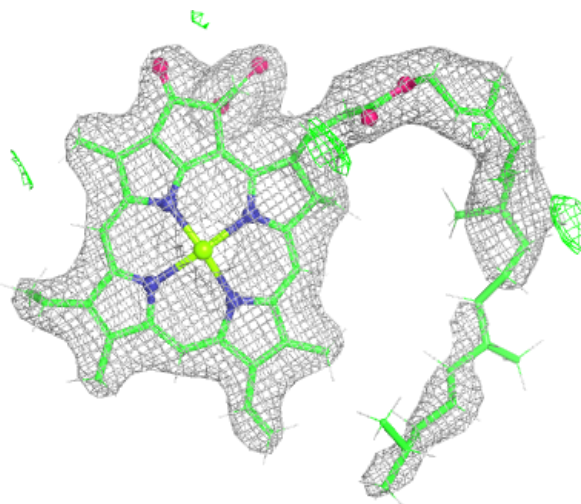
**Electron density around LHG d 407:**

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



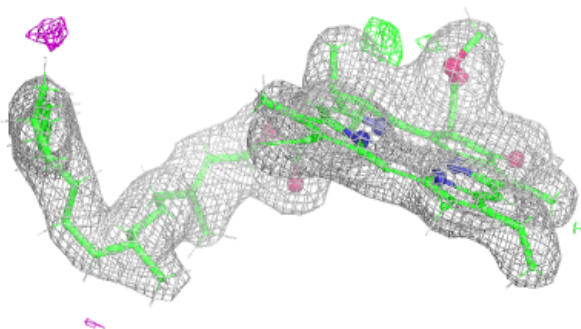
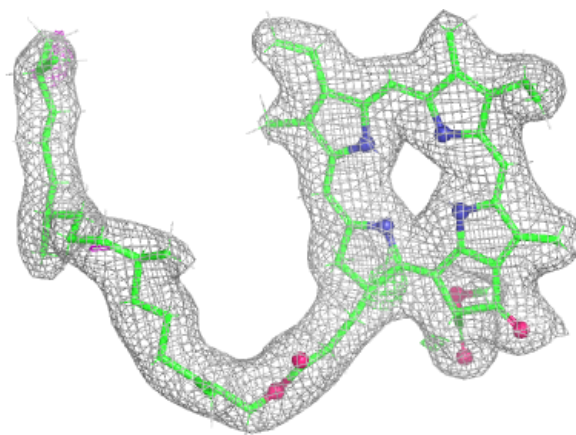
Electron density around CLA C 512:

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

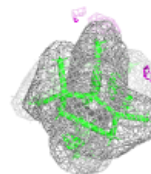
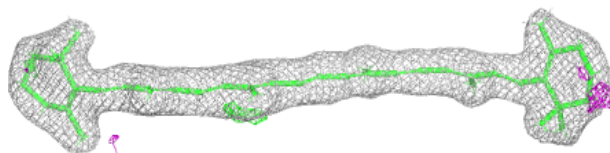
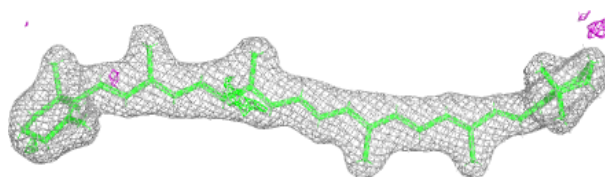


Electron density around PHO d 401:

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

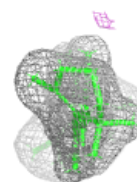
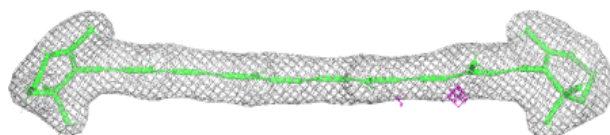
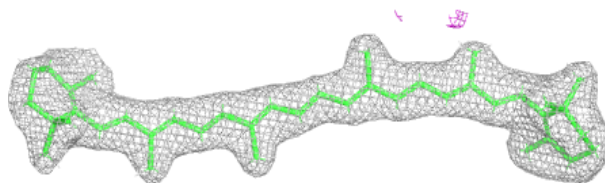
**Electron density around BCR A 610:**

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



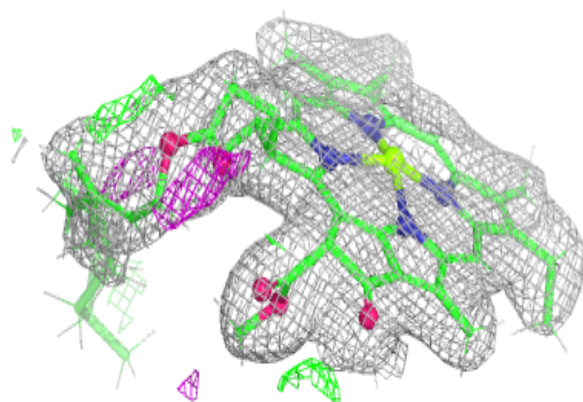
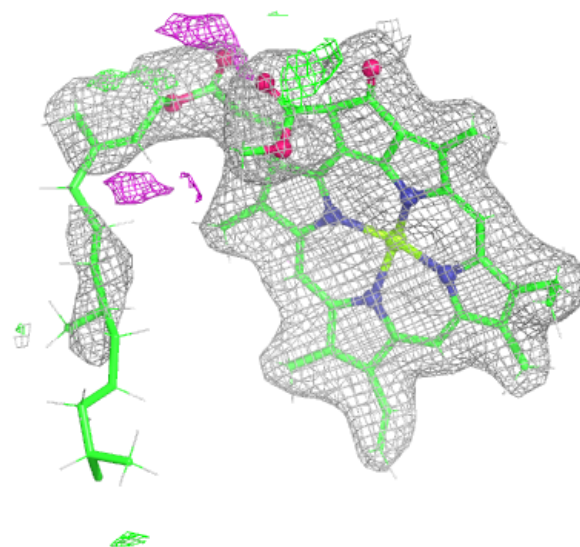
Electron density around BCR b 618:

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



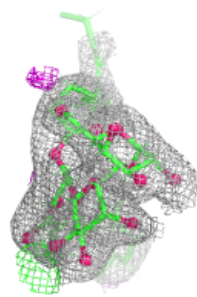
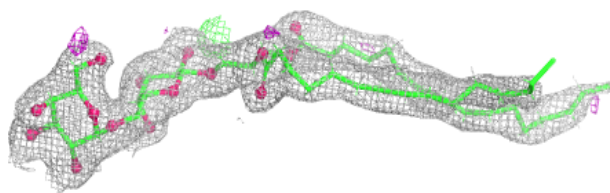
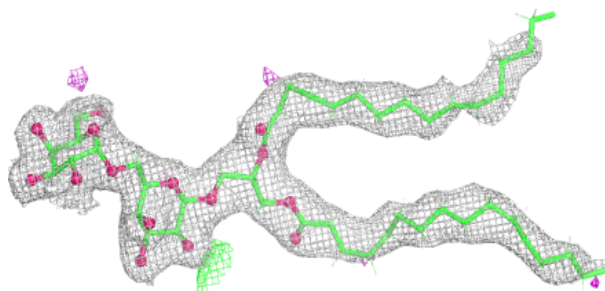
Electron density around CLA b 616:

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

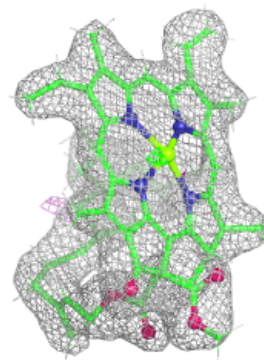
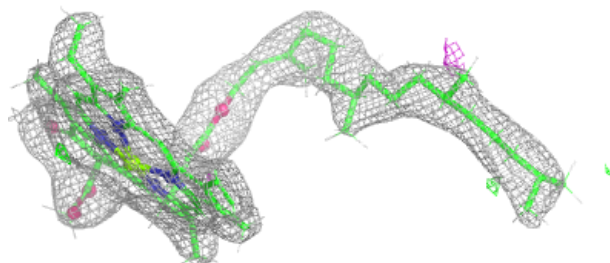
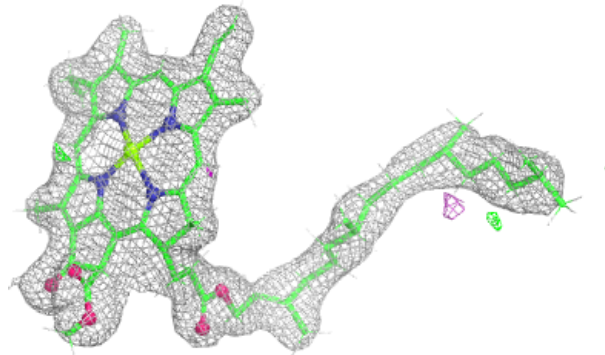


Electron density around DGD C 522:

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

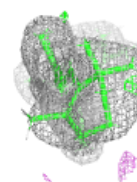
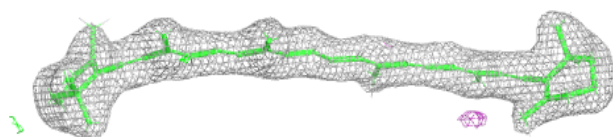
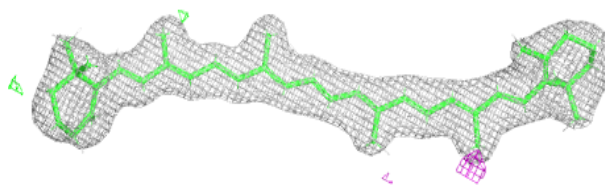
**Electron density around CLA C 511:**

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

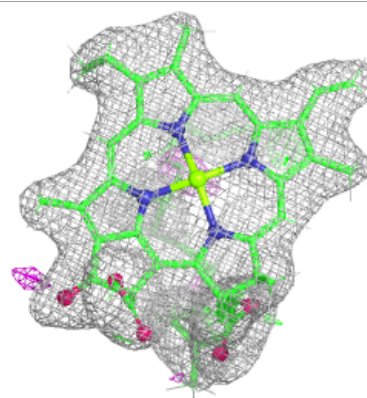
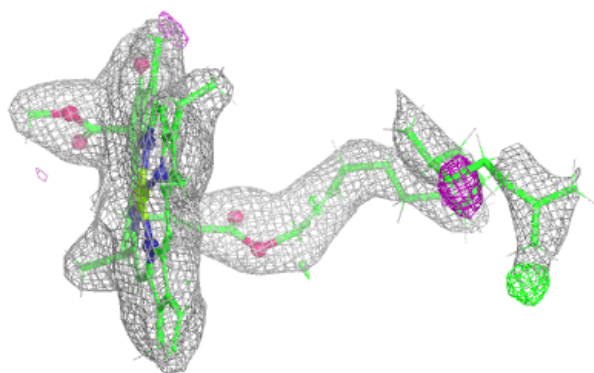
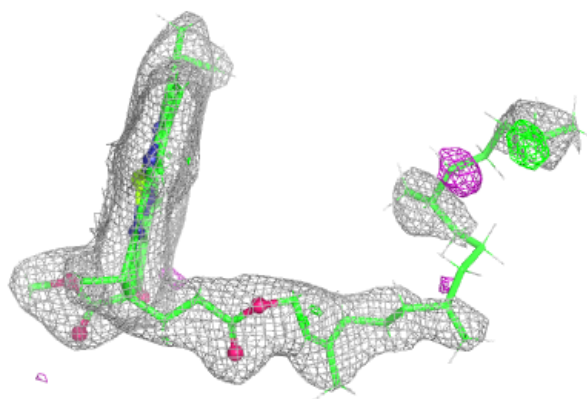


Electron density around BCR B 619:

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

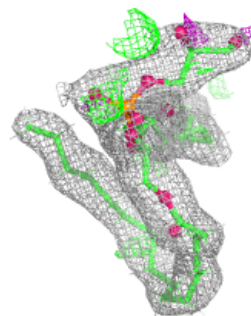
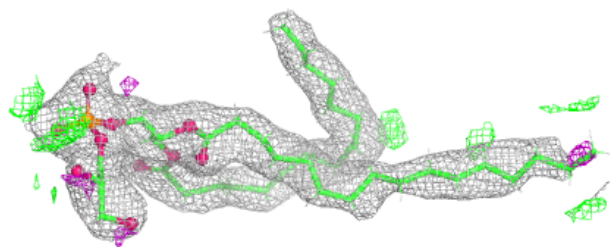
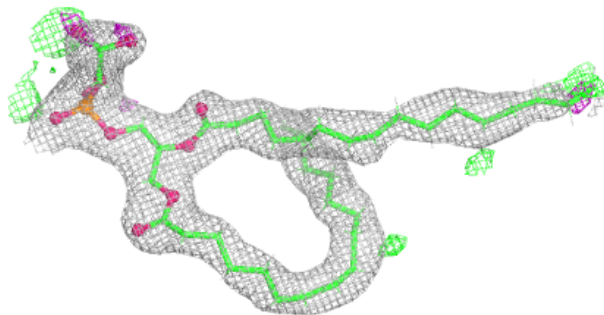
**Electron density around CLA c 506:**

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



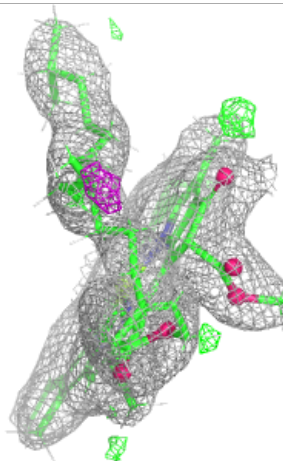
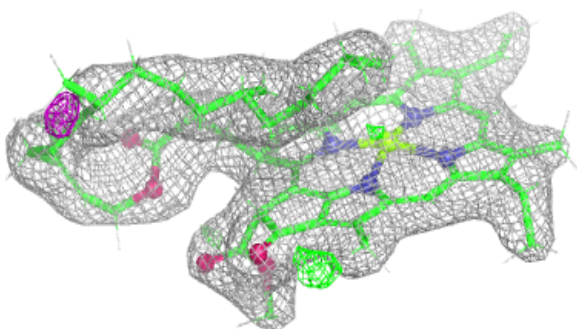
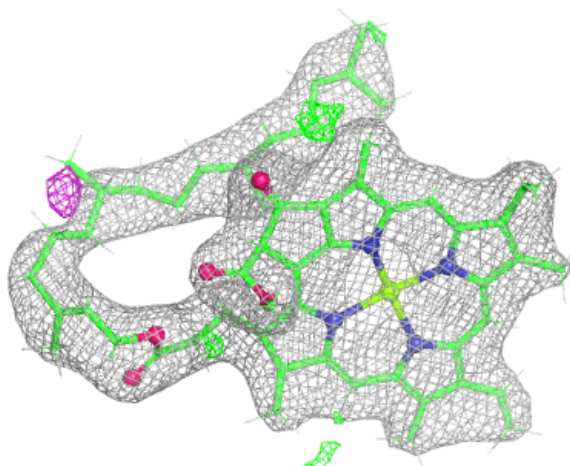
Electron density around LHG B 623:

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



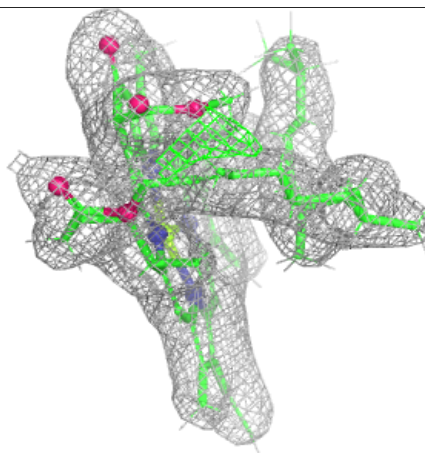
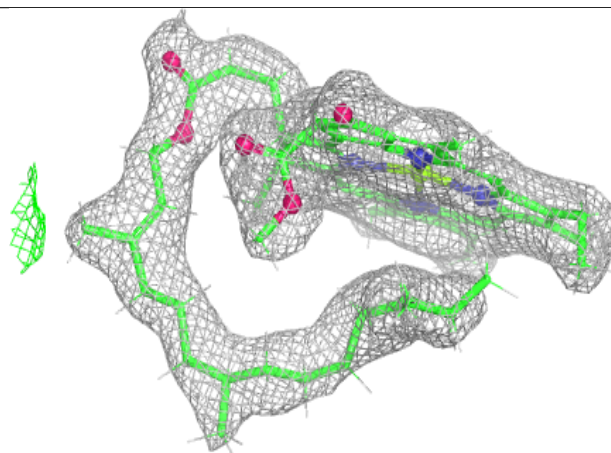
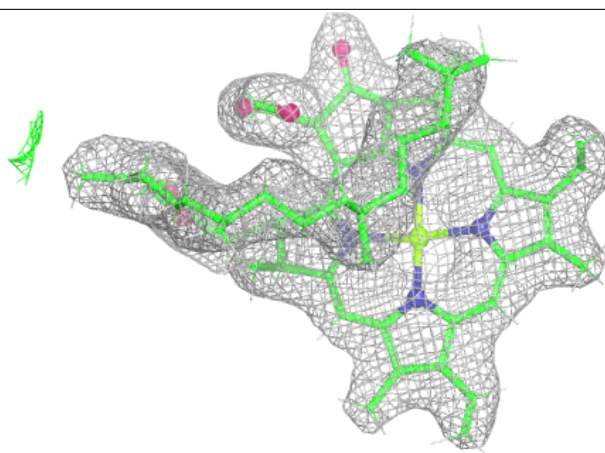
Electron density around CLA c 509:

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

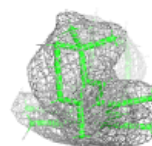
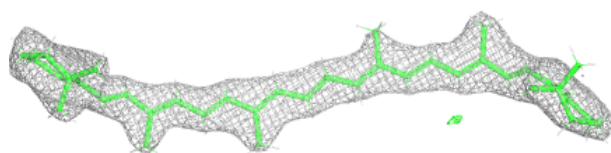
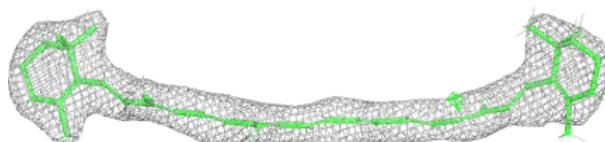


Electron density around CLA C 510:

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

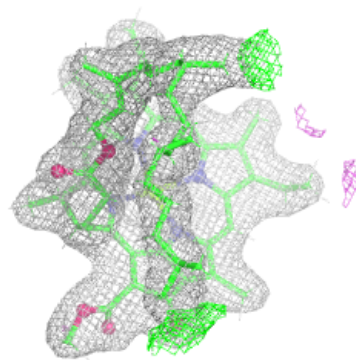
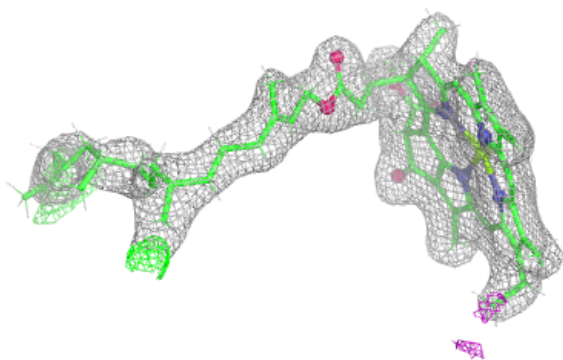
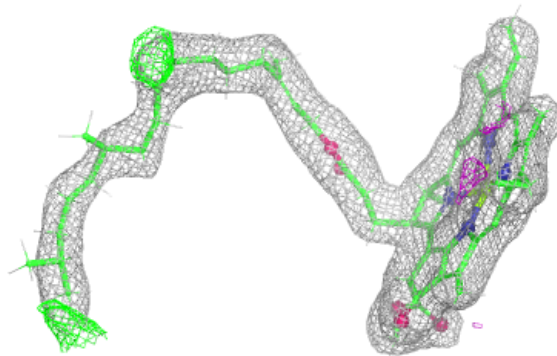
**Electron density around BCR k 102:**

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

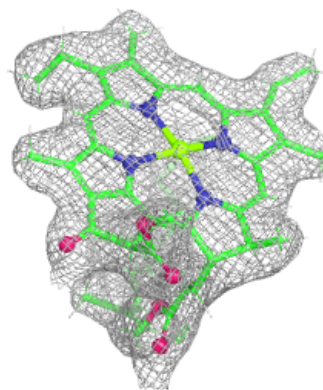
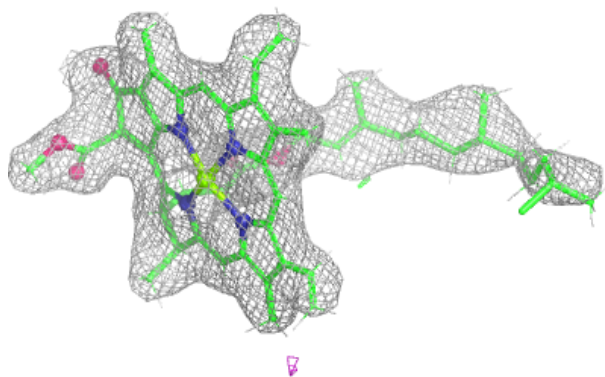
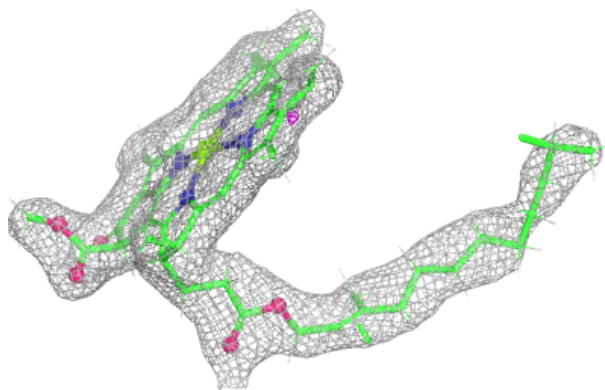


Electron density around CLA b 606:

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

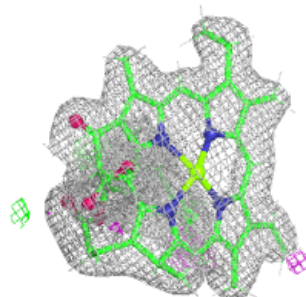
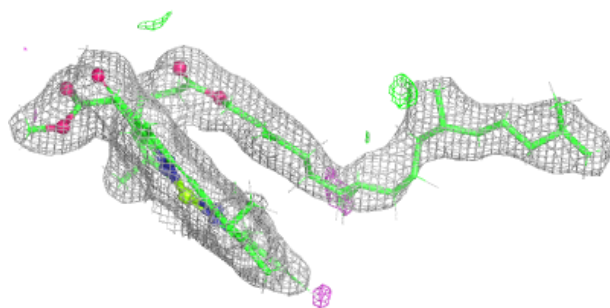
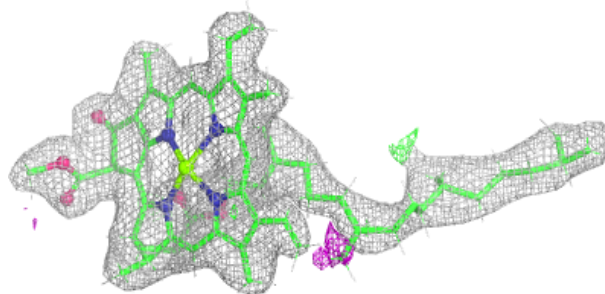
**Electron density around CLA c 504:**

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

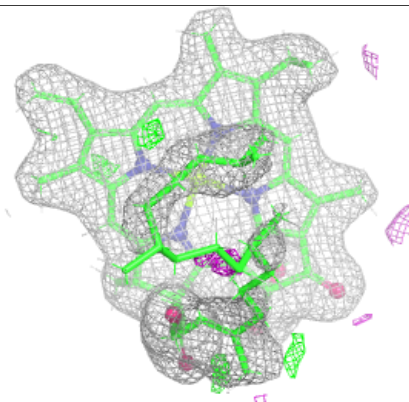
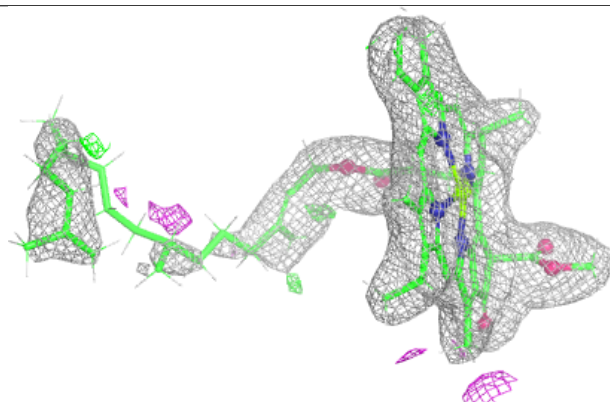
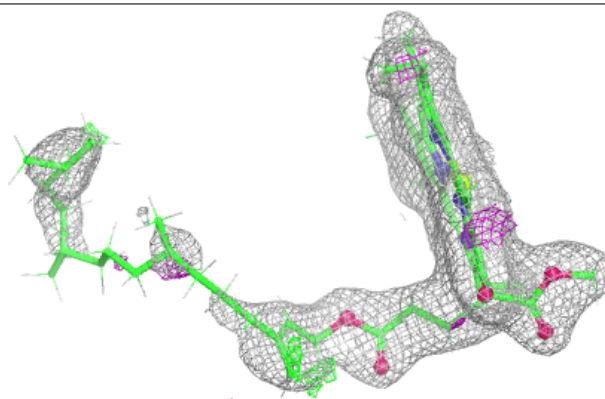


Electron density around CLA c 505:

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

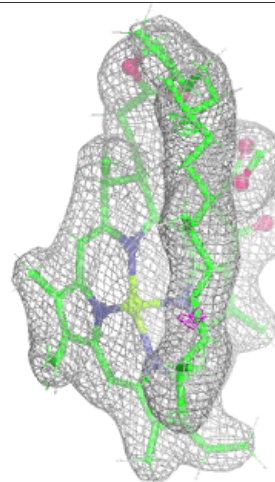
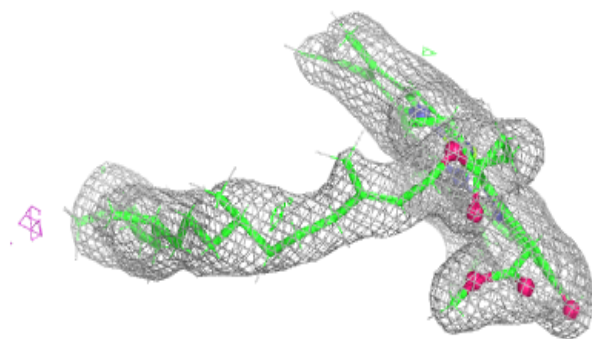
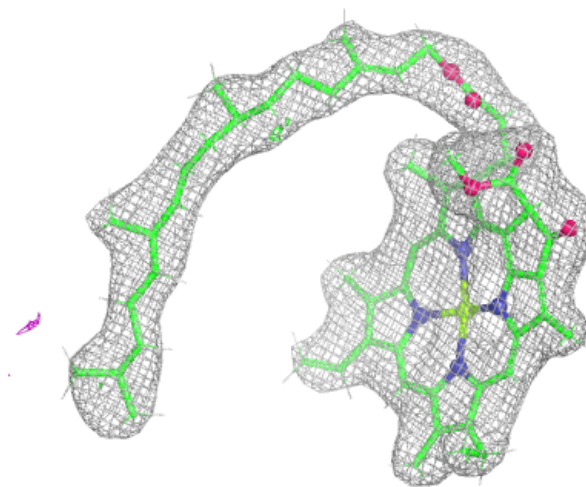
**Electron density around CLA C 506:**

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



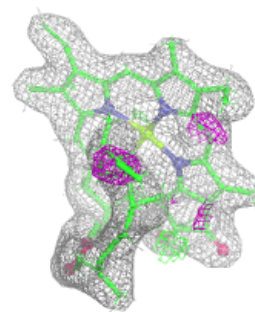
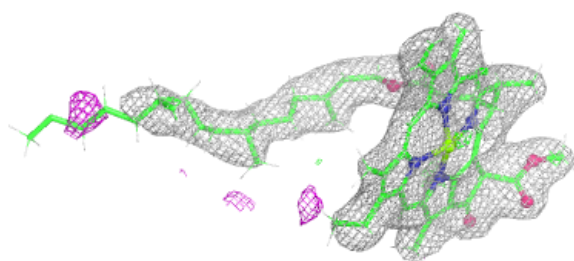
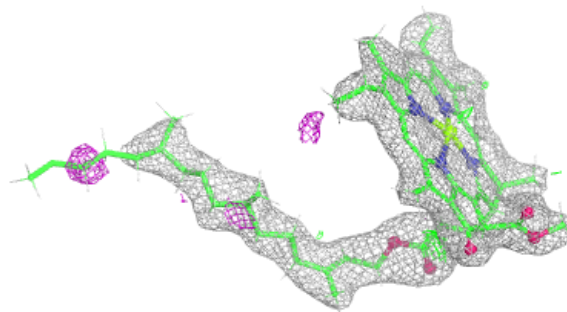
Electron density around CLA c 507:

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

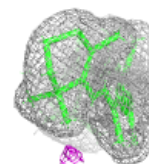
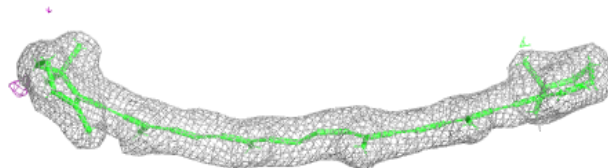
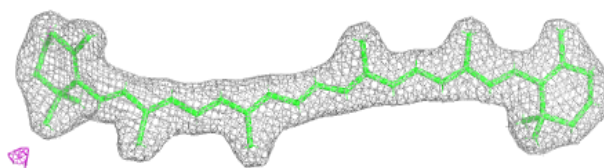


Electron density around CLA c 508:

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

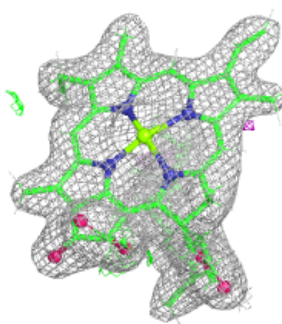
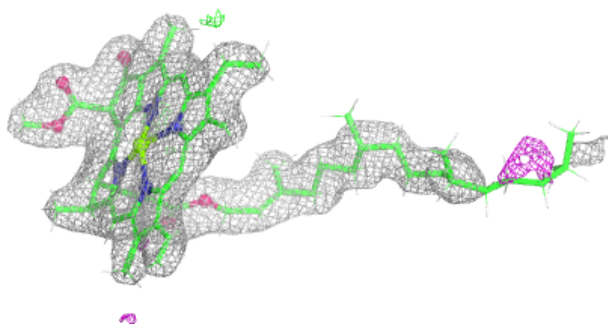
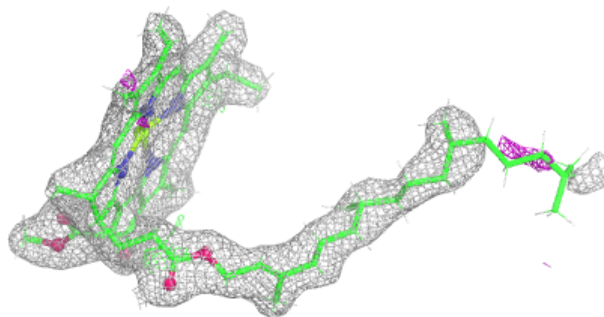
**Electron density around BCR t 101:**

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

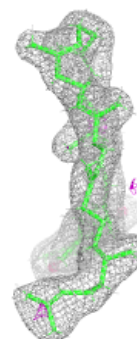
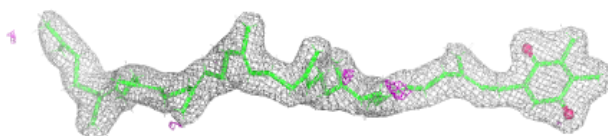
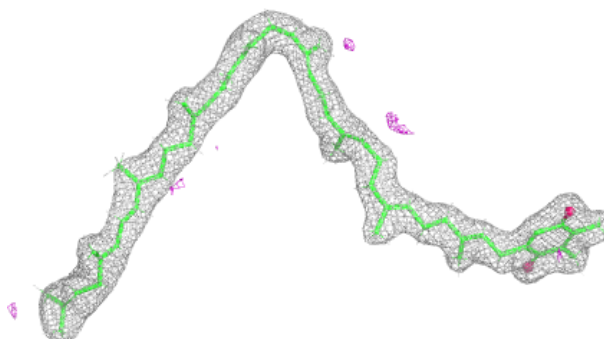


Electron density around CLA C 508:

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

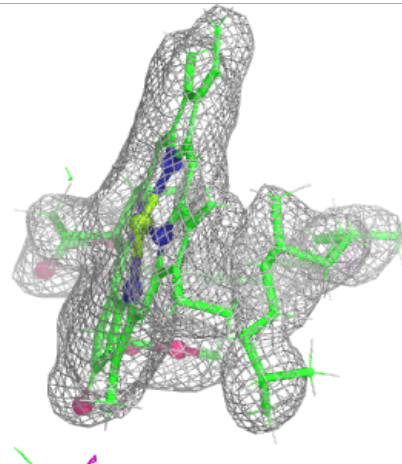
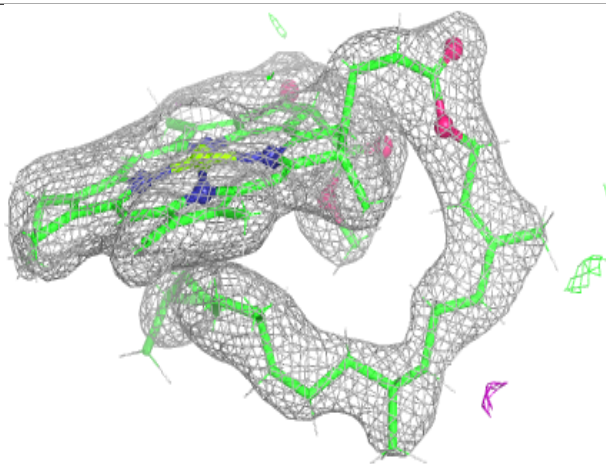
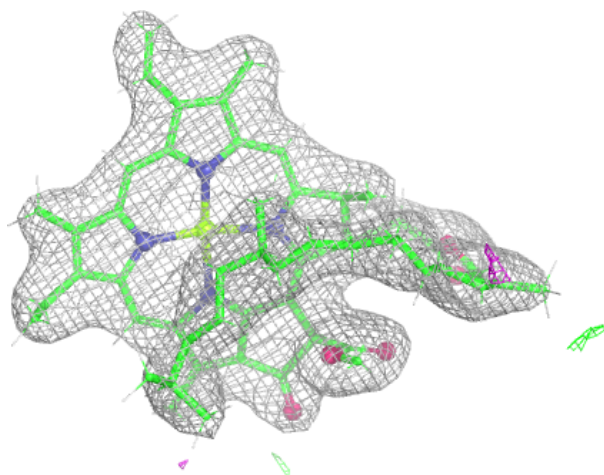
**Electron density around PL9 D 405:**

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



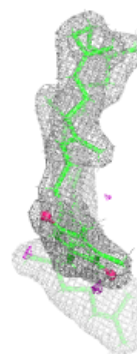
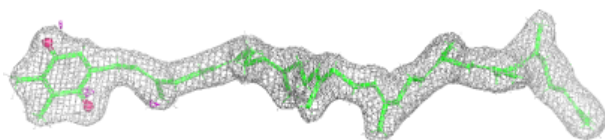
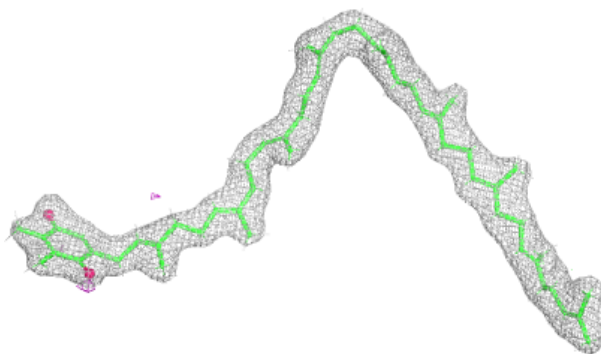
Electron density around CLA c 510:

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

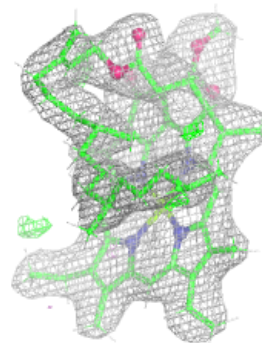
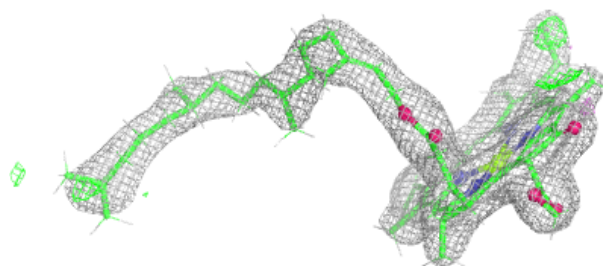
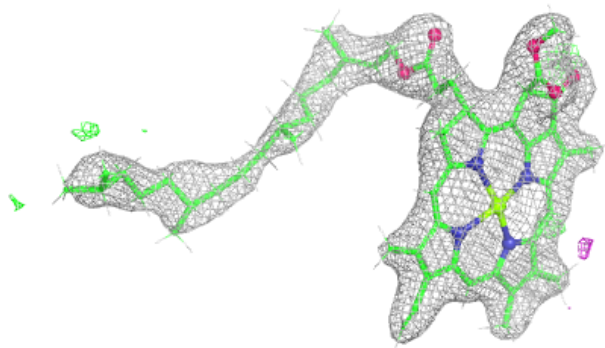


Electron density around PL9 d 405:

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

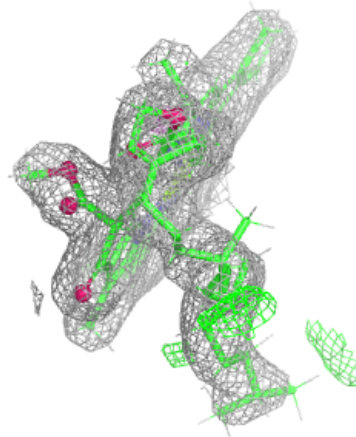
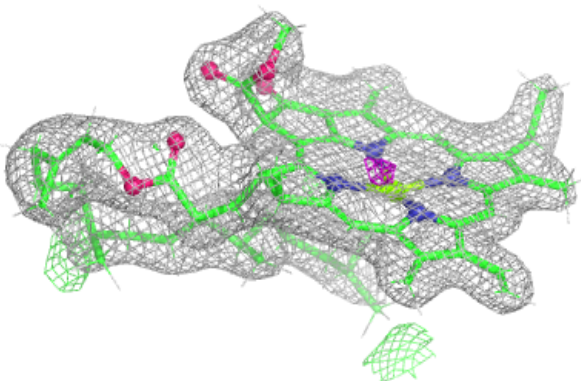
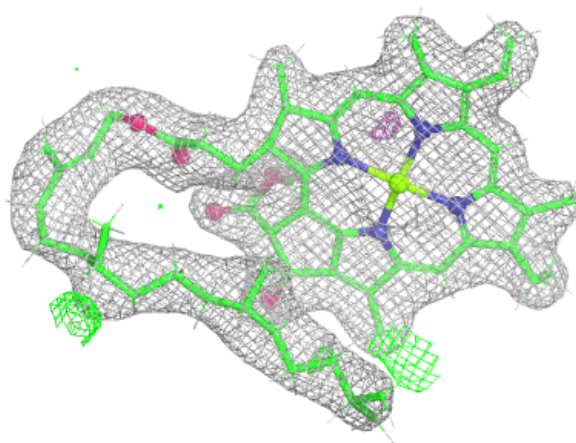
**Electron density around CLA c 511:**

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



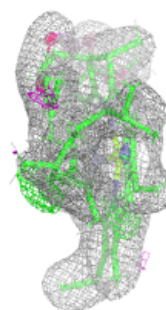
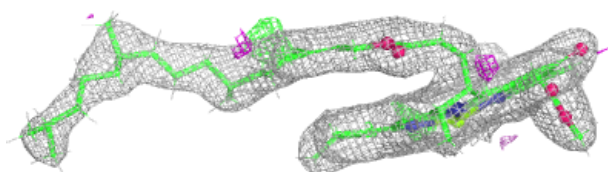
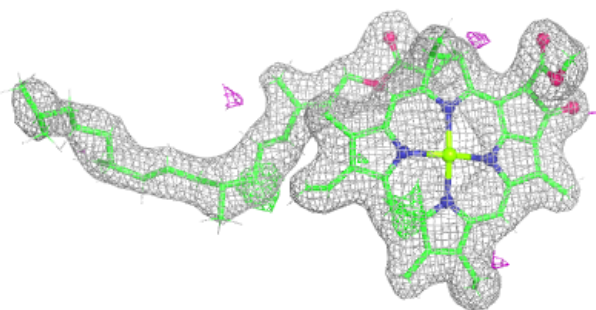
Electron density around CLA C 509:

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

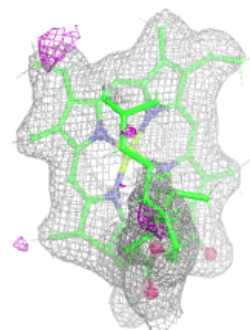
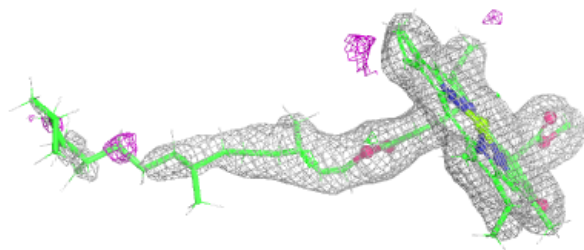
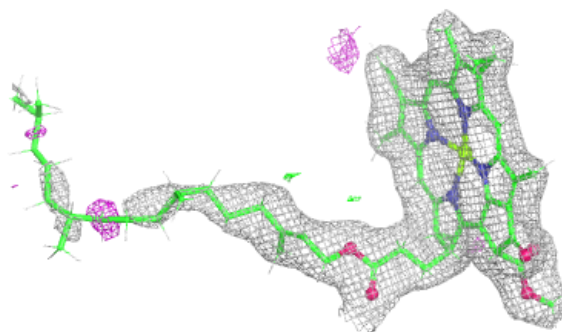


Electron density around CLA B 603:

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

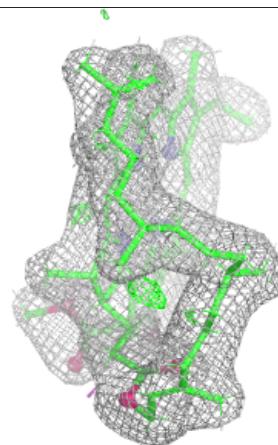
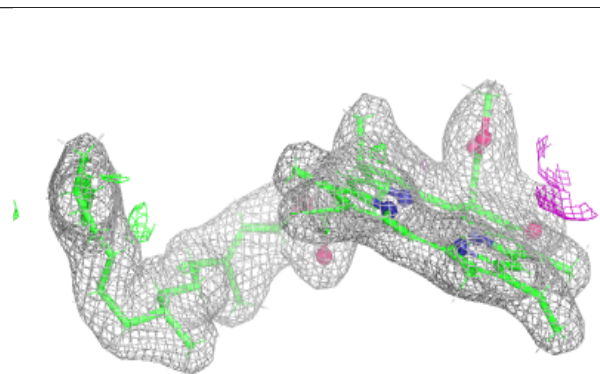
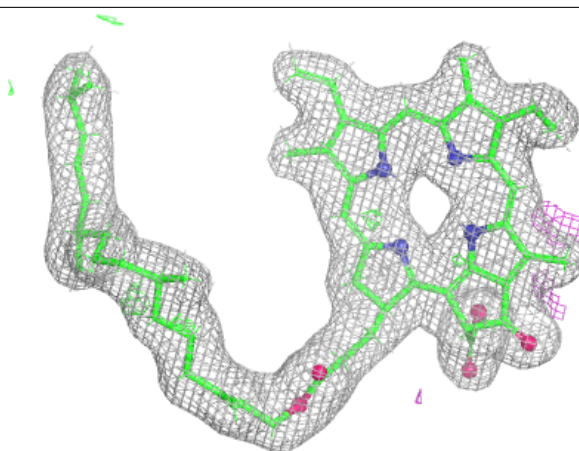
**Electron density around CLA d 403:**

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



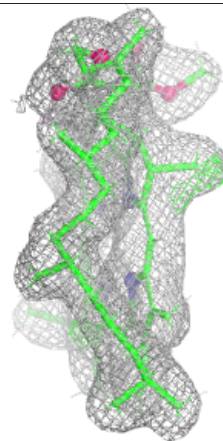
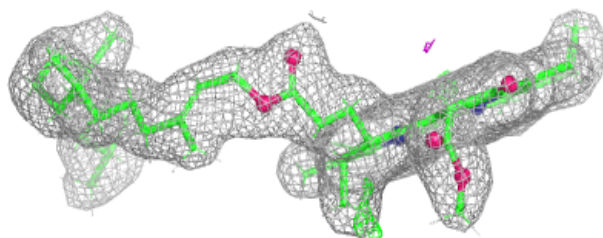
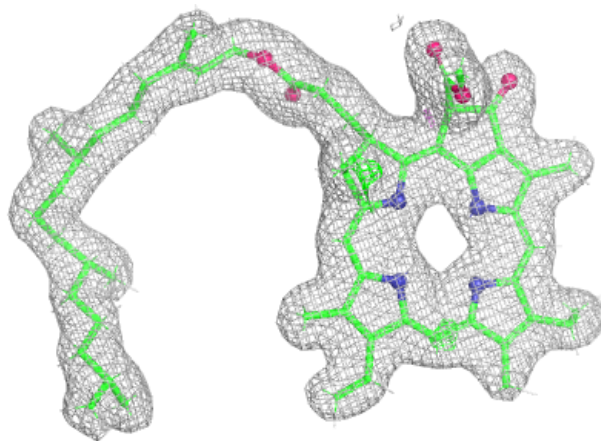
Electron density around PHO A 608:

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



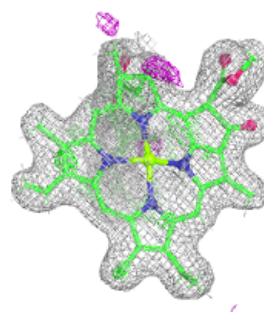
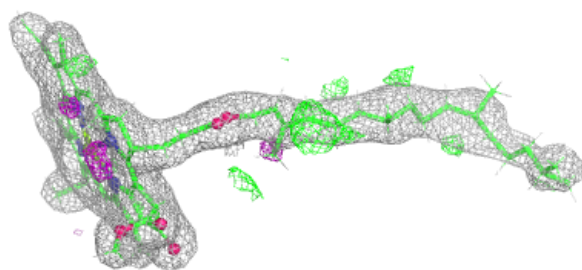
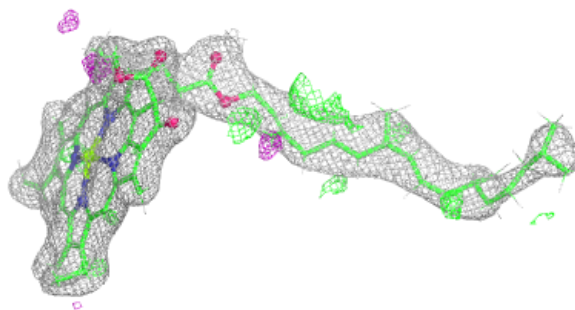
Electron density around PHO a 608:

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



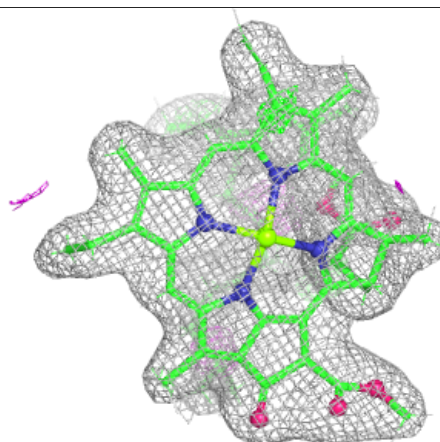
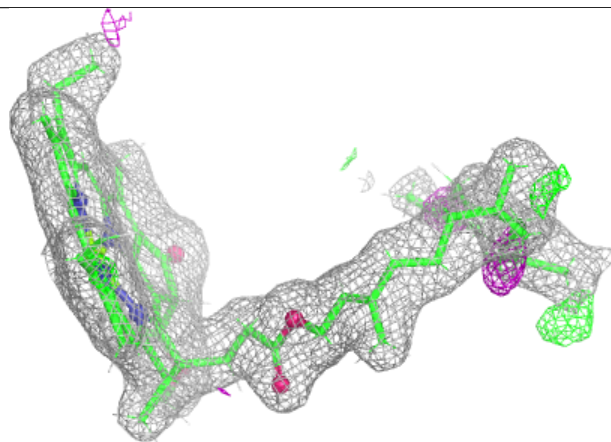
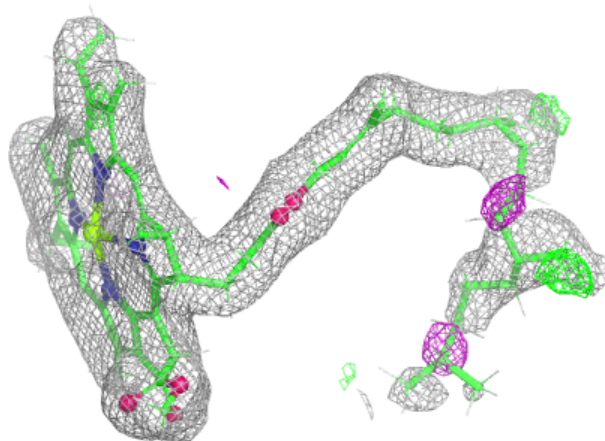
Electron density around CLA B 604:

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

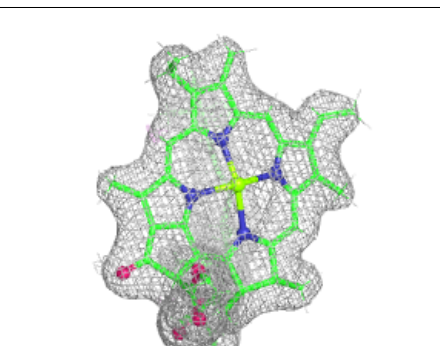
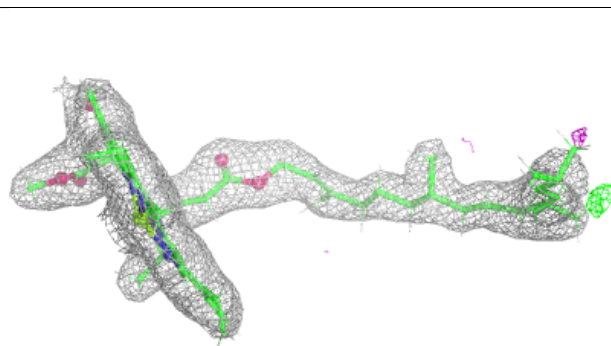
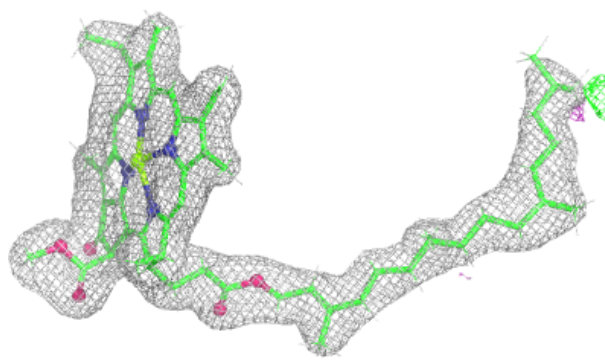


Electron density around CLA B 606:

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

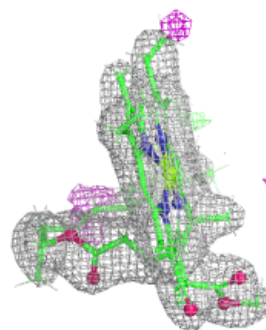
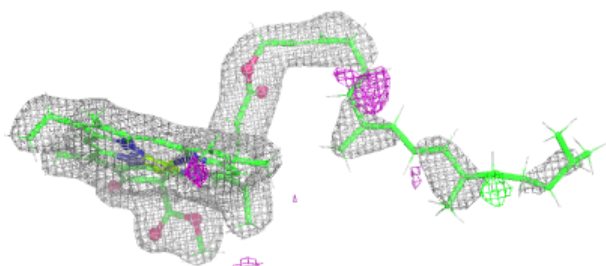
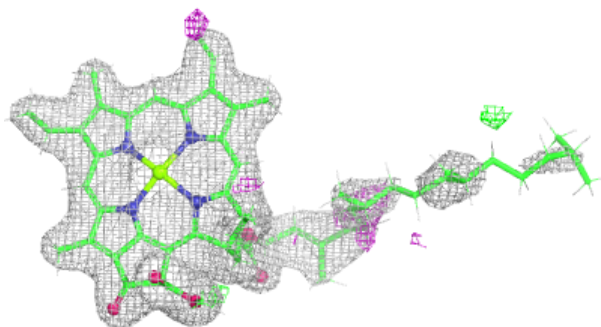
**Electron density around CLA B 609:**

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

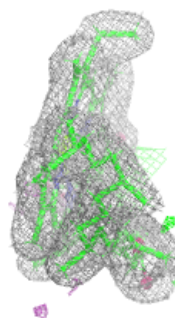
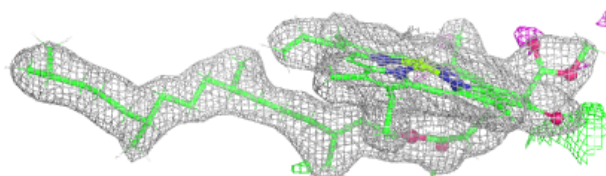
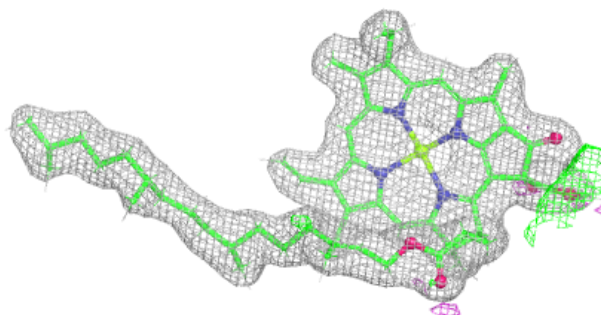


Electron density around CLA a 607:

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

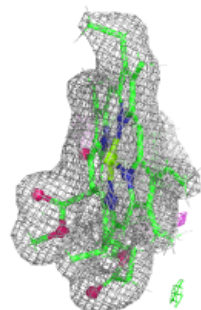
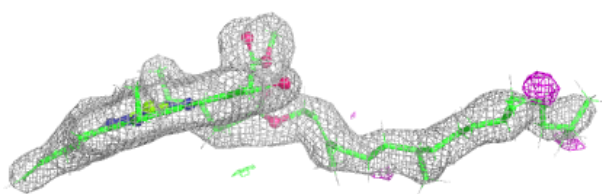
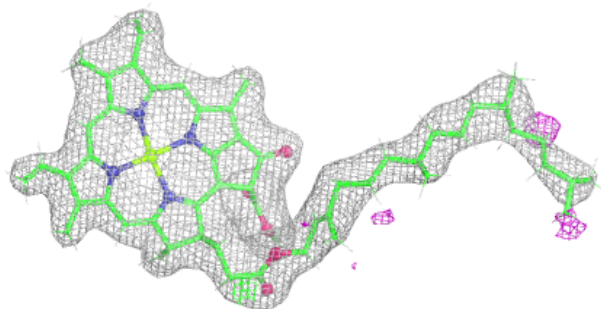
**Electron density around CLA C 501:**

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

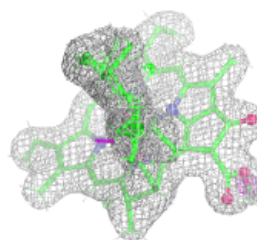
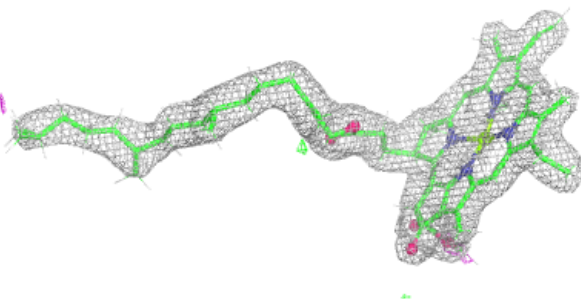
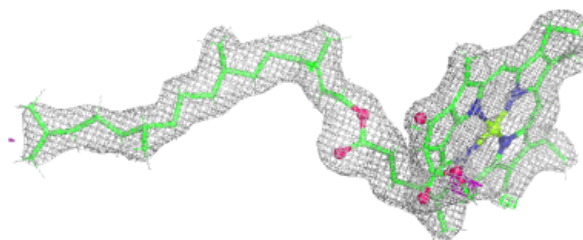


Electron density around CLA b 602:

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

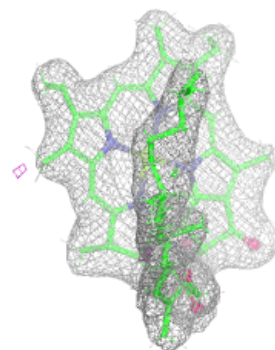
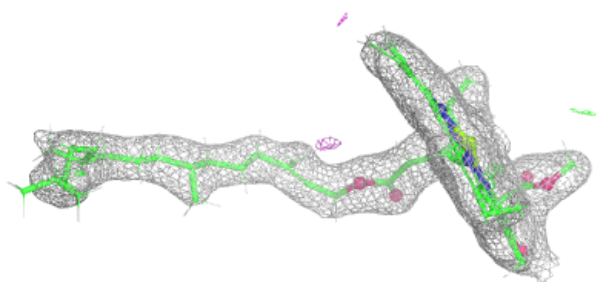
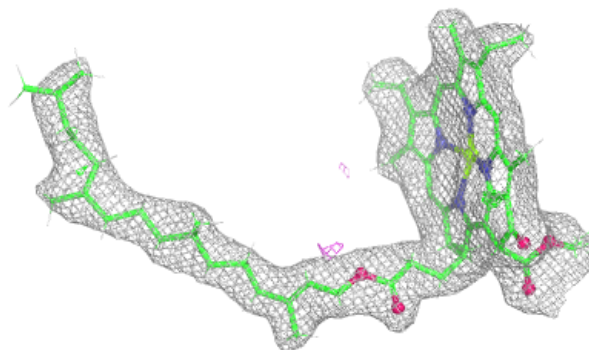
**Electron density around CLA C 502:**

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

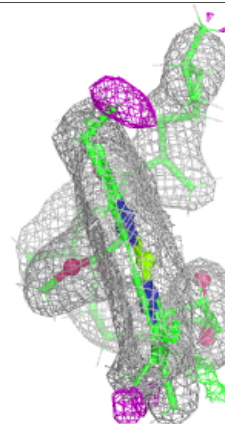
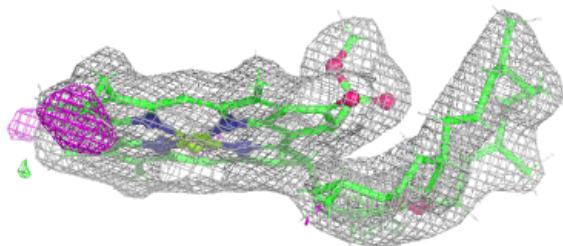
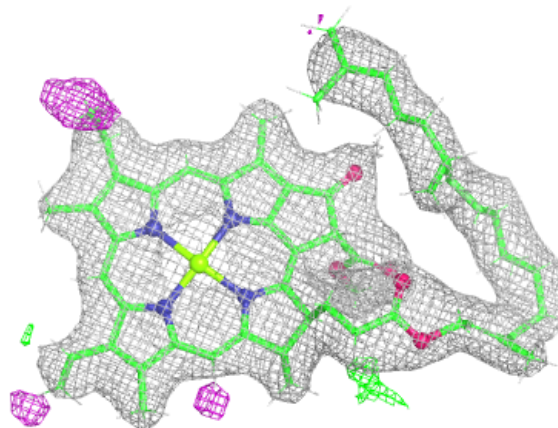


Electron density around CLA b 609:

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

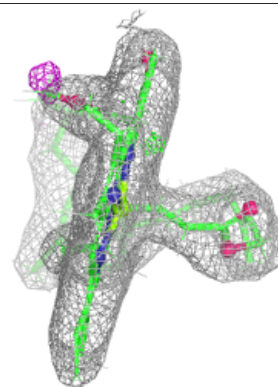
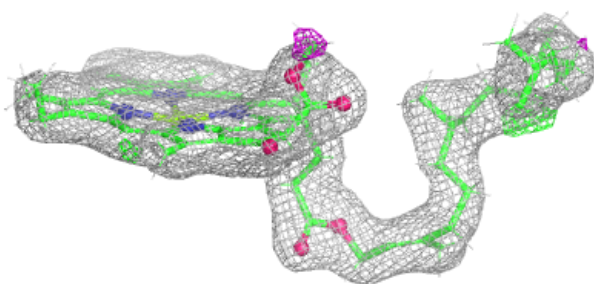
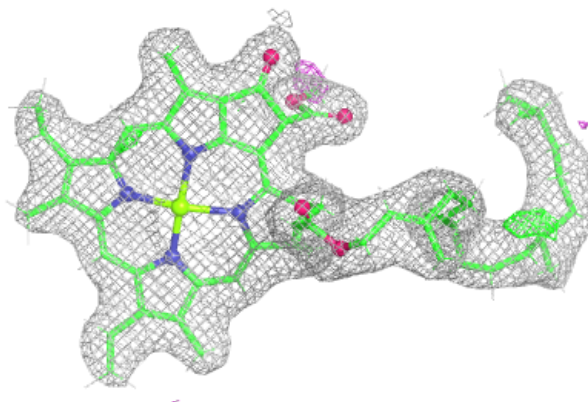
**Electron density around CLA b 610:**

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

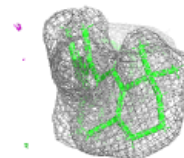
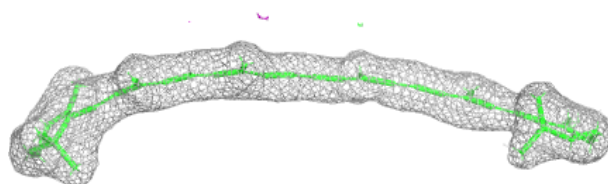
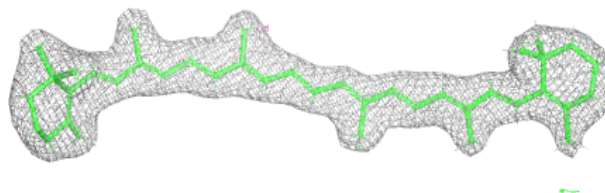


Electron density around CLA b 612:

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

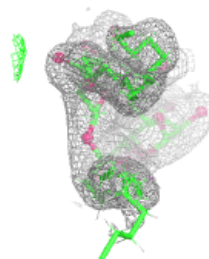
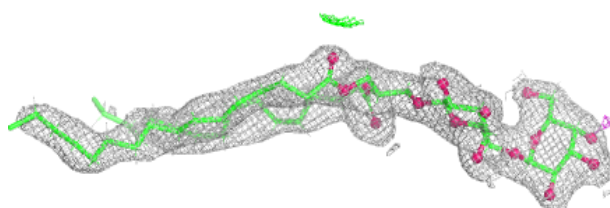
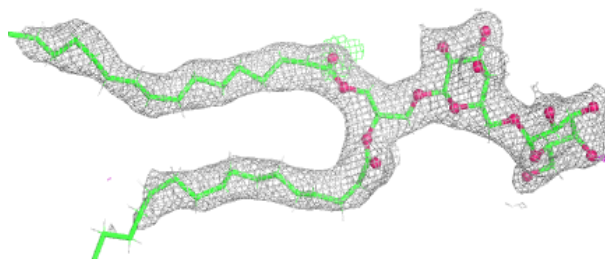
**Electron density around BCR T 101:**

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

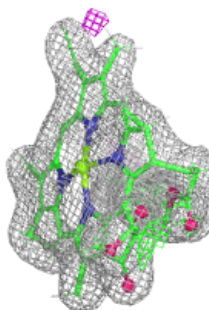
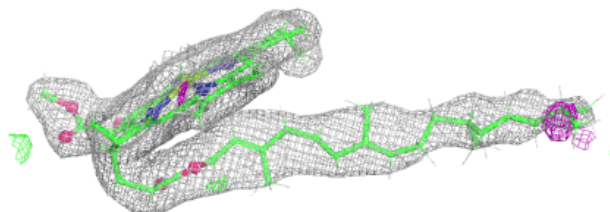
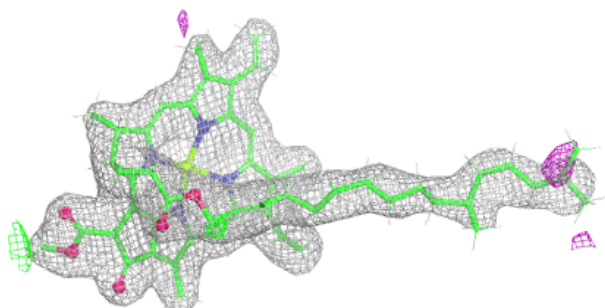


Electron density around DGD c 521:

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

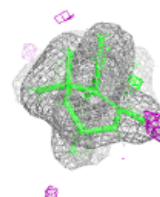
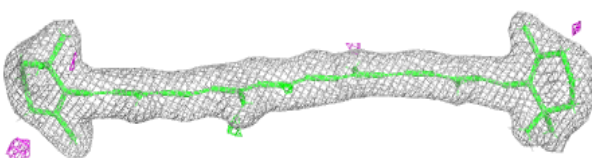
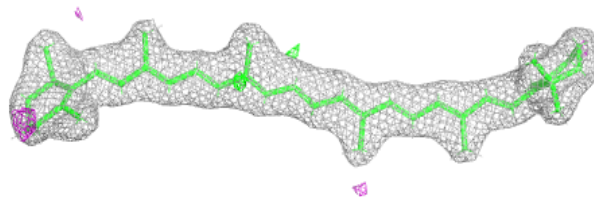
**Electron density around CLA b 614:**

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

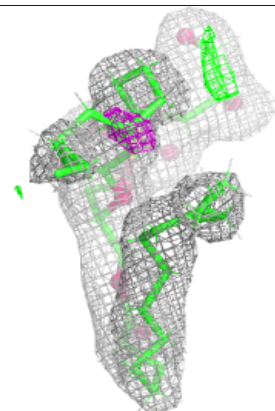
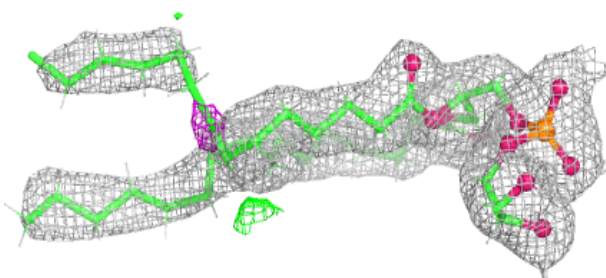
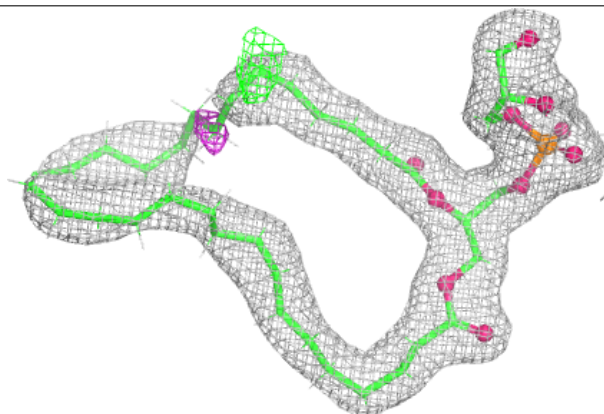


Electron density around BCR a 610:

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

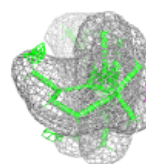
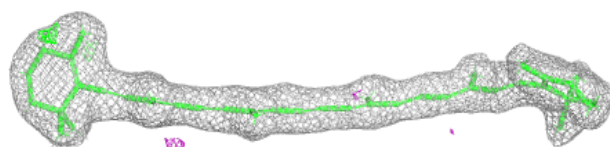
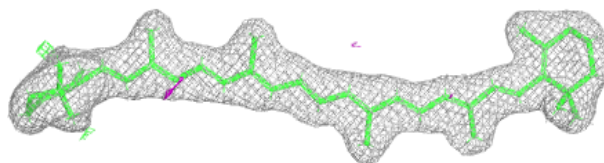
**Electron density around LHG D 410:**

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



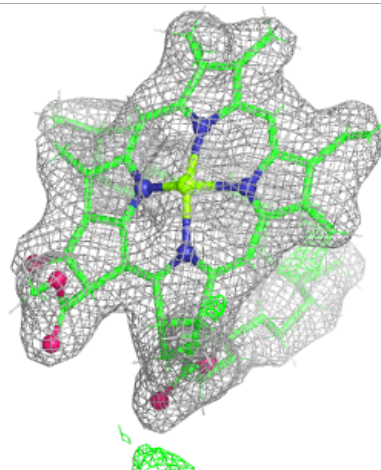
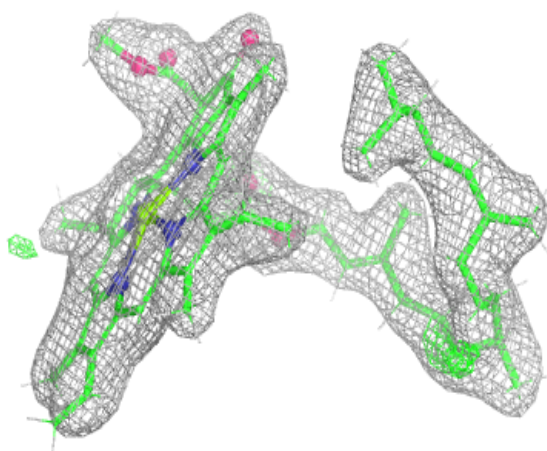
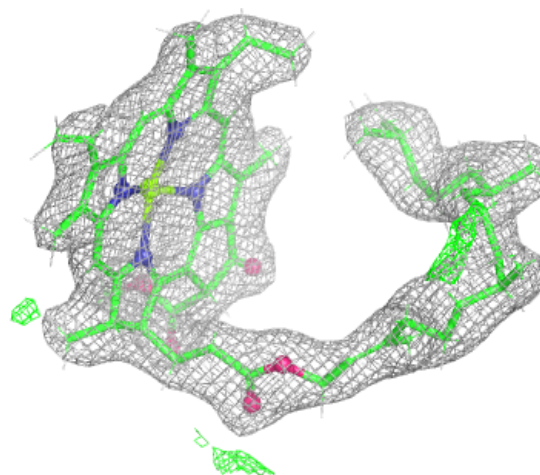
Electron density around BCR b 617:

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



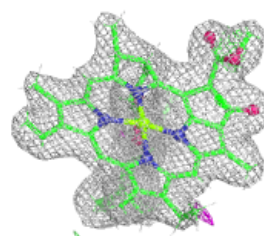
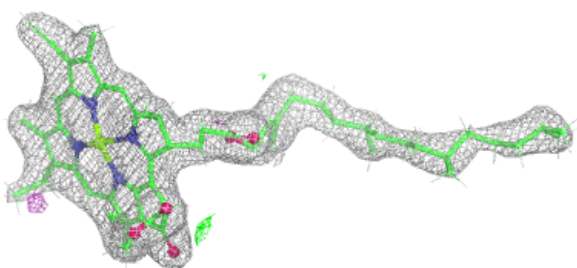
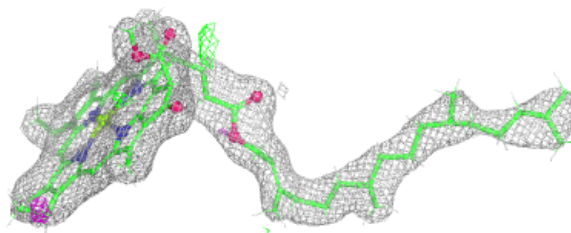
Electron density around CLA C 503:

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



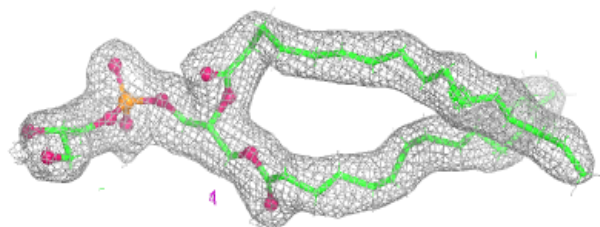
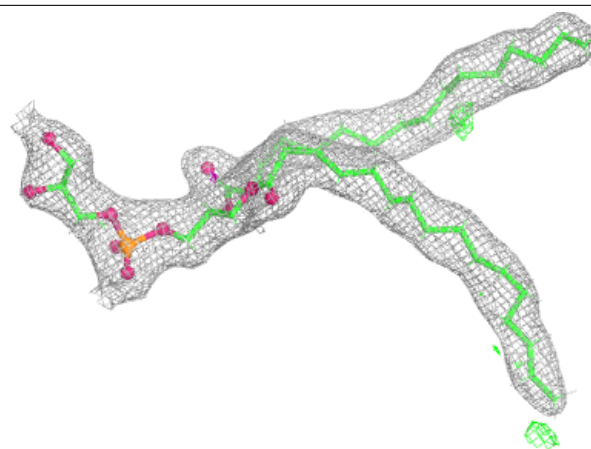
Electron density around CLA c 502:

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

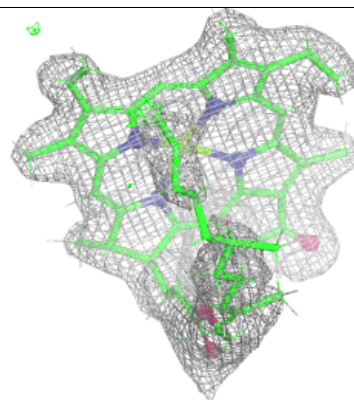
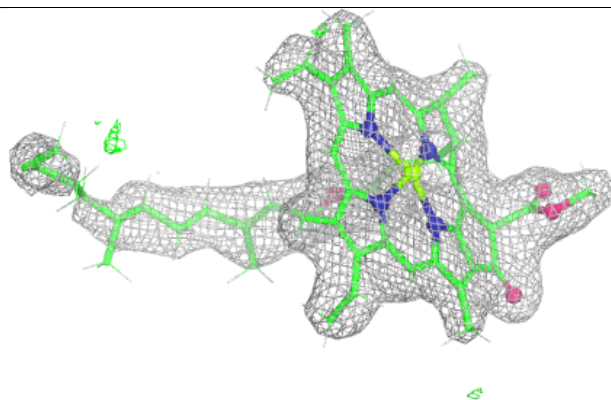
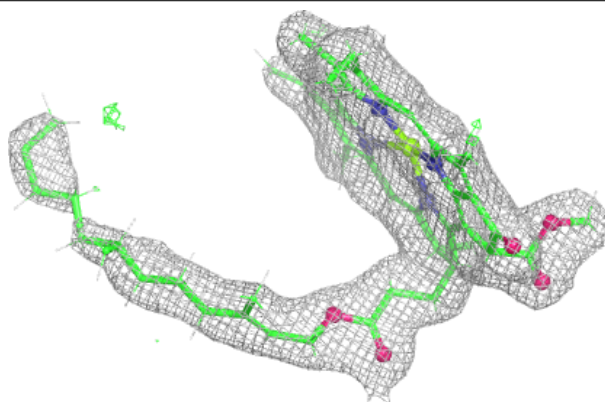


Electron density around LHG d 408:

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

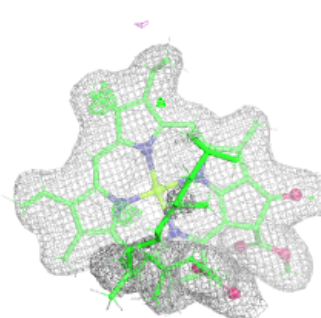
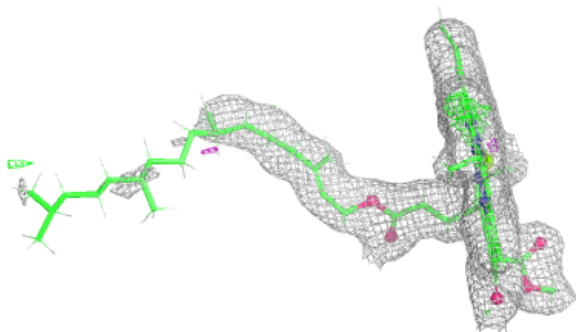
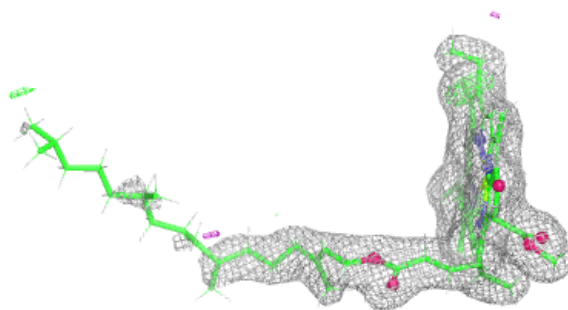
**Electron density around CLA C 504:**

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

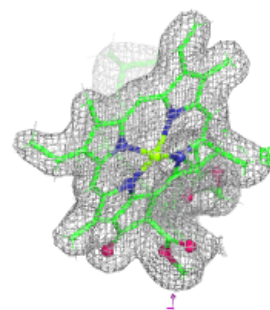
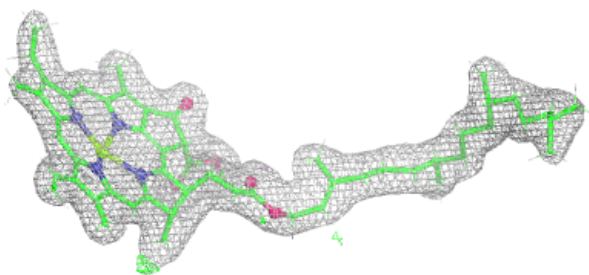
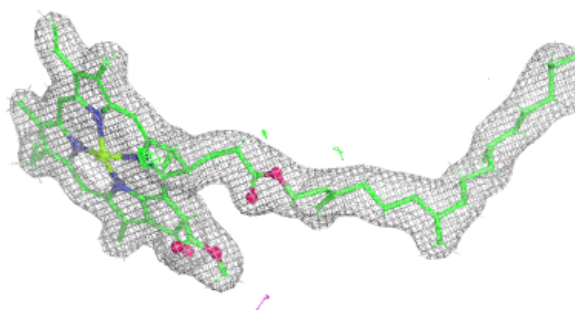


Electron density around CLA D 403:

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

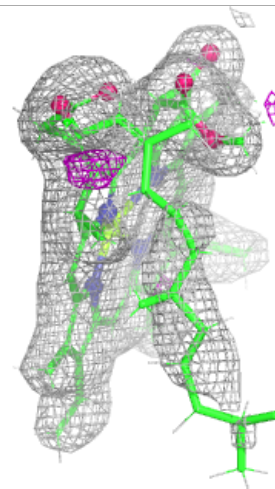
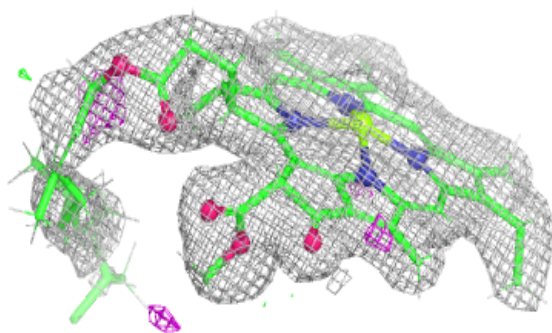
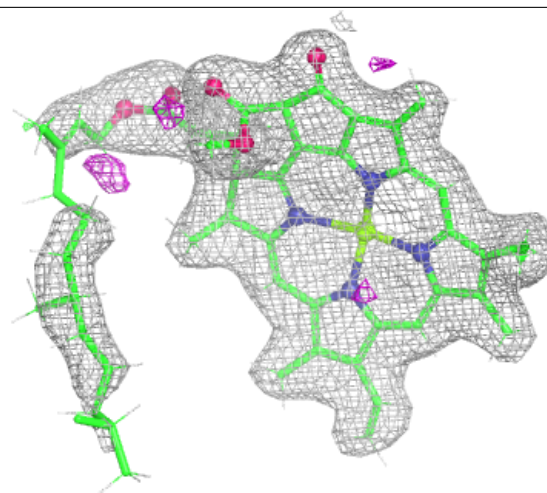
**Electron density around CLA a 606:**

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



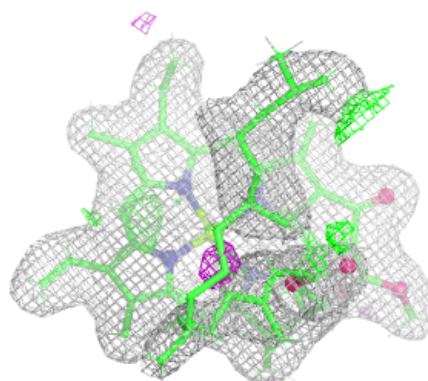
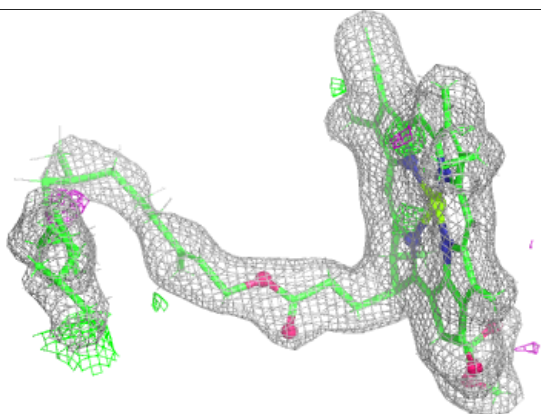
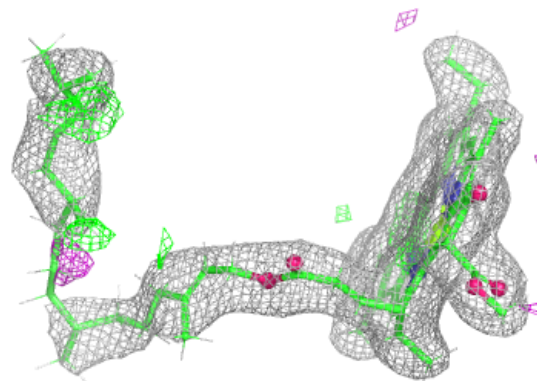
Electron density around CLA B 616:

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

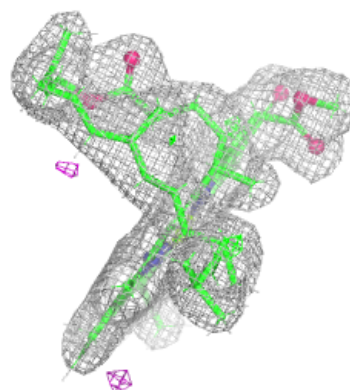
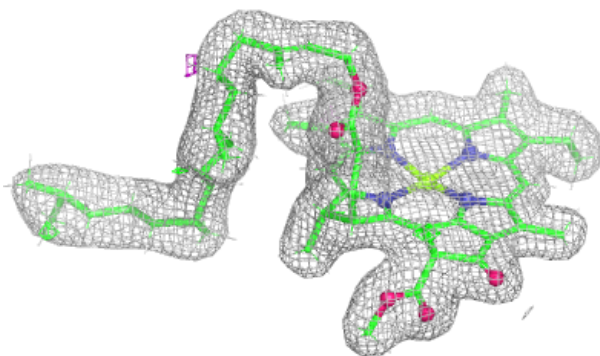
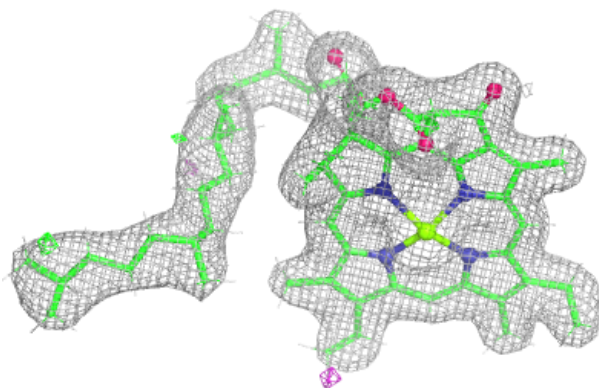


Electron density around CLA a 609:

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

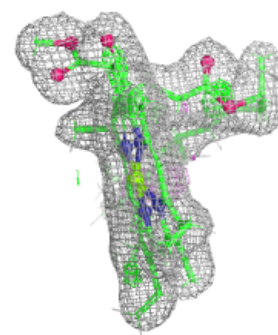
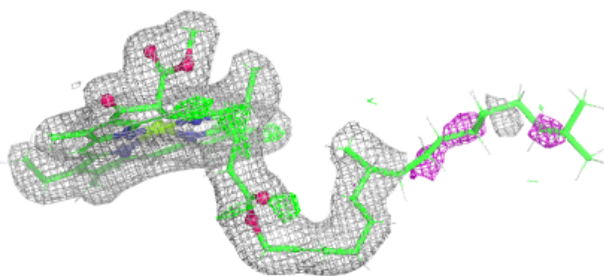
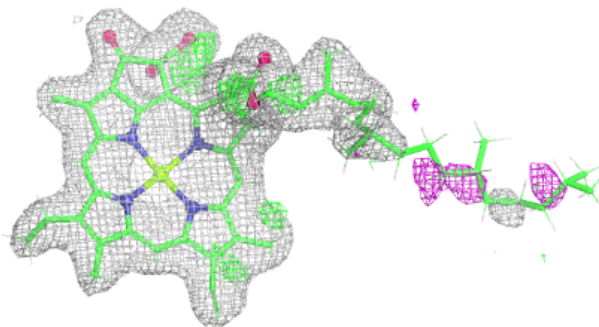
**Electron density around CLA a 612:**

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

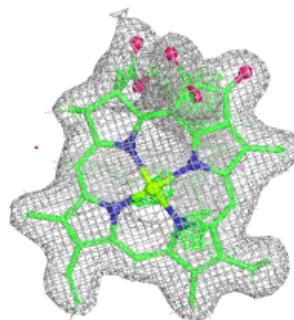
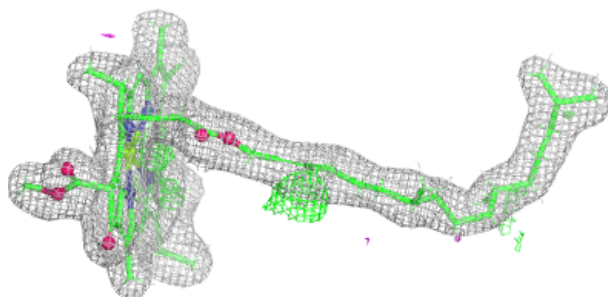
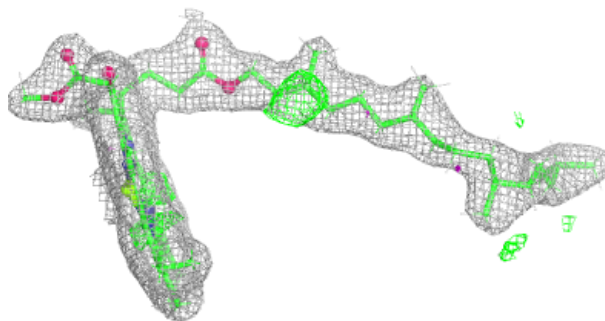


Electron density around CLA A 607:

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

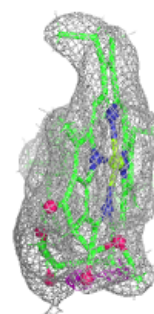
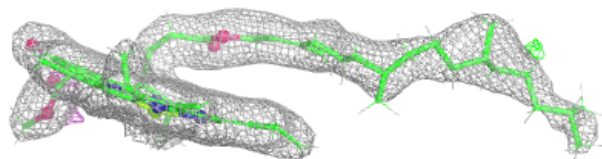
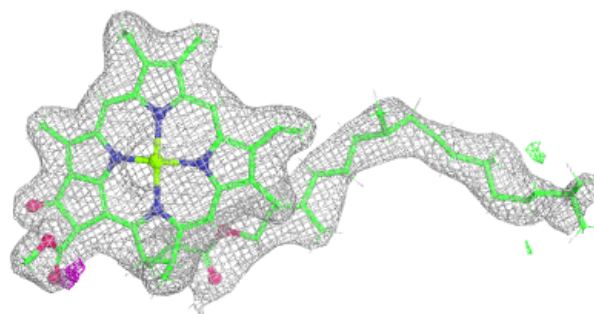
**Electron density around CLA B 605:**

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

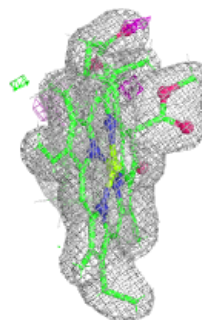
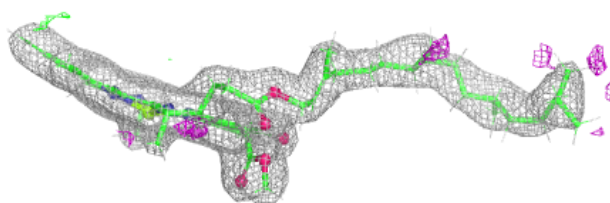
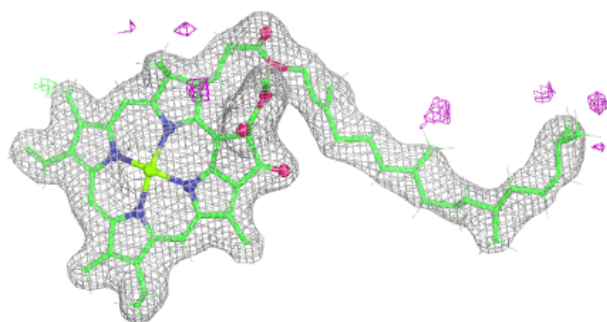


Electron density around CLA b 603:

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

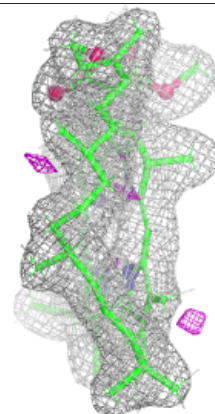
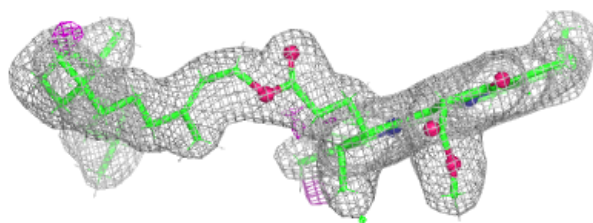
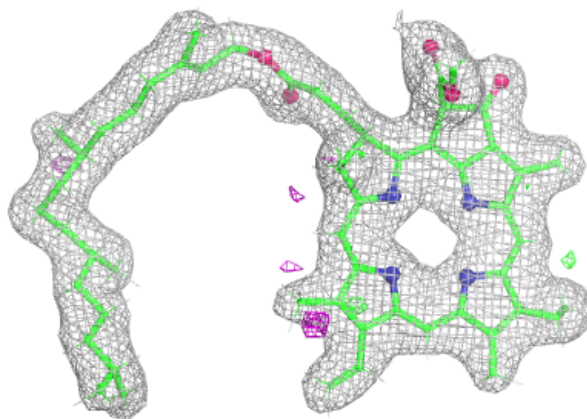
**Electron density around CLA B 602:**

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

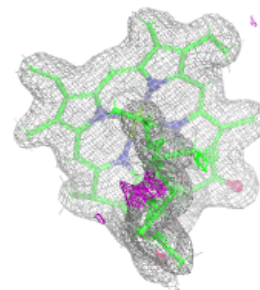
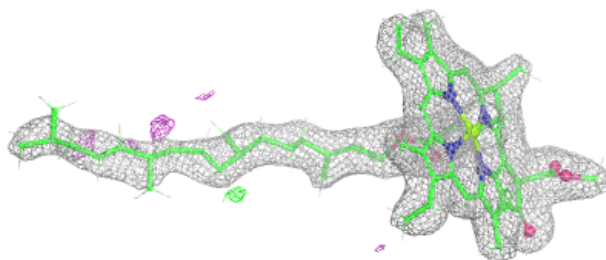
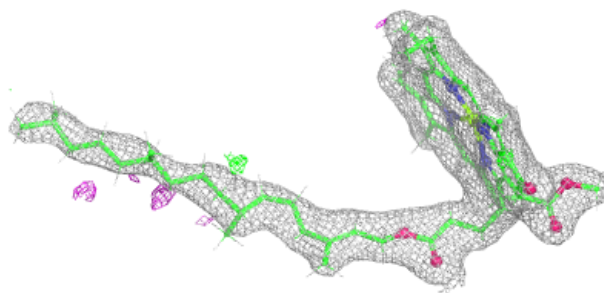


Electron density around PHO D 401:

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

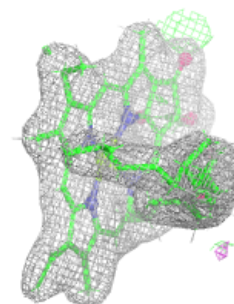
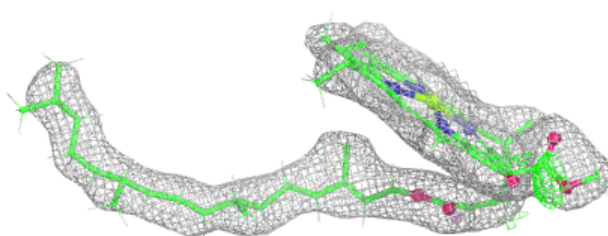
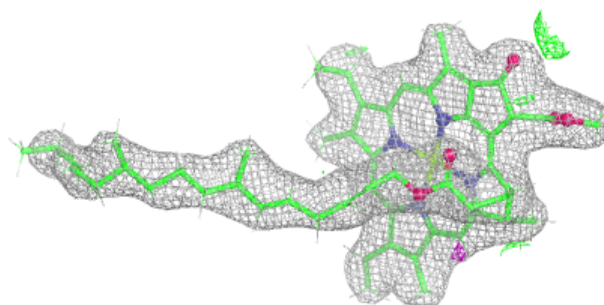
**Electron density around CLA b 607:**

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

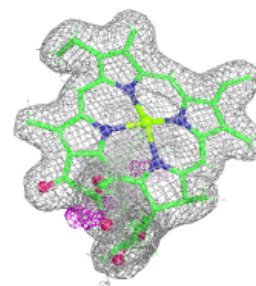
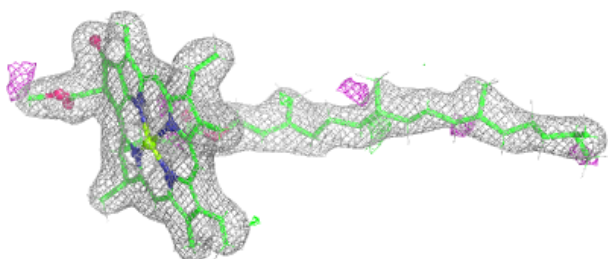
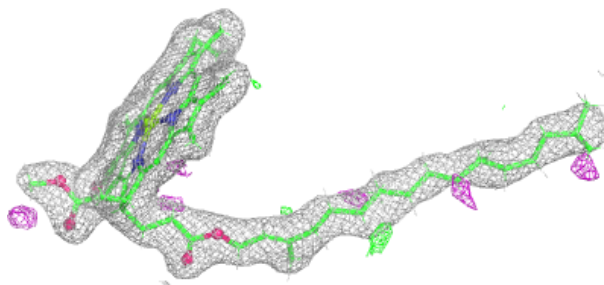


Electron density around CLA b 608:

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

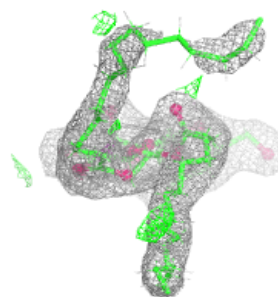
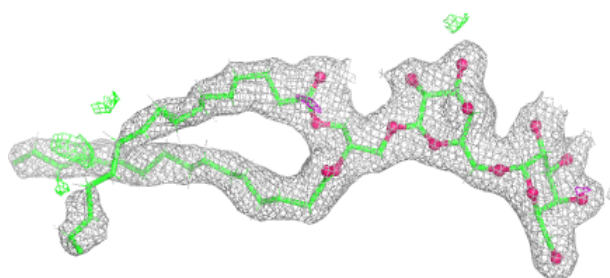
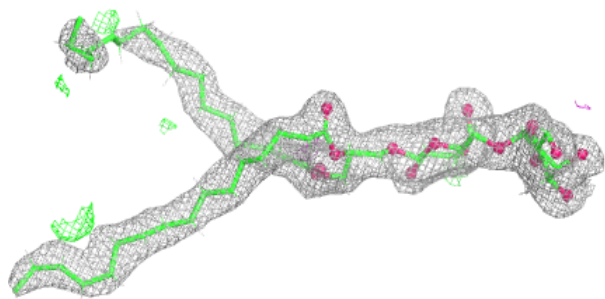
**Electron density around CLA B 607:**

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

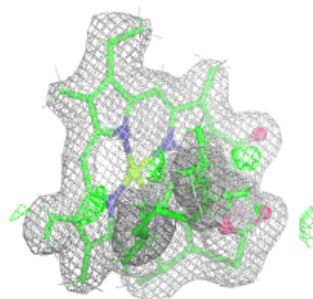
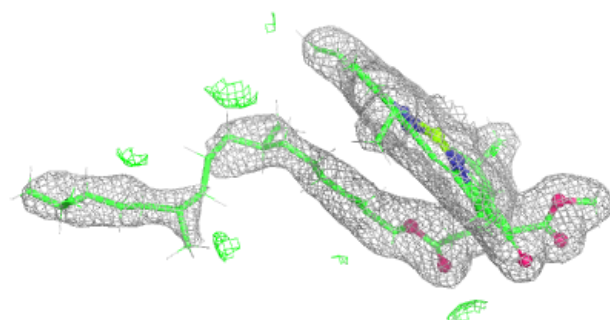
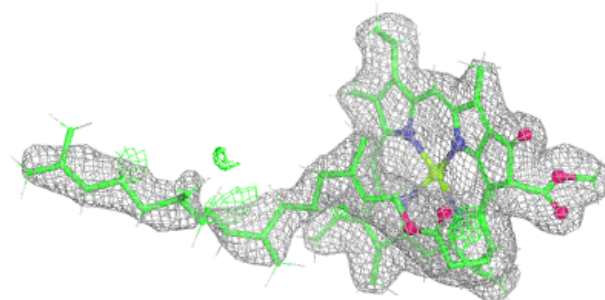


Electron density around DGD C 520:

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

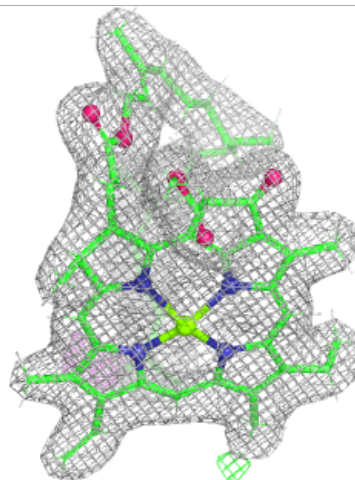
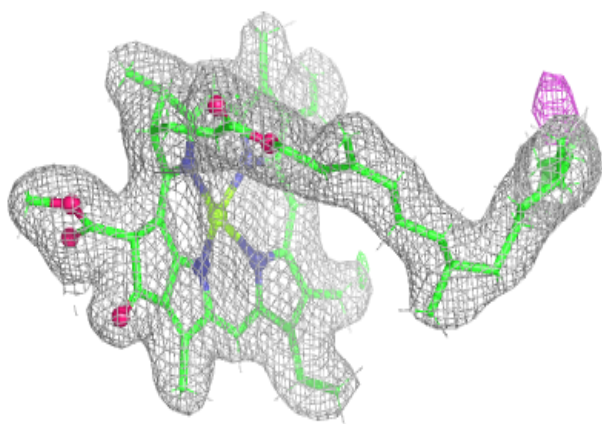
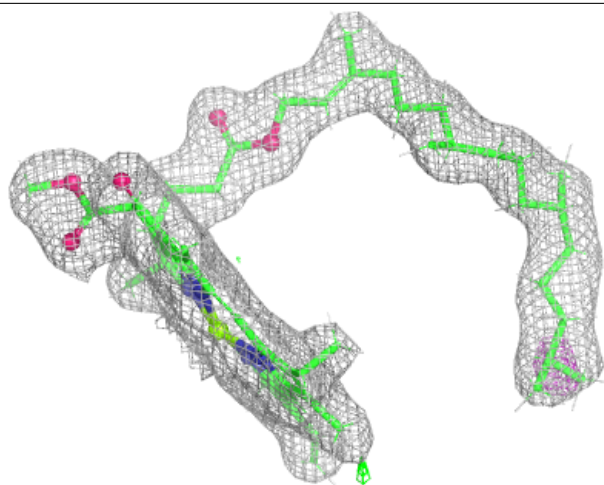
**Electron density around CLA C 505:**

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



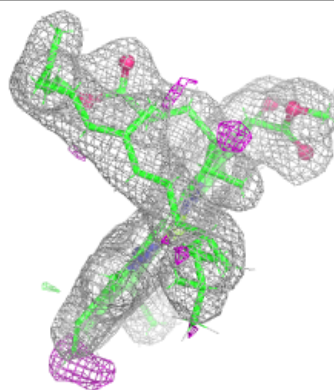
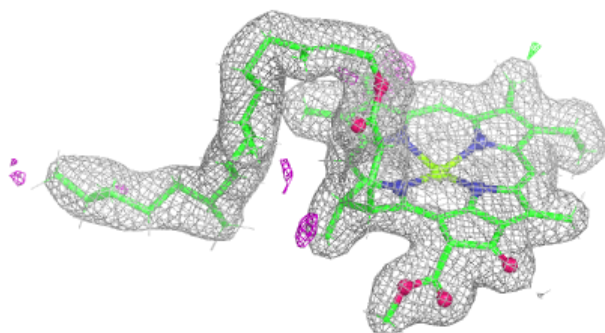
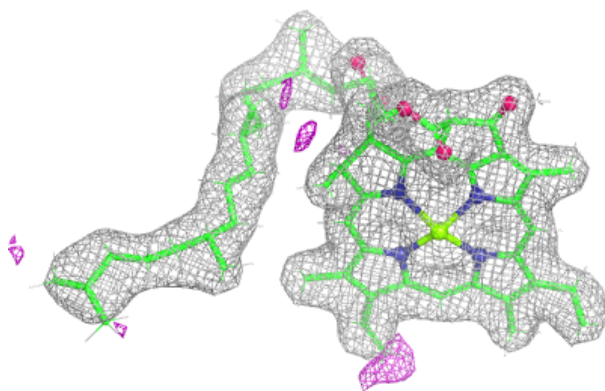
Electron density around CLA b 611:

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

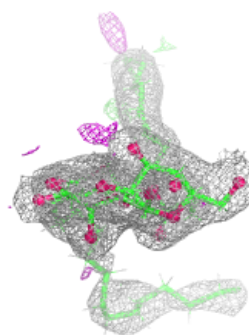
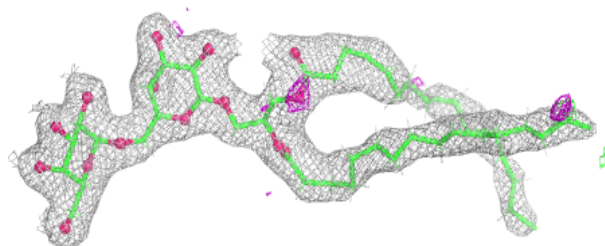
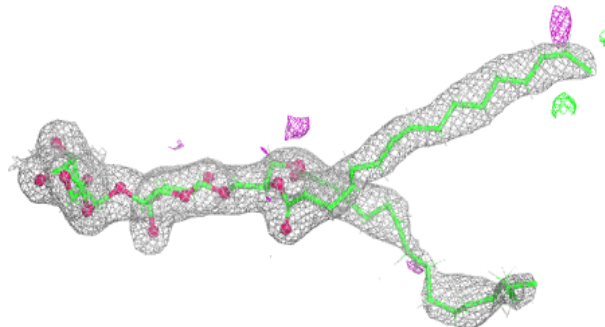


Electron density around CLA A 613:

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

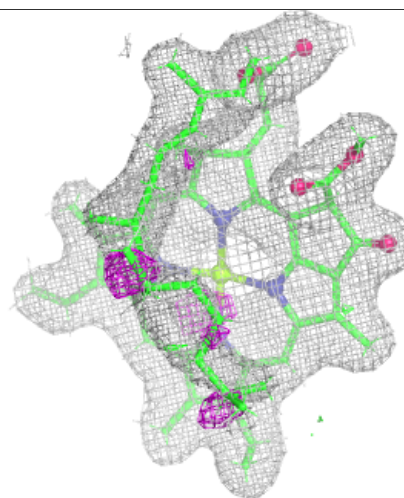
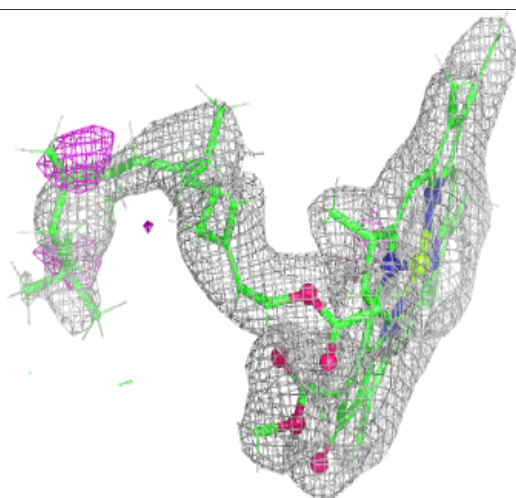
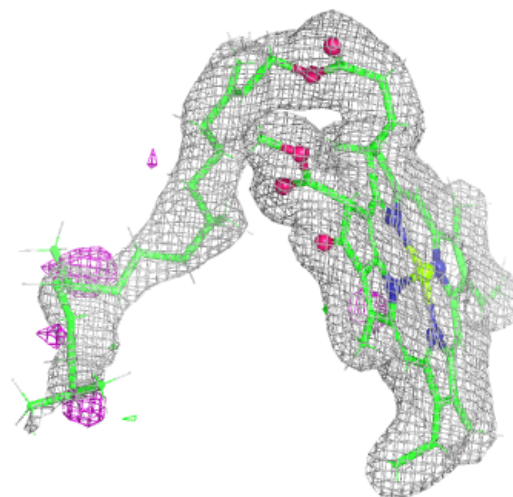
**Electron density around DGD c 519:**

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



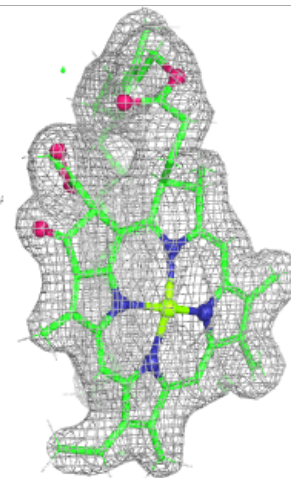
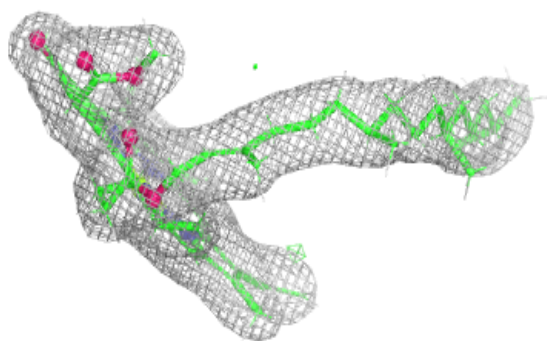
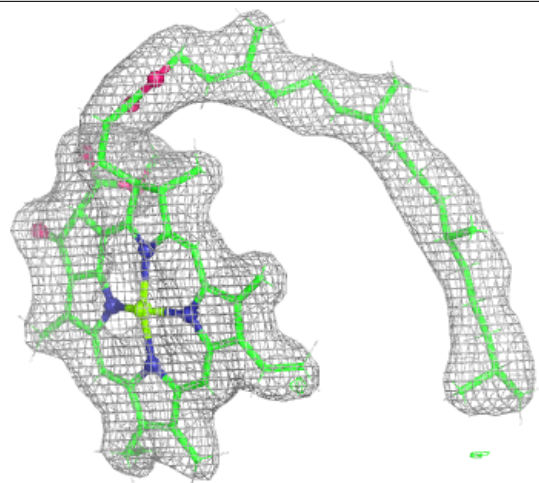
Electron density around CLA b 613:

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



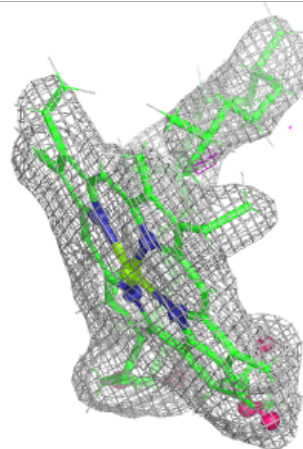
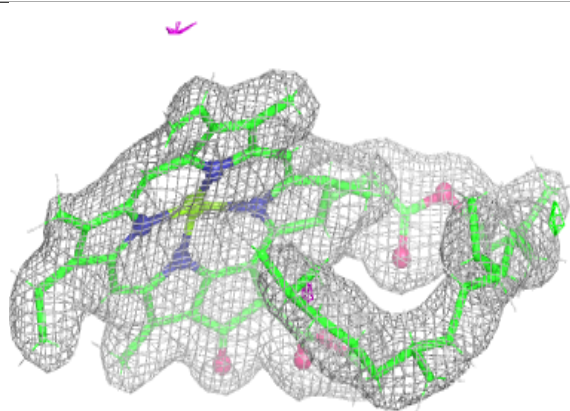
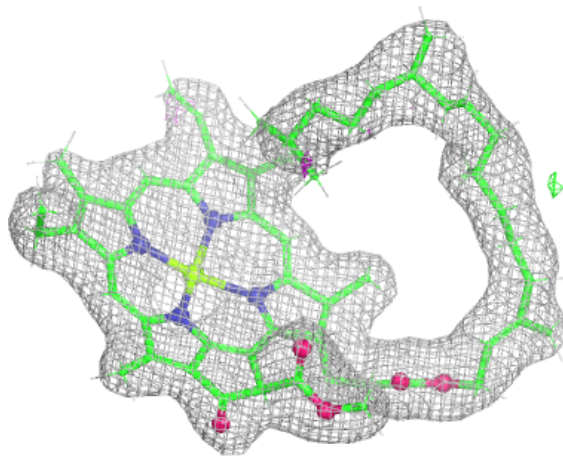
Electron density around CLA C 507:

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



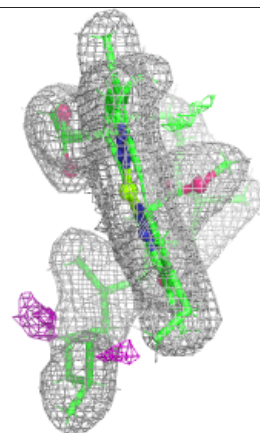
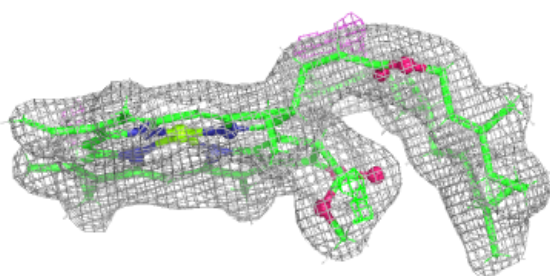
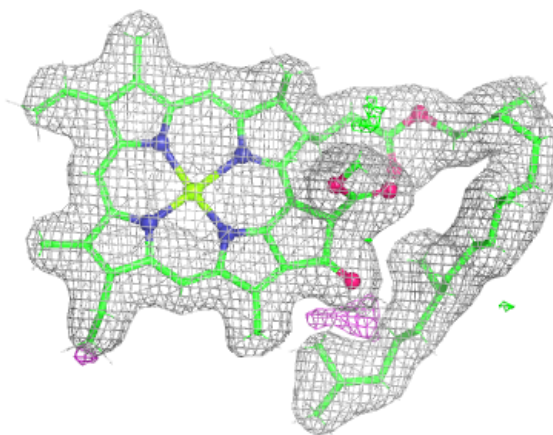
Electron density around CLA b 615:

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

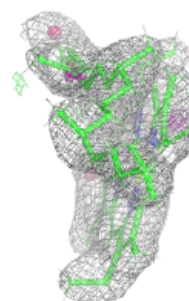
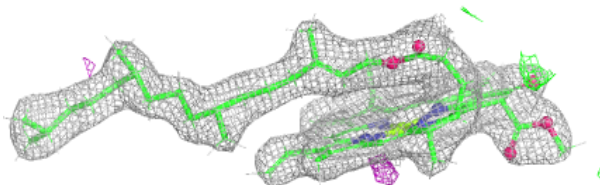
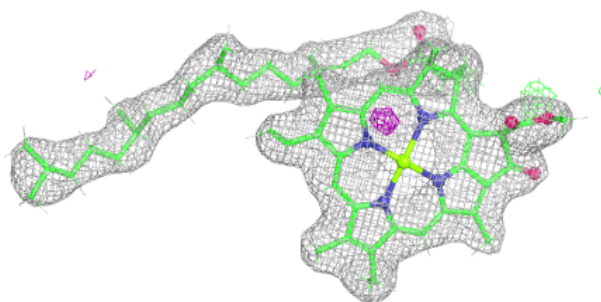


Electron density around CLA B 610:

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

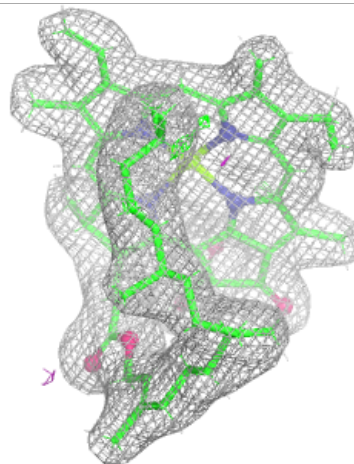
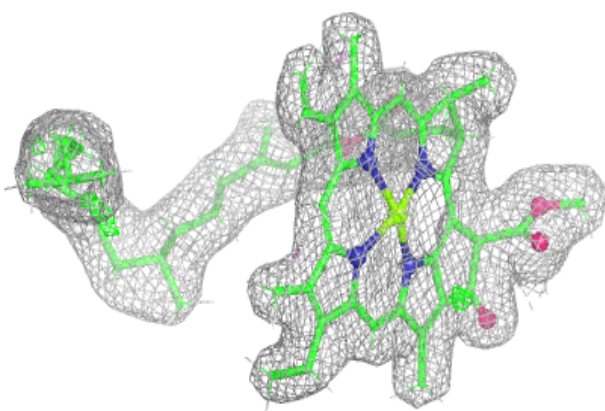
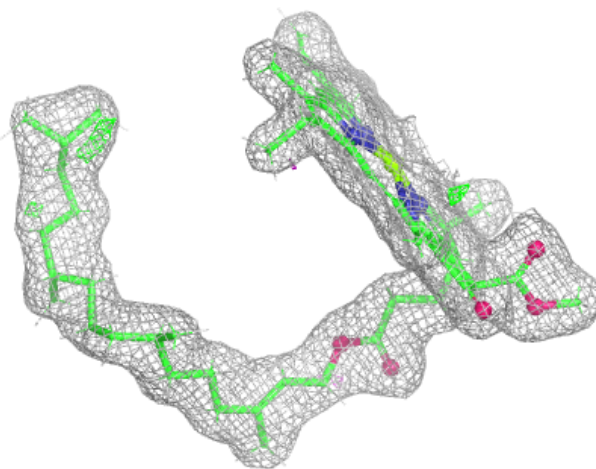
**Electron density around CLA c 501:**

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



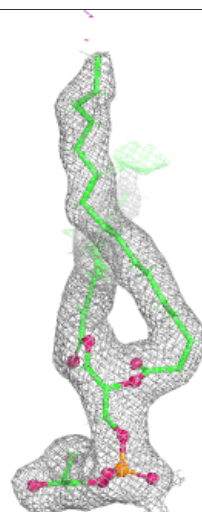
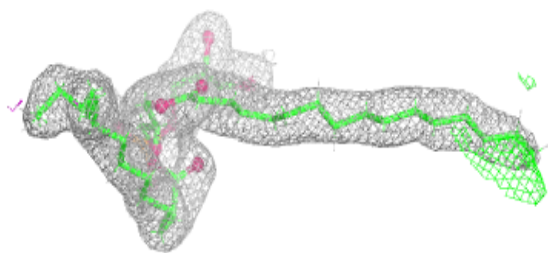
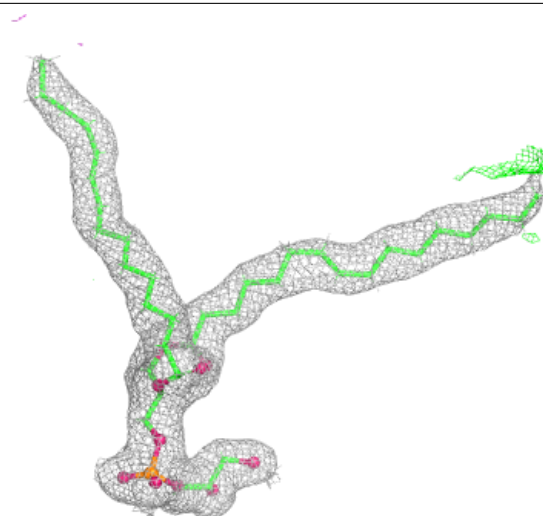
Electron density around CLA B 611:

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



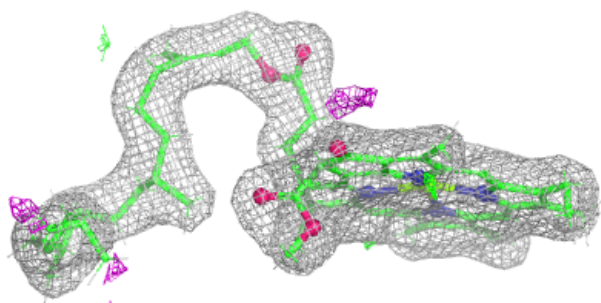
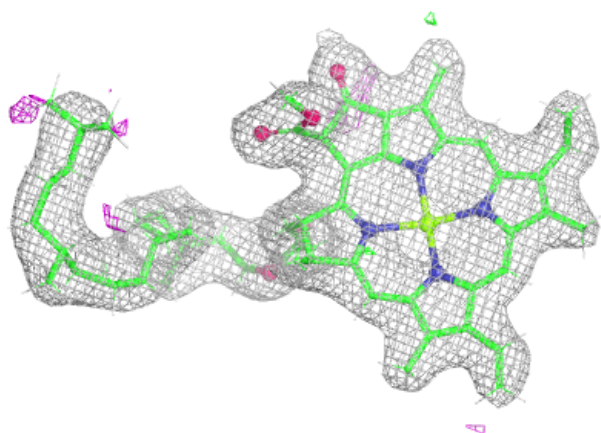
Electron density around LHG L 101:

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



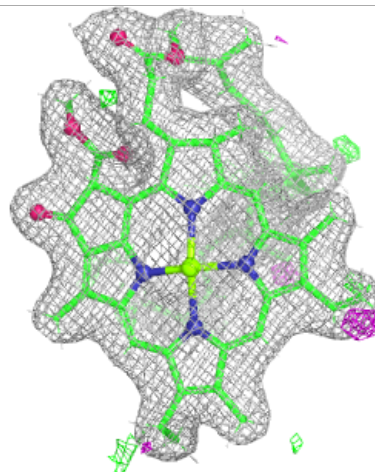
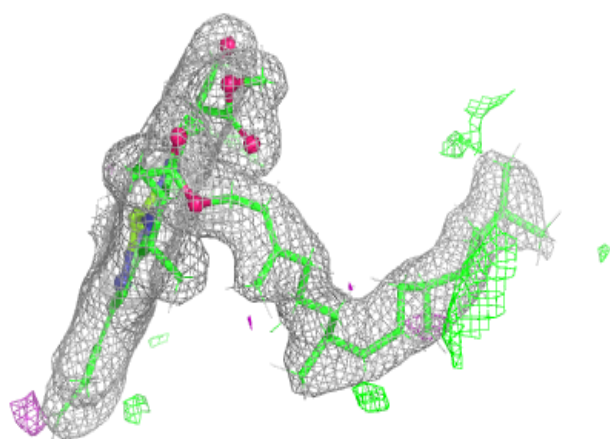
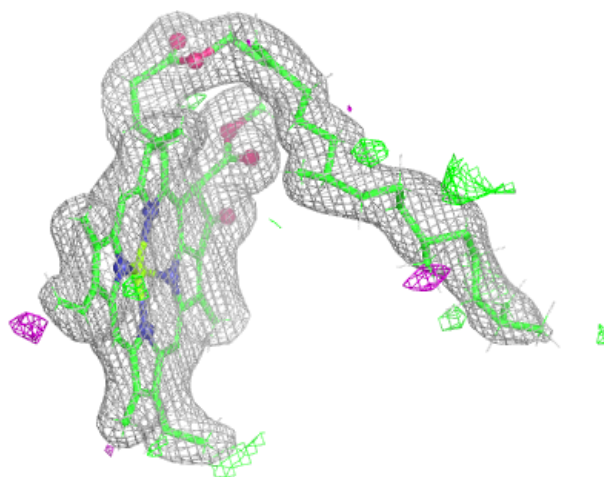
Electron density around CLA B 612:

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



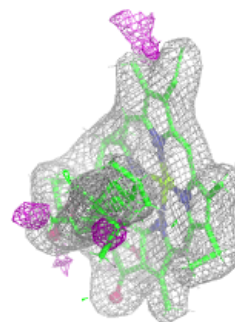
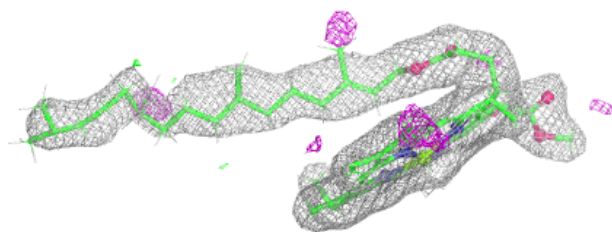
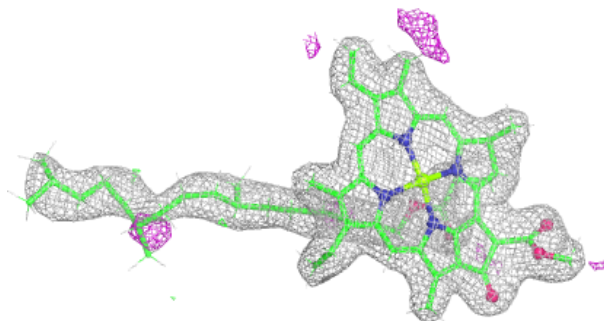
Electron density around CLA B 613:

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



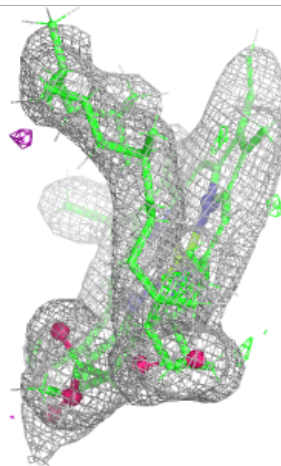
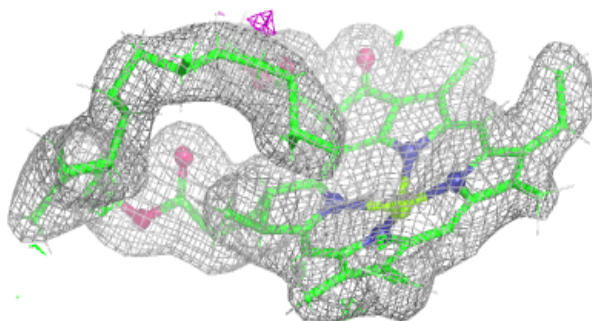
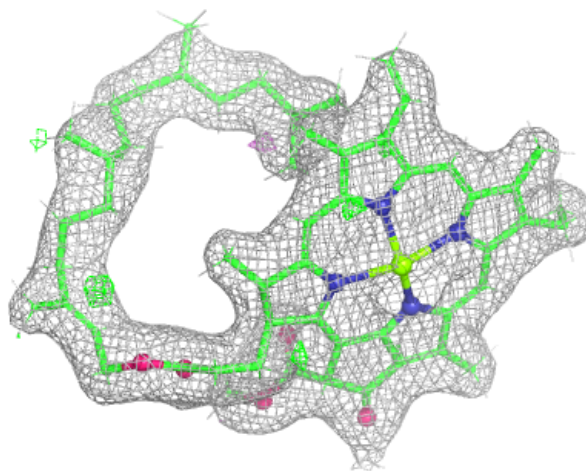
Electron density around CLA B 614:

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



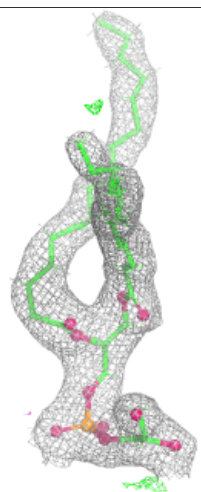
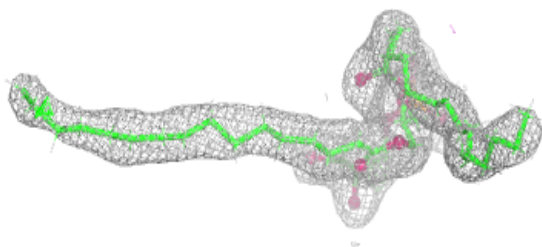
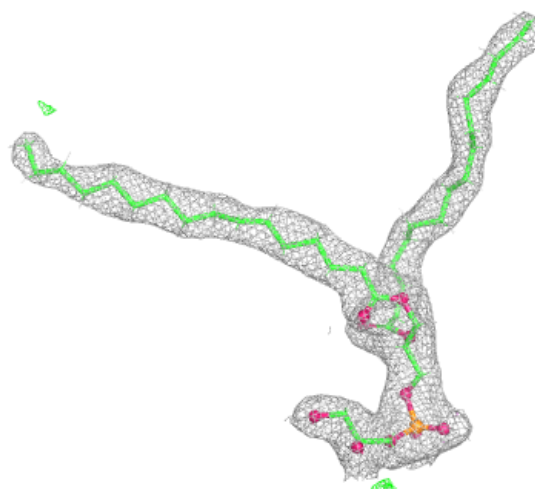
Electron density around CLA B 615:

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



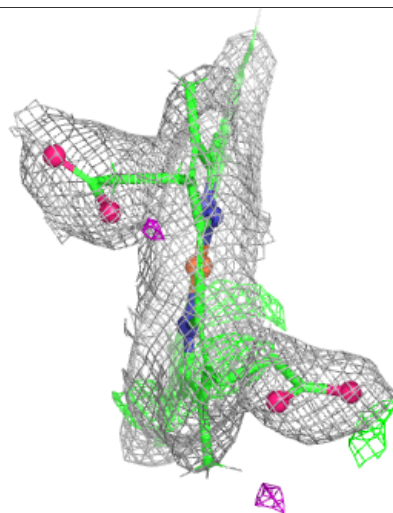
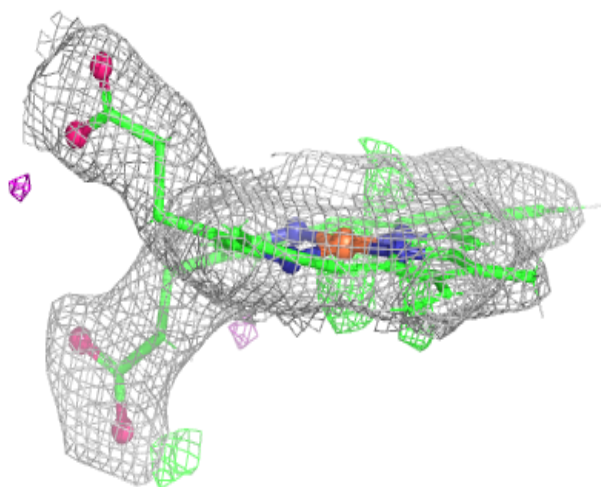
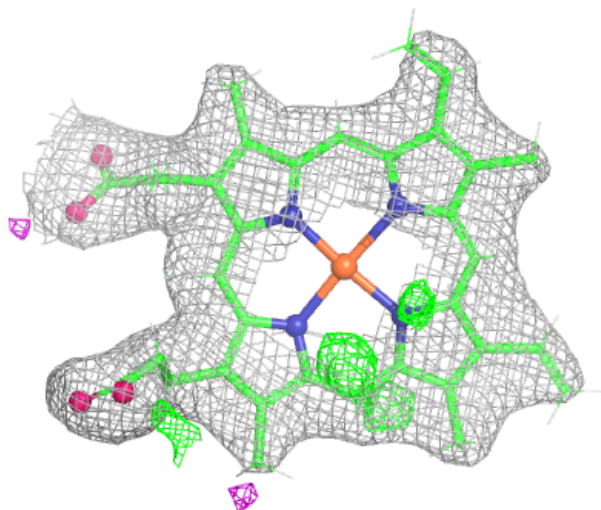
Electron density around LHG 1 101:

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



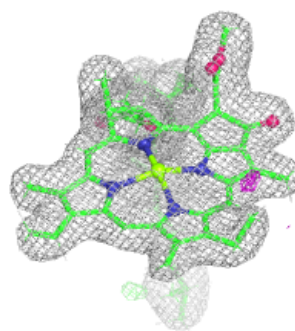
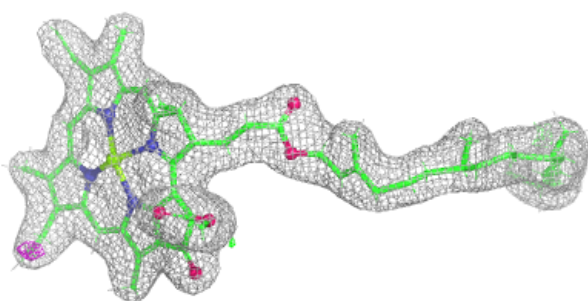
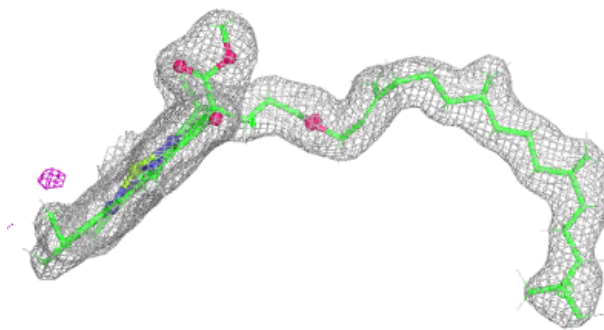
Electron density around HEM F 101:

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

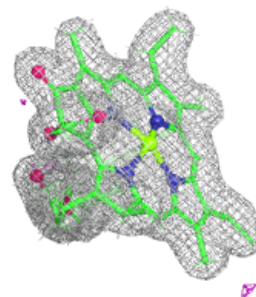
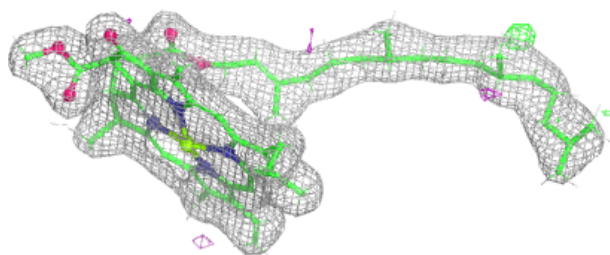
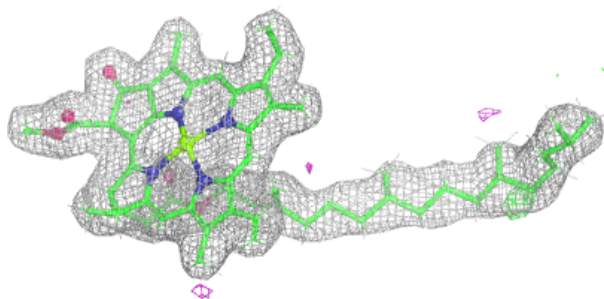


Electron density around CLA D 402:

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

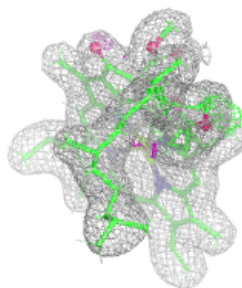
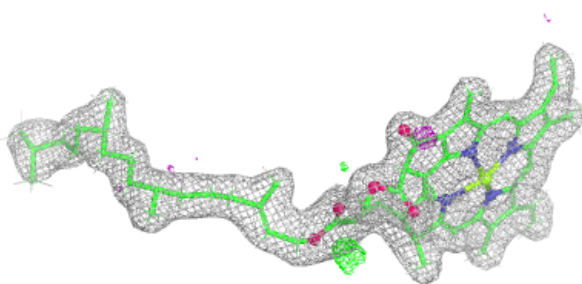
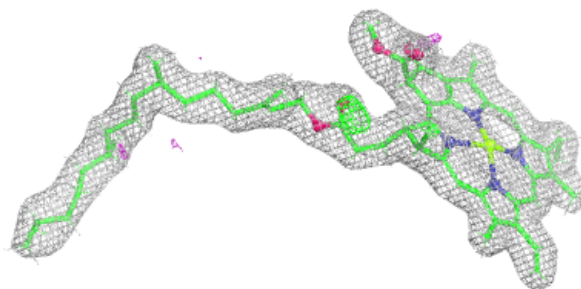
**Electron density around CLA B 608:**

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

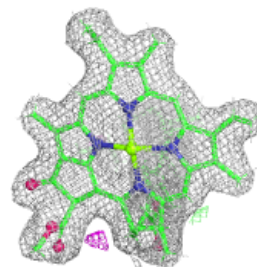
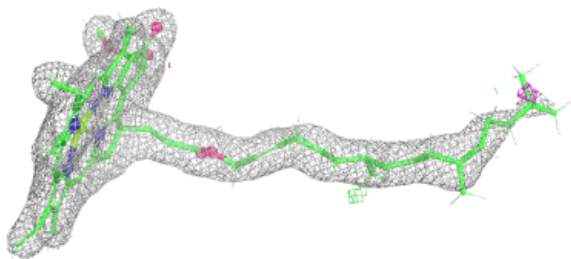
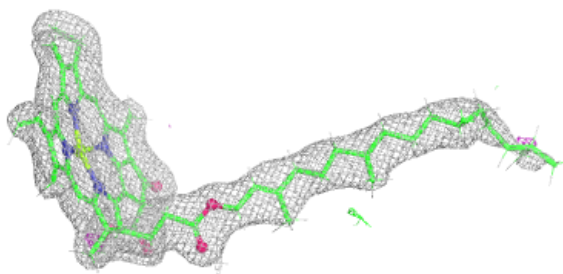


Electron density around CLA A 606:

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

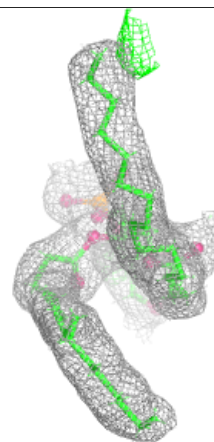
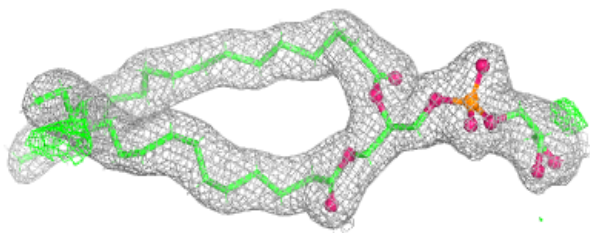
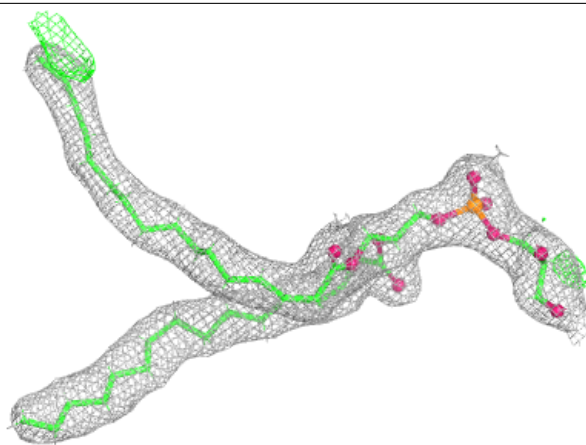
**Electron density around CLA b 604:**

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



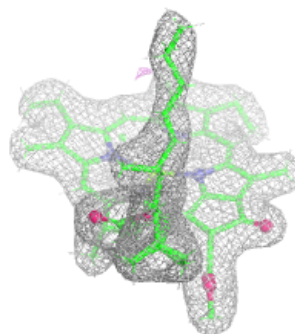
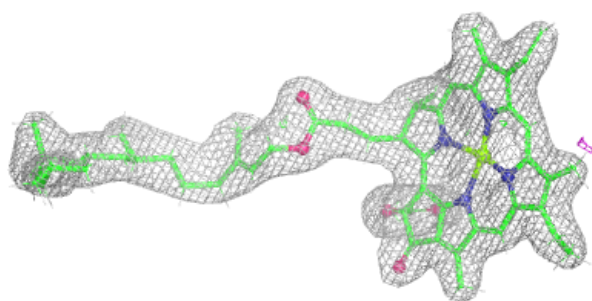
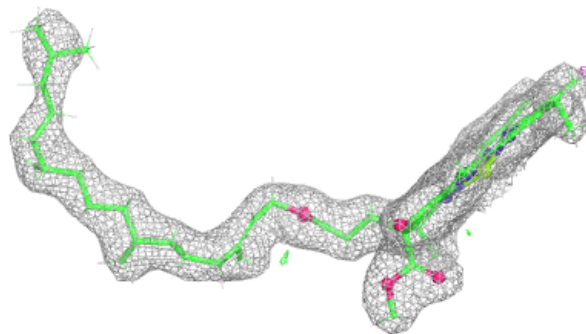
Electron density around LHG D 409:

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

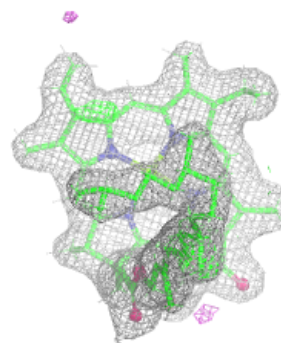
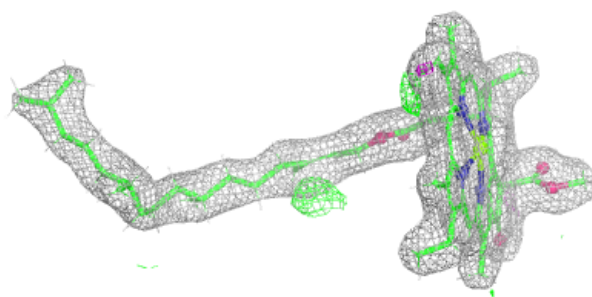
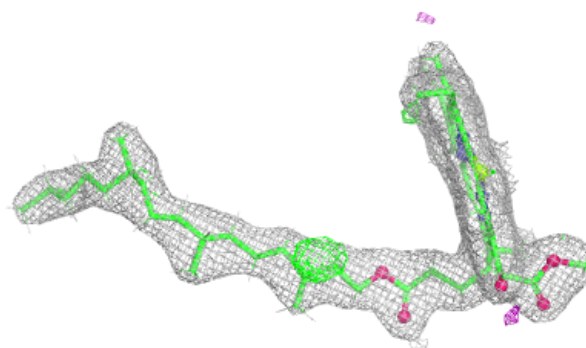


Electron density around CLA d 402:

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

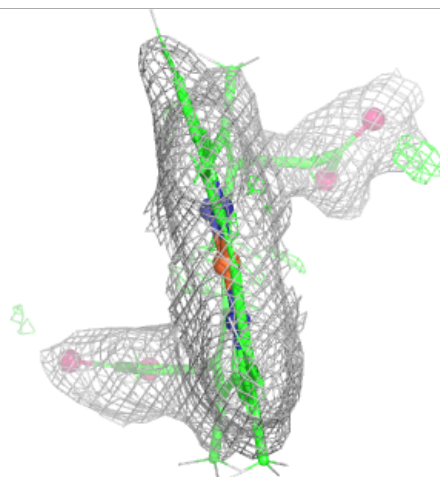
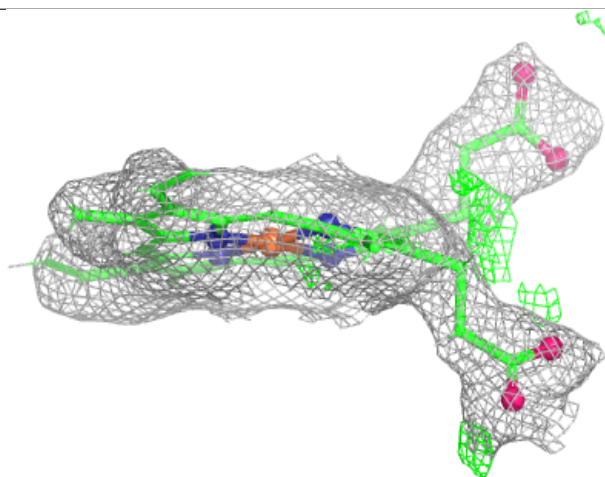
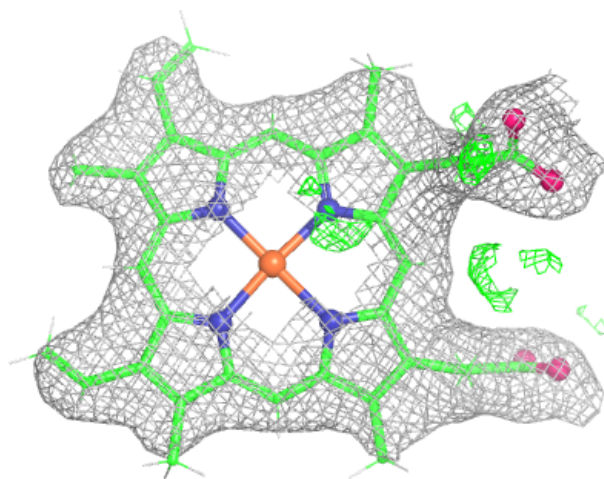
**Electron density around CLA b 605:**

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



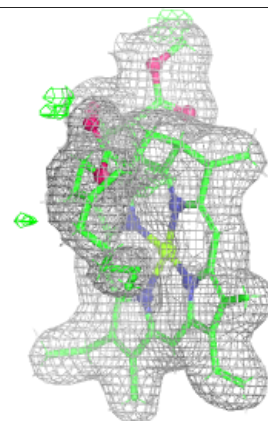
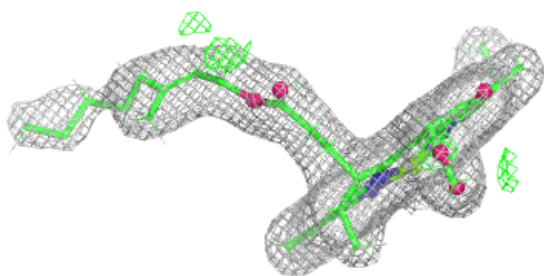
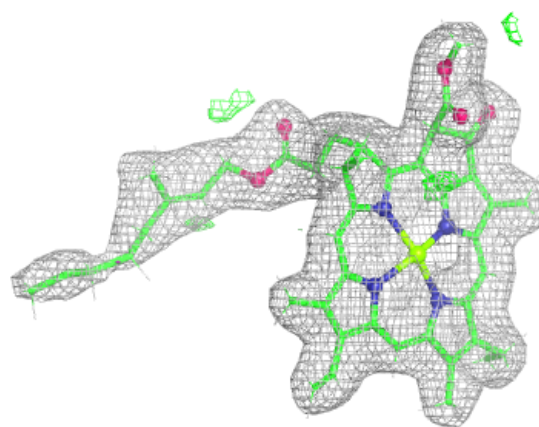
Electron density around HEM e 102:

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



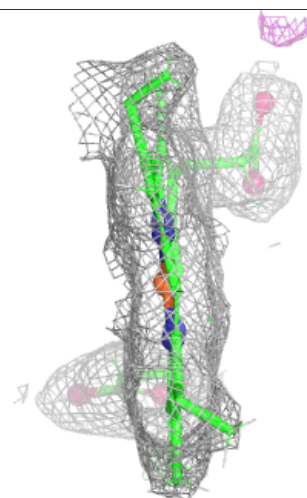
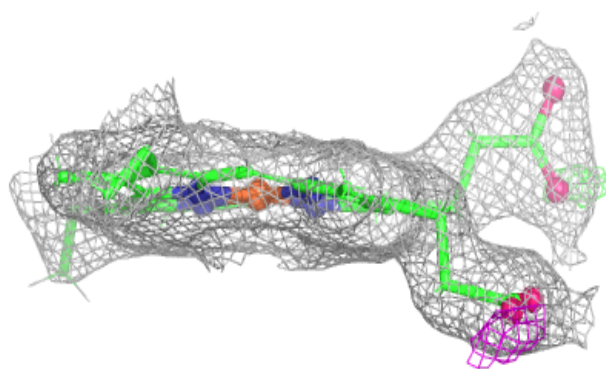
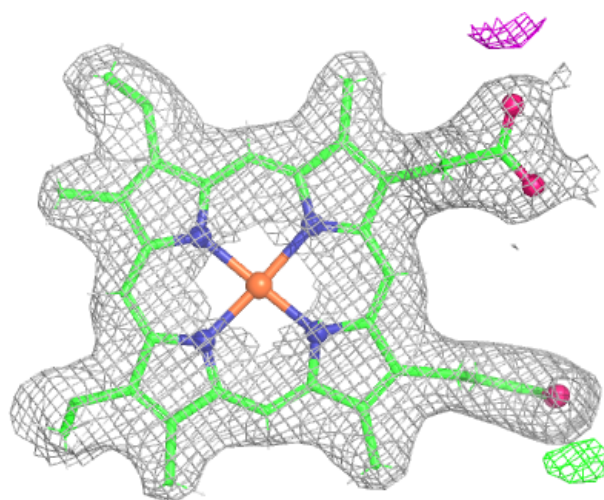
Electron density around CLA A 609:

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



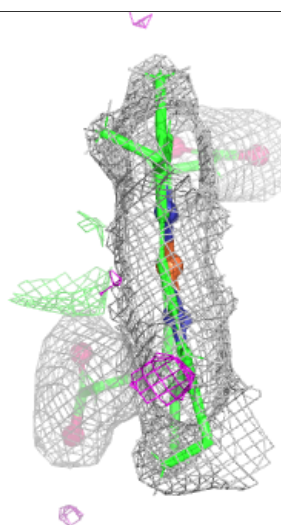
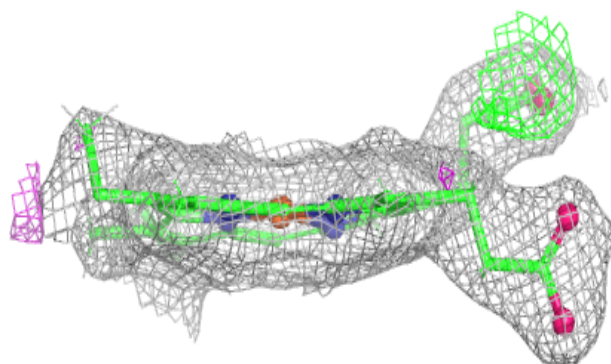
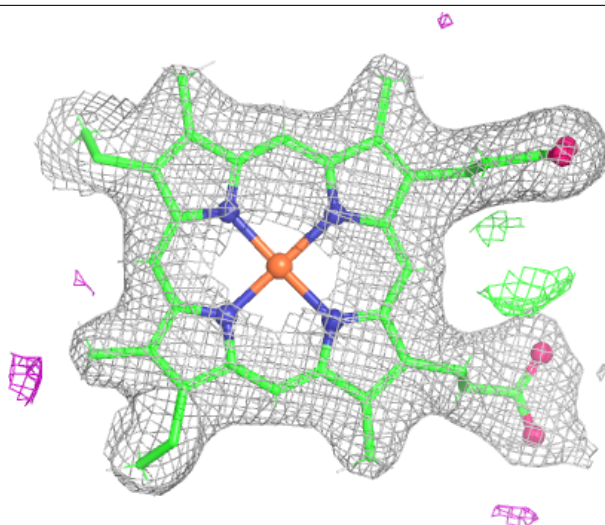
Electron density around HEC V 201:

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



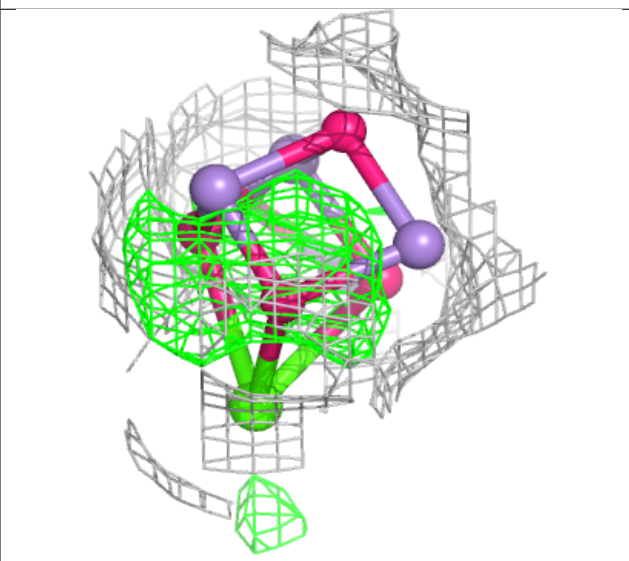
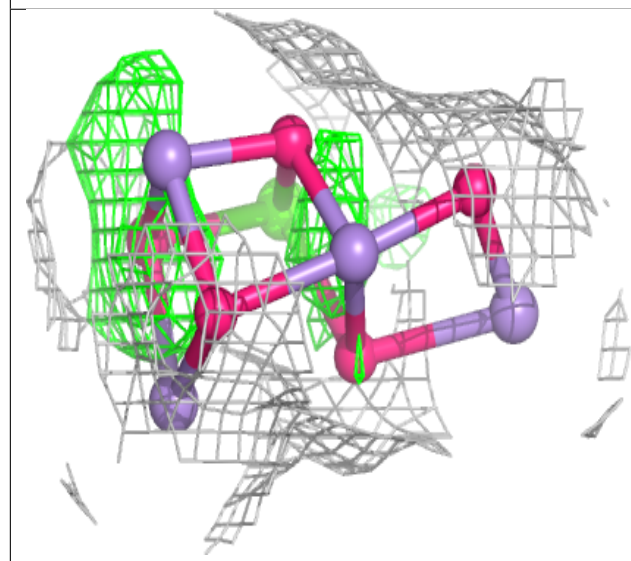
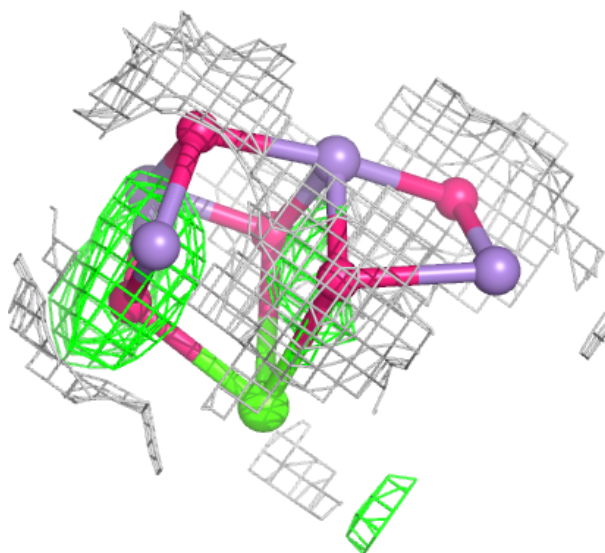
Electron density around HEC v 201:

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



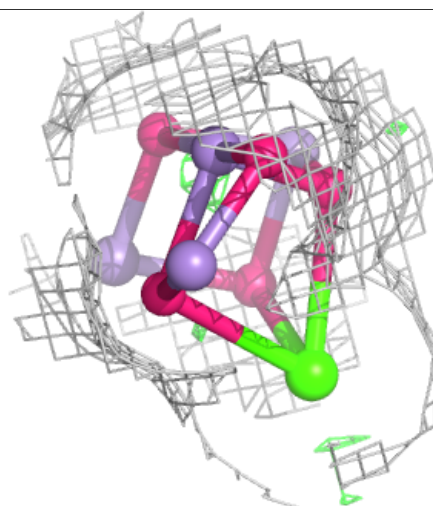
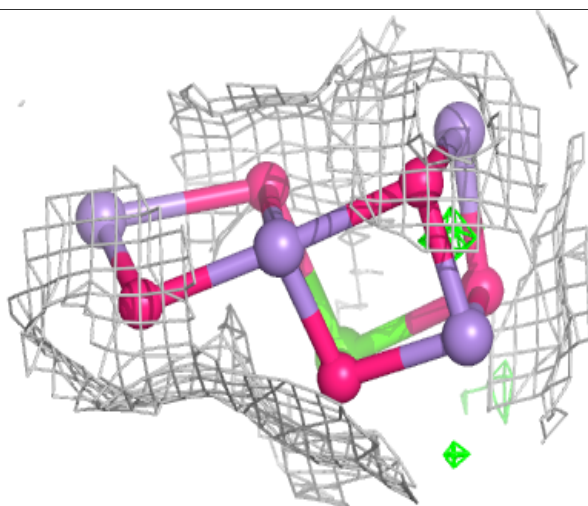
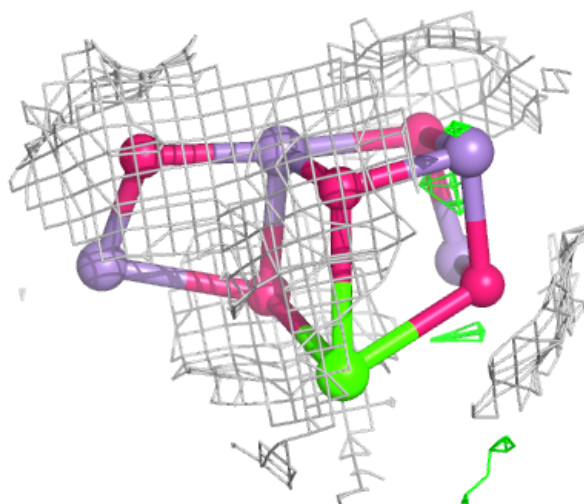
Electron density around OEX A 601:

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



Electron density around OEX a 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.