



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 23, 2023 – 05:37 PM EDT

PDB ID : 5TIS

Title : Room temperature XFEL structure of the native, doubly-illuminated photo-system II complex

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Deposited on : 2016-10-03

Resolution : 2.25 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>.

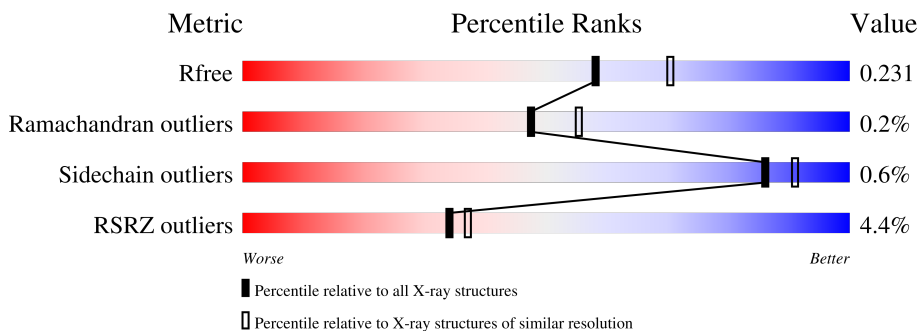
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)


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.

MolProbity	: 4.02b-467
Mogul	: 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	: 1.13
EDS	: 2.35.1
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	: 5.8.0158
CCP4	: 7.0.044 (Gargrove)
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.35.1

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	97%
2	B	510	98%
2	b	510	99%
3	C	461	97%
3	c	461	97%
4	D	352	97%
4	d	352	97%
5	E	84	94%
5	e	84	95%
6	F	45	76% 24%
6	f	45	76% 24%
7	H	66	95%
7	h	66	94% 5%
8	I	38	95%
8	i	38	95% 5%
9	J	40	90% 10%
9	j	40	90% 10%
10	K	46	78% 20%
10	k	46	78% 20%
11	L	37	100%
11	l	37	100%
12	M	36	89% 8%
12	m	36	92% 8%
13	O	272	89% 10%
13	o	272	88% 10%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	615	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606[A]	X	-	-	-
25	CLA	b	606[B]	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 51757 atoms, of which 0 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
			Total	C	N	O	S			
1	A	334	Total 2625	C 1719	N 431	O 460	S 15	0	1	0
1	a	334	Total 2622	C 1717	N 431	O 459	S 15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	Total 4005	C 2629	N 667	O 696	S 13	0	5	0
2	b	504	Total 3982	C 2613	N 665	O 691	S 13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3494	C 2287	N 585	O 609	S 13	0	1	0
3	c	451	Total 3494	C 2286	N 587	O 608	S 13	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2717	C 1800	N 444	O 461	S 12	0	0	0
4	d	341	Total 2716	C 1800	N 444	O 460	S 12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			670	437	109	124			
5	e	82	Total	C	N	O	0	1	0
			671	438	108	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	293	204	43	46	0	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
11	l	37	304	202	48	53	1	0	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	269	178	39	51	1	0	1	0
12	m	33	260	173	38	48	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1888	1179	320	385	4	0	2	0
13	o	244	1888	1179	320	385	4	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0
14	t	30	258	181	36	39	2	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
15	U	97	774	491	129	154	0	0	0
15	u	97	774	491	129	154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	Total 1064	C 675	N 177	O 208	S 4	0	0	0
16	v	137	Total 1070	C 680	N 178	O 208	S 4	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	27	Total 200	C 131	N 35	O 31	S 3	0	0	0
17	y	30	Total 224	C 147	N 38	O 36	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	X	38	Total 281	C 188	N 45	O 48		0	0	0
18	x	38	Total 285	C 192	N 46	O 47		0	1	0

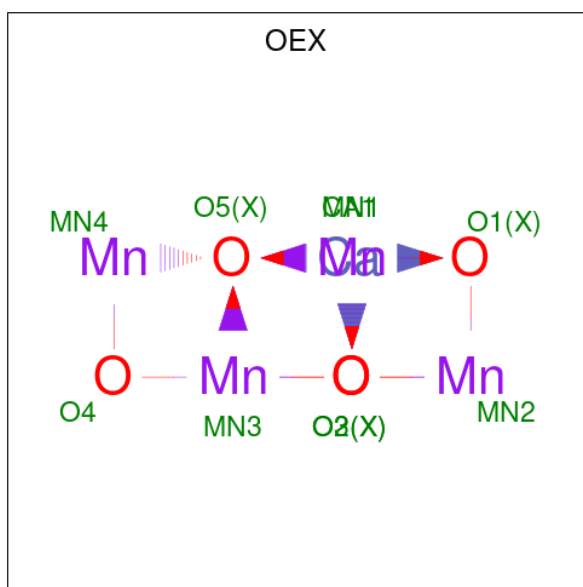
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	Total 479	C 328	N 72	O 77	S 2	0	0	0
19	z	62	Total 478	C 328	N 72	O 76	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	34	Total 273	C 186	N 47	O 40		0	0	0
20	r	34	Total 270	C 183	N 47	O 40		0	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

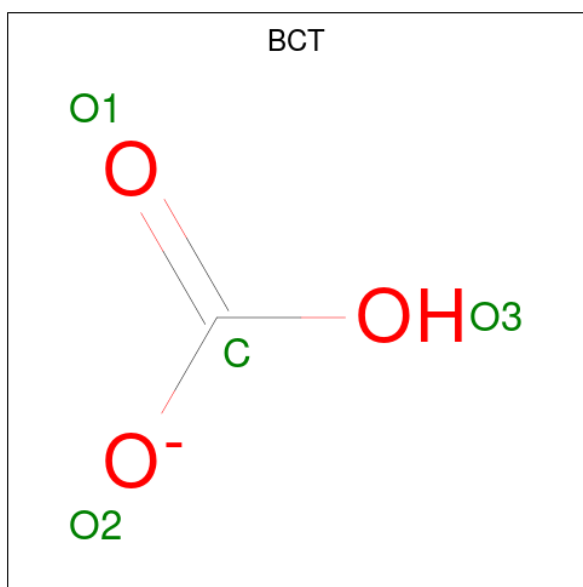
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

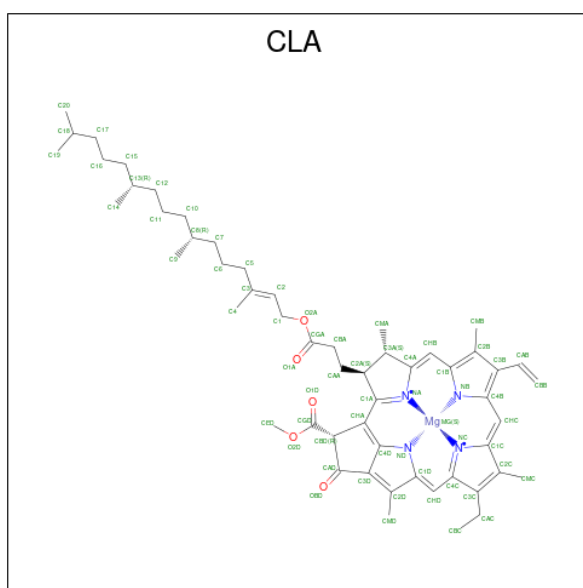
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
23	A	2	2	2	0	0
23	a	2	2	2	0	0

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 4 1 3	0	0
24	a	1	Total C O 4 1 3	0	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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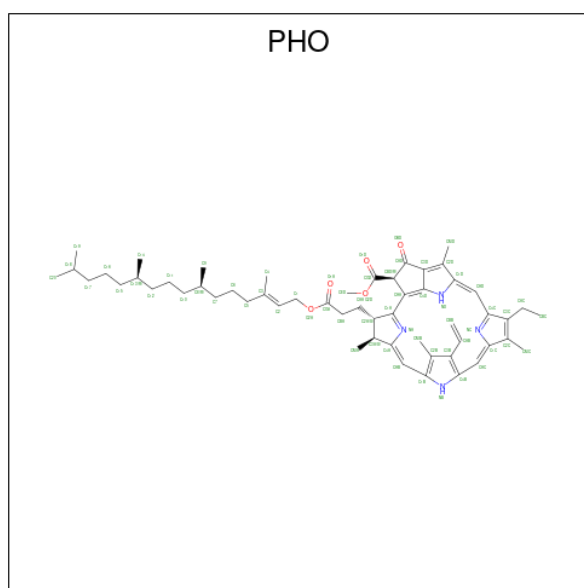
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	b	1	129	110	1	8	10	0	1
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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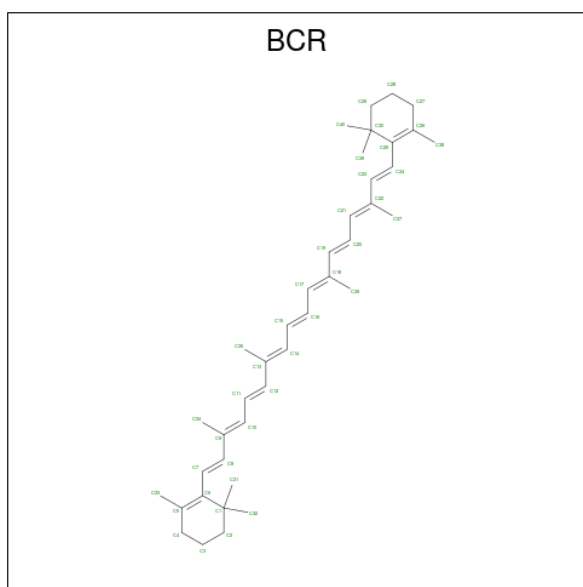
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



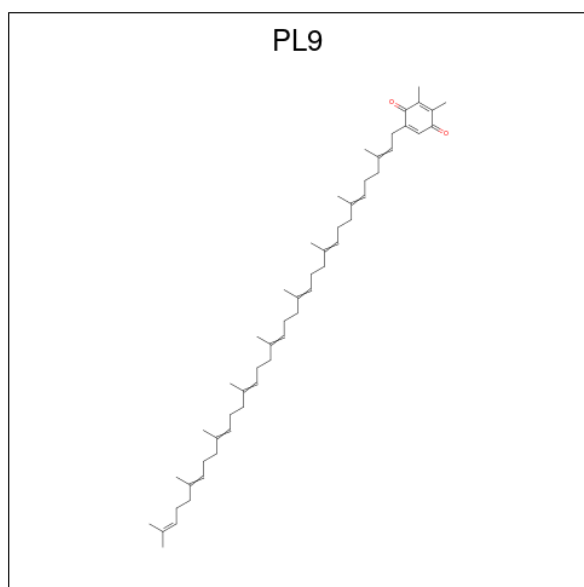
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

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



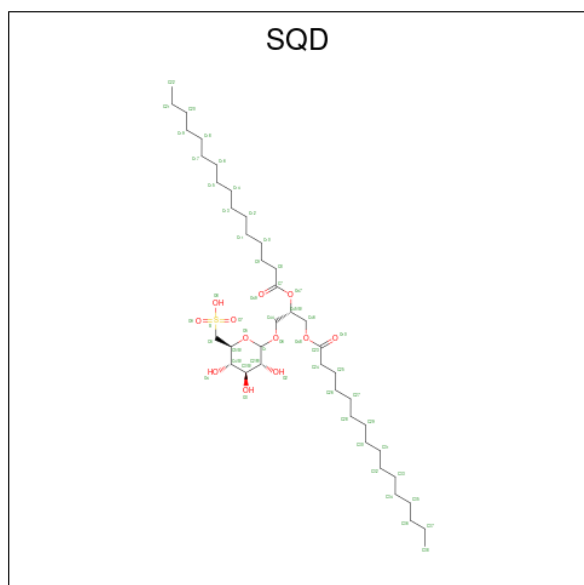
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



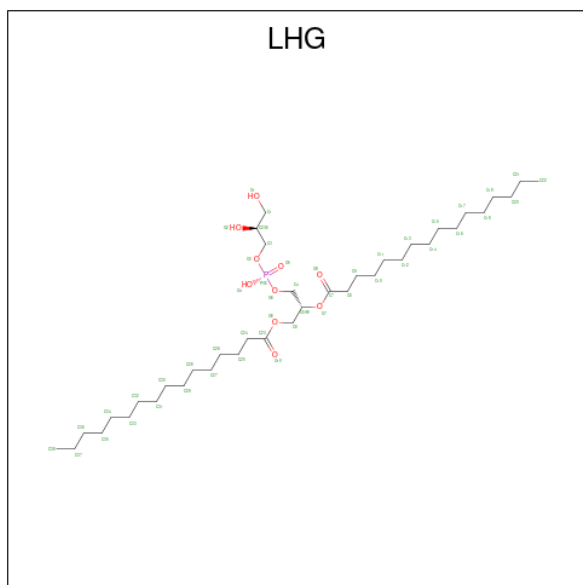
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	D	1	Total	C	O	S	0	0
			47	34	12	1		
29	L	1	Total	C	O	S	0	0
			49	36	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O		0	0
			40	35	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	f	1	41	28	12	1	0	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).

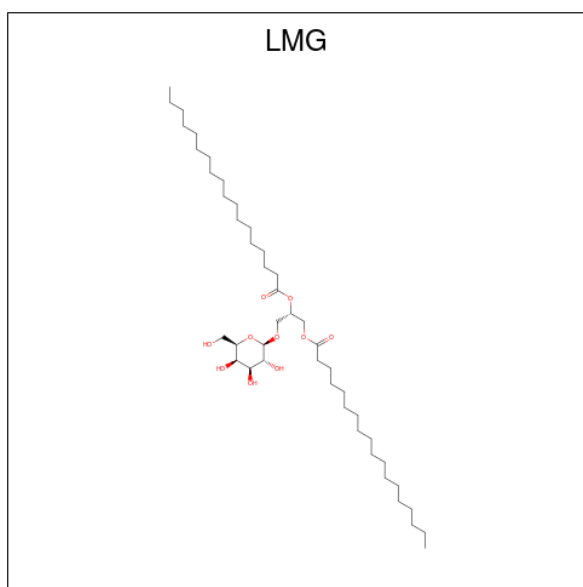


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
30	A	1	47	36	10	1	0	0
30	A	1	49	38	10	1	0	0
30	B	1	49	38	10	1	0	0
30	D	1	49	38	10	1	0	0
30	L	1	49	38	10	1	0	0
30	a	1	39	28	10	1	0	0
30	a	1	42	31	10	1	0	0
30	d	1	49	38	10	1	0	0
30	d	1	49	38	10	1	0	0
30	l	1	49	38	10	1	0	0

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

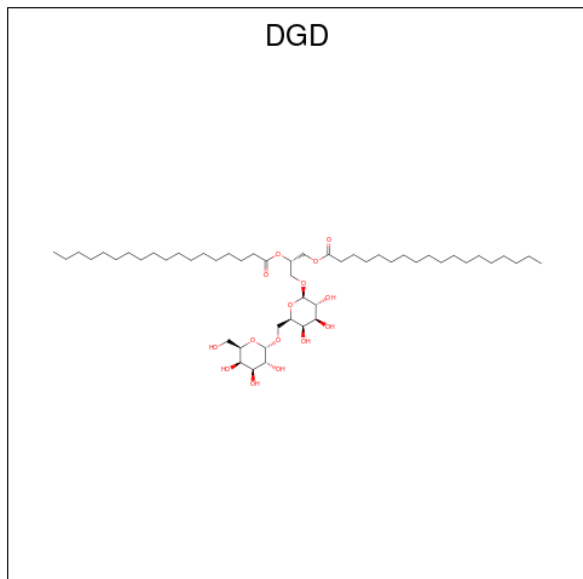
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	2	Total C O 29 27 2	0	0
31	B	2	Total C 26 26	0	0
31	C	2	Total C O 33 31 2	0	0
31	D	2	Total C 28 28	0	0
31	E	1	Total C O 12 10 2	0	0
31	H	1	Total C 7 7	0	0
31	I	2	Total C O 27 25 2	0	0
31	J	2	Total C O 23 21 2	0	0
31	M	2	Total C O 32 30 2	0	0
31	T	2	Total C 26 26	0	0
31	a	2	Total C O 29 27 2	0	0
31	b	2	Total C 28 28	0	0
31	c	3	Total C O 40 34 6	0	0
31	d	1	Total C 17 17	0	0
31	i	1	Total C O 20 18 2	0	0
31	j	2	Total C O 27 25 2	0	0
31	m	2	Total C O 25 23 2	0	0
31	t	1	Total C 18 18	0	0
31	x	1	Total C 16 16	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	b	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			34	24	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			38	36	2		
32	m	1	Total	C	O	0	0
			51	41	10		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	C	1	62	47	15	0	0
33	C	1	62	47	15	0	0
33	C	1	62	47	15	0	0
33	H	1	62	47	15	0	0
33	c	1	62	47	15	0	0
33	c	1	62	47	15	0	0
33	c	1	62	47	15	0	0
33	h	1	62	47	15	0	0

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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	86	Total O 86 86	0	0
36	B	109	Total O 109 109	0	0
36	C	95	Total O 95 95	0	0
36	D	82	Total O 82 82	0	0
36	E	14	Total O 14 14	0	0
36	F	3	Total O 3 3	0	0
36	H	11	Total O 11 11	0	0
36	I	3	Total O 3 3	0	0
36	J	5	Total O 5 5	0	0
36	K	2	Total O 2 2	0	0
36	L	3	Total O 3 3	0	0
36	M	5	Total O 5 5	0	0
36	O	72	Total O 72 72	0	0
36	T	9	Total O 9 9	0	0
36	U	22	Total O 22 22	0	0
36	V	42	Total O 42 42	0	0
36	X	5	Total O 5 5	0	0
36	Z	3	Total O 3 3	0	0
36	a	90	Total O 90 90	0	0
36	b	129	Total O 129 129	0	0
36	c	95	Total O 95 95	0	0

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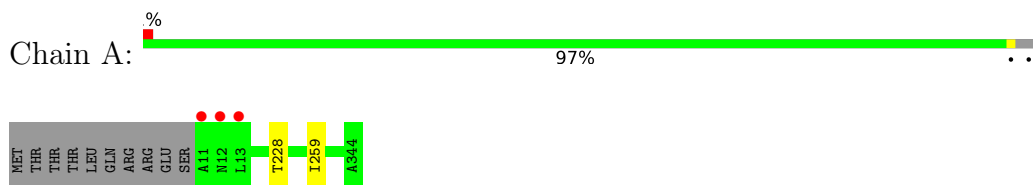
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	87	Total O 87 87	0	0
36	e	9	Total O 9 9	0	0
36	f	2	Total O 2 2	0	0
36	h	13	Total O 13 13	0	0
36	i	6	Total O 6 6	0	0
36	j	2	Total O 2 2	0	0
36	k	4	Total O 4 4	0	0
36	l	10	Total O 10 10	0	0
36	m	10	Total O 10 10	0	0
36	o	69	Total O 69 69	0	0
36	t	4	Total O 4 4	0	0
36	u	34	Total O 34 34	0	0
36	v	37	Total O 37 37	0	0
36	y	1	Total O 1 1	0	0
36	x	4	Total O 4 4	0	0
36	z	1	Total O 1 1	0	0
36	r	1	Total O 1 1	0	0

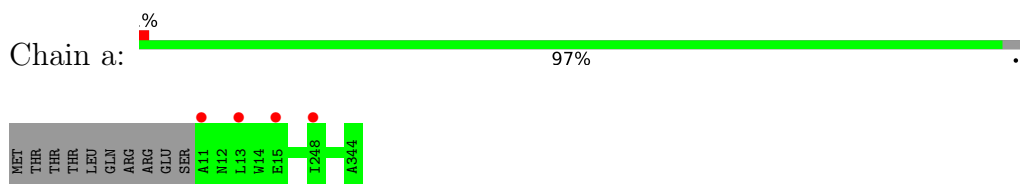
3 Residue-property plots [i](#)

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

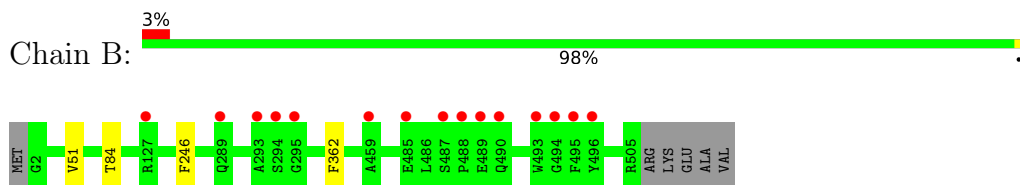
- Molecule 1: Photosystem II protein D1 1



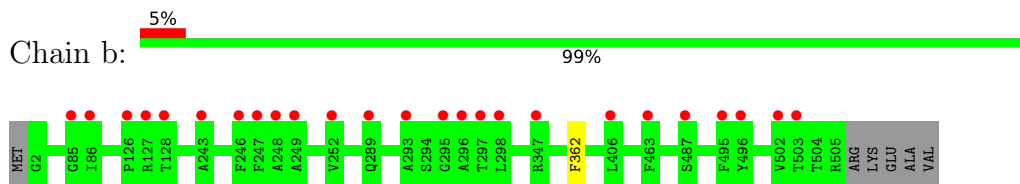
- Molecule 1: Photosystem II protein D1 1



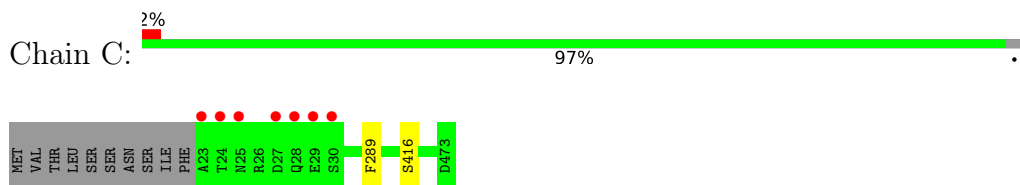
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



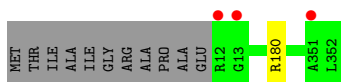
- Molecule 3: Photosystem II CP43 reaction center protein



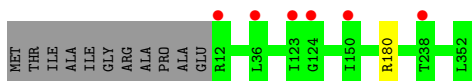
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



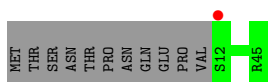
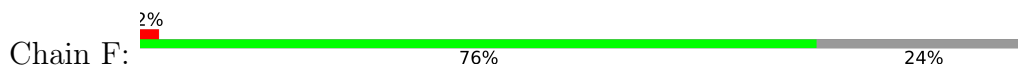
- Molecule 5: Cytochrome b559 subunit alpha



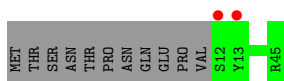
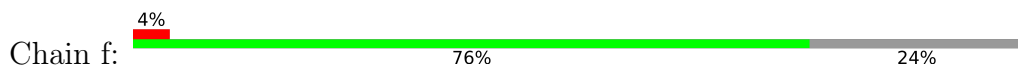
- Molecule 5: Cytochrome b559 subunit alpha



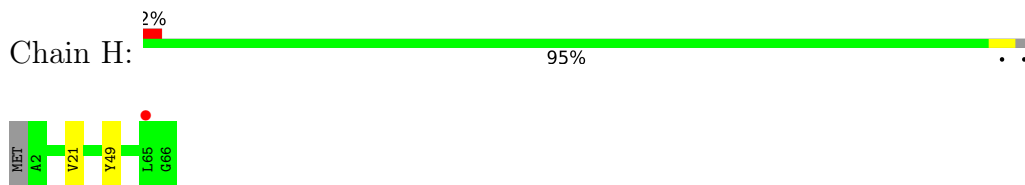
- Molecule 6: Cytochrome b559 subunit beta



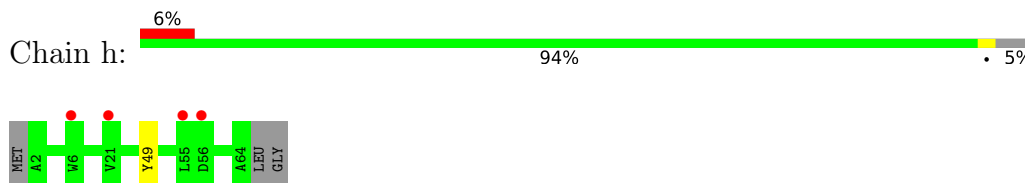
- Molecule 6: Cytochrome b559 subunit beta



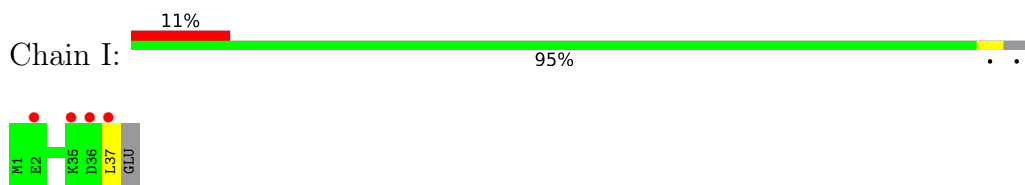
- Molecule 7: Photosystem II reaction center protein H



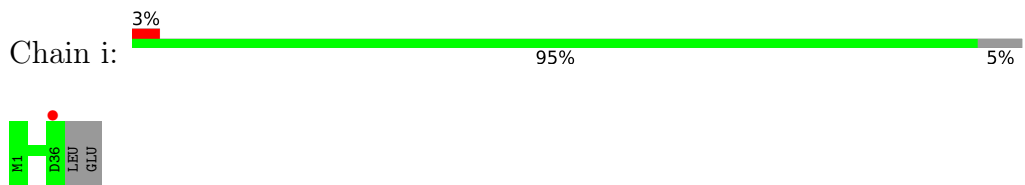
- Molecule 7: Photosystem II reaction center protein H



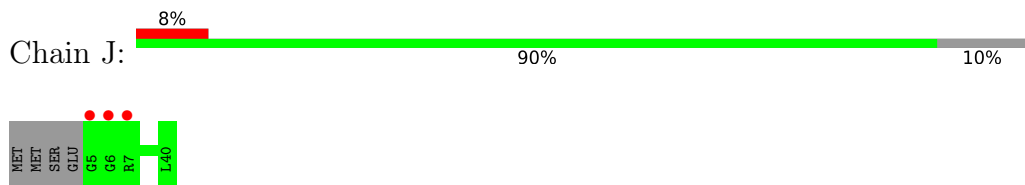
- Molecule 8: Photosystem II reaction center protein I



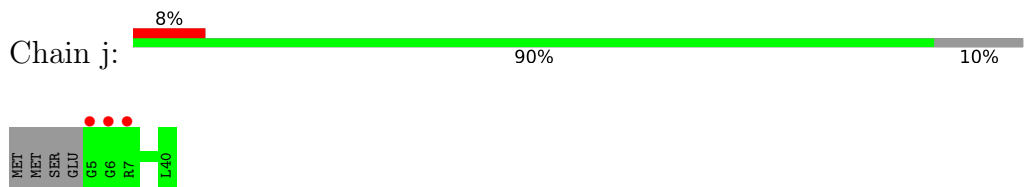
- Molecule 8: Photosystem II reaction center protein I



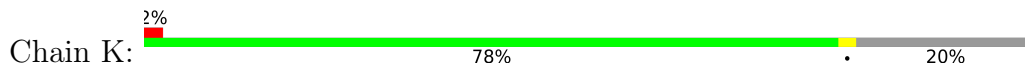
- Molecule 9: Photosystem II reaction center protein J

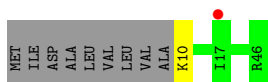


- Molecule 9: Photosystem II reaction center protein J

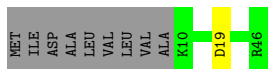
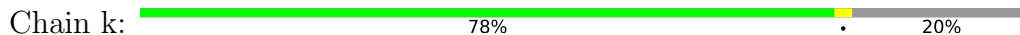


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

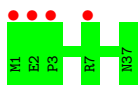


- Molecule 11: Photosystem II reaction center protein L

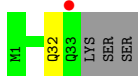
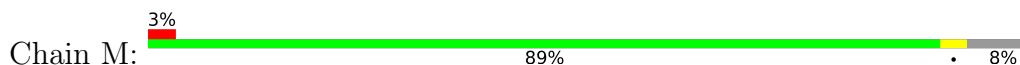


There are no outlier residues recorded for this chain.

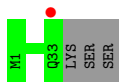
- Molecule 11: Photosystem II reaction center protein L



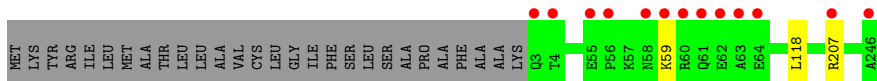
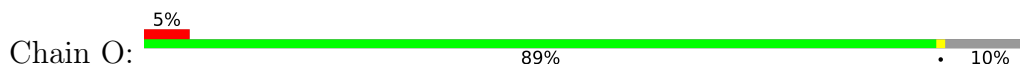
- Molecule 12: Photosystem II reaction center protein M



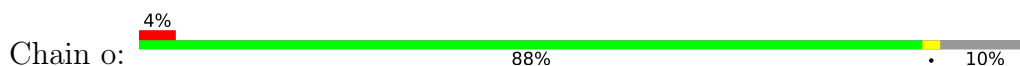
- Molecule 12: Photosystem II reaction center protein M

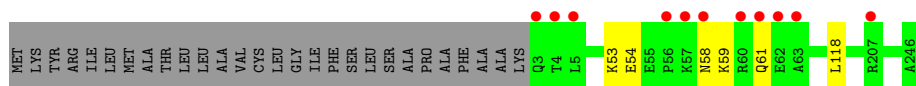


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

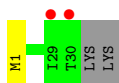
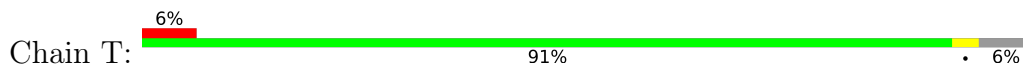


- Molecule 13: Photosystem II manganese-stabilizing polypeptide





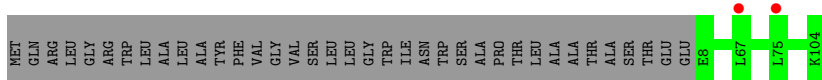
- Molecule 14: Photosystem II reaction center protein T



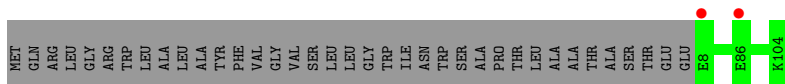
- Molecule 14: Photosystem II reaction center protein T



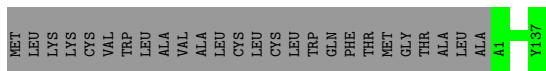
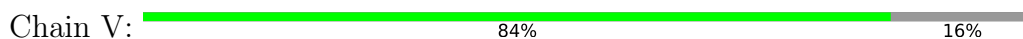
- Molecule 15: Photosystem II 12 kDa extrinsic protein



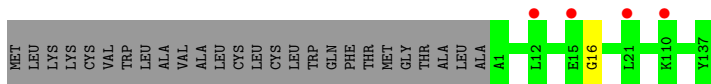
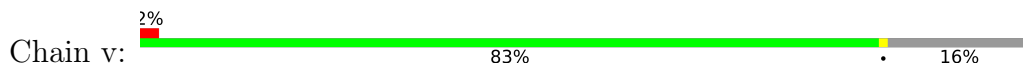
- Molecule 15: Photosystem II 12 kDa extrinsic protein



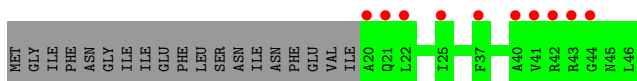
- Molecule 16: Cytochrome c-550



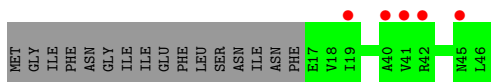
- Molecule 16: Cytochrome c-550



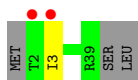
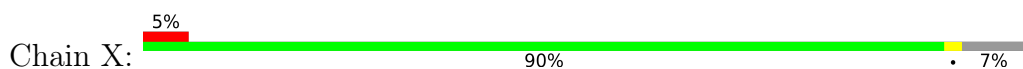
- Molecule 17: Photosystem II reaction center protein Ycf12



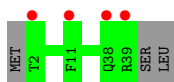
- Molecule 17: Photosystem II reaction center protein Ycf12



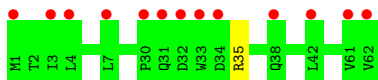
- Molecule 18: Photosystem II reaction center X protein



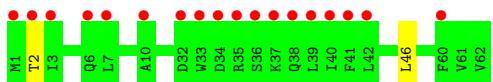
- Molecule 18: Photosystem II reaction center X protein



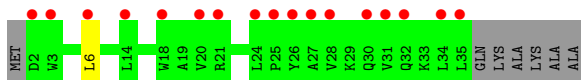
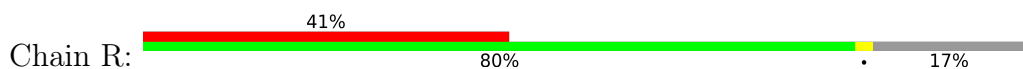
- Molecule 19: Photosystem II reaction center protein Z



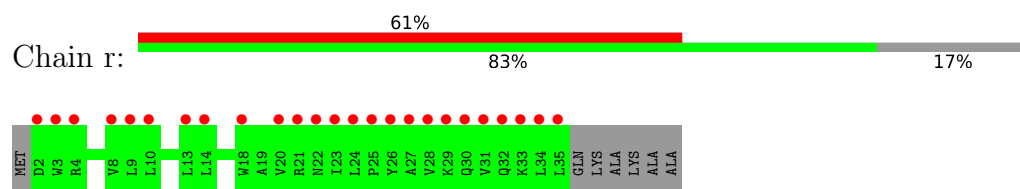
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.87Å 223.14Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 2.25 44.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.28-2.25) 90.6 (44.28-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.24Å)	Xtrriage
Refinement program	PHENIX dev_2481	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.231	Depositor DCC
R_{free} test set	3426 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.255	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: OEX, CLA, PL9, PHO, FME, BCT, HEC, DGD, LHG, FE2, UNL, CL, HEM, SQD, BCR, LMG

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	0.25	0/2713	0.40	0/3700
1	a	0.25	0/2707	0.40	0/3692
2	B	0.25	0/4155	0.40	0/5661
2	b	0.25	0/4125	0.40	0/5621
3	C	0.25	0/3607	0.40	0/4911
3	c	0.25	0/3610	0.40	0/4914
4	D	0.26	0/2812	0.41	0/3832
4	d	0.25	0/2811	0.41	0/3830
5	E	0.23	0/689	0.37	0/940
5	e	0.30	1/693 (0.1%)	0.38	0/945
6	F	0.24	0/284	0.36	0/387
6	f	0.24	0/284	0.35	0/387
7	H	0.25	0/523	0.41	0/713
7	h	0.24	0/511	0.39	0/697
8	I	0.25	0/301	0.43	0/407
8	i	0.26	0/293	0.38	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.25	0/263	0.39	0/356
10	K	0.26	0/303	0.39	0/416
10	k	0.26	0/303	0.37	0/416
11	L	0.24	0/311	0.37	0/422
11	l	0.24	0/311	0.37	0/422
12	M	0.24	0/262	0.34	0/358
12	m	0.24	0/253	0.35	0/346
13	O	0.24	0/1925	0.46	0/2610
13	o	0.25	0/1925	0.47	0/2609
14	T	0.27	0/257	0.34	0/349
14	t	0.27	0/257	0.36	0/349
15	U	0.24	0/785	0.42	0/1064
15	u	0.24	0/785	0.42	0/1064
16	V	0.23	0/1085	0.41	0/1473
16	v	0.23	0/1094	0.40	0/1484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.24	0/201	0.39	0/268
17	y	0.24	0/225	0.37	0/301
18	X	0.24	0/284	0.37	0/384
18	x	0.24	0/291	0.38	0/392
19	Z	0.24	0/490	0.35	0/669
19	z	0.24	0/489	0.36	0/669
20	R	0.22	0/279	0.40	0/383
20	r	0.22	0/276	0.36	0/379
All	All	0.25	1/43035 (0.0%)	0.40	0/58572

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	5.06	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	333/344 (97%)	327 (98%)	5 (2%)	1 (0%)	41	46
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	504/510 (99%)	491 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	450/461 (98%)	439 (98%)	10 (2%)	1 (0%)	47	55
3	c	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	47	55
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	8
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	35/38 (92%)	32 (91%)	3 (9%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	30 (94%)	1 (3%)	1 (3%)	4	1
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	244/272 (90%)	235 (96%)	8 (3%)	1 (0%)	34	37
13	o	244/272 (90%)	229 (94%)	11 (4%)	4 (2%)	9	5
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	136/163 (83%)	130 (96%)	5 (4%)	1 (1%)	22	21
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	1 (3%)	1 (3%)	5	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	4
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5700 (92%)	5108 (97%)	137 (3%)	13 (0%)	47	55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	53	LYS
13	o	58	ASN
3	C	416	SER
3	c	416	SER
13	o	59	LYS

5.3.2 Protein sidechains [i](#)

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	271/280 (97%)	270 (100%)	1 (0%)	91	94
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	407/407 (100%)	403 (99%)	4 (1%)	76	84
2	b	403/407 (99%)	402 (100%)	1 (0%)	93	96
3	C	353/362 (98%)	352 (100%)	1 (0%)	92	95
3	c	353/362 (98%)	349 (99%)	4 (1%)	73	82
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	94
4	d	276/283 (98%)	275 (100%)	1 (0%)	91	94
5	E	73/73 (100%)	72 (99%)	1 (1%)	67	76
5	e	73/73 (100%)	72 (99%)	1 (1%)	67	76
6	F	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	40
7	h	53/55 (96%)	52 (98%)	1 (2%)	57	66
8	I	33/34 (97%)	32 (97%)	1 (3%)	41	50
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	46
10	k	30/37 (81%)	29 (97%)	1 (3%)	38	46
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	209/228 (92%)	207 (99%)	2 (1%)	76	84
13	o	209/228 (92%)	207 (99%)	2 (1%)	76	84
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	118/138 (86%)	118 (100%)	0	100	100
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	66
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	66
20	R	29/33 (88%)	28 (97%)	1 (3%)	37	45
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4359/4654 (94%)	4331 (99%)	28 (1%)	86	91

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	35	ARG
19	z	46	LEU
3	c	29	GLU
10	k	19	ASP
2	b	362	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	409	GLN
5	e	74	GLN
16	v	25	GLN
13	o	200	ASN
13	O	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.86	0
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.90	0
14	FME	t	1	14	8,9,10	0.96	0	7,9,11	0.93	0
12	FME	m	1	12	8,9,10	0.94	0	7,9,11	0.84	0
14	FME	T	1	14	8,9,10	0.91	0	7,9,11	1.20	1 (14%)
8	FME	i	1	8	8,9,10	0.95	0	7,9,11	0.84	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	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
14	T	1	FME	C-CA-N	2.29	113.87	109.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic and 33 are unknown - leaving 151 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
25	CLA	A	607	36	65,73,73	1.47	5 (7%)	76,113,113	1.27	10 (13%)
25	CLA	A	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.24	9 (11%)
25	CLA	B	607	36	65,73,73	1.46	5 (7%)	76,113,113	1.24	8 (10%)
26	PHO	a	609	-	51,69,69	0.98	3 (5%)	47,99,99	1.16	5 (10%)
25	CLA	C	502	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	b	606[A]	-	65,73,73	1.46	5 (7%)	76,113,113	1.27	7 (9%)
25	CLA	c	502	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	7 (9%)
25	CLA	c	506	-	65,73,73	1.47	5 (7%)	76,113,113	1.29	7 (9%)
27	BCR	b	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	c	504	36	60,68,73	1.51	5 (8%)	70,107,113	1.34	8 (11%)
30	LHG	a	617	-	41,41,48	0.67	1 (2%)	44,47,54	1.32	6 (13%)
27	BCR	c	522	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	c	508	-	64,72,73	1.47	5 (7%)	74,111,113	1.35	9 (12%)
27	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
30	LHG	l	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	6 (11%)
32	LMG	a	614	-	51,51,55	0.73	0	59,59,63	1.33	7 (11%)
32	LMG	d	408	-	36,36,55	0.30	0	35,35,63	1.38	3 (8%)
25	CLA	c	510	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
25	CLA	D	402	-	65,73,73	1.46	6 (9%)	76,113,113	1.27	7 (9%)
29	SQD	D	409	-	46,47,54	1.02	5 (10%)	55,58,65	1.58	9 (16%)
28	PL9	A	611	-	55,55,55	0.98	3 (5%)	68,69,69	1.51	12 (17%)
25	CLA	d	401	-	65,73,73	1.47	5 (7%)	76,113,113	1.25	8 (10%)
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
27	BCR	C	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
27	BCR	d	403	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	4 (7%)
25	CLA	C	511	-	65,73,73	1.46	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	D	403	-	65,73,73	1.46	5 (7%)	76,113,113	1.38	10 (13%)
28	PL9	d	404	-	55,55,55	0.94	4 (7%)	68,69,69	1.49	10 (14%)
29	SQD	b	621	-	39,39,54	0.87	2 (5%)	41,41,65	1.14	2 (4%)
30	LHG	d	406	-	48,48,48	0.60	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	C	513	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	10 (13%)
33	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.35	10 (12%)
25	CLA	b	616	-	47,55,73	1.71	6 (12%)	54,91,113	1.53	8 (14%)
32	LMG	D	407	-	51,51,55	0.72	0	59,59,63	1.31	5 (8%)
34	HEM	E	101	6,5	41,50,50	1.51	5 (12%)	45,82,82	1.31	6 (13%)
25	CLA	b	606[B]	-	65,73,73	1.47	5 (7%)	76,113,113	1.27	7 (9%)
21	OEX	A	601	1,3,36	0,15,15	-	-	-	-	-
29	SQD	A	612	-	51,52,54	0.97	5 (9%)	60,63,65	1.50	9 (15%)
27	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	6 (10%)
29	SQD	A	616	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
25	CLA	B	602	-	65,73,73	1.46	5 (7%)	76,113,113	1.31	9 (11%)
25	CLA	C	504	-	65,73,73	1.47	5 (7%)	76,113,113	1.35	8 (10%)
25	CLA	a	610	-	65,73,73	1.47	5 (7%)	76,113,113	1.32	7 (9%)
25	CLA	b	608	-	65,73,73	1.46	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	C	505	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
30	LHG	B	623	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	C	506	-	65,73,73	1.46	6 (9%)	76,113,113	1.32	7 (9%)
32	LMG	C	520	-	48,48,55	0.76	0	56,56,63	1.32	6 (10%)
25	CLA	c	507	36	65,73,73	1.47	5 (7%)	76,113,113	1.36	8 (10%)
29	SQD	f	101	-	40,41,54	1.09	5 (12%)	49,52,65	1.58	9 (18%)
25	CLA	C	508	36	65,73,73	1.46	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	B	612	-	65,73,73	1.43	6 (9%)	76,113,113	1.37	9 (11%)
25	CLA	b	613	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
33	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.38	10 (12%)
27	BCR	C	515	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	4 (7%)
25	CLA	B	605	-	65,73,73	1.45	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	b	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.33	8 (10%)
33	DGD	c	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.37	7 (9%)
25	CLA	A	613	36	65,73,73	1.46	5 (7%)	76,113,113	1.25	8 (10%)
25	CLA	B	613	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	9 (11%)
27	BCR	K	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
25	CLA	c	509	-	65,73,73	1.44	5 (7%)	76,113,113	1.37	8 (10%)
25	CLA	b	605	-	65,73,73	1.47	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	B	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.24	9 (11%)
27	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	615	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	614	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
27	BCR	a	611	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	5 (8%)
32	LMG	c	519	-	37,37,55	0.86	0	45,45,63	1.34	6 (13%)
27	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	5 (8%)
32	LMG	c	520	-	34,34,55	0.86	0	42,42,63	1.24	5 (11%)
25	CLA	b	607	36	65,73,73	1.45	6 (9%)	76,113,113	1.27	8 (10%)
30	LHG	d	405	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	C	512	3	65,73,73	1.46	5 (7%)	76,113,113	1.27	9 (11%)
25	CLA	B	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
35	HEC	v	201	16	32,50,50	1.99	4 (12%)	24,82,82	1.75	5 (20%)
25	CLA	d	402	-	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	a	615	36	65,73,73	1.47	5 (7%)	76,113,113	1.26	7 (9%)
25	CLA	B	610	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
29	SQD	B	625	-	53,54,54	0.96	5 (9%)	62,65,65	1.49	8 (12%)
30	LHG	a	616	-	38,38,48	0.68	1 (2%)	41,44,54	1.16	3 (7%)
32	LMG	b	620	-	51,51,55	0.71	0	59,59,63	1.34	7 (11%)
33	DGD	C	517	-	63,63,67	0.83	0	77,77,81	1.35	9 (11%)
27	BCR	c	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.14	5 (8%)
25	CLA	b	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.27	8 (10%)
25	CLA	C	509	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
25	CLA	B	604	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
25	CLA	b	602	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
25	CLA	C	514	-	65,73,73	1.45	5 (7%)	76,113,113	1.32	8 (10%)
27	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
34	HEM	e	101	6,5	41,50,50	1.53	4 (9%)	45,82,82	1.50	7 (15%)
33	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.41	10 (12%)
25	CLA	C	507	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
25	CLA	c	503	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	9 (11%)
32	LMG	B	626	-	51,51,55	0.72	1 (1%)	59,59,63	1.30	5 (8%)
25	CLA	C	503	-	65,73,73	1.45	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	b	604	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
32	LMG	B	621	-	51,51,55	0.72	0	59,59,63	1.32	6 (10%)
25	CLA	B	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.34	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	m	102	-	51,51,55	0.72	0	59,59,63	1.36	7 (11%)
25	CLA	B	601	36	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
33	DGD	c	518	-	63,63,67	0.84	1 (1%)	77,77,81	1.36	9 (11%)
25	CLA	C	510	-	65,73,73	1.44	5 (7%)	76,113,113	1.37	8 (10%)
25	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.29	8 (10%)
33	DGD	h	102	-	63,63,67	0.88	0	77,77,81	1.35	8 (10%)
25	CLA	b	601	36	65,73,73	1.46	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	c	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.36	9 (11%)
27	BCR	t	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
30	LHG	A	614	-	46,46,48	0.62	1 (2%)	49,52,54	1.24	5 (10%)
25	CLA	a	607	36	65,73,73	1.46	5 (7%)	76,113,113	1.26	9 (11%)
32	LMG	C	521	-	51,51,55	0.78	1 (1%)	59,59,63	1.35	6 (10%)
28	PL9	a	612	-	55,55,55	0.98	3 (5%)	68,69,69	1.53	12 (17%)
32	LMG	C	501	-	48,48,55	0.73	0	56,56,63	1.30	4 (7%)
29	SQD	D	408	-	42,43,54	1.06	5 (11%)	51,54,65	1.64	11 (21%)
25	CLA	b	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
35	HEC	V	201	16	32,50,50	2.00	4 (12%)	24,82,82	1.74	5 (20%)
26	PHO	A	608	-	51,69,69	0.98	3 (5%)	47,99,99	1.12	5 (10%)
25	CLA	c	511	3	65,73,73	1.45	5 (7%)	76,113,113	1.28	9 (11%)
26	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.09	4 (8%)
25	CLA	A	609	-	54,62,73	1.60	5 (9%)	62,99,113	1.42	9 (14%)
27	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	4 (7%)
27	BCR	D	404	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	5 (8%)
29	SQD	L	101	-	48,49,54	0.99	5 (10%)	57,60,65	1.58	10 (17%)
30	LHG	D	406	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)
25	CLA	B	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.28	7 (9%)
25	CLA	b	610	36	65,73,73	1.46	5 (7%)	76,113,113	1.31	9 (11%)
24	BCT	a	605	22	2,3,3	1.27	0	2,3,3	1.86	1 (50%)
25	CLA	B	606	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)
24	BCT	A	605	22	2,3,3	1.27	0	2,3,3	1.87	1 (50%)
29	SQD	a	613	-	53,54,54	0.95	5 (9%)	62,65,65	1.48	9 (14%)
27	BCR	Y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	4 (7%)
25	CLA	c	501	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
27	BCR	H	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	4 (7%)
26	PHO	a	608	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	616	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	8 (10%)
27	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	6 (10%)
30	LHG	L	102	-	48,48,48	0.62	1 (2%)	51,54,54	1.23	6 (11%)
32	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
32	LMG	d	407	-	51,51,55	0.73	0	59,59,63	1.33	6 (10%)
25	CLA	a	606	-	65,73,73	1.43	5 (7%)	76,113,113	1.25	9 (11%)
27	BCR	A	610	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	c	505	-	65,73,73	1.46	6 (9%)	76,113,113	1.31	7 (9%)
21	OEX	a	601	1,3,36	0,15,15	-	-	-	-	-
30	LHG	A	618	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
25	CLA	c	513	-	65,73,73	1.45	5 (7%)	76,113,113	1.30	7 (9%)
27	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
28	PL9	D	405	-	55,55,55	0.94	2 (3%)	68,69,69	1.52	14 (20%)
25	CLA	B	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.24	8 (10%)
29	SQD	B	624	-	53,54,54	0.95	5 (9%)	62,65,65	1.62	10 (16%)

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
25	CLA	A	607	36	1/1/15/20	8/37/115/115	-
25	CLA	A	606	-	1/1/15/20	10/37/115/115	-
25	CLA	B	607	36	1/1/15/20	9/37/115/115	-
26	PHO	a	609	-	-	11/37/103/103	0/5/6/6
25	CLA	C	502	-	1/1/15/20	14/37/115/115	-
25	CLA	b	606[A]	-	1/1/15/20	13/37/115/115	-
25	CLA	c	502	-	1/1/15/20	11/37/115/115	-
25	CLA	c	506	-	1/1/15/20	20/37/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	c	504	36	1/1/14/20	4/31/109/115	-
30	LHG	a	617	-	-	19/46/46/53	-
27	BCR	c	522	-	-	4/29/63/63	0/2/2/2
25	CLA	c	508	-	1/1/14/20	9/36/114/115	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	l	101	-	-	20/53/53/53	-
32	LMG	a	614	-	-	18/46/66/70	0/1/1/1
32	LMG	d	408	-	-	18/32/32/70	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
25	CLA	D	402	-	1/1/15/20	5/37/115/115	-
29	SQD	D	409	-	-	19/42/62/69	0/1/1/1
28	PL9	A	611	-	-	13/53/73/73	0/1/1/1
25	CLA	d	401	-	1/1/15/20	7/37/115/115	-
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
27	BCR	C	516	-	-	4/29/63/63	0/2/2/2
27	BCR	d	403	-	-	6/29/63/63	0/2/2/2
25	CLA	C	511	-	1/1/15/20	10/37/115/115	-
25	CLA	D	403	-	1/1/15/20	9/37/115/115	-
28	PL9	d	404	-	-	9/53/73/73	0/1/1/1
29	SQD	b	621	-	-	9/41/41/69	-
30	LHG	d	406	-	-	24/53/53/53	-
25	CLA	C	513	-	1/1/15/20	14/37/115/115	-
25	CLA	b	611	-	1/1/15/20	8/37/115/115	-
33	DGD	H	102	-	-	11/51/91/95	0/2/2/2
25	CLA	b	616	-	1/1/11/20	3/16/94/115	-
32	LMG	D	407	-	-	14/46/66/70	0/1/1/1
34	HEM	E	101	6,5	-	2/12/54/54	-
25	CLA	b	606[B]	-	1/1/15/20	5/37/115/115	-
29	SQD	A	612	-	-	12/47/67/69	0/1/1/1
27	BCR	T	101	-	-	9/29/63/63	0/2/2/2
29	SQD	A	616	-	-	14/49/69/69	0/1/1/1
25	CLA	B	602	-	1/1/15/20	4/37/115/115	-
25	CLA	C	504	-	1/1/15/20	8/37/115/115	-
25	CLA	a	610	-	1/1/15/20	6/37/115/115	-
25	CLA	b	608	-	1/1/15/20	5/37/115/115	-
25	CLA	C	505	36	1/1/15/20	5/37/115/115	-
30	LHG	B	623	-	-	19/53/53/53	-
25	CLA	C	506	-	1/1/15/20	9/37/115/115	-
32	LMG	C	520	-	-	22/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	507	36	1/1/15/20	11/37/115/115	-
29	SQD	f	101	-	-	7/36/56/69	0/1/1/1
25	CLA	C	508	36	1/1/15/20	13/37/115/115	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
25	CLA	b	613	-	1/1/15/20	12/37/115/115	-
33	DGD	C	519	-	-	17/51/91/95	0/2/2/2
27	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	7/37/115/115	-
25	CLA	b	612	-	1/1/15/20	14/37/115/115	-
33	DGD	c	517	-	-	21/51/91/95	0/2/2/2
25	CLA	A	613	36	1/1/15/20	4/37/115/115	-
25	CLA	B	613	-	1/1/15/20	13/37/115/115	-
27	BCR	K	101	-	-	4/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
25	CLA	b	605	-	1/1/15/20	8/37/115/115	-
25	CLA	B	614	-	1/1/15/20	22/37/115/115	-
27	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	5/37/115/115	-
25	CLA	b	614	-	1/1/15/20	20/37/115/115	-
27	BCR	a	611	-	-	4/29/63/63	0/2/2/2
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
32	LMG	c	520	-	-	18/29/49/70	0/1/1/1
25	CLA	b	607	36	1/1/15/20	12/37/115/115	-
30	LHG	d	405	-	-	23/53/53/53	-
25	CLA	C	512	3	1/1/15/20	9/37/115/115	-
25	CLA	B	609	-	1/1/15/20	11/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
25	CLA	d	402	-	1/1/15/20	7/37/115/115	-
25	CLA	a	615	36	1/1/15/20	10/37/115/115	-
25	CLA	B	610	36	1/1/15/20	6/37/115/115	-
29	SQD	B	625	-	-	24/49/69/69	0/1/1/1
30	LHG	a	616	-	-	18/43/43/53	-
32	LMG	b	620	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	C	517	-	-	24/51/91/95	0/2/2/2
27	BCR	c	521	-	-	7/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	13/37/115/115	-
25	CLA	C	509	-	1/1/15/20	10/37/115/115	-
25	CLA	B	604	-	1/1/15/20	7/37/115/115	-
25	CLA	b	602	-	1/1/15/20	9/37/115/115	-
25	CLA	C	514	-	1/1/15/20	13/37/115/115	-
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
34	HEM	e	101	6,5	-	3/12/54/54	-
33	DGD	c	516	-	-	19/51/91/95	0/2/2/2
25	CLA	C	507	-	1/1/15/20	12/37/115/115	-
25	CLA	c	503	-	1/1/15/20	13/37/115/115	-
33	DGD	C	518	-	-	22/51/91/95	0/2/2/2
32	LMG	B	626	-	-	25/46/66/70	0/1/1/1
25	CLA	C	503	-	1/1/15/20	8/37/115/115	-
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
32	LMG	B	621	-	-	21/46/66/70	0/1/1/1
25	CLA	B	611	-	1/1/15/20	9/37/115/115	-
32	LMG	m	102	-	-	23/46/66/70	0/1/1/1
25	CLA	B	601	36	1/1/15/20	21/37/115/115	-
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	CLA	C	510	-	1/1/15/20	5/37/115/115	-
25	CLA	b	615	-	1/1/15/20	3/37/115/115	-
33	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	CLA	b	601	36	1/1/15/20	14/37/115/115	-
25	CLA	c	512	-	1/1/15/20	12/37/115/115	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
30	LHG	A	614	-	-	16/51/51/53	-
25	CLA	a	607	36	1/1/15/20	9/37/115/115	-
32	LMG	C	521	-	-	21/46/66/70	0/1/1/1
28	PL9	a	612	-	-	3/53/73/73	0/1/1/1
32	LMG	C	501	-	-	23/43/63/70	0/1/1/1
29	SQD	D	408	-	-	9/38/58/69	0/1/1/1
25	CLA	b	609	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	V	201	16	-	2/10/54/54	-
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
25	CLA	c	511	3	1/1/15/20	11/37/115/115	-
26	PHO	D	401	-	-	5/37/103/103	0/5/6/6
25	CLA	A	609	-	1/1/12/20	4/24/102/115	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
27	BCR	D	404	-	-	4/29/63/63	0/2/2/2
29	SQD	L	101	-	-	21/44/64/69	0/1/1/1
30	LHG	D	406	-	-	18/53/53/53	-
25	CLA	B	608	-	1/1/15/20	10/37/115/115	-
25	CLA	b	610	36	1/1/15/20	10/37/115/115	-
25	CLA	B	606	-	1/1/15/20	16/37/115/115	-
29	SQD	a	613	-	-	22/49/69/69	0/1/1/1
27	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/37/115/115	-
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
26	PHO	a	608	-	-	7/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/15/20	12/37/115/115	-
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
30	LHG	L	102	-	-	19/53/53/53	-
32	LMG	B	620	-	-	17/46/66/70	0/1/1/1
32	LMG	d	407	-	-	18/46/66/70	0/1/1/1
25	CLA	a	606	-	1/1/15/20	3/37/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	15/37/115/115	-
30	LHG	A	618	-	-	21/53/53/53	-
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
28	PL9	D	405	-	-	9/53/73/73	0/1/1/1
25	CLA	B	603	-	1/1/15/20	9/37/115/115	-
29	SQD	B	624	-	-	26/49/69/69	0/1/1/1

The worst 5 of 532 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	C4B-NB	7.60	1.42	1.35
25	b	609	CLA	C4B-NB	7.52	1.41	1.35
25	B	614	CLA	C4B-NB	7.49	1.41	1.35
25	b	605	CLA	C4B-NB	7.46	1.41	1.35
25	b	606[B]	CLA	C4B-NB	7.44	1.41	1.35

The worst 5 of 1076 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	B	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	c	503	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	C	508	CLA	C4A-NA-C1A	6.32	109.55	106.71
25	c	507	CLA	C4A-NA-C1A	6.31	109.54	106.71

5 of 71 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	613	CLA	ND
25	B	601	CLA	ND

5 of 1663 torsion outliers are listed below:

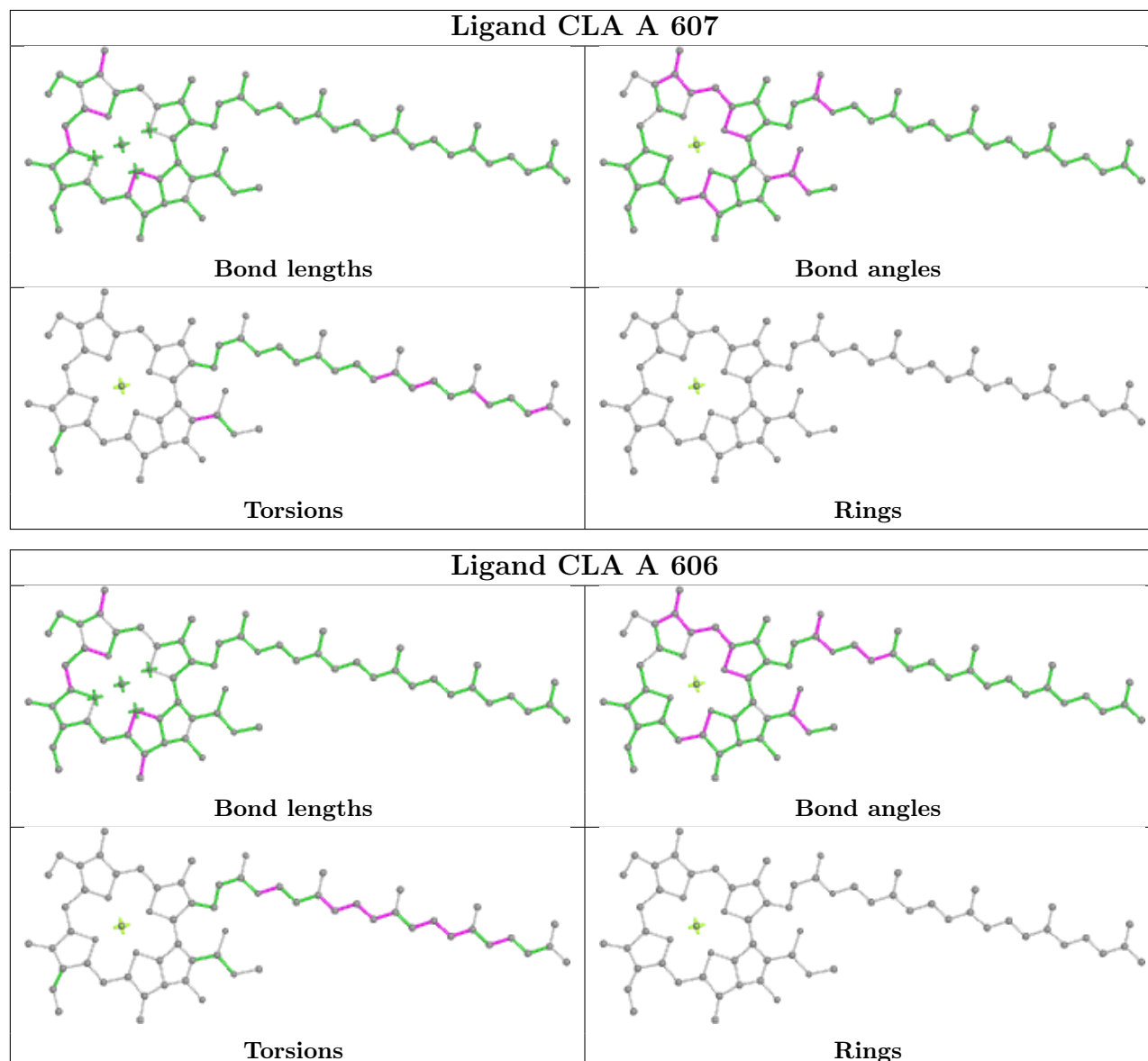
Mol	Chain	Res	Type	Atoms
25	A	613	CLA	CHA-CBD-CGD-O1D
25	A	613	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	608	CLA	C6-C7-C8-C9

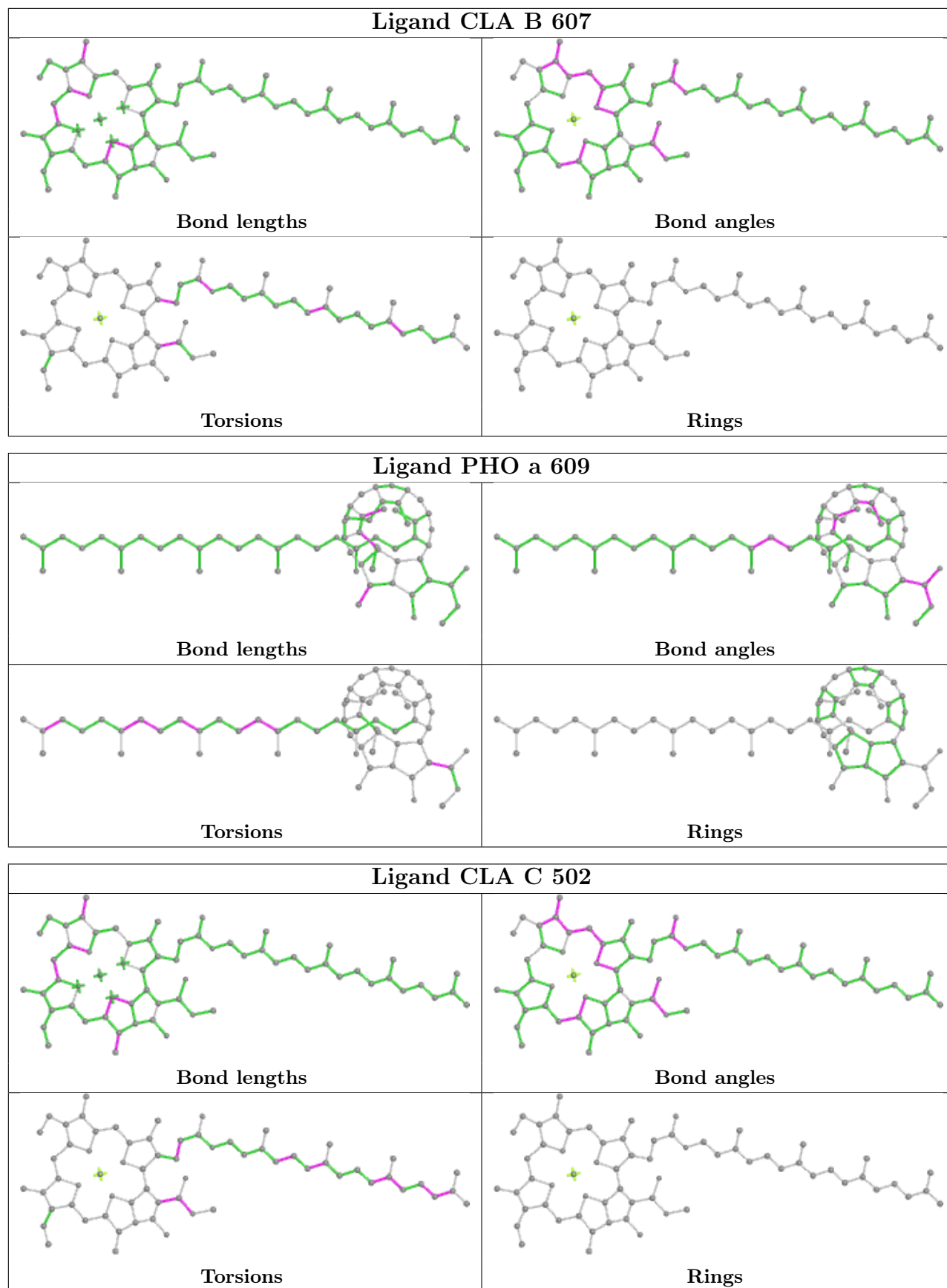
There are no ring outliers.

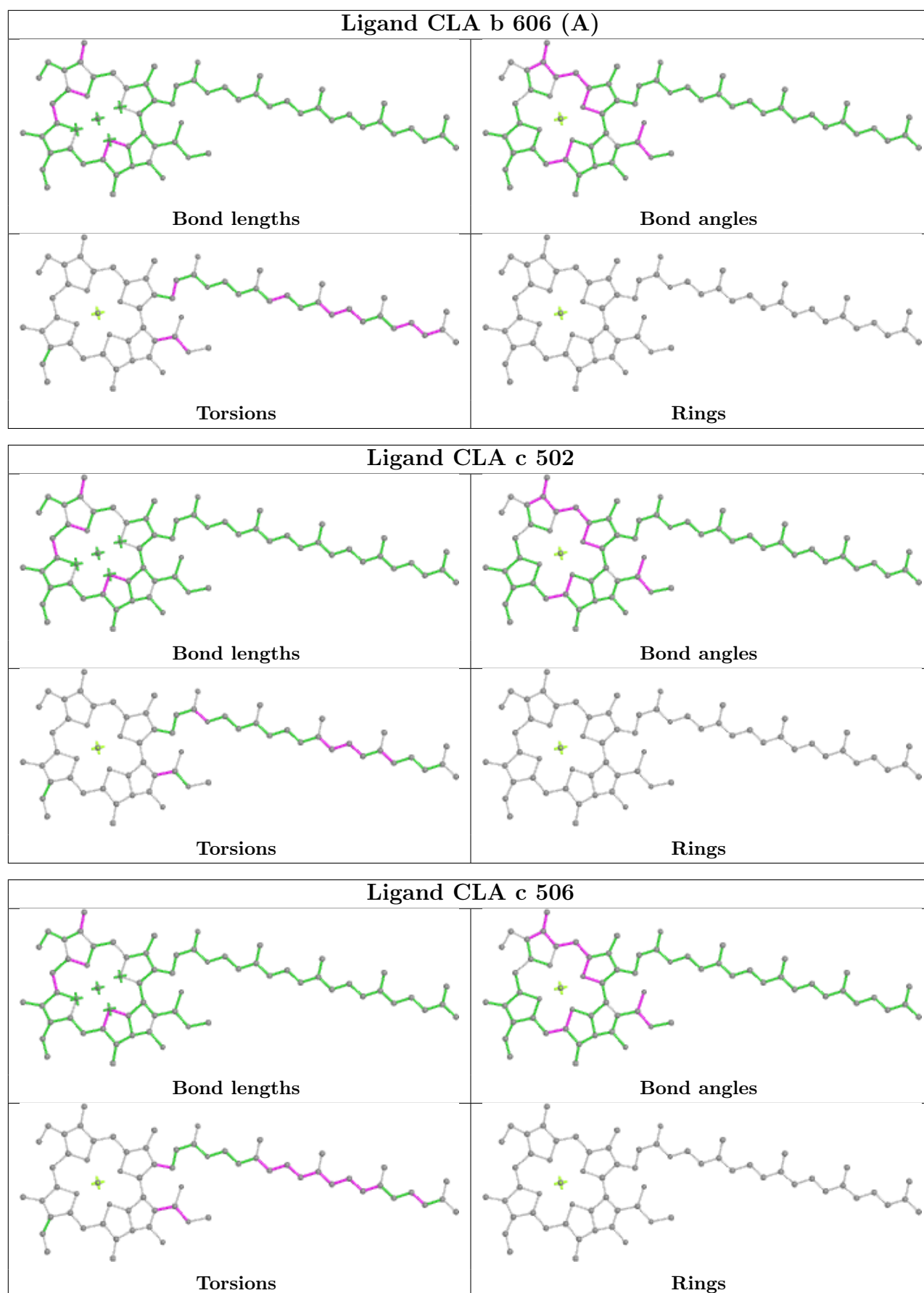
No monomer is involved in short contacts.

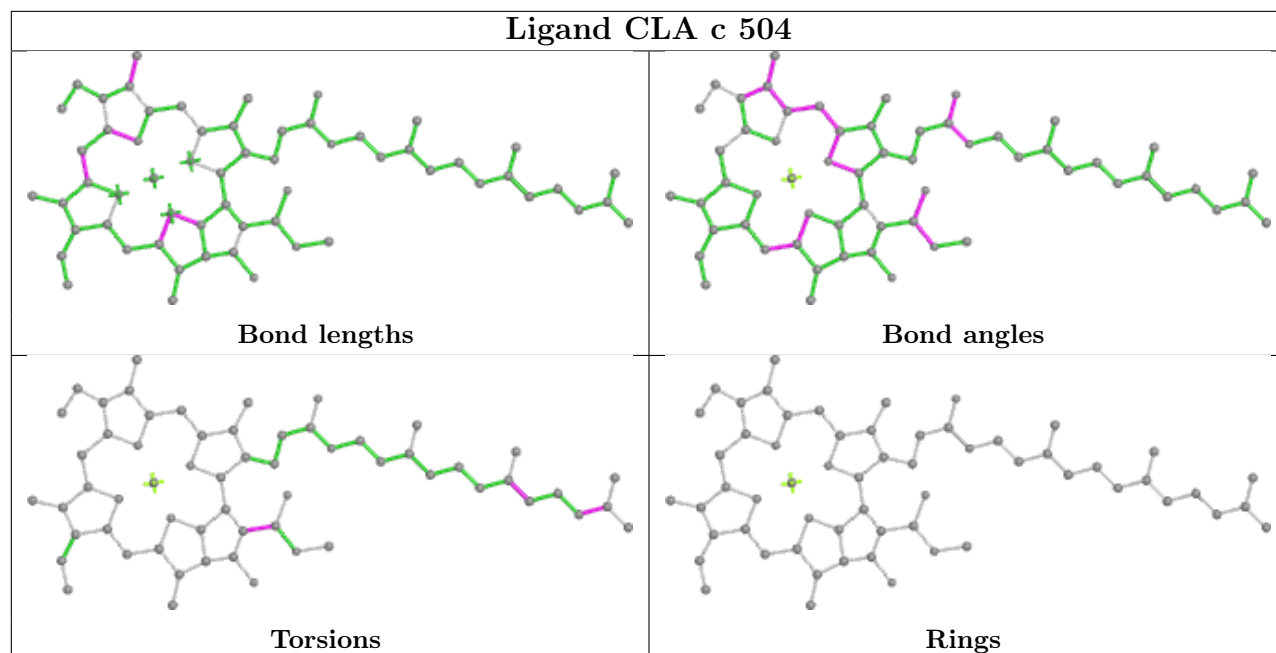
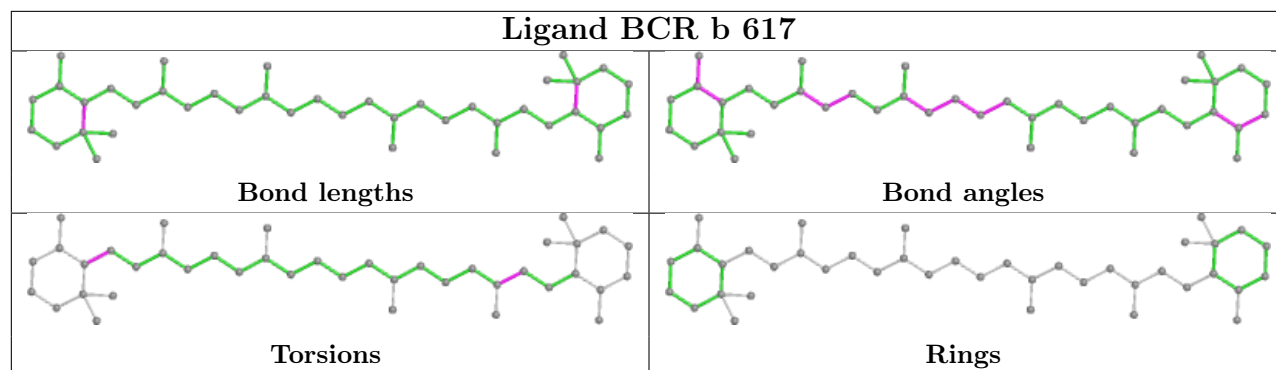
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

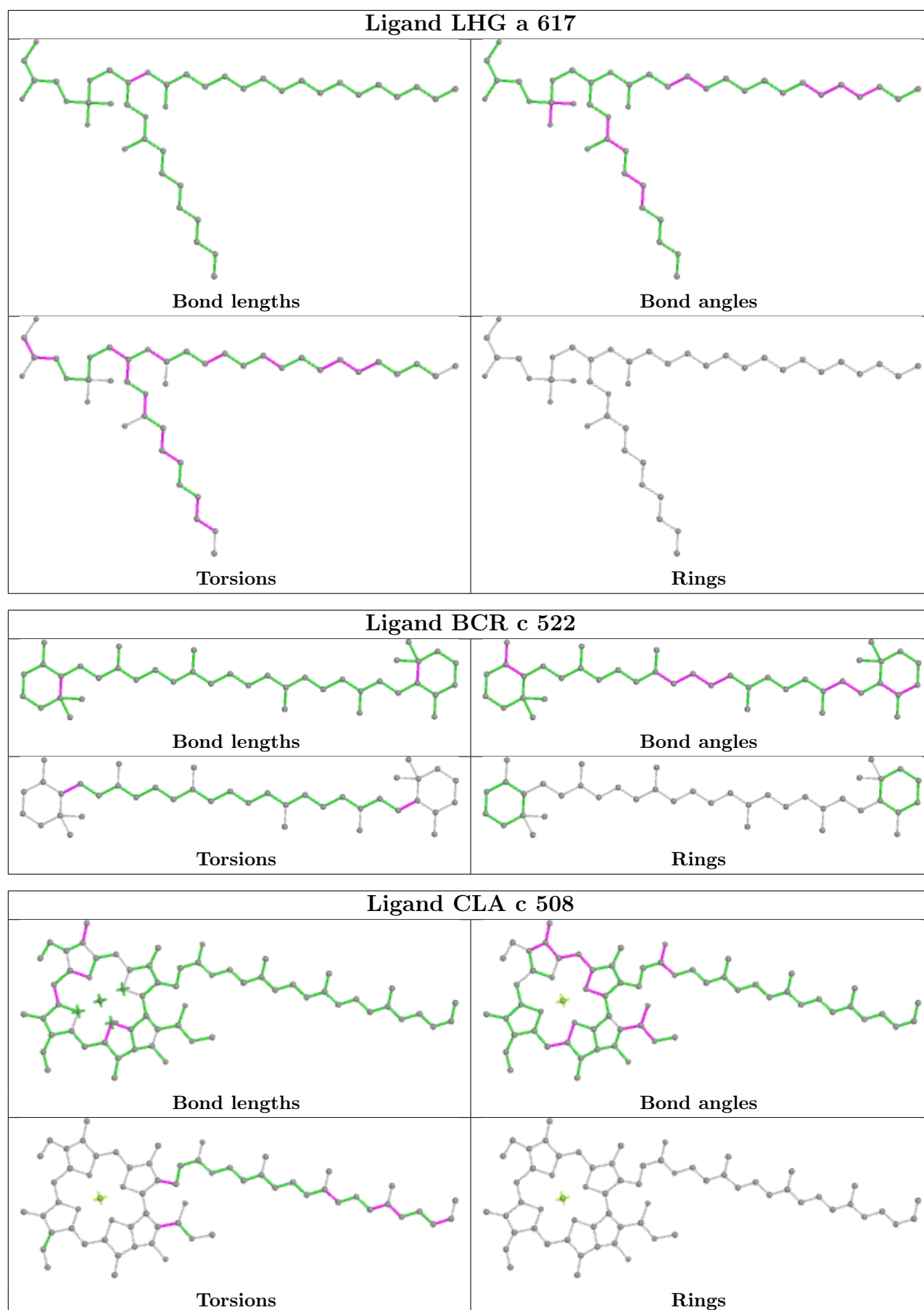
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

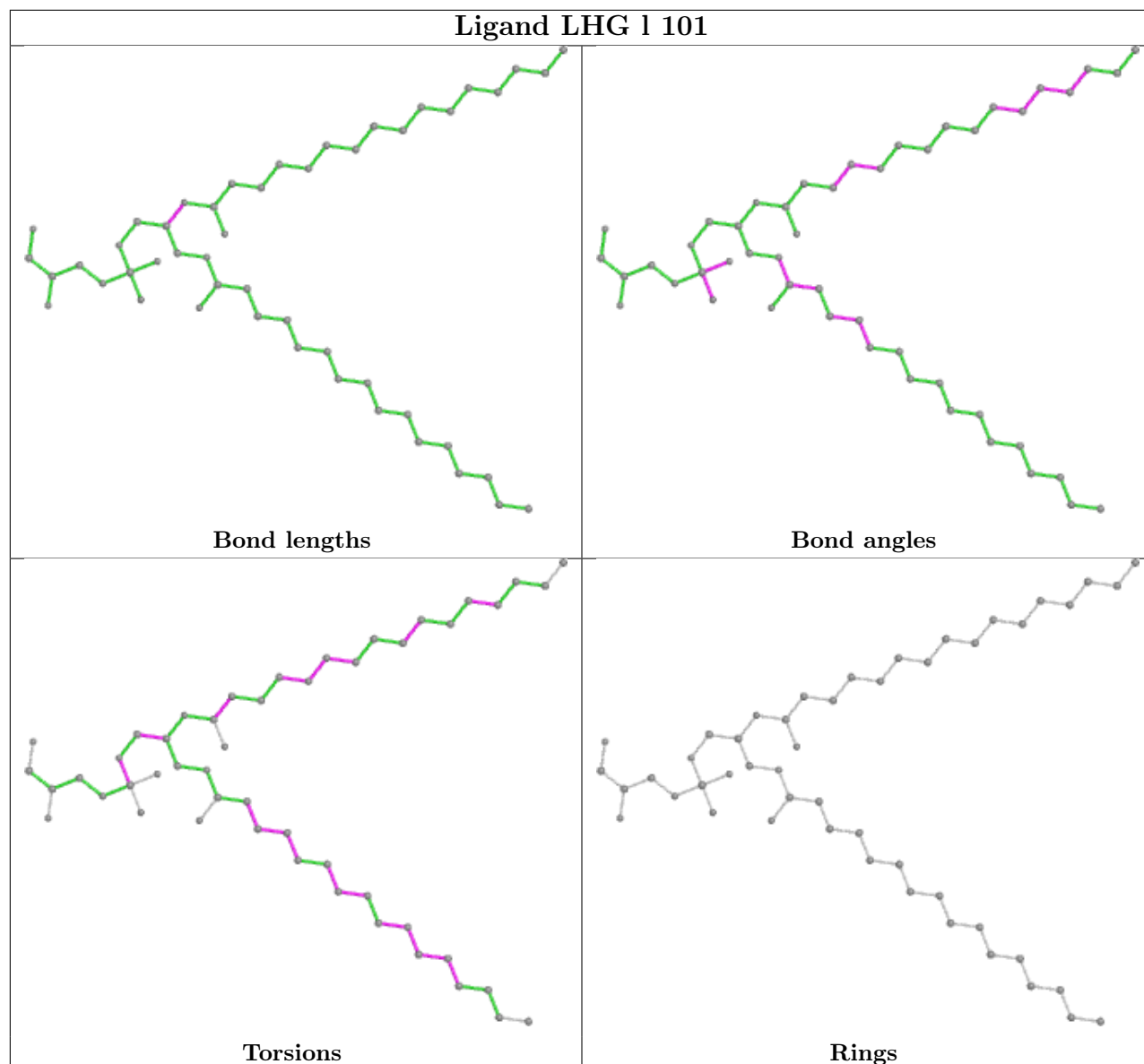
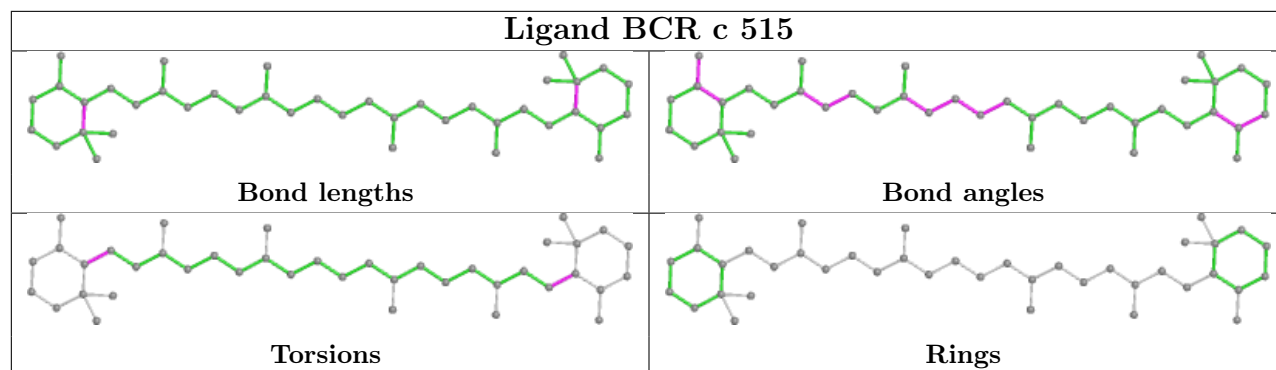


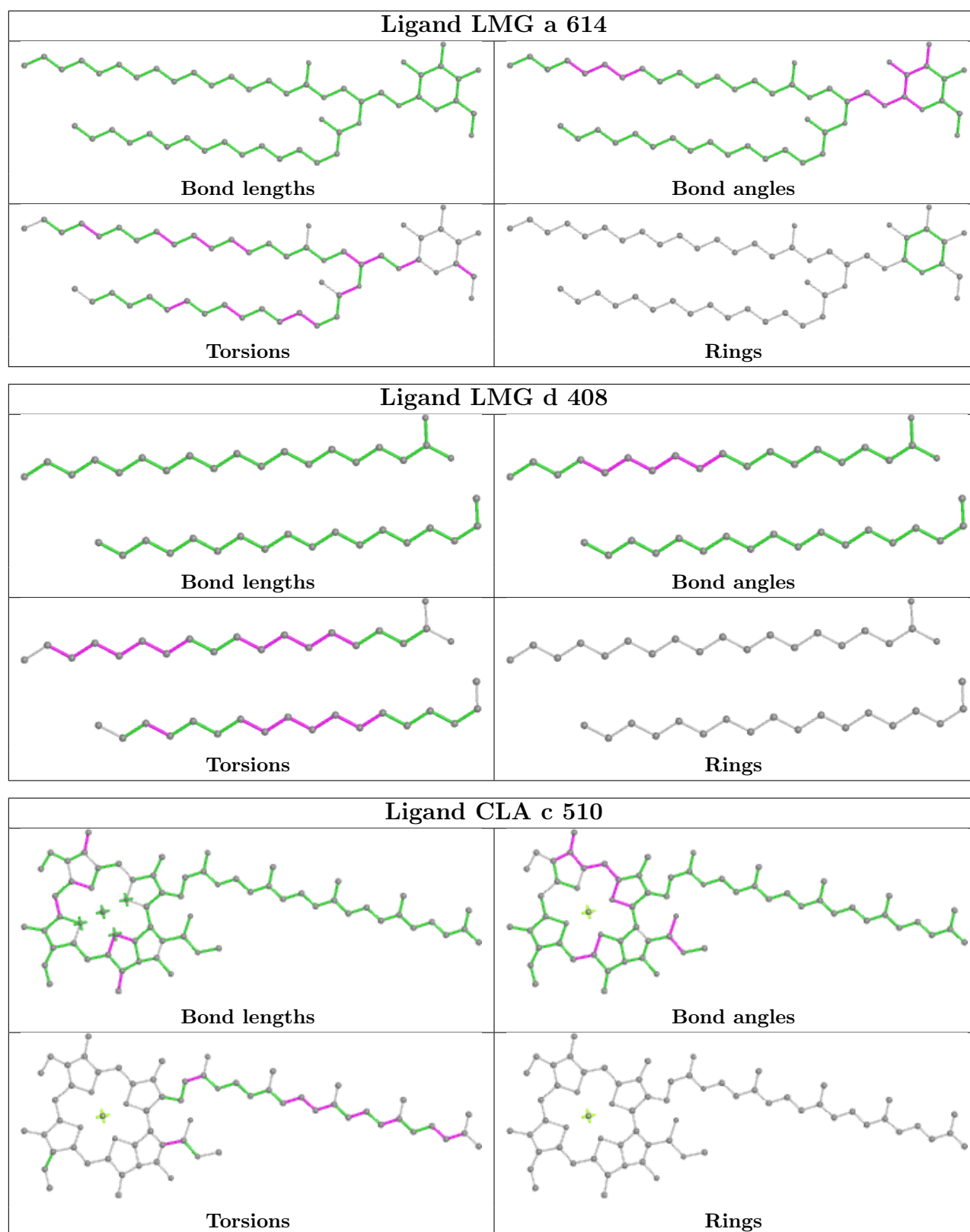


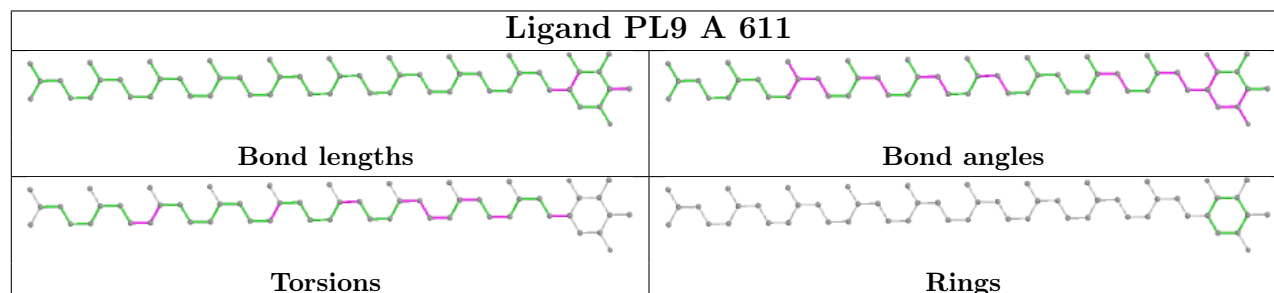
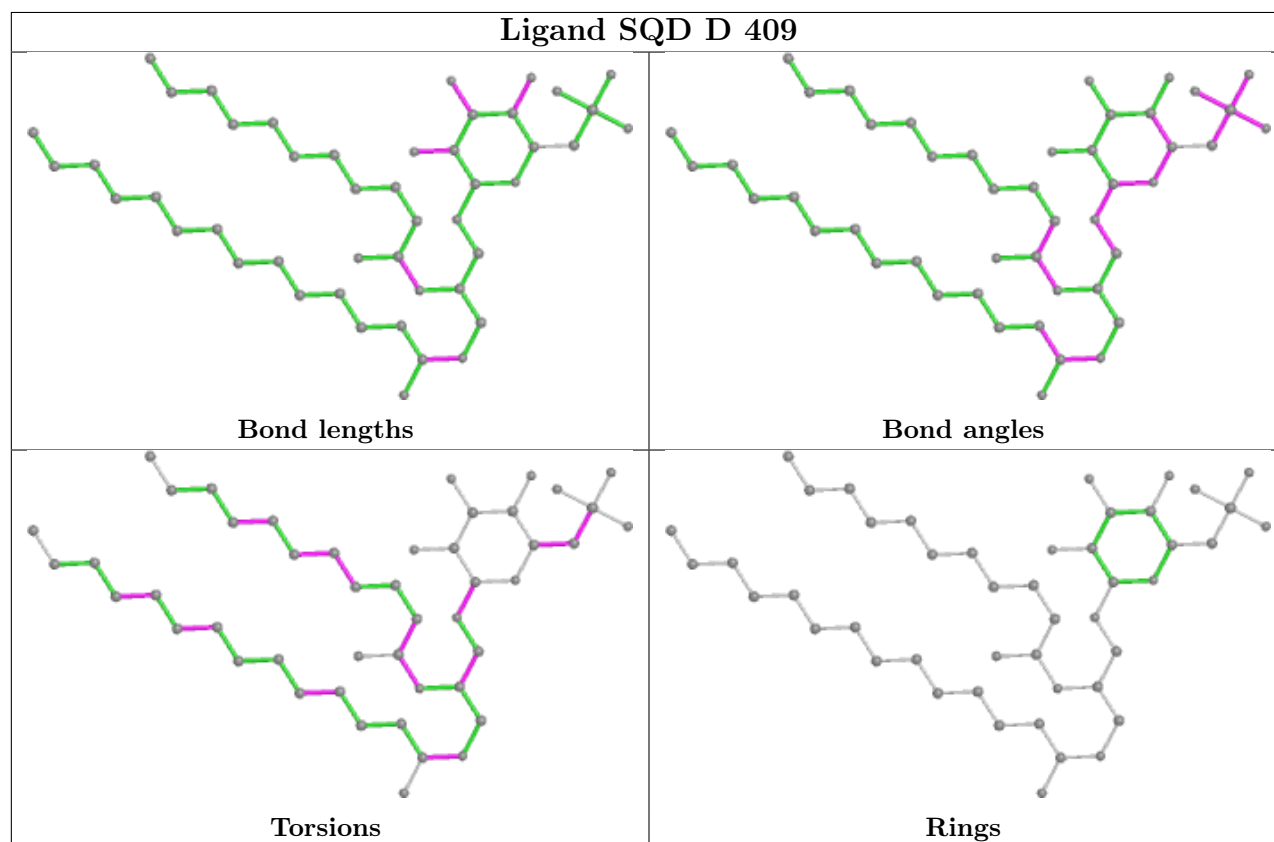
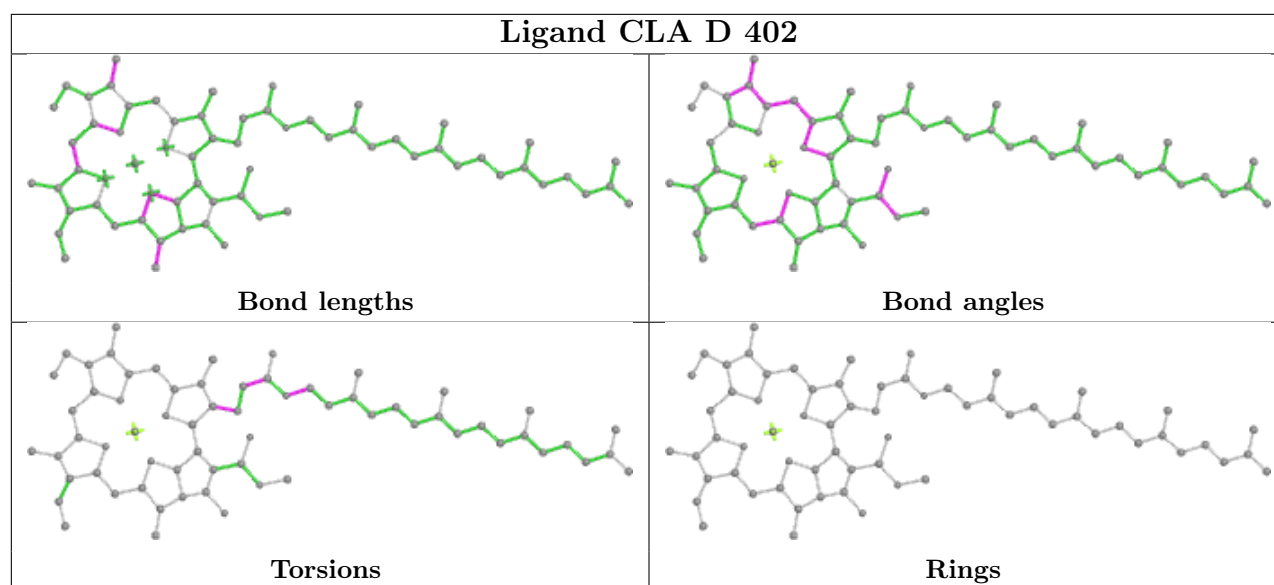


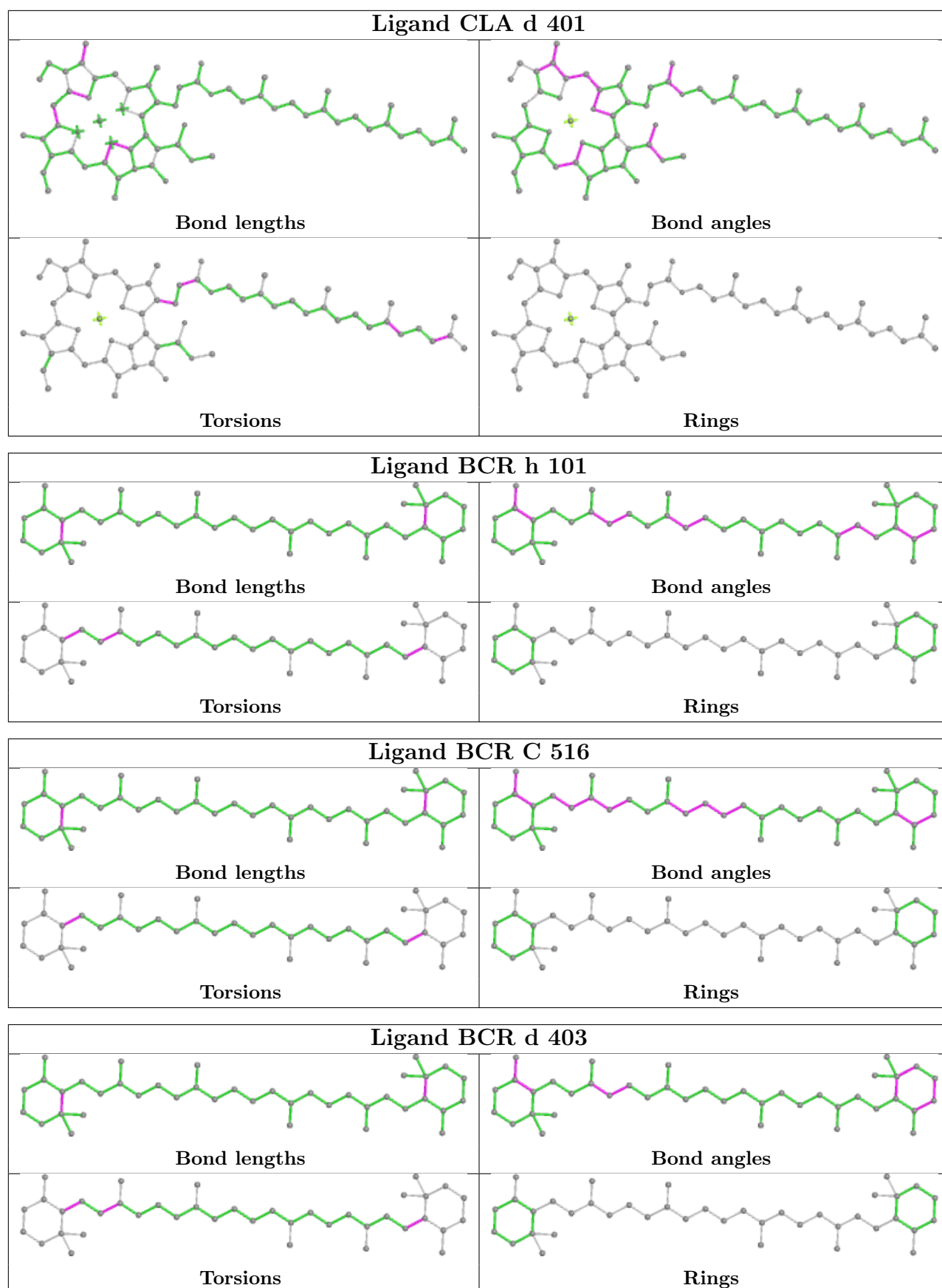


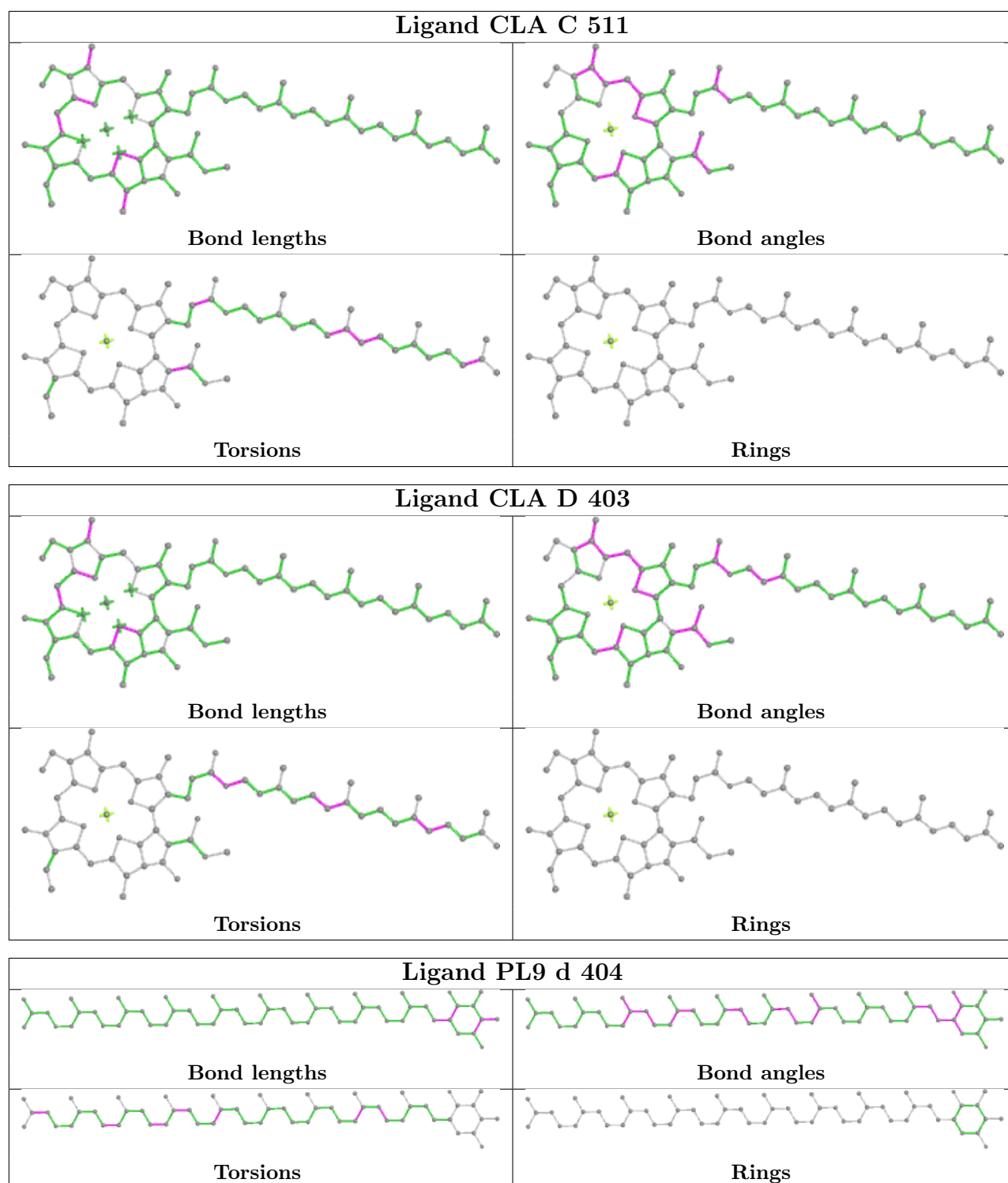


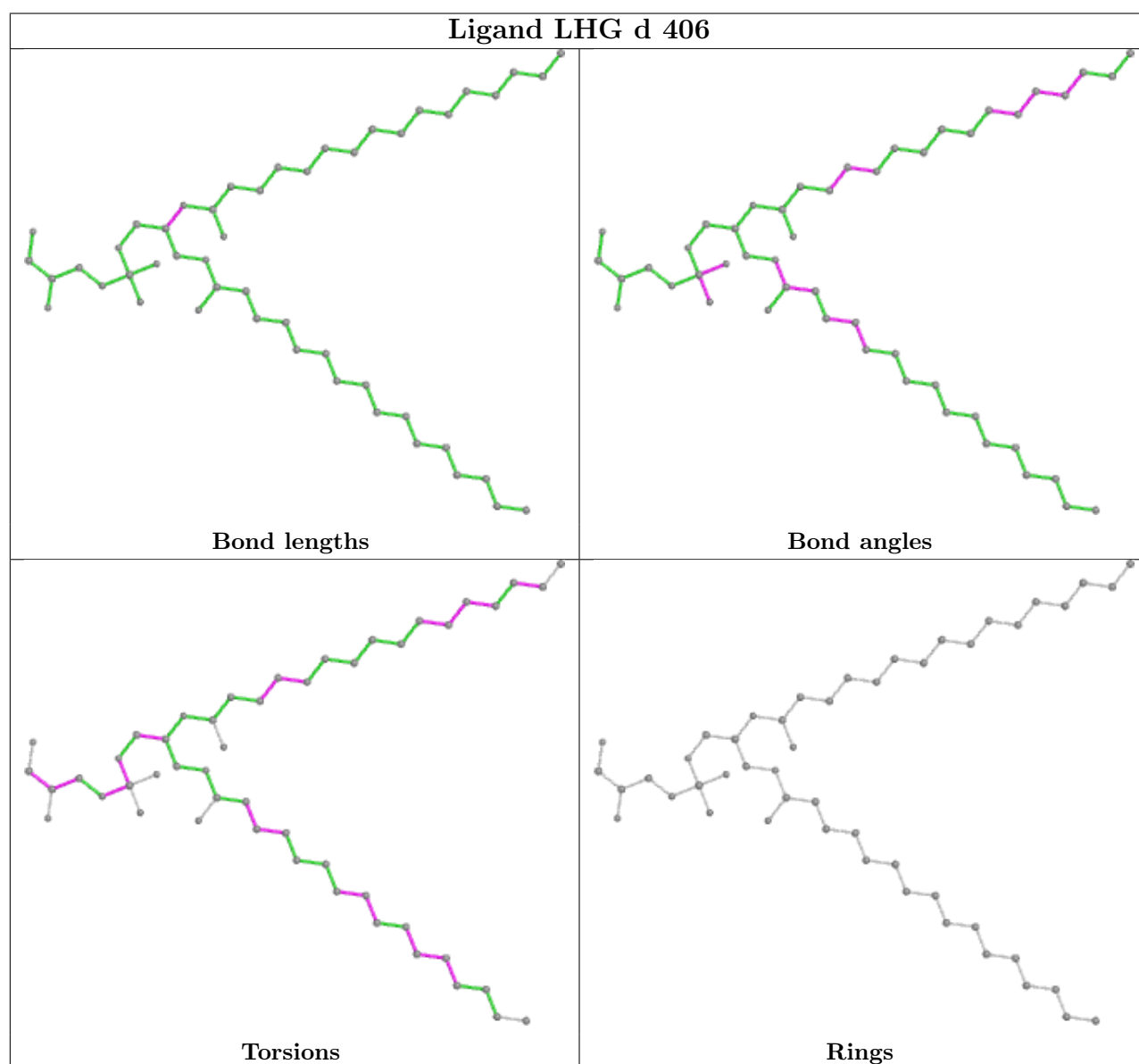
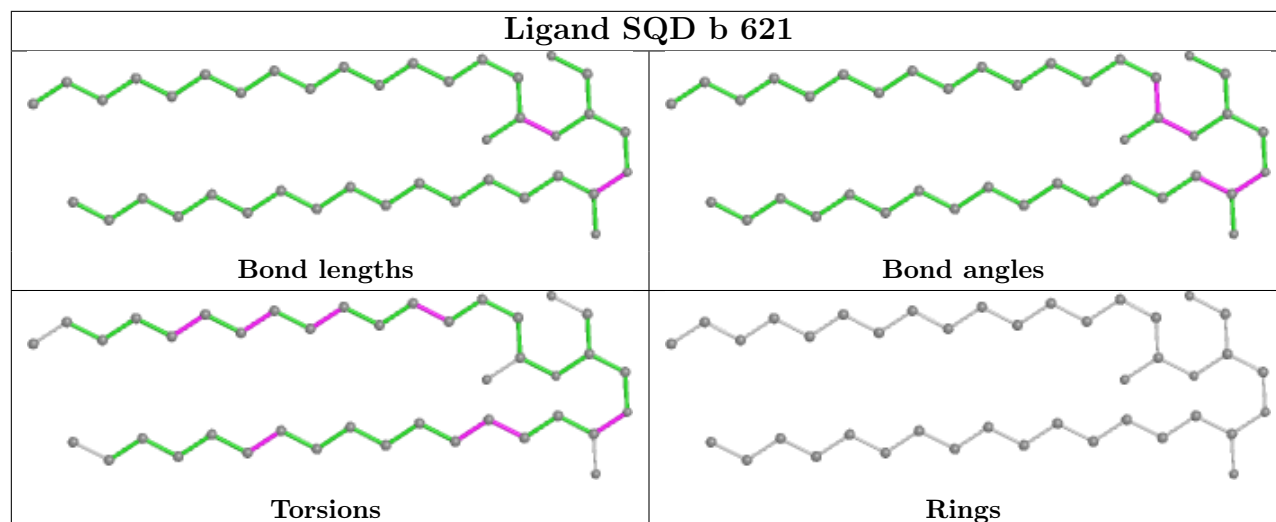


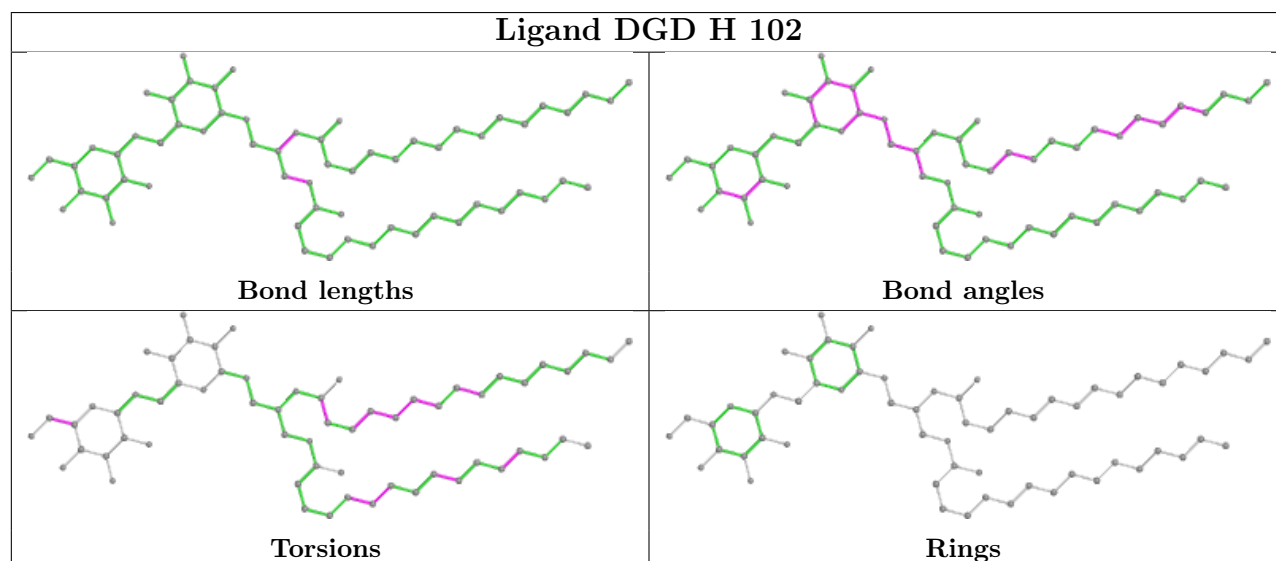
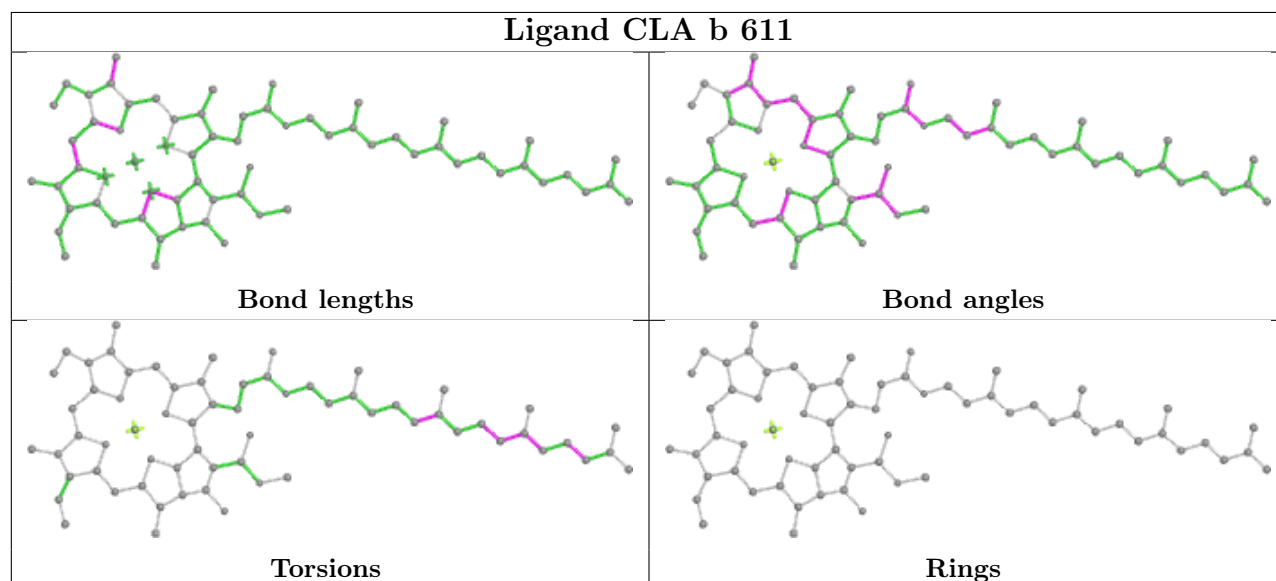
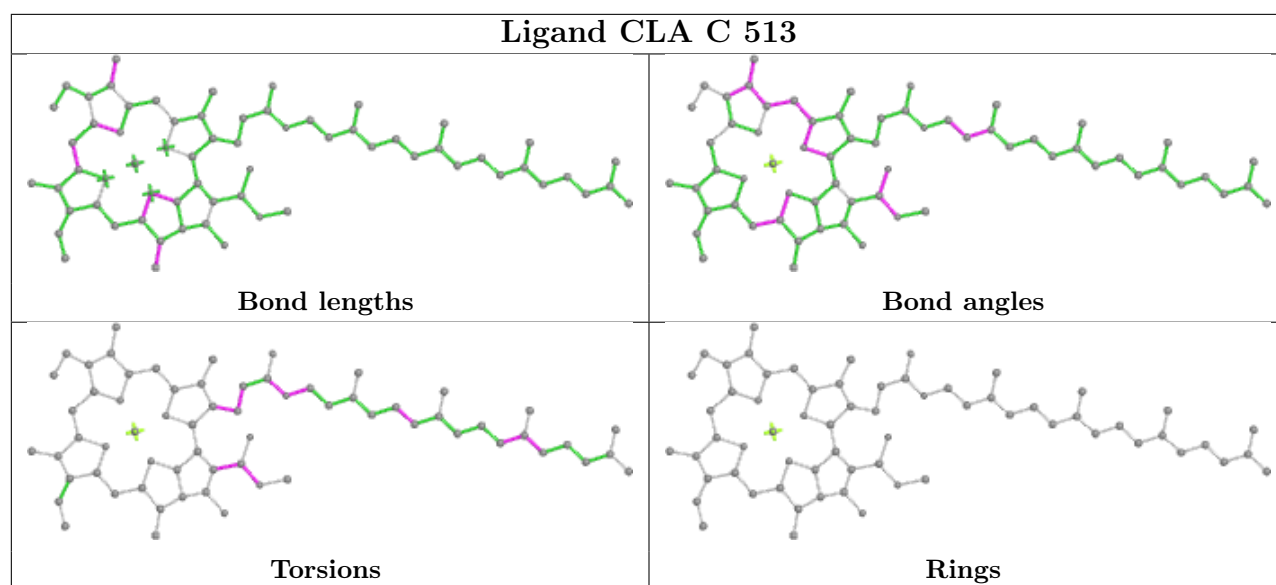


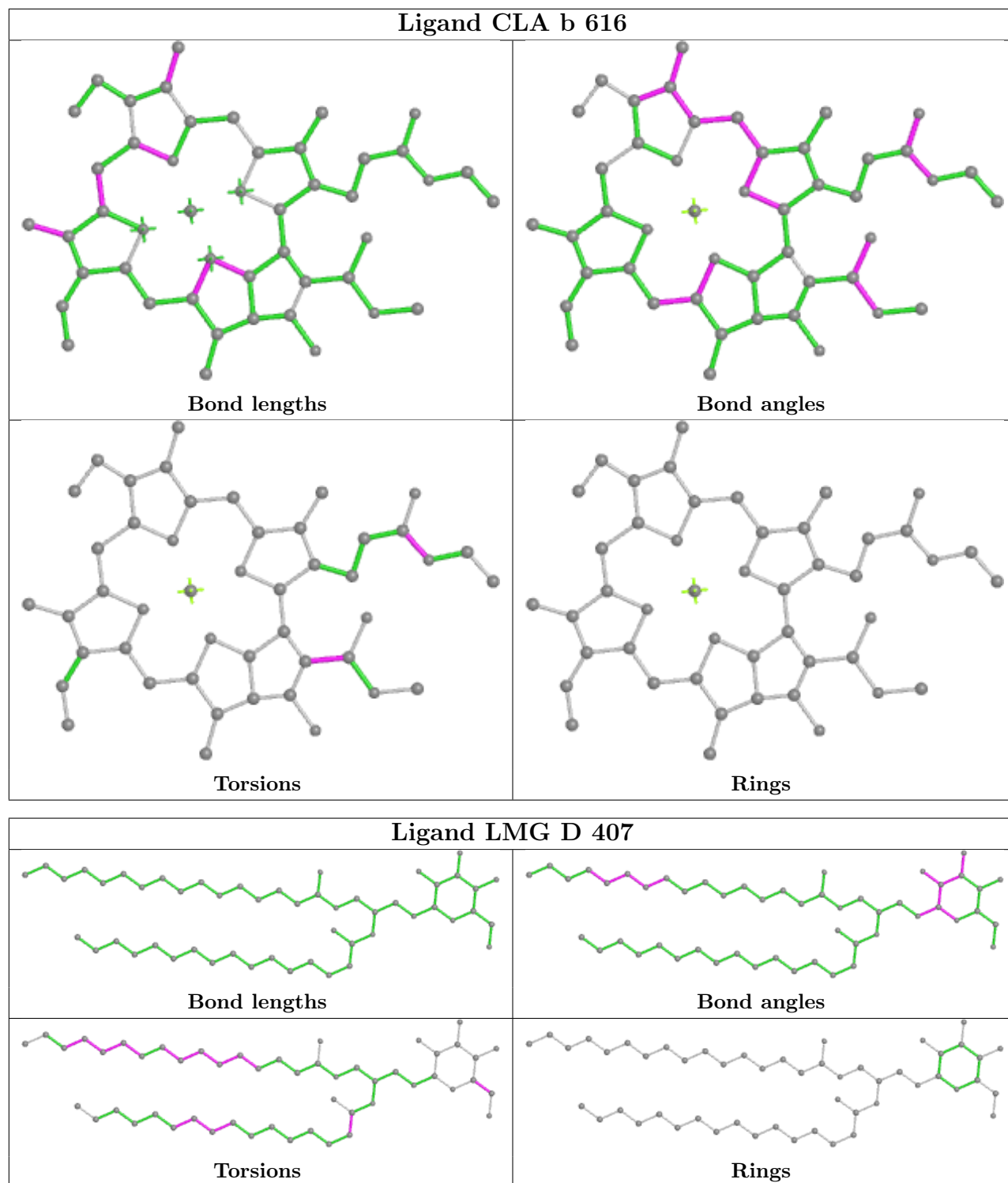


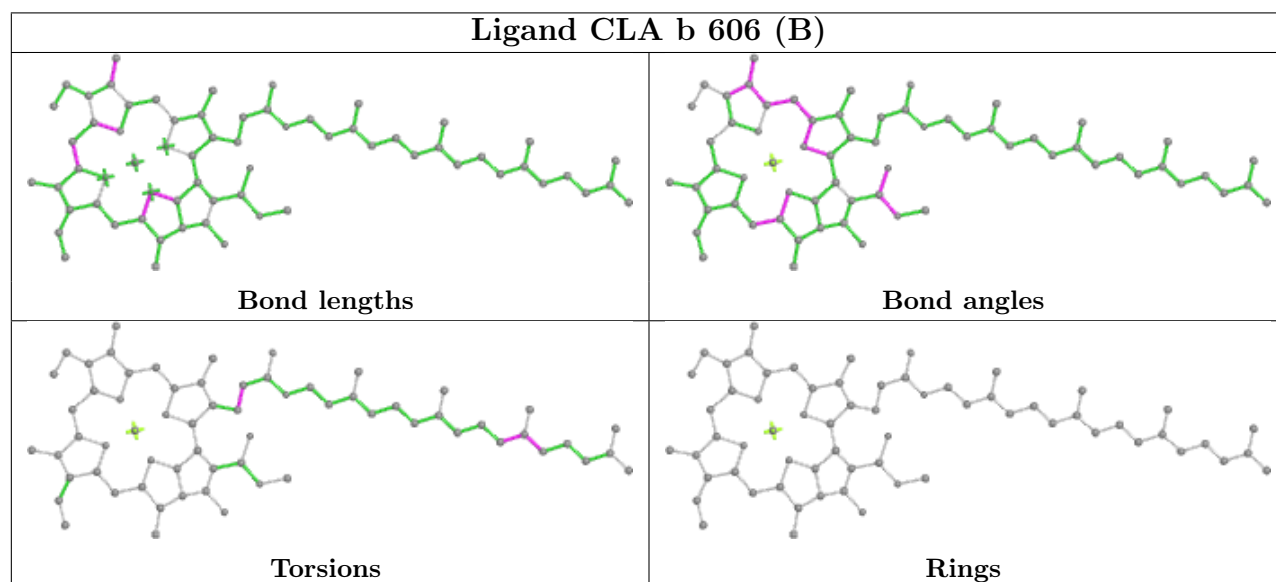
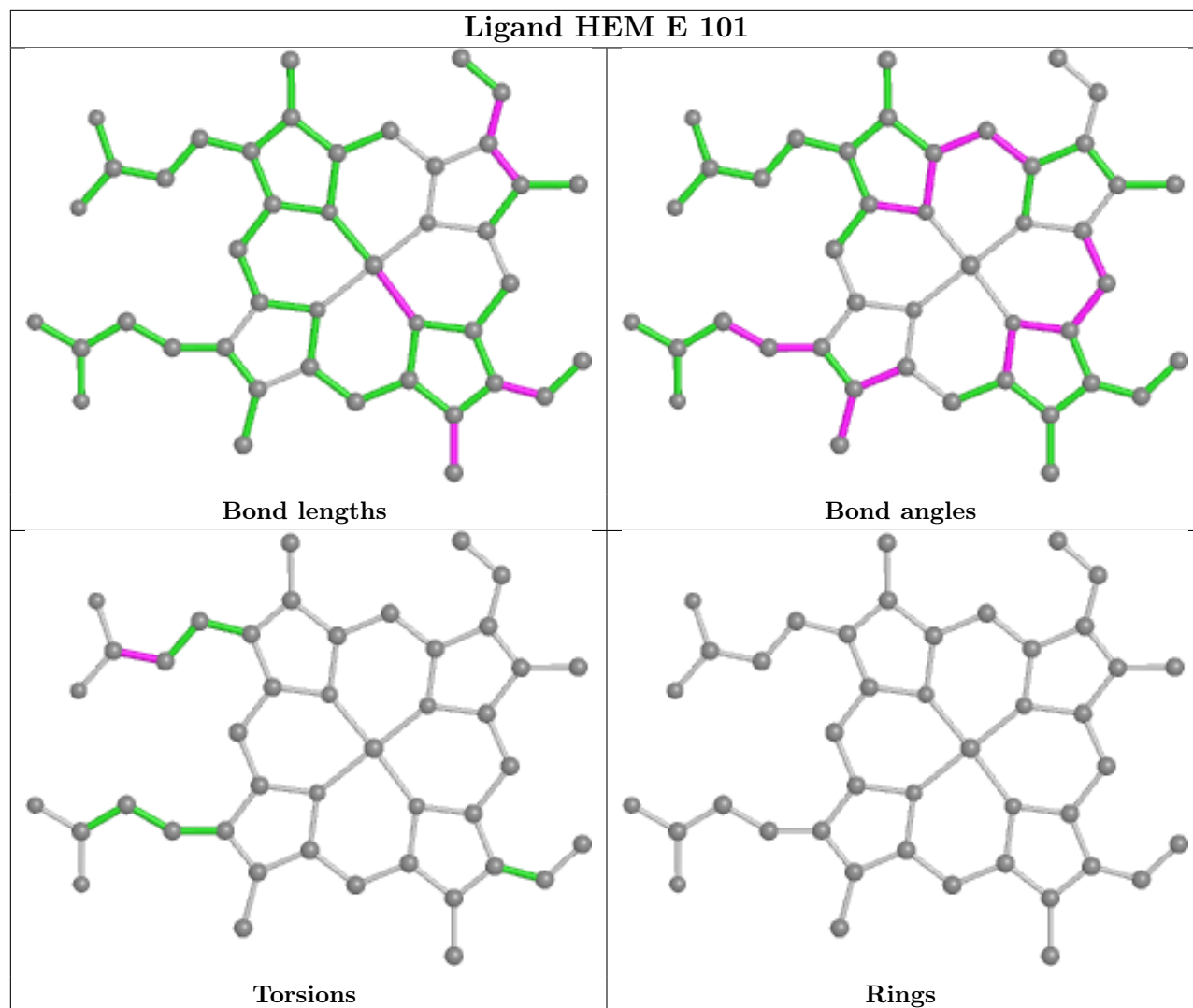


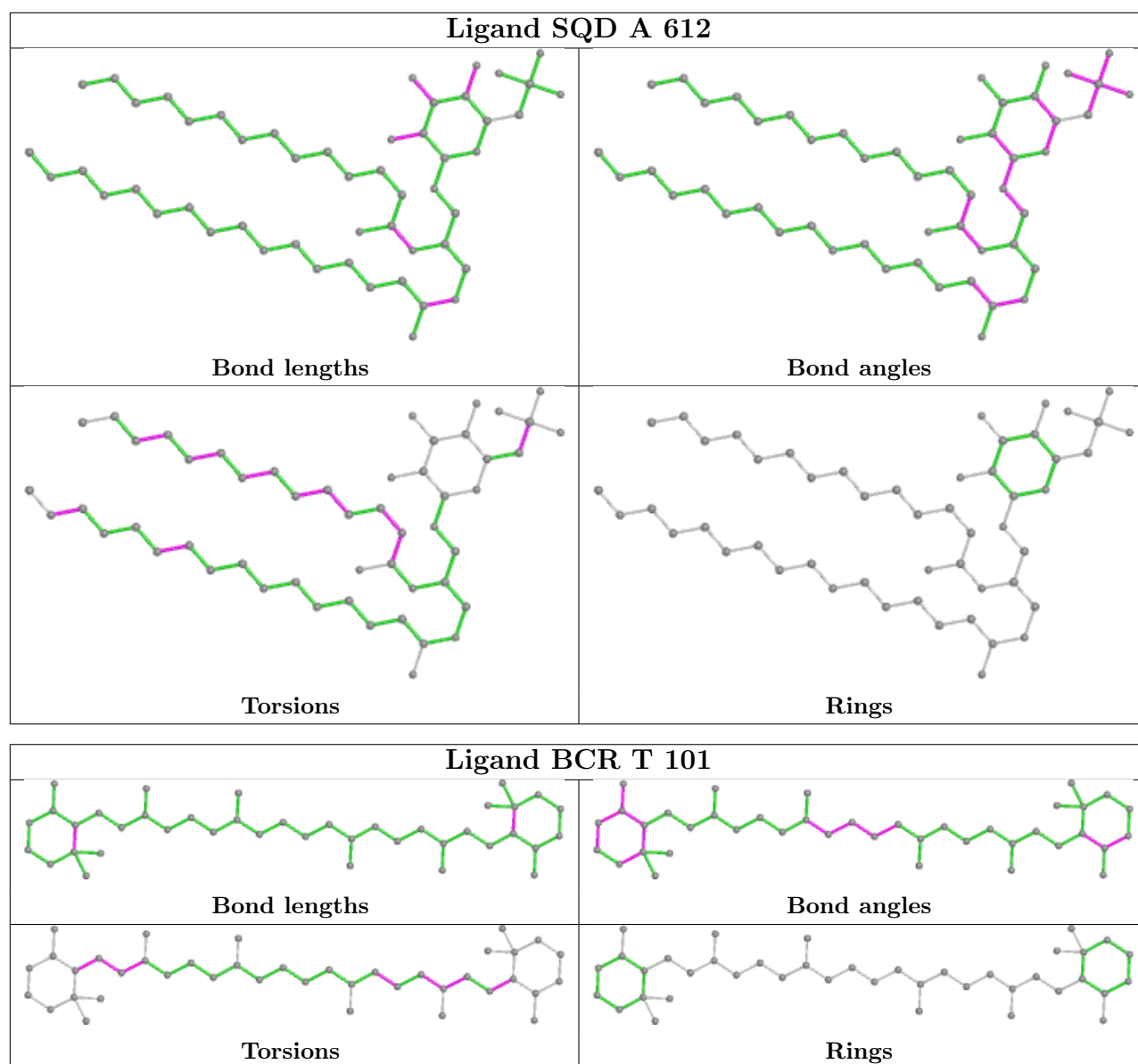


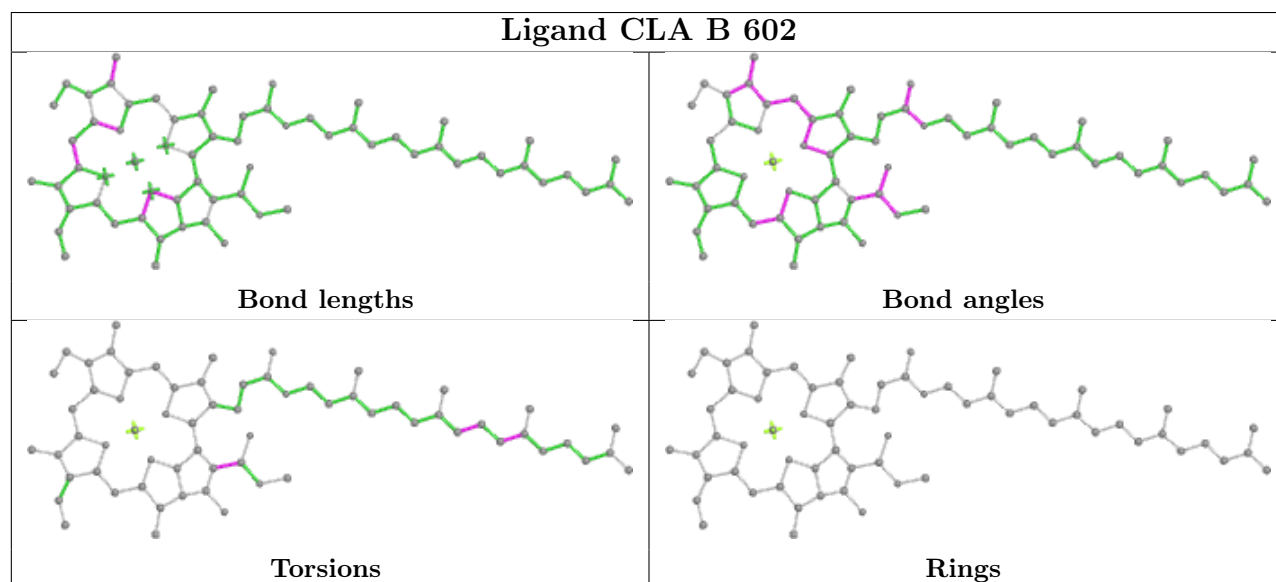
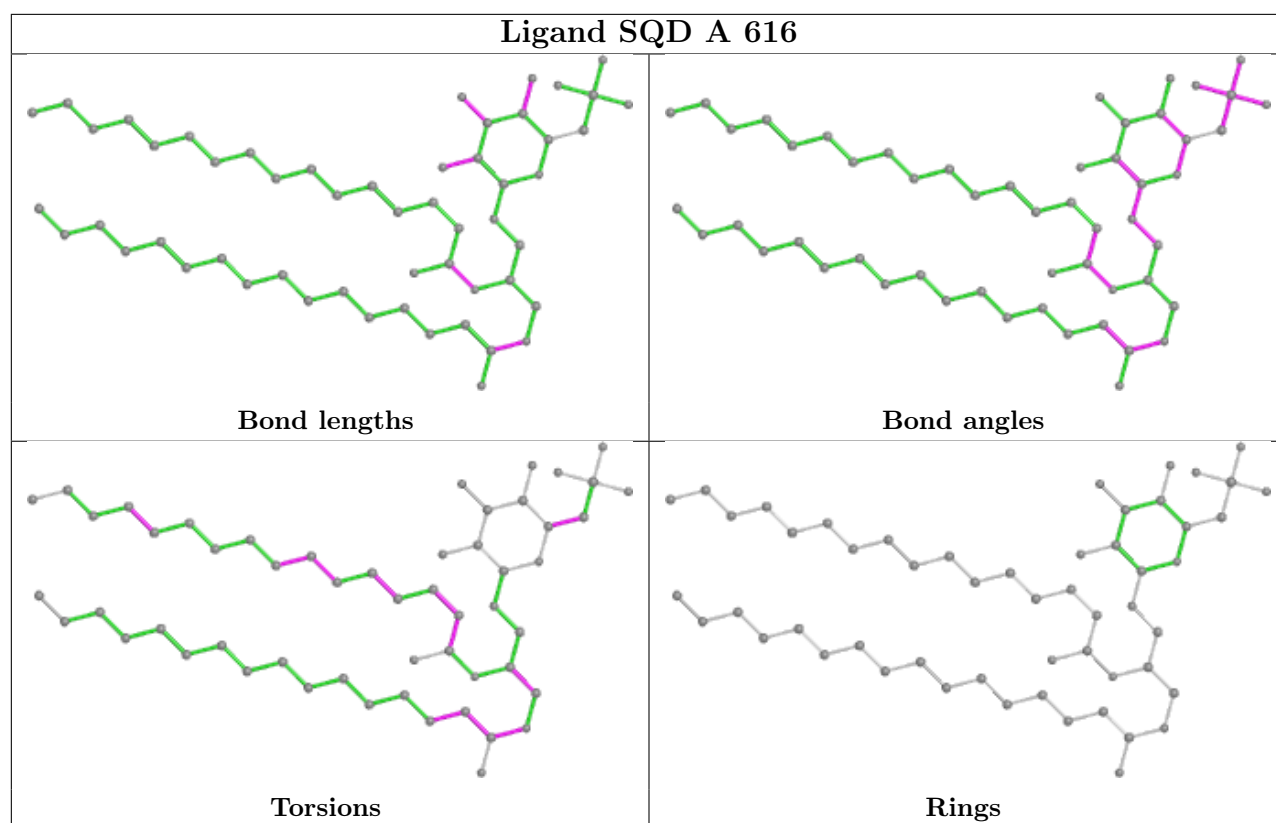


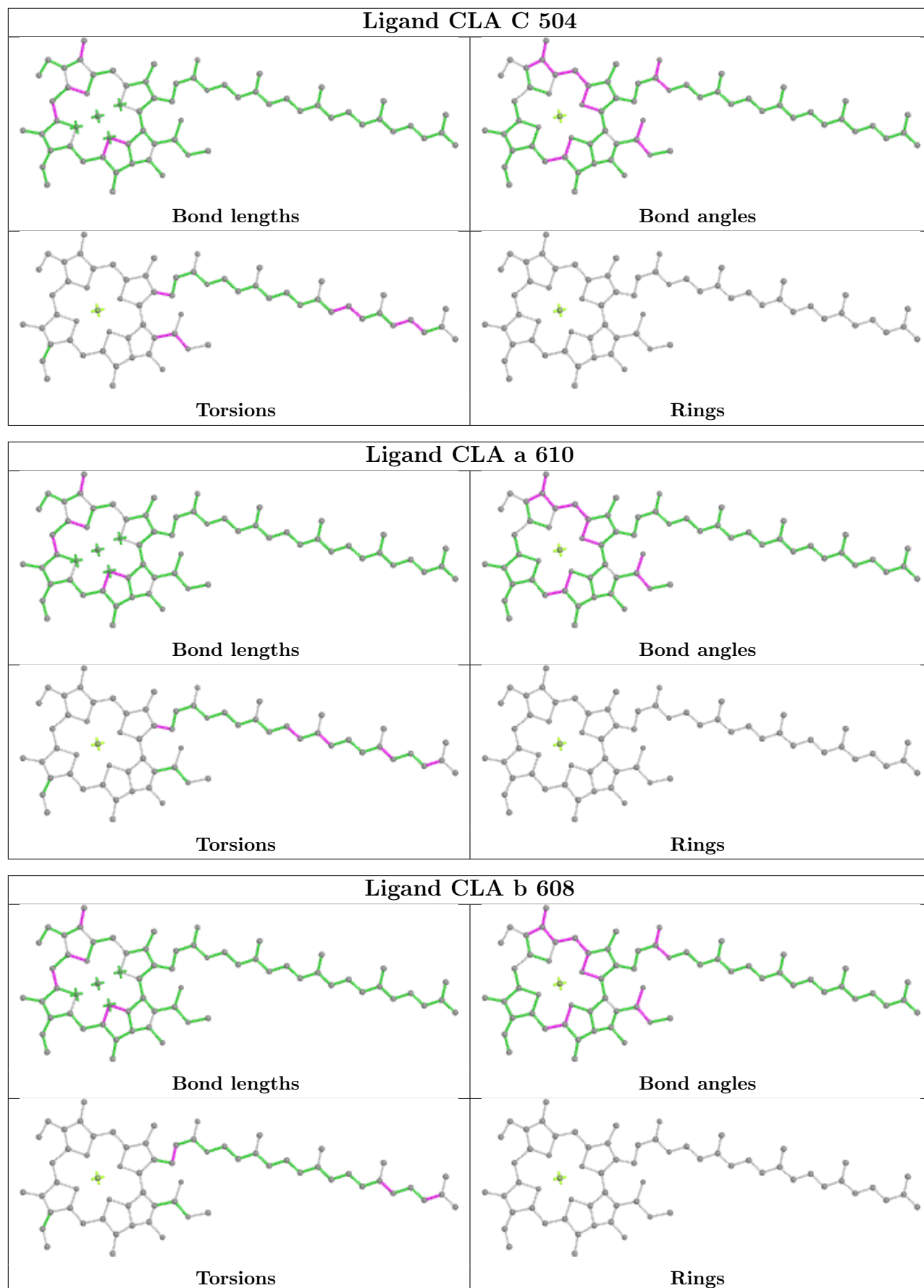


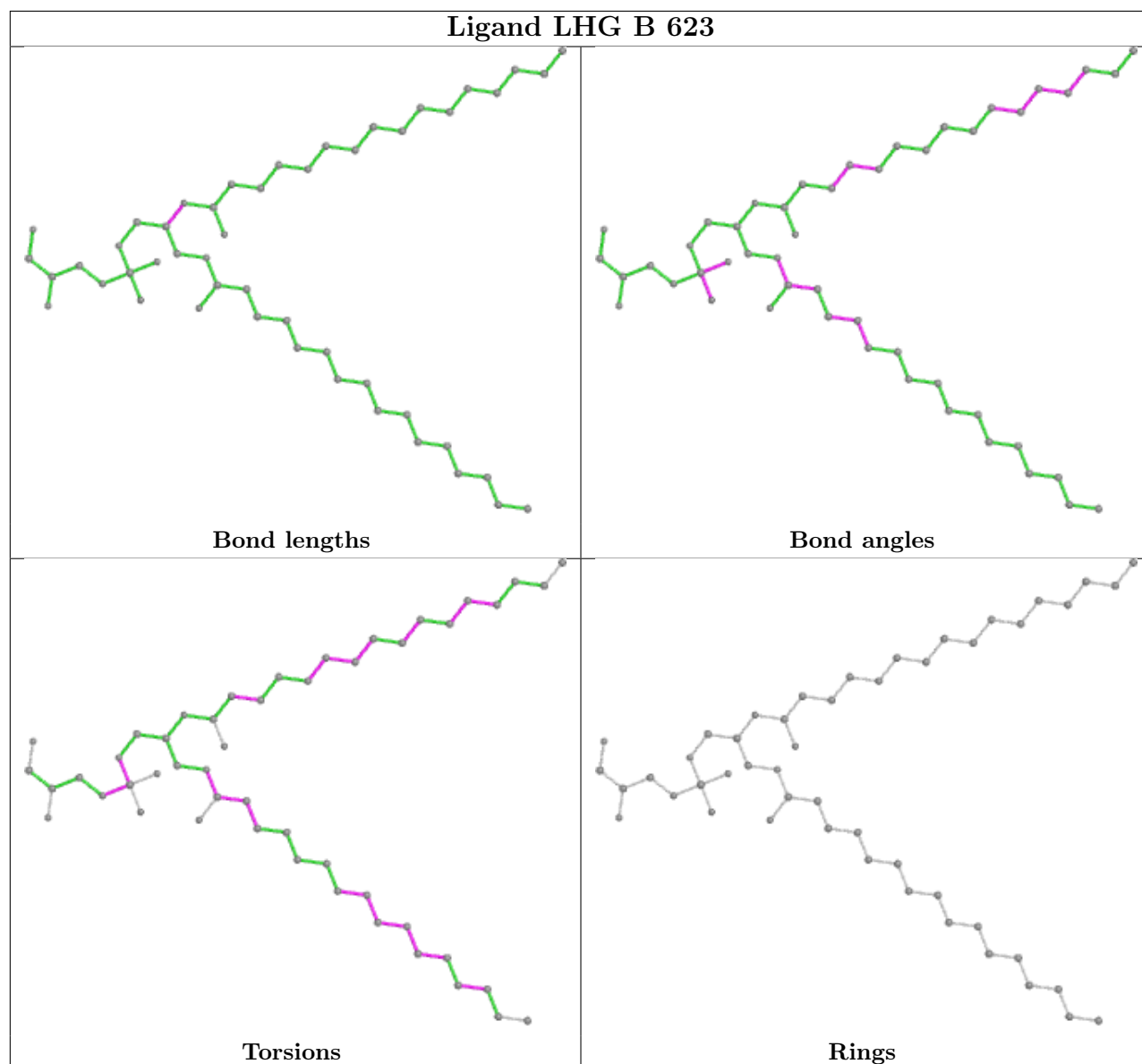
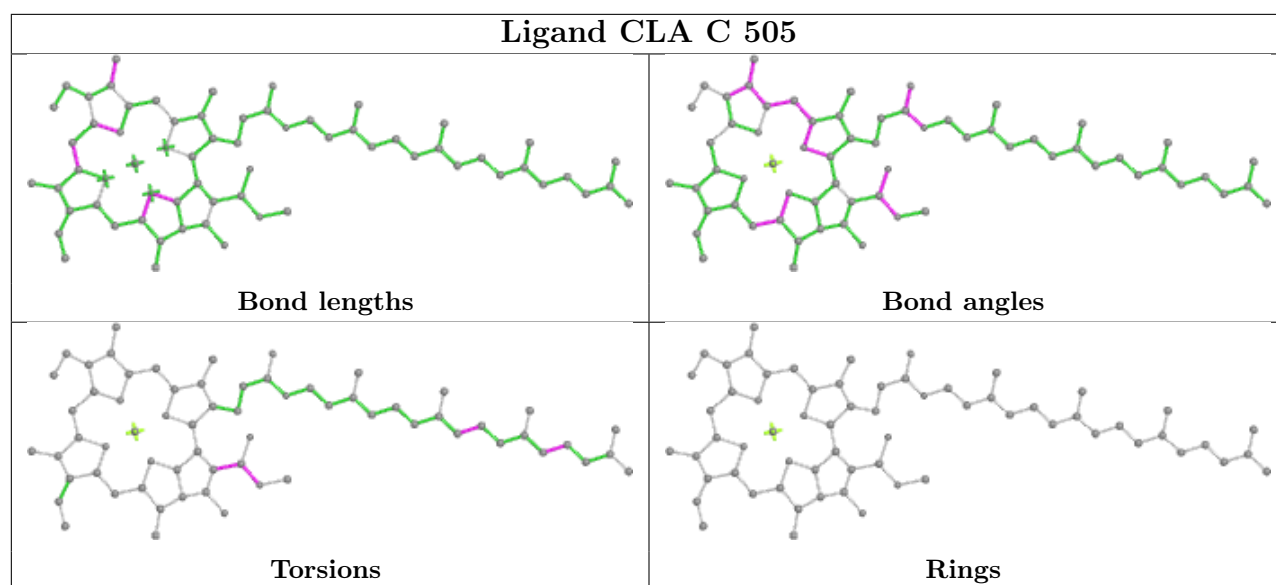


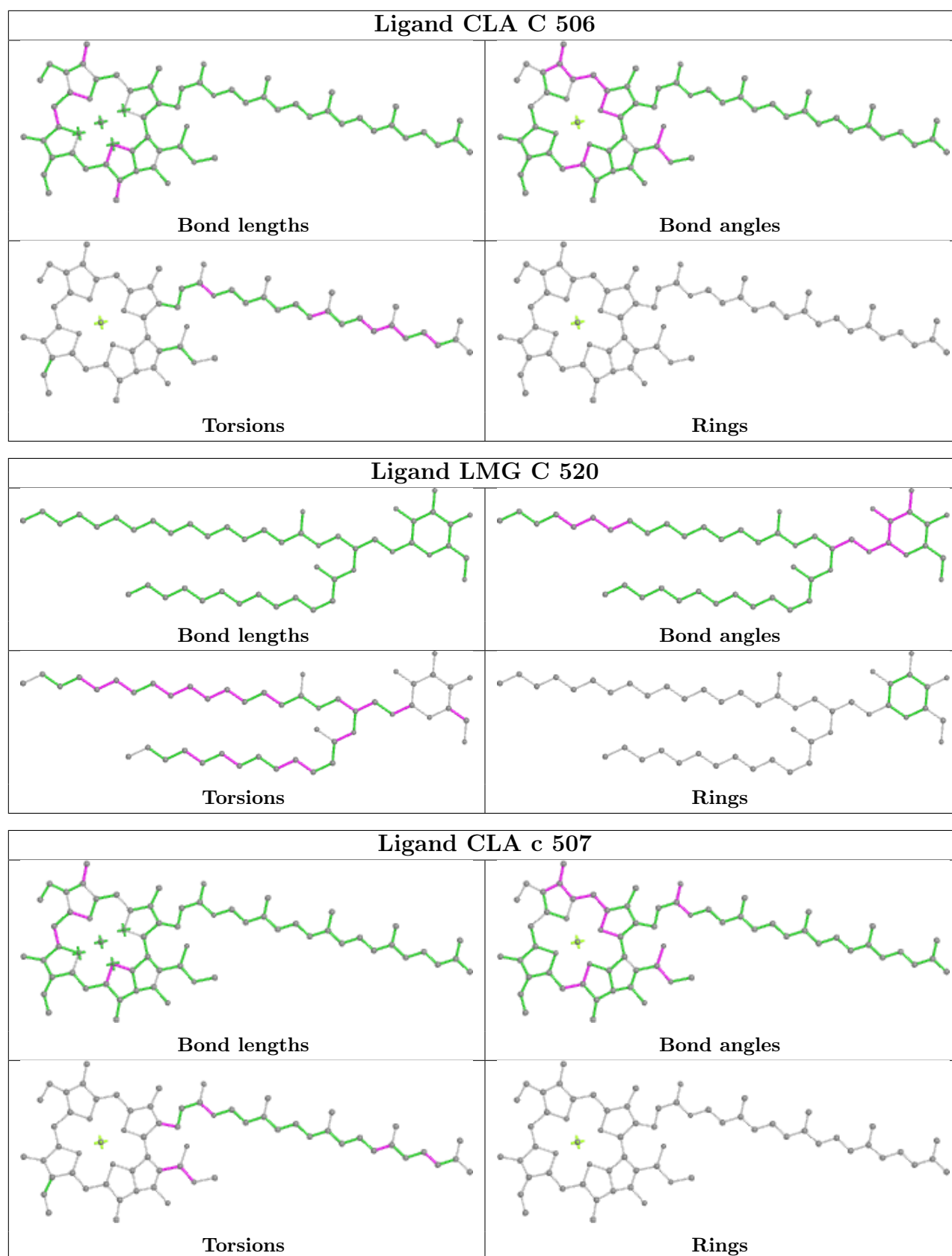


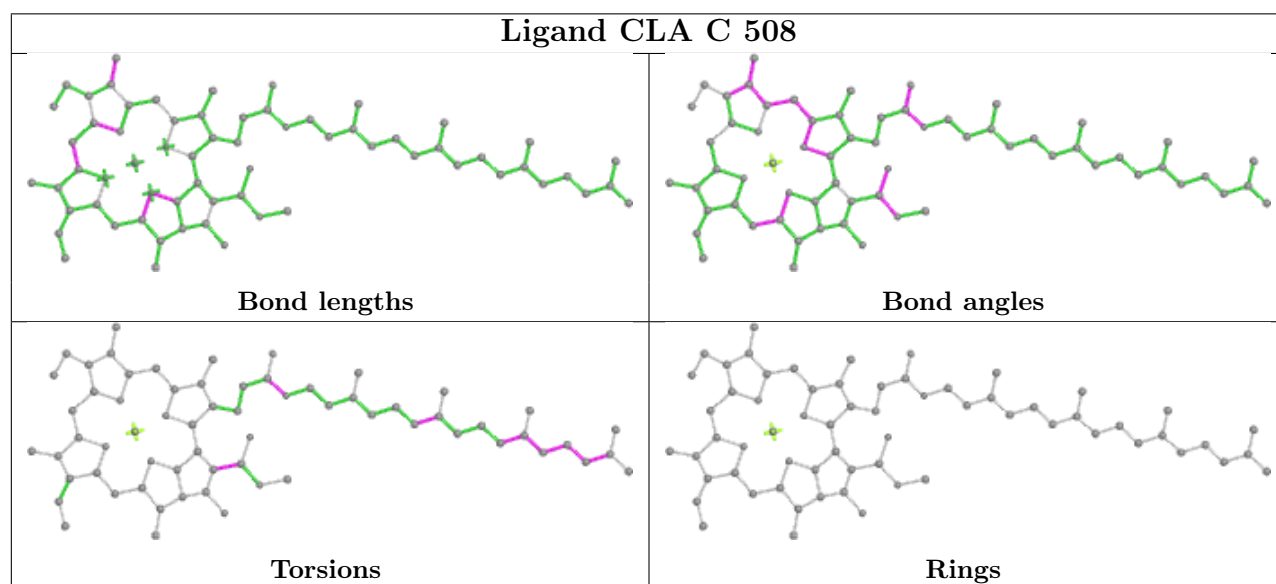
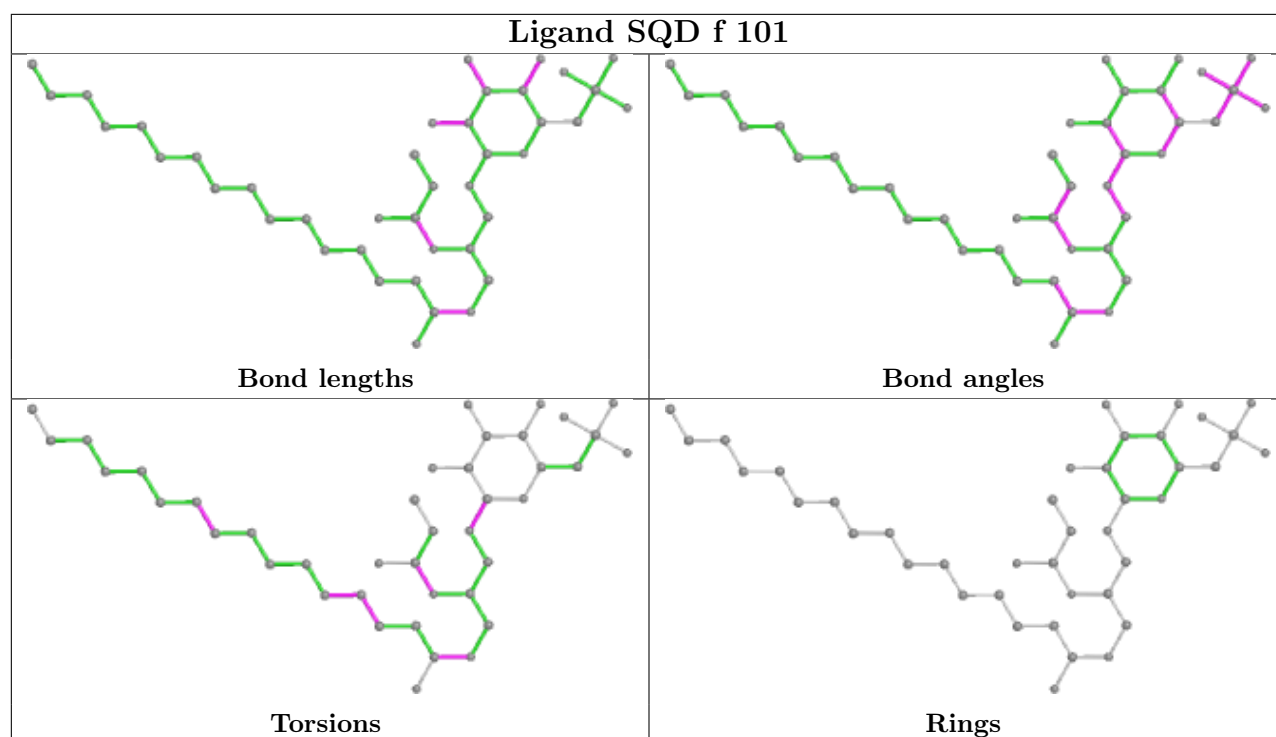


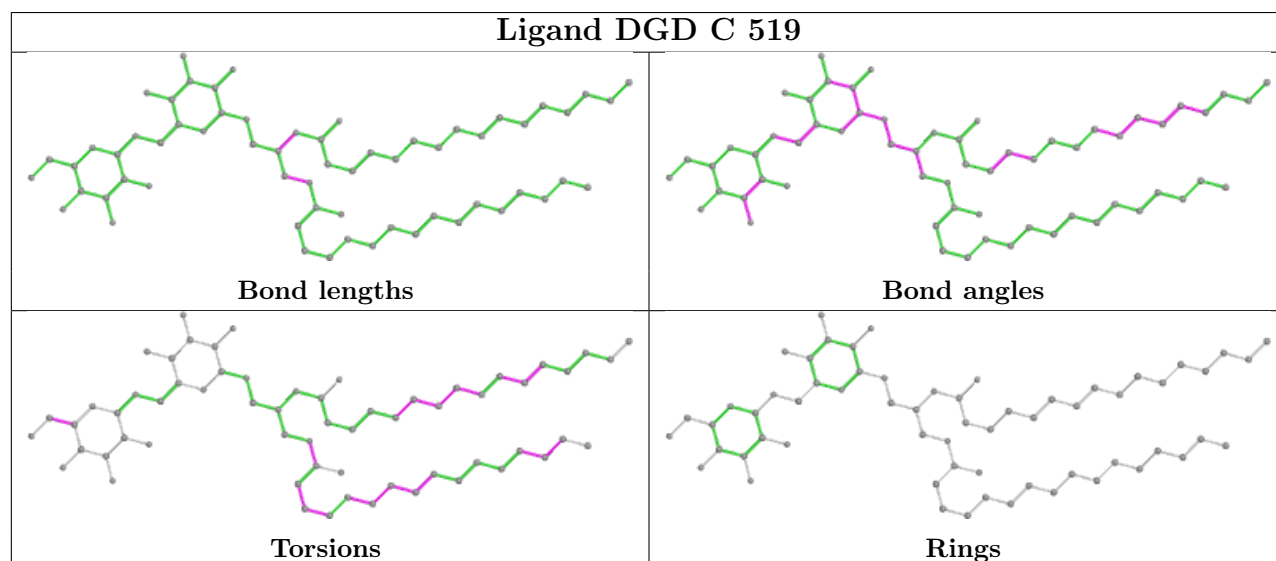
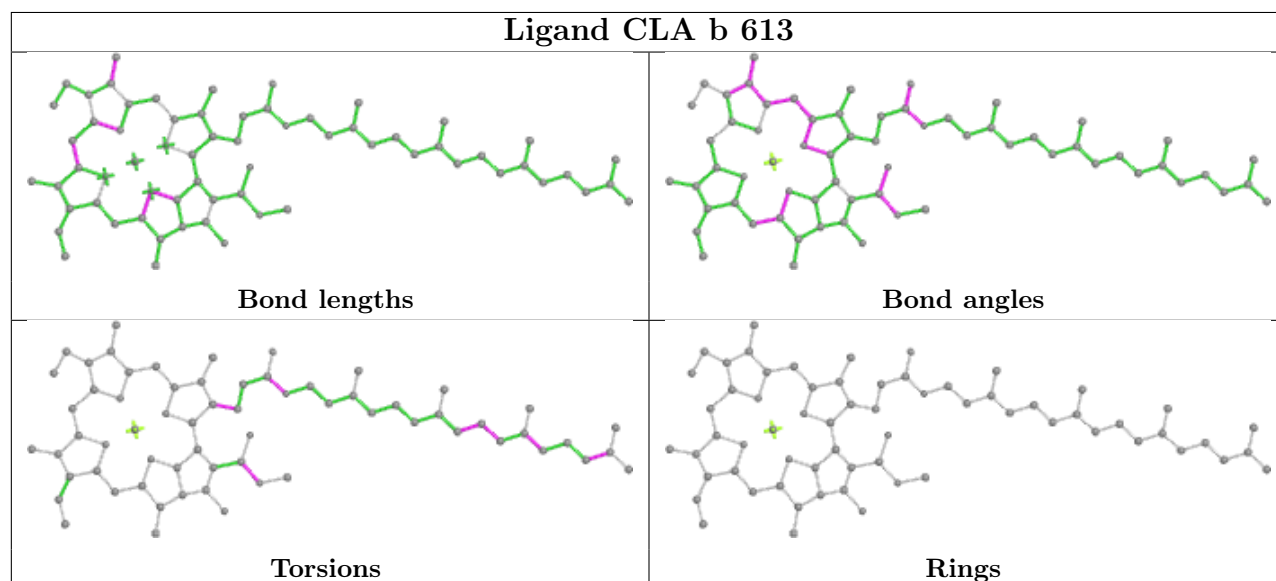
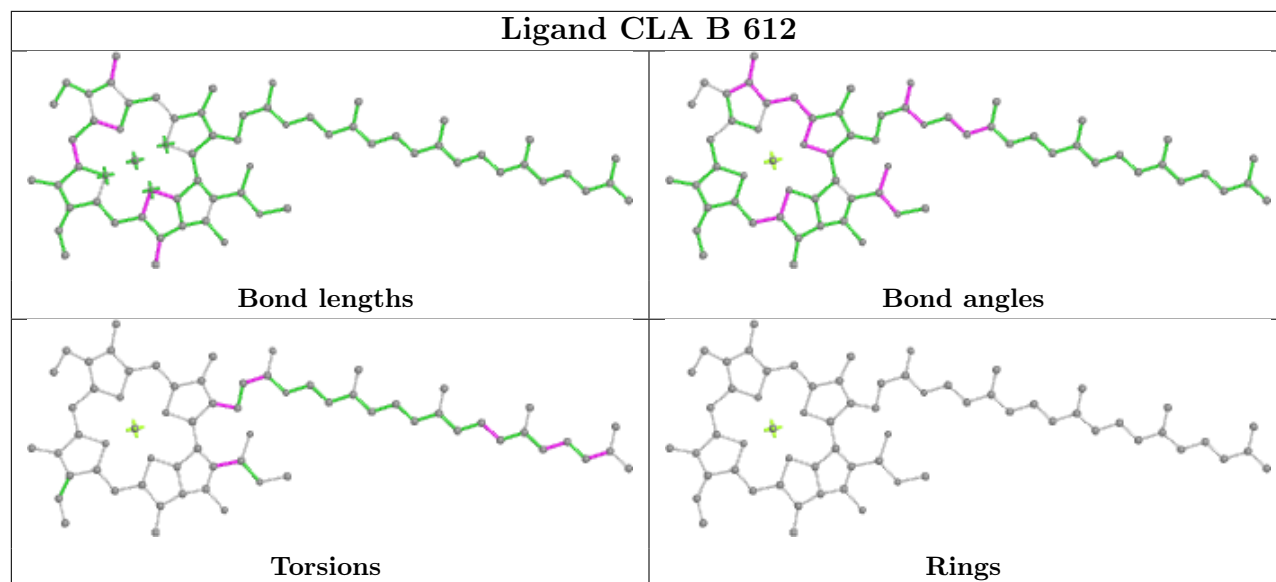


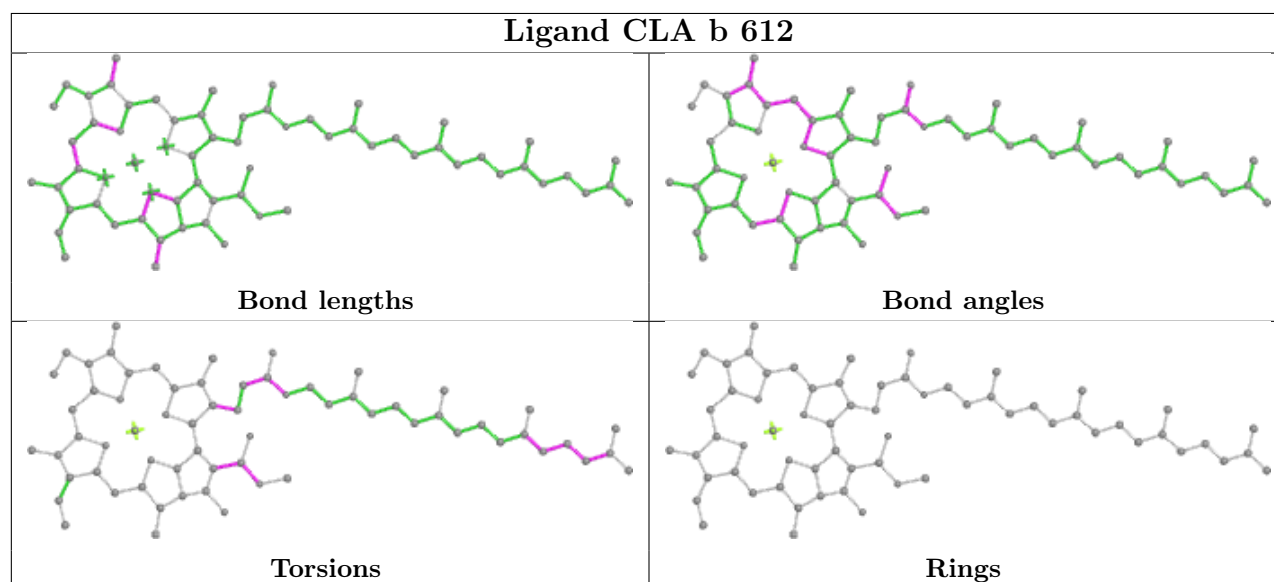
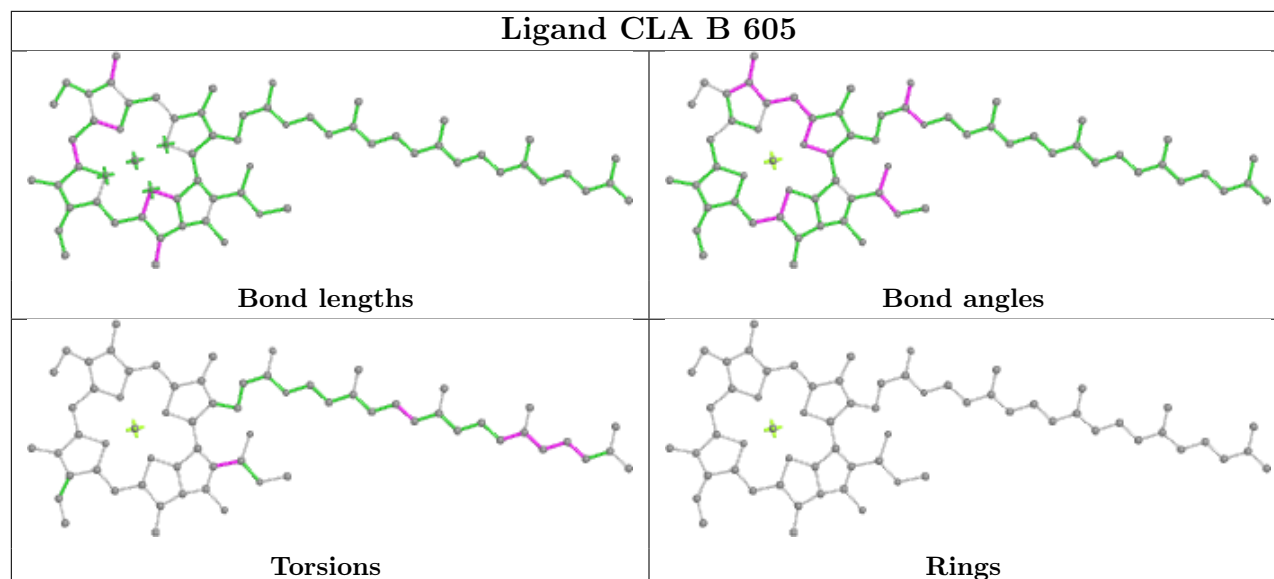
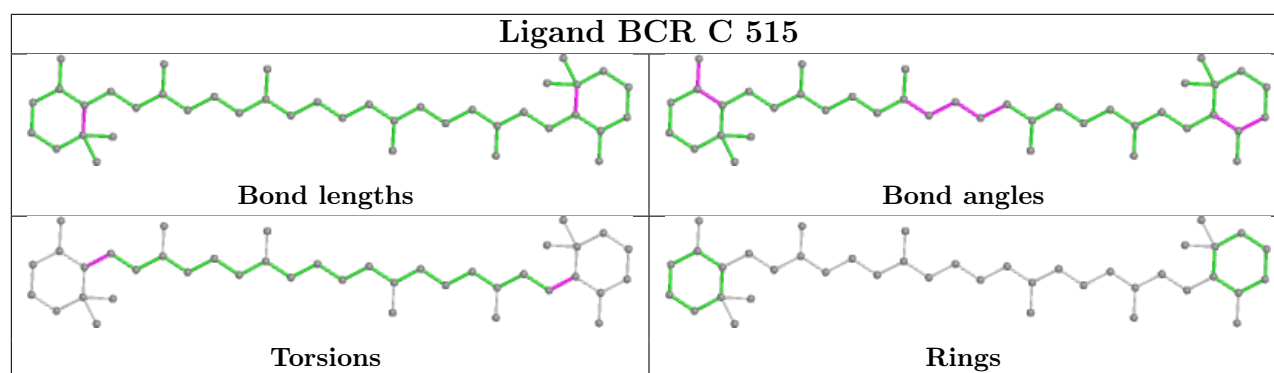


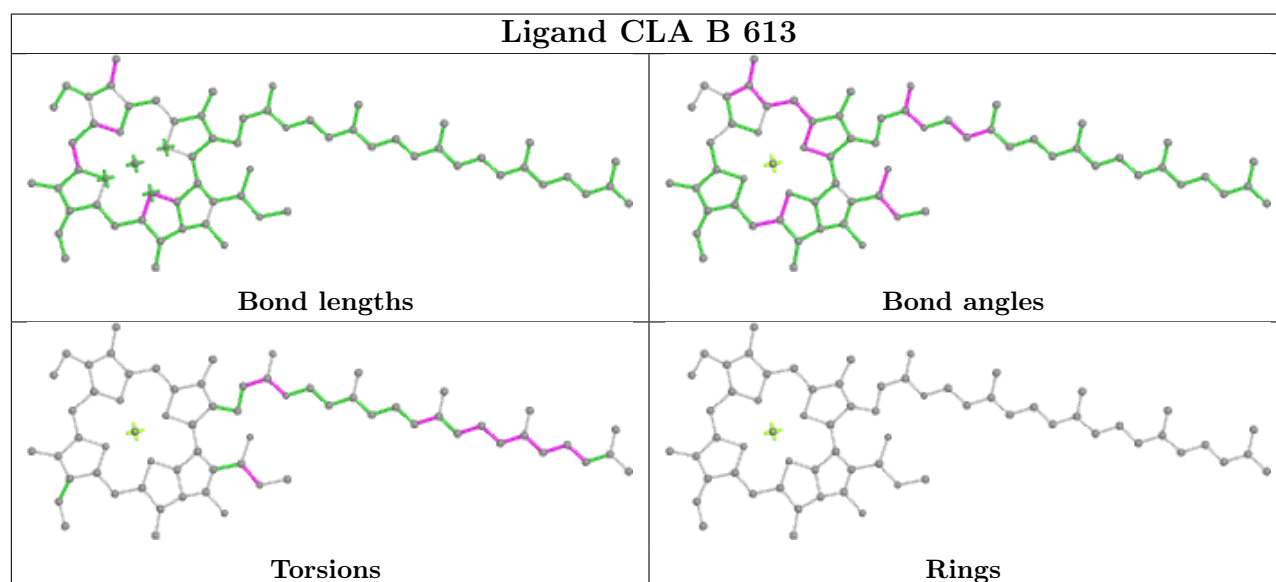
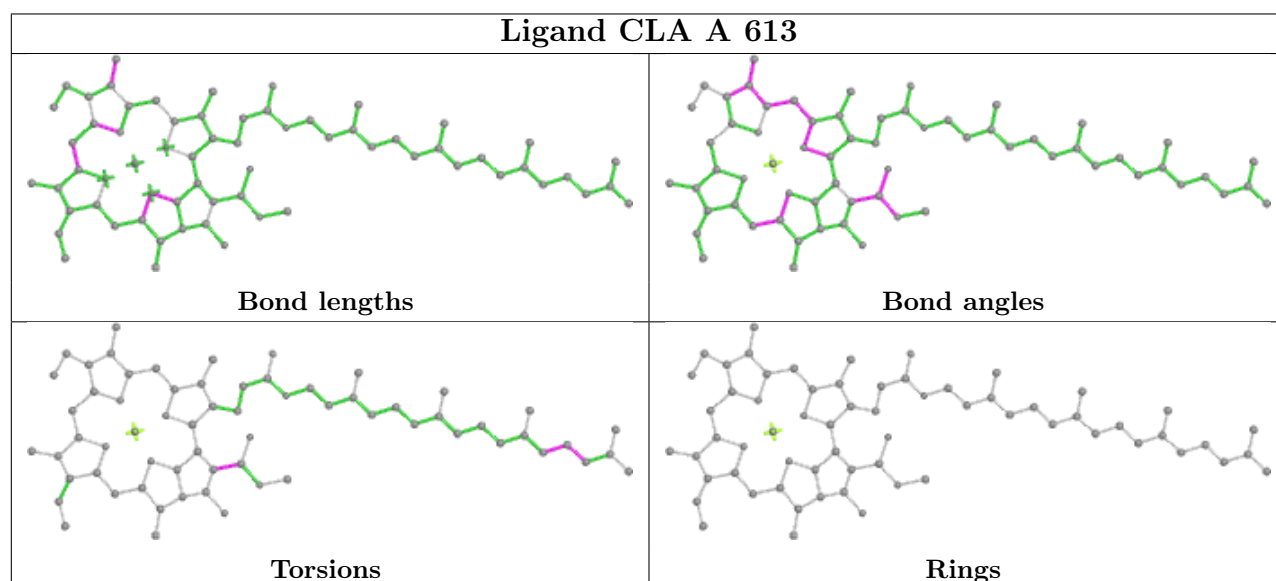
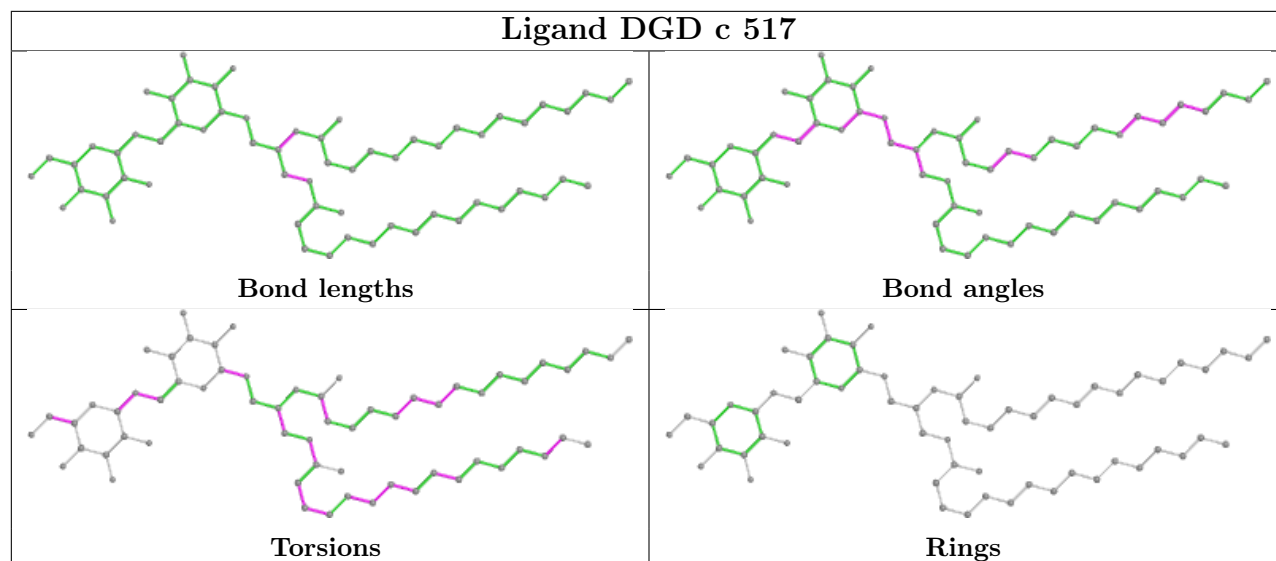


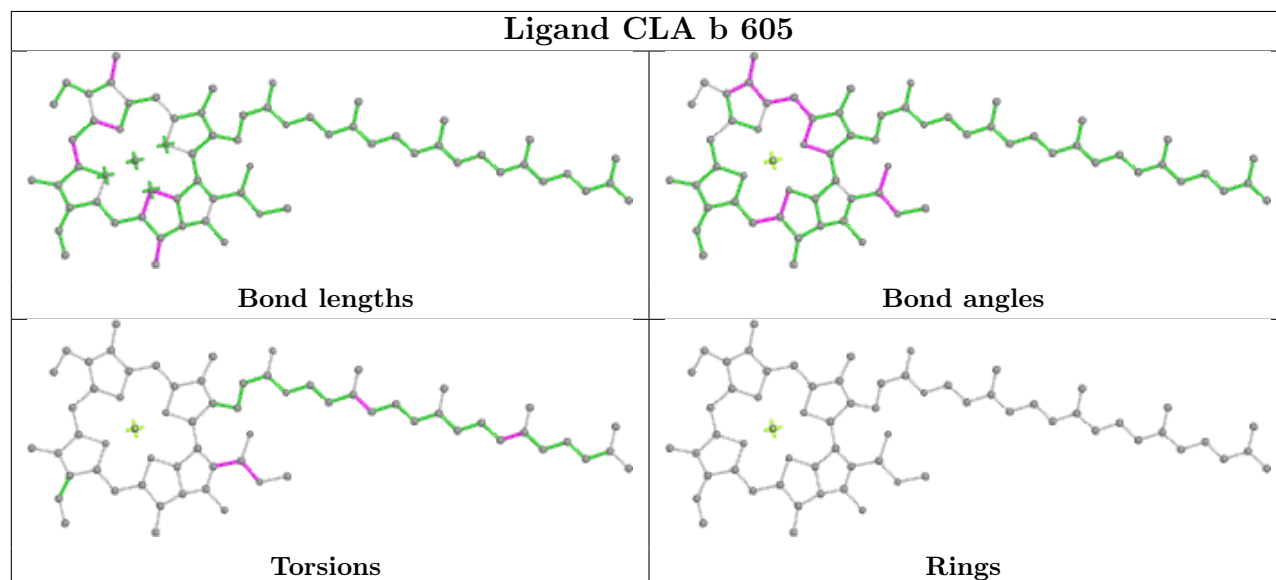
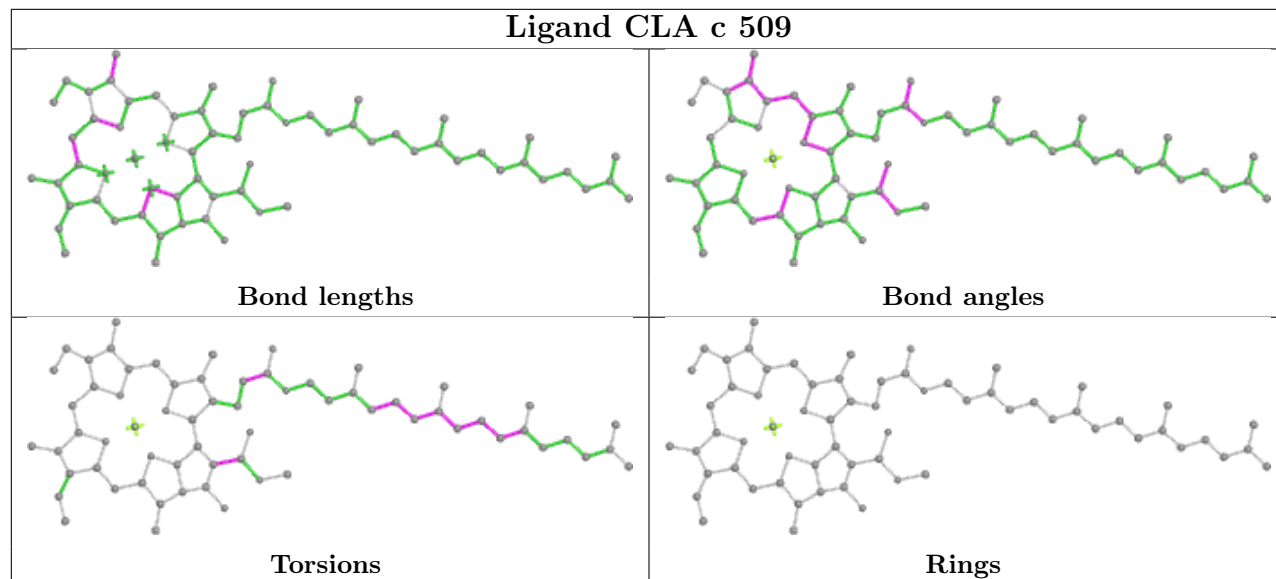
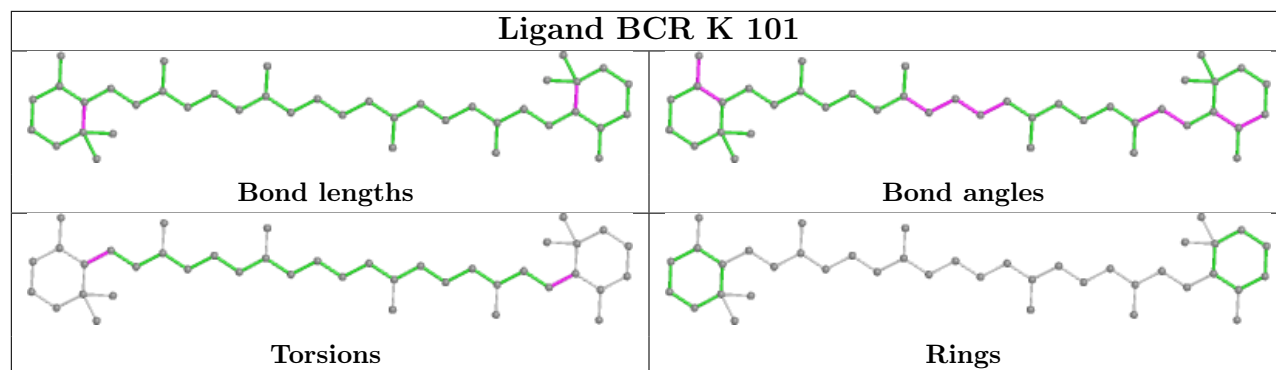


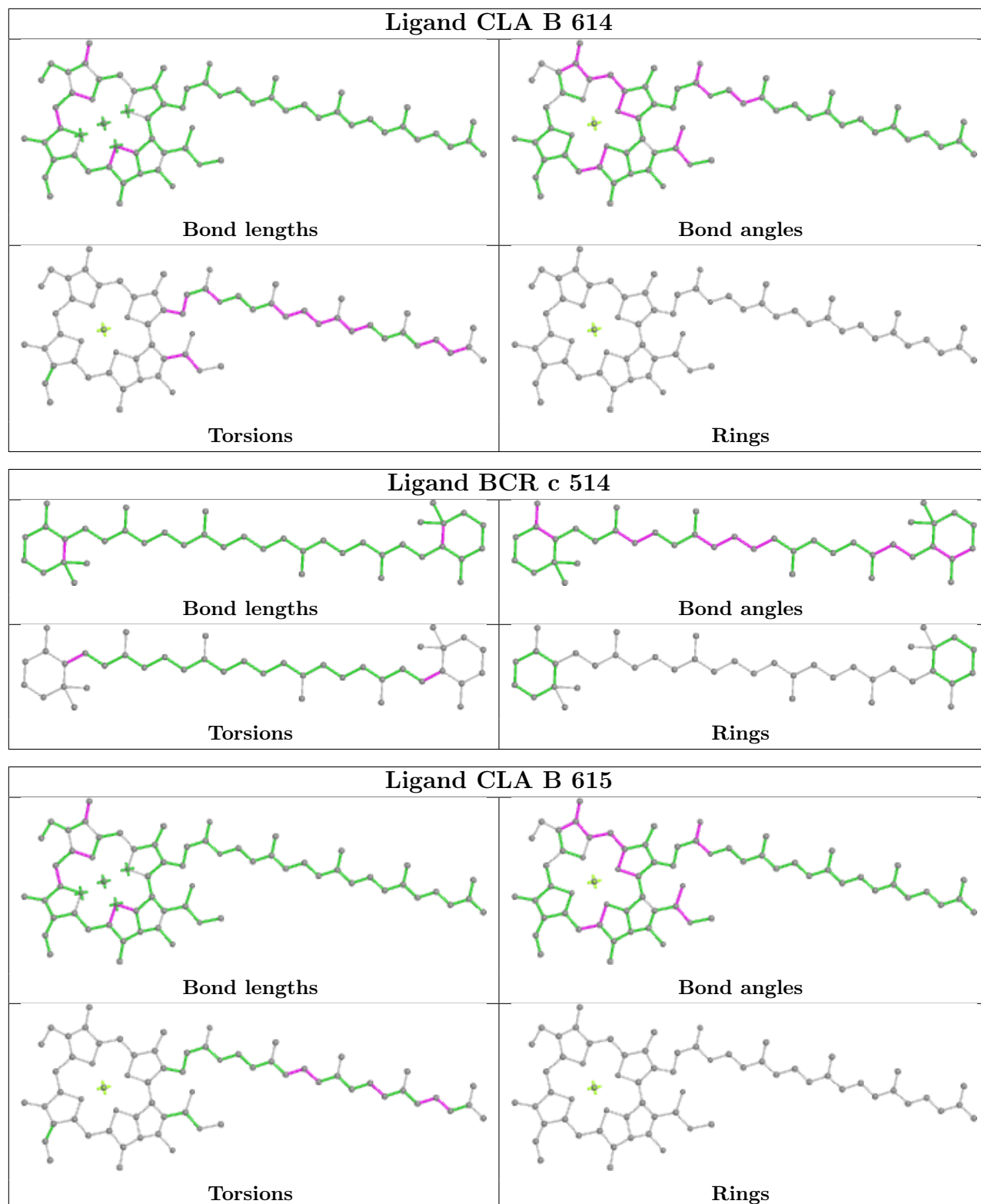


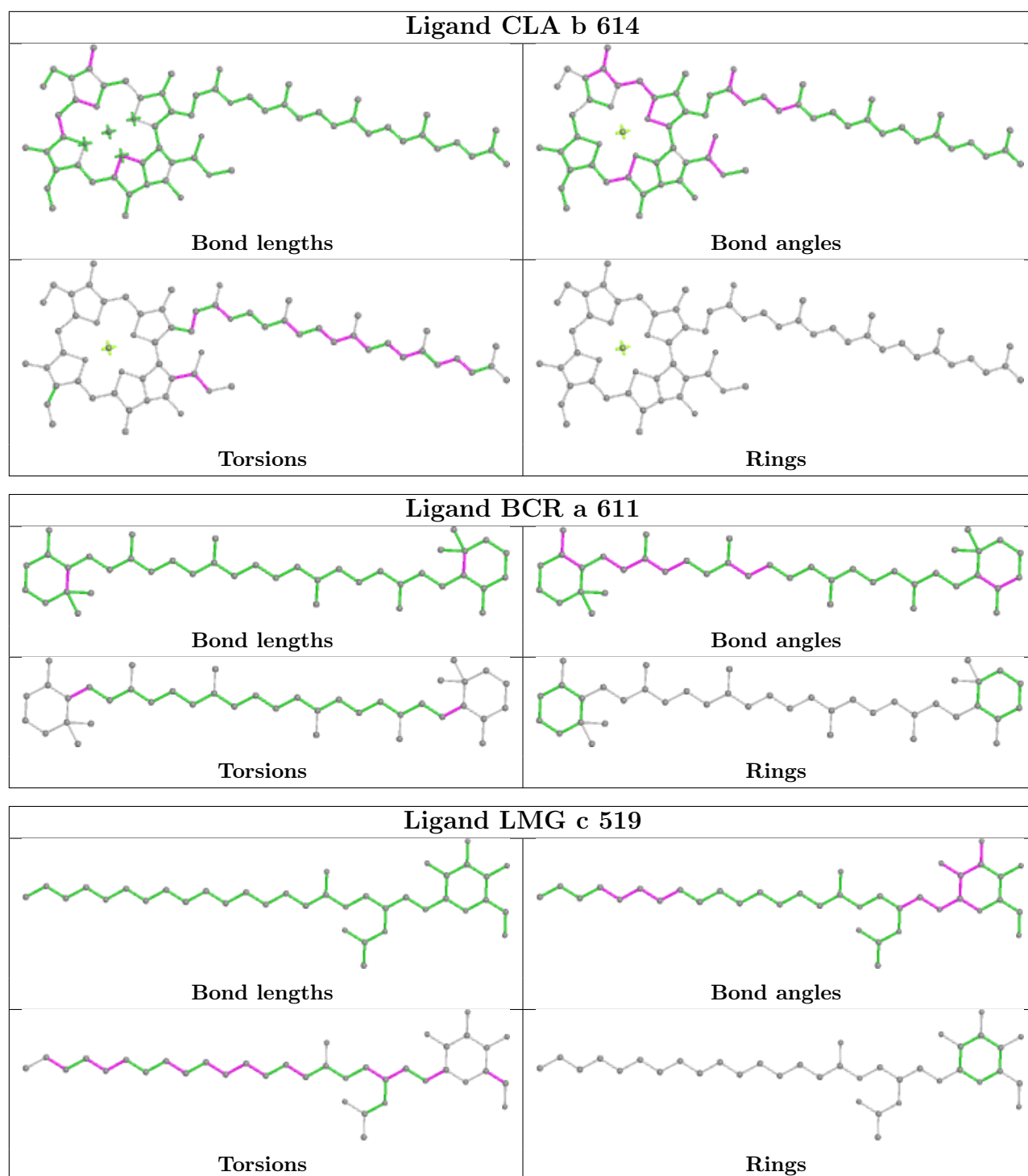


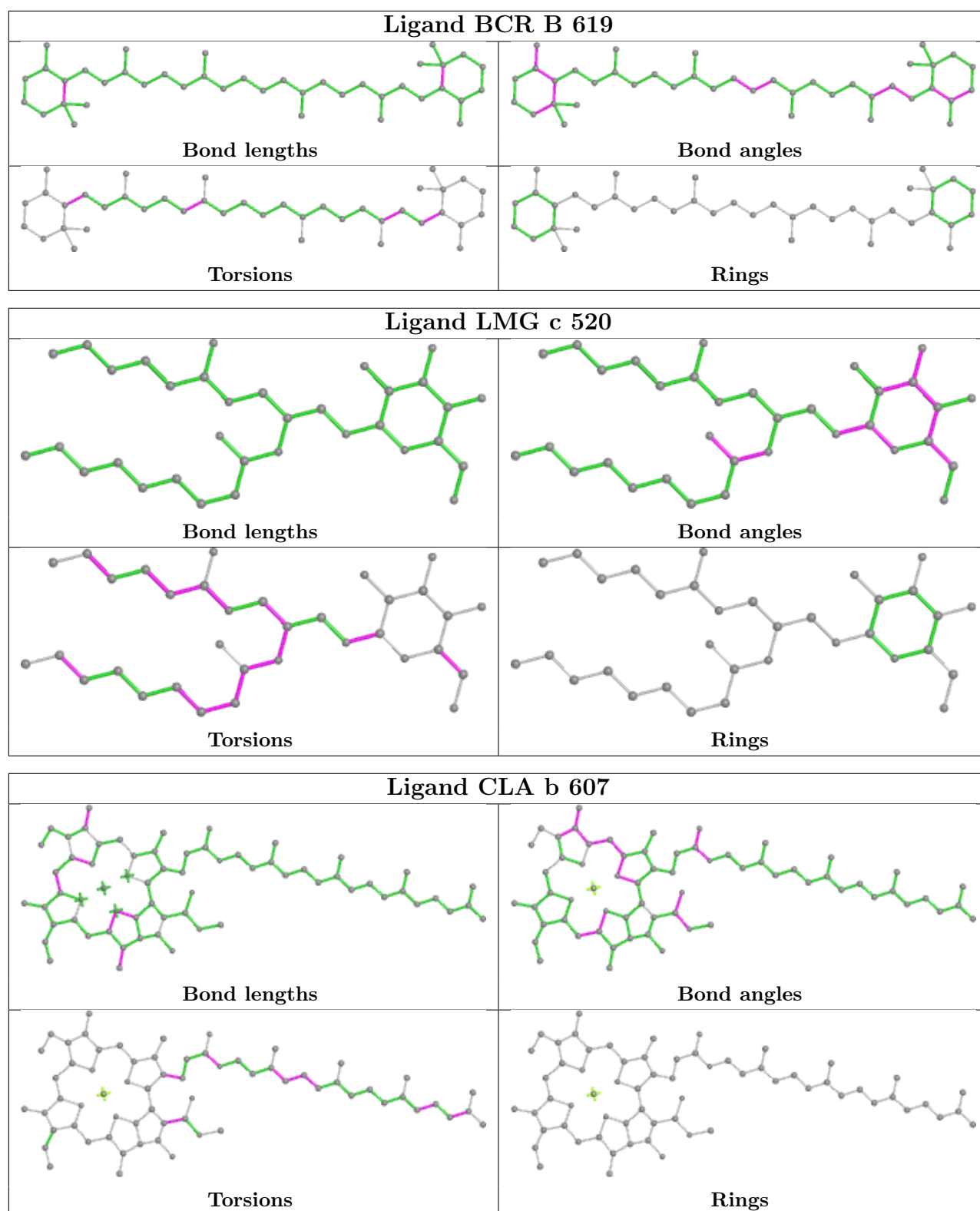


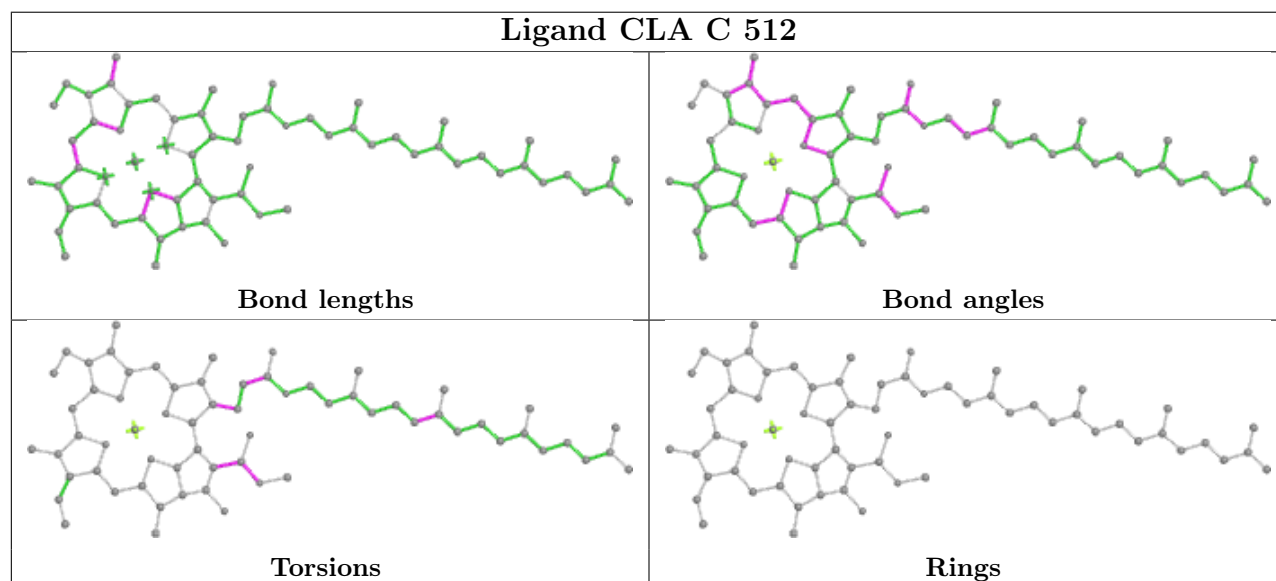
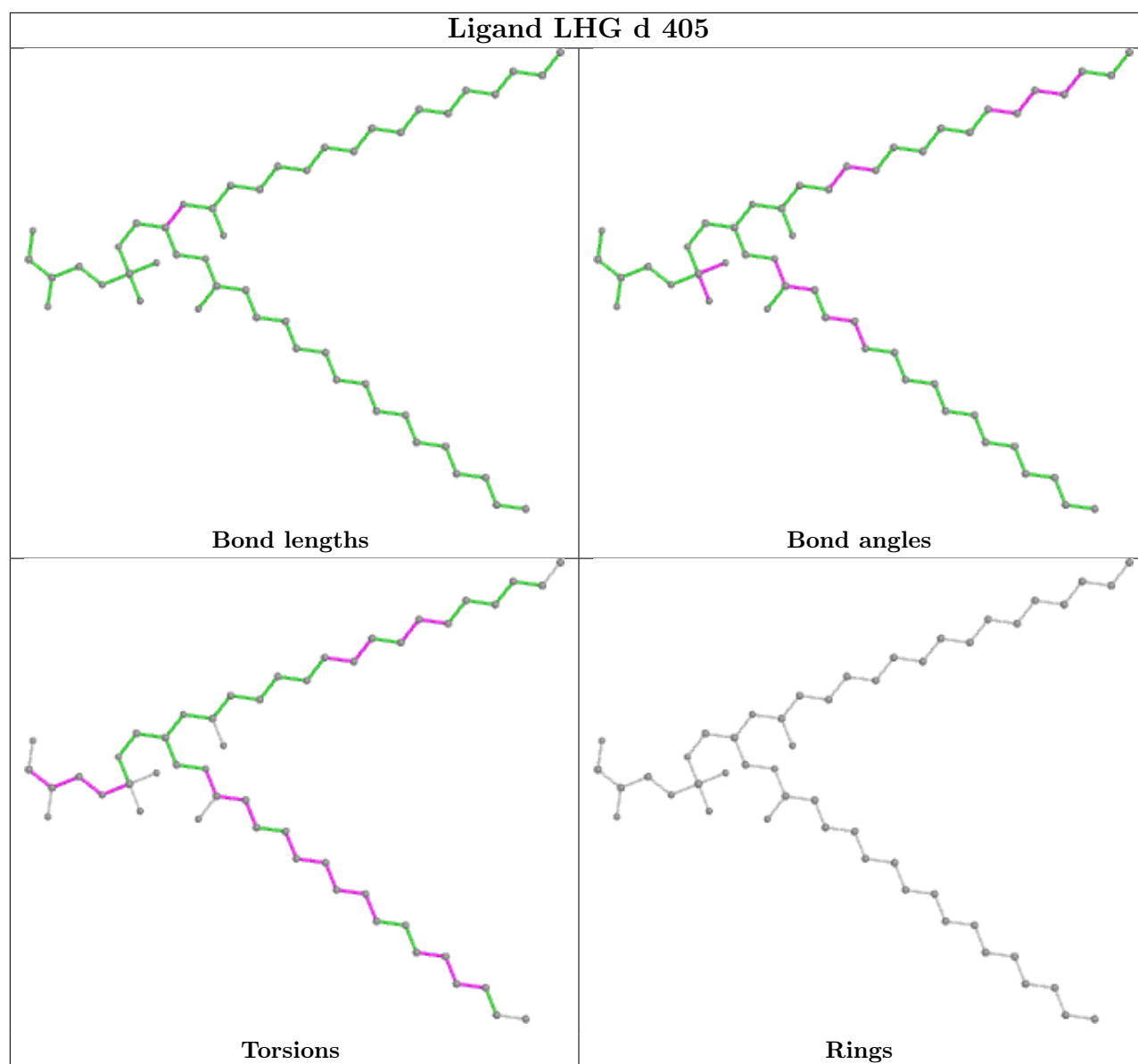


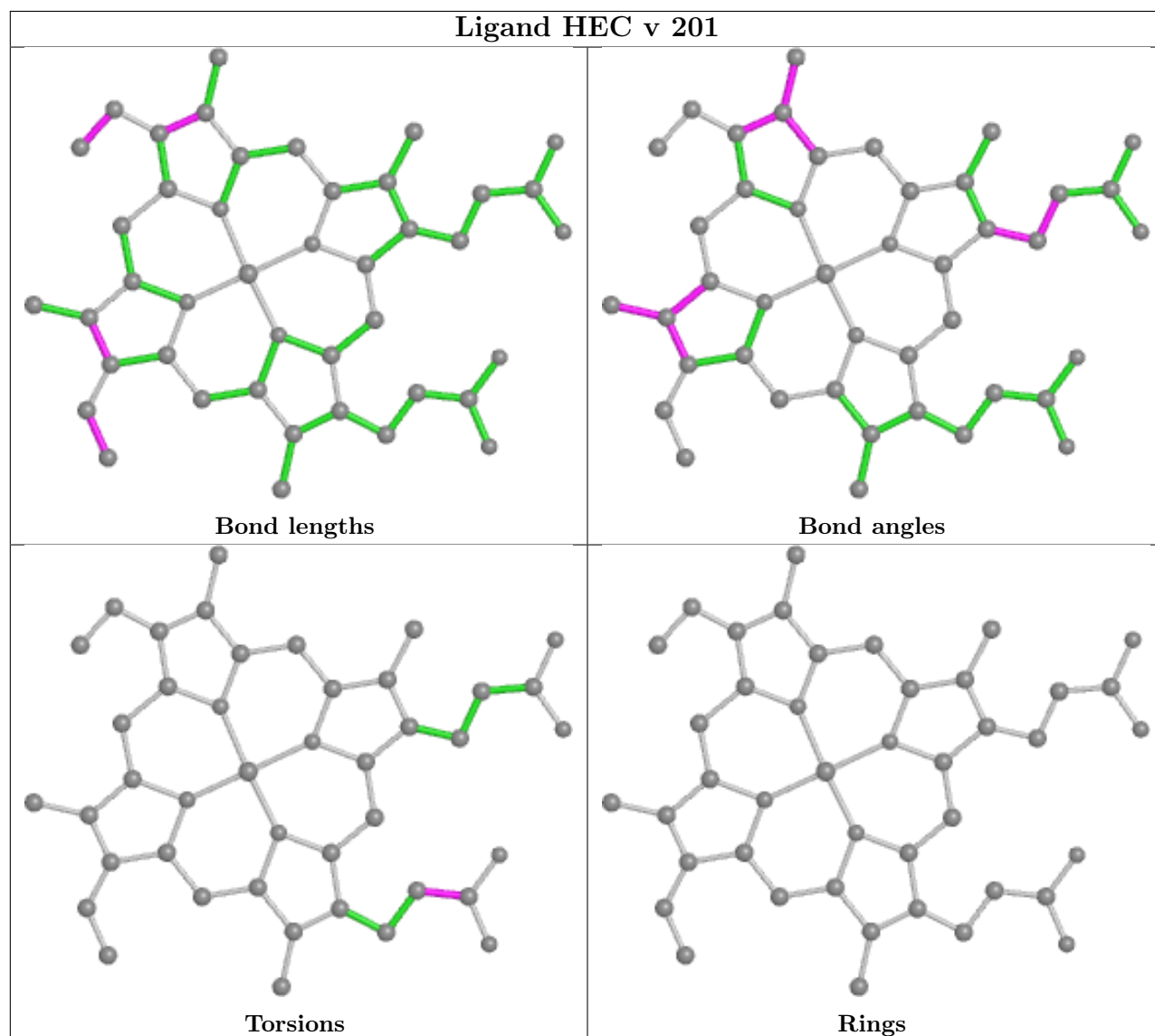
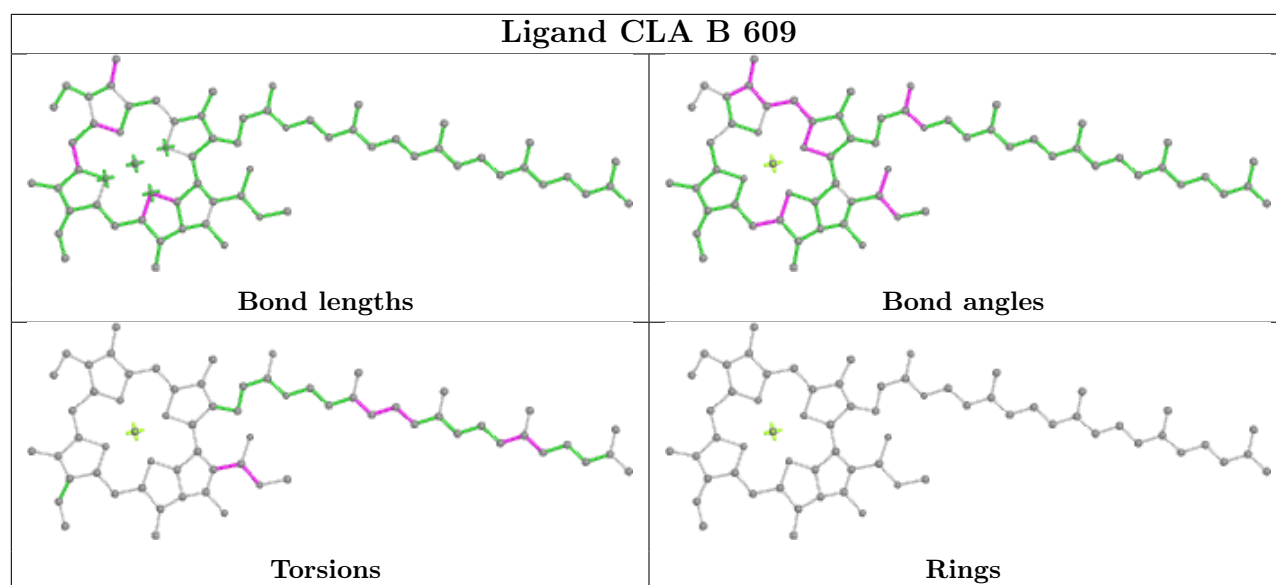


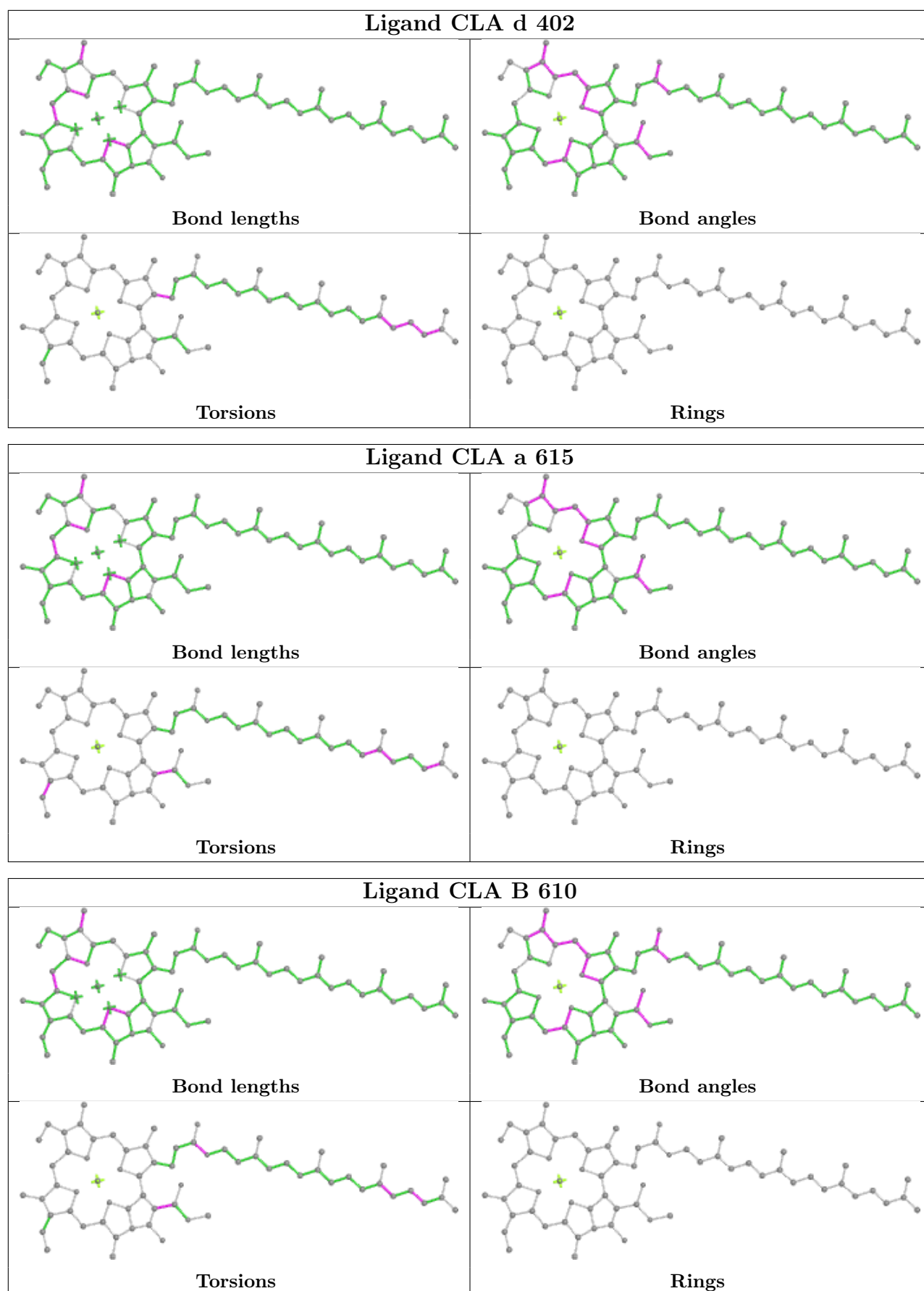


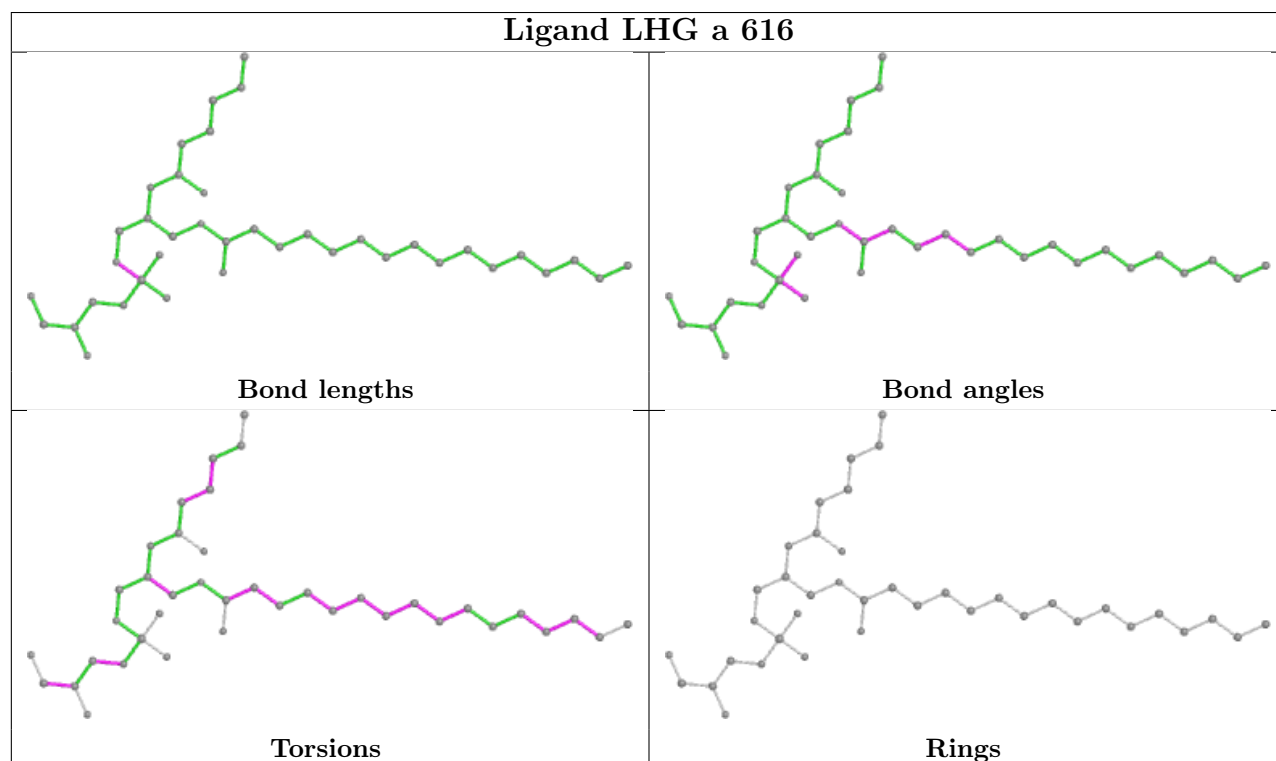
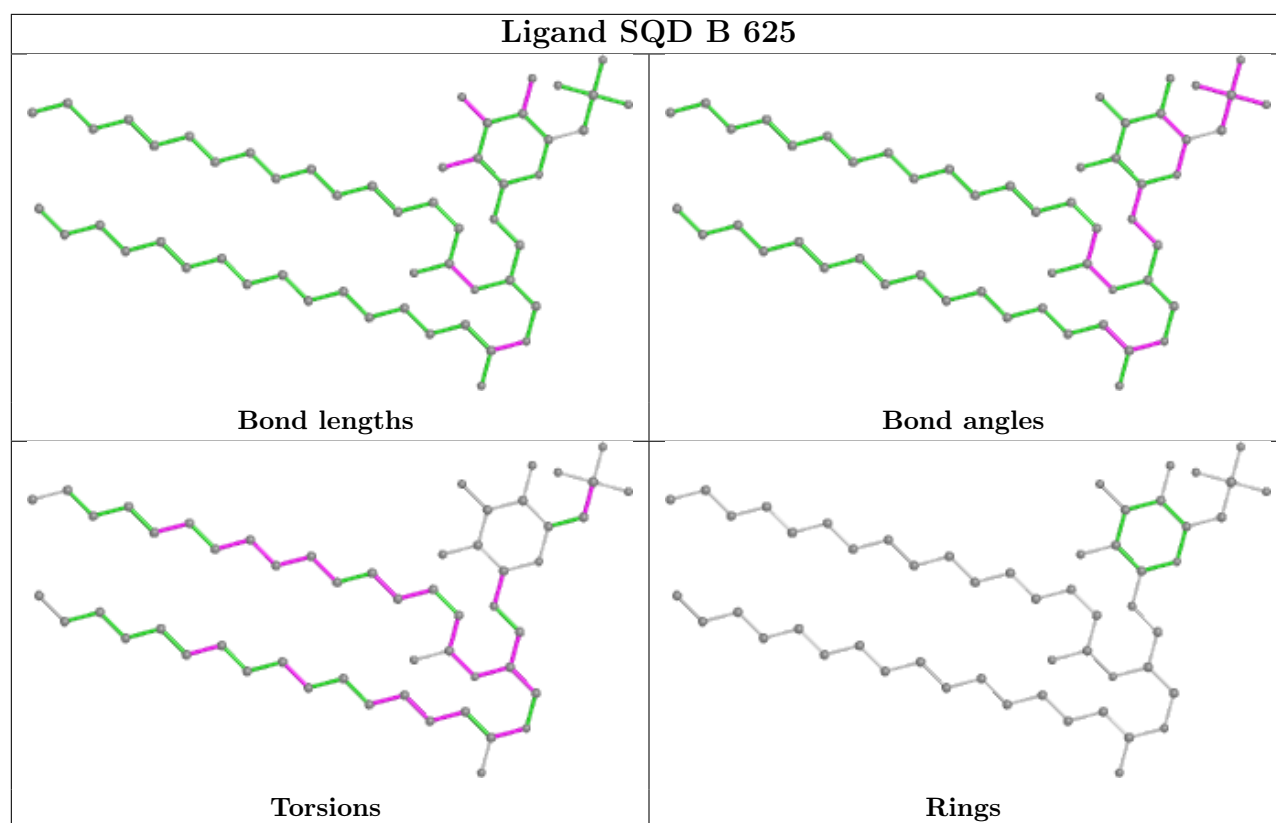


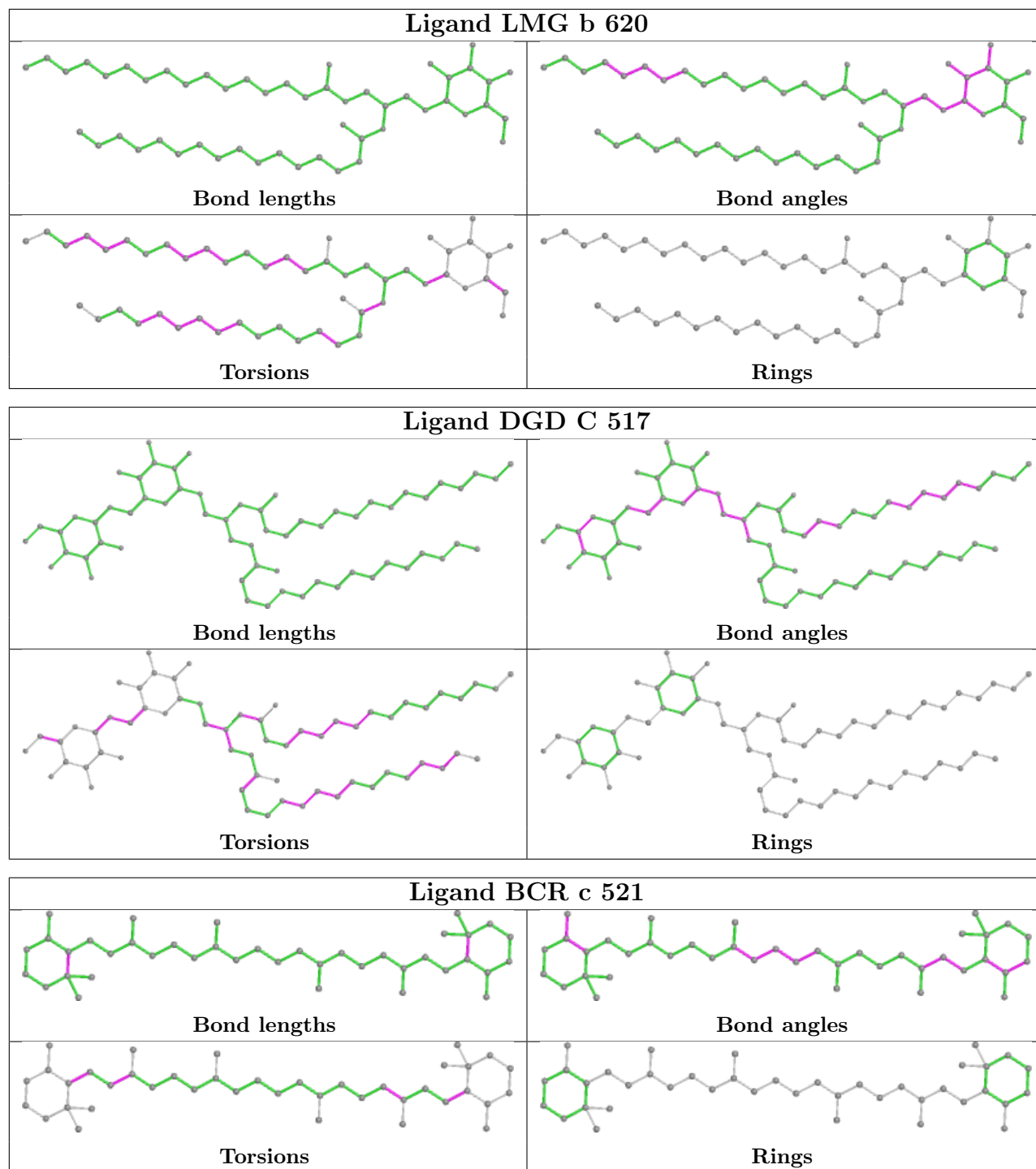


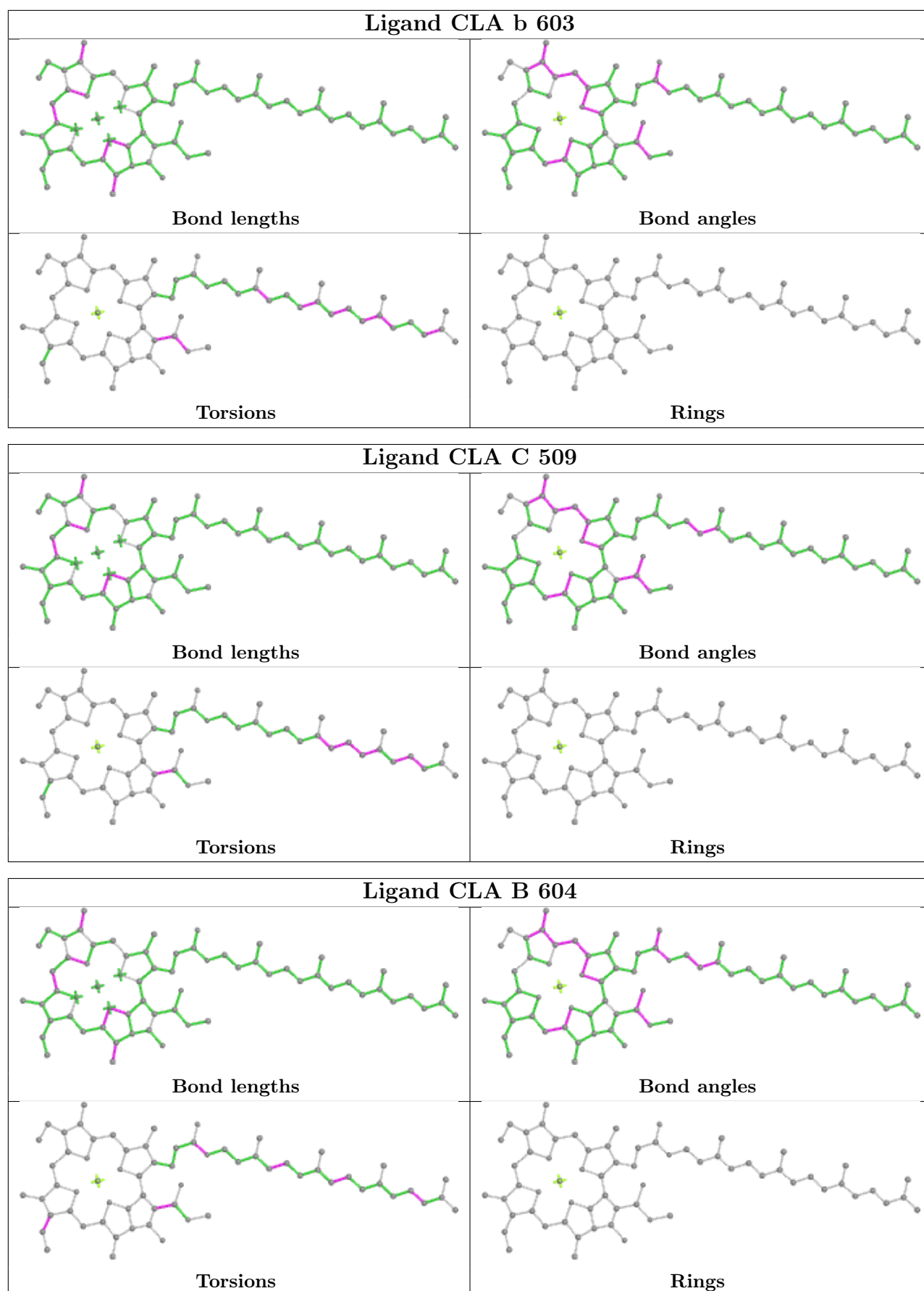


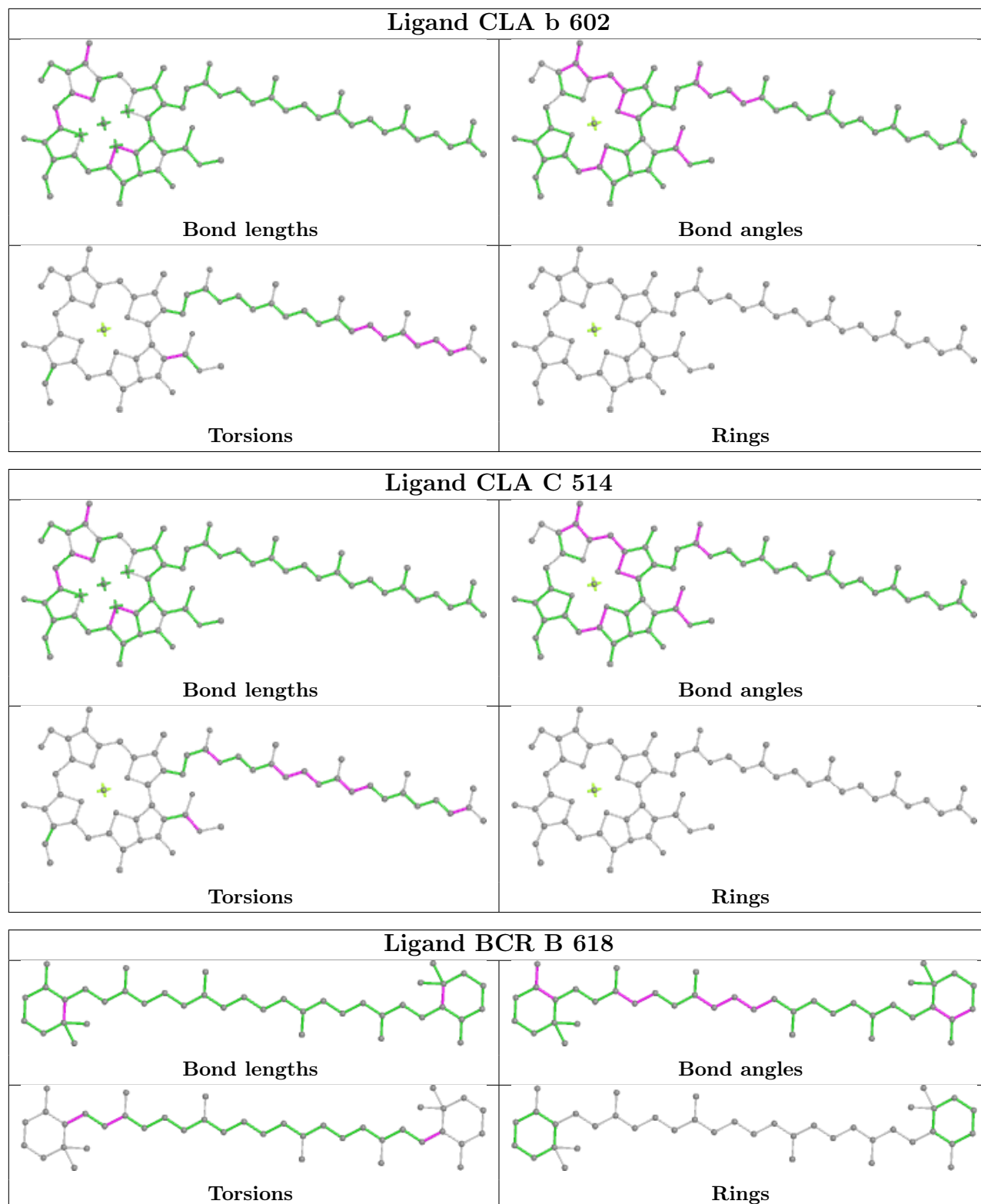


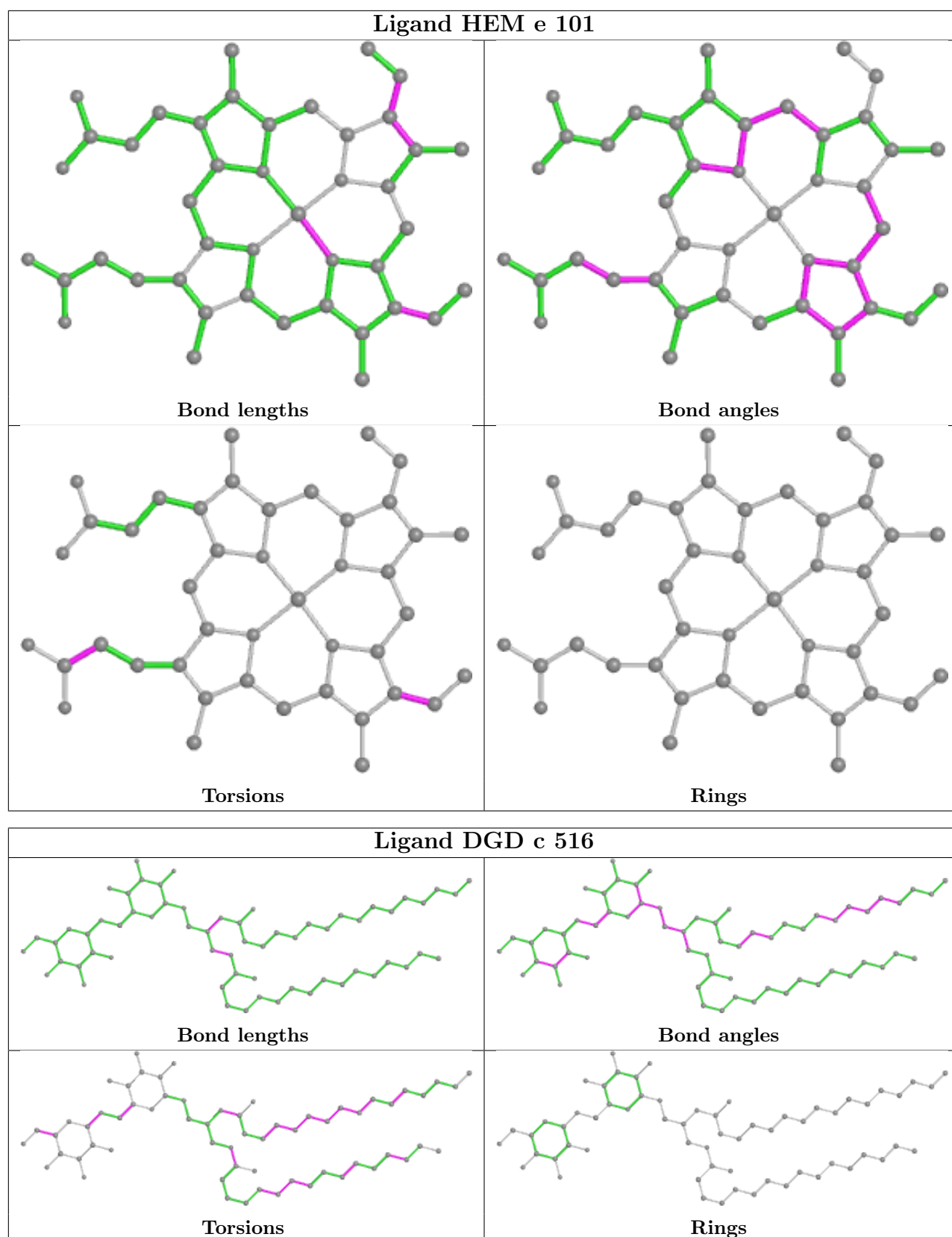


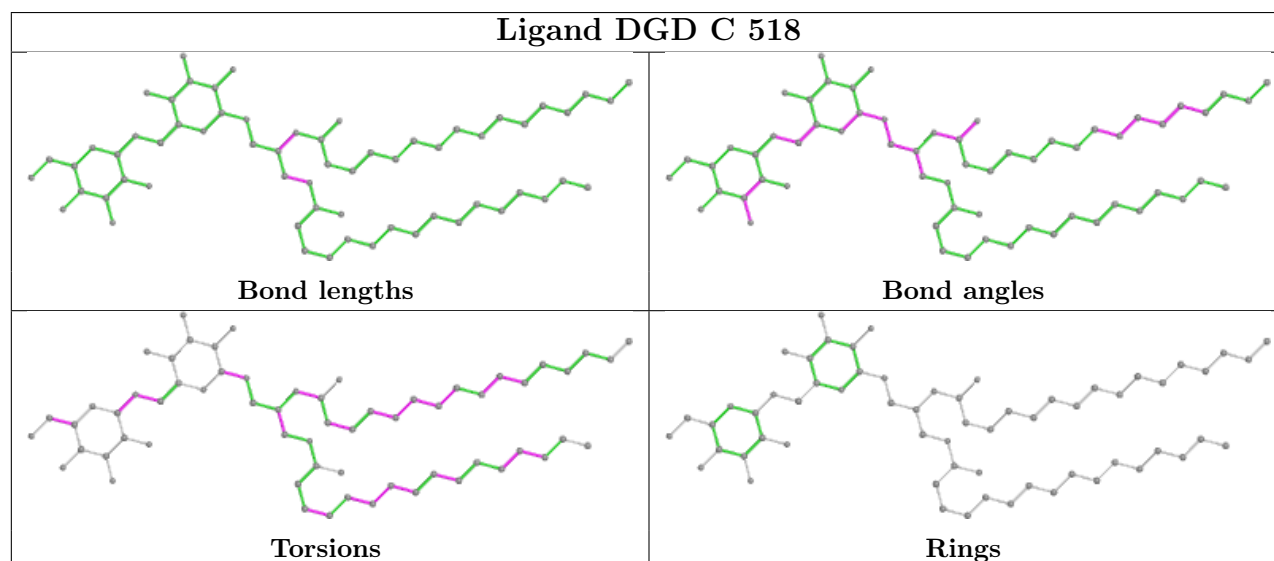
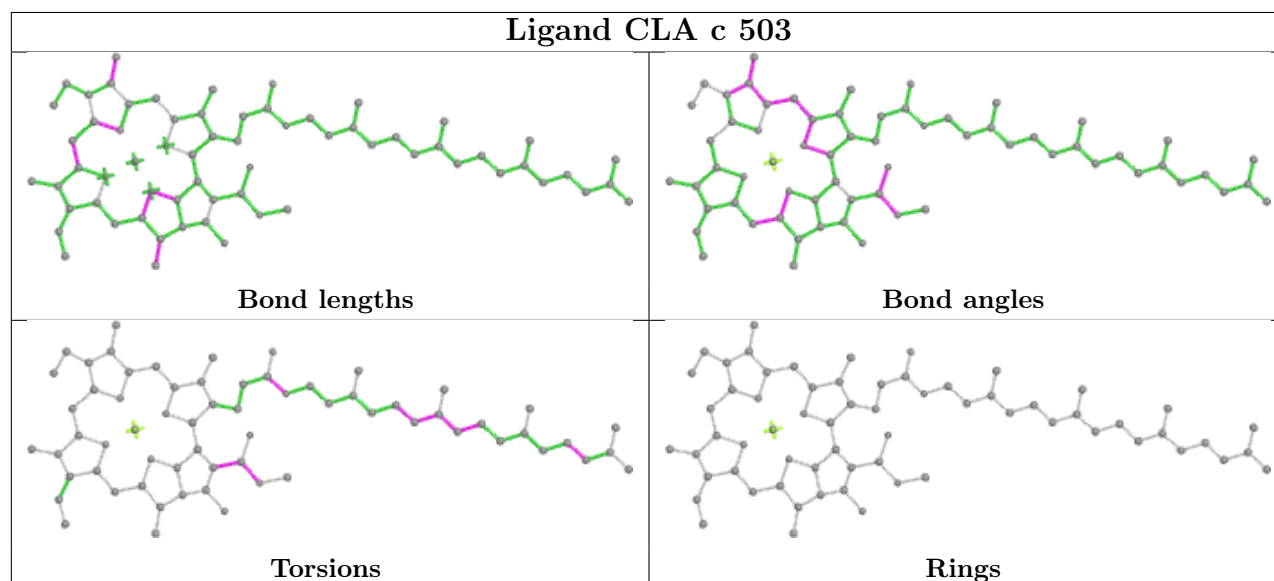
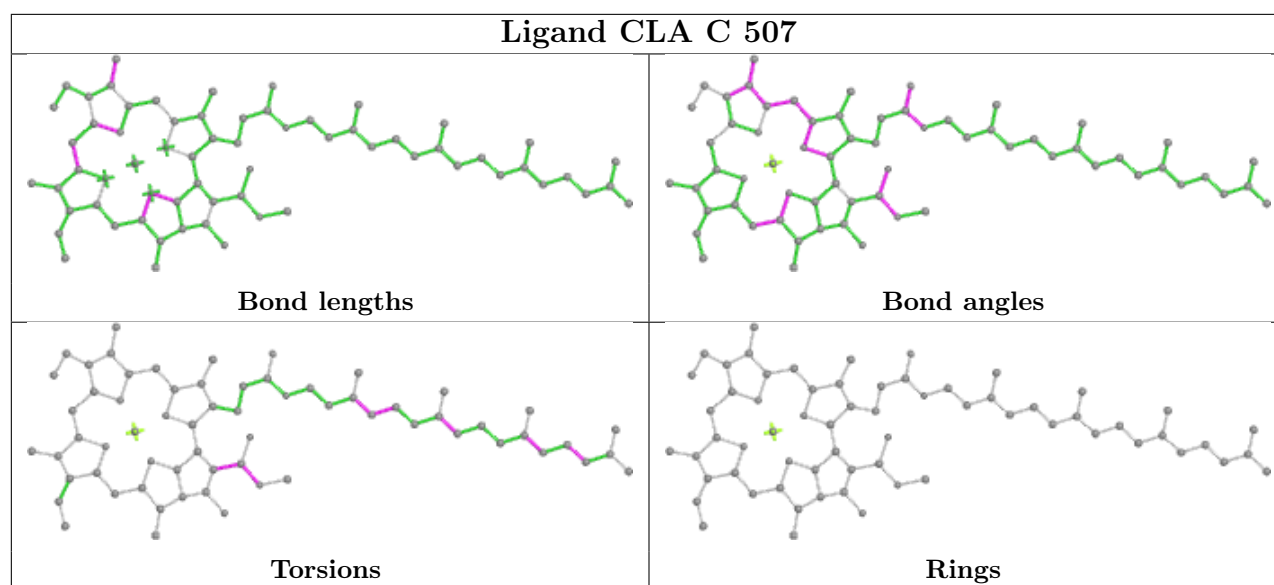


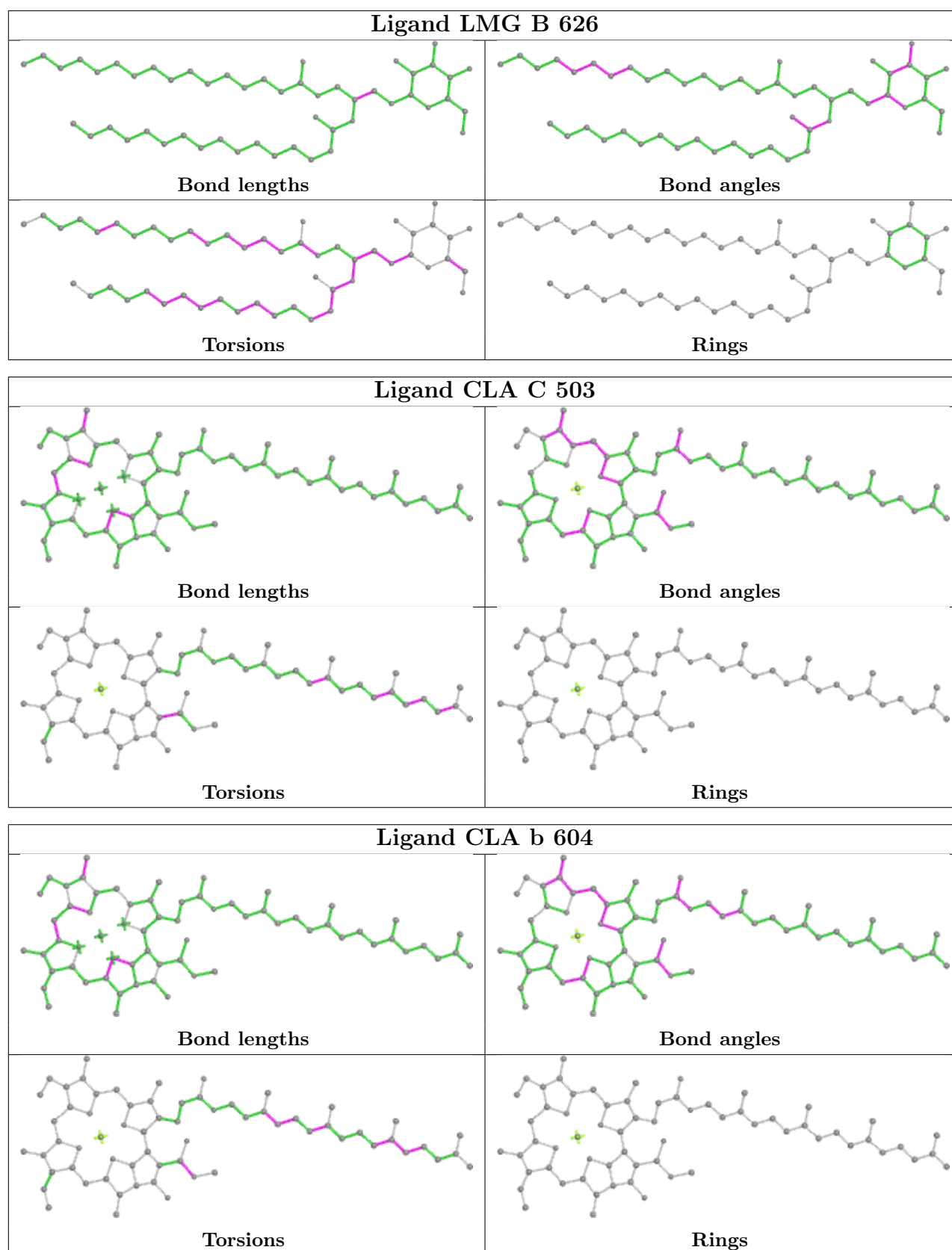


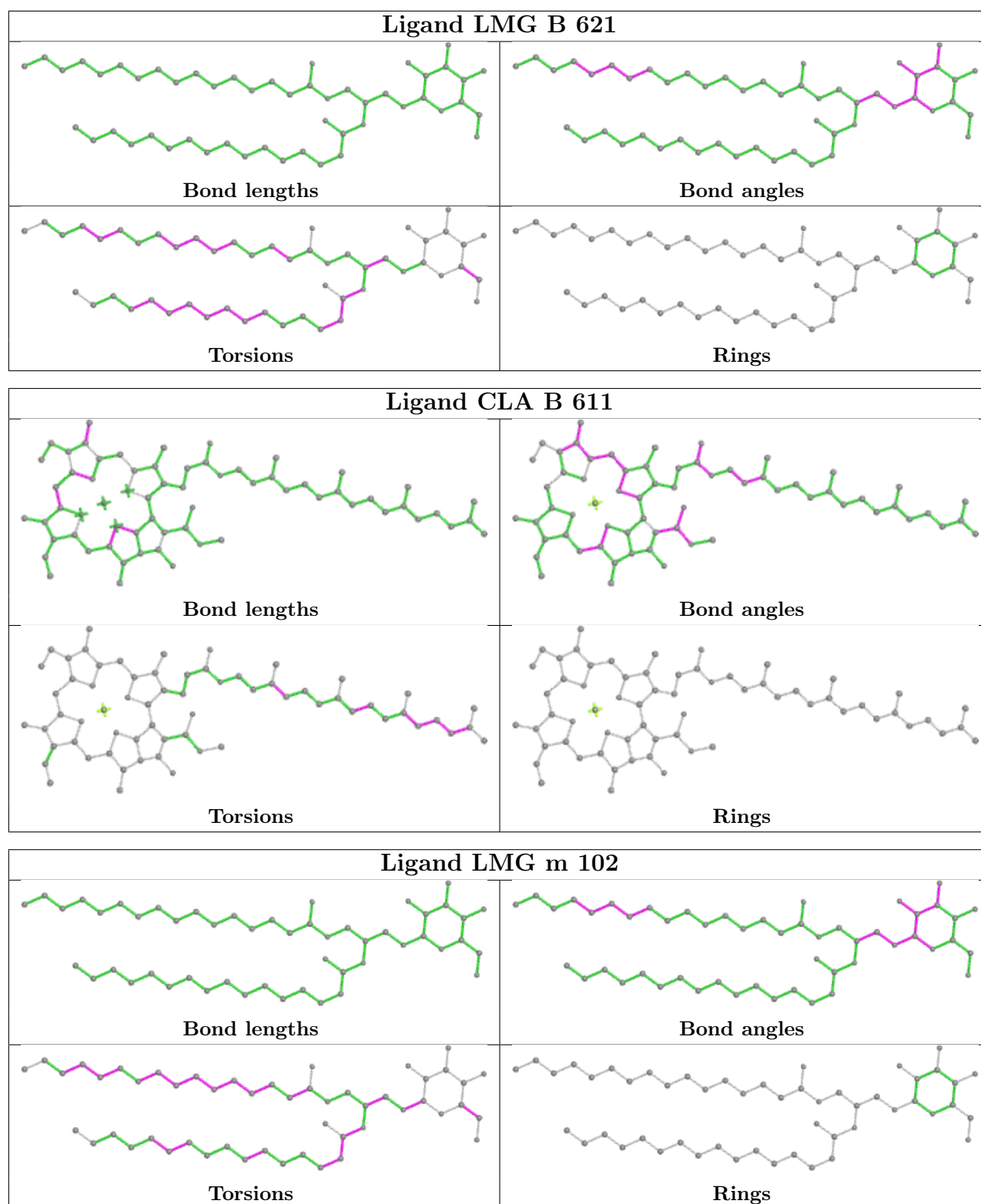


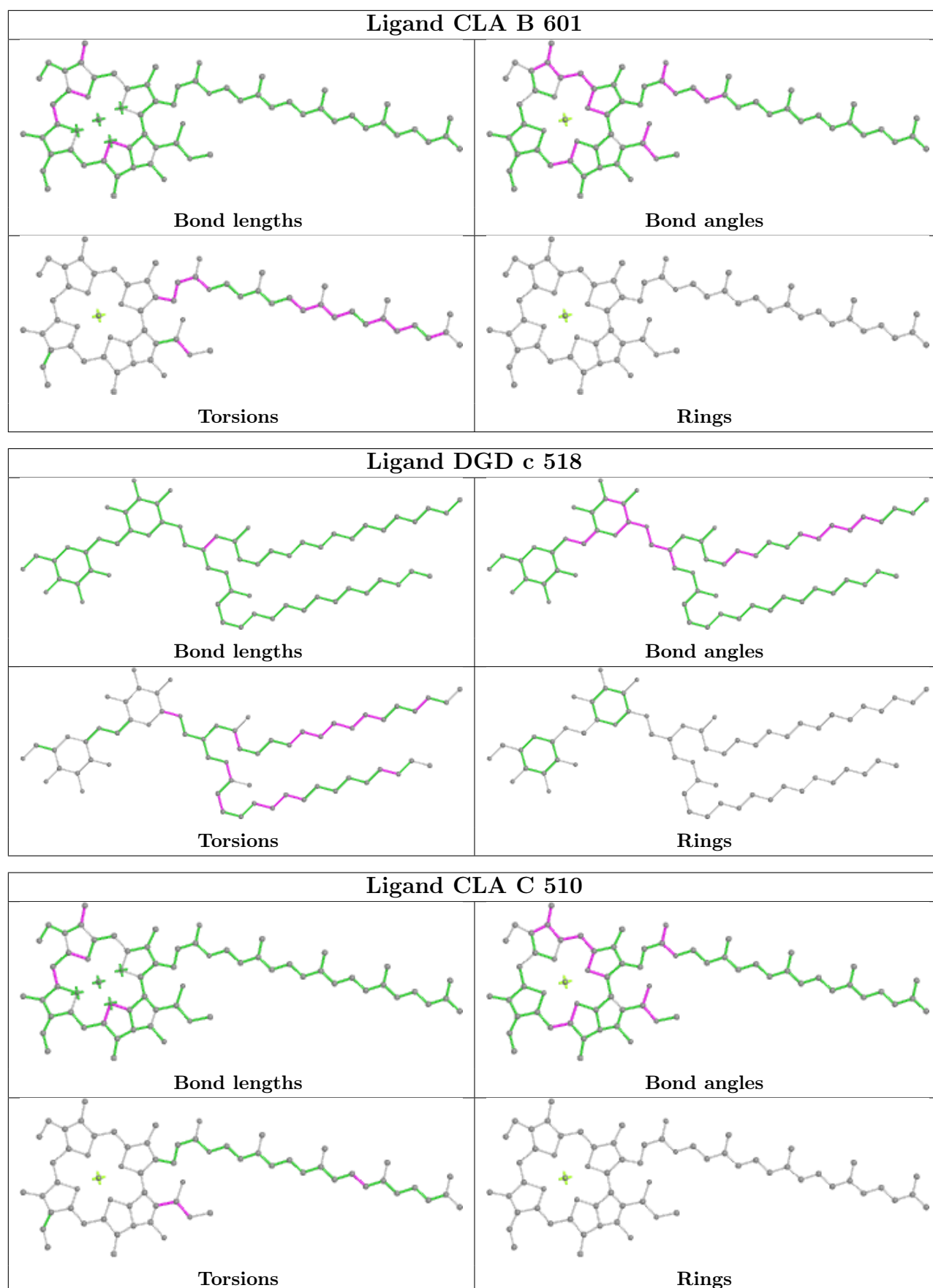


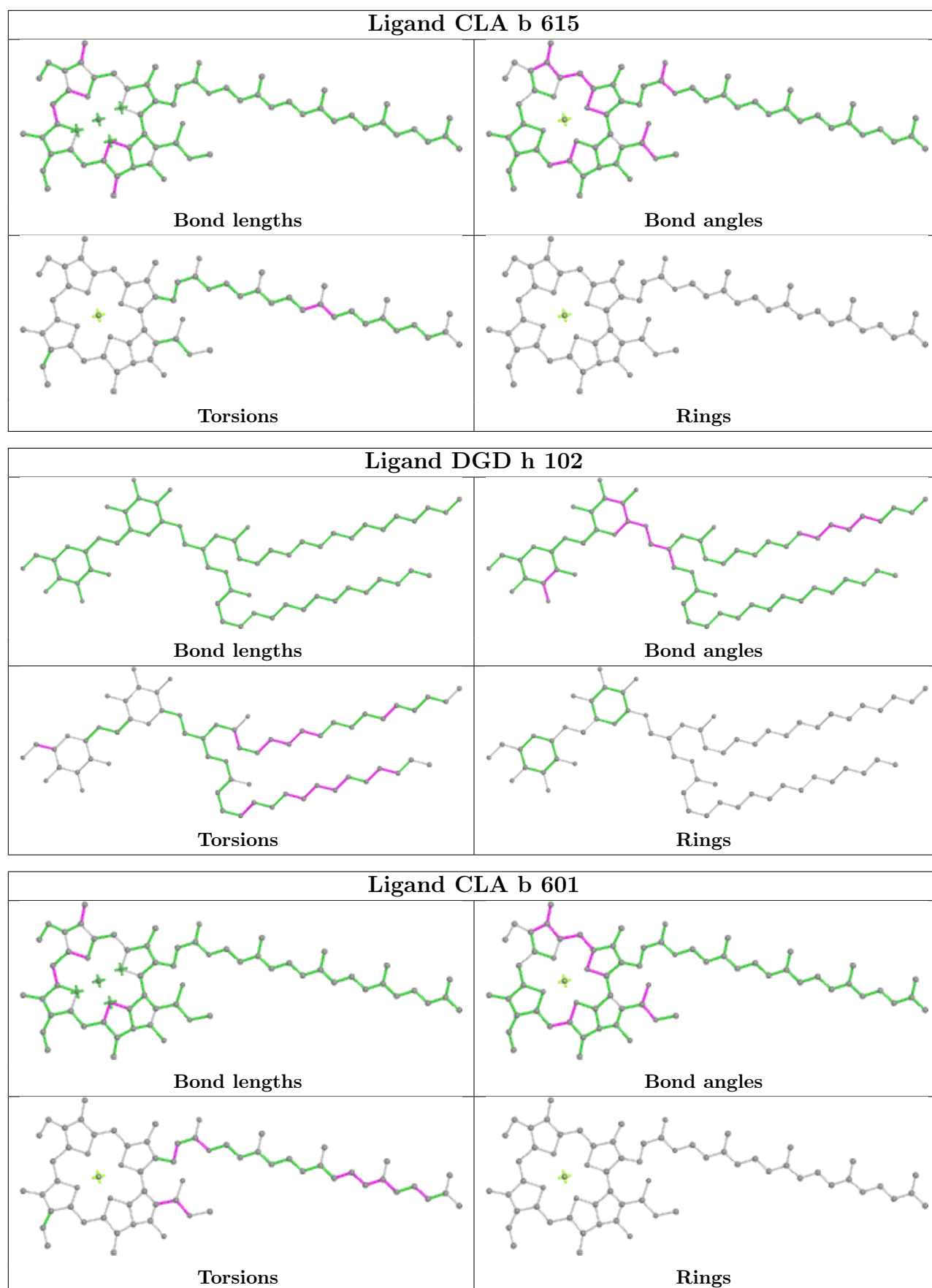


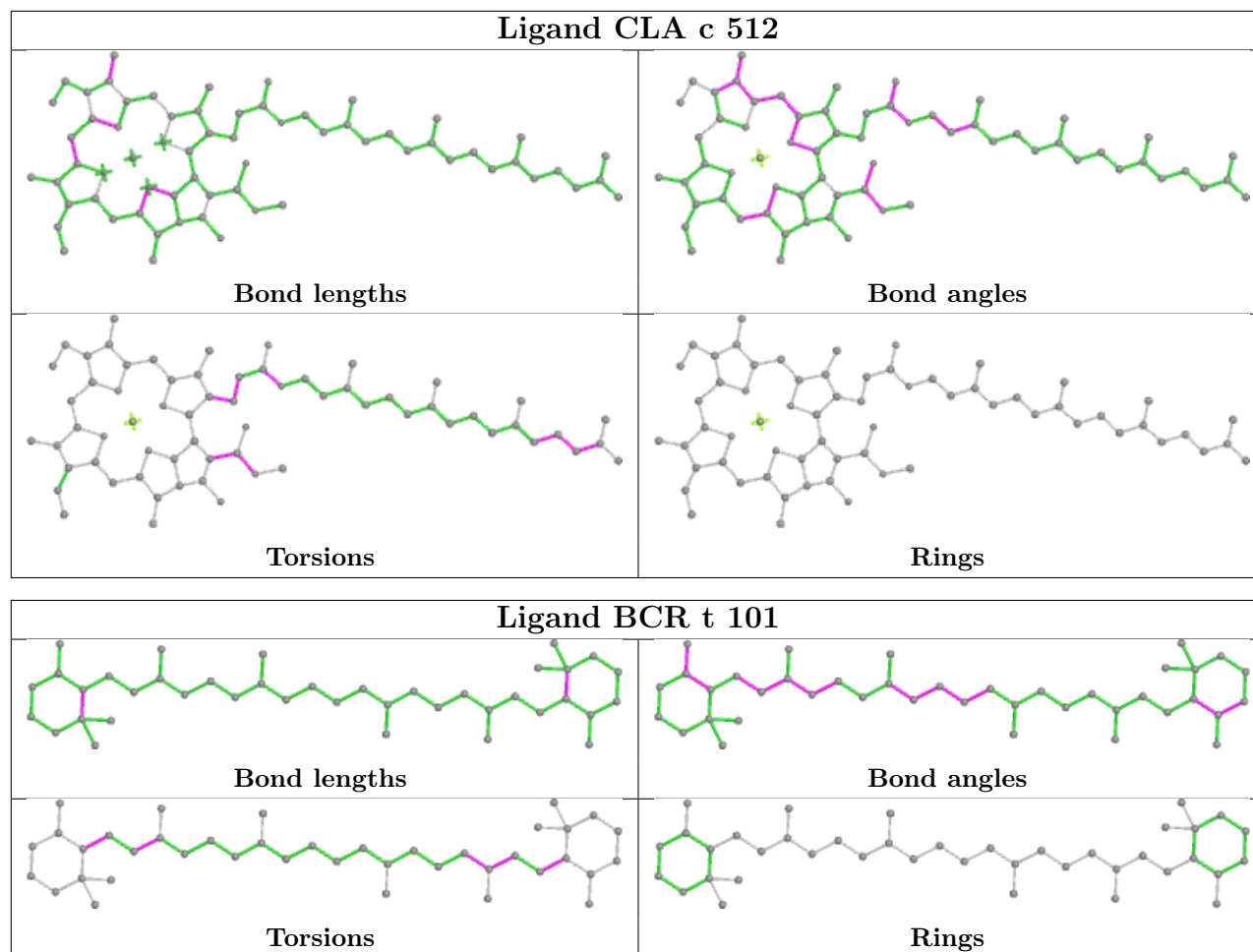


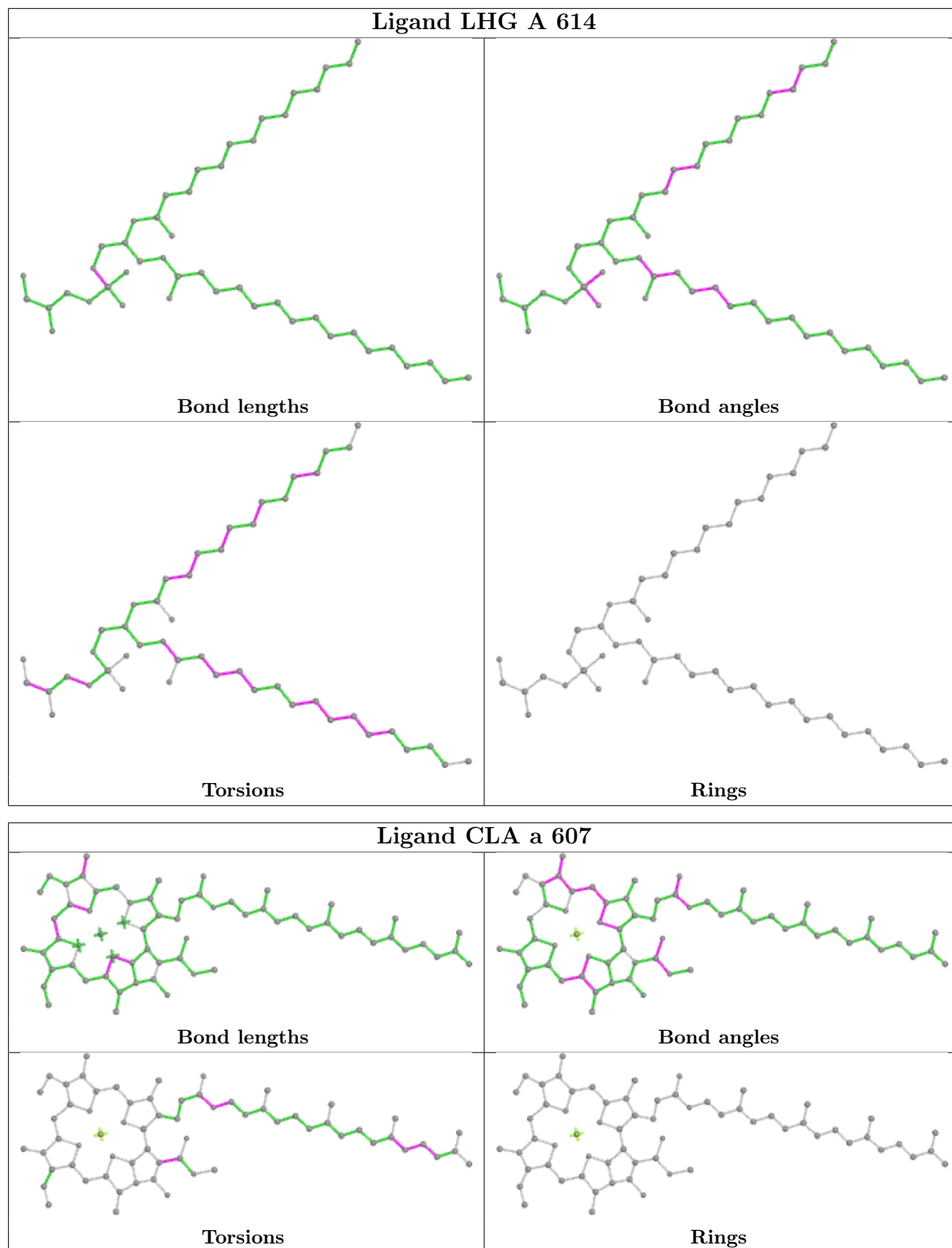


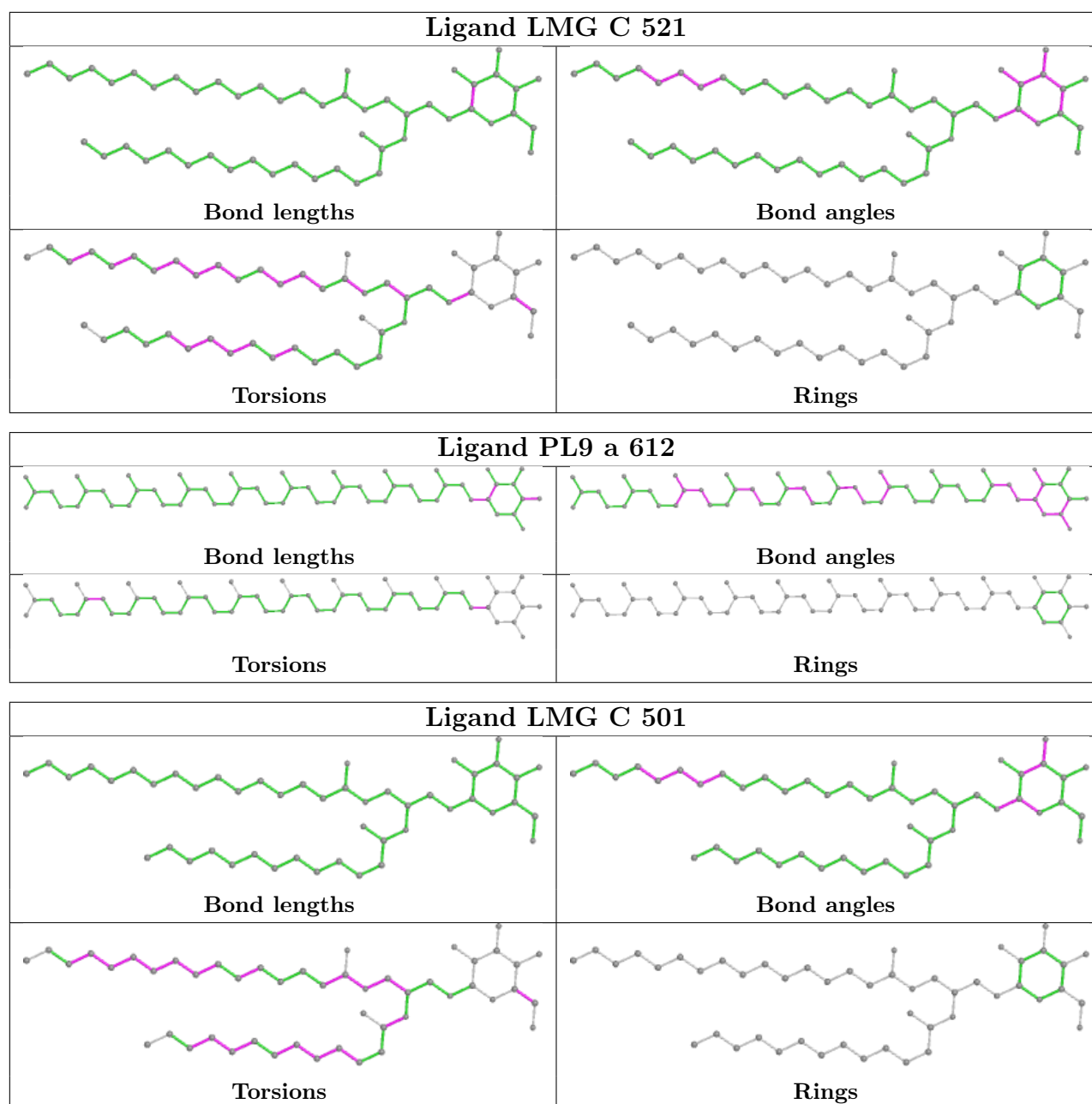


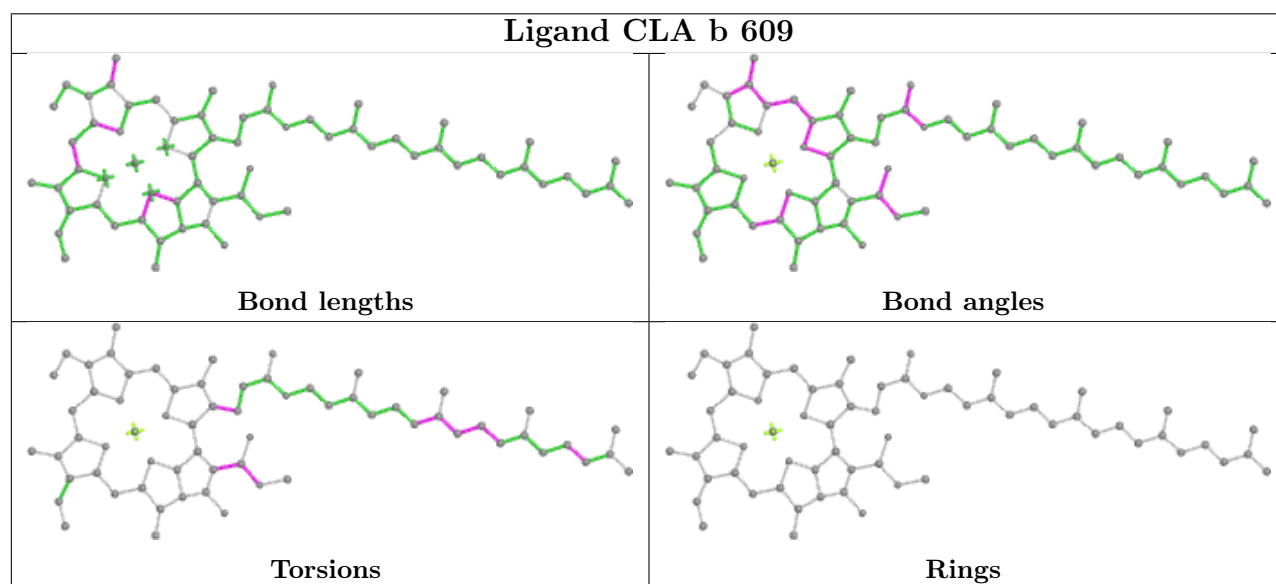
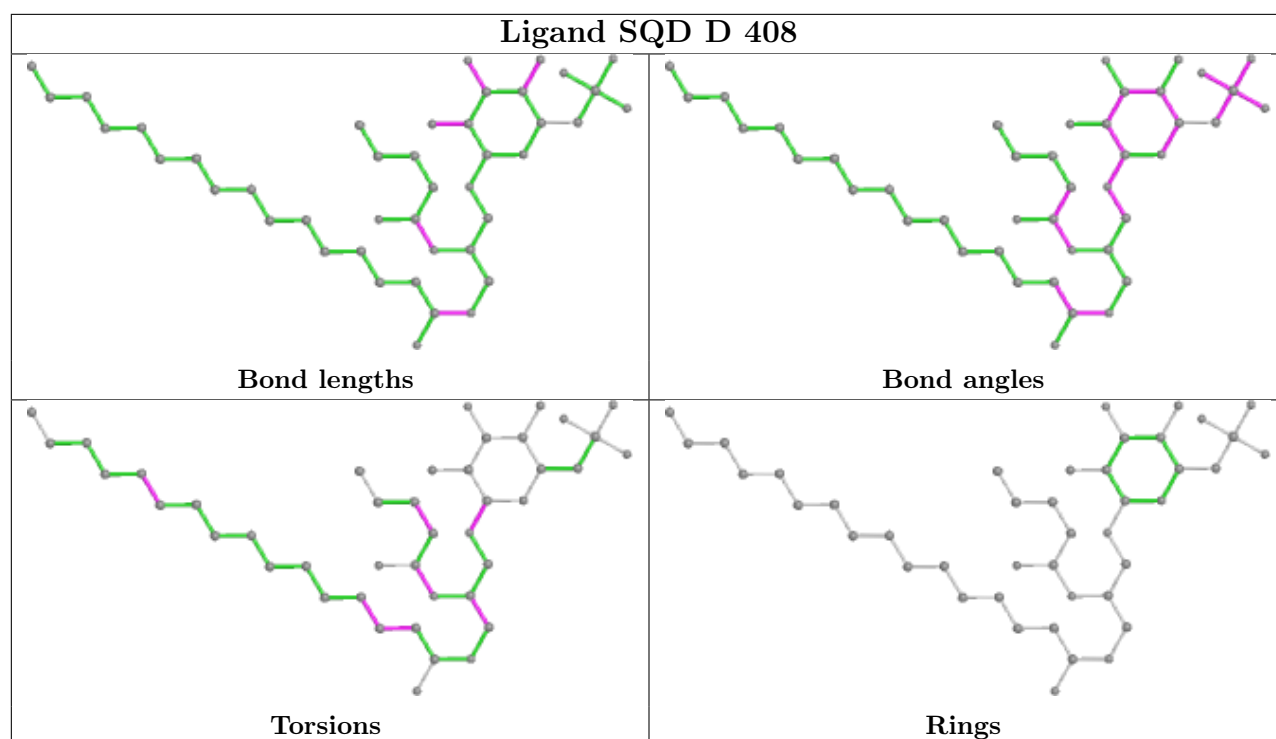


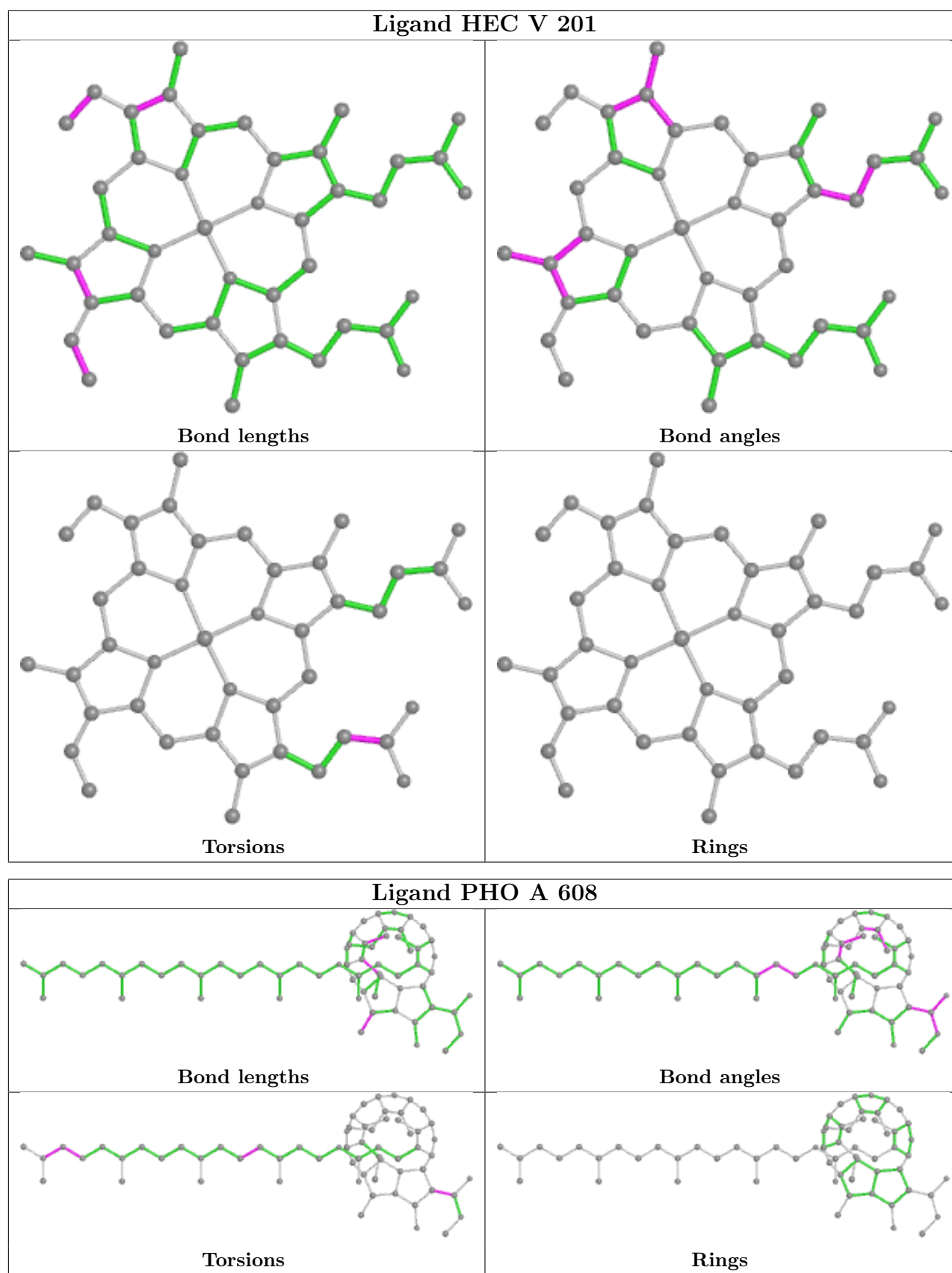


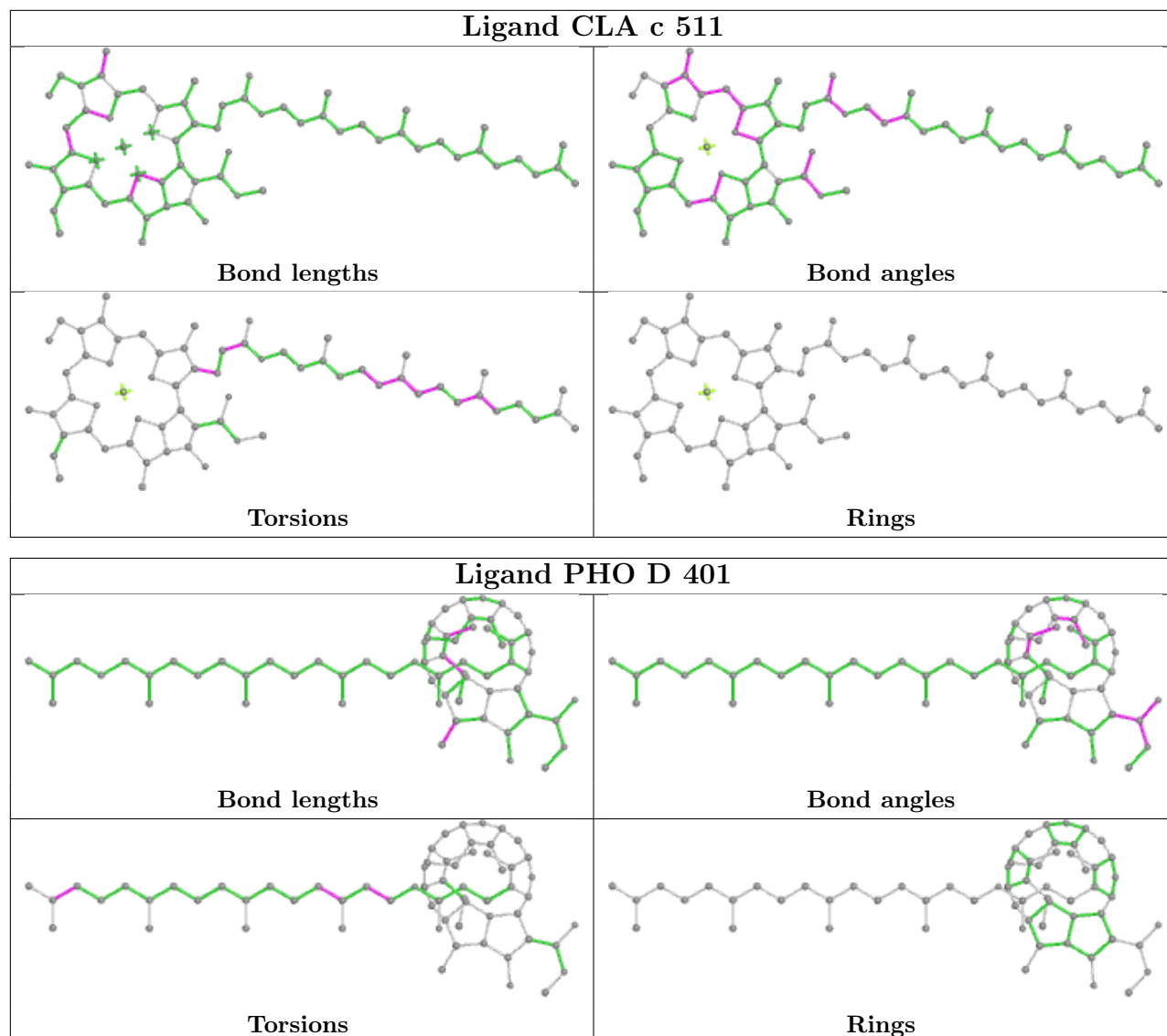


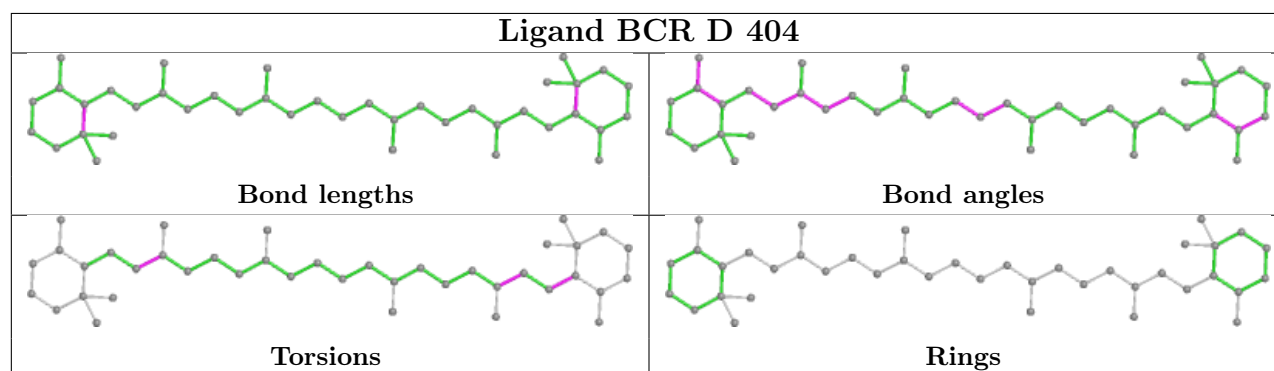
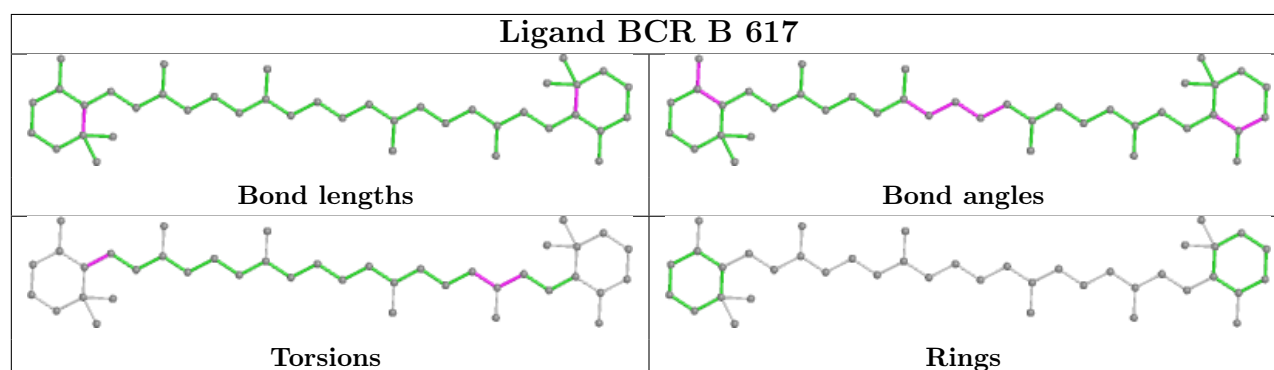
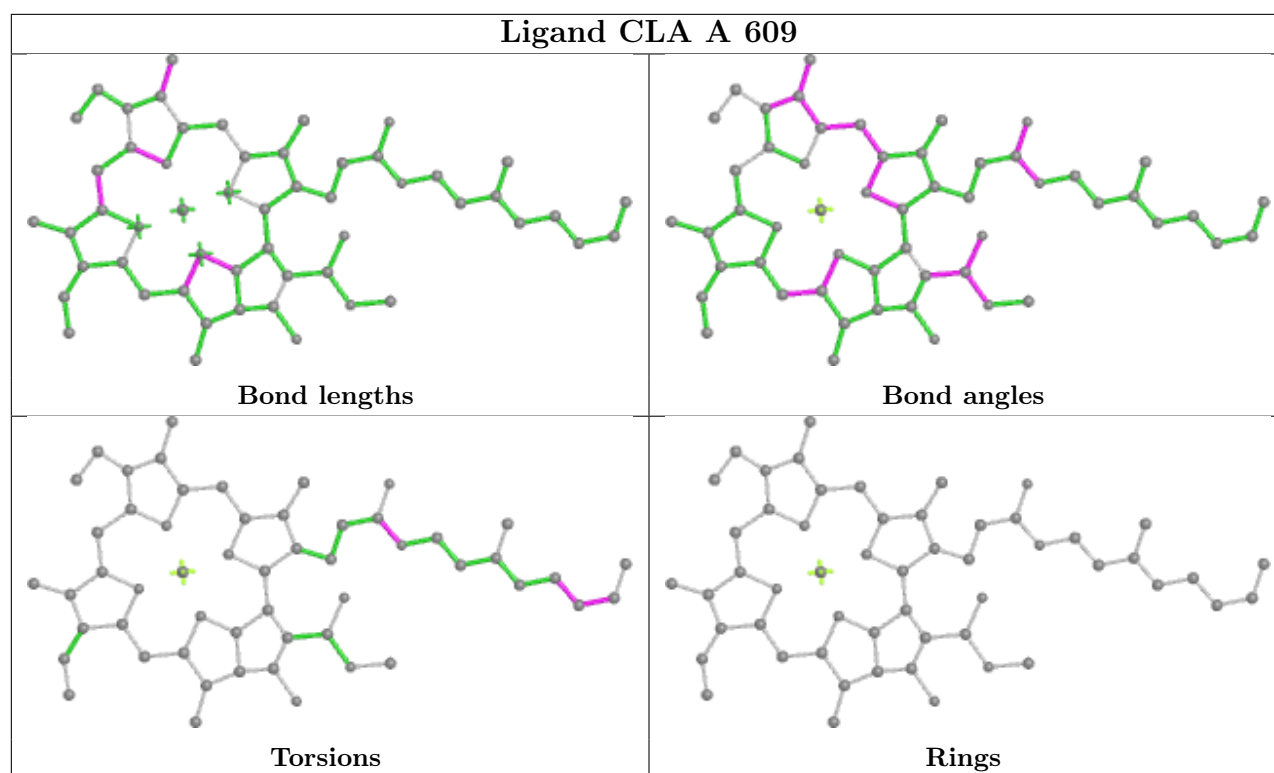


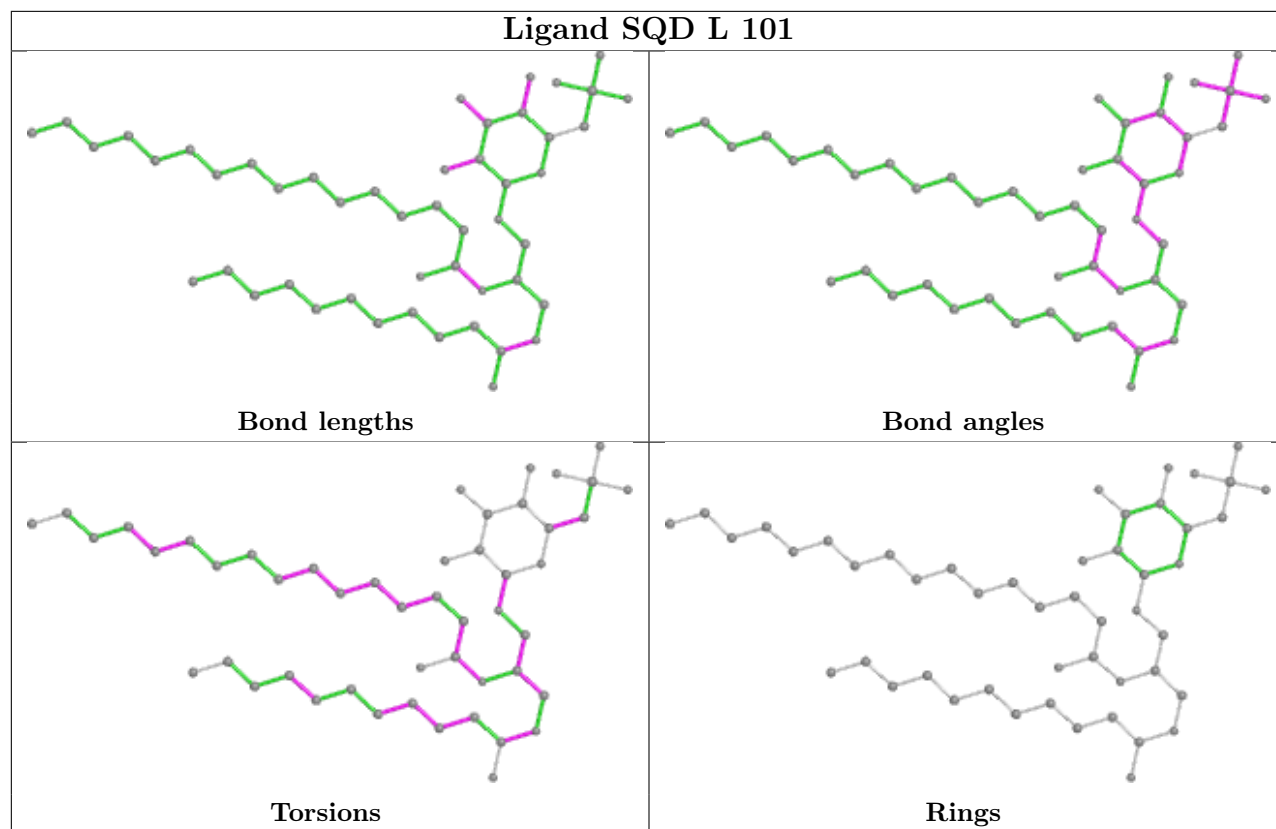


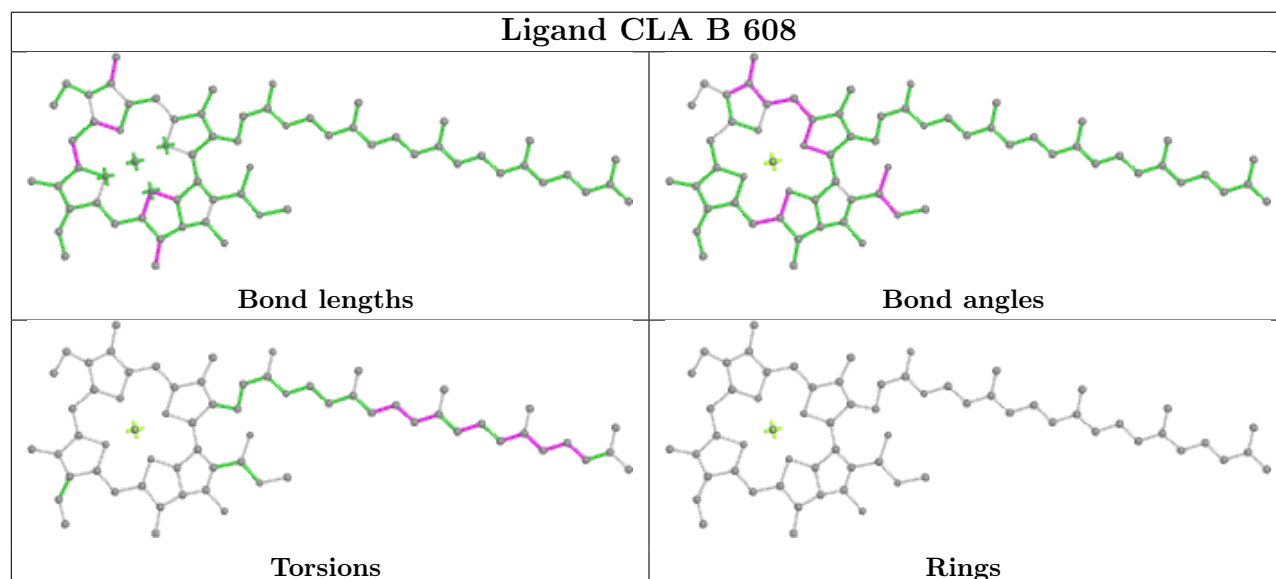
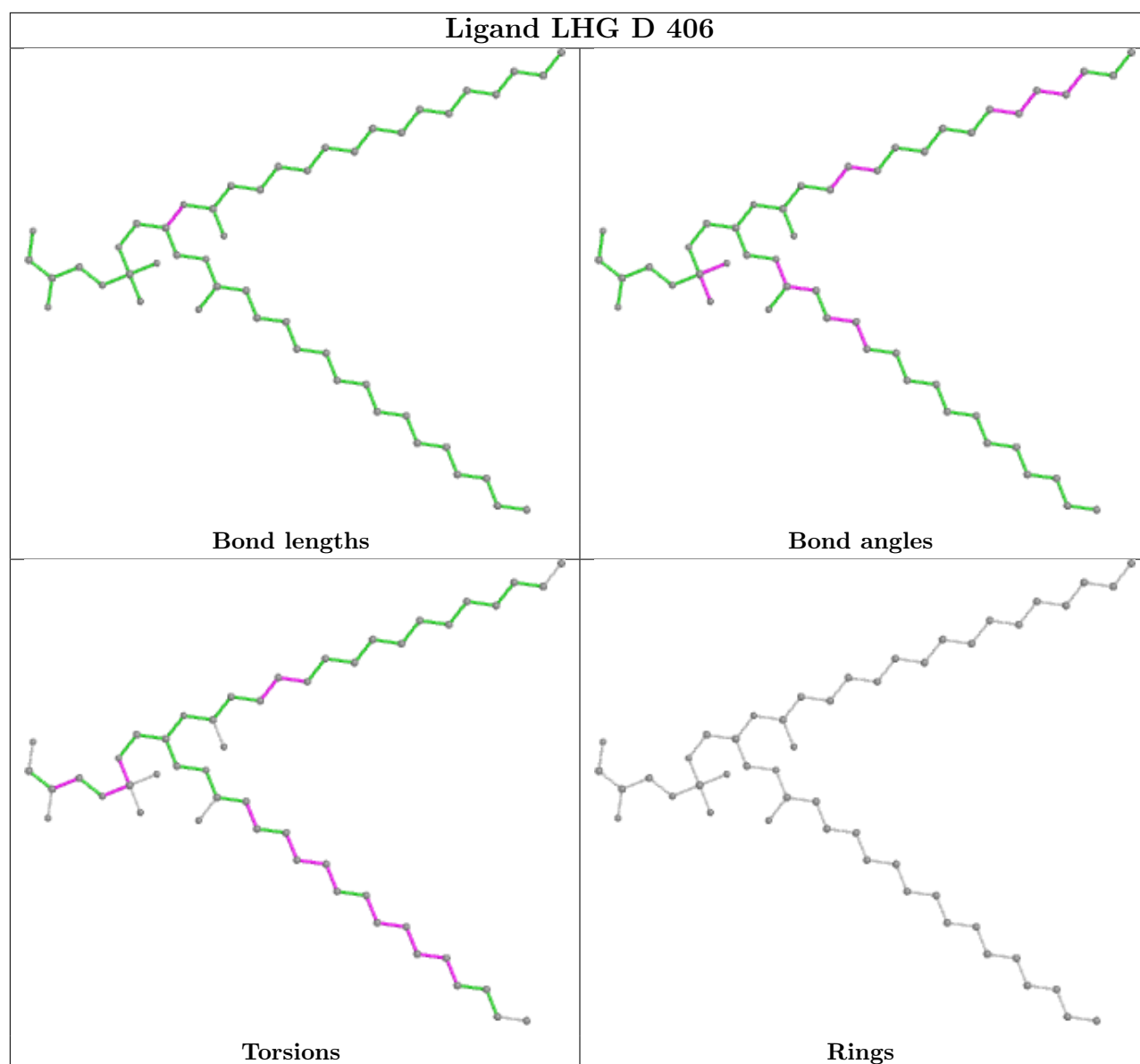


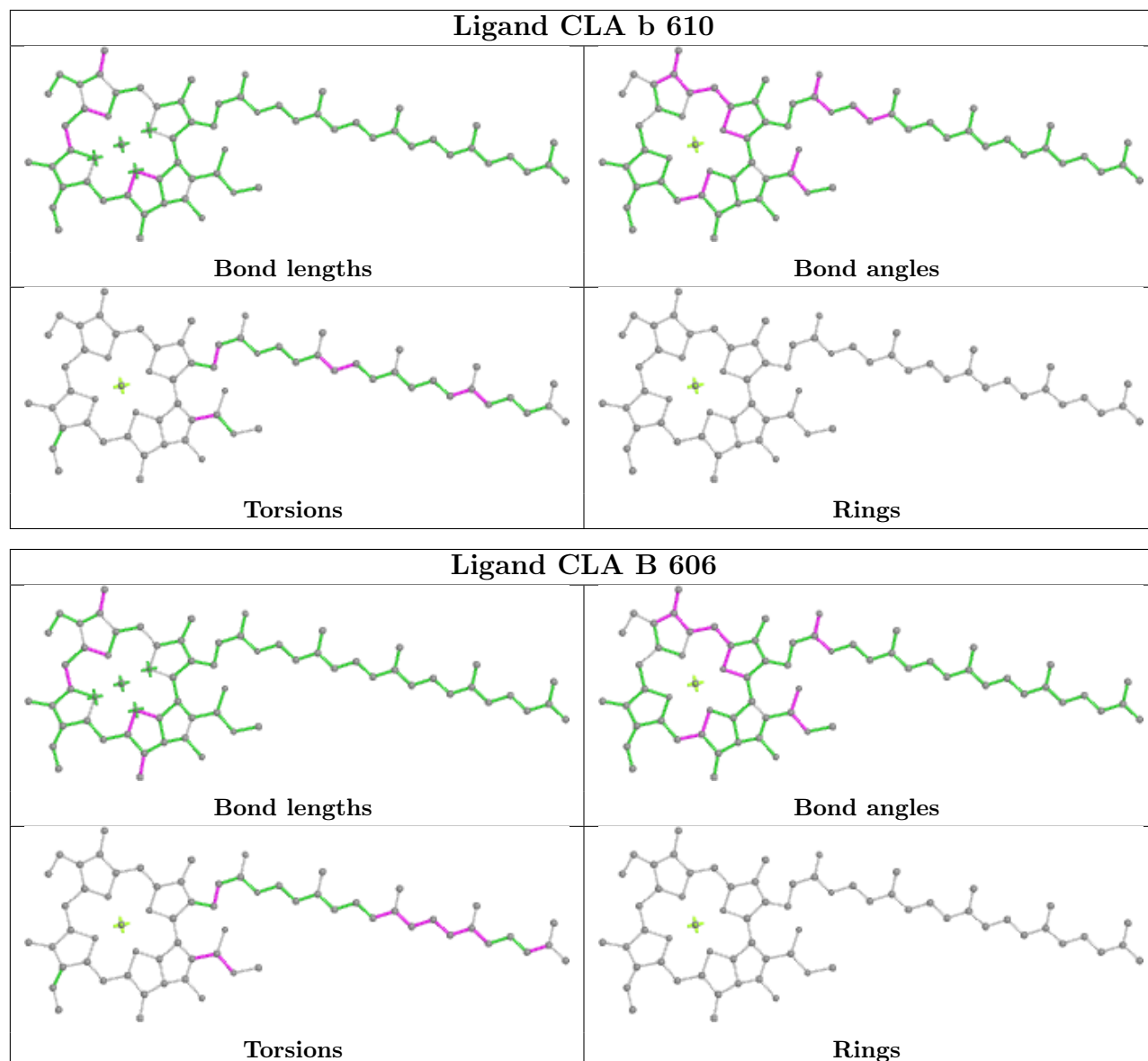


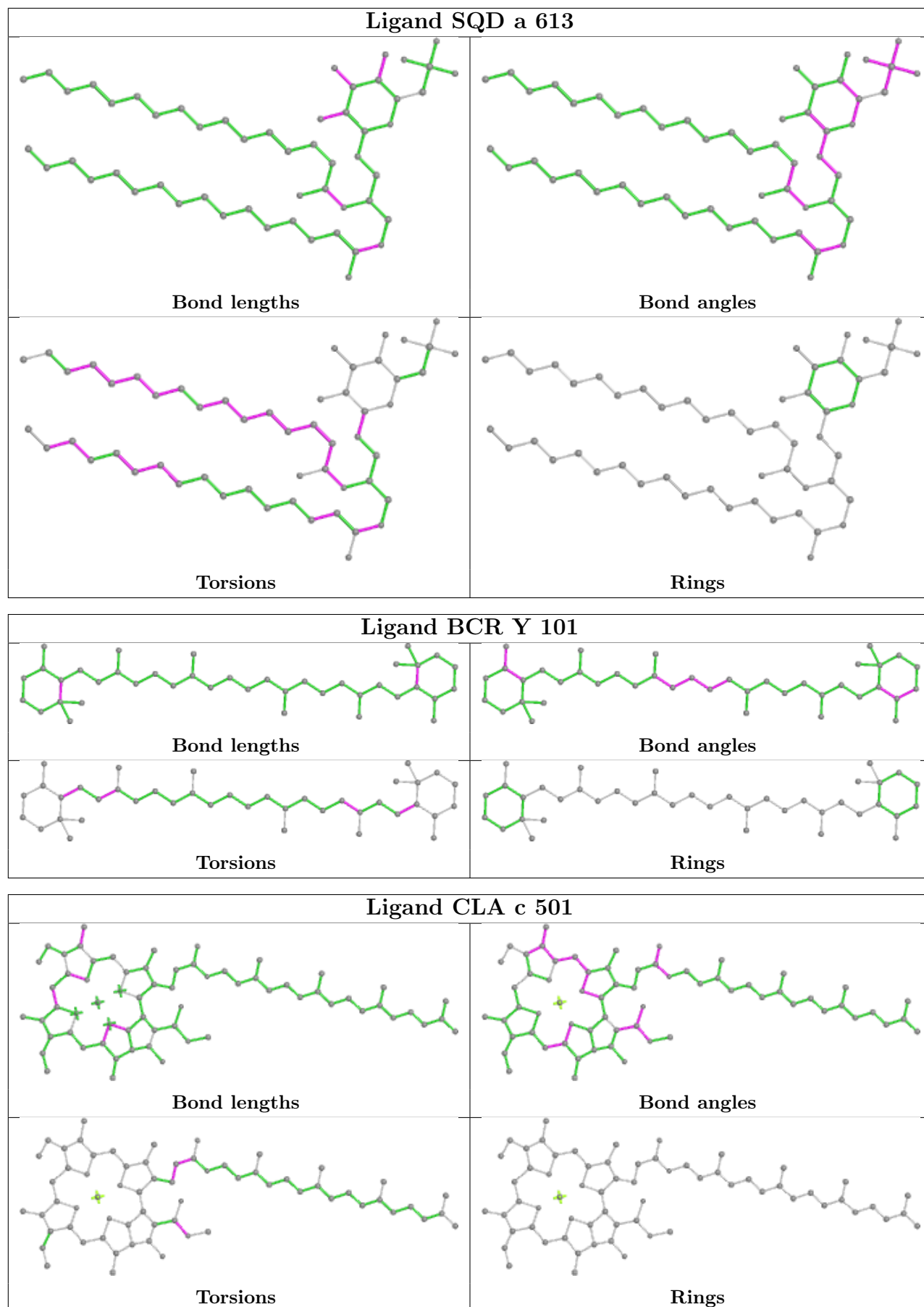


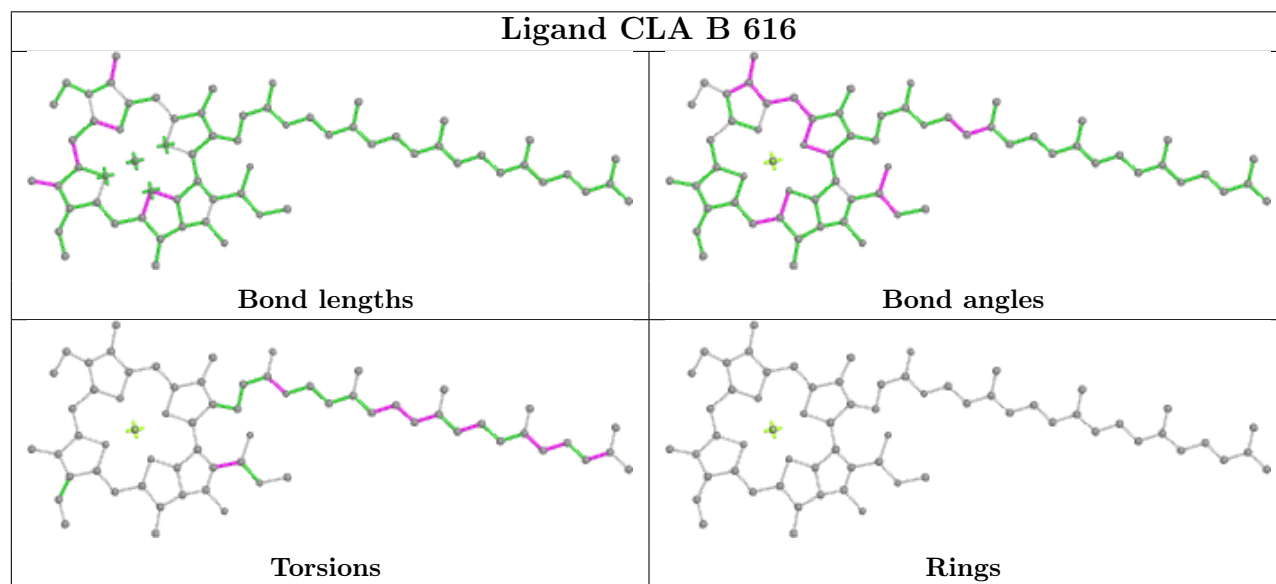
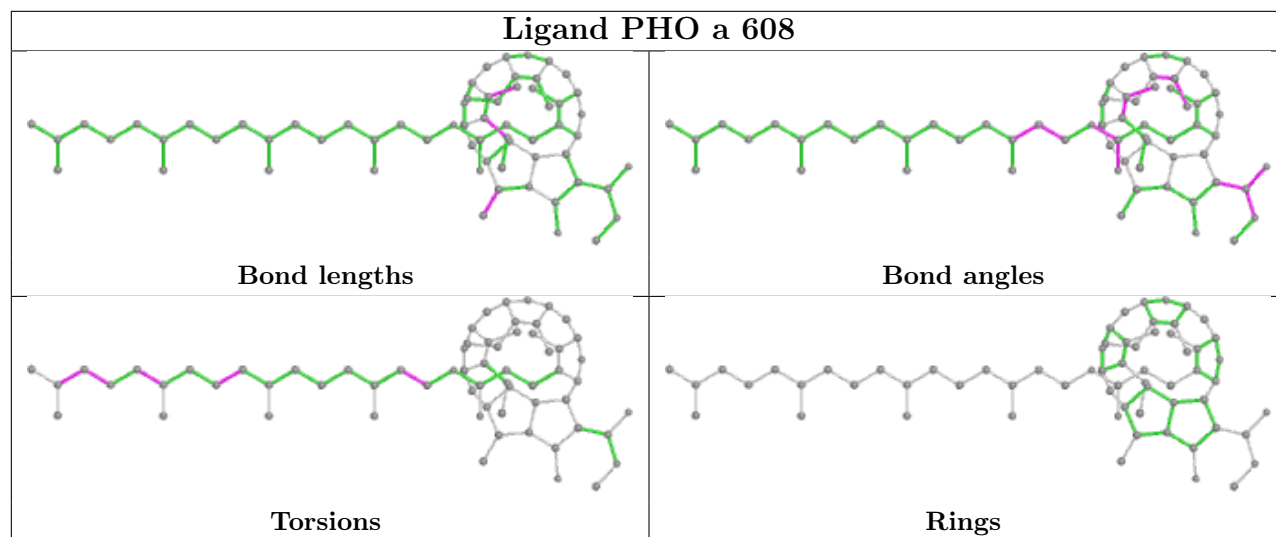
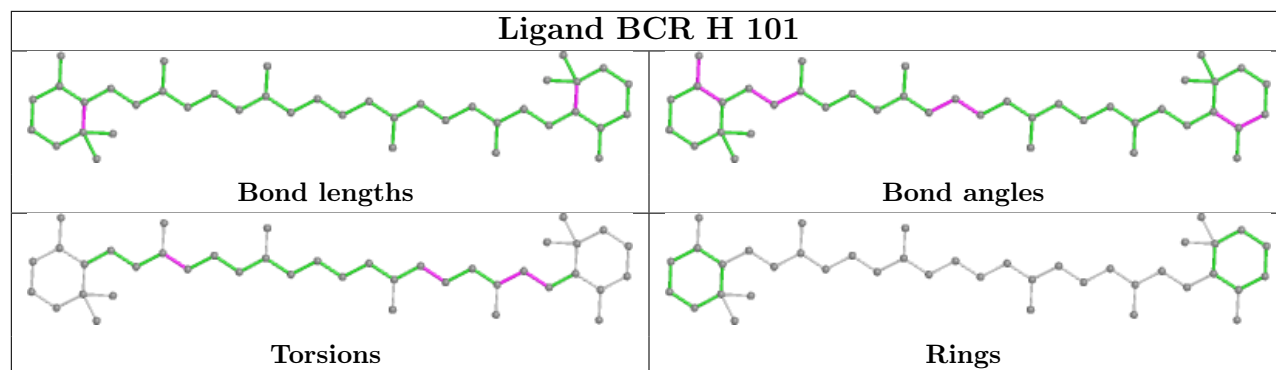


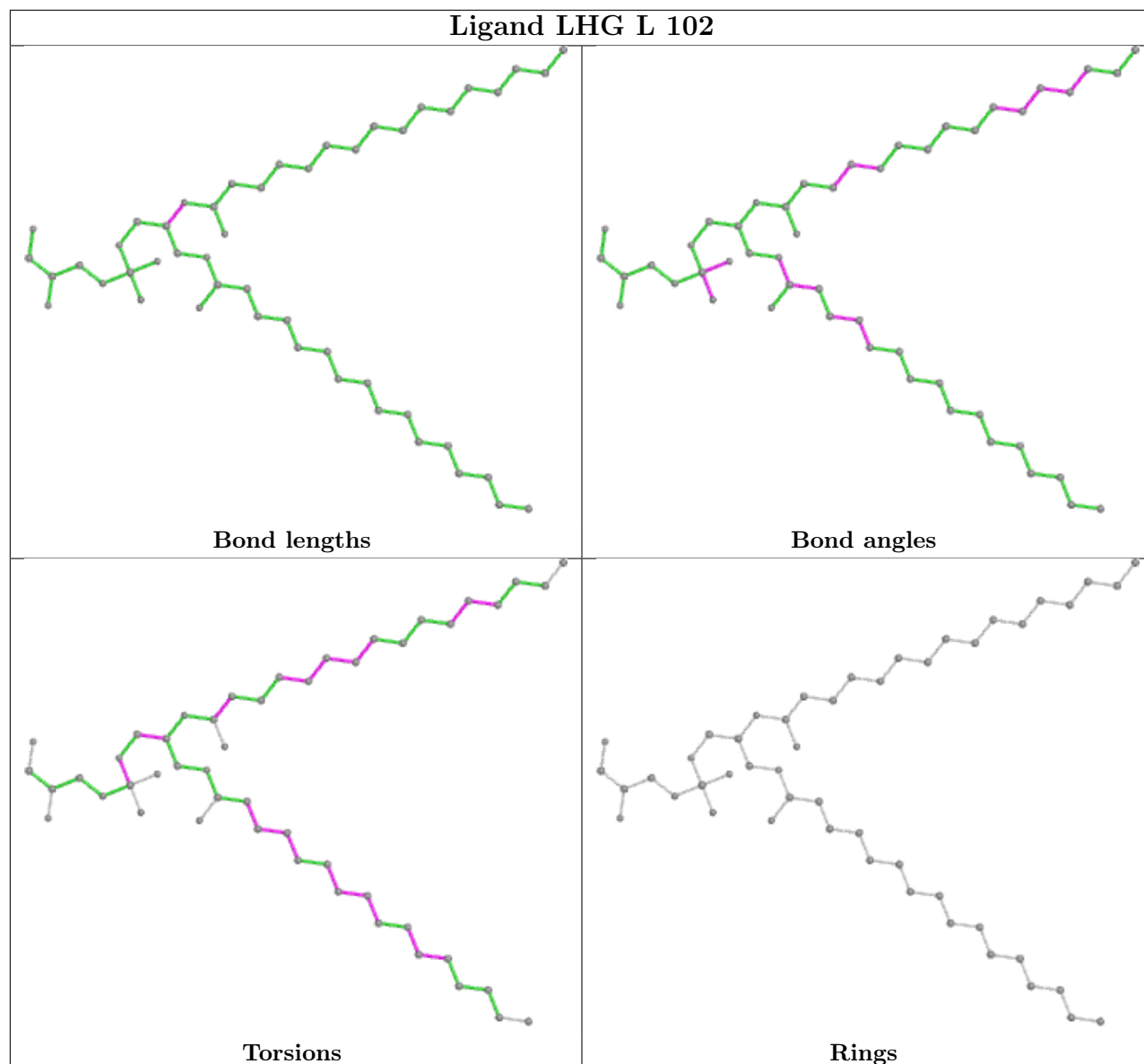
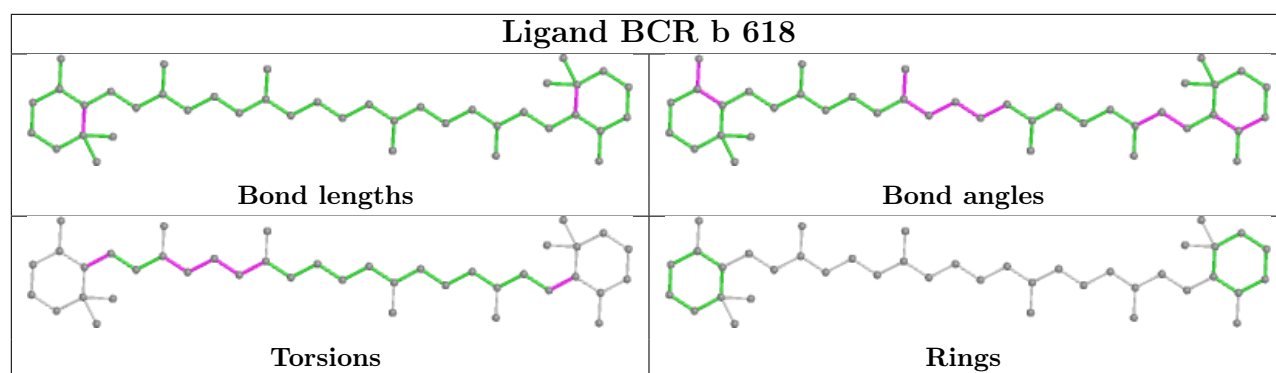


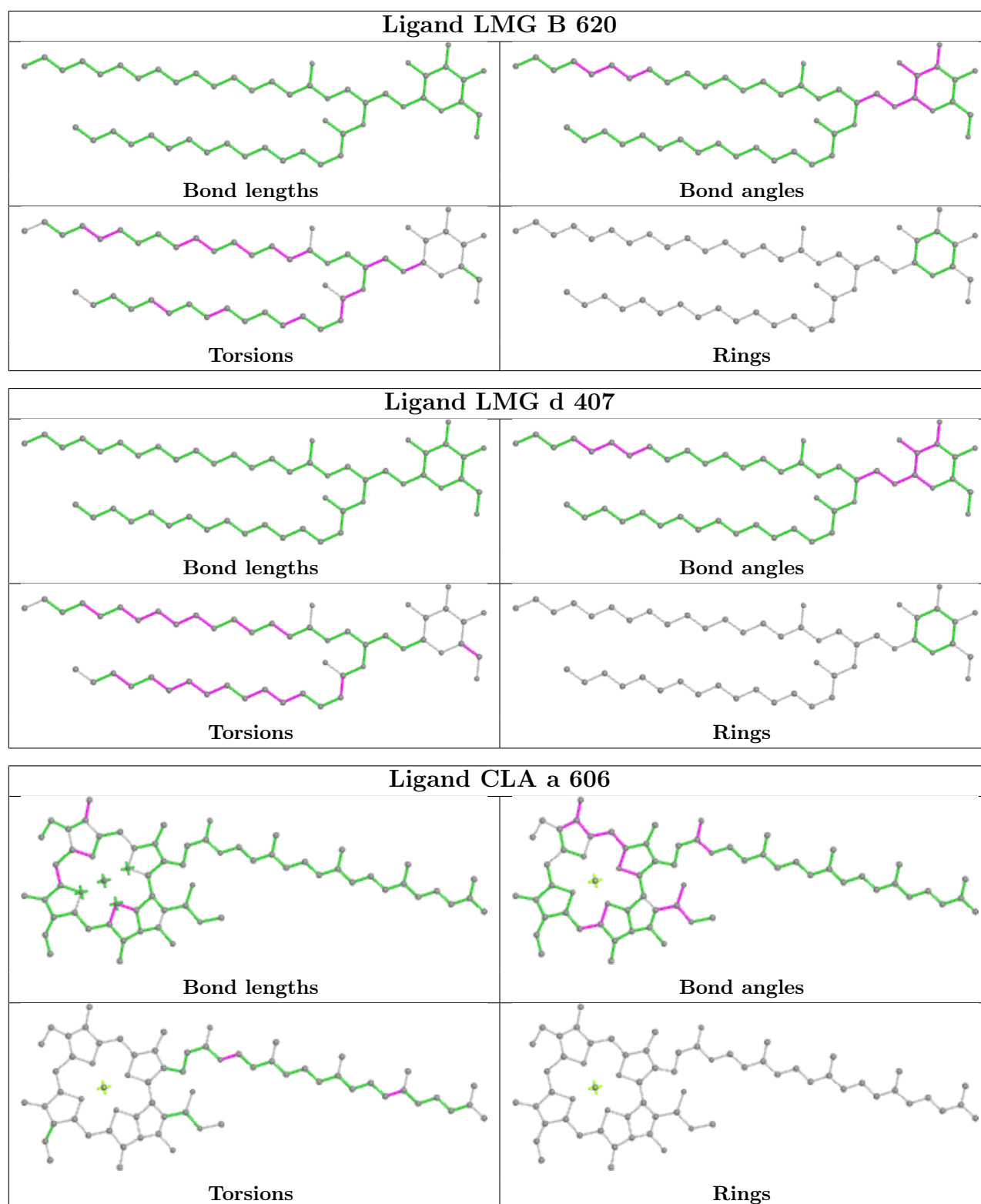


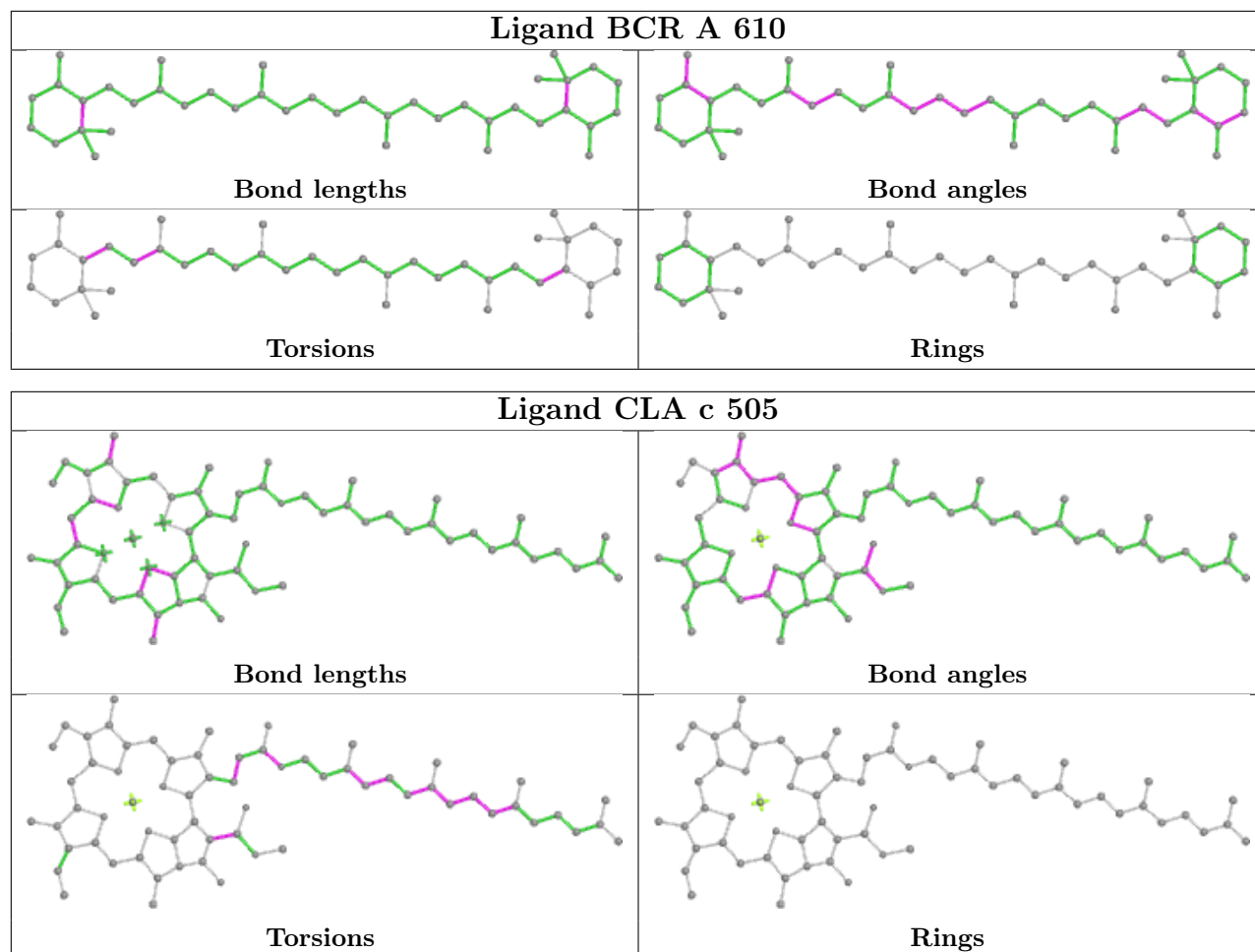


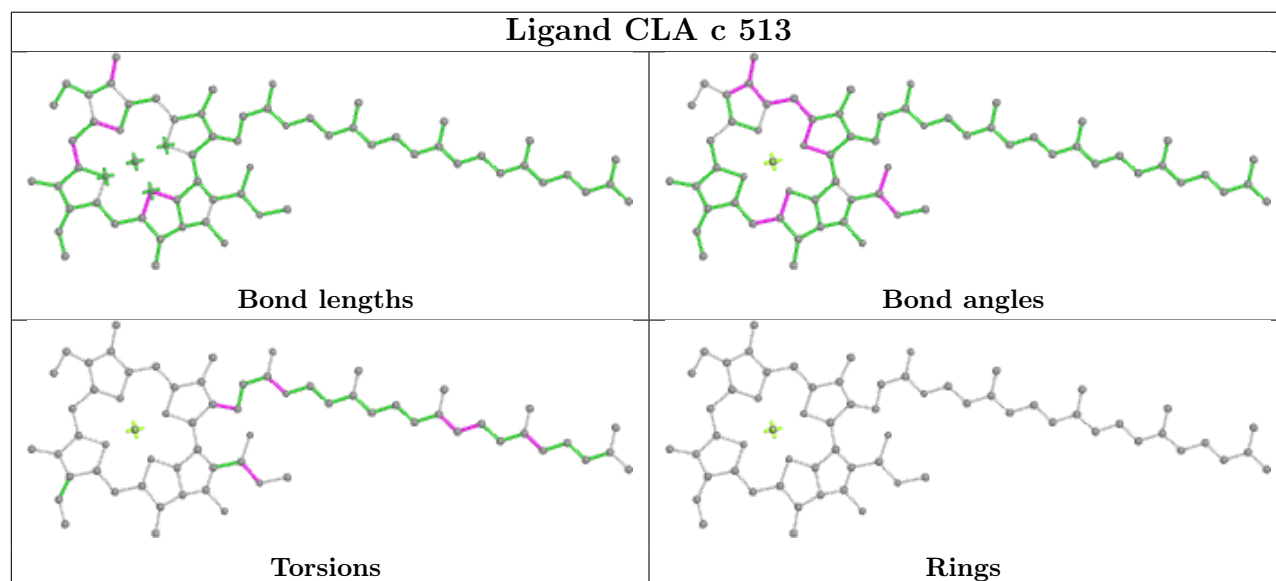
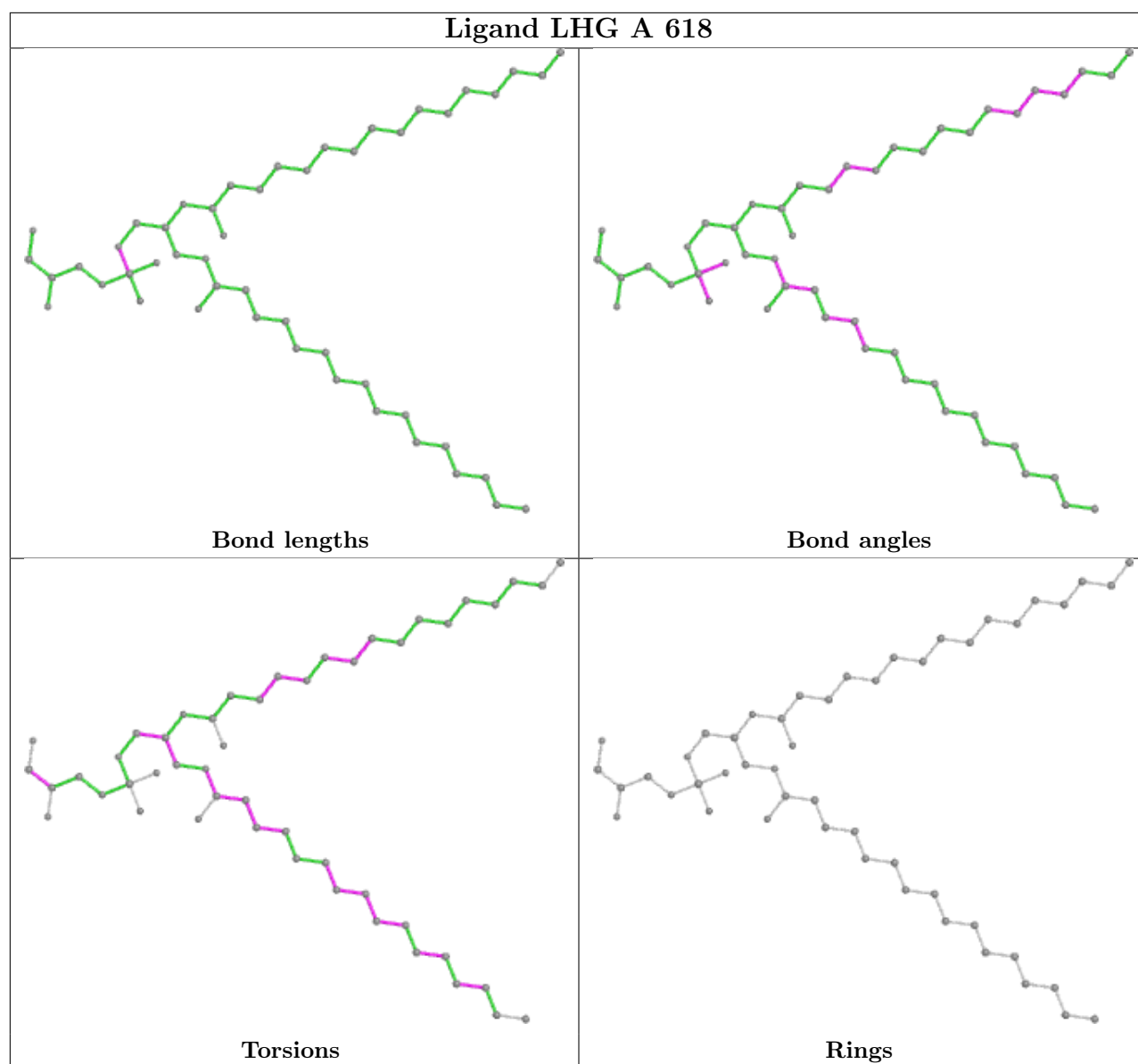


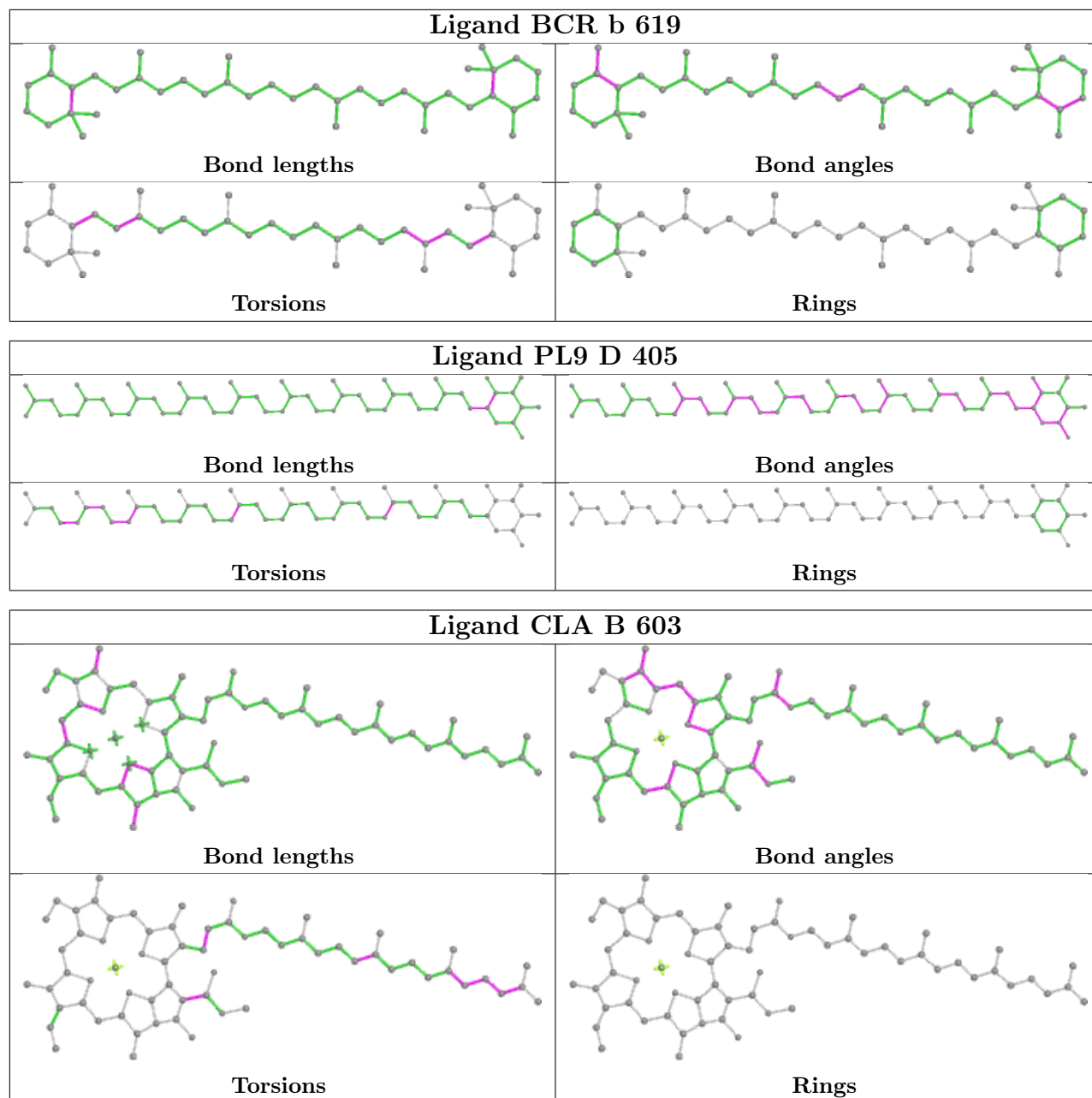


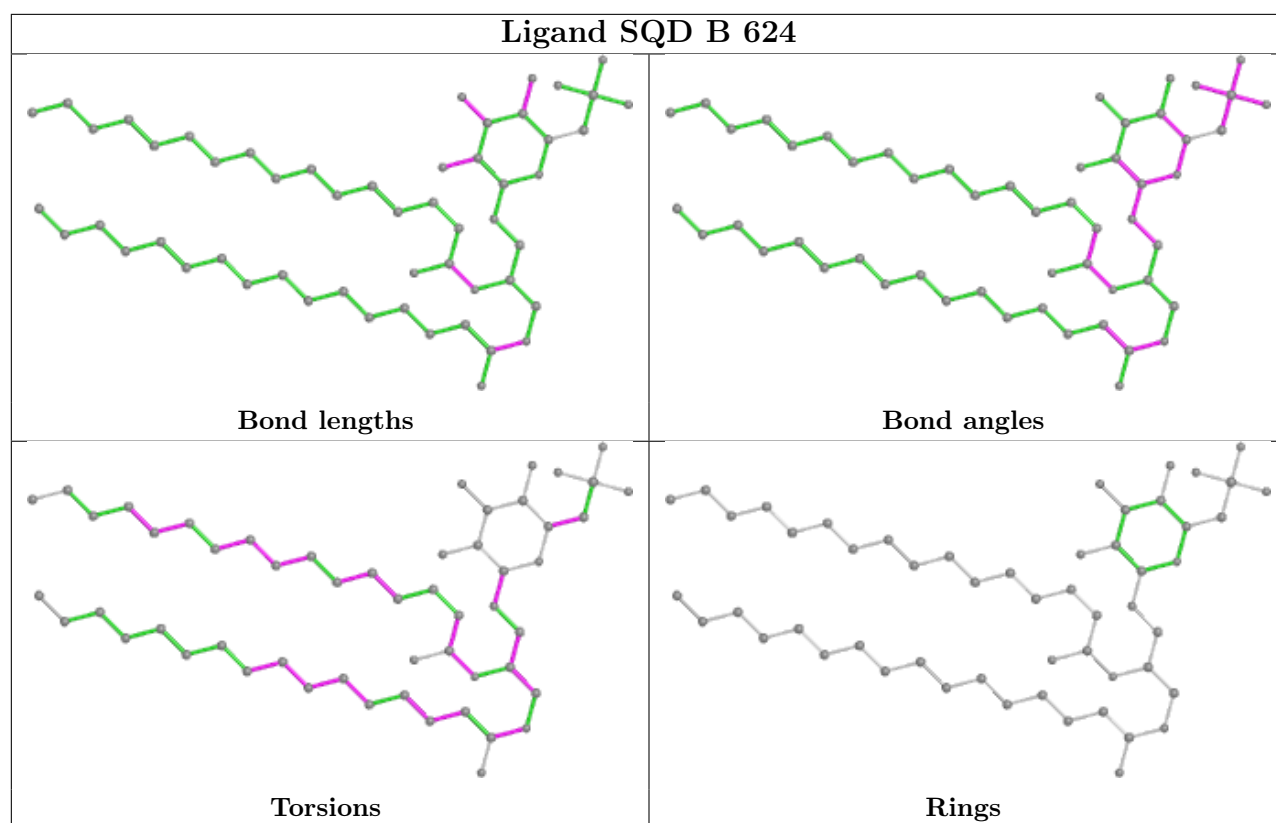












5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.36	3 (0%) 84 85	28, 34, 52, 81	0
1	a	334/344 (97%)	-0.21	4 (1%) 79 81	28, 36, 63, 83	0
2	B	504/510 (98%)	-0.30	15 (2%) 50 53	28, 38, 65, 97	0
2	b	504/510 (98%)	-0.10	25 (4%) 28 31	29, 41, 76, 102	0
3	C	451/461 (97%)	-0.20	7 (1%) 72 74	30, 41, 61, 101	0
3	c	451/461 (97%)	-0.15	7 (1%) 72 74	31, 44, 65, 97	0
4	D	341/352 (96%)	-0.34	3 (0%) 84 85	28, 35, 52, 92	0
4	d	341/352 (96%)	-0.18	6 (1%) 68 71	28, 39, 61, 98	0
5	E	81/84 (96%)	0.12	5 (6%) 20 22	37, 55, 75, 97	0
5	e	82/84 (97%)	0.53	5 (6%) 21 23	42, 61, 83, 99	0
6	F	34/45 (75%)	-0.45	1 (2%) 51 55	41, 48, 70, 82	0
6	f	34/45 (75%)	-0.08	2 (5%) 22 24	44, 55, 83, 91	0
7	H	65/66 (98%)	-0.32	1 (1%) 73 75	36, 44, 61, 93	0
7	h	63/66 (95%)	0.14	4 (6%) 20 22	42, 51, 66, 70	0
8	I	36/38 (94%)	0.39	4 (11%) 5 5	36, 44, 78, 90	0
8	i	35/38 (92%)	-0.22	1 (2%) 51 55	36, 45, 72, 94	0
9	J	36/40 (90%)	-0.18	3 (8%) 11 12	39, 54, 81, 88	0
9	j	36/40 (90%)	0.15	3 (8%) 11 12	41, 57, 87, 96	0
10	K	37/46 (80%)	-0.03	1 (2%) 54 57	47, 56, 76, 83	0
10	k	37/46 (80%)	-0.21	0 100 100	52, 58, 74, 89	0
11	L	37/37 (100%)	-0.16	0 100 100	31, 34, 67, 72	0
11	l	37/37 (100%)	-0.17	4 (10%) 5 5	30, 37, 80, 104	0
12	M	32/36 (88%)	-0.36	1 (3%) 49 52	34, 39, 69, 93	0
12	m	32/36 (88%)	-0.46	1 (3%) 49 52	34, 40, 60, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.12	13 (5%) 26 29	28, 46, 84, 131	0
13	o	244/272 (89%)	-0.06	11 (4%) 33 36	30, 46, 85, 133	0
14	T	29/32 (90%)	0.30	2 (6%) 16 18	33, 37, 58, 84	0
14	t	29/32 (90%)	-0.12	1 (3%) 45 47	32, 37, 71, 88	0
15	U	97/134 (72%)	0.11	2 (2%) 63 66	36, 47, 74, 103	0
15	u	97/134 (72%)	-0.24	2 (2%) 63 66	34, 44, 62, 102	0
16	V	137/163 (84%)	-0.43	0 100 100	35, 44, 60, 85	0
16	v	137/163 (84%)	0.08	4 (2%) 51 55	37, 50, 71, 92	0
17	Y	27/46 (58%)	1.63	10 (37%) 0 0	57, 75, 102, 112	0
17	y	30/46 (65%)	0.42	5 (16%) 1 1	59, 74, 88, 97	0
18	X	38/41 (92%)	0.00	2 (5%) 26 29	43, 51, 76, 83	0
18	x	38/41 (92%)	0.51	4 (10%) 6 6	48, 60, 81, 100	0
19	Z	62/62 (100%)	1.15	13 (20%) 1 1	57, 72, 113, 123	0
19	z	62/62 (100%)	1.48	18 (29%) 0 0	59, 74, 111, 124	0
20	R	34/41 (82%)	1.79	17 (50%) 0 0	64, 76, 94, 102	0
20	r	34/41 (82%)	3.50	25 (73%) 0 0	75, 91, 109, 110	0
All	All	5313/5700 (93%)	-0.08	235 (4%) 34 37	28, 42, 78, 133	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	11.2
8	I	37	LEU	10.7
13	o	61	GLN	9.8
2	b	127	ARG	8.7
20	r	35	LEU	8.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.93	0.18	45,53,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.94	0.14	41,53,62,63	0
14	FME	T	1	10/11	0.95	0.10	32,40,59,74	0
8	FME	I	1	10/11	0.96	0.17	45,49,54,55	0
12	FME	m	1	10/11	0.96	0.14	39,51,70,77	0
14	FME	t	1	10/11	0.96	0.10	31,38,58,64	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
31	UNL	E	102	12/-	0.49	0.26	63,85,93,95	0
31	UNL	J	102	12/-	0.62	0.39	61,79,84,86	0
32	LMG	B	626	51/55	0.62	0.31	55,76,89,91	0
31	UNL	A	617	20/-	0.65	0.23	58,66,76,77	0
31	UNL	j	802	12/-	0.66	0.21	62,72,86,89	0
31	UNL	D	410	18/-	0.66	0.20	41,53,74,74	0
31	UNL	C	523	16/-	0.68	0.22	55,71,94,101	0
32	LMG	d	408	38/55	0.69	0.27	58,68,101,106	0
31	UNL	I	102	20/-	0.73	0.22	46,64,81,84	0
29	SQD	D	409	47/54	0.74	0.21	41,59,109,125	0
29	SQD	B	625	54/54	0.74	0.26	52,72,92,105	0
29	SQD	b	621	40/54	0.75	0.20	48,58,68,70	0
28	PL9	a	612	55/55	0.77	0.28	51,67,89,96	0
31	UNL	J	101	11/-	0.77	0.23	48,61,68,68	0
31	UNL	a	619	12/-	0.78	0.26	60,65,71,76	0
31	UNL	c	525	12/-	0.79	0.25	50,62,73,73	0
32	LMG	C	501	48/55	0.79	0.20	46,61,76,89	0
31	UNL	x	101	16/-	0.79	0.22	41,51,65,68	0
28	PL9	A	611	55/55	0.80	0.27	42,60,82,88	55
30	LHG	A	618	49/49	0.80	0.27	56,90,112,115	0
29	SQD	A	616	54/54	0.80	0.21	50,70,96,103	0
31	UNL	a	618	17/-	0.80	0.16	46,57,71,72	0
31	UNL	I	101	7/-	0.80	0.19	53,57,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	UNL	c	523	8/-	0.80	0.15	49,59,77,84	0
29	SQD	B	624	54/54	0.81	0.20	43,62,96,106	0
31	UNL	c	524	20/-	0.81	0.18	45,67,82,83	0
31	UNL	M	102	17/-	0.81	0.21	52,61,73,74	0
32	LMG	C	520	48/55	0.81	0.19	47,69,88,95	0
31	UNL	b	622	17/-	0.81	0.19	47,53,63,65	0
27	BCR	h	101	40/40	0.82	0.17	40,48,64,68	0
32	LMG	C	521	51/55	0.82	0.27	45,65,116,118	0
31	UNL	C	522	17/-	0.82	0.21	42,56,67,75	0
32	LMG	b	620	51/55	0.83	0.27	55,72,98,110	0
30	LHG	a	617	42/49	0.83	0.30	67,88,102,111	0
31	UNL	b	623	11/-	0.84	0.18	59,66,68,71	0
32	LMG	a	614	51/55	0.84	0.19	41,60,74,80	0
29	SQD	L	101	49/54	0.84	0.18	41,66,96,109	0
32	LMG	B	620	51/55	0.84	0.18	32,57,73,77	0
31	UNL	B	627	15/-	0.85	0.19	48,55,65,68	0
31	UNL	m	101	9/-	0.85	0.18	51,53,61,62	0
31	UNL	m	103	16/-	0.85	0.16	39,51,73,76	0
31	UNL	t	102	18/-	0.86	0.18	43,56,65,66	0
31	UNL	D	411	10/-	0.86	0.20	49,55,72,79	0
31	UNL	T	103	12/-	0.87	0.13	42,54,59,61	0
27	BCR	H	101	40/40	0.87	0.14	36,50,64,65	0
31	UNL	d	409	17/-	0.87	0.28	51,58,67,70	0
32	LMG	c	520	34/55	0.87	0.26	58,66,78,88	0
25	CLA	b	601	65/65	0.87	0.21	40,61,83,94	0
31	UNL	M	101	15/-	0.88	0.14	42,52,63,75	0
32	LMG	B	621	51/55	0.88	0.23	54,71,102,110	0
31	UNL	i	101	20/-	0.88	0.23	51,59,77,79	0
32	LMG	c	519	37/55	0.88	0.15	48,67,76,77	0
31	UNL	j	801	15/-	0.88	0.18	50,60,77,77	0
31	UNL	B	622	11/-	0.88	0.15	41,47,60,61	0
25	CLA	d	402	65/65	0.89	0.17	36,43,83,90	0
31	UNL	H	103	7/-	0.89	0.15	48,53,60,61	0
29	SQD	a	613	54/54	0.89	0.14	40,62,72,76	0
25	CLA	C	513	65/65	0.89	0.17	41,54,81,86	0
27	BCR	d	403	40/40	0.89	0.15	41,54,79,82	0
25	CLA	C	508	65/65	0.89	0.18	30,42,59,78	0
25	CLA	c	512	65/65	0.89	0.15	45,57,89,94	0
32	LMG	m	102	51/55	0.89	0.16	43,56,69,77	0
33	DGD	h	102	62/66	0.89	0.21	38,51,60,64	0
31	UNL	T	102	14/-	0.90	0.16	36,53,63,67	0
29	SQD	f	101	41/54	0.90	0.20	59,84,105,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	c	513	65/65	0.90	0.18	48,63,86,90	0
27	BCR	T	101	40/40	0.91	0.17	35,46,57,68	0
27	BCR	Y	101	40/40	0.91	0.12	43,51,62,68	0
27	BCR	b	617	40/40	0.91	0.14	33,44,52,52	0
27	BCR	b	618	40/40	0.91	0.17	33,44,56,59	0
27	BCR	c	521	40/40	0.91	0.12	49,59,72,73	0
31	UNL	A	615	9/-	0.91	0.17	41,52,68,70	0
27	BCR	c	522	40/40	0.91	0.14	42,54,63,69	0
25	CLA	a	610	65/65	0.91	0.15	24,32,77,81	0
25	CLA	C	504	65/65	0.91	0.17	36,44,50,59	0
25	CLA	b	609	65/65	0.91	0.14	35,46,60,66	0
25	CLA	c	506	65/65	0.91	0.15	33,48,82,95	0
25	CLA	B	601	65/65	0.91	0.15	39,54,81,87	0
25	CLA	B	609	65/65	0.91	0.12	28,39,58,69	0
25	CLA	C	514	65/65	0.91	0.23	49,60,136,139	0
29	SQD	D	408	43/54	0.91	0.22	54,76,105,108	0
27	BCR	D	404	40/40	0.91	0.16	31,44,82,86	0
33	DGD	H	102	62/66	0.91	0.16	39,47,63,65	0
25	CLA	D	403	65/65	0.91	0.19	31,37,89,99	0
25	CLA	c	507	65/65	0.92	0.14	36,46,62,72	0
27	BCR	C	515	40/40	0.92	0.13	44,53,65,67	0
25	CLA	c	510	65/65	0.92	0.16	36,46,61,72	0
27	BCR	c	514	40/40	0.92	0.13	49,58,62,64	0
29	SQD	A	612	52/54	0.92	0.16	48,63,85,91	0
25	CLA	B	606	65/65	0.92	0.13	28,37,63,74	0
33	DGD	c	517	62/66	0.92	0.13	39,52,81,86	0
25	CLA	b	602	65/65	0.92	0.17	33,41,59,66	0
25	CLA	B	604	65/65	0.93	0.16	27,33,72,81	0
25	CLA	C	510	65/65	0.93	0.17	32,42,66,70	0
30	LHG	d	405	49/49	0.93	0.15	43,53,68,72	0
25	CLA	C	512	65/65	0.93	0.13	39,52,67,71	0
25	CLA	b	606[A]	65/65	0.93	0.15	37,43,52,55	64
27	BCR	B	619	40/40	0.93	0.10	34,45,56,58	0
25	CLA	b	606[B]	65/65	0.93	0.15	37,43,52,58	64
27	BCR	C	516	40/40	0.93	0.14	34,44,55,57	0
25	CLA	C	503	65/65	0.93	0.19	28,39,53,65	0
25	CLA	b	615	65/65	0.93	0.11	33,44,62,69	0
27	BCR	K	101	40/40	0.93	0.14	37,52,63,66	0
25	CLA	c	502	65/65	0.93	0.18	31,41,55,63	0
25	CLA	c	503	65/65	0.93	0.15	36,45,50,57	0
25	CLA	A	606	65/65	0.93	0.12	23,32,50,59	0
33	DGD	C	518	62/66	0.93	0.15	40,50,89,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	C	507	65/65	0.93	0.12	34,46,77,89	0
27	BCR	b	619	40/40	0.93	0.10	32,48,60,61	0
25	CLA	c	509	65/65	0.93	0.15	37,45,61,64	0
25	CLA	c	501	65/65	0.94	0.15	29,38,53,56	0
25	CLA	C	506	65/65	0.94	0.12	27,40,65,70	0
25	CLA	a	606	65/65	0.94	0.12	26,33,42,58	0
30	LHG	B	623	49/49	0.94	0.17	36,47,63,70	0
30	LHG	D	406	49/49	0.94	0.18	32,40,56,74	0
30	LHG	a	616	39/49	0.94	0.13	39,48,66,71	0
27	BCR	a	611	40/40	0.94	0.11	26,37,49,54	0
25	CLA	c	505	65/65	0.94	0.12	32,41,69,76	0
30	LHG	l	101	49/49	0.94	0.12	37,49,62,76	0
25	CLA	B	611	65/65	0.94	0.15	25,34,48,52	0
25	CLA	B	614	65/65	0.94	0.13	25,37,75,81	0
25	CLA	C	509	65/65	0.94	0.12	31,41,86,89	0
27	BCR	c	515	40/40	0.94	0.12	30,46,51,63	0
25	CLA	b	604	65/65	0.94	0.18	25,35,69,82	0
25	CLA	c	511	65/65	0.94	0.12	40,54,66,73	0
25	CLA	B	616	65/65	0.94	0.15	29,39,96,102	0
25	CLA	C	502	65/65	0.94	0.17	31,37,50,59	0
27	BCR	t	101	40/40	0.94	0.15	33,43,53,62	0
25	CLA	B	607	65/65	0.94	0.16	27,36,63,71	0
32	LMG	D	407	51/55	0.94	0.14	32,52,72,82	0
26	PHO	a	608	64/64	0.94	0.14	28,34,42,49	0
28	PL9	d	404	55/55	0.94	0.14	27,39,50,54	0
26	PHO	a	609	64/64	0.94	0.17	34,40,49,52	0
27	BCR	B	617	40/40	0.94	0.13	29,45,53,57	0
32	LMG	d	407	51/55	0.94	0.15	38,58,88,93	0
27	BCR	B	618	40/40	0.94	0.16	30,44,55,60	0
25	CLA	b	610	65/65	0.94	0.15	31,40,51,66	0
25	CLA	b	611	65/65	0.94	0.12	29,36,55,66	0
33	DGD	C	519	62/66	0.94	0.12	33,50,79,84	0
25	CLA	b	614	65/65	0.94	0.13	31,39,75,79	0
25	CLA	A	607	65/65	0.94	0.16	25,35,123,129	0
33	DGD	c	518	62/66	0.94	0.12	34,48,73,77	0
25	CLA	b	616	47/65	0.94	0.09	31,42,53,57	0
25	CLA	b	613	65/65	0.95	0.18	29,38,74,89	0
27	BCR	A	610	40/40	0.95	0.09	31,37,41,41	0
28	PL9	D	405	55/55	0.95	0.13	25,35,47,49	0
25	CLA	B	608	65/65	0.95	0.18	30,38,57,60	0
25	CLA	a	607	65/65	0.95	0.12	28,43,84,90	0
25	CLA	B	615	65/65	0.95	0.11	28,40,58,66	0

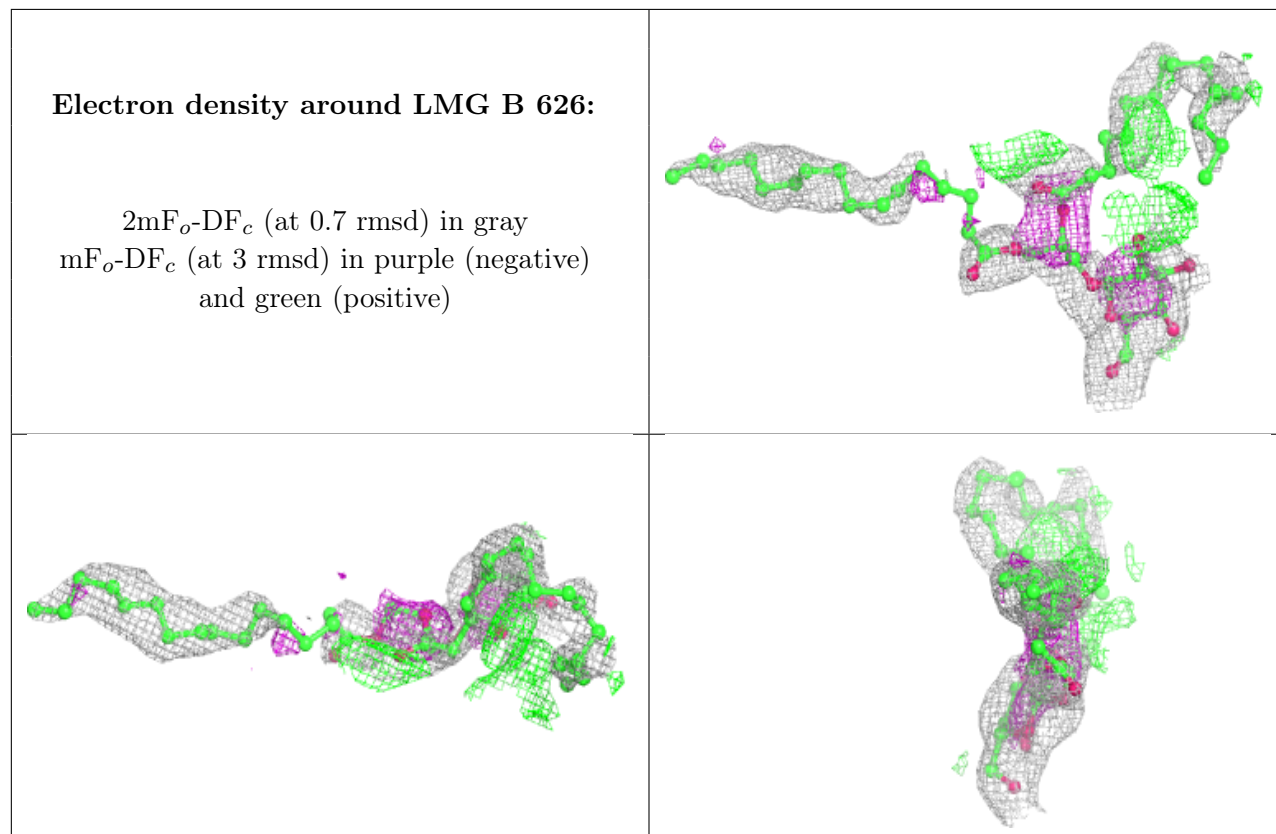
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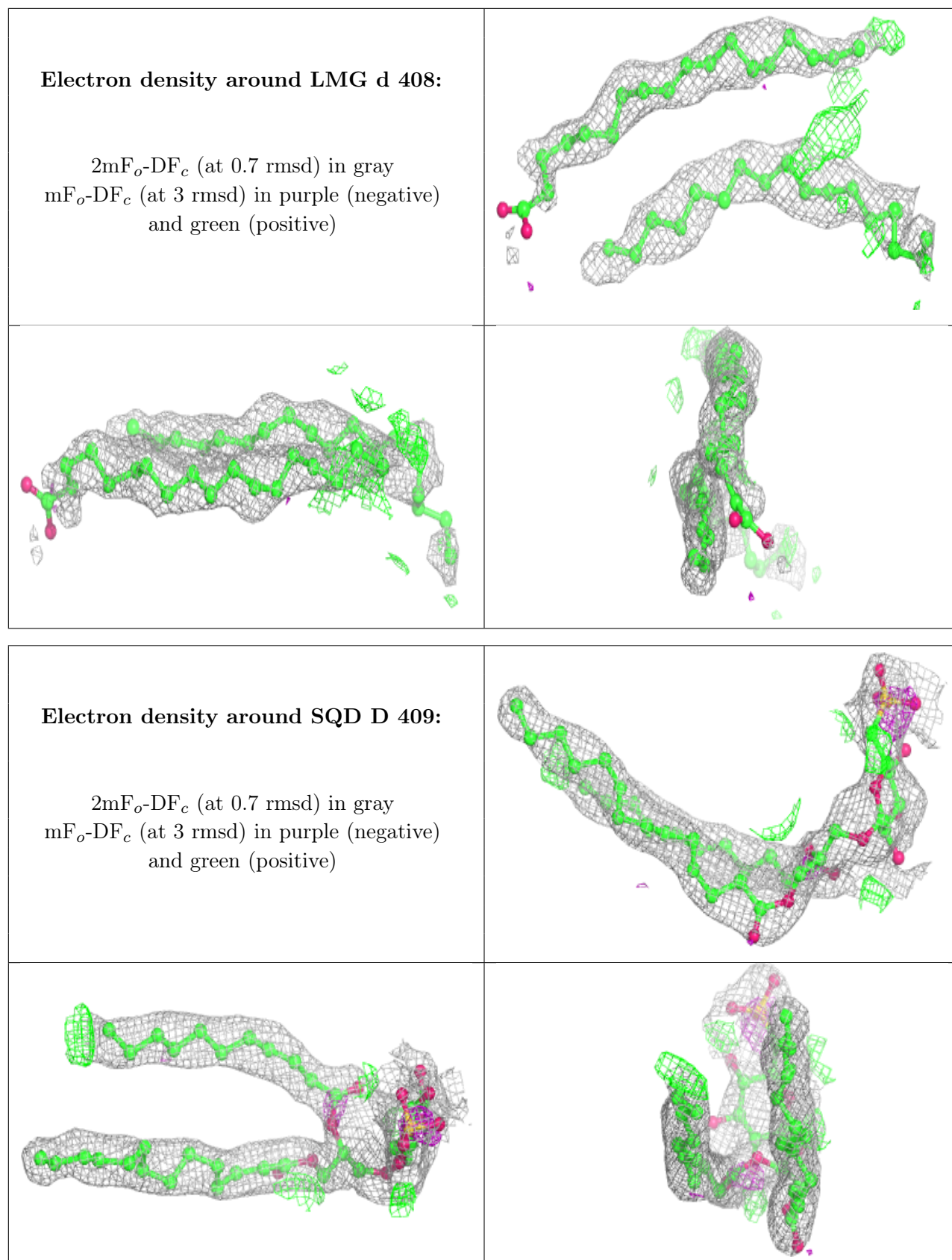
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	a	615	65/65	0.95	0.13	24,34,52,62	0
24	BCT	a	605	4/4	0.95	0.14	37,45,46,53	2
25	CLA	B	610	65/65	0.95	0.13	26,37,47,55	0
25	CLA	c	504	60/65	0.95	0.12	34,47,69,77	0
25	CLA	C	511	65/65	0.95	0.18	30,43,58,70	0
25	CLA	b	605	65/65	0.95	0.14	25,37,46,52	0
25	CLA	A	613	65/65	0.95	0.13	25,33,44,53	0
25	CLA	c	508	64/65	0.95	0.11	36,45,82,87	0
25	CLA	B	612	65/65	0.95	0.15	25,33,42,45	0
30	LHG	A	614	47/49	0.95	0.13	33,44,73,76	0
25	CLA	b	607	65/65	0.95	0.12	29,37,62,68	0
25	CLA	b	608	65/65	0.95	0.22	32,41,56,60	0
25	CLA	C	505	65/65	0.95	0.17	34,42,80,85	0
30	LHG	L	102	49/49	0.95	0.15	35,42,50,58	0
33	DGD	C	517	62/66	0.95	0.16	29,42,72,81	0
25	CLA	D	402	65/65	0.95	0.12	21,31,54,78	0
25	CLA	d	401	65/65	0.95	0.12	25,34,55,69	0
25	CLA	B	613	65/65	0.95	0.20	26,33,63,76	0
33	DGD	c	516	62/66	0.95	0.17	28,44,67,72	0
30	LHG	d	406	49/49	0.95	0.17	31,44,55,64	0
26	PHO	A	608	64/64	0.95	0.15	29,37,43,46	0
25	CLA	b	612	65/65	0.95	0.14	26,38,49,56	0
34	HEM	e	101	43/43	0.95	0.13	47,58,73,80	0
25	CLA	A	609	54/65	0.96	0.12	25,32,72,78	0
25	CLA	B	605	65/65	0.96	0.14	26,33,48,53	0
25	CLA	b	603	65/65	0.96	0.16	29,38,57,62	0
26	PHO	D	401	64/64	0.96	0.14	23,33,38,44	0
25	CLA	B	602	65/65	0.96	0.12	26,36,57,66	0
34	HEM	E	101	43/43	0.96	0.11	43,49,57,65	0
25	CLA	B	603	65/65	0.96	0.15	25,36,56,63	0
35	HEC	V	201	43/43	0.97	0.09	29,36,44,46	0
35	HEC	v	201	43/43	0.97	0.12	31,40,47,54	0
24	BCT	A	605	4/4	0.98	0.07	42,43,44,53	0
23	CL	a	603	1/1	0.98	0.07	33,33,33,33	0
21	OEX	a	601	10/10	0.99	0.11	28,32,35,42	0
22	FE2	A	602	1/1	0.99	0.04	36,36,36,36	0
22	FE2	a	602	1/1	0.99	0.05	43,43,43,43	0
23	CL	A	603	1/1	0.99	0.06	32,32,32,32	0
23	CL	A	604	1/1	0.99	0.13	33,33,33,33	0
21	OEX	A	601	10/10	0.99	0.11	32,34,40,41	1
23	CL	a	604	1/1	0.99	0.08	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all

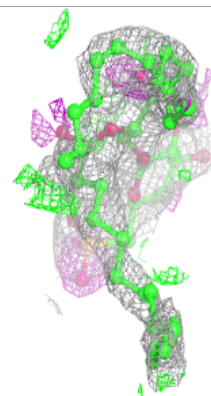
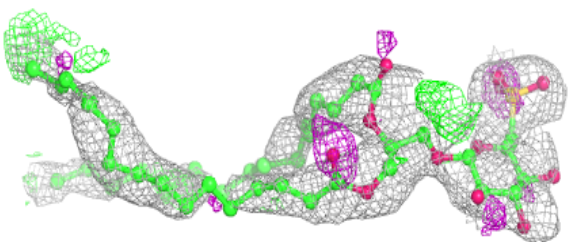
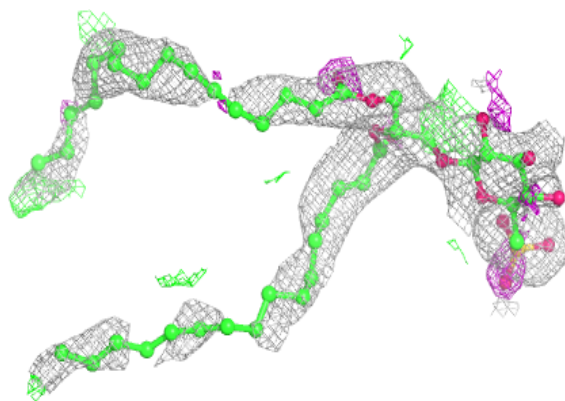
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



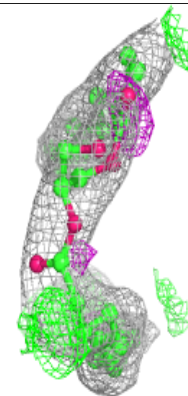
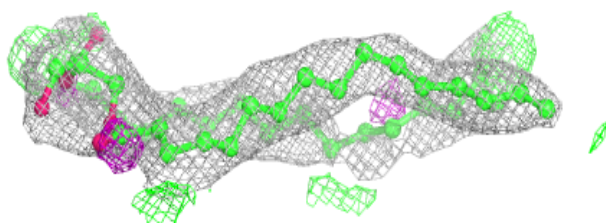
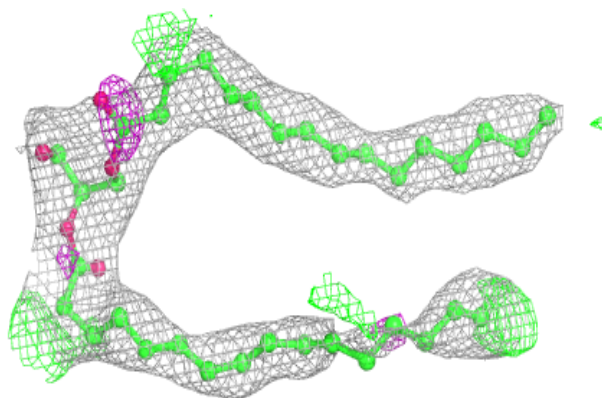


Electron density around SQD B 625:

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

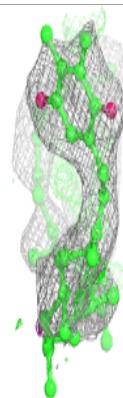
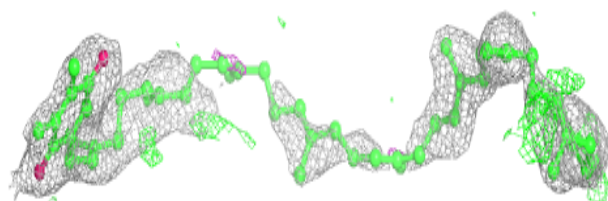
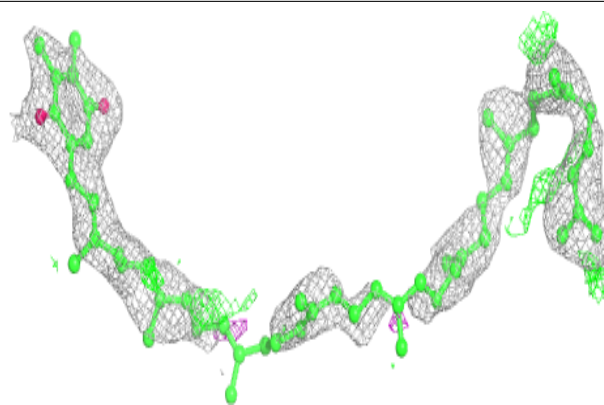
**Electron density around SQD b 621:**

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

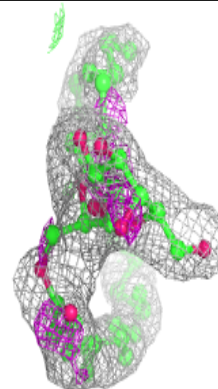
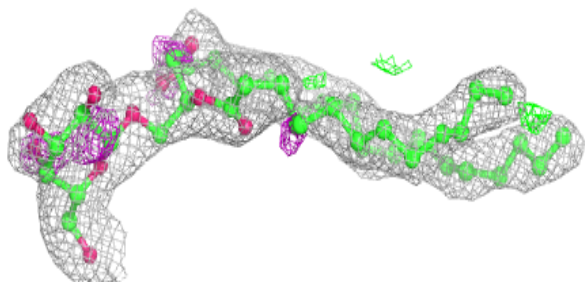
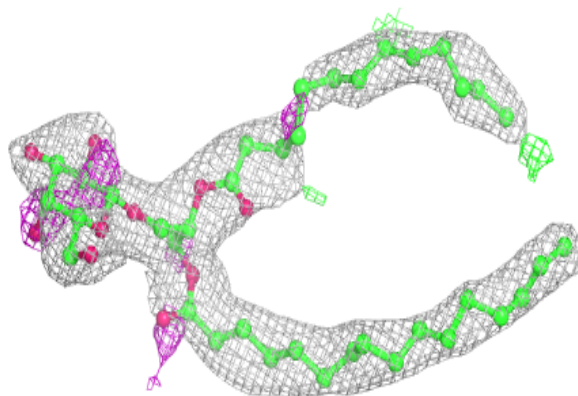


Electron density around PL9 a 612:

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

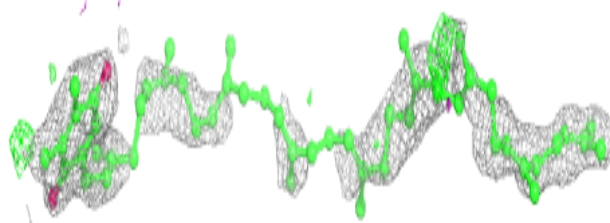
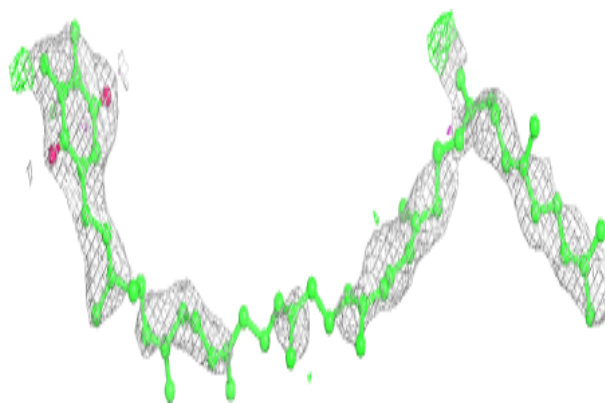
**Electron density around LMG C 501:**

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

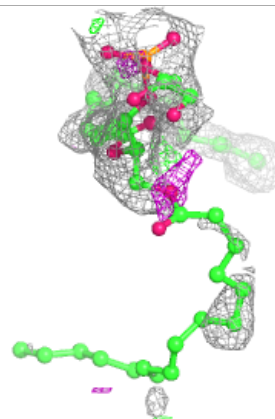
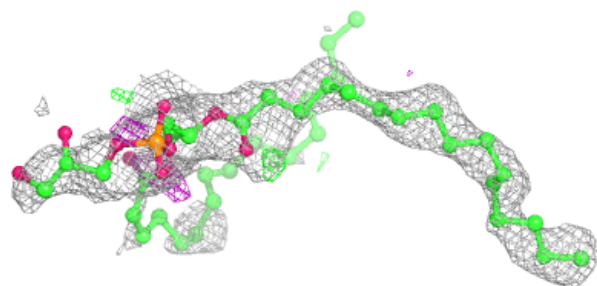
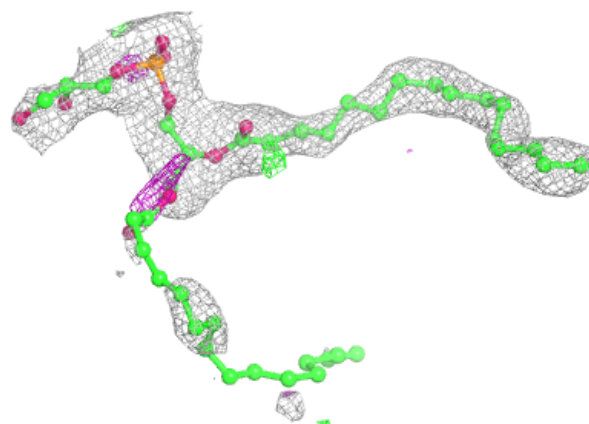


Electron density around PL9 A 611:

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

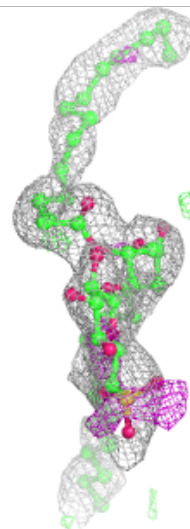
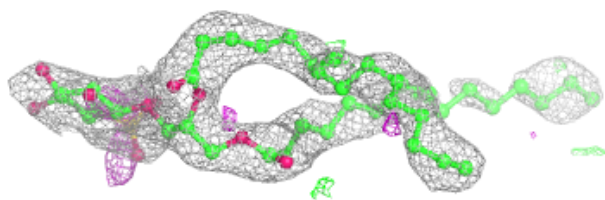
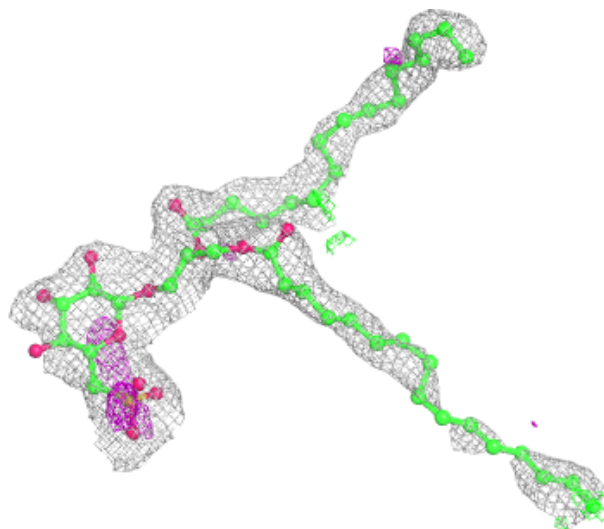
**Electron density around LHG A 618:**

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



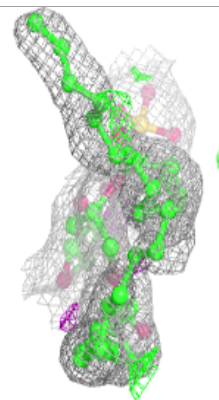
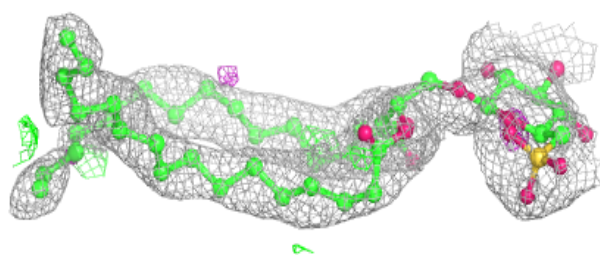
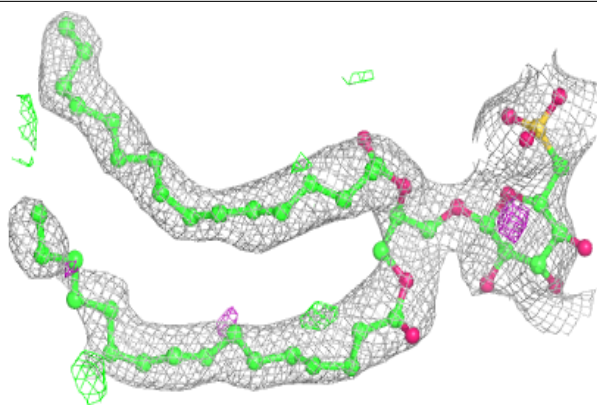
Electron density around SQD A 616:

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

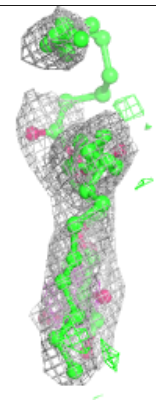
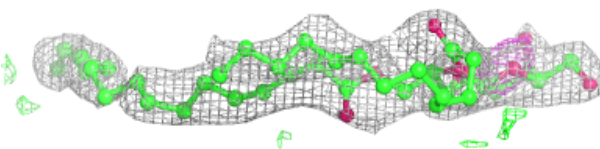
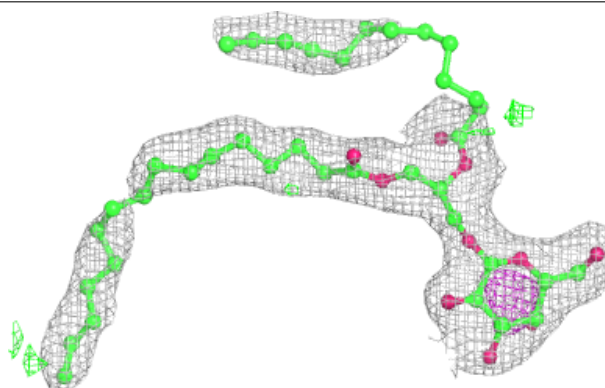


Electron density around SQD B 624:

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

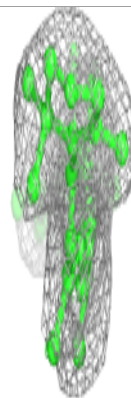
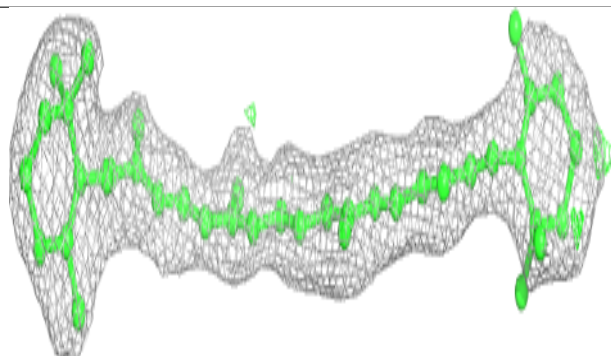
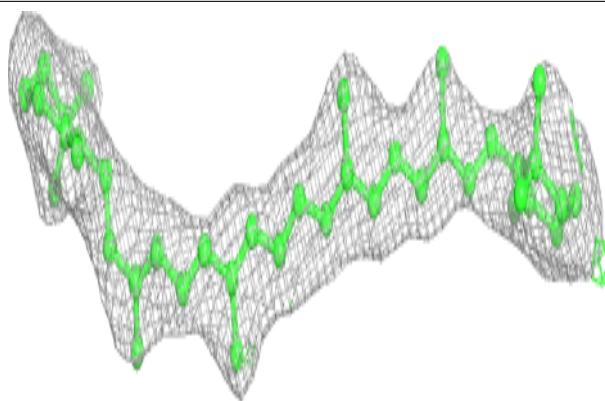
**Electron density around LMG C 520:**

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

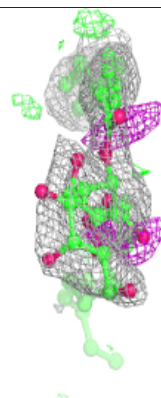
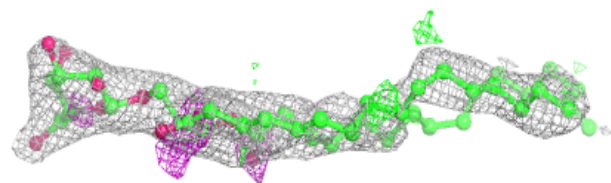
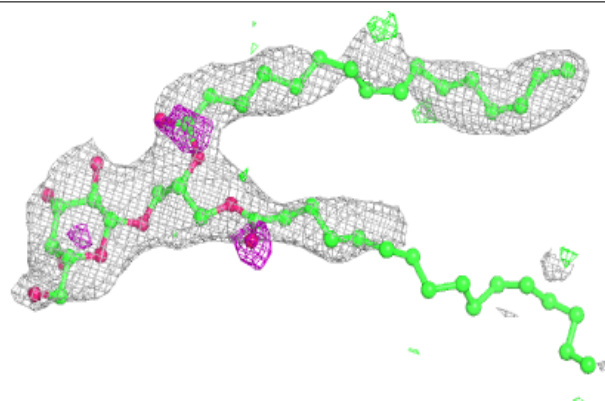


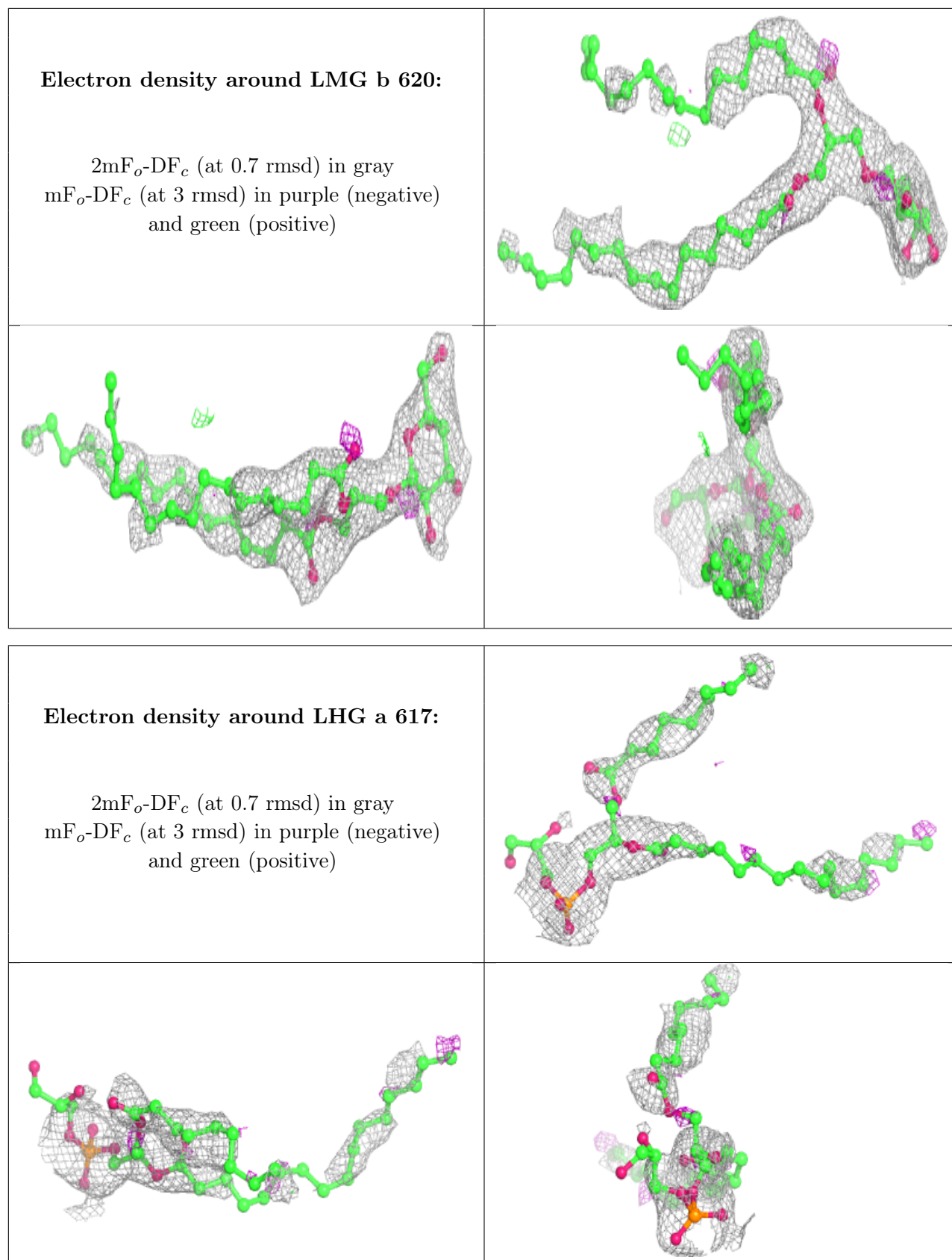
Electron density around BCR h 101:

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

**Electron density around LMG C 521:**

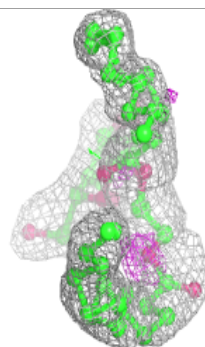
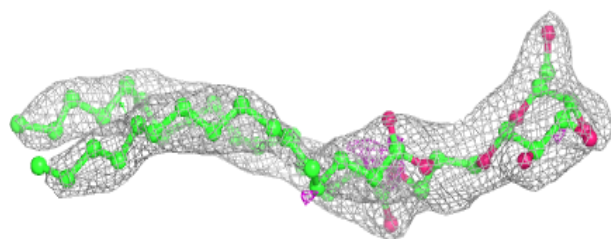
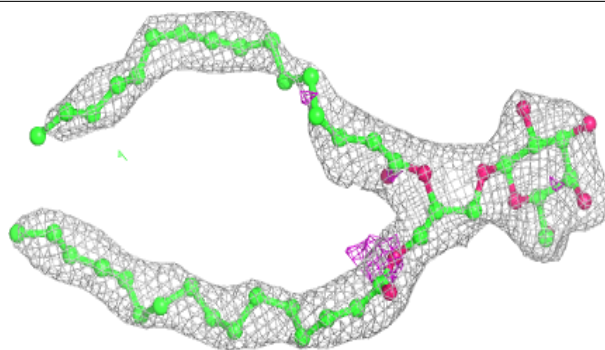
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



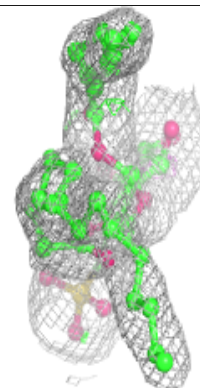
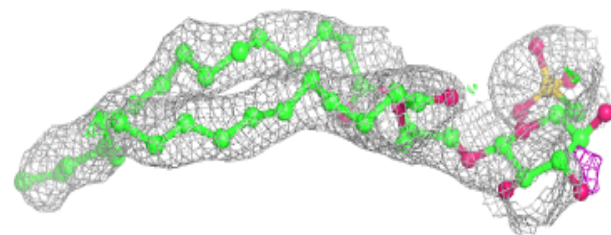
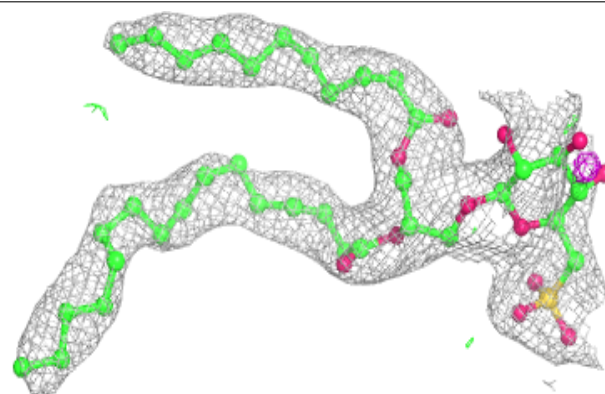


Electron density around LMG a 614:

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

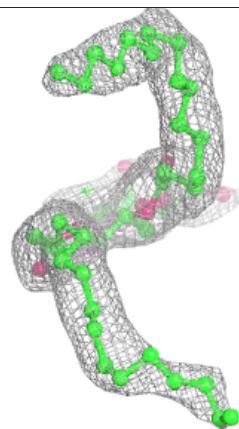
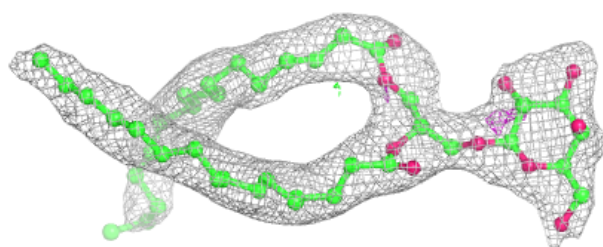
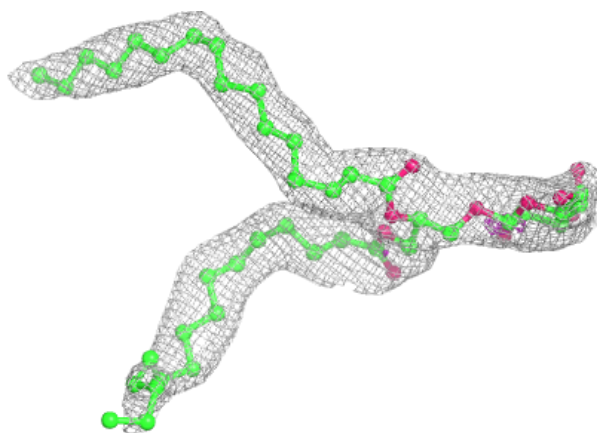
**Electron density around SQD L 101:**

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

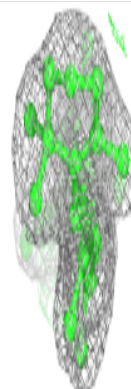
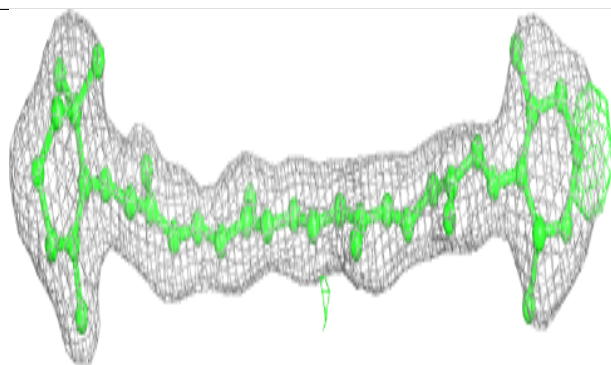
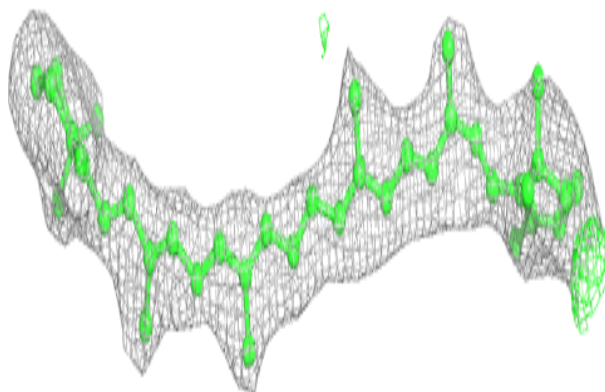


Electron density around LMG B 620:

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

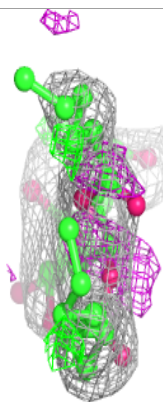
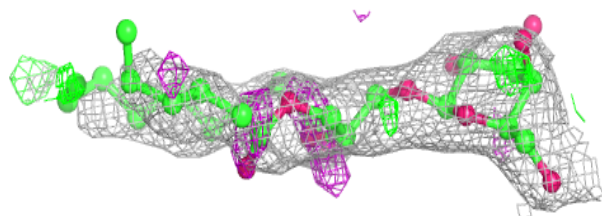
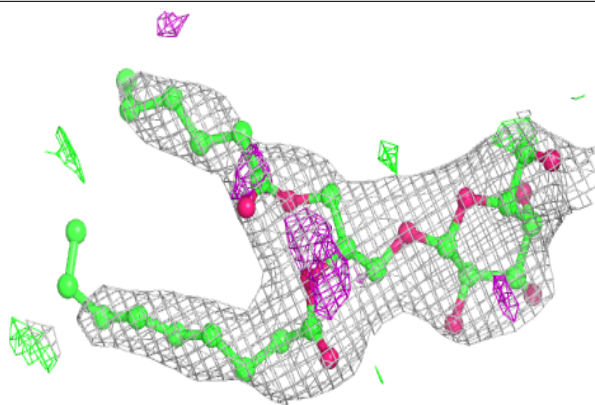
**Electron density around BCR H 101:**

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

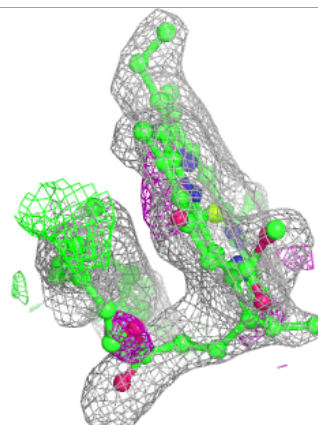
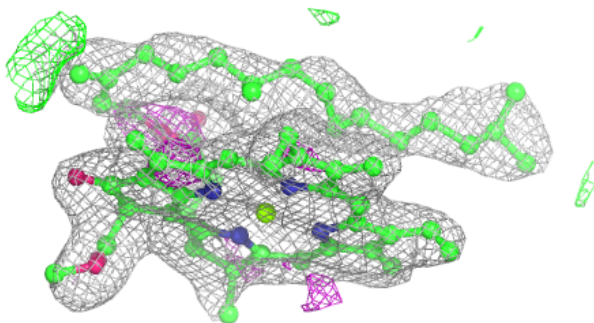
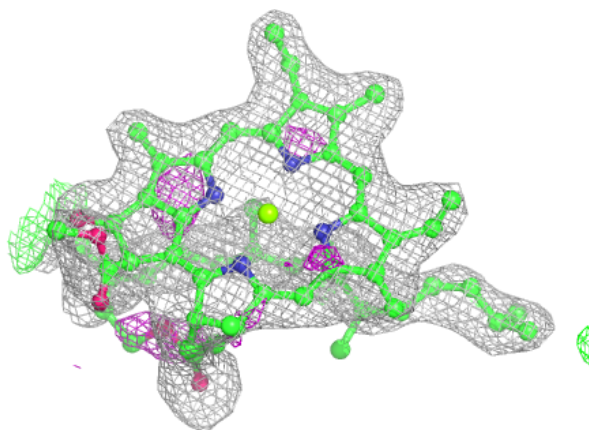


Electron density around LMG c 520:

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

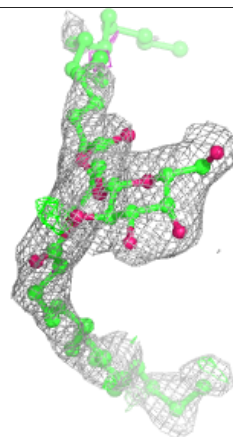
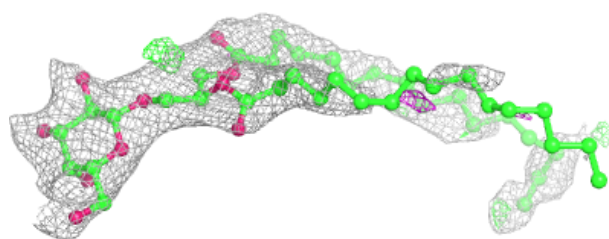
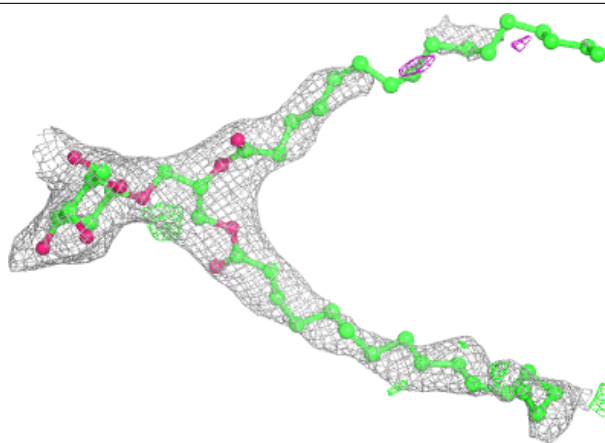
**Electron density around CLA b 601:**

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

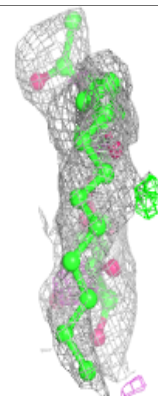
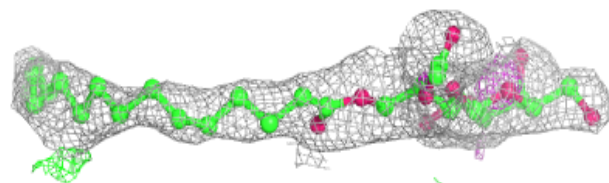
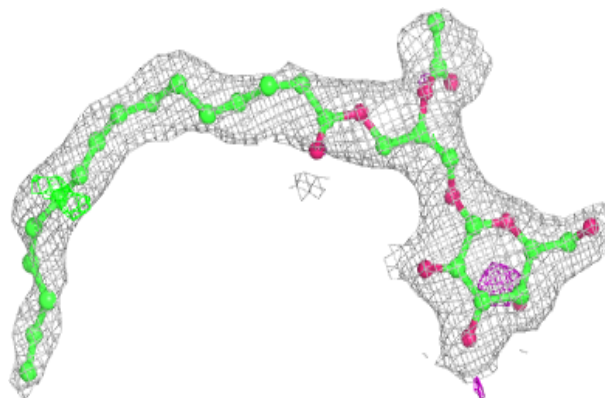


Electron density around LMG B 621:

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

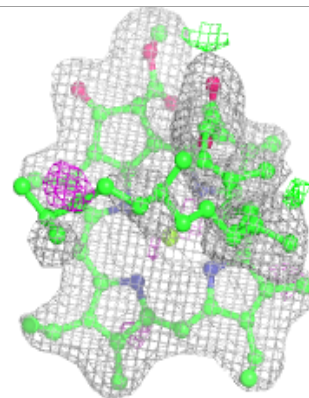
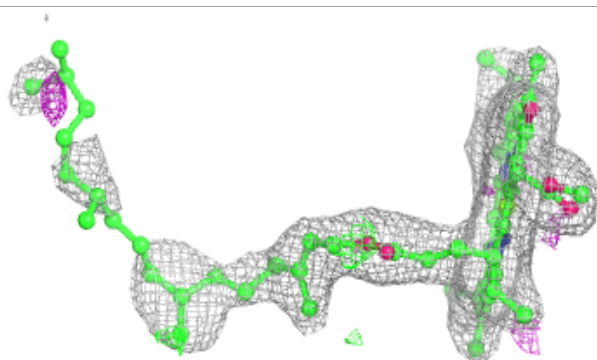
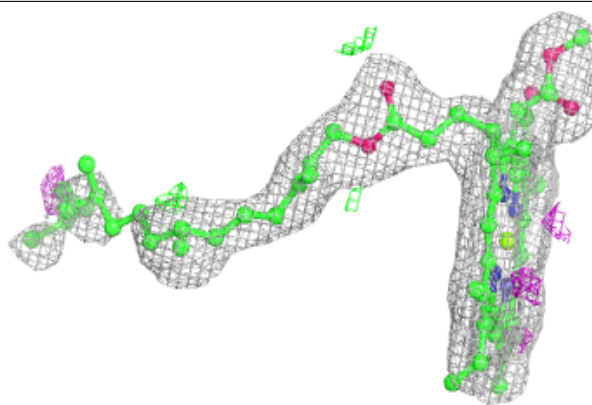
**Electron density around LMG c 519:**

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



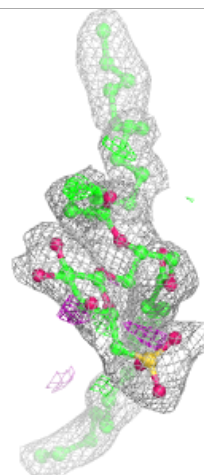
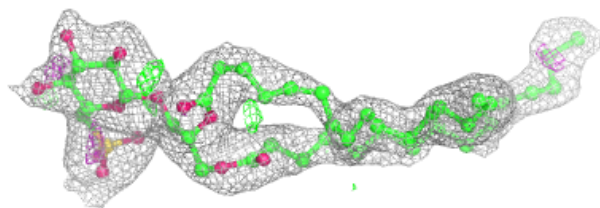
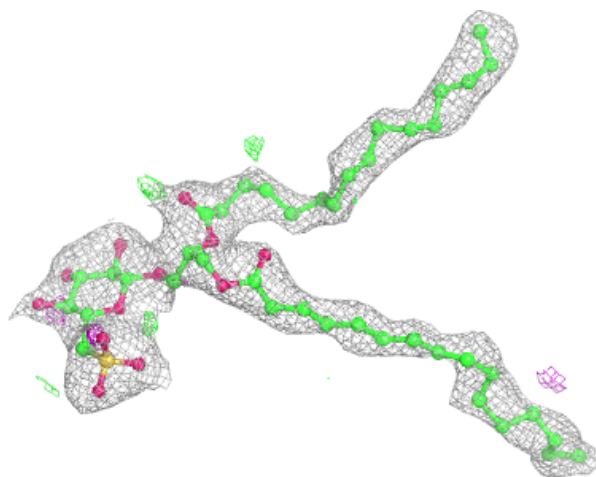
Electron density around CLA d 402:

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



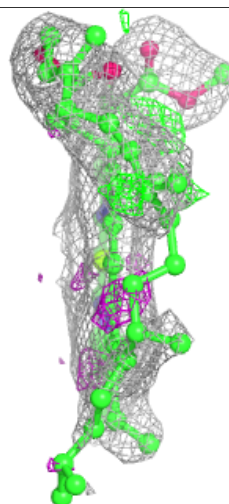
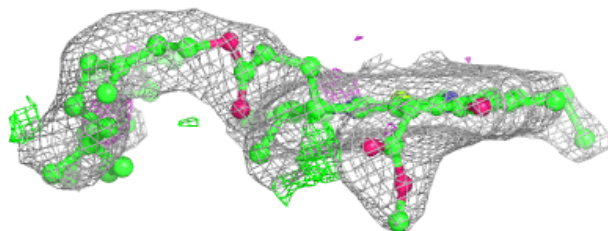
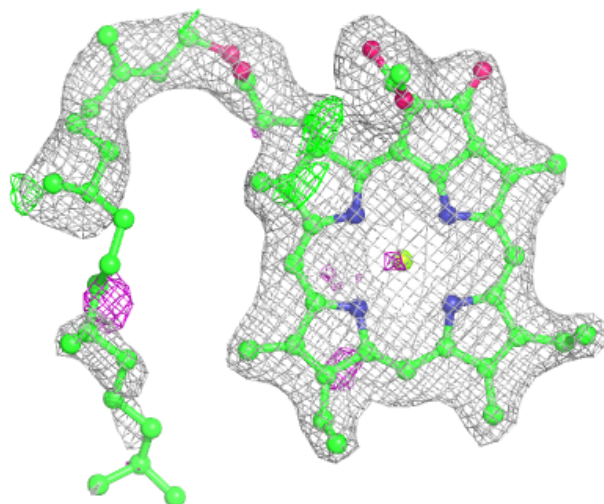
Electron density around SQD a 613:

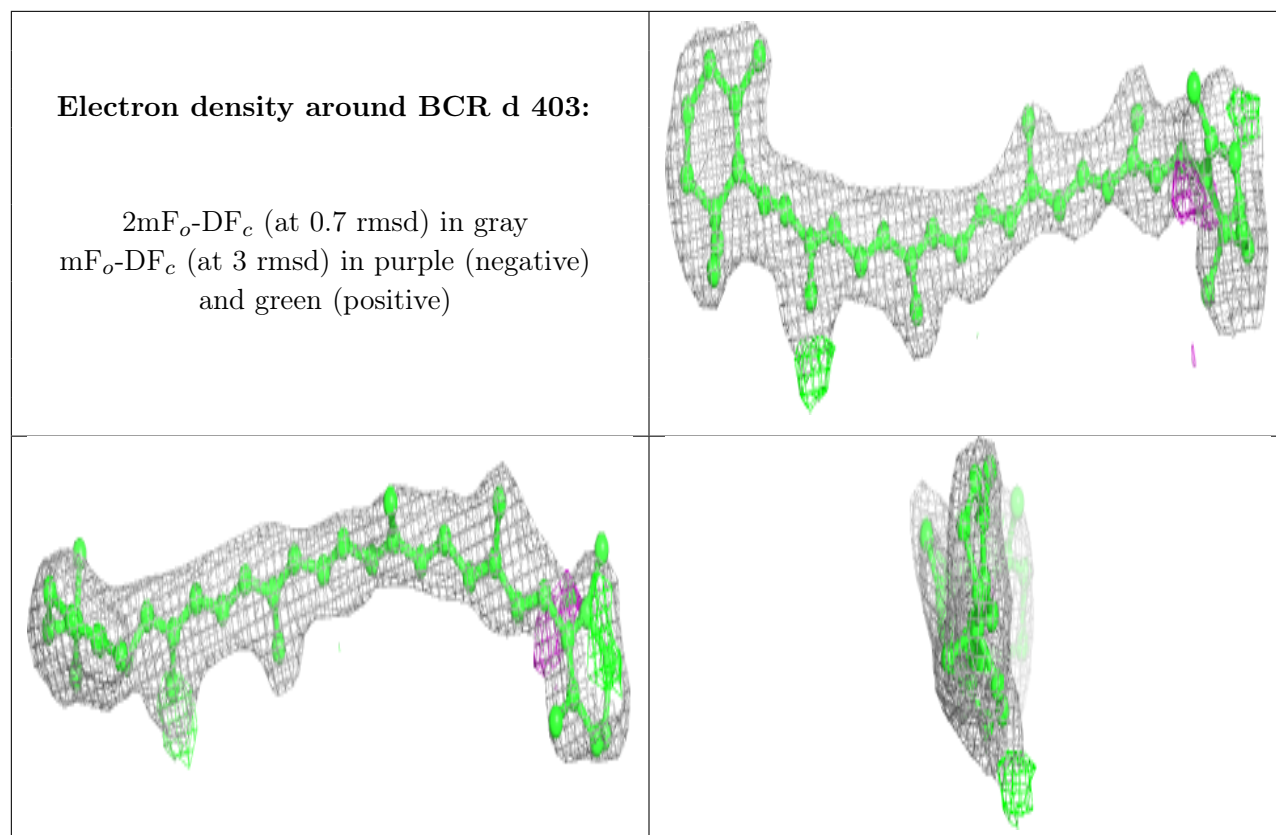
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 513:

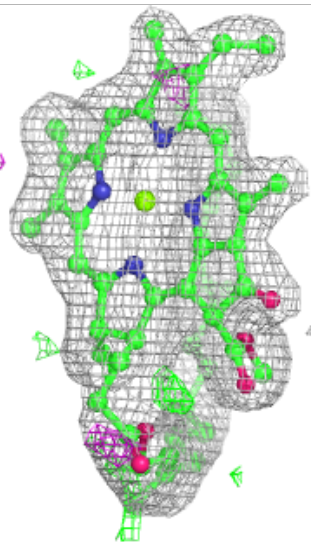
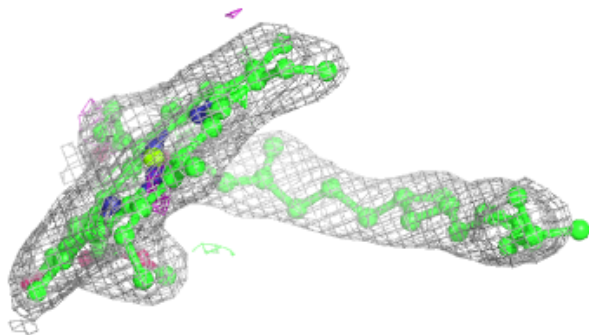
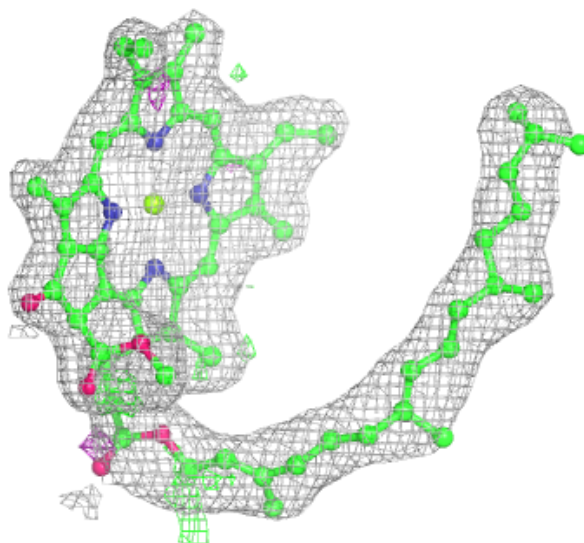
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





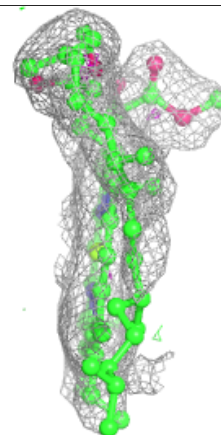
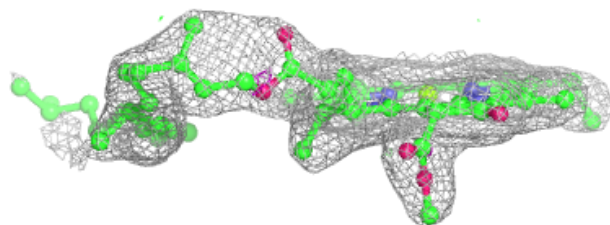
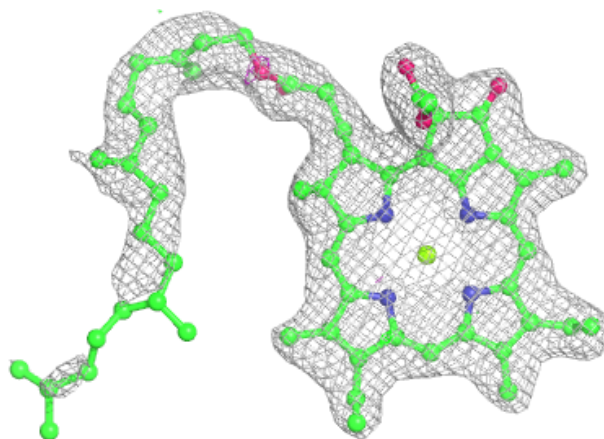
Electron density around CLA C 508:

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

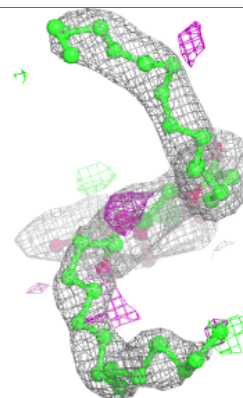
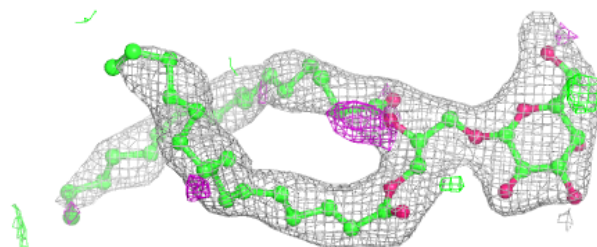
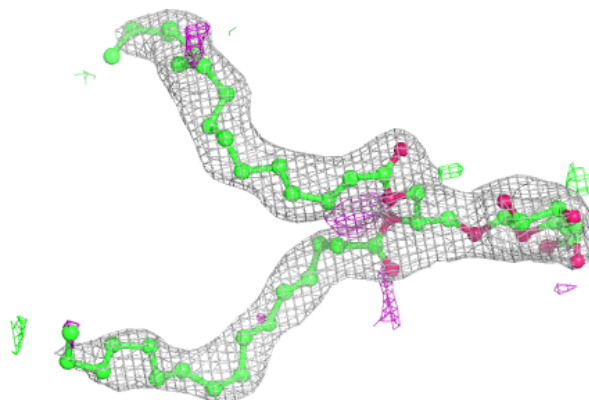


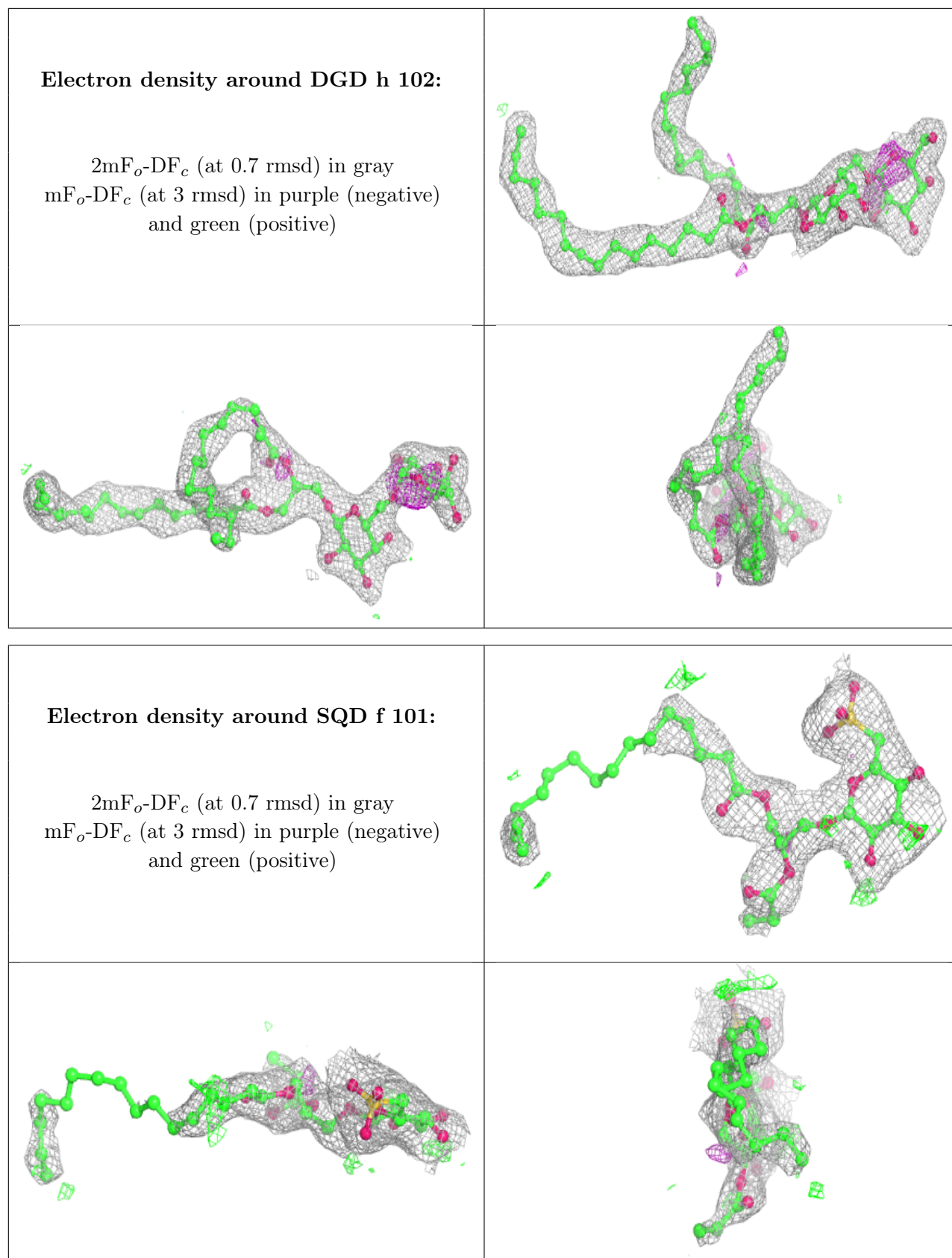
Electron density around CLA c 512:

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

**Electron density around LMG m 102:**

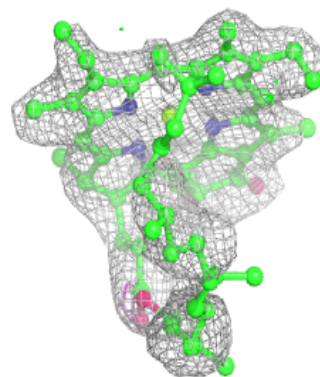
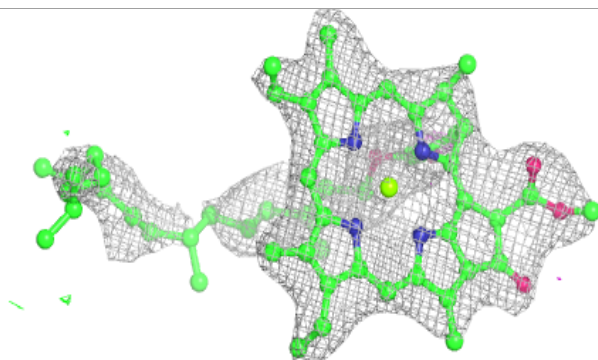
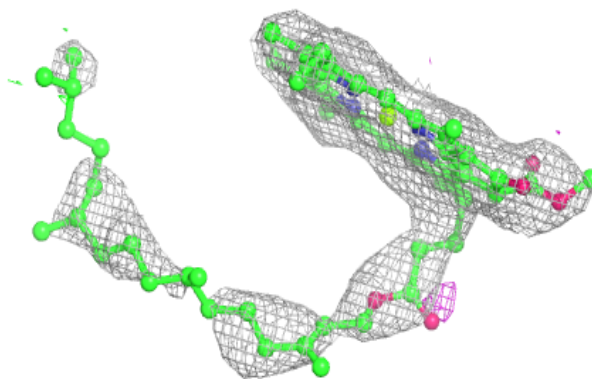
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



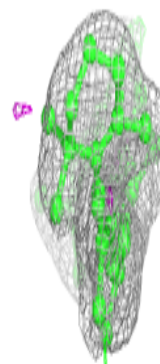
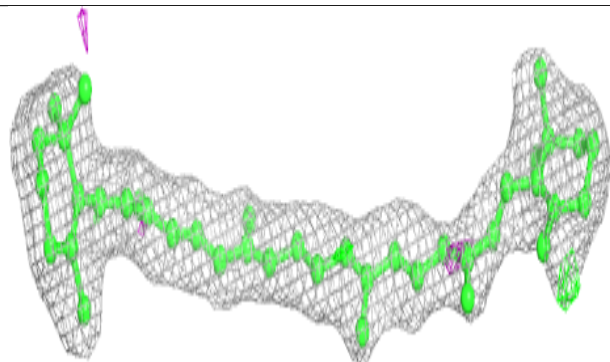
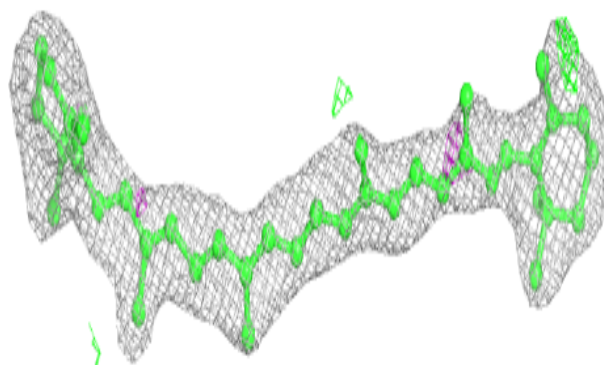


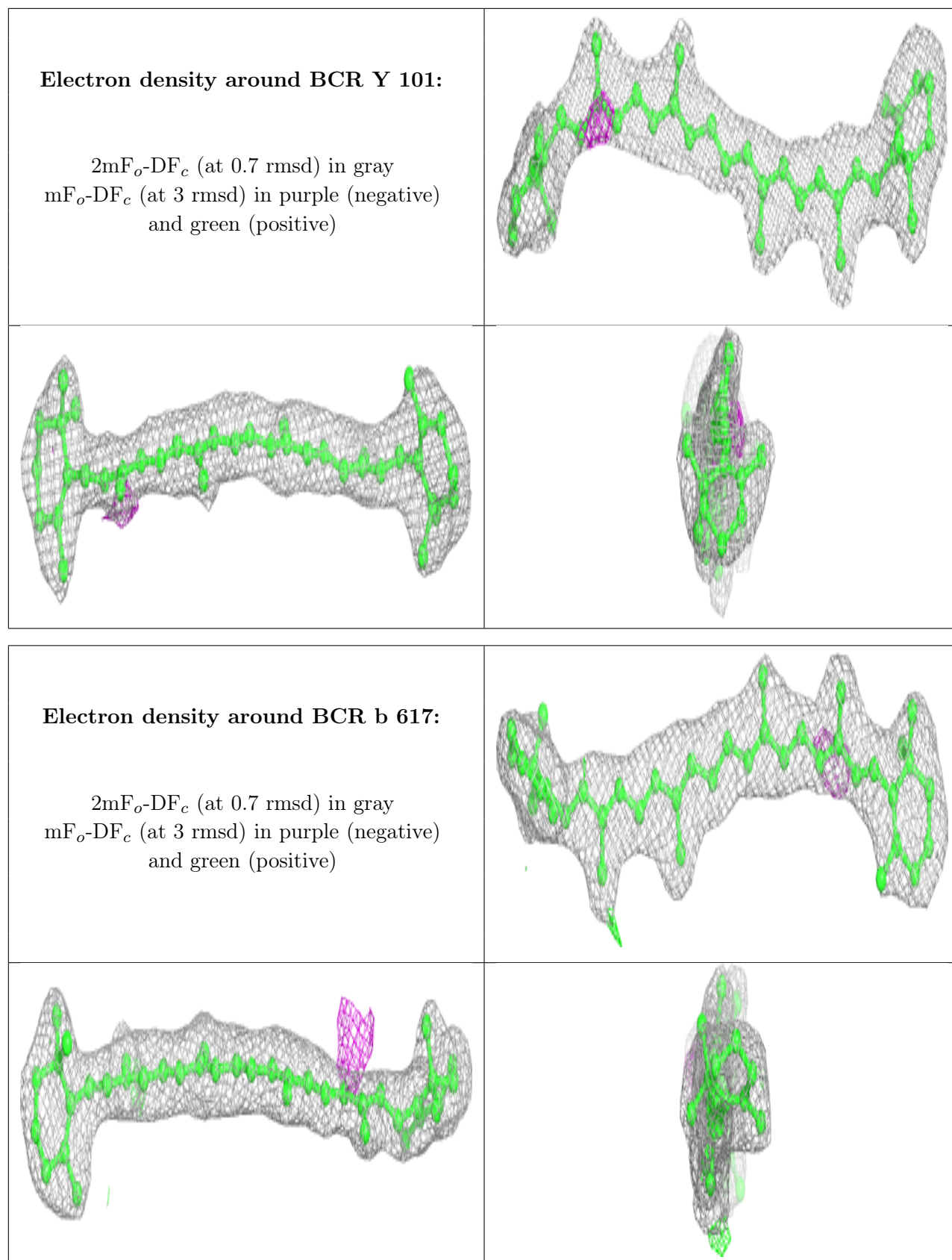
Electron density around CLA c 513:

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

**Electron density around BCR T 101:**

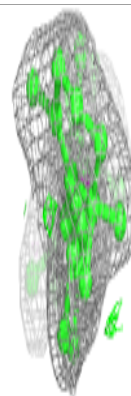
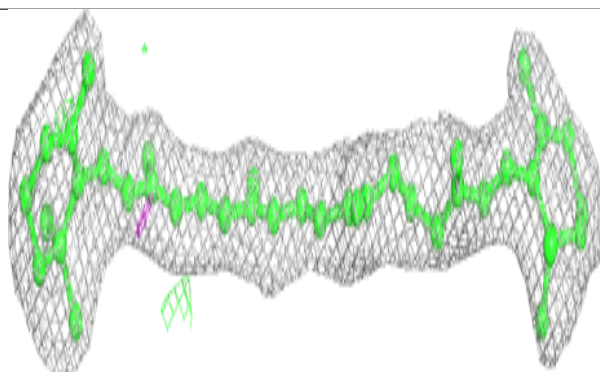
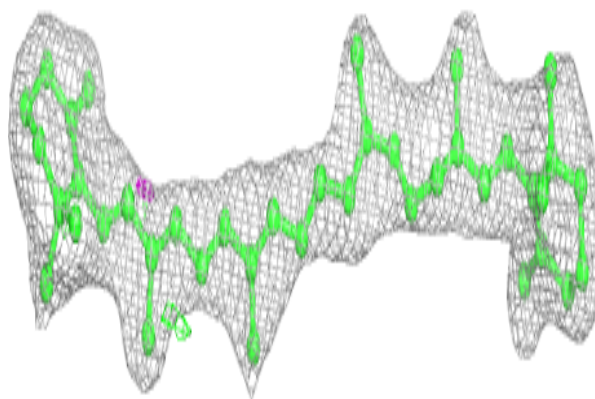
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



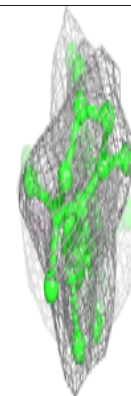
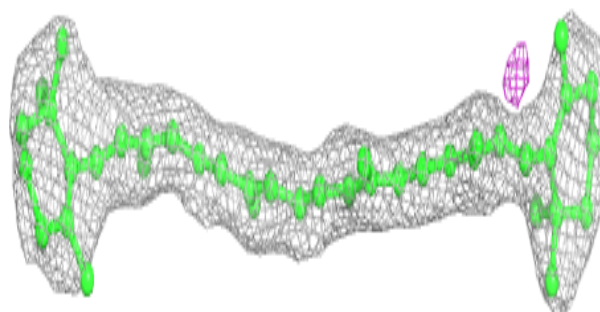
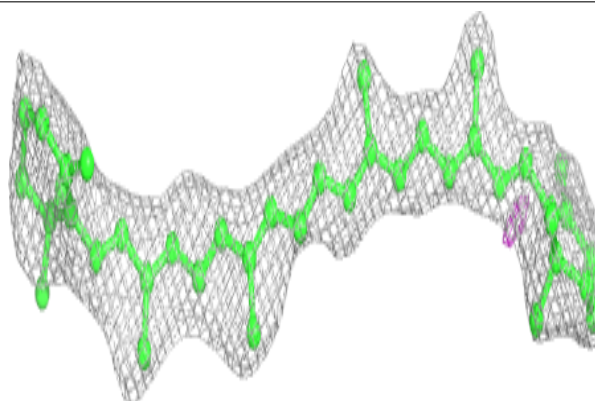


Electron density around BCR b 618:

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

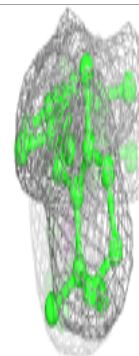
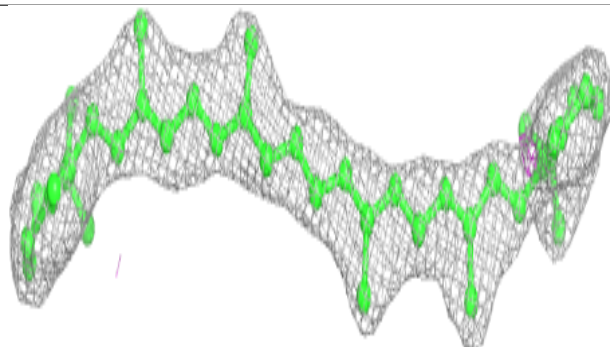
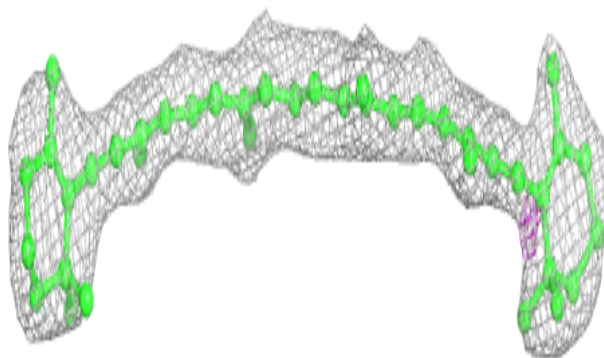
**Electron density around BCR c 521:**

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



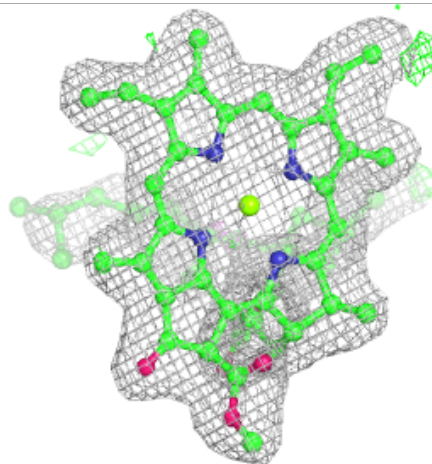
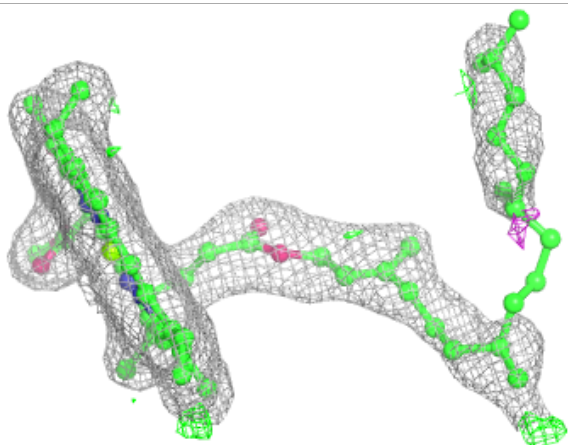
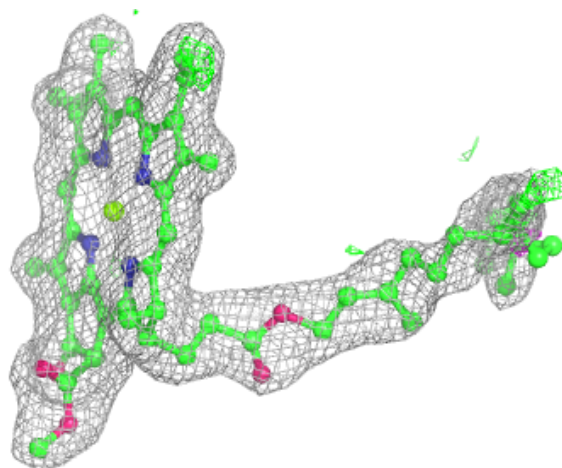
Electron density around BCR c 522:

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



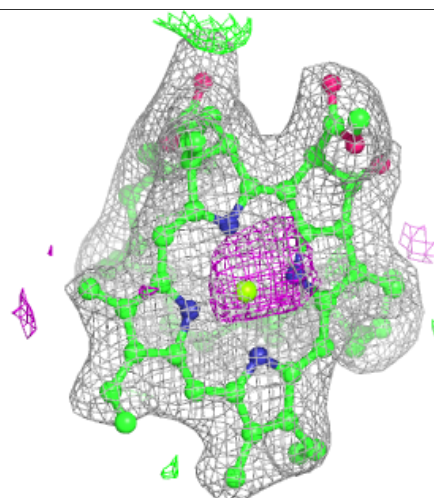
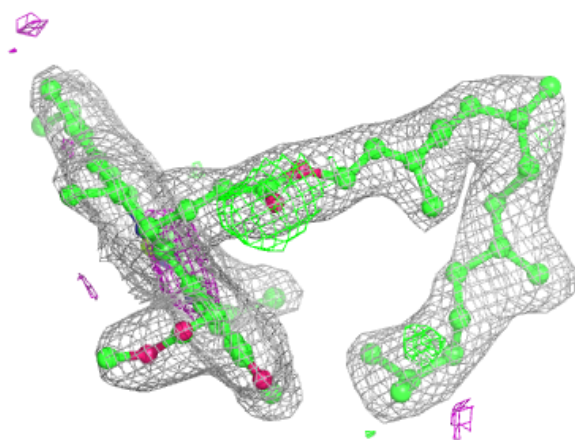
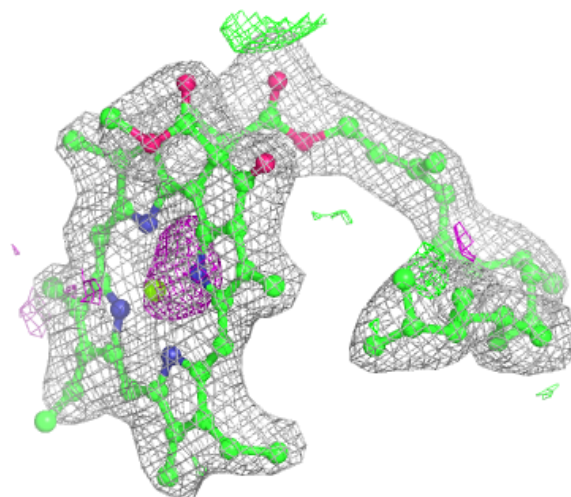
Electron density around CLA a 610:

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



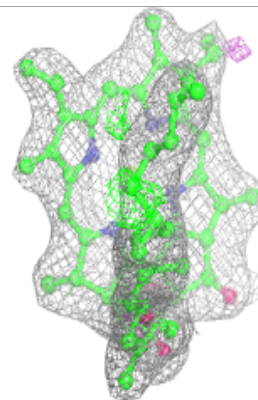
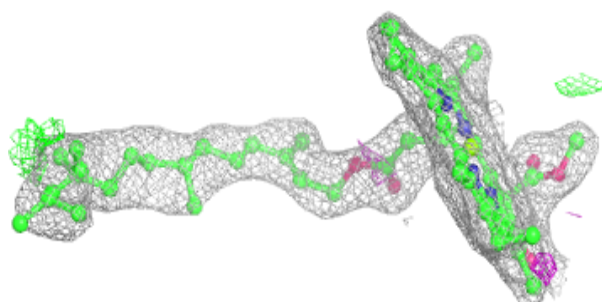
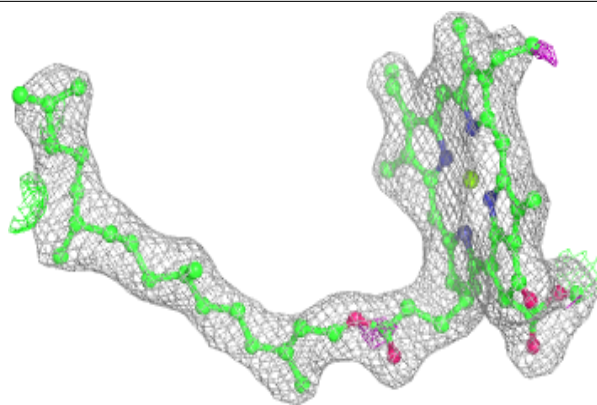
Electron density around CLA C 504:

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

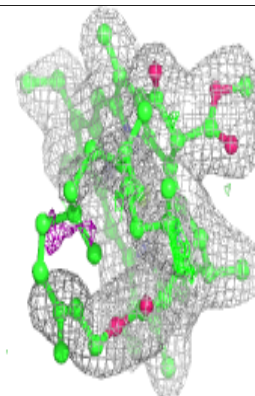
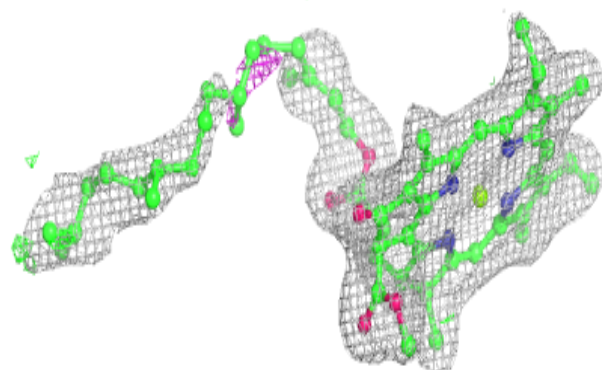
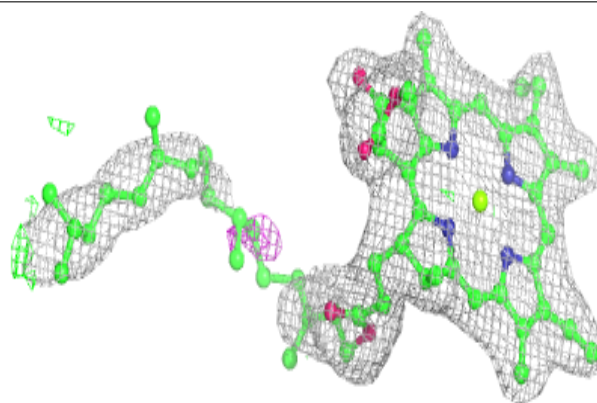


Electron density around CLA b 609:

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

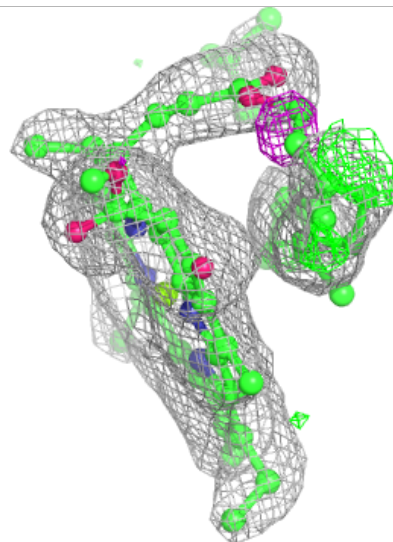
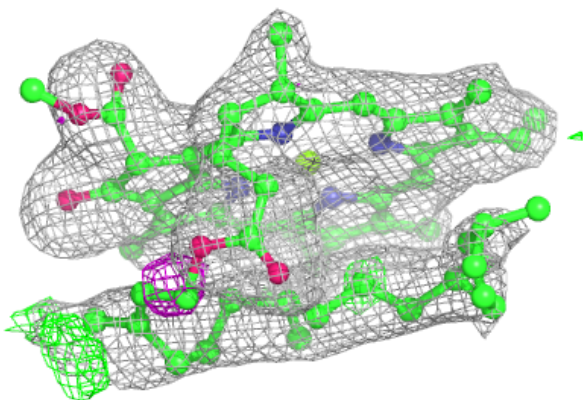
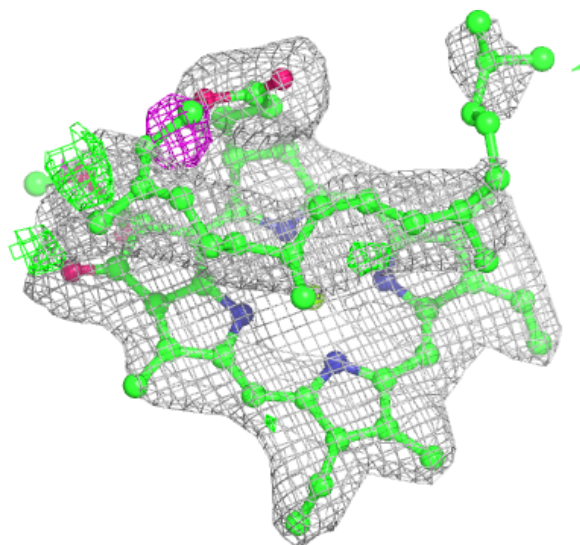
**Electron density around CLA c 506:**

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



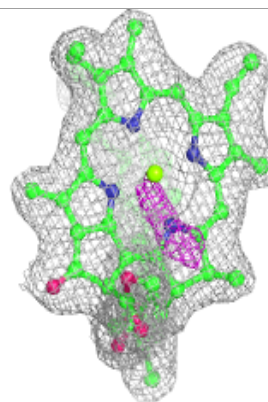
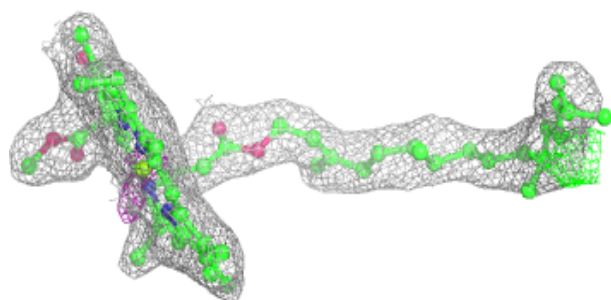
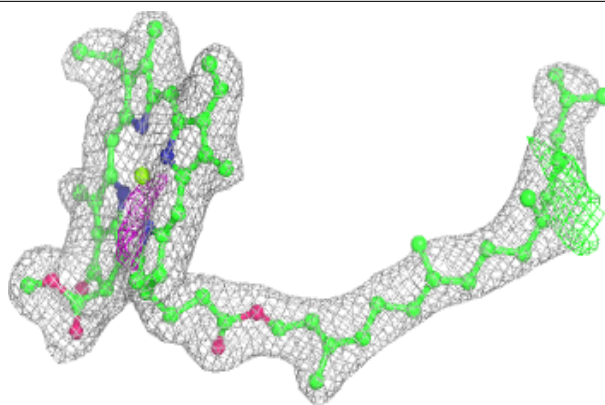
Electron density around CLA B 601:

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

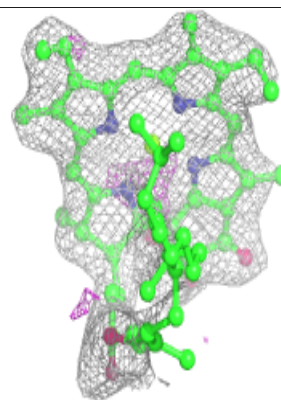
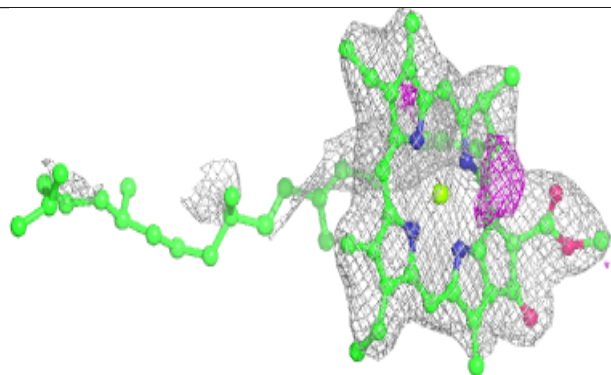
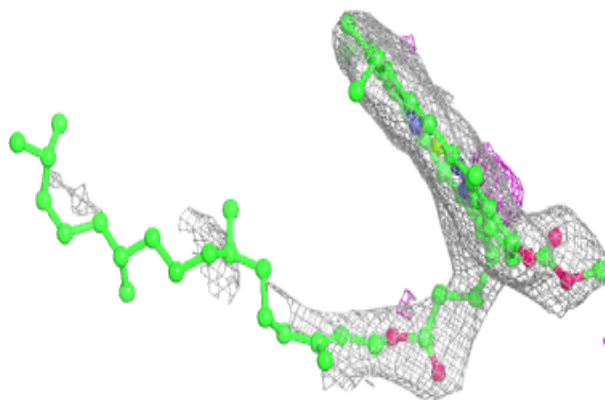


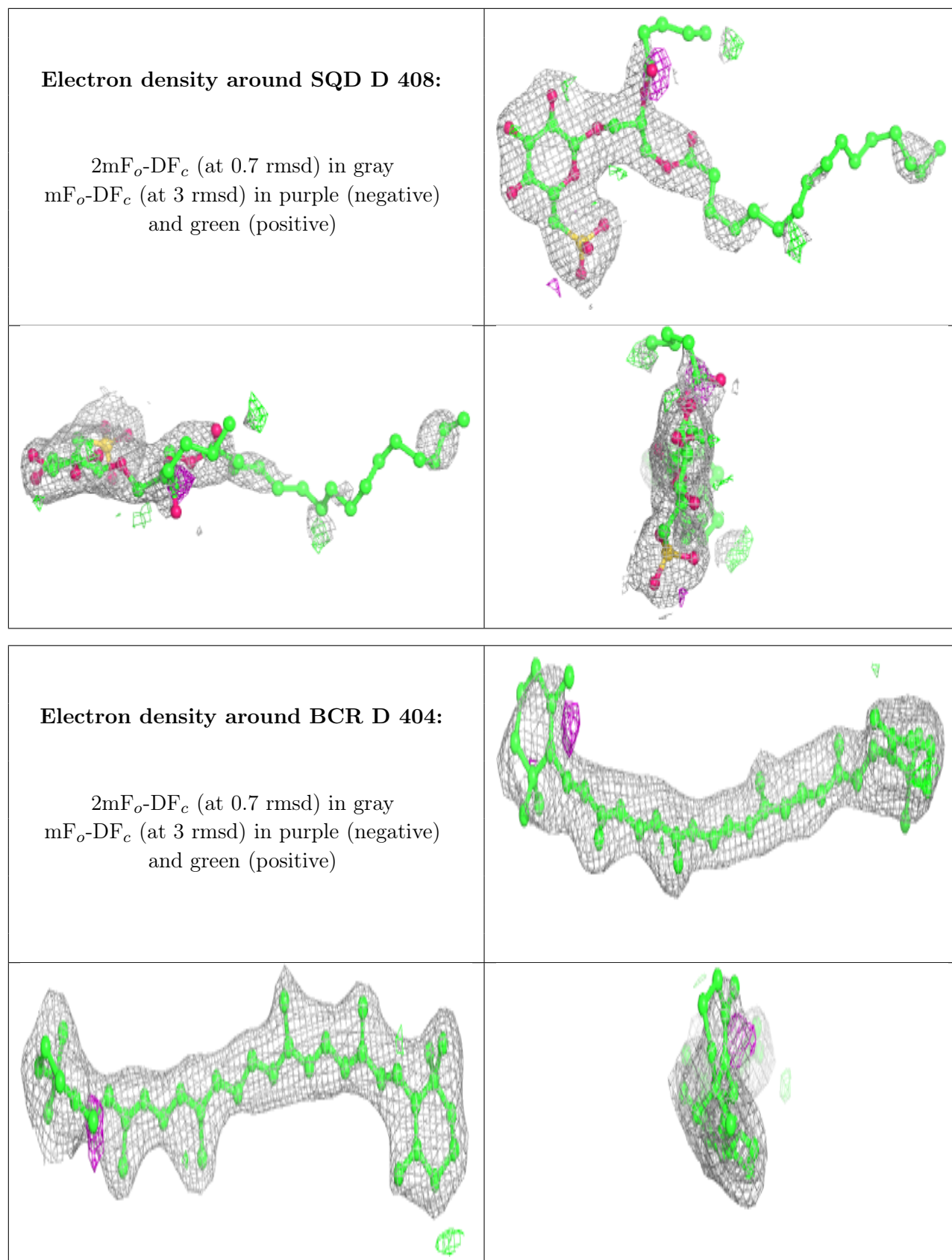
Electron density around CLA B 609:

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

**Electron density around CLA C 514:**

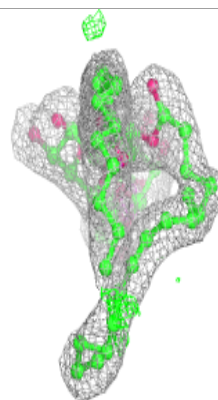
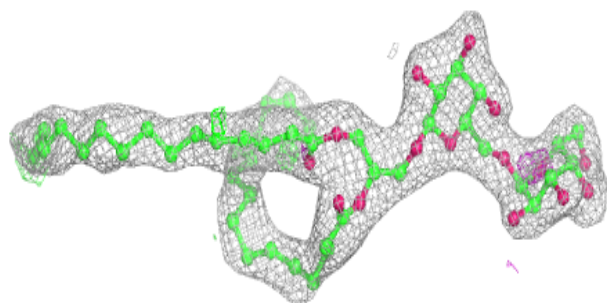
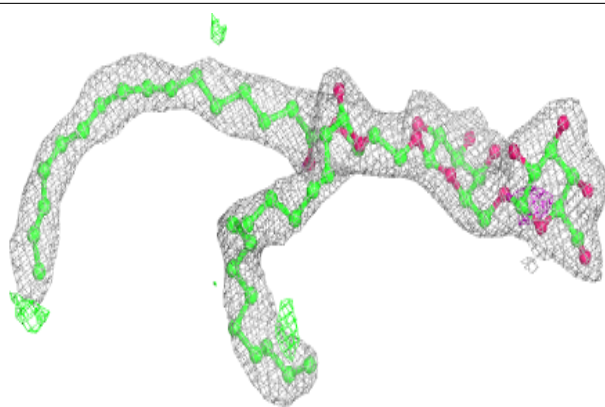
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



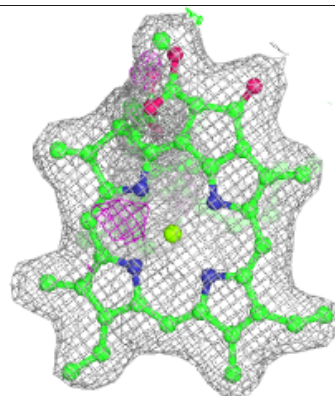
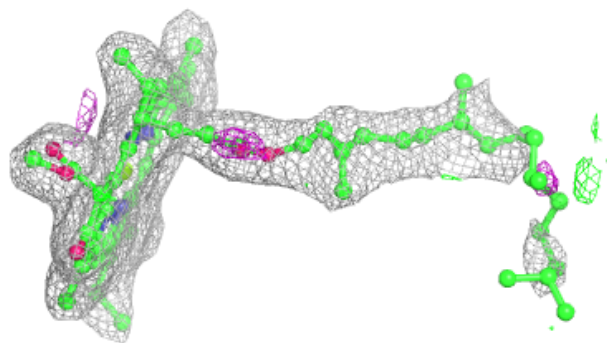
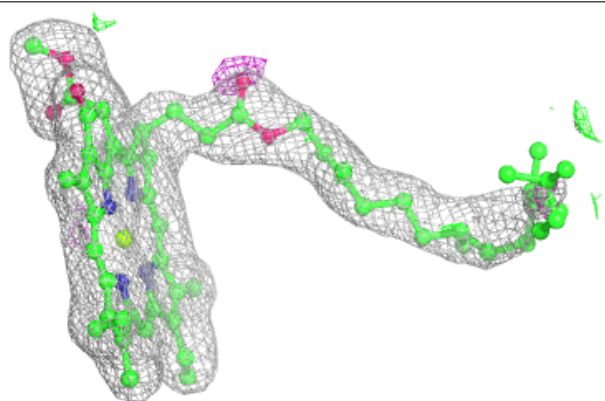


Electron density around DGD H 102:

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

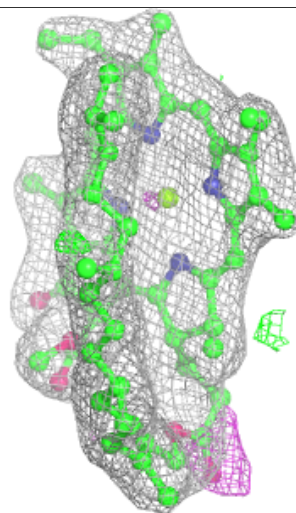
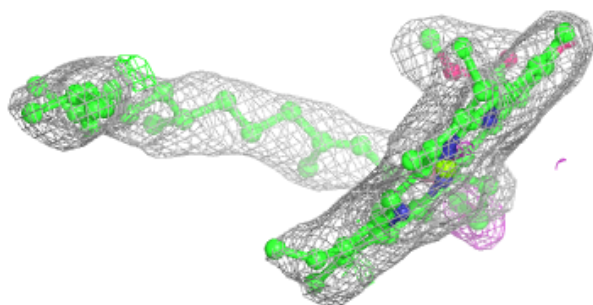
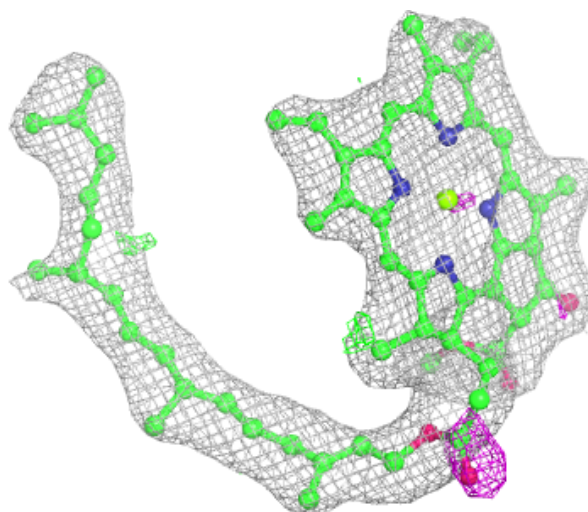
**Electron density around CLA D 403:**

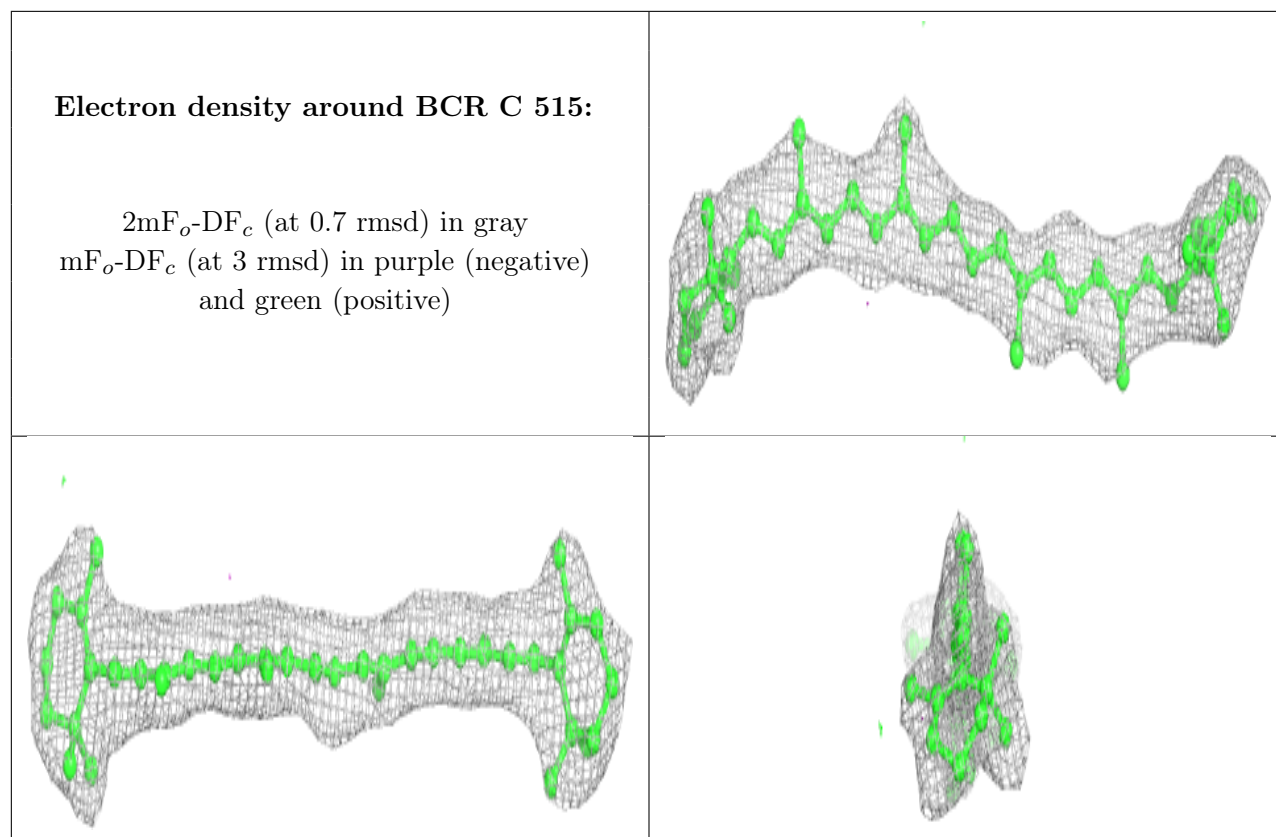
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 507:

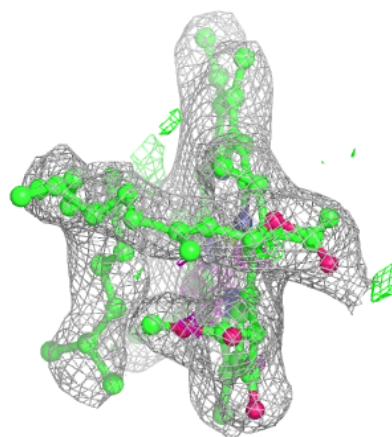
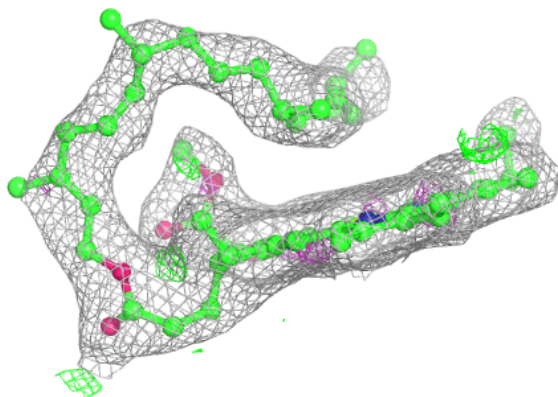
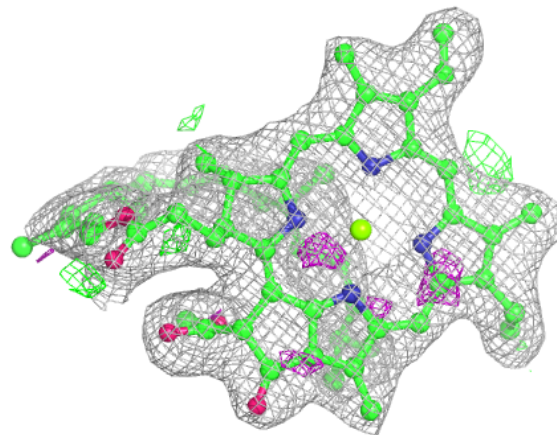
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





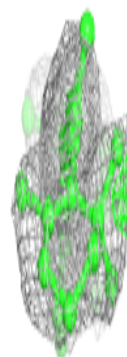
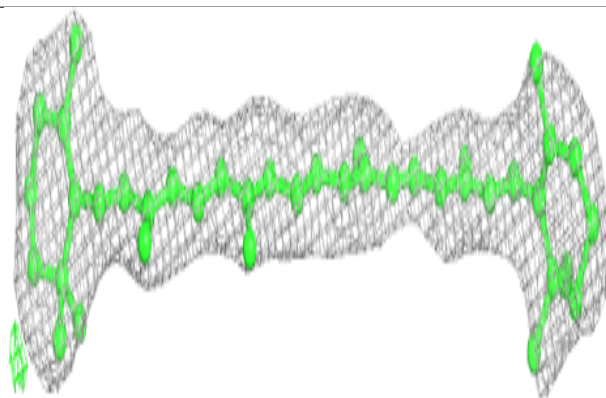
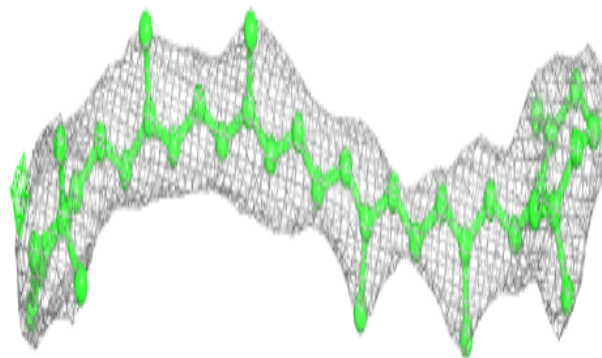
Electron density around CLA c 510:

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

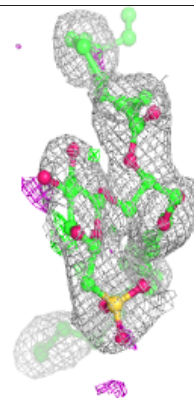
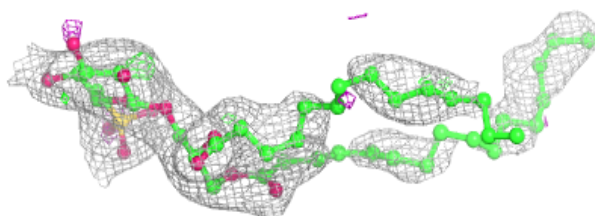
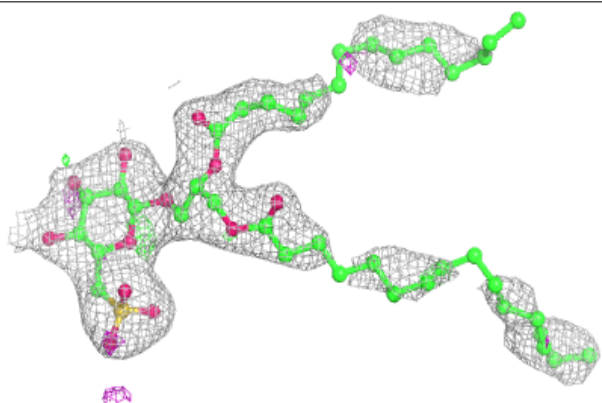


Electron density around BCR c 514:

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

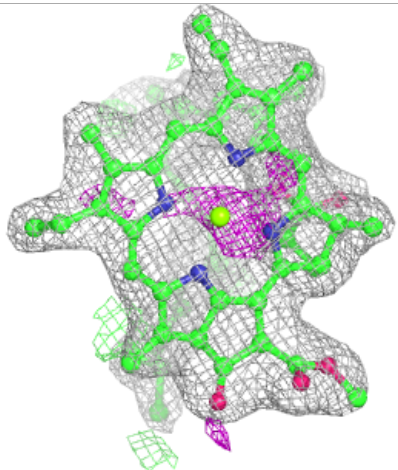
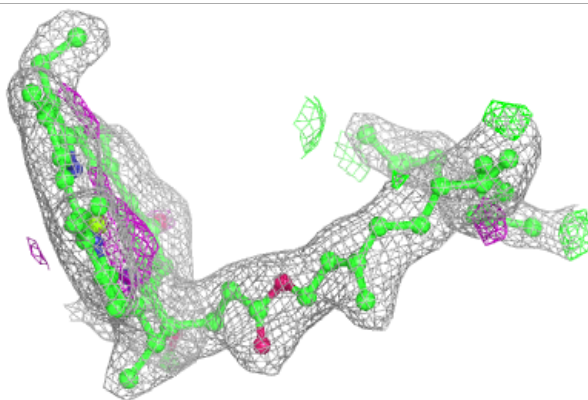
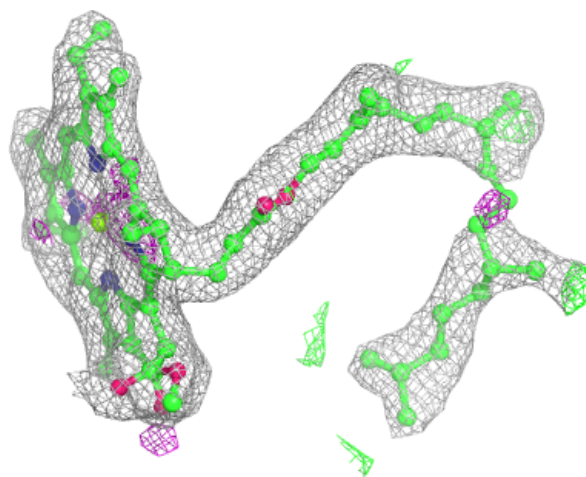
**Electron density around SQD A 612:**

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



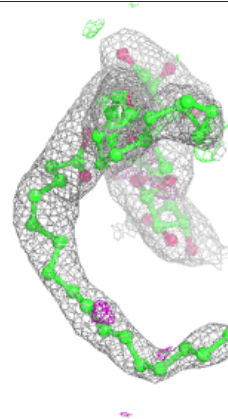
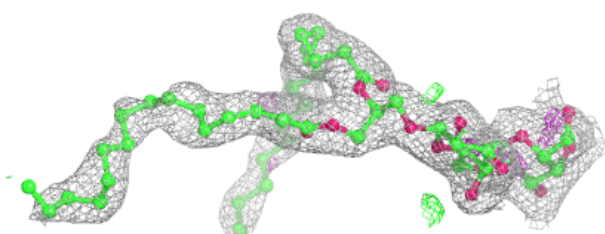
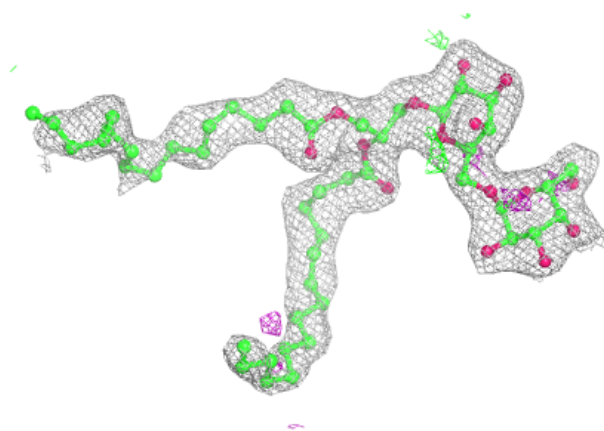
Electron density around CLA B 606:

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

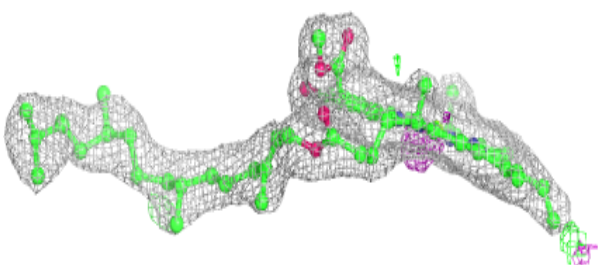
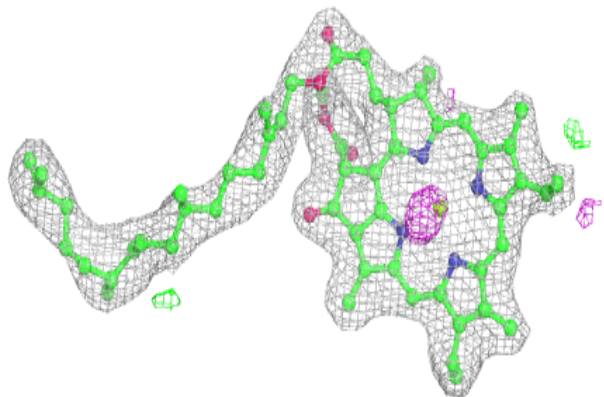


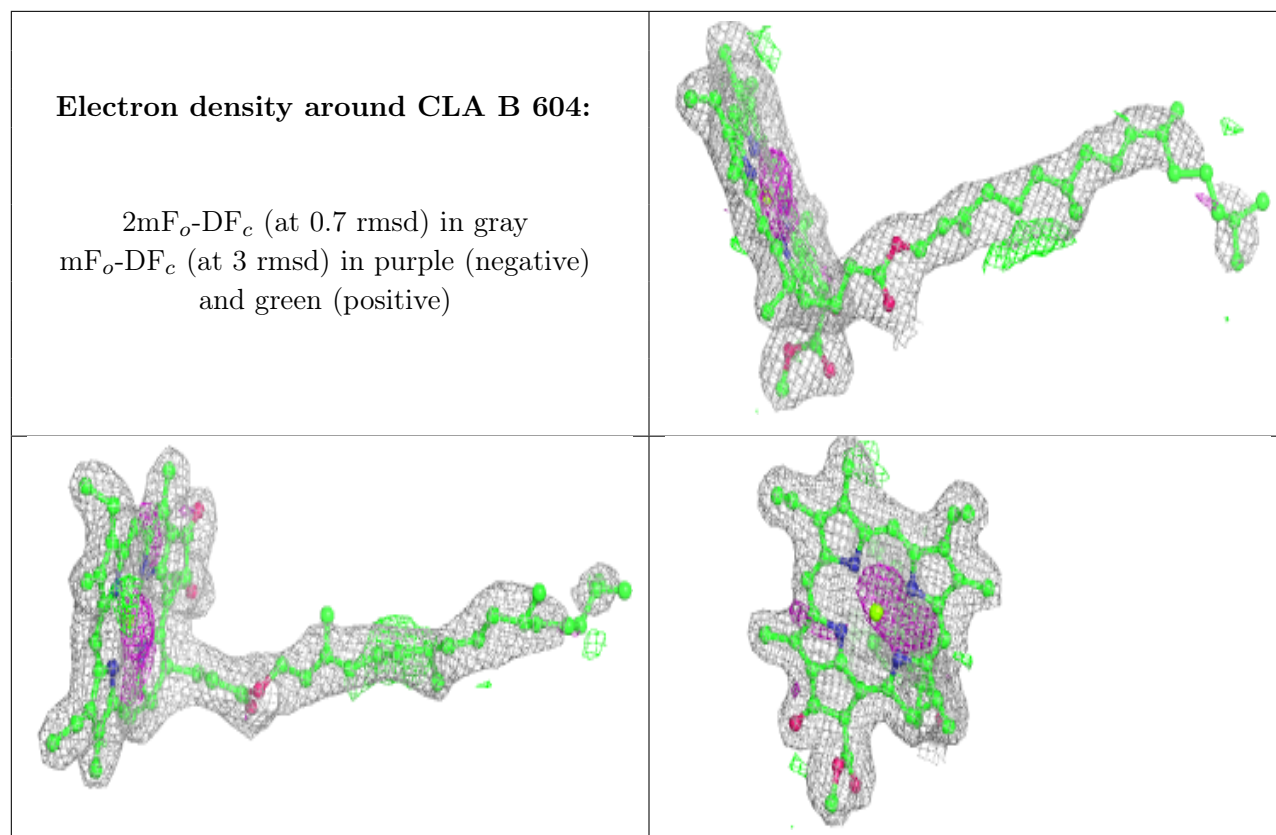
Electron density around DGD c 517:

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

**Electron density around CLA b 602:**

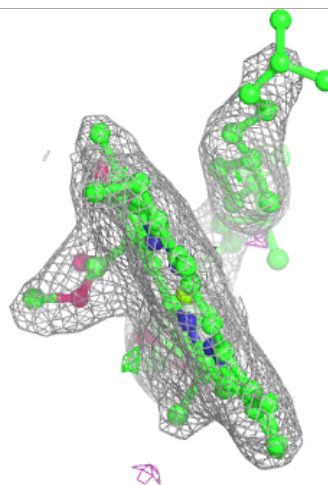
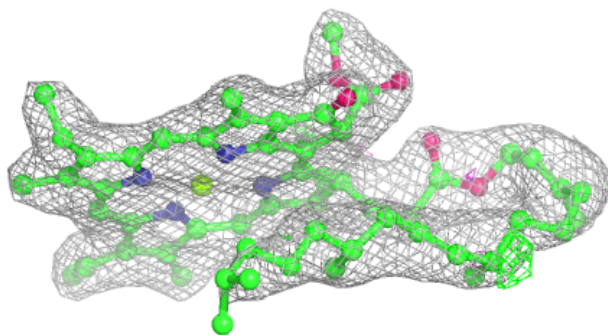
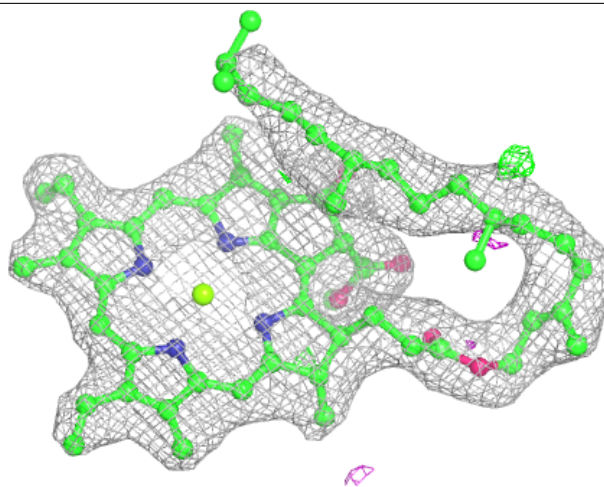
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





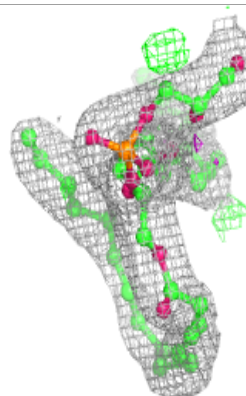
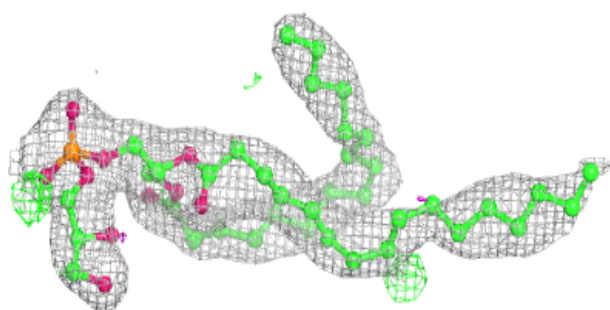
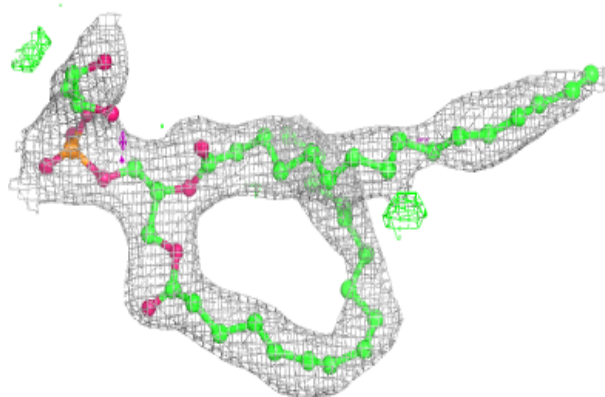
Electron density around CLA C 510:

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

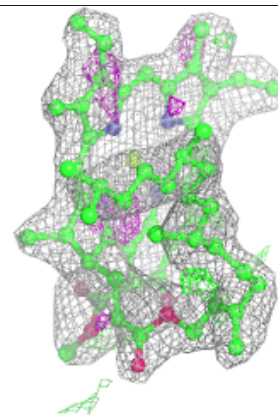
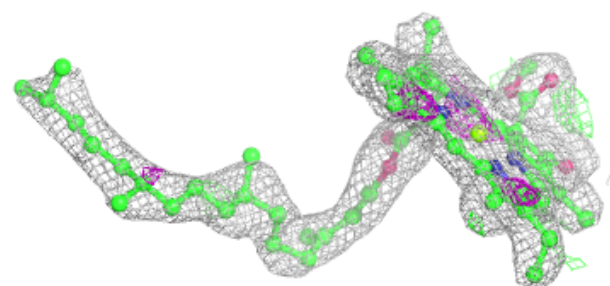
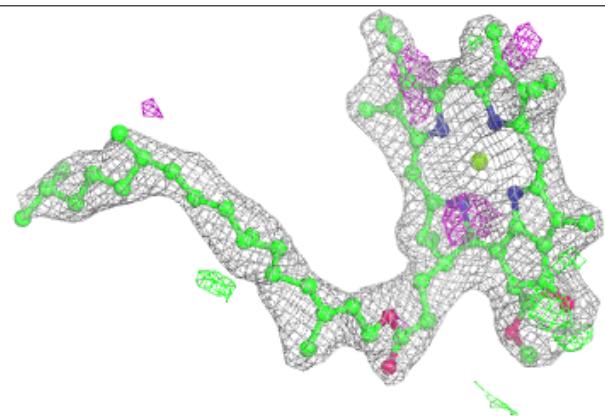


Electron density around LHG d 405:

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

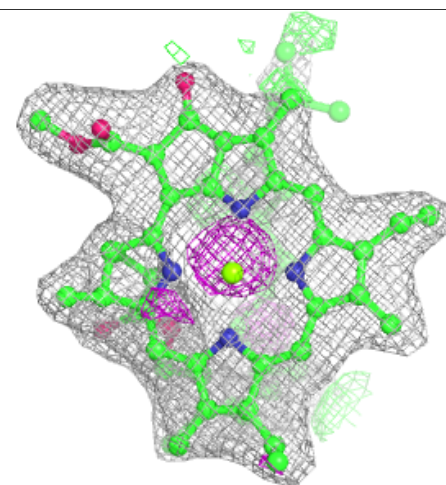
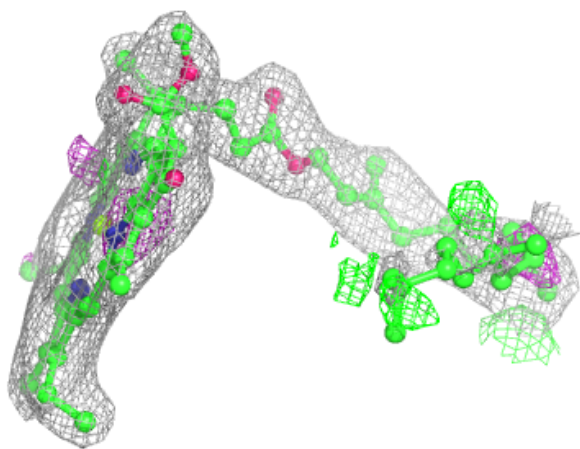
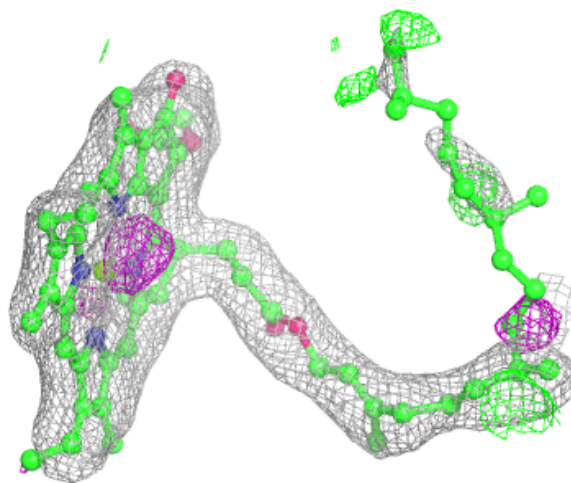
**Electron density around CLA C 512:**

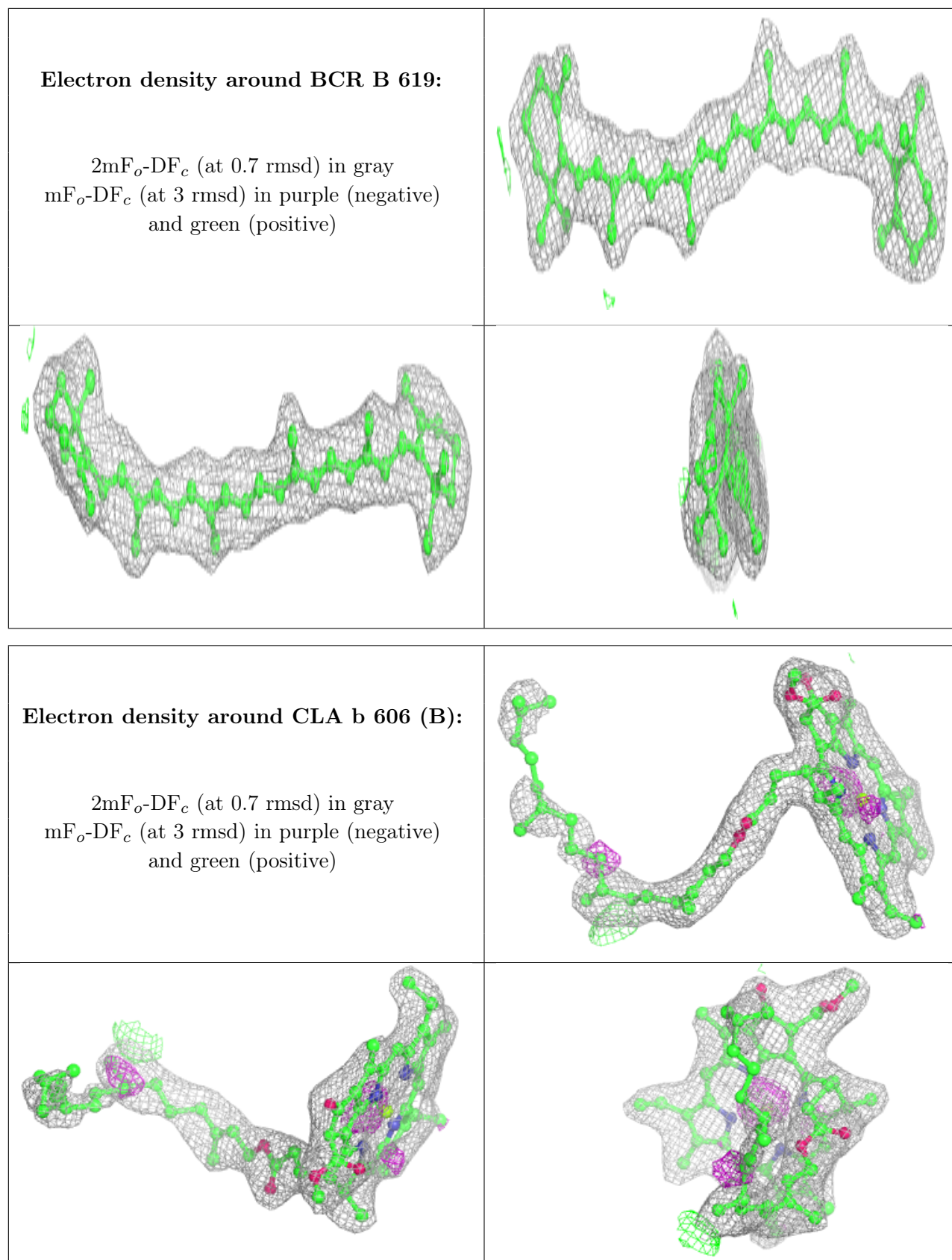
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

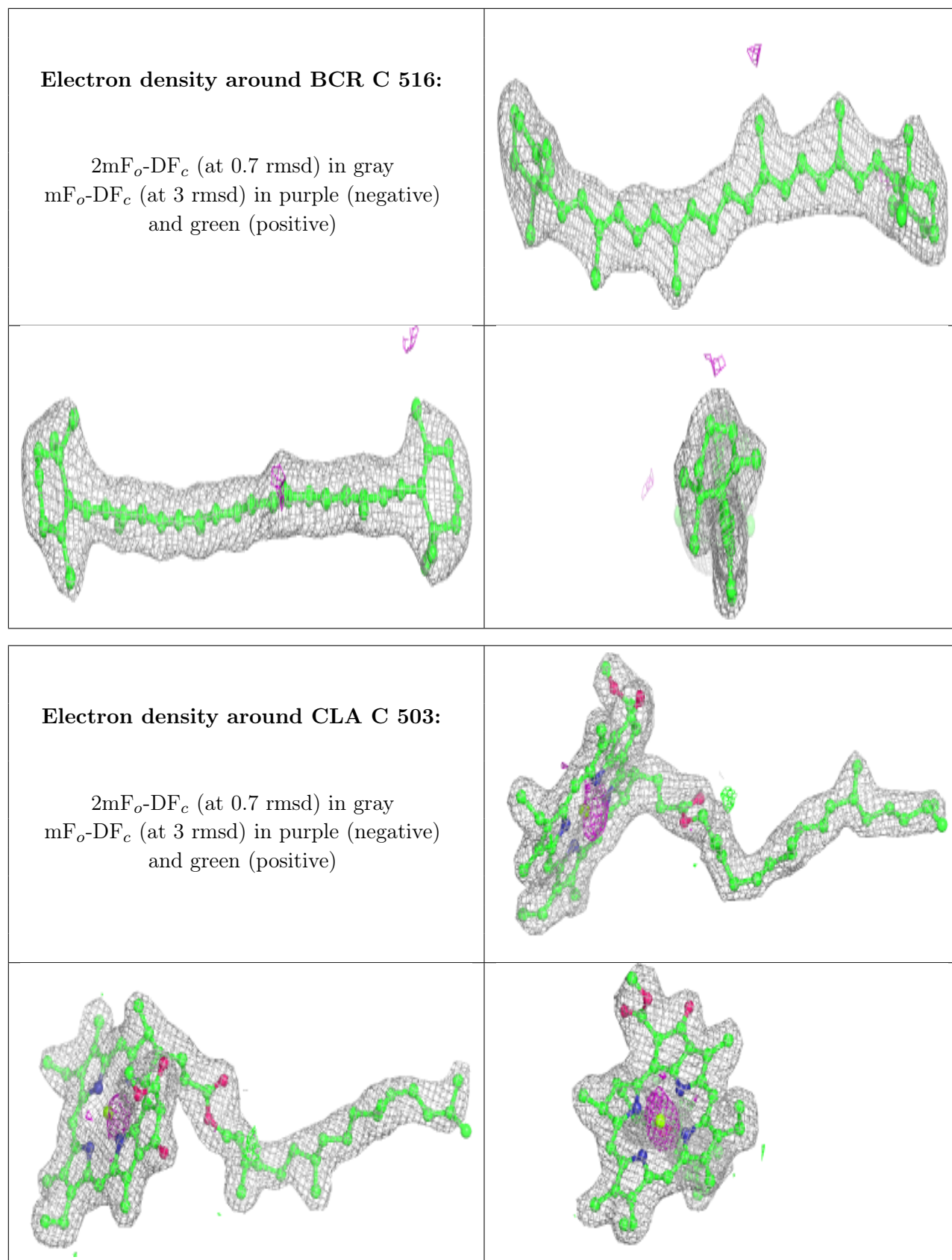


Electron density around CLA b 606 (A):

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

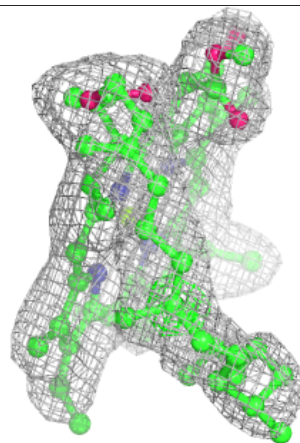
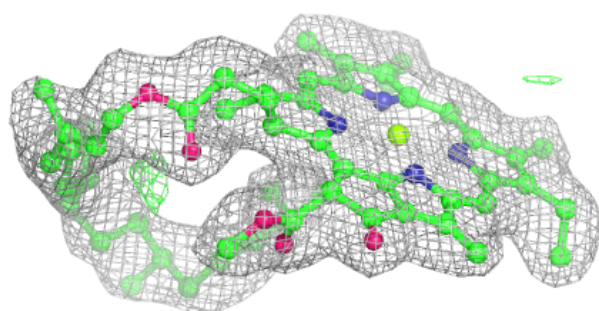
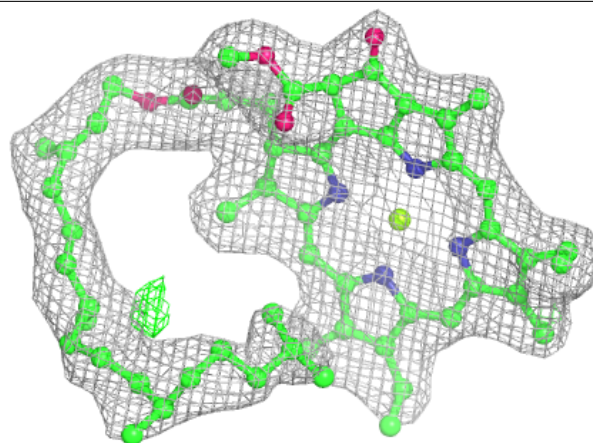




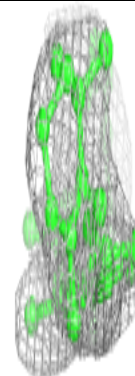
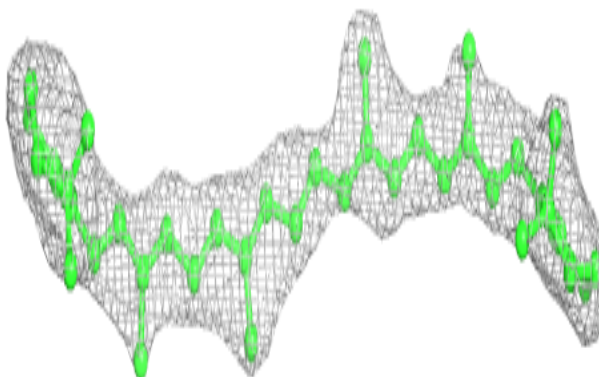
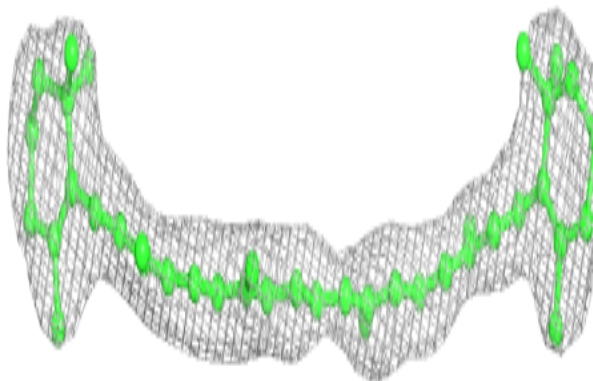


Electron density around CLA b 615:

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

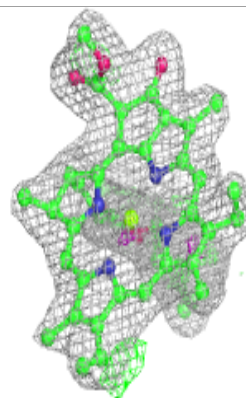
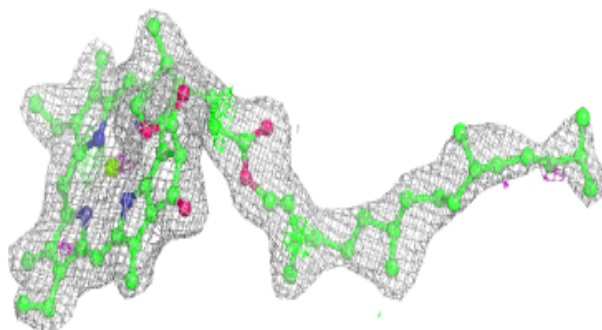
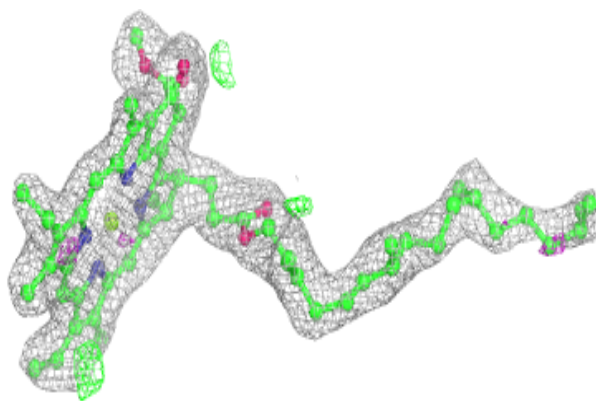
**Electron density around BCR K 101:**

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



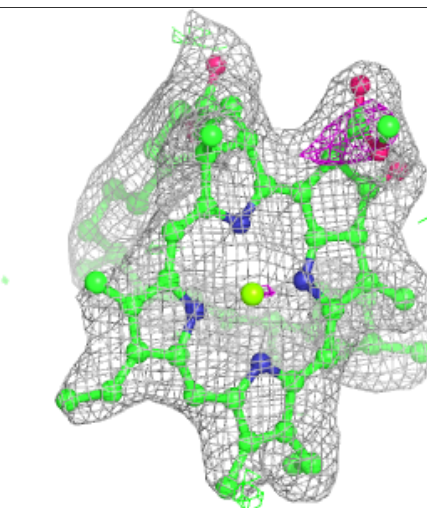
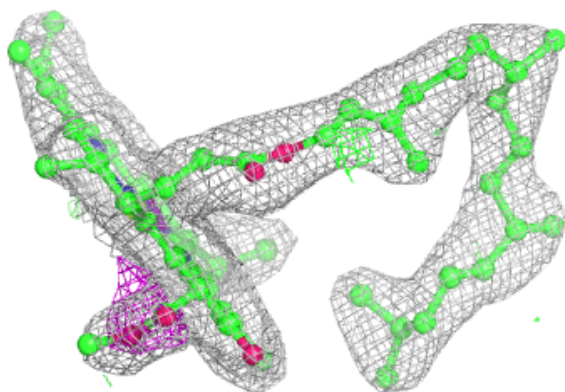
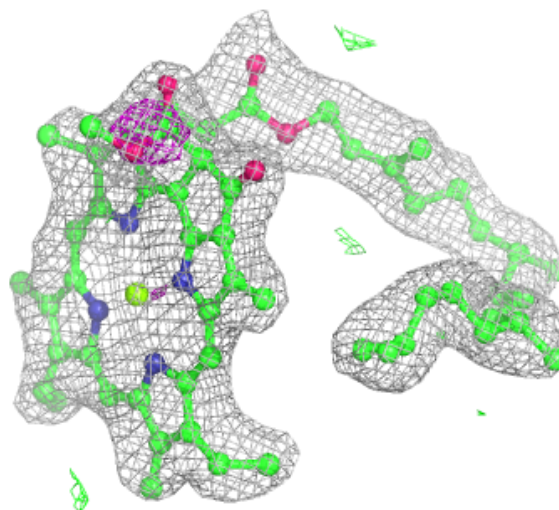
Electron density around CLA c 502:

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



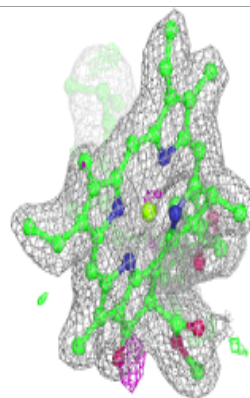
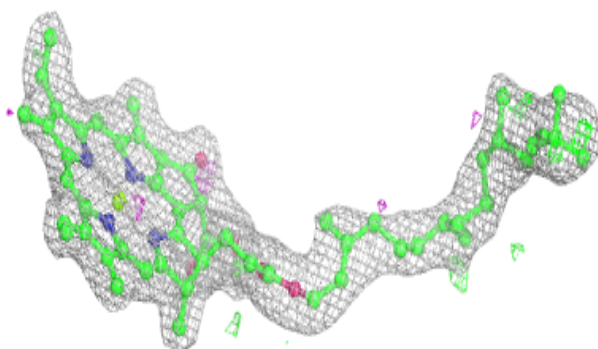
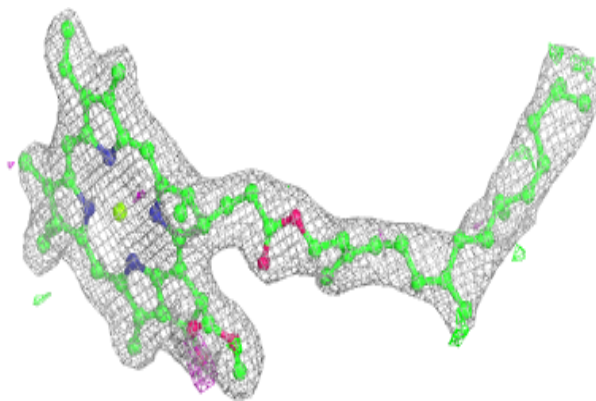
Electron density around CLA c 503:

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

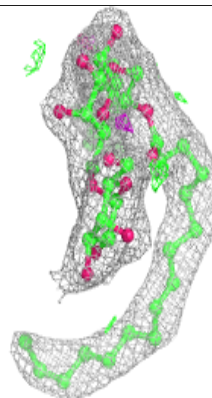
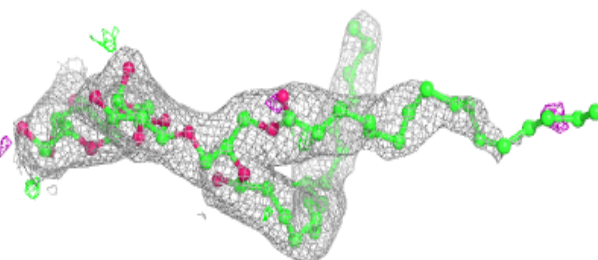
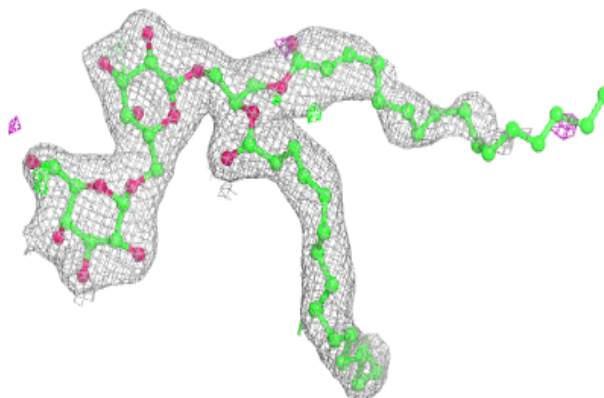


Electron density around CLA A 606:

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

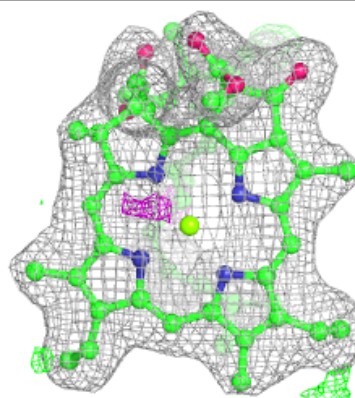
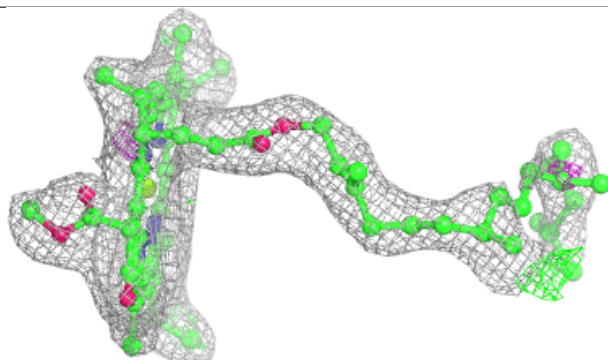
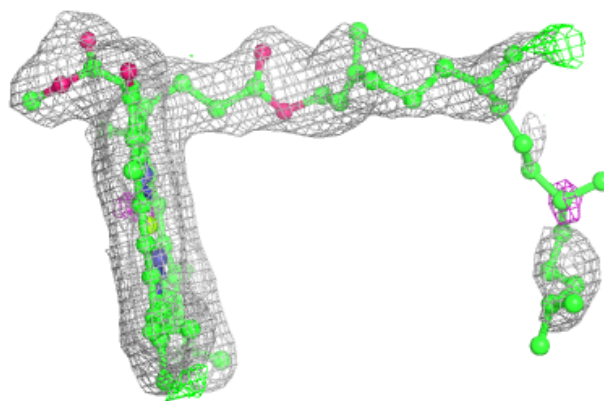
**Electron density around DGD C 518:**

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

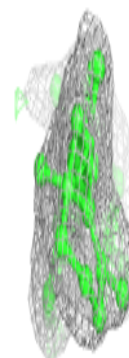
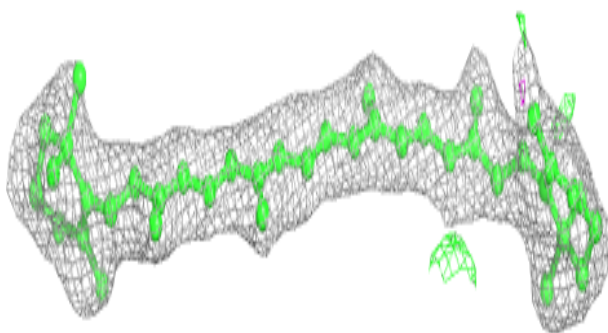
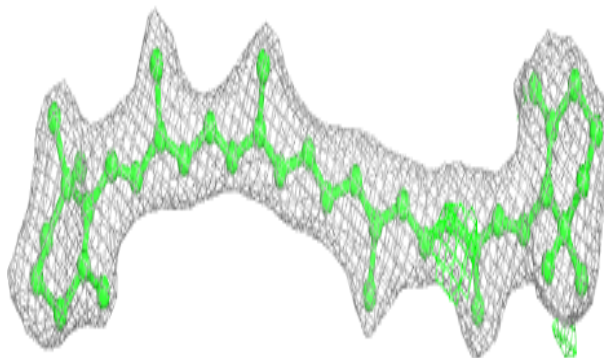


Electron density around CLA C 507:

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

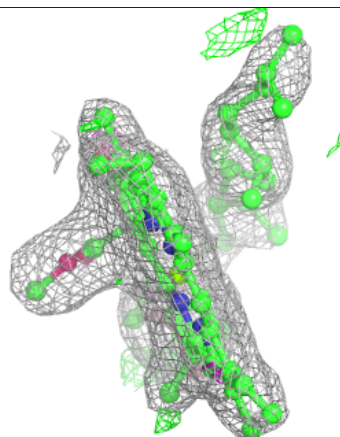
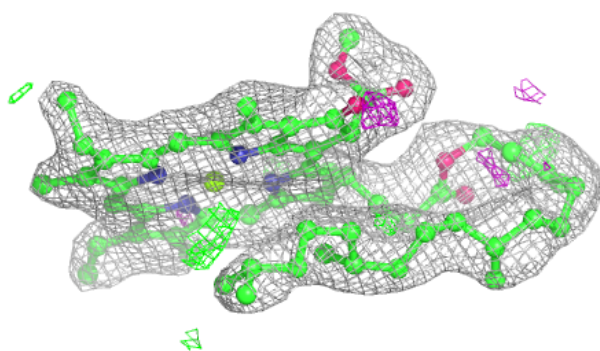
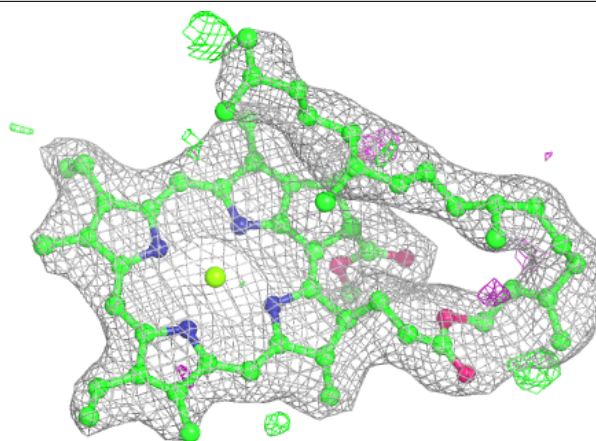
**Electron density around BCR b 619:**

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

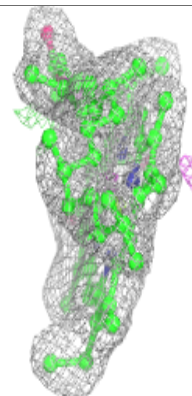
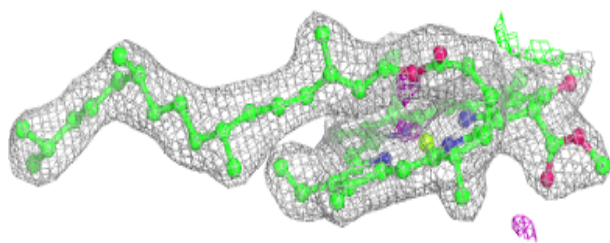
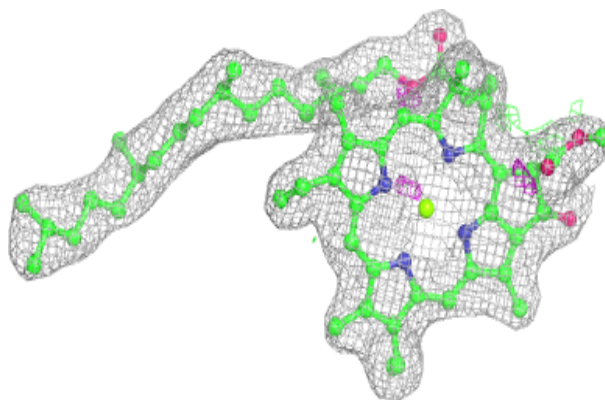


Electron density around CLA c 509:

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

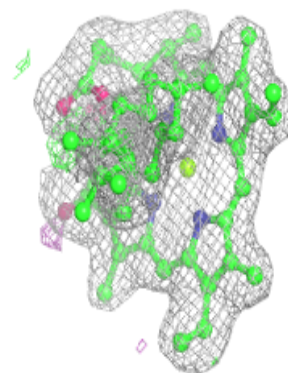
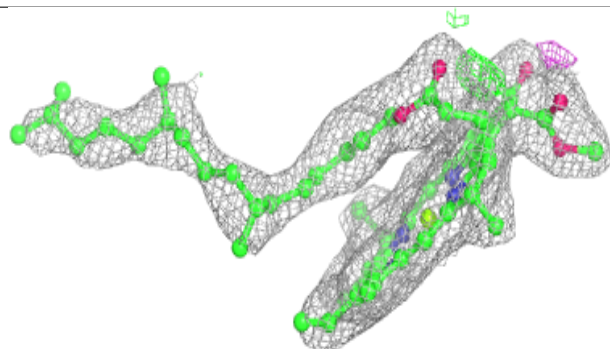
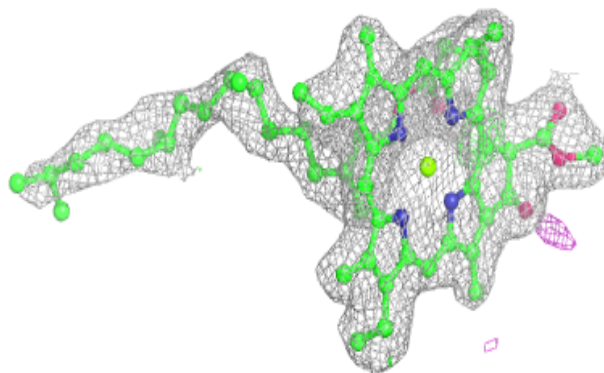
**Electron density around CLA c 501:**

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

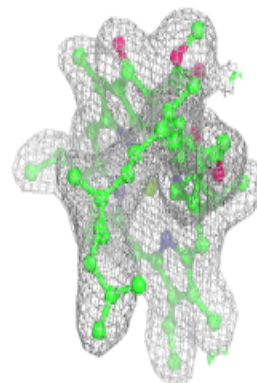
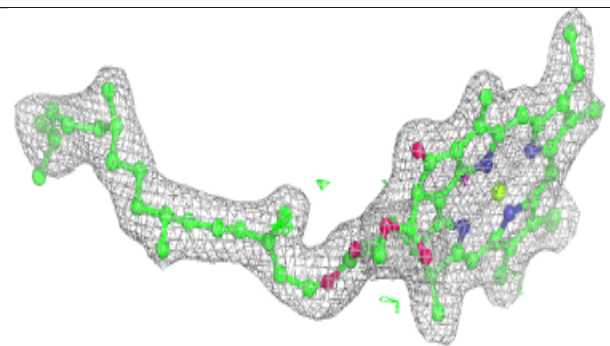
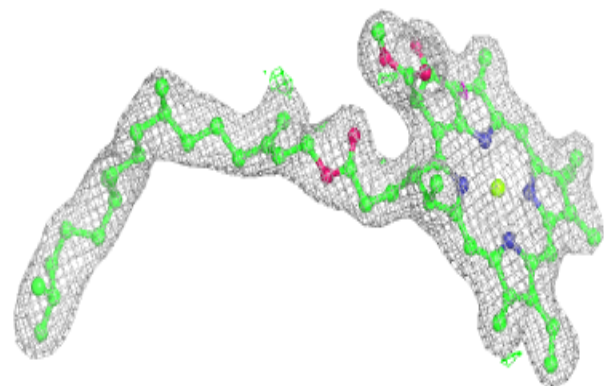


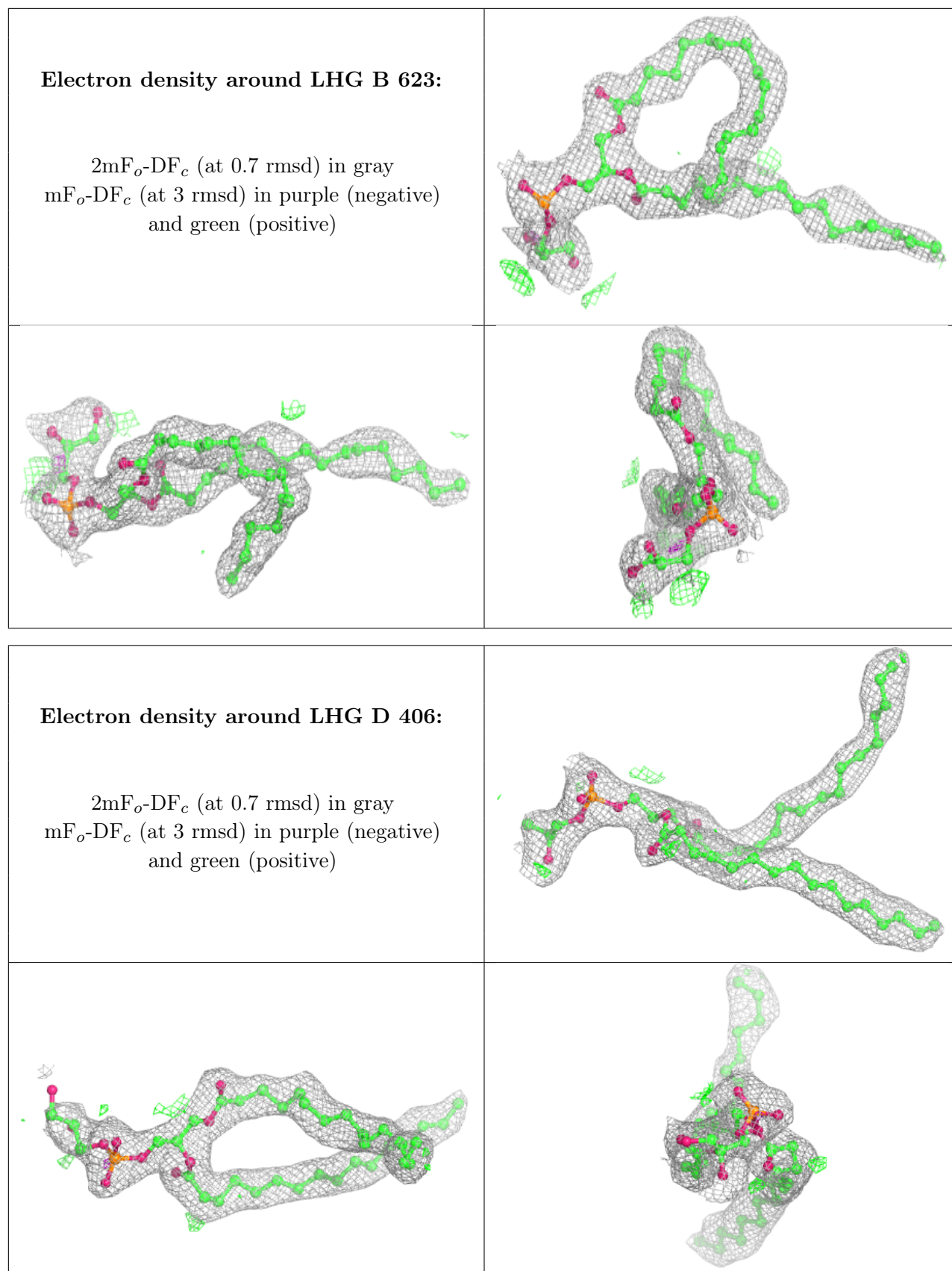
Electron density around CLA C 506:

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

**Electron density around CLA a 606:**

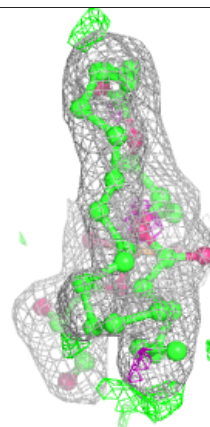
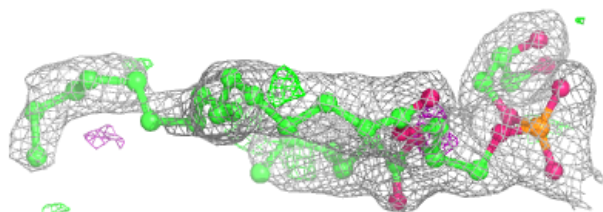
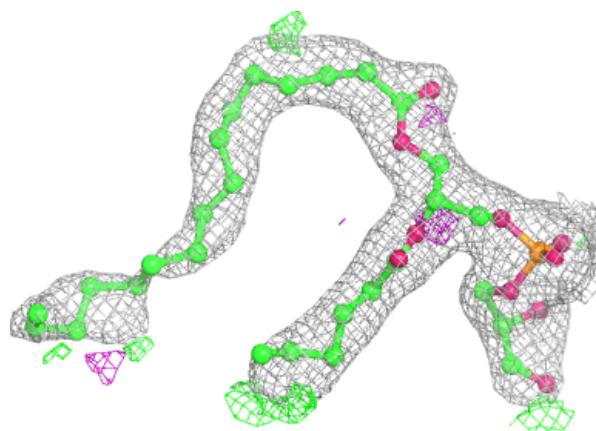
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



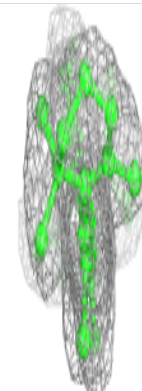
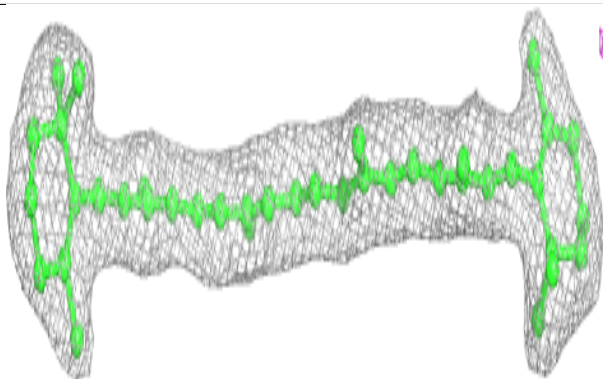
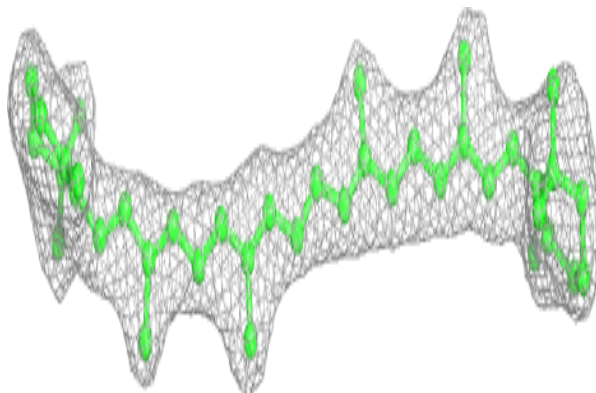


Electron density around LHG a 616:

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

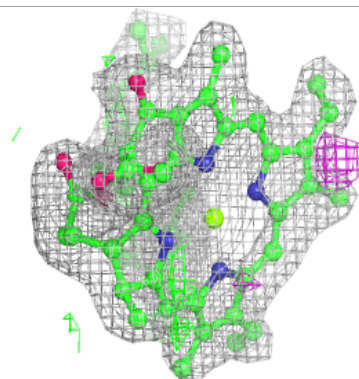
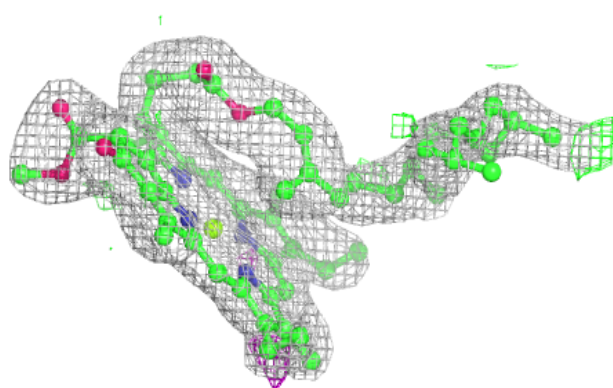
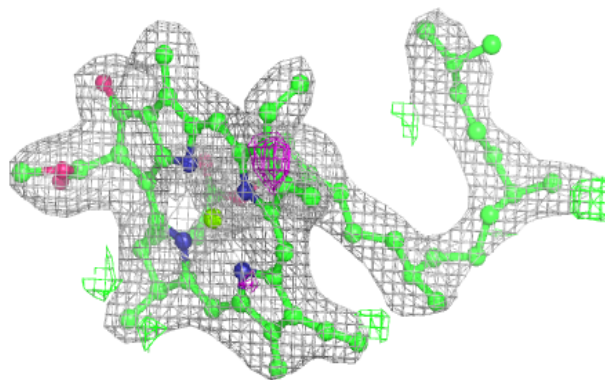
**Electron density around BCR a 611:**

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



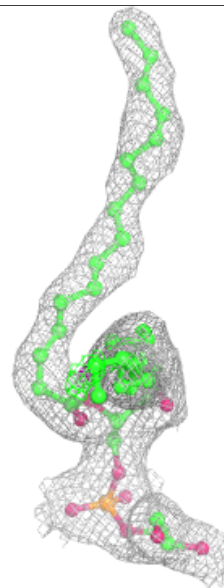
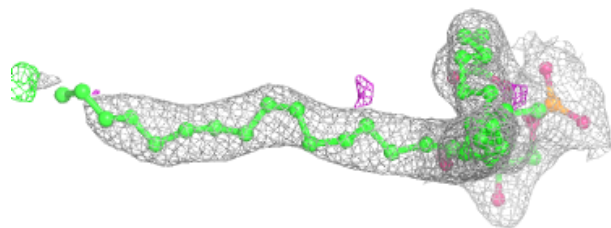
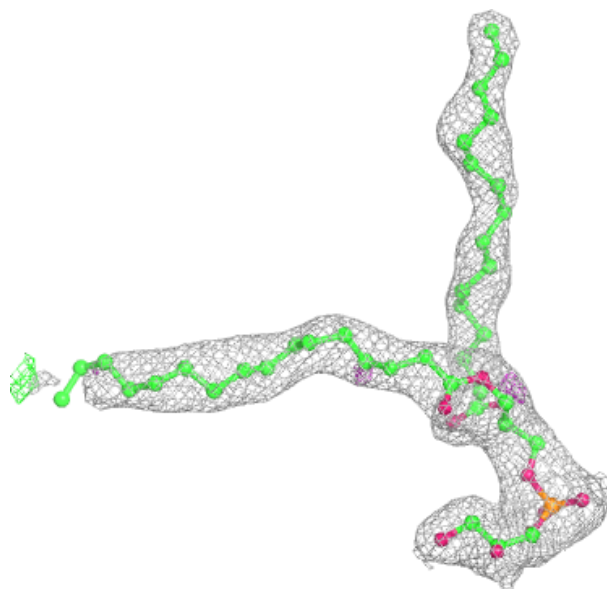
Electron density around CLA c 505:

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



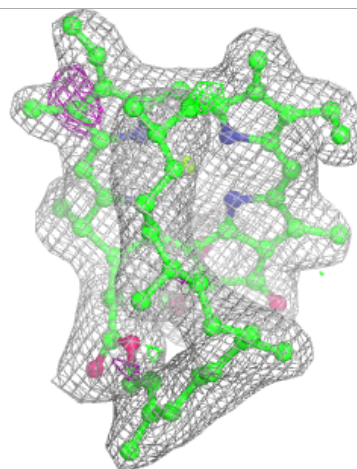
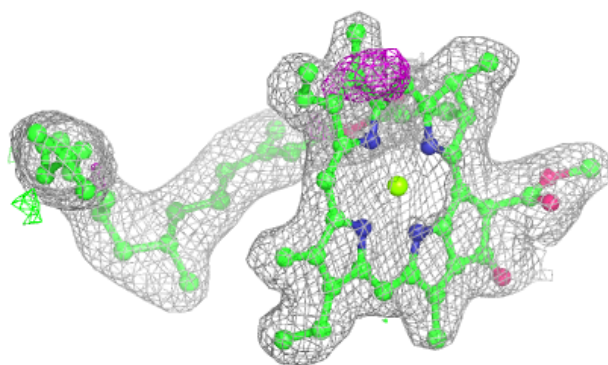
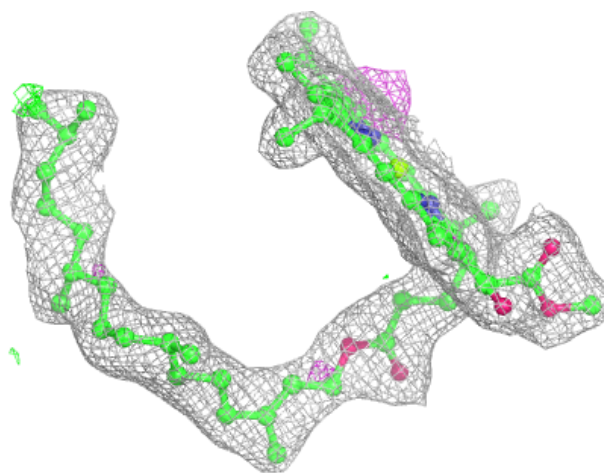
Electron density around LHG 1 101:

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



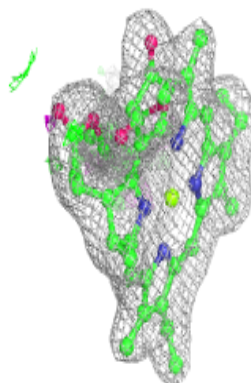
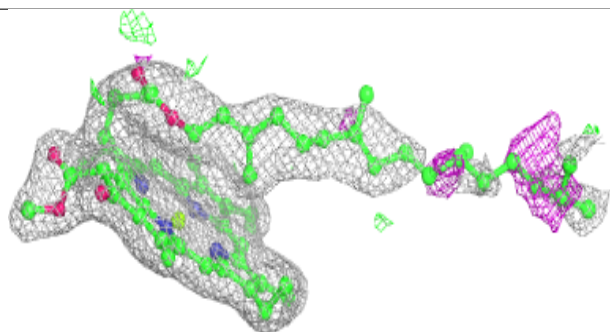
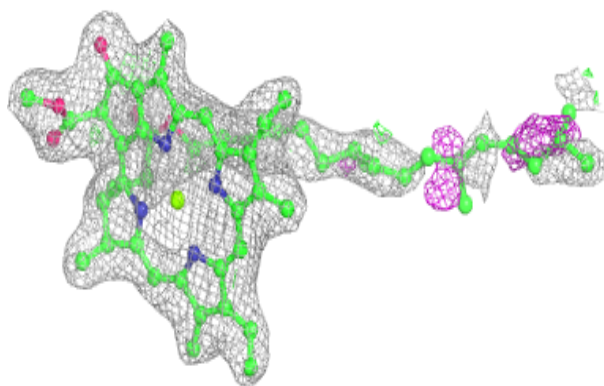
Electron density around CLA B 611:

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

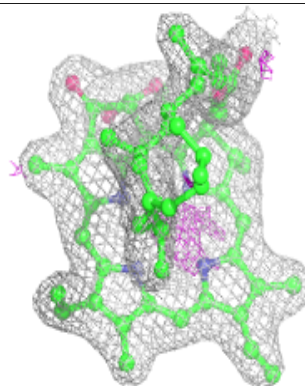
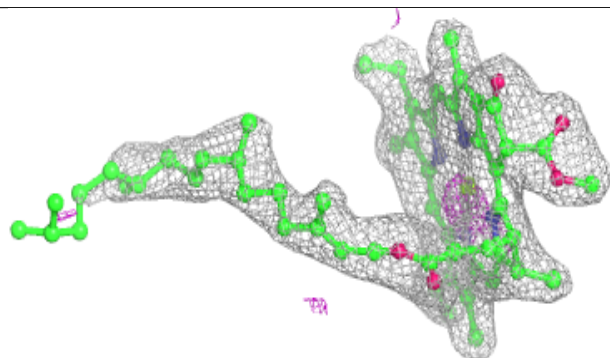
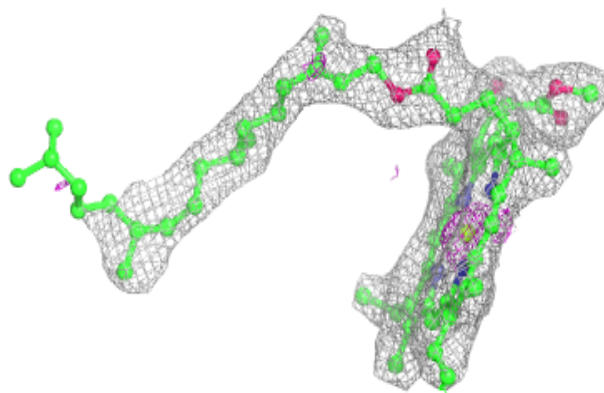


Electron density around CLA B 614:

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

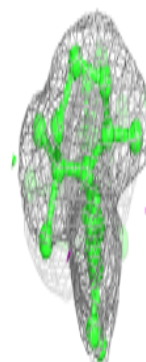
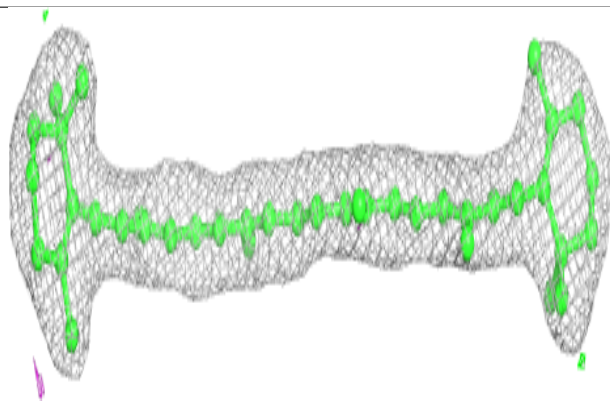
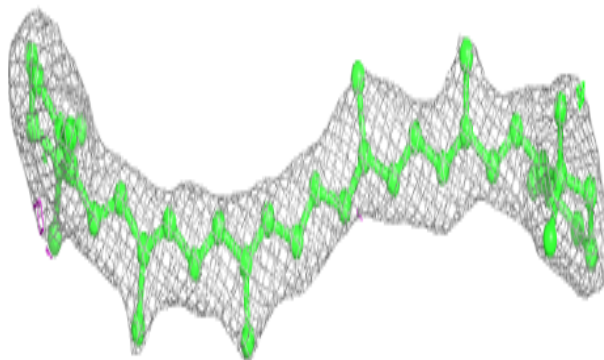
**Electron density around CLA C 509:**

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

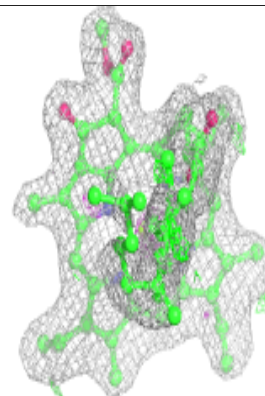
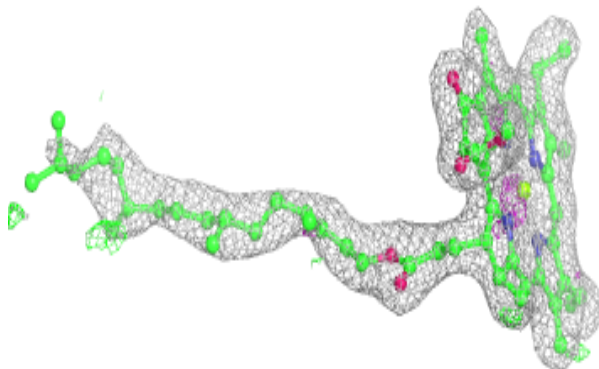
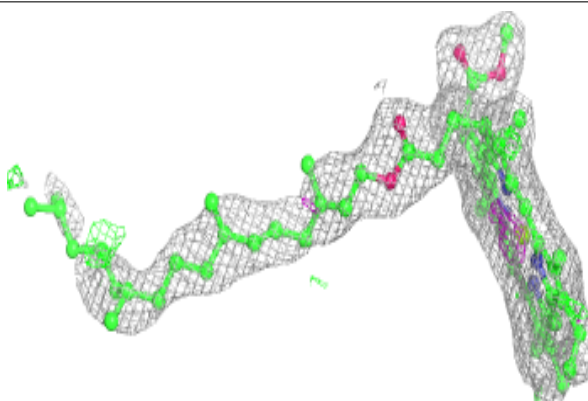


Electron density around BCR c 515:

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

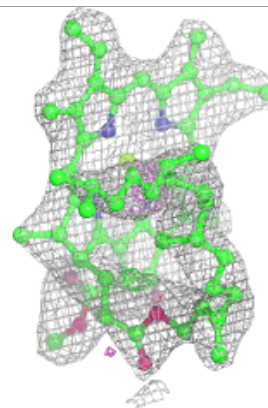
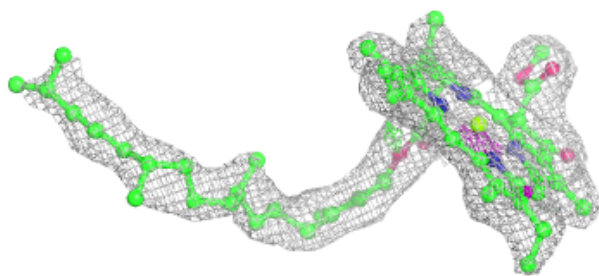
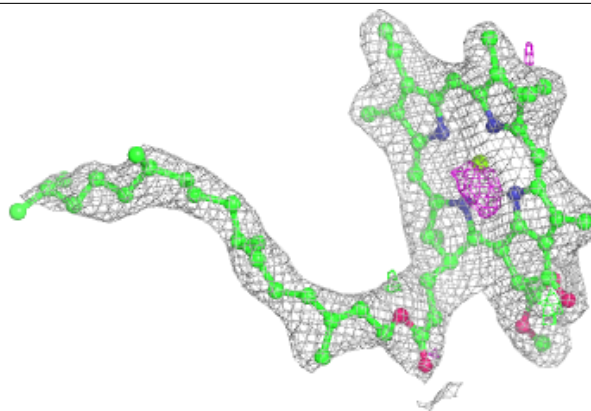
**Electron density around CLA b 604:**

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



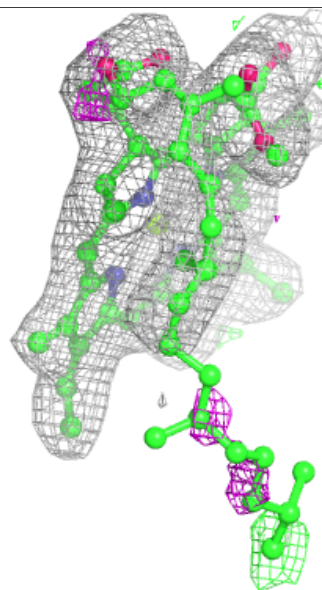
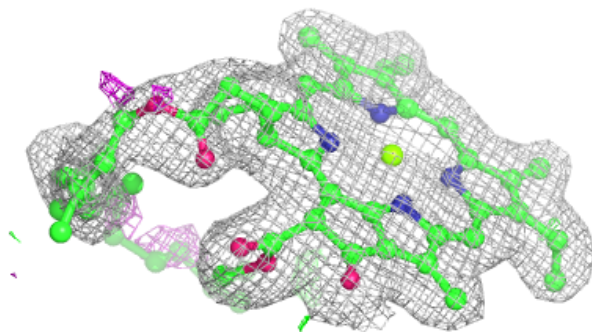
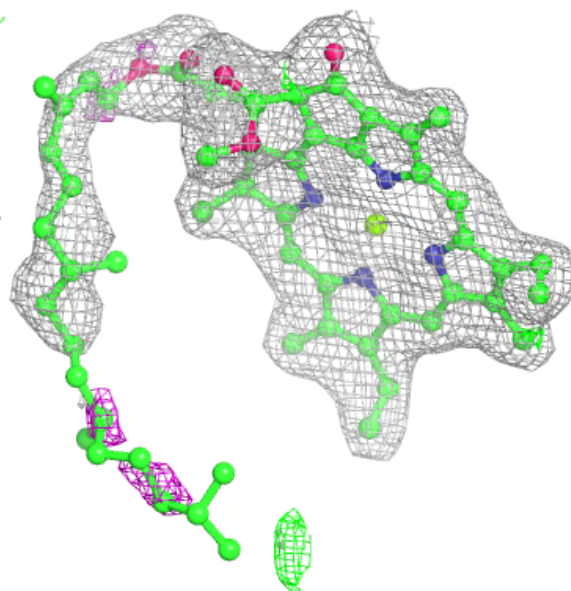
Electron density around CLA c 511:

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



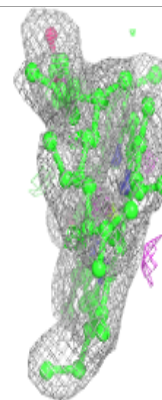
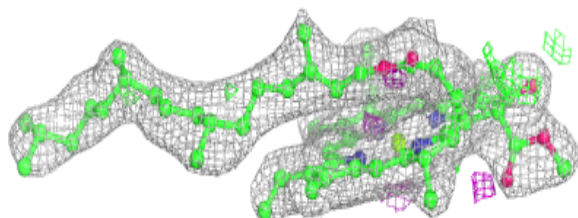
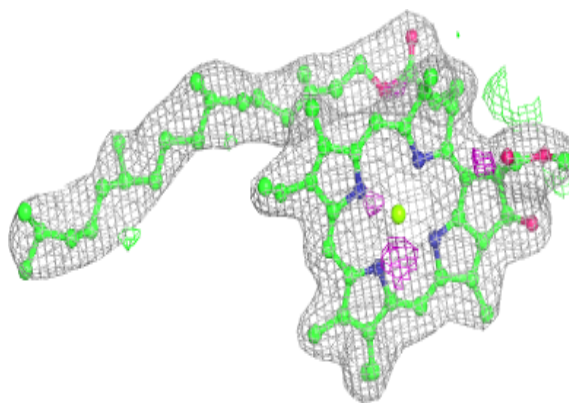
Electron density around CLA B 616:

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

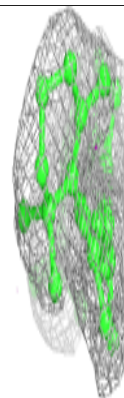
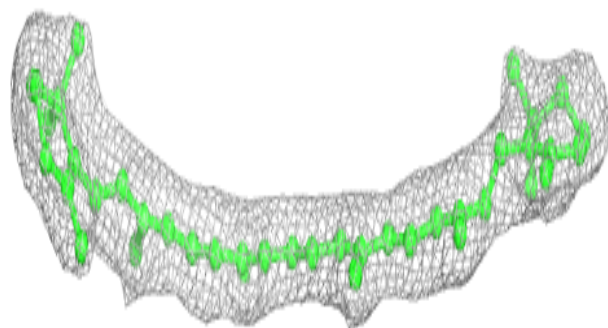
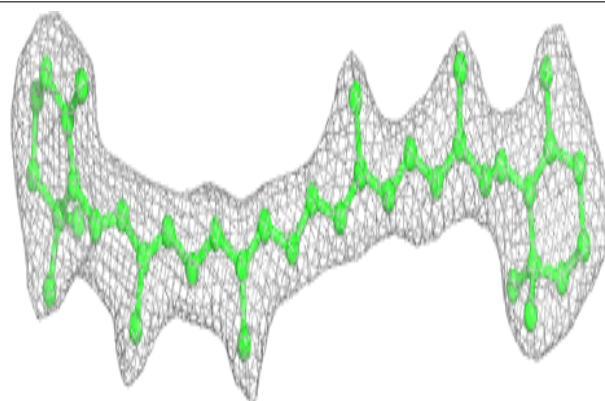


Electron density around CLA C 502:

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

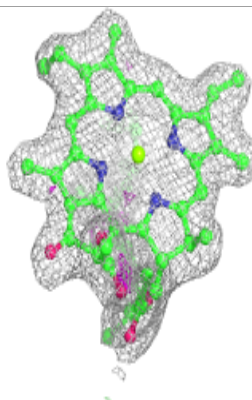
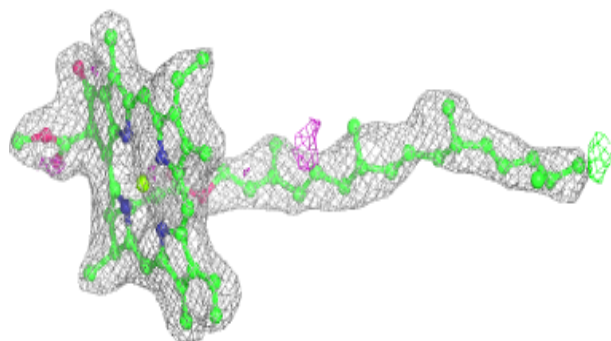
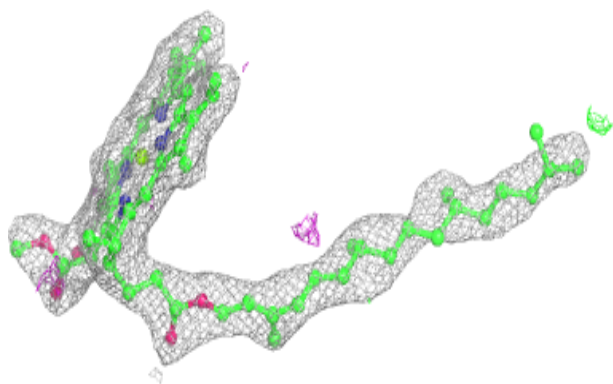
**Electron density around BCR t 101:**

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

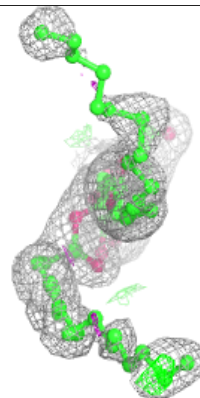
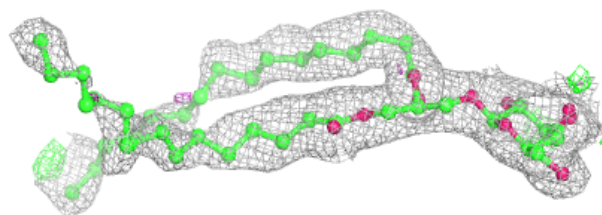
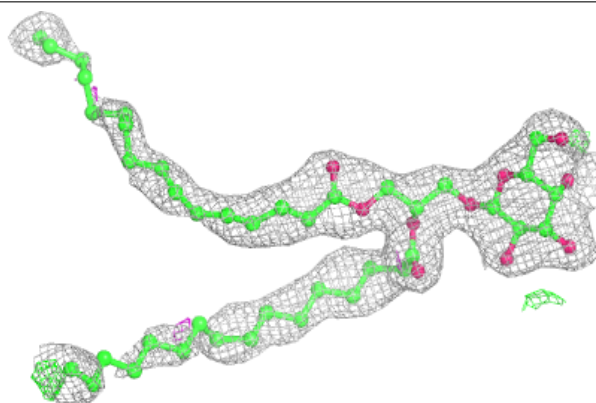


Electron density around CLA B 607:

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

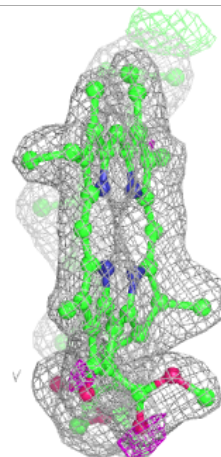
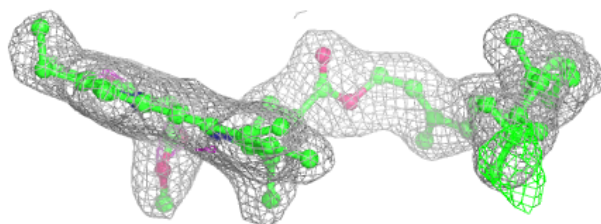
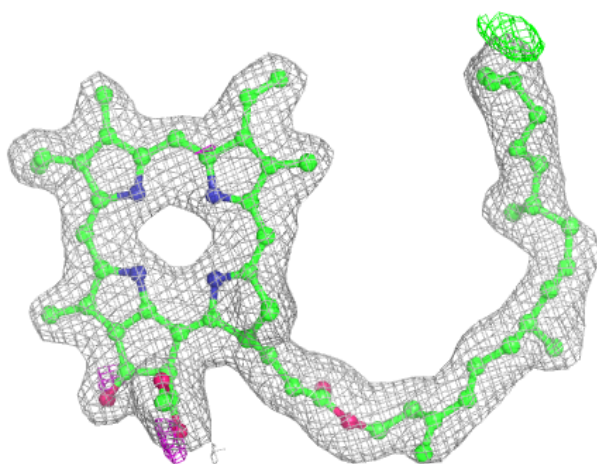
**Electron density around LMG D 407:**

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



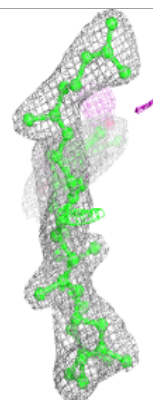
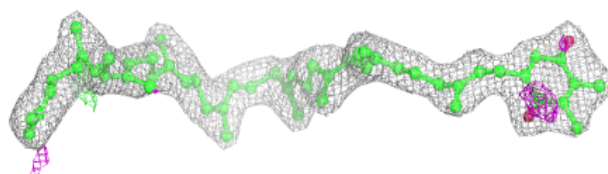
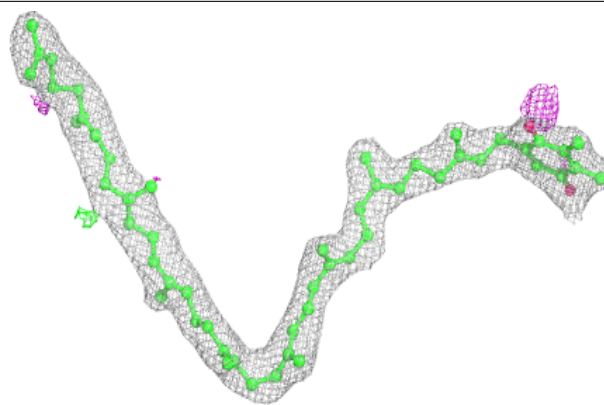
Electron density around PHO a 608:

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

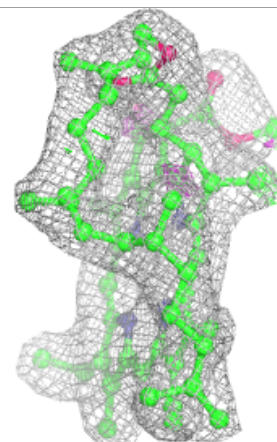
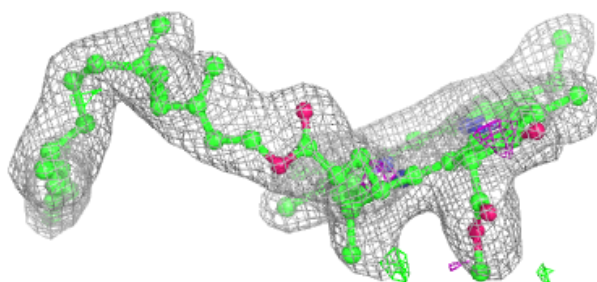
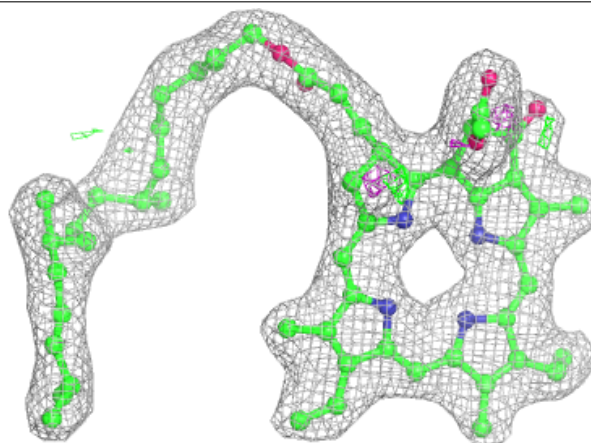


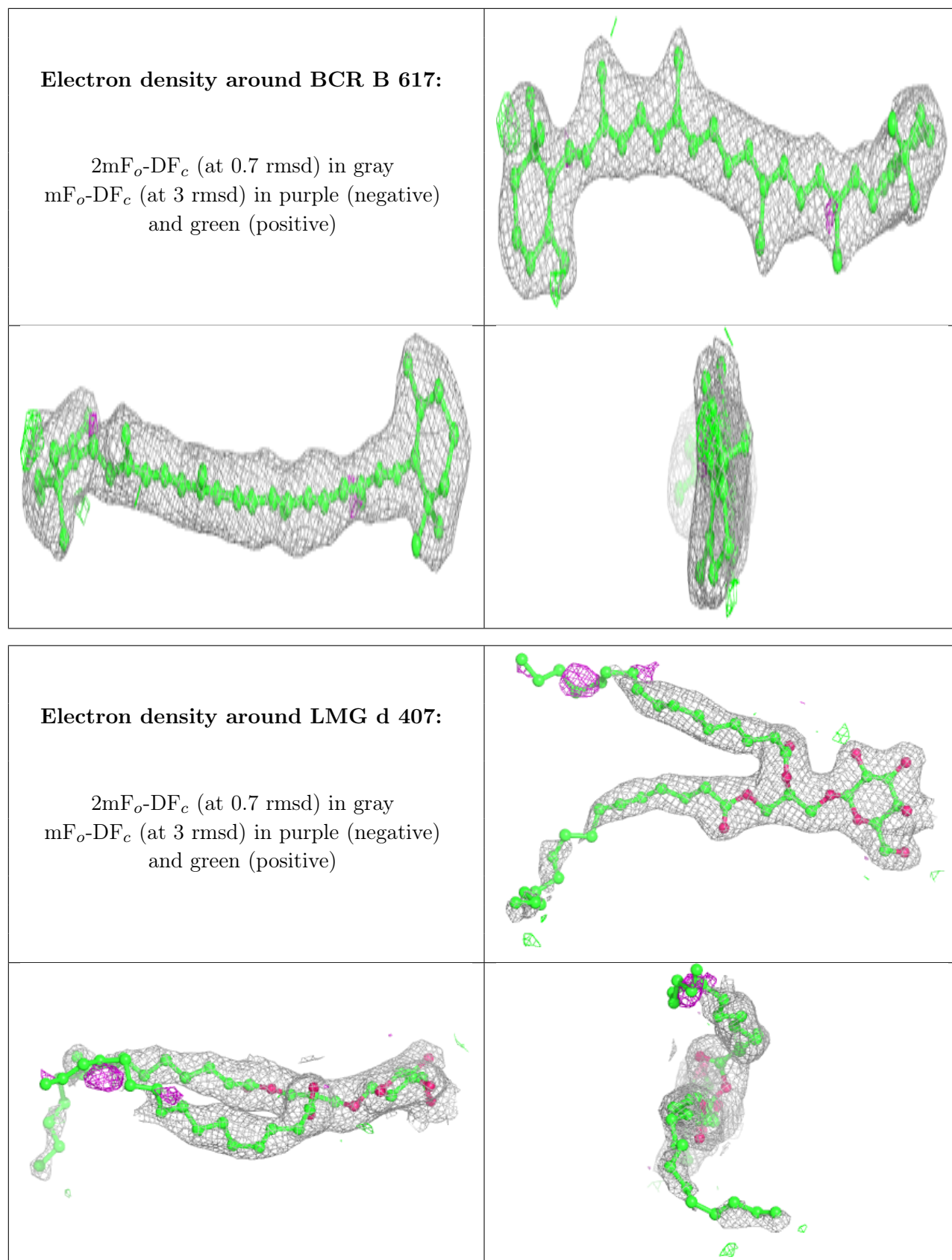
Electron density around PL9 d 404:

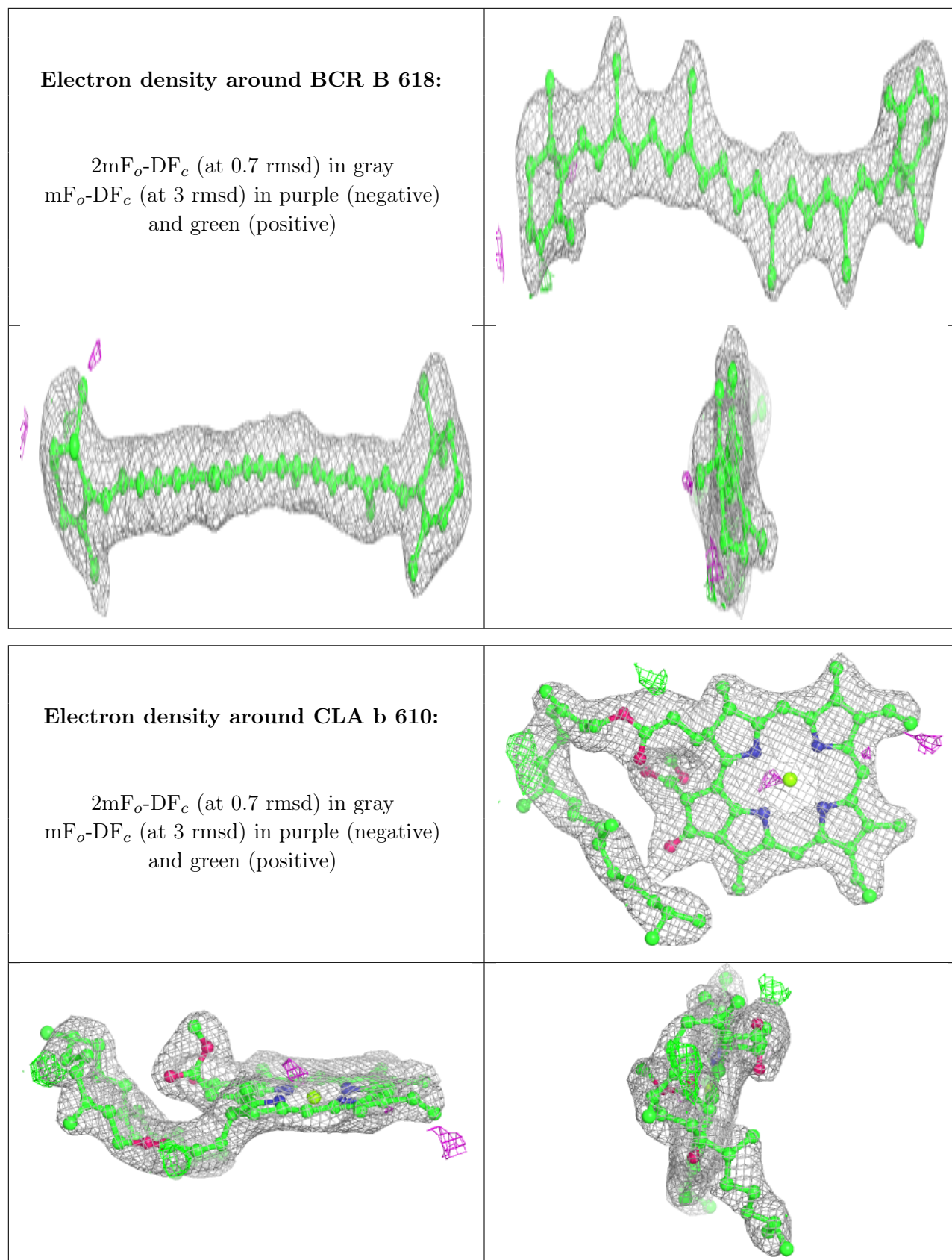
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PHO a 609:**

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

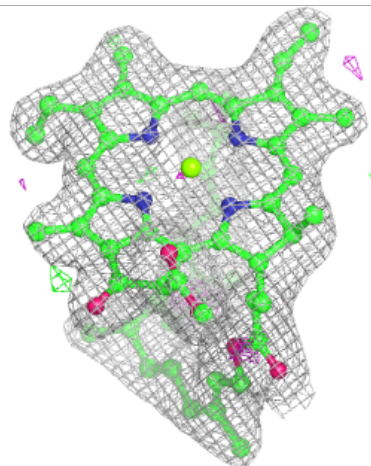
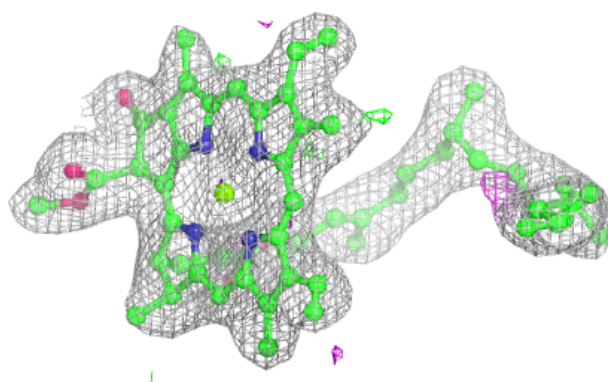
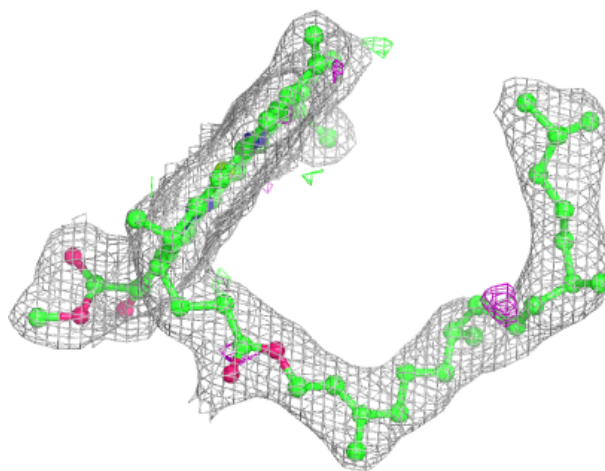






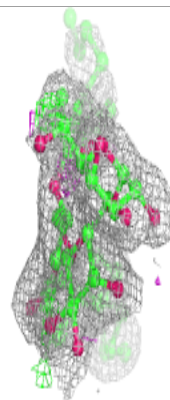
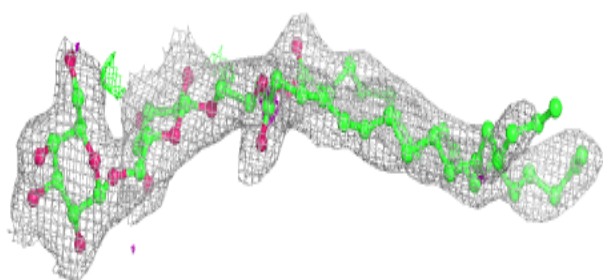
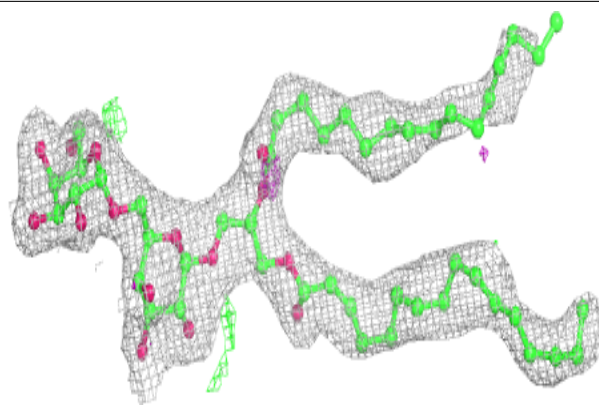
Electron density around CLA b 611:

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

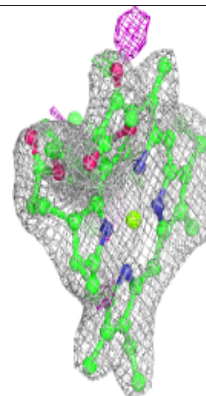
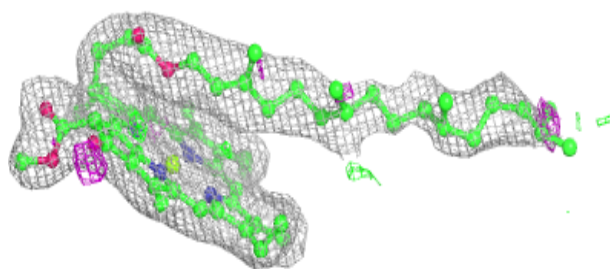
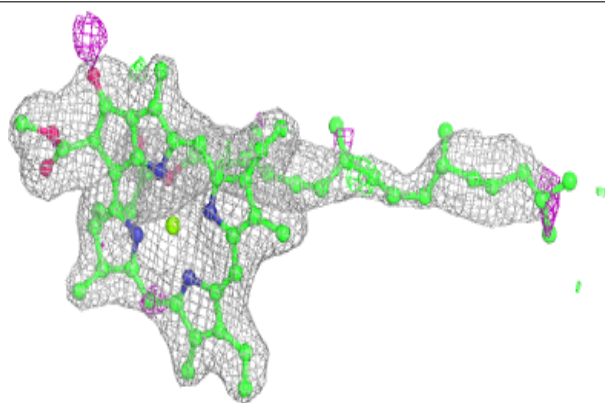


Electron density around DGD C 519:

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

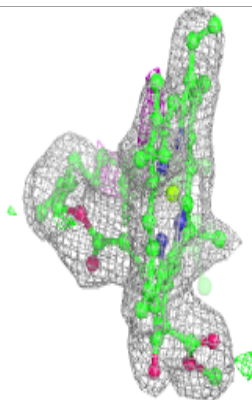
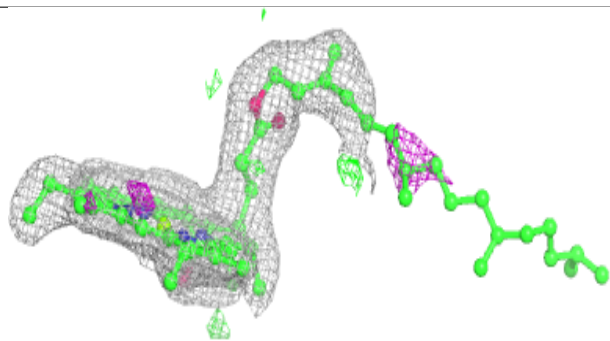
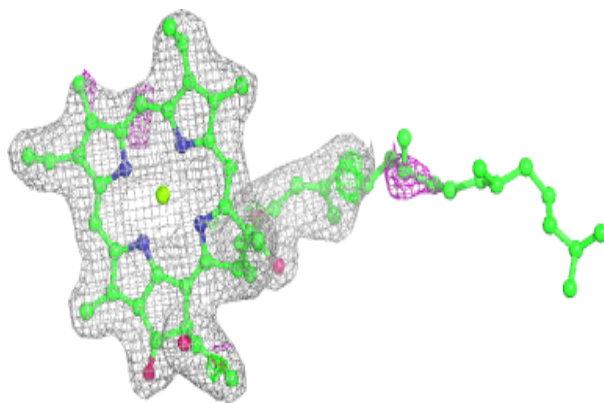
**Electron density around CLA b 614:**

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

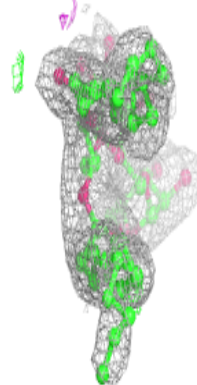
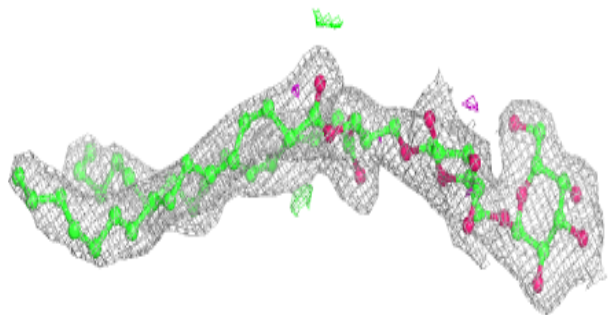
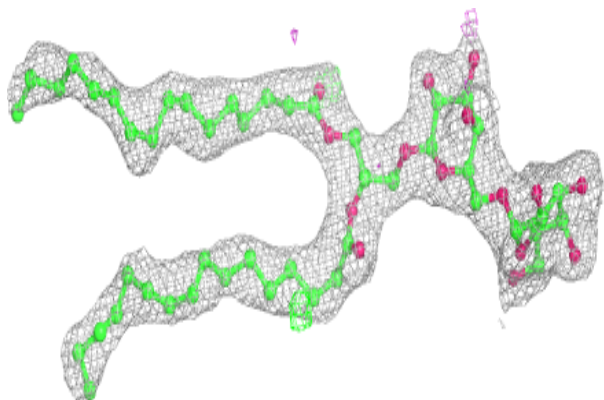


Electron density around CLA A 607:

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

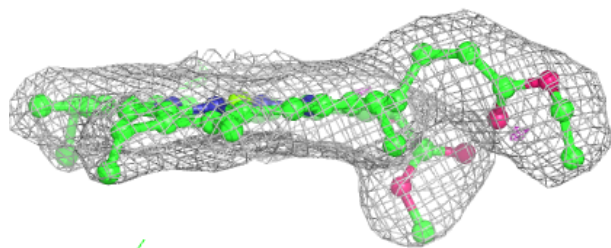
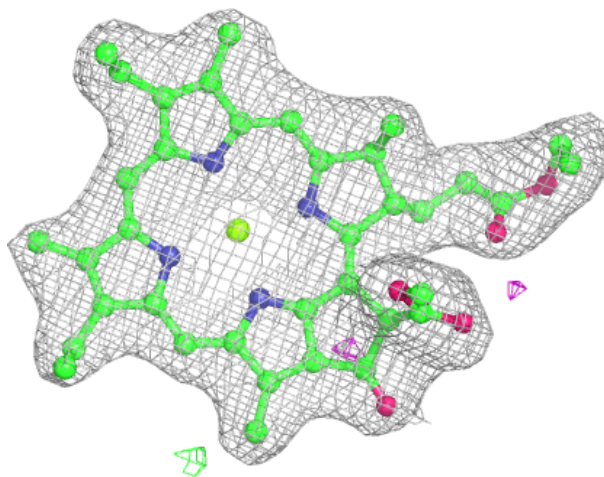
**Electron density around DGD c 518:**

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



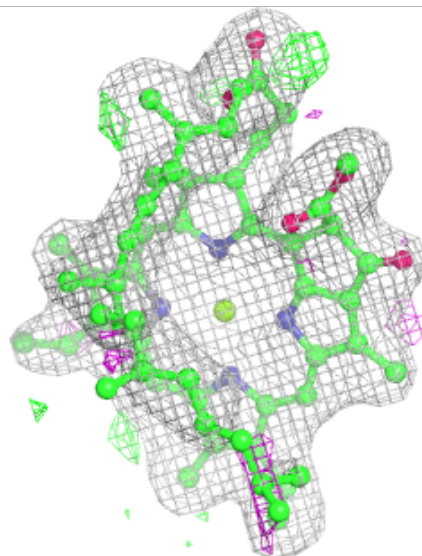
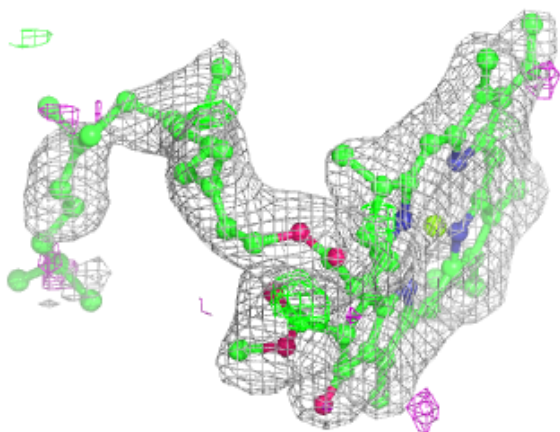
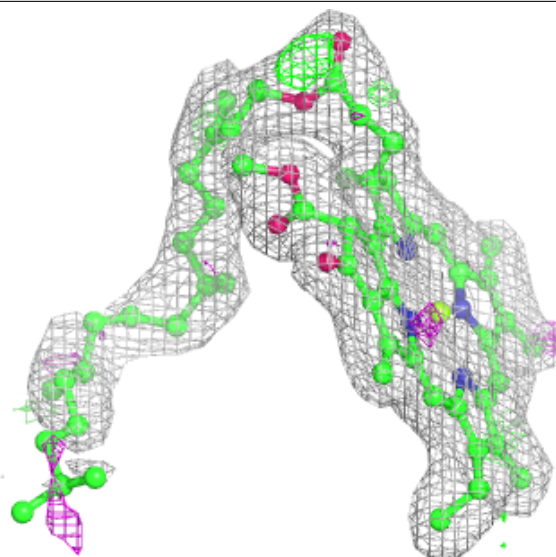
Electron density around CLA b 616:

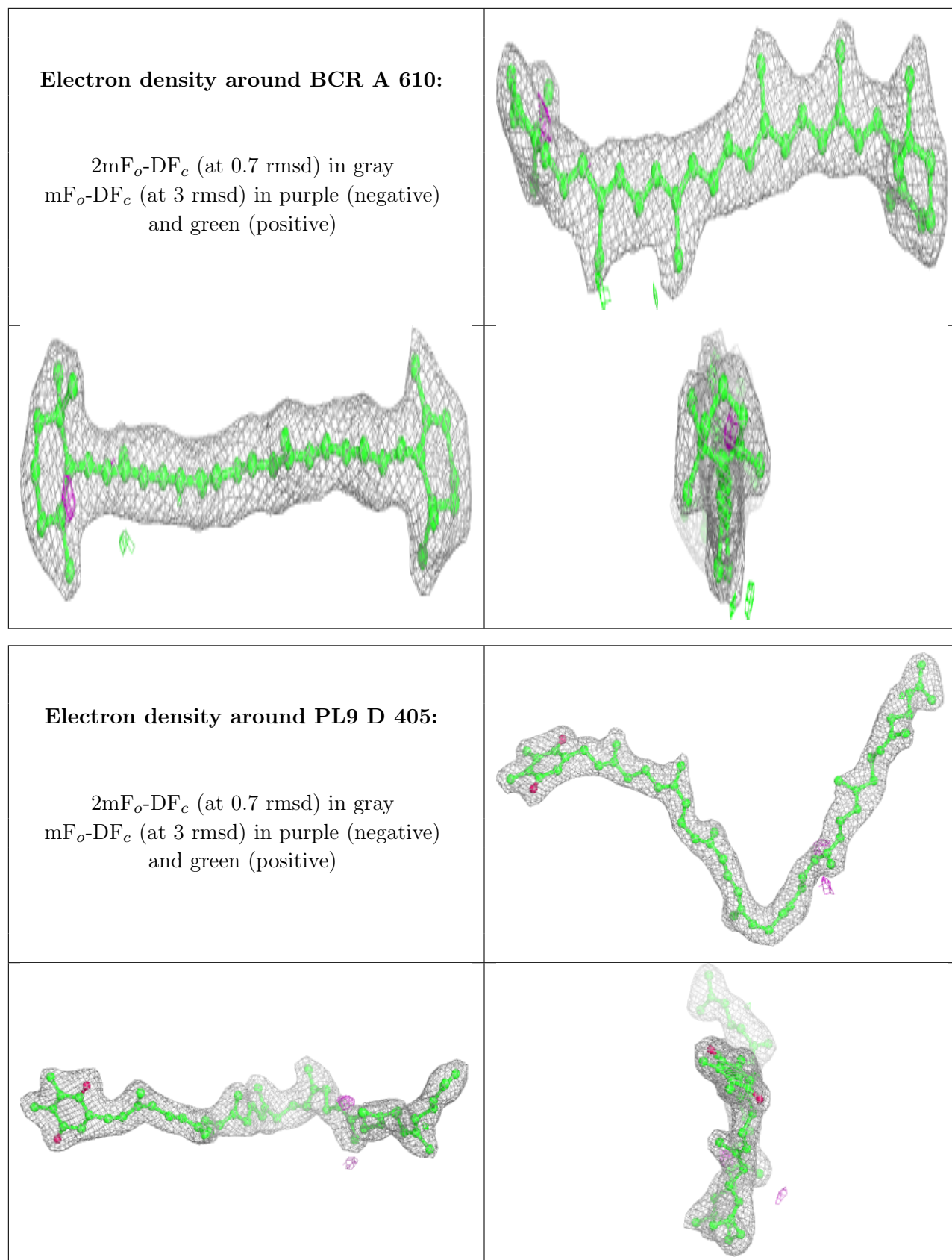
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 613:

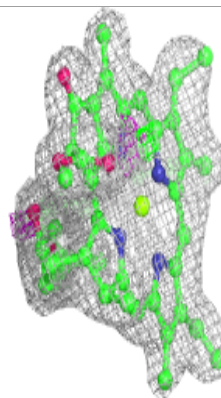
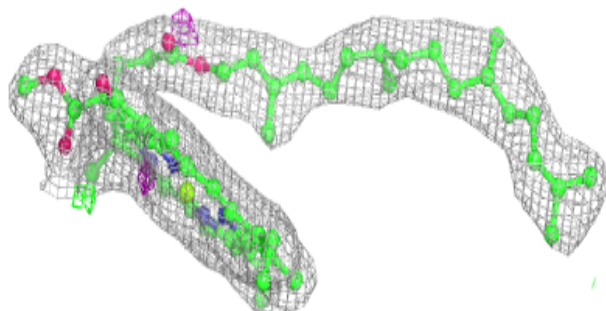
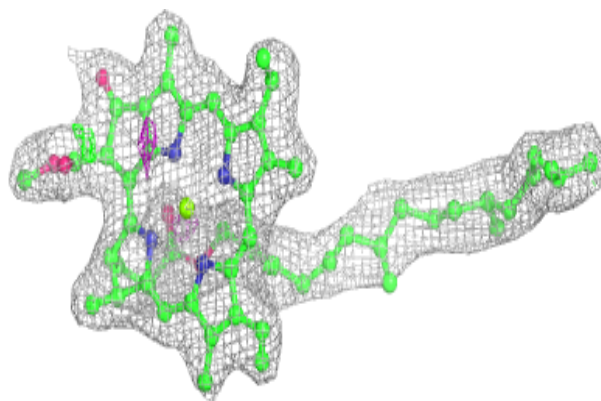
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



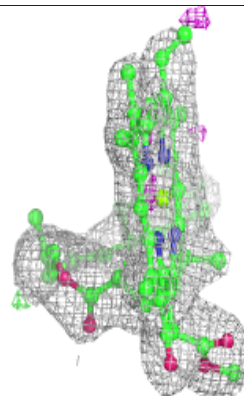
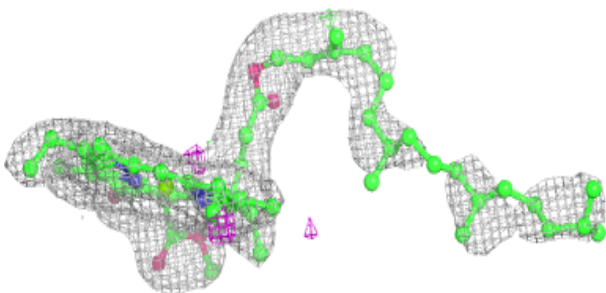
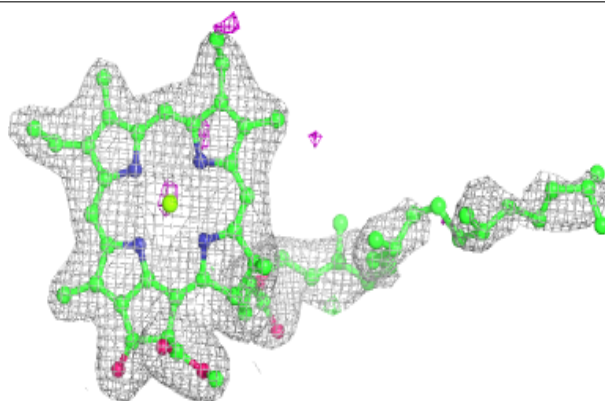


Electron density around CLA B 608:

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

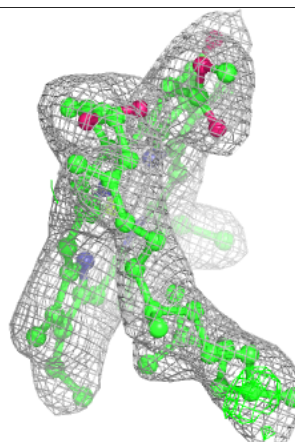
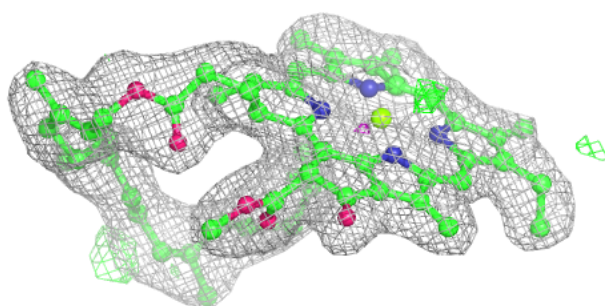
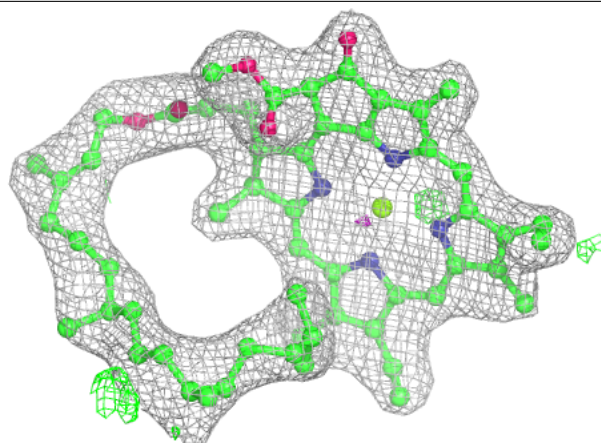
**Electron density around CLA a 607:**

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

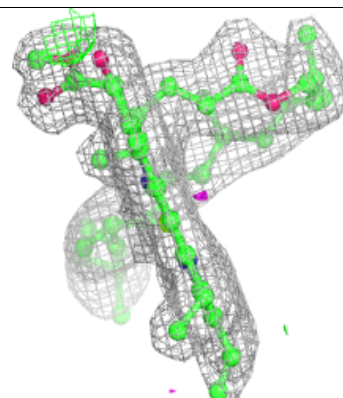
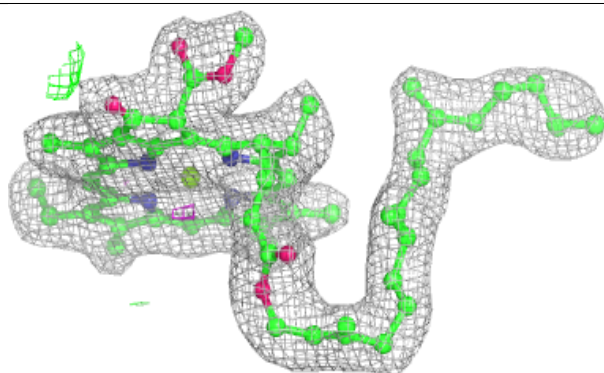
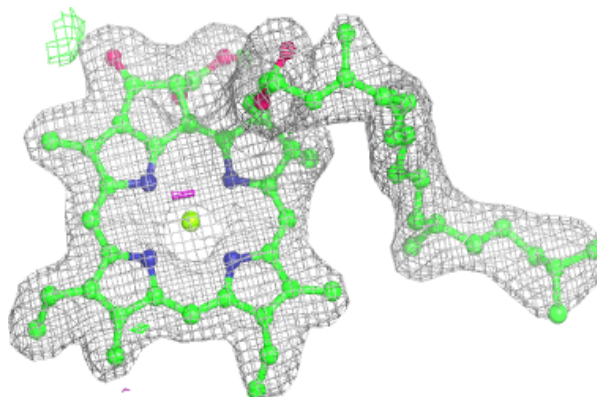


Electron density around CLA B 615:

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

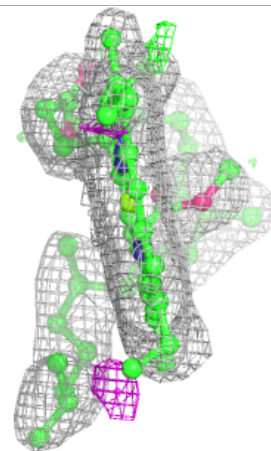
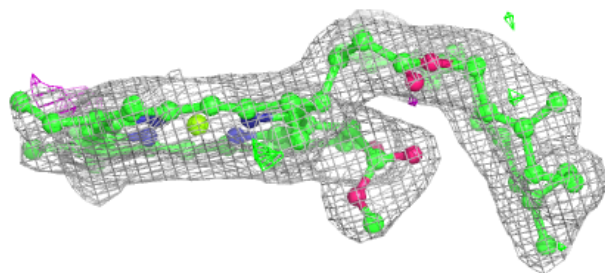
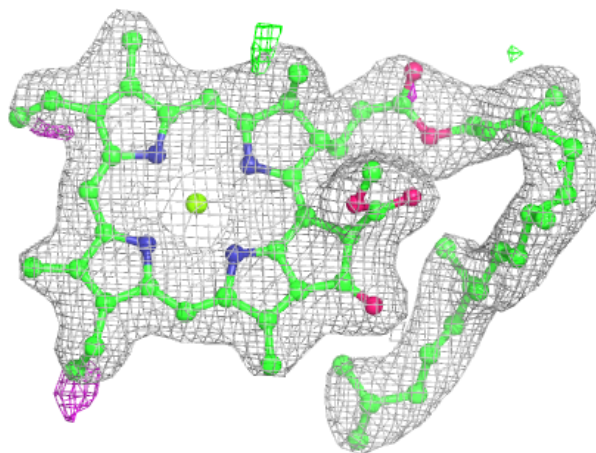
**Electron density around CLA a 615:**

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



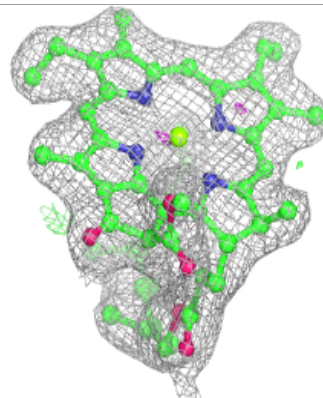
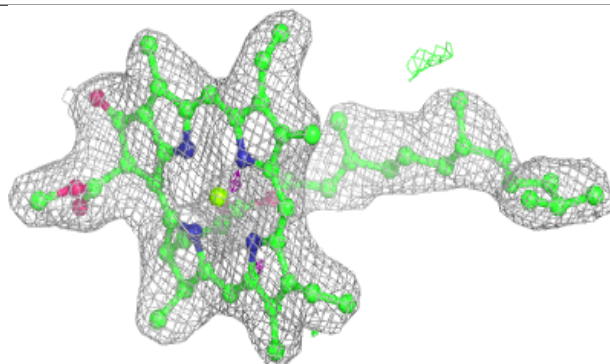
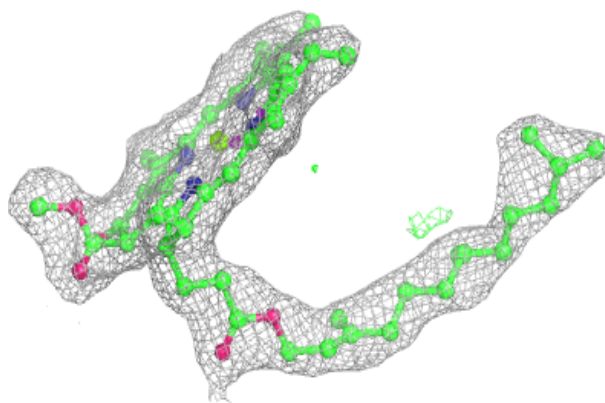
Electron density around CLA B 610:

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



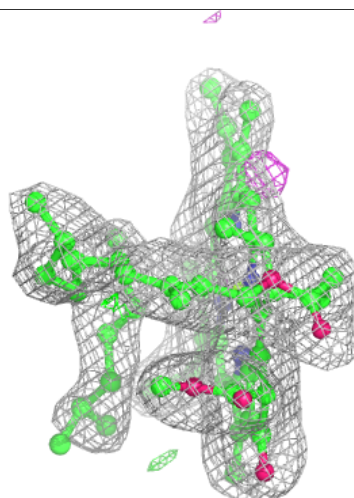
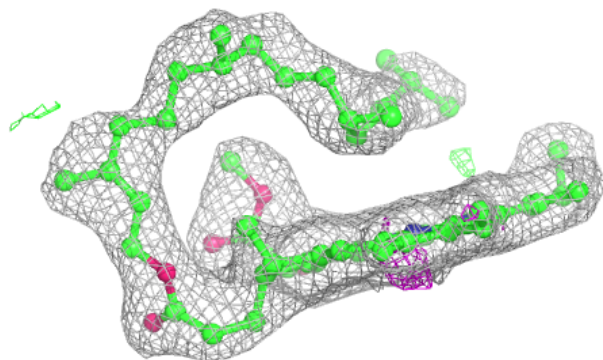
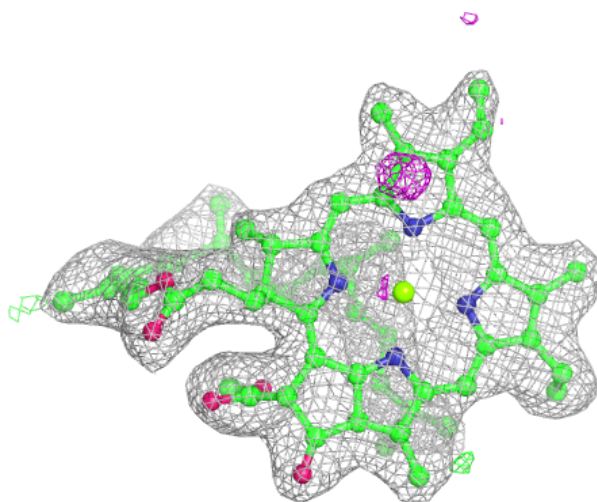
Electron density around CLA c 504:

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



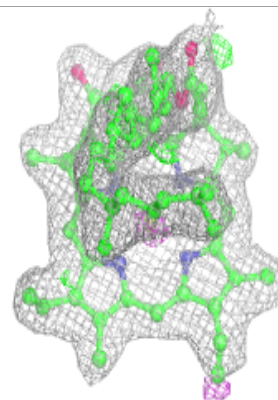
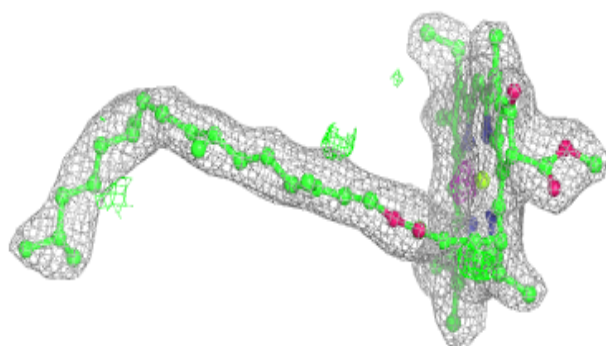
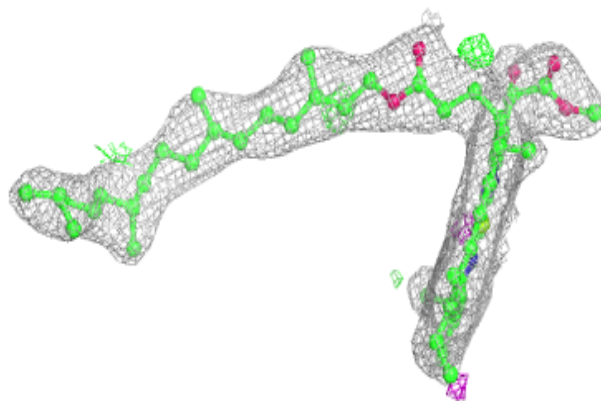
Electron density around CLA C 511:

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

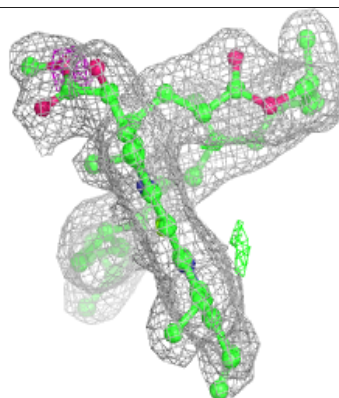
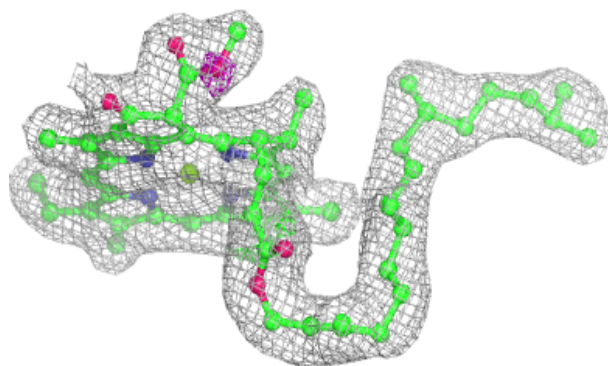
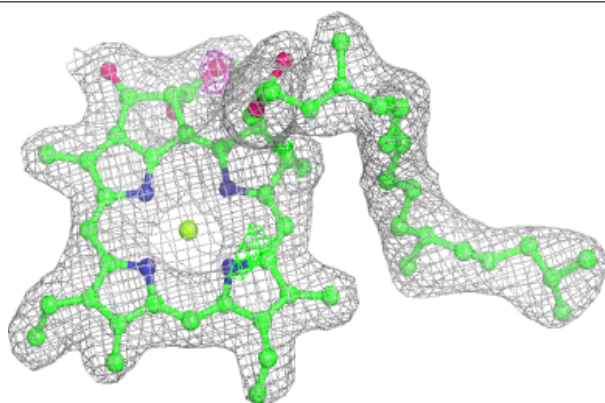


Electron density around CLA b 605:

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

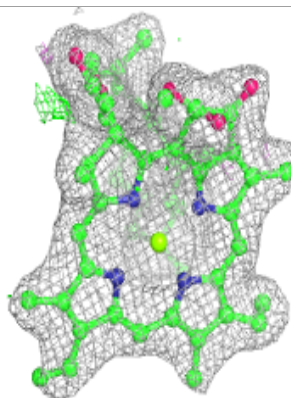
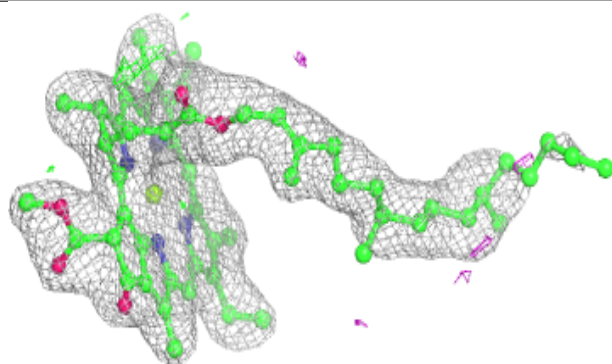
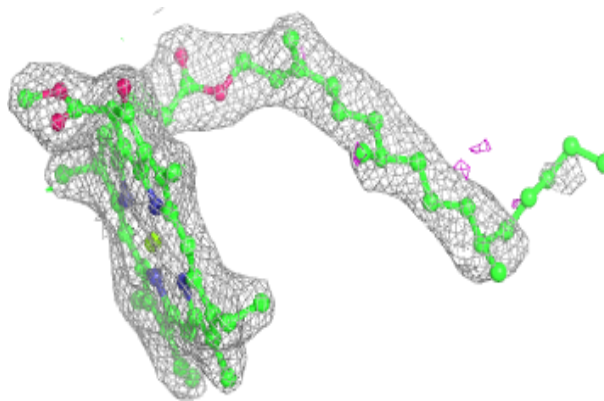
**Electron density around CLA A 613:**

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

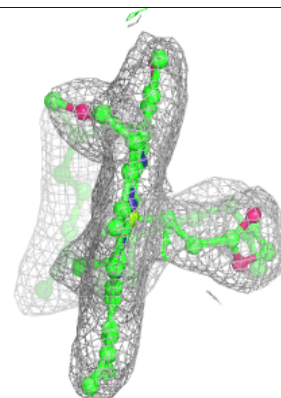
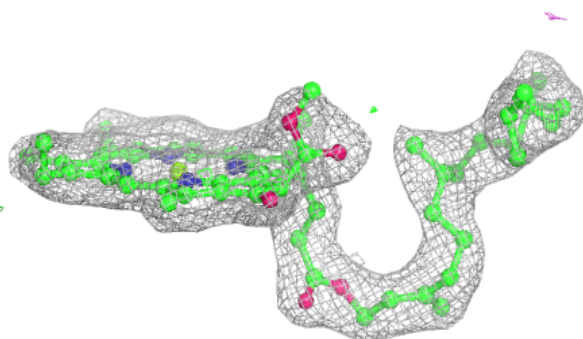
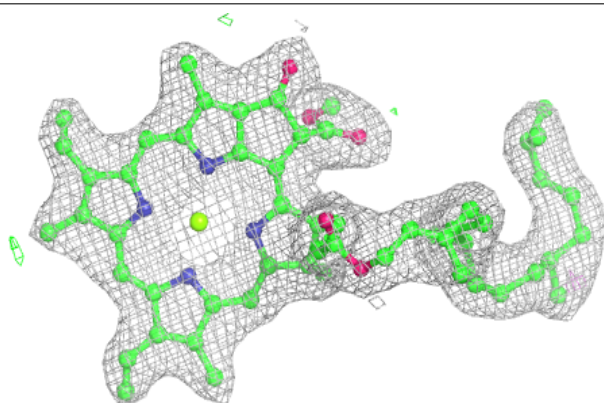


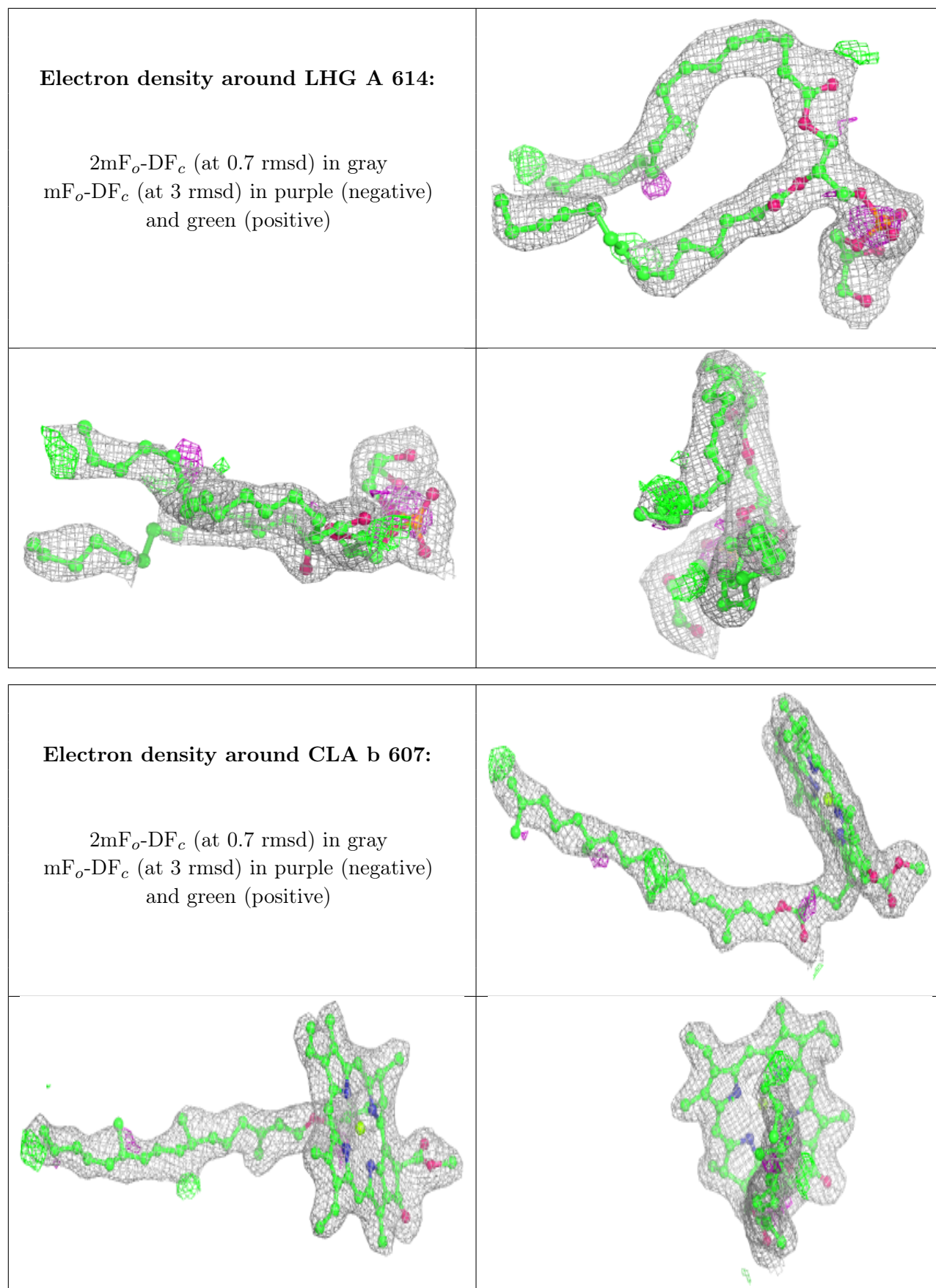
Electron density around CLA c 508:

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

**Electron density around CLA B 612:**

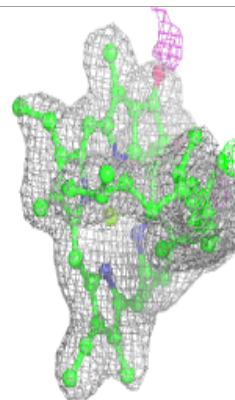
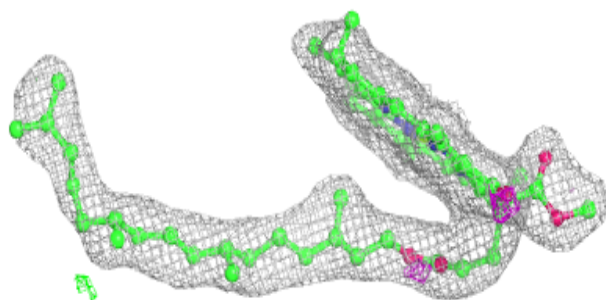
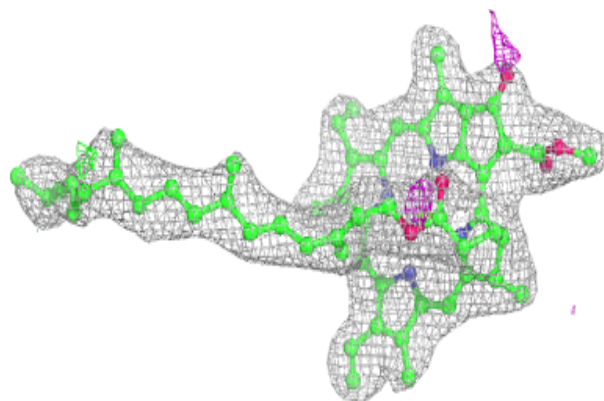
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



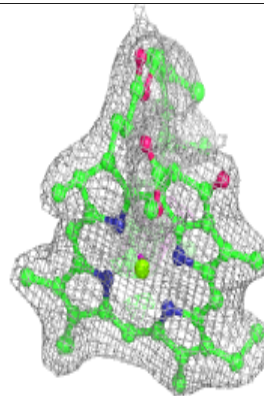
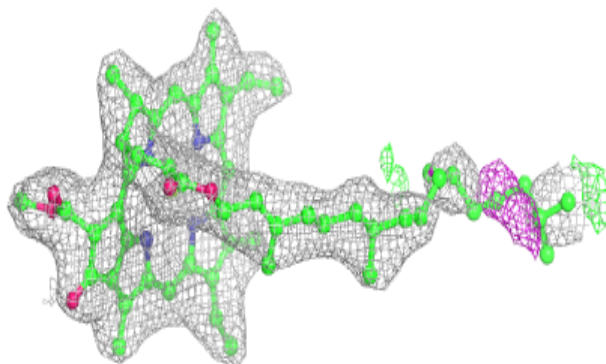
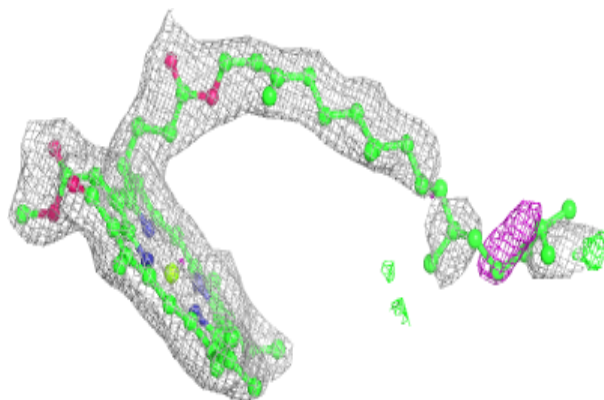


Electron density around CLA b 608:

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

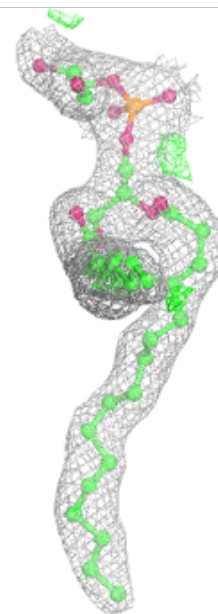
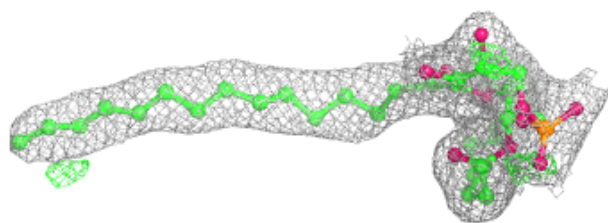
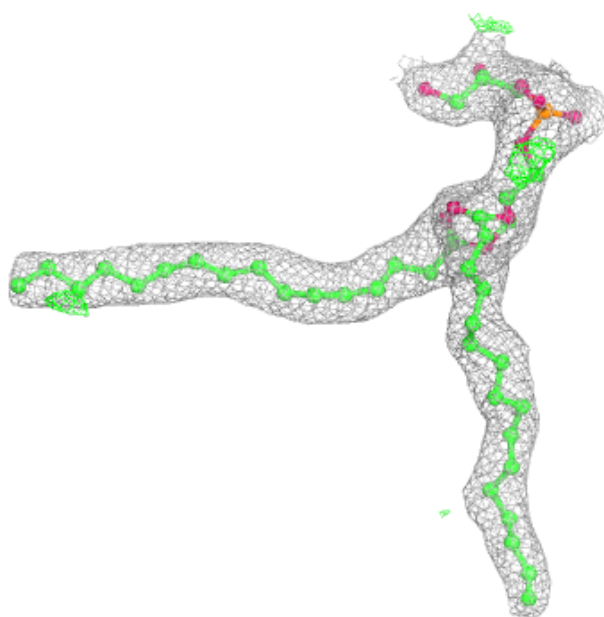
**Electron density around CLA C 505:**

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



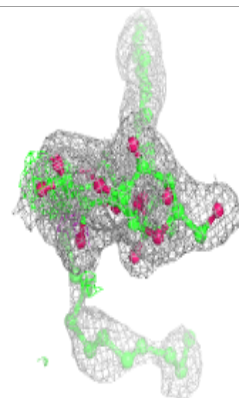
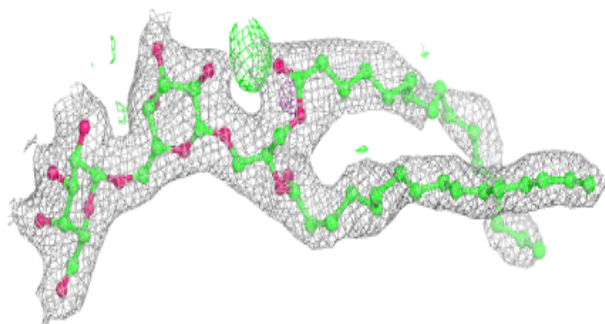
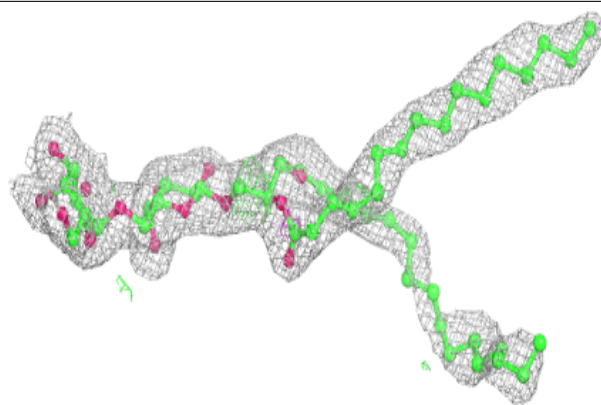
Electron density around LHG L 102:

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

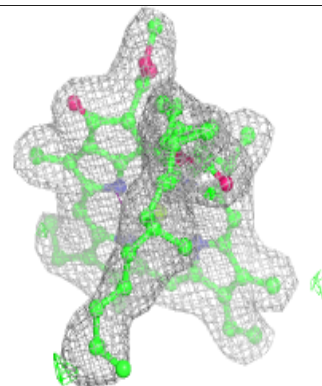
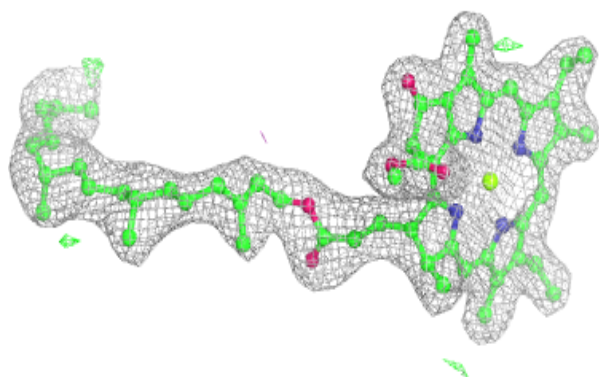
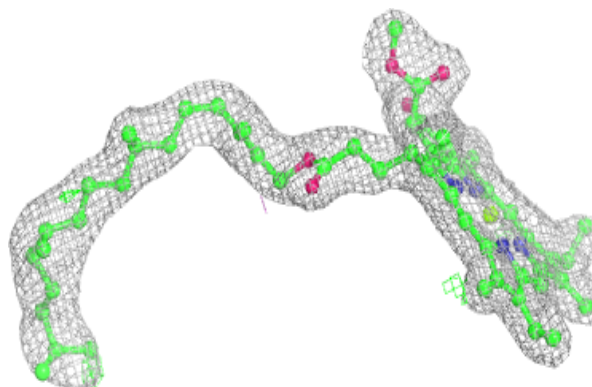


Electron density around DGD C 517:

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

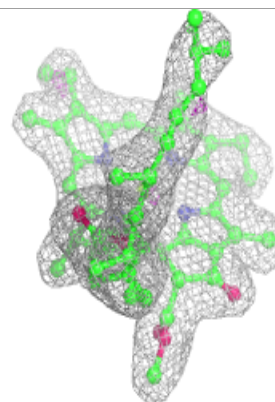
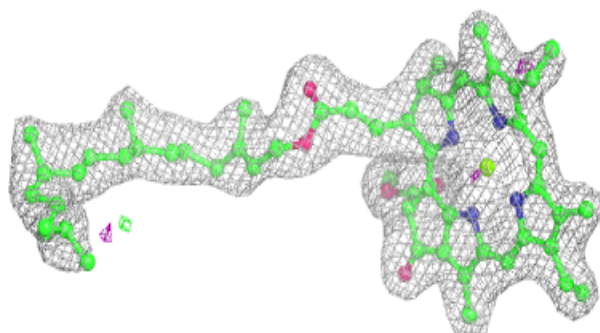
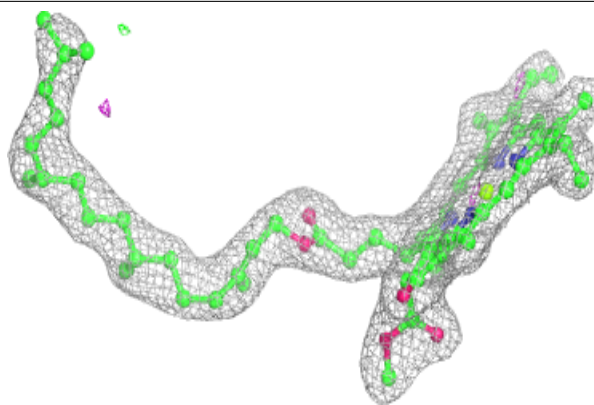
**Electron density around CLA D 402:**

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



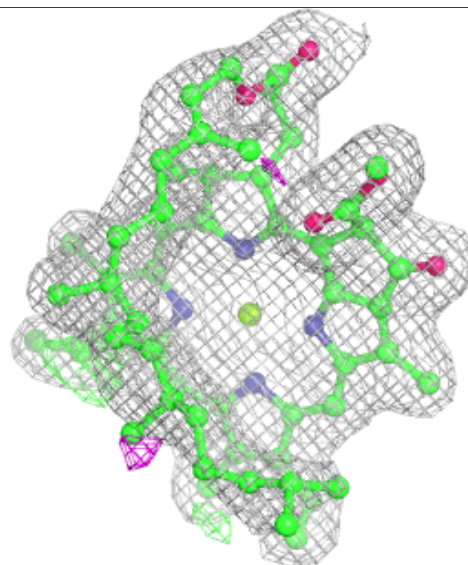
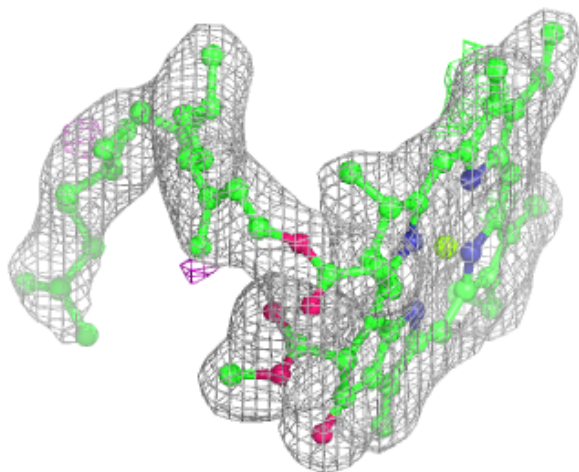
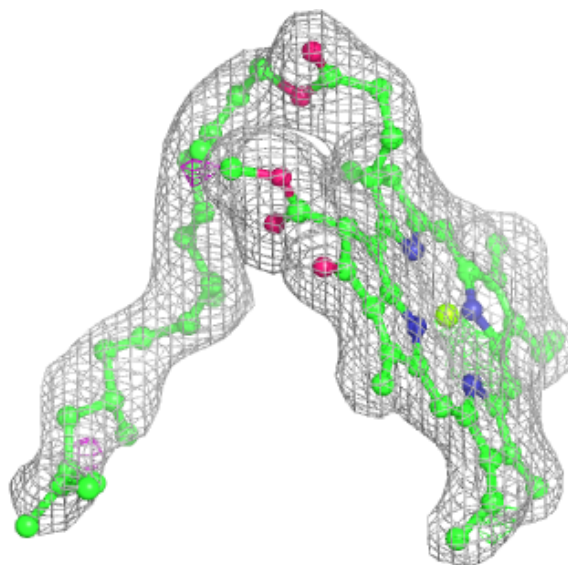
Electron density around CLA d 401:

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



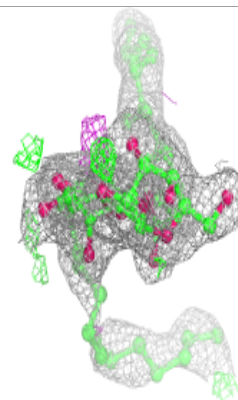
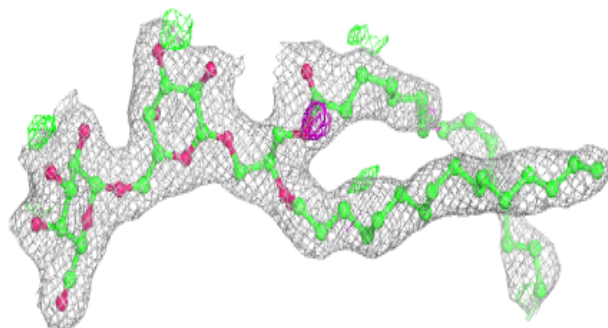
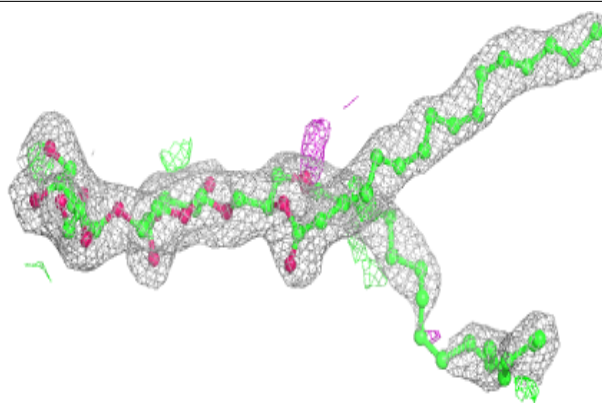
Electron density around CLA B 613:

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

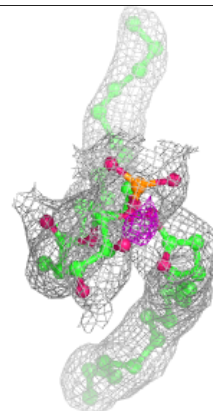
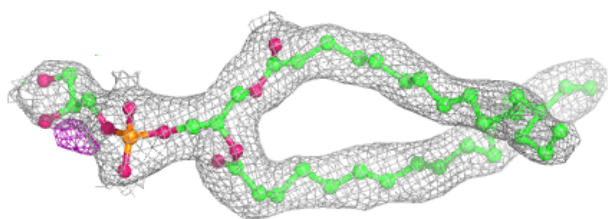
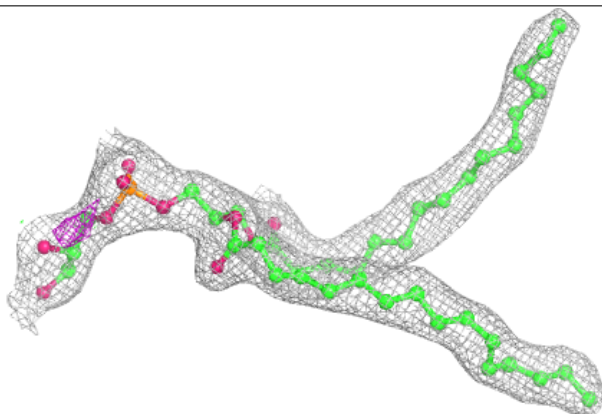


Electron density around DGD c 516:

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

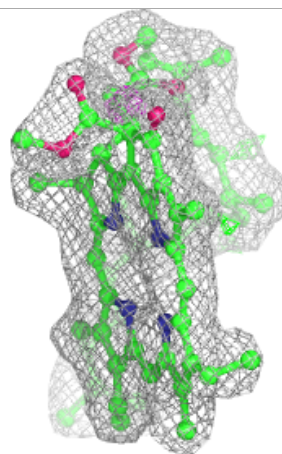
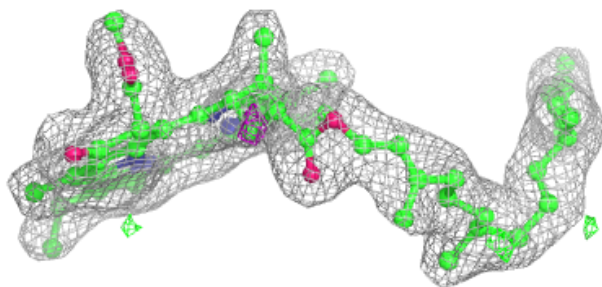
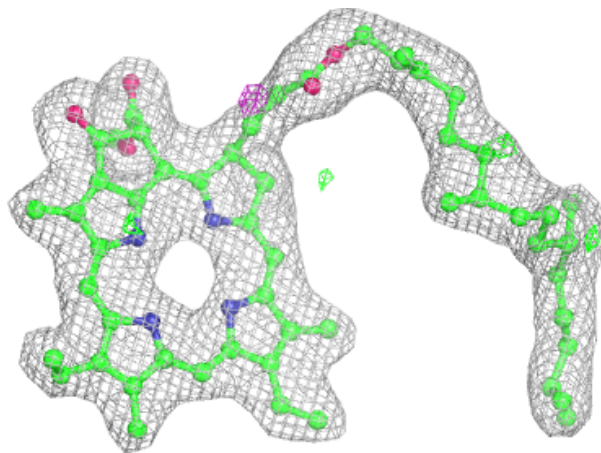
**Electron density around LHG d 406:**

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



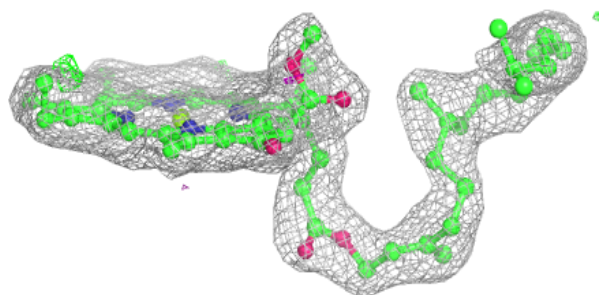
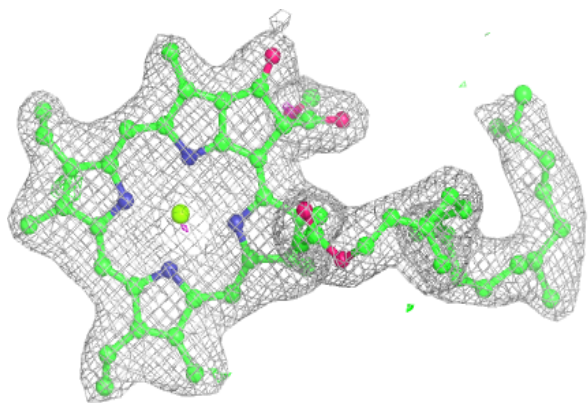
Electron density around PHO A 608:

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



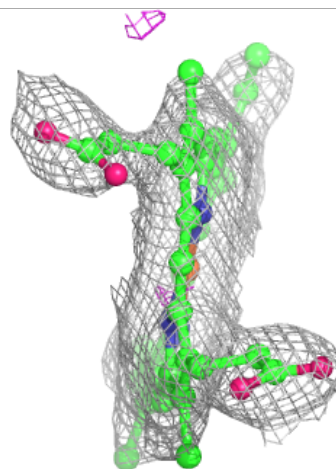
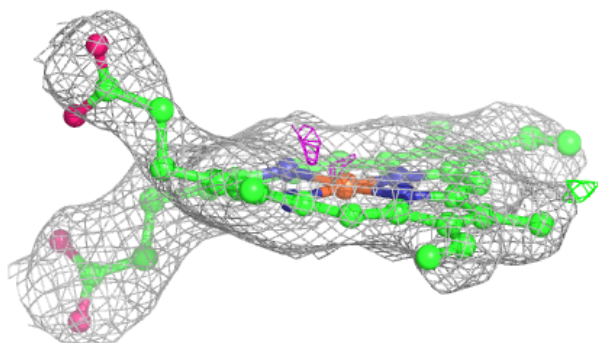
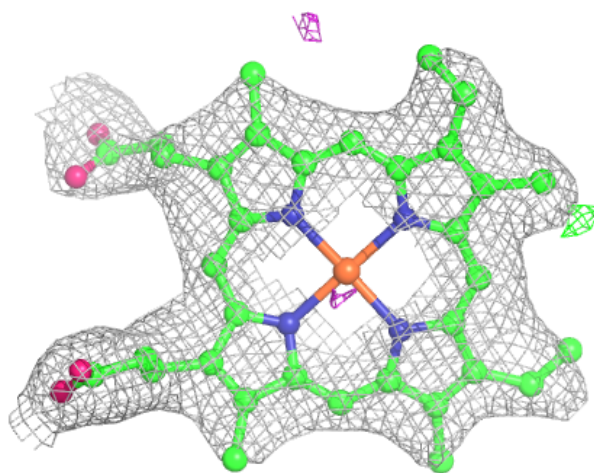
Electron density around CLA b 612:

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



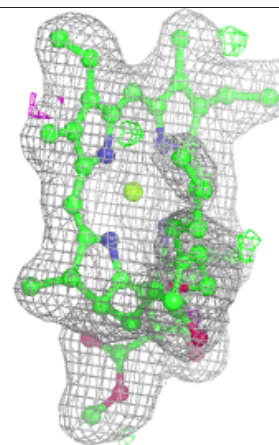
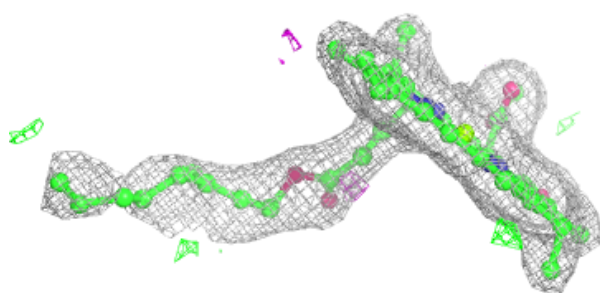
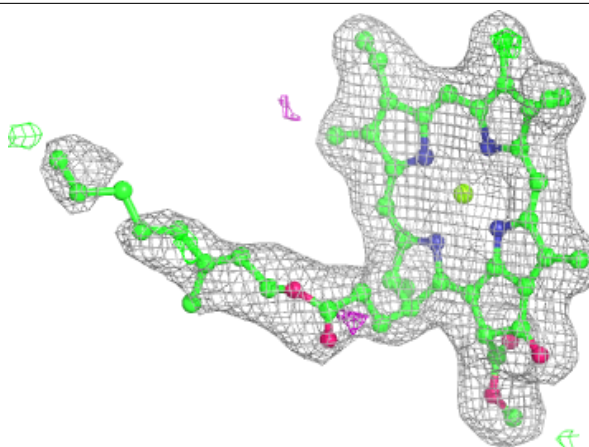
Electron density around HEM e 101:

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

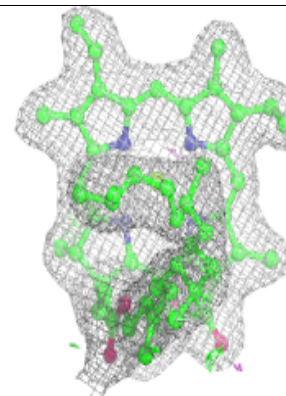
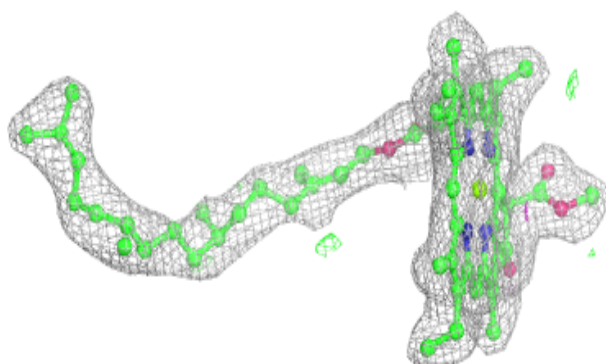
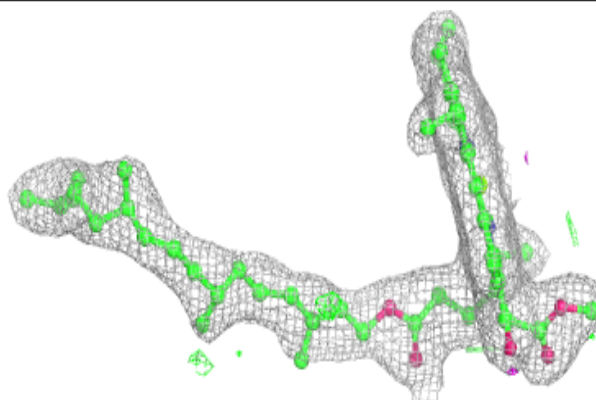


Electron density around CLA A 609:

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

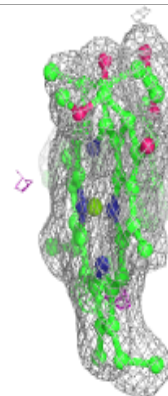
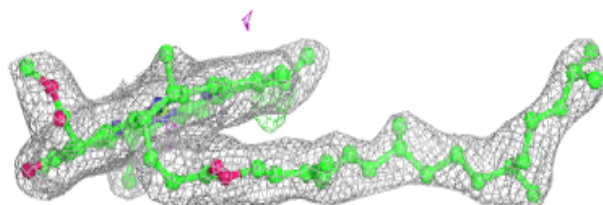
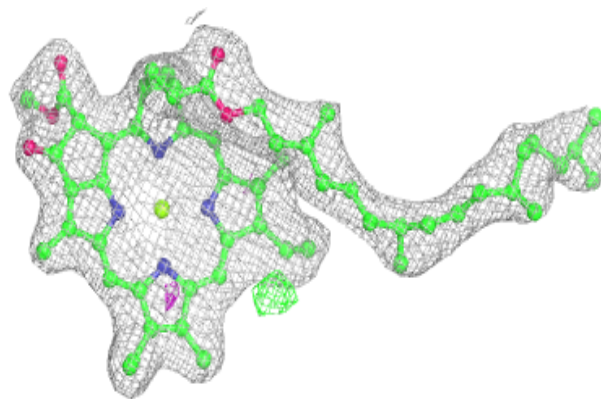
**Electron density around CLA B 605:**

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

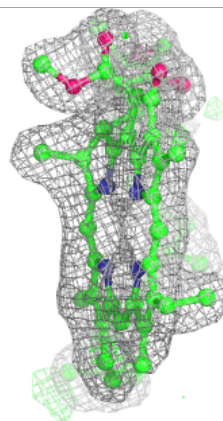
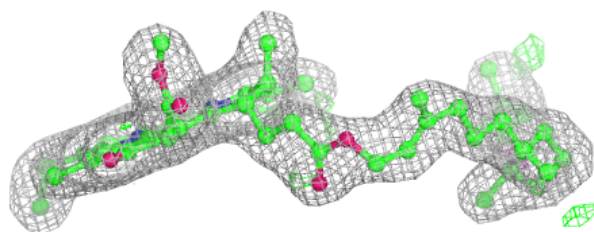
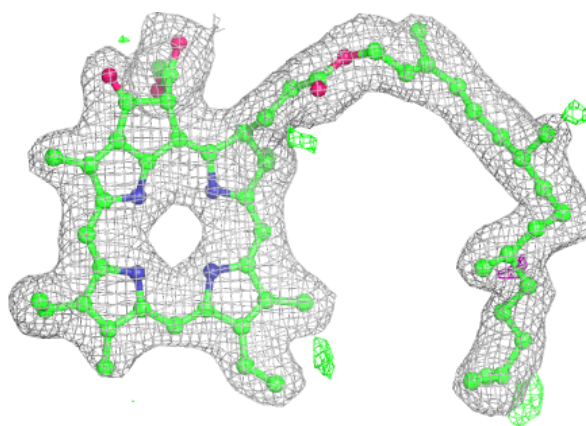


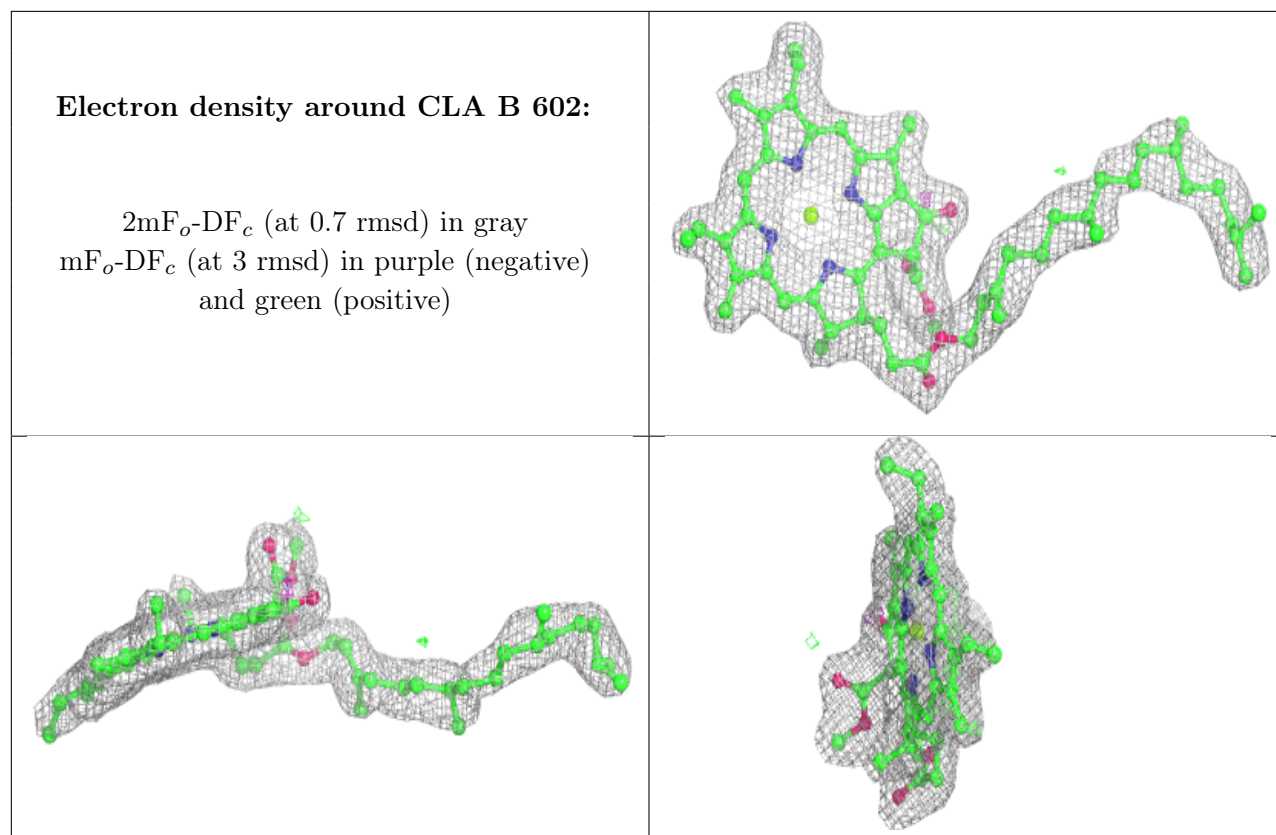
Electron density around CLA b 603:

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

**Electron density around PHO D 401:**

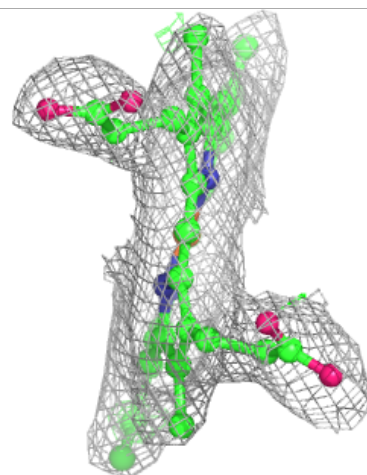
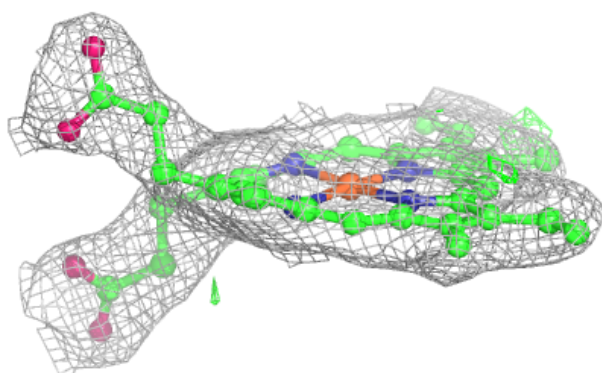
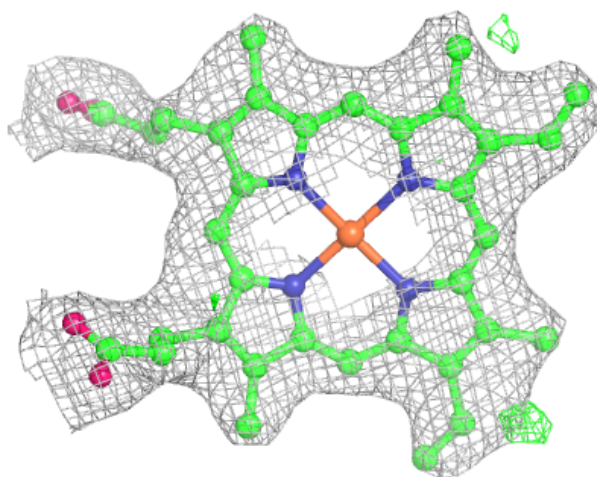
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





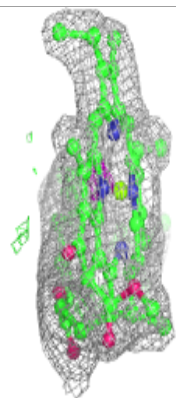
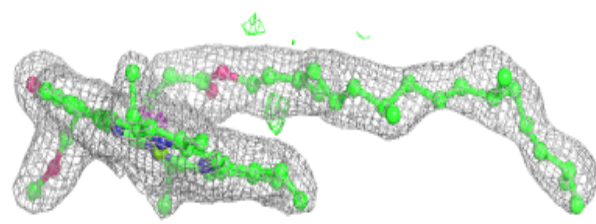
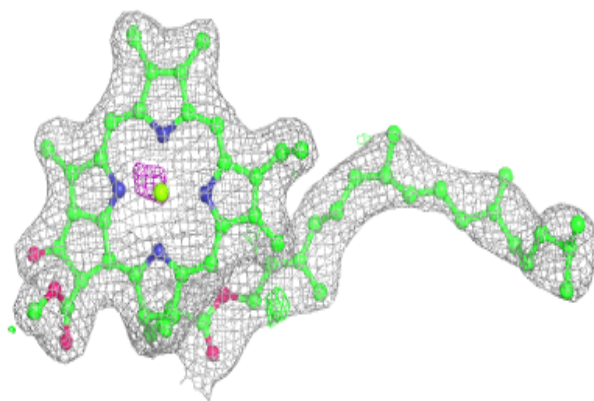
Electron density around HEM E 101:

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

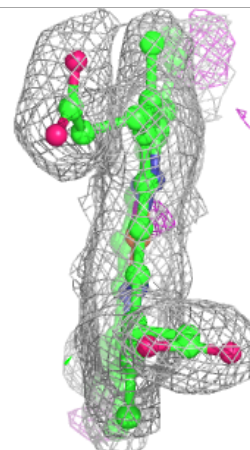
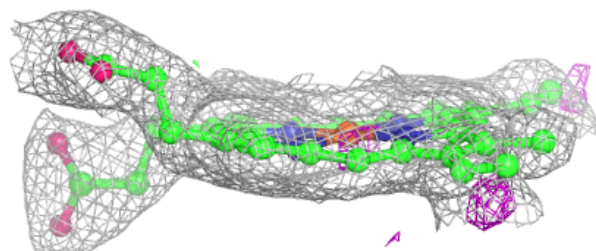
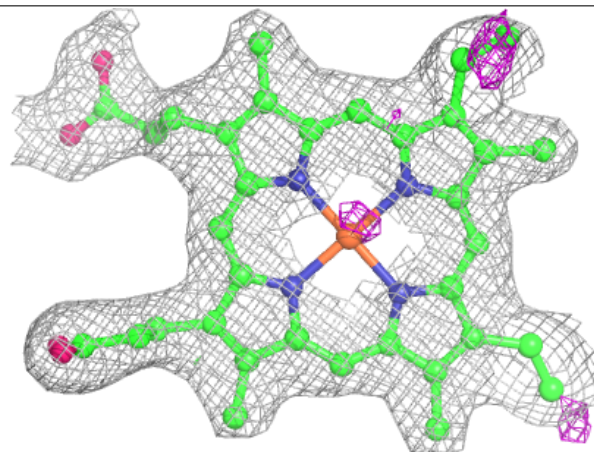


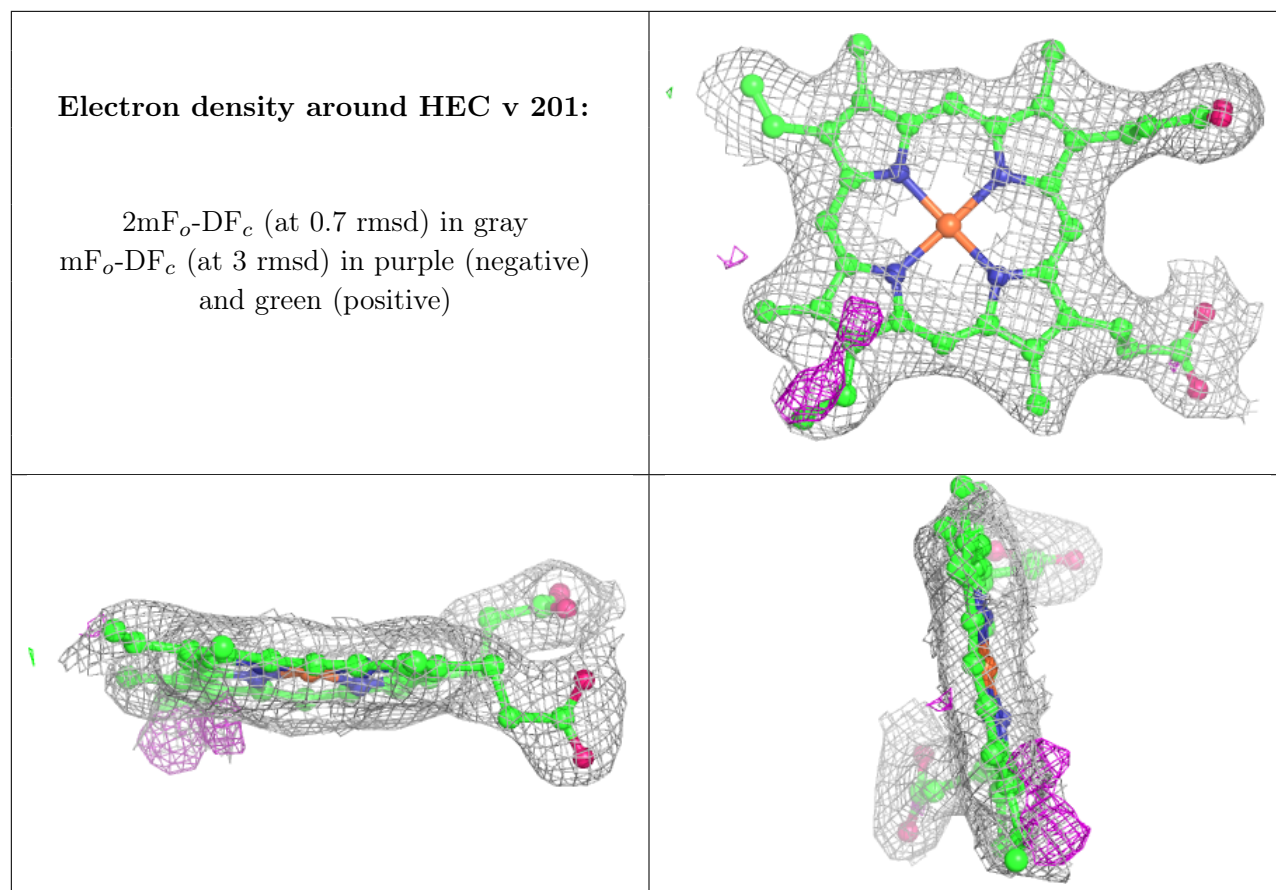
Electron density around CLA B 603:

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

**Electron density around HEC V 201:**

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





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

There are no such residues in this entry.