



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 7, 2023 – 10:22 am GMT

PDB ID : 5E79
Title : Macromolecular diffractive imaging using imperfect crystals
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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)

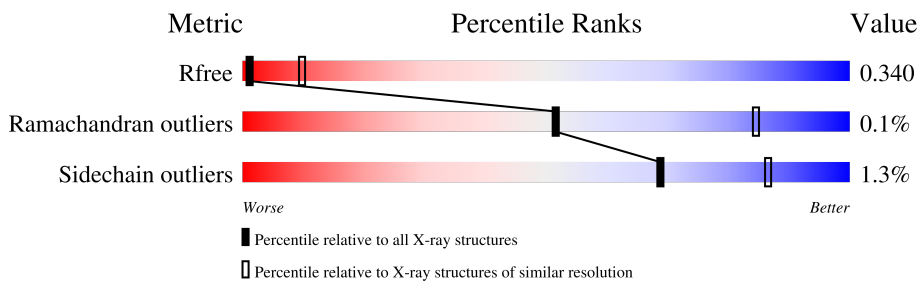
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

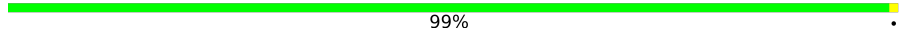
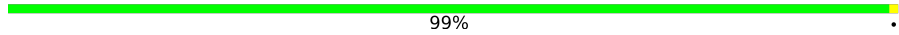
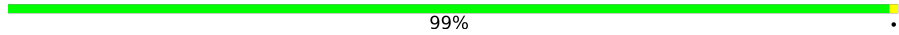
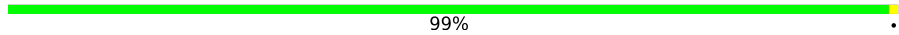
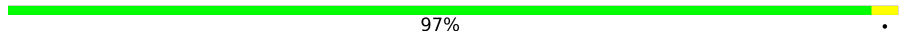
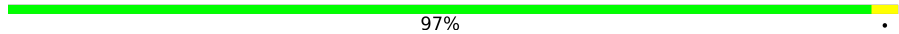
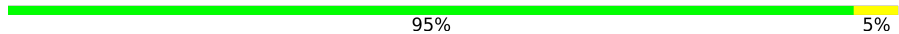
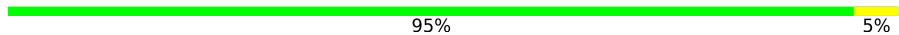
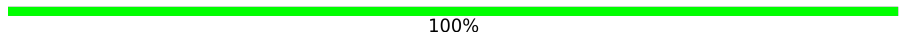
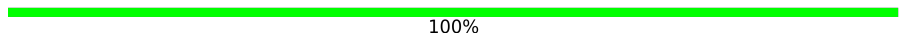
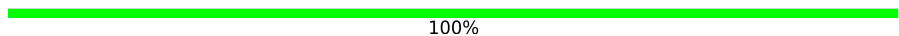
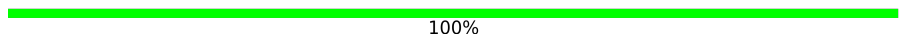
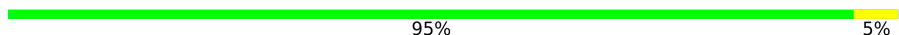

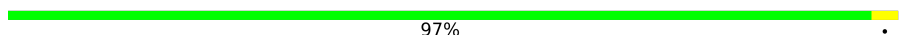
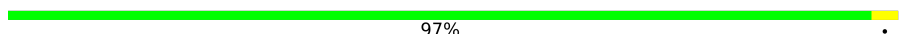
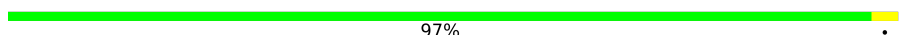
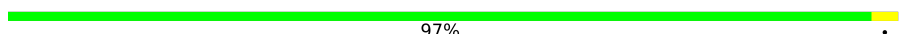
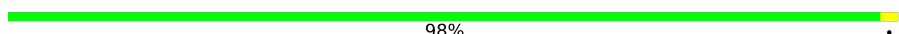
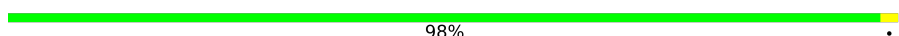
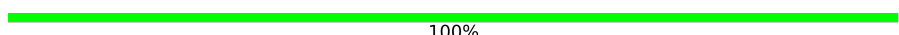
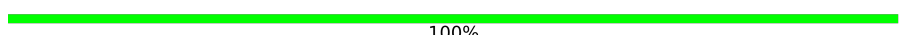
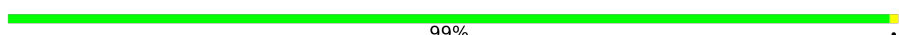
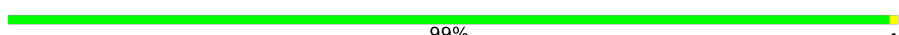
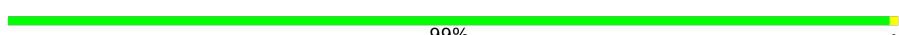
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	334	100%
1	a	334	100%
2	B	504	99% .
2	b	504	99% .
3	C	451	99% .
3	c	451	99% .

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
4	D	342	 99%
4	d	342	 99%
5	E	81	 99%
5	e	81	 99%
6	F	34	 97%
6	f	34	 97%
7	H	65	 95% 5%
7	h	65	 95% 5%
8	I	38	 100%
8	i	38	 100%
9	J	38	 100%
9	j	38	 100%
10	K	37	 95% 5%
10	k	37	 92% 8%
11	L	37	 97%
11	l	37	 97%
12	M	34	 97%
12	m	34	 97%
13	O	243	 98%
13	o	243	 98%
14	T	30	 100%
14	t	30	 100%
15	U	97	 99%
15	u	97	 99%
16	V	137	 99%

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Mol	Chain	Length	Quality of chain
16	v	137	99%
17	Y	29	97%
17	y	29	97%
18	X	39	100%
18	x	39	100%
19	Z	62	98%
19	z	62	98%

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
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607[A]	X	-	-	-
24	CLA	B	607[B]	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	609	X	-	-	-
24	CLA	a	615	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608[A]	X	-	-	-
24	CLA	b	608[B]	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	-	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	-	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	-	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-
26	BCR	c	515	-	X	-	-
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	-	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	-	-
27	PL9	D	405	-	X	-	-
27	PL9	d	404	-	X	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 50074 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	2637	1730	432	460	15	0	4	0
1	a	334	2637	1730	432	460	15	3	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- 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	4024	2641	668	702	13	0	10	0
2	b	504	4024	2641	668	702	13	0	10	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	3506	2296	584	613	13	0	5	0
3	c	451	3506	2296	584	613	13	0	5	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	342	2726	1805	445	464	12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

- 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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			668	436	107	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	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

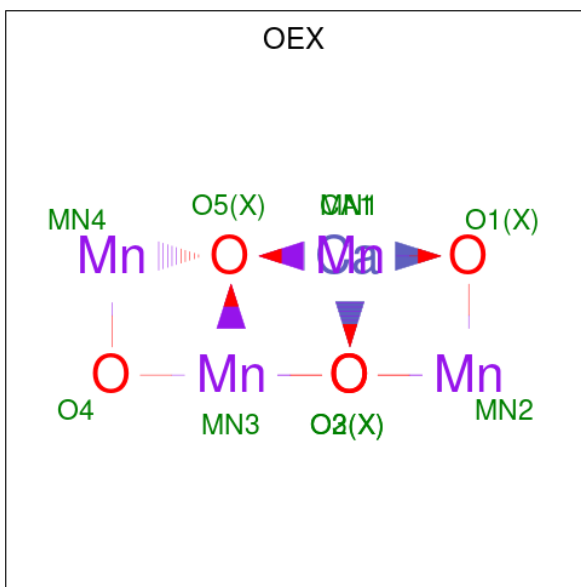
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn₄O₅).



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

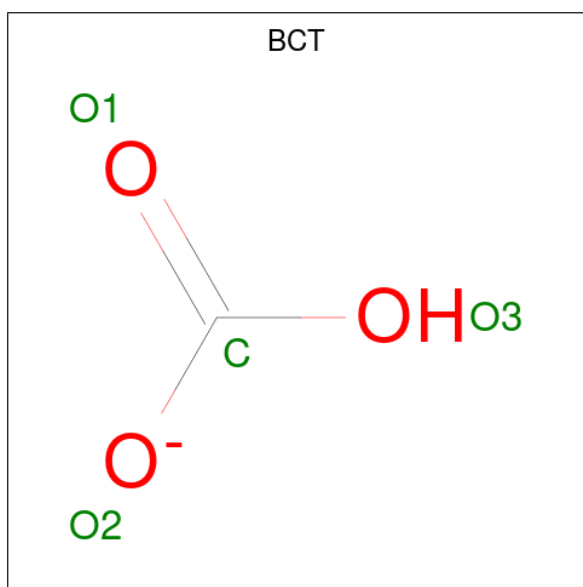
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

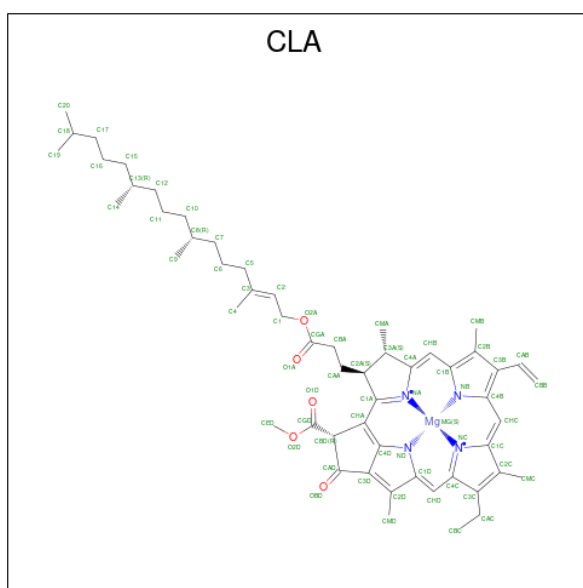
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	A	2	2	2	0	0
22	U	1	1	1	0	0
22	a	2	2	2	0	0
22	u	1	1	1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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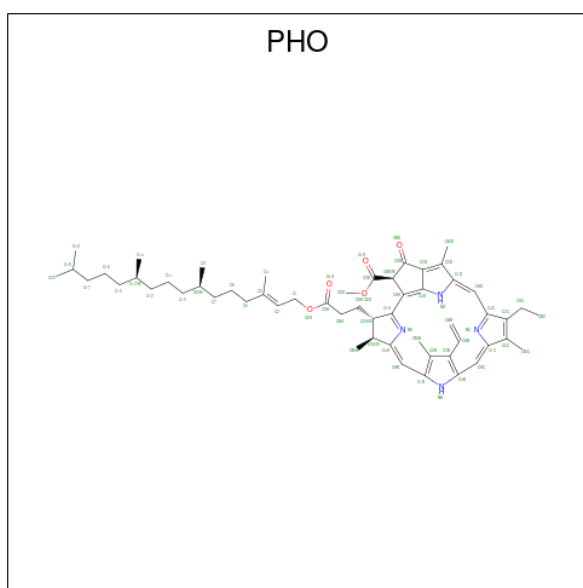
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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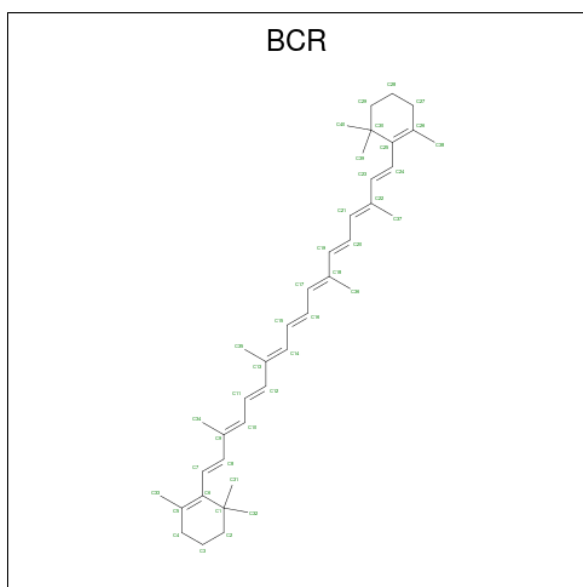
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



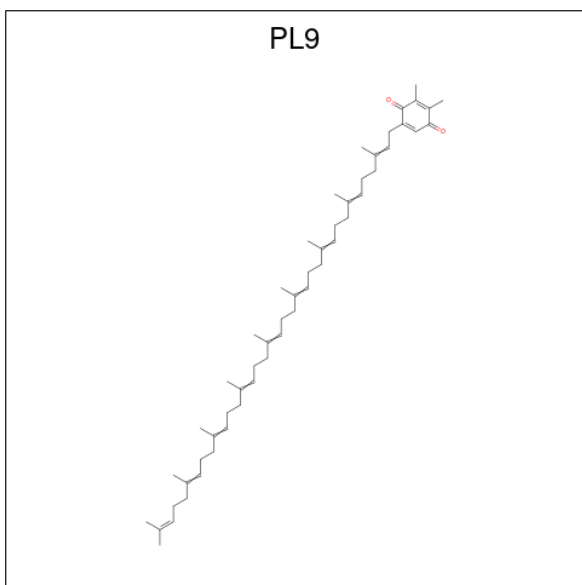
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

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



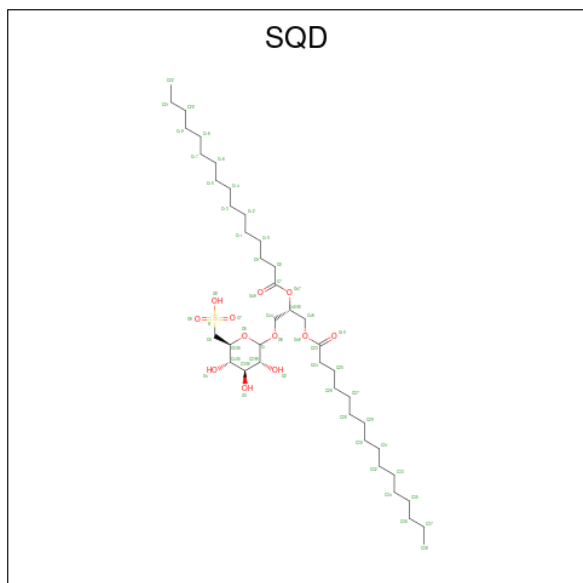
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



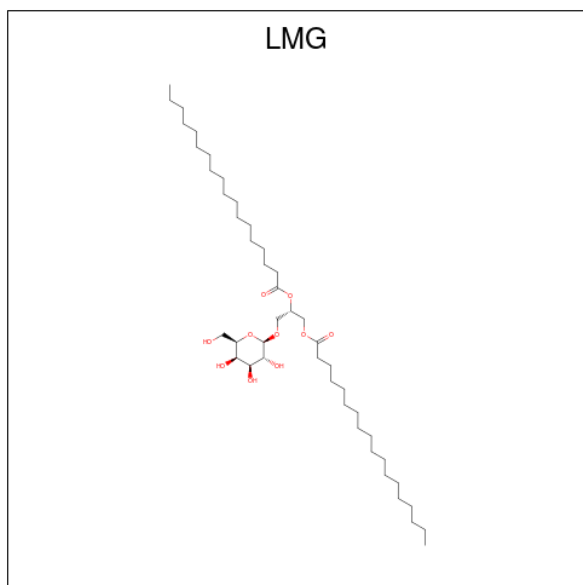
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	X	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
28	x	1	43	30	12	1	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



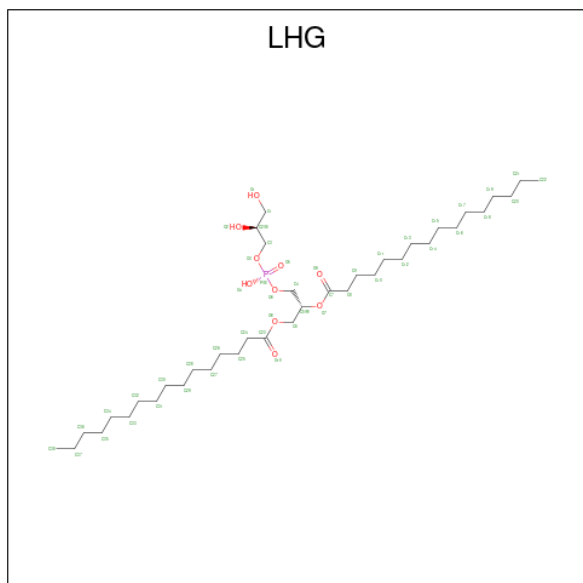
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	51	41	10	0	0
29	B	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	D	1	51	41	10	0	0
29	Z	1	37	27	10	0	0
29	a	1	51	41	10	0	0
29	b	1	51	41	10	0	0
29	c	1	51	41	10	0	0
29	c	1	51	41	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	j	1	Total	C	O	0	0
			51	41	10		
29	z	1	Total	C	O	0	0
			37	27	10		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{76}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	E	1	Total	C	O	P	0	0
			42	31	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	e	1	Total	C	O	P	0	0
			42	31	10	1		

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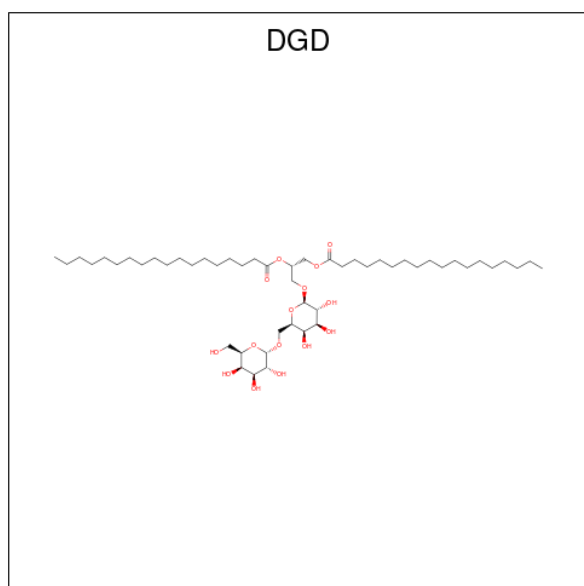
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total	Ca	0	0
			1	1		
31	F	1	Total	Ca	0	0
			1	1		
31	O	1	Total	Ca	0	0
			1	1		
31	b	1	Total	Ca	0	0
			1	1		
31	f	1	Total	Ca	0	0
			1	1		
31	o	1	Total	Ca	0	0
			1	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGD) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



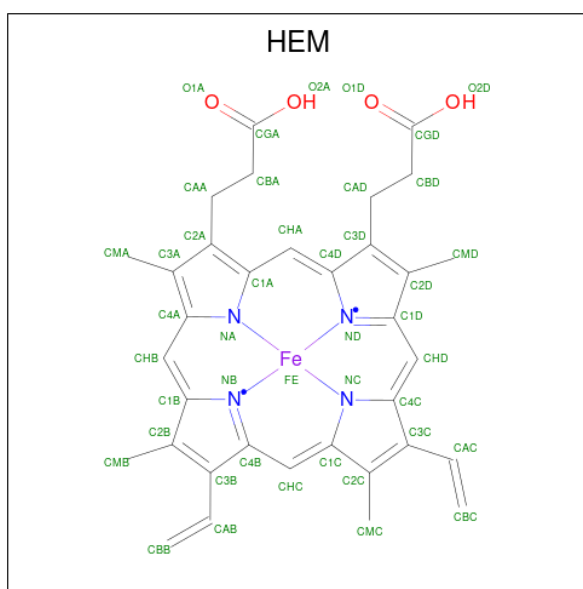
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
33	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
33	v	1	43	34	1	4	4	0	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

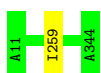
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1 1

Chain A:  100%



- Molecule 1: Photosystem II protein D1 1

Chain a:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  99%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  99%



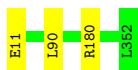
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  99%



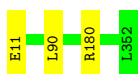
- Molecule 4: Photosystem II D2 protein

Chain D: 99%



- Molecule 4: Photosystem II D2 protein

Chain d: 99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 99%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 97%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 97%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 95% 5%



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J



There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L





- Molecule 11: Photosystem II reaction center protein L

Chain l: 97%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 97%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 97%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 98%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 98%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 100%

There are no outlier residues recorded for this chain.

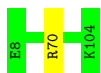
- Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

There are no outlier residues recorded for this chain.

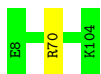
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  99%



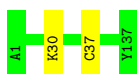
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  99%



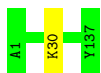
- Molecule 16: Cytochrome c-550

Chain V:  99%



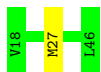
- Molecule 16: Cytochrome c-550

Chain v:  99%



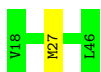
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  97%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  97%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain x:  100%

There are no outlier residues recorded for this chain.

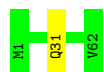
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  98% .



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  98% .



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 250.80 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 100.0 (250.80-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.324 , 0.331 0.343 , 0.340	Depositor DCC
R_{free} test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: PHO, LHG, CA, LMG, FE2, MG, PL9, CLA, HEM, DGD, SQD, BCR, CL, OEX, BCT

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	0.56	0/2734	0.68	0/3727
1	a	0.49	0/2734	0.64	0/3727
2	B	0.51	0/4194	0.65	1/5713 (0.0%)
2	b	0.48	0/4194	0.63	1/5713 (0.0%)
3	C	0.51	0/3634	0.64	0/4947
3	c	0.47	0/3634	0.60	0/4947
4	D	0.53	0/2821	0.65	0/3844
4	d	0.48	0/2821	0.60	0/3844
5	E	0.46	0/693	0.63	0/944
5	e	0.43	0/693	0.58	0/944
6	F	0.51	0/284	0.61	0/387
6	f	0.41	0/284	0.56	0/387
7	H	0.47	0/544	0.64	0/739
7	h	0.46	0/544	0.66	0/739
8	I	0.52	0/327	0.68	0/439
8	i	0.46	0/327	0.60	0/439
9	J	0.46	0/278	0.59	0/376
9	j	0.43	0/278	0.53	0/376
10	K	0.48	0/303	0.70	0/416
10	k	0.55	0/303	0.79	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.48	0/319	0.62	0/433
12	M	0.52	0/278	0.74	0/378
12	m	0.49	0/278	0.69	0/378
13	O	0.46	0/1926	0.65	0/2611
13	o	0.41	0/1926	0.61	0/2611
14	T	0.60	0/282	0.68	0/382
14	t	0.49	0/282	0.60	0/382
15	U	0.48	0/785	0.64	0/1064
15	u	0.46	0/785	0.63	0/1064
16	V	0.52	1/1096 (0.1%)	0.66	0/1487
16	v	0.42	0/1096	0.62	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/216	0.61	0/289
17	y	0.44	0/216	0.59	0/289
18	X	0.43	0/298	0.53	0/403
18	x	0.44	0/298	0.54	0/403
19	Z	0.44	0/490	0.58	0/669
19	z	0.46	0/490	0.56	0/669
All	All	0.49	1/43004 (0.0%)	0.63	2/58496 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	37	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	127	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	39	LEU	CA-CB-CG	-5.25	103.23	115.30

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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	41	75
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	34	72
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	34	72
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	4	31
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	72
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	72
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	51	81

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

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	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	408 (99%)	4 (1%)	76	88
2	b	412/402 (102%)	410 (100%)	2 (0%)	88	94
3	C	357/352 (101%)	351 (98%)	6 (2%)	60	82
3	c	357/352 (101%)	353 (99%)	4 (1%)	73	88
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	88
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	88
5	E	74/72 (103%)	73 (99%)	1 (1%)	67	85
5	e	74/72 (103%)	73 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	66
6	f	28/28 (100%)	27 (96%)	1 (4%)	35	66
7	H	56/54 (104%)	52 (93%)	4 (7%)	14	46
7	h	56/54 (104%)	52 (93%)	4 (7%)	14	46
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	48
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	48
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	72
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	72
12	M	32/31 (103%)	31 (97%)	1 (3%)	40	70
12	m	32/31 (103%)	31 (97%)	1 (3%)	40	70
13	O	210/206 (102%)	206 (98%)	4 (2%)	57	80
13	o	210/206 (102%)	206 (98%)	4 (2%)	57	80
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	71	87
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	87
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	91
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/22 (100%)	21 (96%)	1 (4%)	27	61
17	y	22/22 (100%)	21 (96%)	1 (4%)	27	61
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	80
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	80
All	All	4370/4302 (102%)	4312 (99%)	58 (1%)	69	86

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	30	LYS
16	v	30	LYS
3	c	315	MET
15	u	70	ARG
12	m	9	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	409	GLN
4	d	197	HIS
15	u	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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	$\# Z > 2$
29	LMG	z	101	-	37,37,55	1.40	4 (10%)	45,45,63	1.22	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	H	102	-	63,63,67	1.69	14 (22%)	77,77,81	1.02	4 (5%)
26	BCR	B	618	-	41,41,41	8.92	29 (70%)	56,56,56	5.95	31 (55%)
27	PL9	A	611	-	55,55,55	4.17	20 (36%)	68,69,69	3.92	34 (50%)
26	BCR	B	620	-	41,41,41	9.12	29 (70%)	56,56,56	5.77	33 (58%)
24	CLA	A	606	-	65,73,73	3.71	30 (46%)	76,113,113	1.97	18 (23%)
24	CLA	c	509	-	65,73,73	3.53	30 (46%)	76,113,113	1.82	16 (21%)
24	CLA	B	615	-	65,73,73	3.58	29 (44%)	76,113,113	1.85	15 (19%)
24	CLA	D	404	-	65,73,73	3.59	30 (46%)	76,113,113	2.00	18 (23%)
24	CLA	b	606	-	65,73,73	3.63	27 (41%)	76,113,113	1.94	16 (21%)
30	LHG	e	101	-	41,41,48	1.23	3 (7%)	44,47,54	1.05	2 (4%)
24	CLA	c	506	-	65,73,73	3.54	27 (41%)	76,113,113	1.86	14 (18%)
24	CLA	D	402	-	65,73,73	3.71	32 (49%)	76,113,113	1.83	20 (26%)
24	CLA	b	608[A]	-	65,73,73	3.57	29 (44%)	76,113,113	1.86	18 (23%)
29	LMG	j	101	34	51,51,55	1.31	5 (9%)	59,59,63	0.87	4 (6%)
32	DGD	E	101	-	63,63,67	1.73	15 (23%)	77,77,81	1.23	10 (12%)
30	LHG	D	406	-	48,48,48	1.13	2 (4%)	51,54,54	0.97	4 (7%)
25	PHO	A	608	-	51,69,69	0.99	2 (3%)	47,99,99	1.21	6 (12%)
24	CLA	b	610	-	65,73,73	3.52	29 (44%)	76,113,113	1.86	17 (22%)
24	CLA	B	603	-	65,73,73	3.59	31 (47%)	76,113,113	1.87	19 (25%)
26	BCR	t	101	-	41,41,41	9.01	30 (73%)	56,56,56	5.95	34 (60%)
24	CLA	A	609	-	65,73,73	3.66	30 (46%)	76,113,113	1.80	18 (23%)
24	CLA	B	604	-	65,73,73	3.59	30 (46%)	76,113,113	1.80	17 (22%)
24	CLA	C	507	-	65,73,73	3.49	29 (44%)	76,113,113	2.03	17 (22%)
27	PL9	D	405	-	55,55,55	4.19	20 (36%)	68,69,69	3.80	36 (52%)
30	LHG	L	101	-	48,48,48	1.10	2 (4%)	51,54,54	0.90	3 (5%)
32	DGD	h	102	-	63,63,67	1.68	15 (23%)	77,77,81	1.21	8 (10%)
30	LHG	d	407	-	48,48,48	1.15	3 (6%)	51,54,54	1.09	3 (5%)
27	PL9	a	611	-	55,55,55	4.18	21 (38%)	68,69,69	3.89	34 (50%)
26	BCR	c	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.91	34 (60%)
24	CLA	a	607	-	65,73,73	3.60	27 (41%)	76,113,113	1.86	18 (23%)
28	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	1.45	7 (13%)
33	HEM	E	103	5,6	41,50,50	2.02	7 (17%)	45,82,82	1.42	6 (13%)
26	BCR	b	620	-	41,41,41	8.87	29 (70%)	56,56,56	5.73	31 (55%)
26	BCR	C	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.93	33 (58%)
28	SQD	a	612	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	505	-	65,73,73	3.59	27 (41%)	76,113,113	1.84	14 (18%)
26	BCR	H	101	-	41,41,41	9.06	30 (73%)	56,56,56	5.72	30 (53%)
24	CLA	c	510	-	65,73,73	3.58	29 (44%)	76,113,113	1.81	16 (21%)
24	CLA	B	608	-	65,73,73	3.66	28 (43%)	76,113,113	1.90	19 (25%)
26	BCR	K	101	-	41,41,41	9.12	31 (75%)	56,56,56	5.42	29 (51%)
29	LMG	b	622	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	5 (8%)
24	CLA	C	510	-	65,73,73	3.57	30 (46%)	76,113,113	1.85	16 (21%)
24	CLA	a	615	-	65,73,73	3.70	29 (44%)	76,113,113	1.94	20 (26%)
24	CLA	c	503	-	65,73,73	3.58	30 (46%)	76,113,113	1.74	14 (18%)
28	SQD	A	612	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
24	CLA	c	502	-	65,73,73	3.56	28 (43%)	76,113,113	1.81	16 (21%)
23	BCT	a	605	21	2,3,3	0.96	0	2,3,3	3.74	2 (100%)
30	LHG	l	102	-	48,48,48	1.18	2 (4%)	51,54,54	0.92	2 (3%)
24	CLA	b	609	-	65,73,73	3.63	28 (43%)	76,113,113	1.90	17 (22%)
33	HEM	e	102	5,6	41,50,50	1.99	8 (19%)	45,82,82	1.49	5 (11%)
33	HEM	v	201	16	41,50,50	2.05	6 (14%)	45,82,82	1.70	8 (17%)
24	CLA	c	507	-	65,73,73	3.52	28 (43%)	76,113,113	2.01	16 (21%)
28	SQD	L	102	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	9 (14%)
29	LMG	c	519	-	51,51,55	1.38	5 (9%)	59,59,63	1.06	5 (8%)
30	LHG	a	616	-	48,48,48	1.10	2 (4%)	51,54,54	1.17	6 (11%)
24	CLA	b	612	-	65,73,73	3.60	28 (43%)	76,113,113	1.88	19 (25%)
20	OEX	A	601	3,1	0,15,15	-	-	-	-	-
26	BCR	F	101	-	41,41,41	9.04	26 (63%)	56,56,56	6.08	27 (48%)
24	CLA	B	613	-	65,73,73	3.68	28 (43%)	76,113,113	1.96	19 (25%)
26	BCR	c	515	-	41,41,41	9.15	31 (75%)	56,56,56	5.57	27 (48%)
26	BCR	h	101	-	41,41,41	9.16	30 (73%)	56,56,56	5.68	33 (58%)
24	CLA	b	603	-	65,73,73	3.60	28 (43%)	76,113,113	1.82	16 (21%)
26	BCR	k	101	-	41,41,41	9.22	31 (75%)	56,56,56	5.67	28 (50%)
32	DGD	C	517	-	63,63,67	1.66	15 (23%)	77,77,81	1.14	6 (7%)
24	CLA	c	513	-	65,73,73	3.48	30 (46%)	76,113,113	1.80	16 (21%)
24	CLA	c	512	-	65,73,73	3.60	29 (44%)	76,113,113	1.82	18 (23%)
24	CLA	C	504	-	65,73,73	3.57	29 (44%)	76,113,113	1.91	18 (23%)
33	HEM	V	201	16	41,50,50	2.01	8 (19%)	45,82,82	1.58	7 (15%)
26	BCR	K	102	-	41,41,41	9.13	29 (70%)	56,56,56	5.63	25 (44%)
24	CLA	B	616	-	65,73,73	3.55	29 (44%)	76,113,113	1.73	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.89	3 (5%)
30	LHG	A	615	-	48,48,48	1.11	3 (6%)	51,54,54	1.30	5 (9%)
28	SQD	x	101	-	42,43,54	1.20	4 (9%)	51,54,65	1.46	7 (13%)
24	CLA	b	618	-	65,73,73	3.64	28 (43%)	76,113,113	1.81	18 (23%)
24	CLA	B	612	-	65,73,73	3.66	29 (44%)	76,113,113	1.86	18 (23%)
24	CLA	b	611	-	65,73,73	3.57	26 (40%)	76,113,113	1.78	16 (21%)
24	CLA	B	611	-	65,73,73	3.55	31 (47%)	76,113,113	1.81	19 (25%)
24	CLA	B	607[B]	-	65,73,73	3.60	28 (43%)	76,113,113	1.88	18 (23%)
25	PHO	d	401	-	51,69,69	0.97	0	47,99,99	1.40	6 (12%)
24	CLA	B	610	-	65,73,73	3.69	27 (41%)	76,113,113	1.81	19 (25%)
26	BCR	T	101	-	41,41,41	9.04	30 (73%)	56,56,56	6.12	32 (57%)
24	CLA	B	606	-	65,73,73	3.56	28 (43%)	76,113,113	1.78	14 (18%)
24	CLA	b	613	-	65,73,73	3.71	29 (44%)	76,113,113	1.91	19 (25%)
32	DGD	c	516	-	63,63,67	1.70	15 (23%)	77,77,81	1.09	7 (9%)
24	CLA	b	615	-	65,73,73	3.63	29 (44%)	76,113,113	1.75	16 (21%)
24	CLA	b	617	-	65,73,73	3.54	30 (46%)	76,113,113	1.77	15 (19%)
24	CLA	a	606	-	65,73,73	3.64	28 (43%)	76,113,113	1.90	19 (25%)
24	CLA	b	605	-	65,73,73	3.70	29 (44%)	76,113,113	1.90	19 (25%)
32	DGD	c	517	-	63,63,67	1.62	16 (25%)	77,77,81	1.11	9 (11%)
24	CLA	c	508	-	65,73,73	3.60	28 (43%)	76,113,113	1.94	17 (22%)
24	CLA	A	607	-	65,73,73	3.59	29 (44%)	76,113,113	1.99	19 (25%)
27	PL9	d	404	-	55,55,55	4.15	20 (36%)	68,69,69	3.85	34 (50%)
24	CLA	C	509	-	65,73,73	3.58	30 (46%)	76,113,113	1.86	16 (21%)
24	CLA	C	511	3	65,73,73	3.63	29 (44%)	76,113,113	1.93	20 (26%)
24	CLA	b	607	-	65,73,73	3.57	29 (44%)	76,113,113	1.80	14 (18%)
24	CLA	B	605	-	65,73,73	3.59	27 (41%)	76,113,113	1.91	17 (22%)
26	BCR	A	610	-	41,41,41	9.17	30 (73%)	56,56,56	5.54	27 (48%)
24	CLA	c	501	-	65,73,73	3.56	30 (46%)	76,113,113	1.87	20 (26%)
24	CLA	c	504	-	65,73,73	3.63	31 (47%)	76,113,113	1.96	22 (28%)
26	BCR	f	101	-	41,41,41	8.99	29 (70%)	56,56,56	5.59	26 (46%)
24	CLA	C	505	-	65,73,73	3.53	27 (41%)	76,113,113	1.86	15 (19%)
24	CLA	D	403	-	65,73,73	3.65	28 (43%)	76,113,113	1.73	18 (23%)
26	BCR	b	621	-	41,41,41	9.05	31 (75%)	56,56,56	6.43	31 (55%)
29	LMG	A	613	-	51,51,55	1.33	4 (7%)	59,59,63	0.91	4 (6%)
28	SQD	B	622	-	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	c	518	-	63,63,67	1.68	15 (23%)	77,77,81	1.25	8 (10%)
20	OEX	a	601	3,1	0,15,15	-	-	-	-	-
24	CLA	C	502	-	65,73,73	3.55	28 (43%)	76,113,113	1.85	16 (21%)
24	CLA	B	609	-	65,73,73	3.52	27 (41%)	76,113,113	1.97	23 (30%)
24	CLA	B	617	-	65,73,73	3.57	28 (43%)	76,113,113	1.79	16 (21%)
25	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.48	8 (17%)
30	LHG	d	406	-	48,48,48	1.11	2 (4%)	51,54,54	1.02	3 (5%)
29	LMG	C	518	-	51,51,55	1.42	6 (11%)	59,59,63	1.29	10 (16%)
32	DGD	d	405	-	63,63,67	1.71	16 (25%)	77,77,81	1.16	9 (11%)
24	CLA	d	403	-	65,73,73	3.53	29 (44%)	76,113,113	1.87	19 (25%)
28	SQD	l	101	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
24	CLA	B	602	-	65,73,73	3.52	29 (44%)	76,113,113	1.77	13 (17%)
26	BCR	b	619	-	41,41,41	9.23	29 (70%)	56,56,56	5.80	28 (50%)
29	LMG	C	519	-	51,51,55	1.33	5 (9%)	59,59,63	1.02	4 (6%)
29	LMG	c	520	-	51,51,55	1.37	5 (9%)	59,59,63	1.12	4 (6%)
24	CLA	B	607[A]	-	65,73,73	3.59	27 (41%)	76,113,113	1.90	19 (25%)
24	CLA	a	609	-	65,73,73	3.61	28 (43%)	76,113,113	1.83	17 (22%)
30	LHG	E	102	-	41,41,48	1.22	3 (7%)	44,47,54	0.99	3 (6%)
24	CLA	C	506	-	65,73,73	3.53	28 (43%)	76,113,113	1.90	16 (21%)
24	CLA	b	608[B]	-	65,73,73	3.58	28 (43%)	76,113,113	1.84	19 (25%)
29	LMG	Z	101	-	37,37,55	1.44	4 (10%)	45,45,63	1.34	6 (13%)
24	CLA	C	508	-	65,73,73	3.70	30 (46%)	76,113,113	1.81	16 (21%)
24	CLA	B	614	-	65,73,73	3.63	29 (44%)	76,113,113	1.78	15 (19%)
24	CLA	d	402	-	65,73,73	3.61	30 (46%)	76,113,113	1.83	18 (23%)
24	CLA	C	503	-	65,73,73	3.60	30 (46%)	76,113,113	1.72	14 (18%)
29	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	1.01	3 (5%)
26	BCR	c	521	-	41,41,41	9.34	29 (70%)	56,56,56	5.62	26 (46%)
26	BCR	I	101	-	41,41,41	9.05	31 (75%)	56,56,56	5.91	30 (53%)
29	LMG	D	408	-	51,51,55	1.34	5 (9%)	59,59,63	1.10	7 (11%)
28	SQD	a	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	c	511	3	65,73,73	3.57	28 (43%)	76,113,113	1.85	16 (21%)
25	PHO	a	608	-	51,69,69	1.01	3 (5%)	47,99,99	1.21	5 (10%)
29	LMG	a	613	-	51,51,55	1.33	5 (9%)	59,59,63	0.99	3 (5%)
32	DGD	C	515	-	63,63,67	1.70	15 (23%)	77,77,81	1.03	5 (6%)
26	BCR	B	619	-	41,41,41	8.94	30 (73%)	56,56,56	5.62	29 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	616	-	65,73,73	3.58	29 (44%)	76,113,113	1.85	16 (21%)
32	DGD	C	516	-	63,63,67	1.67	15 (23%)	77,77,81	1.21	10 (12%)
24	CLA	C	512	-	65,73,73	3.53	30 (46%)	76,113,113	1.88	20 (26%)
24	CLA	b	604	-	65,73,73	3.64	28 (43%)	76,113,113	1.92	16 (21%)
23	BCT	A	605	21	2,3,3	0.95	0	2,3,3	2.68	2 (100%)
28	SQD	A	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	b	614	-	65,73,73	3.68	28 (43%)	76,113,113	1.88	18 (23%)
24	CLA	C	513	-	65,73,73	3.51	27 (41%)	76,113,113	1.88	19 (25%)
24	CLA	C	501	-	65,73,73	3.54	28 (43%)	76,113,113	1.90	20 (26%)
28	SQD	b	601	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
26	BCR	a	610	-	41,41,41	8.98	30 (73%)	56,56,56	5.53	24 (42%)

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
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
26	BCR	B	618	-	-	23/29/63/63	0/2/2/2
27	PL9	A	611	-	-	25/53/73/73	0/1/1/1
26	BCR	B	620	-	-	19/29/63/63	0/2/2/2
24	CLA	A	606	-	1/1/15/20	1/37/115/115	-
24	CLA	c	509	-	1/1/15/20	11/37/115/115	-
24	CLA	B	615	-	1/1/15/20	15/37/115/115	-
24	CLA	D	404	-	1/1/15/20	13/37/115/115	-
24	CLA	b	606	-	1/1/15/20	10/37/115/115	-
30	LHG	e	101	-	-	24/46/46/53	-
24	CLA	c	506	-	1/1/15/20	13/37/115/115	-
24	CLA	D	402	-	1/1/15/20	6/37/115/115	-
24	CLA	b	608[A]	-	1/1/15/20	8/37/115/115	-
29	LMG	j	101	34	-	17/46/66/70	0/1/1/1
32	DGD	E	101	-	-	35/51/91/95	0/2/2/2
30	LHG	D	406	-	-	19/53/53/53	-
25	PHO	A	608	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	610	-	1/1/15/20	5/37/115/115	-
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
26	BCR	t	101	-	-	26/29/63/63	0/2/2/2
24	CLA	A	609	-	1/1/15/20	19/37/115/115	-
24	CLA	B	604	-	1/1/15/20	6/37/115/115	-
24	CLA	C	507	-	1/1/15/20	9/37/115/115	-
27	PL9	D	405	-	-	26/53/73/73	0/1/1/1
30	LHG	L	101	-	-	19/53/53/53	-
32	DGD	h	102	-	-	17/51/91/95	0/2/2/2
30	LHG	d	407	-	-	18/53/53/53	-
27	PL9	a	611	-	-	24/53/73/73	0/1/1/1
26	BCR	c	514	-	-	24/29/63/63	0/2/2/2
24	CLA	a	607	-	1/1/15/20	11/37/115/115	-
28	SQD	X	101	-	-	16/38/58/69	0/1/1/1
33	HEM	E	103	5,6	-	3/12/54/54	-
26	BCR	b	620	-	-	19/29/63/63	0/2/2/2
26	BCR	C	514	-	-	25/29/63/63	0/2/2/2
28	SQD	a	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	505	-	1/1/15/20	8/37/115/115	-
26	BCR	H	101	-	-	21/29/63/63	0/2/2/2
24	CLA	c	510	-	1/1/15/20	11/37/115/115	-
24	CLA	B	608	-	1/1/15/20	7/37/115/115	-
26	BCR	K	101	-	-	19/29/63/63	0/2/2/2
29	LMG	b	622	-	-	19/46/66/70	0/1/1/1
24	CLA	C	510	-	1/1/15/20	12/37/115/115	-
24	CLA	a	615	-	1/1/15/20	7/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
28	SQD	A	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	502	-	1/1/15/20	10/37/115/115	-
30	LHG	l	102	-	-	23/53/53/53	-
24	CLA	b	609	-	1/1/15/20	4/37/115/115	-
33	HEM	e	102	5,6	-	3/12/54/54	-
33	HEM	v	201	16	-	2/12/54/54	-
24	CLA	c	507	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	L	102	-	-	28/49/69/69	0/1/1/1
29	LMG	c	519	-	-	21/46/66/70	0/1/1/1
30	LHG	a	616	-	-	17/53/53/53	-
24	CLA	b	612	-	1/1/15/20	10/37/115/115	-
26	BCR	F	101	-	-	21/29/63/63	0/2/2/2
26	BCR	h	101	-	-	25/29/63/63	0/2/2/2
24	CLA	B	613	-	1/1/15/20	7/37/115/115	-
26	BCR	c	515	-	-	20/29/63/63	0/2/2/2
26	BCR	k	101	-	-	20/29/63/63	0/2/2/2
24	CLA	b	603	-	1/1/15/20	19/37/115/115	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
24	CLA	c	513	-	1/1/15/20	10/37/115/115	-
24	CLA	c	512	-	1/1/15/20	7/37/115/115	-
24	CLA	C	504	-	1/1/15/20	12/37/115/115	-
33	HEM	V	201	16	-	2/12/54/54	-
26	BCR	K	102	-	-	20/29/63/63	0/2/2/2
24	CLA	B	616	-	1/1/15/20	13/37/115/115	-
30	LHG	D	407	-	-	19/53/53/53	-
30	LHG	A	615	-	-	16/53/53/53	-
28	SQD	x	101	-	-	16/38/58/69	0/1/1/1
24	CLA	b	618	-	1/1/15/20	14/37/115/115	-
24	CLA	B	612	-	1/1/15/20	5/37/115/115	-
24	CLA	b	611	-	1/1/15/20	5/37/115/115	-
24	CLA	B	611	-	1/1/15/20	9/37/115/115	-
24	CLA	B	607[B]	-	1/1/15/20	10/37/115/115	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
24	CLA	B	610	-	1/1/15/20	6/37/115/115	-
26	BCR	T	101	-	-	25/29/63/63	0/2/2/2
24	CLA	B	606	-	1/1/15/20	7/37/115/115	-
24	CLA	b	613	-	1/1/15/20	4/37/115/115	-
32	DGD	c	516	-	-	22/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	5/37/115/115	-
24	CLA	b	617	-	1/1/15/20	11/37/115/115	-
24	CLA	a	606	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	605	-	1/1/15/20	7/37/115/115	-
32	DGD	c	517	-	-	26/51/91/95	0/2/2/2
24	CLA	c	508	-	1/1/15/20	4/37/115/115	-
24	CLA	A	607	-	1/1/15/20	11/37/115/115	-
27	PL9	d	404	-	-	26/53/73/73	0/1/1/1
24	CLA	C	509	-	1/1/15/20	7/37/115/115	-
24	CLA	C	511	3	1/1/15/20	6/37/115/115	-
24	CLA	b	607	-	1/1/15/20	6/37/115/115	-
24	CLA	B	605	-	1/1/15/20	9/37/115/115	-
26	BCR	A	610	-	-	23/29/63/63	0/2/2/2
24	CLA	c	501	-	1/1/15/20	11/37/115/115	-
24	CLA	c	504	-	1/1/15/20	11/37/115/115	-
26	BCR	f	101	-	-	18/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	7/37/115/115	-
24	CLA	D	403	-	1/1/15/20	6/37/115/115	-
26	BCR	b	621	-	-	20/29/63/63	0/2/2/2
29	LMG	A	613	-	-	32/46/66/70	0/1/1/1
28	SQD	B	622	-	-	29/49/69/69	0/1/1/1
32	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	C	502	-	1/1/15/20	9/37/115/115	-
24	CLA	B	609	-	1/1/15/20	4/37/115/115	-
24	CLA	B	617	-	1/1/15/20	14/37/115/115	-
25	PHO	D	401	-	-	4/37/103/103	0/5/6/6
30	LHG	d	406	-	-	15/53/53/53	-
29	LMG	C	518	-	-	22/46/66/70	0/1/1/1
32	DGD	d	405	-	-	34/51/91/95	0/2/2/2
24	CLA	d	403	-	1/1/15/20	14/37/115/115	-
28	SQD	l	101	-	-	28/49/69/69	0/1/1/1
24	CLA	B	602	-	1/1/15/20	21/37/115/115	-
26	BCR	b	619	-	-	21/29/63/63	0/2/2/2
29	LMG	C	519	-	-	20/46/66/70	0/1/1/1
29	LMG	c	520	-	-	22/46/66/70	0/1/1/1
24	CLA	B	607[A]	-	1/1/15/20	9/37/115/115	-
24	CLA	a	609	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	E	102	-	-	26/46/46/53	-
24	CLA	C	506	-	1/1/15/20	17/37/115/115	-
24	CLA	b	608[B]	-	1/1/15/20	10/37/115/115	-
29	LMG	Z	101	-	-	17/31/51/70	0/1/1/1
24	CLA	C	508	-	1/1/15/20	6/37/115/115	-
24	CLA	B	614	-	1/1/15/20	3/37/115/115	-
24	CLA	d	402	-	1/1/15/20	3/37/115/115	-
24	CLA	C	503	-	1/1/15/20	6/37/115/115	-
29	LMG	B	621	-	-	21/46/66/70	0/1/1/1
26	BCR	c	521	-	-	22/29/63/63	0/2/2/2
26	BCR	I	101	-	-	21/29/63/63	0/2/2/2
29	LMG	D	408	-	-	20/46/66/70	0/1/1/1
28	SQD	a	614	-	-	23/49/69/69	0/1/1/1
24	CLA	c	511	3	1/1/15/20	4/37/115/115	-
25	PHO	a	608	-	-	3/37/103/103	0/5/6/6
29	LMG	a	613	-	-	30/46/66/70	0/1/1/1
32	DGD	C	515	-	-	23/51/91/95	0/2/2/2
26	BCR	B	619	-	-	23/29/63/63	0/2/2/2
24	CLA	b	616	-	1/1/15/20	13/37/115/115	-
32	DGD	C	516	-	-	31/51/91/95	0/2/2/2
24	CLA	C	512	-	1/1/15/20	9/37/115/115	-
24	CLA	b	604	-	1/1/15/20	5/37/115/115	-
28	SQD	A	614	-	-	23/49/69/69	0/1/1/1
24	CLA	b	614	-	1/1/15/20	7/37/115/115	-
24	CLA	C	513	-	1/1/15/20	12/37/115/115	-
24	CLA	C	501	-	1/1/15/20	12/37/115/115	-
28	SQD	b	601	-	-	29/49/69/69	0/1/1/1
26	BCR	a	610	-	-	22/29/63/63	0/2/2/2

The worst 5 of 3107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C14-C13	28.80	1.74	1.35
26	F	101	BCR	C14-C13	27.15	1.71	1.35
26	c	515	BCR	C14-C13	27.13	1.71	1.35
26	K	102	BCR	C14-C13	26.70	1.71	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	620	BCR	C14-C13	26.66	1.71	1.35

The worst 5 of 2340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	621	BCR	C15-C16-C17	25.00	174.68	123.47
26	k	101	BCR	C15-C16-C17	24.97	174.62	123.47
26	T	101	BCR	C15-C16-C17	24.91	174.50	123.47
26	t	101	BCR	C15-C16-C17	24.76	174.19	123.47
26	A	610	BCR	C15-C16-C17	23.82	172.26	123.47

5 of 72 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	ND
24	A	607	CLA	ND
24	A	609	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 2162 torsion outliers are listed below:

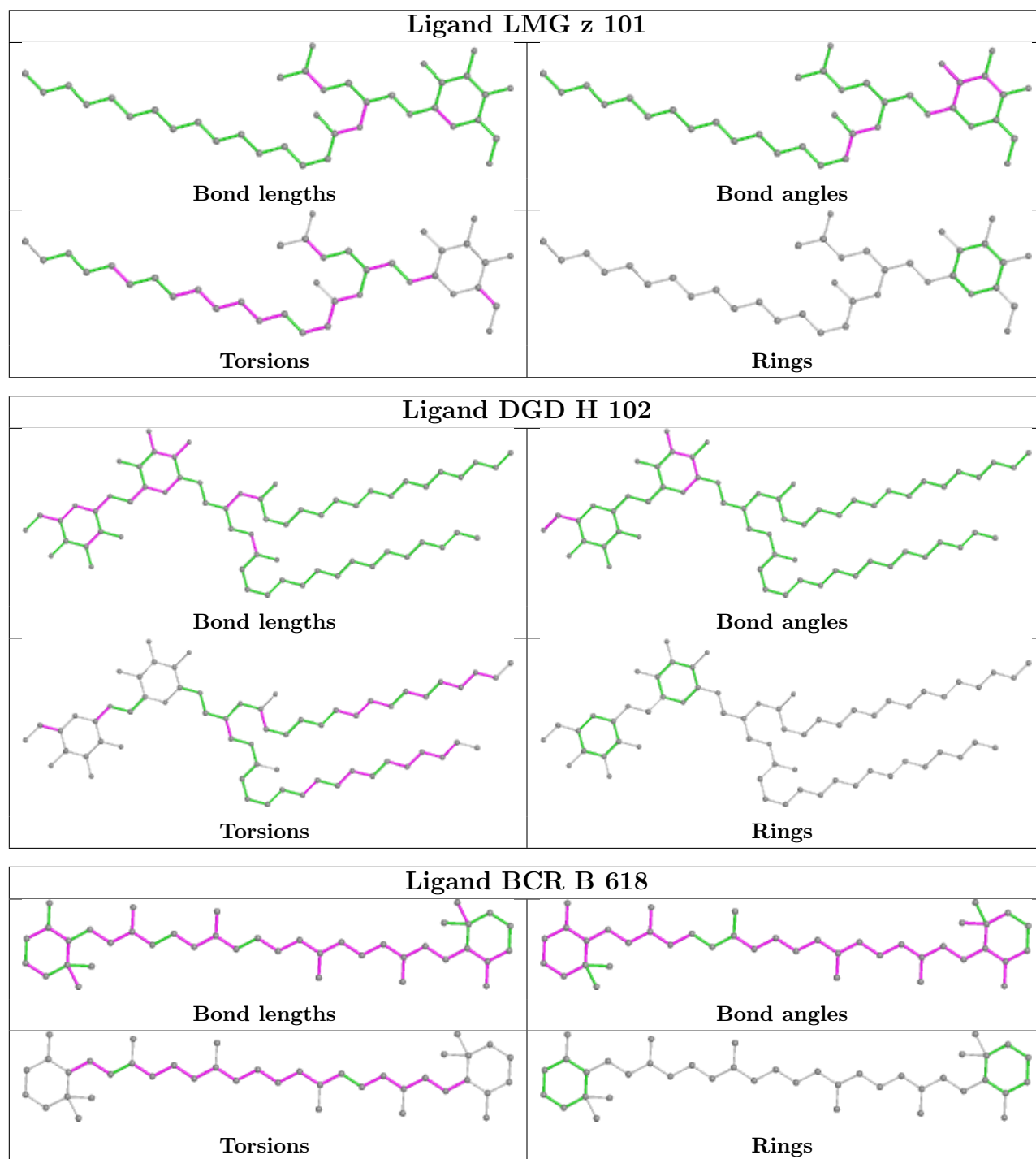
Mol	Chain	Res	Type	Atoms
24	A	607	CLA	CHA-CBD-CGD-O2D
24	A	609	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O2D

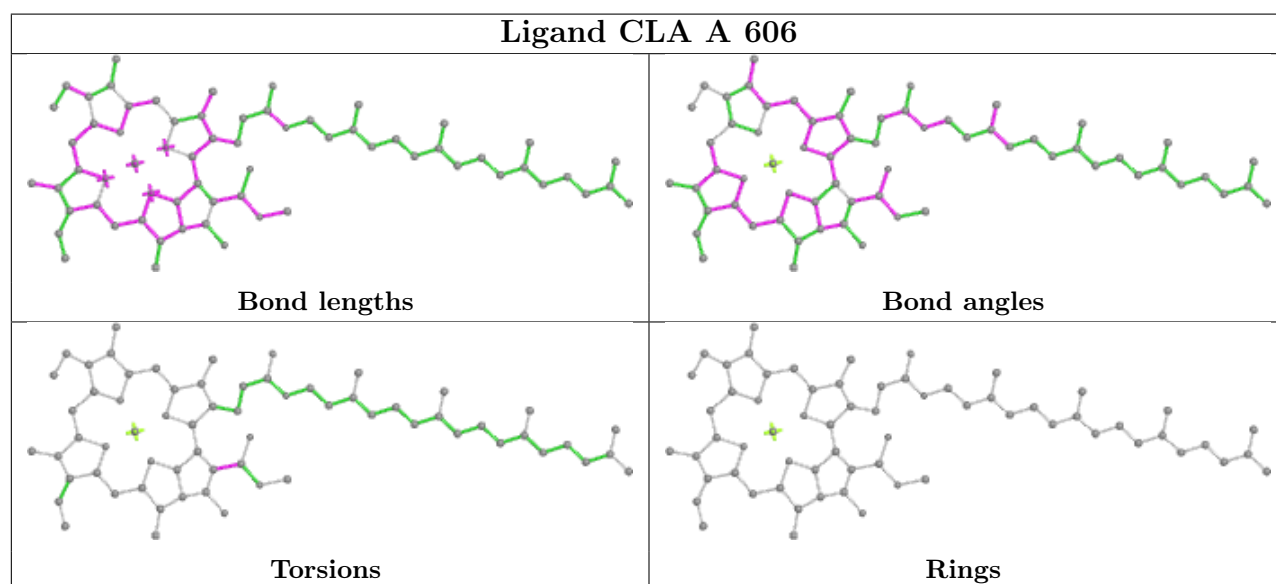
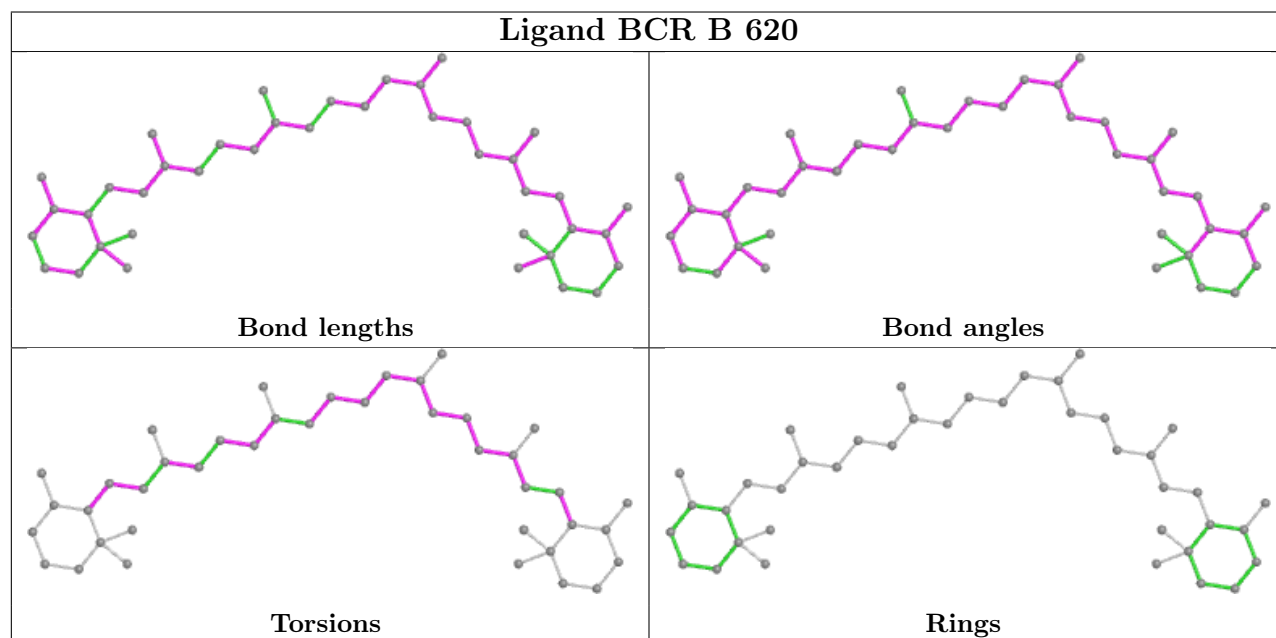
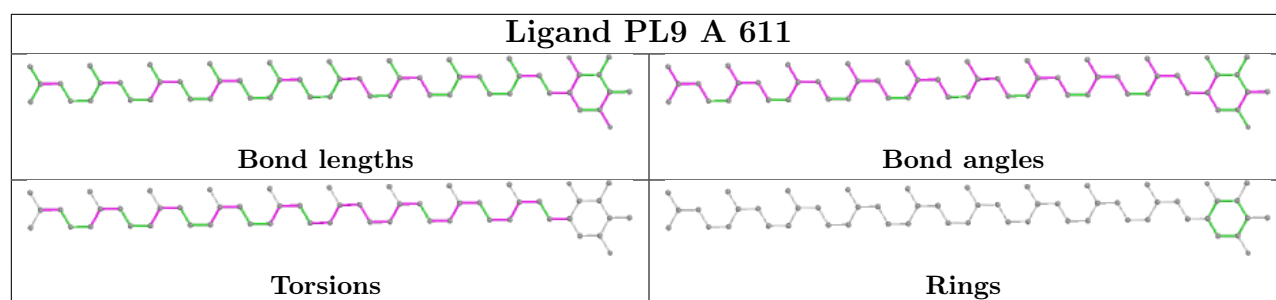
There are no ring outliers.

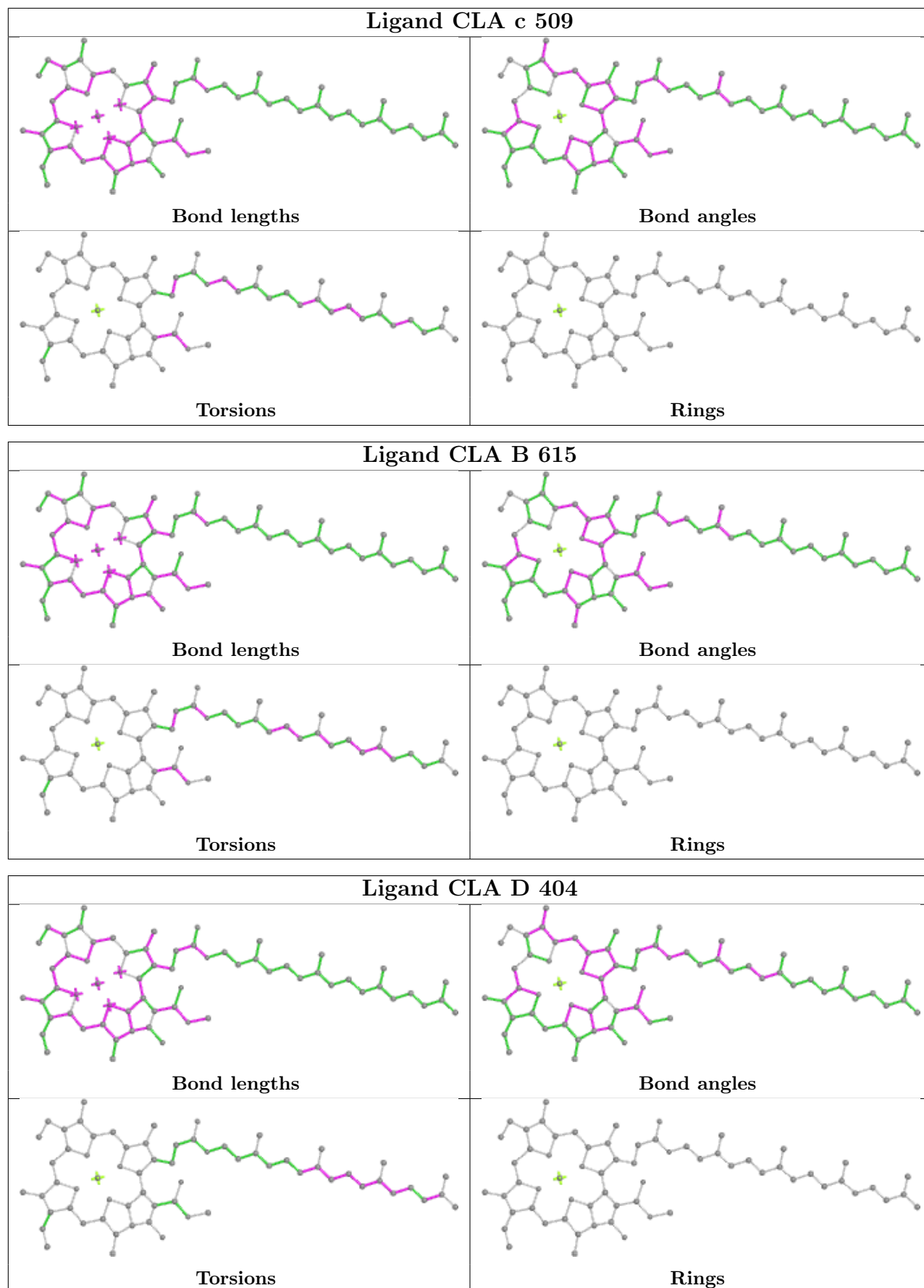
No monomer is involved in short contacts.

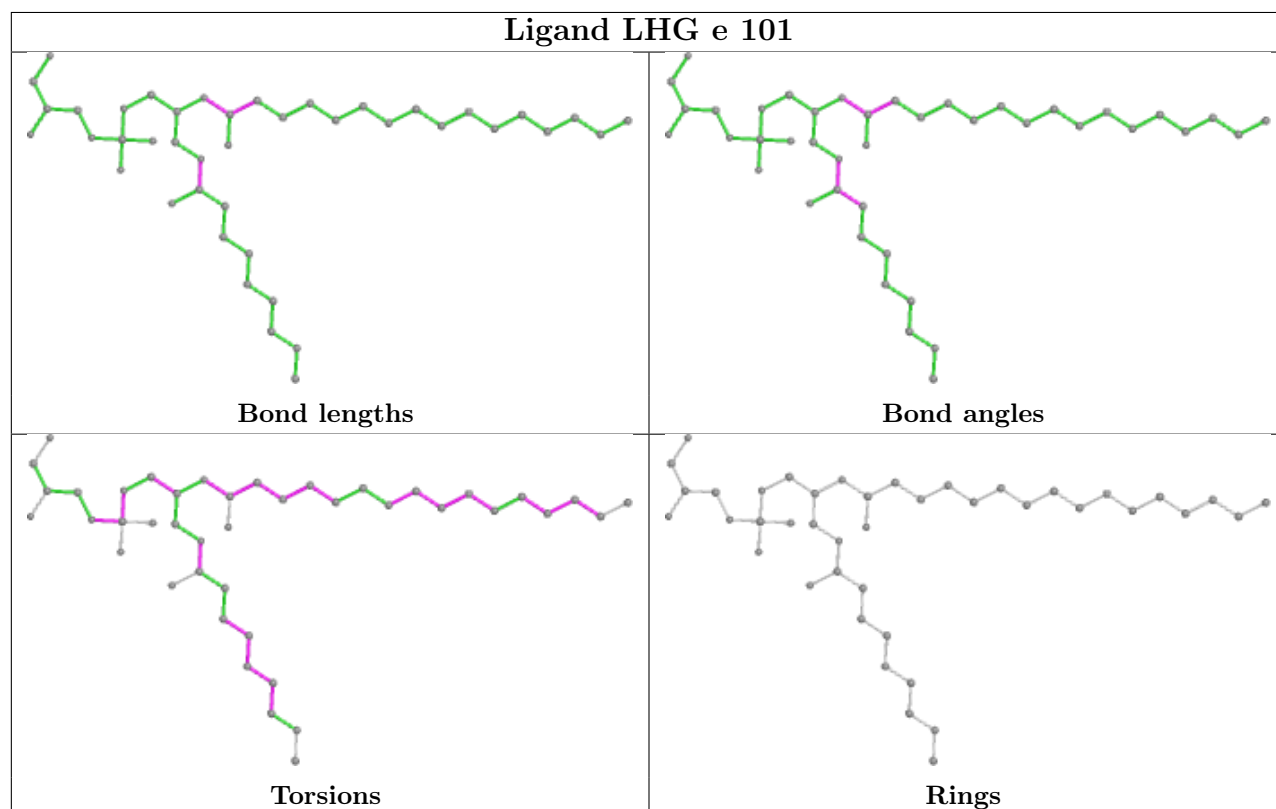
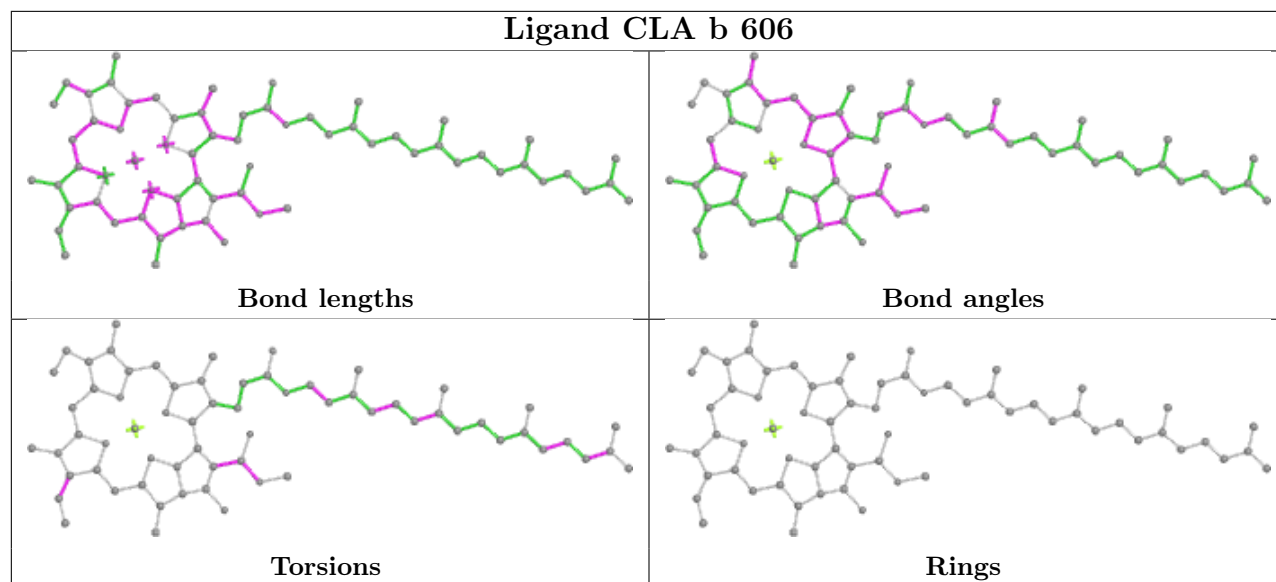
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

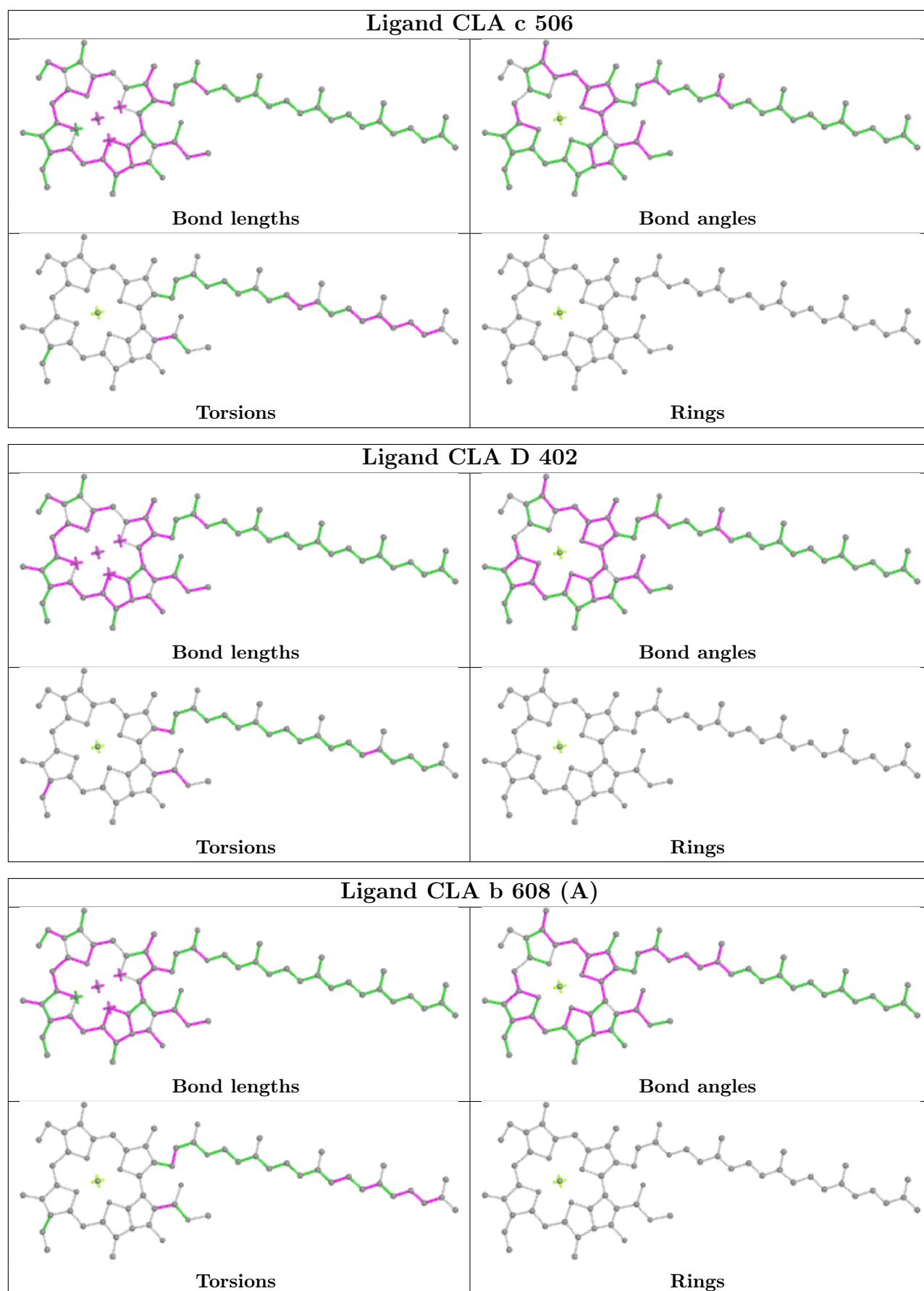
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

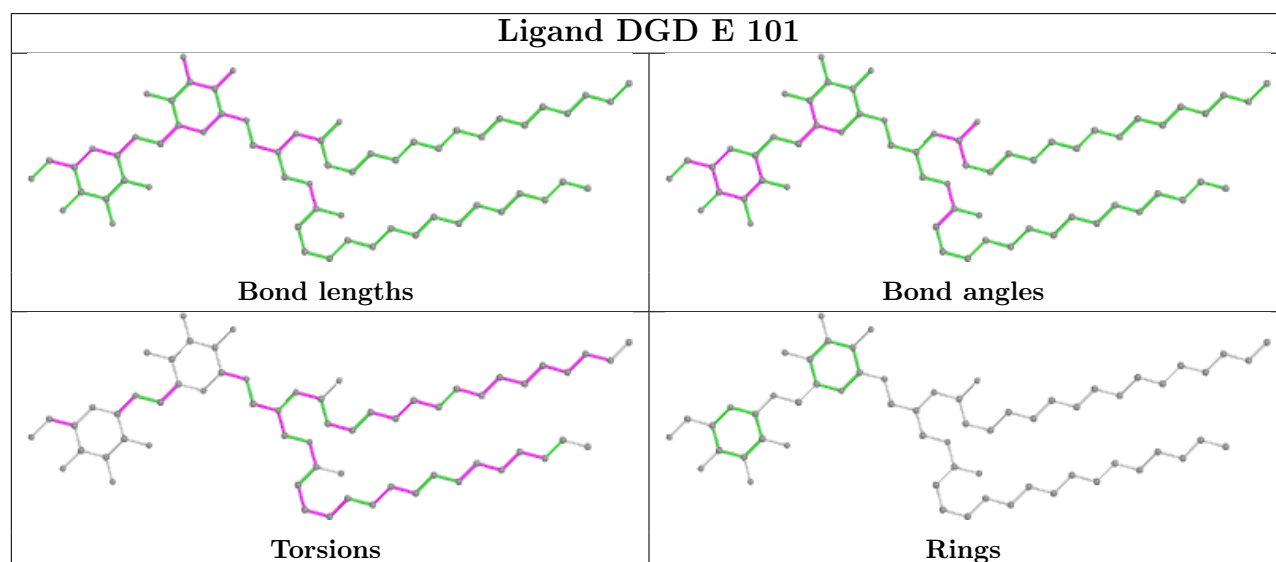
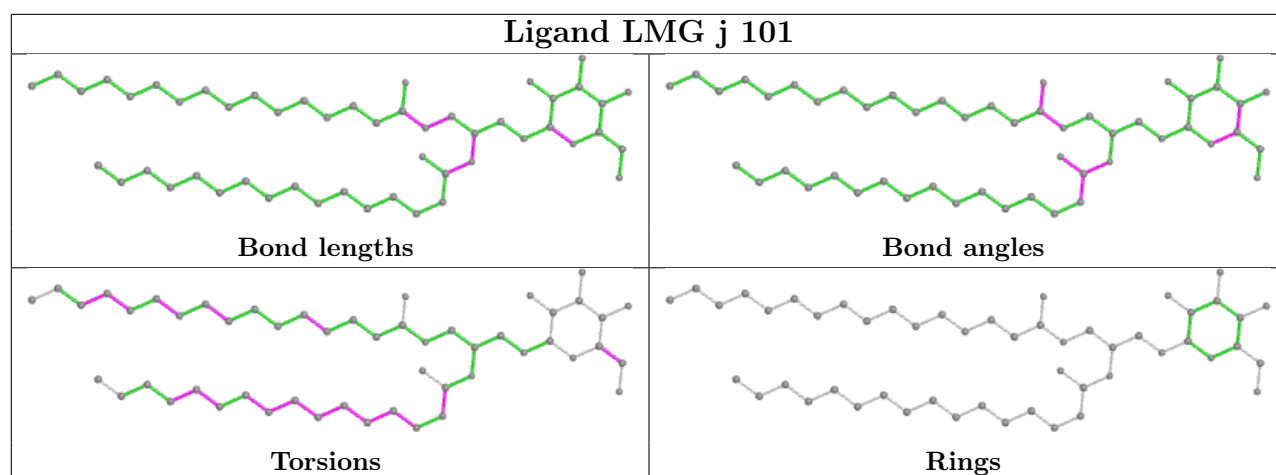


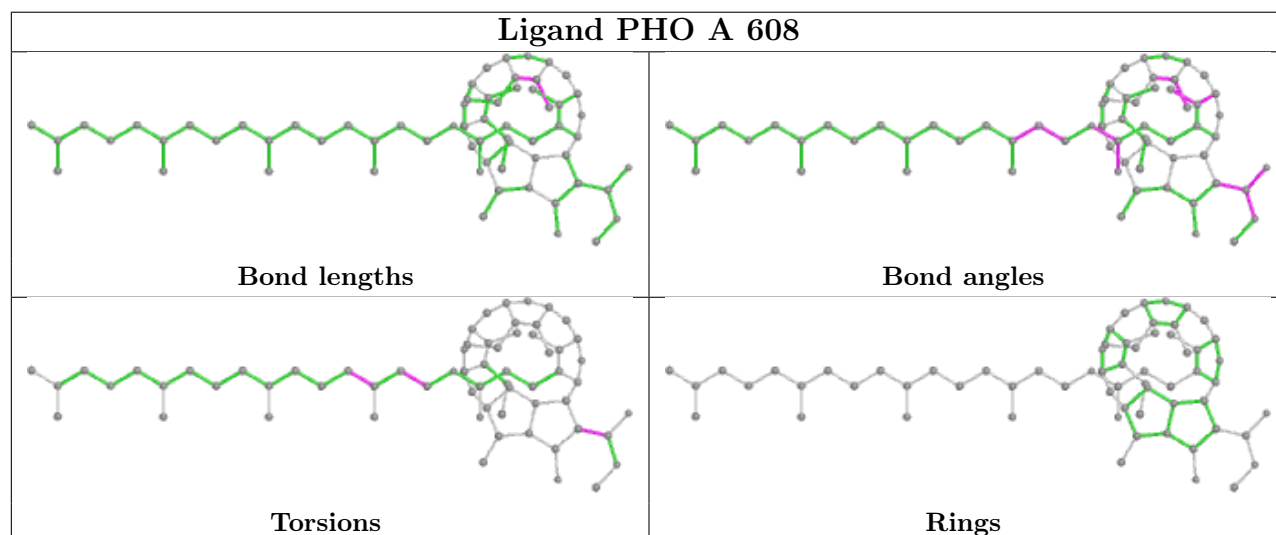
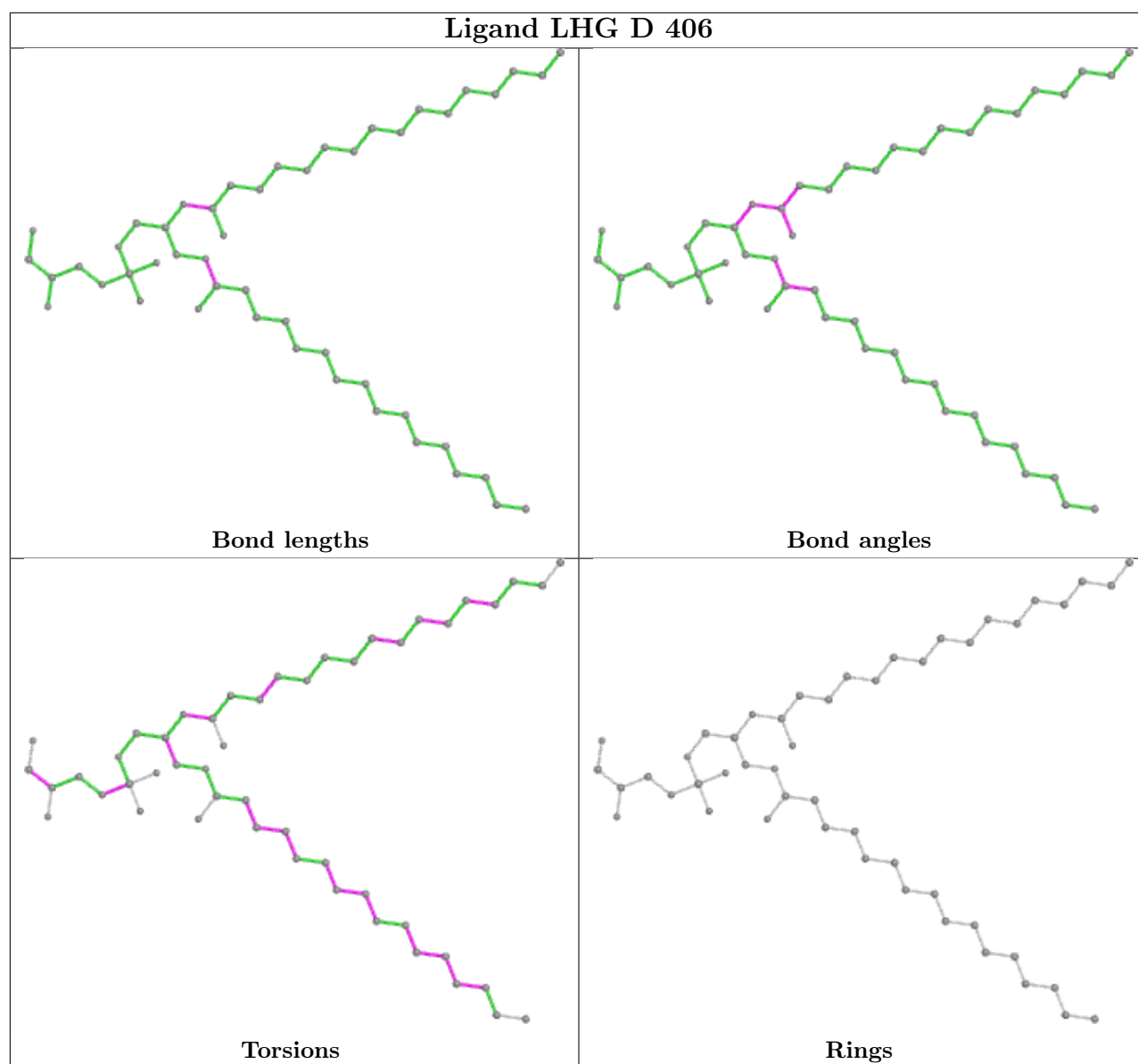


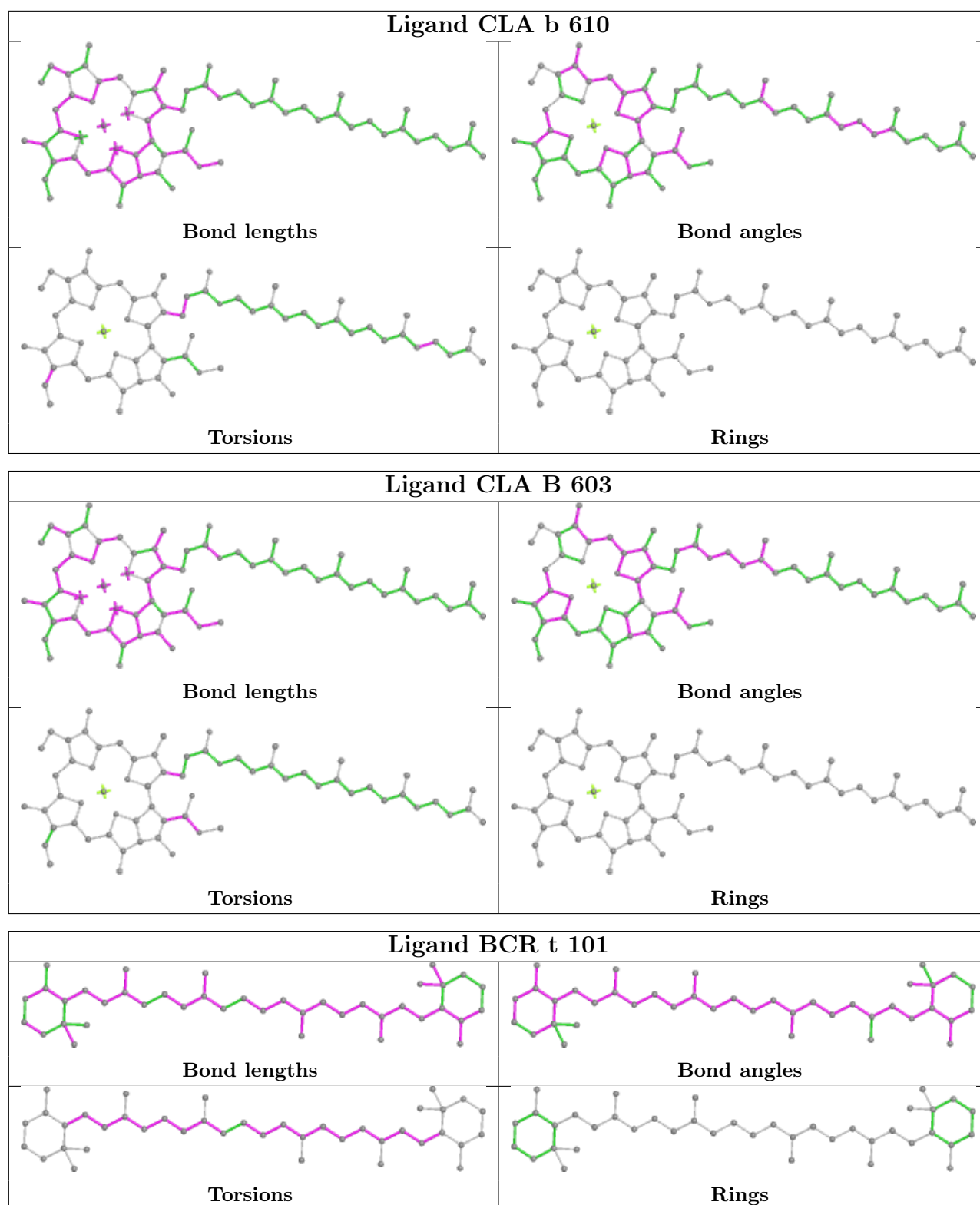


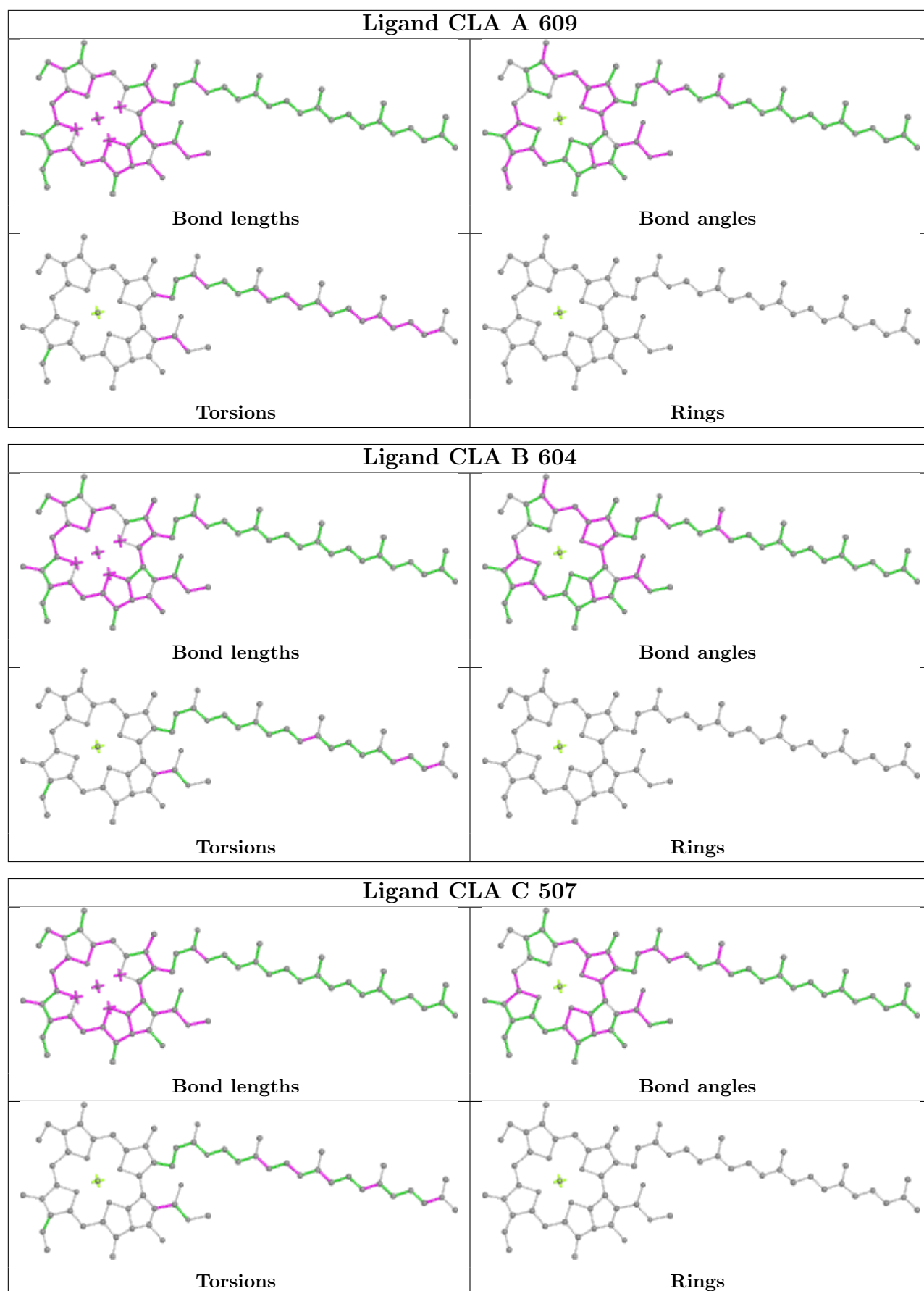


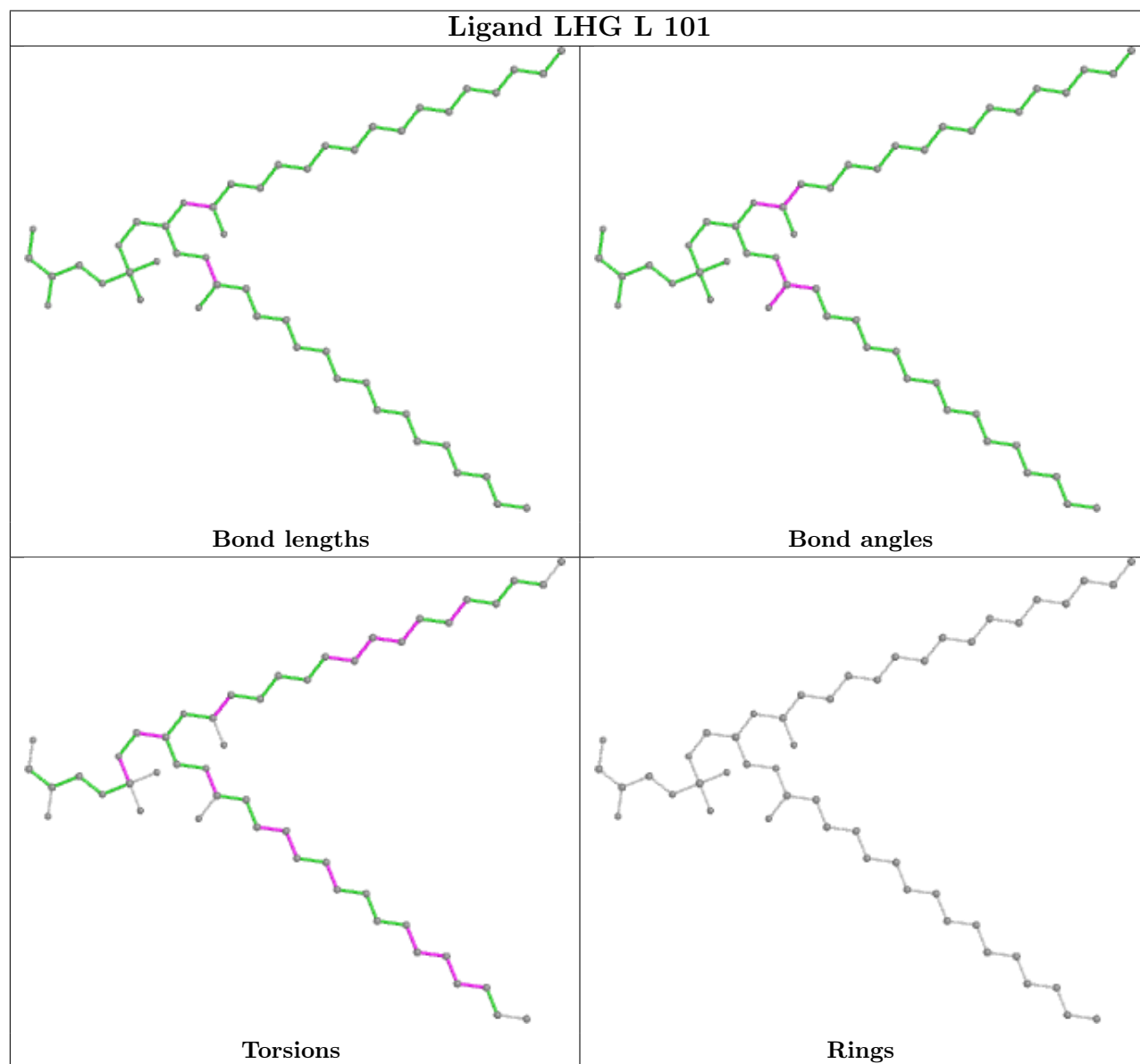
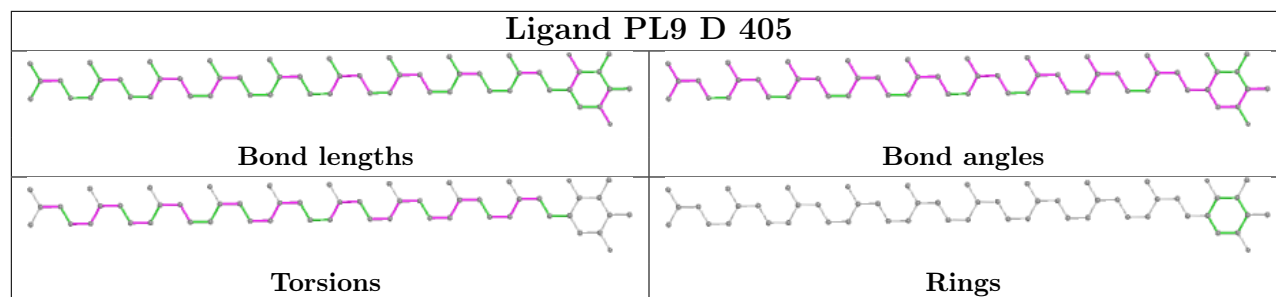


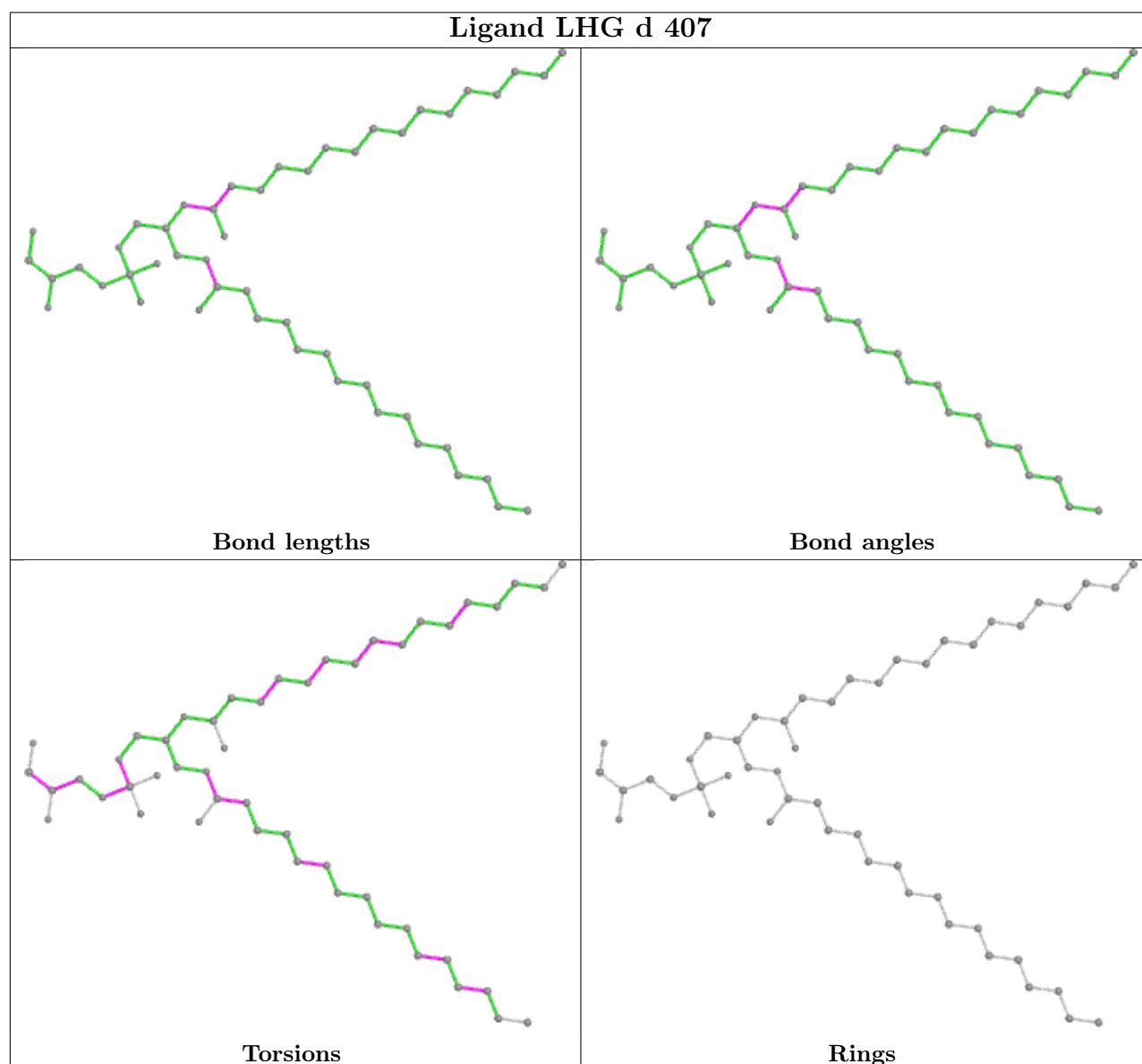
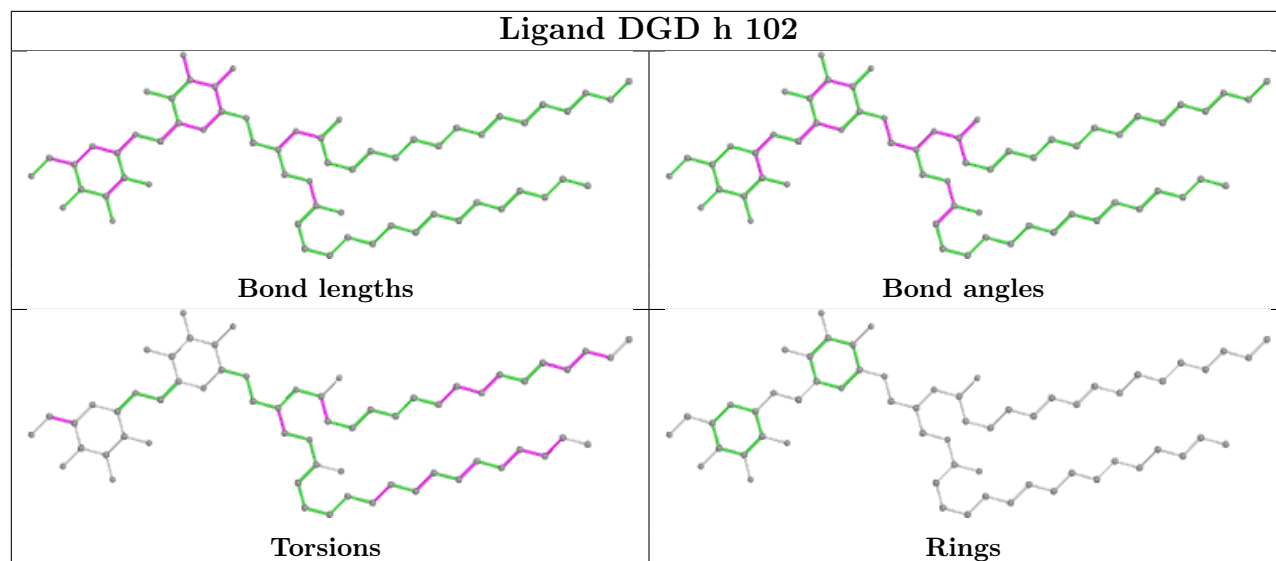


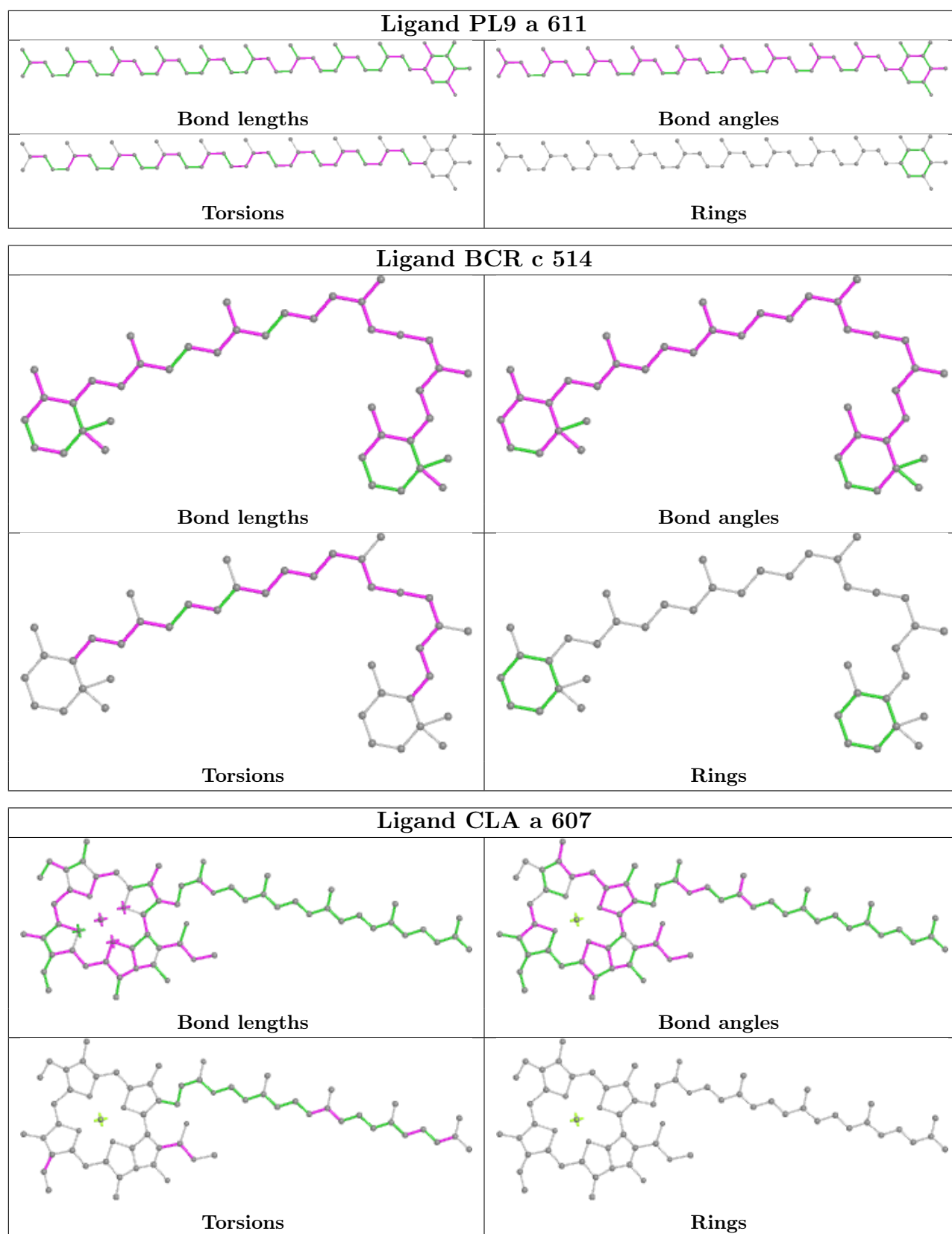


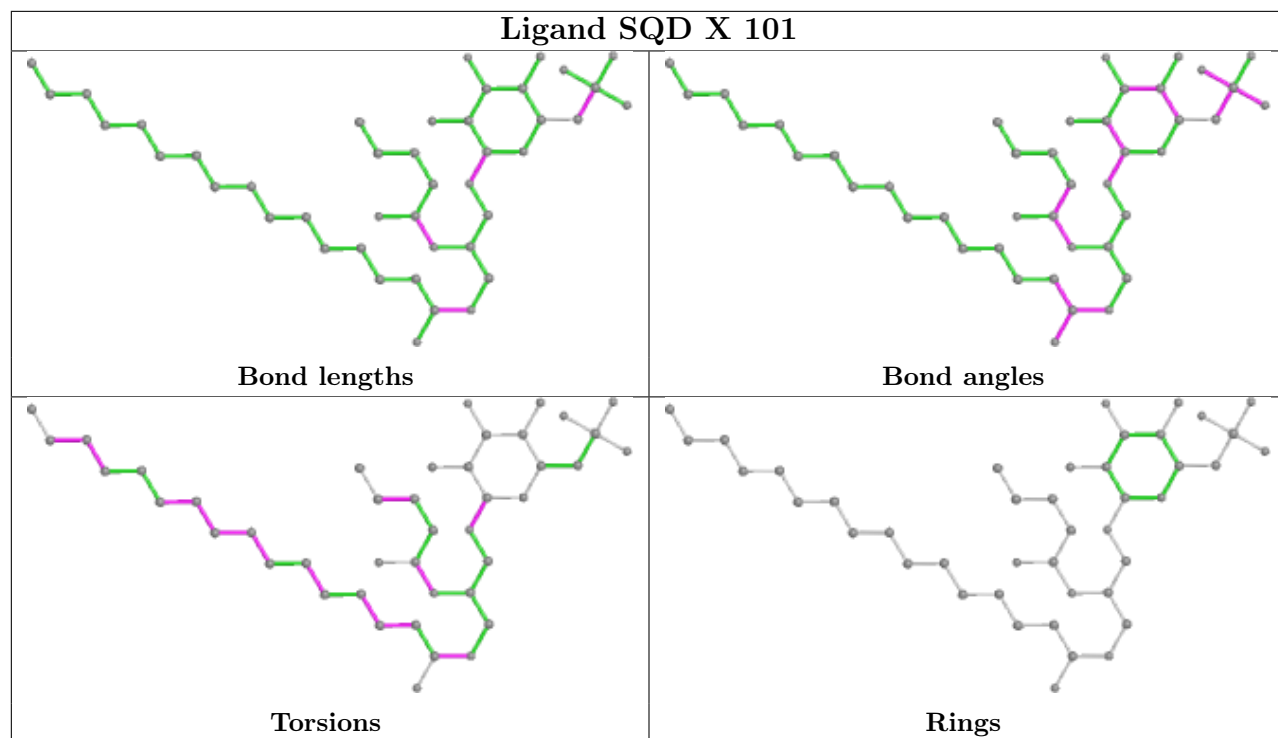


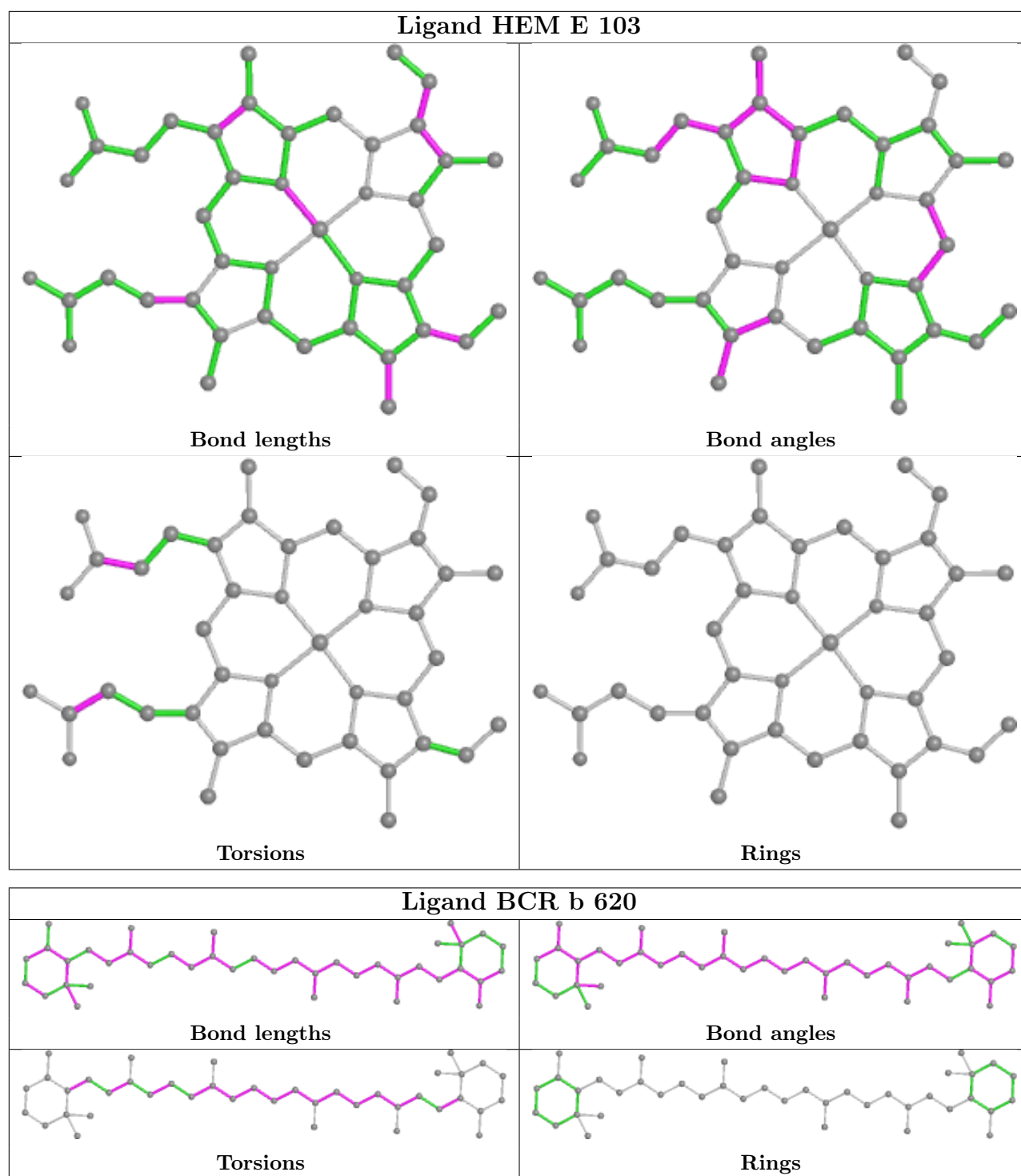


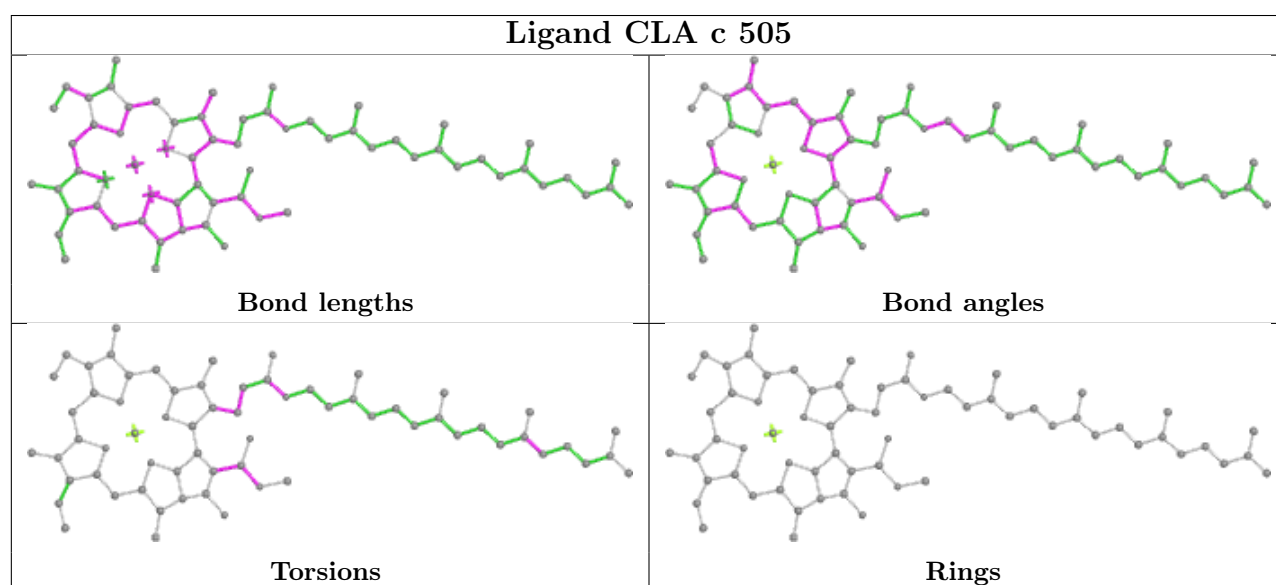
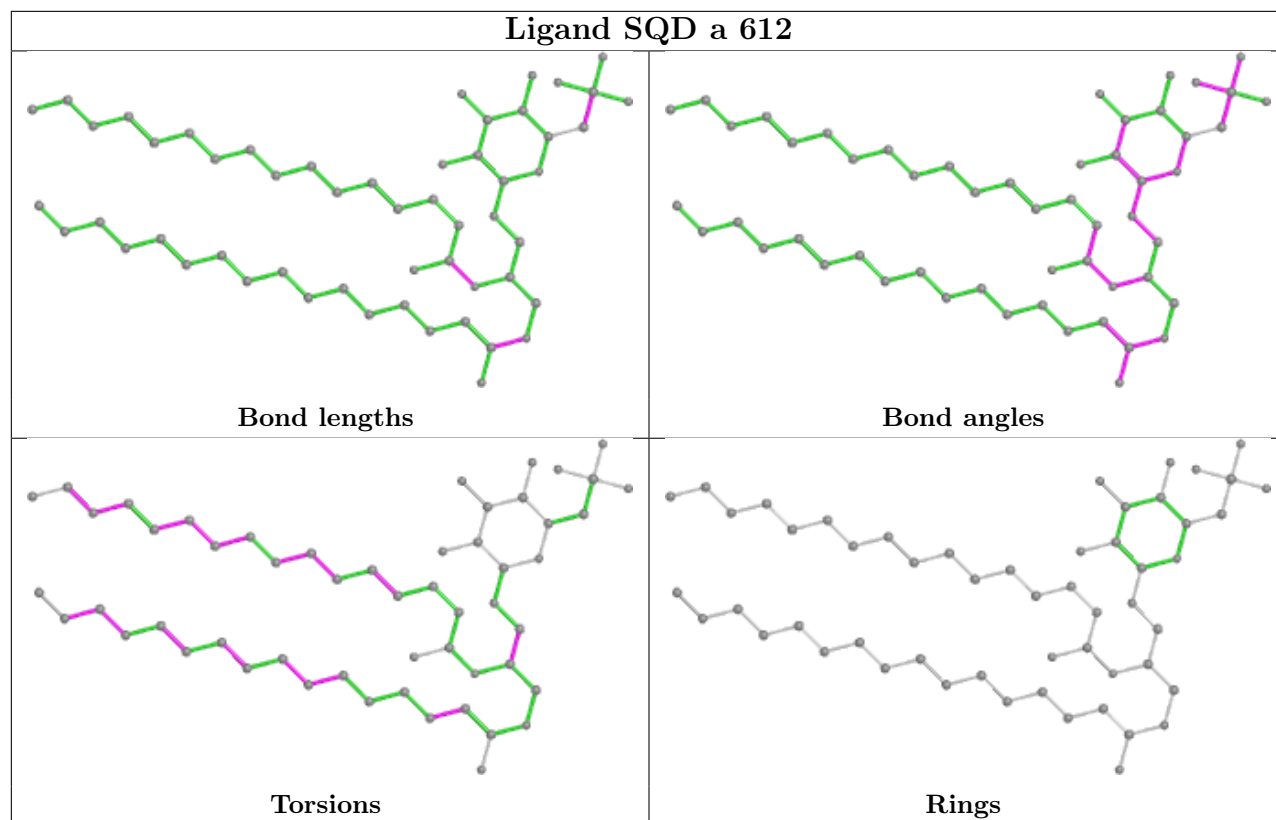
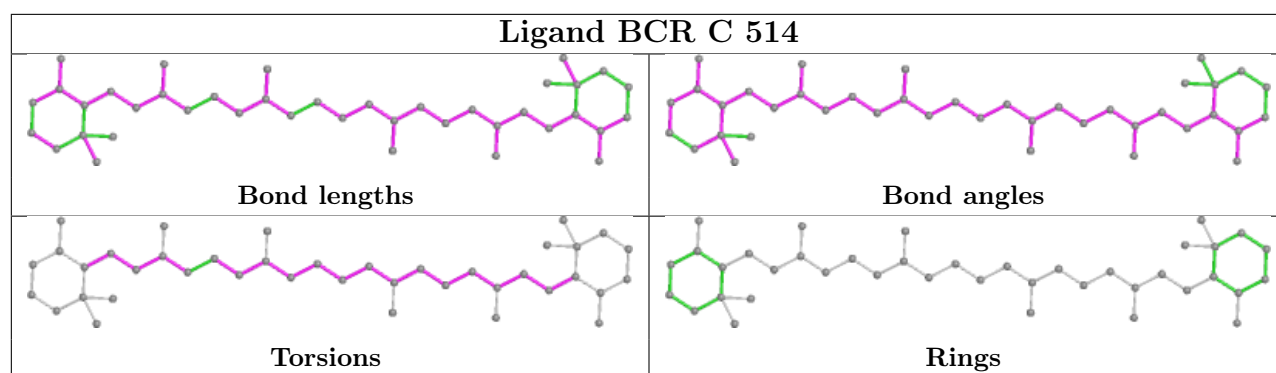


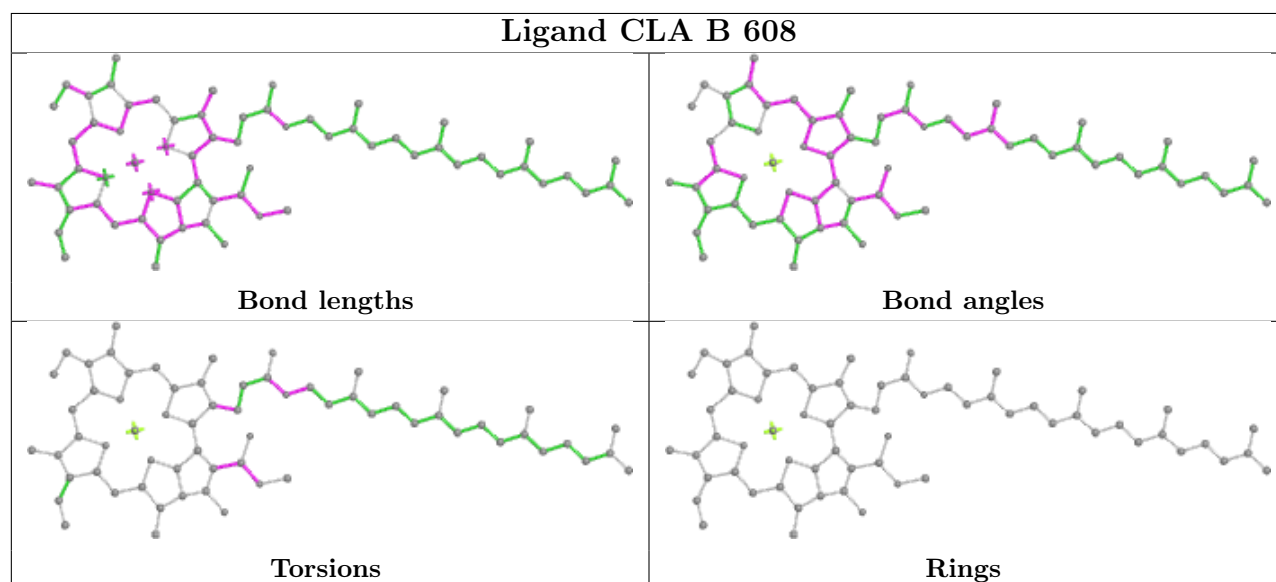
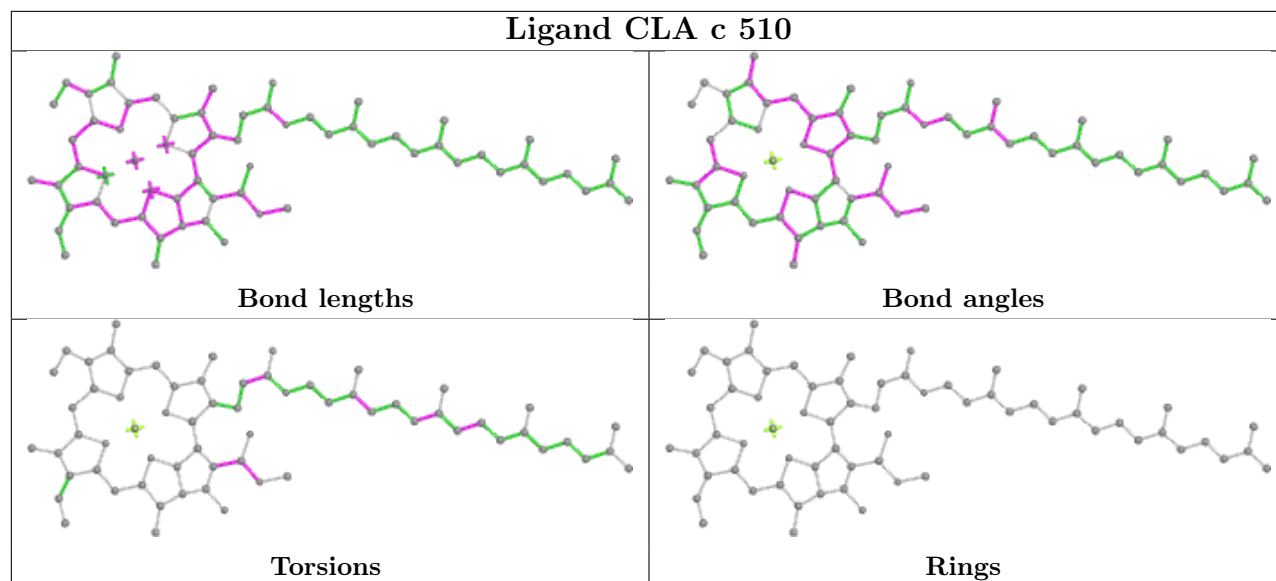
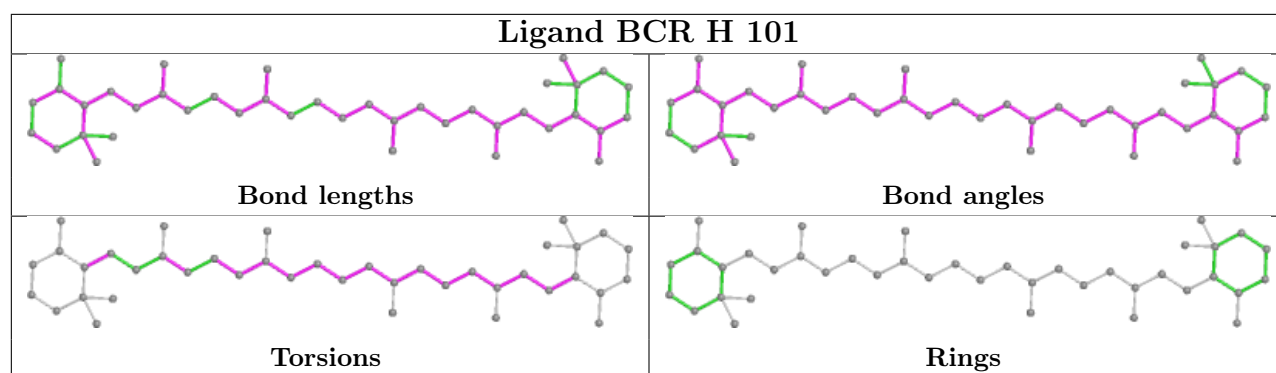


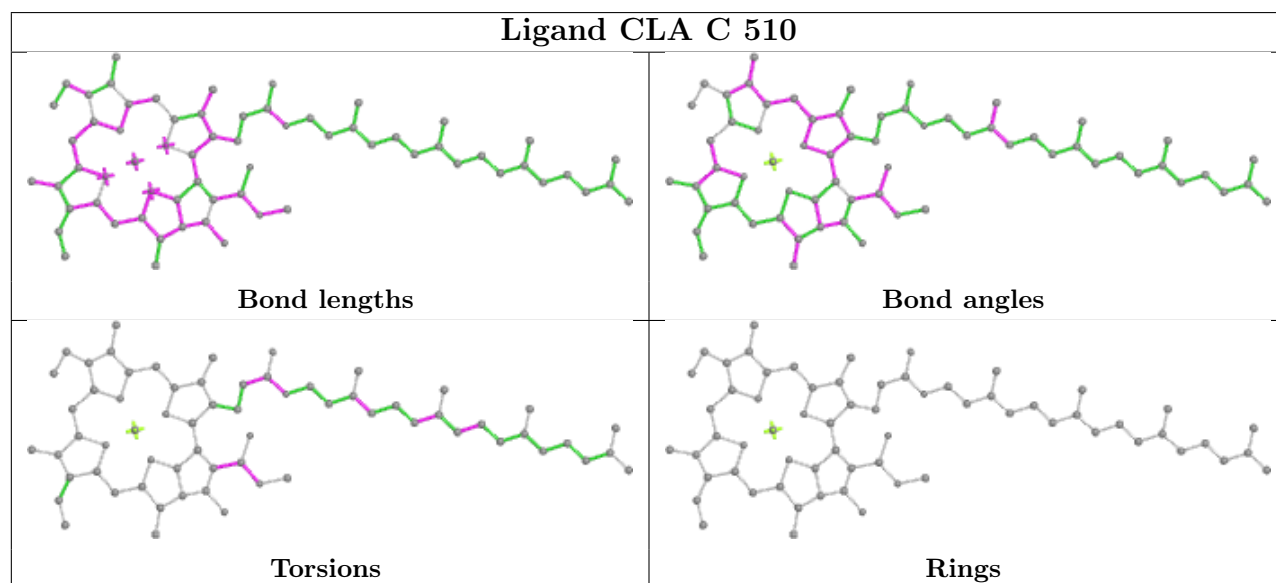
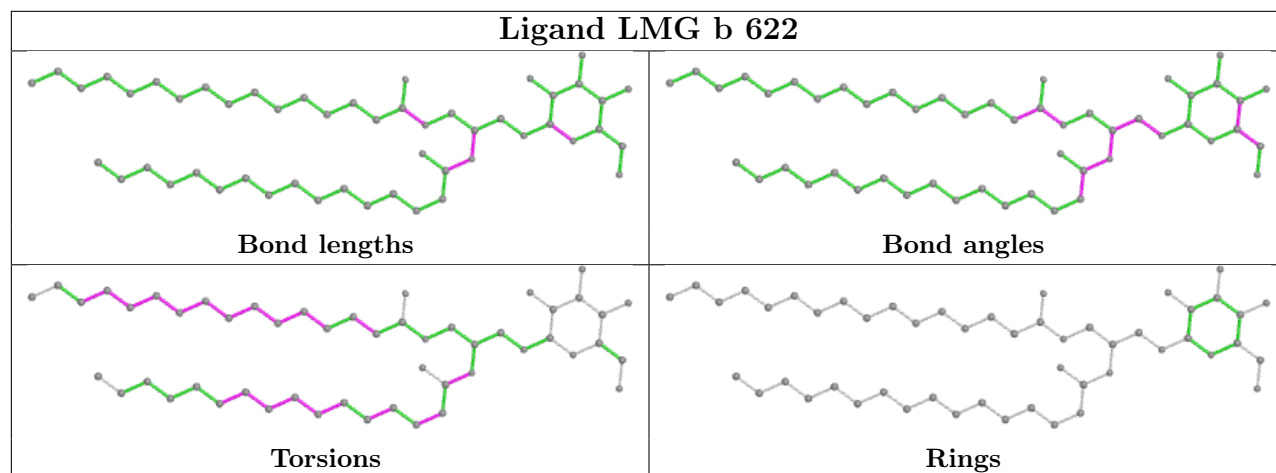
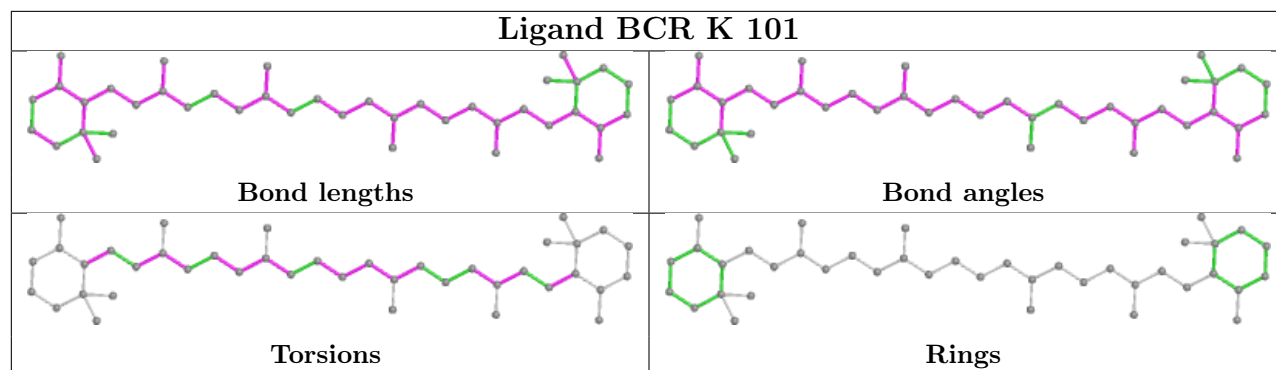


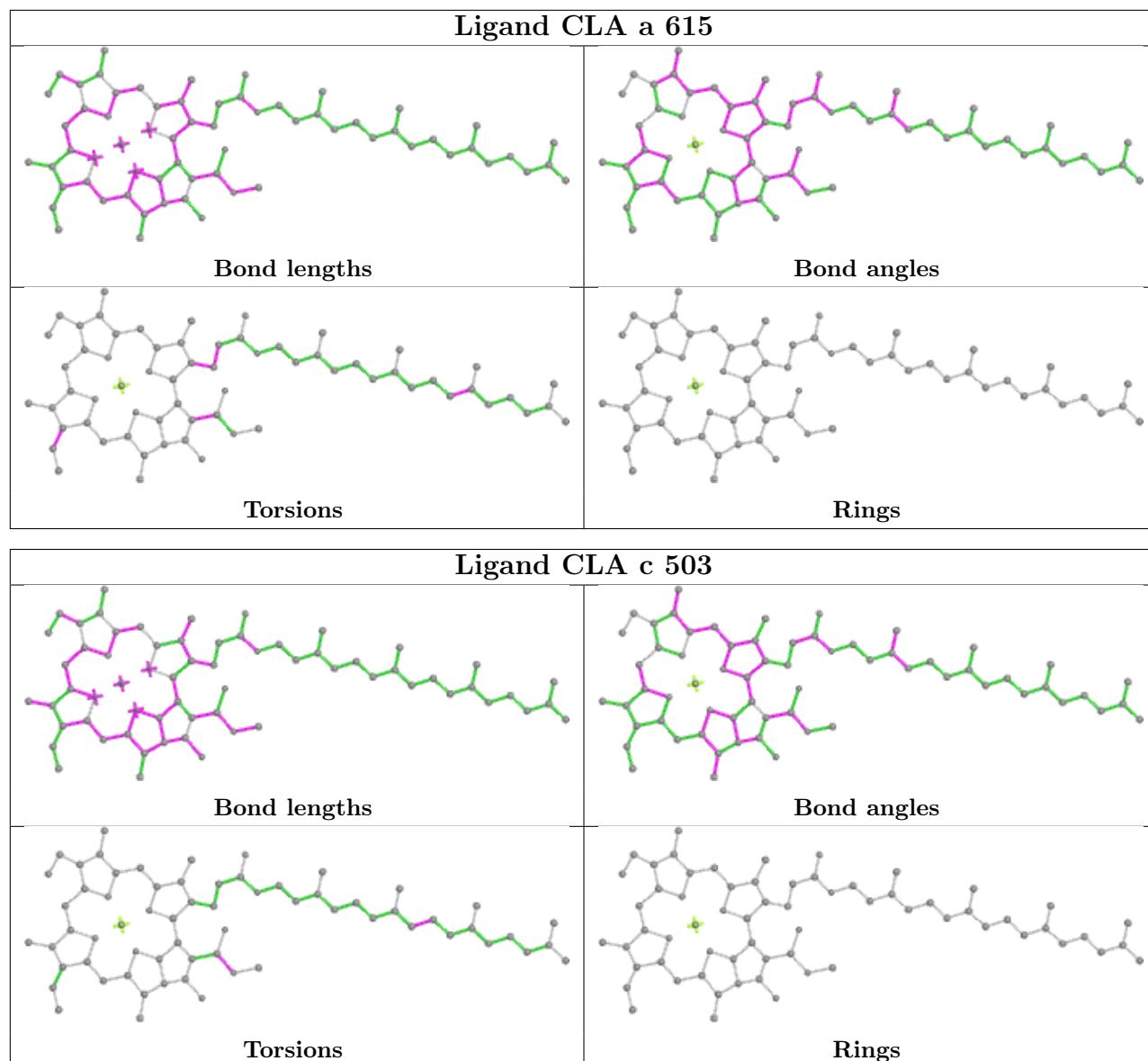


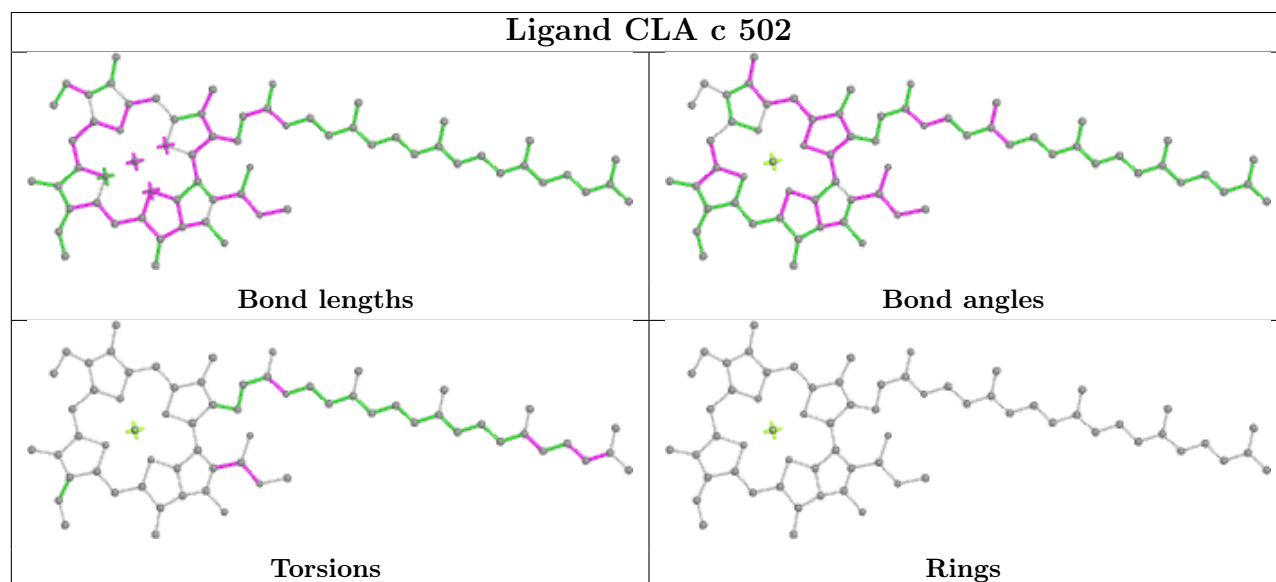
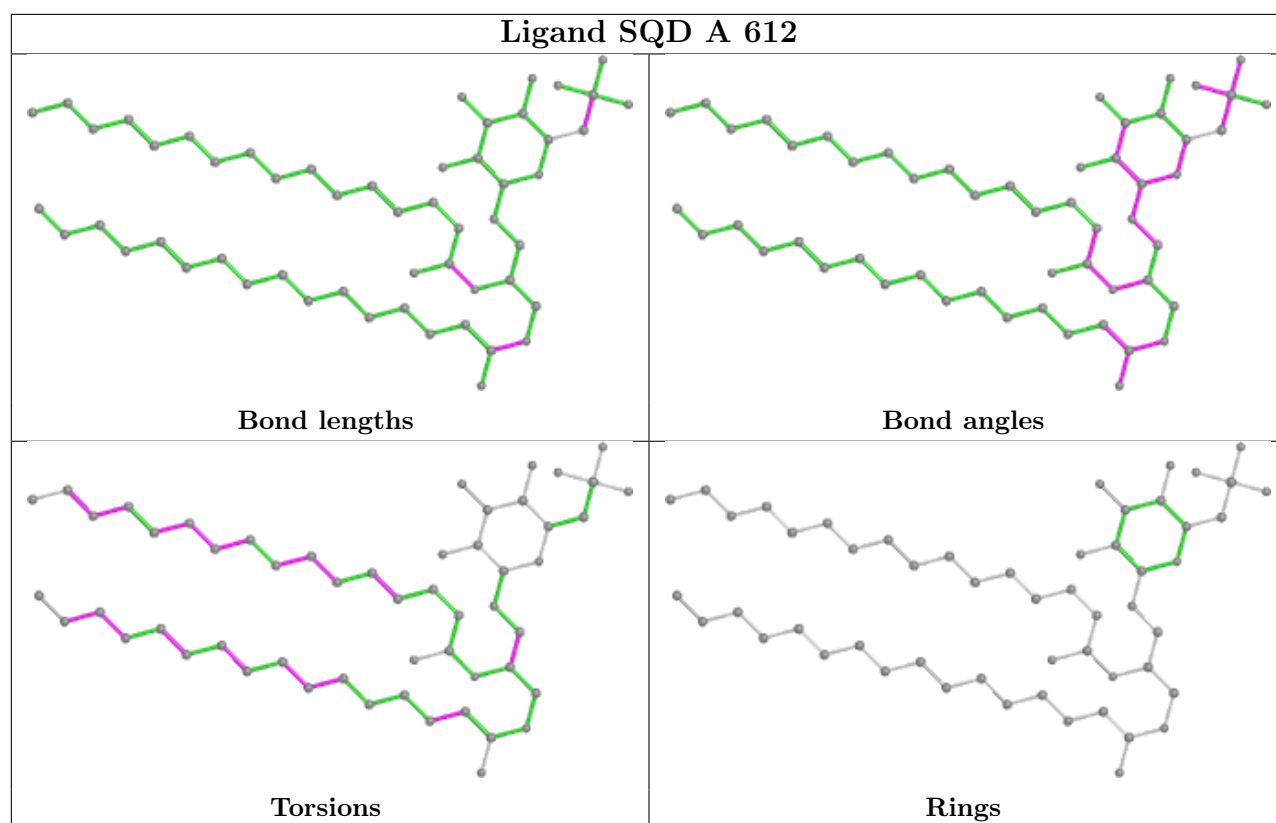


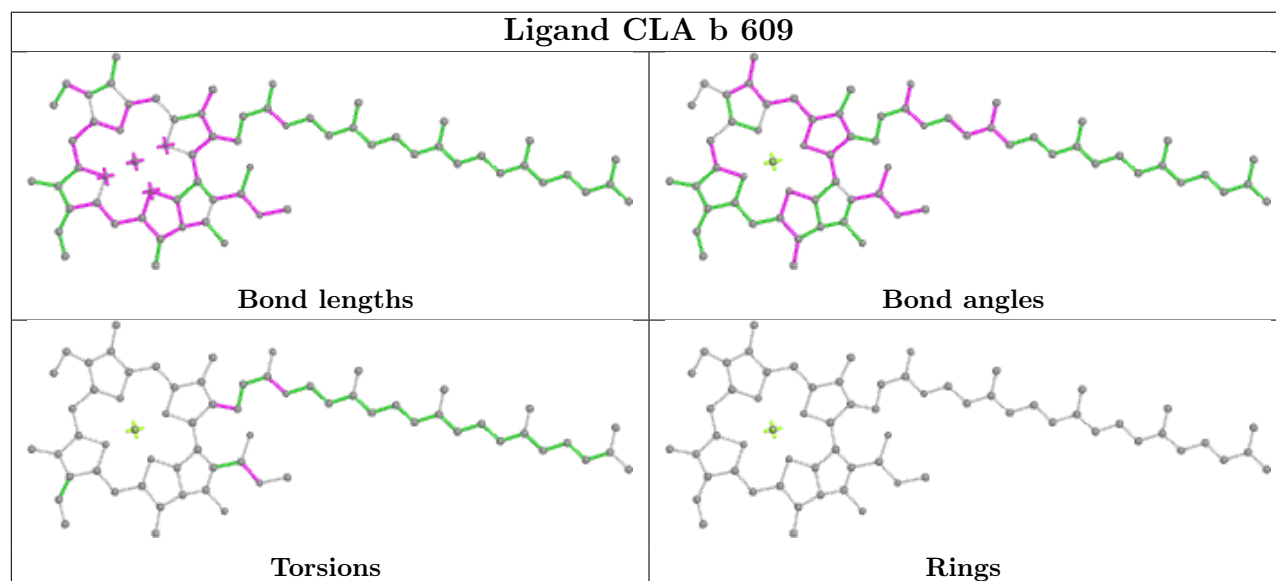
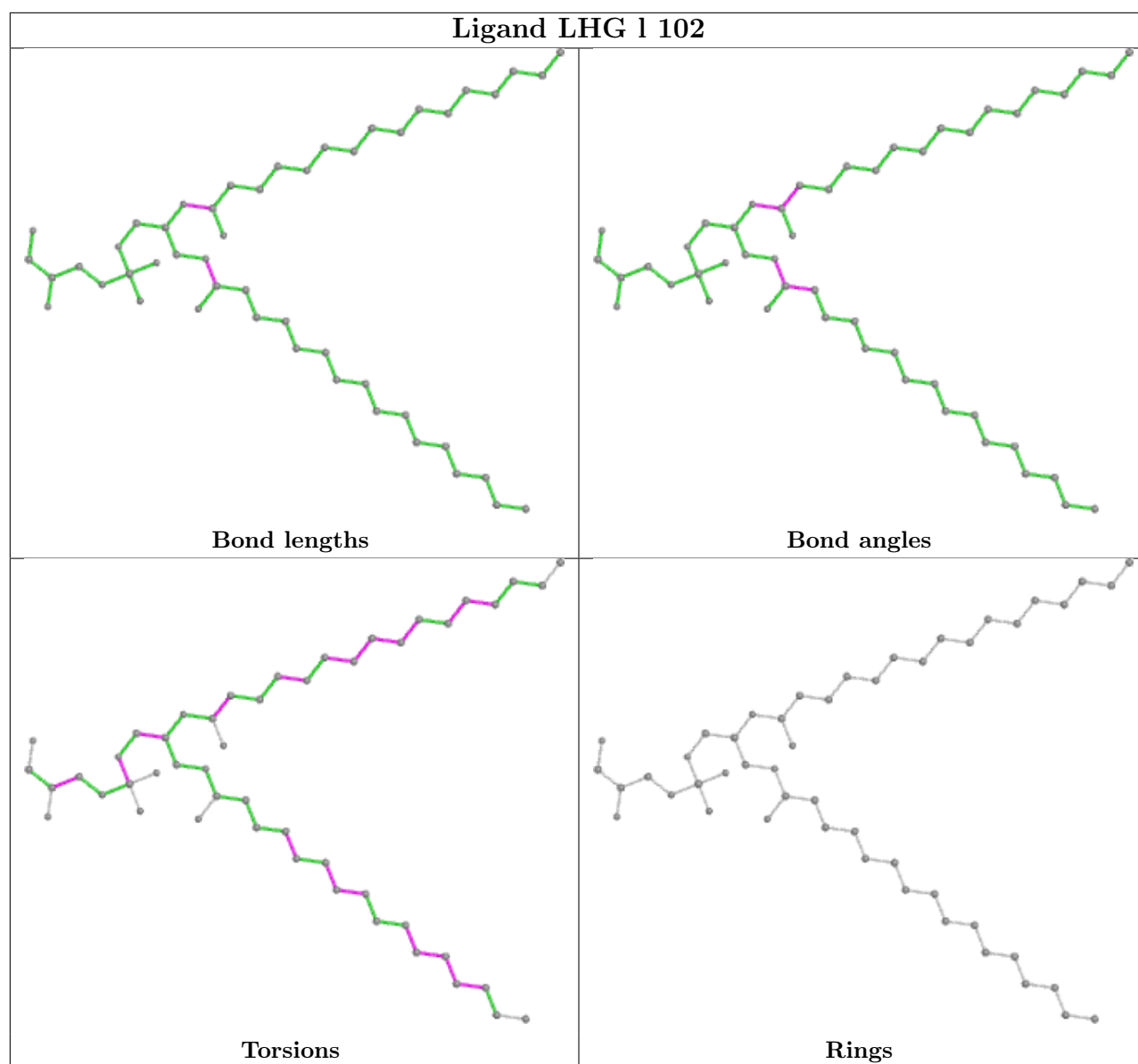


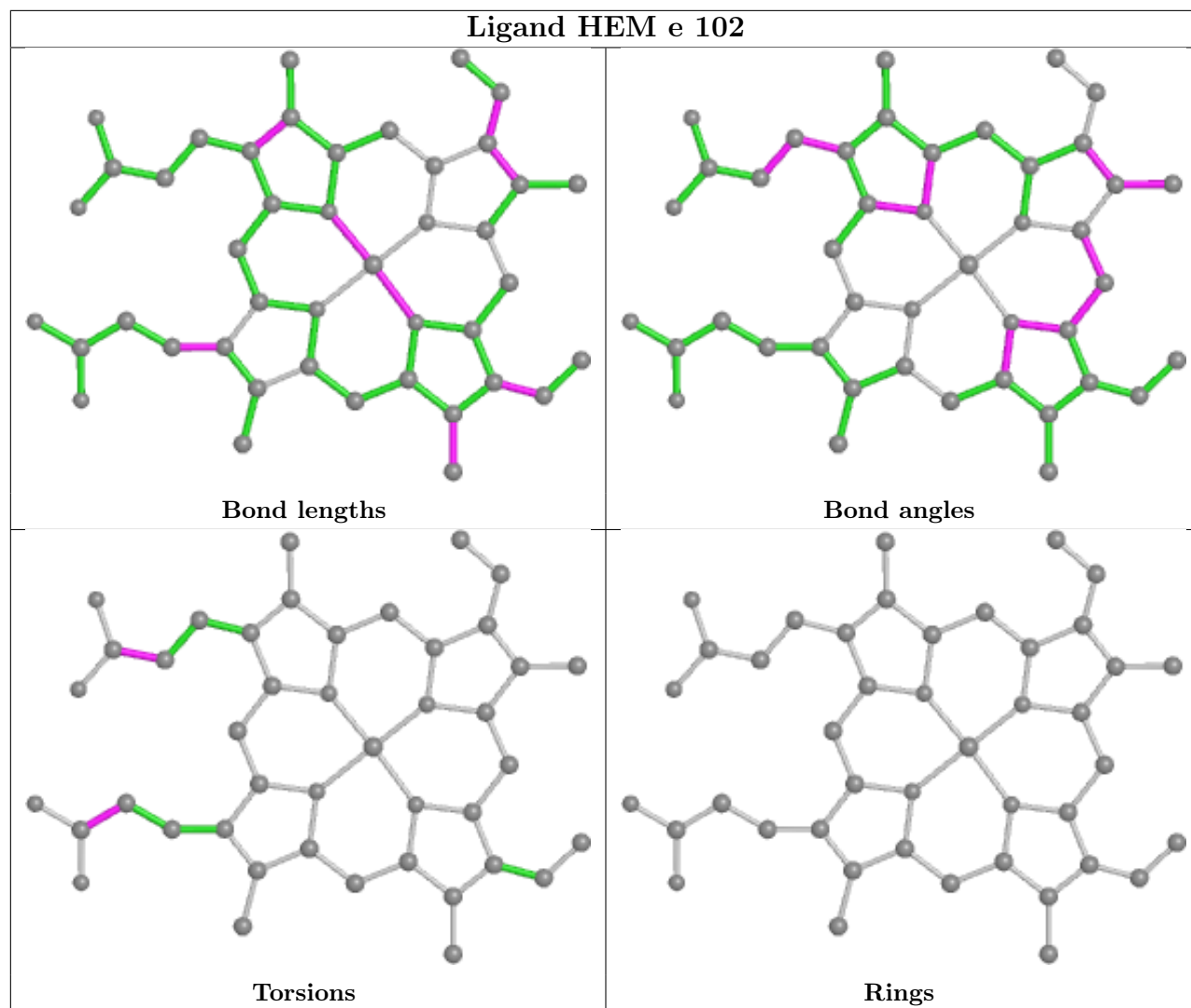


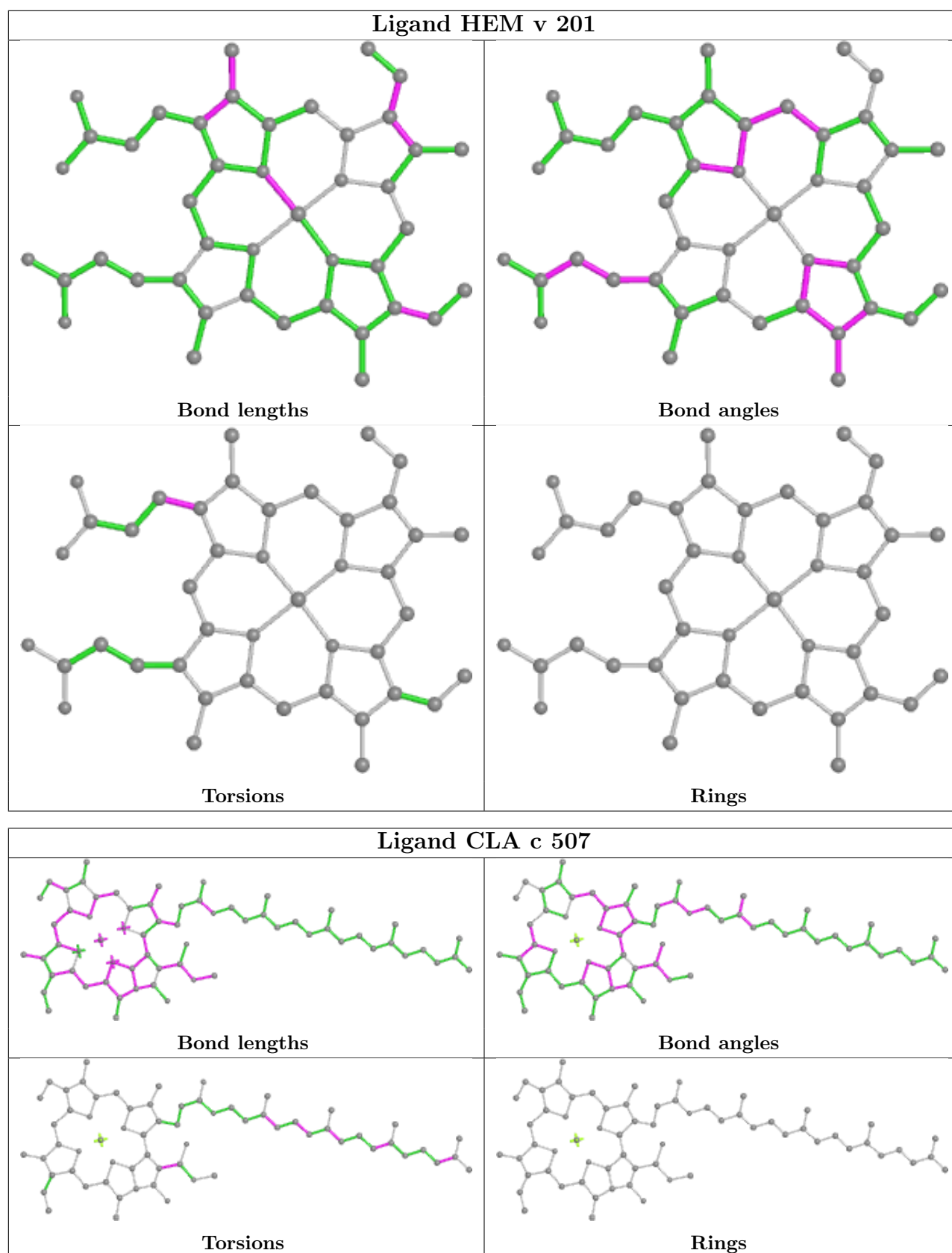


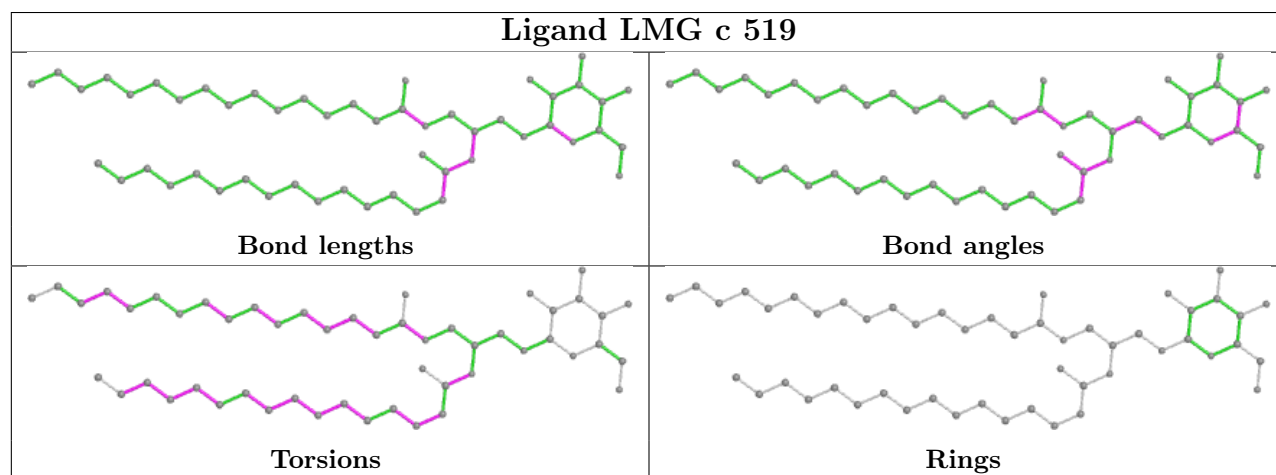
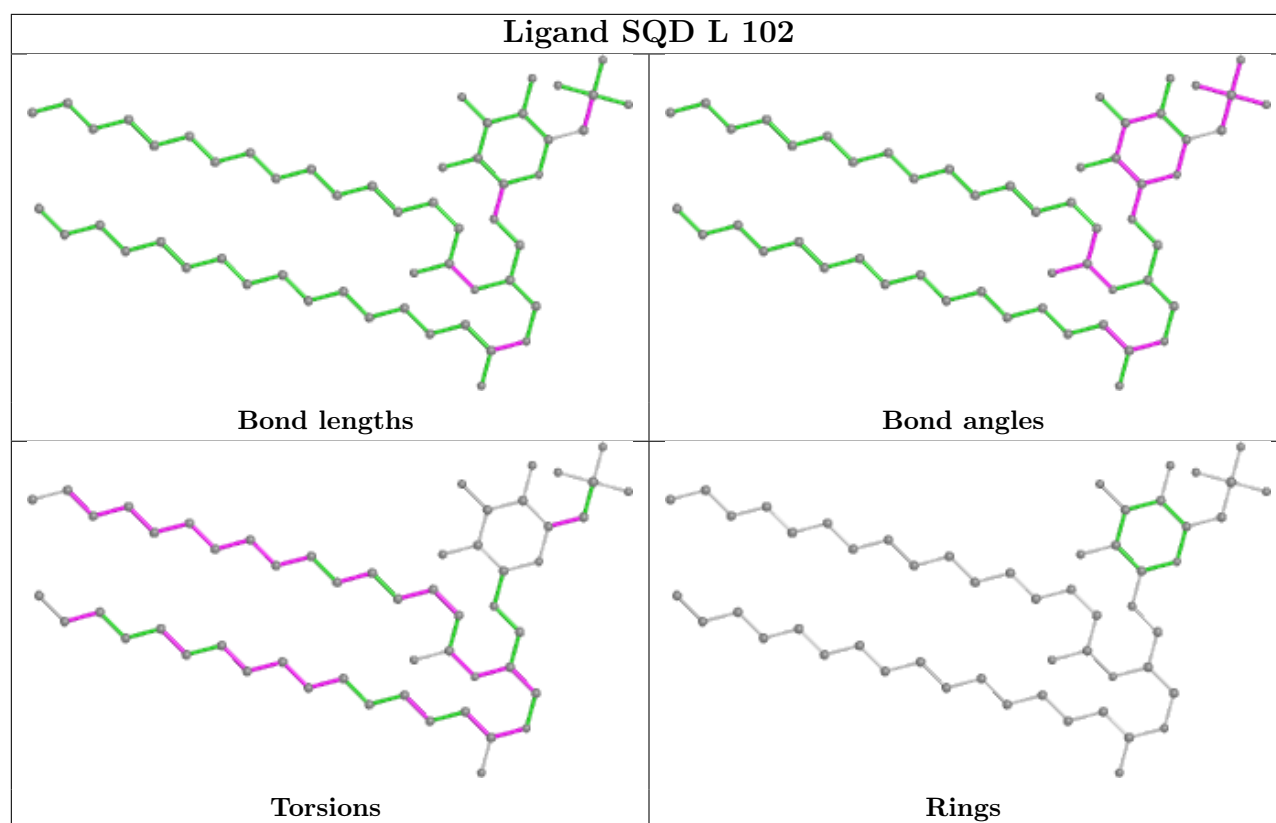


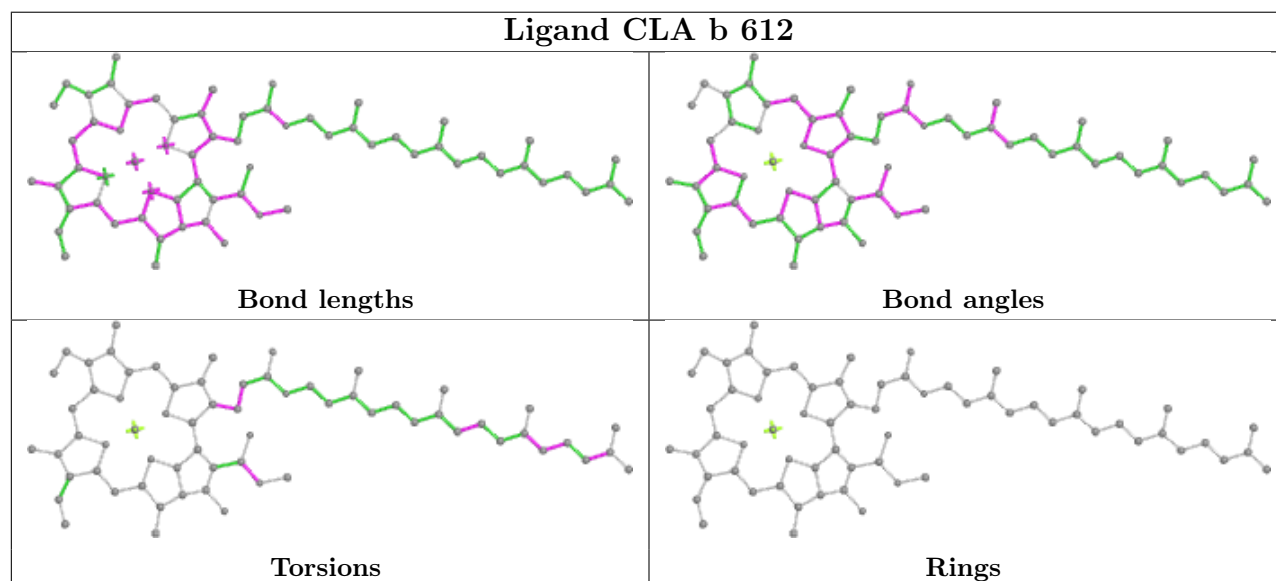
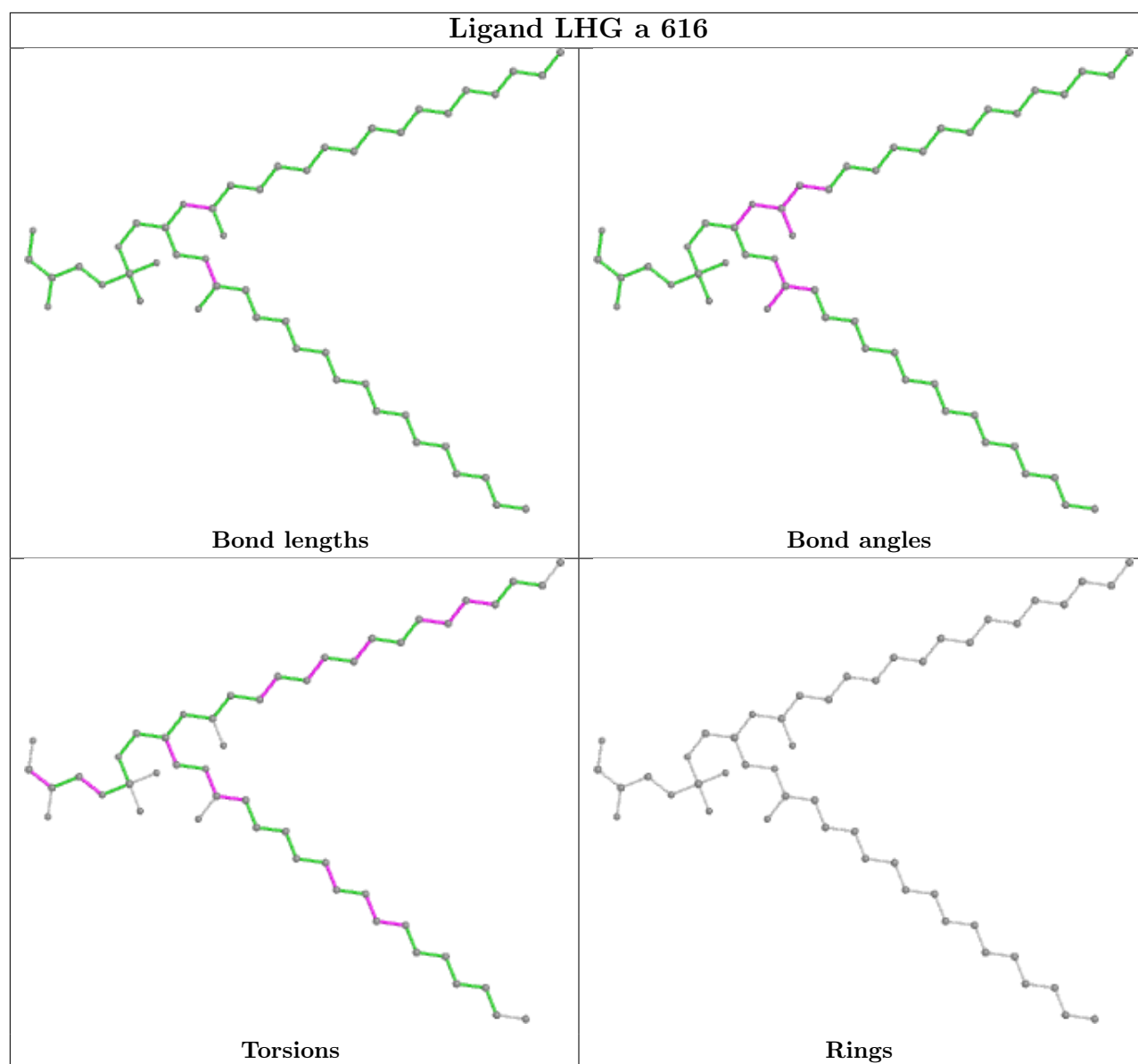


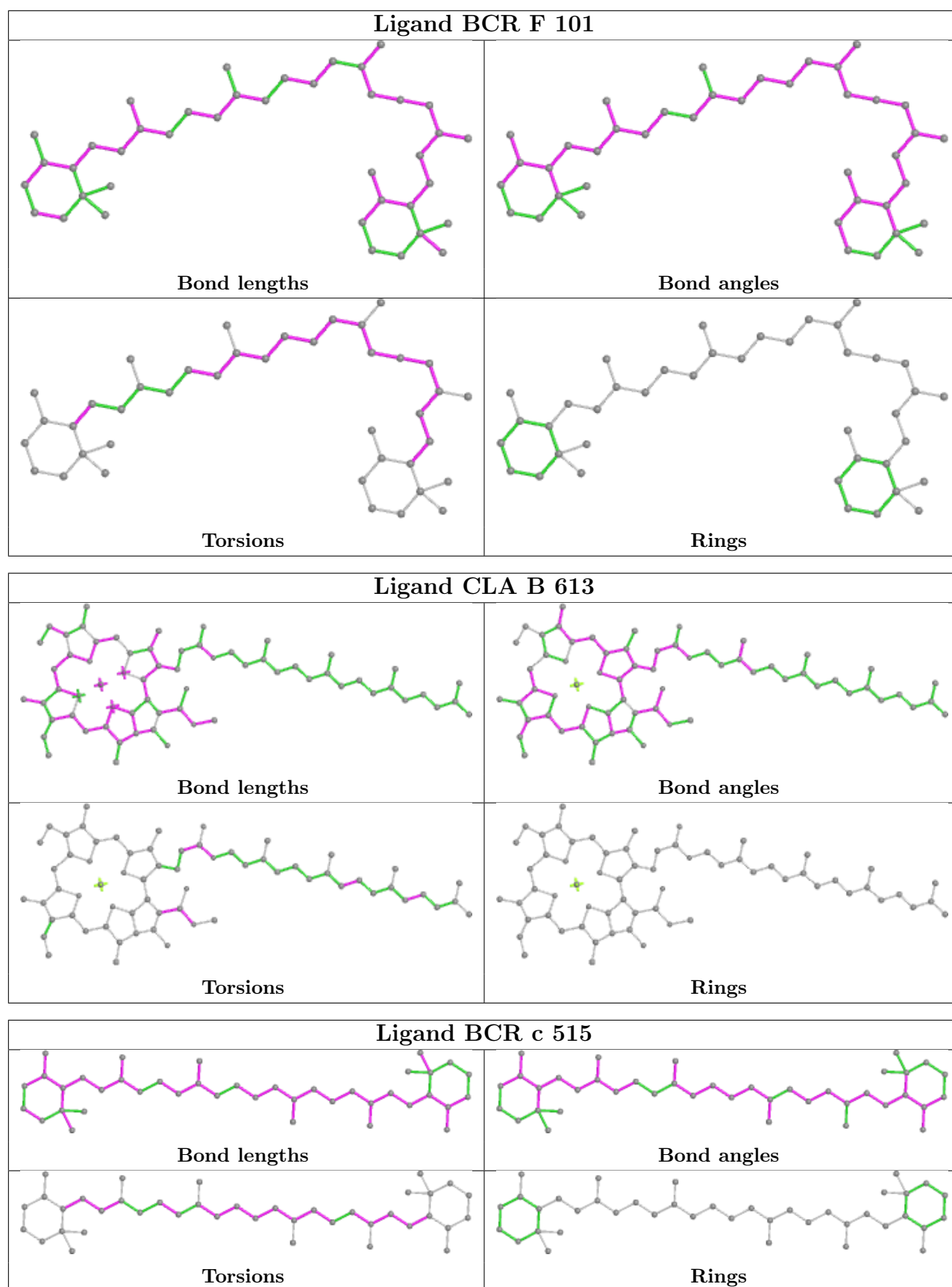


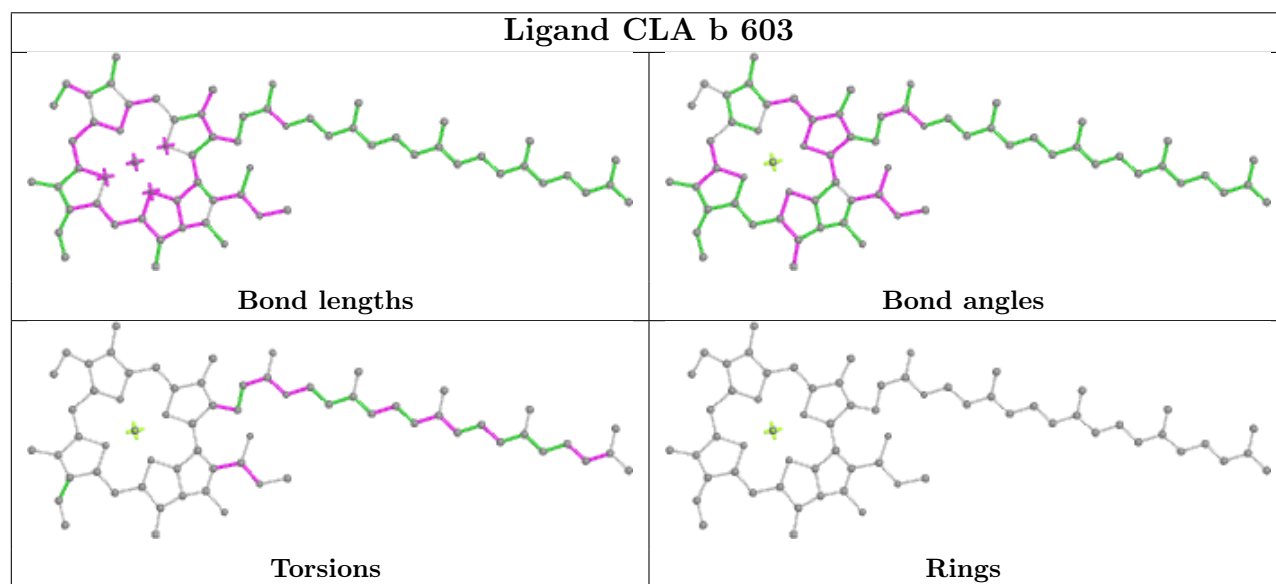
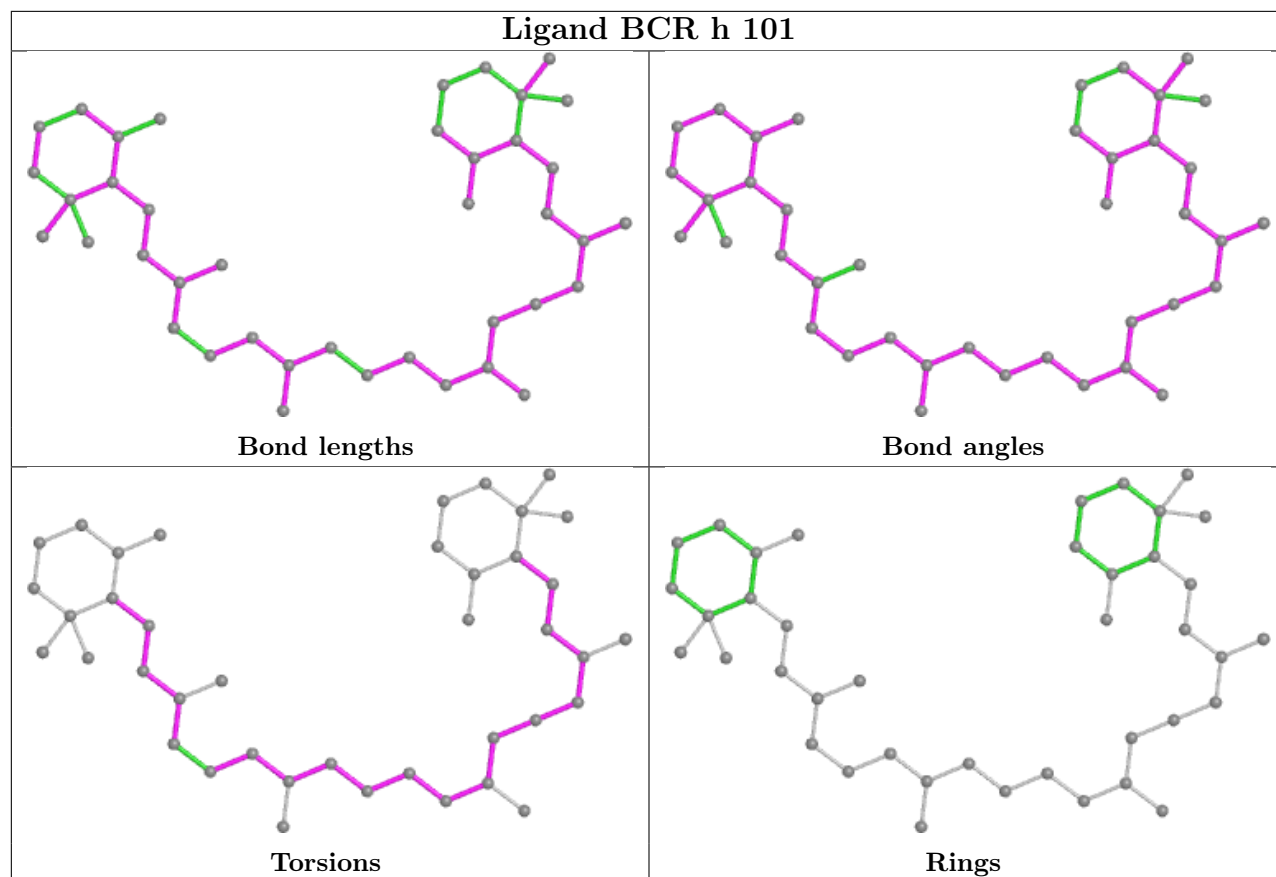


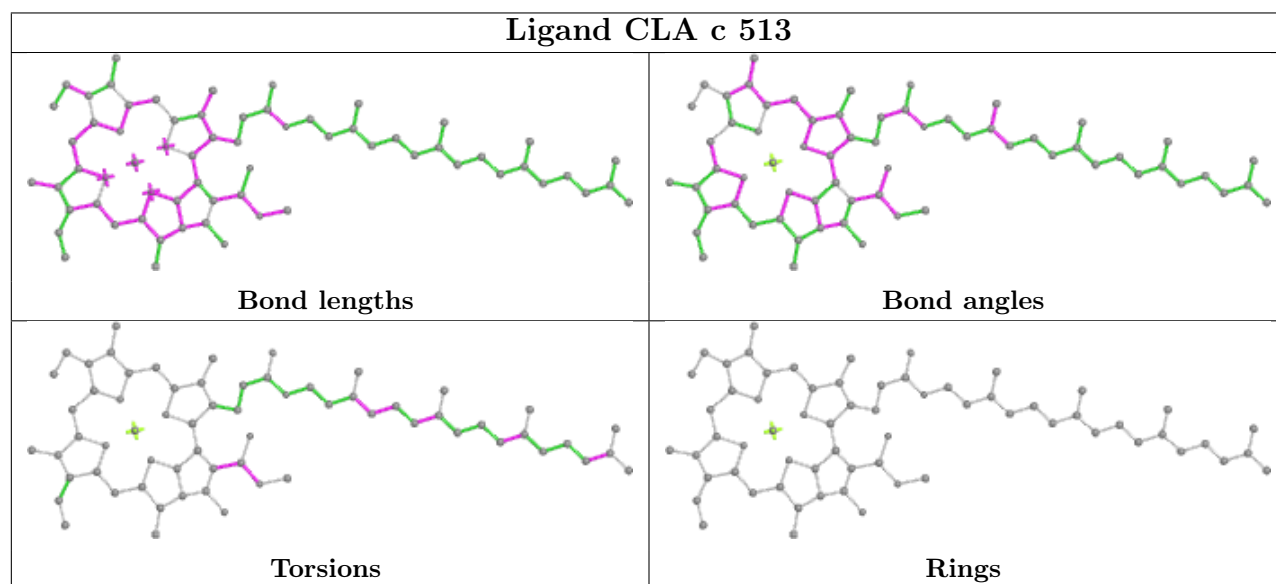
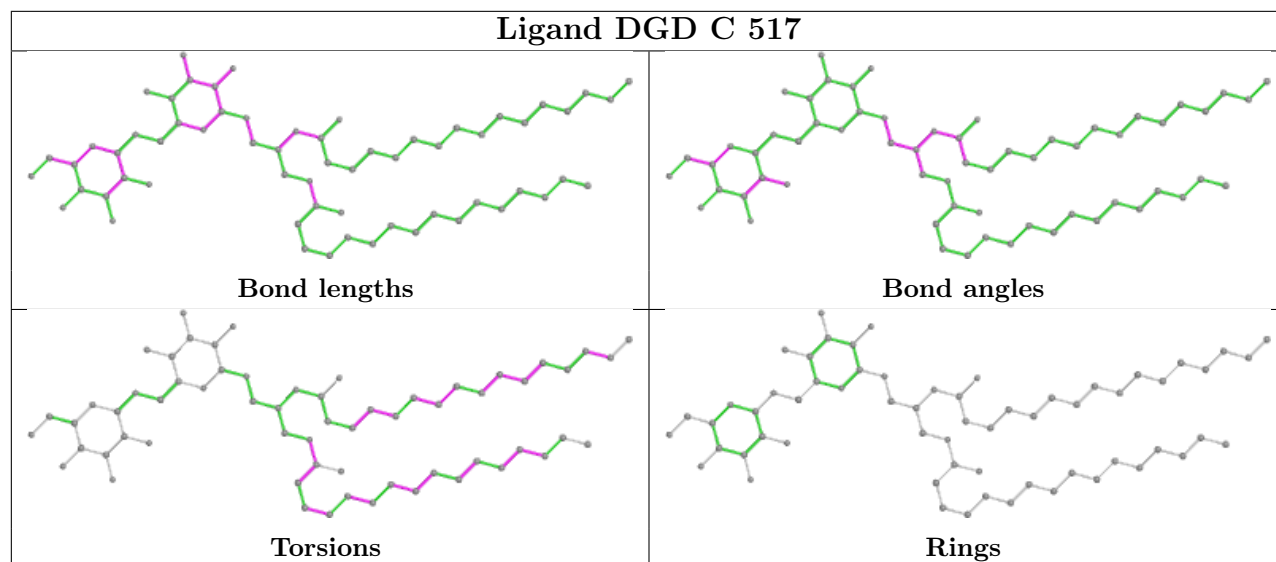
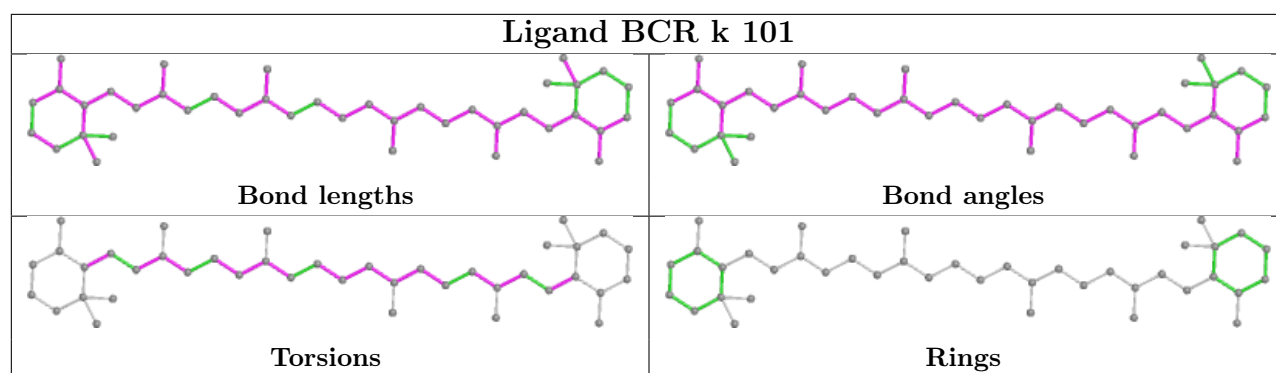


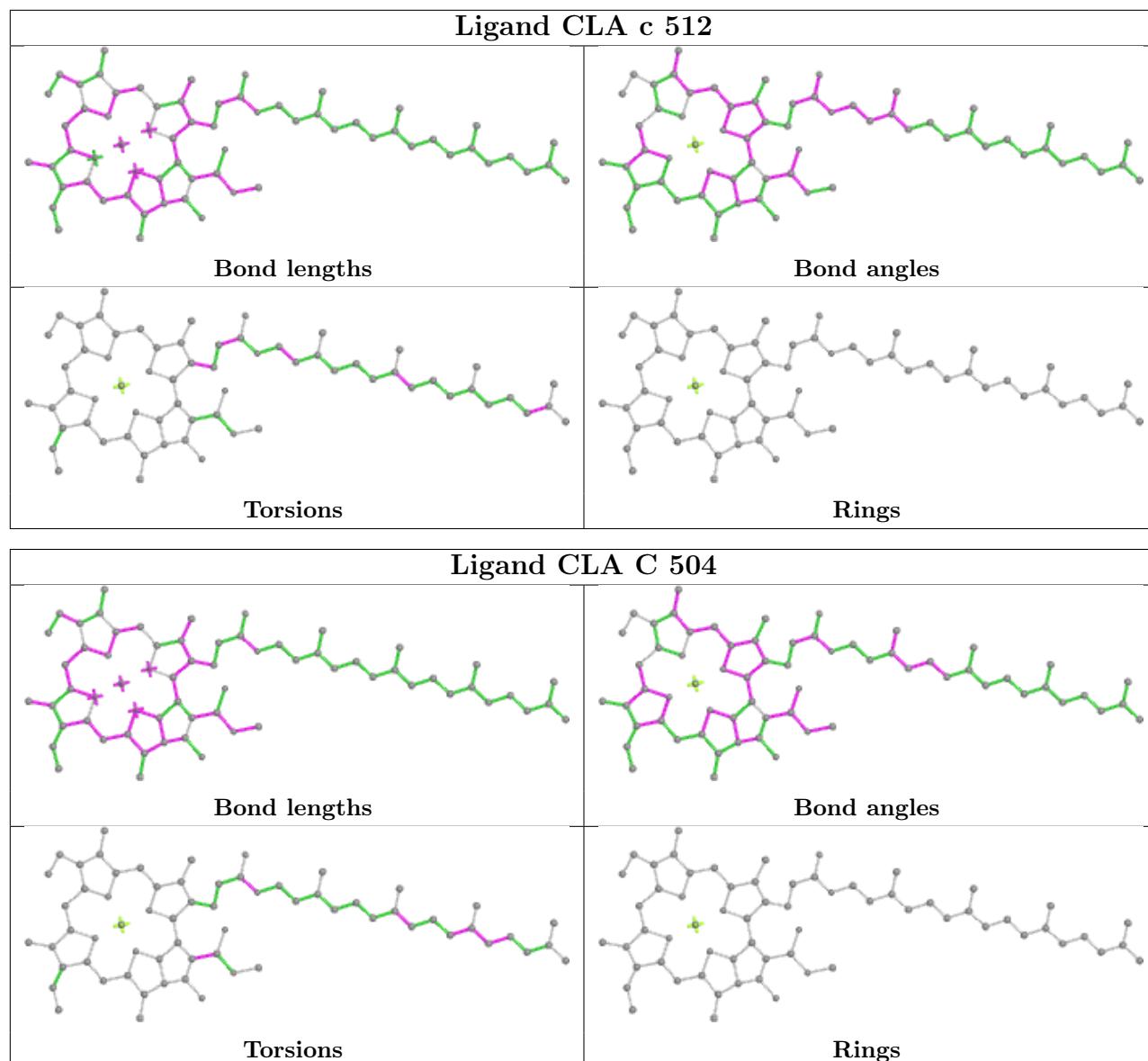


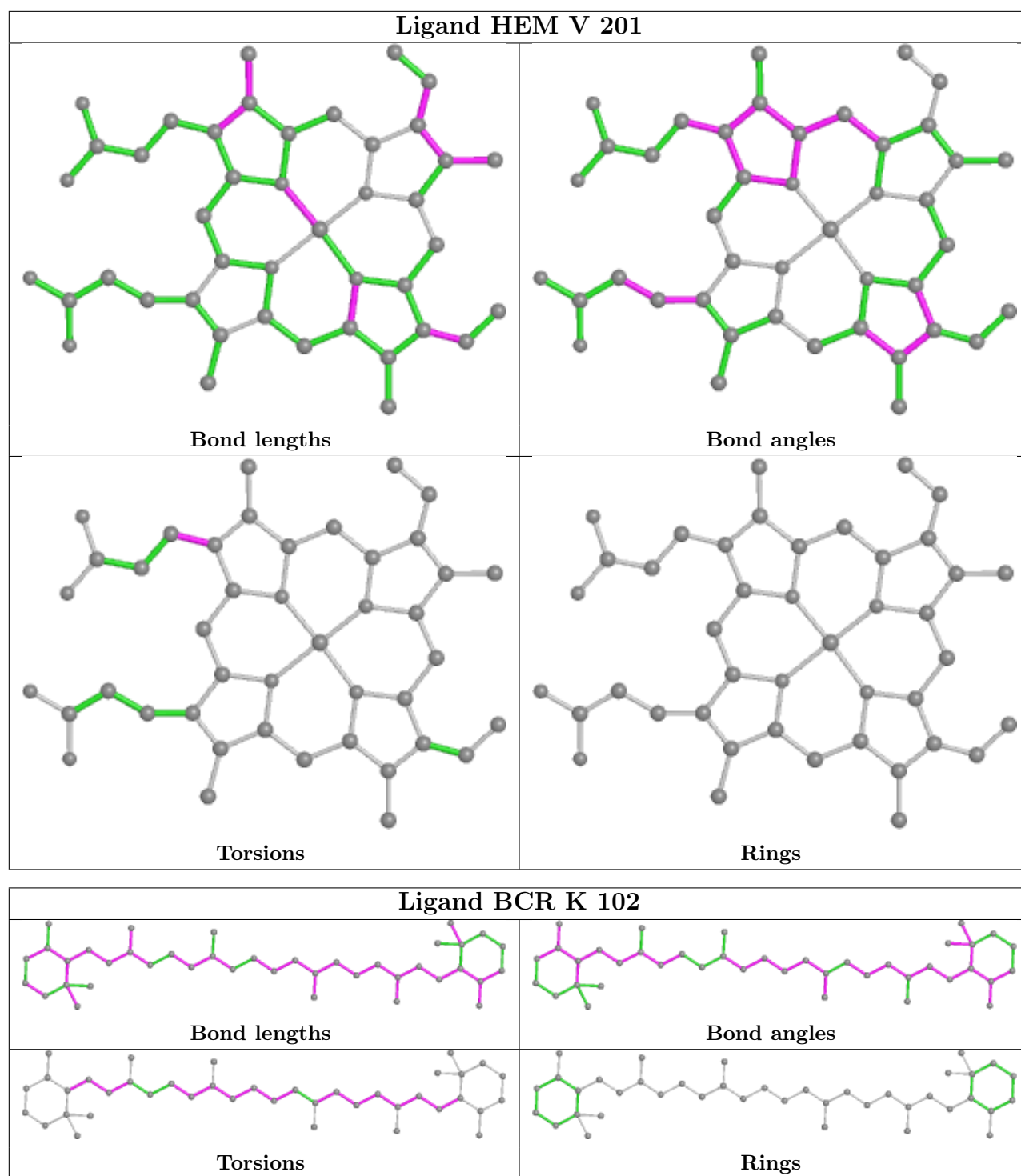


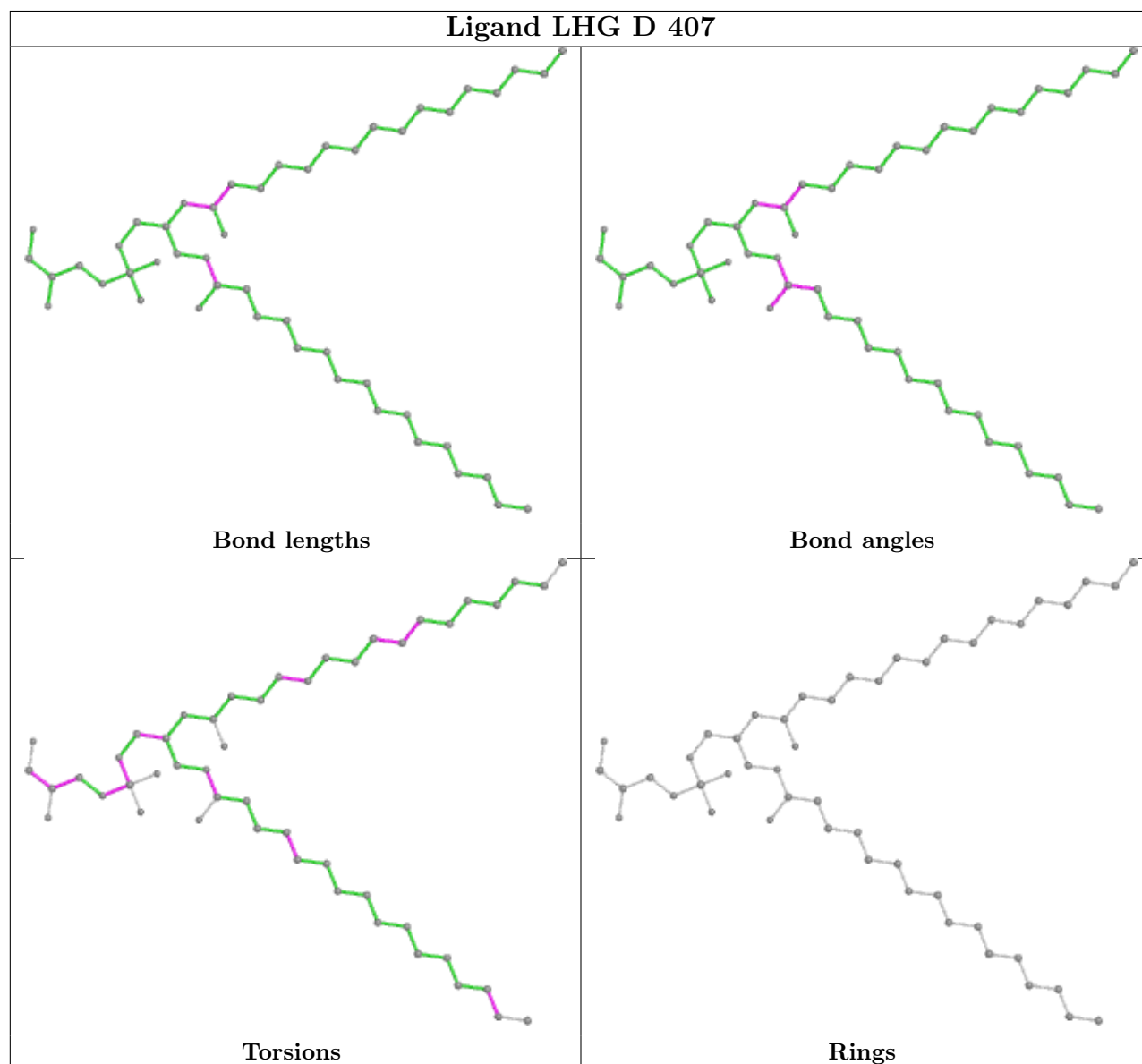
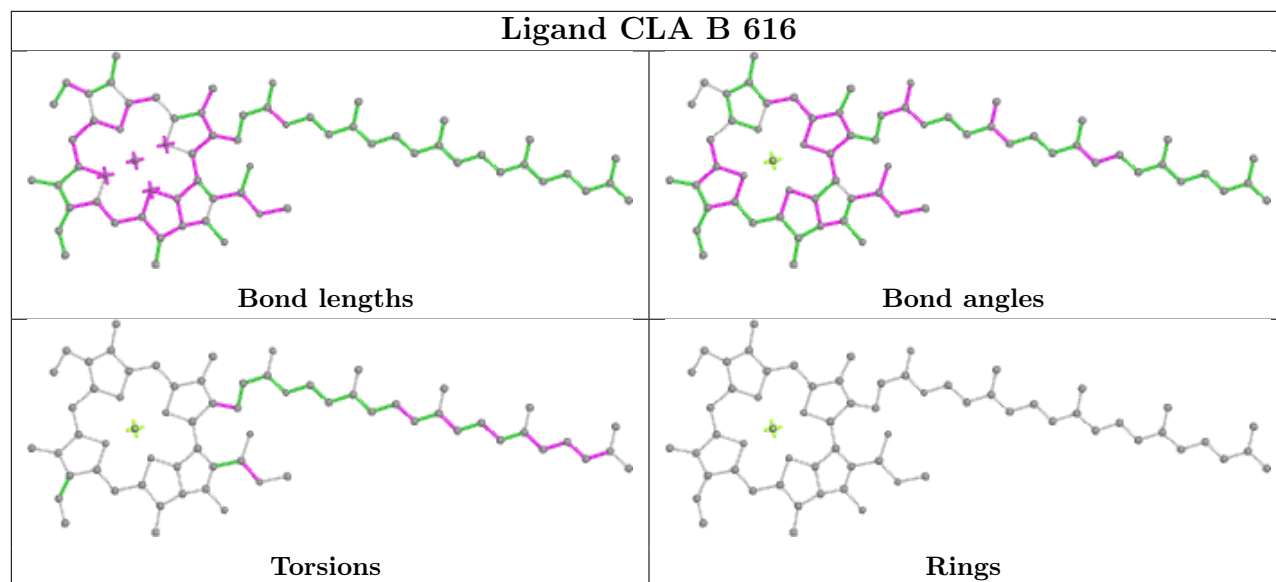


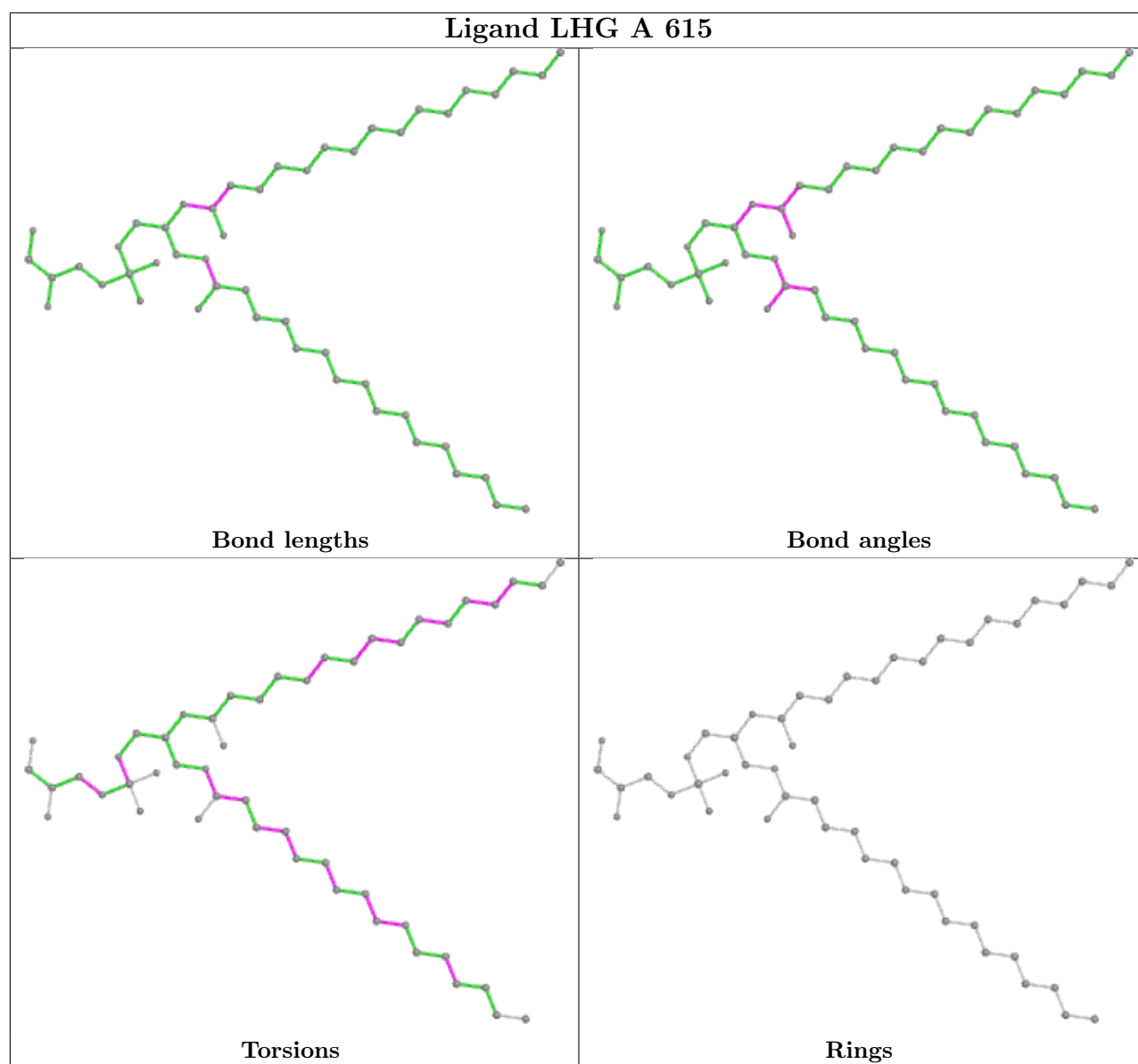


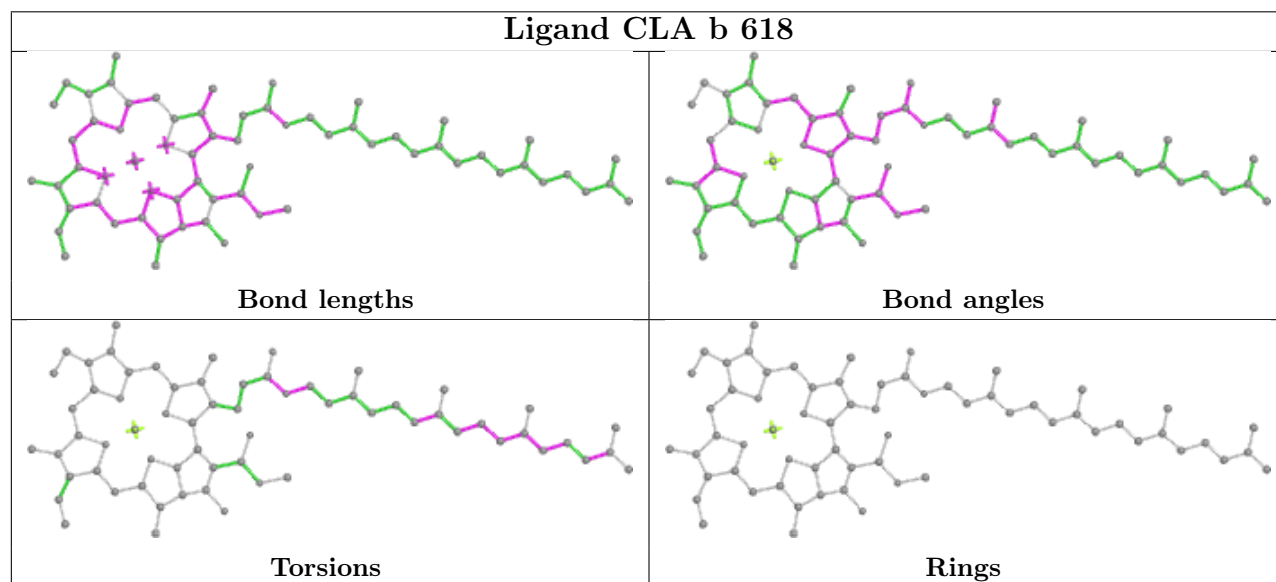
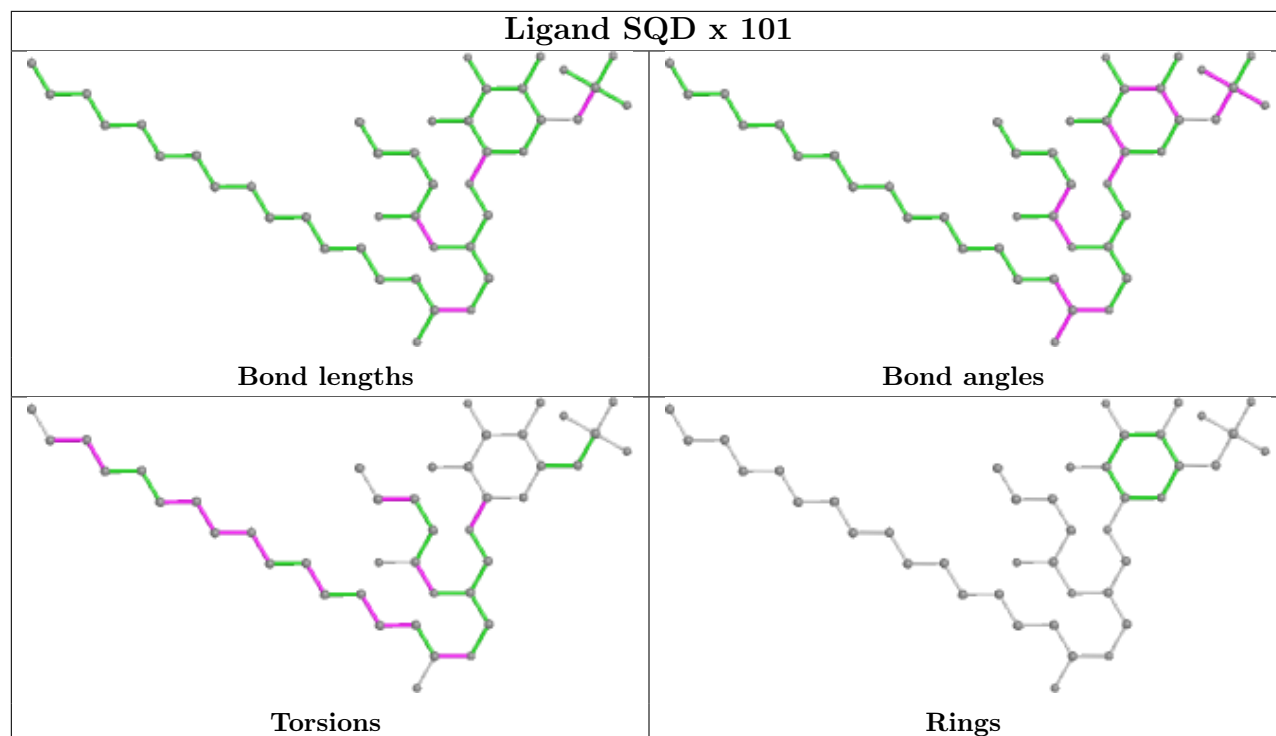


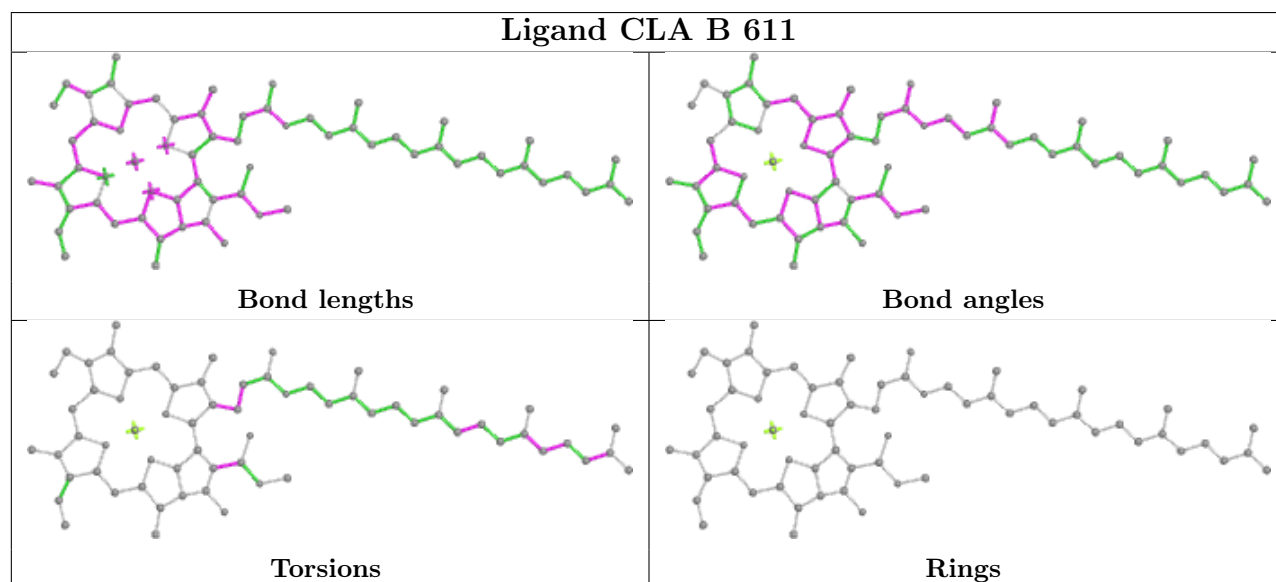
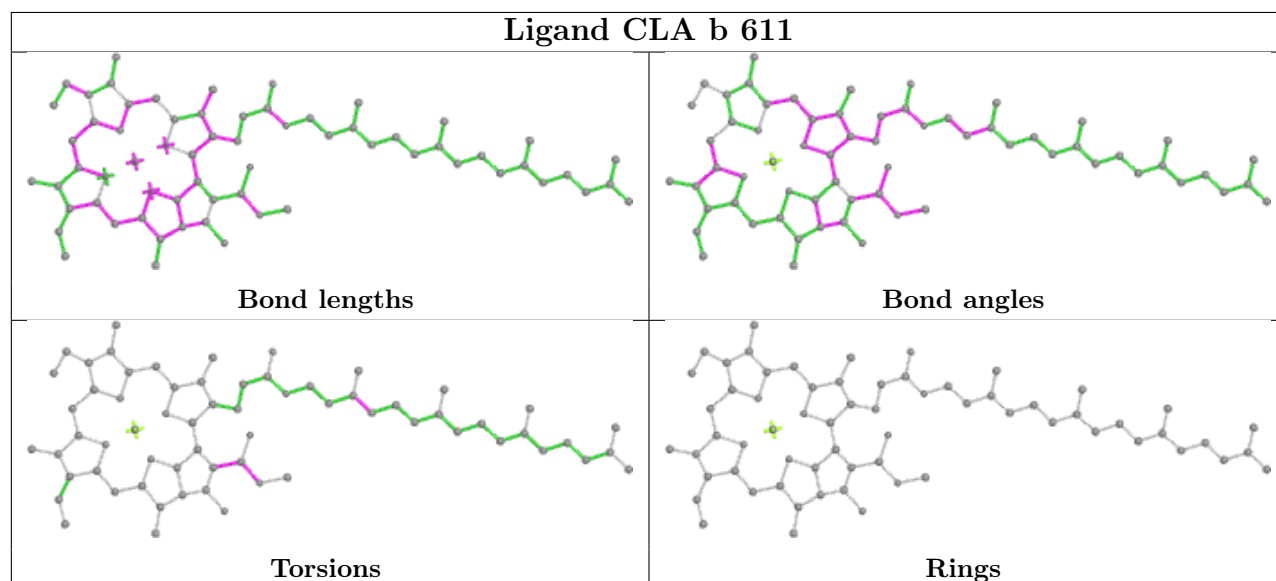
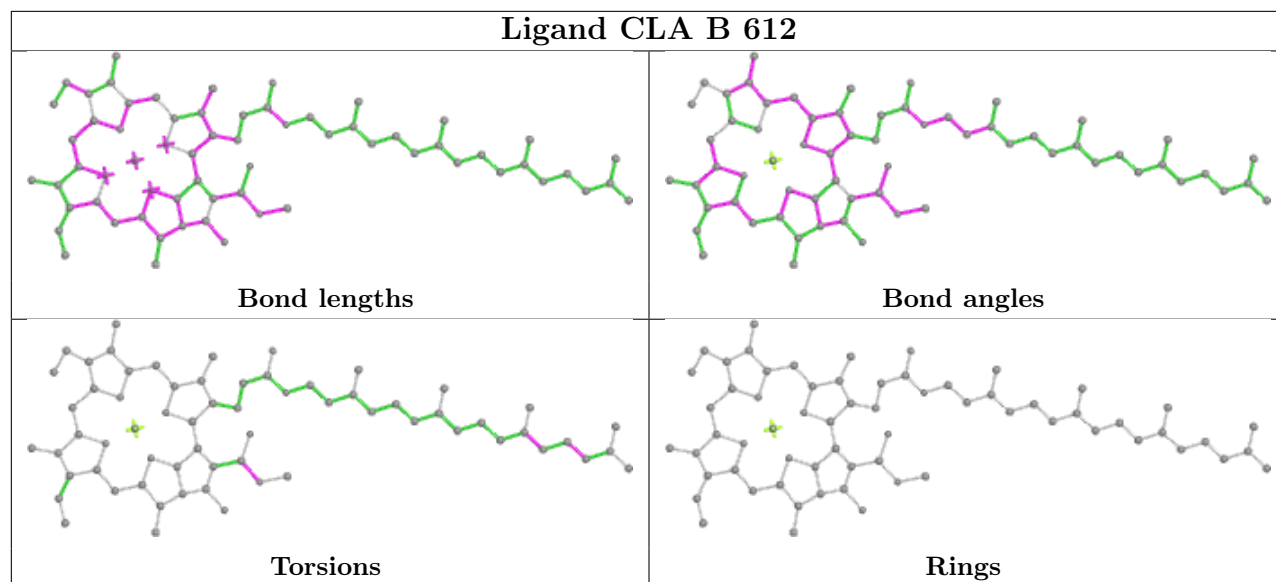


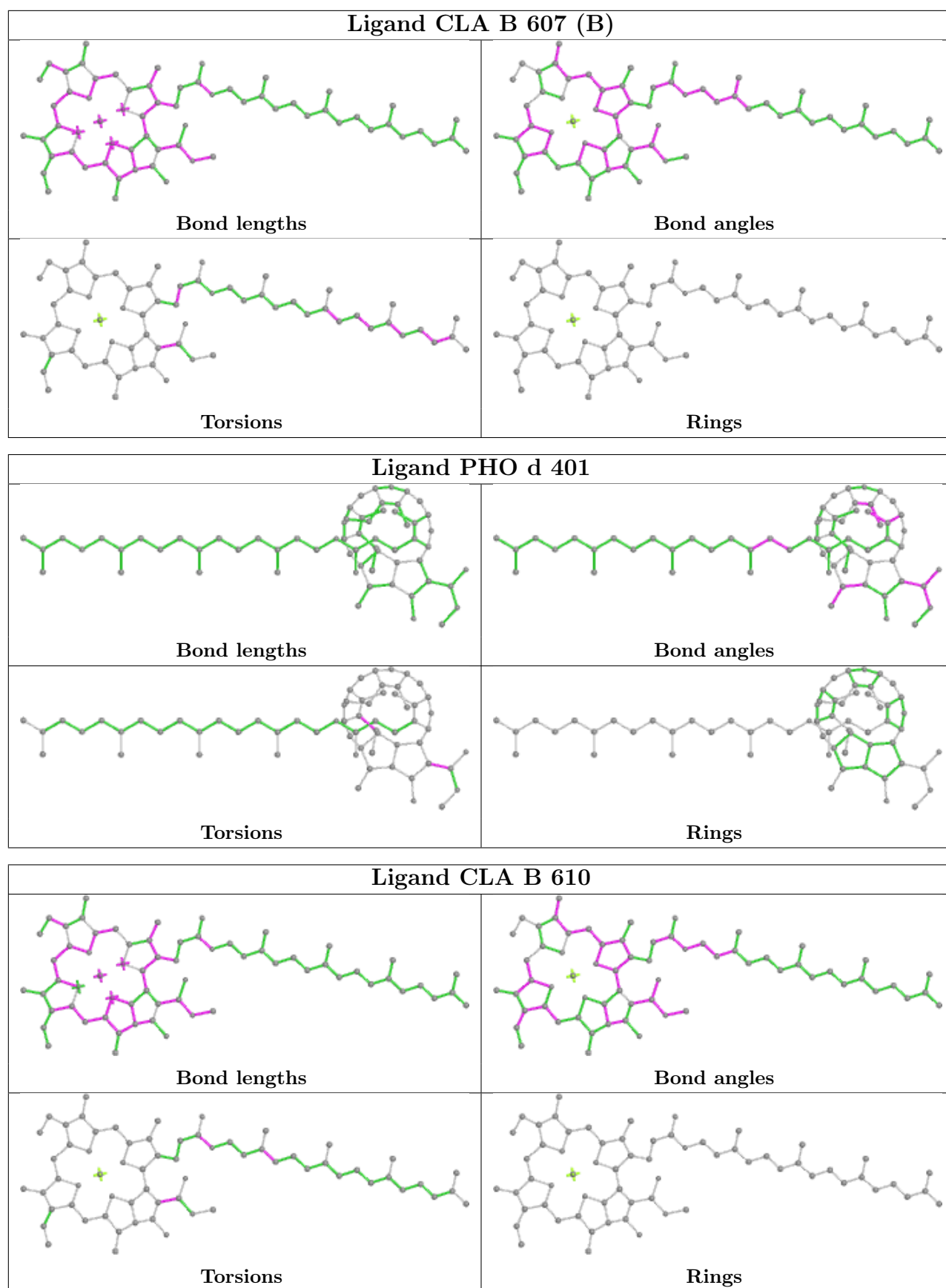


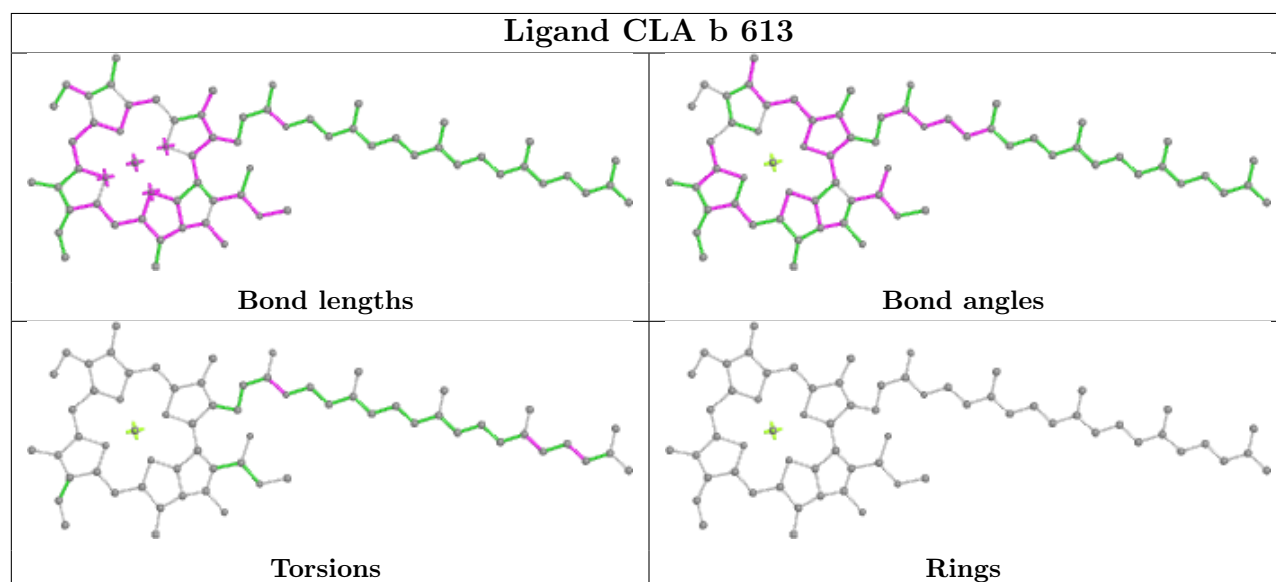
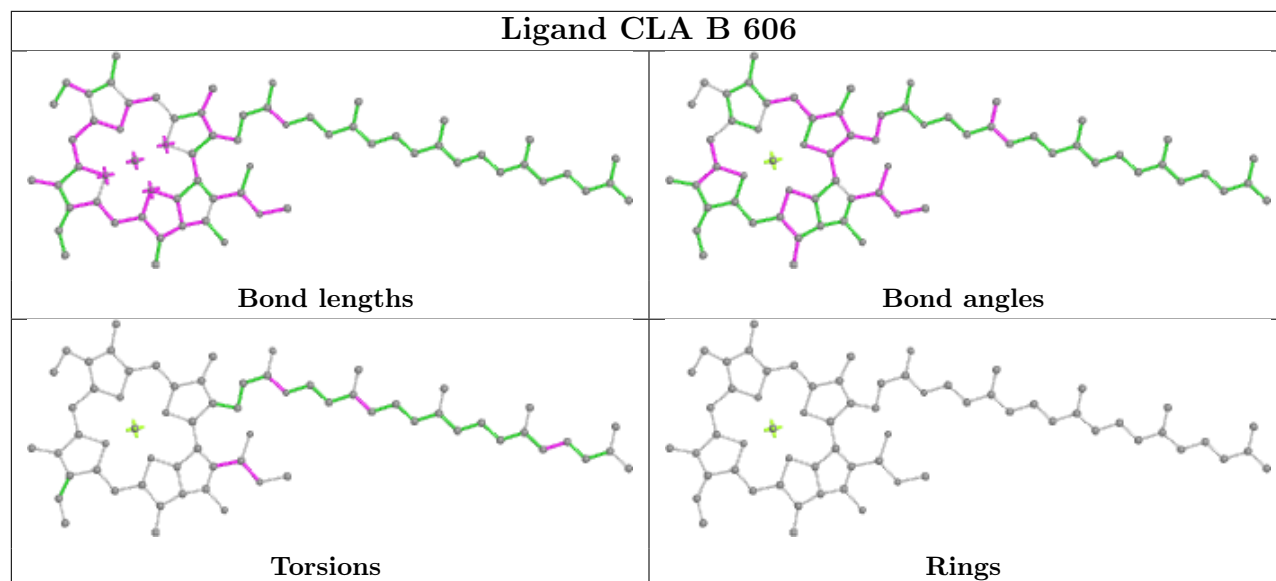
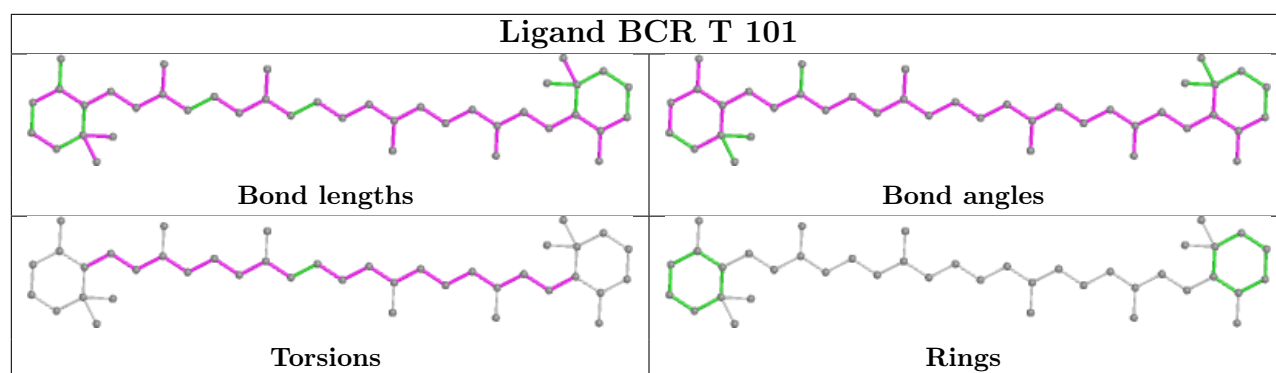


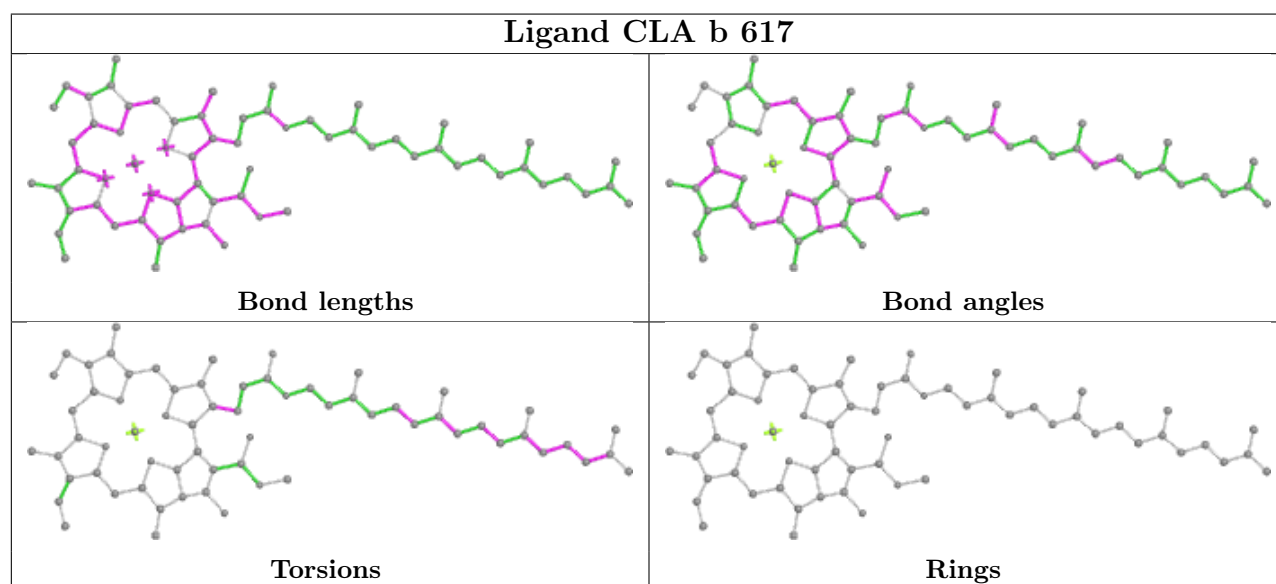
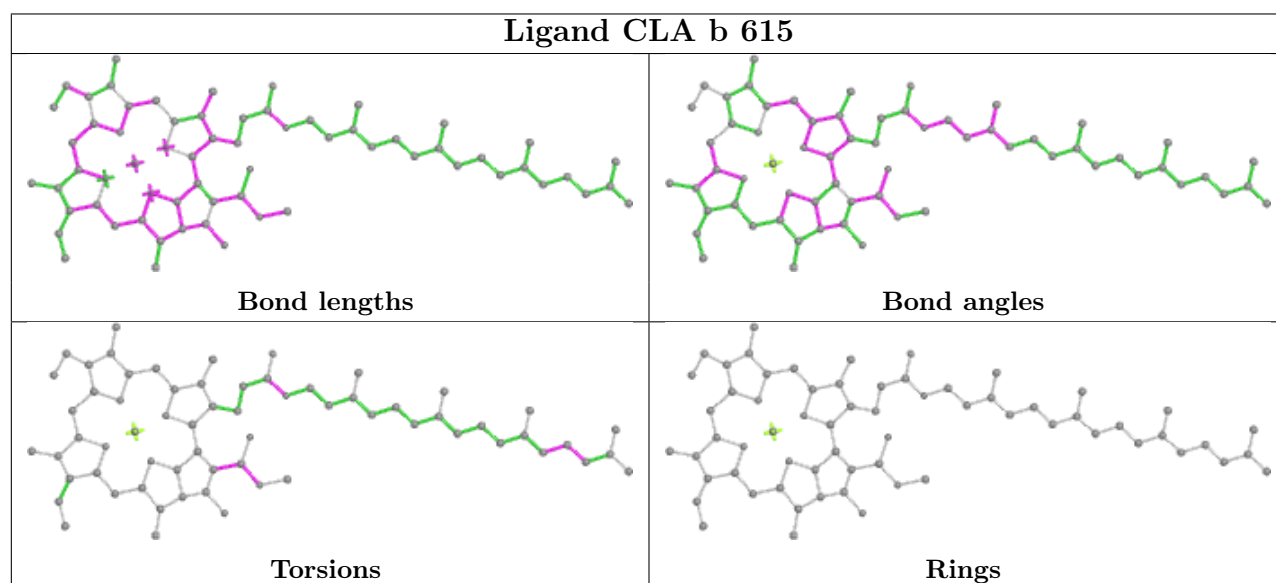
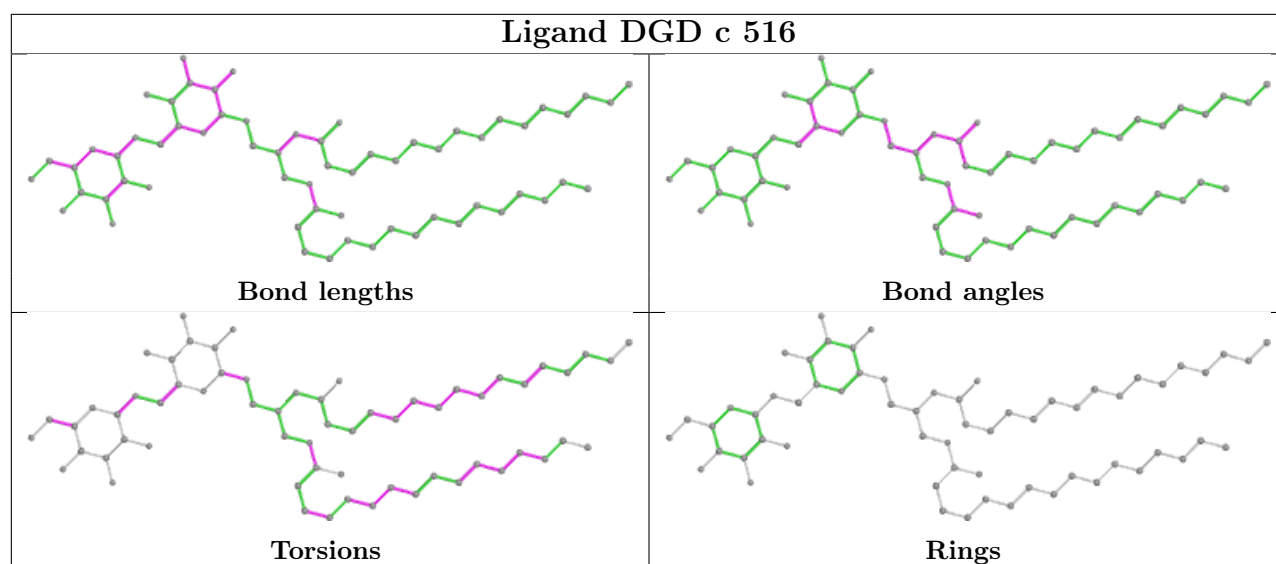


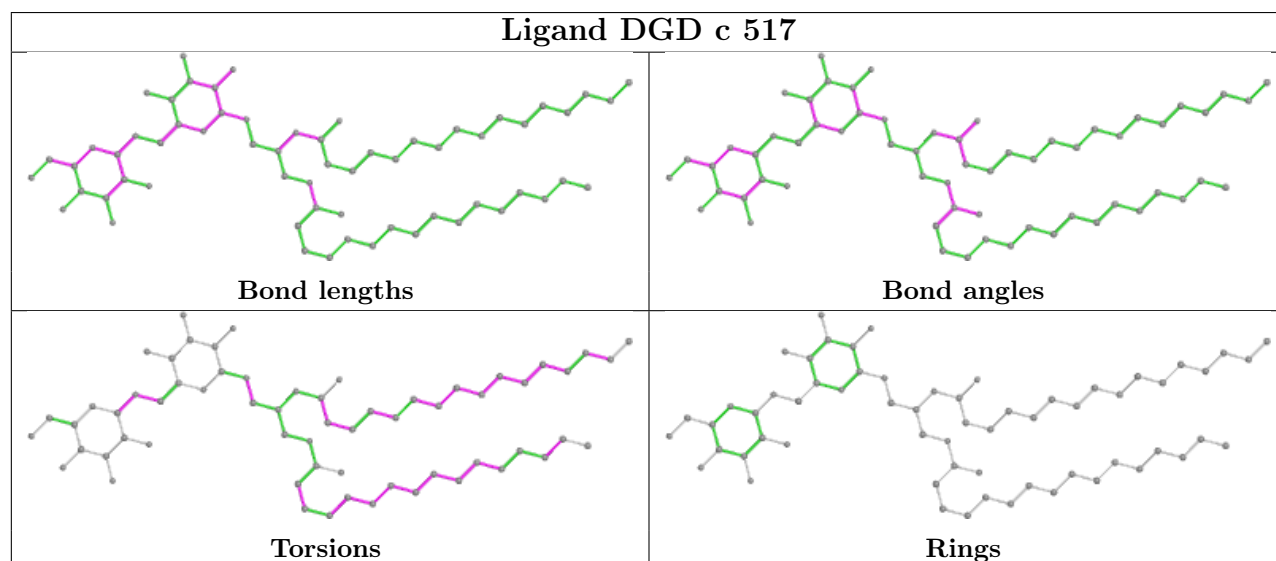
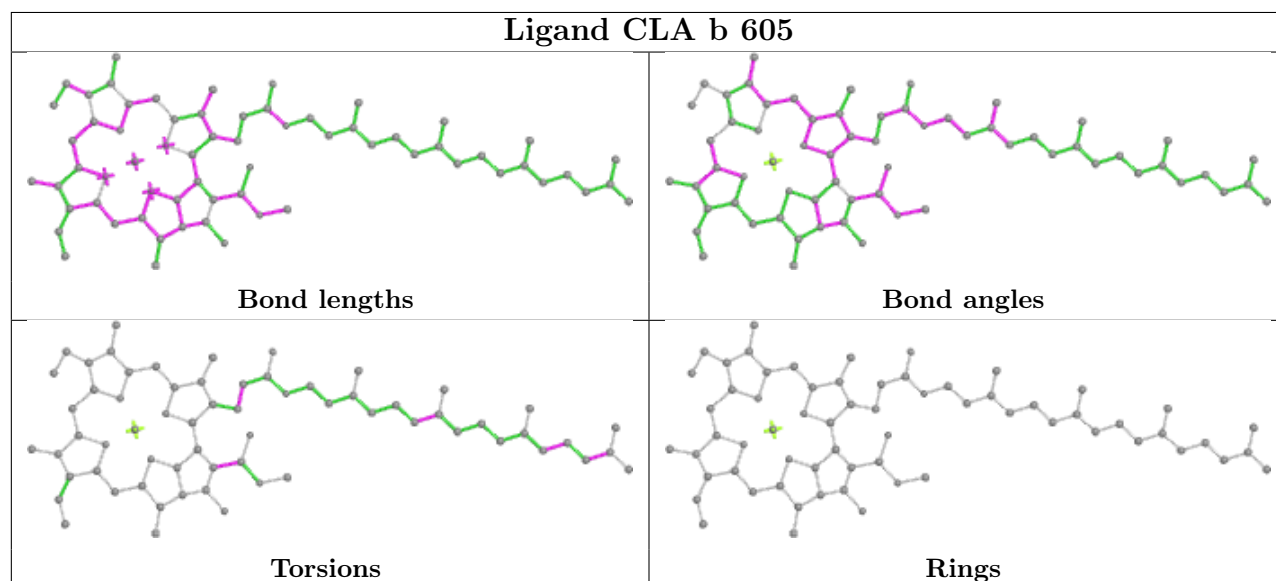
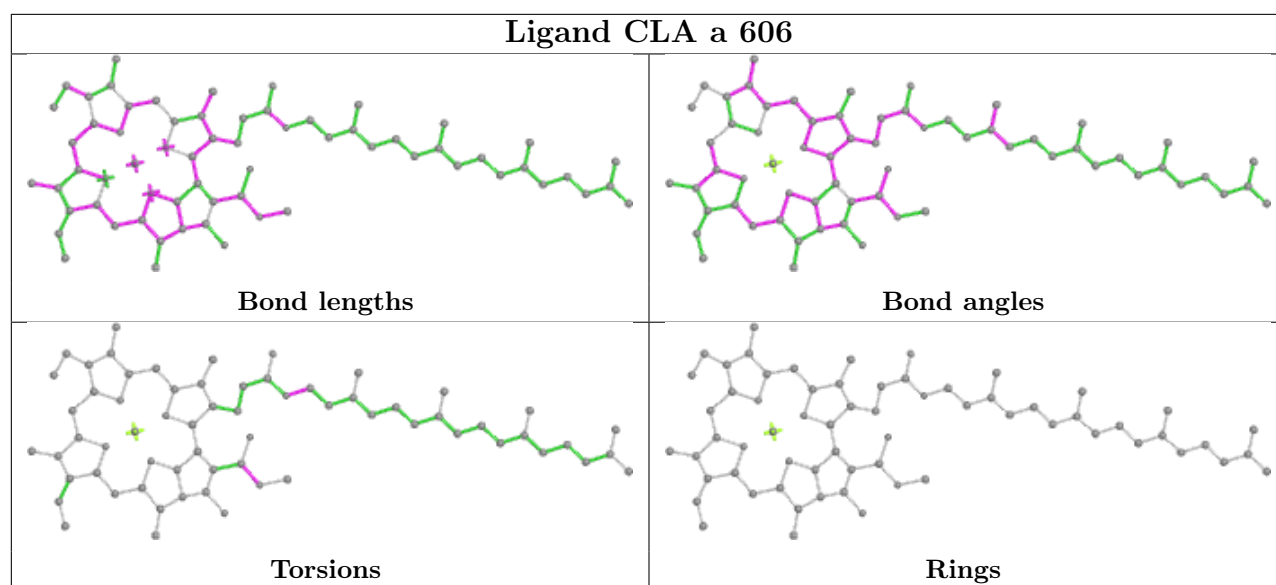


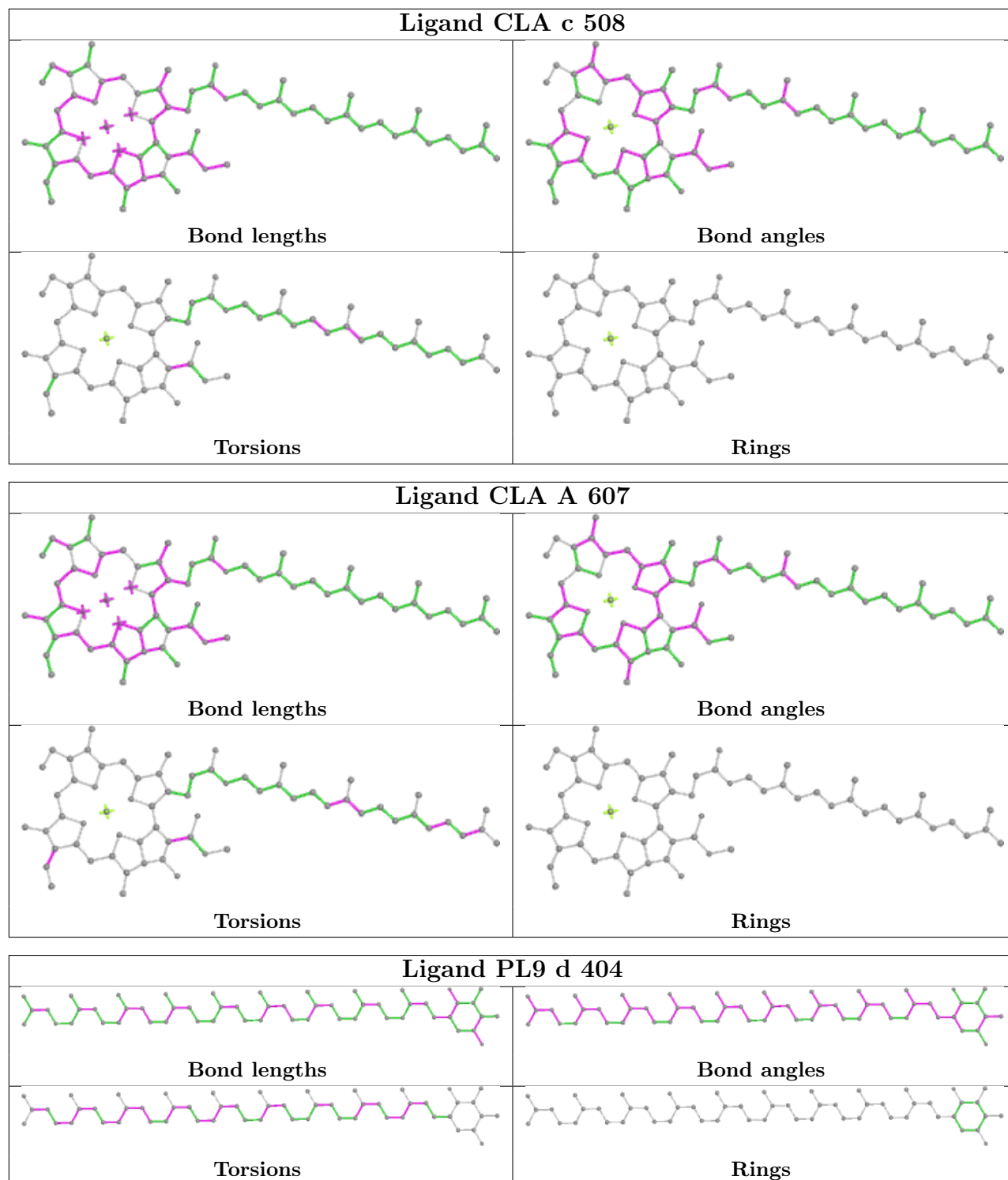


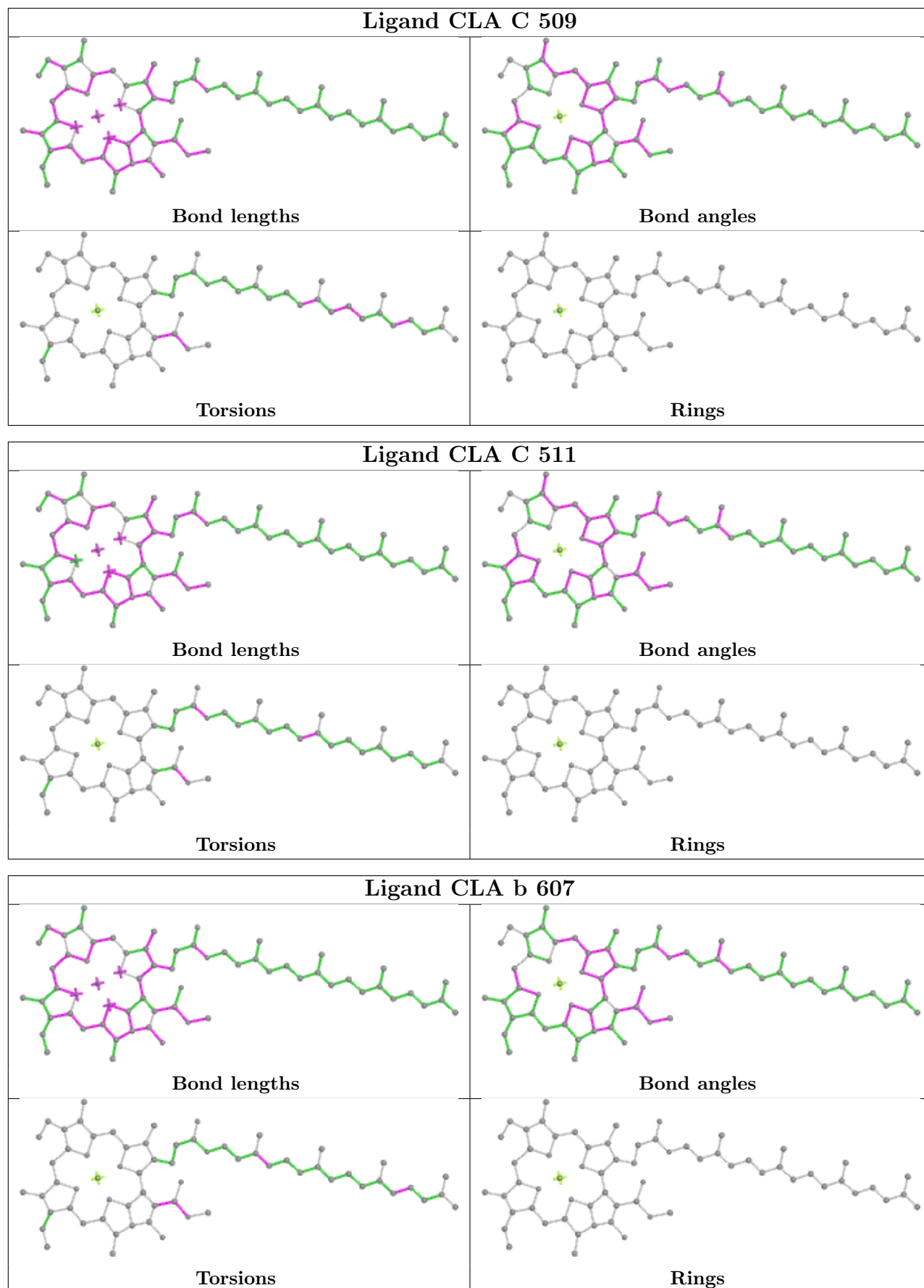


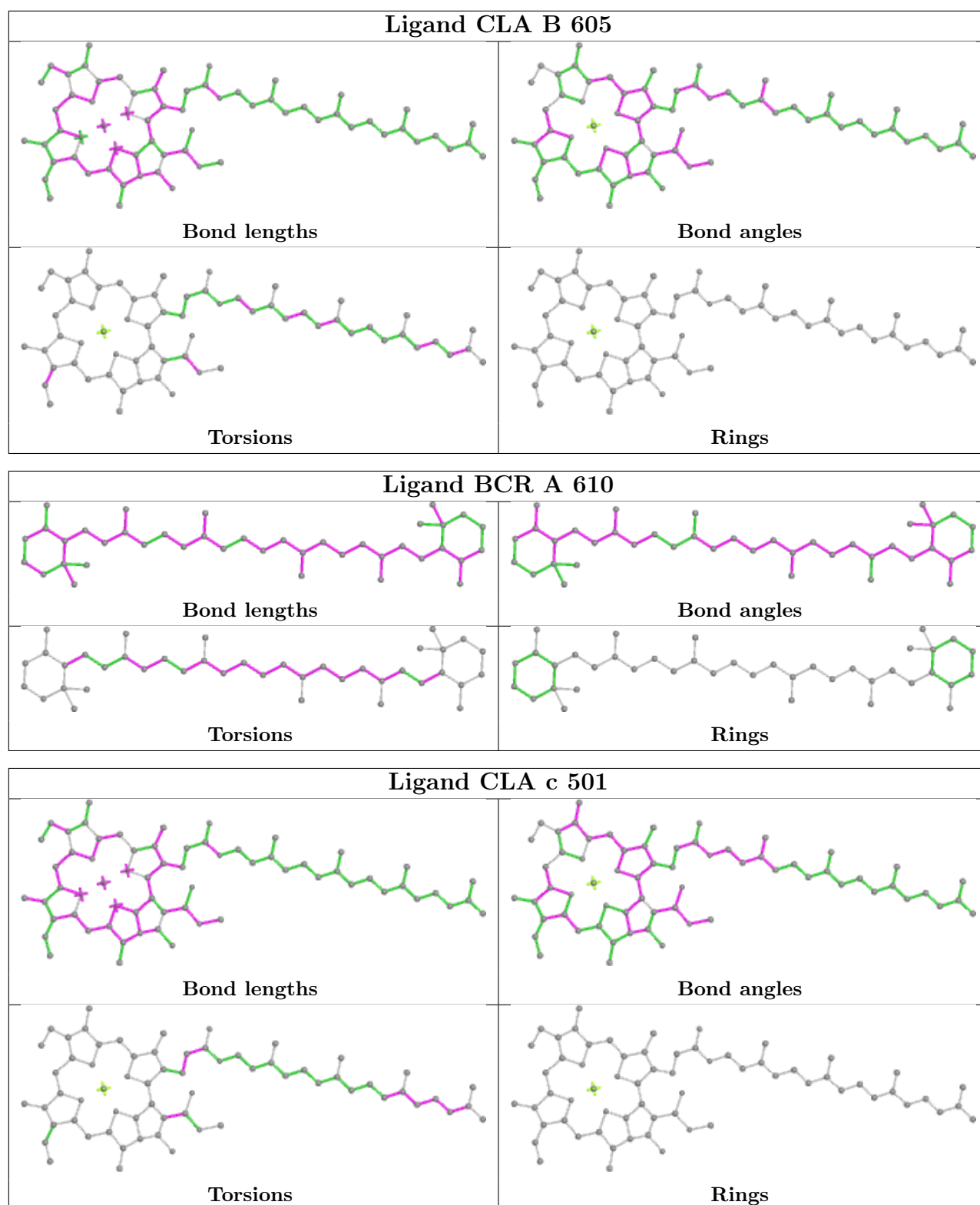


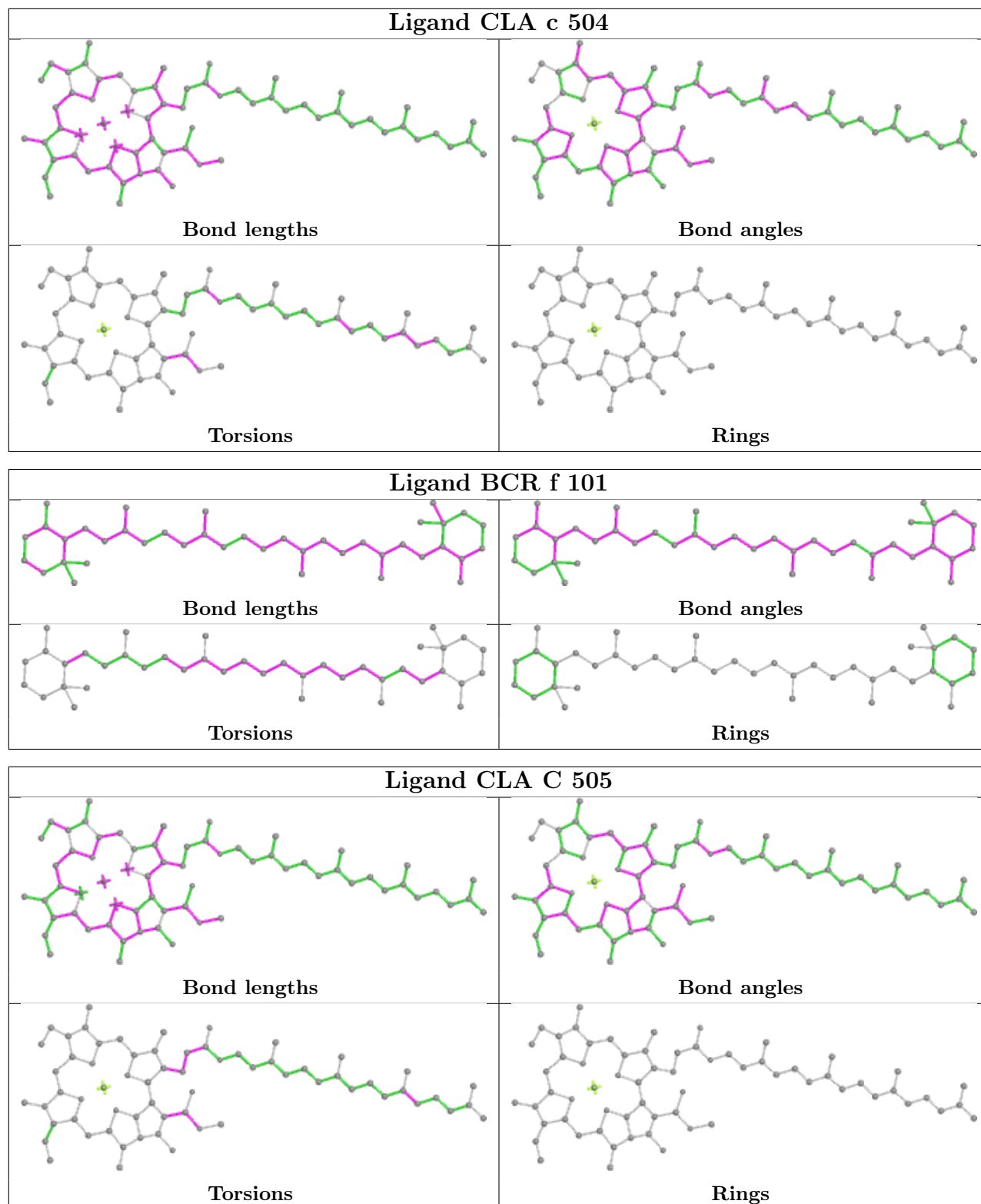


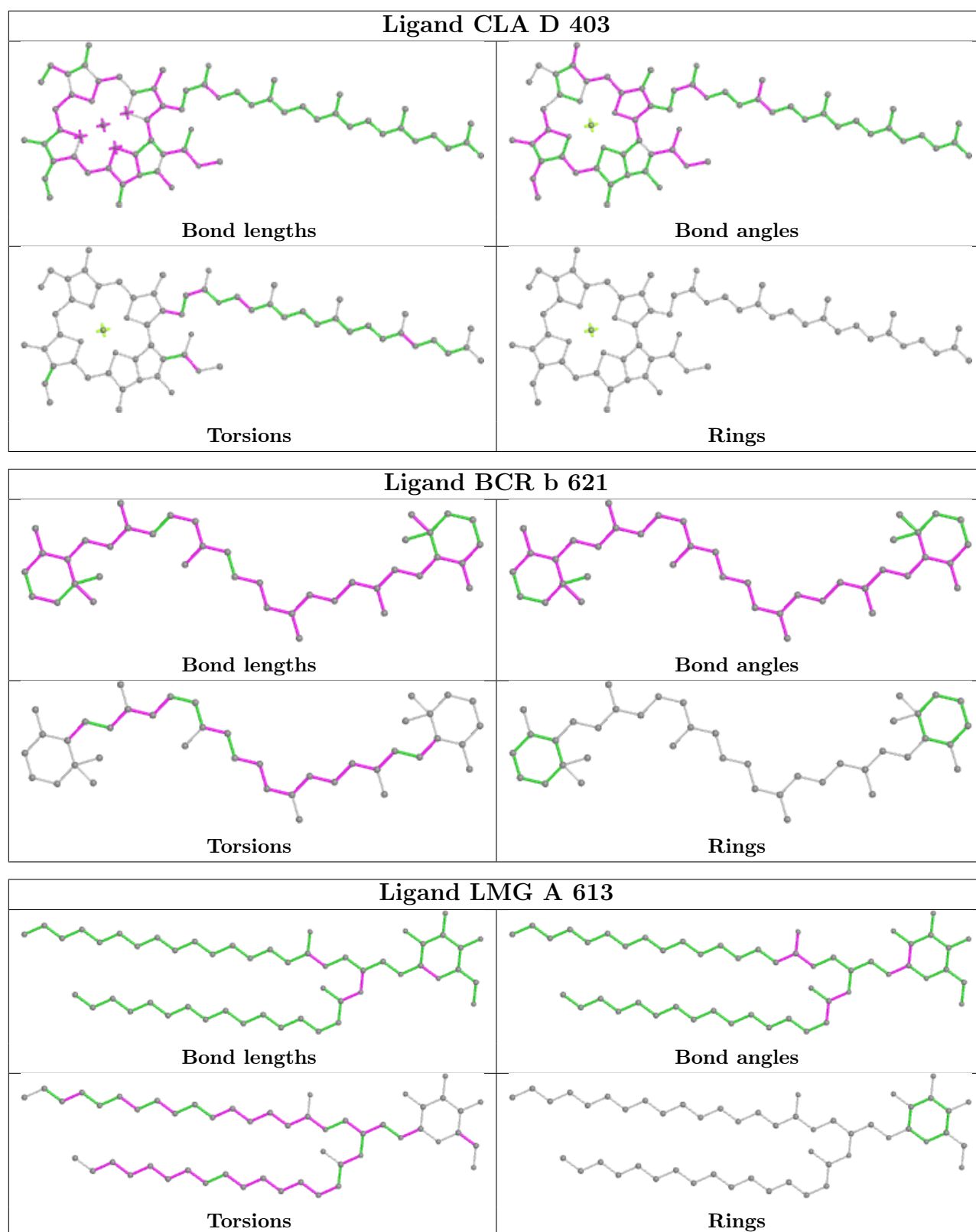


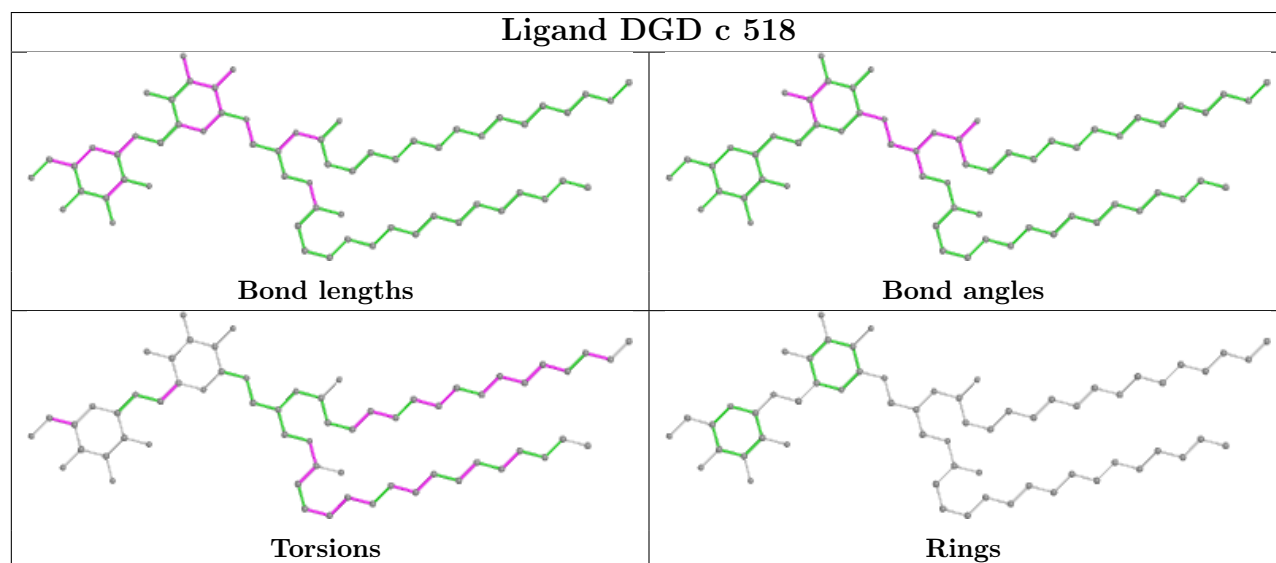
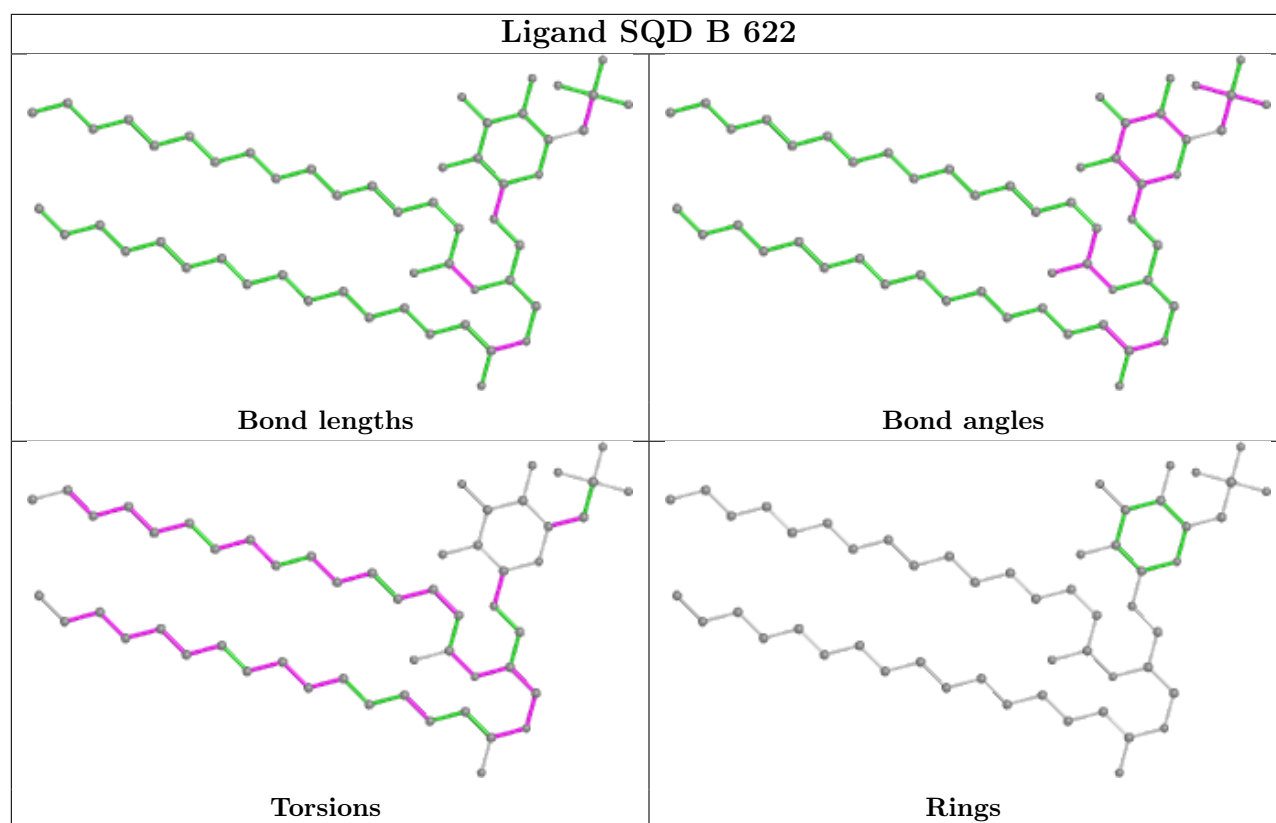


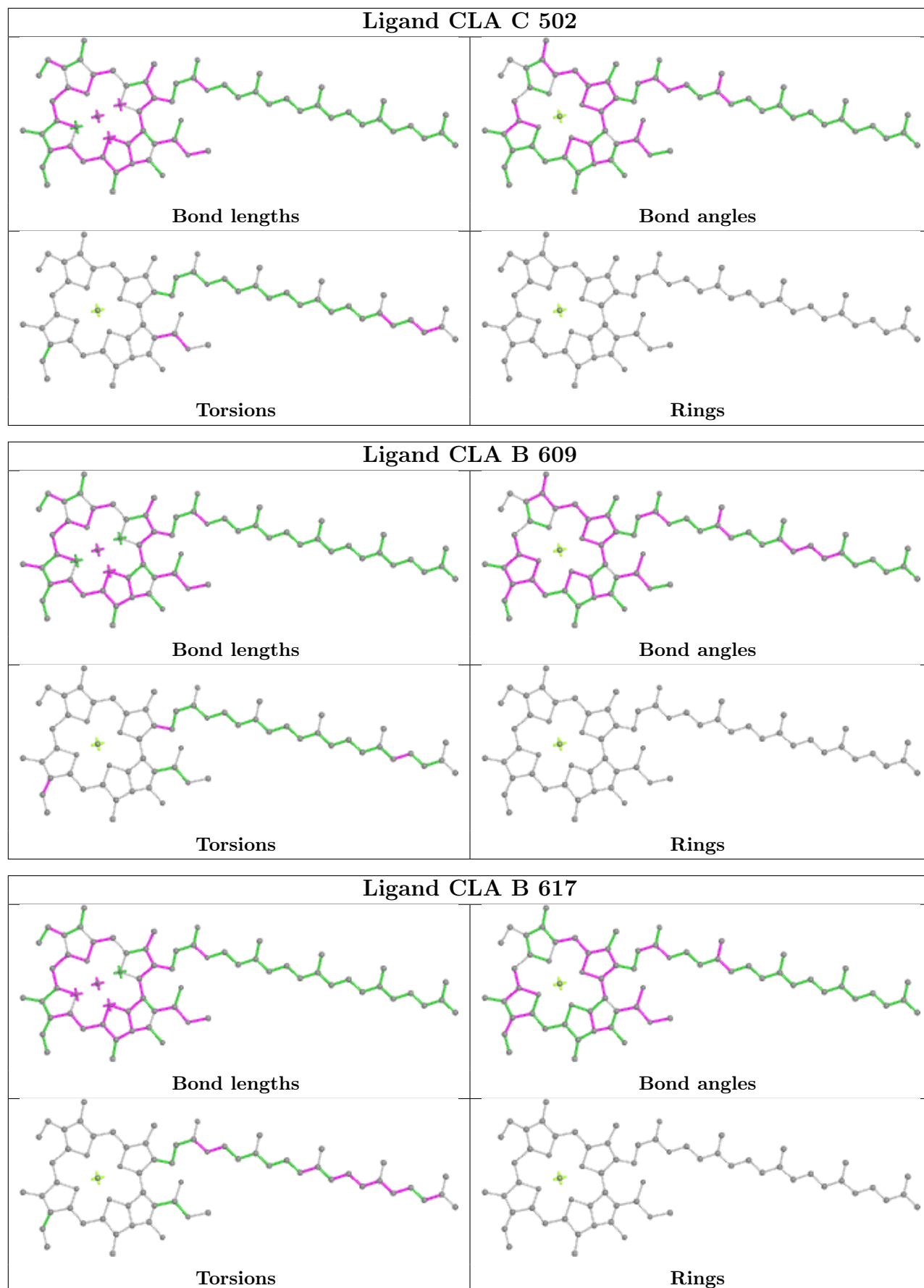


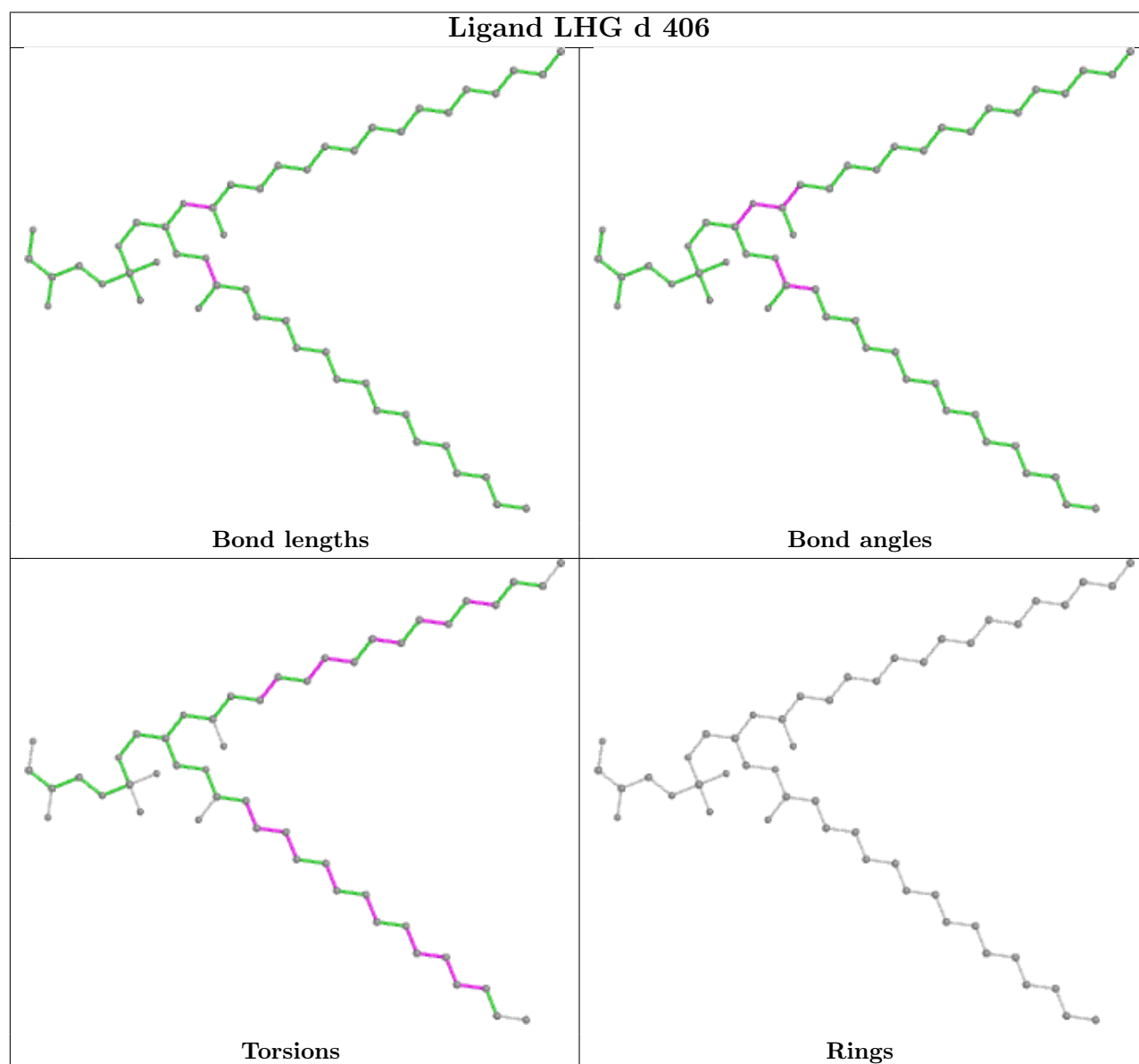
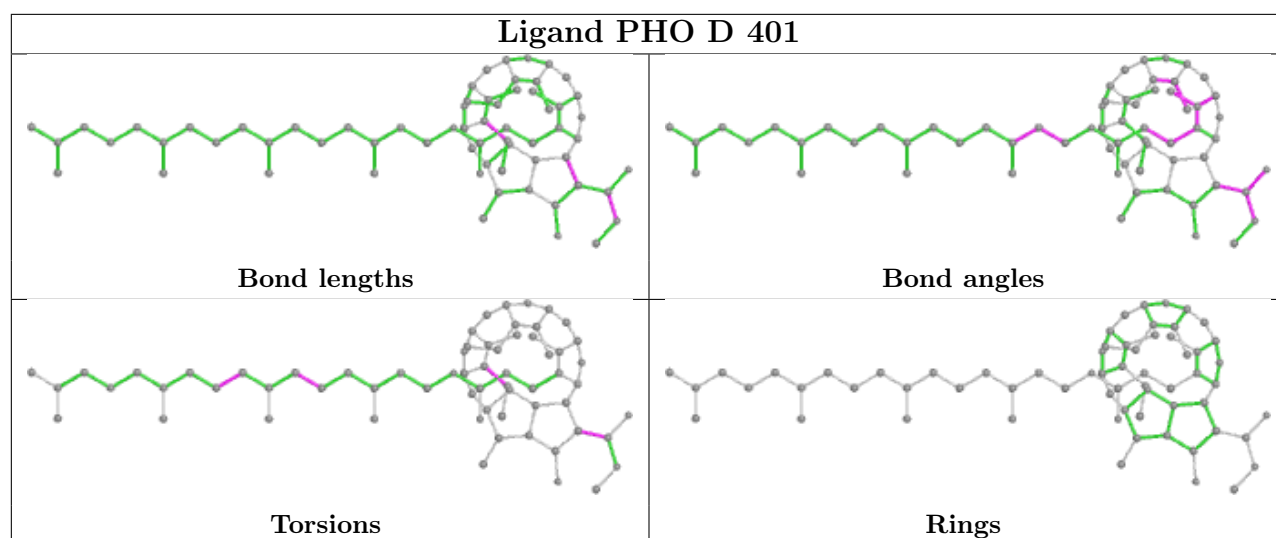


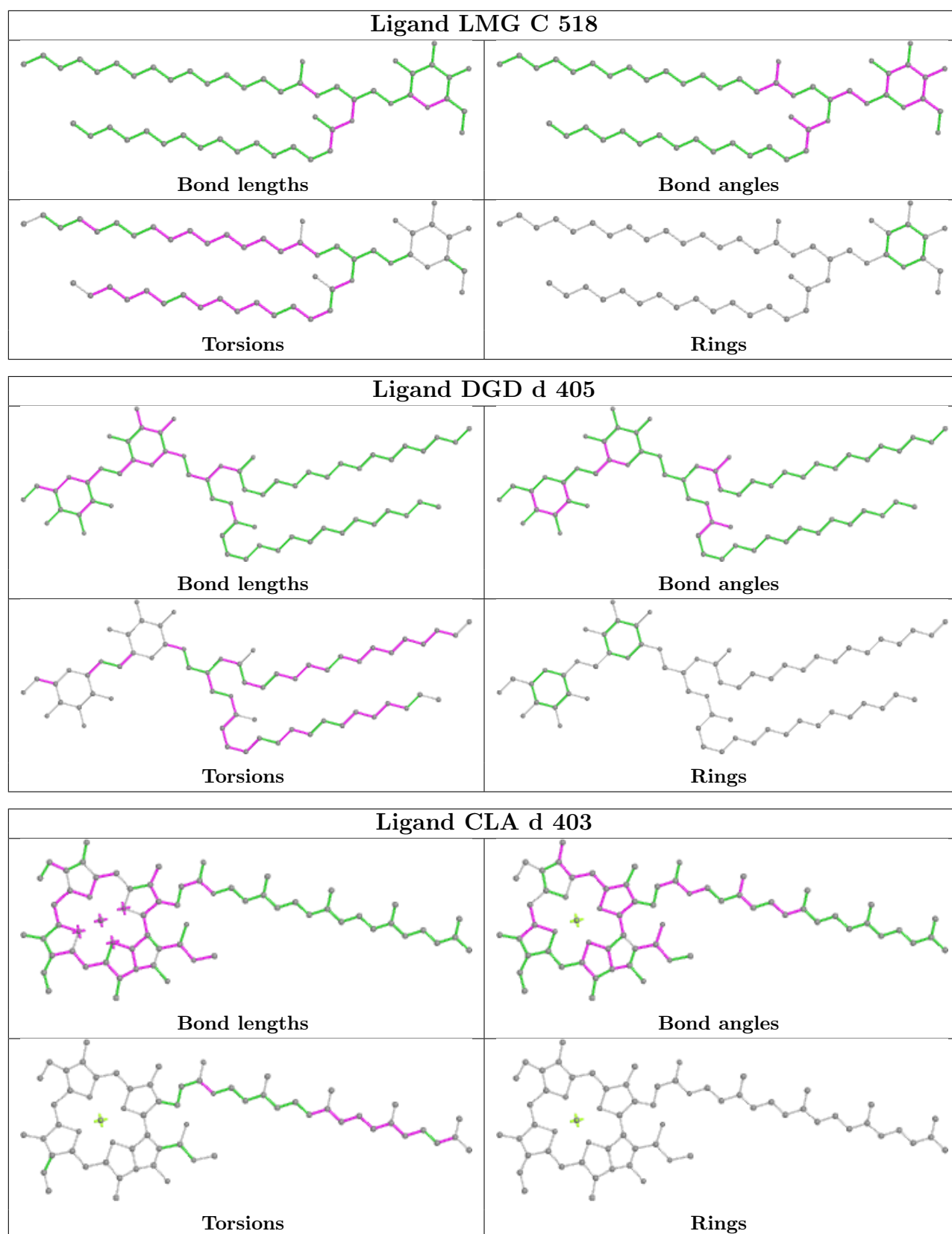


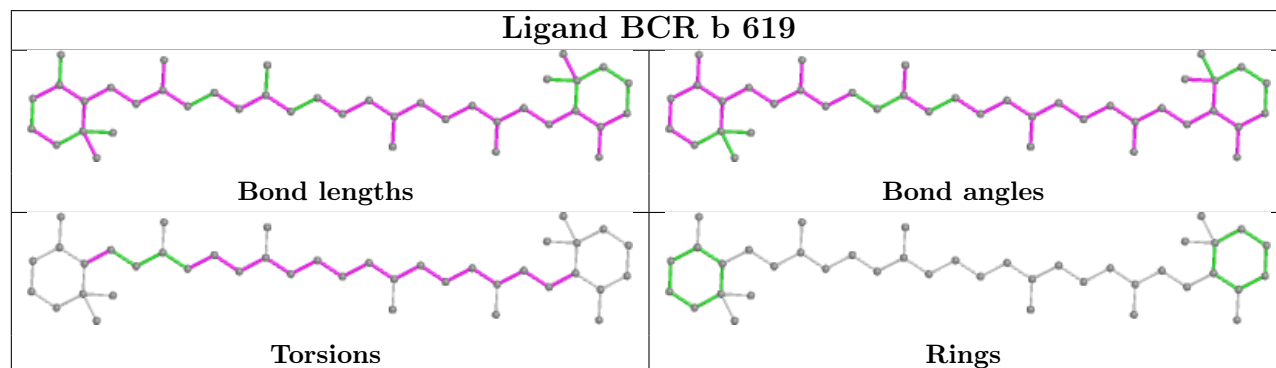
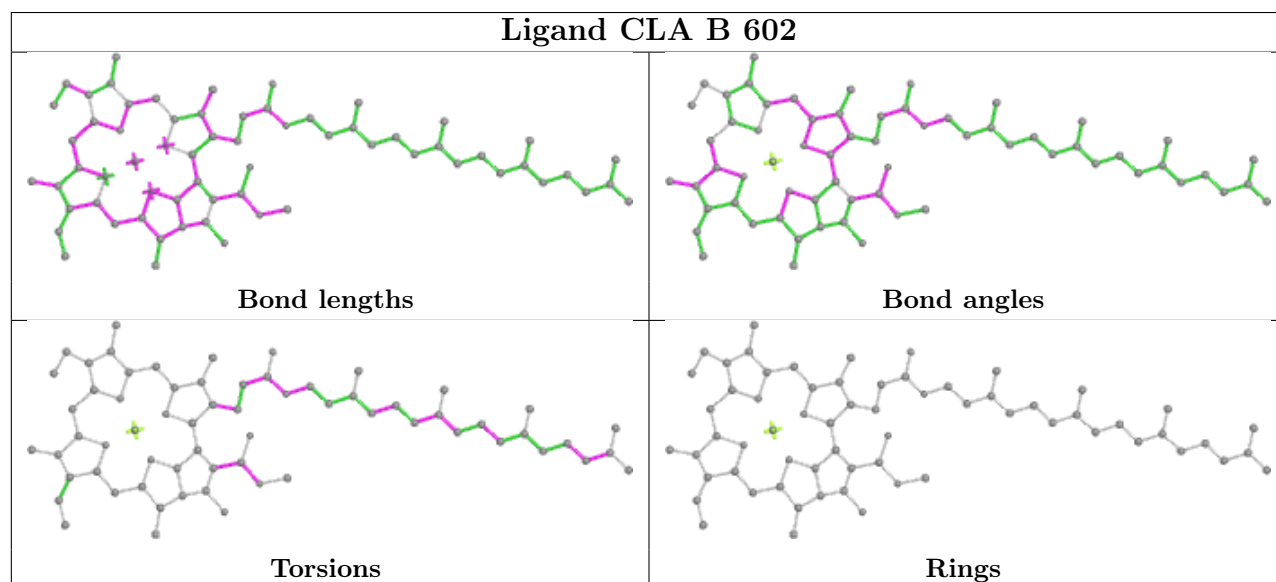
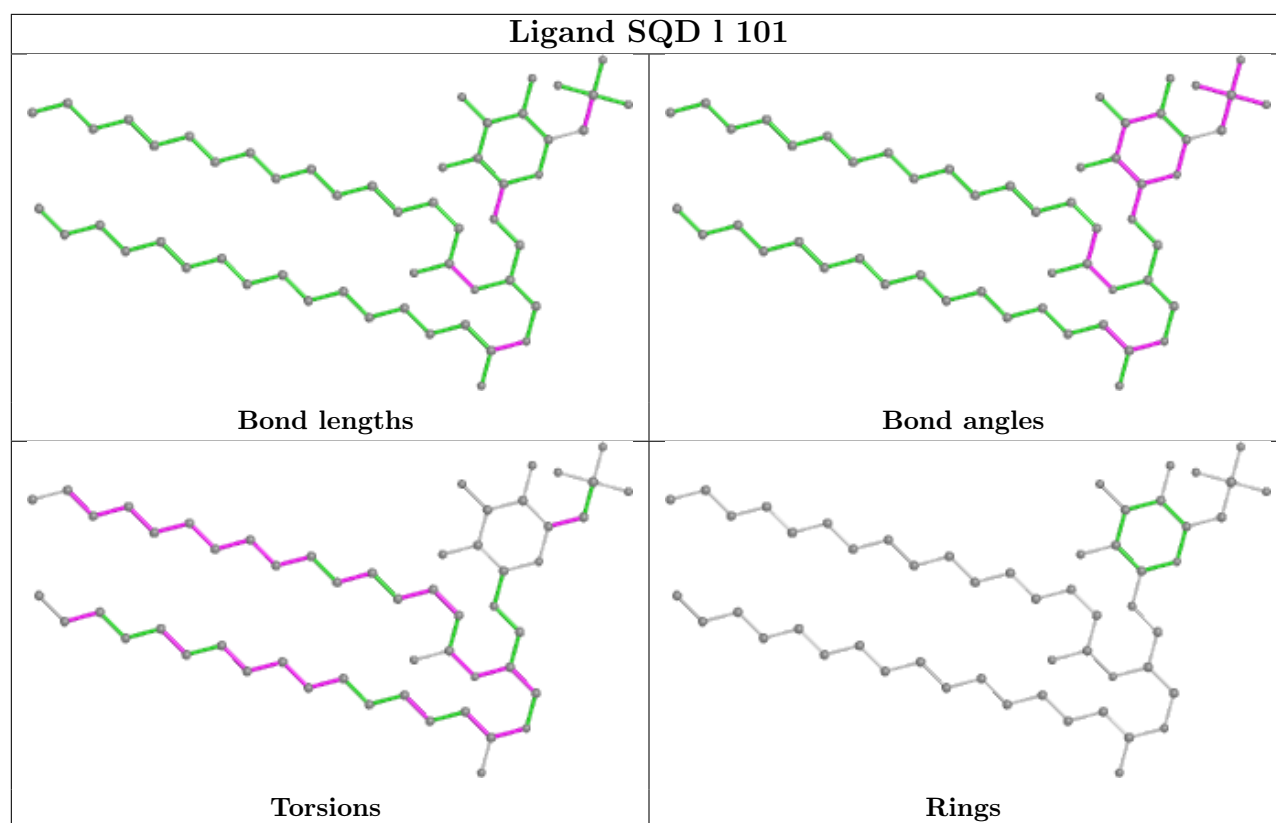


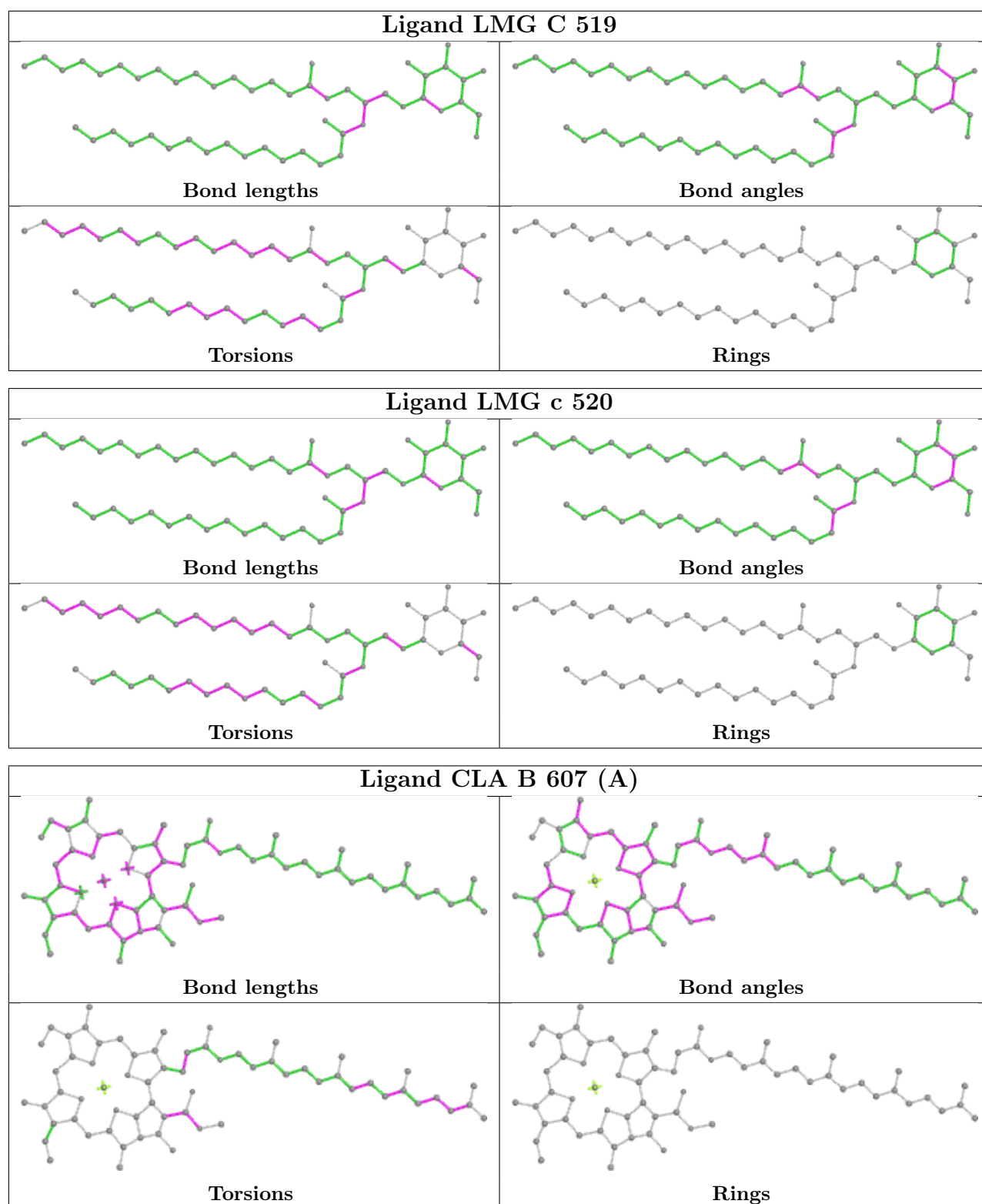


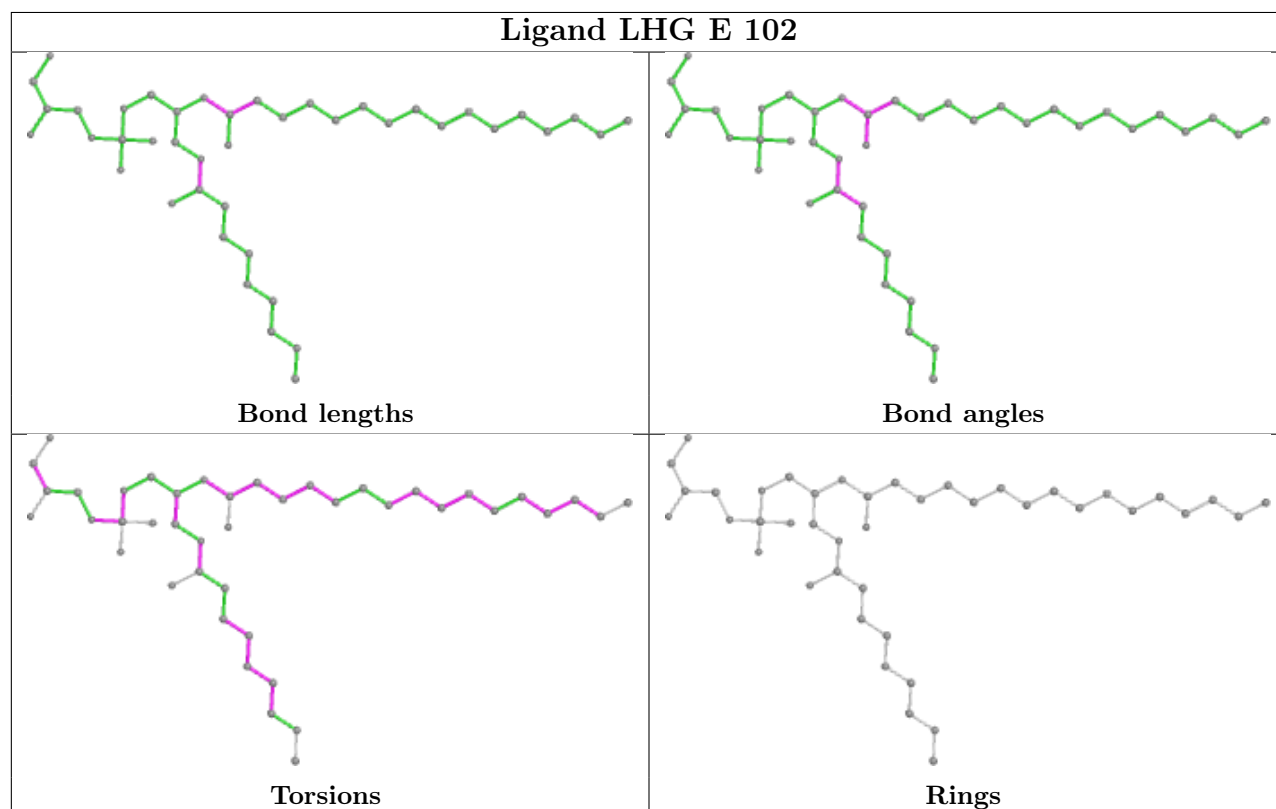
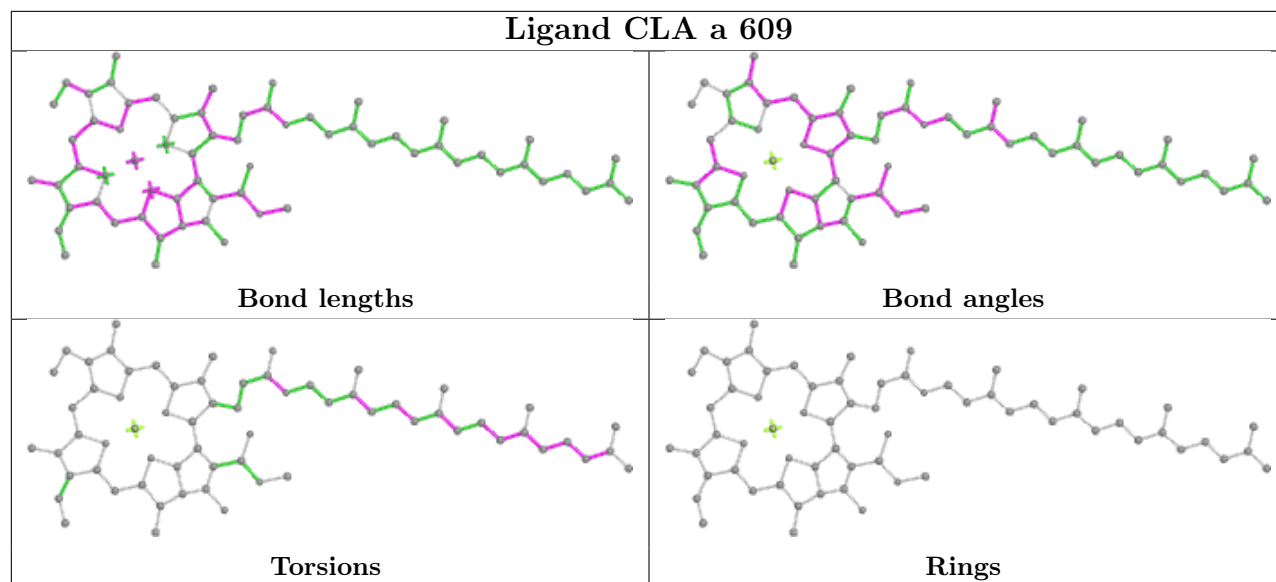


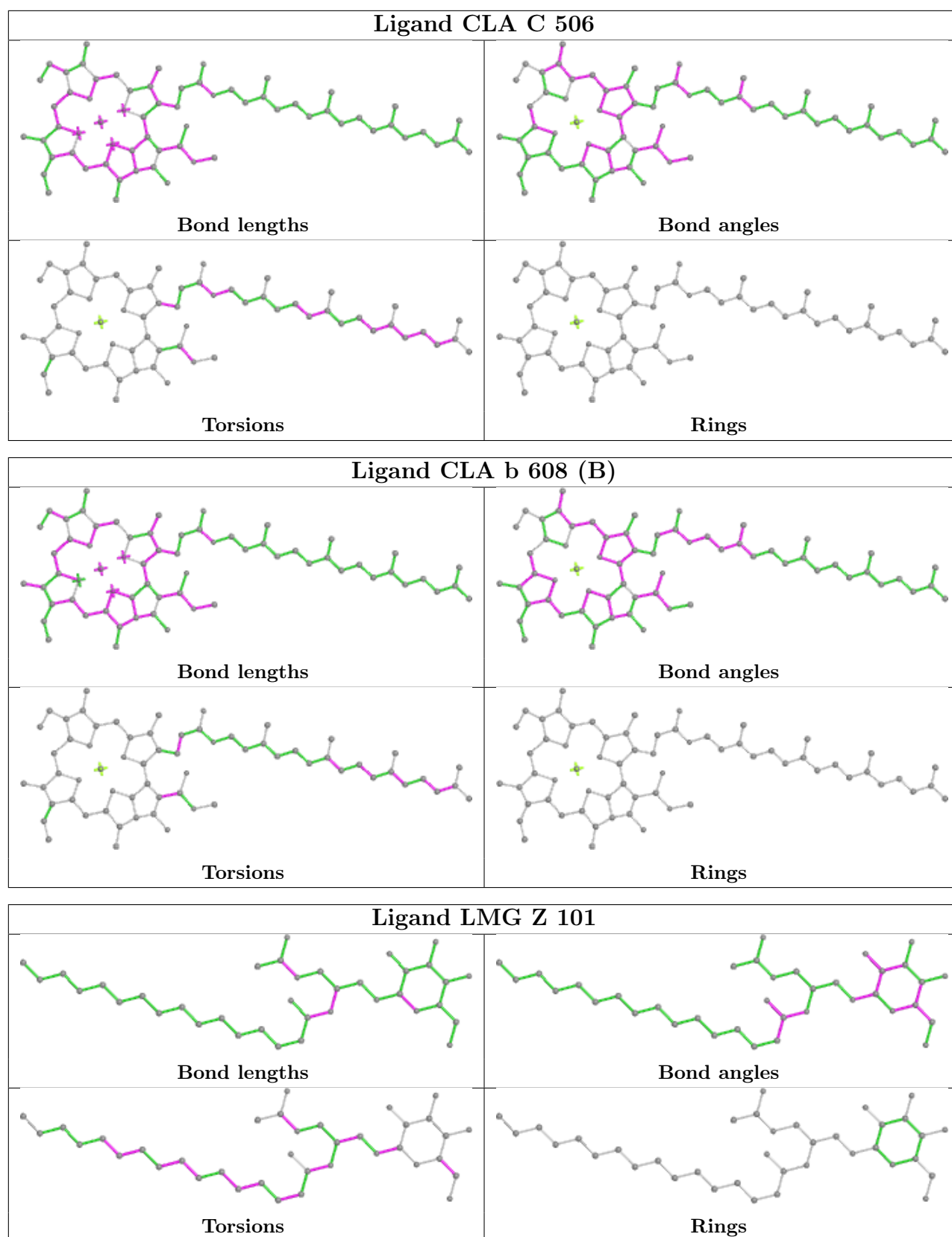


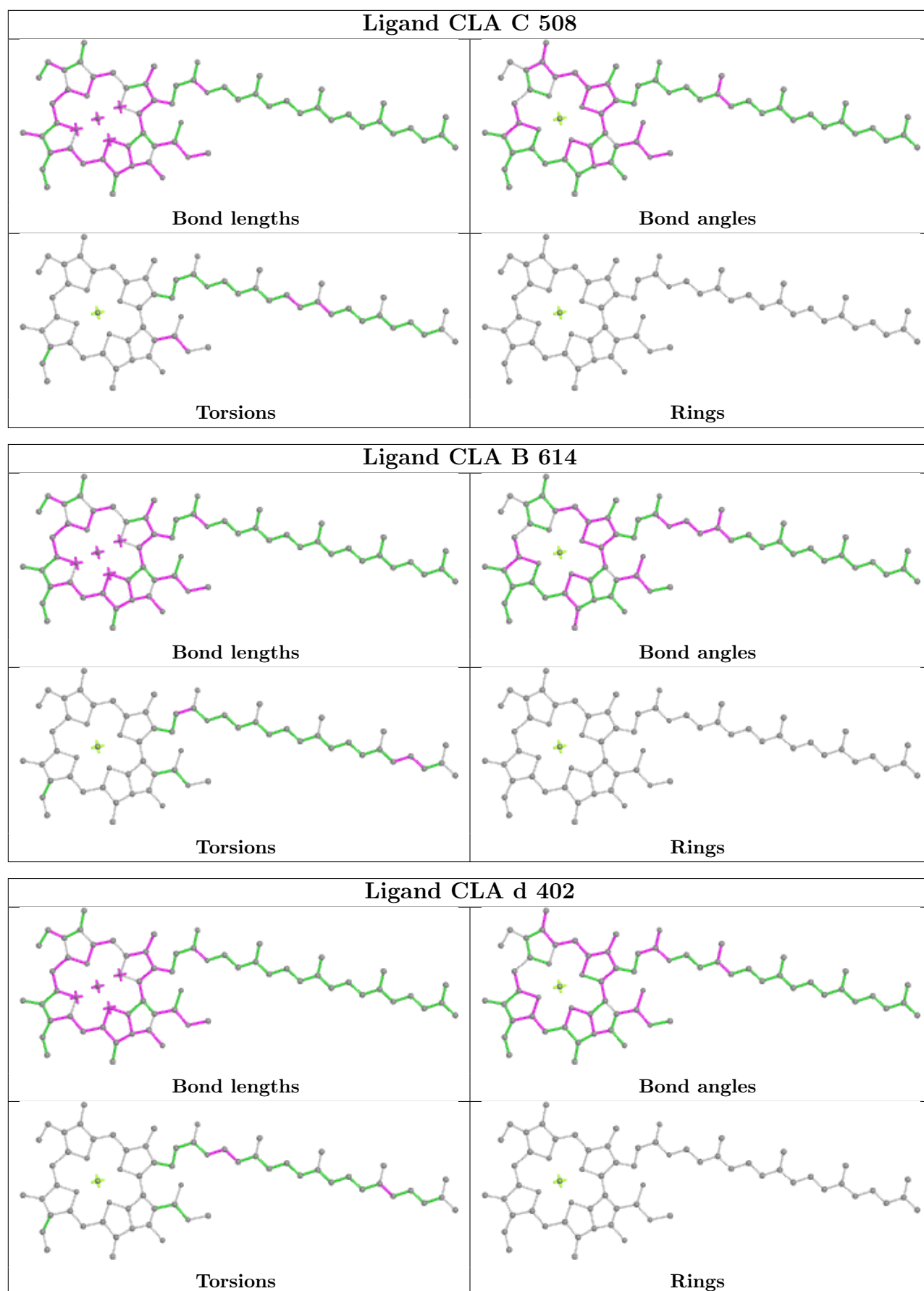


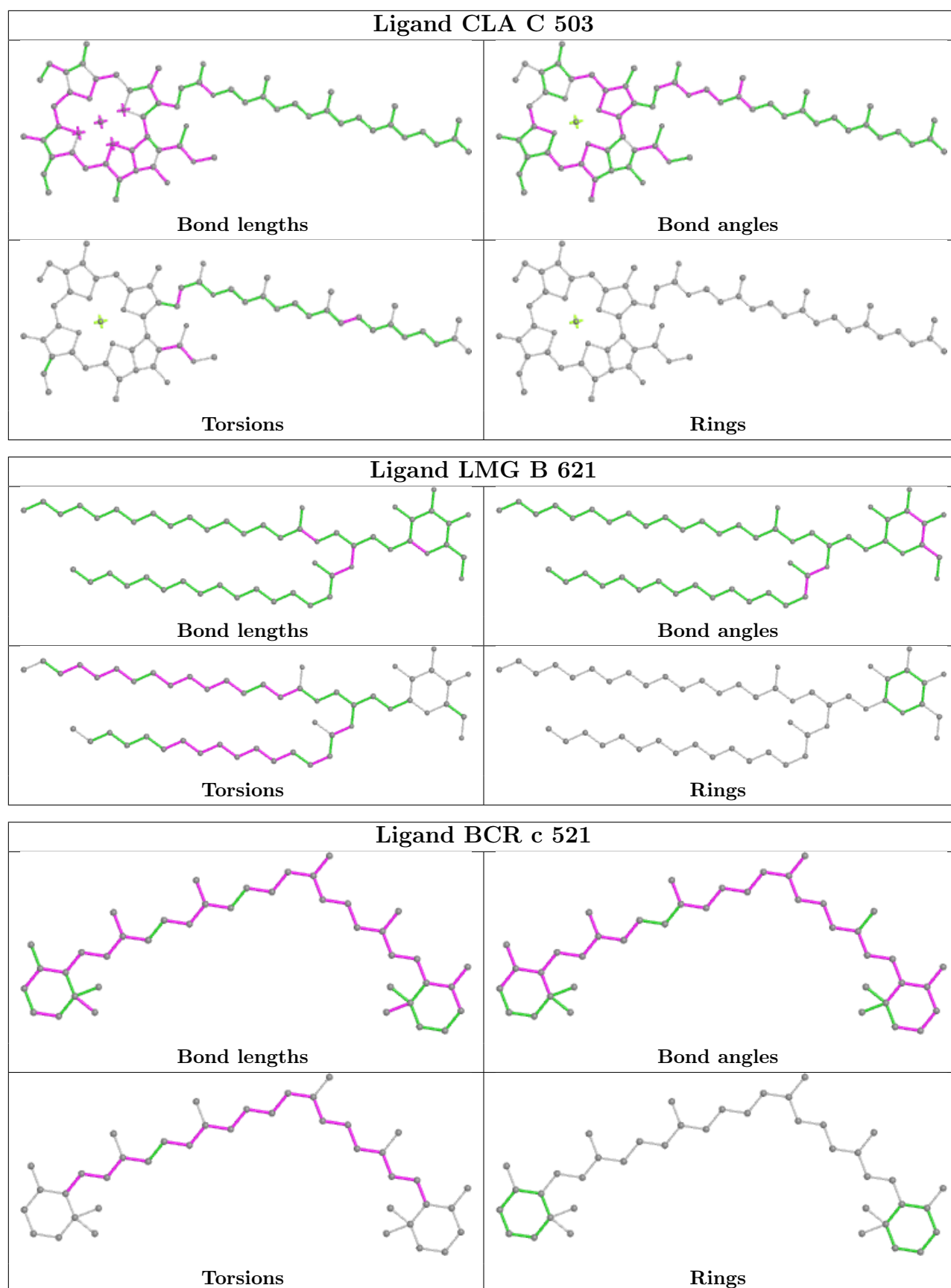


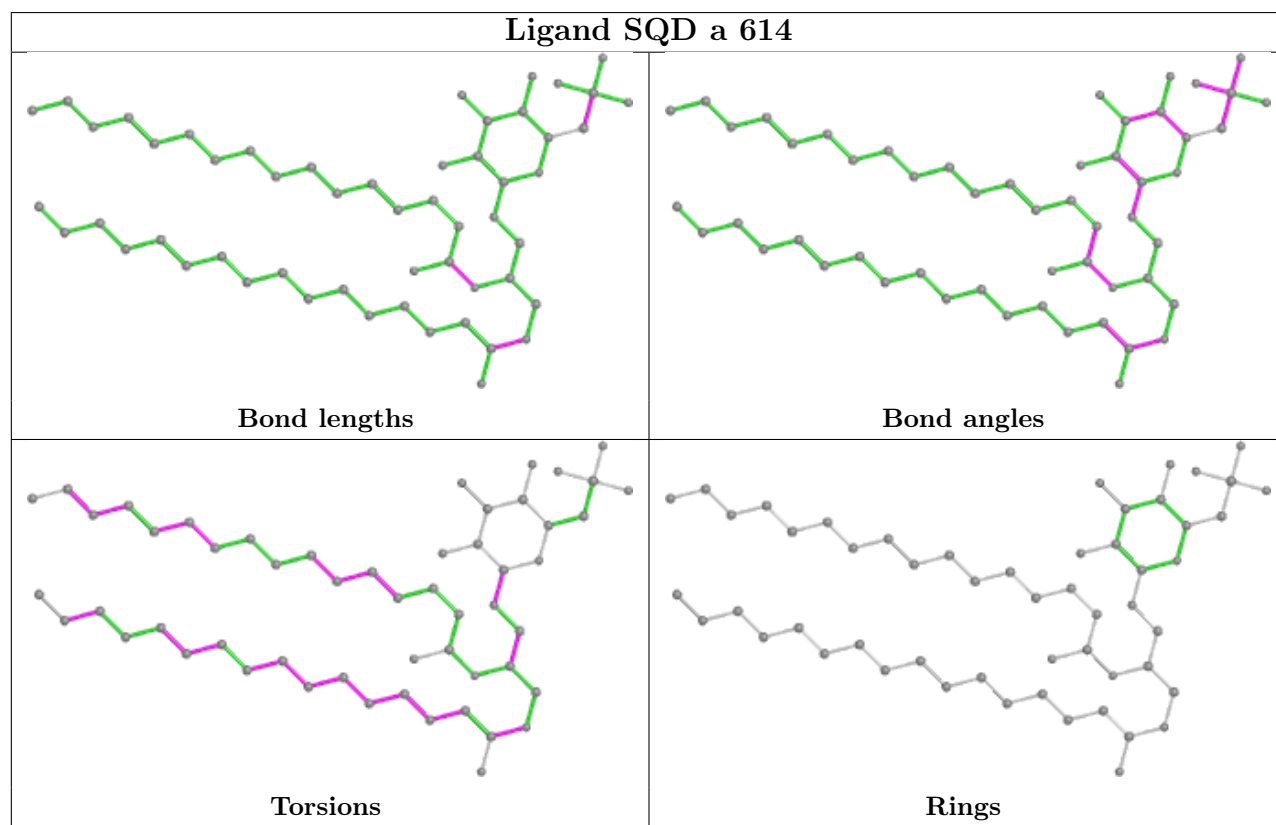
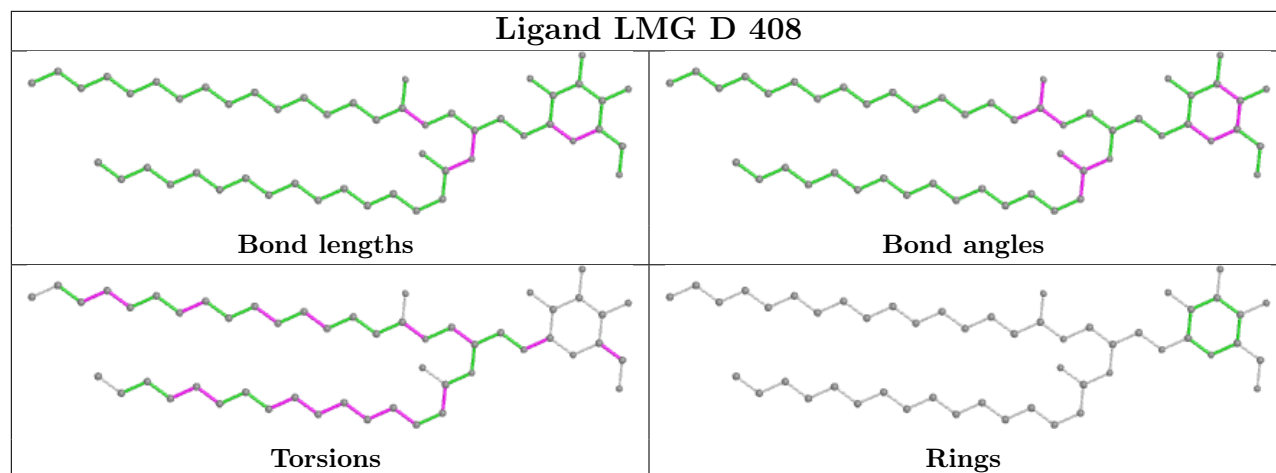
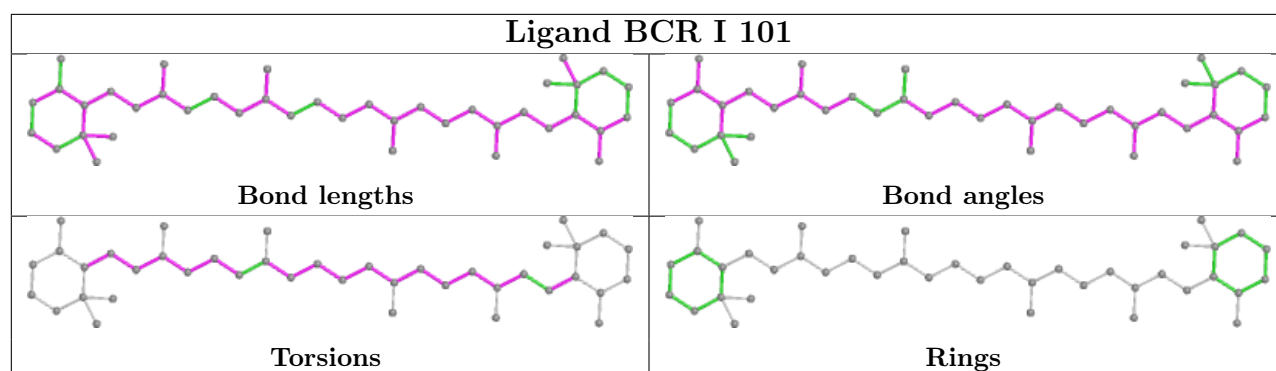


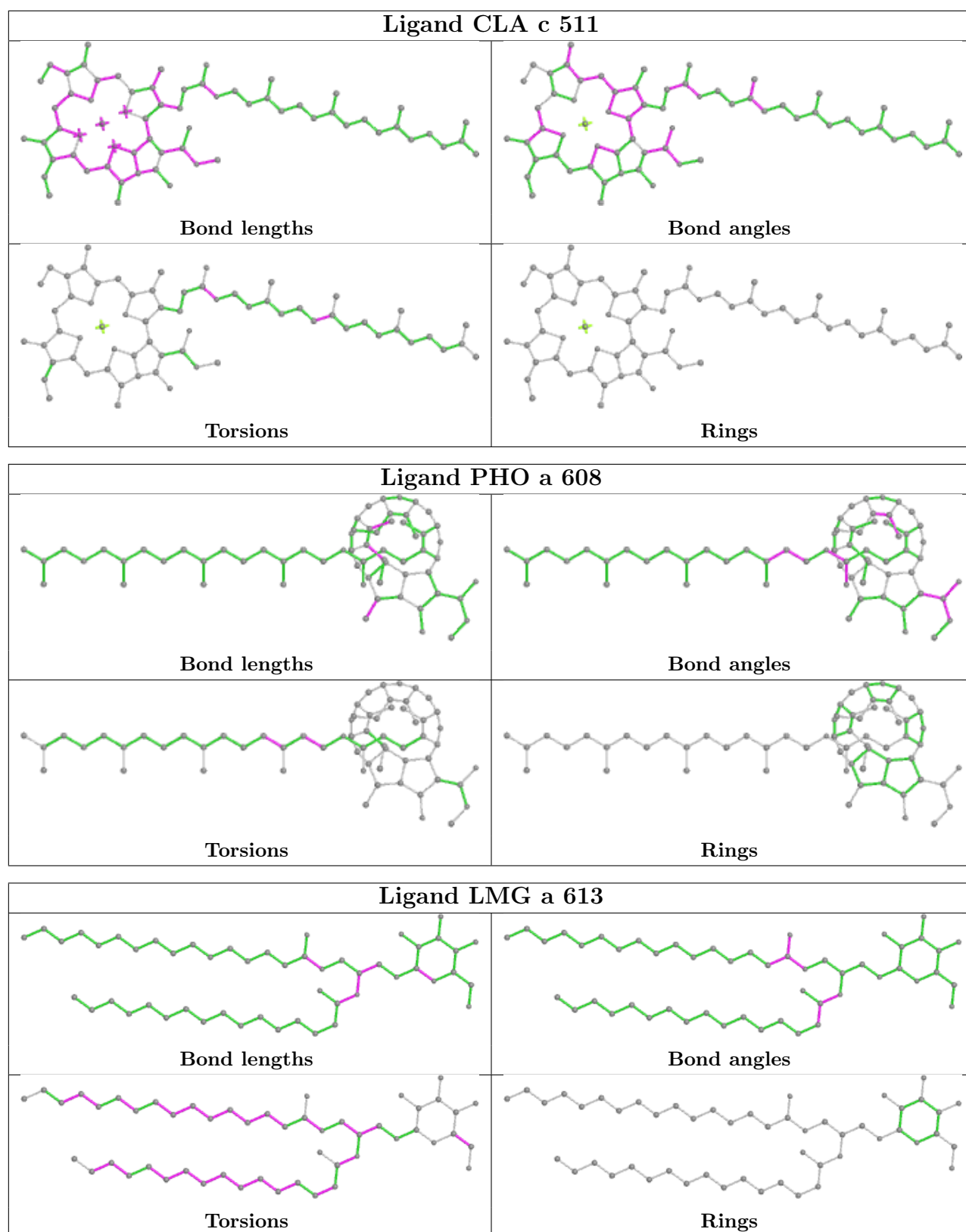


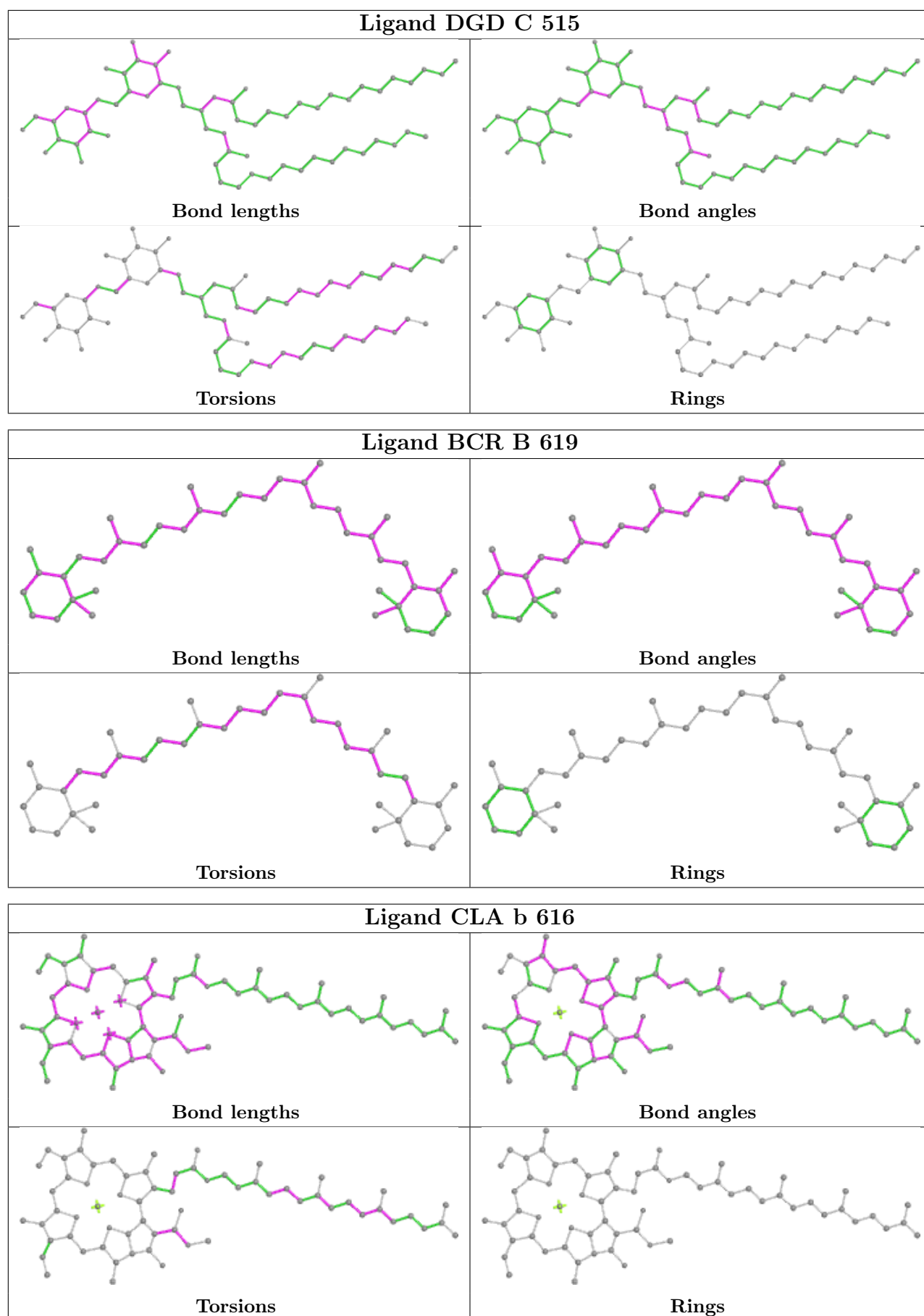


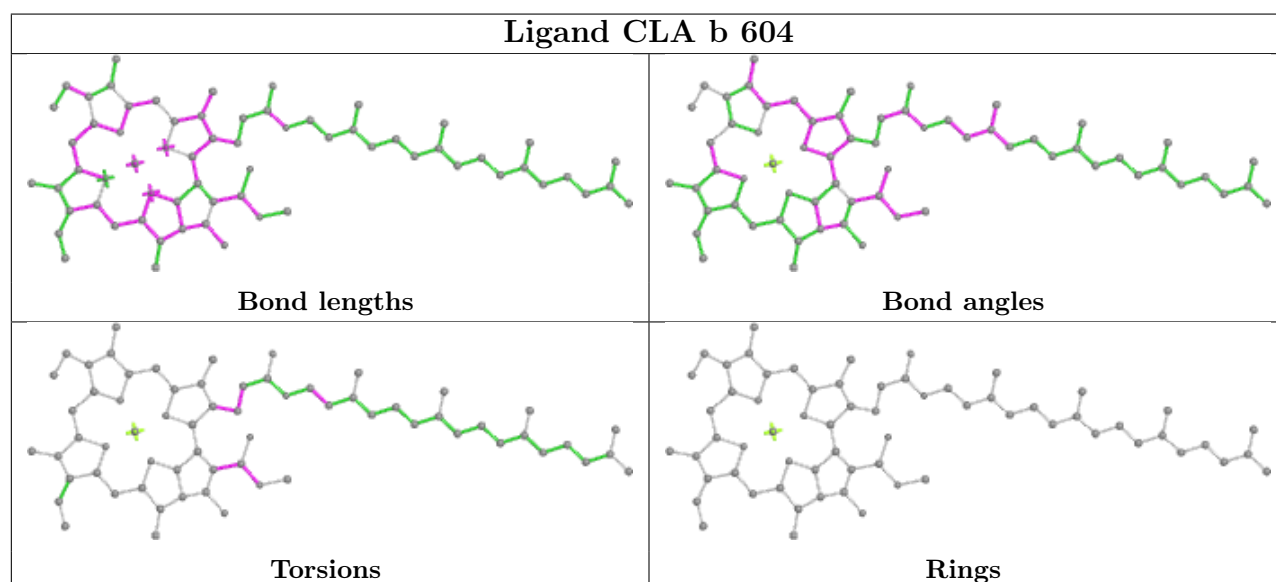
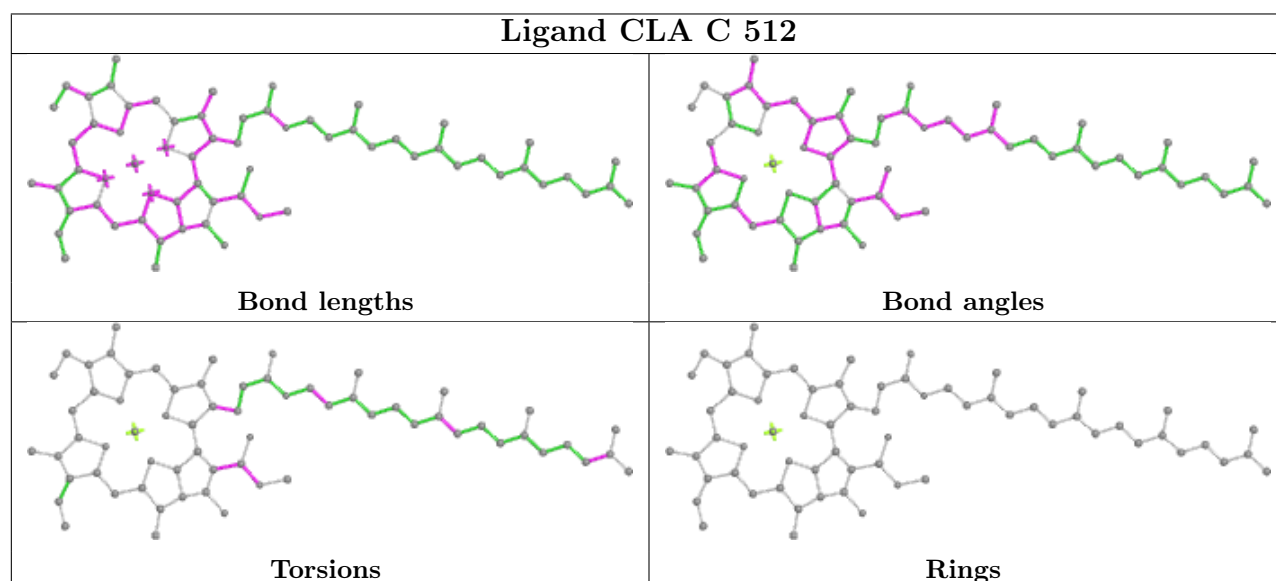
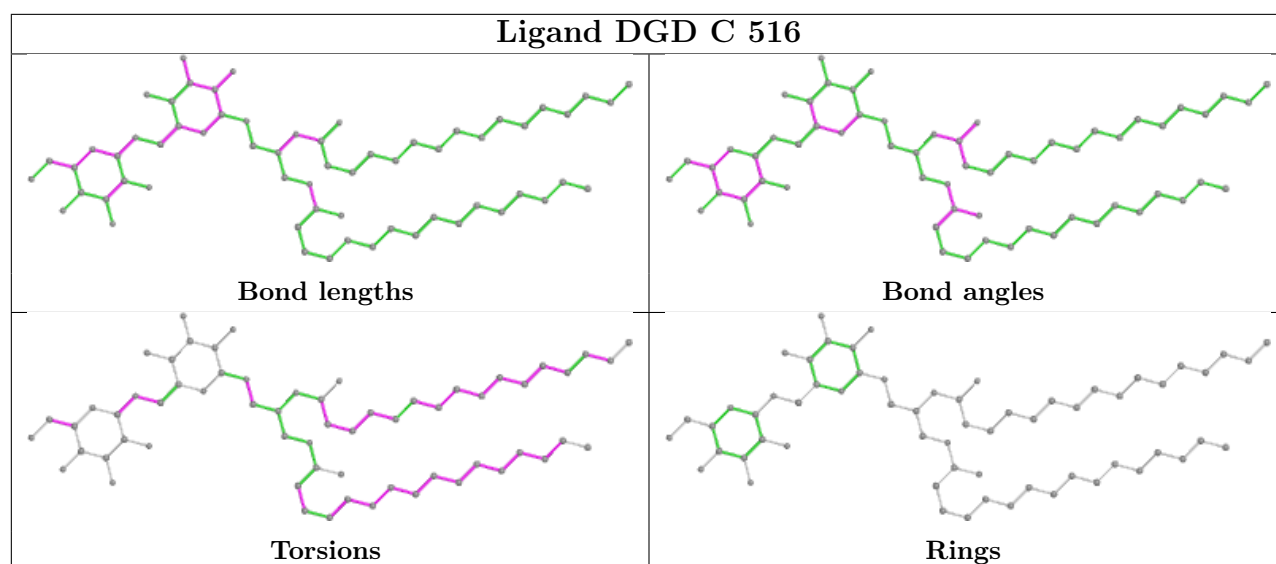


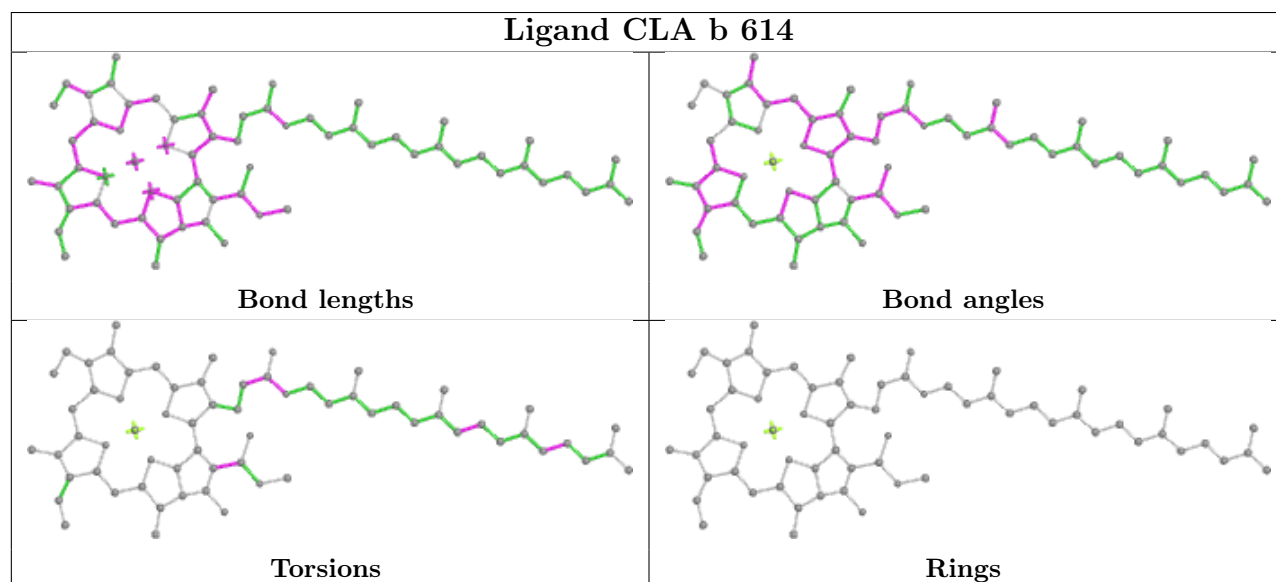
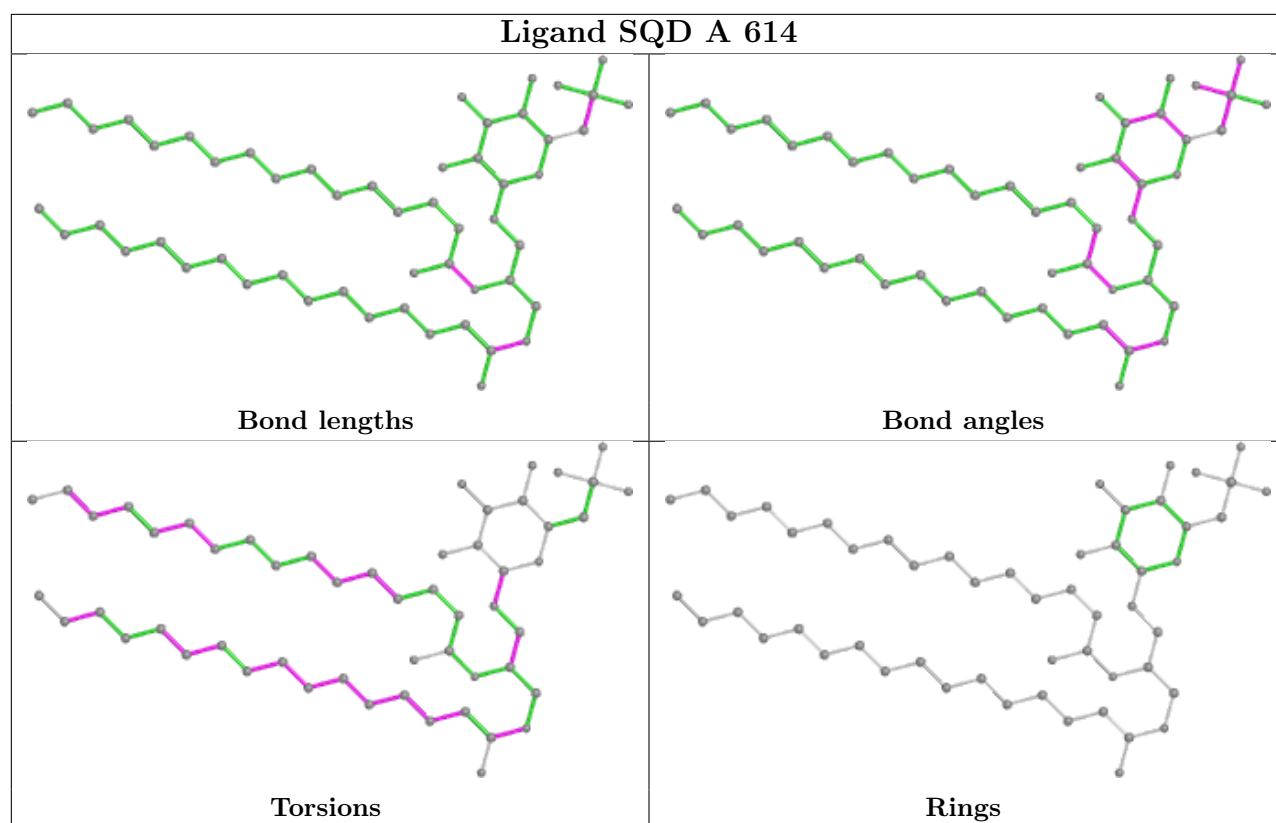


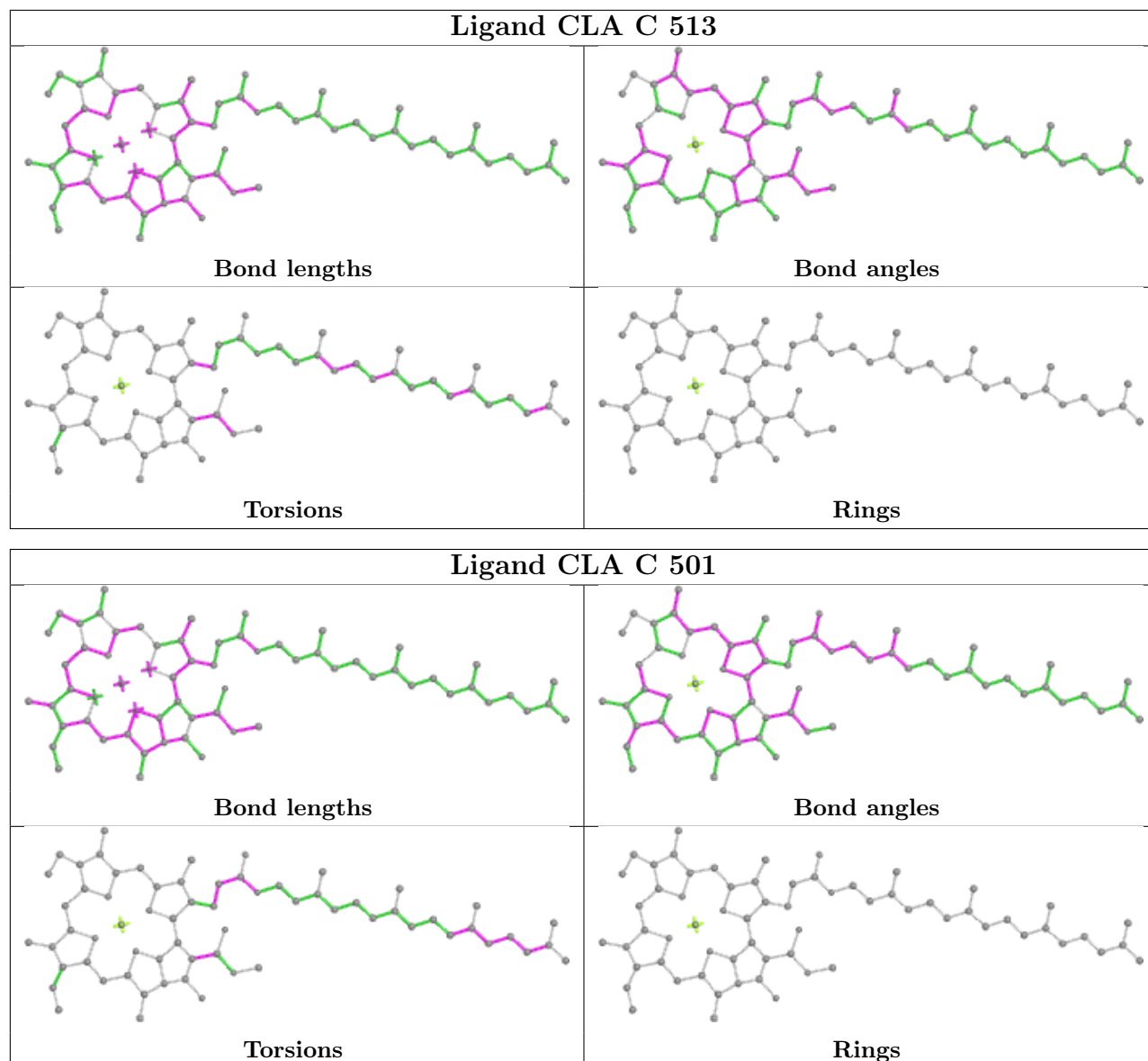


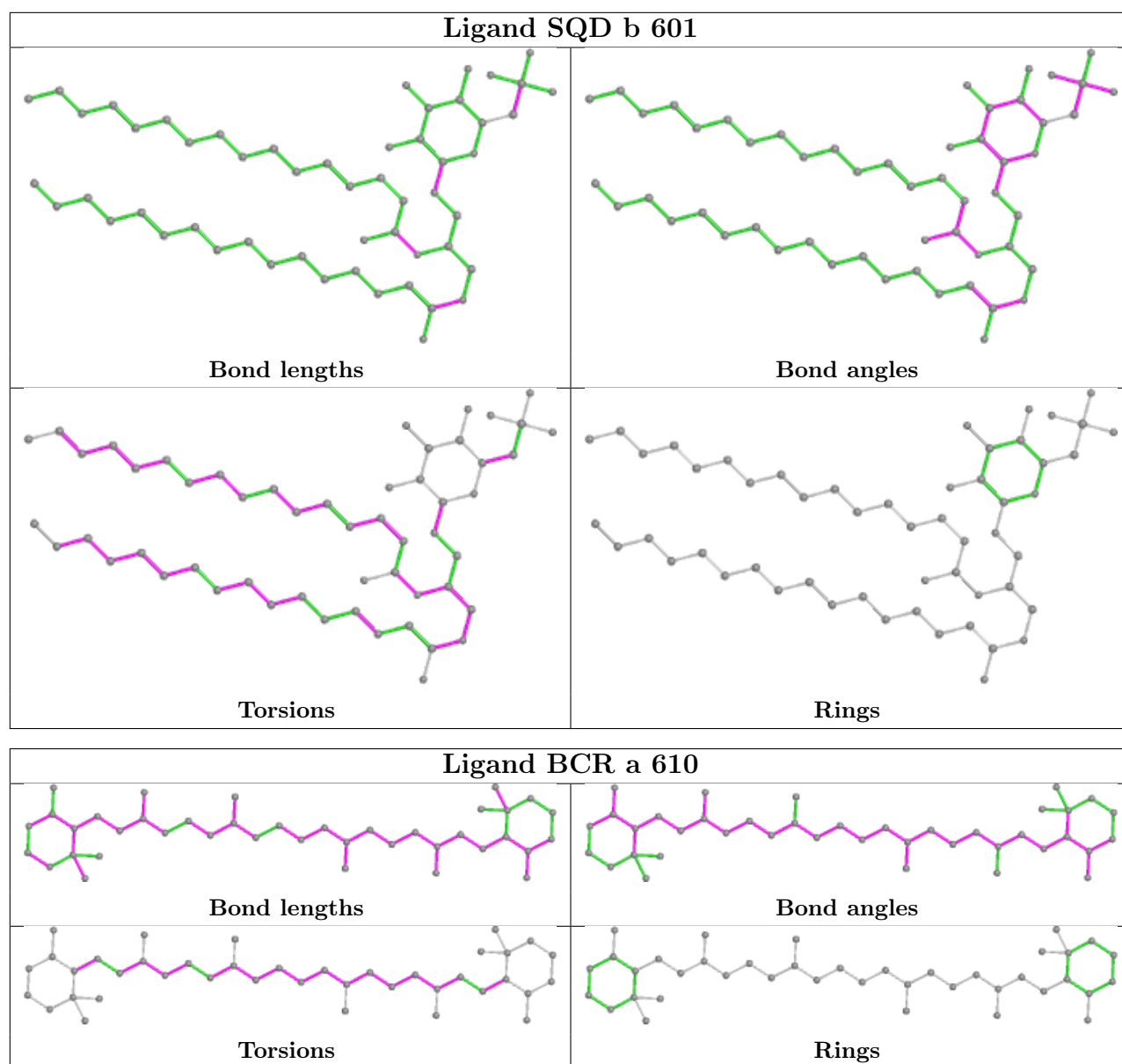












5.7 Other polymers [\(i\)](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

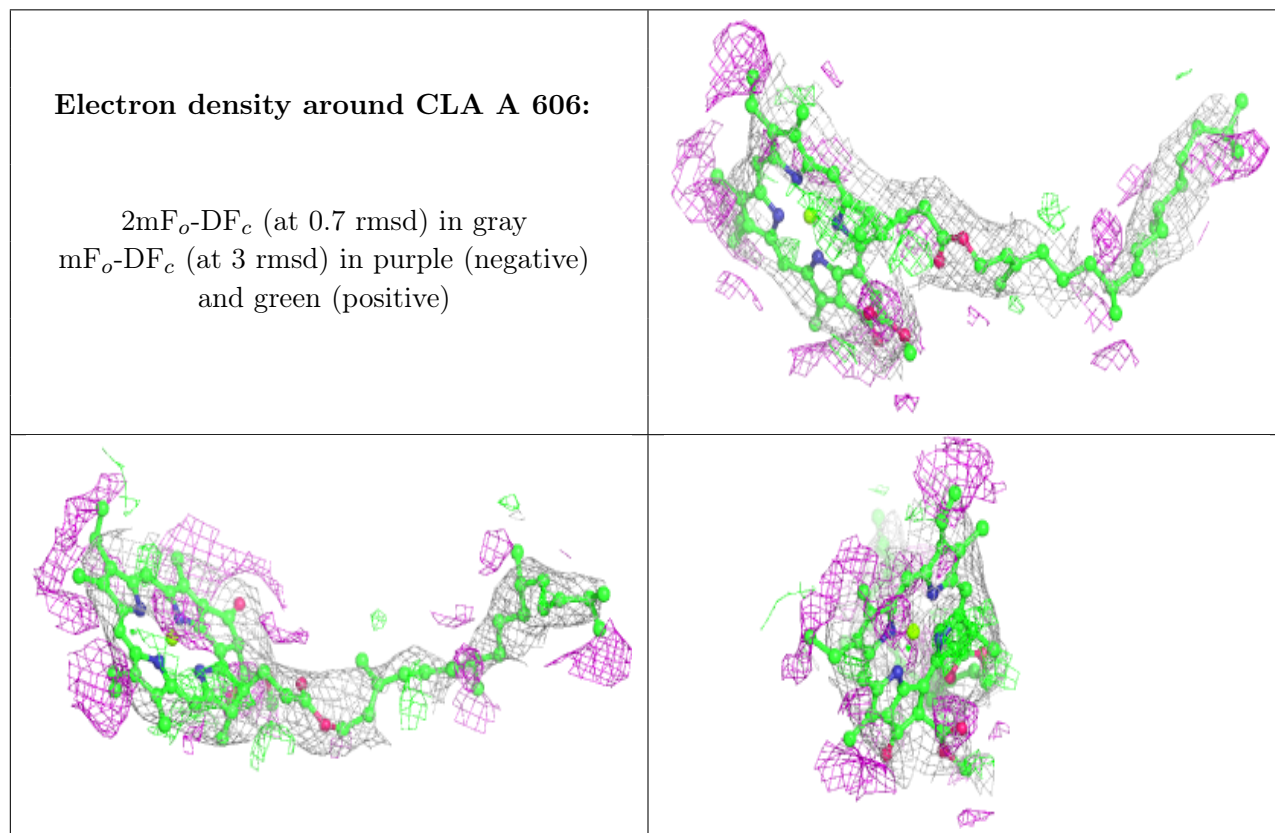
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

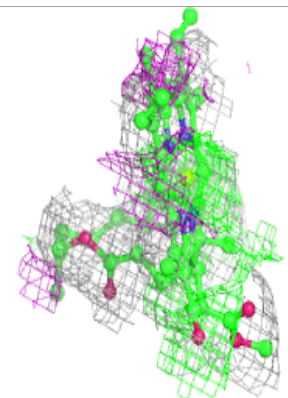
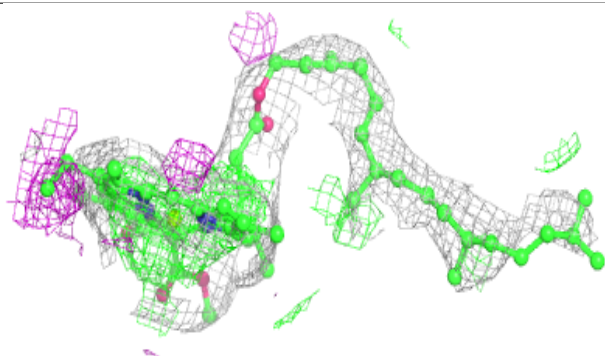
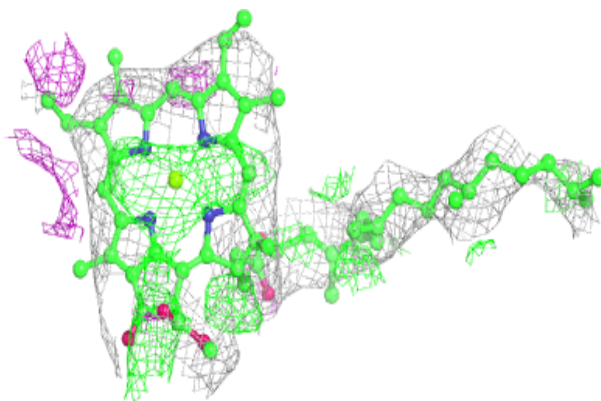
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

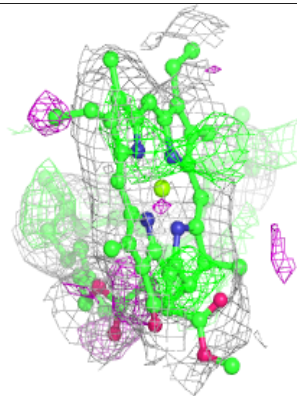
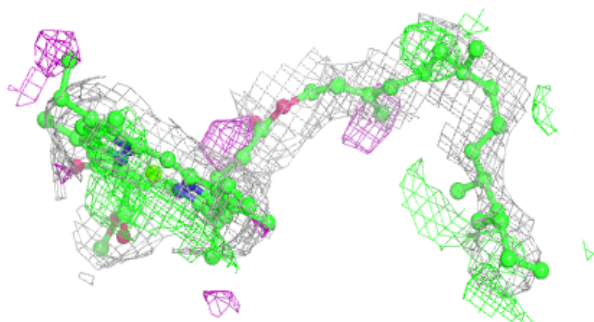
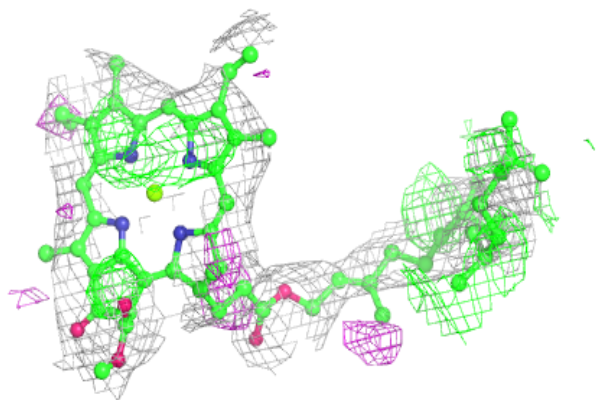


Electron density around CLA A 607:

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

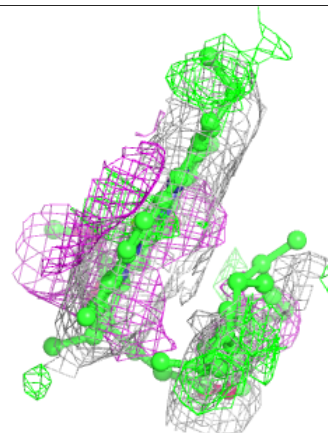
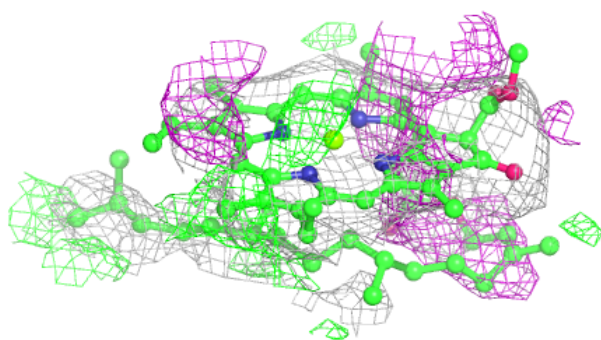
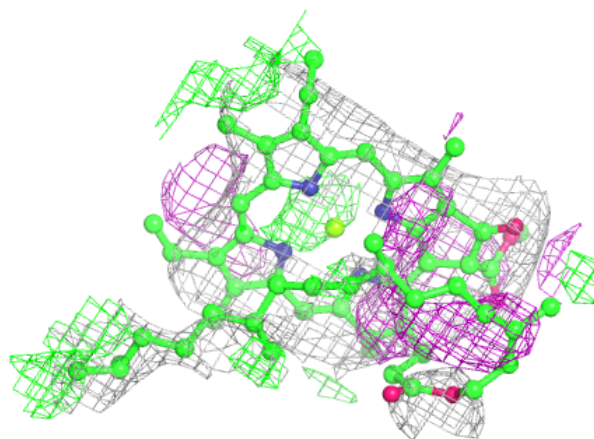
**Electron density around CLA A 609:**

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

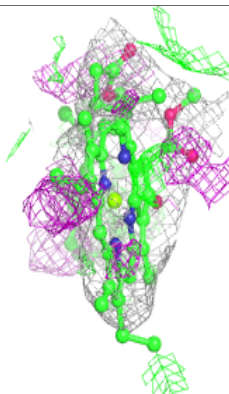
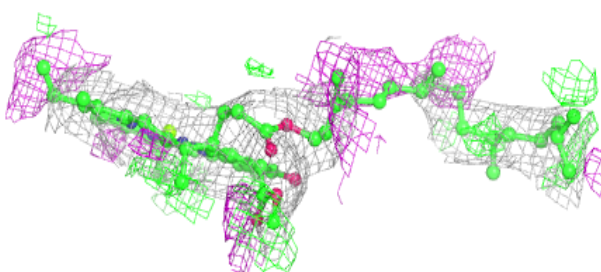
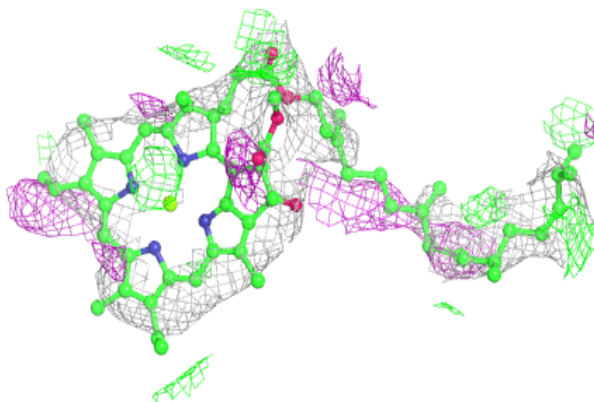


Electron density around CLA B 602:

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

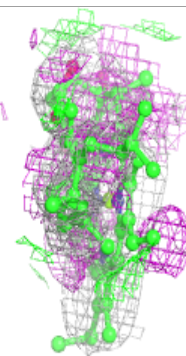
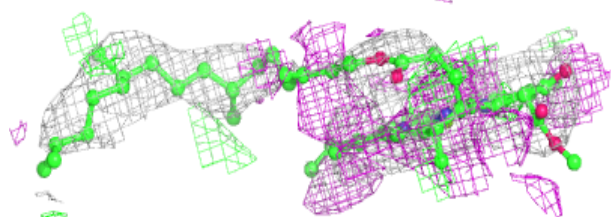
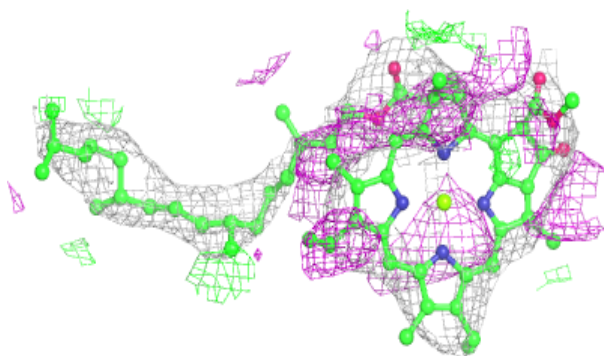
**Electron density around CLA B 603:**

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

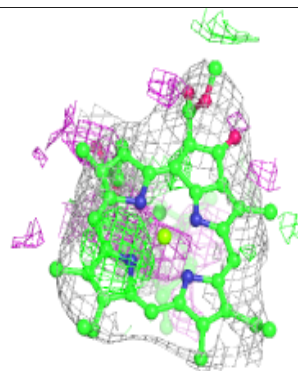
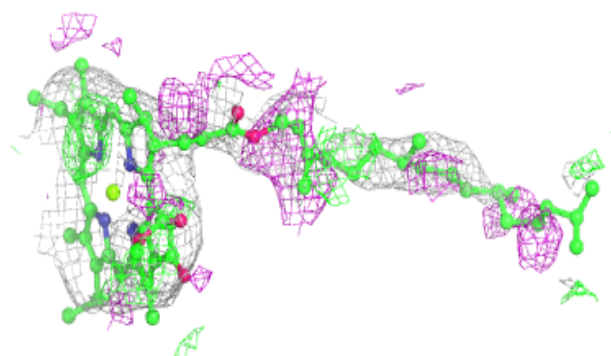
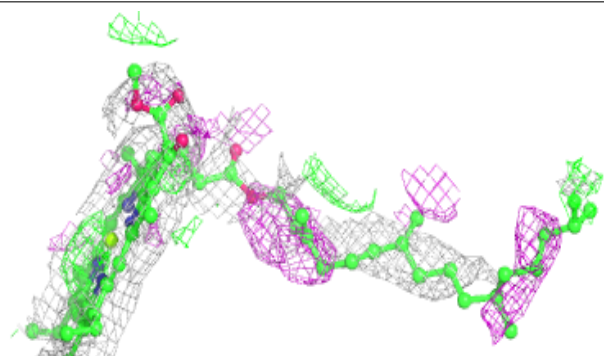


Electron density around CLA B 604:

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

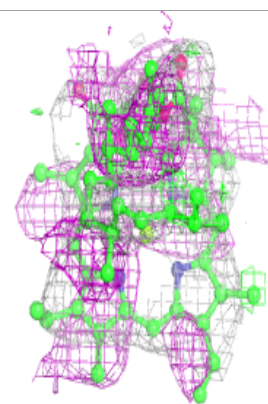
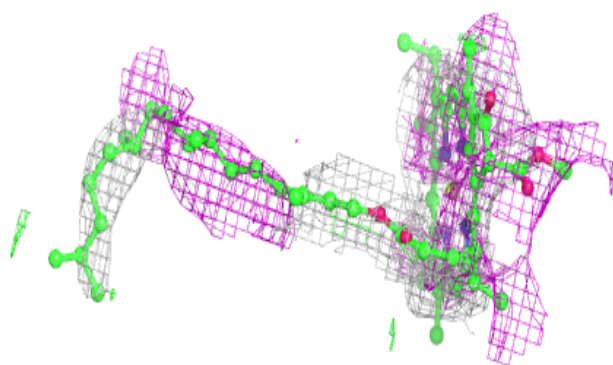
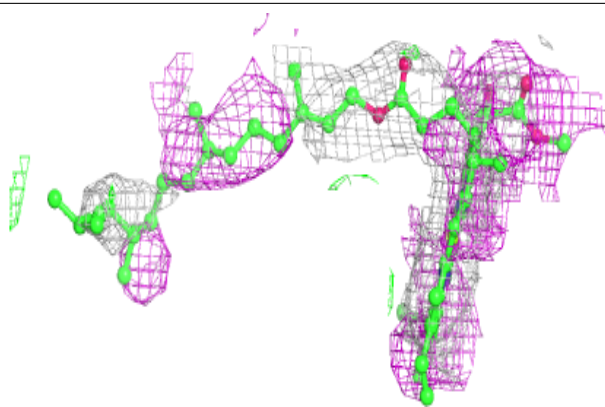
**Electron density around CLA B 605:**

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

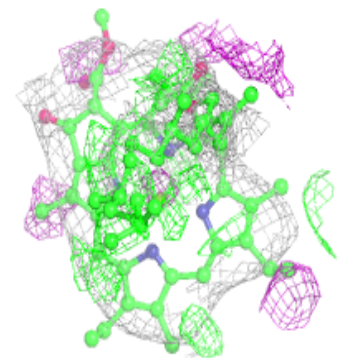
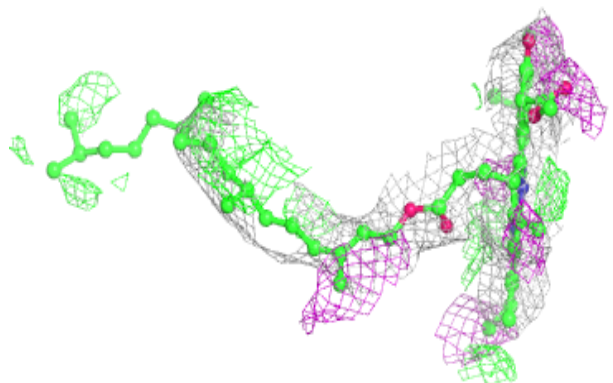
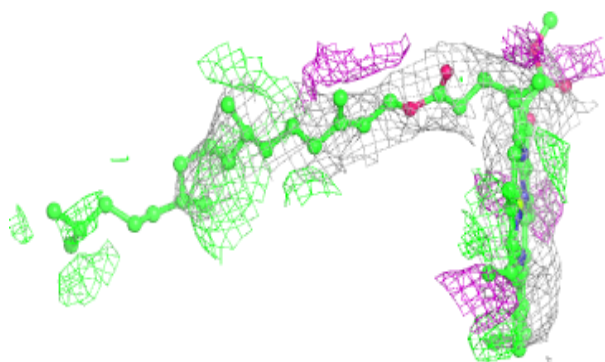


Electron density around CLA B 606:

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

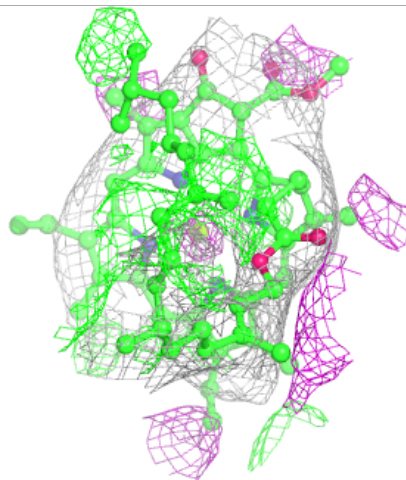
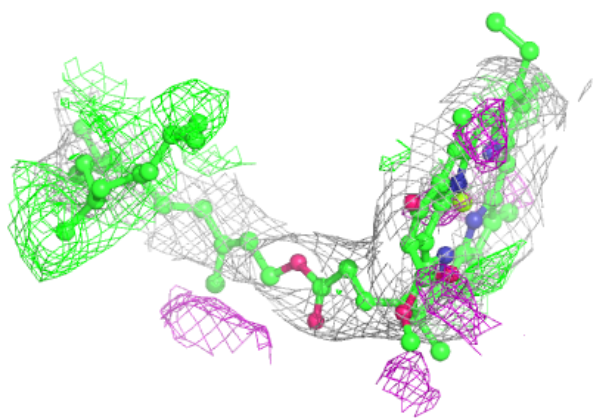
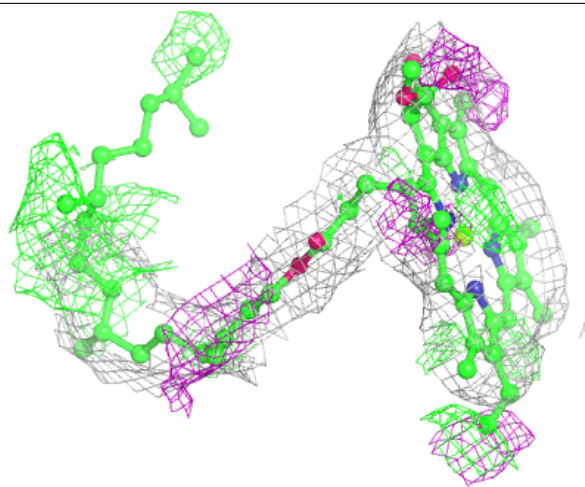
**Electron density around CLA B 607 (A):**

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



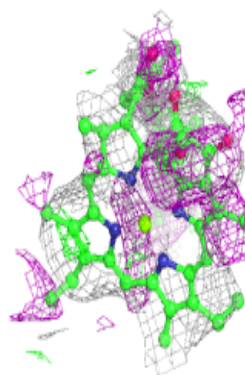
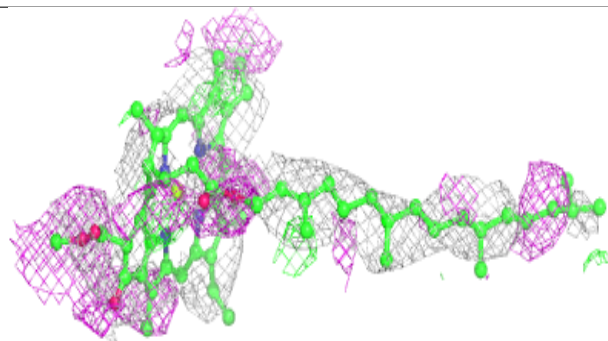
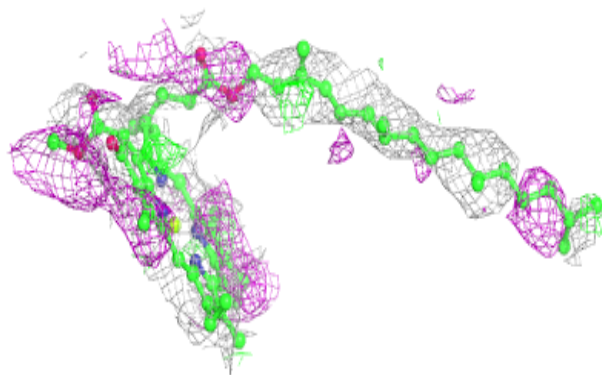
Electron density around CLA B 607 (B):

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

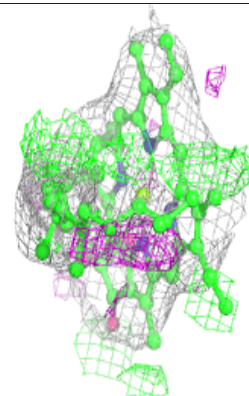
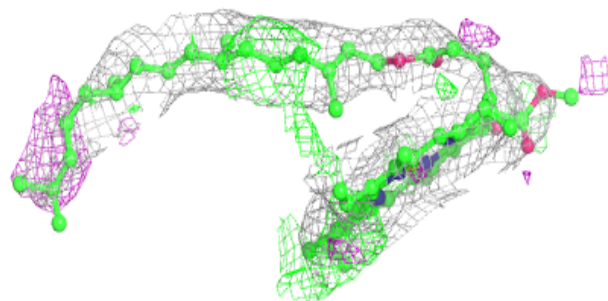
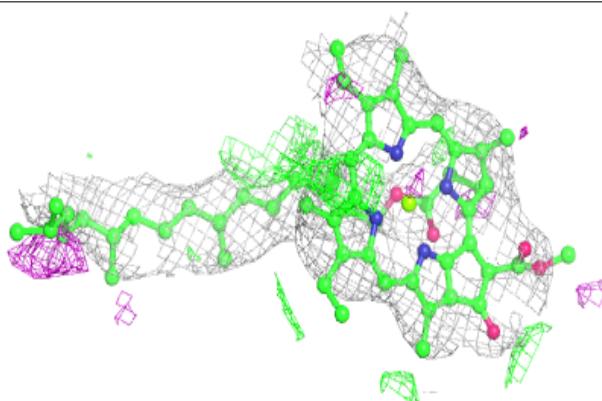


Electron density around CLA B 608:

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

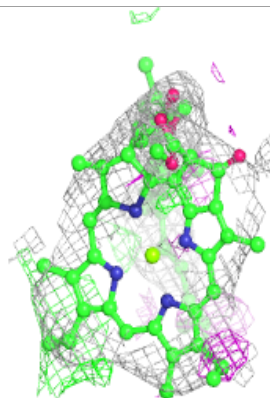
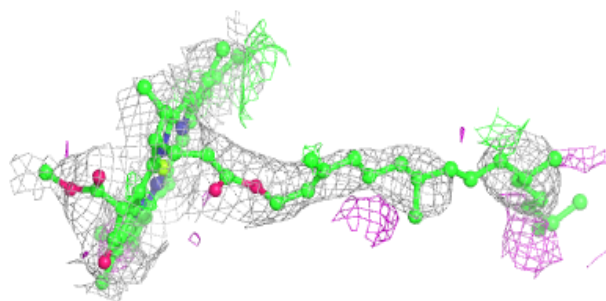
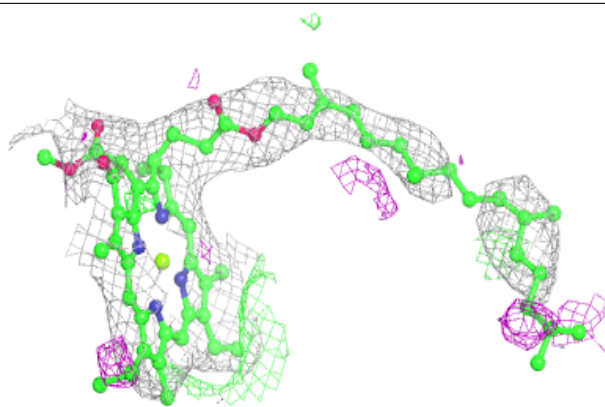
**Electron density around CLA B 609:**

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

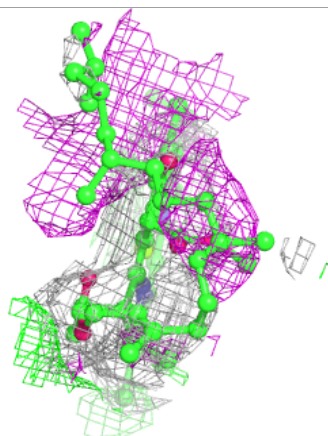
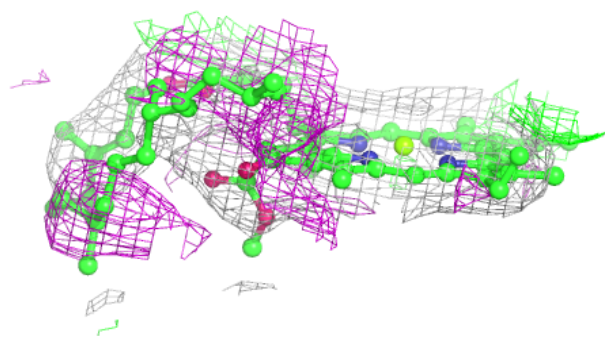
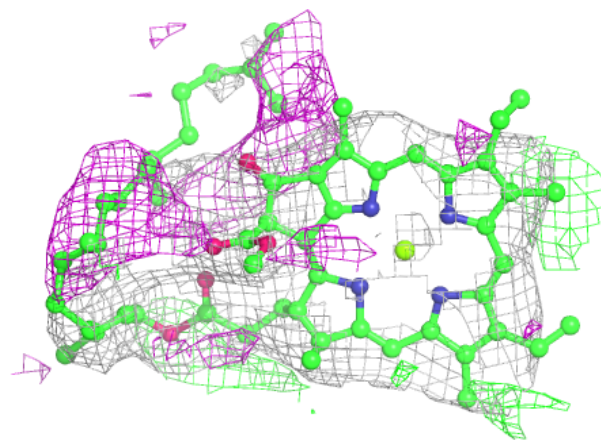


Electron density around CLA B 610:

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

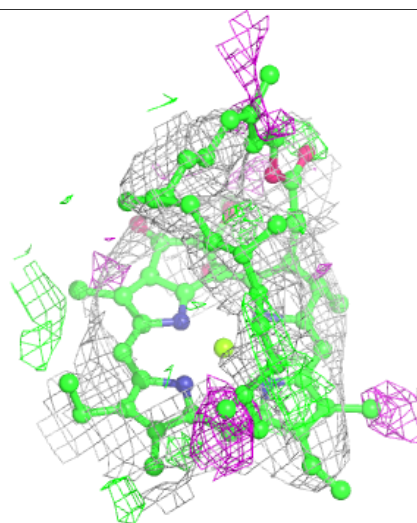
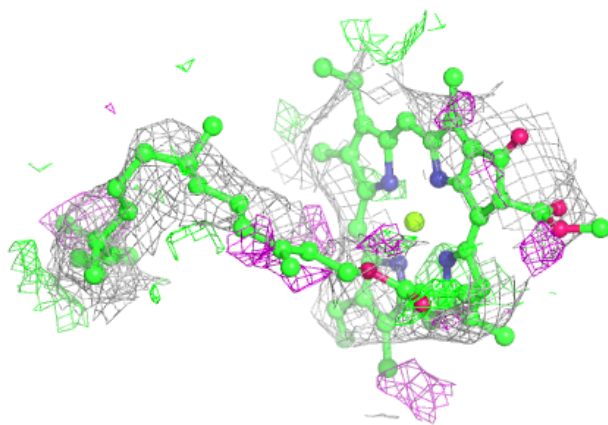
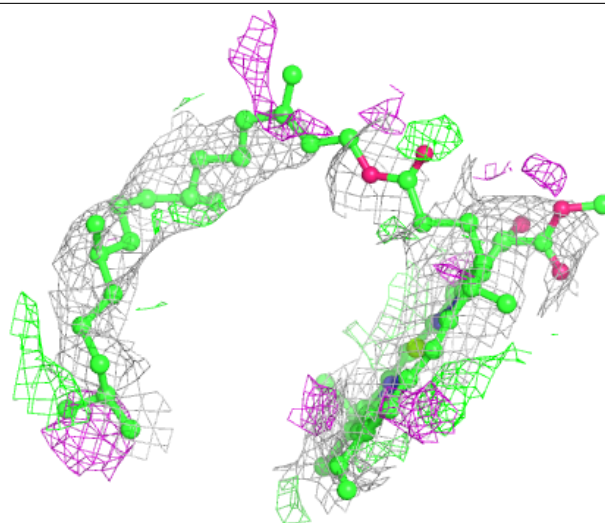
**Electron density around CLA B 611:**

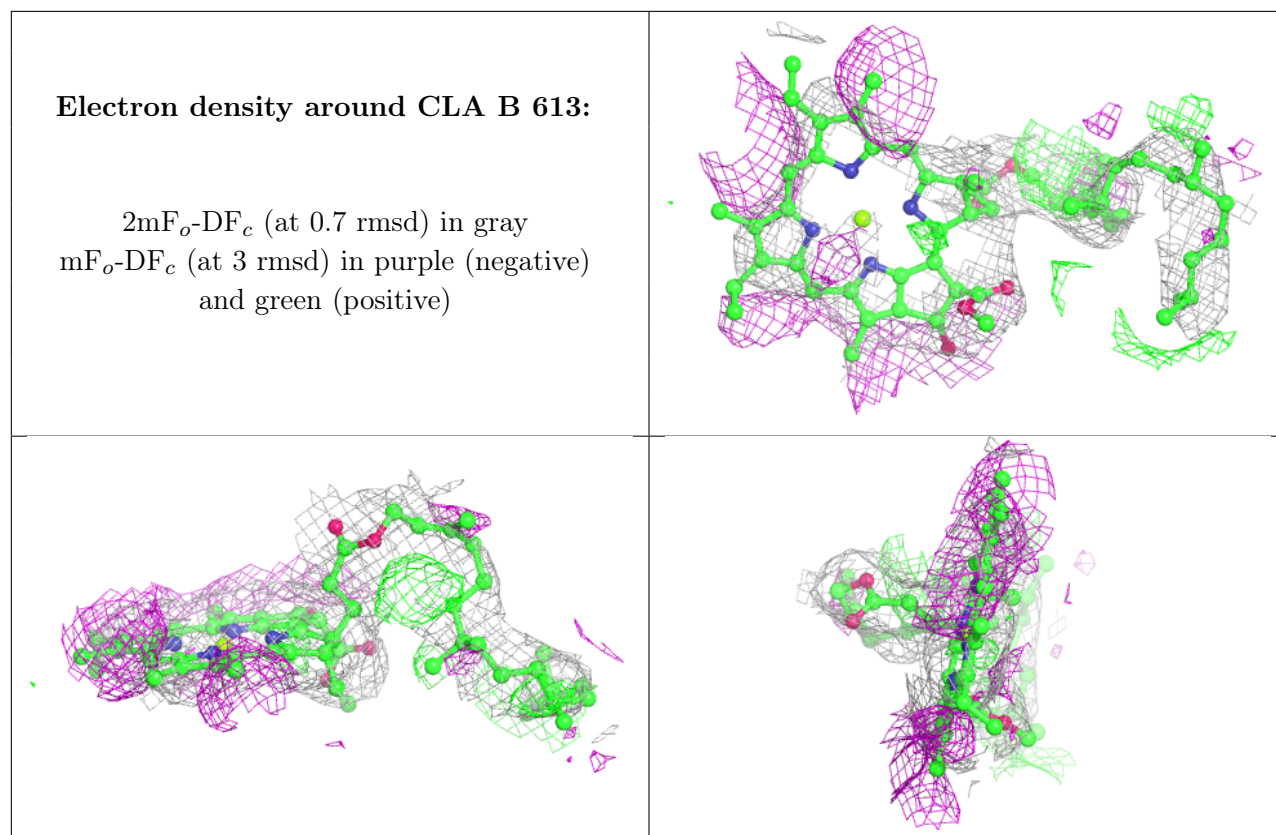
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 612:

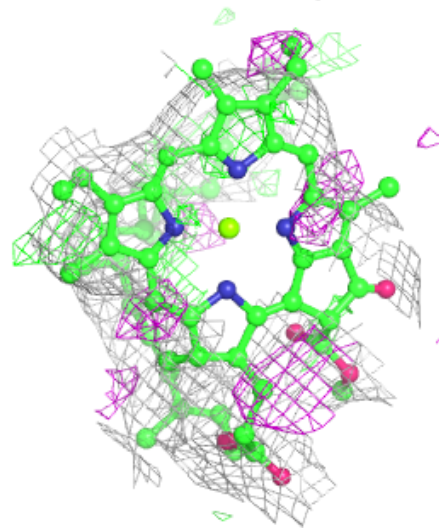
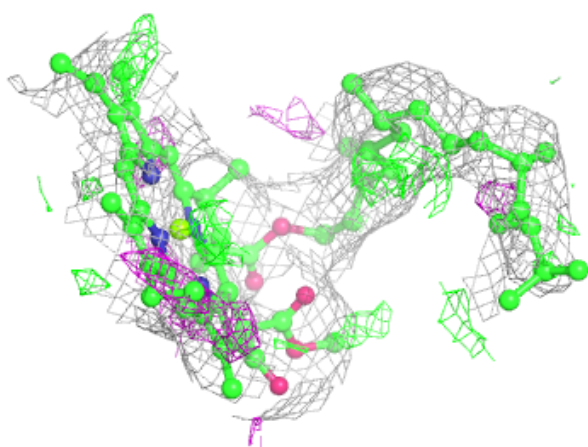
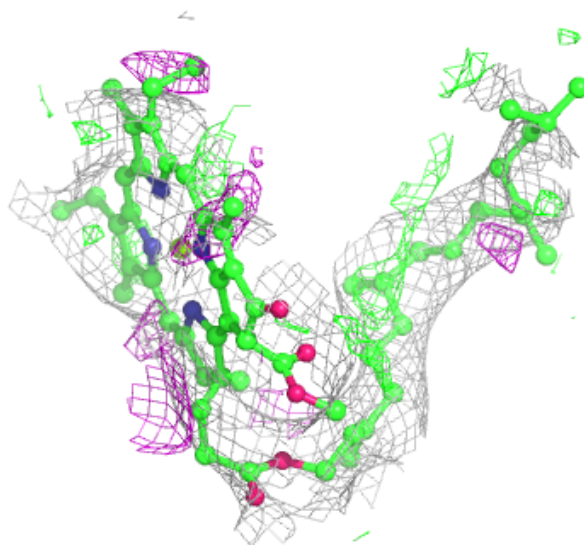
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





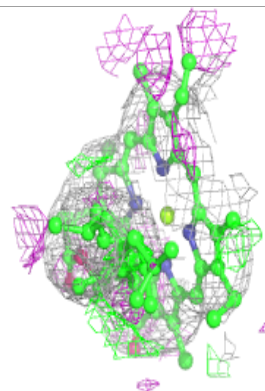
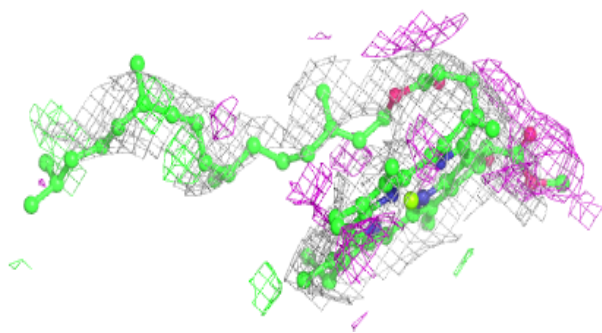
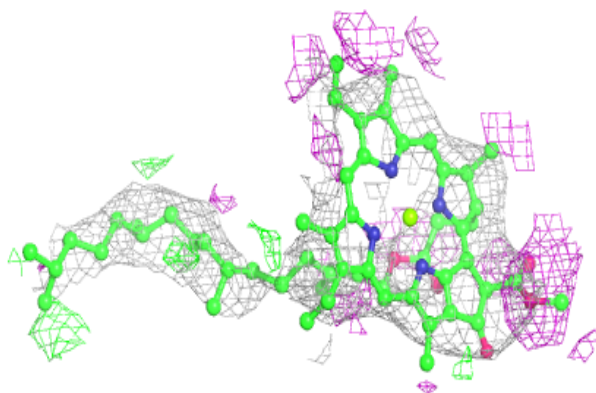
Electron density around CLA B 614:

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

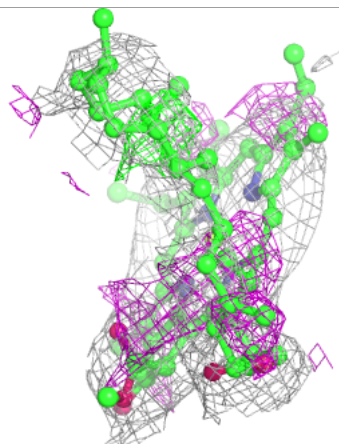
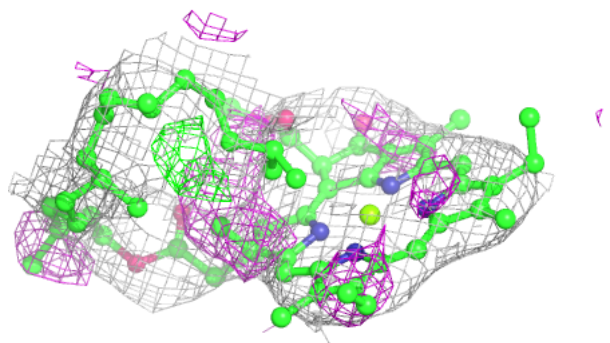
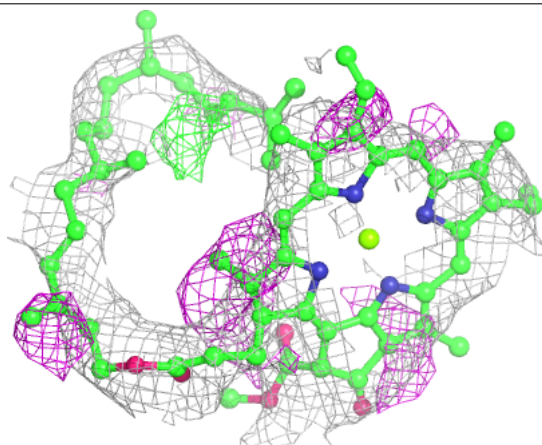


Electron density around CLA B 615:

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

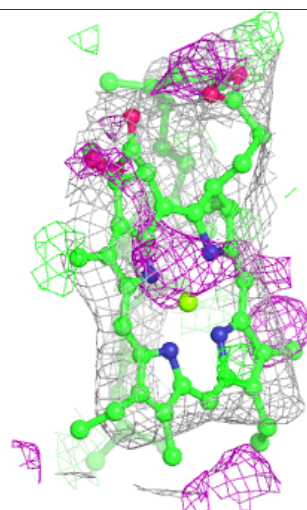
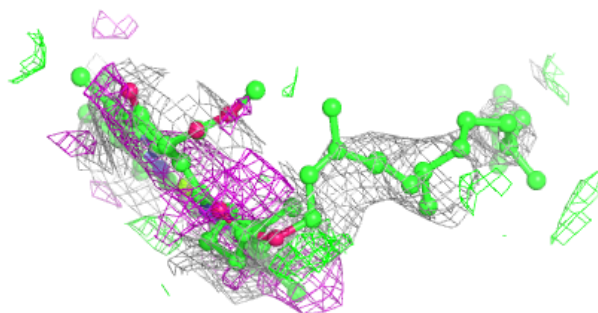
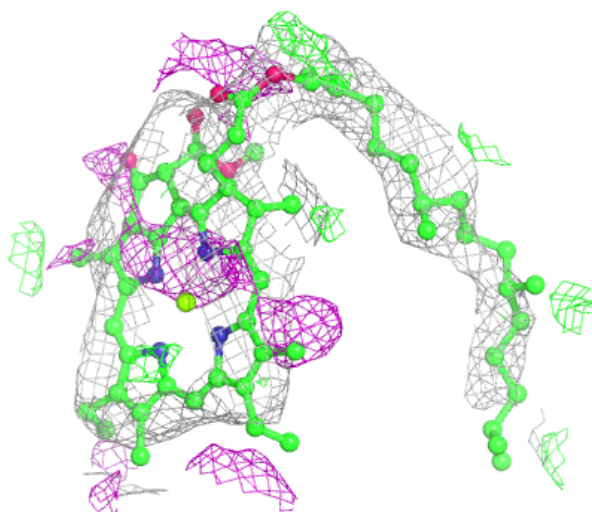
**Electron density around CLA B 616:**

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



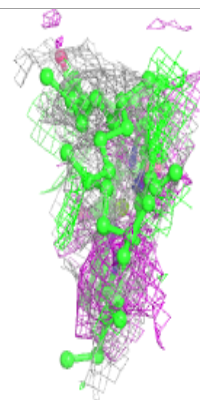
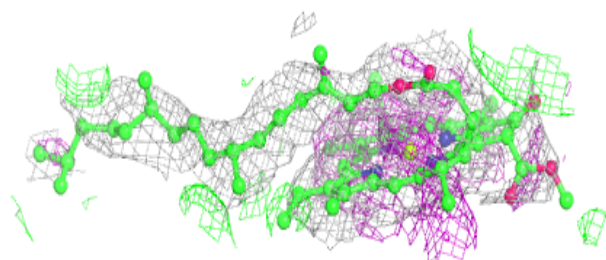
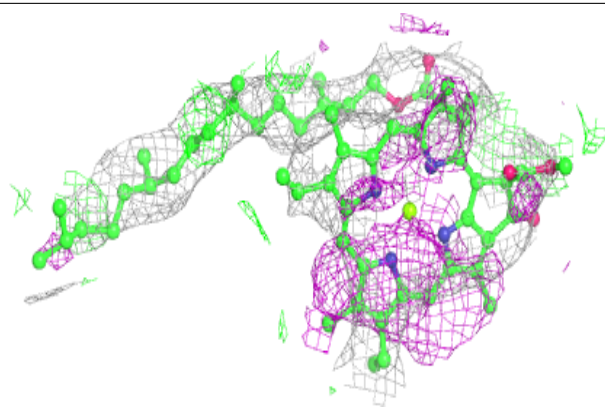
Electron density around CLA B 617:

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

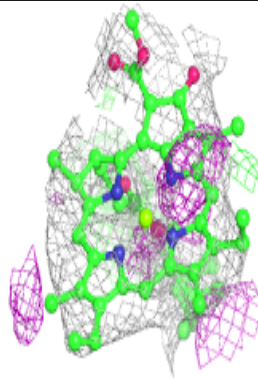
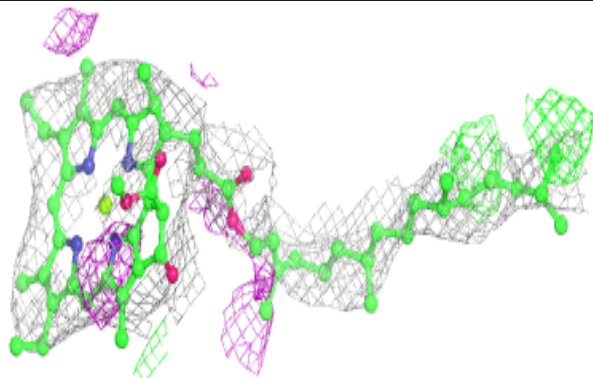
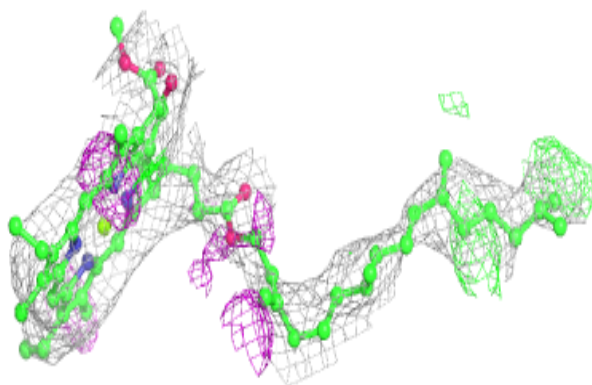


Electron density around CLA C 501:

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

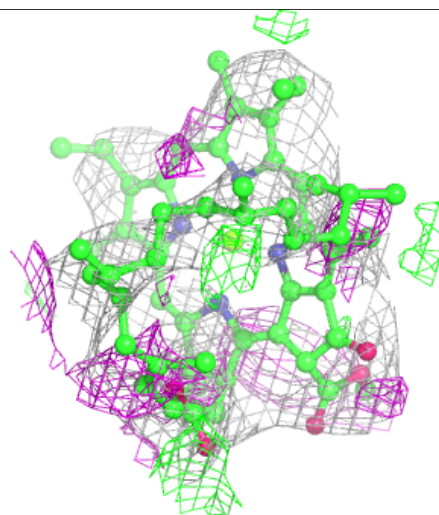
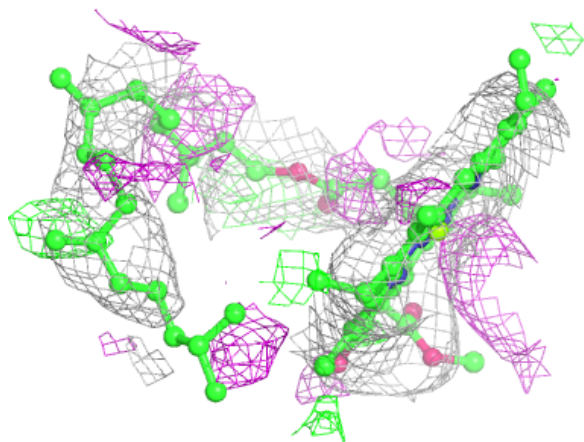
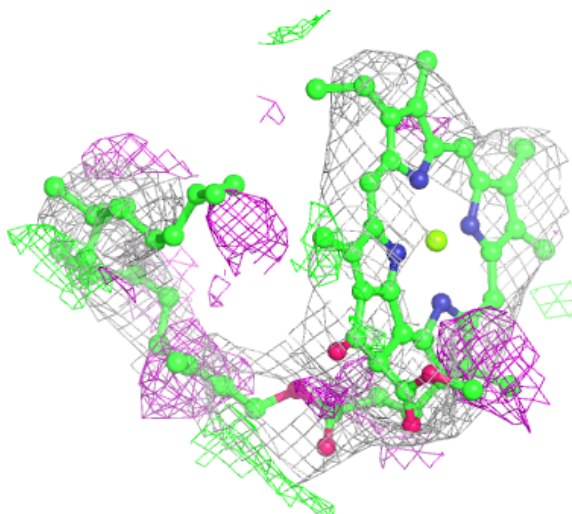
**Electron density around CLA C 502:**

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



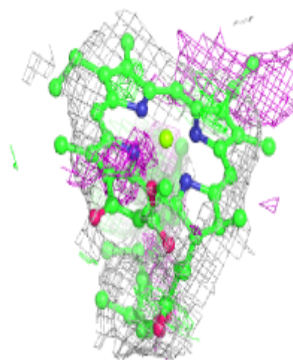
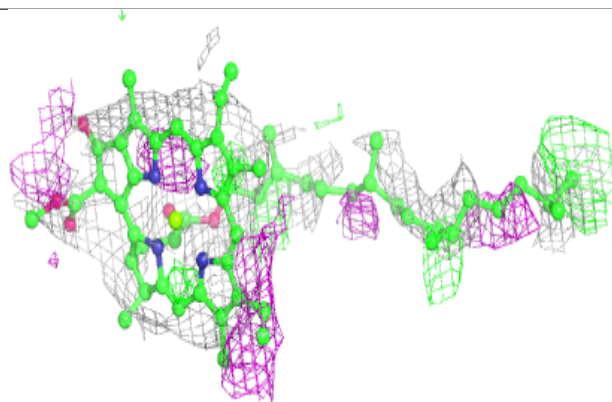
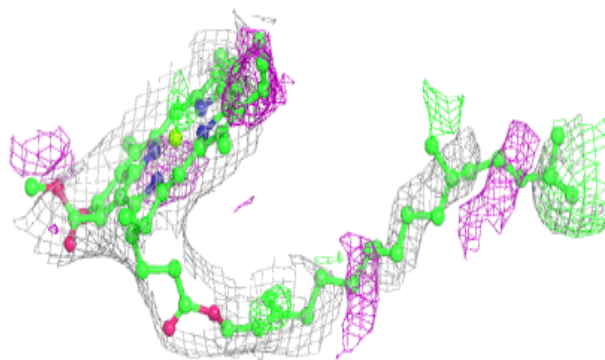
Electron density around CLA C 503:

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

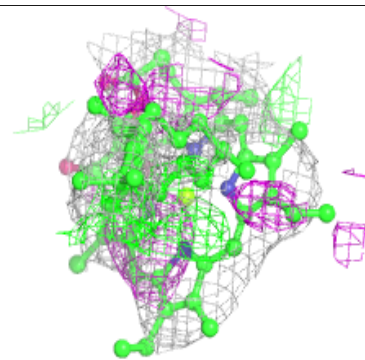
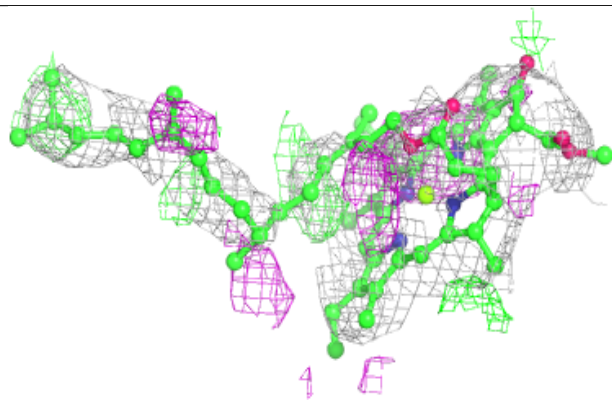
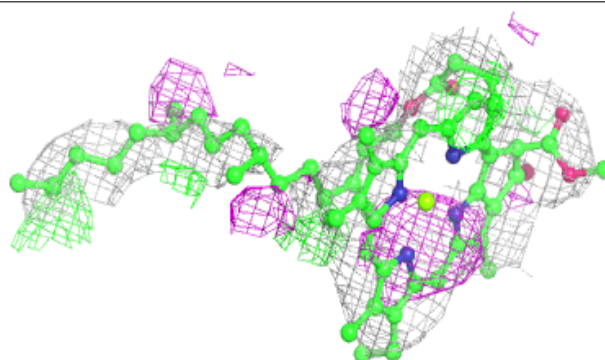


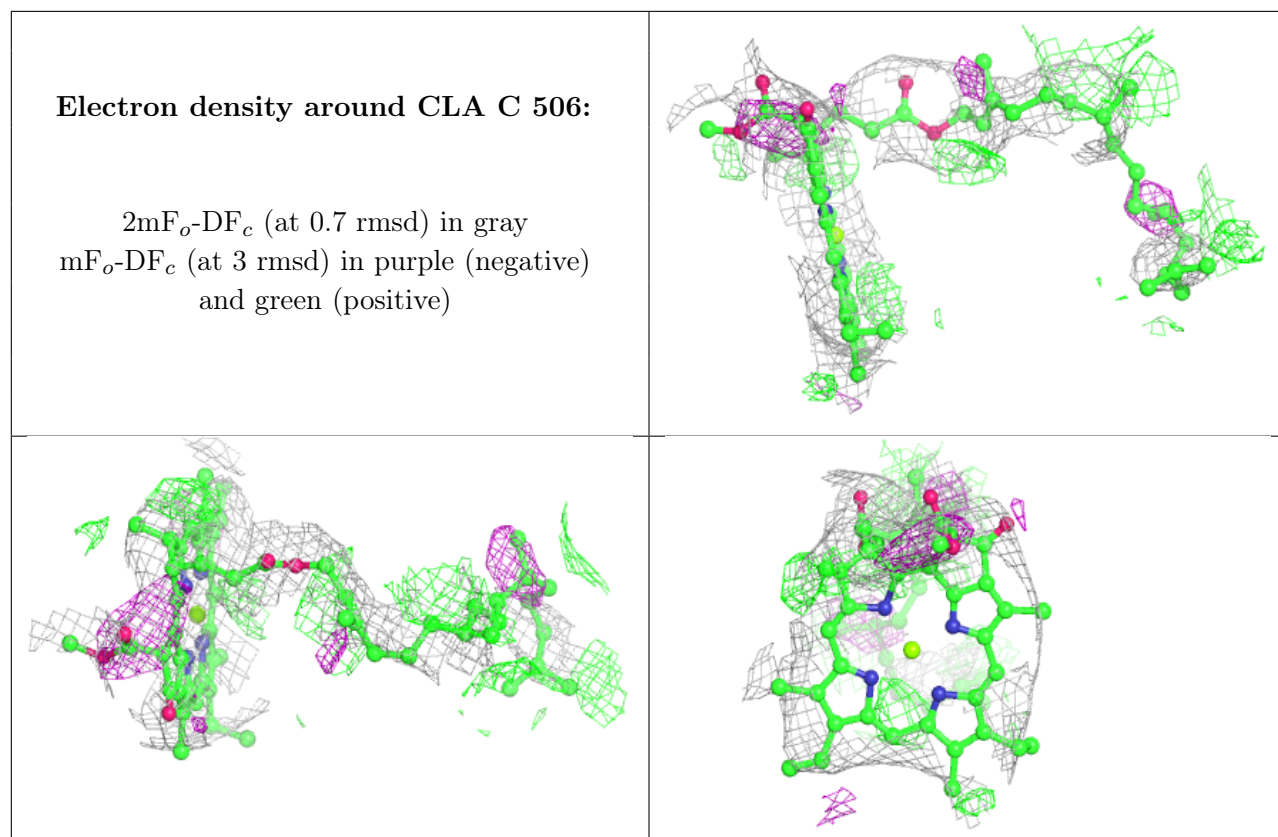
Electron density around CLA C 504:

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

**Electron density around CLA C 505:**

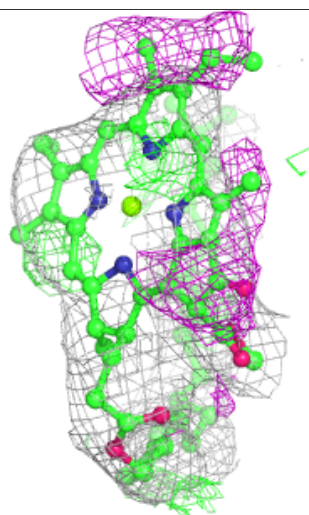
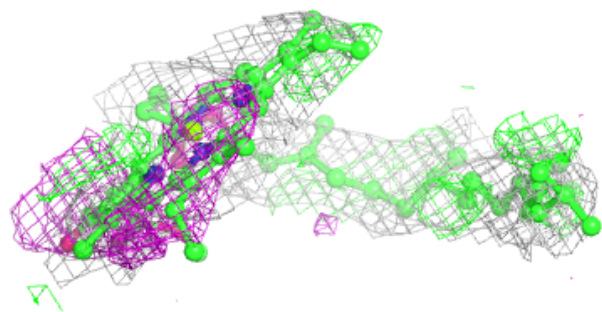
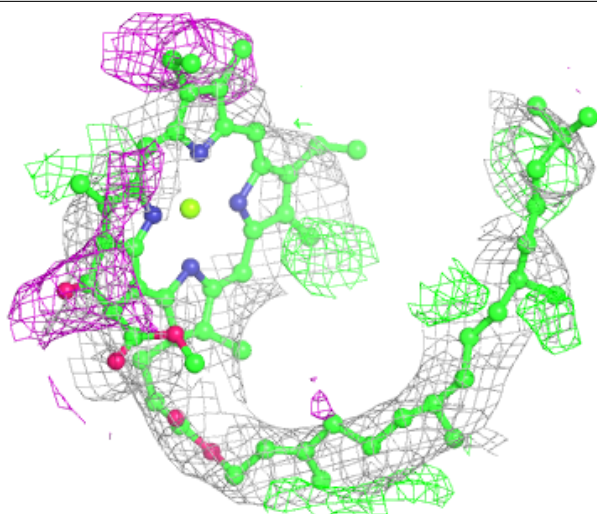
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

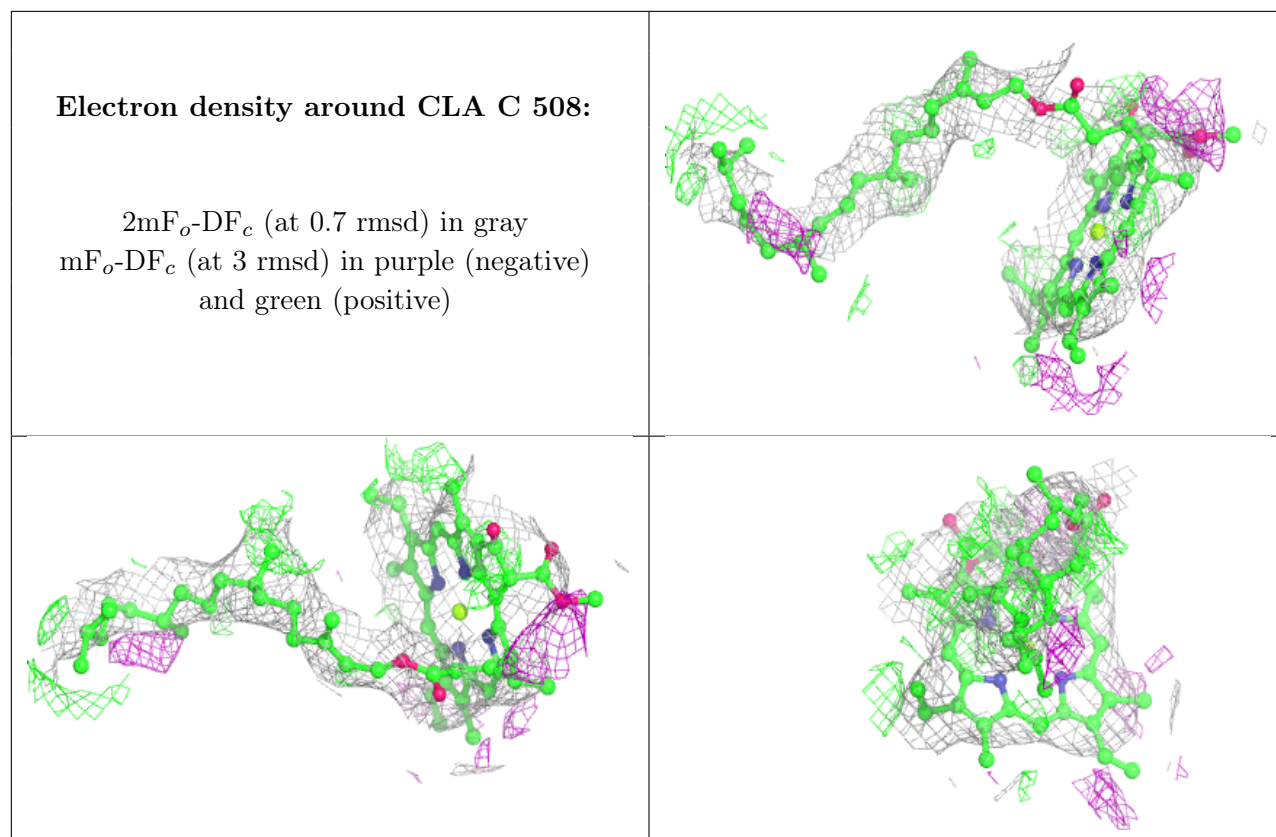




Electron density around CLA C 507:

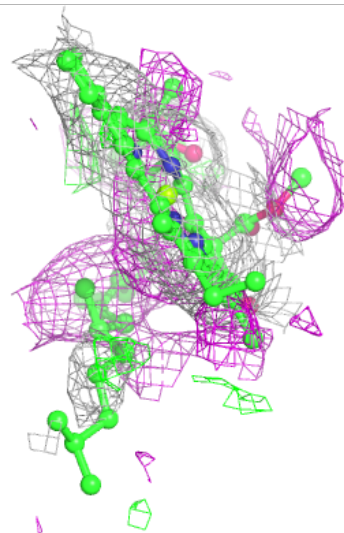
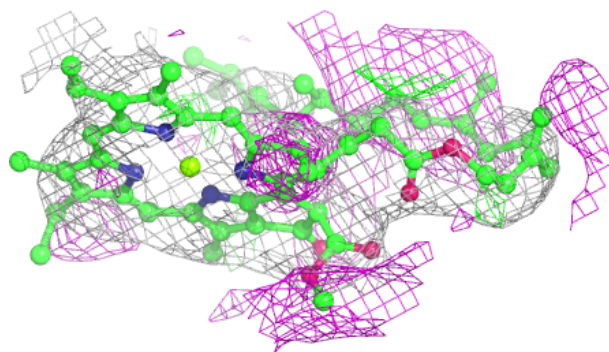
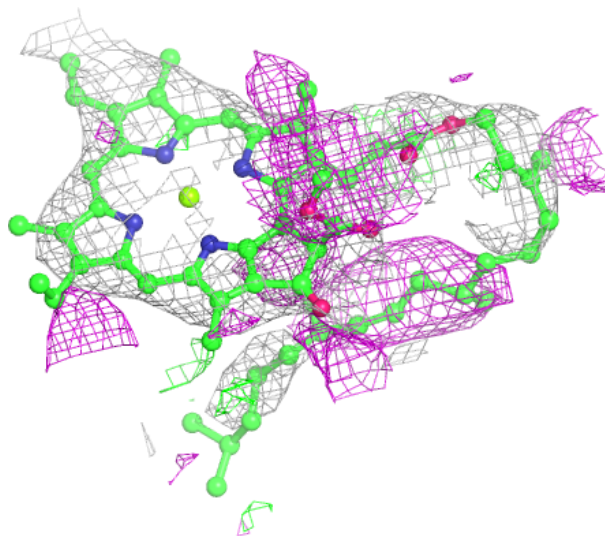
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





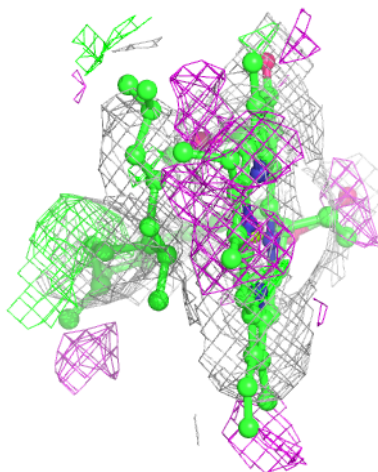
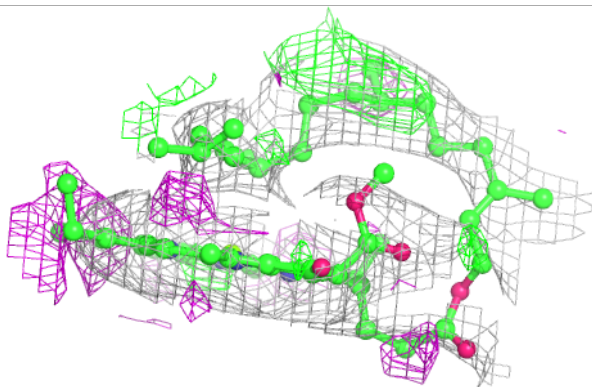
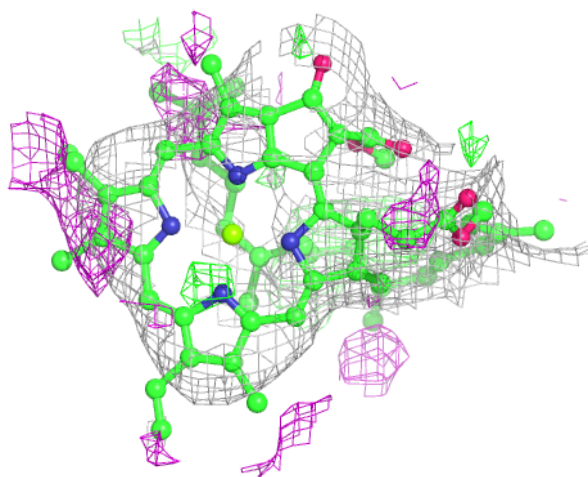
Electron density around CLA C 509:

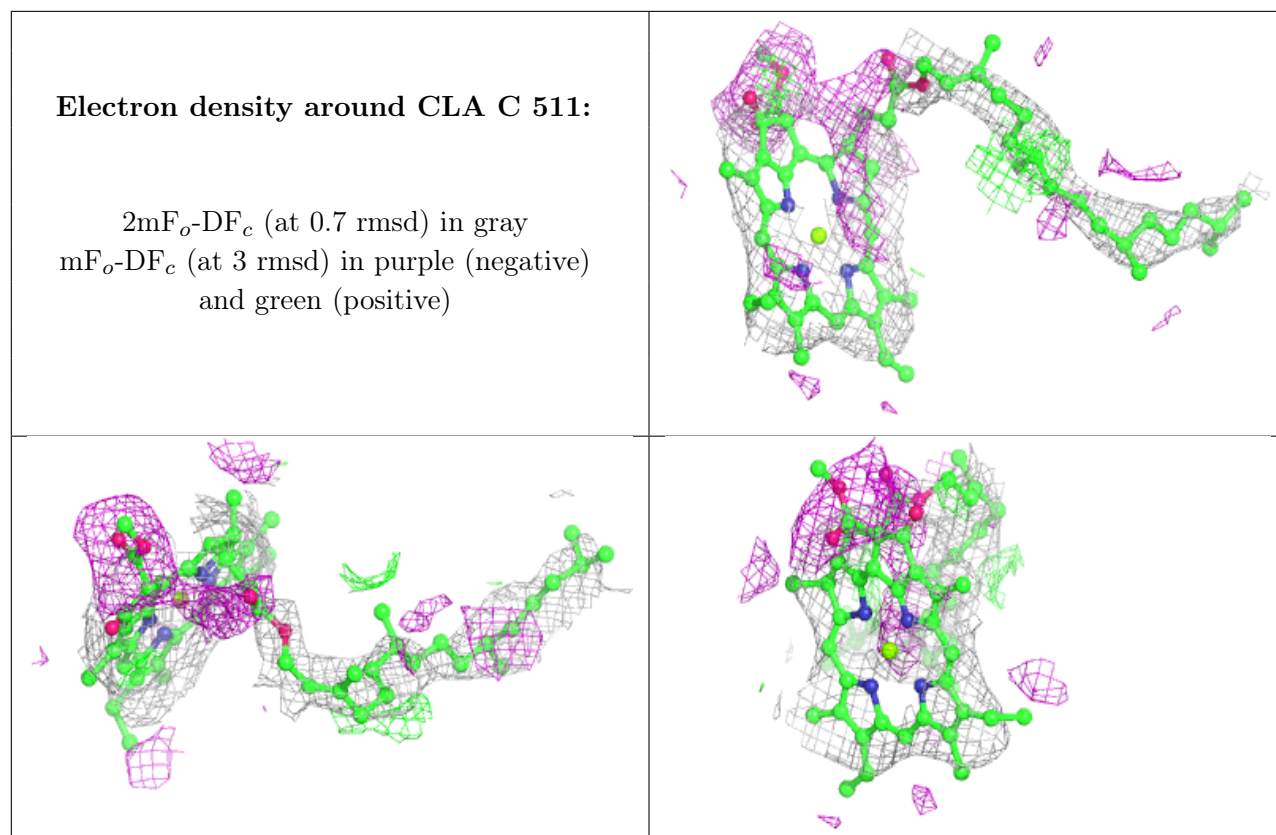
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 510:

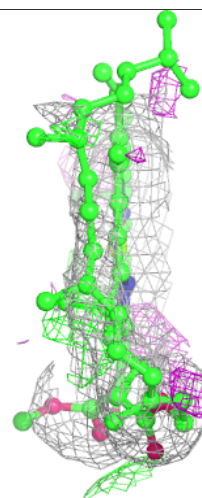
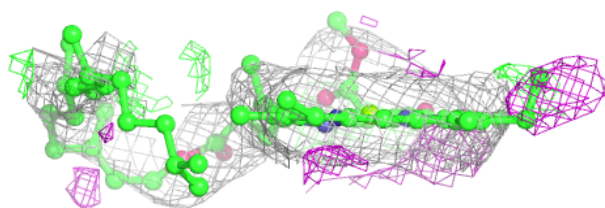
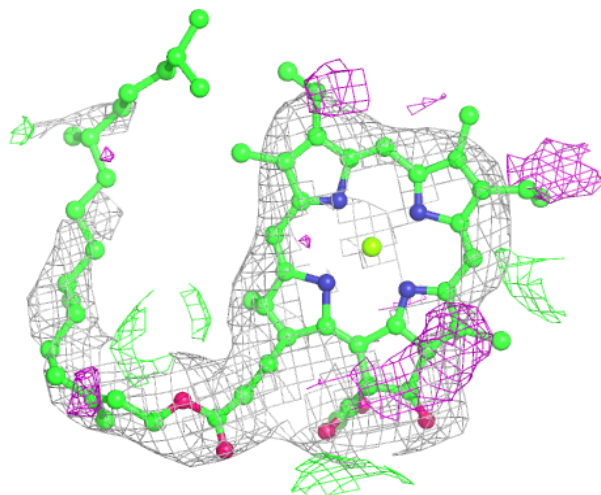
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





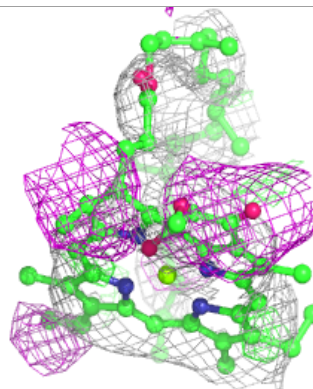
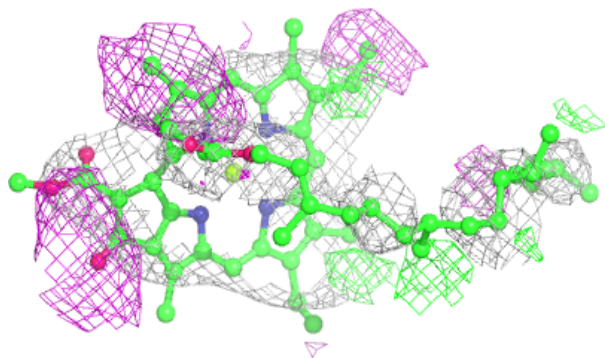
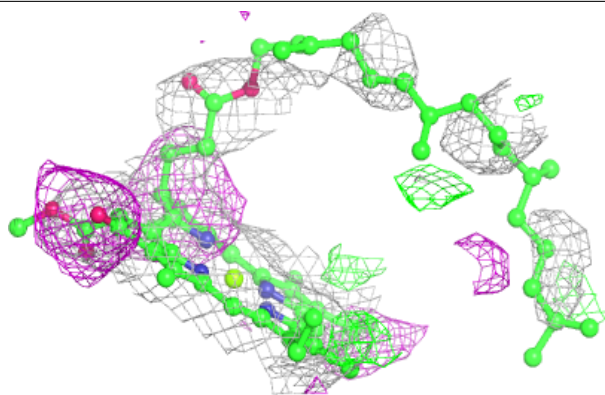
Electron density around CLA C 512:

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

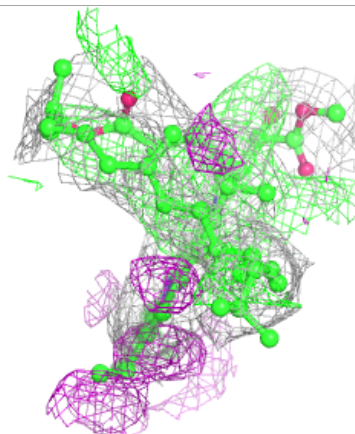
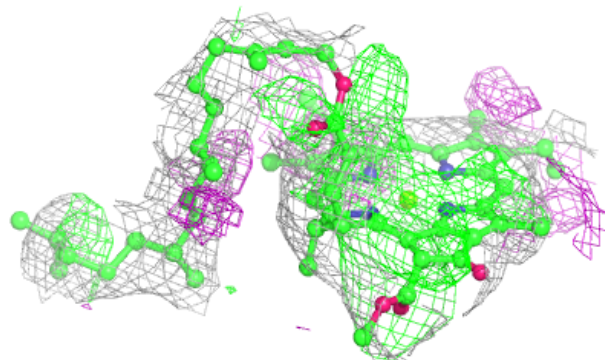
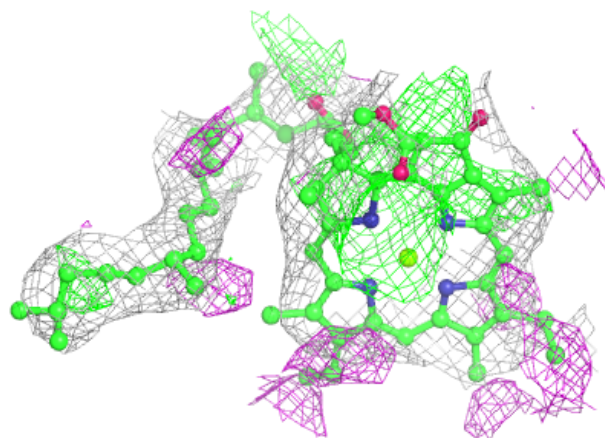


Electron density around CLA C 513:

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

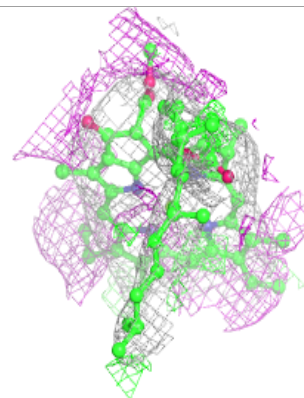
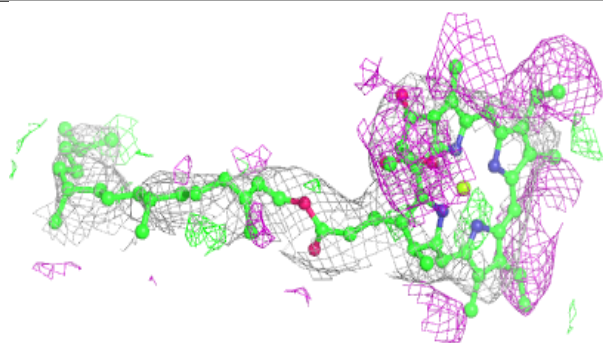
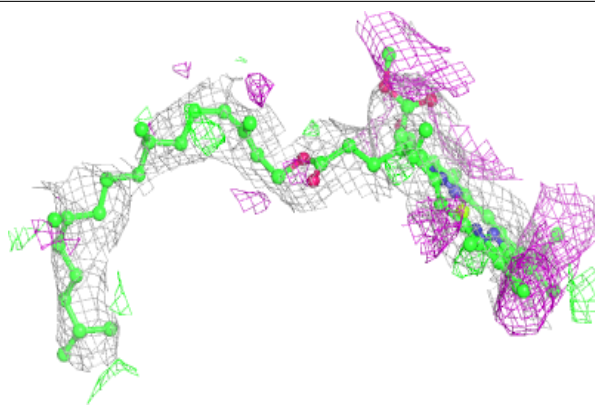
**Electron density around CLA D 402:**

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

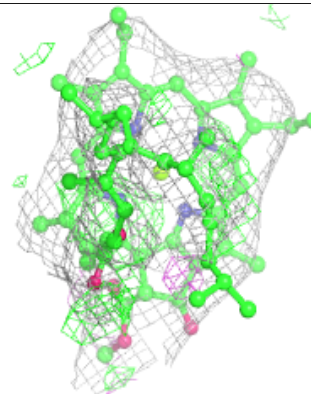
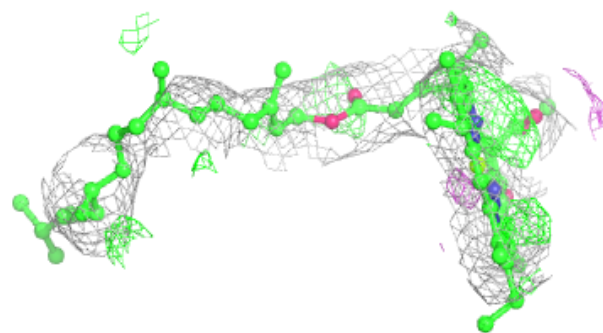
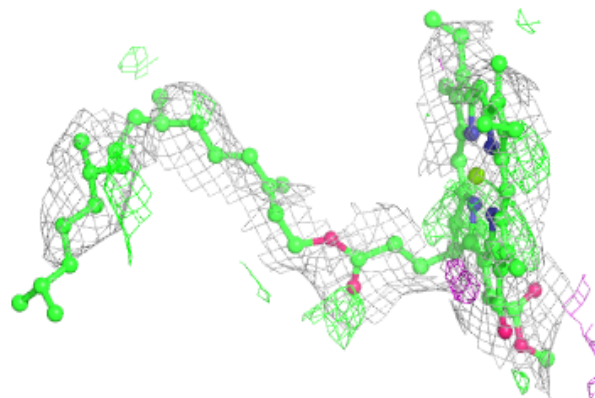


Electron density around CLA D 403:

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

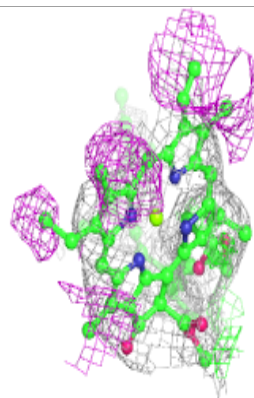
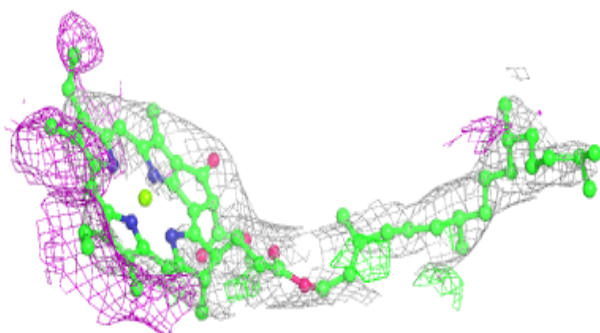
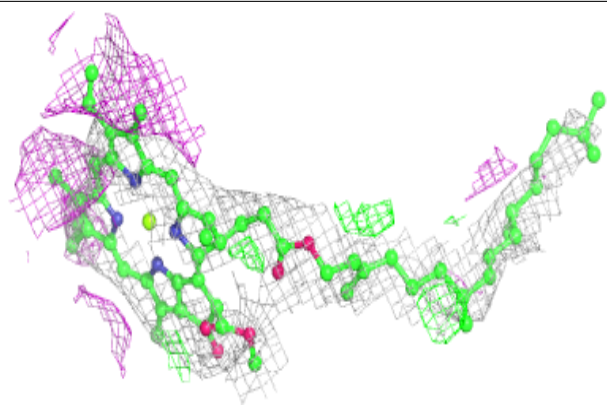
**Electron density around CLA D 404:**

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

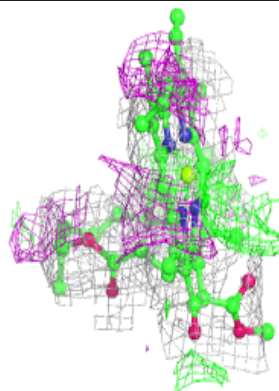
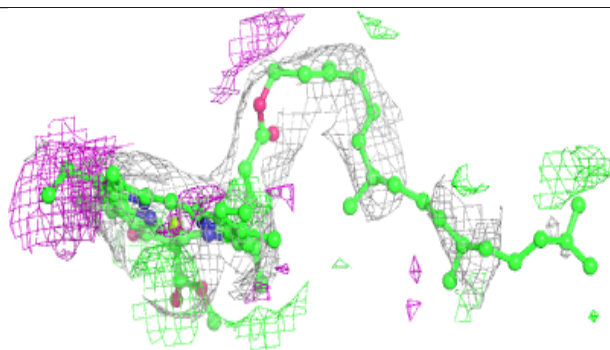
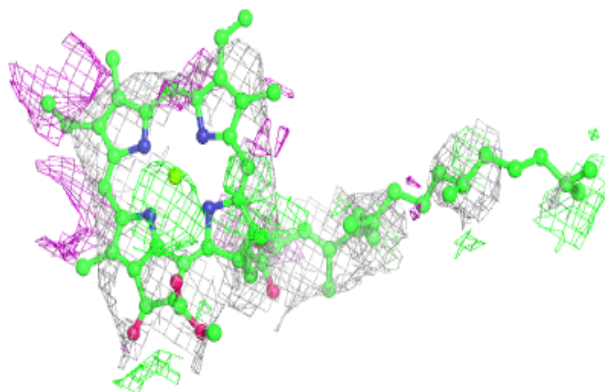


Electron density around CLA a 606:

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

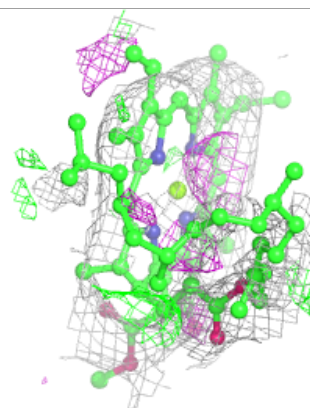
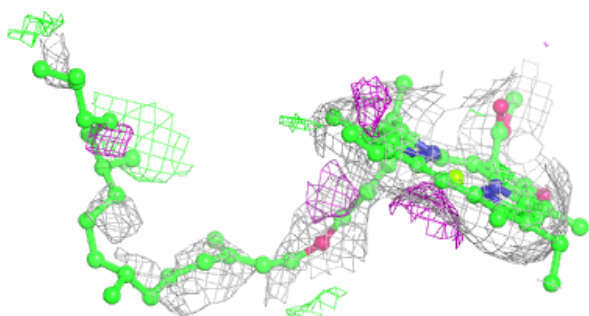
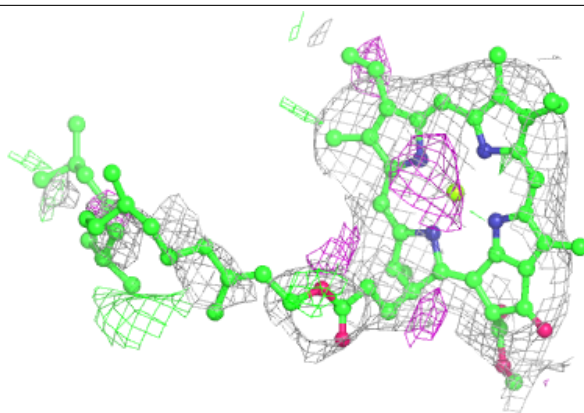
**Electron density around CLA a 607:**

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

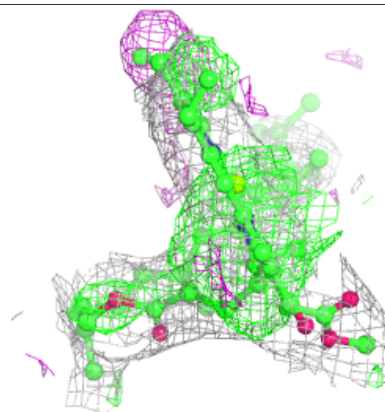
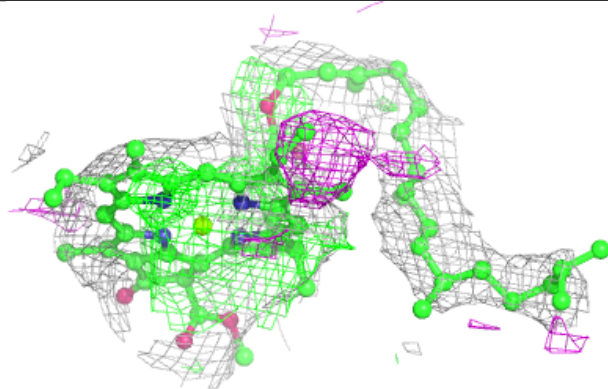
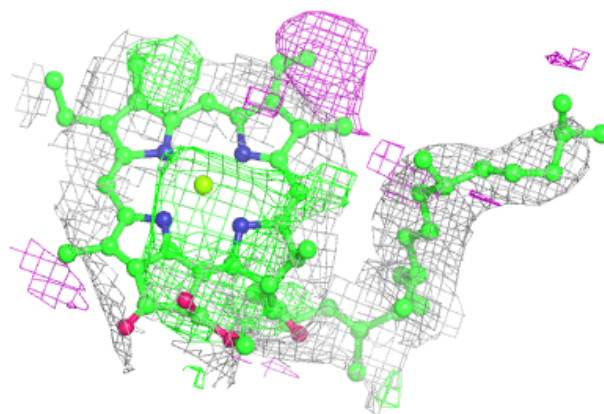


Electron density around CLA a 609:

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

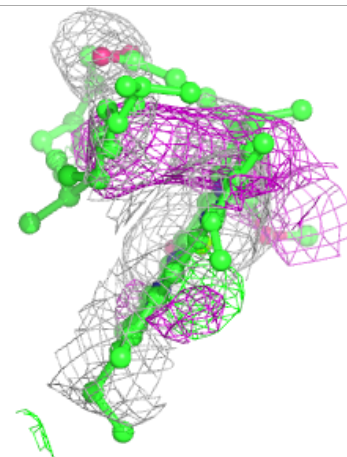
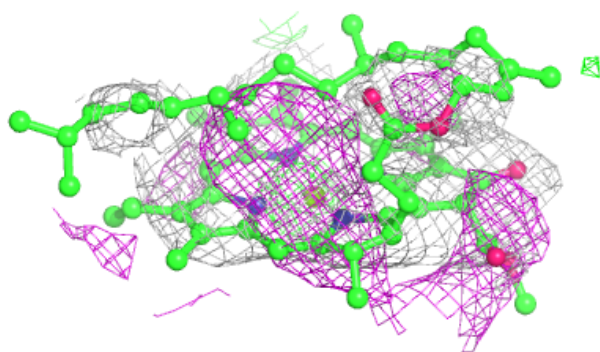
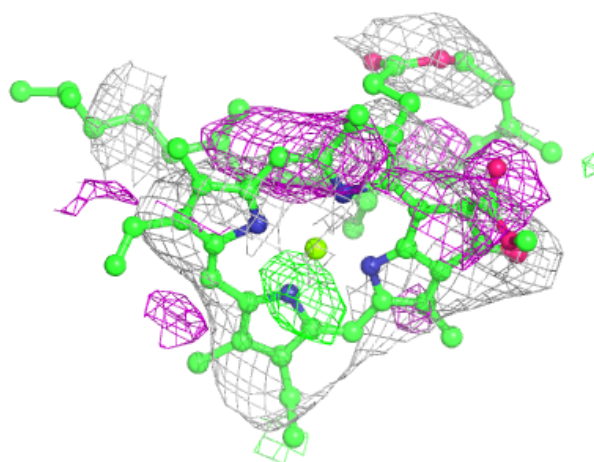
**Electron density around CLA a 615:**

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



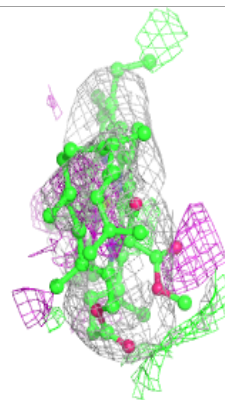
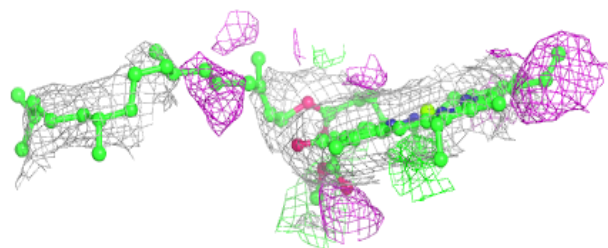
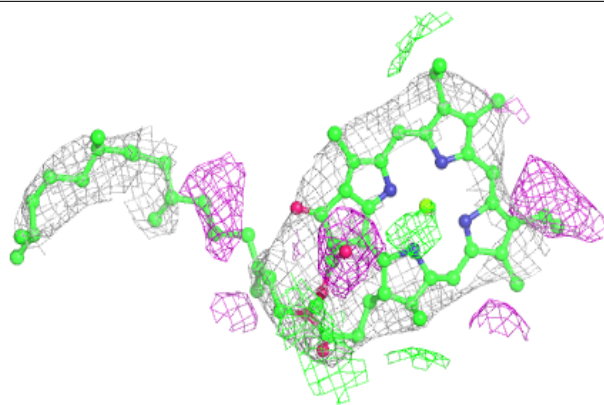
Electron density around CLA b 603:

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

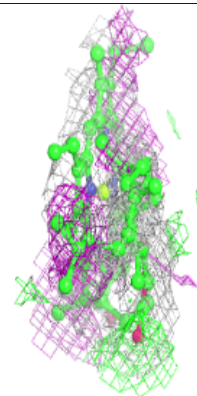
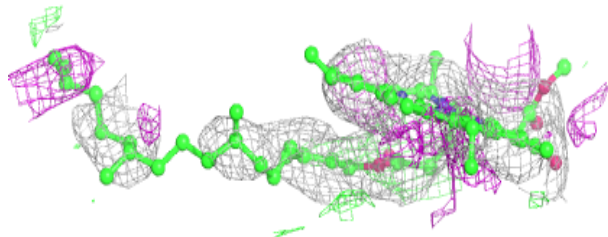
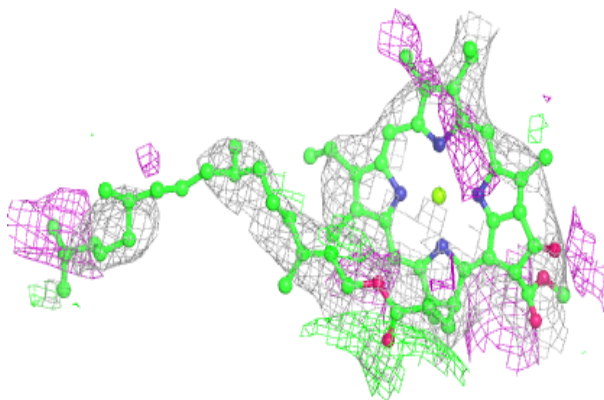


Electron density around CLA b 604:

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

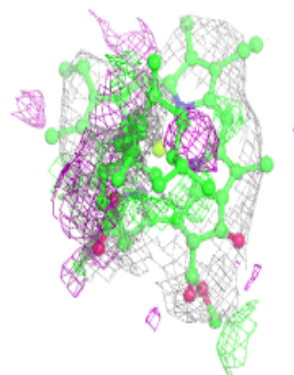
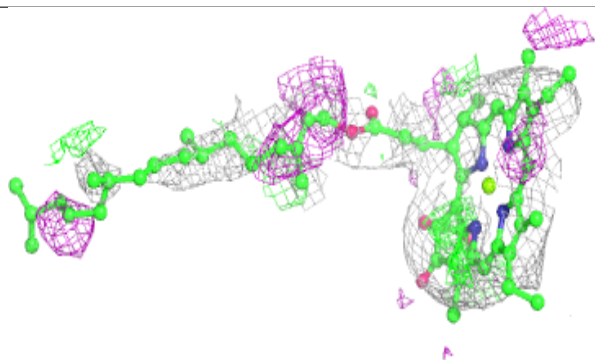
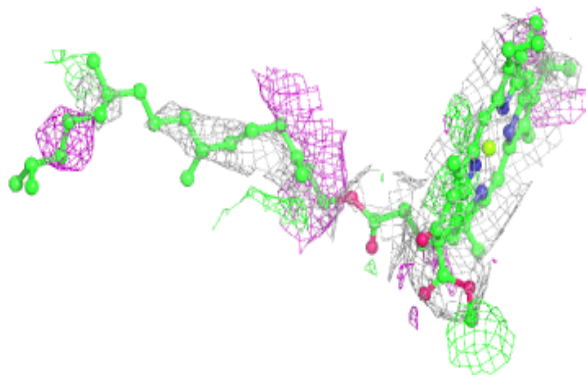
**Electron density around CLA b 605:**

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

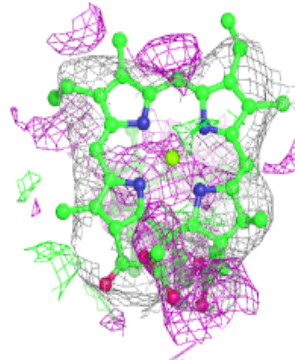
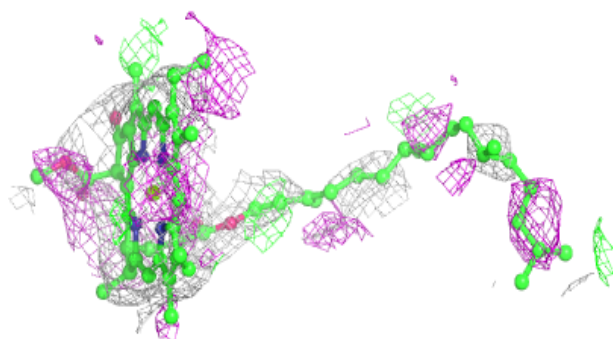
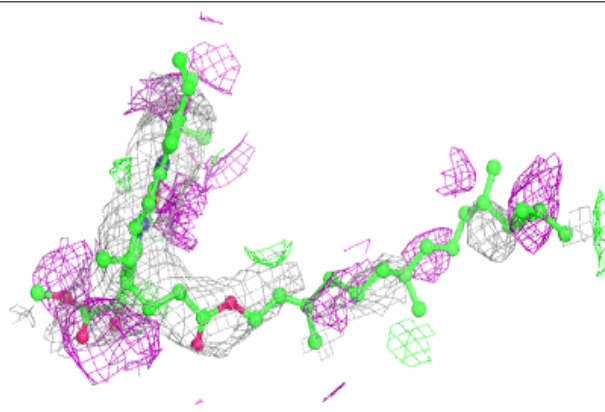


Electron density around CLA b 606:

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

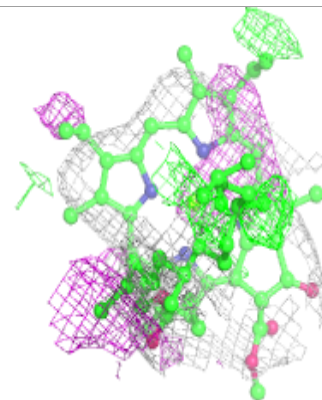
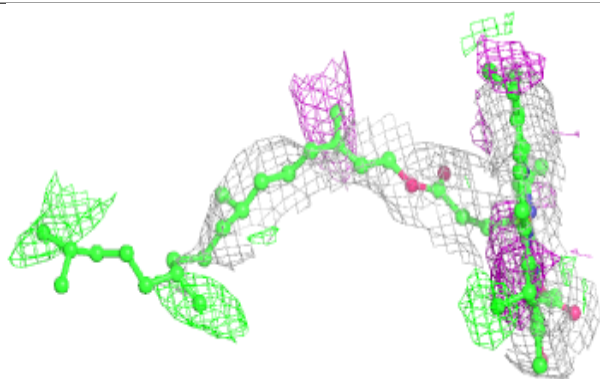
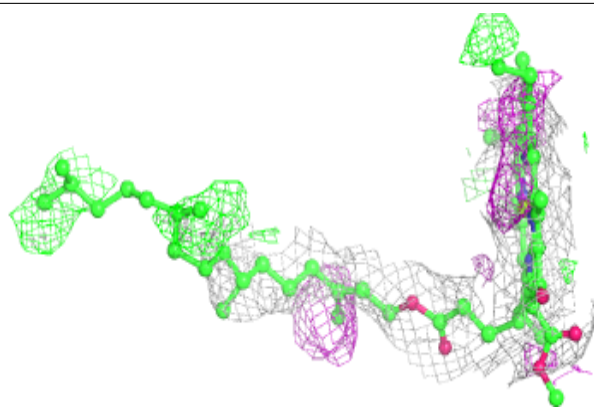
**Electron density around CLA b 607:**

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



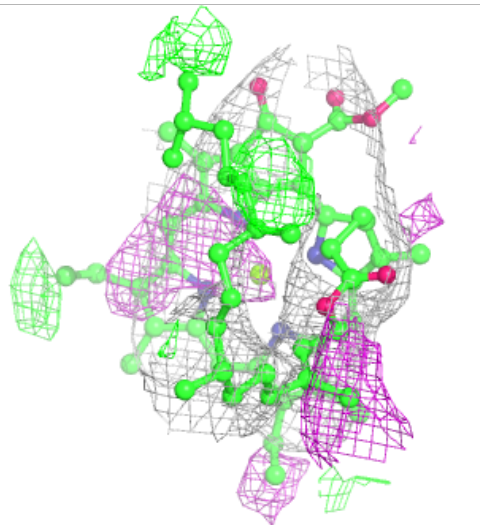
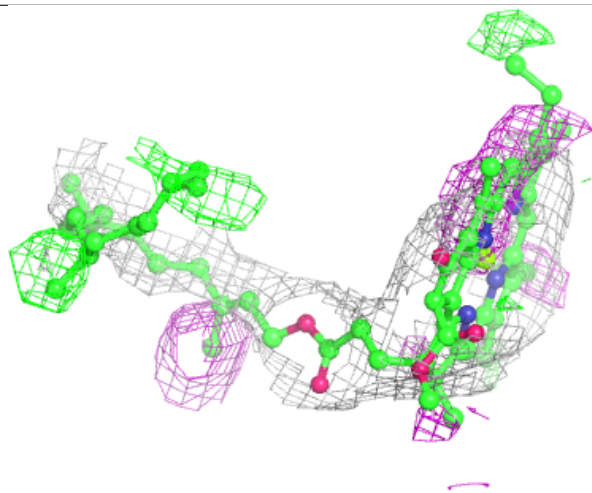
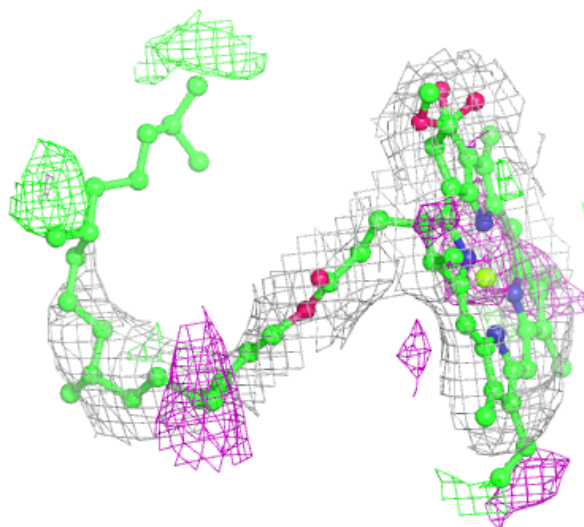
Electron density around CLA b 608 (A):

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



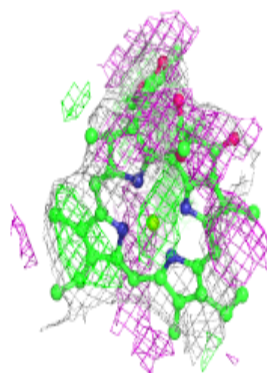
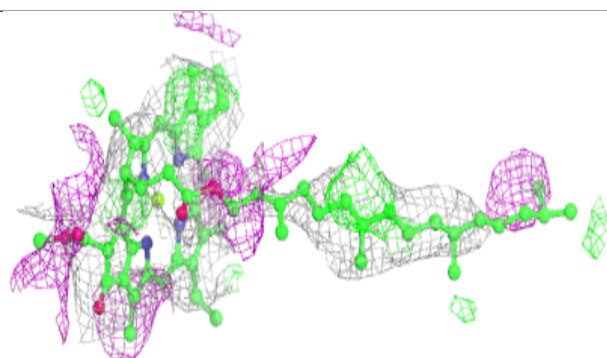
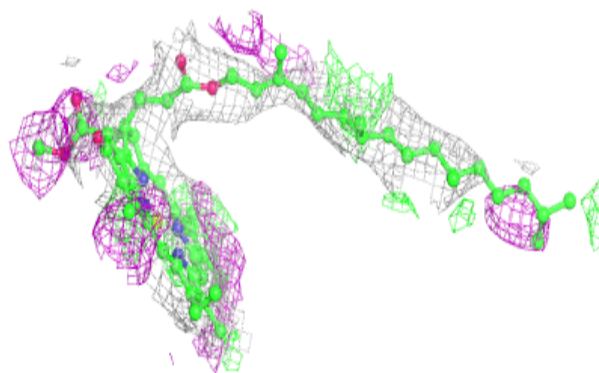
Electron density around CLA b 608 (B):

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

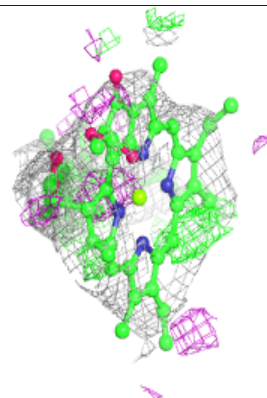
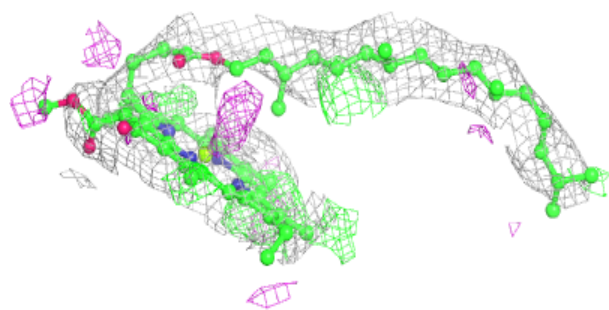
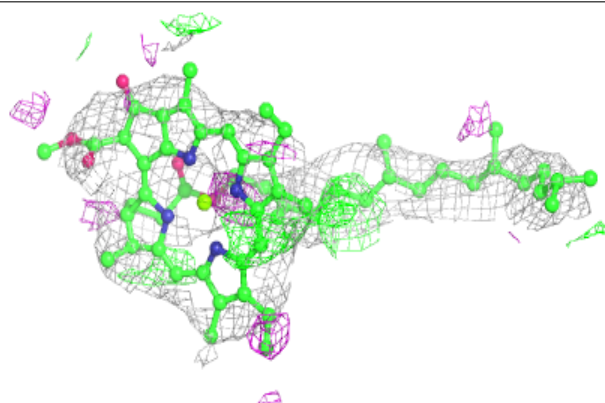


Electron density around CLA b 609:

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

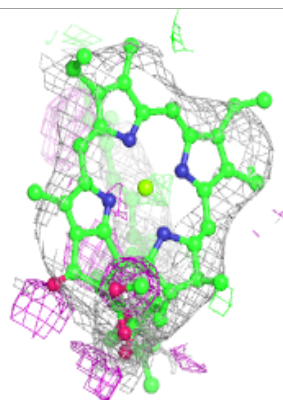
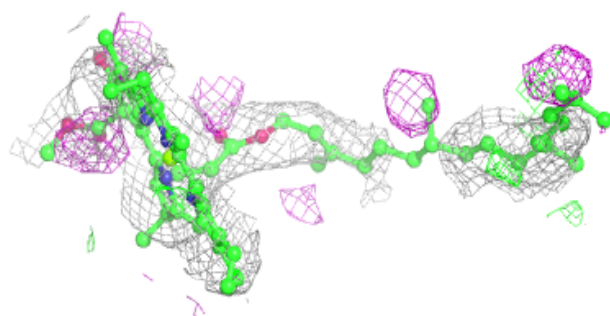
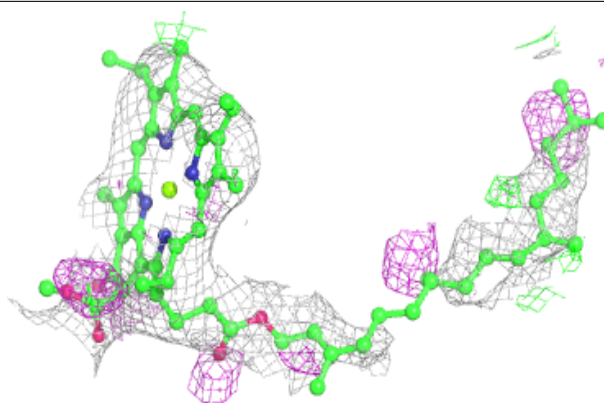
**Electron density around CLA b 610:**

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

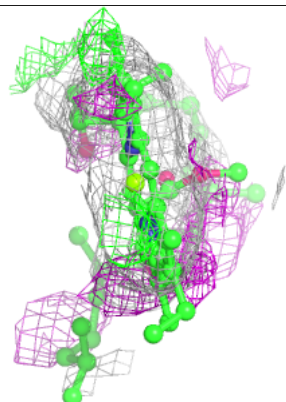
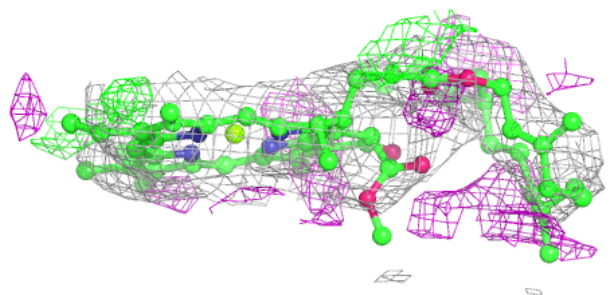
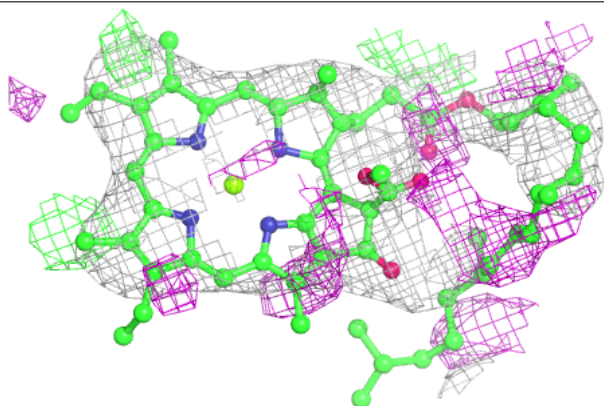


Electron density around CLA b 611:

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

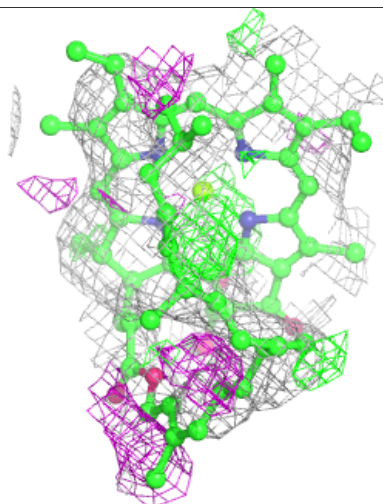
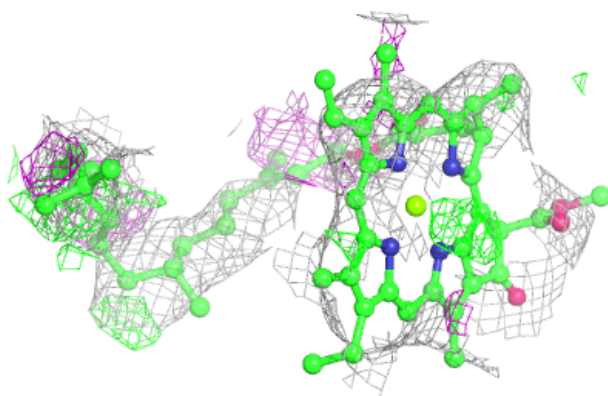
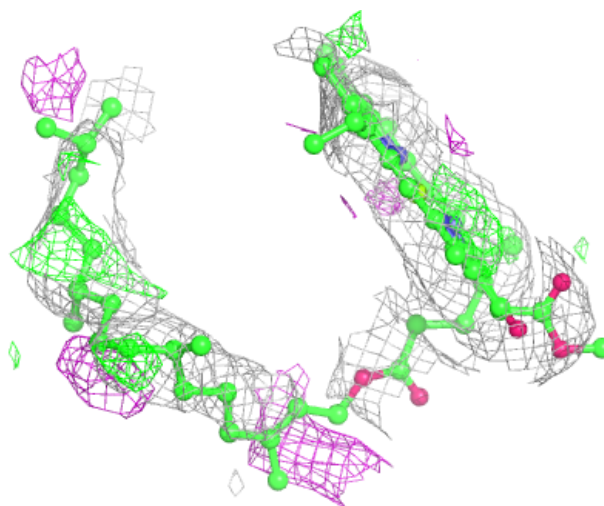
**Electron density around CLA b 612:**

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



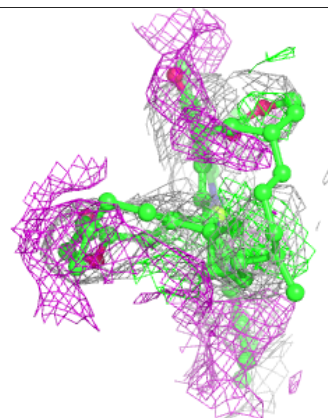
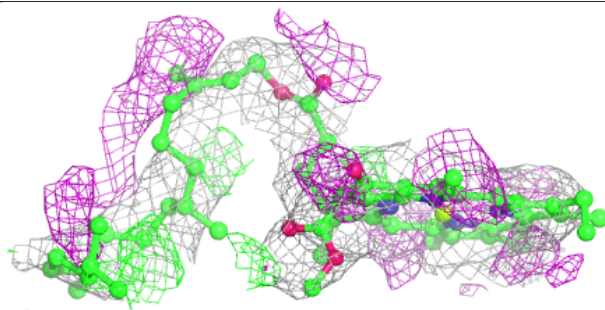
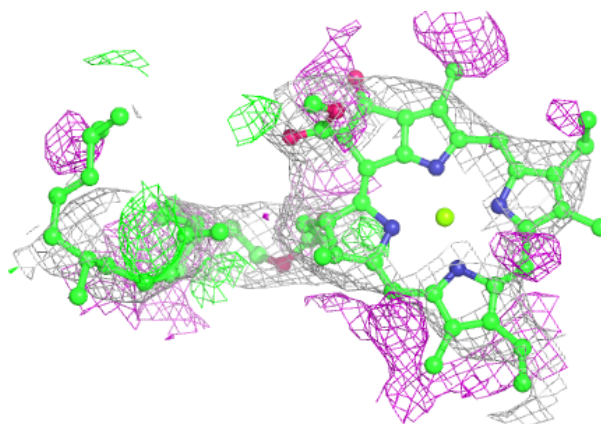
Electron density around CLA b 613:

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



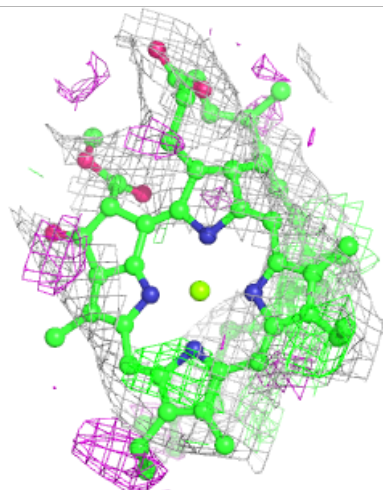
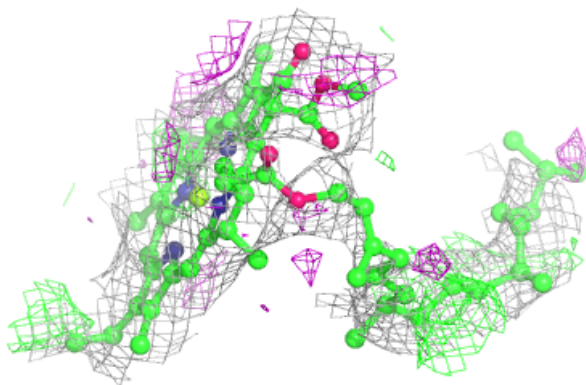
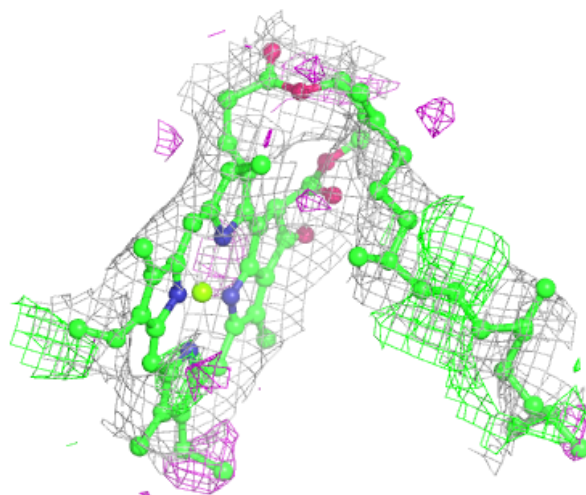
Electron density around CLA b 614:

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



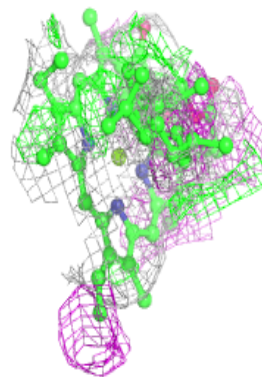
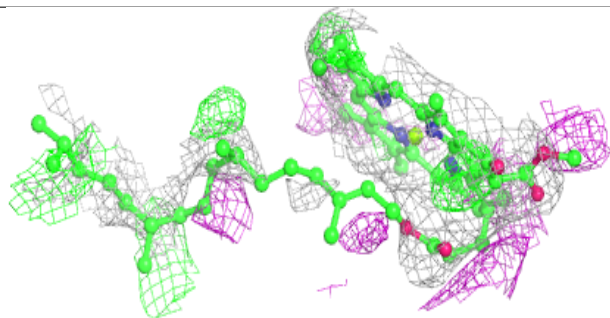
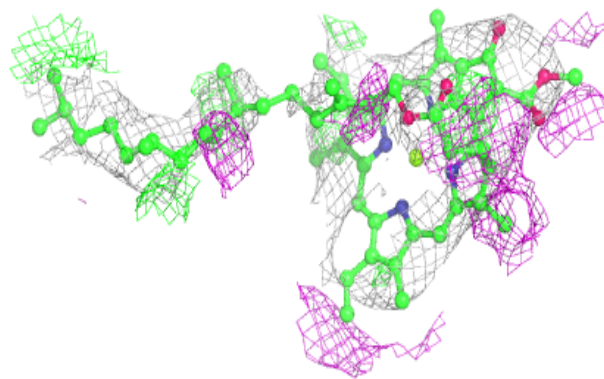
Electron density around CLA b 615:

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



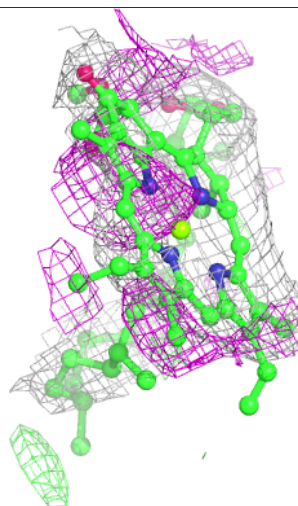
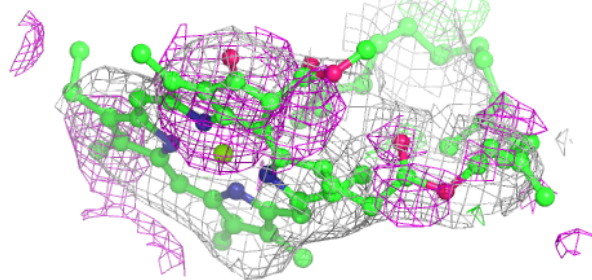
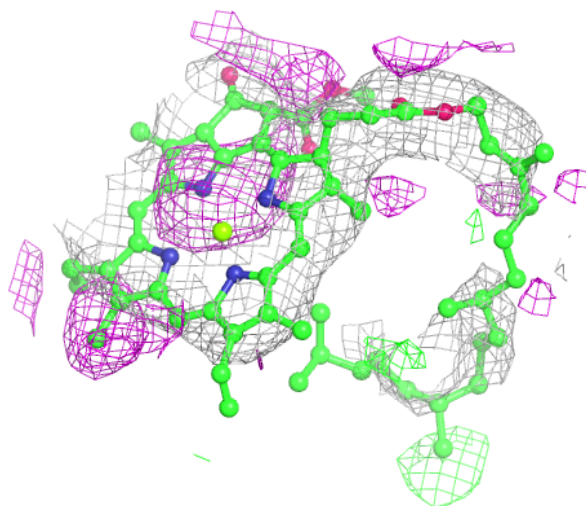
Electron density around CLA b 616:

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



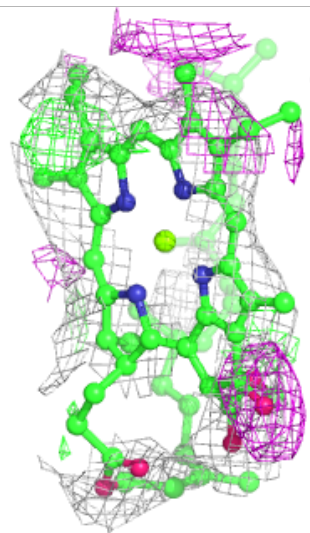
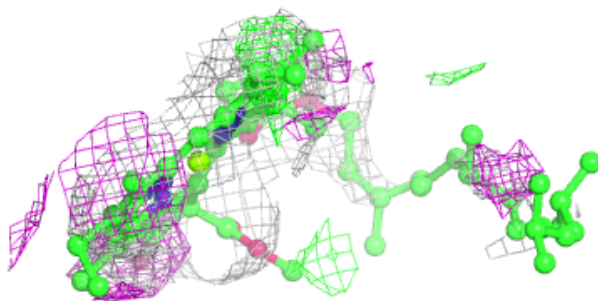
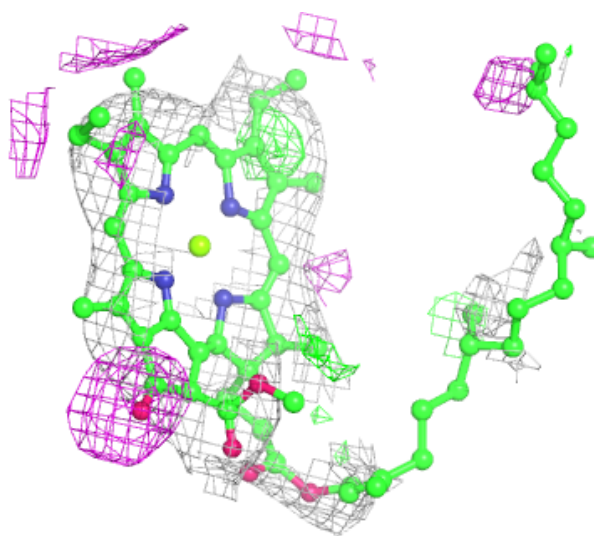
Electron density around CLA b 617:

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



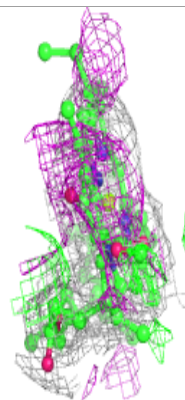
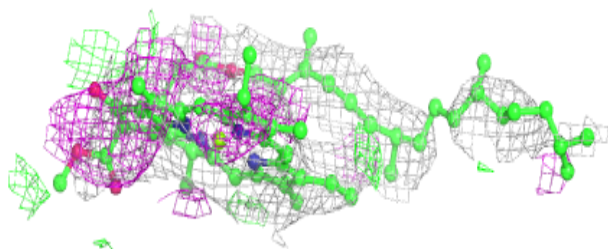
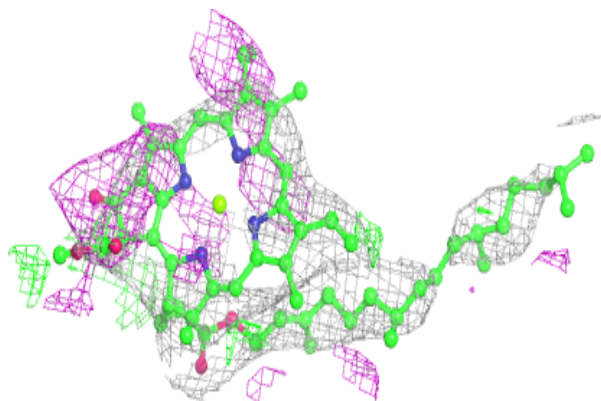
Electron density around CLA b 618:

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

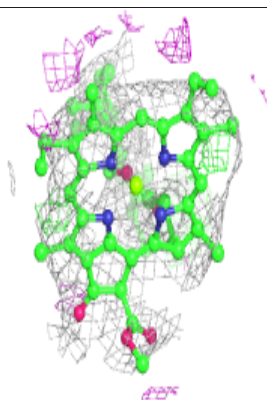
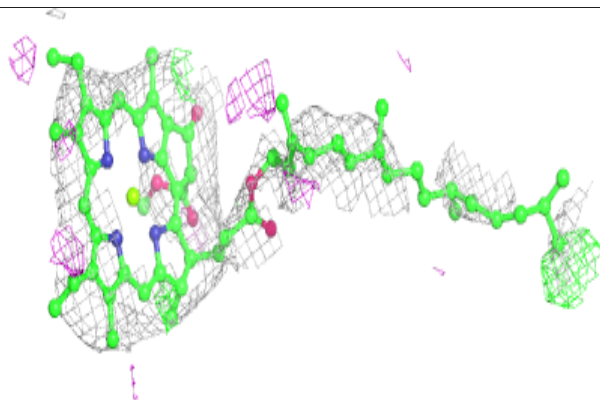
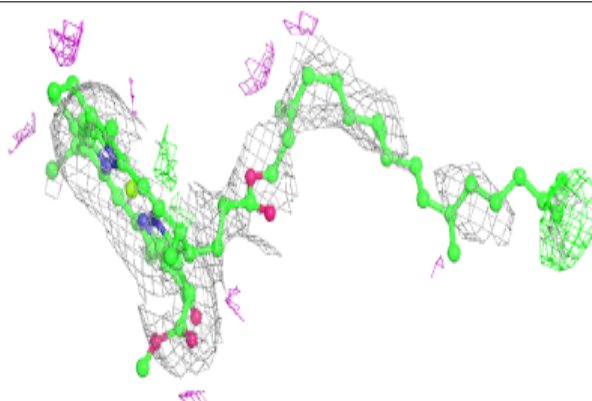


Electron density around CLA c 501:

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

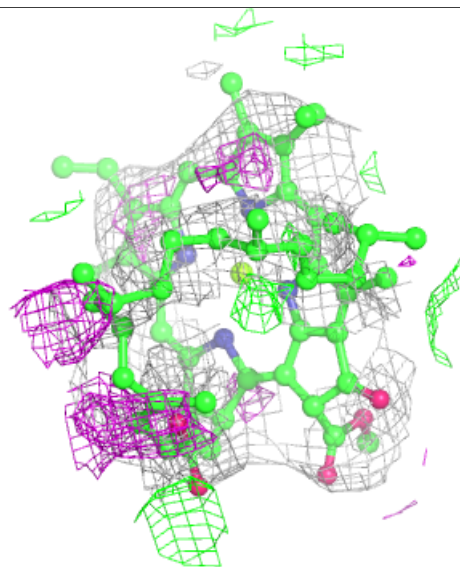
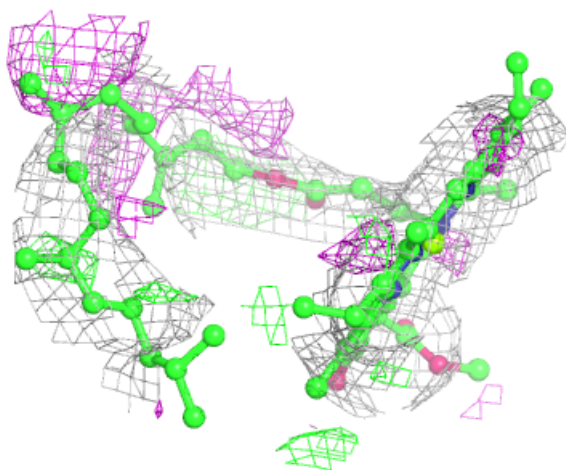
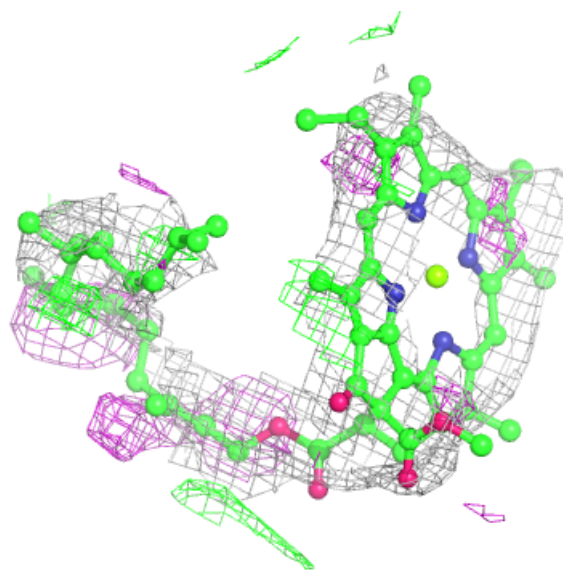
**Electron density around CLA c 502:**

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



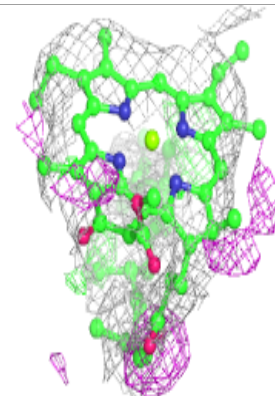
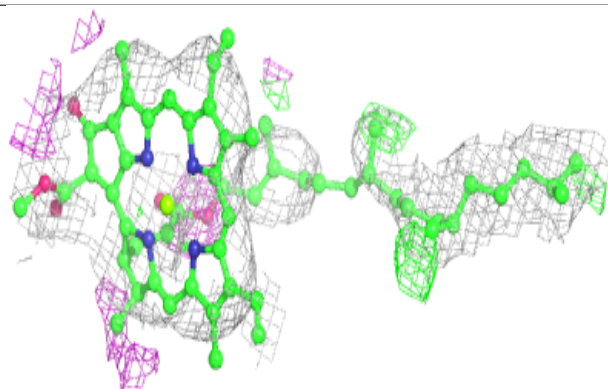
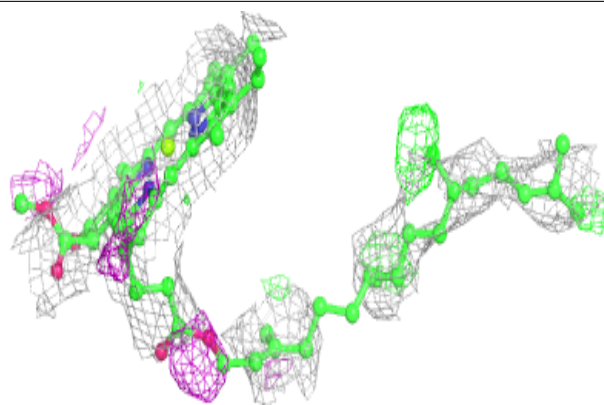
Electron density around CLA c 503:

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

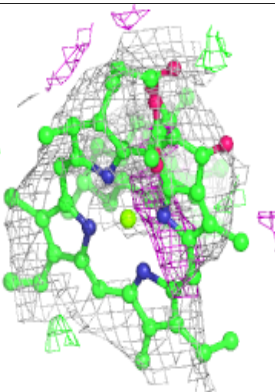
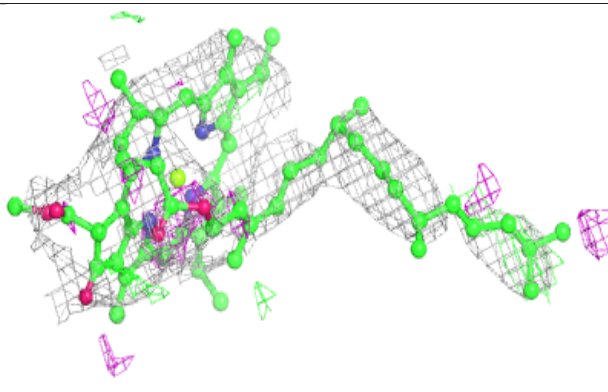
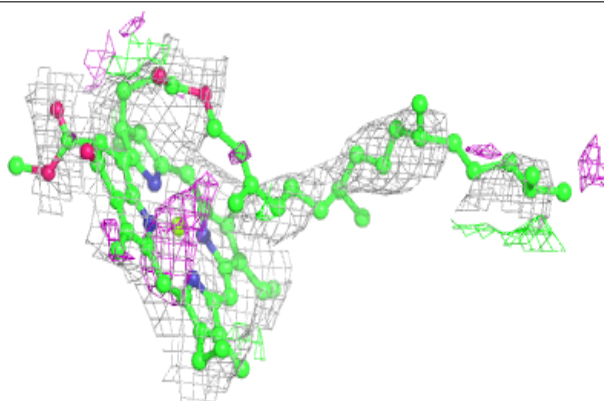


Electron density around CLA c 504:

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

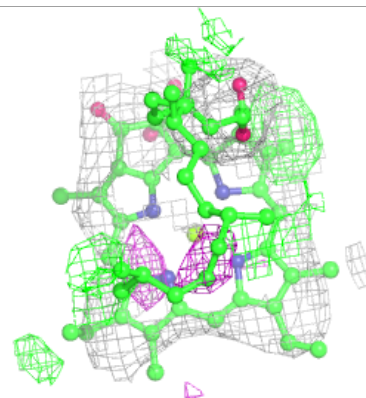
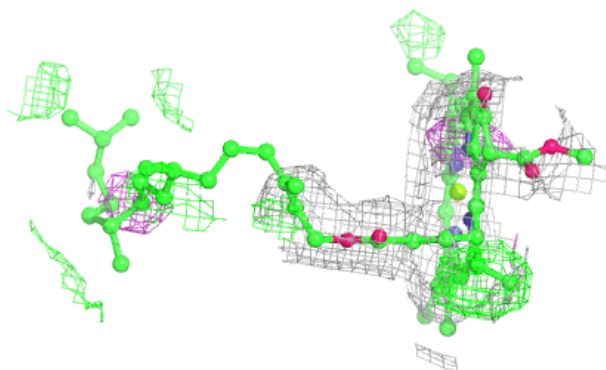
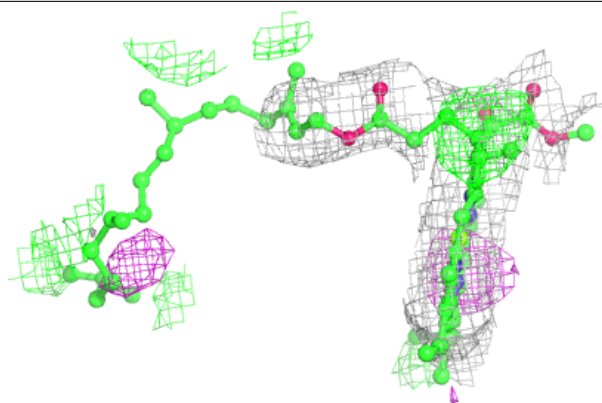
**Electron density around CLA c 505:**

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



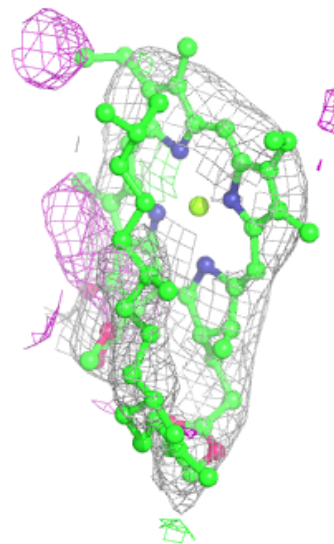
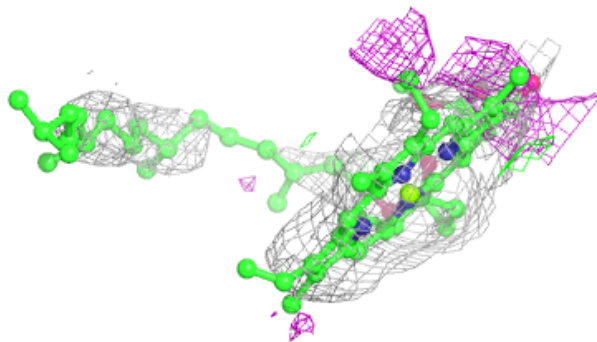
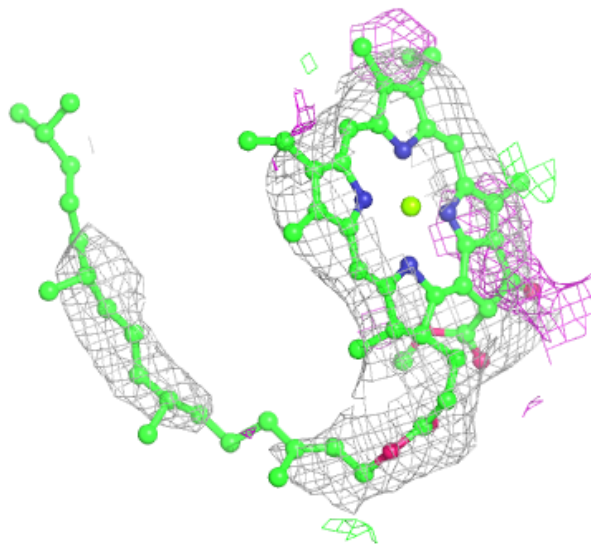
Electron density around CLA c 506:

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



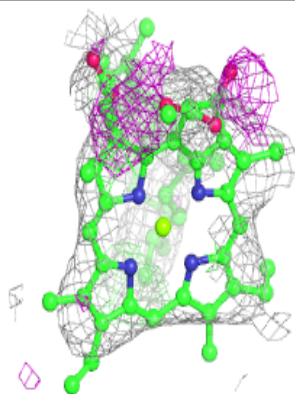
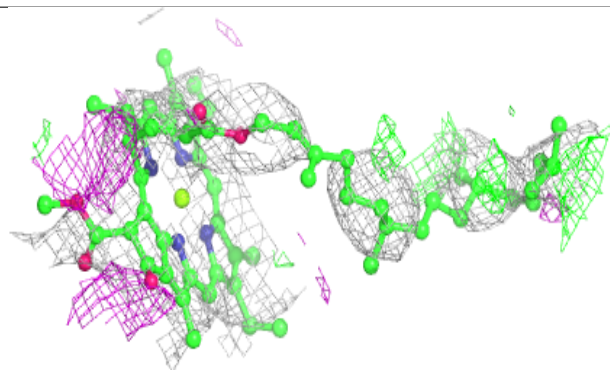
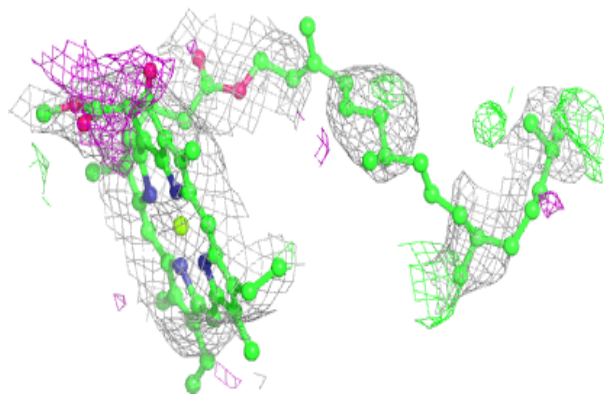
Electron density around CLA c 507:

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



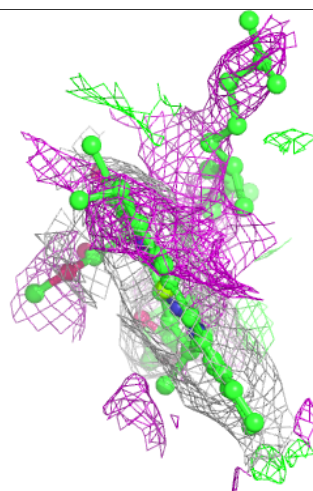
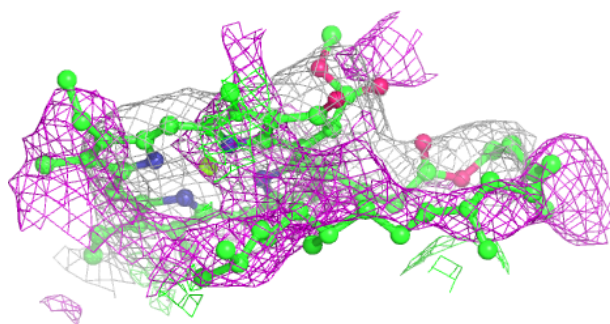
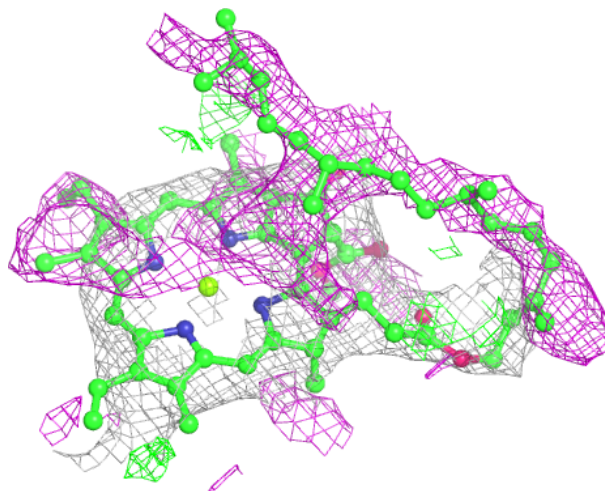
Electron density around CLA c 508:

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



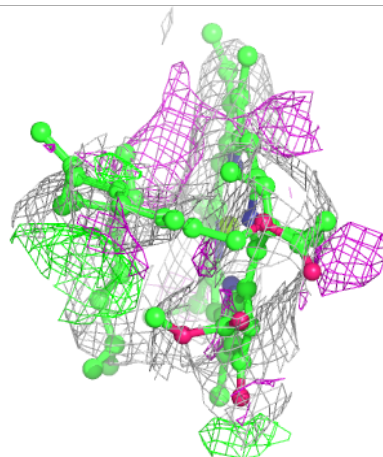
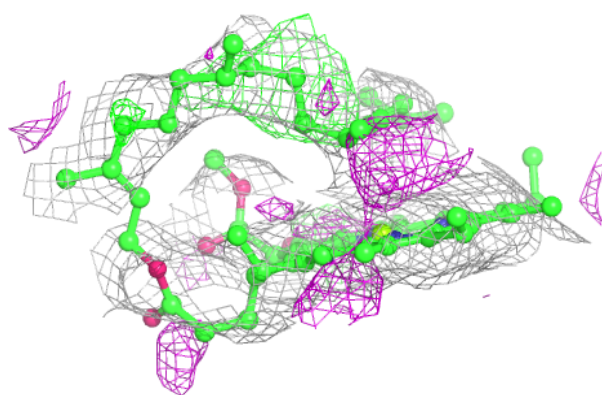
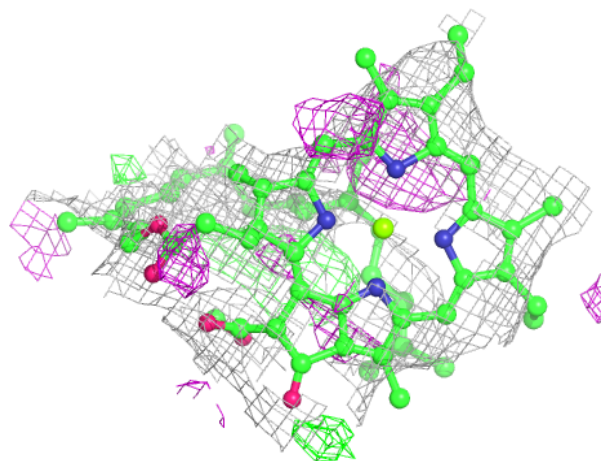
Electron density around CLA c 509:

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



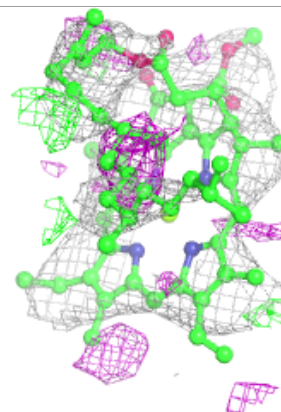
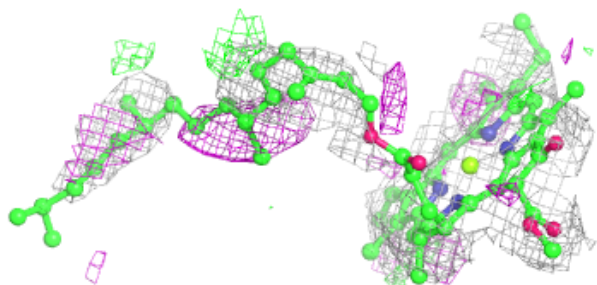
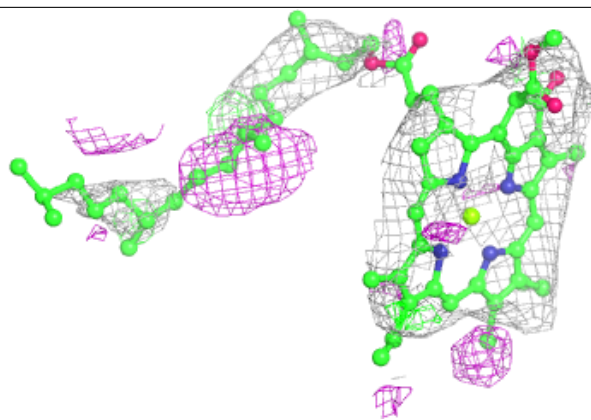
Electron density around CLA c 510:

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



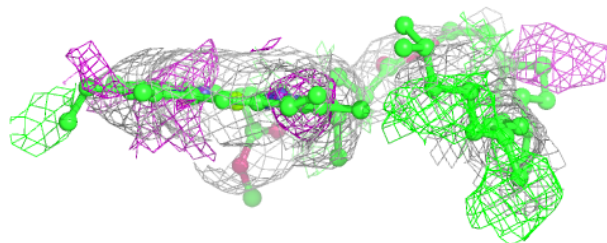
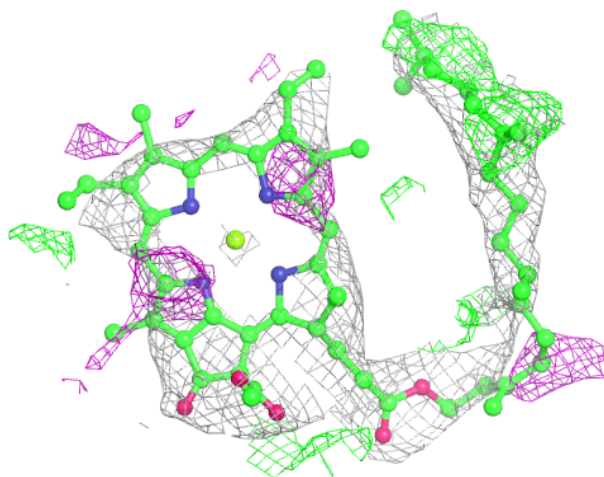
Electron density around CLA c 511:

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



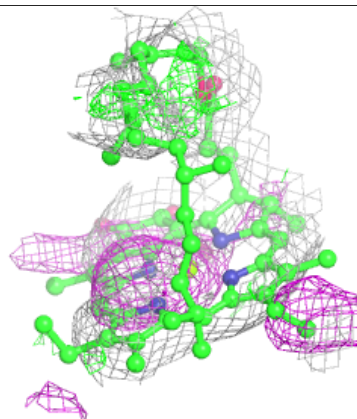
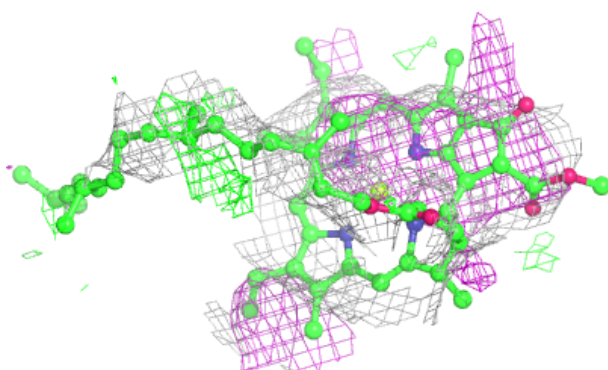
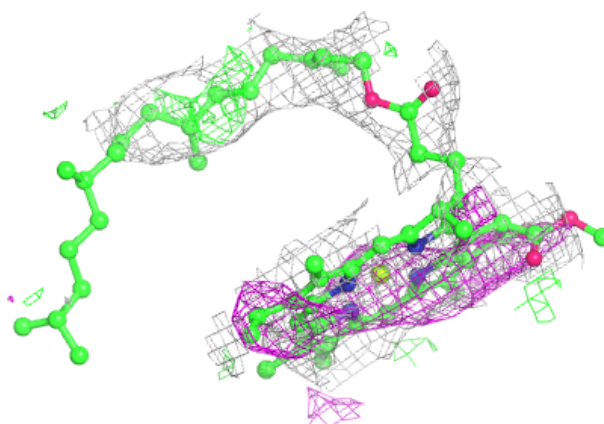
Electron density around CLA c 512:

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

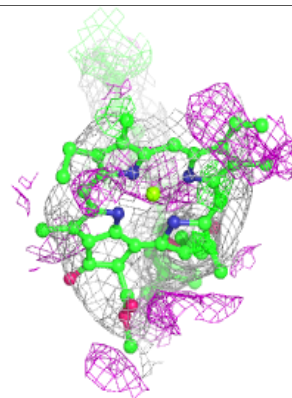
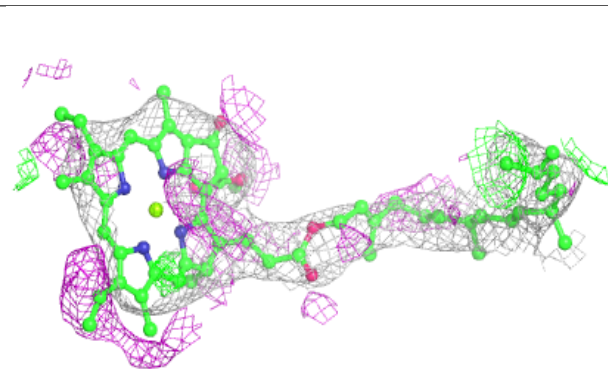
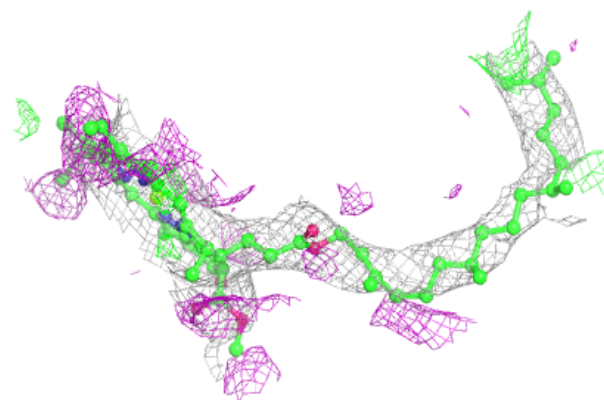


Electron density around CLA c 513:

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

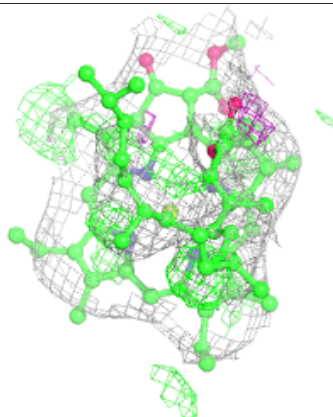
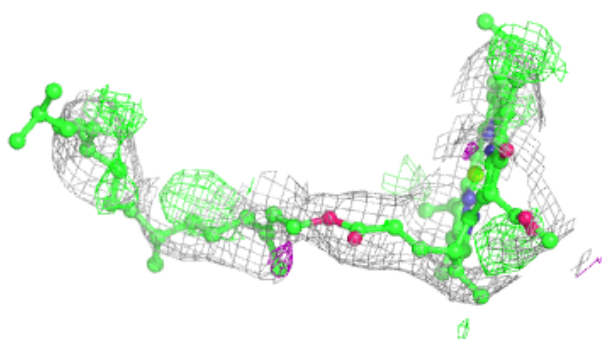
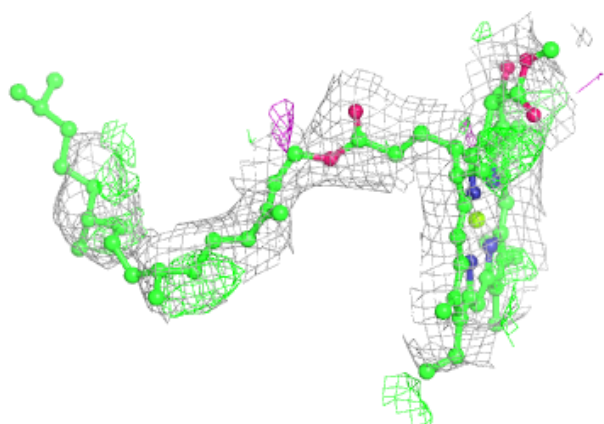
**Electron density around CLA d 402:**

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



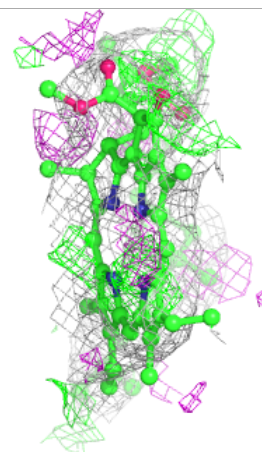
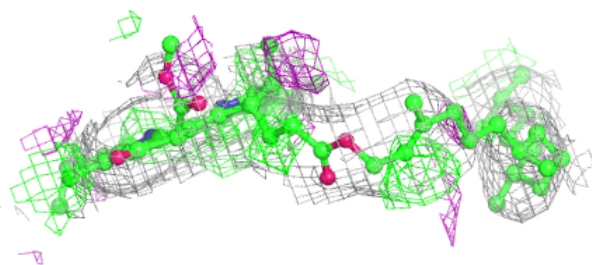
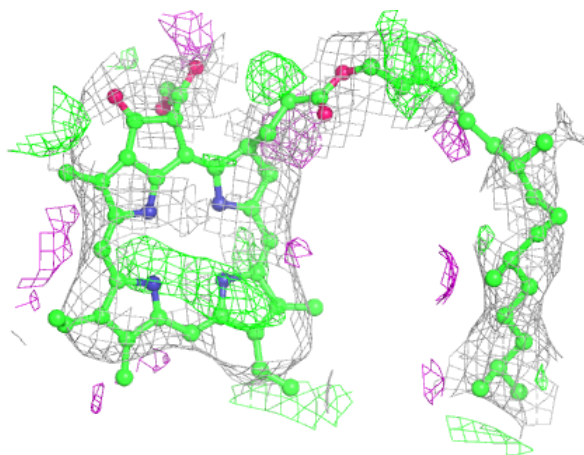
Electron density around CLA d 403:

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



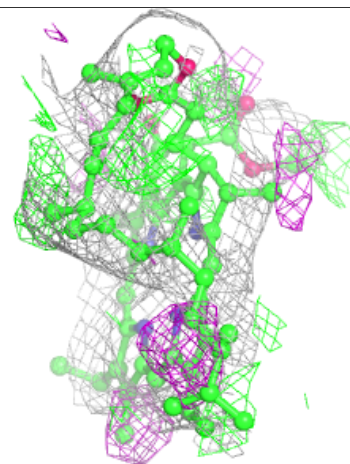
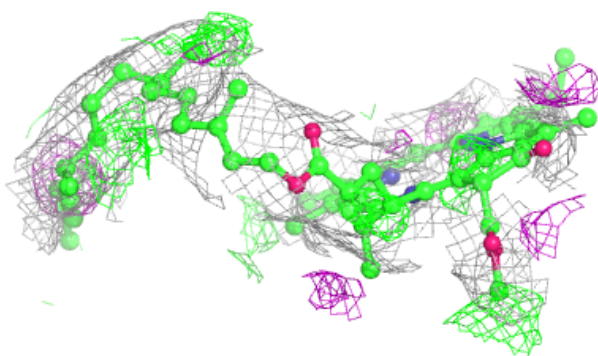
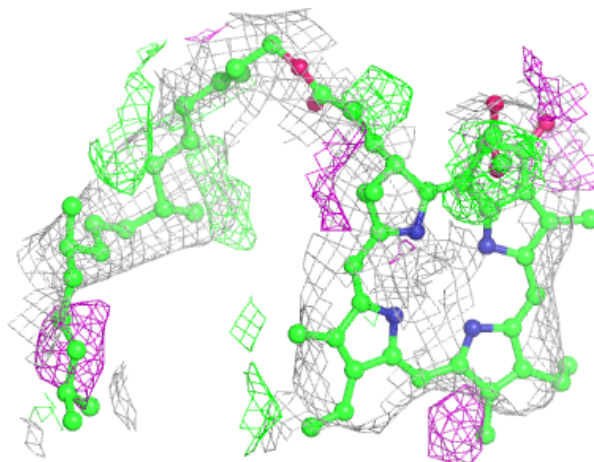
Electron density around PHO A 608:

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



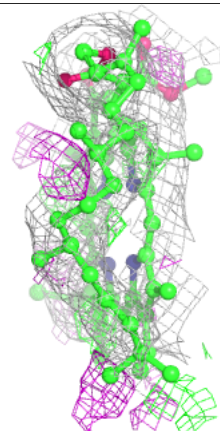
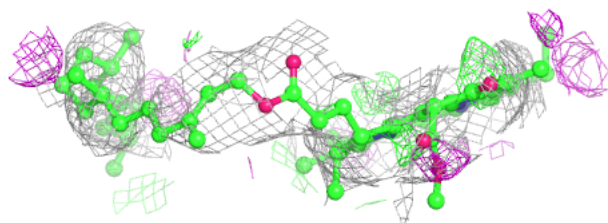
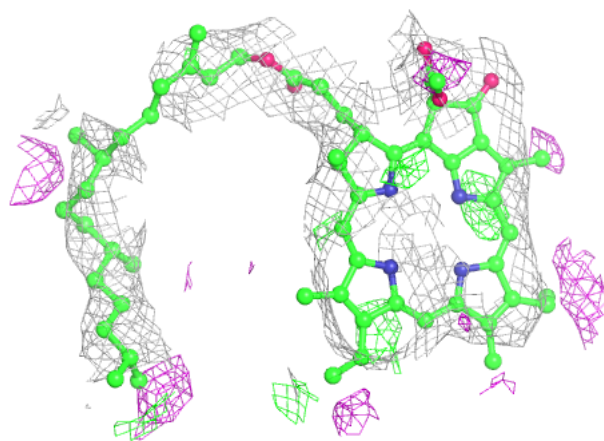
Electron density around PHO D 401:

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



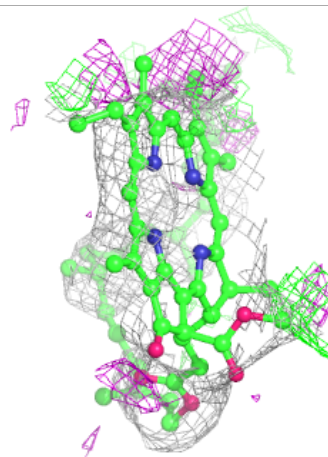
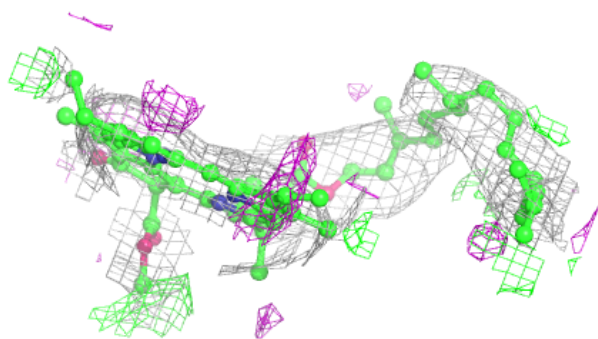
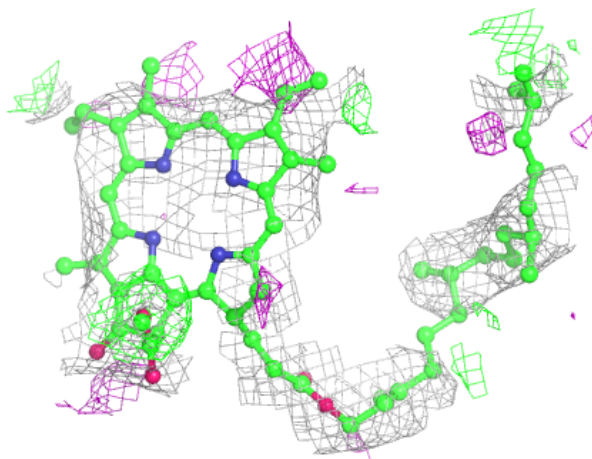
Electron density around PHO a 608:

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



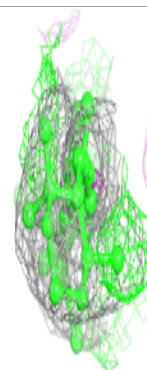
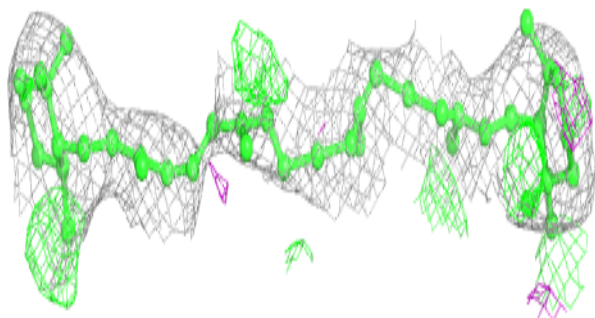
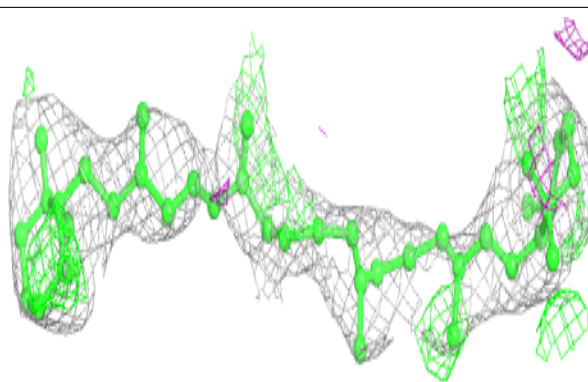
Electron density around PHO d 401:

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

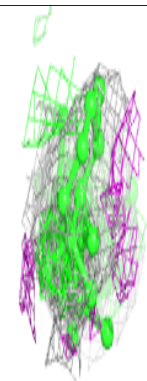
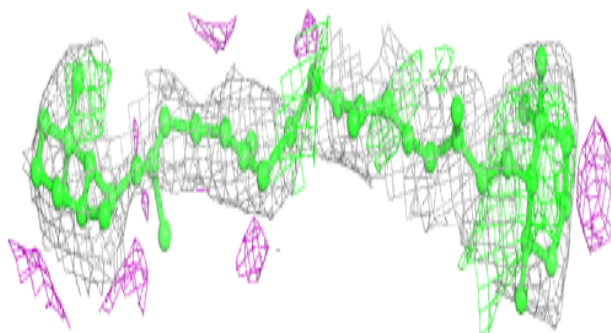
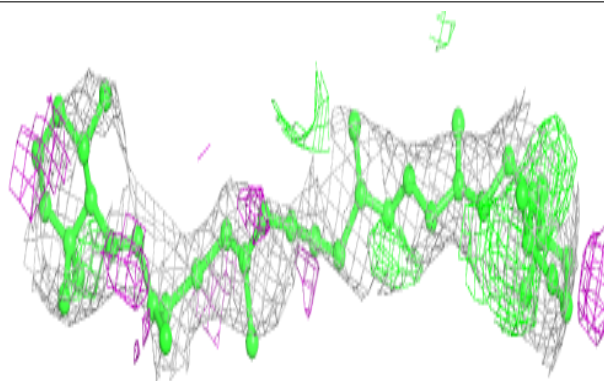


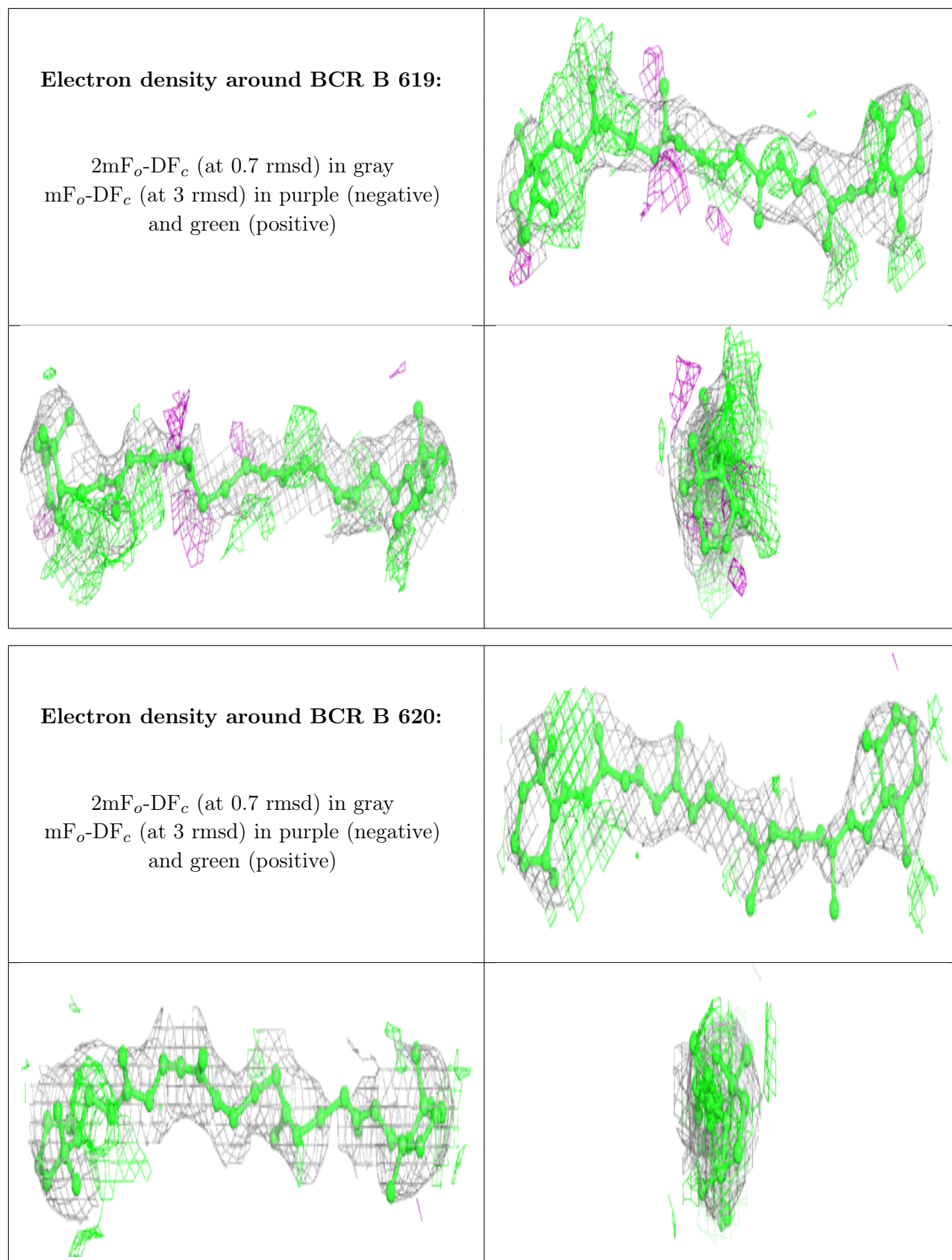
Electron density around BCR A 610:

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

**Electron density around BCR B 618:**

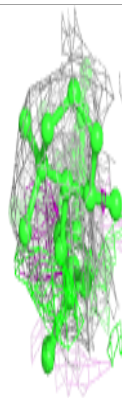
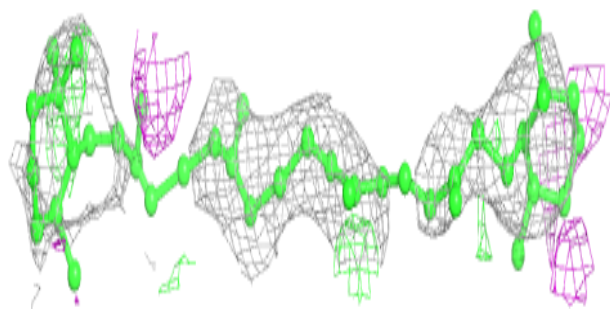
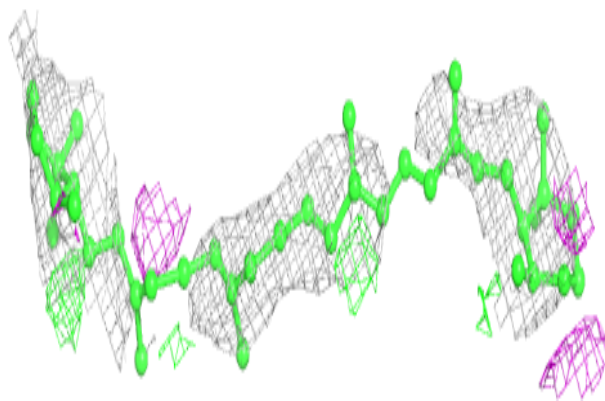
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



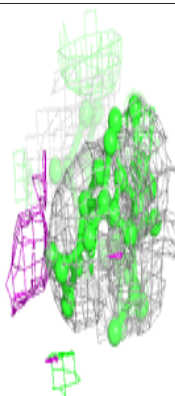
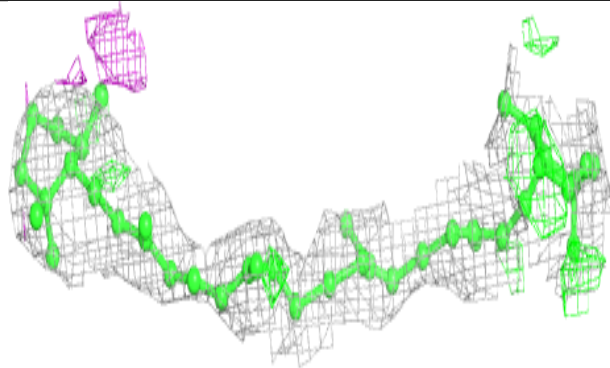
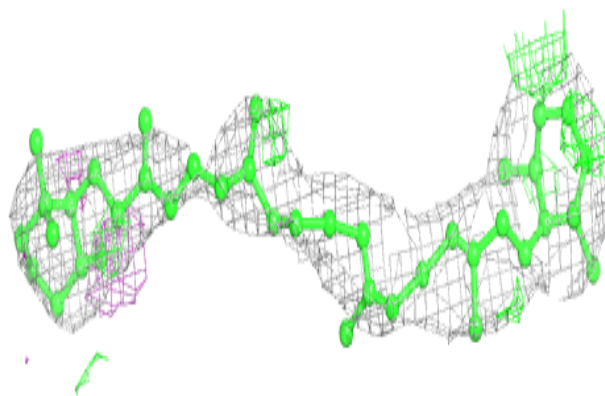


Electron density around BCR C 514:

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

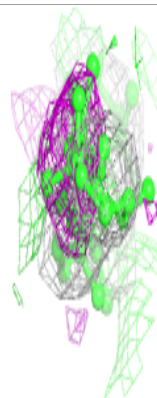
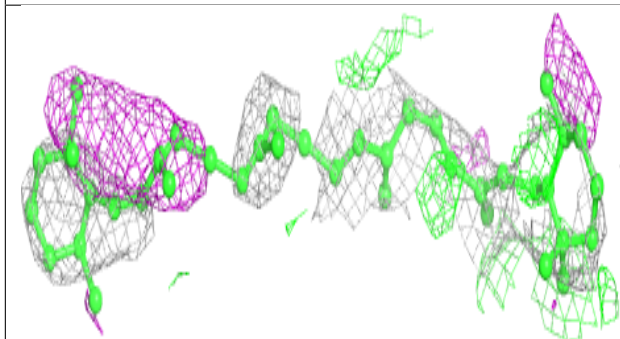
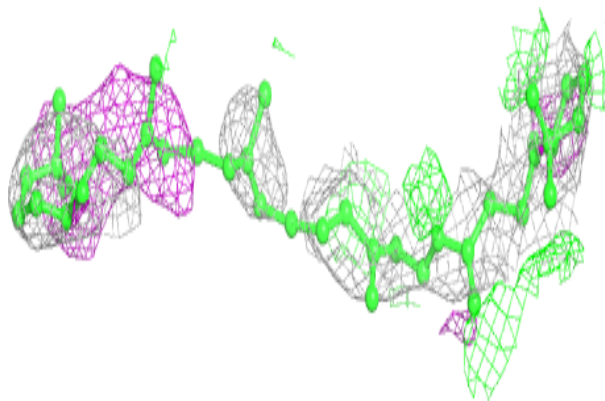
**Electron density around BCR F 101:**

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

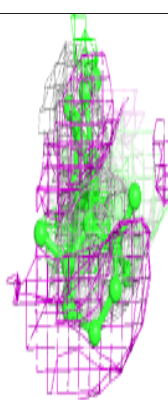
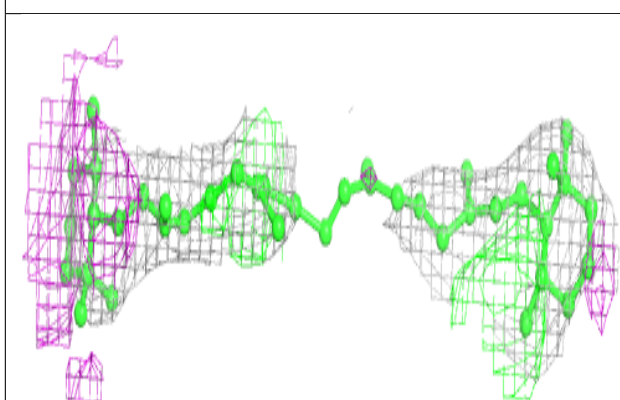
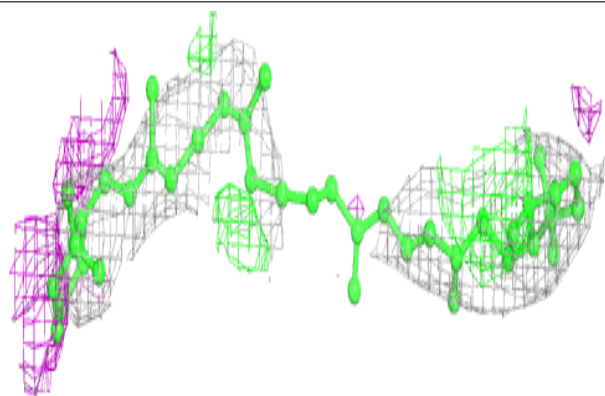


Electron density around BCR H 101:

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

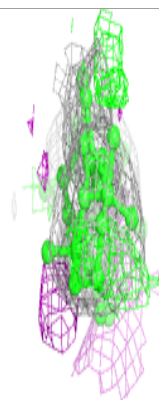
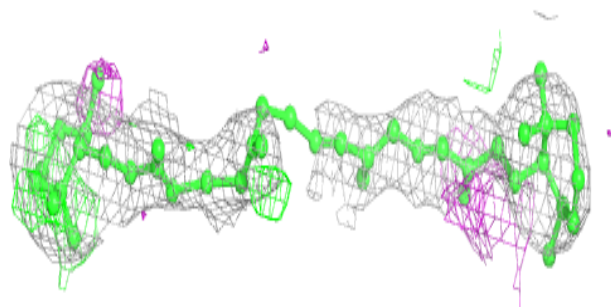
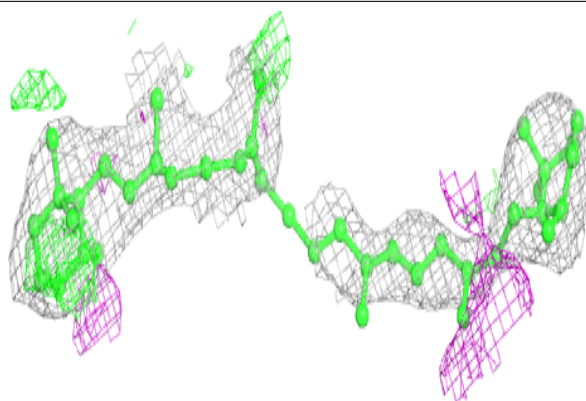
**Electron density around BCR I 101:**

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

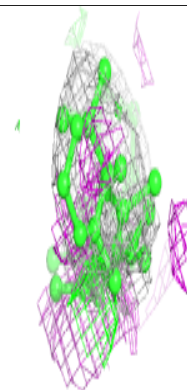
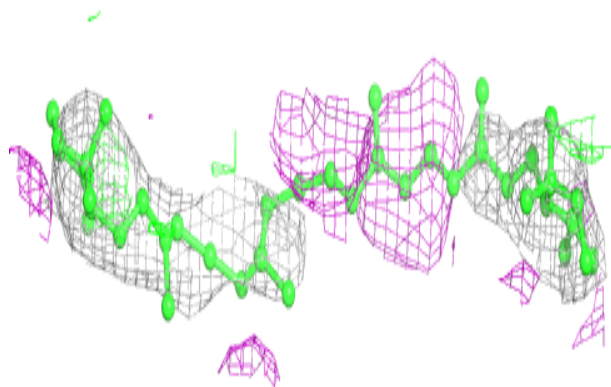
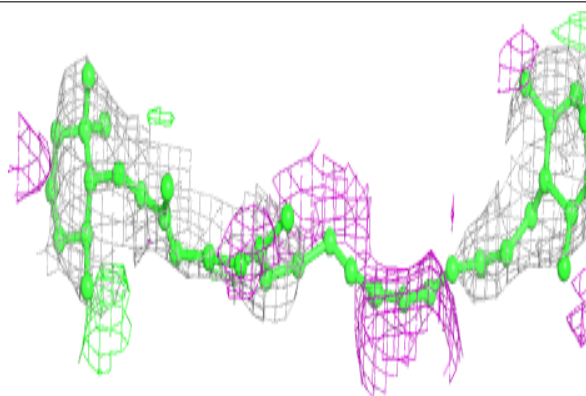


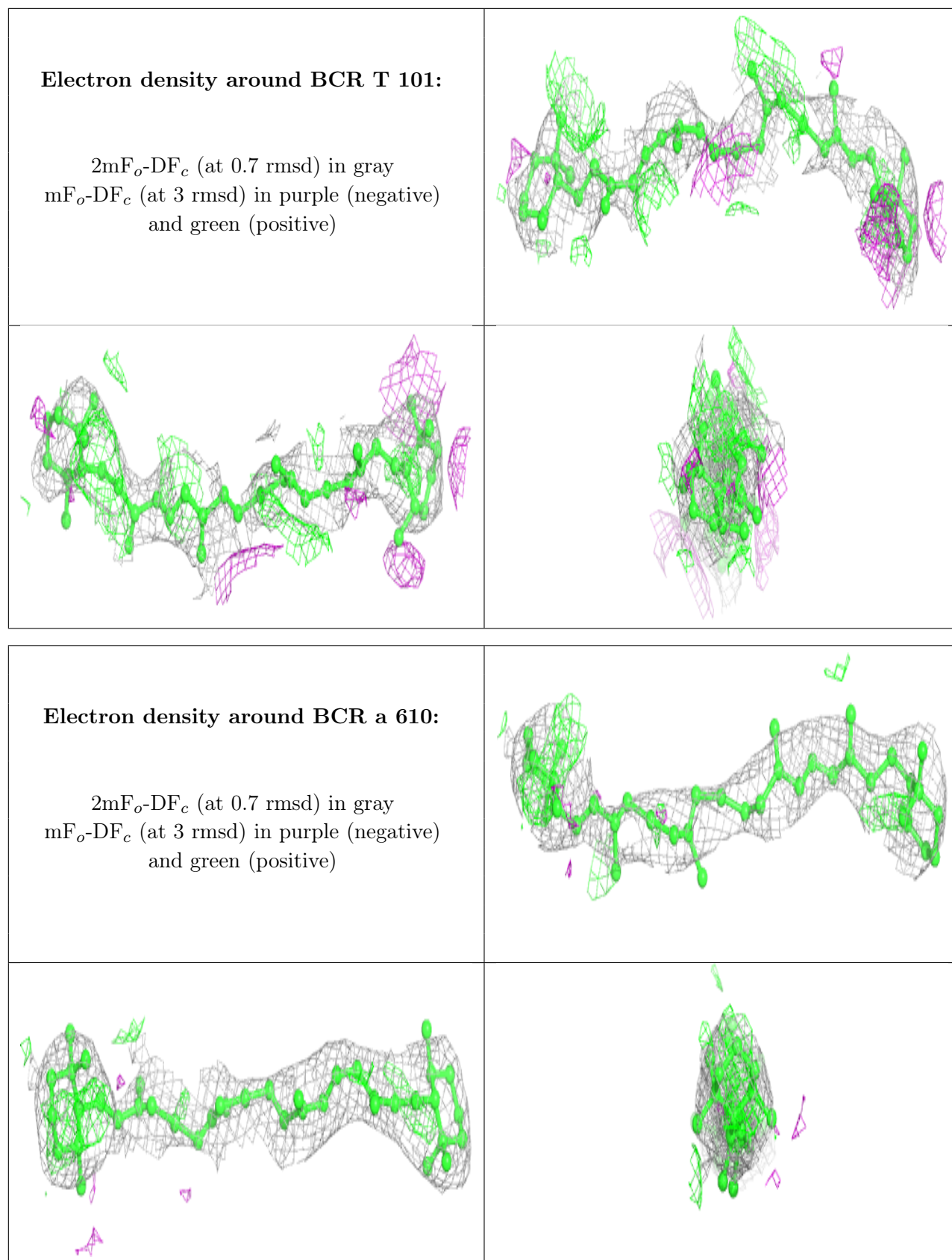
Electron density around BCR K 101:

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

**Electron density around BCR K 102:**

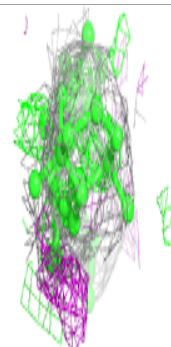
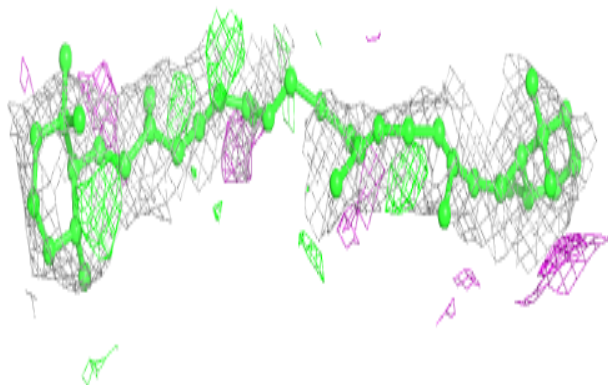
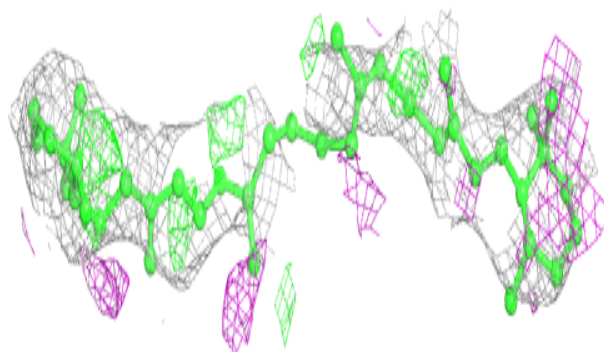
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



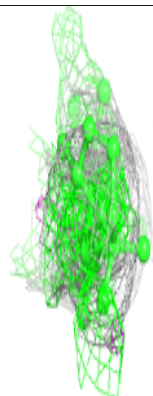
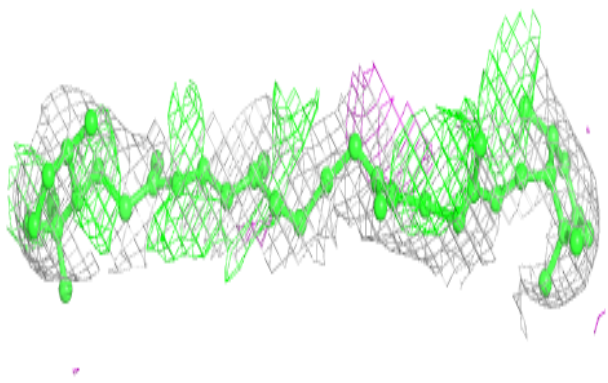
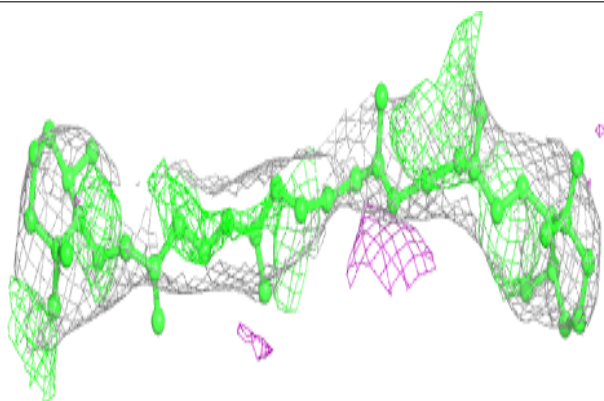


Electron density around BCR b 619:

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

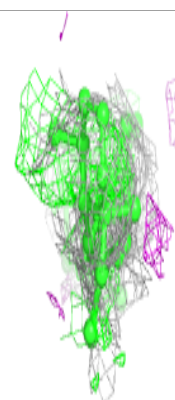
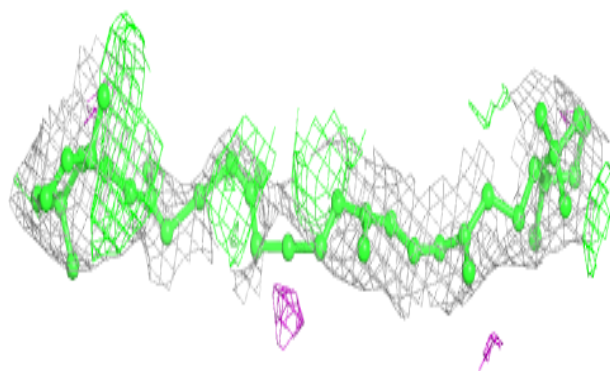
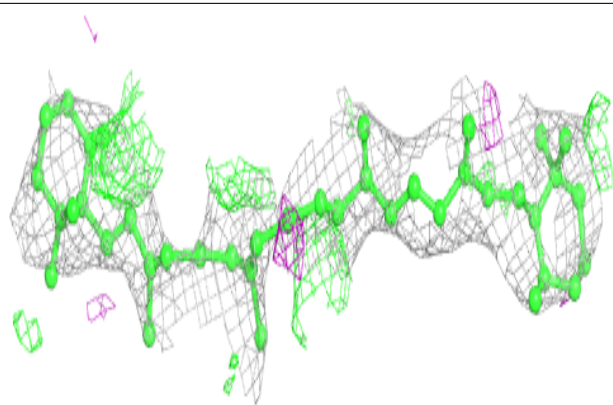
**Electron density around BCR b 620:**

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

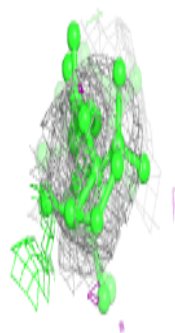
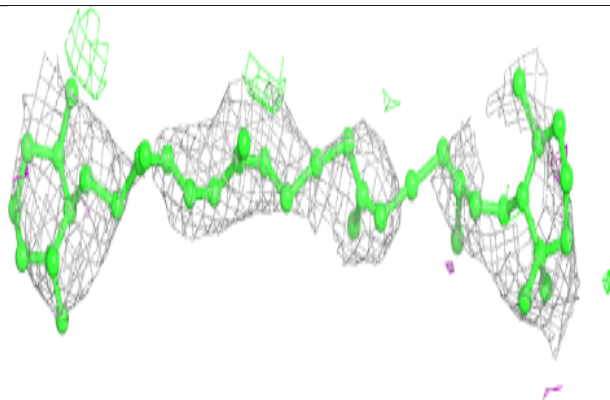
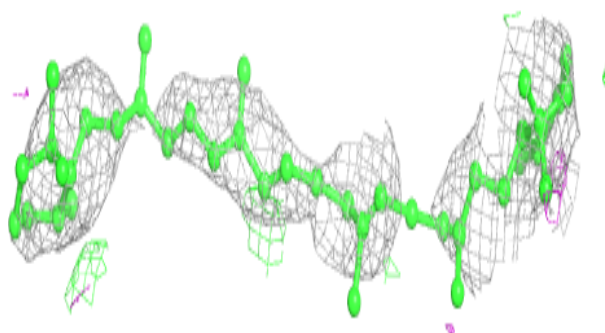


Electron density around BCR b 621:

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

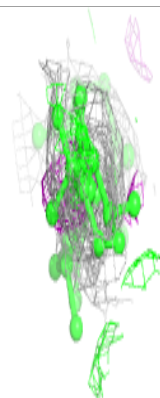
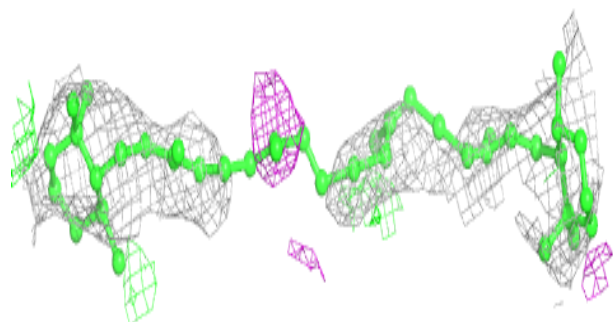
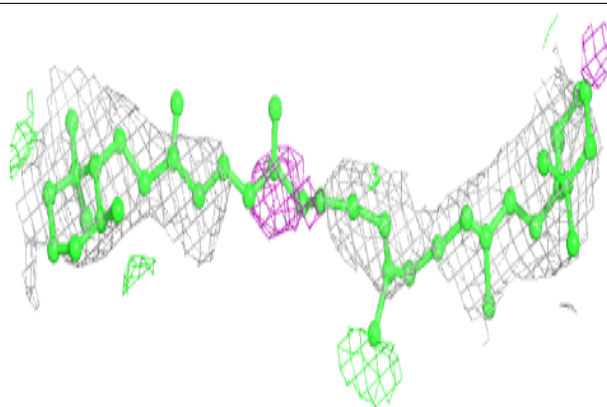
**Electron density around BCR c 514:**

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

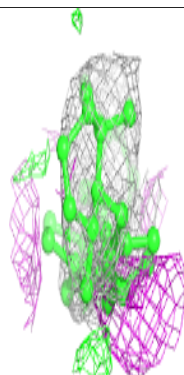
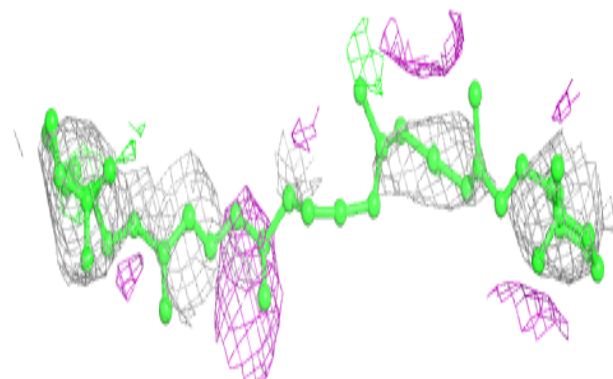
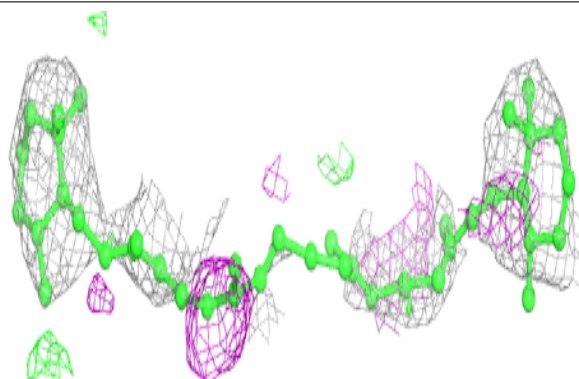


Electron density around BCR c 515:

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

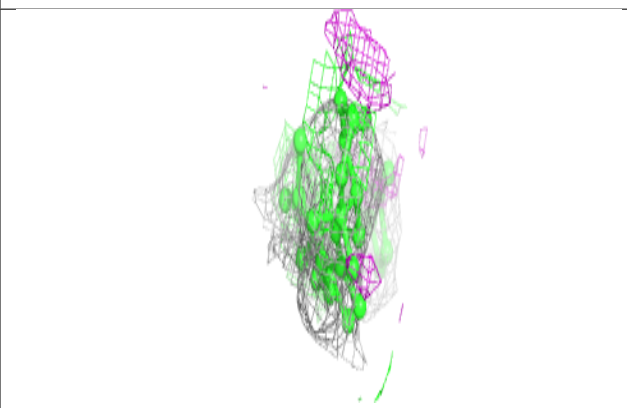
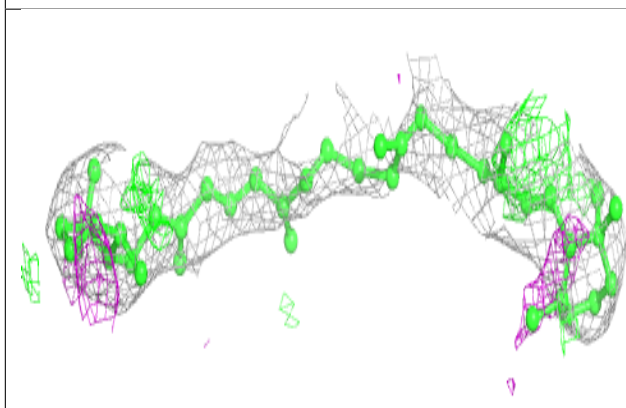
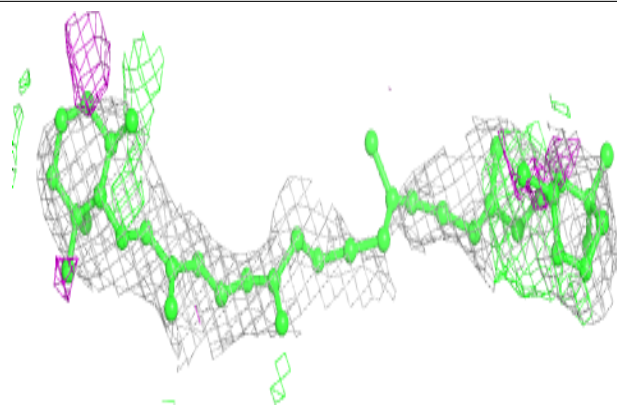
**Electron density around BCR c 521:**

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

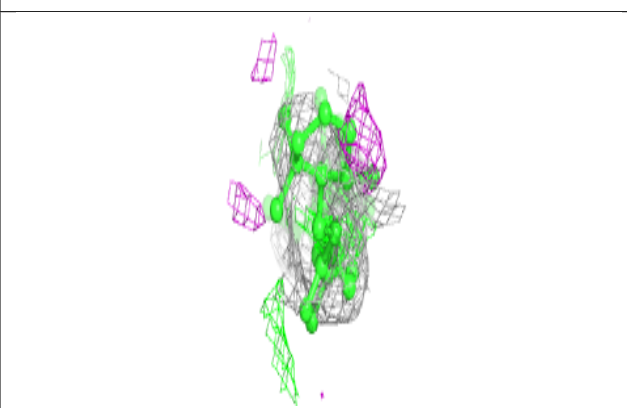
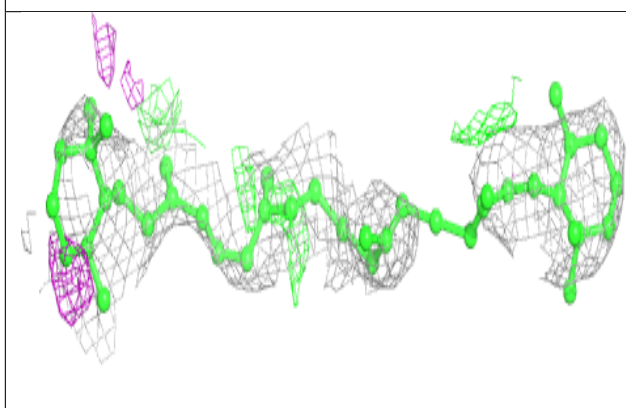
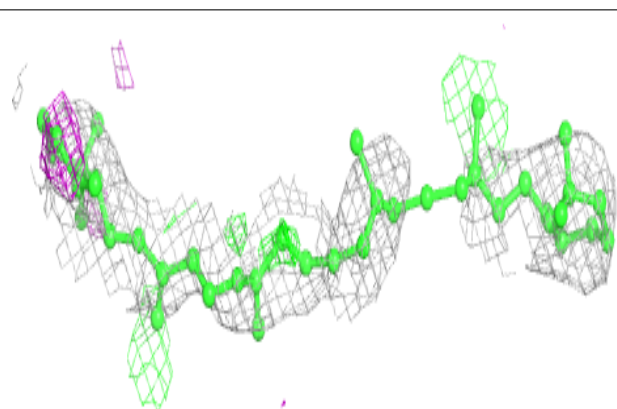


Electron density around BCR f 101:

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

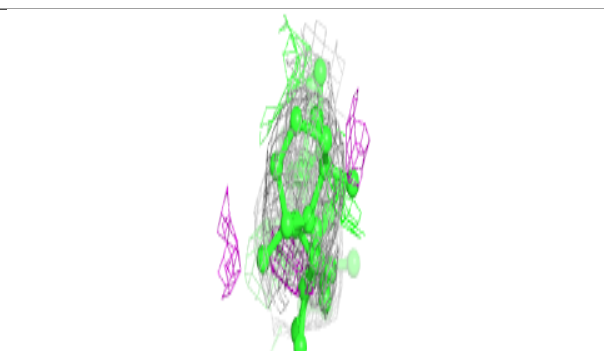
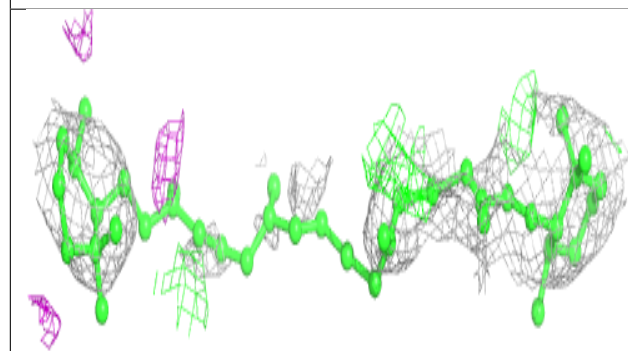
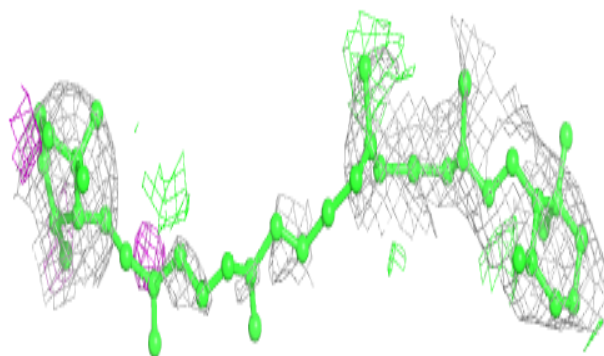
**Electron density around BCR h 101:**

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

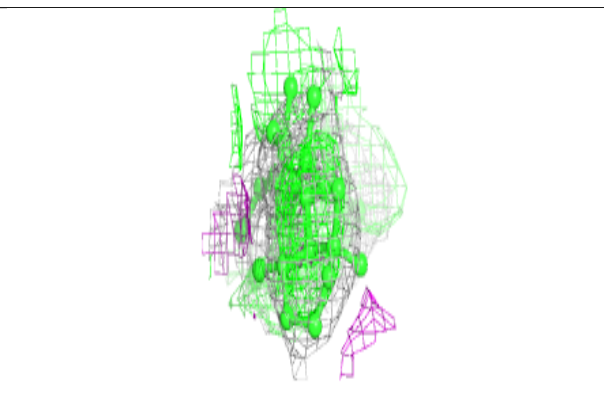
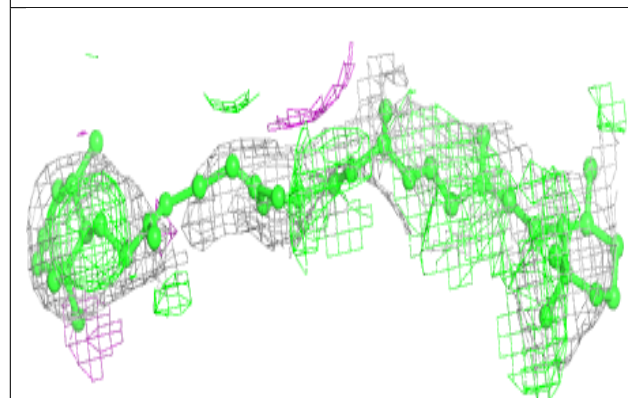
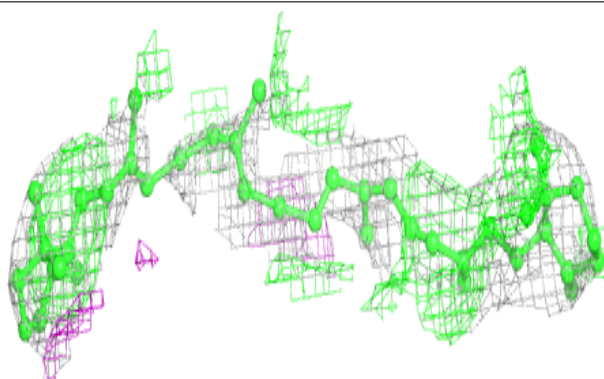


Electron density around BCR k 101:

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

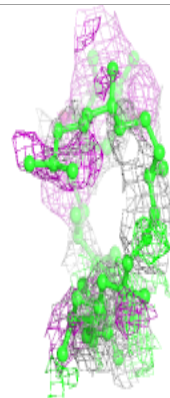
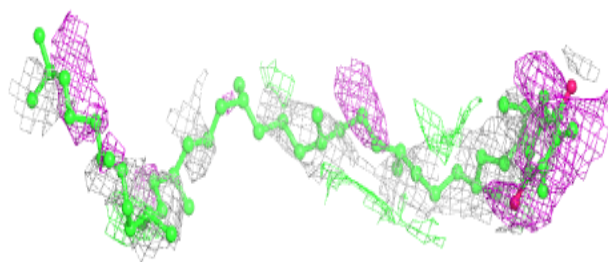
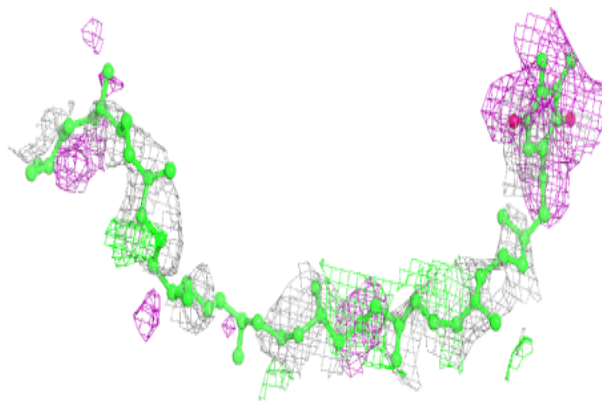
**Electron density around BCR t 101:**

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

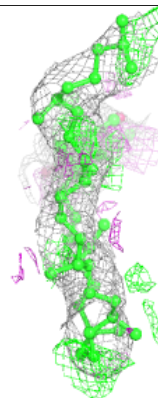
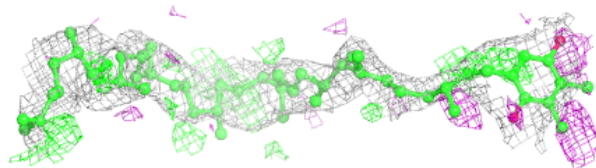
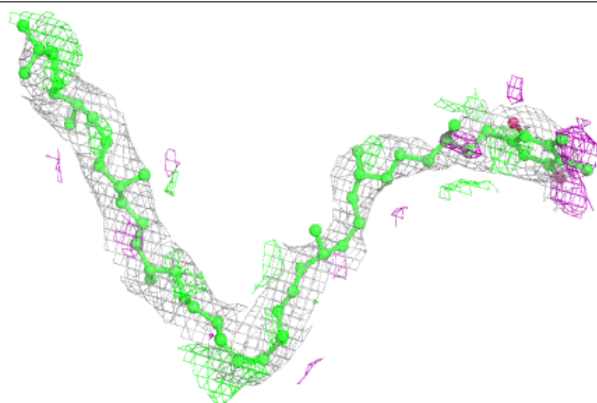


Electron density around PL9 A 611:

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

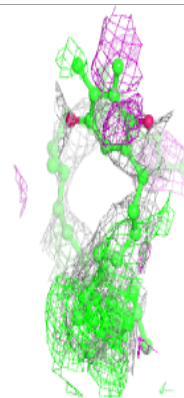
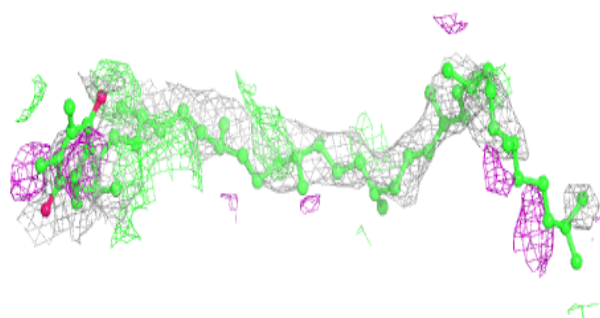
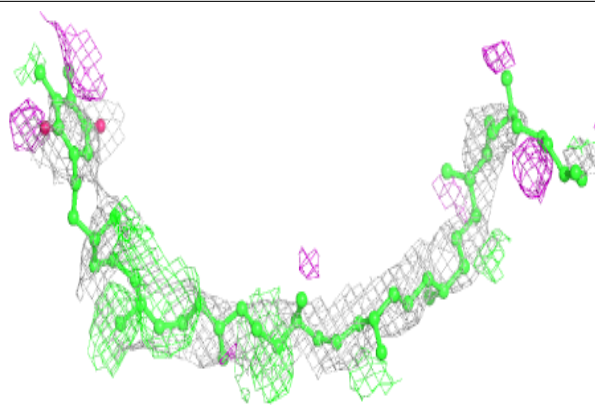
**Electron density around PL9 D 405:**

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

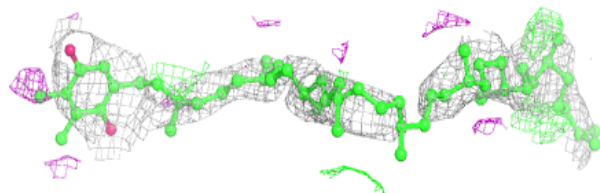
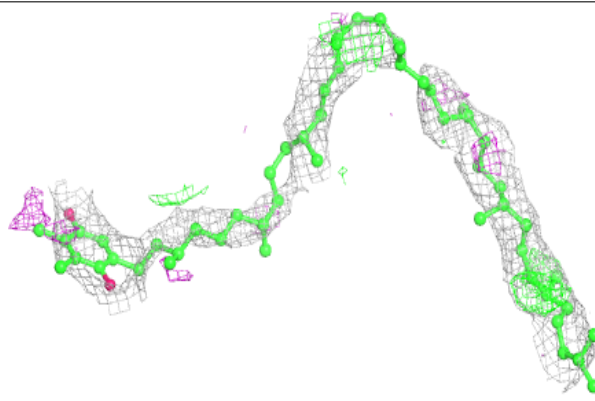


Electron density around PL9 a 611:

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

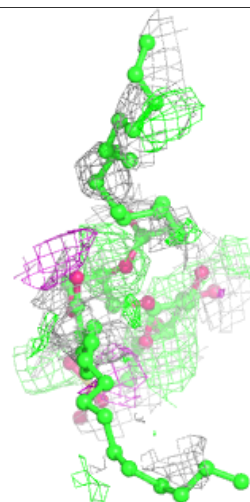
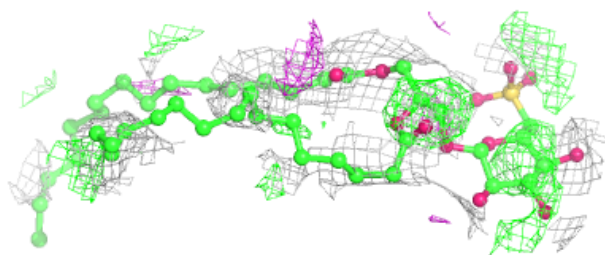
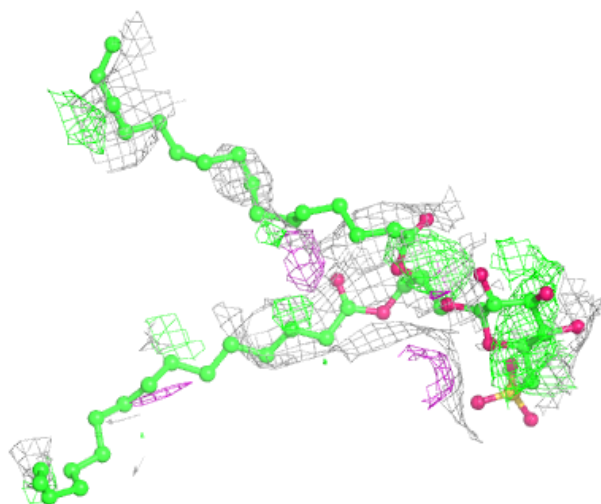
**Electron density around PL9 d 404:**

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



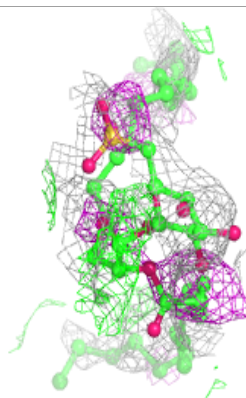
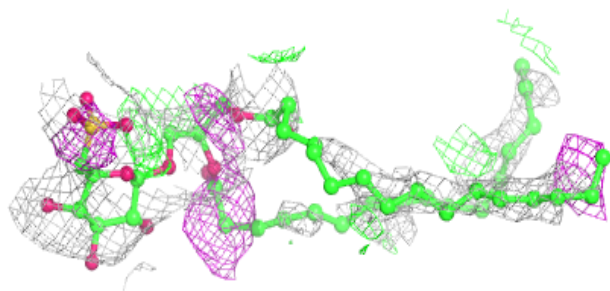
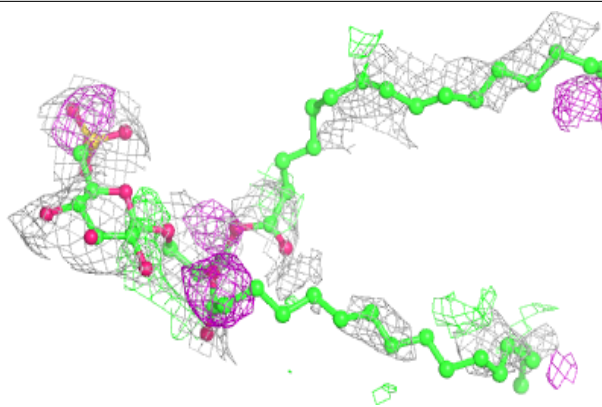
Electron density around SQD A 612:

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

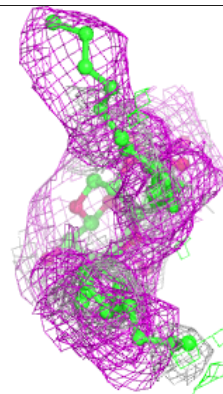
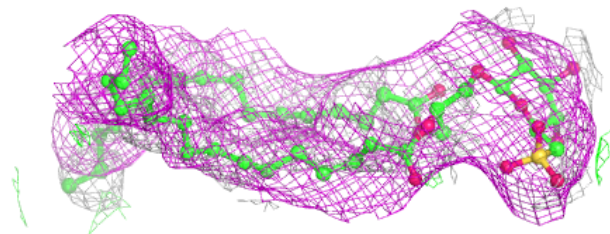
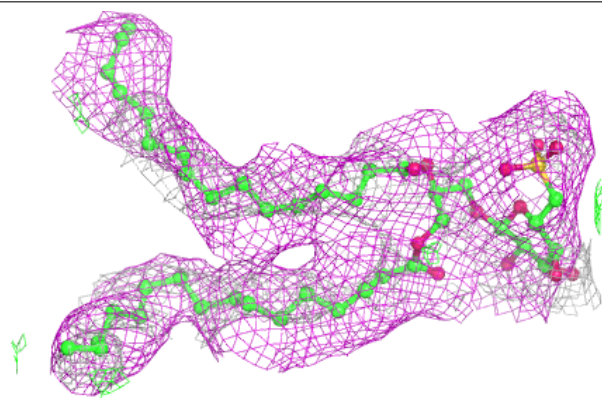


Electron density around SQD A 614:

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

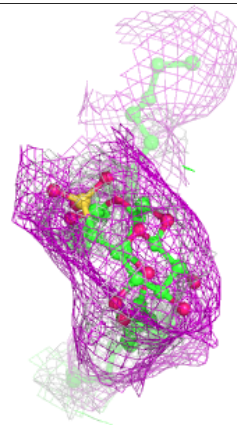
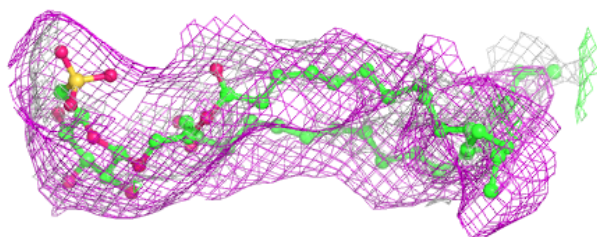
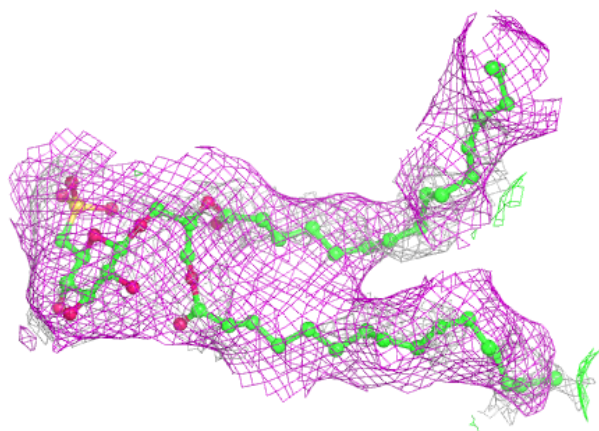
**Electron density around SQD B 622:**

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

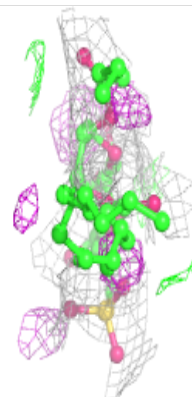
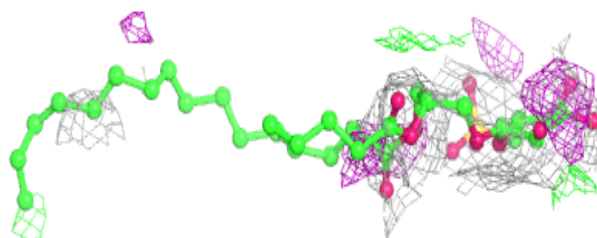
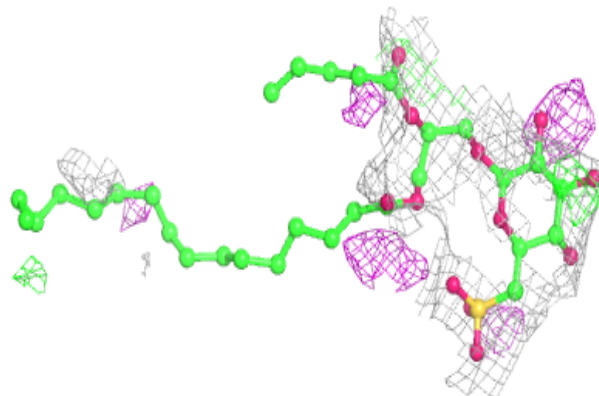


Electron density around SQD L 102:

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

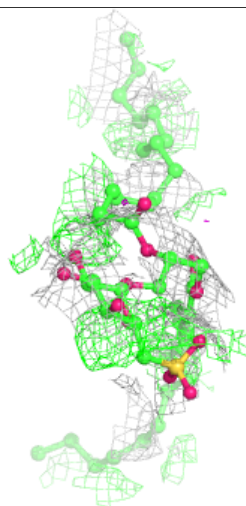
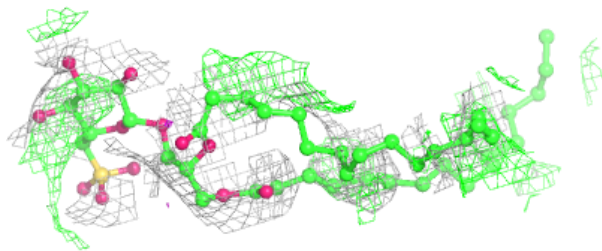
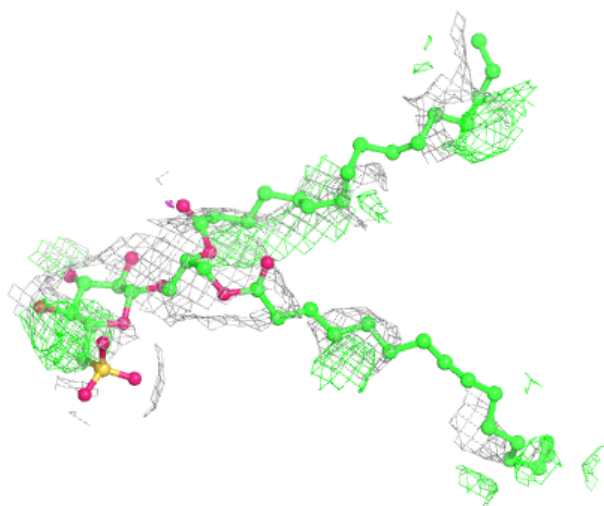
**Electron density around SQD X 101:**

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



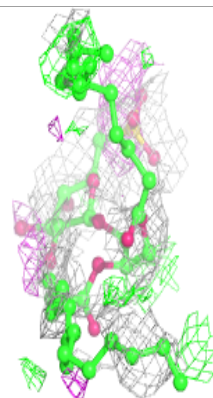
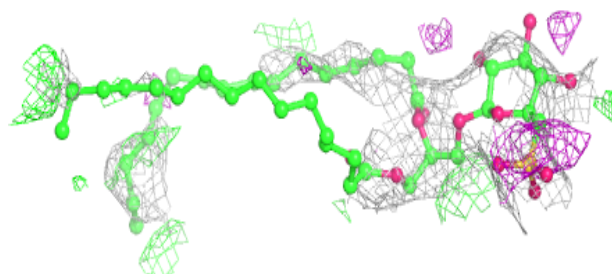
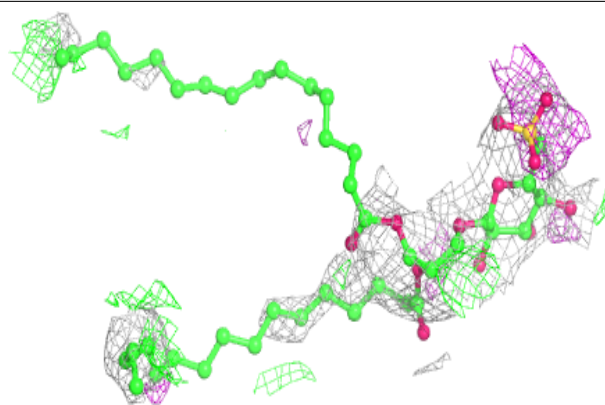
Electron density around SQD a 612:

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

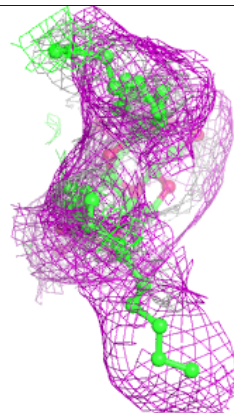
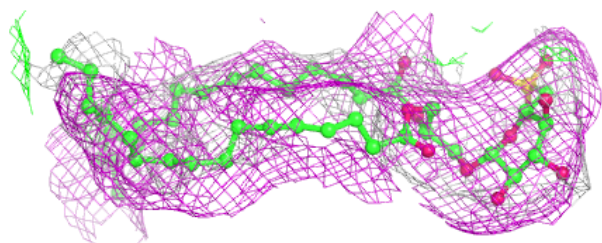
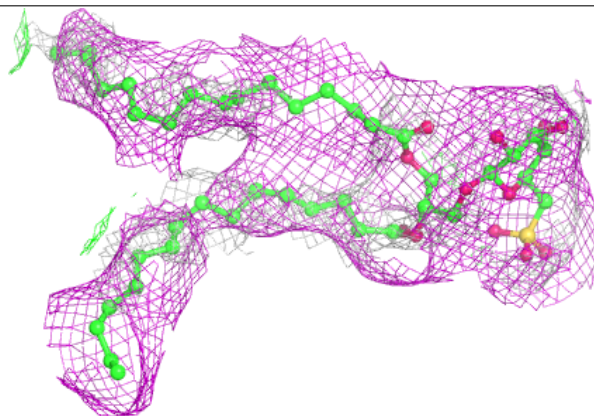


Electron density around SQD a 614:

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

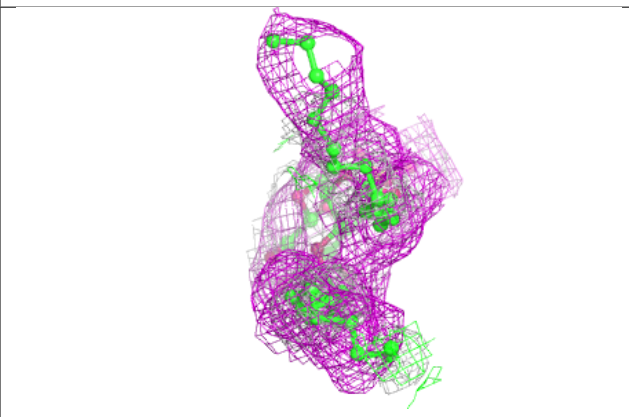
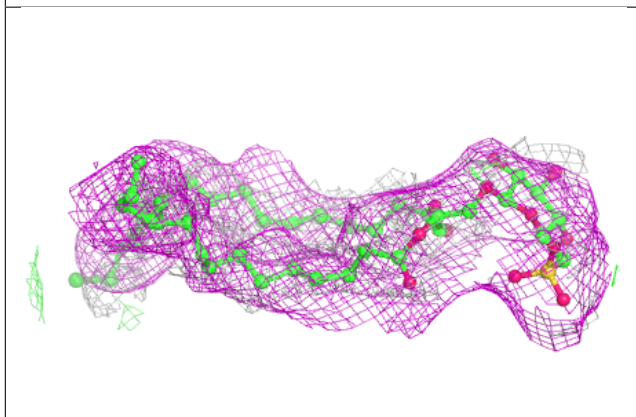
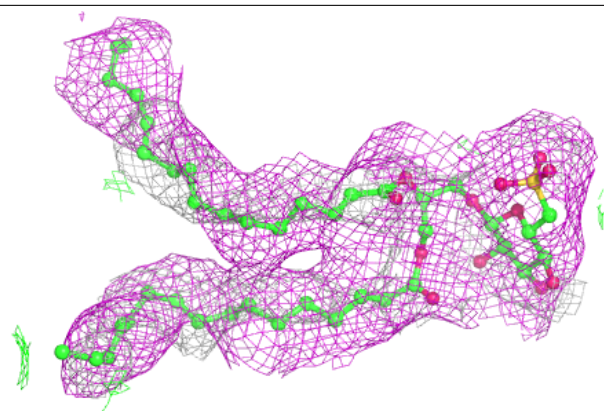
**Electron density around SQD b 601:**

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

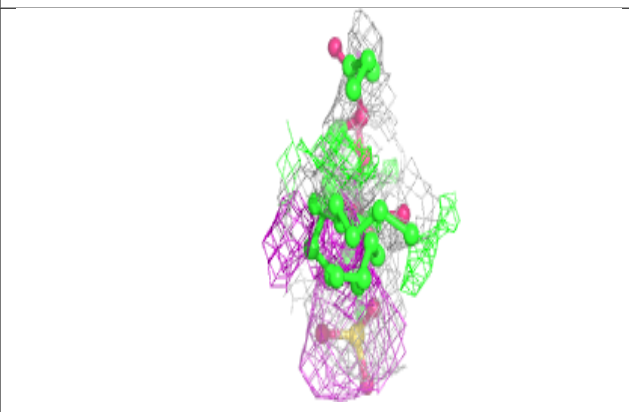
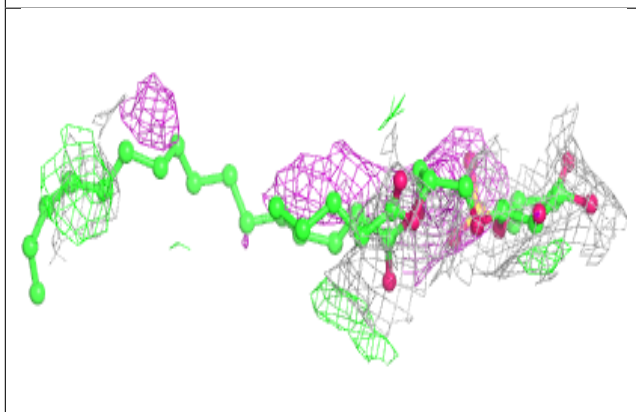
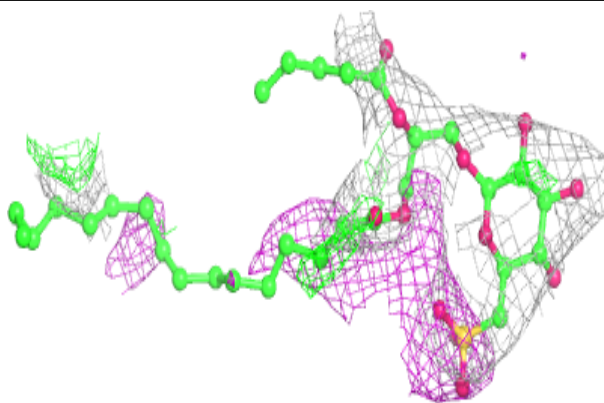


Electron density around SQD 1 101:

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

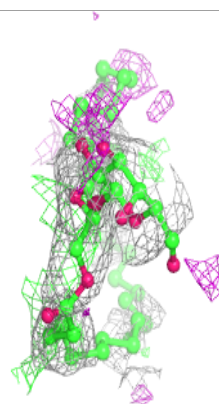
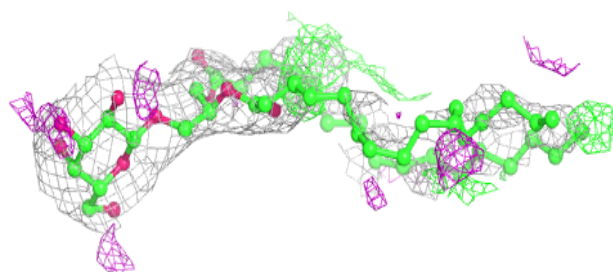
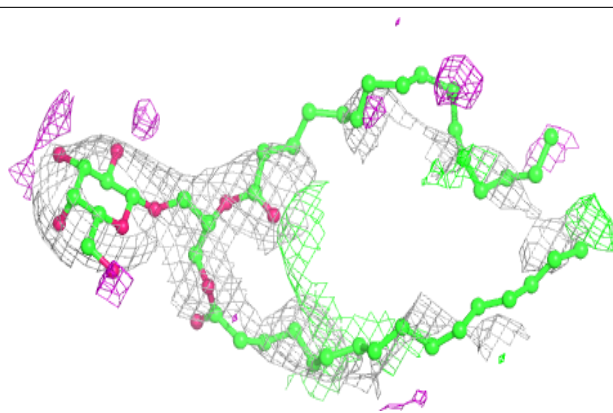
**Electron density around SQD x 101:**

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

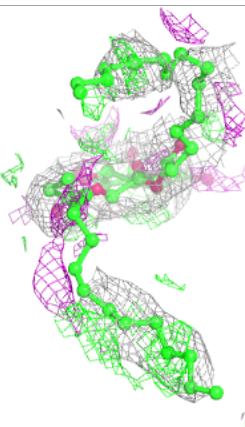
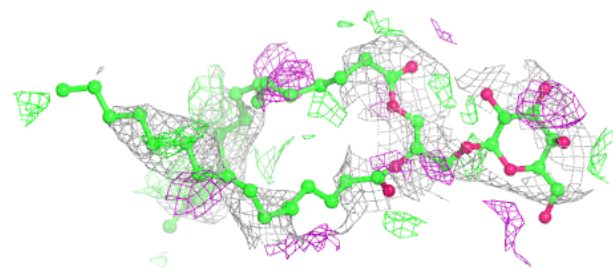
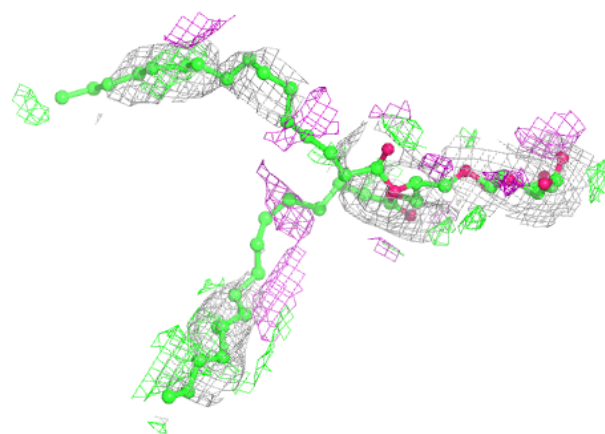


Electron density around LMG A 613:

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

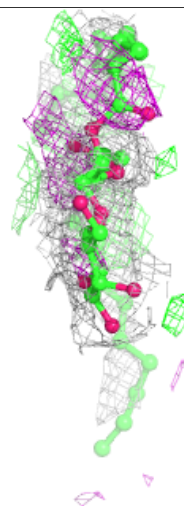
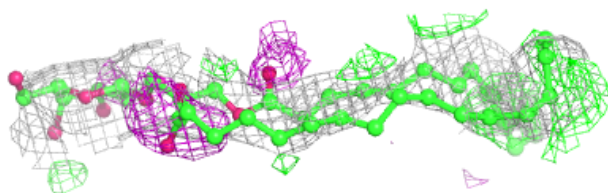
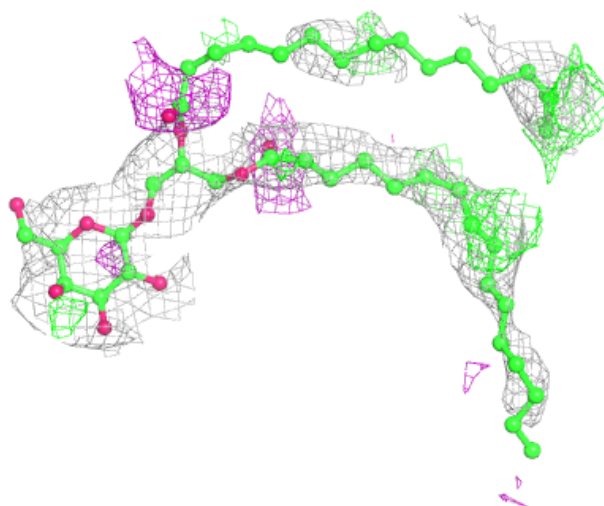
**Electron density around LMG B 621:**

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



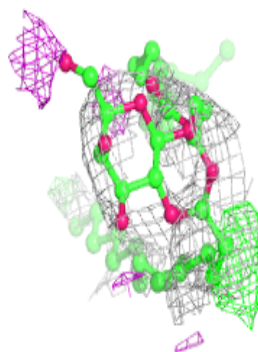
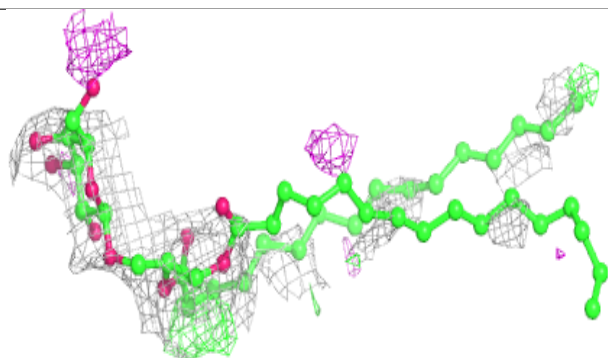
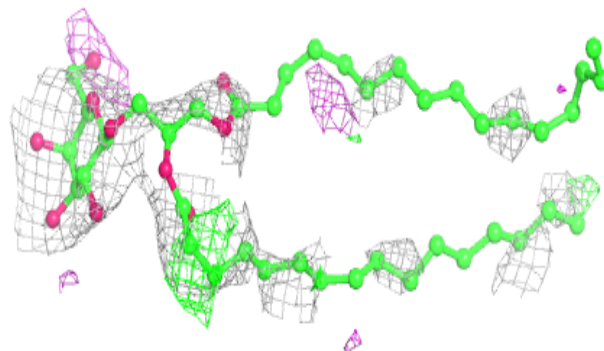
Electron density around LMG C 518:

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

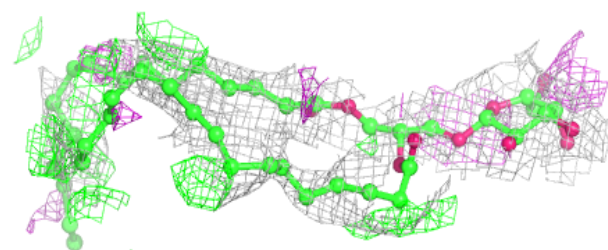
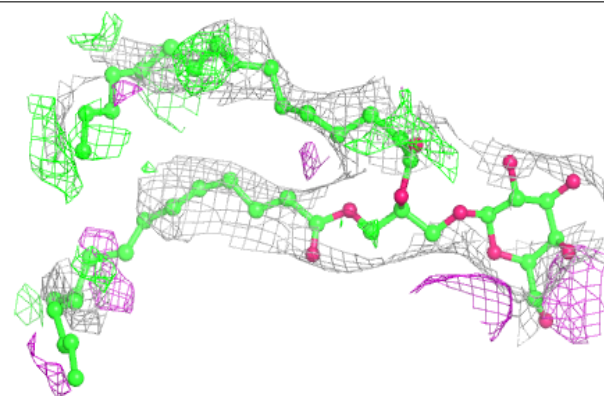


Electron density around LMG C 519:

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

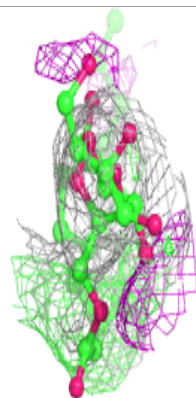
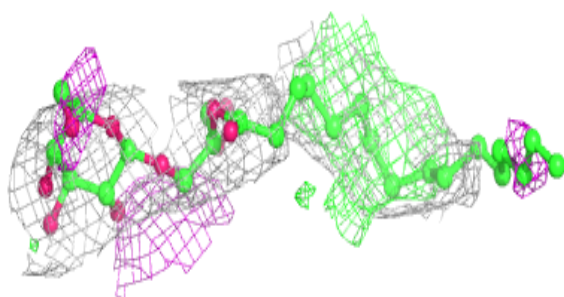
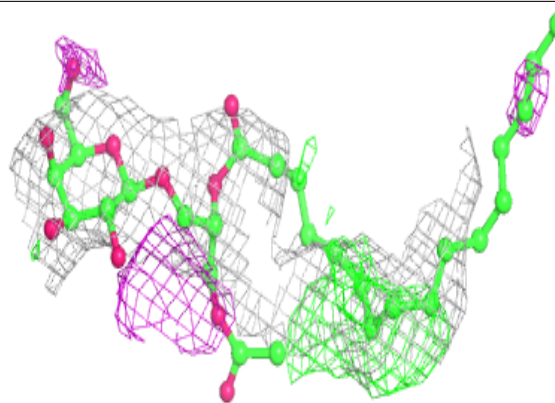
**Electron density around LMG D 408:**

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

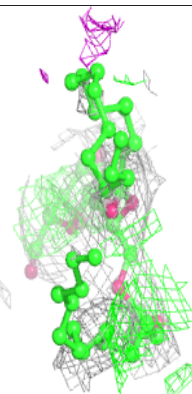
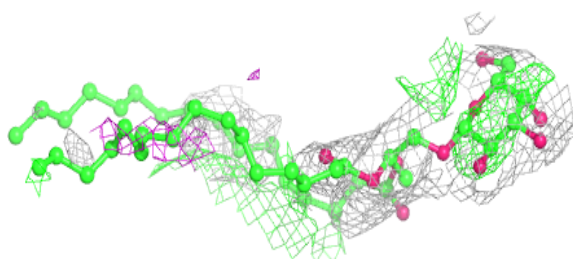
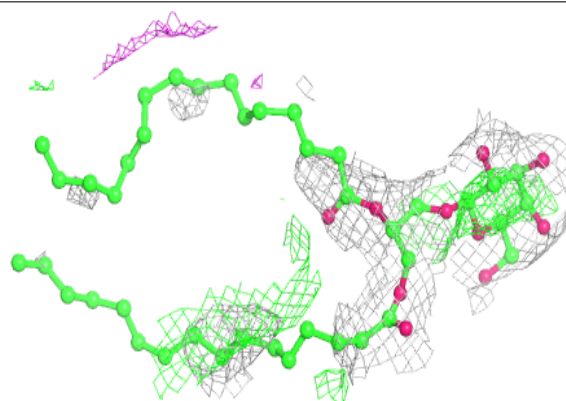


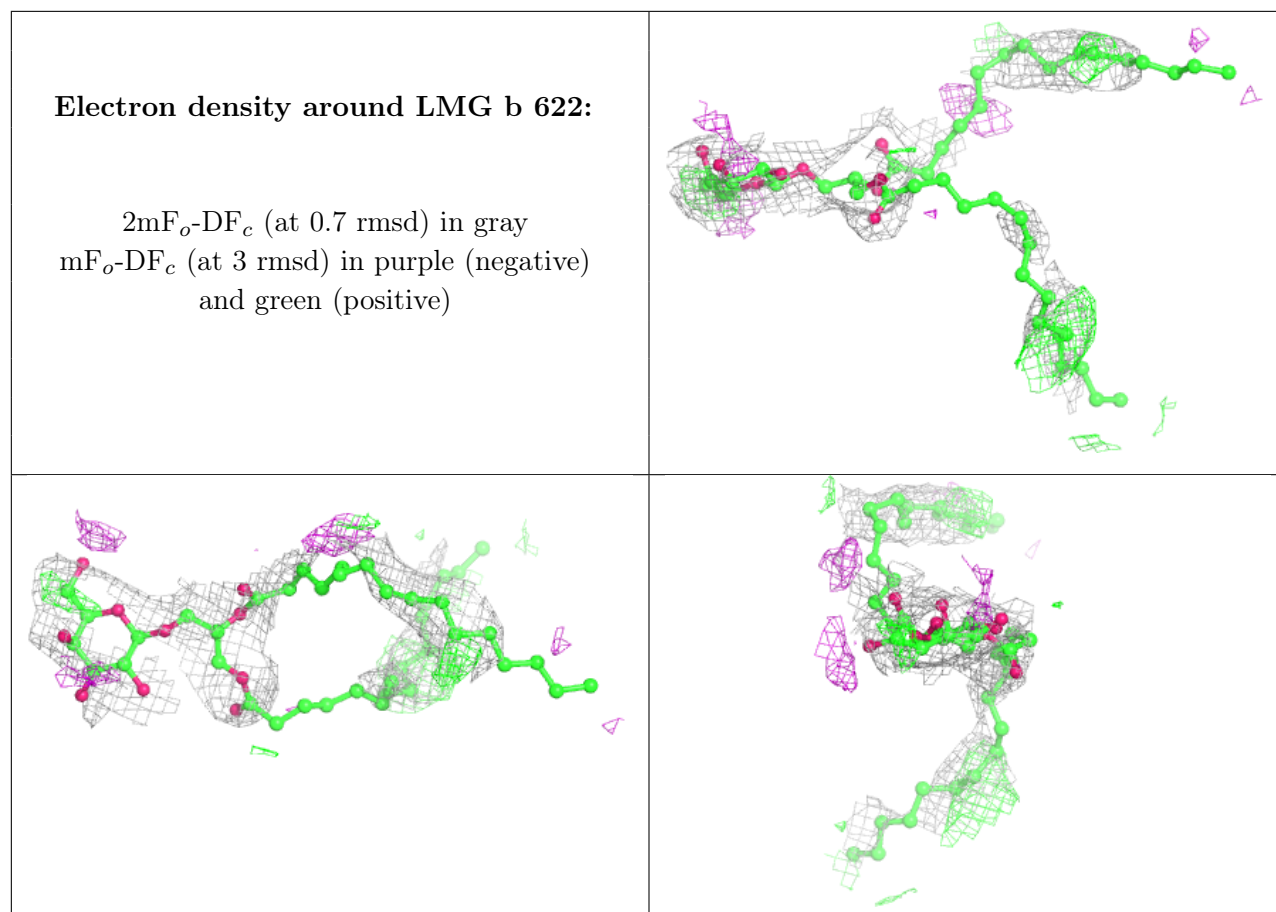
Electron density around LMG Z 101:

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

**Electron density around LMG a 613:**

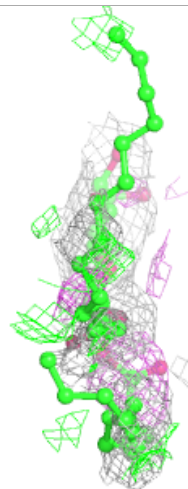
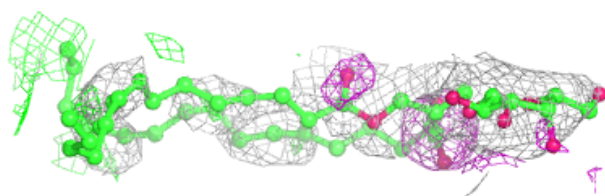
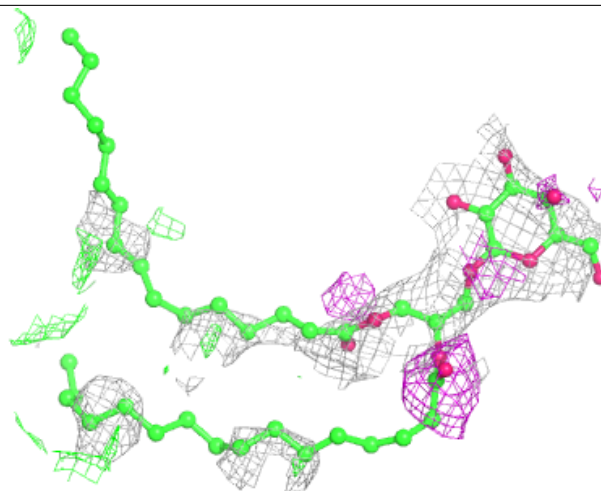
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





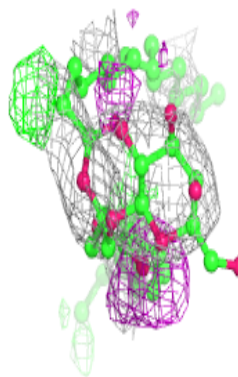
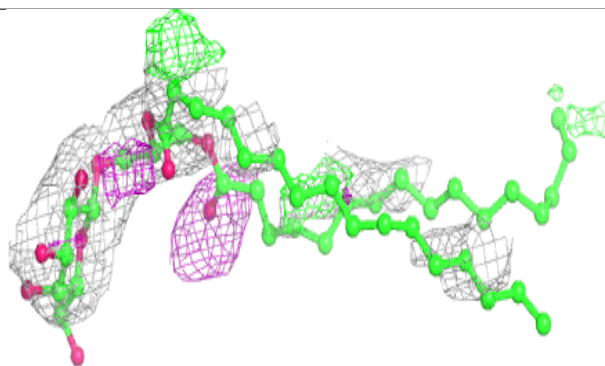
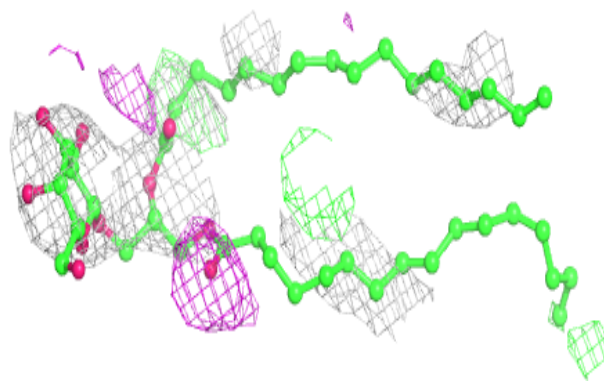
Electron density around LMG c 519:

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

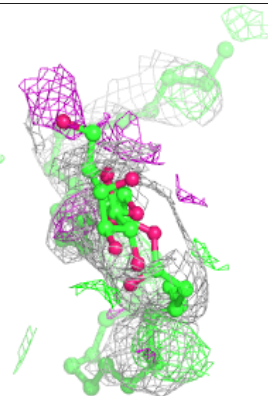
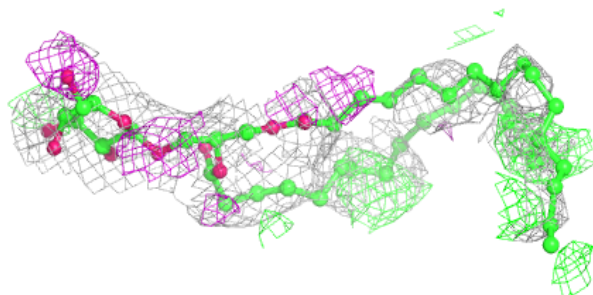
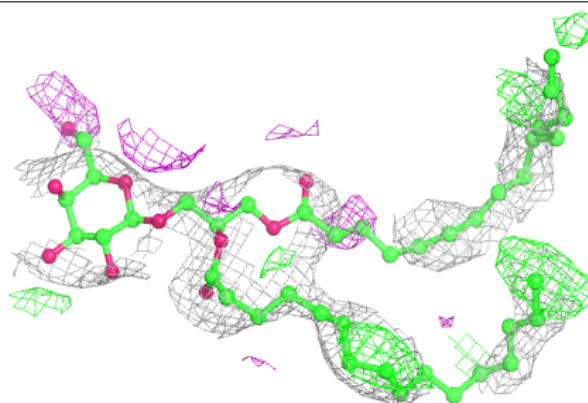


Electron density around LMG c 520:

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

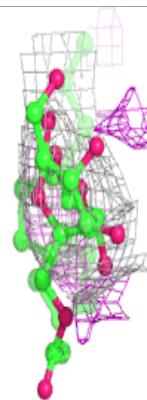
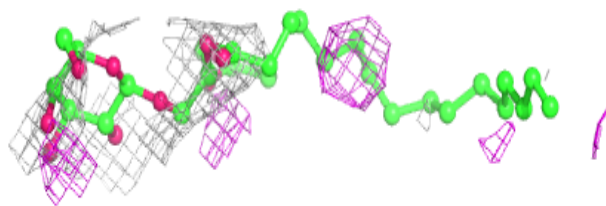
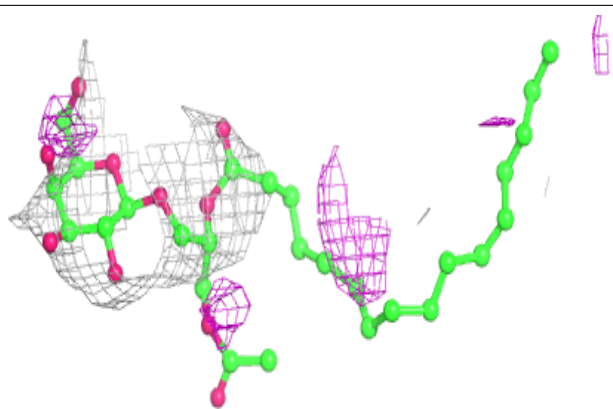
**Electron density around LMG j 101:**

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

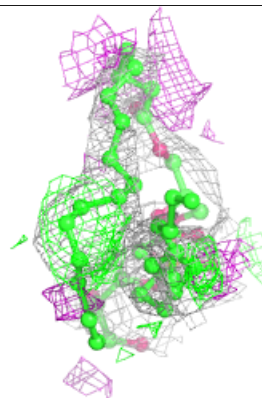
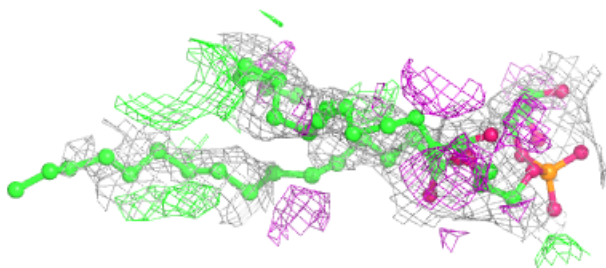
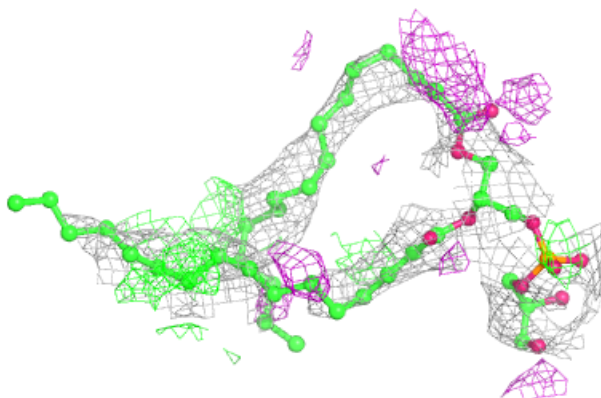


Electron density around LMG z 101:

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

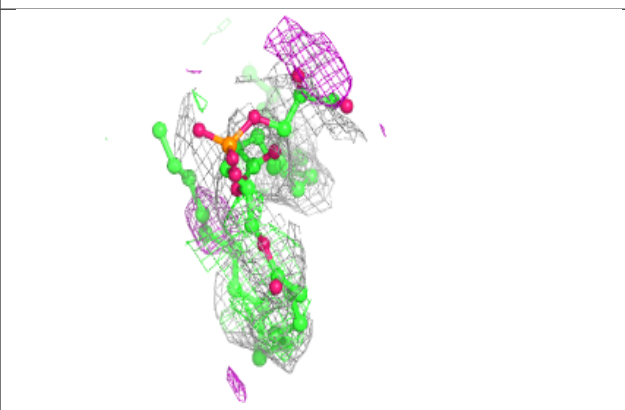
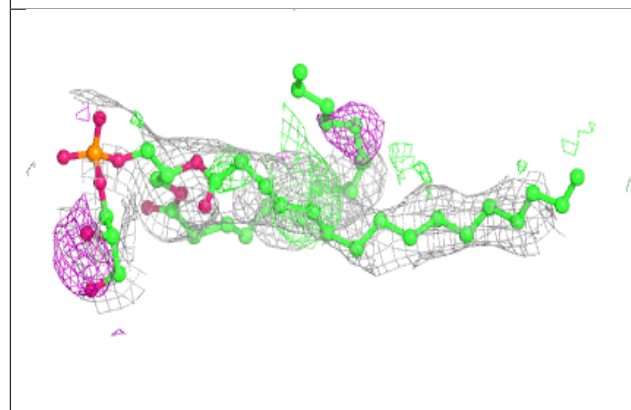
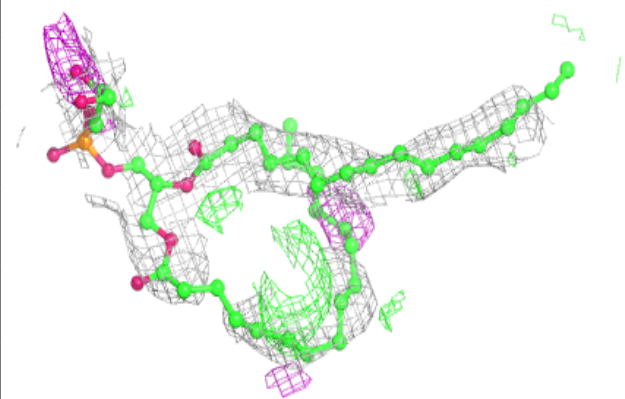
**Electron density around LHG A 615:**

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

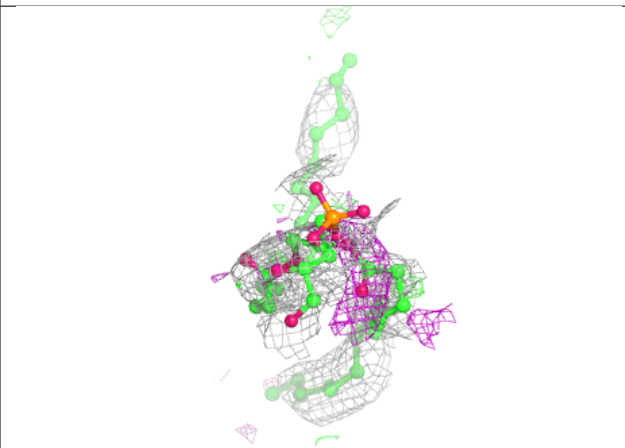
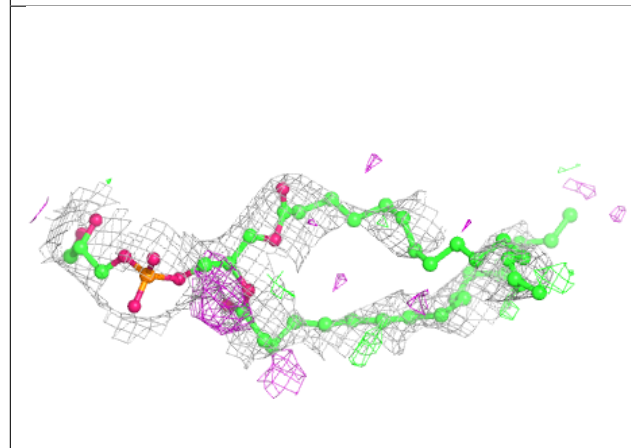
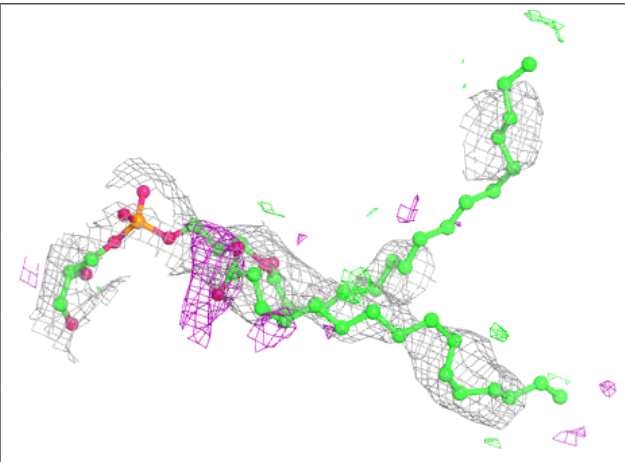


Electron density around LHG D 406:

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

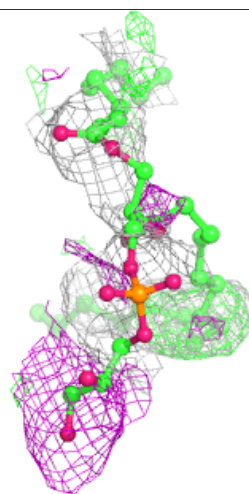
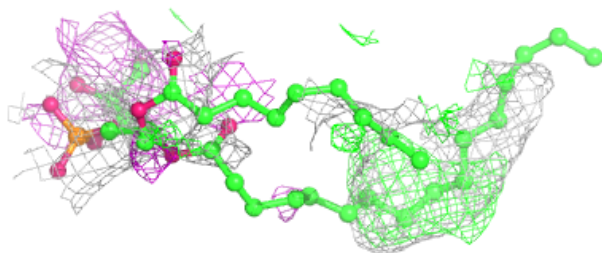
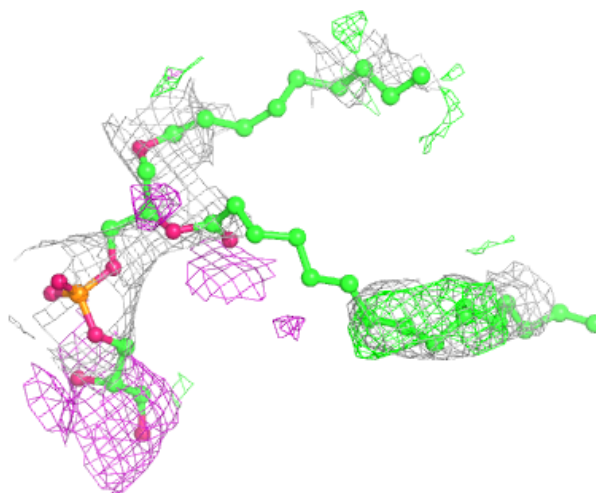
**Electron density around LHG D 407:**

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



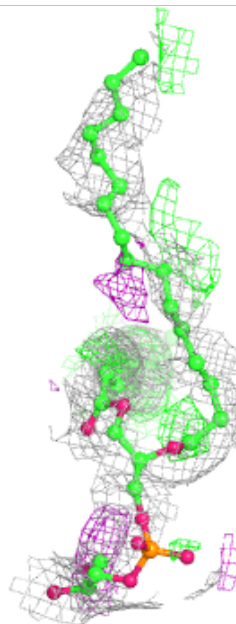
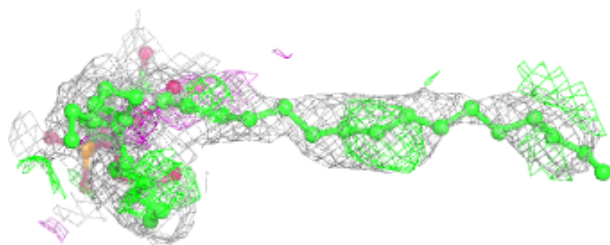
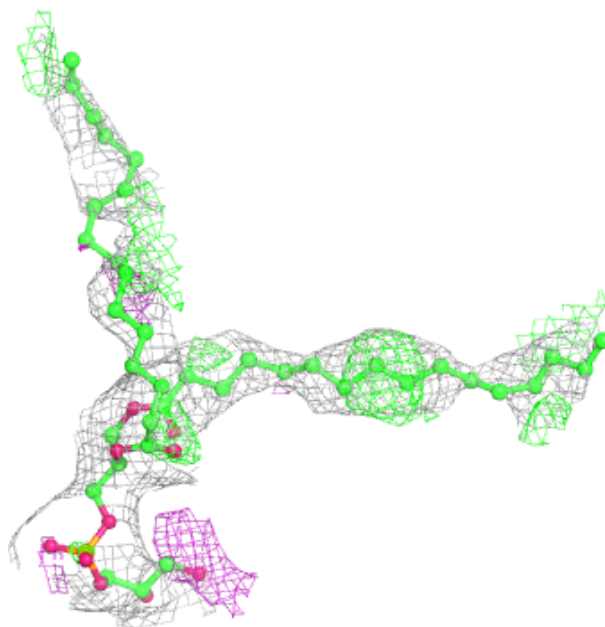
Electron density around LHG E 102:

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



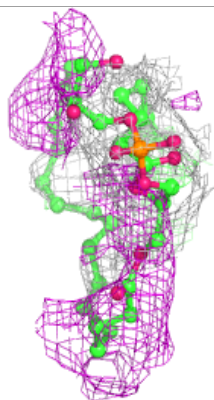
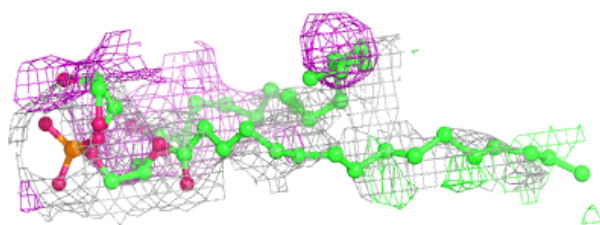
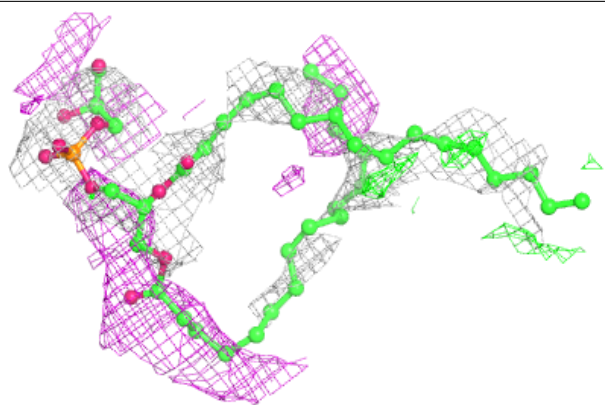
Electron density around LHG L 101:

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

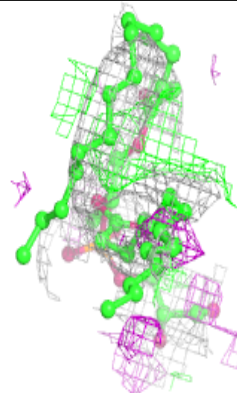
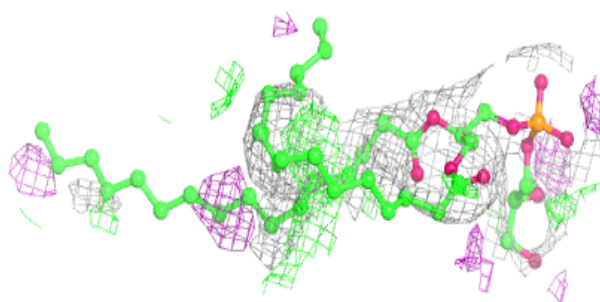
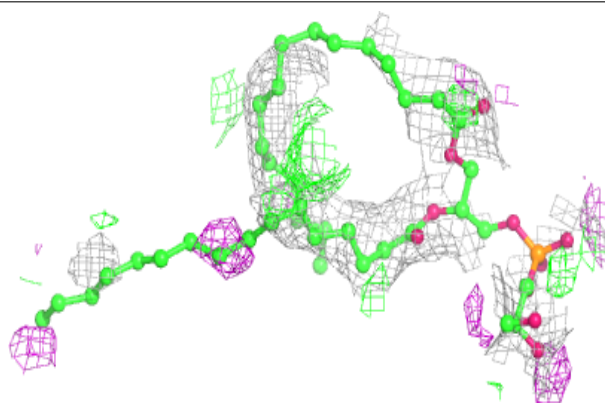


Electron density around LHG a 616:

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

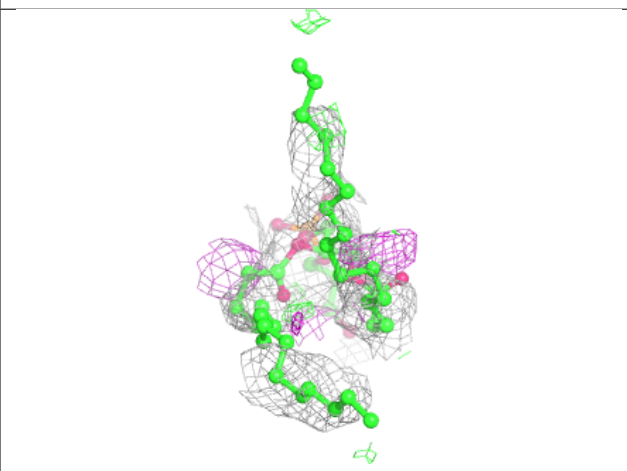
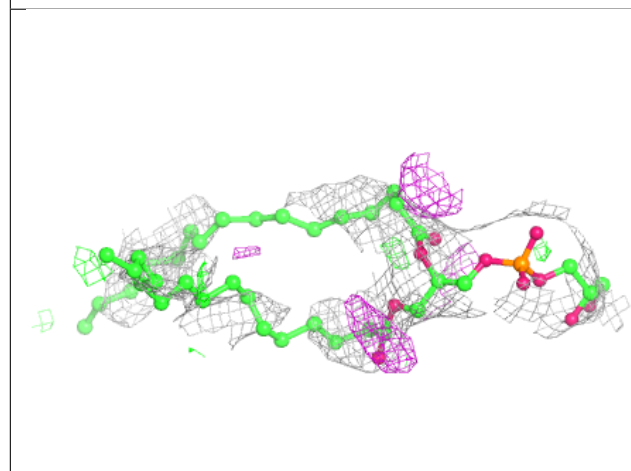
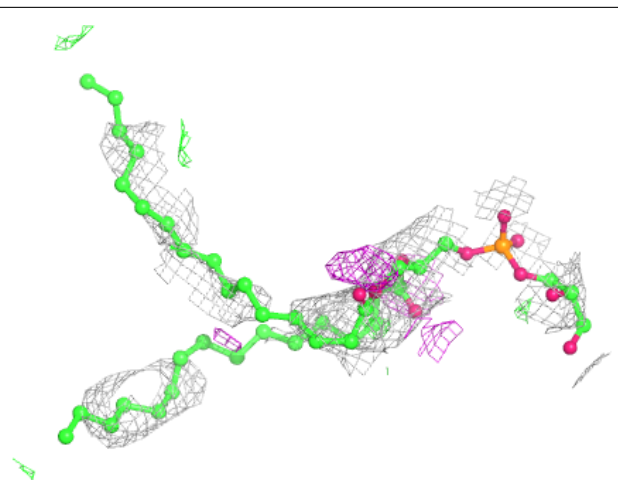
**Electron density around LHG d 406:**

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



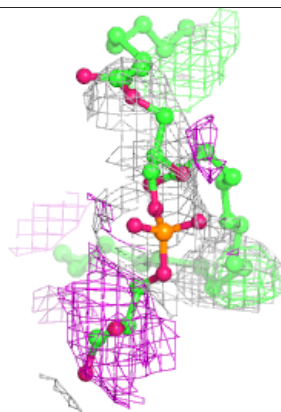
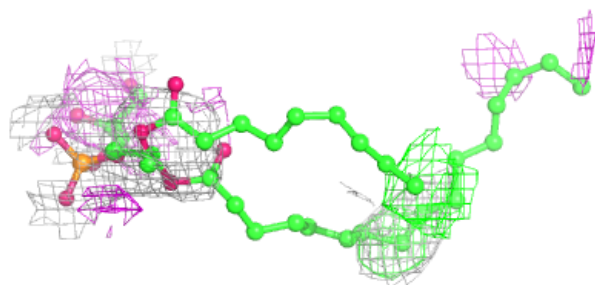
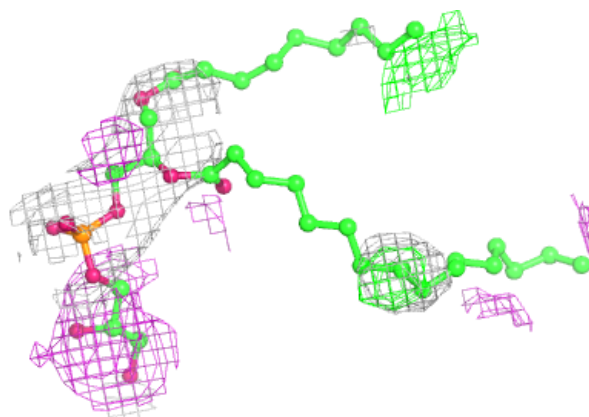
Electron density around LHG d 407:

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



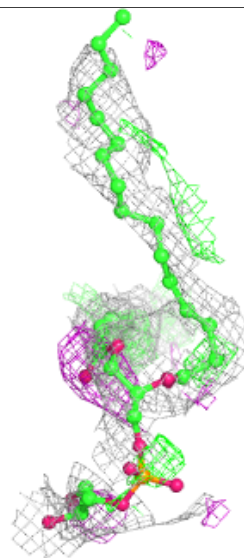
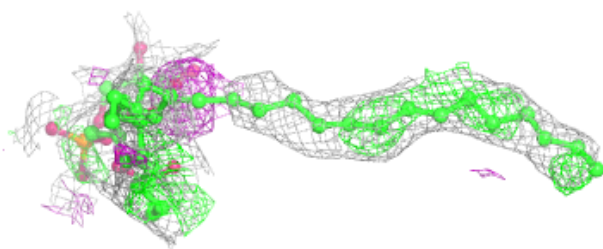
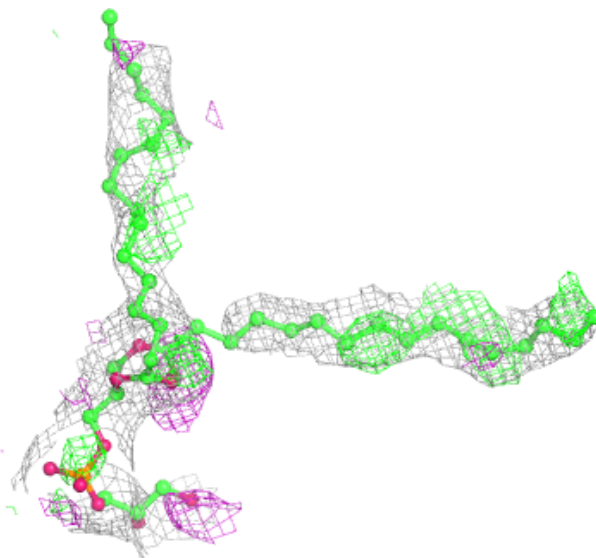
Electron density around LHG e 101:

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



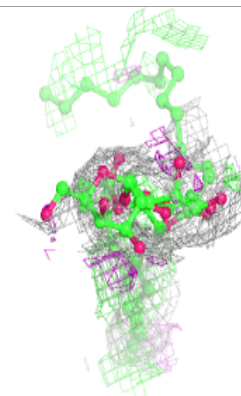
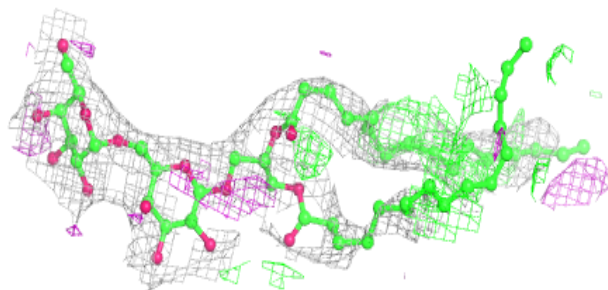
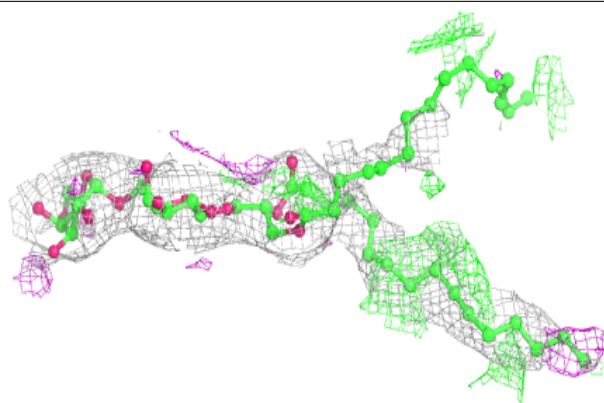
Electron density around LHG 1 102:

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

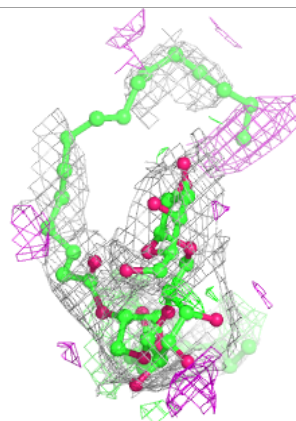
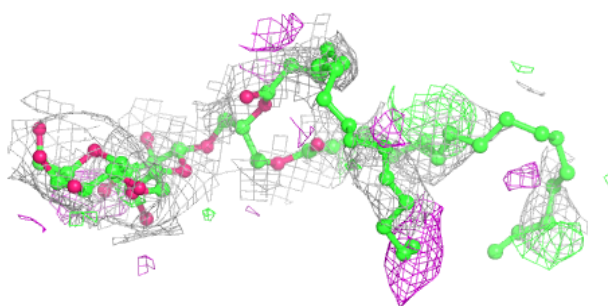
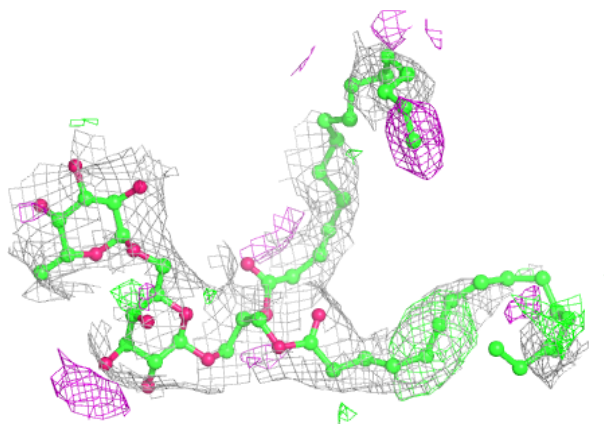


Electron density around DGD C 515:

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

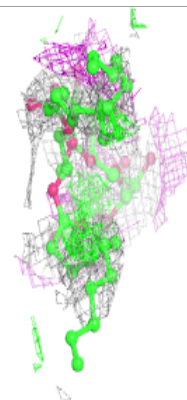
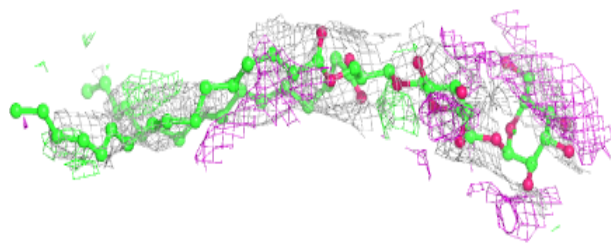
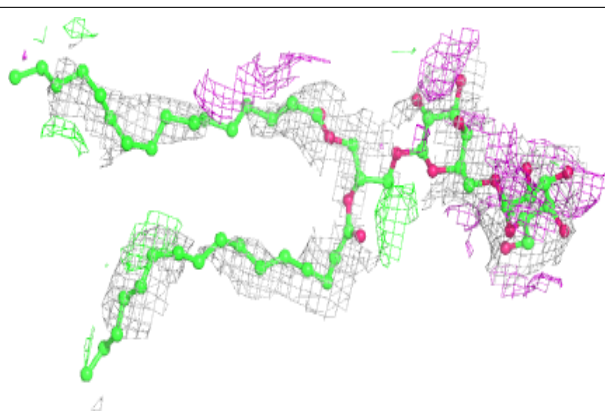
**Electron density around DGD C 516:**

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

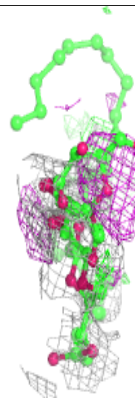
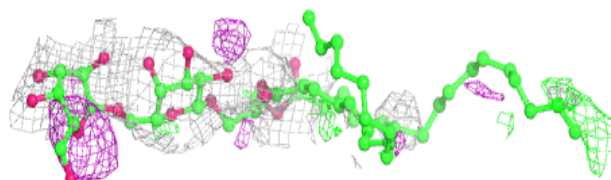
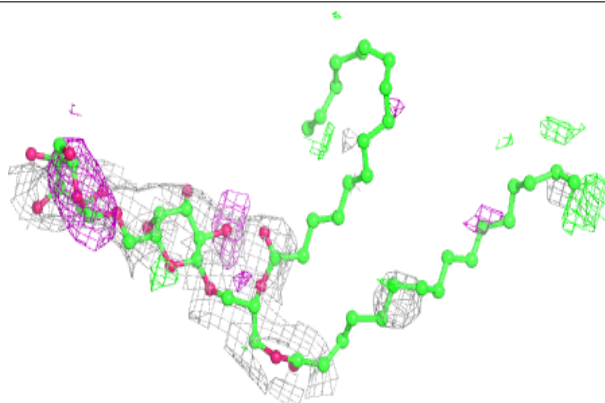


Electron density around DGD C 517:

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

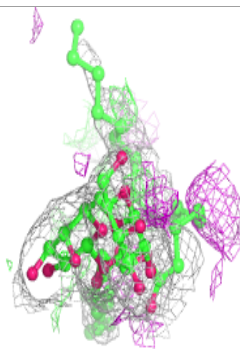
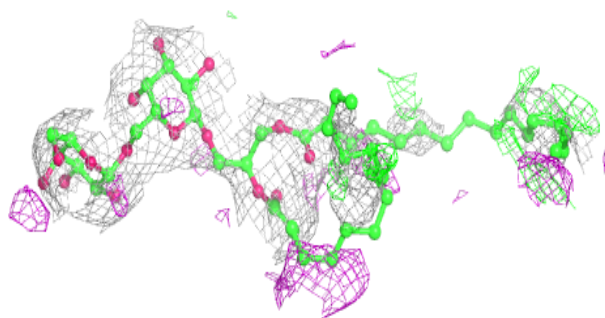
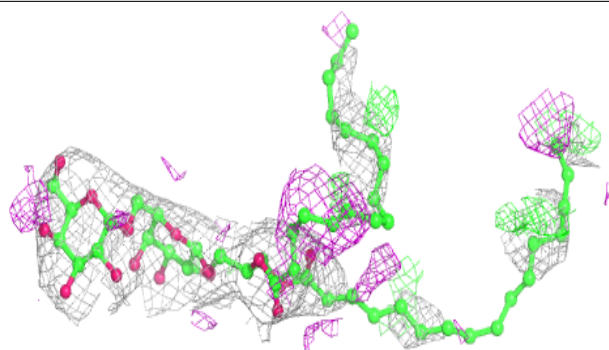
**Electron density around DGD E 101:**

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

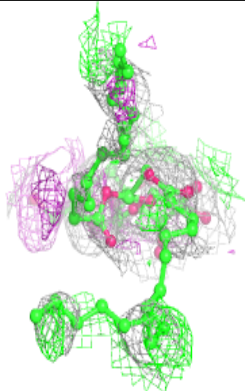
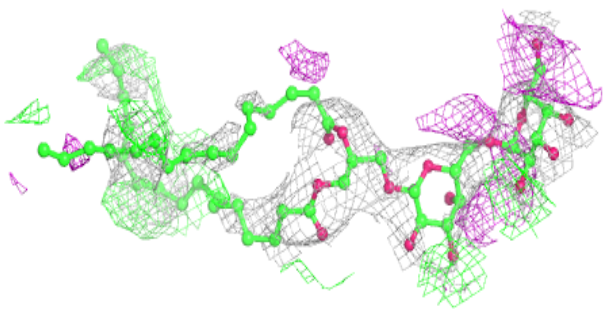
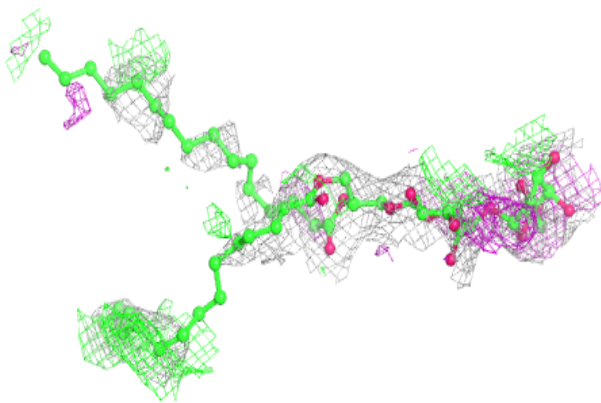


Electron density around DGD H 102:

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

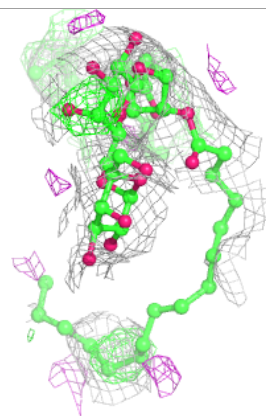
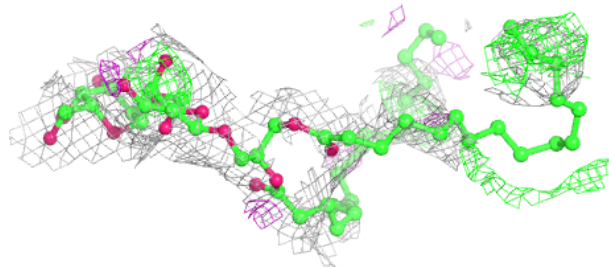
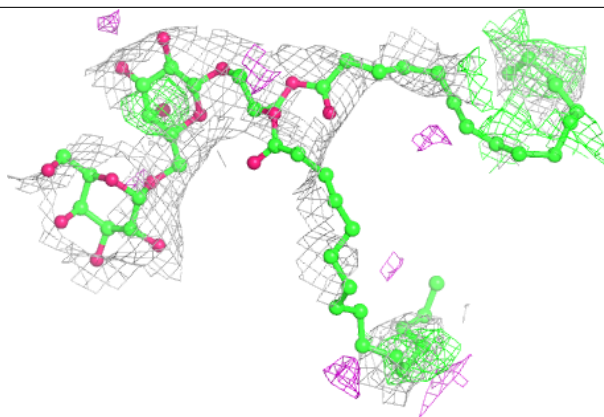
**Electron density around DGD c 516:**

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

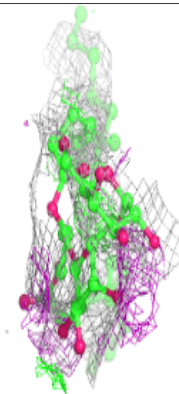
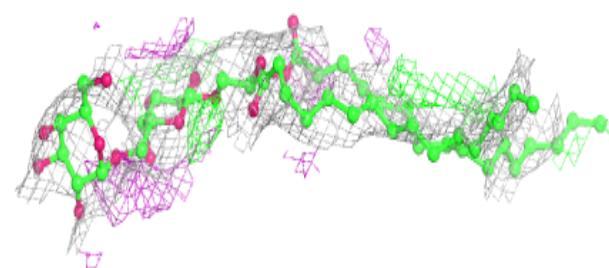
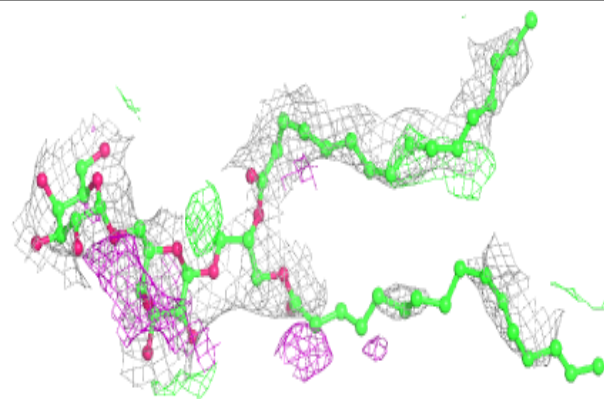


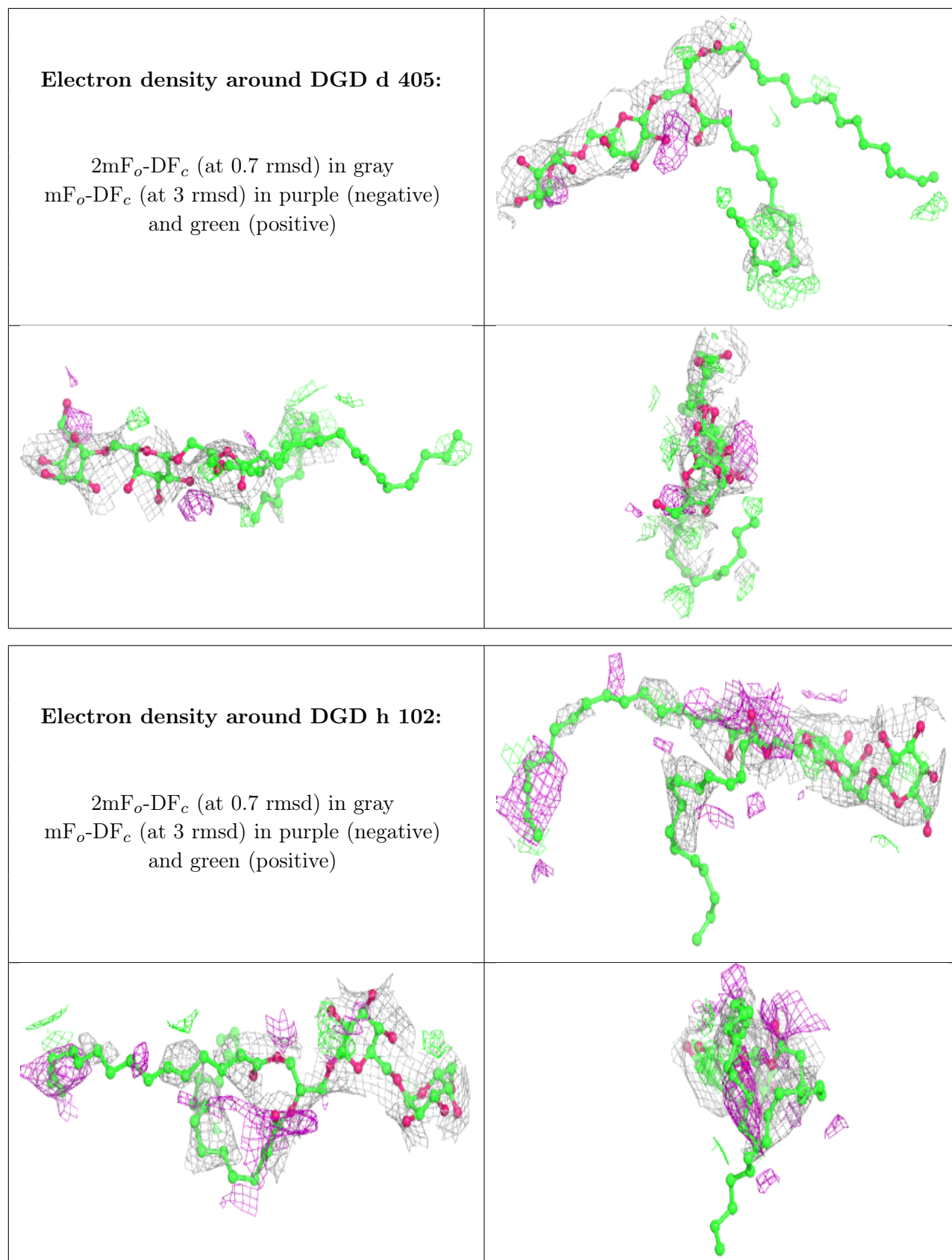
Electron density around DGD c 517:

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

**Electron density around DGD c 518:**

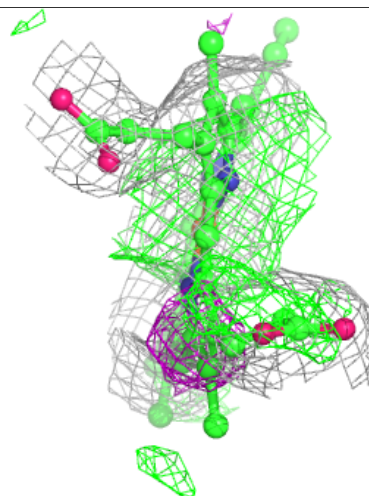
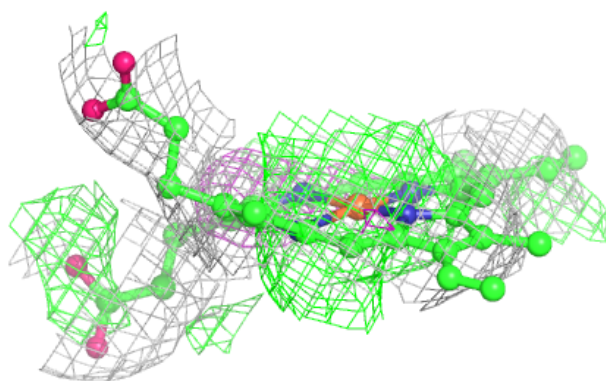
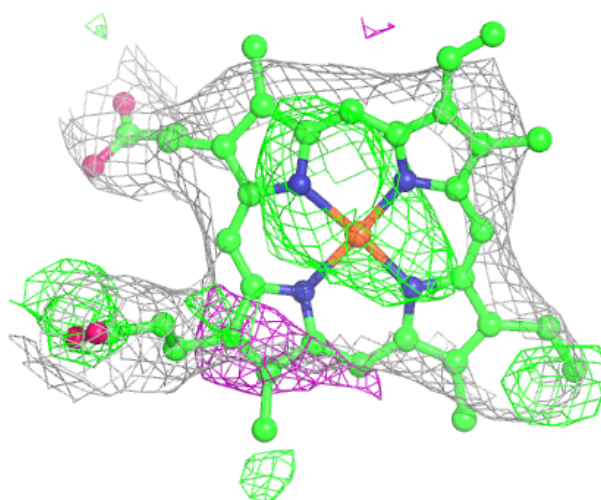
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





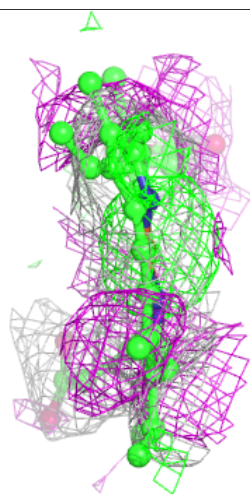
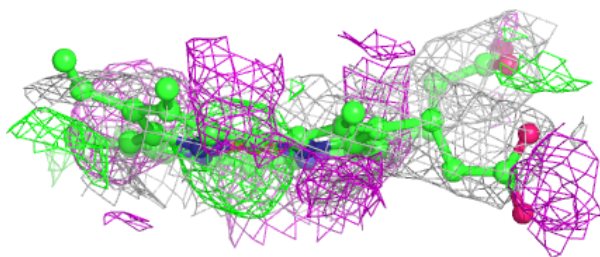
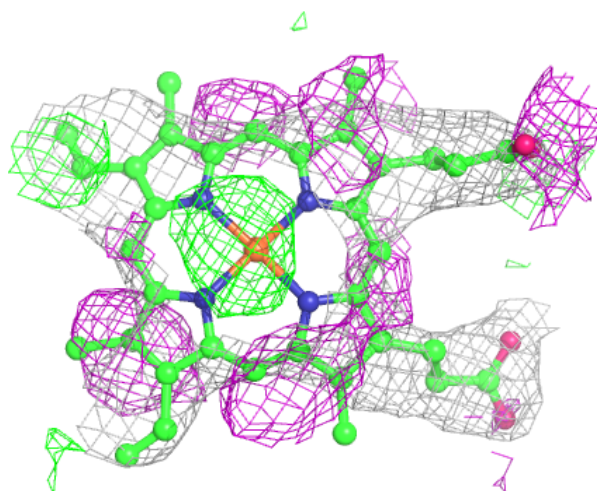
Electron density around HEM E 103:

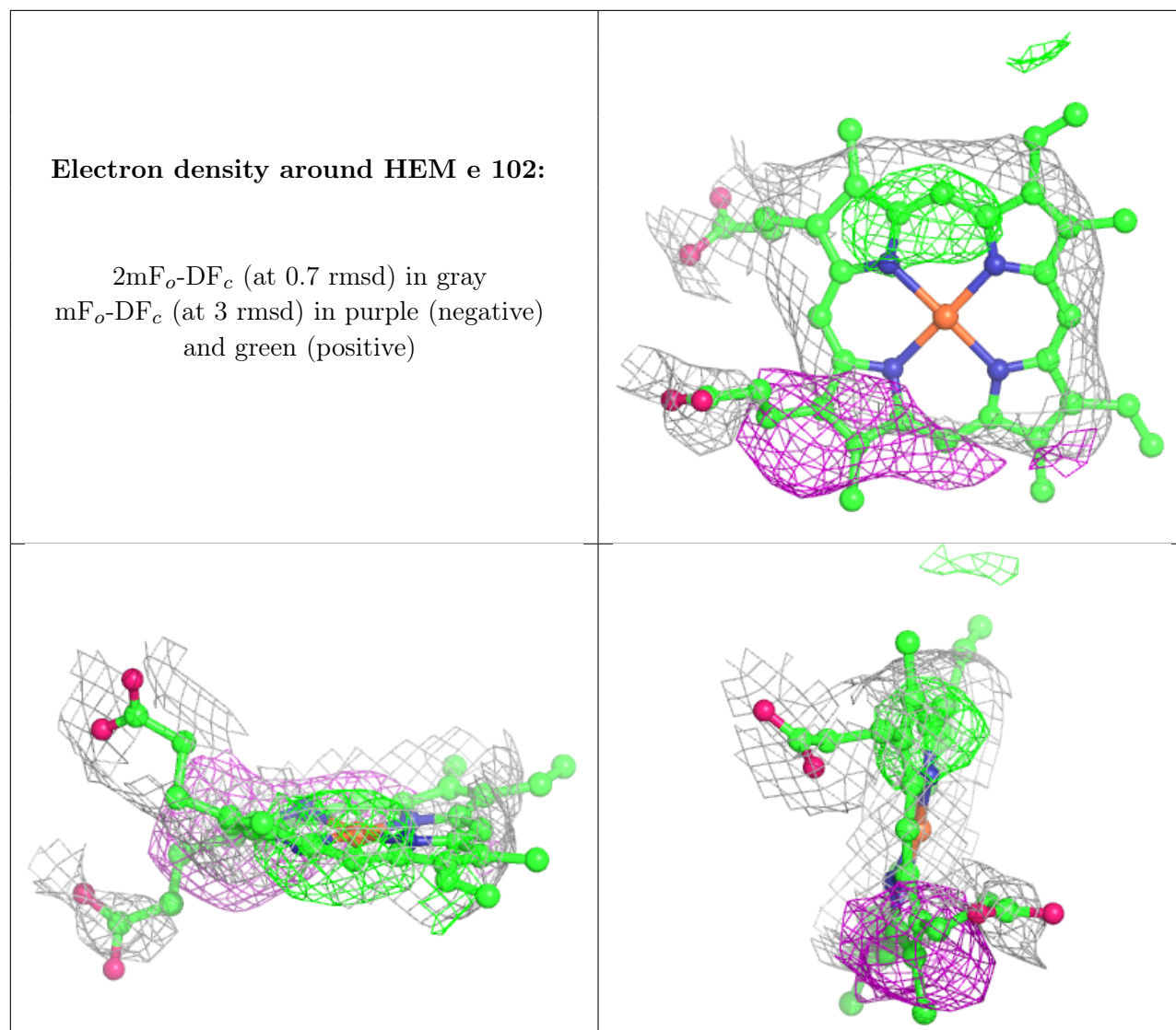
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

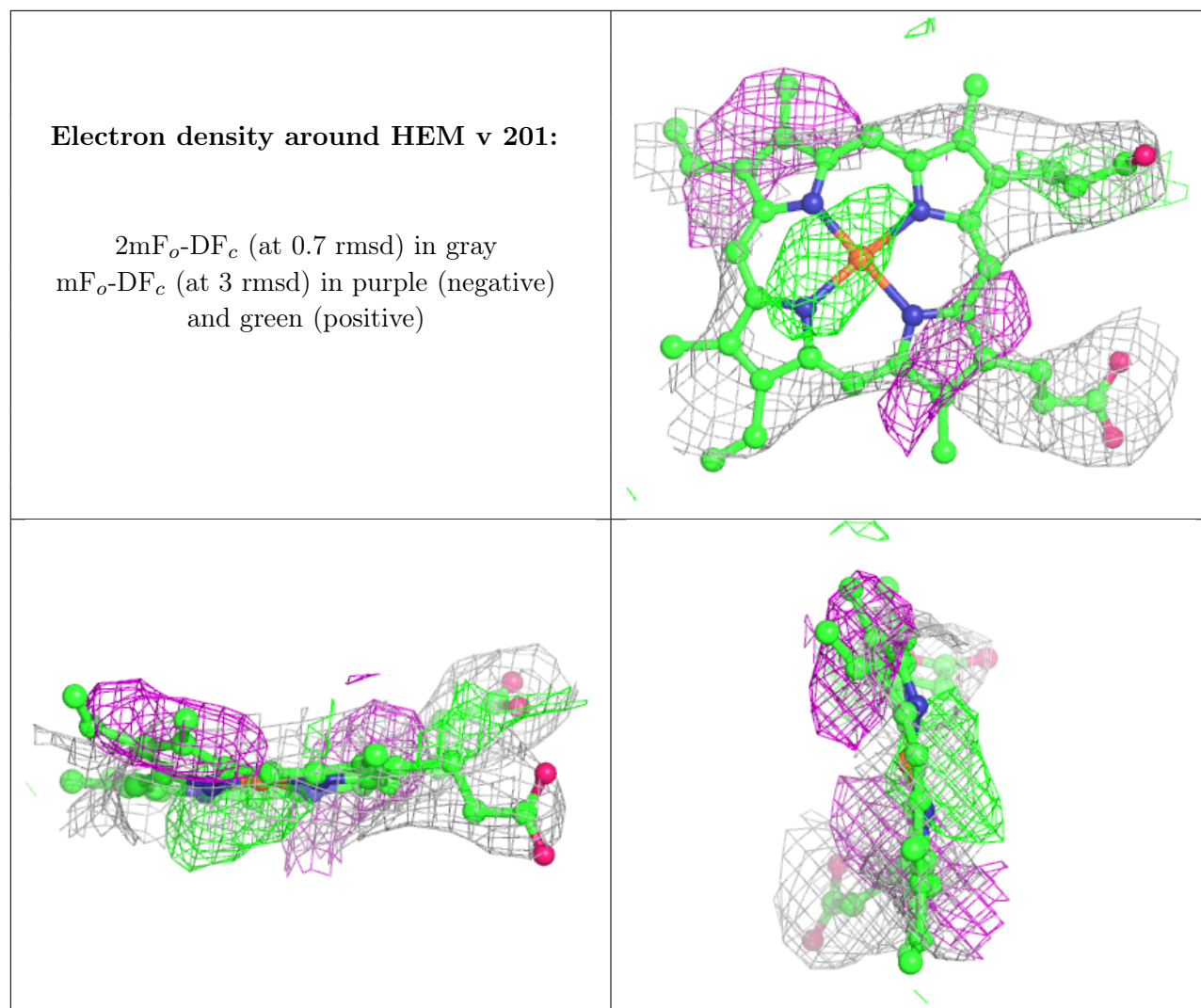


Electron density around HEM V 201:

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







6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.