



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2026 – 02:24 PM EDT

PDB ID : 9Z69 / pdb_00009z69
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2 rich) at 1.98 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 : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

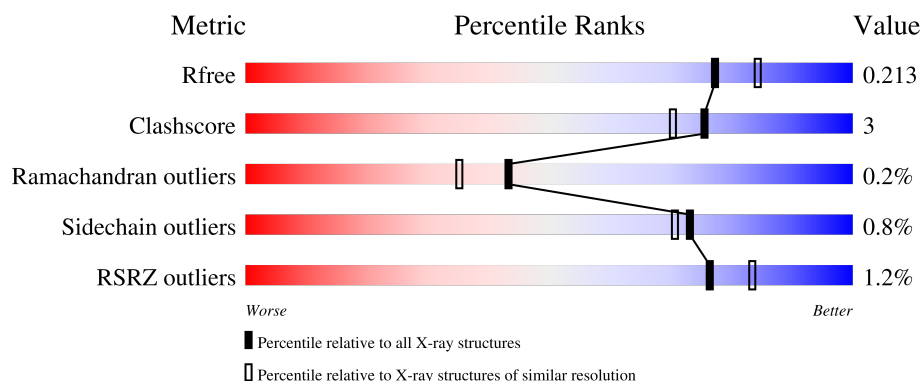
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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.



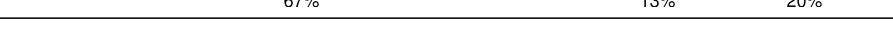
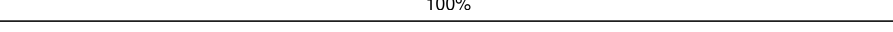
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	
1	a	344	
2	B	510	
2	b	510	

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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

There are 36 unique types of molecules in this entry. The entry contains 104563 atoms, of which 52080 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
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	12			

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

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

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

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

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

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

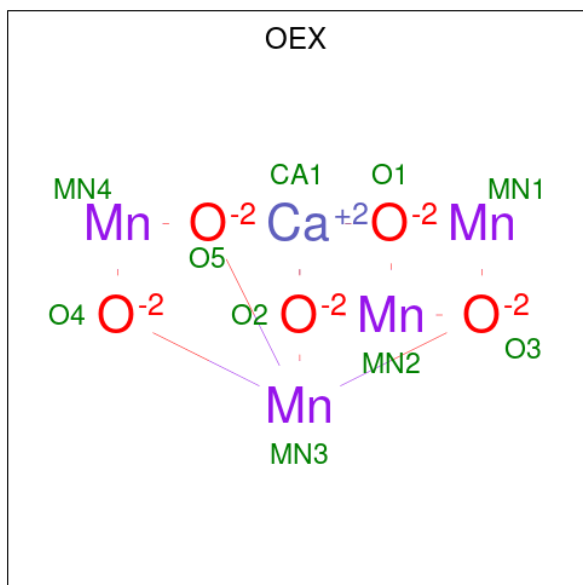
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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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).

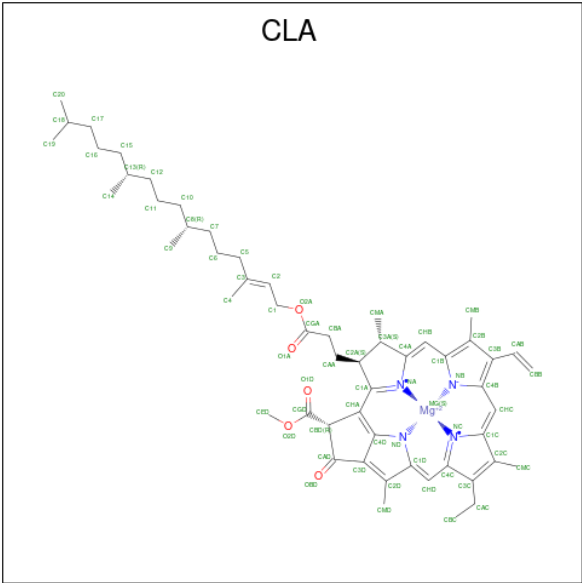
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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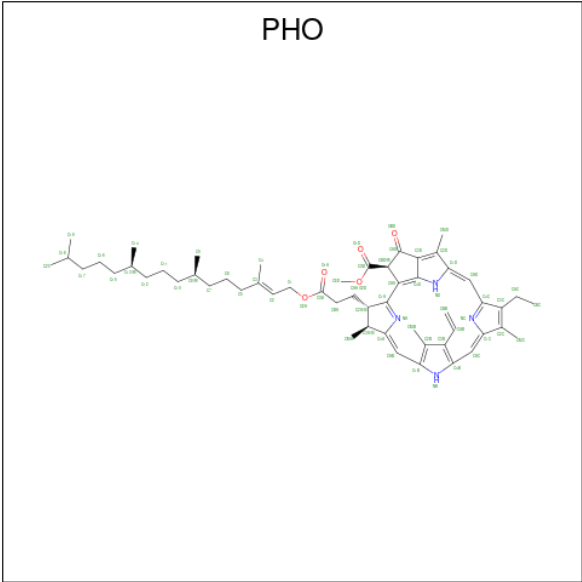
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24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg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

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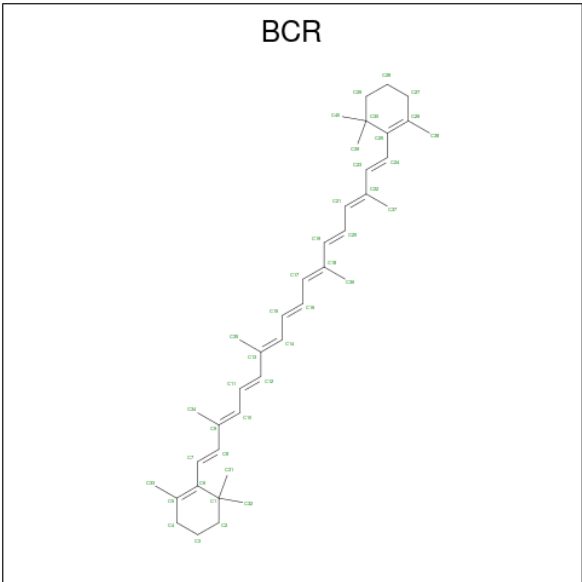
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	c	1	Total 137	C 55	H 72	Mg 1	N 4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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



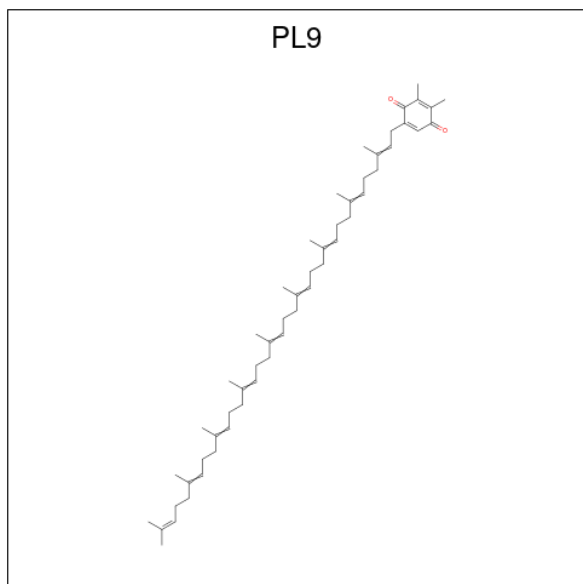
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



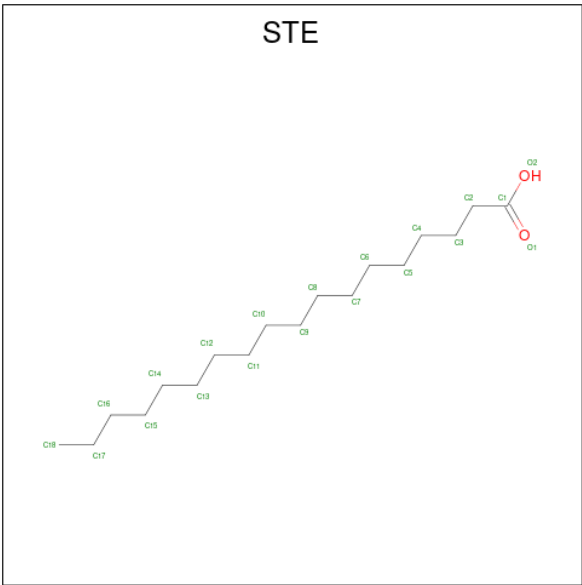
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total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

- Molecule 27 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
27	A	1	Total	C	H	O	0	0
			135	53	80	2		
27	D	1	Total	C	H	O	0	0
			135	53	80	2		
27	a	1	Total	C	H	O	0	0
			135	53	80	2		
27	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H		0	0
			23	9	14			
28	A	1	Total	C	H		0	0
			23	8	15			
28	A	1	Total	C	H		0	0
			50	17	33			
28	A	1	Total	C	H		0	0
			32	11	21			
28	B	1	Total	C	H	O	0	0
			43	15	26	2		
28	B	1	Total	C	H	O	0	0
			46	16	28	2		
28	B	1	Total	C	H	O	0	0
			28	10	16	2		
28	B	1	Total	C	H		0	0
			41	15	26			
28	C	1	Total	C	H	O	0	0
			34	12	20	2		
28	C	1	Total	C	H		0	0
			11	5	6			
28	C	1	Total	C	H		0	0
			17	7	10			
28	C	1	Total	C	H		0	0
			26	10	16			
28	C	1	Total	C	H	O	0	0
			28	10	16	2		
28	C	1	Total	C	H		0	0
			47	16	31			

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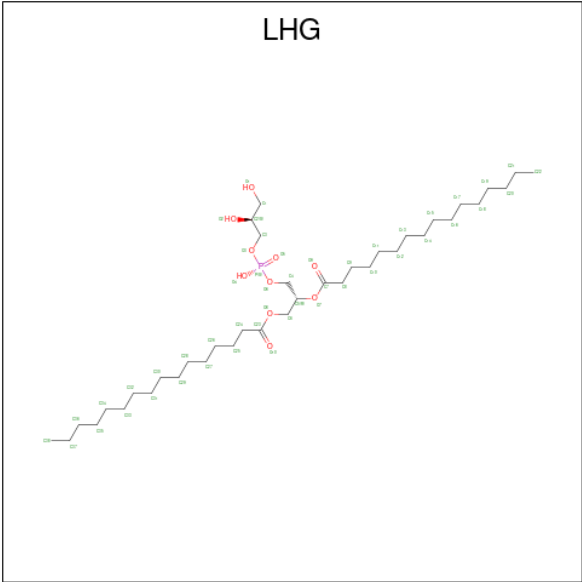
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C H 41 14 27	0	0
28	D	1	Total C H O 55 18 35 2	0	0
28	E	1	Total C H 35 12 23	0	0
28	E	1	Total C H O 55 18 35 2	0	0
28	H	1	Total C H 53 18 35	0	0
28	H	1	Total C H 26 9 17	0	0
28	I	1	Total C H O 43 15 26 2	0	0
28	I	1	Total C H O 37 13 22 2	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	K	1	Total C H 41 14 27	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	M	1	Total C H 44 15 29	0	0
28	T	1	Total C H 47 16 31	0	0
28	Z	1	Total C H 50 17 33	0	0
28	R	1	Total C H O 28 10 16 2	0	0
28	a	1	Total C H O 28 10 16 2	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H O 40 14 24 2	0	0
28	b	1	Total C H 26 10 16	0	0
28	b	1	Total C H 32 11 21	0	0

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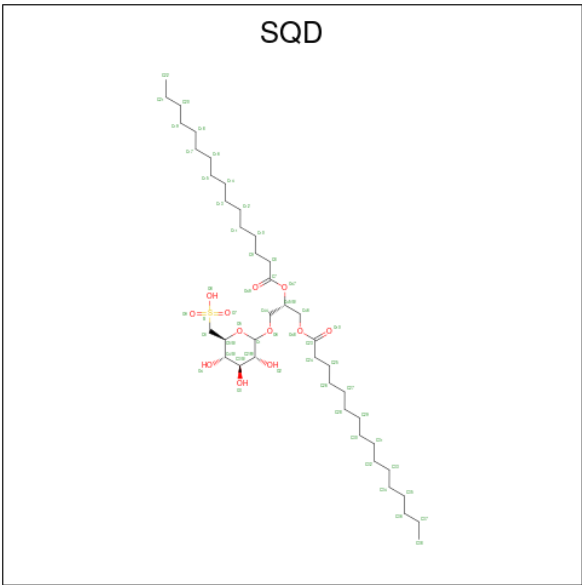
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total	C	H		0	0
			35	13	22			
28	c	1	Total	C	H		0	0
			53	18	35			
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	d	1	Total	C	H	O	0	0
			55	18	35	2		
28	e	1	Total	C	H		0	0
			26	9	17			
28	e	1	Total	C	H		0	0
			26	9	17			
28	e	1	Total	C	H	O	0	0
			31	11	18	2		
28	f	1	Total	C	H		0	0
			23	8	15			
28	h	1	Total	C	H		0	0
			29	10	19			
28	i	1	Total	C	H	O	0	0
			28	10	16	2		
28	i	1	Total	C	H		0	0
			14	6	8			
28	j	1	Total	C	H	O	0	0
			28	10	16	2		
28	j	1	Total	C	H		0	0
			47	16	31			
28	k	1	Total	C	H	O	0	0
			34	12	20	2		
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	m	1	Total	C	H		0	0
			53	18	35			
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	t	1	Total	C	H		0	0
			26	10	16			
28	z	1	Total	C	H		0	0
			23	9	14			

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



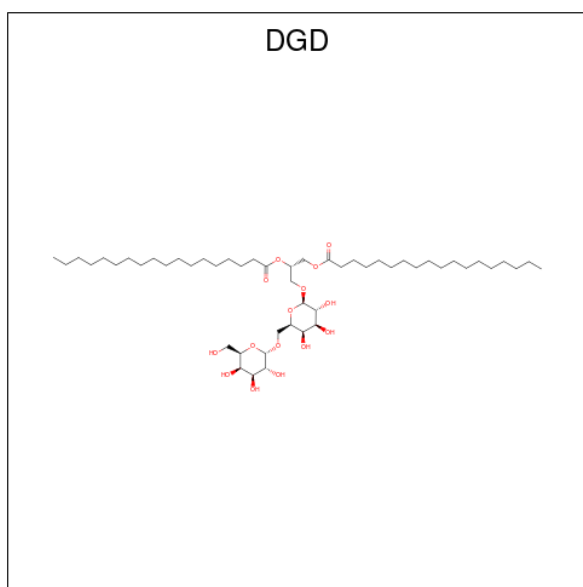
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



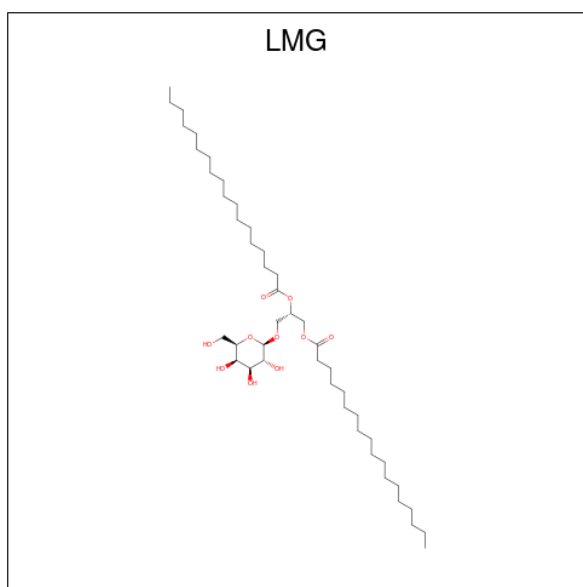
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
30	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
30	D	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



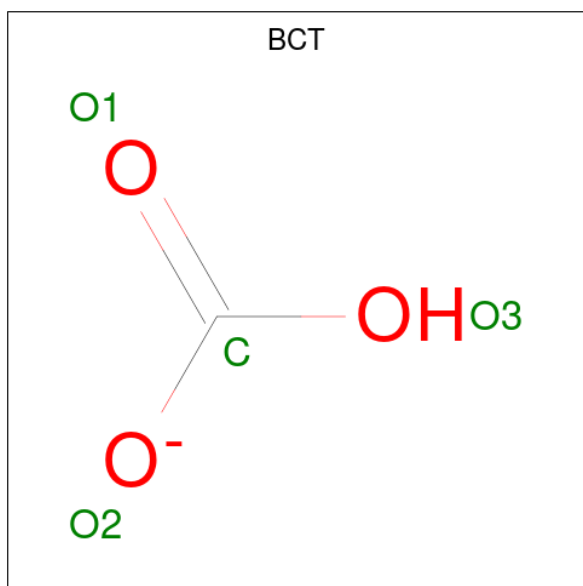
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			105	35	60	10		
32	C	1	Total	C	H	O	0	0
			76	26	40	10		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			120	40	70	10		
32	D	1	Total	C	H	O	0	0
			123	41	72	10		
32	M	1	Total	C	H	O	0	0
			123	41	72	10		
32	a	1	Total	C	H	O	0	0
			141	45	86	10		
32	a	1	Total	C	H	O	0	0
			117	39	68	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			71	25	41	5		
32	c	1	Total	C	H	O	0	0
			108	36	62	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		
32	d	1	Total	C	H	O	0	0
			102	34	58	10		

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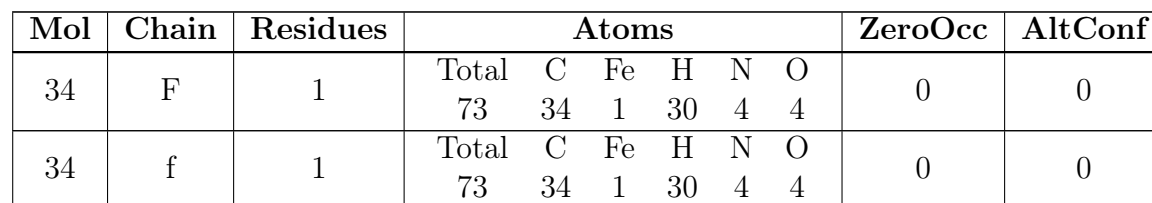
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	m	1	Total	C	H	O	0	0
			123	41	72	10		

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



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

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



- [illegible]

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	130	Total O 130 130	0	0
36	B	208	Total O 208 208	0	0
36	C	180	Total O 180 180	0	0
36	D	137	Total O 137 137	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	30	Total O 30 30	0	0
36	I	17	Total O 17 17	0	0
36	J	14	Total O 14 14	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	5	Total O 5 5	0	0
36	O	100	Total O 100 100	0	0
36	T	8	Total O 8 8	0	0
36	U	46	Total O 46 46	0	0
36	V	71	Total O 71 71	0	0
36	X	18	Total O 18 18	0	0
36	R	3	Total O 3 3	0	0
36	a	119	Total O 119 119	0	0
36	b	190	Total O 190 190	0	0
36	c	158	Total O 158 158	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	d	126	Total 126	O 126	0	0
36	e	19	Total 19	O 19	0	0
36	f	6	Total 6	O 6	0	0
36	h	20	Total 20	O 20	0	0
36	i	12	Total 12	O 12	0	0
36	j	7	Total 7	O 7	0	0
36	k	8	Total 8	O 8	0	0
36	l	11	Total 11	O 11	0	0
36	m	9	Total 9	O 9	0	0
36	o	109	Total 109	O 109	0	0
36	t	9	Total 9	O 9	0	0
36	u	53	Total 53	O 53	0	0
36	v	52	Total 52	O 52	0	0
36	y	3	Total 3	O 3	0	0
36	x	10	Total 10	O 10	0	0
36	z	3	Total 3	O 3	0	0
36	r	4	Total 4	O 4	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: 

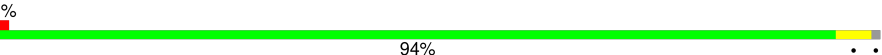


- Molecule 1: Photosystem II protein D1 1

Chain a: 

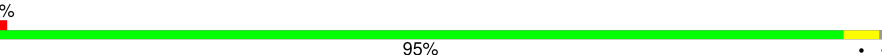


- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



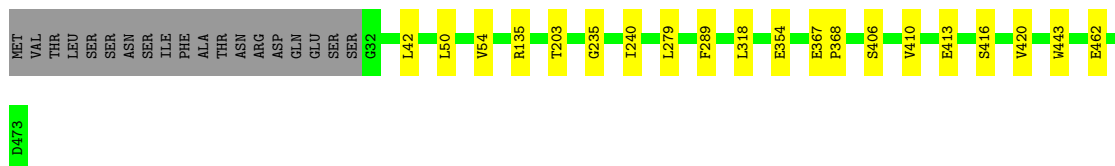
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 

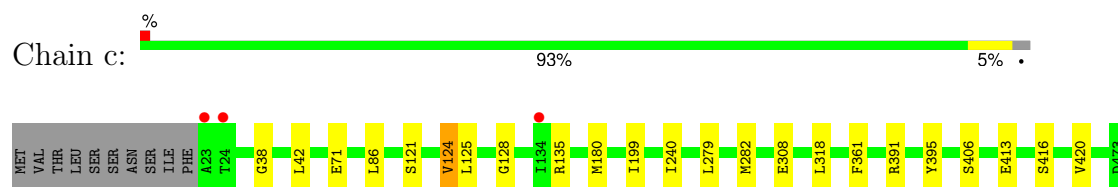


- Molecule 3: Photosystem II CP43 reaction center protein

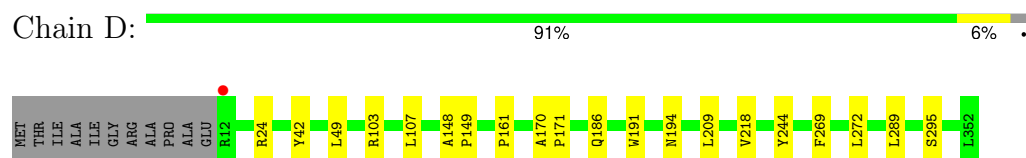
Chain C: 



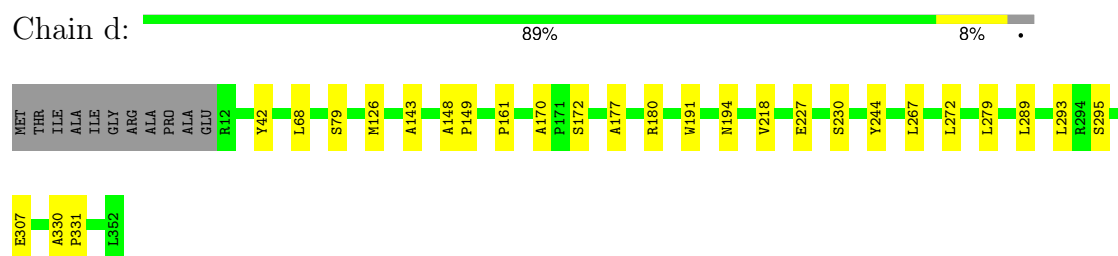
- Molecule 3: Photosystem II CP43 reaction center protein



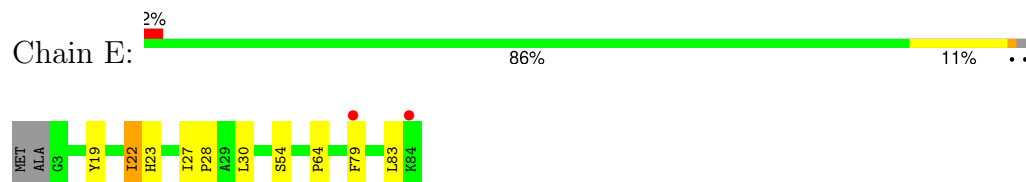
- Molecule 4: Photosystem II D2 protein



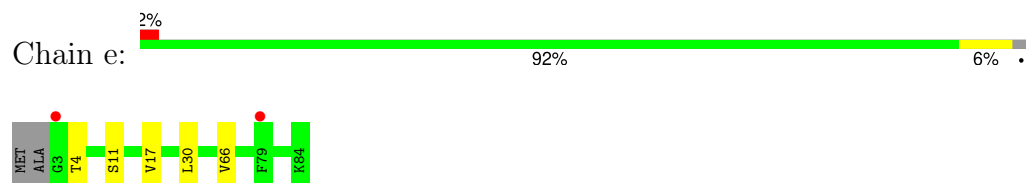
- Molecule 4: Photosystem II D2 protein



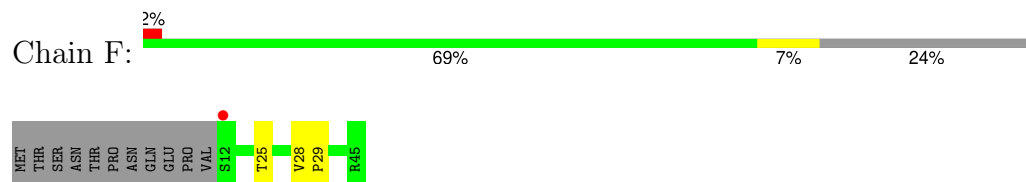
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

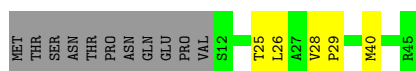


- Molecule 6: Cytochrome b559 subunit beta

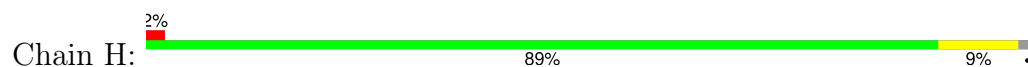


- Molecule 6: Cytochrome b559 subunit beta

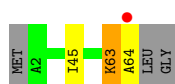
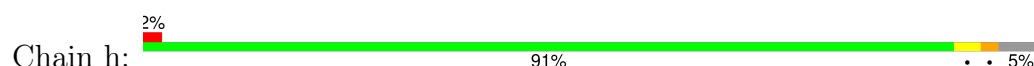




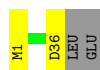
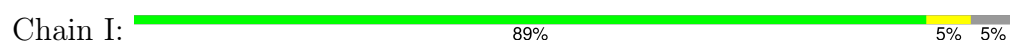
- Molecule 7: Photosystem II reaction center protein H



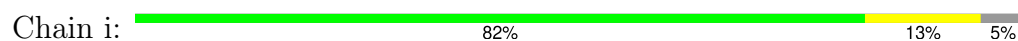
- Molecule 7: Photosystem II reaction center protein H



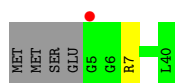
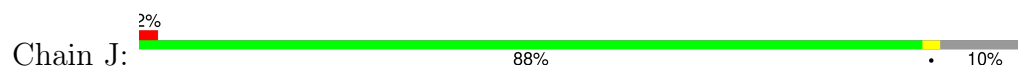
- Molecule 8: Photosystem II reaction center protein I



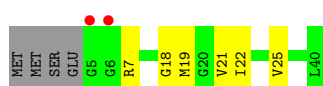
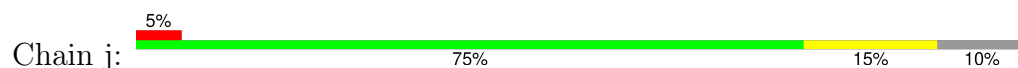
- Molecule 8: Photosystem II reaction center protein I



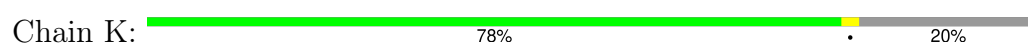
- Molecule 9: Photosystem II reaction center protein J

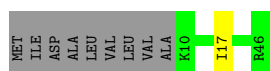


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





• Molecule 10: Photosystem II reaction center protein K

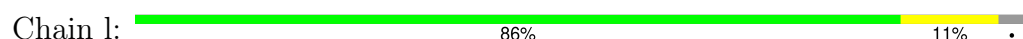


• Molecule 11: Photosystem II reaction center protein L

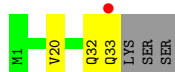
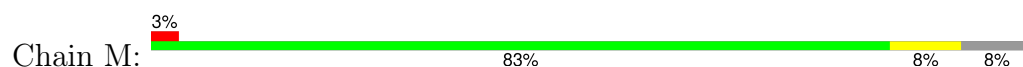


There are no outlier residues recorded for this chain.

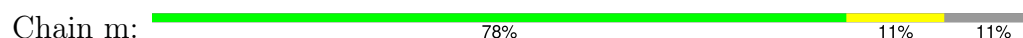
• Molecule 11: Photosystem II reaction center protein L



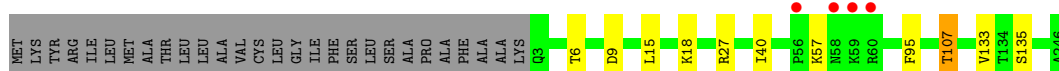
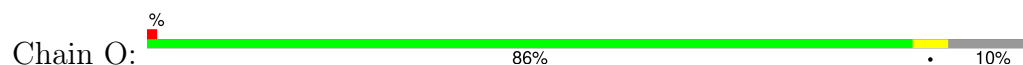
• Molecule 12: Photosystem II reaction center protein M



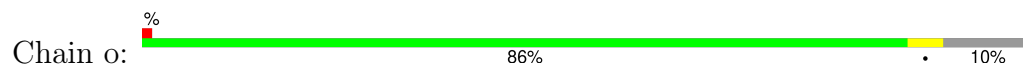
• Molecule 12: Photosystem II reaction center protein M



• Molecule 13: Photosystem II manganese-stabilizing polypeptide



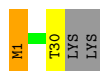
• Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 14: Photosystem II reaction center protein T

Chain T: 88% 6%



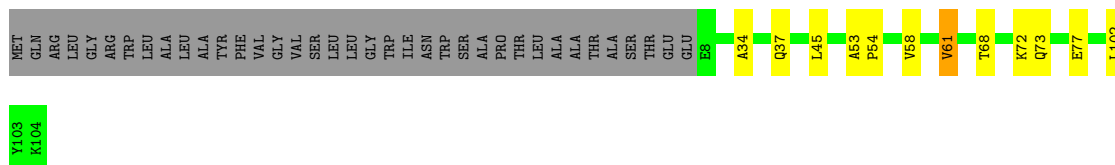
- Molecule 14: Photosystem II reaction center protein T

Chain t: 91% 6%



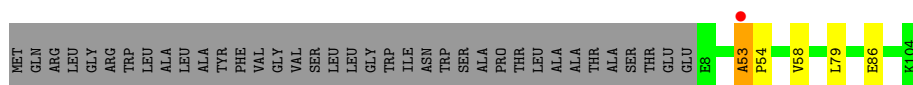
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 63% 8% 28%



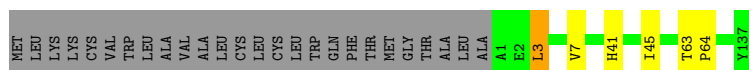
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 69% 8% 28%



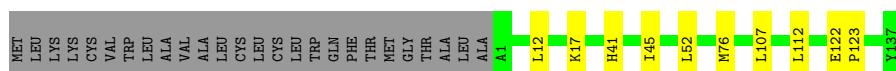
- Molecule 16: Cytochrome c-550

Chain V: 80% 6% 16%

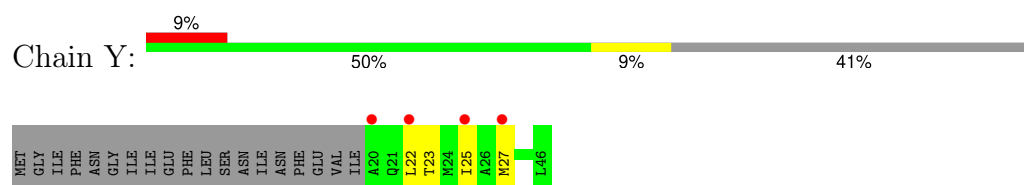


- Molecule 16: Cytochrome c-550

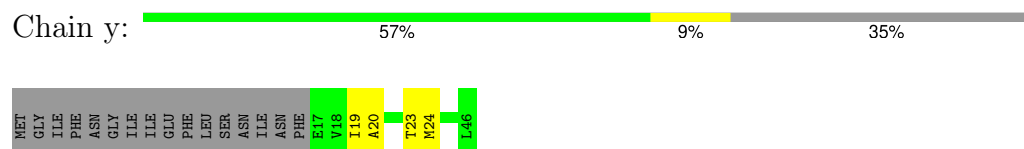
Chain v: 78% 6% 16%



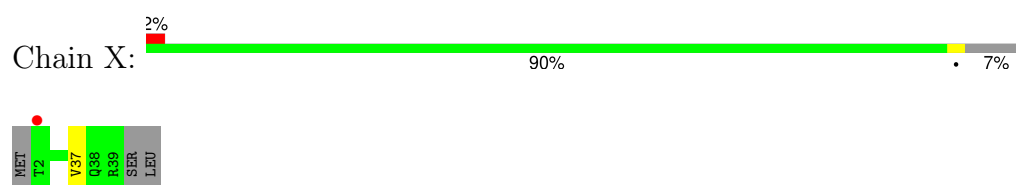
- Molecule 17: Photosystem II reaction center protein Ycf12



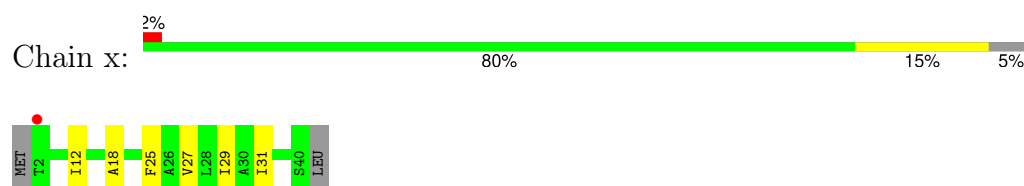
- Molecule 17: Photosystem II reaction center protein Ycf12



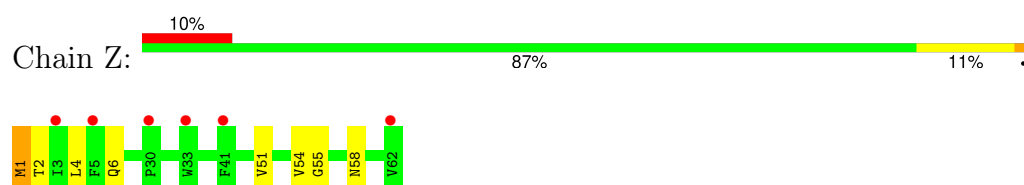
- Molecule 18: Photosystem II reaction center X protein



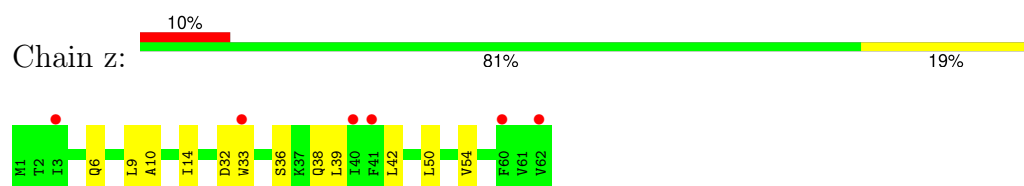
- Molecule 18: Photosystem II reaction center X protein



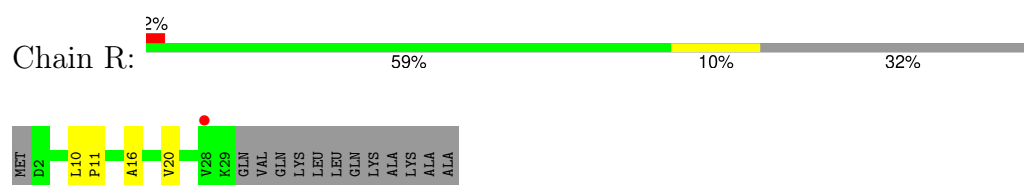
- Molecule 19: Photosystem II reaction center protein Z



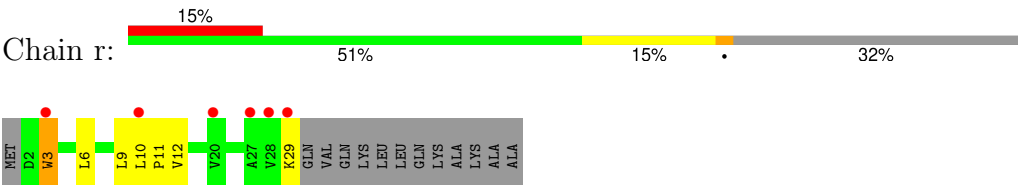
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.55Å 222.83Å 309.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 1.98 37.44 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.44-1.98) 86.3 (37.44-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 1.98Å)	Xtriage
Refinement program	PHENIX 2.0_5848	Depositor
R, R_{free}	0.173 , 0.213 0.173 , 0.213	Depositor DCC
R_{free} test set	4966 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	104563	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/2707	0.59	0/3692
1	a	0.36	0/2704	0.58	0/3688
2	B	0.35	0/4179	0.54	0/5693
2	b	0.32	0/4127	0.53	0/5623
3	C	0.34	0/3547	0.54	0/4830
3	c	0.32	0/3619	0.53	0/4926
4	D	0.35	0/2812	0.57	0/3832
4	d	0.33	0/2821	0.54	0/3844
5	E	0.29	0/688	0.51	0/940
5	e	0.27	0/683	0.48	0/932
6	F	0.28	0/284	0.48	0/387
6	f	0.28	0/284	0.52	0/387
7	H	0.32	0/517	0.53	0/705
7	h	0.28	0/505	0.49	0/689
8	I	0.31	0/293	0.51	0/396
8	i	0.33	0/293	0.45	0/396
9	J	0.28	0/263	0.44	0/356
9	j	0.28	0/263	0.46	0/356
10	K	0.28	0/303	0.50	0/416
10	k	0.25	0/303	0.43	0/416
11	L	0.37	0/311	0.54	0/422
11	l	0.35	0/303	0.49	0/412
12	M	0.36	0/249	0.59	0/341
12	m	0.37	0/244	0.52	0/334
13	O	0.34	0/1904	0.55	0/2585
13	o	0.36	0/1905	0.57	0/2583
14	T	0.37	0/257	0.55	0/349
14	t	0.34	0/255	0.48	0/346
15	U	0.31	0/785	0.54	0/1064
15	u	0.34	0/785	0.57	0/1064
16	V	0.35	0/1085	0.57	0/1473
16	v	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.27	0/197	0.39	0/264
17	y	0.22	0/219	0.45	0/294
18	X	0.28	0/284	0.50	0/384
18	x	0.24	0/289	0.42	0/391
19	Z	0.24	0/490	0.47	0/669
19	z	0.23	0/488	0.39	0/666
20	R	0.24	0/227	0.41	0/313
20	r	0.24	0/227	0.47	0/313
All	All	0.33	0/42784	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
13	o	0	1
16	V	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain

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	11	0
1	a	2619	2462	2510	15	0
2	B	4016	3887	3871	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3984	3842	3842	12	0
3	C	3426	3347	3343	11	1
3	c	3500	3418	3426	14	0
4	D	2717	2621	2621	16	0
4	d	2723	2627	2627	17	0
5	E	666	651	651	7	0
5	e	664	648	648	4	0
6	F	275	282	282	2	0
6	f	275	282	282	6	0
7	H	505	528	528	6	1
7	h	493	514	514	2	0
8	I	296	311	311	1	0
8	i	296	311	311	2	0
9	J	257	268	268	0	0
9	j	257	268	268	4	0
10	K	293	305	305	4	0
10	k	293	305	305	7	0
11	L	304	316	316	0	0
11	l	296	304	304	1	0
12	M	256	267	269	3	0
12	m	251	267	267	5	0
13	O	1870	1830	1830	7	0
13	o	1874	1846	1846	6	0
14	T	258	261	261	2	0
14	t	256	256	256	1	0
15	U	774	773	773	6	0
15	u	774	773	773	5	0
16	V	1064	1071	1073	2	0
16	v	1064	1071	1073	4	0
17	Y	196	217	217	2	0
17	y	218	241	241	2	0
18	X	281	312	312	1	0
18	x	286	316	314	5	0
19	Z	479	516	516	5	0
19	z	477	509	509	9	0
20	R	221	238	238	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	2	0	0	0	0
24	A	249	264	264	6	0
24	B	1035	1139	1139	17	0
24	C	839	922	922	9	0
24	D	130	144	144	1	0
24	a	260	288	288	2	0
24	b	1035	1139	1139	13	0
24	c	839	919	919	9	0
24	d	130	144	144	1	0
25	A	64	74	74	0	0
25	D	64	74	74	0	0
25	a	64	74	74	0	0
25	d	64	74	74	1	0
26	A	40	56	56	1	0
26	B	120	168	168	3	0
26	C	80	112	112	4	0
26	D	40	56	56	5	0
26	H	40	56	56	4	0
26	K	80	112	112	2	0
26	T	40	56	56	4	0
26	a	40	56	56	0	0
26	b	120	168	168	4	0
26	c	80	112	112	0	0
26	d	40	56	56	5	0
26	h	40	56	56	5	0
26	k	80	112	112	4	0
26	t	40	56	56	2	0
27	A	55	80	80	2	0
27	D	55	80	80	0	0
27	a	55	80	80	2	0
27	d	55	80	80	0	0
28	A	45	83	83	2	0
28	B	62	96	96	0	0
28	C	78	126	126	0	0
28	D	20	35	35	0	0
28	E	32	58	58	0	0
28	H	27	52	52	1	0
28	I	32	48	48	0	0
28	J	12	16	16	0	0
28	K	14	27	27	0	0
28	M	40	67	67	0	0
28	R	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	T	16	31	31	1	0
28	Z	17	33	33	0	0
28	a	12	16	16	0	0
28	b	57	96	96	2	0
28	c	31	57	57	1	0
28	d	60	105	105	3	0
28	e	31	52	52	0	0
28	f	8	15	15	0	0
28	h	10	19	19	0	0
28	i	18	24	24	0	0
28	j	28	47	47	0	0
28	k	14	20	20	0	0
28	m	30	51	51	0	0
28	t	24	36	36	0	0
28	z	9	14	14	0	0
29	A	49	74	74	1	0
29	D	145	215	215	2	0
29	L	49	74	74	3	0
29	d	137	199	199	1	0
29	e	42	57	57	1	0
29	l	49	74	74	1	0
30	A	43	52	53	0	0
30	B	54	77	78	2	0
30	D	88	115	117	1	0
30	a	108	154	156	1	0
30	b	49	64	65	0	0
30	f	41	48	49	0	0
31	A	66	96	96	1	0
31	C	186	246	246	0	0
31	H	62	82	82	0	0
31	c	186	246	246	1	0
31	h	62	82	82	0	0
32	B	45	60	60	2	0
32	C	132	172	172	2	0
32	D	101	142	142	6	0
32	M	51	72	72	1	0
32	a	104	154	154	2	0
32	b	55	86	86	0	0
32	c	124	172	172	1	0
32	d	44	58	58	0	0
32	m	51	72	72	4	0
33	D	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	d	4	1	1	0	0
34	F	43	30	30	4	0
34	f	43	30	30	4	0
35	V	43	30	30	0	0
35	v	43	30	30	0	0
36	A	130	0	0	2	0
36	B	208	0	0	0	0
36	C	180	0	0	0	0
36	D	137	0	0	2	0
36	E	26	0	0	0	0
36	F	8	0	0	0	0
36	H	30	0	0	0	0
36	I	17	0	0	0	0
36	J	14	0	0	0	0
36	K	8	0	0	0	0
36	L	8	0	0	0	0
36	M	5	0	0	0	0
36	O	100	0	0	1	0
36	R	3	0	0	0	0
36	T	8	0	0	1	0
36	U	46	0	0	0	0
36	V	71	0	0	0	0
36	X	18	0	0	0	0
36	a	119	0	0	0	0
36	b	190	0	0	2	0
36	c	158	0	0	1	0
36	d	126	0	0	1	0
36	e	19	0	0	0	0
36	f	6	0	0	0	0
36	h	20	0	0	0	0
36	i	12	0	0	1	0
36	j	7	0	0	0	0
36	k	8	0	0	0	0
36	l	11	0	0	0	0
36	m	9	0	0	1	0
36	o	109	0	0	1	0
36	r	4	0	0	0	0
36	t	9	0	0	0	0
36	u	53	0	0	0	0
36	v	52	0	0	0	0
36	x	10	0	0	0	0
36	y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	3	0	0	0	0
All	All	52483	52080	52178	312	1

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

The worst 5 of 312 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)
24:b:613:CLA:H192	29:d:408:LHG:H223	1.38	1.05
26:t:101:BCR:HC8	26:t:101:BCR:H311	1.61	0.83
34:f:101:HEM:HHD	34:f:101:HEM:HBC2	1.65	0.79
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.66	0.78
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.66	0.77

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:462:GLU:OE2	7:H:3:ARG:NH1[4_557]	2.17	0.03

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%)	327 (98%)	4 (1%)	1 (0%)	36	27
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	510/510 (100%)	503 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	497 (99%)	7 (1%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	43	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	35
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	2 (3%)	1 (2%)	7	2
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	0
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	30 (100%)	0	0	100	100
13	O	243/272 (89%)	231 (95%)	11 (4%)	1 (0%)	30	20
13	o	242/272 (89%)	236 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	4
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	9
16	v	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
20	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
All	All	5234/5700 (92%)	5111 (98%)	115 (2%)	8 (0%)	43	35

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	c	416	SER
3	C	416	SER
7	h	63	LYS
15	u	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	82
1	a	269/280 (96%)	266 (99%)	3 (1%)	65	61
2	B	410/407 (101%)	408 (100%)	2 (0%)	81	79
2	b	403/407 (99%)	401 (100%)	2 (0%)	81	79
3	C	346/362 (96%)	343 (99%)	3 (1%)	70	67
3	c	354/362 (98%)	349 (99%)	5 (1%)	59	54
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	277/283 (98%)	273 (99%)	4 (1%)	59	54
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	29
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	29
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	32/34 (94%)	32 (100%)	0	100	100
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%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	23
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	8
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%)	205 (100%)	1 (0%)	81	79
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	79
14	T	26/28 (93%)	26 (100%)	0	100	100
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%)	115 (98%)	2 (2%)	53	48
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%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	44
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	20 (91%)	2 (9%)	9	2
All	All	4324/4654 (93%)	4286 (99%)	38 (1%)	73	67

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	4	THR
16	v	107	LEU
5	e	66	VAL
11	l	30	LEU
20	r	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
18	x	33	GLN
7	h	59	ASN
12	m	32	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.41	0	8,9,11	0.91	1 (12%)
14	FME	t	1	14	8,9,10	0.50	0	8,9,11	1.02	0
14	FME	T	1	14	8,9,10	0.40	0	8,9,11	1.11	1 (12%)
8	FME	i	1	8	8,9,10	0.42	0	8,9,11	0.87	1 (12%)
12	FME	m	1	12	8,9,10	0.41	0	8,9,11	0.87	0
12	FME	M	1	12	8,9,10	0.43	0	8,9,11	0.70	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	-	3/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CG-CB-CA	2.29	119.87	112.87
8	I	1	FME	O-C-CA	-2.08	119.41	124.77
8	i	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
24	CLA	B	603	2	69,73,73	1.45	7 (10%)	82,113,113	1.40	10 (12%)
31	DGD	h	102	-	63,63,67	0.63	0	77,77,81	0.95	6 (7%)
29	LHG	d	410	-	38,38,48	0.62	0	41,44,54	0.76	0
24	CLA	C	508	3	69,73,73	1.25	8 (11%)	82,113,113	1.27	7 (8%)
26	BCR	h	101	-	41,41,41	0.55	0	56,56,56	0.90	2 (3%)
28	STE	T	102	-	15,15,19	0.46	0	14,14,19	0.55	0
24	CLA	C	502	3	69,73,73	1.28	8 (11%)	82,113,113	1.33	7 (8%)
26	BCR	B	617	-	41,41,41	0.46	0	56,56,56	0.91	2 (3%)
28	STE	m	103	-	17,17,19	0.44	0	16,16,19	0.63	0
35	HEC	v	201	16	50,50,50	1.59	4 (8%)	68,82,82	1.25	7 (10%)
32	LMG	c	518	-	29,29,55	0.49	0	31,31,63	0.72	1 (3%)
32	LMG	D	407	-	50,50,55	0.48	0	58,58,63	1.27	6 (10%)
32	LMG	C	517	-	35,35,55	0.49	0	43,43,63	1.69	9 (20%)
24	CLA	B	613	2	69,73,73	1.36	7 (10%)	82,113,113	1.40	8 (9%)
28	STE	M	102	-	14,14,19	0.72	0	14,14,19	0.99	1 (7%)
28	STE	a	616	-	11,11,19	0.83	0	11,11,19	1.02	1 (9%)
28	STE	B	624	-	11,11,19	0.70	0	11,11,19	1.24	1 (9%)
29	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.68	0
26	BCR	b	618	-	41,41,41	0.52	0	56,56,56	0.93	3 (5%)
31	DGD	H	102	-	63,63,67	0.56	0	77,77,81	0.95	6 (7%)
24	CLA	C	506	3	69,73,73	1.29	11 (15%)	82,113,113	1.13	6 (7%)
24	CLA	c	502	3	69,73,73	1.13	5 (7%)	82,113,113	1.29	8 (9%)
28	STE	C	519	-	6,6,19	0.44	0	5,5,19	0.53	0
24	CLA	D	403	4	69,73,73	1.16	8 (11%)	82,113,113	1.12	8 (9%)
24	CLA	c	505	3	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
28	STE	k	103	-	13,13,19	0.69	0	13,13,19	1.06	0
30	SQD	b	620	-	47,49,54	1.67	10 (21%)	57,60,65	2.03	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	614	2	69,73,73	1.32	10 (14%)	82,113,113	1.30	7 (8%)
26	BCR	B	618	-	41,41,41	0.56	0	56,56,56	0.88	2 (3%)
24	CLA	c	508	3	68,72,73	1.32	9 (13%)	80,111,113	1.31	7 (8%)
28	STE	z	101	-	8,8,19	0.45	0	7,7,19	0.56	0
25	PHO	A	607	-	58,69,69	1.92	11 (18%)	55,99,99	1.59	7 (12%)
31	DGD	c	521	-	63,63,67	0.54	1 (1%)	77,77,81	0.79	2 (2%)
28	STE	Z	101	-	16,16,19	0.47	0	15,15,19	0.54	0
26	BCR	b	617	-	41,41,41	0.48	0	56,56,56	0.98	2 (3%)
24	CLA	C	512	3	69,73,73	1.52	10 (14%)	82,113,113	1.40	10 (12%)
32	LMG	d	412	-	44,44,55	0.51	0	52,52,63	0.72	1 (1%)
28	STE	A	617	-	16,16,19	0.45	0	15,15,19	0.57	0
32	LMG	C	525	-	48,48,55	0.50	0	56,56,63	0.71	1 (1%)
28	STE	K	103	-	13,13,19	0.37	0	12,12,19	0.77	0
32	LMG	b	622	-	55,55,55	0.50	0	63,63,63	1.19	9 (14%)
24	CLA	B	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.32	11 (13%)
28	STE	j	101	-	11,11,19	0.85	0	11,11,19	1.35	2 (18%)
24	CLA	B	607	36	69,73,73	1.31	8 (11%)	82,113,113	1.31	6 (7%)
24	CLA	b	613	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	9 (10%)
24	CLA	C	509	3	69,73,73	1.13	5 (7%)	82,113,113	1.26	6 (7%)
24	CLA	C	503	3	69,73,73	1.27	9 (13%)	82,113,113	1.43	8 (9%)
24	CLA	b	601	36	69,73,73	1.27	7 (10%)	82,113,113	1.31	5 (6%)
27	PL9	d	406	-	55,55,55	1.17	5 (9%)	68,69,69	1.68	13 (19%)
24	CLA	C	501	3	69,73,73	1.39	8 (11%)	82,113,113	1.48	8 (9%)
27	PL9	D	406	-	55,55,55	1.30	7 (12%)	68,69,69	1.52	12 (17%)
28	STE	C	526	-	11,11,19	0.79	0	11,11,19	1.35	2 (18%)
24	CLA	C	507	36	69,73,73	1.07	4 (5%)	82,113,113	1.40	8 (9%)
28	STE	b	623	-	15,15,19	0.78	0	15,15,19	1.07	2 (13%)
24	CLA	B	604	2	69,73,73	1.39	9 (13%)	82,113,113	1.54	7 (8%)
24	CLA	b	616	2	64,68,73	1.21	6 (9%)	76,107,113	1.40	8 (10%)
28	STE	M	103	-	9,9,19	0.41	0	8,8,19	0.63	0
28	STE	b	624	-	9,9,19	0.37	0	8,8,19	0.72	0
24	CLA	d	404	4	69,73,73	1.34	7 (10%)	82,113,113	1.15	8 (9%)
28	STE	c	517	-	17,17,19	0.46	0	16,16,19	0.54	0
27	PL9	A	610	-	55,55,55	0.98	0	68,69,69	1.47	8 (11%)
24	CLA	A	612	36	69,73,73	1.26	8 (11%)	82,113,113	1.16	6 (7%)
24	CLA	c	512	3	69,73,73	1.19	9 (13%)	82,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	c	523	-	48,48,55	0.51	0	56,56,63	0.72	0
28	STE	e	101	-	8,8,19	0.48	0	7,7,19	0.42	0
28	STE	B	625	-	14,14,19	0.41	0	13,13,19	0.72	0
24	CLA	a	605	1	69,73,73	1.34	9 (13%)	82,113,113	1.49	9 (10%)
26	BCR	a	609	-	41,41,41	0.48	0	56,56,56	0.88	2 (3%)
28	STE	d	413	-	19,19,19	0.68	0	19,19,19	0.88	0
28	STE	I	101	-	16,16,19	0.84	0	16,16,19	0.92	1 (6%)
30	SQD	a	612	-	52,54,54	1.52	8 (15%)	62,65,65	2.07	12 (19%)
24	CLA	c	501	3	69,73,73	1.10	4 (5%)	82,113,113	1.23	6 (7%)
26	BCR	b	619	-	41,41,41	0.49	0	56,56,56	0.97	3 (5%)
28	STE	C	527	-	15,15,19	0.37	0	14,14,19	0.74	0
32	LMG	a	615	-	49,49,55	0.56	1 (2%)	57,57,63	0.92	3 (5%)
24	CLA	C	511	3	69,73,73	1.41	7 (10%)	82,113,113	1.36	4 (4%)
28	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.23	1 (9%)
28	STE	b	625	-	10,10,19	0.45	0	9,9,19	0.66	0
29	LHG	A	613	-	48,48,48	0.58	0	51,54,54	0.58	1 (1%)
26	BCR	D	405	-	41,41,41	0.49	0	56,56,56	0.84	1 (1%)
24	CLA	b	606	2	69,73,73	1.50	5 (7%)	82,113,113	1.42	6 (7%)
28	STE	j	102	-	15,15,19	0.50	0	14,14,19	0.50	0
24	CLA	C	504	36	63,67,73	1.27	7 (11%)	74,105,113	1.26	11 (14%)
26	BCR	K	102	-	41,41,41	0.44	0	56,56,56	1.02	3 (5%)
26	BCR	C	515	-	41,41,41	0.42	0	56,56,56	0.70	0
28	STE	m	102	-	11,11,19	0.70	0	11,11,19	1.17	0
24	CLA	c	510	3	69,73,73	1.27	8 (11%)	82,113,113	1.25	8 (9%)
26	BCR	H	101	-	41,41,41	0.50	0	56,56,56	0.99	2 (3%)
28	STE	R	101	-	11,11,19	0.82	0	11,11,19	1.10	1 (9%)
28	STE	I	102	-	14,14,19	0.78	0	14,14,19	0.97	0
32	LMG	M	101	-	51,51,55	0.52	0	59,59,63	0.95	1 (1%)
28	STE	A	616	-	7,7,19	0.37	0	6,6,19	0.63	0
24	CLA	C	505	3	69,73,73	1.15	7 (10%)	82,113,113	1.40	9 (10%)
30	SQD	B	622	-	52,54,54	1.59	10 (19%)	62,65,65	1.97	15 (24%)
28	STE	f	103	-	7,7,19	0.41	0	6,6,19	0.60	0
24	CLA	b	612	2	69,73,73	1.28	8 (11%)	82,113,113	1.18	7 (8%)
29	LHG	d	408	-	48,48,48	0.55	0	51,54,54	0.75	1 (1%)
30	SQD	a	613	-	52,54,54	1.61	8 (15%)	62,65,65	1.37	8 (12%)
31	DGD	C	522	-	63,63,67	0.60	1 (1%)	77,77,81	0.97	5 (6%)
30	SQD	f	102	-	39,41,54	1.69	7 (17%)	49,52,65	2.04	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	e	102	-	41,41,48	0.60	0	44,47,54	0.58	0
24	CLA	B	601	36	69,73,73	1.53	9 (13%)	82,113,113	1.45	7 (8%)
24	CLA	B	606	2	69,73,73	1.45	7 (10%)	82,113,113	1.39	9 (10%)
26	BCR	k	102	-	41,41,41	0.49	0	56,56,56	0.89	1 (1%)
28	STE	C	516	-	13,13,19	0.83	0	13,13,19	0.85	0
24	CLA	b	609	2	69,73,73	1.18	6 (8%)	82,113,113	1.36	11 (13%)
28	STE	i	101	-	11,11,19	0.75	0	11,11,19	1.05	0
28	STE	A	611	-	8,8,19	0.43	0	7,7,19	0.58	0
26	BCR	c	515	-	41,41,41	0.44	0	56,56,56	0.87	2 (3%)
30	SQD	D	412	-	50,52,54	1.61	8 (16%)	60,63,65	1.97	13 (21%)
32	LMG	D	408	-	51,51,55	0.49	0	59,59,63	0.77	0
31	DGD	C	524	-	63,63,67	0.60	1 (1%)	77,77,81	0.80	2 (2%)
28	STE	E	102	-	19,19,19	0.68	0	19,19,19	0.90	1 (5%)
33	BCT	D	401	22	3,3,3	0.79	0	2,3,3	2.49	1 (50%)
27	PL9	a	610	-	55,55,55	1.02	4 (7%)	68,69,69	1.56	11 (16%)
28	STE	B	623	-	17,17,19	0.65	0	17,17,19	1.02	0
28	STE	t	103	-	9,9,19	0.43	0	8,8,19	0.64	0
28	STE	D	414	-	19,19,19	0.61	0	19,19,19	1.16	0
30	SQD	A	614	-	41,43,54	1.80	9 (21%)	51,54,65	1.56	8 (15%)
35	HEC	V	201	16	50,50,50	1.56	4 (8%)	68,82,82	1.32	8 (11%)
24	CLA	b	607	36	69,73,73	1.36	6 (8%)	82,113,113	1.20	6 (7%)
24	CLA	b	608	2	69,73,73	1.10	8 (11%)	82,113,113	1.13	4 (4%)
24	CLA	B	605	2	69,73,73	1.23	6 (8%)	82,113,113	1.28	10 (12%)
24	CLA	c	509	3	69,73,73	1.12	6 (8%)	82,113,113	1.44	5 (6%)
34	HEM	F	101	5,6	50,50,50	1.35	6 (12%)	67,82,82	1.12	5 (7%)
31	DGD	c	519	-	63,63,67	0.61	0	77,77,81	0.85	3 (3%)
28	STE	H	104	-	8,8,19	0.41	0	7,7,19	0.49	0
24	CLA	C	513	3	69,73,73	1.47	9 (13%)	82,113,113	1.37	7 (8%)
25	PHO	d	402	-	58,69,69	2.20	13 (22%)	55,99,99	1.68	10 (18%)
24	CLA	B	616	2	64,68,73	1.30	6 (9%)	76,107,113	1.47	10 (13%)
24	CLA	c	507	36	69,73,73	1.11	6 (8%)	82,113,113	1.34	8 (9%)
29	LHG	D	413	-	48,48,48	0.56	0	51,54,54	0.94	3 (5%)
28	STE	c	516	-	12,12,19	0.44	0	11,11,19	0.62	0
24	CLA	a	611	36	69,73,73	1.32	8 (11%)	82,113,113	1.27	9 (10%)
32	LMG	B	620	-	45,45,55	0.51	0	53,53,63	0.92	2 (3%)
24	CLA	c	511	3	69,73,73	1.50	6 (8%)	82,113,113	1.46	7 (8%)
24	CLA	A	608	1	58,62,73	1.28	7 (12%)	68,99,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	612	2	69,73,73	1.24	9 (13%)	82,113,113	1.37	9 (10%)
28	STE	C	520	-	9,9,19	0.44	0	8,8,19	0.60	0
24	CLA	c	503	3	69,73,73	1.32	6 (8%)	82,113,113	1.38	6 (7%)
32	LMG	C	521	-	48,48,55	0.53	0	56,56,63	0.83	1 (1%)
21	OEX	A	601	36,3,1	0,14,14	-	-	-		
24	CLA	b	604	2	69,73,73	1.13	6 (8%)	82,113,113	1.49	14 (17%)
24	CLA	b	615	2	69,73,73	1.42	9 (13%)	82,113,113	1.32	7 (8%)
24	CLA	b	602	2	69,73,73	1.17	8 (11%)	82,113,113	1.39	10 (12%)
28	STE	t	102	-	13,13,19	0.67	0	13,13,19	1.31	2 (15%)
29	LHG	D	410	-	48,48,48	0.63	1 (2%)	51,54,54	0.87	0
21	OEX	a	601	36,3,1	0,14,14	-	-	-		
24	CLA	a	606	36	69,73,73	1.17	7 (10%)	82,113,113	1.26	8 (9%)
26	BCR	C	514	-	41,41,41	0.42	0	56,56,56	0.75	1 (1%)
28	STE	d	407	-	19,19,19	0.74	0	19,19,19	0.87	1 (5%)
31	DGD	C	523	-	63,63,67	0.64	1 (1%)	77,77,81	0.78	1 (1%)
28	STE	A	618	-	10,10,19	0.37	0	9,9,19	0.77	0
30	SQD	D	409	-	34,36,54	1.55	4 (11%)	42,45,65	2.10	9 (21%)
24	CLA	D	404	4	69,73,73	1.30	9 (13%)	82,113,113	1.26	7 (8%)
28	STE	h	103	-	9,9,19	0.43	0	8,8,19	0.63	0
28	STE	e	103	-	8,8,19	0.42	0	7,7,19	0.61	0
26	BCR	k	101	-	41,41,41	0.46	0	56,56,56	0.77	1 (1%)
24	CLA	b	610	36	69,73,73	1.39	7 (10%)	82,113,113	1.20	9 (10%)
24	CLA	b	603	2	69,73,73	1.18	6 (8%)	82,113,113	1.47	11 (13%)
26	BCR	t	101	-	41,41,41	0.51	0	56,56,56	1.14	4 (7%)
24	CLA	B	602	2	69,73,73	1.21	7 (10%)	82,113,113	1.29	6 (7%)
24	CLA	c	506	3	69,73,73	1.34	11 (15%)	82,113,113	1.13	7 (8%)
29	LHG	D	411	-	46,46,48	0.57	0	49,52,54	0.67	2 (4%)
28	STE	e	104	-	12,12,19	0.71	0	12,12,19	1.10	1 (8%)
26	BCR	c	514	-	41,41,41	0.41	0	56,56,56	0.72	0
28	STE	E	101	-	11,11,19	0.40	0	10,10,19	0.62	0
34	HEM	f	101	5,6	50,50,50	1.47	8 (16%)	67,82,82	1.33	7 (10%)
26	BCR	A	609	-	41,41,41	0.44	0	56,56,56	0.71	0
24	CLA	c	504	36	64,68,73	1.25	9 (14%)	76,107,113	1.34	10 (13%)
25	PHO	a	607	-	58,69,69	2.06	11 (18%)	55,99,99	1.64	13 (23%)
29	LHG	L	101	-	48,48,48	0.54	0	51,54,54	0.85	2 (3%)
31	DGD	A	615	-	67,67,67	0.53	0	81,81,81	1.12	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	a	614	-	55,55,55	0.58	0	63,63,63	1.40	10 (15%)
29	LHG	d	409	-	48,48,48	0.54	0	51,54,54	0.73	2 (3%)
24	CLA	d	403	4	69,73,73	1.21	7 (10%)	82,113,113	1.30	5 (6%)
24	CLA	B	608	2	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
28	STE	b	621	-	19,19,19	0.63	0	19,19,19	0.98	1 (5%)
24	CLA	B	610	36	69,73,73	1.33	7 (10%)	82,113,113	1.44	10 (12%)
26	BCR	T	101	-	41,41,41	0.54	0	56,56,56	0.89	1 (1%)
28	STE	H	103	-	17,17,19	0.43	0	16,16,19	0.69	0
24	CLA	b	611	2	69,73,73	1.20	7 (10%)	82,113,113	1.28	7 (8%)
28	STE	C	518	-	4,4,19	0.46	0	3,3,19	0.36	0
24	CLA	c	513	3	69,73,73	1.21	7 (10%)	82,113,113	1.16	7 (8%)
33	BCT	d	401	22	3,3,3	0.79	0	2,3,3	2.17	1 (50%)
24	CLA	a	608	1	69,73,73	1.15	6 (8%)	82,113,113	1.21	8 (9%)
26	BCR	d	405	-	41,41,41	0.54	0	56,56,56	0.95	4 (7%)
24	CLA	A	606	36	69,73,73	1.21	6 (8%)	82,113,113	1.36	8 (9%)
28	STE	i	102	-	5,5,19	0.38	0	4,4,19	0.49	0
24	CLA	C	510	3	69,73,73	1.27	9 (13%)	82,113,113	1.43	8 (9%)
28	STE	d	411	-	19,19,19	0.66	0	19,19,19	0.83	0
32	LMG	m	101	-	51,51,55	0.51	0	59,59,63	0.96	4 (6%)
31	DGD	c	520	-	63,63,67	0.53	0	77,77,81	0.80	3 (3%)
32	LMG	c	522	-	46,46,55	0.50	0	54,54,63	0.66	0
28	STE	C	528	-	13,13,19	0.44	0	12,12,19	0.57	0
28	STE	M	104	-	14,14,19	0.37	0	13,13,19	0.76	0
26	BCR	B	619	-	41,41,41	0.41	0	56,56,56	0.80	1 (1%)
24	CLA	B	609	2	69,73,73	1.19	4 (5%)	82,113,113	1.31	7 (8%)
28	STE	B	621	-	16,16,19	0.68	0	16,16,19	1.08	0
25	PHO	D	402	-	58,69,69	1.99	10 (17%)	55,99,99	1.69	10 (18%)
24	CLA	B	615	2	69,73,73	1.64	10 (14%)	82,113,113	1.36	5 (6%)
24	CLA	A	605	1	69,73,73	1.20	5 (7%)	82,113,113	1.13	7 (8%)
24	CLA	B	611	2	69,73,73	1.24	9 (13%)	82,113,113	1.25	6 (7%)
24	CLA	b	605	2	69,73,73	1.09	6 (8%)	82,113,113	1.32	9 (10%)
26	BCR	K	101	-	41,41,41	0.47	0	56,56,56	0.86	1 (1%)

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
24	CLA	B	603	2	-	2/39/115/115	-
31	DGD	h	102	-	-	17/51/91/95	0/2/2/2
29	LHG	d	410	-	-	8/43/43/53	-
24	CLA	C	508	3	-	3/39/115/115	-
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
28	STE	T	102	-	-	7/13/13/17	-
24	CLA	C	502	3	-	6/39/115/115	-
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
28	STE	m	103	-	-	7/15/15/17	-
35	HEC	v	201	16	1/1/7/7	4/14/54/54	-
32	LMG	c	518	-	-	7/31/31/70	-
32	LMG	D	407	-	-	16/45/65/70	0/1/1/1
32	LMG	C	517	-	-	13/30/50/70	0/1/1/1
24	CLA	B	613	2	-	10/39/115/115	-
28	STE	M	102	-	-	4/12/12/17	-
28	STE	a	616	-	-	4/9/9/17	-
28	STE	B	624	-	-	3/9/9/17	-
29	LHG	l	101	-	-	18/53/53/53	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
24	CLA	C	506	3	-	12/39/115/115	-
24	CLA	c	502	3	-	6/39/115/115	-
28	STE	C	519	-	-	0/4/4/17	-
24	CLA	D	403	4	-	3/39/115/115	-
24	CLA	c	505	3	-	6/39/115/115	-
28	STE	k	103	-	-	4/11/11/17	-
30	SQD	b	620	-	-	16/44/64/69	0/1/1/1
24	CLA	b	614	2	-	13/39/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	CLA	c	508	3	-	2/38/114/115	-
28	STE	z	101	-	-	3/6/6/17	-
25	PHO	A	607	-	-	1/37/103/103	0/5/6/6
31	DGD	c	521	-	-	15/51/91/95	0/2/2/2
28	STE	Z	101	-	-	3/14/14/17	-
26	BCR	b	617	-	-	0/29/63/63	0/2/2/2
24	CLA	C	512	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	d	412	-	-	10/39/59/70	0/1/1/1
28	STE	A	617	-	-	9/14/14/17	-
32	LMG	C	525	-	-	11/43/63/70	0/1/1/1
28	STE	K	103	-	-	7/11/11/17	-
32	LMG	b	622	-	-	25/50/70/70	0/1/1/1
24	CLA	B	614	2	-	10/39/115/115	-
28	STE	j	101	-	-	3/9/9/17	-
24	CLA	B	607	36	-	2/39/115/115	-
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	C	509	3	-	11/39/115/115	-
24	CLA	C	503	3	-	1/39/115/115	-
24	CLA	b	601	36	-	14/39/115/115	-
27	PL9	d	406	-	-	8/53/73/73	0/1/1/1
24	CLA	C	501	3	-	4/39/115/115	-
27	PL9	D	406	-	-	6/53/73/73	0/1/1/1
28	STE	C	526	-	-	2/9/9/17	-
24	CLA	C	507	36	-	9/39/115/115	-
28	STE	b	623	-	-	4/13/13/17	-
24	CLA	B	604	2	-	6/39/115/115	-
24	CLA	b	616	2	-	5/33/109/115	-
28	STE	M	103	-	-	5/7/7/17	-
28	STE	b	624	-	-	3/7/7/17	-
24	CLA	d	404	4	-	9/39/115/115	-
28	STE	c	517	-	-	8/15/15/17	-
27	PL9	A	610	-	-	22/53/73/73	0/1/1/1
24	CLA	A	612	36	-	3/39/115/115	-
24	CLA	c	512	3	-	15/39/115/115	-
32	LMG	c	523	-	-	15/43/63/70	0/1/1/1
28	STE	e	101	-	-	3/6/6/17	-
28	STE	B	625	-	-	4/12/12/17	-
24	CLA	a	605	1	-	5/39/115/115	-
26	BCR	a	609	-	-	0/29/63/63	0/2/2/2
28	STE	d	413	-	-	8/17/17/17	-
28	STE	I	101	-	-	6/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	612	-	-	20/49/69/69	0/1/1/1
24	CLA	c	501	3	-	2/39/115/115	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
28	STE	C	527	-	-	4/13/13/17	-
32	LMG	a	615	-	-	18/44/64/70	0/1/1/1
24	CLA	C	511	3	-	2/39/115/115	-
28	STE	J	101	-	-	4/9/9/17	-
28	STE	b	625	-	-	4/8/8/17	-
29	LHG	A	613	-	-	14/53/53/53	-
26	BCR	D	405	-	-	2/29/63/63	0/2/2/2
24	CLA	b	606	2	-	6/39/115/115	-
28	STE	j	102	-	-	6/13/13/17	-
24	CLA	C	504	36	-	8/32/108/115	-
26	BCR	K	102	-	-	4/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
28	STE	m	102	-	-	4/9/9/17	-
24	CLA	c	510	3	-	7/39/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	STE	R	101	-	-	4/9/9/17	-
28	STE	I	102	-	-	4/12/12/17	-
32	LMG	M	101	-	-	20/46/66/70	0/1/1/1
28	STE	A	616	-	-	3/5/5/17	-
24	CLA	C	505	3	-	9/39/115/115	-
30	SQD	B	622	-	-	23/49/69/69	0/1/1/1
28	STE	f	103	-	-	4/5/5/17	-
24	CLA	b	612	2	-	4/39/115/115	-
29	LHG	d	408	-	-	19/53/53/53	-
30	SQD	a	613	-	-	20/49/69/69	0/1/1/1
31	DGD	C	522	-	-	18/51/91/95	0/2/2/2
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
29	LHG	e	102	-	-	22/46/46/53	-
24	CLA	B	601	36	-	12/39/115/115	-
24	CLA	B	606	2	-	8/39/115/115	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	C	516	-	-	7/11/11/17	-
24	CLA	b	609	2	-	3/39/115/115	-
28	STE	i	101	-	-	6/9/9/17	-
28	STE	A	611	-	-	3/6/6/17	-
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
30	SQD	D	412	-	-	18/47/67/69	0/1/1/1
32	LMG	D	408	-	-	13/46/66/70	0/1/1/1
31	DGD	C	524	-	-	12/51/91/95	0/2/2/2
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
28	STE	E	102	-	-	10/17/17/17	-
27	PL9	a	610	-	-	14/53/73/73	0/1/1/1
28	STE	B	623	-	-	11/15/15/17	-
28	STE	t	103	-	-	2/7/7/17	-
28	STE	D	414	-	-	6/17/17/17	-
30	SQD	A	614	-	-	14/38/58/69	0/1/1/1
24	CLA	b	607	36	-	9/39/115/115	-
24	CLA	b	608	2	-	7/39/115/115	-
24	CLA	B	605	2	-	6/39/115/115	-
24	CLA	c	509	3	-	13/39/115/115	-
34	HEM	F	101	5,6	-	3/14/54/54	-
31	DGD	c	519	-	-	24/51/91/95	0/2/2/2
28	STE	H	104	-	-	4/6/6/17	-
24	CLA	C	513	3	-	11/39/115/115	-
25	PHO	d	402	-	-	0/37/103/103	0/5/6/6
24	CLA	B	616	2	-	6/33/109/115	-
24	CLA	c	507	36	-	7/39/115/115	-
29	LHG	D	413	-	-	20/53/53/53	-
28	STE	c	516	-	-	6/10/10/17	-
24	CLA	a	611	36	-	4/39/115/115	-
32	LMG	B	620	-	-	15/40/60/70	0/1/1/1
24	CLA	c	511	3	-	4/39/115/115	-
24	CLA	A	608	1	-	3/26/102/115	-
24	CLA	B	612	2	-	7/39/115/115	-
28	STE	C	520	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	3	-	6/39/115/115	-
32	LMG	C	521	-	-	18/43/63/70	0/1/1/1
24	CLA	b	604	2	-	8/39/115/115	-
24	CLA	b	615	2	-	2/39/115/115	-
24	CLA	b	602	2	-	4/39/115/115	-
28	STE	t	102	-	-	3/11/11/17	-
29	LHG	D	410	-	-	15/53/53/53	-
24	CLA	a	606	36	-	4/39/115/115	-
26	BCR	C	514	-	-	3/29/63/63	0/2/2/2
28	STE	d	407	-	-	7/17/17/17	-
31	DGD	C	523	-	-	17/51/91/95	0/2/2/2
28	STE	A	618	-	-	5/8/8/17	-
30	SQD	D	409	-	-	18/28/48/69	0/1/1/1
24	CLA	D	404	4	-	4/39/115/115	-
28	STE	h	103	-	-	3/7/7/17	-
28	STE	e	103	-	-	3/6/6/17	-
26	BCR	k	101	-	-	4/29/63/63	0/2/2/2
24	CLA	b	610	36	-	5/39/115/115	-
24	CLA	b	603	2	-	6/39/115/115	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	602	2	-	3/39/115/115	-
24	CLA	c	506	3	-	12/39/115/115	-
29	LHG	D	411	-	-	15/51/51/53	-
28	STE	e	104	-	-	3/10/10/17	-
26	BCR	c	514	-	-	3/29/63/63	0/2/2/2
28	STE	E	101	-	-	4/9/9/17	-
34	HEM	f	101	5,6	-	4/14/54/54	-
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
24	CLA	c	504	36	-	6/33/109/115	-
25	PHO	a	607	-	-	3/37/103/103	0/5/6/6
29	LHG	L	101	-	-	12/53/53/53	-
31	DGD	A	615	-	-	24/55/95/95	0/2/2/2
32	LMG	a	614	-	-	21/50/70/70	0/1/1/1
29	LHG	d	409	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	403	4	-	7/39/115/115	-
24	CLA	B	608	2	-	2/39/115/115	-
28	STE	b	621	-	-	8/17/17/17	-
24	CLA	B	610	36	-	6/39/115/115	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
28	STE	H	103	-	-	8/15/15/17	-
24	CLA	b	611	2	-	7/39/115/115	-
28	STE	C	518	-	-	1/2/2/17	-
24	CLA	c	513	3	-	13/39/115/115	-
24	CLA	a	608	1	-	12/39/115/115	-
26	BCR	d	405	-	-	0/29/63/63	0/2/2/2
24	CLA	A	606	36	-	5/39/115/115	-
28	STE	i	102	-	-	1/3/3/17	-
24	CLA	C	510	3	-	9/39/115/115	-
28	STE	d	411	-	-	8/17/17/17	-
32	LMG	m	101	-	-	14/46/66/70	0/1/1/1
31	DGD	c	520	-	-	17/51/91/95	0/2/2/2
32	LMG	c	522	-	-	17/41/61/70	0/1/1/1
28	STE	C	528	-	-	6/11/11/17	-
28	STE	M	104	-	-	7/12/12/17	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	2	-	4/39/115/115	-
28	STE	B	621	-	-	5/14/14/17	-
25	PHO	D	402	-	-	1/37/103/103	0/5/6/6
24	CLA	B	615	2	-	15/39/115/115	-
24	CLA	A	605	1	-	6/39/115/115	-
24	CLA	B	611	2	-	4/39/115/115	-
24	CLA	b	605	2	-	6/39/115/115	-
26	BCR	K	101	-	-	4/29/63/63	0/2/2/2

The worst 5 of 667 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C1B-C2B	10.33	1.50	1.39
25	a	607	PHO	C1B-C2B	9.10	1.49	1.39
25	d	402	PHO	C3B-C4B	8.91	1.50	1.41
24	b	606	CLA	MG-NA	8.89	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	PHO	C1B-C2B	8.50	1.48	1.39

The worst 5 of 894 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	8.66	121.42	108.27
24	B	601	CLA	C4A-NA-C1A	8.42	110.52	106.68
24	C	510	CLA	C4A-NA-C1A	8.40	110.51	106.68
24	B	604	CLA	C4A-NA-C1A	8.23	110.44	106.68
24	a	605	CLA	C4A-NA-C1A	8.21	110.42	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 1528 torsion outliers are listed below:

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

There are no ring outliers.

88 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	508	CLA	1	0
26	h	101	BCR	5	0
28	T	102	STE	1	0
24	C	502	CLA	1	0
26	B	617	BCR	1	0
32	D	407	LMG	3	0
32	C	517	LMG	1	0
24	B	613	CLA	1	0
29	l	101	LHG	1	0
26	b	618	BCR	1	0
24	D	403	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	505	CLA	2	0
24	b	614	CLA	4	0
26	B	618	BCR	1	0
31	c	521	DGD	1	0
26	b	617	BCR	2	0
24	C	512	CLA	1	0
28	A	617	STE	2	0
24	B	614	CLA	1	0
24	b	613	CLA	2	0
24	C	509	CLA	3	0
24	B	604	CLA	1	0
24	d	404	CLA	1	0
28	c	517	STE	1	0
27	A	610	PL9	2	0
32	c	523	LMG	1	0
24	a	605	CLA	2	0
28	d	413	STE	1	0
24	c	501	CLA	1	0
26	b	619	BCR	1	0
24	C	511	CLA	1	0
28	b	625	STE	2	0
29	A	613	LHG	1	0
26	D	405	BCR	5	0
26	C	515	BCR	1	0
26	H	101	BCR	4	0
32	M	101	LMG	1	0
24	C	505	CLA	2	0
30	B	622	SQD	2	0
29	d	408	LHG	1	0
30	a	613	SQD	1	0
29	e	102	LHG	1	0
24	B	601	CLA	6	0
26	k	102	BCR	3	0
24	b	609	CLA	1	0
32	D	408	LMG	3	0
27	a	610	PL9	2	0
24	B	605	CLA	3	0
24	c	509	CLA	1	0
34	F	101	HEM	4	0
24	C	513	CLA	1	0
25	d	402	PHO	1	0
24	c	507	CLA	1	0

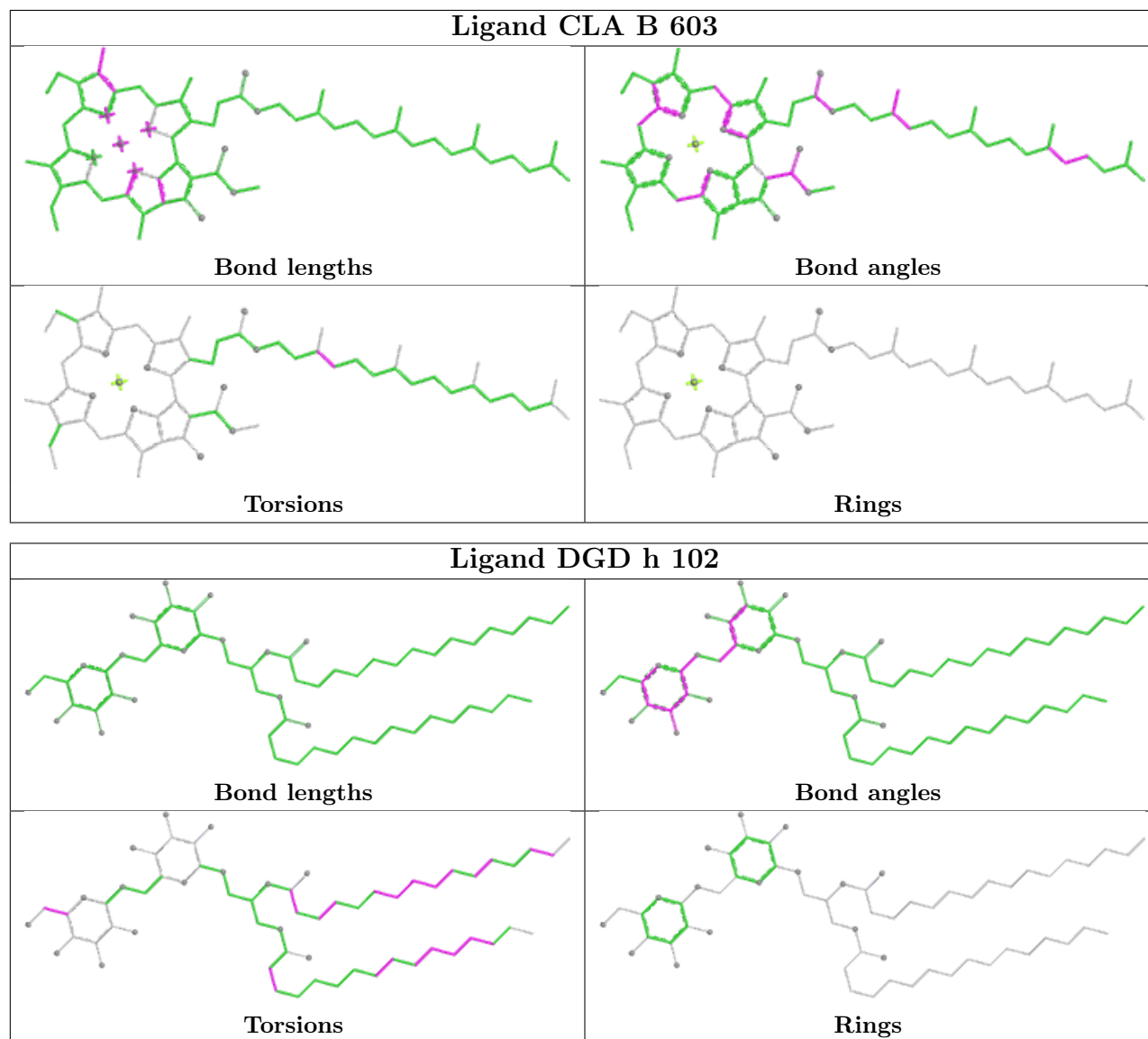
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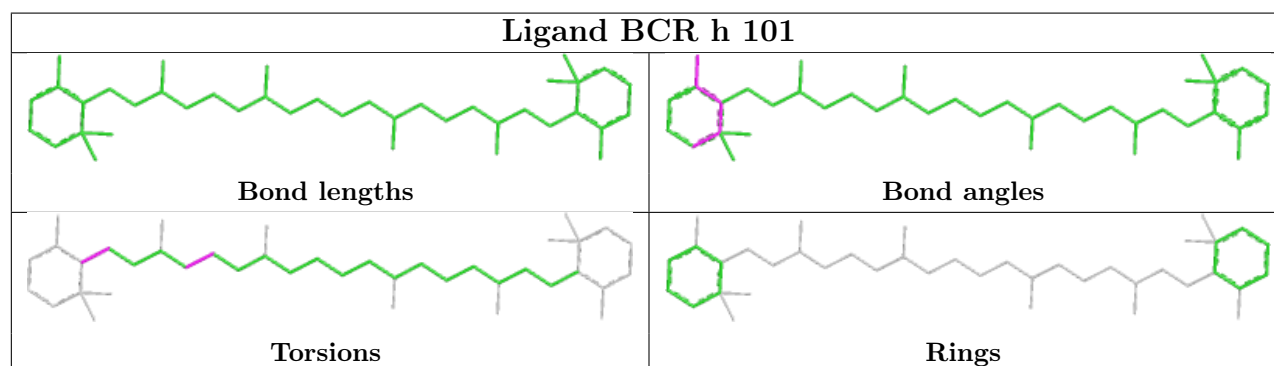
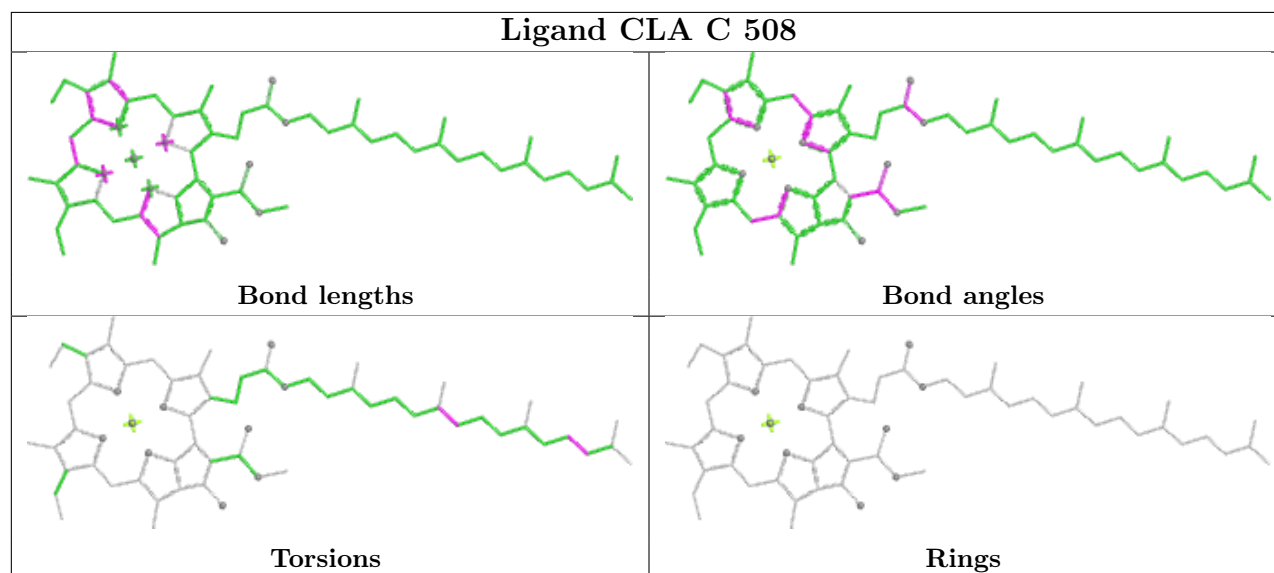
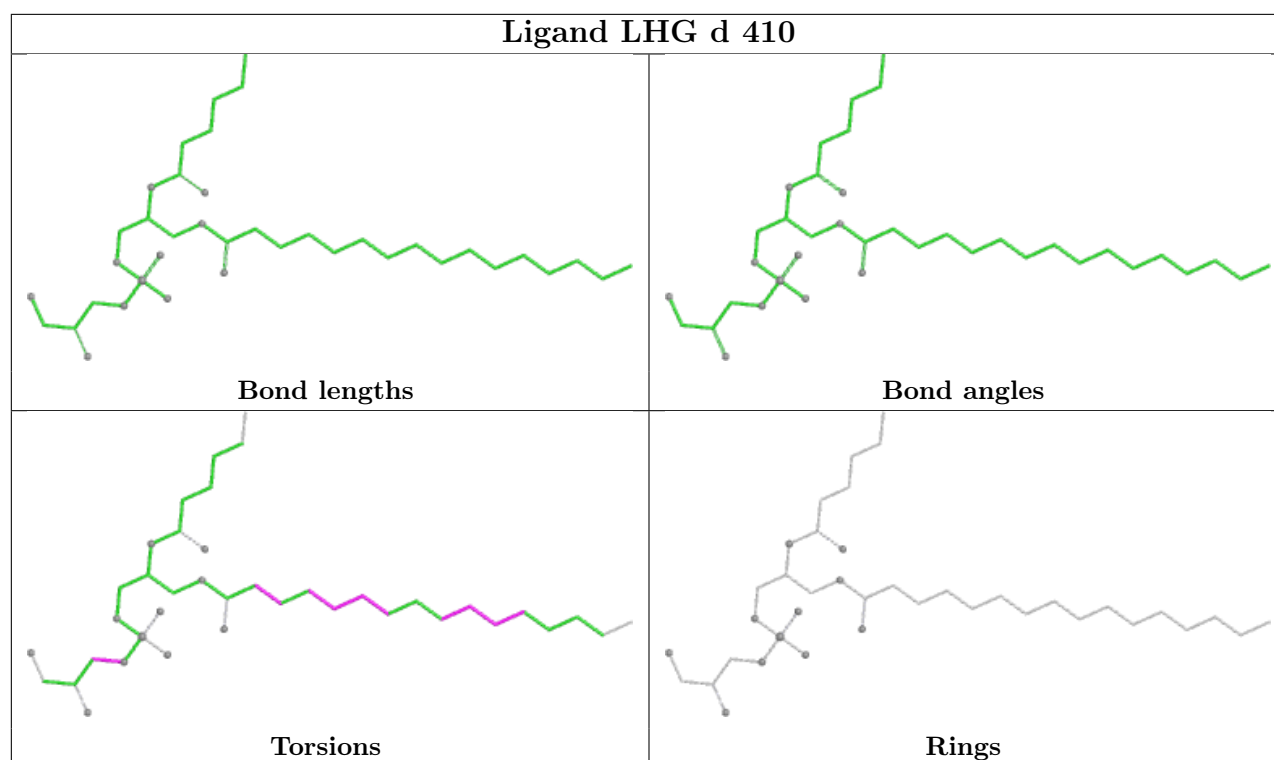
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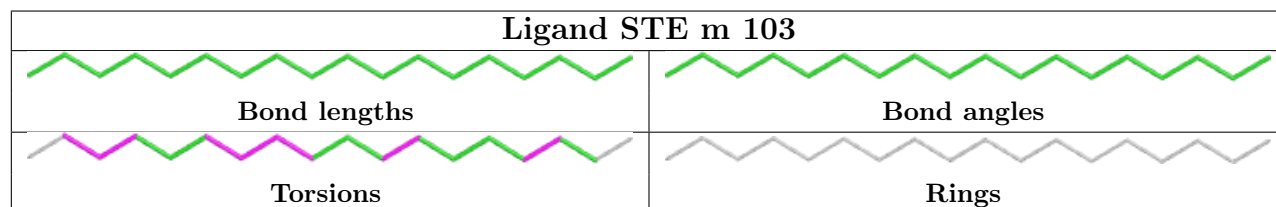
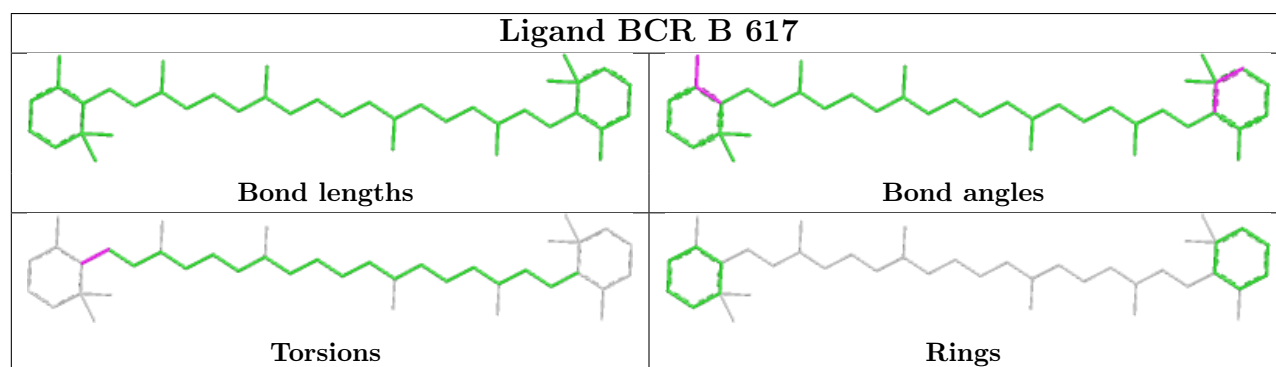
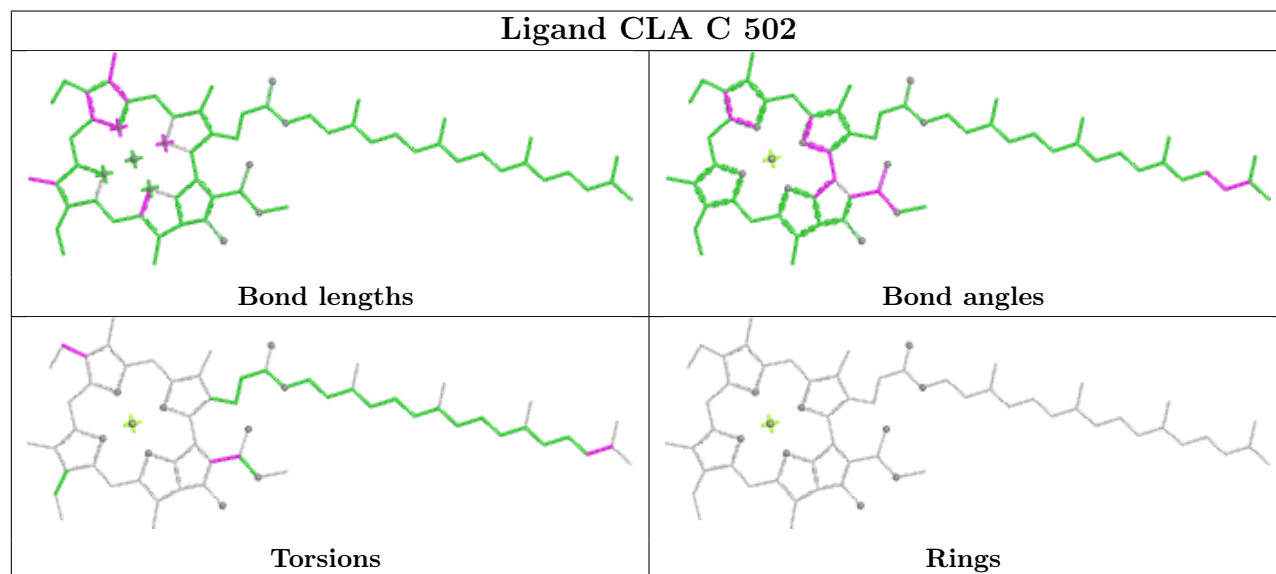
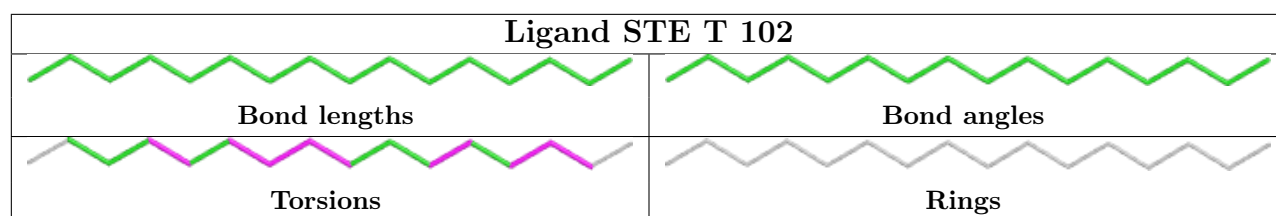
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	413	LHG	1	0
32	B	620	LMG	2	0
24	c	511	CLA	2	0
24	A	608	CLA	1	0
24	B	612	CLA	3	0
32	C	521	LMG	1	0
24	b	615	CLA	1	0
24	b	602	CLA	1	0
29	D	410	LHG	1	0
26	C	514	BCR	3	0
28	A	618	STE	2	0
30	D	409	SQD	1	0
26	k	101	BCR	2	0
24	b	610	CLA	1	0
24	b	603	CLA	2	0
26	t	101	BCR	2	0
24	B	602	CLA	1	0
34	f	101	HEM	4	0
26	A	609	BCR	1	0
29	L	101	LHG	3	0
31	A	615	DGD	1	0
32	a	614	LMG	2	0
24	B	610	CLA	1	0
26	T	101	BCR	4	0
28	H	103	STE	1	0
24	c	513	CLA	3	0
26	d	405	BCR	5	0
24	A	606	CLA	2	0
28	d	411	STE	2	0
32	m	101	LMG	4	0
26	B	619	BCR	1	0
24	A	605	CLA	3	0
24	B	611	CLA	2	0
24	b	605	CLA	2	0
26	K	101	BCR	2	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

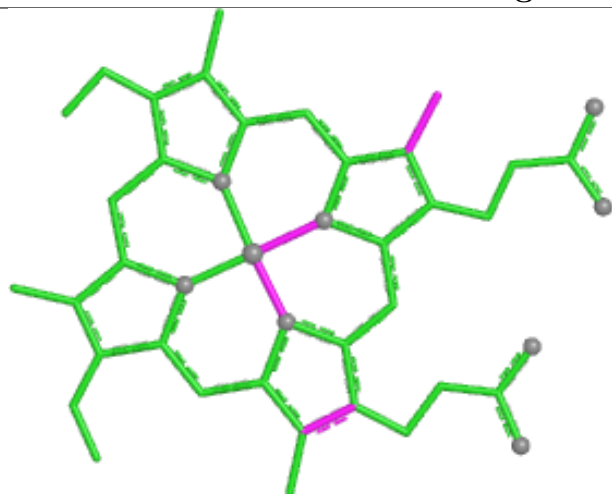
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



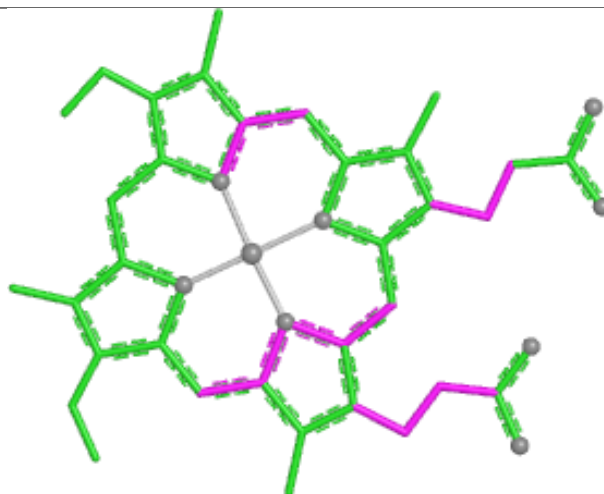




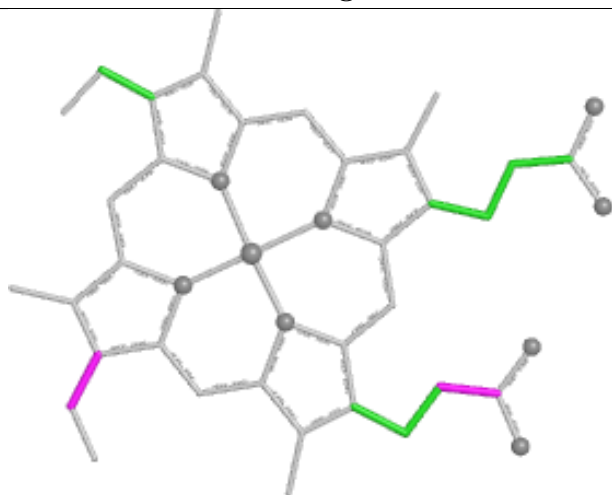
Ligand HEC v 201



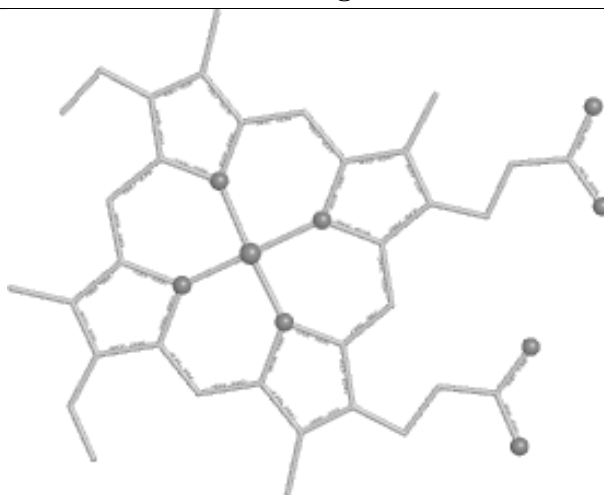
Bond lengths



Bond angles



Torsions

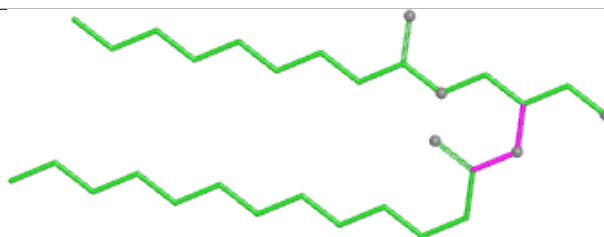


Rings

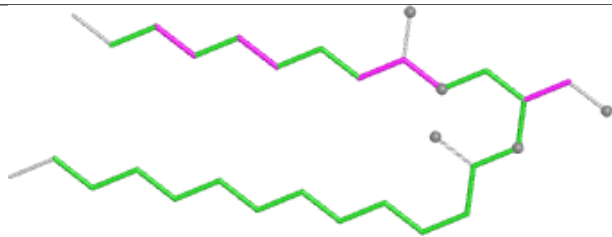
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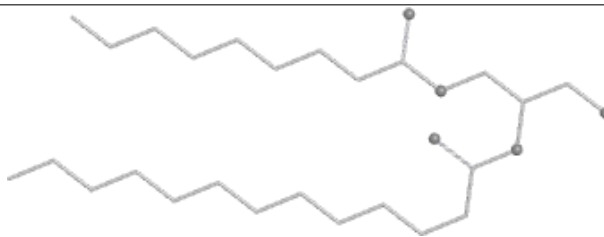
Bond lengths



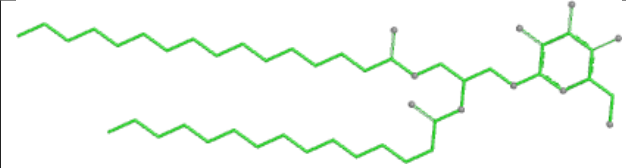
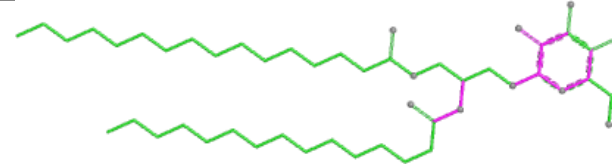
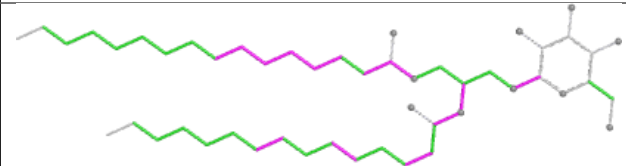
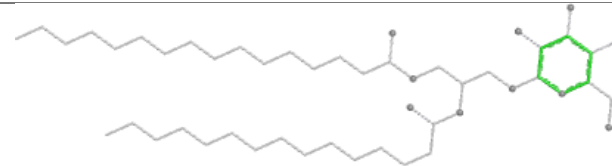
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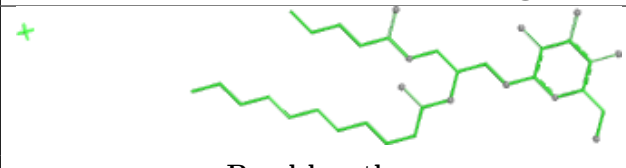


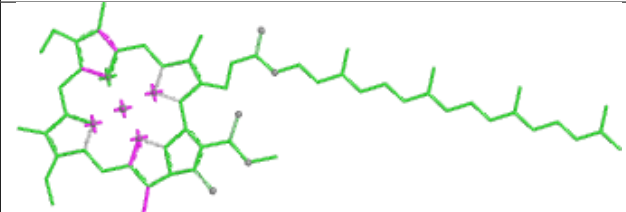
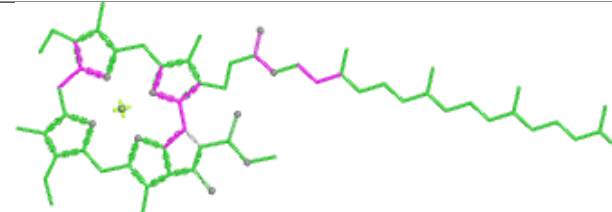
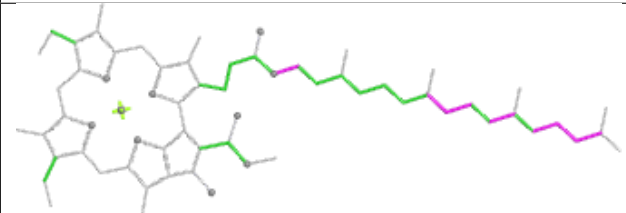
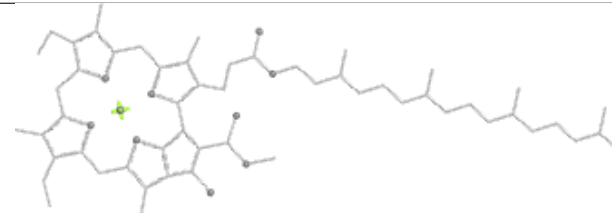
Torsions

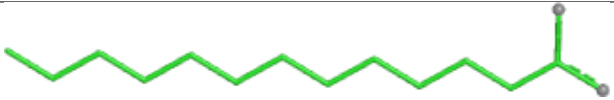
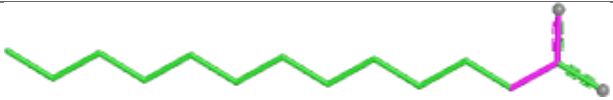
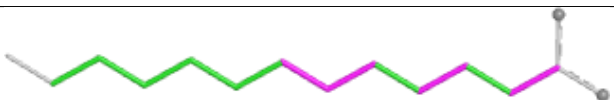
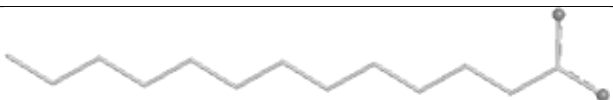


Rings

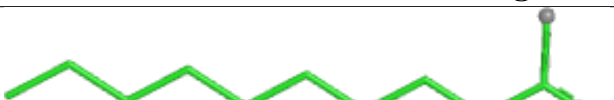
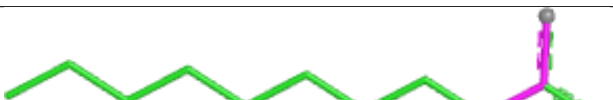
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

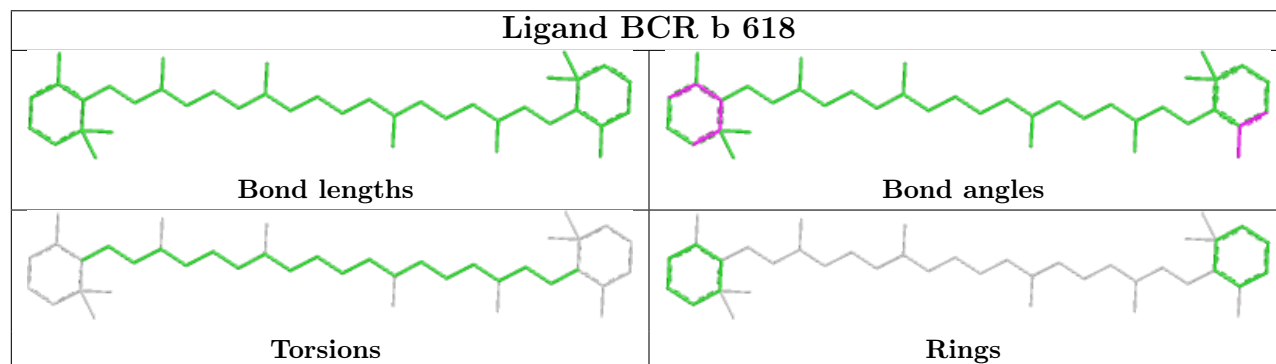
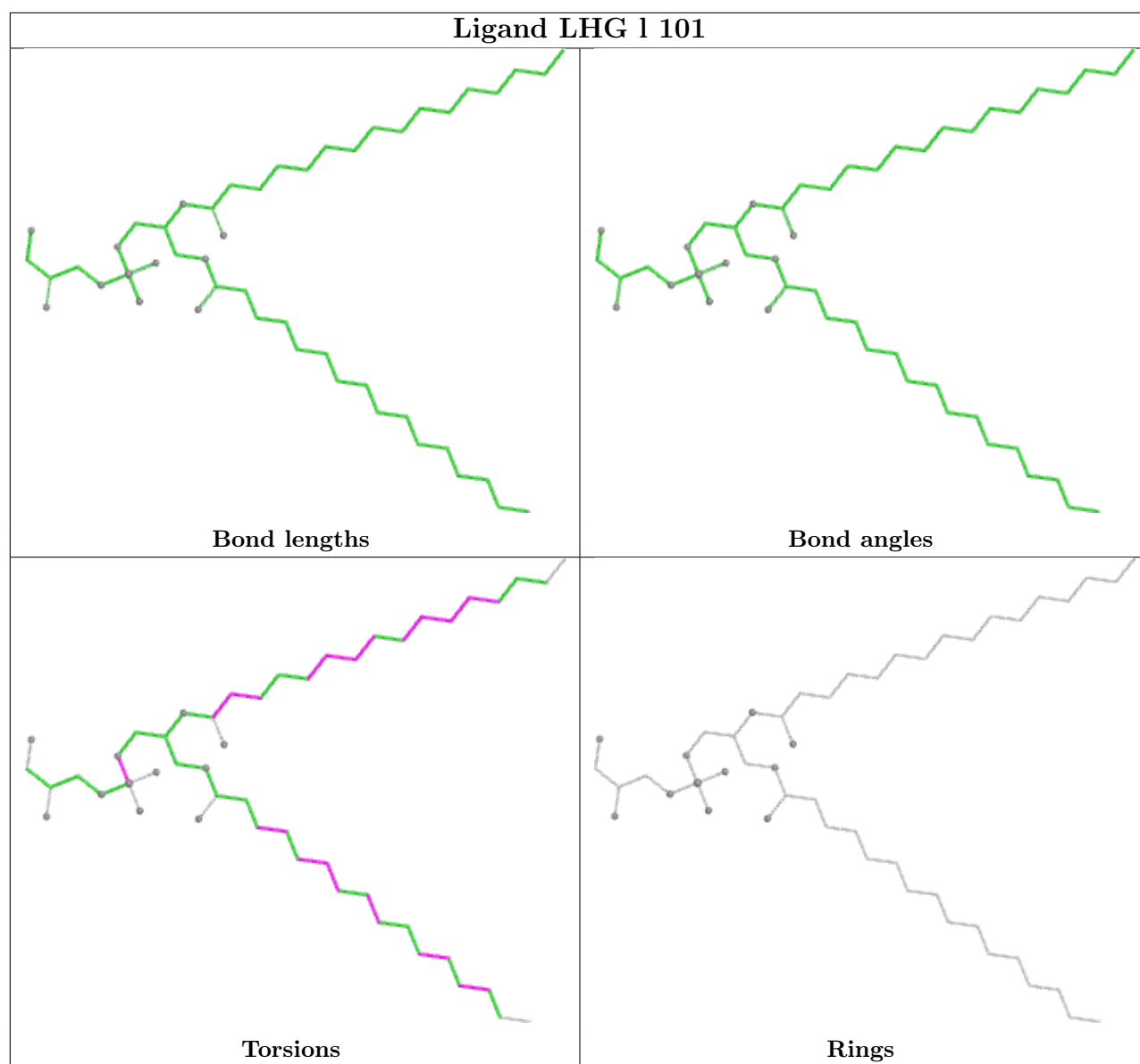
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Bond lengths	Bond angles
	
Torsions	Rings

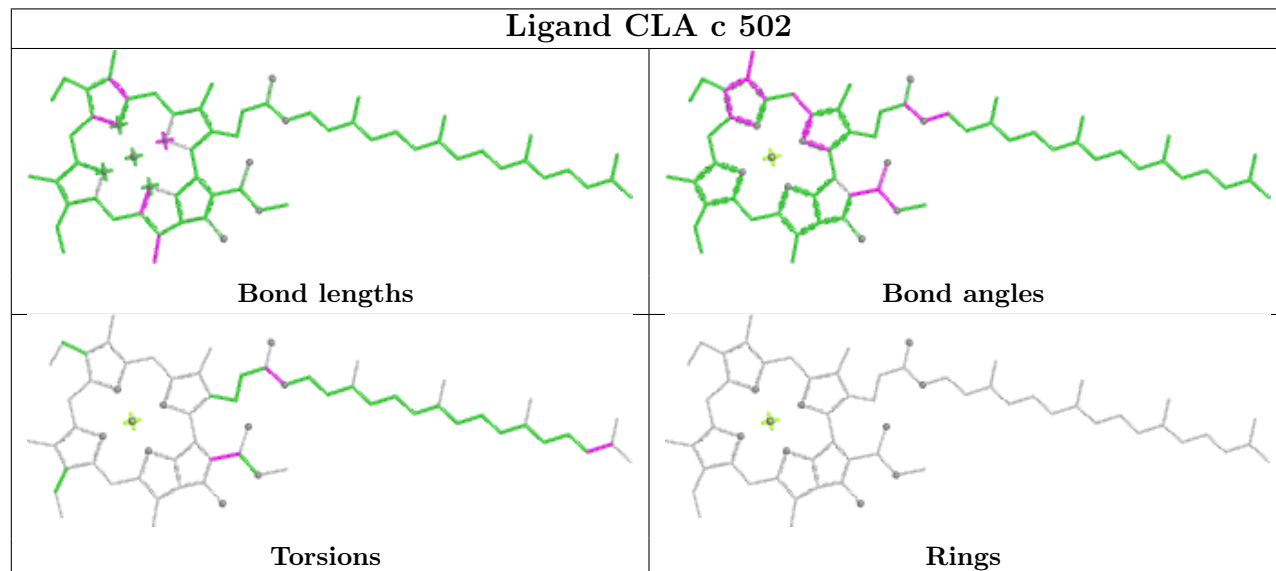
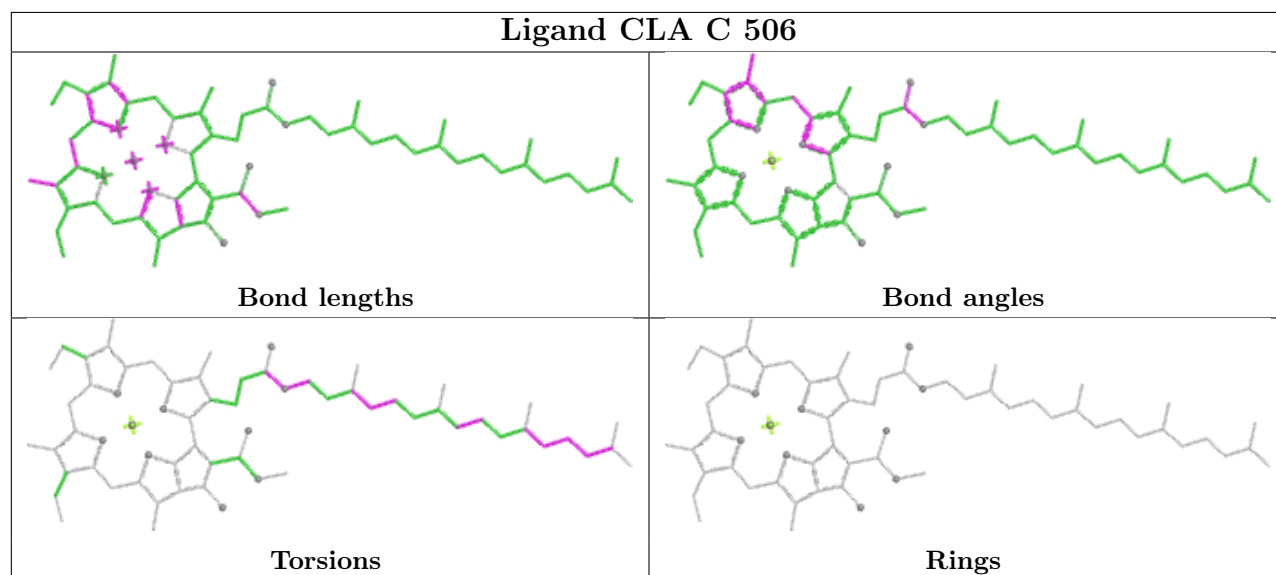
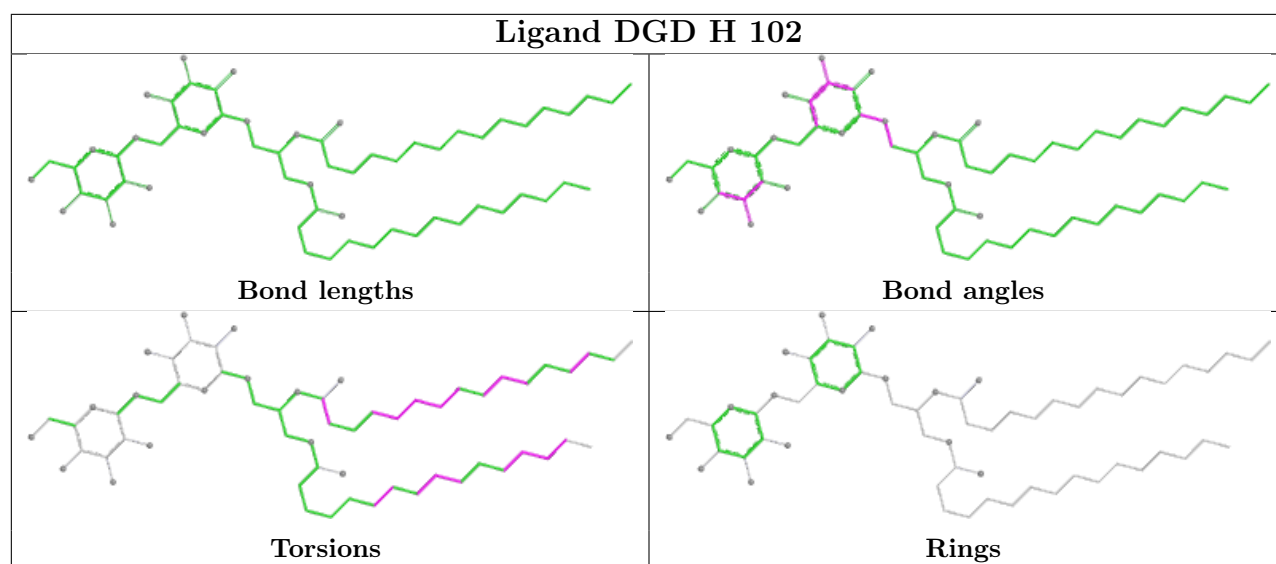
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

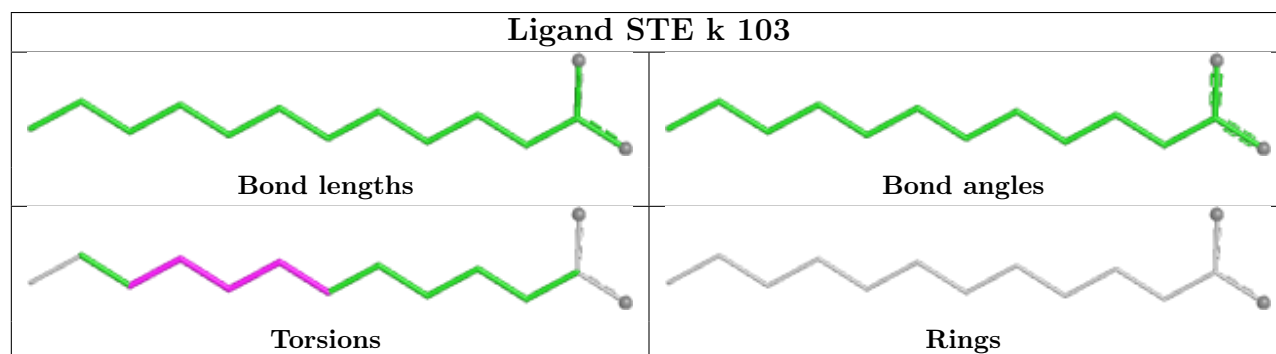
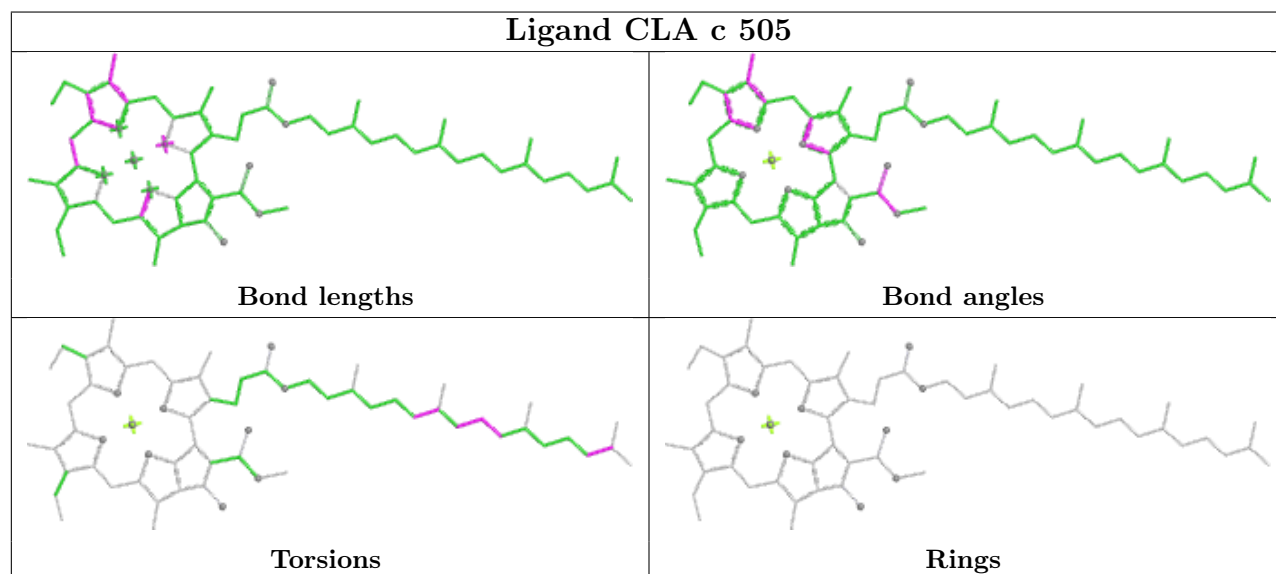
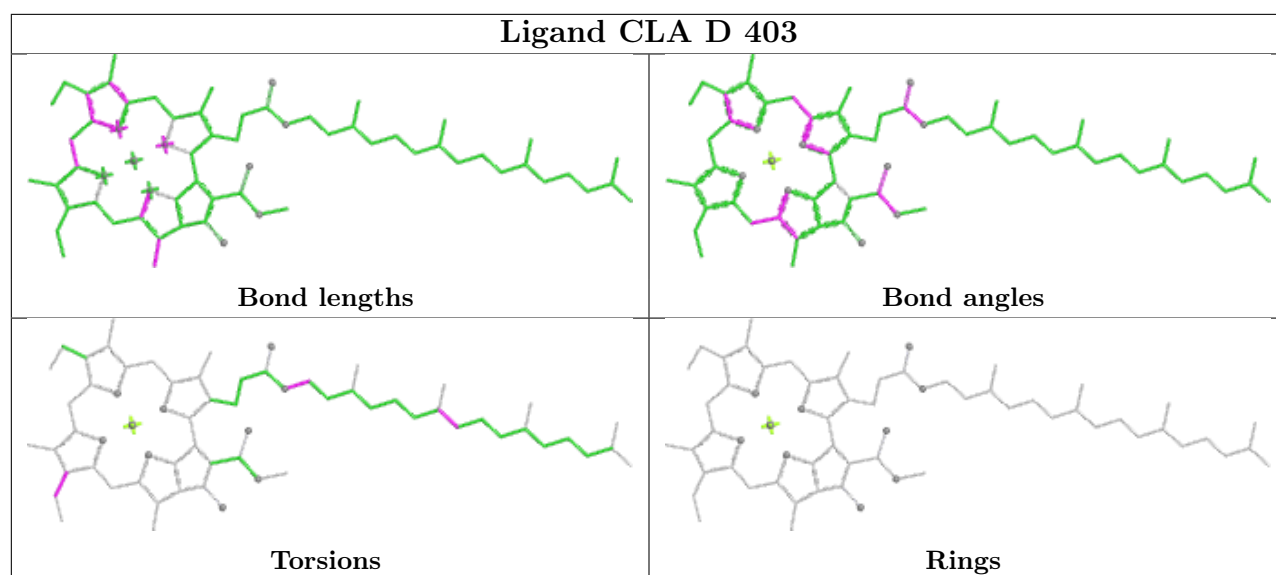
Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

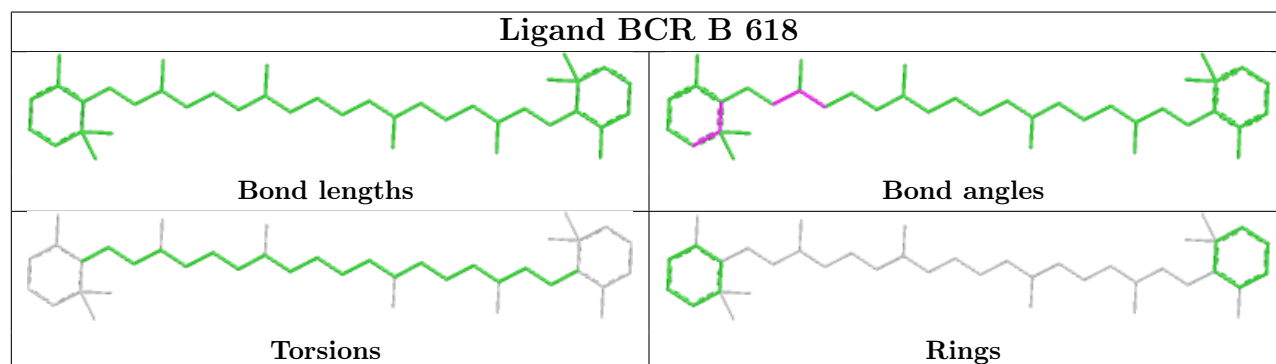
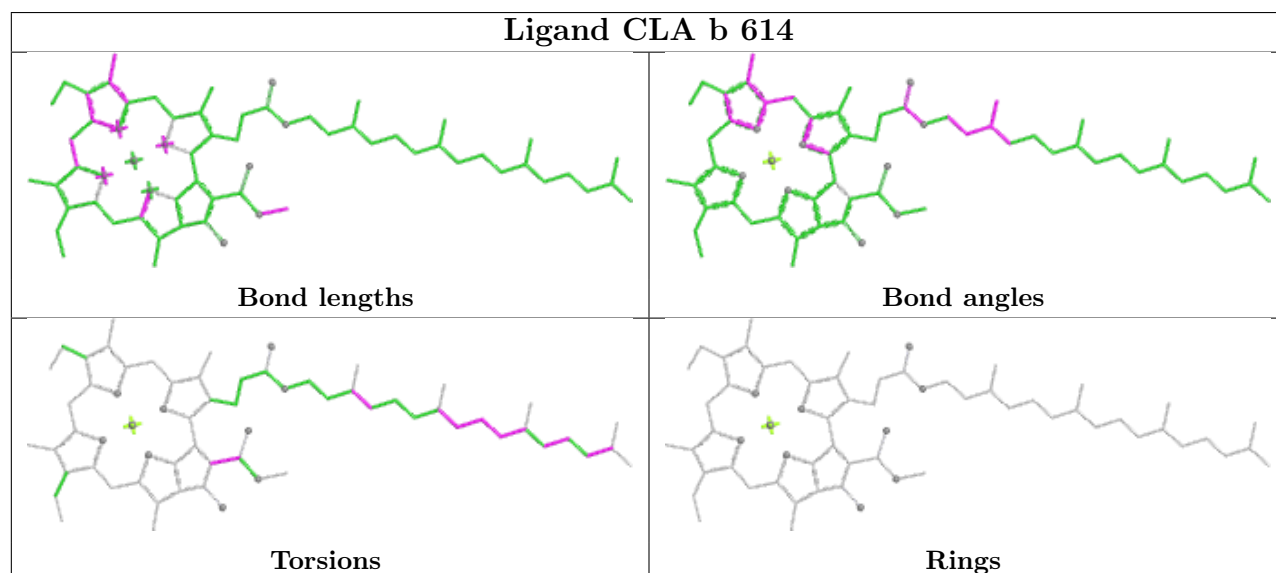
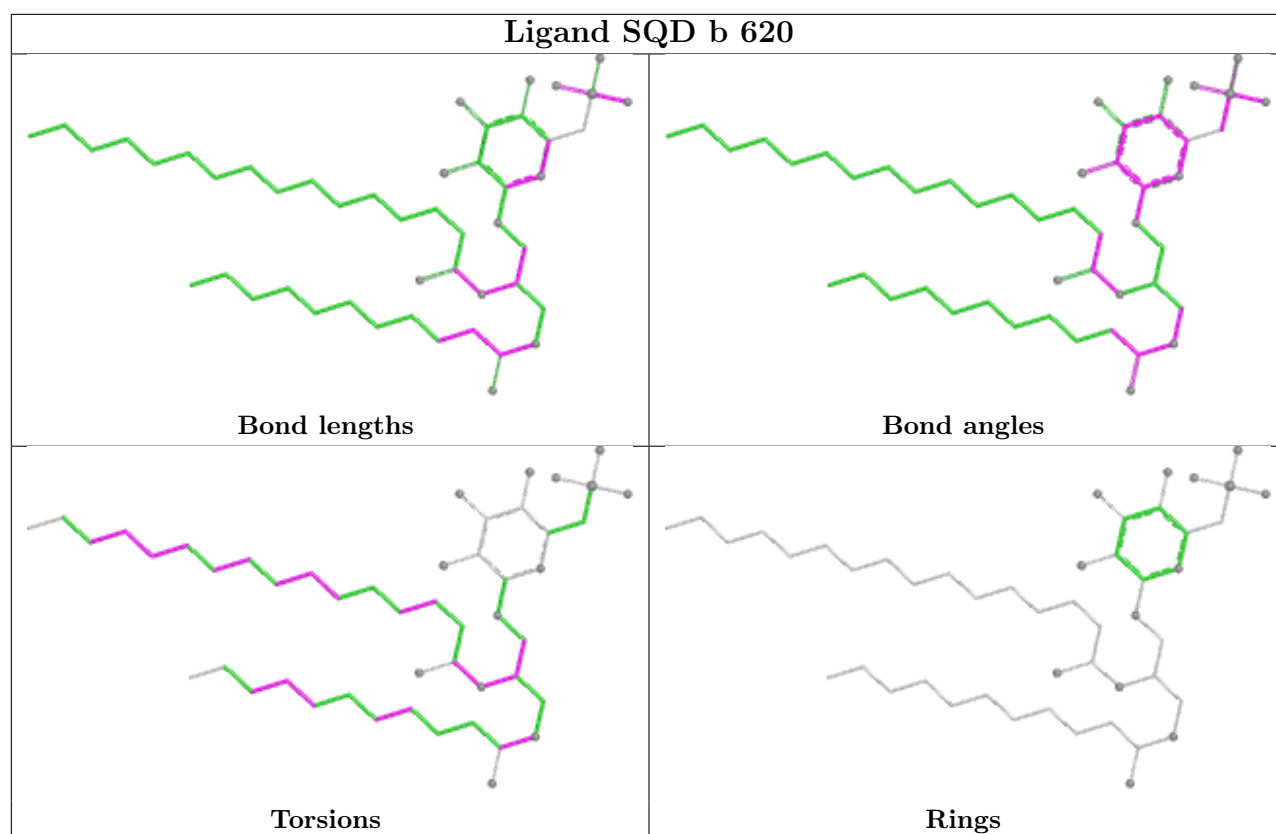
Ligand STE a 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

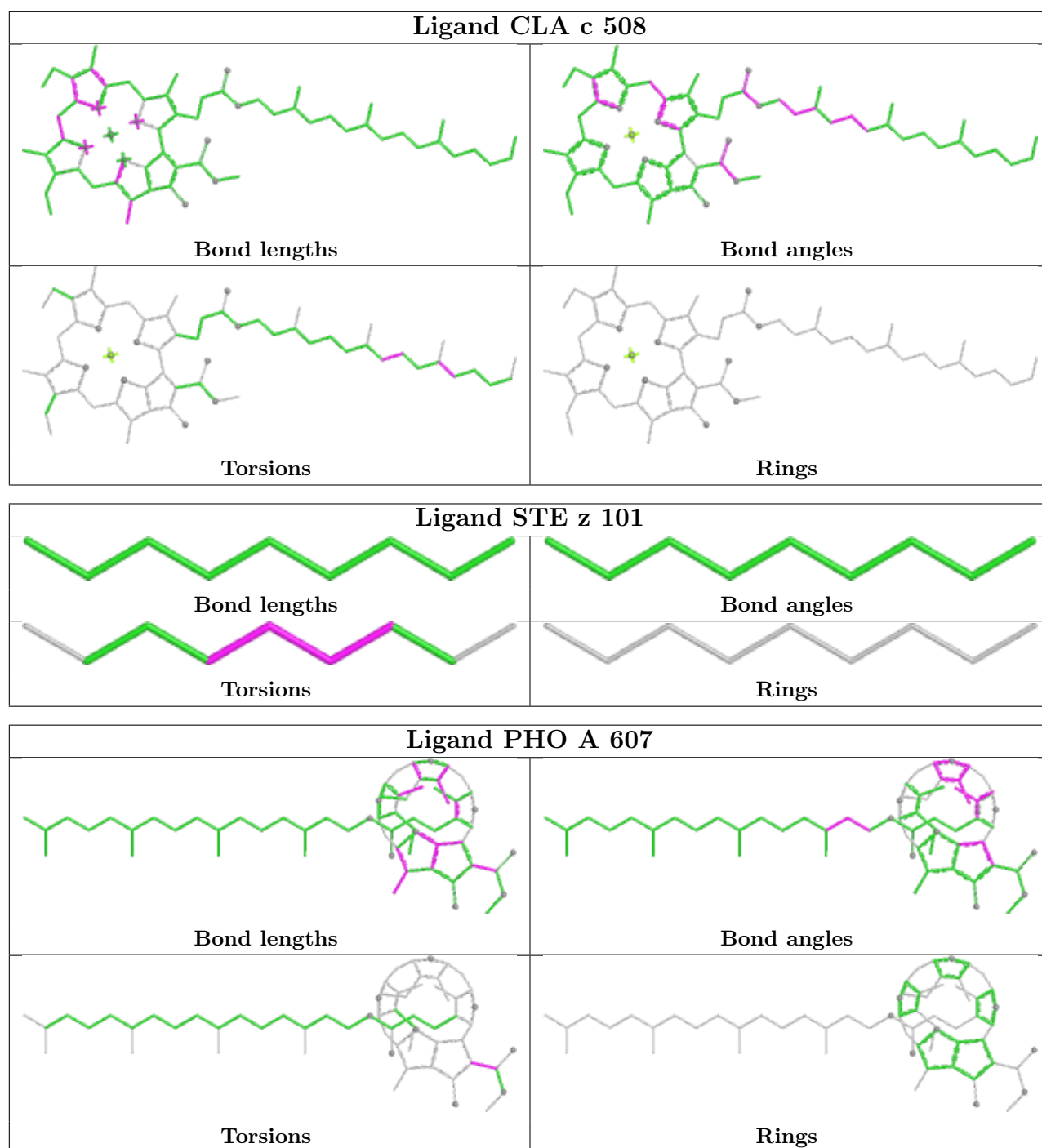
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 Bond lengths	 Bond angles
 Torsions	 Rings

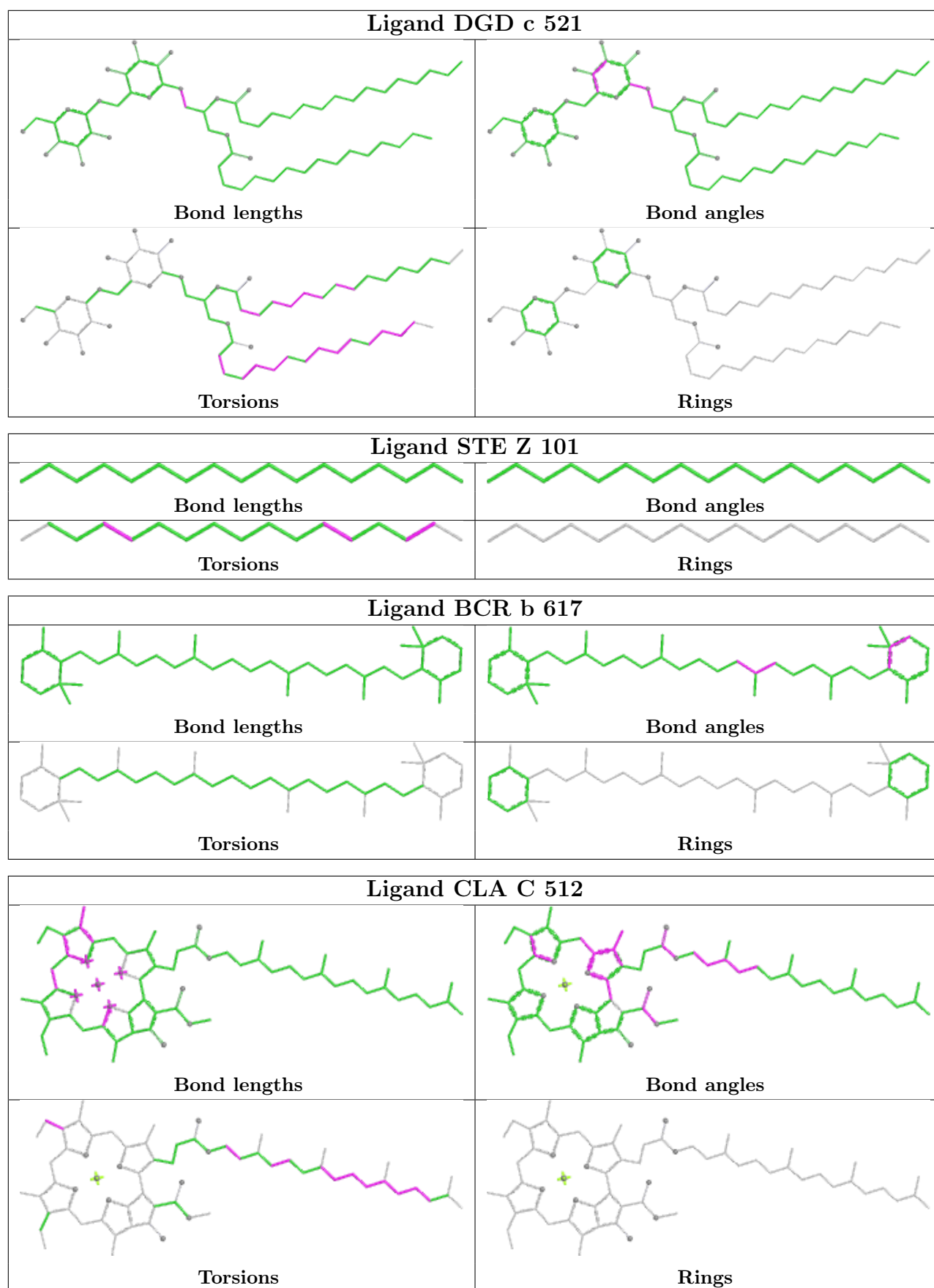


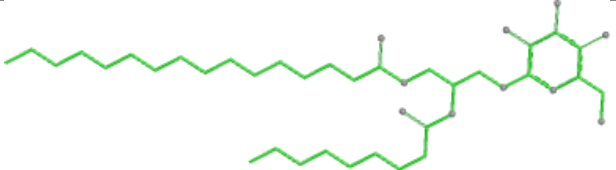
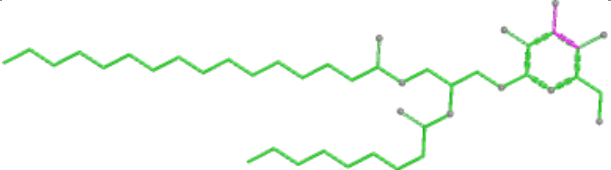
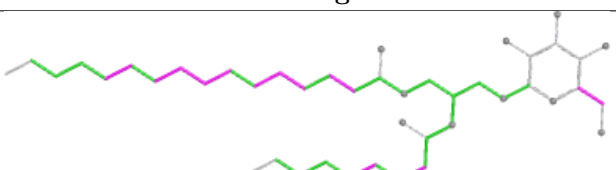
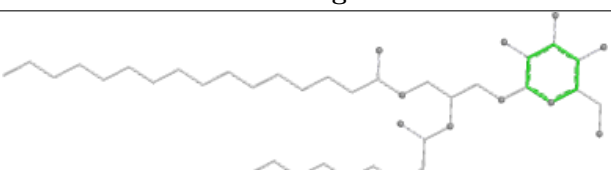




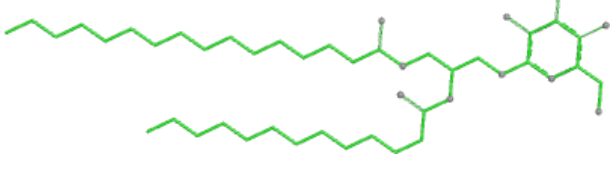
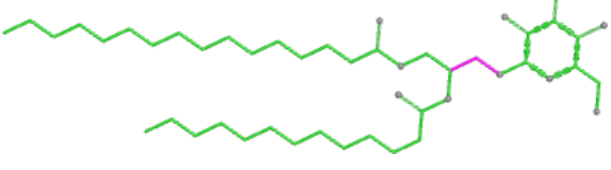
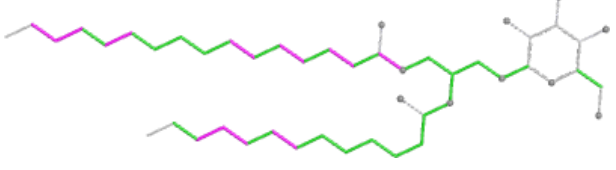
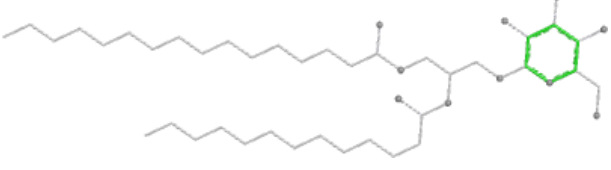


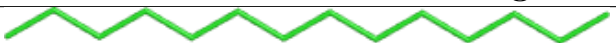
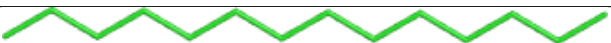


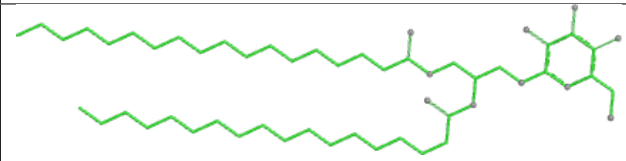
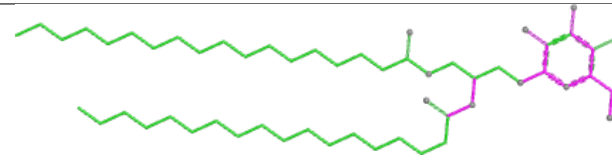
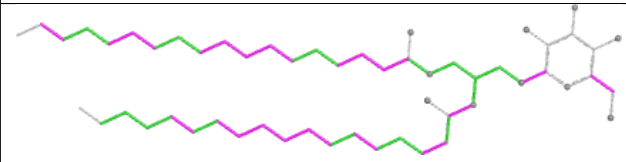
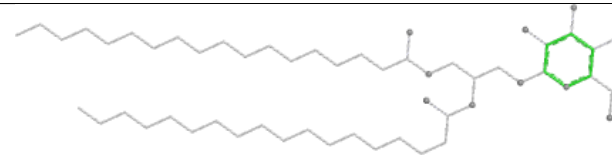
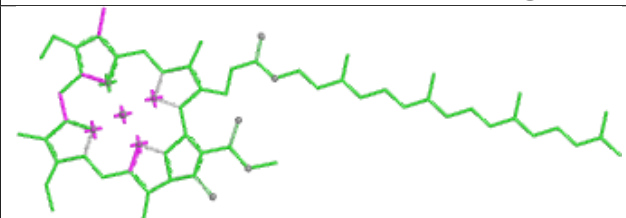
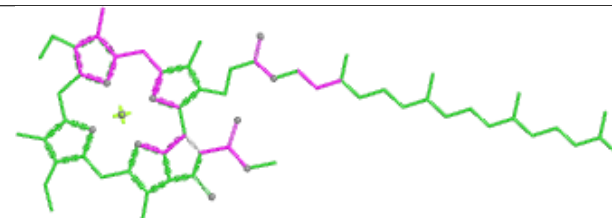
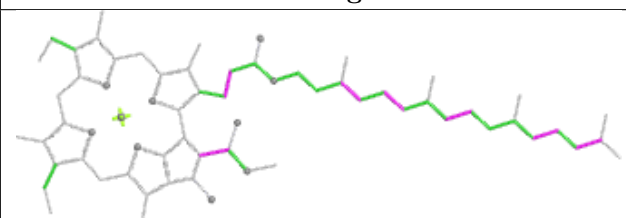
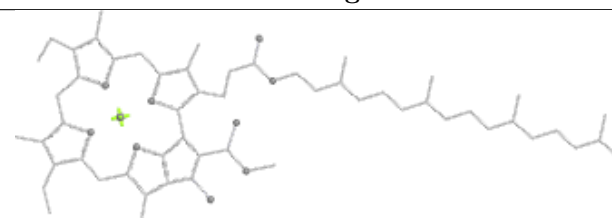
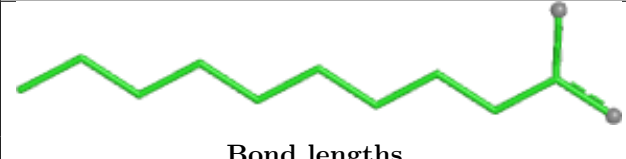
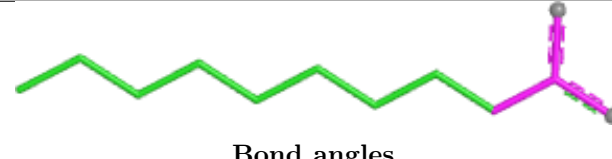


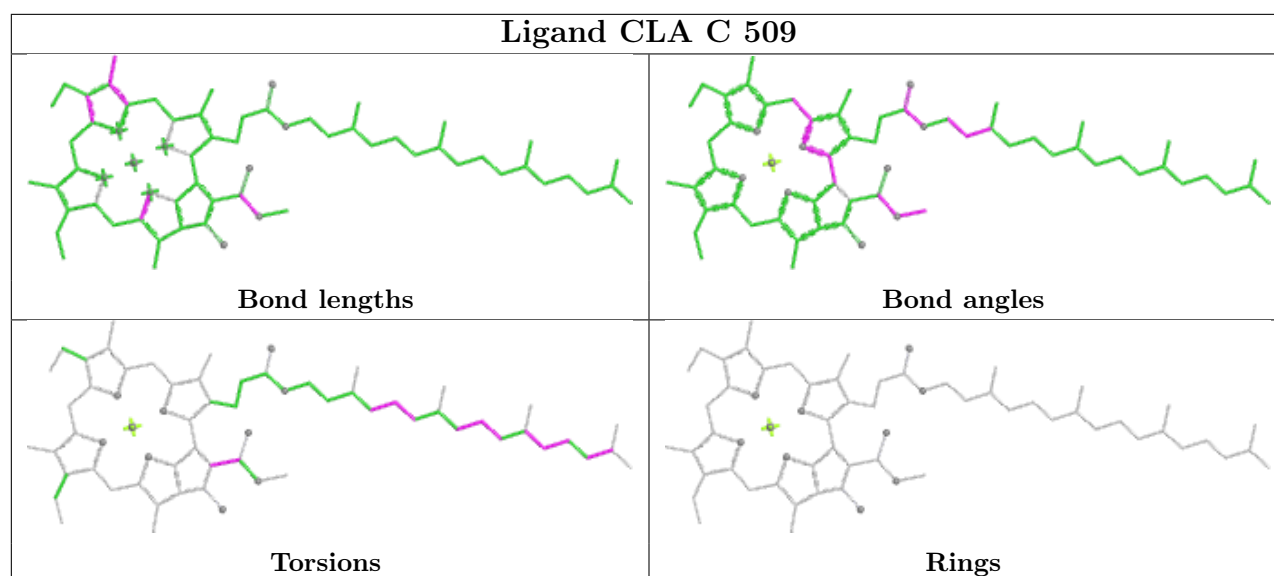
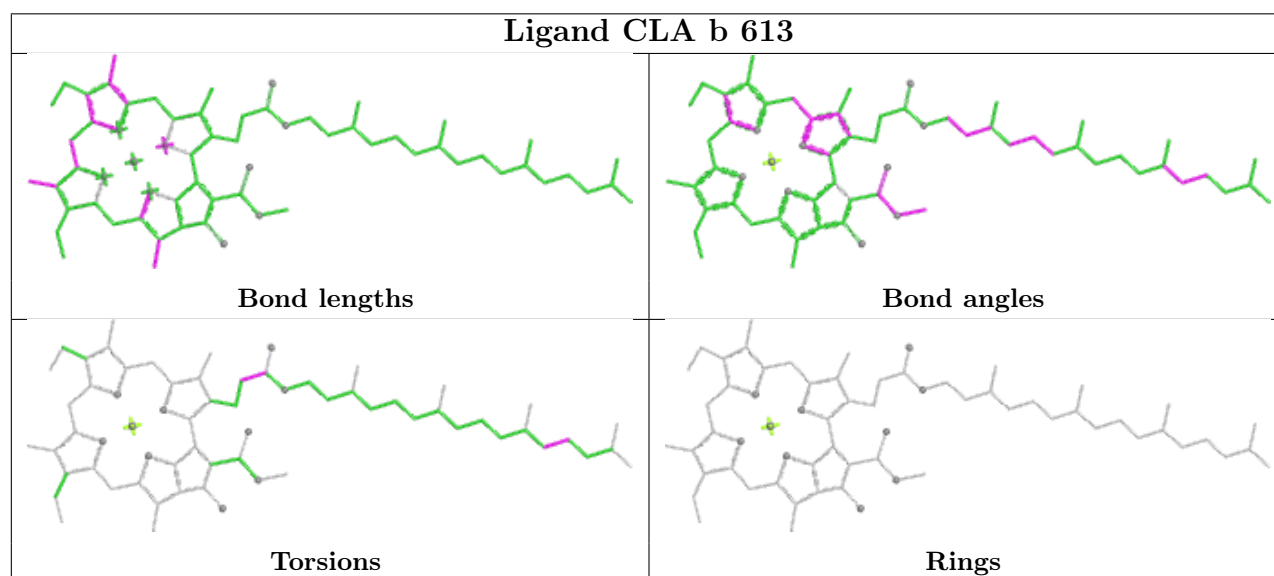
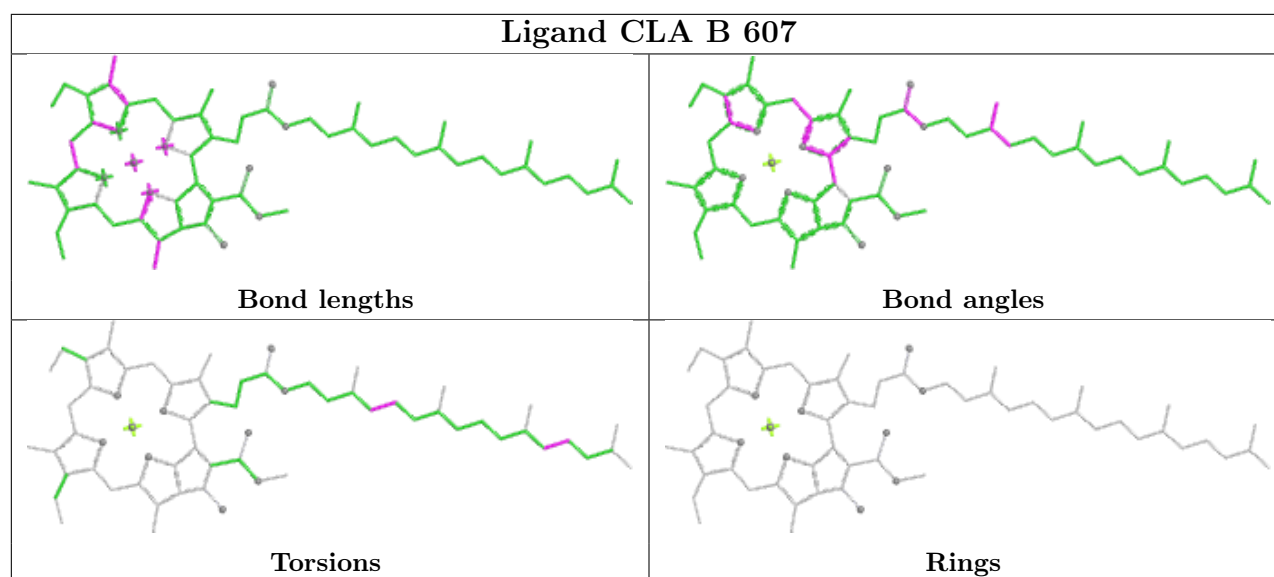
Ligand LMG d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

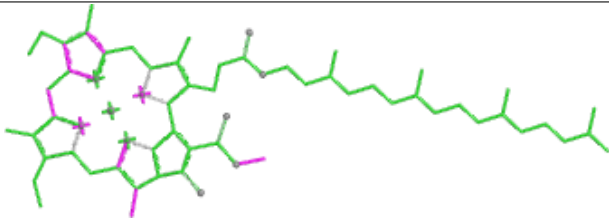
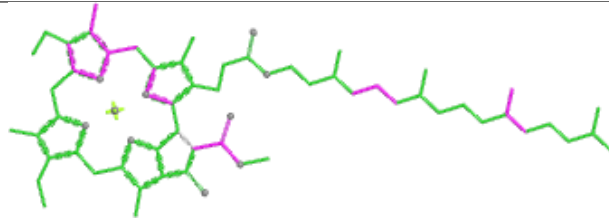
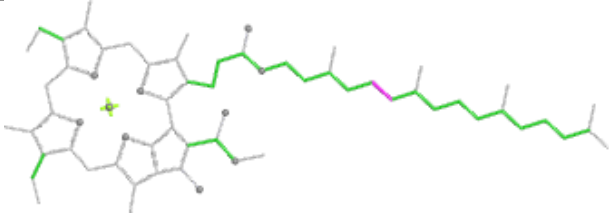
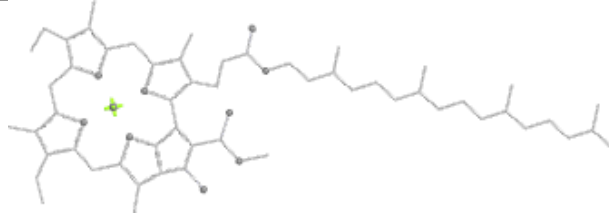
Ligand STE A 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

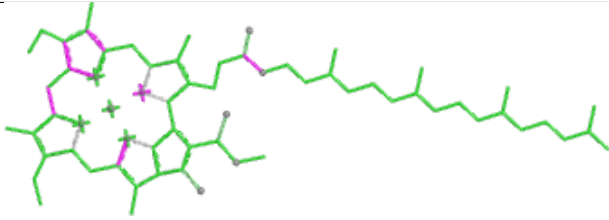
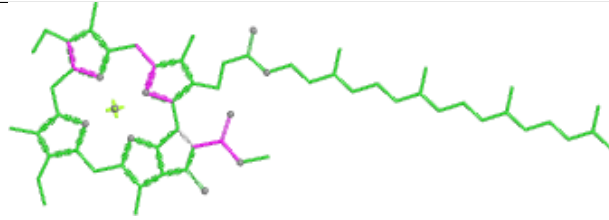
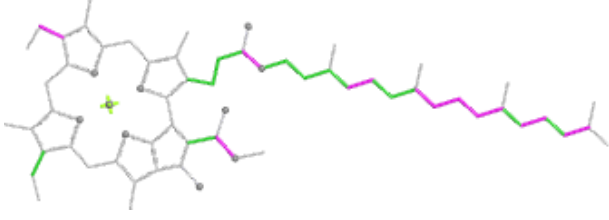
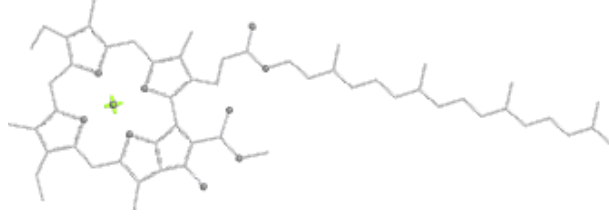
Ligand LMG C 525	
 Bond lengths	 Bond angles
 Torsions	 Rings

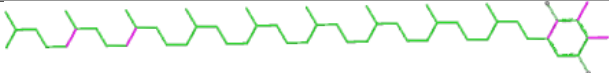
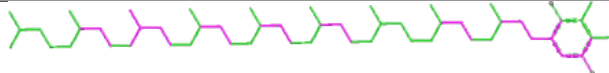
Ligand STE K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

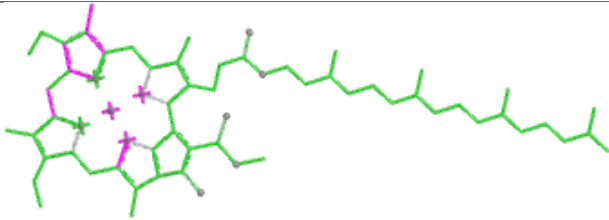
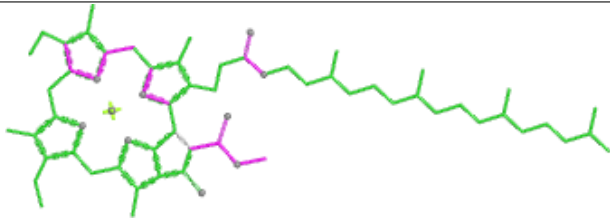
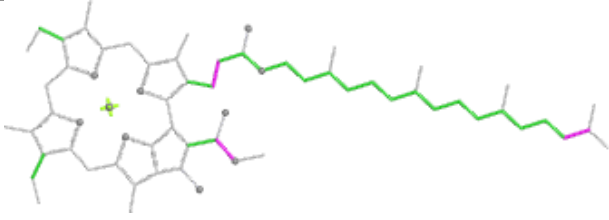
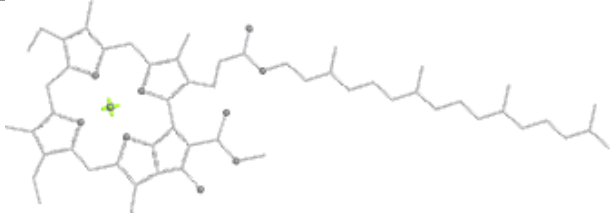
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

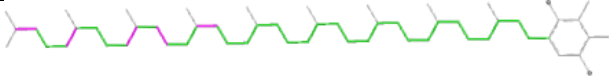
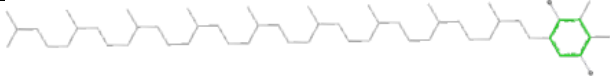


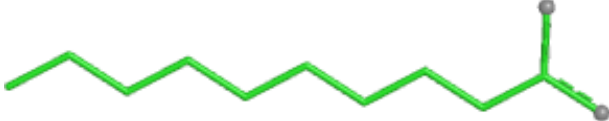
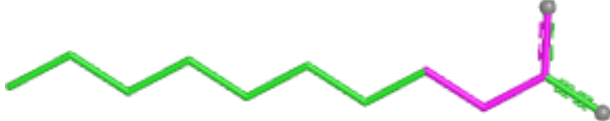
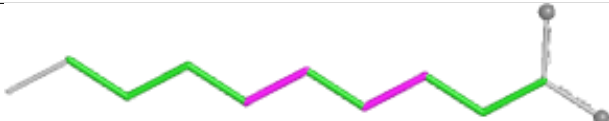
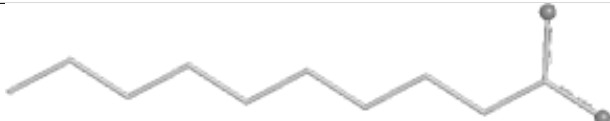
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

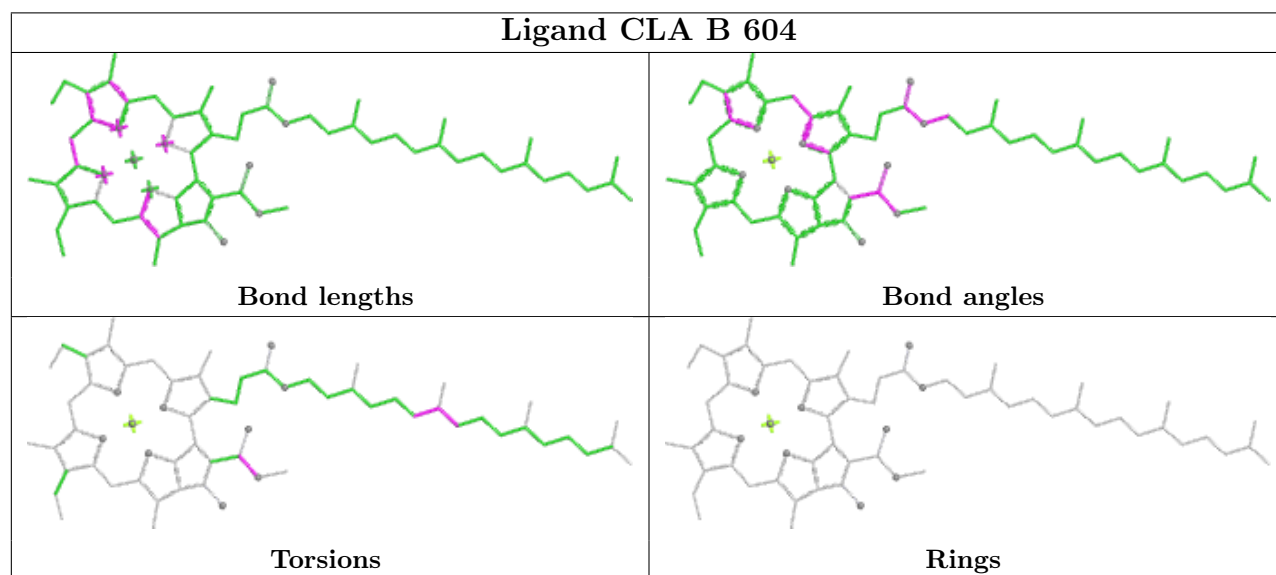
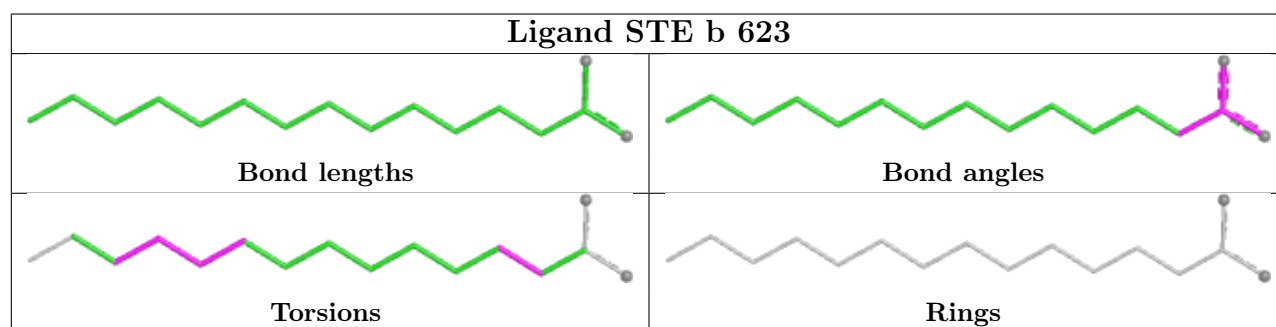
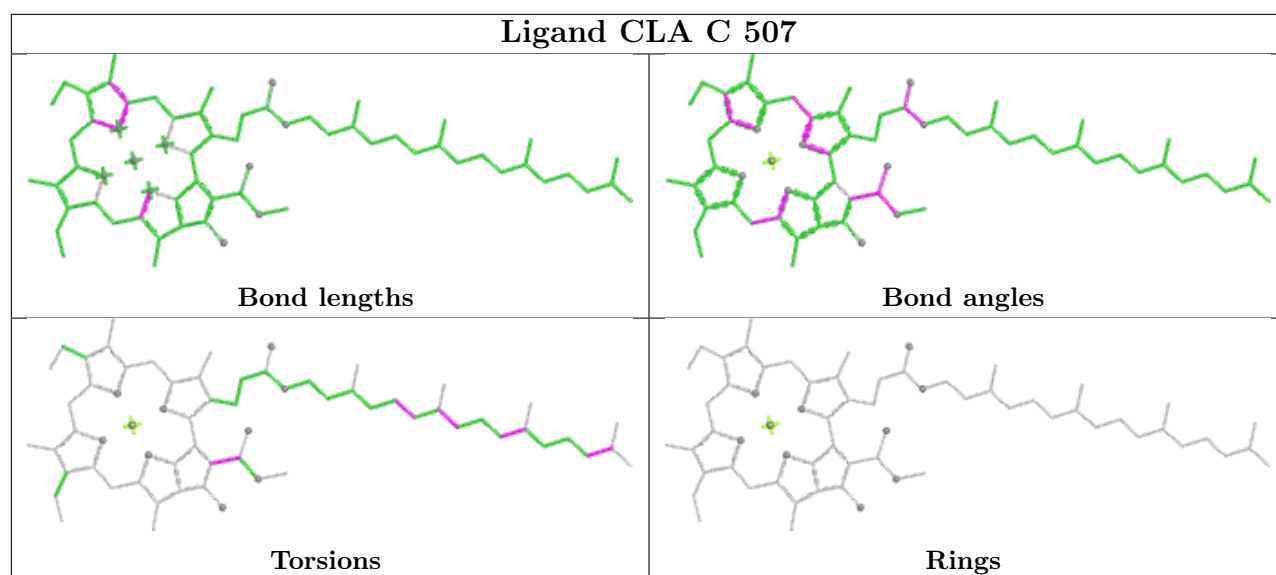
Ligand CLA b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

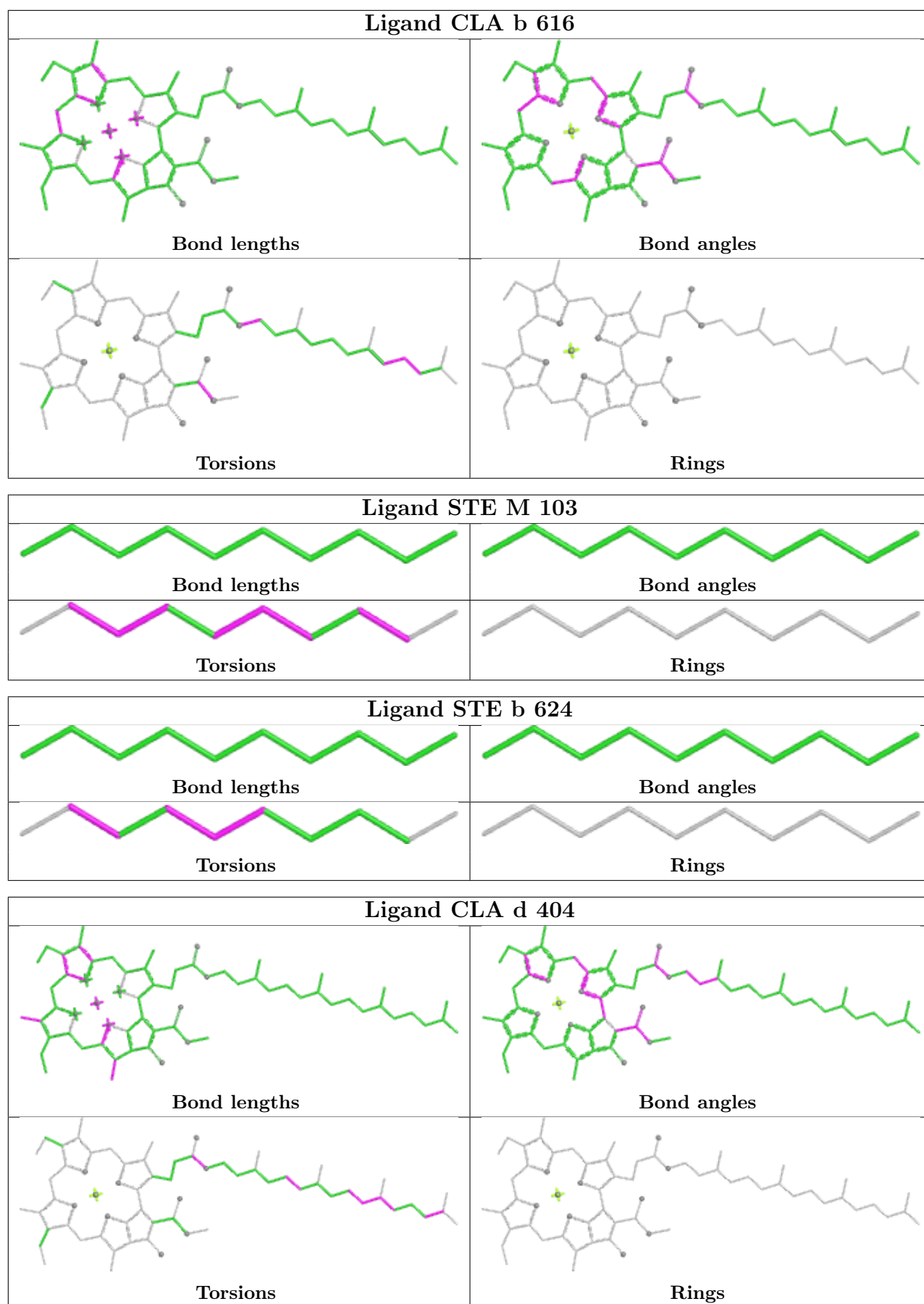
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

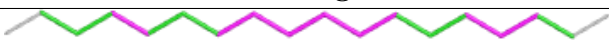
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Bond lengths	Bond angles
	
Torsions	Rings

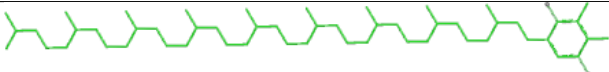
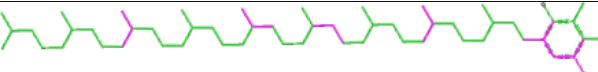
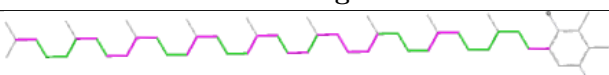
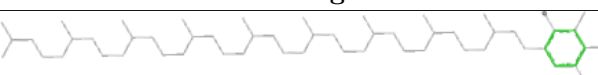
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Bond lengths	Bond angles
	
Torsions	Rings

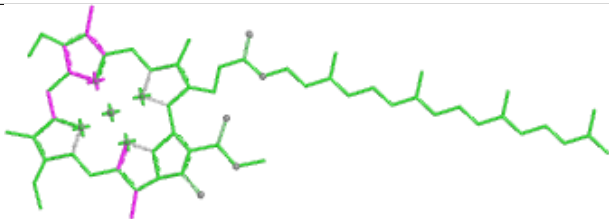
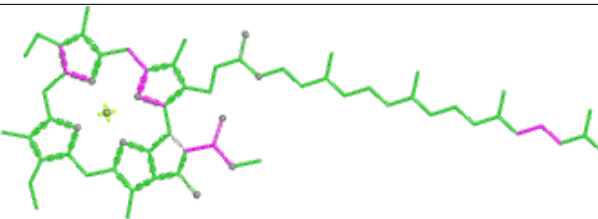
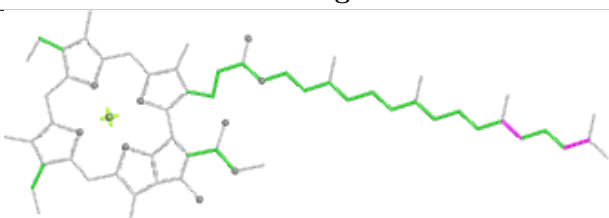
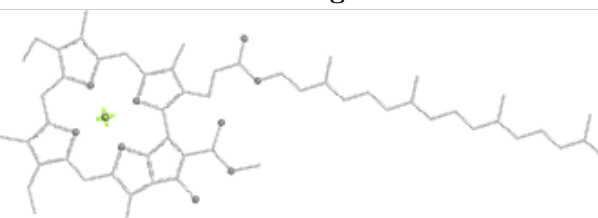
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Bond lengths	Bond angles
	
Torsions	Rings

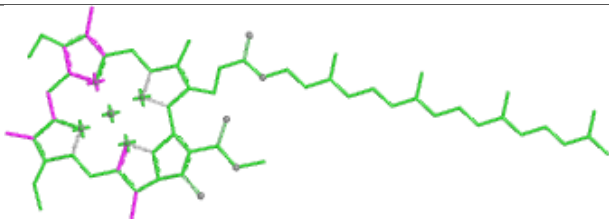
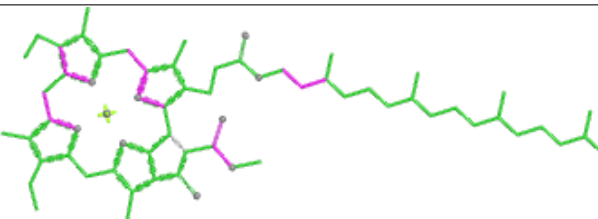
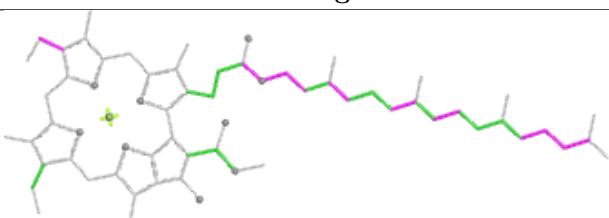
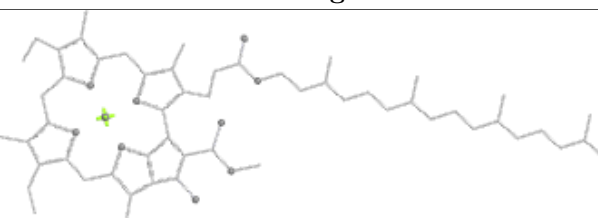


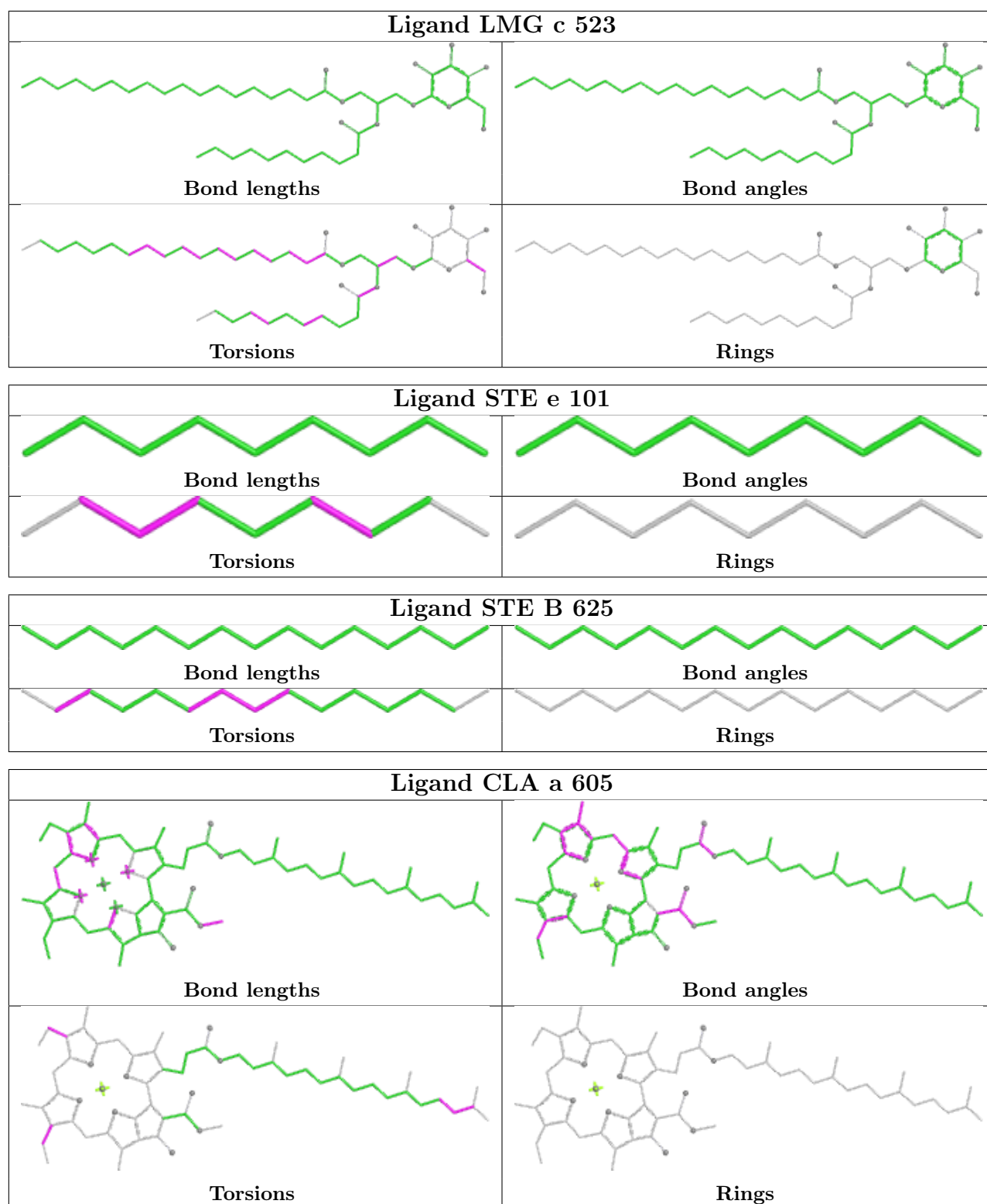


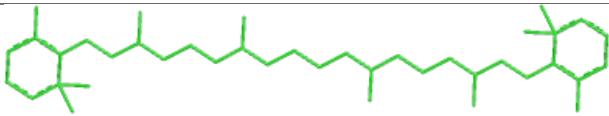
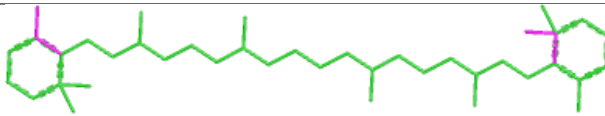
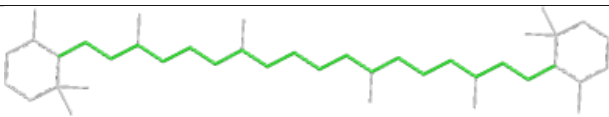
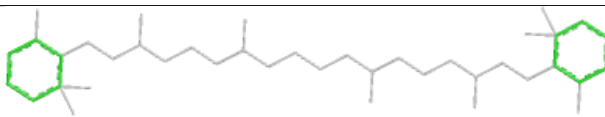
Ligand STE c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

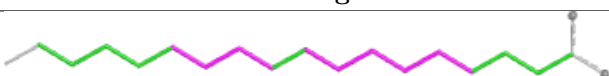
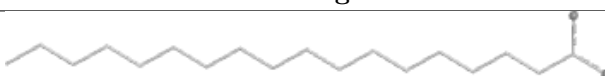
Ligand PL9 A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

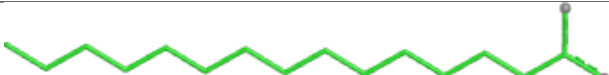
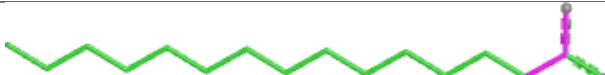
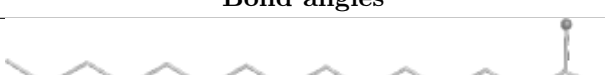
Ligand CLA A 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

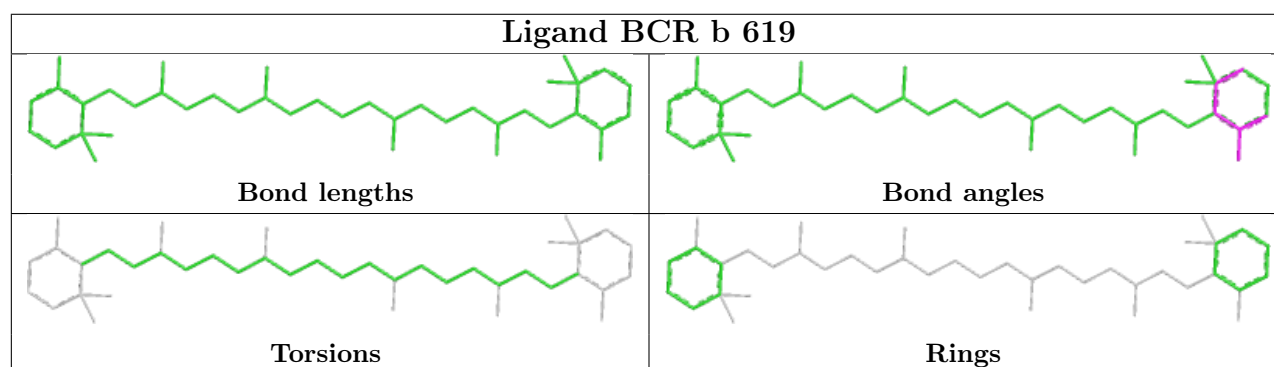
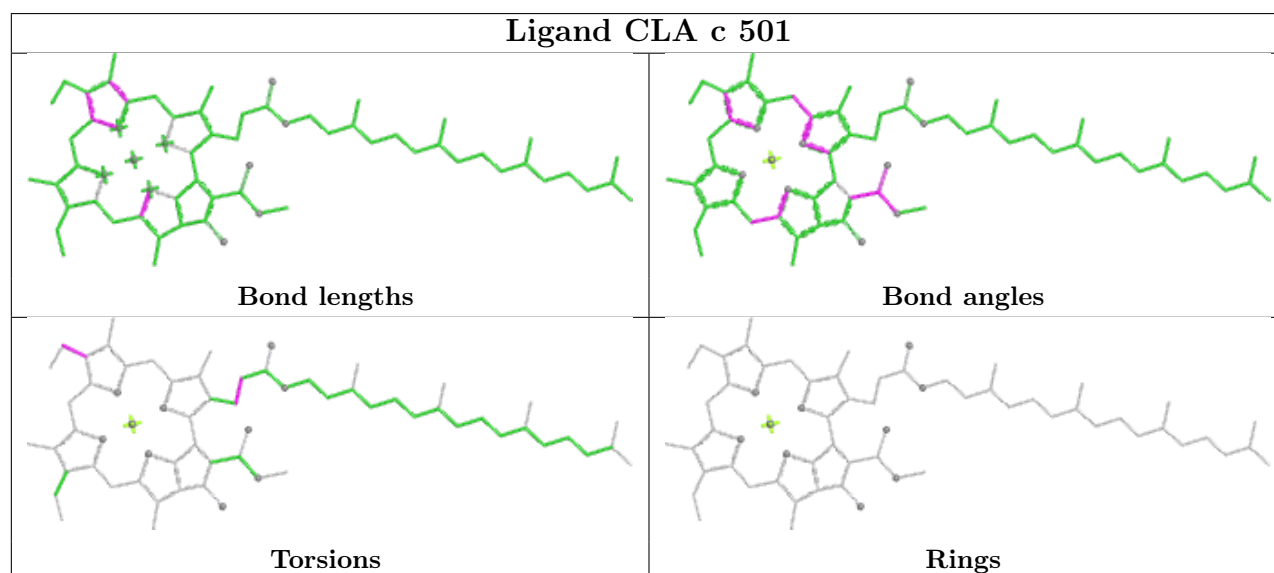
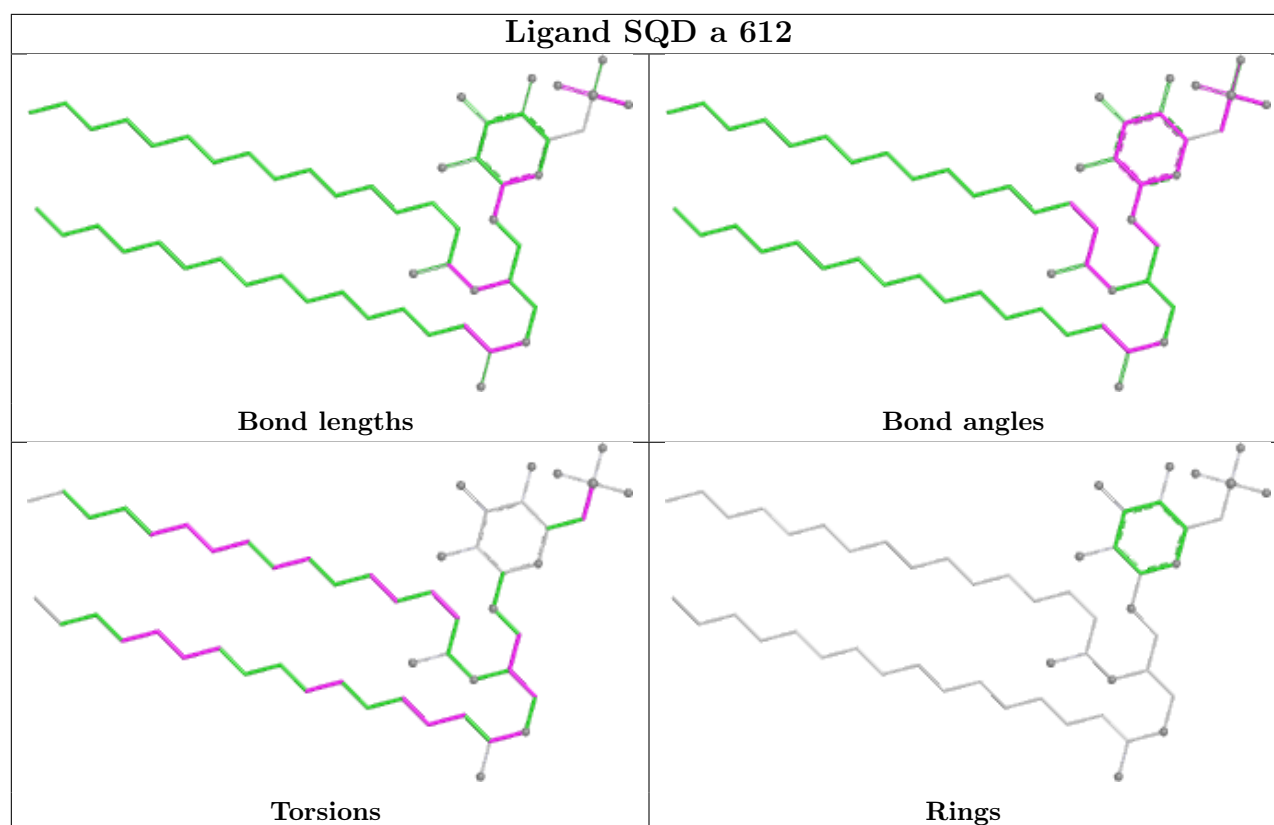
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

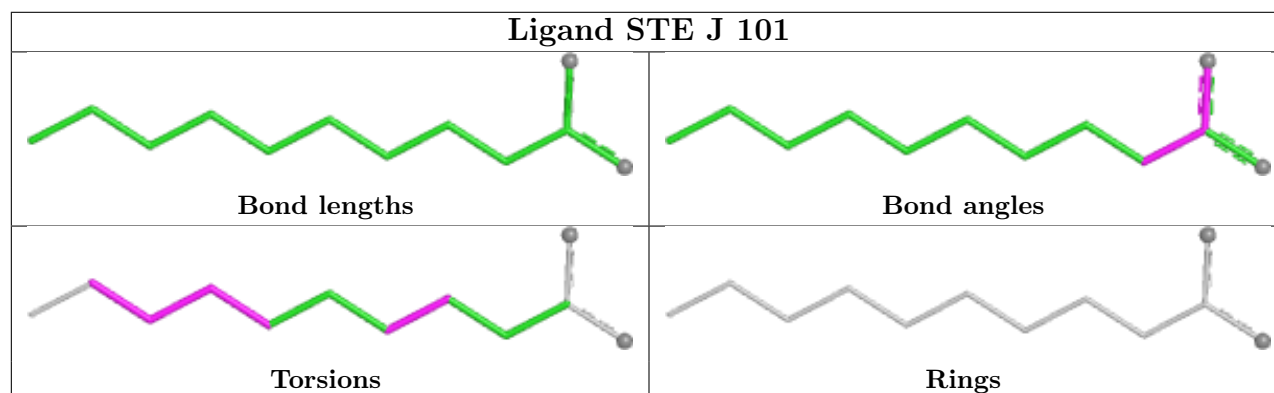
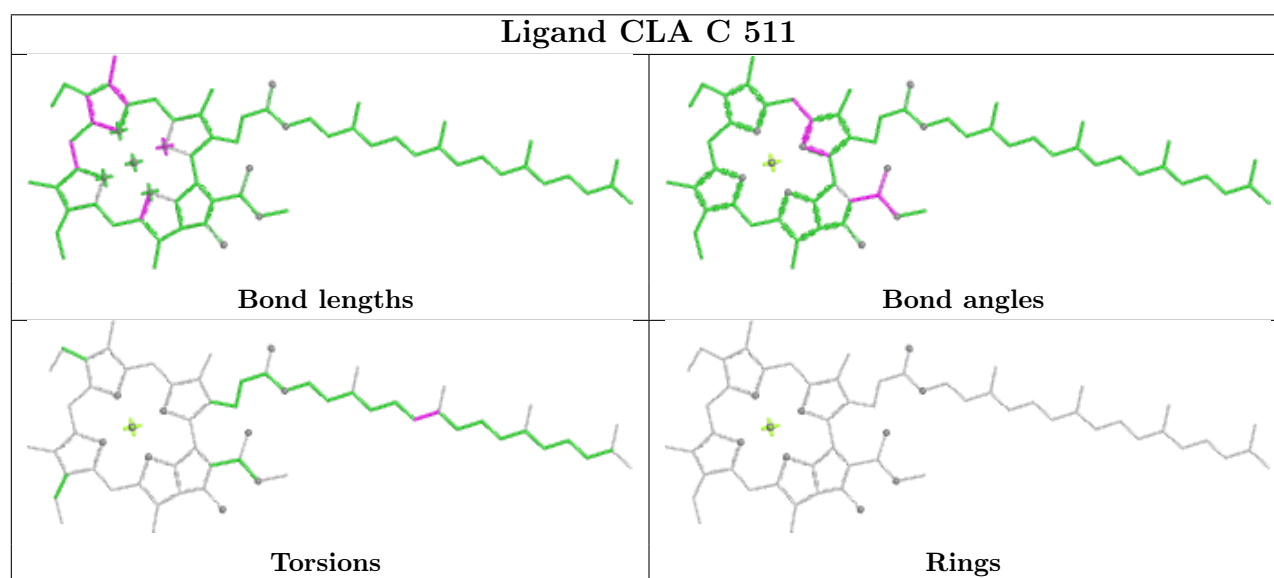
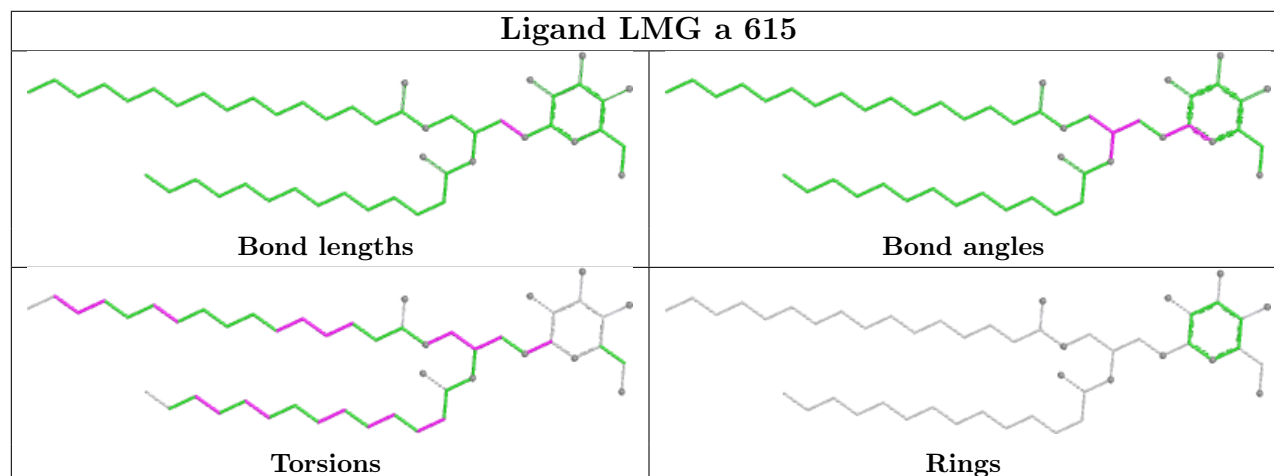
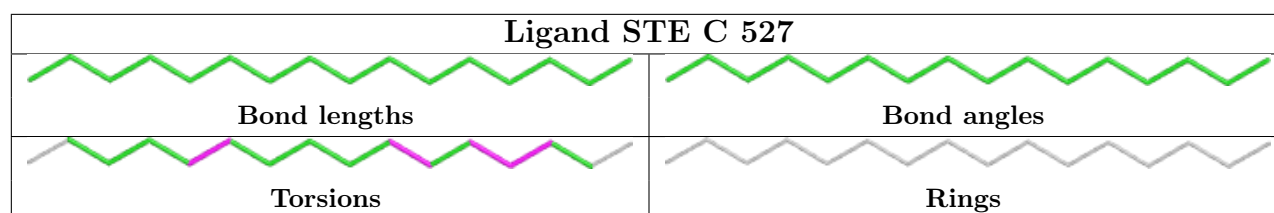


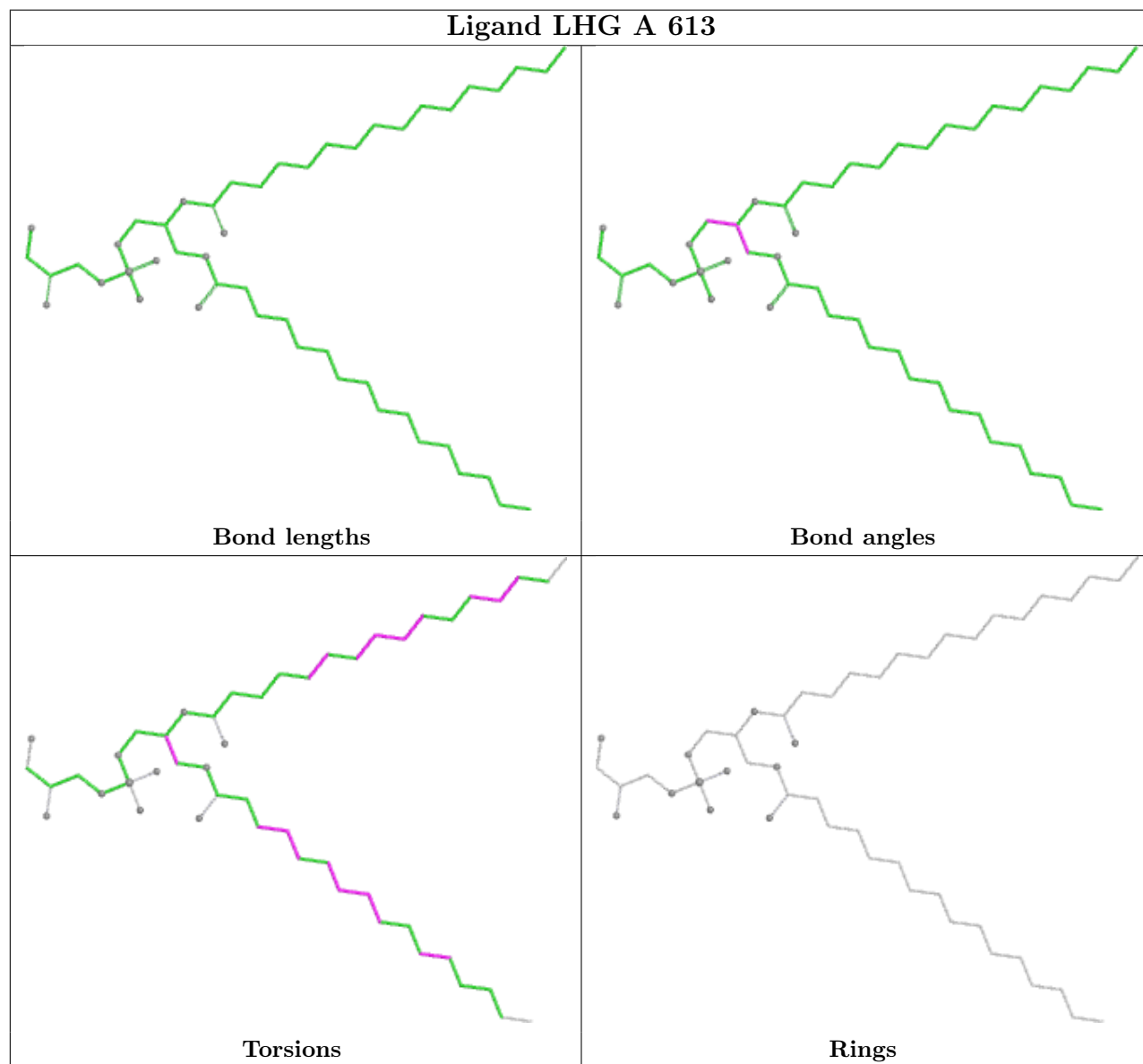
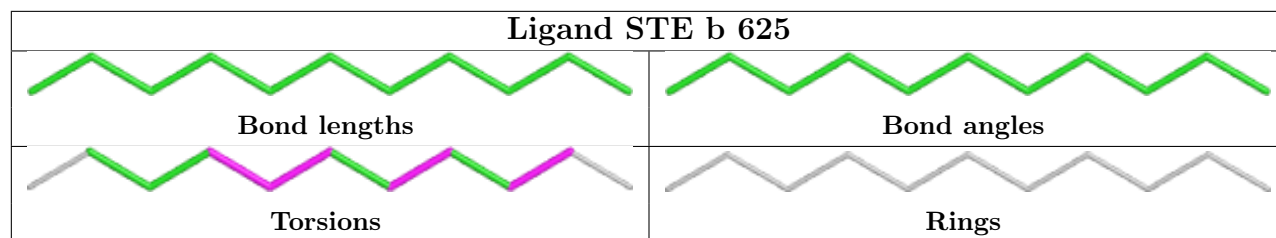
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Bond lengths	Bond angles
	
Torsions	Rings

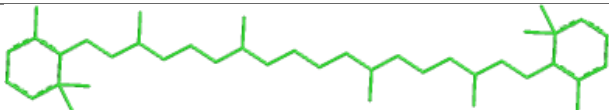
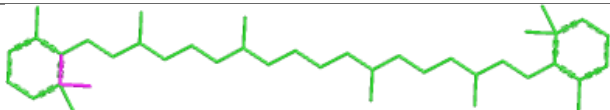
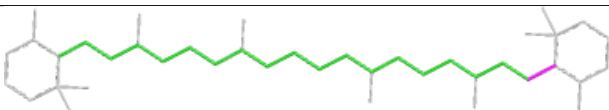
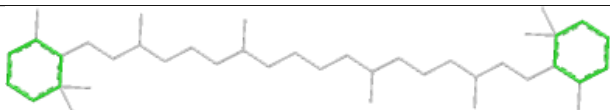
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Bond lengths	Bond angles
	
Torsions	Rings

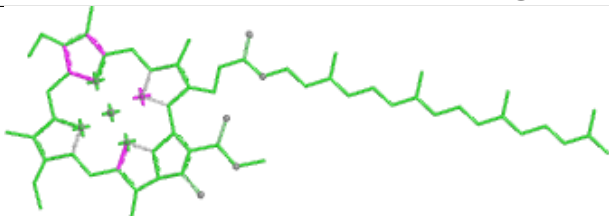
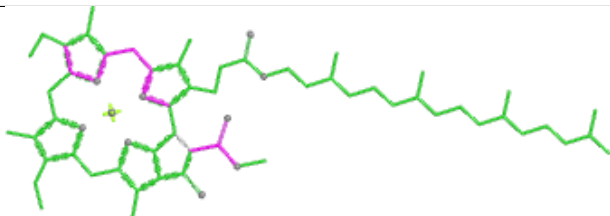
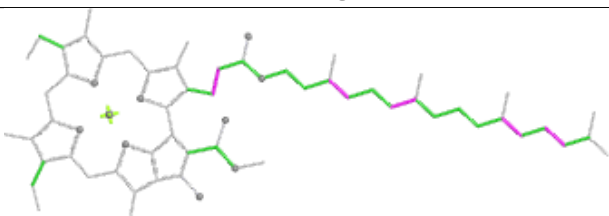
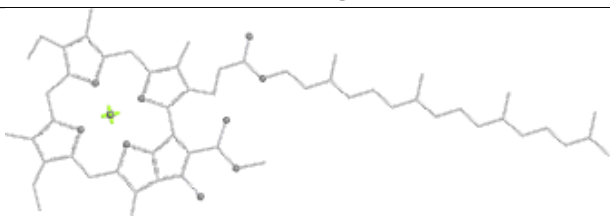
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Bond lengths	Bond angles
	
Torsions	Rings

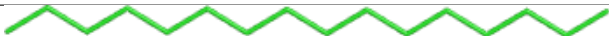
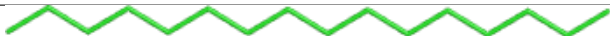
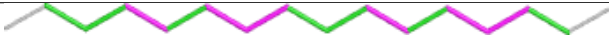


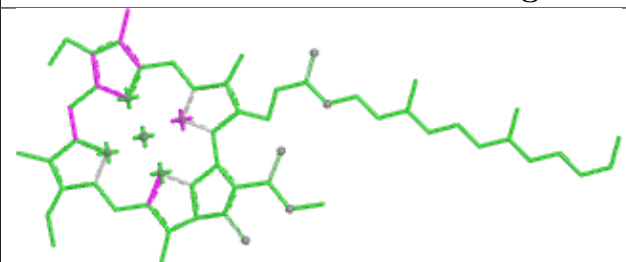
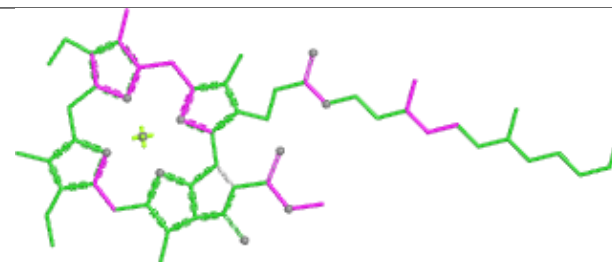
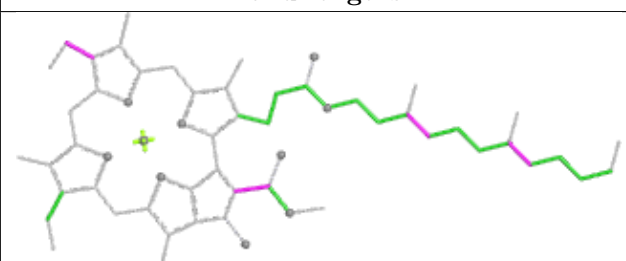
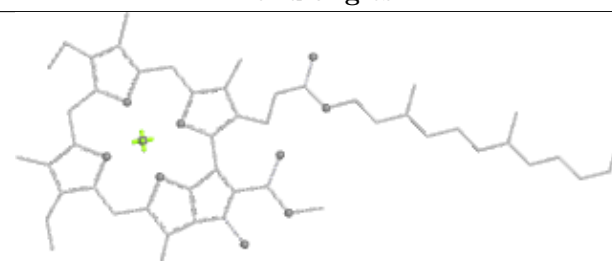


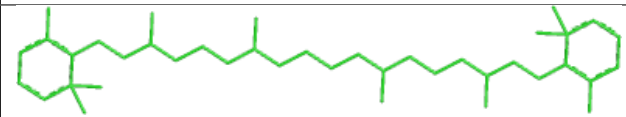
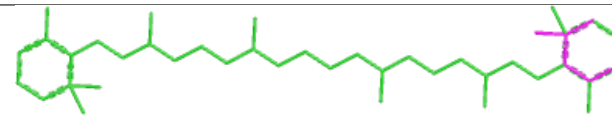
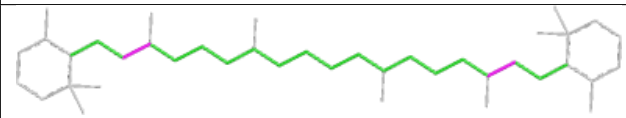
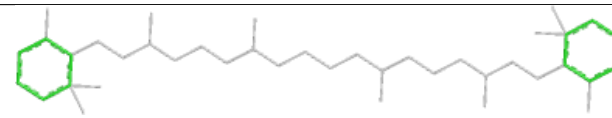


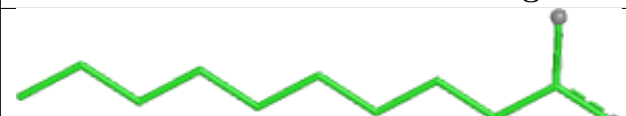
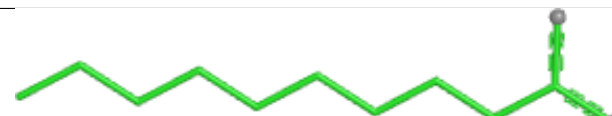
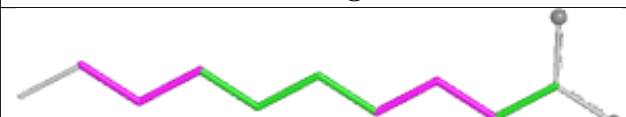
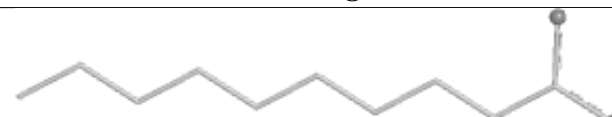
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

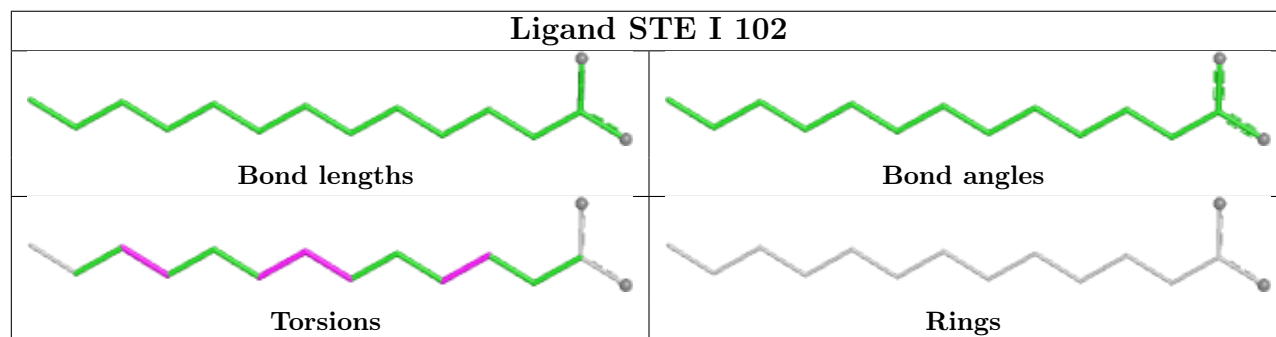
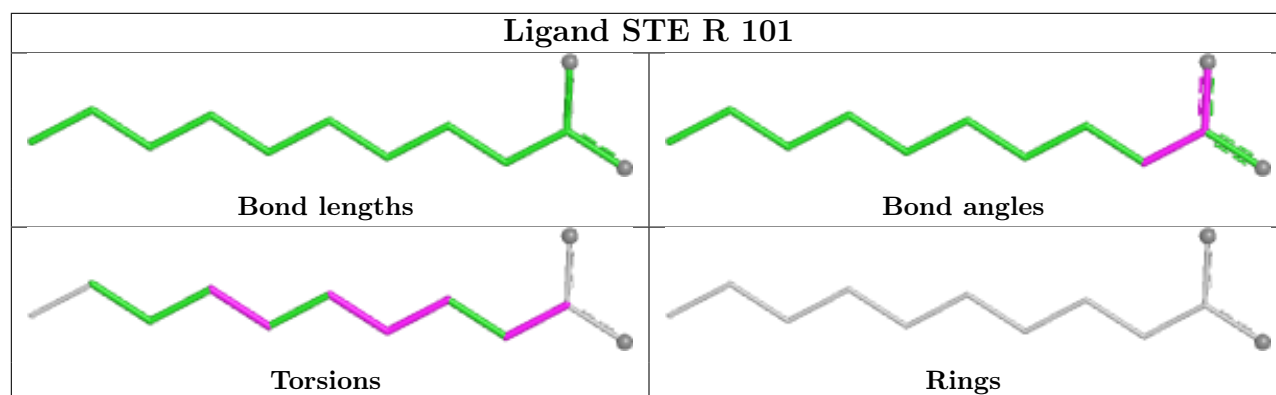
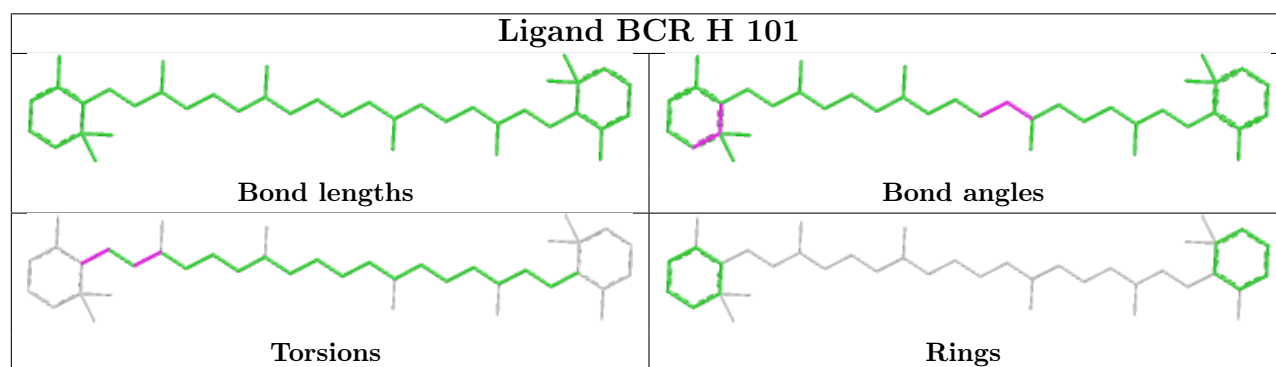
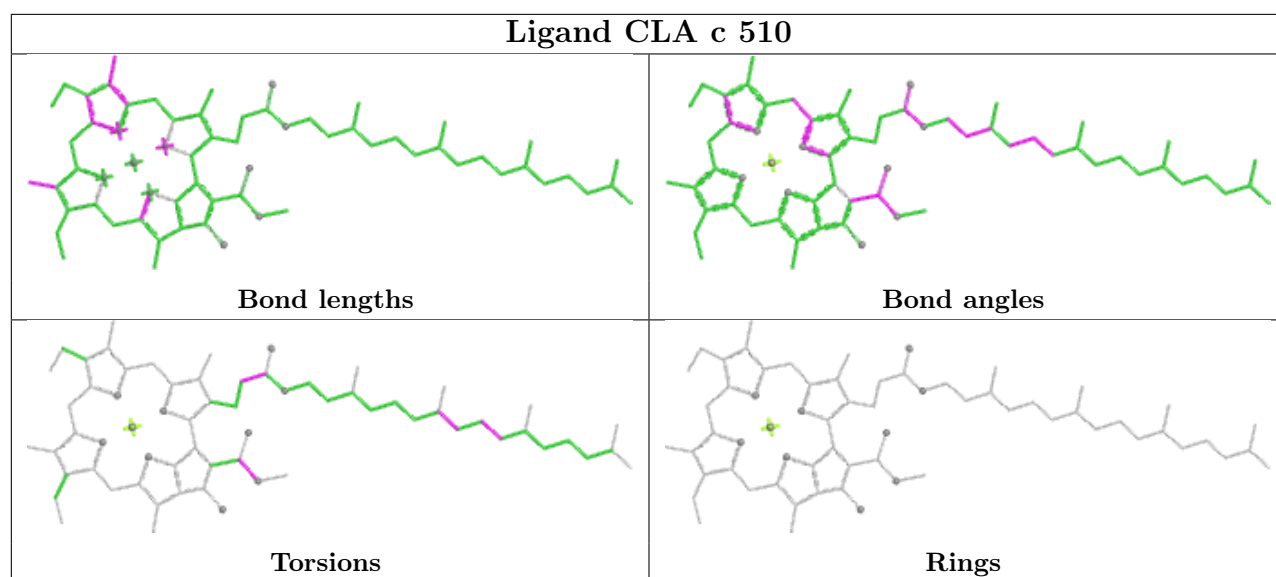
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

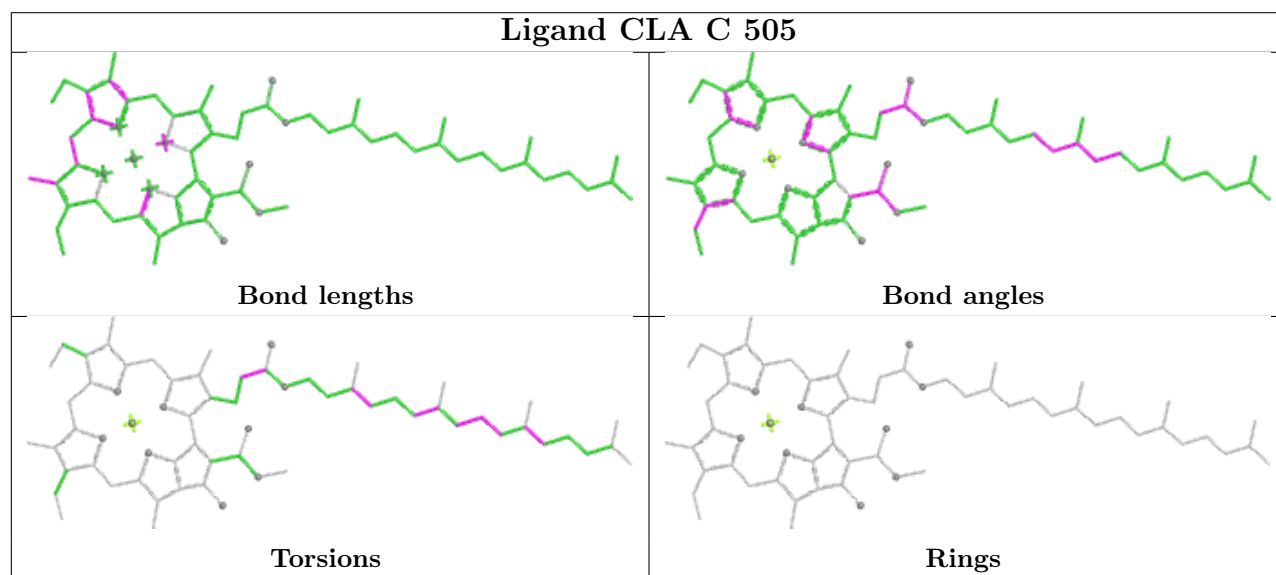
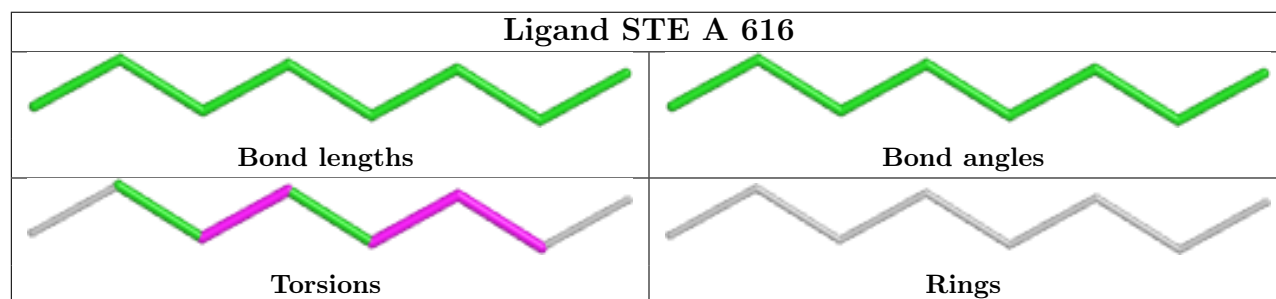
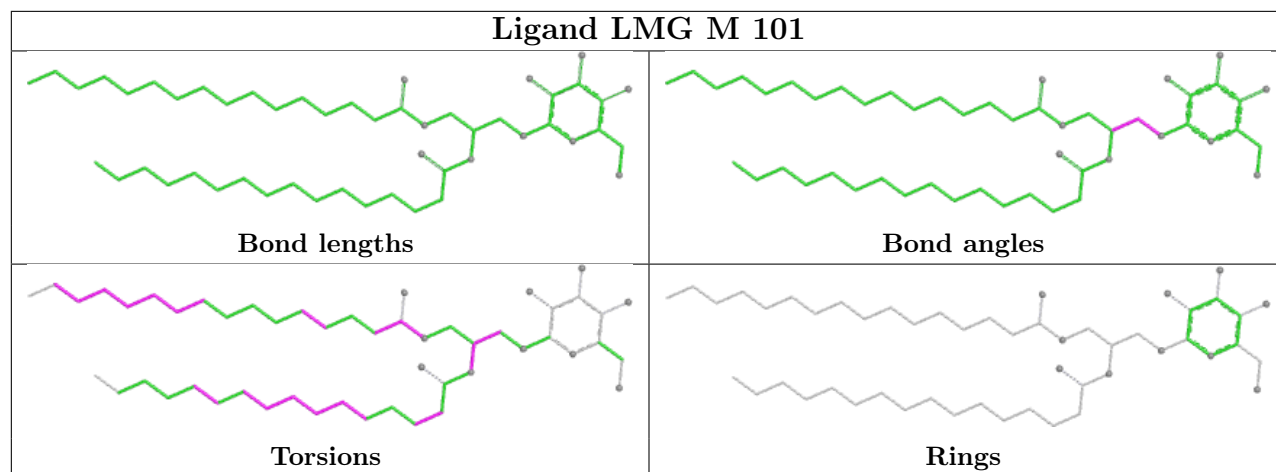
Ligand STE j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

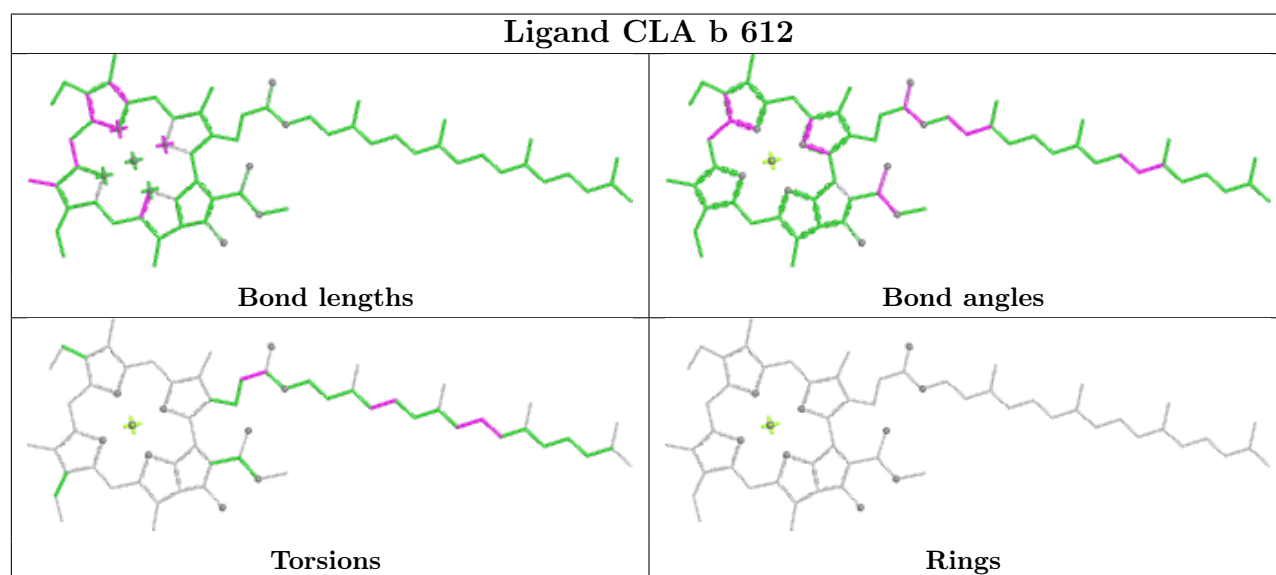
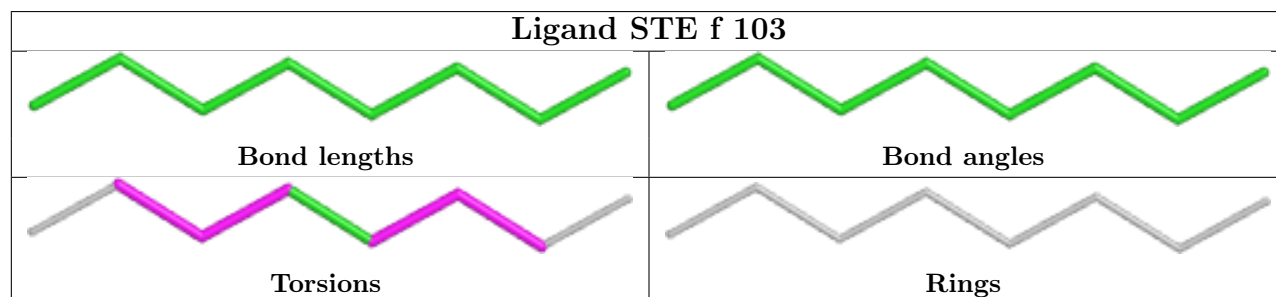
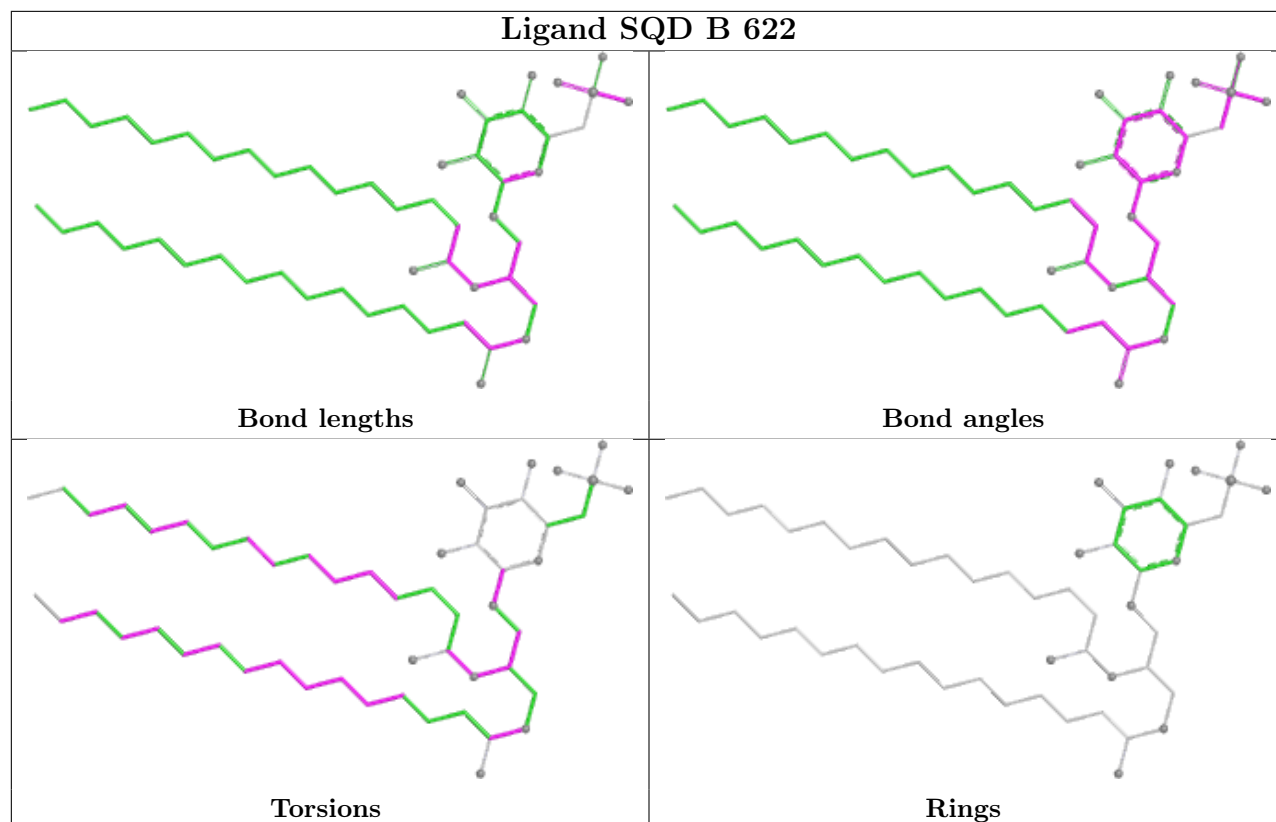
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Bond lengths	Bond angles
	
Torsions	Rings

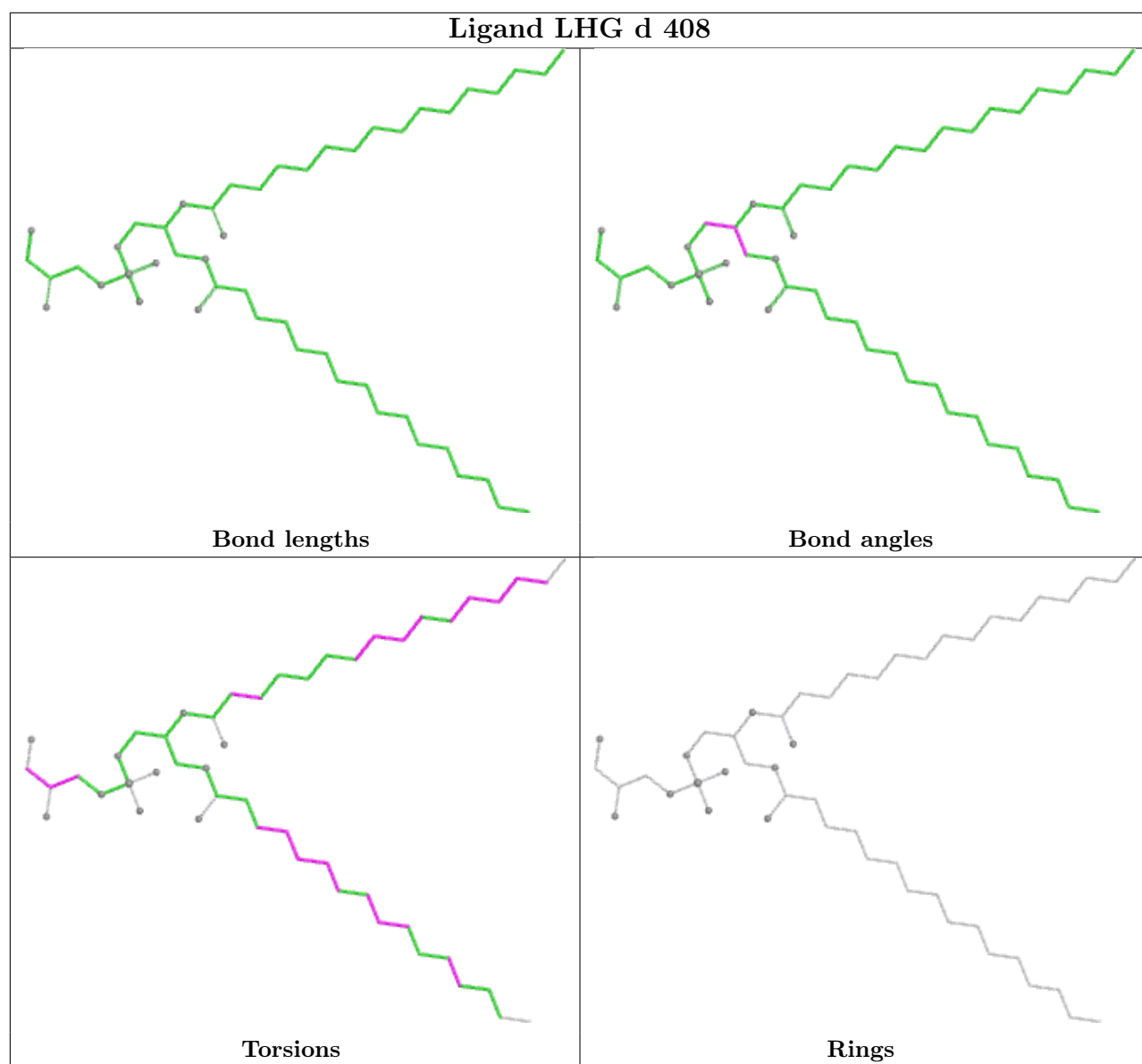
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

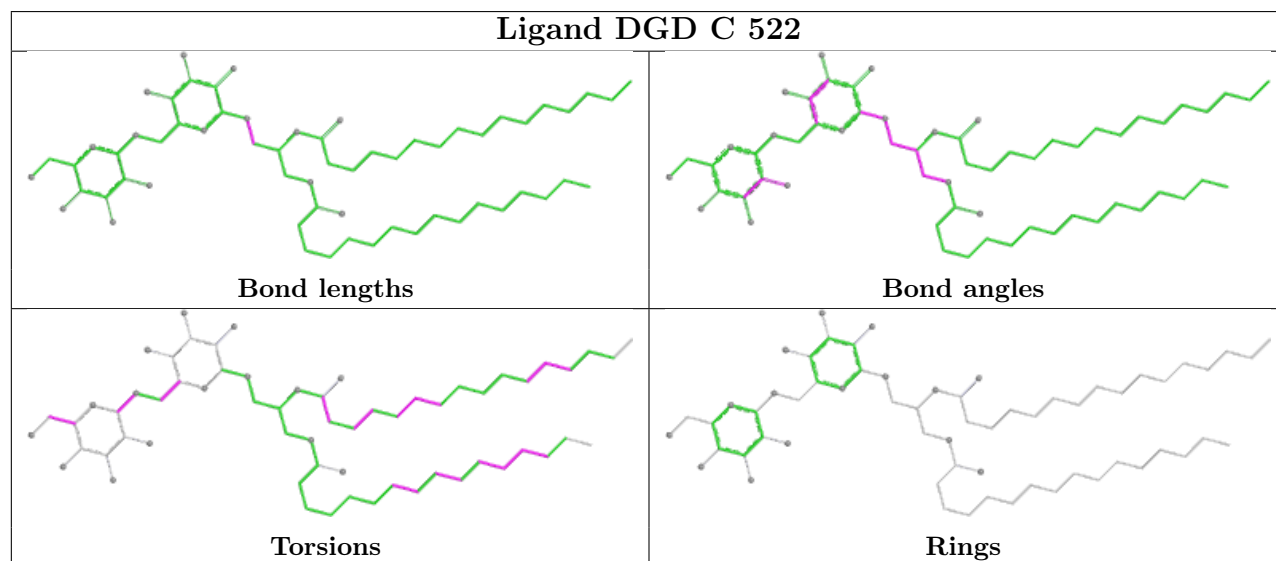
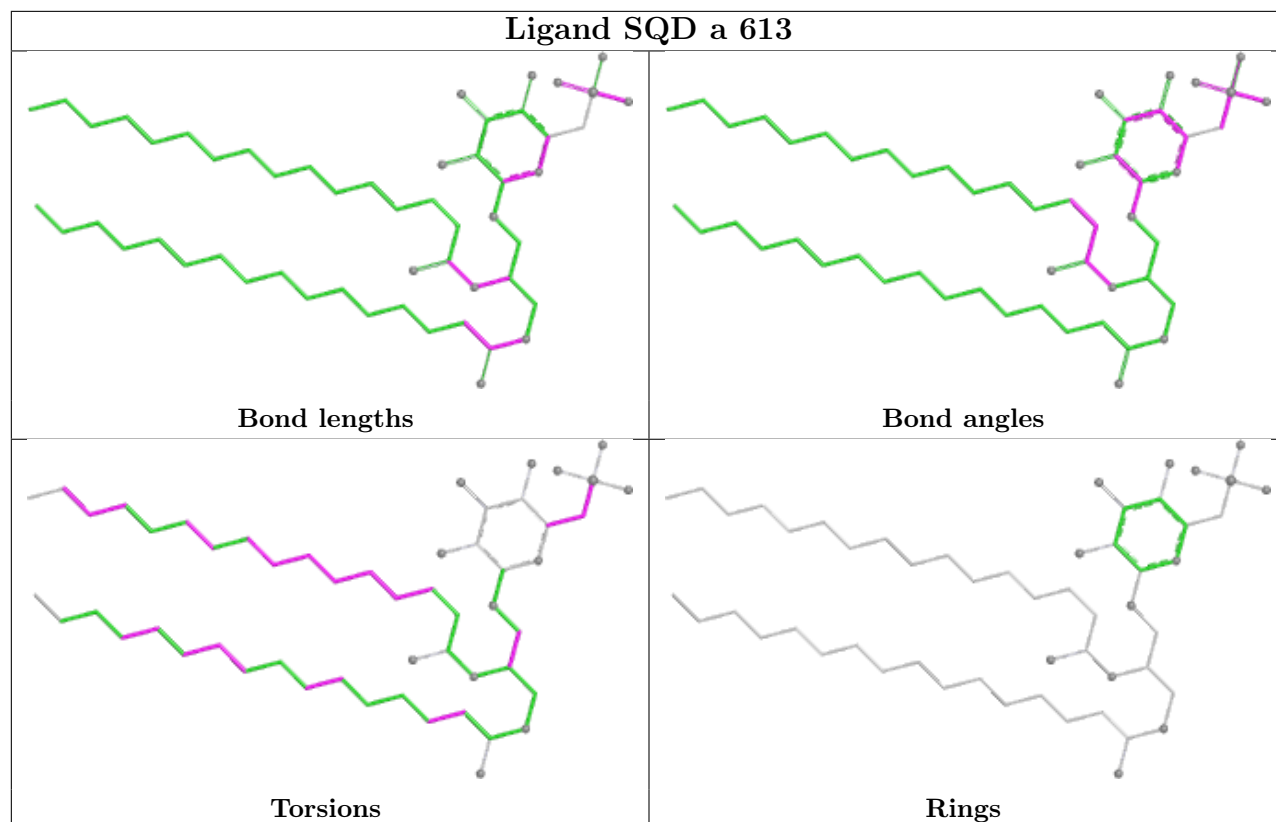
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Bond lengths	Bond angles
	
Torsions	Rings

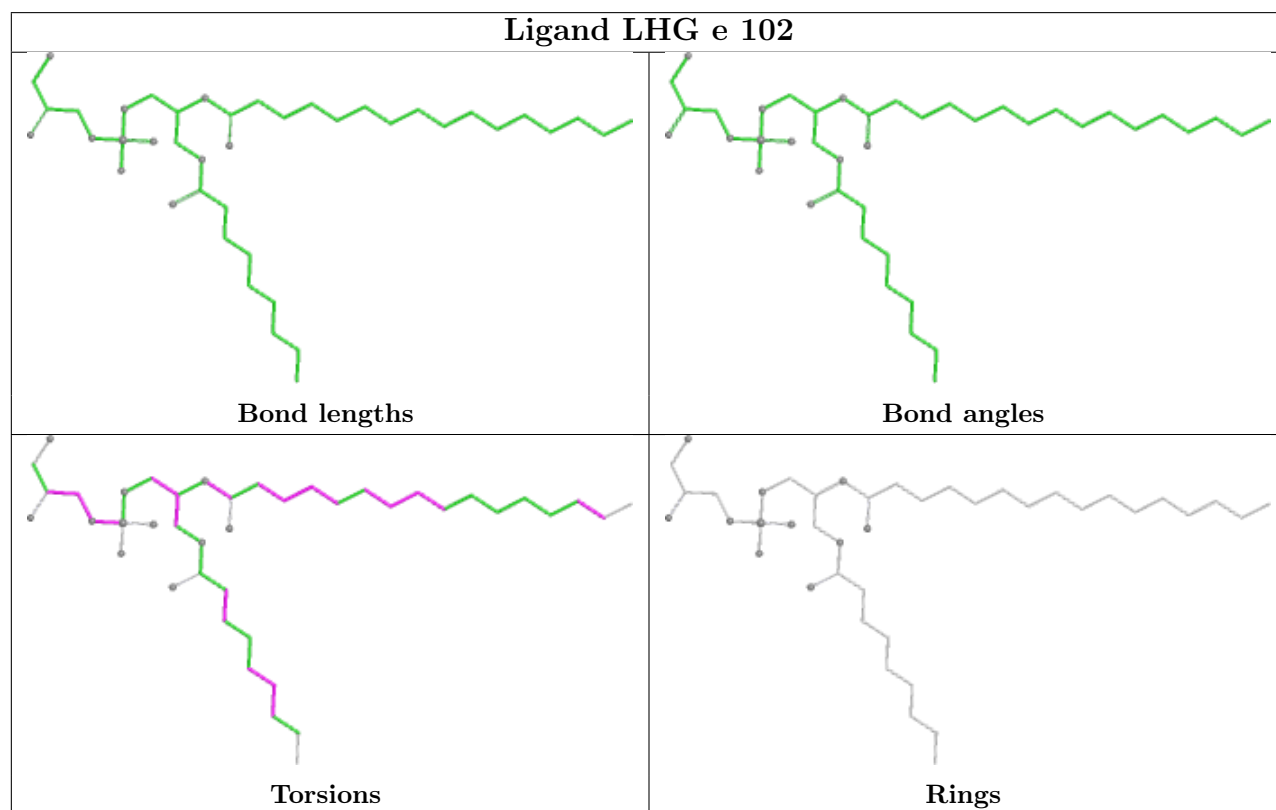
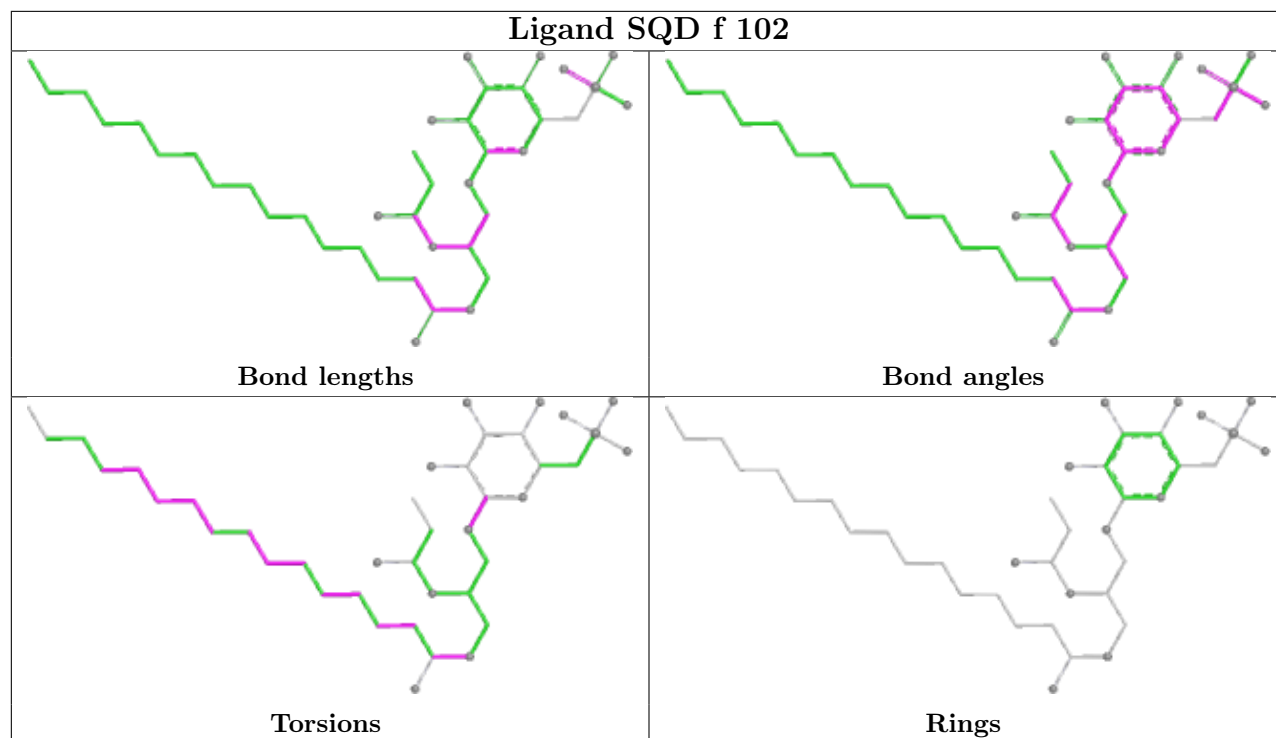


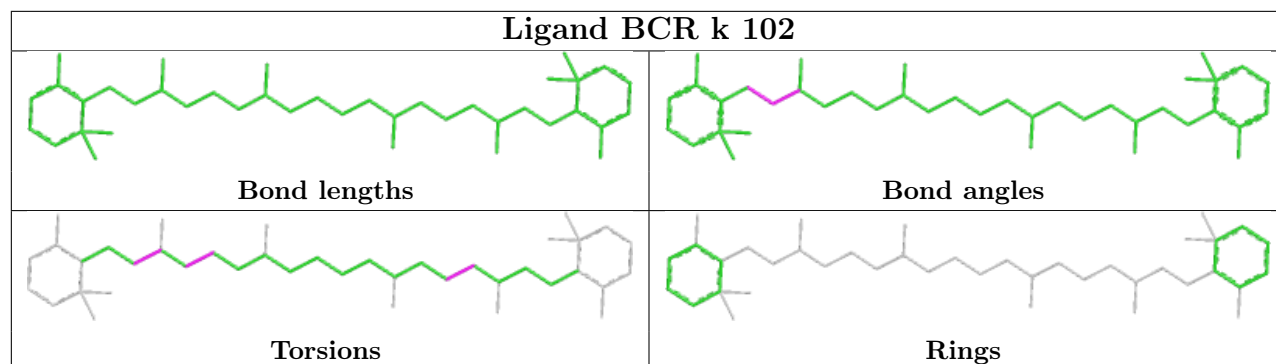
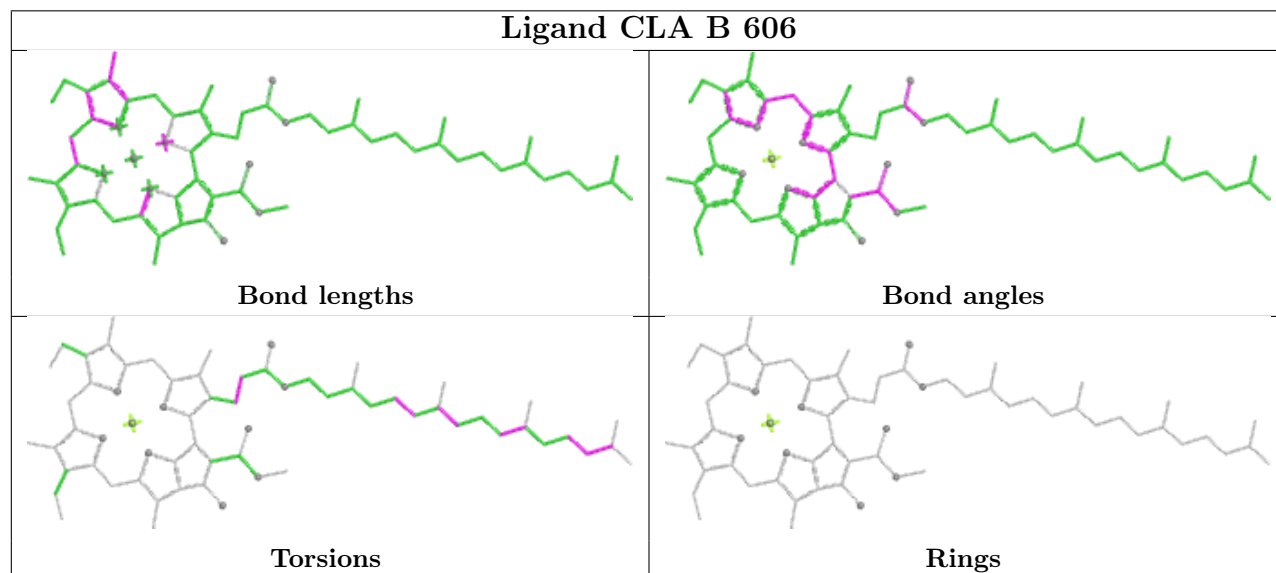
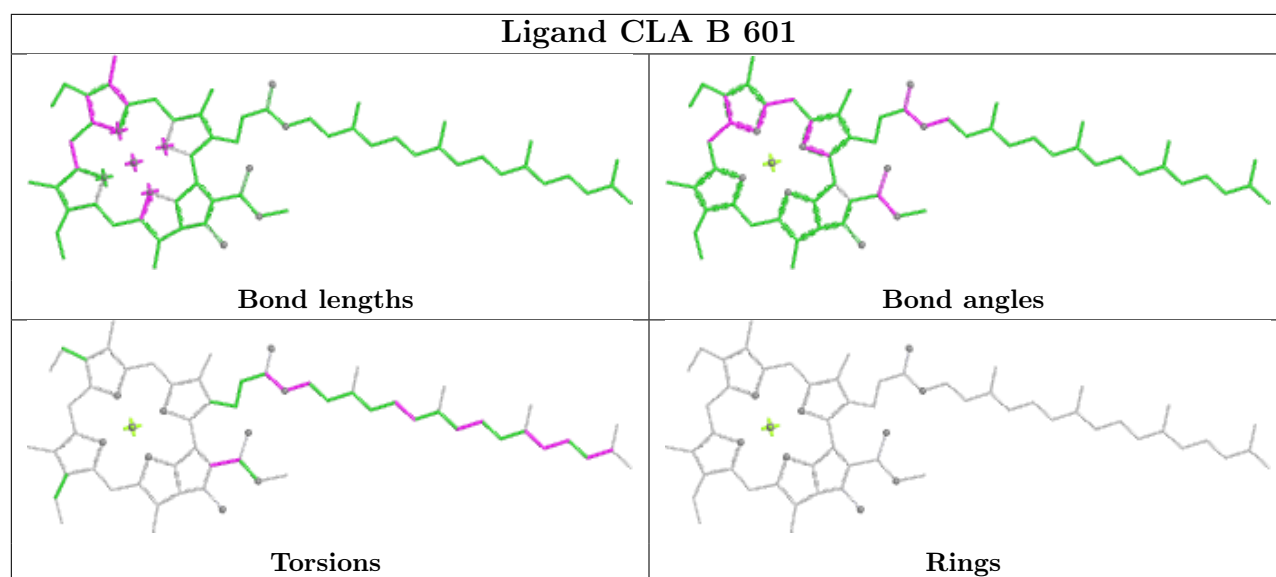


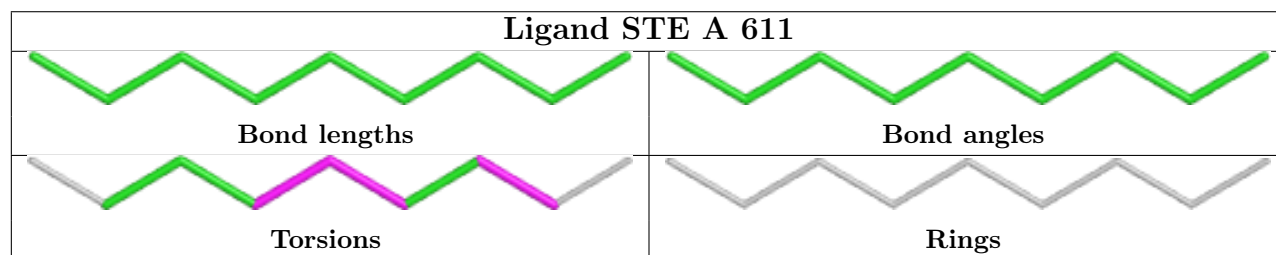
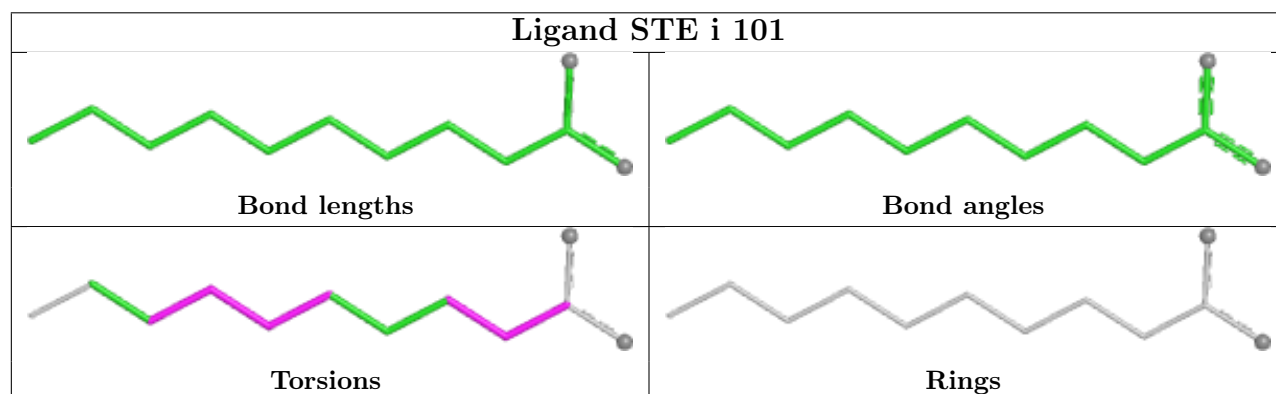
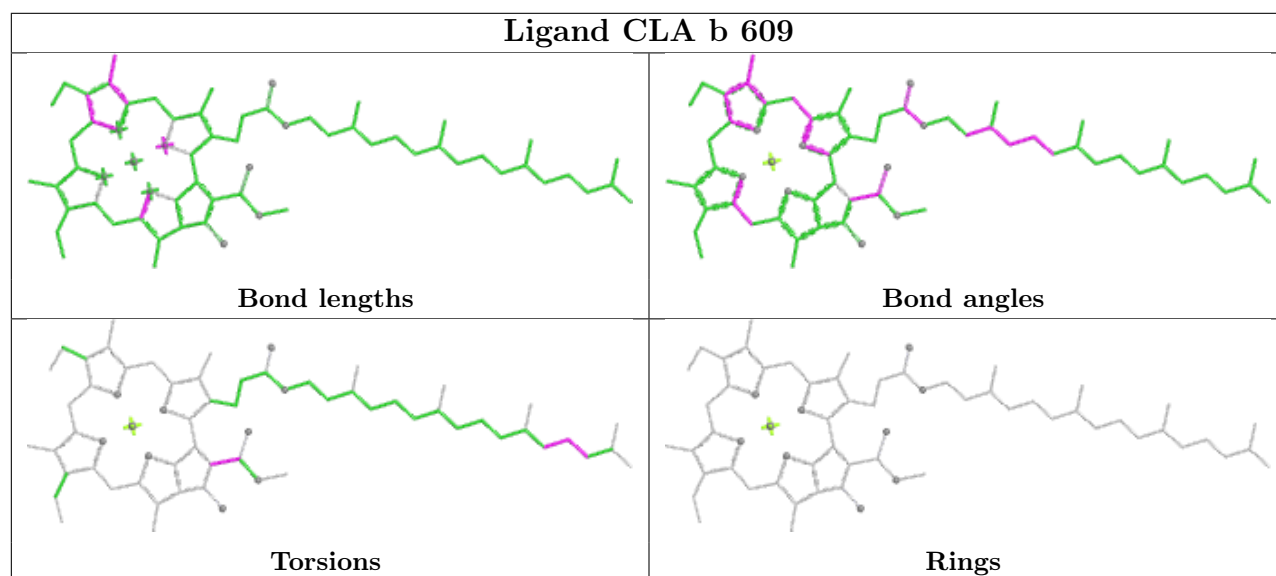
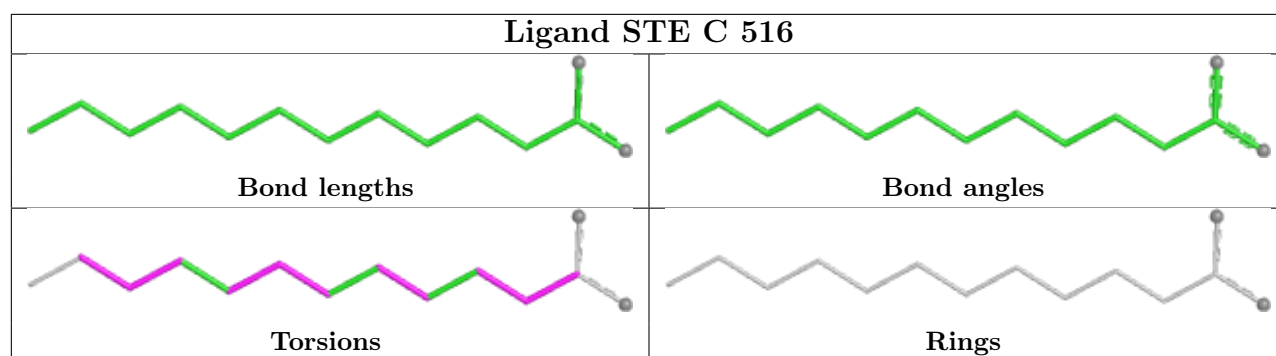


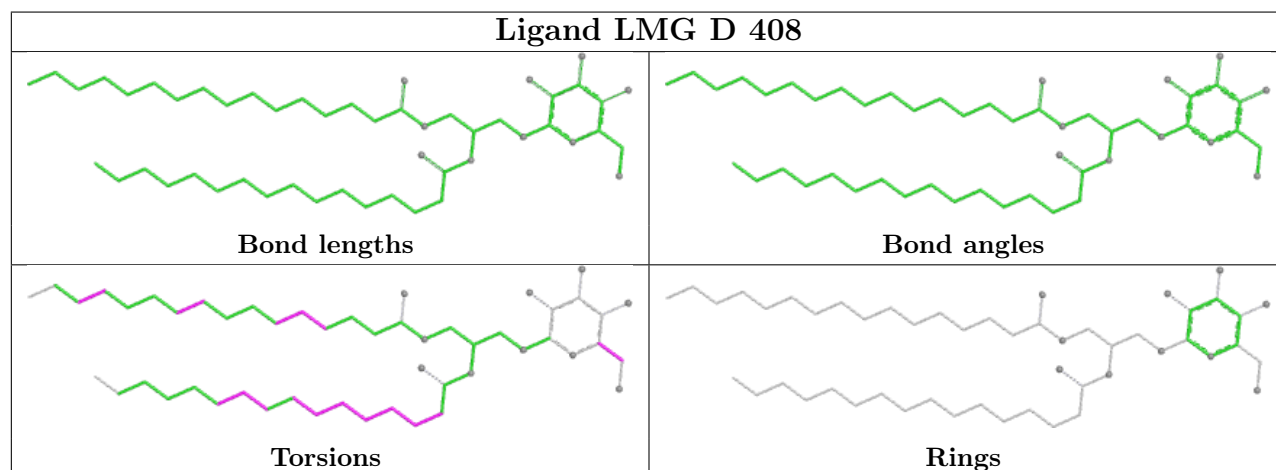
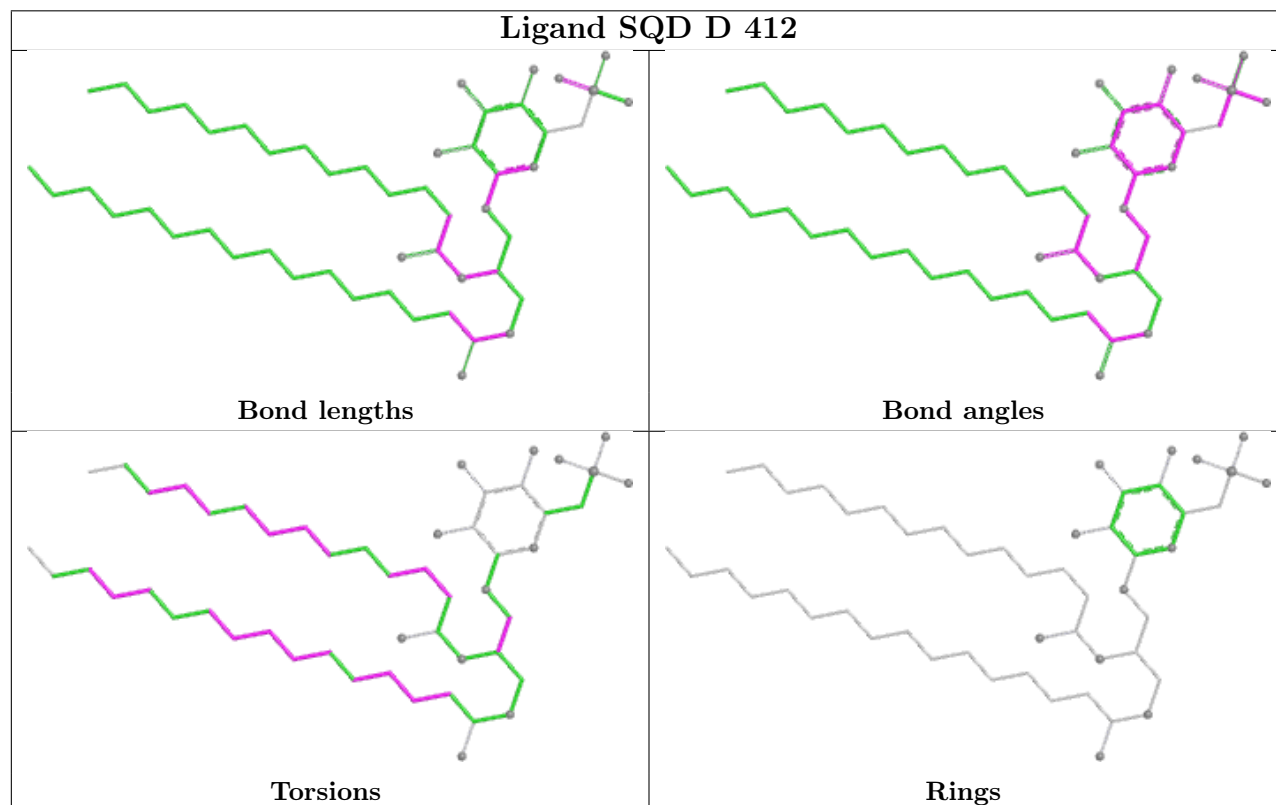
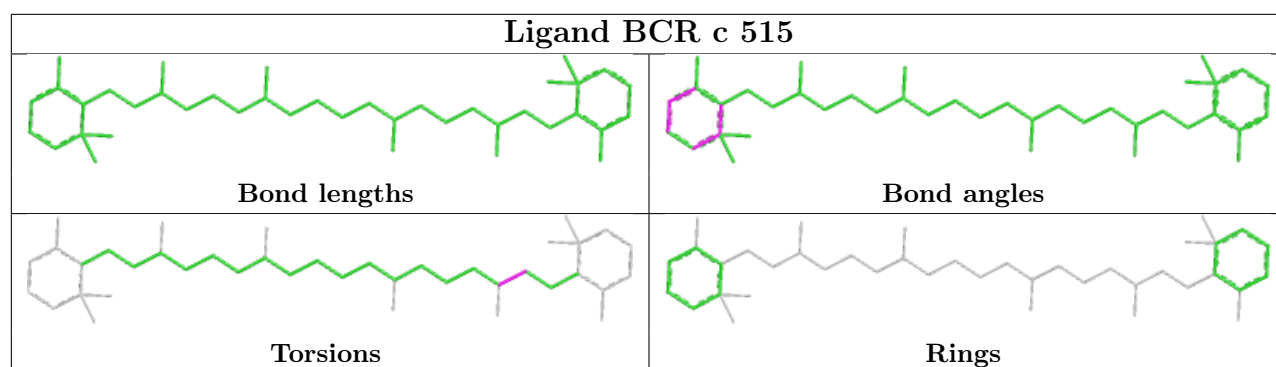


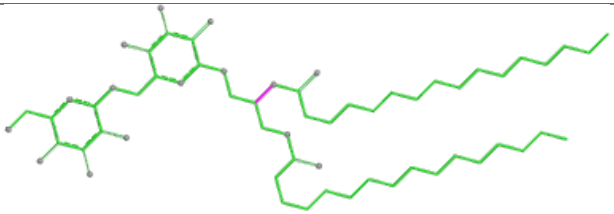
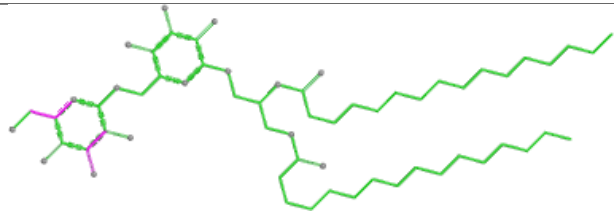
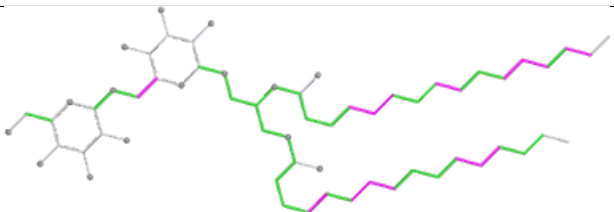
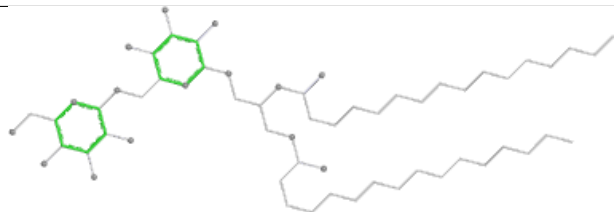


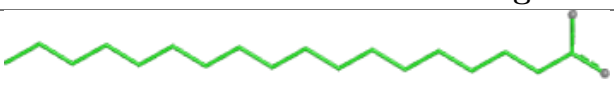
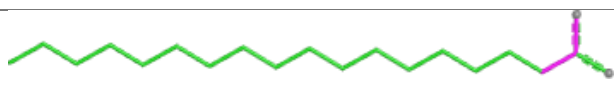
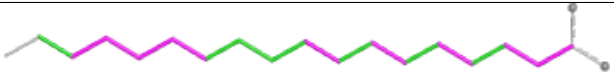
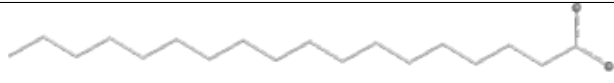


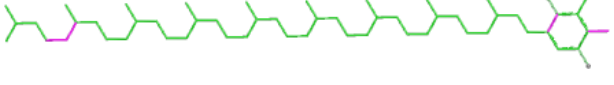
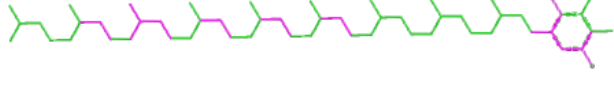
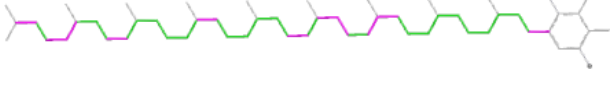
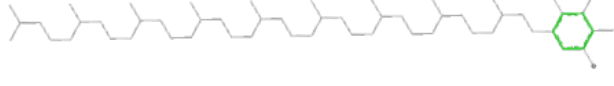


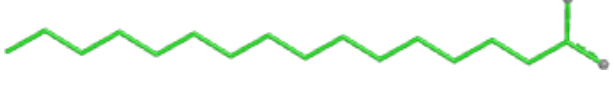
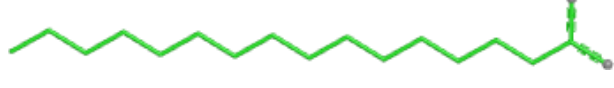
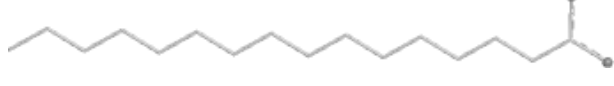




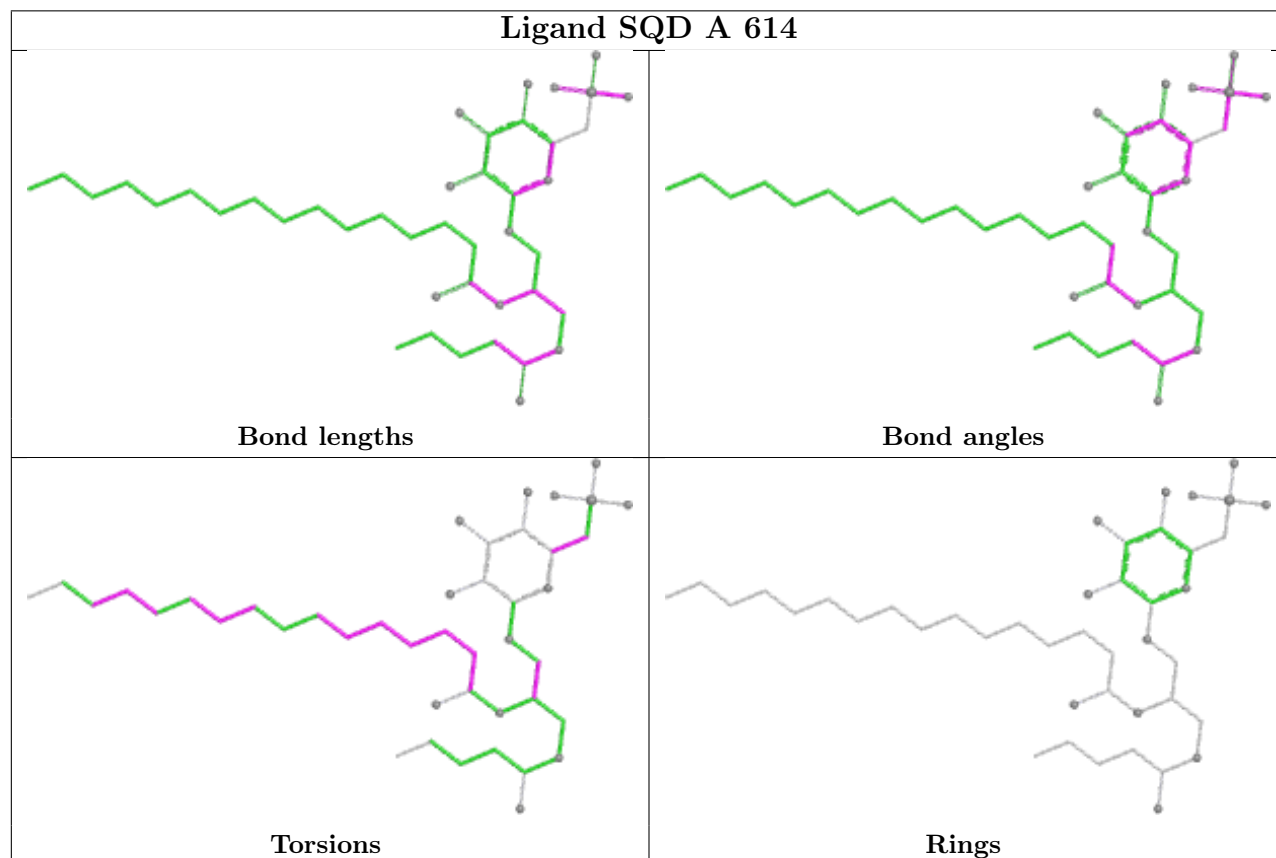
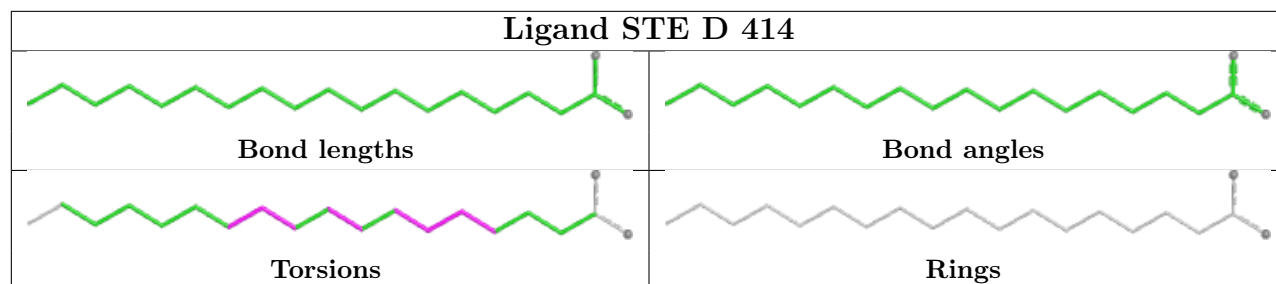
Ligand DGD C 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE E 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

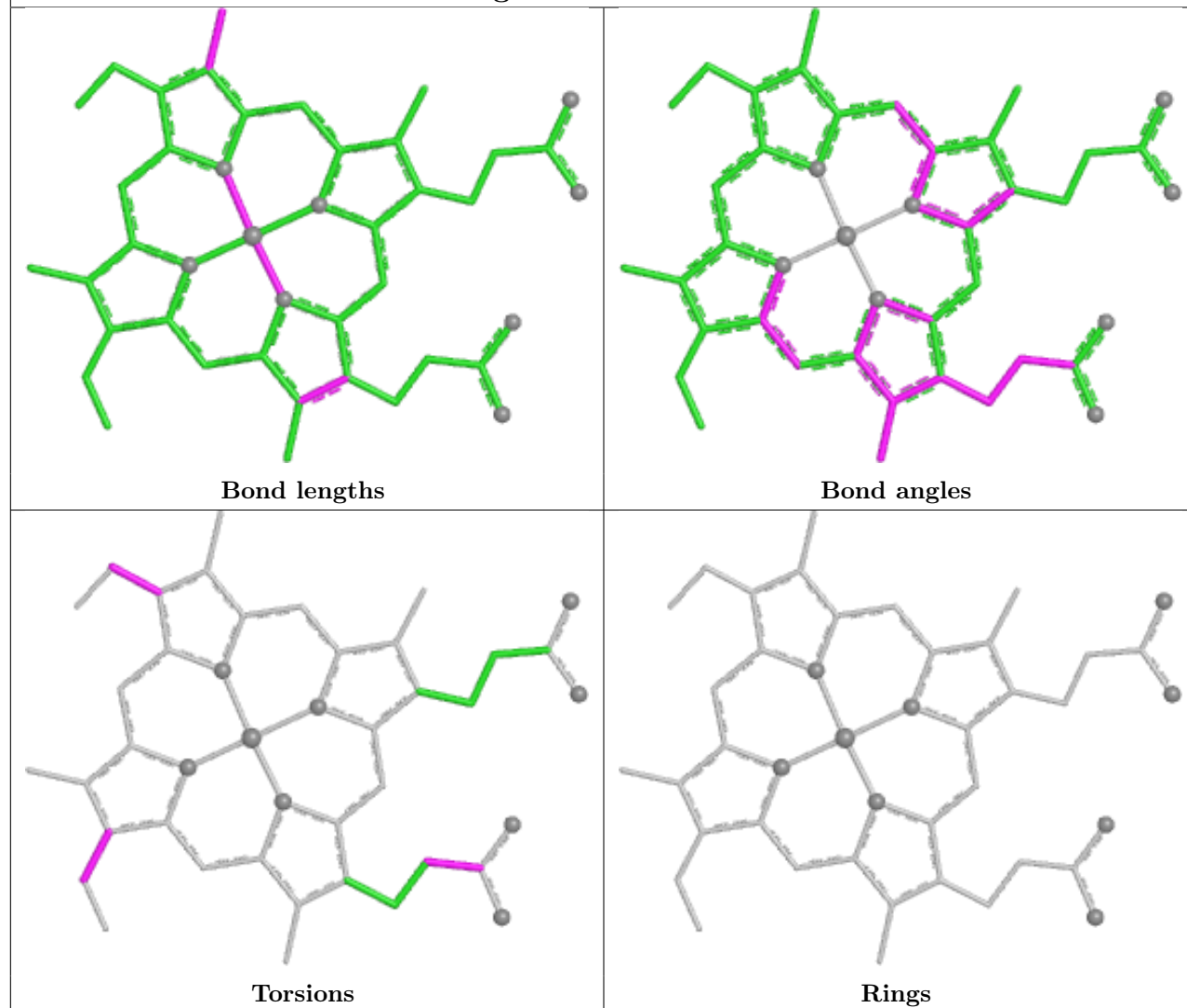
Ligand PL9 a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

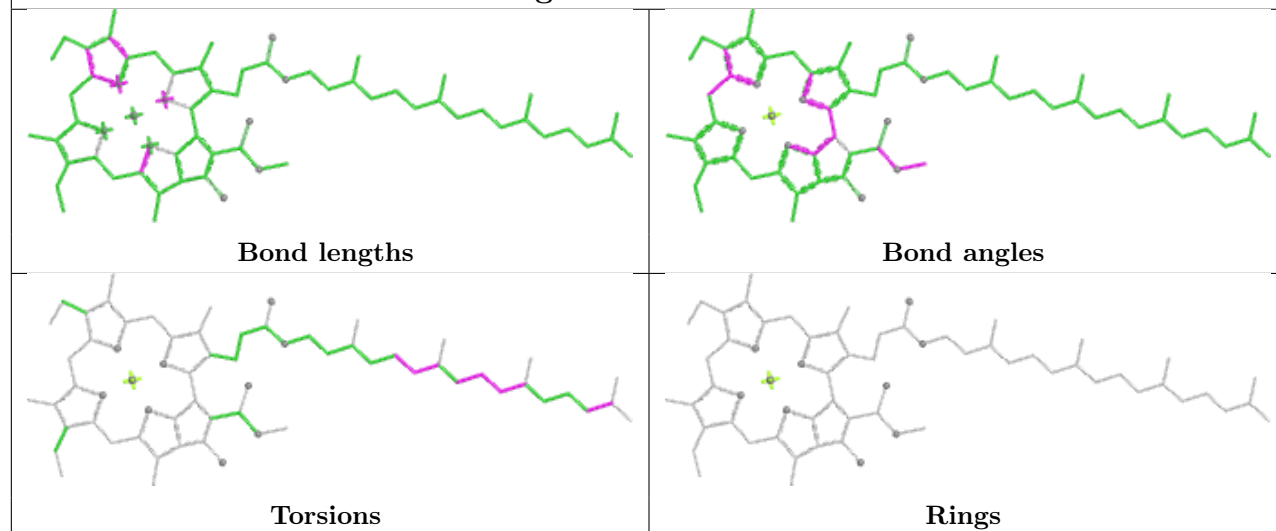
Ligand STE t 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

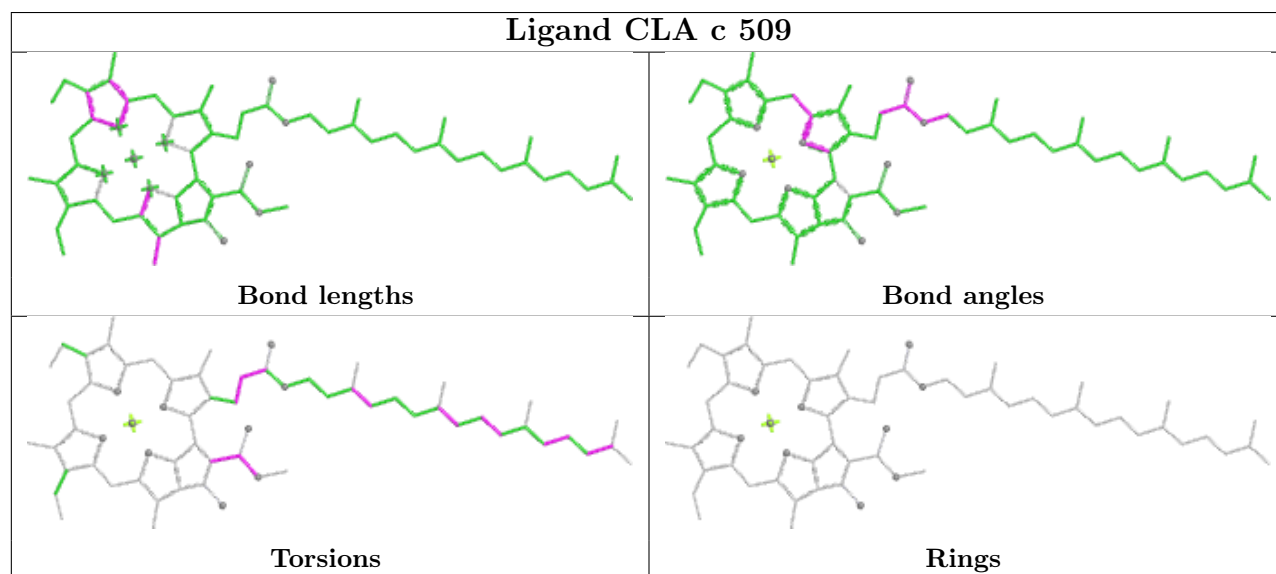
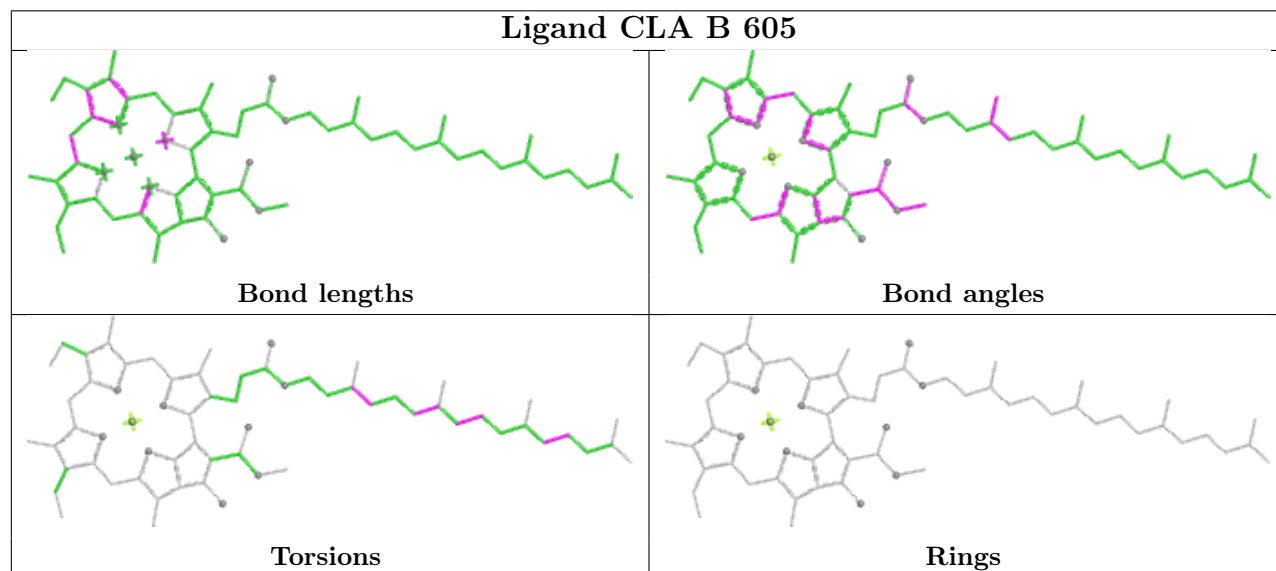
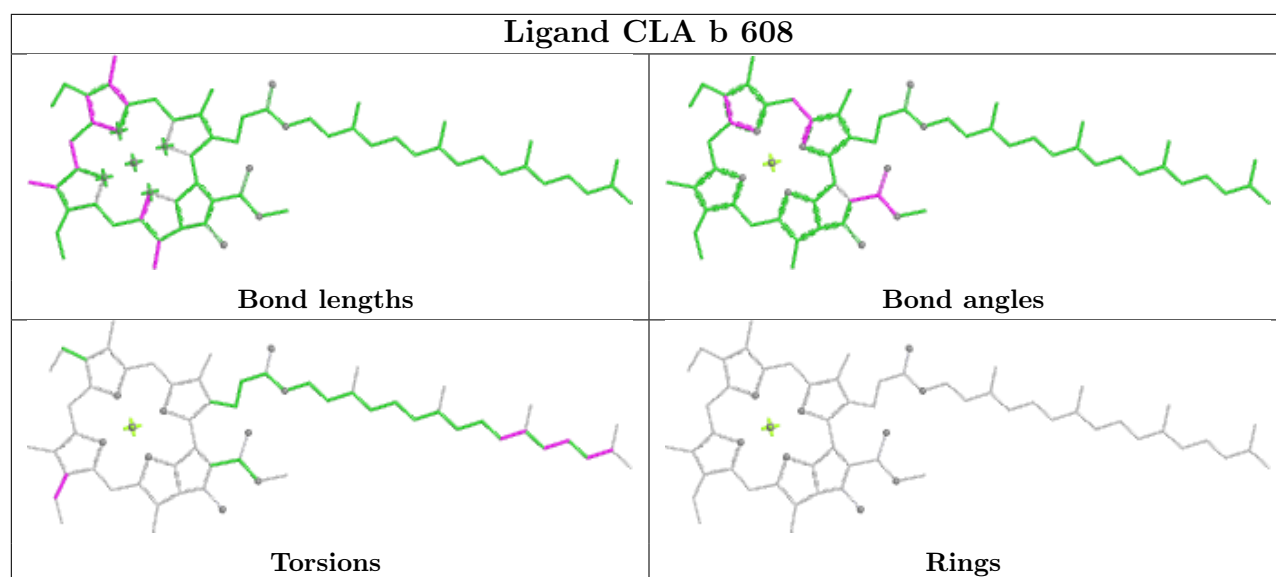


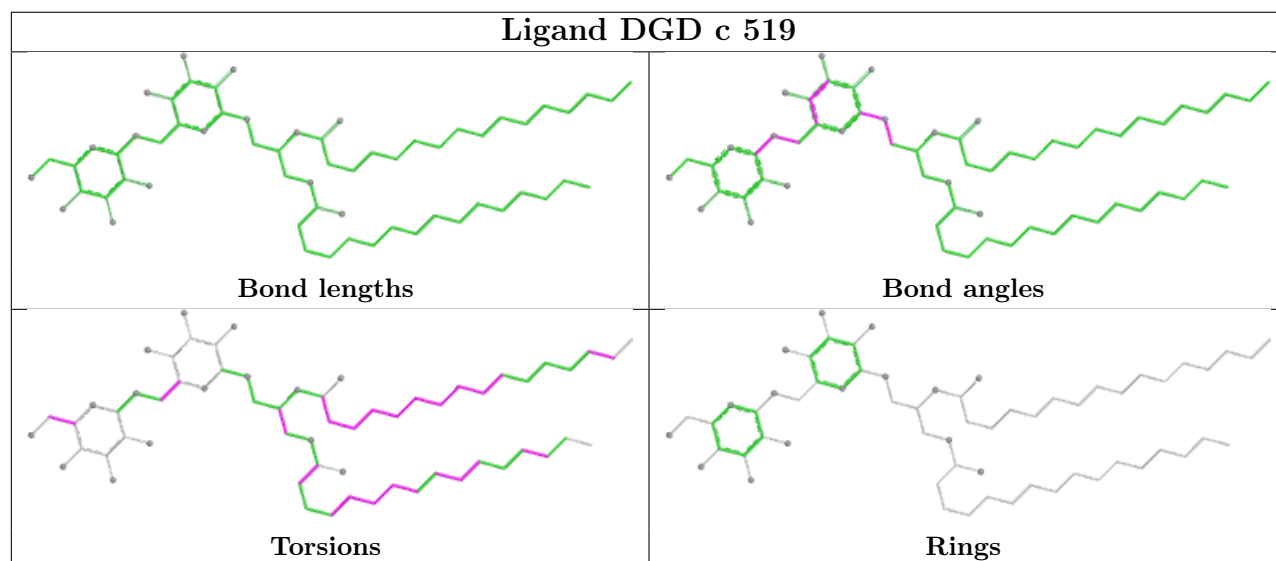
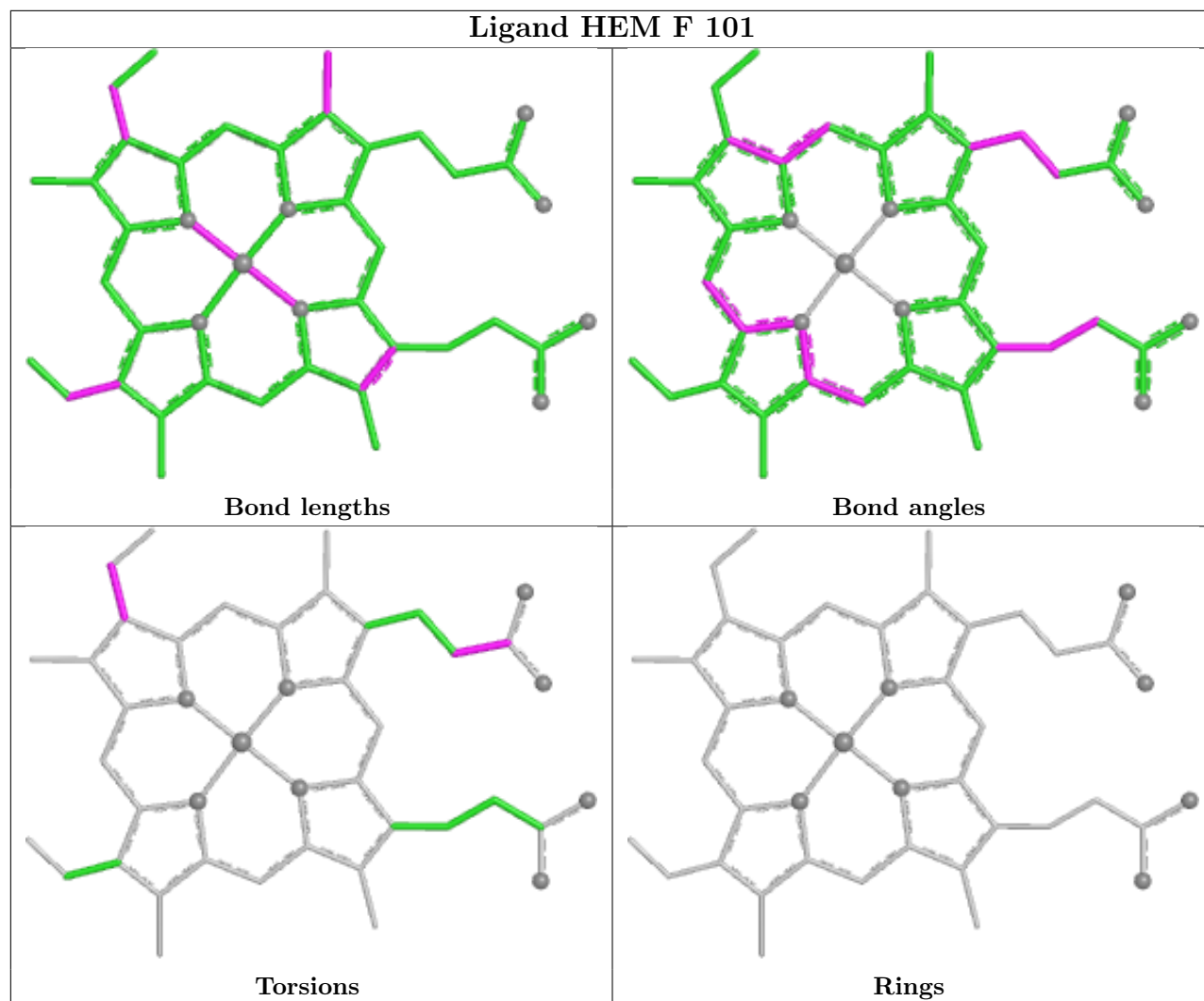
Ligand HEC V 201

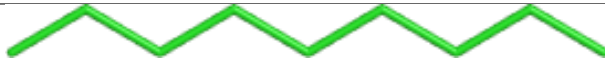


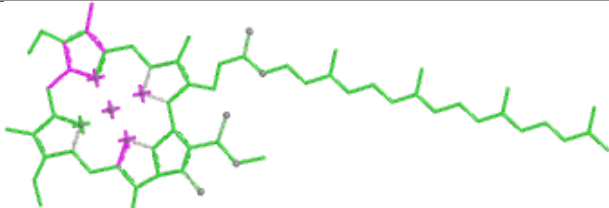
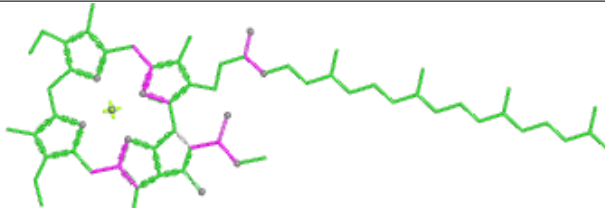
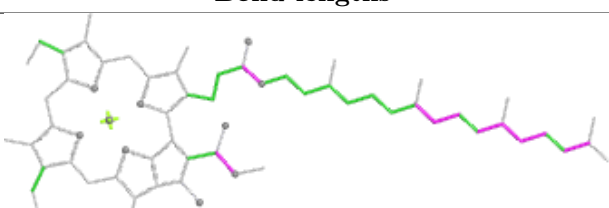
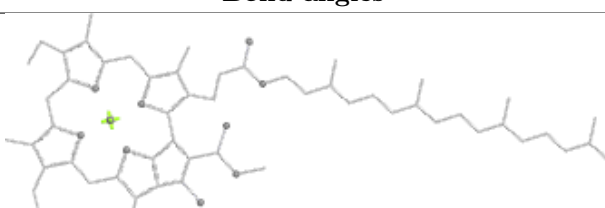
Ligand CLA b 607

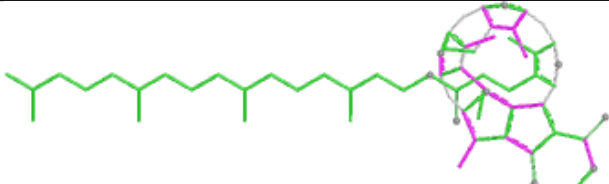
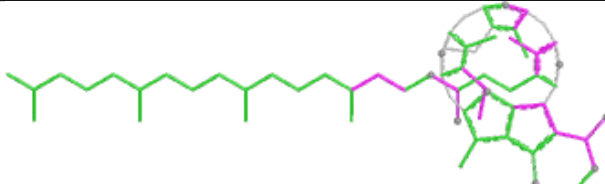
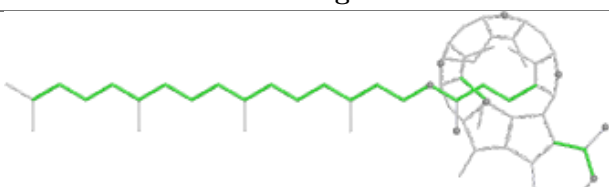
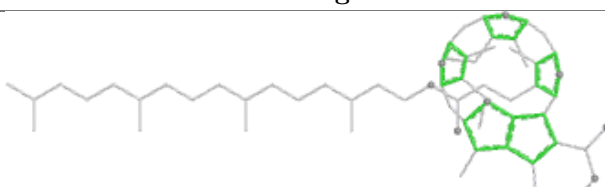


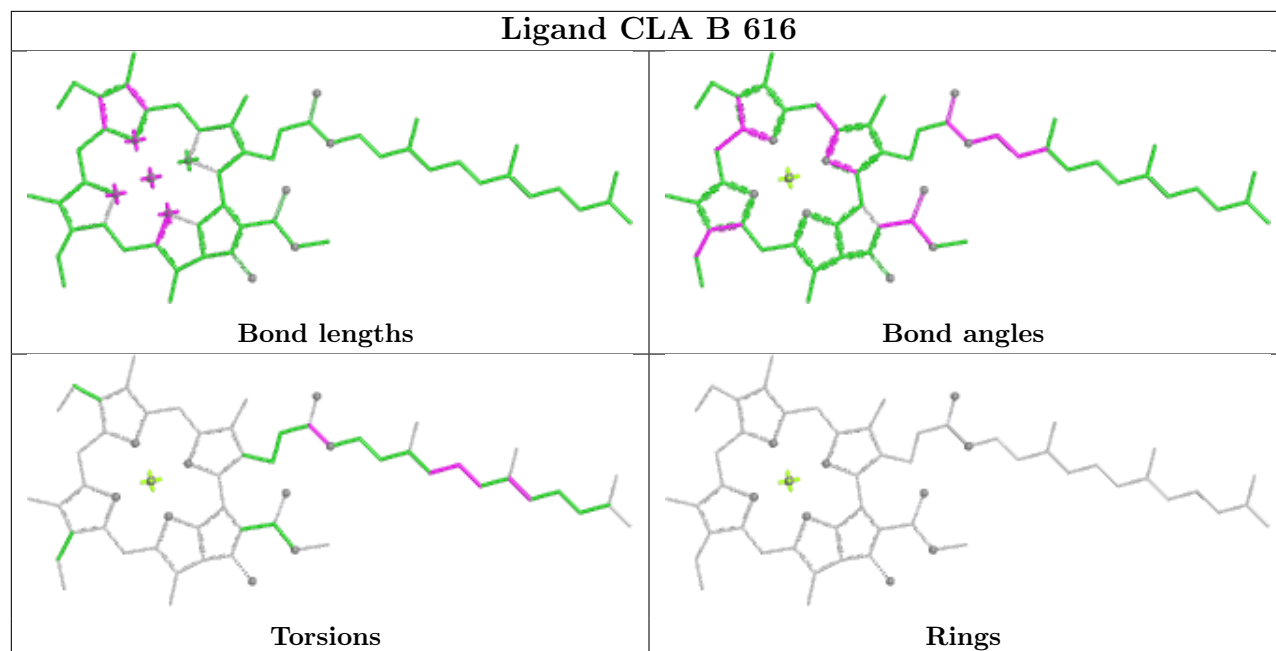
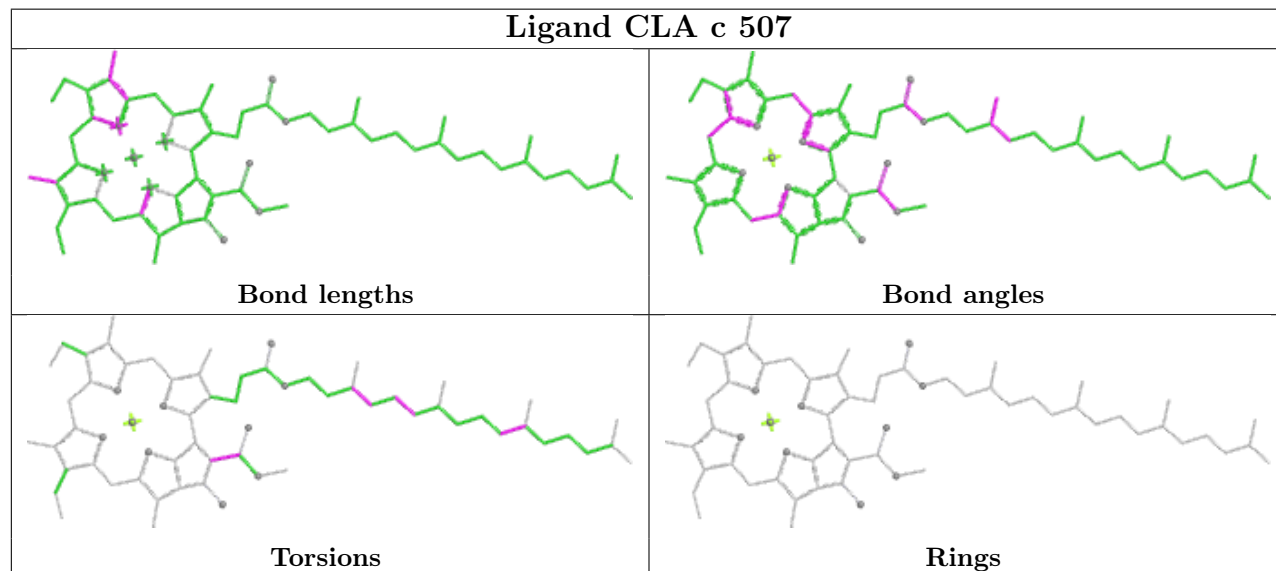


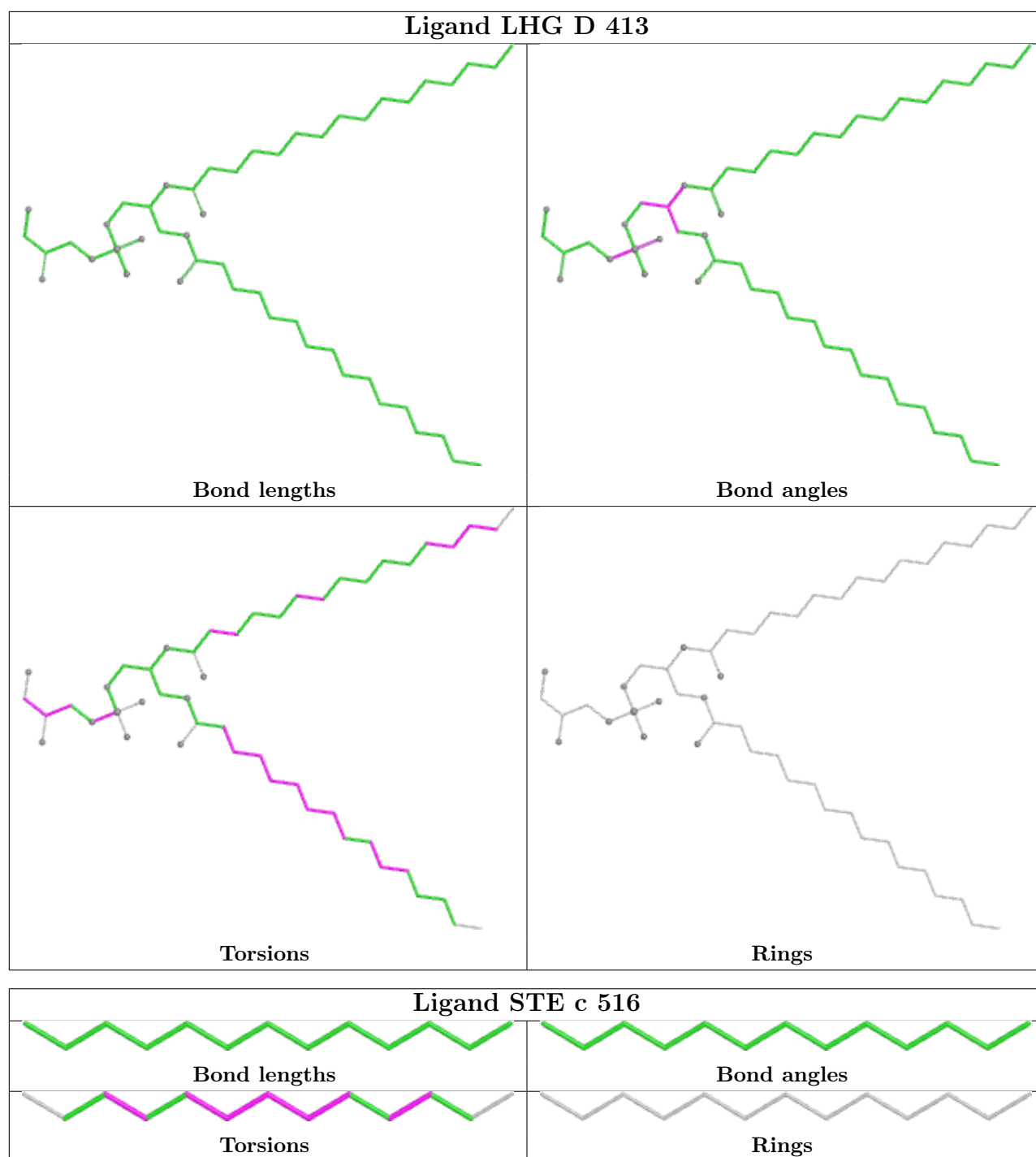


Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

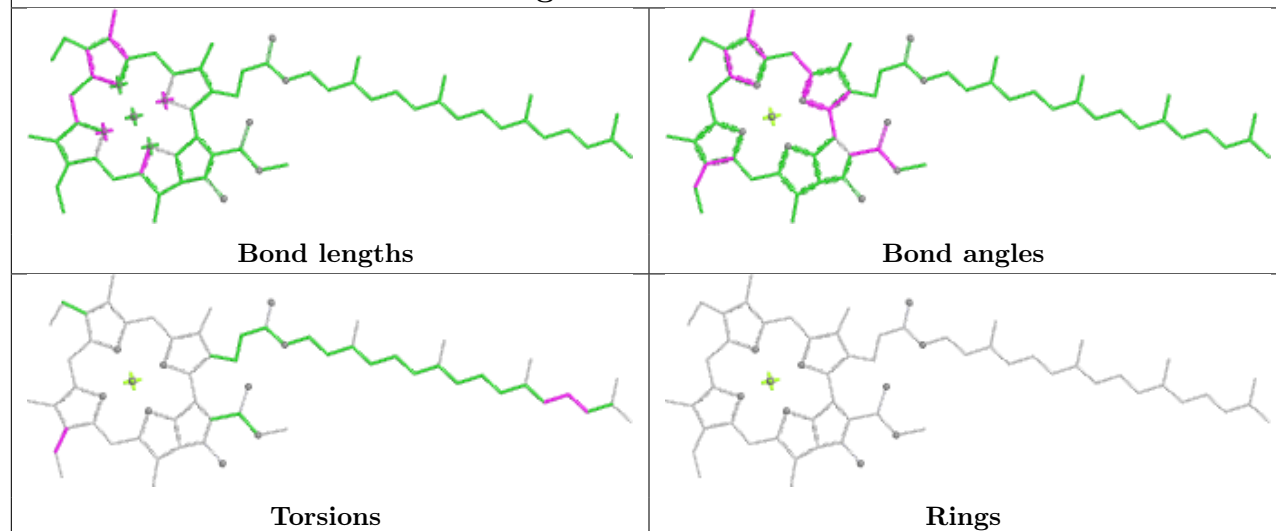
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO d 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 616**Ligand CLA c 507**



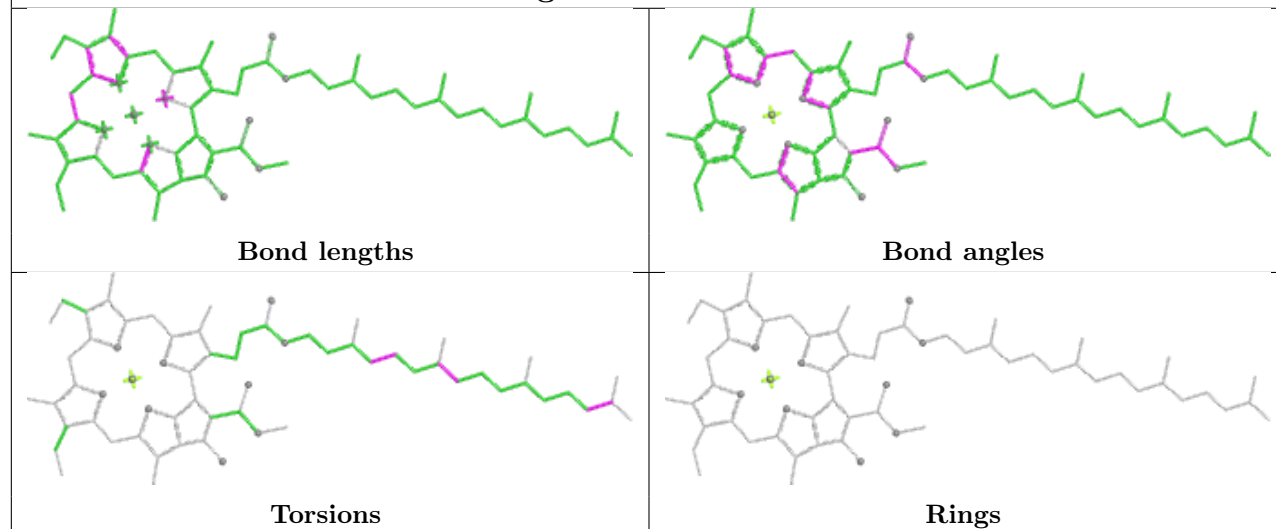
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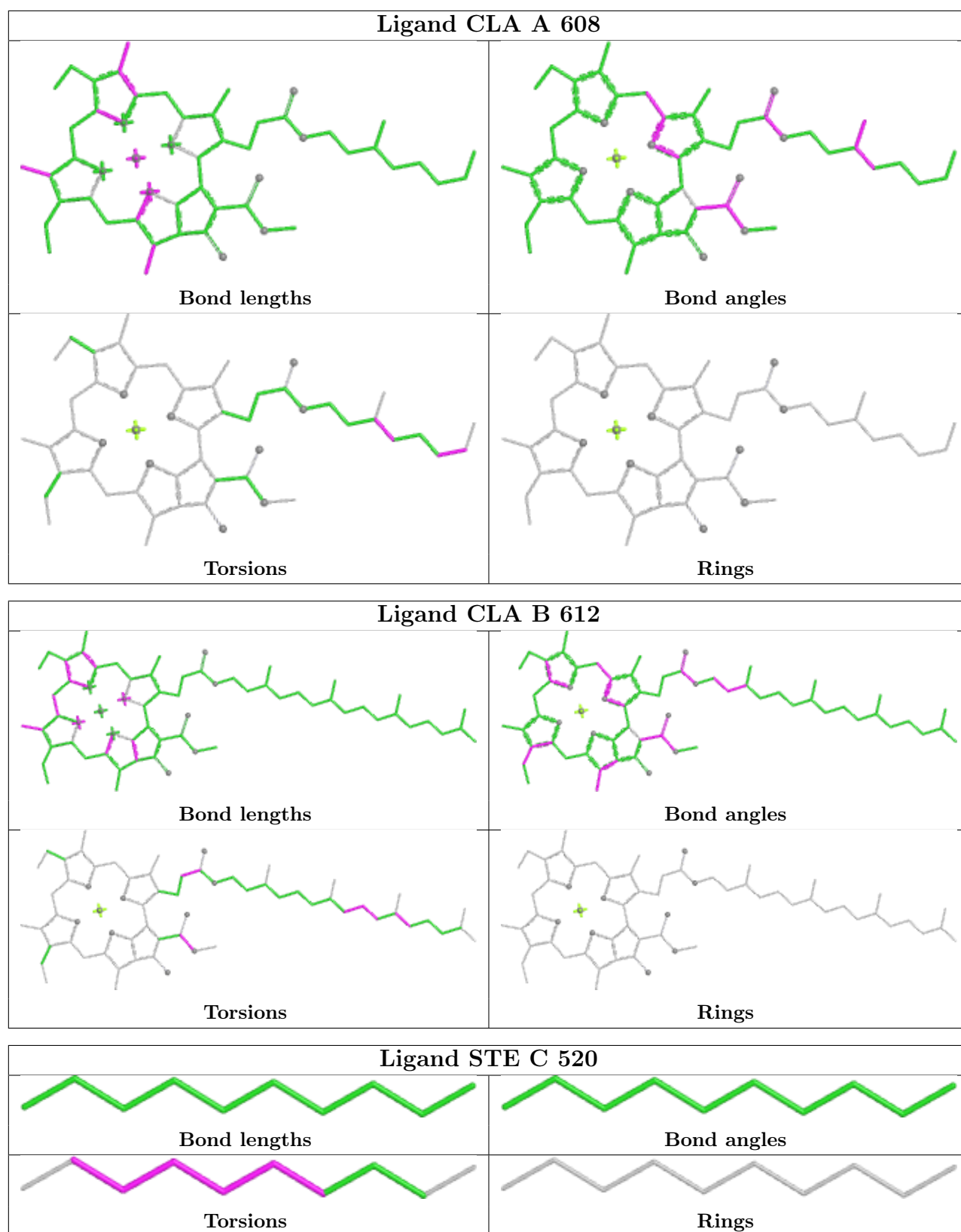


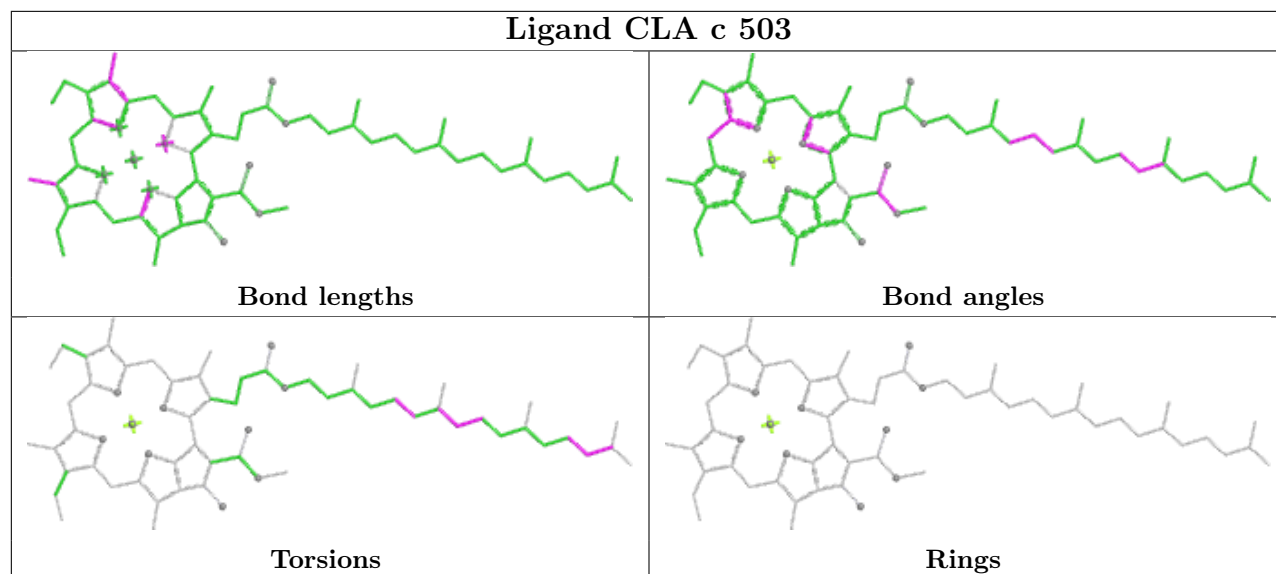
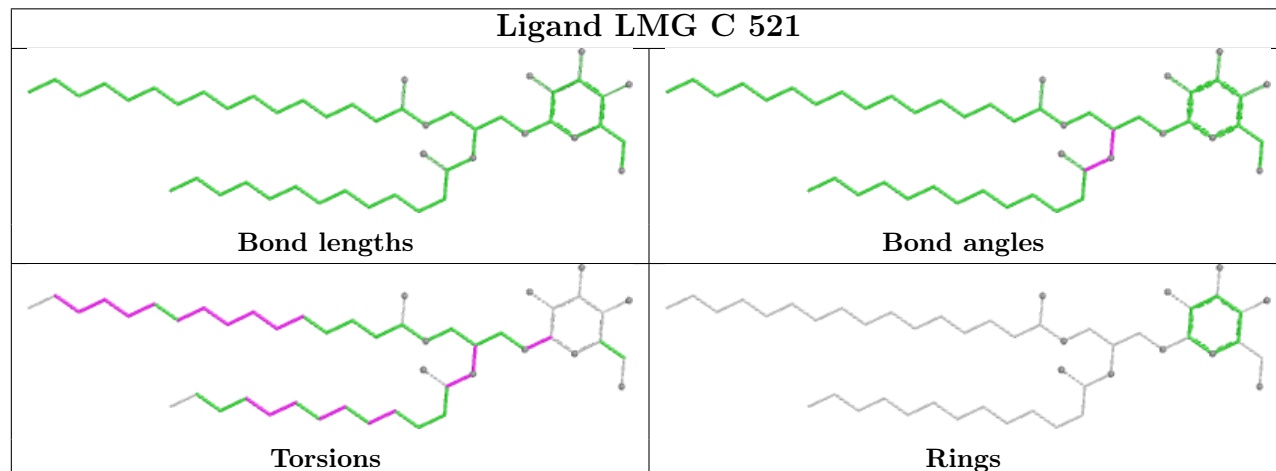
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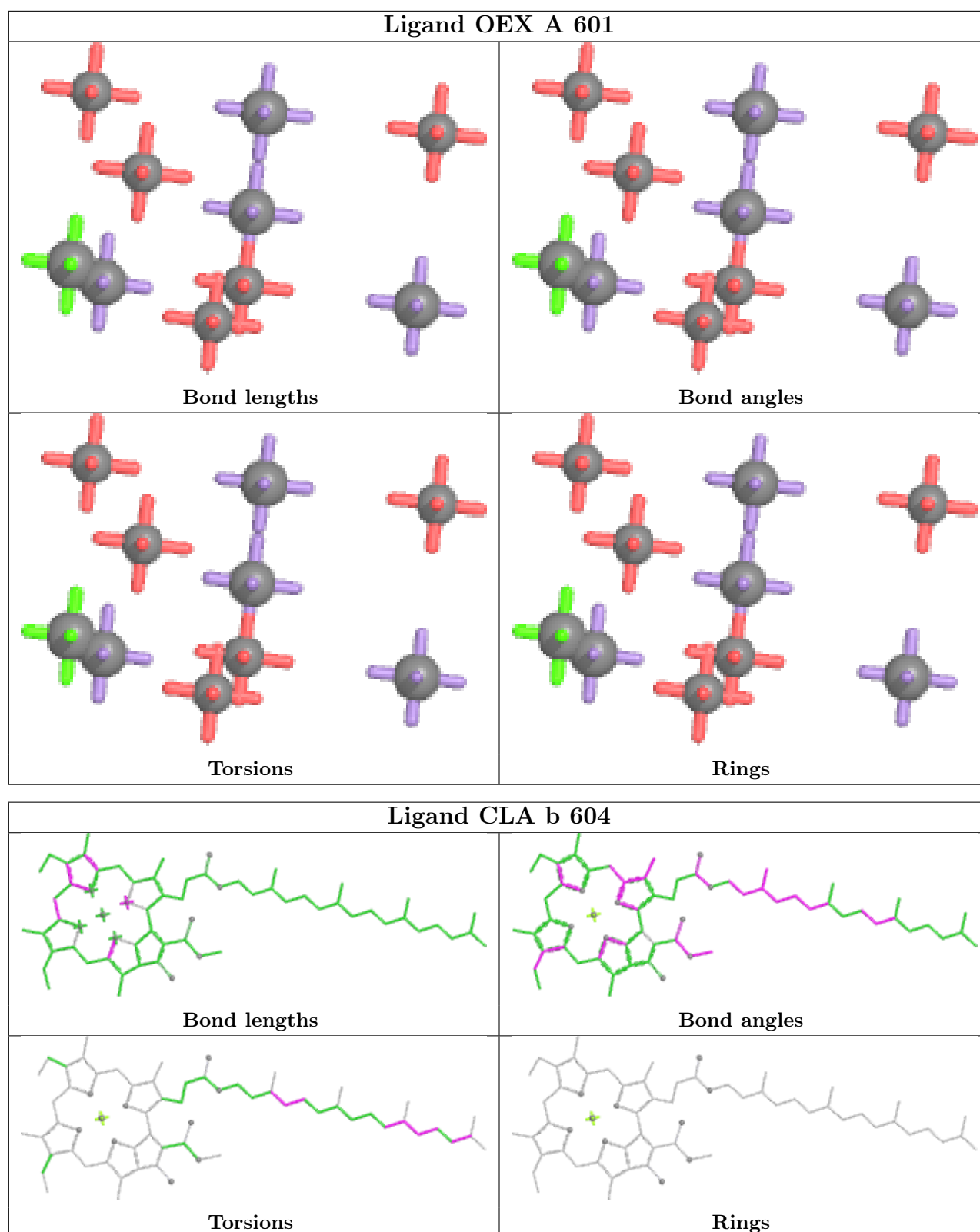


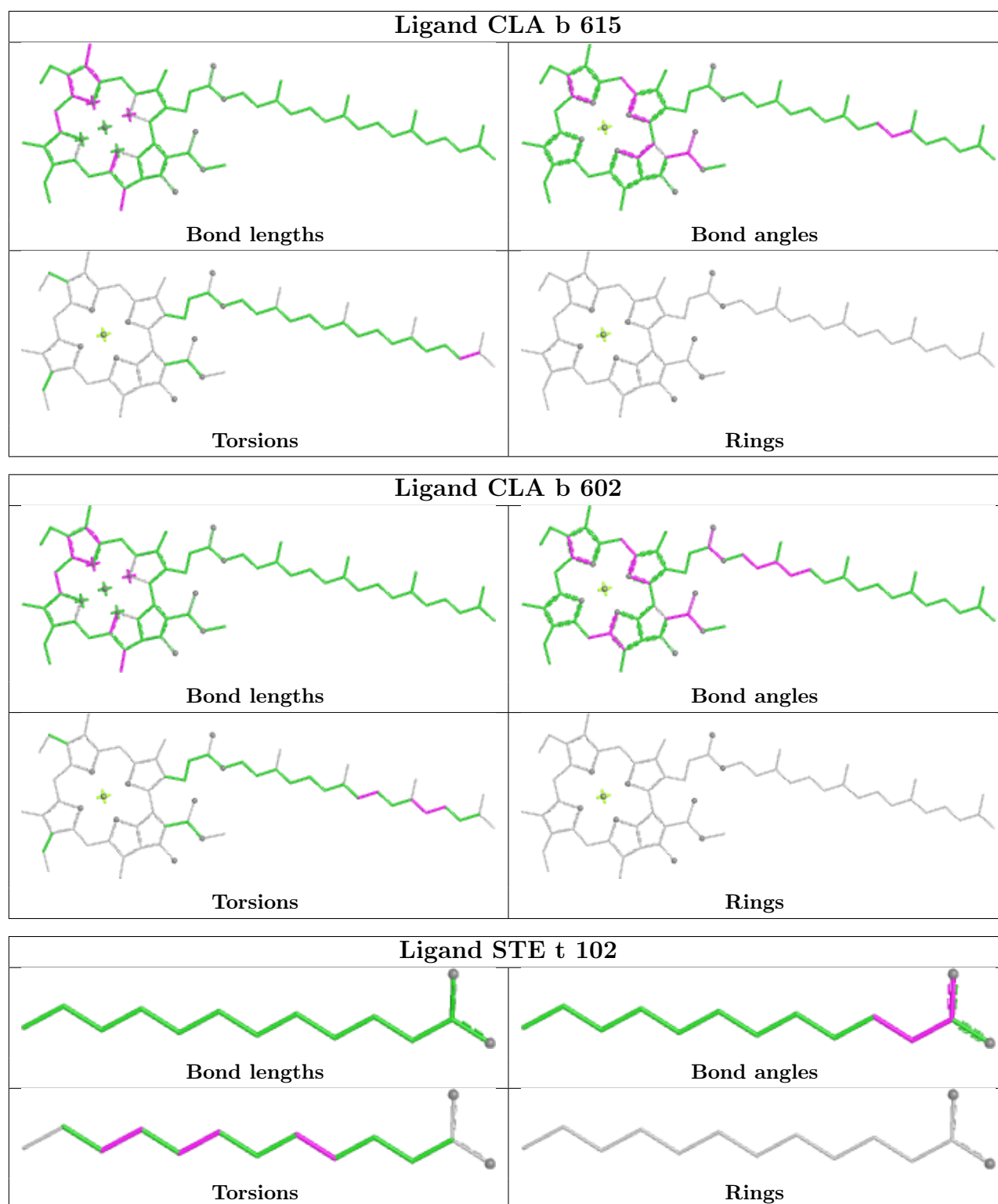
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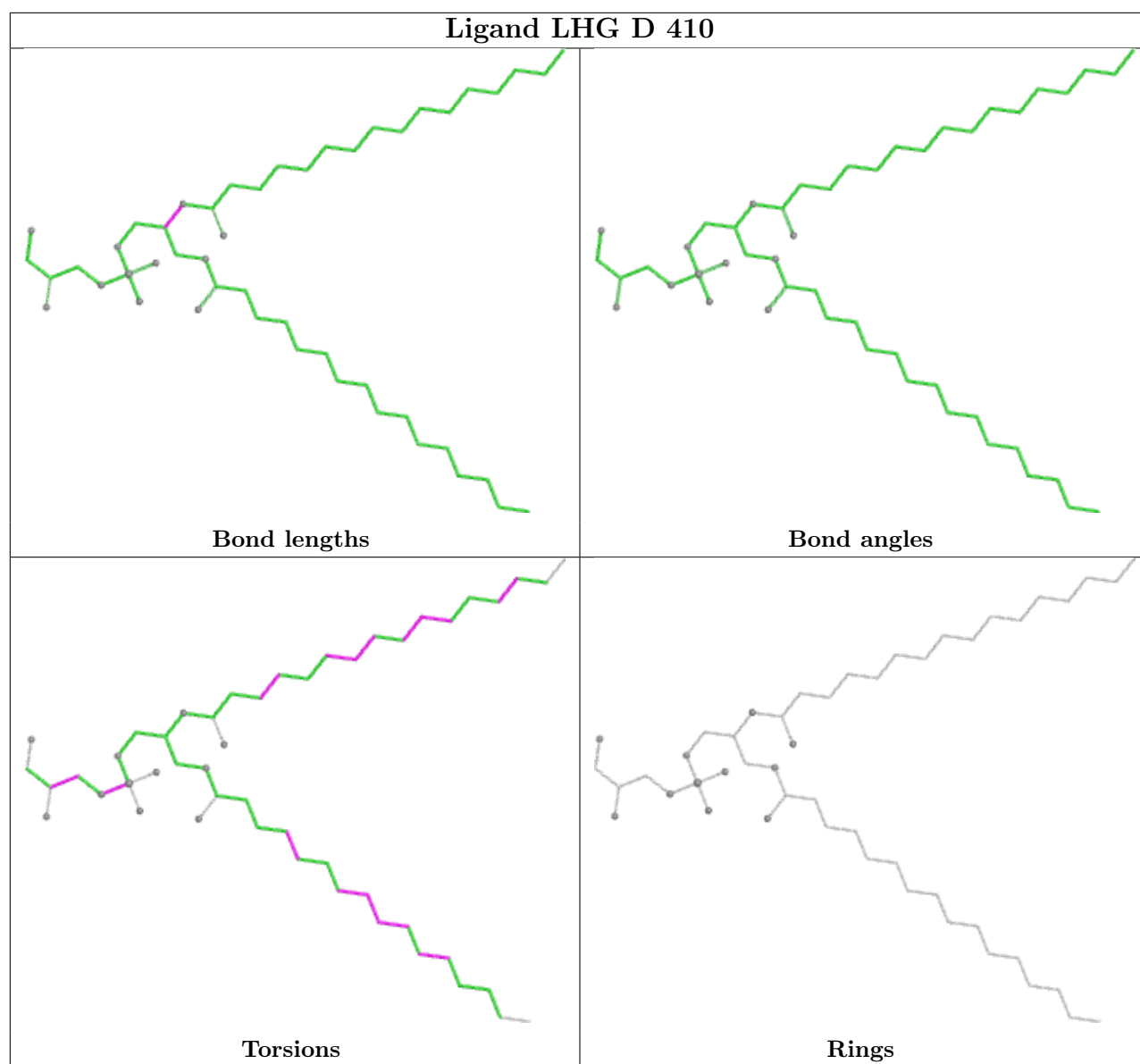


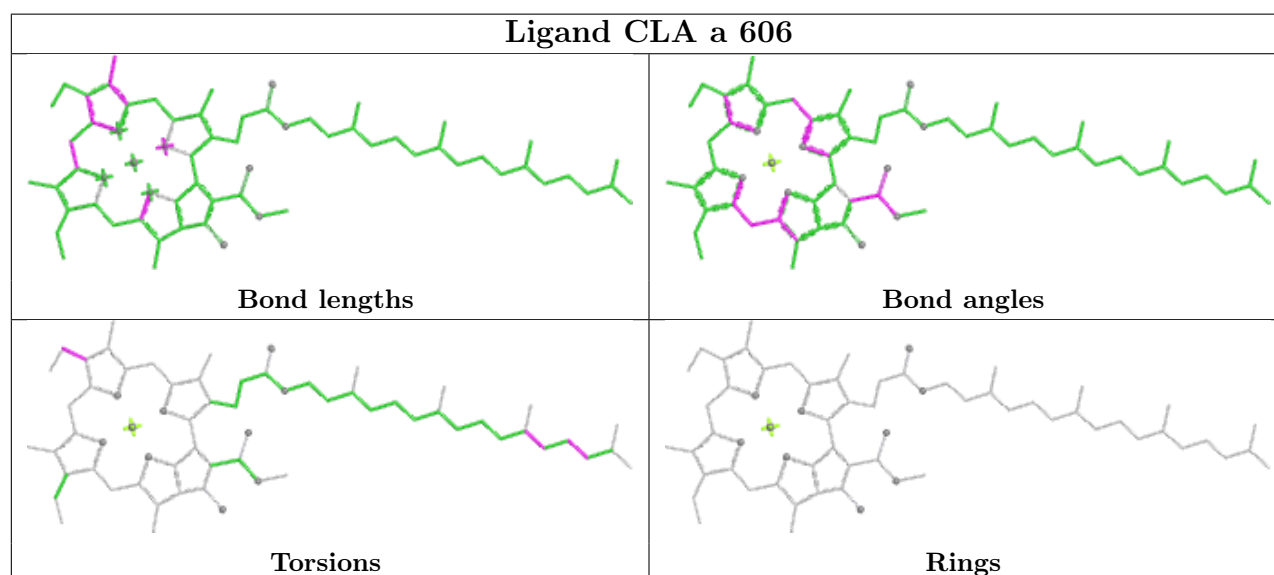
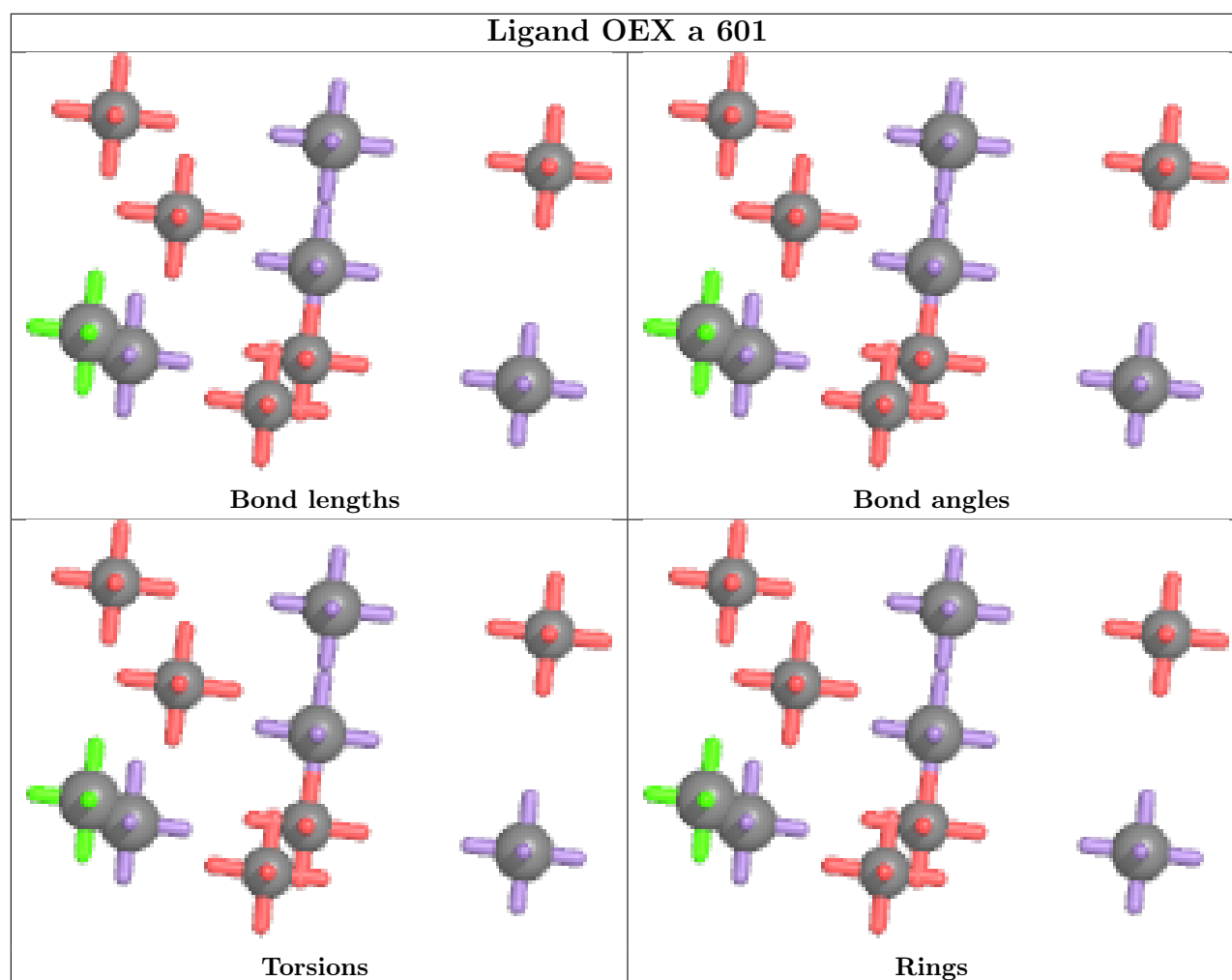


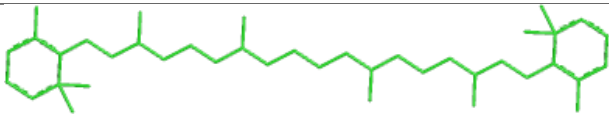
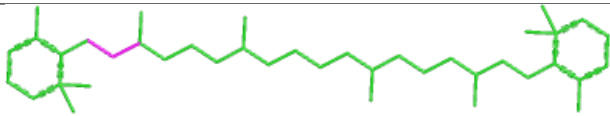
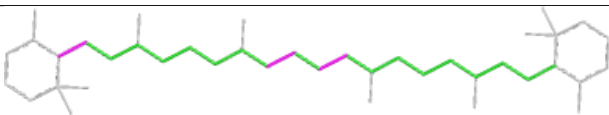
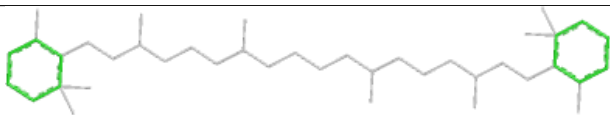
Ligand CLA c 503**Ligand LMG C 521**

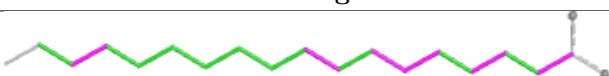
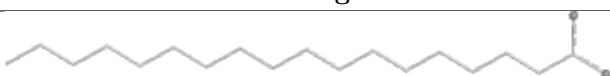


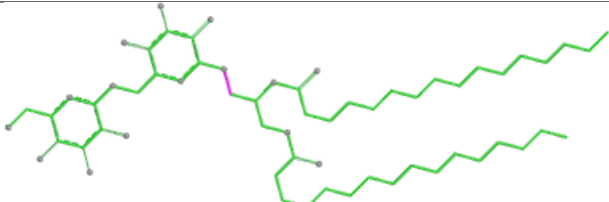
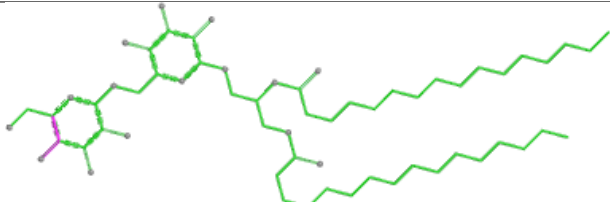
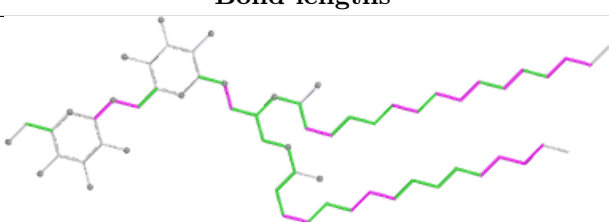
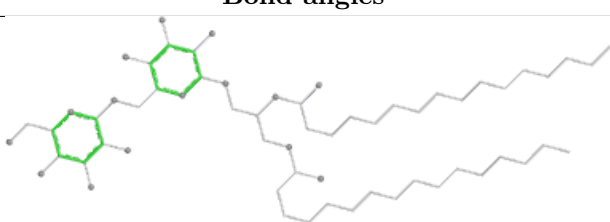


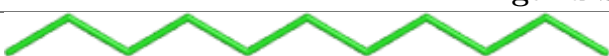
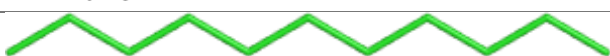
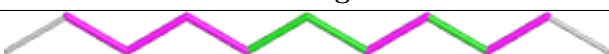


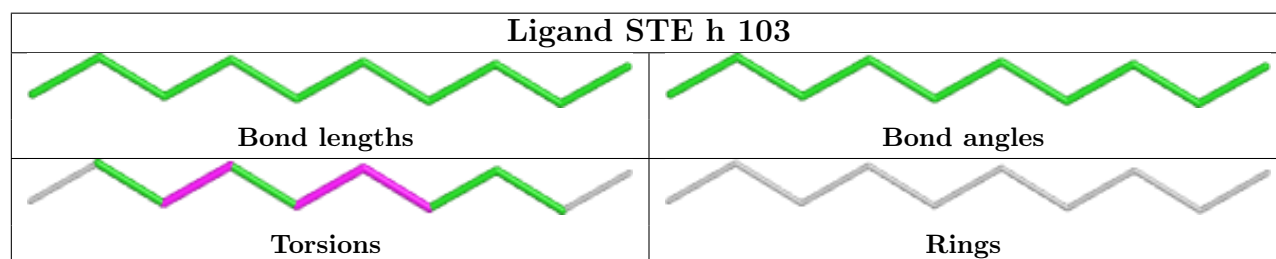
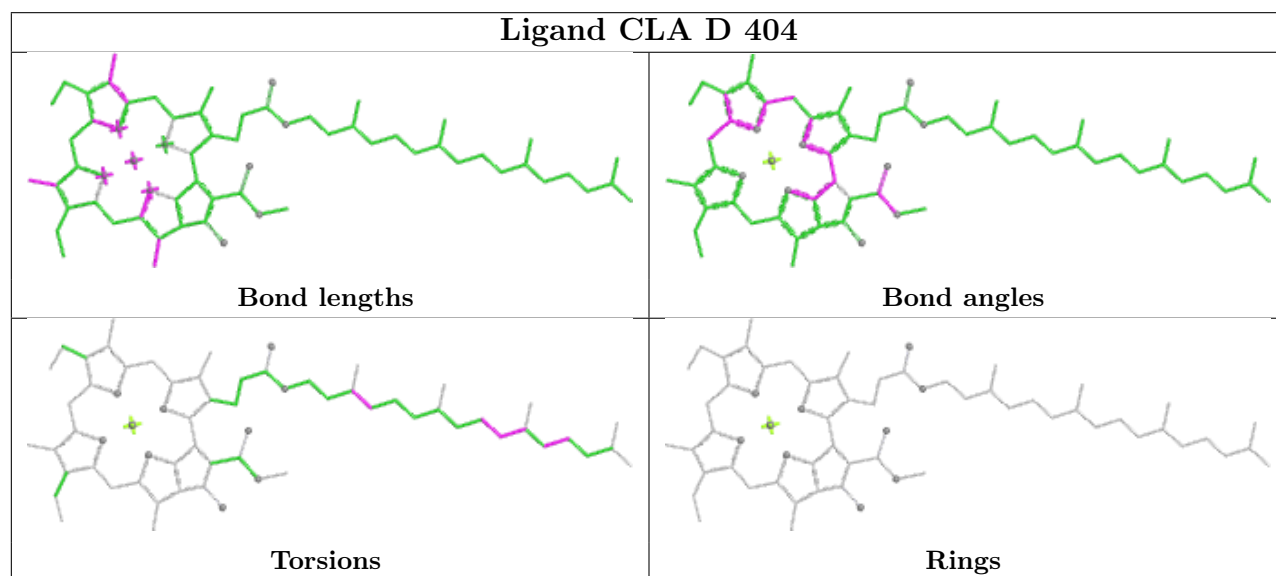
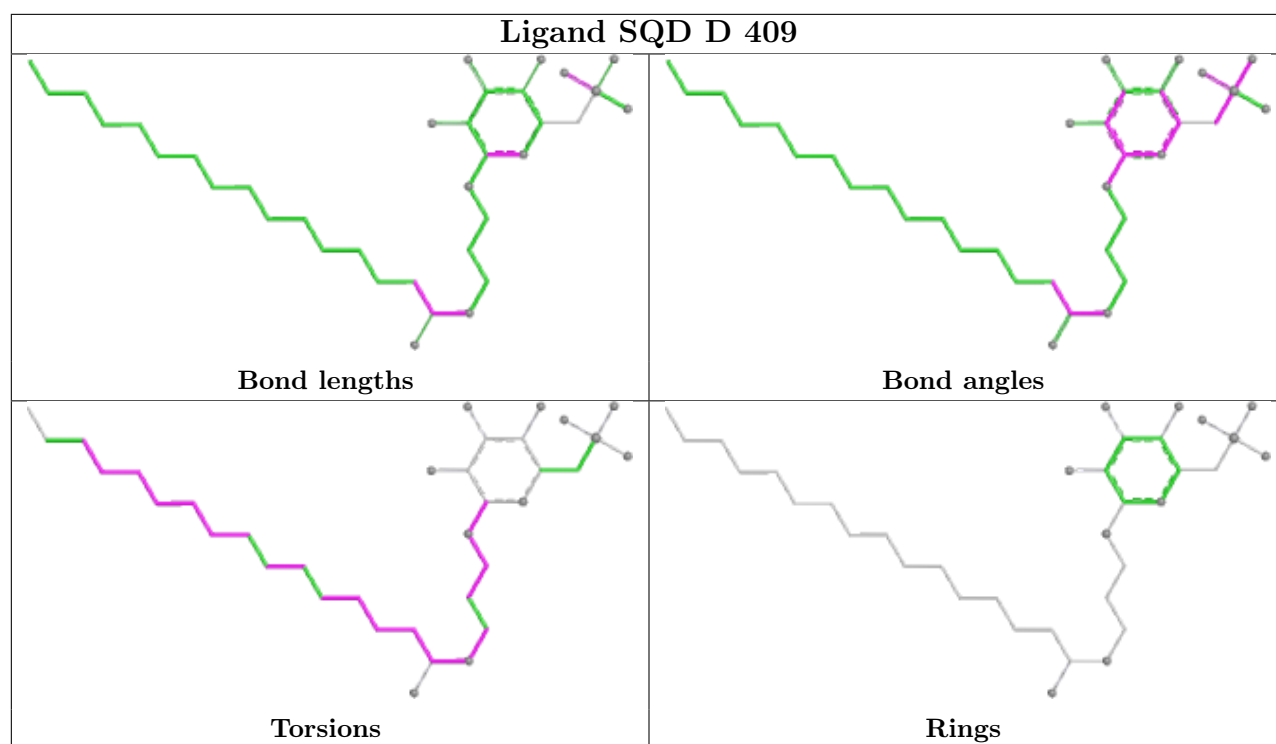


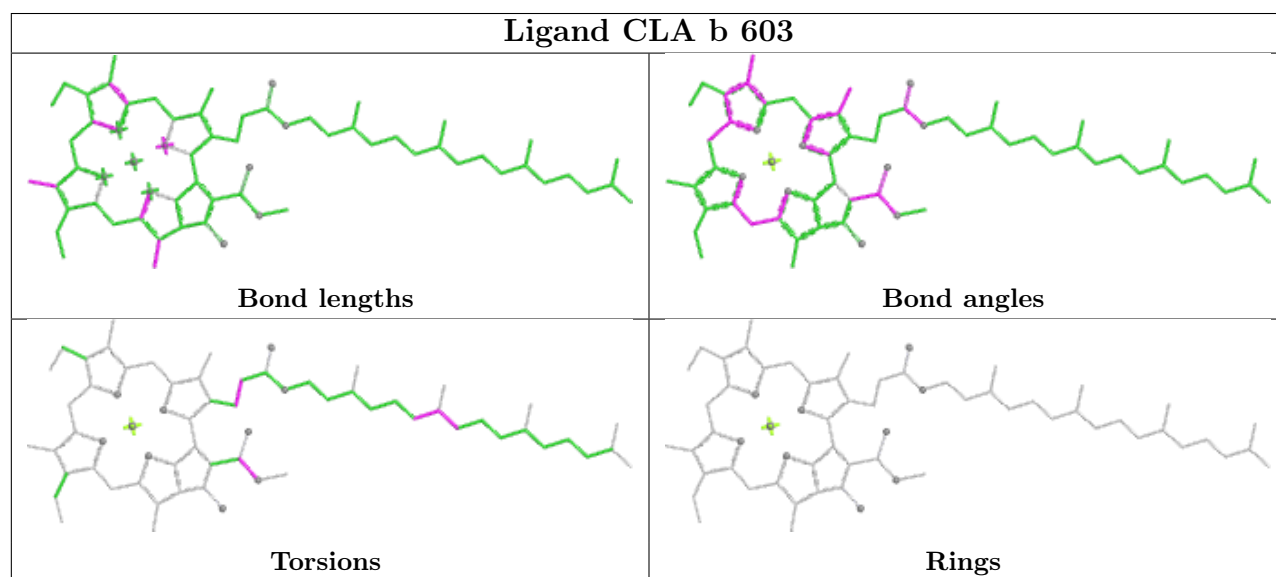
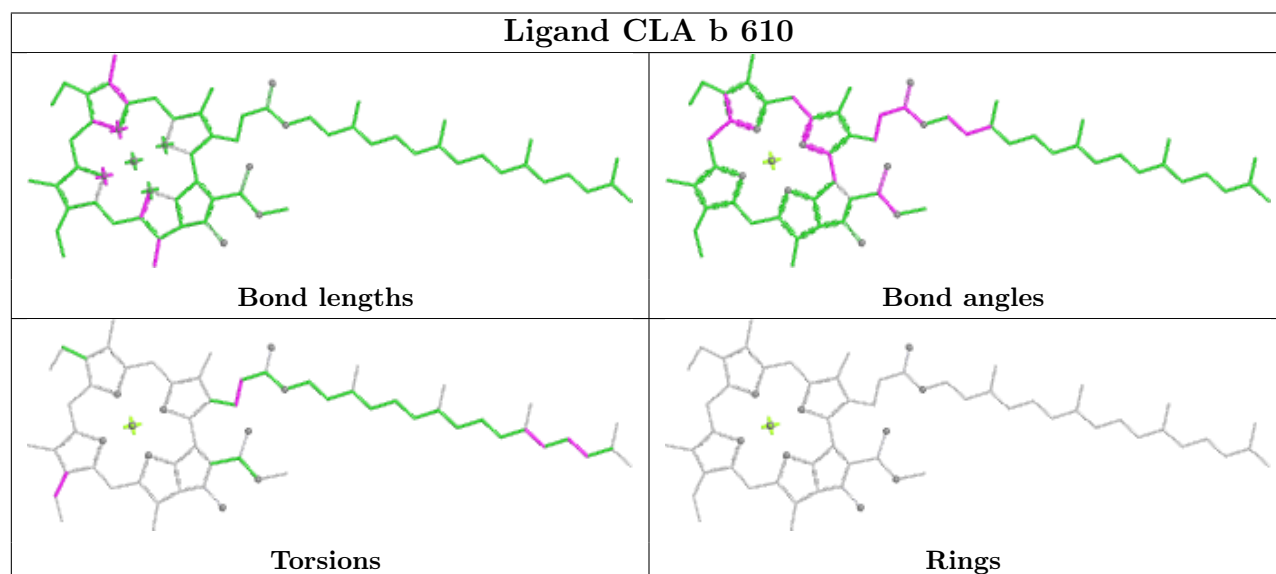
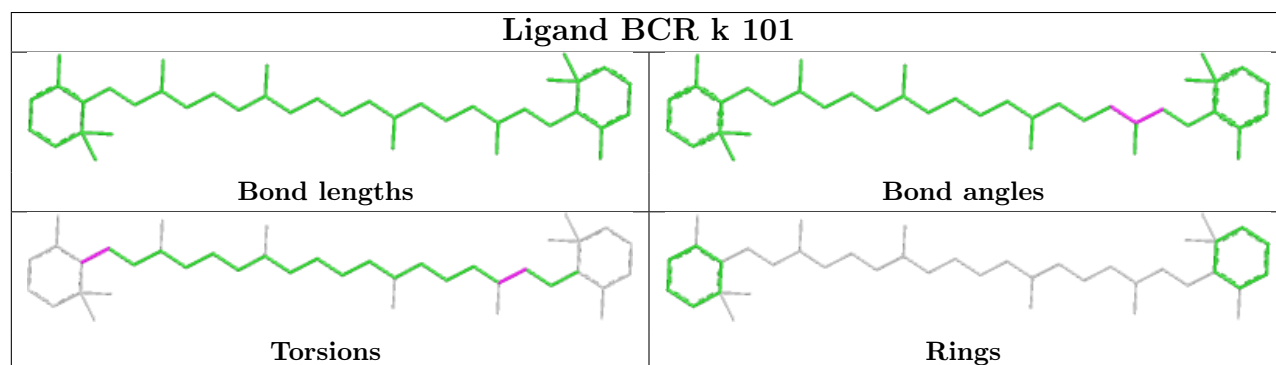
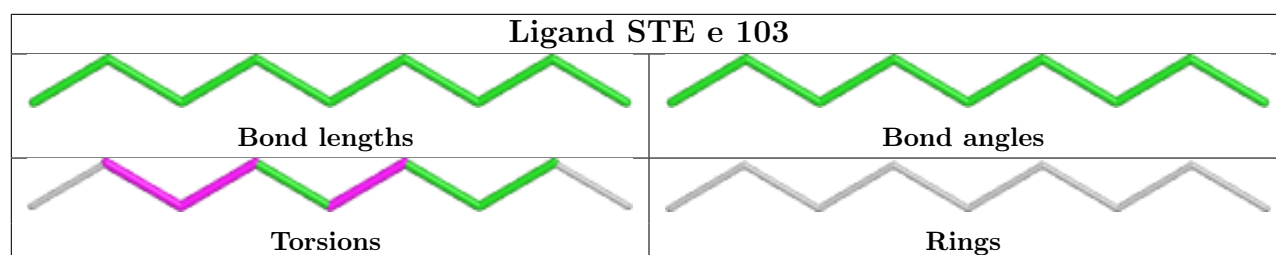
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

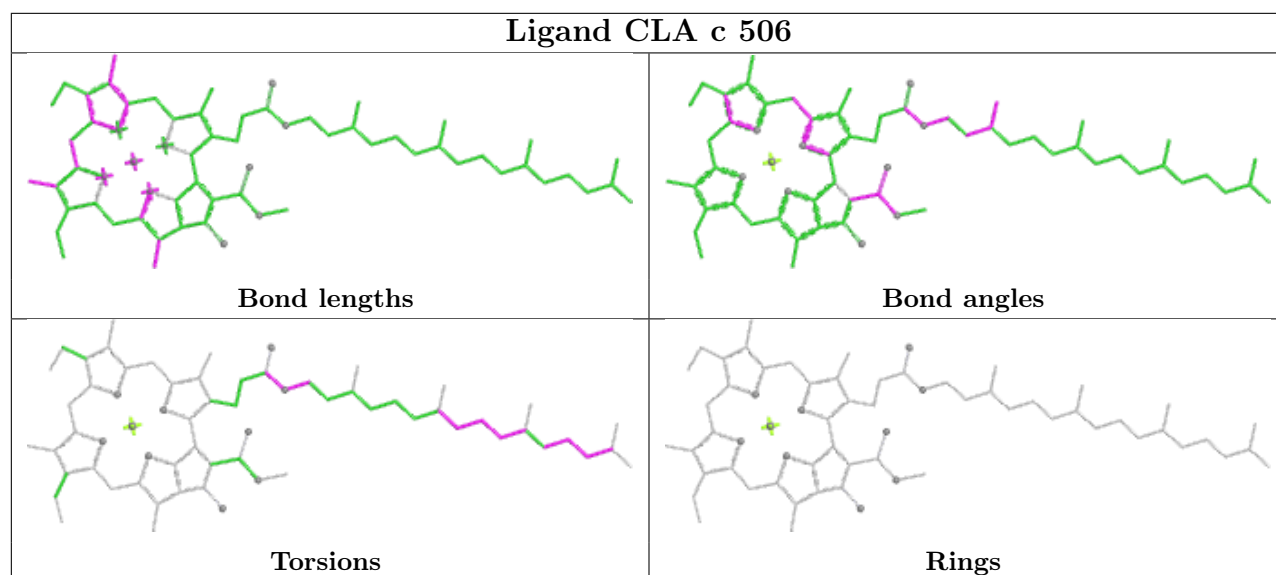
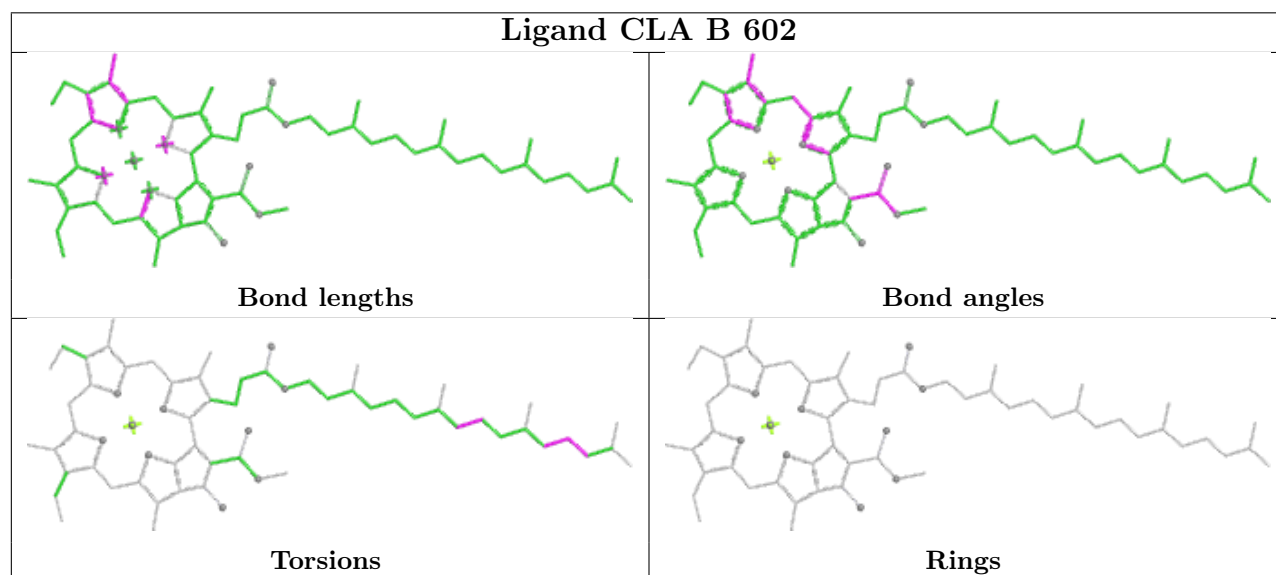
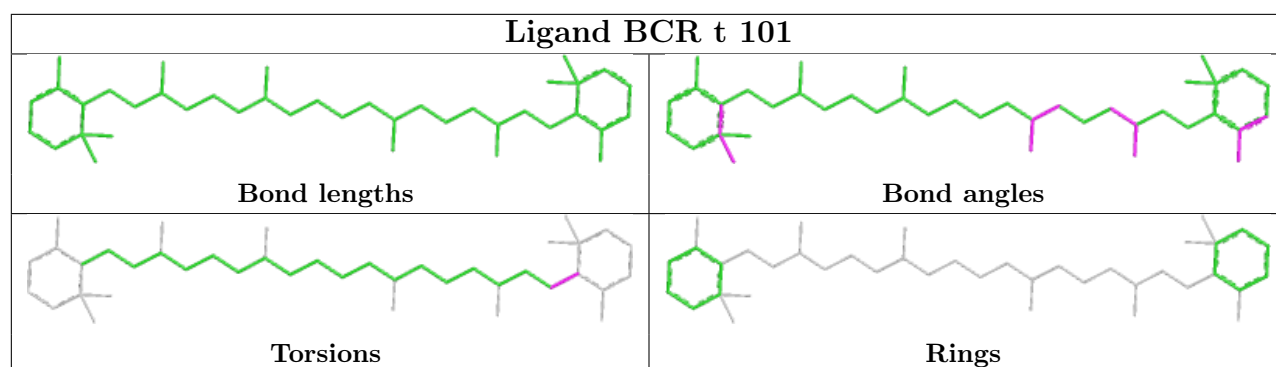
Ligand STE d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

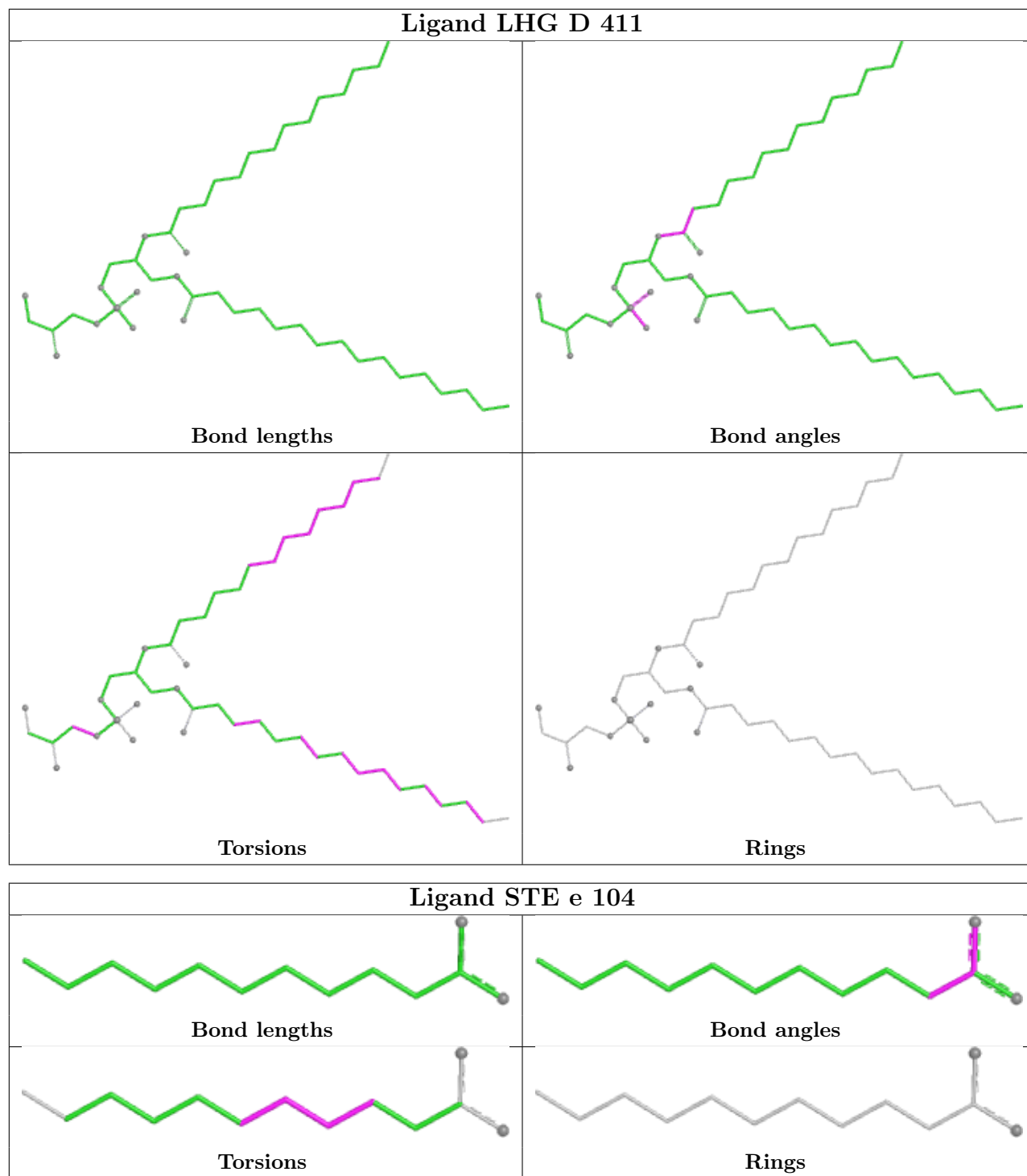
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Bond lengths	Bond angles
	
Torsions	Rings

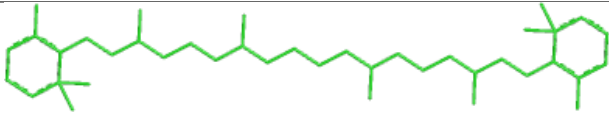
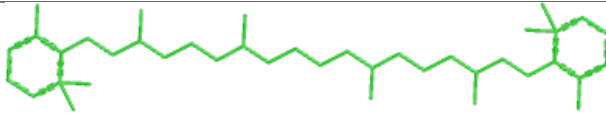
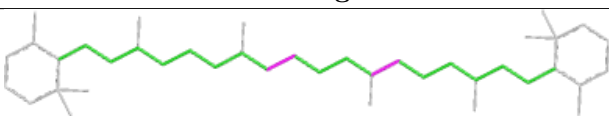
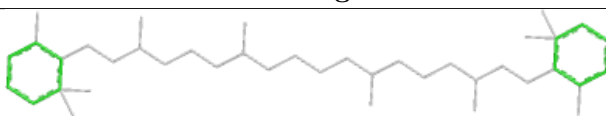
Ligand STE A 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



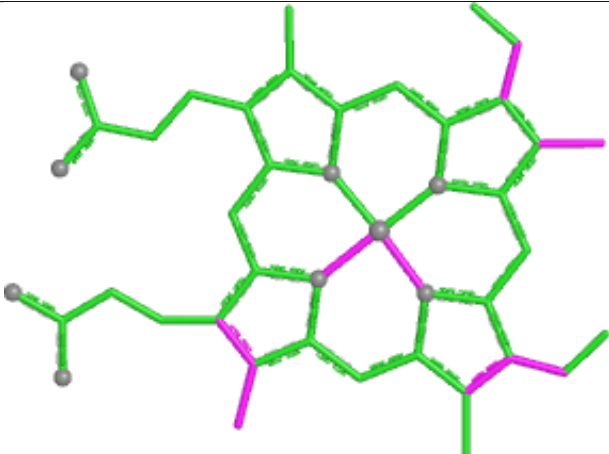
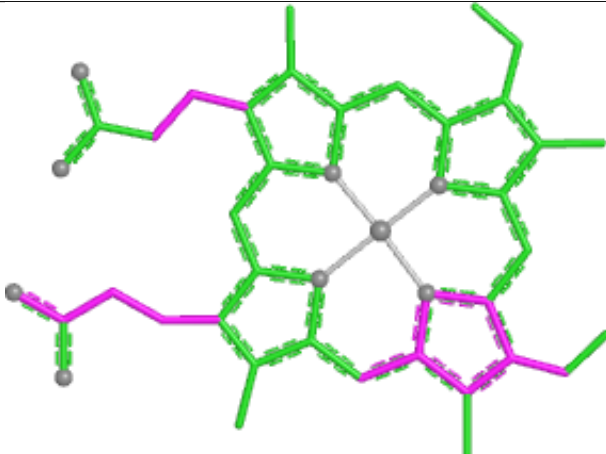
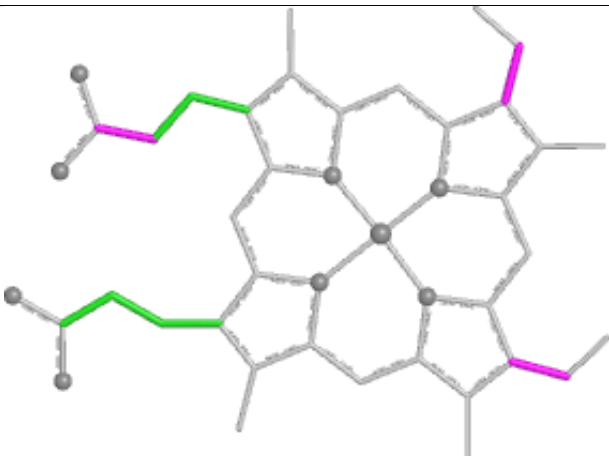
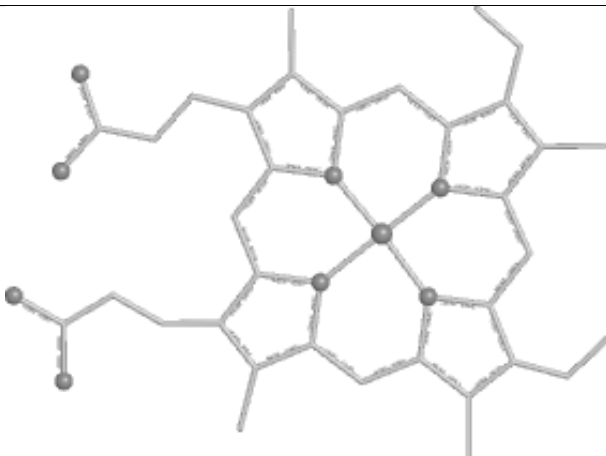


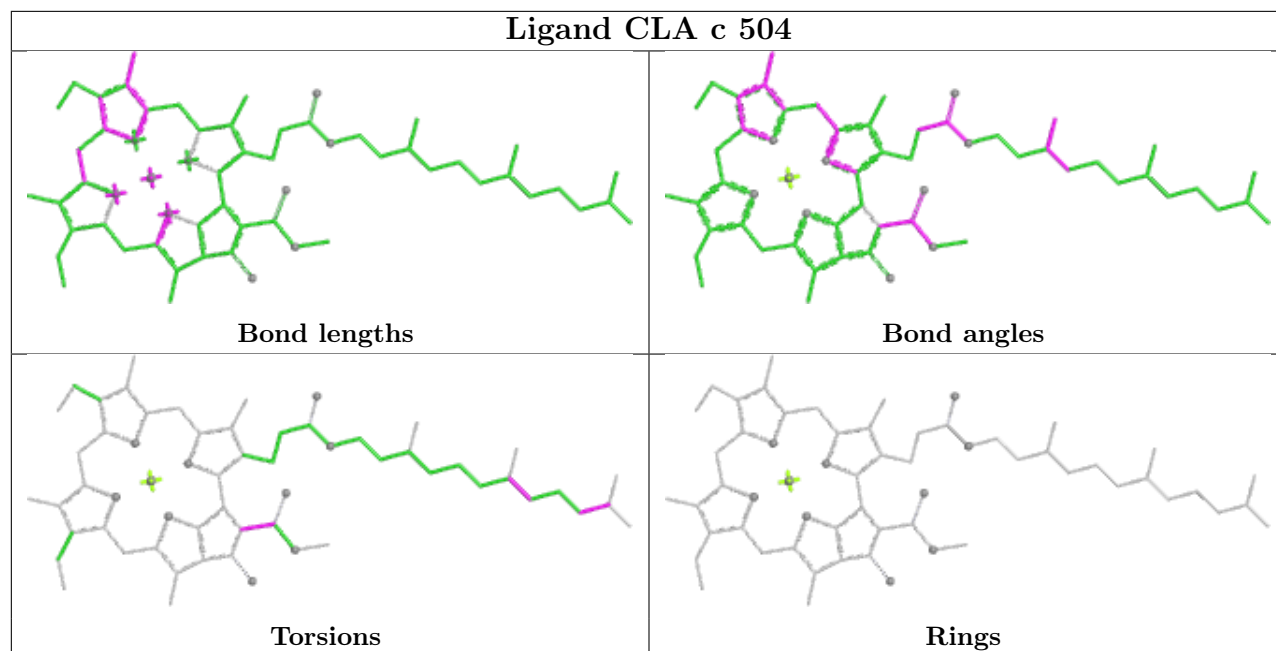
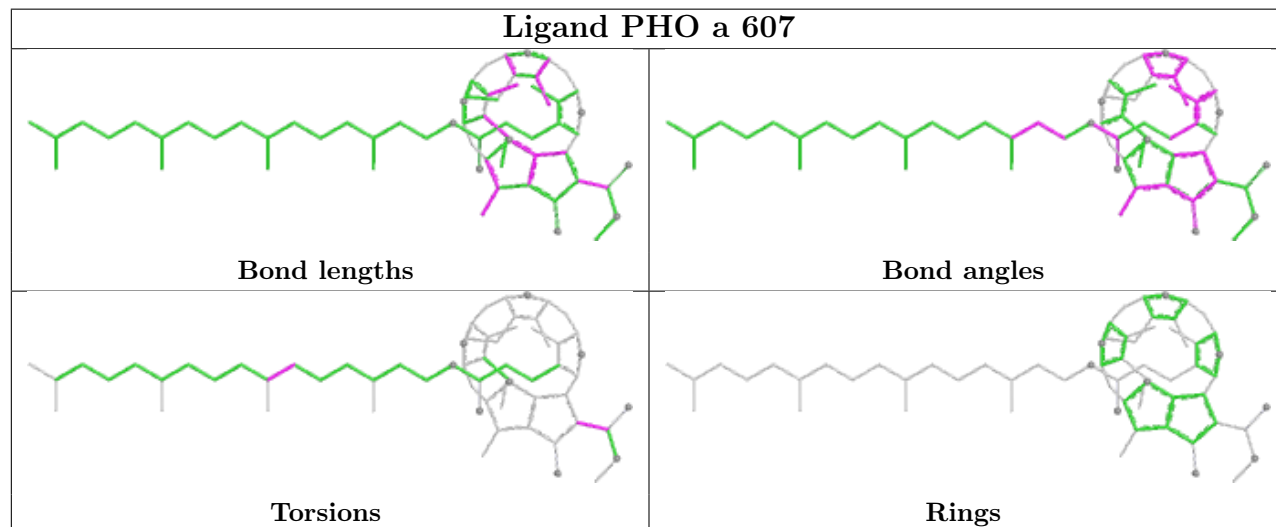


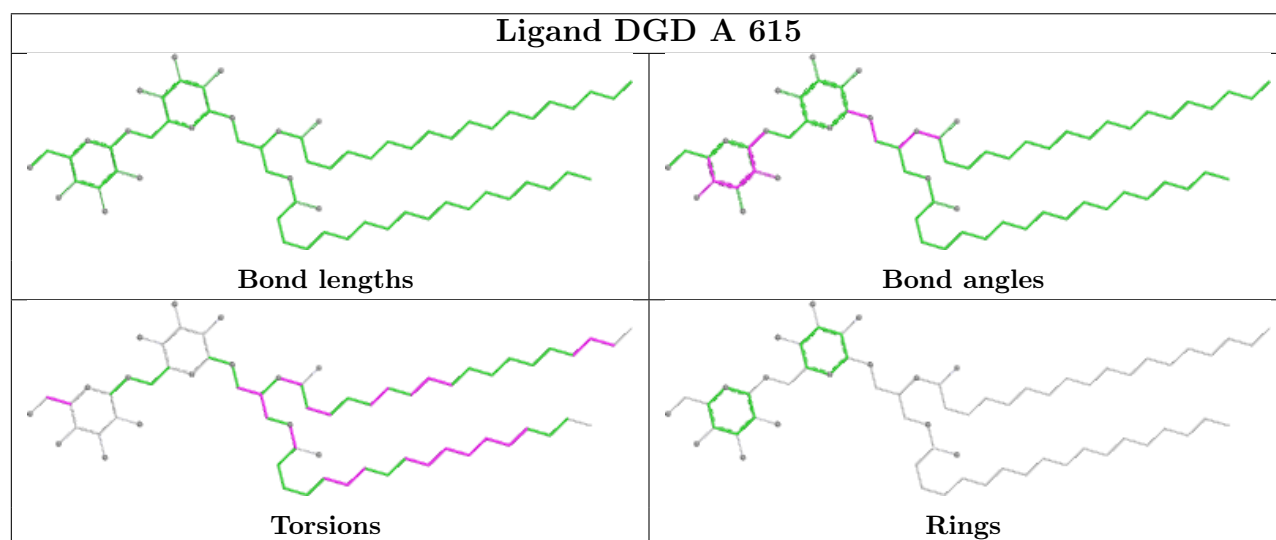
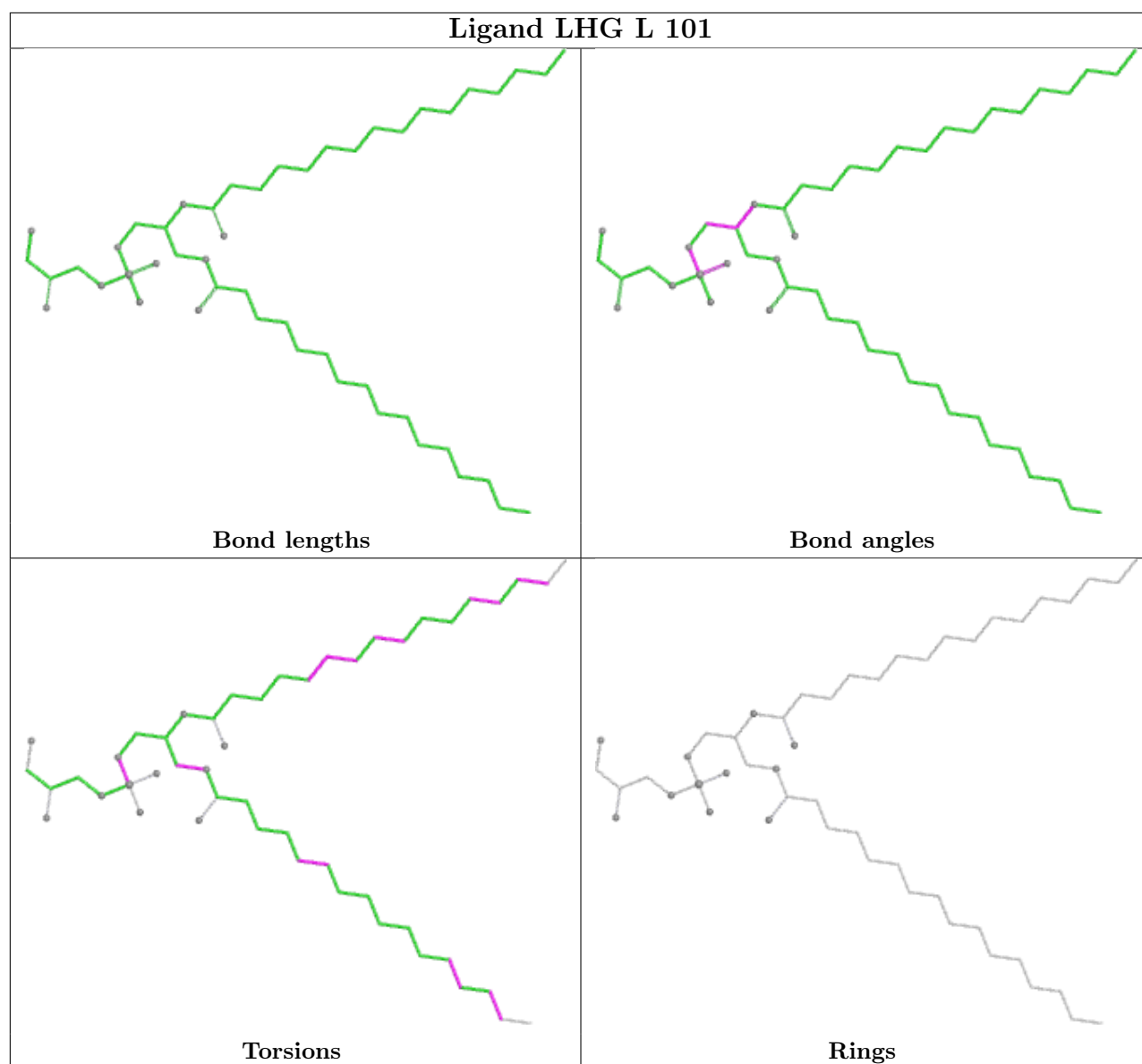


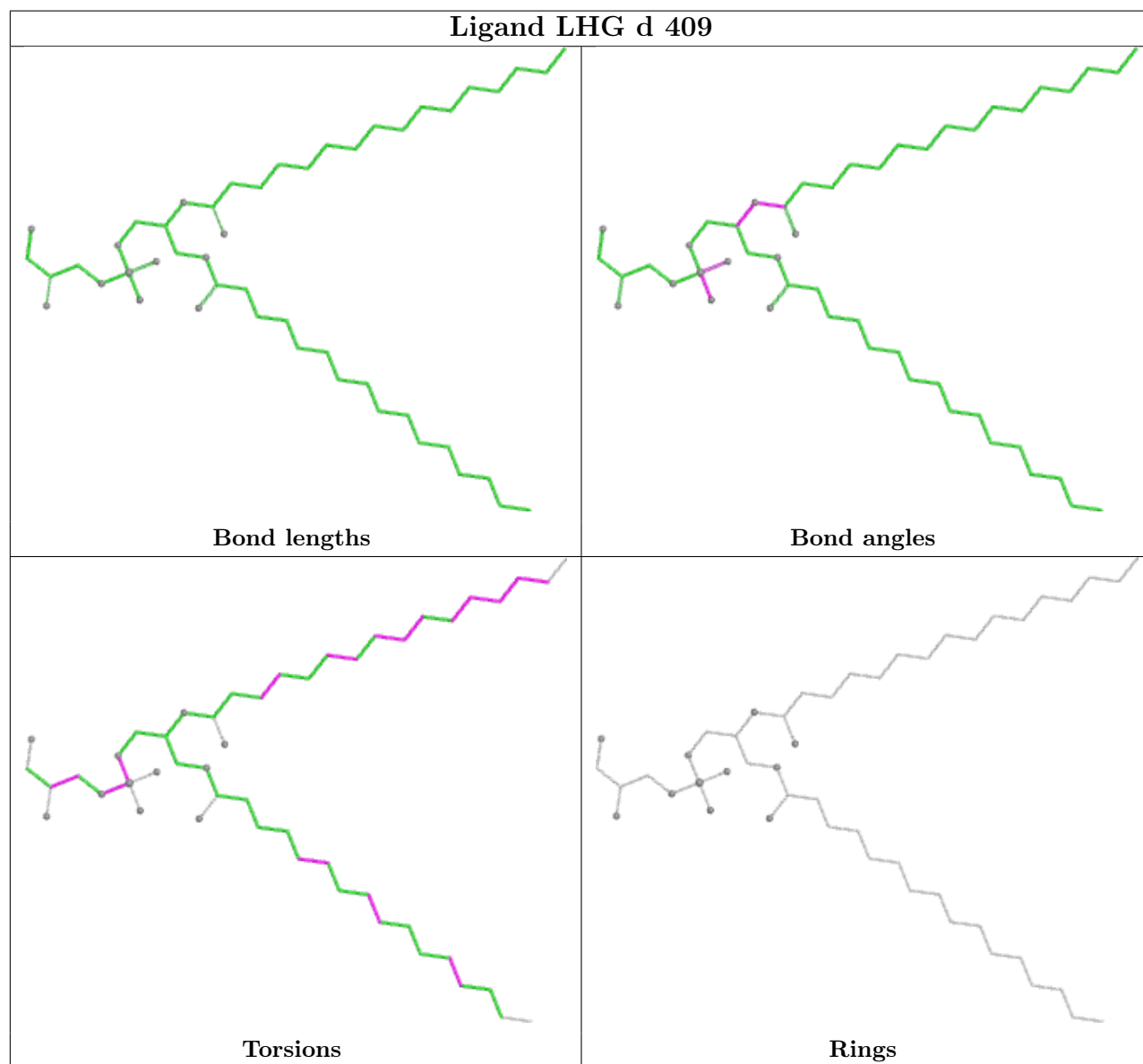
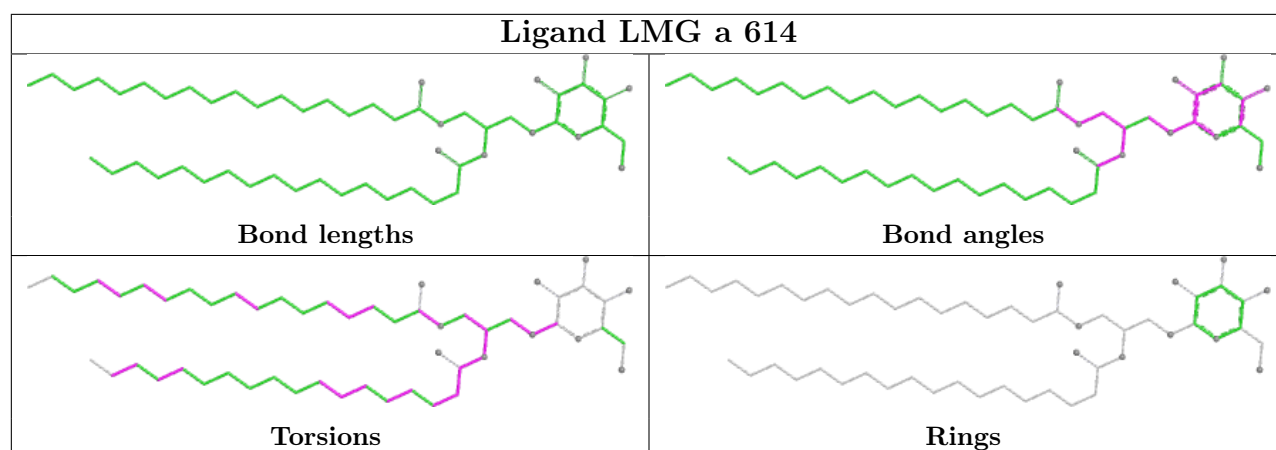
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE E 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

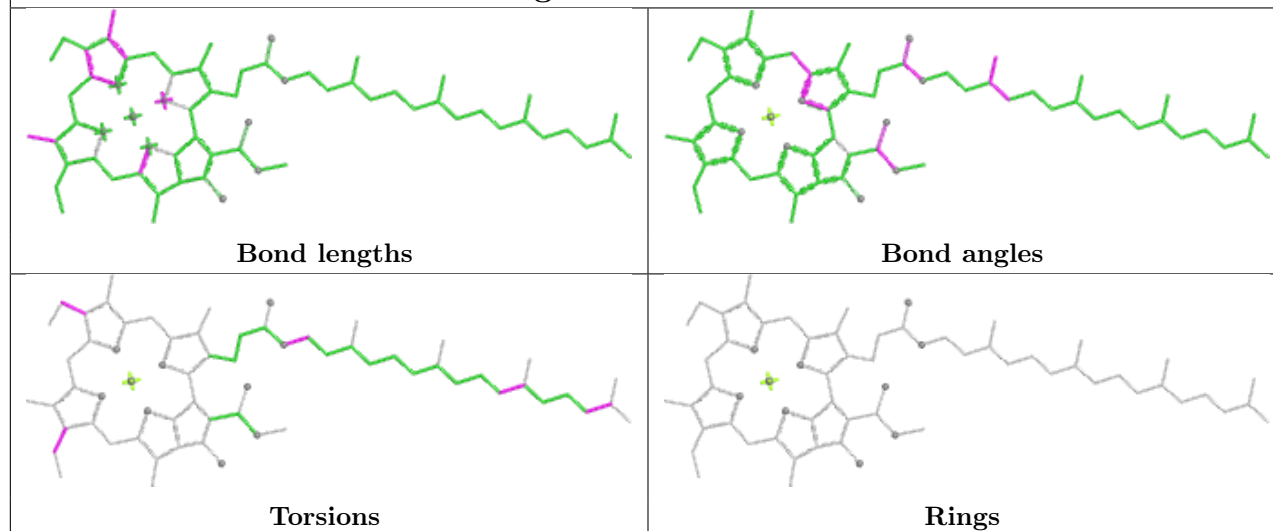
Ligand HEM f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 504**Ligand PHO a 607**

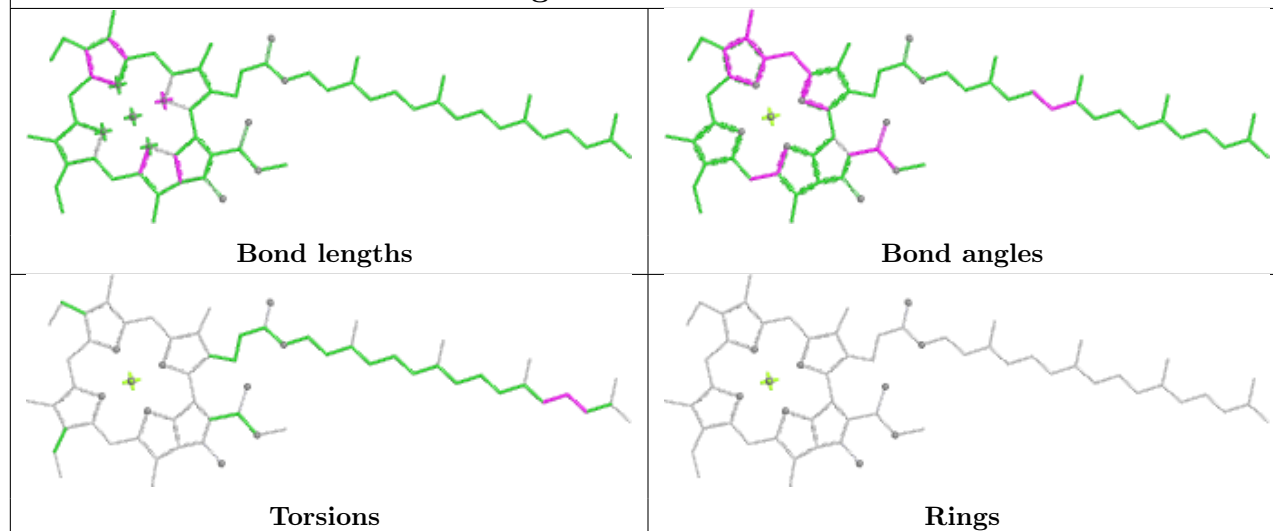




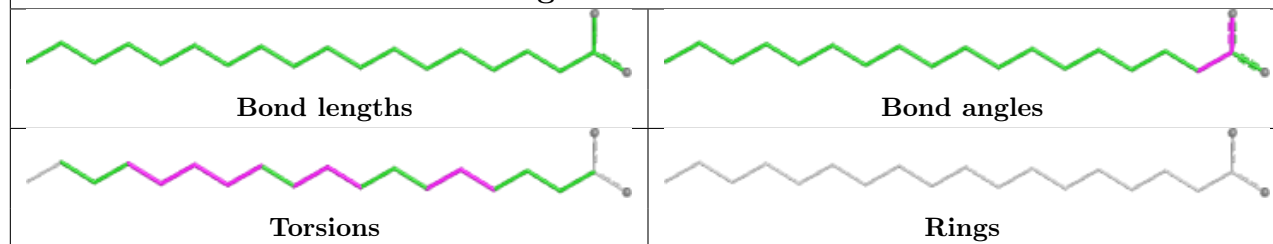
Ligand CLA d 403

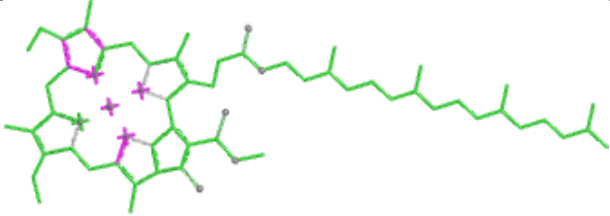
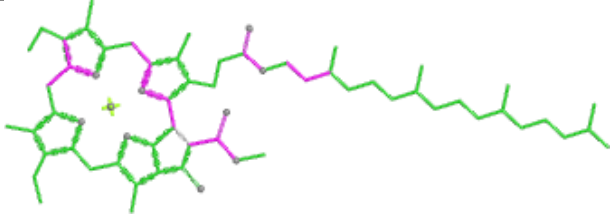
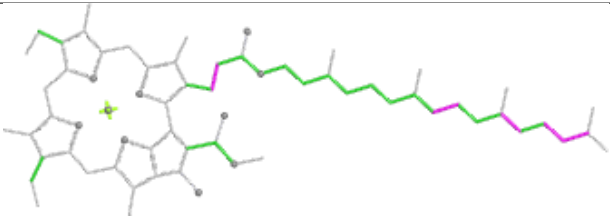
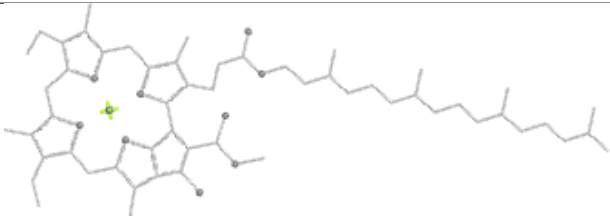
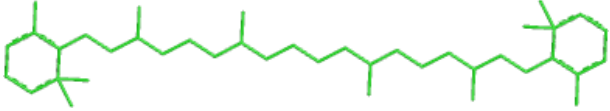
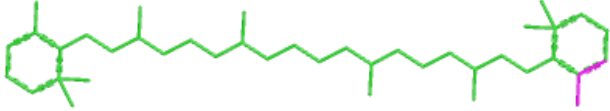
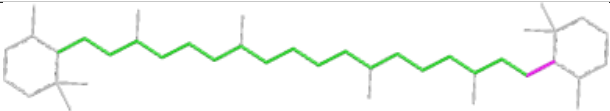
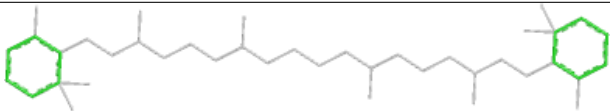
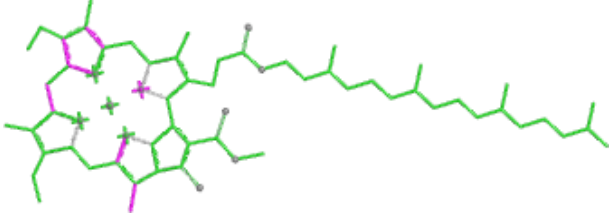
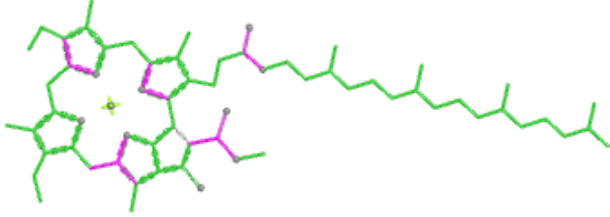
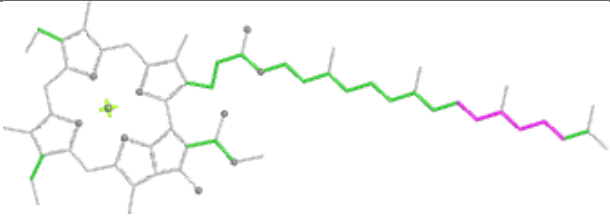
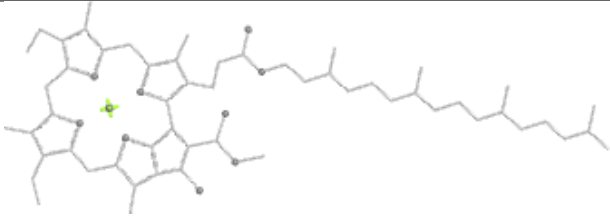


Ligand CLA B 608

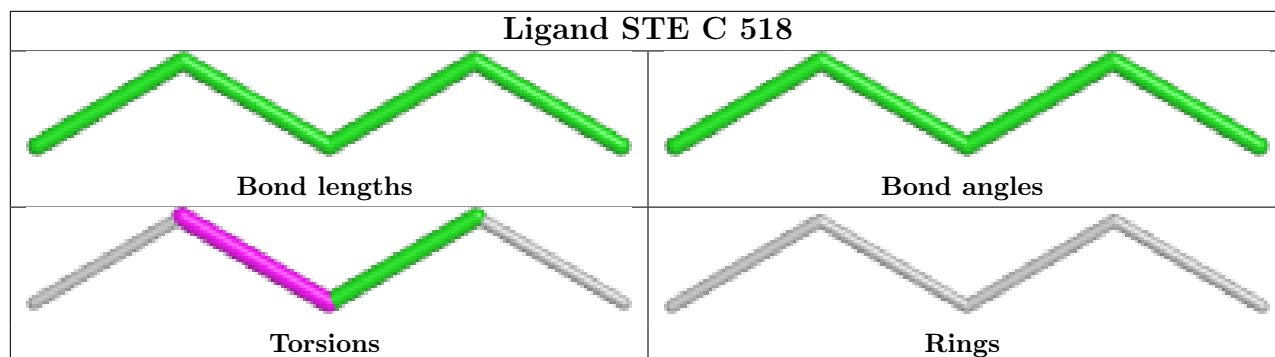


Ligand STE b 621

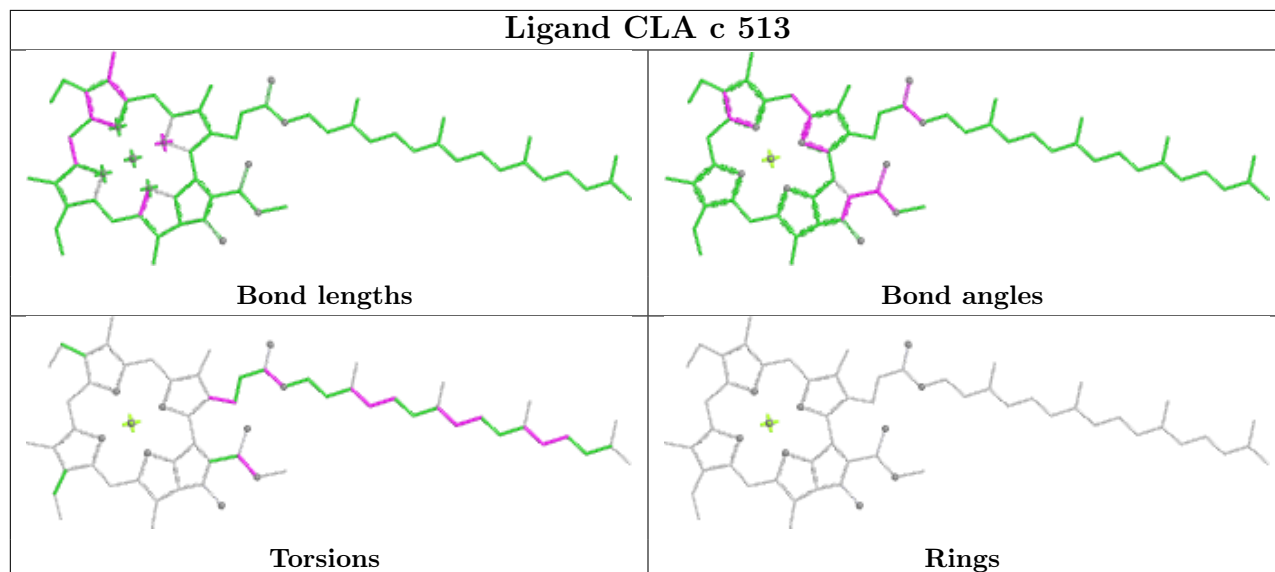


Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

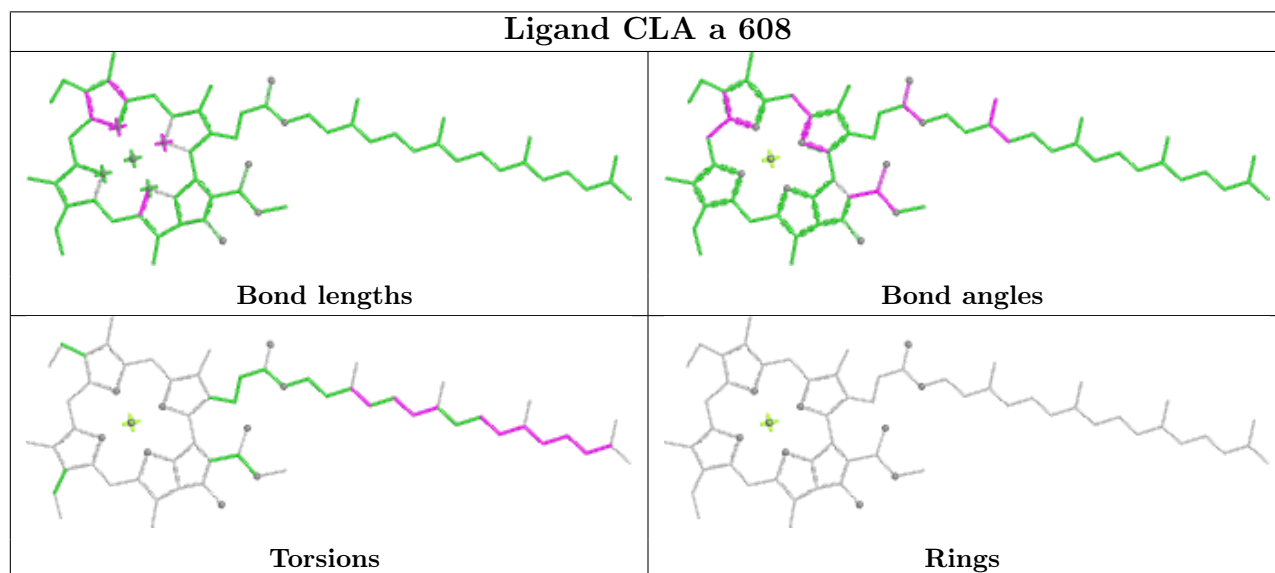
Ligand STE C 518

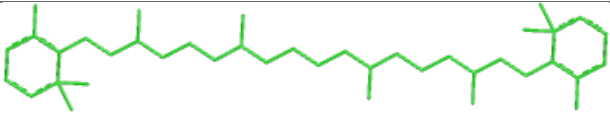
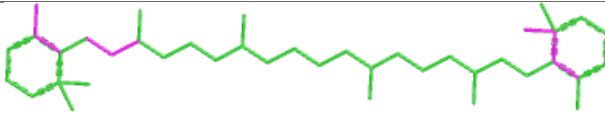
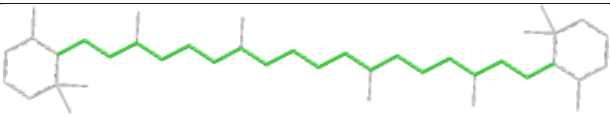
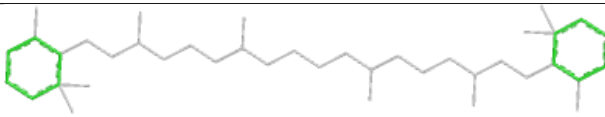
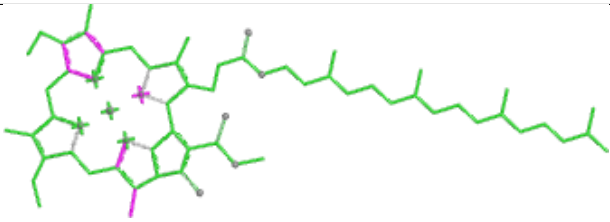
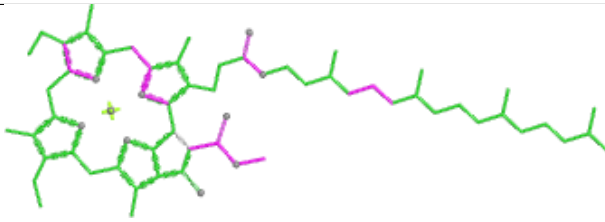
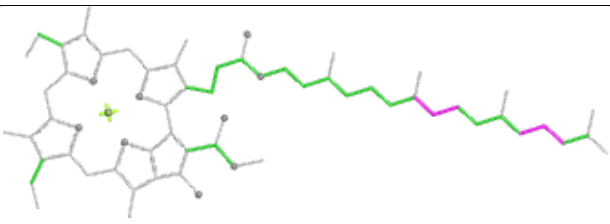
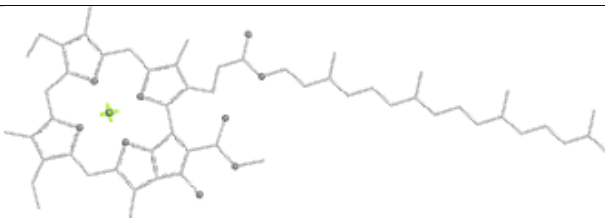
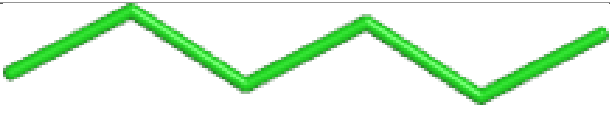
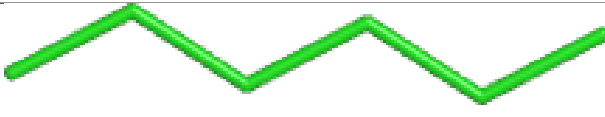


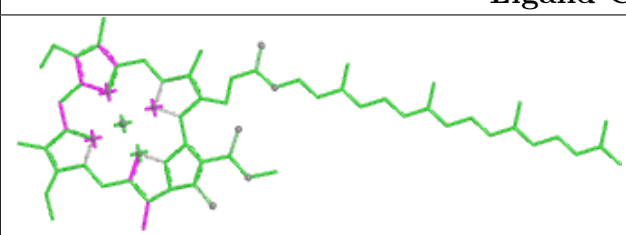
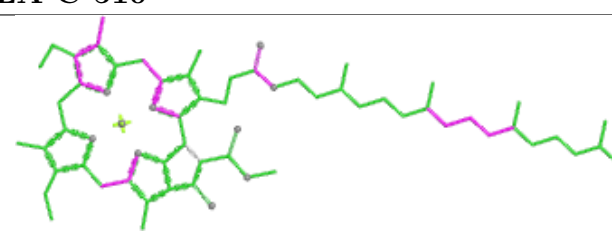
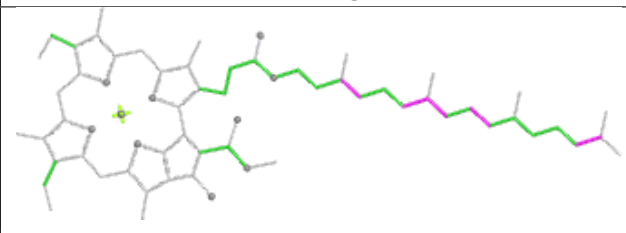
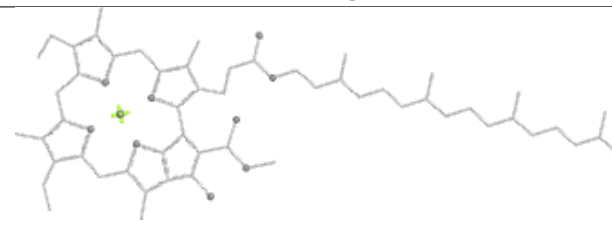
Ligand CLA c 513

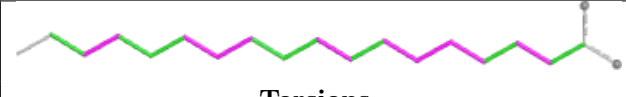
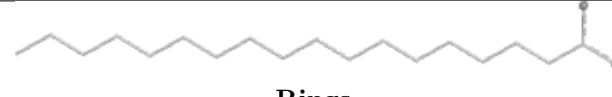


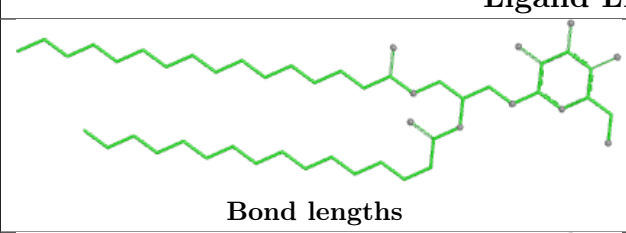
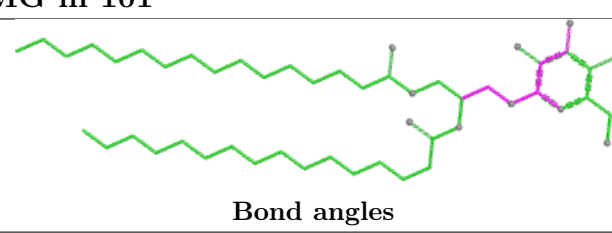
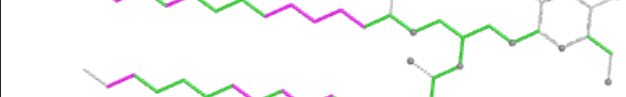
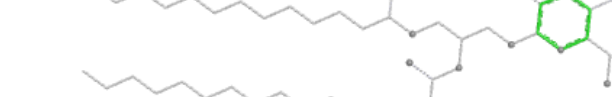
Ligand CLA a 608

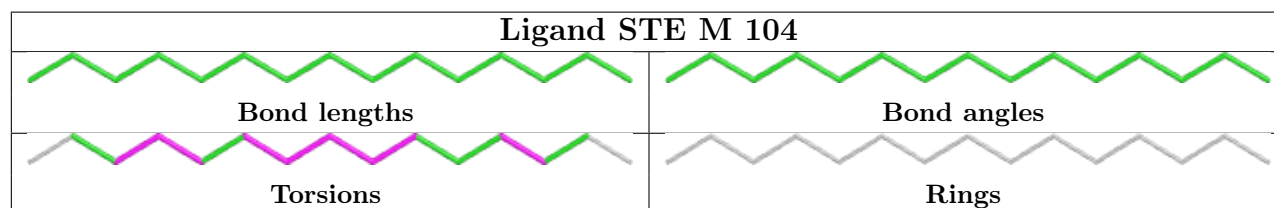
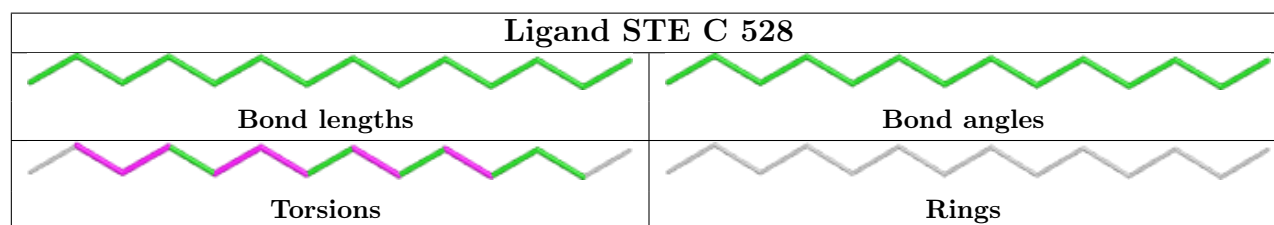
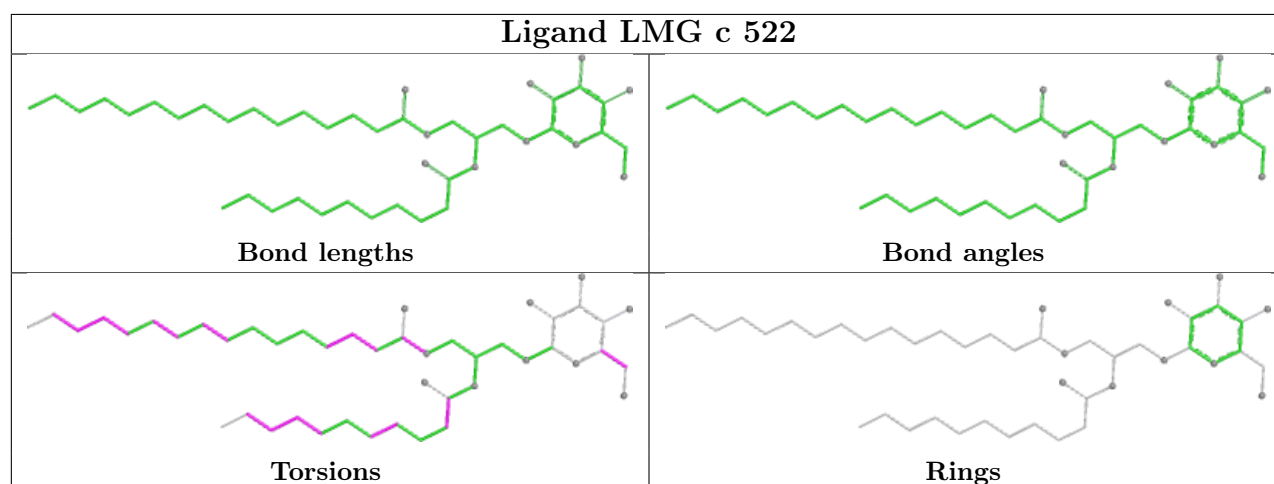
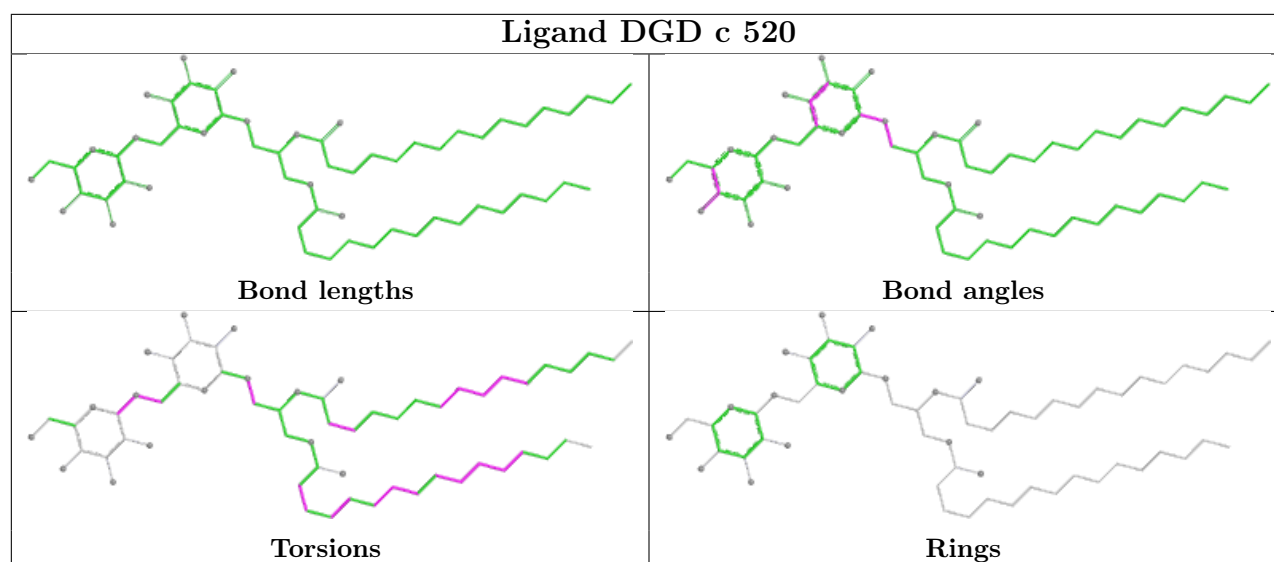


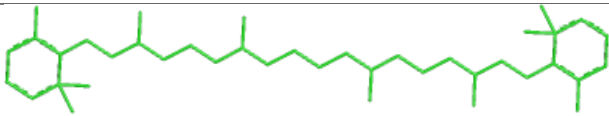
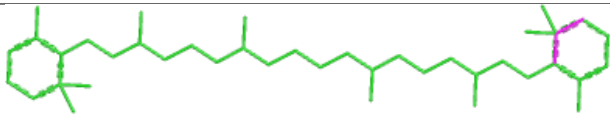
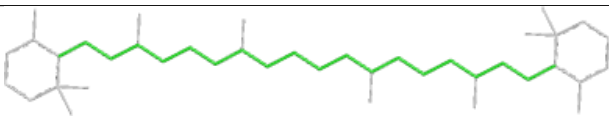
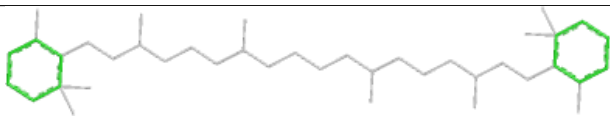
Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

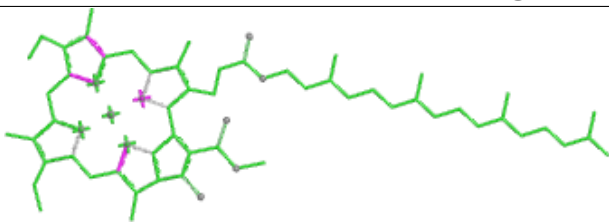
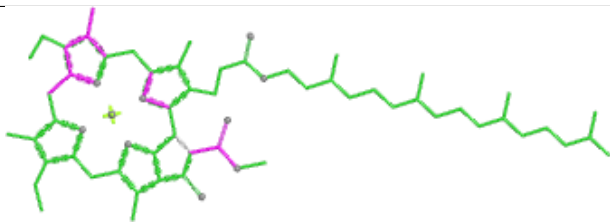
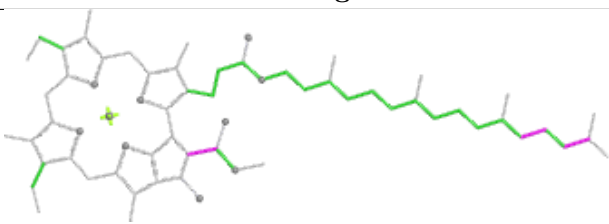
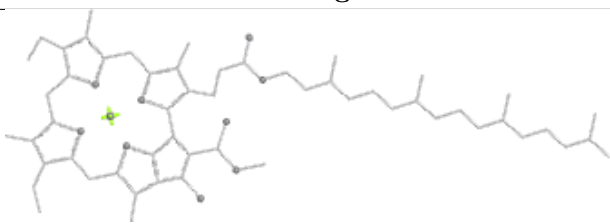
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

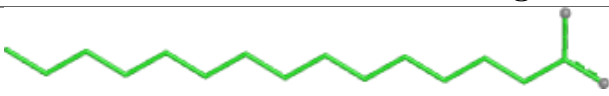
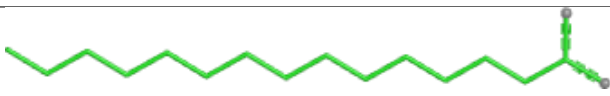
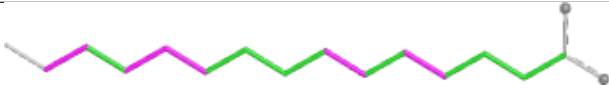
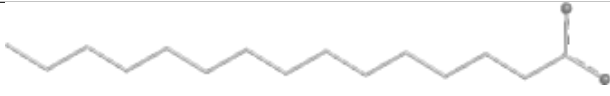
Ligand STE d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

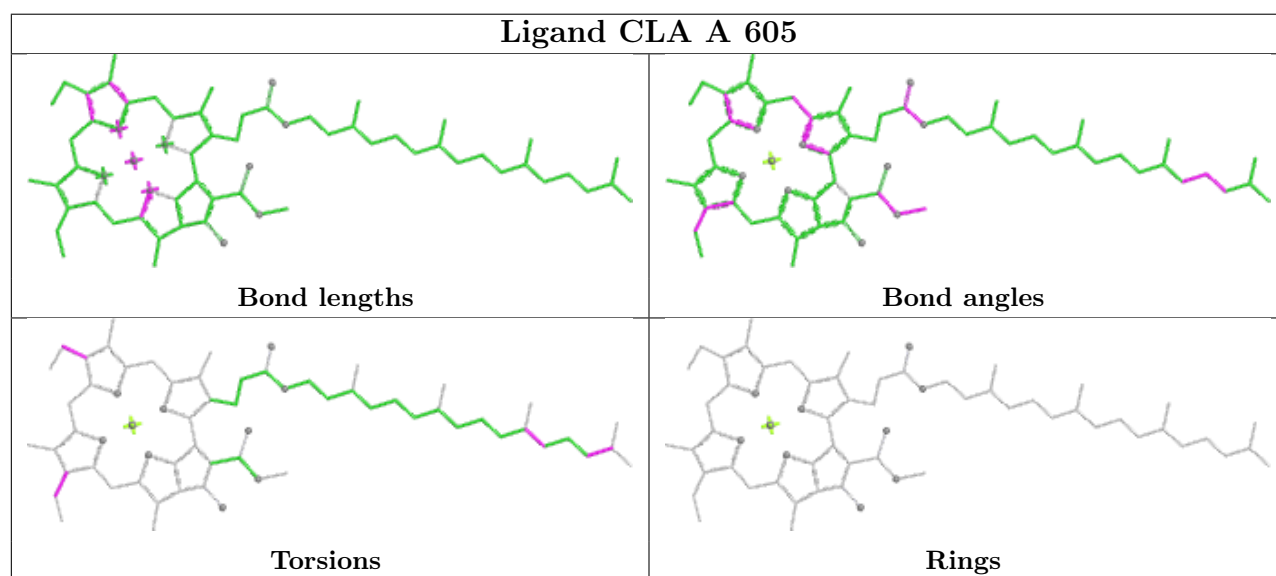
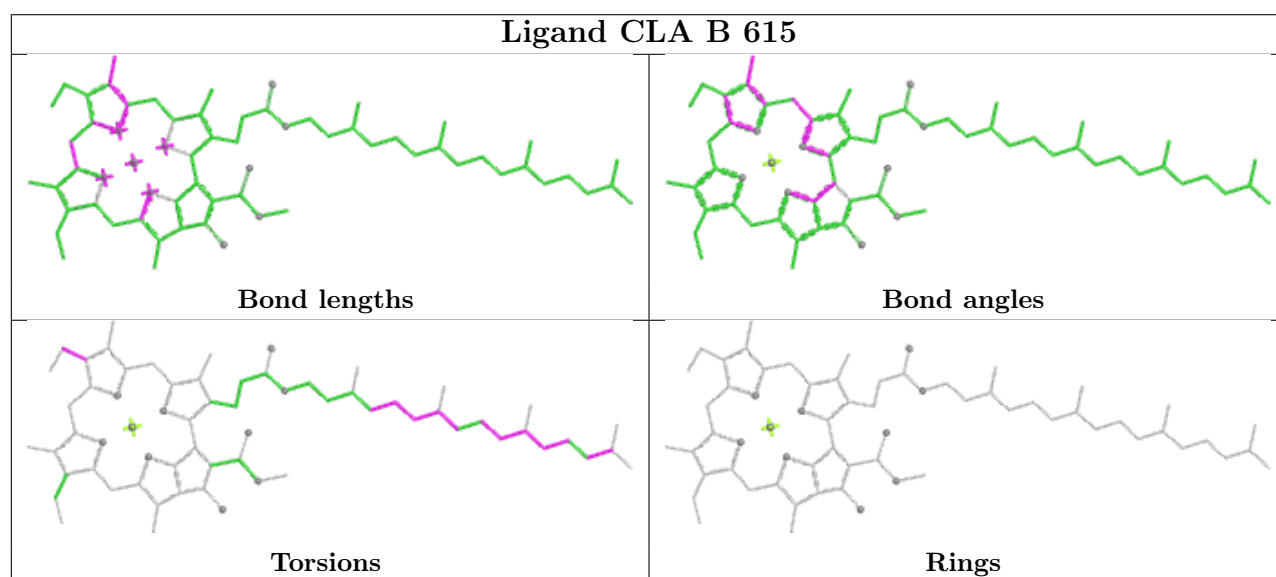
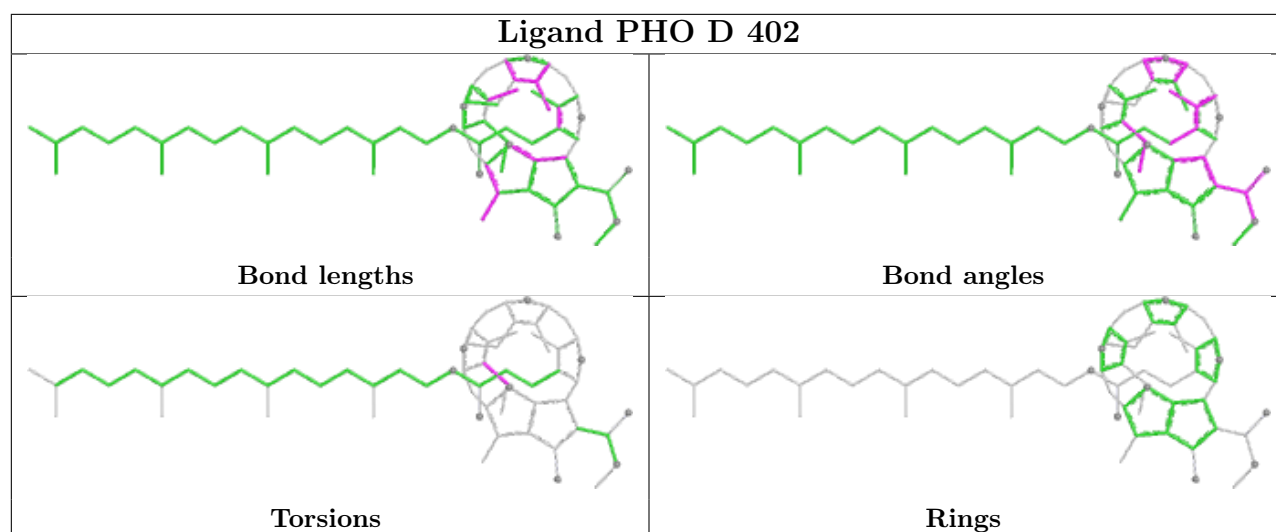
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

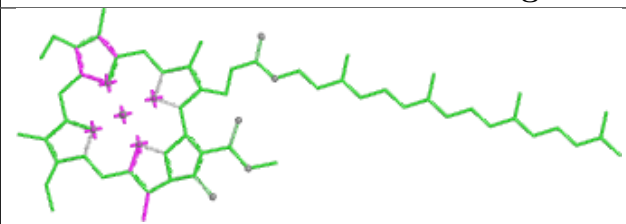
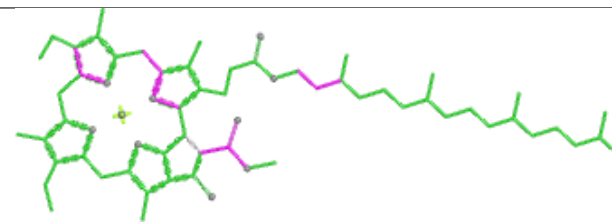
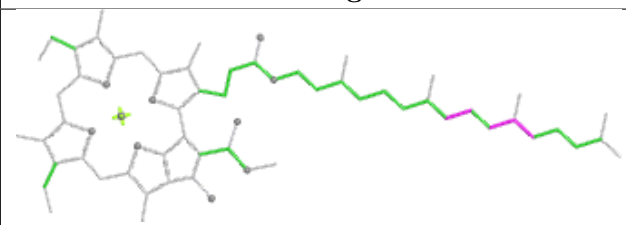
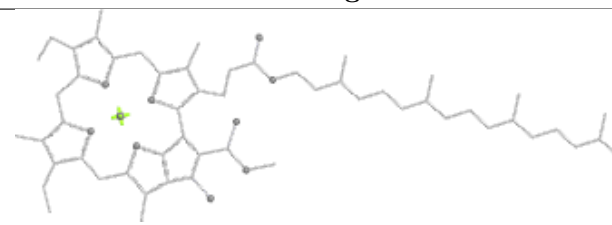
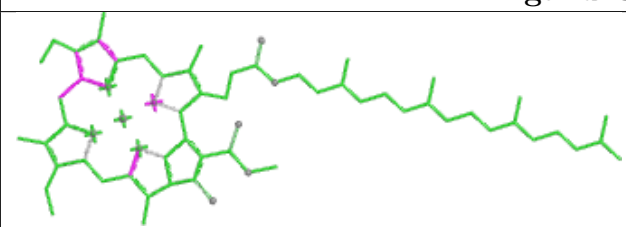
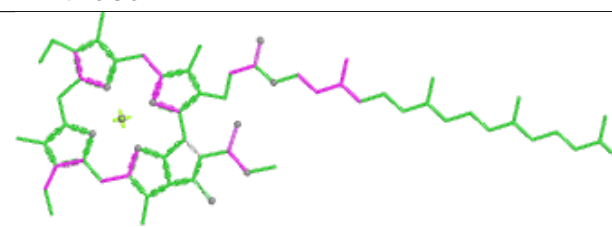
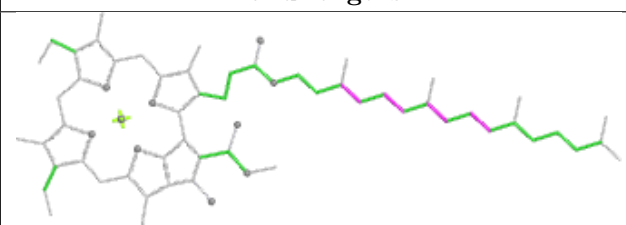
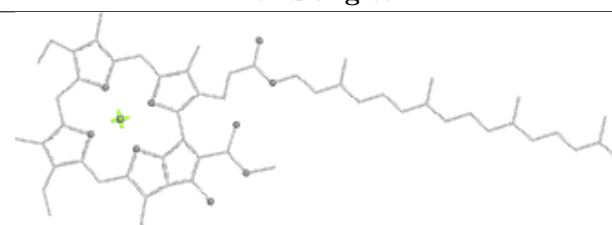
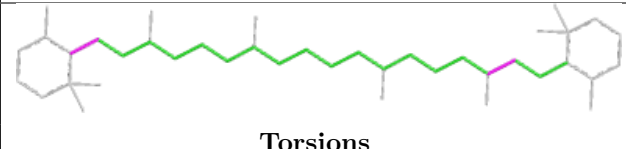
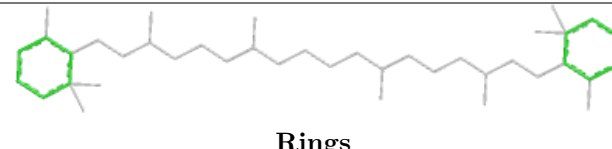


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.61	1 (0%) 90 93	26, 32, 50, 87	0
1	a	334/344 (97%)	-0.46	1 (0%) 90 93	26, 35, 58, 82	0
2	B	505/510 (99%)	-0.37	5 (0%) 79 86	20, 36, 62, 99	5 (0%)
2	b	505/510 (99%)	-0.26	3 (0%) 85 90	28, 40, 72, 104	1 (0%)
3	C	442/461 (95%)	-0.37	0 100 100	18, 39, 55, 84	1 (0%)
3	c	451/461 (97%)	-0.17	3 (0%) 84 89	21, 44, 64, 104	2 (0%)
4	D	341/352 (96%)	-0.59	1 (0%) 90 93	25, 33, 49, 80	0
4	d	341/352 (96%)	-0.42	0 100 100	27, 38, 61, 81	1 (0%)
5	E	82/84 (97%)	0.37	2 (2%) 59 69	31, 54, 69, 85	1 (1%)
5	e	82/84 (97%)	0.41	2 (2%) 59 69	44, 62, 80, 96	0
6	F	34/45 (75%)	-0.03	1 (2%) 53 63	38, 45, 64, 88	0
6	f	34/45 (75%)	0.29	0 100 100	47, 53, 79, 93	0
7	H	65/66 (98%)	-0.17	1 (1%) 72 80	34, 44, 62, 77	0
7	h	63/66 (95%)	0.26	1 (1%) 70 79	42, 53, 68, 71	0
8	I	35/38 (92%)	-0.30	0 100 100	36, 43, 70, 80	0
8	i	35/38 (92%)	-0.07	0 100 100	37, 46, 79, 96	0
9	J	36/40 (90%)	0.13	1 (2%) 55 65	37, 52, 83, 102	0
9	j	36/40 (90%)	0.33	2 (5%) 30 38	43, 59, 94, 97	0
10	K	37/46 (80%)	0.14	0 100 100	44, 54, 73, 77	0
10	k	37/46 (80%)	0.23	0 100 100	50, 59, 74, 85	0
11	L	37/37 (100%)	-0.53	0 100 100	29, 34, 67, 72	0
11	l	36/37 (97%)	-0.51	0 100 100	29, 35, 74, 83	0
12	M	32/36 (88%)	-0.19	1 (3%) 51 61	32, 37, 59, 77	0
12	m	31/36 (86%)	-0.34	0 100 100	32, 39, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.14	4 (1%) 70 79	26, 45, 82, 139	1 (0%)
13	o	244/272 (89%)	-0.09	4 (1%) 70 79	29, 44, 84, 134	0
14	T	29/32 (90%)	-0.45	0 100 100	30, 36, 59, 78	0
14	t	29/32 (90%)	-0.26	2 (6%) 23 30	30, 36, 69, 84	0
15	U	97/134 (72%)	-0.13	0 100 100	34, 46, 71, 100	0
15	u	97/134 (72%)	-0.17	1 (1%) 79 86	33, 44, 63, 93	0
16	V	137/163 (84%)	-0.32	0 100 100	31, 43, 58, 75	0
16	v	137/163 (84%)	-0.06	0 100 100	36, 50, 72, 89	0
17	Y	27/46 (58%)	1.25	4 (14%) 5 7	57, 75, 99, 106	0
17	y	30/46 (65%)	0.66	0 100 100	61, 75, 94, 95	0
18	X	38/41 (92%)	0.20	1 (2%) 57 67	42, 53, 74, 87	0
18	x	39/41 (95%)	0.27	1 (2%) 57 67	49, 62, 84, 96	0
19	Z	62/62 (100%)	0.92	6 (9%) 13 19	56, 70, 117, 128	0
19	z	62/62 (100%)	0.84	6 (9%) 13 19	59, 74, 117, 135	0
20	R	28/41 (68%)	0.76	1 (3%) 46 56	60, 74, 84, 103	0
20	r	28/41 (68%)	1.43	6 (21%) 2 2	71, 90, 107, 110	0
All	All	5293/5700 (92%)	-0.21	61 (1%) 76 83	18, 41, 75, 139	12 (0%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	6.2
20	r	29	LYS	4.5
19	Z	62	VAL	4.4
14	t	30	THR	4.4
19	z	33	TRP	4.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	34,49,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.95	0.07	31,46,65,65	0
12	FME	M	1	10/11	0.96	0.09	37,46,66,72	0
8	FME	i	1	10/11	0.97	0.07	38,47,58,62	0
8	FME	I	1	10/11	0.97	0.07	39,49,64,65	0
12	FME	m	1	10/11	0.98	0.06	35,47,71,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	C	520	10/20	0.55	0.25	51,79,95,97	0
28	STE	j	102	16/20	0.63	0.23	60,80,105,106	0
28	STE	e	101	9/20	0.64	0.25	60,78,92,94	0
28	STE	i	101	12/20	0.66	0.14	63,95,115,122	0
28	STE	K	103	14/20	0.68	0.17	59,76,99,101	0
28	STE	I	101	17/20	0.68	0.16	53,76,84,88	0
28	STE	c	517	18/20	0.70	0.19	61,83,102,103	0
28	STE	C	528	14/20	0.71	0.19	60,85,108,109	0
28	STE	A	617	17/20	0.72	0.14	54,74,81,88	0
28	STE	C	518	5/20	0.72	0.24	54,61,73,73	0
28	STE	b	625	11/20	0.74	0.20	54,68,82,82	0
28	STE	C	519	7/20	0.75	0.21	57,68,79,79	0
28	STE	H	103	18/20	0.75	0.17	48,74,94,95	0
28	STE	A	618	11/20	0.75	0.15	56,72,88,88	0
32	LMG	c	518	30/55	0.75	0.17	45,80,107,111	0
28	STE	E	101	12/20	0.76	0.19	63,80,107,108	0
29	LHG	e	102	42/49	0.76	0.17	59,85,116,130	0
32	LMG	D	407	50/55	0.76	0.15	41,72,115,121	0
28	STE	b	624	10/20	0.76	0.18	51,61,69,73	0
28	STE	E	102	20/20	0.78	0.14	47,69,87,96	0
28	STE	A	611	9/20	0.78	0.17	62,76,86,93	0
28	STE	Z	101	17/20	0.78	0.20	51,74,99,102	0
28	STE	C	516	14/20	0.79	0.17	53,69,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	B	625	15/20	0.79	0.21	47,64,79,94	0
28	STE	I	102	15/20	0.80	0.18	50,64,85,88	0
28	STE	a	616	12/20	0.80	0.13	51,76,81,91	0
28	STE	T	102	16/20	0.80	0.17	42,58,96,100	0
32	LMG	C	517	36/55	0.80	0.14	49,63,81,87	0
28	STE	e	103	9/20	0.80	0.16	53,72,83,87	0
32	LMG	b	622	55/55	0.80	0.16	50,74,94,104	0
28	STE	h	103	10/20	0.80	0.18	63,77,88,91	0
32	LMG	c	523	48/55	0.80	0.15	53,80,104,114	0
29	LHG	A	613	49/49	0.81	0.14	51,74,109,113	0
28	STE	b	623	16/20	0.81	0.17	49,63,85,91	0
28	STE	i	102	6/20	0.81	0.17	55,73,76,76	0
28	STE	c	516	13/20	0.81	0.16	56,75,83,84	0
32	LMG	a	614	55/55	0.81	0.14	41,64,84,96	0
28	STE	k	103	14/20	0.81	0.13	57,74,93,94	0
28	STE	t	103	10/20	0.81	0.18	48,69,77,80	0
28	STE	z	101	9/20	0.81	0.22	56,70,80,82	0
28	STE	e	104	13/20	0.82	0.17	73,88,96,99	0
32	LMG	B	620	45/55	0.82	0.15	38,59,98,116	0
27	PL9	a	610	55/55	0.83	0.16	38,70,87,91	0
28	STE	f	103	8/20	0.83	0.17	56,69,79,81	0
28	STE	d	411	20/20	0.83	0.13	50,68,91,92	0
27	PL9	A	610	55/55	0.84	0.16	35,68,88,90	0
28	STE	H	104	9/20	0.84	0.14	53,66,82,83	0
31	DGD	A	615	66/66	0.84	0.13	50,69,105,114	0
28	STE	B	624	12/20	0.84	0.13	52,68,78,81	0
28	STE	j	101	12/20	0.84	0.14	49,64,71,72	0
28	STE	C	526	12/20	0.85	0.15	40,52,63,63	0
28	STE	M	104	15/20	0.85	0.15	46,63,93,95	0
28	STE	R	101	12/20	0.85	0.15	57,74,87,87	0
30	SQD	a	613	54/54	0.85	0.12	45,63,101,118	0
30	SQD	A	614	43/54	0.86	0.11	44,61,102,117	0
28	STE	d	407	20/20	0.86	0.12	42,58,81,82	0
28	STE	M	103	10/20	0.87	0.14	45,57,64,75	0
28	STE	A	616	8/20	0.87	0.14	47,63,74,74	0
24	CLA	b	601	65/65	0.87	0.12	49,68,91,108	0
28	STE	M	102	15/20	0.87	0.10	38,50,65,70	0
32	LMG	C	521	48/55	0.87	0.12	43,60,74,84	0
28	STE	m	103	18/20	0.88	0.14	40,53,84,90	0
32	LMG	a	615	49/55	0.88	0.12	42,64,86,92	0
28	STE	J	101	12/20	0.88	0.12	49,62,66,70	0
28	STE	C	527	16/20	0.88	0.12	42,53,70,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMG	M	101	51/55	0.88	0.10	34,53,72,80	0
30	SQD	f	102	41/54	0.89	0.13	55,80,98,102	0
28	STE	b	621	20/20	0.89	0.11	37,59,72,76	0
28	STE	B	621	17/20	0.89	0.11	40,57,75,80	0
28	STE	d	413	20/20	0.89	0.11	39,57,70,72	0
28	STE	B	623	18/20	0.89	0.11	46,61,80,83	0
30	SQD	b	620	49/54	0.89	0.10	44,61,83,88	0
32	LMG	m	101	51/55	0.89	0.10	37,57,71,84	0
30	SQD	B	622	54/54	0.90	0.09	41,61,86,91	0
32	LMG	c	522	46/55	0.90	0.11	40,70,86,87	0
28	STE	t	102	14/20	0.91	0.09	42,52,67,67	0
28	STE	m	102	12/20	0.91	0.11	47,58,76,77	0
32	LMG	C	525	48/55	0.91	0.12	44,74,96,99	0
26	BCR	C	514	40/40	0.92	0.10	48,60,71,76	0
26	BCR	d	405	40/40	0.92	0.10	39,53,89,94	0
30	SQD	a	612	54/54	0.92	0.11	43,68,96,100	0
24	CLA	B	601	65/65	0.92	0.10	35,59,96,98	0
24	CLA	c	513	65/65	0.92	0.11	48,70,99,103	0
28	STE	D	414	20/20	0.93	0.09	36,50,73,81	0
26	BCR	k	102	40/40	0.93	0.10	43,55,71,74	0
26	BCR	B	618	40/40	0.93	0.08	27,41,53,55	0
24	CLA	c	512	65/65	0.93	0.10	43,60,92,94	0
30	SQD	D	409	36/54	0.93	0.11	43,71,90,93	0
30	SQD	D	412	52/54	0.93	0.10	31,61,87,94	0
26	BCR	H	101	40/40	0.93	0.08	32,45,59,62	0
26	BCR	K	101	40/40	0.93	0.09	40,54,72,76	0
26	BCR	c	514	40/40	0.93	0.10	51,64,76,76	0
24	CLA	C	513	65/65	0.93	0.09	43,66,99,103	0
26	BCR	h	101	40/40	0.93	0.09	41,53,72,73	0
26	BCR	k	101	40/40	0.93	0.09	46,59,71,75	0
31	DGD	c	520	62/66	0.94	0.09	35,53,94,100	0
31	DGD	h	102	62/66	0.94	0.08	35,50,62,64	0
26	BCR	C	515	40/40	0.94	0.08	28,42,54,60	0
29	LHG	d	408	49/49	0.94	0.10	38,53,74,82	0
26	BCR	c	515	40/40	0.94	0.09	32,47,63,63	0
26	BCR	b	619	40/40	0.94	0.09	32,49,67,70	0
31	DGD	C	523	62/66	0.94	0.10	32,50,107,118	0
32	LMG	D	408	51/55	0.94	0.11	30,61,87,92	0
26	BCR	B	617	40/40	0.95	0.07	29,41,52,55	0
27	PL9	d	406	55/55	0.95	0.07	27,38,45,47	0
24	CLA	B	606	65/65	0.95	0.08	25,37,76,81	0
26	BCR	B	619	40/40	0.95	0.07	30,45,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	510	65/65	0.95	0.07	33,44,64,77	0
24	CLA	b	606	65/65	0.95	0.08	29,41,79,85	0
26	BCR	D	405	40/40	0.95	0.10	33,47,83,99	0
31	DGD	H	102	62/66	0.95	0.08	31,45,60,67	0
24	CLA	b	616	60/65	0.95	0.09	32,45,90,94	0
24	CLA	c	503	65/65	0.95	0.07	35,46,56,59	0
26	BCR	K	102	40/40	0.95	0.08	42,53,70,70	0
26	BCR	T	101	40/40	0.95	0.07	30,40,59,59	0
26	BCR	b	617	40/40	0.95	0.07	30,43,53,57	0
26	BCR	b	618	40/40	0.95	0.07	28,44,59,63	0
24	CLA	c	506	65/65	0.95	0.09	36,51,96,103	0
24	CLA	c	509	65/65	0.95	0.08	34,48,65,68	0
24	CLA	c	511	65/65	0.95	0.08	40,56,72,75	0
29	LHG	D	413	49/49	0.95	0.09	31,47,72,76	0
24	CLA	C	511	65/65	0.95	0.08	32,51,65,71	0
29	LHG	d	410	39/49	0.95	0.09	32,48,71,80	0
24	CLA	C	512	65/65	0.95	0.08	39,54,89,99	0
24	CLA	d	404	65/65	0.95	0.09	33,49,94,97	0
25	PHO	D	402	64/64	0.95	0.06	24,33,40,45	0
32	LMG	d	412	44/55	0.95	0.09	37,55,83,94	0
25	PHO	d	402	64/64	0.95	0.07	30,38,46,53	0
24	CLA	C	504	59/65	0.96	0.07	29,42,92,96	0
29	LHG	D	411	47/49	0.96	0.09	31,52,87,94	0
24	CLA	c	504	60/65	0.96	0.07	33,44,82,87	0
24	CLA	c	505	65/65	0.96	0.07	29,44,75,85	0
29	LHG	d	409	49/49	0.96	0.07	30,44,58,69	0
24	CLA	C	505	65/65	0.96	0.07	27,40,69,81	0
24	CLA	c	507	65/65	0.96	0.07	33,47,61,64	0
24	CLA	c	508	64/65	0.96	0.09	35,46,98,111	0
26	BCR	t	101	40/40	0.96	0.06	27,41,53,58	0
24	CLA	C	506	65/65	0.96	0.10	31,46,93,100	0
27	PL9	D	406	55/55	0.96	0.06	22,34,46,51	0
24	CLA	c	510	65/65	0.96	0.07	33,47,63,68	0
24	CLA	C	507	65/65	0.96	0.06	27,42,61,66	0
24	CLA	C	509	65/65	0.96	0.07	31,45,61,74	0
24	CLA	B	609	65/65	0.96	0.06	27,37,57,66	0
24	CLA	B	610	65/65	0.96	0.06	23,34,43,46	0
31	DGD	C	522	62/66	0.96	0.08	24,44,90,94	0
25	PHO	A	607	64/64	0.96	0.06	21,30,38,44	0
31	DGD	C	524	62/66	0.96	0.08	29,51,86,98	0
24	CLA	B	614	65/65	0.96	0.07	24,37,81,95	0
31	DGD	c	519	62/66	0.96	0.09	24,45,81,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PHO	a	607	64/64	0.96	0.06	24,32,40,44	0
31	DGD	c	521	62/66	0.96	0.09	31,54,91,96	0
24	CLA	B	616	60/65	0.96	0.08	27,40,94,104	0
26	BCR	A	609	40/40	0.96	0.06	27,39,46,49	0
24	CLA	a	606	65/65	0.96	0.09	28,42,101,108	0
24	CLA	a	608	65/65	0.96	0.09	23,37,83,96	0
24	CLA	C	501	65/65	0.96	0.06	27,38,52,58	0
24	CLA	b	602	65/65	0.96	0.08	28,44,62,67	0
24	CLA	b	605	65/65	0.96	0.06	26,37,51,54	0
24	CLA	C	502	65/65	0.96	0.06	29,40,55,61	0
24	CLA	b	608	65/65	0.96	0.06	30,43,62,66	0
24	CLA	b	609	65/65	0.96	0.07	32,47,68,72	0
24	CLA	b	610	65/65	0.96	0.07	30,41,51,52	0
24	CLA	b	614	65/65	0.96	0.08	28,40,85,92	0
26	BCR	a	609	40/40	0.96	0.06	27,37,49,51	0
24	CLA	b	615	65/65	0.96	0.07	27,44,68,77	0
24	CLA	C	503	65/65	0.96	0.06	33,42,50,57	0
24	CLA	c	502	65/65	0.96	0.07	30,43,60,69	0
33	BCT	D	401	4/4	0.96	0.07	28,32,36,43	0
24	CLA	B	612	65/65	0.97	0.07	21,34,47,56	0
24	CLA	b	611	65/65	0.97	0.06	25,36,56,59	0
24	CLA	b	612	65/65	0.97	0.06	25,37,49,54	0
24	CLA	b	613	65/65	0.97	0.07	25,36,82,86	0
24	CLA	B	613	65/65	0.97	0.06	22,33,75,80	0
24	CLA	B	603	65/65	0.97	0.07	25,35,64,65	0
24	CLA	B	615	65/65	0.97	0.07	26,40,62,69	0
24	CLA	c	501	65/65	0.97	0.07	31,43,56,60	0
24	CLA	B	604	65/65	0.97	0.07	22,34,74,82	0
24	CLA	D	404	65/65	0.97	0.08	27,42,115,134	0
24	CLA	a	605	65/65	0.97	0.06	22,31,50,60	0
24	CLA	B	605	65/65	0.97	0.06	22,34,49,51	0
29	LHG	D	410	49/49	0.97	0.06	27,41,52,55	0
24	CLA	A	612	65/65	0.97	0.06	22,29,49,58	0
24	CLA	a	611	65/65	0.97	0.06	23,31,49,56	0
29	LHG	L	101	49/49	0.97	0.07	30,44,63,75	0
24	CLA	B	607	65/65	0.97	0.07	22,36,64,77	0
24	CLA	B	608	65/65	0.97	0.06	25,36,58,62	0
24	CLA	b	603	65/65	0.97	0.06	28,38,67,74	0
24	CLA	b	604	65/65	0.97	0.07	24,37,79,98	0
29	LHG	l	101	49/49	0.97	0.07	30,48,67,75	0
24	CLA	A	605	65/65	0.97	0.05	20,29,53,59	0
24	CLA	B	602	65/65	0.97	0.06	26,37,56,62	0

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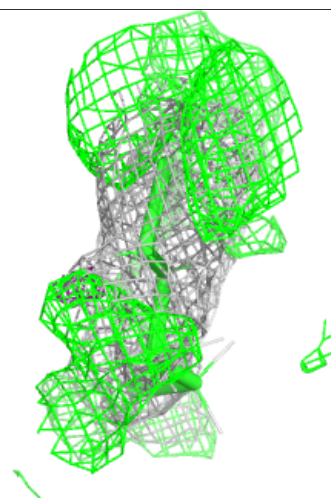
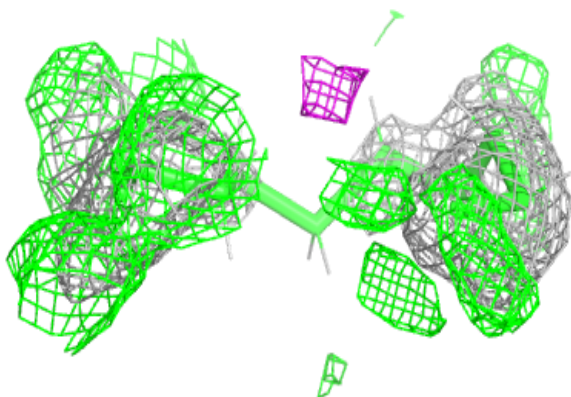
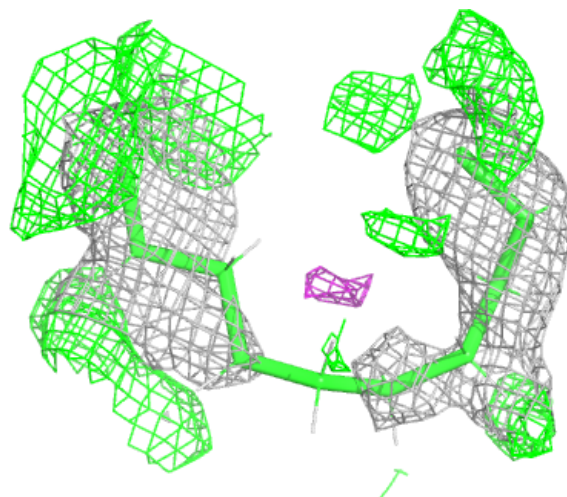
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	d	403	65/65	0.97	0.06	23,35,64,67	0
24	CLA	b	607	65/65	0.97	0.08	25,38,66,73	0
24	CLA	B	611	65/65	0.97	0.05	23,32,49,55	0
24	CLA	C	508	65/65	0.97	0.07	30,42,111,122	0
33	BCT	d	401	4/4	0.97	0.06	33,36,47,56	0
34	HEM	F	101	43/43	0.97	0.07	40,47,61,61	0
34	HEM	f	101	43/43	0.97	0.08	47,57,73,73	0
24	CLA	D	403	65/65	0.98	0.05	21,30,62,70	0
24	CLA	A	606	65/65	0.98	0.07	24,37,100,111	0
24	CLA	A	608	54/65	0.98	0.05	22,35,67,78	0
23	CL	a	603	1/1	0.99	0.03	29,29,29,29	0
35	HEC	V	201	43/43	0.99	0.05	27,34,41,42	0
35	HEC	v	201	43/43	0.99	0.05	30,37,49,49	0
21	OEX	a	601	10/10	1.00	0.02	24,27,30,31	0
22	FE2	A	602	1/1	1.00	0.01	29,29,29,29	0
22	FE2	a	602	1/1	1.00	0.03	35,35,35,35	0
23	CL	A	603	1/1	1.00	0.04	28,28,28,28	0
23	CL	A	604	1/1	1.00	0.03	29,29,29,29	0
21	OEX	A	601	10/10	1.00	0.02	25,27,30,32	0
23	CL	a	604	1/1	1.00	0.04	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.

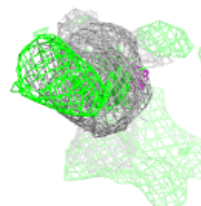
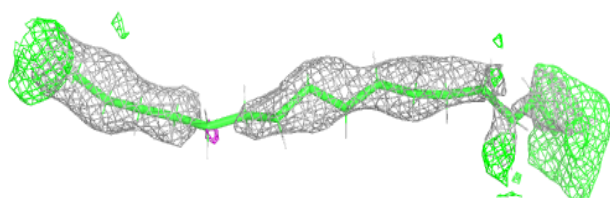
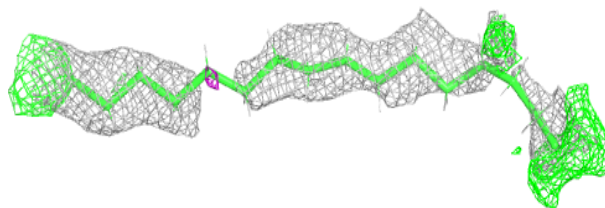
Electron density around STE C 520:

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

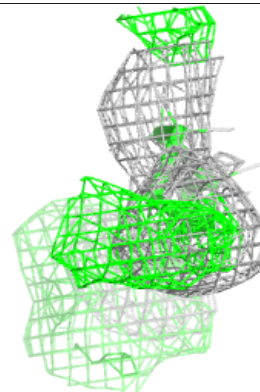
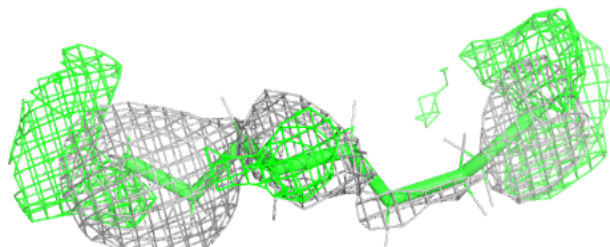
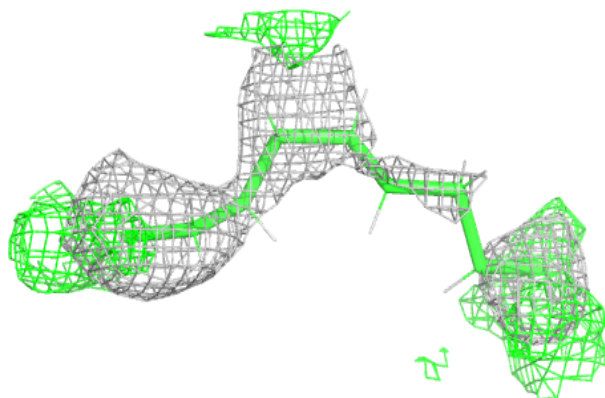


Electron density around STE j 102:

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

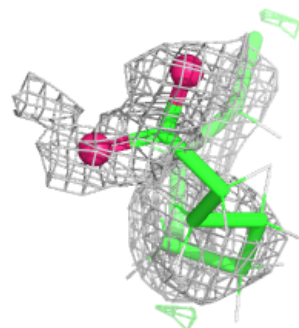
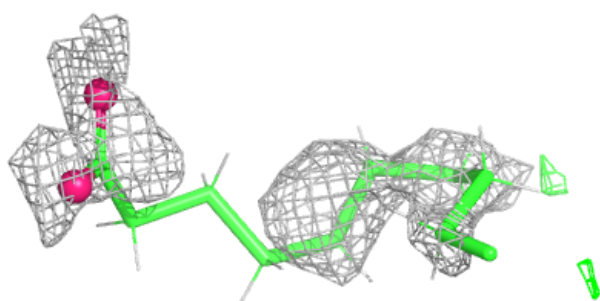
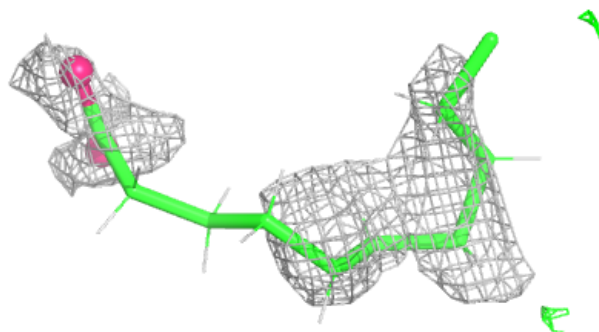
**Electron density around STE e 101:**

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

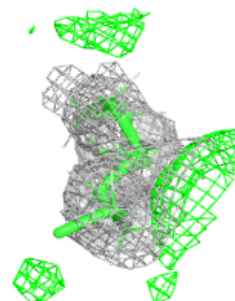
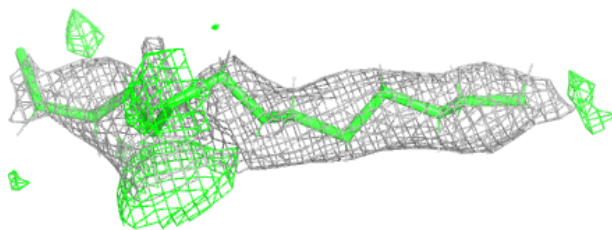
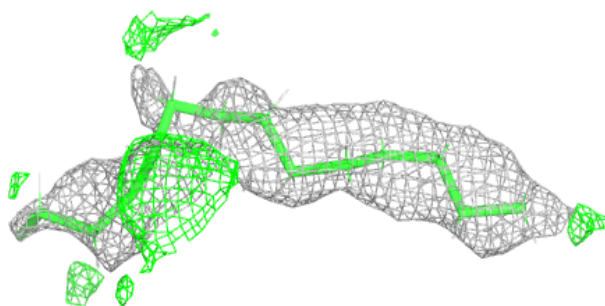


Electron density around STE i 101:

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

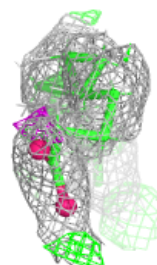
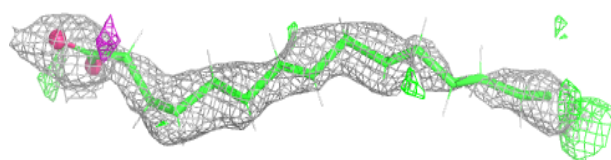
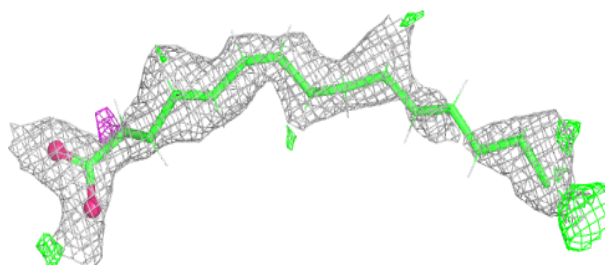
**Electron density around STE K 103:**

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

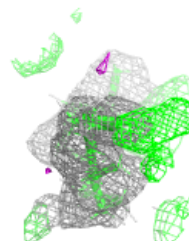
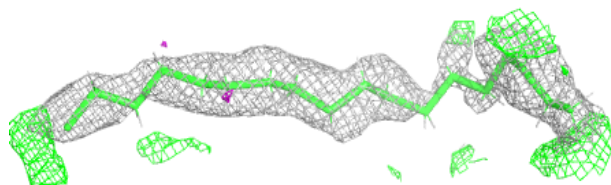
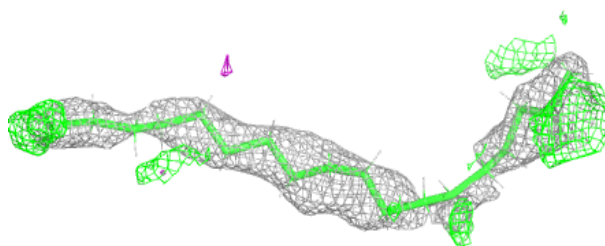


Electron density around STE I 101:

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

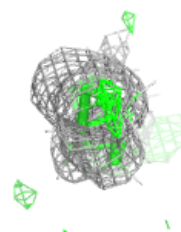
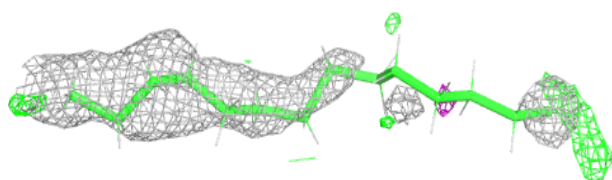
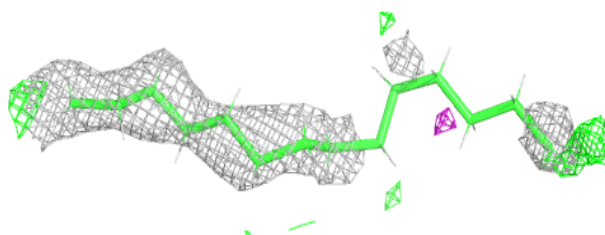
**Electron density around STE c 517:**

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

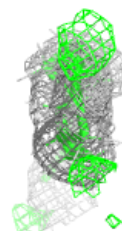
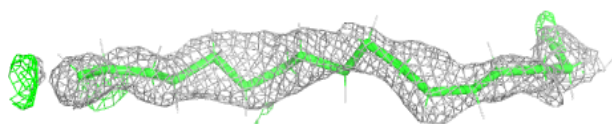
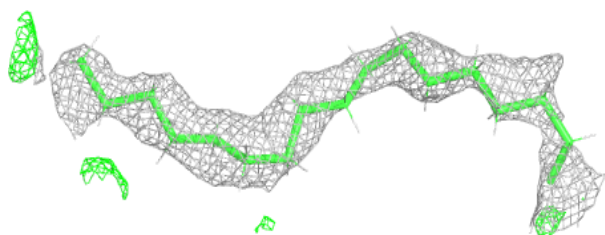


Electron density around STE C 528:

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

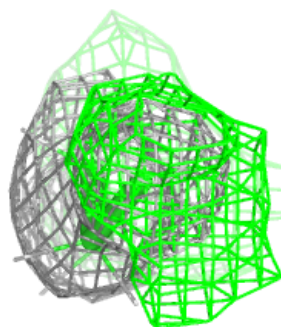
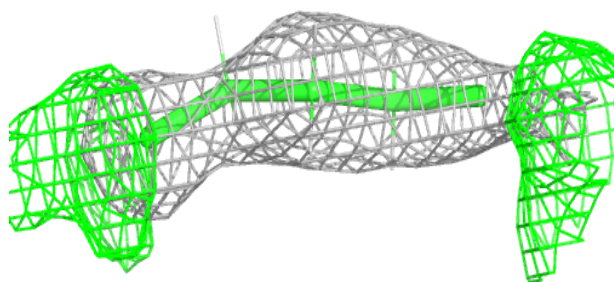
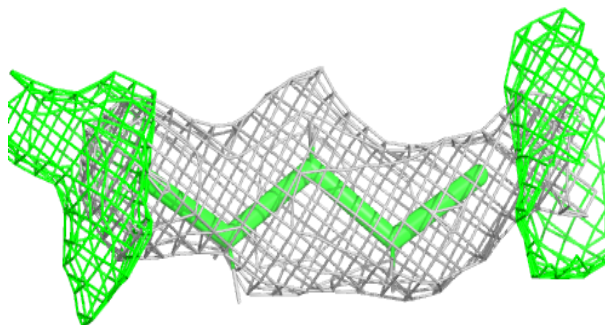
**Electron density around STE A 617:**

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

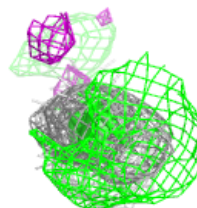
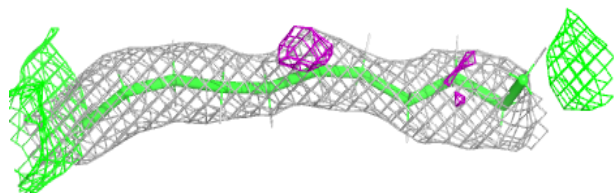
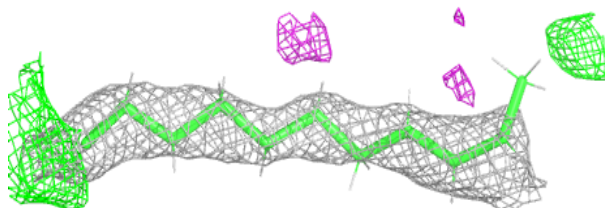


Electron density around STE C 518:

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

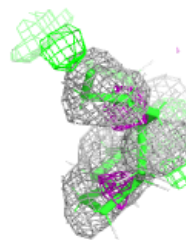
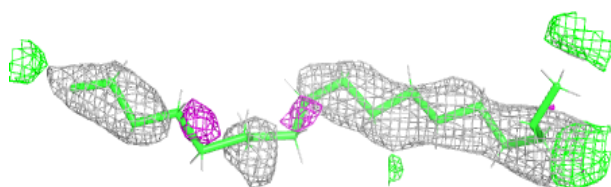
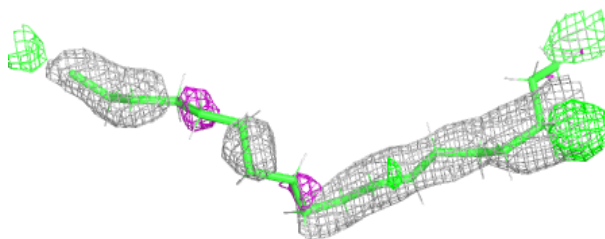
**Electron density around STE b 625:**

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

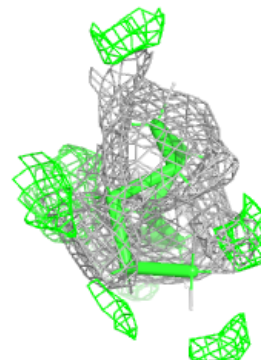
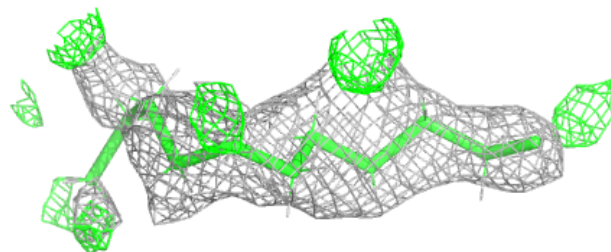
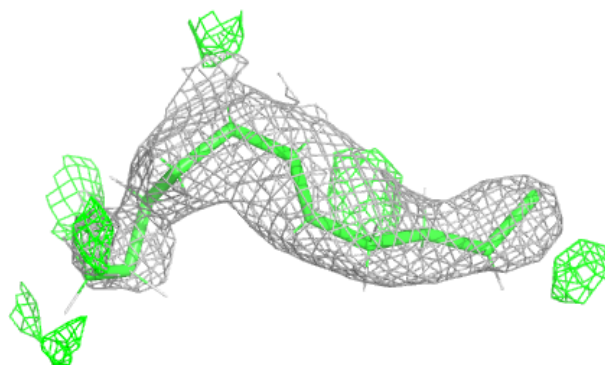


Electron density around STE H 103:

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

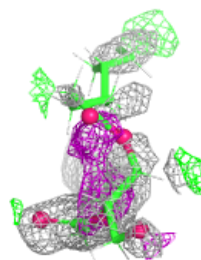
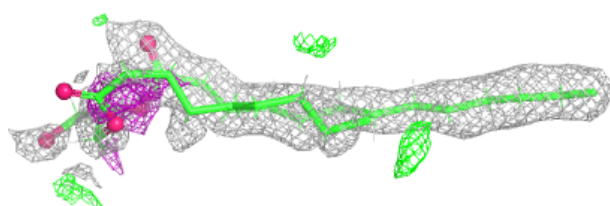
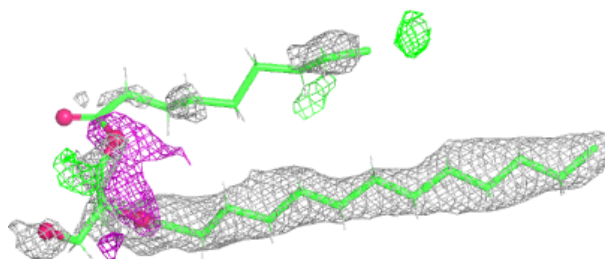
**Electron density around STE A 618:**

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

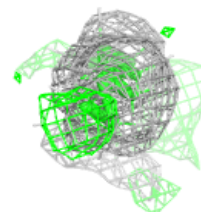
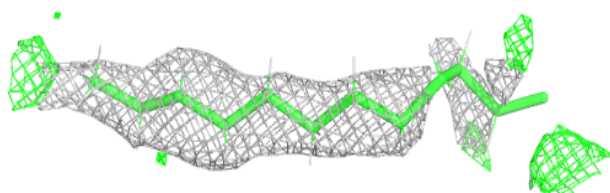
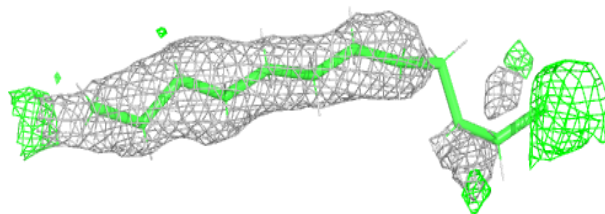


Electron density around LMG c 518:

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

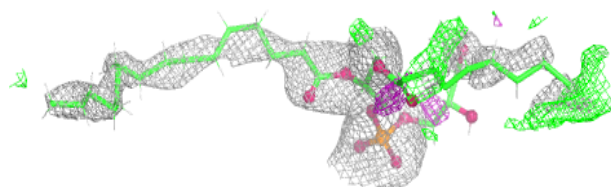
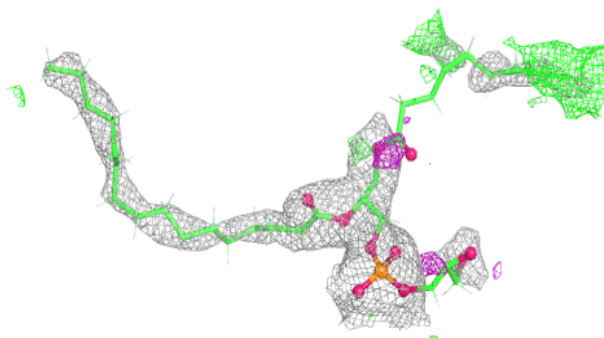
**Electron density around STE E 101:**

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

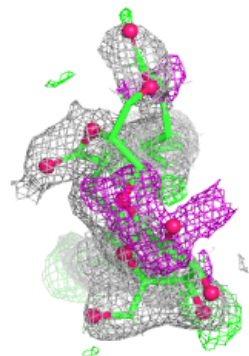
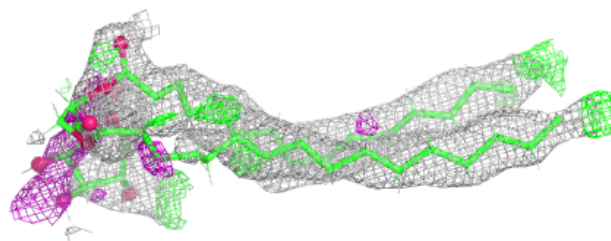
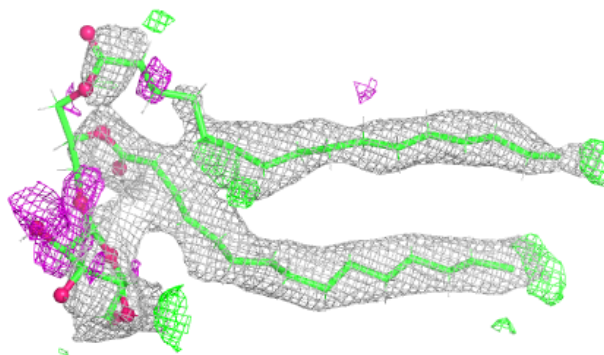


Electron density around LHG e 102:

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

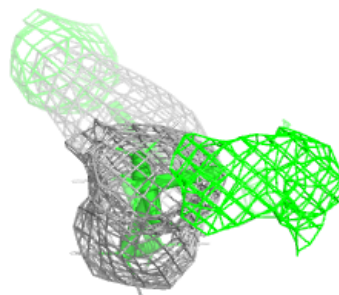
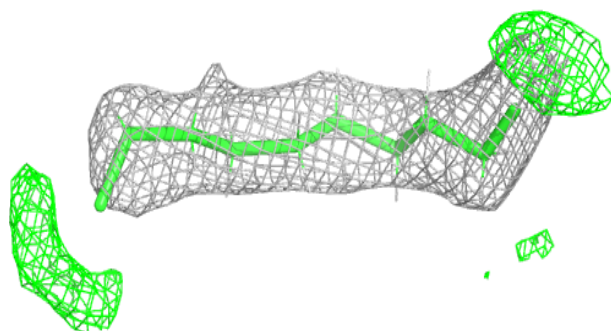
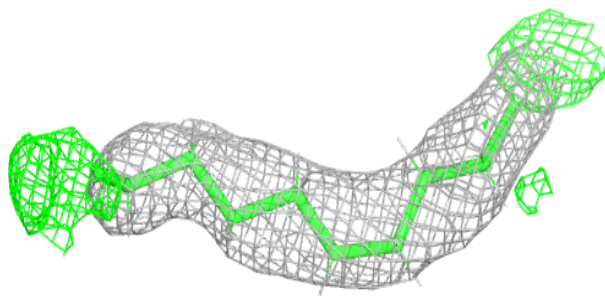
**Electron density around LMG D 407:**

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

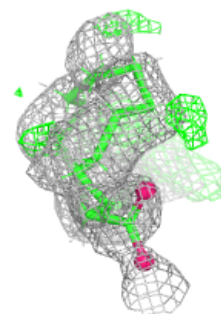
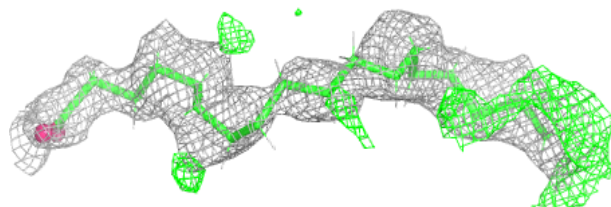
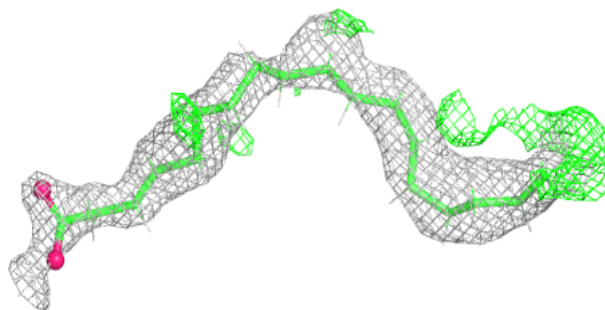


Electron density around STE b 624:

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

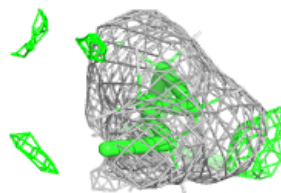
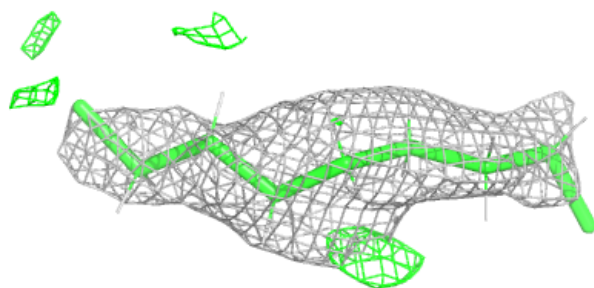
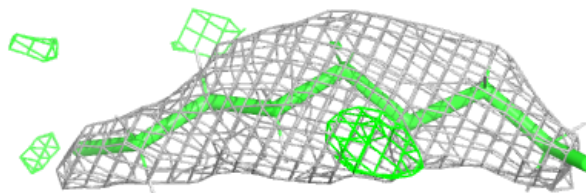
**Electron density around STE E 102:**

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

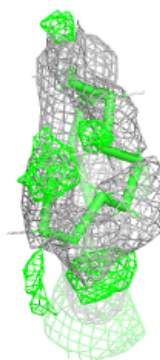
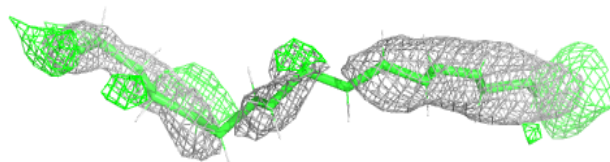
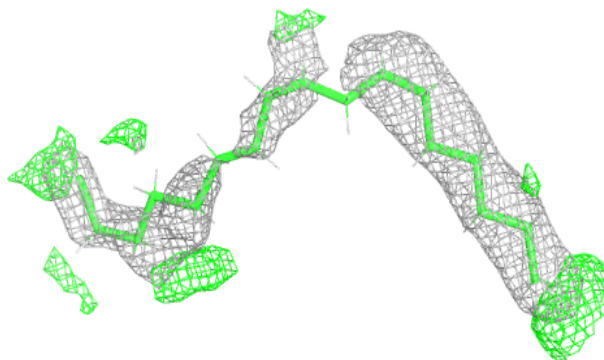


Electron density around STE A 611:

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

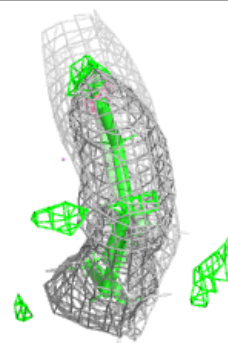
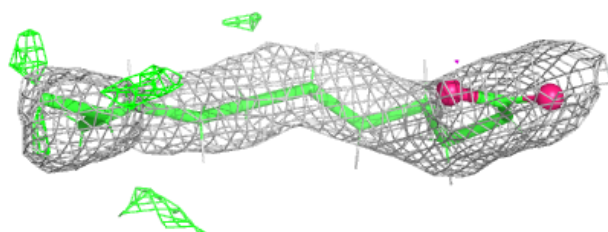
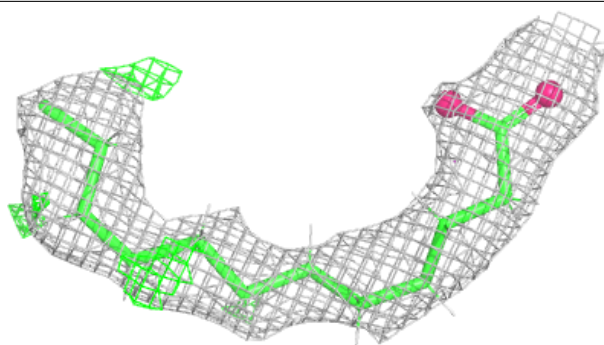
**Electron density around STE Z 101:**

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

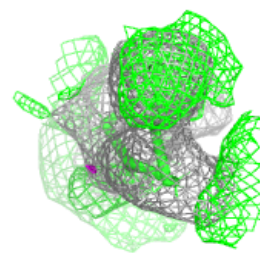
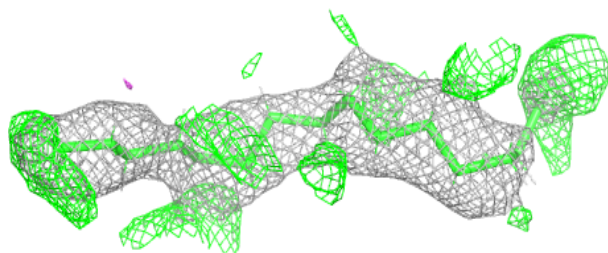
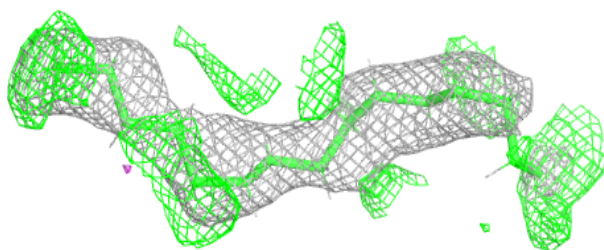


Electron density around STE C 516:

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

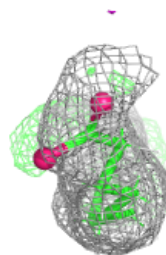
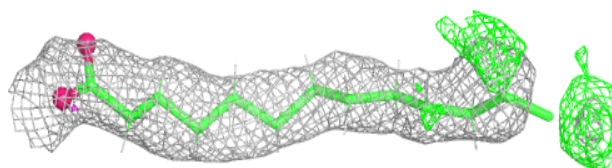
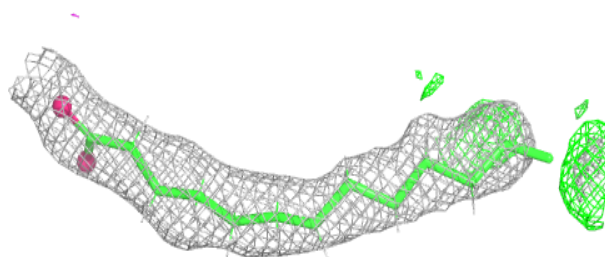
**Electron density around STE B 625:**

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

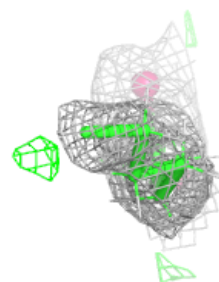
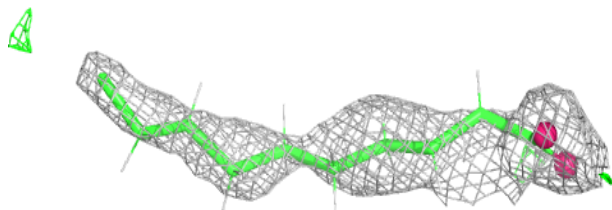
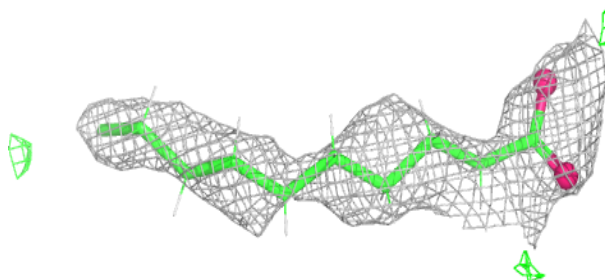


Electron density around STE I 102:

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

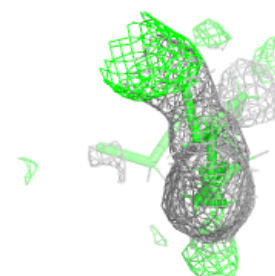
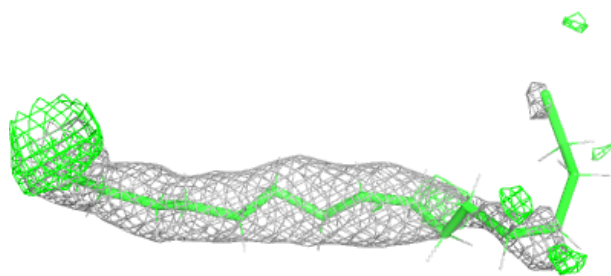
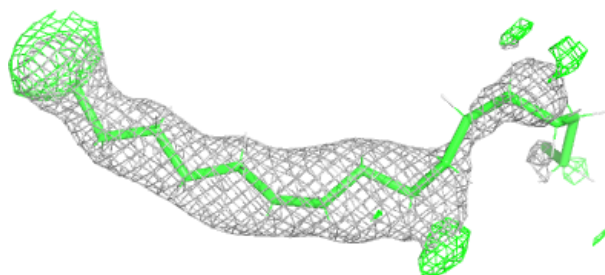
**Electron density around STE a 616:**

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

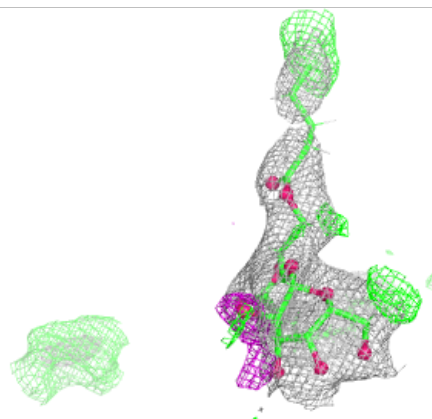
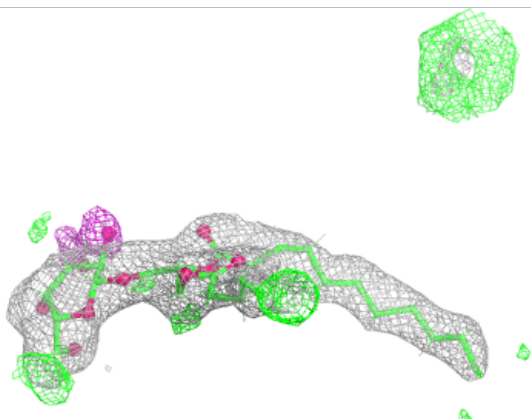
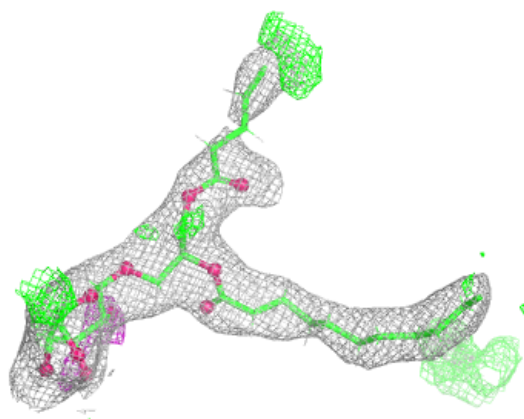


Electron density around STE T 102:

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

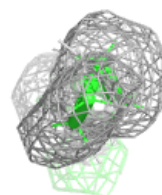
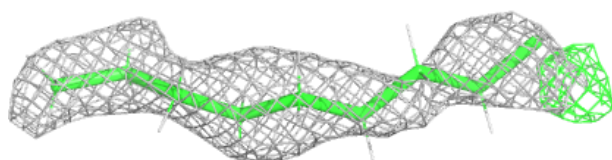
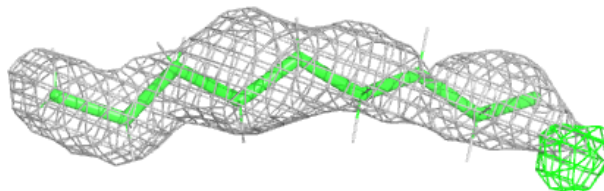
**Electron density around LMG C 517:**

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

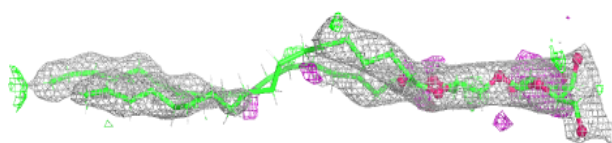
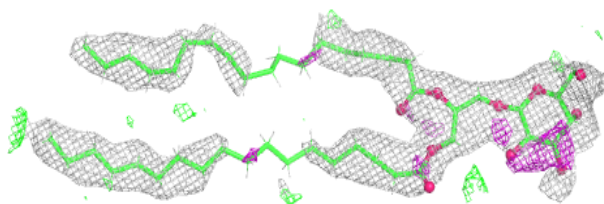


Electron density around STE e 103:

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

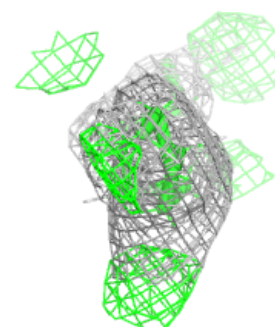
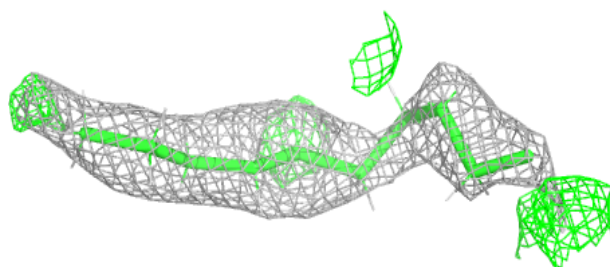
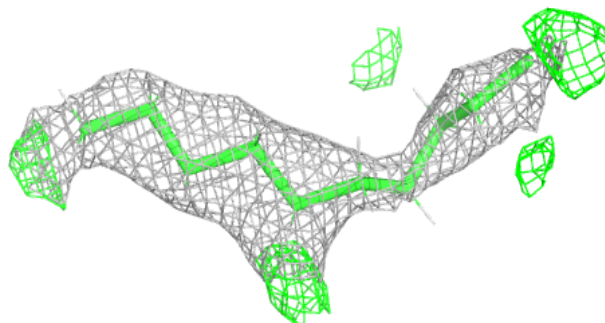
**Electron density around LMG b 622:**

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

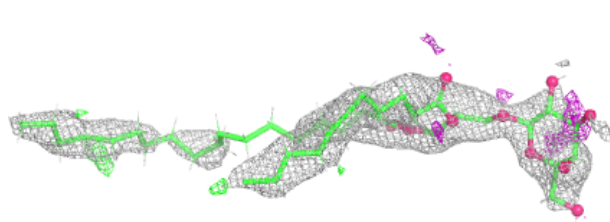
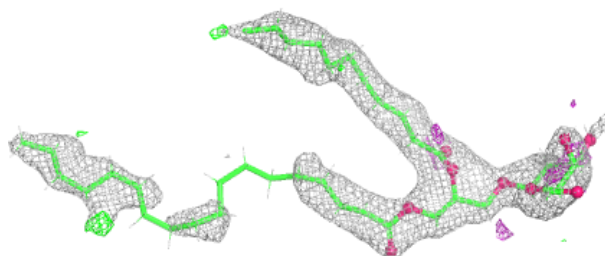


Electron density around STE h 103:

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

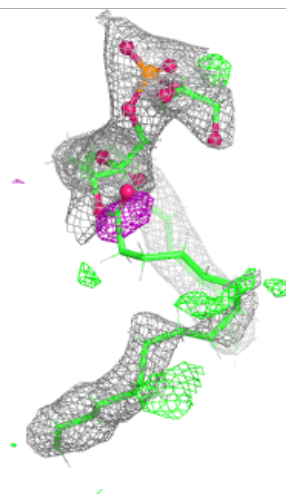
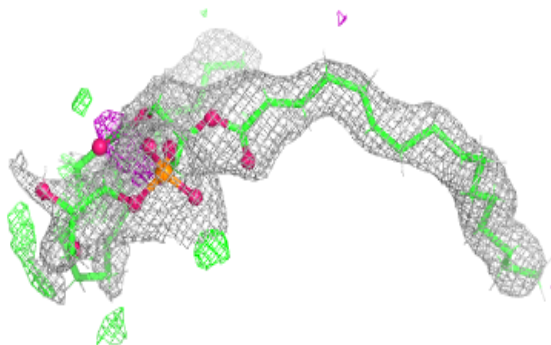
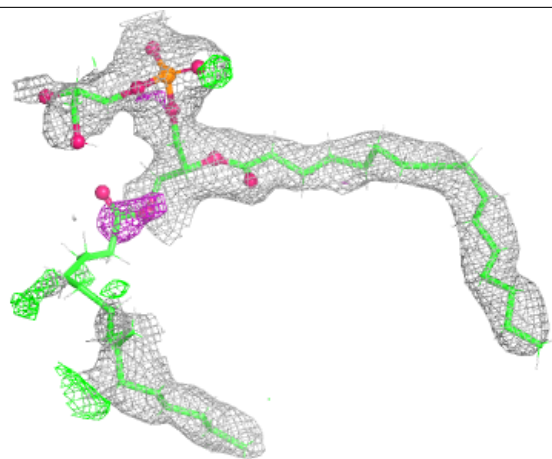
**Electron density around LMG c 523:**

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



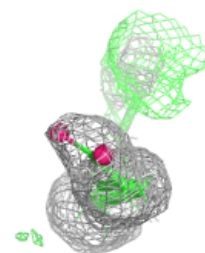
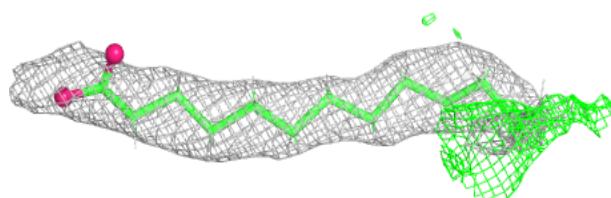
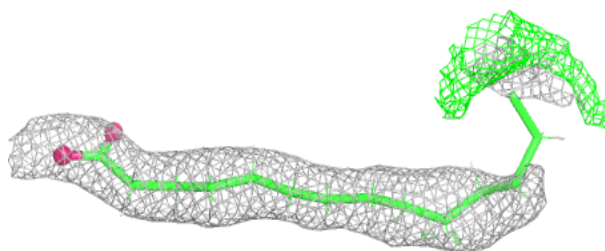
Electron density around LHG A 613:

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

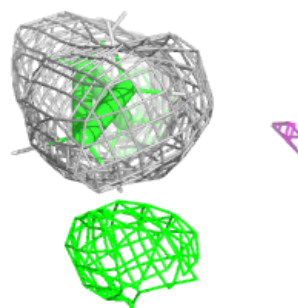
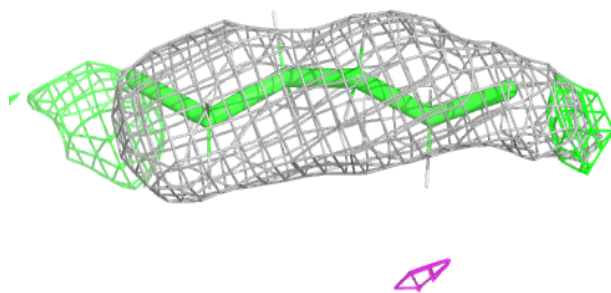
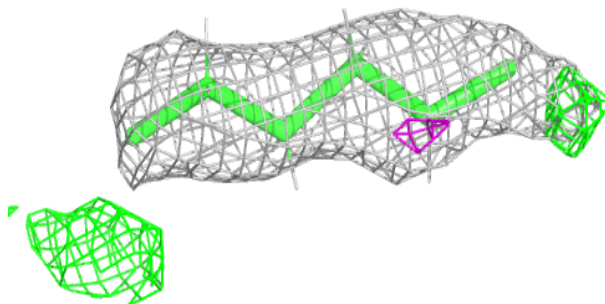


Electron density around STE b 623:

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

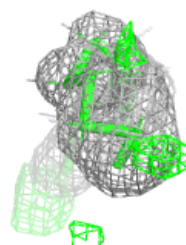
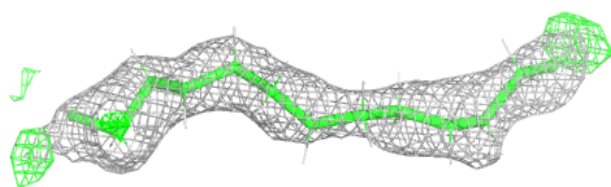
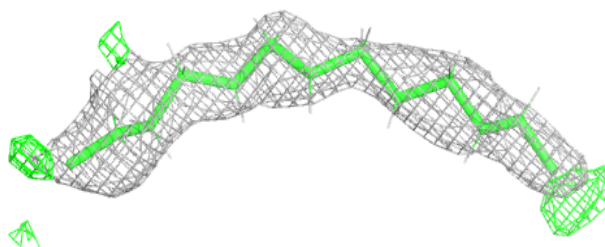
**Electron density around STE i 102:**

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

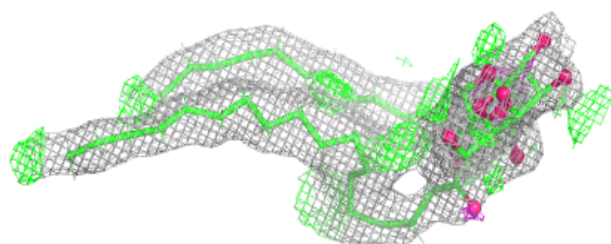
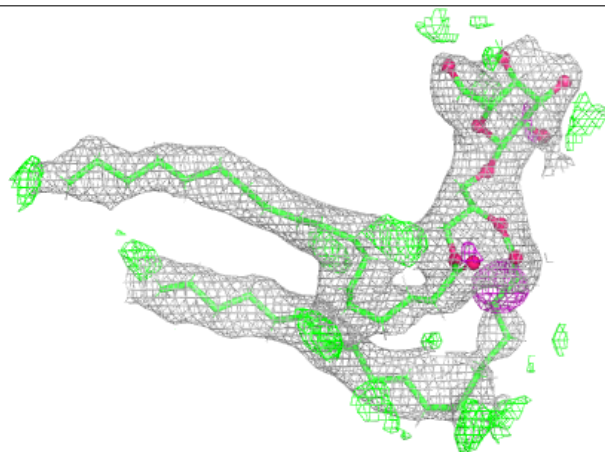


Electron density around STE c 516:

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

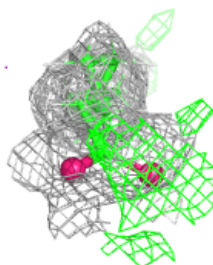
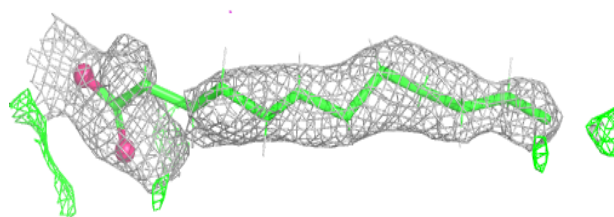
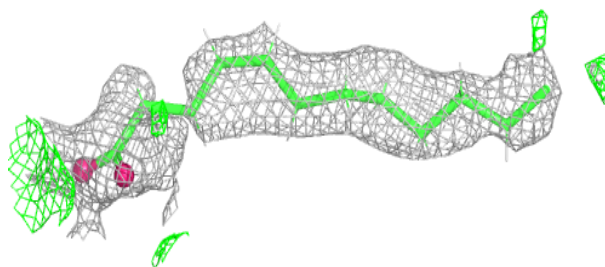
**Electron density around LMG a 614:**

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

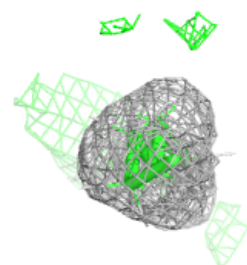
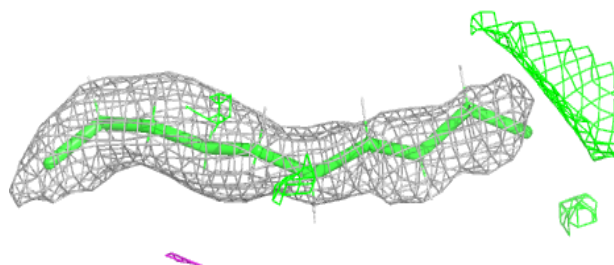
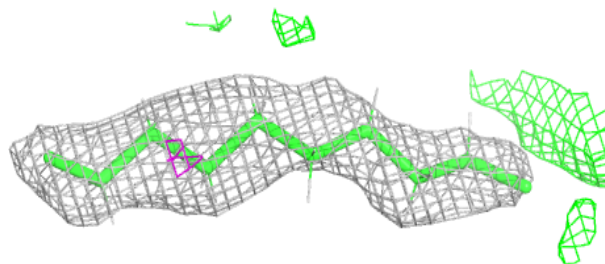


Electron density around STE k 103:

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

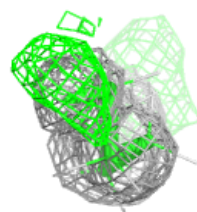
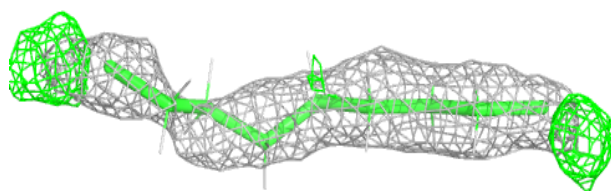
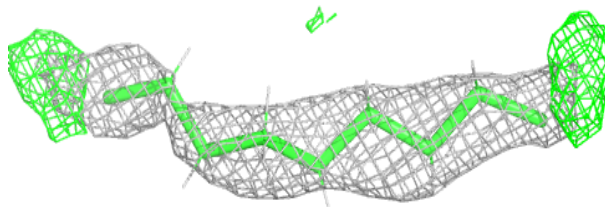
**Electron density around STE t 103:**

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

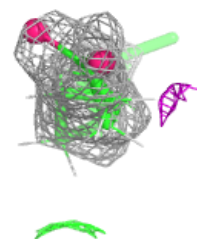
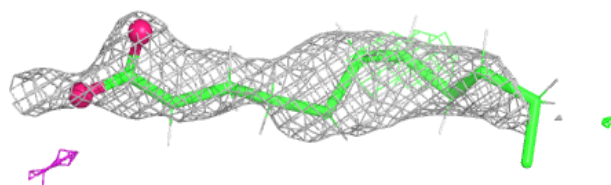
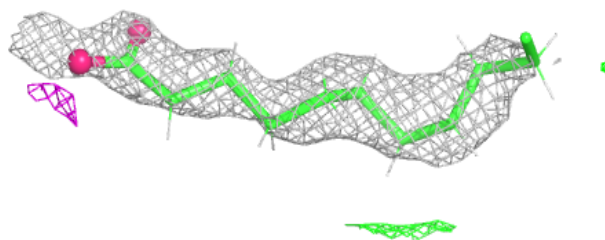


Electron density around STE z 101:

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

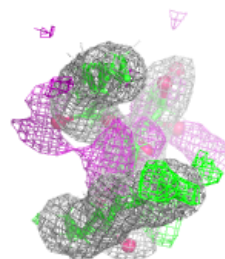
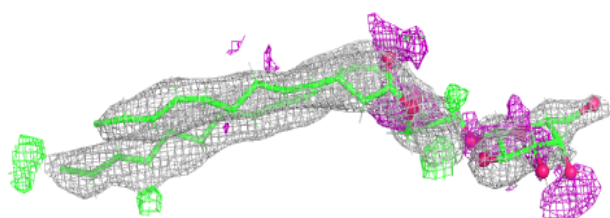
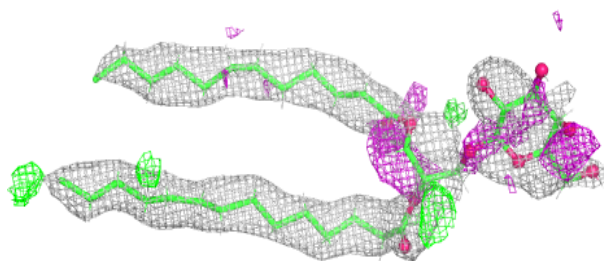
**Electron density around STE e 104:**

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

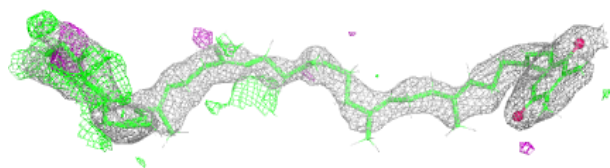
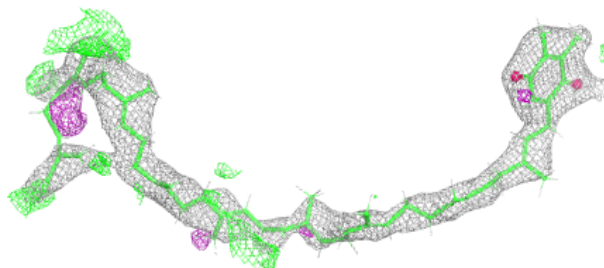


Electron density around LMG B 620:

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

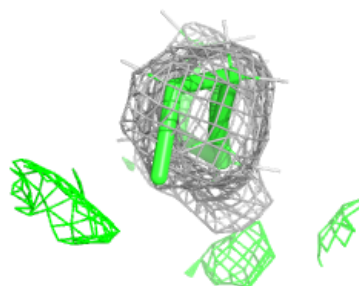
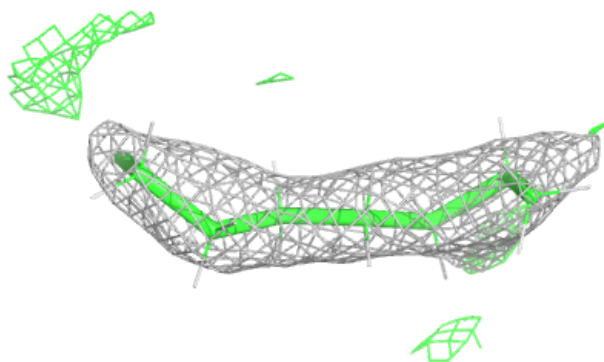
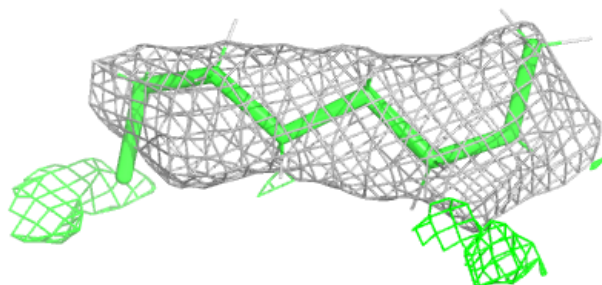
**Electron density around PL9 a 610:**

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

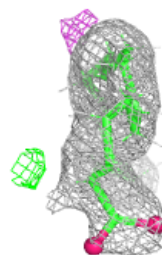
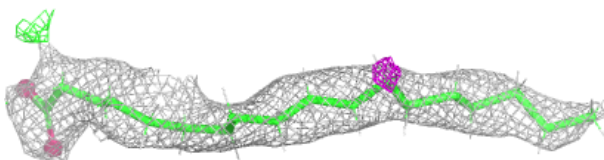
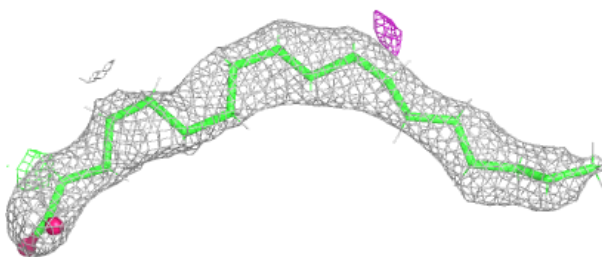


Electron density around STE f 103:

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

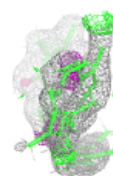
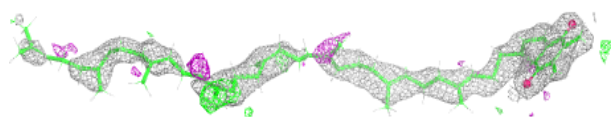
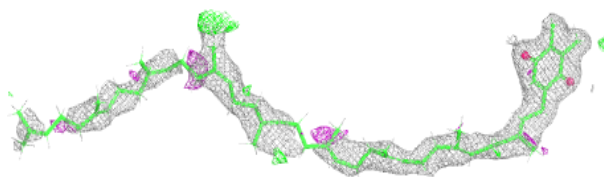
**Electron density around STE d 411:**

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

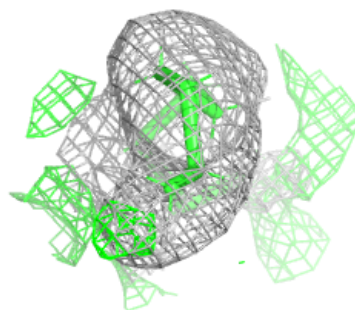
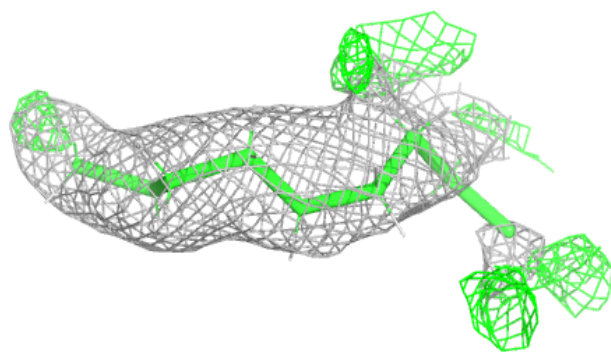
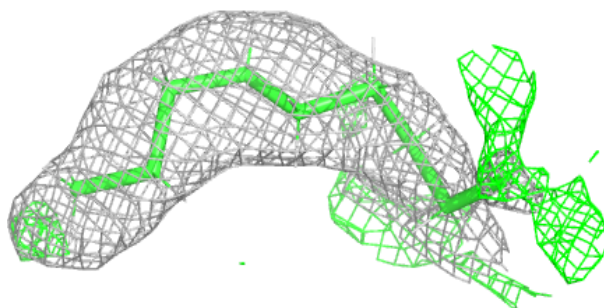


Electron density around PL9 A 610:

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

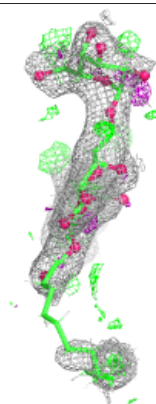
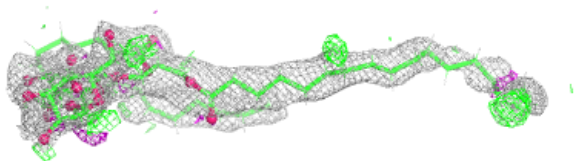
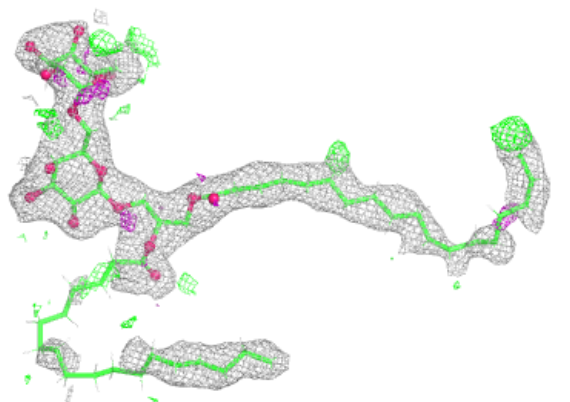
**Electron density around STE H 104:**

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

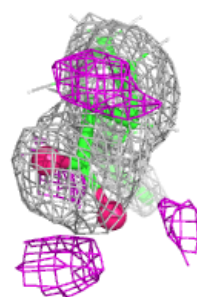
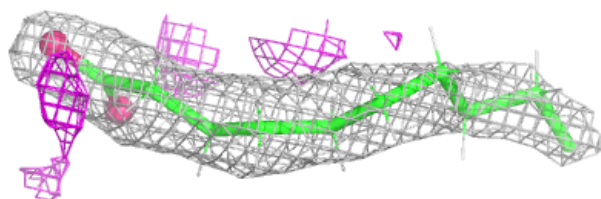
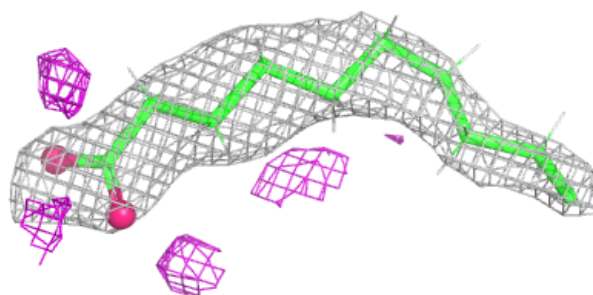


Electron density around DGD A 615:

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

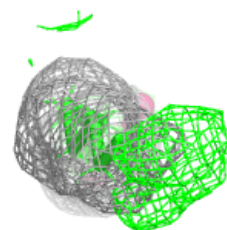
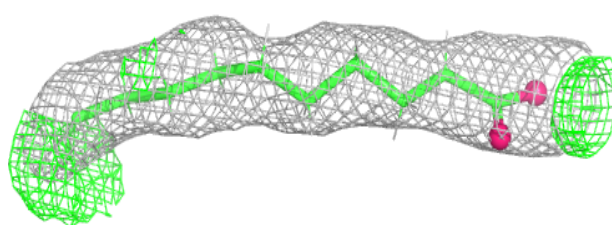
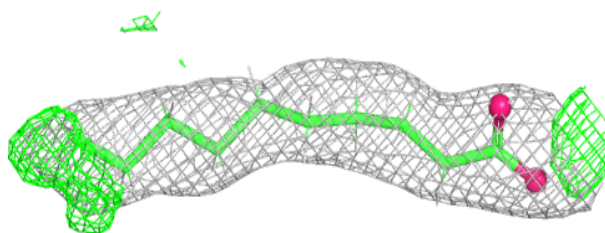
**Electron density around STE B 624:**

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

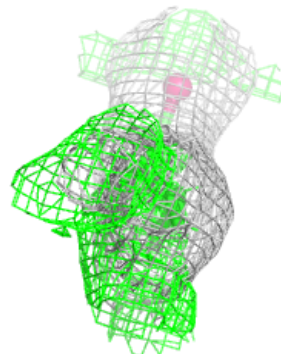
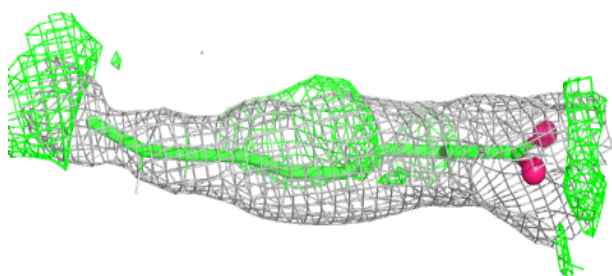
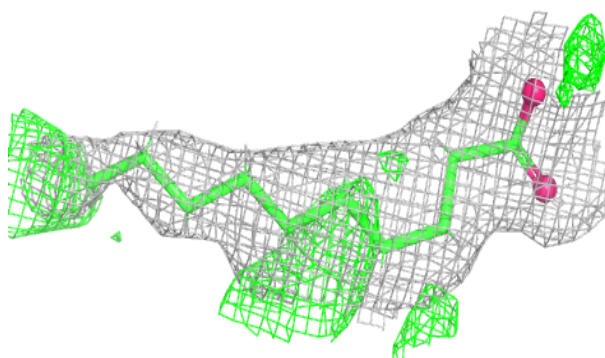


Electron density around STE j 101:

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

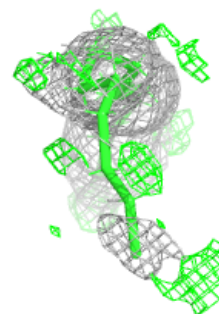
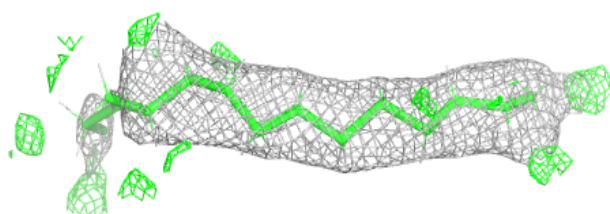
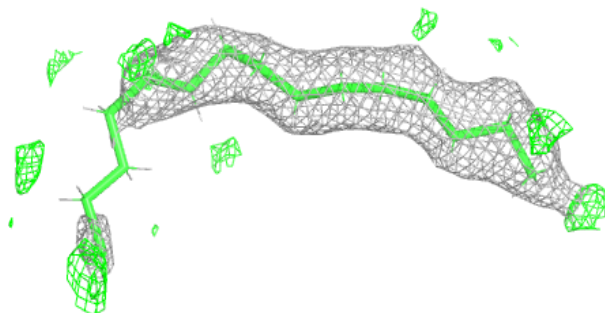
**Electron density around STE C 526:**

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

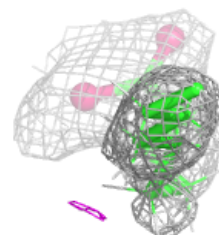
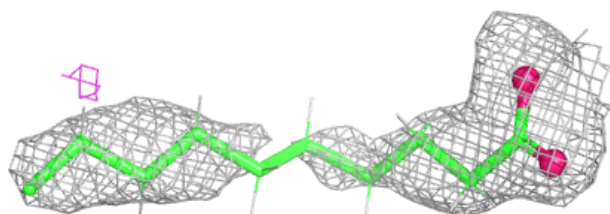
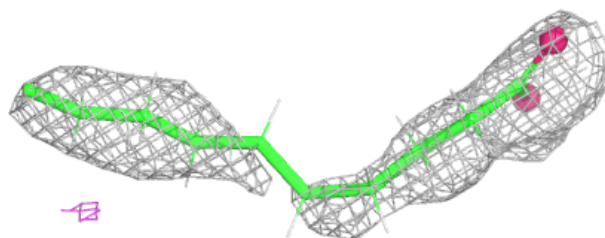


Electron density around STE M 104:

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

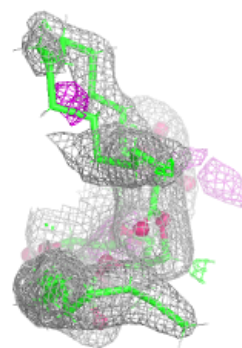
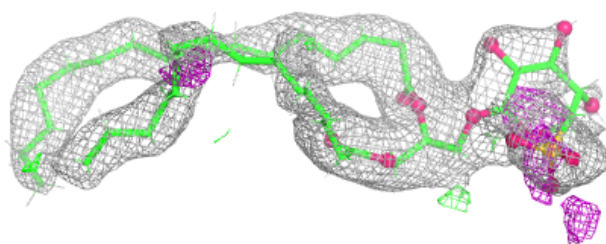
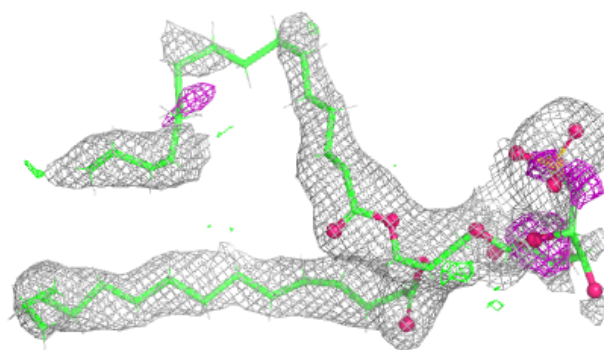
**Electron density around STE R 101:**

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

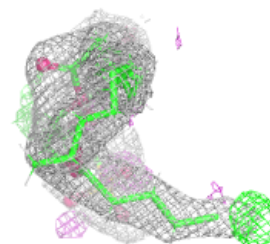
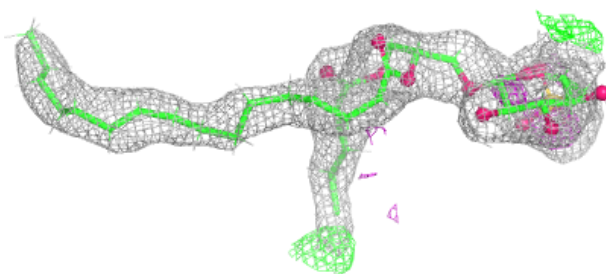
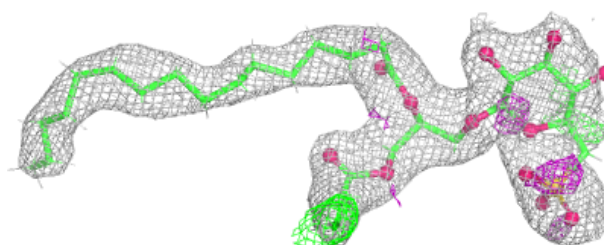


Electron density around SQD a 613:

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

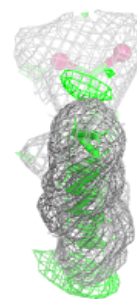
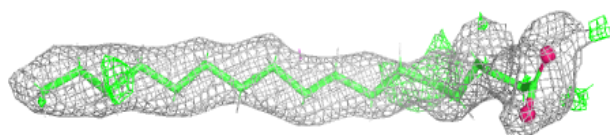
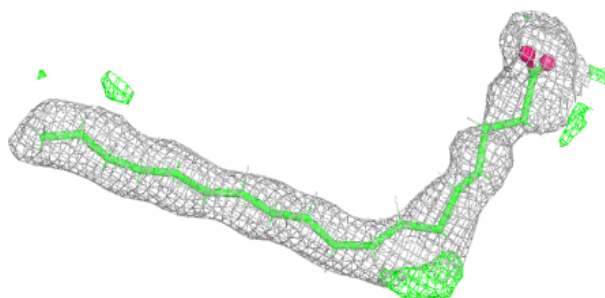
**Electron density around SQD A 614:**

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

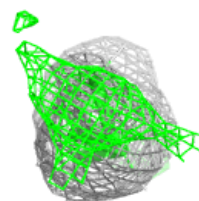
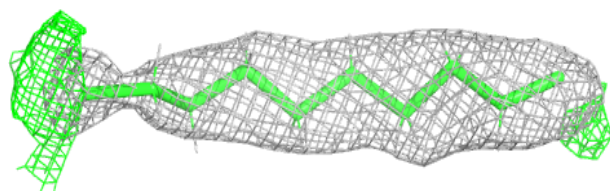
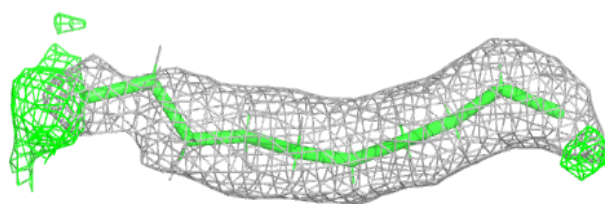


Electron density around STE d 407:

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

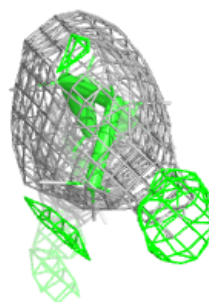
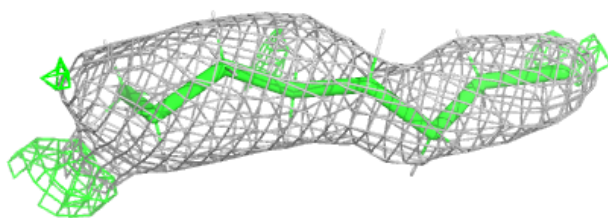
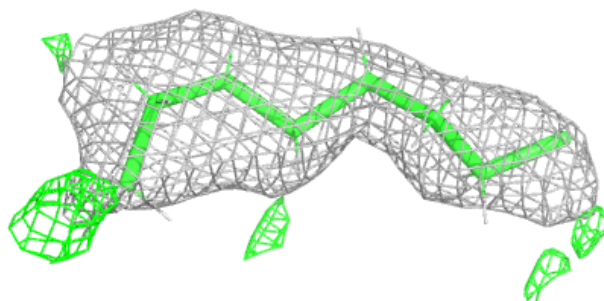
**Electron density around STE M 103:**

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

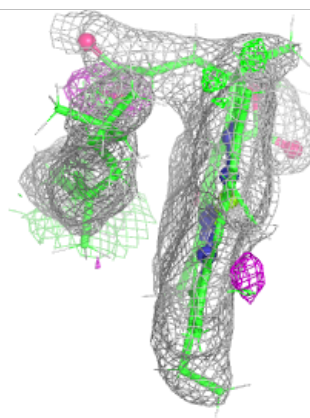
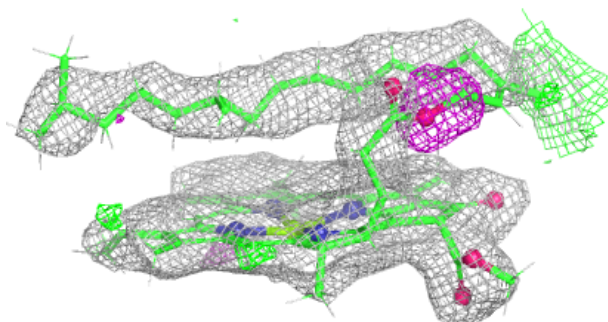
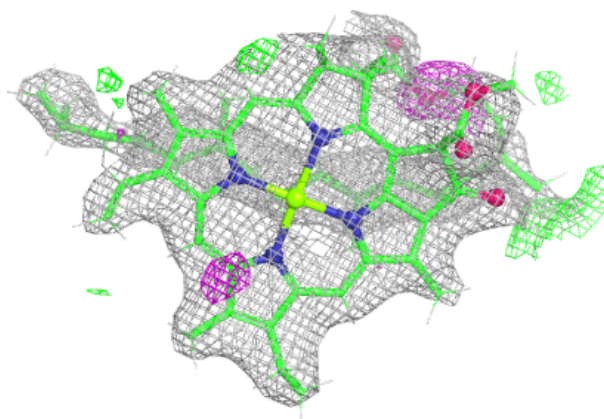


Electron density around STE A 616:

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

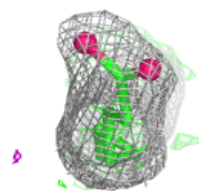
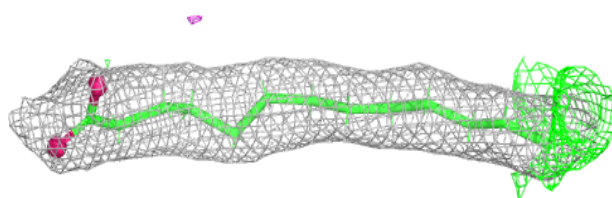
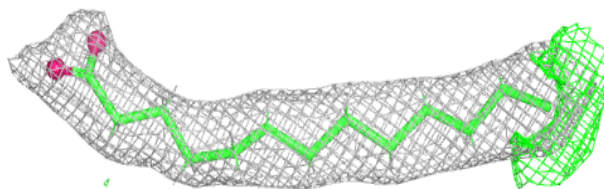
**Electron density around CLA b 601:**

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

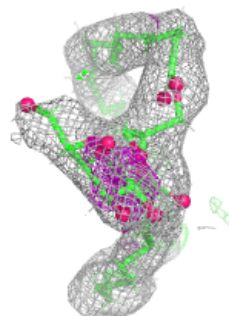
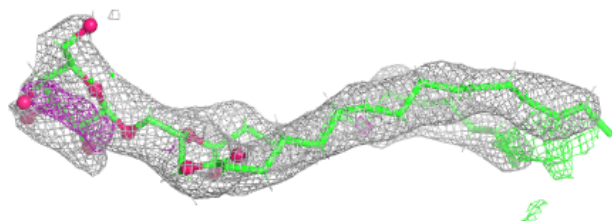
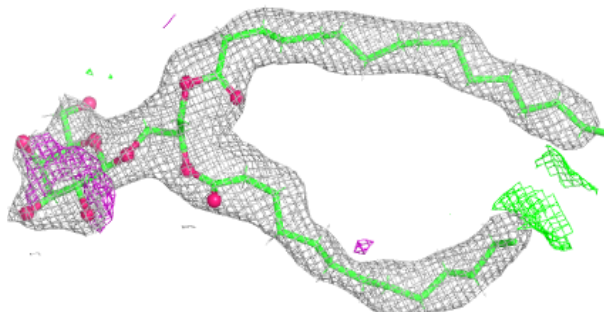


Electron density around STE M 102:

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

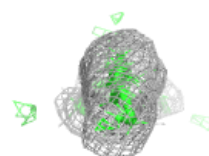
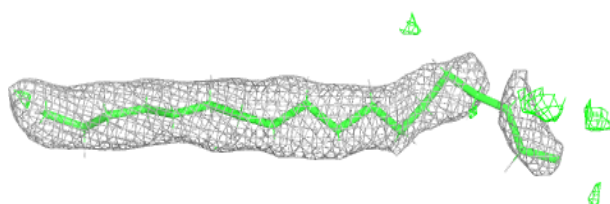
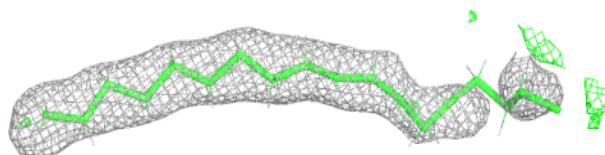
**Electron density around LMG C 521:**

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

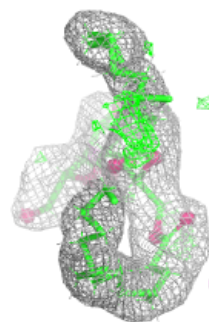
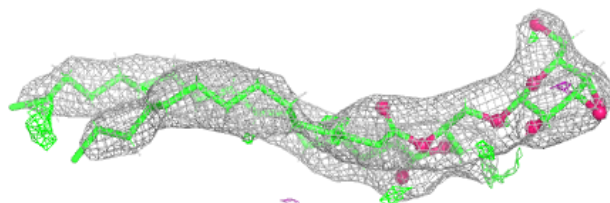
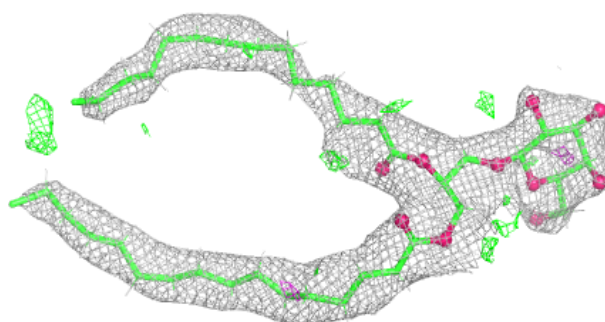


Electron density around STE m 103:

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

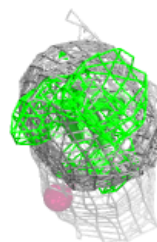
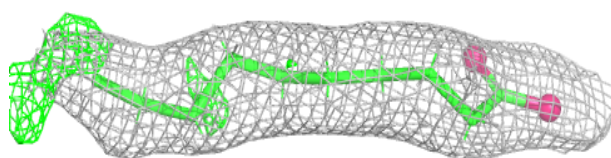
**Electron density around LMG a 615:**

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

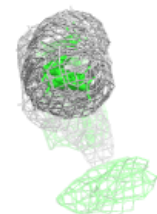
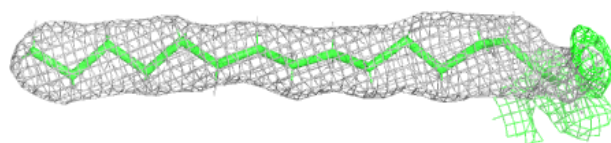
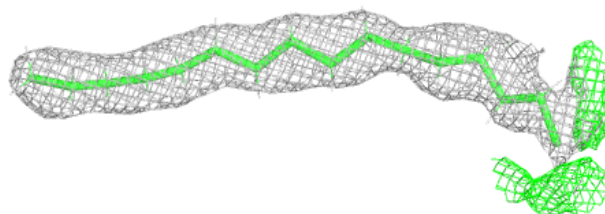


Electron density around STE J 101:

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

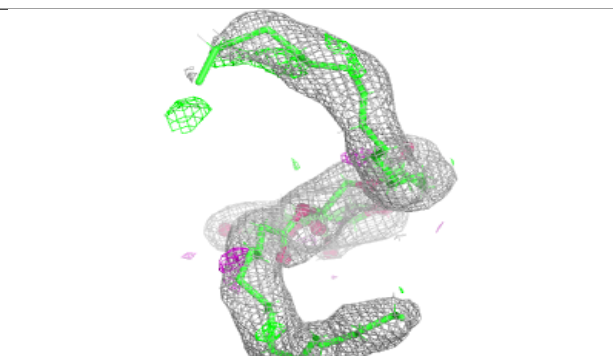
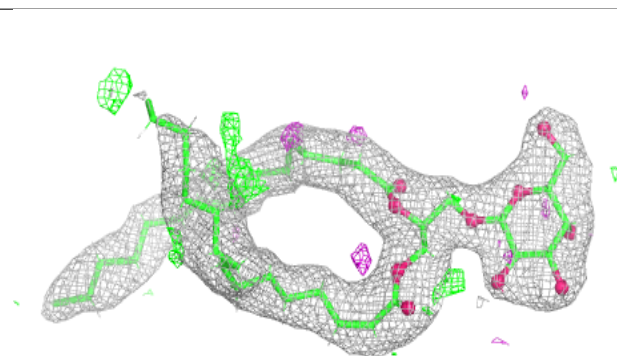
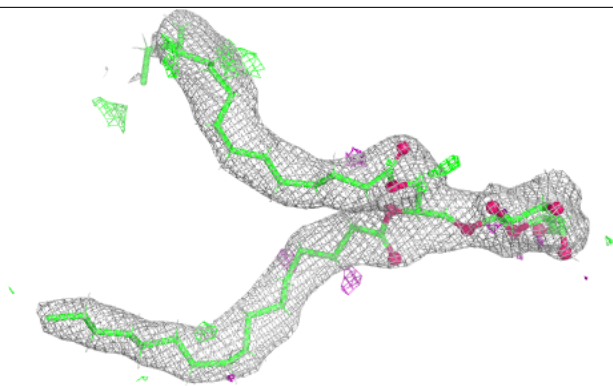
**Electron density around STE C 527:**

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

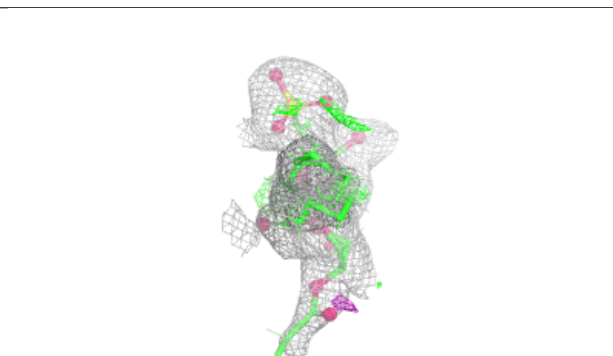
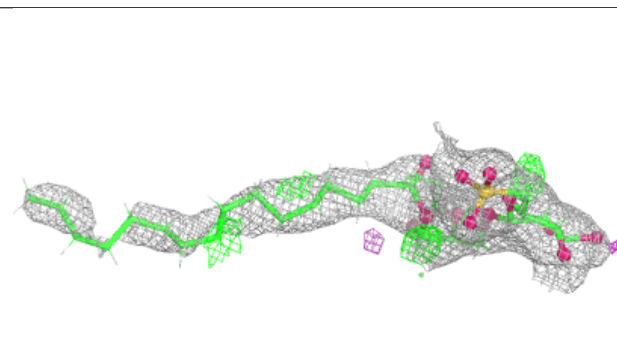
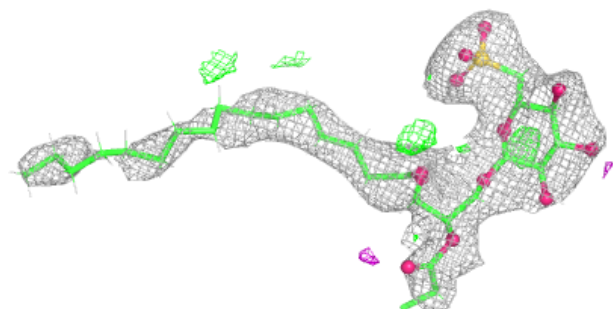


Electron density around LMG M 101:

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

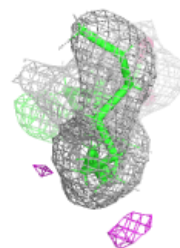
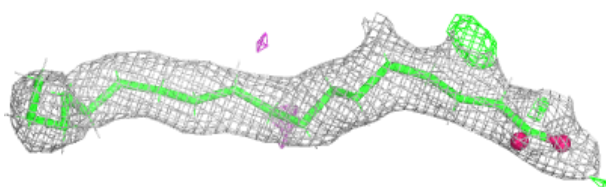
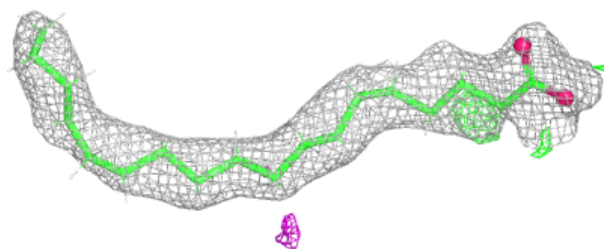
**Electron density around SQD f 102:**

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

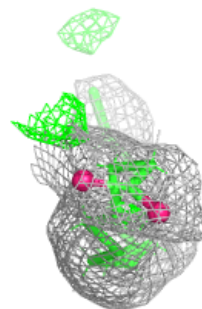
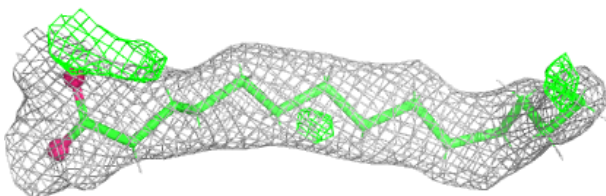
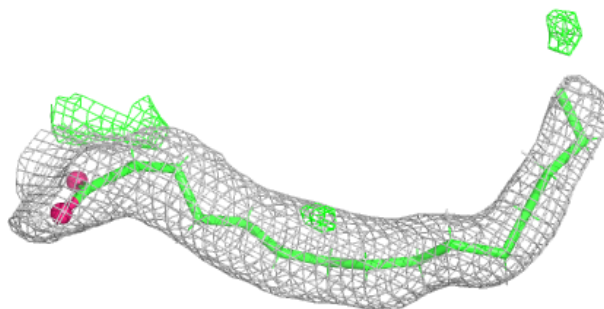


Electron density around STE b 621:

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

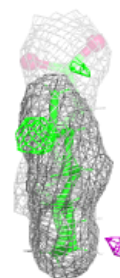
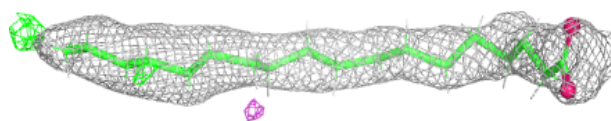
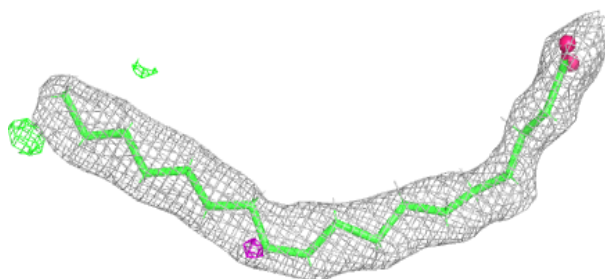
**Electron density around STE B 621:**

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

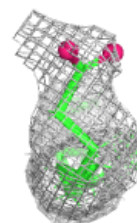
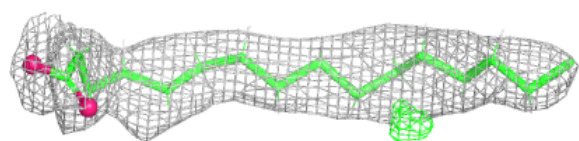
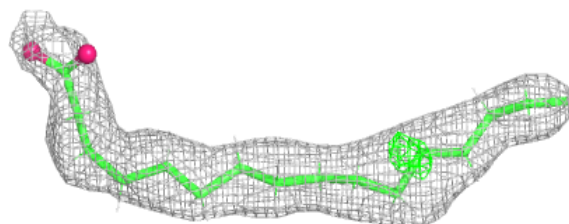


Electron density around STE d 413:

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

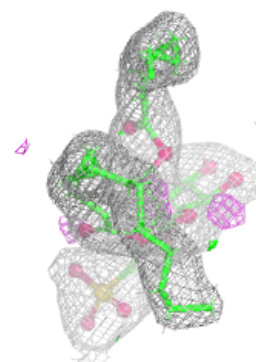
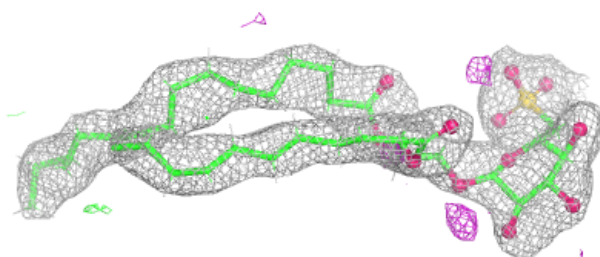
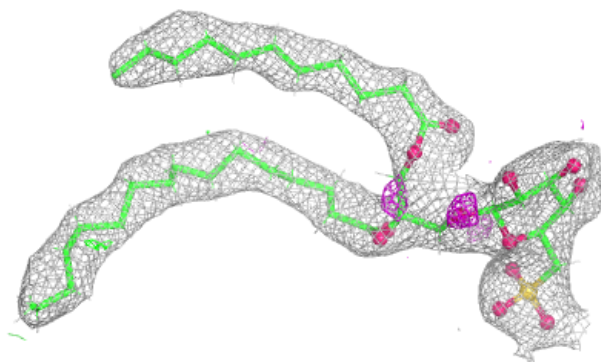
**Electron density around STE B 623:**

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

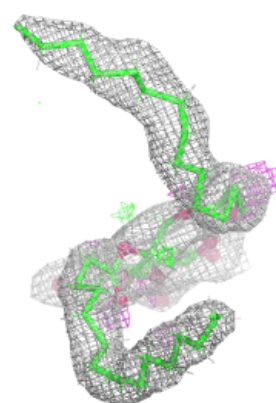
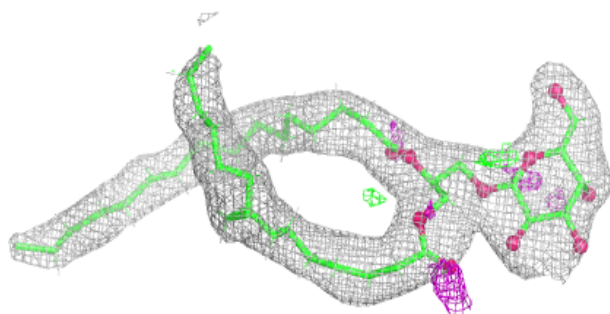
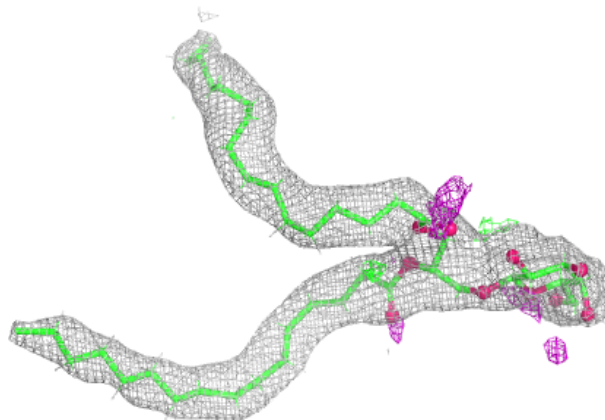


Electron density around SQD b 620:

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

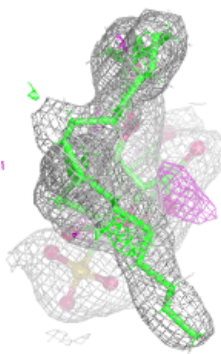
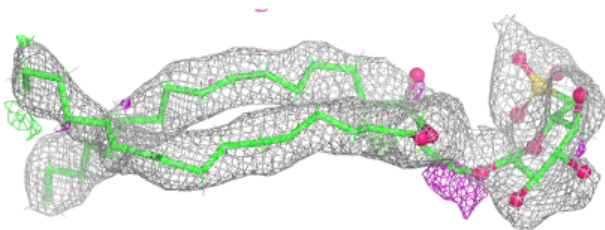
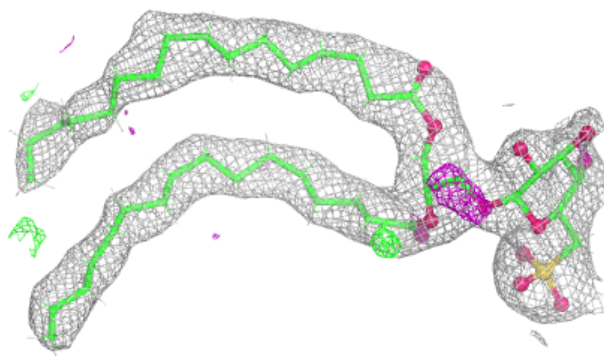
**Electron density around LMG m 101:**

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

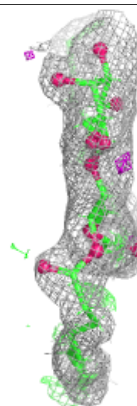
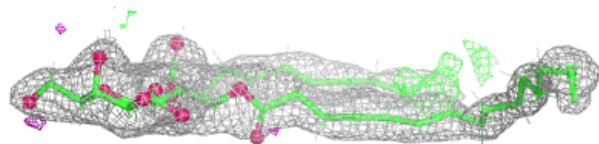
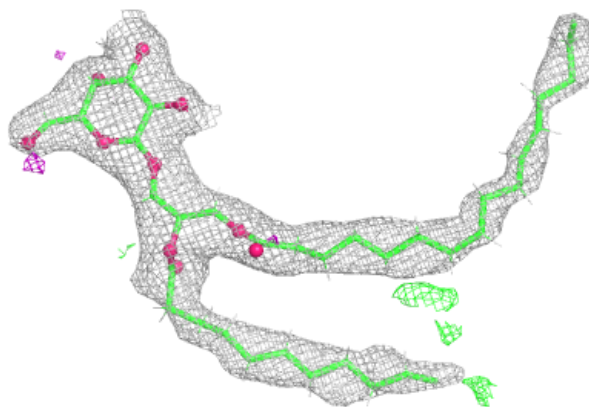


Electron density around SQD B 622:

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

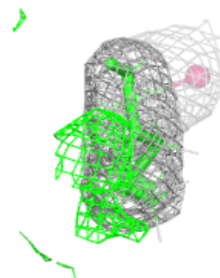
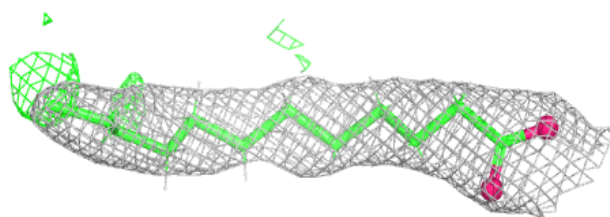
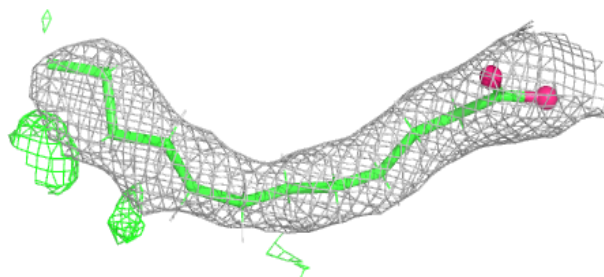
**Electron density around LMG c 522:**

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

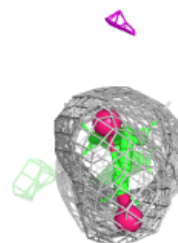
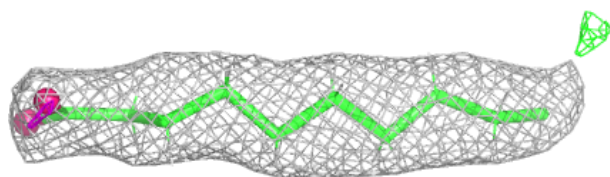
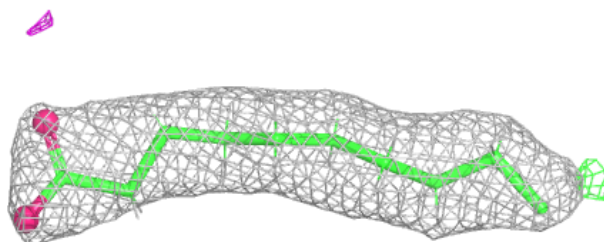


Electron density around STE t 102:

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

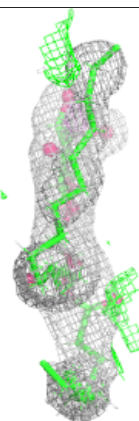
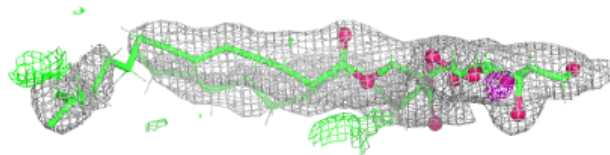
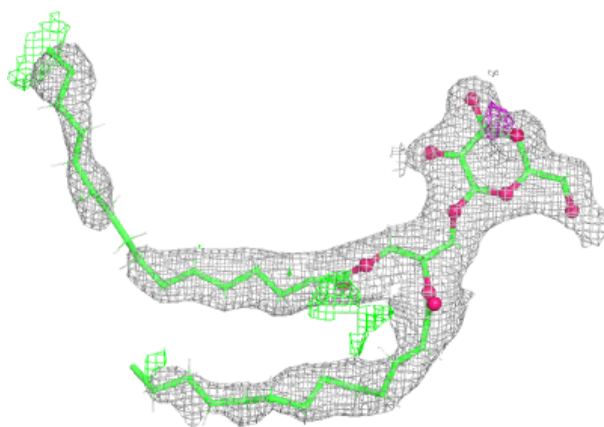
**Electron density around STE m 102:**

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

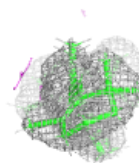
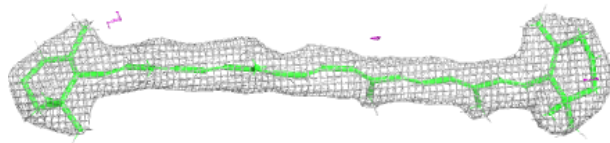
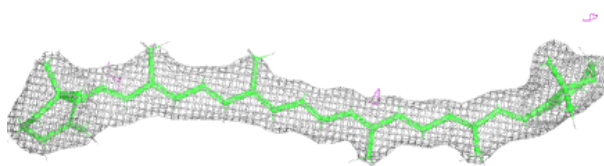


Electron density around LMG C 525:

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

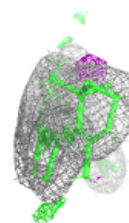
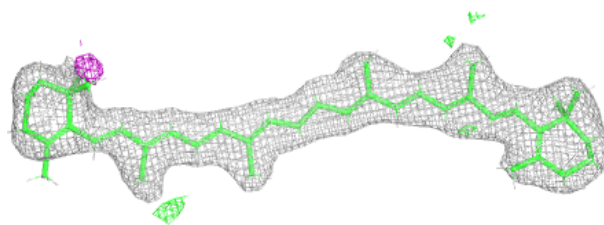
**Electron density around BCR C 514:**

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



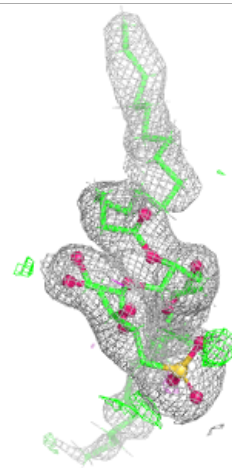
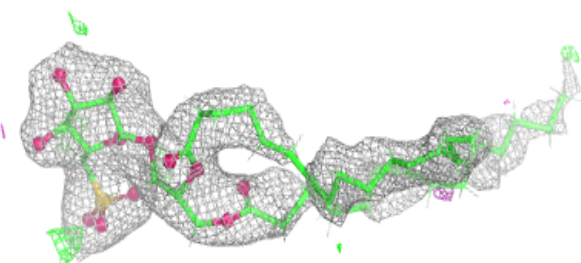
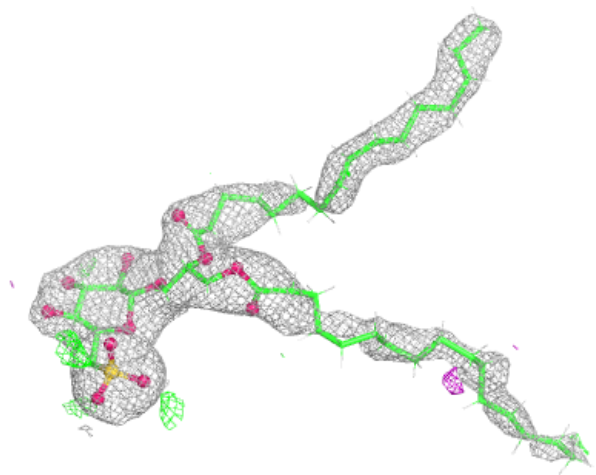
Electron density around BCR d 405:

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



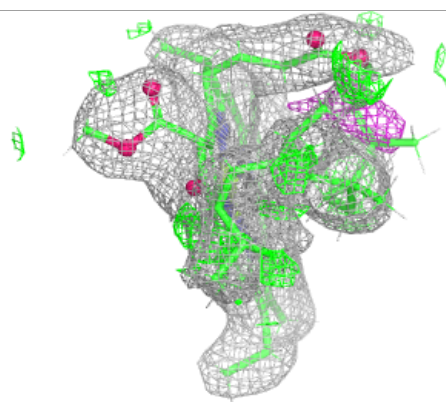
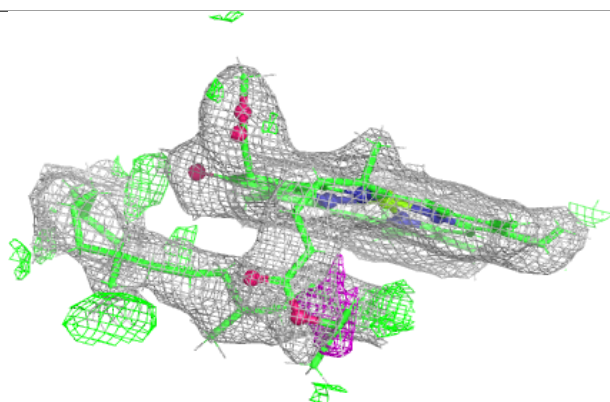
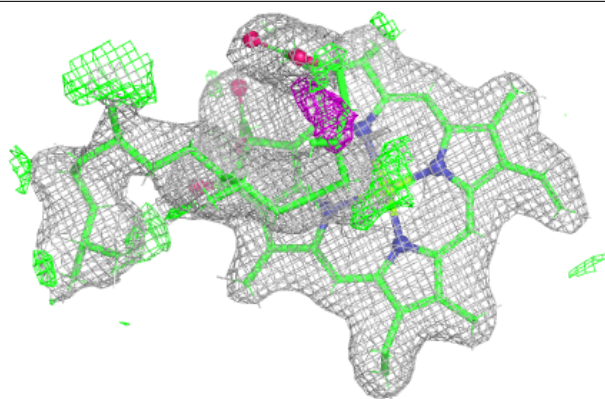
Electron density around SQD a 612:

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

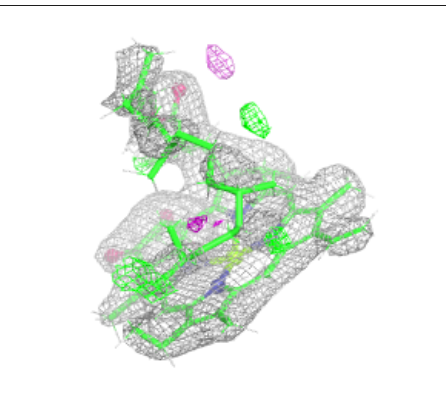
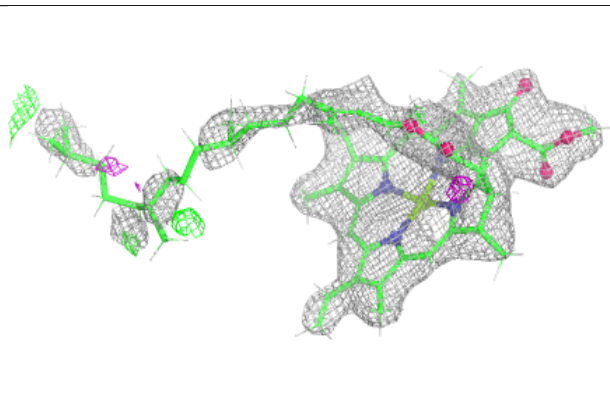
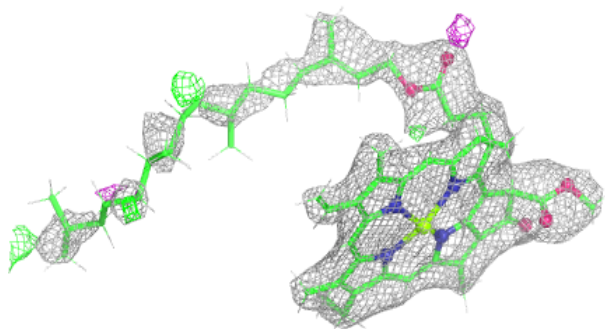


Electron density around CLA B 601:

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

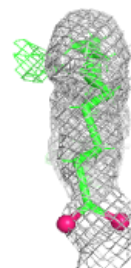
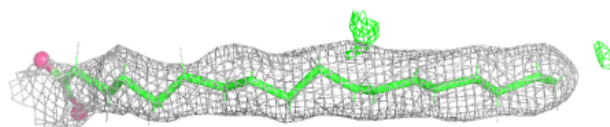
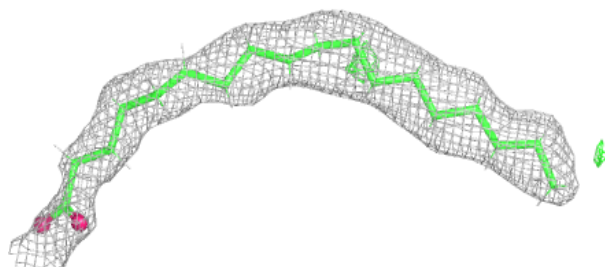
**Electron density around CLA c 513:**

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

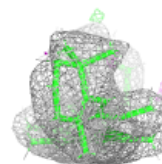
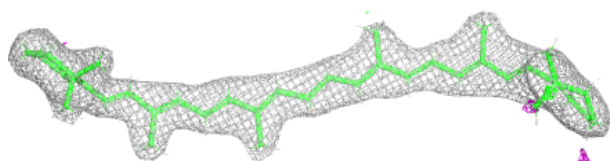
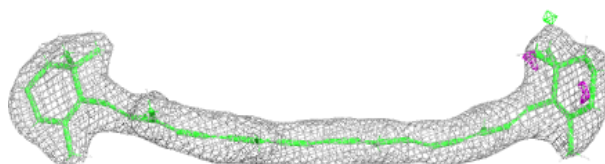


Electron density around STE D 414:

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

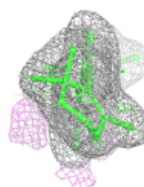
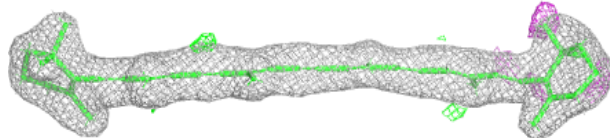
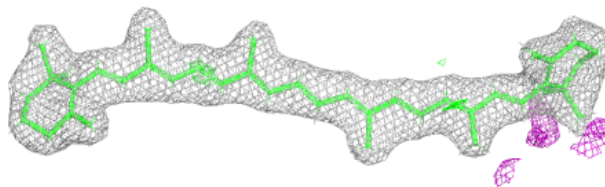
**Electron density around BCR k 102:**

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



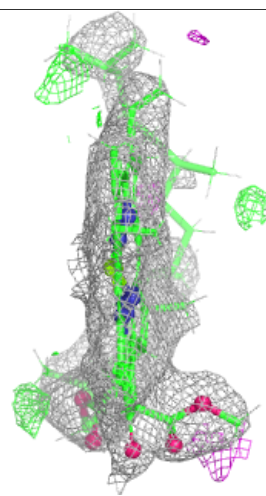
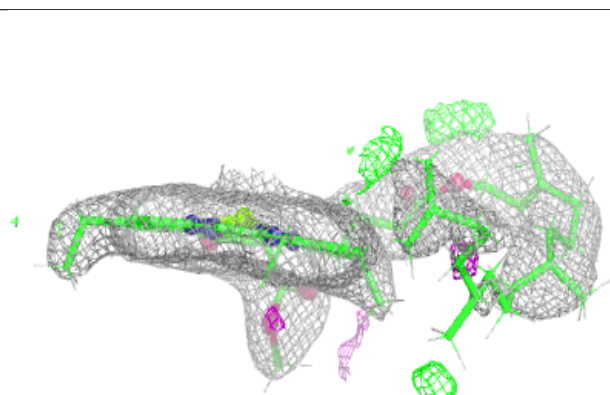
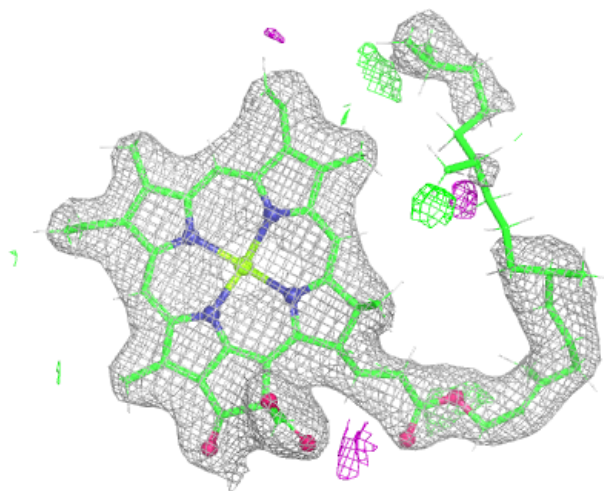
Electron density around BCR B 618:

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



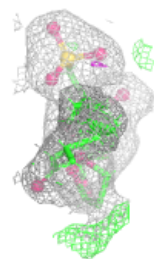
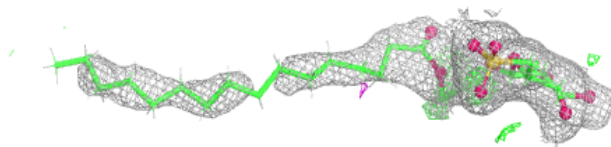
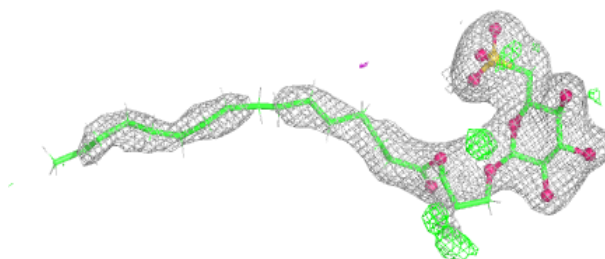
Electron density around CLA c 512:

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



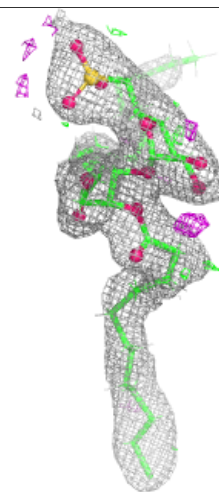
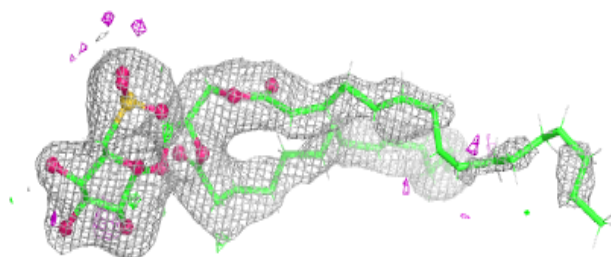
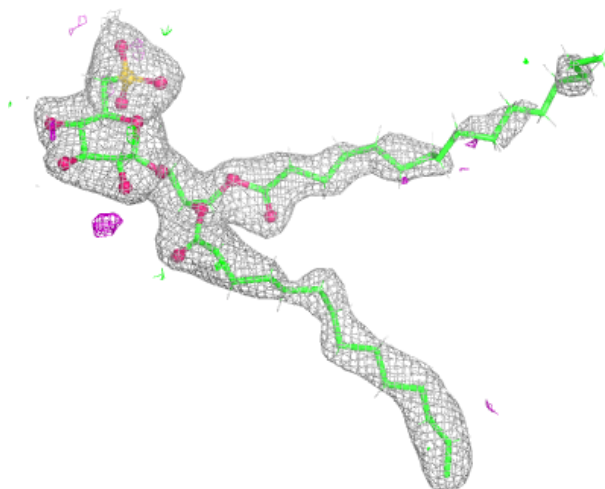
Electron density around SQD D 409:

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



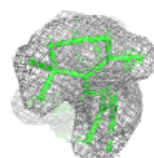
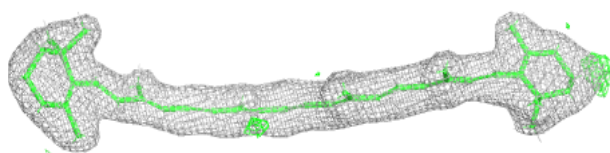
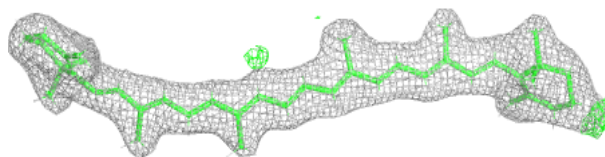
Electron density around SQD D 412:

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

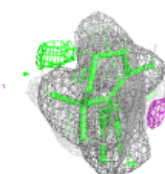
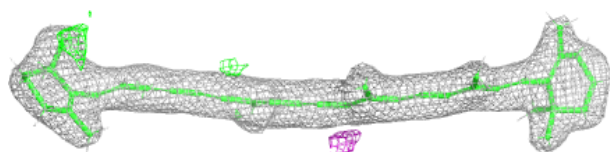
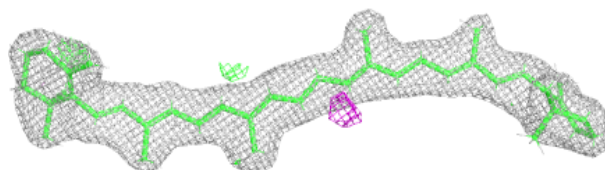


Electron density around BCR H 101:

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

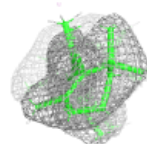
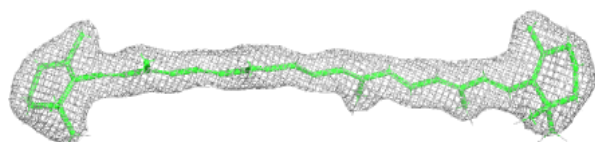
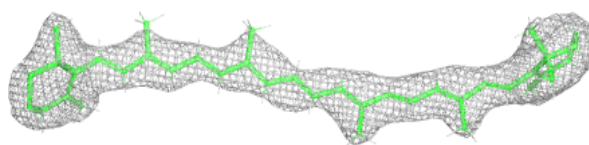
**Electron density around BCR K 101:**

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

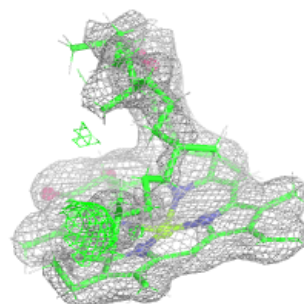
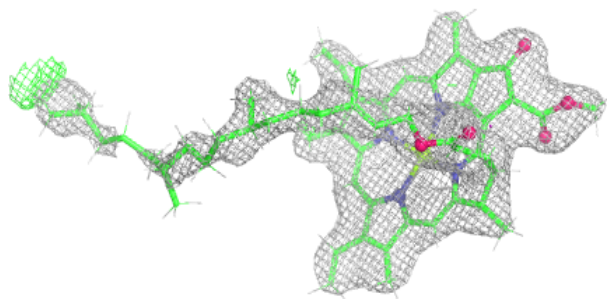
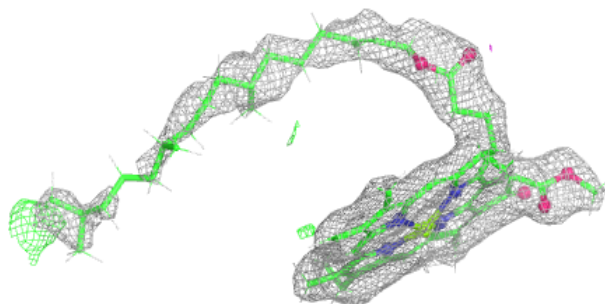


Electron density around BCR c 514:

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

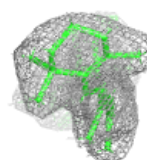
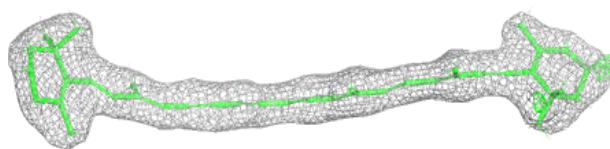
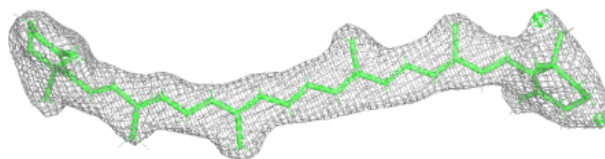
**Electron density around CLA C 513:**

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

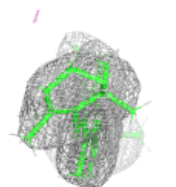
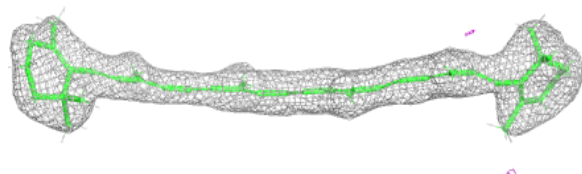
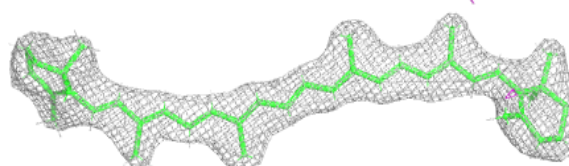


Electron density around BCR h 101:

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

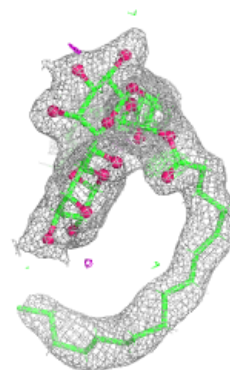
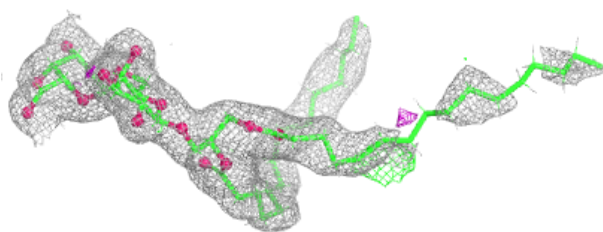
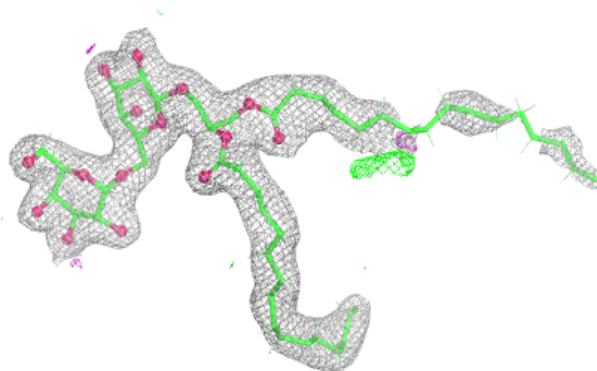
**Electron density around BCR k 101:**

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

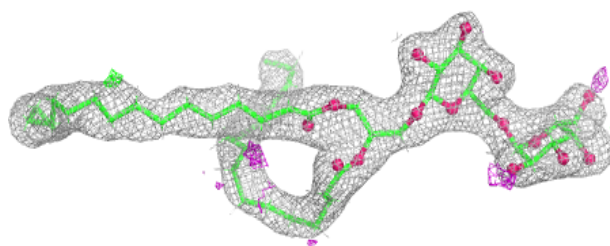
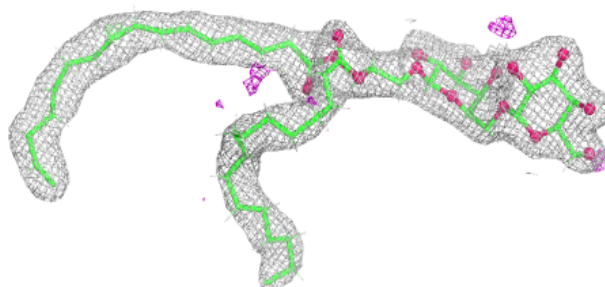


Electron density around DGD c 520:

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

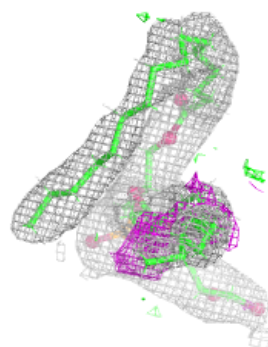
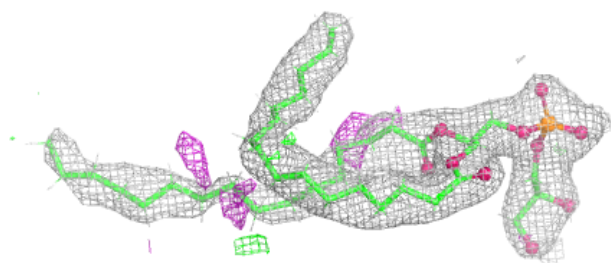
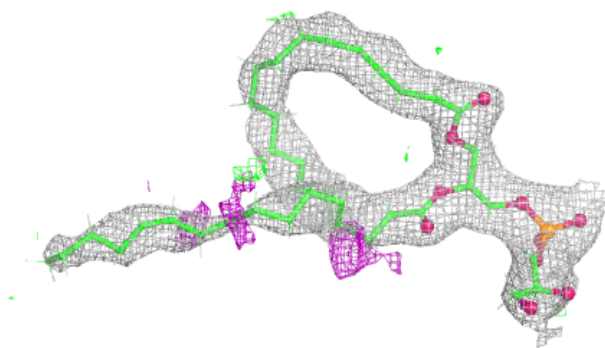
**Electron density around DGD h 102:**

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

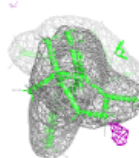
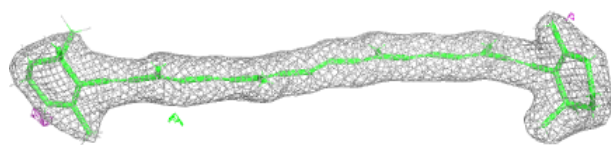
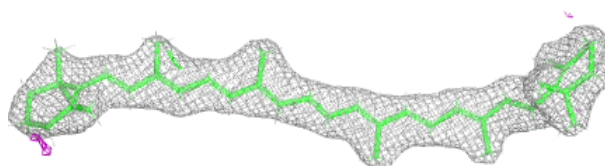


Electron density around LHG d 408:

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

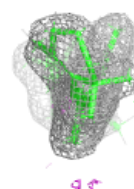
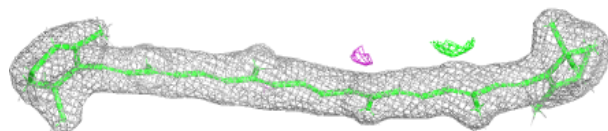
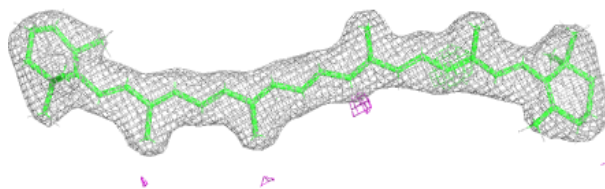
**Electron density around BCR c 515:**

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



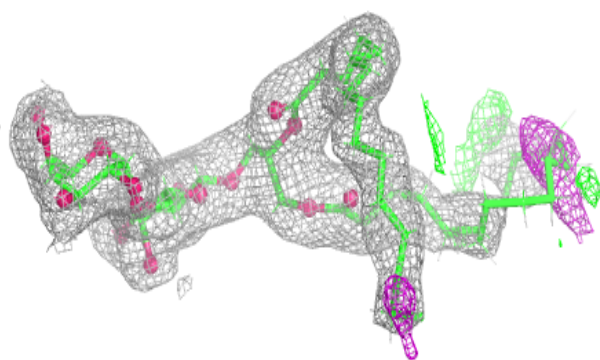
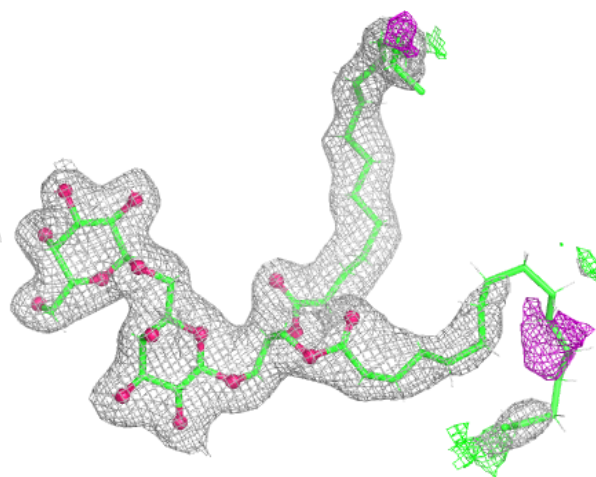
Electron density around BCR b 619:

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



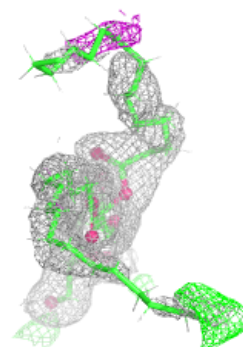
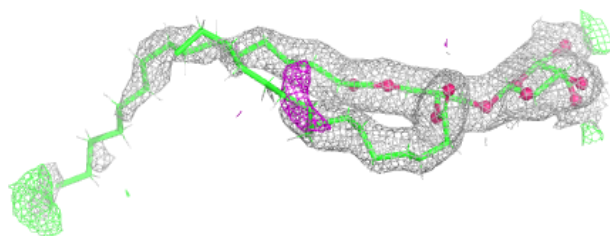
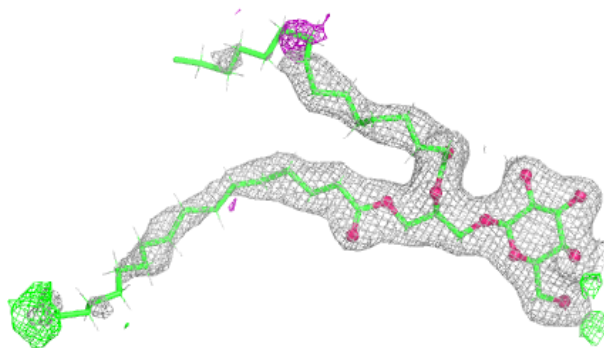
Electron density around DGD C 523:

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

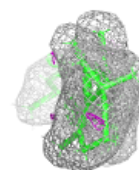
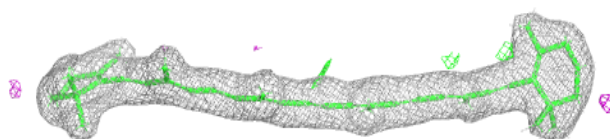
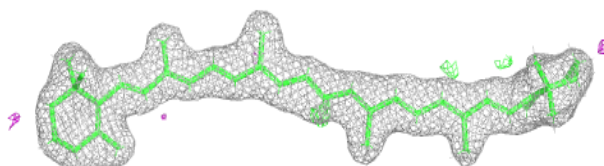


Electron density around LMG D 408:

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

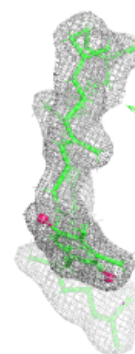
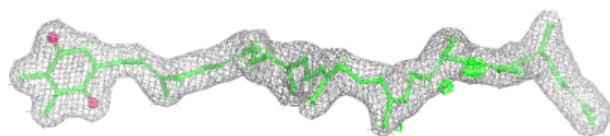
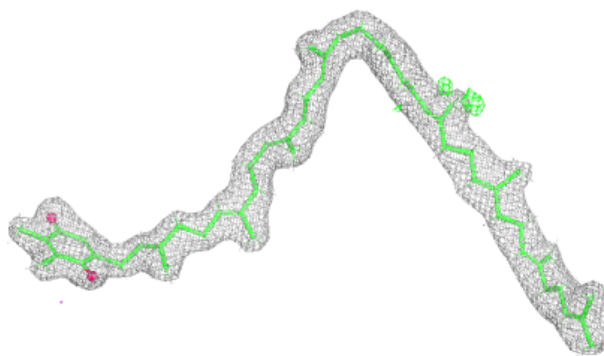
**Electron density around BCR B 617:**

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



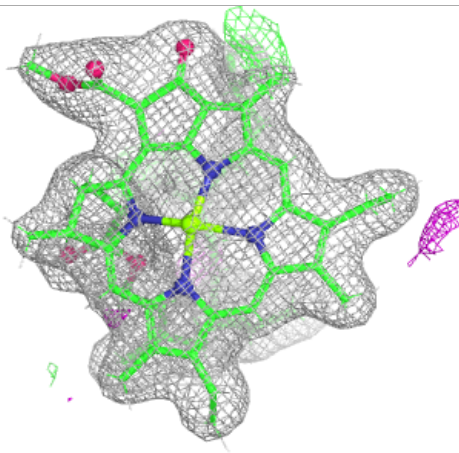
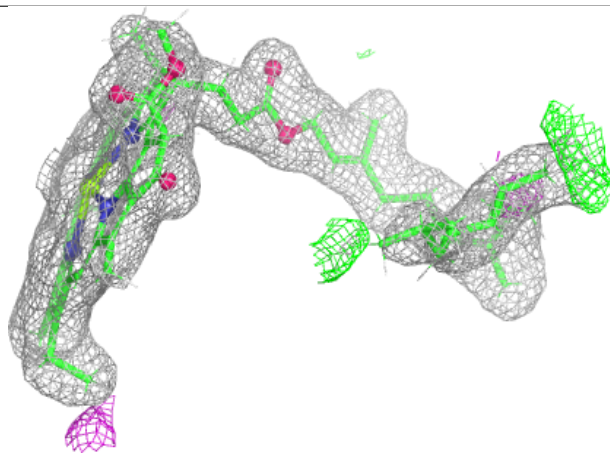
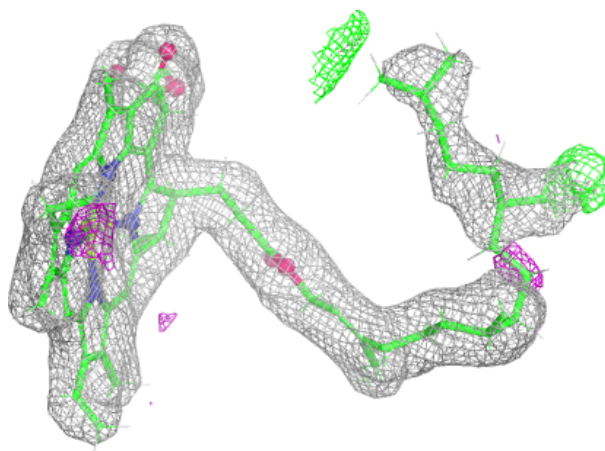
Electron density around PL9 d 406:

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



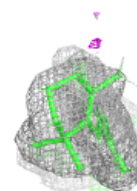
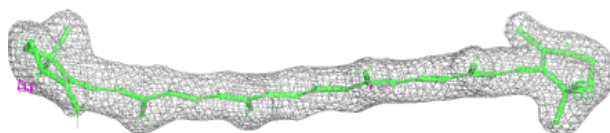
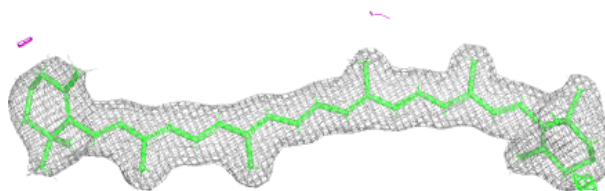
Electron density around CLA B 606:

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



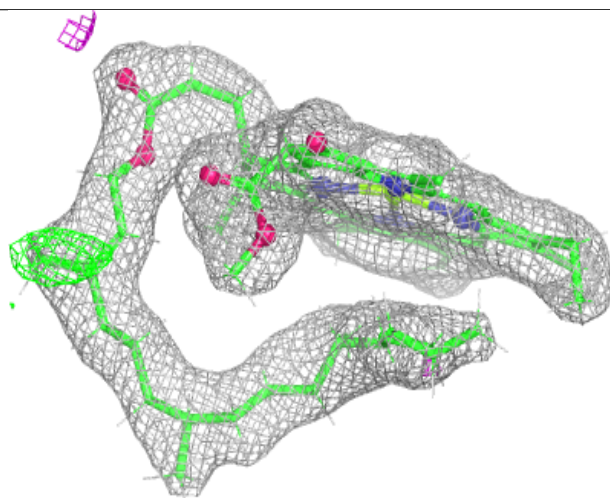
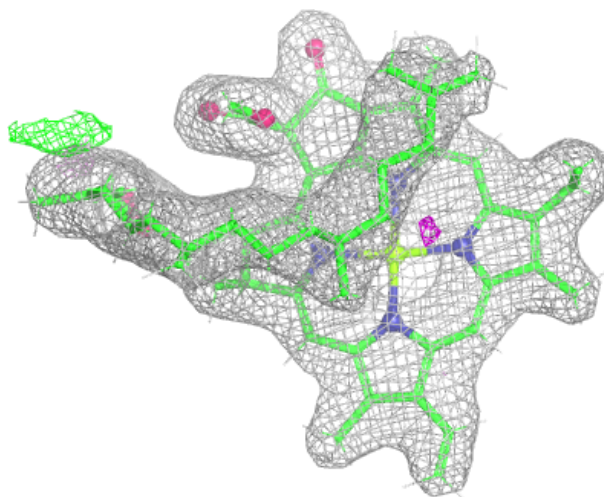
Electron density around BCR B 619:

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



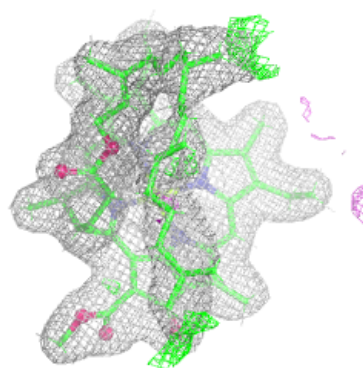
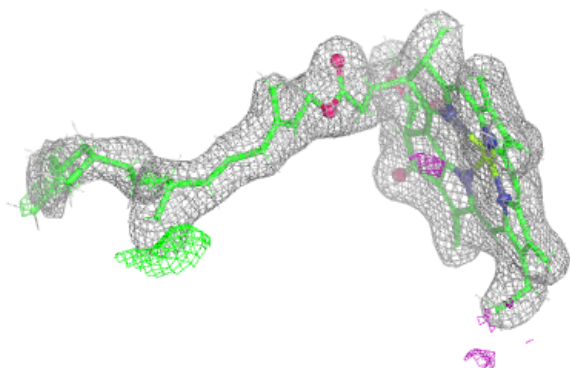
Electron density around CLA C 510:

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

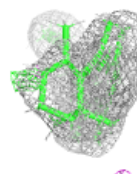
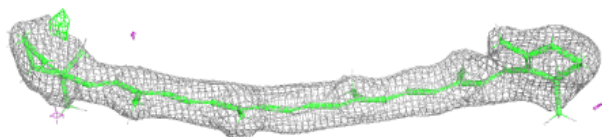
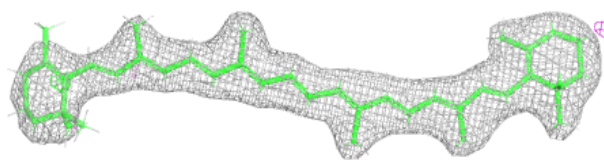


Electron density around CLA b 606:

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

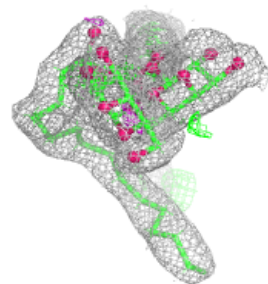
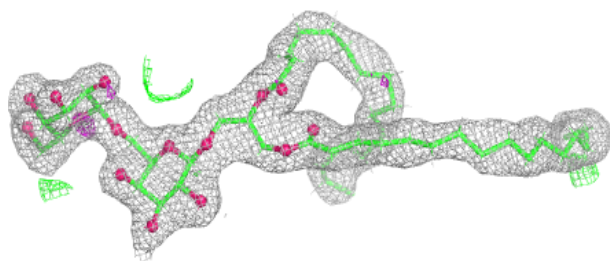
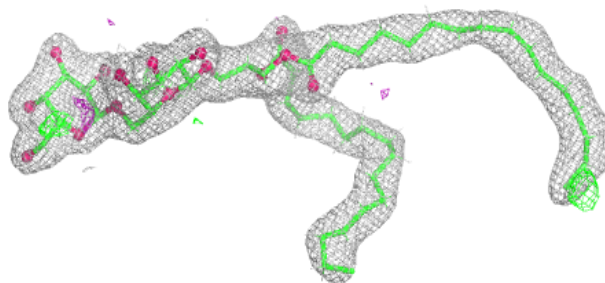
**Electron density around BCR D 405:**

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



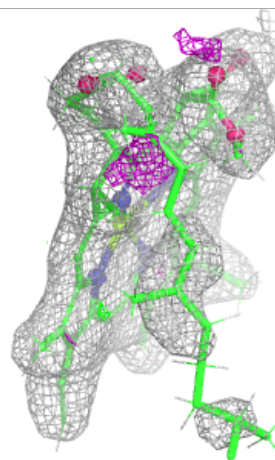
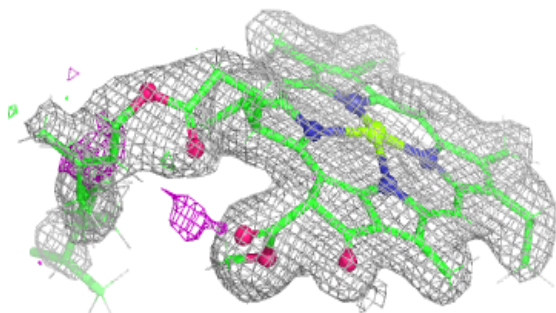
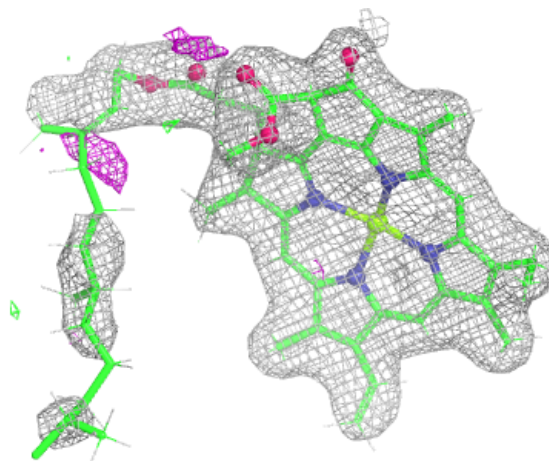
Electron density around DGD H 102:

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



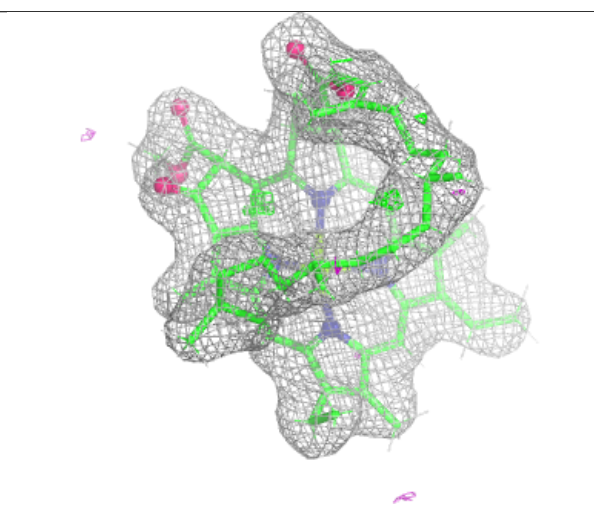
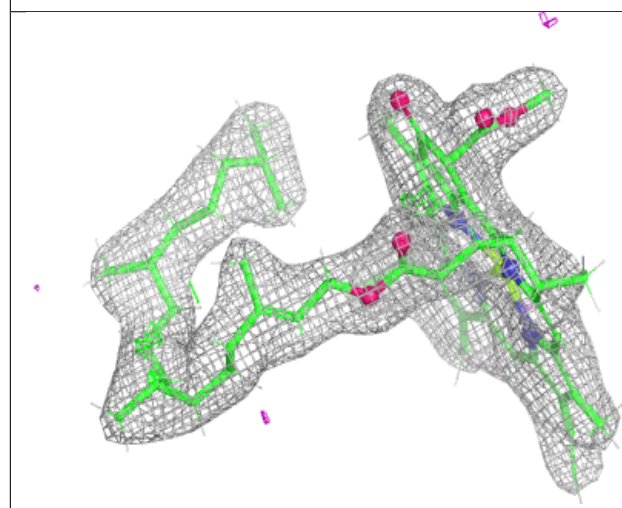
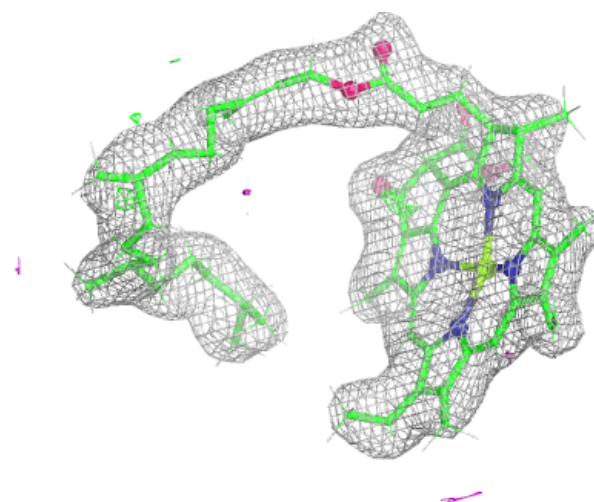
Electron density around CLA b 616:

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



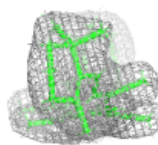
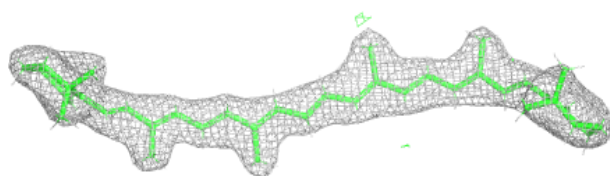
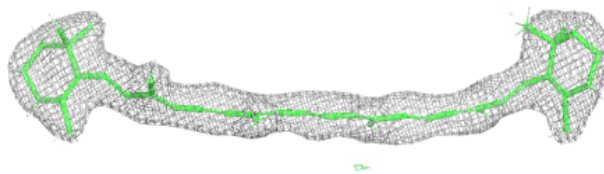
Electron density around CLA c 503:

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

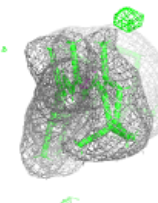
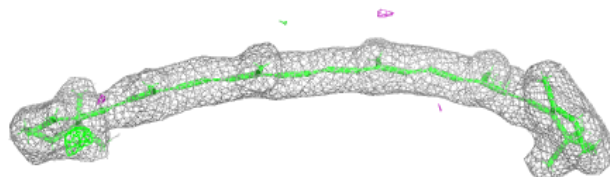
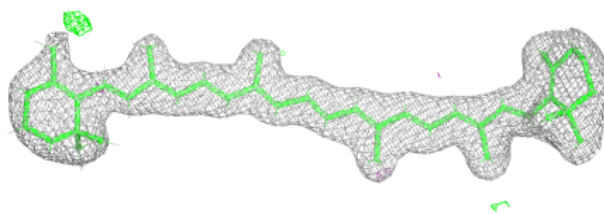


Electron density around BCR K 102:

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

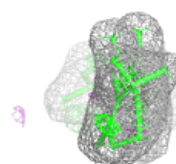
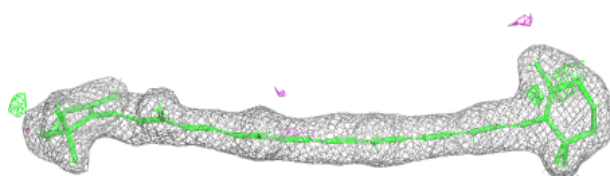
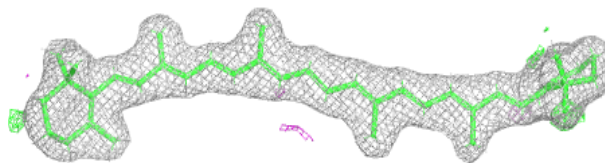
**Electron density around BCR T 101:**

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

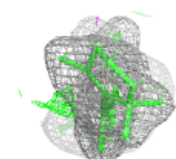
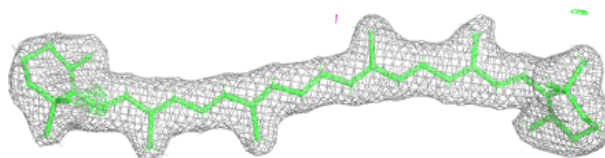


Electron density around BCR b 617:

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

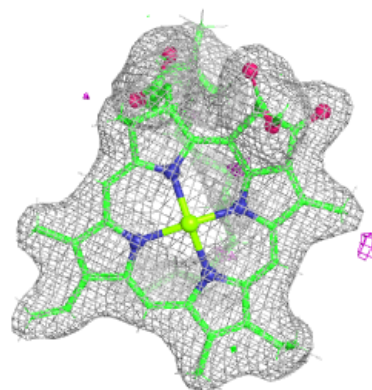
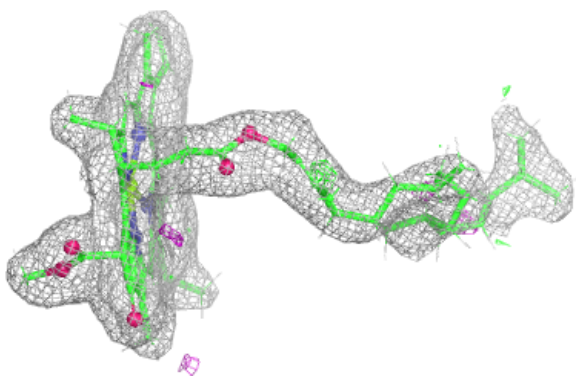
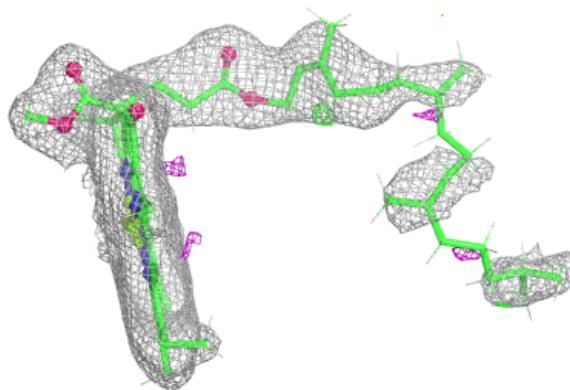
**Electron density around BCR b 618:**

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



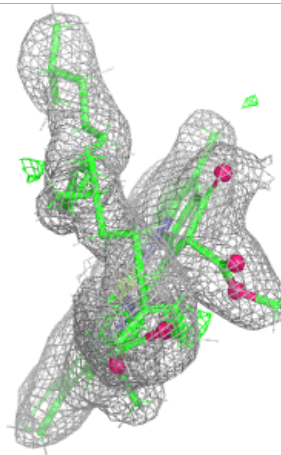
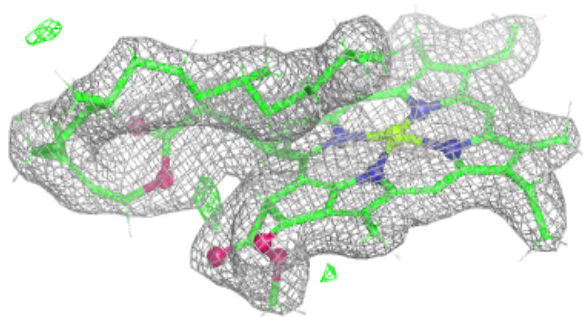
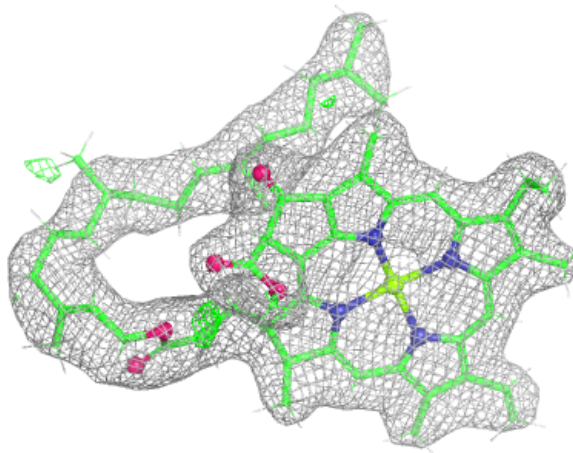
Electron density around CLA c 506:

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



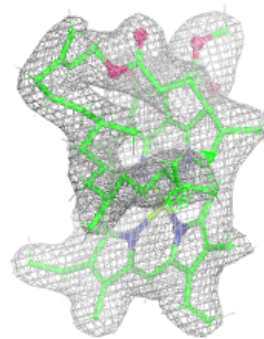
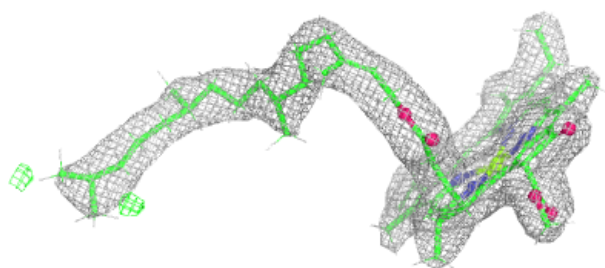
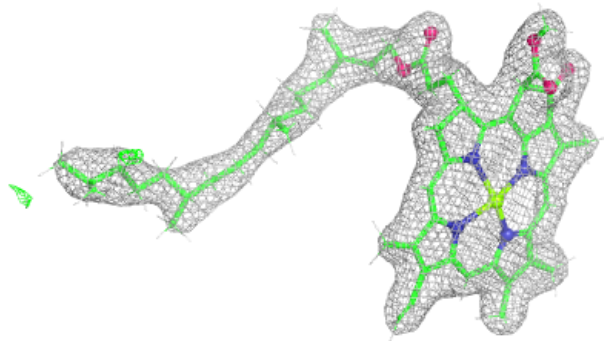
Electron density around CLA c 509:

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

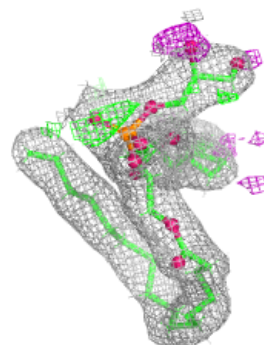
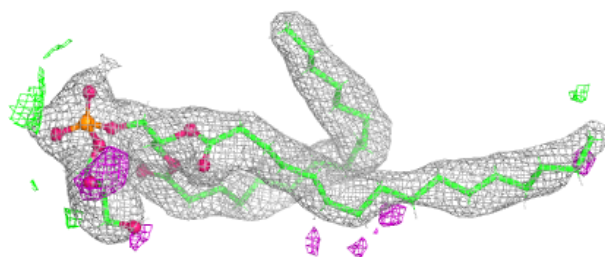
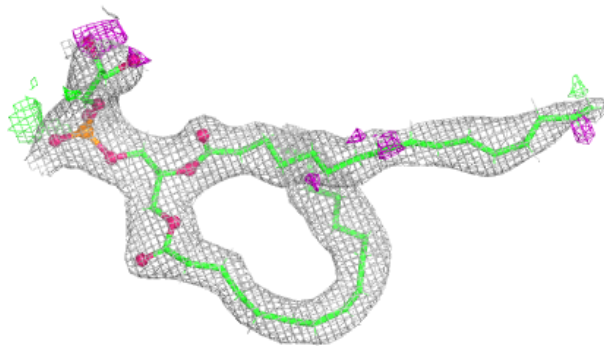


Electron density around CLA c 511:

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

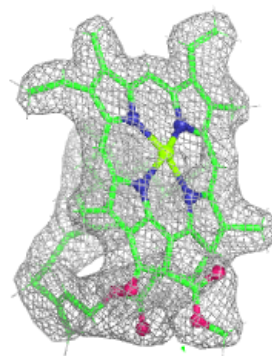
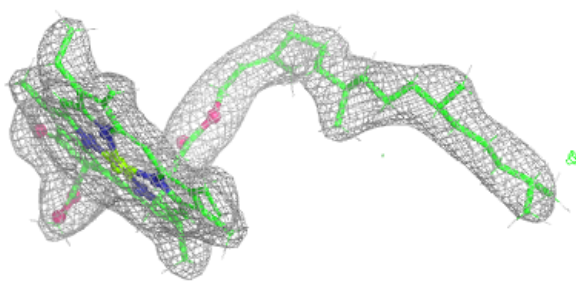
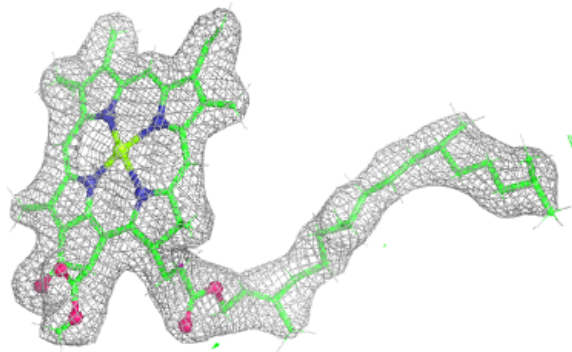
**Electron density around LHG D 413:**

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

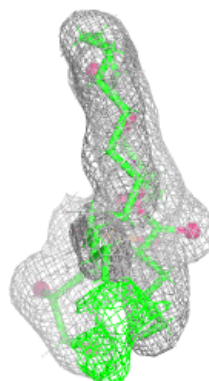
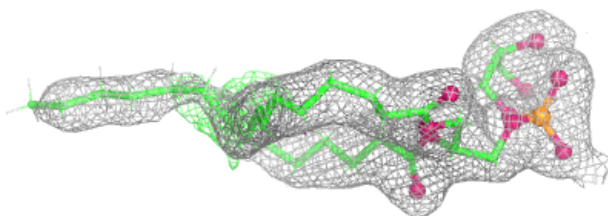
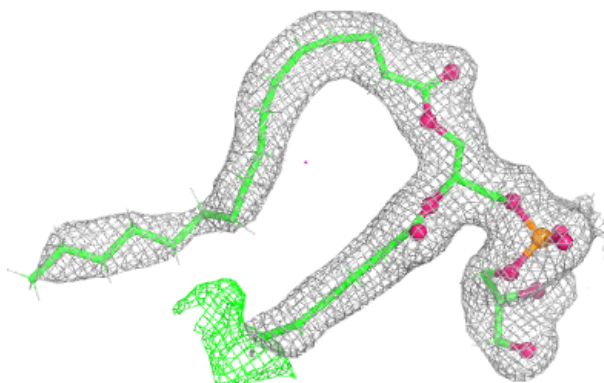


Electron density around CLA C 511:

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

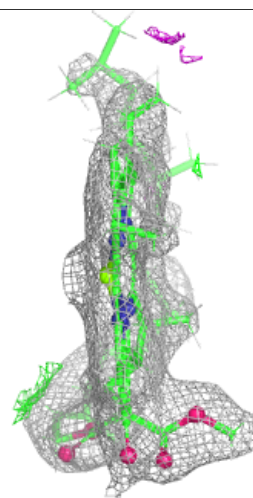
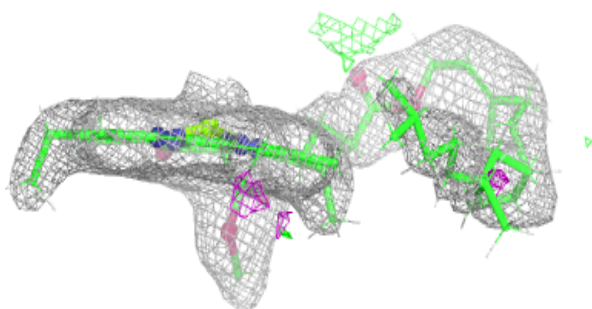
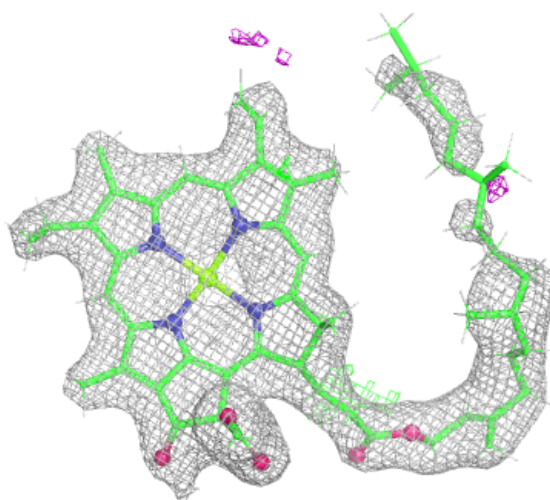
**Electron density around LHG d 410:**

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



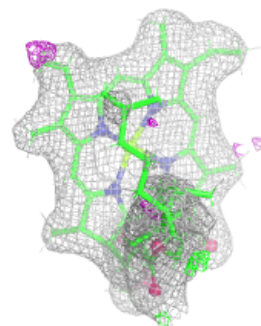
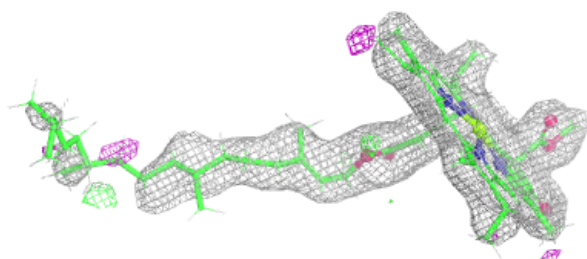
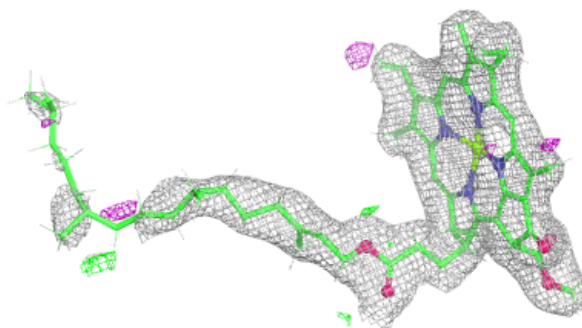
Electron density around CLA C 512:

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



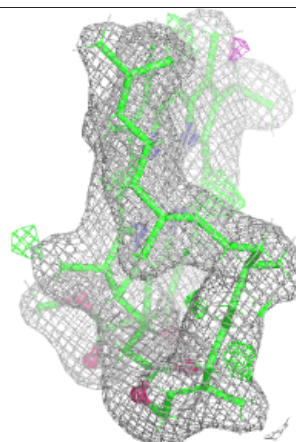
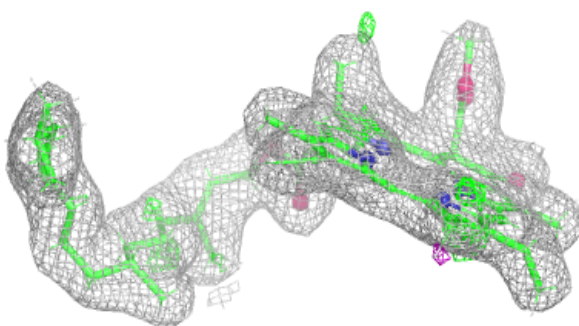
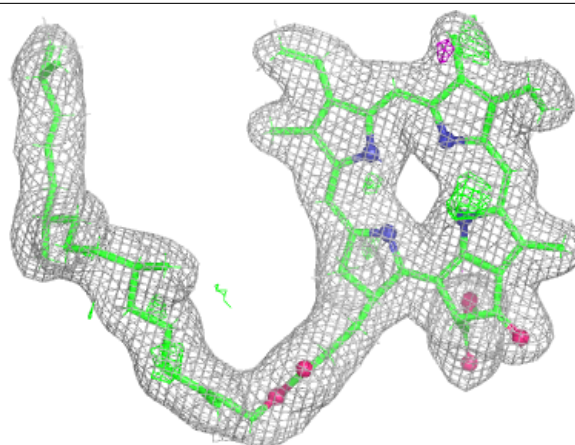
Electron density around CLA d 404:

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

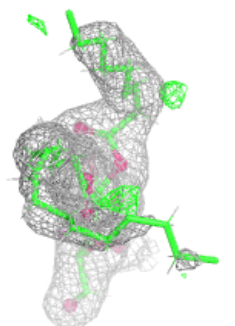
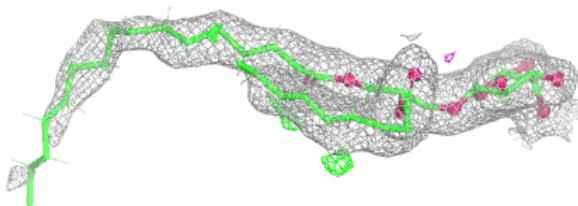
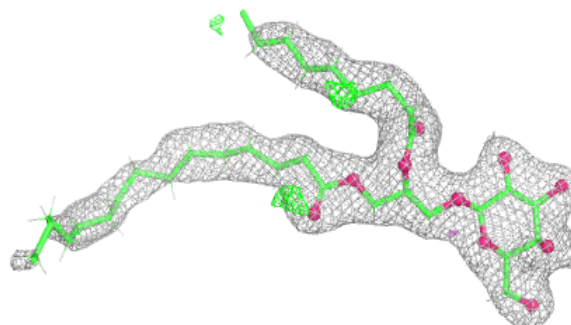


Electron density around PHO D 402:

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

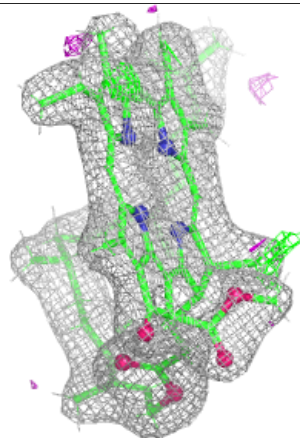
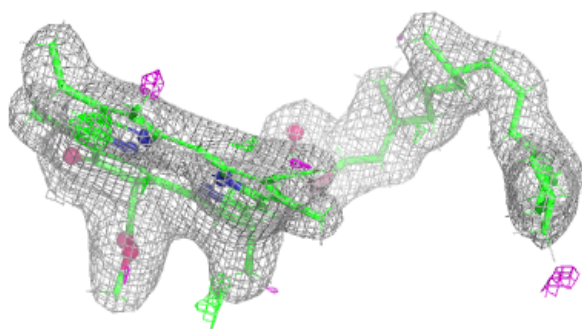
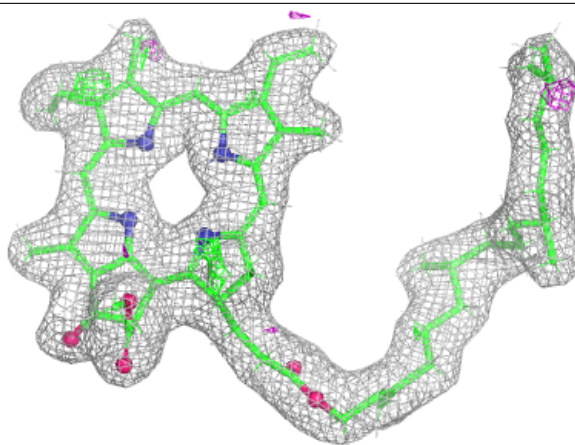
**Electron density around LMG d 412:**

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

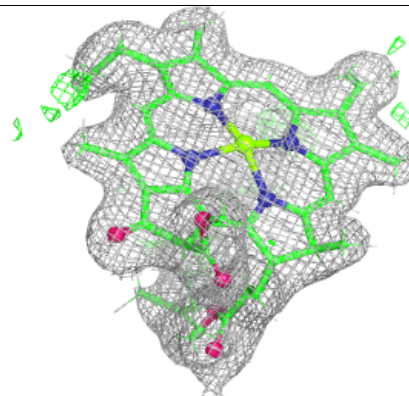
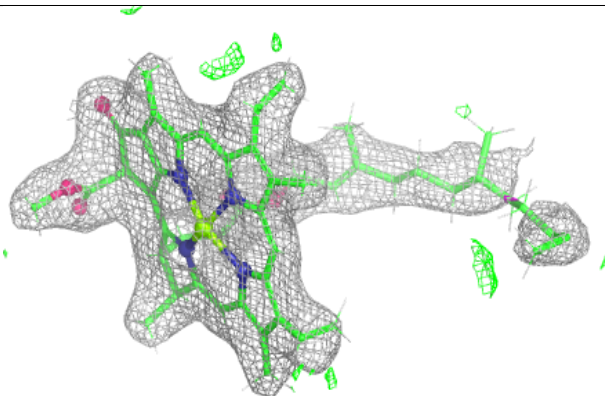
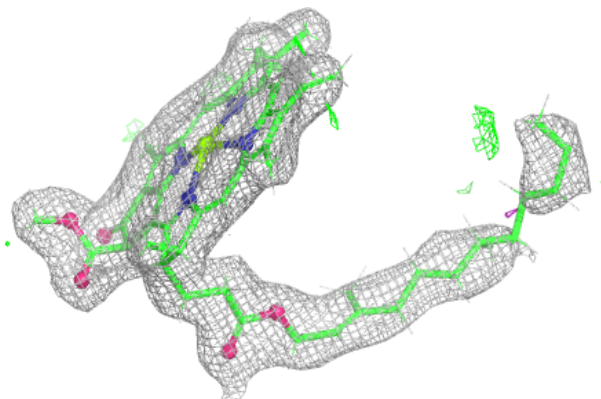


Electron density around PHO d 402:

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

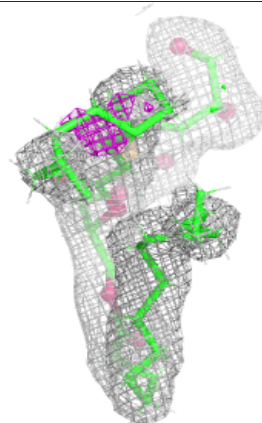
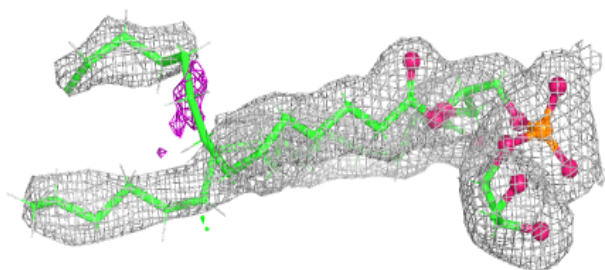
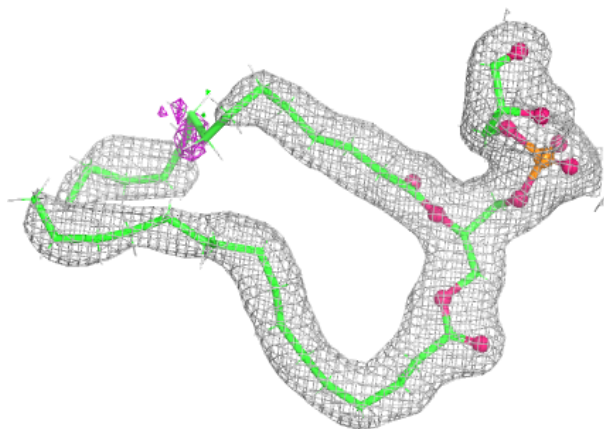
**Electron density around CLA C 504:**

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

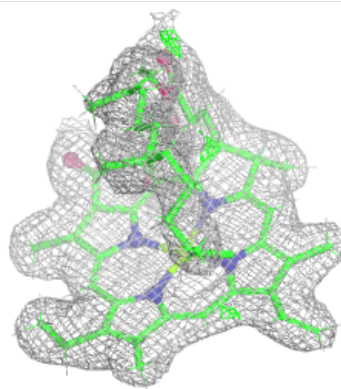
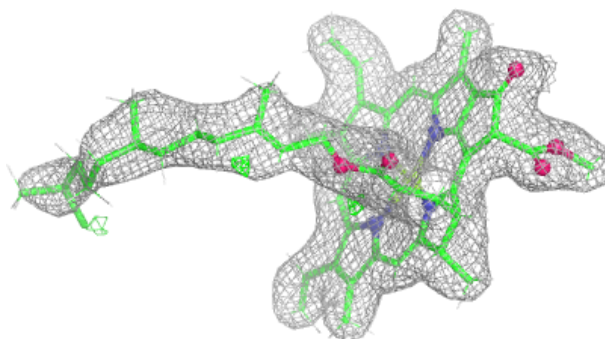
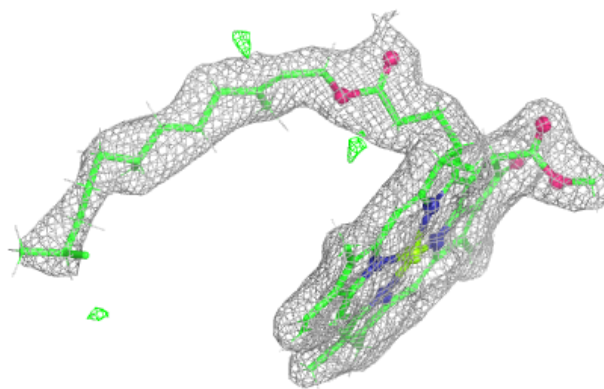


Electron density around LHG D 411:

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

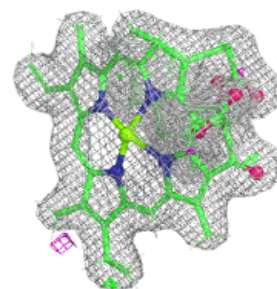
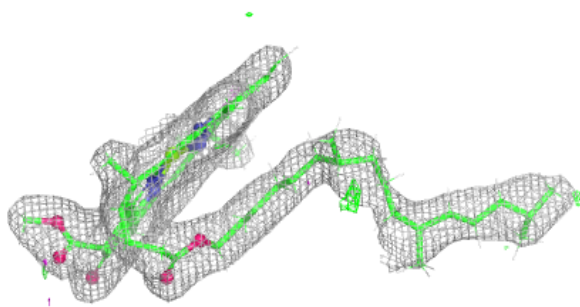
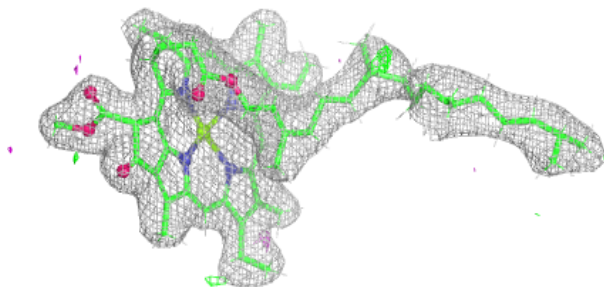
**Electron density around CLA c 504:**

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

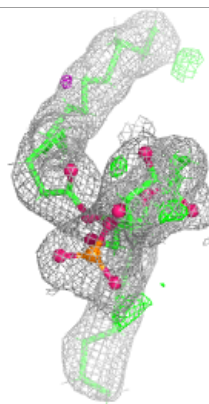
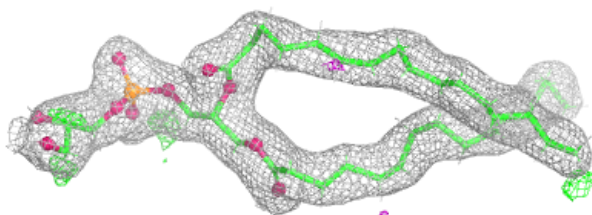
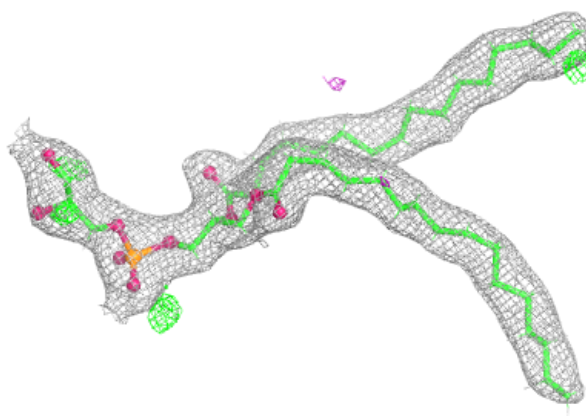


Electron density around CLA c 505:

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

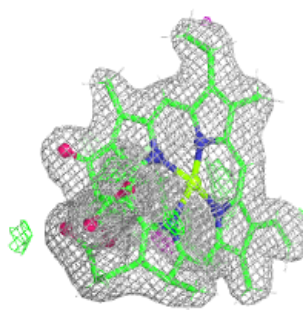
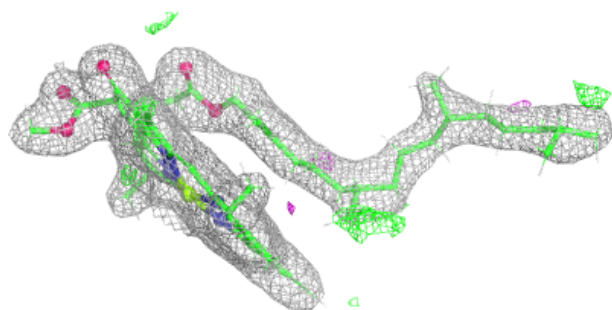
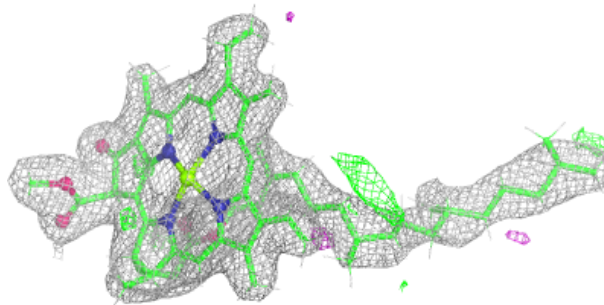
**Electron density around LHG d 409:**

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



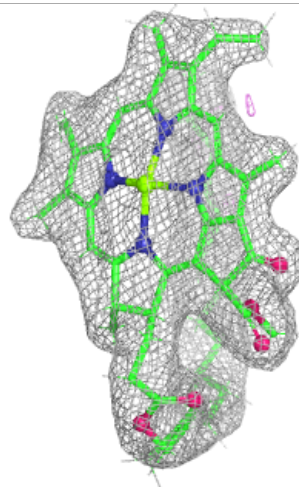
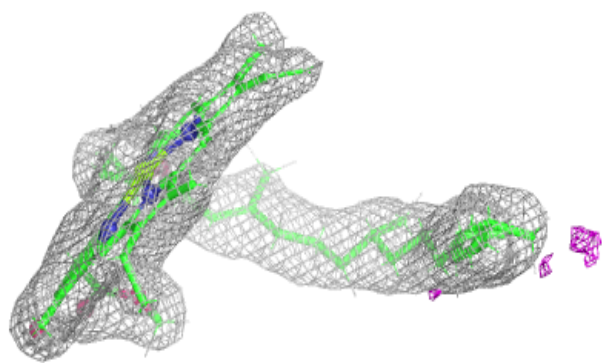
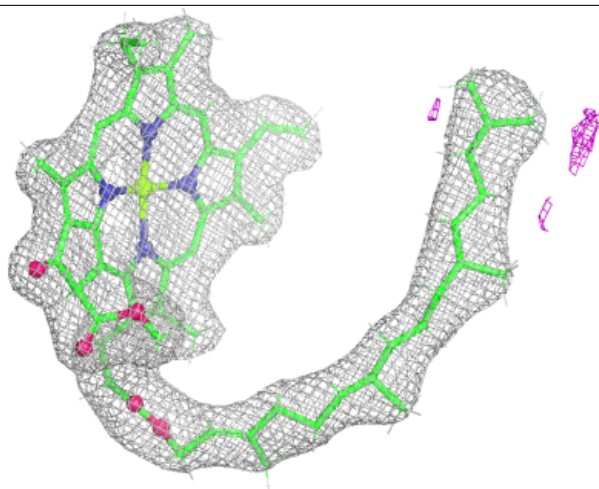
Electron density around CLA C 505:

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



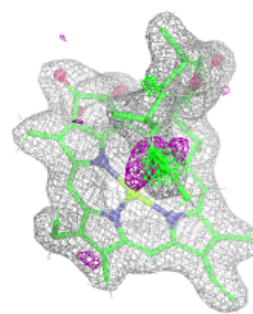
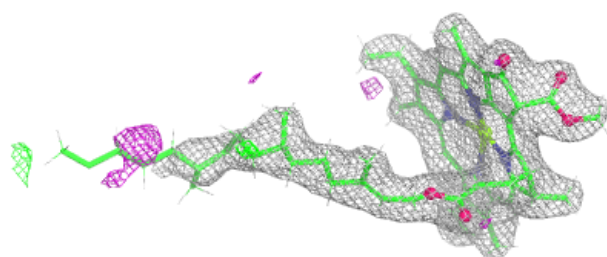
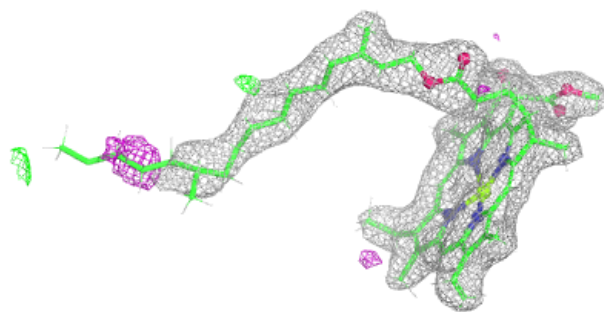
Electron density around CLA c 507:

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

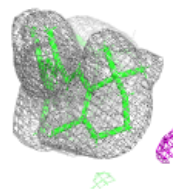
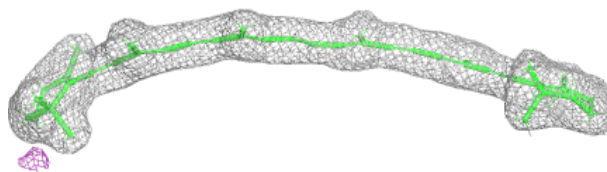
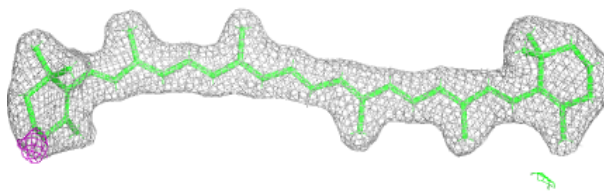


Electron density around CLA c 508:

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

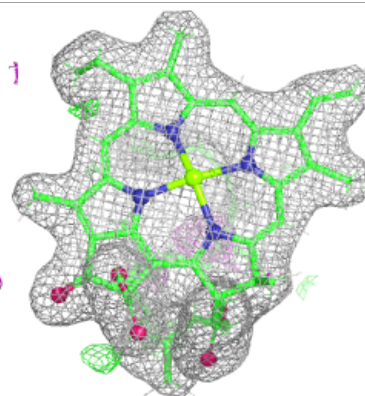
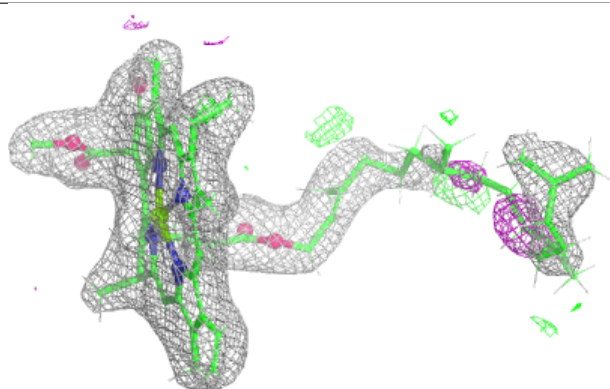
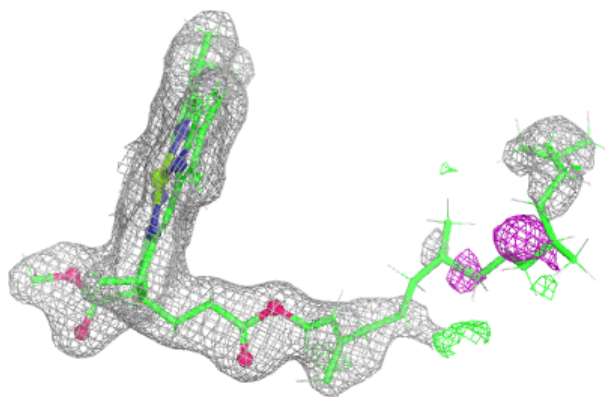
**Electron density around BCR t 101:**

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

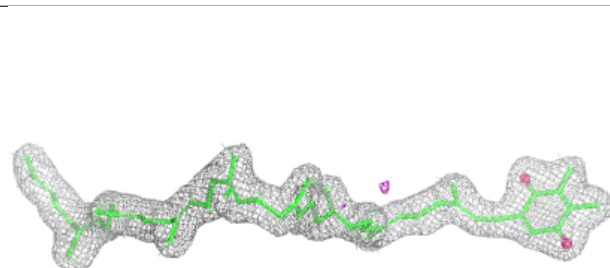
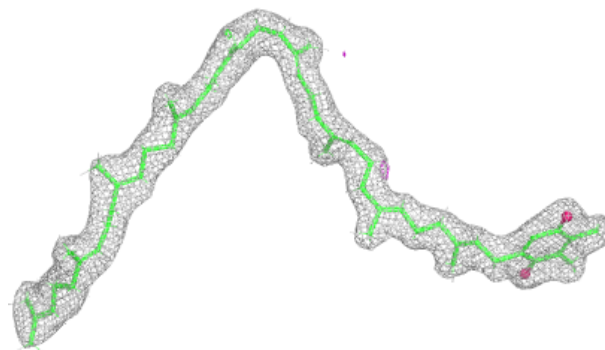


Electron density around CLA C 506:

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

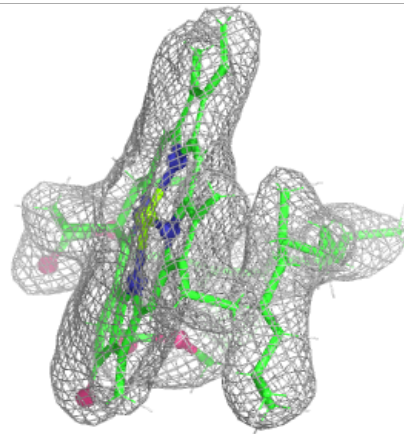
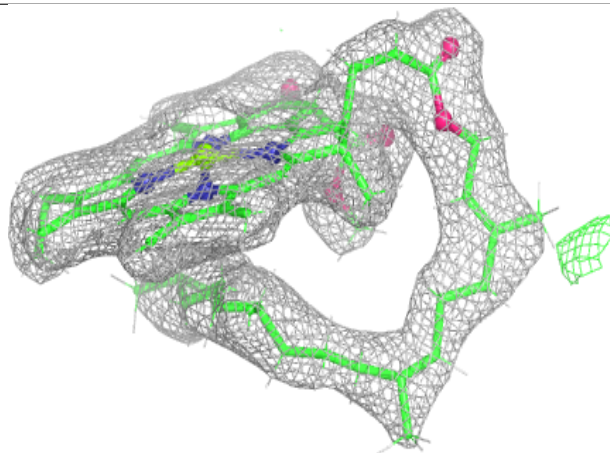
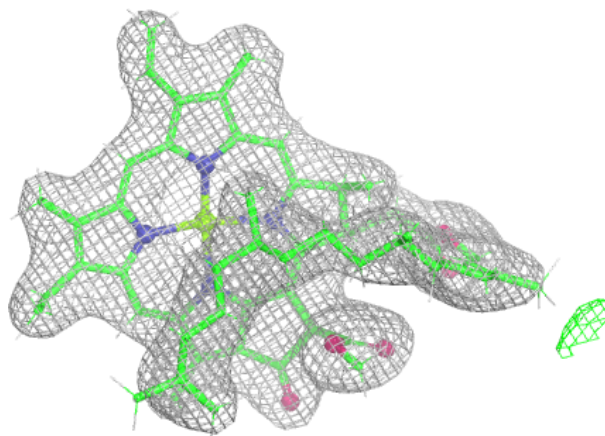
**Electron density around PL9 D 406:**

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



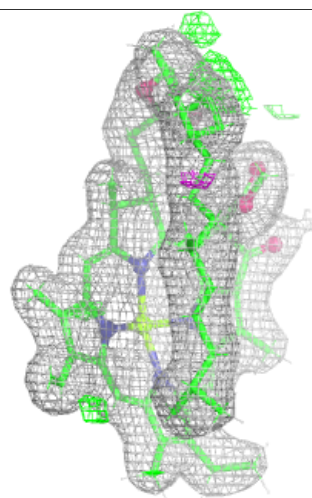
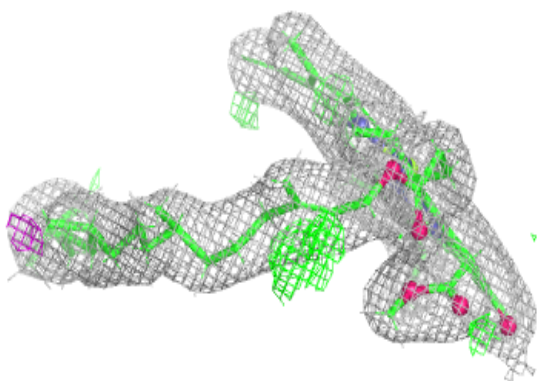
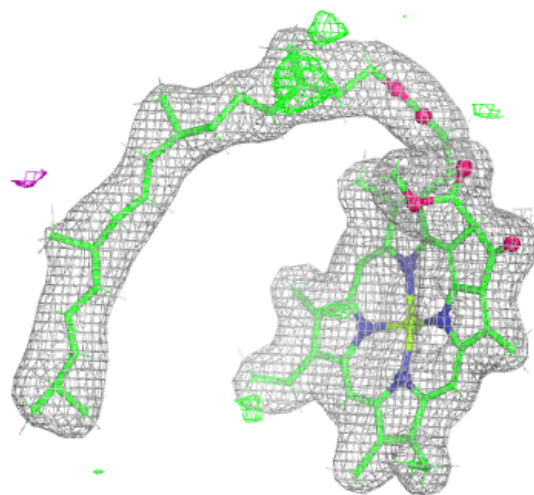
Electron density around CLA c 510:

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



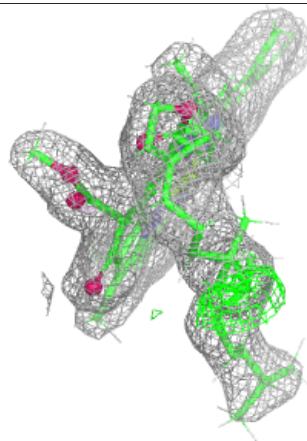
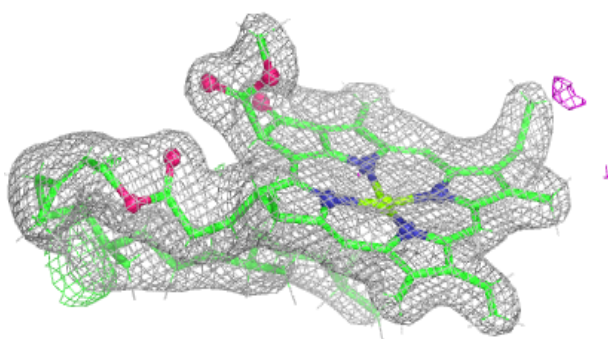
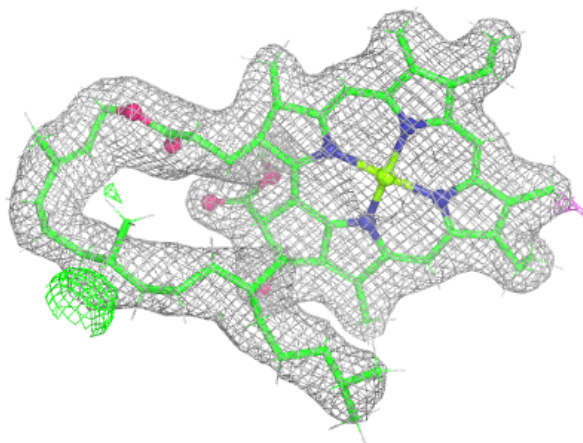
Electron density around CLA C 507:

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



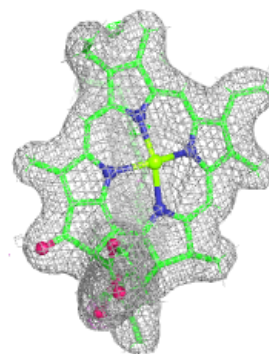
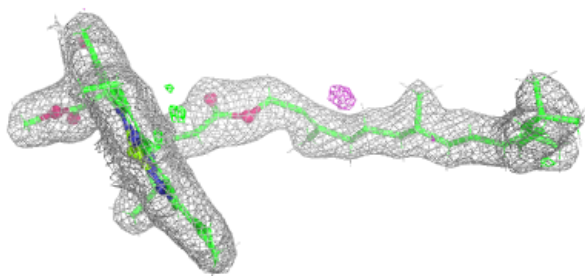
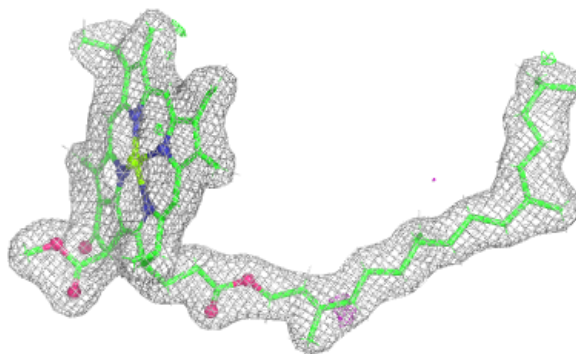
Electron density around CLA C 509:

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



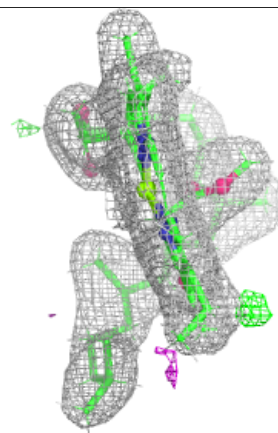
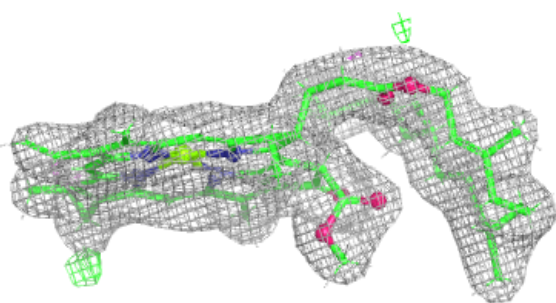
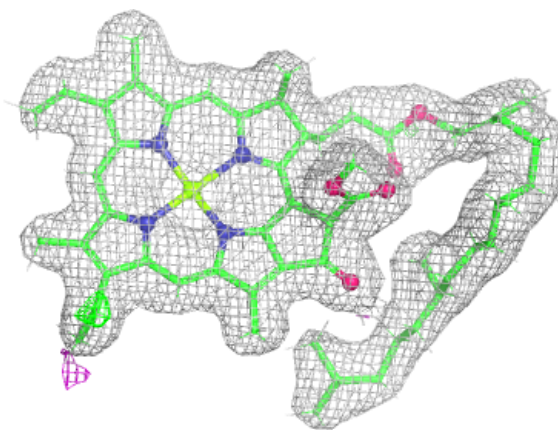
Electron density around CLA B 609:

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

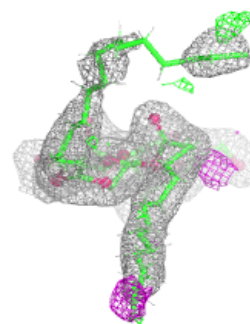
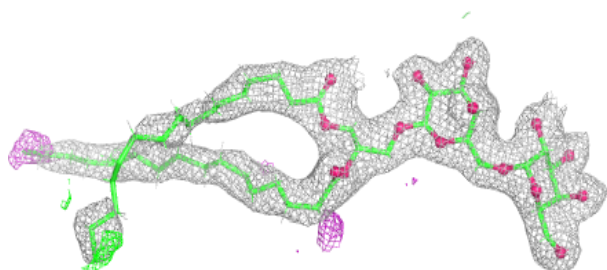
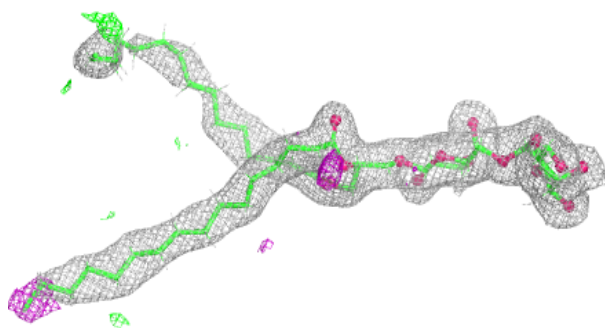


Electron density around CLA B 610:

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

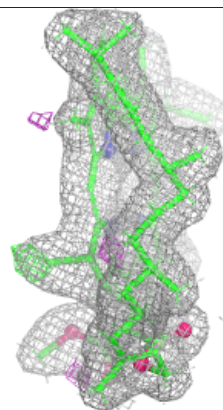
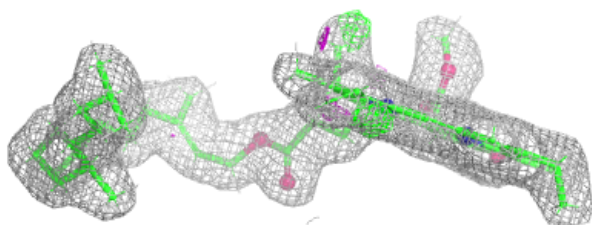
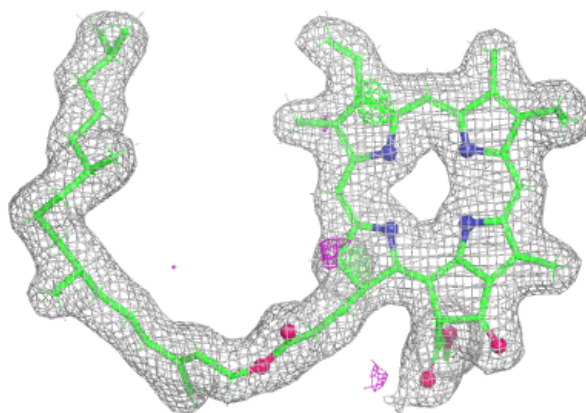
**Electron density around DGD C 522:**

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

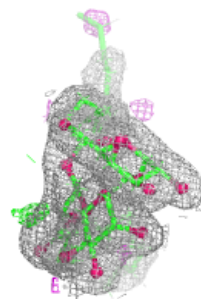
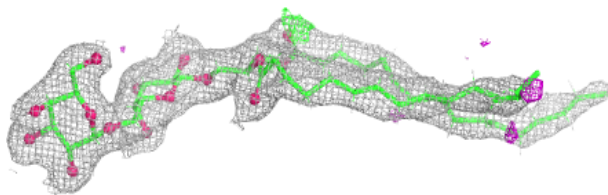
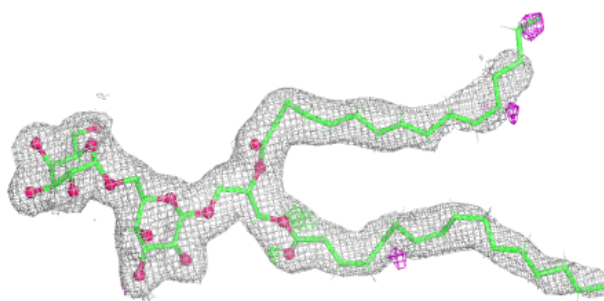


Electron density around PHO A 607:

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

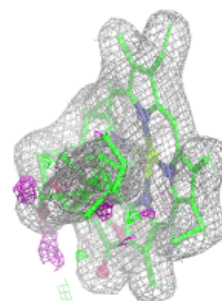
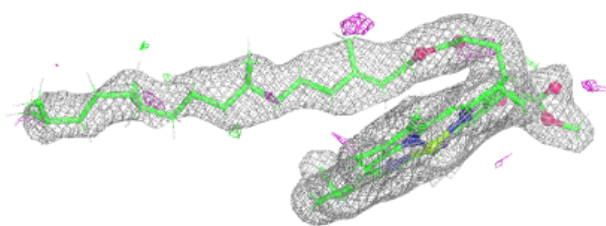
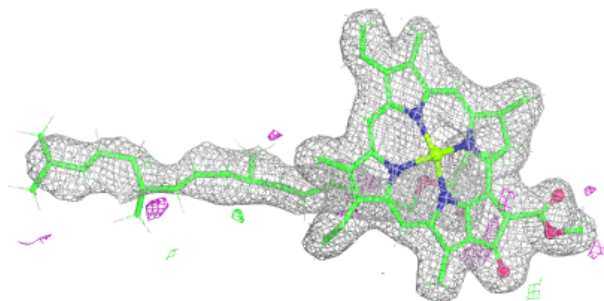
**Electron density around DGD C 524:**

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

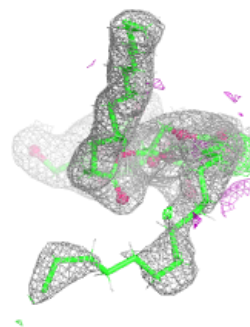
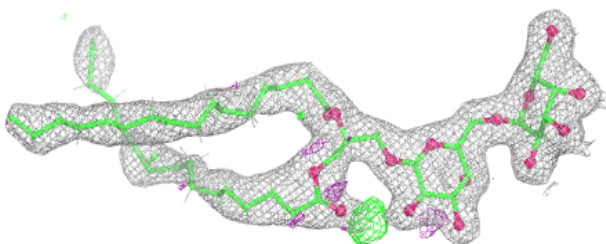
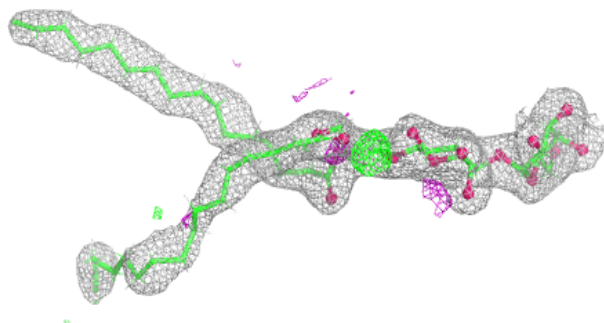


Electron density around CLA B 614:

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

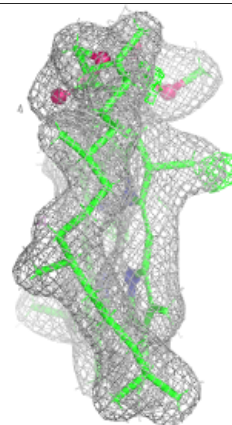
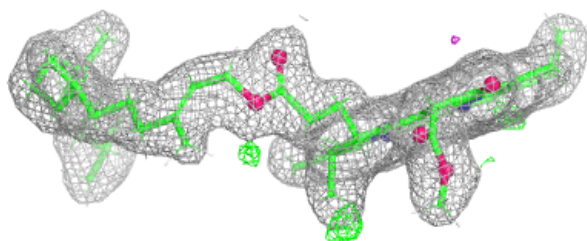
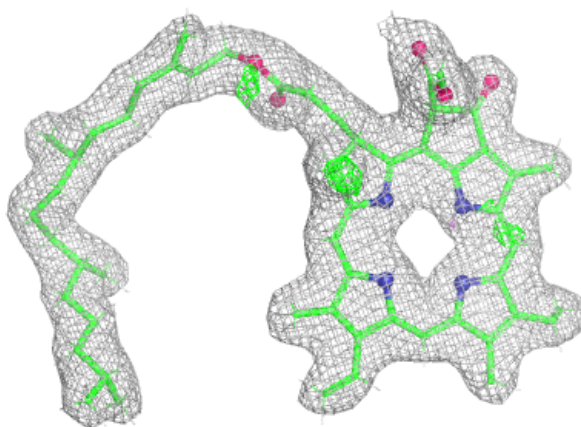
**Electron density around DGD c 519:**

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

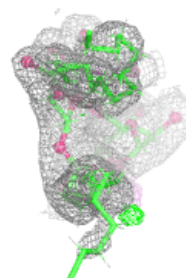
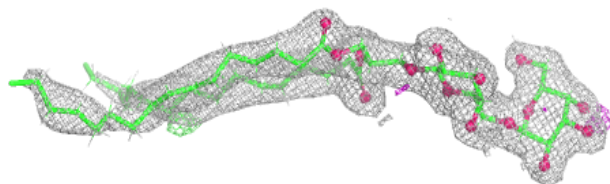
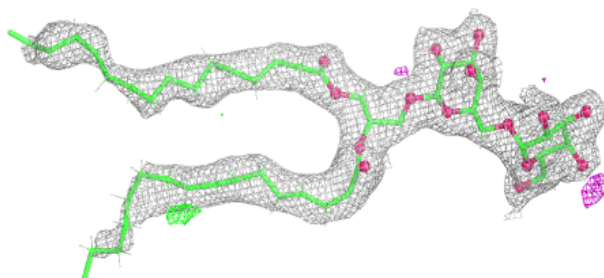


Electron density around PHO a 607:

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

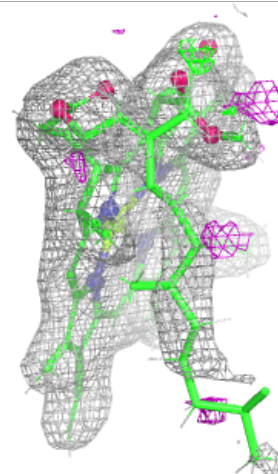
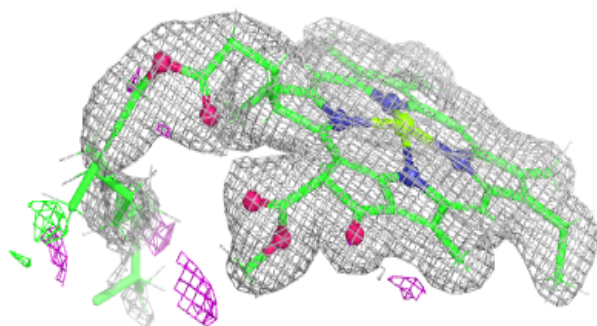
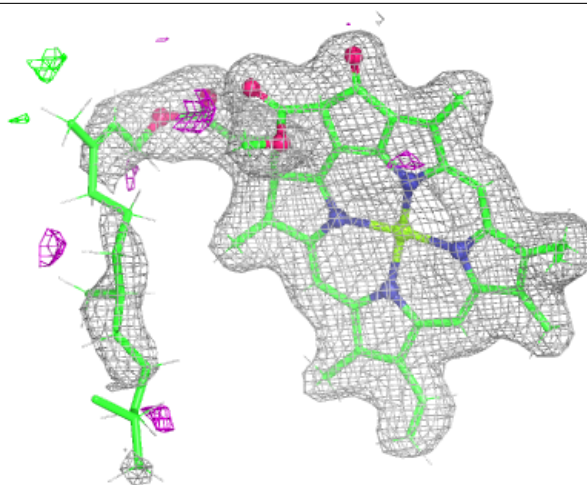
**Electron density around DGD c 521:**

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



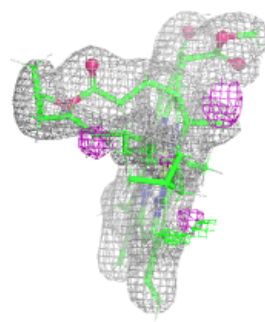
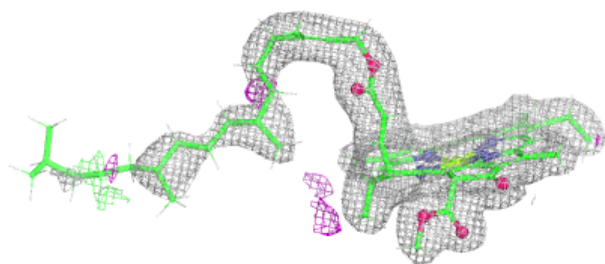
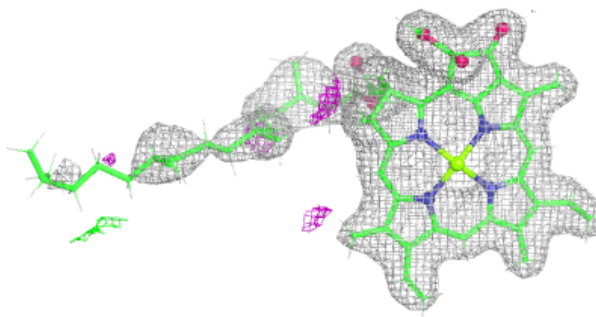
Electron density around CLA B 616:

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

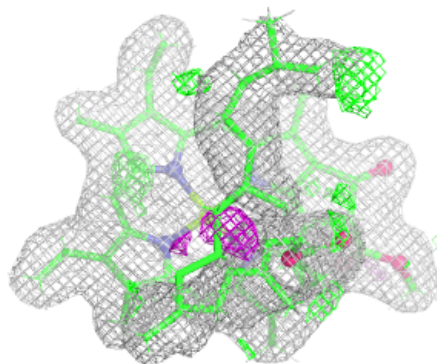
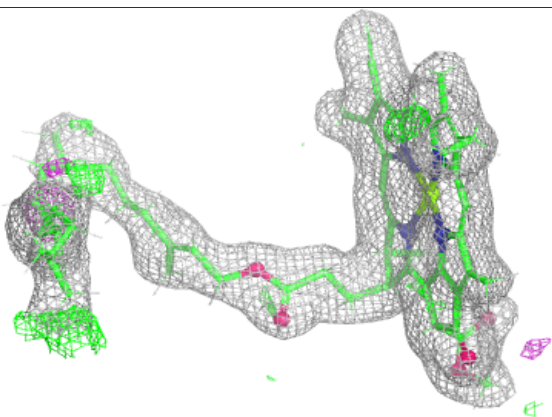
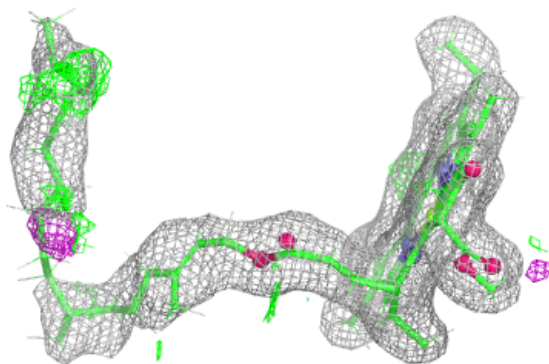


Electron density around CLA a 606:

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

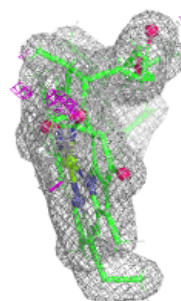
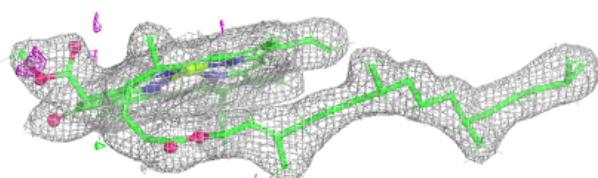
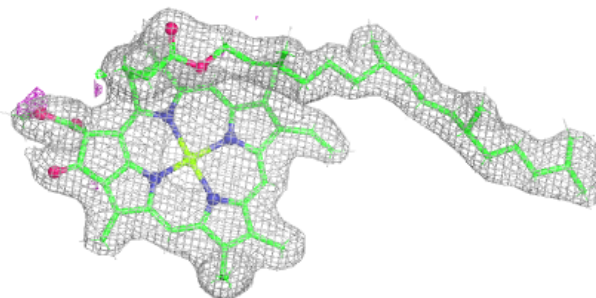
**Electron density around CLA a 608:**

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

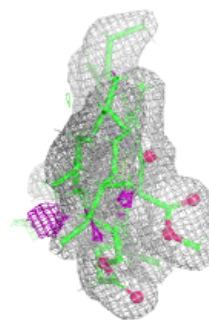
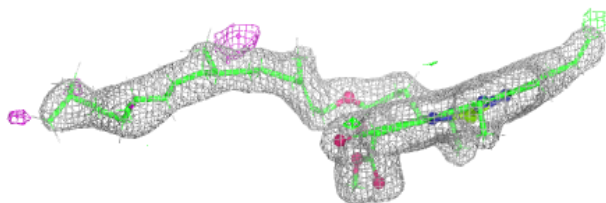
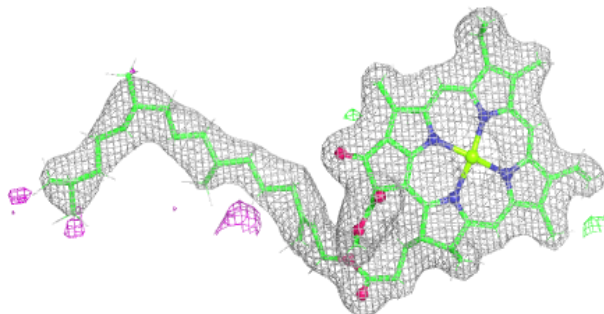


Electron density around CLA C 501:

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

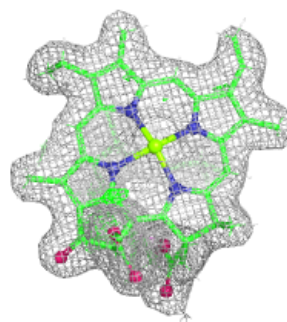
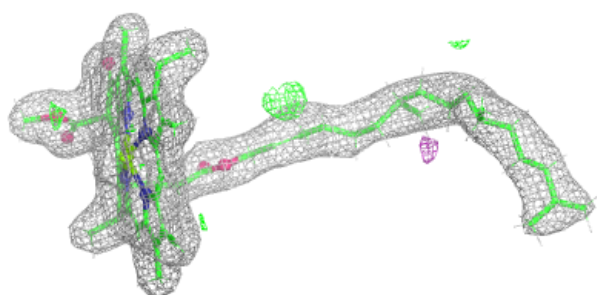
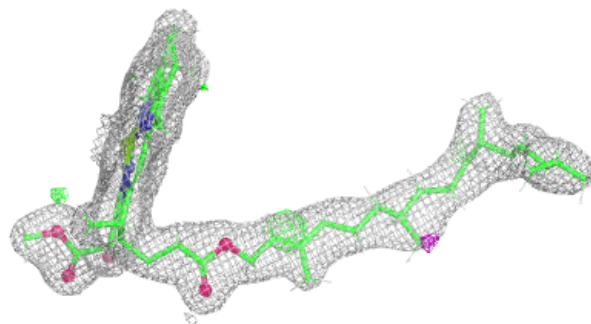
**Electron density around CLA b 602:**

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

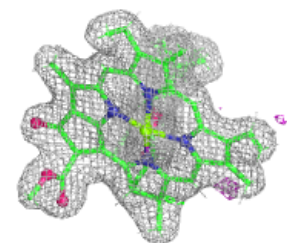
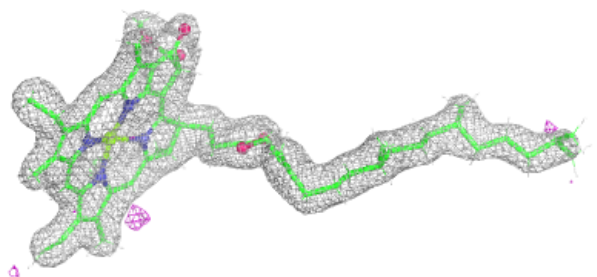
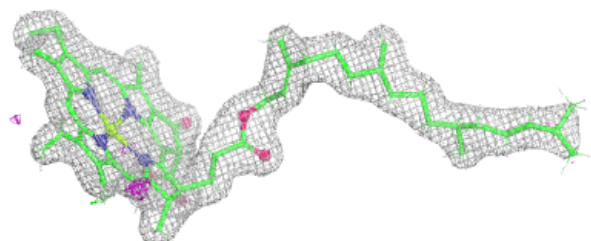


Electron density around CLA b 605:

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

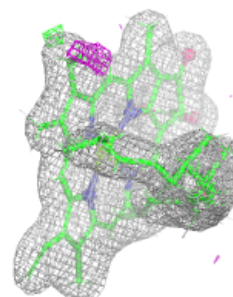
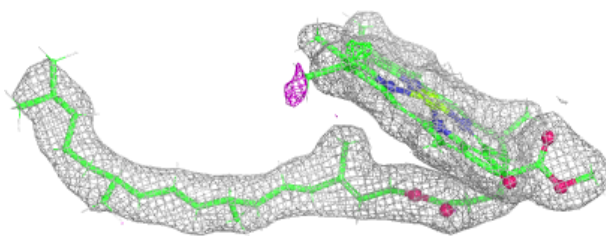
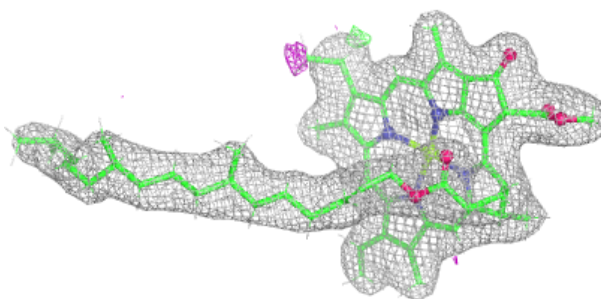
**Electron density around CLA C 502:**

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

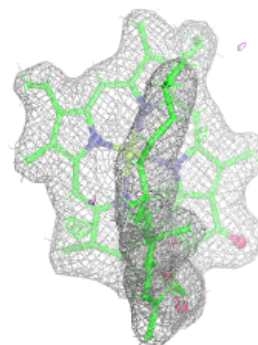
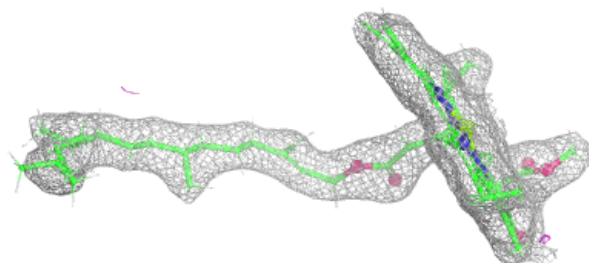
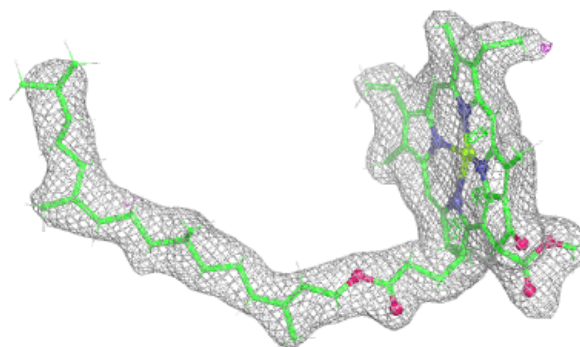


Electron density around CLA b 608:

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

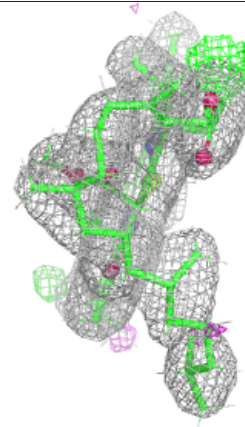
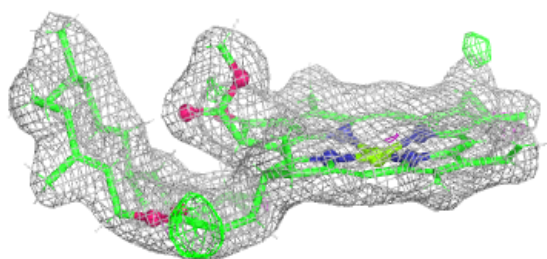
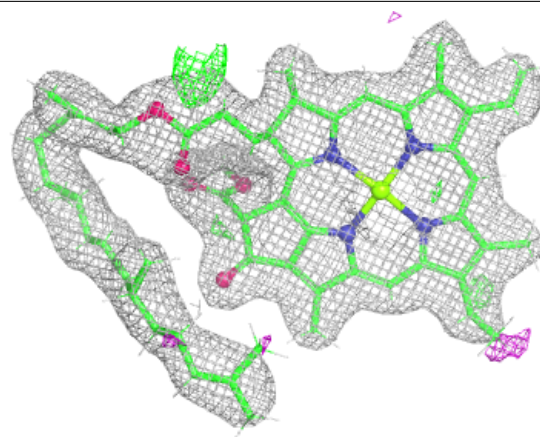
**Electron density around CLA b 609:**

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

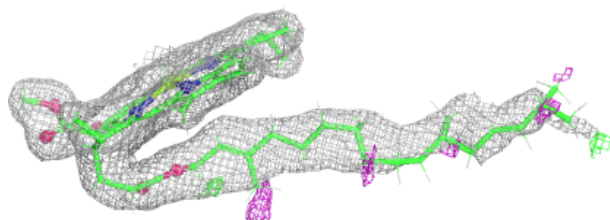
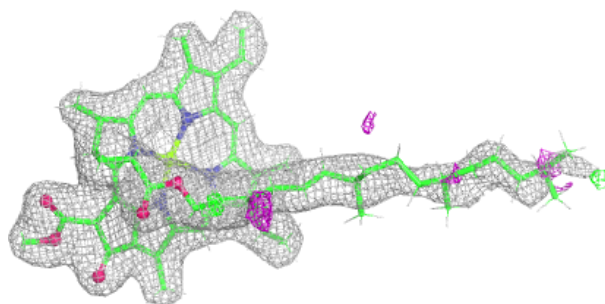


Electron density around CLA b 610:

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

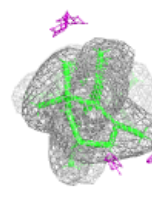
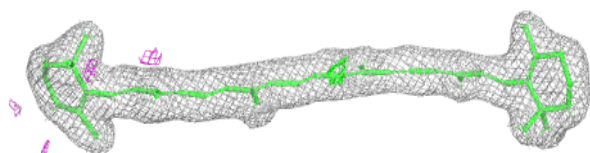
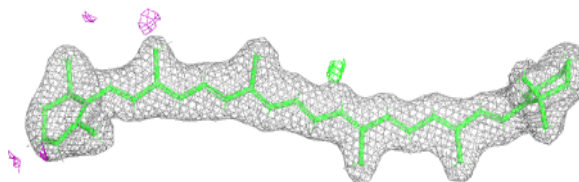
**Electron density around CLA b 614:**

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



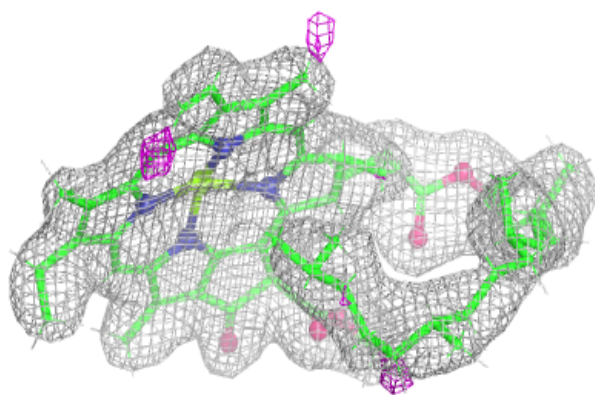
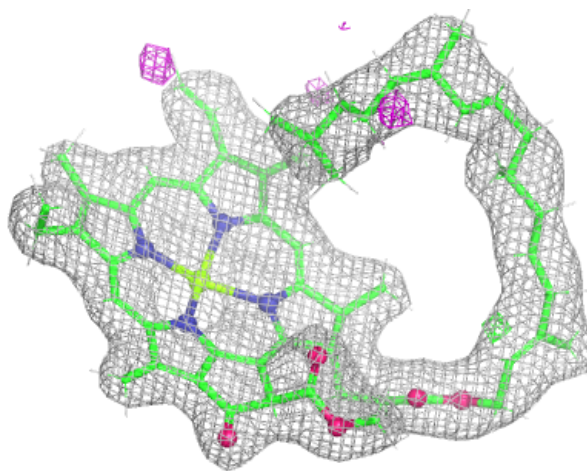
Electron density around BCR a 609:

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



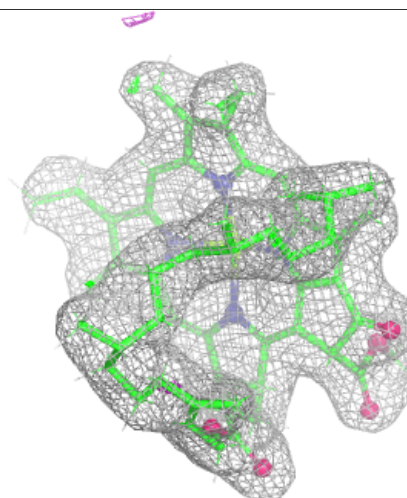
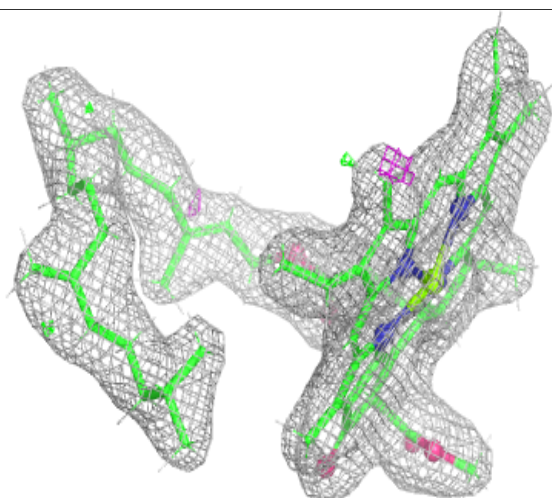
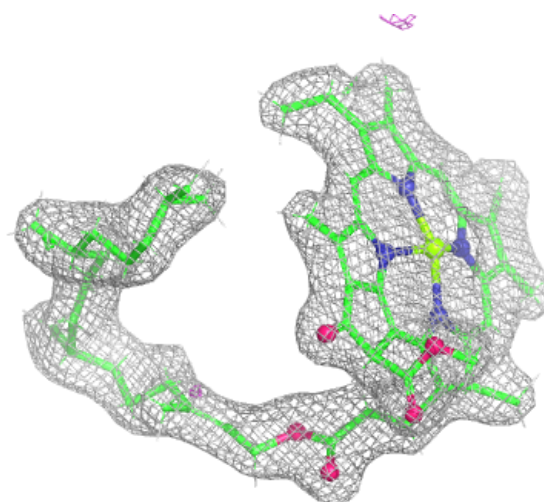
Electron density around CLA b 615:

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



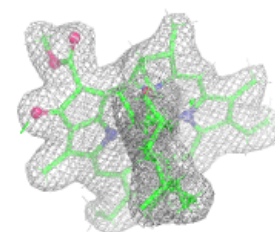
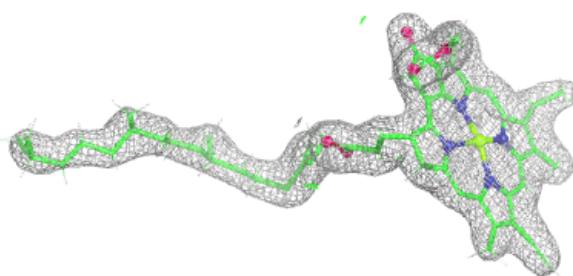
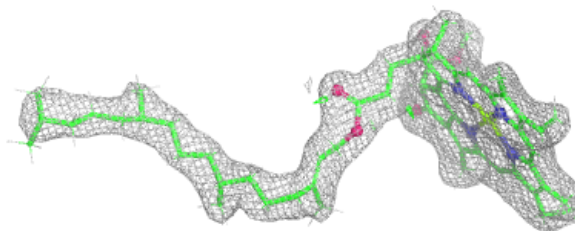
Electron density around CLA C 503:

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

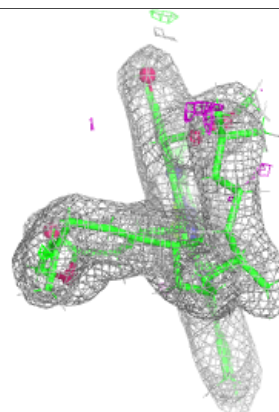
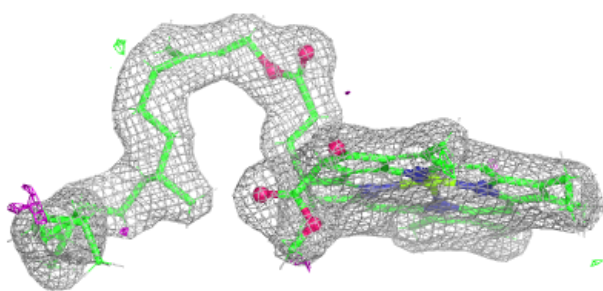
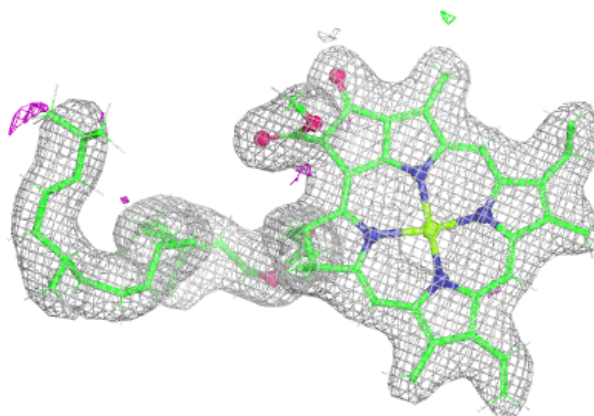


Electron density around CLA c 502:

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

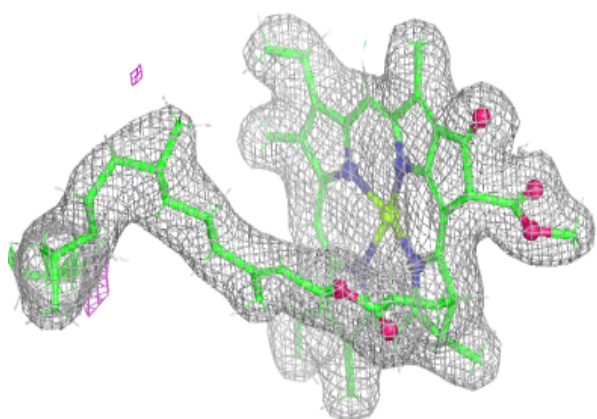
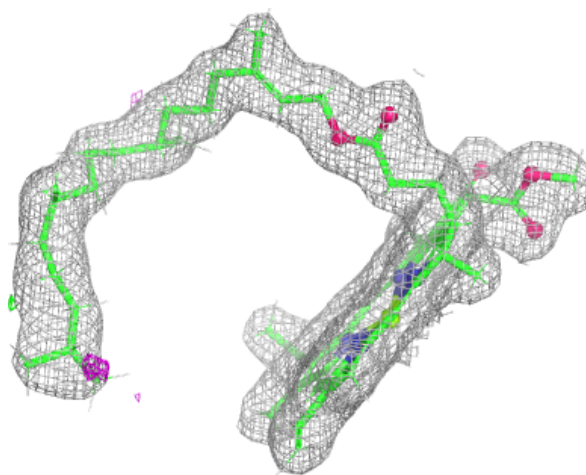
**Electron density around CLA B 612:**

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



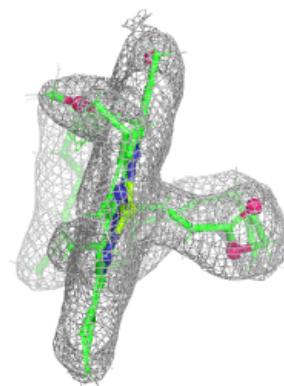
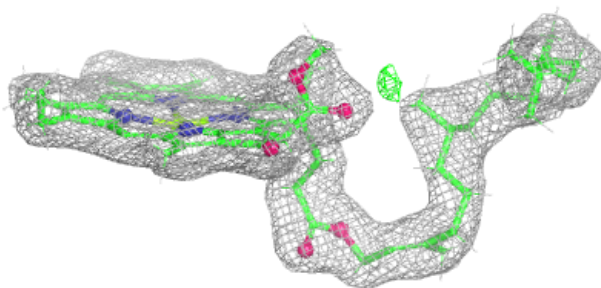
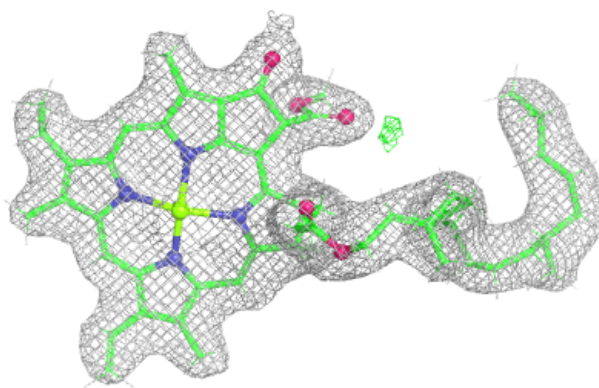
Electron density around CLA b 611:

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



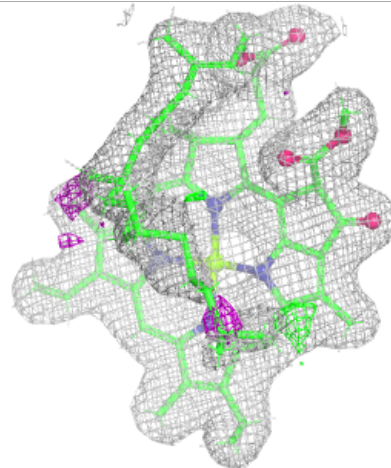
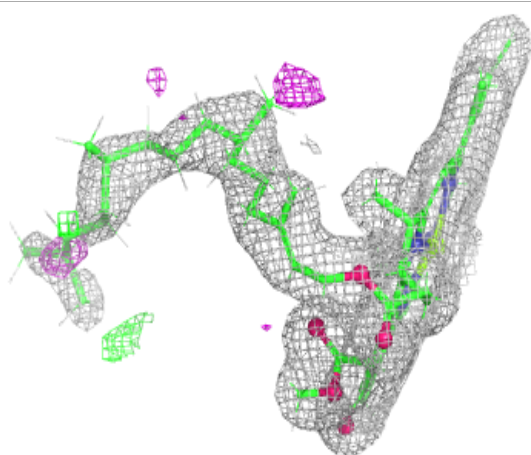
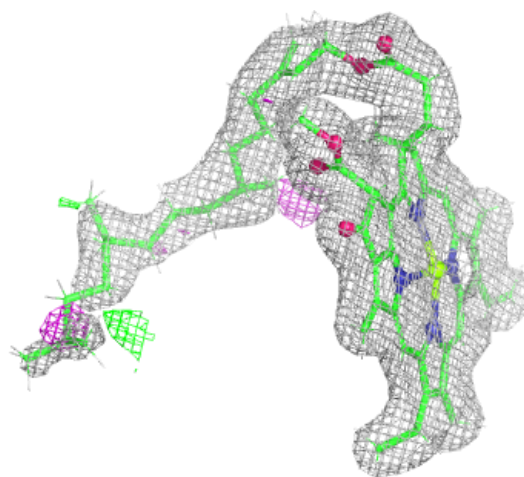
Electron density around CLA b 612:

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



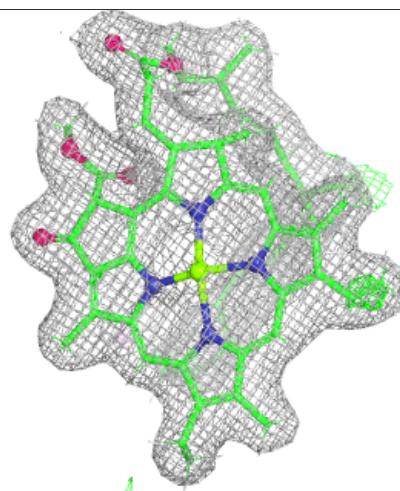
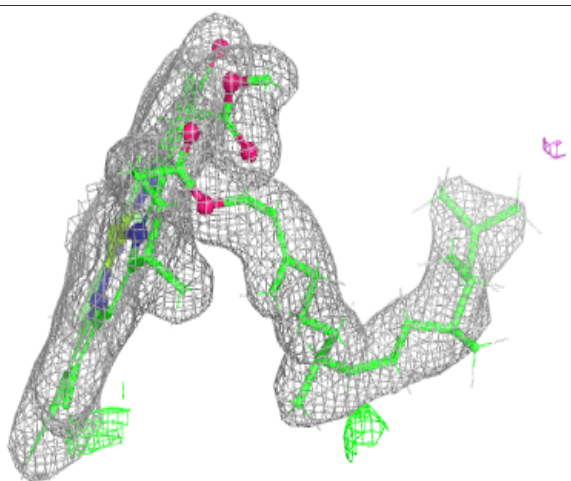
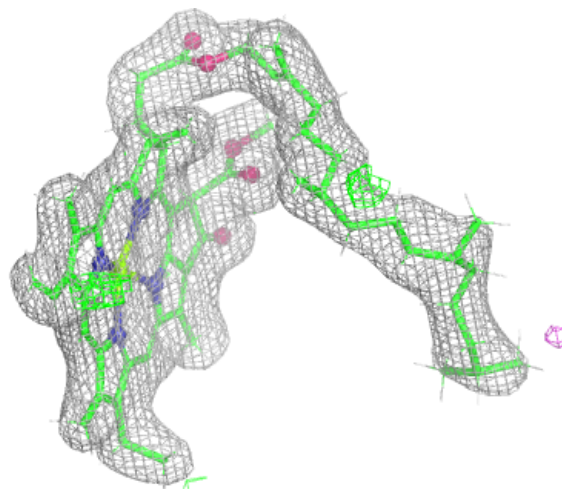
Electron density around CLA b 613:

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



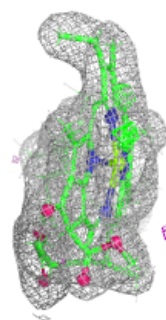
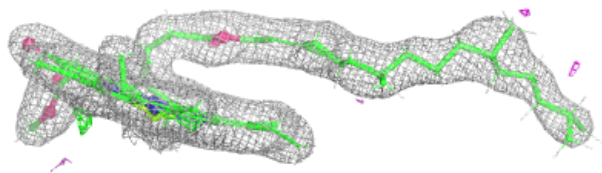
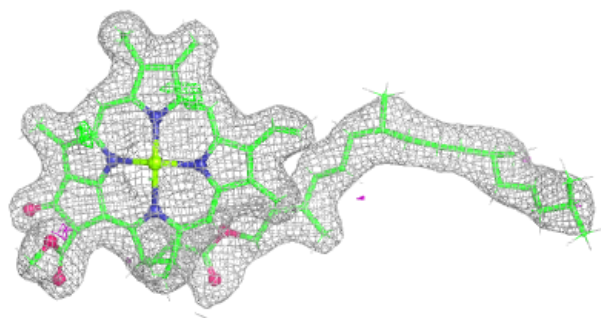
Electron density around CLA B 613:

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



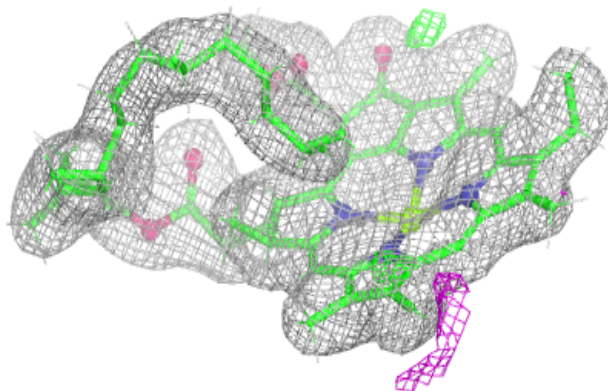
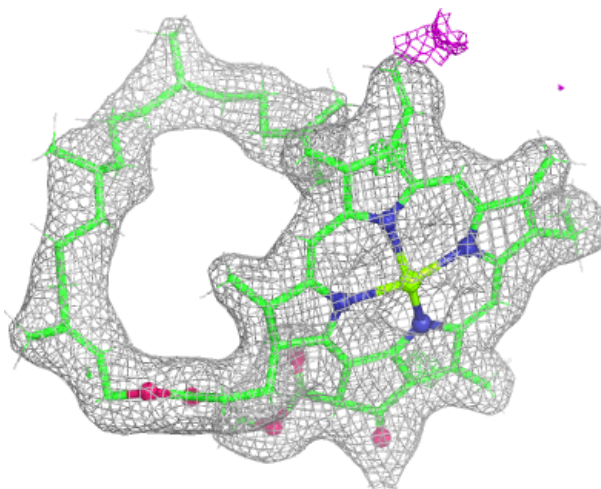
Electron density around CLA B 603:

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



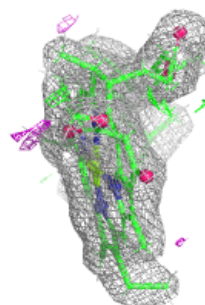
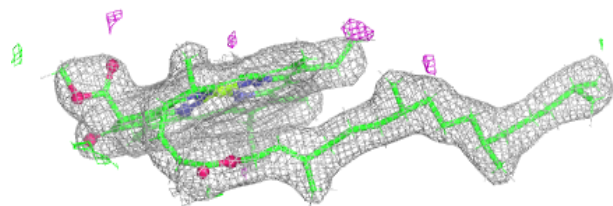
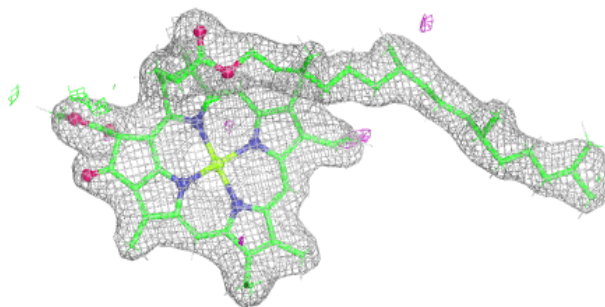
Electron density around CLA B 615:

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

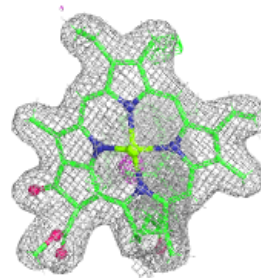
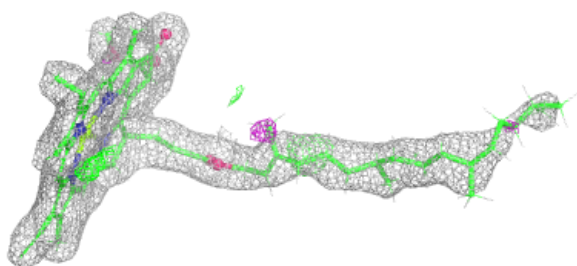
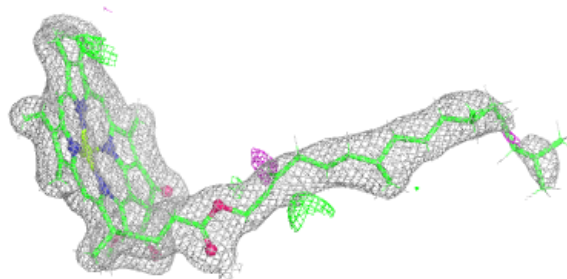


Electron density around CLA c 501:

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

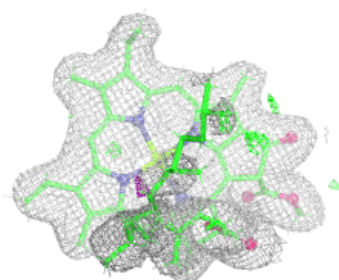
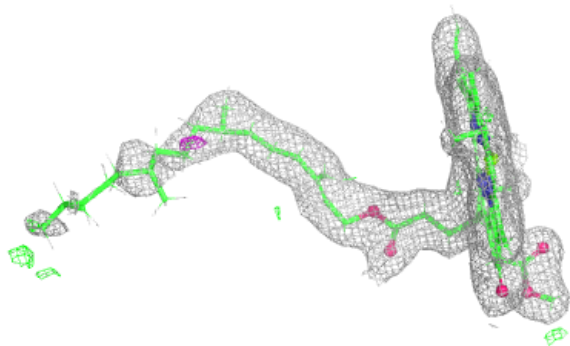
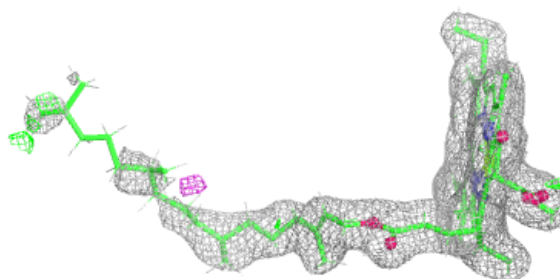
**Electron density around CLA B 604:**

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

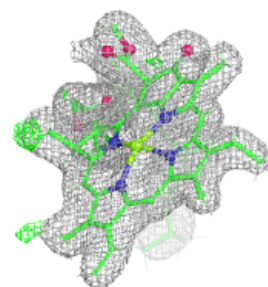
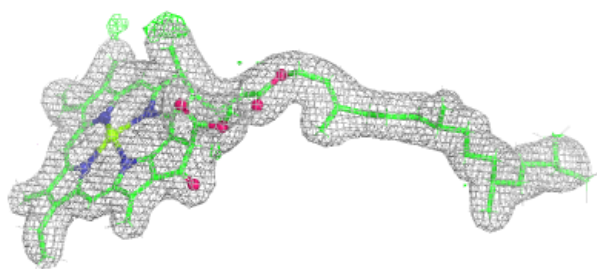
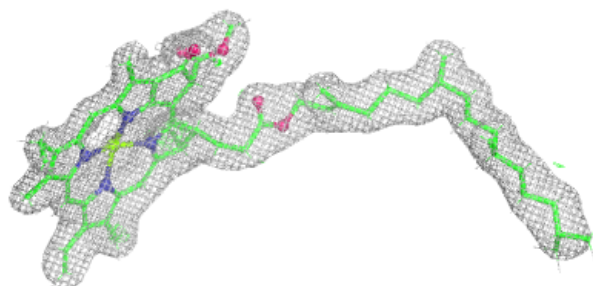


Electron density around CLA D 404:

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

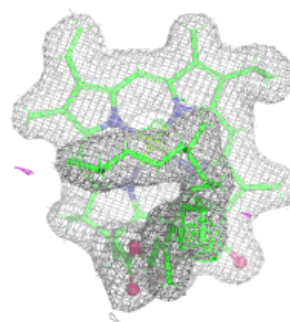
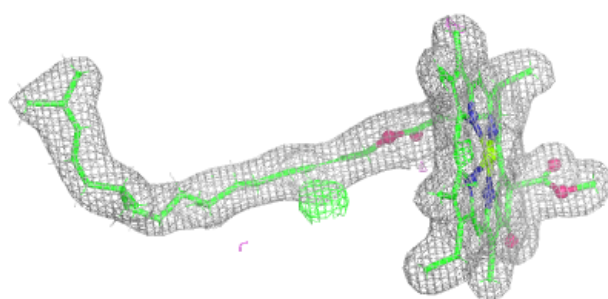
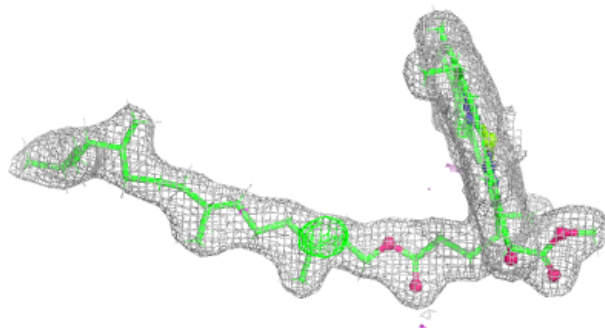
**Electron density around CLA a 605:**

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

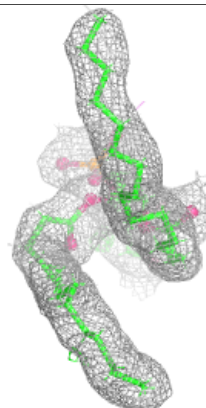
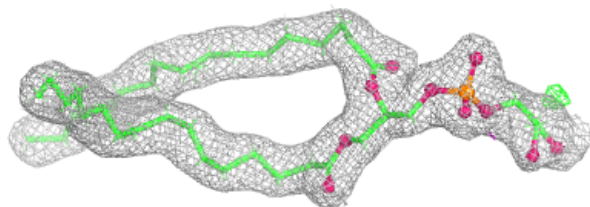
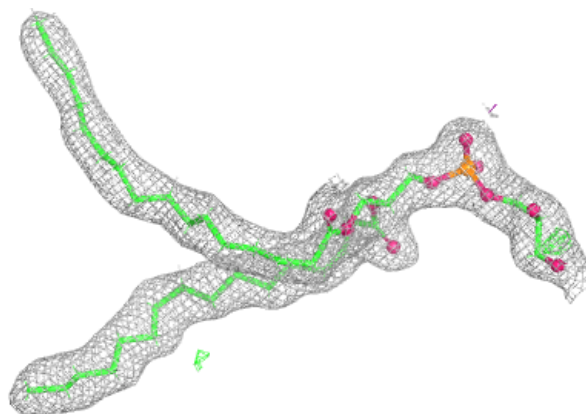


Electron density around CLA B 605:

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

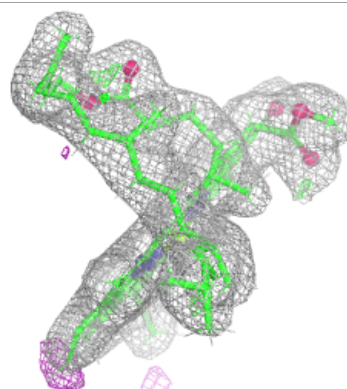
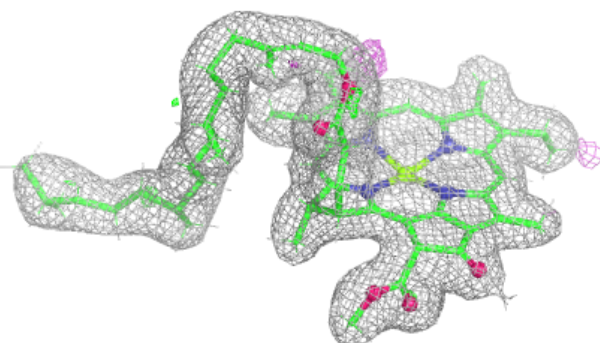
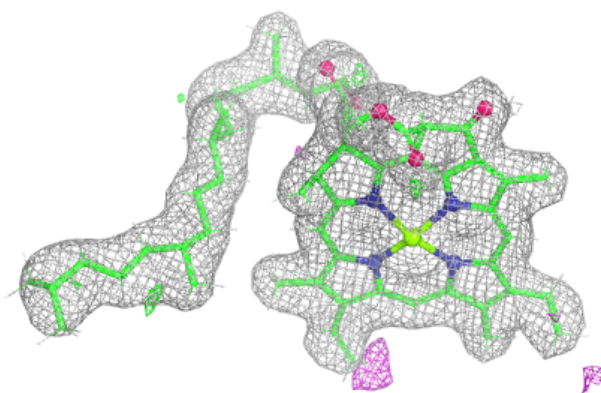
**Electron density around LHG D 410:**

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

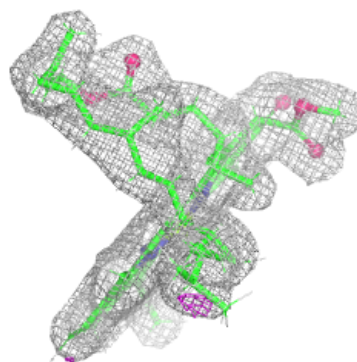
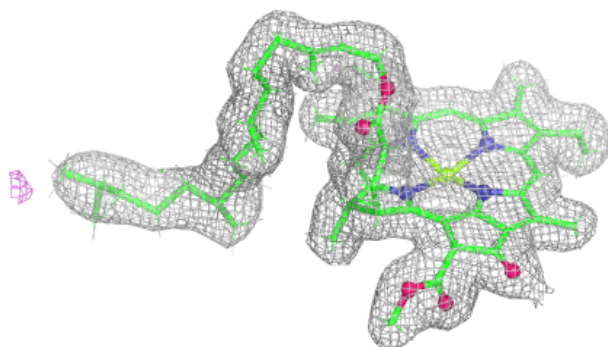
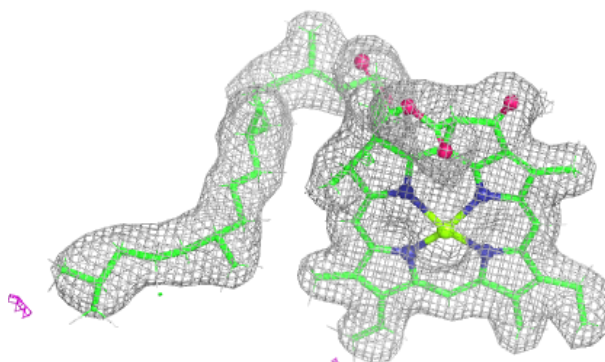


Electron density around CLA A 612:

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

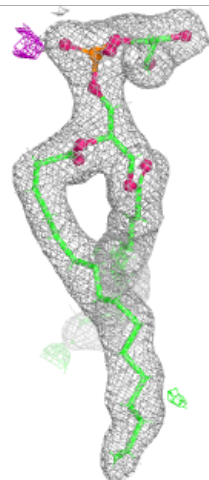
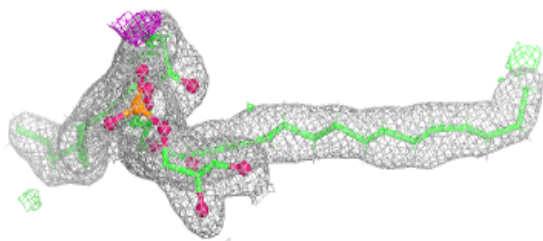
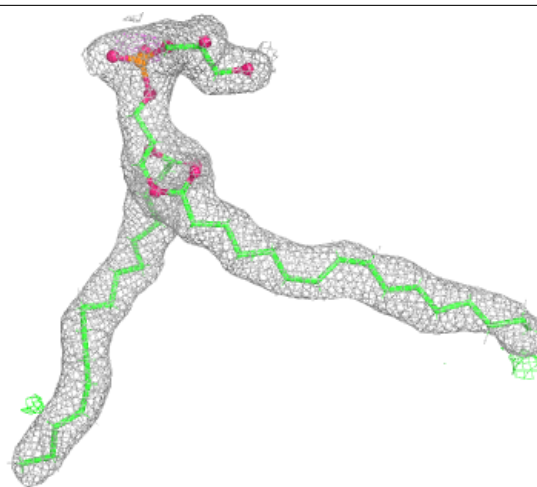
**Electron density around CLA a 611:**

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



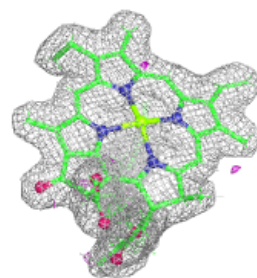
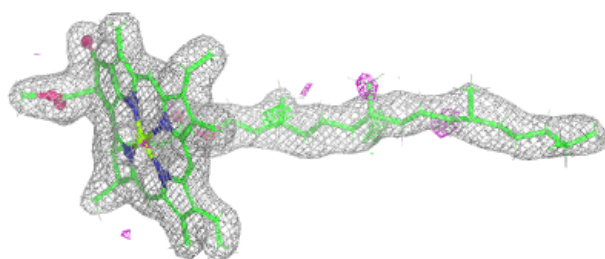
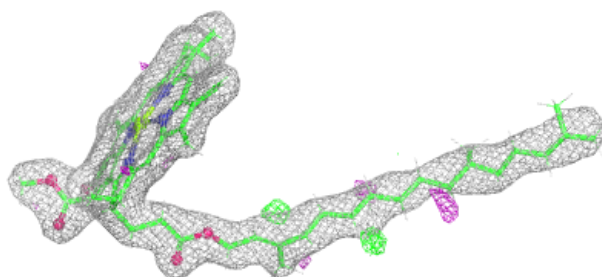
Electron density around LHG L 101:

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

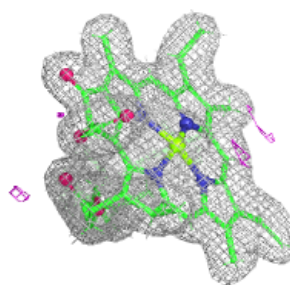
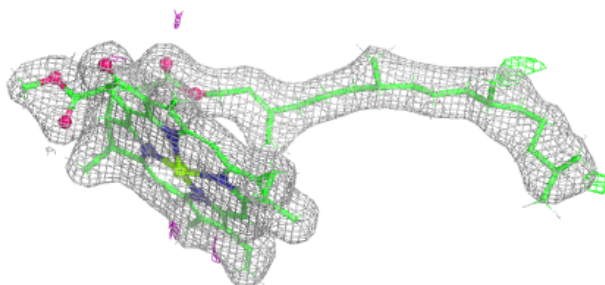
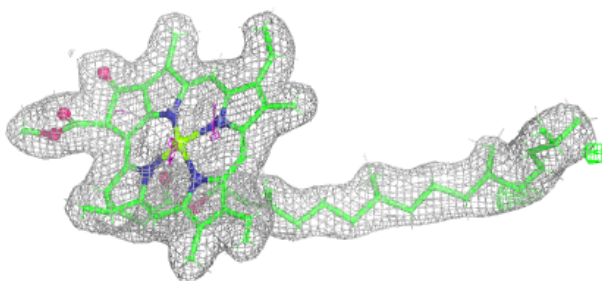


Electron density around CLA B 607:

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

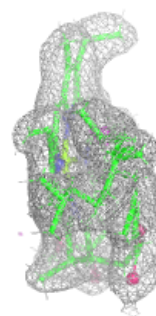
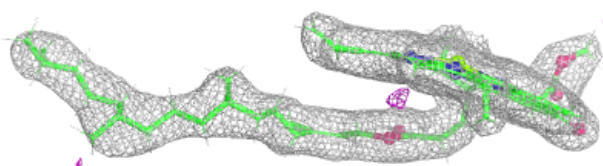
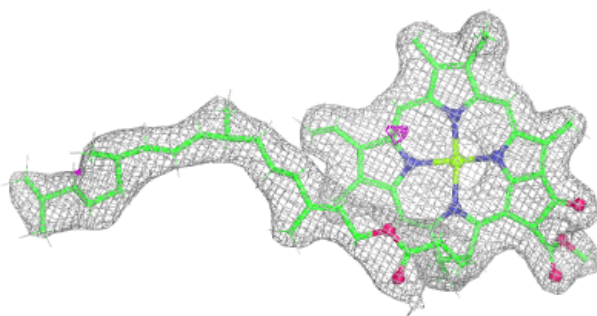
**Electron density around CLA B 608:**

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

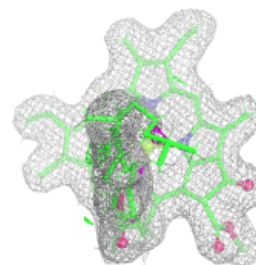
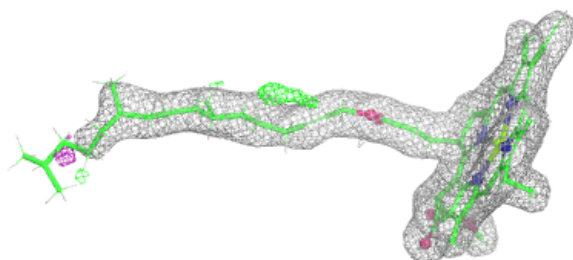
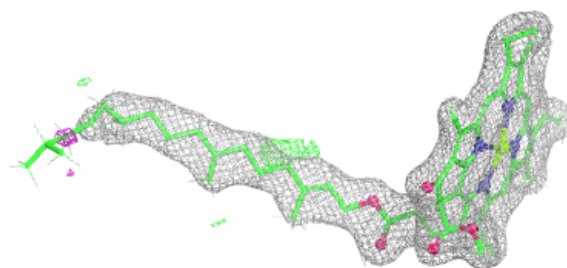


Electron density around CLA b 603:

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

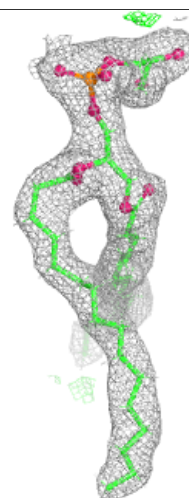
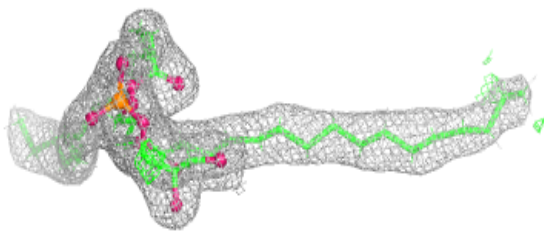
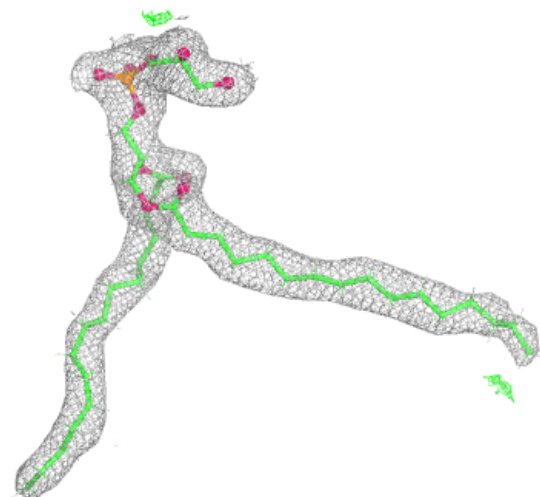
**Electron density around CLA b 604:**

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



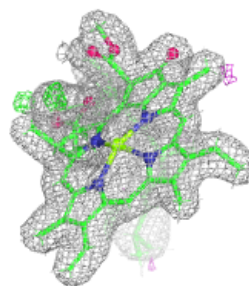
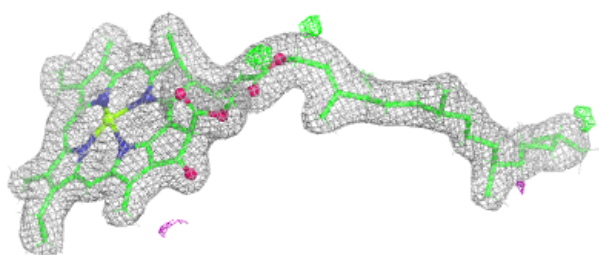
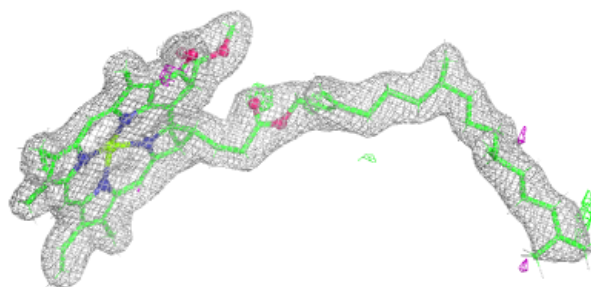
Electron density around LHG 1 101:

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

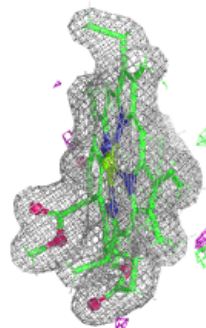
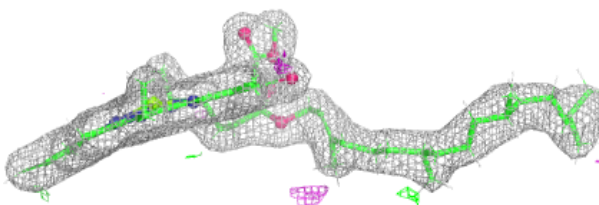
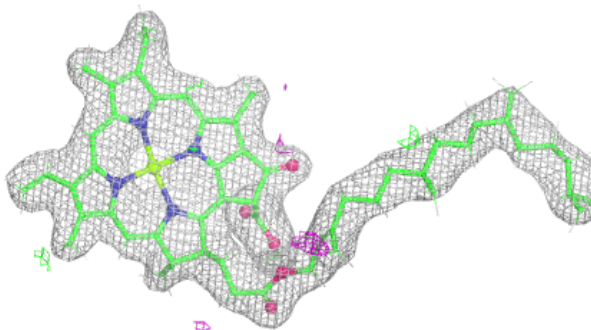


Electron density around CLA A 605:

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

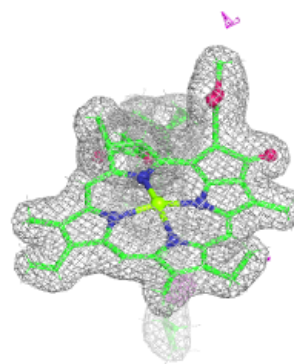
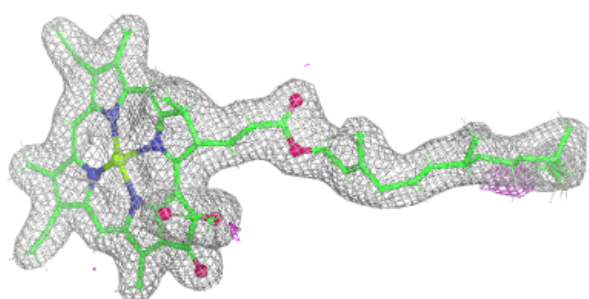
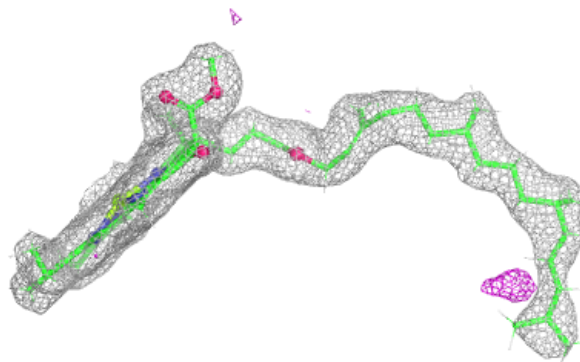
**Electron density around CLA B 602:**

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

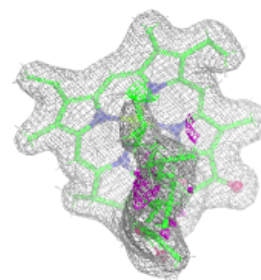
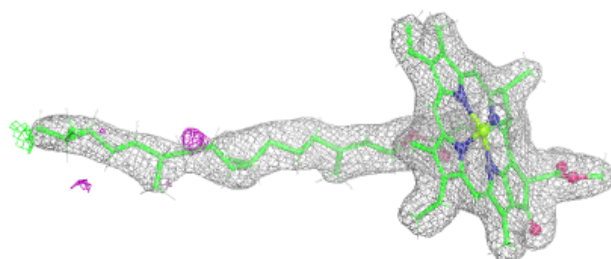
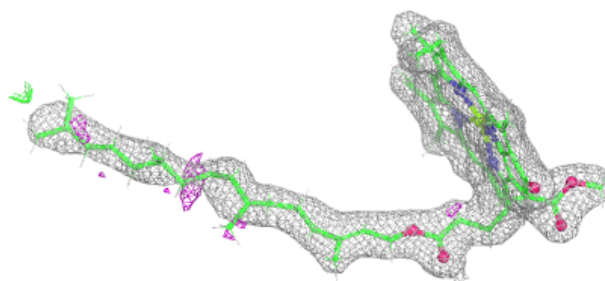


Electron density around CLA d 403:

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

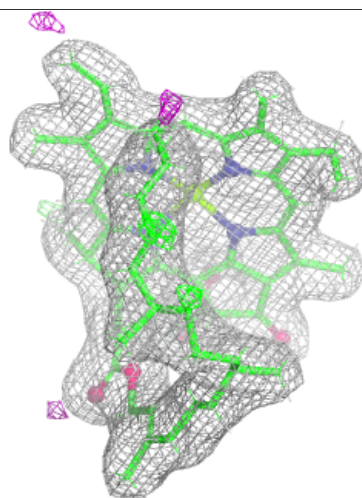
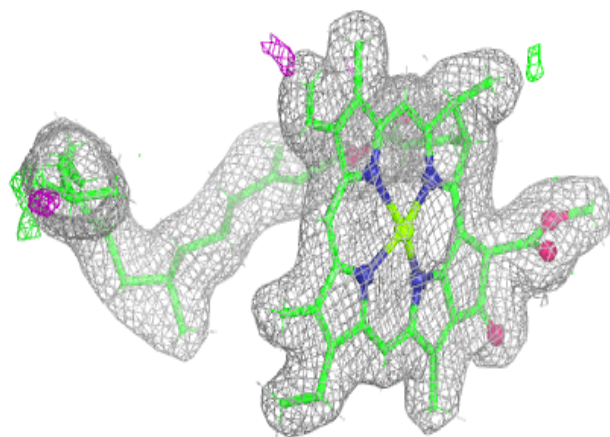
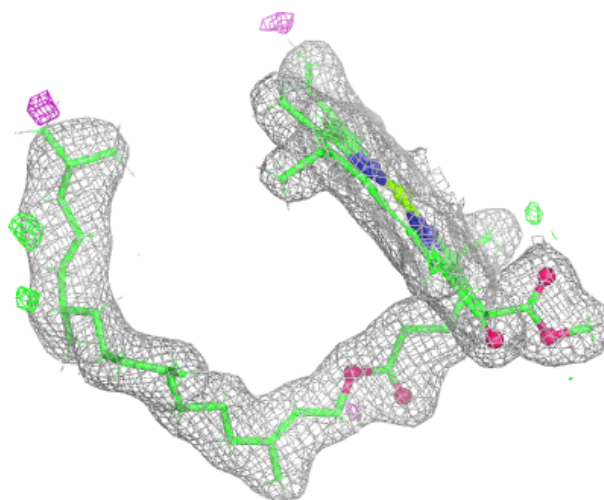
**Electron density around CLA b 607:**

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



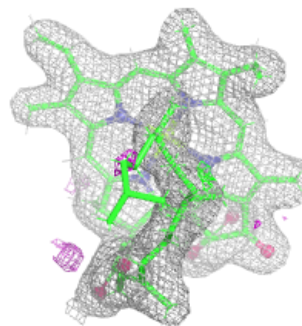
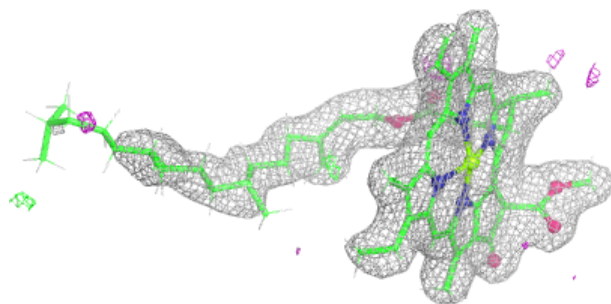
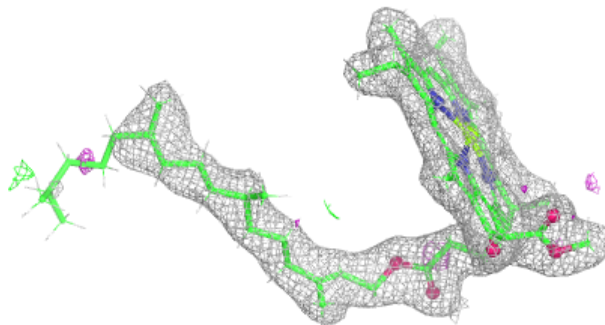
Electron density around CLA B 611:

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



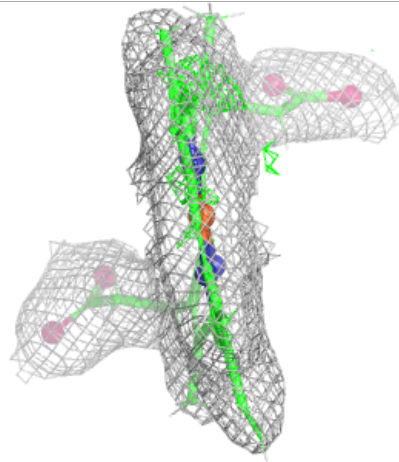
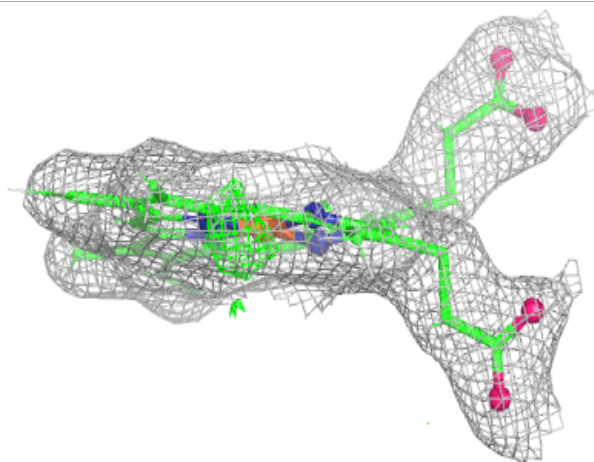
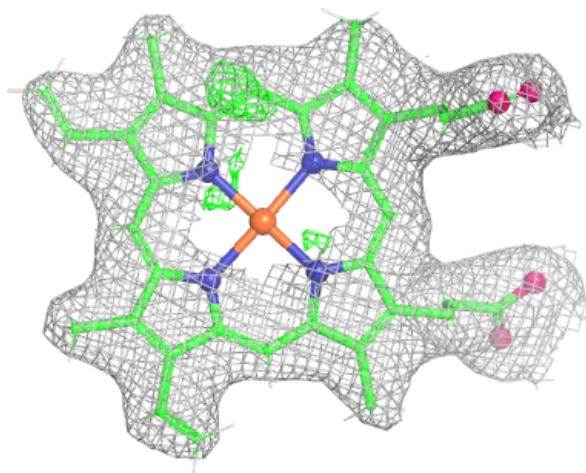
Electron density around CLA C 508:

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



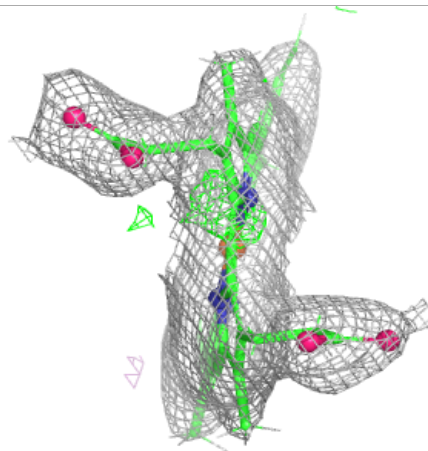
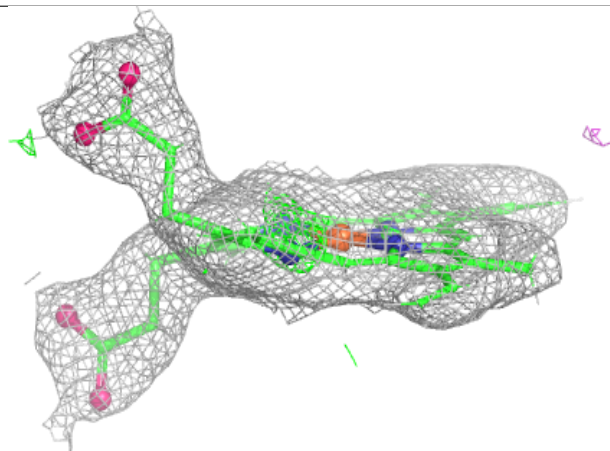
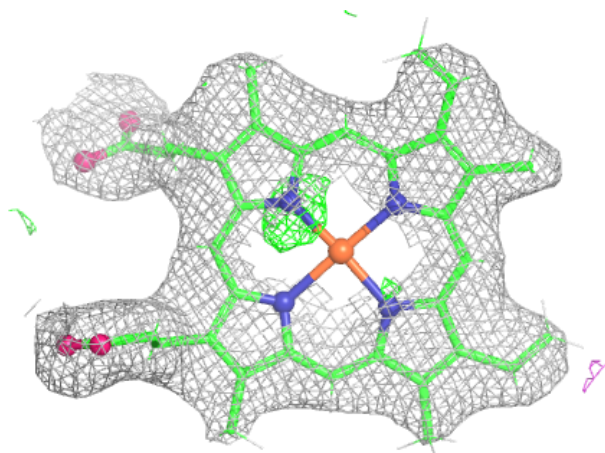
Electron density around HEM F 101:

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



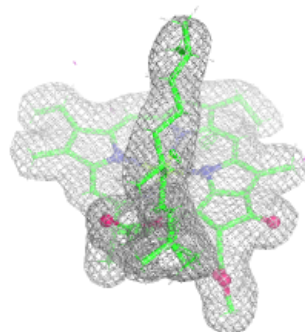
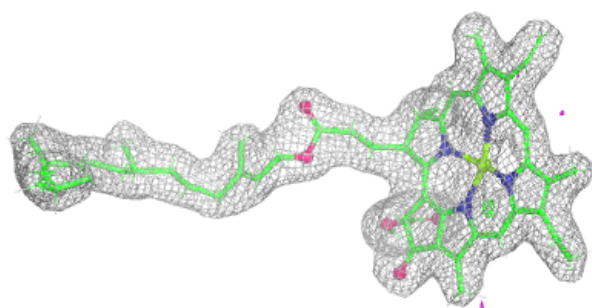
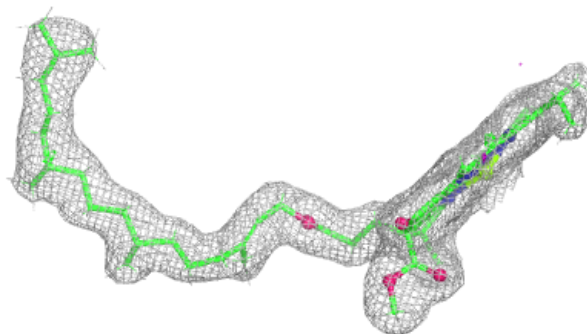
Electron density around HEM f 101:

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

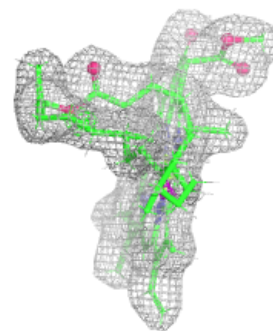
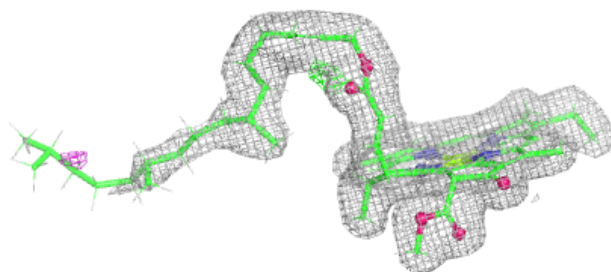
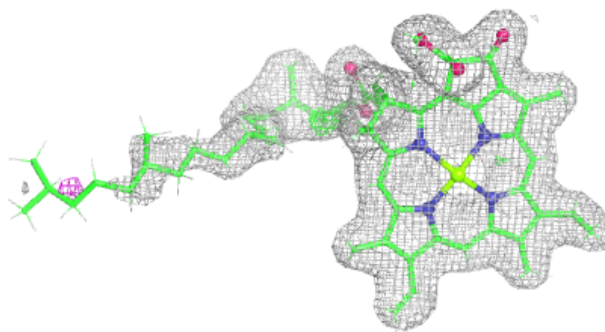


Electron density around CLA D 403:

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

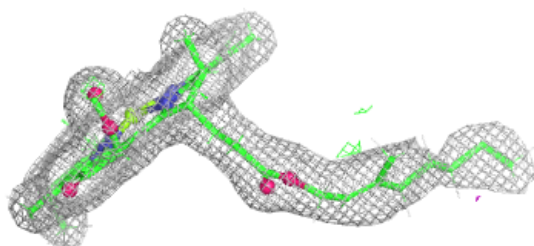
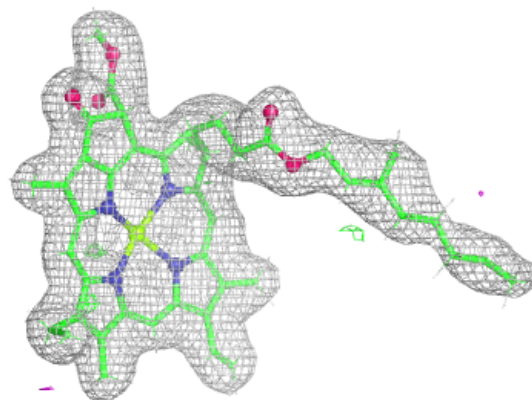
**Electron density around CLA A 606:**

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



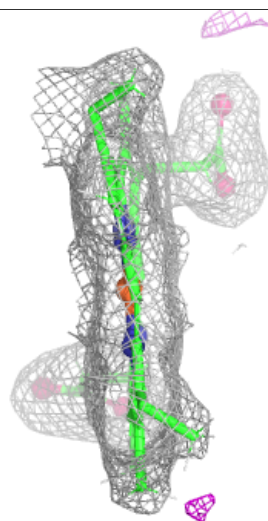
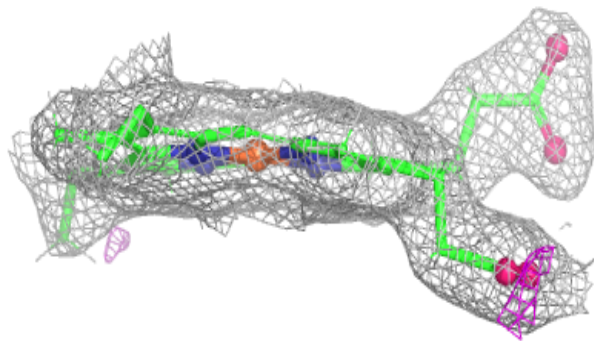
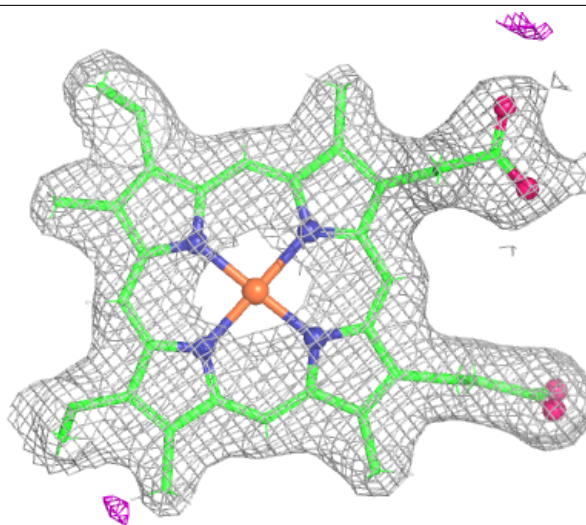
Electron density around CLA A 608:

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



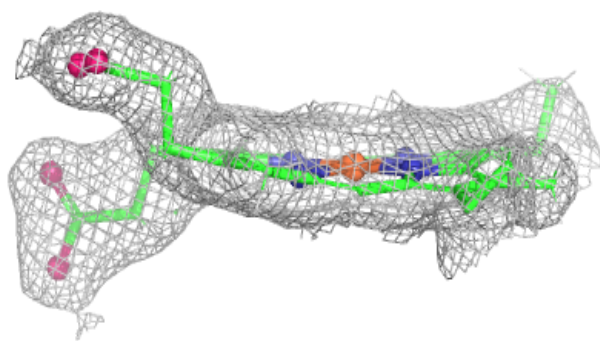
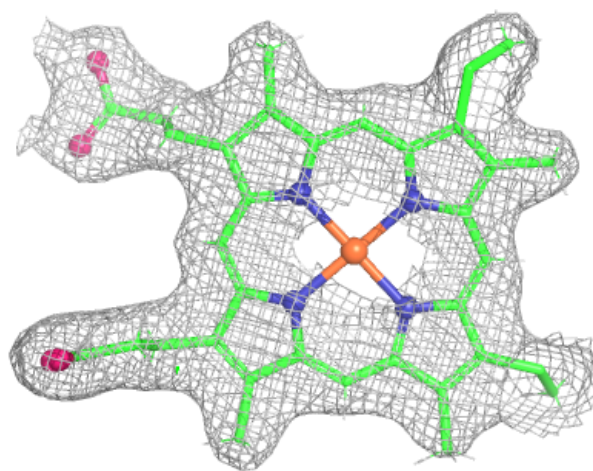
Electron density around HEC V 201:

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



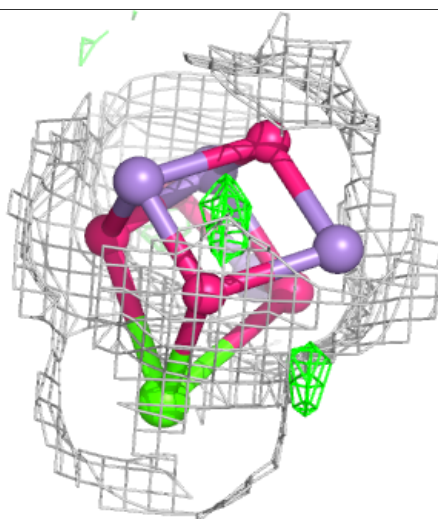
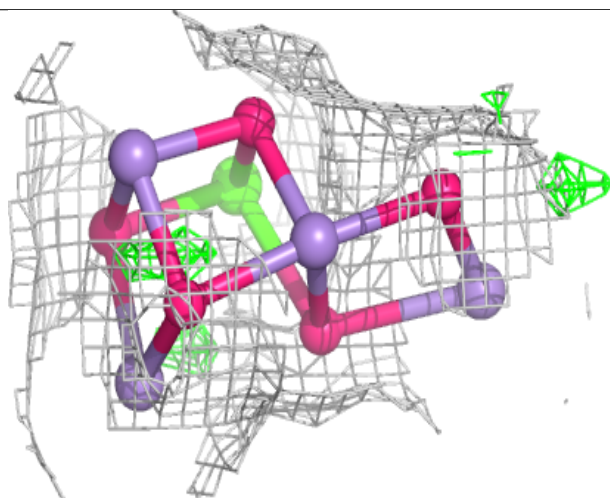
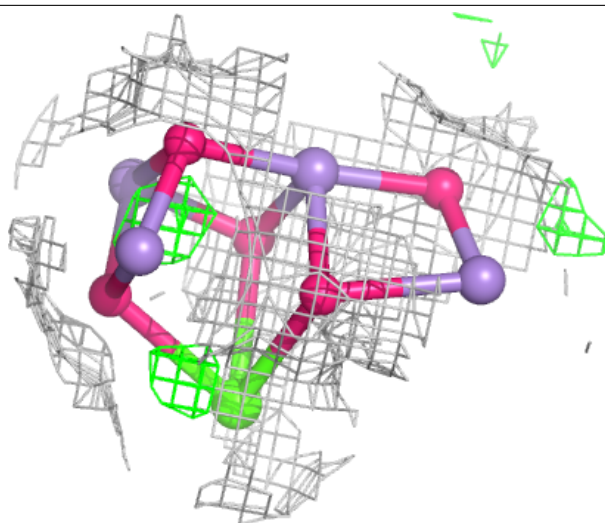
Electron density around HEC v 201:

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



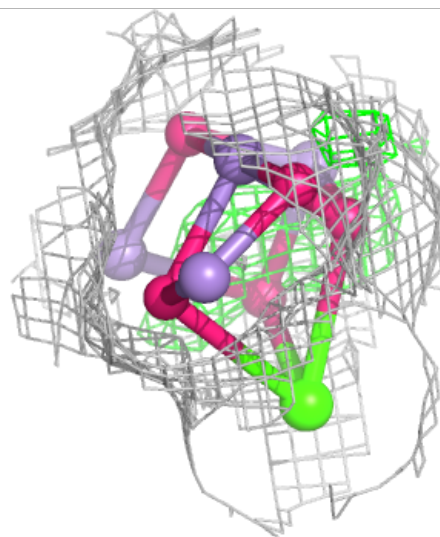
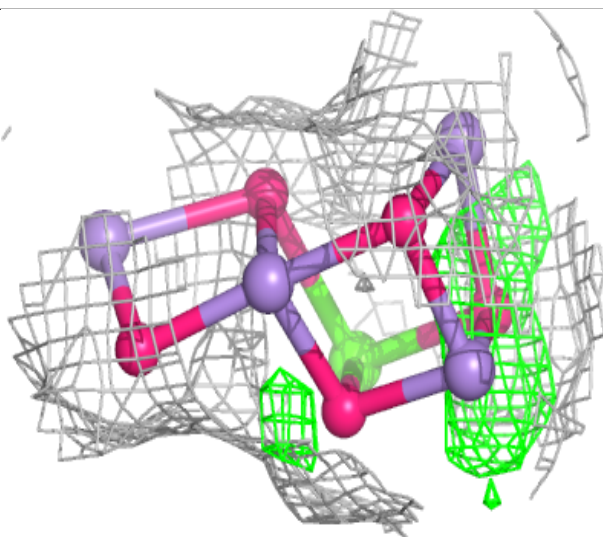
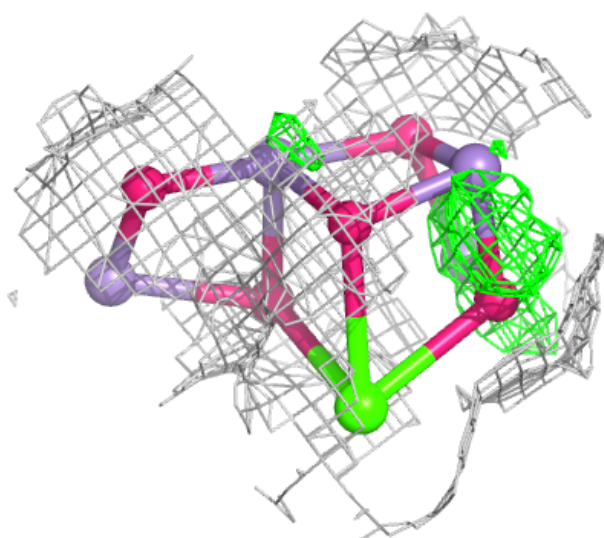
Electron density around OEX a 601:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.