



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 07:27 AM EDT

PDB ID : 2AXT  
Title : Crystal Structure of Photosystem II from *Thermosynechococcus elongatus*  
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.  
Deposited on : 2005-09-06  
Resolution : 3.00 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

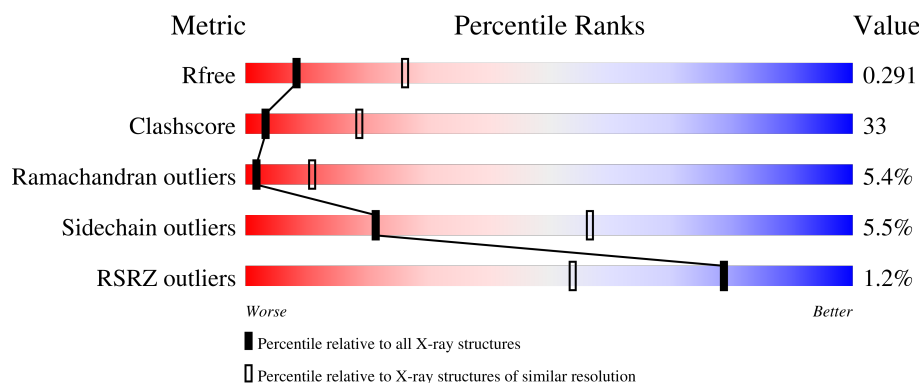
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.






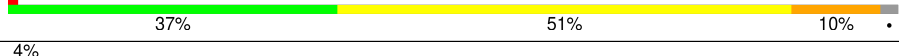
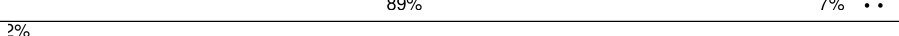
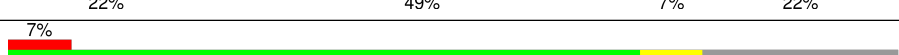
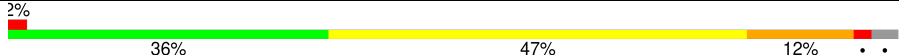
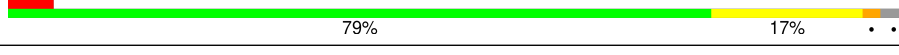
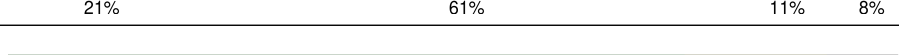
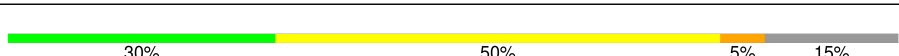
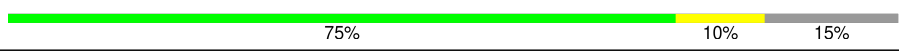
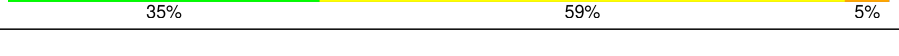
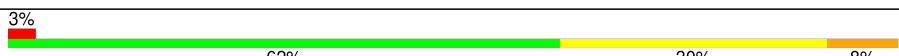


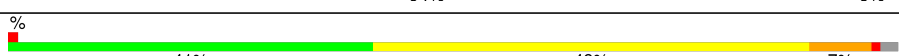


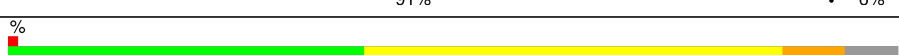




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	473	

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Mol	Chain	Length	Quality of chain
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	z	62	

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
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	X
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	498	X	-	-	-
20	CLA	C	499	X	-	-	-
20	CLA	C	500	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	D	354	X	-	-	-
20	CLA	D	355	X	-	-	-
20	CLA	a	5558	X	-	-	-
20	CLA	a	5559	X	-	-	-
20	CLA	a	5560	X	-	-	-
20	CLA	a	5563	X	-	-	-
20	CLA	b	5511	X	-	-	-
20	CLA	b	5512	X	-	-	-
20	CLA	b	5513	X	-	-	-
20	CLA	b	5514	X	-	-	-
20	CLA	b	5515	X	-	-	-
20	CLA	b	5516	X	-	-	-
20	CLA	b	5517	X	-	-	-
20	CLA	b	5518	X	-	-	-
20	CLA	b	5519	X	-	-	-
20	CLA	b	5520	X	-	-	-
20	CLA	b	5521	X	-	-	-
20	CLA	b	5522	X	-	-	-
20	CLA	b	5523	X	-	-	-
20	CLA	b	5524	X	-	-	-
20	CLA	b	5525	X	-	-	-
20	CLA	b	5526	X	-	-	-
20	CLA	c	5491	X	-	-	-
20	CLA	c	5492	X	-	-	-
20	CLA	c	5493	X	-	-	-
20	CLA	c	5494	X	-	-	-
20	CLA	c	5495	X	-	-	-
20	CLA	c	5496	X	-	-	-
20	CLA	c	5497	X	-	-	-
20	CLA	c	5498	X	-	-	-
20	CLA	c	5499	X	-	-	-
20	CLA	c	5500	X	-	-	-
20	CLA	c	5501	X	-	-	-
20	CLA	c	5502	X	-	-	-
20	CLA	c	5503	X	-	-	-
20	CLA	d	5354	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	X	-	-	-
24	BCR	x	5130	-	-	-	X
27	LMT	A	569	-	-	-	X
27	LMT	t	5217	-	-	-	X
29	UNK	C	489	-	-	-	X
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	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
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

- 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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

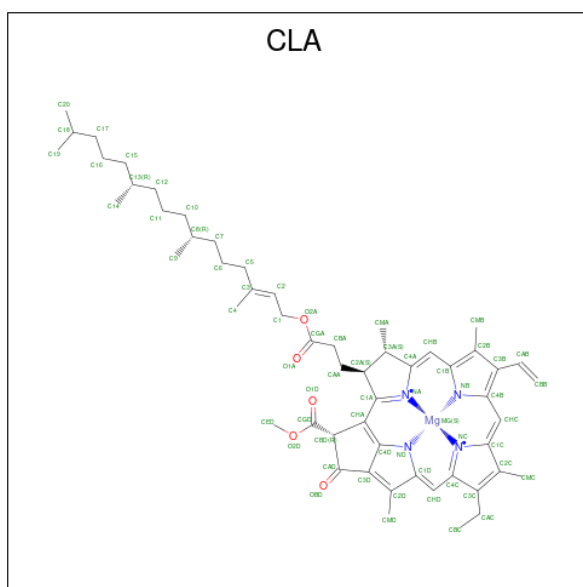
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

- Molecule 19 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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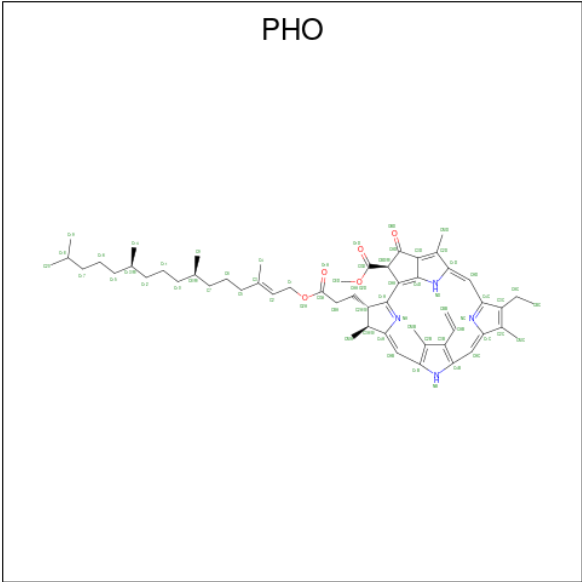
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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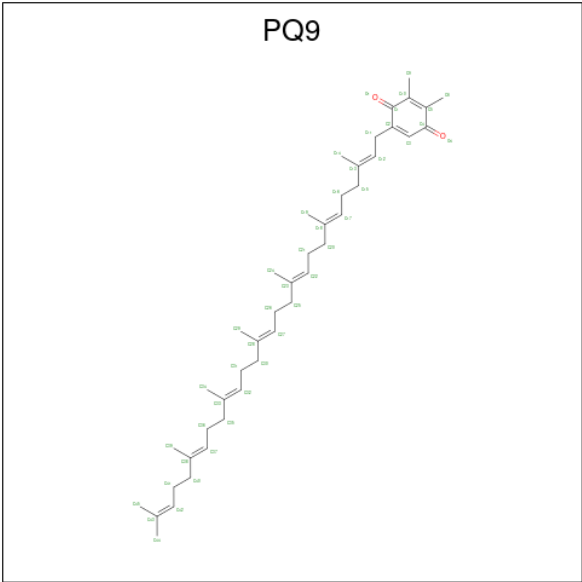
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



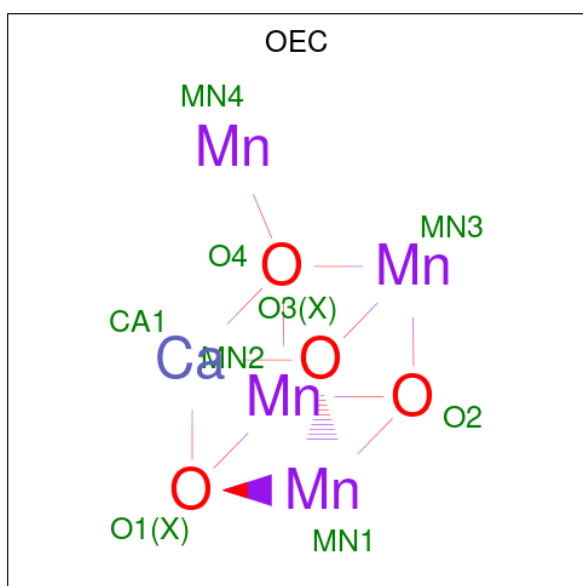
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: C<sub>43</sub>H<sub>64</sub>O<sub>2</sub>).



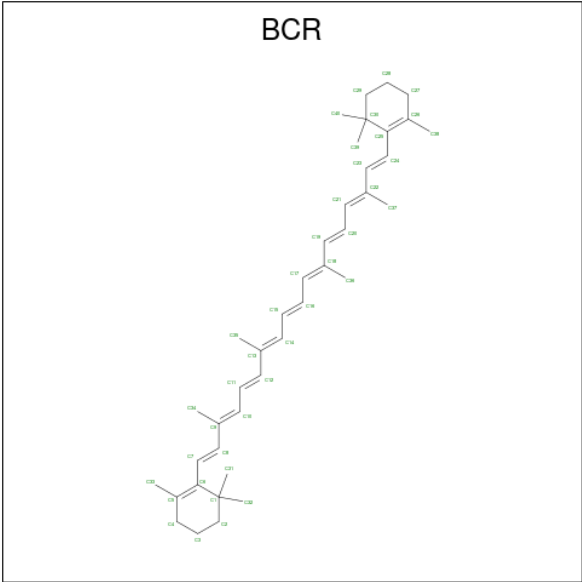
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Ca	Mn	0	0
			5	1	4		
23	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).



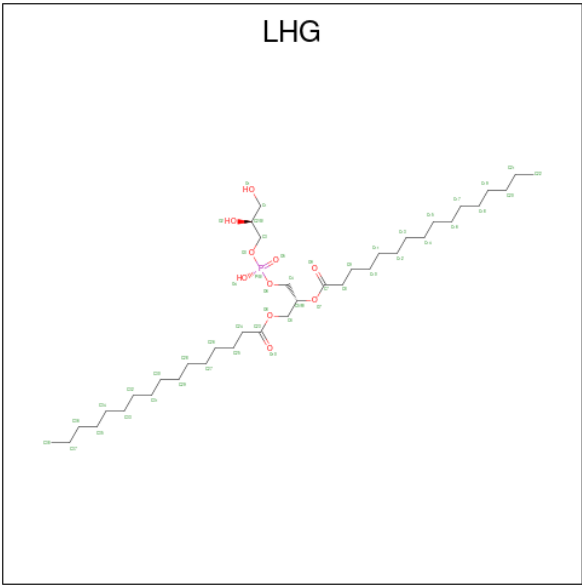
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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

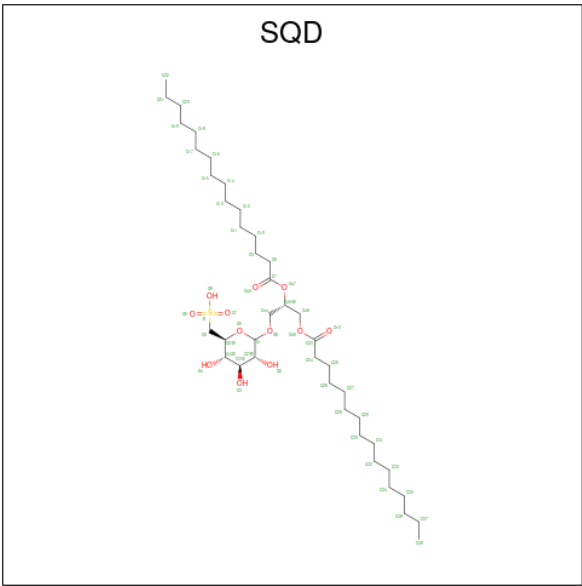
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 39 28 10 1	0	0
25	a	1	Total C O P 39 28 10 1	0	0

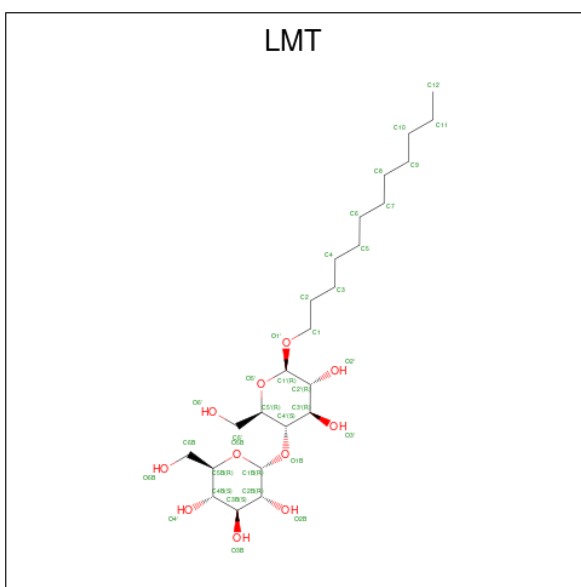
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

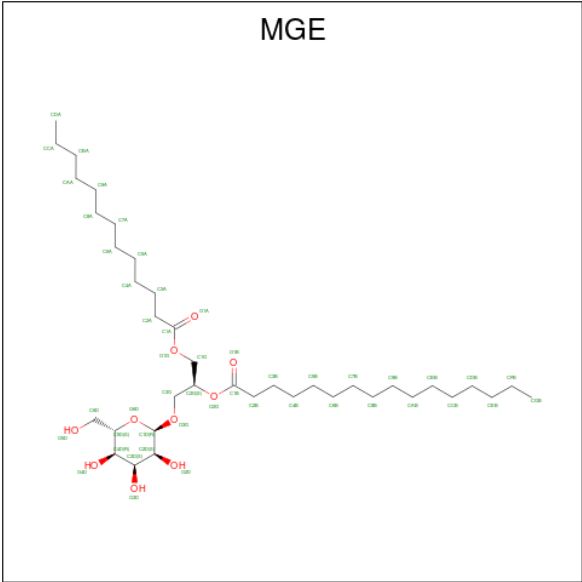
- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total 35	C 24	O 11	0	0
27	M	1	Total 35	C 24	O 11	0	0
27	T	1	Total 35	C 24	O 11	0	0
27	a	1	Total 35	C 24	O 11	0	0
27	m	1	Total 35	C 24	O 11	0	0
27	t	1	Total 35	C 24	O 11	0	0

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula:  $C_{38}H_{72}O_{10}$ ).



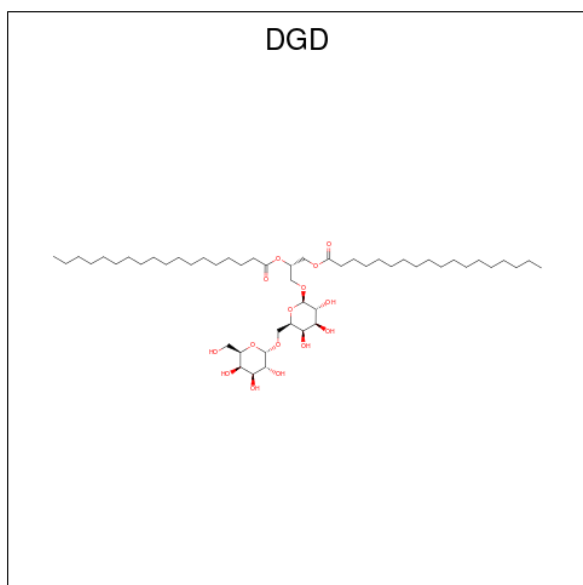


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	C	O	0	0
			47	37	10		
28	d	1	Total	C	O	0	0
			41	31	10		
28	d	1	Total	C	O	0	0
			48	38	10		
28	i	1	Total	C	O	0	0
			48	38	10		
28	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).

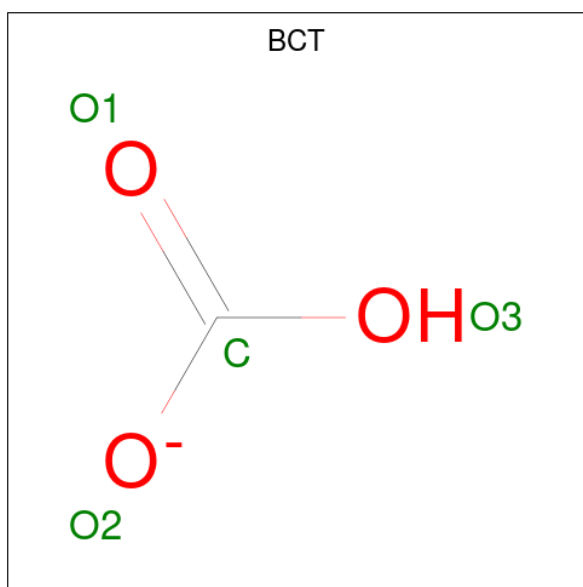
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



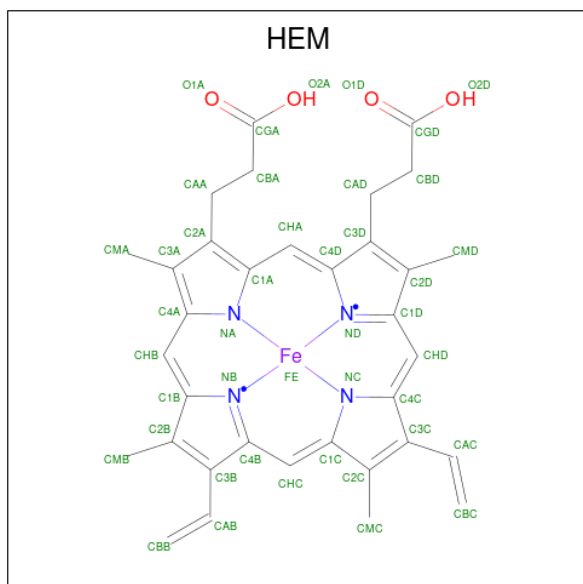
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total	C	O	0	0
			54	39	15		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		
31	d	1	Total	C	O	0	0
			4	1	3		

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



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

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

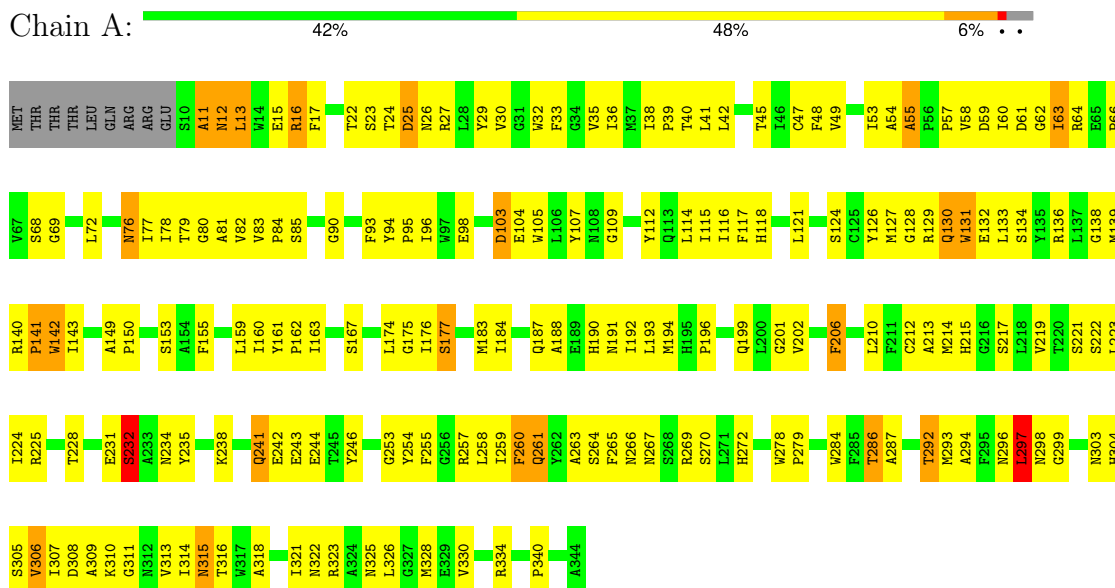
- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total 1	Ca 1	0	0
33	k	1	Total 1	Ca 1	0	0

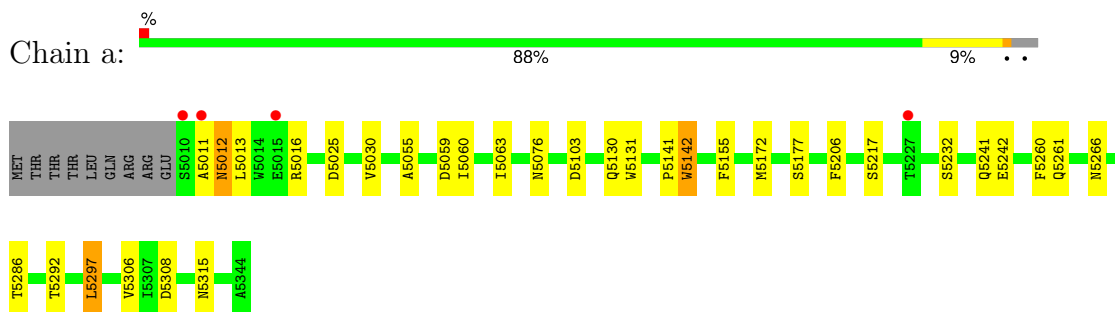
### 3 Residue-property plots

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

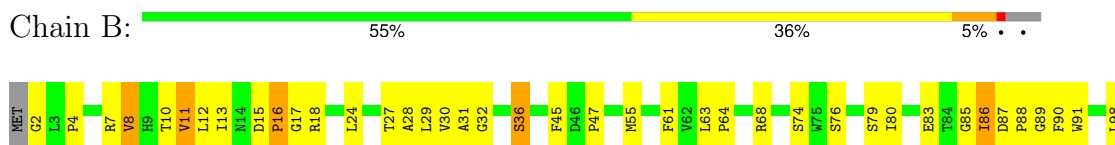
#### • Molecule 1: Photosystem Q(B) protein

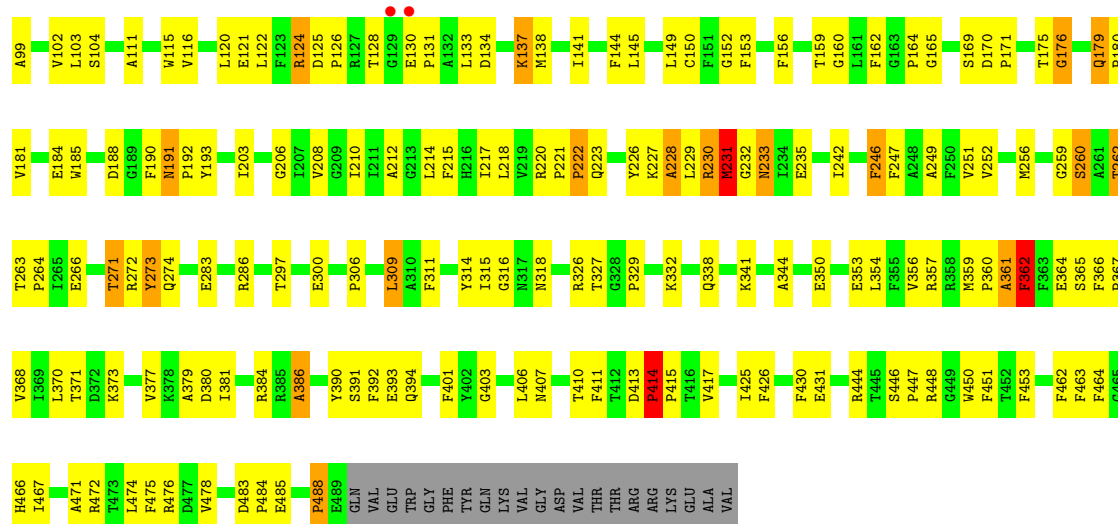


#### • Molecule 1: Photosystem Q(B) protein



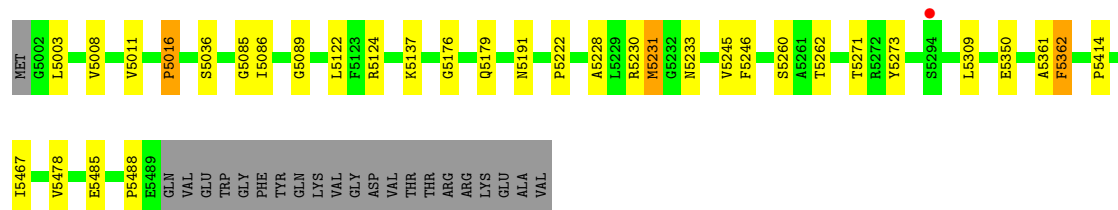
#### • Molecule 2: CP47 protein





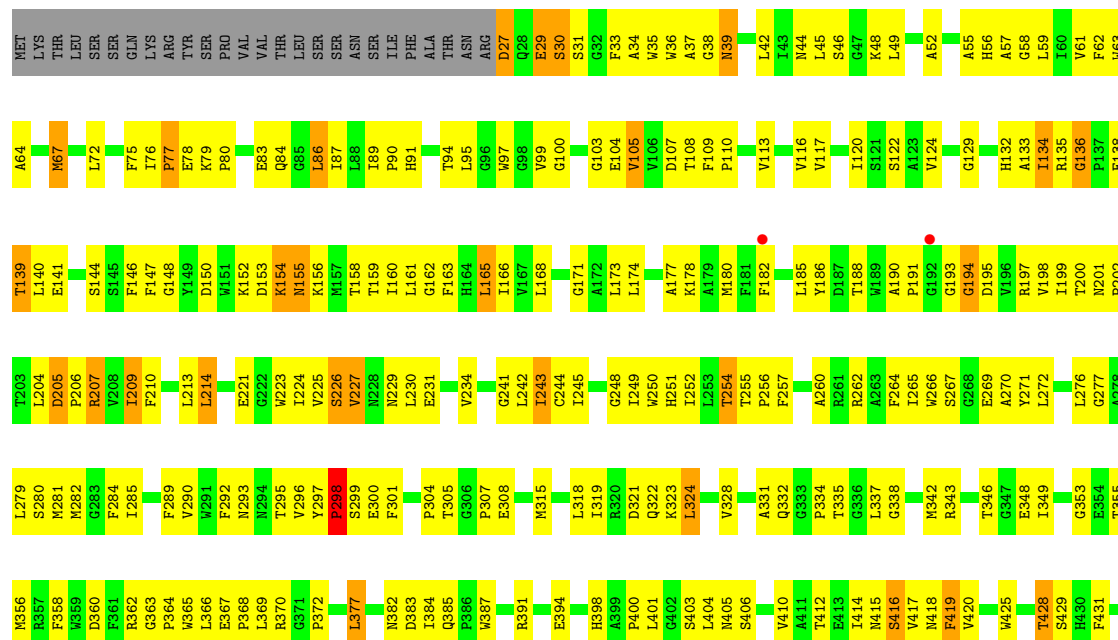
### • Molecule 2: CP47 protein

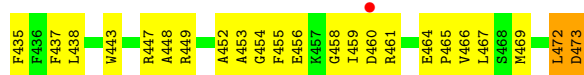
Chain b: 89% 6% . .



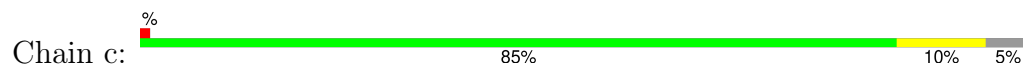
### • Molecule 3: photosystem II CP43 protein

Chain C: 40% 48% 6% 5%

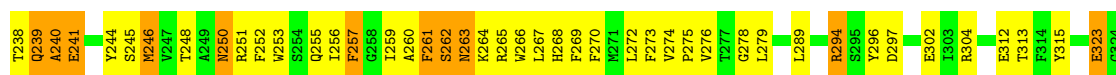
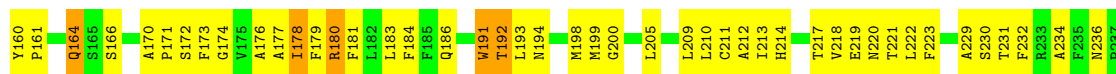
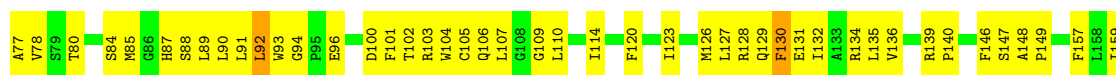
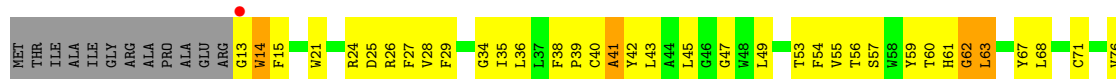




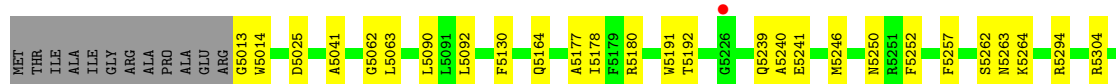
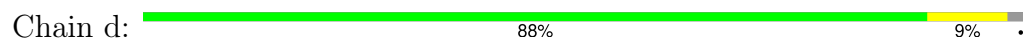
• Molecule 3: photosystem II CP43 protein



• Molecule 4: photosystem II reaction center D2 protein



• Molecule 4: photosystem II reaction center D2 protein



• Molecule 5: Cytochrome b559 alpha subunit

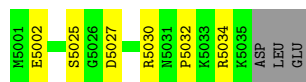







- Molecule 8: Photosystem II reaction center I protein

Chain i:  76% 16% 8%



- Molecule 9: Photosystem II reaction center J protein

Chain J:  30% 50% 5% 15%



- Molecule 9: Photosystem II reaction center J protein

Chain j:  75% 10% 15%




- Molecule 10: Photosystem II reaction center protein K

Chain K:  35% 59% 5%



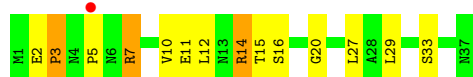
- Molecule 10: Photosystem II reaction center protein K

Chain k:  89% 11%




- Molecule 11: Photosystem II reaction center L protein

Chain L:  3% 62% 30% 8%

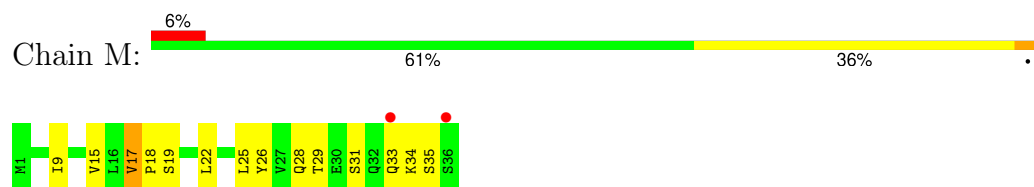


- Molecule 11: Photosystem II reaction center L protein

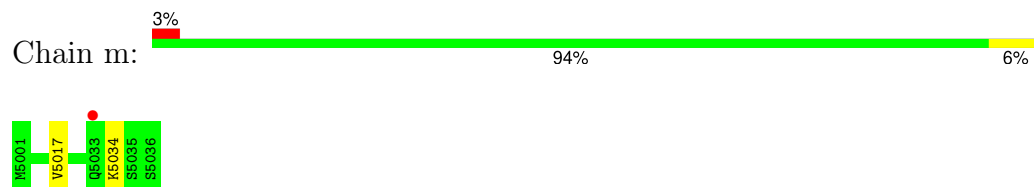
Chain l:  5% 84% 16%



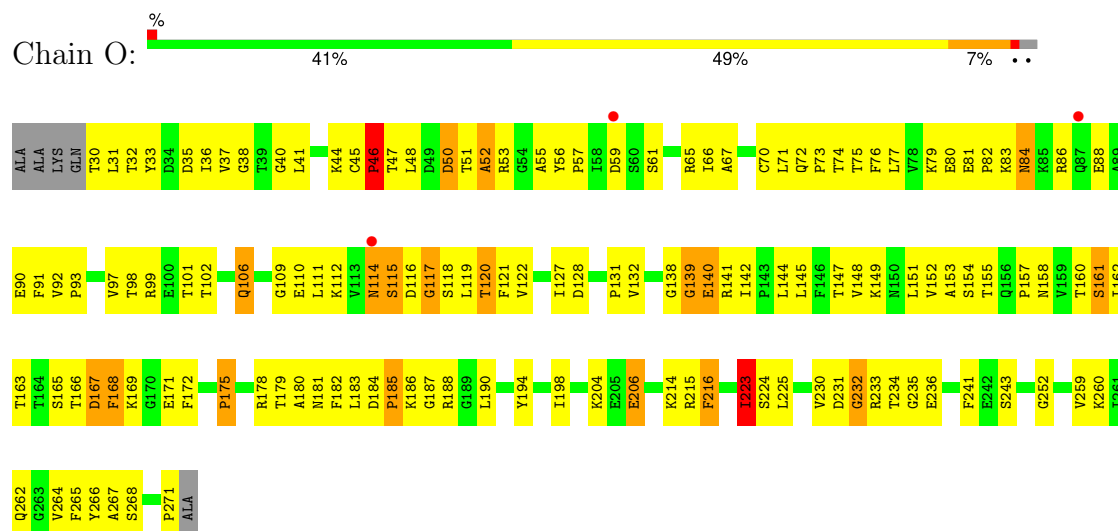
- Molecule 12: Photosystem II reaction center M protein



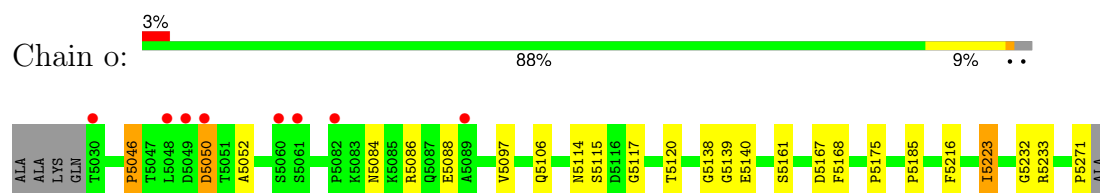
- Molecule 12: Photosystem II reaction center M protein



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



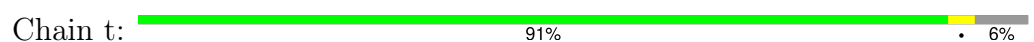
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center T protein

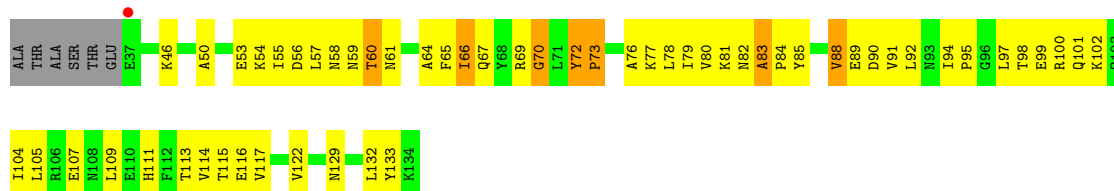


- Molecule 14: Photosystem II reaction center T protein

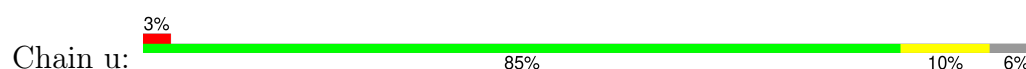




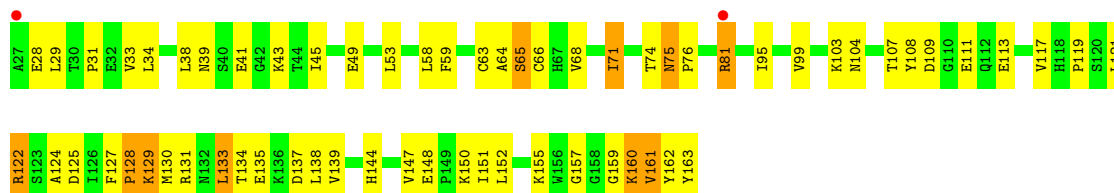
- Molecule 15: Photosystem II 12 kDa extrinsic protein



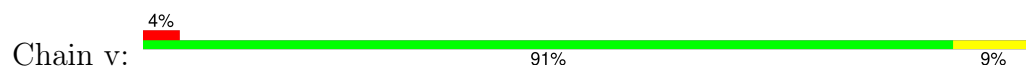
- Molecule 15: Photosystem II 12 kDa extrinsic protein



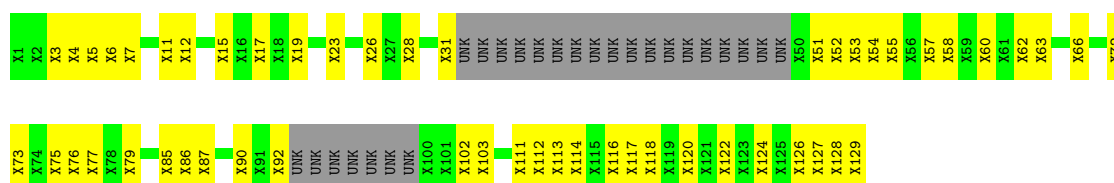
- Molecule 16: Cytochrome c-550



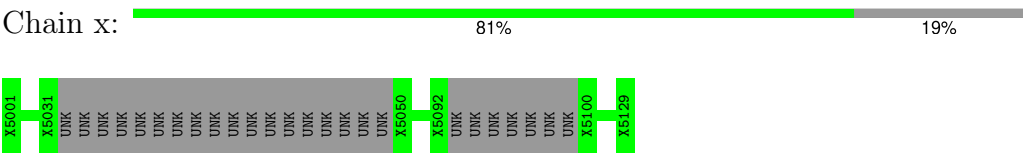
- Molecule 16: Cytochrome c-550



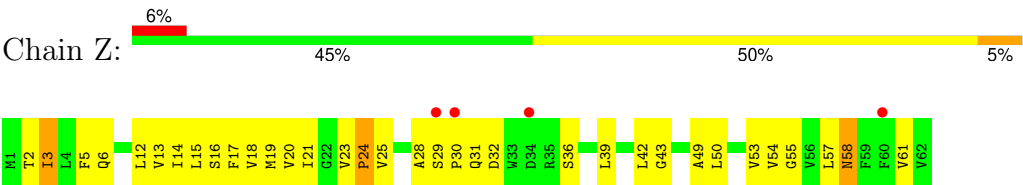
- Molecule 17: Unassigned subunits



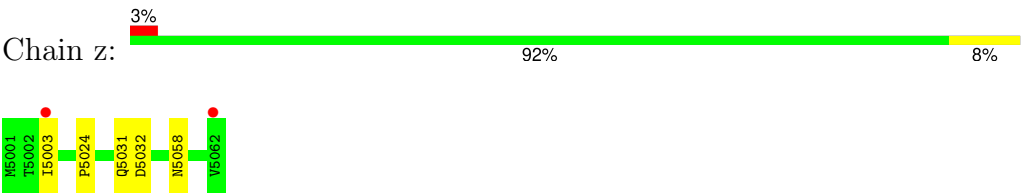
• Molecule 17: Unassigned subunits



• Molecule 18: Photosystem II reaction center Z protein



• Molecule 18: Photosystem II reaction center Z protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.234 , 0.286 0.241 , 0.291	Depositor DCC
$R_{free}$ test set	1908 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BCT, SQD, DGD, LHG, MGE, CLA, CA, PHO, LMT, BCR, PQ9, FE2, OEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	57	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	A	1	0	0	0	0
19	a	1	0	0	0	0
20	A	250	0	265	15	0
20	B	1007	0	1088	74	0
20	C	774	0	783	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	115	0	111	8	0
20	a	250	0	265	0	0
20	b	1007	0	1088	0	0
20	c	774	0	783	0	0
20	d	115	0	111	0	0
21	A	128	0	148	12	0
21	a	128	0	148	0	0
22	A	30	0	37	2	0
22	D	30	0	37	7	0
22	a	30	0	37	0	0
22	d	30	0	37	0	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	6	0
24	C	120	0	168	20	0
24	D	40	0	56	4	0
24	H	40	0	56	3	0
24	T	40	0	56	5	0
24	X	40	0	56	9	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	t	40	0	56	0	0
24	x	40	0	56	0	0
25	A	39	0	51	4	0
25	a	39	0	51	0	0
26	A	80	0	92	0	0
26	L	47	0	60	0	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	0	0
27	A	35	0	46	0	0
27	M	35	0	46	0	0
27	T	35	0	46	3	0
27	a	35	0	46	0	0
27	m	35	0	46	0	0
27	t	35	0	46	0	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	0	0
28	d	136	0	194	0	0
28	i	48	0	72	0	0
28	l	48	0	72	0	0
29	C	152	0	17	2	0
29	c	152	0	17	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	0	0
32	v	43	0	30	0	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47107	1538	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 1538 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:NE2	17:X:26:UNK:CD	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	2	14
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	12
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	3	17
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	3	20
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	10
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	1	10
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	2	14
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	16
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	5
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	5
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	0	2
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	0	2
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	0	3
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	0	3
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	10
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	10
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	9
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	1	9
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	5
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	1	5
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1	5
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	12
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	12
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	6
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	6
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	2	11

5 of 269 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	251 (93%)	18 (7%)	16	49
1	a	269/280 (96%)	252 (94%)	17 (6%)	18	51
2	B	378/407 (93%)	361 (96%)	17 (4%)	27	64
2	b	378/407 (93%)	360 (95%)	18 (5%)	25	62
3	C	341/374 (91%)	320 (94%)	21 (6%)	18	52
3	c	341/374 (91%)	320 (94%)	21 (6%)	18	52
4	D	273/283 (96%)	259 (95%)	14 (5%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	273/283 (96%)	258 (94%)	15 (6%)	21	57
5	E	68/73 (93%)	65 (96%)	3 (4%)	28	65
5	e	68/73 (93%)	66 (97%)	2 (3%)	42	76
6	F	27/39 (69%)	26 (96%)	1 (4%)	34	70
6	f	27/39 (69%)	26 (96%)	1 (4%)	34	70
7	H	50/55 (91%)	42 (84%)	8 (16%)	2	12
7	h	50/55 (91%)	43 (86%)	7 (14%)	3	16
8	I	32/35 (91%)	27 (84%)	5 (16%)	2	13
8	i	32/35 (91%)	27 (84%)	5 (16%)	2	13
9	J	22/28 (79%)	21 (96%)	1 (4%)	27	64
9	j	22/28 (79%)	21 (96%)	1 (4%)	27	64
10	K	29/30 (97%)	28 (97%)	1 (3%)	37	72
10	k	29/30 (97%)	28 (97%)	1 (3%)	37	72
11	L	34/35 (97%)	31 (91%)	3 (9%)	10	36
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	36
12	M	32/33 (97%)	32 (100%)	0	100	100
12	m	32/33 (97%)	32 (100%)	0	100	100
13	O	181/208 (87%)	171 (94%)	10 (6%)	21	57
13	o	181/208 (87%)	172 (95%)	9 (5%)	24	60
14	T	26/29 (90%)	25 (96%)	1 (4%)	33	69
14	t	26/29 (90%)	25 (96%)	1 (4%)	33	69
15	U	83/89 (93%)	80 (96%)	3 (4%)	35	70
15	u	83/89 (93%)	80 (96%)	3 (4%)	35	70
16	V	117/117 (100%)	113 (97%)	4 (3%)	37	72
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	60
18	Z	43/52 (83%)	42 (98%)	1 (2%)	50	80
18	z	43/52 (83%)	42 (98%)	1 (2%)	50	80
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	21	57

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	5030	VAL

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Mol	Chain	Res	Type
18	z	5058	ASN
2	b	5362	PHE
16	v	5122	ARG
11	l	5010	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	5296	ASN
3	c	5201	ASN
1	a	5304	HIS
2	b	5233	ASN
3	c	5398	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 180 ligands modelled in this entry, 4 are monoatomic and 34 are unknown - leaving 142 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	h	5107	-	41,41,41	2.04	7 (17%)	56,56,56	2.30	25 (44%)
31	BCT	d	5353	19	3,3,3	2.70	1 (33%)	2,3,3	0.35	0
24	BCR	B	527	-	41,41,41	1.74	8 (19%)	56,56,56	2.08	16 (28%)
20	CLA	B	512	2	63,73,73	1.67	7 (11%)	74,113,113	1.73	12 (16%)
20	CLA	b	5526	-	63,73,73	2.01	11 (17%)	74,113,113	1.86	11 (14%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	1.00	3 (6%)
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.55	8 (11%)
22	PQ9	d	5356	-	30,30,45	0.82	0	38,39,57	1.66	6 (15%)
24	BCR	t	104	-	41,41,41	1.67	10 (24%)	56,56,56	2.28	23 (41%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.46	6 (8%)
21	PHO	A	561	-	50,69,69	1.12	3 (6%)	48,99,99	1.69	12 (25%)
28	MGE	L	210	-	48,48,48	0.99	3 (6%)	56,56,56	1.15	5 (8%)
20	CLA	b	5514	2	63,73,73	1.99	9 (14%)	74,113,113	1.92	10 (13%)
32	HEM	V	552	16	42,50,50	2.00	14 (33%)	46,82,82	2.34	13 (28%)
20	CLA	A	560	-	63,73,73	1.74	9 (14%)	74,113,113	1.82	12 (16%)
24	BCR	C	504	-	41,41,41	1.87	6 (14%)	56,56,56	2.21	22 (39%)
24	BCR	d	5357	-	41,41,41	2.02	8 (19%)	56,56,56	2.33	21 (37%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.07	4 (7%)
20	CLA	B	526	-	63,73,73	1.94	14 (22%)	74,113,113	1.84	10 (13%)
20	CLA	c	5495	-	63,73,73	2.06	9 (14%)	74,113,113	1.95	13 (17%)
26	SQD	a	212	-	24,26,54	3.09	13 (54%)	34,37,65	2.73	13 (38%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.12	4 (7%)
24	BCR	D	357	-	41,41,41	1.96	8 (19%)	56,56,56	2.27	20 (35%)
24	BCR	c	5505	-	41,41,41	2.01	8 (19%)	56,56,56	2.14	19 (33%)
28	MGE	i	5201	-	48,48,48	1.24	7 (14%)	56,56,56	1.08	4 (7%)
24	BCR	a	5566	-	41,41,41	1.68	7 (17%)	56,56,56	2.14	23 (41%)
24	BCR	H	107	-	41,41,41	2.11	6 (14%)	56,56,56	2.29	24 (42%)
32	HEM	f	5051	5,6	42,50,50	2.08	14 (33%)	46,82,82	2.49	14 (30%)
20	CLA	B	524	2	54,64,73	2.01	6 (11%)	63,102,113	2.04	9 (14%)
24	BCR	C	505	-	41,41,41	1.98	9 (21%)	56,56,56	2.13	18 (32%)
24	BCR	b	5528	-	41,41,41	1.74	6 (14%)	56,56,56	2.06	17 (30%)
27	LMT	M	5216	-	36,36,36	1.45	8 (22%)	47,47,47	0.92	2 (4%)
20	CLA	C	498	3	63,73,73	1.69	6 (9%)	74,113,113	1.84	10 (13%)
24	BCR	c	5504	-	41,41,41	2.18	5 (12%)	56,56,56	2.18	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	525	-	63,73,73	1.82	7 (11%)	74,113,113	1.84	9 (12%)
20	CLA	c	5494	-	44,54,73	2.00	6 (13%)	51,90,113	2.05	9 (17%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.67	11 (17%)
24	BCR	B	529	-	41,41,41	1.79	6 (14%)	56,56,56	2.22	21 (37%)
20	CLA	c	5503	3	48,58,73	2.38	9 (18%)	56,95,113	2.08	6 (10%)
20	CLA	C	501	3	63,73,73	2.06	9 (14%)	74,113,113	1.94	11 (14%)
28	MGE	d	5360	-	41,41,48	1.19	6 (14%)	49,49,56	1.05	4 (8%)
20	CLA	a	5560	-	63,73,73	1.78	9 (14%)	74,113,113	1.84	11 (14%)
24	BCR	x	5130	-	41,41,41	1.95	9 (21%)	56,56,56	2.52	24 (42%)
20	CLA	b	5513	2	63,73,73	1.70	9 (14%)	74,113,113	1.73	14 (18%)
20	CLA	A	563	-	53,63,73	1.82	10 (18%)	62,101,113	1.86	11 (17%)
20	CLA	b	5519	-	63,73,73	1.92	8 (12%)	74,113,113	1.81	12 (16%)
27	LMT	a	5568	-	36,36,36	1.46	6 (16%)	47,47,47	1.09	1 (2%)
20	CLA	C	494	-	44,54,73	1.97	7 (15%)	51,90,113	2.23	9 (17%)
20	CLA	c	5493	3	63,73,73	1.81	7 (11%)	74,113,113	1.90	13 (17%)
24	BCR	b	5529	-	41,41,41	1.66	6 (14%)	56,56,56	2.15	21 (37%)
25	LHG	a	5567	-	38,38,48	2.02	5 (13%)	41,44,54	1.46	4 (9%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.56	9 (13%)
20	CLA	B	519	-	63,73,73	2.00	8 (12%)	74,113,113	1.82	11 (14%)
20	CLA	b	5512	2	63,73,73	1.67	7 (11%)	74,113,113	1.69	10 (13%)
24	BCR	b	5527	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
21	PHO	a	5561	-	50,69,69	1.13	5 (10%)	48,99,99	1.57	11 (22%)
20	CLA	c	5500	-	63,73,73	1.76	8 (12%)	74,113,113	1.79	12 (16%)
27	LMT	A	569	-	36,36,36	1.54	6 (16%)	47,47,47	1.07	1 (2%)
20	CLA	b	5520	-	63,73,73	1.81	11 (17%)	74,113,113	1.75	11 (14%)
22	PQ9	D	356	-	30,30,45	0.91	1 (3%)	38,39,57	1.68	9 (23%)
20	CLA	d	5354	4	63,73,73	1.64	10 (15%)	74,113,113	1.75	11 (14%)
20	CLA	C	496	3	63,73,73	1.89	11 (17%)	74,113,113	1.87	13 (17%)
20	CLA	b	5516	-	63,73,73	1.94	7 (11%)	74,113,113	1.94	8 (10%)
20	CLA	c	5501	3	63,73,73	1.89	7 (11%)	74,113,113	1.91	8 (10%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.47	7 (10%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.06	2 (3%)
20	CLA	c	5498	3	63,73,73	1.86	8 (12%)	74,113,113	1.88	12 (16%)
20	CLA	C	500	-	63,73,73	1.66	10 (15%)	74,113,113	1.78	12 (16%)
30	DGD	c	5508	-	48,48,67	1.48	8 (16%)	62,62,81	1.71	10 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	C	495	-	63,73,73	2.08	11 (17%)	74,113,113	1.92	12 (16%)
24	BCR	A	566	-	41,41,41	1.63	8 (19%)	56,56,56	2.14	22 (39%)
20	CLA	a	5558	1	63,73,73	1.67	11 (17%)	74,113,113	1.66	12 (16%)
20	CLA	C	491	3	63,73,73	1.76	7 (11%)	74,113,113	1.70	8 (10%)
20	CLA	d	5355	-	48,58,73	2.30	9 (18%)	56,95,113	2.05	9 (16%)
32	HEM	F	51	5,6	42,50,50	2.06	15 (35%)	46,82,82	2.41	15 (32%)
20	CLA	b	5515	-	63,73,73	1.71	11 (17%)	74,113,113	1.83	15 (20%)
24	BCR	T	5104	-	41,41,41	1.55	9 (21%)	56,56,56	2.31	25 (44%)
20	CLA	c	5496	-	63,73,73	1.78	9 (14%)	74,113,113	1.81	11 (14%)
20	CLA	b	5518	2	63,73,73	1.91	6 (9%)	74,113,113	1.89	11 (14%)
20	CLA	c	5499	-	45,55,73	2.04	8 (17%)	52,91,113	2.04	8 (15%)
20	CLA	B	523	-	63,73,73	1.98	8 (12%)	74,113,113	1.86	11 (14%)
20	CLA	a	5563	-	53,63,73	1.84	9 (16%)	62,101,113	1.80	11 (17%)
24	BCR	C	506	-	41,41,41	1.74	8 (19%)	56,56,56	2.23	21 (37%)
20	CLA	C	493	3	63,73,73	1.81	8 (12%)	74,113,113	1.91	13 (17%)
20	CLA	A	559	-	63,73,73	1.73	7 (11%)	74,113,113	1.72	8 (10%)
20	CLA	b	5524	2	54,64,73	1.91	6 (11%)	63,102,113	1.93	8 (12%)
25	LHG	A	567	-	38,38,48	1.98	5 (13%)	41,44,54	1.51	4 (9%)
27	LMT	m	216	-	36,36,36	1.45	7 (19%)	47,47,47	0.98	3 (6%)
20	CLA	B	521	2	63,73,73	1.85	9 (14%)	74,113,113	1.90	11 (14%)
20	CLA	C	502	-	49,59,73	2.16	10 (20%)	56,96,113	2.13	11 (19%)
26	SQD	t	213	-	45,47,54	2.81	23 (51%)	55,58,65	2.49	14 (25%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.11	6 (10%)
32	HEM	v	5552	16	42,50,50	2.11	15 (35%)	46,82,82	2.34	15 (32%)
20	CLA	B	511	-	39,49,73	2.25	11 (28%)	46,84,113	2.11	9 (19%)
31	BCT	D	353	19	3,3,3	2.28	1 (33%)	2,3,3	0.32	0
30	DGD	c	5509	-	58,58,67	1.35	7 (12%)	72,72,81	1.39	6 (8%)
26	SQD	A	5212	-	24,26,54	2.85	13 (54%)	34,37,65	2.65	11 (32%)
20	CLA	D	354	4	63,73,73	1.70	8 (12%)	74,113,113	1.68	10 (13%)
20	CLA	D	355	-	48,58,73	2.30	11 (22%)	56,95,113	2.07	11 (19%)
20	CLA	b	5511	-	39,49,73	2.46	10 (25%)	46,84,113	2.18	9 (19%)
27	LMT	T	217	-	36,36,36	1.40	5 (13%)	47,47,47	1.03	4 (8%)
20	CLA	B	514	2	63,73,73	1.98	9 (14%)	74,113,113	1.89	10 (13%)
20	CLA	C	499	-	45,55,73	2.28	9 (20%)	52,91,113	2.09	10 (19%)
20	CLA	B	513	2	63,73,73	1.87	11 (17%)	74,113,113	1.76	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	b	5523	-	63,73,73	1.87	10 (15%)	74,113,113	1.89	11 (14%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	4 (8%)
20	CLA	b	5521	2	63,73,73	1.56	6 (9%)	74,113,113	1.84	12 (16%)
26	SQD	A	568	-	52,54,54	2.59	31 (59%)	62,65,65	2.55	18 (29%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.96	3 (5%)
22	PQ9	A	564	-	30,30,45	0.85	0	38,39,57	1.50	8 (21%)
20	CLA	B	516	-	63,73,73	1.82	6 (9%)	74,113,113	1.90	8 (10%)
20	CLA	B	515	-	63,73,73	1.78	10 (15%)	74,113,113	1.86	14 (18%)
26	SQD	d	5358	-	52,54,54	2.58	29 (55%)	62,65,65	2.53	18 (29%)
20	CLA	a	5559	-	63,73,73	1.61	6 (9%)	74,113,113	1.75	10 (13%)
20	CLA	B	518	2	63,73,73	1.91	6 (9%)	74,113,113	1.91	9 (12%)
20	CLA	B	517	-	63,73,73	2.03	7 (11%)	74,113,113	1.96	12 (16%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.16	6 (10%)
21	PHO	A	562	-	50,69,69	1.12	3 (6%)	48,99,99	1.66	10 (20%)
20	CLA	c	5491	3	63,73,73	1.90	7 (11%)	74,113,113	1.91	10 (13%)
24	BCR	c	5506	-	41,41,41	1.95	7 (17%)	56,56,56	2.16	20 (35%)
20	CLA	c	5492	3	58,68,73	1.76	9 (15%)	68,107,113	1.93	9 (13%)
30	DGD	C	509	-	58,58,67	1.12	7 (12%)	72,72,81	1.40	5 (6%)
20	CLA	C	497	-	63,73,73	1.78	9 (14%)	74,113,113	1.95	11 (14%)
20	CLA	B	520	-	63,73,73	1.71	10 (15%)	74,113,113	1.76	12 (16%)
20	CLA	b	5522	-	63,73,73	1.87	8 (12%)	74,113,113	1.76	7 (9%)
21	PHO	a	5562	-	50,69,69	1.09	3 (6%)	48,99,99	1.64	11 (22%)
20	CLA	C	503	3	48,58,73	2.28	8 (16%)	56,95,113	2.08	10 (17%)
22	PQ9	a	5564	-	30,30,45	0.86	1 (3%)	38,39,57	1.46	6 (15%)
20	CLA	B	522	-	63,73,73	1.83	7 (11%)	74,113,113	1.75	9 (12%)
24	BCR	B	528	-	41,41,41	1.93	6 (14%)	56,56,56	2.02	17 (30%)
28	MGE	l	5210	-	48,48,48	0.90	4 (8%)	56,56,56	1.12	5 (8%)
24	BCR	X	130	-	41,41,41	1.93	8 (19%)	56,56,56	2.54	23 (41%)
20	CLA	c	5502	-	49,59,73	2.29	10 (20%)	56,96,113	2.17	11 (19%)
20	CLA	c	5497	-	63,73,73	1.81	10 (15%)	74,113,113	1.85	11 (14%)
20	CLA	b	5525	-	63,73,73	1.85	6 (9%)	74,113,113	1.87	9 (12%)
26	SQD	L	5213	-	45,47,54	2.81	24 (53%)	55,58,65	2.42	12 (21%)
20	CLA	C	492	3	58,68,73	1.75	9 (15%)	68,107,113	1.91	11 (16%)
20	CLA	A	558	1	63,73,73	1.70	8 (12%)	74,113,113	1.71	10 (13%)
20	CLA	b	5517	-	63,73,73	1.82	8 (12%)	74,113,113	1.86	9 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	B	512	2	1/1/15/20	10/37/115/115	-
20	CLA	b	5526	-	1/1/15/20	10/37/115/115	-
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	A	561	-	-	12/37/103/103	0/5/6/6
28	MGE	L	210	-	-	23/43/63/63	0/1/1/1
20	CLA	b	5514	2	1/1/15/20	12/37/115/115	-
32	HEM	V	552	16	-	4/12/54/54	-
20	CLA	A	560	-	1/1/15/20	7/37/115/115	-
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
28	MGE	d	5359	-	-	13/42/62/63	0/1/1/1
28	MGE	I	201	-	-	24/43/63/63	0/1/1/1
20	CLA	B	526	-	1/1/15/20	10/37/115/115	-
20	CLA	c	5495	-	1/1/15/20	16/37/115/115	-
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
32	HEM	f	5051	5,6	-	2/12/54/54	-
20	CLA	B	524	2	1/1/13/20	7/27/105/115	-
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	C	498	3	1/1/15/20	16/37/115/115	-
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
20	CLA	B	525	-	1/1/15/20	12/37/115/115	-
20	CLA	c	5494	-	1/1/11/20	7/15/93/115	-
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
24	BCR	B	529	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5503	3	1/1/12/20	5/19/97/115	-
20	CLA	C	501	3	1/1/15/20	13/37/115/115	-
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
20	CLA	a	5560	-	1/1/15/20	7/37/115/115	-
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5513	2	1/1/15/20	10/37/115/115	-
20	CLA	A	563	-	1/1/13/20	5/25/103/115	-
20	CLA	b	5519	-	1/1/15/20	11/37/115/115	-
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
20	CLA	C	494	-	1/1/11/20	7/15/93/115	-
20	CLA	c	5493	3	1/1/15/20	10/37/115/115	-
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
25	LHG	a	5567	-	-	14/43/43/53	-
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	B	519	-	1/1/15/20	11/37/115/115	-
20	CLA	b	5512	2	1/1/15/20	10/37/115/115	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
21	PHO	a	5561	-	-	12/37/103/103	0/5/6/6
20	CLA	c	5500	-	1/1/15/20	11/37/115/115	-
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
20	CLA	b	5520	-	1/1/15/20	11/37/115/115	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
20	CLA	d	5354	4	1/1/15/20	8/37/115/115	-
20	CLA	C	496	3	1/1/15/20	11/37/115/115	-
20	CLA	b	5516	-	1/1/15/20	13/37/115/115	-
20	CLA	c	5501	3	1/1/15/20	11/37/115/115	-
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	5498	3	1/1/15/20	16/37/115/115	-
20	CLA	C	500	-	1/1/15/20	11/37/115/115	-
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
20	CLA	C	495	-	1/1/15/20	16/37/115/115	-
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
20	CLA	a	5558	1	1/1/15/20	9/37/115/115	-
20	CLA	C	491	3	1/1/15/20	7/37/115/115	-
20	CLA	d	5355	-	1/1/12/20	9/19/97/115	-
32	HEM	F	51	5,6	-	2/12/54/54	-
20	CLA	b	5515	-	1/1/15/20	17/37/115/115	-
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5496	-	1/1/15/20	11/37/115/115	-
20	CLA	b	5518	2	1/1/15/20	14/37/115/115	-
20	CLA	c	5499	-	1/1/11/20	6/16/94/115	-
20	CLA	B	523	-	1/1/15/20	13/37/115/115	-
20	CLA	a	5563	-	1/1/13/20	5/25/103/115	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
20	CLA	C	493	3	1/1/15/20	10/37/115/115	-
20	CLA	A	559	-	1/1/15/20	12/37/115/115	-
20	CLA	b	5524	2	1/1/13/20	7/27/105/115	-
25	LHG	A	567	-	-	16/43/43/53	-
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	B	521	2	1/1/15/20	7/37/115/115	-
20	CLA	C	502	-	1/1/12/20	7/21/99/115	-
26	SQD	t	213	-	-	20/42/62/69	0/1/1/1
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
32	HEM	v	5552	16	-	4/12/54/54	-
20	CLA	B	511	-	1/1/10/20	2/8/86/115	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
26	SQD	A	5212	-	-	5/19/39/69	0/1/1/1
20	CLA	D	354	4	1/1/15/20	10/37/115/115	-
20	CLA	D	355	-	1/1/12/20	9/19/97/115	-
20	CLA	b	5511	-	1/1/10/20	2/8/86/115	-
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	514	2	1/1/15/20	11/37/115/115	-
20	CLA	C	499	-	1/1/11/20	6/16/94/115	-
20	CLA	B	513	2	1/1/15/20	12/37/115/115	-
20	CLA	b	5523	-	1/1/15/20	13/37/115/115	-
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
20	CLA	b	5521	2	1/1/15/20	7/37/115/115	-
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	516	-	1/1/15/20	13/37/115/115	-
20	CLA	B	515	-	1/1/15/20	17/37/115/115	-
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
20	CLA	a	5559	-	1/1/15/20	12/37/115/115	-
20	CLA	B	518	2	1/1/15/20	14/37/115/115	-
20	CLA	B	517	-	1/1/15/20	12/37/115/115	-
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
21	PHO	A	562	-	-	9/37/103/103	0/5/6/6
20	CLA	c	5491	3	1/1/15/20	9/37/115/115	-
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5492	3	1/1/14/20	9/31/109/115	-
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
20	CLA	C	497	-	1/1/15/20	7/37/115/115	-
20	CLA	B	520	-	1/1/15/20	13/37/115/115	-
20	CLA	b	5522	-	1/1/15/20	12/37/115/115	-
21	PHO	a	5562	-	-	9/37/103/103	0/5/6/6
20	CLA	C	503	3	1/1/12/20	5/19/97/115	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	522	-	1/1/15/20	12/37/115/115	-
24	BCR	B	528	-	-	1/29/63/63	0/2/2/2
28	MGE	l	5210	-	-	23/43/63/63	0/1/1/1
24	BCR	X	130	-	-	5/29/63/63	0/2/2/2
20	CLA	c	5502	-	1/1/12/20	6/21/99/115	-
20	CLA	c	5497	-	1/1/15/20	8/37/115/115	-
20	CLA	b	5525	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	L	5213	-	-	21/42/62/69	0/1/1/1
20	CLA	C	492	3	1/1/14/20	9/31/109/115	-
20	CLA	A	558	1	1/1/15/20	8/37/115/115	-
20	CLA	b	5517	-	1/1/15/20	12/37/115/115	-

The worst 5 of 1145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	523	CLA	CHB-C4A	11.56	1.43	1.33
20	C	501	CLA	CHB-C4A	11.29	1.43	1.33
20	b	5525	CLA	CHB-C4A	11.17	1.43	1.33
20	C	495	CLA	CHB-C4A	11.16	1.43	1.33
20	b	5511	CLA	CHB-C4A	10.99	1.43	1.33

The worst 5 of 1544 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5501	CLA	C4A-NA-C1A	12.96	112.59	106.68
20	b	5514	CLA	C4A-NA-C1A	12.90	112.56	106.68
20	C	501	CLA	C4A-NA-C1A	12.84	112.54	106.68
20	B	514	CLA	C4A-NA-C1A	12.74	112.49	106.68
20	B	524	CLA	C4A-NA-C1A	12.52	112.39	106.68

5 of 94 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	558	CLA	ND
20	A	559	CLA	ND
20	A	560	CLA	ND
20	A	563	CLA	ND
20	B	511	CLA	ND

5 of 1400 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	511	CLA	CBD-CGD-O2D-CED
20	B	515	CLA	C2-C3-C5-C6
20	B	515	CLA	C4-C3-C5-C6
20	B	516	CLA	C1A-C2A-CAA-CBA
20	B	516	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	527	BCR	2	0
20	B	512	CLA	2	0
30	H	208	DGD	3	0
21	A	561	PHO	7	0
28	L	210	MGE	2	0
32	V	552	HEM	2	0
20	A	560	CLA	1	0
24	C	504	BCR	7	0
28	I	201	MGE	1	0
20	B	526	CLA	2	0
28	D	360	MGE	7	0
24	D	357	BCR	4	0
24	H	107	BCR	3	0
20	B	524	CLA	4	0
24	C	505	BCR	6	0
20	C	498	CLA	6	0
20	B	525	CLA	4	0
30	C	508	DGD	2	0
24	B	529	BCR	2	0
20	C	501	CLA	13	0
20	C	494	CLA	2	0
20	B	519	CLA	5	0
22	D	356	PQ9	7	0
20	C	496	CLA	2	0
30	C	507	DGD	6	0
20	C	500	CLA	3	0
20	C	495	CLA	9	0
24	A	566	BCR	1	0
20	C	491	CLA	4	0
32	F	51	HEM	3	0
24	T	5104	BCR	5	0
20	B	523	CLA	2	0
24	C	506	BCR	7	0
20	C	493	CLA	7	0
20	A	559	CLA	5	0
25	A	567	LHG	4	0
20	B	521	CLA	2	0
20	C	502	CLA	2	0
20	B	511	CLA	1	0
20	D	354	CLA	5	0

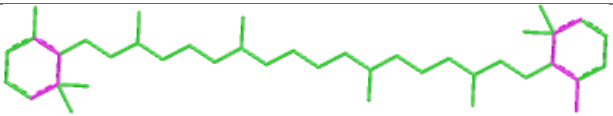
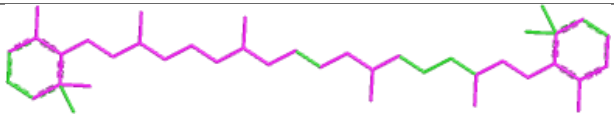
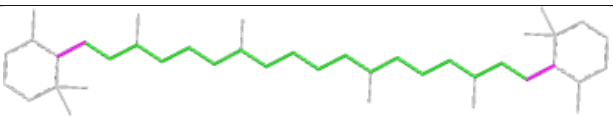
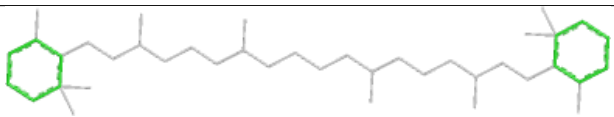
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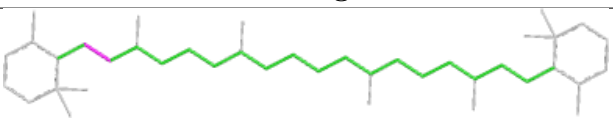
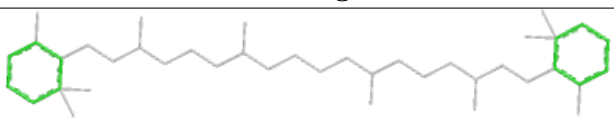


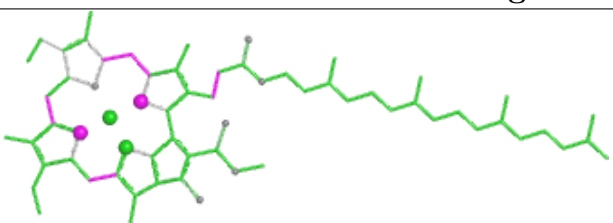
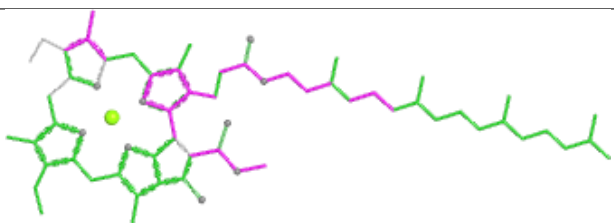
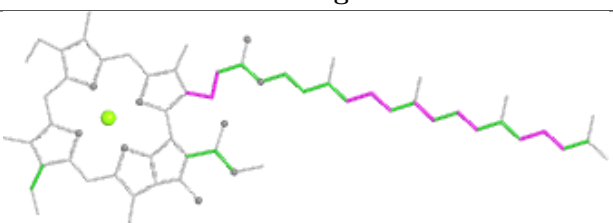
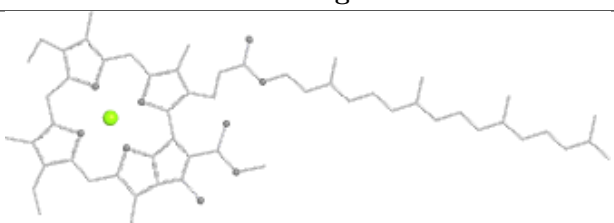
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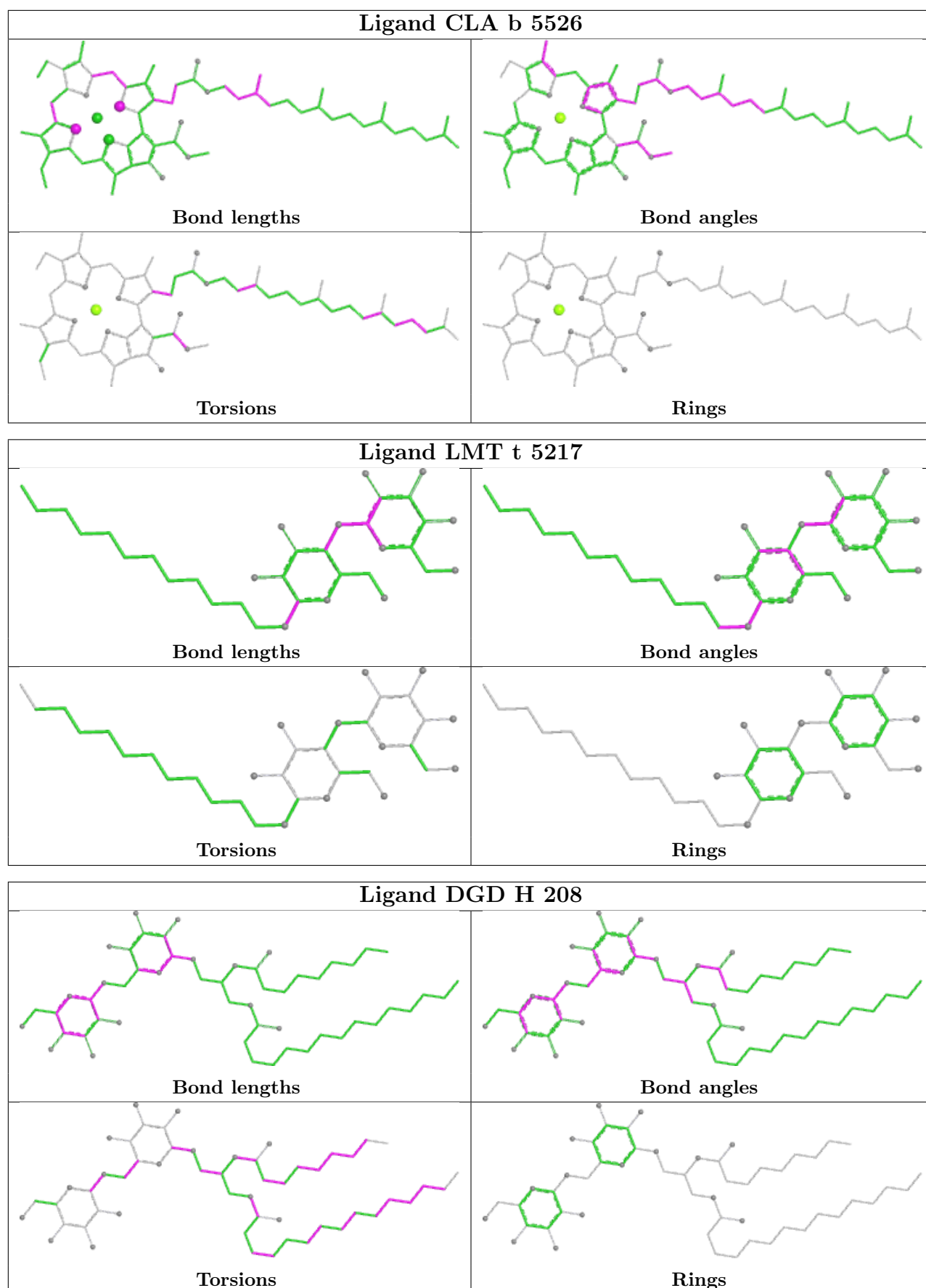
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	355	CLA	3	0
27	T	217	LMT	3	0
20	B	514	CLA	5	0
20	C	499	CLA	2	0
20	B	513	CLA	8	0
28	D	359	MGE	1	0
28	D	358	MGE	2	0
22	A	564	PQ9	2	0
20	B	516	CLA	6	0
20	B	515	CLA	12	0
20	B	518	CLA	11	0
20	B	517	CLA	9	0
28	B	530	MGE	1	0
21	A	562	PHO	5	0
30	C	509	DGD	10	0
20	C	497	CLA	5	0
20	B	520	CLA	6	0
20	C	503	CLA	1	0
20	B	522	CLA	4	0
24	B	528	BCR	2	0
24	X	130	BCR	9	0
20	C	492	CLA	2	0
20	A	558	CLA	10	0

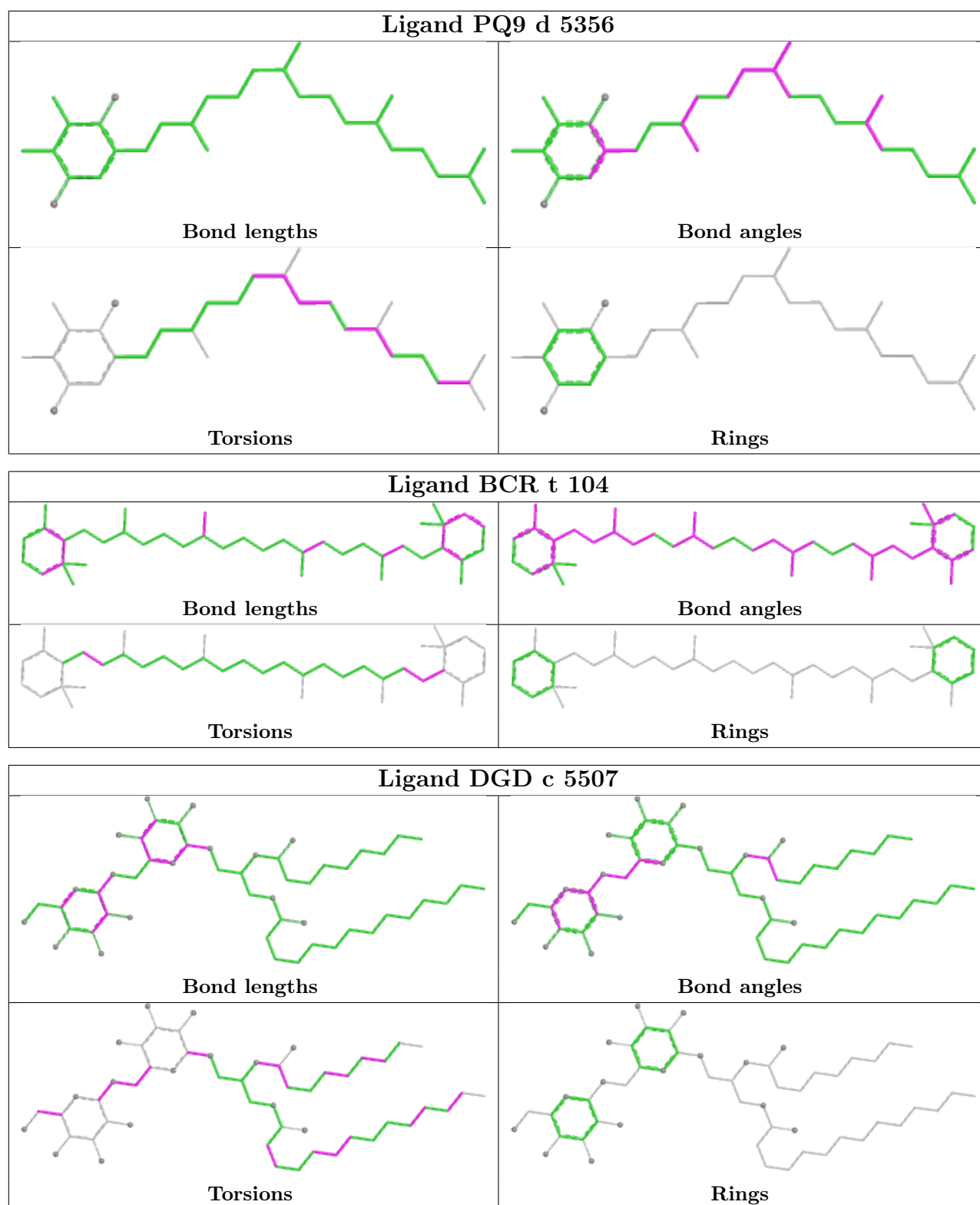
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

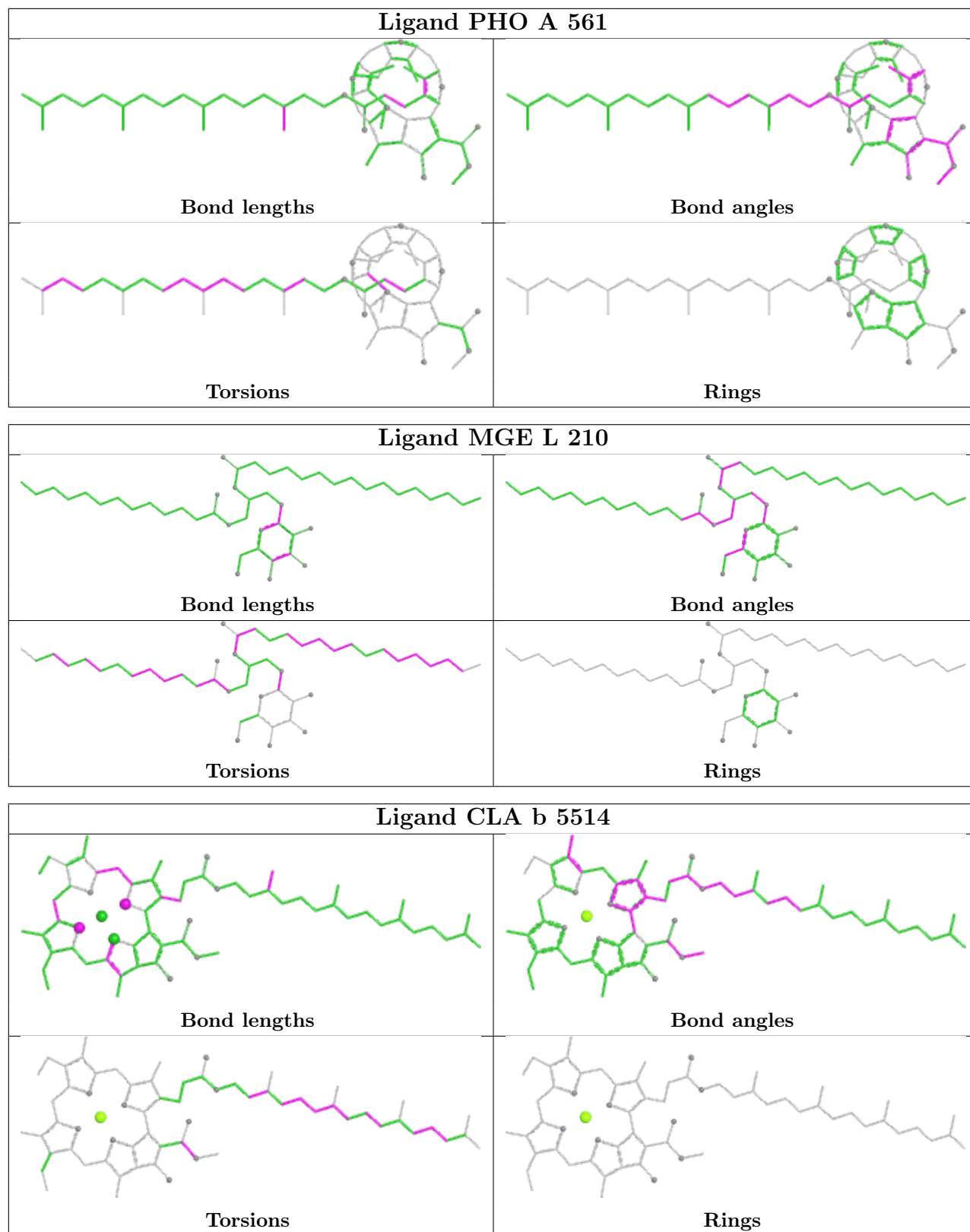
Ligand BCR h 5107	
	
Bond lengths	Bond angles
	
Torsions	Rings

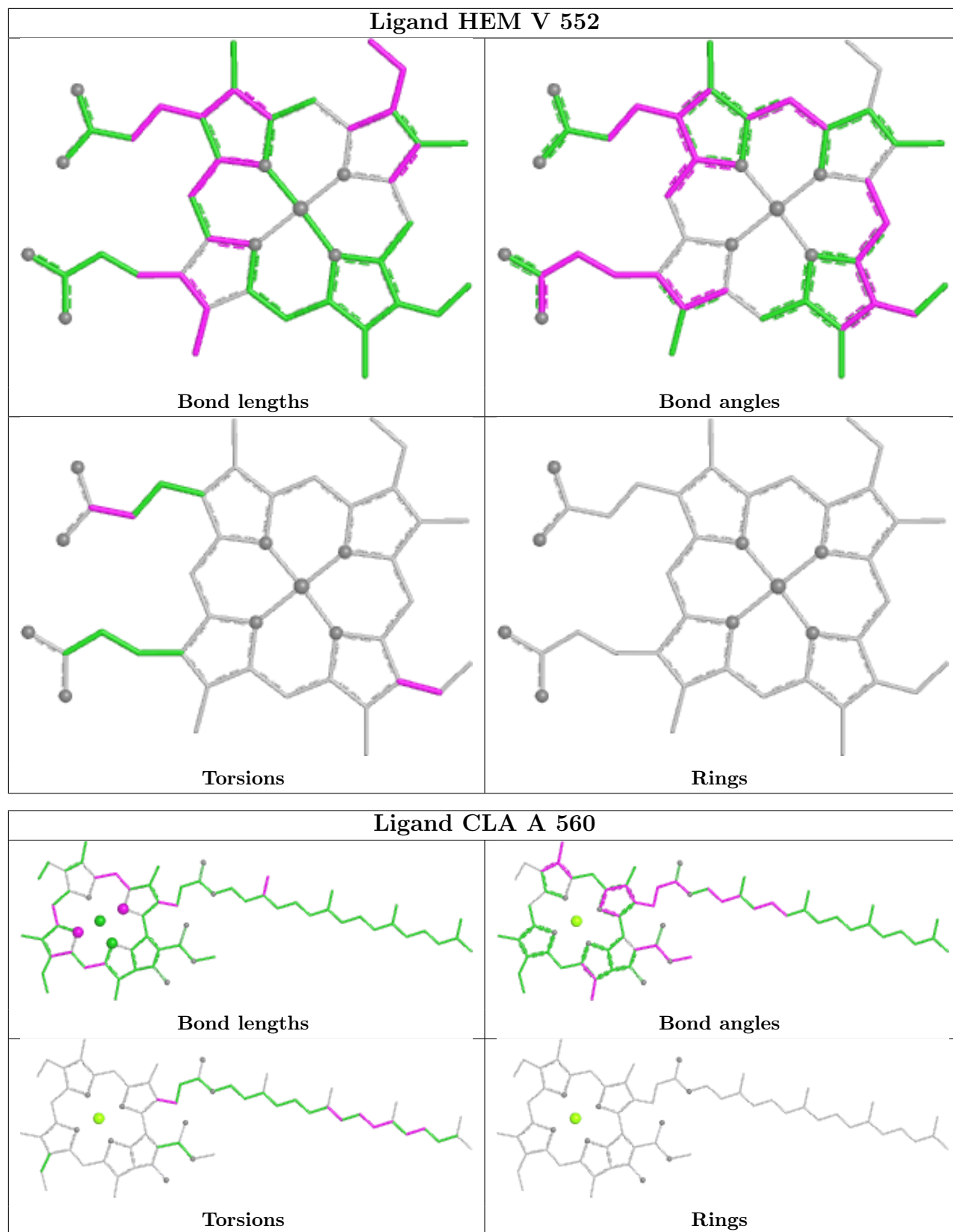
Ligand BCR B 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

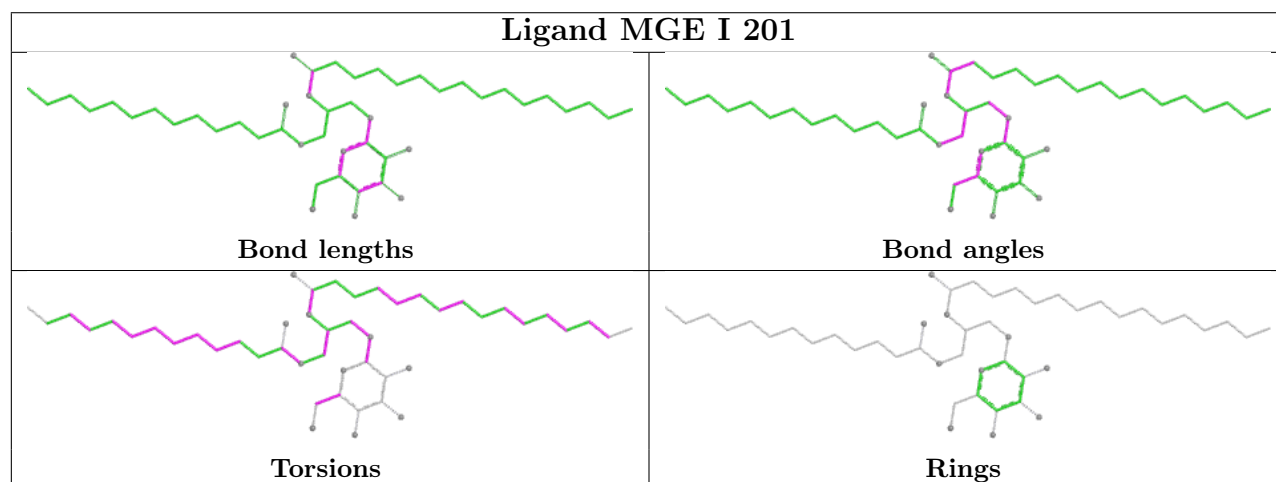
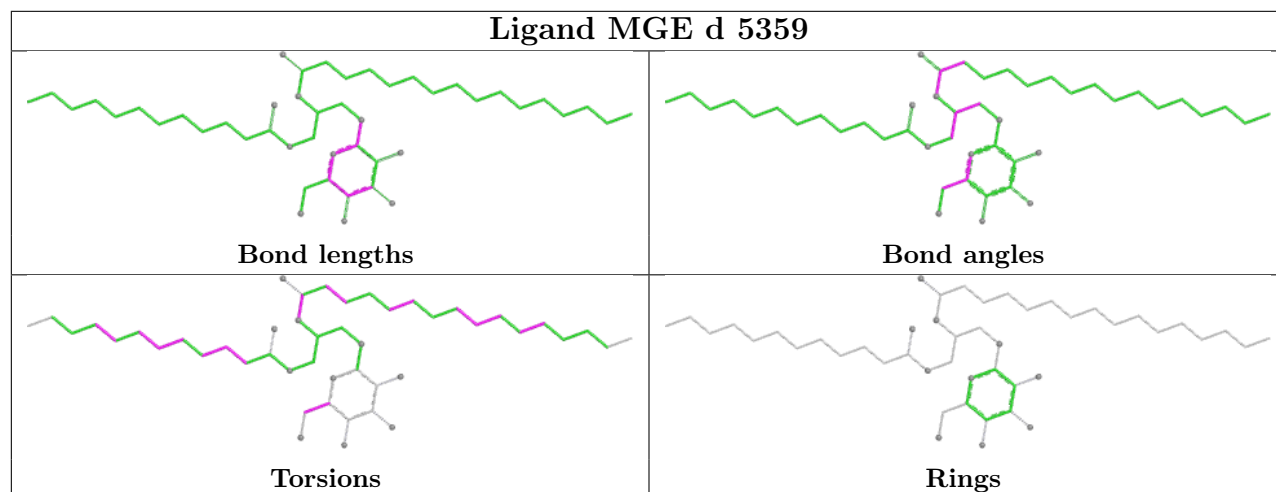
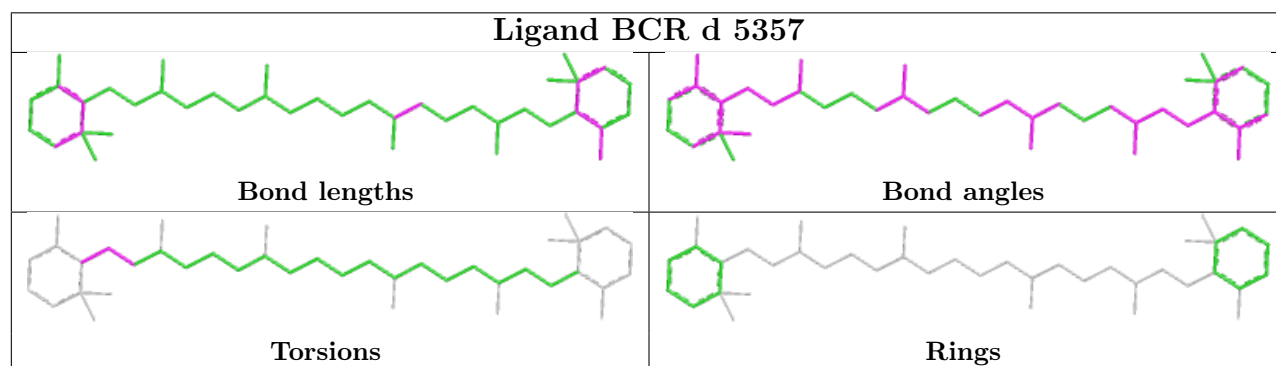
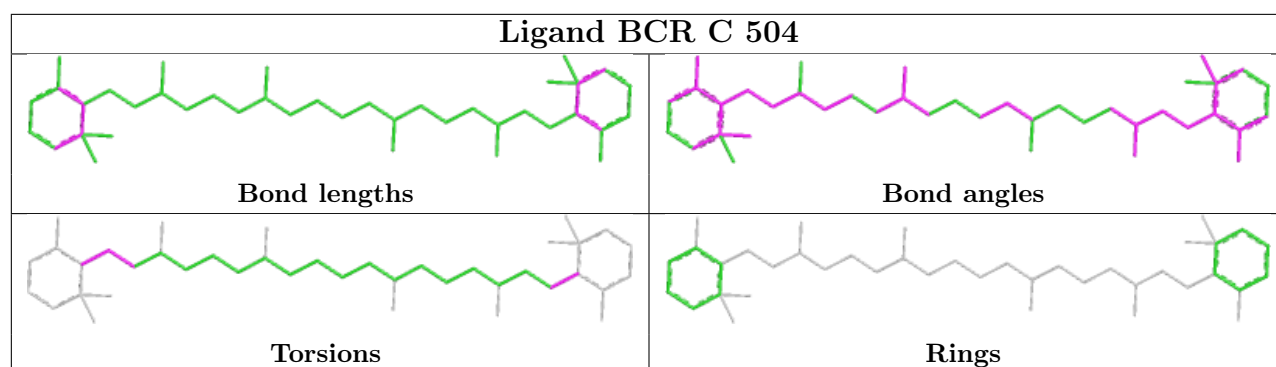
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Bond lengths	Bond angles
	
Torsions	Rings

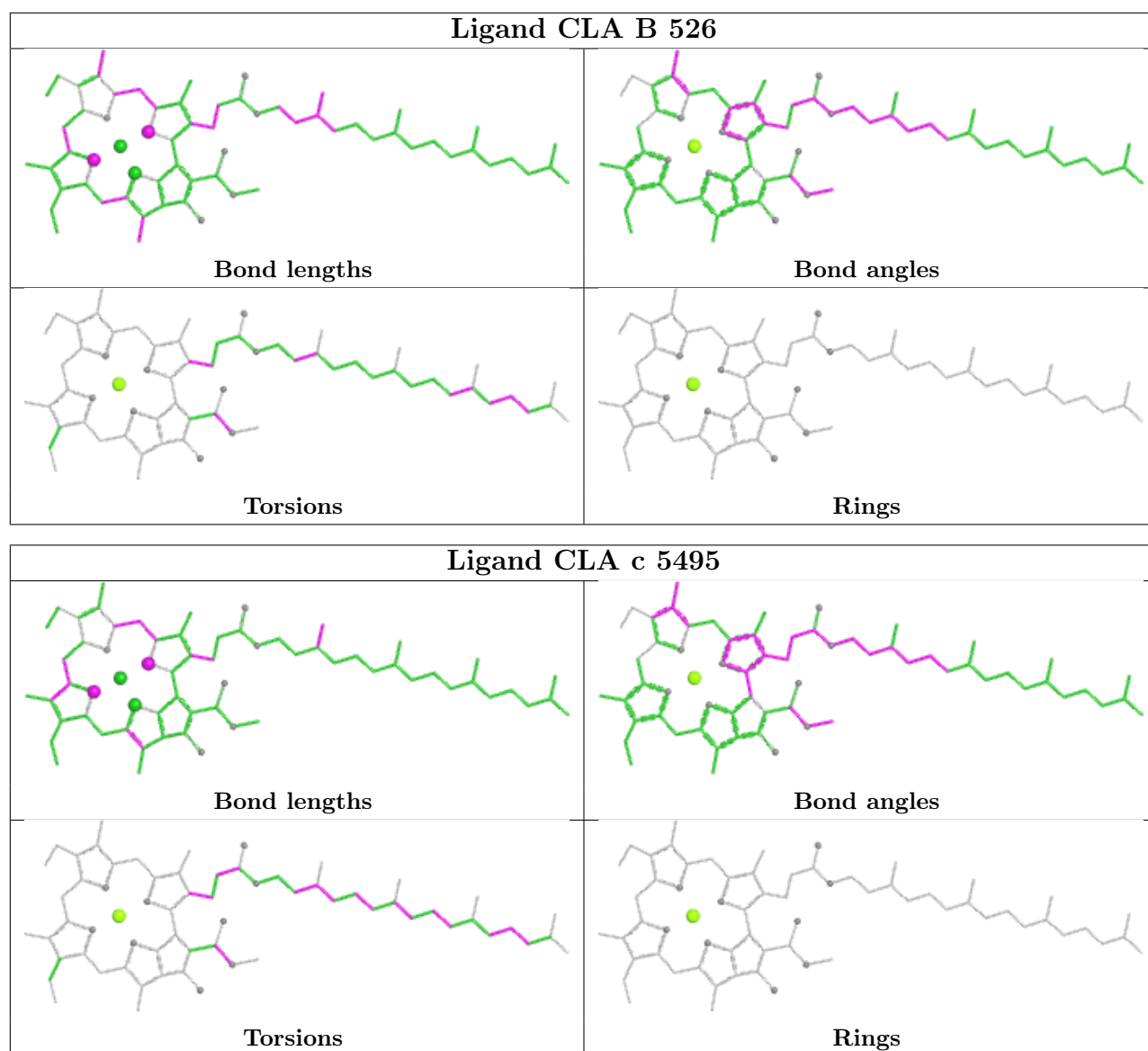




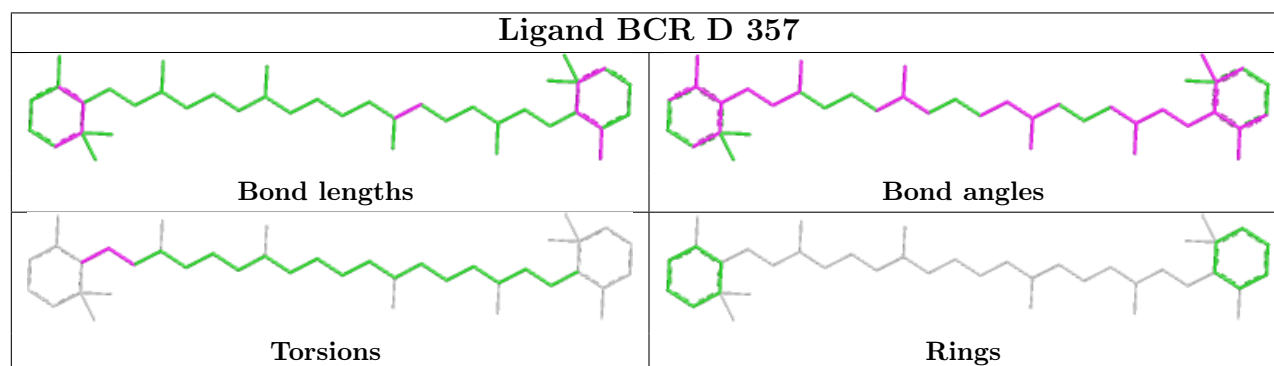
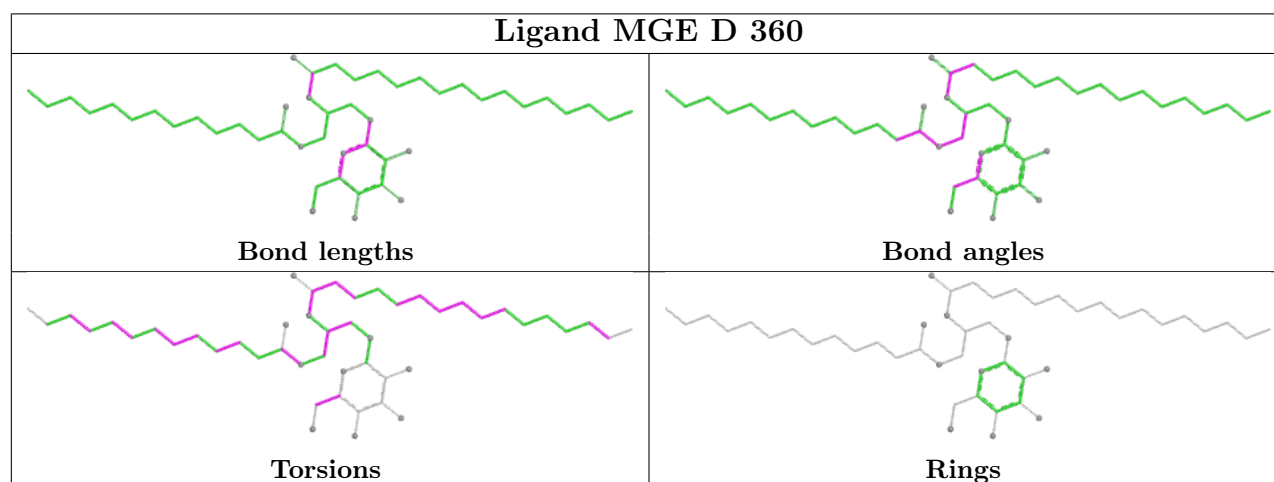
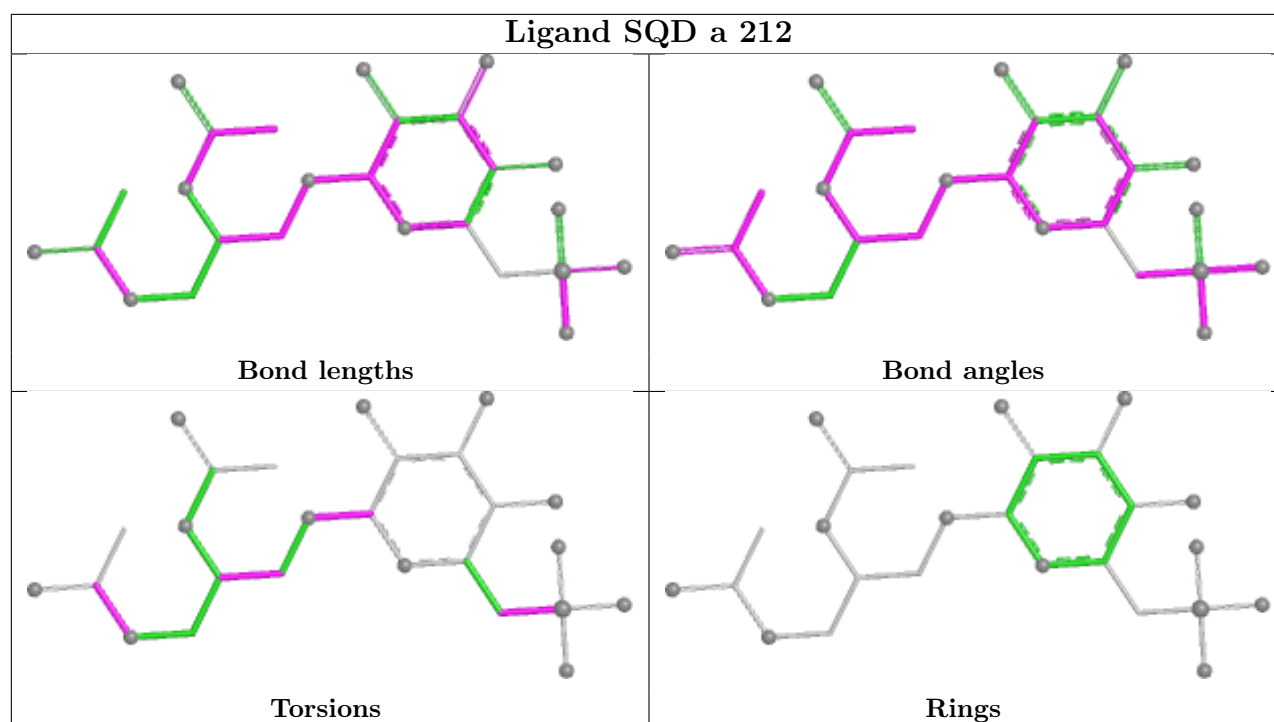


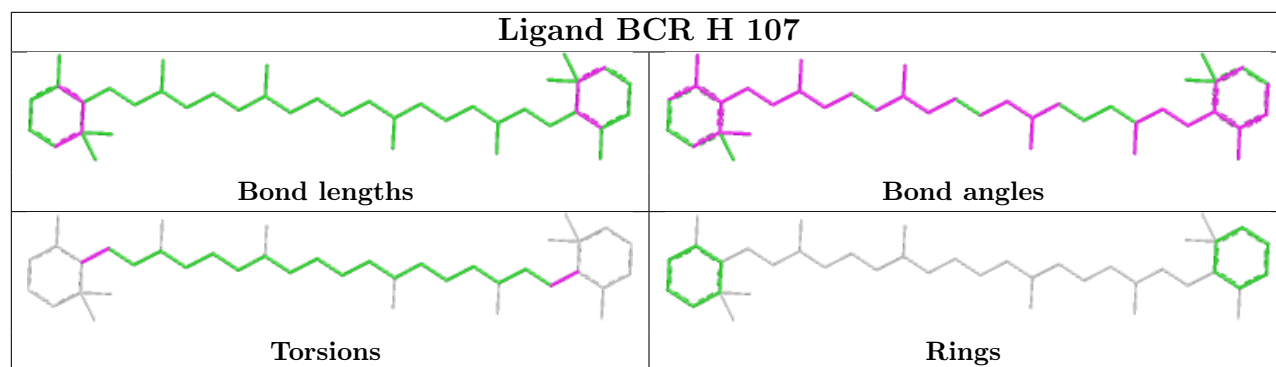
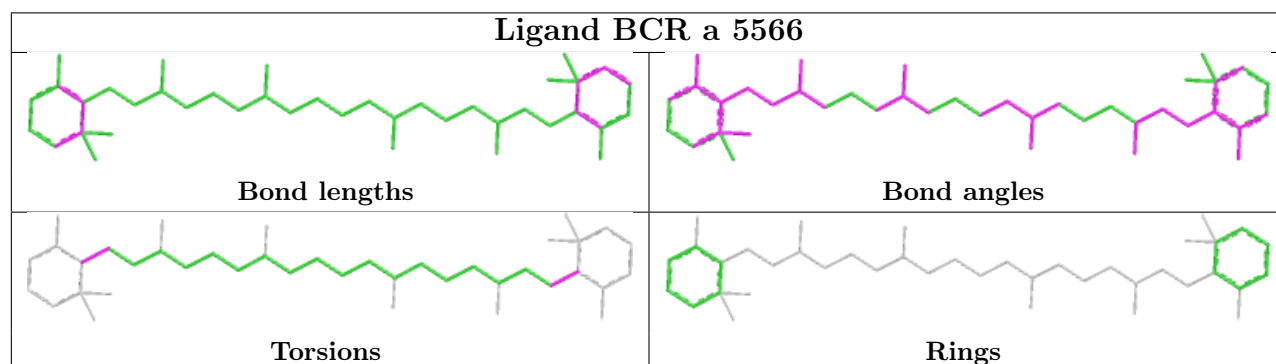
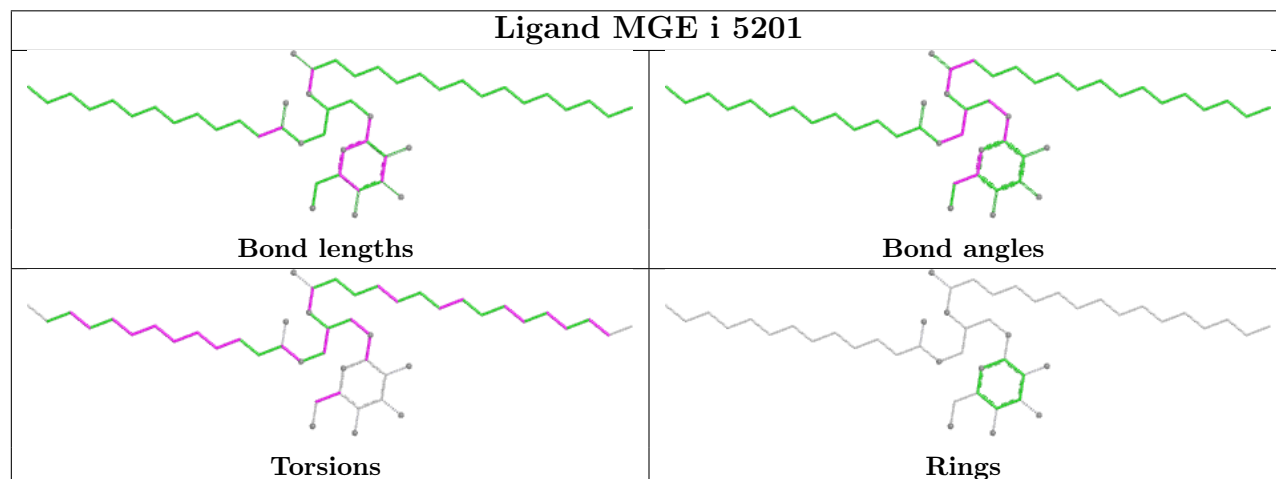
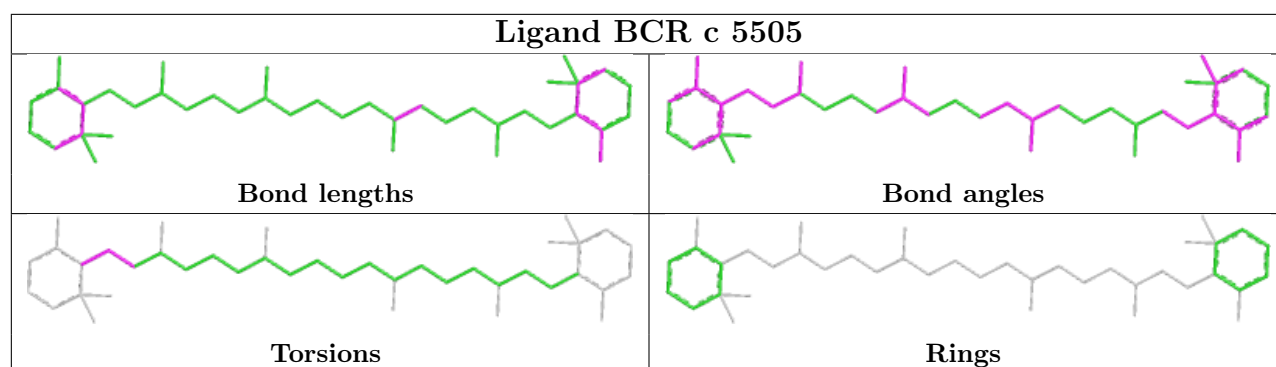


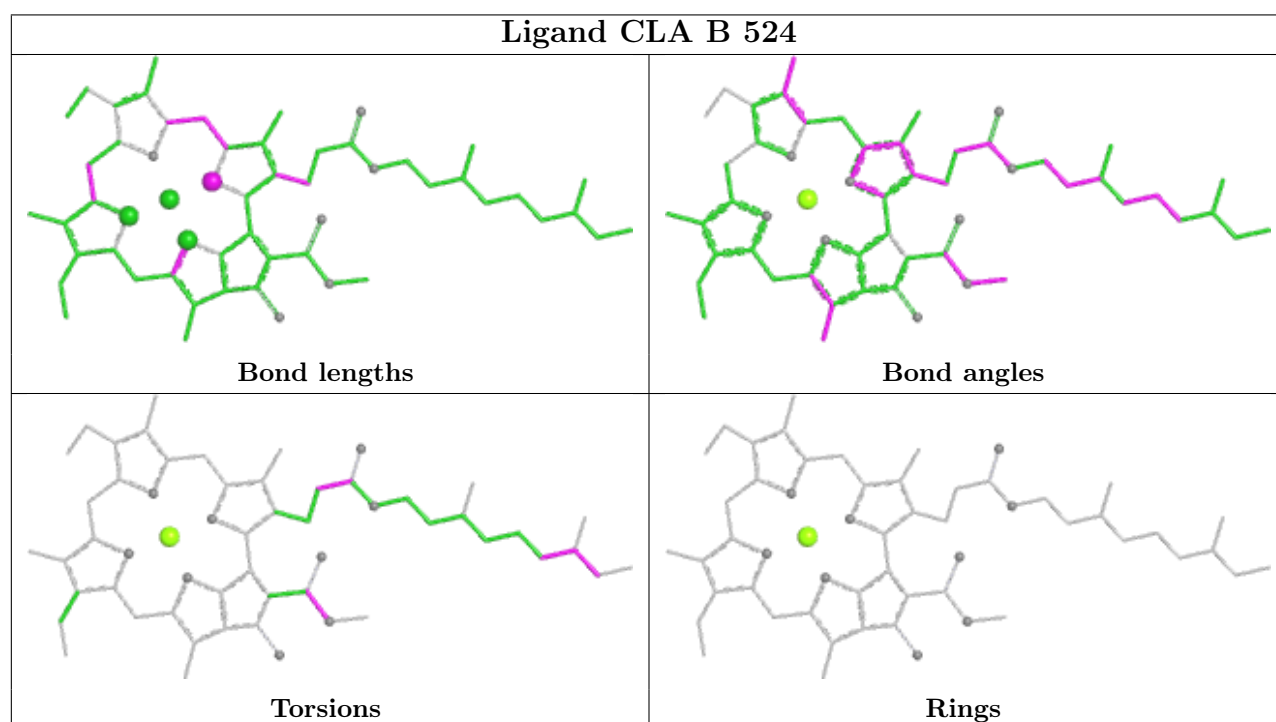
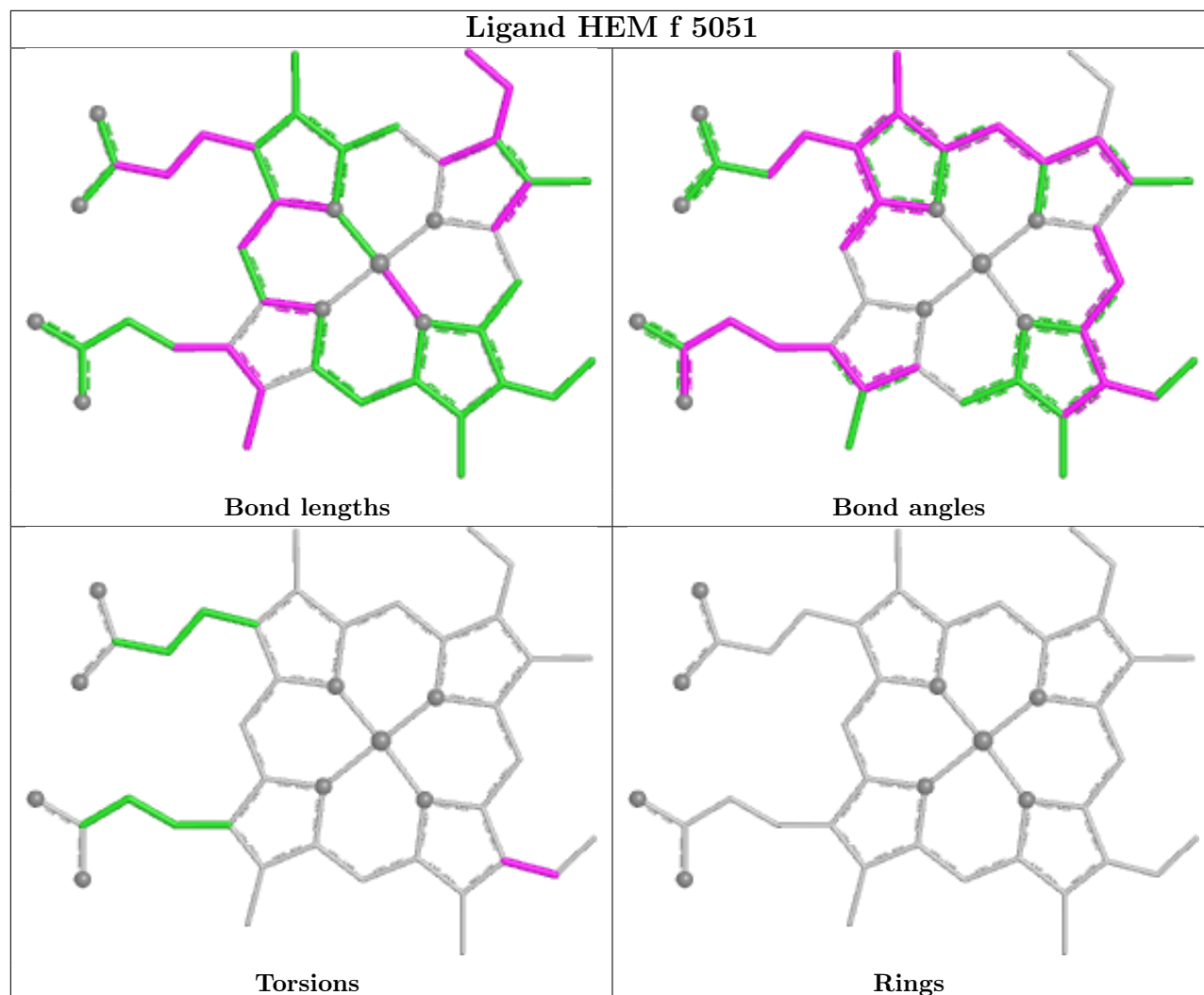


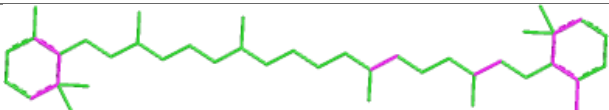
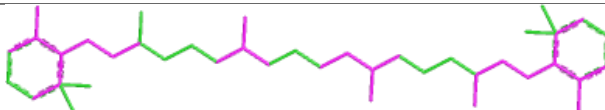
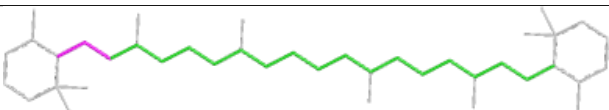
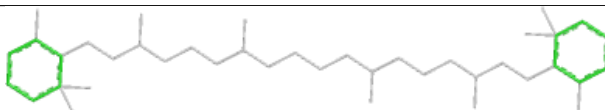




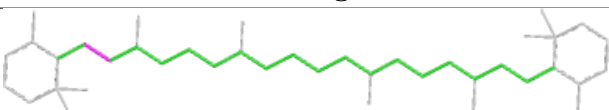
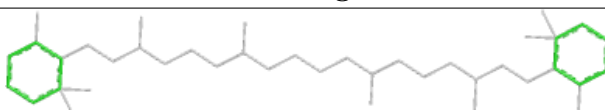


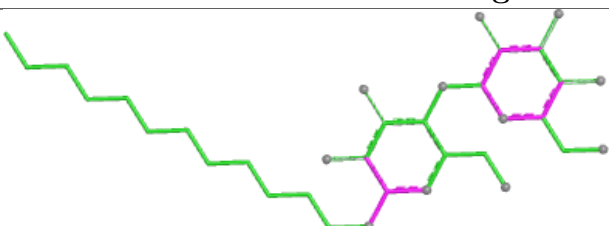
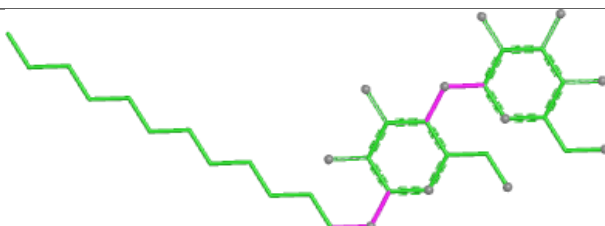
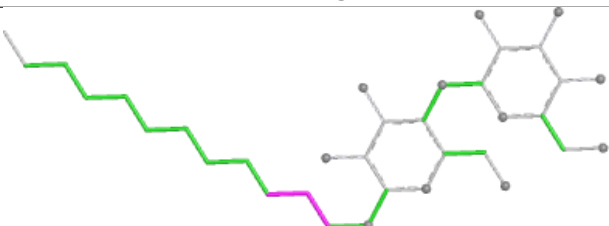
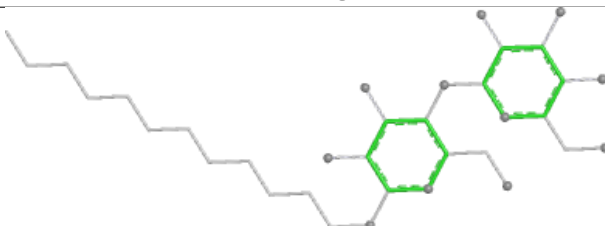


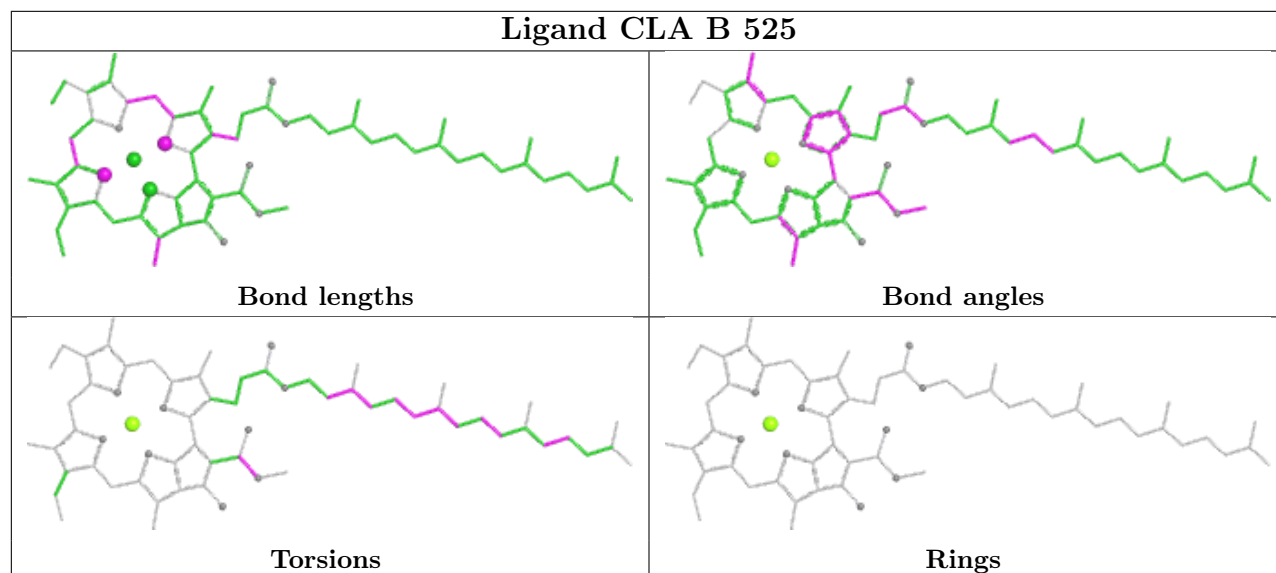
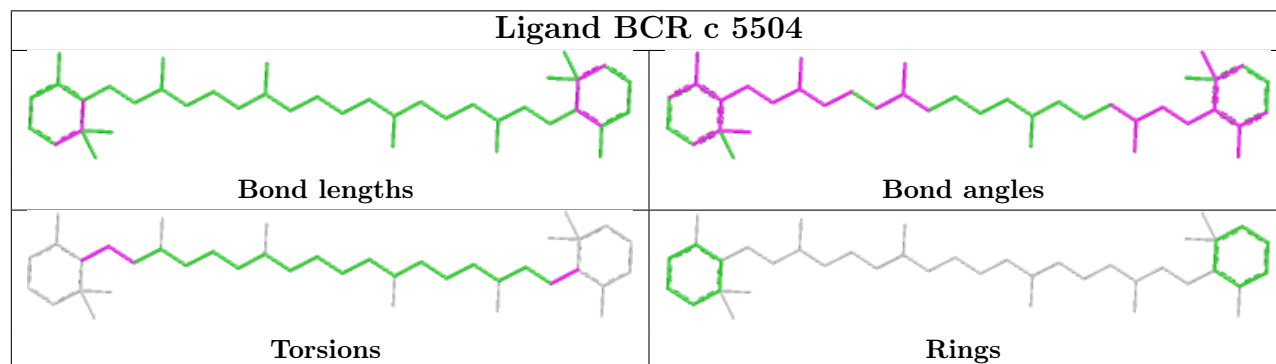
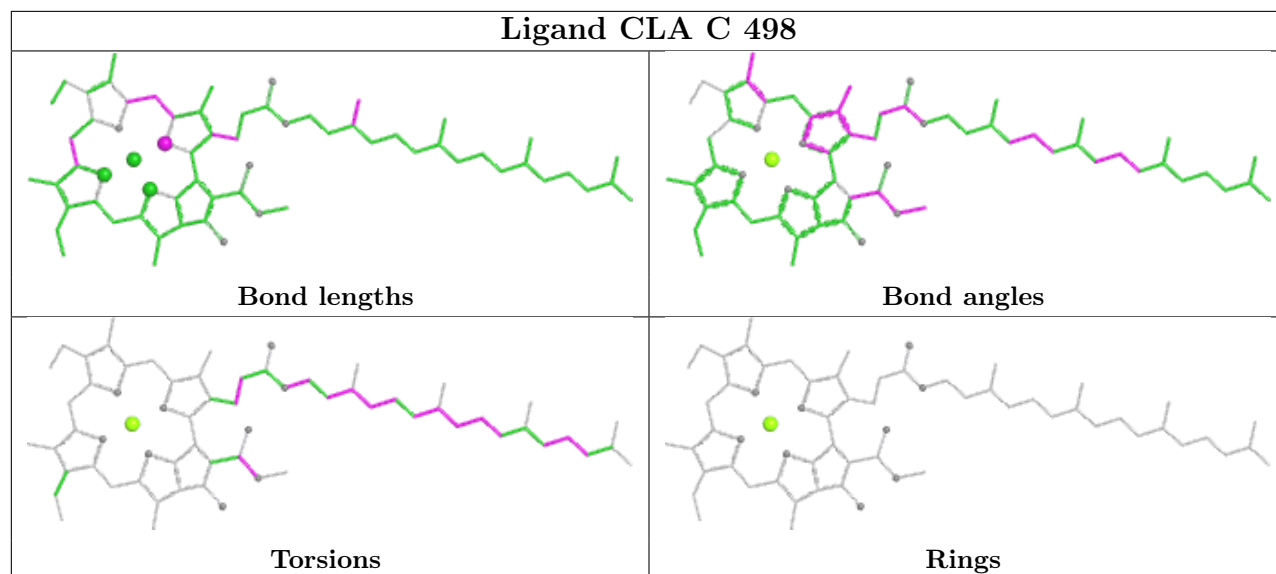


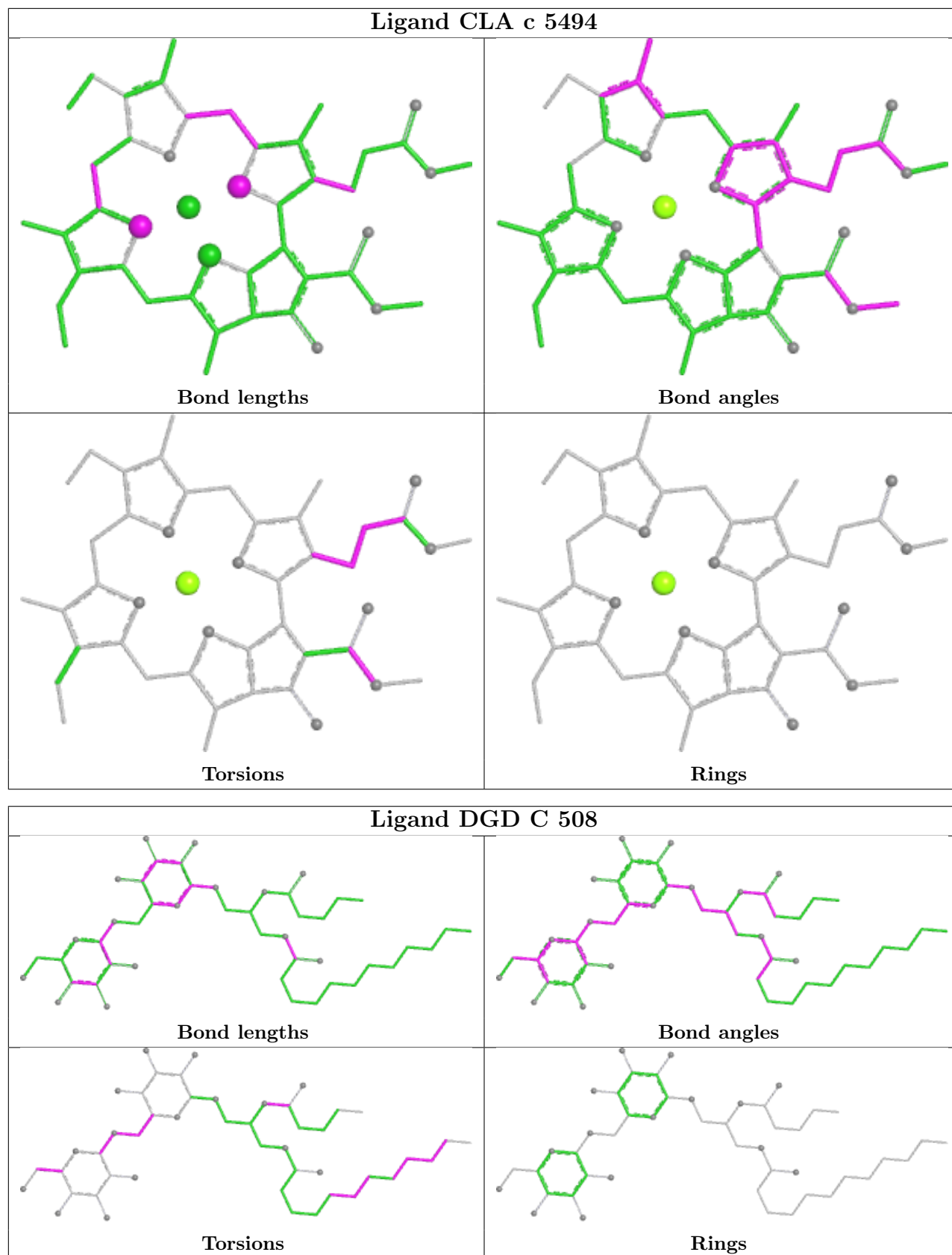


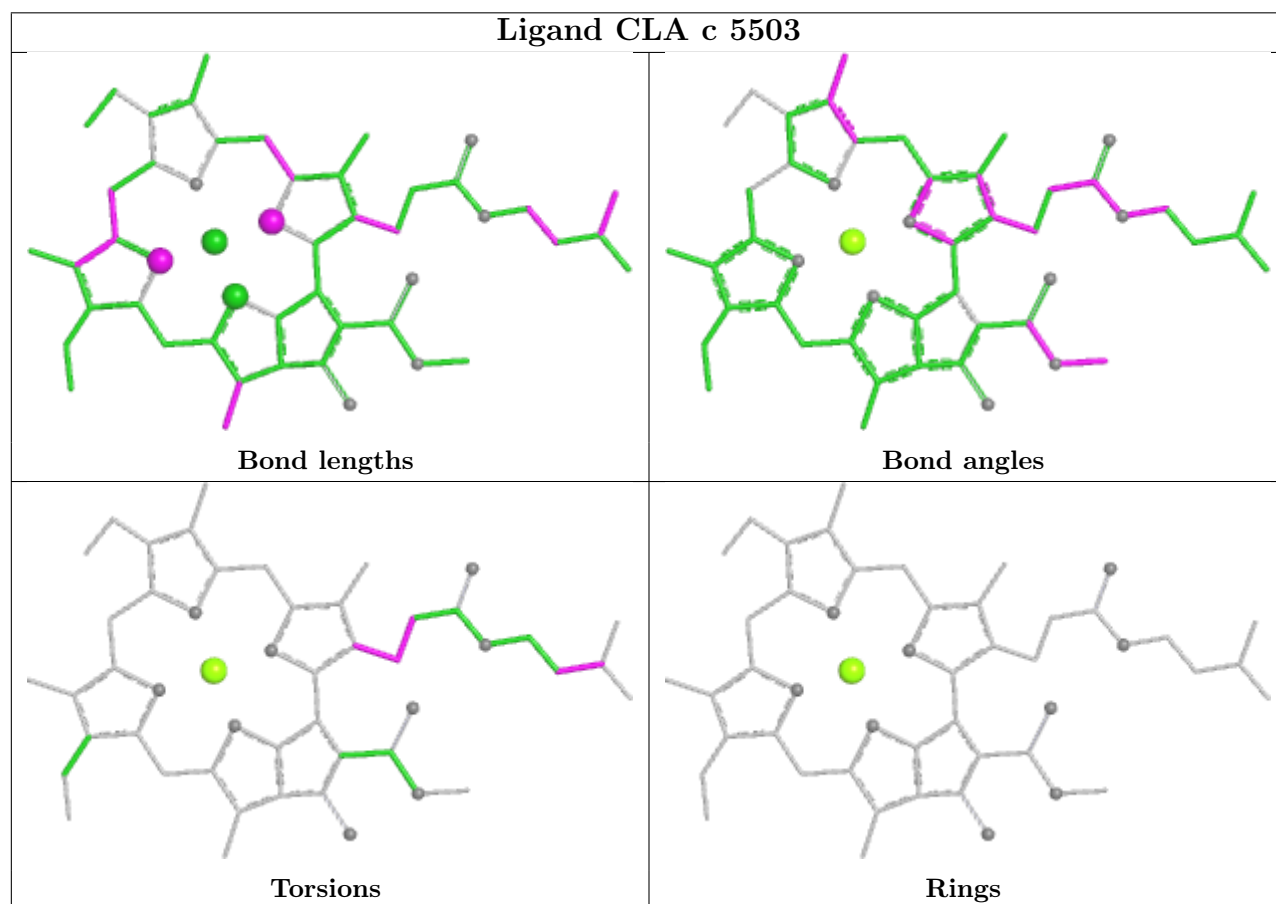
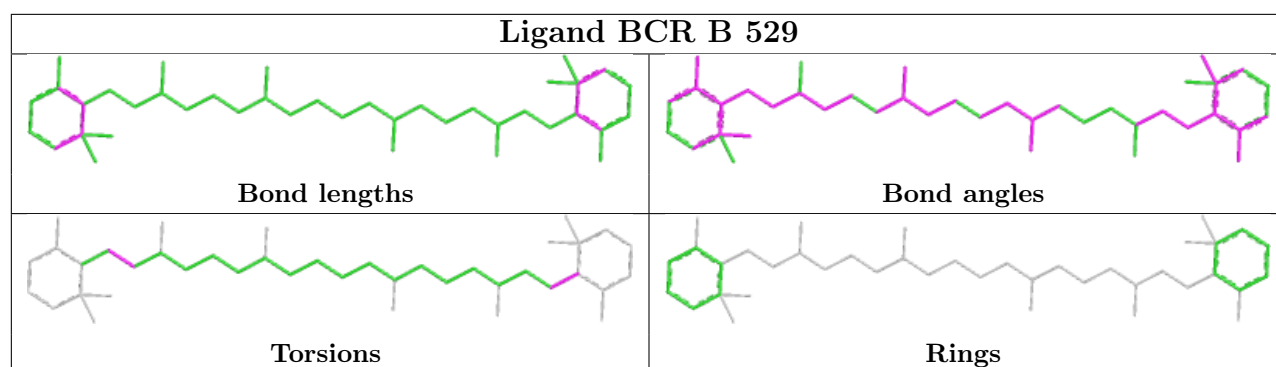
Ligand BCR C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

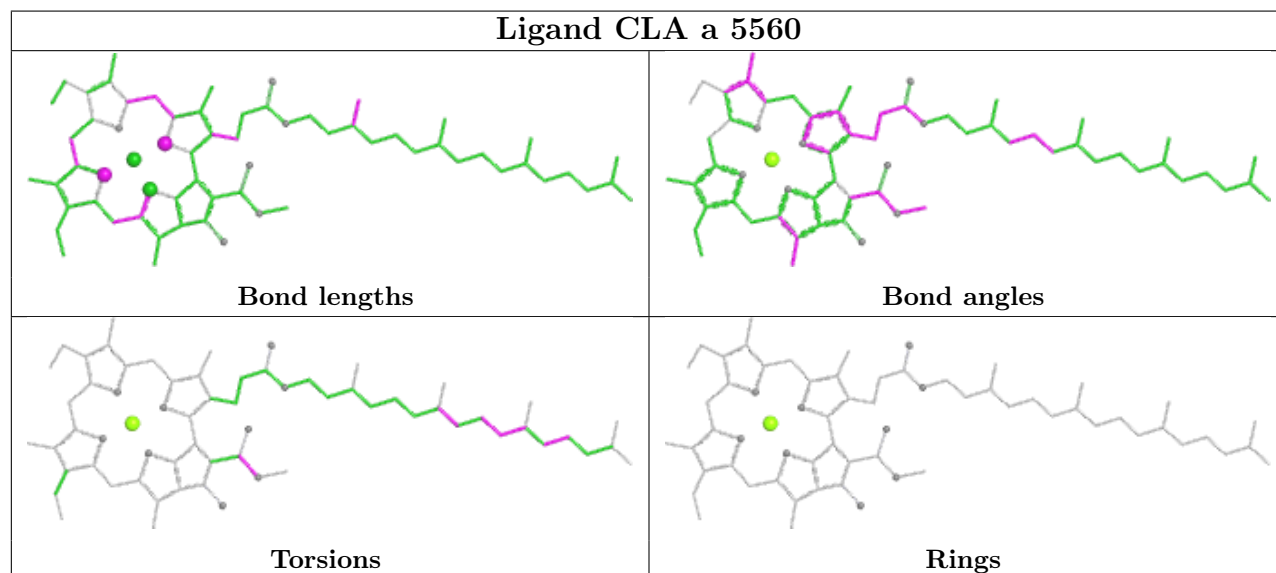
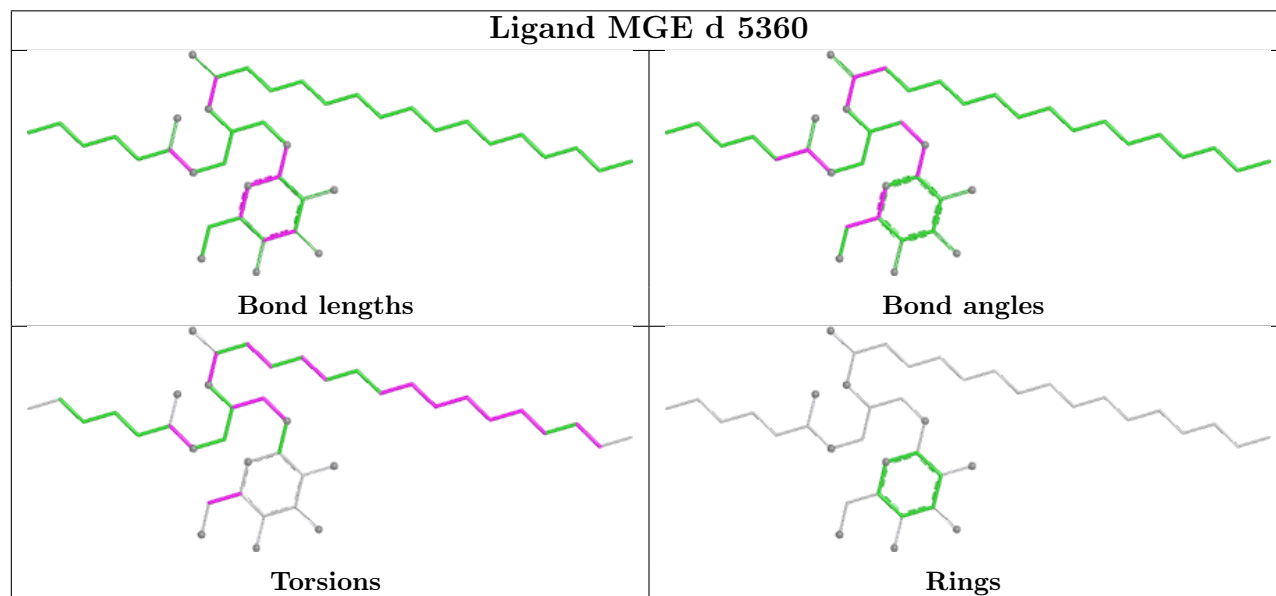
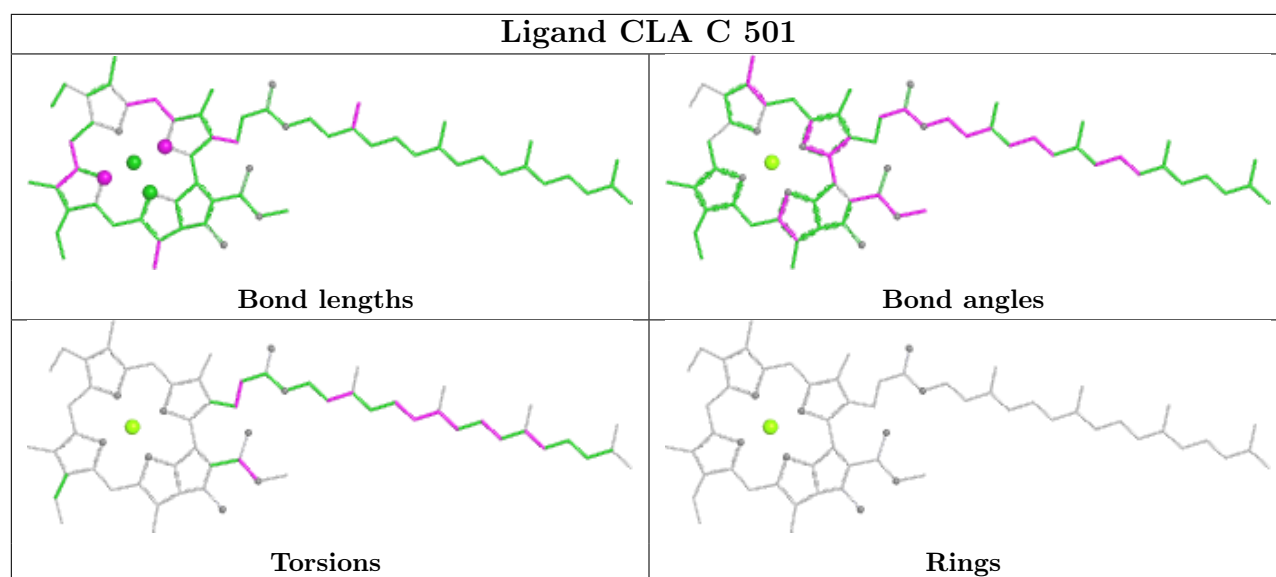
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT M 5216	
	
Bond lengths	Bond angles
	
Torsions	Rings

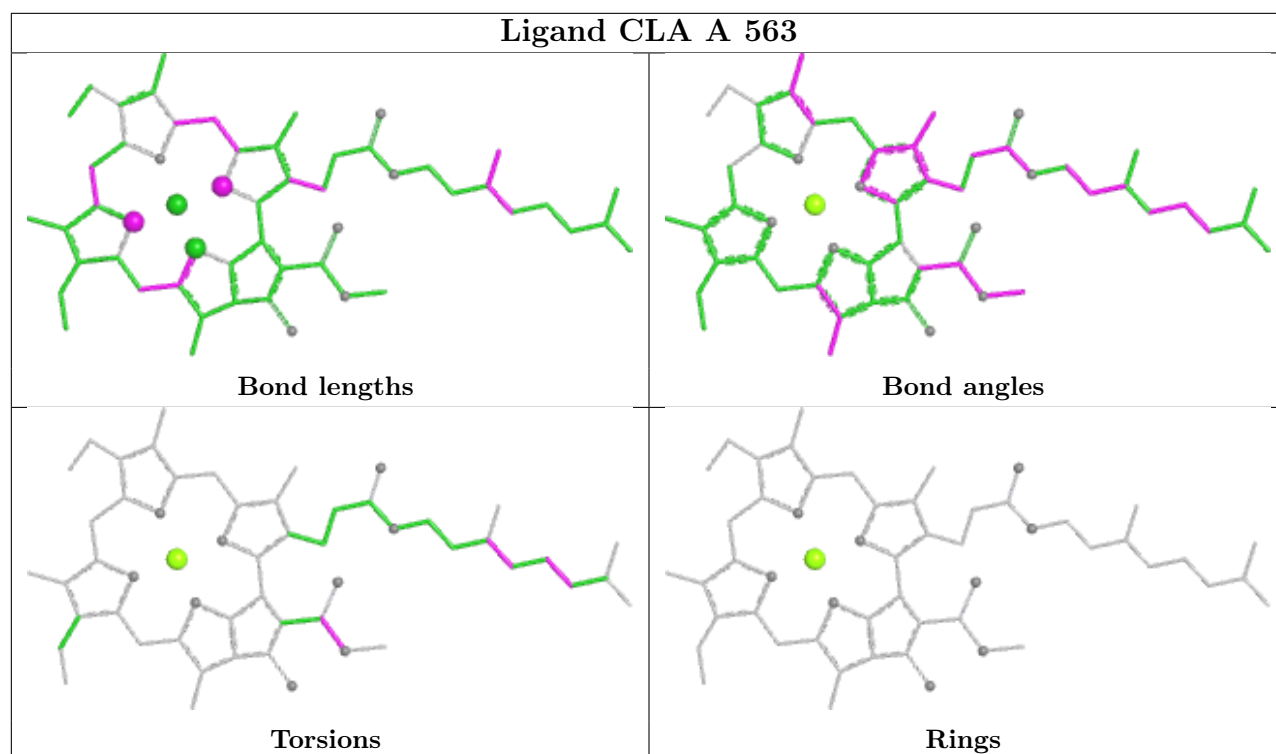
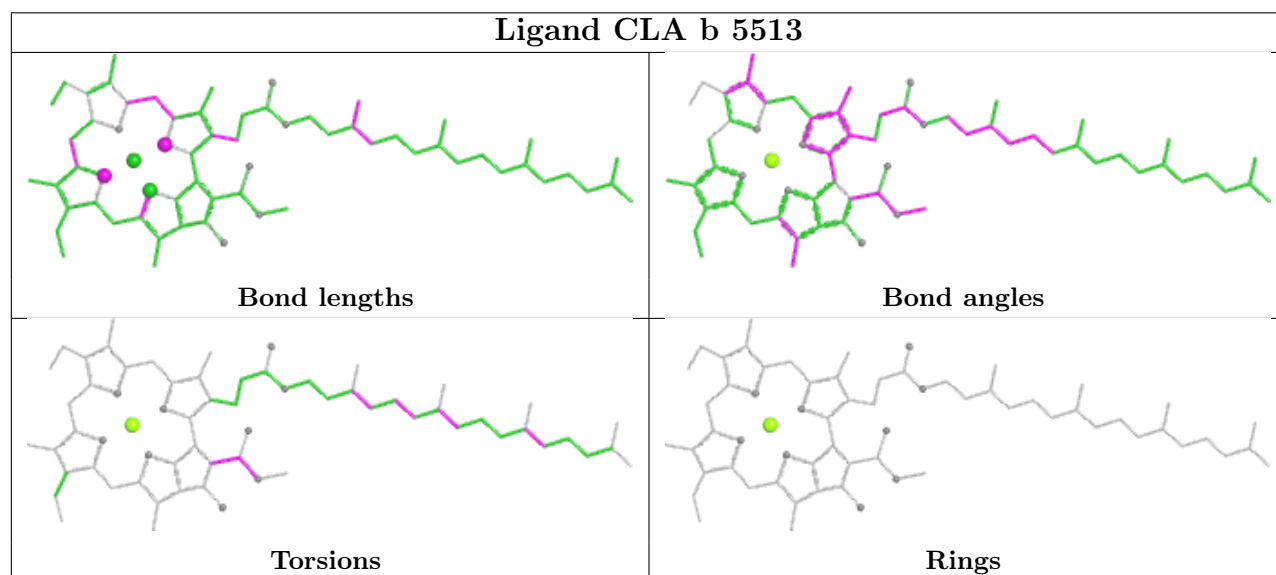
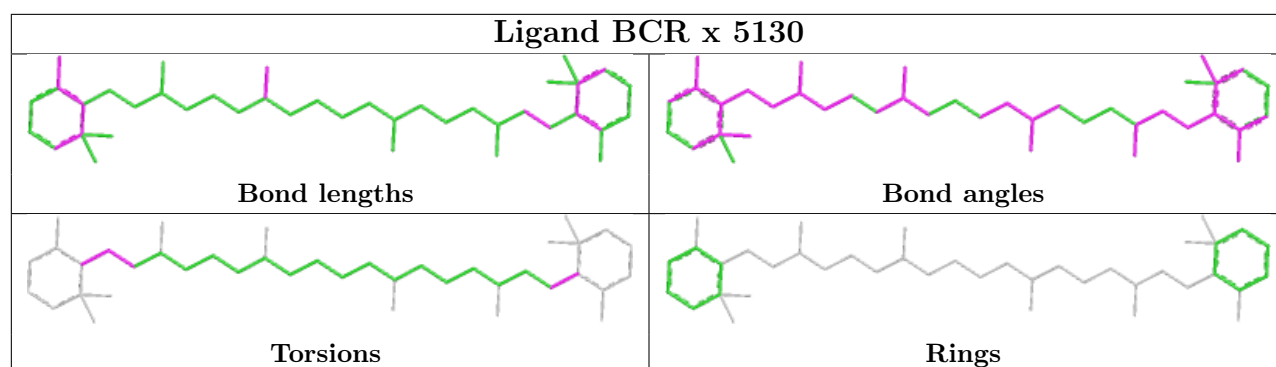


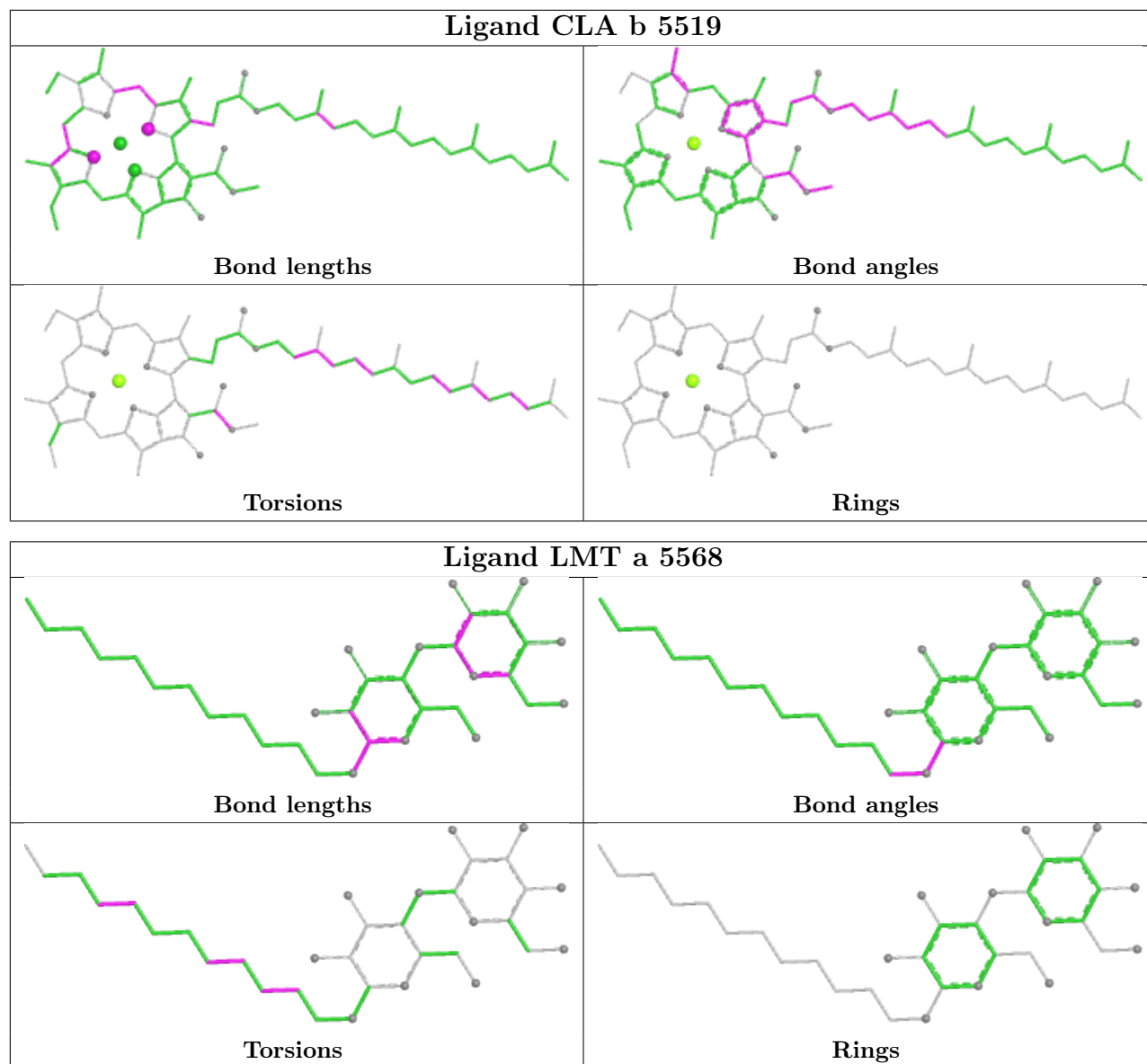




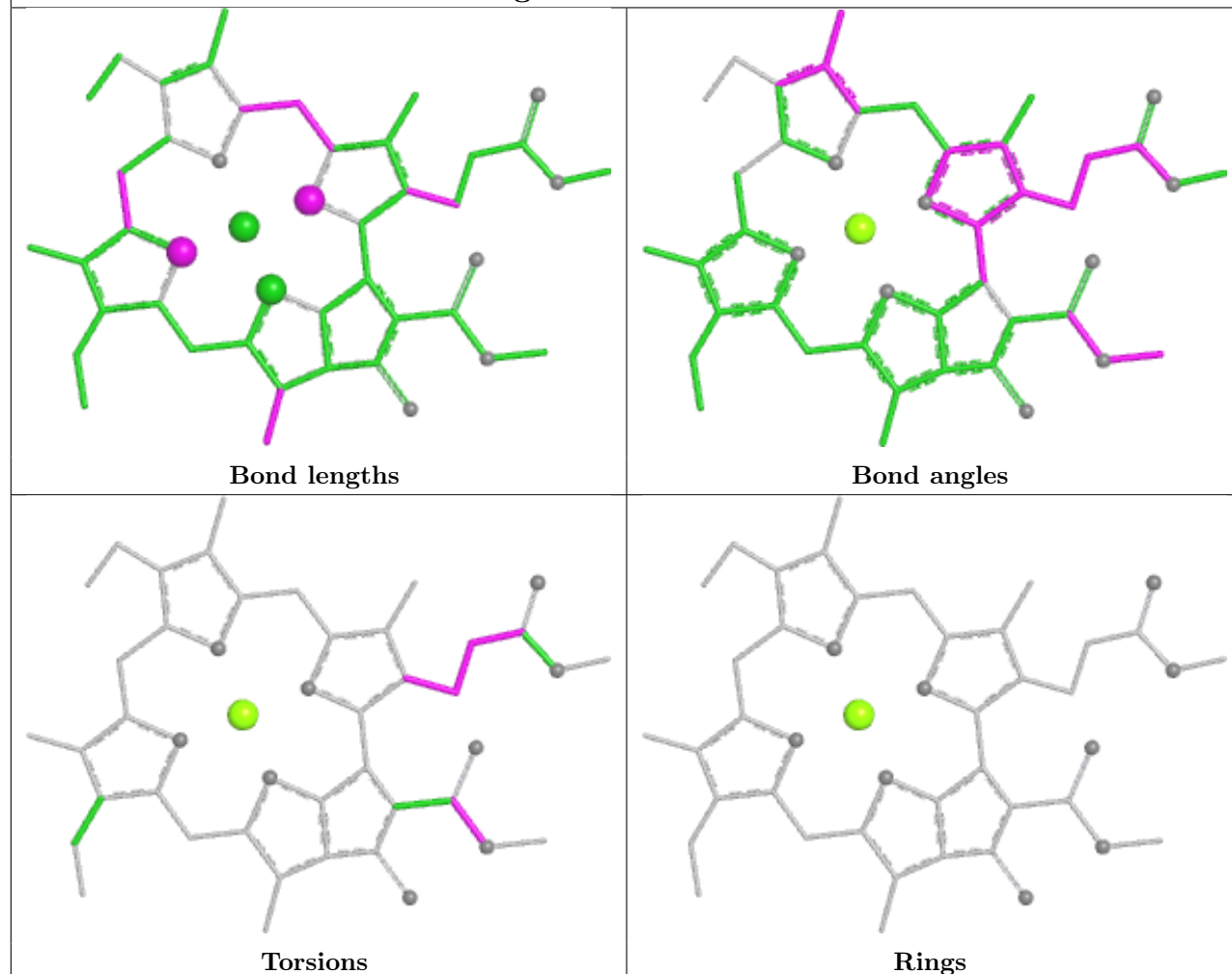




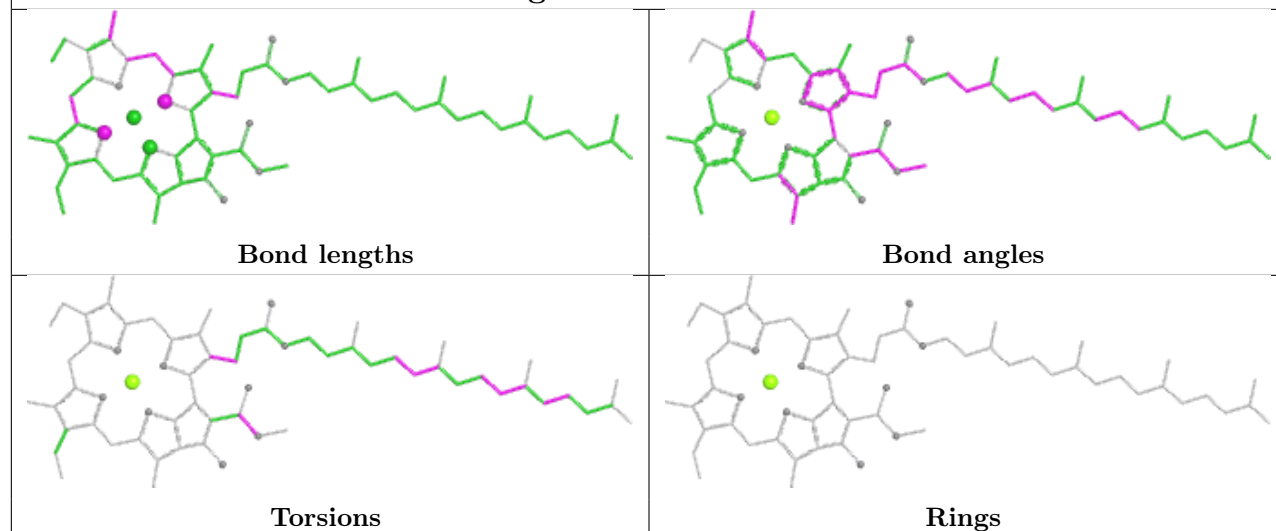


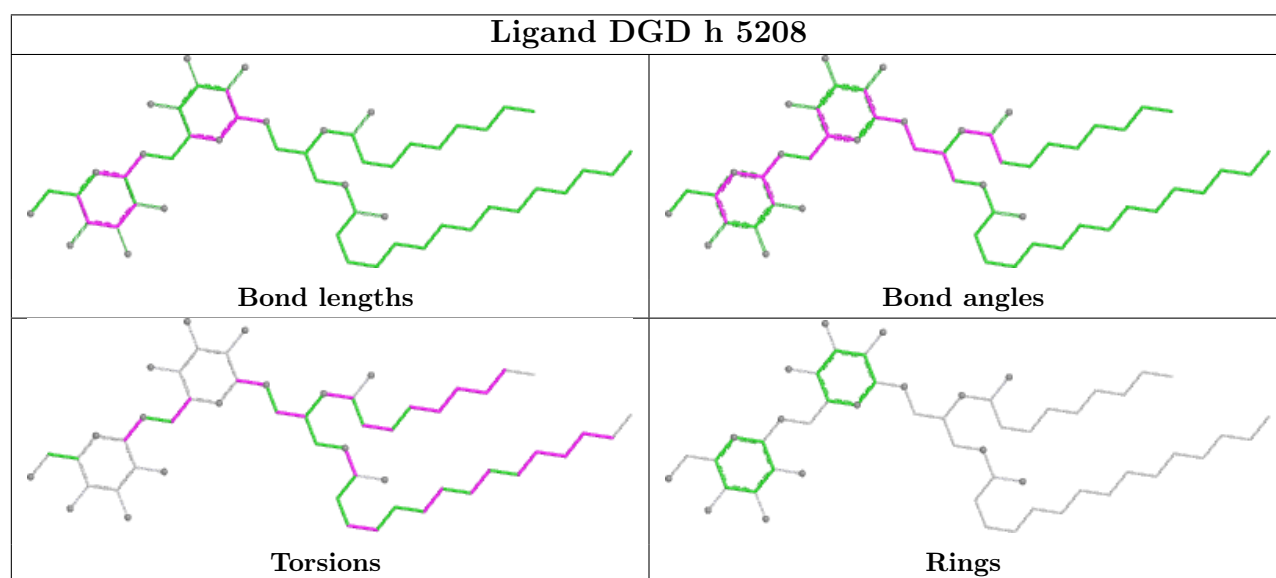
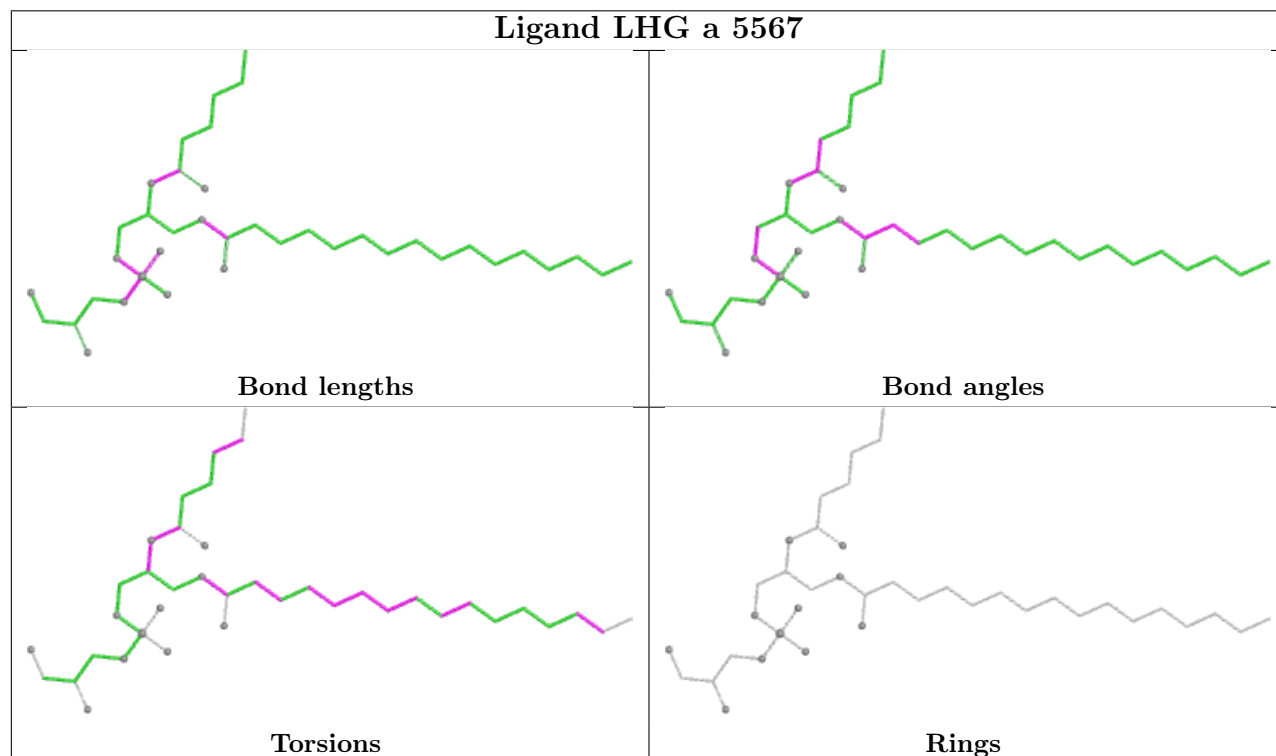
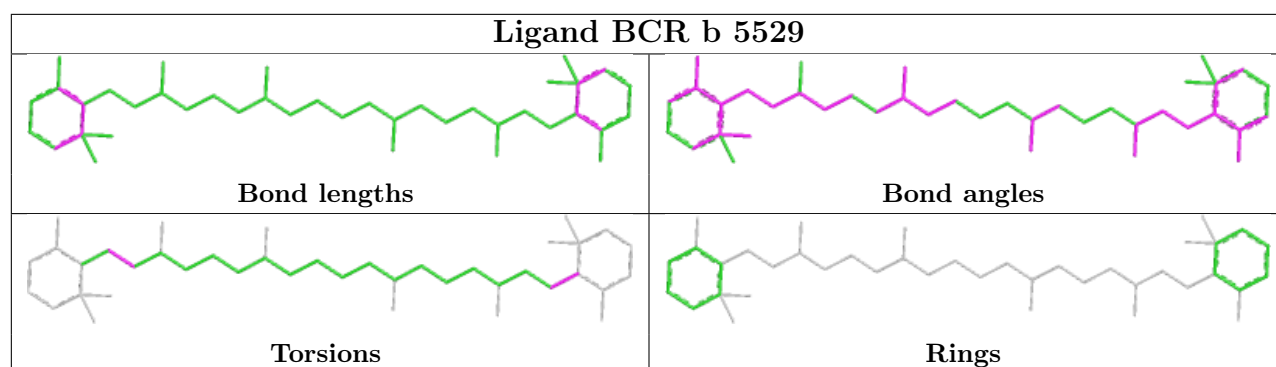


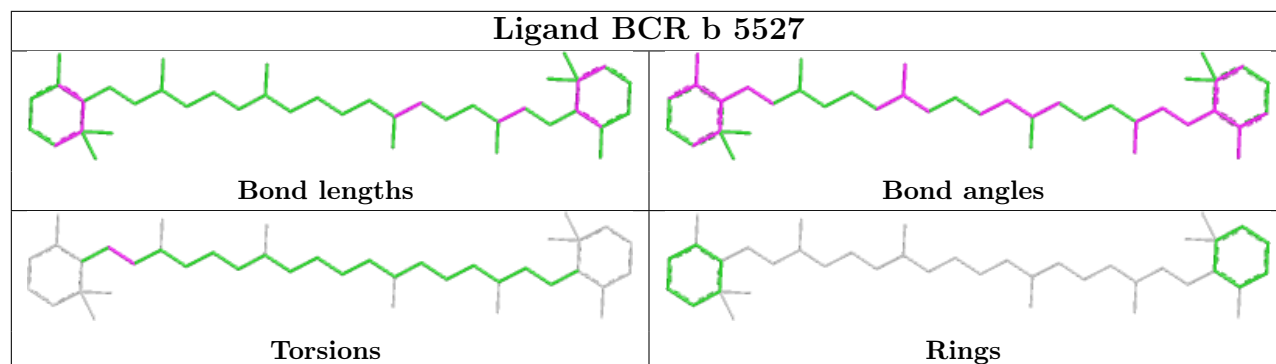
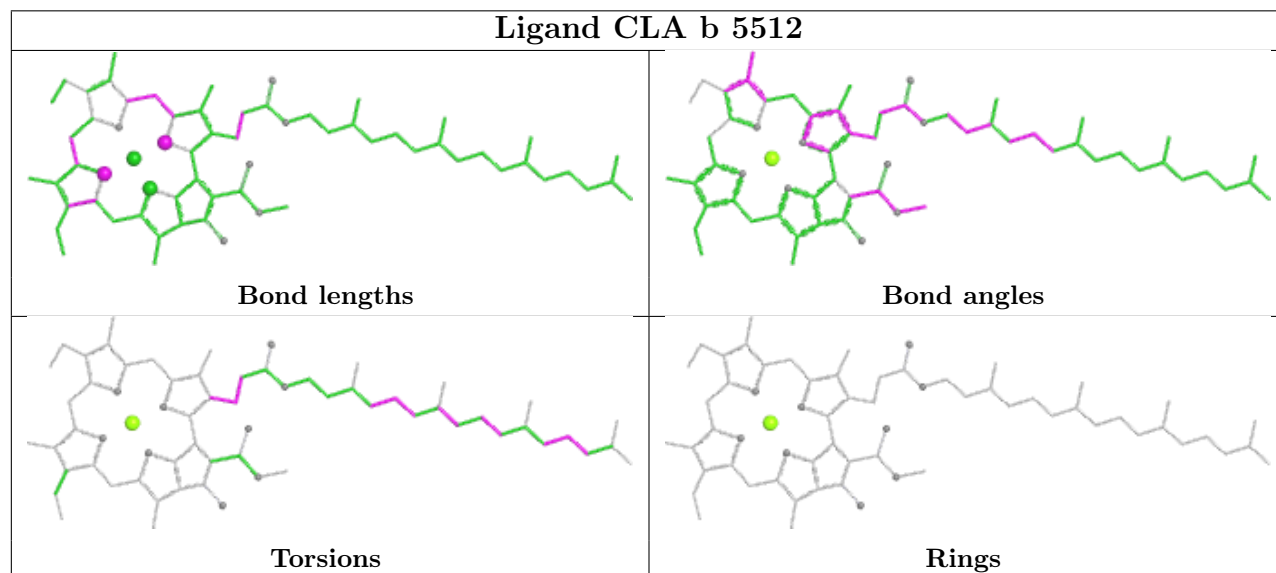
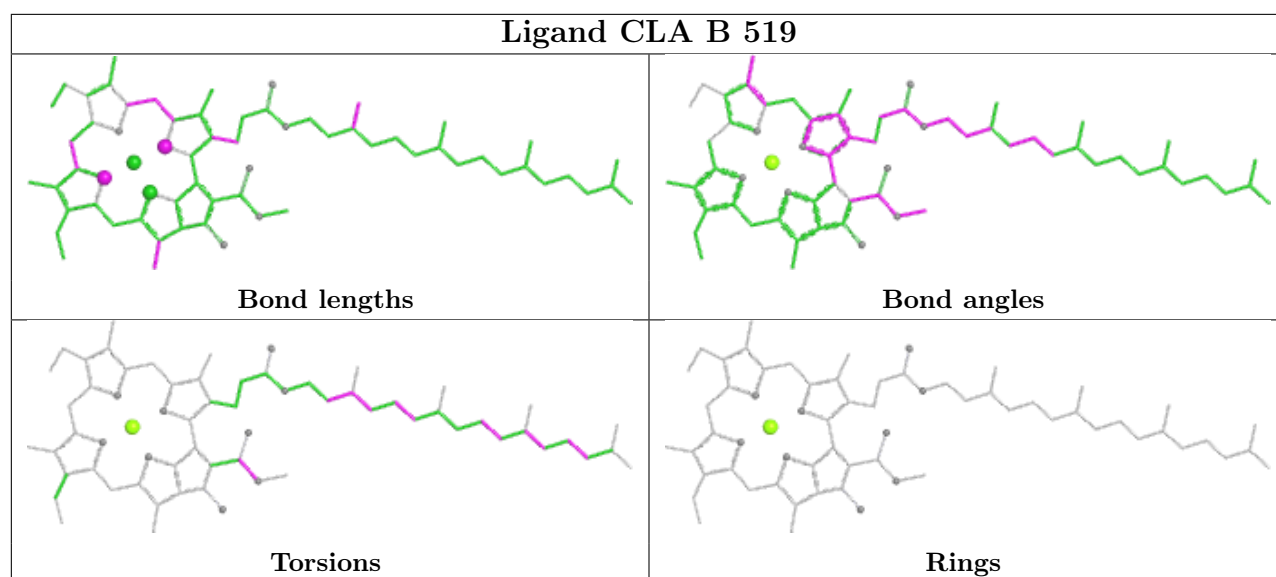
## Ligand CLA C 494

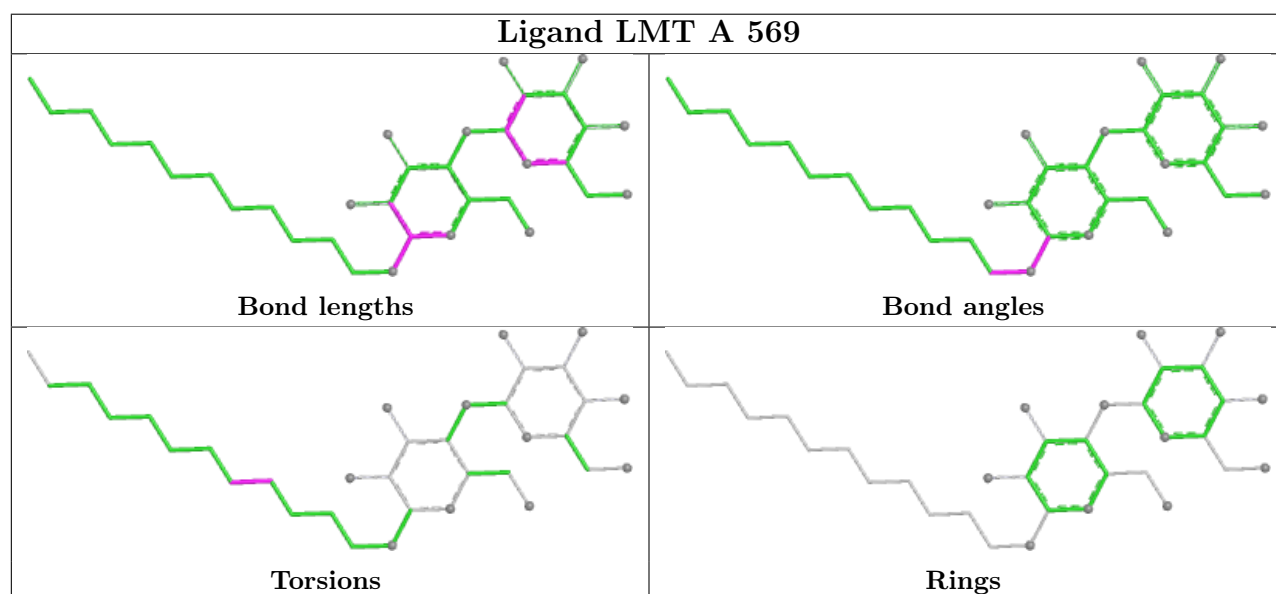
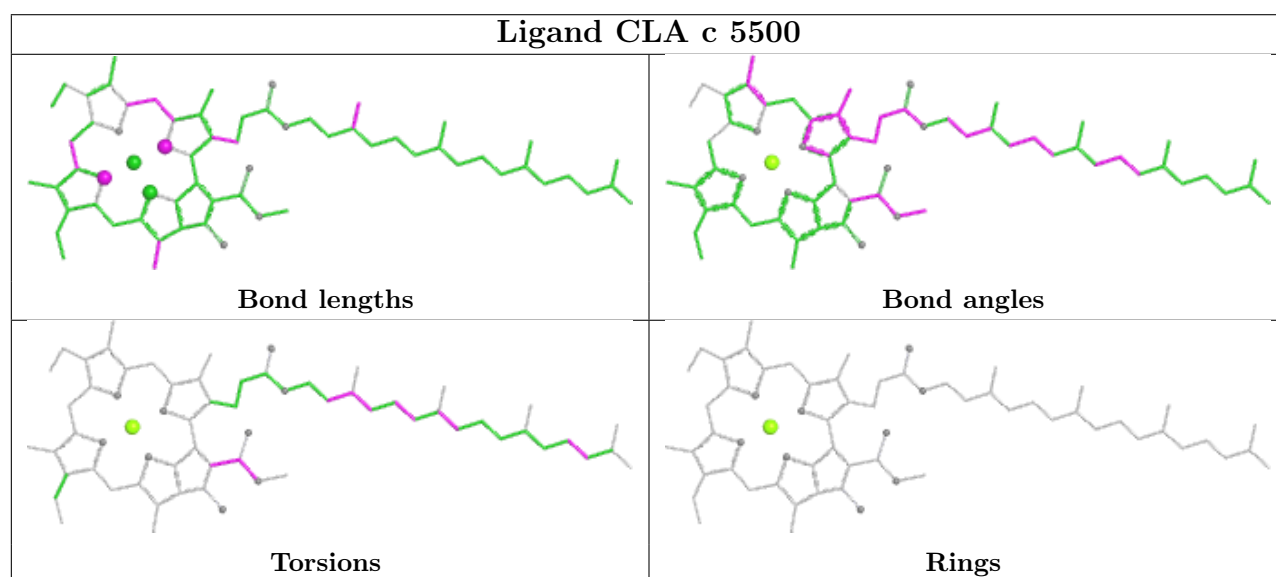
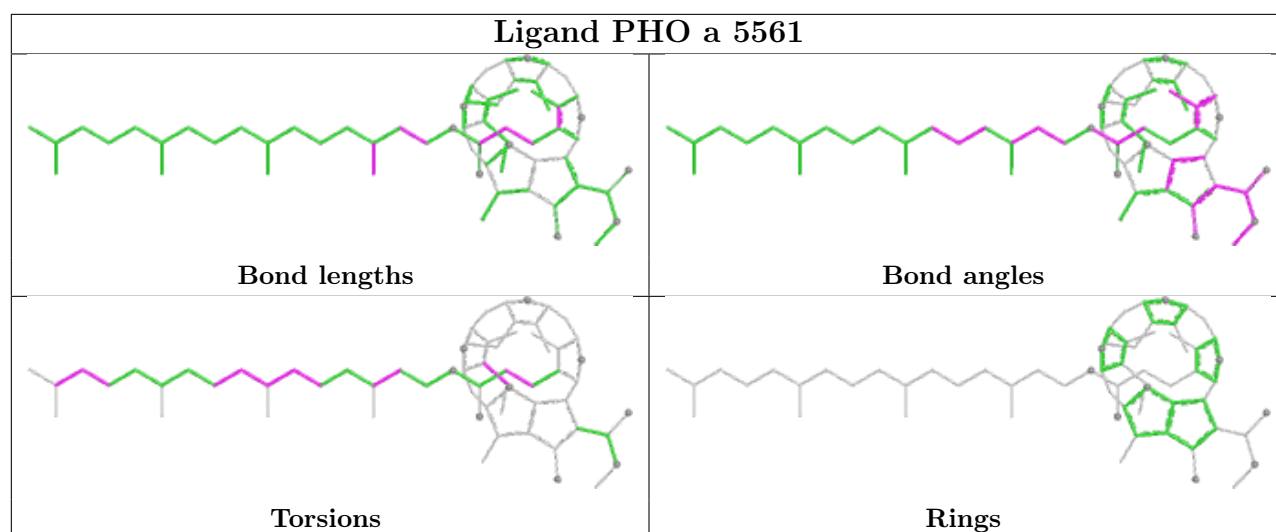


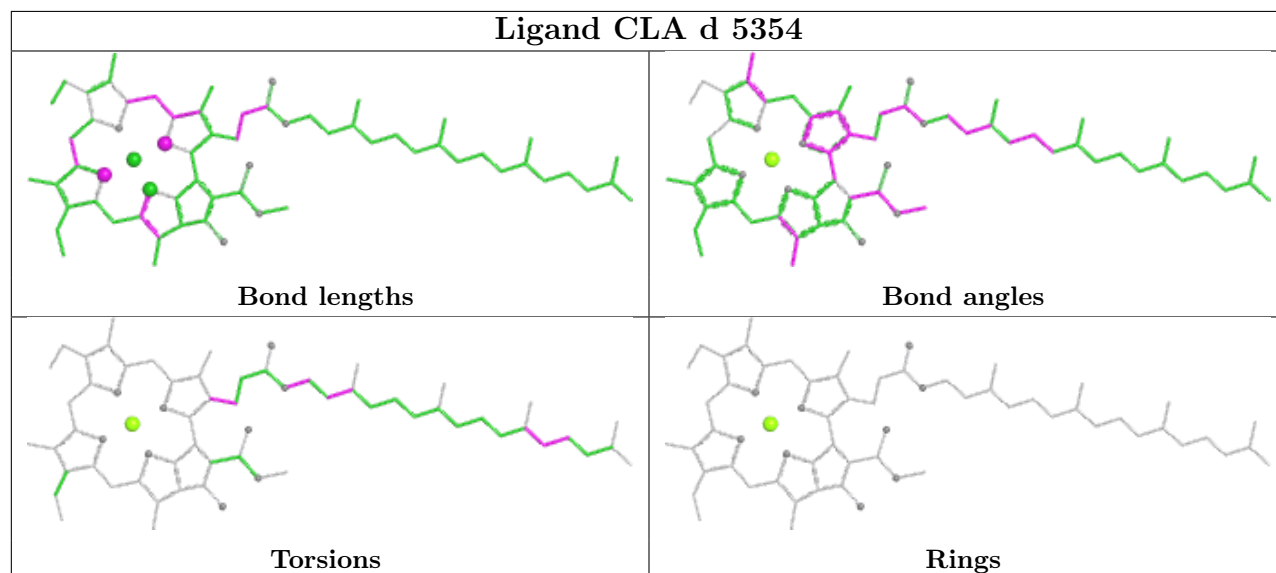
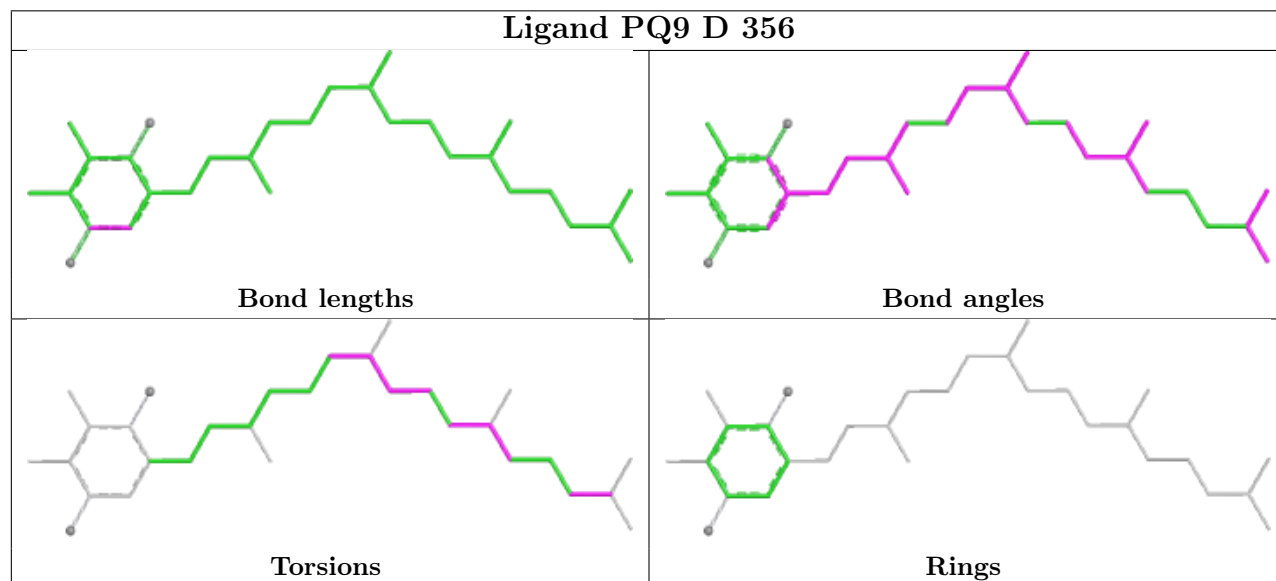
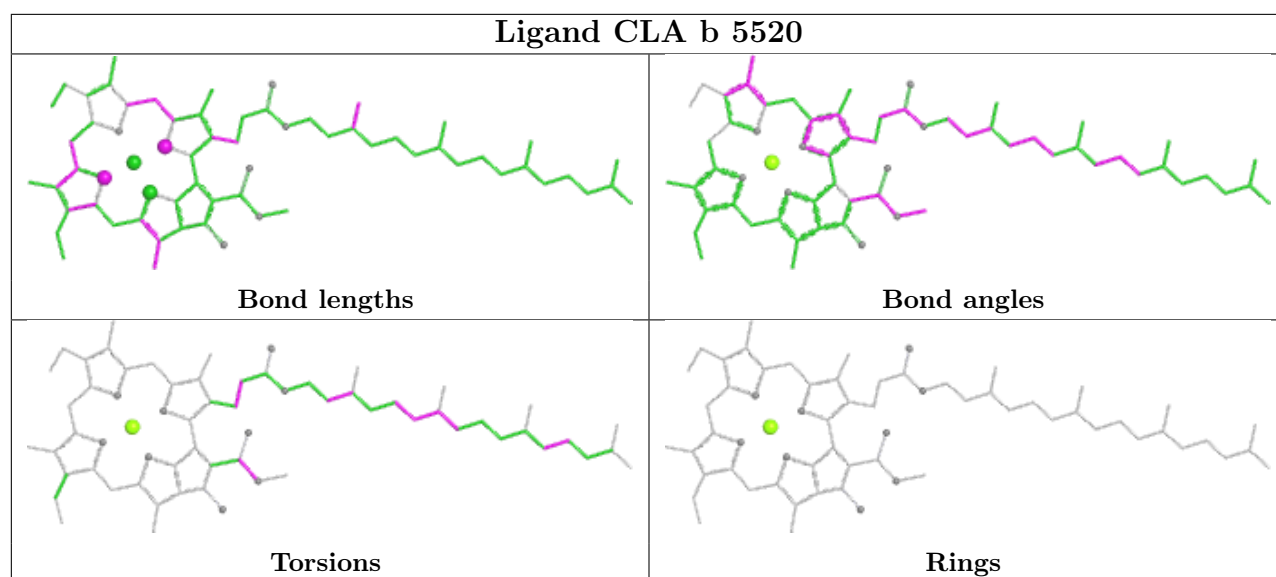
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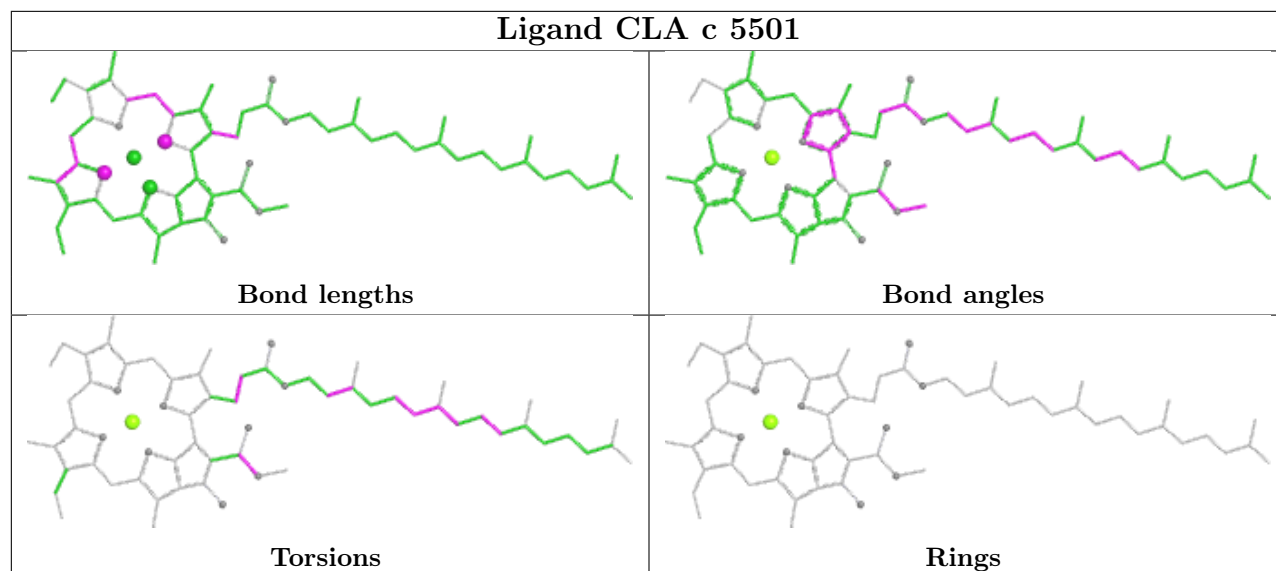
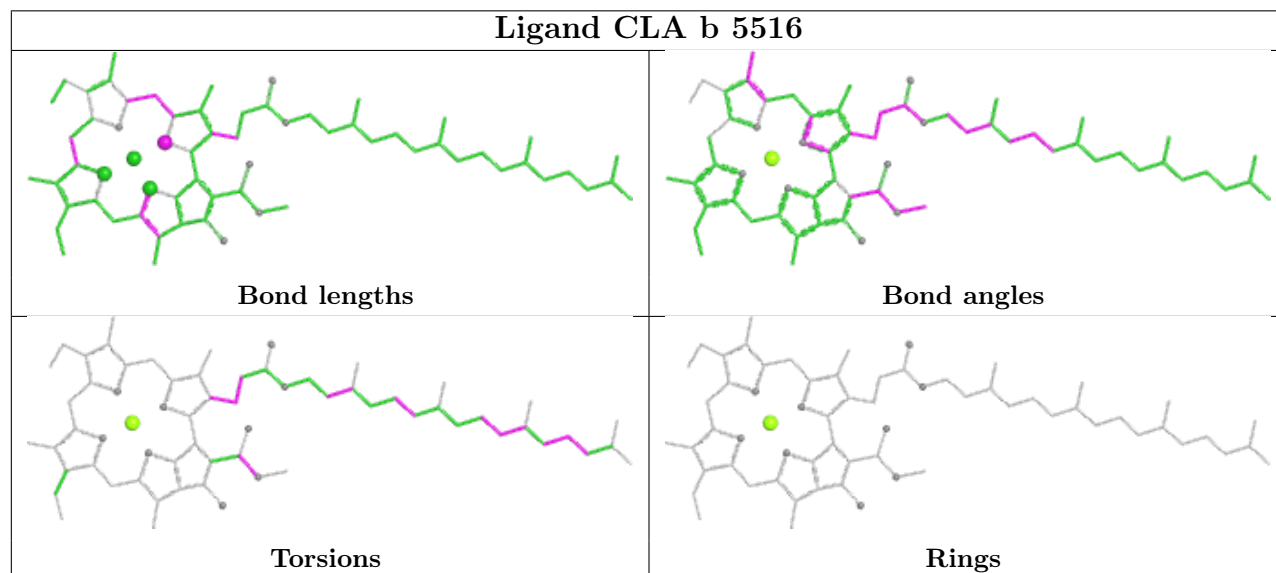
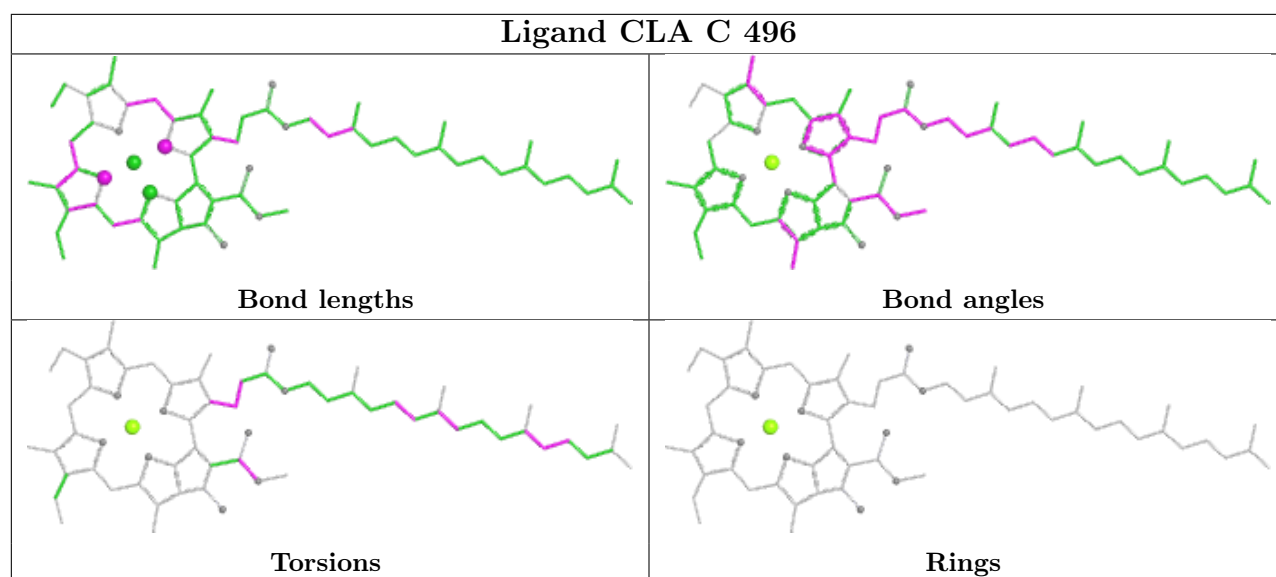




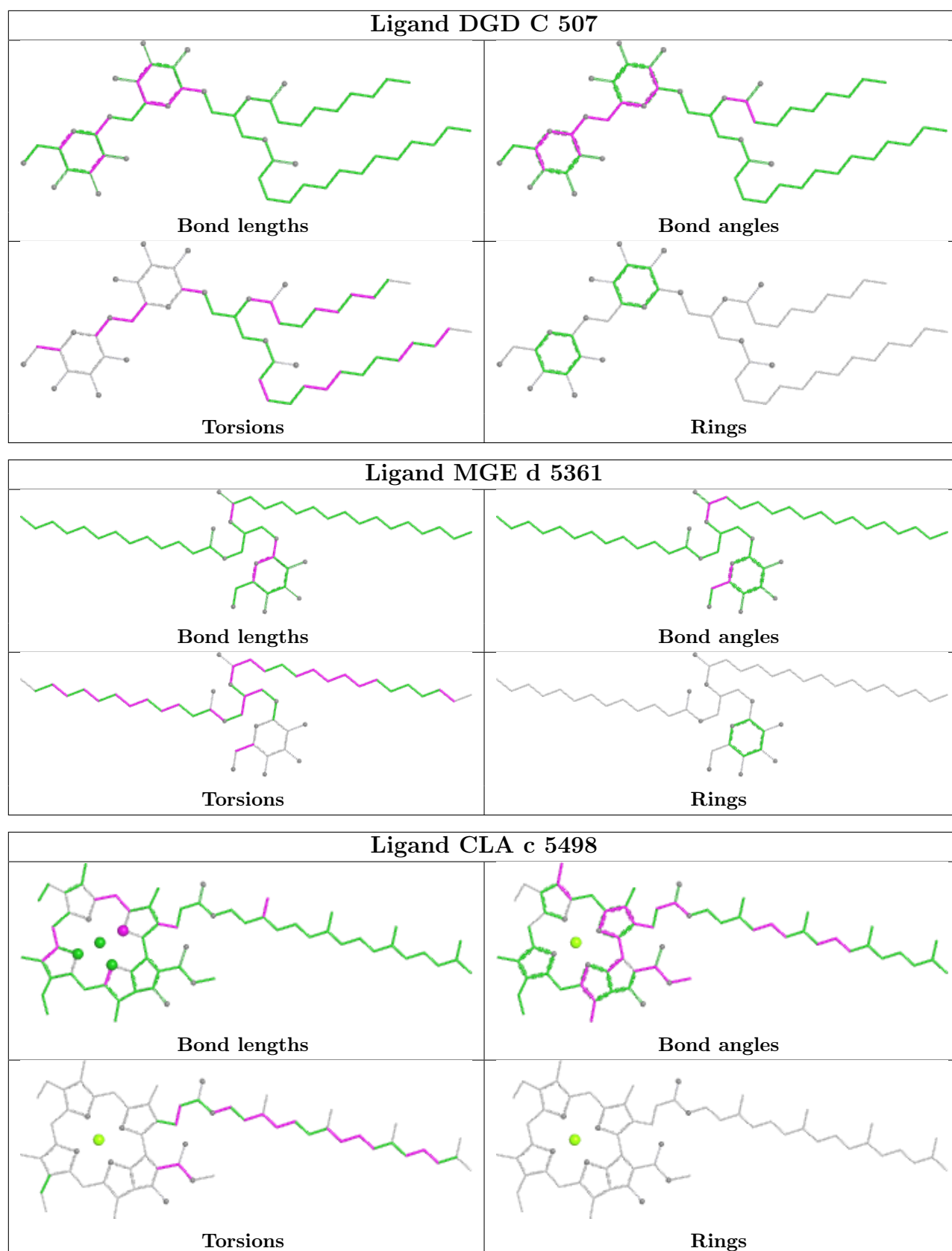


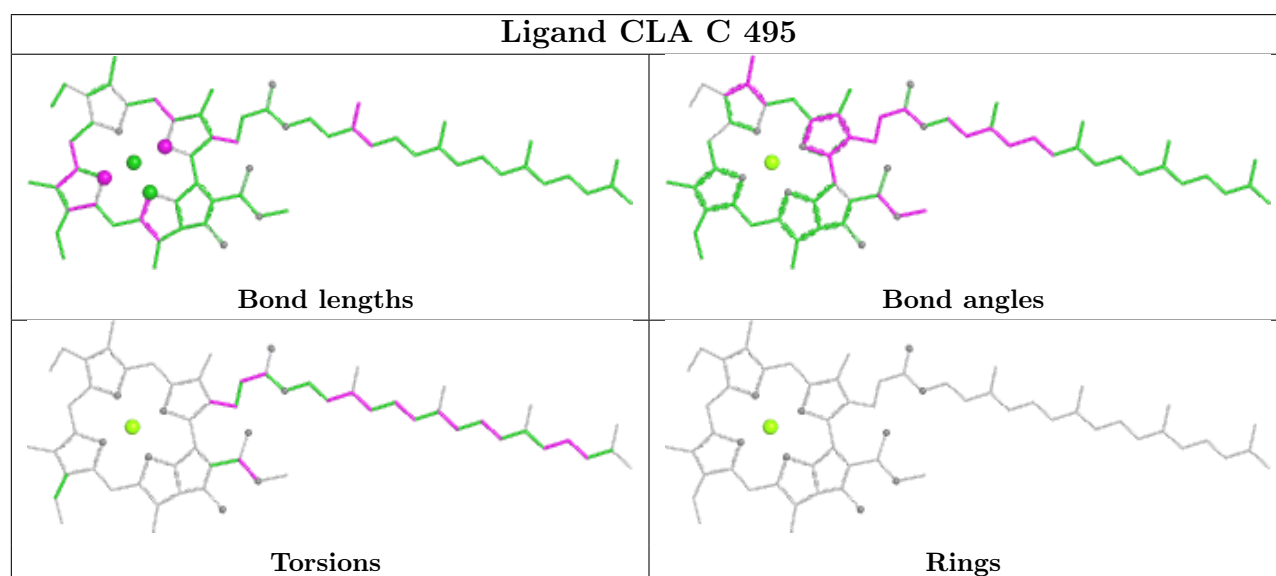
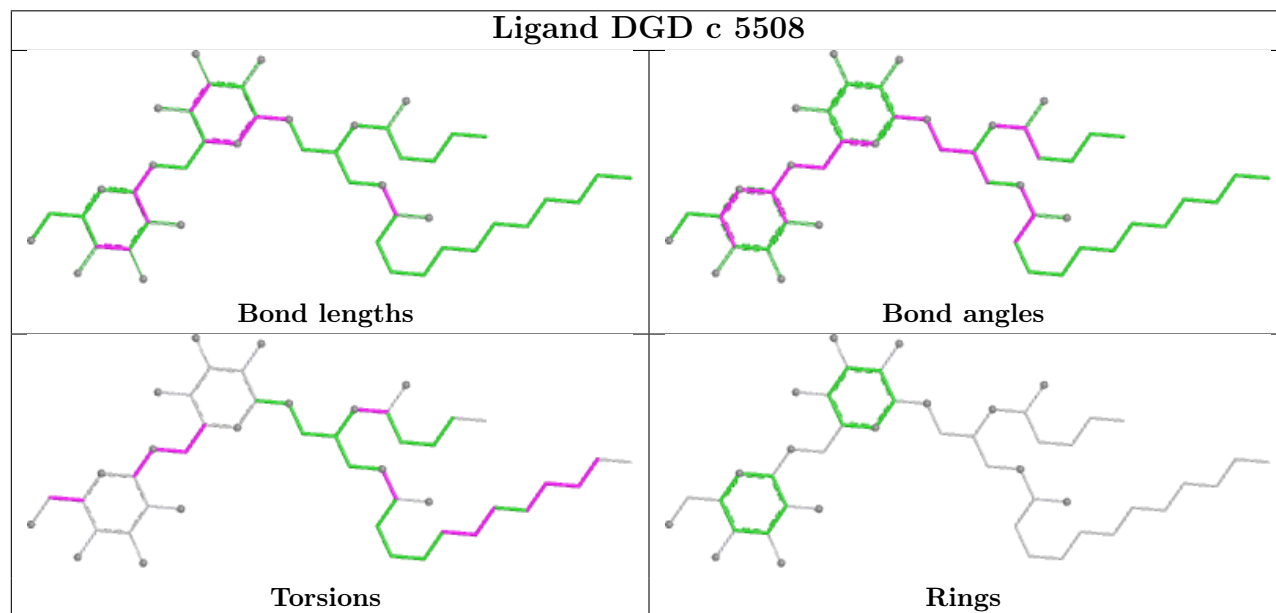
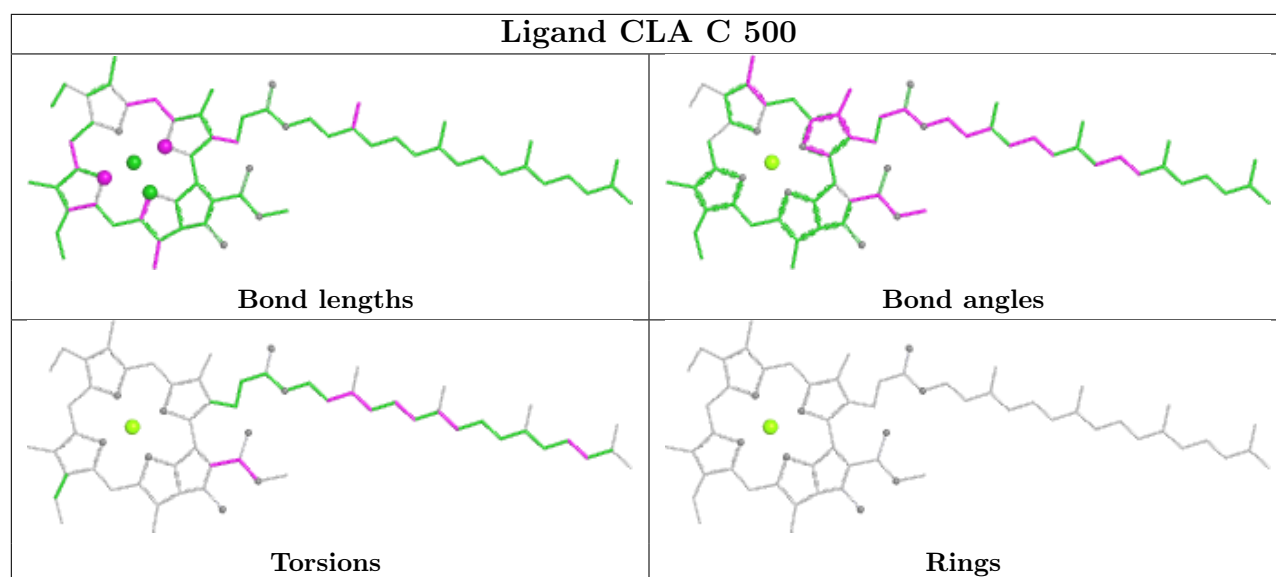


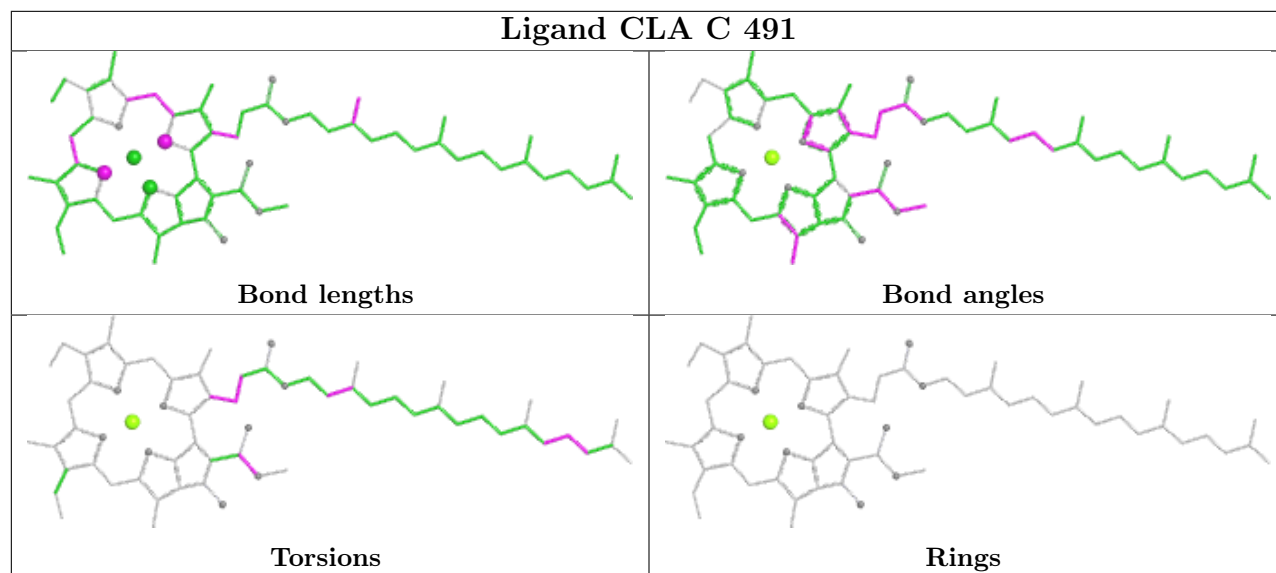
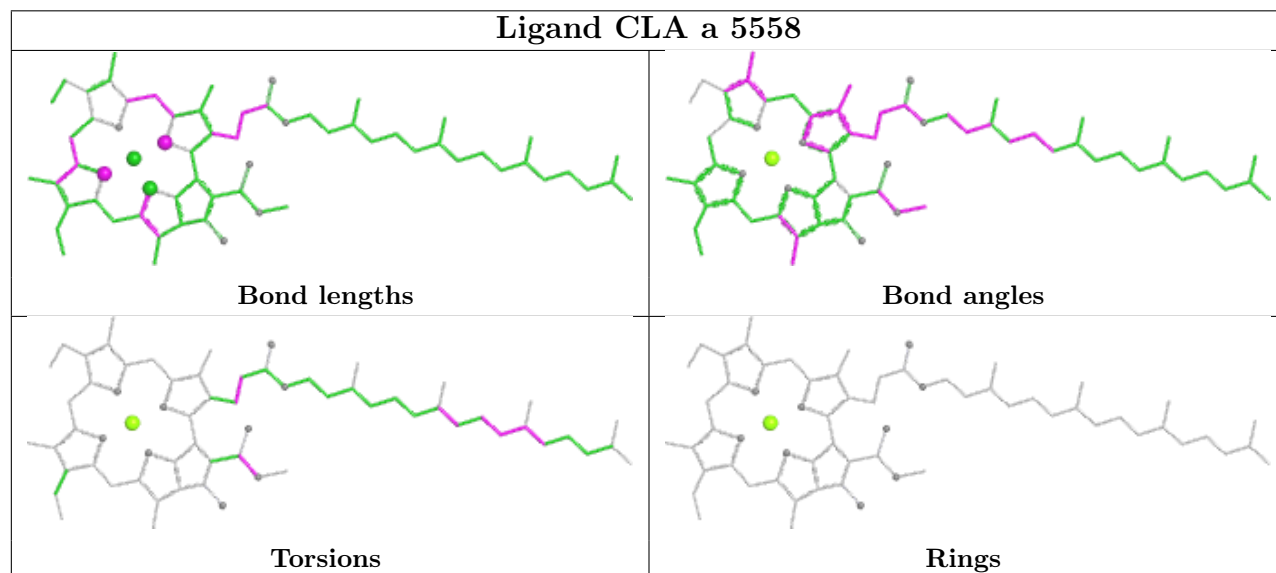
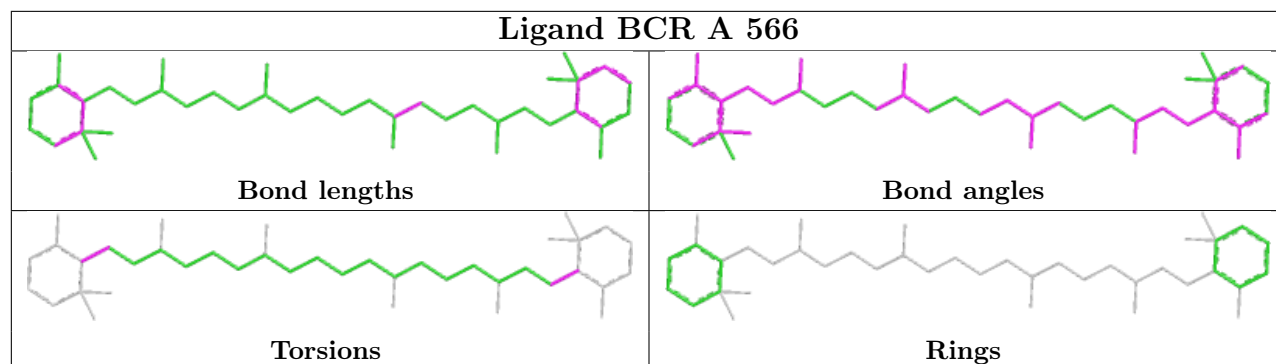


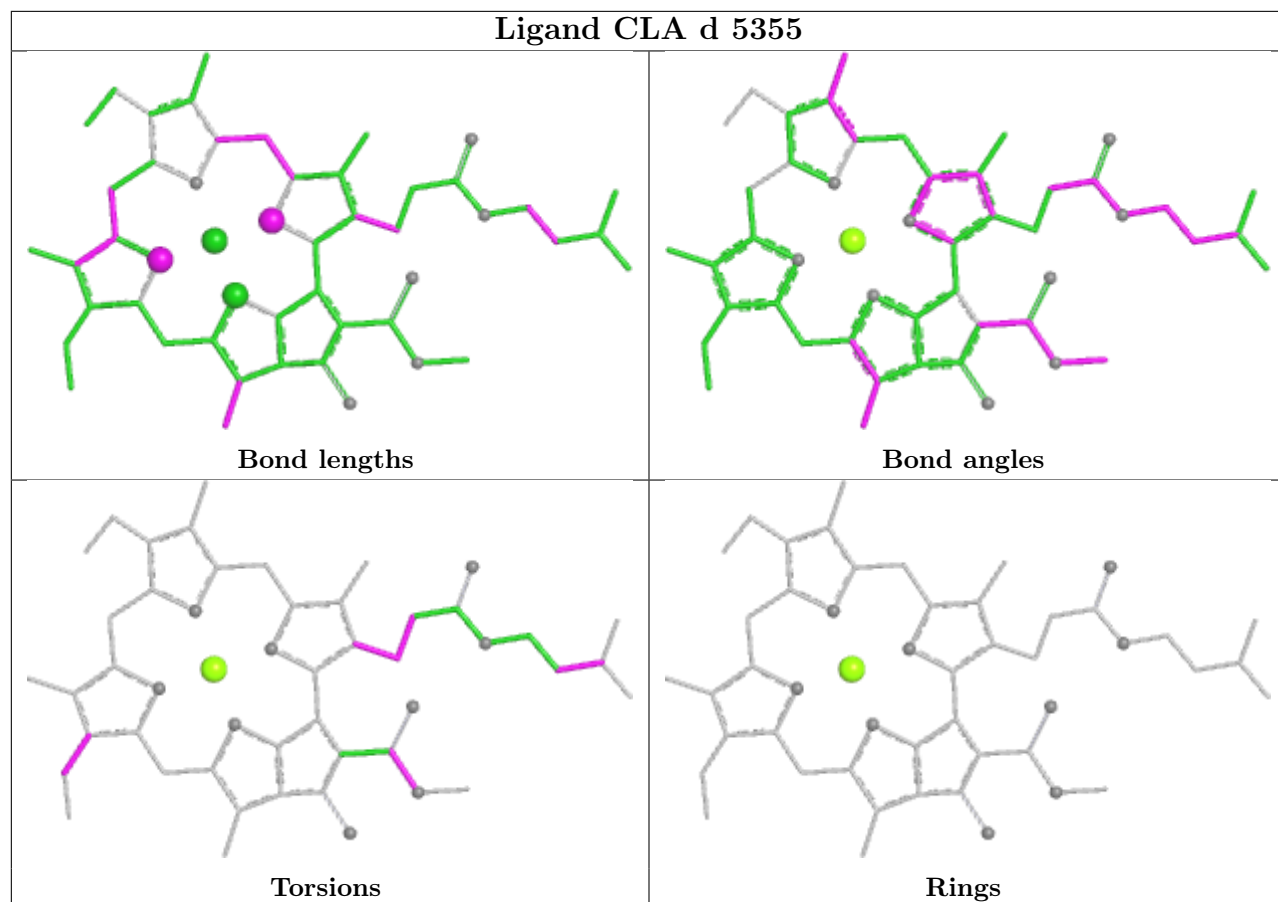




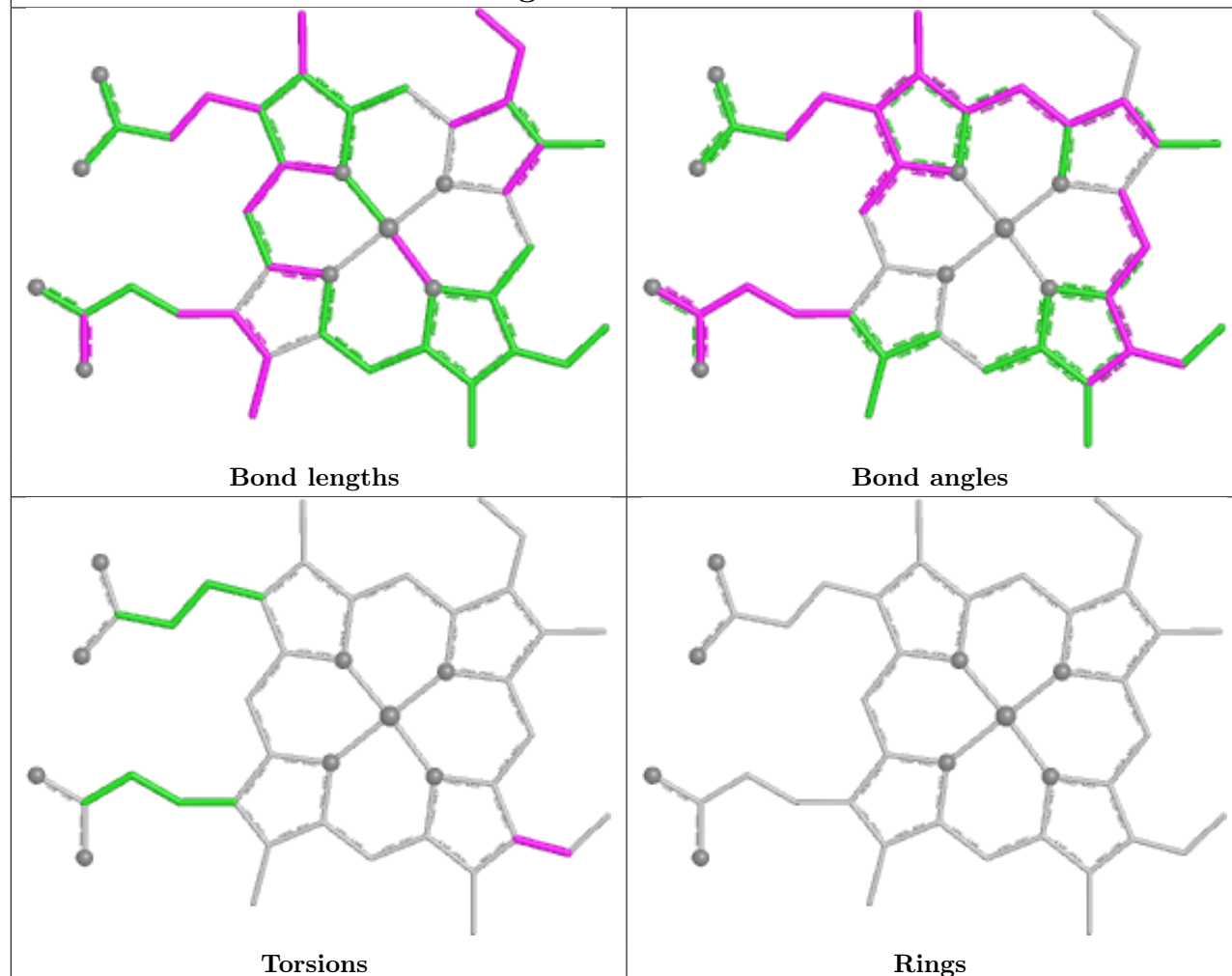




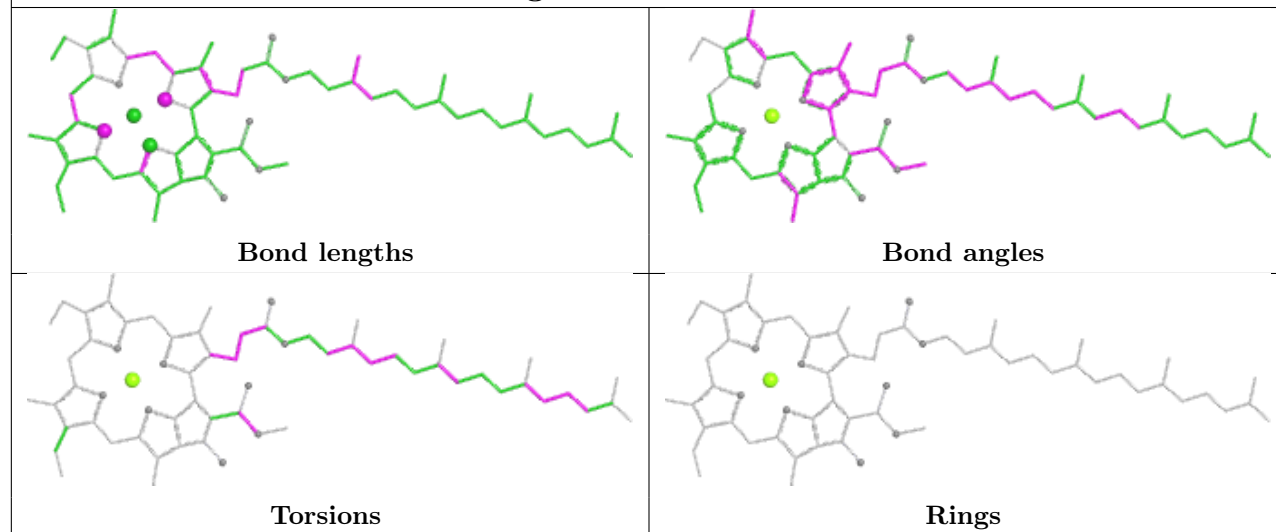


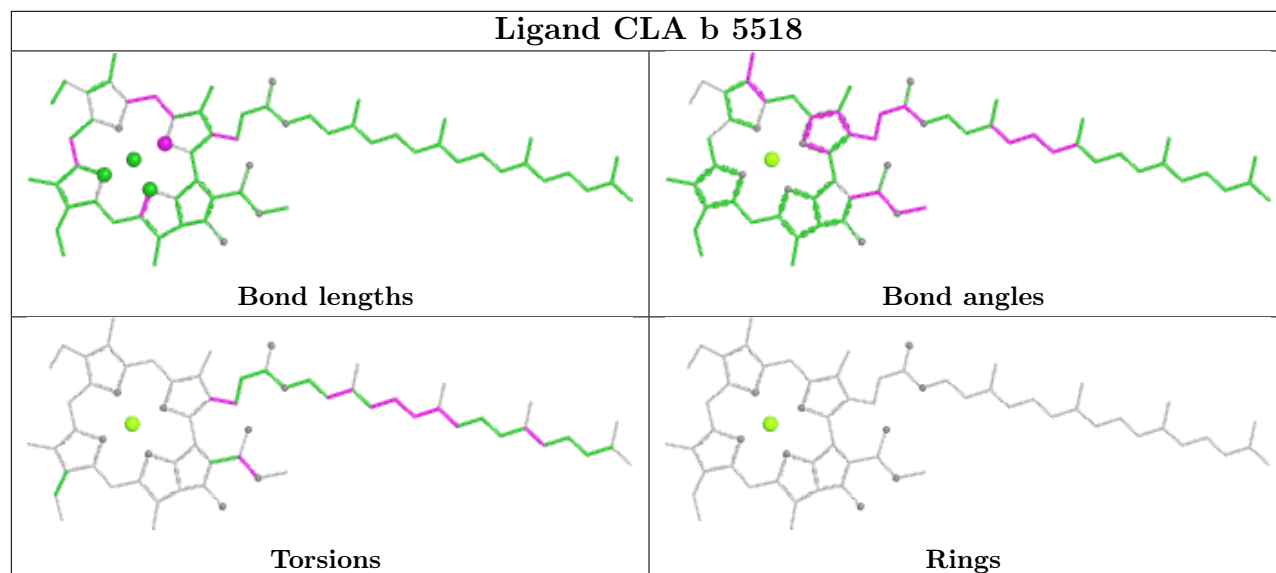
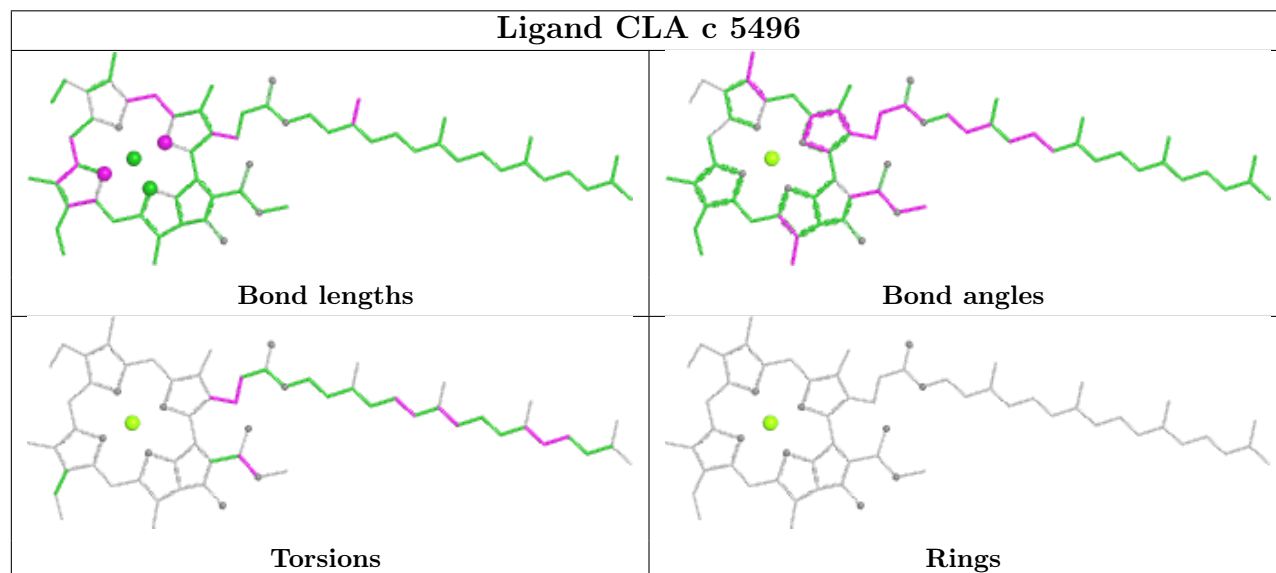
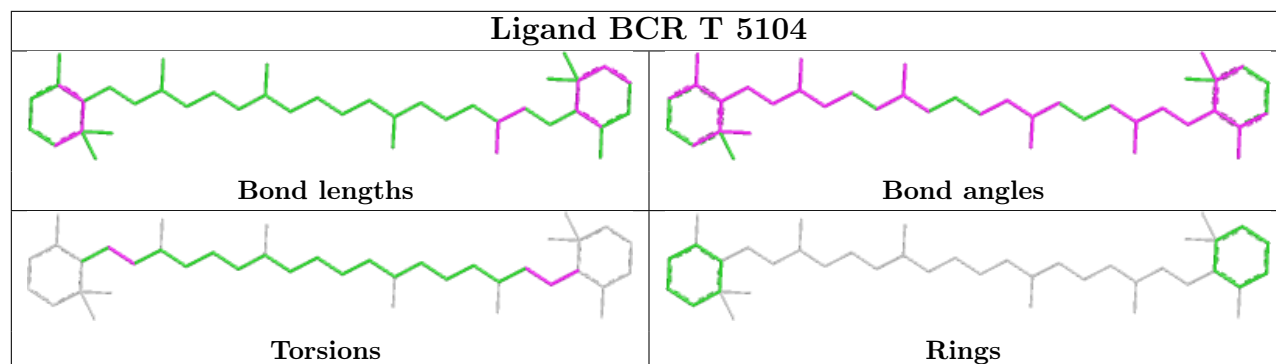


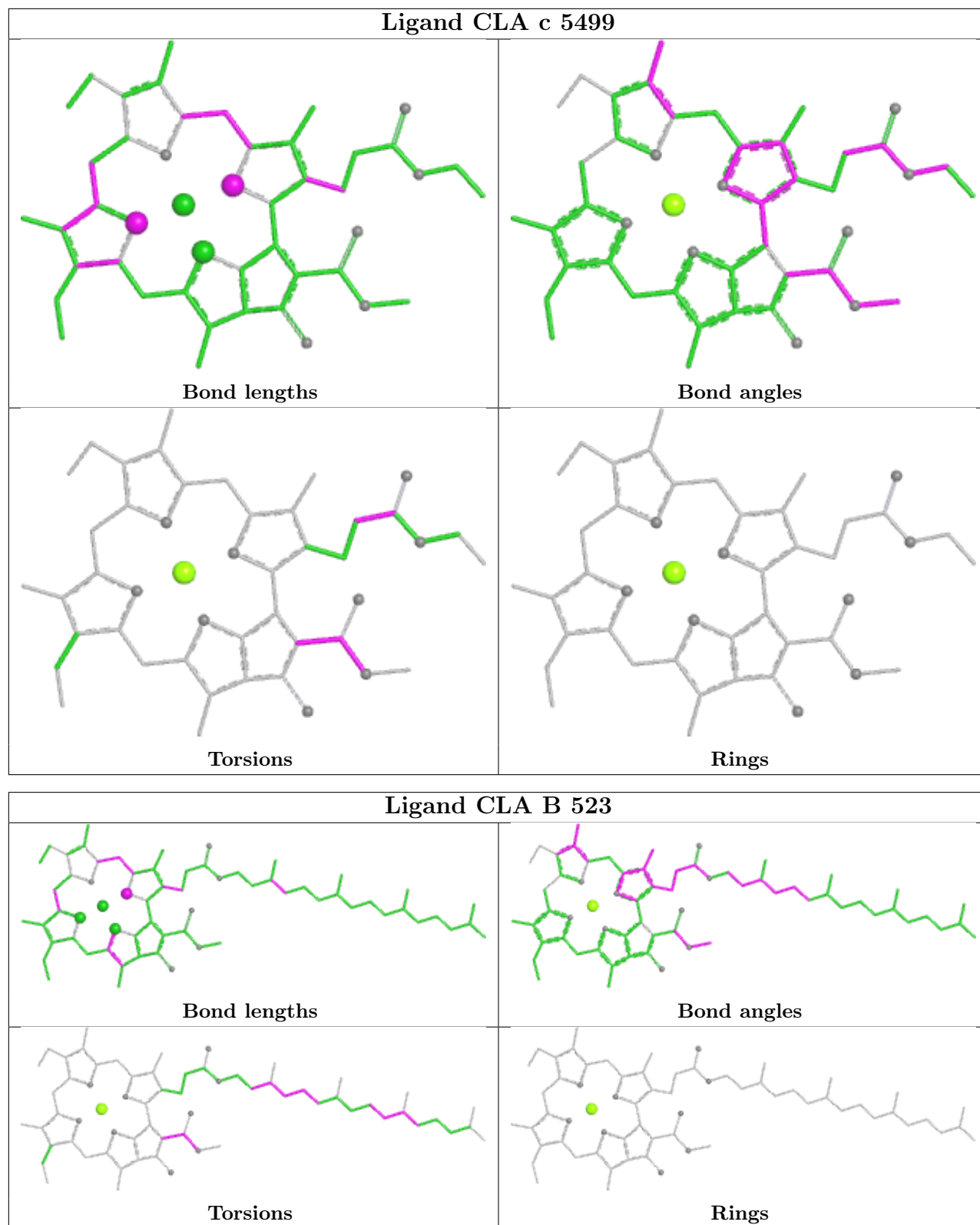
## Ligand HEM F 51

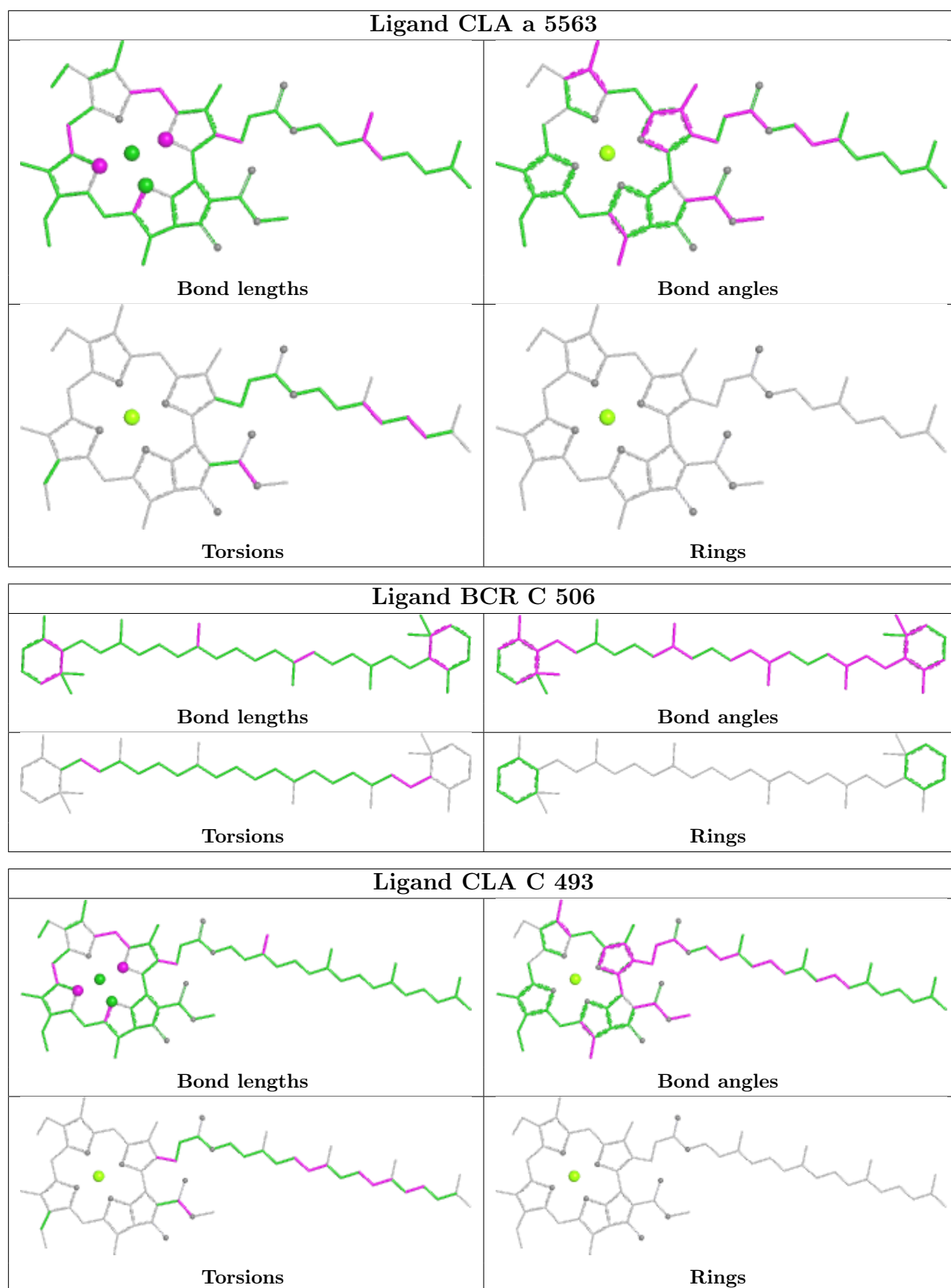


## Ligand CLA b 5515

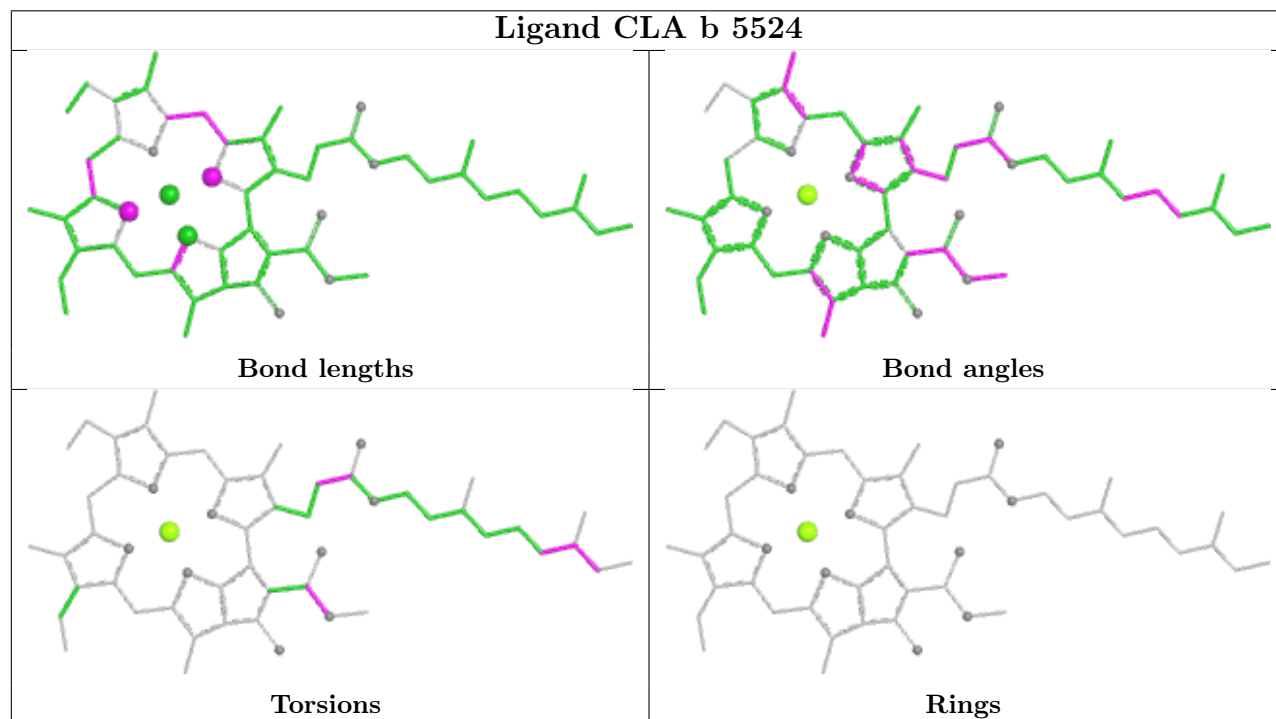
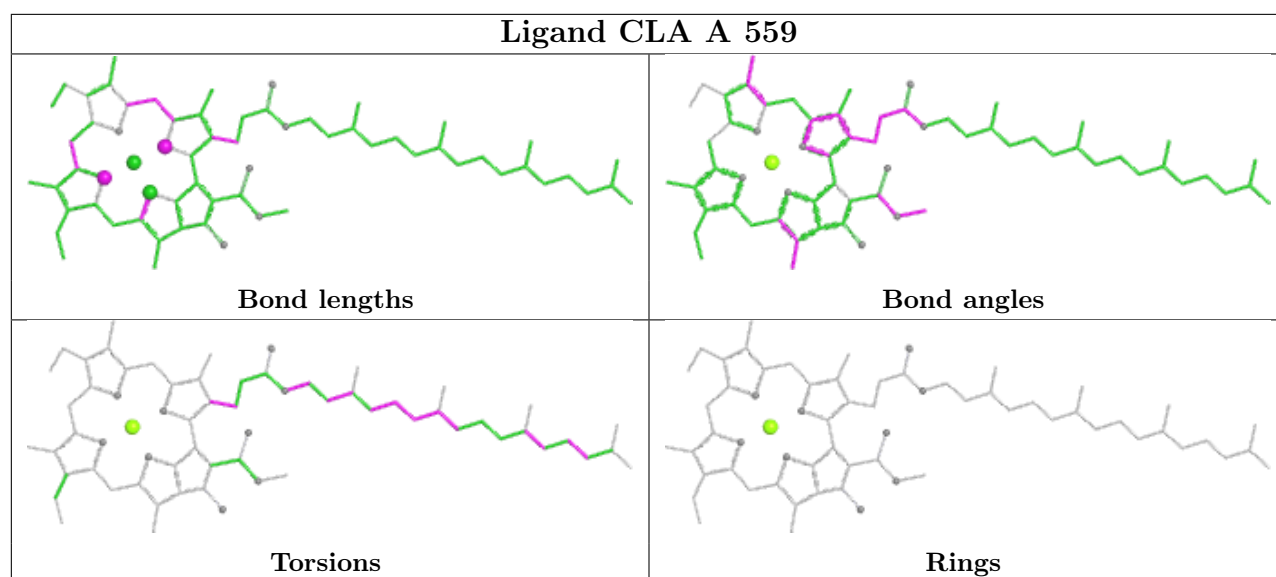


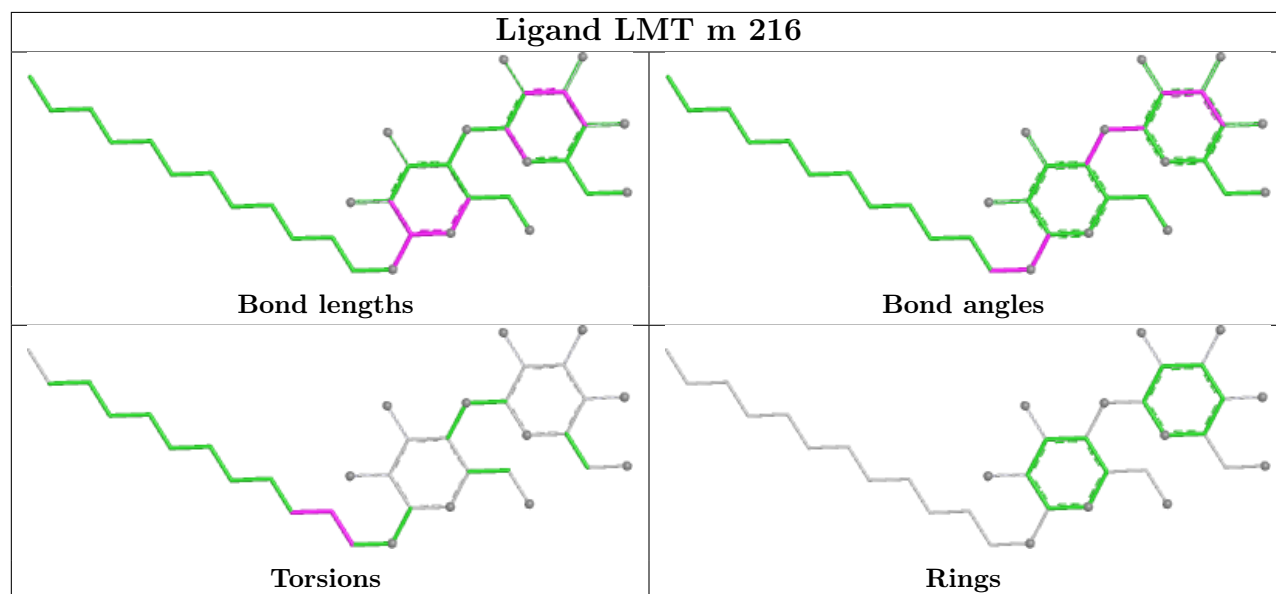
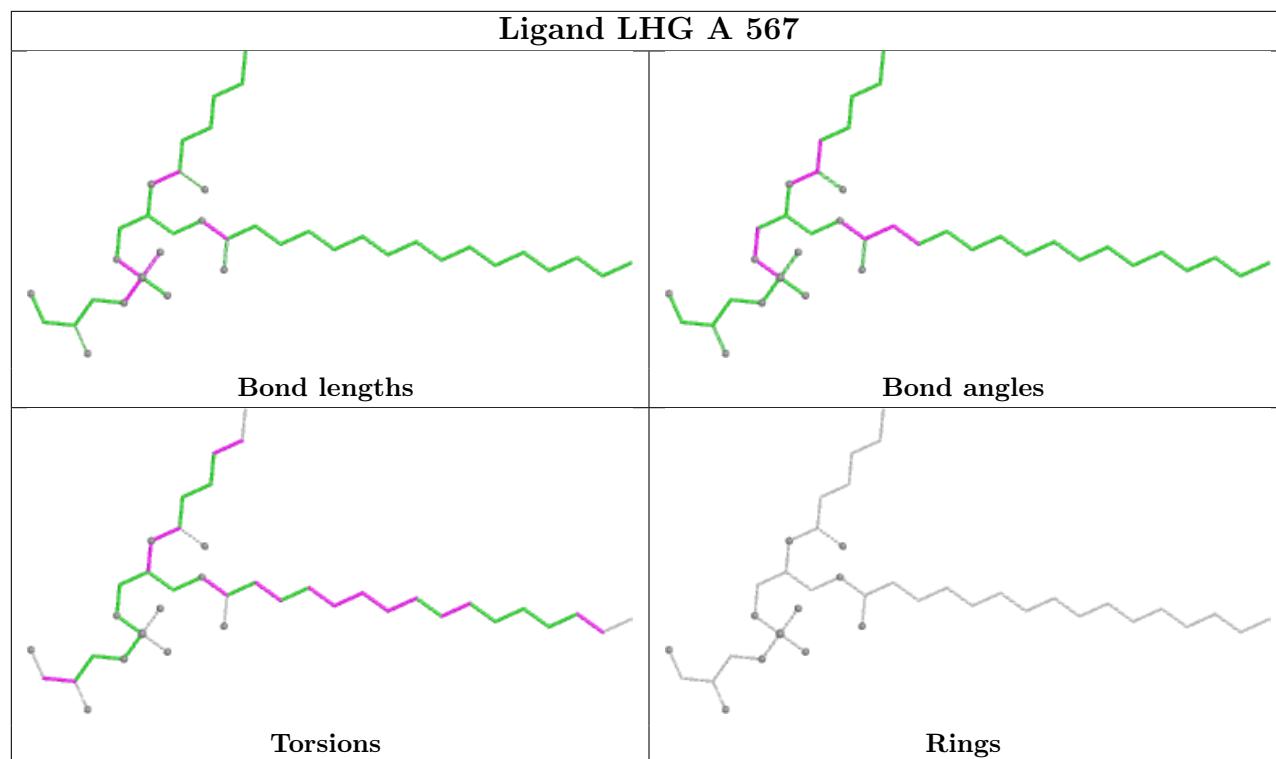




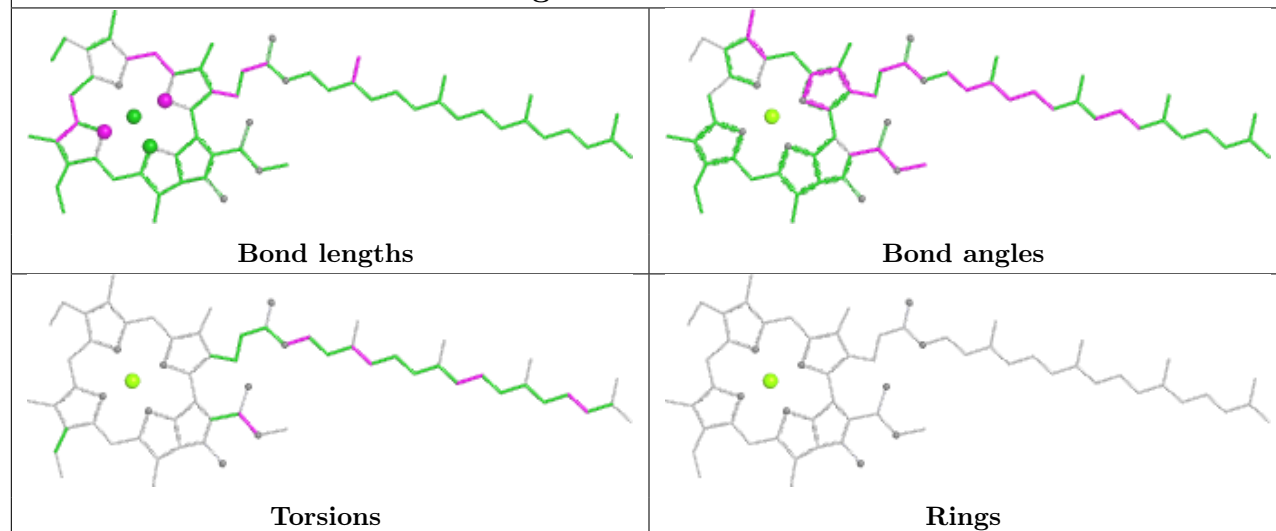




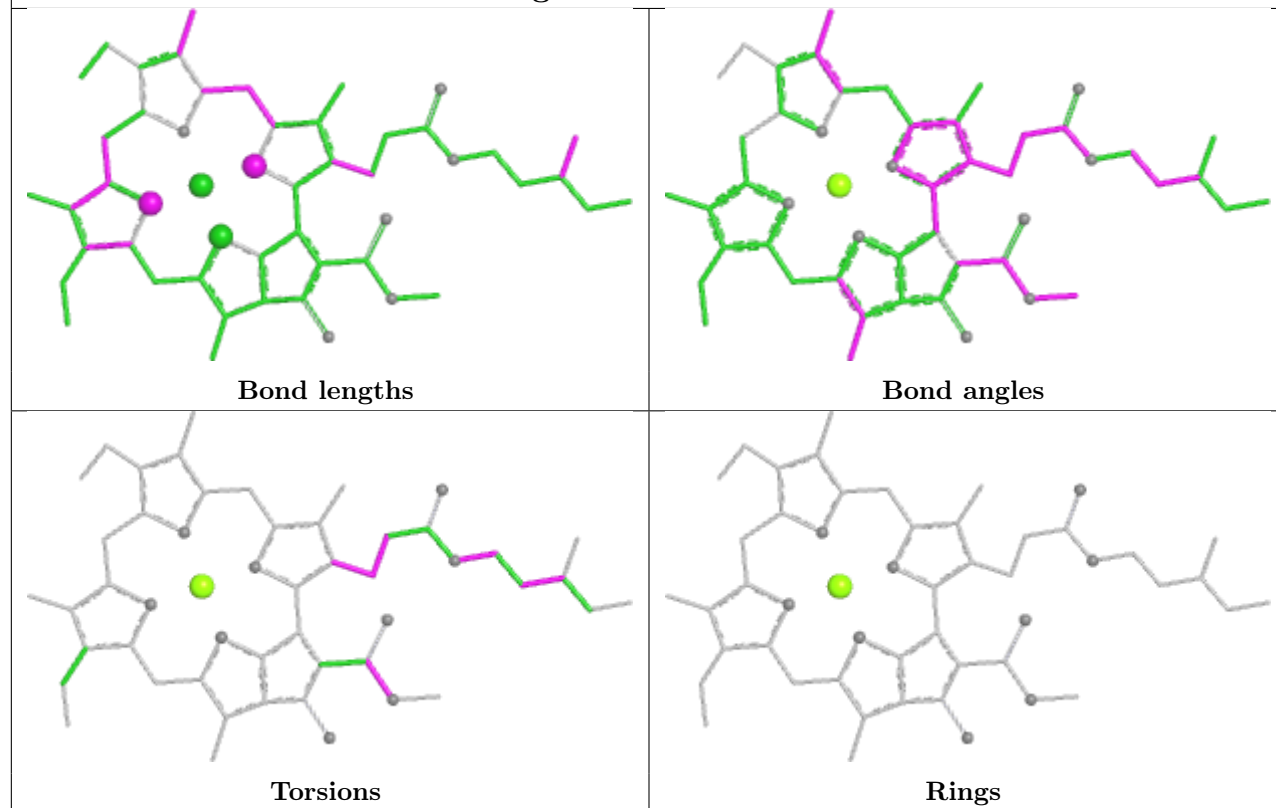


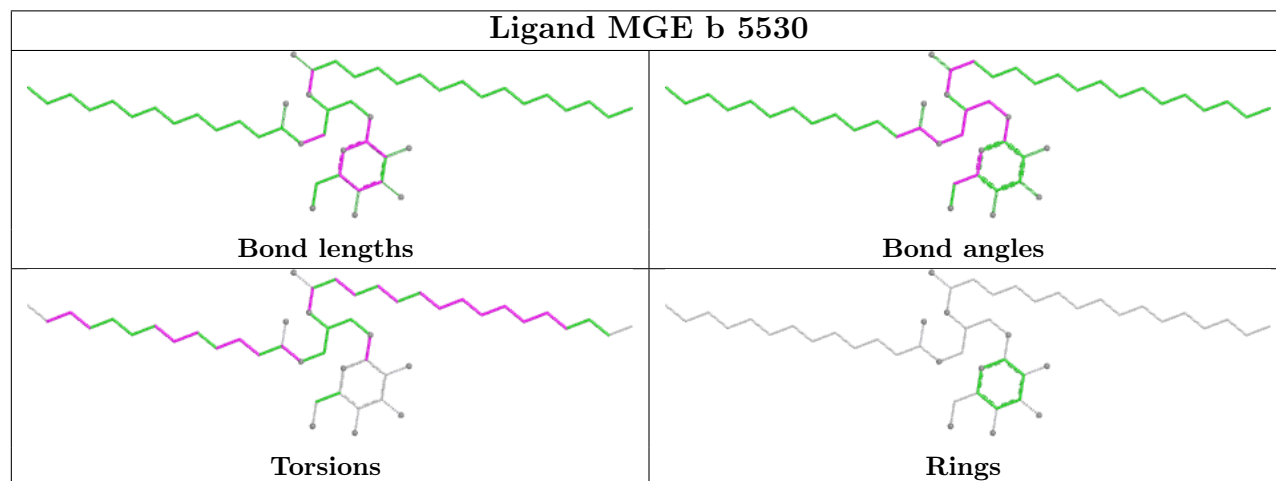
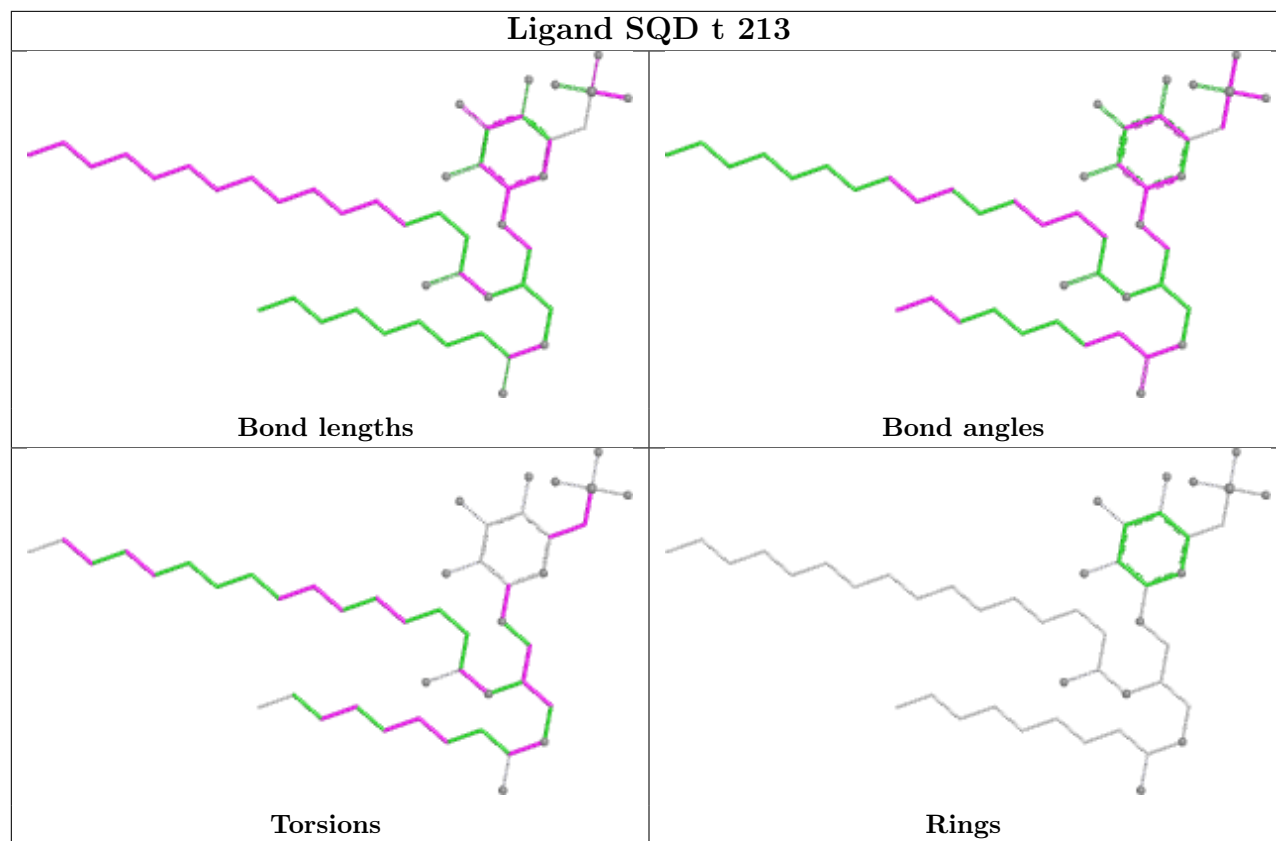


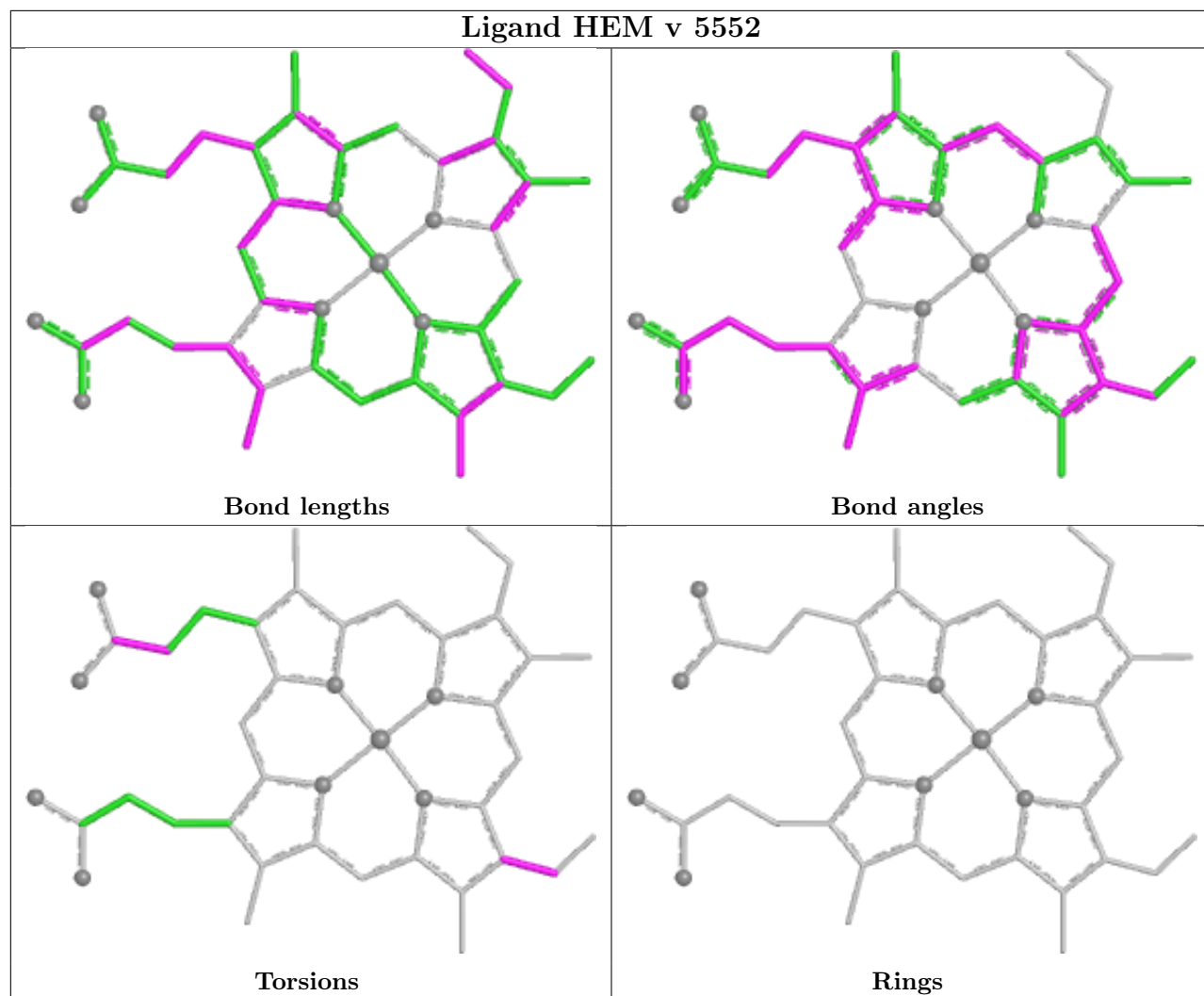
## Ligand CLA B 521



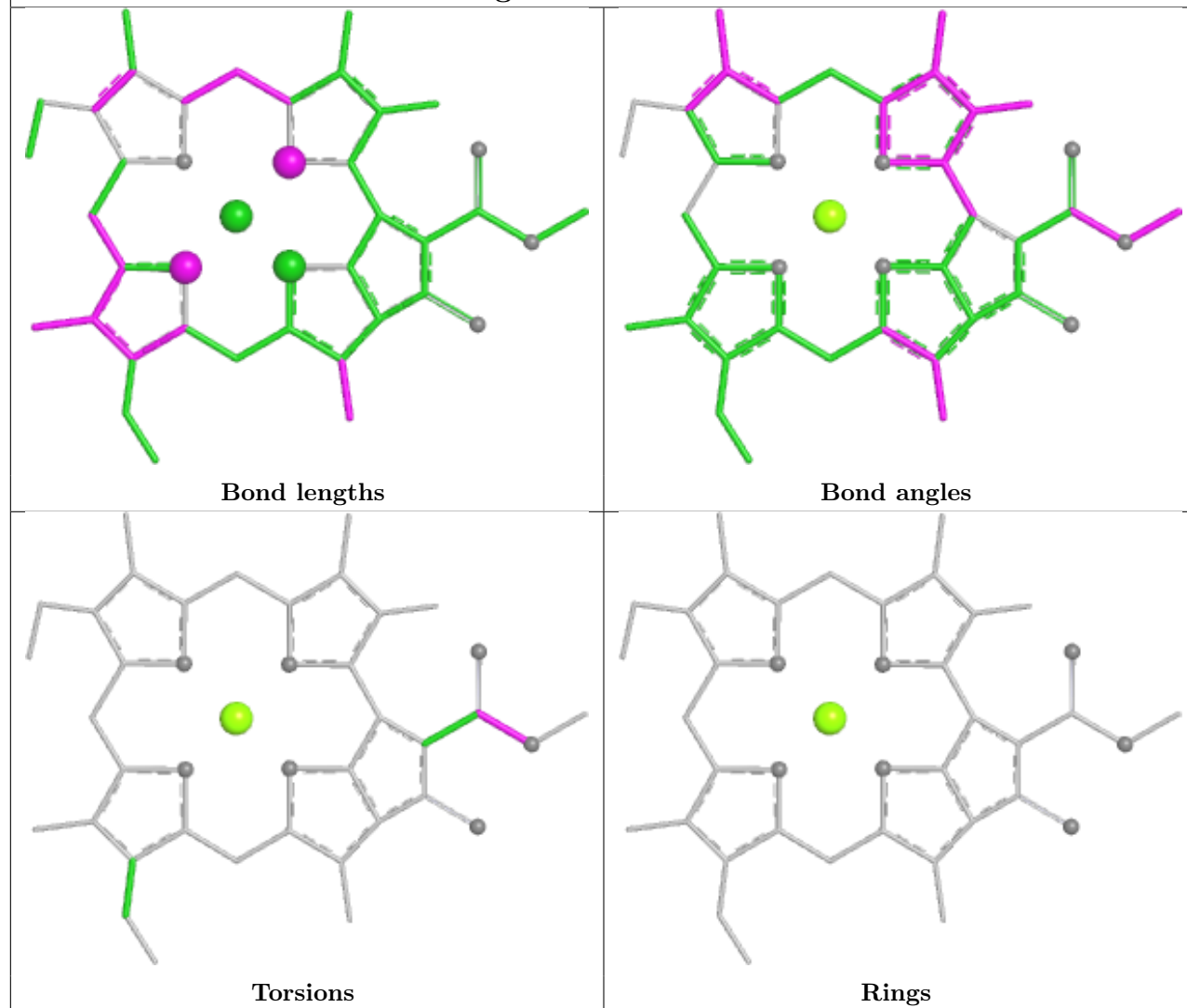
## Ligand CLA C 502



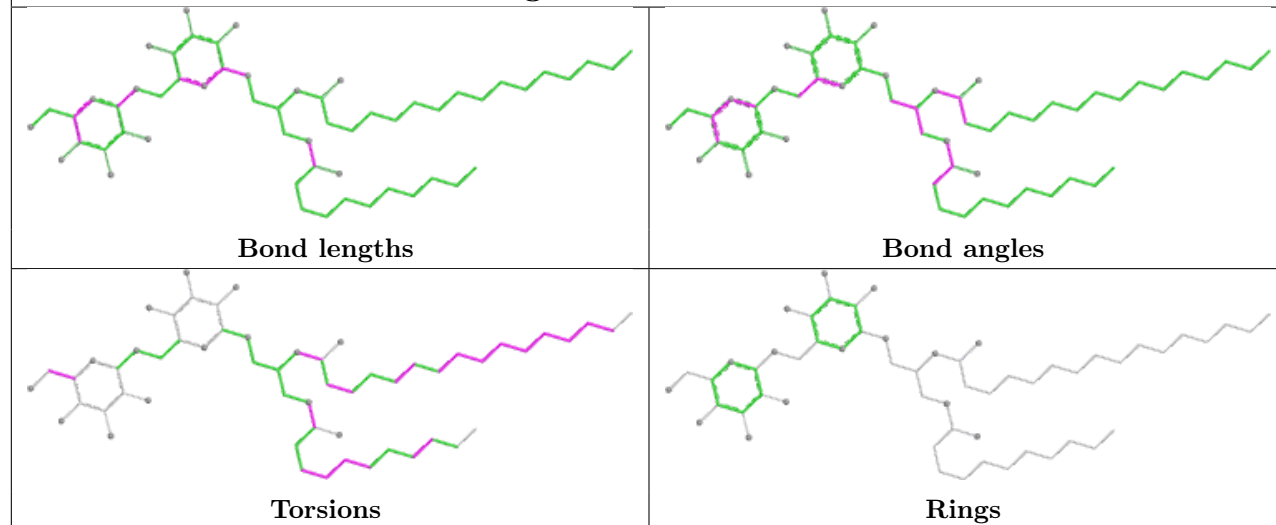


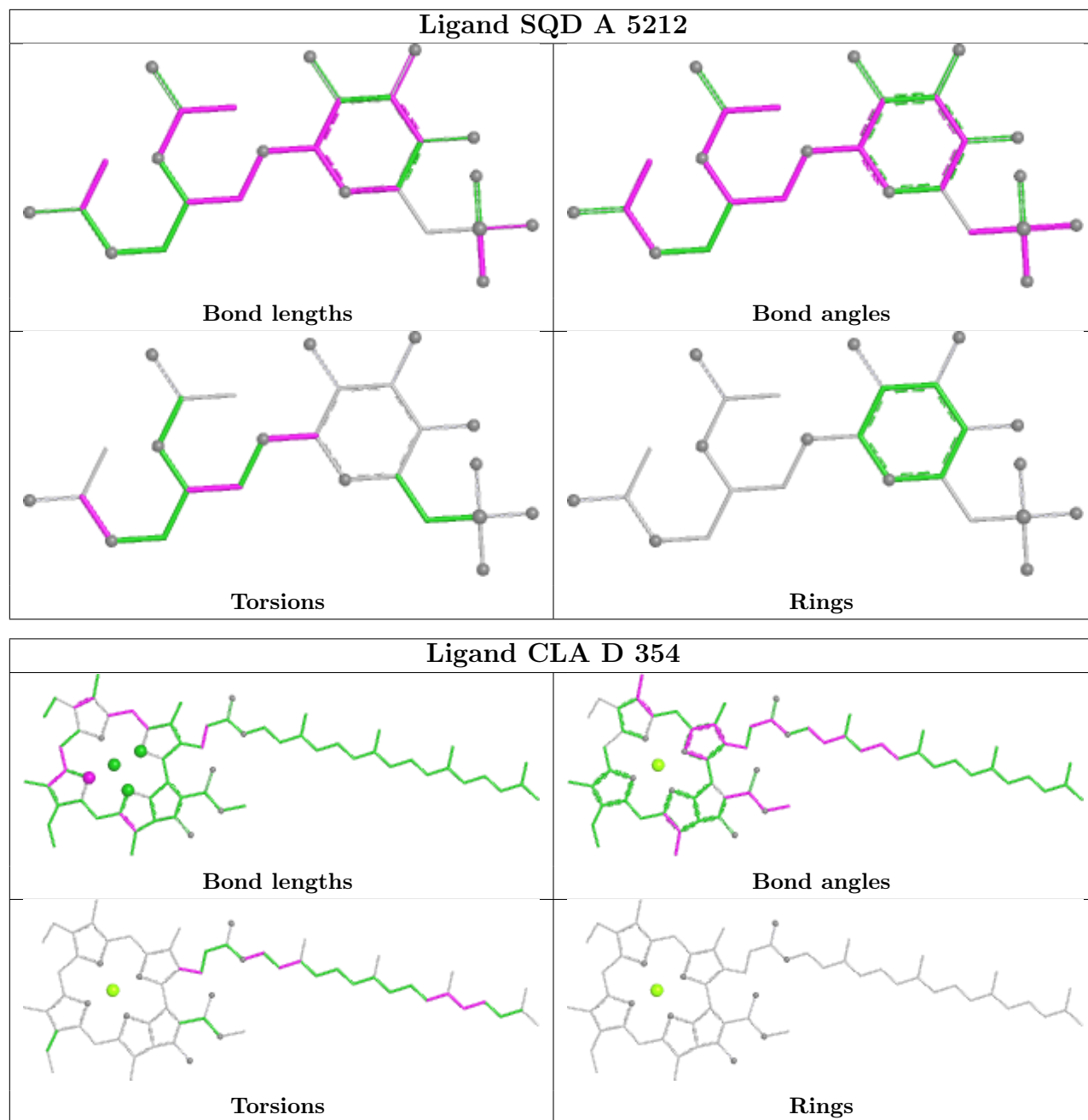


## Ligand CLA B 511

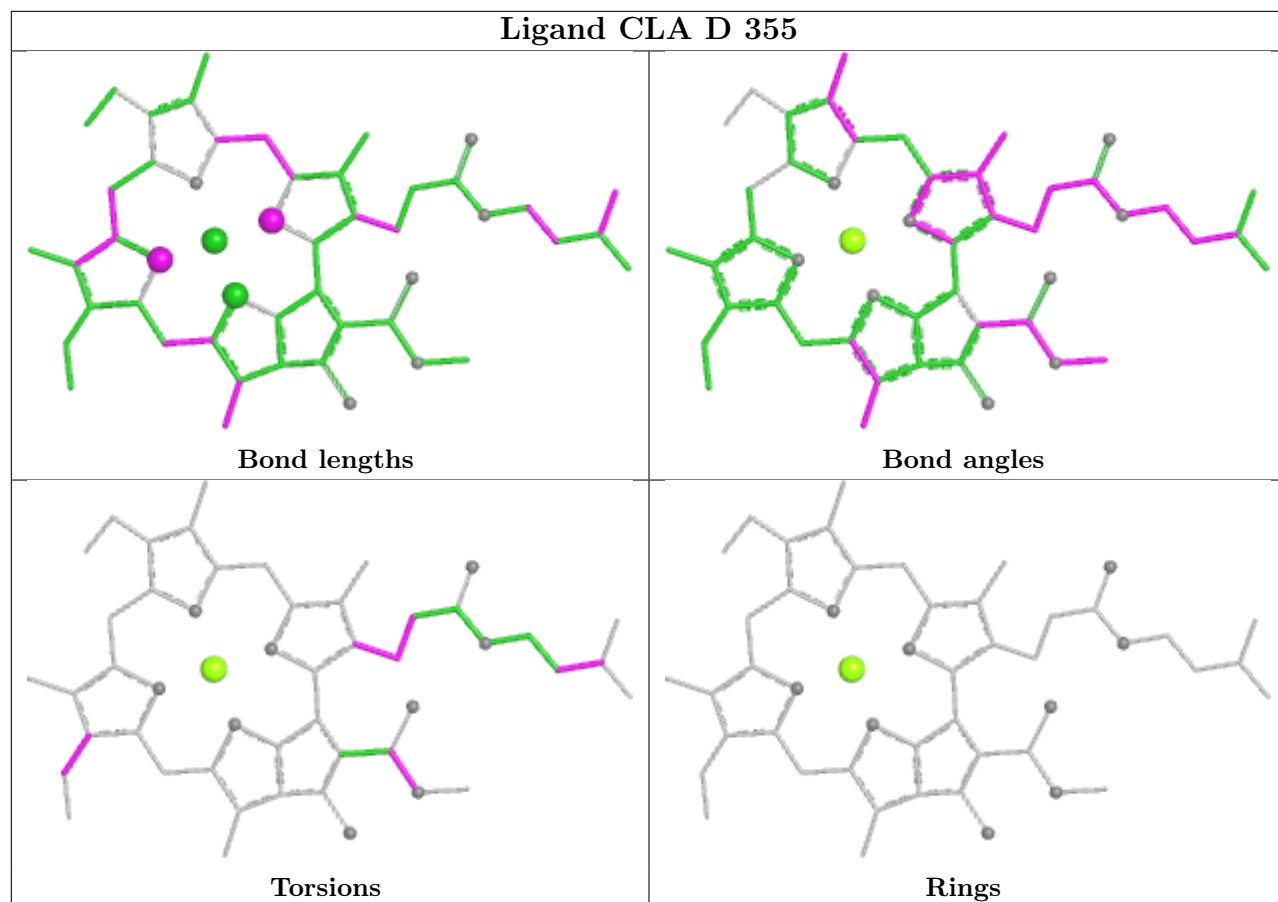


## Ligand DGD c 5509

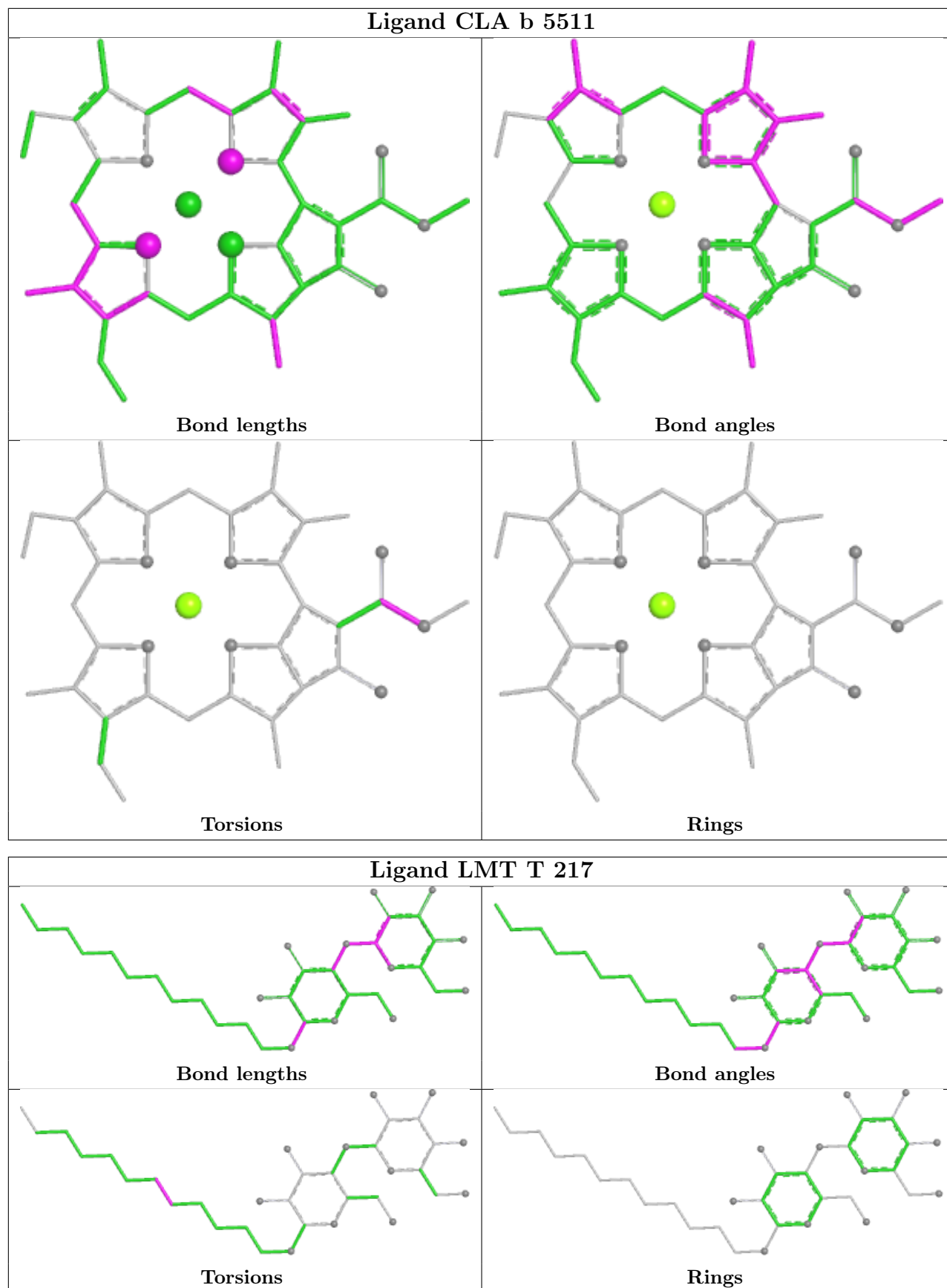




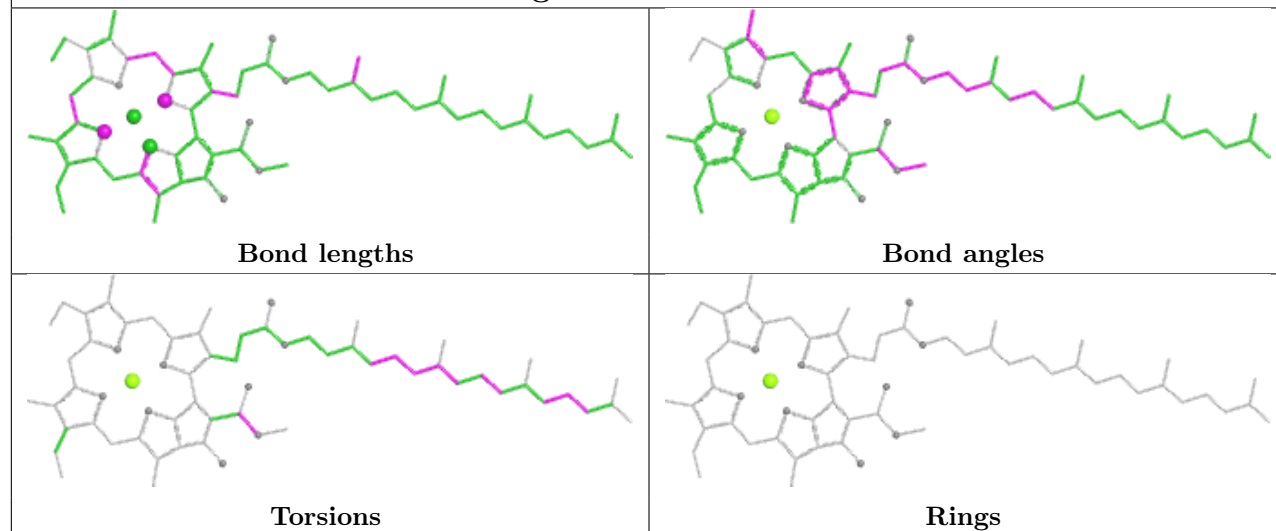
## Ligand CLA D 355



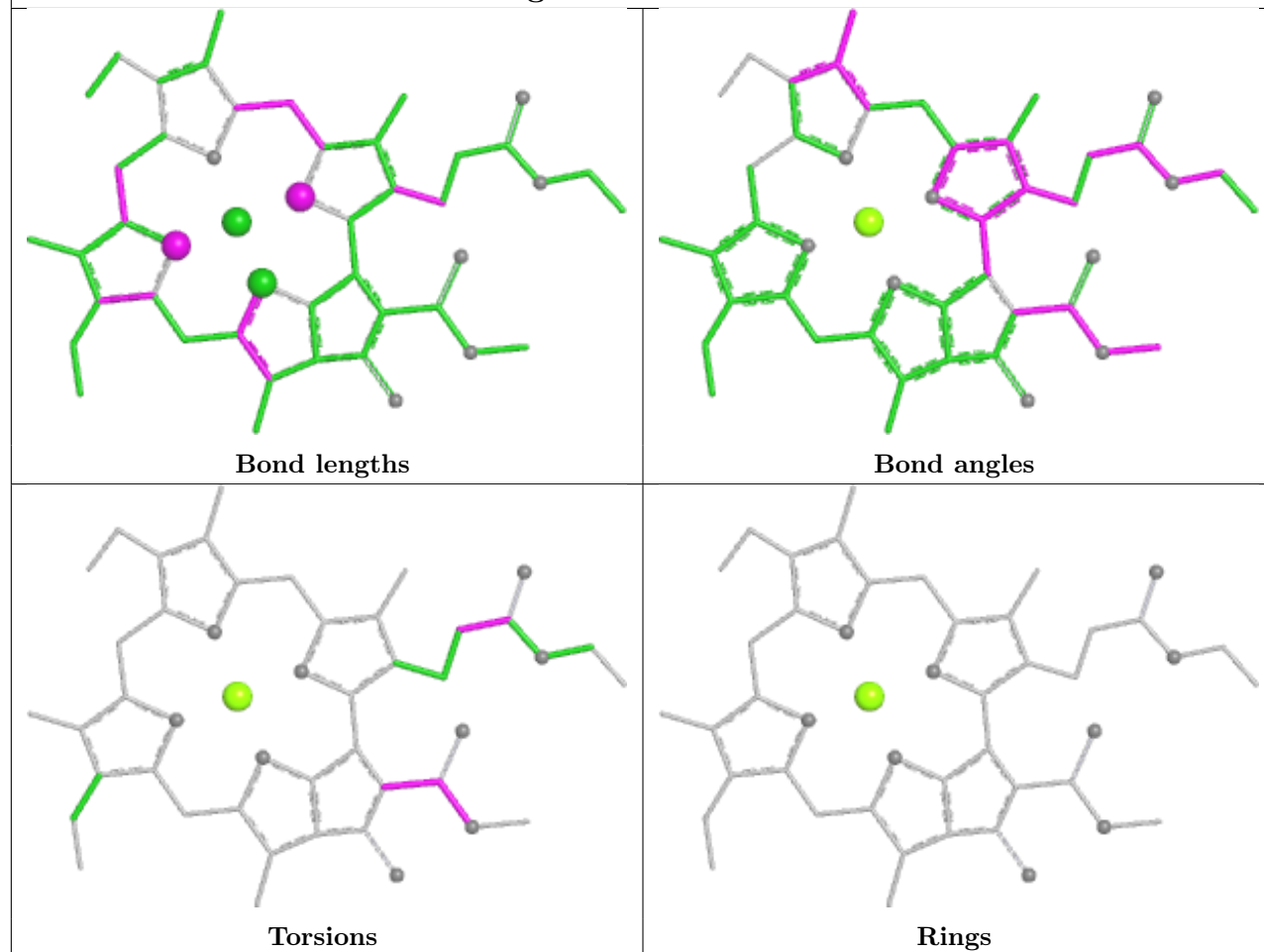


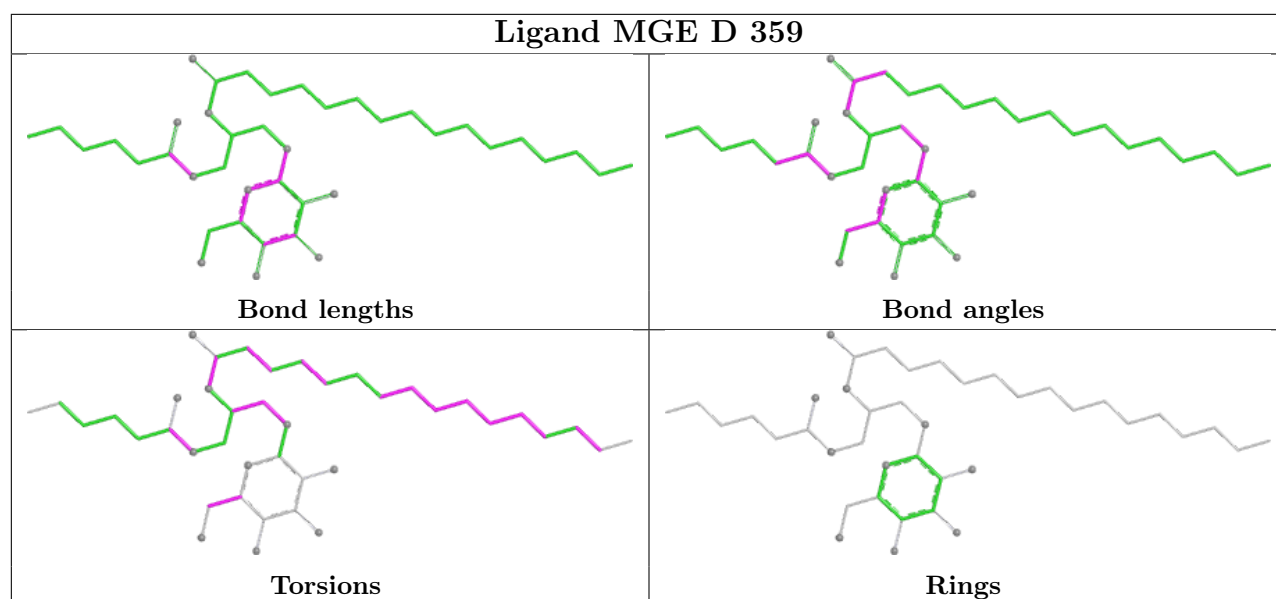
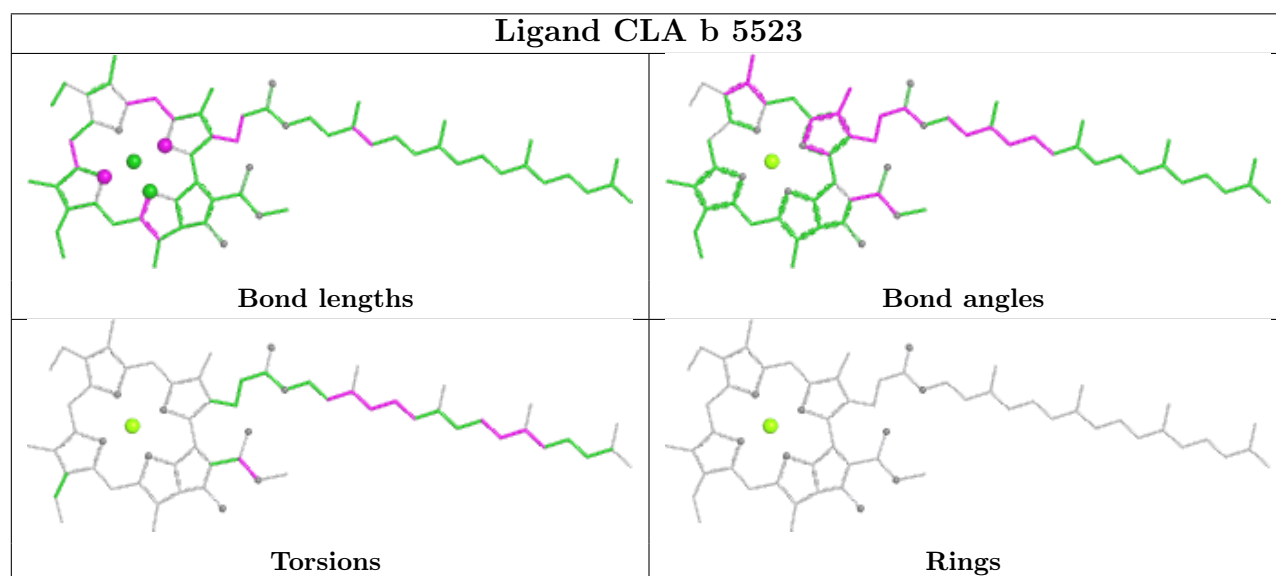
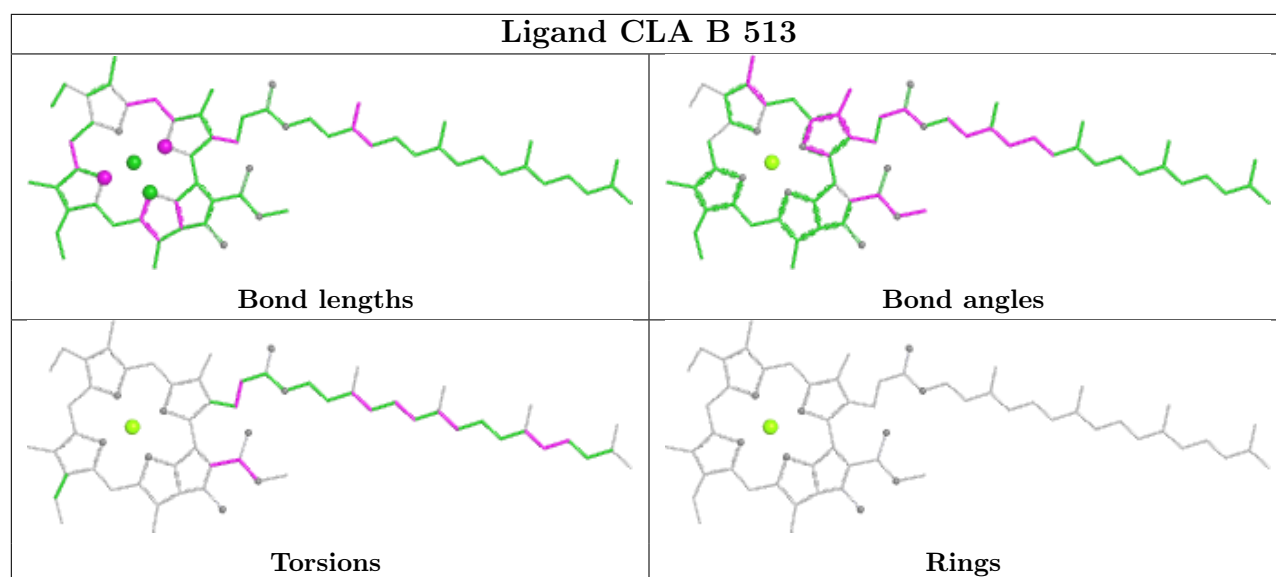


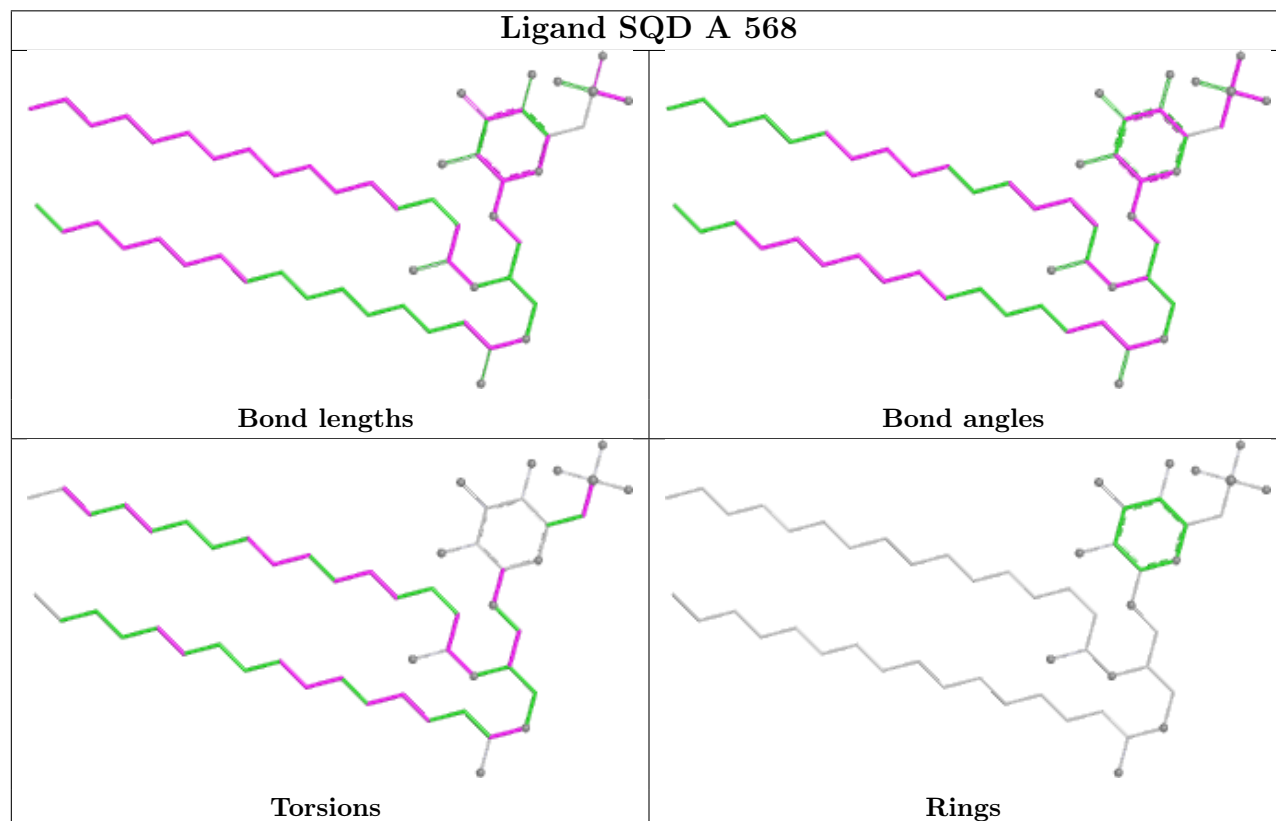
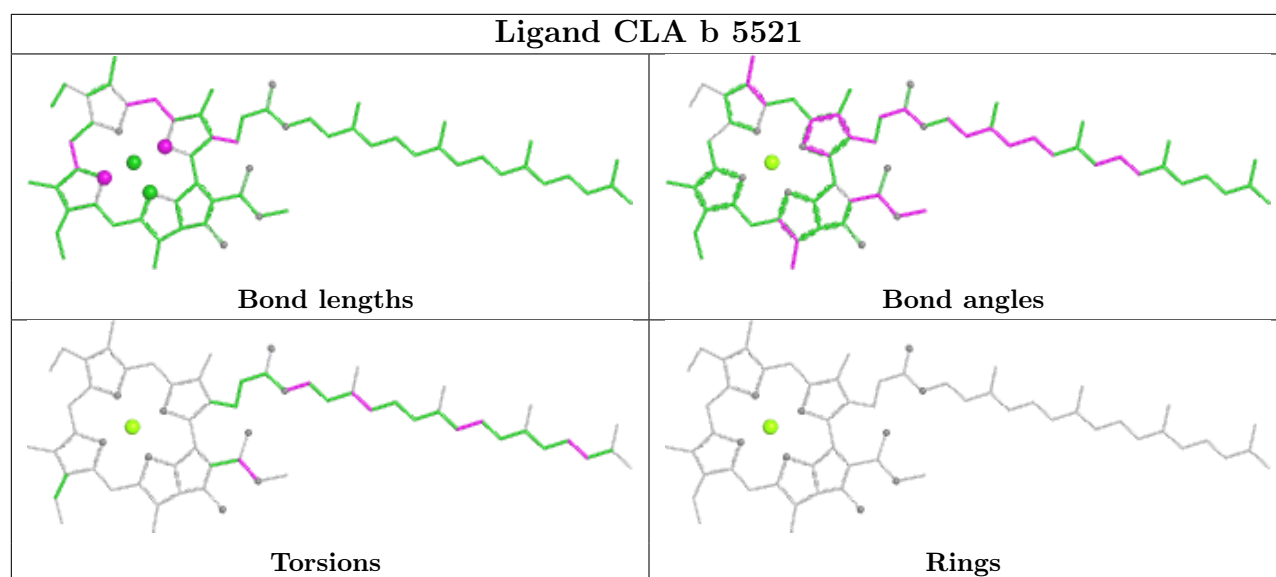
## Ligand CLA B 514

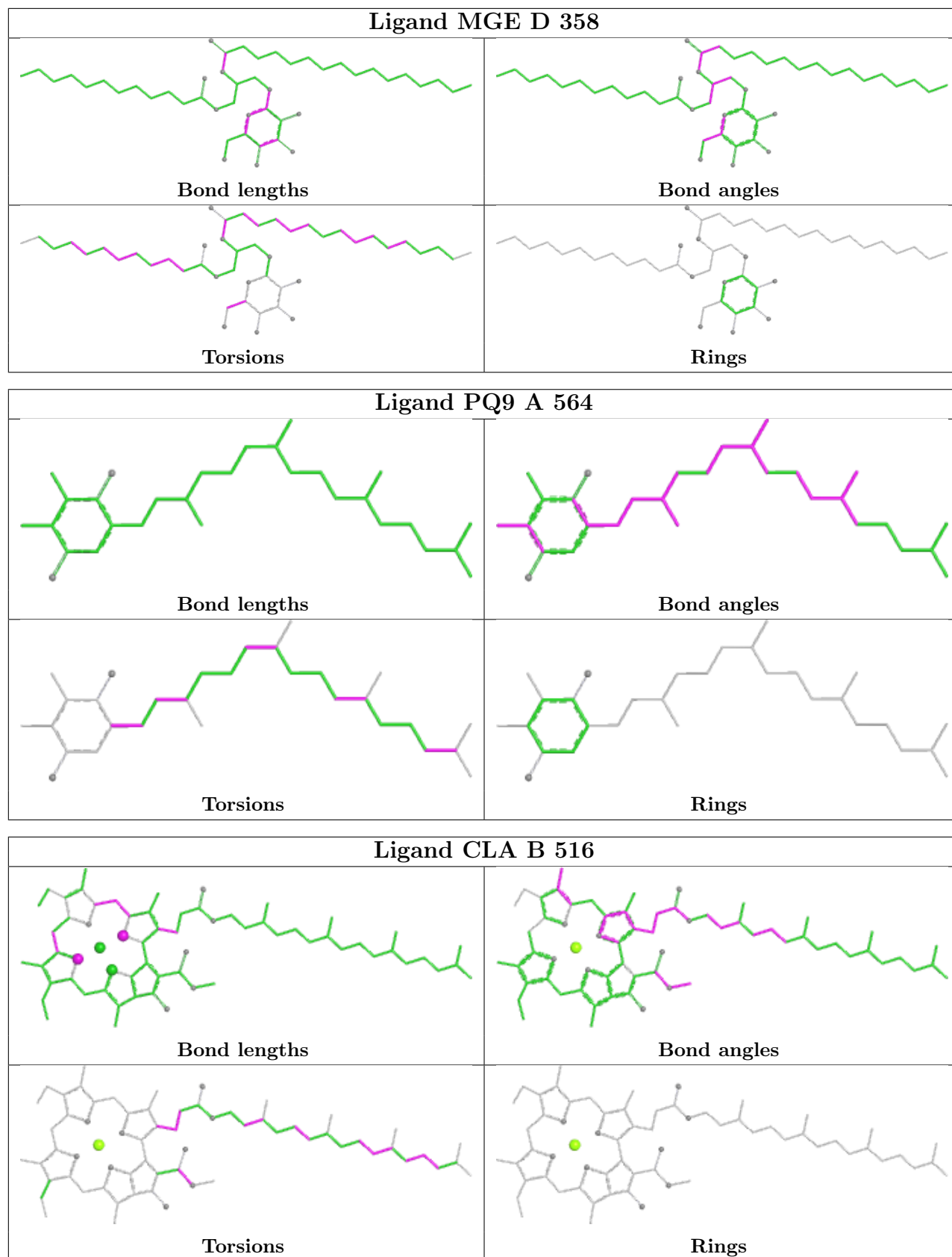


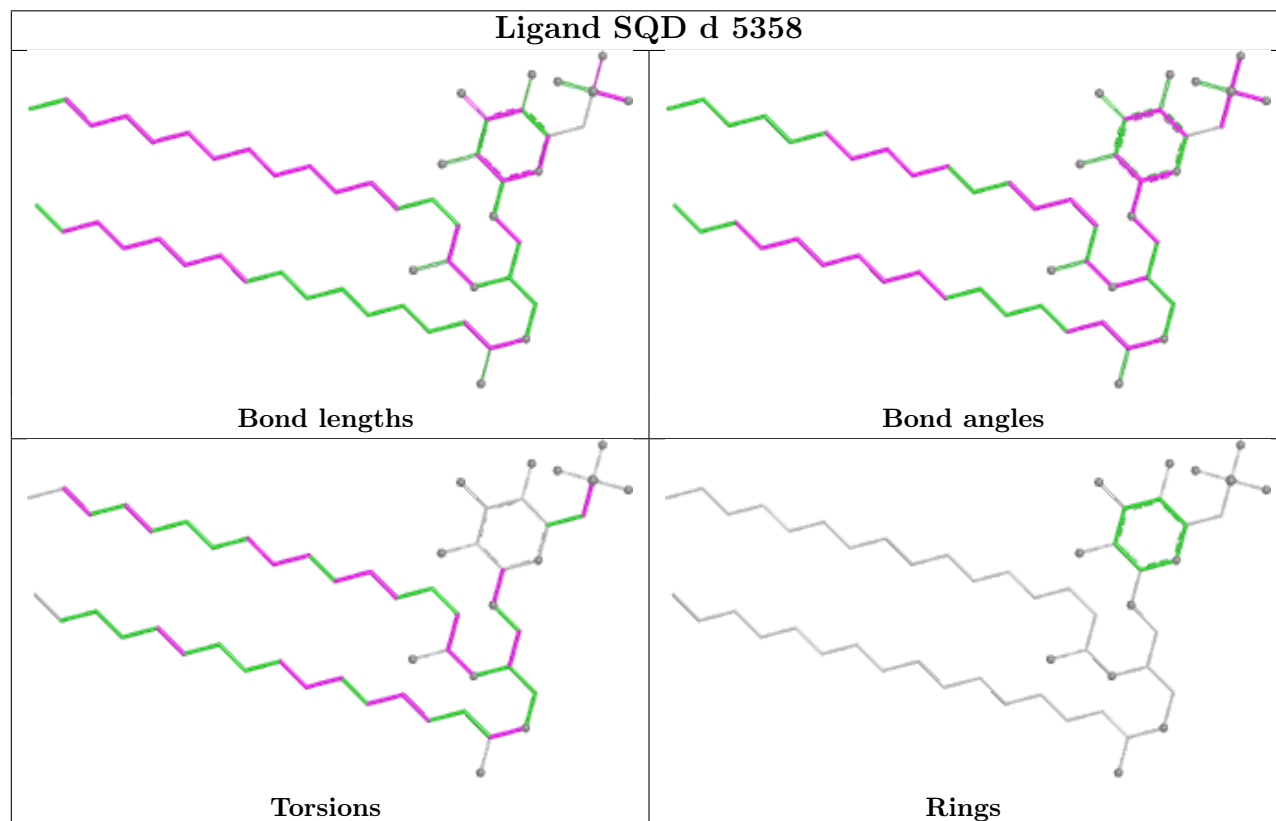
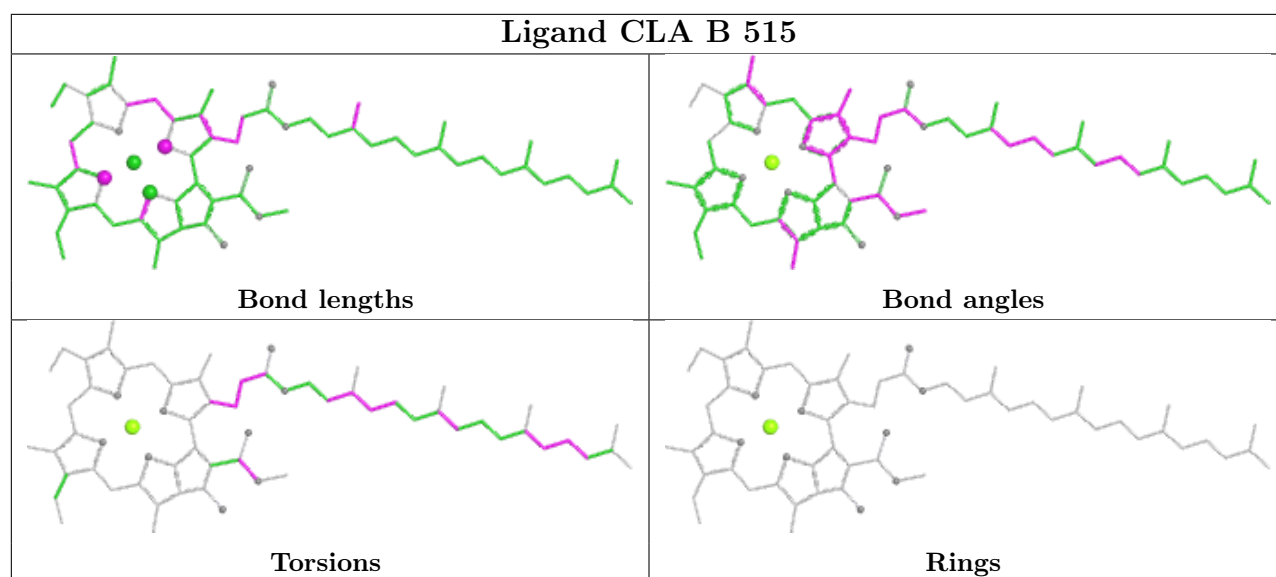
## Ligand CLA C 499

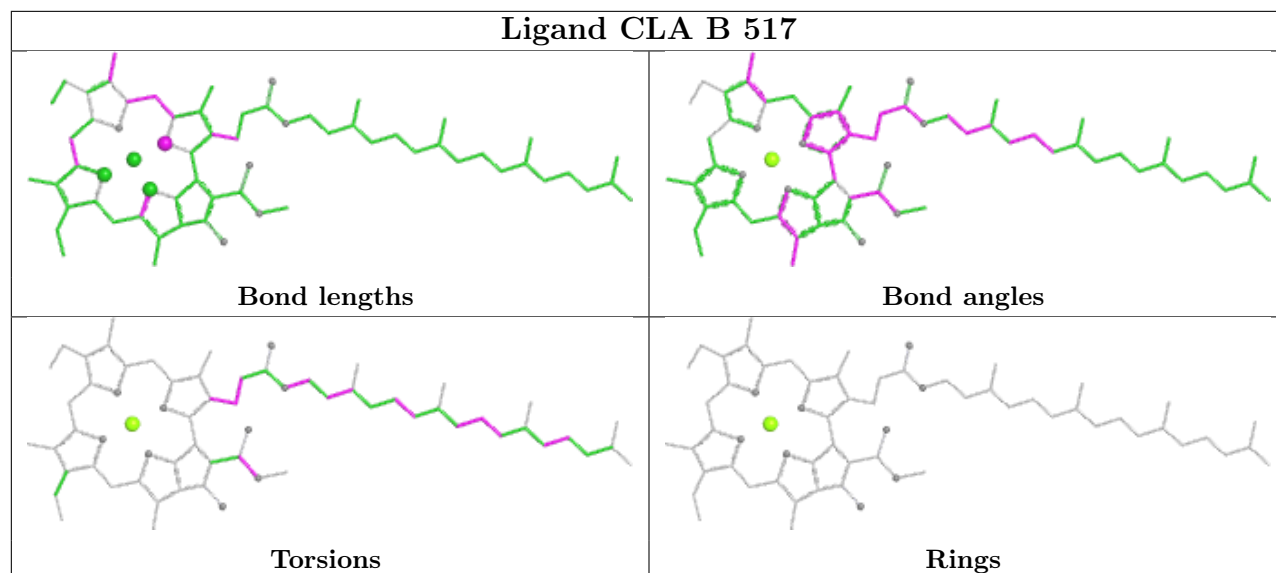
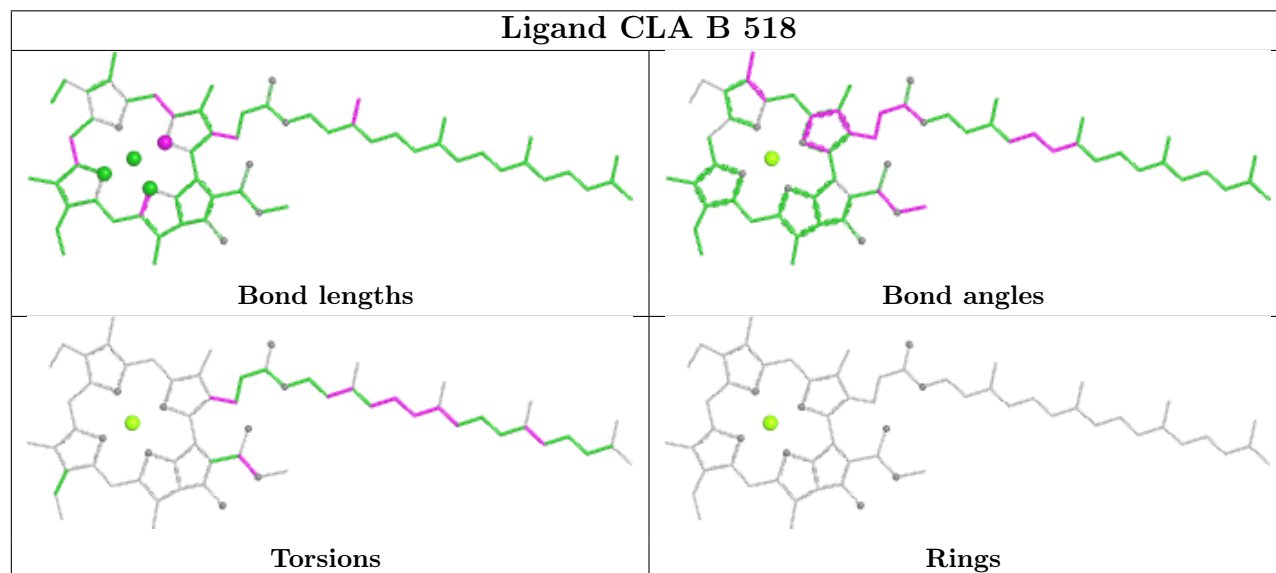
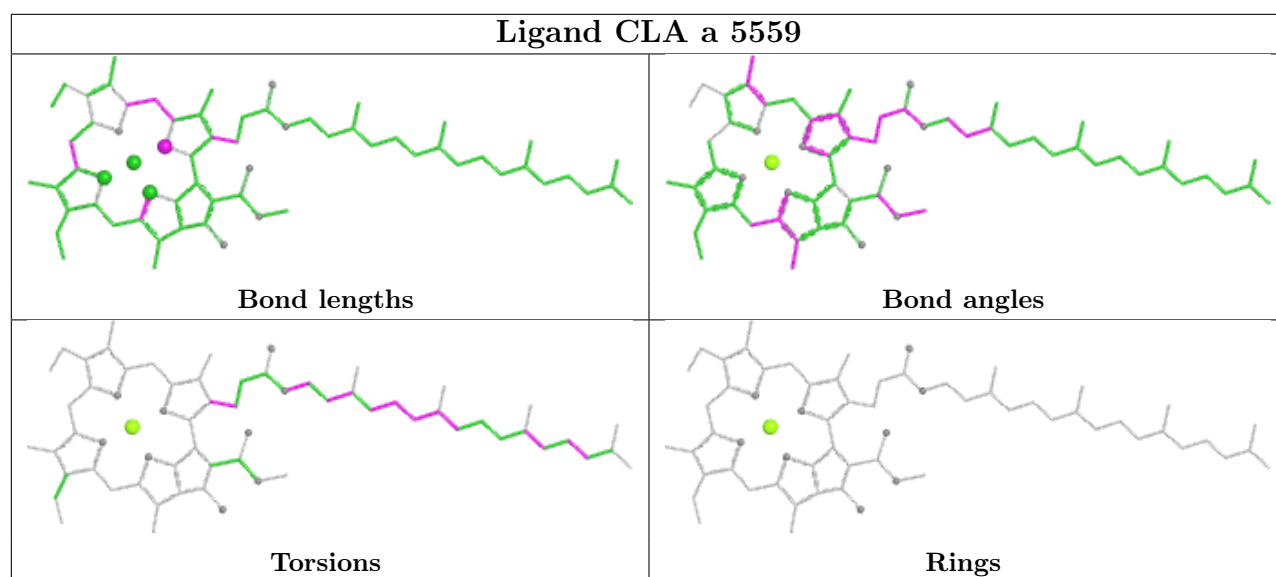


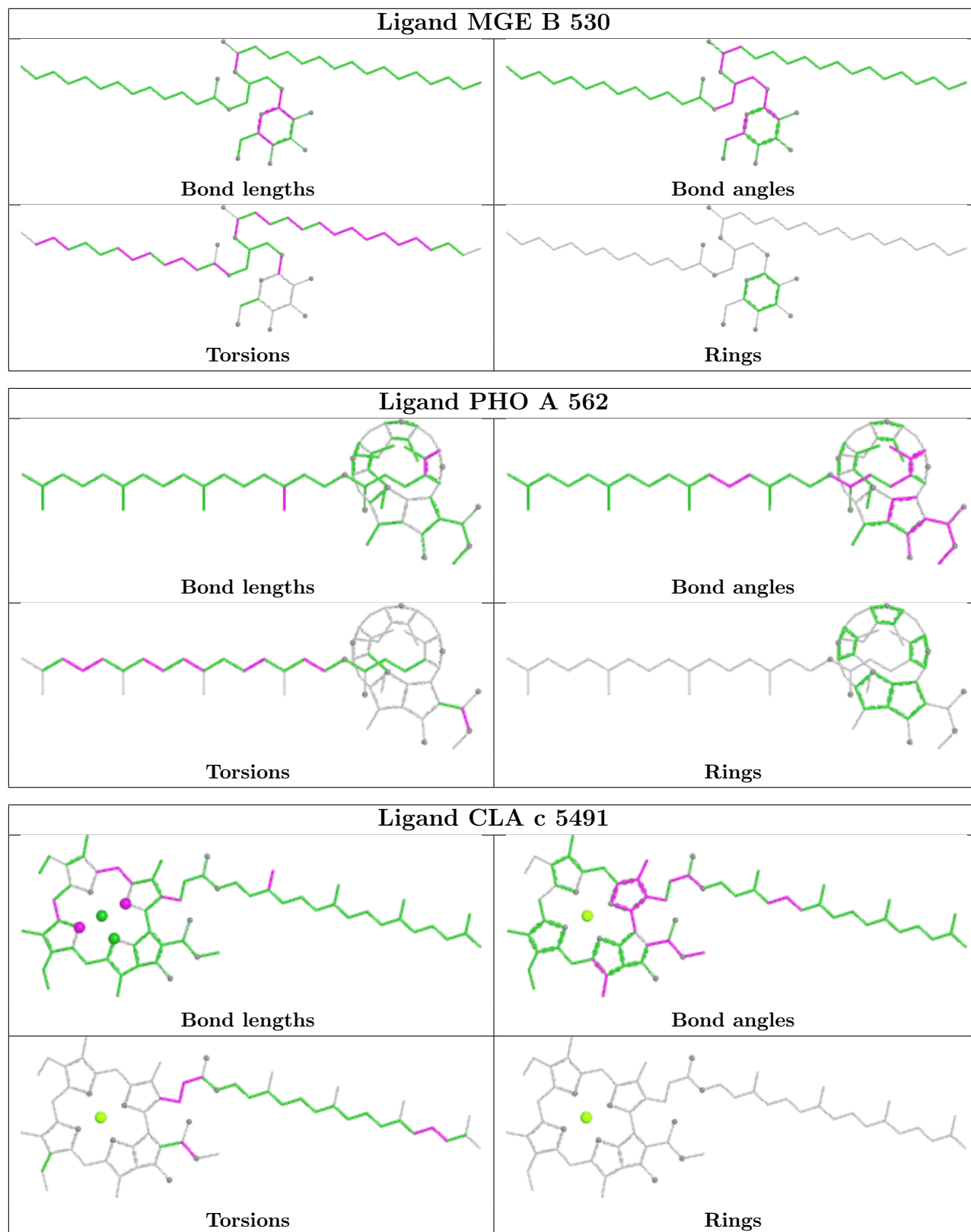




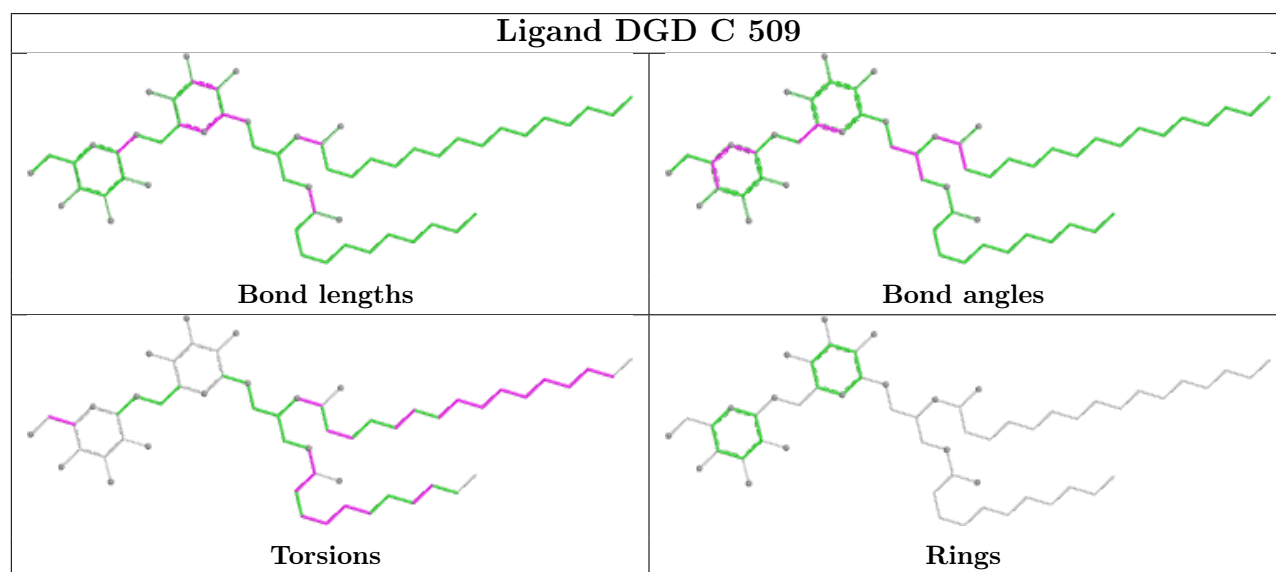
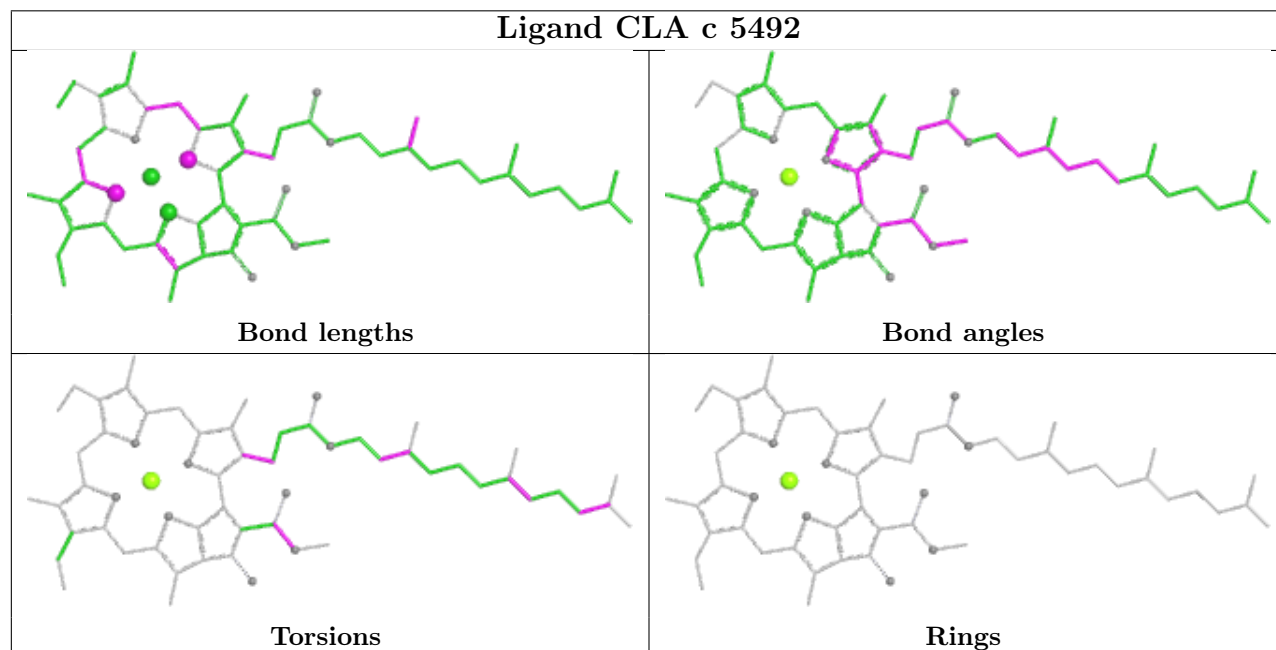
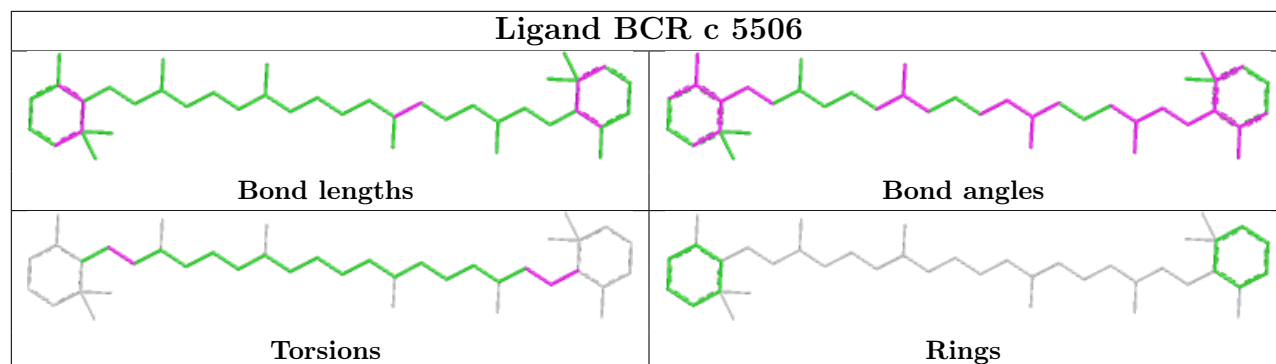


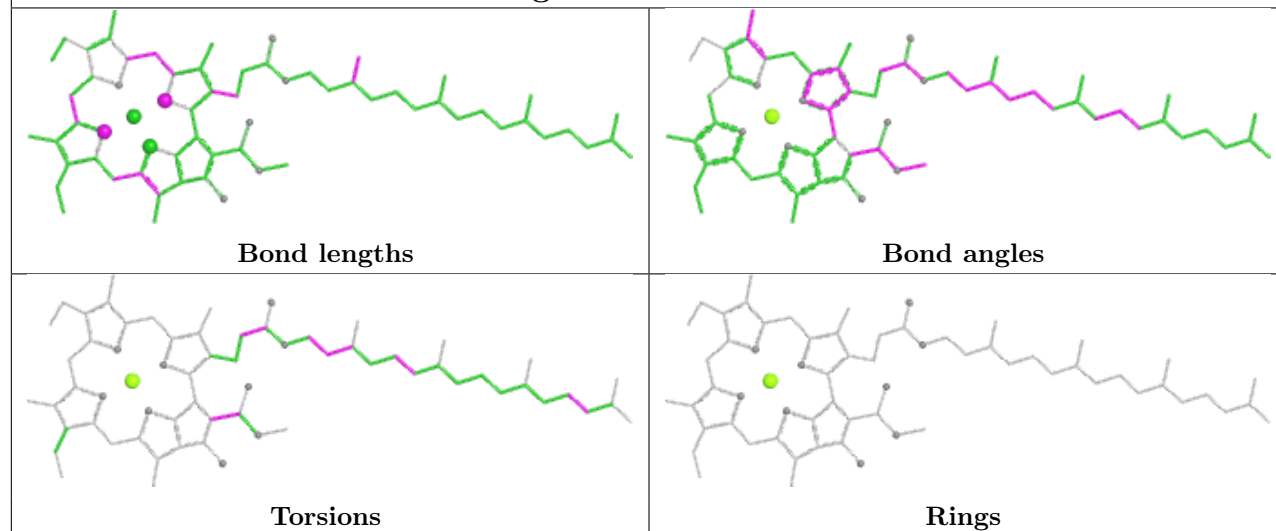
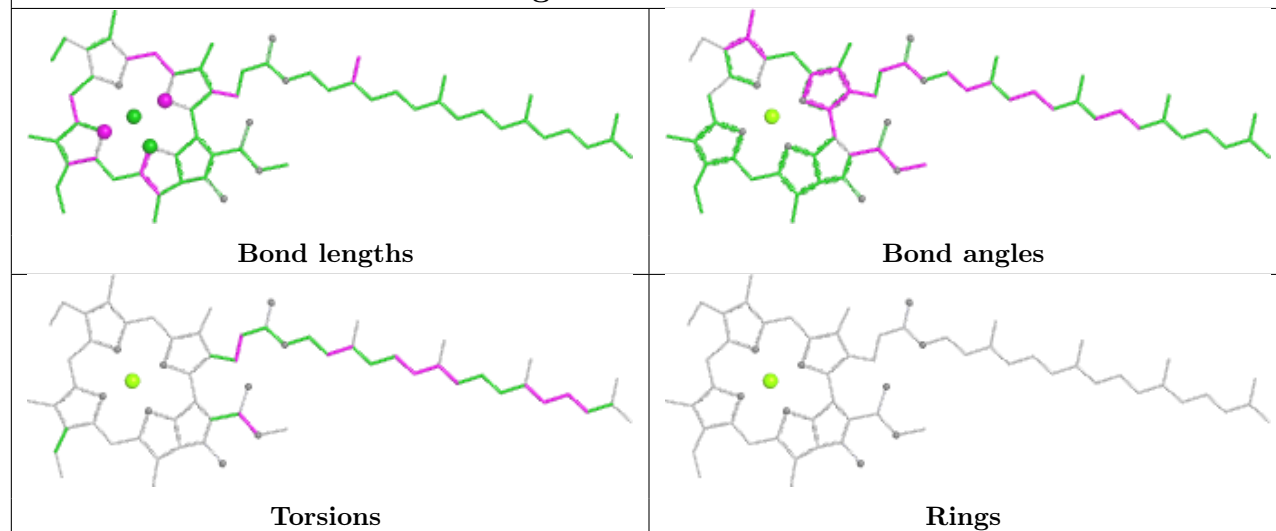
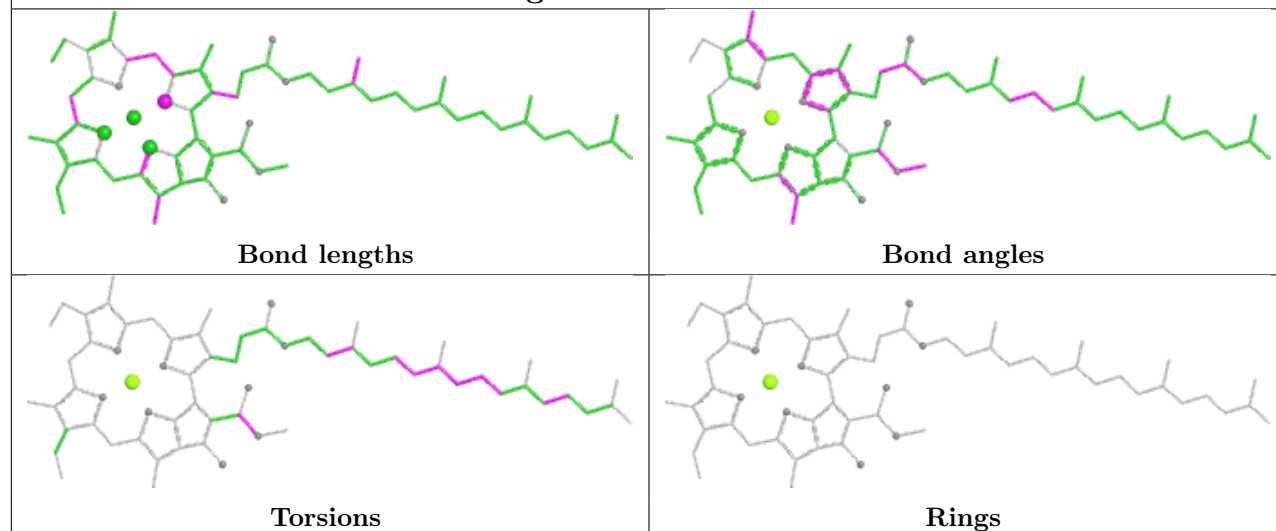


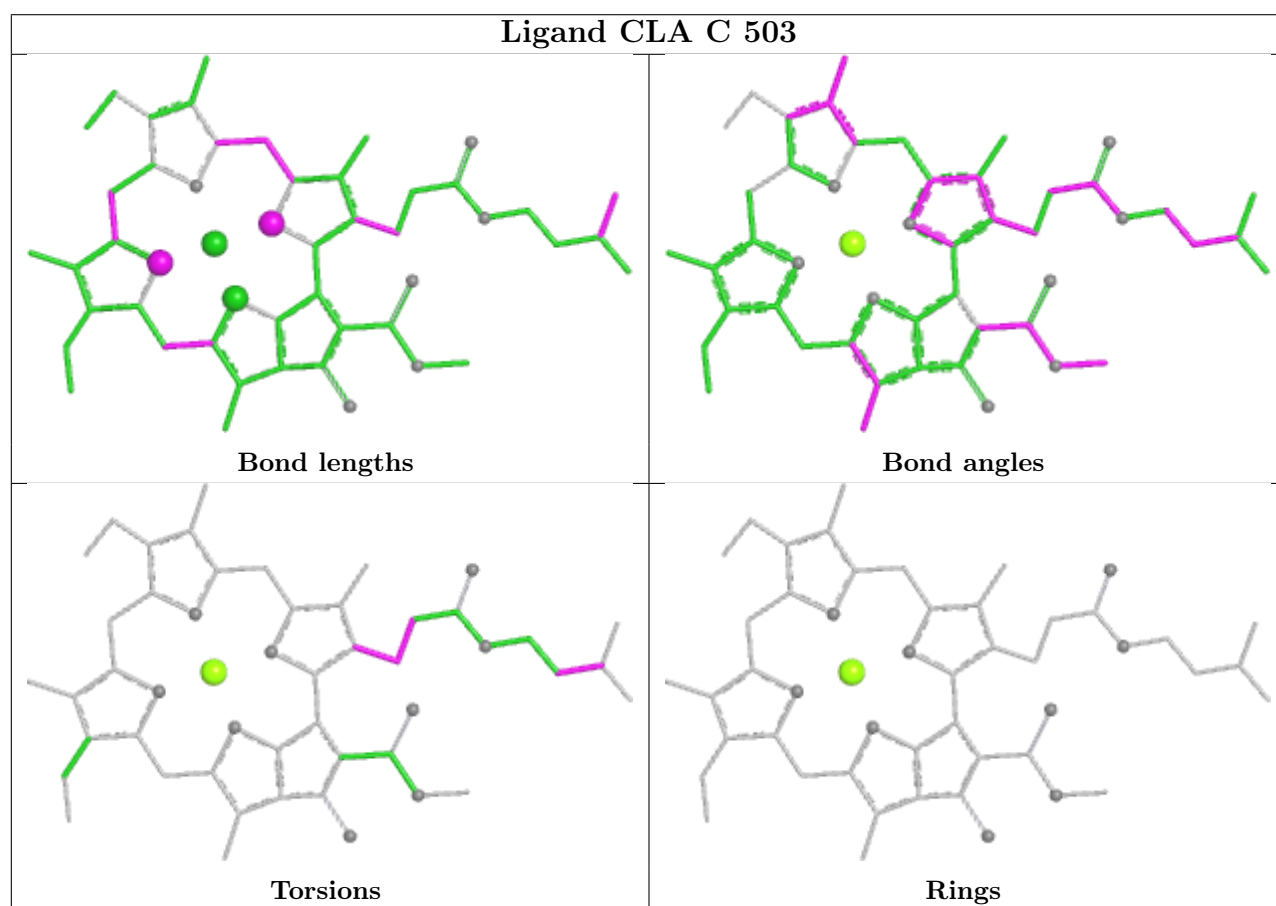
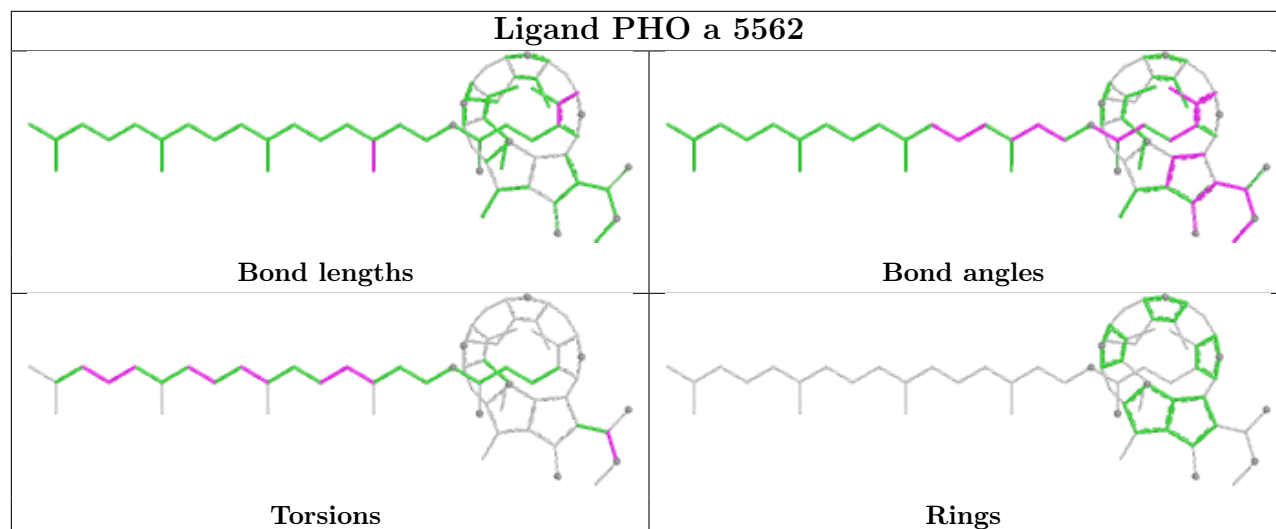


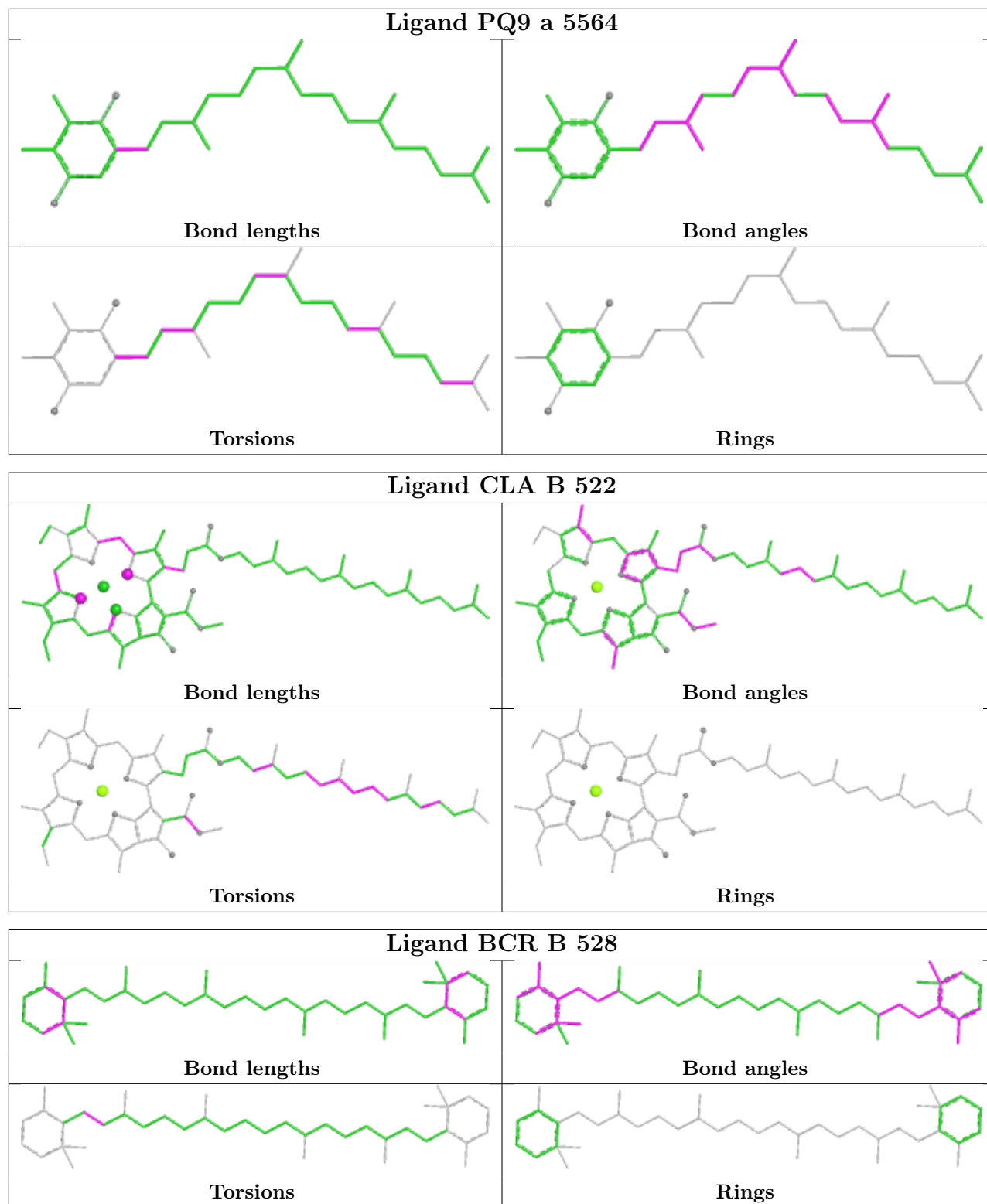


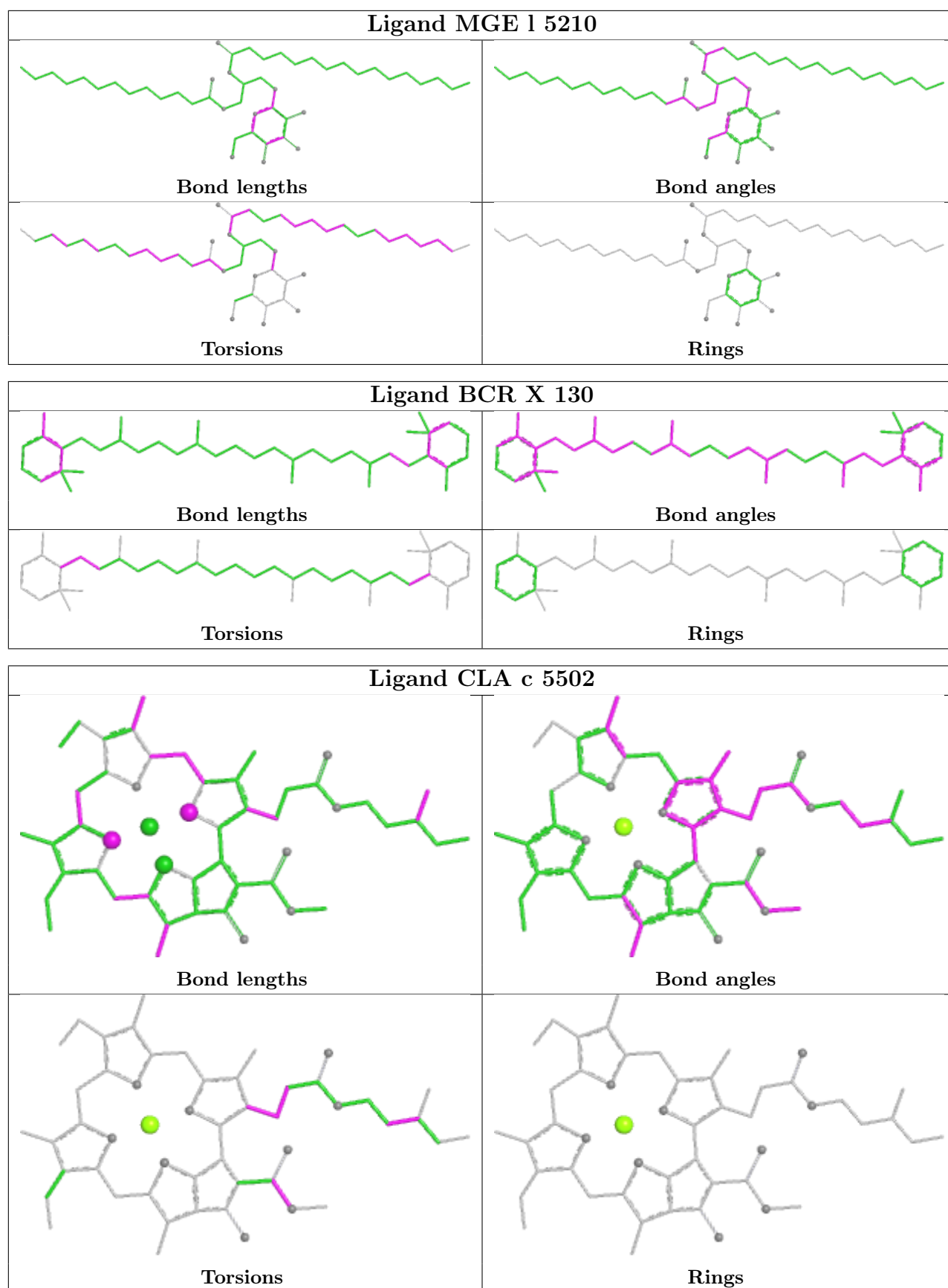


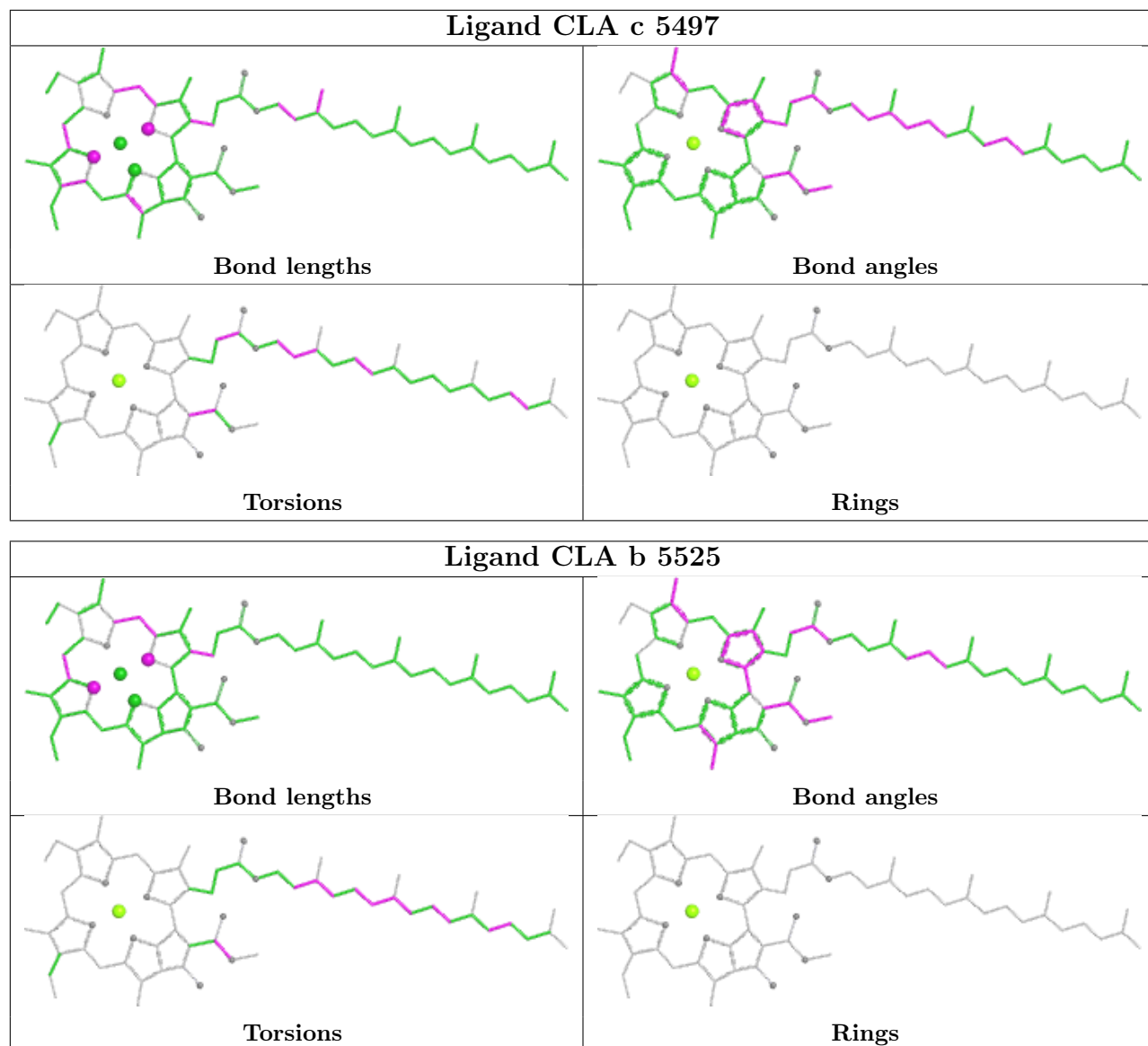


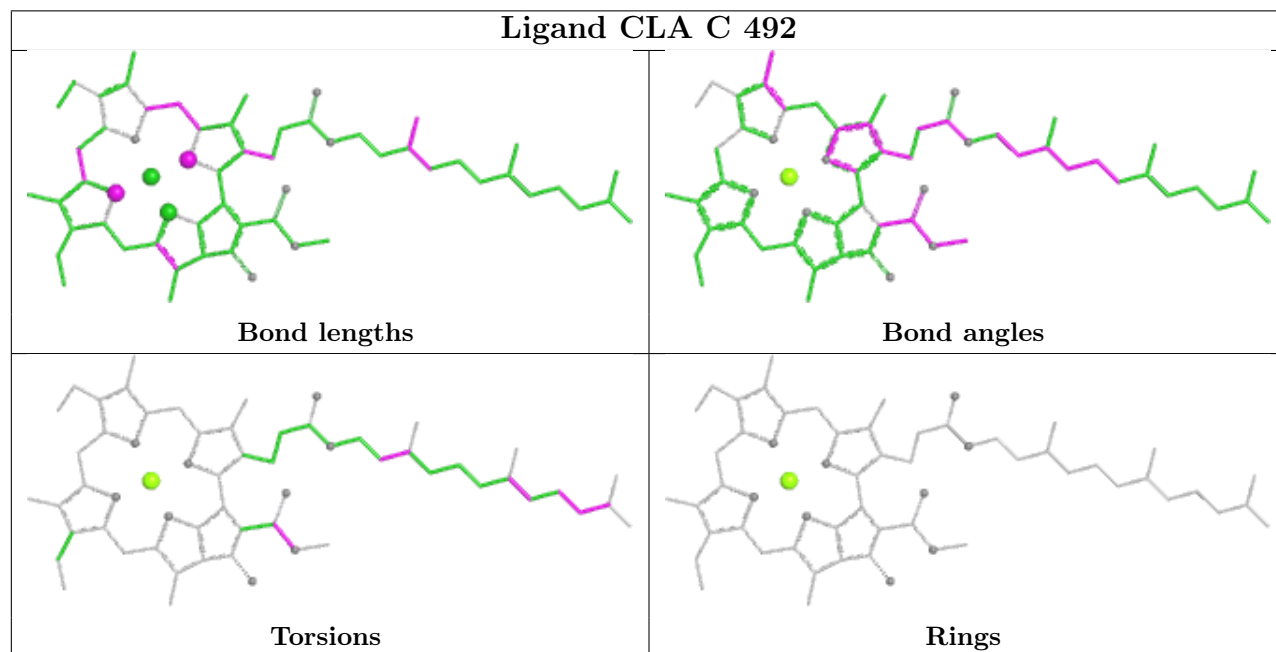
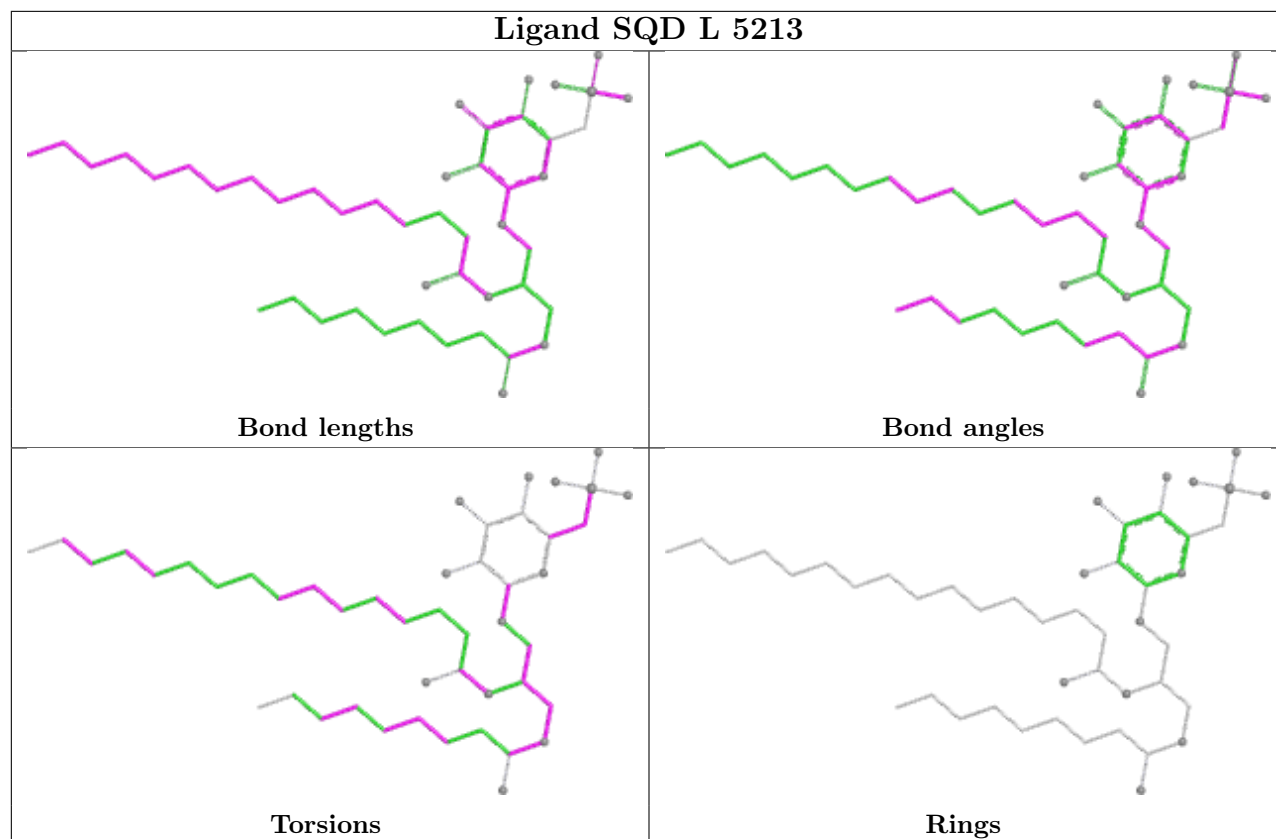
**Ligand CLA C 497****Ligand CLA B 520****Ligand CLA b 5522**

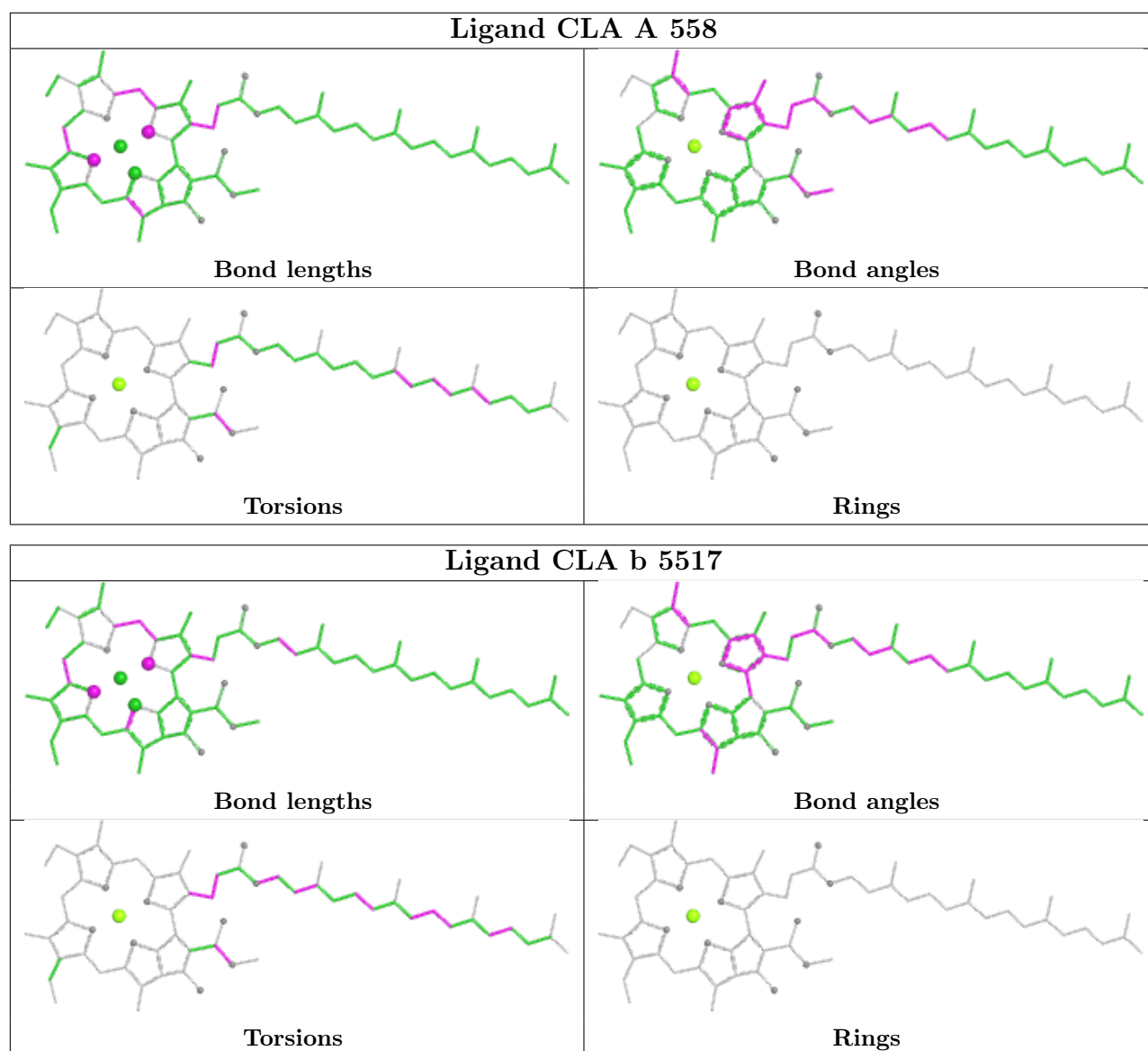












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	-0.59	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.53	4 (1%) 79 54	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.53	2 (0%) 92 79	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.50	1 (0%) 95 87	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.52	3 (0%) 87 69	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.35	5 (1%) 80 56	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 94 84	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.57	1 (0%) 94 84	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.20	1 (1%) 79 54	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.01	3 (3%) 41 17	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.25	1 (2%) 51 23	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	3 (8%) 10 3	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.37	1 (1%) 72 44	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.19	3 (4%) 31 11	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	0 100 100	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.34	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.60	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.52	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.53	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.40	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.15	1 (2%) 54 26	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.36	2 (5%) 25 9	45, 56, 86, 91	0
12	M	36/36 (100%)	-0.42	2 (5%) 24 8	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.34	1 (2%) 53 25	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/247 (97%)	-0.39	3 (1%) 79 54	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.30	8 (3%) 46 20	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.48	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.73	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.39	1 (1%) 82 59	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.42	3 (3%) 49 21	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.48	2 (1%) 73 46	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.24	5 (3%) 42 17	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.25	4 (6%) 18 5	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.20	2 (3%) 47 20	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.45	63 (1%) 79 54	35, 66, 85, 101	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5473	ASP	4.5
1	a	5010	SER	4.4
13	o	5049	ASP	4.3
4	D	13	GLY	4.2
11	l	5001	MET	4.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	b	5511	41/65	0.64	0.39	88,92,95,96	0
27	LMT	t	5217	35/35	0.69	0.45	76,95,104,105	0
29	UNK	c	5478	11/-	0.70	0.40	76,79,81,81	0
29	UNK	c	5490	4/-	0.71	0.33	91,92,92,92	0
29	UNK	C	481	13/-	0.72	0.37	61,64,68,69	0
27	LMT	A	569	35/35	0.73	0.47	80,89,92,93	0
20	CLA	B	511	41/65	0.73	0.41	88,90,92,98	0
29	UNK	C	475	12/-	0.73	0.32	68,69,72,73	0
29	UNK	c	5475	12/-	0.74	0.35	74,78,84,84	0
27	LMT	T	217	35/35	0.75	0.32	83,93,96,97	0
28	MGE	d	5359	47/48	0.76	0.30	72,81,96,98	0
24	BCR	c	5506	40/40	0.77	0.32	75,81,86,86	0
22	PQ9	A	564	30/45	0.77	0.37	54,57,63,64	30
24	BCR	x	5130	40/40	0.78	0.44	77,81,85,86	0
27	LMT	M	5216	35/35	0.78	0.31	58,83,90,90	0
29	UNK	C	489	7/-	0.79	0.42	75,76,77,78	0
26	SQD	a	212	26/54	0.79	0.26	82,94,101,103	0
26	SQD	d	5358	54/54	0.79	0.29	74,85,106,107	0
29	UNK	c	5489	7/-	0.79	0.39	73,73,74,74	0
20	CLA	b	5526	65/65	0.79	0.28	66,71,92,95	0
26	SQD	L	5213	47/54	0.80	0.27	52,85,106,108	0
20	CLA	B	526	65/65	0.80	0.28	71,82,97,98	0
29	UNK	c	5476	9/-	0.80	0.32	58,60,62,62	0
27	LMT	a	5568	35/35	0.81	0.43	79,92,94,96	0
29	UNK	C	486	8/-	0.81	0.36	55,56,59,60	0
27	LMT	m	216	35/35	0.81	0.28	62,87,89,91	0
20	CLA	b	5516	65/65	0.81	0.28	62,66,84,86	0
28	MGE	D	358	47/48	0.81	0.24	65,72,79,81	0
24	BCR	C	505	40/40	0.81	0.43	75,81,91,92	0
26	SQD	A	5212	26/54	0.81	0.23	75,100,107,107	0
29	UNK	C	476	9/-	0.81	0.29	61,62,63,64	0
24	BCR	d	5357	40/40	0.82	0.37	61,72,86,88	0
20	CLA	c	5496	65/65	0.82	0.27	79,83,95,97	0
24	BCR	H	107	40/40	0.82	0.30	77,83,88,89	0
20	CLA	B	516	65/65	0.82	0.27	61,76,92,97	0
29	UNK	c	5485	5/-	0.83	0.41	68,69,69,70	0
29	UNK	C	478	11/-	0.84	0.24	58,65,66,66	0
20	CLA	C	496	65/65	0.84	0.26	71,78,88,89	0
29	UNK	c	5484	5/-	0.84	0.52	69,69,70,72	0
26	SQD	A	568	54/54	0.84	0.32	76,82,90,90	0
24	BCR	B	528	40/40	0.84	0.25	54,68,74,75	0
20	CLA	a	5563	55/65	0.84	0.32	59,65,102,103	0
24	BCR	X	130	40/40	0.85	0.32	68,71,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	c	5498	65/65	0.85	0.25	81,90,93,93	0
28	MGE	i	5201	48/48	0.85	0.27	67,83,88,90	0
20	CLA	c	5503	50/65	0.85	0.28	88,91,92,93	0
24	BCR	h	5107	40/40	0.85	0.28	74,79,82,83	0
29	UNK	c	5479	11/-	0.85	0.24	76,77,77,77	0
20	CLA	C	503	50/65	0.85	0.27	83,86,88,94	0
29	UNK	C	479	11/-	0.85	0.26	58,64,67,67	0
26	SQD	t	213	47/54	0.85	0.27	61,95,116,117	0
29	UNK	C	482	13/-	0.85	0.25	64,66,67,67	0
24	BCR	b	5529	40/40	0.86	0.35	69,72,74,74	0
29	UNK	C	487	7/-	0.86	0.24	49,52,52,53	0
29	UNK	C	488	5/-	0.86	0.17	41,45,47,47	0
24	BCR	c	5504	40/40	0.86	0.29	73,80,88,89	0
20	CLA	d	5355	50/65	0.86	0.23	74,77,80,81	0
29	UNK	C	484	5/-	0.86	0.21	47,51,52,53	0
30	DGD	c	5509	57/66	0.86	0.28	67,72,77,78	0
20	CLA	c	5502	51/65	0.87	0.23	93,96,97,98	0
28	MGE	D	359	41/48	0.87	0.23	60,67,76,79	0
28	MGE	I	201	48/48	0.87	0.22	73,81,89,90	0
20	CLA	B	519	65/65	0.87	0.26	73,82,85,87	0
29	UNK	c	5481	13/-	0.87	0.22	60,62,66,66	0
24	BCR	C	506	40/40	0.88	0.22	68,72,79,80	0
20	CLA	C	498	65/65	0.88	0.22	64,74,98,101	0
29	UNK	c	5483	13/-	0.88	0.26	71,75,80,82	0
24	BCR	T	5104	40/40	0.88	0.25	67,71,78,79	0
22	PQ9	a	5564	30/45	0.88	0.32	51,55,62,62	30
29	UNK	c	5487	7/-	0.88	0.20	57,57,58,58	0
20	CLA	C	502	51/65	0.88	0.21	74,80,83,84	0
20	CLA	A	563	55/65	0.88	0.26	43,49,75,78	0
24	BCR	c	5505	40/40	0.88	0.31	84,87,91,92	0
29	UNK	C	474	15/-	0.89	0.18	26,37,40,40	0
29	UNK	c	5474	15/-	0.89	0.24	39,50,56,56	0
24	BCR	D	357	40/40	0.89	0.26	61,66,78,80	0
20	CLA	b	5519	65/65	0.89	0.24	70,75,80,81	0
29	UNK	c	5477	7/-	0.89	0.34	67,68,70,70	0
28	MGE	B	530	48/48	0.89	0.19	55,64,70,72	0
20	CLA	c	5501	65/65	0.89	0.26	82,91,94,95	0
29	UNK	c	5480	7/-	0.89	0.26	65,66,66,67	0
20	CLA	C	501	65/65	0.89	0.25	70,78,83,85	0
24	BCR	B	529	40/40	0.89	0.25	62,69,80,80	0
29	UNK	C	483	13/-	0.89	0.23	61,68,78,78	0
28	MGE	L	210	48/48	0.89	0.24	59,68,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNK	c	5486	8/-	0.89	0.30	63,64,65,66	0
29	UNK	C	485	5/-	0.89	0.24	57,59,61,61	0
20	CLA	C	497	65/65	0.89	0.24	74,78,80,82	0
28	MGE	d	5360	41/48	0.89	0.21	68,72,78,80	0
30	DGD	C	507	53/66	0.89	0.25	55,66,86,88	0
30	DGD	c	5507	53/66	0.89	0.23	66,74,90,91	0
20	CLA	c	5497	65/65	0.89	0.24	66,82,84,87	0
25	LHG	a	5567	39/49	0.90	0.26	65,68,74,80	0
20	CLA	c	5493	65/65	0.90	0.21	67,81,86,86	0
28	MGE	d	5361	48/48	0.90	0.21	61,68,78,83	0
20	CLA	a	5560	65/65	0.90	0.22	62,68,100,101	0
28	MGE	l	5210	48/48	0.90	0.21	59,69,78,81	0
24	BCR	a	5566	40/40	0.90	0.25	59,75,78,79	0
20	CLA	b	5520	65/65	0.90	0.24	63,72,74,76	0
20	CLA	B	520	65/65	0.90	0.23	62,67,76,79	0
30	DGD	H	208	54/66	0.90	0.20	61,69,75,76	0
28	MGE	b	5530	48/48	0.90	0.18	59,64,71,73	0
29	UNK	c	5482	13/-	0.90	0.19	60,61,71,72	0
24	BCR	C	504	40/40	0.91	0.27	57,64,70,70	0
20	CLA	A	560	65/65	0.91	0.21	49,57,86,88	0
21	PHO	a	5562	64/64	0.91	0.22	70,75,81,82	0
28	MGE	D	360	48/48	0.91	0.20	52,60,63,68	0
20	CLA	c	5491	65/65	0.91	0.20	70,78,81,86	0
22	PQ9	D	356	30/45	0.91	0.21	49,67,80,83	0
29	UNK	C	480	7/-	0.91	0.22	35,36,38,38	0
24	BCR	t	104	40/40	0.91	0.20	65,72,84,85	0
20	CLA	B	512	65/65	0.91	0.24	68,75,78,79	0
30	DGD	C	508	47/66	0.91	0.19	61,71,80,83	0
30	DGD	C	509	57/66	0.91	0.20	52,60,69,70	0
24	BCR	B	527	40/40	0.91	0.18	58,65,68,69	0
20	CLA	c	5495	65/65	0.91	0.21	74,81,86,88	0
30	DGD	c	5508	47/66	0.91	0.18	66,76,82,84	0
20	CLA	D	355	50/65	0.91	0.22	63,65,68,70	0
29	UNK	c	5488	5/-	0.92	0.21	59,59,59,60	0
20	CLA	b	5512	65/65	0.92	0.23	68,72,75,76	0
22	PQ9	d	5356	30/45	0.92	0.20	51,57,66,66	0
24	BCR	A	566	40/40	0.92	0.24	50,57,64,66	0
20	CLA	c	5499	47/65	0.92	0.20	60,69,76,78	0
20	CLA	c	5500	65/65	0.92	0.20	64,69,82,83	0
20	CLA	C	495	65/65	0.92	0.21	58,68,74,76	0
20	CLA	b	5525	65/65	0.92	0.20	71,77,80,82	0
24	BCR	b	5527	40/40	0.92	0.19	58,63,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	LHG	A	567	39/49	0.92	0.23	57,73,79,81	0
20	CLA	B	525	65/65	0.93	0.20	67,84,91,92	0
20	CLA	B	518	65/65	0.93	0.19	53,64,79,79	0
20	CLA	c	5492	60/65	0.93	0.17	57,61,83,84	0
20	CLA	B	515	65/65	0.93	0.21	55,66,71,72	0
20	CLA	c	5494	46/65	0.93	0.16	72,77,86,88	0
20	CLA	B	514	65/65	0.93	0.21	59,64,82,83	0
24	BCR	b	5528	40/40	0.93	0.18	61,64,72,73	0
20	CLA	B	522	65/65	0.93	0.21	54,65,75,77	0
20	CLA	b	5524	56/65	0.93	0.18	63,68,89,91	0
20	CLA	B	524	56/65	0.93	0.19	67,72,77,80	0
30	DGD	h	5208	54/66	0.93	0.17	57,68,73,75	0
20	CLA	B	513	65/65	0.94	0.18	56,61,67,67	0
20	CLA	C	493	65/65	0.94	0.18	67,71,77,79	0
20	CLA	b	5521	65/65	0.94	0.15	48,57,63,64	0
20	CLA	b	5522	65/65	0.94	0.20	60,66,75,76	0
20	CLA	b	5513	65/65	0.94	0.20	54,61,84,90	0
21	PHO	A	562	64/64	0.94	0.17	47,53,63,66	0
21	PHO	a	5561	64/64	0.94	0.18	51,55,66,68	0
20	CLA	b	5514	65/65	0.94	0.18	41,51,74,75	0
20	CLA	b	5515	65/65	0.94	0.21	46,51,74,76	0
20	CLA	C	500	65/65	0.94	0.16	59,63,73,74	0
32	HEM	f	5051	43/43	0.94	0.28	80,84,97,101	0
33	CA	k	5056	1/1	0.94	0.19	119,119,119,119	0
20	CLA	C	499	47/65	0.95	0.17	57,60,66,69	0
20	CLA	b	5523	65/65	0.95	0.15	45,52,74,75	0
20	CLA	B	521	65/65	0.95	0.17	58,63,66,68	0
20	CLA	C	494	46/65	0.95	0.15	59,66,68,72	0
19	FE2	A	557	1/1	0.95	0.05	60,60,60,60	0
20	CLA	d	5354	65/65	0.95	0.17	39,47,64,65	0
20	CLA	B	523	65/65	0.95	0.16	47,56,73,74	0
21	PHO	A	561	64/64	0.95	0.16	32,52,55,59	0
20	CLA	D	354	65/65	0.95	0.16	35,43,63,66	0
20	CLA	C	491	65/65	0.95	0.18	63,70,77,79	0
20	CLA	b	5517	65/65	0.95	0.15	54,58,66,71	0
20	CLA	b	5518	65/65	0.95	0.17	60,64,69,75	0
20	CLA	a	5558	65/65	0.95	0.16	41,50,55,61	0
32	HEM	F	51	43/43	0.95	0.25	78,84,92,95	0
20	CLA	a	5559	65/65	0.95	0.15	42,49,60,60	0
20	CLA	C	492	60/65	0.95	0.17	53,58,76,77	0
20	CLA	B	517	65/65	0.96	0.14	37,44,56,57	0
20	CLA	A	558	65/65	0.96	0.14	41,46,50,51	0

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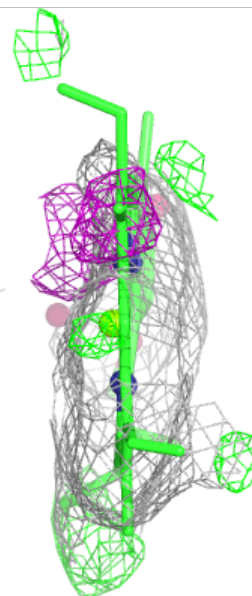
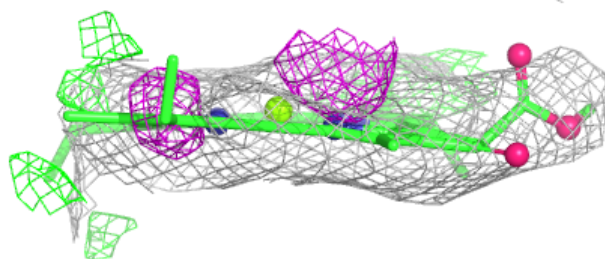
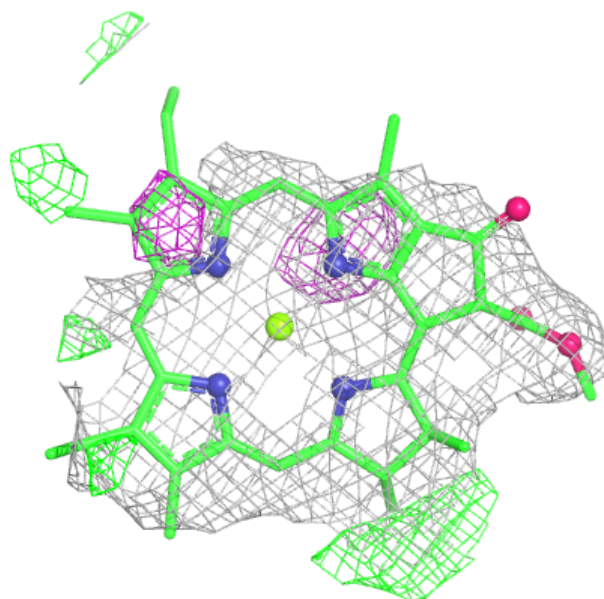
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	OEC	A	565	5/9	0.96	0.13	62,63,65,66	0
23	OEC	a	5565	5/9	0.96	0.13	63,64,71,87	0
31	BCT	D	353	4/4	0.96	0.18	72,73,73,74	0
20	CLA	A	559	65/65	0.96	0.14	39,43,49,52	0
29	UNK	C	477	7/-	0.96	0.16	47,49,51,51	0
32	HEM	v	5552	43/43	0.96	0.21	65,67,70,70	0
33	CA	K	56	1/1	0.96	0.09	119,119,119,119	0
29	UNK	C	490	4/-	0.96	0.15	67,67,68,68	0
32	HEM	V	552	43/43	0.97	0.18	37,54,58,59	0
31	BCT	d	5353	4/4	0.98	0.15	75,75,76,77	0
19	FE2	a	5557	1/1	1.00	0.11	75,75,75,75	0

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



**Electron density around CLA b 5511:**

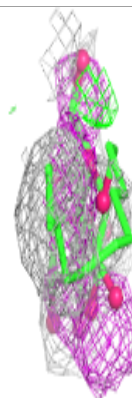
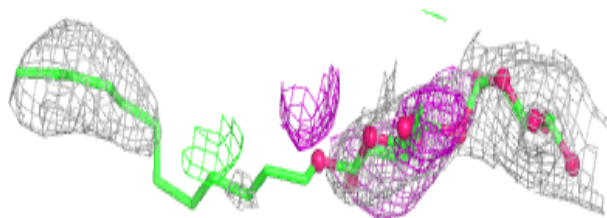
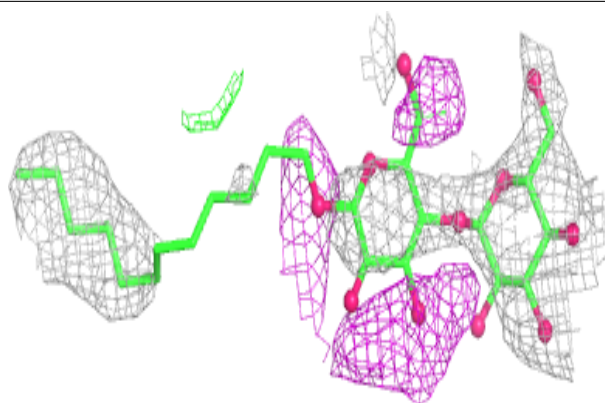
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



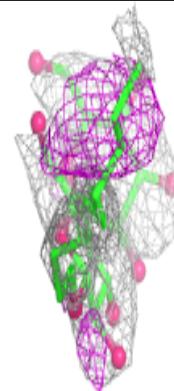
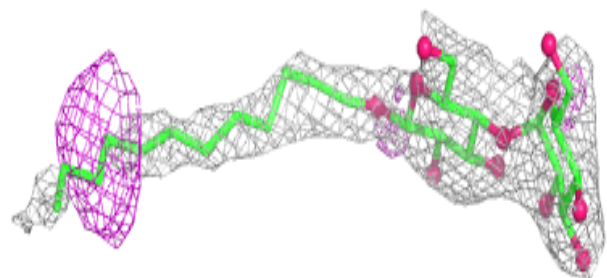
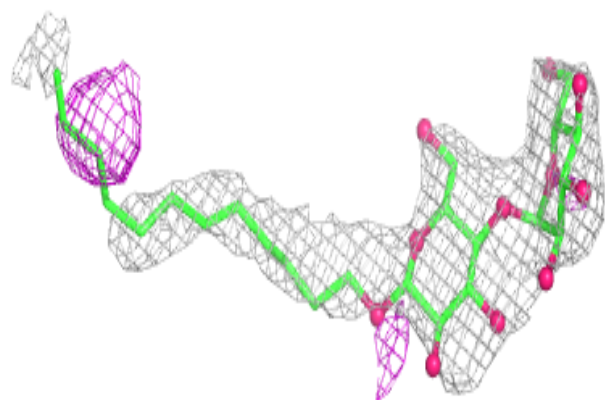


**Electron density around LMT t 5217:**

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

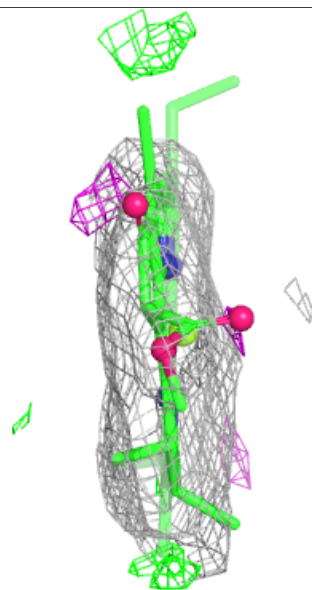
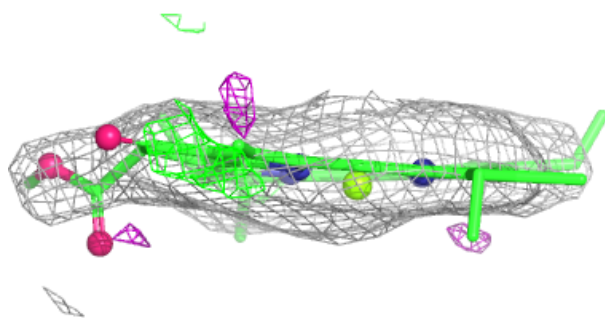
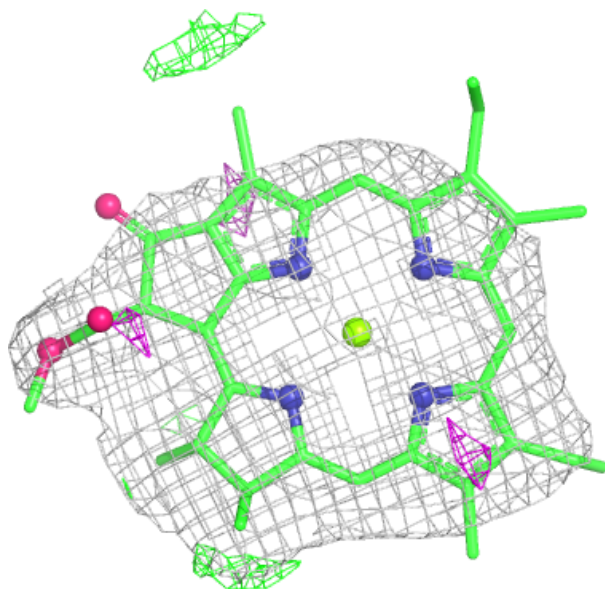
**Electron density around LMT A 569:**

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



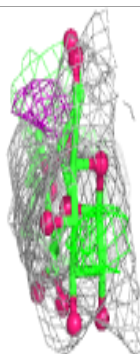
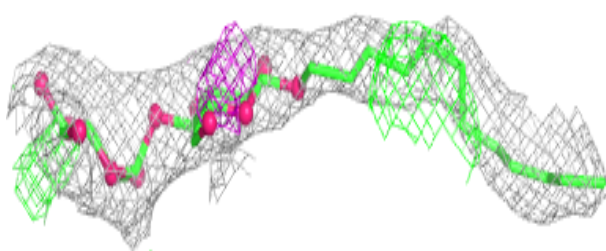
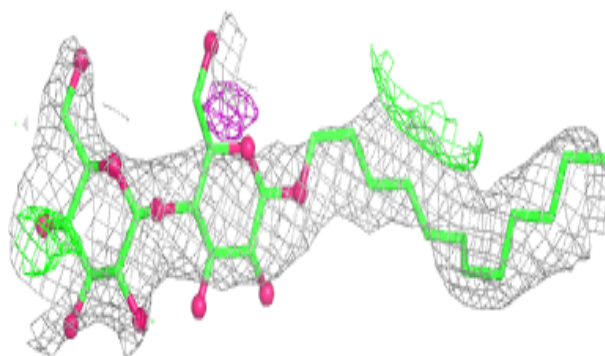
**Electron density around CLA B 511:**

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

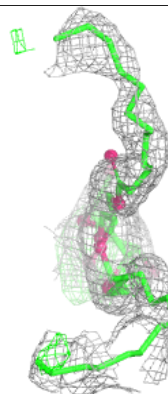
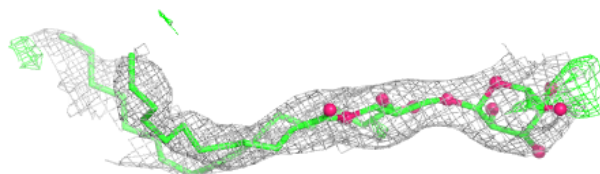
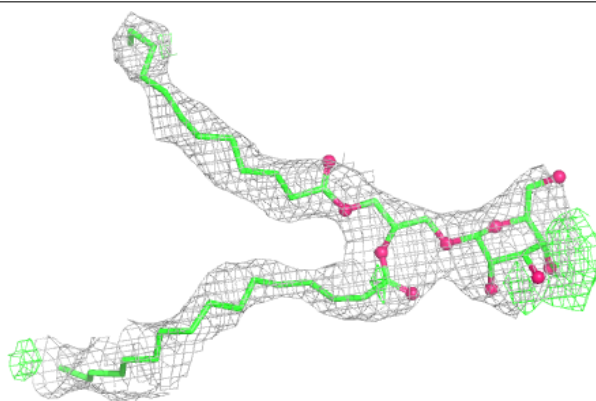


**Electron density around LMT T 217:**

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

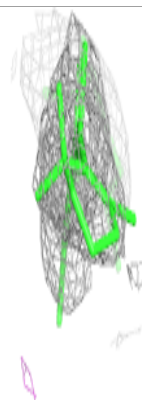
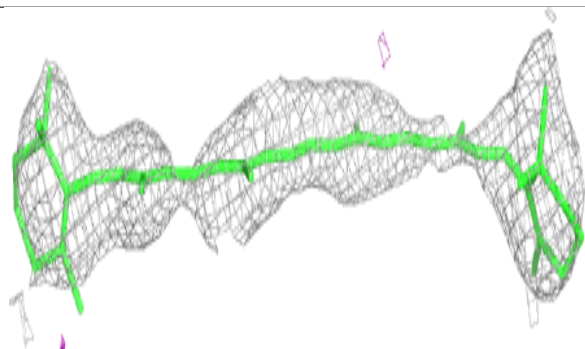
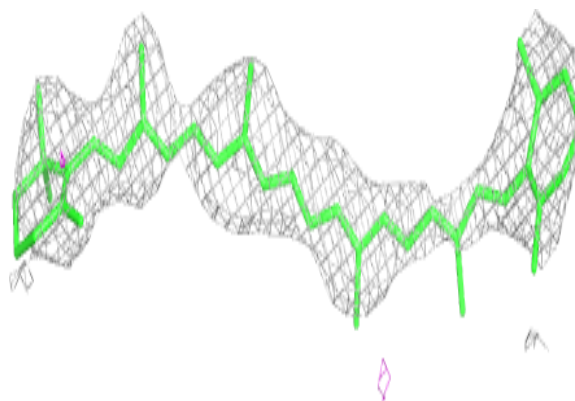
**Electron density around MGE d 5359:**

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

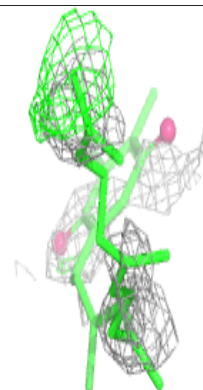
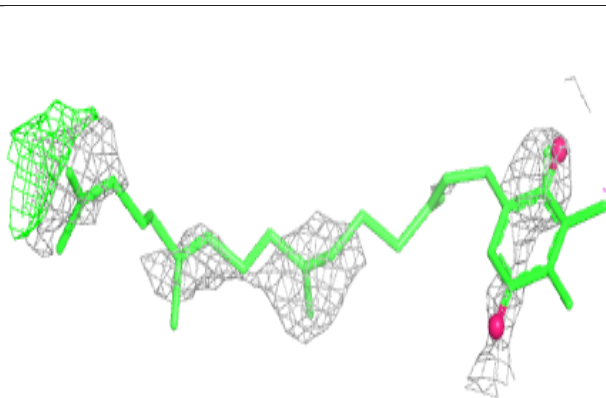
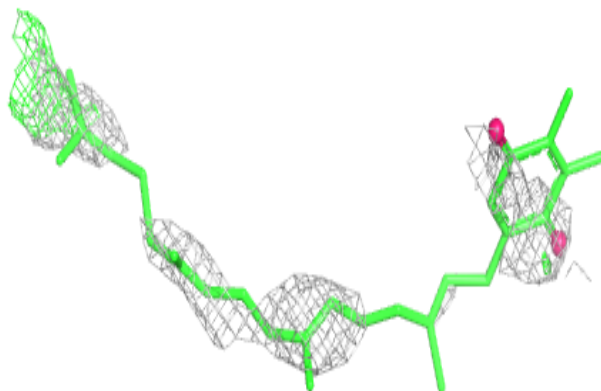


**Electron density around BCR c 5506:**

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

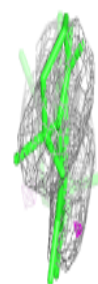
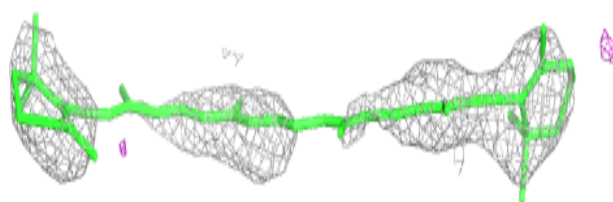
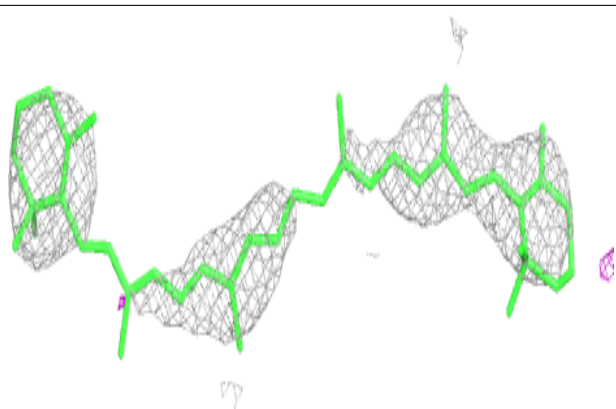
**Electron density around PQ9 A 564:**

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

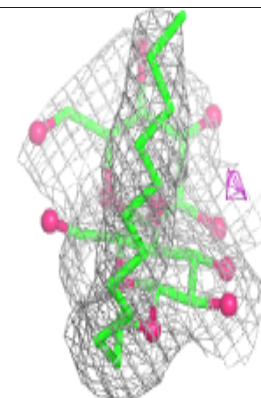
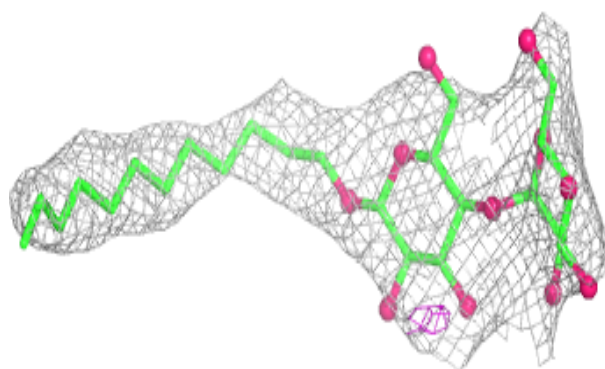
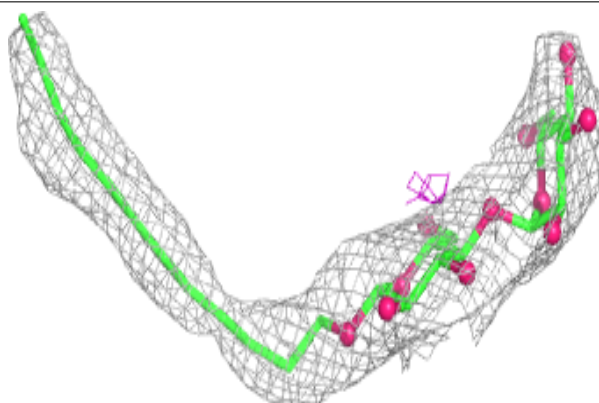


**Electron density around BCR x 5130:**

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

**Electron density around LMT M 5216:**

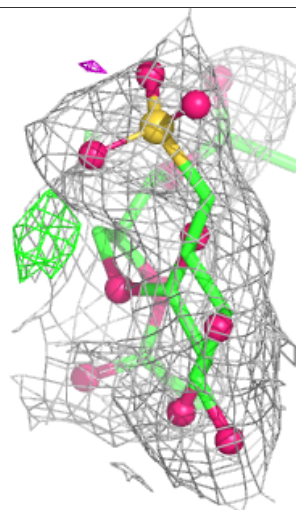
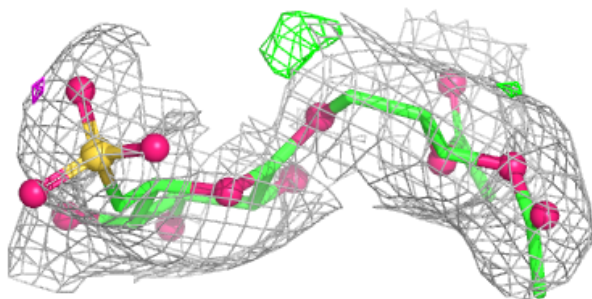
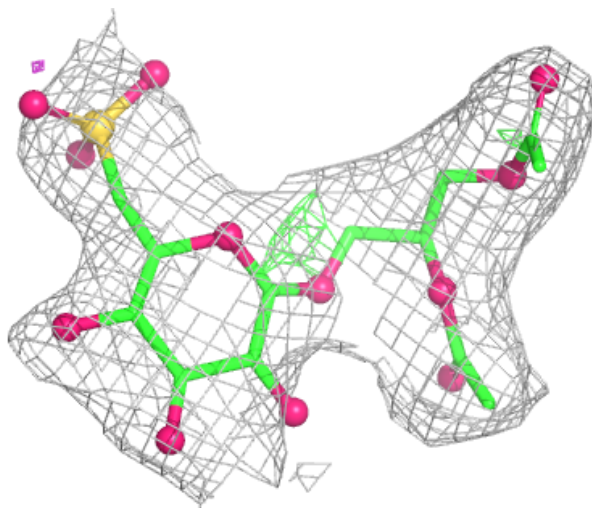
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





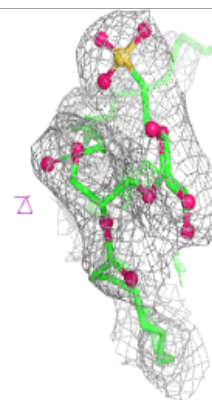
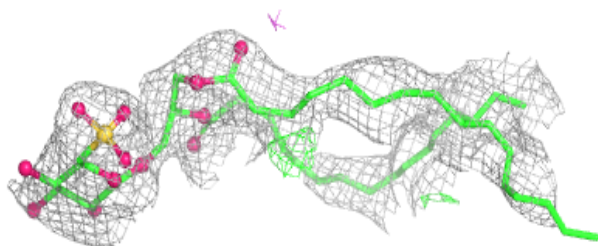
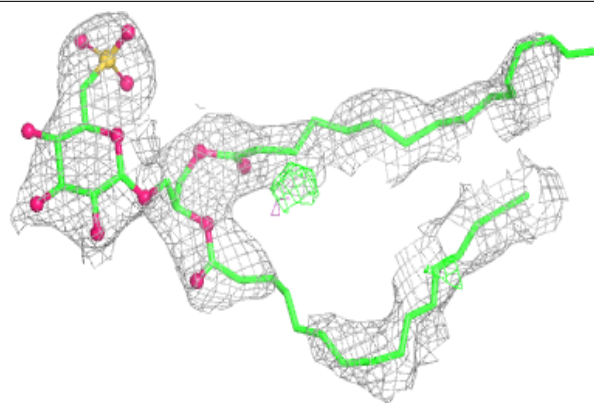
**Electron density around SQD a 212:**

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



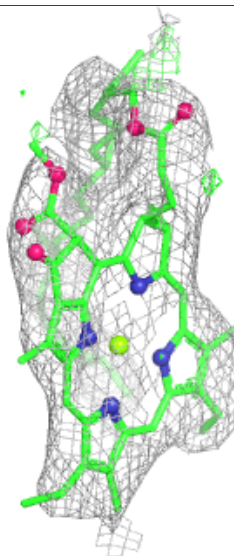
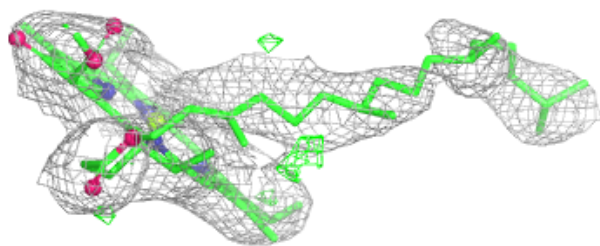
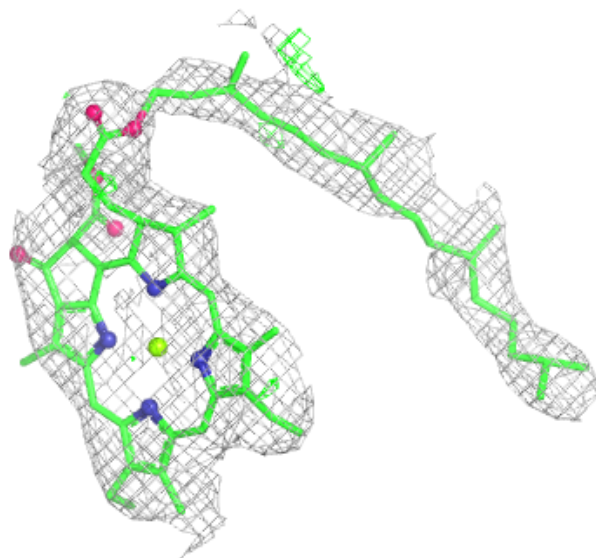
**Electron density around SQD d 5358:**

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



**Electron density around CLA b 5526:**

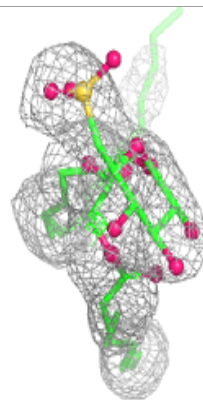
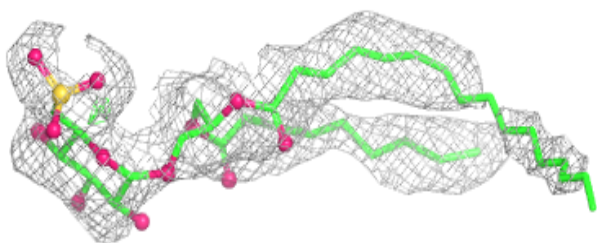
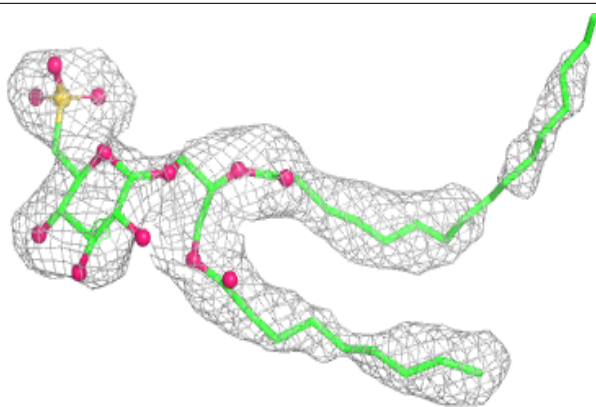
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





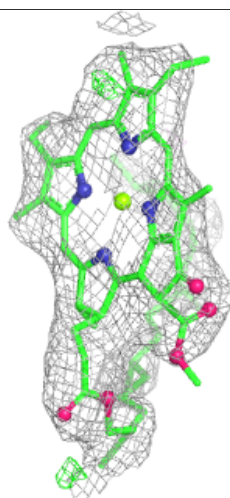
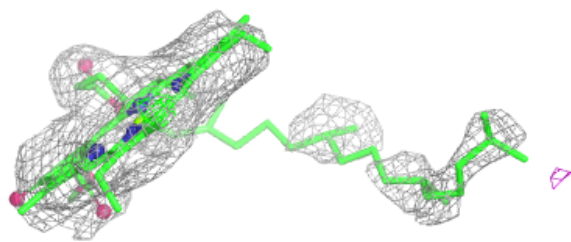
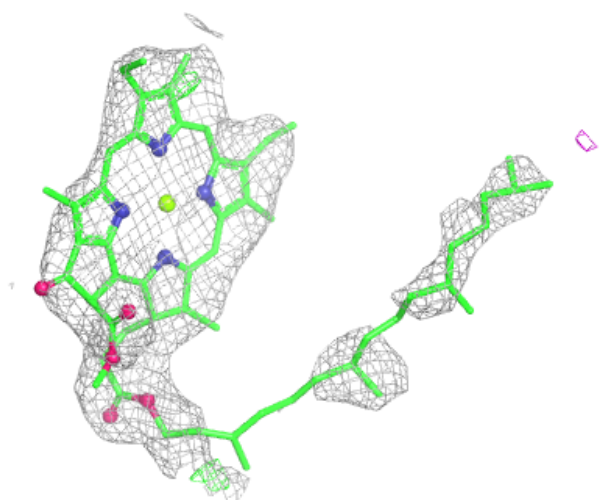
**Electron density around SQD L 5213:**

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



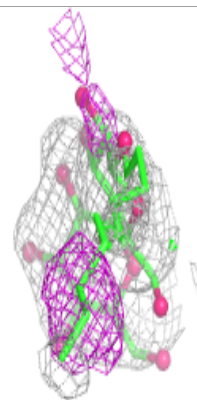
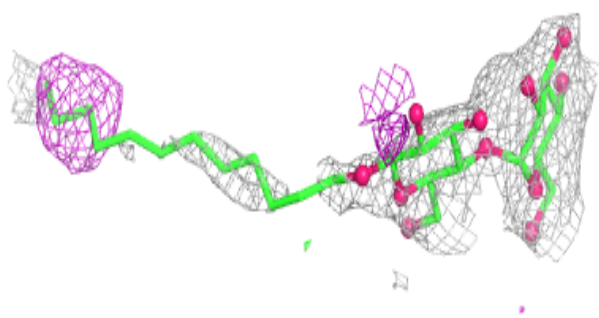
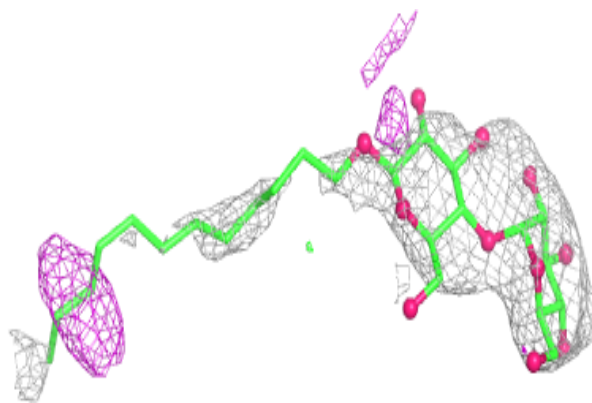
**Electron density around CLA B 526:**

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

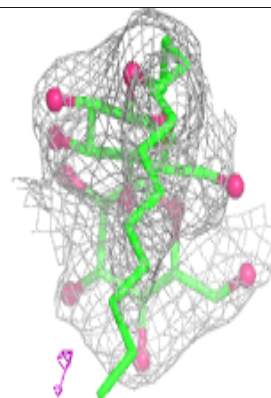
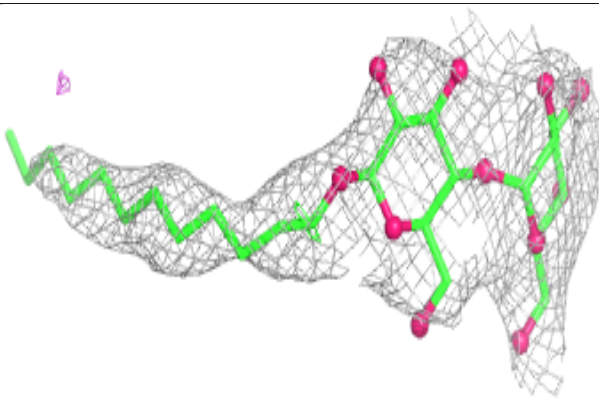
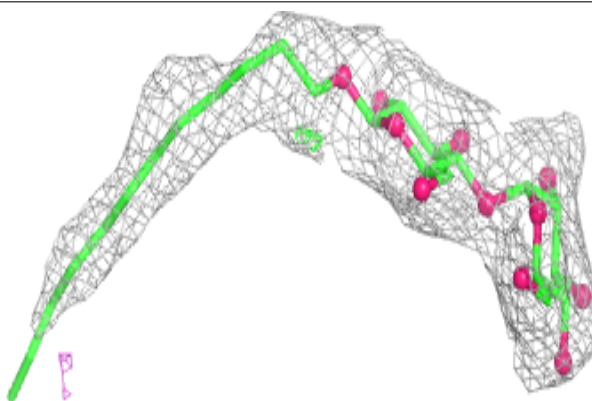


**Electron density around LMT a 5568:**

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

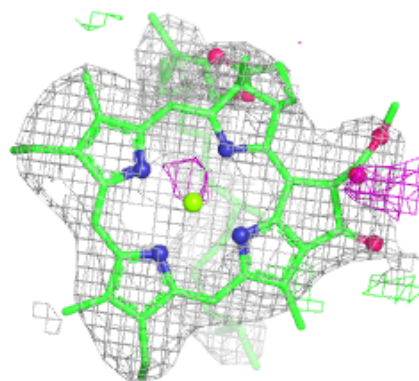
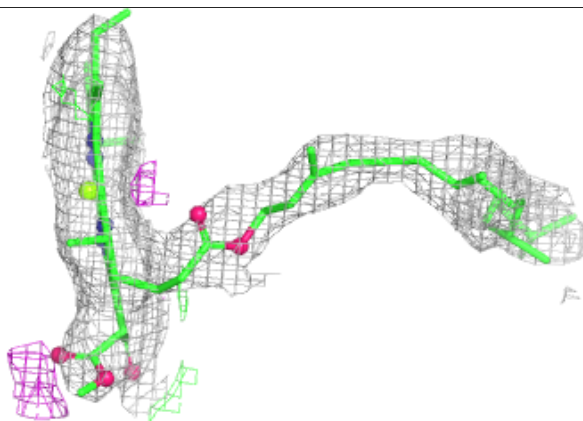
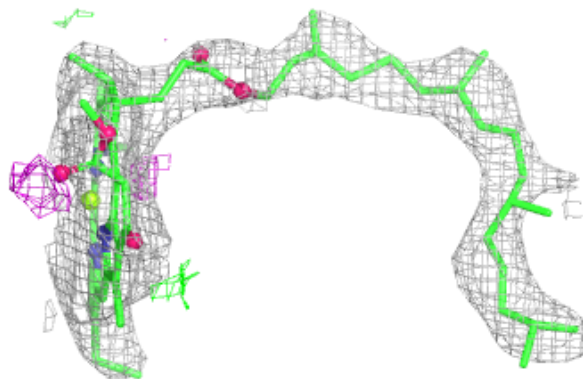
**Electron density around LMT m 216:**

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

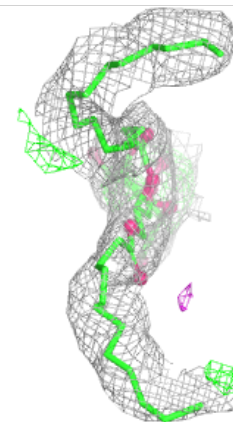
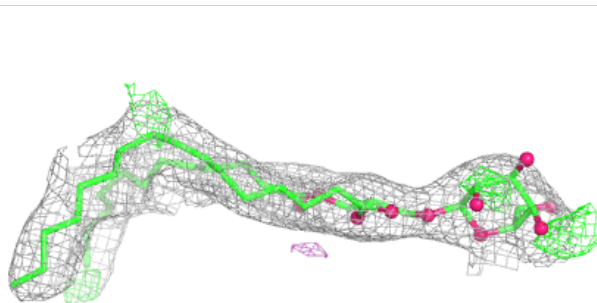
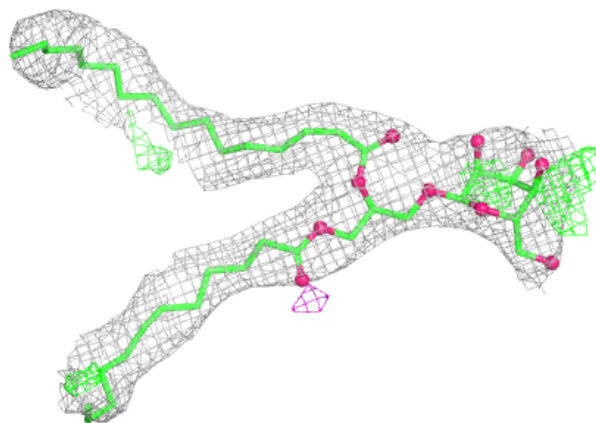


**Electron density around CLA b 5516:**

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

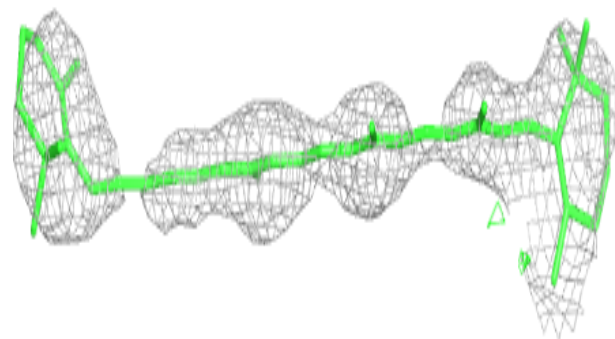
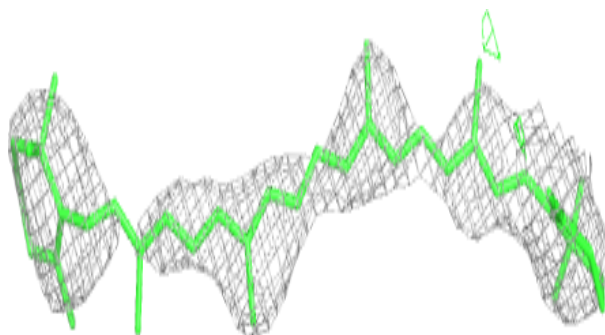
**Electron density around MGE D 358:**

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



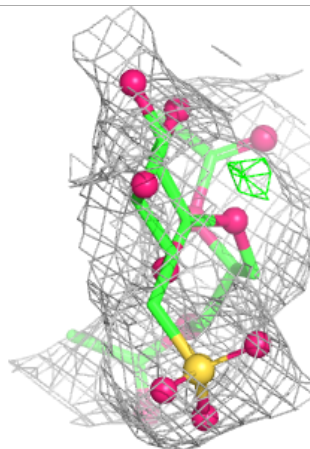
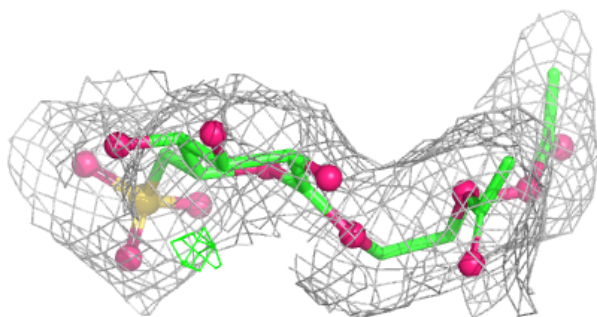
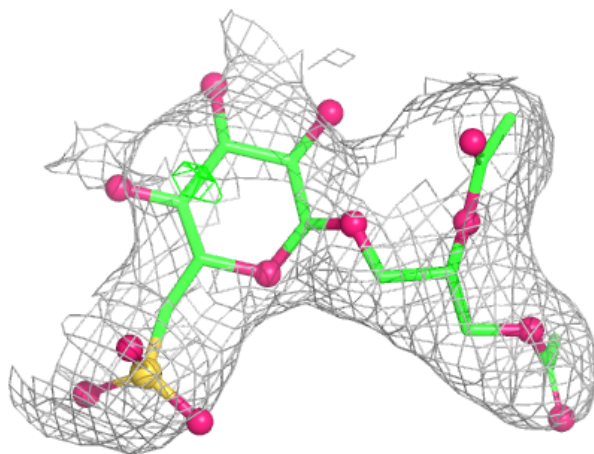
**Electron density around BCR C 505:**

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



**Electron density around SQD A 5212:**

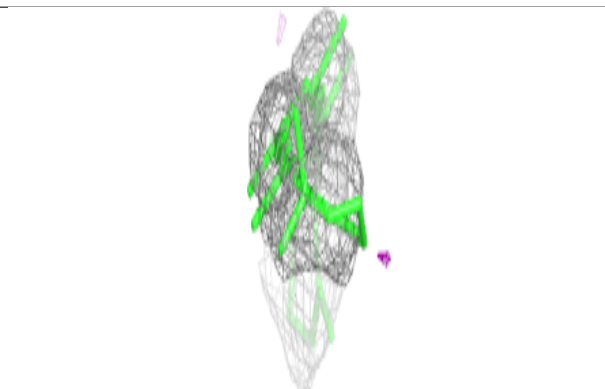
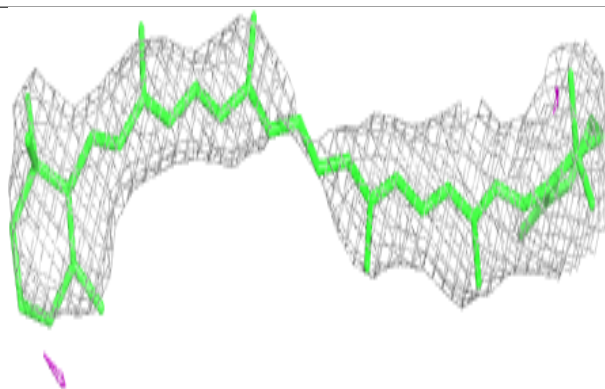
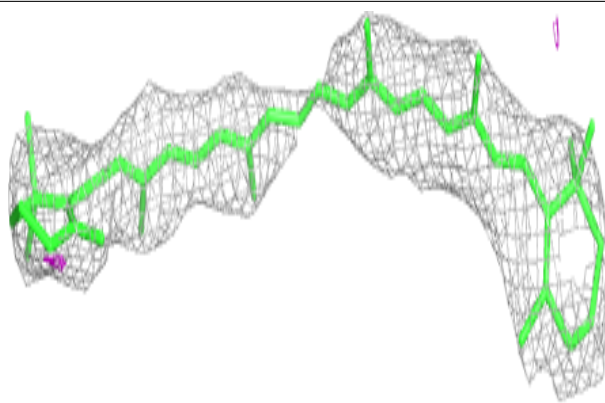
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



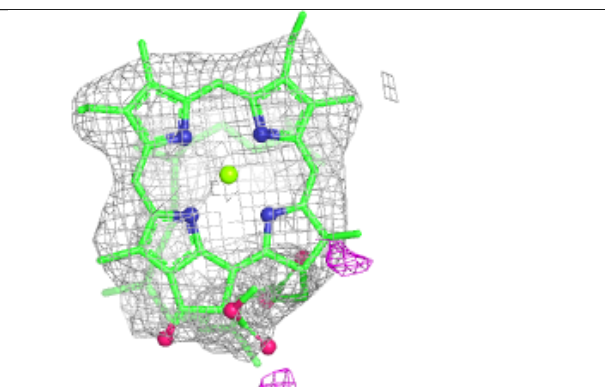
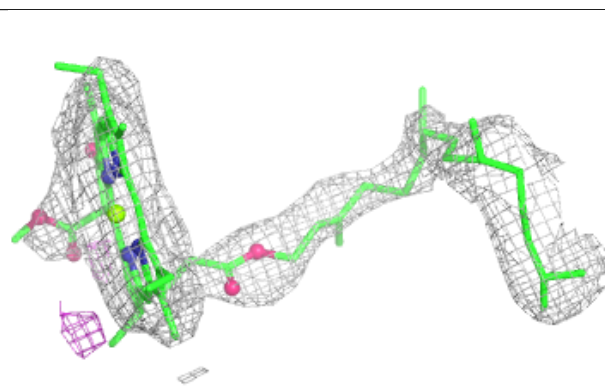
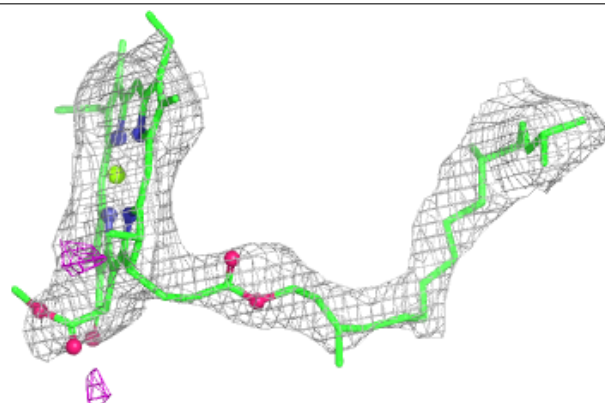


**Electron density around BCR d 5357:**

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

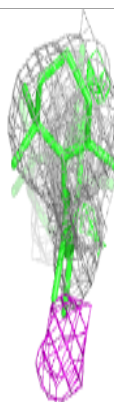
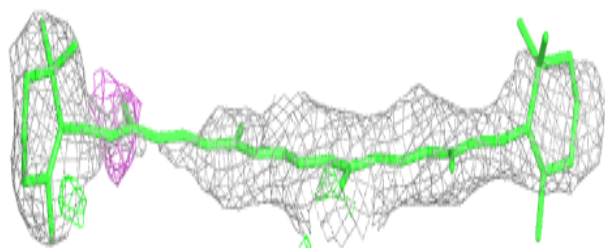
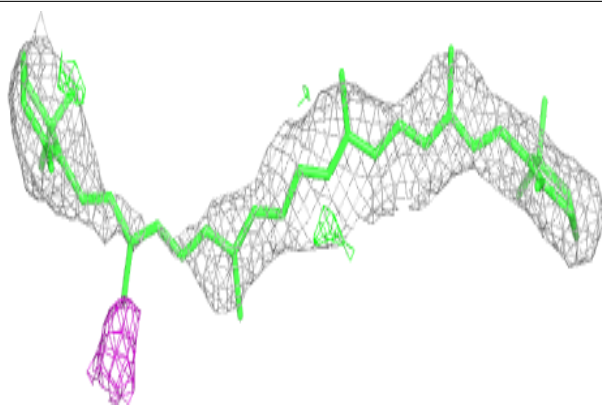
**Electron density around CLA c 5496:**

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



**Electron density around BCR H 107:**

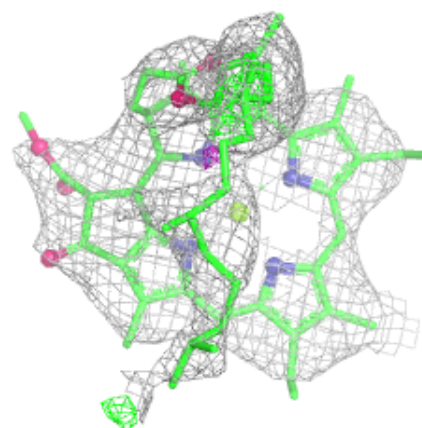
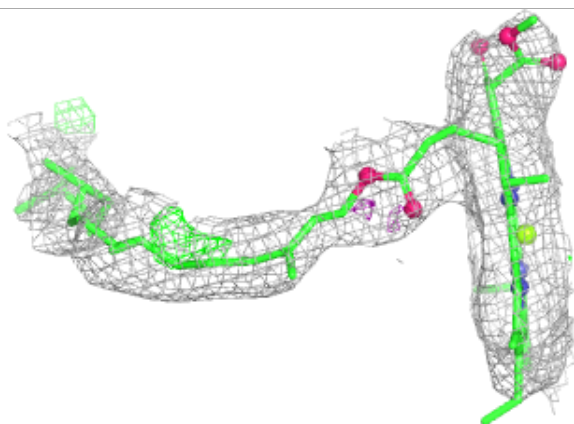
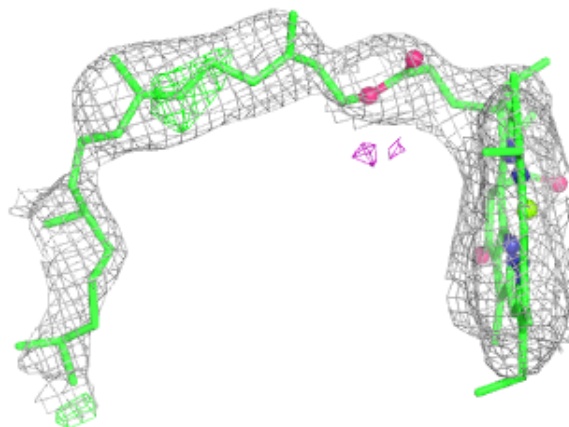
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





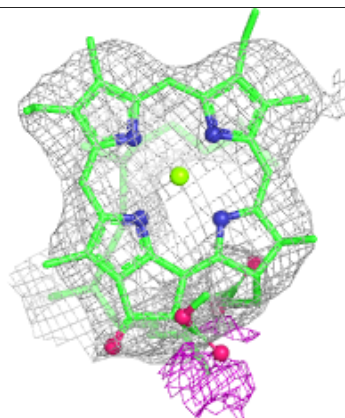
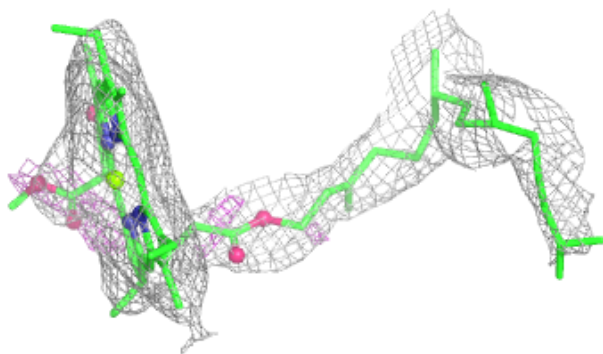
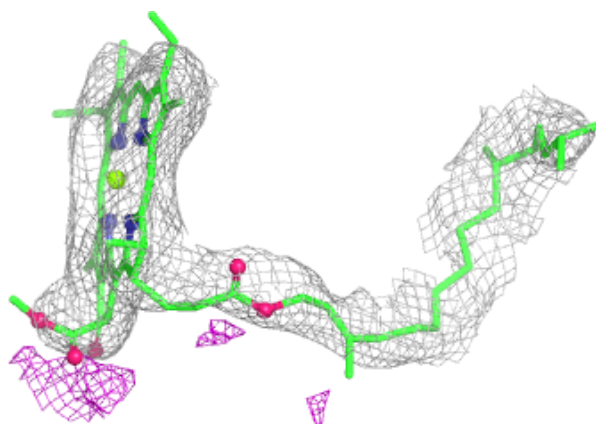
**Electron density around CLA B 516:**

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

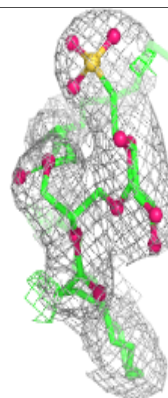
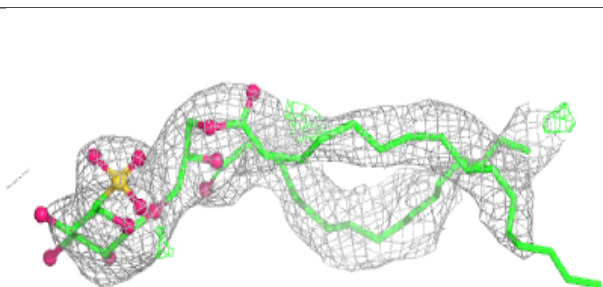
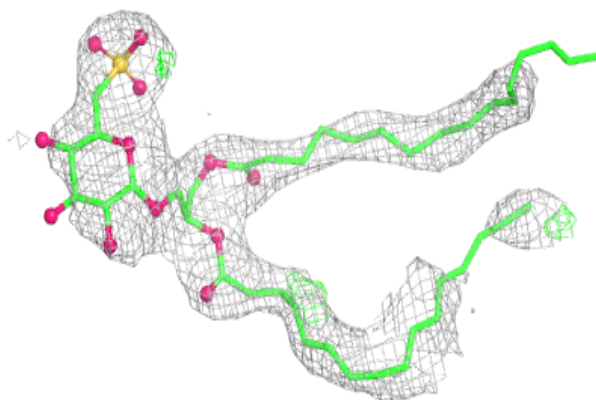


**Electron density around CLA C 496:**

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

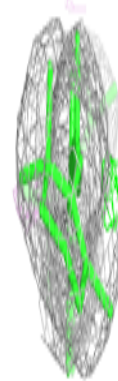
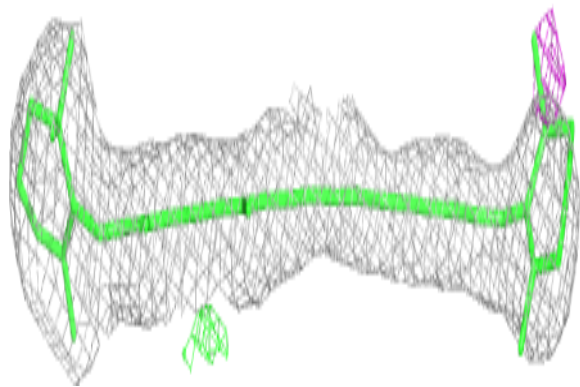
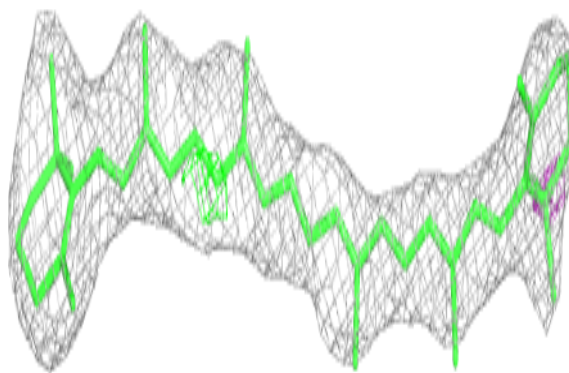
**Electron density around SQD A 568:**

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



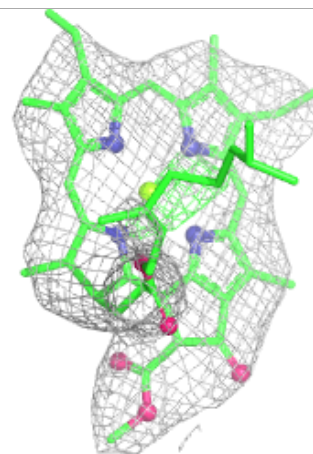
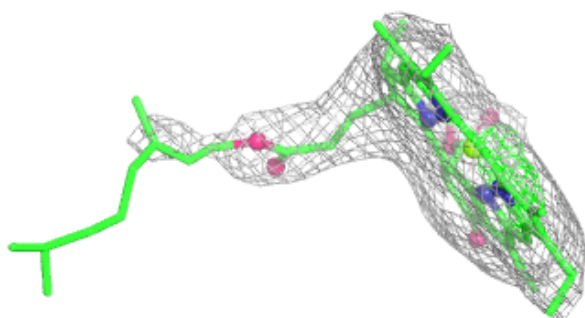
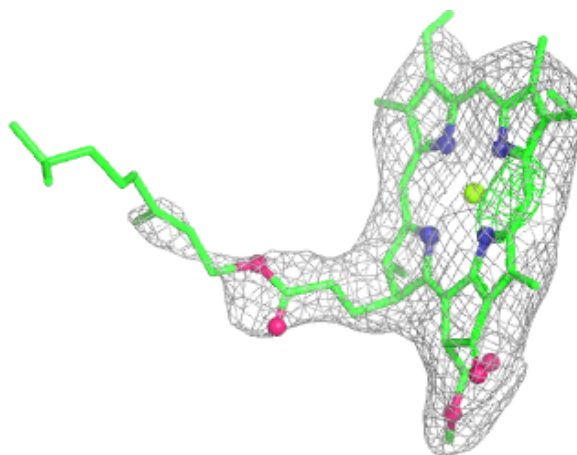
**Electron density around BCR B 528:**

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



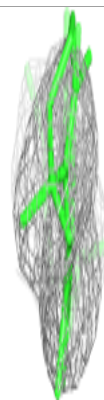
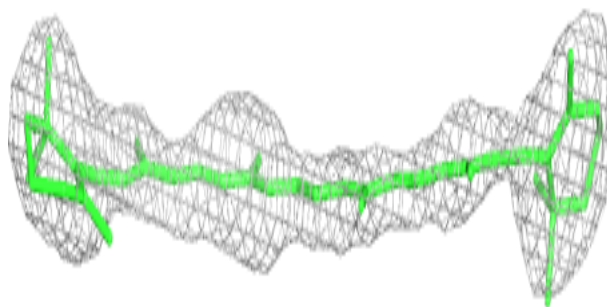
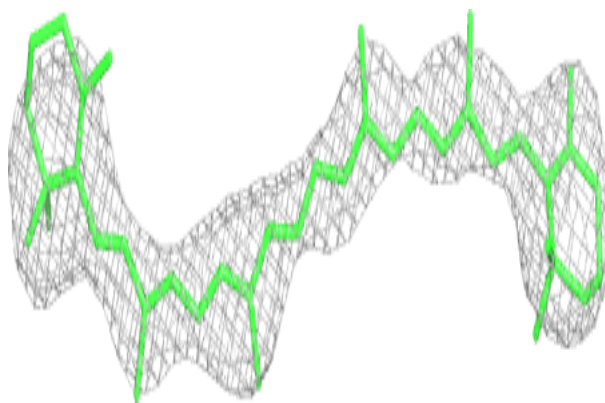
**Electron density around CLA a 5563:**

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

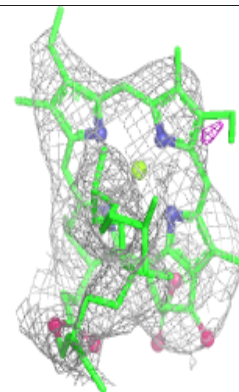
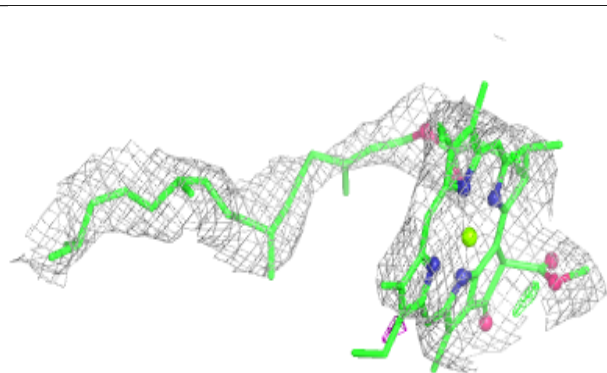
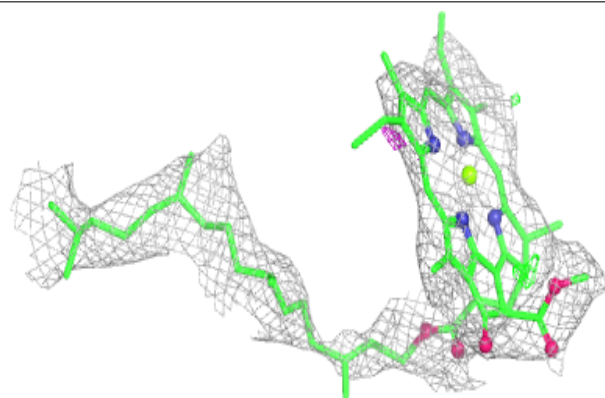


**Electron density around BCR X 130:**

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

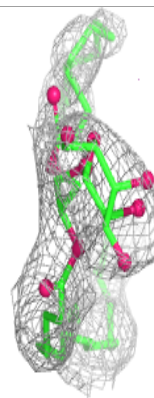
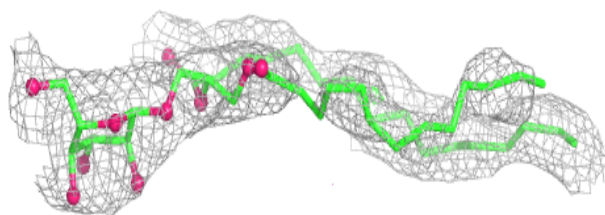
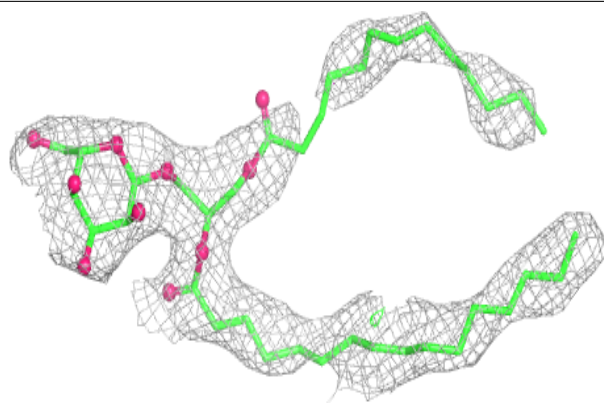
**Electron density around CLA c 5498:**

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



**Electron density around MGE i 5201:**

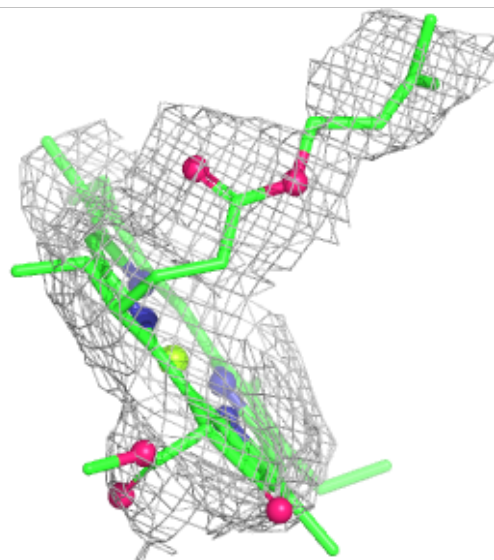
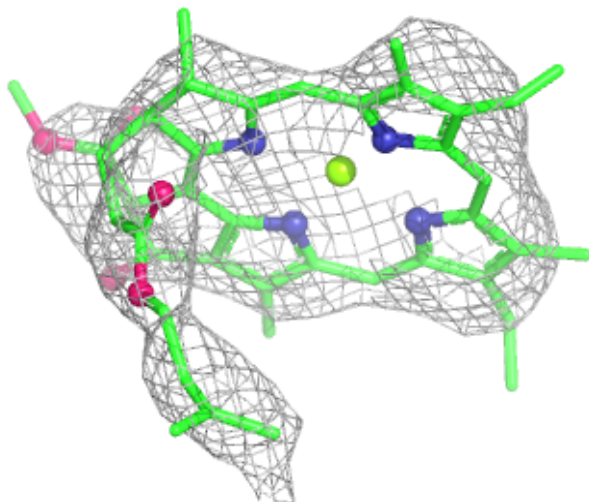
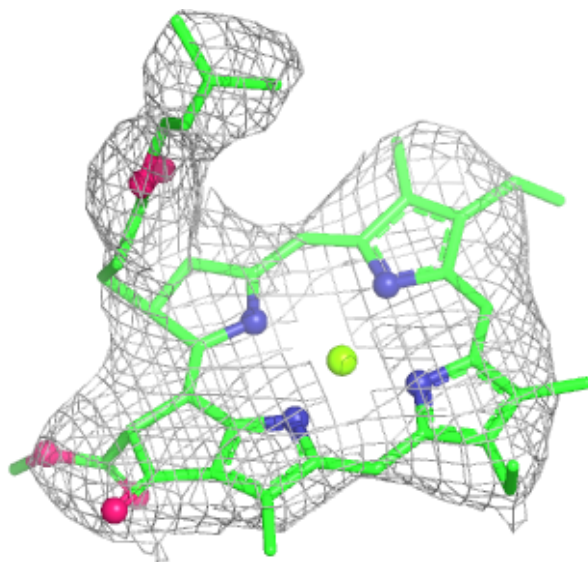
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





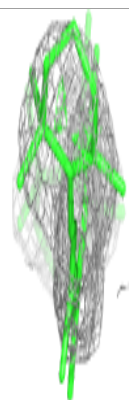
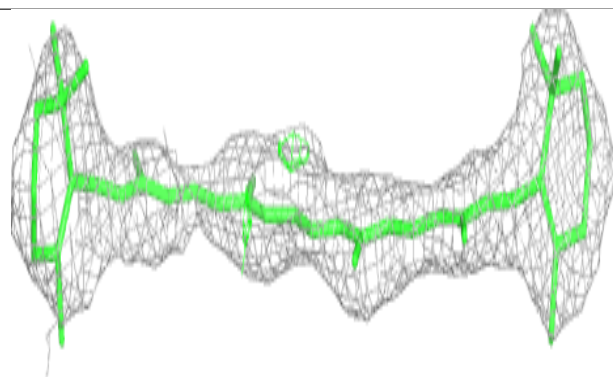
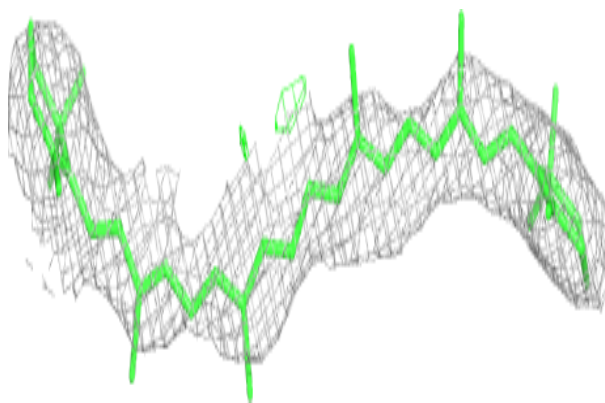
**Electron density around CLA c 5503:**

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



**Electron density around BCR h 5107:**

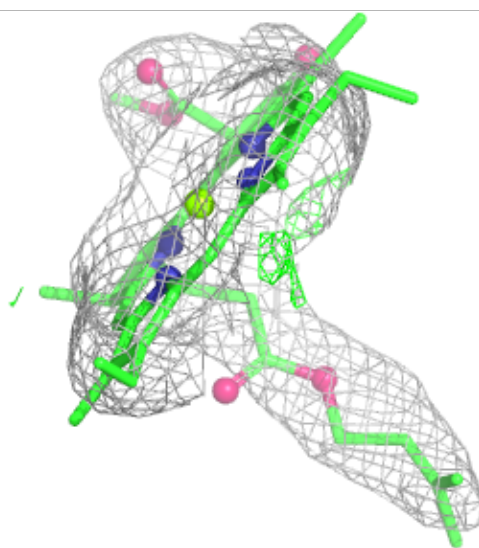
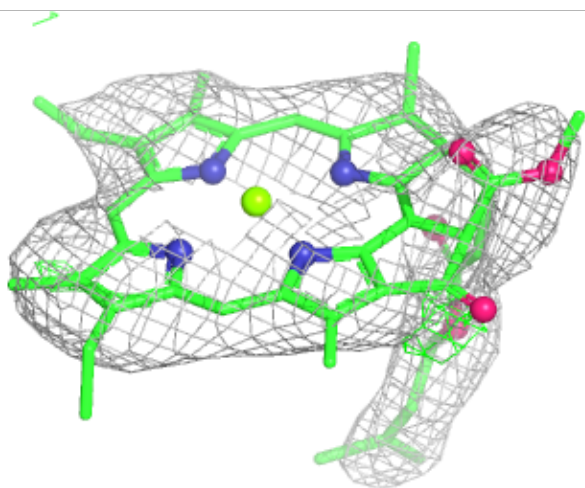
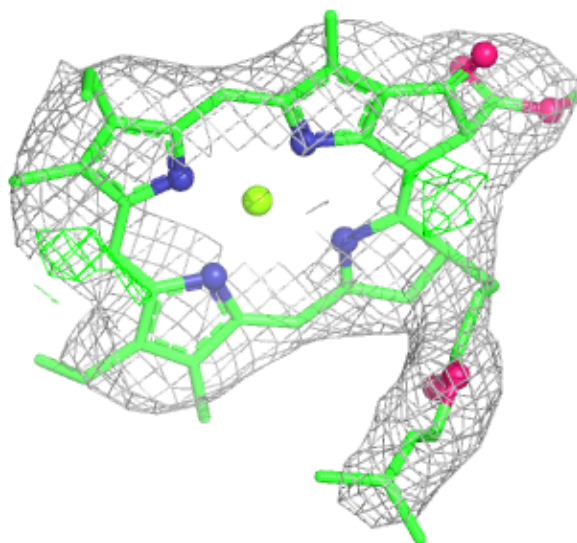
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





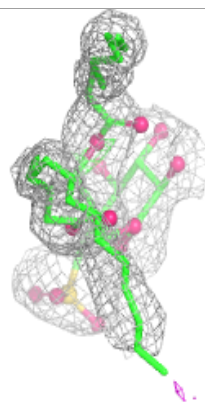
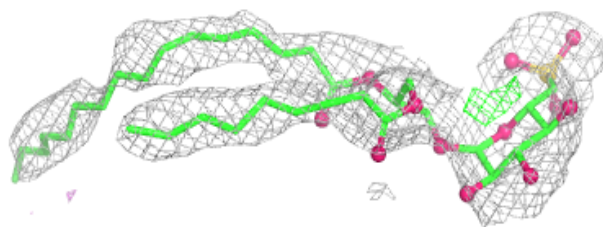
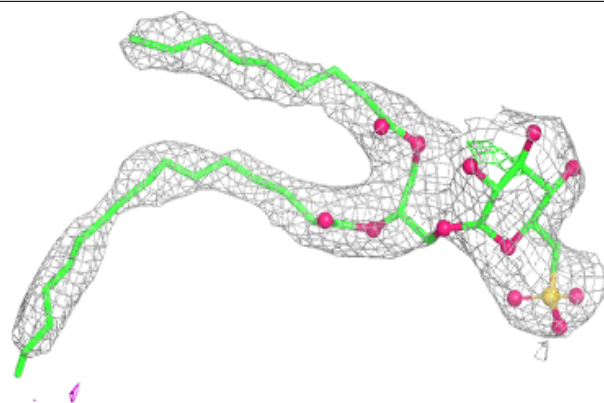
**Electron density around CLA C 503:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

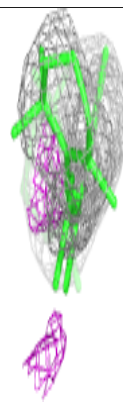
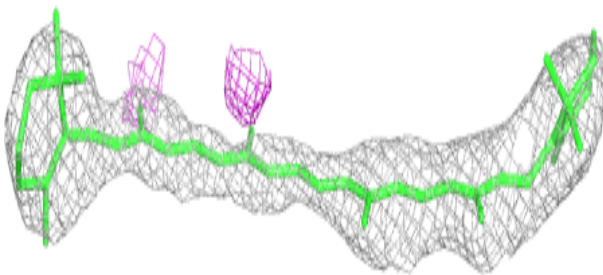
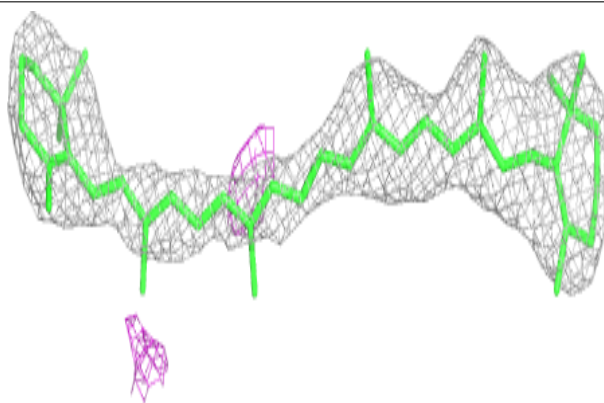


**Electron density around SQD t 213:**

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

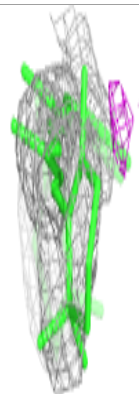
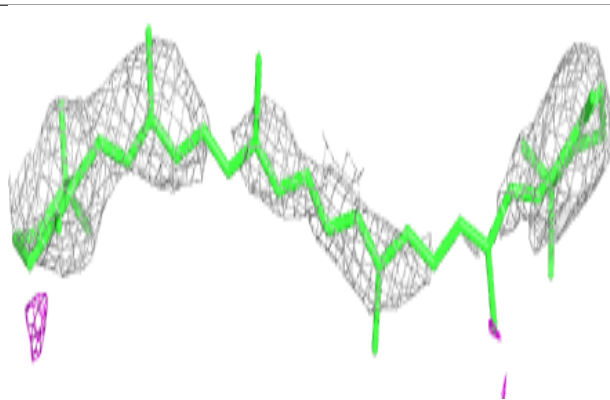
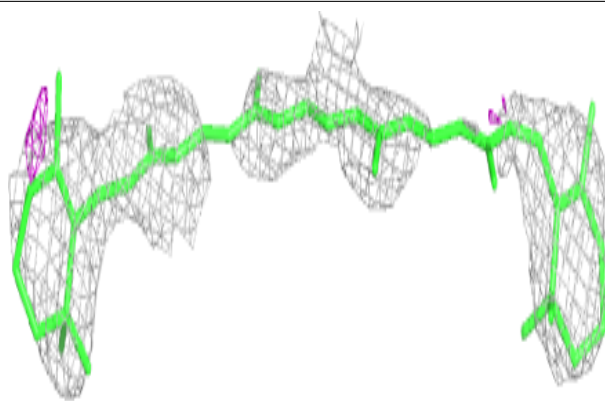
**Electron density around BCR b 5529:**

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



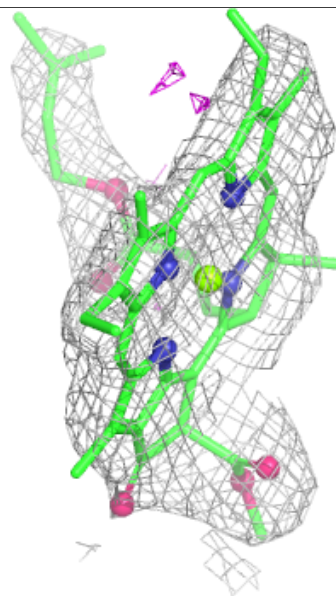
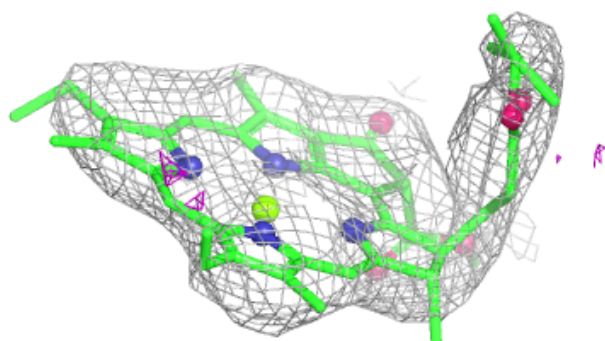
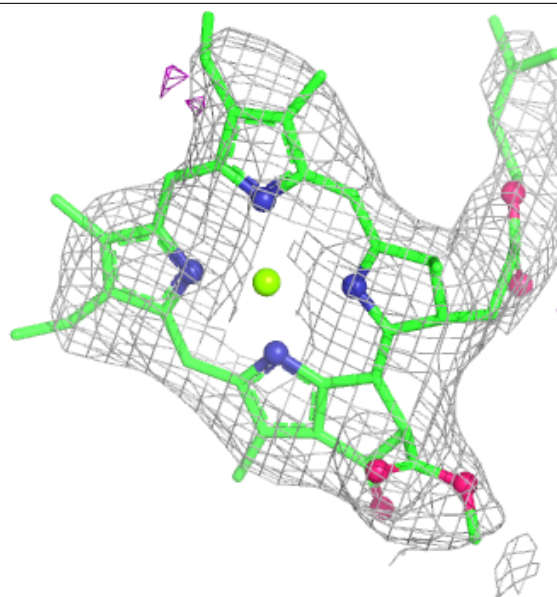
**Electron density around BCR c 5504:**

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



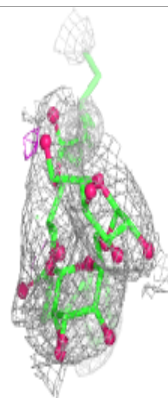
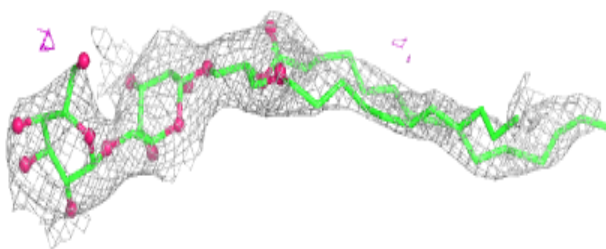
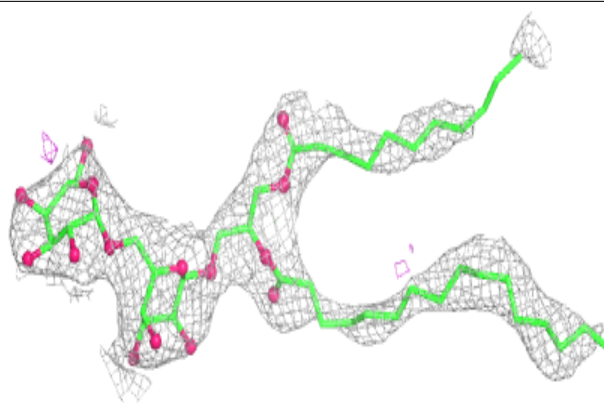
**Electron density around CLA d 5355:**

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

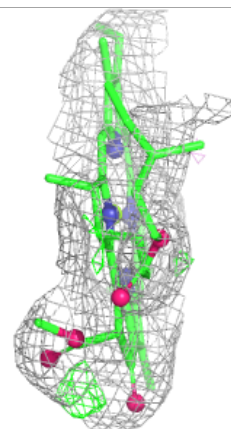
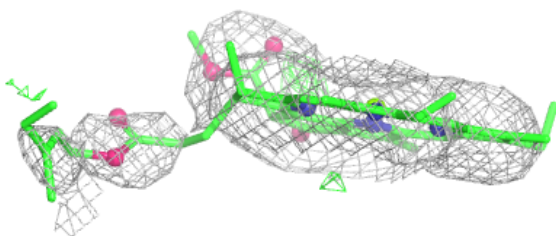
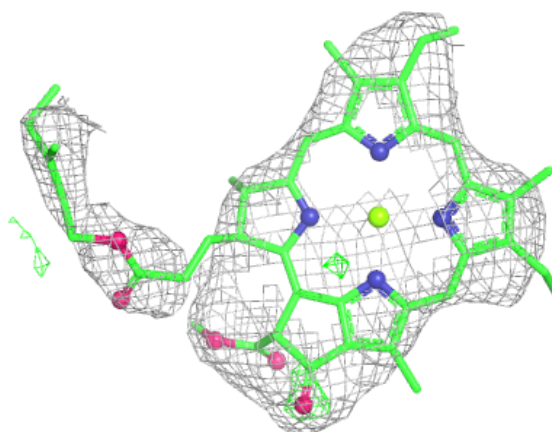


**Electron density around DGD c 5509:**

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

**Electron density around CLA c 5502:**

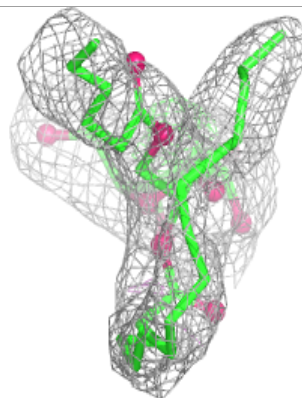
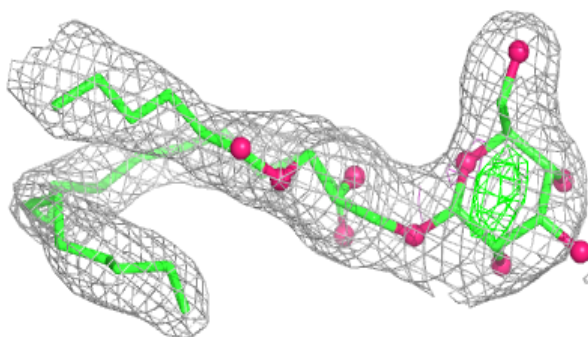
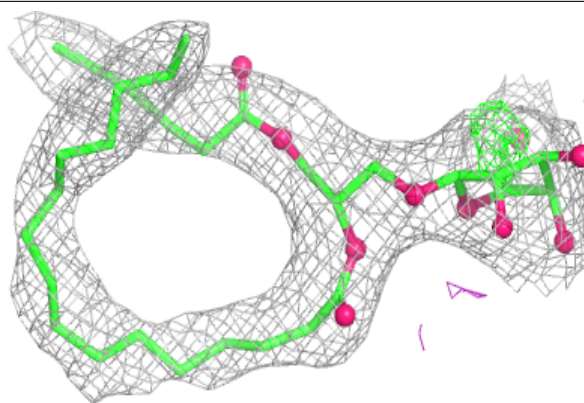
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



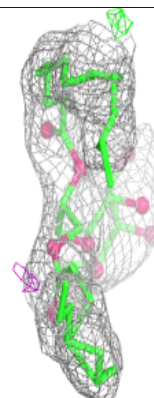
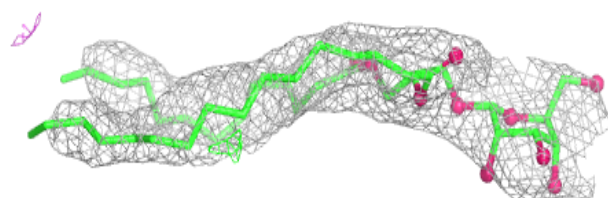
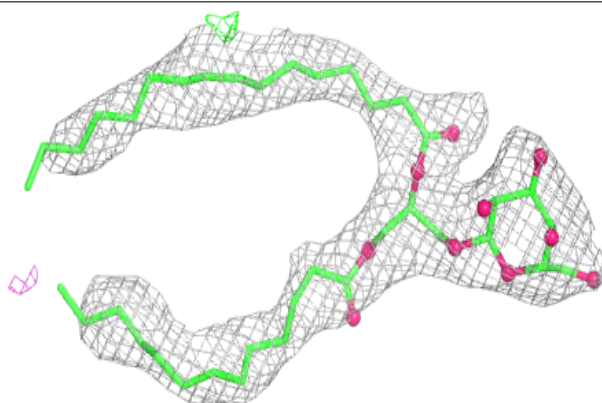


**Electron density around MGE D 359:**

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

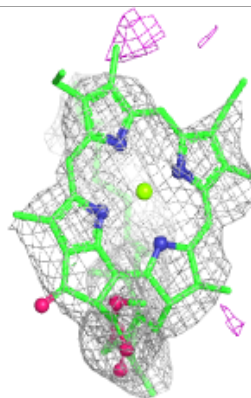
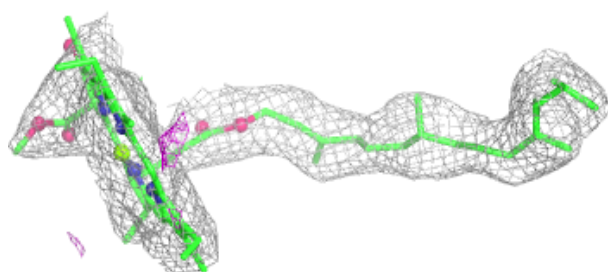
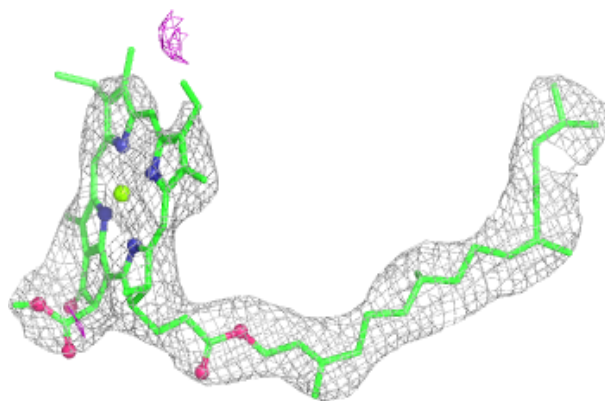
**Electron density around MGE I 201:**

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

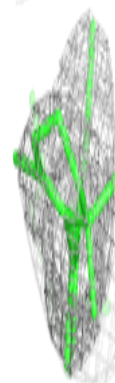
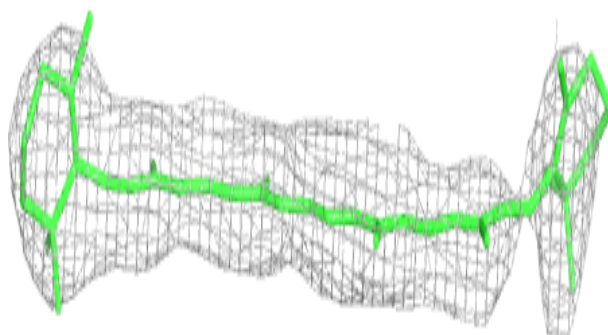
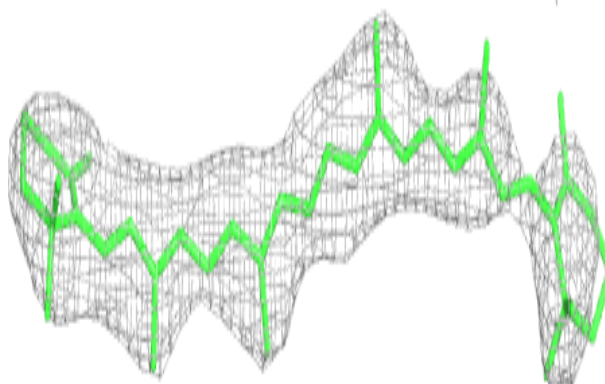


**Electron density around CLA B 519:**

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

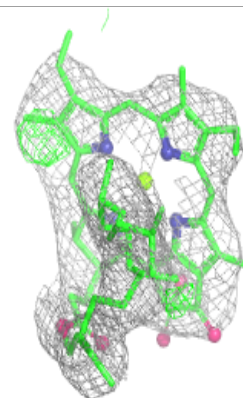
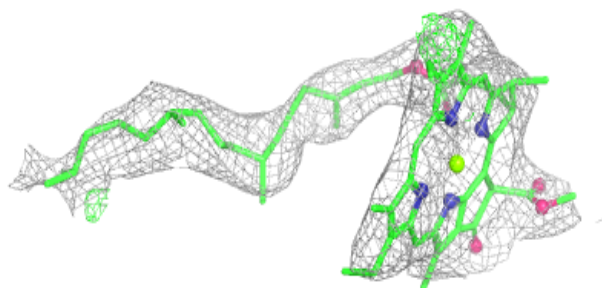
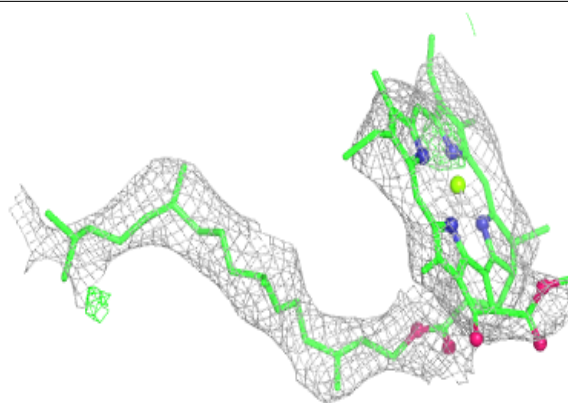
**Electron density around BCR C 506:**

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

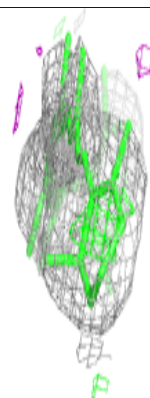
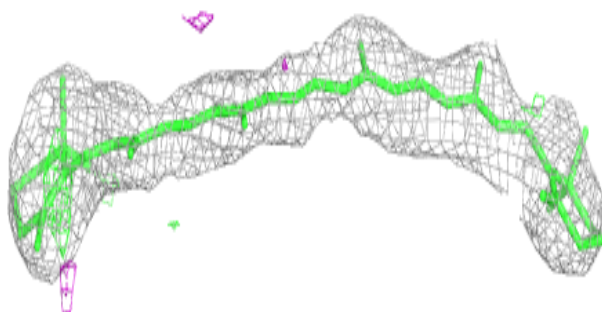
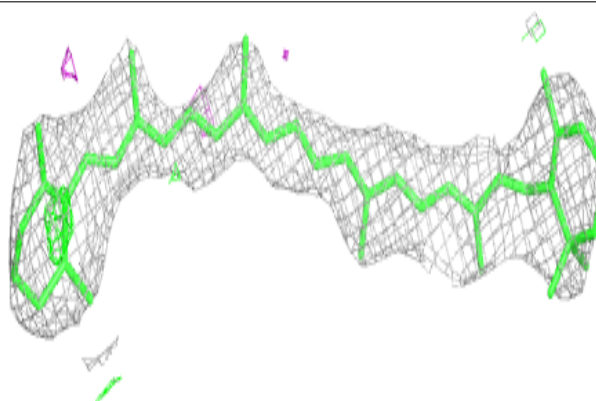


**Electron density around CLA C 498:**

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

**Electron density around BCR T 5104:**

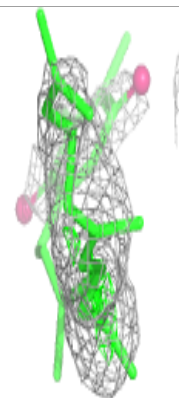
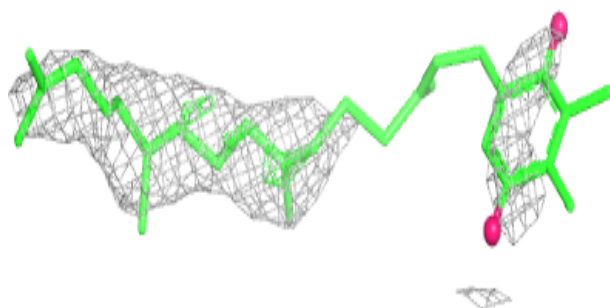
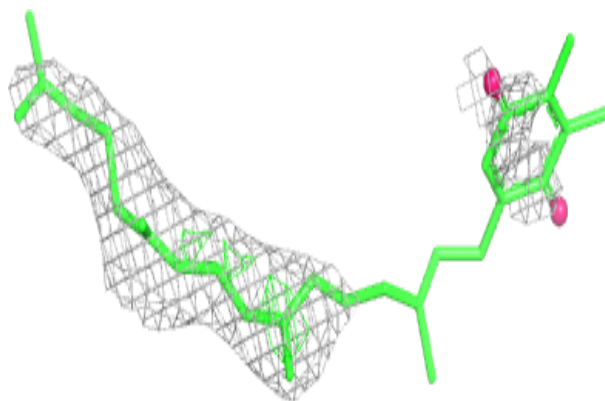
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



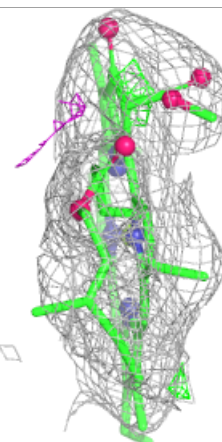
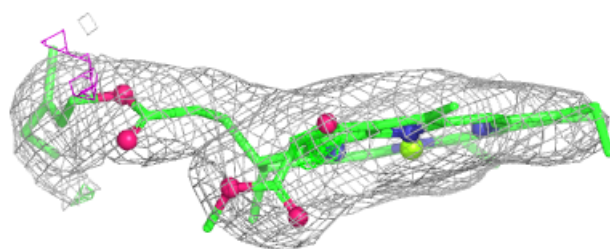
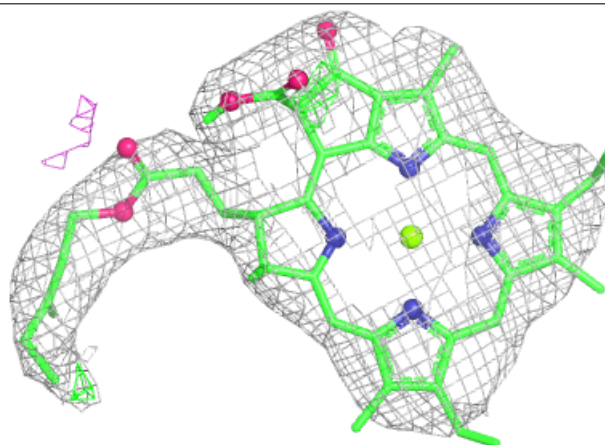


**Electron density around PQ9 a 5564:**

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

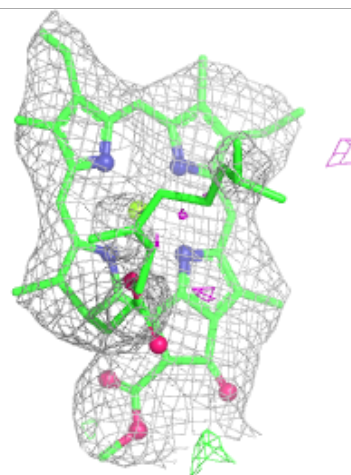
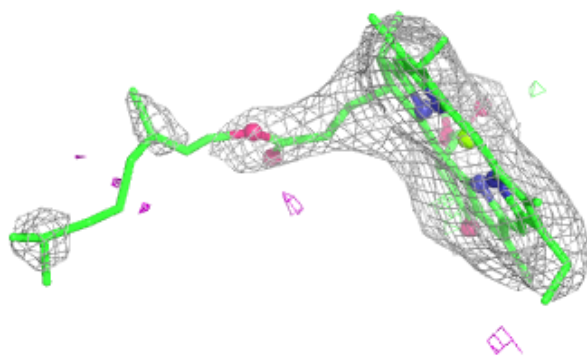
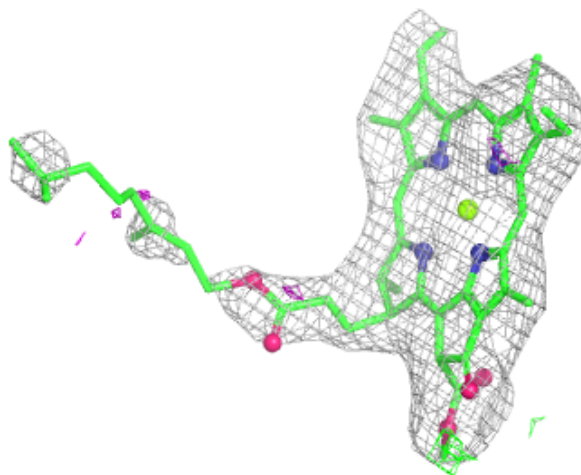
**Electron density around CLA C 502:**

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



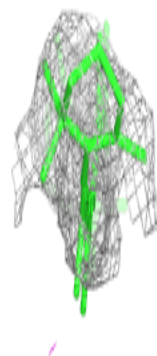
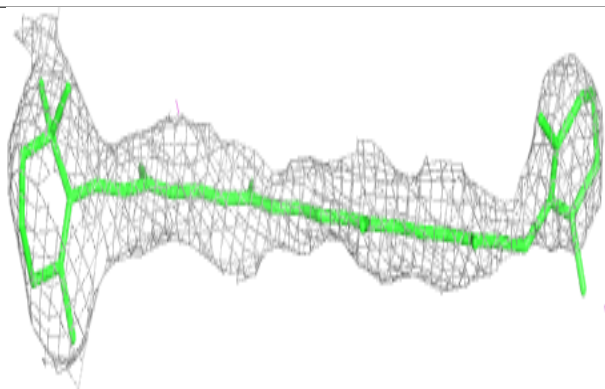
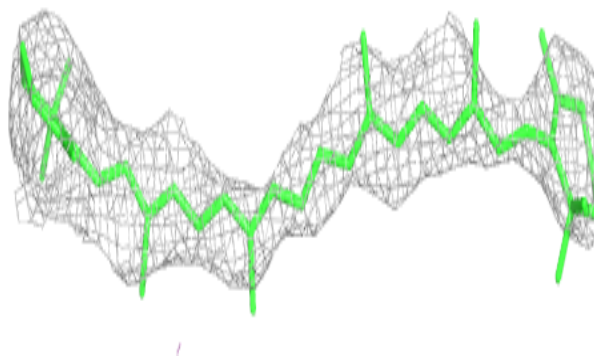
**Electron density around CLA A 563:**

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

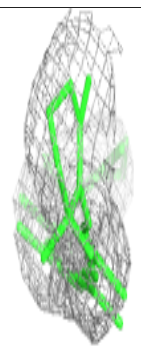
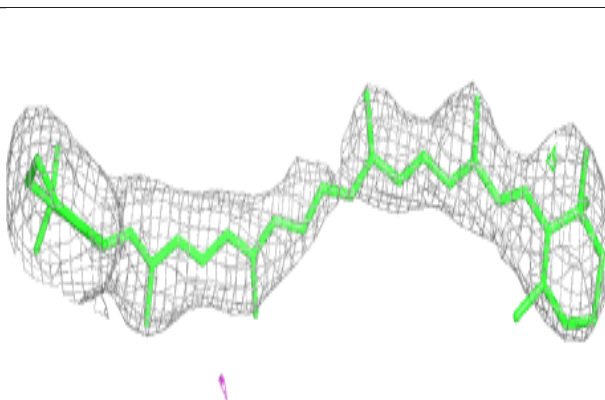
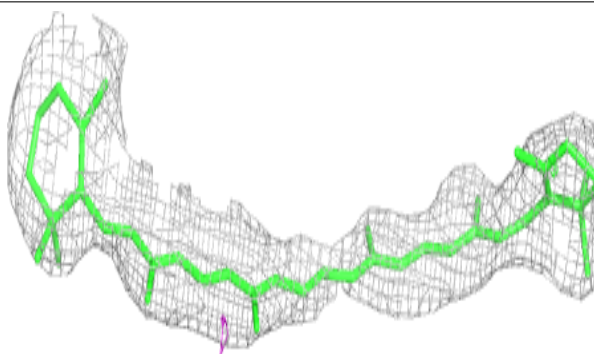


**Electron density around BCR c 5505:**

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

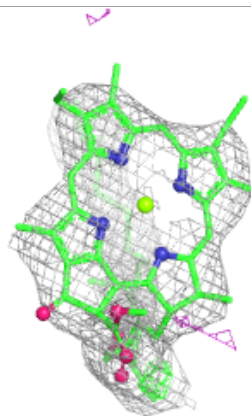
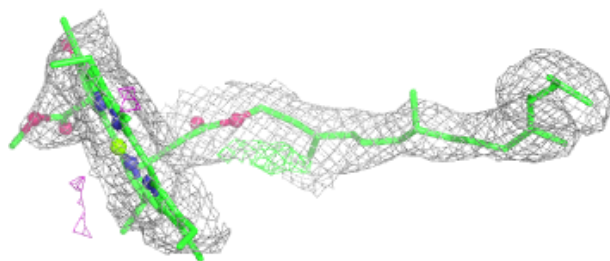
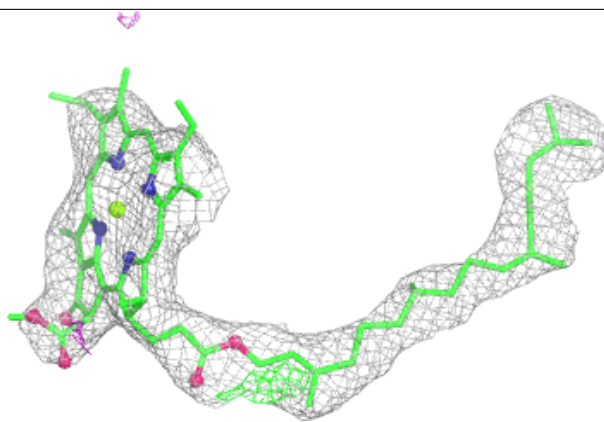
**Electron density around BCR D 357:**

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



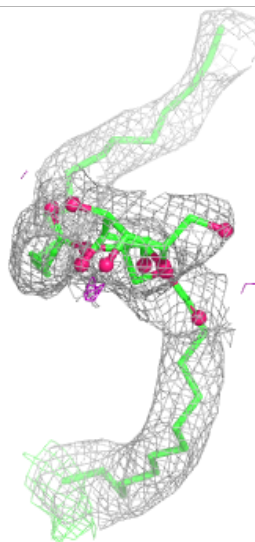
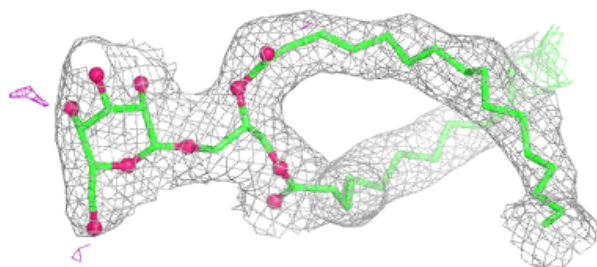
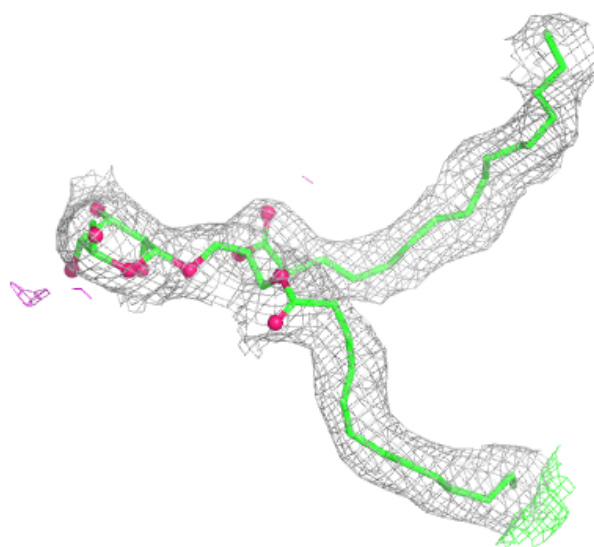
**Electron density around CLA b 5519:**

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



**Electron density around MGE B 530:**

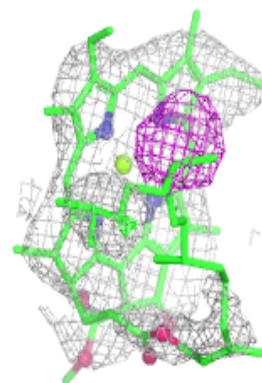
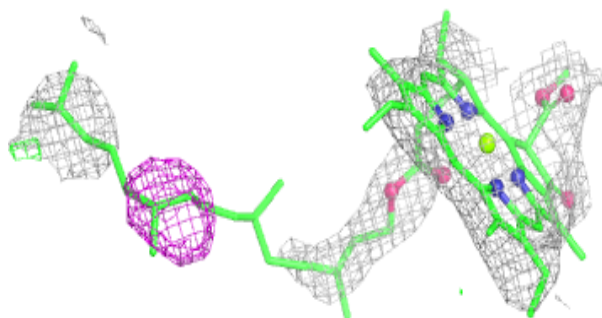
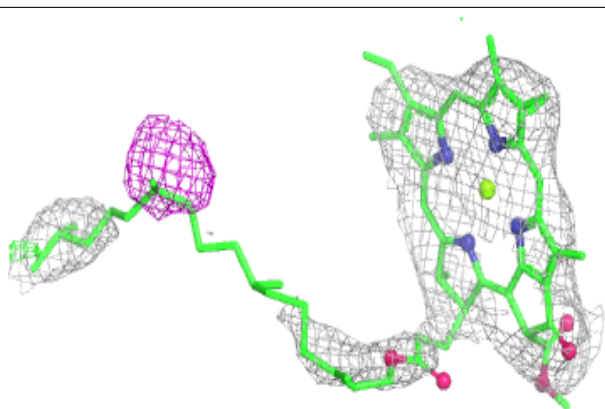
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



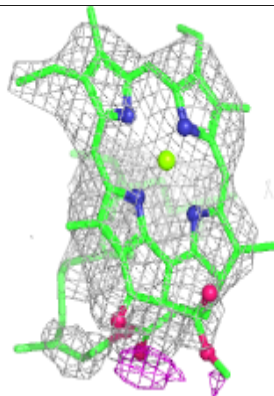
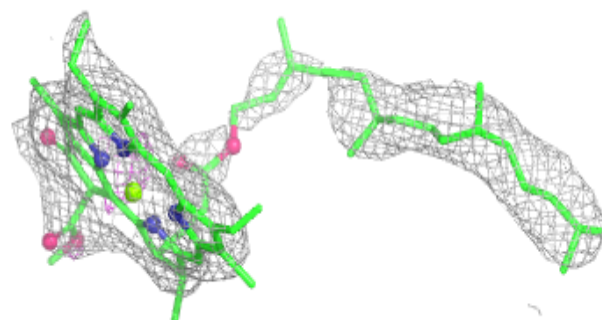
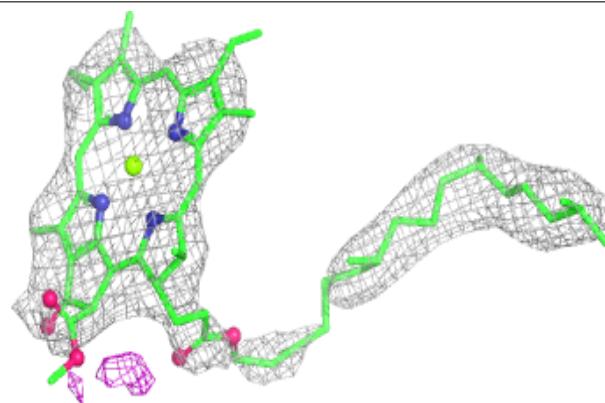


**Electron density around CLA c 5501:**

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

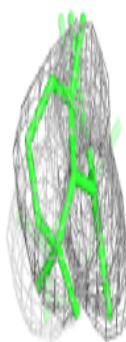
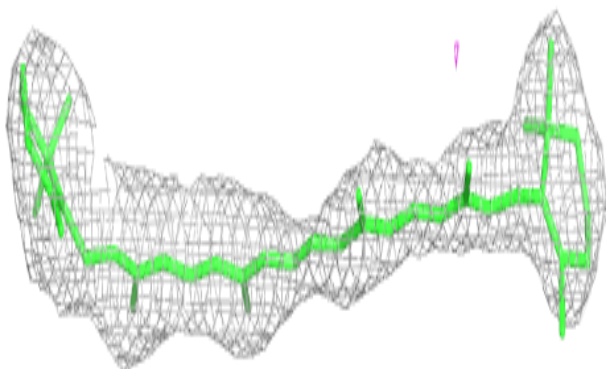
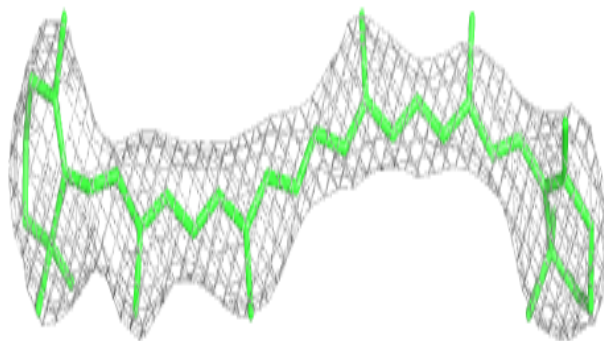
**Electron density around CLA C 501:**

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



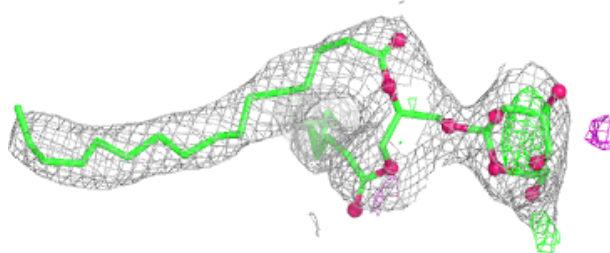
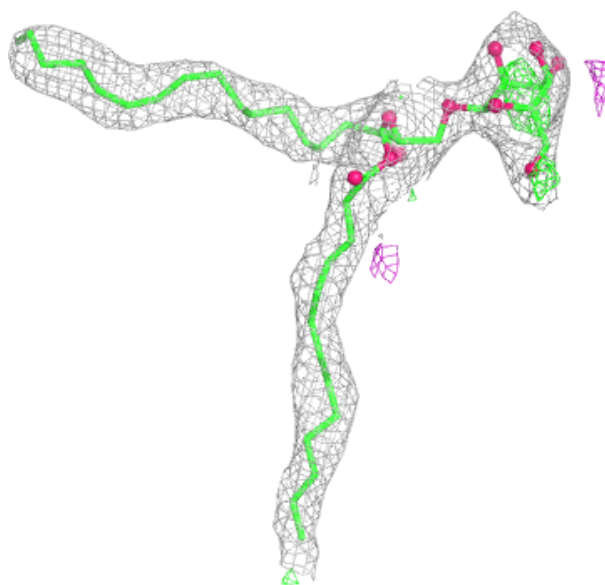
**Electron density around BCR B 529:**

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



**Electron density around MGE L 210:**

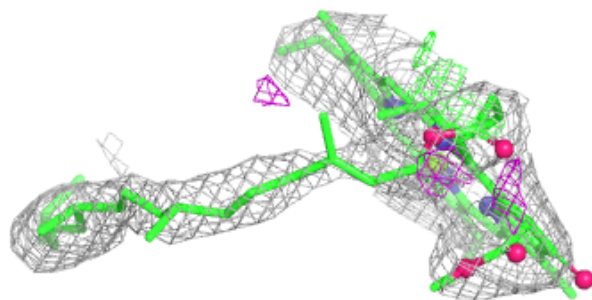
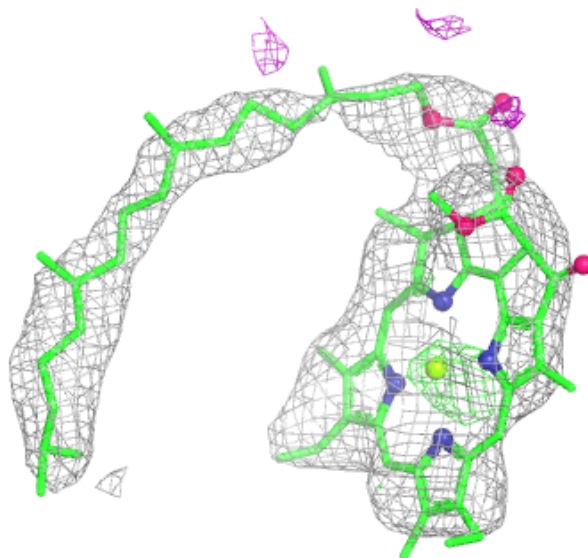
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





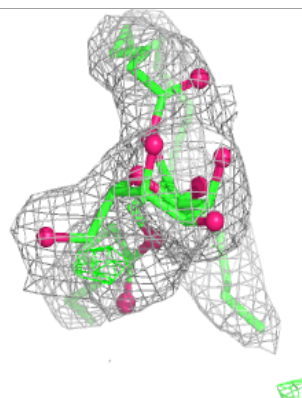
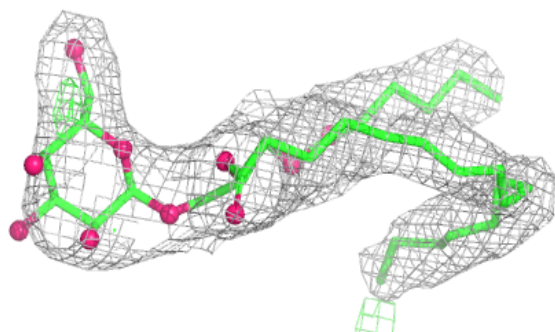
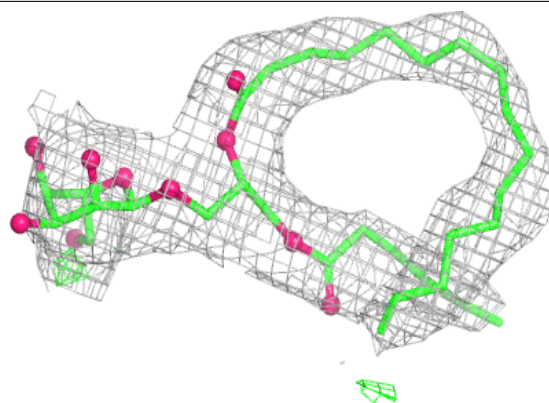
**Electron density around CLA C 497:**

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

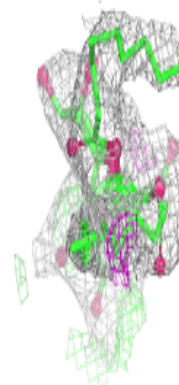
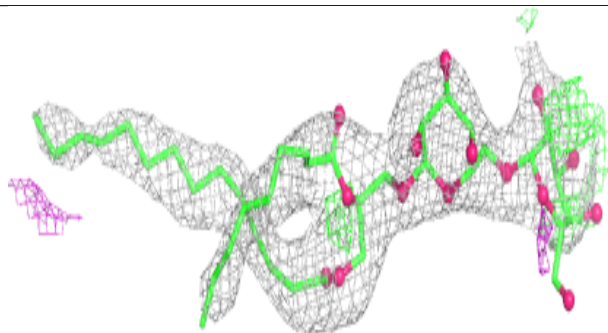
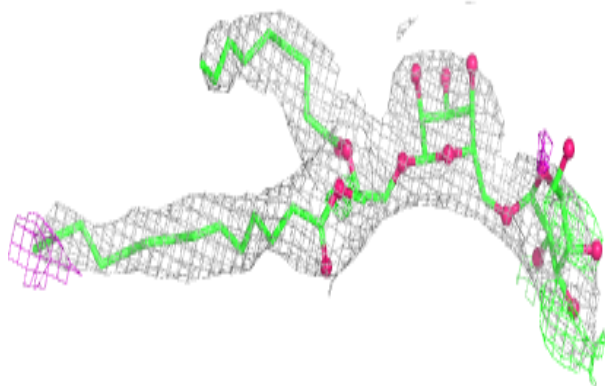


**Electron density around MGE d 5360:**

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

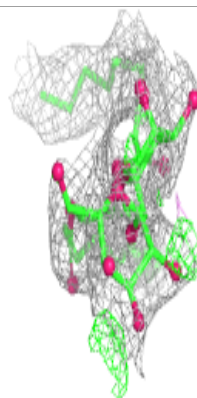
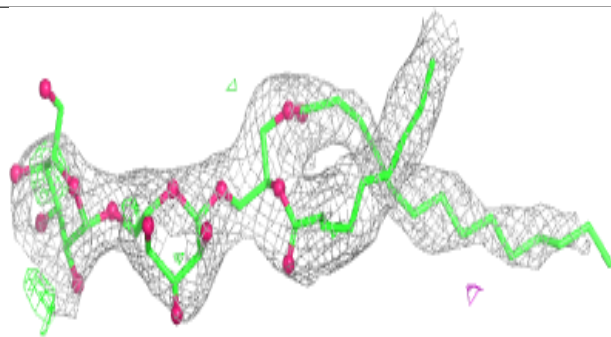
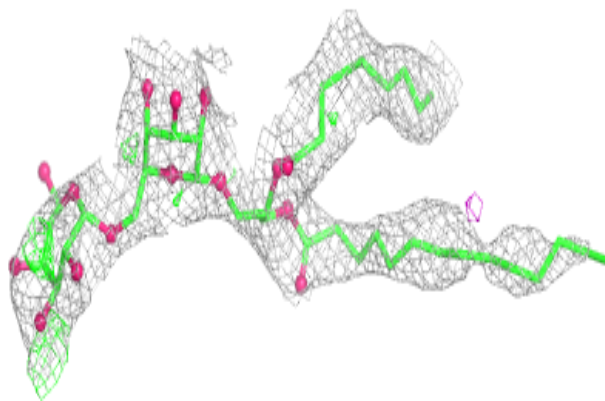
**Electron density around DGD C 507:**

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



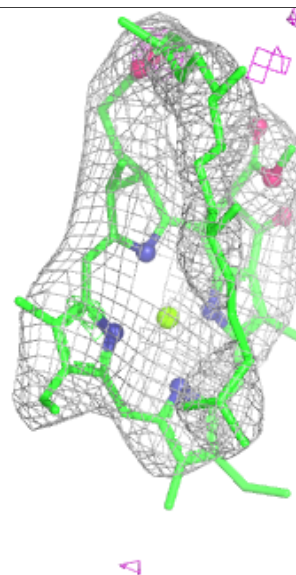
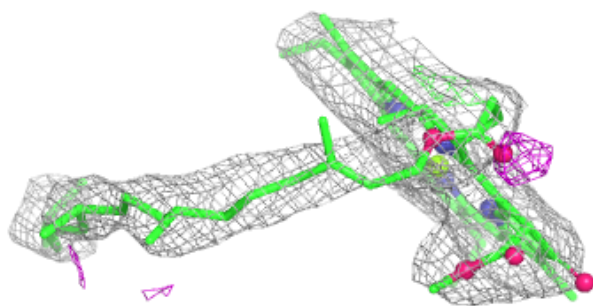
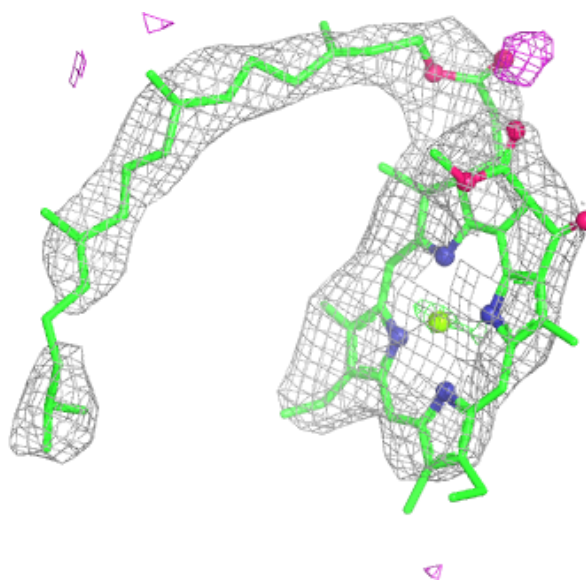
**Electron density around DGD c 5507:**

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



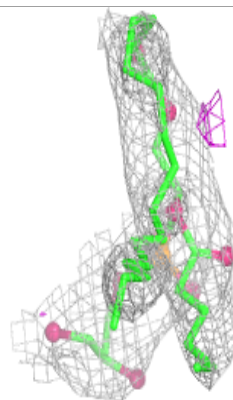
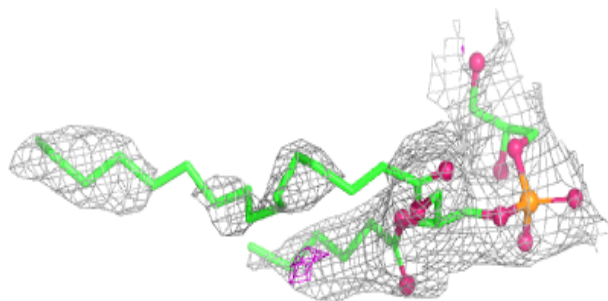
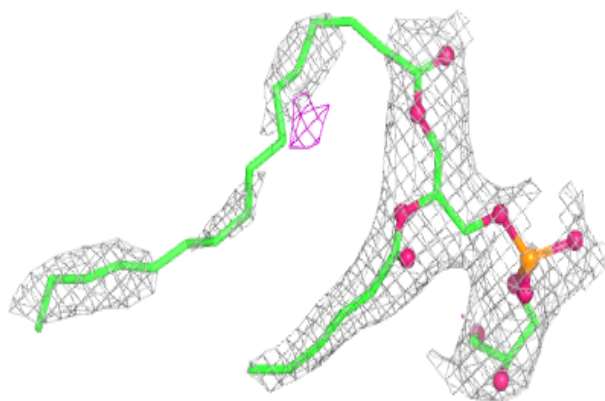
**Electron density around CLA c 5497:**

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



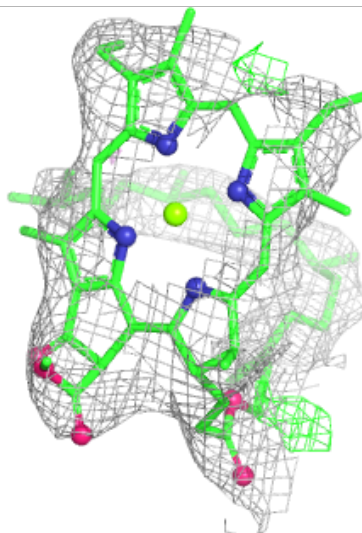
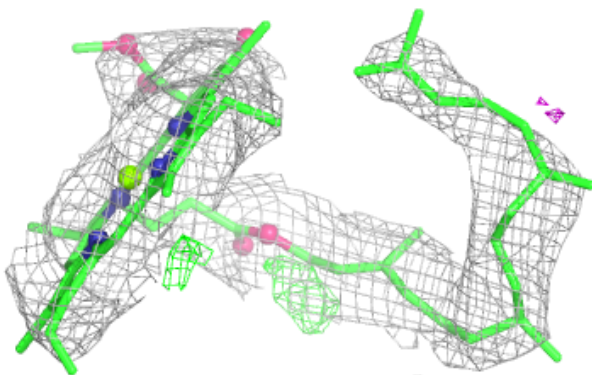
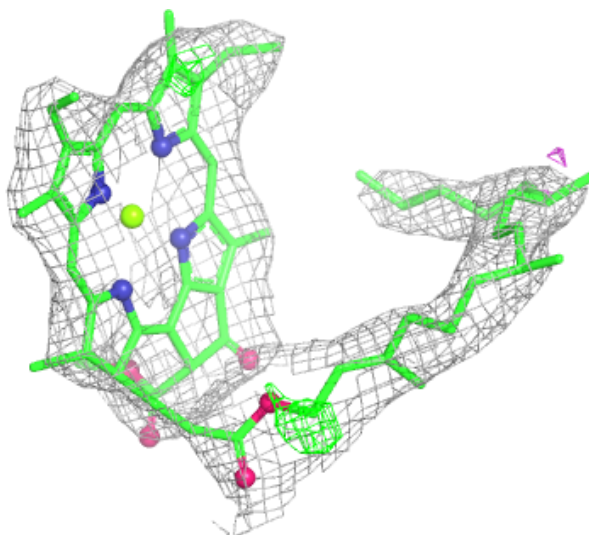
**Electron density around LHG a 5567:**

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



**Electron density around CLA c 5493:**

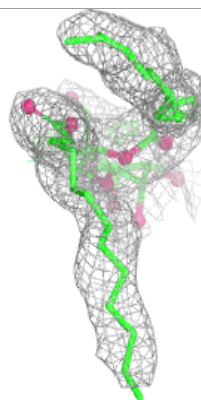
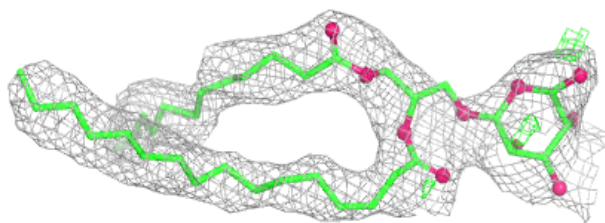
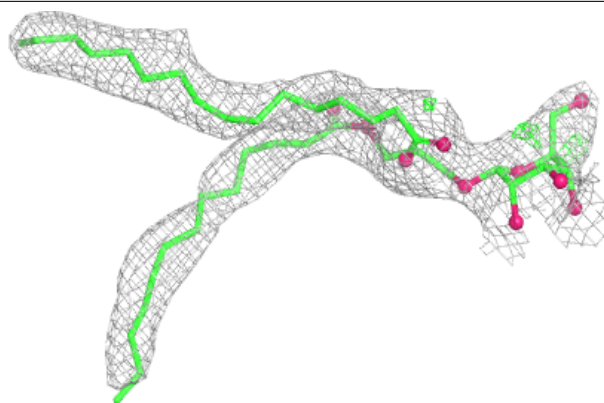
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



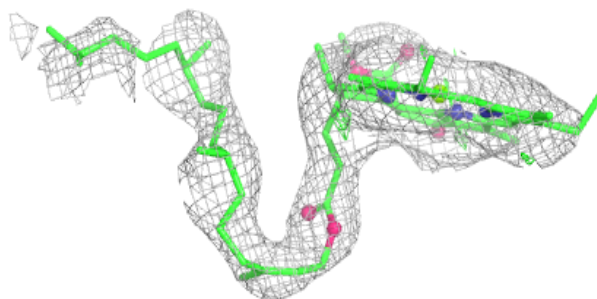
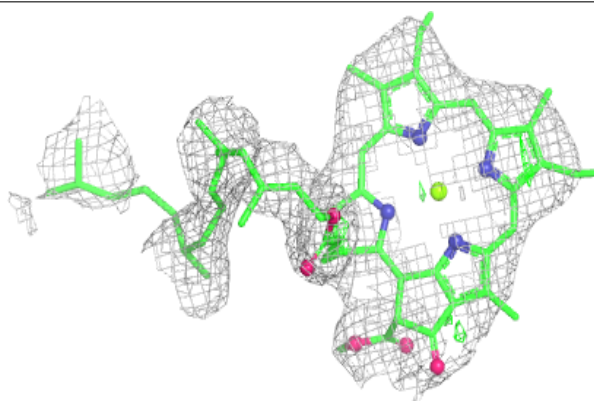


**Electron density around MGE d 5361:**

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

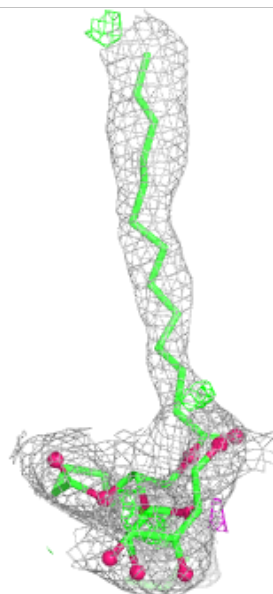
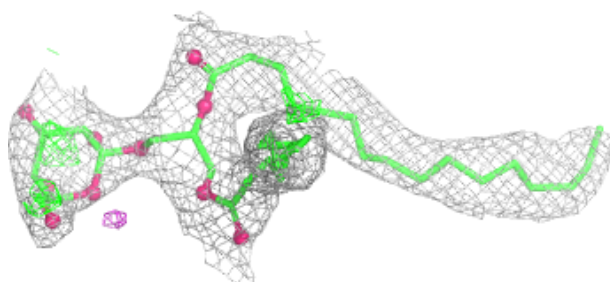
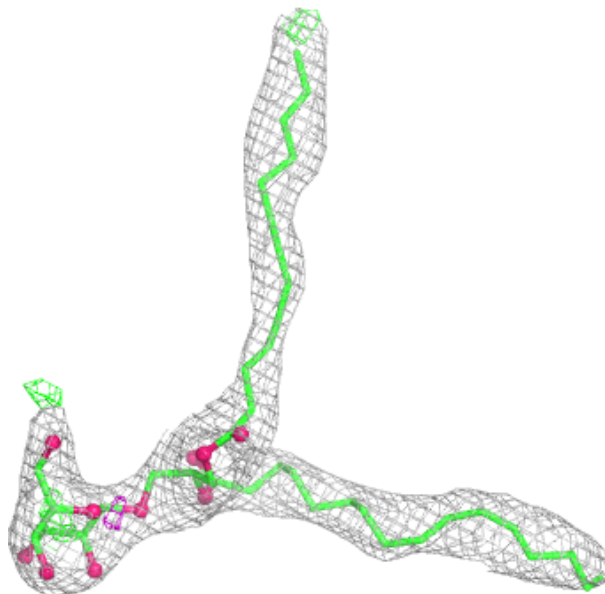
**Electron density around CLA a 5560:**

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



**Electron density around MGE 1 5210:**

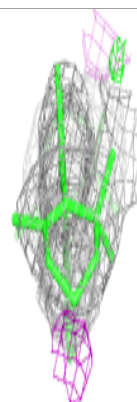
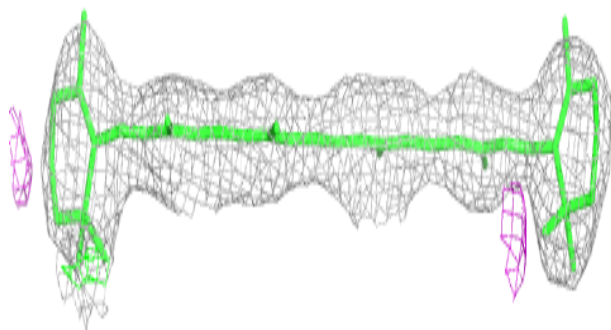
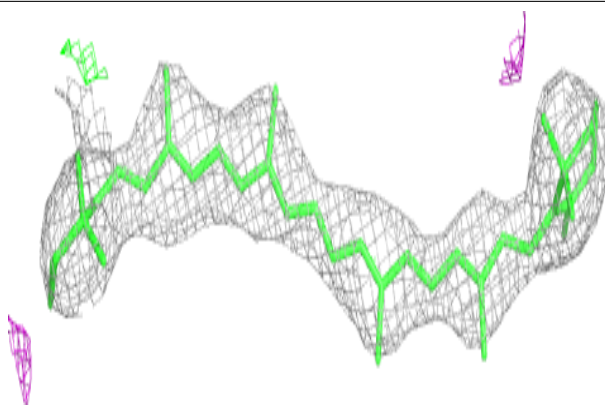
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





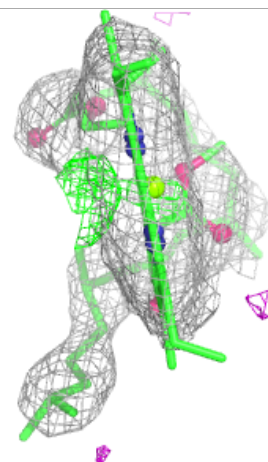
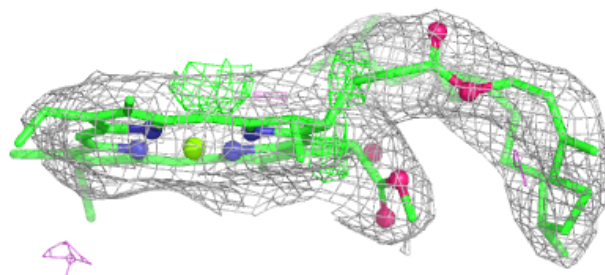
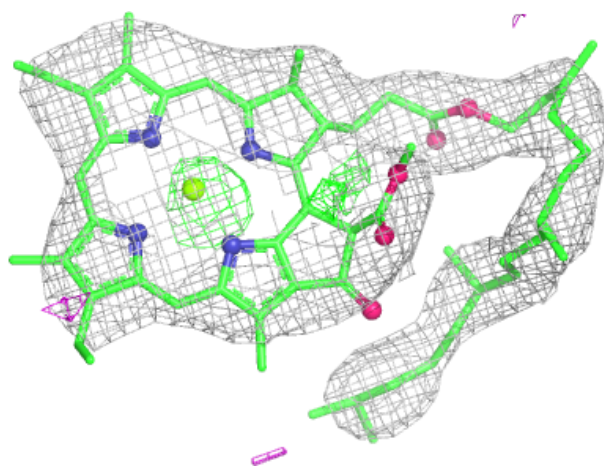
**Electron density around BCR a 5566:**

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



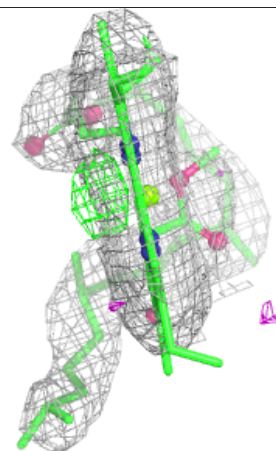
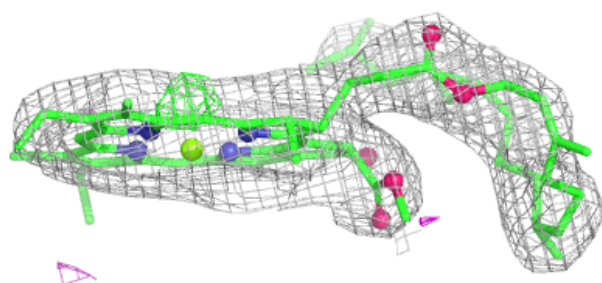
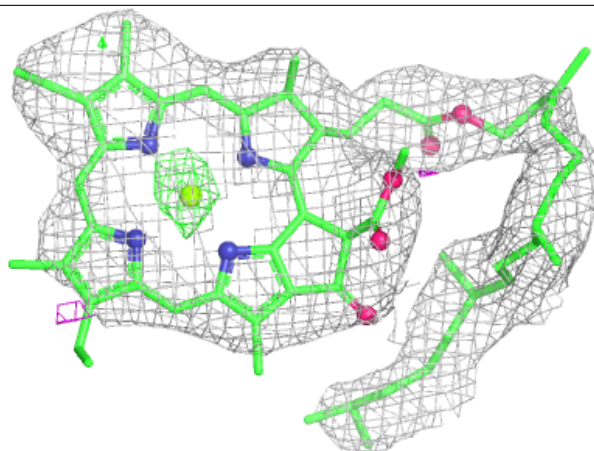
**Electron density around CLA b 5520:**

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

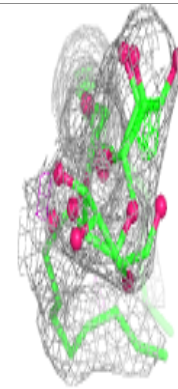
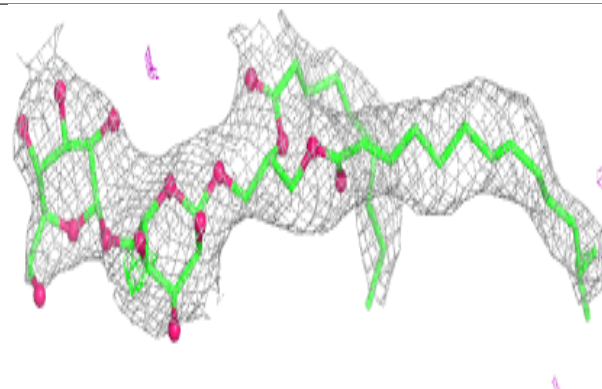


**Electron density around CLA B 520:**

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

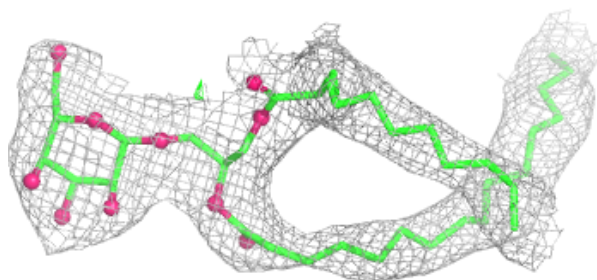
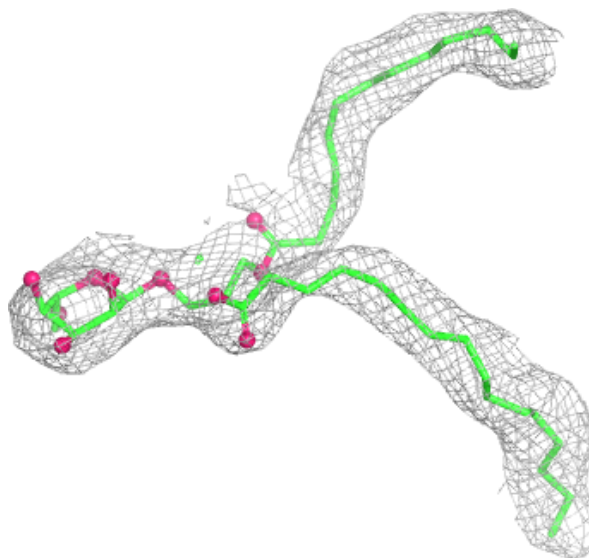
**Electron density around DGD H 208:**

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



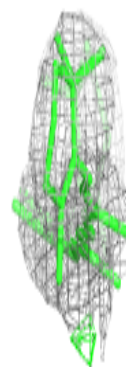
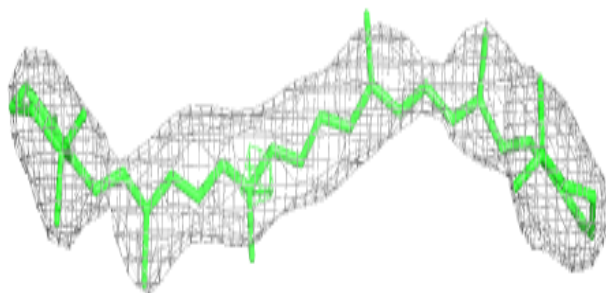
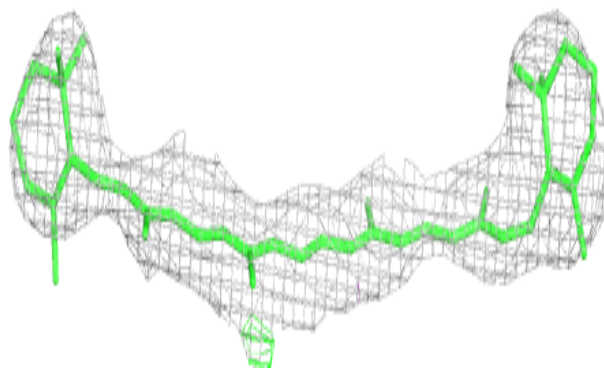
**Electron density around MGE b 5530:**

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

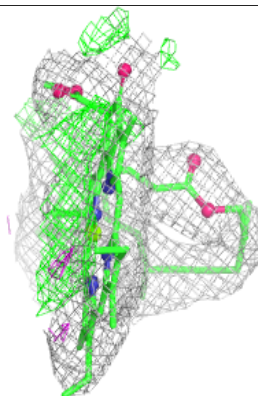
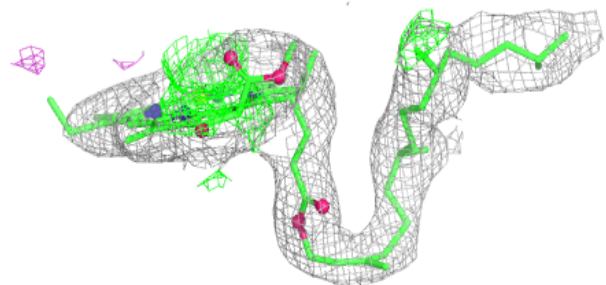
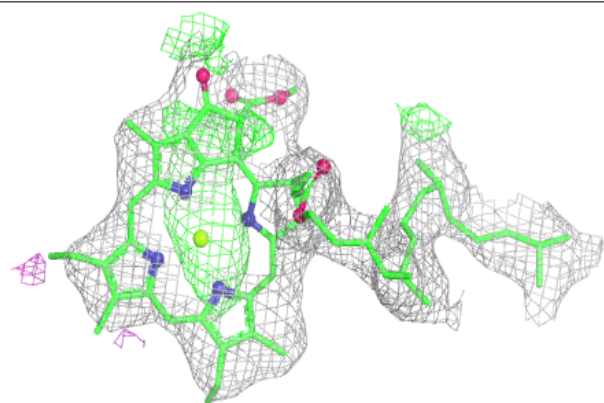


**Electron density around BCR C 504:**

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

**Electron density around CLA A 560:**

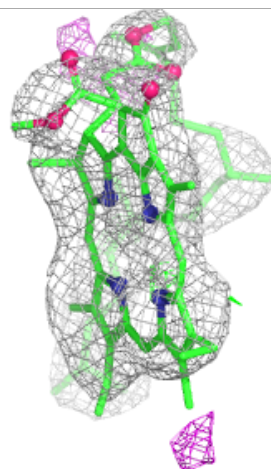
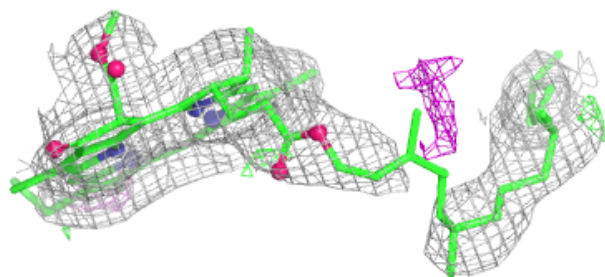
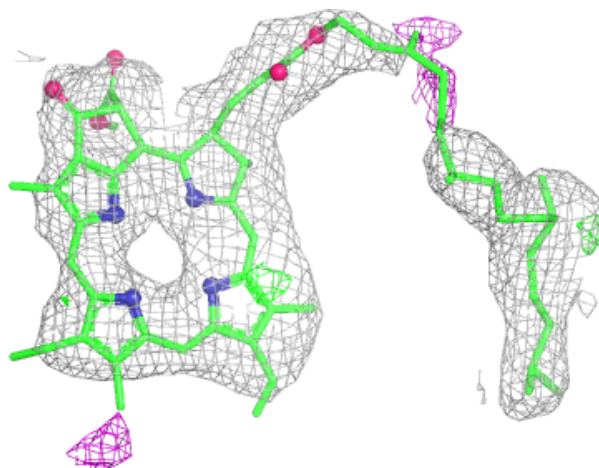
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





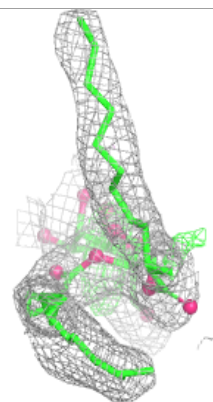
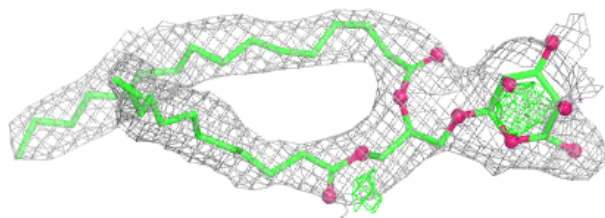
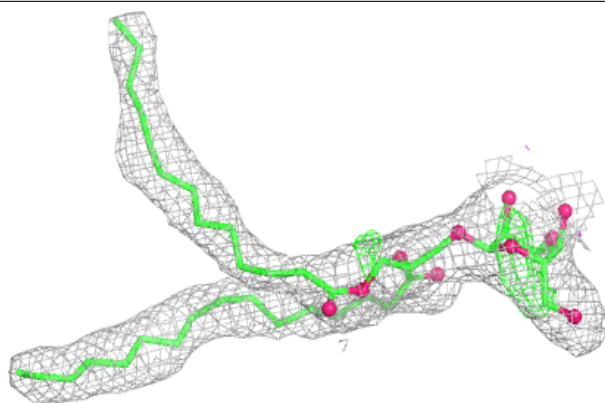
**Electron density around PHO a 5562:**

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

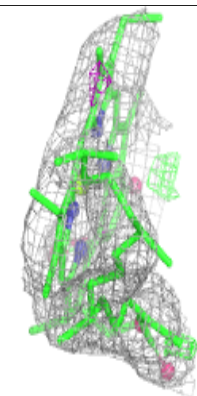
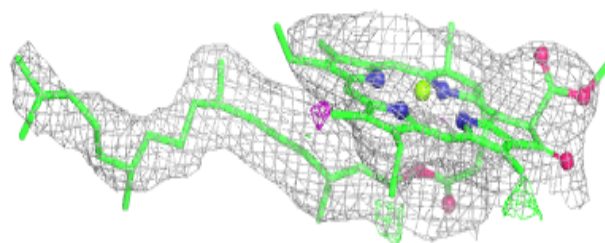
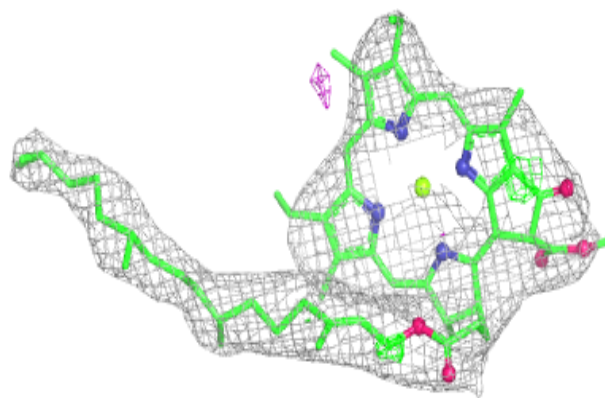


**Electron density around MGE D 360:**

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

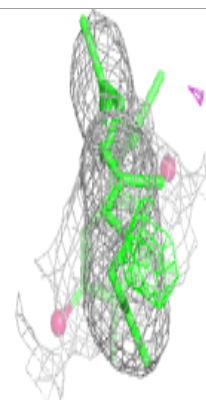
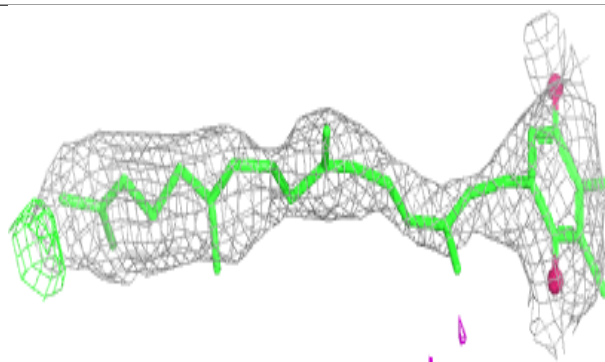
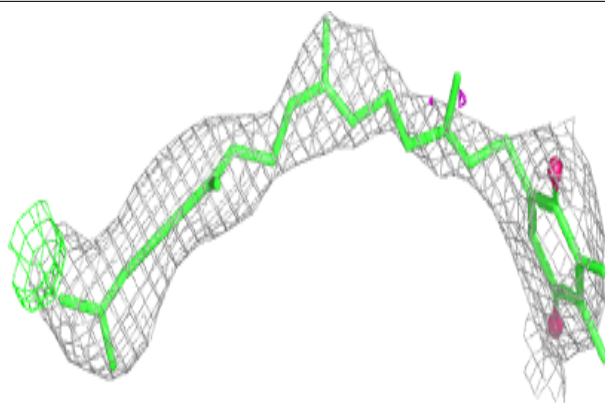
**Electron density around CLA c 5491:**

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

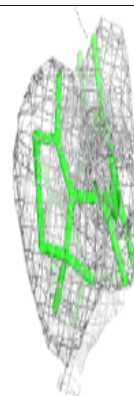
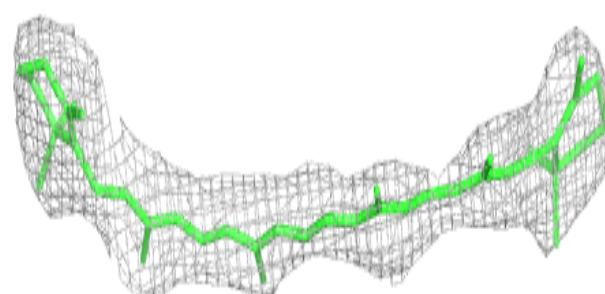
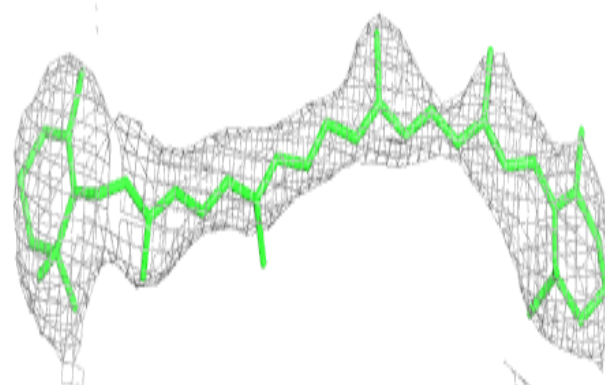


**Electron density around PQ9 D 356:**

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

**Electron density around BCR t 104:**

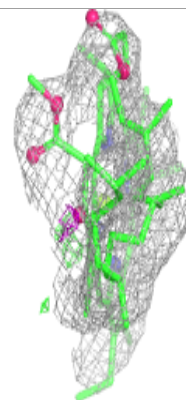
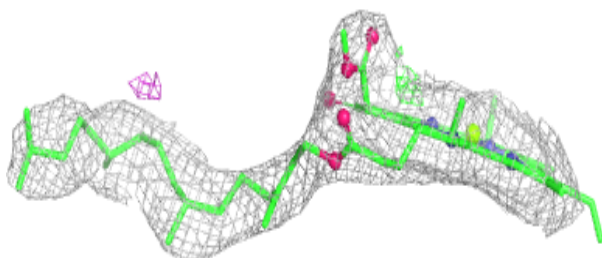
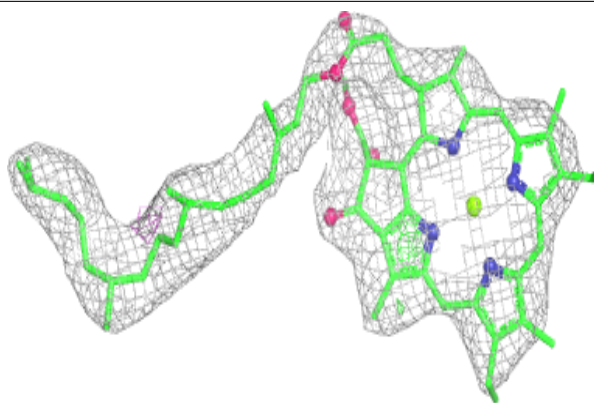
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



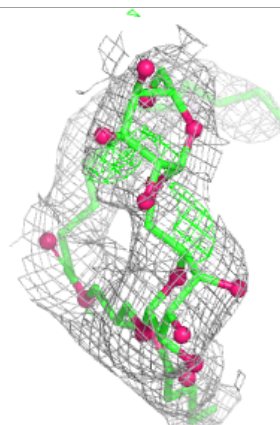
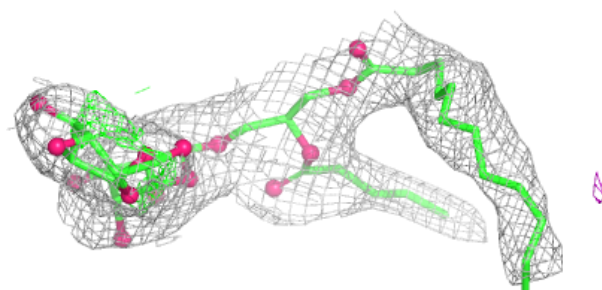
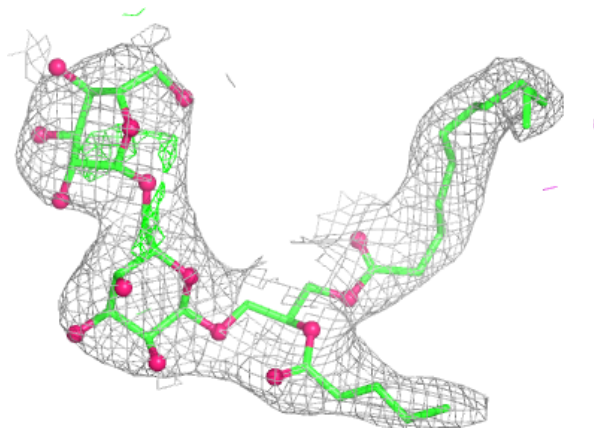


**Electron density around CLA B 512:**

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

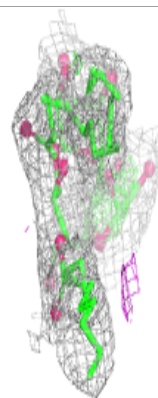
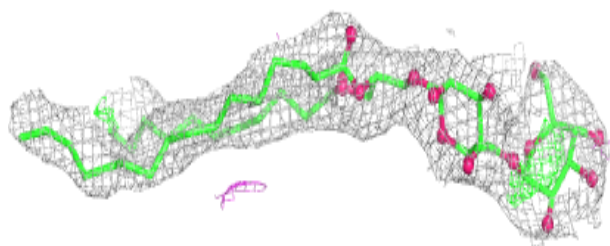
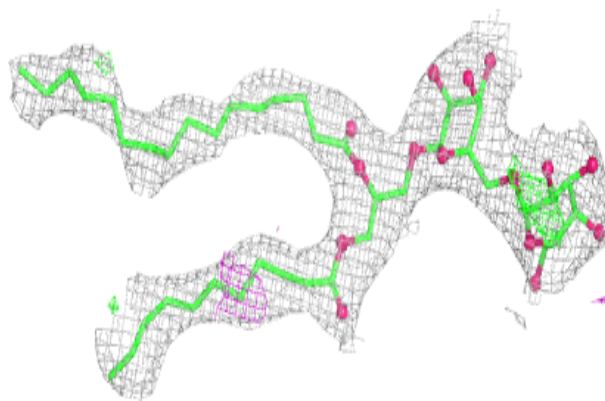
**Electron density around DGD C 508:**

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

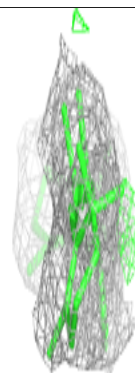
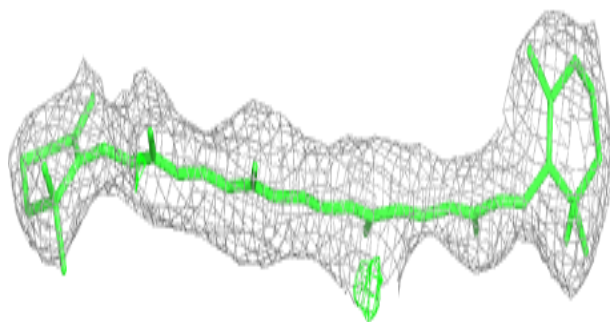
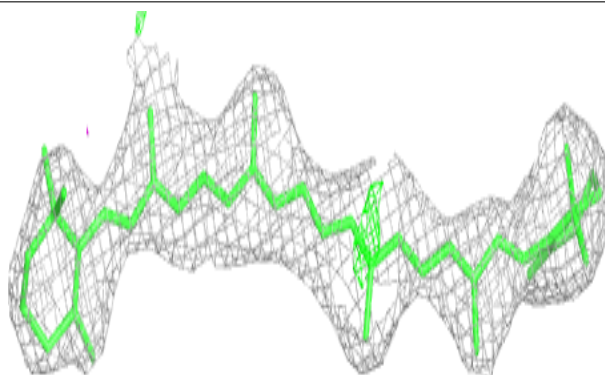


**Electron density around DGD C 509:**

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

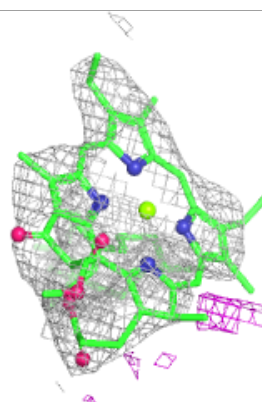
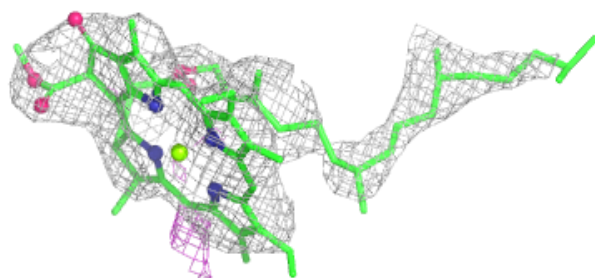
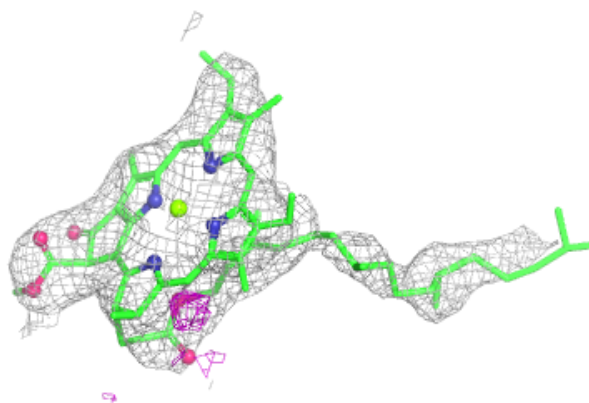
**Electron density around BCR B 527:**

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



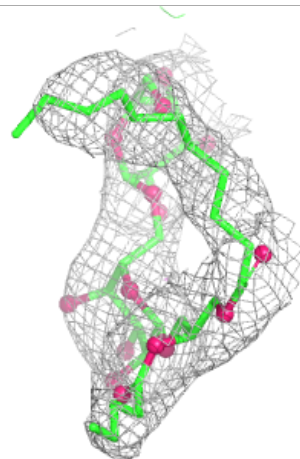
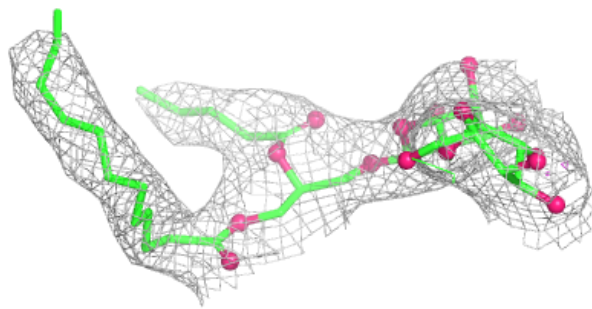
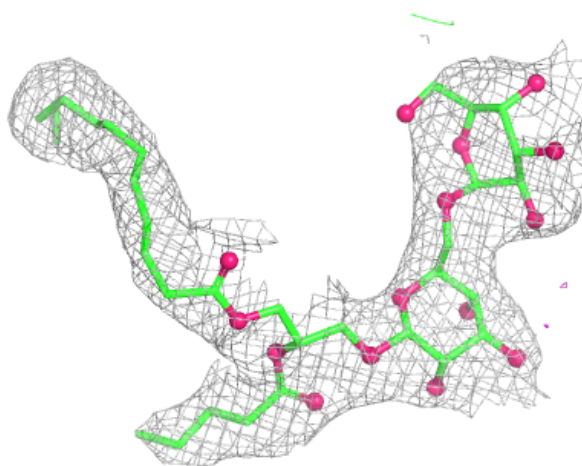
**Electron density around CLA c 5495:**

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



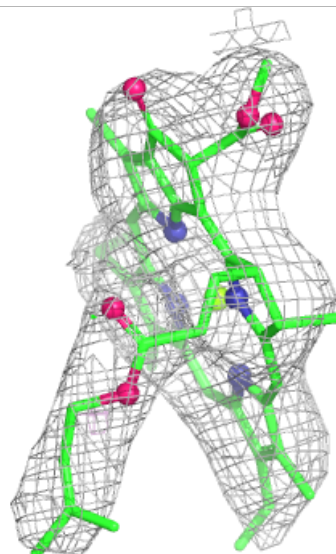
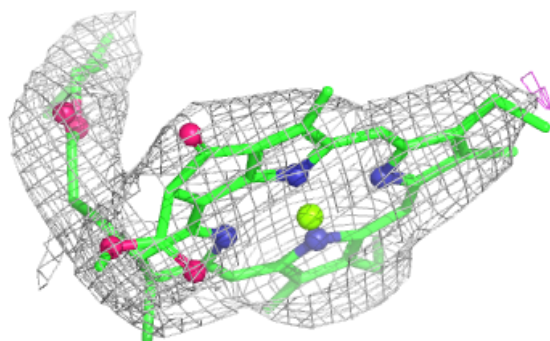
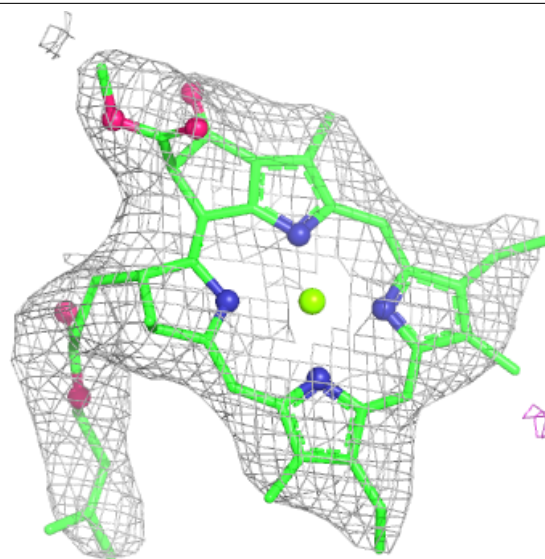
**Electron density around DGD c 5508:**

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



**Electron density around CLA D 355:**

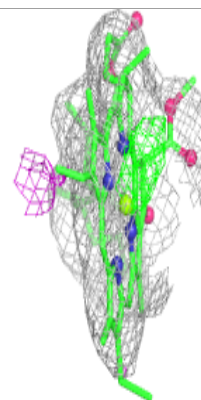
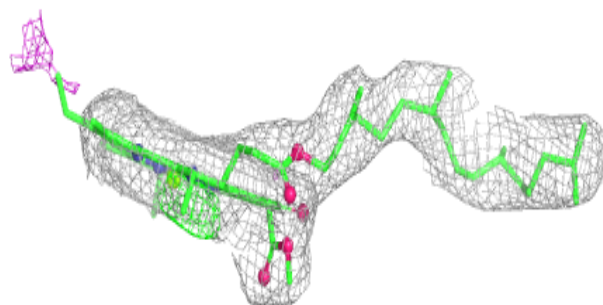
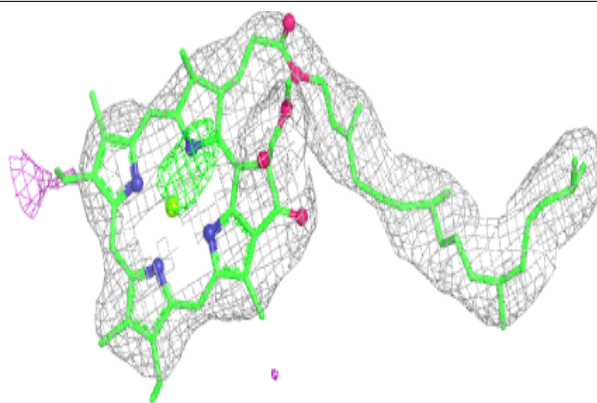
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



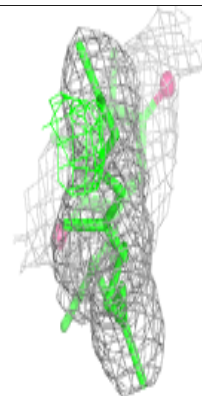
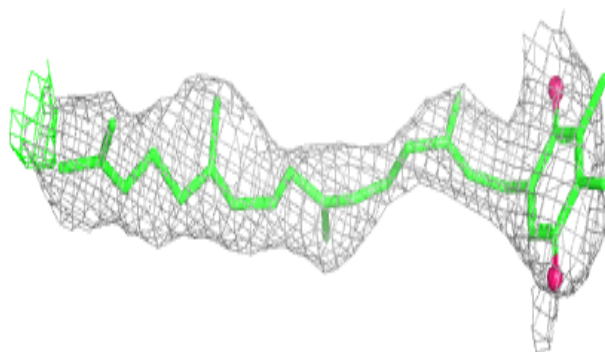
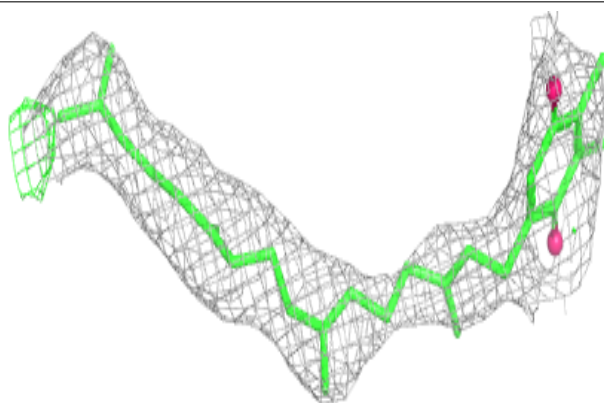


**Electron density around CLA b 5512:**

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

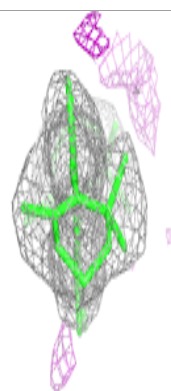
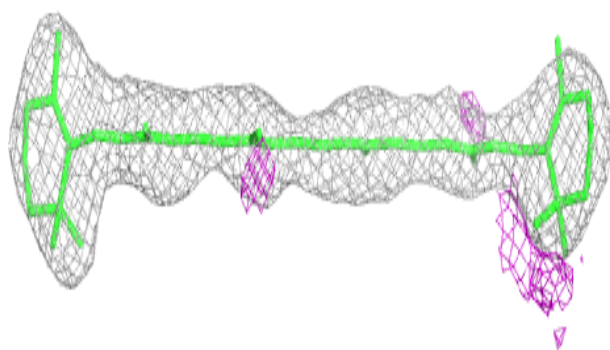
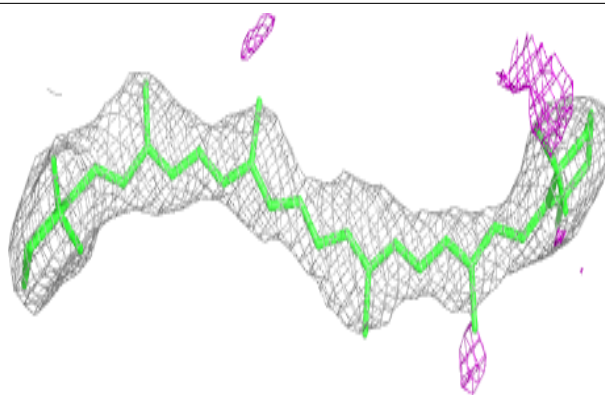
**Electron density around PQ9 d 5356:**

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

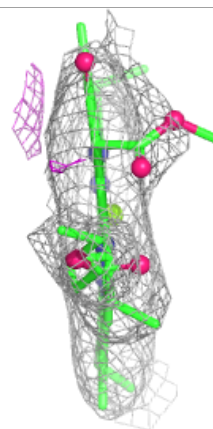
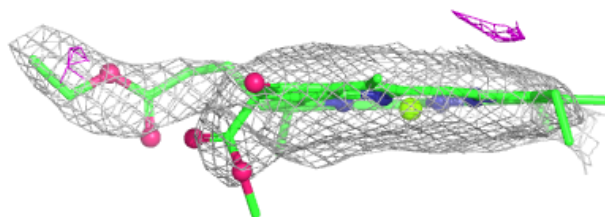
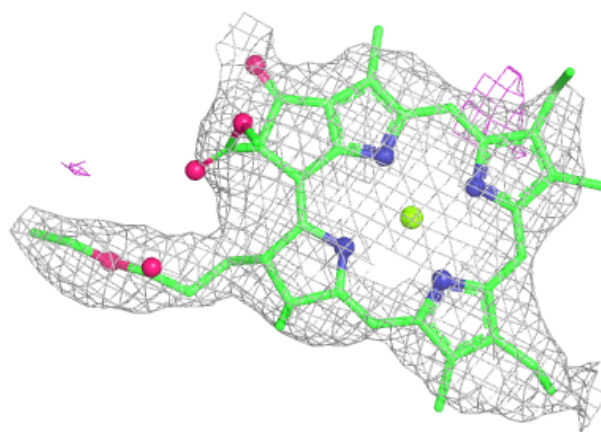


**Electron density around BCR A 566:**

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

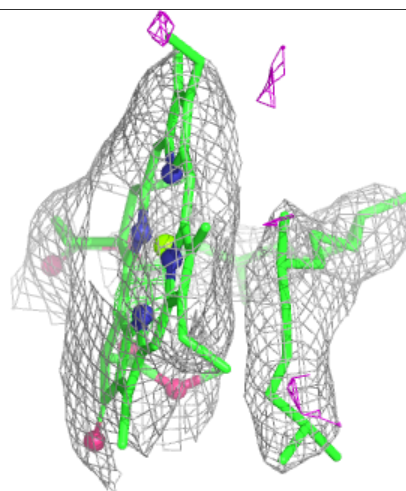
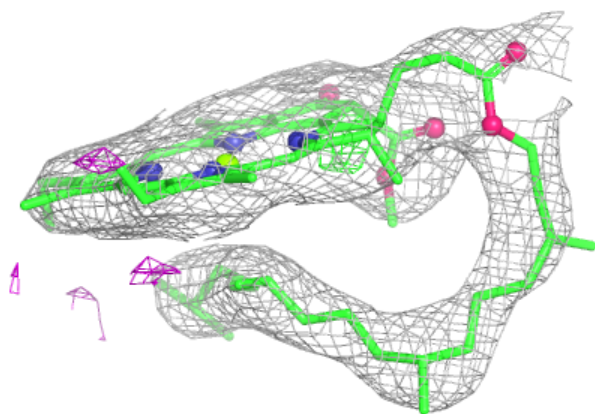
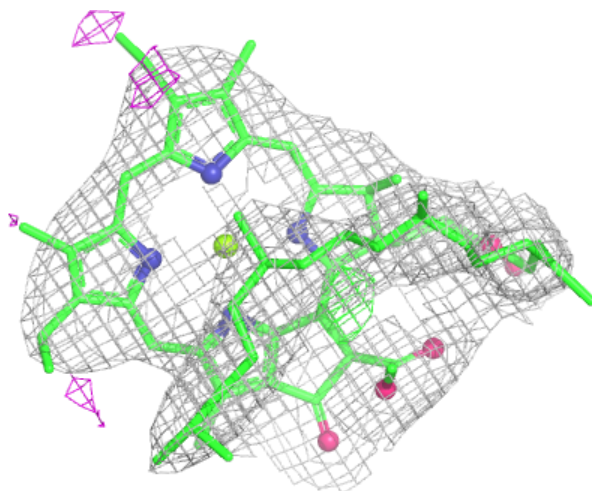
**Electron density around CLA c 5499:**

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



**Electron density around CLA c 5500:**

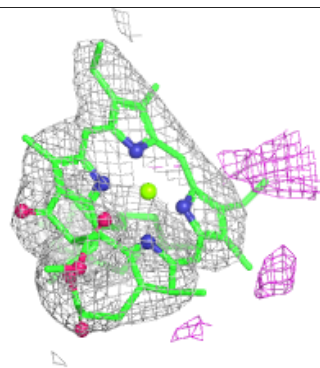
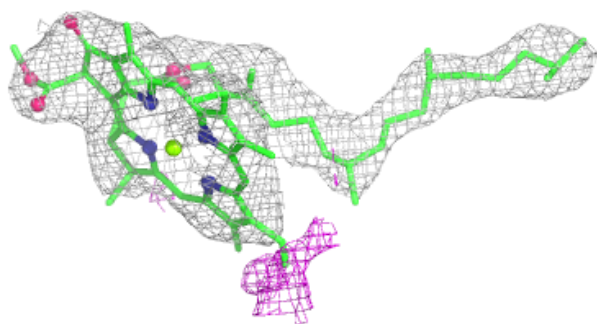
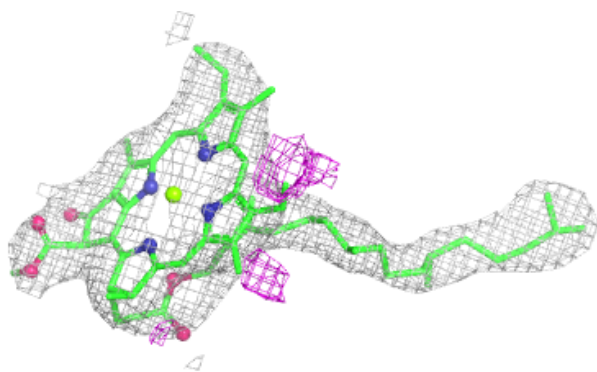
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





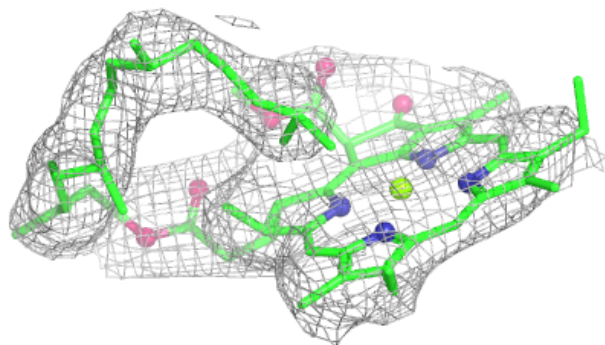
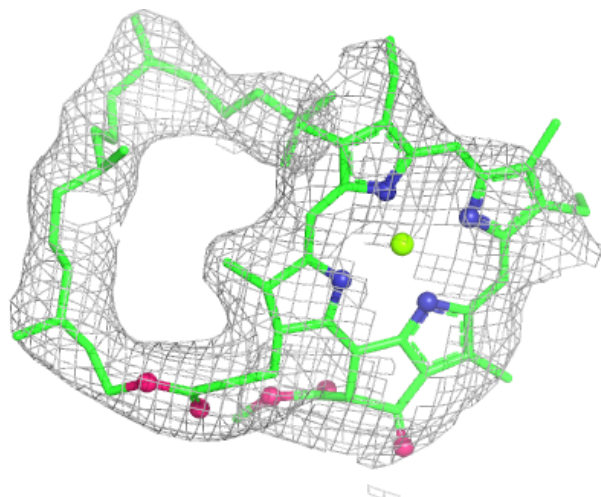
**Electron density around CLA C 495:**

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



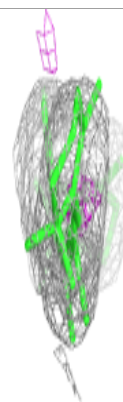
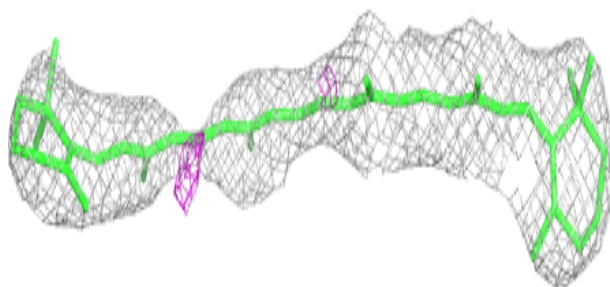
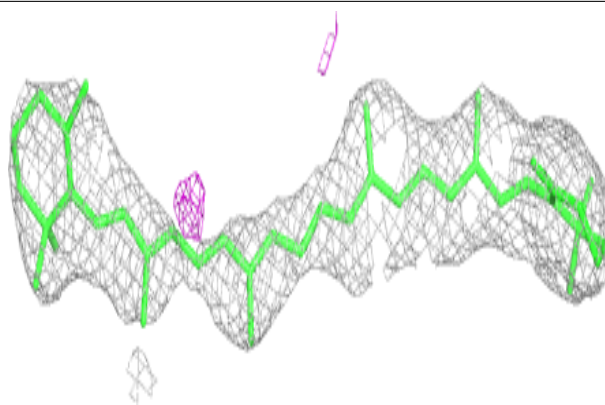
**Electron density around CLA b 5525:**

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

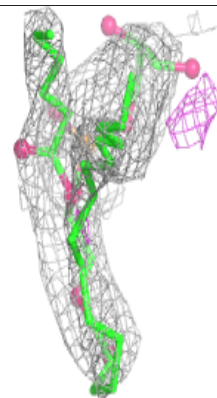
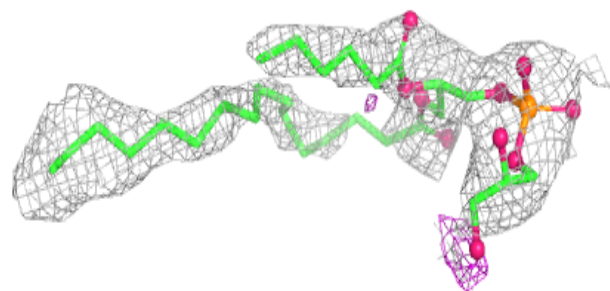
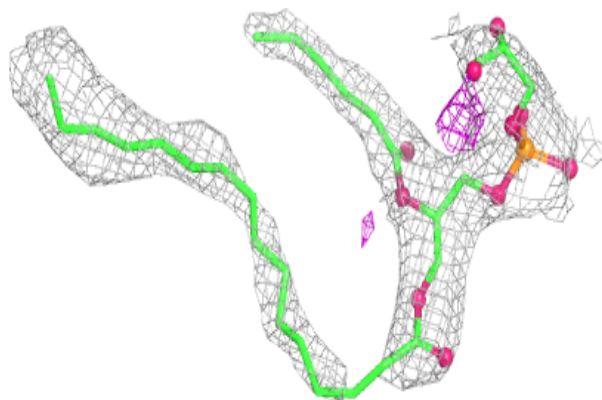


**Electron density around BCR b 5527:**

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

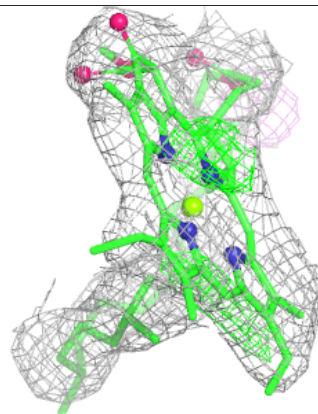
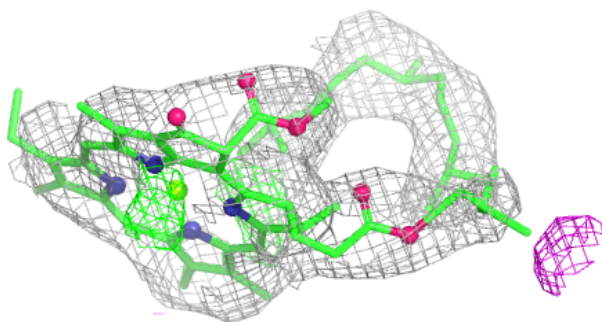
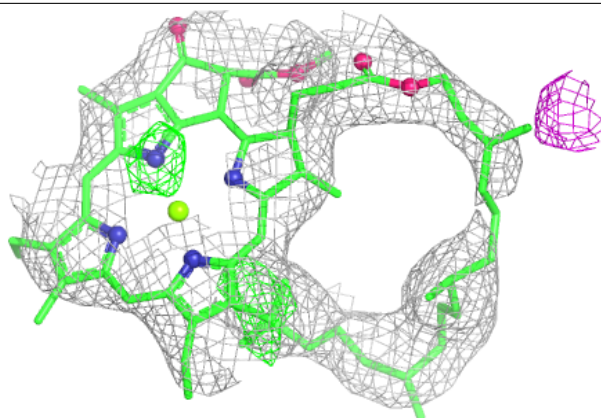
**Electron density around LHG A 567:**

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

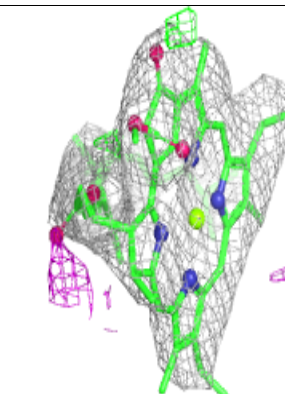
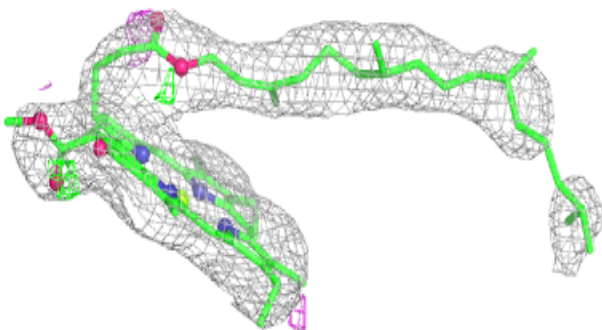
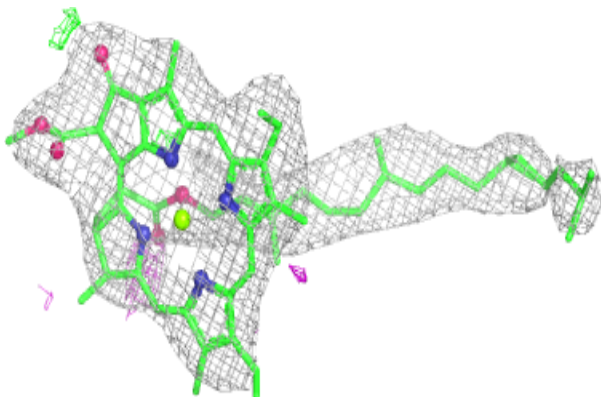


**Electron density around CLA B 525:**

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

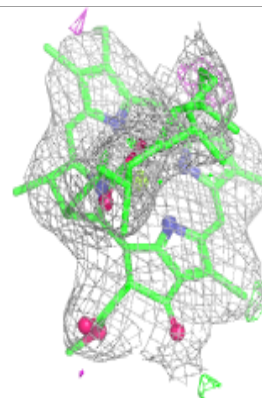
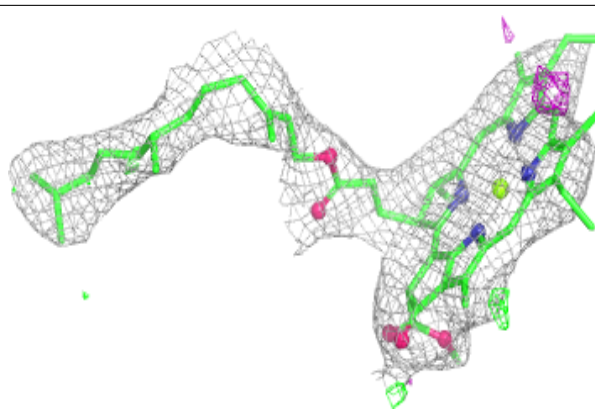
**Electron density around CLA B 518:**

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

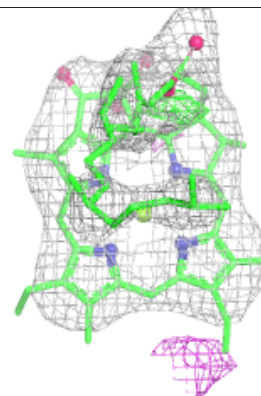
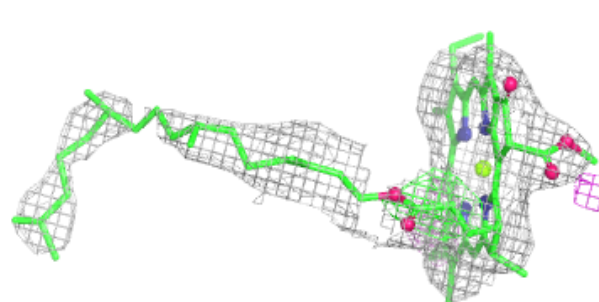
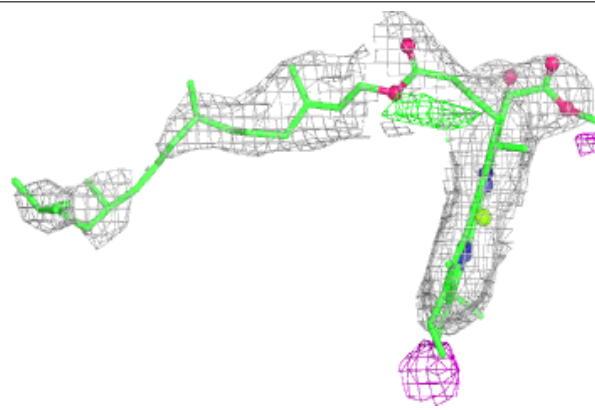


**Electron density around CLA c 5492:**

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

**Electron density around CLA B 515:**

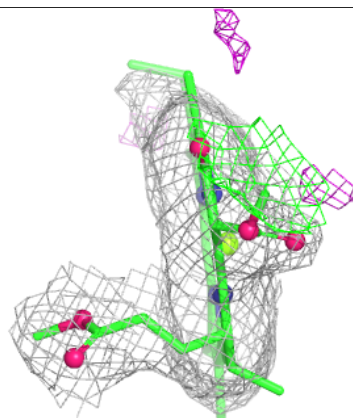
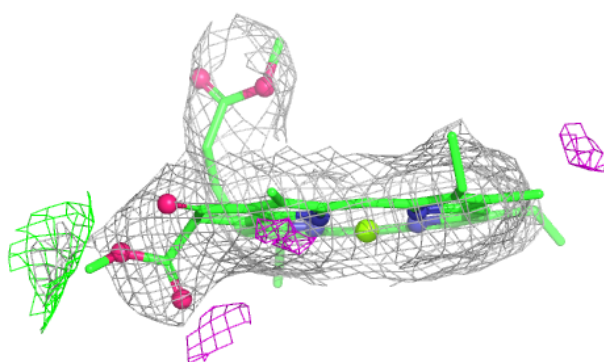
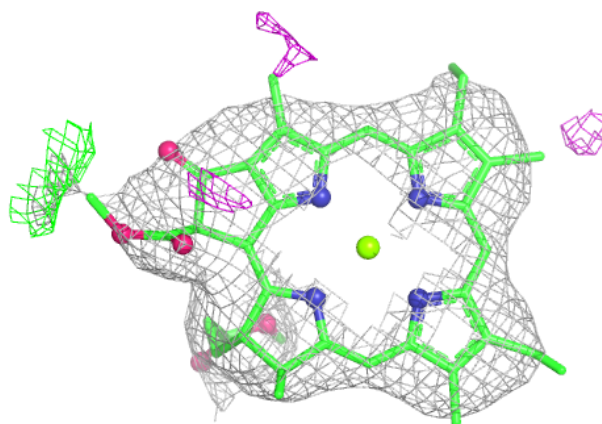
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



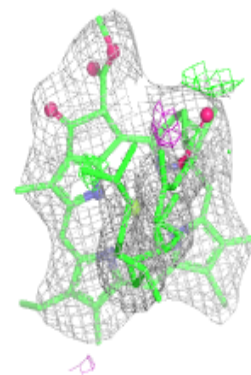
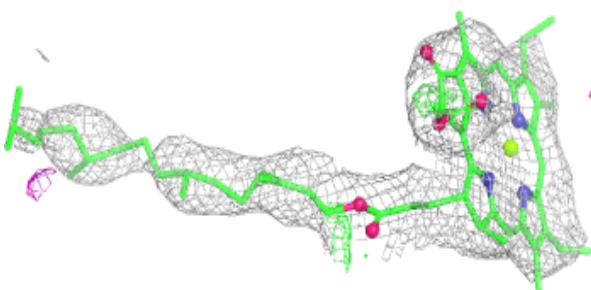
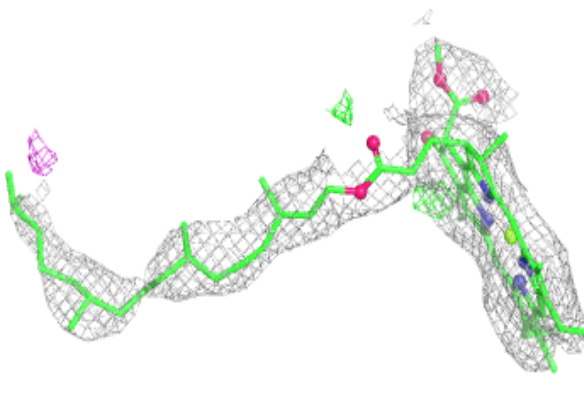


**Electron density around CLA c 5494:**

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

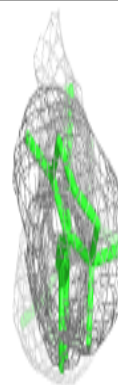
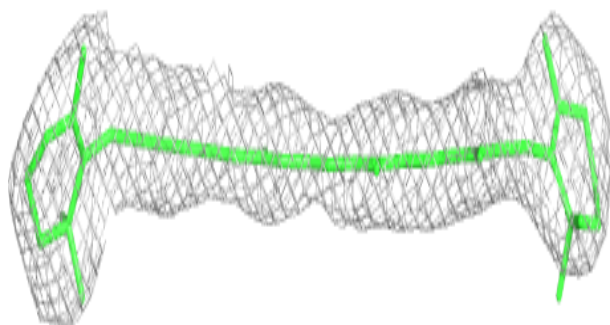
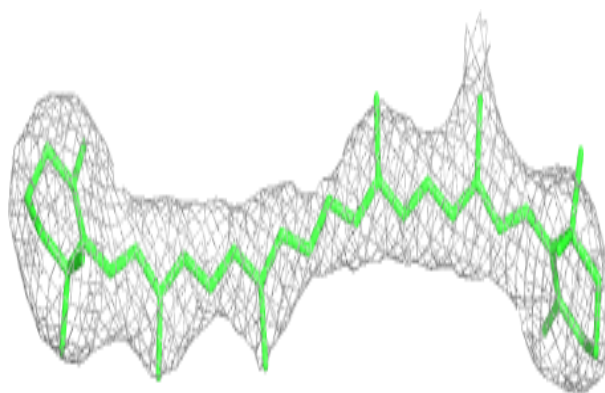
**Electron density around CLA B 514:**

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

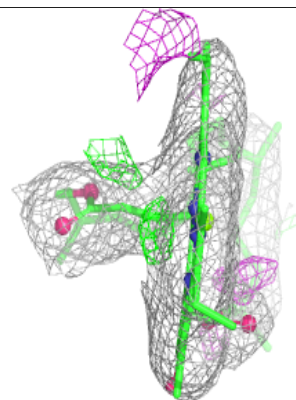
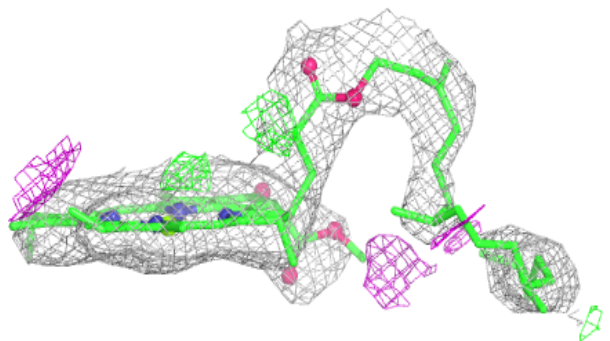
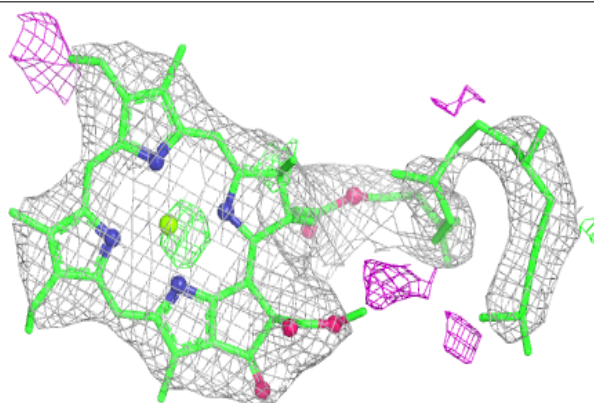


**Electron density around BCR b 5528:**

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

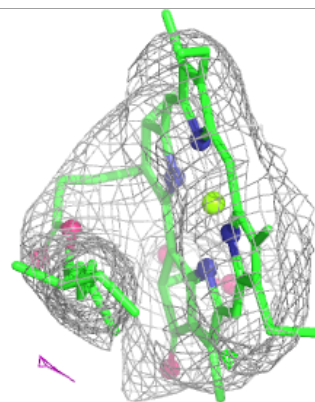
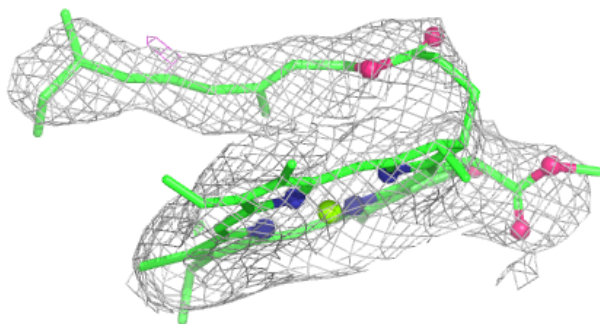
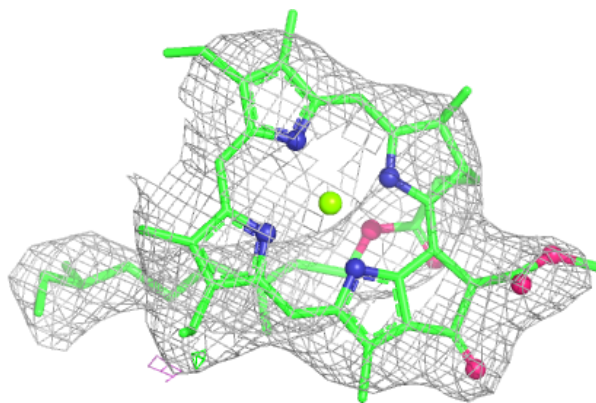
**Electron density around CLA B 522:**

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



**Electron density around CLA b 5524:**

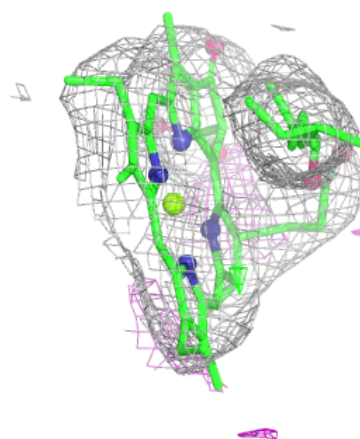
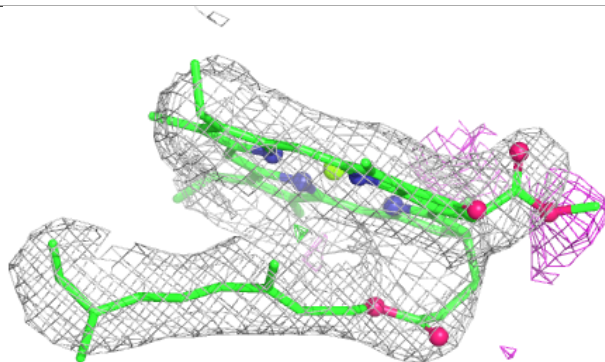
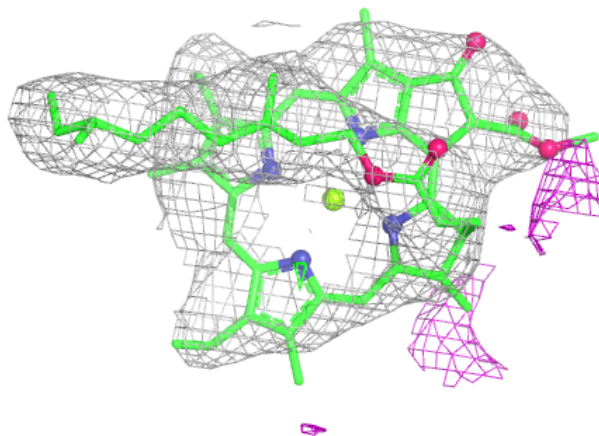
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





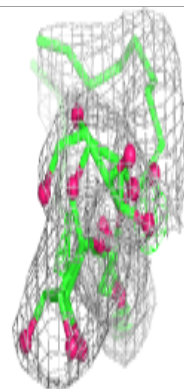
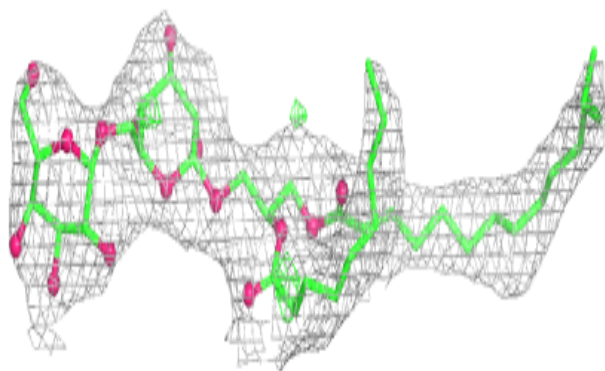
**Electron density around CLA B 524:**

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

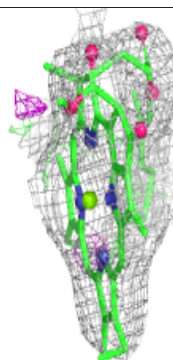
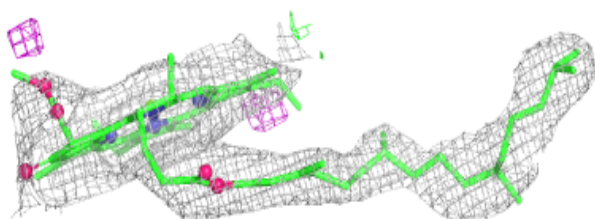
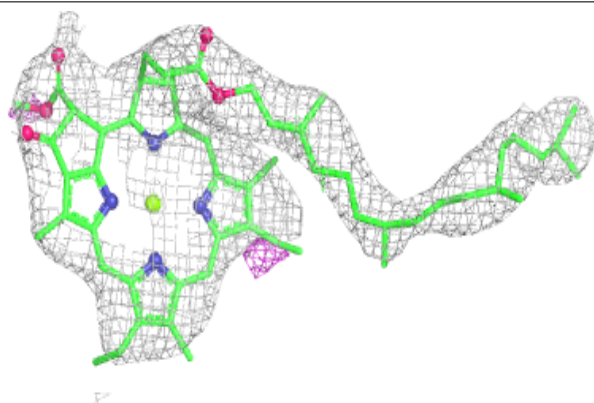


**Electron density around DGD h 5208:**

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

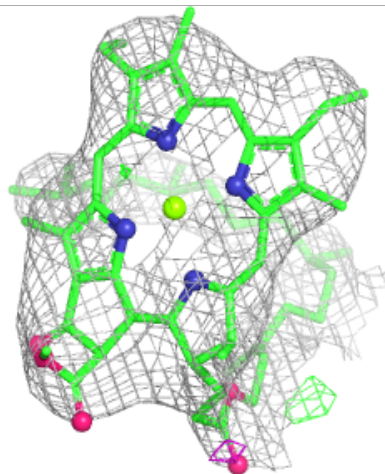
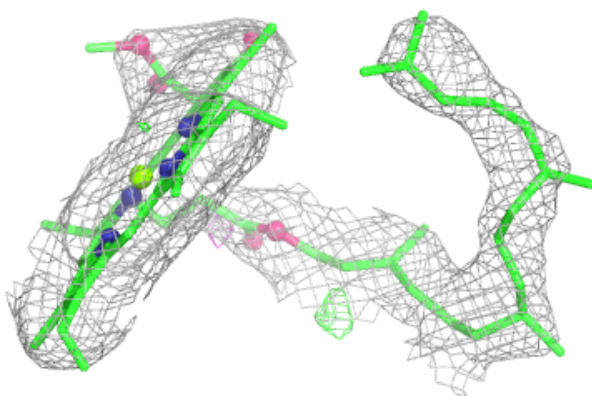
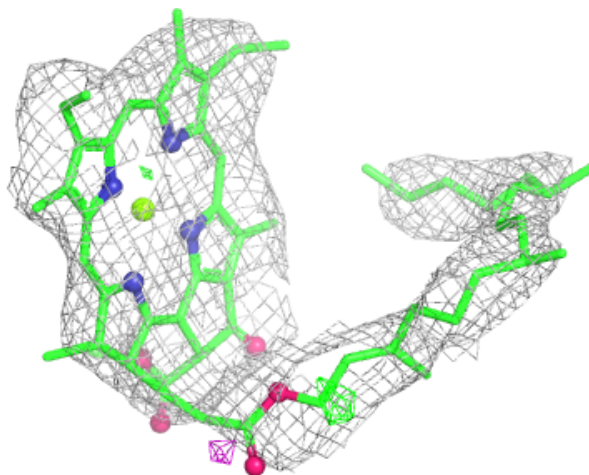
**Electron density around CLA B 513:**

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



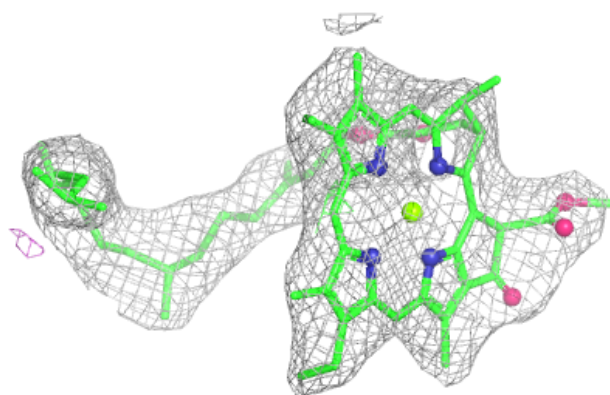
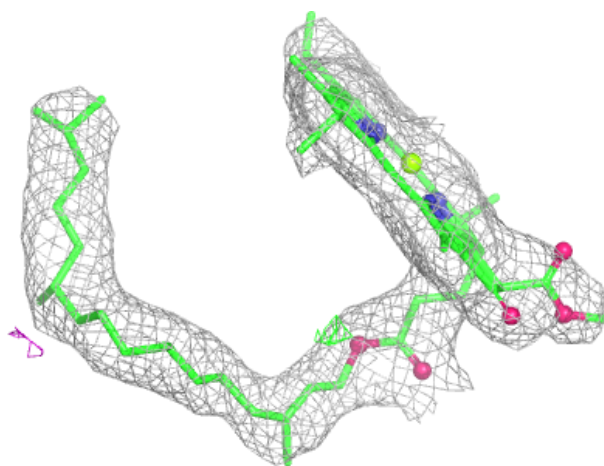
**Electron density around CLA C 493:**

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



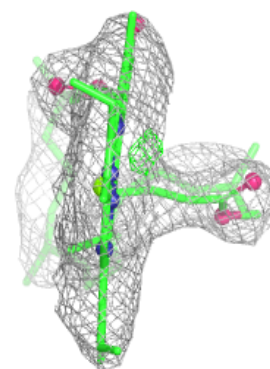
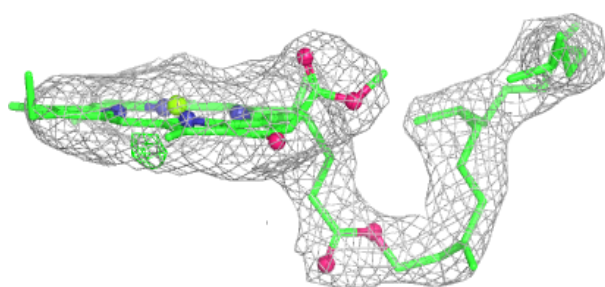
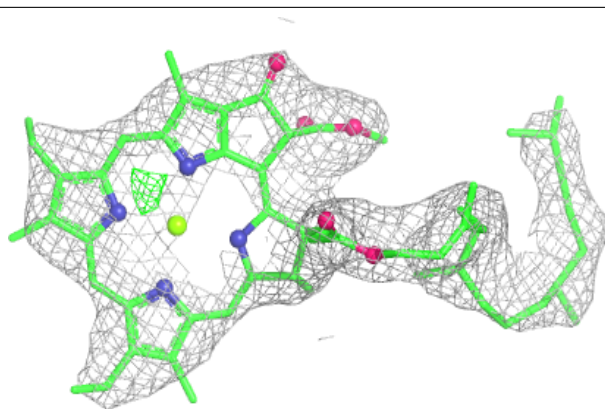
**Electron density around CLA b 5521:**

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

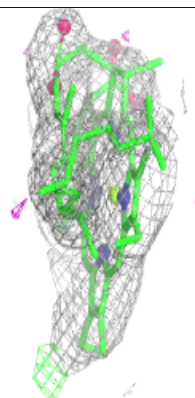
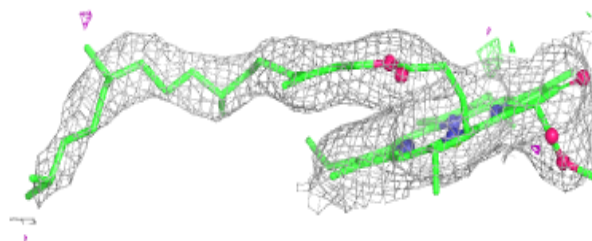
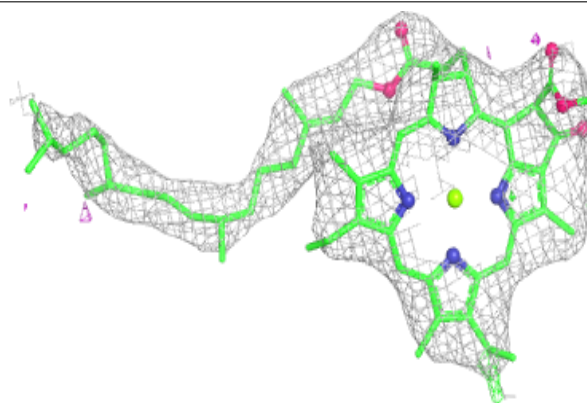


**Electron density around CLA b 5522:**

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

**Electron density around CLA b 5513:**

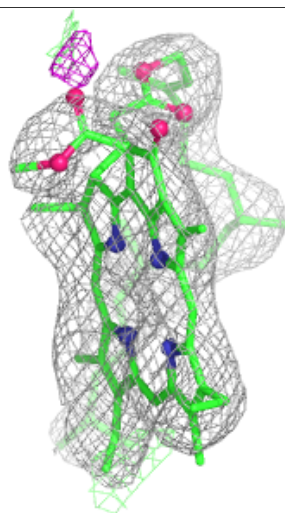
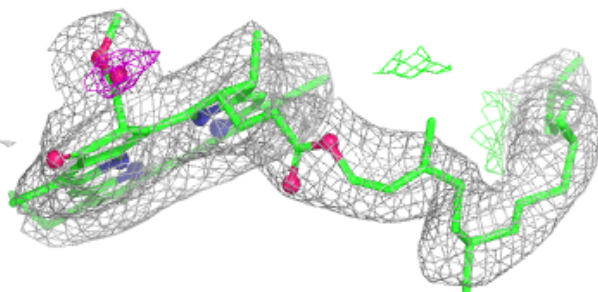
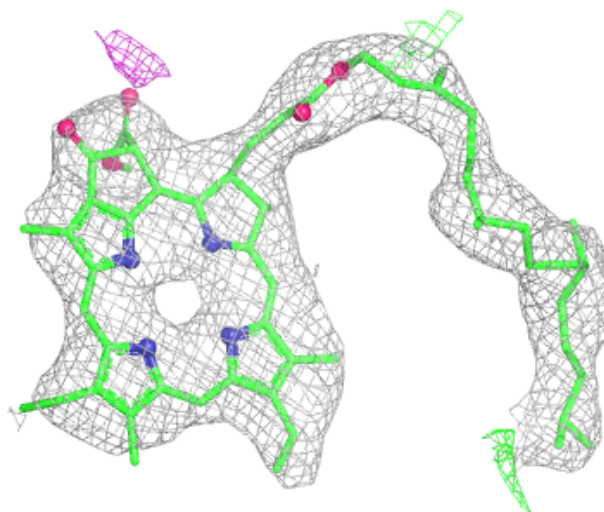
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





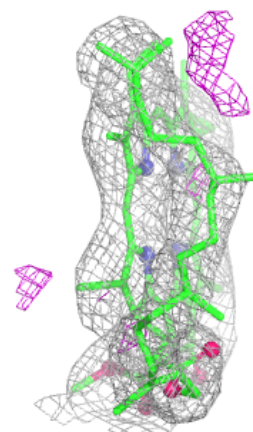
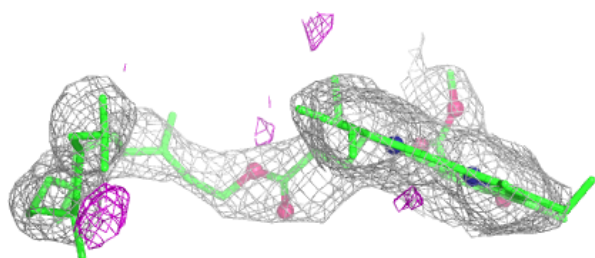
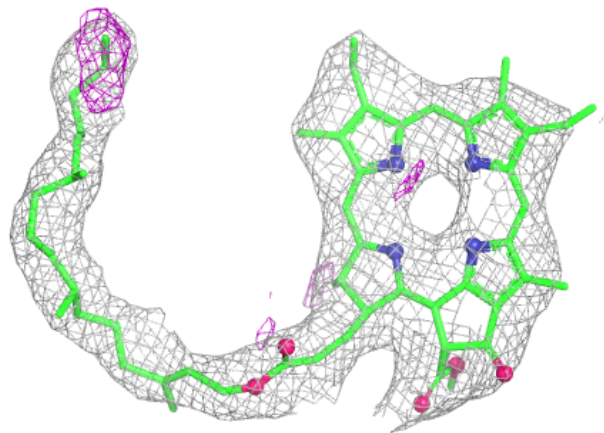
**Electron density around PHO A 562:**

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



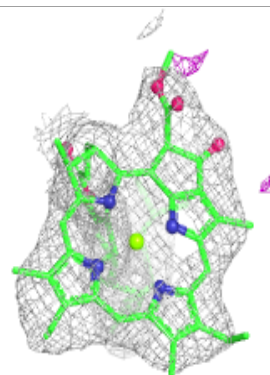
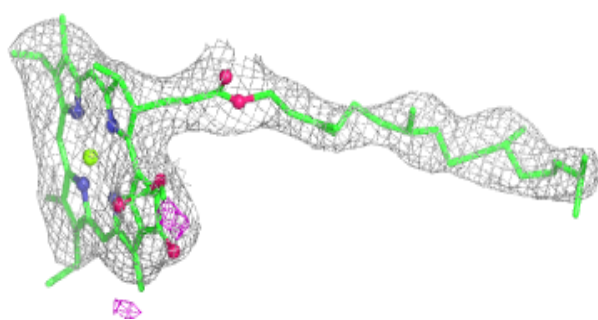
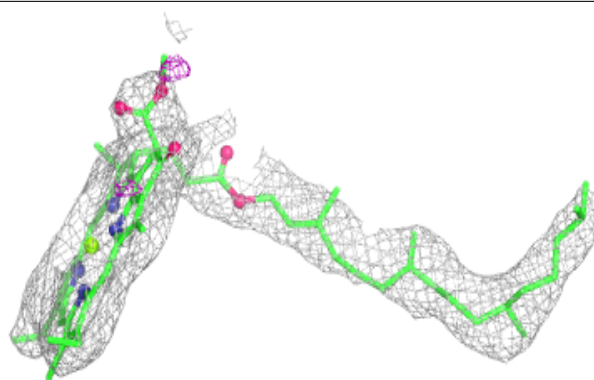
**Electron density around PHO a 5561:**

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

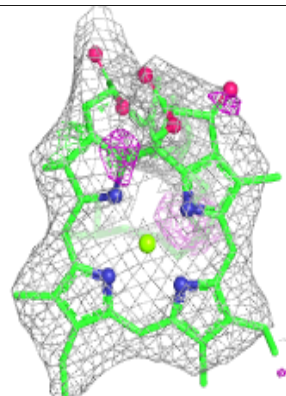
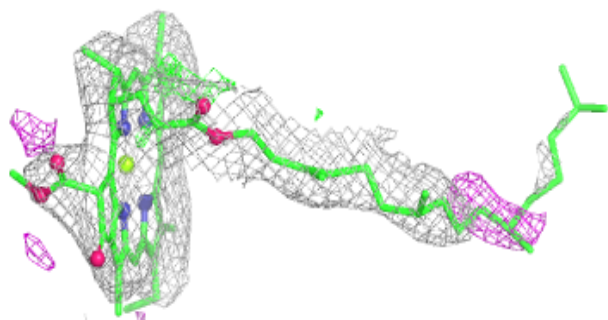
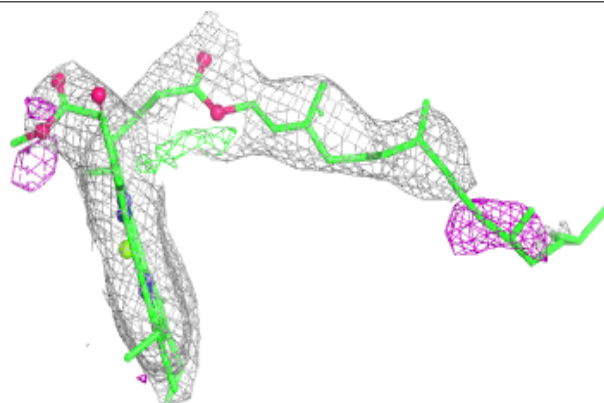


**Electron density around CLA b 5514:**

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

**Electron density around CLA b 5515:**

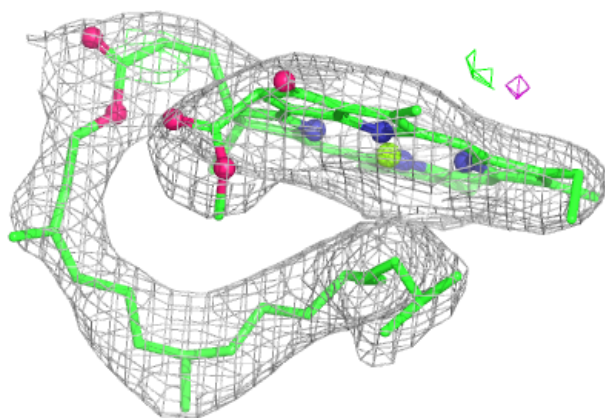
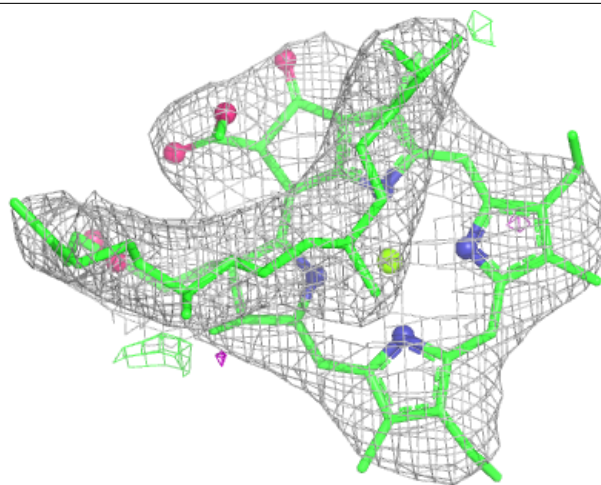
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





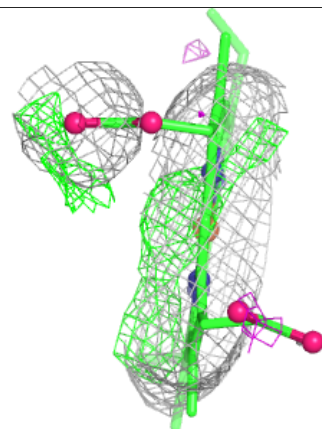
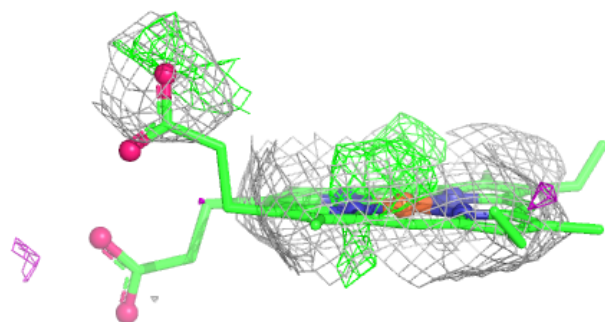
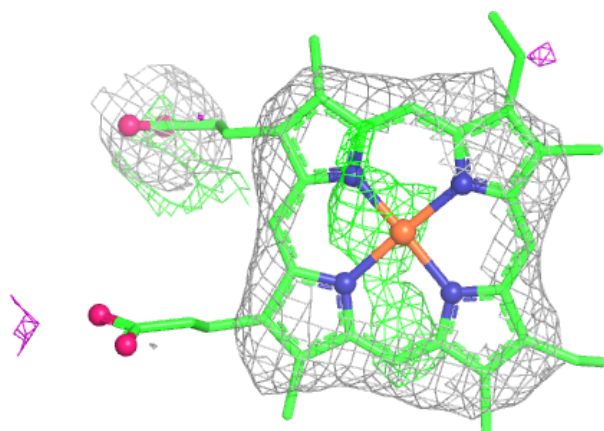
**Electron density around CLA C 500:**

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

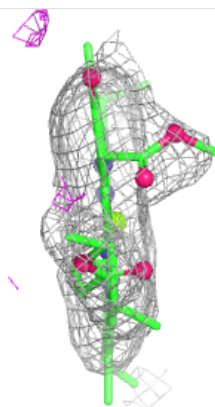
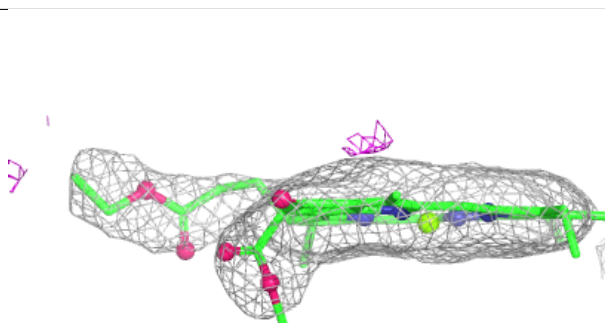
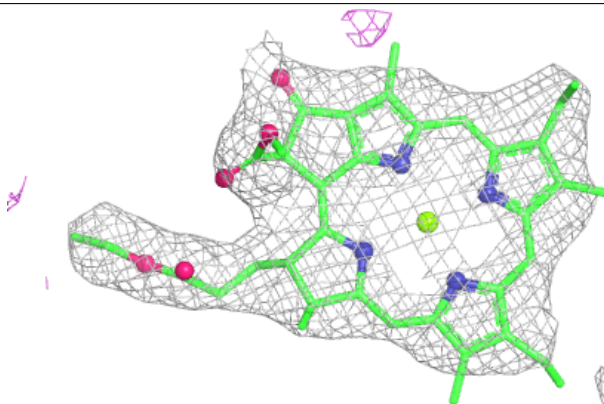


**Electron density around HEM f 5051:**

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

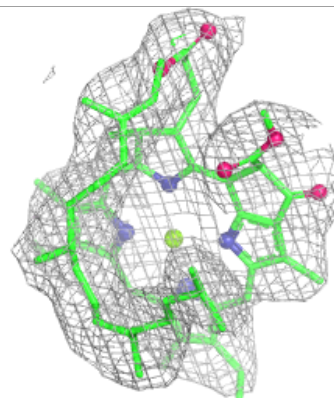
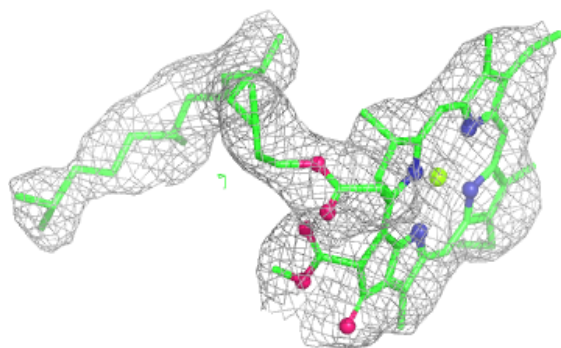
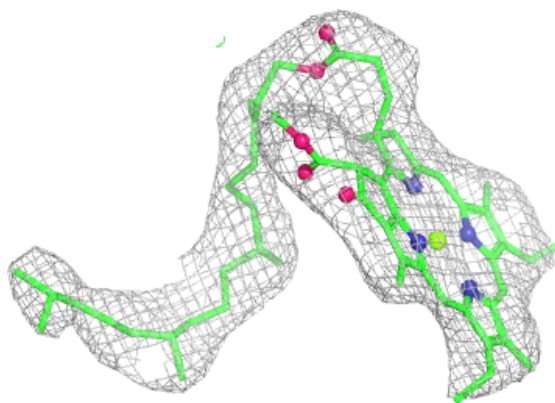
**Electron density around CLA C 499:**

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

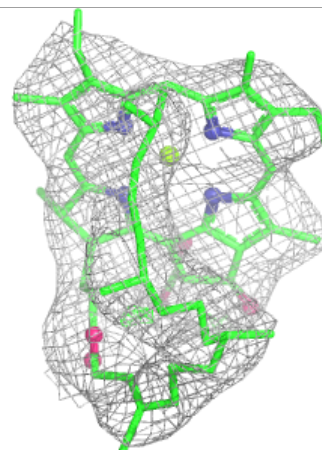
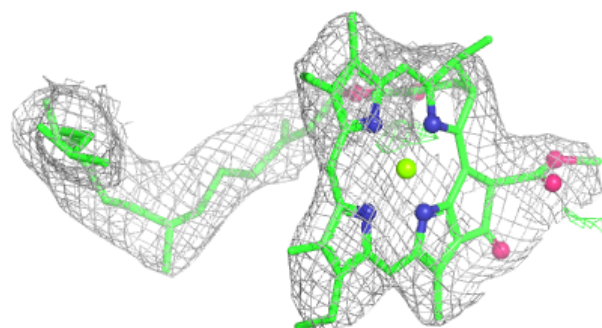
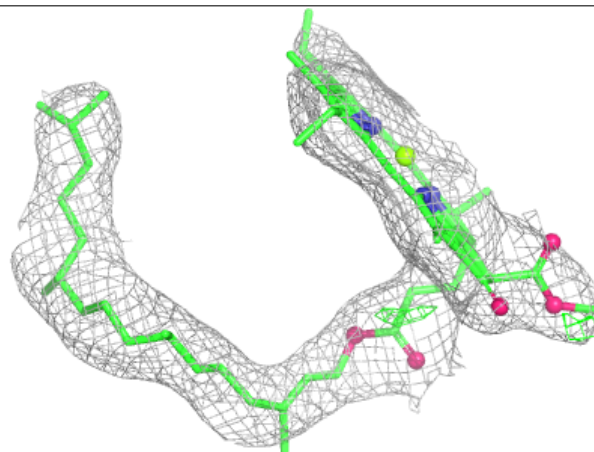


**Electron density around CLA b 5523:**

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

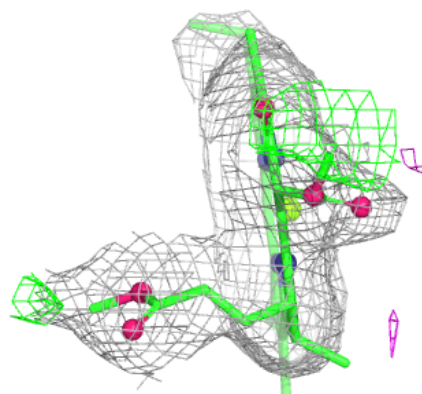
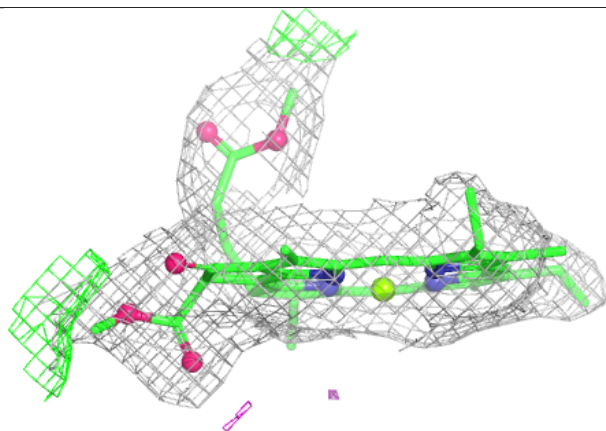
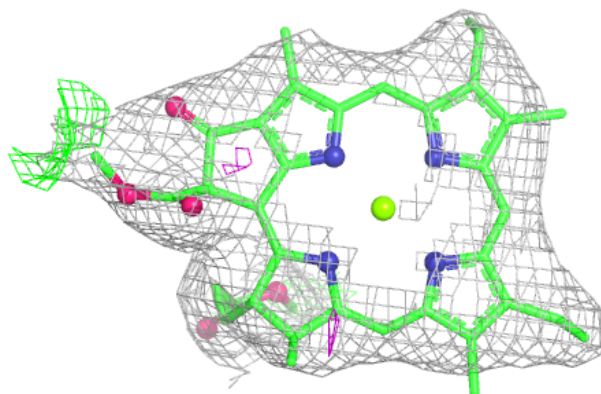
**Electron density around CLA B 521:**

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

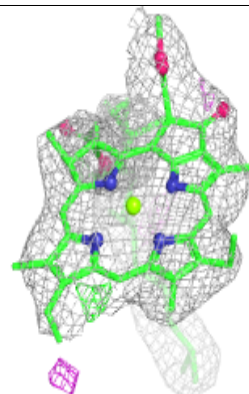
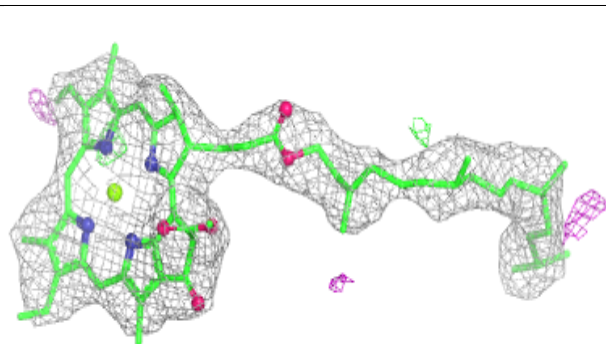
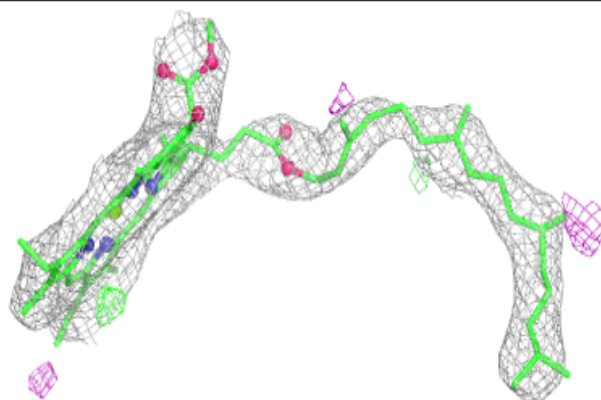


**Electron density around CLA C 494:**

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

**Electron density around CLA d 5354:**

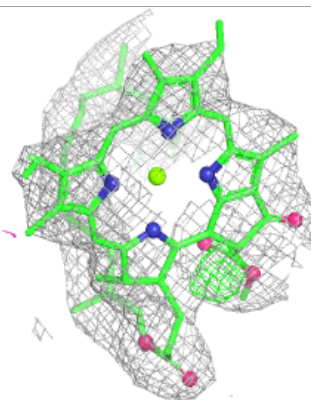
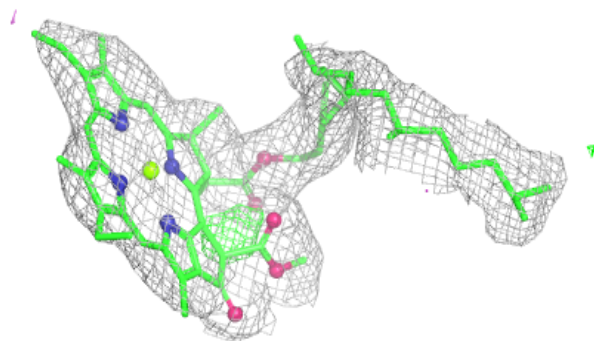
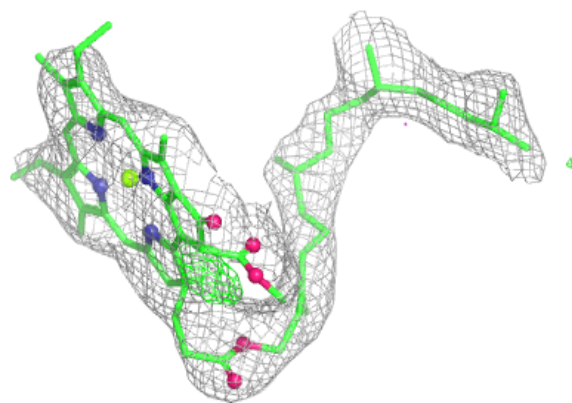
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



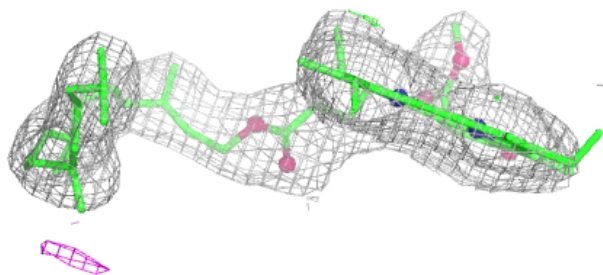
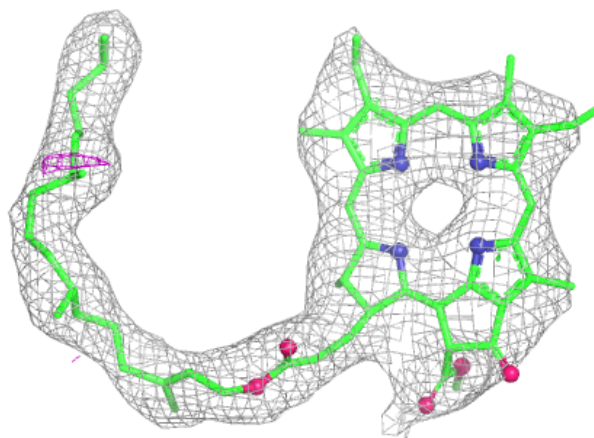


**Electron density around CLA B 523:**

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

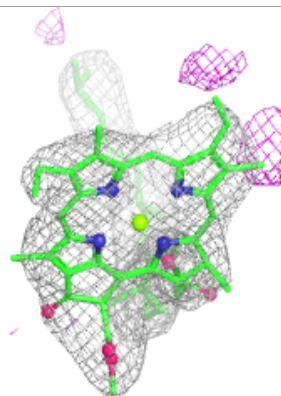
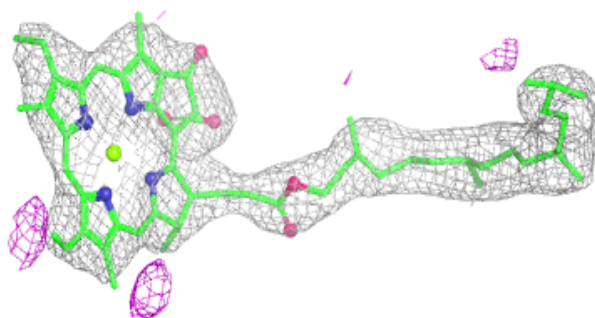
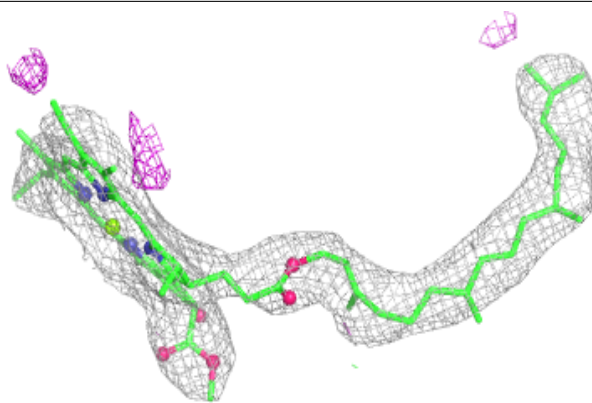
**Electron density around PHO A 561:**

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

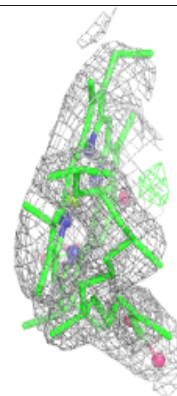
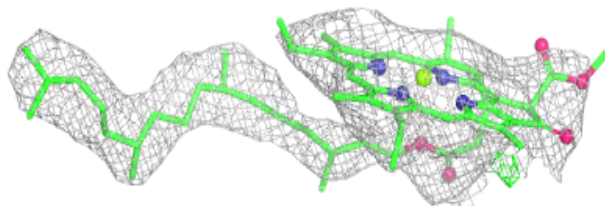
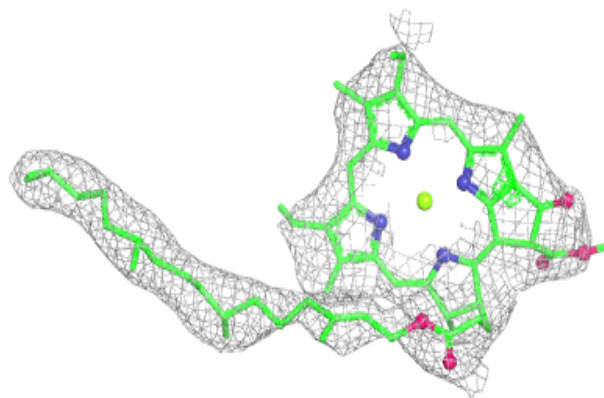


**Electron density around CLA D 354:**

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

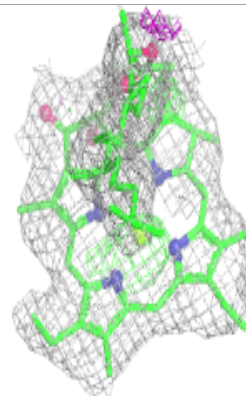
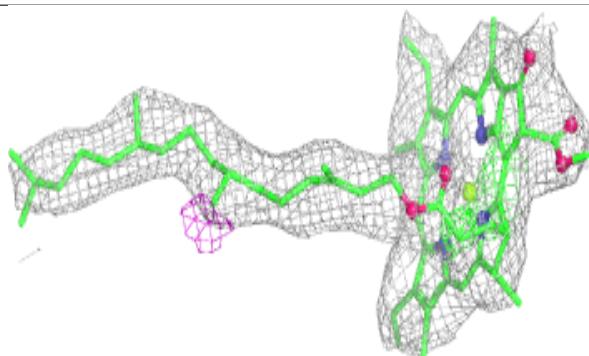
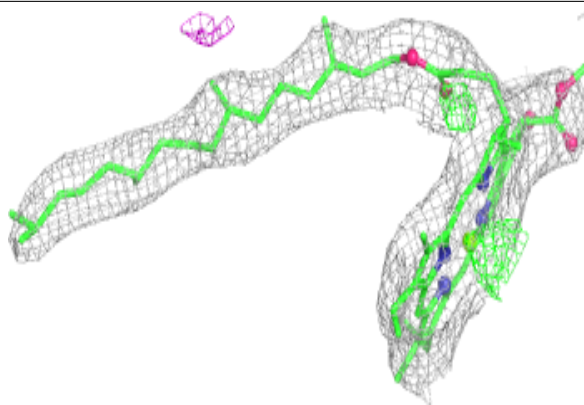
**Electron density around CLA C 491:**

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

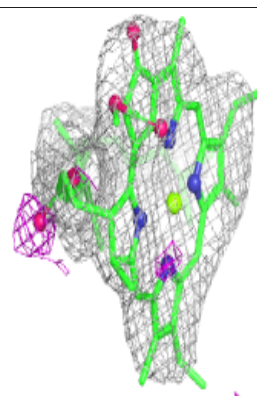
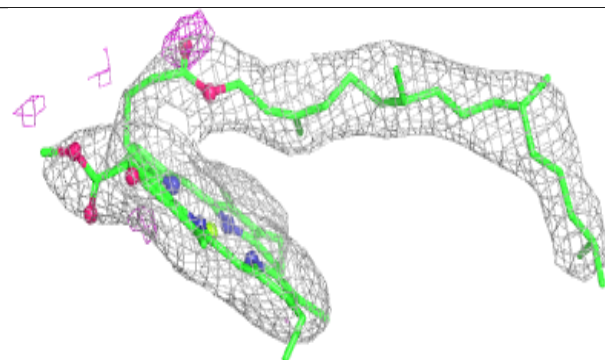
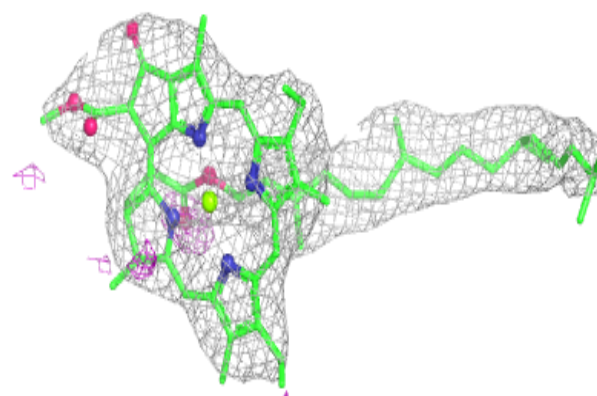


**Electron density around CLA b 5517:**

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

**Electron density around CLA b 5518:**

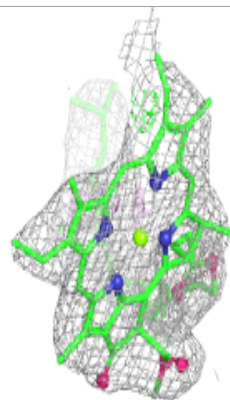
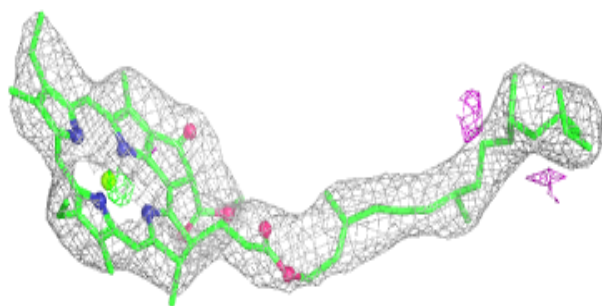
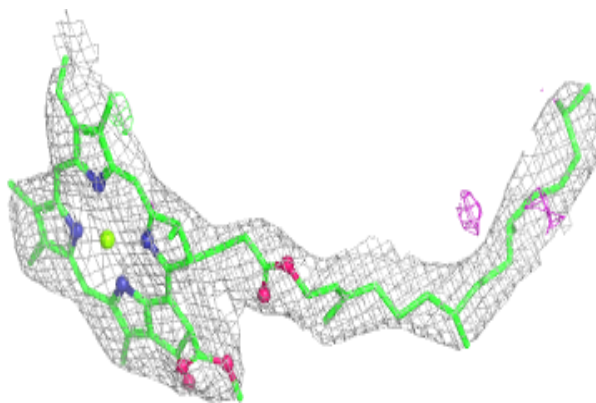
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





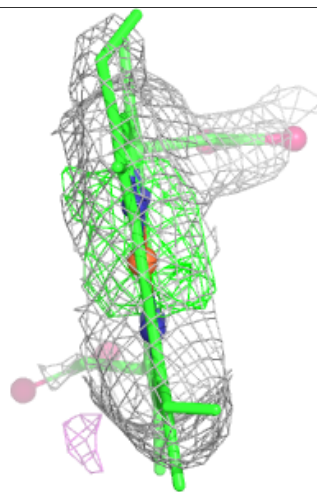
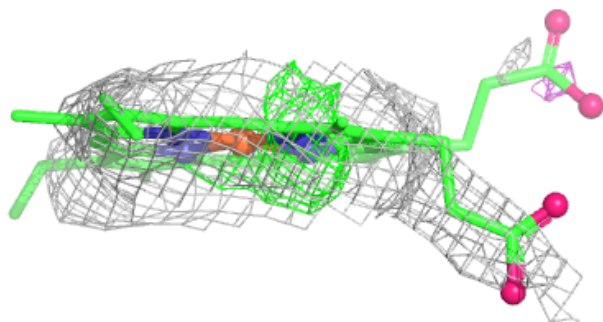
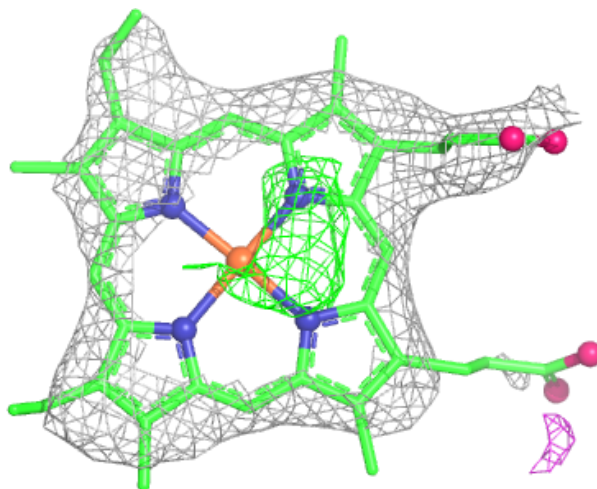
**Electron density around CLA a 5558:**

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



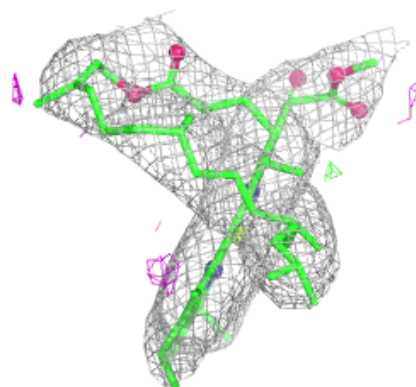
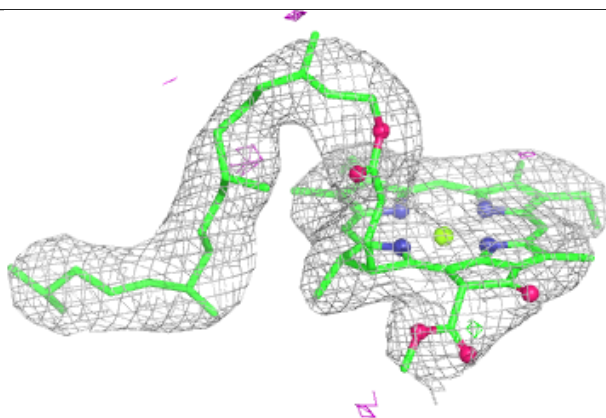
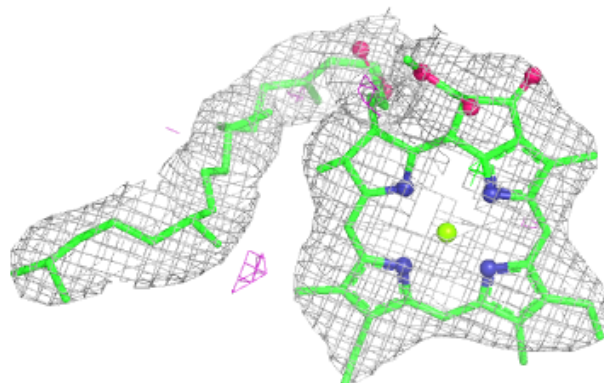
**Electron density around HEM F 51:**

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

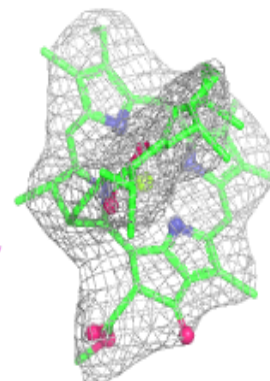
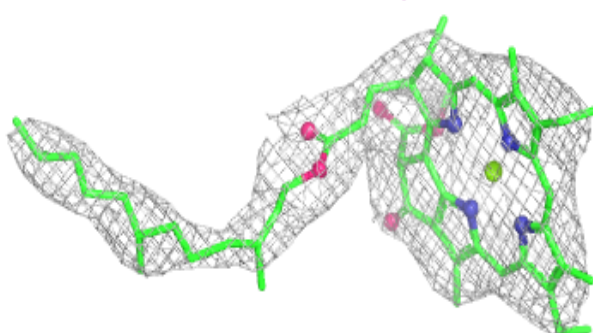
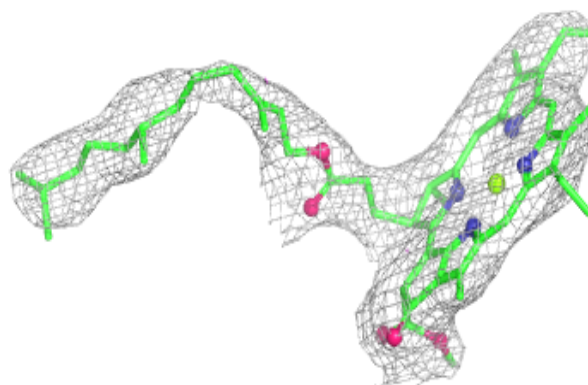


**Electron density around CLA a 5559:**

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

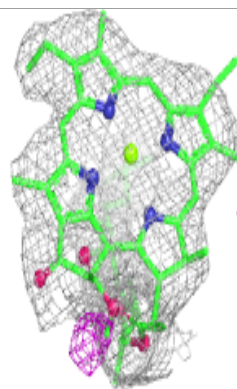
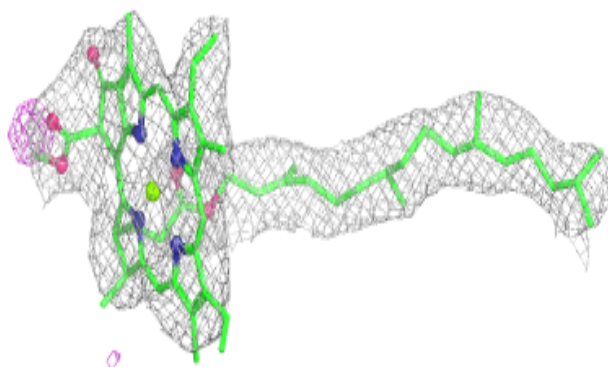
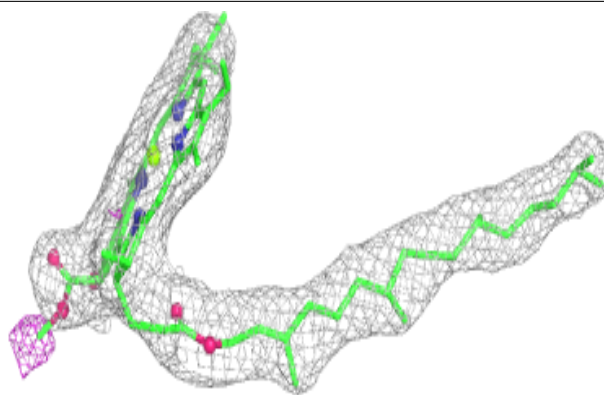
**Electron density around CLA C 492:**

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

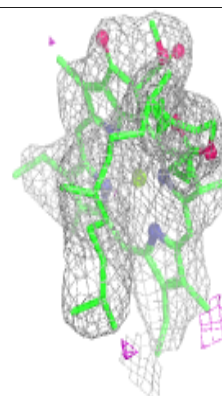
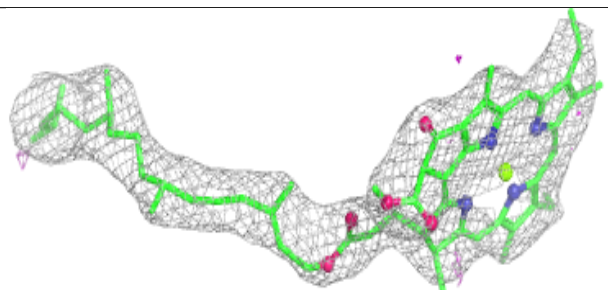
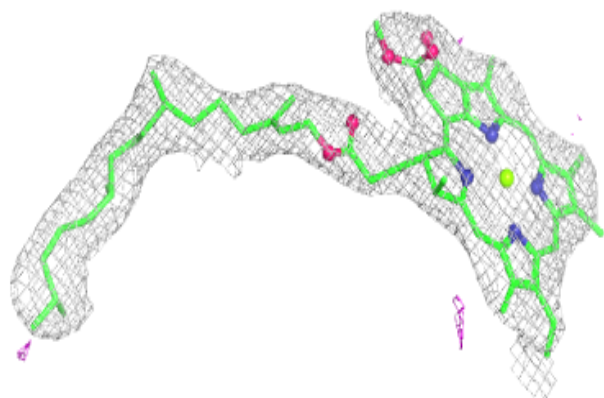


**Electron density around CLA B 517:**

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

**Electron density around CLA A 558:**

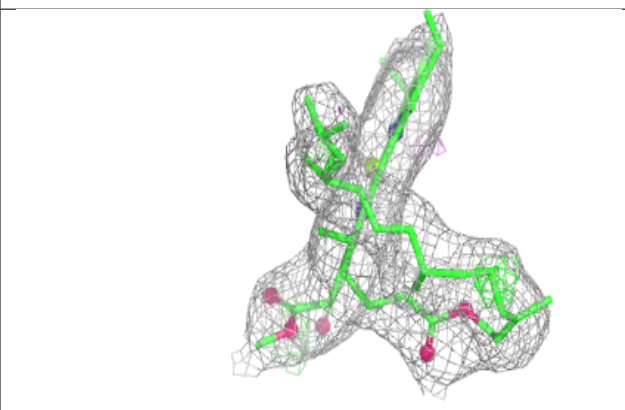
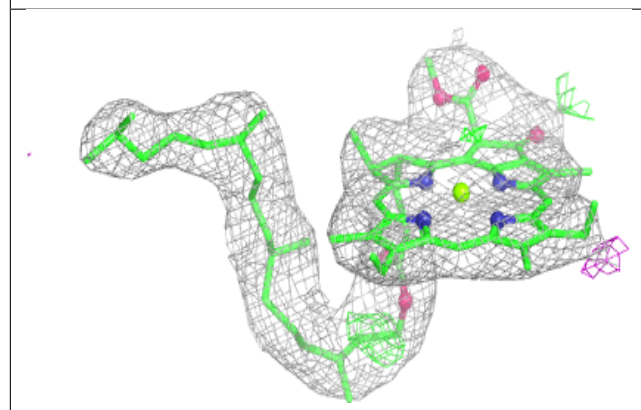
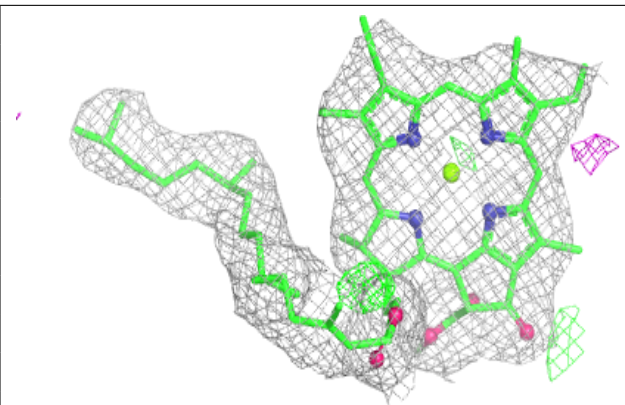
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



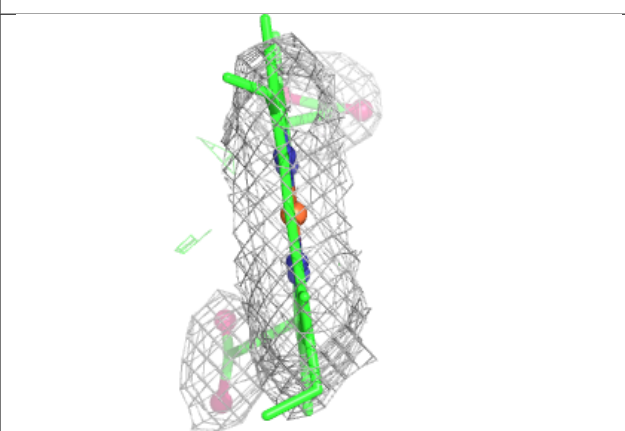
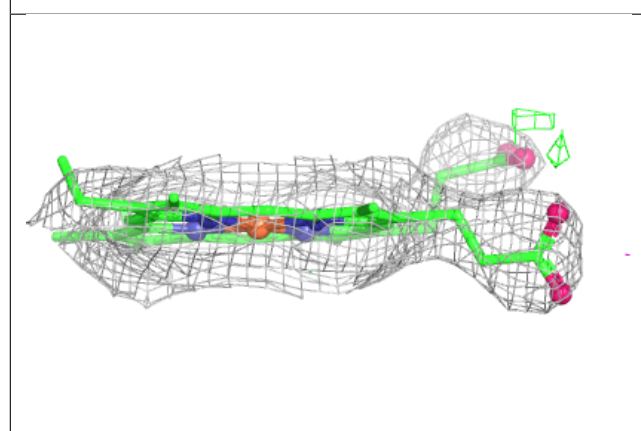
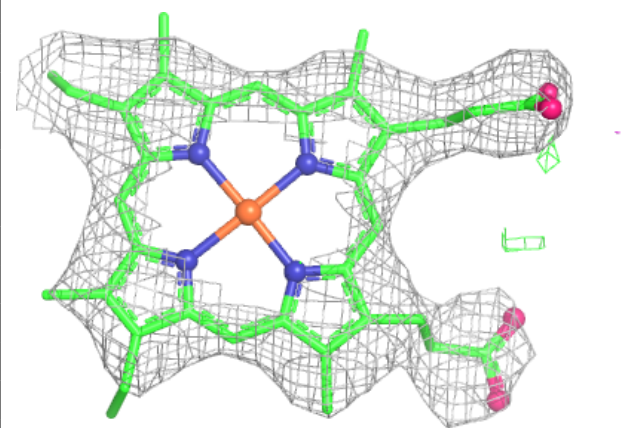


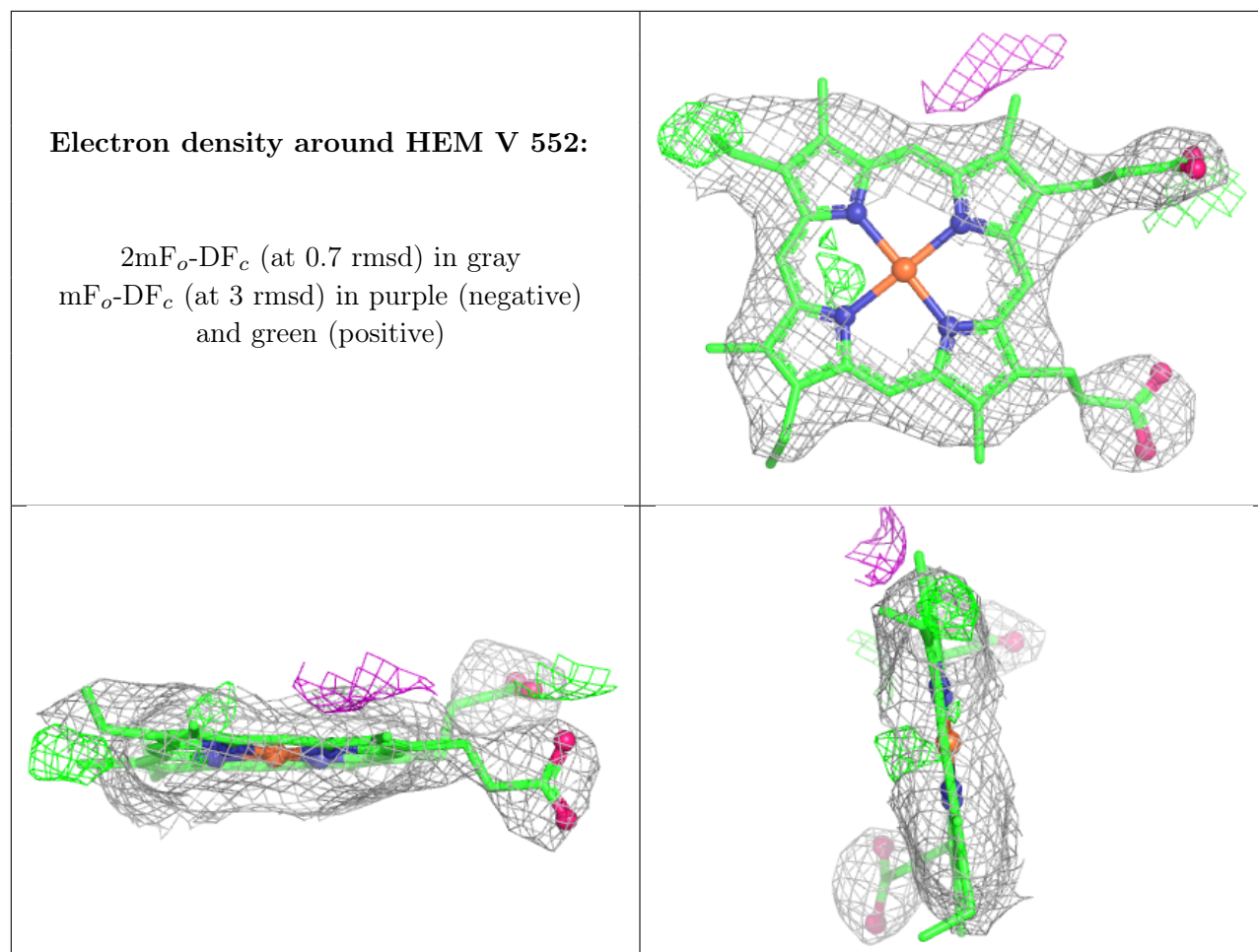
**Electron density around CLA A 559:**

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

**Electron density around HEM v 5552:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.