



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2026 – 01:56 PM EDT

PDB ID : 13CH / pdb_000013ch
Title : RT XFEL structure of one-flash state of Photosystem II (1F, S2 rich) at 2.02 Angstrom
Authors : Bhowmick, A.; Kern, J.; Yano, J.; Yachandra, V.K.; Bogacz, I.; Chatterjee, R.; Zhang, M.
Deposited on : 2026-04-28
Resolution : 2.02 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

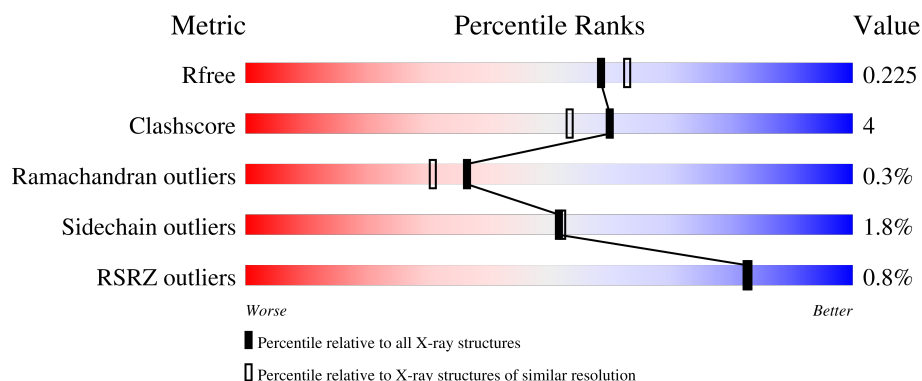
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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.



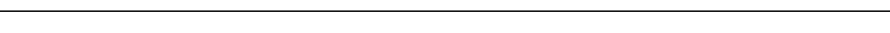
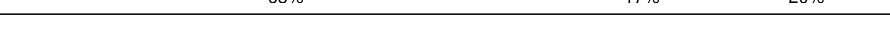
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	89% 8% .
1	a	344	88% 9% ..
2	B	510	92% 7% .
2	b	510	89% 10% .

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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	 % 66% 5% 28%
16	V	163	 76% 8% 16%
16	v	163	 71% 13% 16%
17	Y	46	 7% 46% 13% 41%
17	y	46	 2% 52% 11% 35%
18	X	41	 2% 88% 5% 7%
18	x	41	 2% 80% 12% 5%
19	Z	62	 5% 79% 21%
19	z	62	 6% 77% 21%
20	R	41	 54% 15% 32%
20	r	41	 12% 41% 22% 5% 32%

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

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

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 104064 atoms, of which 51466 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
			4864	1717	2242	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			4851	1714	2232	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
			6707	2244	3290	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6855	2286	3361	587	608	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
			5303	1800	2586	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5315	1804	2592	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
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	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.

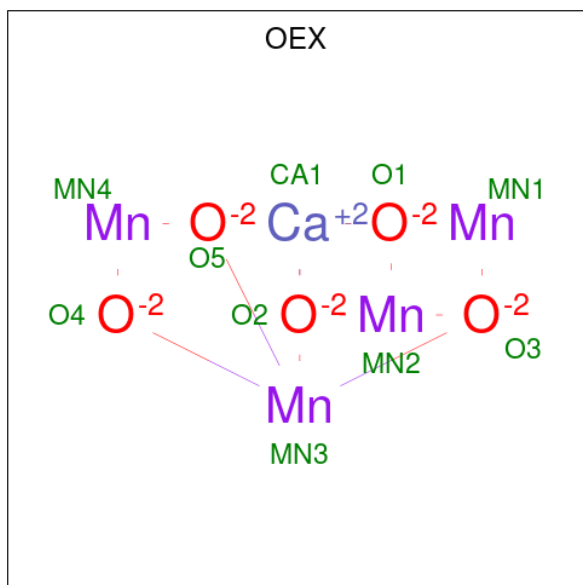
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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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).

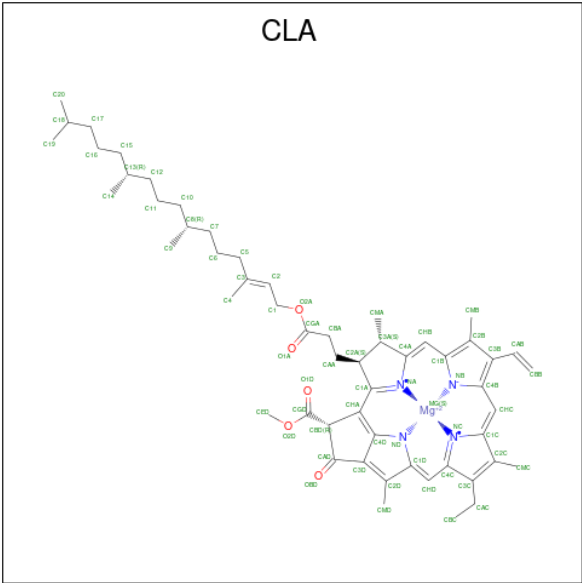
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		

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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
			134	55	69	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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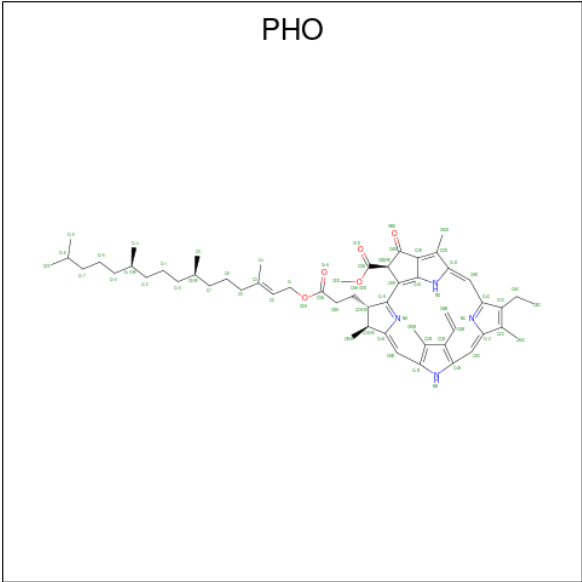
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 134	C 55	H 69	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	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
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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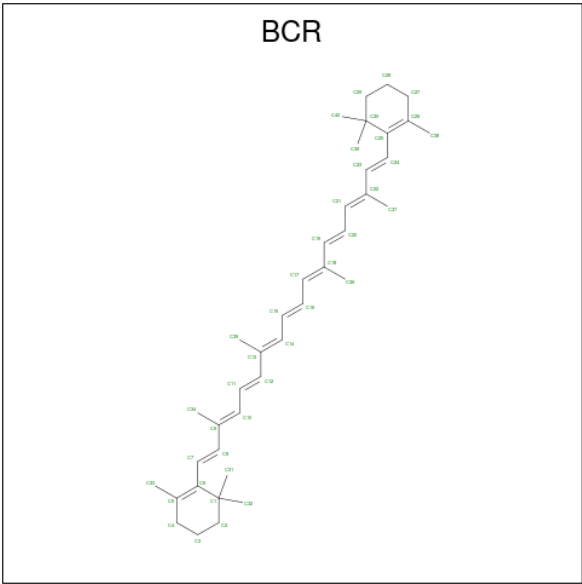
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



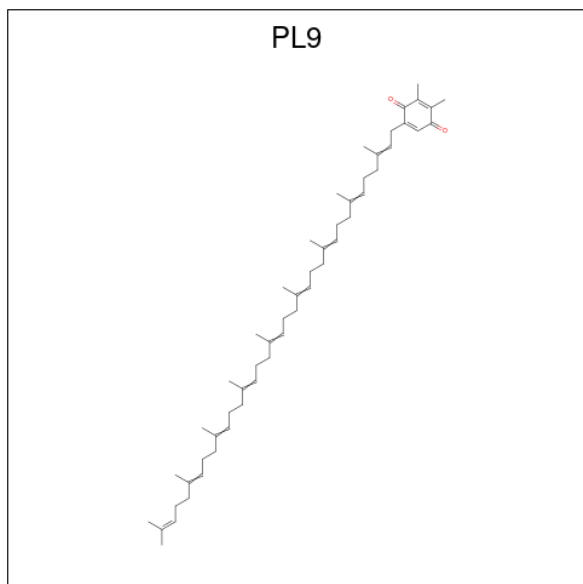
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
25	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



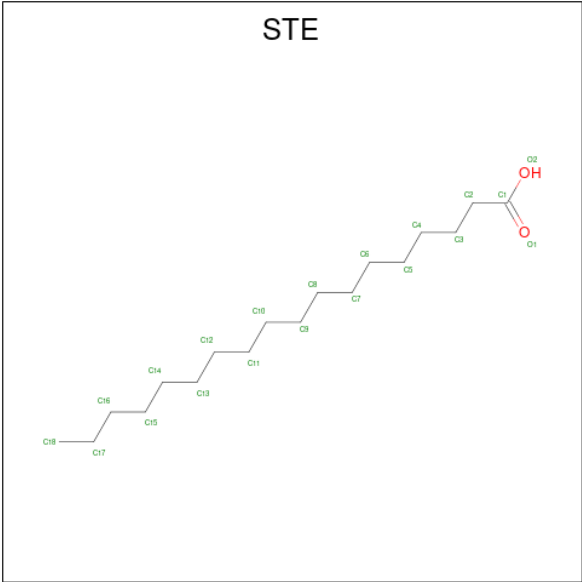
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	H	1	Total	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 23 9 14	0	0
28	A	1	Total C H 50 17 33	0	0
28	A	1	Total C H 32 11 21	0	0
28	B	1	Total C H O 43 15 26 2	0	0
28	B	1	Total C H O 46 16 28 2	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H 41 15 26	0	0
28	C	1	Total C H O 34 12 20 2	0	0
28	C	1	Total C H 11 5 6	0	0
28	C	1	Total C H 17 7 10	0	0
28	C	1	Total C H 26 10 16	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	C	1	Total C H 47 16 31	0	0
28	C	1	Total C H 41 14 27	0	0

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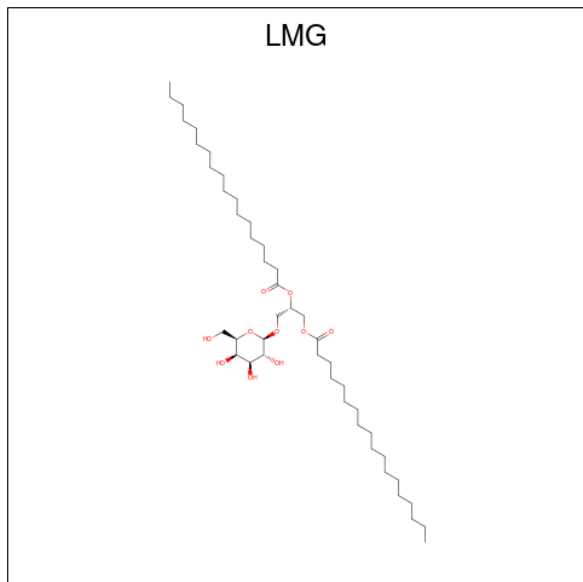
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C H 41 14 27	0	0
28	D	1	Total C H 26 9 17	0	0
28	E	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H 35 12 23	0	0
28	E	1	Total C H O 55 18 35 2	0	0
28	H	1	Total C H 53 18 35	0	0
28	I	1	Total C H O 43 15 26 2	0	0
28	I	1	Total C H O 37 13 22 2	0	0
28	J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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	b	1	Total	C	H		0	0
			32	11	21			
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
			34	12	20	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	l	1	Total	C	H		0	0
			53	18	35			
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	t	1	Total	C	H		0	0
			26	10	16			
28	x	1	Total	C	H	O	0	0
			55	18	35	2		
28	z	1	Total	C	H		0	0
			23	9	14			

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



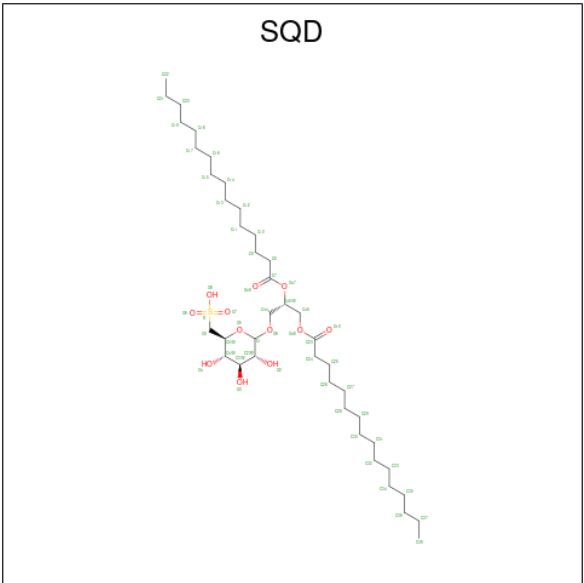
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	B	1	Total	C	H	O	0	0
			105	35	60	10		
29	B	1	Total	C	H	O	0	0
			123	41	72	10		
29	C	1	Total	C	H	O	0	0
			76	26	40	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			120	40	70	10		
29	D	1	Total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

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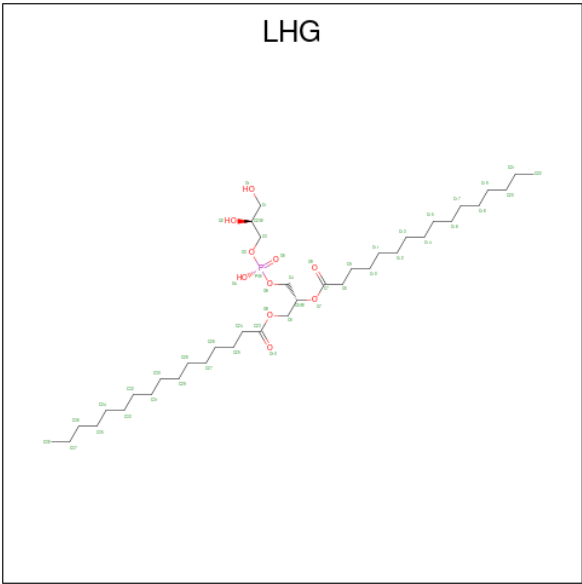
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	d	1	Total	C	H	O	0	0
			102	34	58	10		
29	m	1	Total	C	H	O	0	0
			123	41	72	10		
29	o	1	Total	C	H	O	0	0
			141	45	86	10		

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



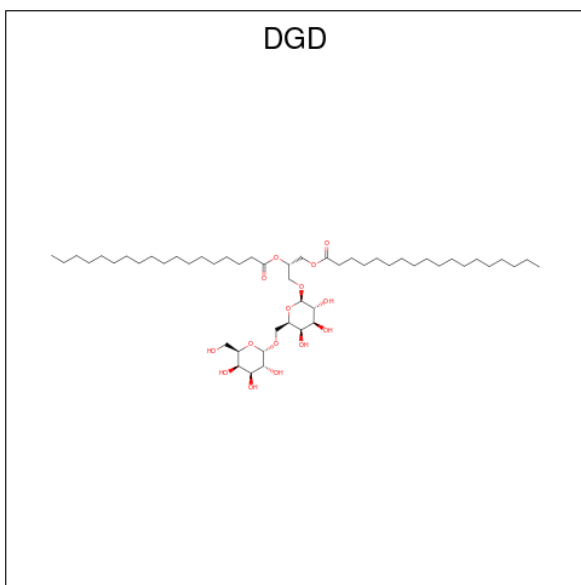
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
30	A	1	Total	C	H	O	S	0	0
			95	30	52	12	1		
30	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
30	a	1	Total	C	H	O	S	0	0
			131	41	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 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



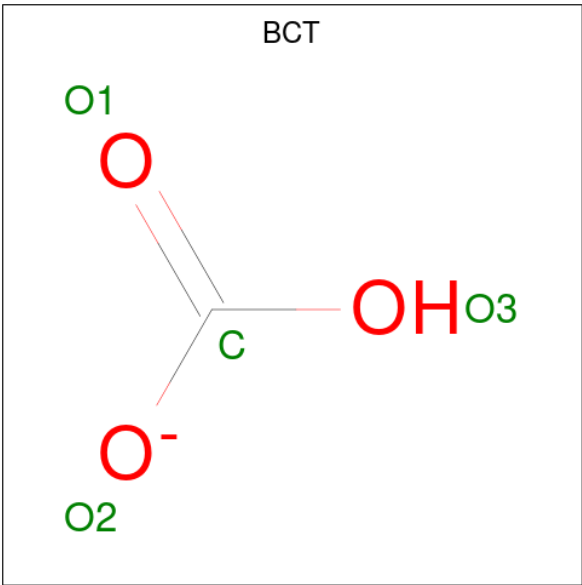
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
31	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
31	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



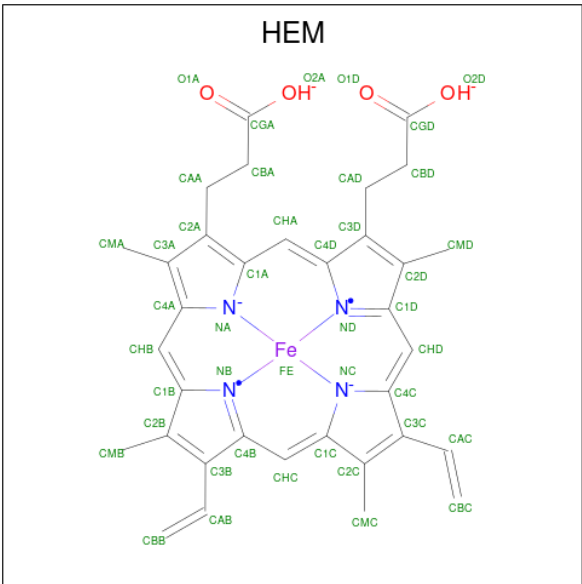
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	H	O	0	0
			162	51	96	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	H	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total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

- Molecule 33 is 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: C₃₄H₃₂FeN₄O₄).



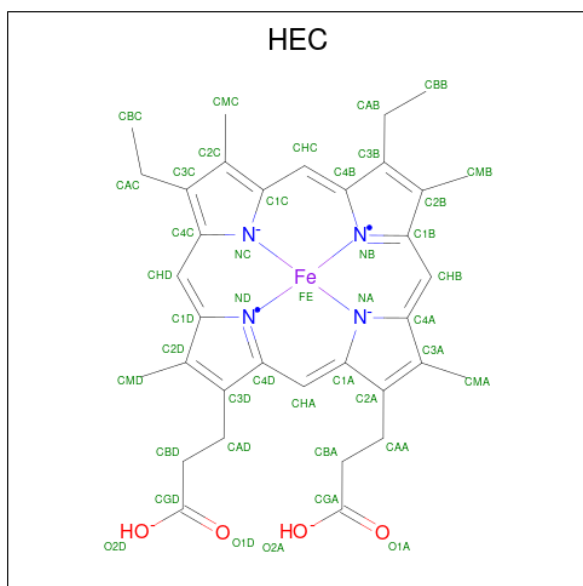
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	221	Total	O	0	0
			221	221		
36	C	187	Total	O	0	0
			187	187		
36	D	134	Total	O	0	0
			134	134		
36	E	29	Total	O	0	0
			29	29		
36	F	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	31	Total O 31 31	0	0
36	I	6	Total O 6 6	0	0
36	J	14	Total O 14 14	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	7	Total O 7 7	0	0
36	O	109	Total O 109 109	0	0
36	T	12	Total O 12 12	0	0
36	U	43	Total O 43 43	0	0
36	V	72	Total O 72 72	0	0
36	Y	1	Total O 1 1	0	0
36	X	17	Total O 17 17	0	0
36	Z	3	Total O 3 3	0	0
36	R	6	Total O 6 6	0	0
36	a	116	Total O 116 116	0	0
36	b	207	Total O 207 207	0	0
36	c	191	Total O 191 191	0	0
36	d	118	Total O 118 118	0	0
36	e	21	Total O 21 21	0	0
36	f	6	Total O 6 6	0	0
36	h	17	Total O 17 17	0	0

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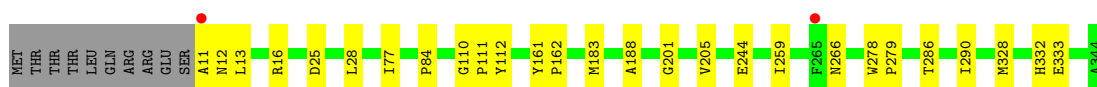
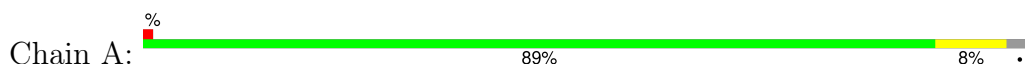
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	i	13	Total 13	O 13	0	0
36	j	7	Total 7	O 7	0	0
36	k	4	Total 4	O 4	0	0
36	l	11	Total 11	O 11	0	0
36	m	6	Total 6	O 6	0	0
36	o	101	Total 101	O 101	0	0
36	t	10	Total 10	O 10	0	0
36	u	74	Total 74	O 74	0	0
36	v	62	Total 62	O 62	0	0
36	y	2	Total 2	O 2	0	0
36	x	15	Total 15	O 15	0	0
36	z	4	Total 4	O 4	0	0
36	r	11	Total 11	O 11	0	0

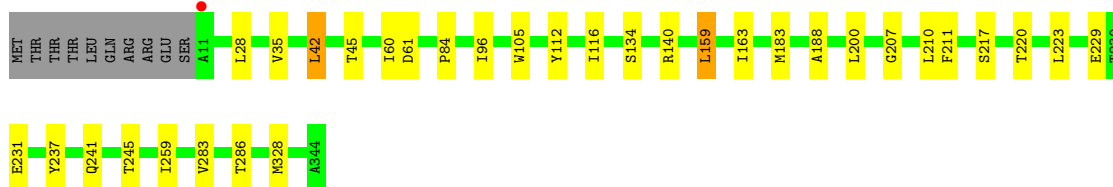
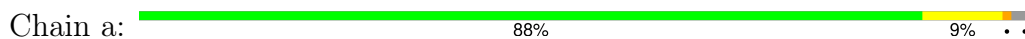
3 Residue-property plots [i](#)

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

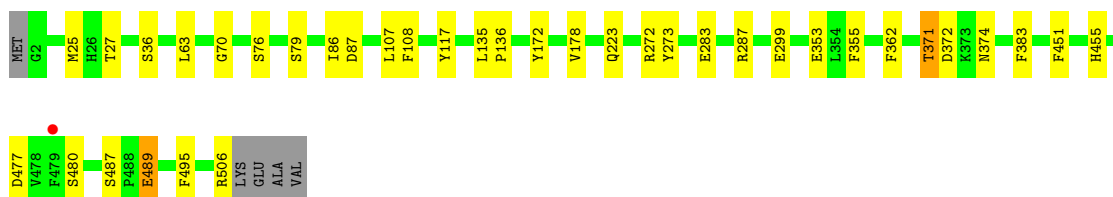
- Molecule 1: Photosystem II protein D1 1



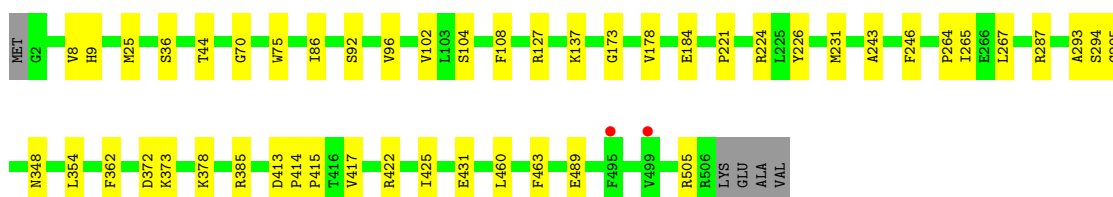
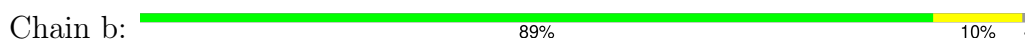
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

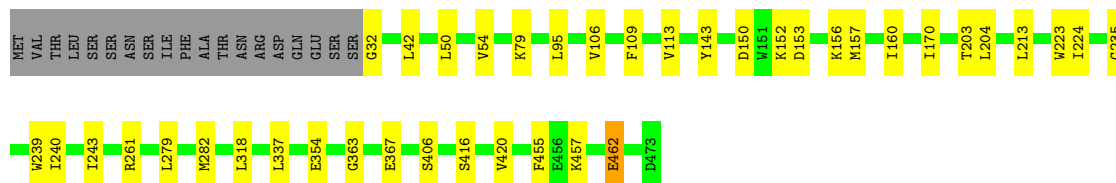


- Molecule 2: Photosystem II CP47 reaction center protein



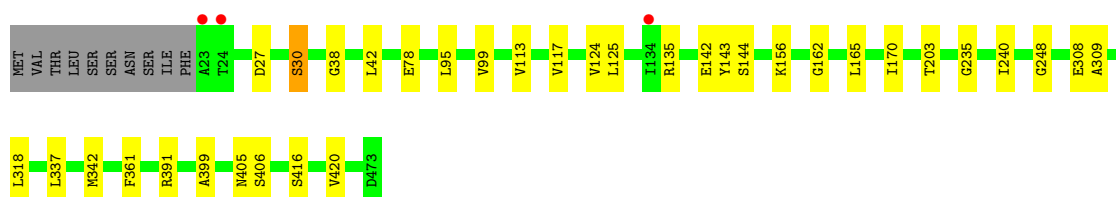
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  90% 7% .



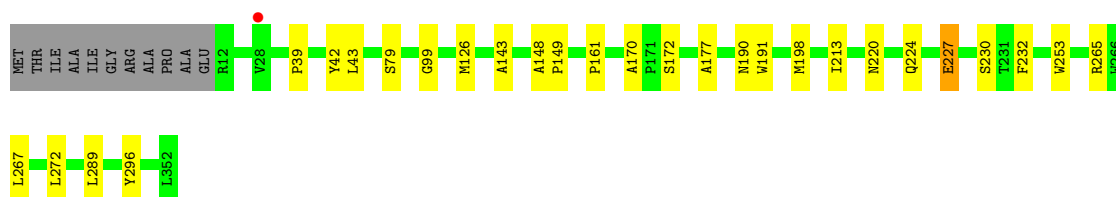
- Molecule 4: Photosystem II D2 protein

Chain D:  90% 7% .



- Molecule 4: Photosystem II D2 protein

Chain d:  89% 8% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  86% 11% .

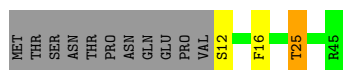


- Molecule 5: Cytochrome b559 subunit alpha

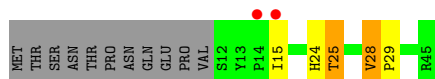
Chain e:  83% 14% .



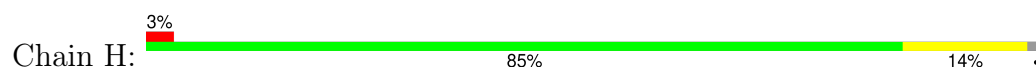
• Molecule 6: Cytochrome b559 subunit beta



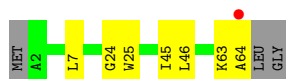
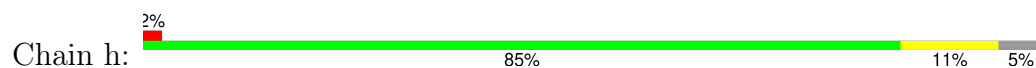
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H



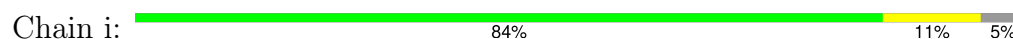
• Molecule 7: Photosystem II reaction center protein H



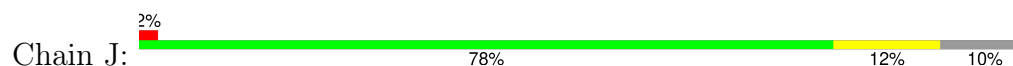
• Molecule 8: Photosystem II reaction center protein I

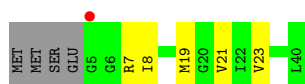


• Molecule 8: Photosystem II reaction center protein I



• Molecule 9: Photosystem II reaction center protein J





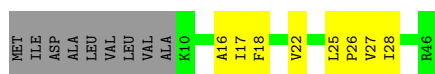
- Molecule 9: Photosystem II reaction center protein J

Chain j: 70% 20% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 63% 17% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 61% 20% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 14%



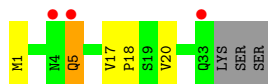
- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 8% 78% 11% 8%

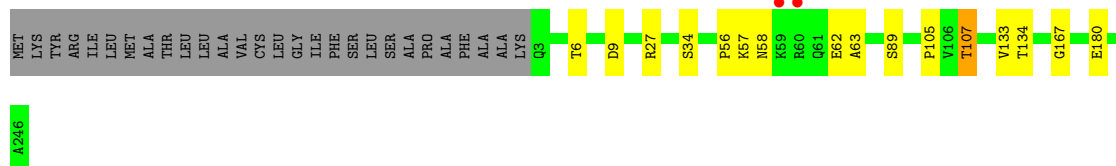
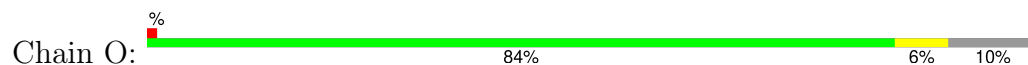


- Molecule 12: Photosystem II reaction center protein M

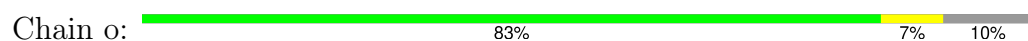
Chain m: 72% 17% 11%



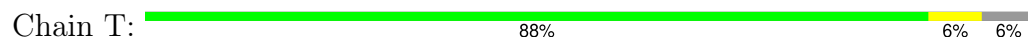
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



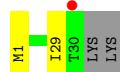
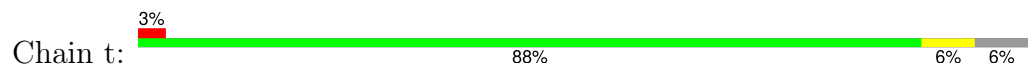
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



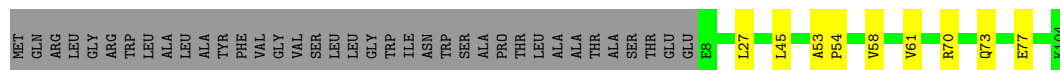
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

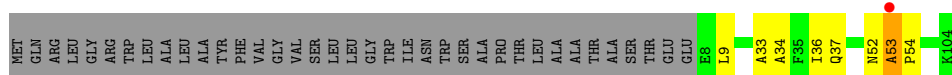


- Molecule 15: Photosystem II 12 kDa extrinsic protein

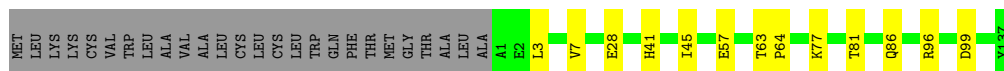


- Molecule 15: Photosystem II 12 kDa extrinsic protein





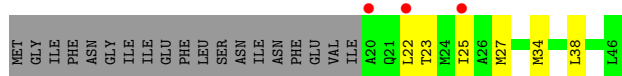
• Molecule 16: Cytochrome c-550



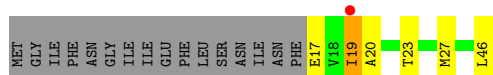
• Molecule 16: Cytochrome c-550



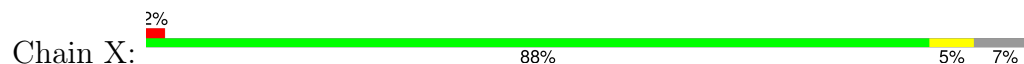
• Molecule 17: Photosystem II reaction center protein Ycf12



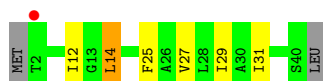
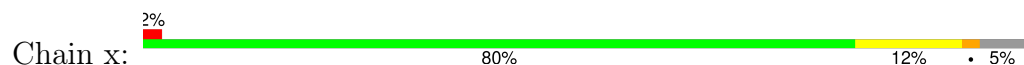
• Molecule 17: Photosystem II reaction center protein Ycf12



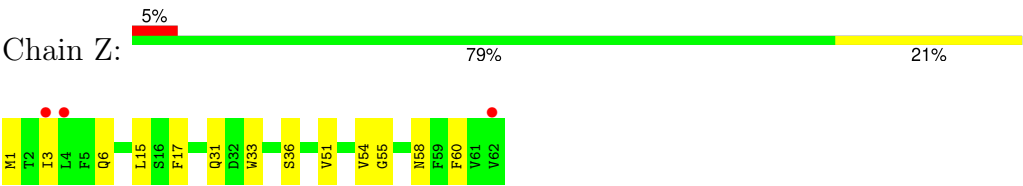
• Molecule 18: Photosystem II reaction center X protein



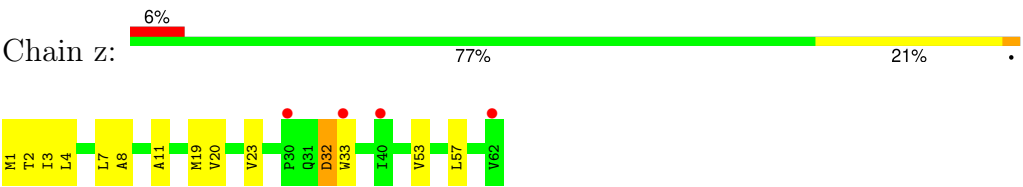
• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



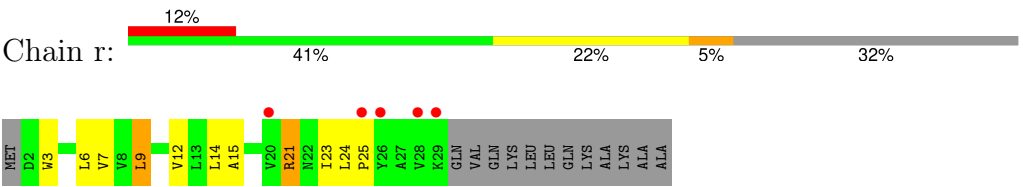
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.54Å 222.87Å 309.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.14 – 2.02 30.14 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.14-2.02) 87.4 (30.14-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.225 0.173 , 0.225	Depositor DCC
R_{free} test set	4689 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	104064	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2707	0.69	0/3692
1	a	0.59	0/2704	0.68	0/3688
2	B	0.55	0/4179	0.64	0/5693
2	b	0.54	0/4127	0.64	0/5623
3	C	0.57	1/3538 (0.0%)	0.65	1/4818 (0.0%)
3	c	0.51	0/3610	0.63	0/4914
4	D	0.59	0/2812	0.65	0/3832
4	d	0.55	0/2821	0.63	0/3844
5	E	0.45	0/688	0.58	0/940
5	e	0.39	0/683	0.53	0/932
6	F	0.41	0/284	0.53	0/387
6	f	0.44	0/284	0.61	0/387
7	H	0.51	0/517	0.62	0/705
7	h	0.42	0/505	0.59	0/689
8	I	0.53	0/293	0.60	0/396
8	i	0.54	0/293	0.58	0/396
9	J	0.49	0/263	0.56	0/356
9	j	0.42	0/263	0.50	0/356
10	K	0.38	0/303	0.51	0/416
10	k	0.40	0/303	0.49	0/416
11	L	0.59	0/311	0.69	0/422
11	l	0.61	0/303	0.64	0/412
12	M	0.56	0/249	0.76	0/341
12	m	0.57	0/244	0.69	0/334
13	O	0.53	0/1904	0.64	0/2585
13	o	0.53	0/1905	0.66	0/2583
14	T	0.53	0/257	0.69	0/349
14	t	0.58	0/255	0.60	0/346
15	U	0.49	0/785	0.60	0/1064
15	u	0.52	0/785	0.68	0/1064
16	V	0.53	0/1085	0.67	0/1473
16	v	0.48	0/1085	0.57	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.36	0/197	0.47	0/264
17	y	0.33	0/219	0.49	0/294
18	X	0.43	0/284	0.58	0/384
18	x	0.38	0/289	0.45	0/391
19	Z	0.34	0/490	0.53	0/669
19	z	0.30	0/488	0.47	0/666
20	R	0.32	0/227	0.48	0/313
20	r	0.26	0/227	0.41	0/313
All	All	0.53	1/42766 (0.0%)	0.63	1/58220 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	462	GLU	CG-CD	-5.70	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	462	GLU	CA-CB-CG	-6.22	101.67	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2242	2519	17	0
1	a	2619	2232	2510	20	0
2	B	4016	3887	3871	23	0
2	b	3984	3842	3842	36	0
3	C	3417	3290	3337	30	3
3	c	3494	3361	3420	22	0
4	D	2717	2586	2621	16	0
4	d	2723	2592	2627	19	0
5	E	666	651	651	8	0
5	e	664	648	648	11	0
6	F	275	282	282	3	0
6	f	275	282	282	4	0
7	H	505	528	528	5	3
7	h	493	514	514	6	0
8	I	296	311	311	4	0
8	i	296	311	311	4	0
9	J	257	268	268	5	0
9	j	257	268	268	7	0
10	K	293	305	305	5	0
10	k	293	305	305	4	0
11	L	304	316	316	4	0
11	l	296	304	304	2	0
12	M	256	267	269	4	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	11	0
13	o	1874	1846	1846	8	0
14	T	258	261	261	2	0
14	t	256	256	256	1	0
15	U	774	773	773	5	0
15	u	774	773	773	5	0
16	V	1064	1070	1073	7	0
16	v	1064	1070	1073	16	0
17	Y	196	217	217	4	0
17	y	218	241	241	5	0
18	X	281	312	312	3	0
18	x	286	316	314	4	0
19	Z	479	516	516	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	477	509	509	8	0
20	R	221	238	238	4	0
20	r	221	238	238	8	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	249	261	264	4	0
24	B	1035	1139	1139	15	0
24	C	839	922	922	17	0
24	D	130	144	144	1	0
24	a	195	213	216	2	0
24	b	1035	1139	1139	20	0
24	c	839	919	919	9	0
24	d	195	216	216	3	0
25	A	64	74	74	0	0
25	D	64	74	74	2	0
25	d	128	148	148	0	0
26	A	40	56	56	2	0
26	B	120	168	168	6	0
26	C	80	112	112	1	0
26	D	40	56	56	5	0
26	H	40	56	56	2	0
26	K	80	112	112	8	0
26	T	40	56	56	5	0
26	a	40	56	56	0	0
26	b	120	168	168	6	0
26	c	80	112	112	6	0
26	d	40	56	56	1	0
26	h	40	56	56	1	0
26	k	80	112	112	3	0
26	t	40	56	56	3	0
27	A	55	80	80	1	0
27	D	55	80	80	1	0
27	a	55	80	80	1	0
27	d	55	80	80	0	0
28	A	37	68	68	1	0
28	B	62	96	96	1	0
28	C	92	153	153	2	0
28	D	9	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	E	44	74	74	1	0
28	H	18	35	35	0	0
28	I	32	48	48	0	0
28	J	12	16	16	0	0
28	M	40	67	67	0	0
28	R	20	35	35	4	0
28	X	20	35	35	1	0
28	Z	17	33	33	0	0
28	a	12	16	16	0	0
28	b	81	142	142	2	0
28	c	31	57	57	1	0
28	d	54	90	90	2	0
28	e	31	52	52	1	0
28	f	8	15	15	0	0
28	h	10	19	19	0	0
28	i	18	24	24	1	0
28	j	28	47	47	0	0
28	l	18	35	35	1	0
28	m	12	16	16	0	0
28	t	24	36	36	2	0
28	x	20	35	35	2	0
28	z	9	14	14	0	0
29	A	48	66	66	0	0
29	B	96	132	132	2	0
29	C	84	106	106	1	0
29	D	101	142	142	1	0
29	b	55	86	86	1	0
29	c	173	240	240	2	0
29	d	44	58	58	1	0
29	m	51	72	72	1	0
29	o	55	86	86	1	0
30	A	95	122	124	1	0
30	B	54	77	78	1	0
30	F	36	45	46	0	0
30	a	108	154	156	3	0
30	b	49	64	65	1	0
30	f	41	48	49	1	0
31	A	49	74	74	2	0
31	D	145	215	214	2	0
31	L	49	74	74	0	0
31	d	137	199	199	8	0
31	e	42	57	57	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	l	49	74	74	0	0
32	A	66	96	96	2	0
32	C	186	246	246	1	0
32	H	62	82	80	0	0
32	c	186	246	243	1	0
32	h	62	82	82	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	F	43	30	30	2	0
34	e	43	30	30	4	0
35	V	43	30	30	0	0
35	v	43	30	30	1	0
36	A	144	0	0	3	0
36	B	221	0	0	4	1
36	C	187	0	0	10	1
36	D	134	0	0	1	0
36	E	29	0	0	0	0
36	F	5	0	0	0	0
36	H	31	0	0	1	0
36	I	6	0	0	0	0
36	J	14	0	0	0	0
36	K	7	0	0	0	0
36	L	11	0	0	0	0
36	M	7	0	0	0	0
36	O	109	0	0	1	0
36	R	6	0	0	0	0
36	T	12	0	0	0	0
36	U	43	0	0	1	0
36	V	72	0	0	1	0
36	X	17	0	0	0	0
36	Y	1	0	0	0	0
36	Z	3	0	0	1	0
36	a	116	0	0	1	0
36	b	207	0	0	8	0
36	c	191	0	0	5	0
36	d	118	0	0	0	0
36	e	21	0	0	1	0
36	f	6	0	0	0	0
36	h	17	0	0	1	0
36	i	13	0	0	2	0
36	j	7	0	0	2	0
36	k	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	11	0	0	0	0
36	m	6	0	0	1	0
36	o	101	0	0	1	0
36	r	11	0	0	1	0
36	t	10	0	0	2	0
36	u	74	0	0	0	0
36	v	62	0	0	2	0
36	x	15	0	0	0	0
36	y	2	0	0	0	0
36	z	4	0	0	0	0
All	All	52598	51466	52195	444	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 444 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)
3:C:153:ASP:N	36:C:601:HOH:O	1.91	1.04
16:v:6:GLU:OE1	36:v:301:HOH:O	1.80	0.98
13:o:84:GLU:OE2	13:o:86:LYS:NZ	1.96	0.97
24:b:613:CLA:H203	31:d:410:LHG:H223	1.48	0.95
13:O:27:ARG:NH1	36:O:301:HOH:O	2.03	0.92

All (4) 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:OE1	7:H:3:ARG:NH1[4_557]	1.45	0.75
3:C:462:GLU:OE1	7:H:3:ARG:HH12[4_557]	1.20	0.40
3:C:462:GLU:OE2	7:H:3:ARG:NH2[4_557]	2.12	0.08
36:B:865:HOH:O	36:C:768:HOH:O[1_455]	2.16	0.04

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	31
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	36	31
2	B	510/510 (100%)	503 (99%)	7 (1%)	0	100	100
2	b	504/510 (99%)	493 (98%)	9 (2%)	2 (0%)	30	22
3	C	441/461 (96%)	432 (98%)	8 (2%)	1 (0%)	43	40
3	c	450/461 (98%)	441 (98%)	7 (2%)	2 (0%)	30	22
4	D	339/352 (96%)	330 (97%)	9 (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%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	229 (94%)	13 (5%)	1 (0%)	30	22
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	16	8
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%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	5
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	10
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	26/41 (63%)	26 (100%)	0	0	100	100
20	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
All	All	5232/5700 (92%)	5091 (97%)	127 (2%)	14 (0%)	36	31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
13	o	58	ASN
15	u	53	ALA
9	J	7	ARG

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%)	268 (99%)	2 (1%)	76	77
1	a	269/280 (96%)	262 (97%)	7 (3%)	40	38
2	B	410/407 (101%)	401 (98%)	9 (2%)	45	45
2	b	403/407 (99%)	402 (100%)	1 (0%)	87	88
3	C	345/362 (95%)	342 (99%)	3 (1%)	70	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	353/362 (98%)	346 (98%)	7 (2%)	48	48
4	D	276/283 (98%)	273 (99%)	3 (1%)	65	68
4	d	277/283 (98%)	274 (99%)	3 (1%)	65	68
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	35
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	61
6	F	28/39 (72%)	26 (93%)	2 (7%)	13	7
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	7
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	50
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	31
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%)	23 (96%)	1 (4%)	26	20
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	32 (94%)	2 (6%)	18	10
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	26
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	202 (98%)	4 (2%)	50	50
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	41
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%)	83 (99%)	1 (1%)	63	65
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	65
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	115 (98%)	2 (2%)	53	53
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	17
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	23
19	z	51/52 (98%)	49 (96%)	2 (4%)	28	22
20	R	22/33 (67%)	22 (100%)	0	100	100
20	r	22/33 (67%)	18 (82%)	4 (18%)	2	0
All	All	4322/4654 (93%)	4243 (98%)	79 (2%)	51	52

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	19	ASP
17	y	19	ILE
10	k	30	VAL
13	o	118	LEU
20	r	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
19	Z	6	GLN
13	o	231	HIS
1	a	165	GLN
19	z	58	ASN
11	l	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	1.07	1 (12%)	8,9,11	1.63	1 (12%)
12	FME	m	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.68	0
12	FME	M	1	12	8,9,10	1.07	1 (12%)	8,9,11	0.68	0
14	FME	T	1	14	8,9,10	0.90	0	8,9,11	1.04	0
8	FME	i	1	8	8,9,10	1.15	0	8,9,11	1.08	0
14	FME	t	1	14	8,9,10	1.15	1 (12%)	8,9,11	1.22	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	-
12	FME	m	1	12	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	FME	CA-N	-2.37	1.43	1.46
12	M	1	FME	CA-N	-2.32	1.43	1.46
14	t	1	FME	CA-N	-2.27	1.43	1.46
12	m	1	FME	CA-N	-2.26	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-3.25	117.82	122.82

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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	$\# Z > 2$
28	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.97	0
28	STE	e	101	-	8,8,19	0.50	0	7,7,19	0.53	0
24	CLA	C	511	3	69,73,73	1.49	11 (15%)	82,113,113	1.36	6 (7%)
24	CLA	b	614	2	69,73,73	1.26	8 (11%)	82,113,113	1.40	12 (14%)
24	CLA	b	608	2	69,73,73	1.18	6 (8%)	82,113,113	1.23	8 (9%)
24	CLA	b	609	2	69,73,73	1.41	10 (14%)	82,113,113	1.42	15 (18%)
28	STE	b	621	-	15,15,19	0.48	0	14,14,19	0.57	0
24	CLA	C	504	36	63,67,73	1.31	7 (11%)	74,105,113	1.42	9 (12%)
28	STE	J	101	-	11,11,19	0.77	0	11,11,19	0.93	0
24	CLA	c	511	3	69,73,73	1.57	7 (10%)	82,113,113	1.54	6 (7%)
24	CLA	d	406	4	69,73,73	1.44	11 (15%)	82,113,113	1.19	8 (9%)
24	CLA	C	507	36	69,73,73	1.27	7 (10%)	82,113,113	1.51	9 (10%)
24	CLA	B	601	36	69,73,73	1.59	10 (14%)	82,113,113	1.51	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	C	524	-	48,48,55	0.99	4 (8%)	56,56,63	1.26	3 (5%)
28	STE	e	104	-	8,8,19	0.45	0	7,7,19	0.64	0
26	BCR	b	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.20	5 (8%)
30	SQD	F	102	-	34,36,54	1.47	5 (14%)	42,45,65	2.13	12 (28%)
31	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.20	5 (9%)
24	CLA	A	606	36	69,73,73	1.16	6 (8%)	82,113,113	1.33	9 (10%)
24	CLA	C	501	3	69,73,73	1.35	7 (10%)	82,113,113	1.48	8 (9%)
28	STE	e	105	-	12,12,19	0.74	0	12,12,19	1.25	2 (16%)
28	STE	E	103	-	19,19,19	0.78	0	19,19,19	0.82	0
24	CLA	C	510	3	69,73,73	1.27	11 (15%)	82,113,113	1.24	4 (4%)
28	STE	t	103	-	9,9,19	0.53	0	8,8,19	0.53	0
24	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.38	8 (9%)
24	CLA	B	611	2	69,73,73	1.43	8 (11%)	82,113,113	1.51	12 (14%)
24	CLA	B	616	2	64,68,73	1.64	9 (14%)	76,107,113	1.51	9 (11%)
28	STE	b	622	-	19,19,19	0.58	0	19,19,19	1.13	0
32	DGD	A	617	-	67,67,67	1.21	8 (11%)	81,81,81	1.38	10 (12%)
32	DGD	C	522	-	63,63,67	1.14	6 (9%)	77,77,81	1.38	10 (12%)
32	DGD	h	102	-	63,63,67	1.14	7 (11%)	77,77,81	1.43	11 (14%)
28	STE	d	415	-	13,13,19	0.73	0	13,13,19	0.99	0
29	LMG	c	522	-	46,46,55	1.08	5 (10%)	54,54,63	1.21	4 (7%)
28	STE	B	625	-	11,11,19	0.86	0	11,11,19	1.30	1 (9%)
25	PHO	A	607	-	58,69,69	1.76	11 (18%)	55,99,99	1.71	9 (16%)
28	STE	C	515	-	13,13,19	0.83	0	13,13,19	0.90	0
24	CLA	B	604	2	69,73,73	1.41	7 (10%)	82,113,113	1.80	6 (7%)
31	LHG	D	411	-	48,48,48	0.90	2 (4%)	51,54,54	1.37	8 (15%)
35	HEC	v	201	16	50,50,50	1.72	5 (10%)	68,82,82	1.35	8 (11%)
25	PHO	D	402	-	58,69,69	1.88	7 (12%)	55,99,99	1.47	8 (14%)
26	BCR	c	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.38	10 (17%)
24	CLA	B	607	36	69,73,73	1.24	6 (8%)	82,113,113	1.44	7 (8%)
24	CLA	C	509	3	69,73,73	1.16	7 (10%)	82,113,113	1.33	9 (10%)
24	CLA	A	605	1	69,73,73	1.22	7 (10%)	82,113,113	1.20	6 (7%)
26	BCR	C	520	-	41,41,41	1.00	2 (4%)	56,56,56	1.21	5 (8%)
24	CLA	C	505	3	69,73,73	1.29	8 (11%)	82,113,113	1.50	6 (7%)
28	STE	t	102	-	13,13,19	0.74	0	13,13,19	1.12	2 (15%)
29	LMG	o	301	-	55,55,55	1.32	6 (10%)	63,63,63	1.55	7 (11%)
24	CLA	c	509	3	69,73,73	1.22	7 (10%)	82,113,113	1.42	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	404	36	69,73,73	1.50	5 (7%)	82,113,113	1.47	8 (9%)
24	CLA	c	505	3	69,73,73	1.12	6 (8%)	82,113,113	1.35	8 (9%)
28	STE	H	103	-	17,17,19	0.55	0	16,16,19	0.58	0
28	STE	B	622	-	16,16,19	0.71	0	16,16,19	1.16	1 (6%)
26	BCR	h	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.32	11 (19%)
28	STE	b	626	-	7,7,19	0.42	0	6,6,19	0.63	0
28	STE	C	528	-	13,13,19	0.46	0	12,12,19	0.61	0
28	STE	m	102	-	11,11,19	0.79	0	11,11,19	1.06	0
30	SQD	A	616	-	41,43,54	1.76	9 (21%)	51,54,65	1.54	9 (17%)
24	CLA	b	605	2	69,73,73	1.30	10 (14%)	82,113,113	1.51	13 (15%)
29	LMG	m	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.51	10 (16%)
24	CLA	b	607	36	69,73,73	1.11	7 (10%)	82,113,113	1.40	6 (7%)
33	BCT	D	401	22	3,3,3	1.11	0	2,3,3	3.45	1 (50%)
31	LHG	D	410	-	46,46,48	1.18	2 (4%)	49,52,54	1.31	4 (8%)
29	LMG	D	407	-	50,50,55	0.90	2 (4%)	58,58,63	1.19	4 (6%)
28	STE	C	526	-	15,15,19	0.35	0	14,14,19	0.88	0
26	BCR	K	102	-	41,41,41	1.05	3 (7%)	56,56,56	1.21	6 (10%)
24	CLA	a	607	1	69,73,73	1.19	7 (10%)	82,113,113	1.39	11 (13%)
29	LMG	c	523	-	48,48,55	0.97	4 (8%)	56,56,63	1.27	7 (12%)
27	PL9	A	610	-	55,55,55	1.26	5 (9%)	68,69,69	1.54	14 (20%)
24	CLA	b	604	2	69,73,73	1.17	6 (8%)	82,113,113	1.46	8 (9%)
27	PL9	D	406	-	55,55,55	1.19	4 (7%)	68,69,69	1.61	15 (22%)
28	STE	M	103	-	14,14,19	0.40	0	13,13,19	0.83	0
28	STE	M	101	-	14,14,19	0.70	0	14,14,19	0.98	0
29	LMG	B	620	-	45,45,55	1.18	3 (6%)	53,53,63	1.29	5 (9%)
24	CLA	b	611	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	11 (13%)
24	CLA	B	612	2	69,73,73	1.17	6 (8%)	82,113,113	1.32	9 (10%)
24	CLA	b	612	2	69,73,73	1.14	8 (11%)	82,113,113	1.40	12 (14%)
26	BCR	t	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	7 (12%)
28	STE	B	624	-	17,17,19	0.66	0	17,17,19	1.00	0
32	DGD	C	521	-	63,63,67	1.08	5 (7%)	77,77,81	1.29	7 (9%)
28	STE	D	412	-	8,8,19	0.48	0	7,7,19	0.58	0
33	BCT	d	401	22	3,3,3	1.04	0	2,3,3	3.11	1 (50%)
24	CLA	d	405	4	69,73,73	1.36	7 (10%)	82,113,113	1.36	8 (9%)
28	STE	j	102	-	15,15,19	0.51	0	14,14,19	0.62	0
24	CLA	c	503	3	69,73,73	1.13	5 (7%)	82,113,113	1.35	8 (9%)
26	BCR	K	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	STE	C	517	-	4,4,19	0.52	0	3,3,19	0.35	0
24	CLA	C	502	3	69,73,73	1.28	7 (10%)	82,113,113	1.44	11 (13%)
24	CLA	A	612	36	69,73,73	1.41	7 (10%)	82,113,113	1.28	8 (9%)
29	LMG	C	516	-	35,35,55	1.51	7 (20%)	43,43,63	1.43	5 (11%)
26	BCR	A	609	-	41,41,41	1.05	3 (7%)	56,56,56	1.29	6 (10%)
28	STE	i	101	-	11,11,19	0.84	0	11,11,19	1.04	1 (9%)
24	CLA	B	608	2	69,73,73	1.23	9 (13%)	82,113,113	1.23	8 (9%)
24	CLA	a	606	36	69,73,73	1.28	9 (13%)	82,113,113	1.40	12 (14%)
31	LHG	L	101	-	48,48,48	1.01	3 (6%)	51,54,54	1.23	4 (7%)
26	BCR	D	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	7 (12%)
28	STE	j	101	-	11,11,19	0.76	0	11,11,19	1.09	1 (9%)
24	CLA	c	512	3	69,73,73	1.29	9 (13%)	82,113,113	1.41	8 (9%)
24	CLA	B	613	2	69,73,73	1.33	10 (14%)	82,113,113	1.26	9 (10%)
26	BCR	T	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.32	8 (14%)
31	LHG	D	409	-	48,48,48	0.99	3 (6%)	51,54,54	1.10	3 (5%)
29	LMG	A	613	-	48,48,55	1.17	8 (16%)	56,56,63	1.41	10 (17%)
32	DGD	C	523	-	63,63,67	0.97	4 (6%)	77,77,81	1.19	6 (7%)
28	STE	C	518	-	6,6,19	0.46	0	5,5,19	0.43	0
28	STE	E	102	-	11,11,19	0.44	0	10,10,19	0.60	0
26	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	7 (12%)
26	BCR	d	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	5 (8%)
31	LHG	A	615	-	48,48,48	1.05	3 (6%)	51,54,54	1.18	3 (5%)
24	CLA	a	605	1	69,73,73	1.35	9 (13%)	82,113,113	1.54	9 (10%)
24	CLA	b	616	2	64,68,73	1.21	8 (12%)	76,107,113	1.36	9 (11%)
28	STE	z	101	-	8,8,19	0.45	0	7,7,19	0.54	0
28	STE	M	102	-	9,9,19	0.42	0	8,8,19	0.76	0
25	PHO	d	402	-	58,69,69	2.25	14 (24%)	55,99,99	1.76	8 (14%)
29	LMG	d	414	-	44,44,55	1.11	4 (9%)	52,52,63	1.31	7 (13%)
29	LMG	c	518	-	29,29,55	1.06	2 (6%)	31,31,63	1.06	2 (6%)
30	SQD	B	623	-	52,54,54	1.52	9 (17%)	62,65,65	1.85	14 (22%)
31	LHG	d	411	-	48,48,48	0.83	2 (4%)	51,54,54	1.26	6 (11%)
29	LMG	D	408	-	51,51,55	0.95	3 (5%)	59,59,63	1.42	8 (13%)
28	STE	f	102	-	7,7,19	0.49	0	6,6,19	0.42	0
27	PL9	a	609	-	55,55,55	1.11	6 (10%)	68,69,69	1.60	13 (19%)
26	BCR	C	514	-	41,41,41	1.25	4 (9%)	56,56,56	1.38	6 (10%)
29	LMG	B	621	-	51,51,55	0.99	5 (9%)	59,59,63	1.46	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HEC	V	201	16	50,50,50	1.57	4 (8%)	68,82,82	1.27	8 (11%)
24	CLA	c	513	3	69,73,73	1.38	9 (13%)	82,113,113	1.24	9 (10%)
28	STE	I	102	-	14,14,19	0.81	0	14,14,19	1.00	1 (7%)
24	CLA	C	512	3	69,73,73	1.38	8 (11%)	82,113,113	1.60	12 (14%)
30	SQD	a	611	-	52,54,54	1.63	8 (15%)	62,65,65	1.69	9 (14%)
34	HEM	e	102	6,5	50,50,50	1.40	8 (16%)	67,82,82	1.37	7 (10%)
24	CLA	b	610	36	69,73,73	1.24	7 (10%)	82,113,113	1.33	11 (13%)
21	OEX	A	601	3,36,1	0,14,14	-	-	-		
28	STE	x	101	-	19,19,19	0.80	1 (5%)	19,19,19	0.99	1 (5%)
24	CLA	b	602	2	69,73,73	1.17	9 (13%)	82,113,113	1.48	14 (17%)
28	STE	C	519	-	9,9,19	0.43	0	8,8,19	0.58	0
28	STE	Z	101	-	16,16,19	0.50	0	15,15,19	0.52	0
26	BCR	k	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.18	4 (7%)
24	CLA	B	614	2	69,73,73	1.51	7 (10%)	82,113,113	1.41	12 (14%)
26	BCR	H	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	5 (8%)
28	STE	c	516	-	12,12,19	0.43	0	11,11,19	0.69	0
26	BCR	B	618	-	41,41,41	0.99	2 (4%)	56,56,56	1.22	5 (8%)
27	PL9	d	408	-	55,55,55	1.64	5 (9%)	68,69,69	1.76	12 (17%)
28	STE	b	624	-	15,15,19	0.84	1 (6%)	15,15,19	1.11	2 (13%)
28	STE	A	618	-	16,16,19	0.48	0	15,15,19	0.56	0
24	CLA	B	602	2	69,73,73	1.19	8 (11%)	82,113,113	1.14	7 (8%)
24	CLA	c	507	36	69,73,73	1.20	7 (10%)	82,113,113	1.26	10 (12%)
26	BCR	b	617	-	41,41,41	1.10	4 (9%)	56,56,56	1.34	6 (10%)
28	STE	b	625	-	9,9,19	0.38	0	8,8,19	0.88	0
28	STE	C	527	-	13,13,19	0.39	0	12,12,19	0.75	0
24	CLA	b	613	2	69,73,73	1.36	7 (10%)	82,113,113	1.19	10 (12%)
28	STE	b	627	-	10,10,19	0.52	0	9,9,19	0.51	0
29	LMG	c	524	-	49,49,55	1.07	6 (12%)	57,57,63	1.35	6 (10%)
24	CLA	b	601	36	69,73,73	1.37	9 (13%)	82,113,113	1.43	6 (7%)
28	STE	h	103	-	9,9,19	0.51	0	8,8,19	0.56	0
31	LHG	e	103	-	41,41,48	1.09	4 (9%)	44,47,54	1.28	4 (9%)
26	BCR	B	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	10 (17%)
24	CLA	c	508	3	68,72,73	1.38	10 (14%)	80,111,113	1.33	8 (10%)
24	CLA	c	506	3	69,73,73	1.23	10 (14%)	82,113,113	1.25	12 (14%)
30	SQD	A	614	-	50,52,54	1.62	7 (14%)	60,63,65	2.11	10 (16%)
28	STE	a	612	-	11,11,19	0.84	0	11,11,19	1.00	0
28	STE	X	101	-	19,19,19	0.74	1 (5%)	19,19,19	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	d	410	-	48,48,48	0.74	1 (2%)	51,54,54	1.35	7 (13%)
24	CLA	B	610	36	69,73,73	1.50	11 (15%)	82,113,113	1.35	9 (10%)
24	CLA	c	510	3	69,73,73	1.15	7 (10%)	82,113,113	1.28	8 (9%)
28	STE	d	413	-	19,19,19	0.65	0	19,19,19	0.77	0
32	DGD	c	521	-	63,63,67	1.00	6 (9%)	77,77,81	1.42	13 (16%)
24	CLA	B	609	2	69,73,73	1.29	6 (8%)	82,113,113	1.34	8 (9%)
26	BCR	a	608	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	7 (12%)
24	CLA	A	608	1	58,62,73	1.37	6 (10%)	68,99,113	1.55	10 (14%)
28	STE	i	102	-	5,5,19	0.45	0	4,4,19	0.42	0
28	STE	A	611	-	8,8,19	0.43	0	7,7,19	0.69	0
24	CLA	b	615	2	69,73,73	1.35	10 (14%)	82,113,113	1.39	10 (12%)
32	DGD	H	102	-	63,63,67	1.15	5 (7%)	77,77,81	1.51	14 (18%)
24	CLA	C	513	3	69,73,73	1.73	8 (11%)	82,113,113	1.43	6 (7%)
25	PHO	d	403	-	58,69,69	2.16	9 (15%)	55,99,99	1.46	7 (12%)
34	HEM	F	101	6,5	50,50,50	1.41	8 (16%)	67,82,82	1.10	3 (4%)
28	STE	c	517	-	17,17,19	0.49	0	16,16,19	0.63	0
28	STE	A	619	-	10,10,19	0.48	0	9,9,19	0.62	0
24	CLA	B	603	2	69,73,73	1.11	7 (10%)	82,113,113	1.49	17 (20%)
24	CLA	B	615	2	69,73,73	1.41	8 (11%)	82,113,113	1.26	8 (9%)
26	BCR	B	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.31	6 (10%)
24	CLA	D	404	4	69,73,73	1.43	11 (15%)	82,113,113	1.26	5 (6%)
29	LMG	b	623	-	55,55,55	1.02	4 (7%)	63,63,63	1.46	7 (11%)
28	STE	I	101	-	16,16,19	0.79	0	16,16,19	0.85	1 (6%)
32	DGD	c	520	-	63,63,67	1.14	10 (15%)	77,77,81	1.35	8 (10%)
28	STE	C	525	-	11,11,19	0.78	0	11,11,19	1.18	1 (9%)
30	SQD	a	610	-	52,54,54	1.43	6 (11%)	62,65,65	2.07	14 (22%)
28	STE	R	101	-	19,19,19	0.74	1 (5%)	19,19,19	1.19	3 (15%)
30	SQD	b	620	-	47,49,54	1.55	7 (14%)	57,60,65	2.04	16 (28%)
24	CLA	c	501	3	69,73,73	1.33	9 (13%)	82,113,113	1.51	7 (8%)
28	STE	B	626	-	14,14,19	0.47	0	13,13,19	0.61	0
24	CLA	b	606	2	69,73,73	1.55	7 (10%)	82,113,113	1.54	9 (10%)
26	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.40	9 (16%)
28	STE	d	409	-	19,19,19	0.78	0	19,19,19	0.88	1 (5%)
30	SQD	f	101	-	39,41,54	1.70	7 (17%)	49,52,65	1.87	11 (22%)
24	CLA	D	403	4	69,73,73	1.27	8 (11%)	82,113,113	1.39	8 (9%)
24	CLA	b	603	2	69,73,73	1.20	9 (13%)	82,113,113	1.46	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	c	519	-	63,63,67	1.27	9 (14%)	77,77,81	1.34	10 (12%)
24	CLA	C	506	3	69,73,73	1.48	10 (14%)	82,113,113	1.24	8 (9%)
26	BCR	k	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.06	3 (5%)
31	LHG	d	412	-	38,38,48	1.15	2 (5%)	41,44,54	1.33	5 (12%)
21	OEX	a	601	3,36,1	0,14,14	-	-	-	-	-
24	CLA	B	606	2	69,73,73	1.41	6 (8%)	82,113,113	1.39	8 (9%)
24	CLA	B	605	2	69,73,73	1.23	5 (7%)	82,113,113	1.34	11 (13%)
28	STE	E	101	-	11,11,19	0.83	0	11,11,19	1.08	1 (9%)
24	CLA	c	502	3	69,73,73	1.24	6 (8%)	82,113,113	1.16	4 (4%)
24	CLA	c	504	36	64,68,73	1.37	9 (14%)	76,107,113	1.37	9 (11%)
24	CLA	C	503	3	69,73,73	1.43	6 (8%)	82,113,113	1.51	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	l	102	-	-	7/15/15/17	-
28	STE	e	101	-	-	2/6/6/17	-
24	CLA	C	511	3	-	2/39/115/115	-
24	CLA	b	614	2	-	12/39/115/115	-
24	CLA	b	608	2	-	1/39/115/115	-
24	CLA	b	609	2	-	6/39/115/115	-
28	STE	b	621	-	-	7/13/13/17	-
24	CLA	C	504	36	-	7/32/108/115	-
28	STE	J	101	-	-	6/9/9/17	-
24	CLA	c	511	3	-	6/39/115/115	-
24	CLA	d	406	4	-	11/39/115/115	-
24	CLA	C	507	36	-	7/39/115/115	-
24	CLA	B	601	36	-	18/39/115/115	-
29	LMG	C	524	-	-	17/43/63/70	0/1/1/1
28	STE	e	104	-	-	3/6/6/17	-
26	BCR	b	619	-	-	7/29/63/63	0/2/2/2
30	SQD	F	102	-	-	12/28/48/69	0/1/1/1
31	LHG	l	101	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	606	36	-	7/39/115/115	-
24	CLA	C	501	3	-	3/39/115/115	-
28	STE	e	105	-	-	5/10/10/17	-
28	STE	E	103	-	-	8/17/17/17	-
24	CLA	C	510	3	-	7/39/115/115	-
28	STE	t	103	-	-	4/7/7/17	-
24	CLA	C	508	3	-	6/39/115/115	-
24	CLA	B	611	2	-	4/39/115/115	-
24	CLA	B	616	2	-	9/33/109/115	-
28	STE	b	622	-	-	7/17/17/17	-
32	DGD	A	617	-	-	24/55/95/95	0/2/2/2
32	DGD	C	522	-	-	17/51/91/95	0/2/2/2
32	DGD	h	102	-	-	16/51/91/95	0/2/2/2
28	STE	d	415	-	-	5/11/11/17	-
29	LMG	c	522	-	-	15/41/61/70	0/1/1/1
28	STE	B	625	-	-	2/9/9/17	-
25	PHO	A	607	-	-	2/37/103/103	0/5/6/6
28	STE	C	515	-	-	4/11/11/17	-
24	CLA	B	604	2	-	8/39/115/115	-
31	LHG	D	411	-	-	16/53/53/53	-
35	HEC	v	201	16	1/1/7/7	6/14/54/54	-
25	PHO	D	402	-	-	2/37/103/103	0/5/6/6
26	BCR	c	515	-	-	4/29/63/63	0/2/2/2
24	CLA	B	607	36	-	9/39/115/115	-
24	CLA	C	509	3	-	12/39/115/115	-
24	CLA	A	605	1	-	1/39/115/115	-
26	BCR	C	520	-	-	5/29/63/63	0/2/2/2
24	CLA	C	505	3	-	9/39/115/115	-
28	STE	t	102	-	-	5/11/11/17	-
29	LMG	o	301	-	-	26/50/70/70	0/1/1/1
24	CLA	c	509	3	-	10/39/115/115	-
24	CLA	d	404	36	-	0/39/115/115	-
24	CLA	c	505	3	-	11/39/115/115	-
28	STE	H	103	-	-	8/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	B	622	-	-	7/14/14/17	-
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
28	STE	b	626	-	-	2/5/5/17	-
28	STE	C	528	-	-	4/11/11/17	-
28	STE	m	102	-	-	2/9/9/17	-
30	SQD	A	616	-	-	14/38/58/69	0/1/1/1
24	CLA	b	605	2	-	5/39/115/115	-
29	LMG	m	101	-	-	18/46/66/70	0/1/1/1
24	CLA	b	607	36	-	14/39/115/115	-
31	LHG	D	410	-	-	15/51/51/53	-
29	LMG	D	407	-	-	21/45/65/70	0/1/1/1
28	STE	C	526	-	-	3/13/13/17	-
26	BCR	K	102	-	-	8/29/63/63	0/2/2/2
24	CLA	a	607	1	-	12/39/115/115	-
29	LMG	c	523	-	-	17/43/63/70	0/1/1/1
27	PL9	A	610	-	-	19/53/73/73	0/1/1/1
24	CLA	b	604	2	-	9/39/115/115	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
28	STE	M	103	-	-	8/12/12/17	-
28	STE	M	101	-	-	7/12/12/17	-
29	LMG	B	620	-	-	16/40/60/70	0/1/1/1
24	CLA	b	611	2	-	7/39/115/115	-
24	CLA	B	612	2	-	8/39/115/115	-
24	CLA	b	612	2	-	3/39/115/115	-
26	BCR	t	101	-	-	4/29/63/63	0/2/2/2
28	STE	B	624	-	-	5/15/15/17	-
32	DGD	C	521	-	-	25/51/91/95	0/2/2/2
28	STE	D	412	-	-	3/6/6/17	-
24	CLA	d	405	4	-	6/39/115/115	-
28	STE	j	102	-	-	6/13/13/17	-
24	CLA	c	503	3	-	9/39/115/115	-
26	BCR	K	101	-	-	5/29/63/63	0/2/2/2
28	STE	C	517	-	-	1/2/2/17	-
24	CLA	C	502	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	612	36	-	4/39/115/115	-
29	LMG	C	516	-	-	11/30/50/70	0/1/1/1
26	BCR	A	609	-	-	3/29/63/63	0/2/2/2
28	STE	i	101	-	-	4/9/9/17	-
24	CLA	B	608	2	-	3/39/115/115	-
24	CLA	a	606	36	-	3/39/115/115	-
31	LHG	L	101	-	-	18/53/53/53	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
28	STE	j	101	-	-	5/9/9/17	-
24	CLA	c	512	3	-	17/39/115/115	-
24	CLA	B	613	2	-	13/39/115/115	-
26	BCR	T	101	-	-	3/29/63/63	0/2/2/2
31	LHG	D	409	-	-	21/53/53/53	-
29	LMG	A	613	-	-	17/43/63/70	0/1/1/1
32	DGD	C	523	-	-	15/51/91/95	0/2/2/2
28	STE	C	518	-	-	2/4/4/17	-
28	STE	E	102	-	-	4/9/9/17	-
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
26	BCR	d	407	-	-	8/29/63/63	0/2/2/2
31	LHG	A	615	-	-	26/53/53/53	-
24	CLA	a	605	1	-	5/39/115/115	-
24	CLA	b	616	2	-	6/33/109/115	-
28	STE	z	101	-	-	4/6/6/17	-
28	STE	M	102	-	-	2/7/7/17	-
25	PHO	d	402	-	-	4/37/103/103	0/5/6/6
29	LMG	d	414	-	-	11/39/59/70	0/1/1/1
29	LMG	c	518	-	-	16/31/31/70	-
30	SQD	B	623	-	-	27/49/69/69	0/1/1/1
31	LHG	d	411	-	-	20/53/53/53	-
29	LMG	D	408	-	-	14/46/66/70	0/1/1/1
28	STE	f	102	-	-	3/5/5/17	-
27	PL9	a	609	-	-	20/53/73/73	0/1/1/1
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	B	621	-	-	20/46/66/70	0/1/1/1
24	CLA	c	513	3	-	11/39/115/115	-
28	STE	I	102	-	-	8/12/12/17	-
24	CLA	C	512	3	-	13/39/115/115	-
30	SQD	a	611	-	-	23/49/69/69	0/1/1/1
34	HEM	e	102	6,5	-	5/14/54/54	-
24	CLA	b	610	36	-	6/39/115/115	-
28	STE	x	101	-	-	9/17/17/17	-
24	CLA	b	602	2	-	5/39/115/115	-
28	STE	C	519	-	-	4/7/7/17	-
28	STE	Z	101	-	-	7/14/14/17	-
26	BCR	k	102	-	-	3/29/63/63	0/2/2/2
24	CLA	B	614	2	-	6/39/115/115	-
26	BCR	H	101	-	-	5/29/63/63	0/2/2/2
28	STE	c	516	-	-	5/10/10/17	-
26	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	PL9	d	408	-	-	10/53/73/73	0/1/1/1
28	STE	b	624	-	-	7/13/13/17	-
28	STE	A	618	-	-	7/14/14/17	-
24	CLA	B	602	2	-	7/39/115/115	-
24	CLA	c	507	36	-	7/39/115/115	-
26	BCR	b	617	-	-	3/29/63/63	0/2/2/2
28	STE	b	625	-	-	2/7/7/17	-
28	STE	C	527	-	-	5/11/11/17	-
24	CLA	b	613	2	-	7/39/115/115	-
28	STE	b	627	-	-	6/8/8/17	-
29	LMG	c	524	-	-	18/44/64/70	0/1/1/1
24	CLA	b	601	36	-	15/39/115/115	-
28	STE	h	103	-	-	4/7/7/17	-
31	LHG	e	103	-	-	21/46/46/53	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
24	CLA	c	508	3	-	8/38/114/115	-
24	CLA	c	506	3	-	12/39/115/115	-
30	SQD	A	614	-	-	19/47/67/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	a	612	-	-	1/9/9/17	-
28	STE	X	101	-	-	6/17/17/17	-
31	LHG	d	410	-	-	15/53/53/53	-
24	CLA	B	610	36	-	3/39/115/115	-
24	CLA	c	510	3	-	6/39/115/115	-
28	STE	d	413	-	-	8/17/17/17	-
32	DGD	c	521	-	-	18/51/91/95	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-
26	BCR	a	608	-	-	4/29/63/63	0/2/2/2
24	CLA	A	608	1	-	4/26/102/115	-
28	STE	i	102	-	-	1/3/3/17	-
28	STE	A	611	-	-	4/6/6/17	-
24	CLA	b	615	2	-	5/39/115/115	-
32	DGD	H	102	-	-	18/51/91/95	0/2/2/2
24	CLA	C	513	3	-	8/39/115/115	-
25	PHO	d	403	-	-	6/37/103/103	0/5/6/6
34	HEM	F	101	6,5	-	3/14/54/54	-
28	STE	c	517	-	-	8/15/15/17	-
28	STE	A	619	-	-	5/8/8/17	-
24	CLA	B	603	2	-	12/39/115/115	-
24	CLA	B	615	2	-	8/39/115/115	-
26	BCR	B	619	-	-	2/29/63/63	0/2/2/2
24	CLA	D	404	4	-	9/39/115/115	-
29	LMG	b	623	-	-	25/50/70/70	0/1/1/1
28	STE	I	101	-	-	6/14/14/17	-
32	DGD	c	520	-	-	19/51/91/95	0/2/2/2
28	STE	C	525	-	-	2/9/9/17	-
30	SQD	a	610	-	-	17/49/69/69	0/1/1/1
28	STE	R	101	-	-	11/17/17/17	-
30	SQD	b	620	-	-	21/44/64/69	0/1/1/1
24	CLA	c	501	3	-	3/39/115/115	-
28	STE	B	626	-	-	8/12/12/17	-
24	CLA	b	606	2	-	6/39/115/115	-
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
28	STE	d	409	-	-	12/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	f	101	-	-	15/36/56/69	0/1/1/1
24	CLA	D	403	4	-	2/39/115/115	-
24	CLA	b	603	2	-	7/39/115/115	-
32	DGD	c	519	-	-	28/51/91/95	0/2/2/2
24	CLA	C	506	3	-	12/39/115/115	-
26	BCR	k	101	-	-	6/29/63/63	0/2/2/2
31	LHG	d	412	-	-	14/43/43/53	-
24	CLA	B	606	2	-	5/39/115/115	-
24	CLA	B	605	2	-	8/39/115/115	-
28	STE	E	101	-	-	5/9/9/17	-
24	CLA	c	502	3	-	4/39/115/115	-
24	CLA	c	504	36	-	4/33/109/115	-
24	CLA	C	503	3	-	6/39/115/115	-

The worst 5 of 901 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C1B-C2B	10.35	1.50	1.39
25	d	403	PHO	C1B-C2B	10.06	1.50	1.39
25	D	402	PHO	C1B-C2B	8.74	1.49	1.39
24	C	513	CLA	MG-ND	8.44	2.22	2.05
24	c	511	CLA	MG-NA	8.20	2.25	2.06

The worst 5 of 1229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C4A-NA-C1A	12.69	112.47	106.68
24	C	507	CLA	C4A-NA-C1A	9.48	111.00	106.68
24	c	511	CLA	C4A-NA-C1A	9.46	110.99	106.68
24	B	601	CLA	C4A-NA-C1A	9.07	110.82	106.68
24	C	505	CLA	C4A-NA-C1A	8.37	110.50	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 1762 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

110 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	l	102	STE	1	0
24	C	511	CLA	1	0
24	b	614	CLA	2	0
24	b	609	CLA	1	0
28	b	621	STE	1	0
24	c	511	CLA	2	0
24	d	406	CLA	1	0
24	B	601	CLA	2	0
26	b	619	BCR	1	0
24	C	501	CLA	1	0
28	e	105	STE	1	0
28	E	103	STE	1	0
24	C	510	CLA	1	0
24	C	508	CLA	1	0
32	A	617	DGD	2	0
24	B	604	CLA	1	0
31	D	411	LHG	1	0
35	v	201	HEC	1	0
25	D	402	PHO	2	0
26	c	515	BCR	3	0
24	B	607	CLA	1	0
24	C	509	CLA	3	0
24	A	605	CLA	2	0
26	C	520	BCR	1	0
24	C	505	CLA	1	0
28	t	102	STE	2	0
29	o	301	LMG	1	0
24	c	509	CLA	1	0
24	d	404	CLA	2	0
28	B	622	STE	1	0
26	h	101	BCR	1	0
30	A	616	SQD	1	0
24	b	605	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	m	101	LMG	1	0
24	b	607	CLA	2	0
29	D	407	LMG	1	0
28	C	526	STE	2	0
26	K	102	BCR	4	0
24	a	607	CLA	1	0
27	A	610	PL9	1	0
24	b	604	CLA	3	0
27	D	406	PL9	1	0
29	B	620	LMG	2	0
24	b	612	CLA	1	0
26	t	101	BCR	3	0
32	C	521	DGD	1	0
26	K	101	BCR	4	0
24	C	502	CLA	1	0
24	A	612	CLA	1	0
29	C	516	LMG	1	0
26	A	609	BCR	2	0
28	i	101	STE	1	0
24	B	608	CLA	1	0
26	D	405	BCR	5	0
24	c	512	CLA	1	0
24	B	613	CLA	1	0
26	T	101	BCR	5	0
31	D	409	LHG	1	0
26	c	514	BCR	3	0
26	d	407	BCR	1	0
31	A	615	LHG	2	0
24	a	605	CLA	1	0
29	d	414	LMG	1	0
29	c	518	LMG	2	0
30	B	623	SQD	1	0
27	a	609	PL9	1	0
24	c	513	CLA	2	0
24	C	512	CLA	4	0
30	a	611	SQD	2	0
34	e	102	HEM	4	0
24	b	610	CLA	2	0
28	x	101	STE	2	0
24	b	602	CLA	2	0
26	k	102	BCR	1	0
24	B	614	CLA	1	0

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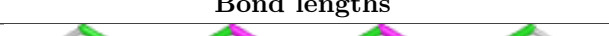
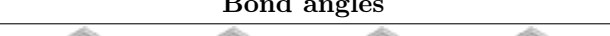
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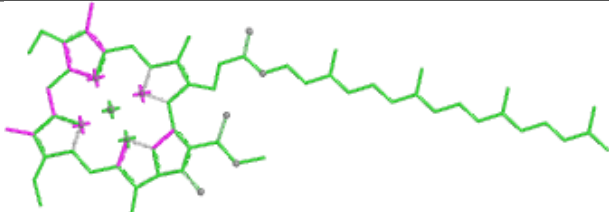
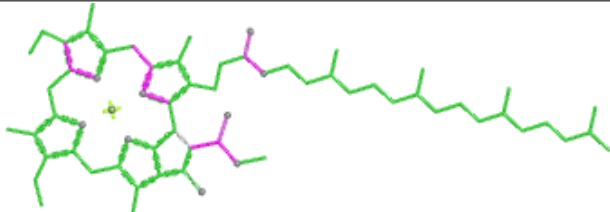
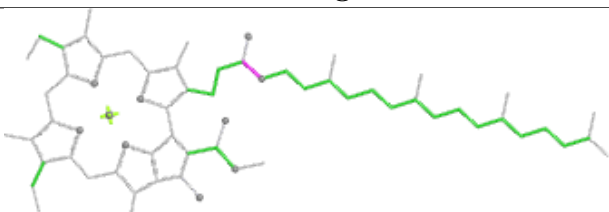
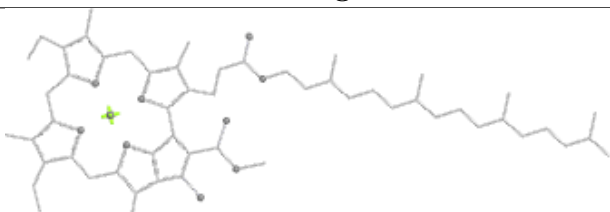
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	H	101	BCR	2	0
26	B	618	BCR	2	0
24	B	602	CLA	1	0
24	c	507	CLA	2	0
24	b	613	CLA	9	0
28	b	627	STE	1	0
31	e	103	LHG	2	0
24	c	508	CLA	1	0
28	X	101	STE	1	0
31	d	410	LHG	8	0
28	d	413	STE	2	0
32	c	521	DGD	1	0
24	B	609	CLA	1	0
24	A	608	CLA	1	0
28	A	611	STE	1	0
24	C	513	CLA	4	0
34	F	101	HEM	2	0
28	c	517	STE	1	0
24	B	603	CLA	1	0
26	B	619	BCR	4	0
24	D	404	CLA	1	0
29	b	623	LMG	1	0
30	a	610	SQD	1	0
28	R	101	STE	4	0
30	b	620	SQD	1	0
24	c	501	CLA	3	0
26	b	618	BCR	5	0
28	d	409	STE	1	0
30	f	101	SQD	1	0
24	b	603	CLA	1	0
24	C	506	CLA	2	0
26	k	101	BCR	2	0
24	B	606	CLA	3	0
24	B	605	CLA	4	0
24	c	504	CLA	1	0

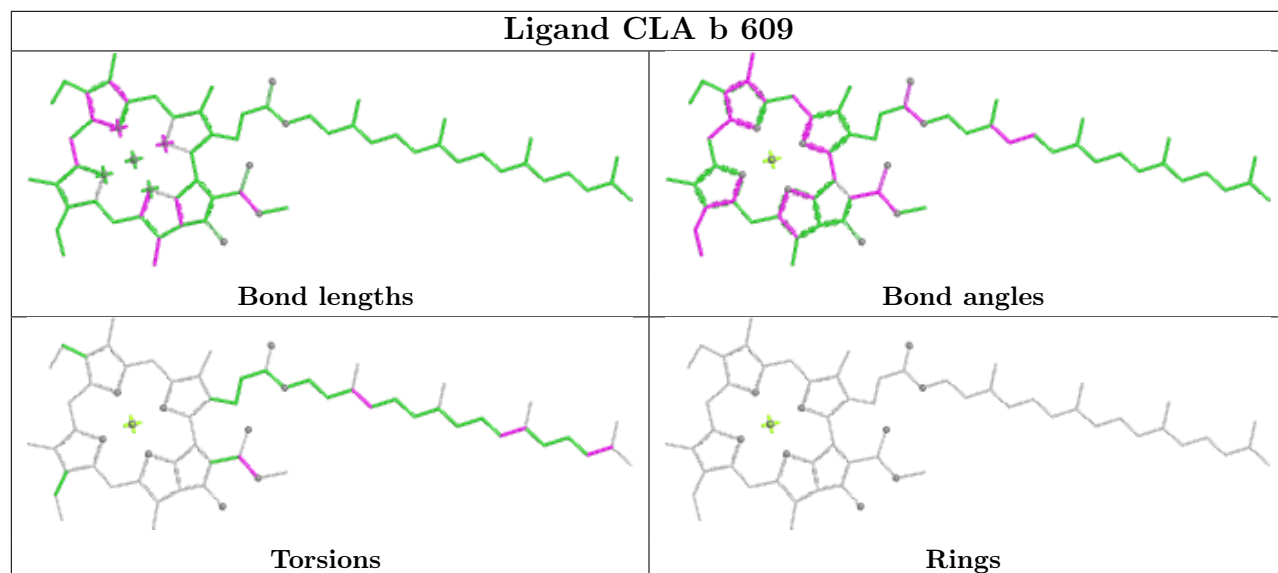
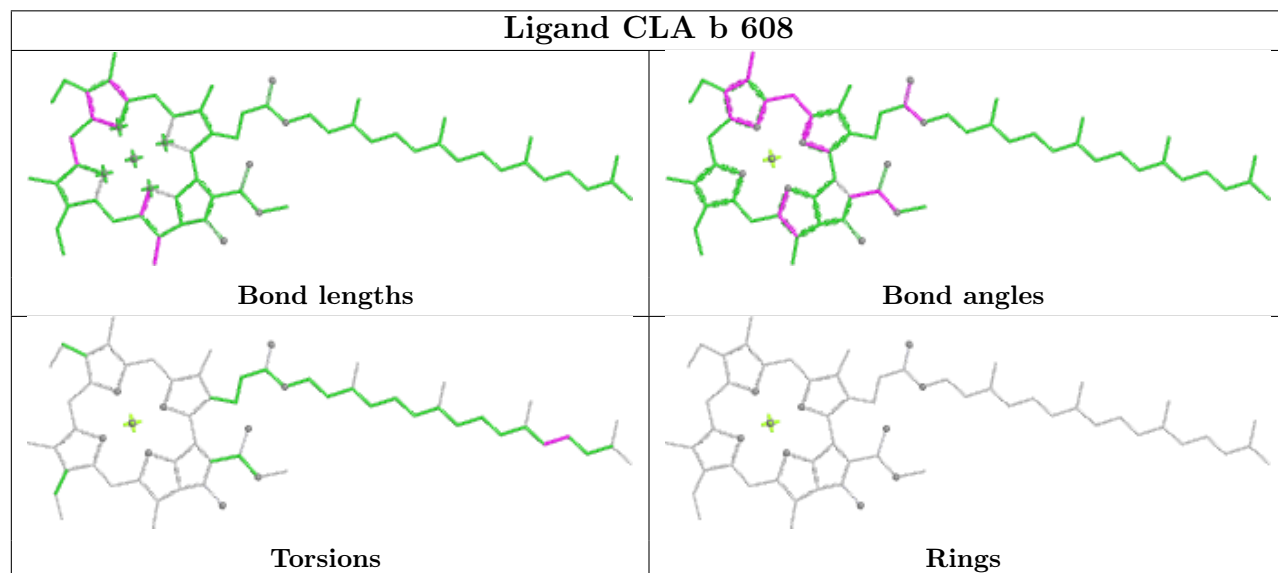
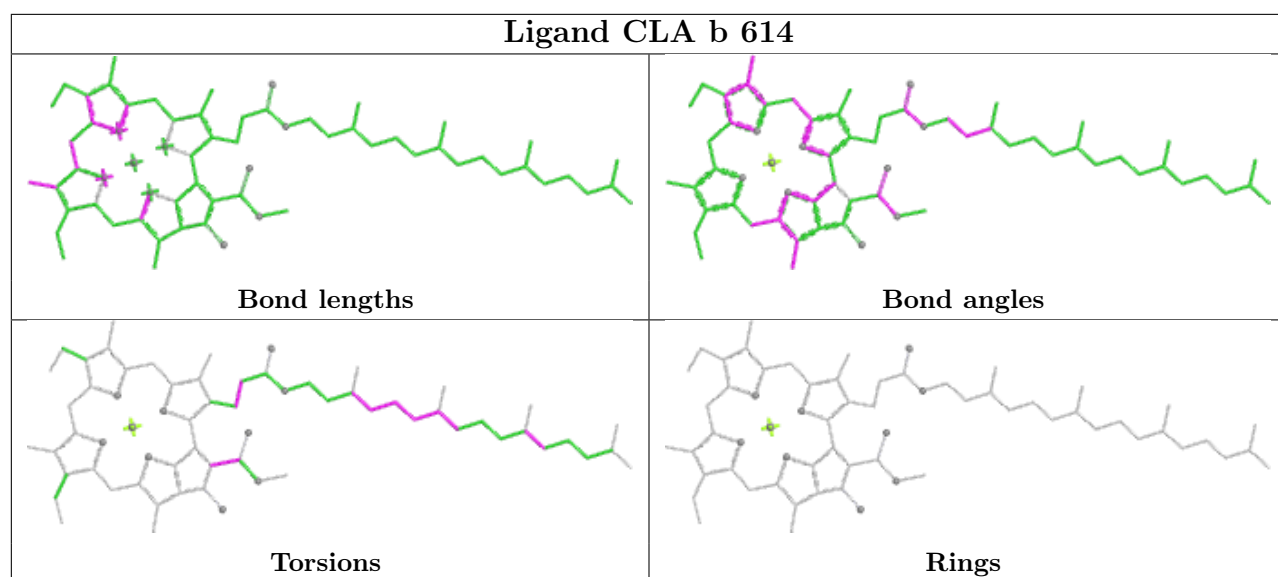
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

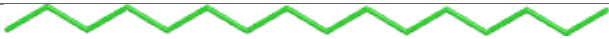
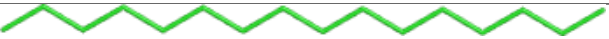
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

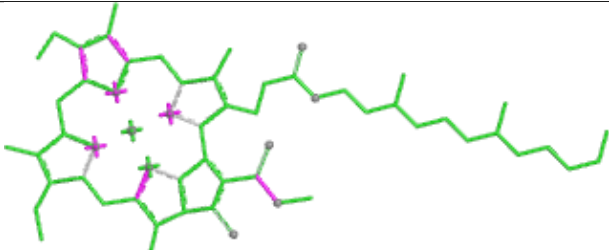
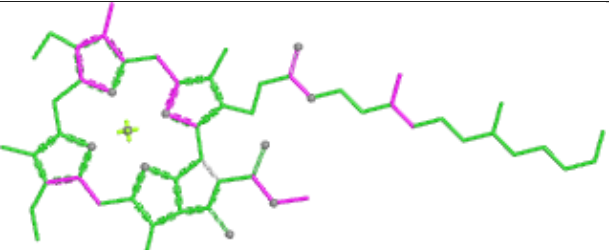
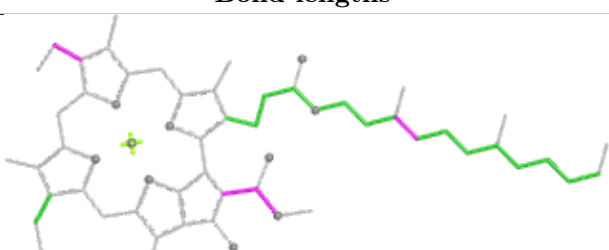
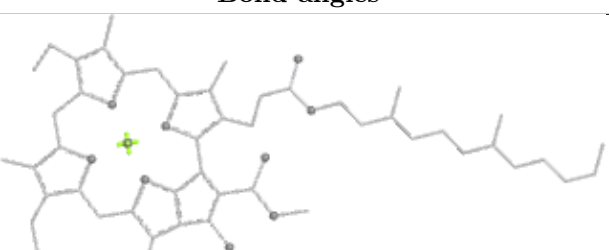
Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

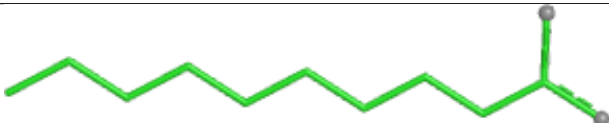
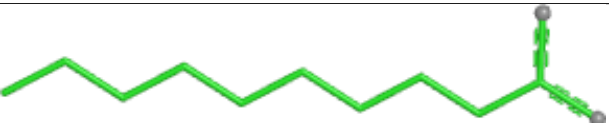
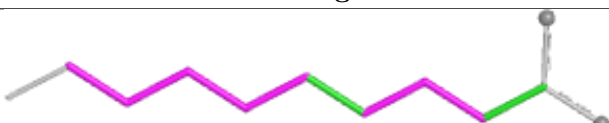
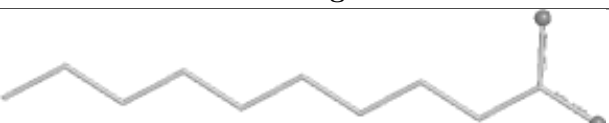
Ligand STE e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

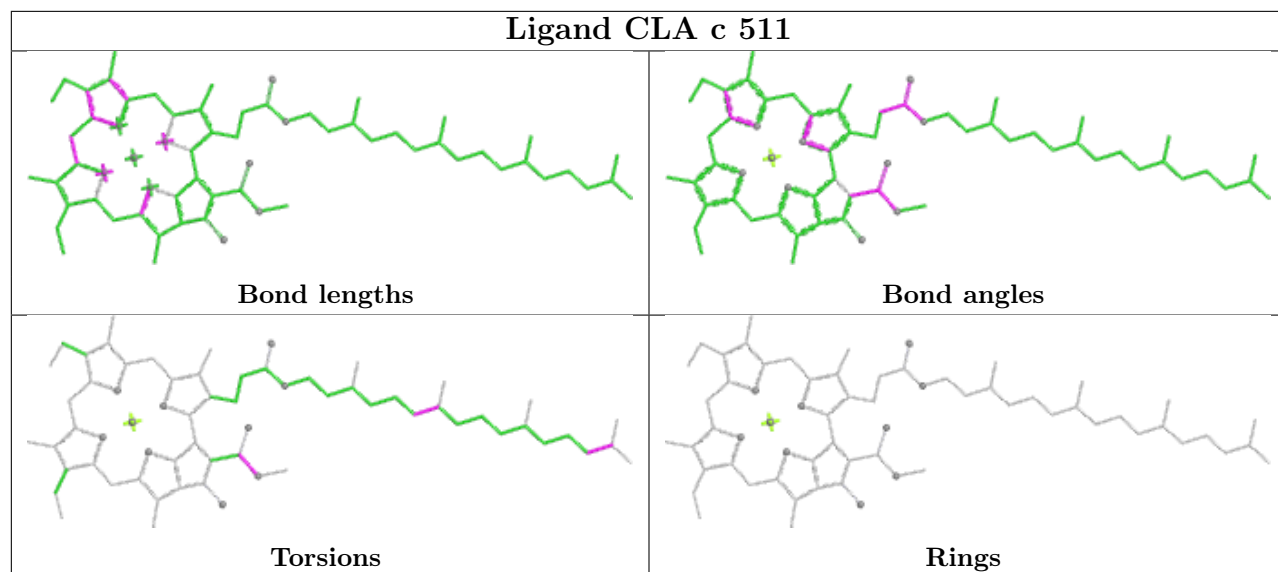


Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

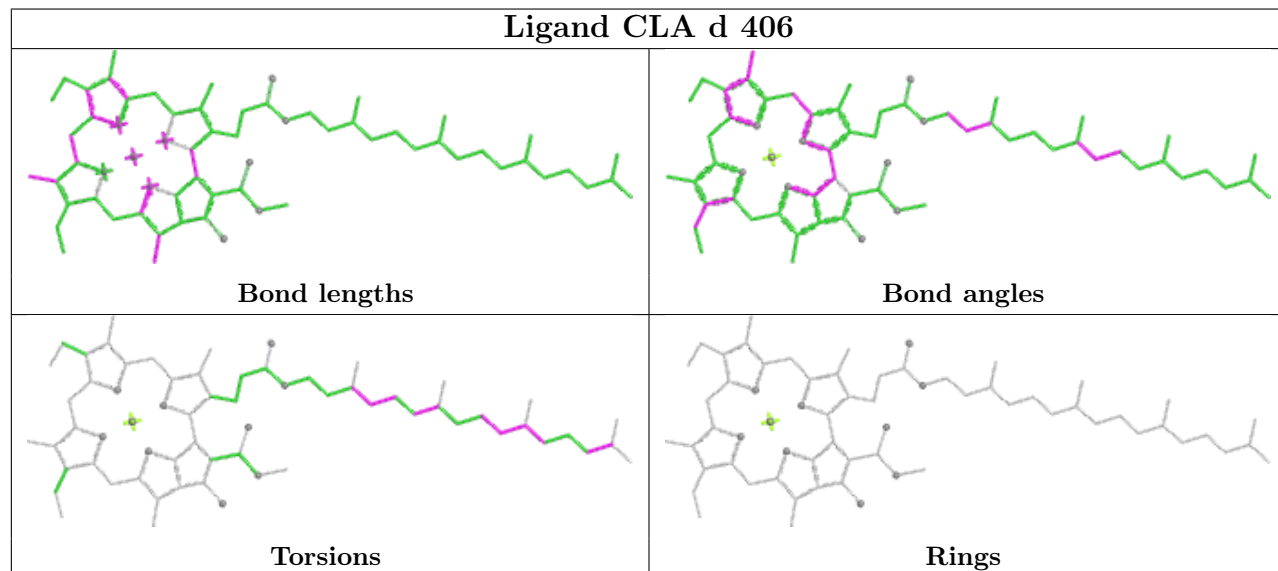
Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

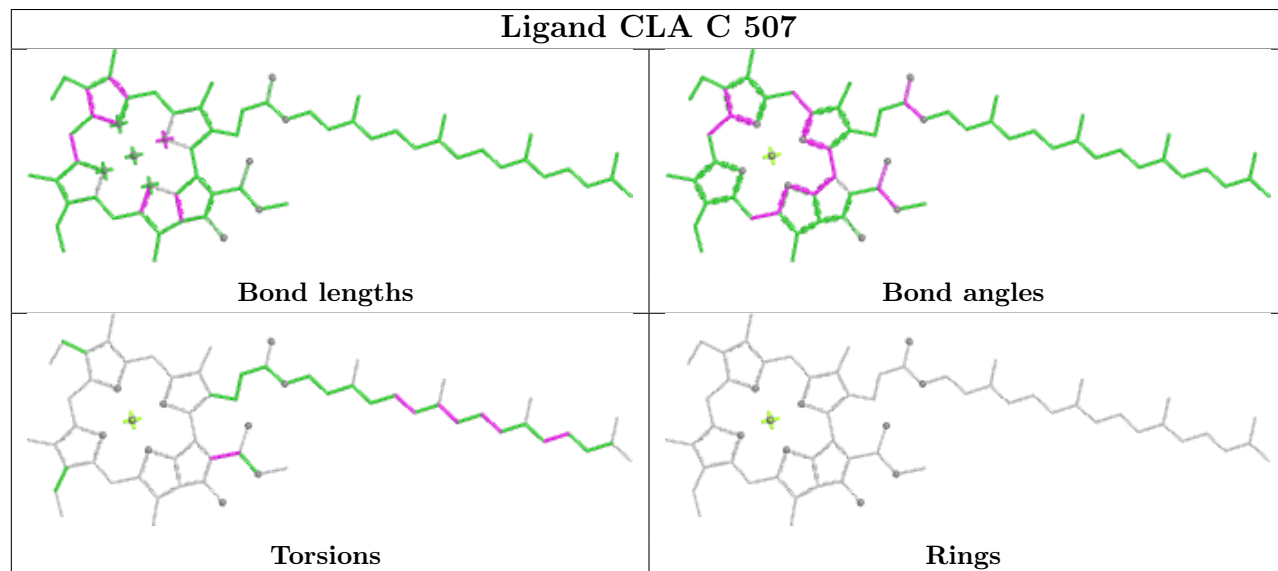
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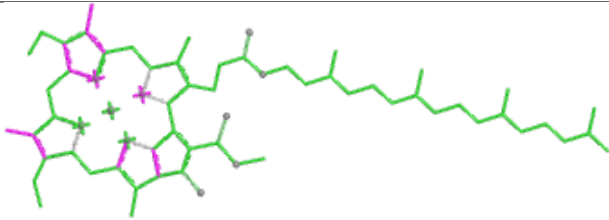
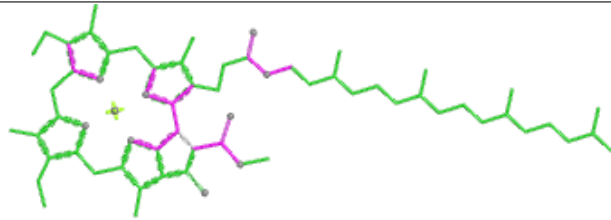
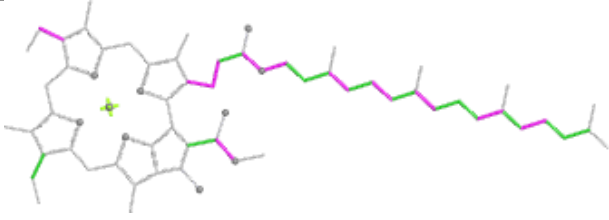
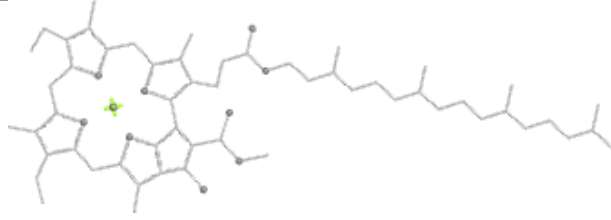


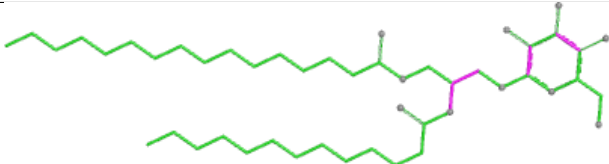
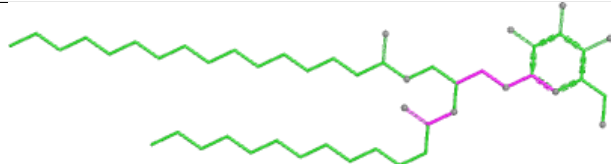
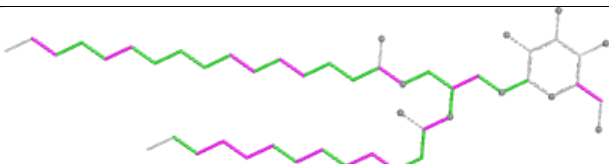
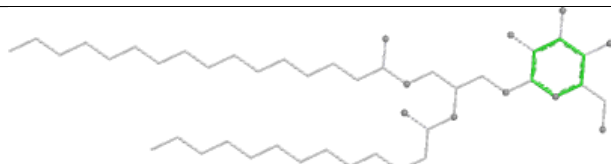
Ligand CLA d 406



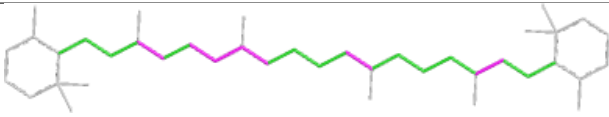
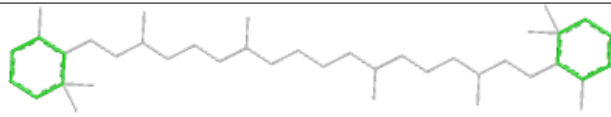
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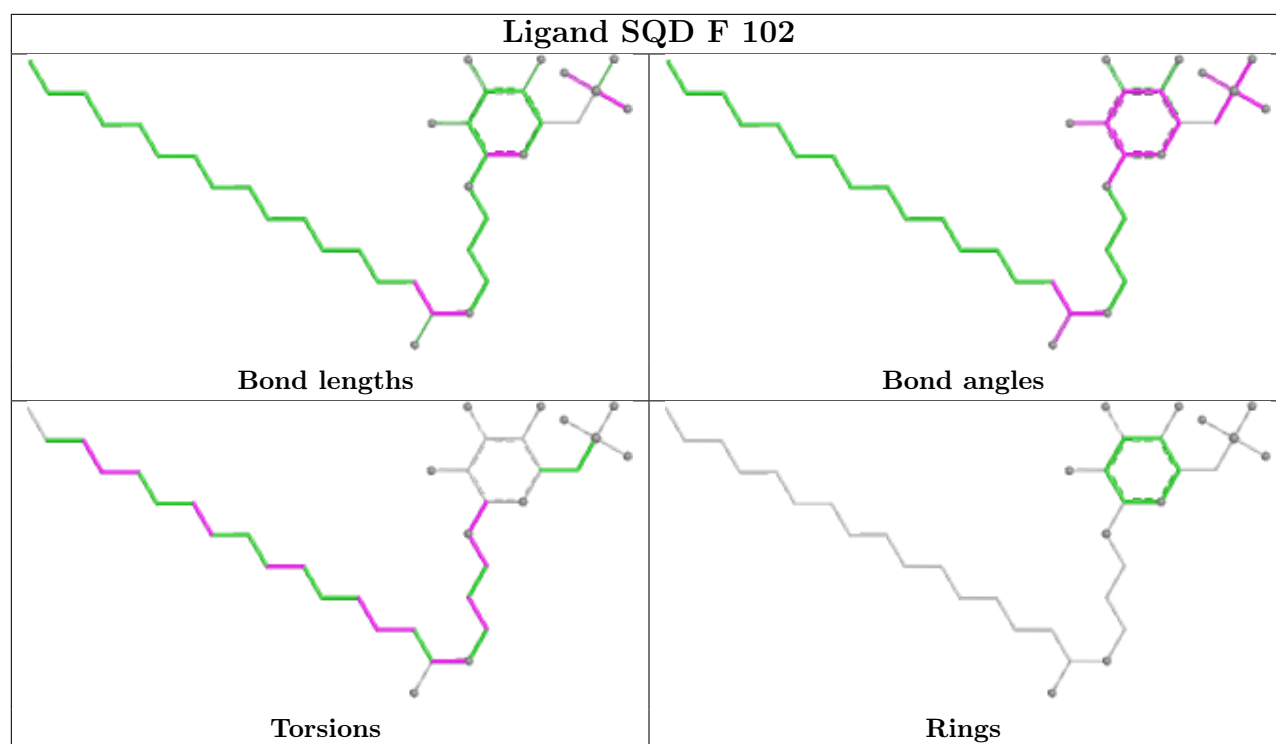


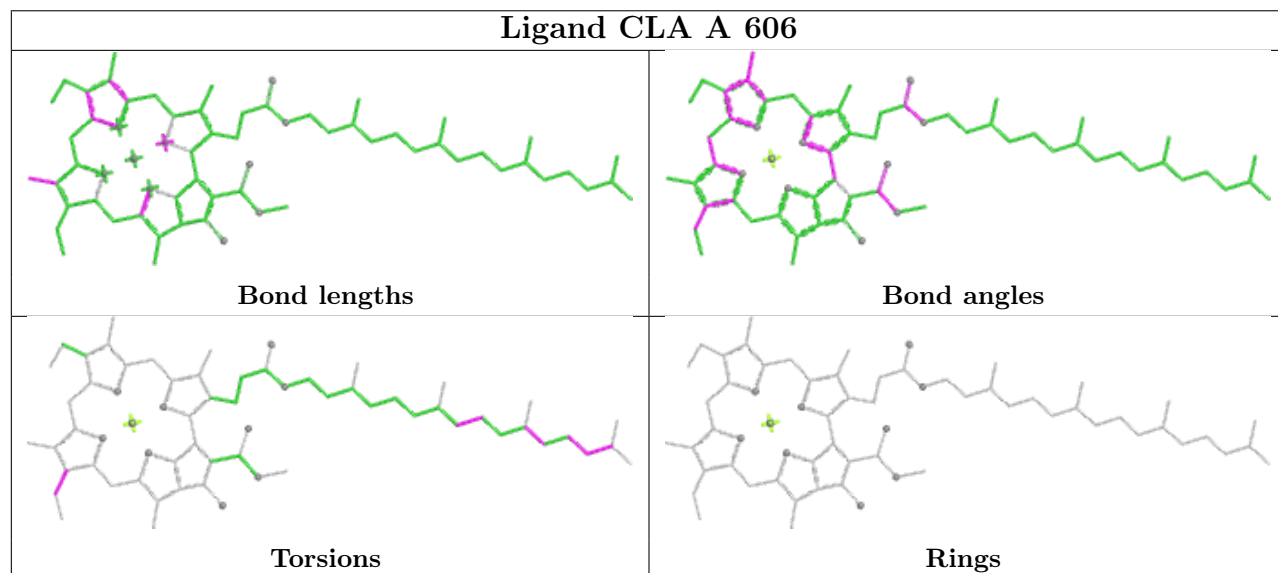
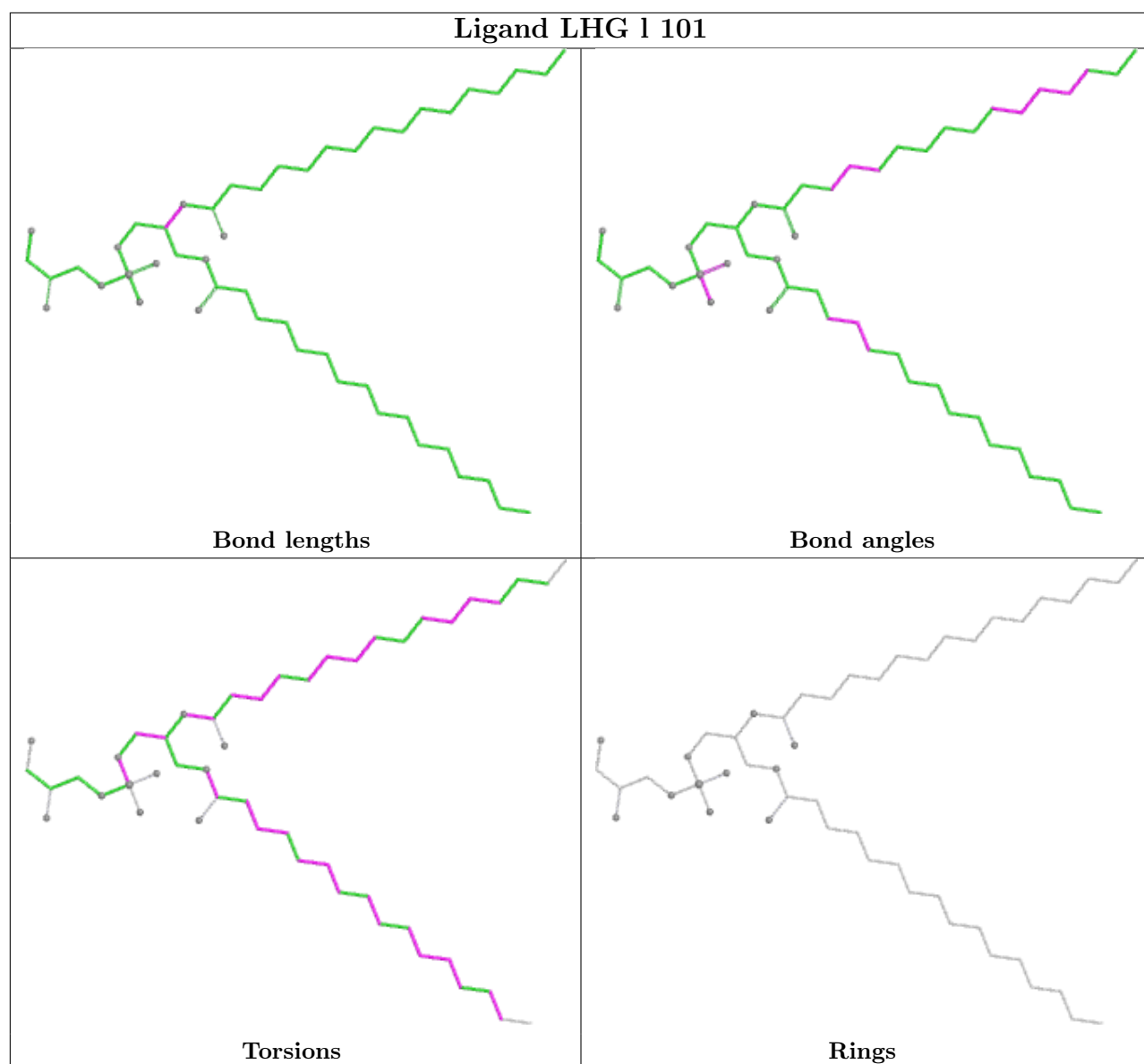
Ligand CLA B 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

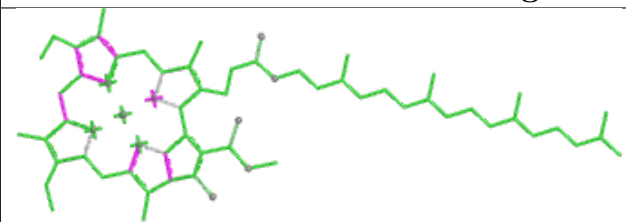
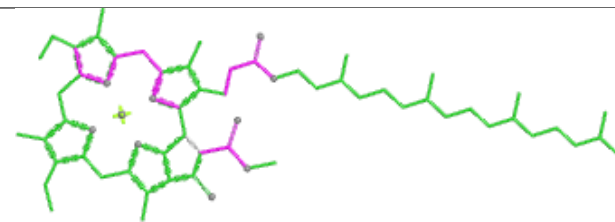
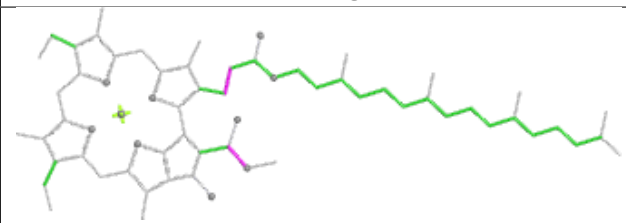
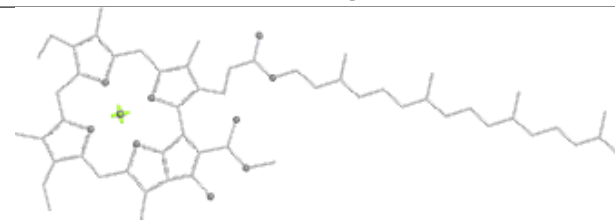
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Bond lengths	Bond angles
	
Torsions	Rings

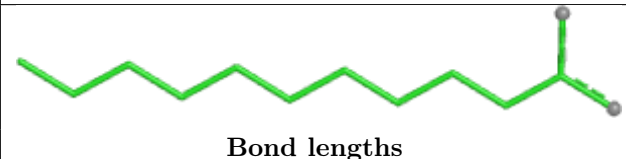
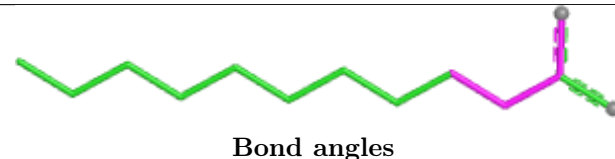
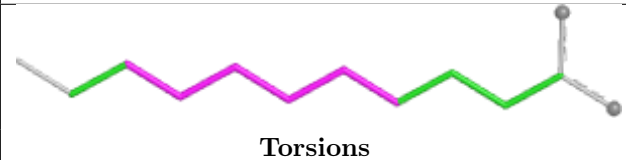
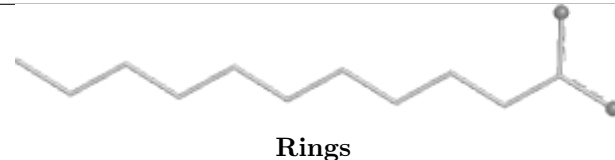
Ligand STE e 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

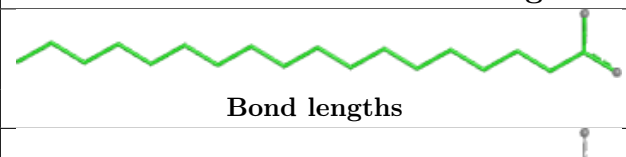
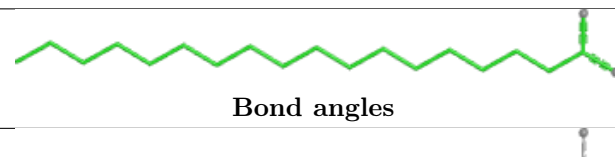
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Bond lengths	Bond angles
	
Torsions	Rings

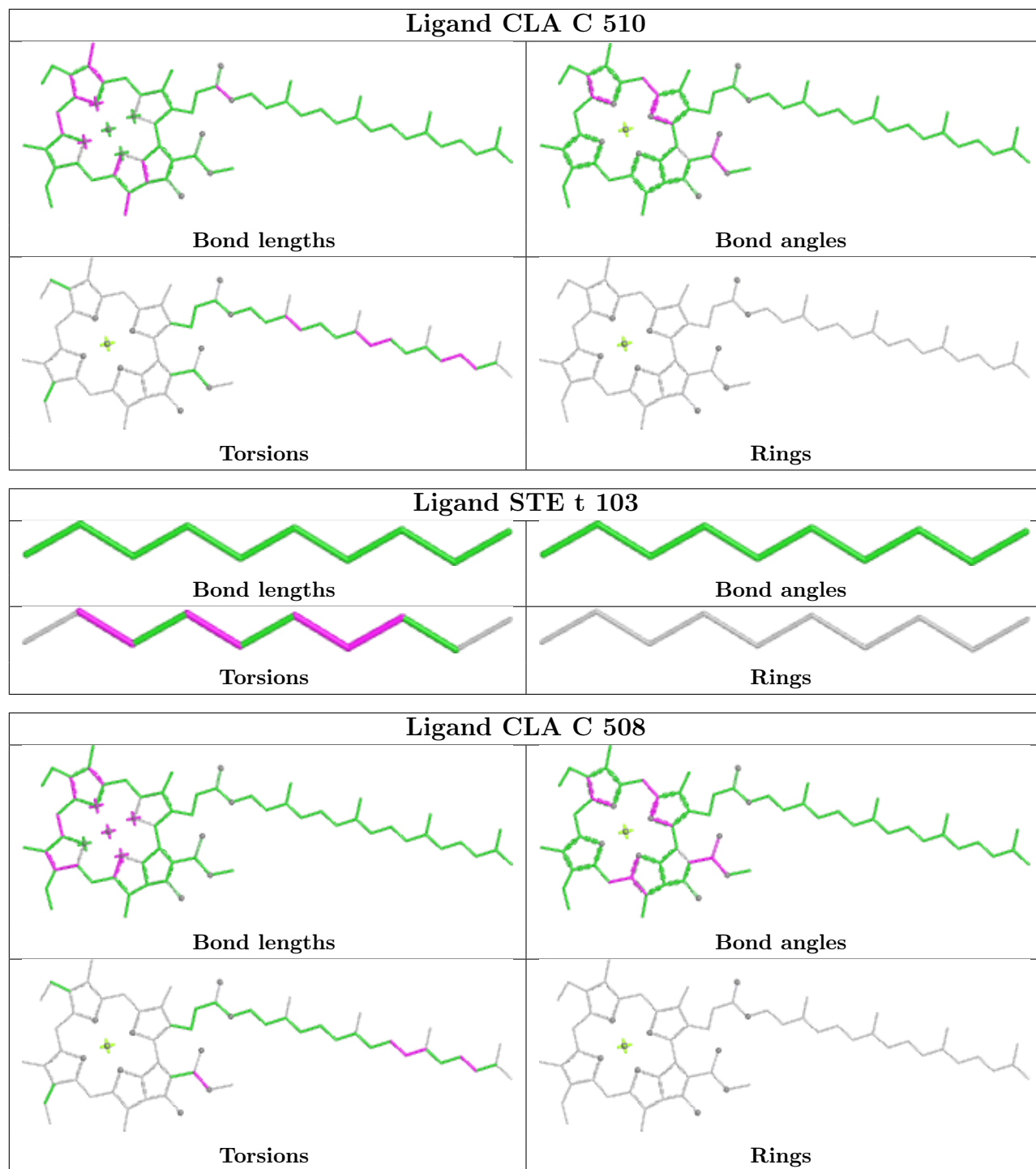


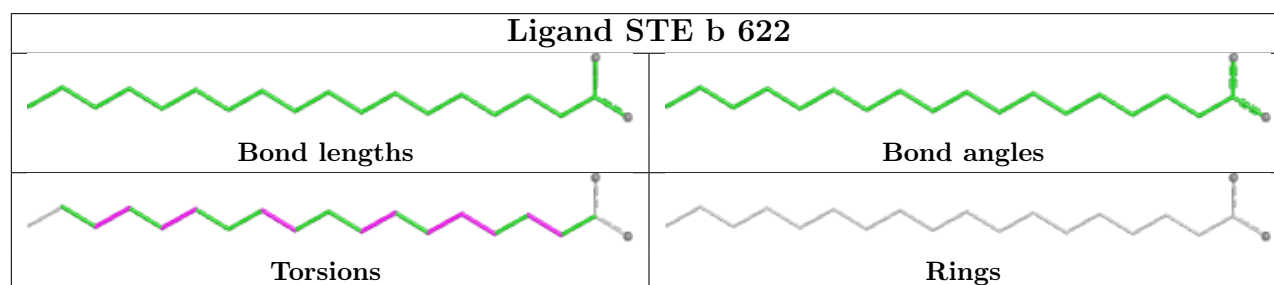
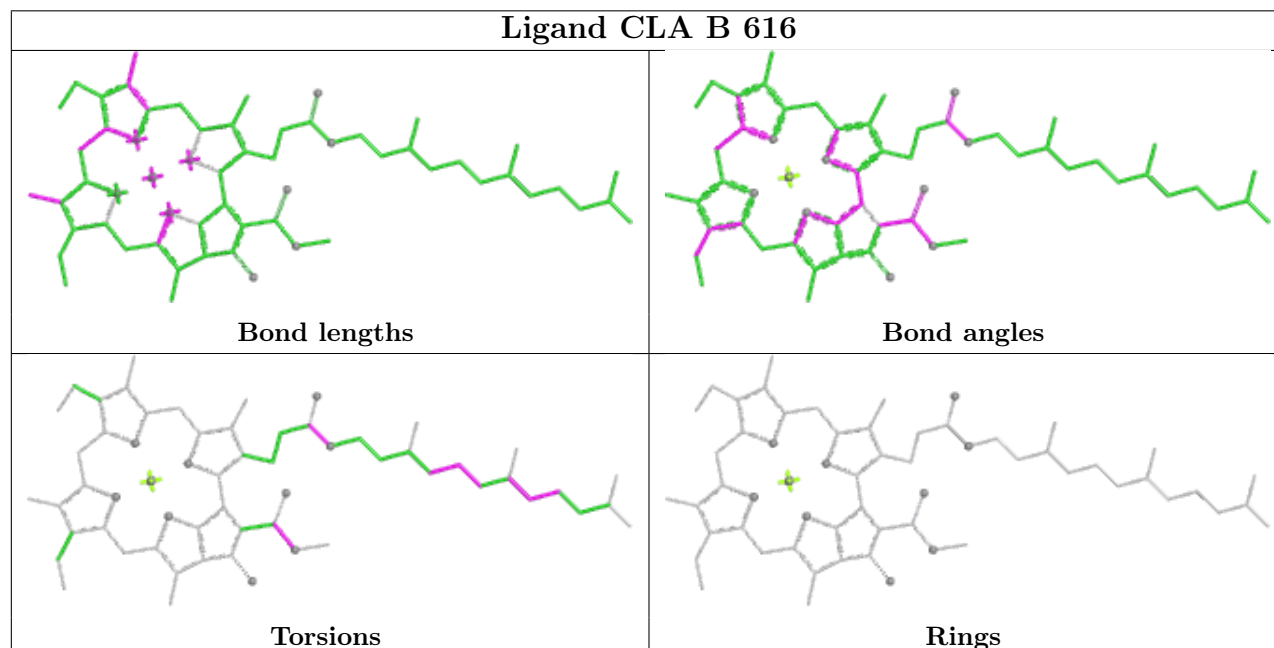
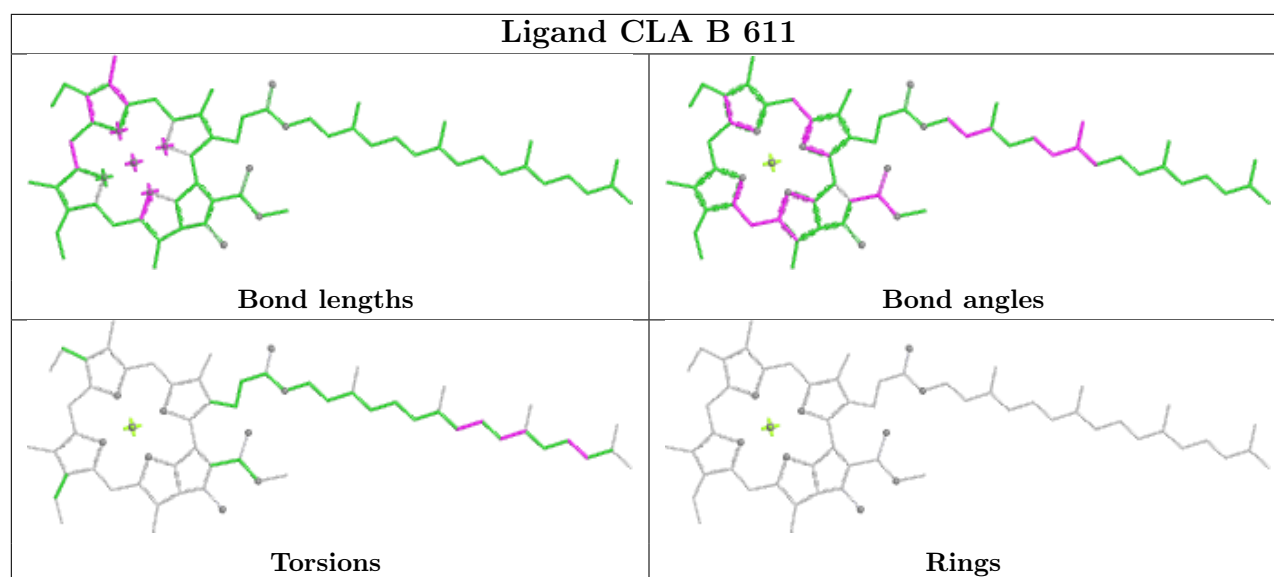


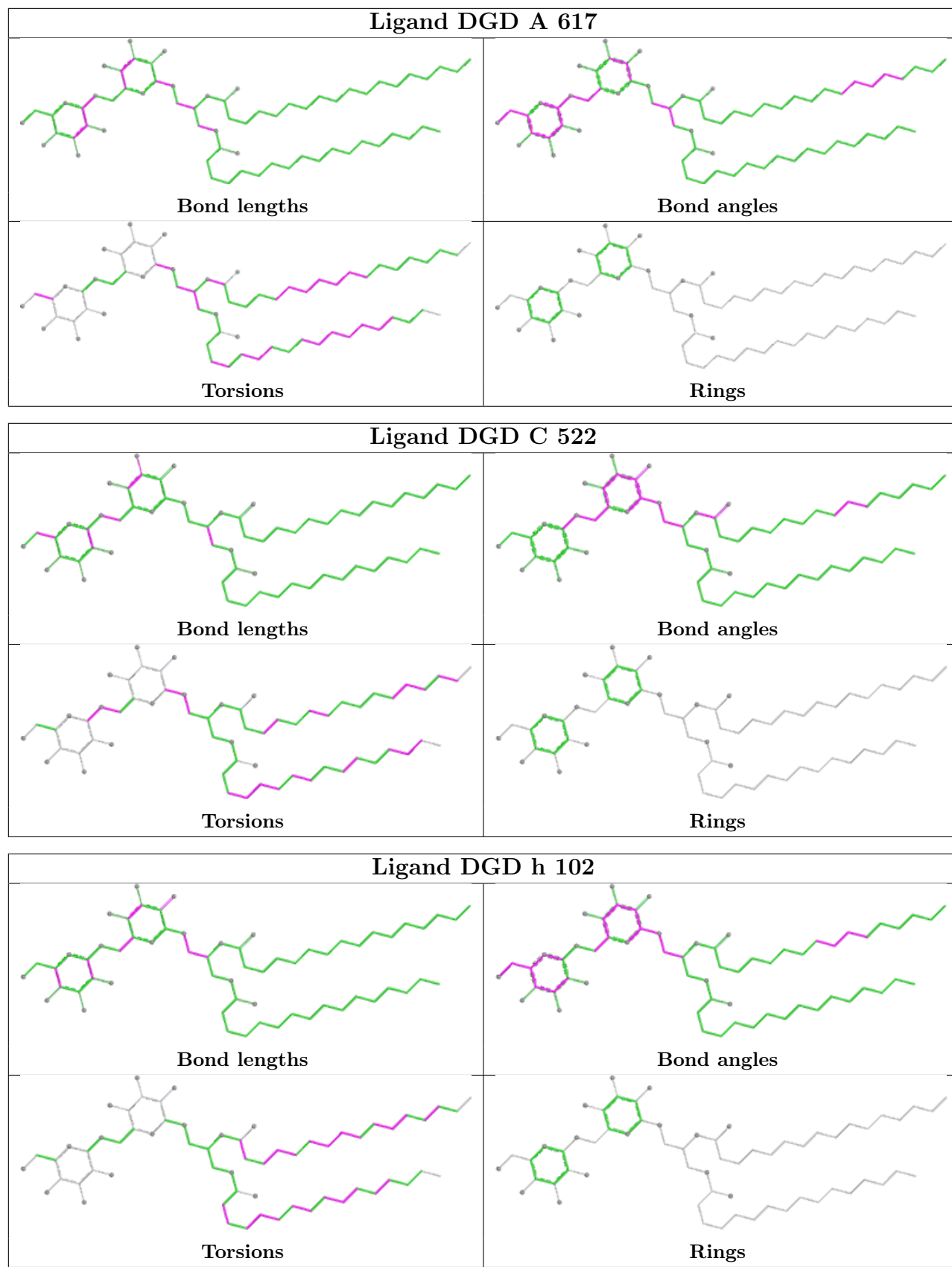
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

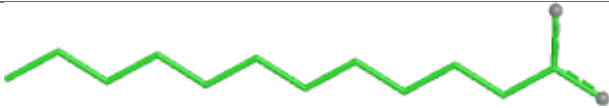
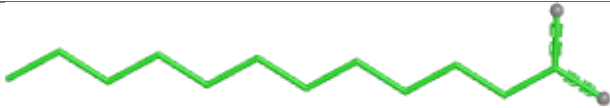
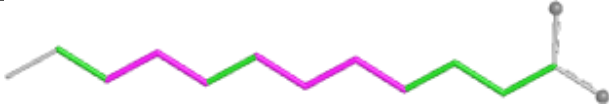
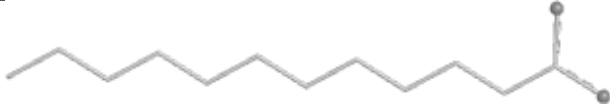
Ligand STE e 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

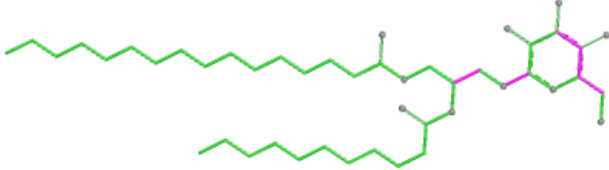
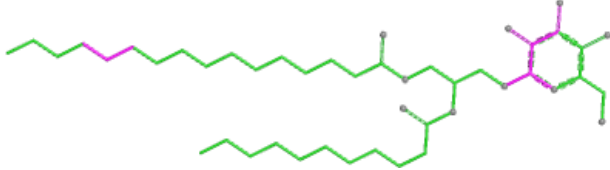
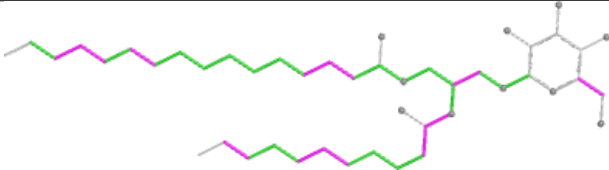
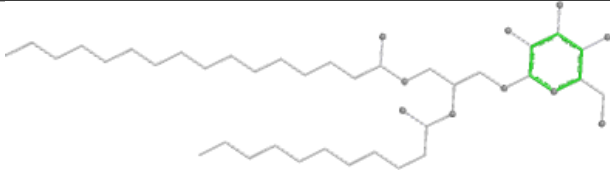
Ligand STE E 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

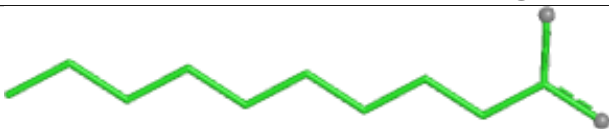
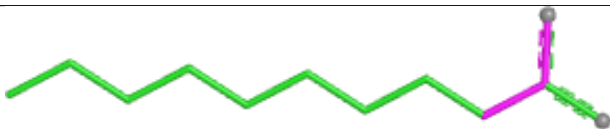
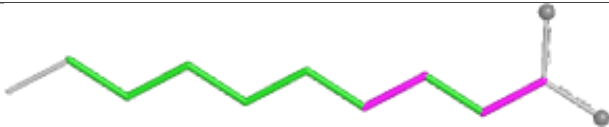
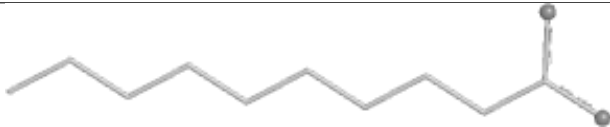


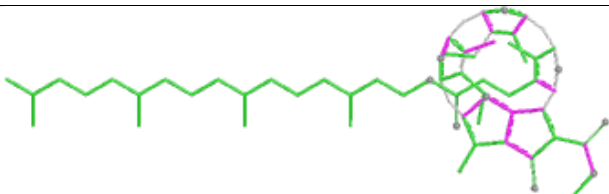
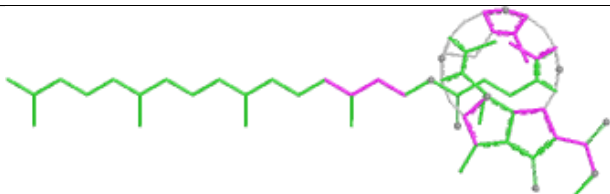
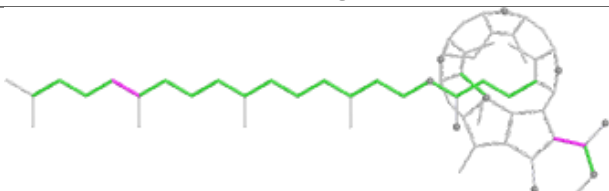
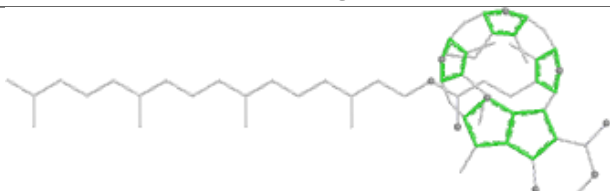


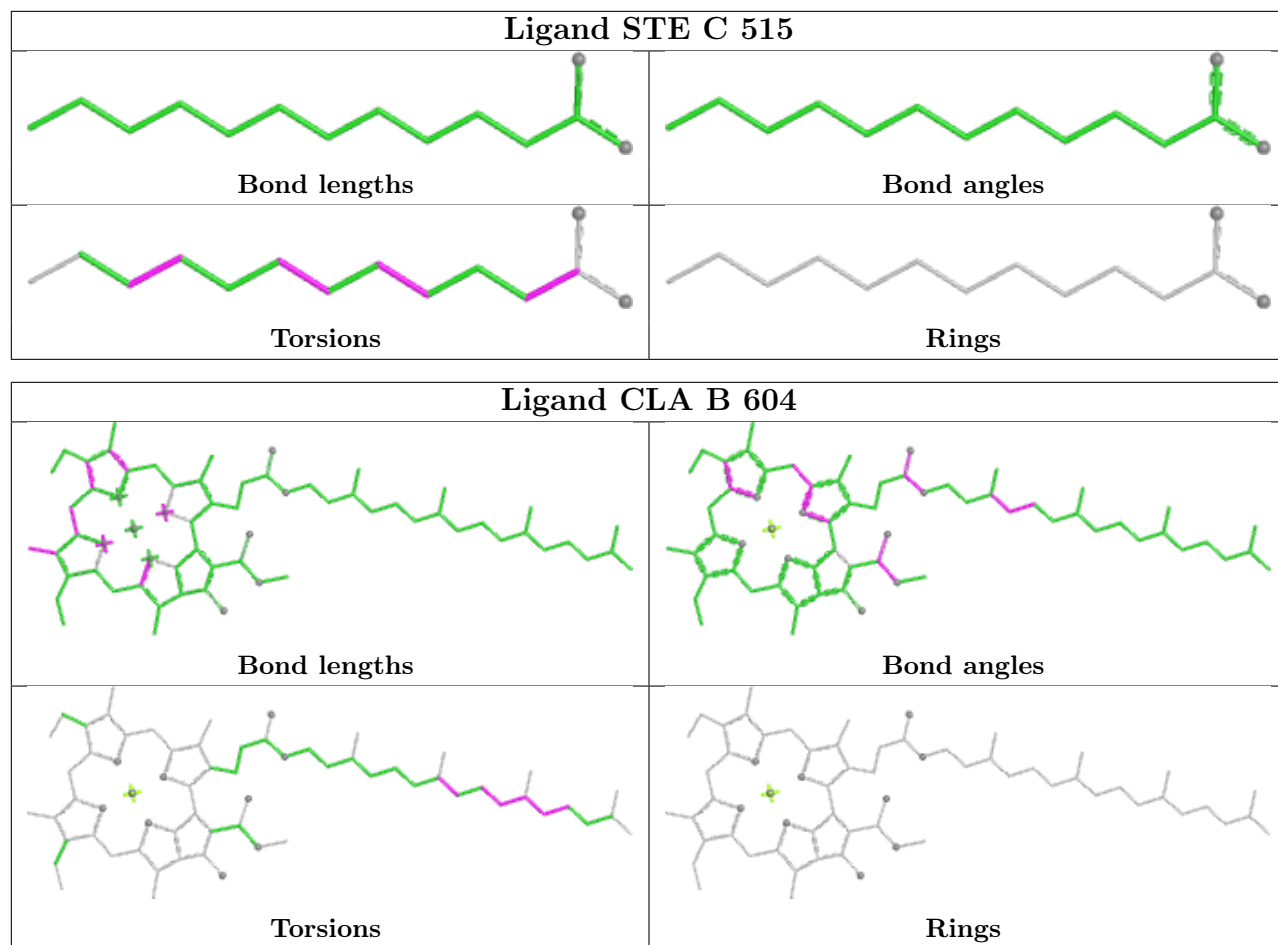


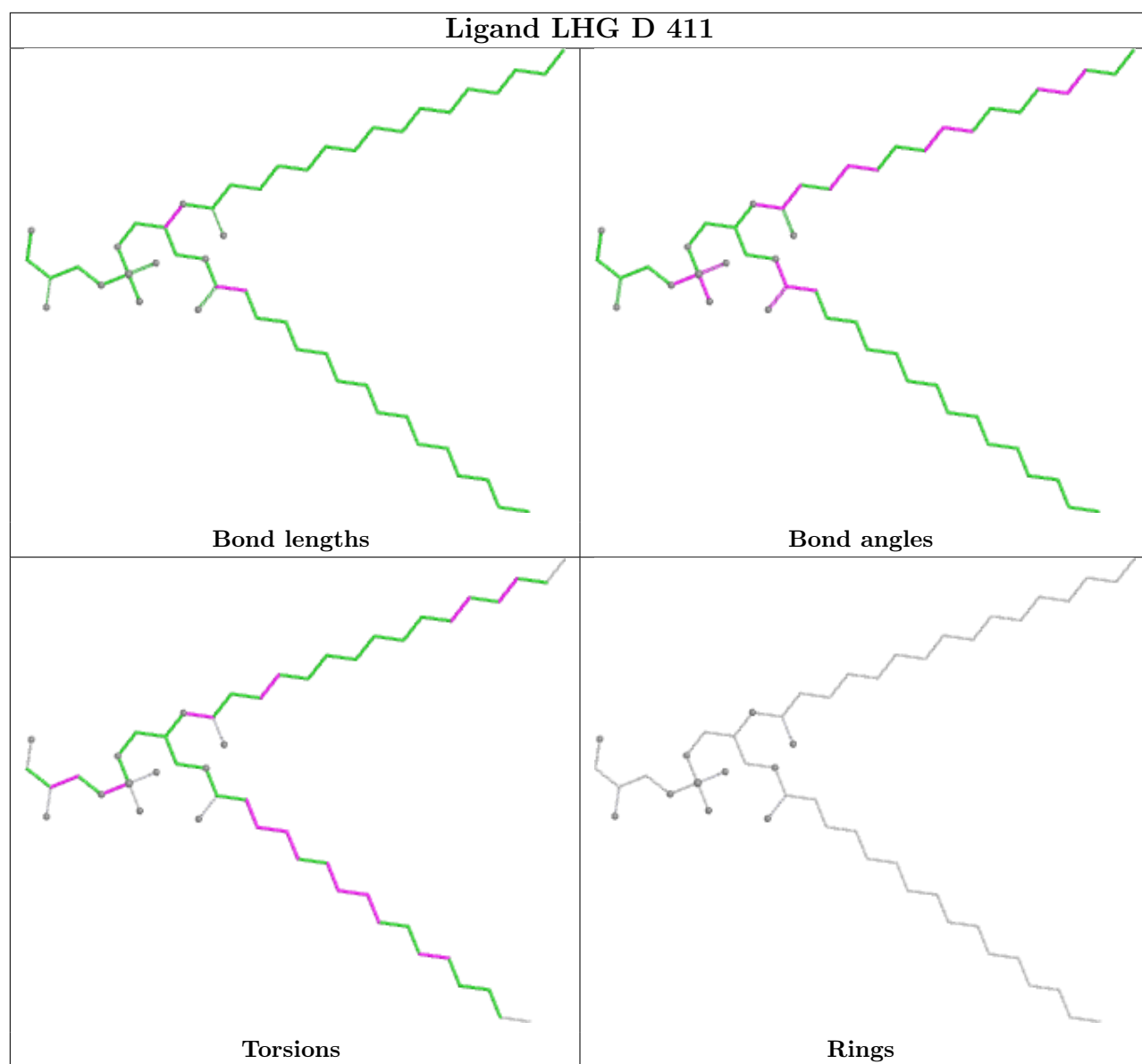
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

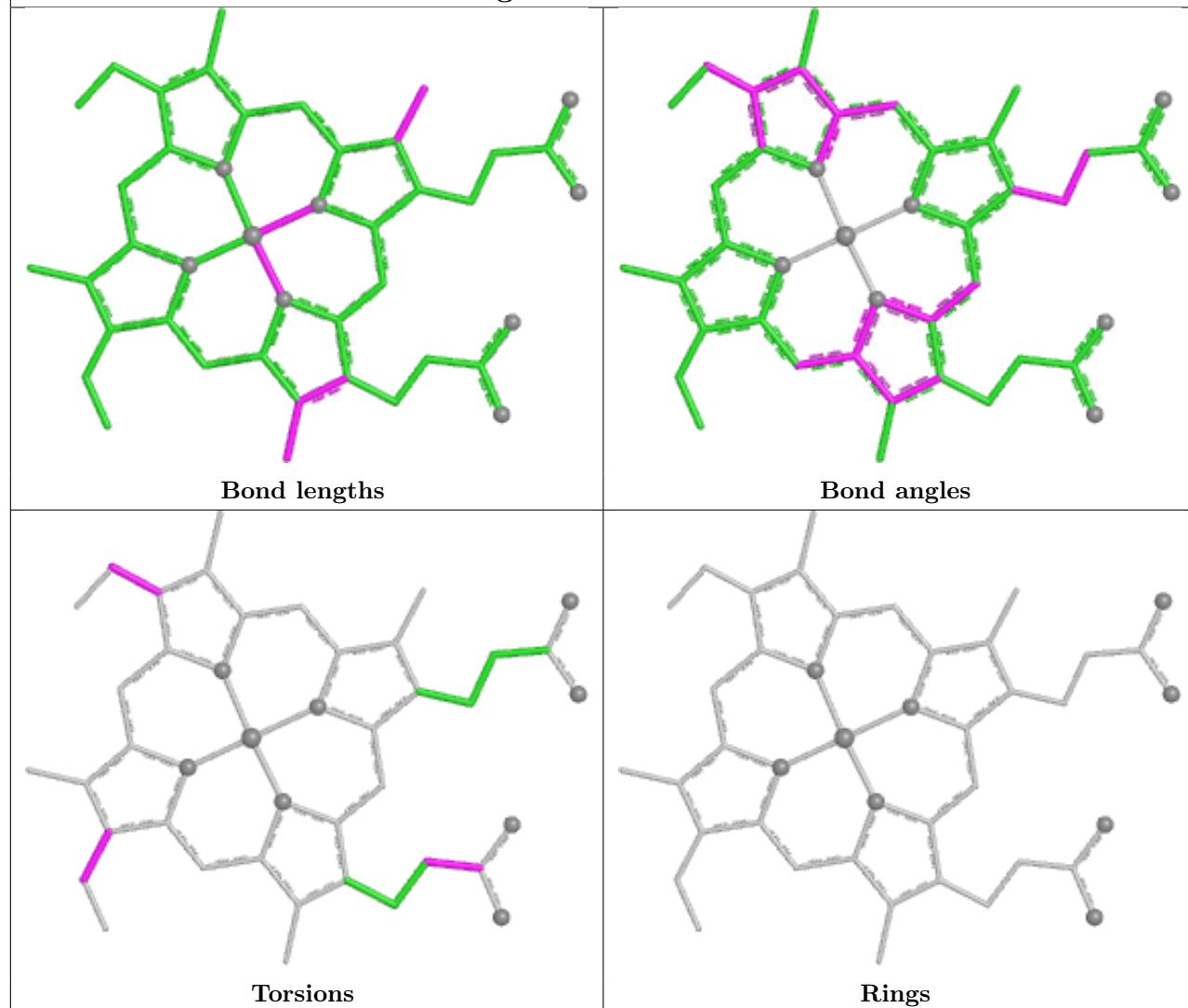
Ligand STE B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

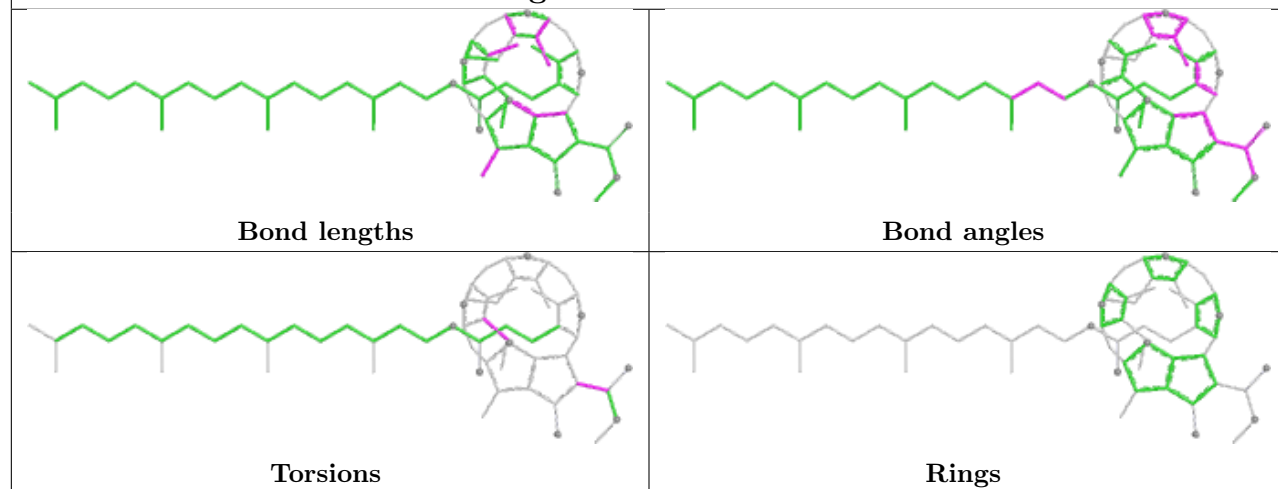


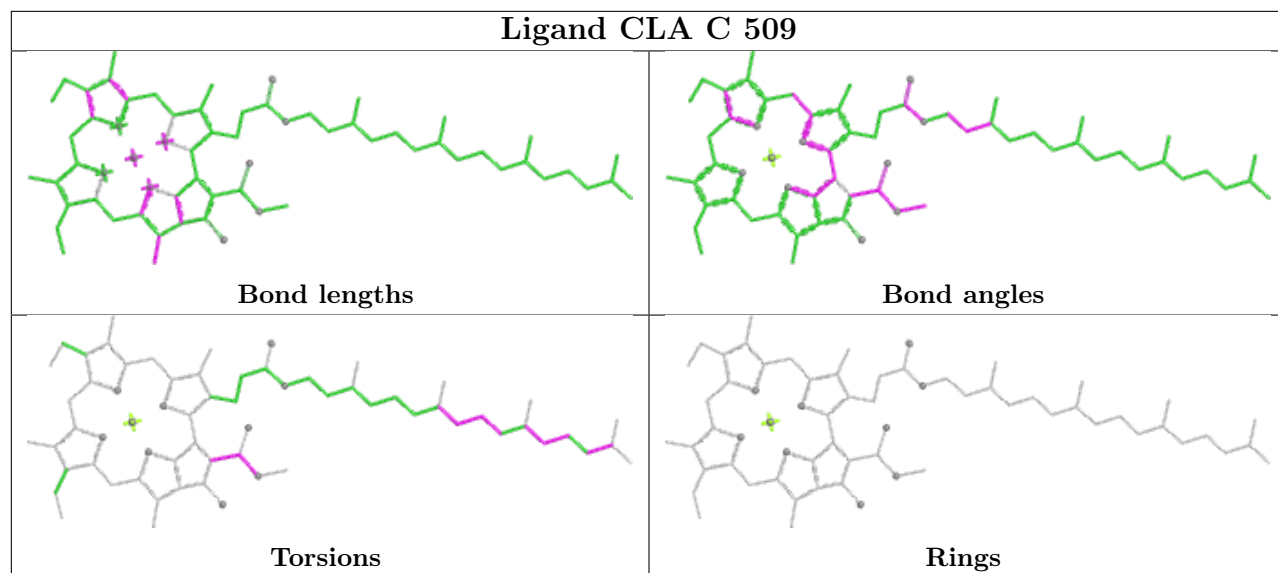
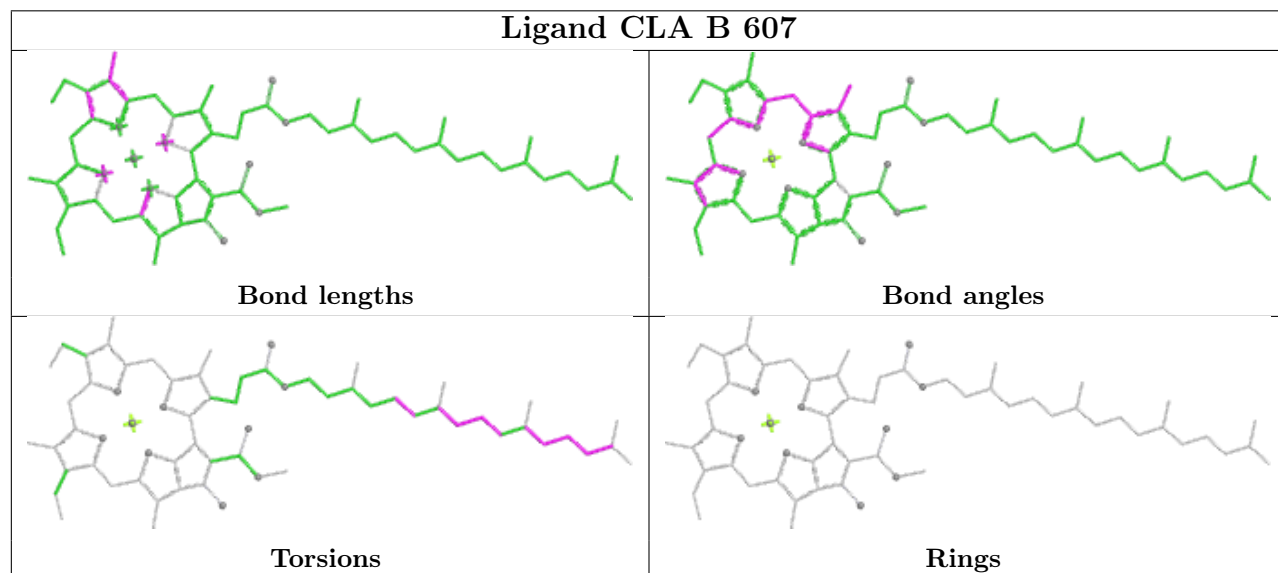
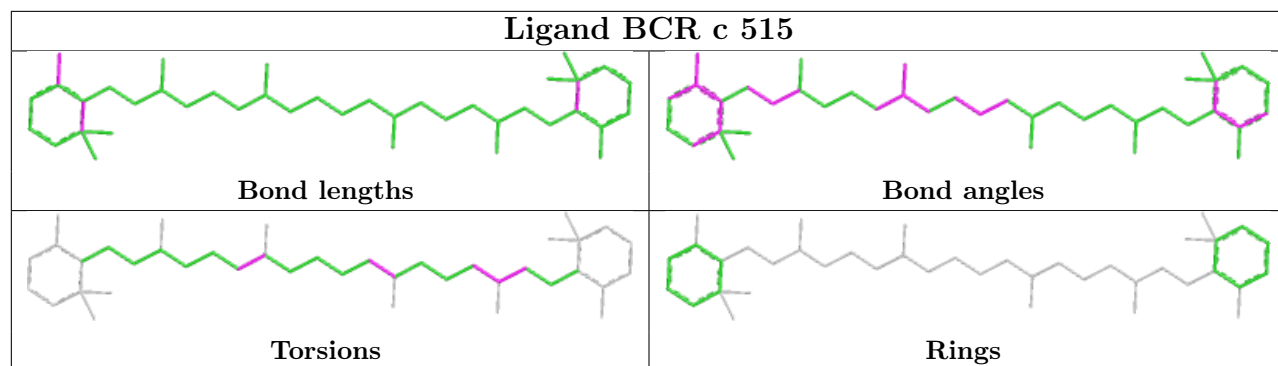


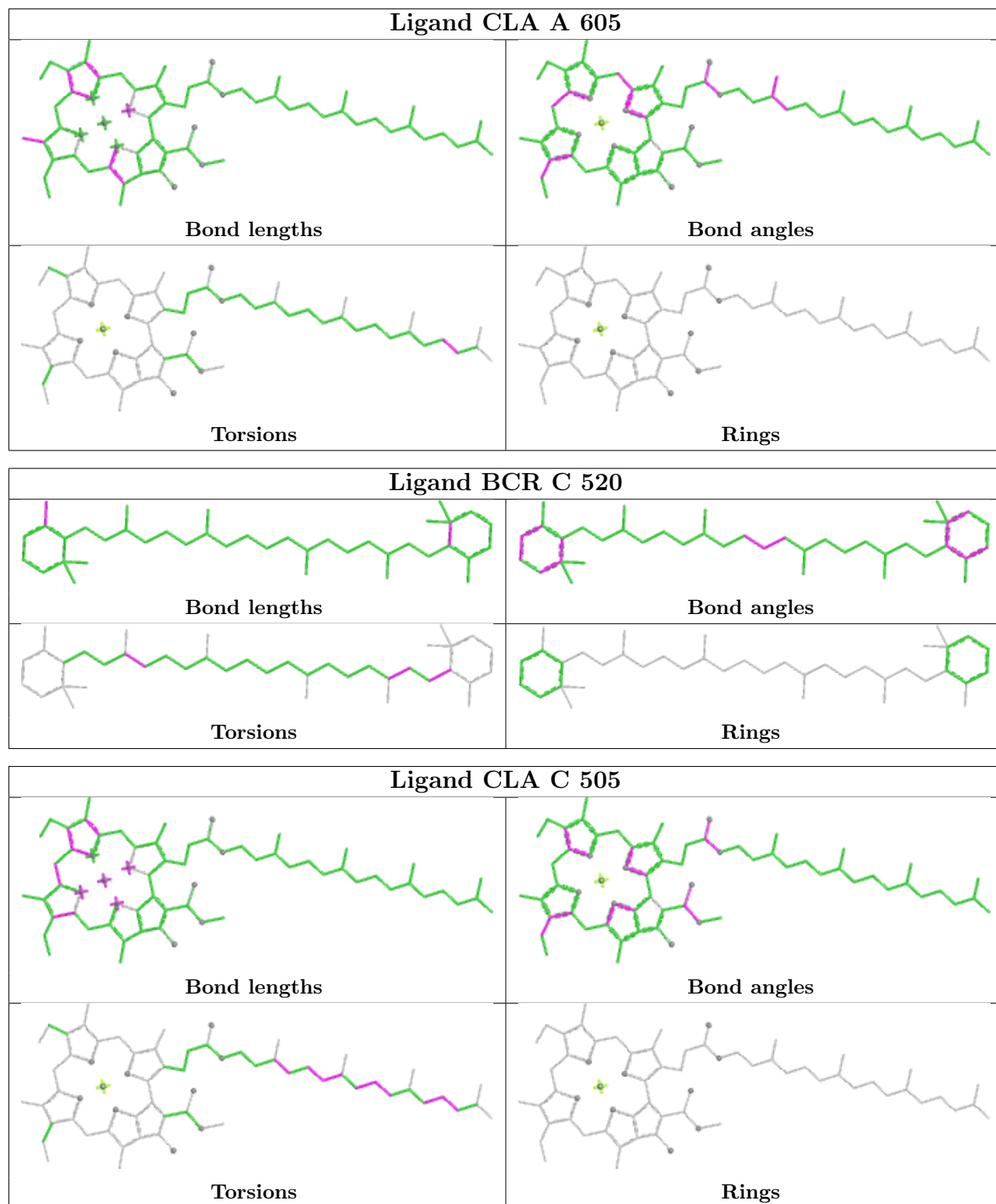
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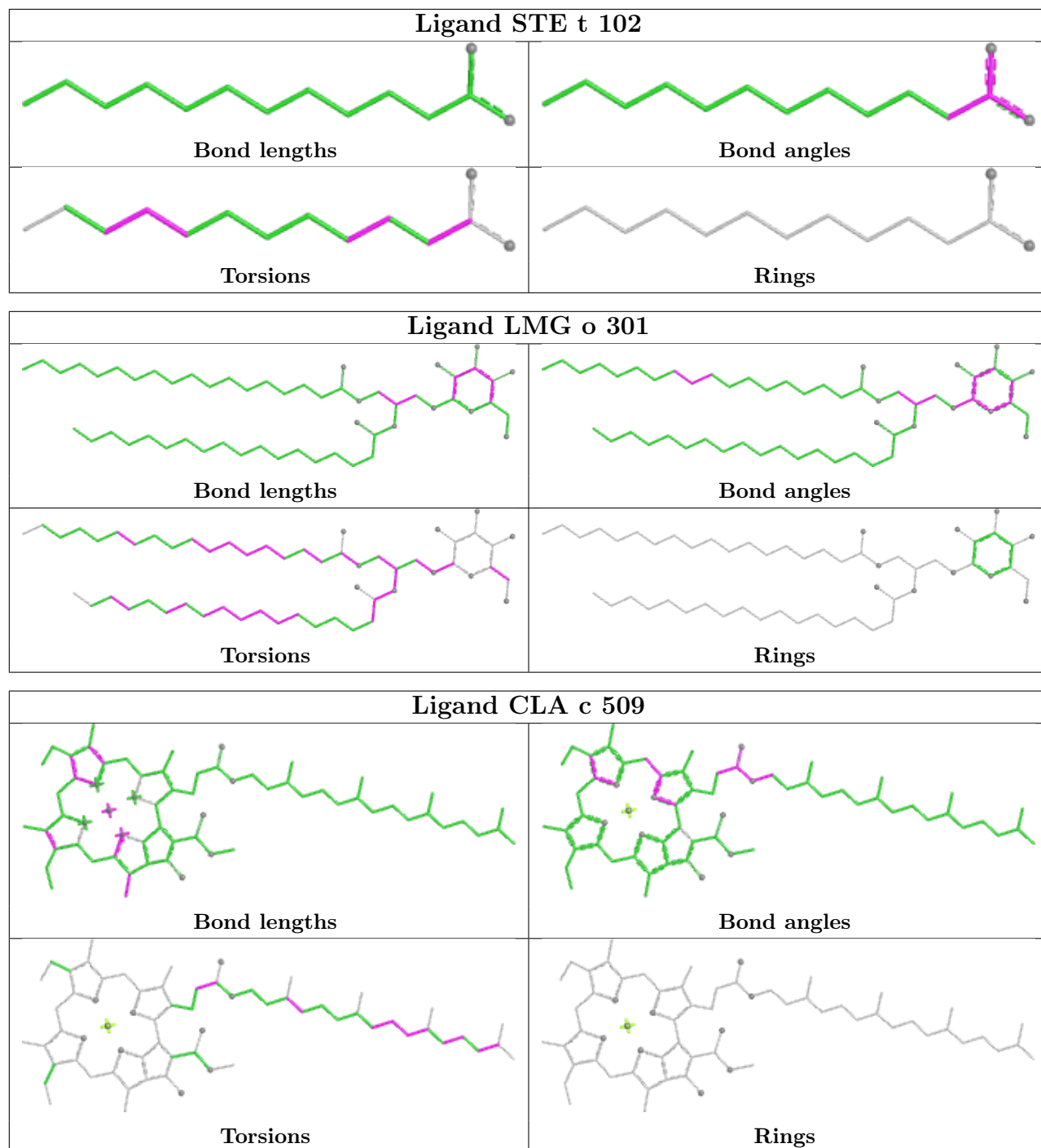


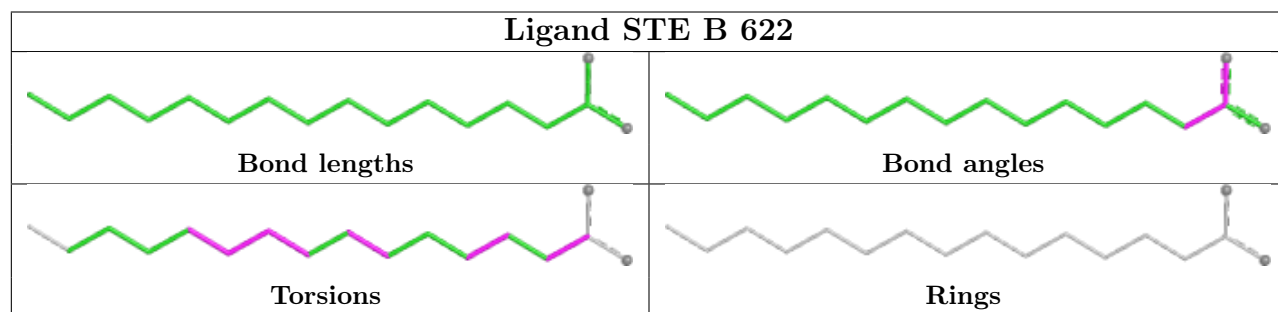
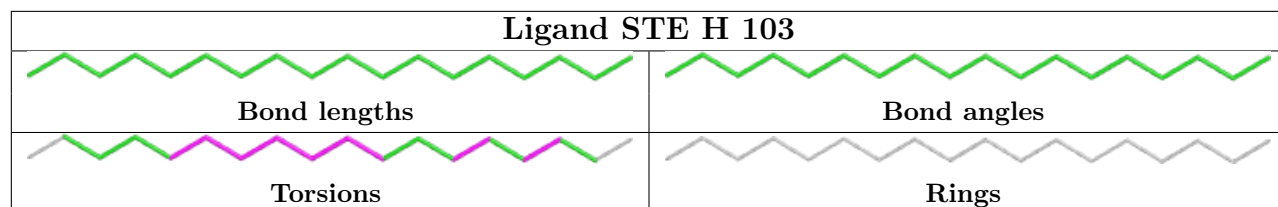
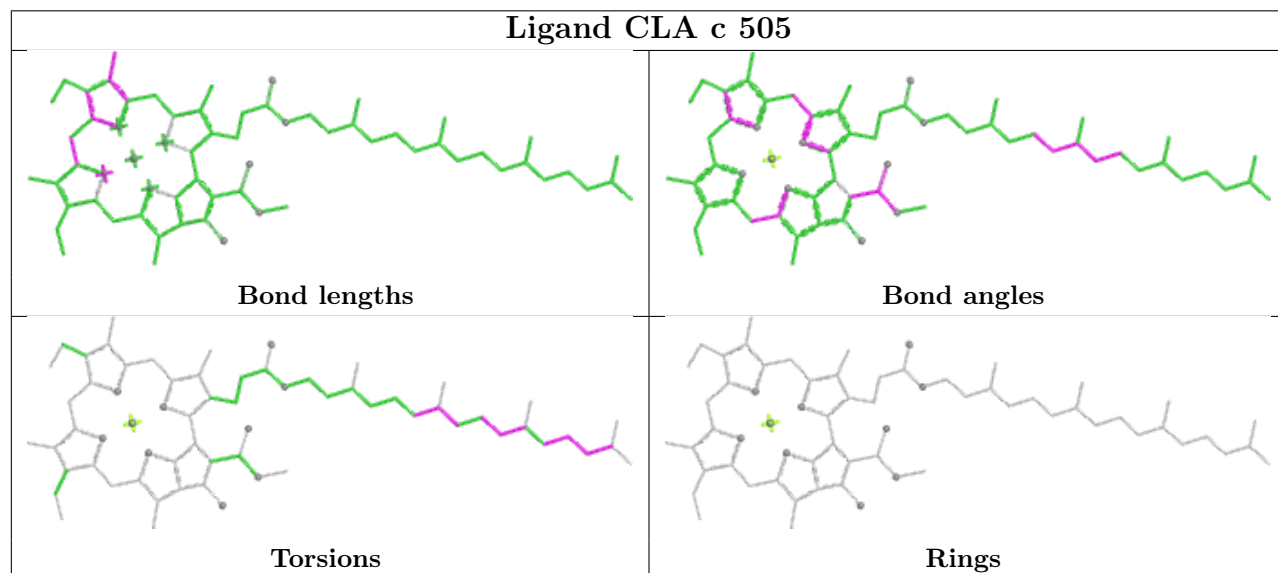
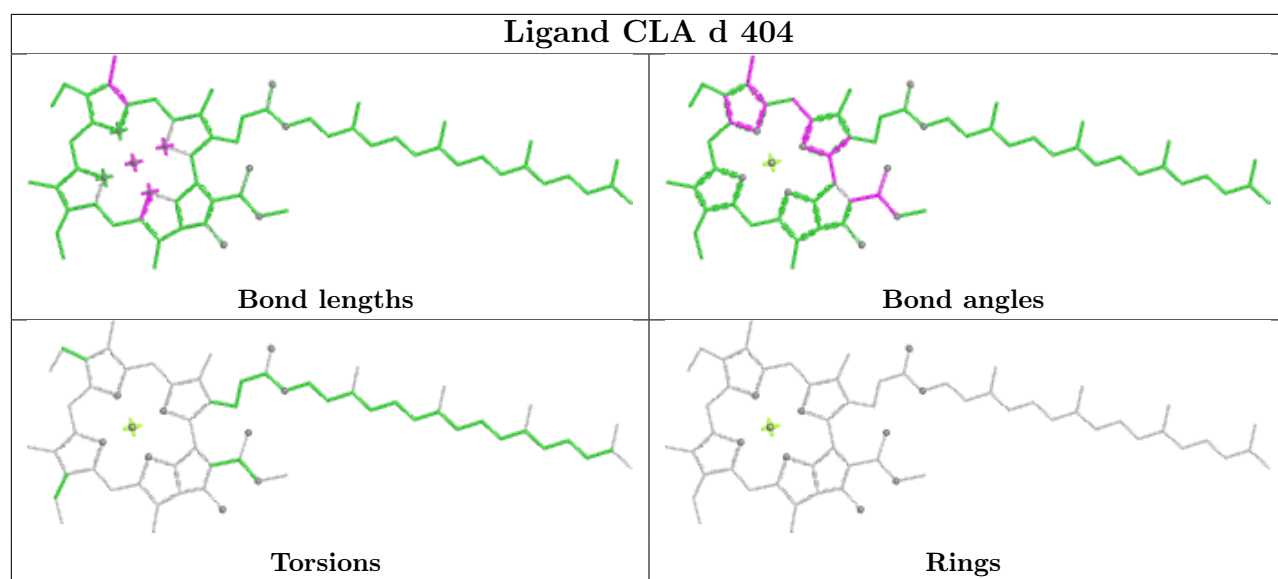
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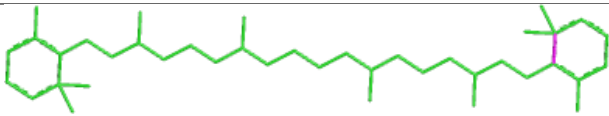
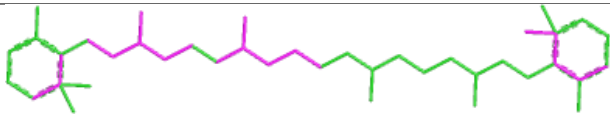
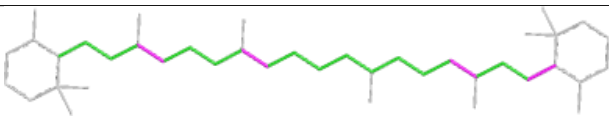
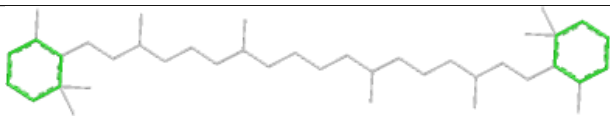


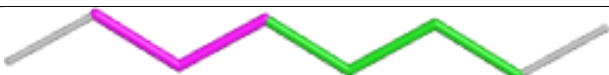


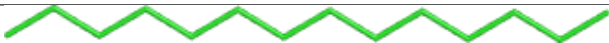
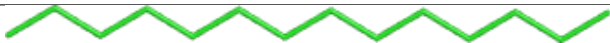


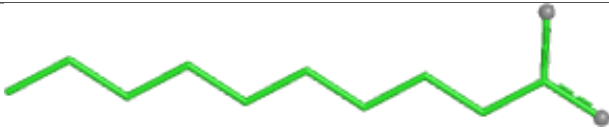
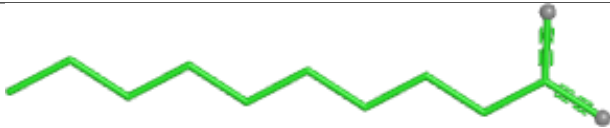
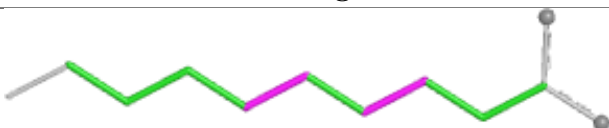
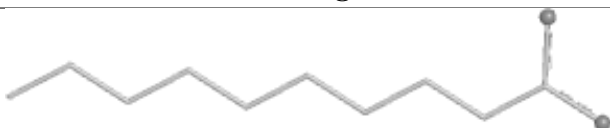


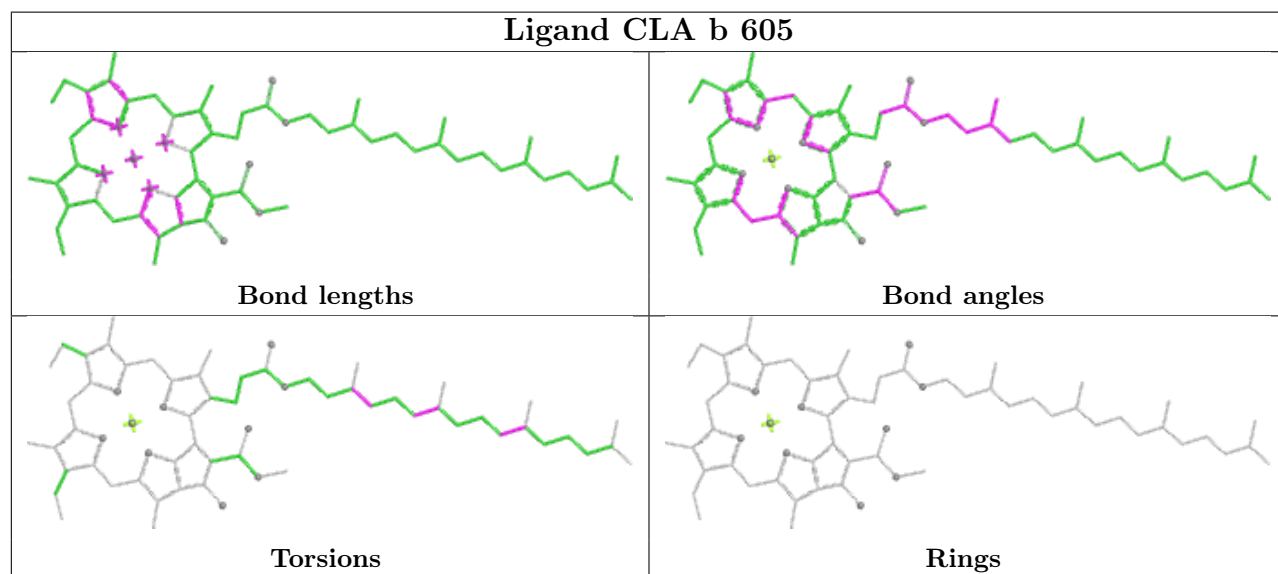
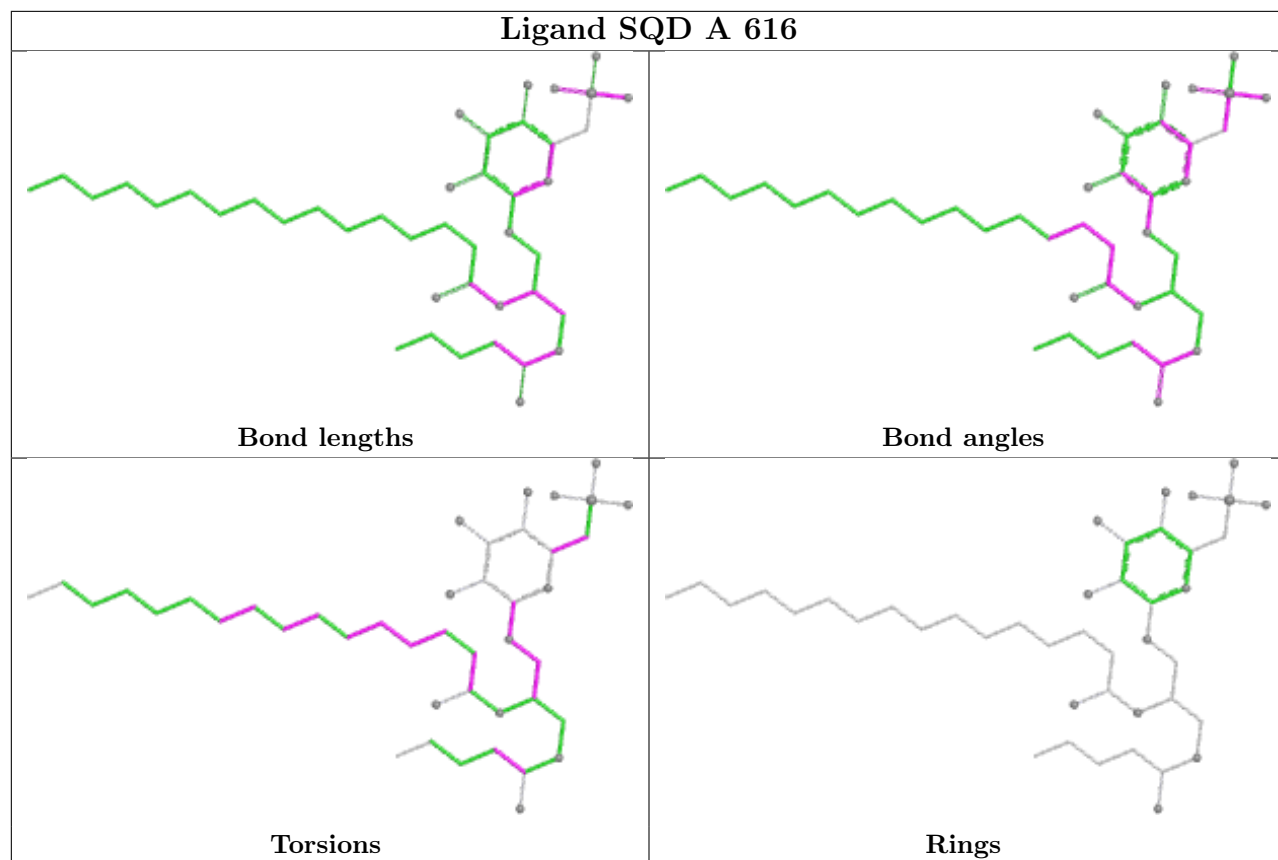


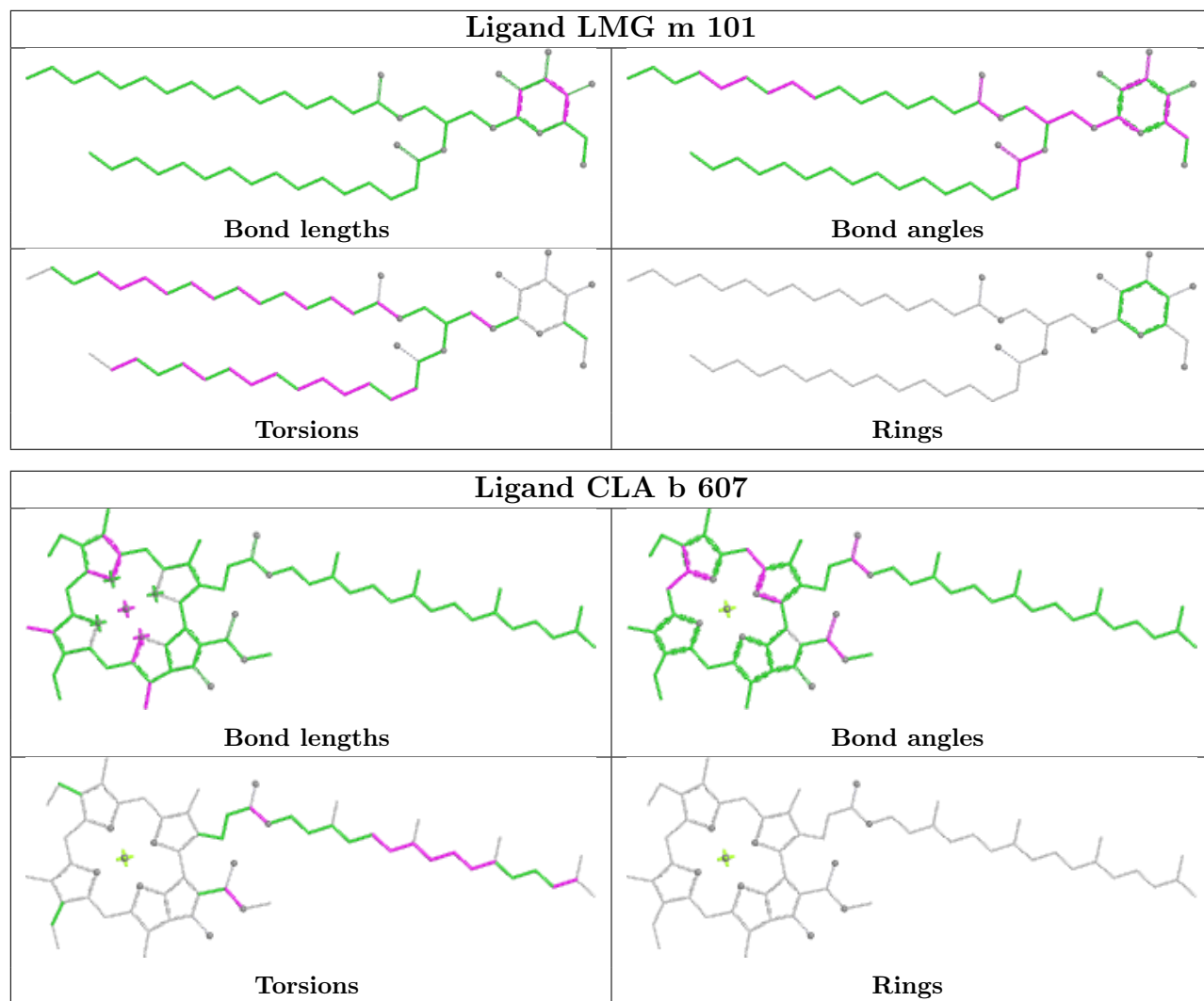
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

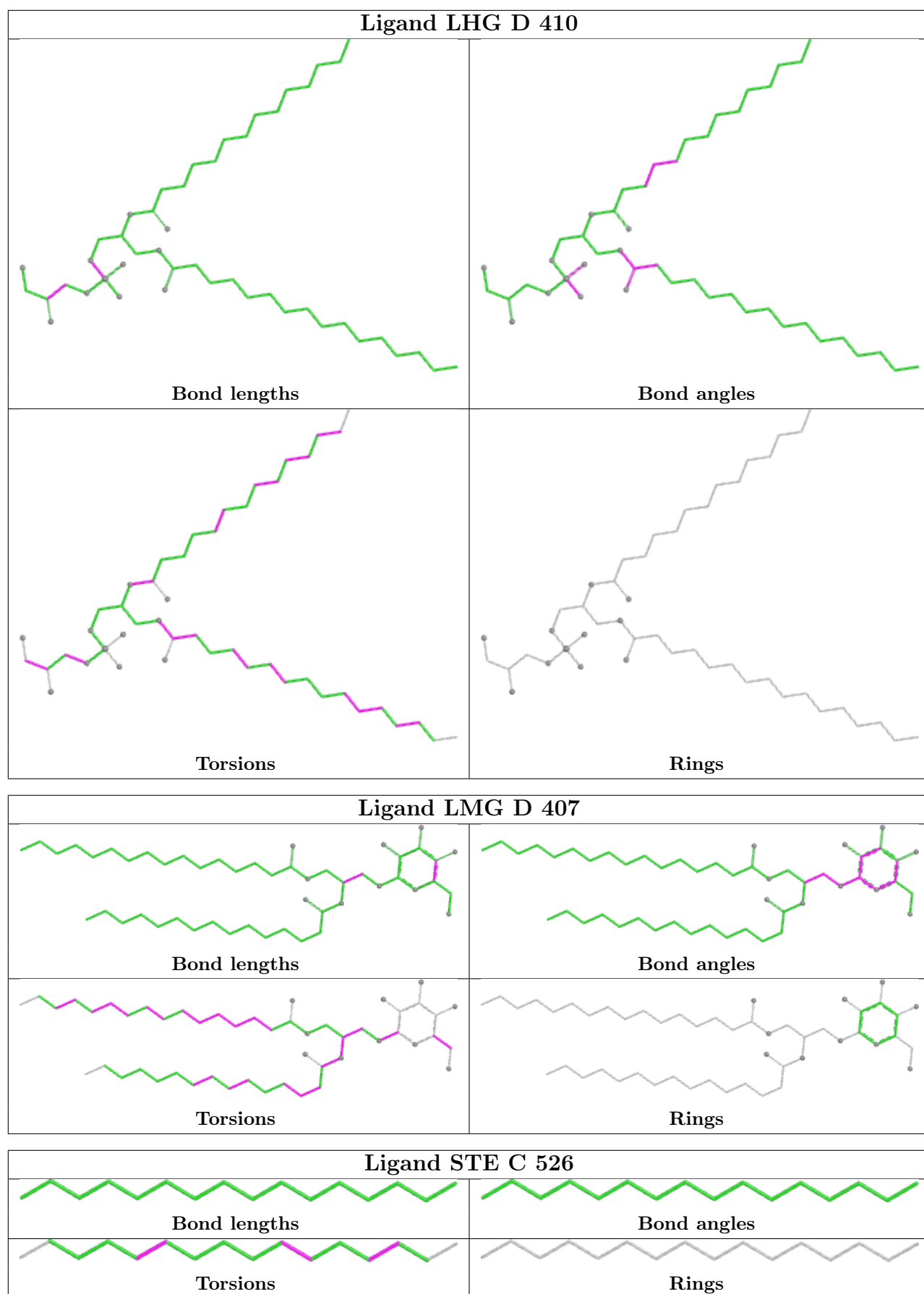
Ligand STE b 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

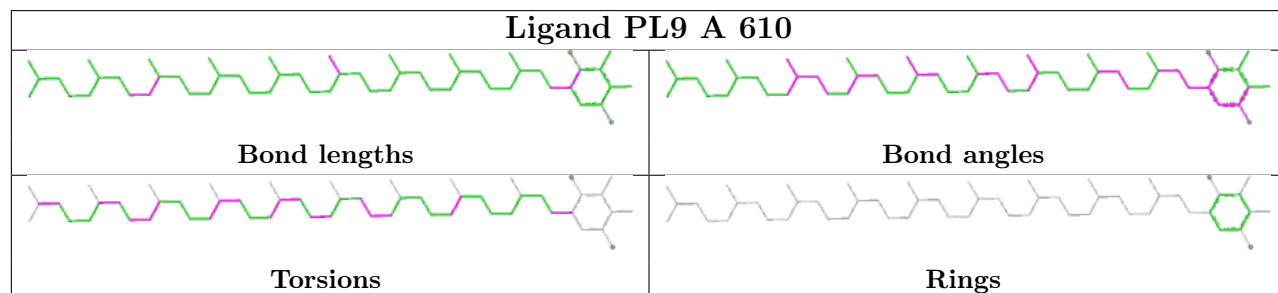
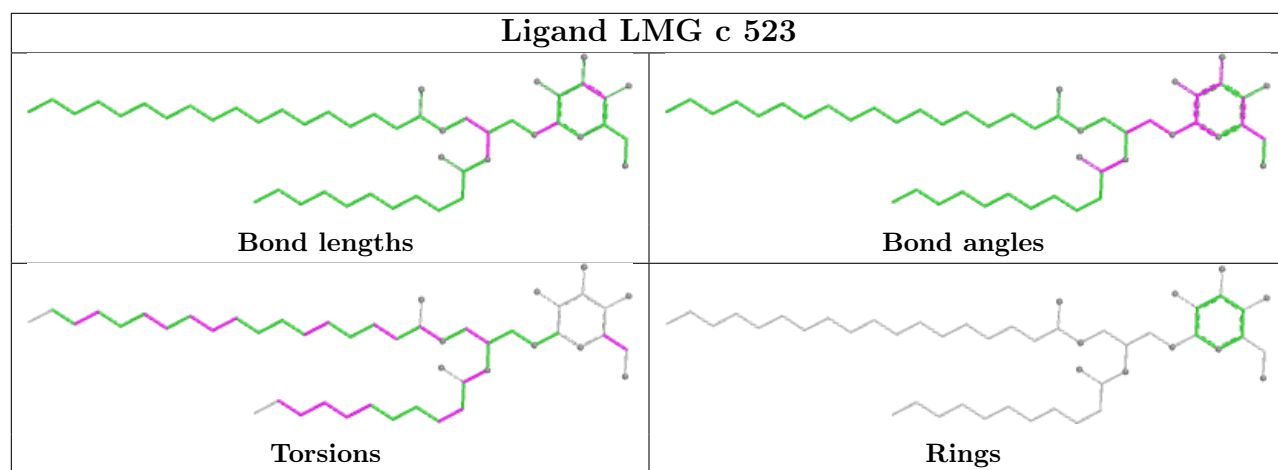
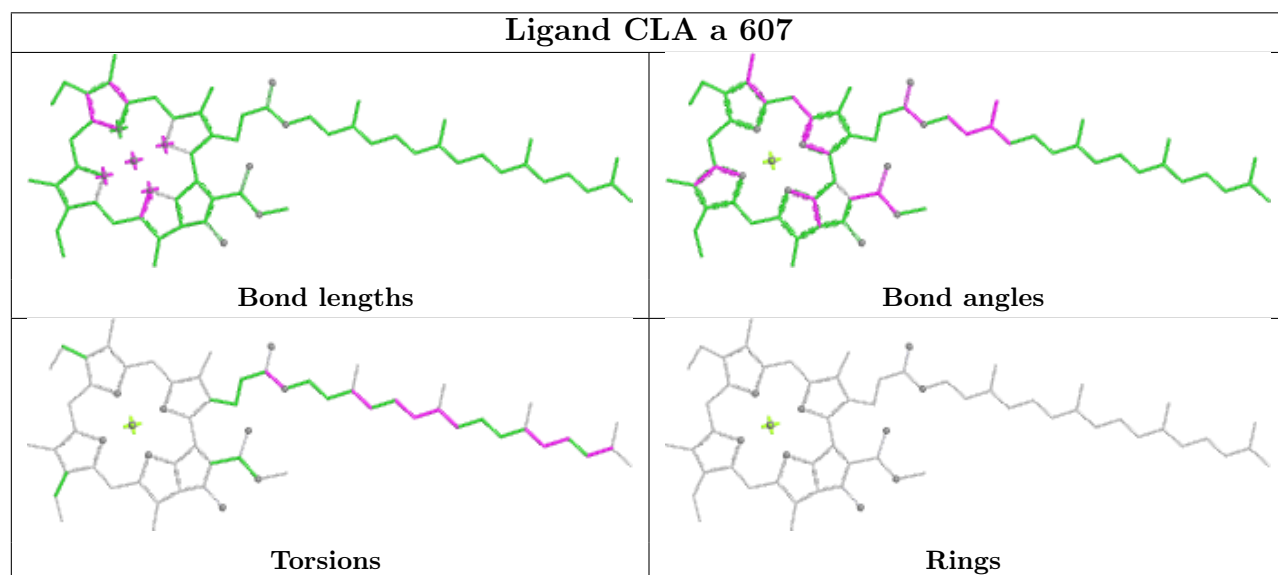
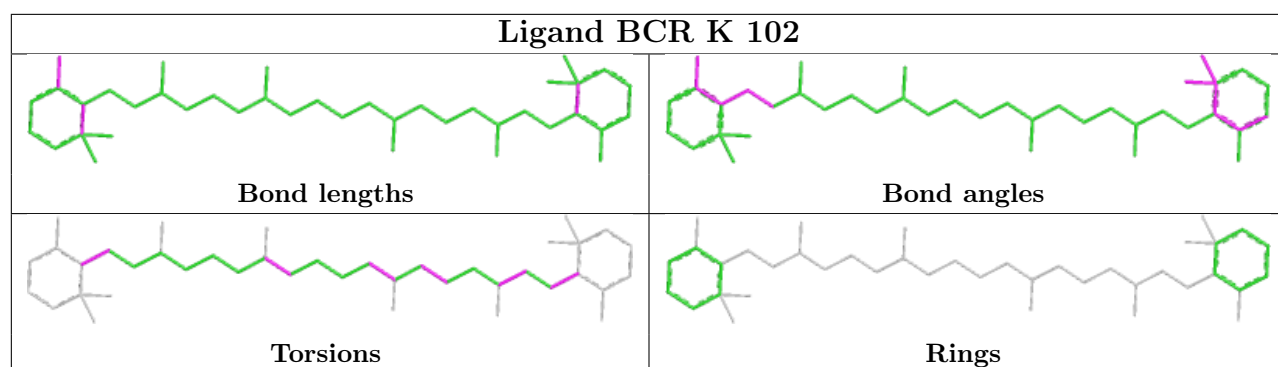
Ligand STE C 528	
	
Bond lengths	Bond angles
	
Torsions	Rings

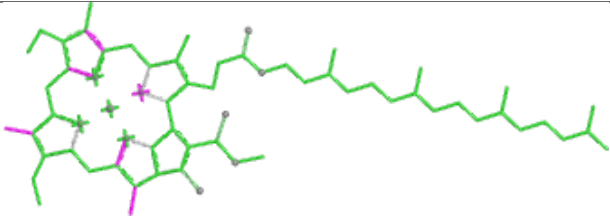
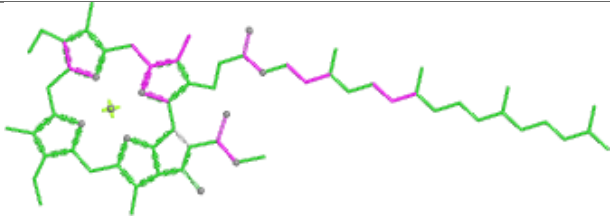
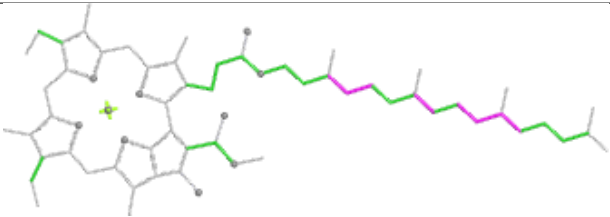
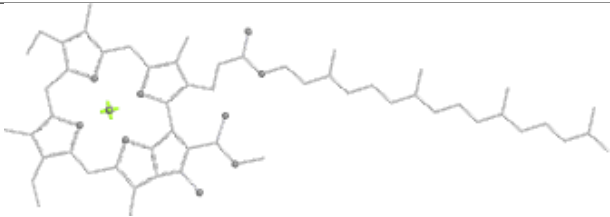
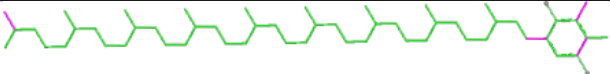
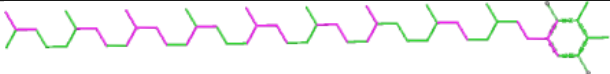
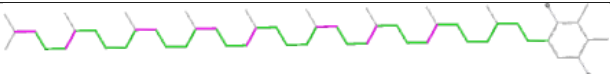
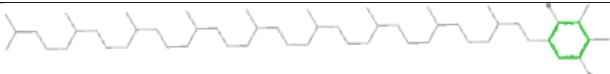
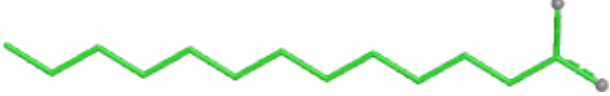
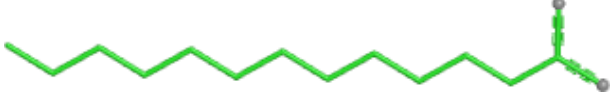
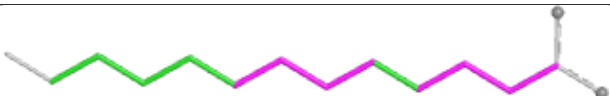
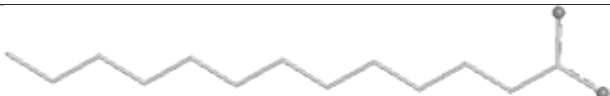
Ligand STE m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

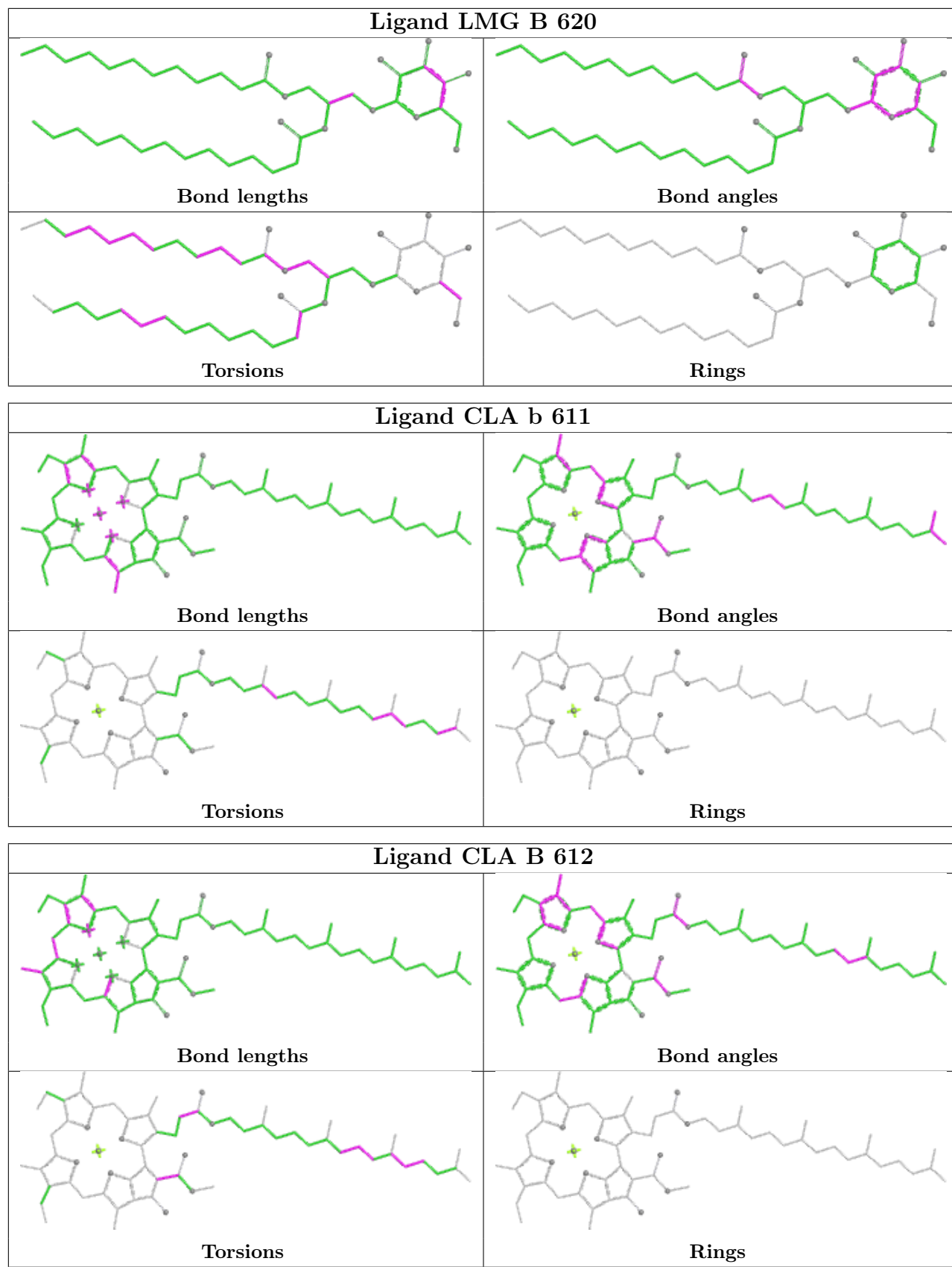


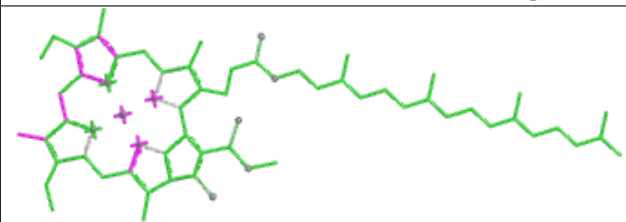
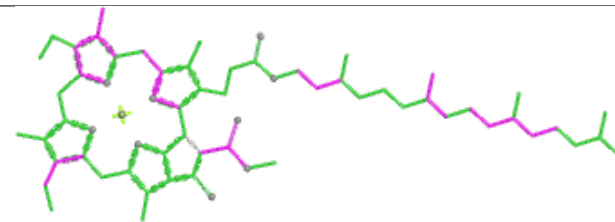
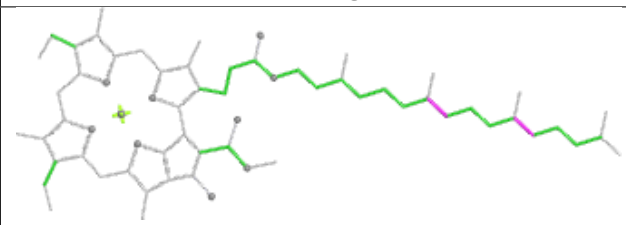
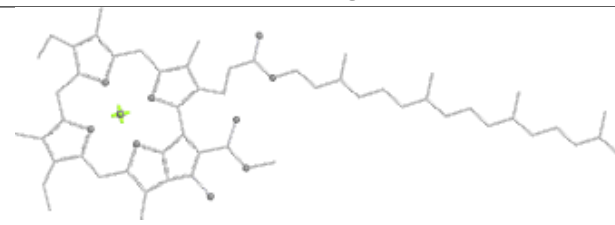


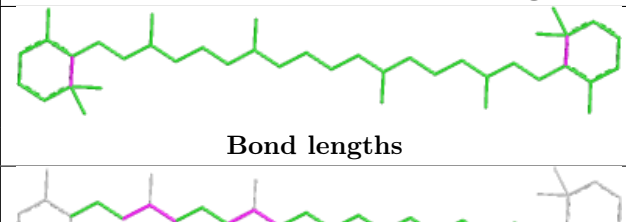
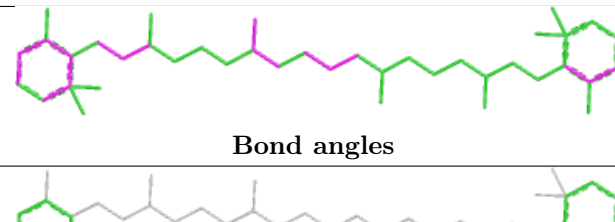
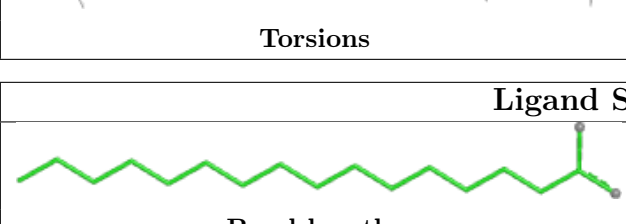
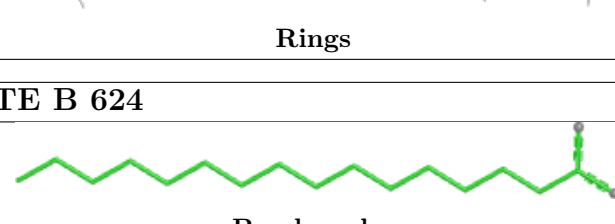


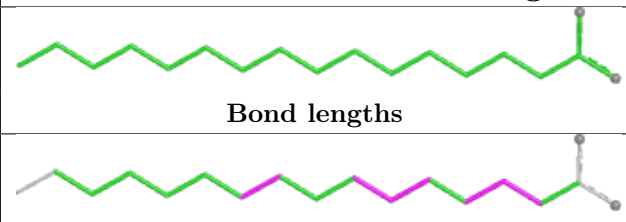
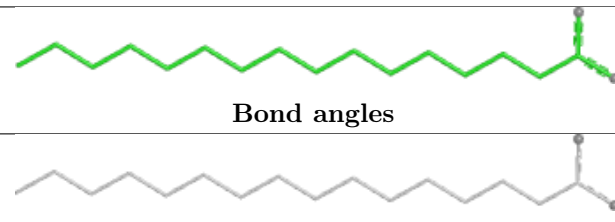
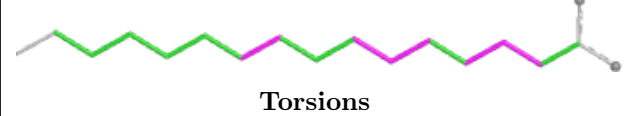
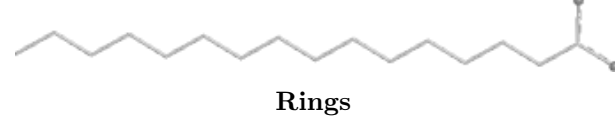


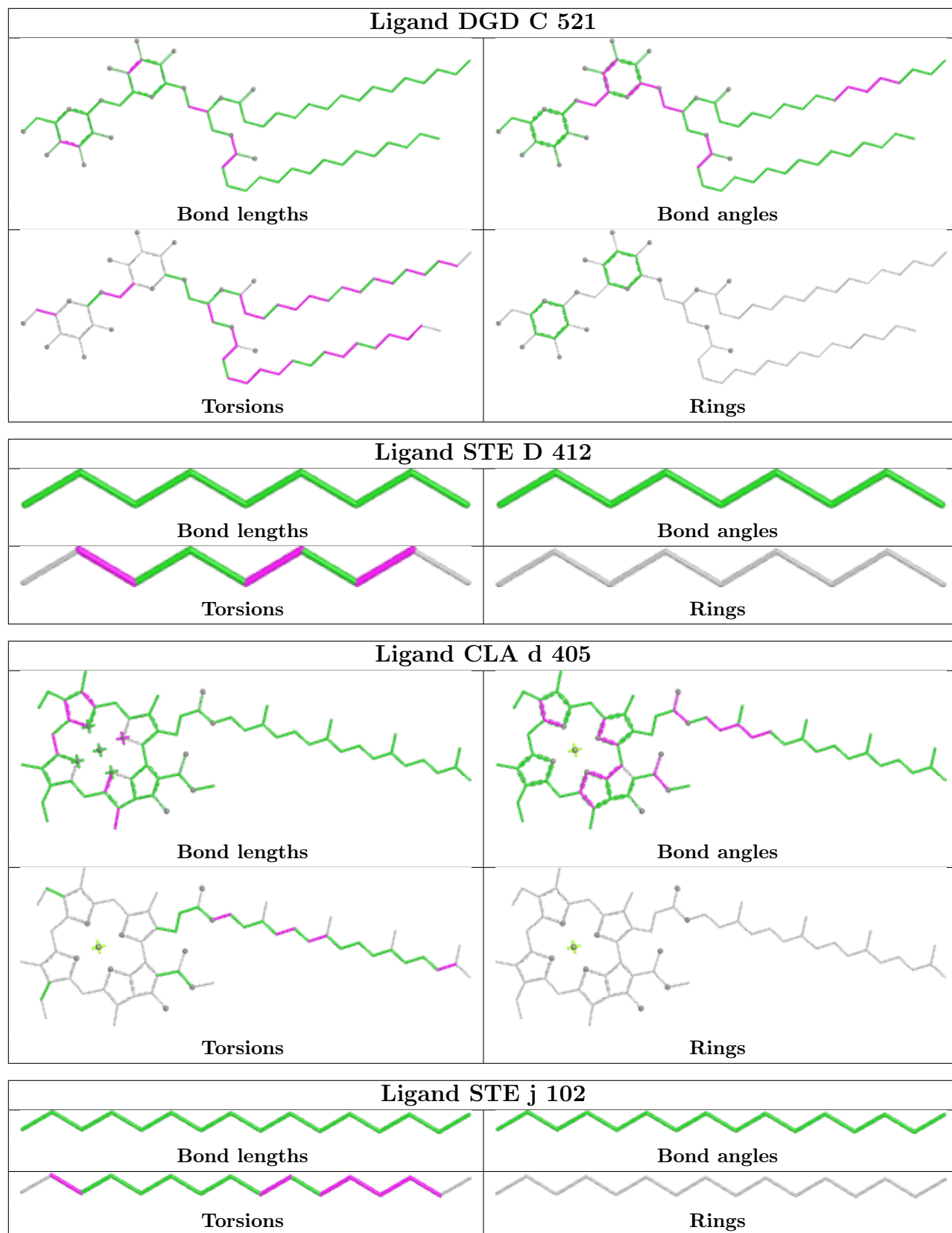
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

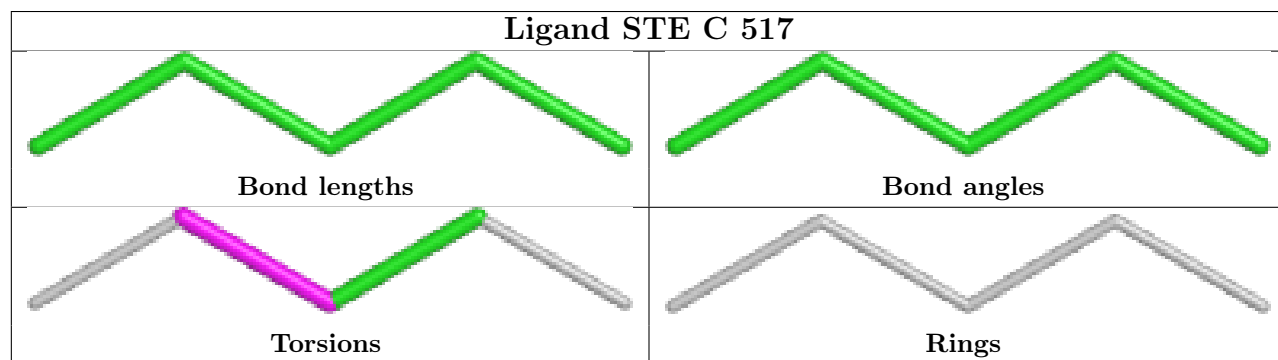
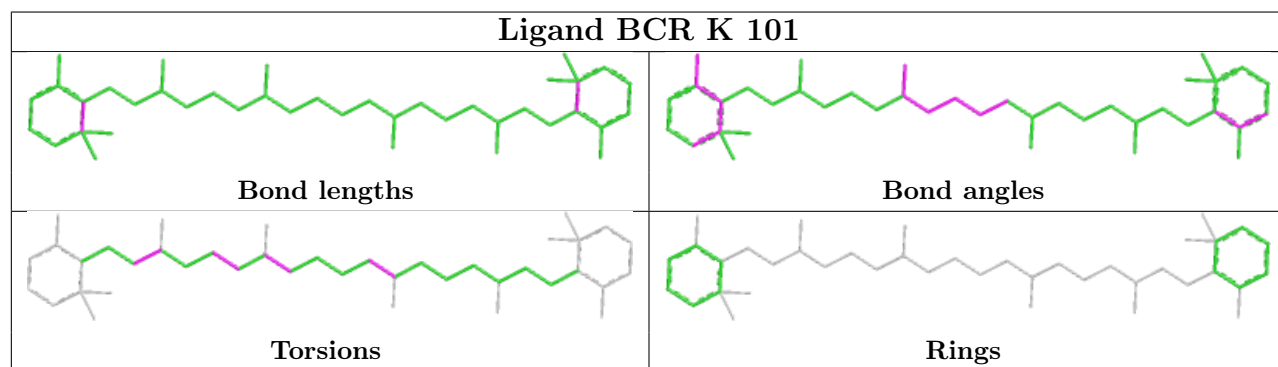
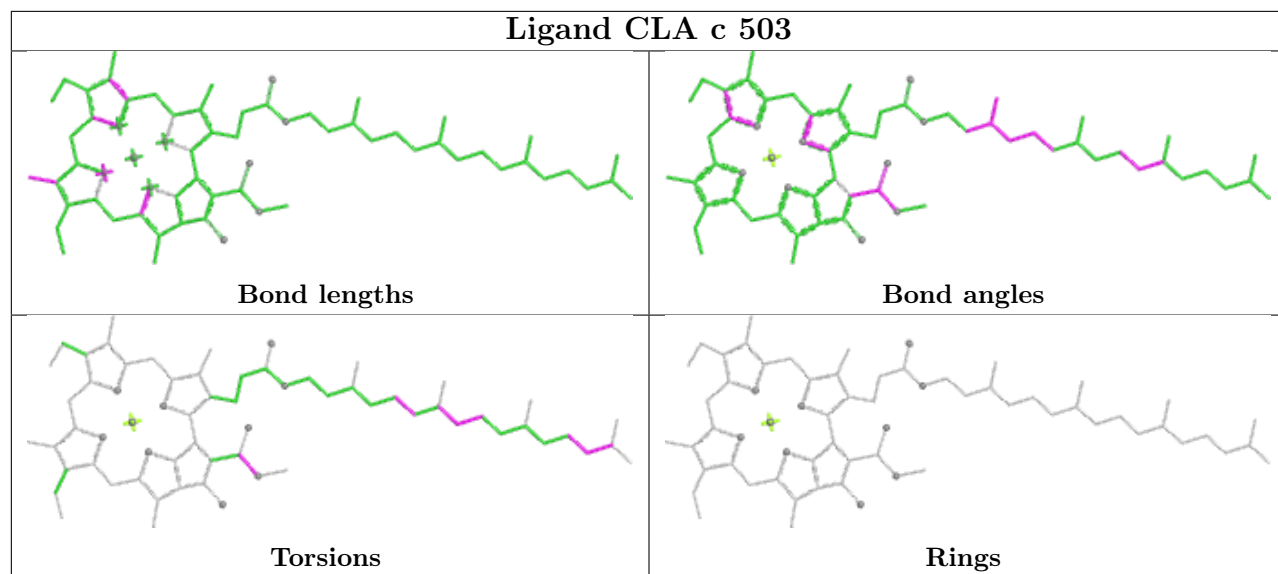


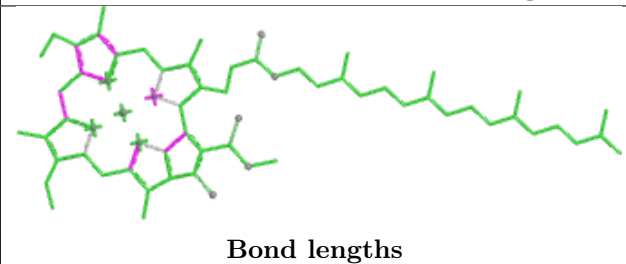
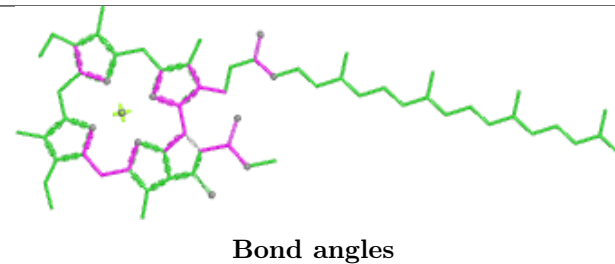
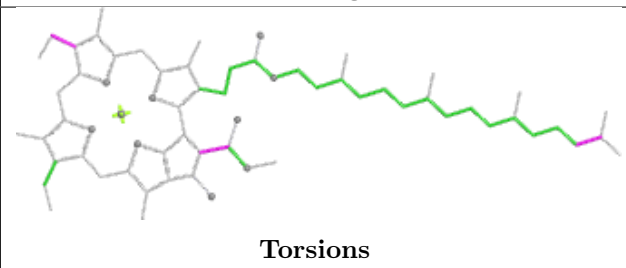
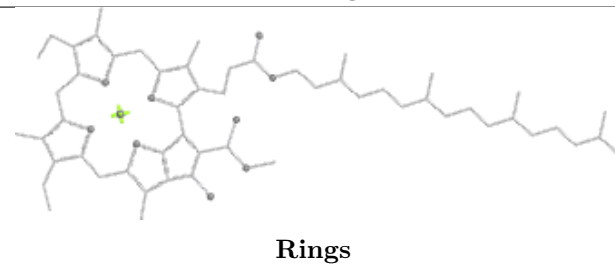
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

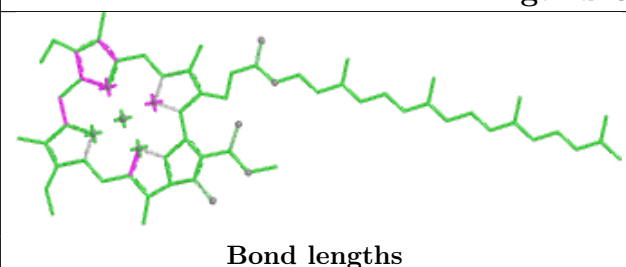
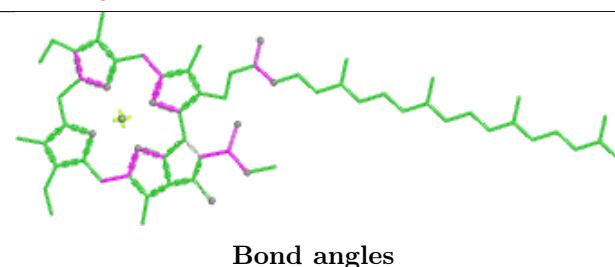
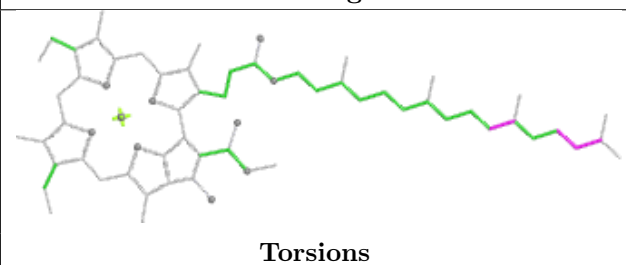
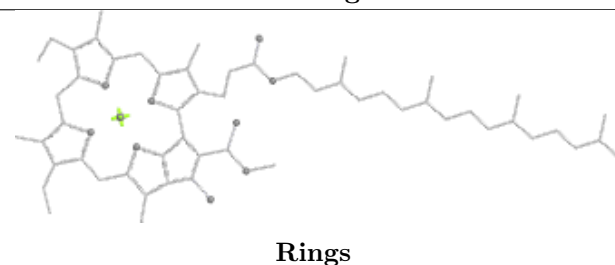
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

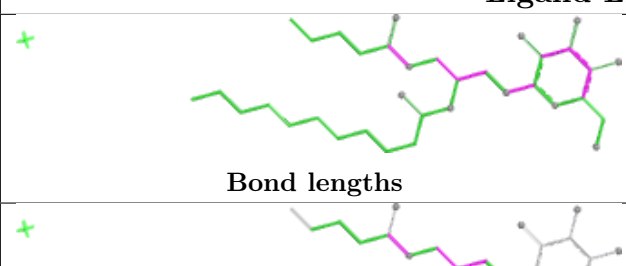
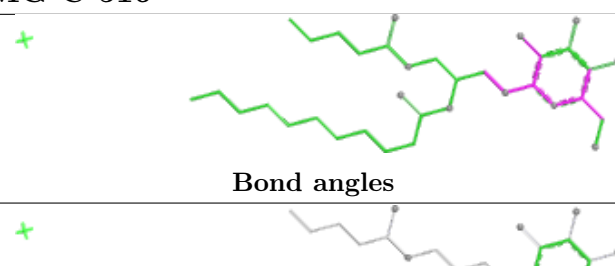
Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

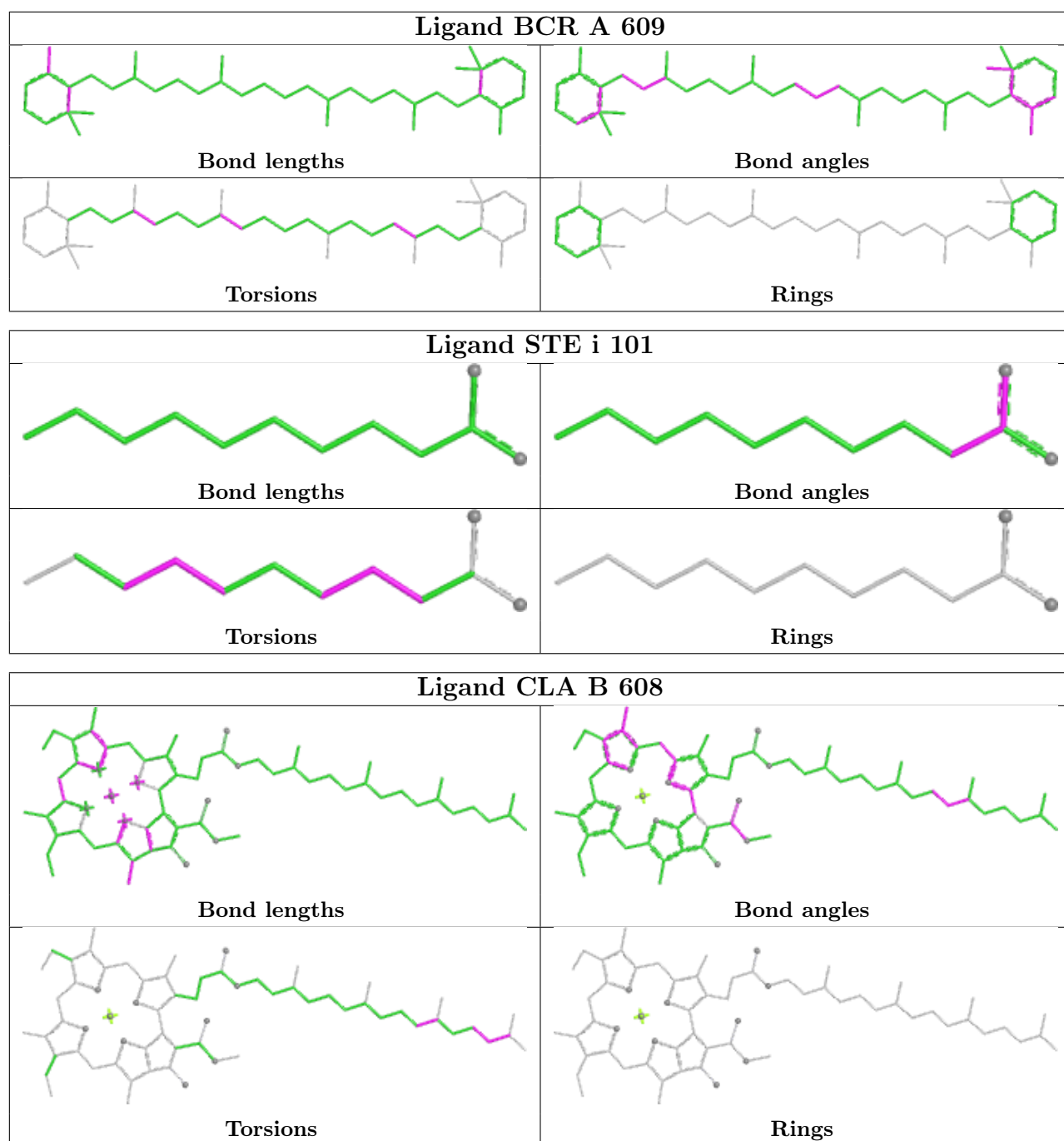




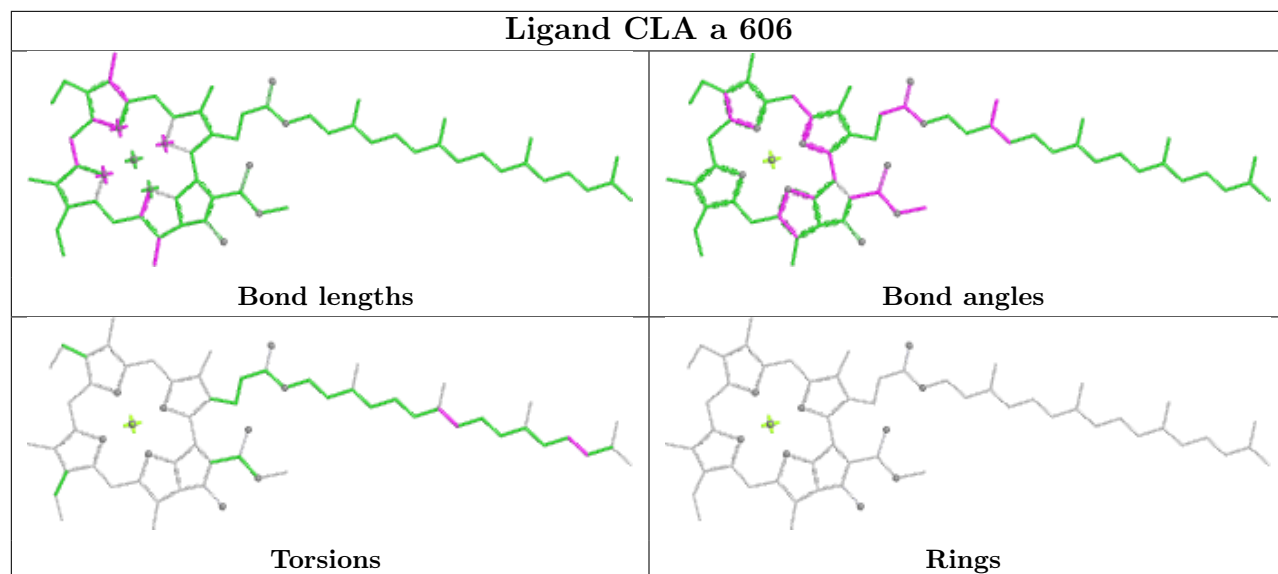
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

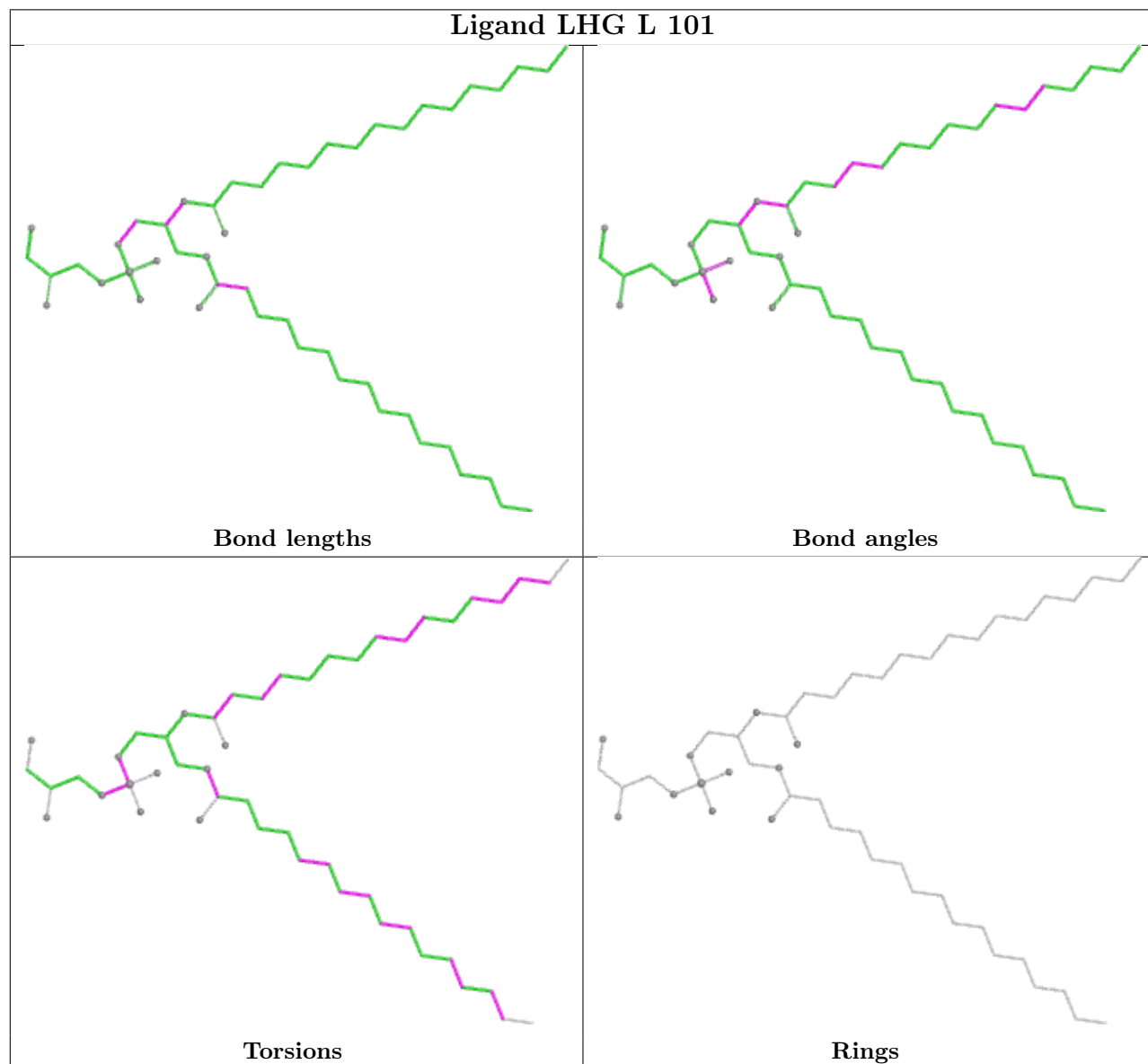
Ligand LMG C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

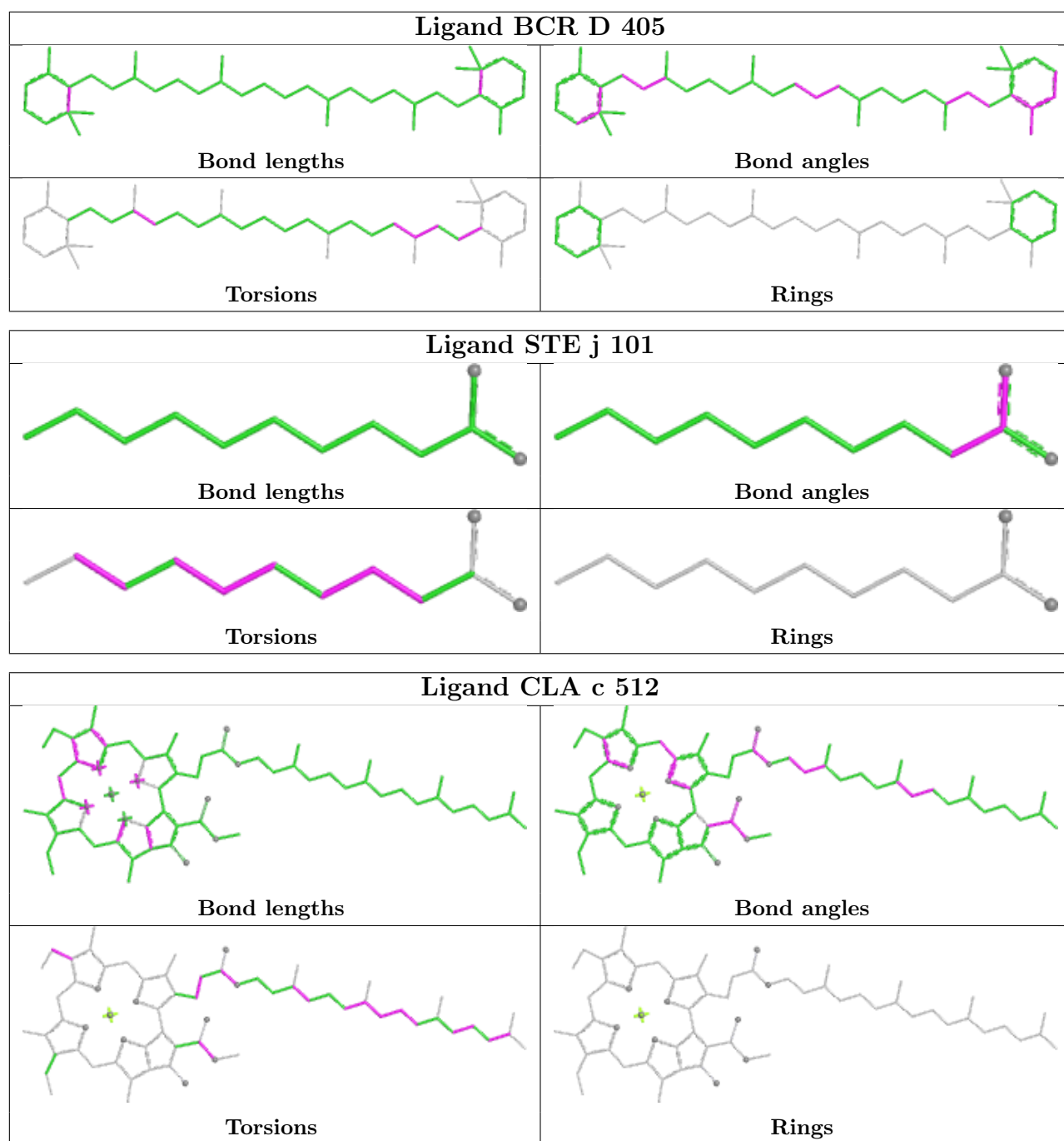


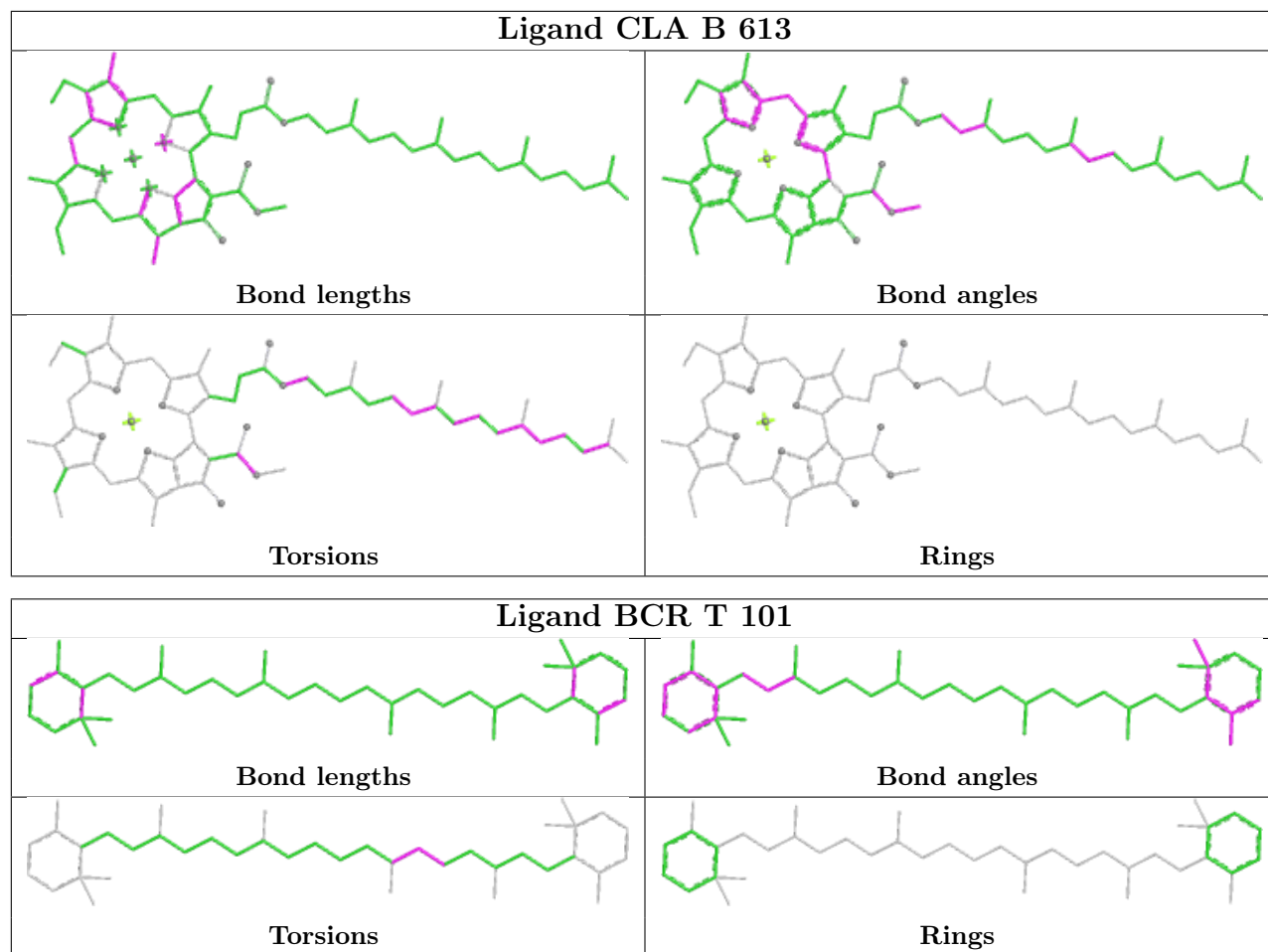
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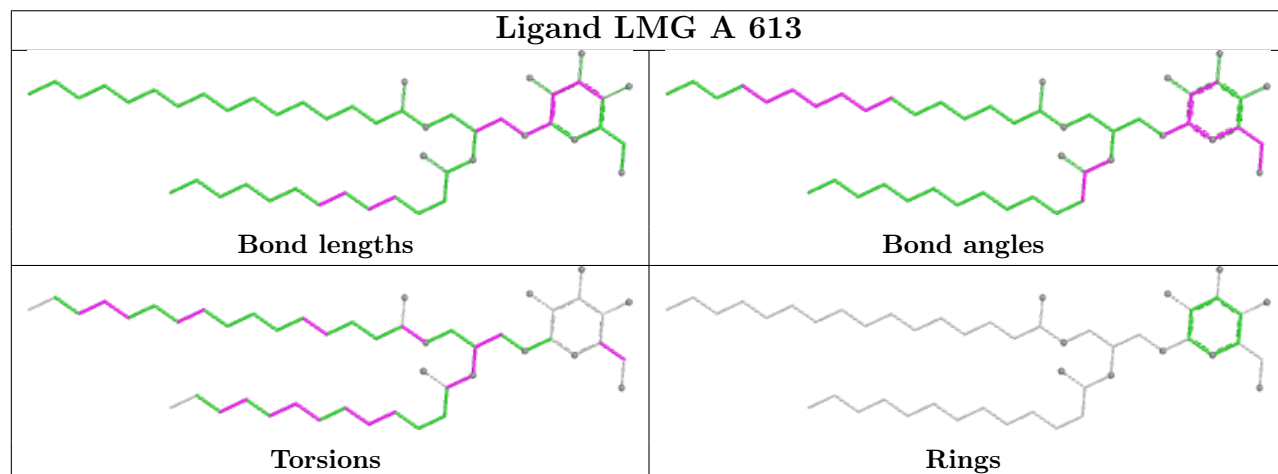
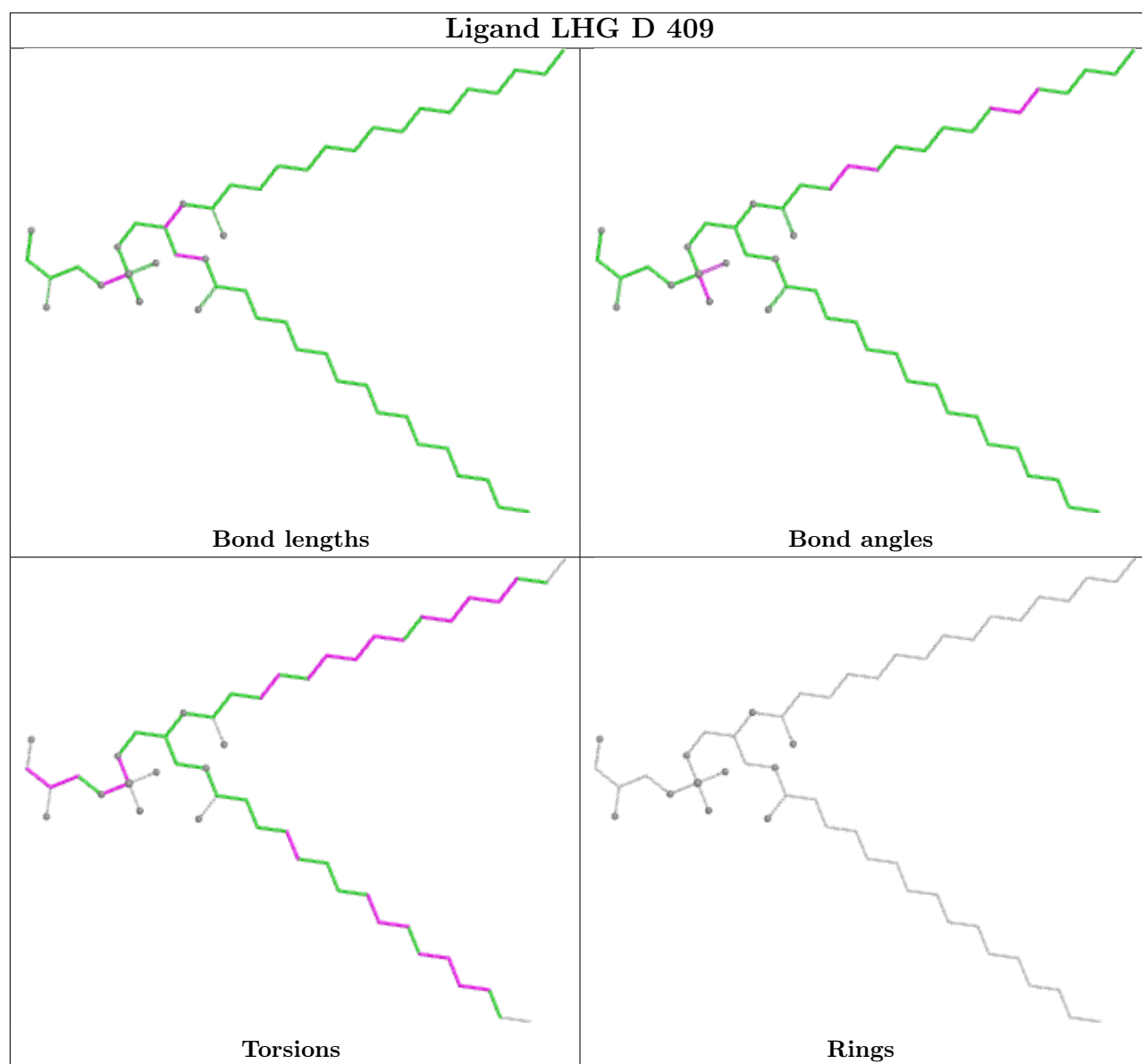


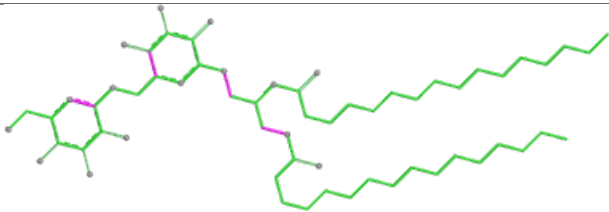
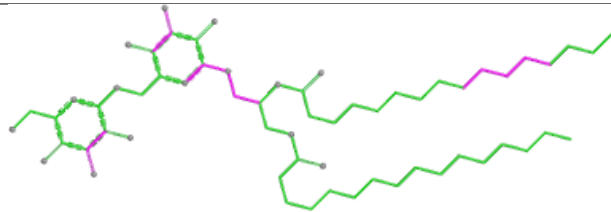
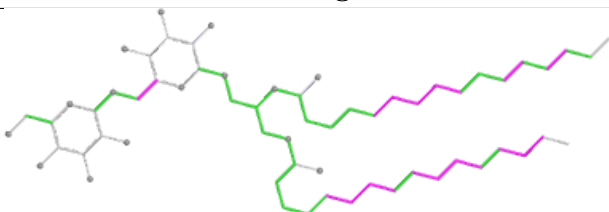
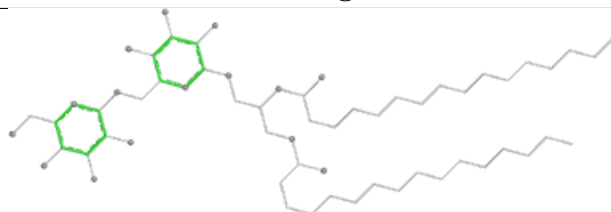
Ligand LHG L 101

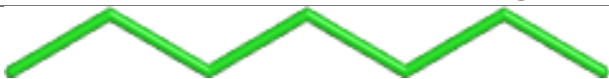
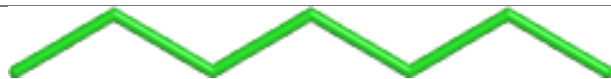
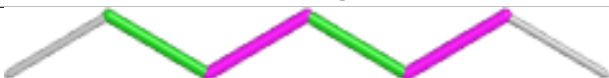




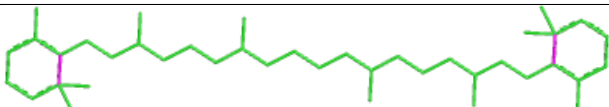
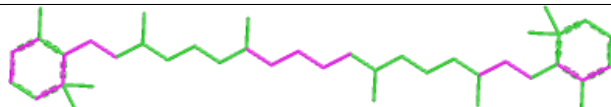
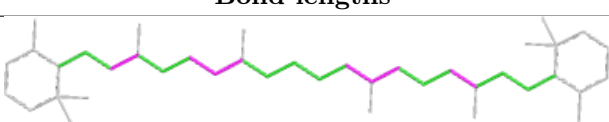
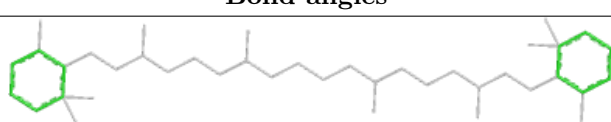


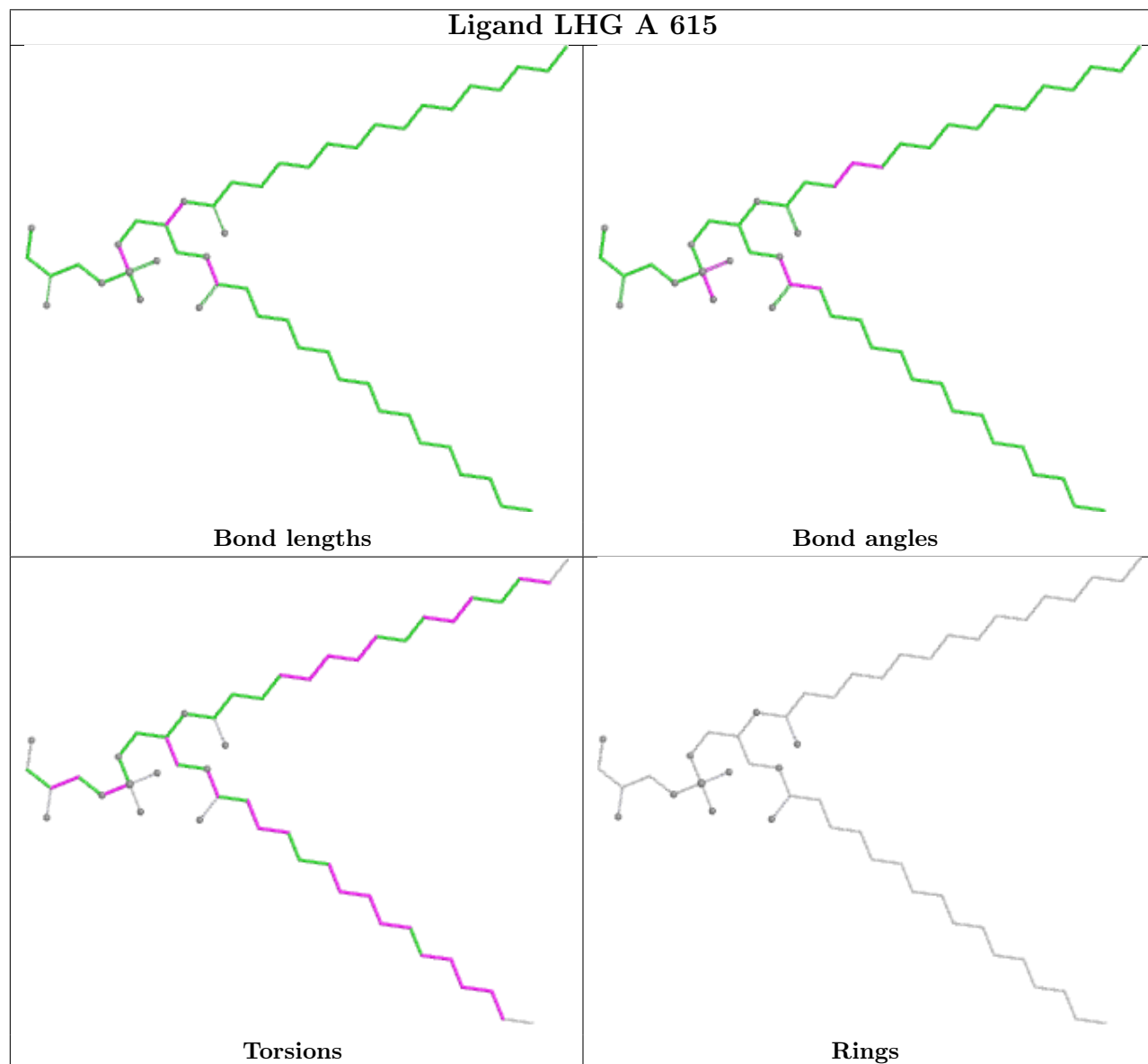
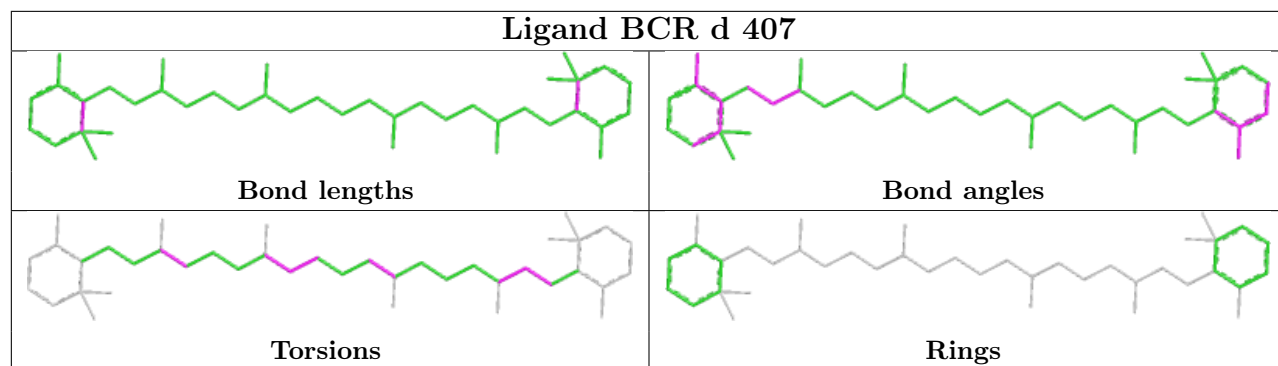


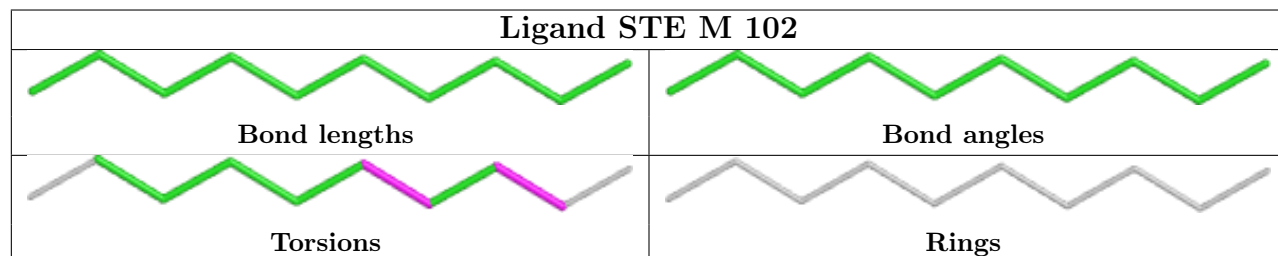
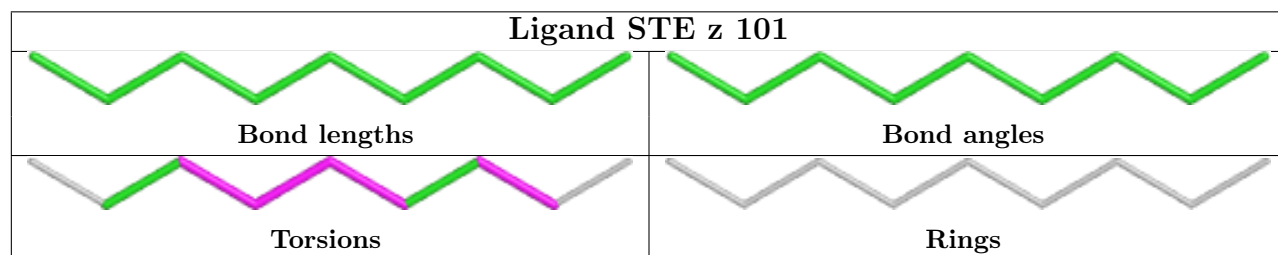
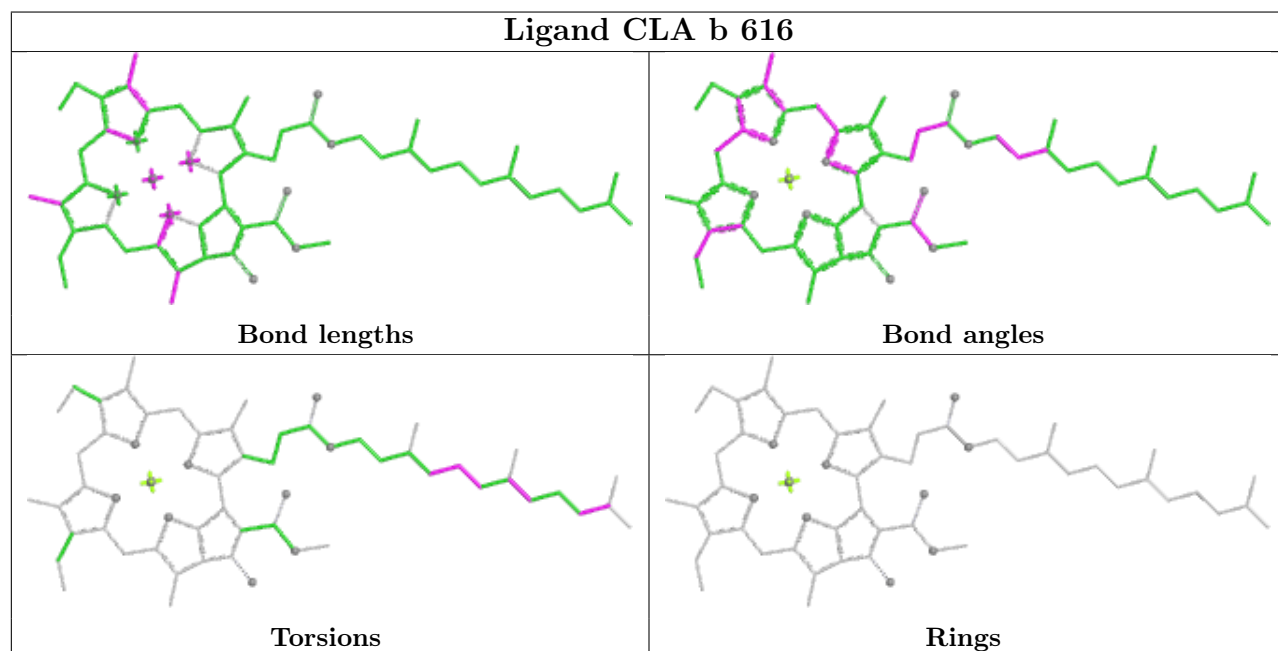
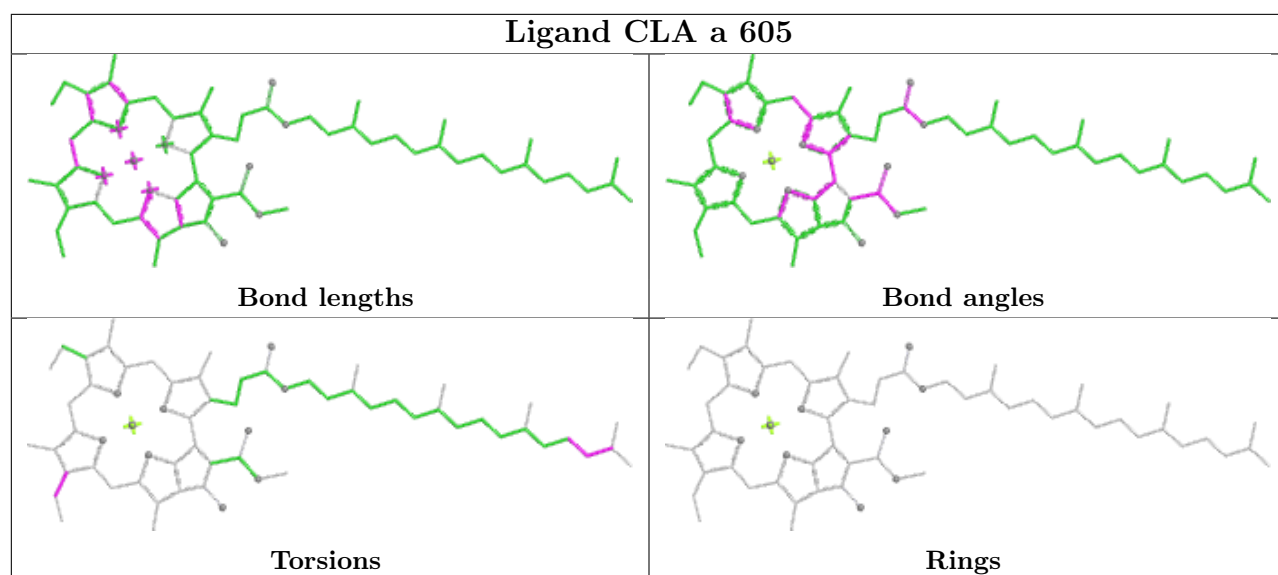
Ligand DGD C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

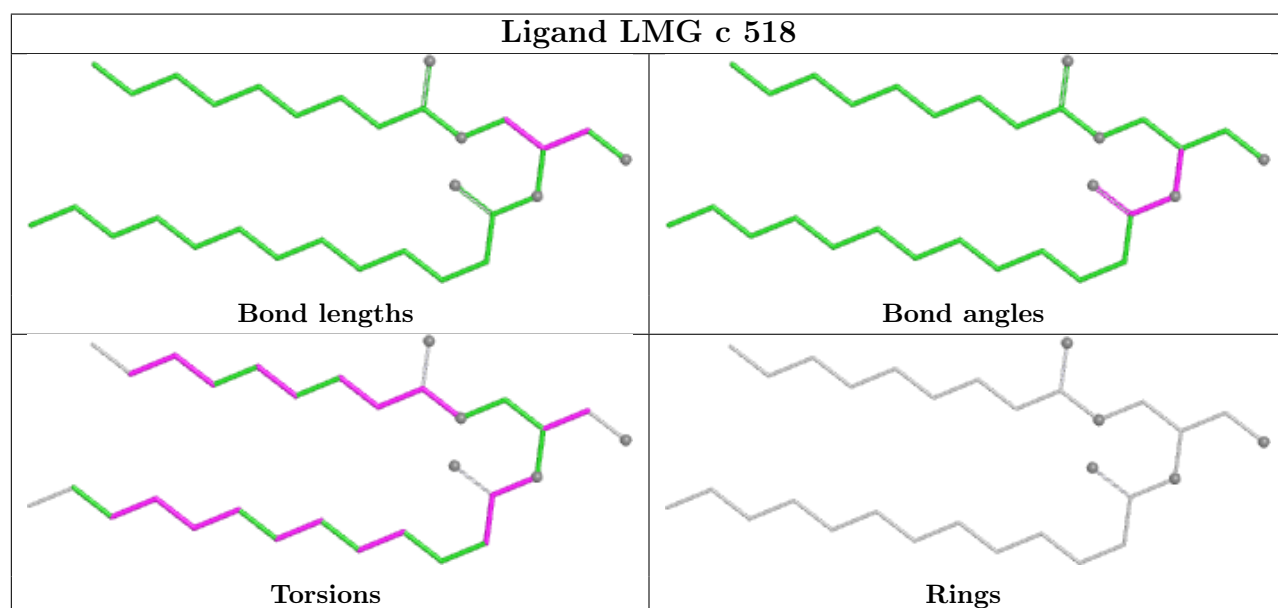
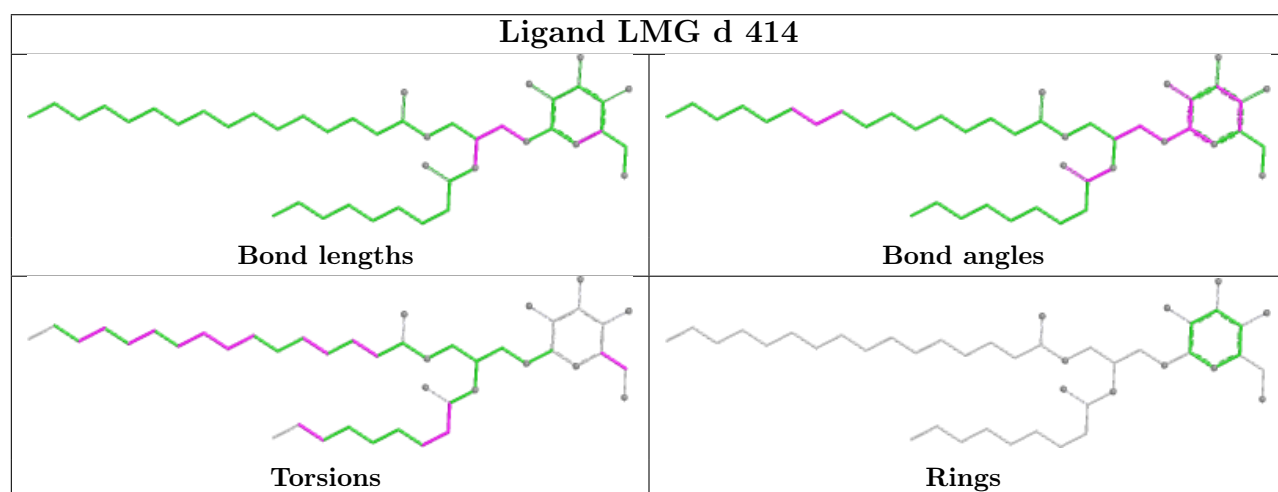
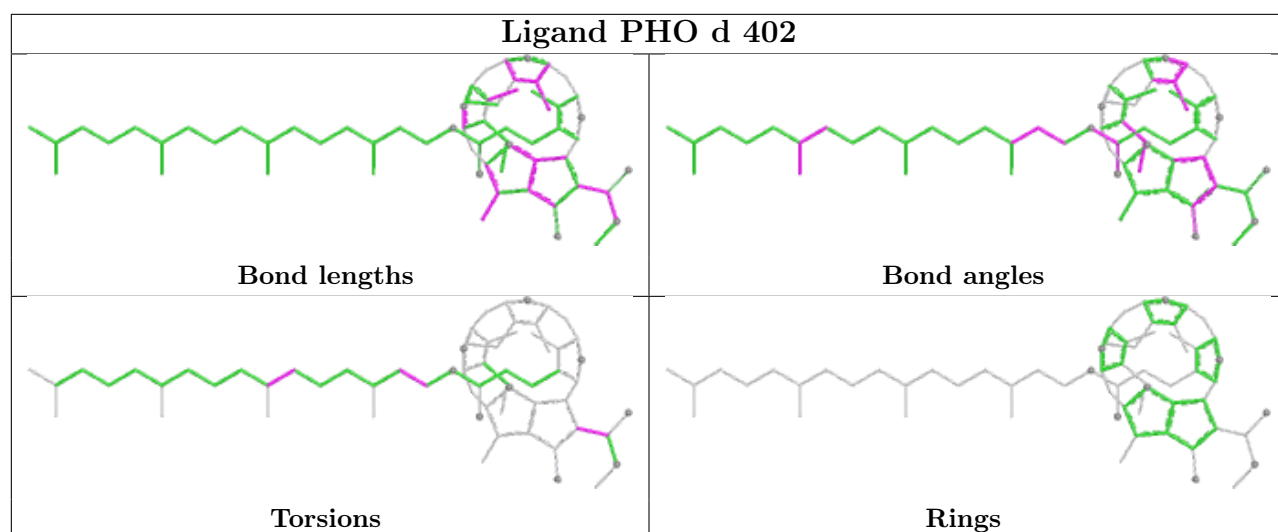
Ligand STE C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

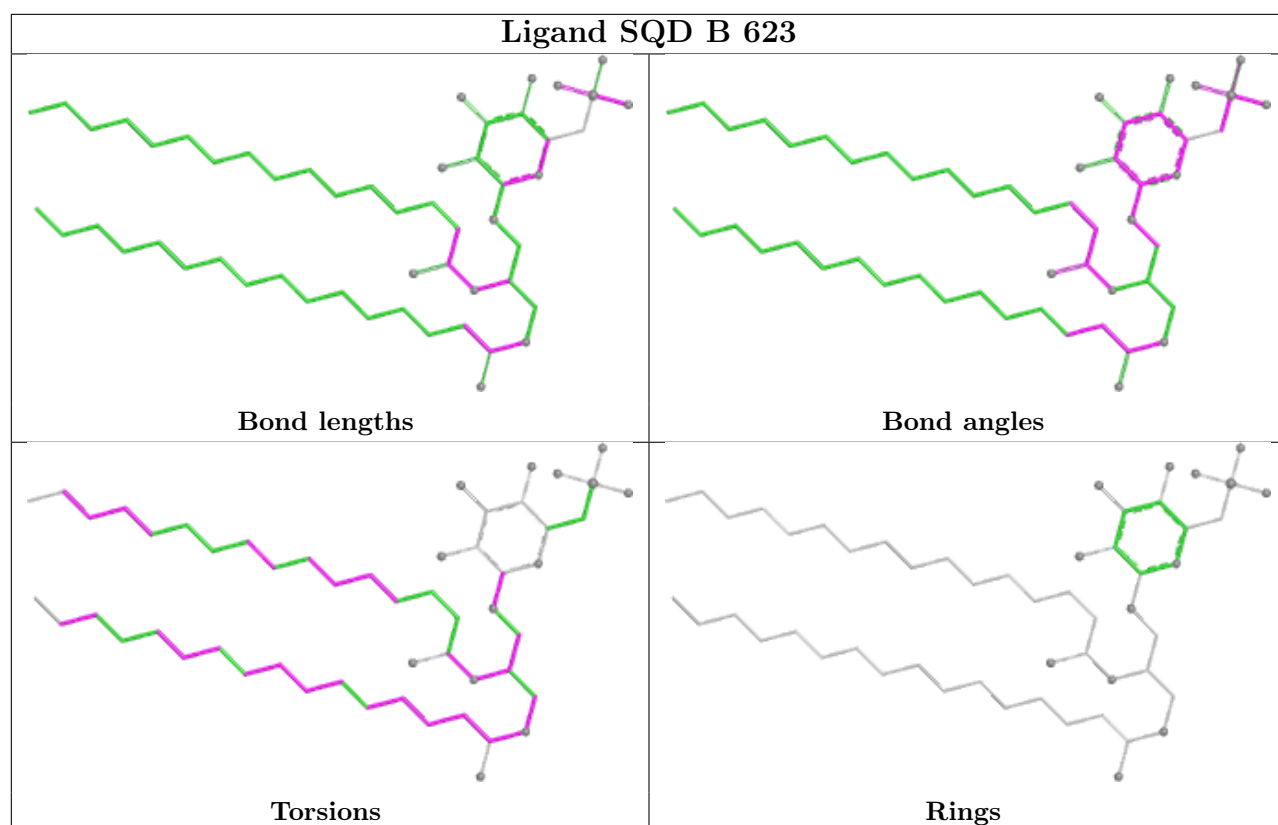
Ligand STE E 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

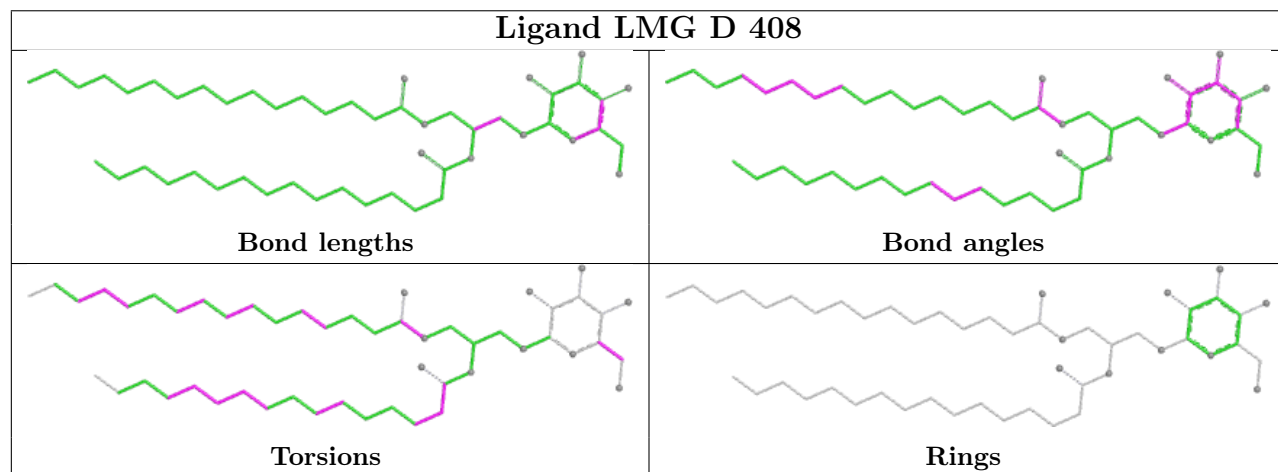
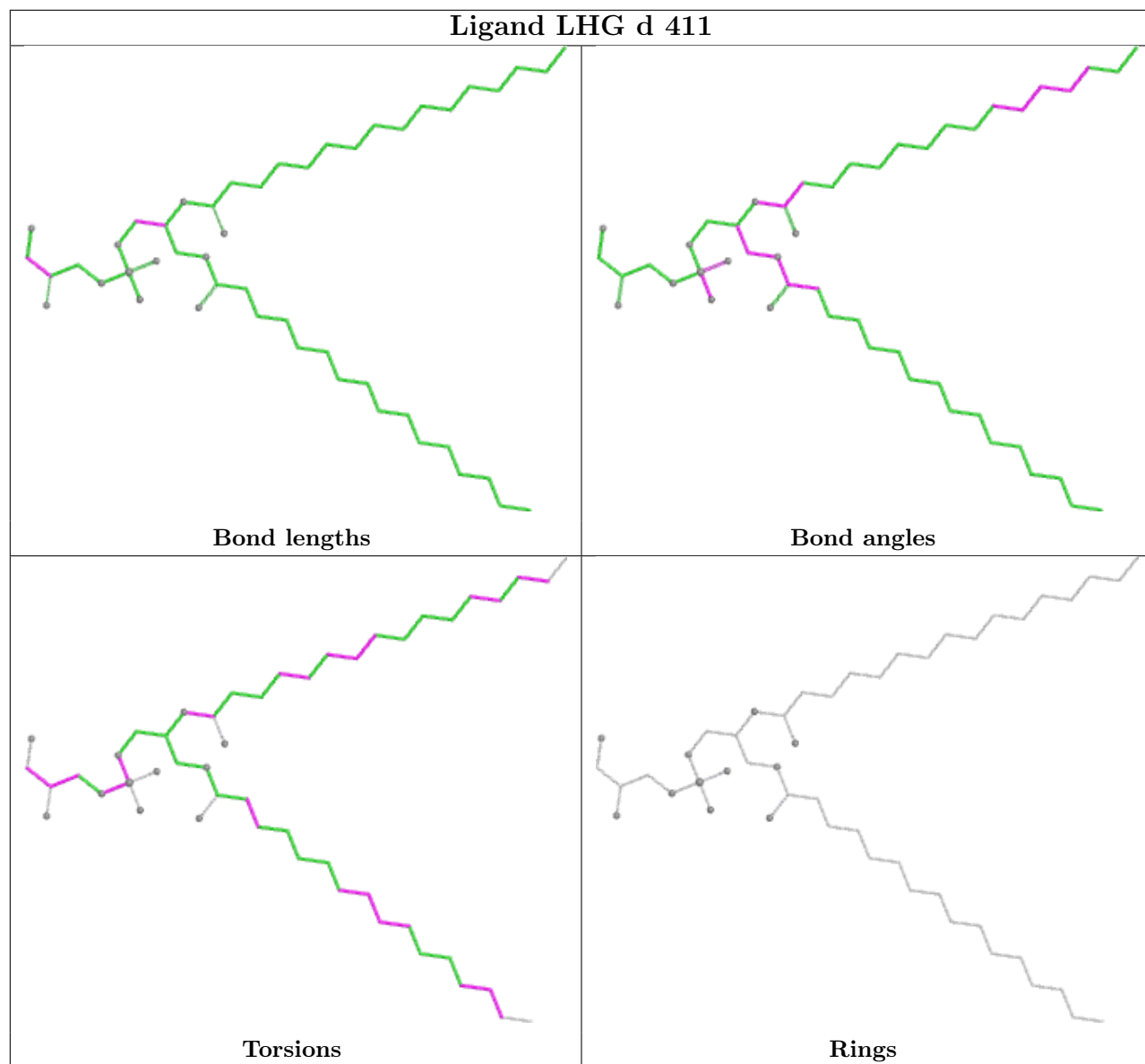
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

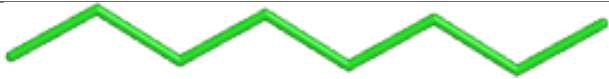
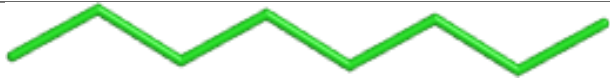


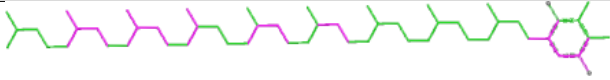
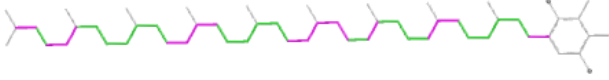
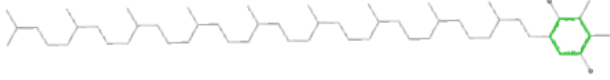


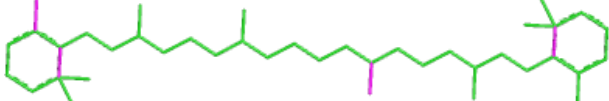
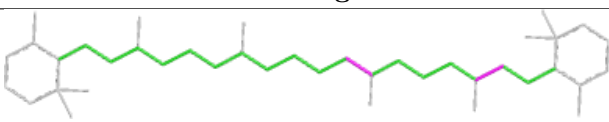
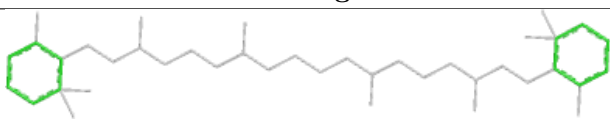


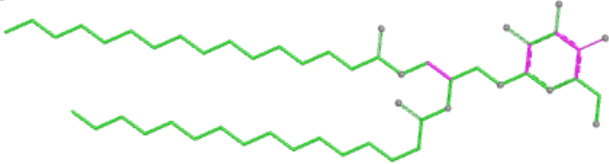
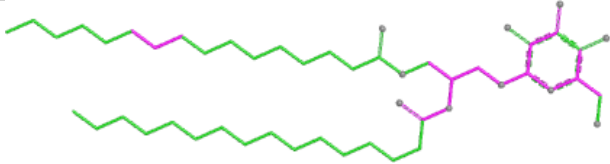
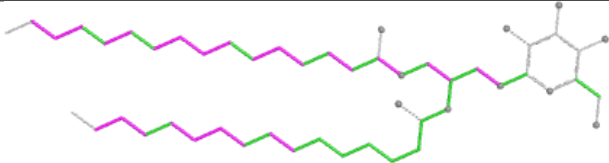
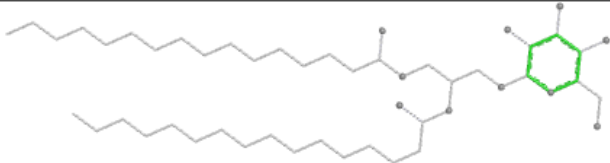




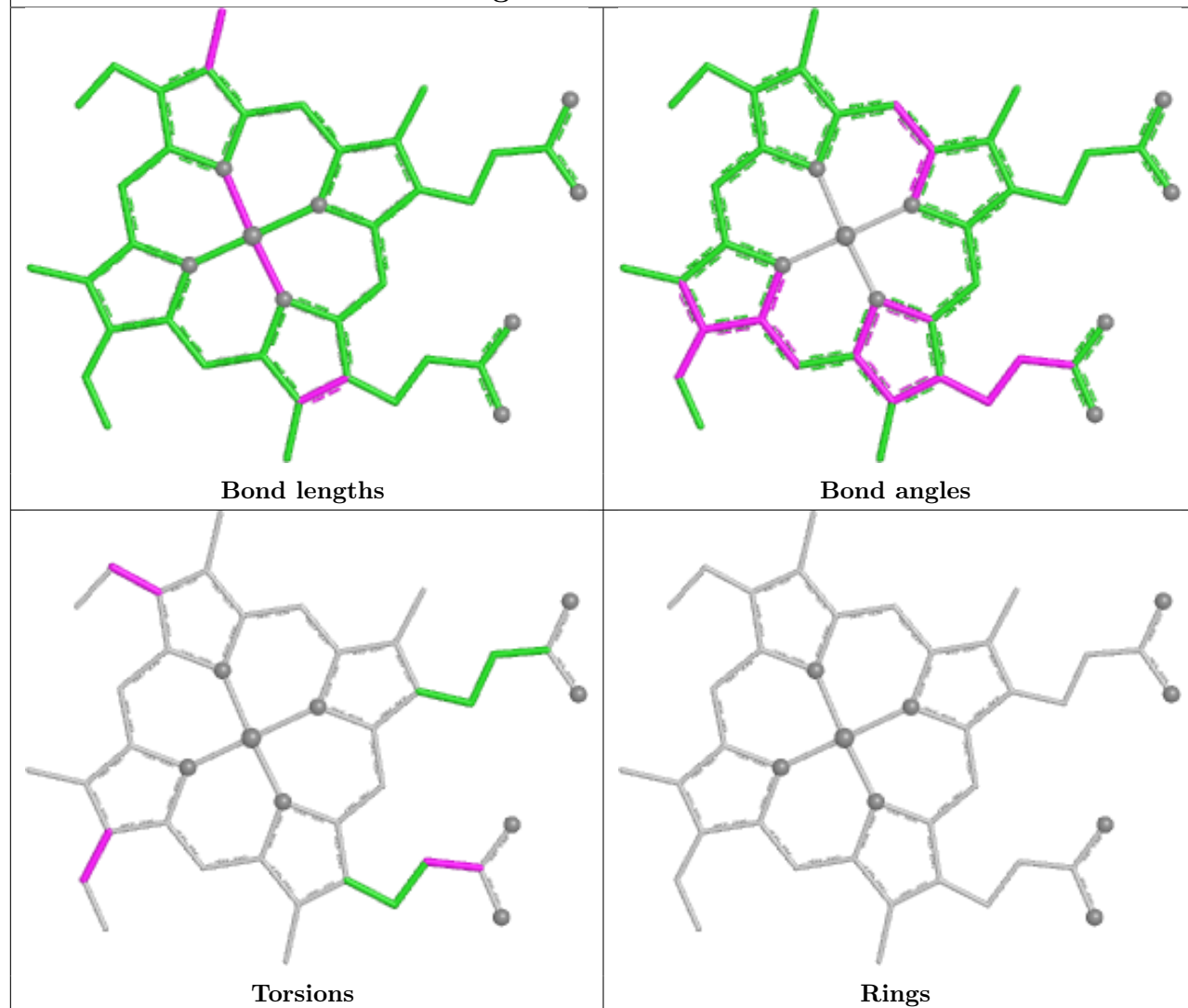
Ligand STE f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 a 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

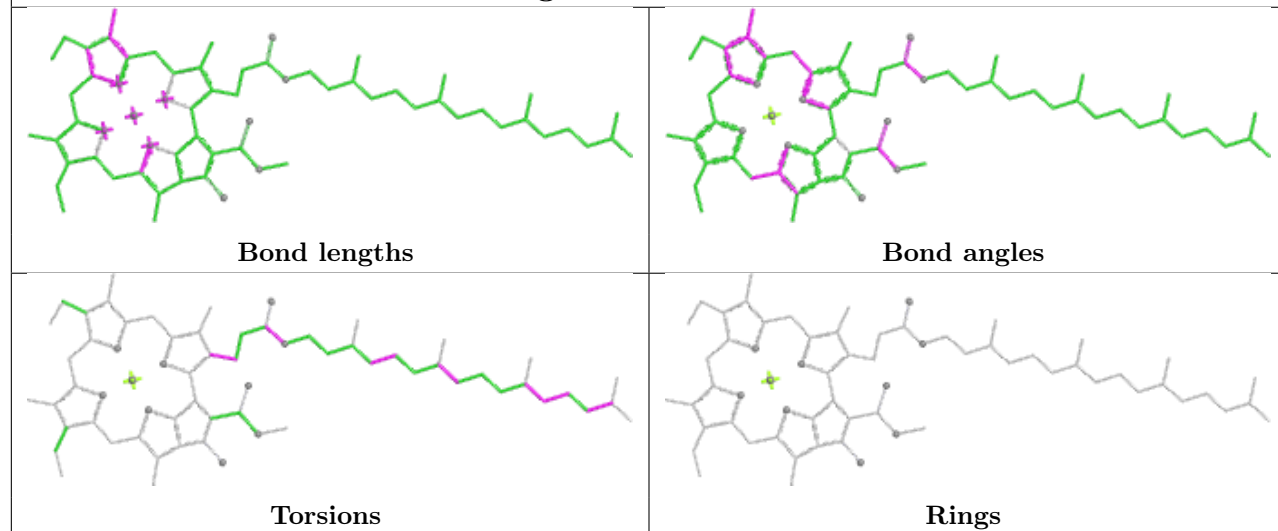
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

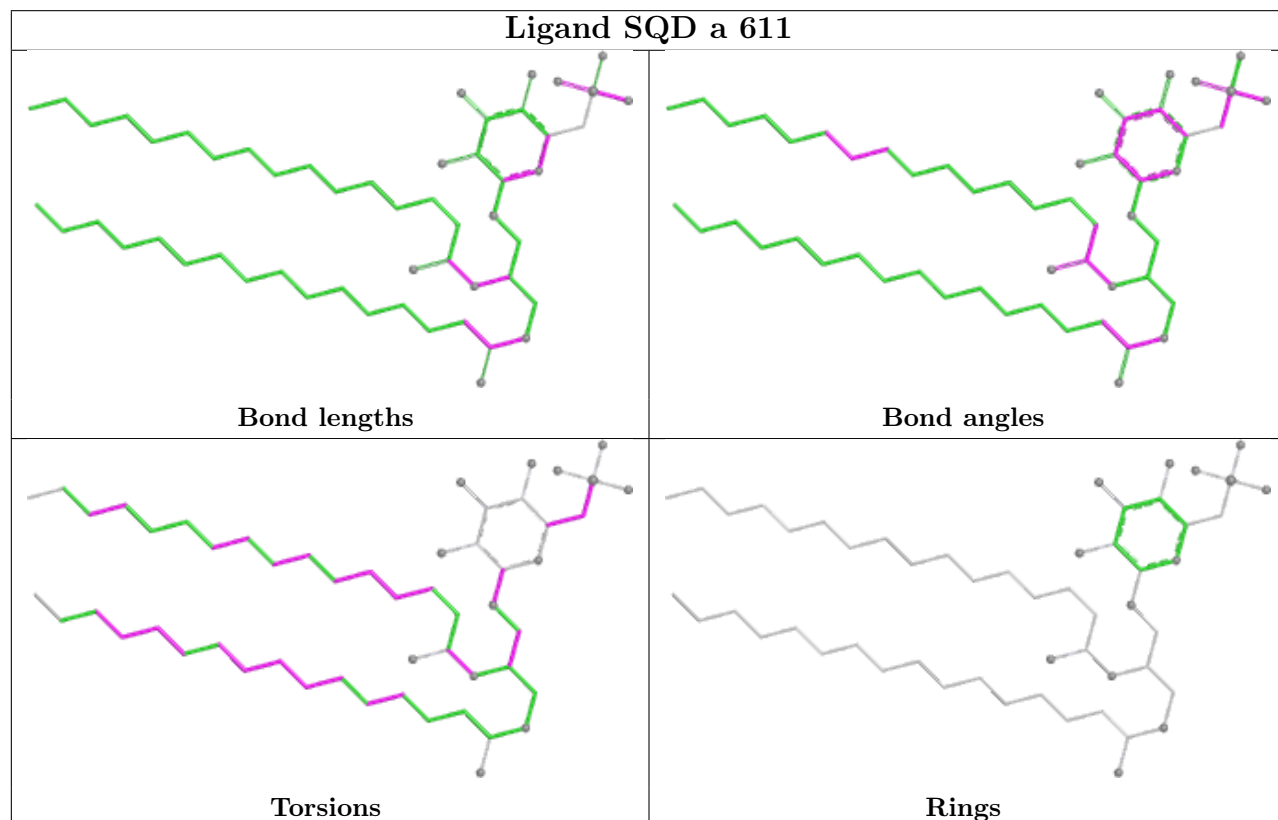
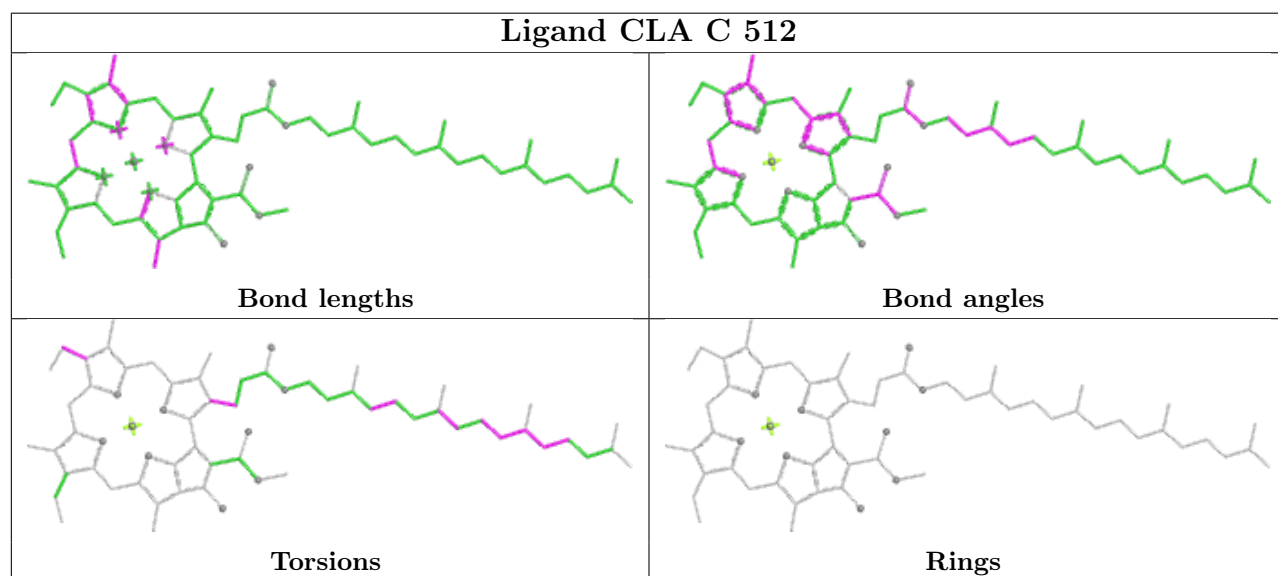
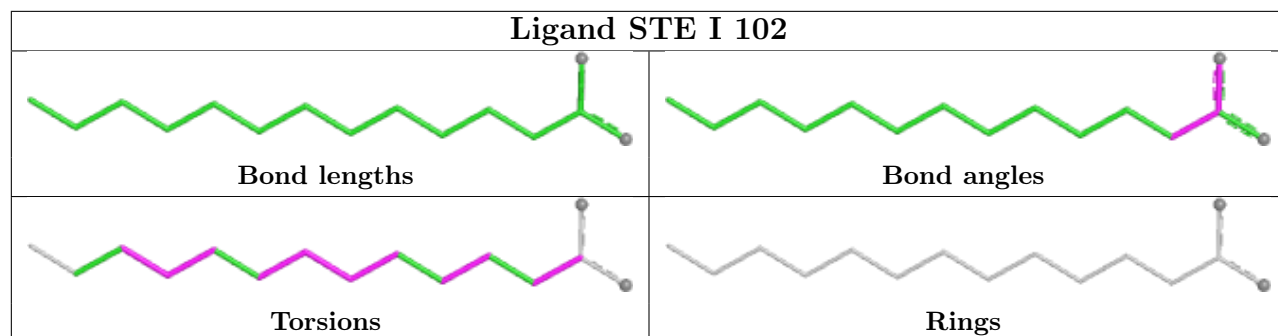
Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC V 201

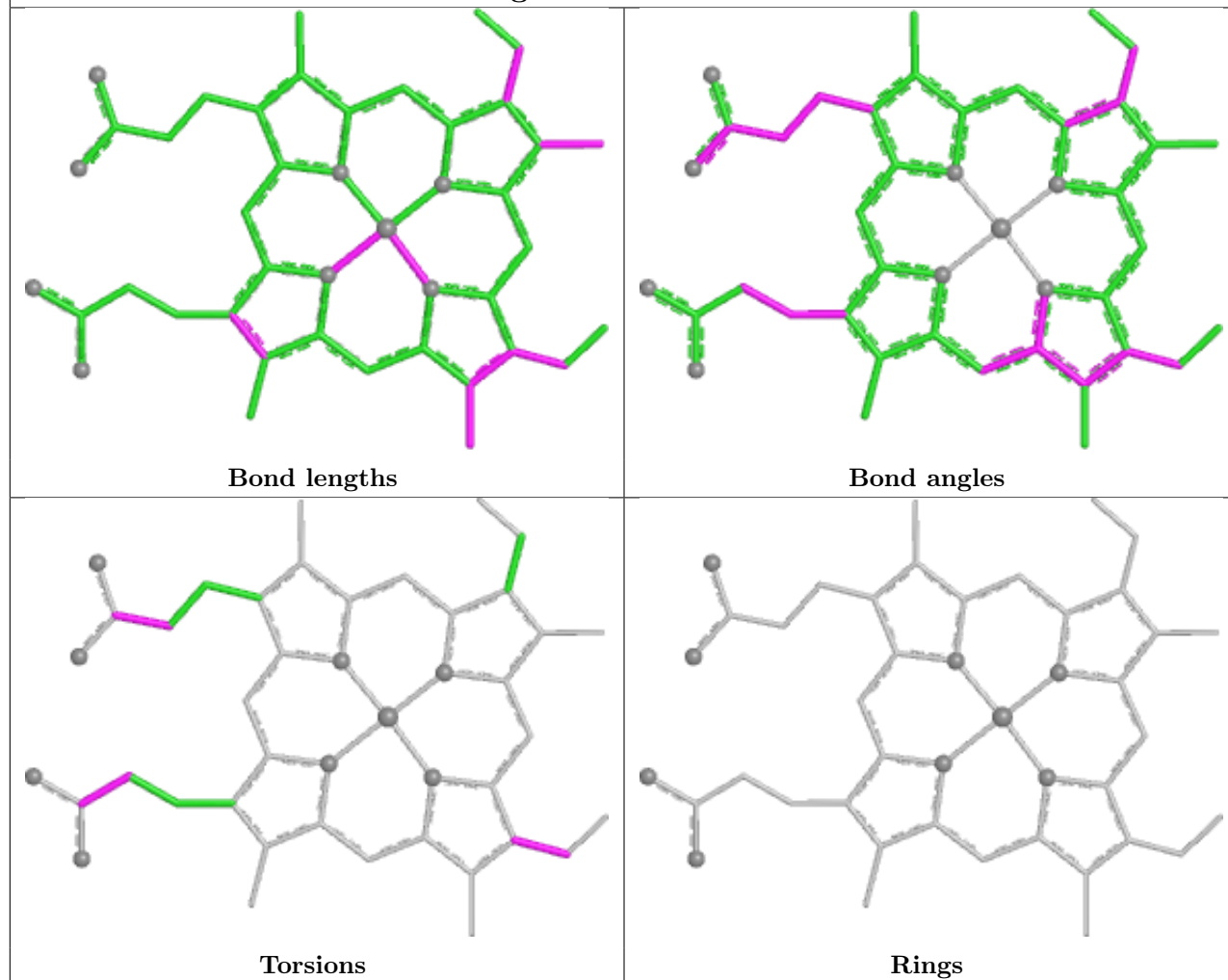


Ligand CLA c 513

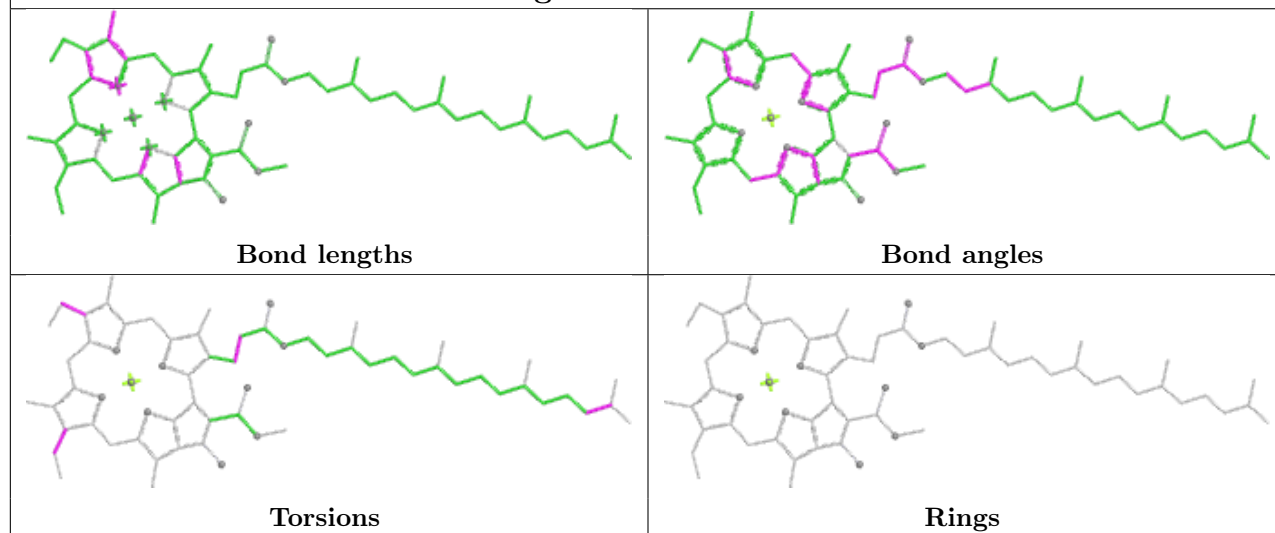


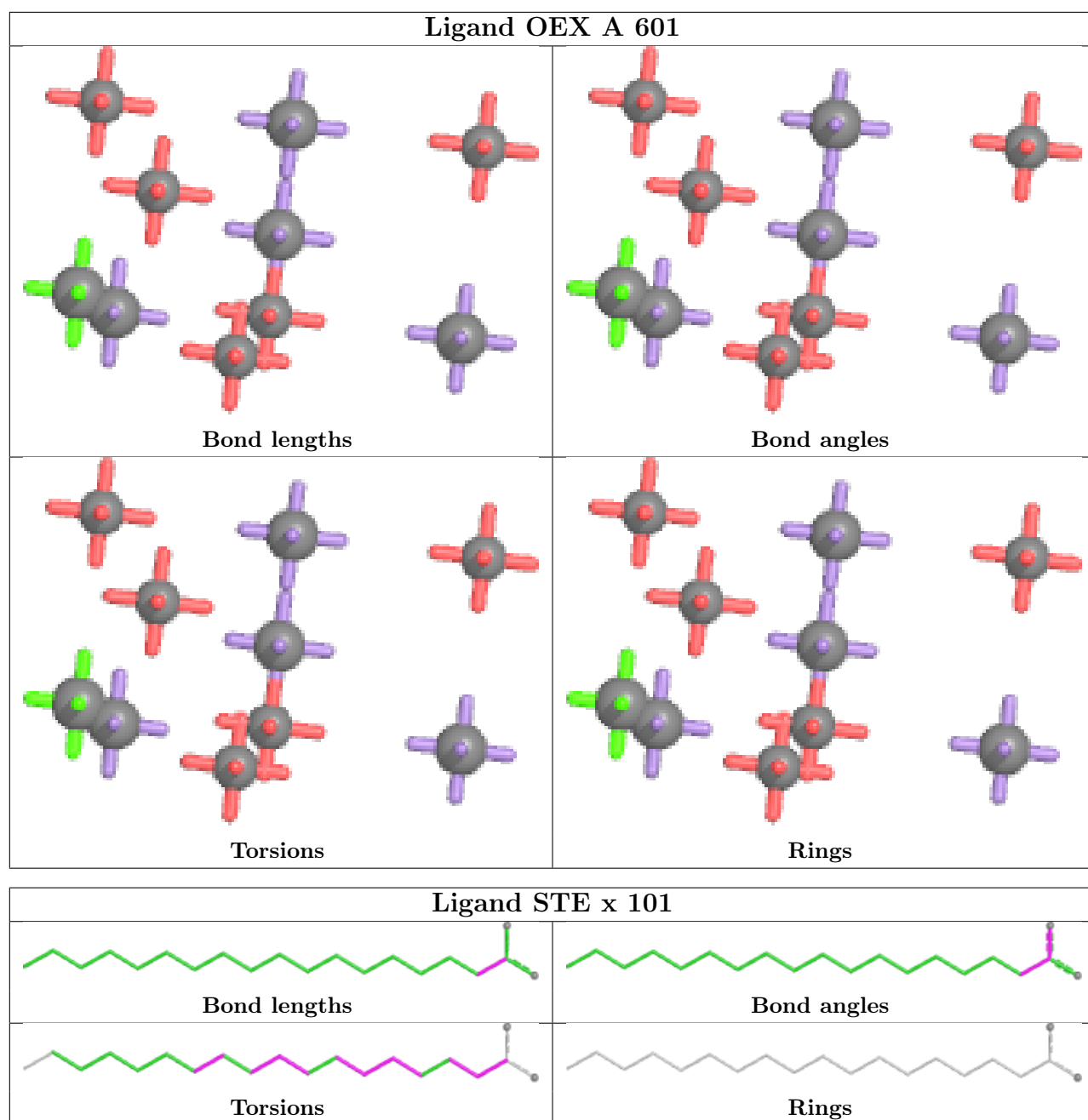


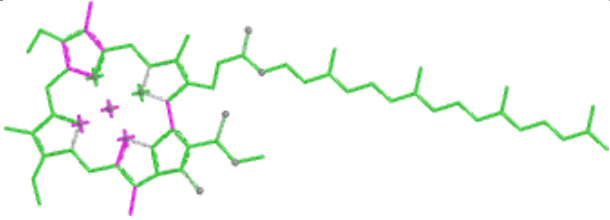
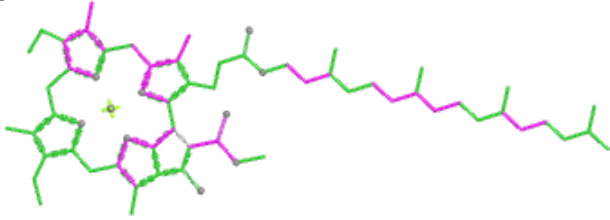
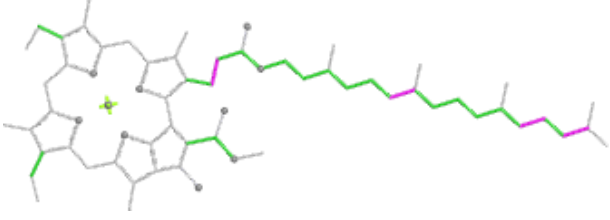
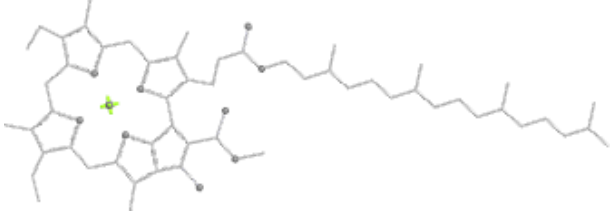
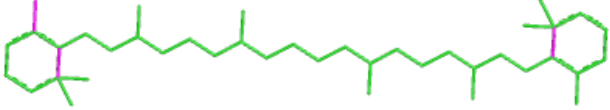
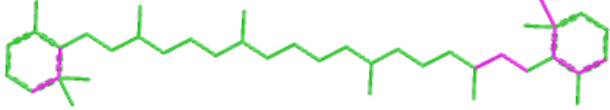
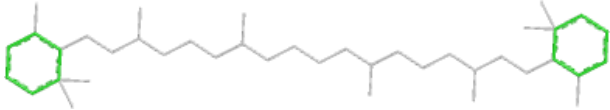
Ligand HEM e 102

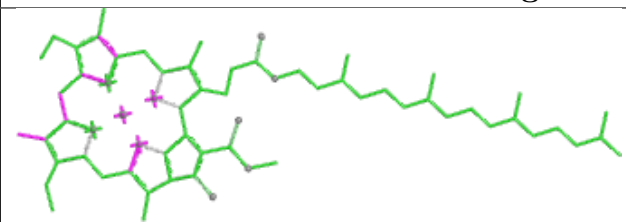
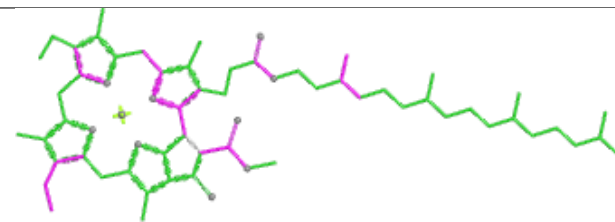
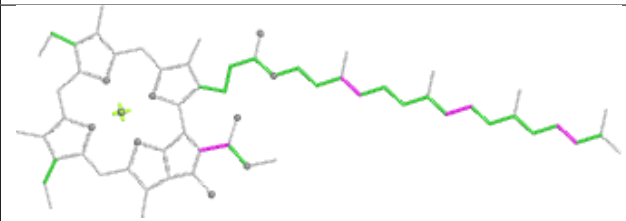
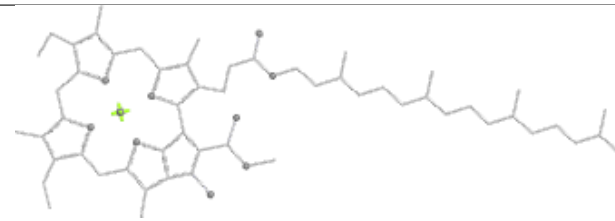


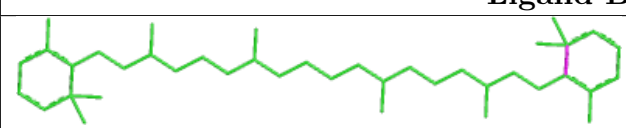
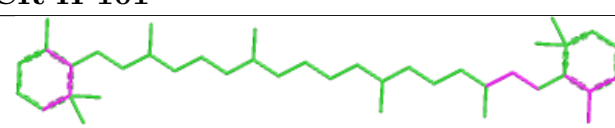
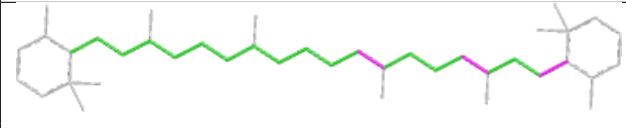
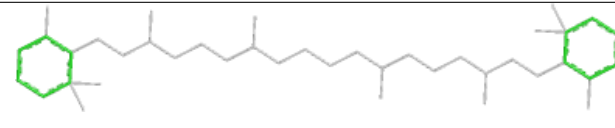
Ligand CLA b 610



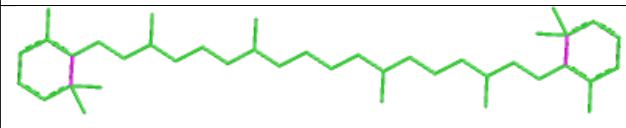
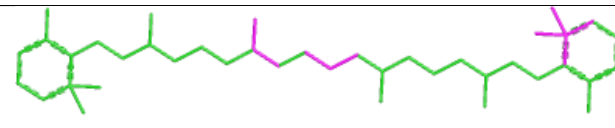
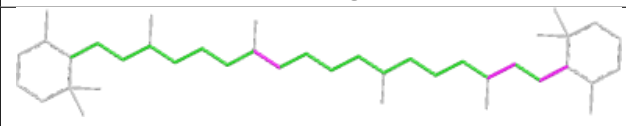
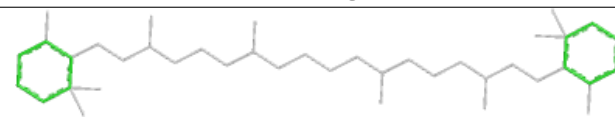


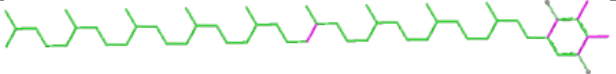
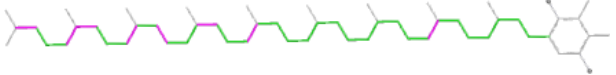
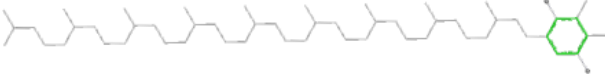
Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

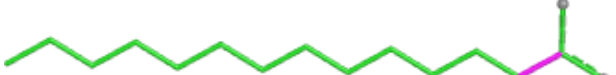
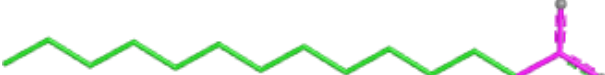
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

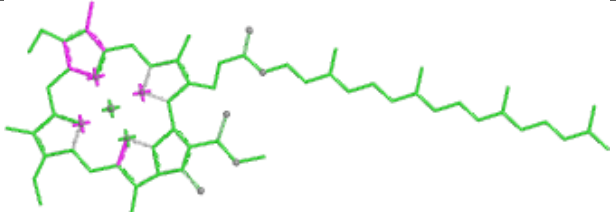
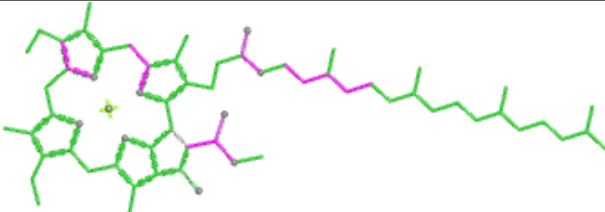
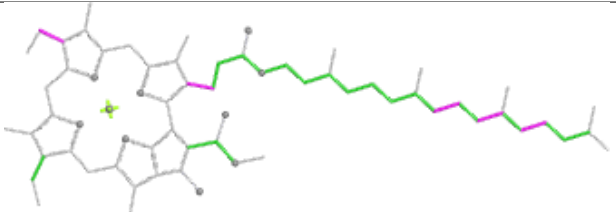
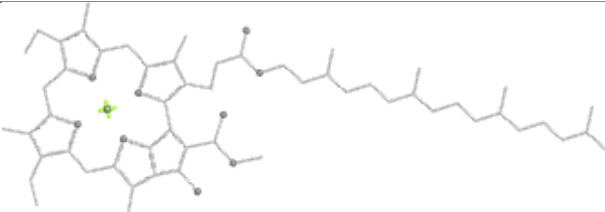
Ligand STE c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

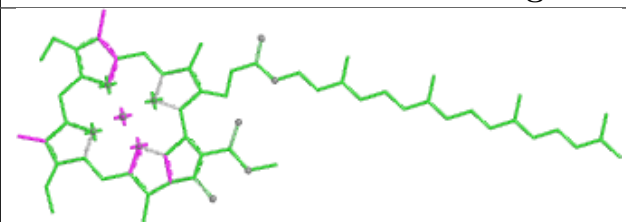
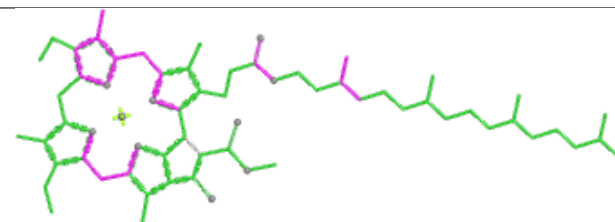
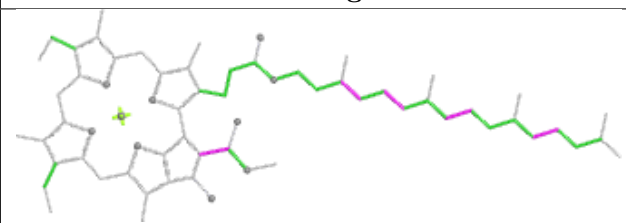
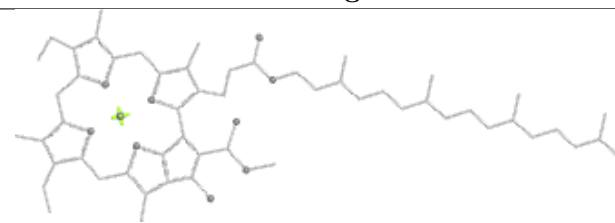
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

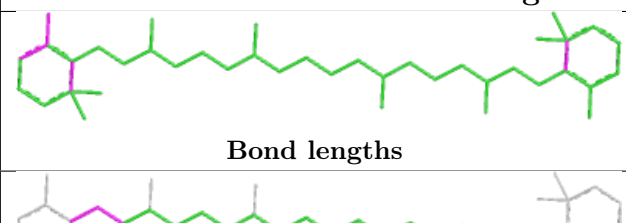
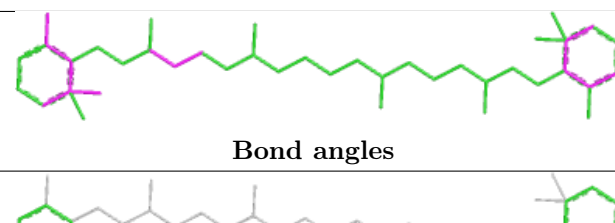
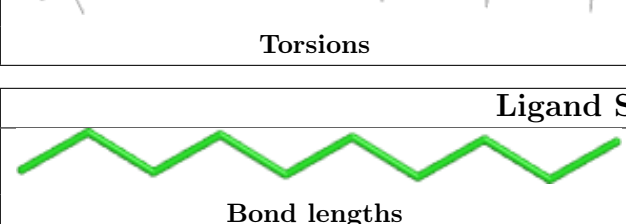
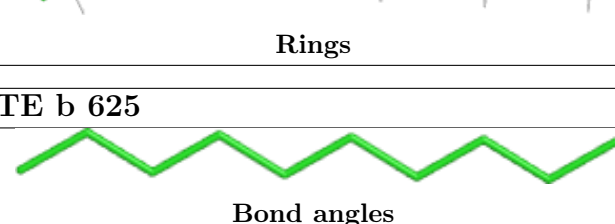
Ligand PL9 d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

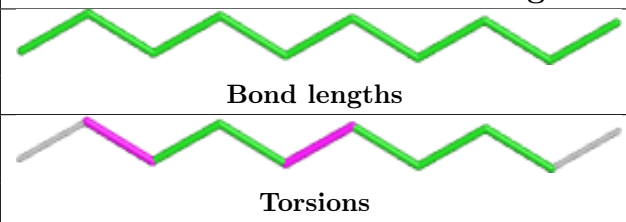
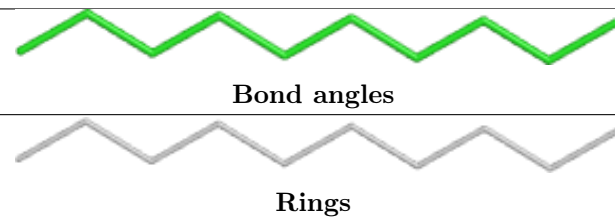
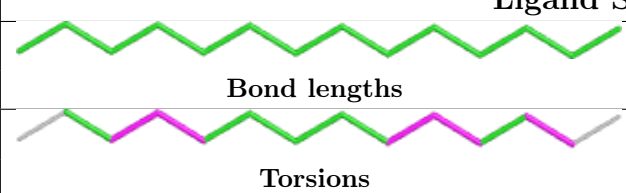
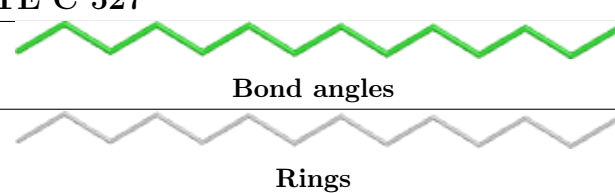
Ligand STE b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

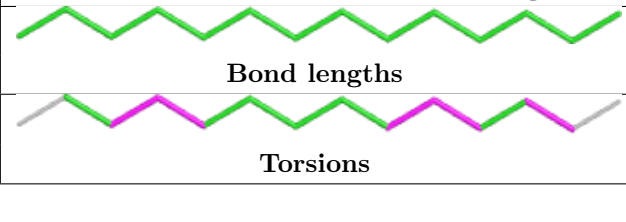
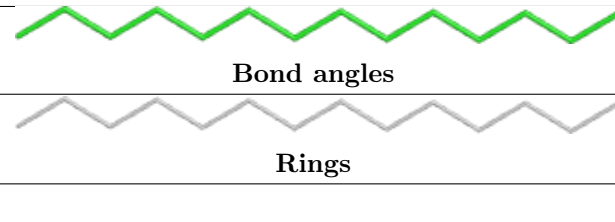
Ligand STE A 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

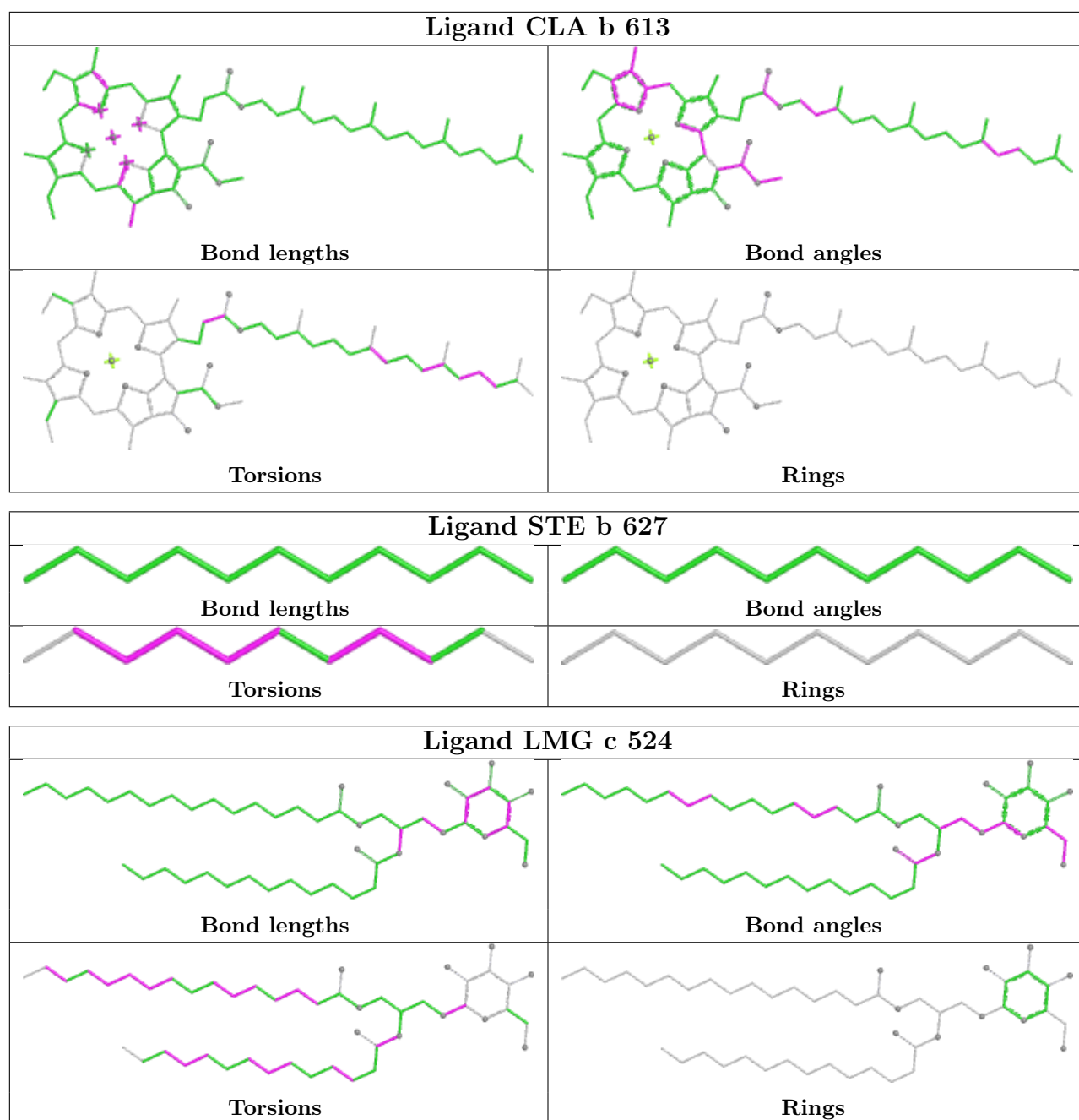
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

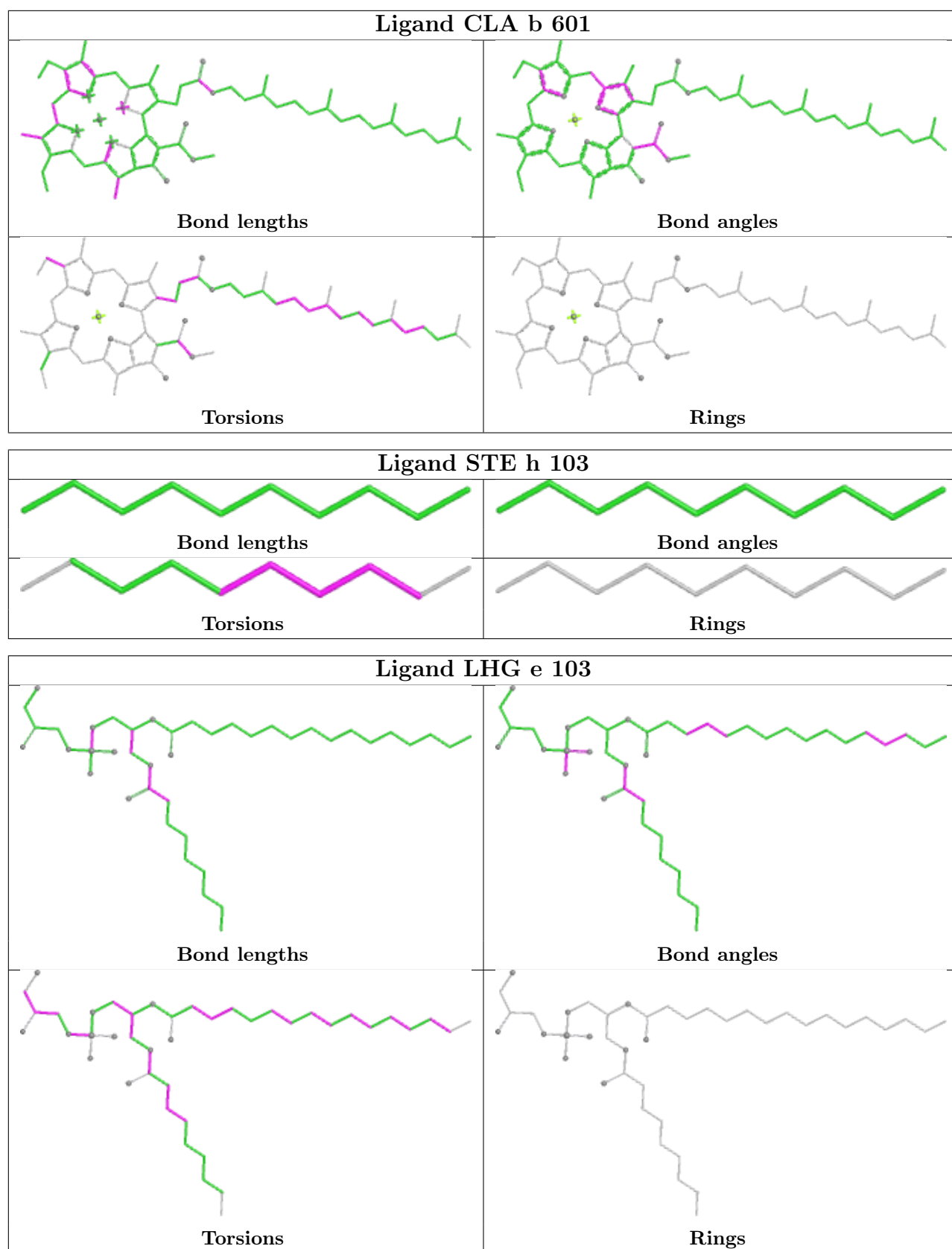
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

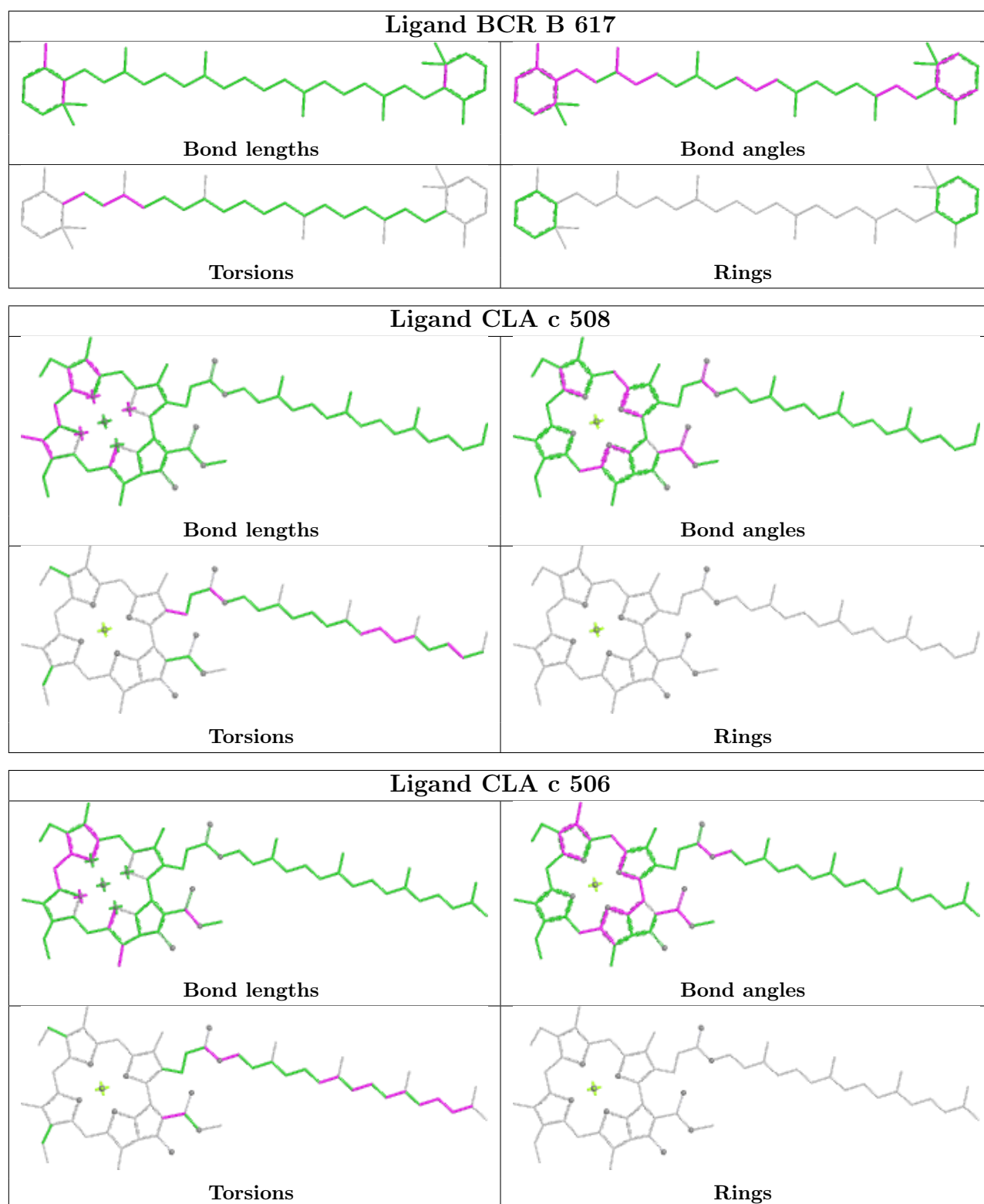
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

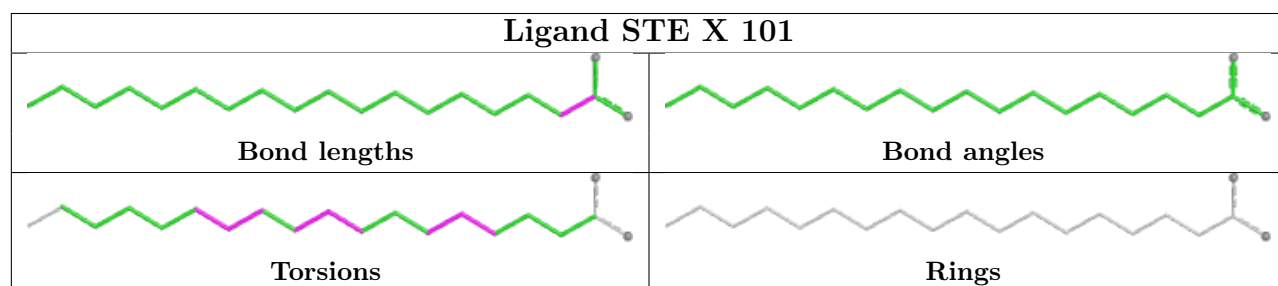
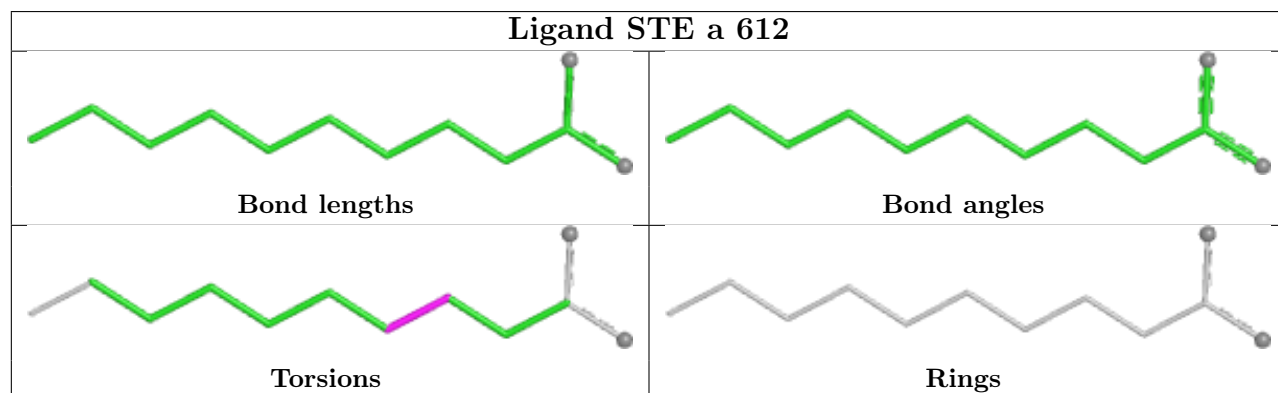
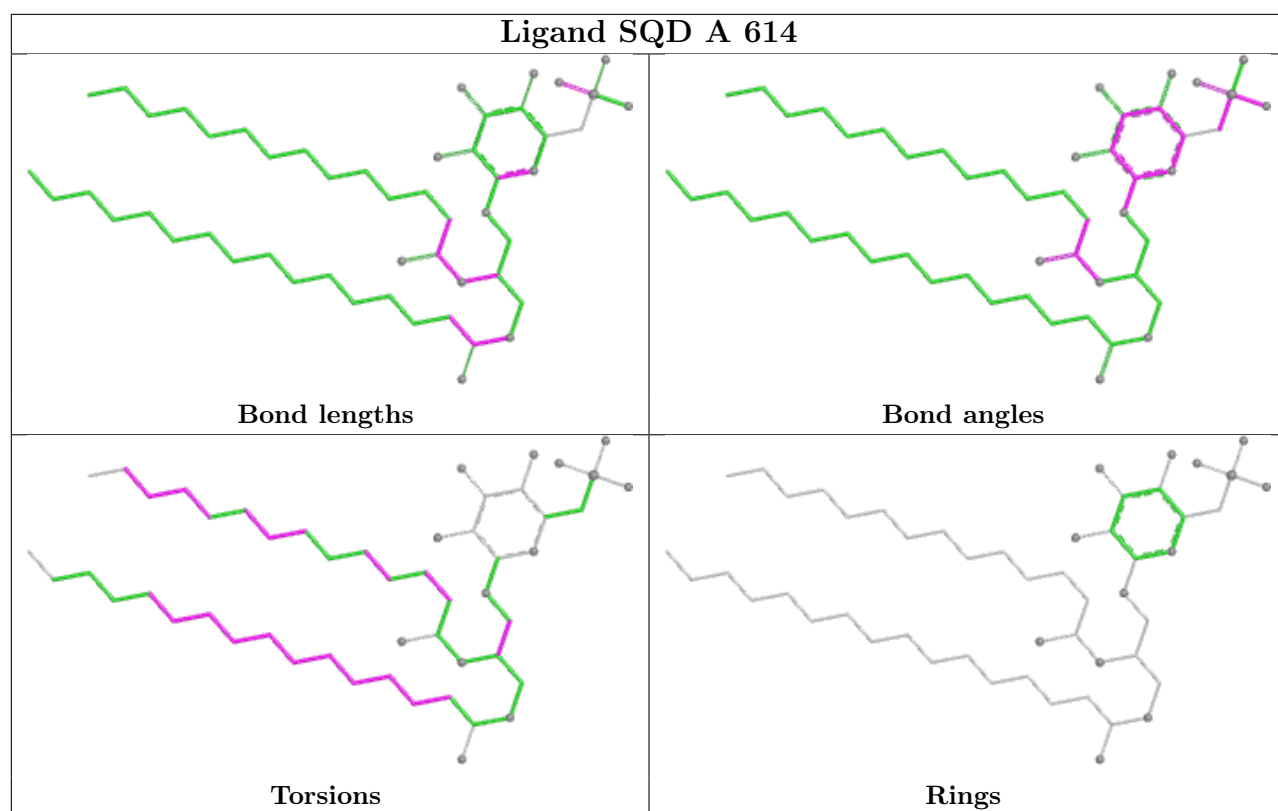
Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

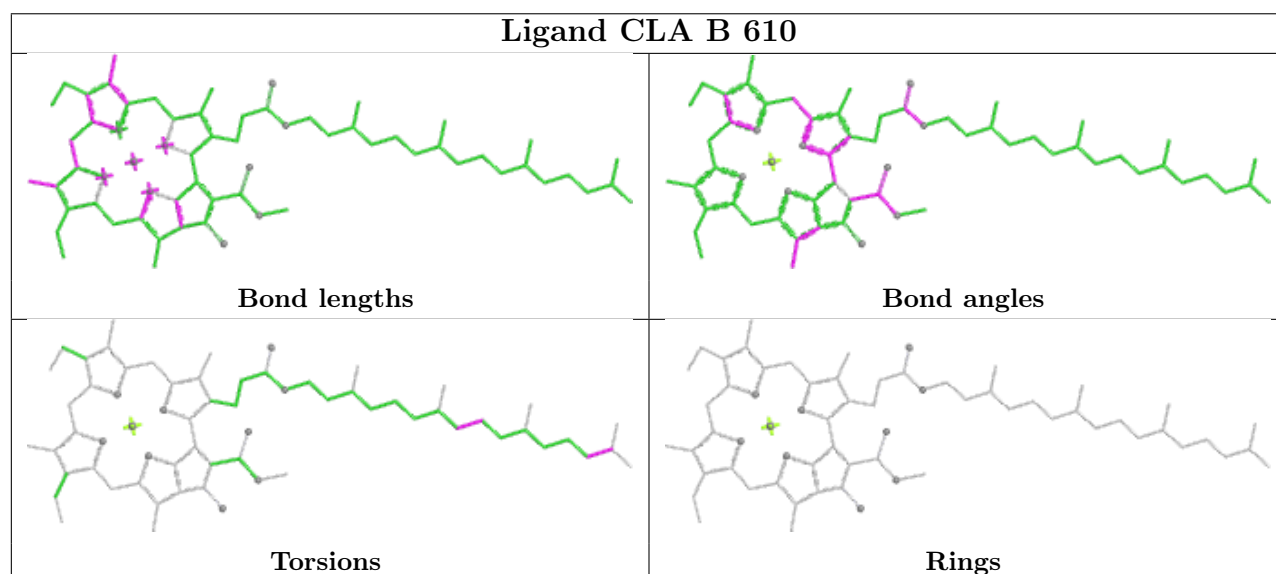
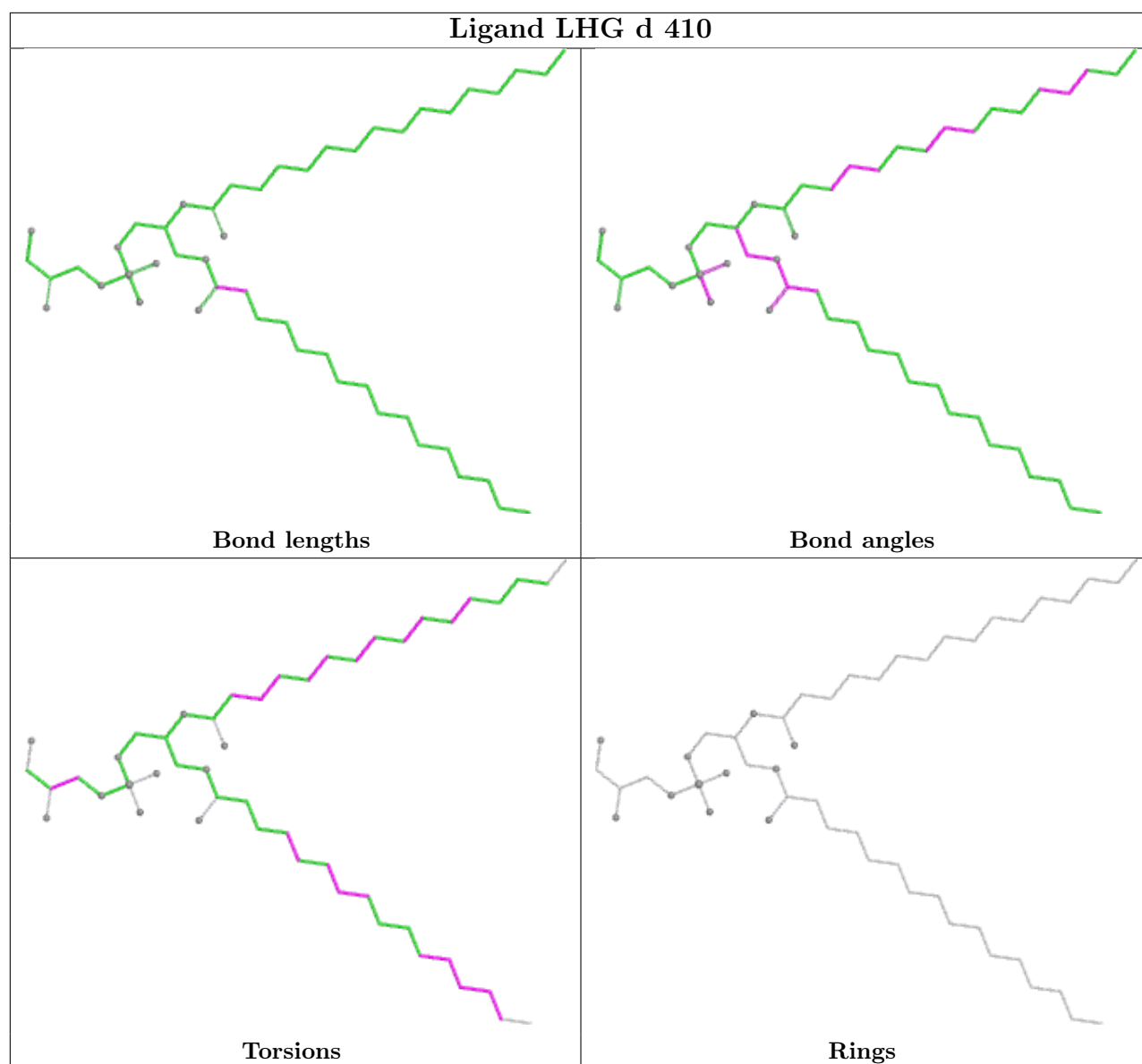
Ligand STE C 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

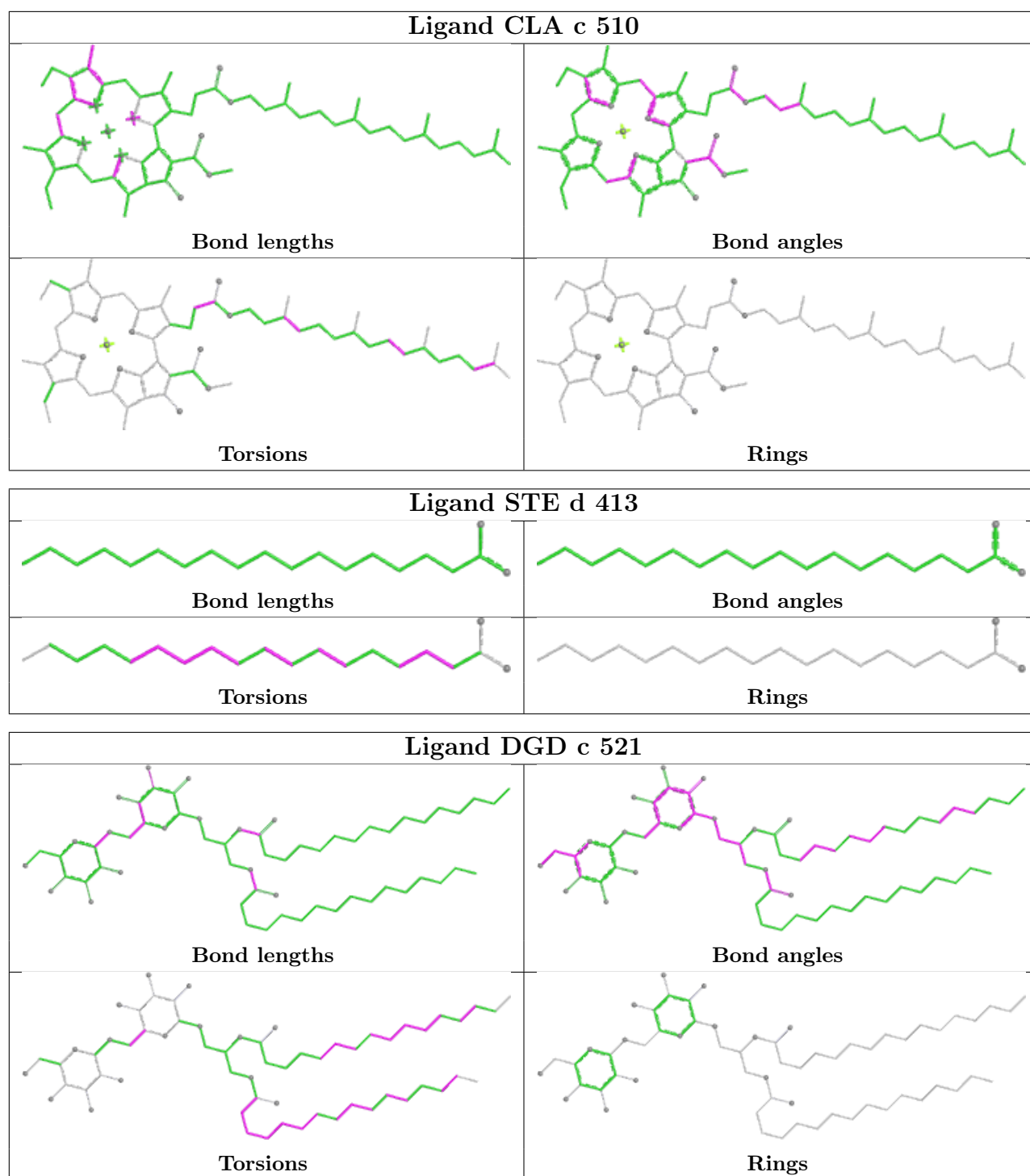


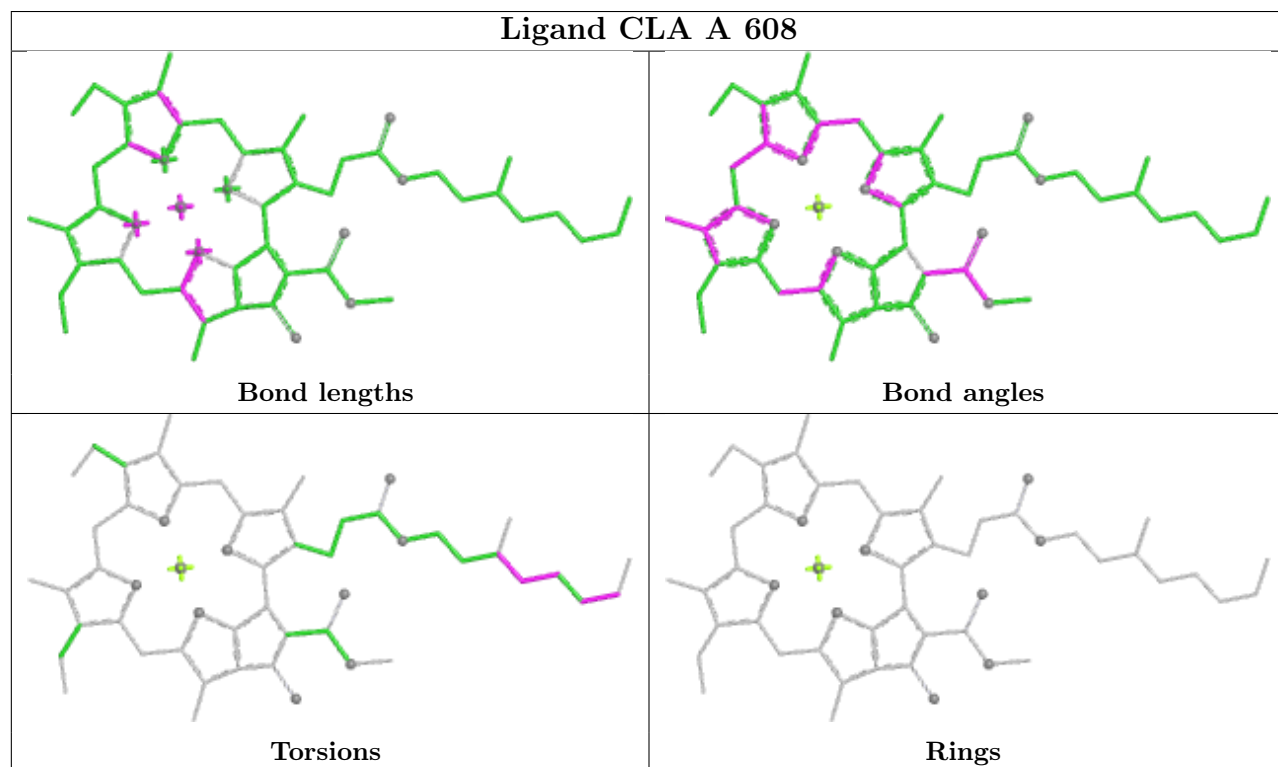
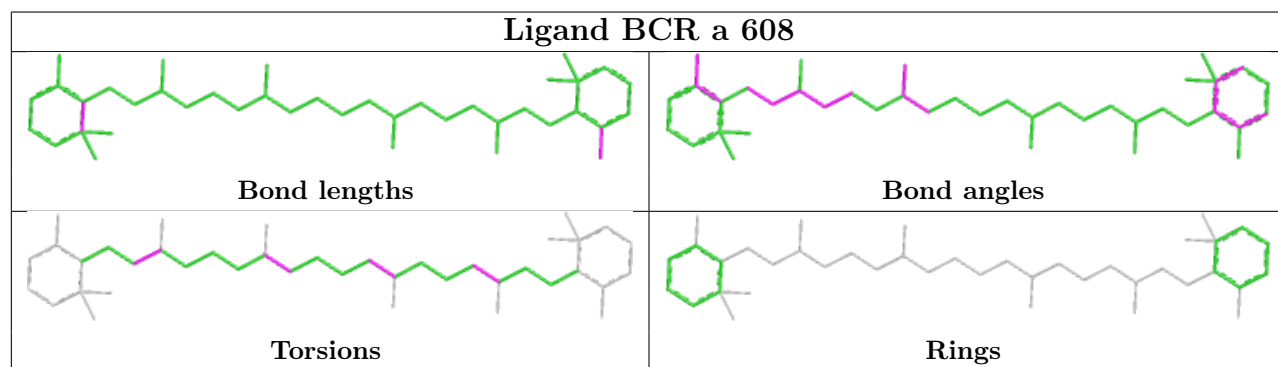
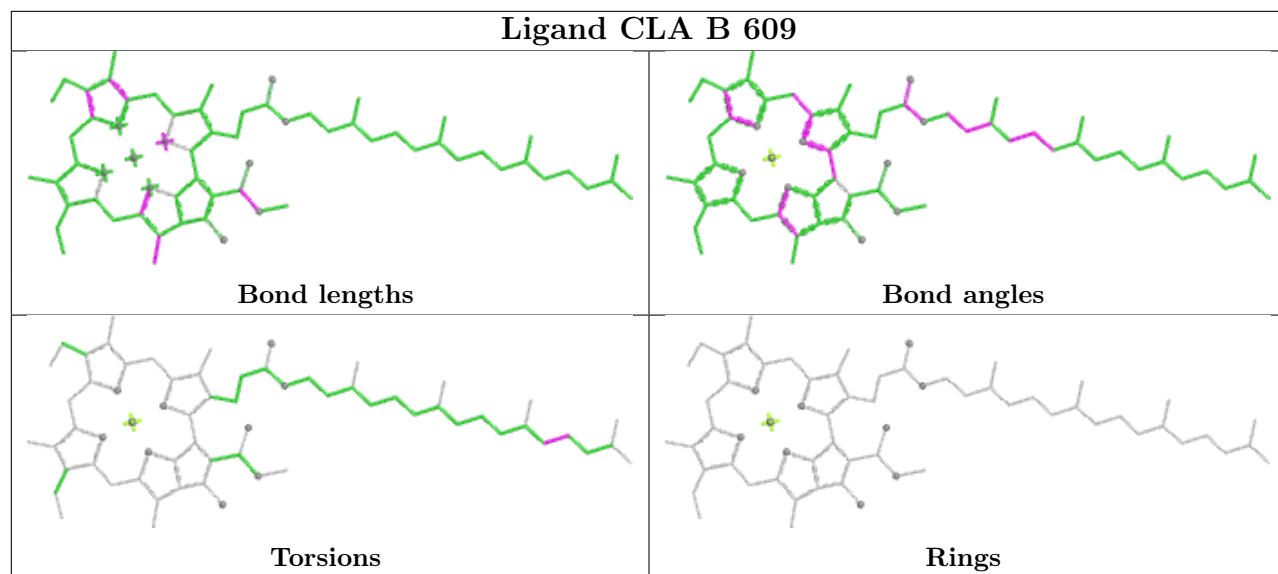


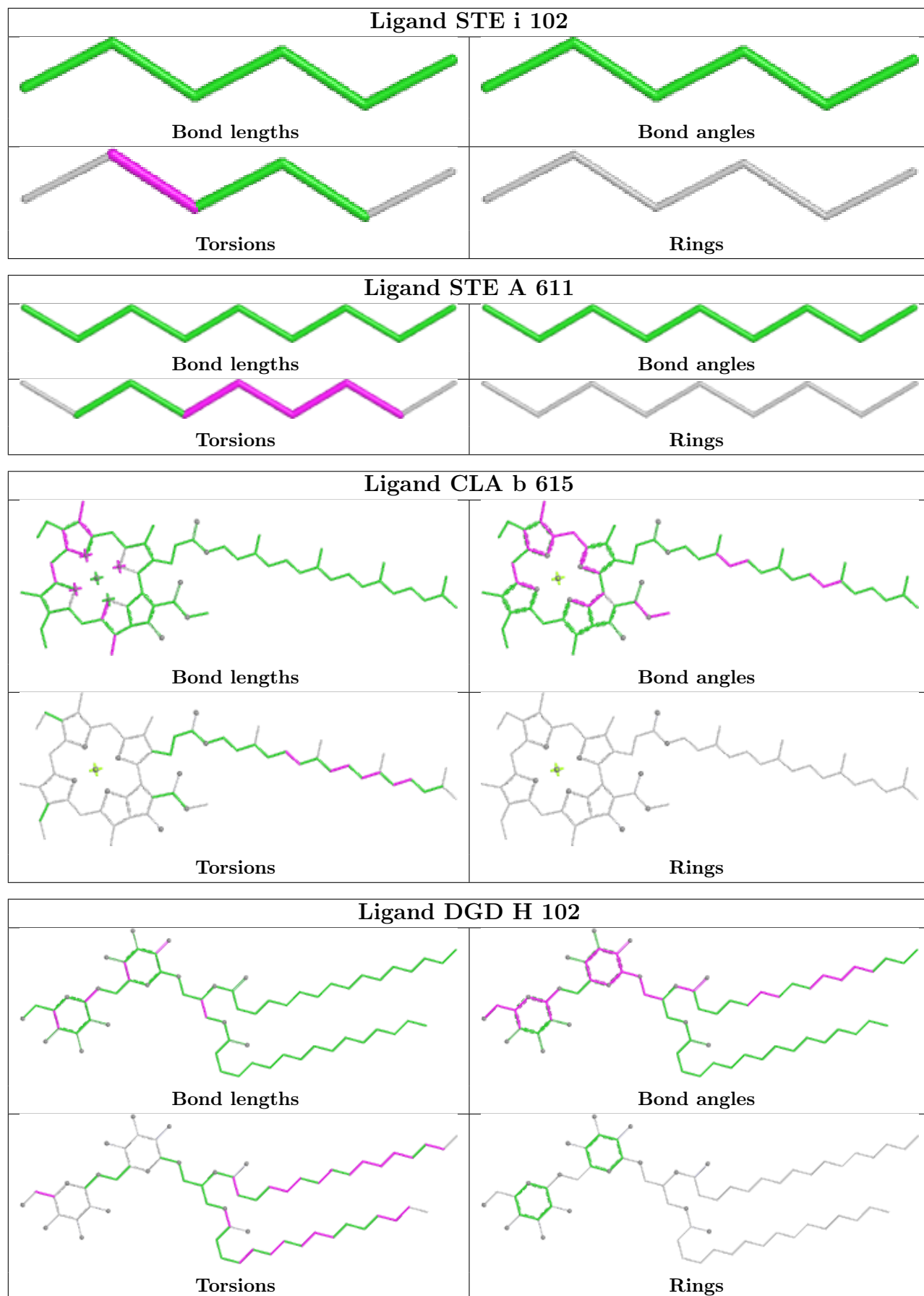


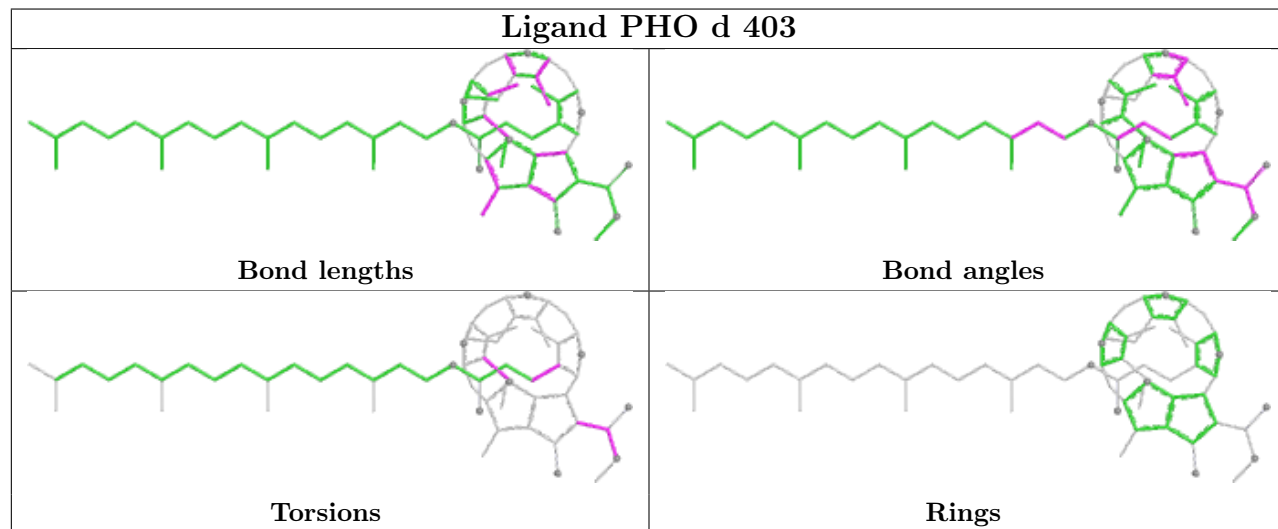
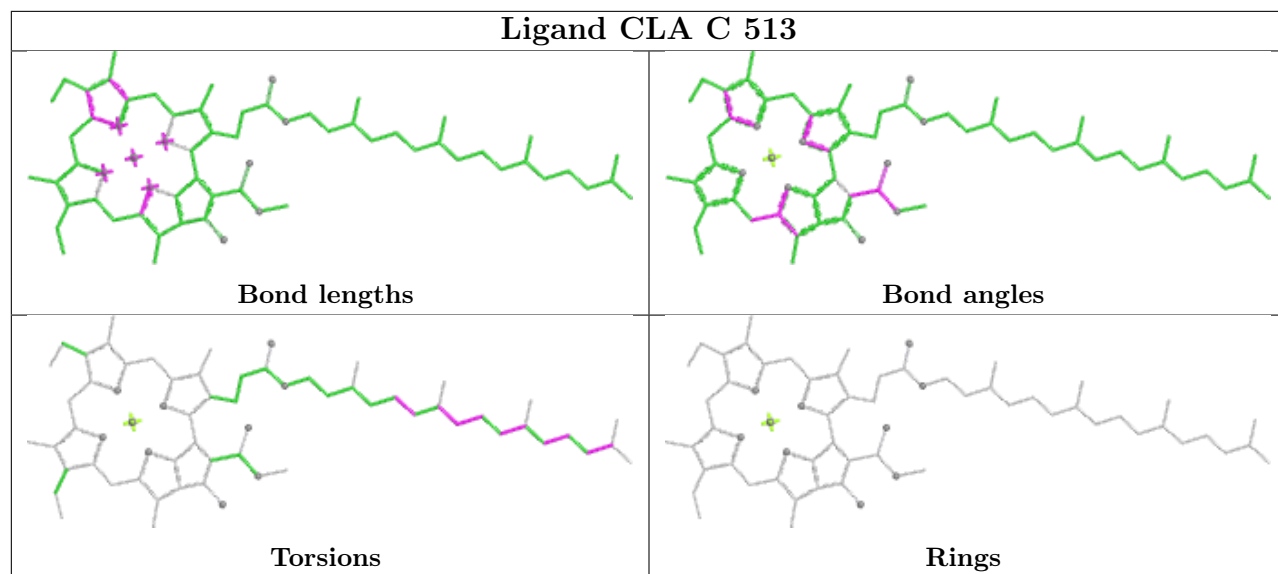


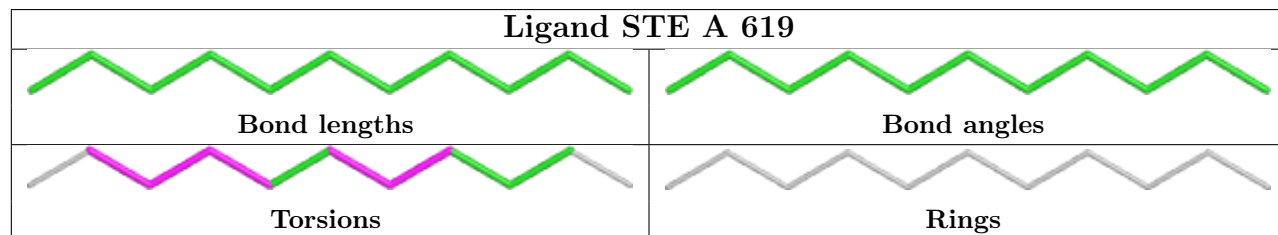
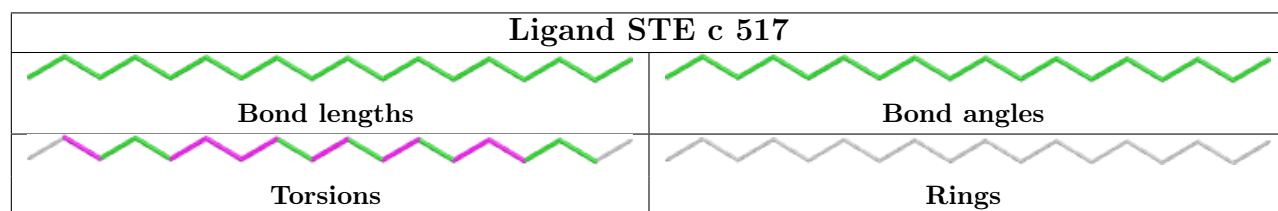
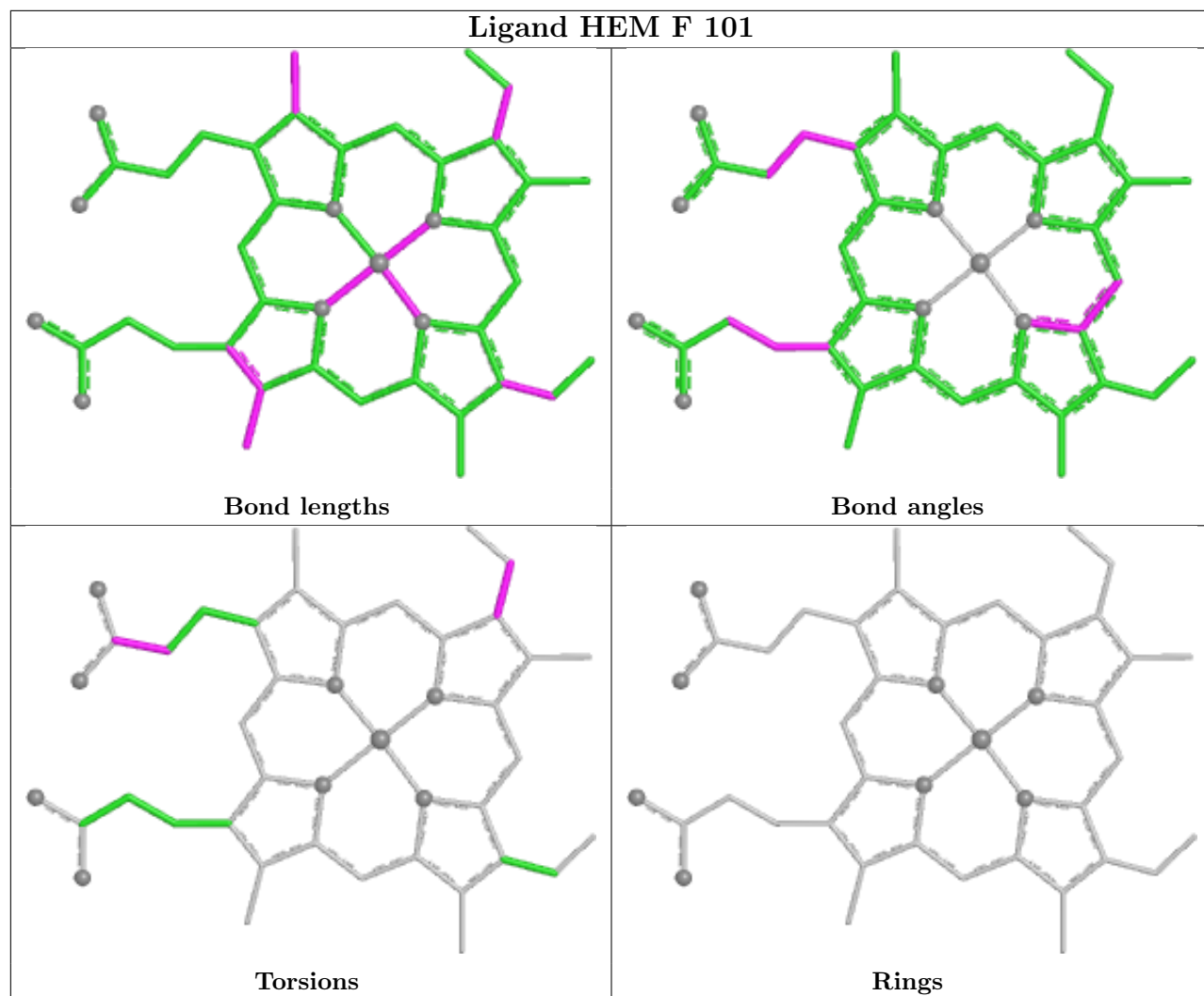


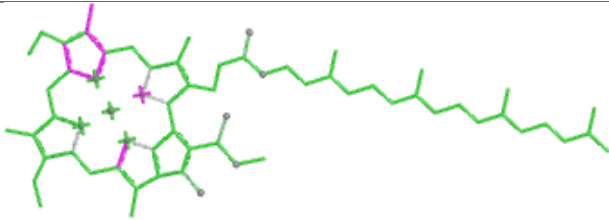
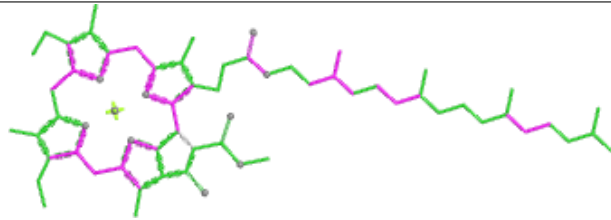
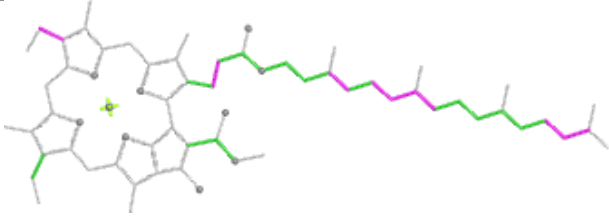
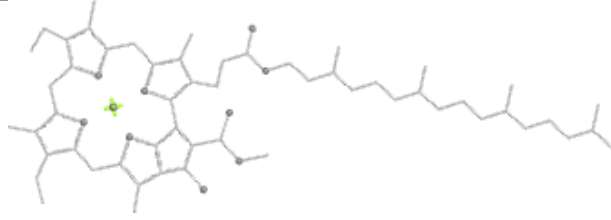


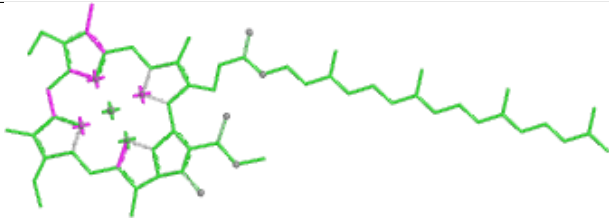
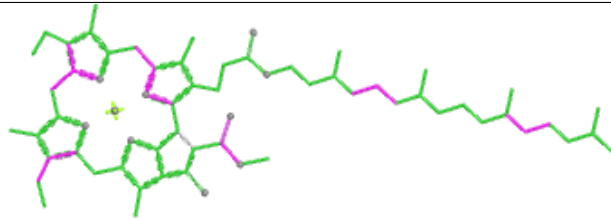
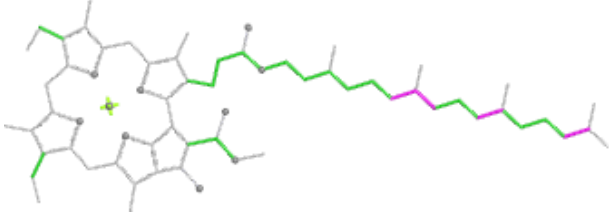
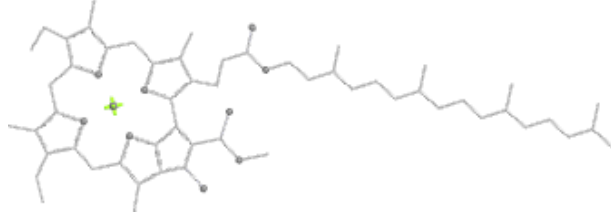


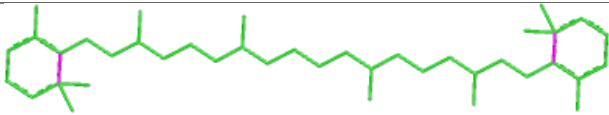
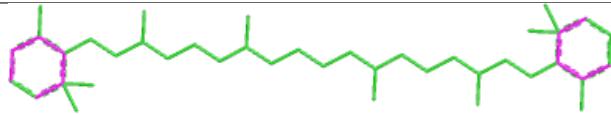
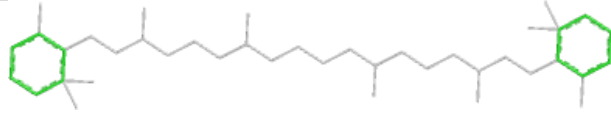


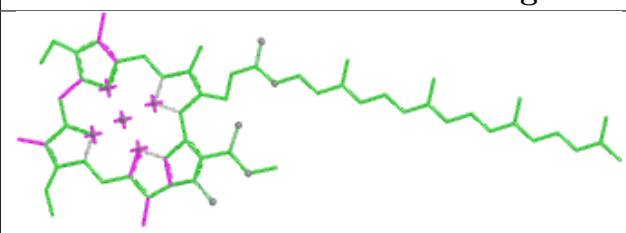
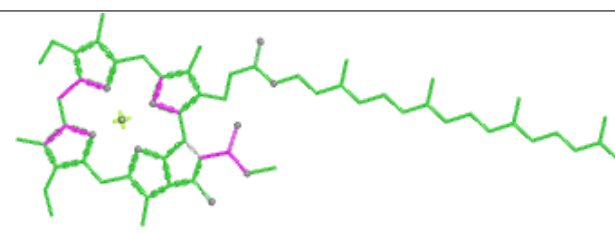
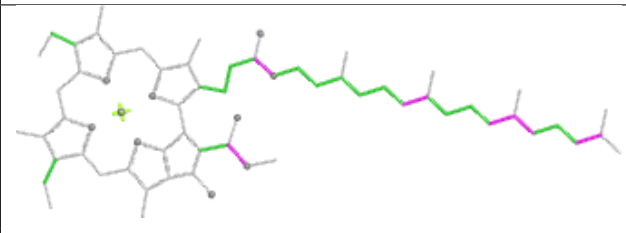
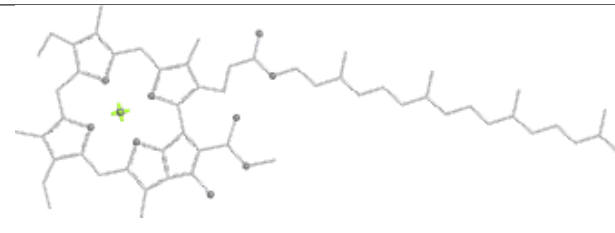


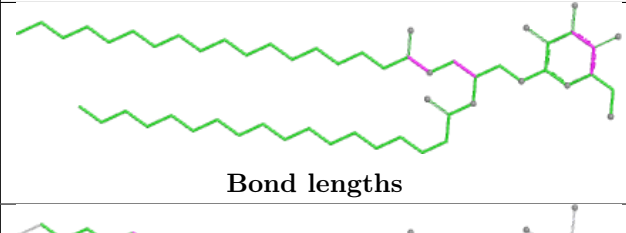
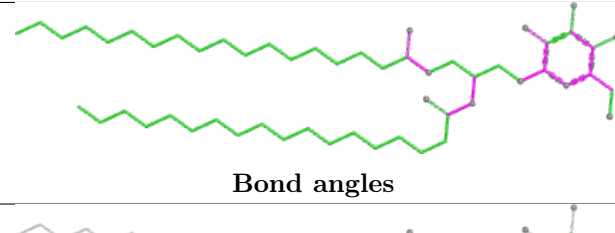
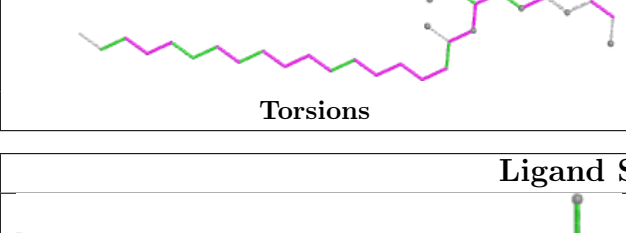
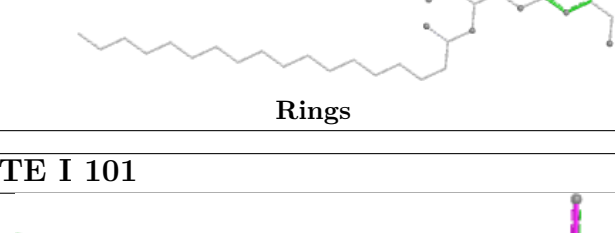


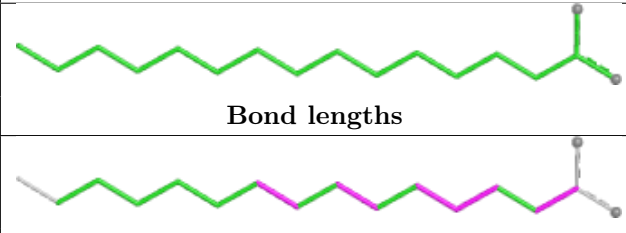
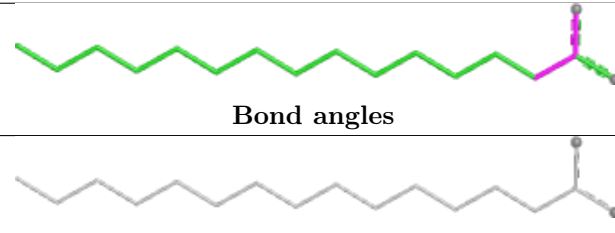
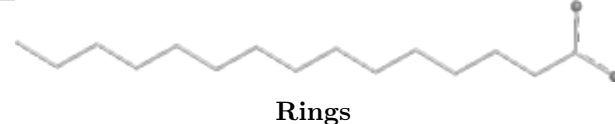
Ligand CLA B 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

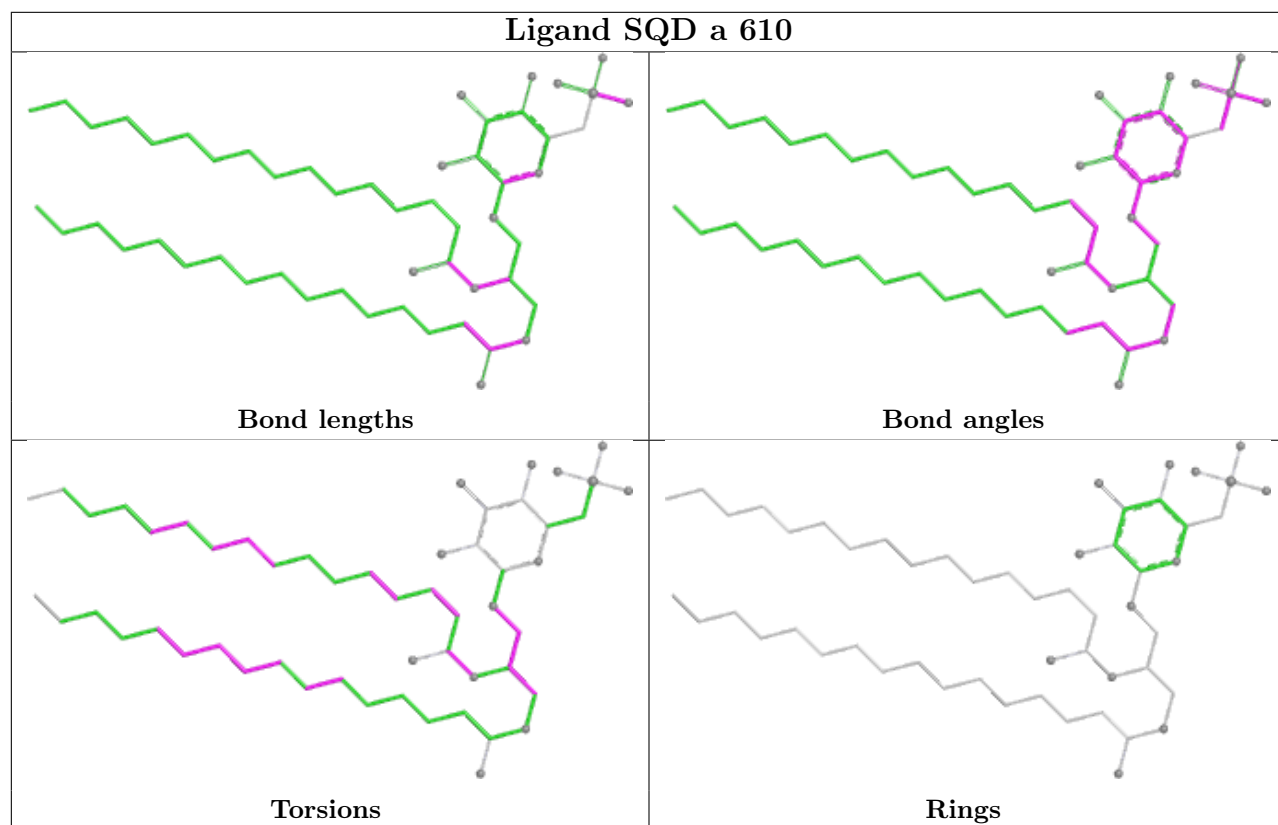
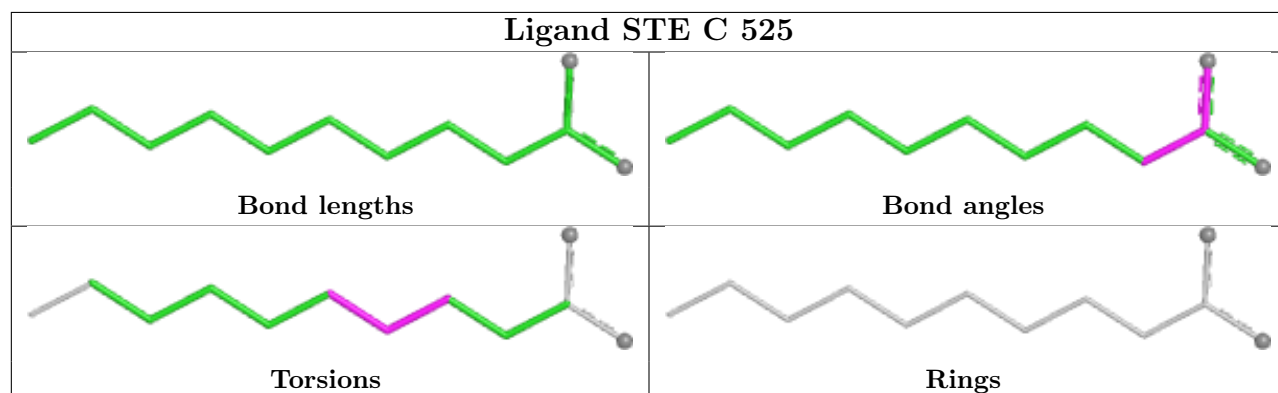
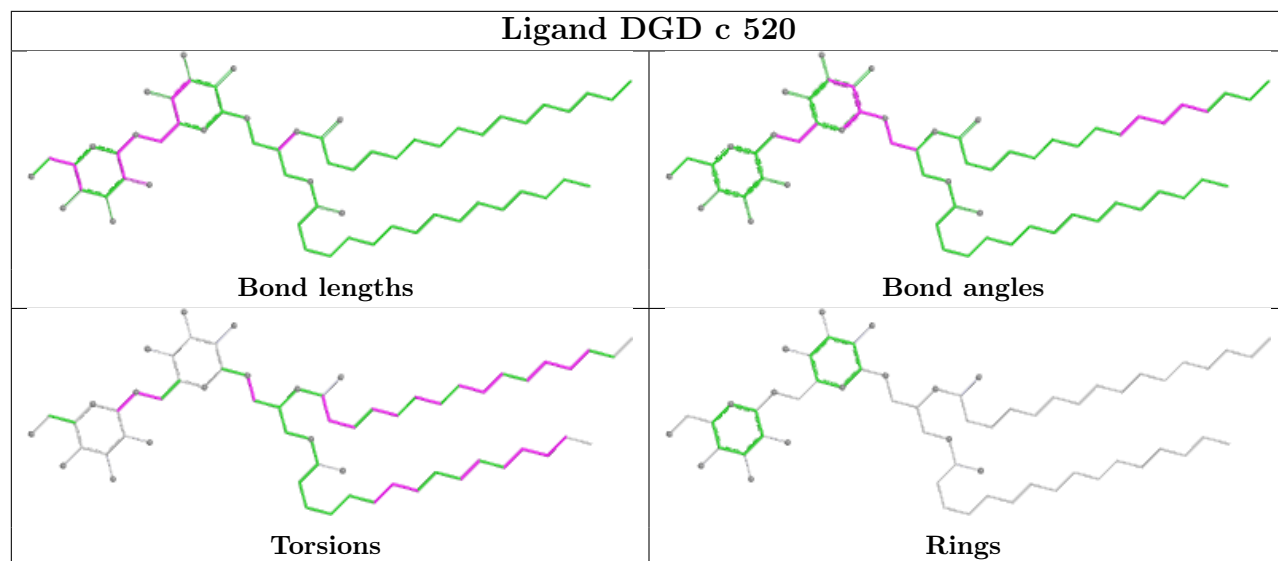
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

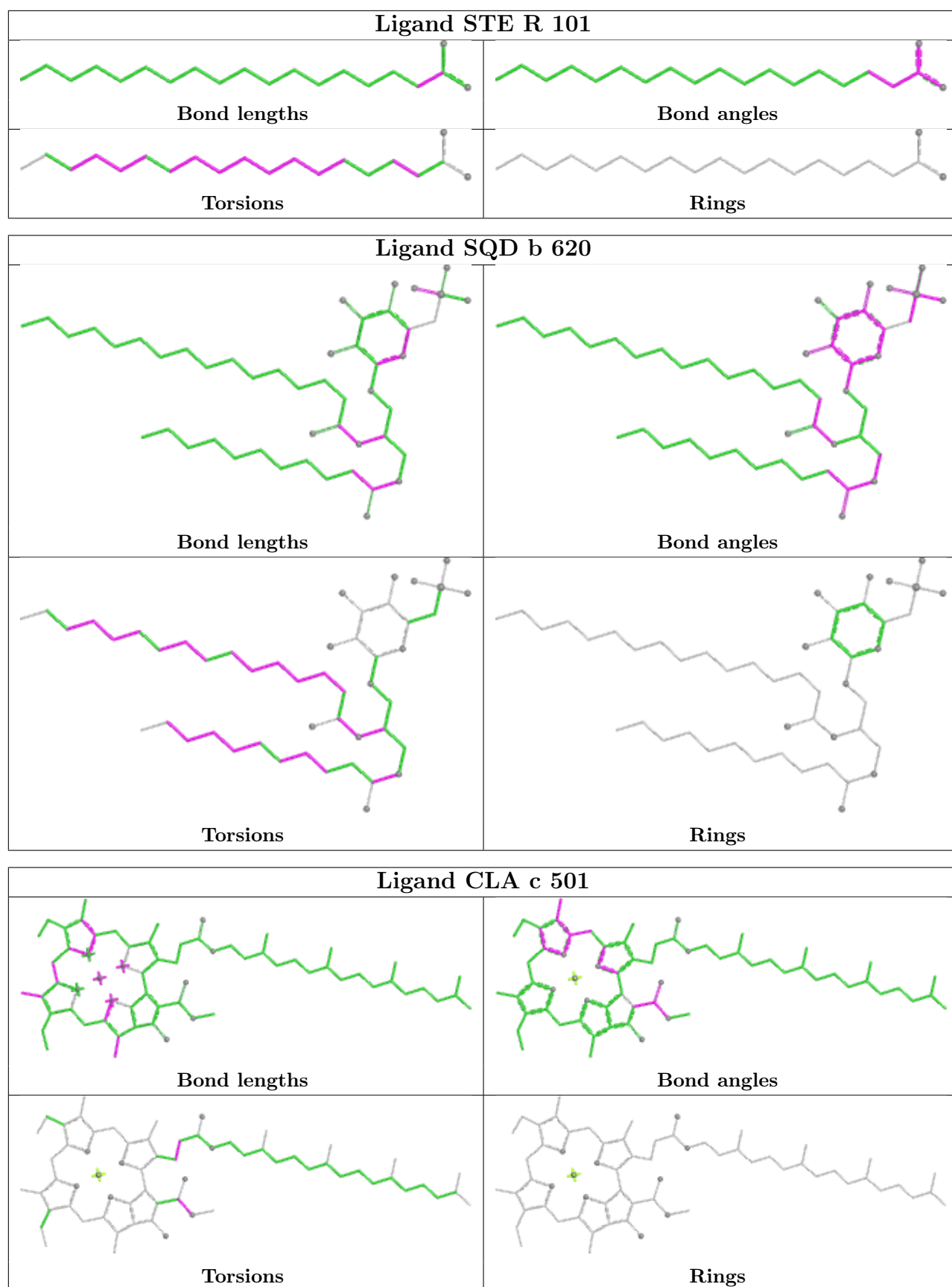
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

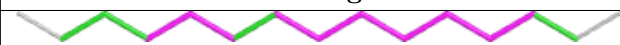
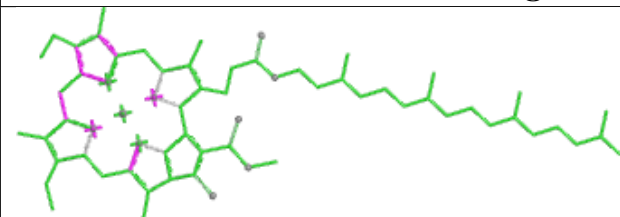
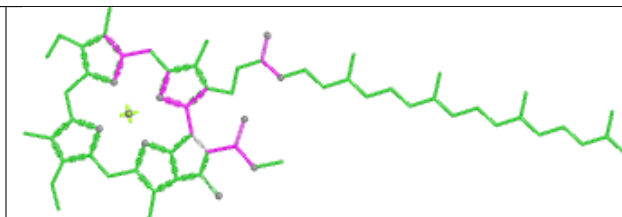
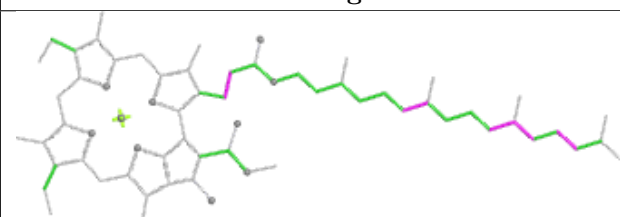
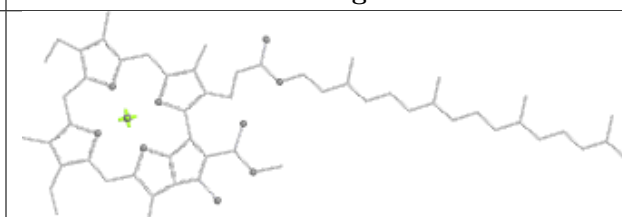
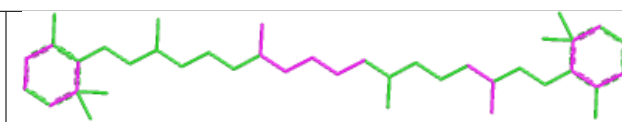
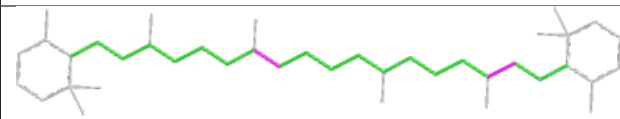
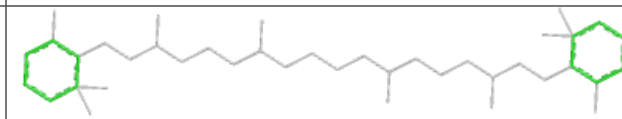
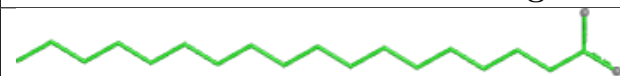
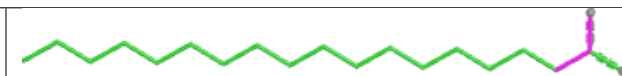
Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

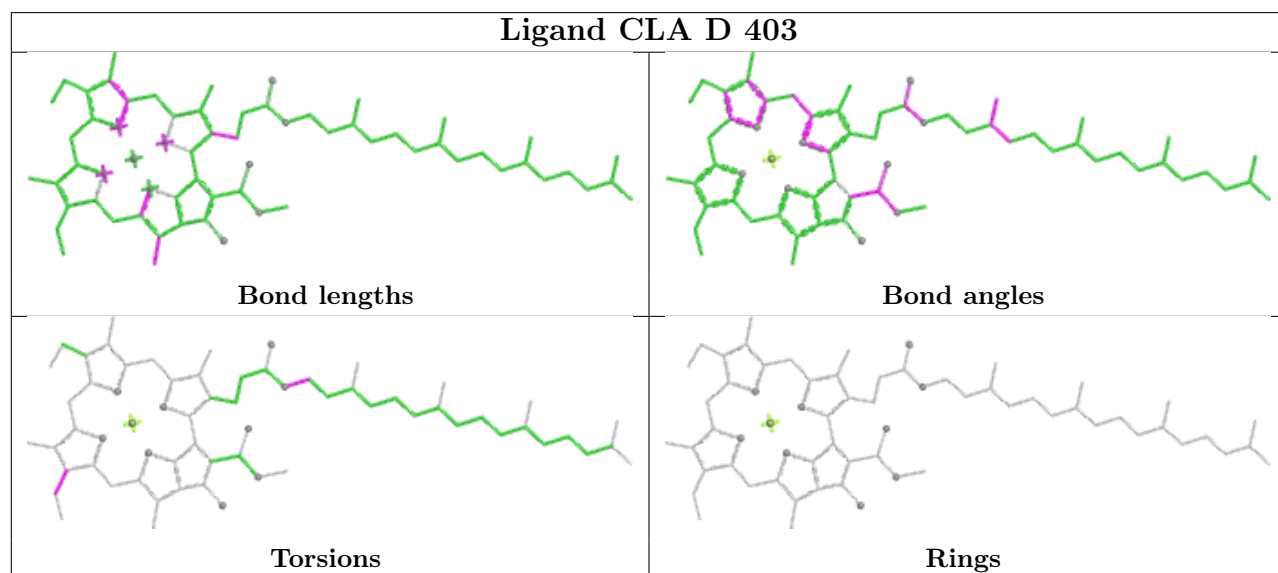
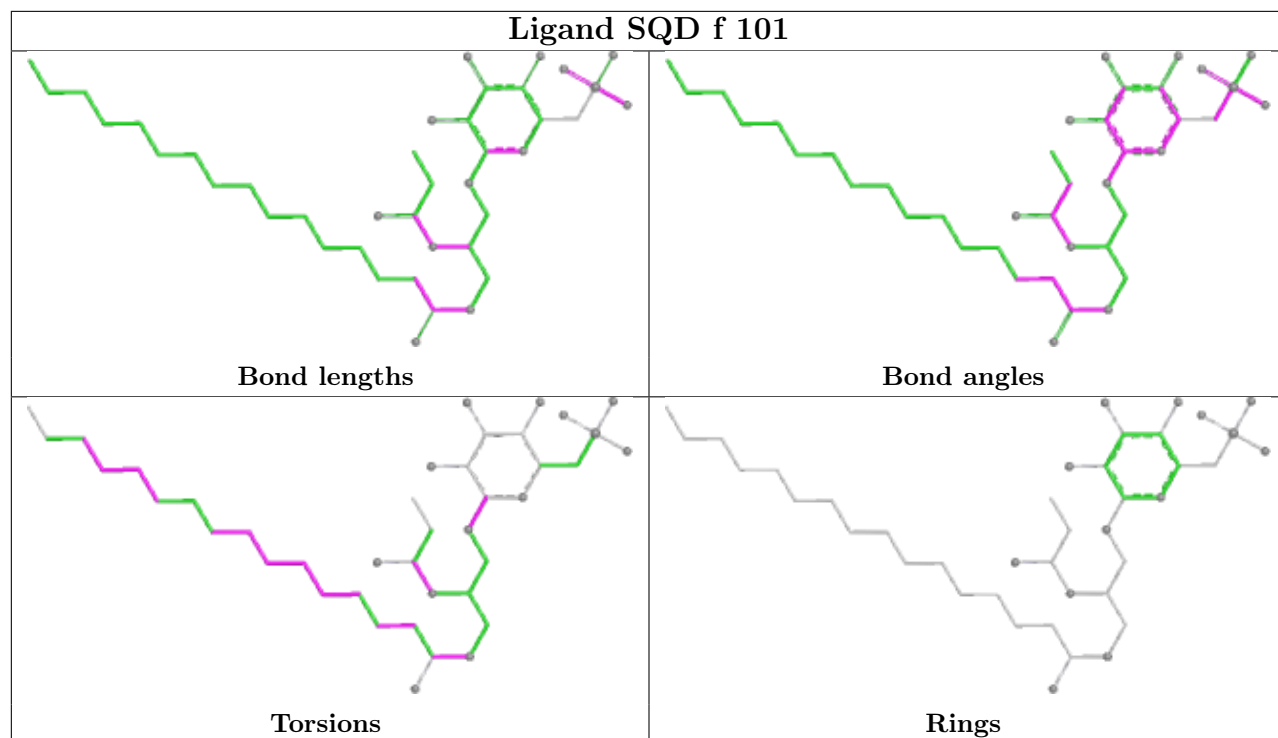
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

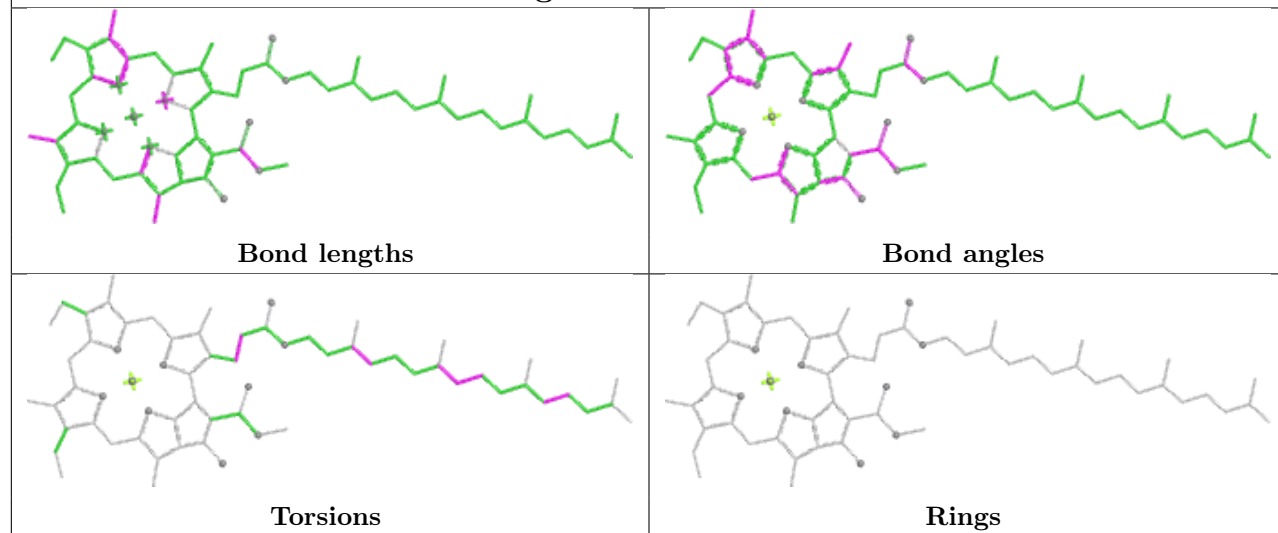




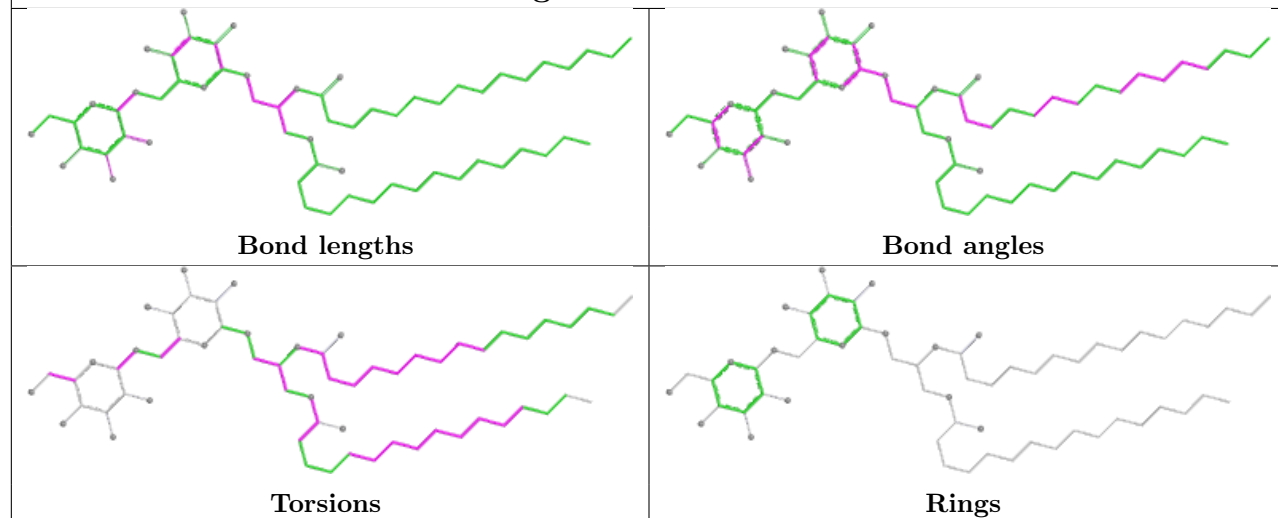
Ligand STE B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings



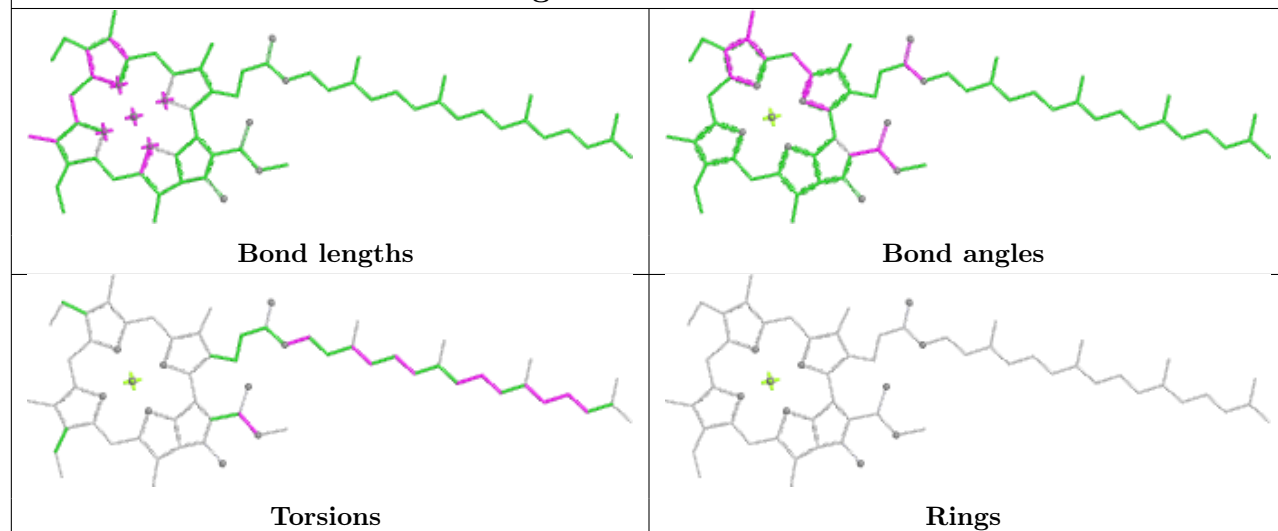
Ligand CLA b 603

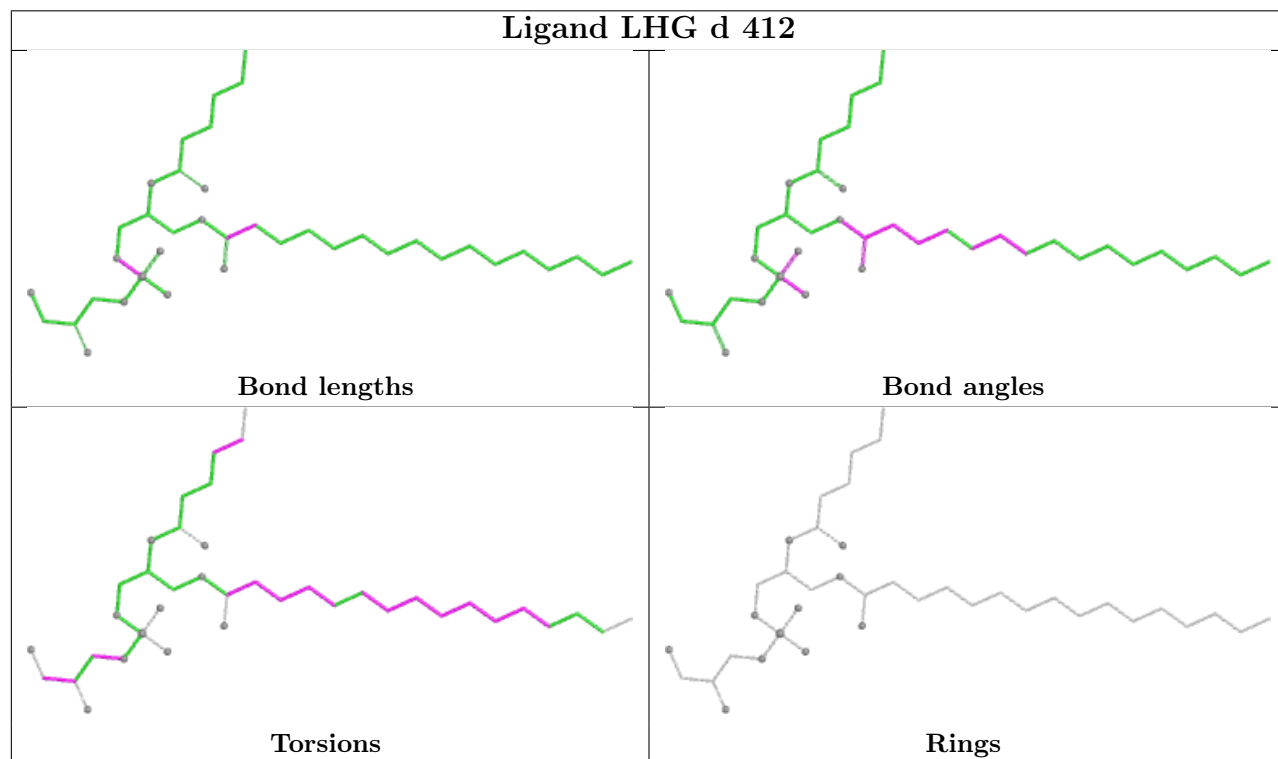
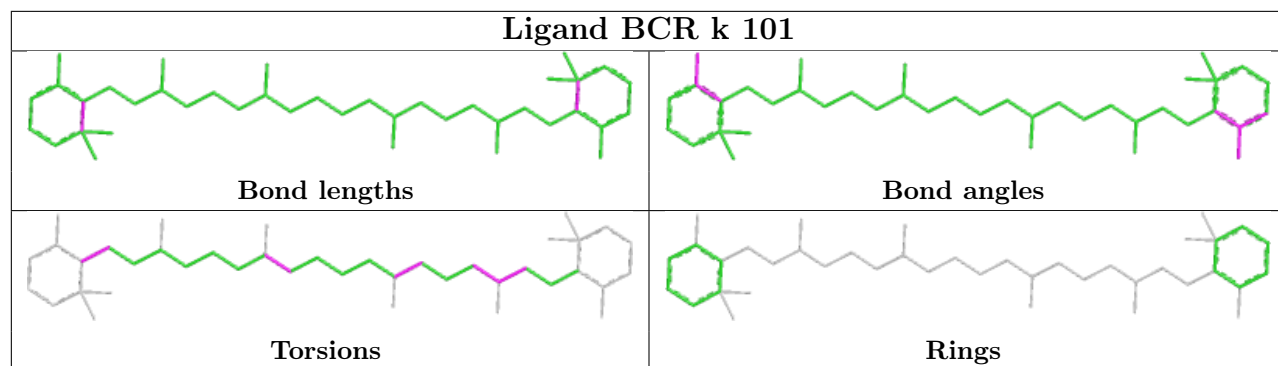


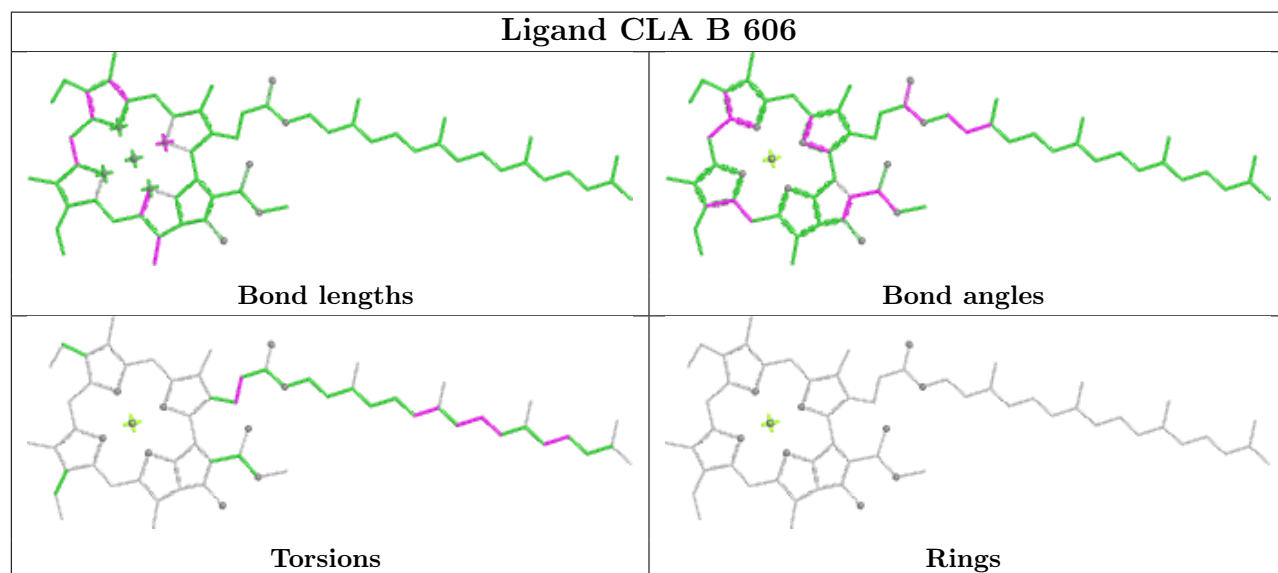
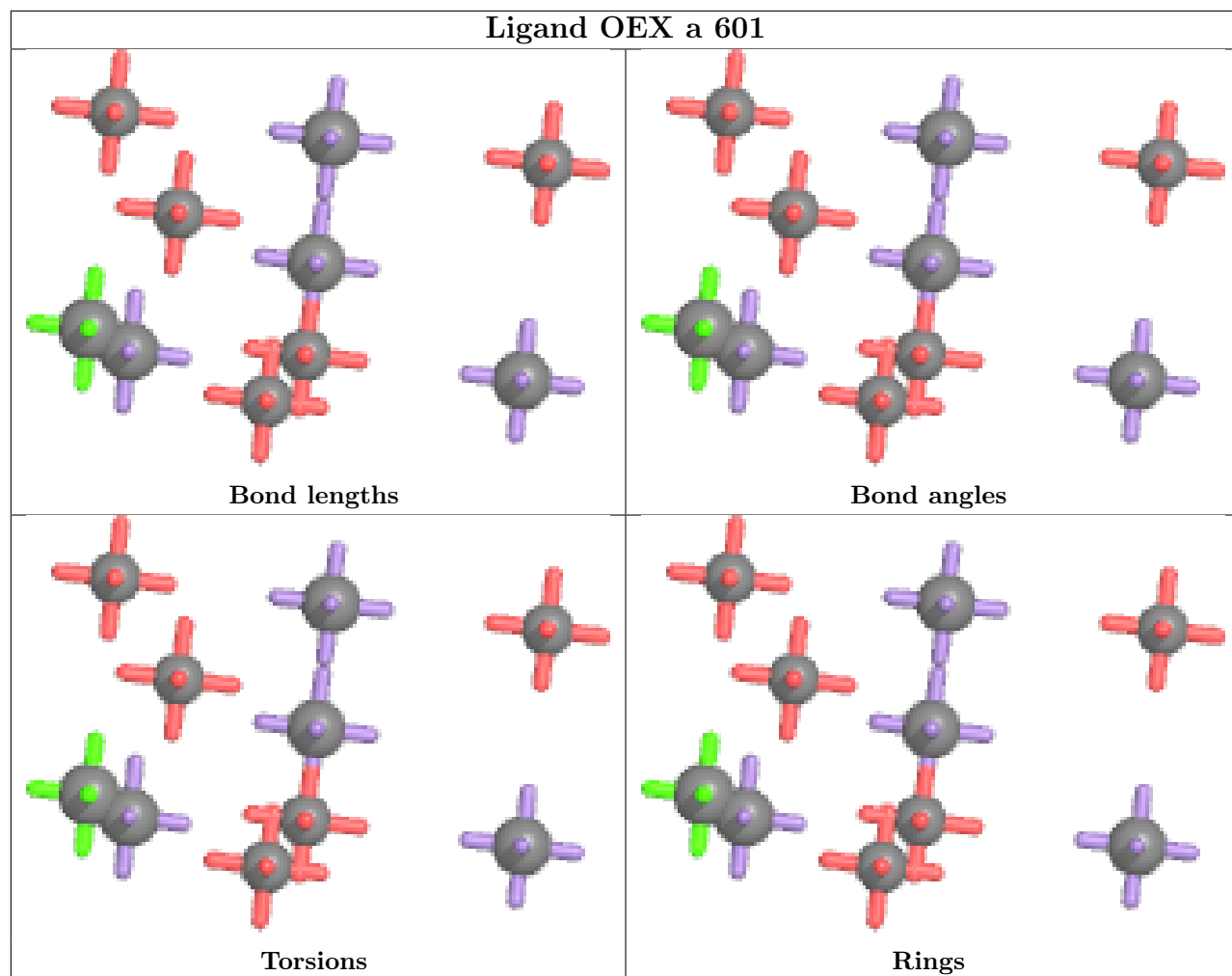
Ligand DGD c 519

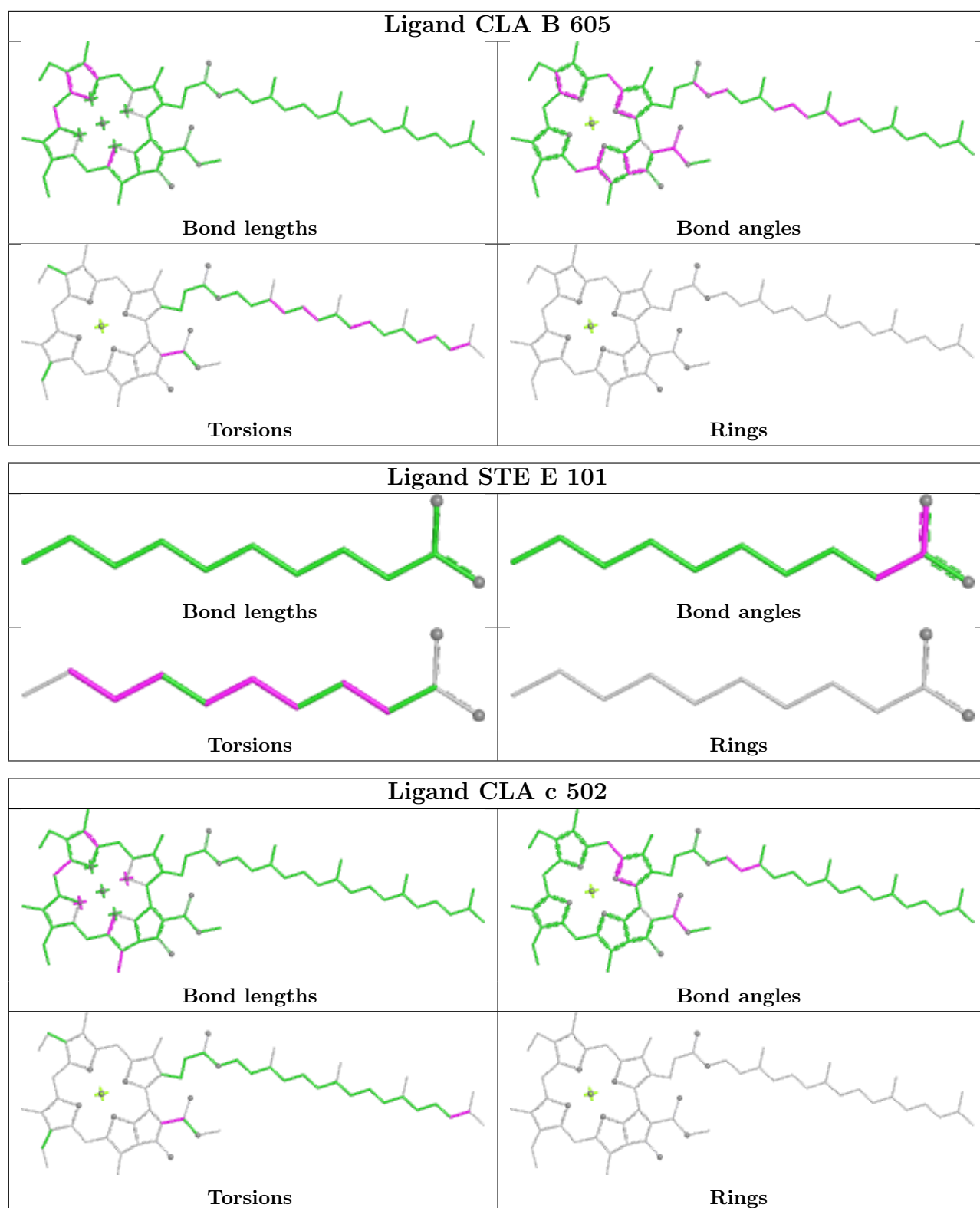


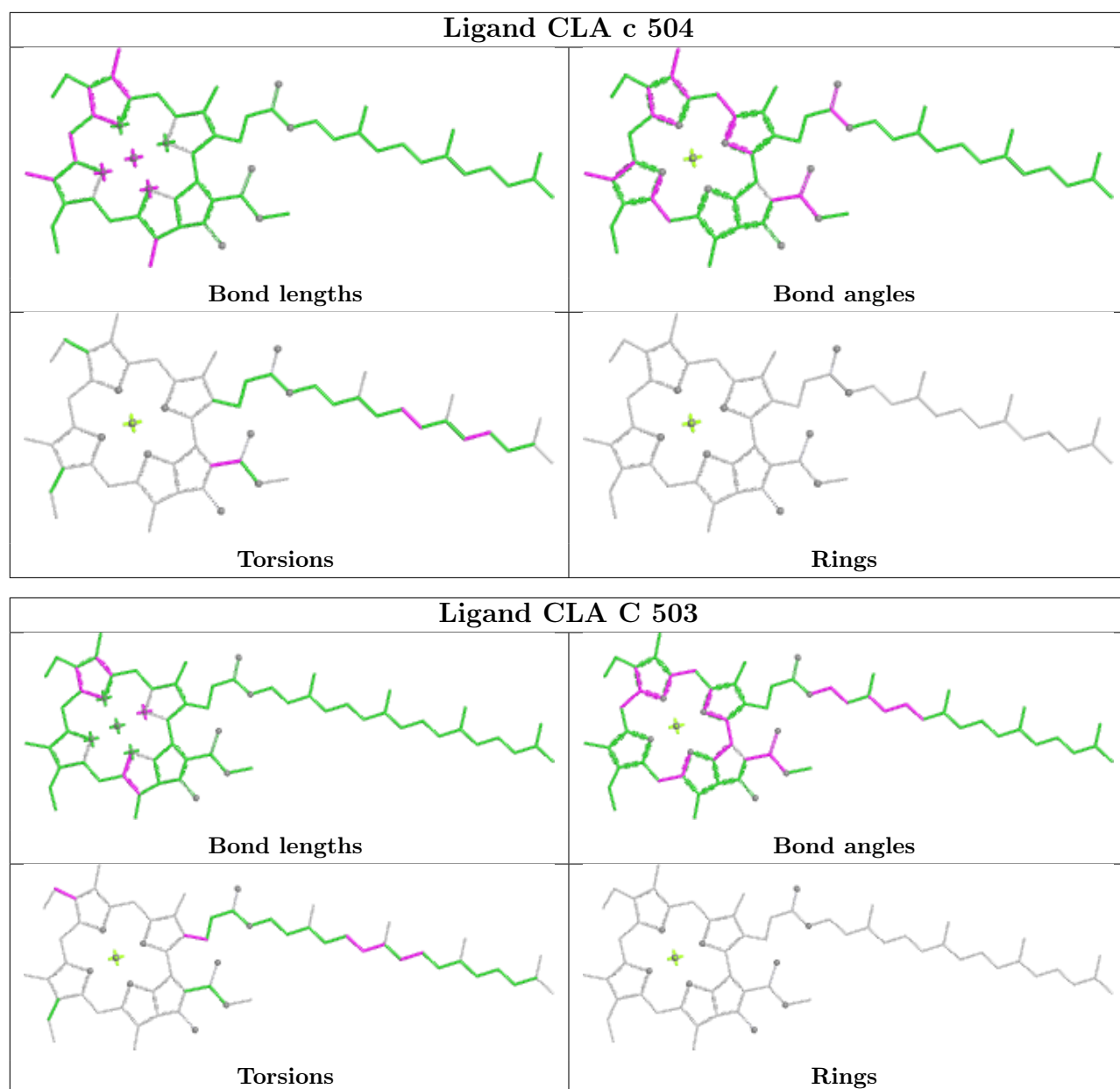
Ligand CLA C 506











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.67	2 (0%) 85 86	23, 30, 52, 81	0
1	a	334/344 (97%)	-0.57	1 (0%) 90 90	22, 32, 63, 77	0
2	B	505/510 (99%)	-0.56	1 (0%) 91 91	18, 35, 68, 96	5 (0%)
2	b	505/510 (99%)	-0.41	2 (0%) 88 89	26, 38, 74, 110	1 (0%)
3	C	442/461 (95%)	-0.53	0 100 100	25, 39, 58, 84	0
3	c	451/461 (97%)	-0.39	3 (0%) 84 84	23, 42, 69, 102	1 (0%)
4	D	341/352 (96%)	-0.69	0 100 100	23, 33, 51, 82	0
4	d	341/352 (96%)	-0.55	1 (0%) 90 90	25, 36, 62, 87	1 (0%)
5	E	82/84 (97%)	0.07	1 (1%) 76 76	31, 54, 73, 87	1 (1%)
5	e	82/84 (97%)	0.25	0 100 100	41, 63, 83, 92	0
6	F	34/45 (75%)	-0.20	0 100 100	39, 46, 64, 84	0
6	f	34/45 (75%)	0.13	2 (5%) 28 27	42, 53, 82, 96	0
7	H	65/66 (98%)	-0.32	2 (3%) 51 51	36, 45, 61, 81	0
7	h	63/66 (95%)	-0.00	1 (1%) 70 70	44, 54, 67, 76	0
8	I	35/38 (92%)	-0.35	0 100 100	32, 42, 76, 81	0
8	i	35/38 (92%)	-0.41	0 100 100	32, 43, 78, 91	0
9	J	36/40 (90%)	0.04	1 (2%) 55 54	39, 54, 80, 99	0
9	j	36/40 (90%)	0.16	0 100 100	39, 60, 91, 97	0
10	K	37/46 (80%)	-0.12	0 100 100	44, 57, 74, 83	0
10	k	37/46 (80%)	0.08	0 100 100	47, 60, 76, 85	0
11	L	37/37 (100%)	-0.69	0 100 100	26, 31, 66, 73	0
11	l	36/37 (97%)	-0.58	0 100 100	27, 33, 70, 82	0
12	M	32/36 (88%)	-0.39	3 (9%) 14 13	28, 36, 66, 80	0
12	m	31/36 (86%)	-0.54	0 100 100	29, 37, 51, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.33	2 (0%) 82 83	26, 44, 86, 128	1 (0%)
13	o	244/272 (89%)	-0.38	1 (0%) 88 89	25, 43, 82, 125	0
14	T	29/32 (90%)	-0.70	0 100 100	27, 34, 65, 78	0
14	t	29/32 (90%)	-0.56	1 (3%) 48 47	28, 35, 80, 90	0
15	U	97/134 (72%)	-0.36	0 100 100	31, 45, 71, 94	0
15	u	97/134 (72%)	-0.38	1 (1%) 79 80	32, 43, 58, 89	0
16	V	137/163 (84%)	-0.49	0 100 100	29, 42, 60, 76	0
16	v	137/163 (84%)	-0.15	0 100 100	35, 49, 74, 90	0
17	Y	27/46 (58%)	0.91	3 (11%) 10 9	56, 79, 105, 108	0
17	y	30/46 (65%)	0.67	1 (3%) 49 48	63, 77, 106, 118	0
18	X	38/41 (92%)	0.01	1 (2%) 57 57	43, 55, 78, 88	0
18	x	39/41 (95%)	0.13	1 (2%) 57 57	50, 65, 85, 94	0
19	Z	62/62 (100%)	0.53	3 (4%) 35 35	58, 72, 109, 126	0
19	z	62/62 (100%)	0.69	4 (6%) 25 24	58, 78, 116, 134	0
20	R	28/41 (68%)	0.60	0 100 100	63, 71, 89, 99	0
20	r	28/41 (68%)	1.07	5 (17%) 3 3	75, 89, 106, 113	0
All	All	5293/5700 (92%)	-0.38	43 (0%) 82 83	18, 40, 77, 134	10 (0%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	3.8
13	o	58	ASN	3.3
12	M	4	ASN	3.2
7	h	64	ALA	2.9
17	Y	20	ALA	2.9

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
8	FME	I	1	10/11	0.95	0.09	36,52,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.95	0.09	39,47,67,72	0
8	FME	i	1	10/11	0.95	0.08	34,47,61,65	0
14	FME	T	1	10/11	0.96	0.08	29,45,68,69	0
14	FME	t	1	10/11	0.96	0.07	29,42,67,67	0
12	FME	m	1	10/11	0.98	0.06	29,45,70,79	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	528	14/20	0.65	0.20	51,82,107,107	0
28	STE	i	101	12/20	0.65	0.17	50,90,107,109	0
28	STE	C	518	7/20	0.66	0.15	47,69,81,81	0
28	STE	j	102	16/20	0.67	0.21	61,82,104,110	0
28	STE	A	619	11/20	0.68	0.18	47,85,112,119	0
28	STE	H	103	18/20	0.68	0.19	49,74,87,88	0
28	STE	E	102	12/20	0.69	0.18	53,83,111,112	0
28	STE	c	517	18/20	0.70	0.18	61,85,105,107	0
28	STE	C	517	5/20	0.71	0.21	47,62,75,75	0
28	STE	I	101	17/20	0.72	0.18	51,76,88,89	0
28	STE	C	519	10/20	0.73	0.15	54,91,107,109	0
28	STE	i	102	6/20	0.74	0.23	45,75,84,84	0
28	STE	e	101	9/20	0.76	0.20	54,75,90,91	0
31	LHG	e	103	42/49	0.76	0.15	61,89,112,130	0
28	STE	e	104	9/20	0.77	0.17	50,69,86,87	0
28	STE	c	516	13/20	0.77	0.14	51,78,88,91	0
28	STE	A	618	17/20	0.77	0.13	48,73,85,88	0
28	STE	d	415	14/20	0.77	0.14	53,74,90,100	0
28	STE	R	101	20/20	0.77	0.15	48,67,81,83	0
29	LMG	D	407	50/55	0.78	0.16	36,71,126,141	0
31	LHG	A	615	49/49	0.78	0.15	50,84,118,128	0
28	STE	B	626	15/20	0.78	0.20	44,64,87,91	0
29	LMG	c	518	30/55	0.79	0.14	45,75,101,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	STE	b	627	11/20	0.79	0.19	56,73,84,88	0
28	STE	f	102	8/20	0.79	0.20	48,76,81,83	0
28	STE	t	103	10/20	0.80	0.13	46,64,69,77	0
28	STE	C	527	14/20	0.80	0.15	55,80,117,121	0
28	STE	A	611	9/20	0.80	0.18	49,71,90,97	0
28	STE	a	612	12/20	0.80	0.14	40,71,77,83	0
28	STE	e	105	13/20	0.80	0.16	71,88,103,104	0
28	STE	h	103	10/20	0.81	0.16	52,75,93,100	0
28	STE	E	101	12/20	0.81	0.14	53,76,89,94	0
29	LMG	b	623	55/55	0.81	0.16	47,73,92,108	0
27	PL9	A	610	55/55	0.82	0.14	39,65,93,97	0
28	STE	z	101	9/20	0.82	0.17	49,74,83,87	0
29	LMG	c	523	48/55	0.82	0.14	53,80,107,118	0
29	LMG	B	620	45/55	0.82	0.14	37,62,110,132	0
28	STE	b	624	16/20	0.82	0.16	49,69,94,101	0
28	STE	b	621	16/20	0.83	0.18	41,55,108,110	0
27	PL9	a	609	55/55	0.83	0.14	41,67,89,96	0
28	STE	b	625	10/20	0.83	0.15	45,60,68,72	0
28	STE	E	103	20/20	0.83	0.13	43,69,84,85	0
29	LMG	o	301	55/55	0.84	0.13	33,62,84,87	0
28	STE	B	625	12/20	0.84	0.13	46,65,77,81	0
28	STE	C	515	14/20	0.84	0.13	53,67,80,81	0
28	STE	M	103	15/20	0.85	0.17	47,62,95,101	0
28	STE	j	101	12/20	0.85	0.12	44,59,73,73	0
28	STE	d	409	20/20	0.85	0.13	39,63,81,82	0
28	STE	d	413	20/20	0.85	0.13	50,72,91,94	0
28	STE	Z	101	17/20	0.85	0.15	48,72,97,99	0
28	STE	C	526	16/20	0.85	0.12	47,60,69,70	0
29	LMG	C	516	36/55	0.85	0.12	40,63,87,99	0
32	DGD	A	617	66/66	0.85	0.12	47,69,90,98	0
30	SQD	a	611	54/54	0.86	0.12	38,64,101,120	0
29	LMG	C	524	48/55	0.86	0.12	48,74,95,104	0
28	STE	I	102	15/20	0.86	0.13	43,59,73,73	0
28	STE	J	101	12/20	0.86	0.12	52,67,75,79	0
29	LMG	A	613	48/55	0.87	0.10	37,58,72,87	0
28	STE	m	102	12/20	0.87	0.14	45,59,79,92	0
28	STE	B	624	18/20	0.87	0.11	48,60,73,74	0
29	LMG	c	522	46/55	0.87	0.12	43,72,90,98	0
28	STE	C	525	12/20	0.87	0.14	37,53,67,68	0
28	STE	x	101	20/20	0.88	0.12	37,57,75,89	0
28	STE	D	412	9/20	0.88	0.12	49,66,75,81	0
28	STE	b	622	20/20	0.88	0.10	41,59,86,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	601	65/65	0.88	0.11	44,68,97,113	0
28	STE	M	102	10/20	0.89	0.13	41,59,67,77	0
30	SQD	B	623	54/54	0.89	0.10	38,61,90,97	0
28	STE	B	622	17/20	0.90	0.11	33,54,75,77	0
30	SQD	A	616	43/54	0.90	0.09	42,61,106,119	0
26	BCR	k	101	40/40	0.90	0.10	45,62,74,82	0
28	STE	M	101	15/20	0.90	0.11	35,51,66,73	0
30	SQD	f	101	41/54	0.90	0.11	51,78,95,100	0
28	STE	b	626	8/20	0.90	0.11	44,60,80,80	0
29	LMG	c	524	49/55	0.90	0.10	35,59,95,115	0
29	LMG	m	101	51/55	0.90	0.09	36,53,67,80	0
26	BCR	K	101	40/40	0.91	0.10	41,58,69,73	0
28	STE	t	102	14/20	0.91	0.09	43,56,64,69	0
28	STE	l	102	18/20	0.91	0.12	34,53,94,94	0
26	BCR	h	101	40/40	0.92	0.09	34,56,80,80	0
29	LMG	B	621	51/55	0.92	0.09	27,51,77,86	0
30	SQD	F	102	36/54	0.92	0.11	42,74,90,102	0
30	SQD	a	610	54/54	0.92	0.10	40,66,93,99	0
24	CLA	B	601	65/65	0.92	0.09	33,61,94,95	0
30	SQD	b	620	49/54	0.92	0.09	41,59,87,98	0
24	CLA	c	513	65/65	0.92	0.10	44,70,95,103	0
24	CLA	C	513	65/65	0.92	0.10	44,65,92,99	0
26	BCR	K	102	40/40	0.92	0.09	40,54,75,77	0
30	SQD	A	614	52/54	0.92	0.09	32,61,90,97	0
32	DGD	H	102	62/66	0.92	0.09	34,50,62,69	0
26	BCR	H	101	40/40	0.93	0.07	32,51,65,69	0
28	STE	X	101	20/20	0.93	0.09	37,51,71,77	0
24	CLA	c	512	65/65	0.93	0.09	37,59,89,98	0
26	BCR	k	102	40/40	0.93	0.10	40,57,69,80	0
26	BCR	D	405	40/40	0.93	0.09	30,46,96,107	0
26	BCR	c	514	40/40	0.93	0.09	46,61,74,79	0
32	DGD	C	522	62/66	0.93	0.09	32,52,103,122	0
26	BCR	d	407	40/40	0.93	0.09	33,54,93,98	0
32	DGD	c	520	62/66	0.93	0.09	32,52,92,101	0
32	DGD	h	102	62/66	0.93	0.09	35,53,68,75	0
29	LMG	D	408	51/55	0.94	0.09	26,58,88,96	0
26	BCR	B	619	40/40	0.94	0.07	24,40,61,68	0
26	BCR	c	515	40/40	0.94	0.08	30,45,67,74	0
26	BCR	C	520	40/40	0.94	0.09	38,53,69,69	0
24	CLA	c	511	65/65	0.94	0.08	39,53,68,81	0
24	CLA	C	512	65/65	0.94	0.09	39,54,98,102	0
31	LHG	d	410	49/49	0.94	0.09	34,54,78,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMG	d	414	44/55	0.94	0.09	33,55,93,100	0
24	CLA	c	509	65/65	0.94	0.09	33,47,67,74	0
26	BCR	B	618	40/40	0.94	0.06	23,40,52,57	0
26	BCR	b	617	40/40	0.94	0.07	27,41,52,60	0
26	BCR	b	618	40/40	0.94	0.06	25,40,61,65	0
26	BCR	b	619	40/40	0.94	0.07	30,46,65,70	0
26	BCR	t	101	40/40	0.95	0.06	29,41,60,64	0
24	CLA	c	504	60/65	0.95	0.07	26,45,83,85	0
24	CLA	c	506	65/65	0.95	0.09	26,49,102,105	0
24	CLA	c	508	64/65	0.95	0.08	29,45,96,112	0
24	CLA	C	511	65/65	0.95	0.07	32,49,68,74	0
26	BCR	T	101	40/40	0.95	0.06	26,39,57,62	0
24	CLA	B	606	65/65	0.95	0.07	21,36,71,79	0
24	CLA	C	503	65/65	0.95	0.07	30,43,53,56	0
24	CLA	C	510	65/65	0.95	0.07	29,45,62,70	0
31	LHG	d	412	39/49	0.95	0.09	31,48,72,82	0
26	BCR	A	609	40/40	0.95	0.06	24,35,46,48	0
31	LHG	l	101	49/49	0.95	0.07	32,46,58,62	0
26	BCR	B	617	40/40	0.95	0.07	25,39,54,58	0
24	CLA	b	609	65/65	0.95	0.07	28,45,65,79	0
32	DGD	C	523	62/66	0.95	0.08	28,50,79,94	0
24	CLA	b	612	65/65	0.95	0.07	22,33,47,55	0
26	BCR	C	514	40/40	0.95	0.07	27,41,55,57	0
24	CLA	c	503	65/65	0.95	0.07	30,44,57,60	0
24	CLA	C	501	65/65	0.96	0.06	24,36,51,61	0
24	CLA	c	510	65/65	0.96	0.07	29,48,68,80	0
24	CLA	B	609	65/65	0.96	0.07	26,38,62,65	0
24	CLA	a	606	65/65	0.96	0.08	23,41,97,103	0
24	CLA	C	504	59/65	0.96	0.07	29,43,89,94	0
24	CLA	d	406	65/65	0.96	0.08	23,50,91,105	0
25	PHO	d	403	64/64	0.96	0.06	26,37,48,58	0
27	PL9	D	406	55/55	0.96	0.06	22,34,47,51	0
24	CLA	b	602	65/65	0.96	0.08	27,45,70,74	0
27	PL9	d	408	55/55	0.96	0.06	23,35,47,47	0
24	CLA	b	606	65/65	0.96	0.07	24,39,74,84	0
24	CLA	b	608	65/65	0.96	0.07	23,43,72,76	0
24	CLA	C	505	65/65	0.96	0.08	24,40,66,71	0
24	CLA	b	610	65/65	0.96	0.07	23,39,52,58	0
24	CLA	C	506	65/65	0.96	0.09	27,43,93,99	0
31	LHG	D	410	47/49	0.96	0.08	27,50,84,101	0
31	LHG	D	411	49/49	0.96	0.08	29,47,73,83	0
24	CLA	b	614	65/65	0.96	0.07	23,39,78,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	d	411	49/49	0.96	0.07	23,44,53,64	0
24	CLA	b	615	65/65	0.96	0.07	25,41,61,73	0
24	CLA	b	616	60/65	0.96	0.08	25,44,86,93	0
24	CLA	c	502	65/65	0.96	0.06	27,43,60,63	0
24	CLA	C	508	65/65	0.96	0.07	28,43,116,126	0
32	DGD	C	521	62/66	0.96	0.08	22,41,85,94	0
26	BCR	a	608	40/40	0.96	0.06	20,33,48,50	0
24	CLA	C	509	65/65	0.96	0.08	24,46,66,74	0
24	CLA	c	505	65/65	0.96	0.07	25,42,67,73	0
32	DGD	c	519	62/66	0.96	0.08	20,42,75,88	0
24	CLA	B	612	65/65	0.96	0.06	19,34,46,53	0
32	DGD	c	521	62/66	0.96	0.08	29,55,80,94	0
24	CLA	B	615	65/65	0.96	0.07	22,39,66,75	0
33	BCT	D	401	4/4	0.96	0.08	28,30,33,40	0
33	BCT	d	401	4/4	0.96	0.08	28,30,46,55	0
24	CLA	a	607	65/65	0.97	0.08	19,33,83,91	0
24	CLA	d	404	65/65	0.97	0.06	20,30,49,52	0
24	CLA	d	405	65/65	0.97	0.06	20,34,62,69	0
24	CLA	B	614	65/65	0.97	0.07	18,37,84,90	0
25	PHO	A	607	64/64	0.97	0.05	18,29,40,43	0
25	PHO	D	402	64/64	0.97	0.05	21,33,43,47	0
25	PHO	d	402	64/64	0.97	0.05	22,31,40,41	0
24	CLA	A	605	65/65	0.97	0.05	17,29,51,60	0
24	CLA	b	603	65/65	0.97	0.06	20,36,73,82	0
24	CLA	b	605	65/65	0.97	0.05	20,35,49,58	0
24	CLA	B	616	60/65	0.97	0.08	20,39,87,102	0
24	CLA	b	607	65/65	0.97	0.06	19,36,70,81	0
24	CLA	B	602	65/65	0.97	0.06	22,37,68,73	0
24	CLA	C	502	65/65	0.97	0.06	26,39,60,72	0
24	CLA	B	603	65/65	0.97	0.06	18,34,67,74	0
31	LHG	D	409	49/49	0.97	0.06	22,40,57,66	0
24	CLA	b	611	65/65	0.97	0.05	22,35,55,61	0
24	CLA	B	604	65/65	0.97	0.07	20,33,74,87	0
31	LHG	L	101	49/49	0.97	0.06	28,43,62,68	0
24	CLA	b	613	65/65	0.97	0.06	20,35,73,90	0
24	CLA	B	605	65/65	0.97	0.06	19,31,49,55	0
24	CLA	A	606	65/65	0.97	0.08	20,36,101,115	0
24	CLA	C	507	65/65	0.97	0.06	24,41,58,61	0
24	CLA	c	501	65/65	0.97	0.06	27,41,56,58	0
24	CLA	B	607	65/65	0.97	0.06	17,31,58,71	0
24	CLA	B	608	65/65	0.97	0.05	20,36,59,69	0
24	CLA	A	608	54/65	0.97	0.06	18,34,58,68	0

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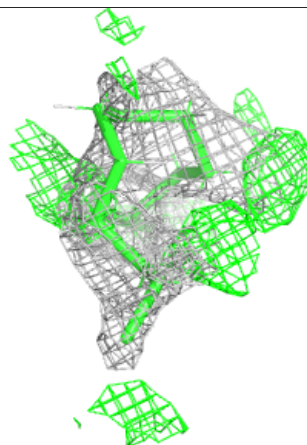
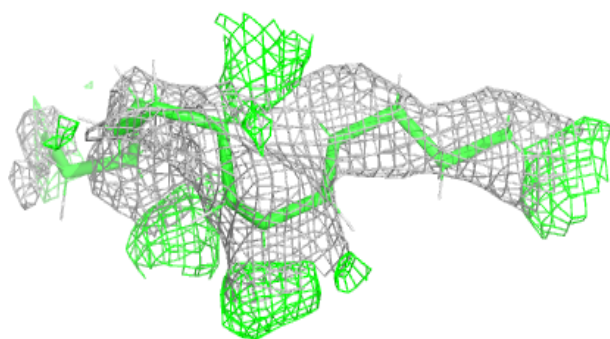
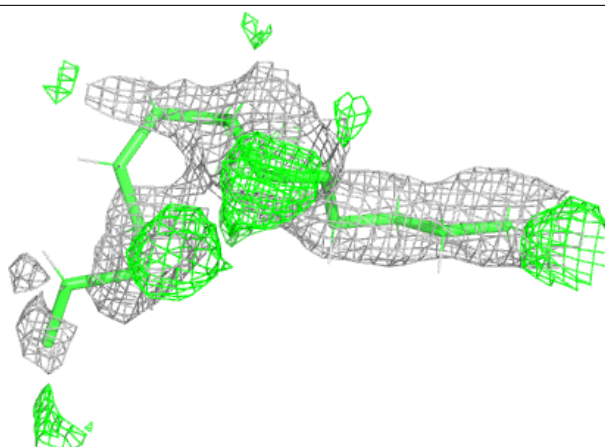
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	610	65/65	0.97	0.06	22,33,45,50	0
24	CLA	B	611	65/65	0.97	0.05	21,30,48,58	0
24	CLA	c	507	65/65	0.97	0.07	25,46,61,66	0
24	CLA	A	612	65/65	0.97	0.06	21,29,55,56	0
24	CLA	D	403	65/65	0.97	0.05	19,31,57,63	0
24	CLA	D	404	65/65	0.97	0.08	21,43,112,127	0
24	CLA	a	605	65/65	0.97	0.05	18,29,49,57	0
24	CLA	B	613	65/65	0.97	0.06	19,32,70,77	0
34	HEM	e	102	43/43	0.97	0.09	45,57,80,83	0
34	HEM	F	101	43/43	0.98	0.08	33,48,65,69	0
24	CLA	b	604	65/65	0.98	0.06	21,34,86,99	0
35	HEC	v	201	43/43	0.98	0.06	30,37,47,52	0
23	CL	A	604	1/1	0.99	0.04	28,28,28,28	0
21	OEX	A	601	10/10	0.99	0.03	26,27,30,30	0
22	FE2	a	602	1/1	0.99	0.02	31,31,31,31	0
35	HEC	V	201	43/43	0.99	0.06	22,32,45,47	0
23	CL	A	603	1/1	0.99	0.03	26,26,26,26	0
22	FE2	A	602	1/1	1.00	0.01	26,26,26,26	0
21	OEX	a	601	10/10	1.00	0.02	23,26,29,31	0
23	CL	a	603	1/1	1.00	0.03	28,28,28,28	0
23	CL	a	604	1/1	1.00	0.04	28,28,28,28	0

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

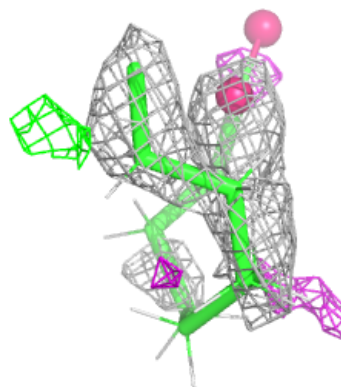
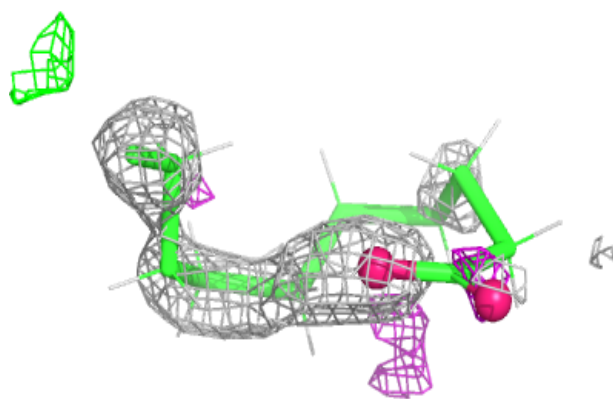
Electron density around STE C 528:

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



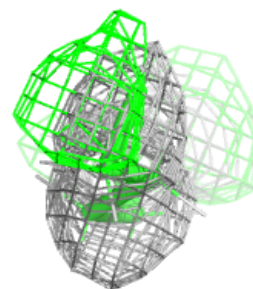
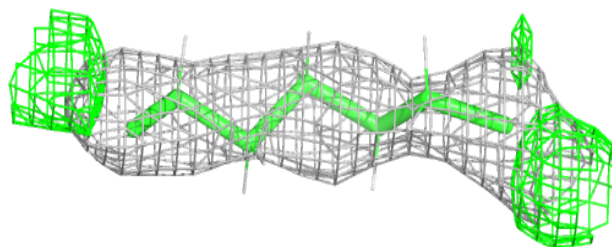
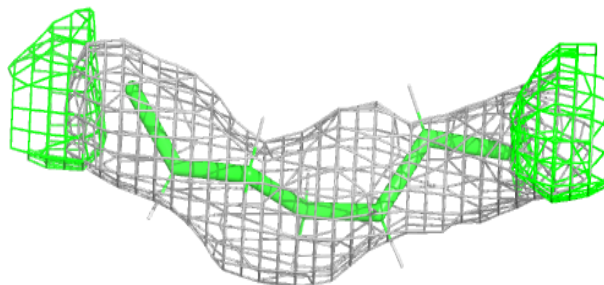
Electron density around STE i 101:

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

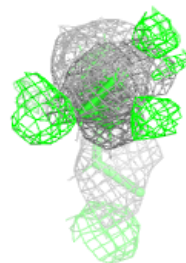
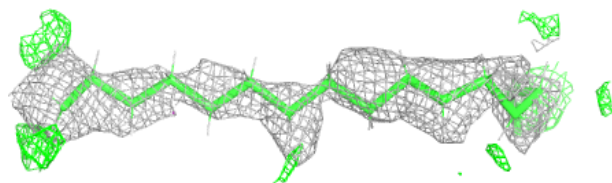
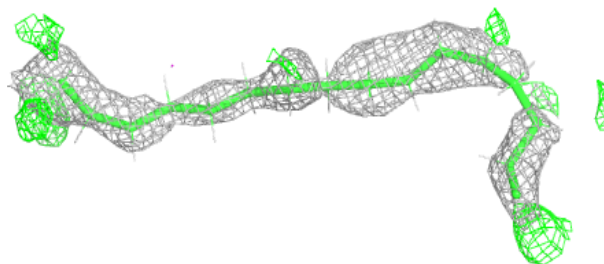


Electron density around STE C 518:

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

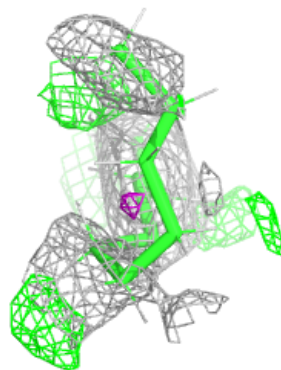
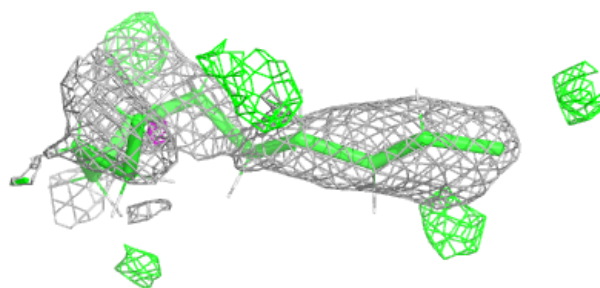
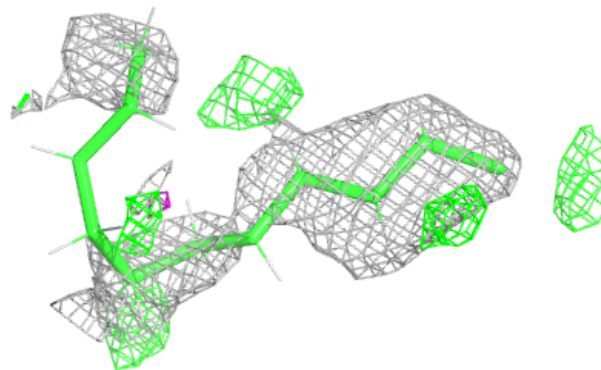
**Electron density around STE j 102:**

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

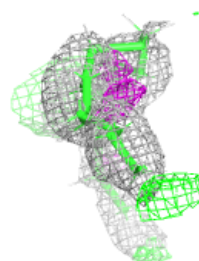
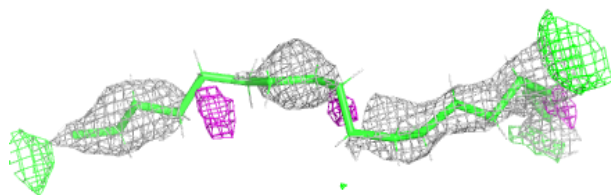
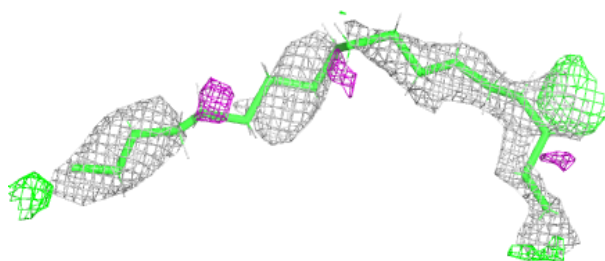


Electron density around STE A 619:

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

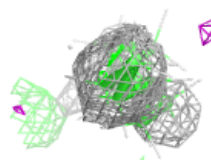
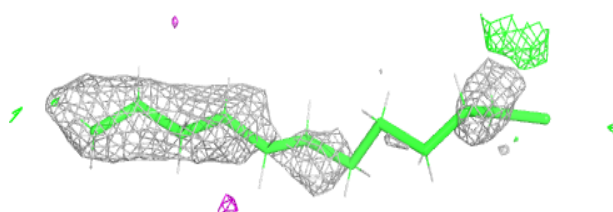
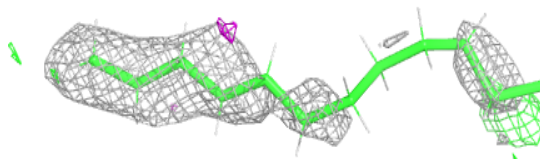
**Electron density around STE H 103:**

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

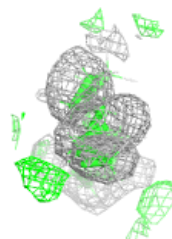
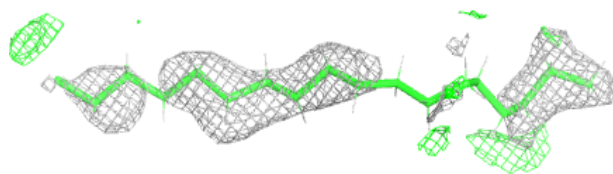
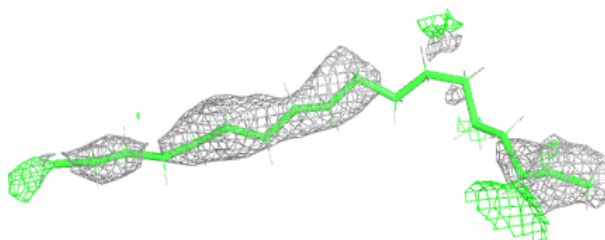


Electron density around STE E 102:

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

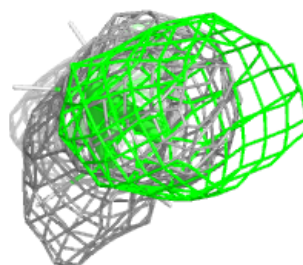
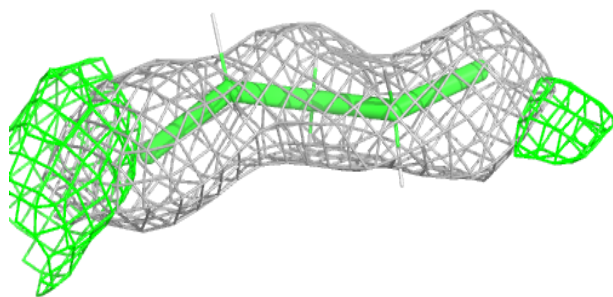
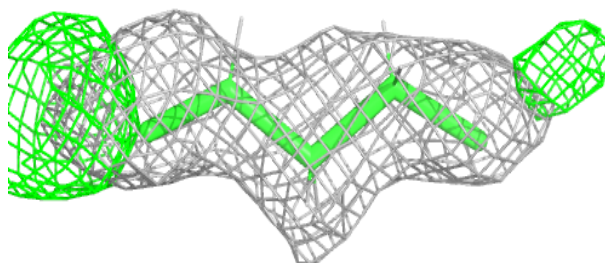
**Electron density around STE c 517:**

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

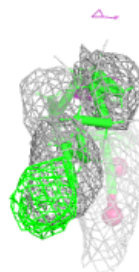
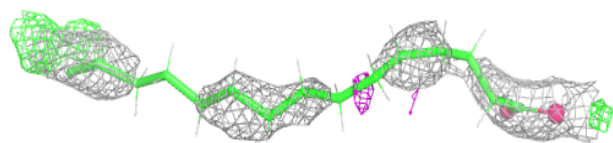
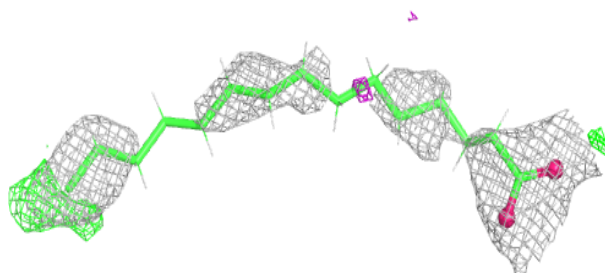


Electron density around STE C 517:

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

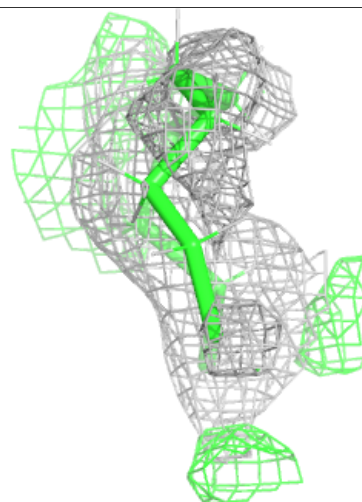
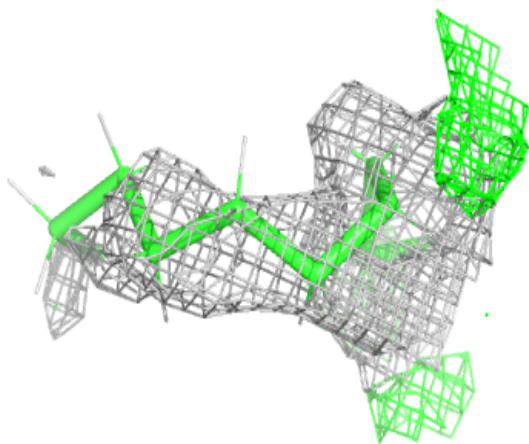
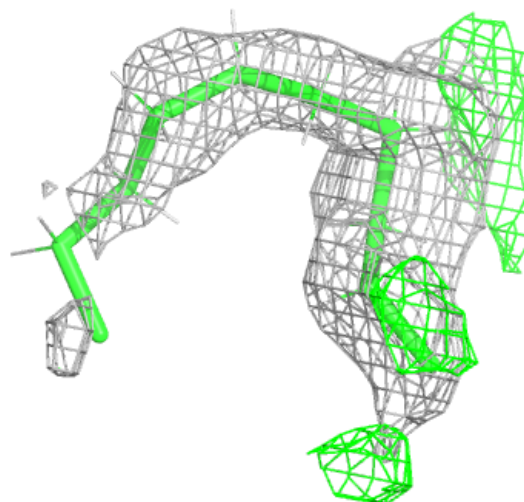
**Electron density around STE I 101:**

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



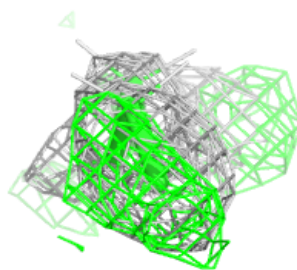
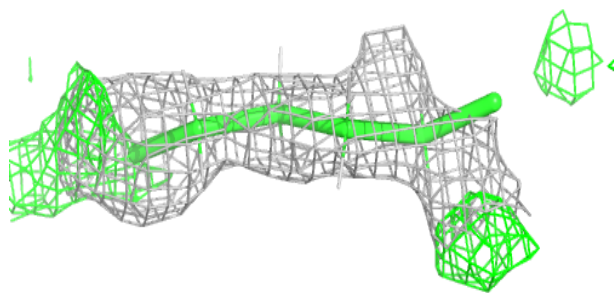
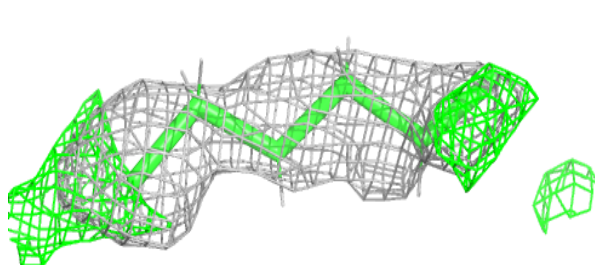
Electron density around STE C 519:

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

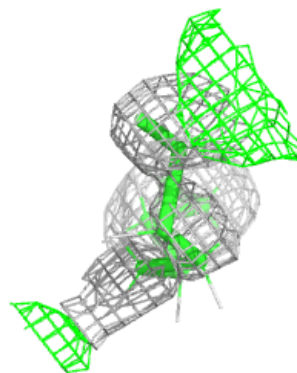
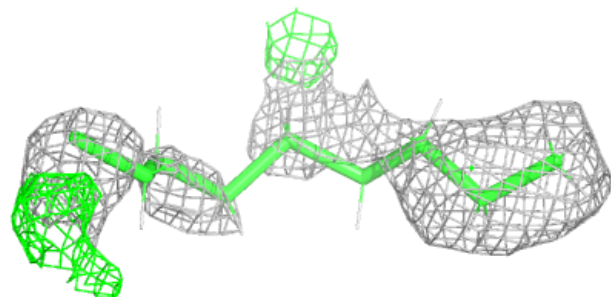
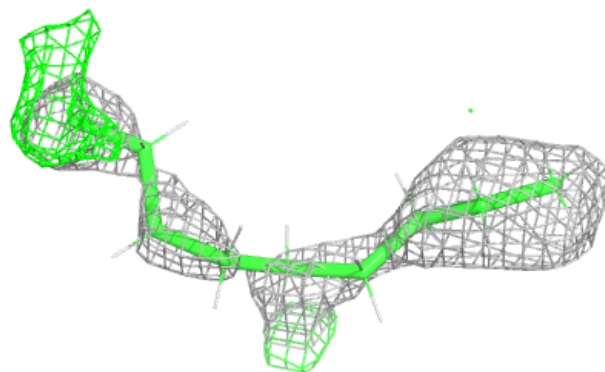


Electron density around STE i 102:

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

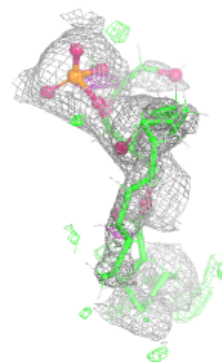
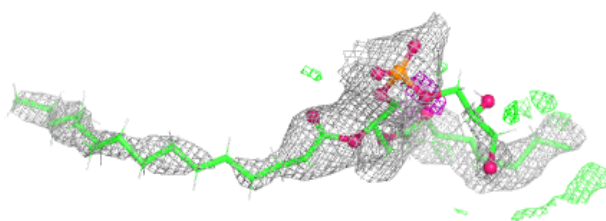
**Electron density around STE e 101:**

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

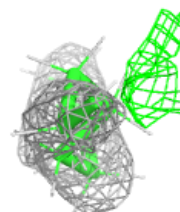
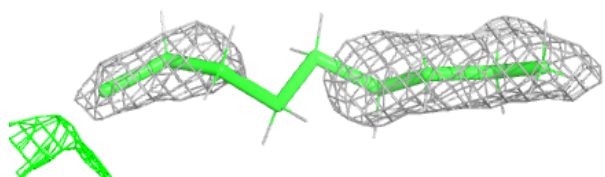
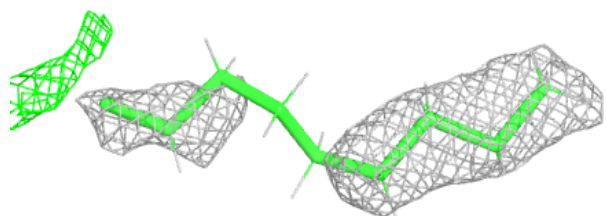


Electron density around LHG e 103:

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

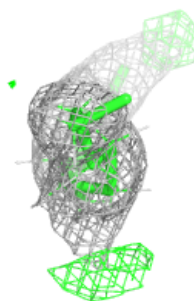
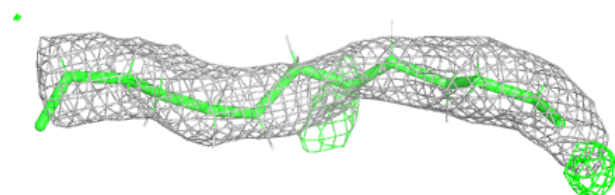
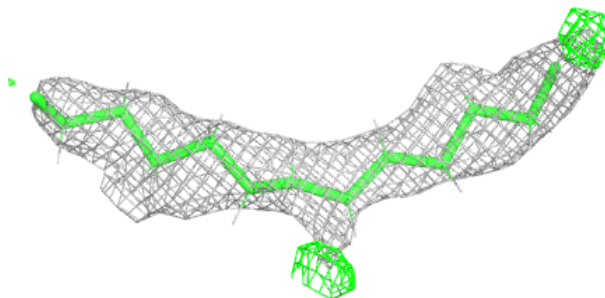
**Electron density around STE e 104:**

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

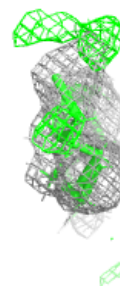
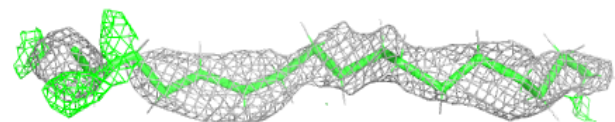
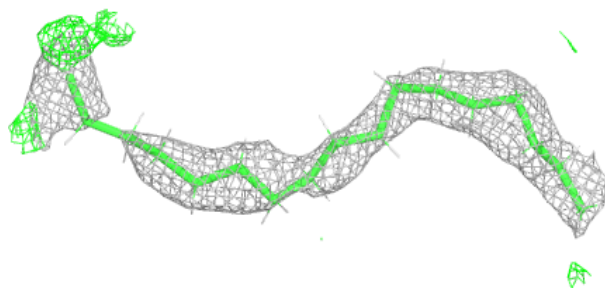


Electron density around STE c 516:

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

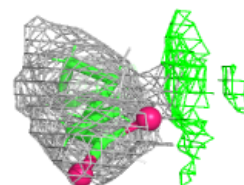
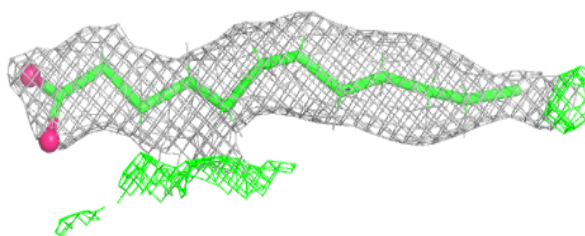
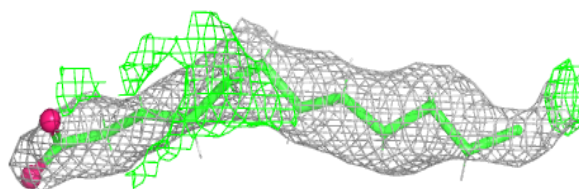
**Electron density around STE A 618:**

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

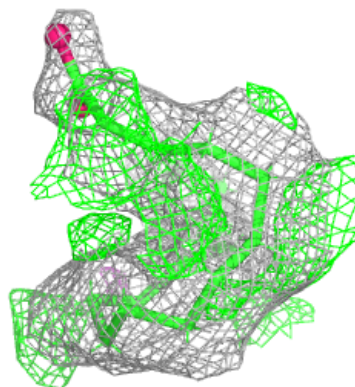
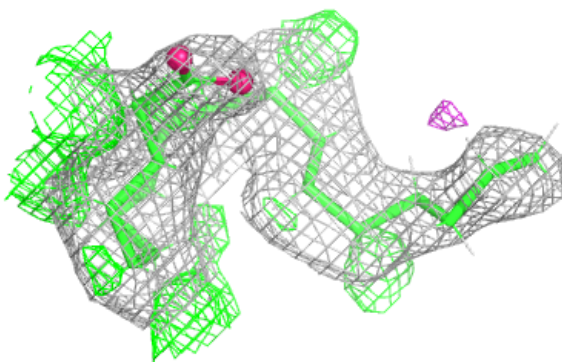
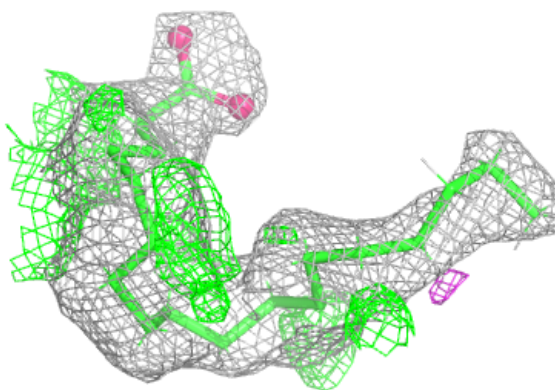


Electron density around STE d 415:

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

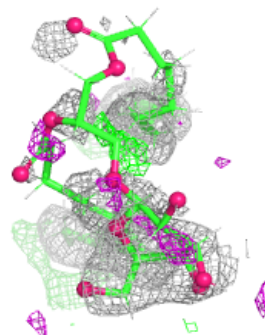
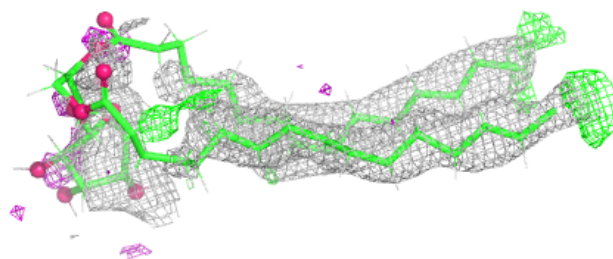
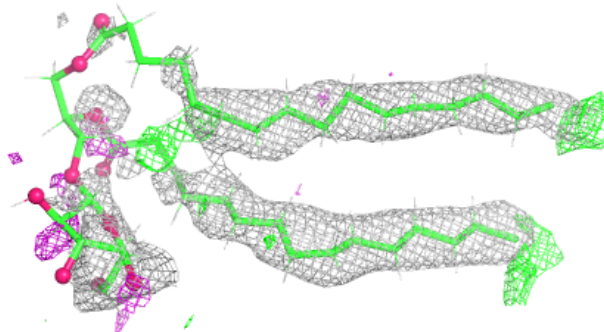
**Electron density around STE R 101:**

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

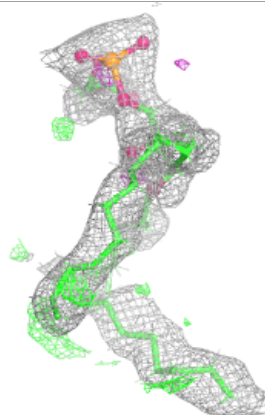
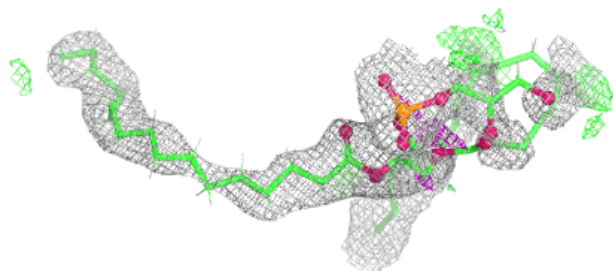
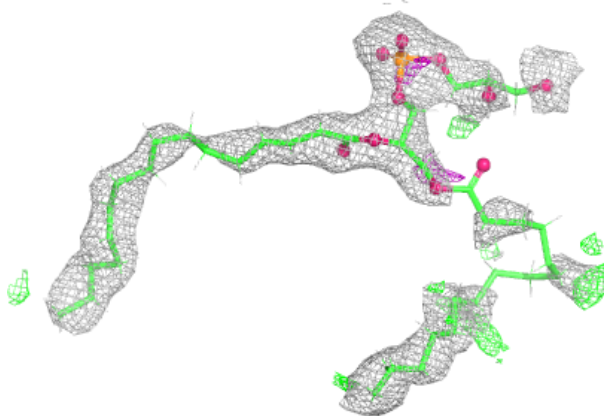


Electron density around LMG D 407:

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

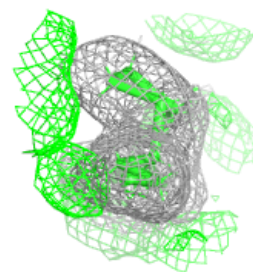
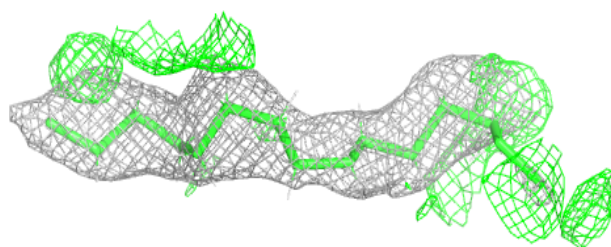
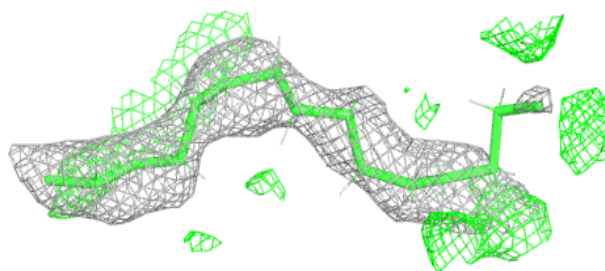
**Electron density around LHG A 615:**

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

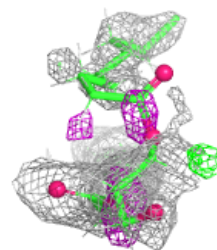
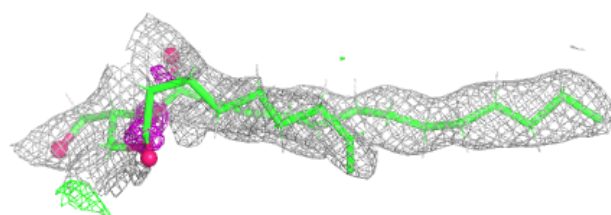
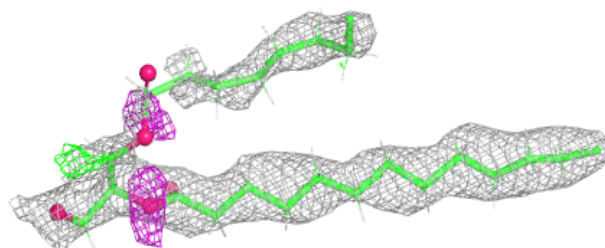


Electron density around STE B 626:

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

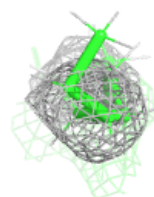
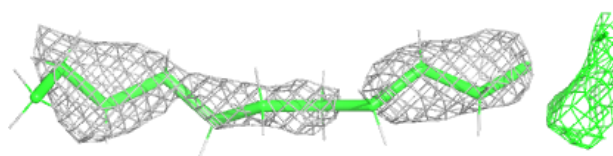
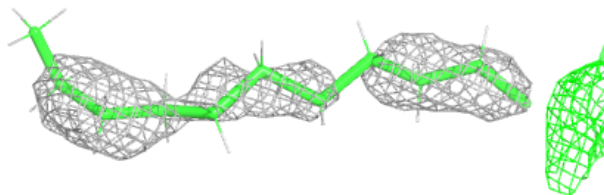
**Electron density around LMG c 518:**

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

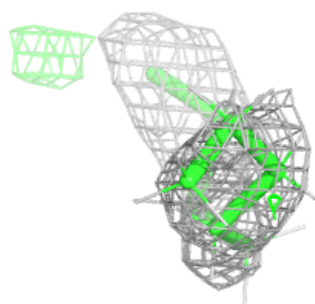
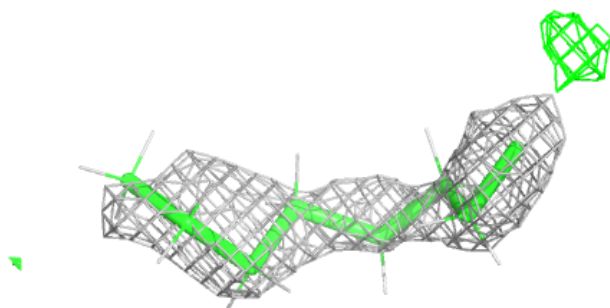
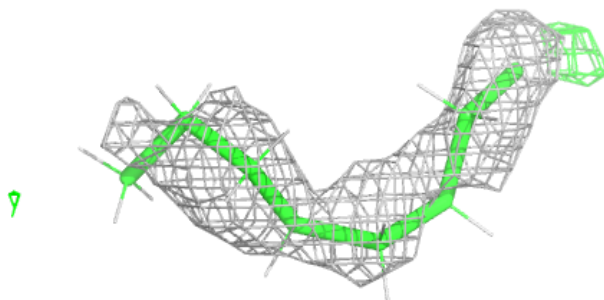


Electron density around STE b 627:

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

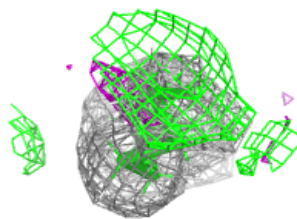
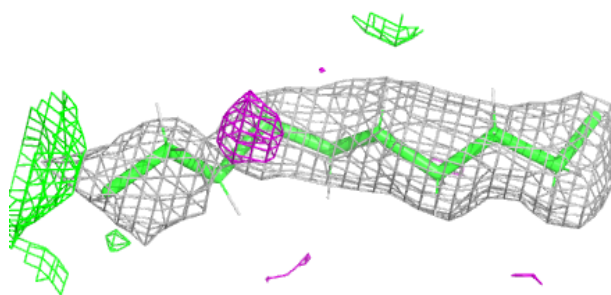
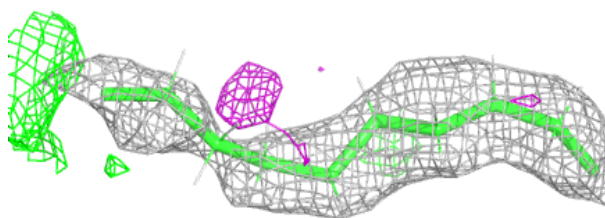
**Electron density around STE f 102:**

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

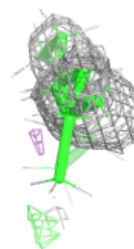
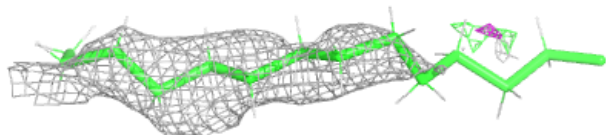
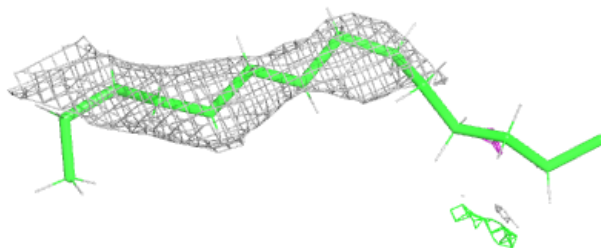


Electron density around STE t 103:

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

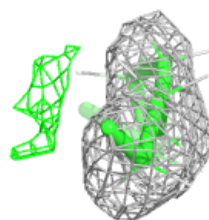
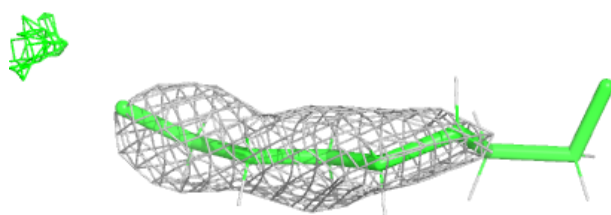
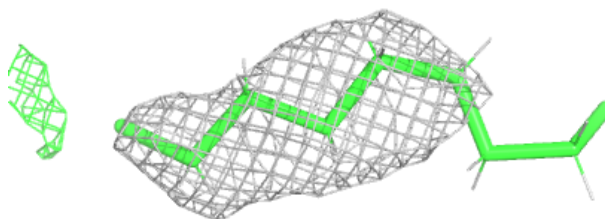
**Electron density around STE C 527:**

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

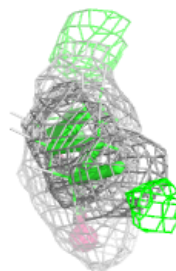
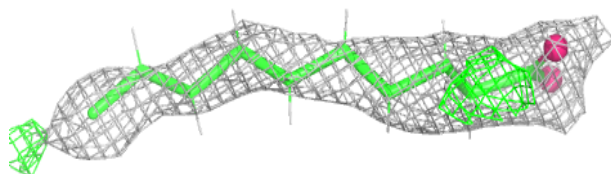
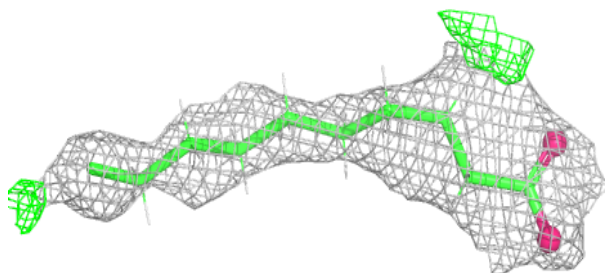


Electron density around STE A 611:

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

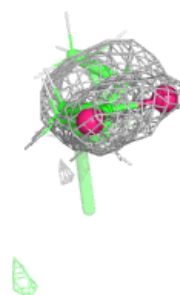
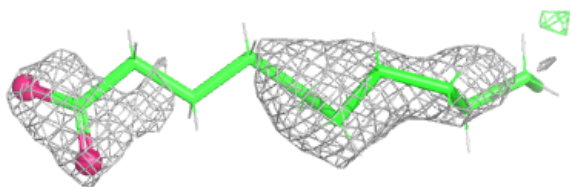
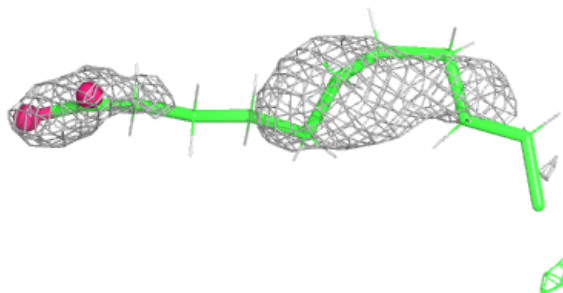
**Electron density around STE a 612:**

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

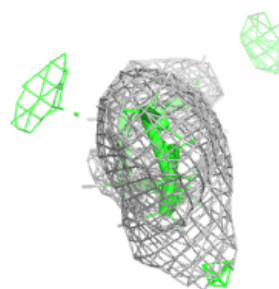
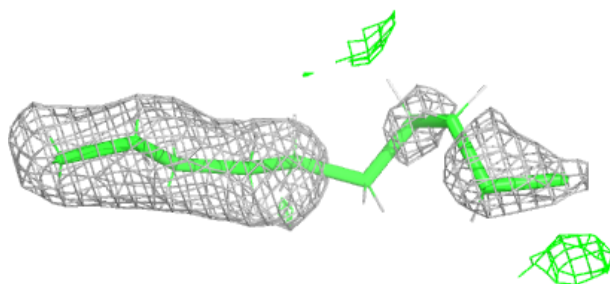
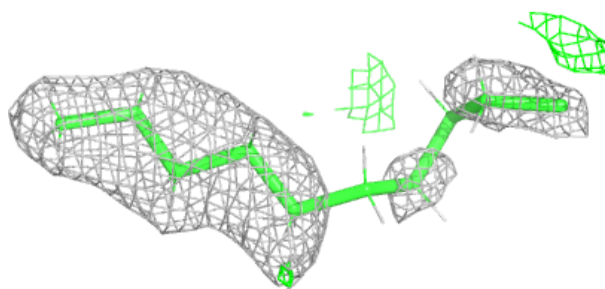


Electron density around STE e 105:

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

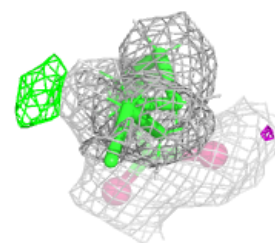
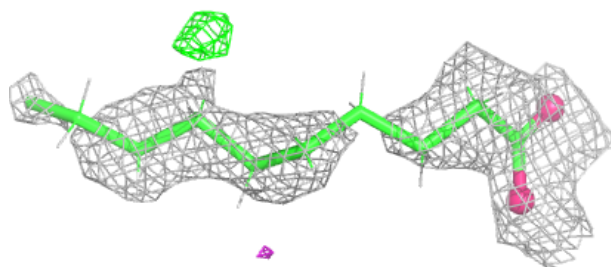
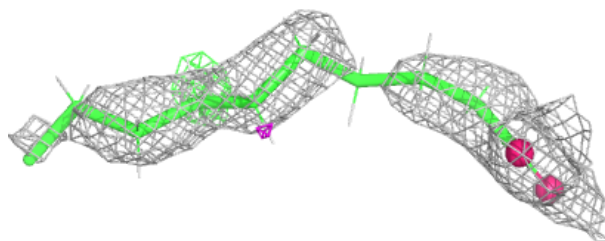
**Electron density around STE h 103:**

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

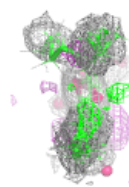
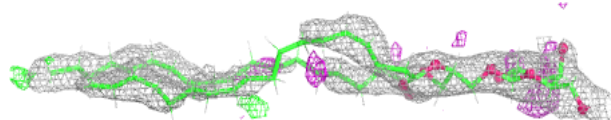
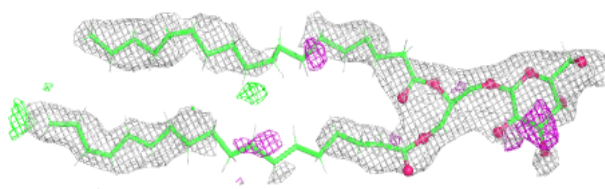


Electron density around STE E 101:

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

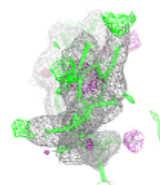
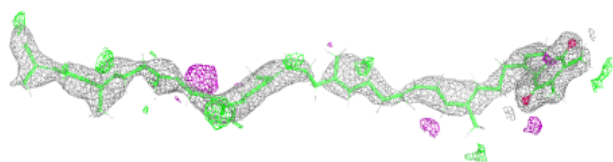
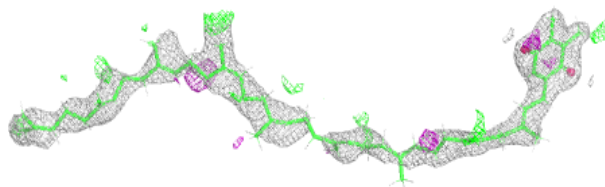
**Electron density around LMG b 623:**

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

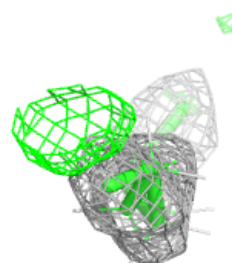
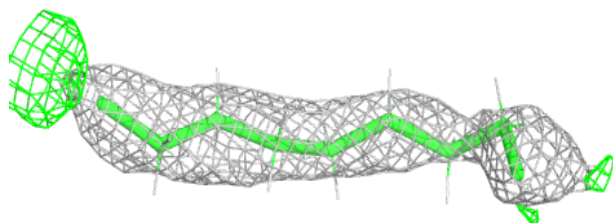
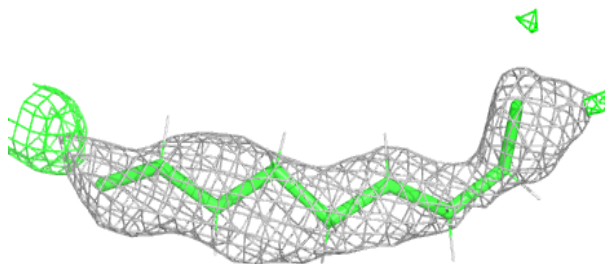


Electron density around PL9 A 610:

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

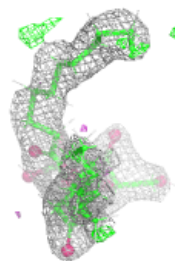
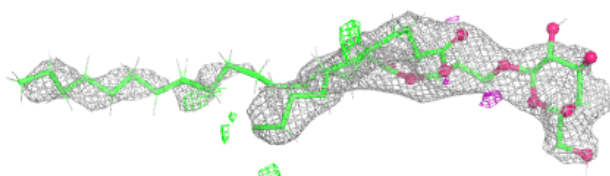
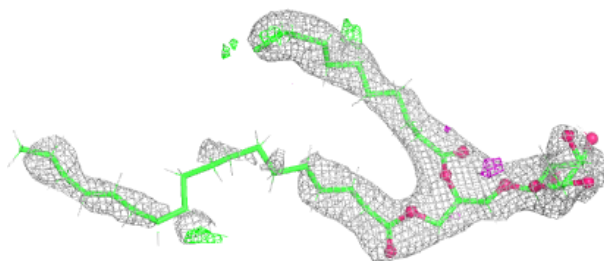
**Electron density around STE z 101:**

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

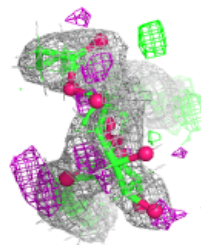
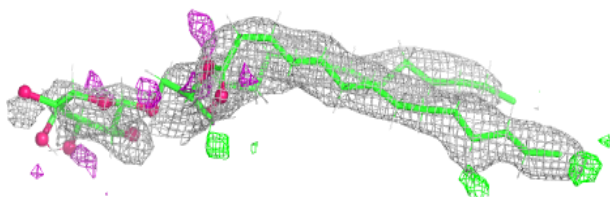
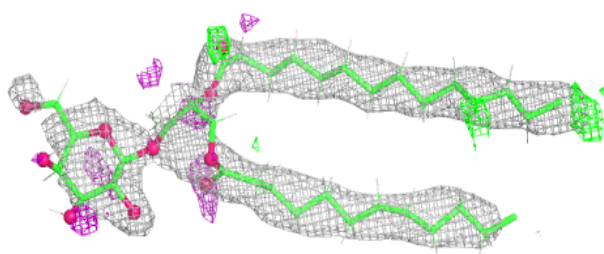


Electron density around LMG c 523:

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

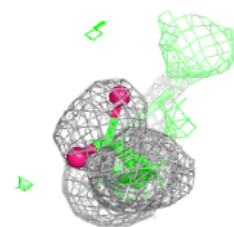
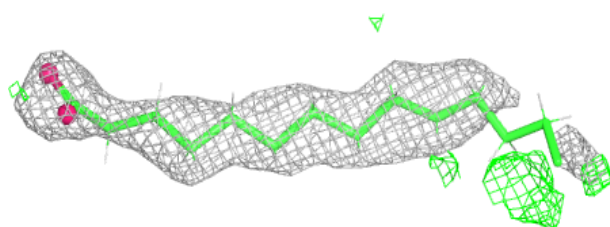
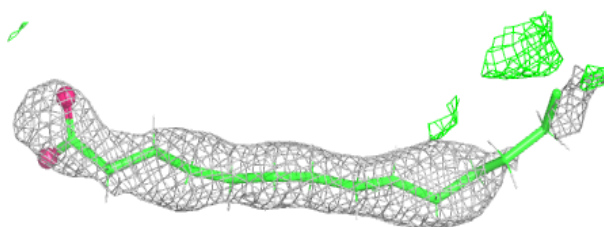
**Electron density around LMG B 620:**

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

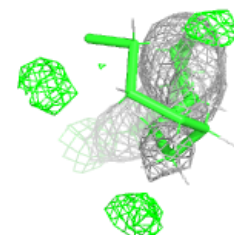
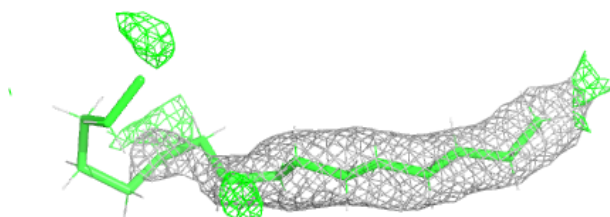
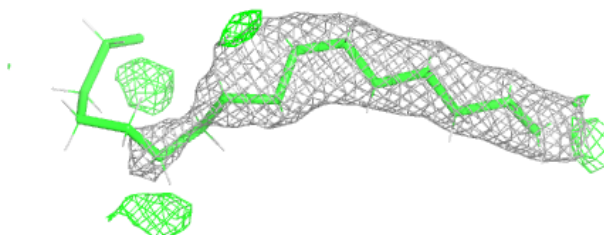


Electron density around STE b 624:

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

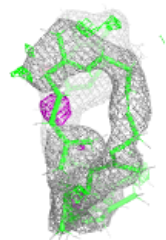
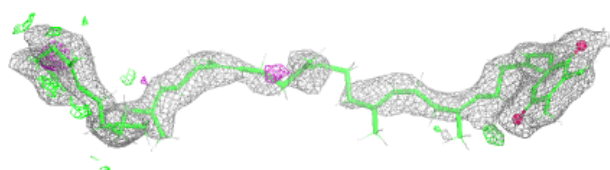
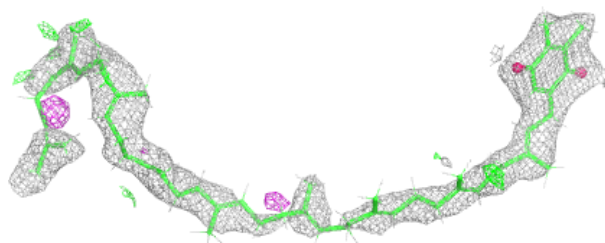
**Electron density around STE b 621:**

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

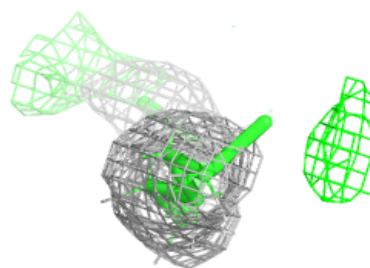
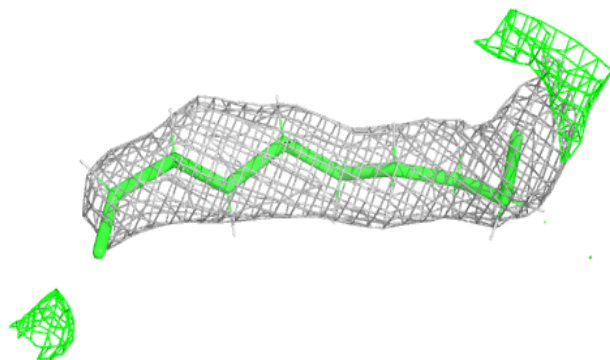
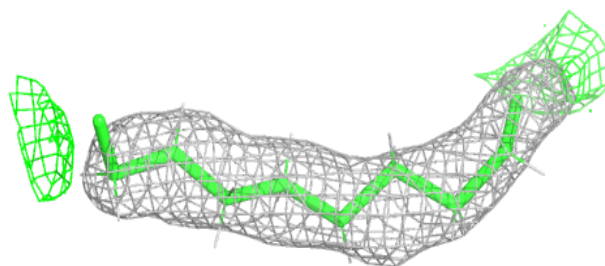


Electron density around PL9 a 609:

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

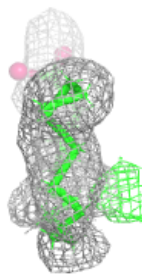
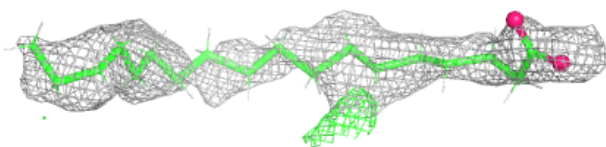
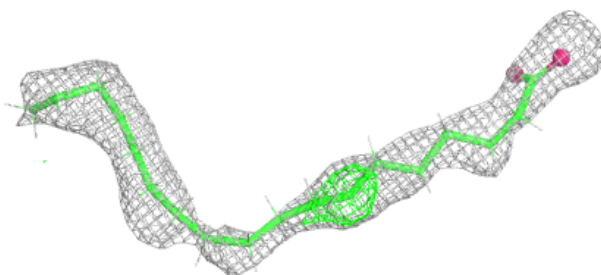
**Electron density around STE b 625:**

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

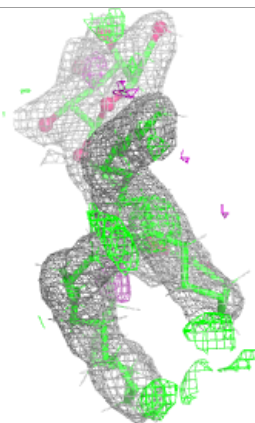
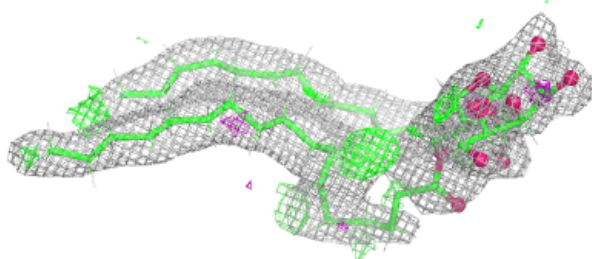
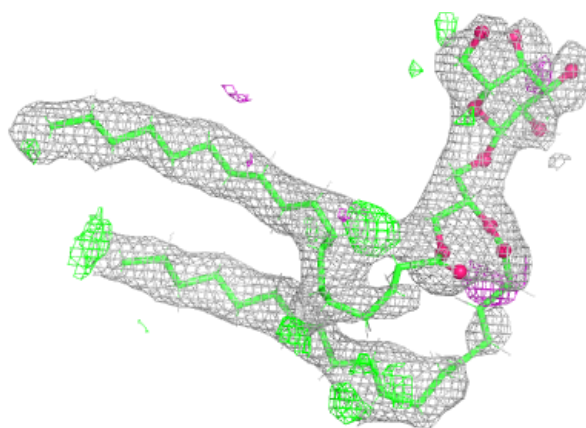


Electron density around STE E 103:

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

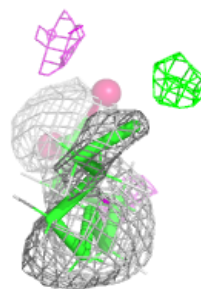
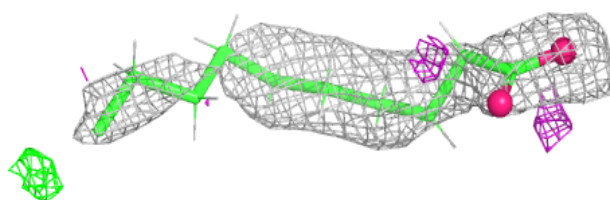
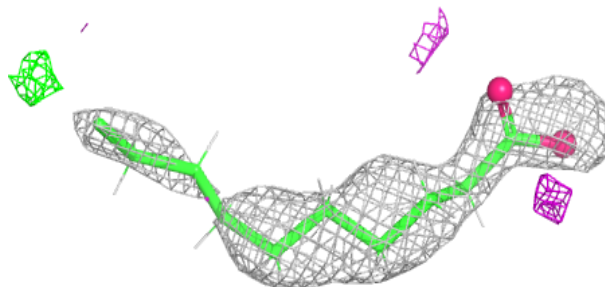
**Electron density around LMG o 301:**

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

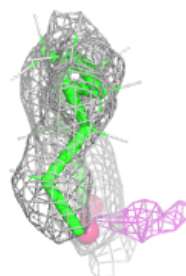
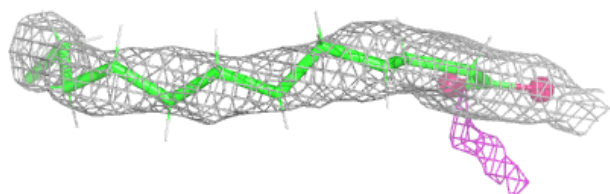
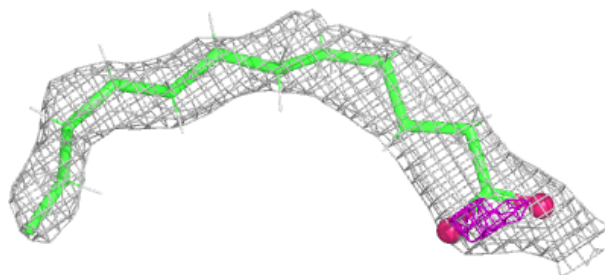


Electron density around STE B 625:

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

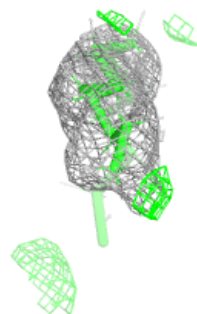
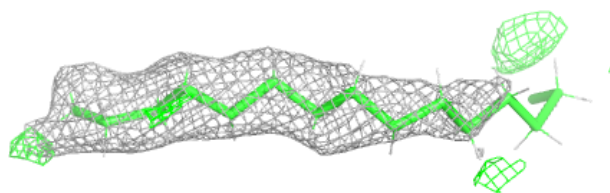
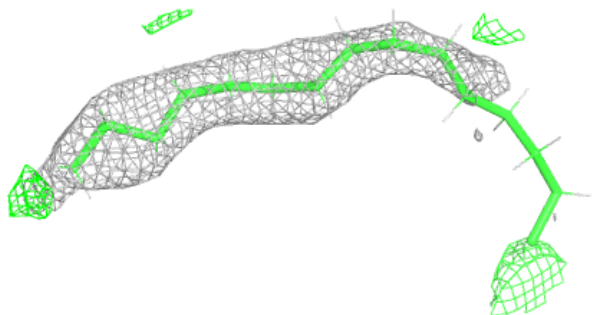
**Electron density around STE C 515:**

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

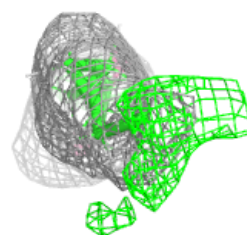
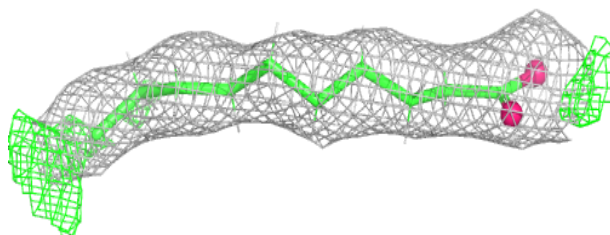
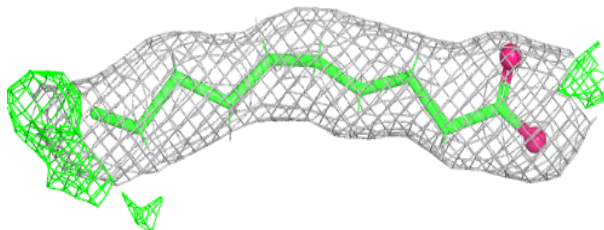


Electron density around STE M 103:

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

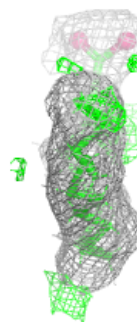
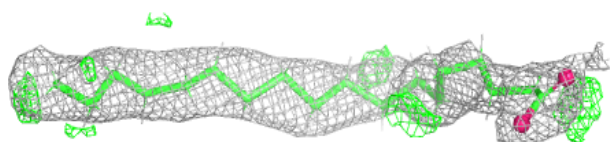
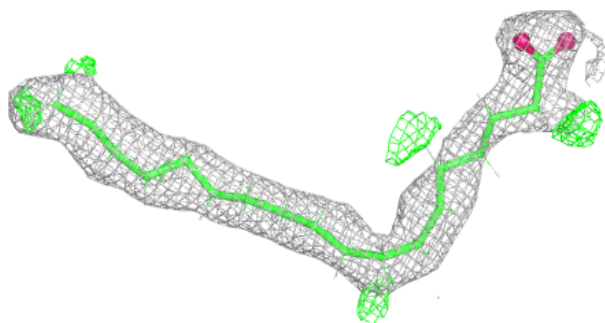
**Electron density around STE j 101:**

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

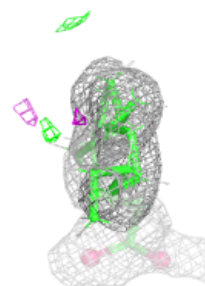
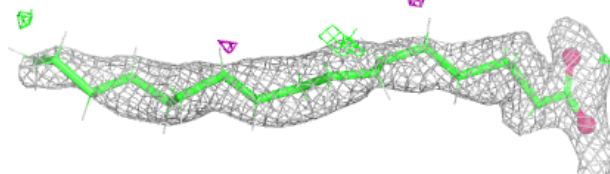
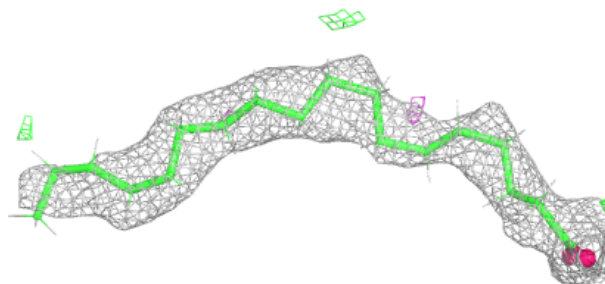


Electron density around STE d 409:

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

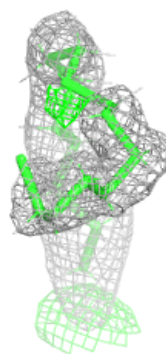
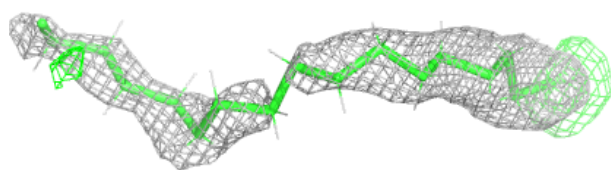
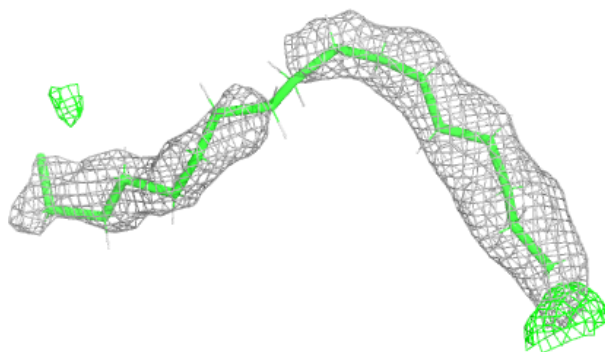
**Electron density around STE d 413:**

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

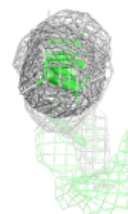
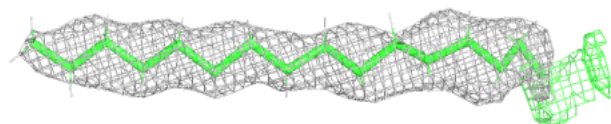
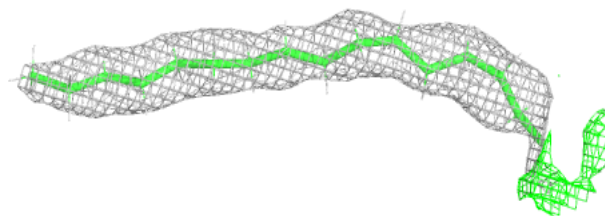


Electron density around STE Z 101:

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

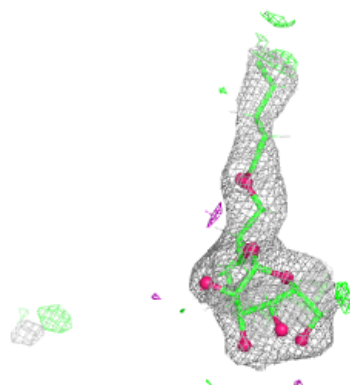
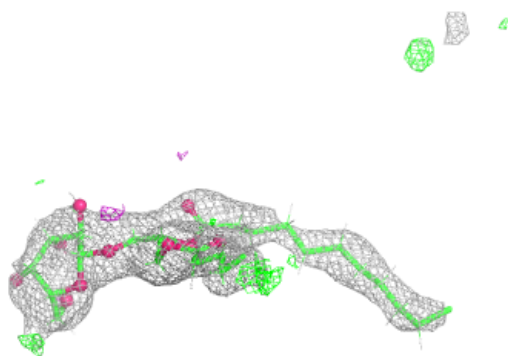
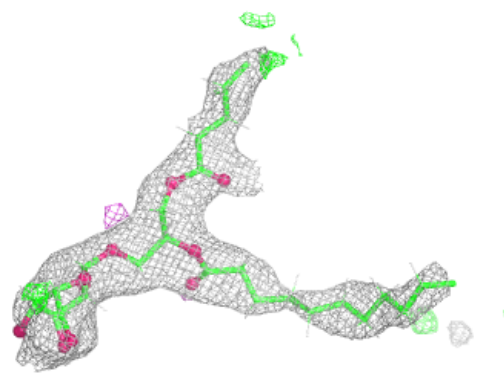
**Electron density around STE C 526:**

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

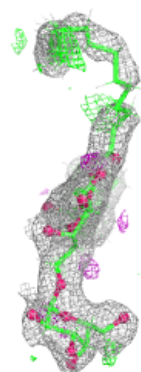
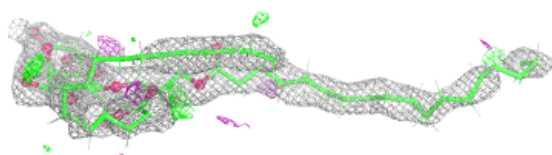
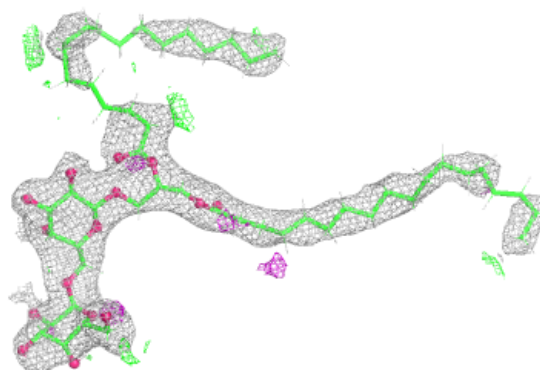


Electron density around LMG C 516:

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

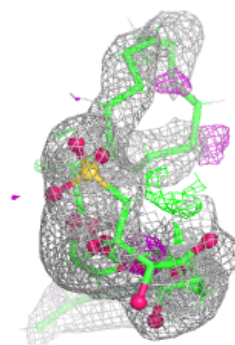
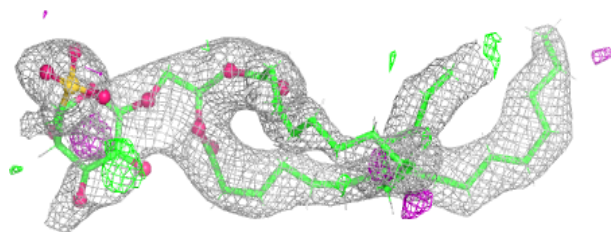
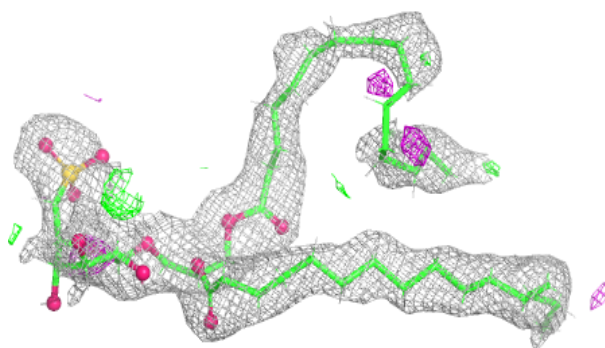
**Electron density around DGD A 617:**

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



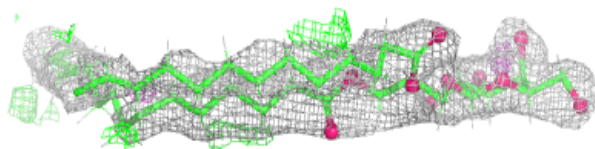
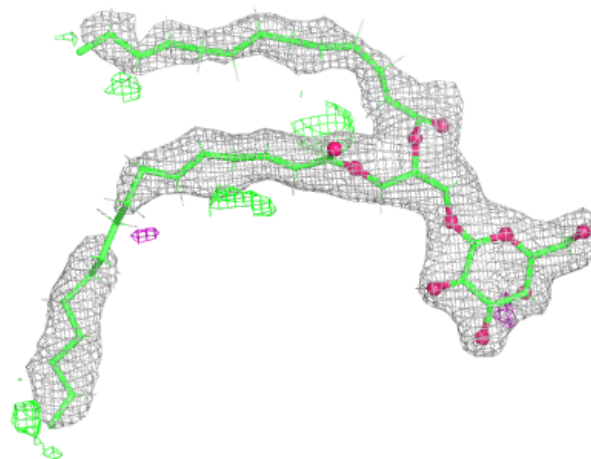
Electron density around SQD a 611:

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



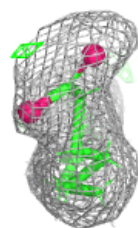
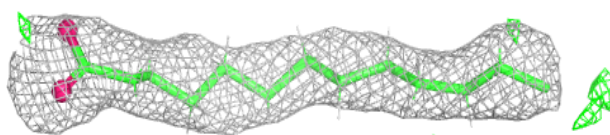
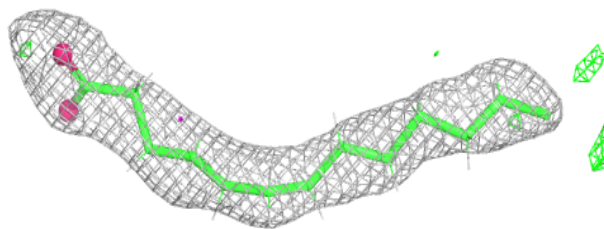
Electron density around LMG C 524:

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

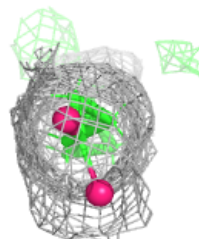
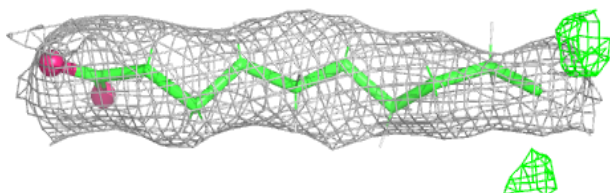
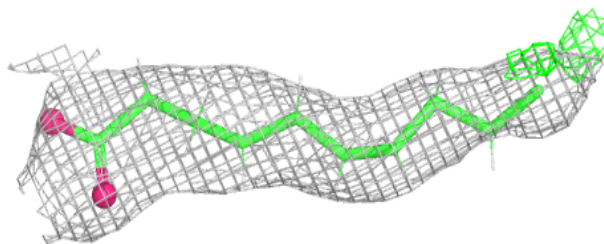


Electron density around STE I 102:

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

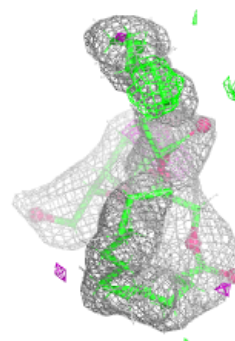
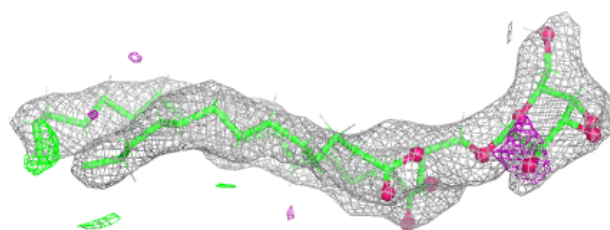
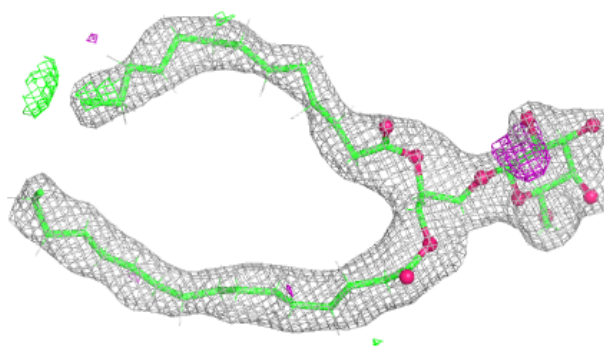
**Electron density around STE J 101:**

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

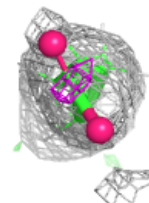
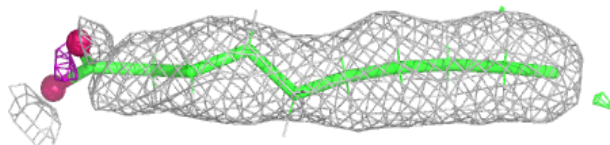
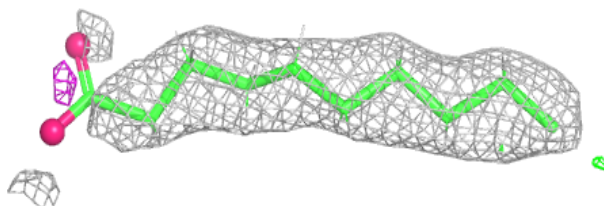


Electron density around LMG A 613:

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

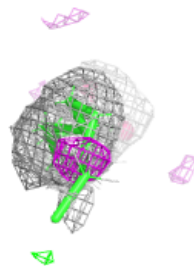
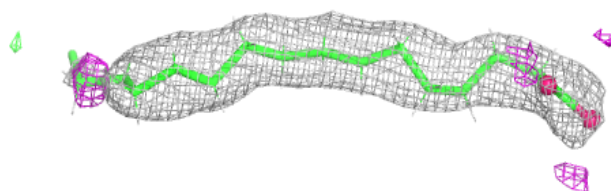
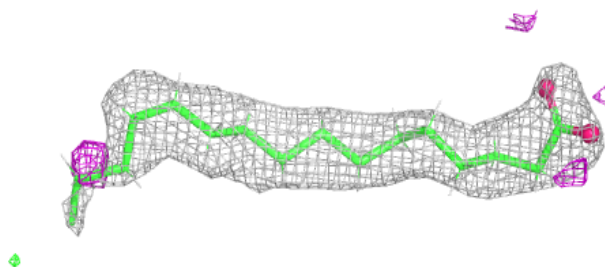
**Electron density around STE m 102:**

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



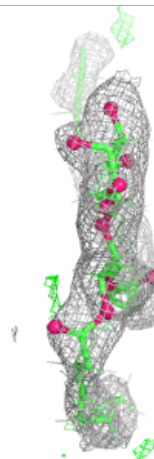
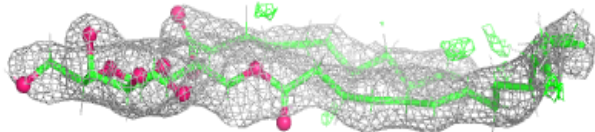
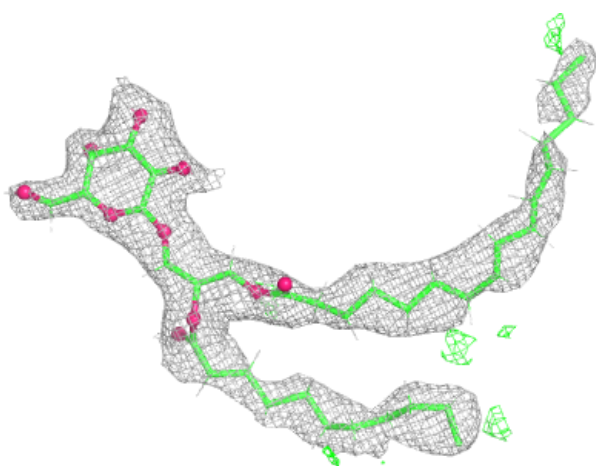
Electron density around STE B 624:

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



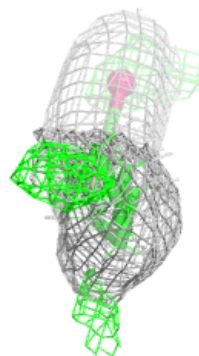
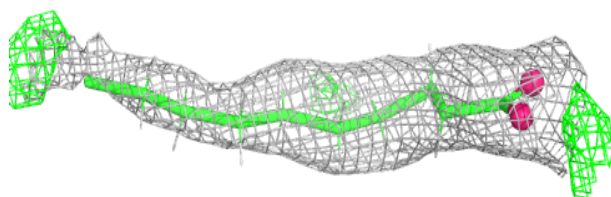
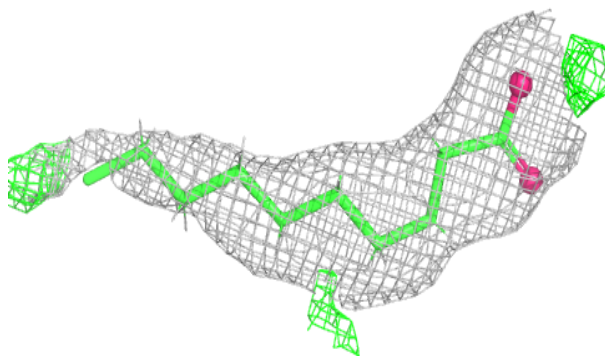
Electron density around LMG c 522:

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

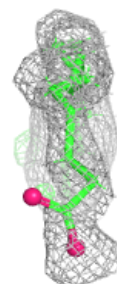
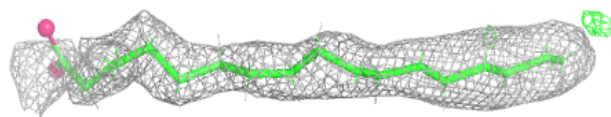
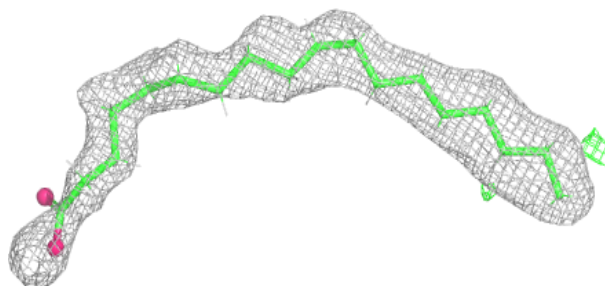


Electron density around STE C 525:

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

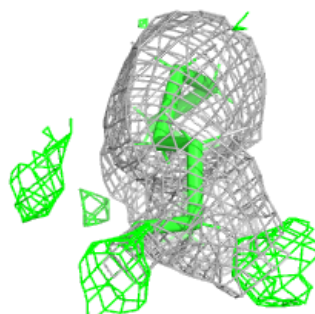
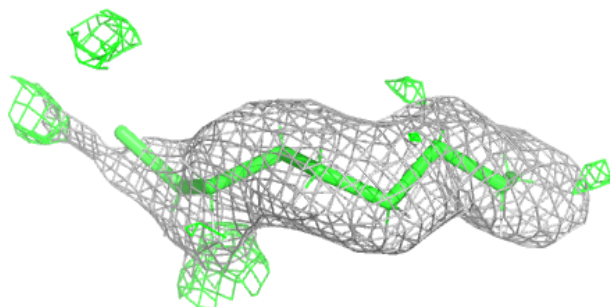
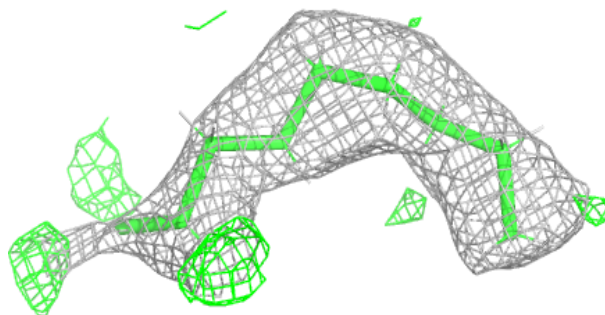
**Electron density around STE x 101:**

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

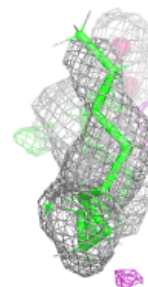
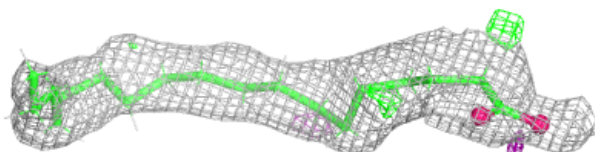
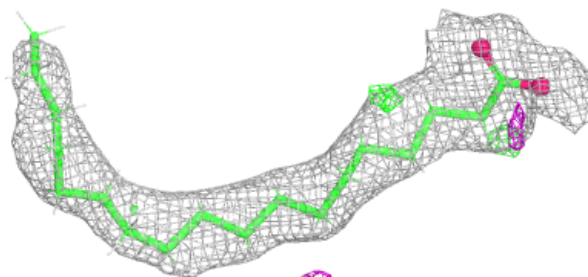


Electron density around STE D 412:

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

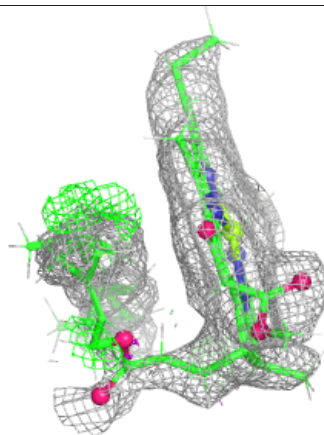
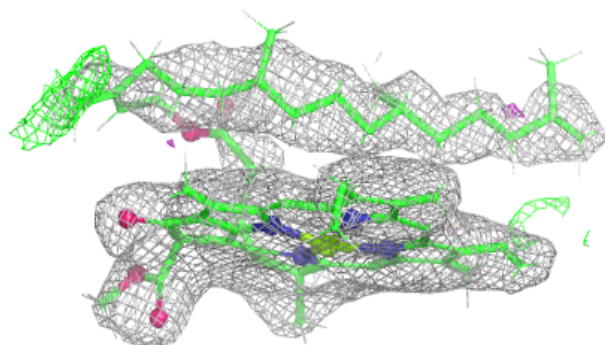
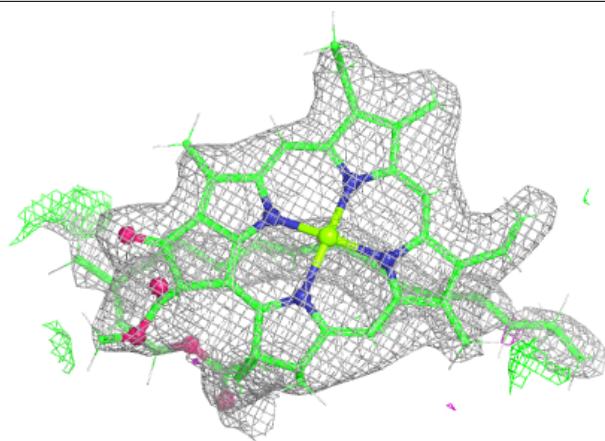
**Electron density around STE b 622:**

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

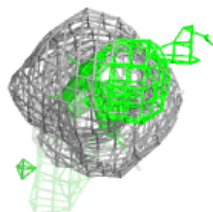
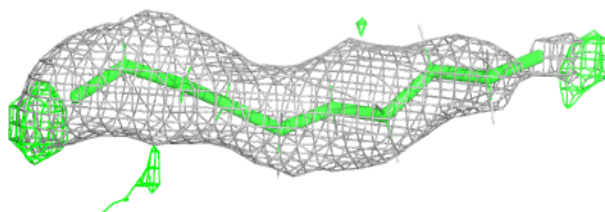
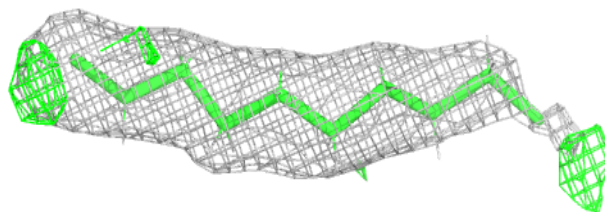


Electron density around CLA b 601:

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

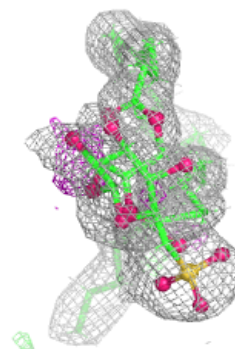
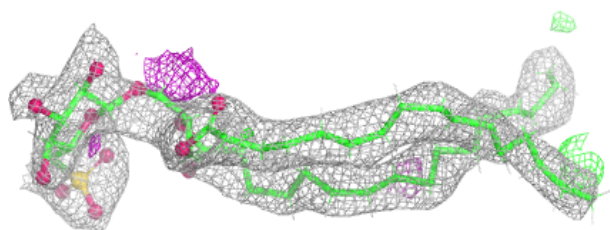
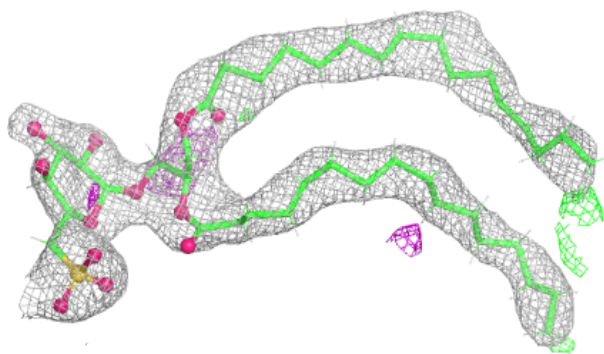
**Electron density around STE M 102:**

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

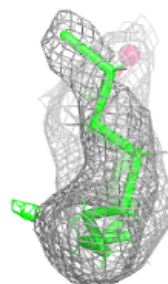
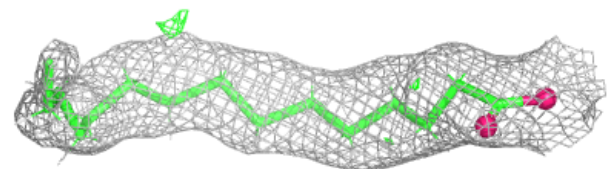
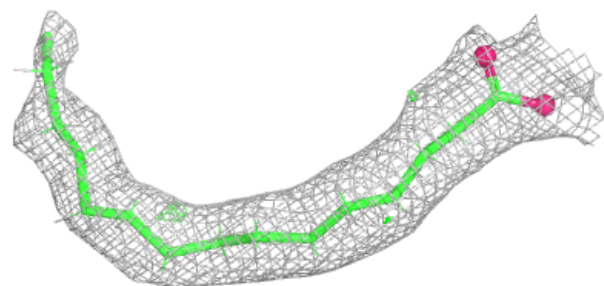


Electron density around SQD B 623:

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

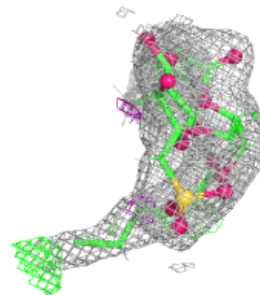
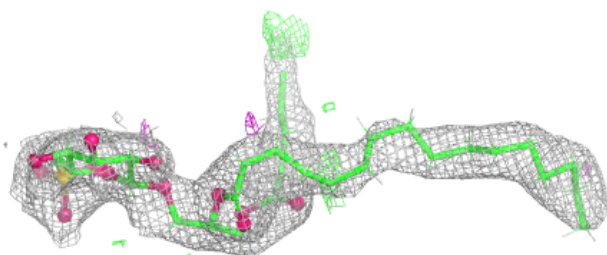
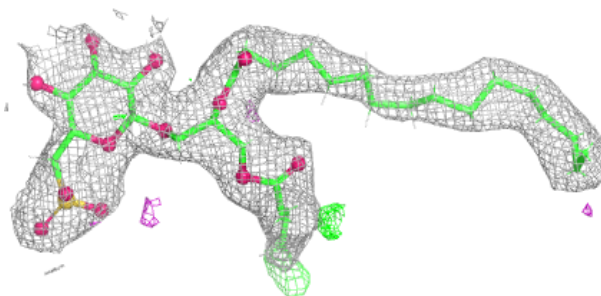
**Electron density around STE B 622:**

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

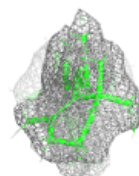
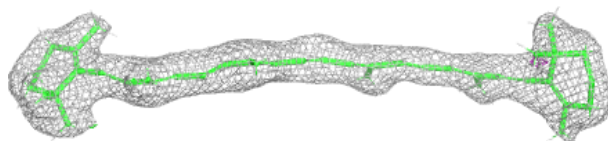
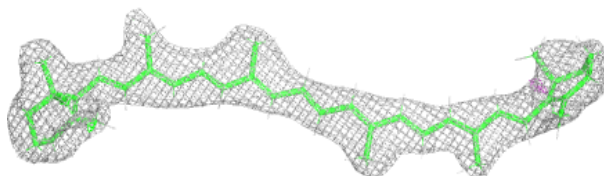


Electron density around SQD A 616:

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

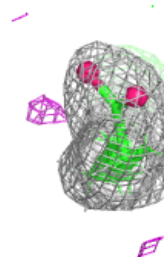
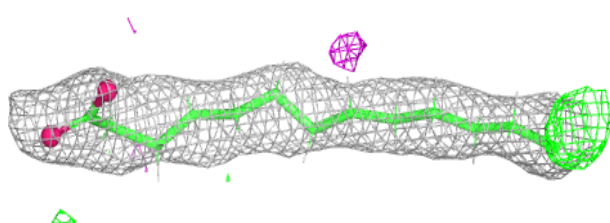
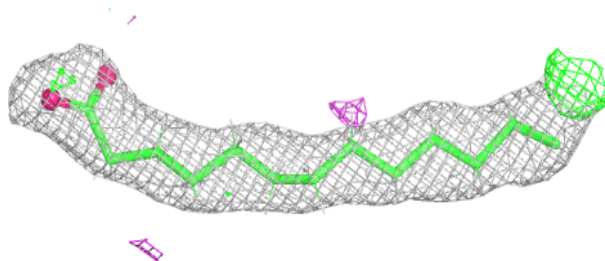
**Electron density around BCR k 101:**

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

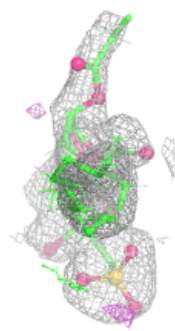
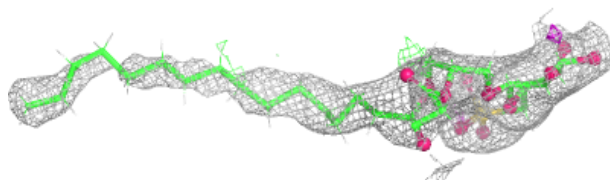
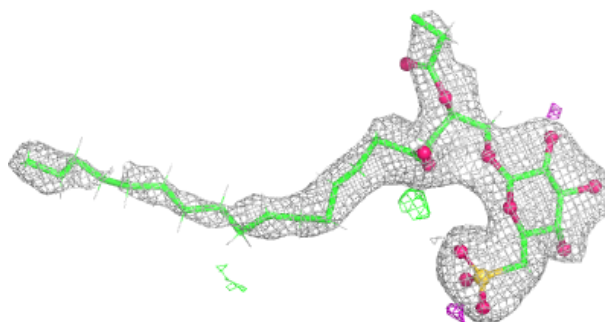


Electron density around STE M 101:

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

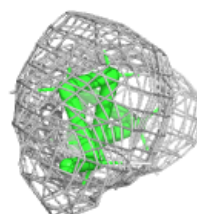
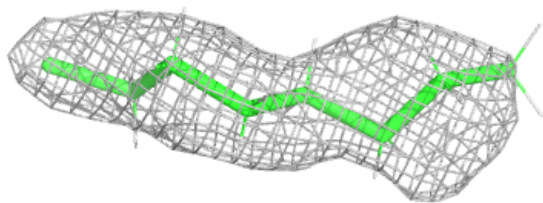
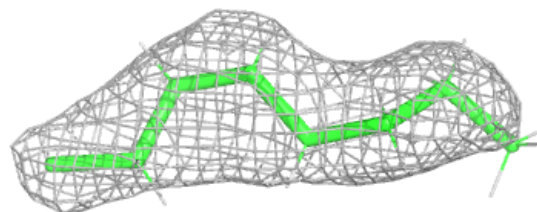
**Electron density around SQD f 101:**

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

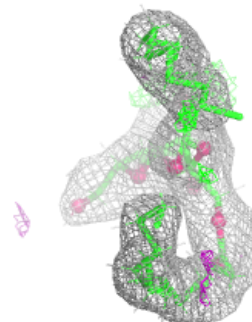
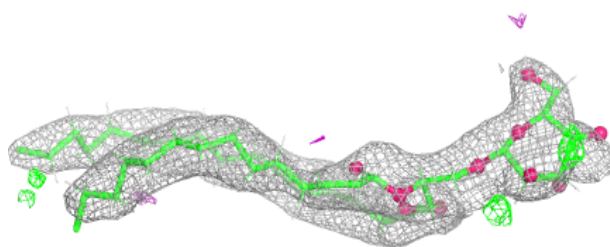
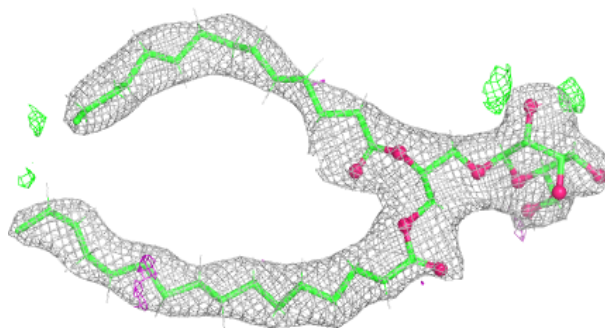


Electron density around STE b 626:

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

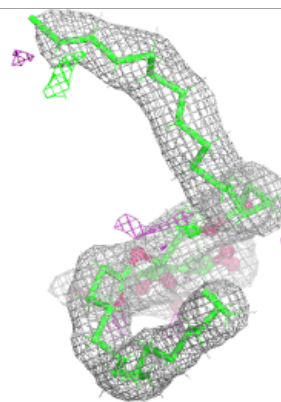
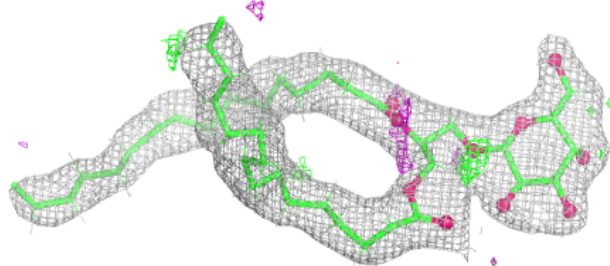
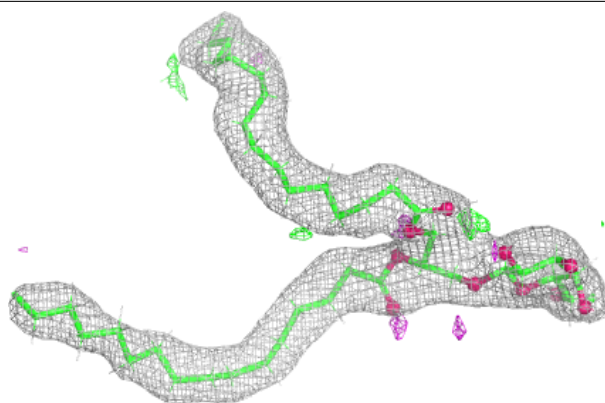
**Electron density around LMG c 524:**

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

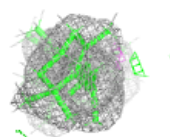
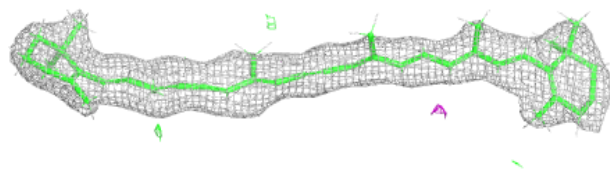
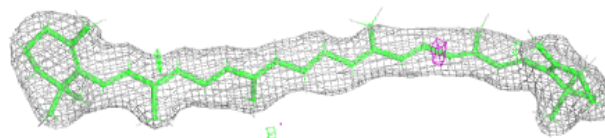


Electron density around LMG m 101:

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

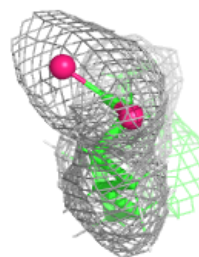
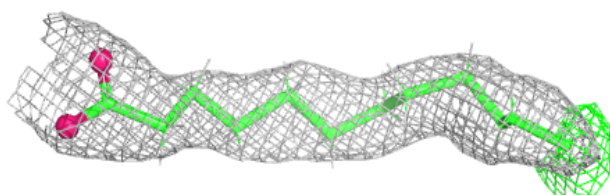
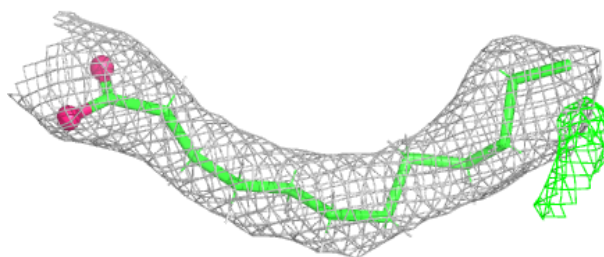
**Electron density around BCR K 101:**

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

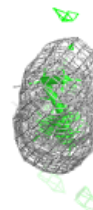
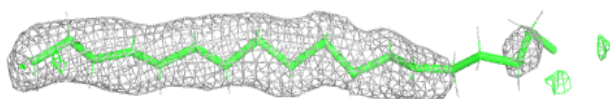
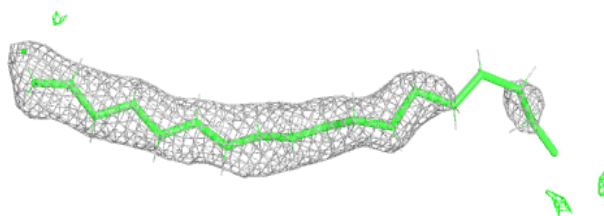


Electron density around STE t 102:

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

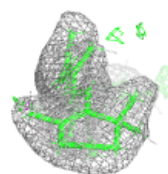
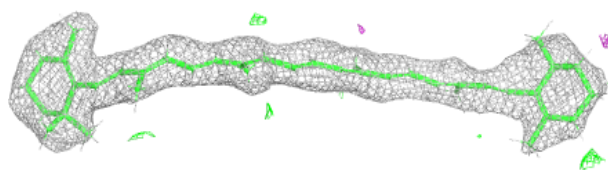
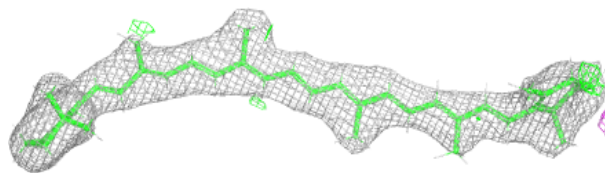
**Electron density around STE l 102:**

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

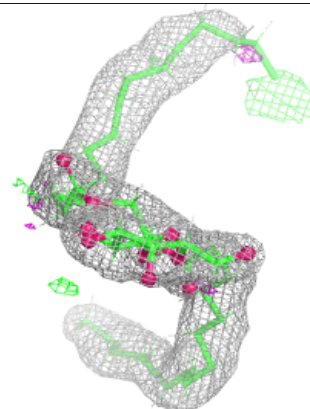
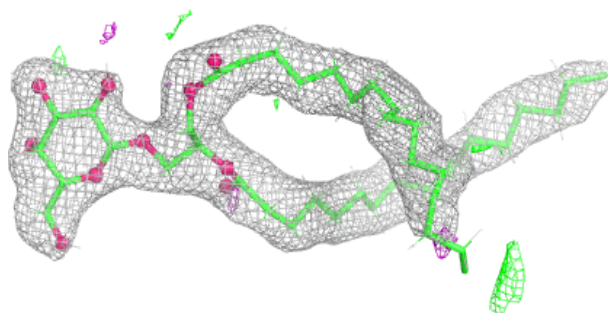
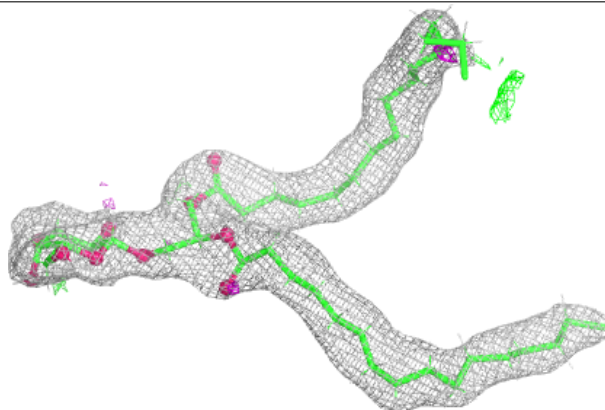


Electron density around BCR h 101:

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

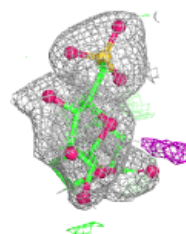
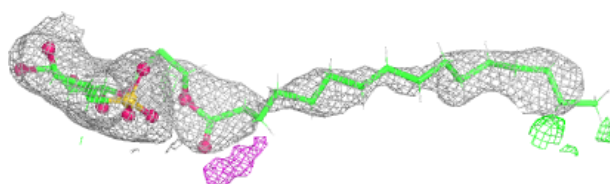
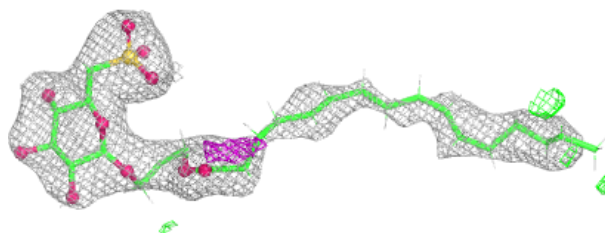
**Electron density around LMG B 621:**

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



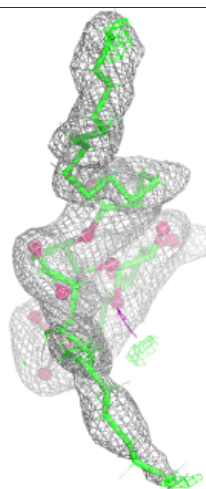
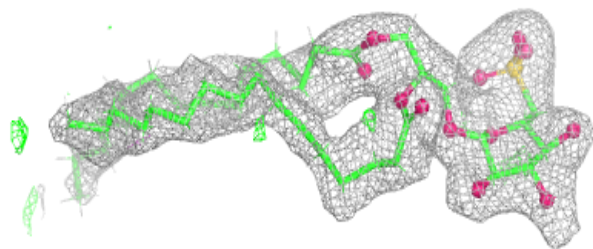
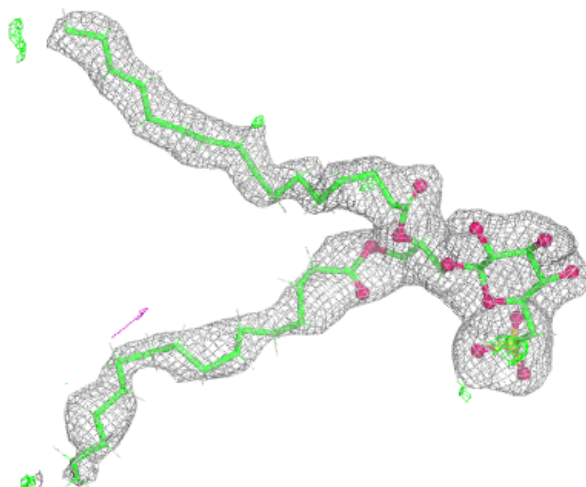
Electron density around SQD F 102:

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



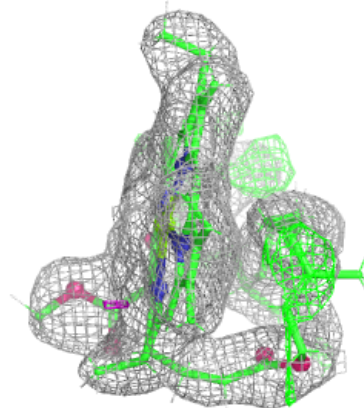
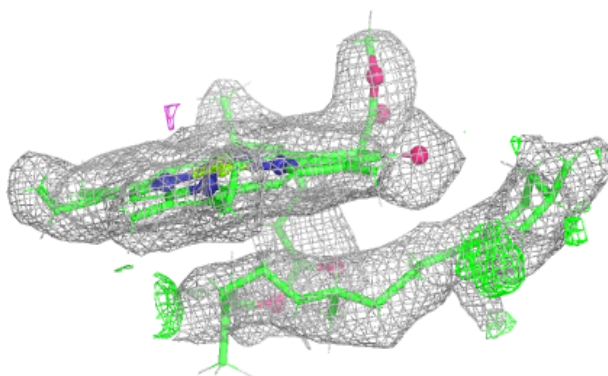
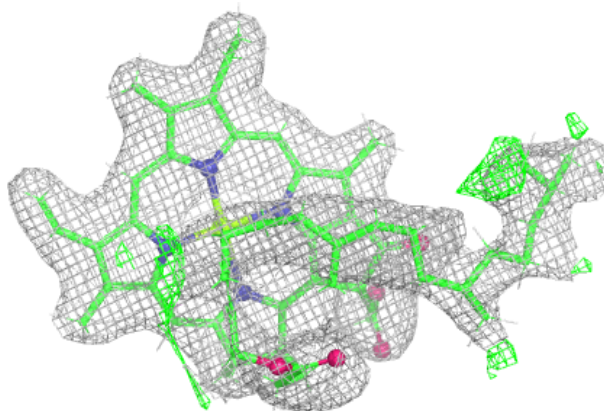
Electron density around SQD a 610:

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

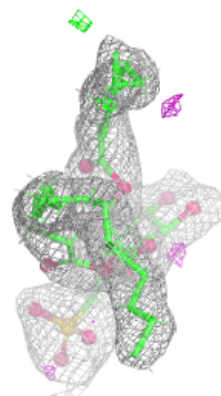
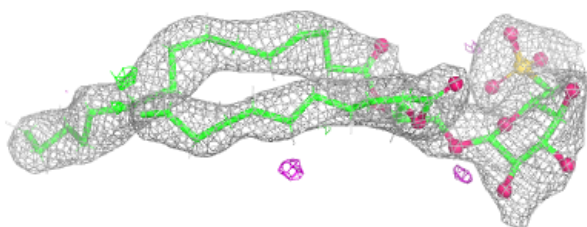
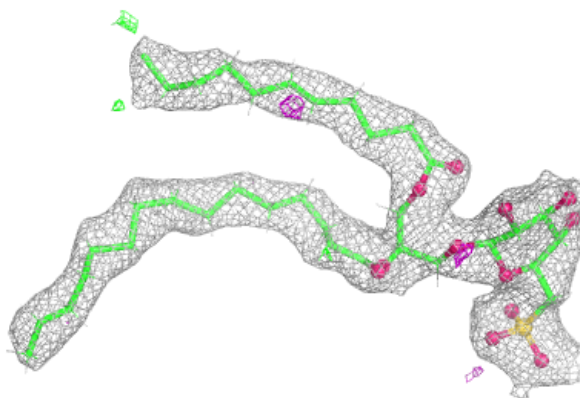


Electron density around CLA B 601:

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

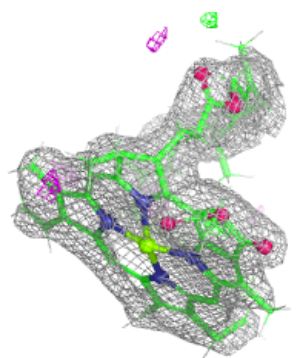
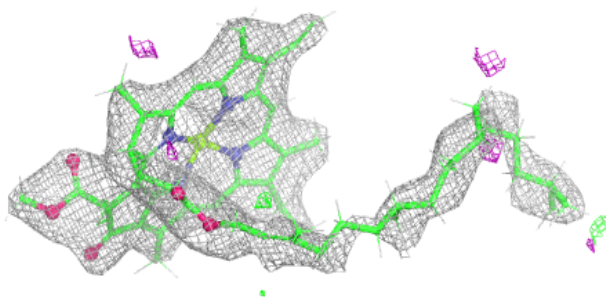
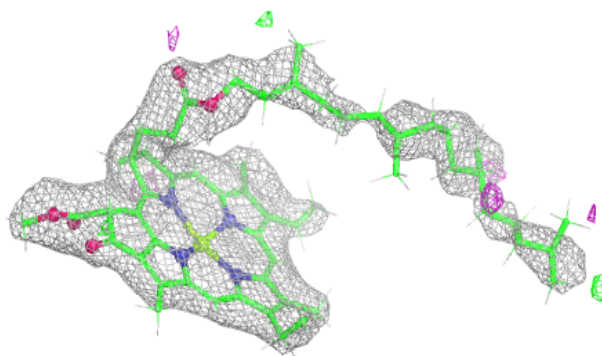
**Electron density around SQD b 620:**

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

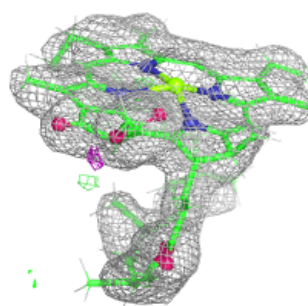
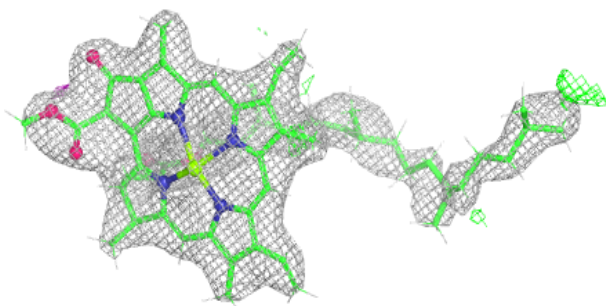
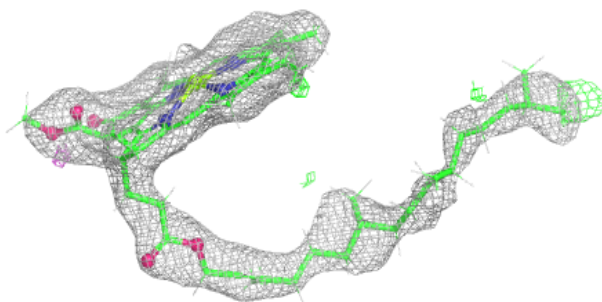


Electron density around CLA c 513:

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

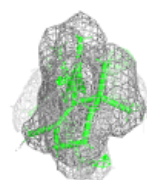
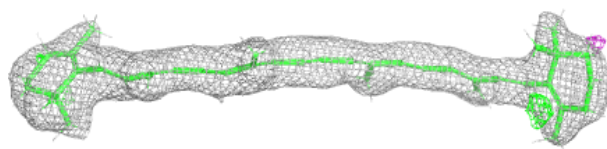
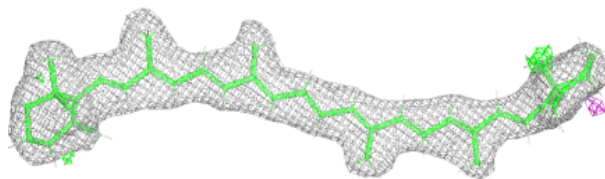
**Electron density around CLA C 513:**

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



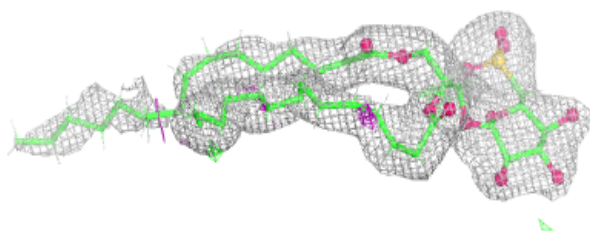
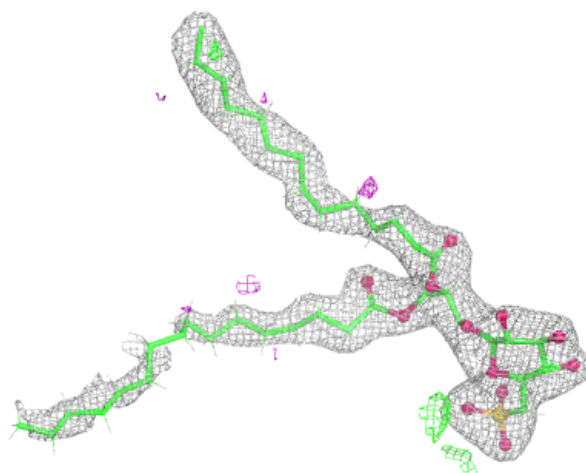
Electron density around BCR K 102:

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



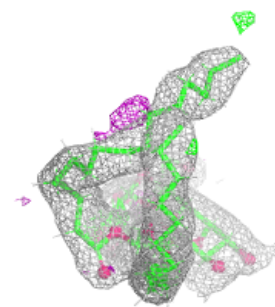
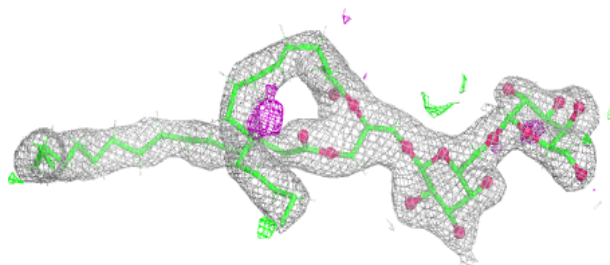
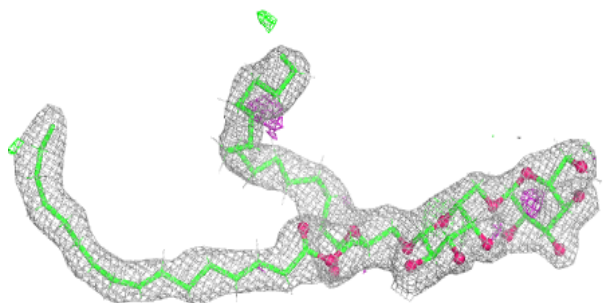
Electron density around SQD A 614:

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

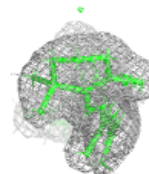
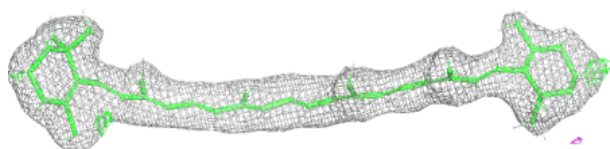
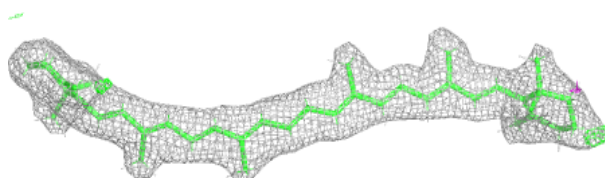


Electron density around DGD H 102:

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

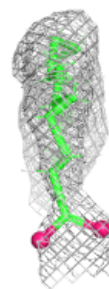
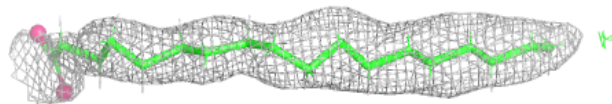
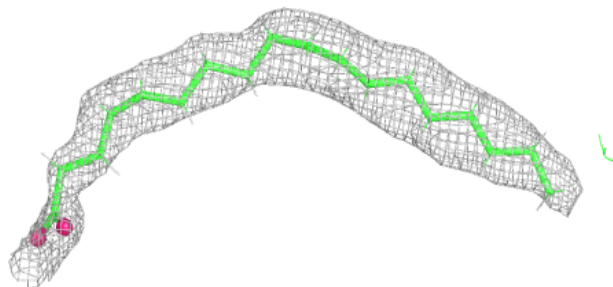
**Electron density around BCR H 101:**

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



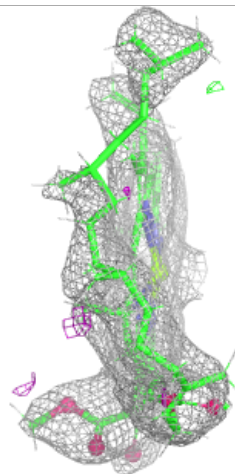
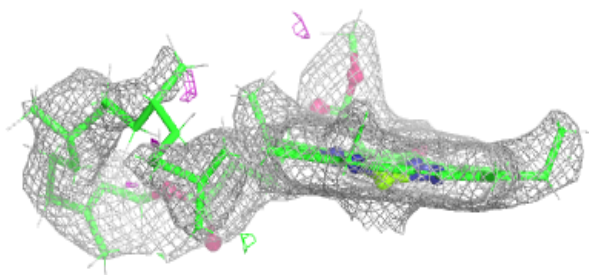
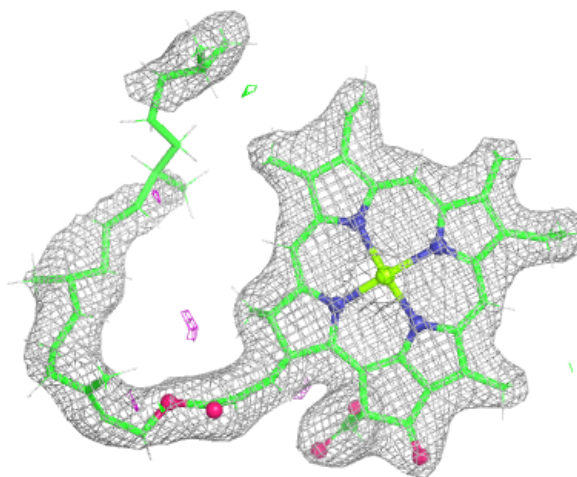
Electron density around STE X 101:

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



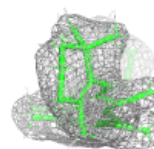
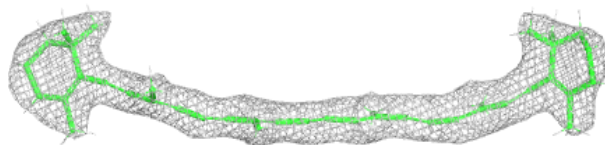
Electron density around CLA c 512:

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

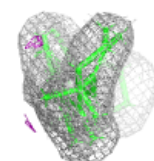
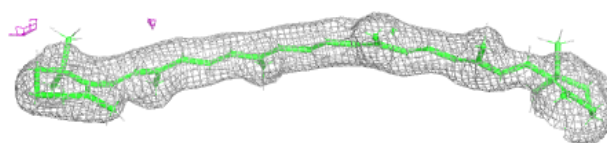


Electron density around BCR k 102:

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

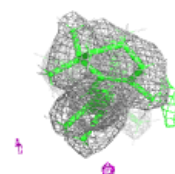
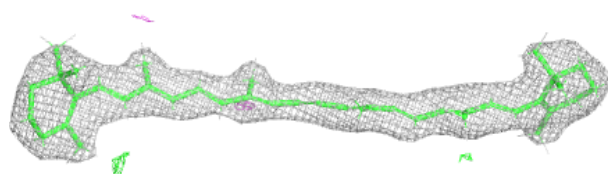
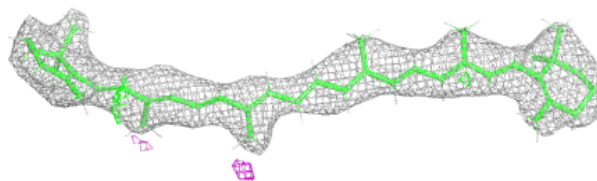
**Electron density around BCR D 405:**

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

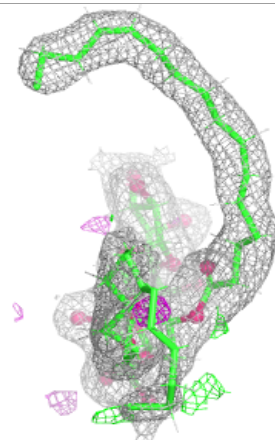
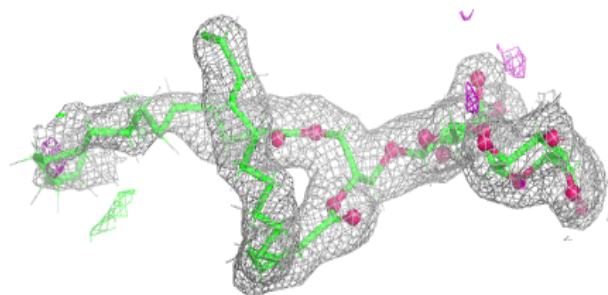
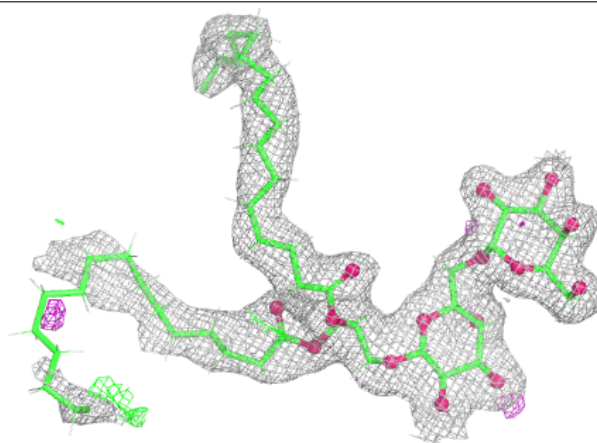


Electron density around BCR c 514:

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

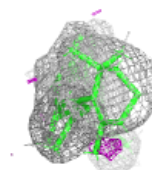
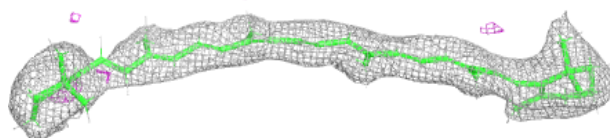
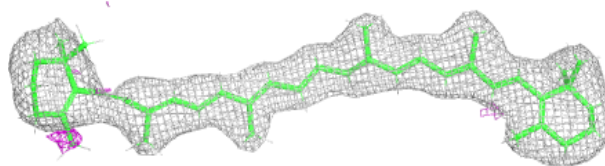
**Electron density around DGD C 522:**

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

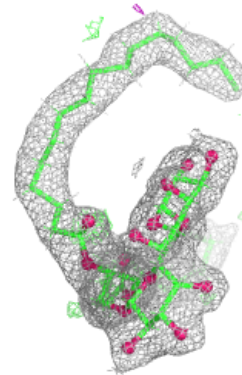
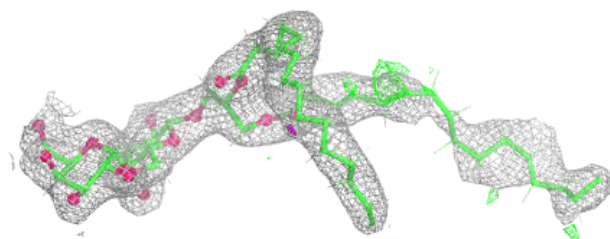
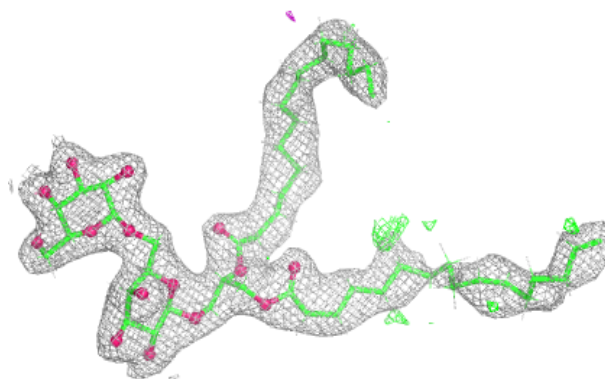


Electron density around BCR d 407:

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

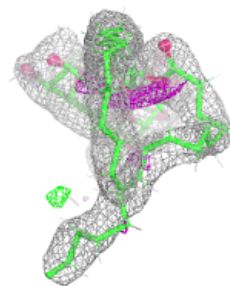
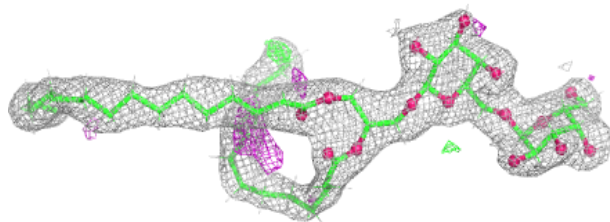
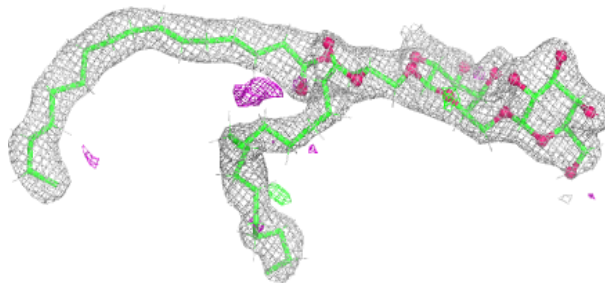
**Electron density around DGD c 520:**

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

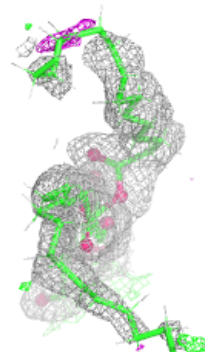
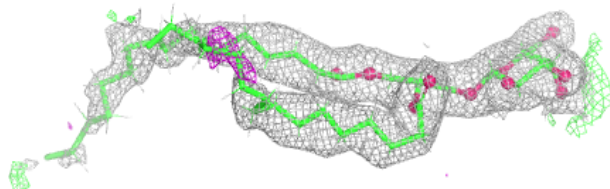
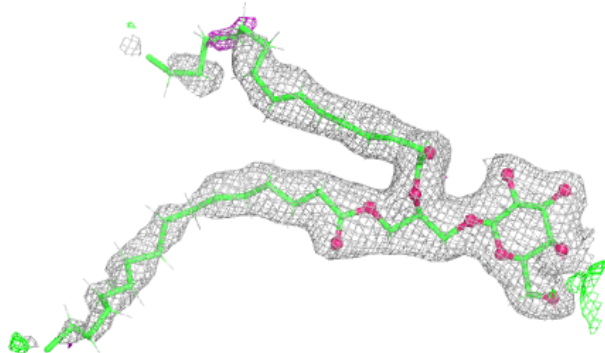


Electron density around DGD h 102:

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

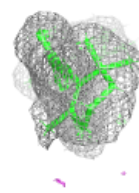
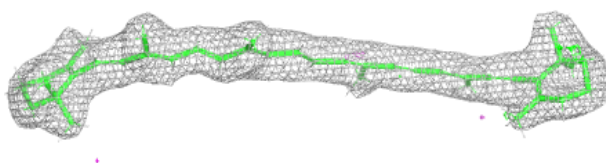
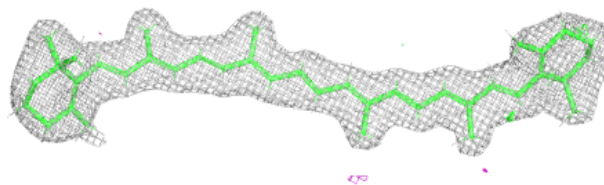
**Electron density around LMG D 408:**

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

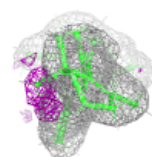
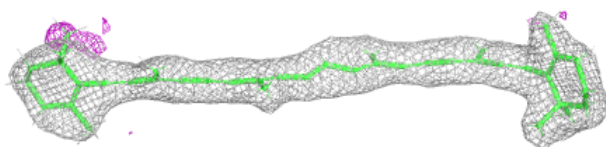
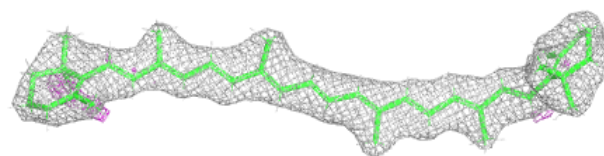


Electron density around BCR B 619:

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

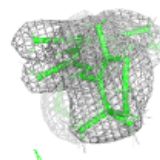
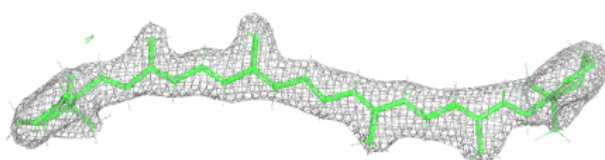
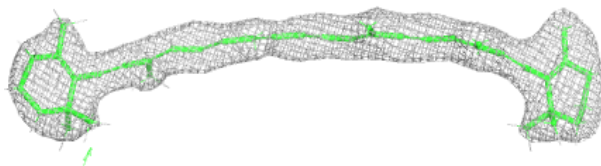
**Electron density around BCR c 515:**

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

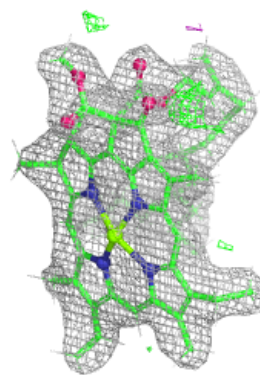
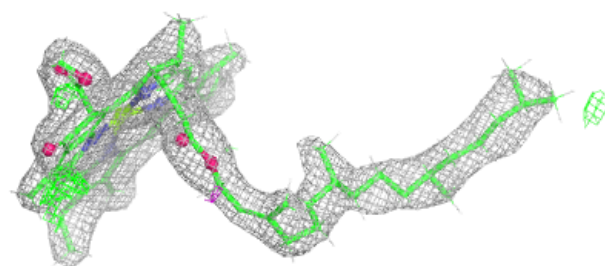
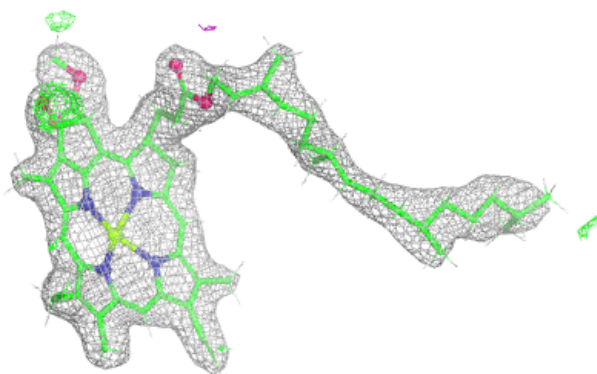


Electron density around BCR C 520:

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

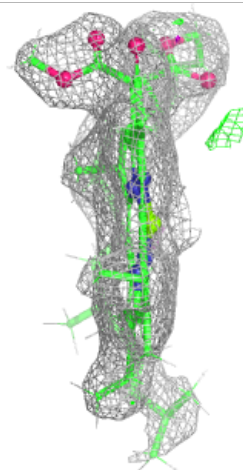
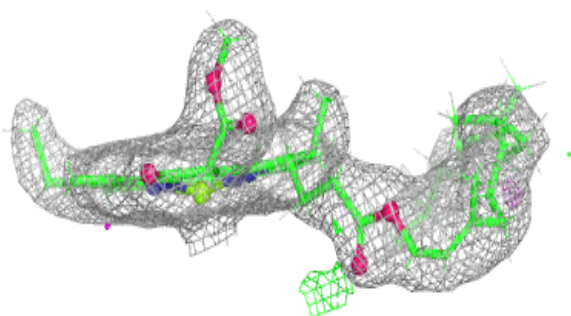
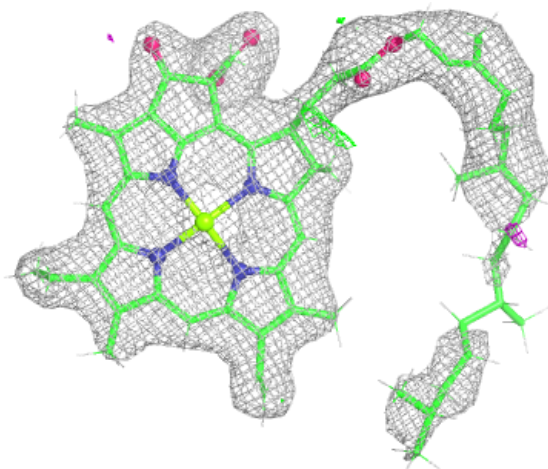
**Electron density around CLA c 511:**

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



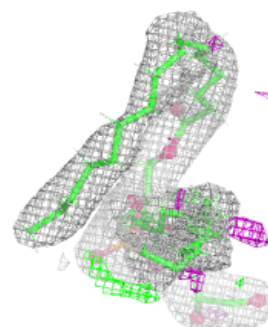
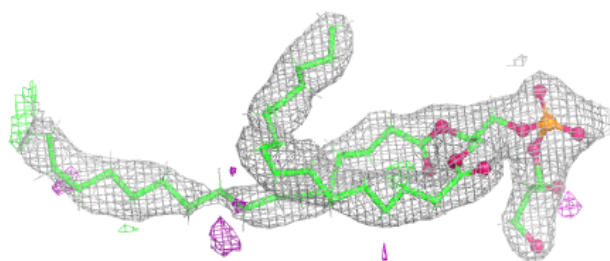
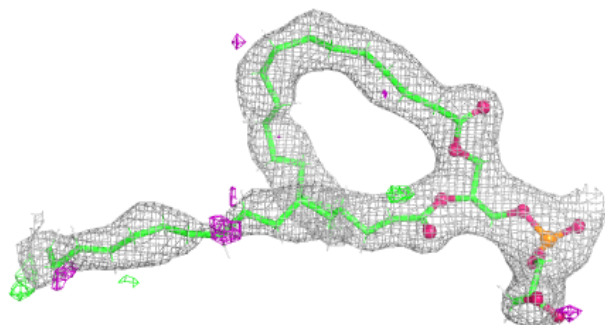
Electron density around CLA C 512:

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

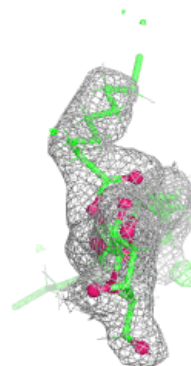
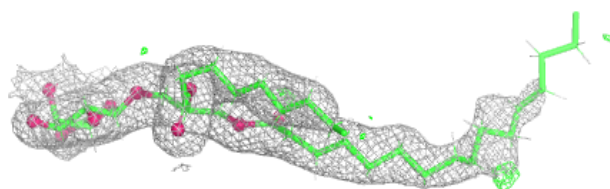
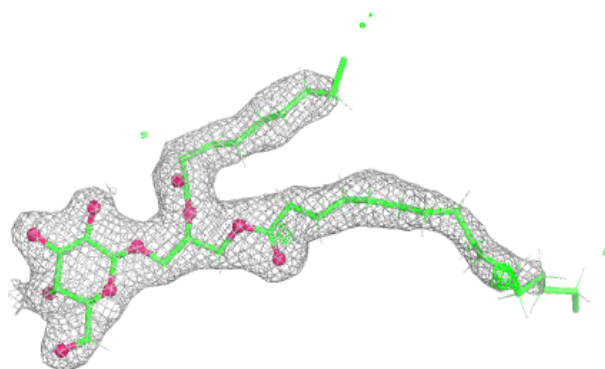


Electron density around LHG d 410:

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

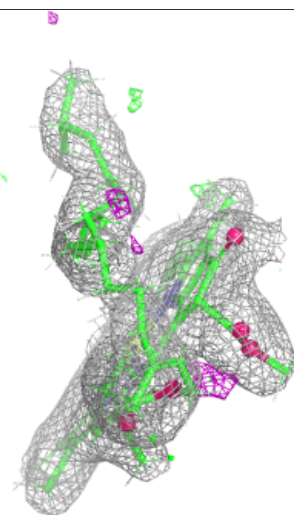
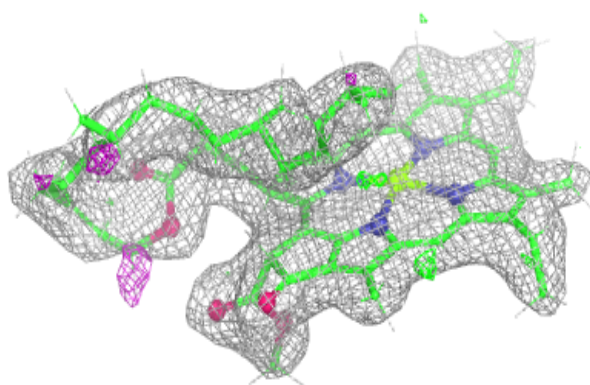
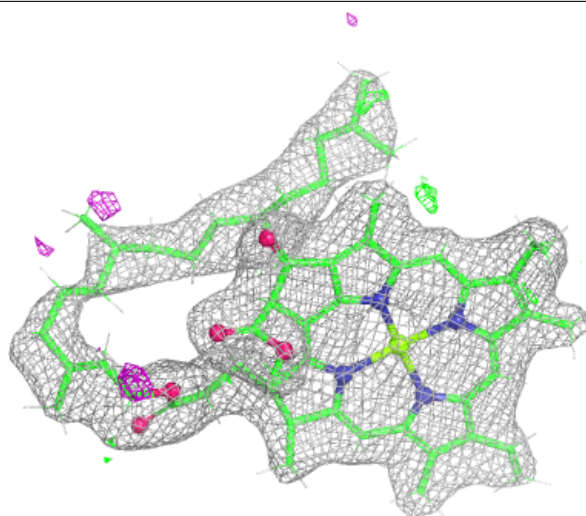
**Electron density around LMG d 414:**

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



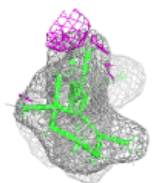
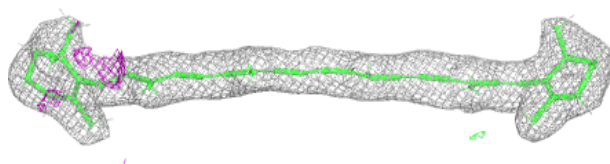
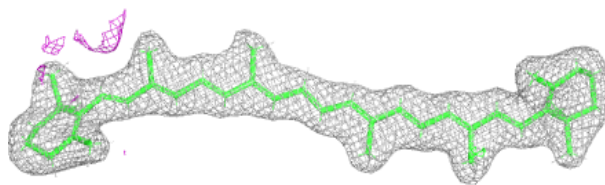
Electron density around CLA c 509:

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

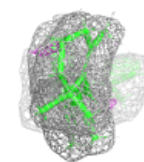
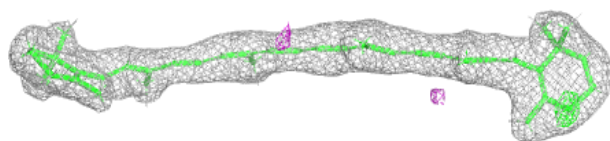
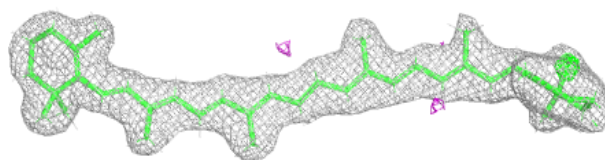


Electron density around BCR B 618:

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

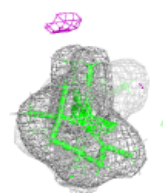
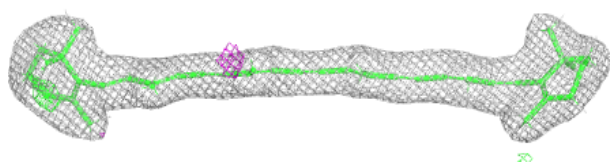
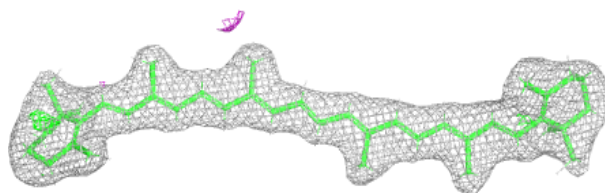
**Electron density around BCR b 617:**

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

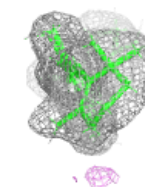
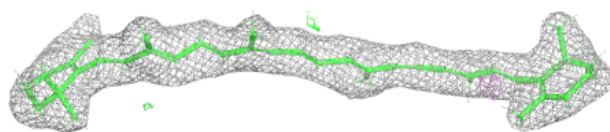
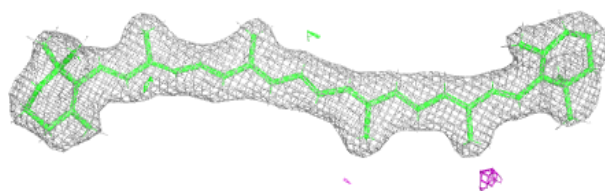


Electron density around BCR b 618:

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

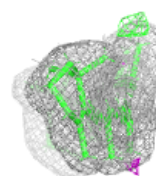
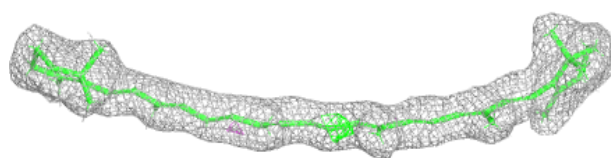
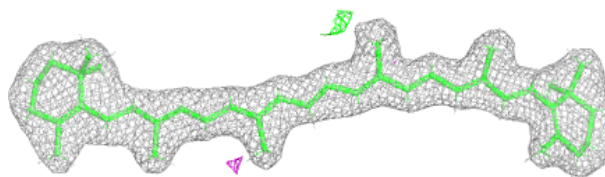
**Electron density around BCR b 619:**

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

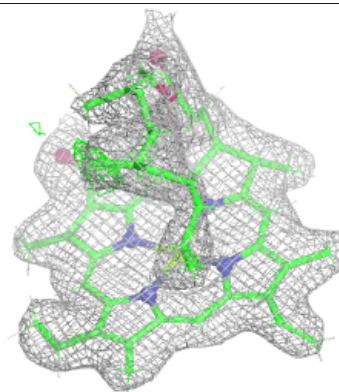
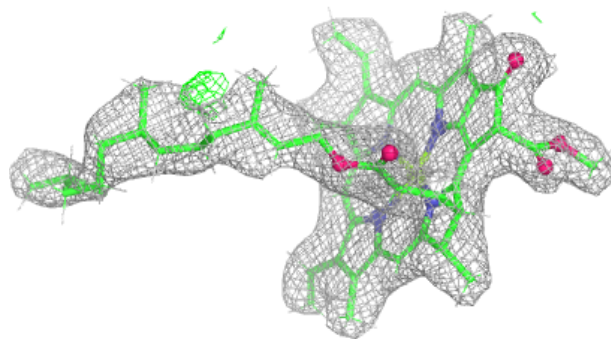
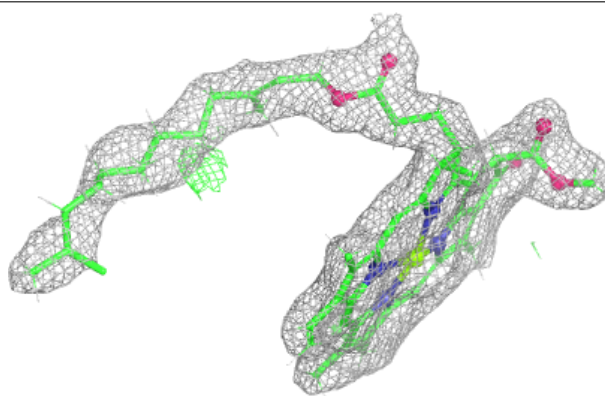


Electron density around BCR t 101:

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

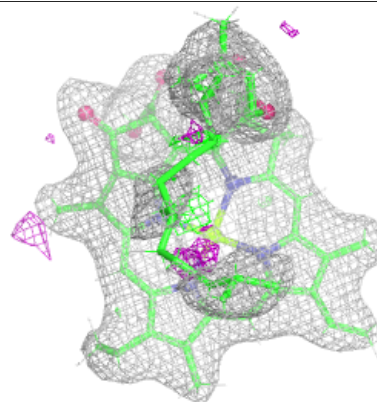
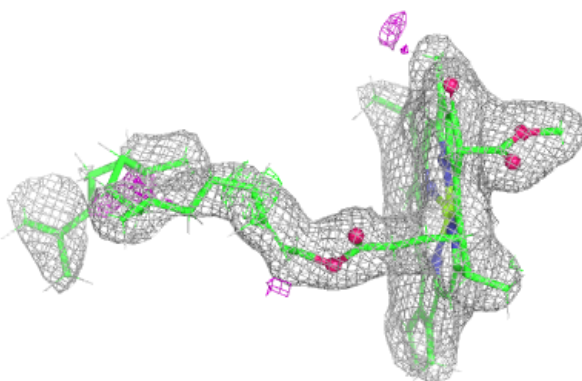
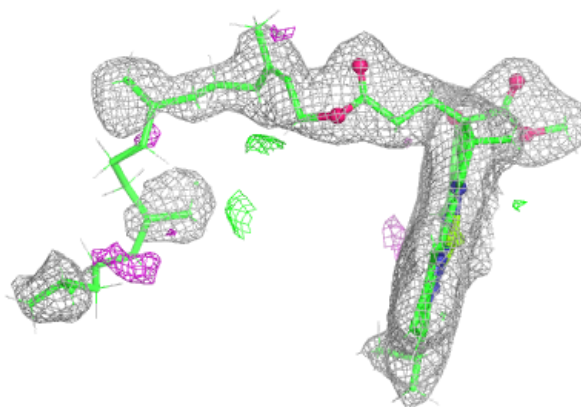
**Electron density around CLA c 504:**

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

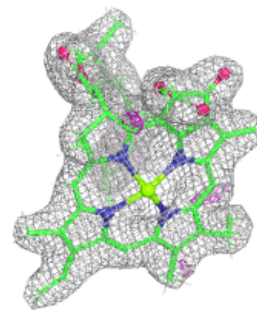
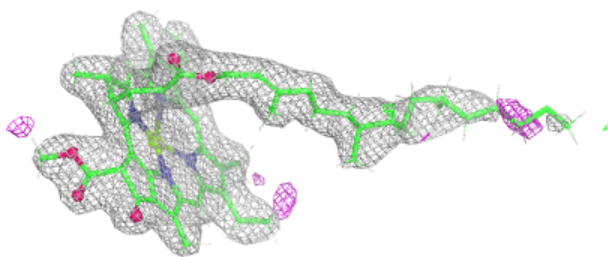
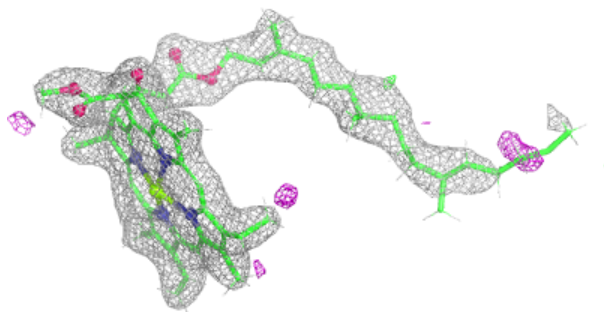


Electron density around CLA c 506:

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

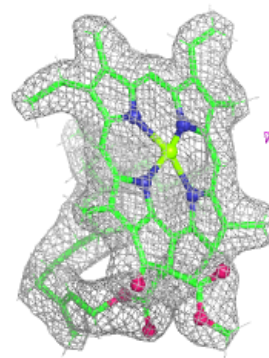
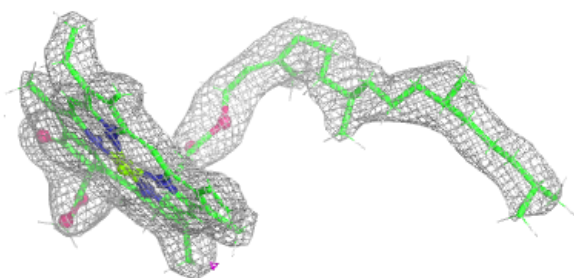
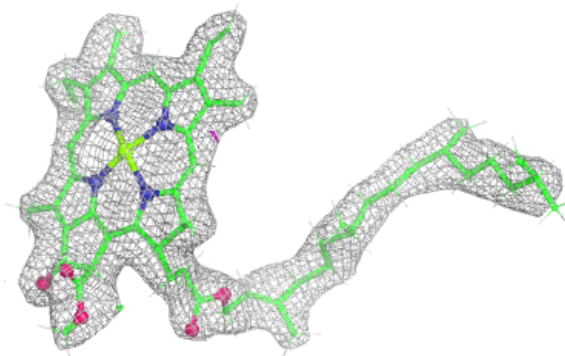
**Electron density around CLA c 508:**

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

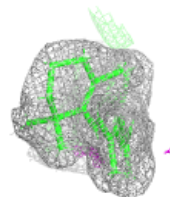
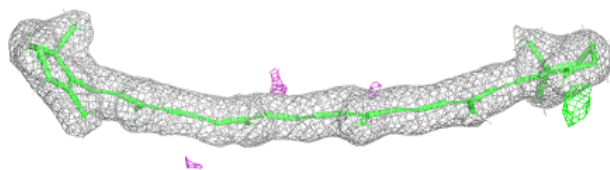
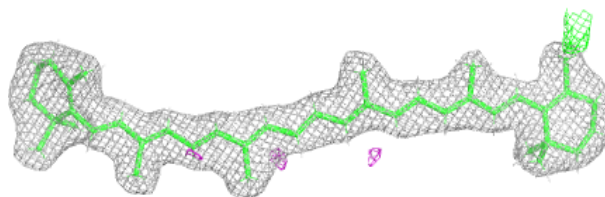


Electron density around CLA C 511:

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

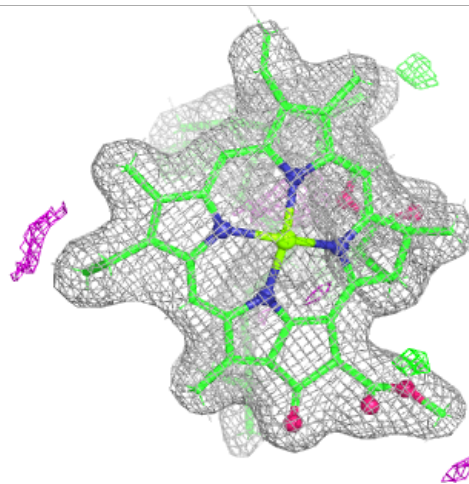
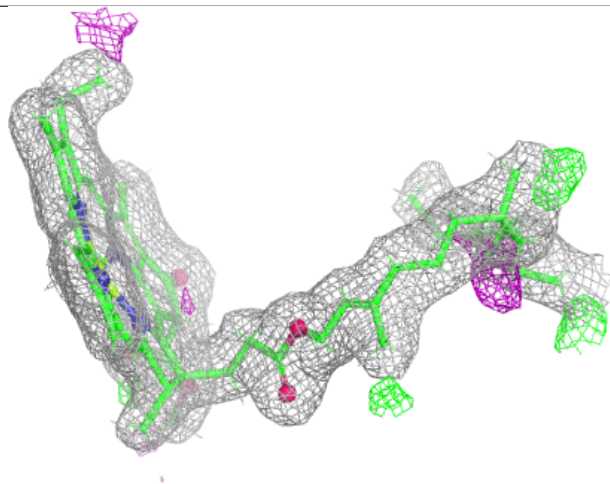
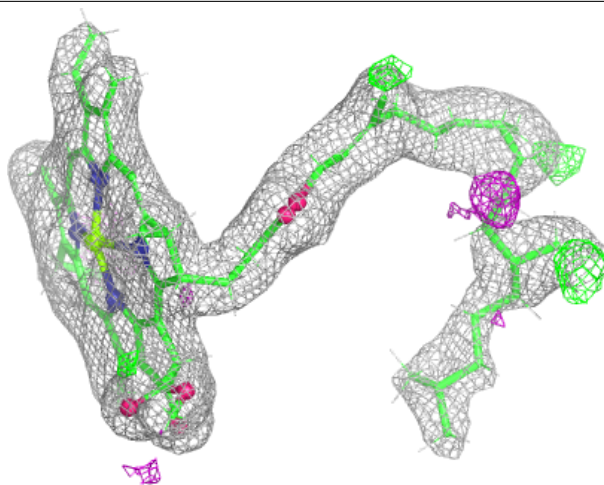
**Electron density around BCR T 101:**

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



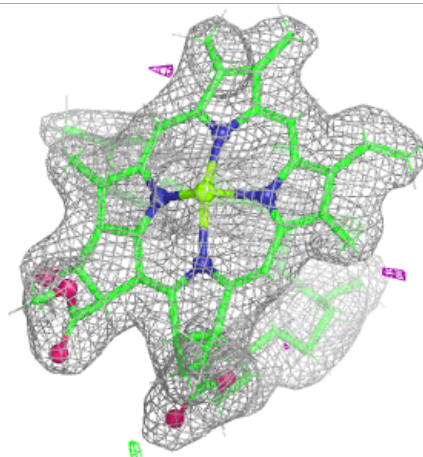
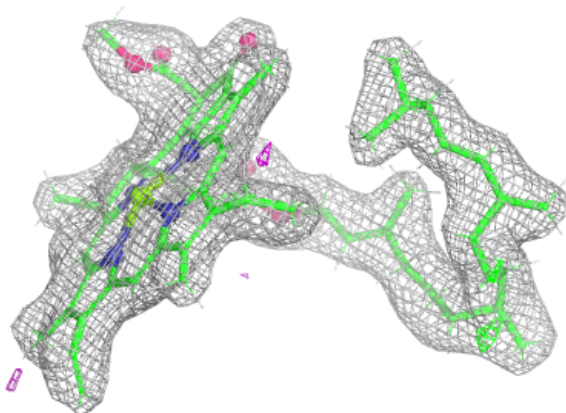
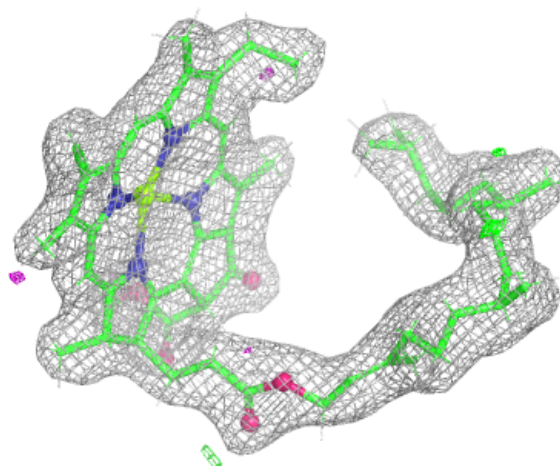
Electron density around CLA B 606:

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



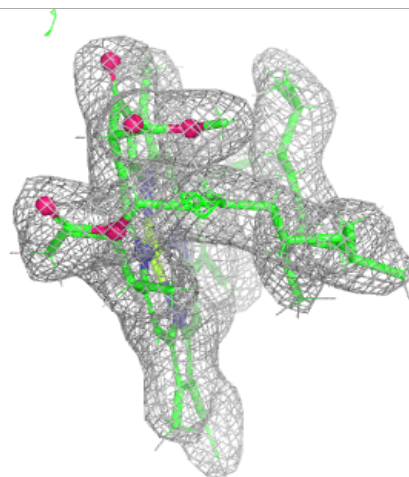
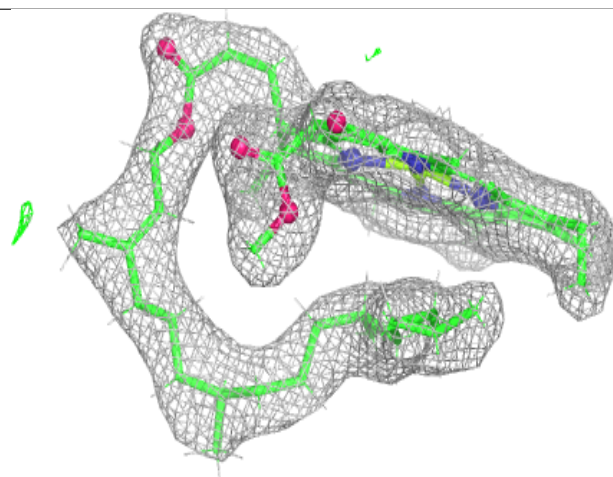
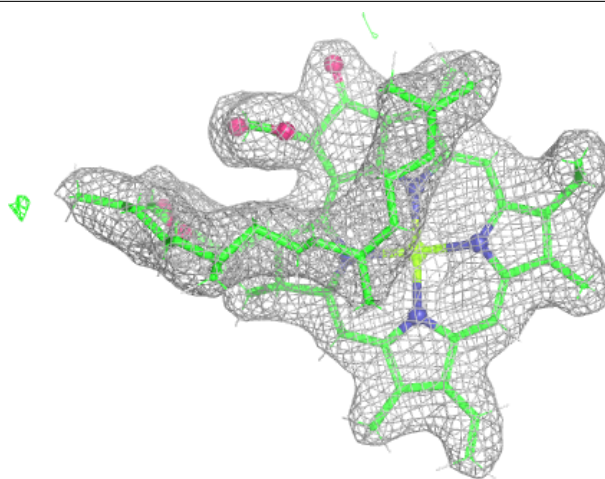
Electron density around CLA C 503:

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



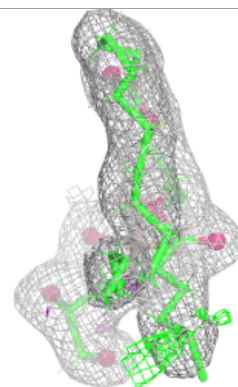
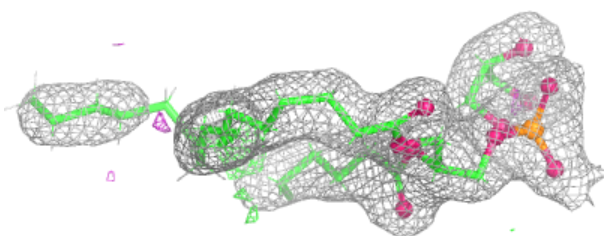
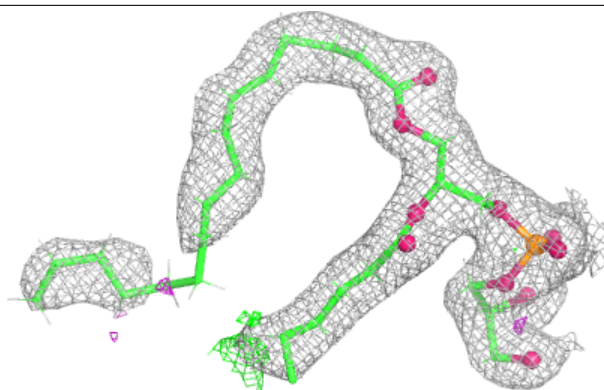
Electron density around CLA C 510:

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

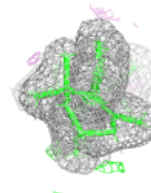
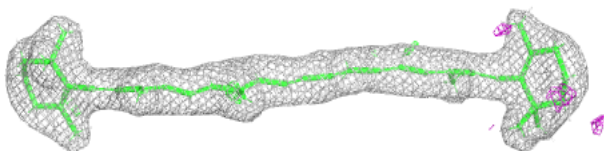
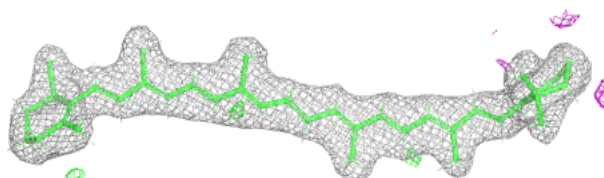


Electron density around LHG d 412:

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

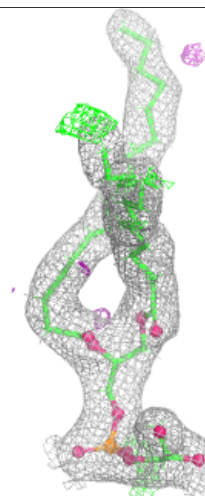
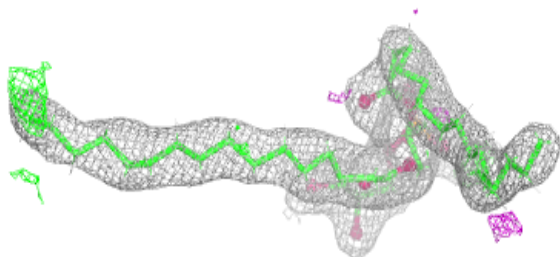
**Electron density around BCR A 609:**

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



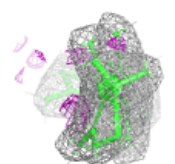
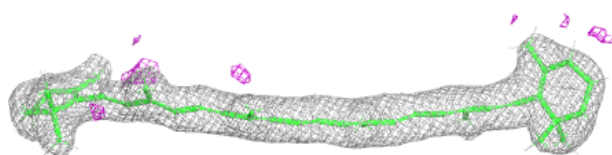
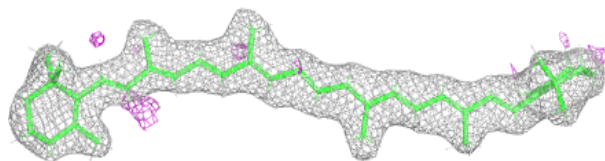
Electron density around LHG 1 101:

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

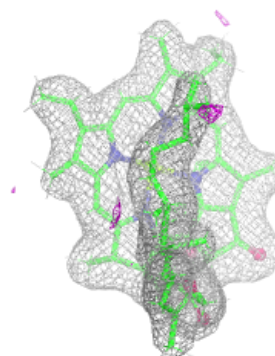
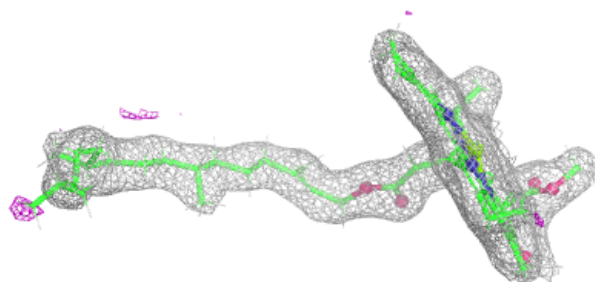
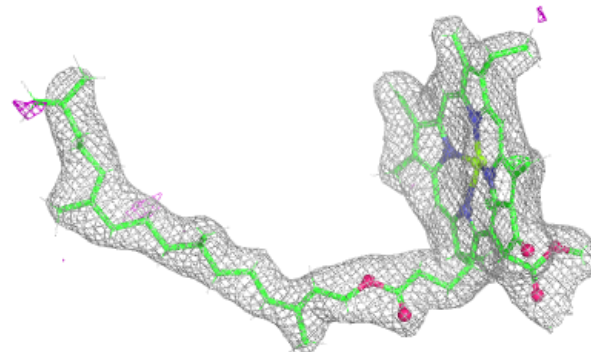


Electron density around BCR B 617:

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

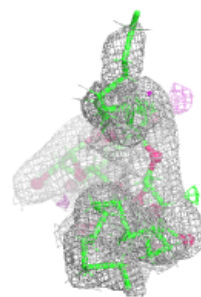
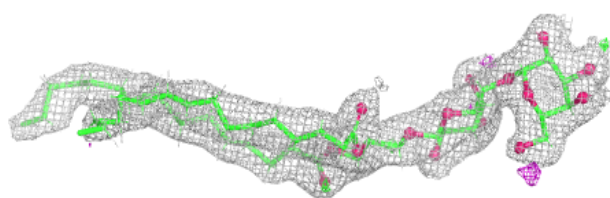
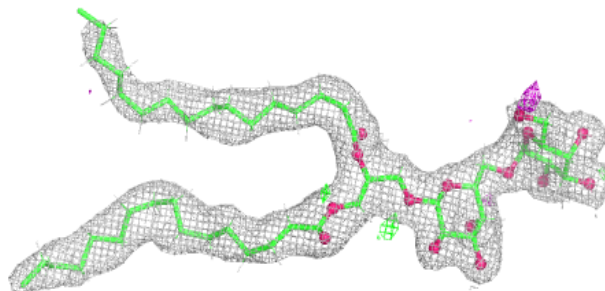
**Electron density around CLA b 609:**

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

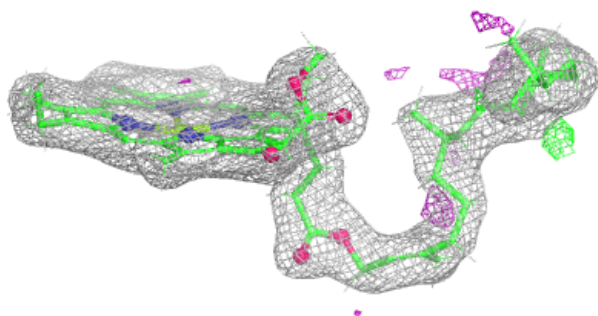
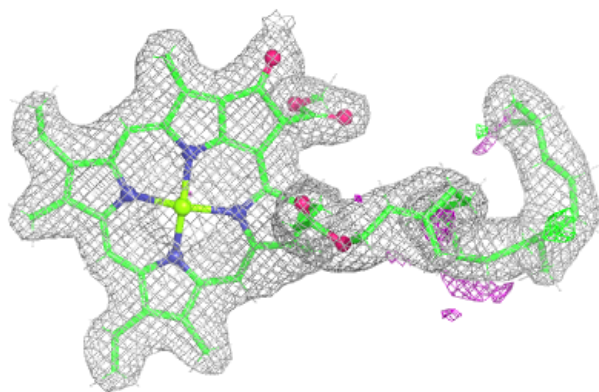


Electron density around DGD C 523:

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

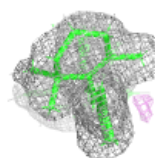
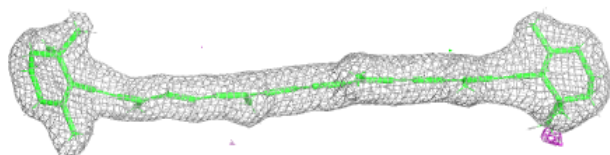
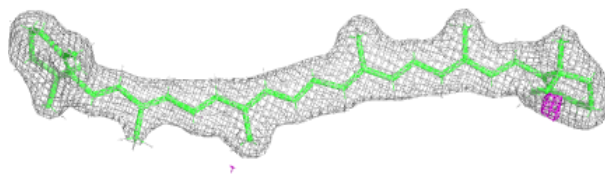
**Electron density around CLA b 612:**

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



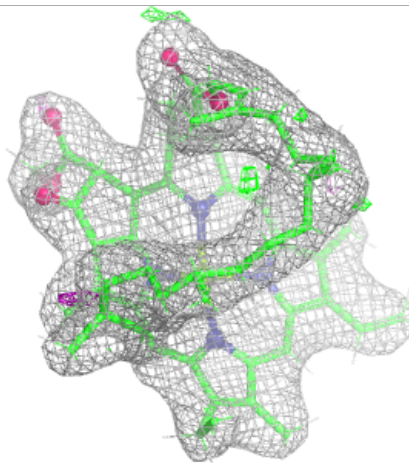
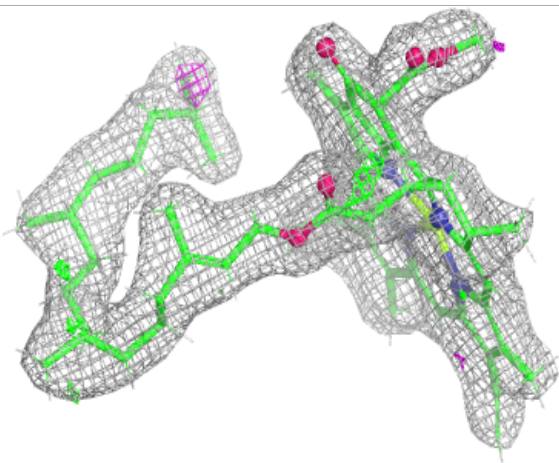
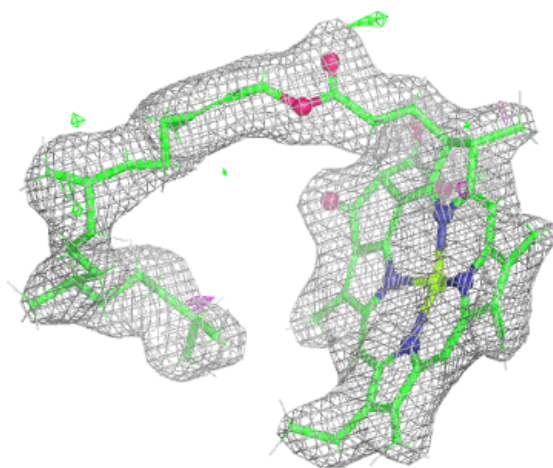
Electron density around BCR C 514:

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



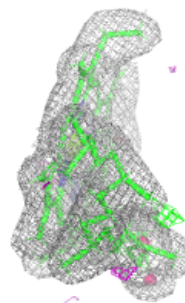
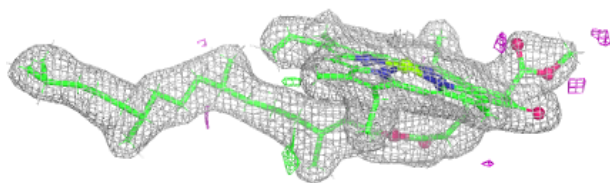
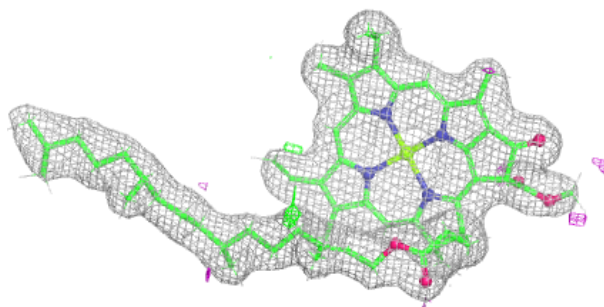
Electron density around CLA c 503:

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



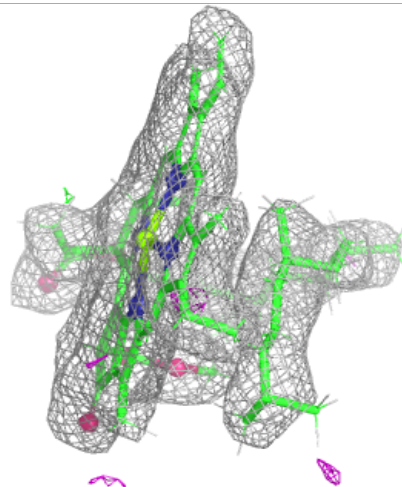
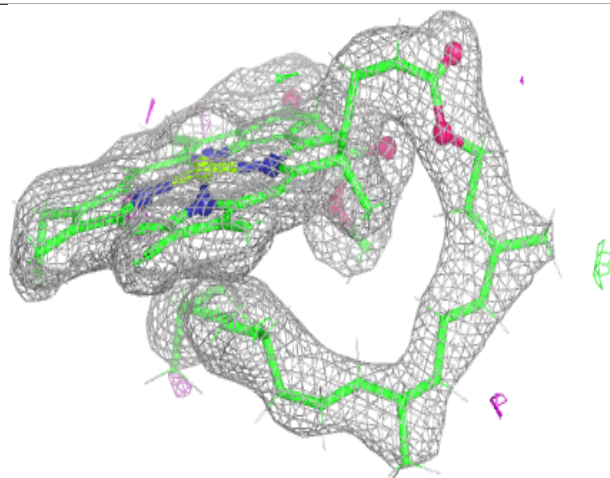
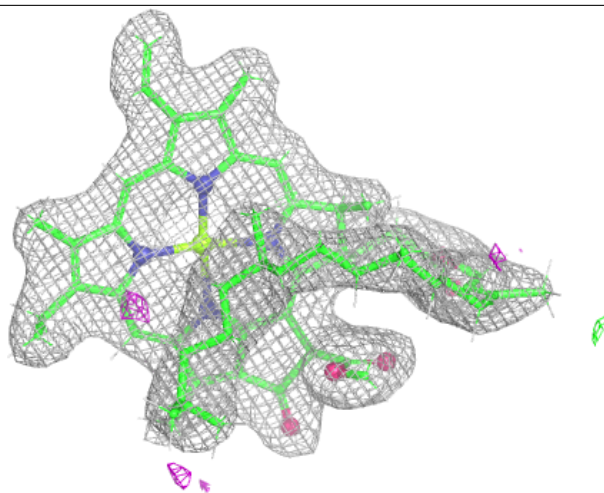
Electron density around CLA C 501:

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



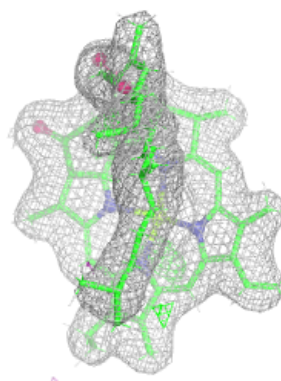
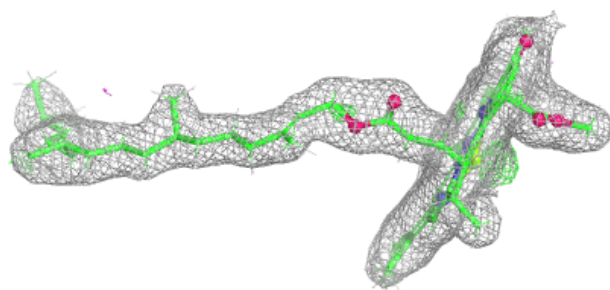
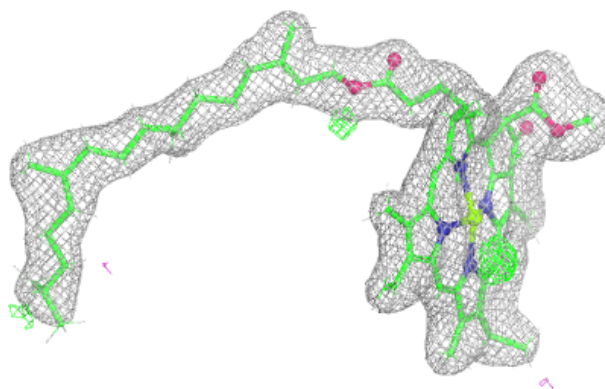
Electron density around CLA c 510:

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

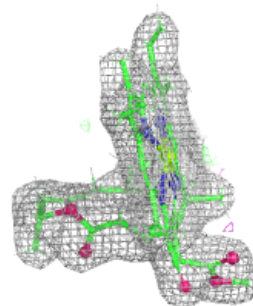
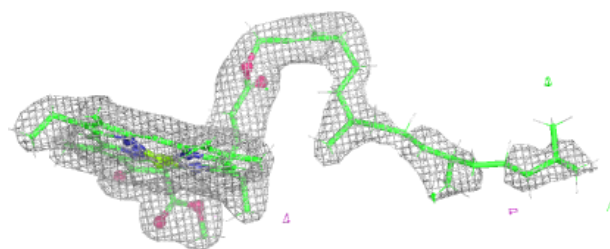
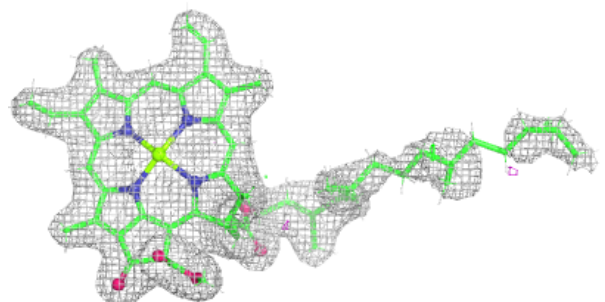


Electron density around CLA B 609:

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

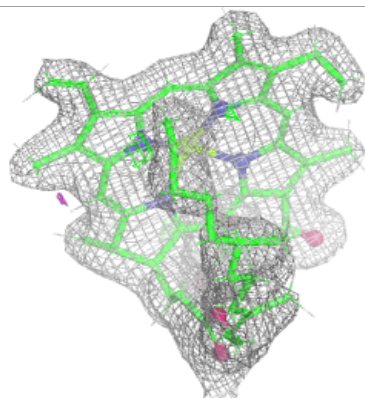
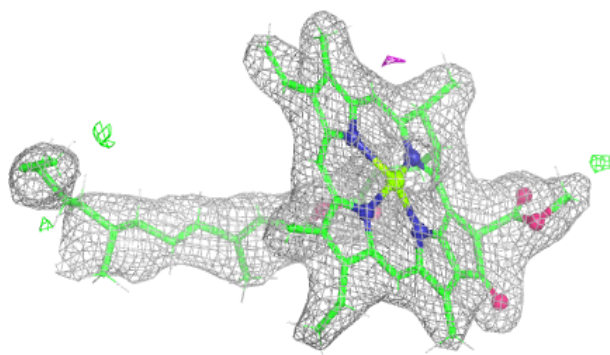
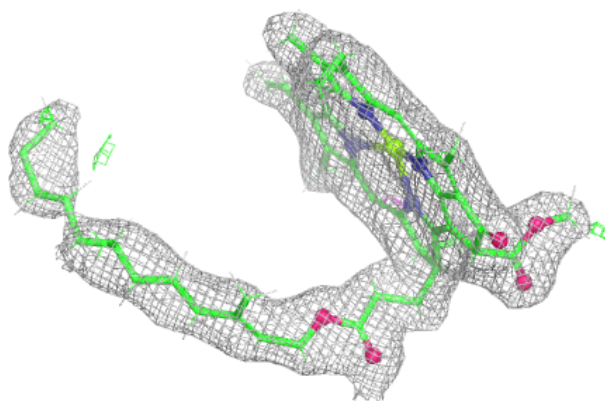
**Electron density around CLA a 606:**

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

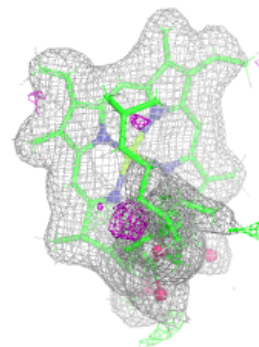
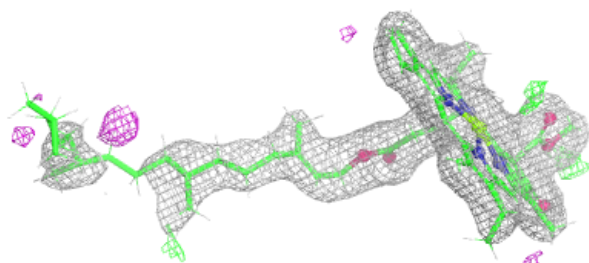
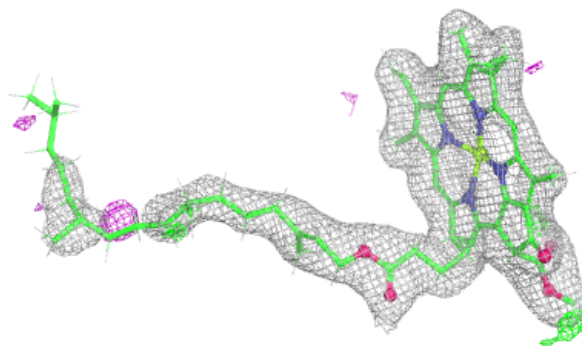


Electron density around CLA C 504:

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

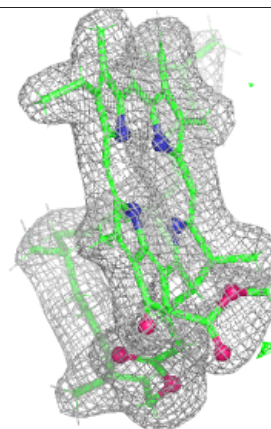
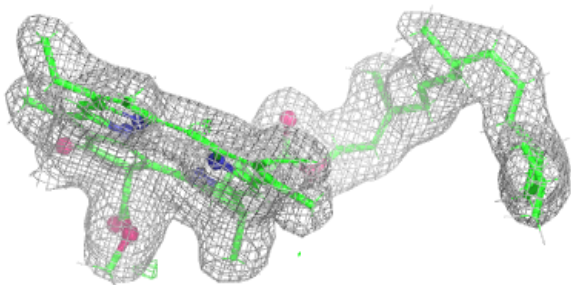
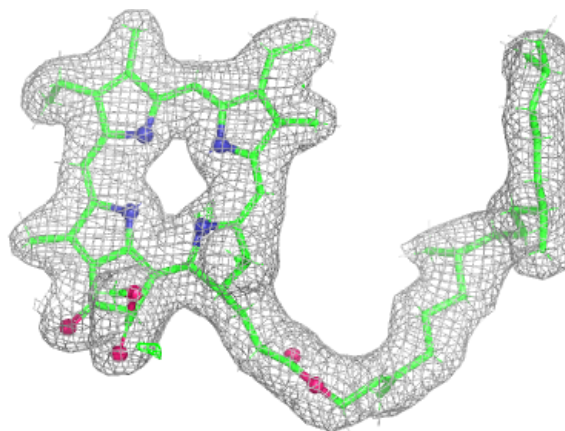
**Electron density around CLA d 406:**

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

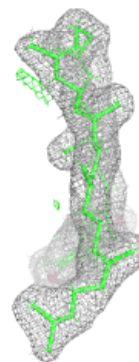
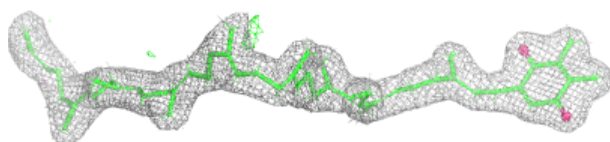
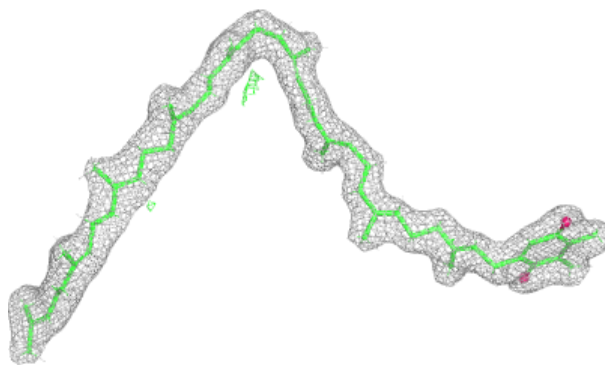


Electron density around PHO d 403:

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

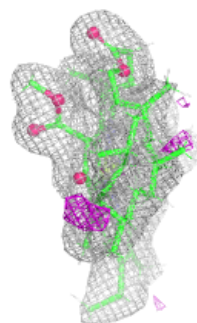
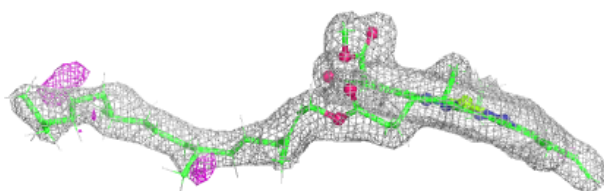
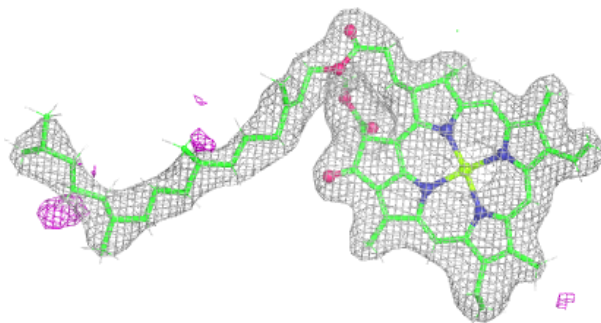
**Electron density around PL9 D 406:**

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

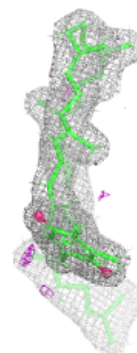
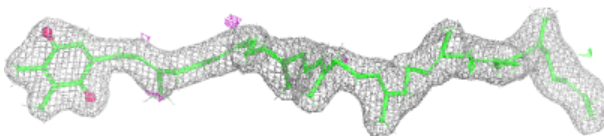
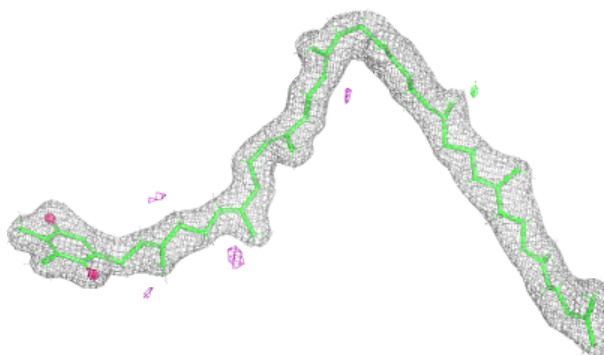


Electron density around CLA b 602:

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

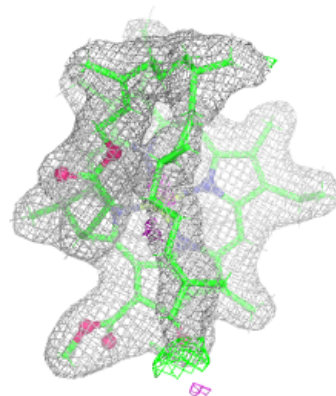
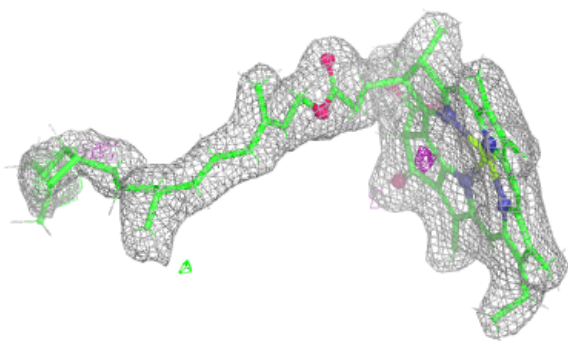
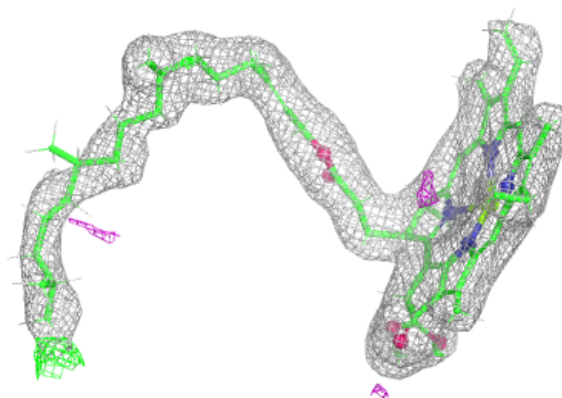
**Electron density around PL9 d 408:**

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

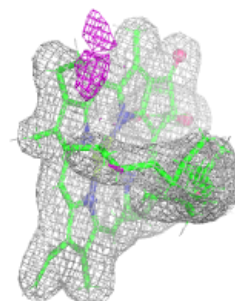
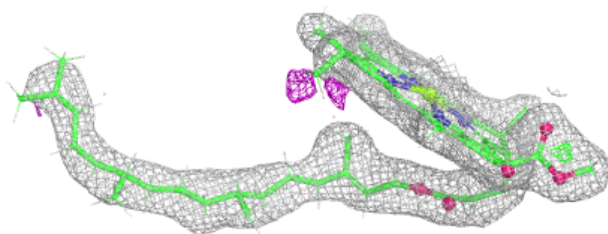
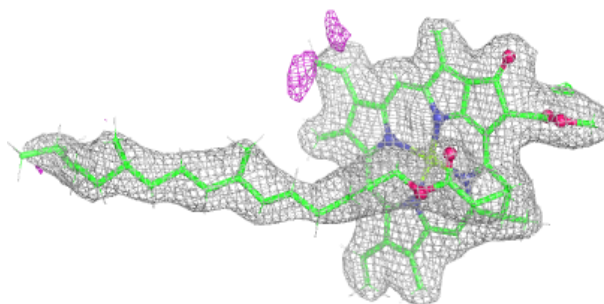


Electron density around CLA b 606:

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

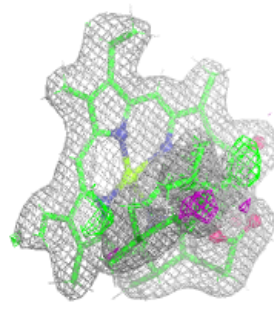
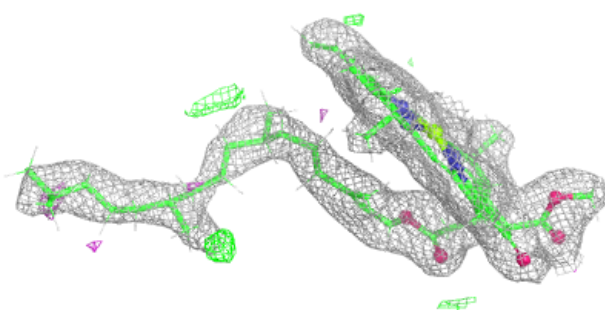
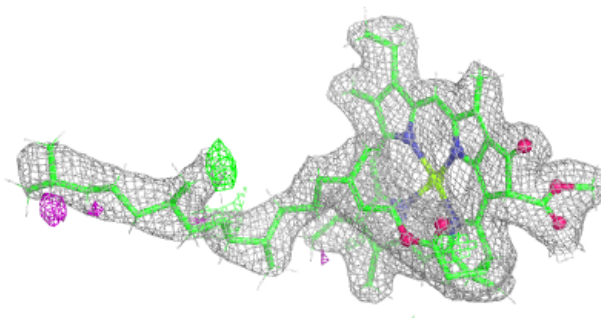
**Electron density around CLA b 608:**

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

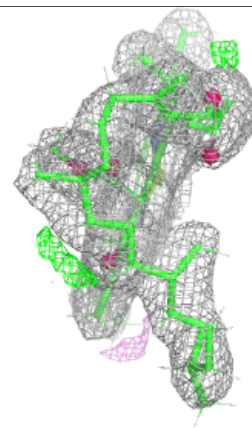
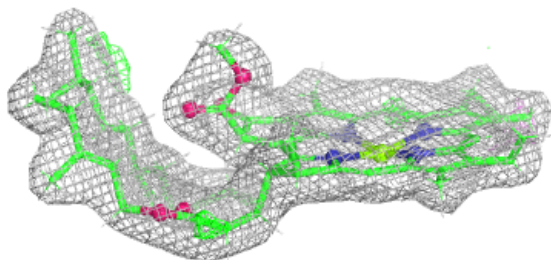
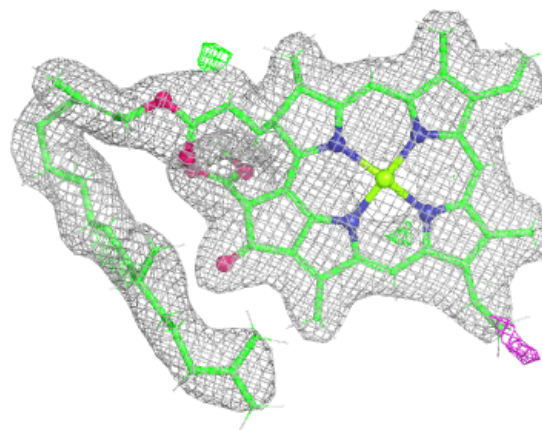


Electron density around CLA C 505:

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

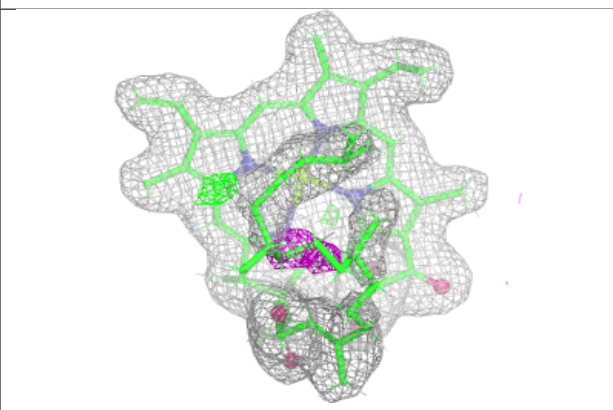
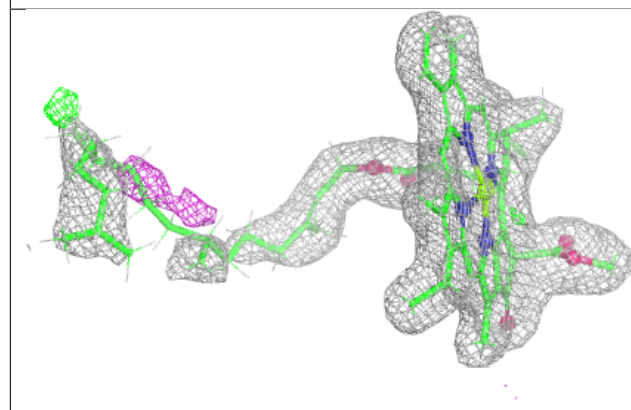
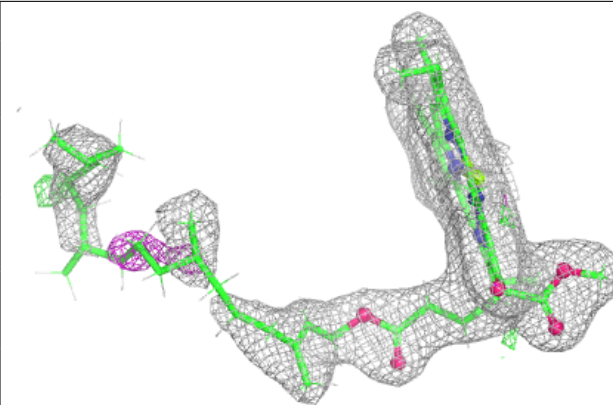
**Electron density around CLA b 610:**

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

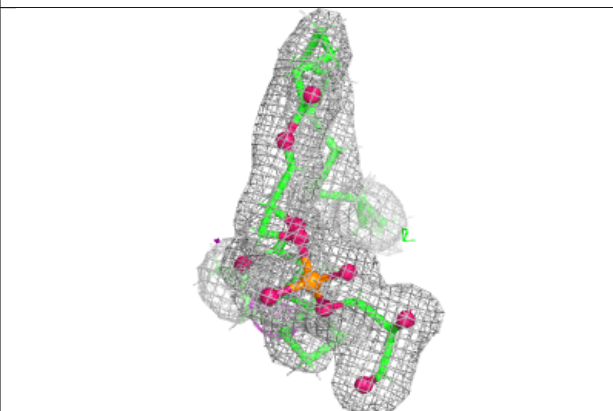
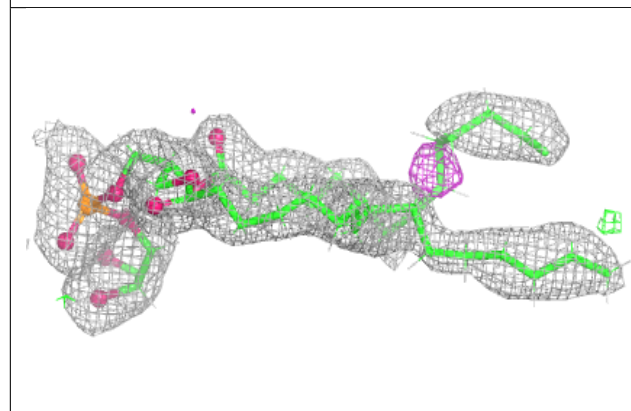
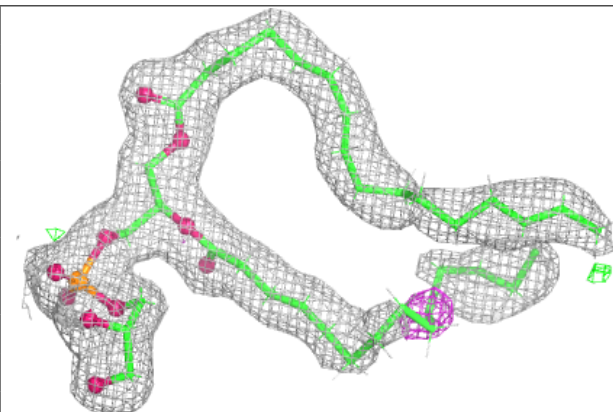


Electron density around CLA C 506:

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

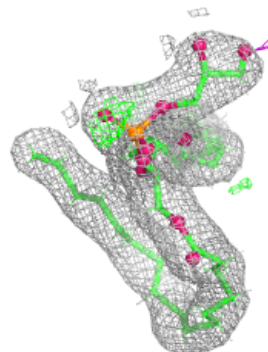
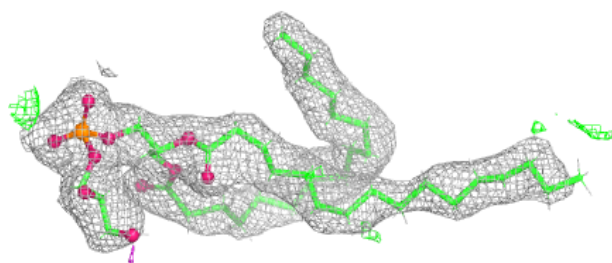
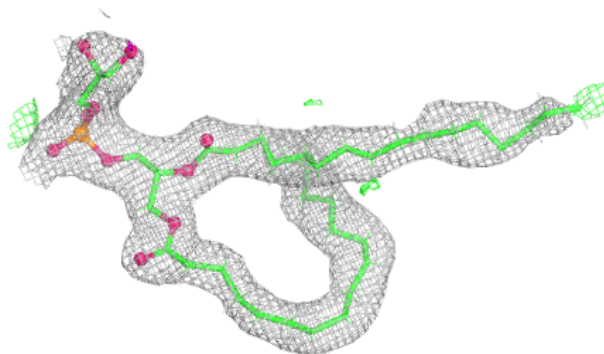
**Electron density around LHG D 410:**

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

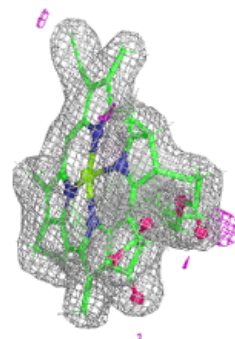
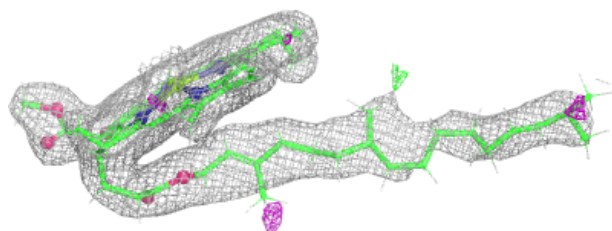
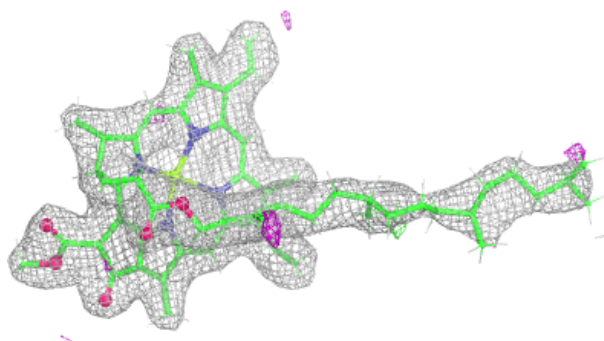


Electron density around LHG D 411:

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

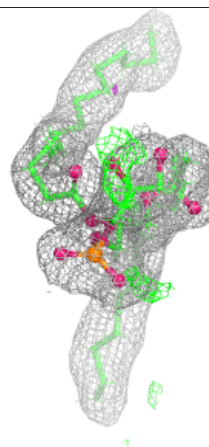
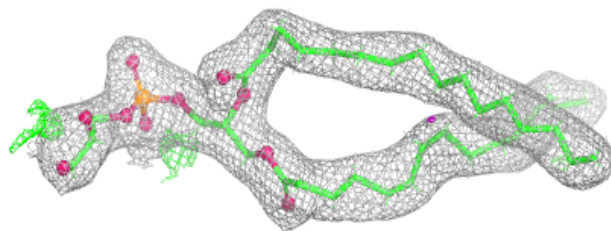
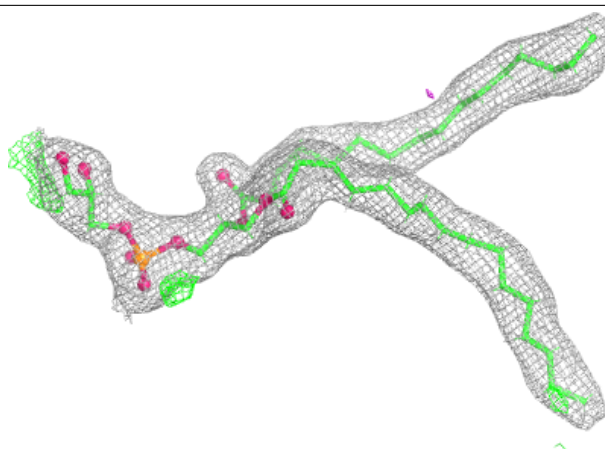
**Electron density around CLA b 614:**

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



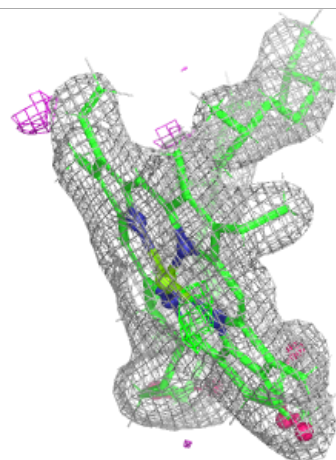
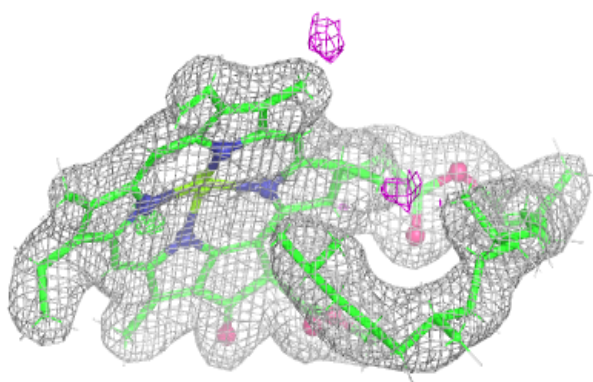
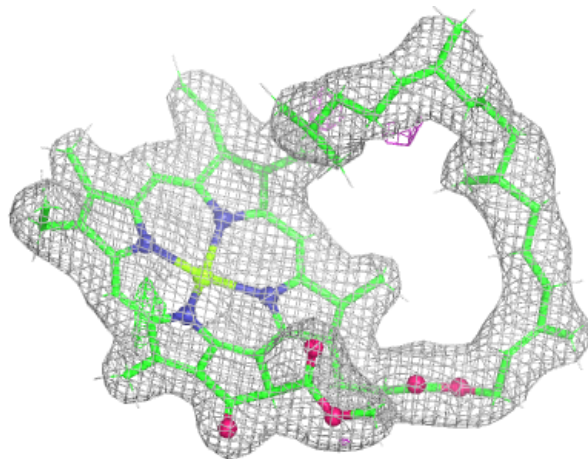
Electron density around LHG d 411:

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



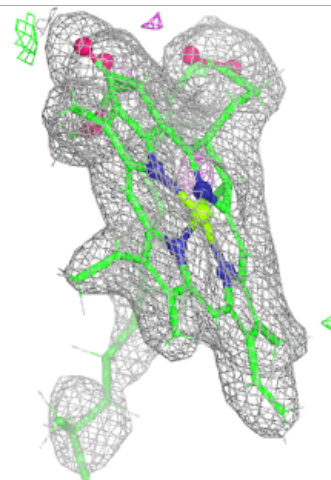
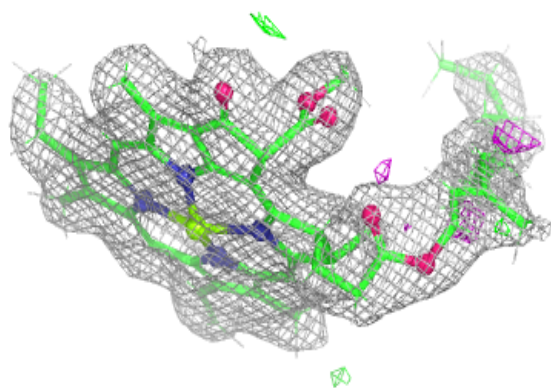
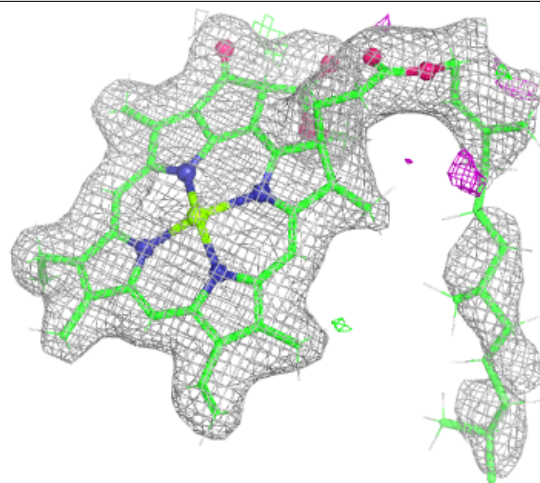
Electron density around CLA b 615:

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



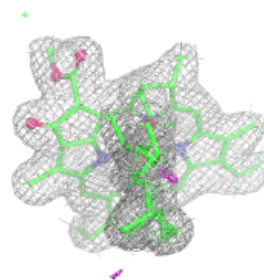
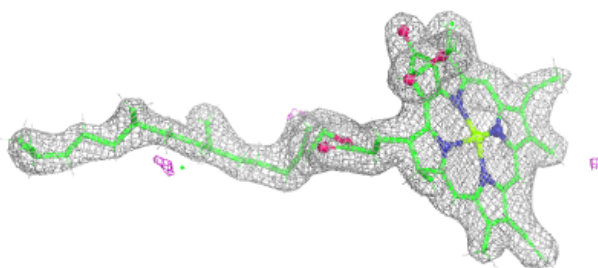
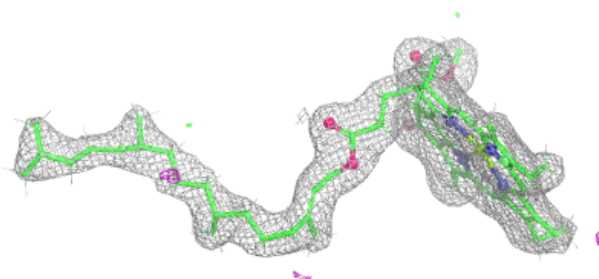
Electron density around CLA b 616:

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

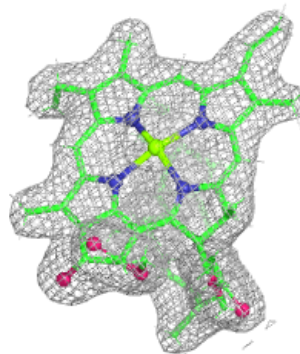
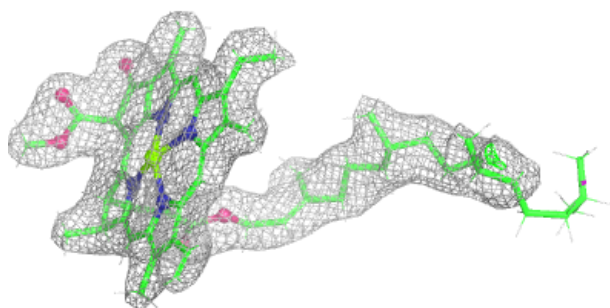
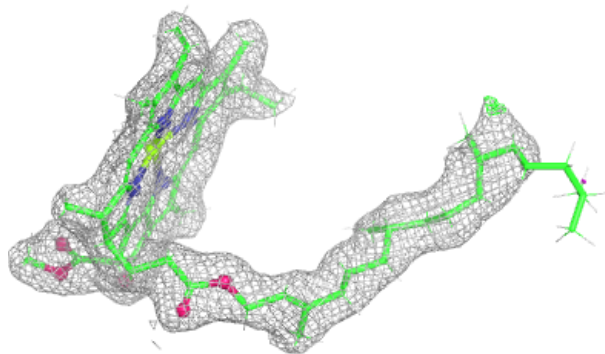


Electron density around CLA c 502:

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

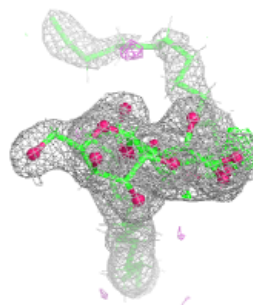
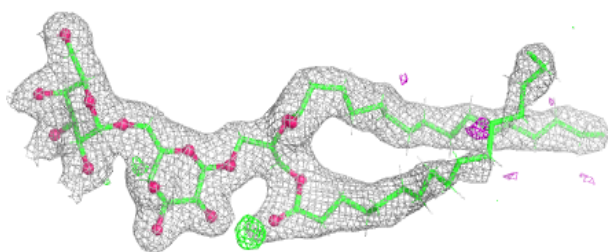
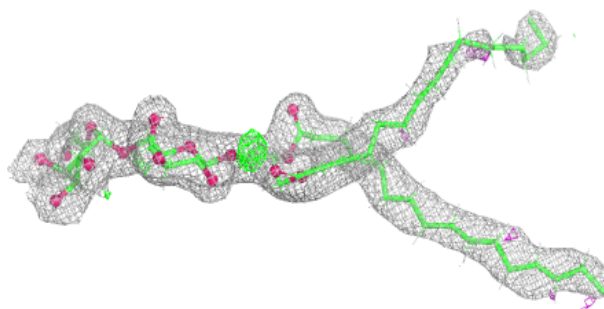
**Electron density around CLA C 508:**

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

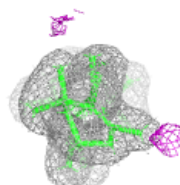
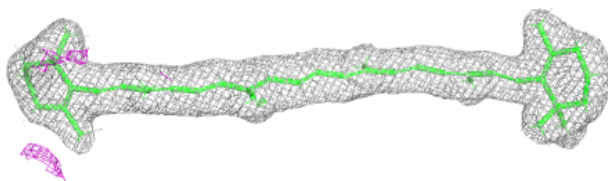
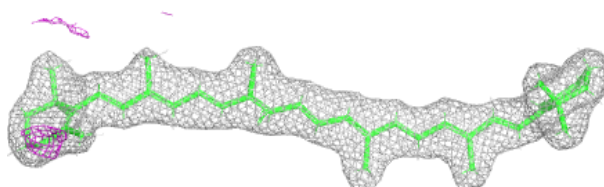


Electron density around DGD C 521:

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

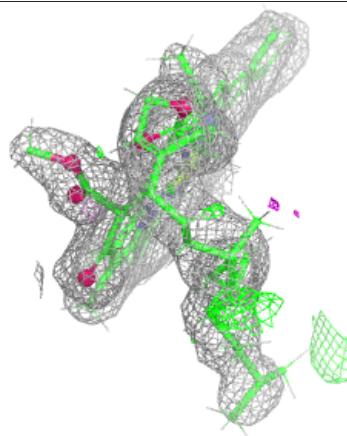
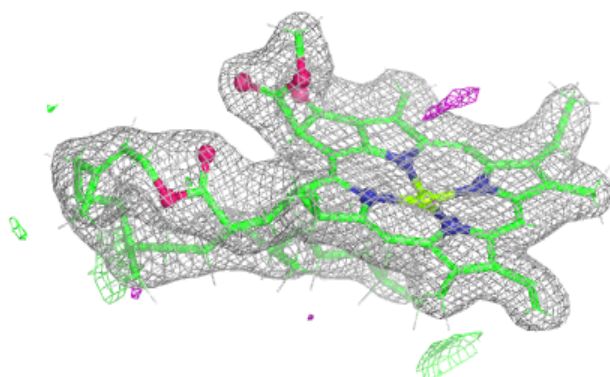
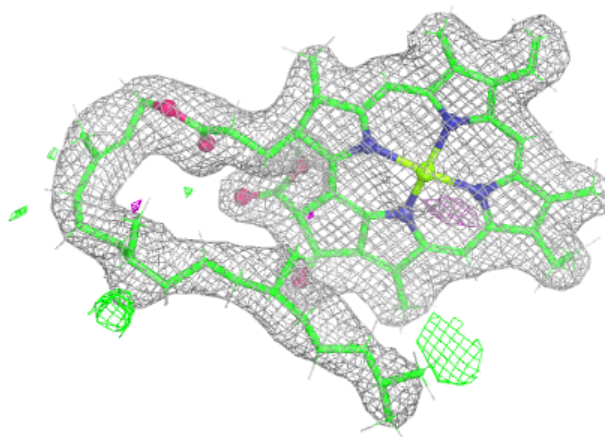
**Electron density around BCR a 608:**

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

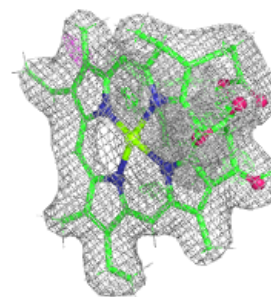
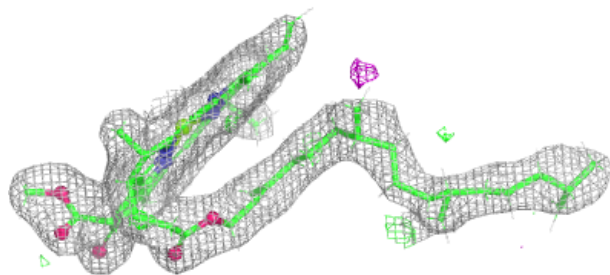
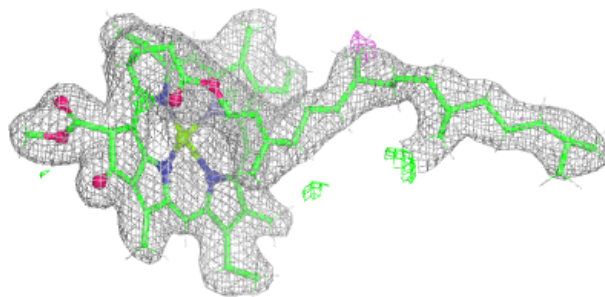


Electron density around CLA C 509:

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

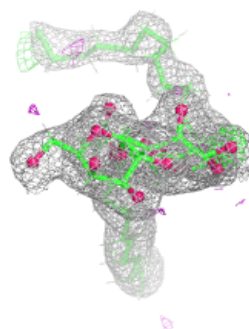
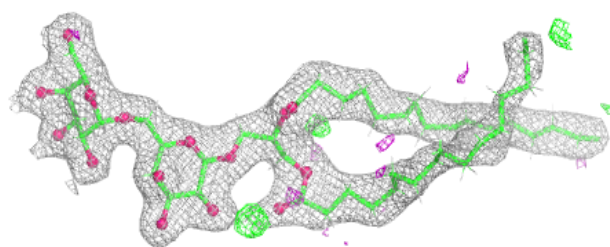
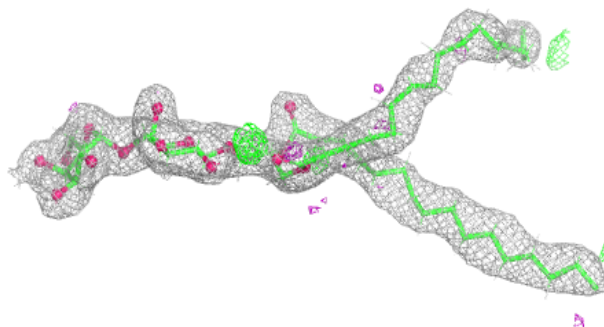
**Electron density around CLA c 505:**

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

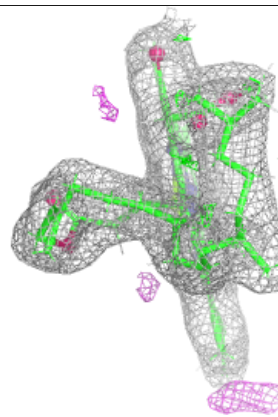
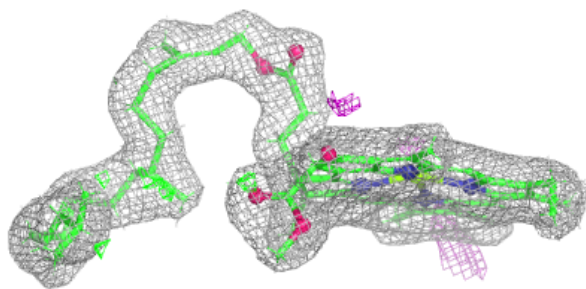
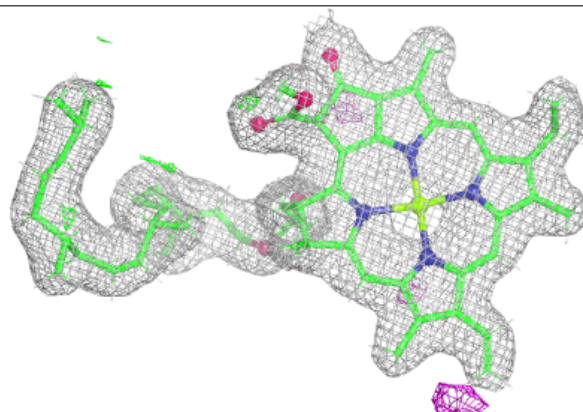


Electron density around DGD c 519:

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

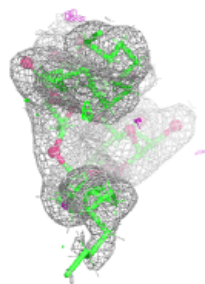
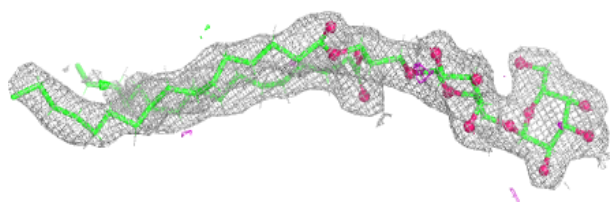
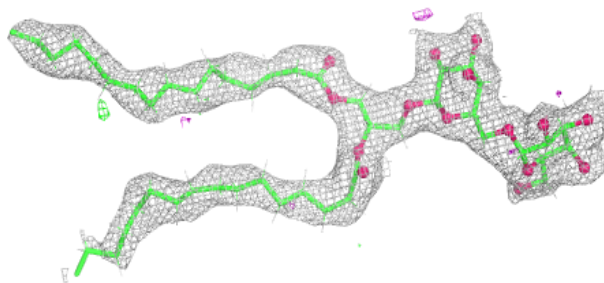
**Electron density around CLA B 612:**

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



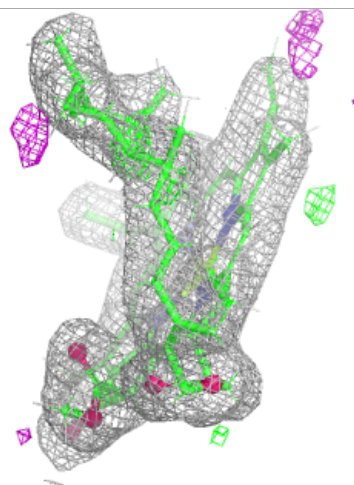
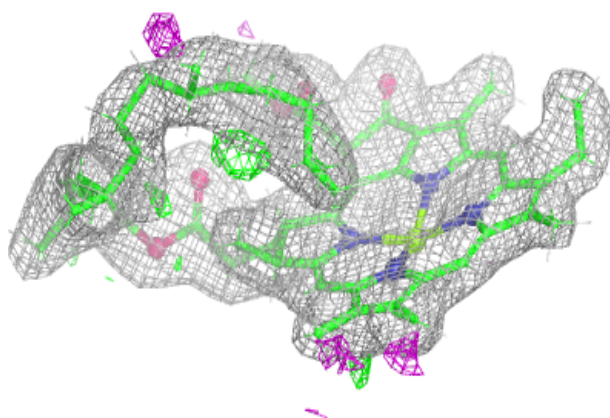
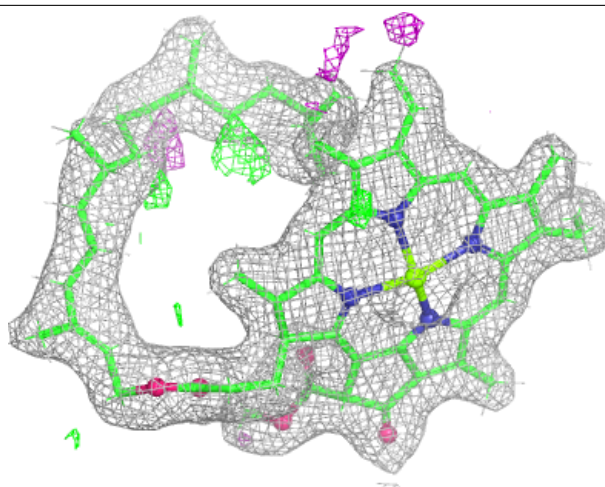
Electron density around DGD c 521:

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



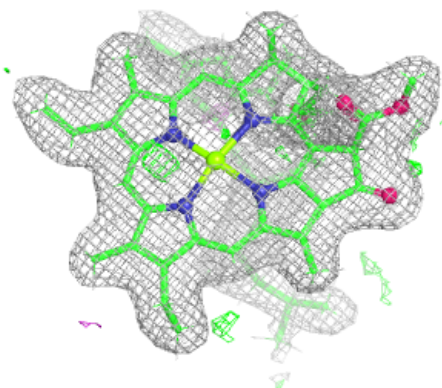
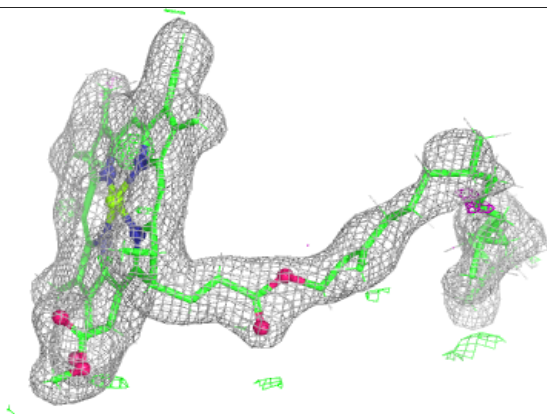
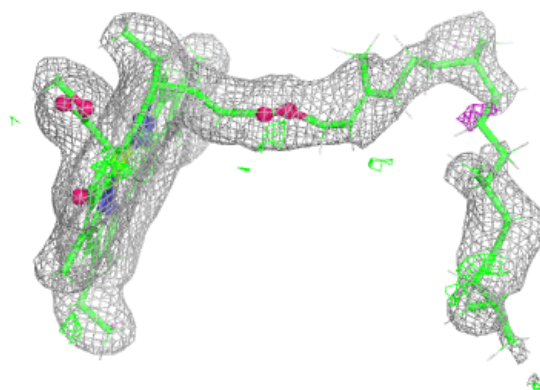
Electron density around CLA B 615:

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

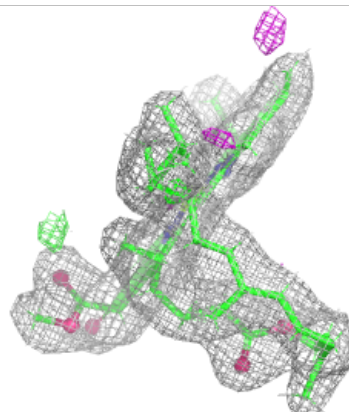
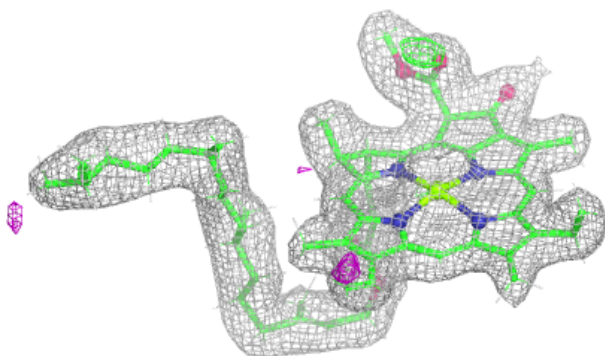
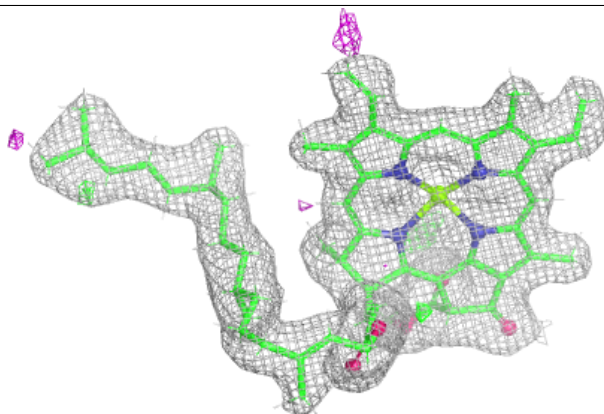


Electron density around CLA a 607:

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

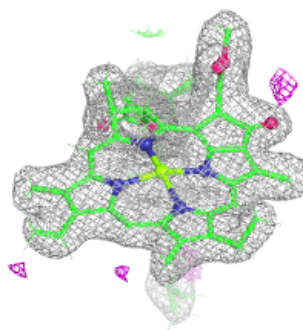
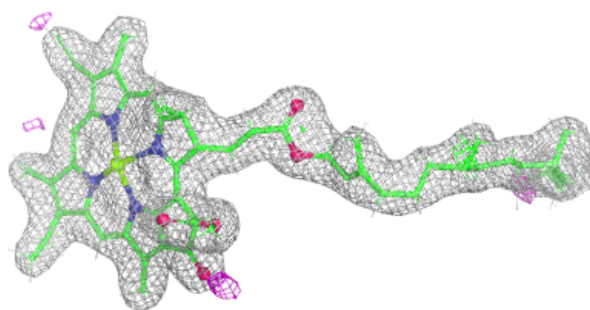
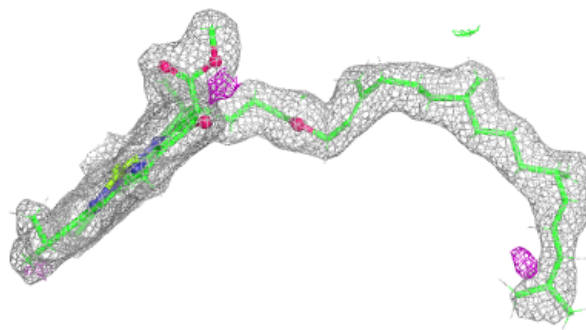
**Electron density around CLA d 404:**

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

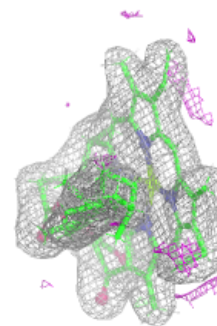
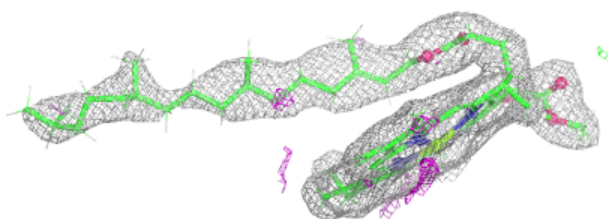
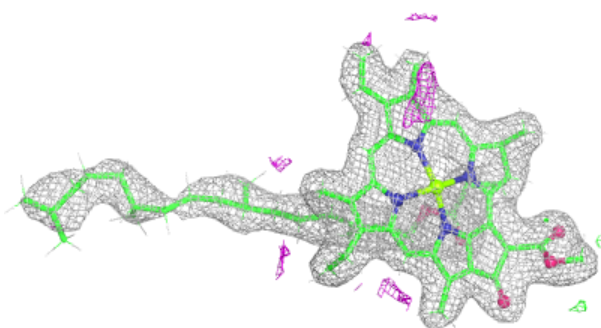


Electron density around CLA d 405:

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

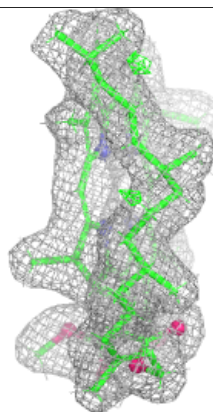
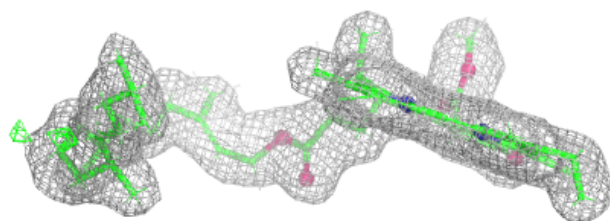
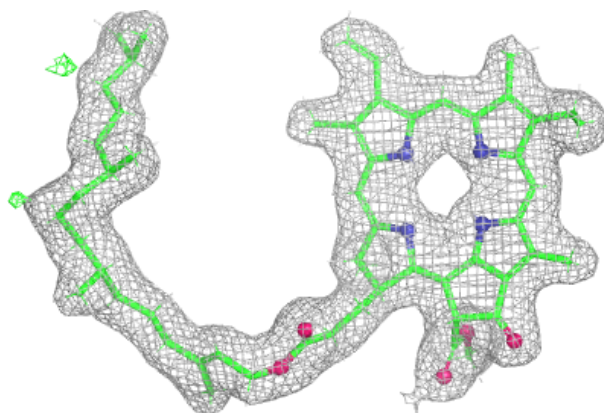
**Electron density around CLA B 614:**

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



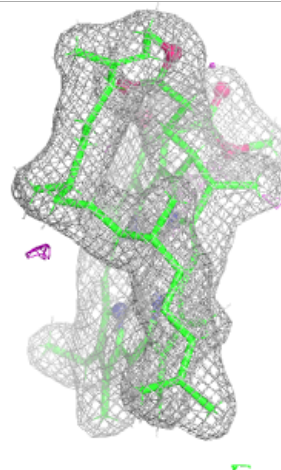
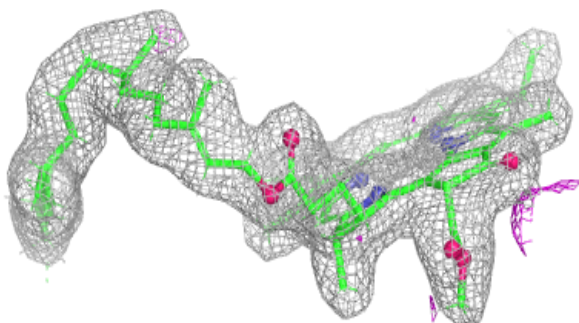
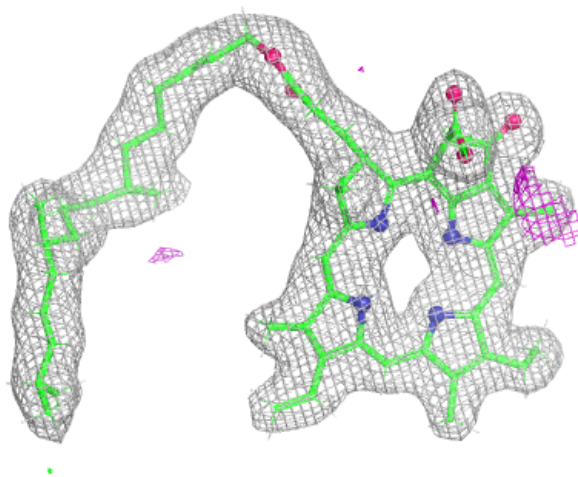
Electron density around PHO A 607:

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



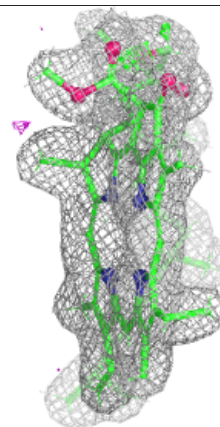
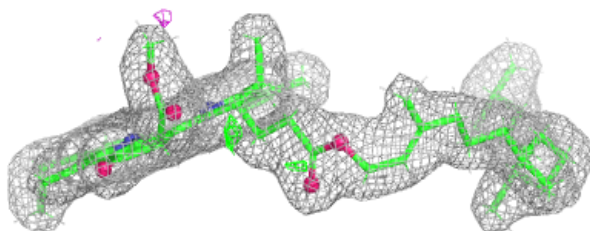
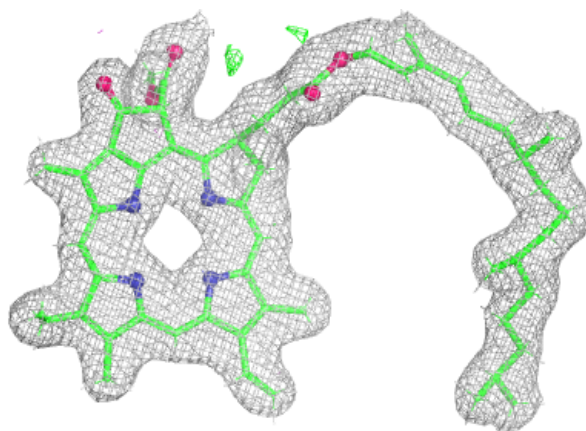
Electron density around PHO D 402:

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

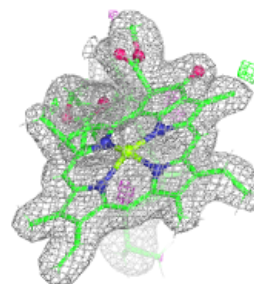
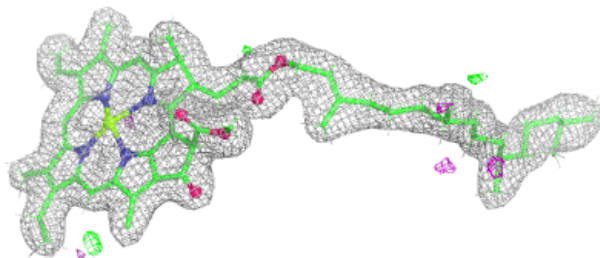
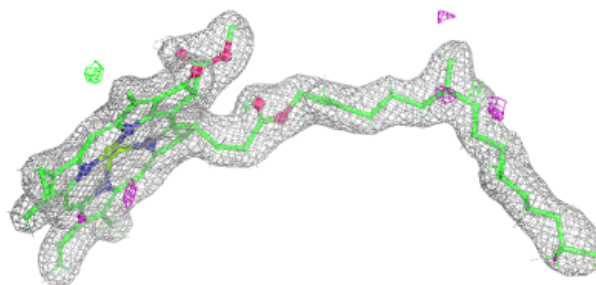


Electron density around PHO d 402:

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

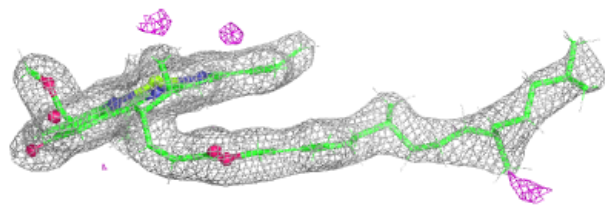
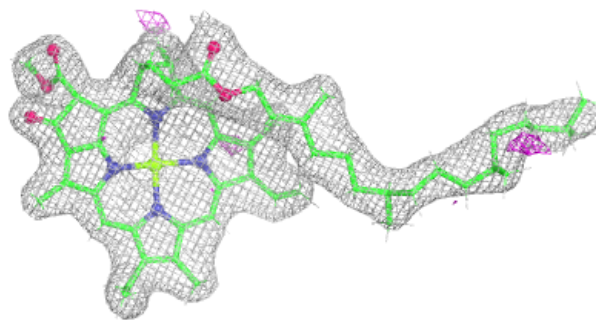
**Electron density around CLA A 605:**

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

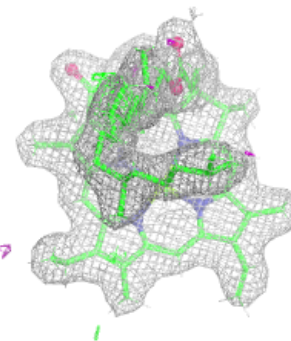
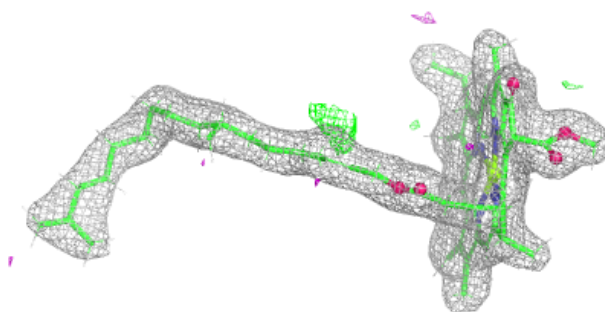
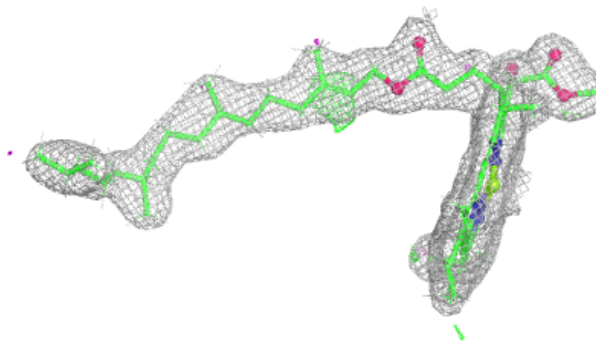


Electron density around CLA b 603:

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

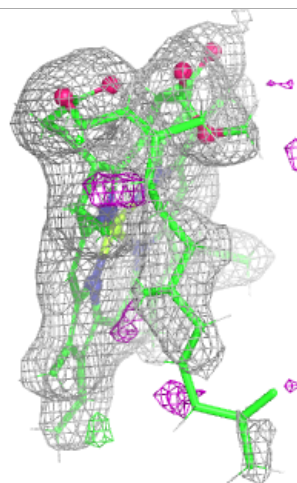
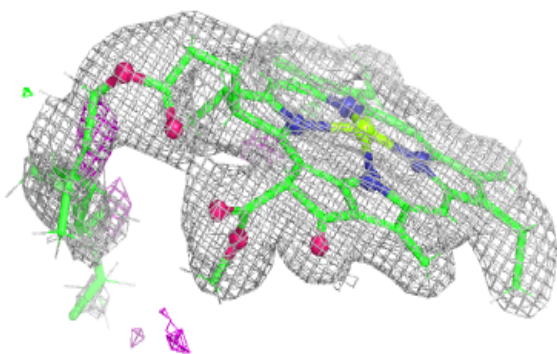
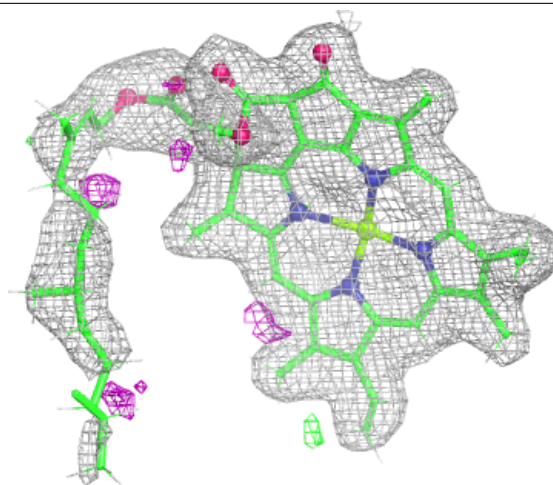
**Electron density around CLA b 605:**

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



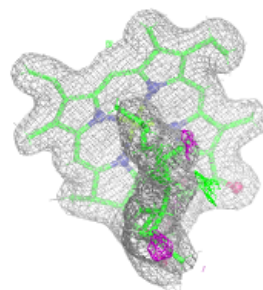
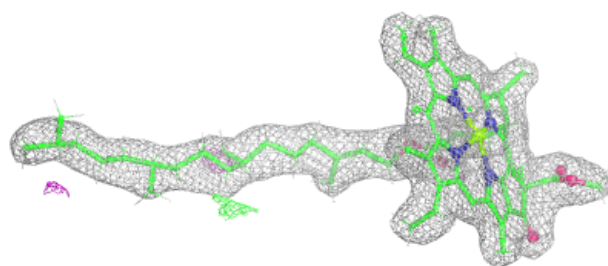
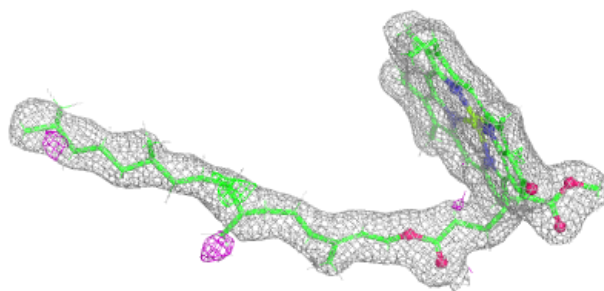
Electron density around CLA B 616:

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

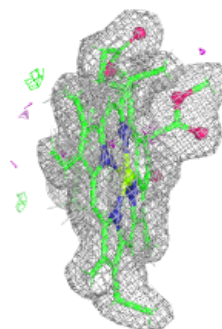
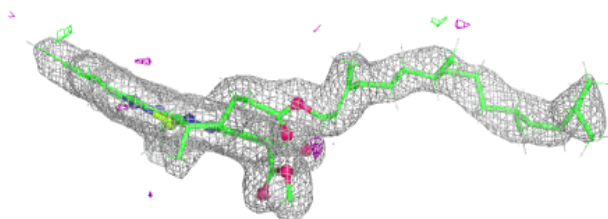
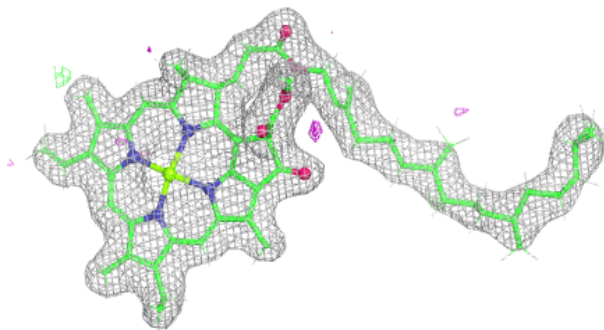


Electron density around CLA b 607:

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

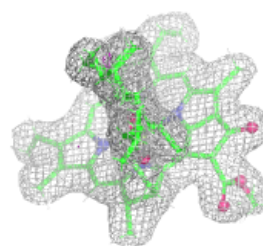
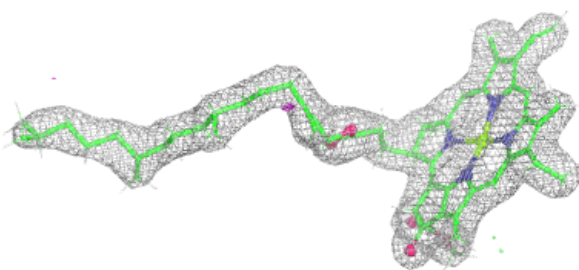
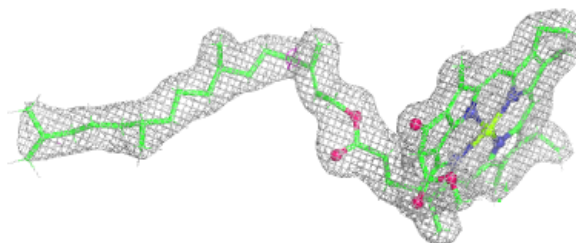
**Electron density around CLA B 602:**

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

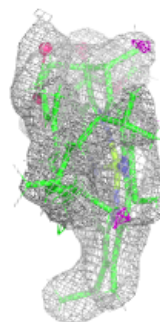
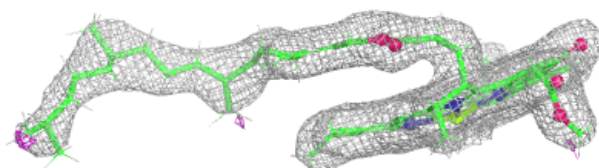
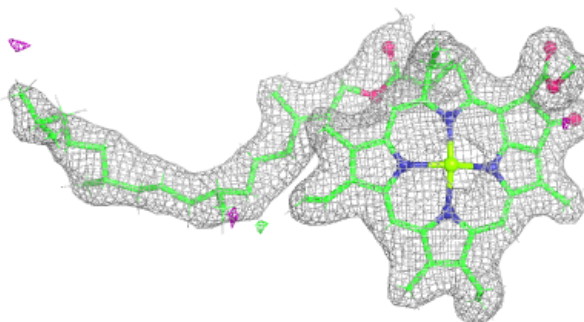


Electron density around CLA C 502:

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

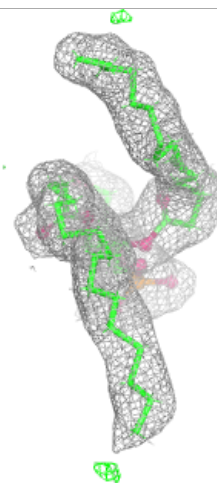
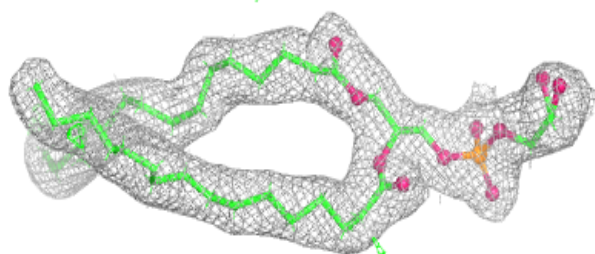
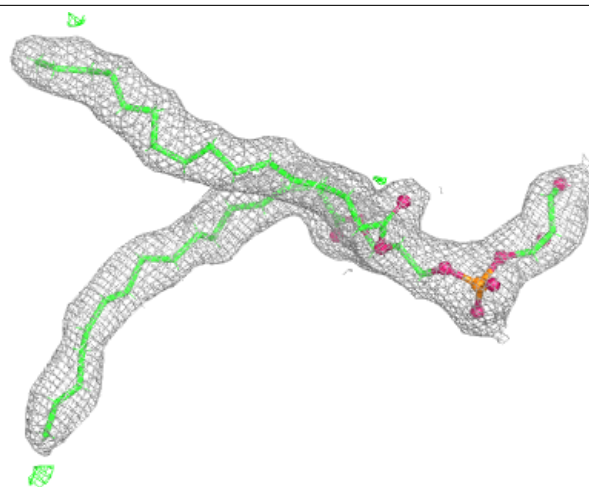
**Electron density around CLA B 603:**

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



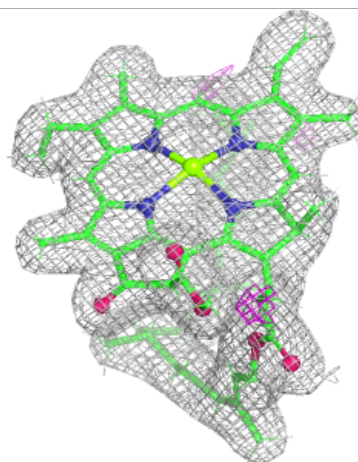
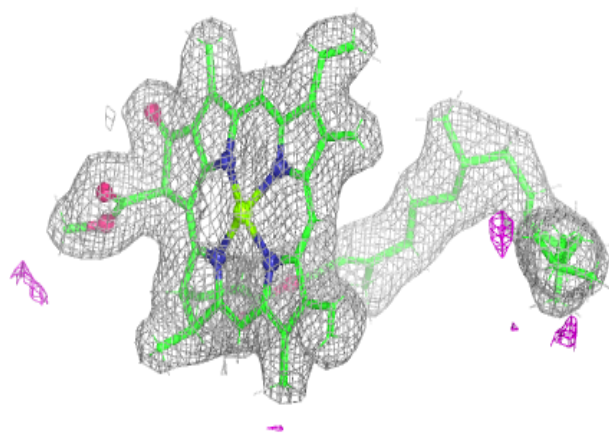
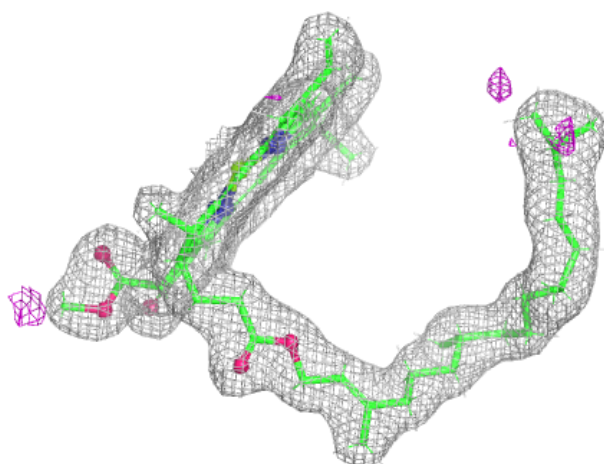
Electron density around LHG D 409:

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



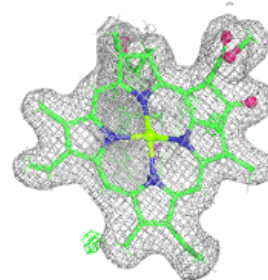
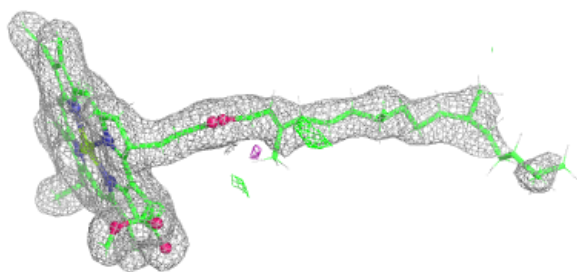
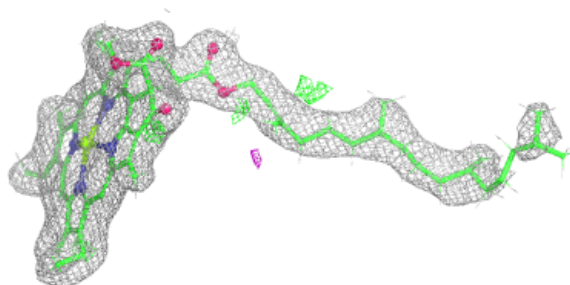
Electron density around CLA b 611:

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



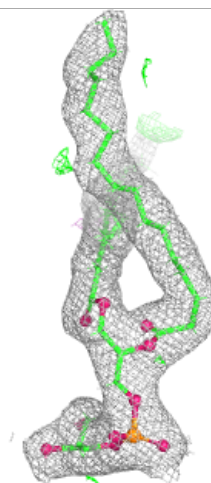
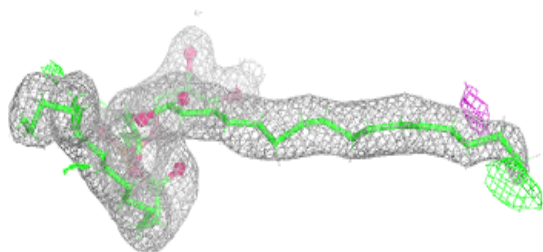
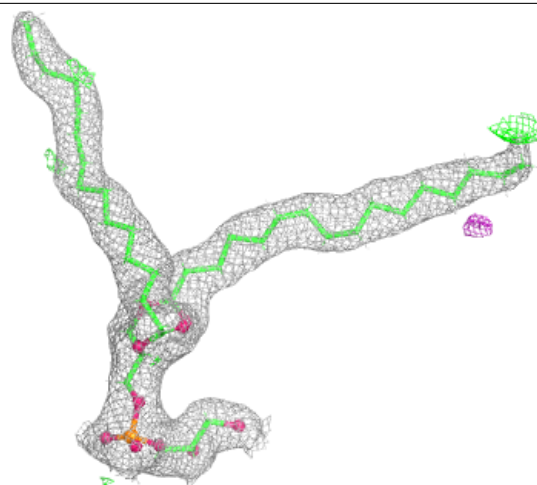
Electron density around CLA B 604:

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



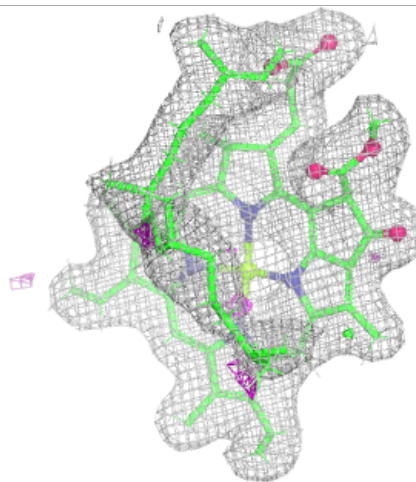
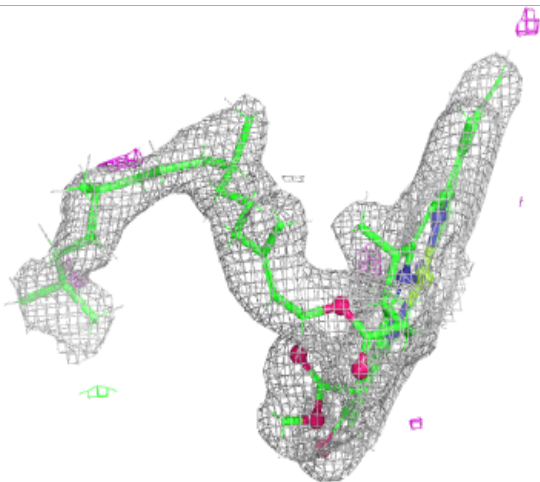
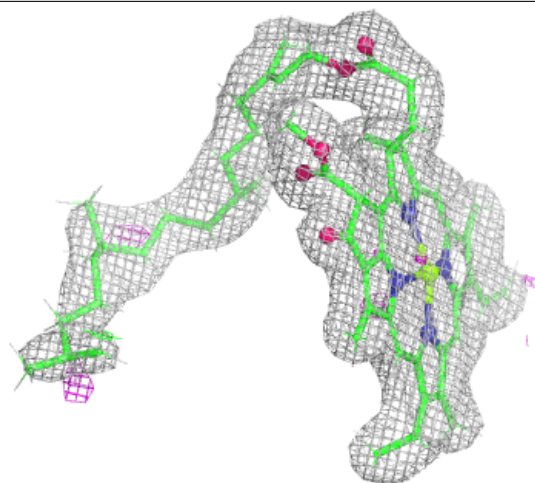
Electron density around LHG L 101:

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



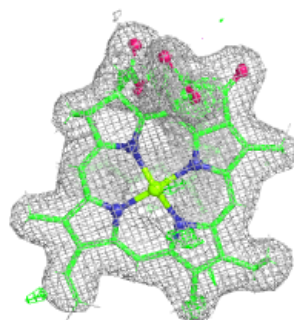
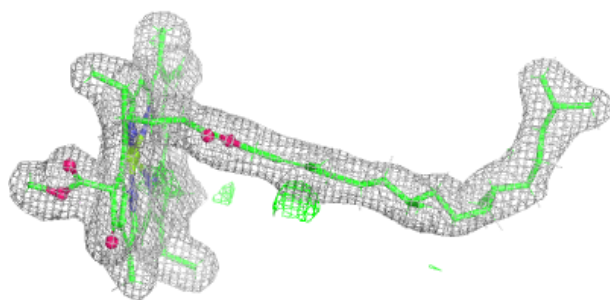
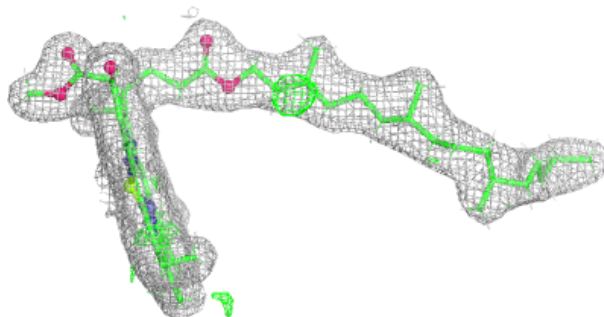
Electron density around CLA b 613:

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

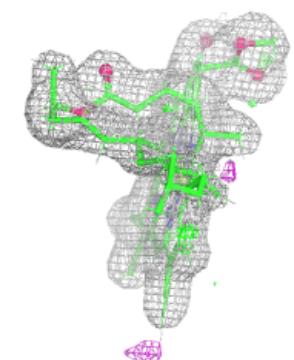
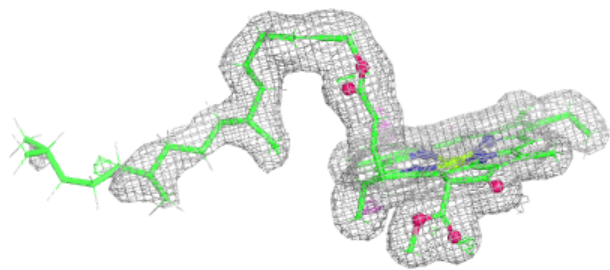
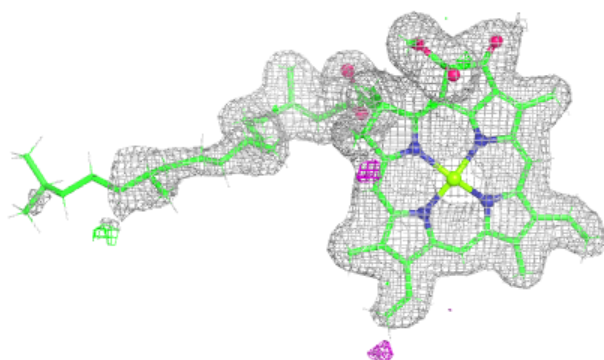


Electron density around CLA B 605:

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

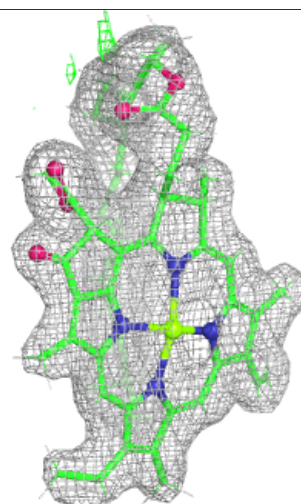
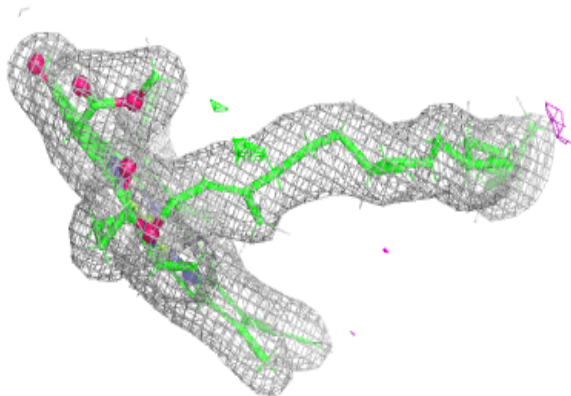
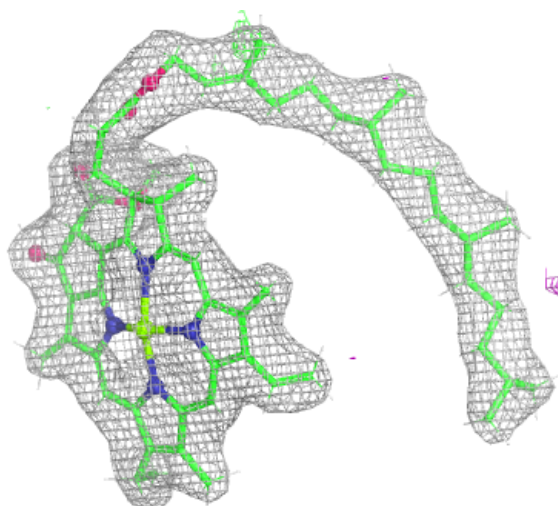
**Electron density around CLA A 606:**

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



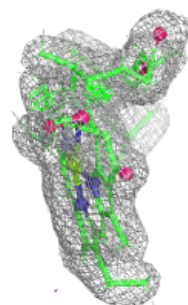
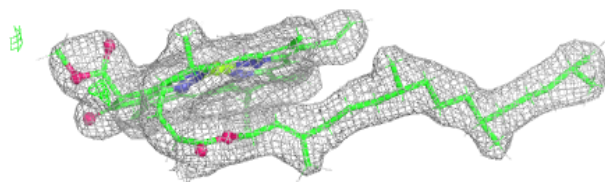
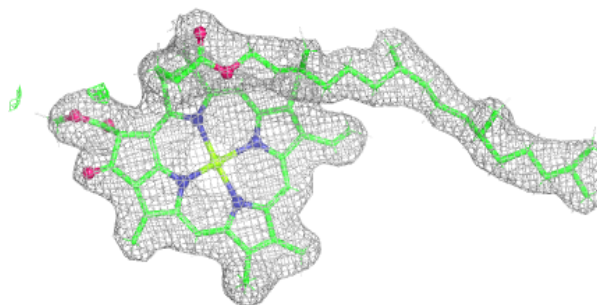
Electron density around CLA C 507:

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

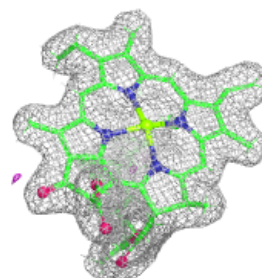
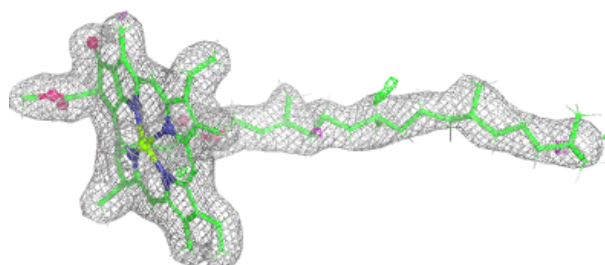
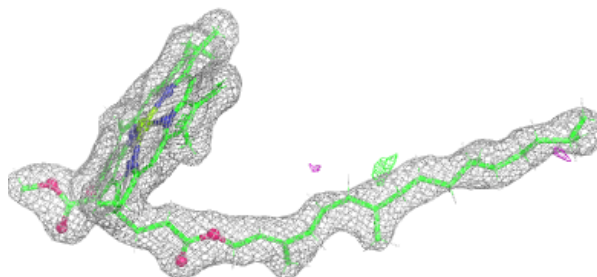


Electron density around CLA c 501:

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

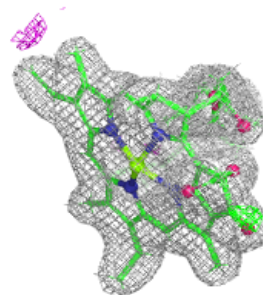
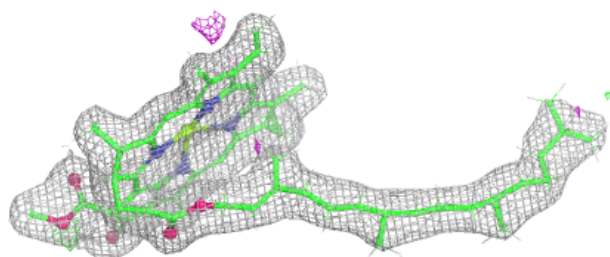
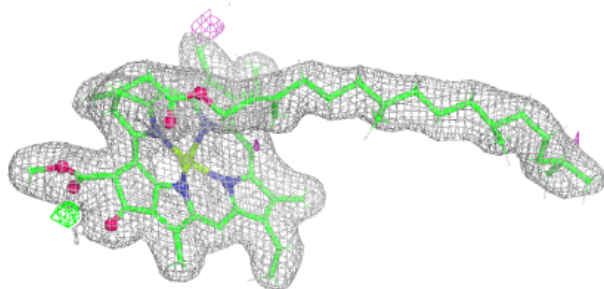
**Electron density around CLA B 607:**

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

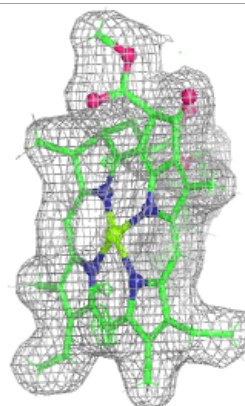
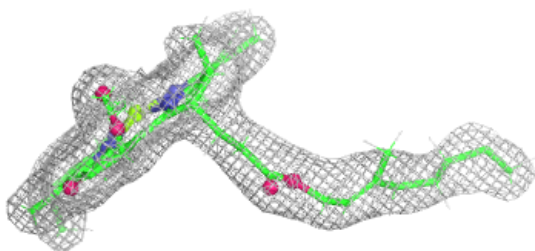
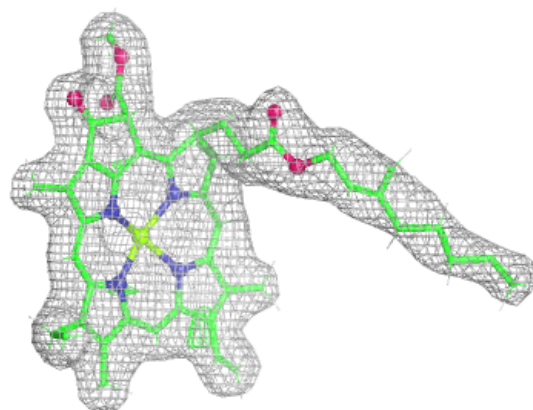


Electron density around CLA B 608:

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

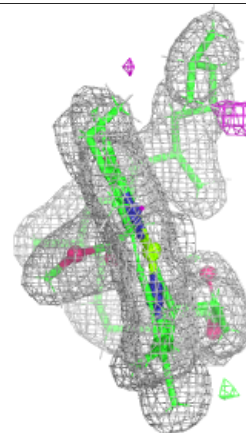
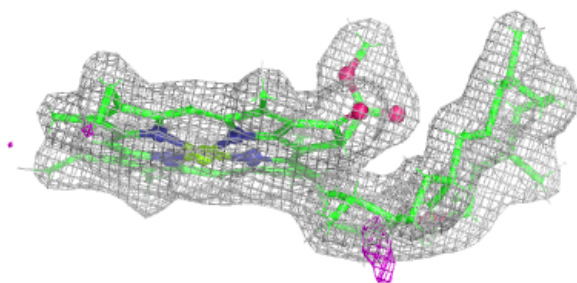
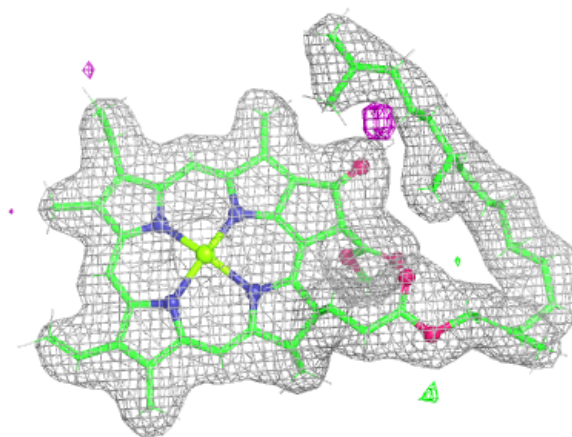
**Electron density around CLA A 608:**

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



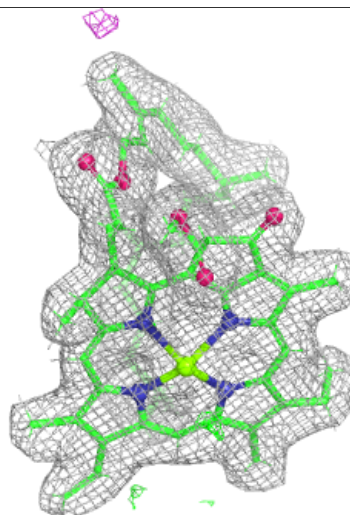
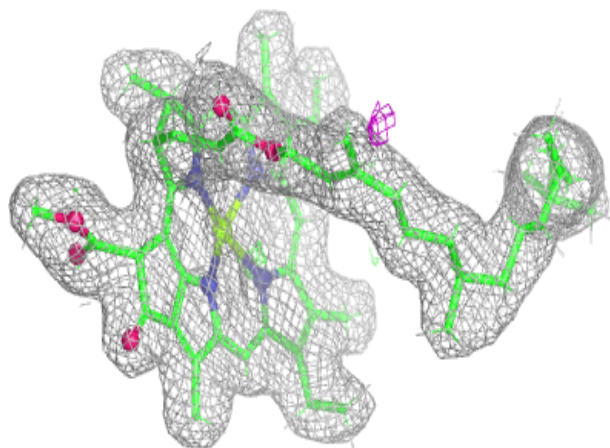
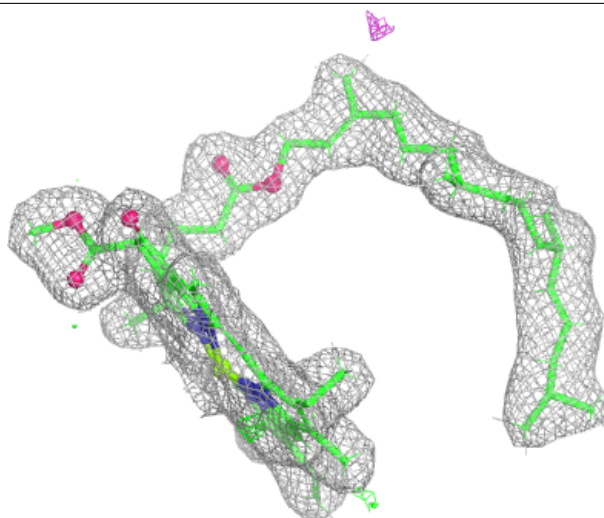
Electron density around CLA B 610:

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



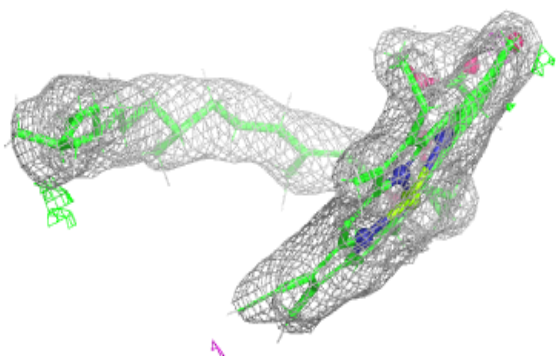
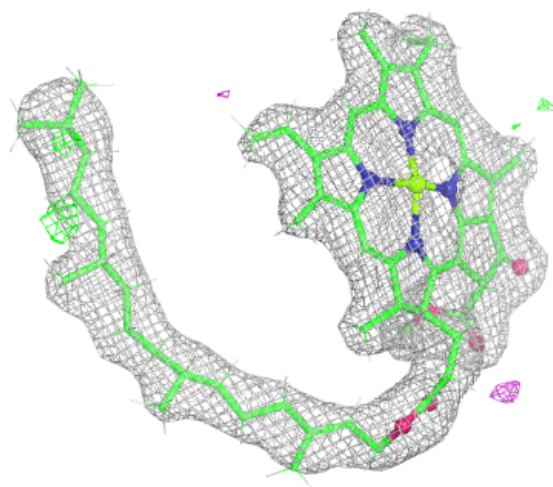
Electron density around CLA B 611:

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



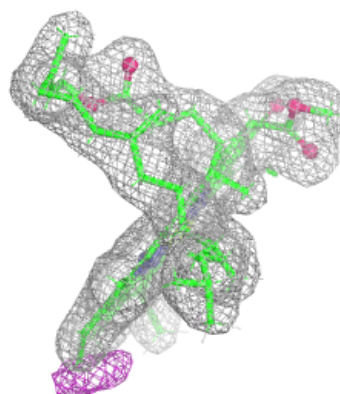
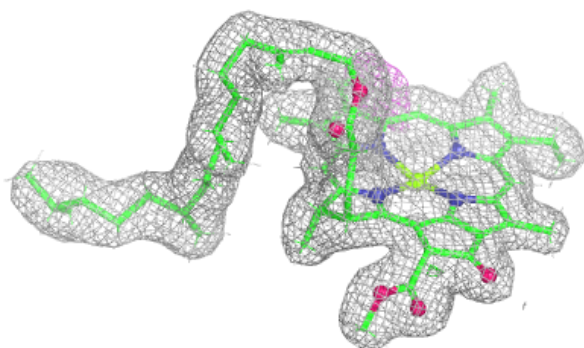
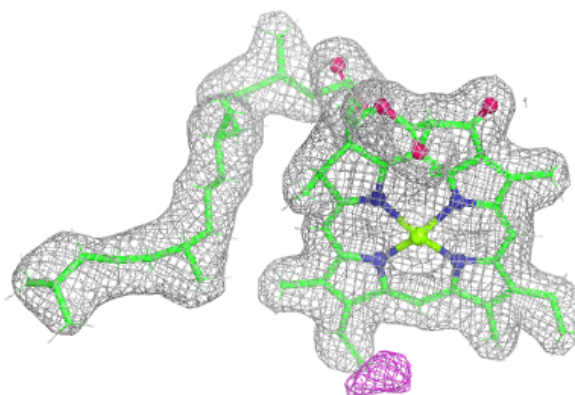
Electron density around CLA c 507:

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

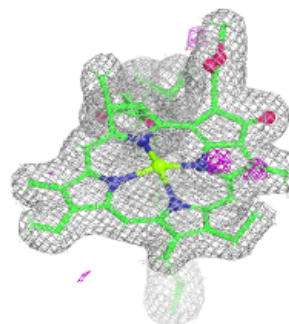
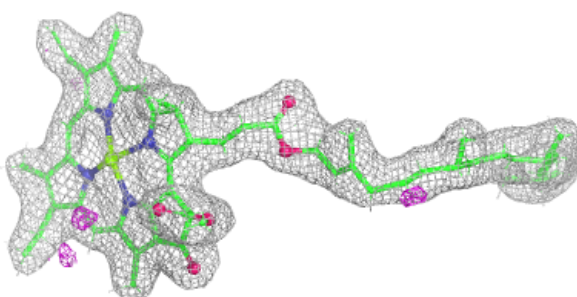
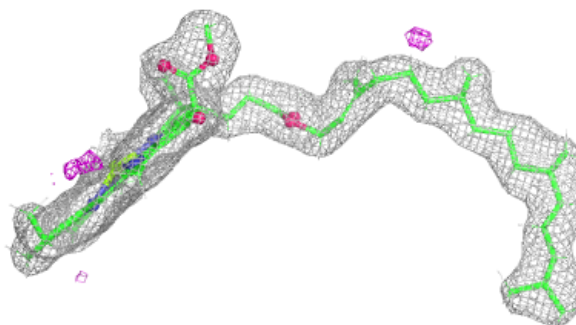


Electron density around CLA A 612:

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

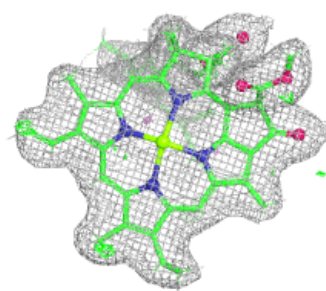
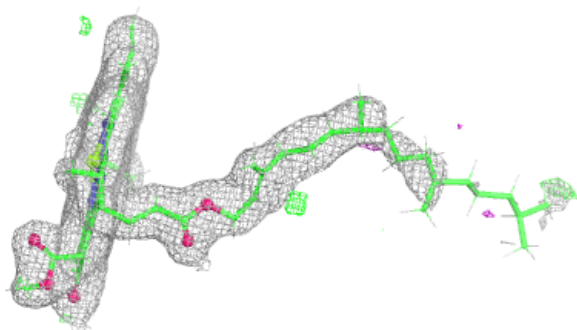
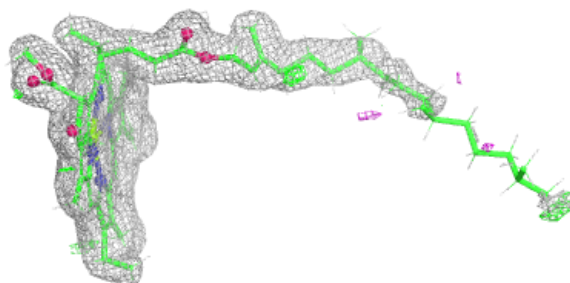
**Electron density around CLA D 403:**

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

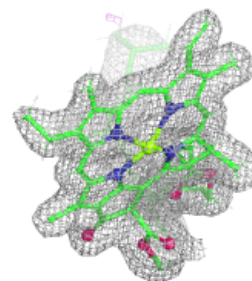
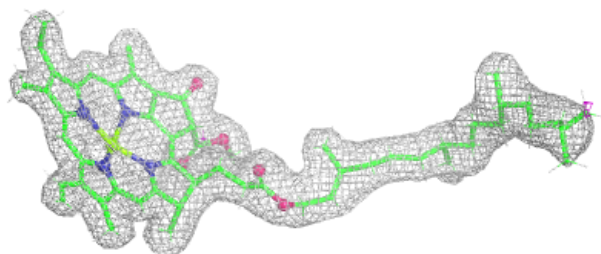
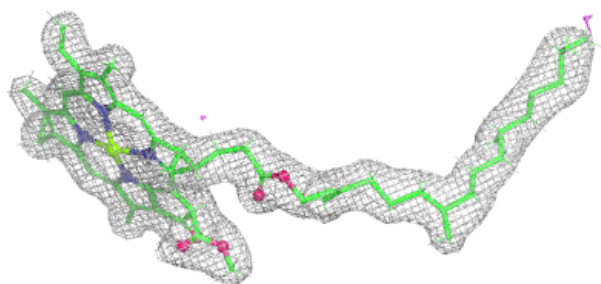


Electron density around CLA D 404:

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

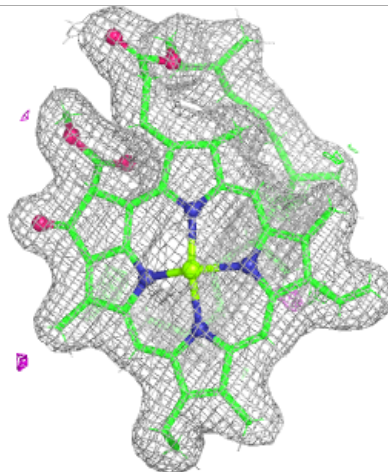
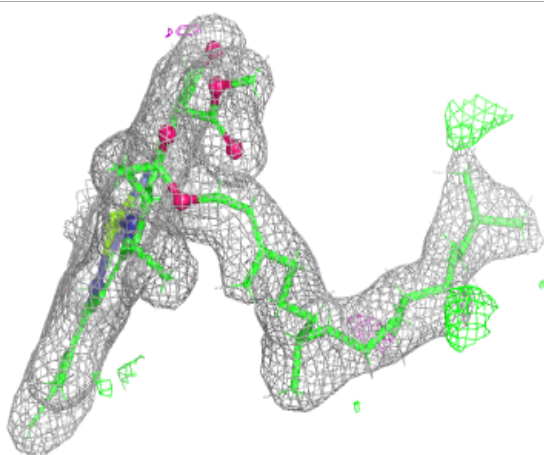
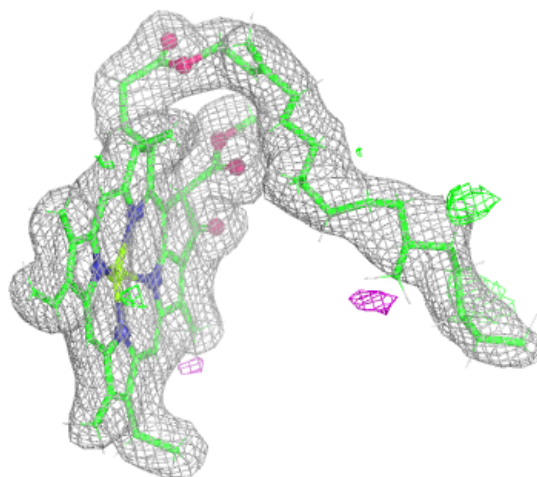
**Electron density around CLA a 605:**

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



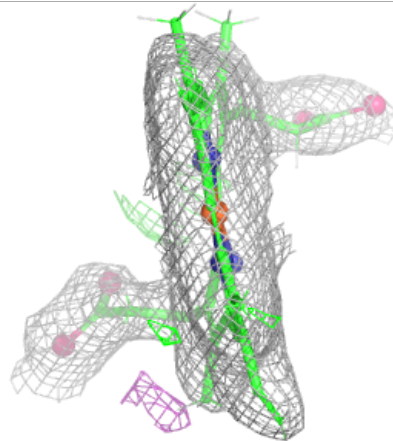
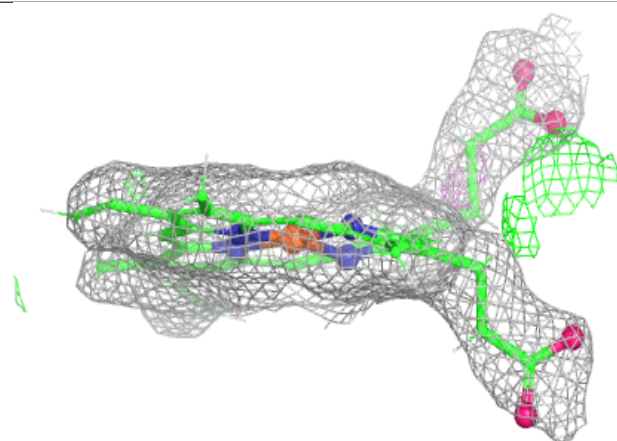
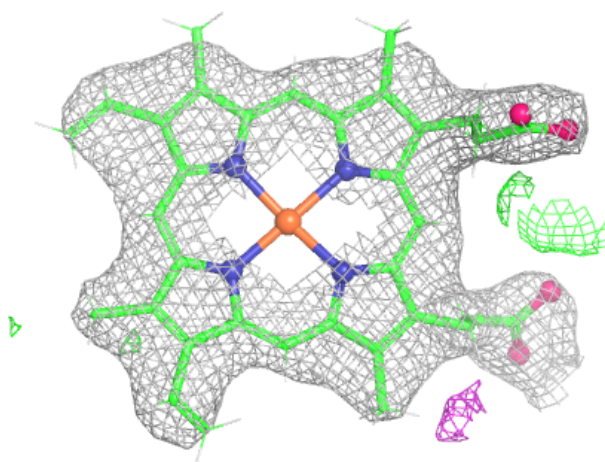
Electron density around CLA B 613:

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



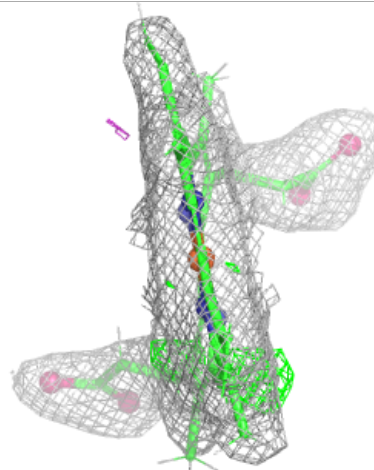
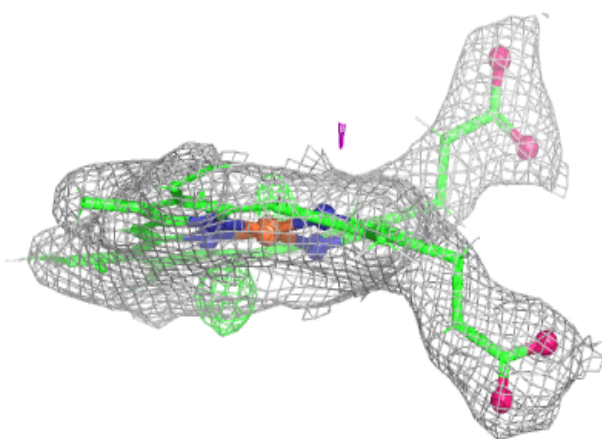
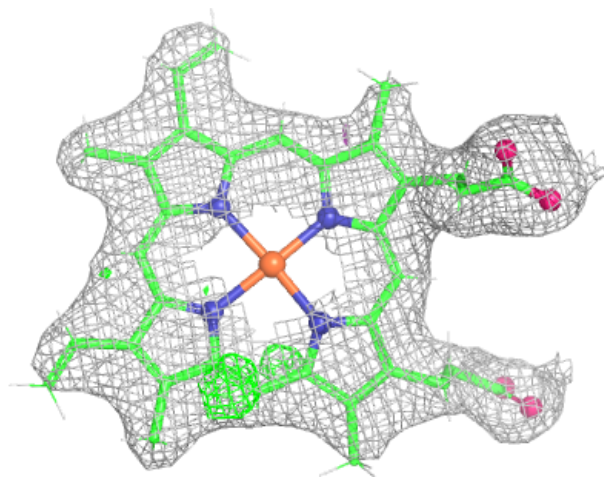
Electron density around HEM e 102:

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



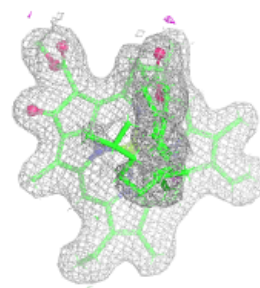
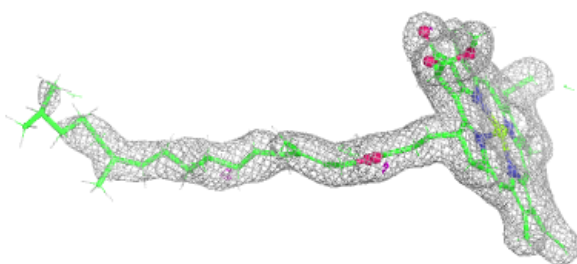
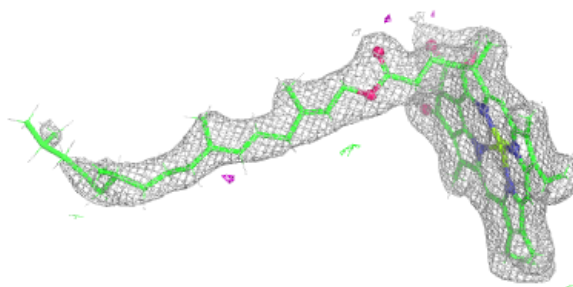
Electron density around HEM F 101:

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



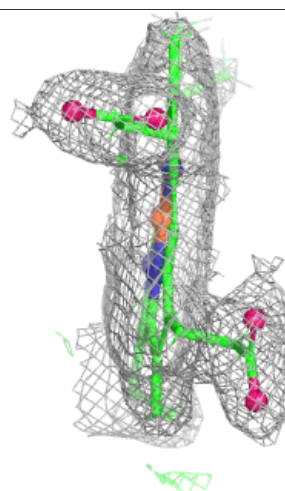
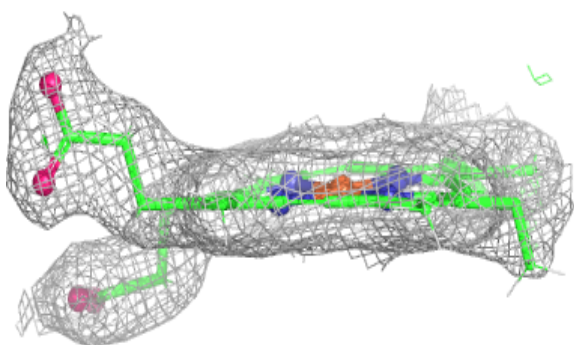
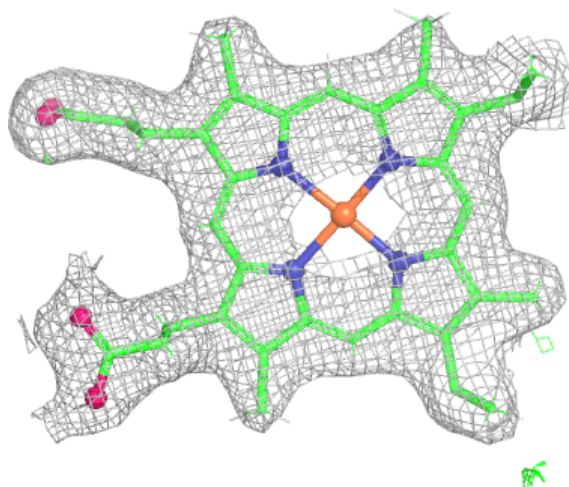
Electron density around CLA b 604:

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



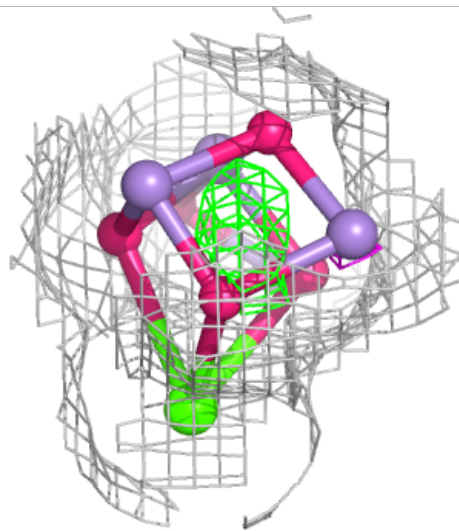
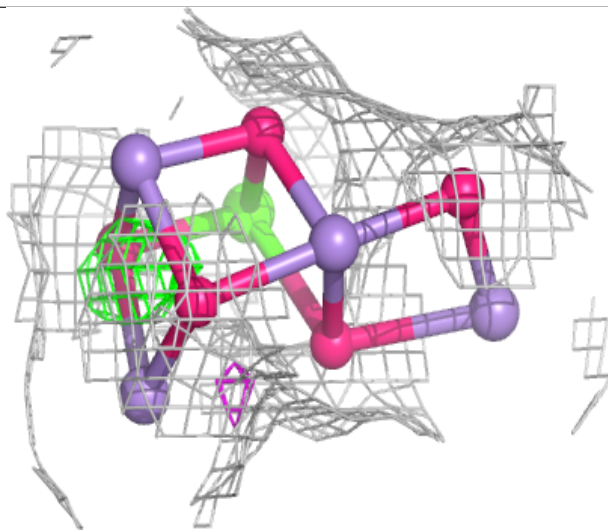
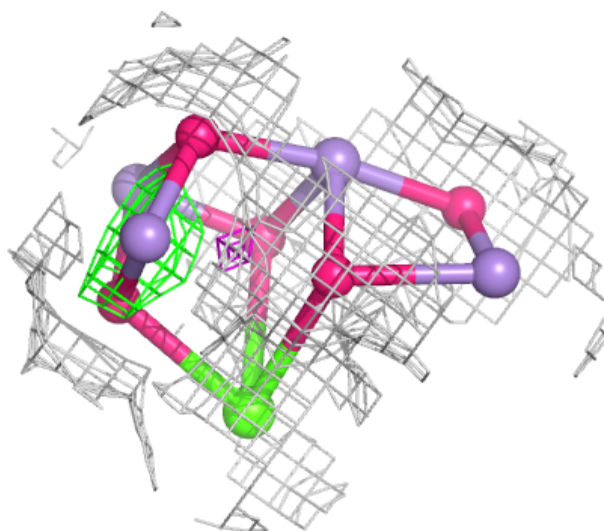
Electron density around HEC v 201:

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



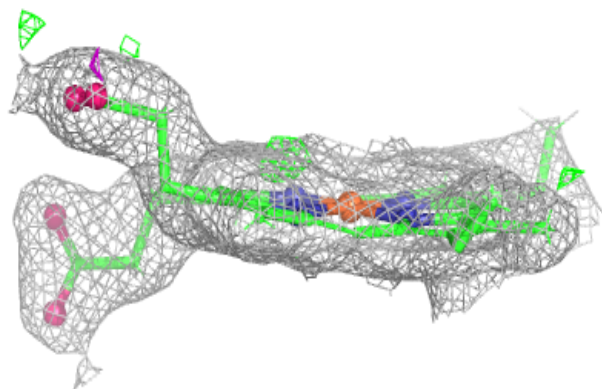
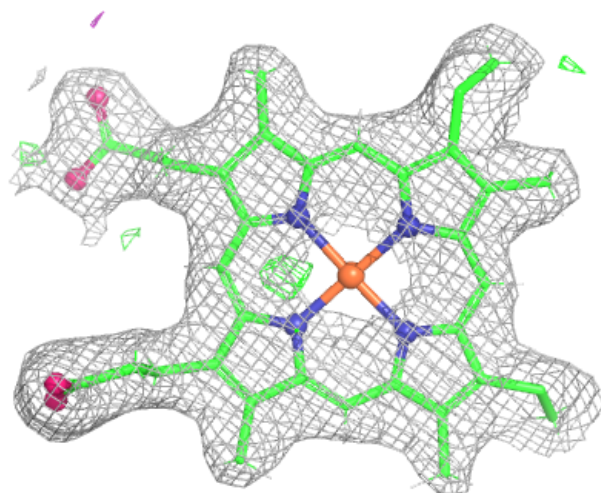
Electron density around OEX A 601:

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



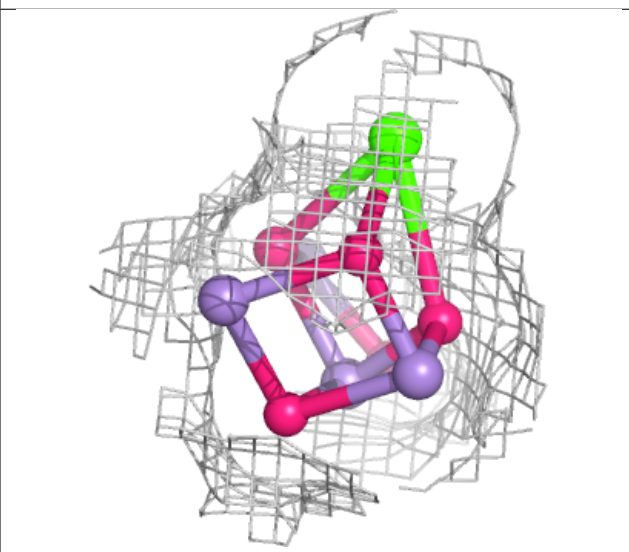
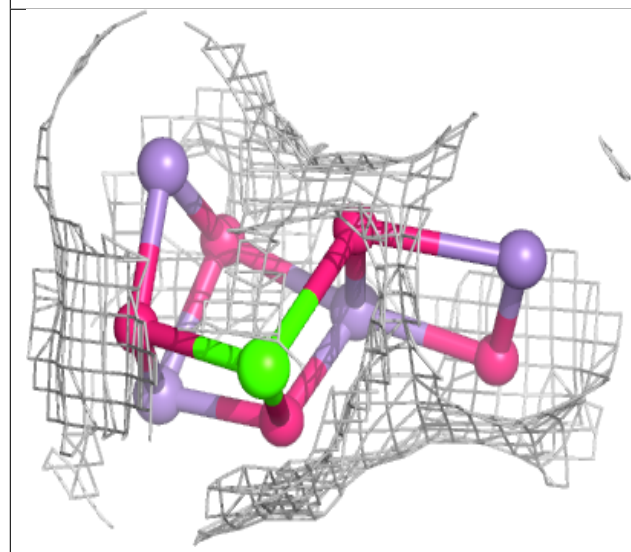
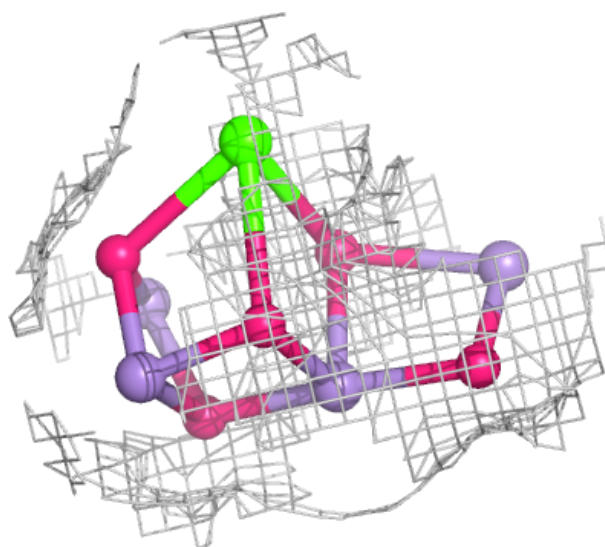
Electron density around HEC V 201:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.