



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2025 – 12:26 AM EST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

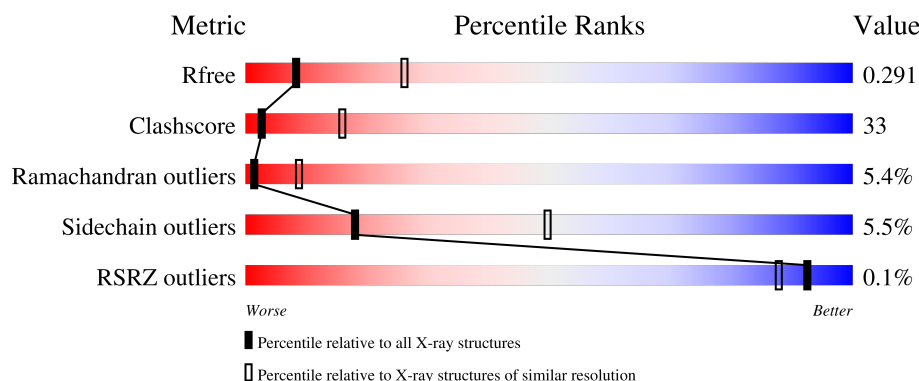
1 Overall quality at a glance ⓘ

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.






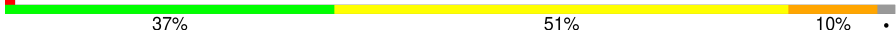

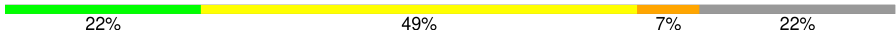

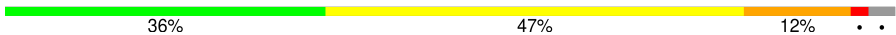

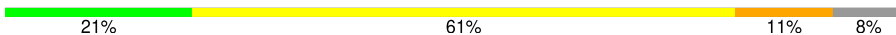

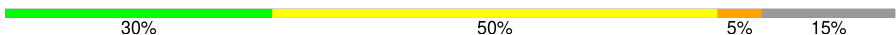

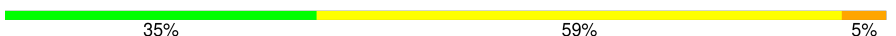




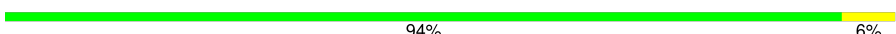






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 ≥ 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	<div> <div>42%</div> <div>48%</div> <div>6%</div> <div>...</div> </div>
1	a	344	<div> <div>88%</div> <div>9%</div> <div>...</div> </div>
2	B	510	<div> <div>55%</div> <div>36%</div> <div>5%</div> <div>...</div> </div>
2	b	510	<div> <div>89%</div> <div>6%</div> <div>...</div> </div>
3	C	473	<div> <div>40%</div> <div>48%</div> <div>6%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	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			

Continued on next page...

Continued from previous page...

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			

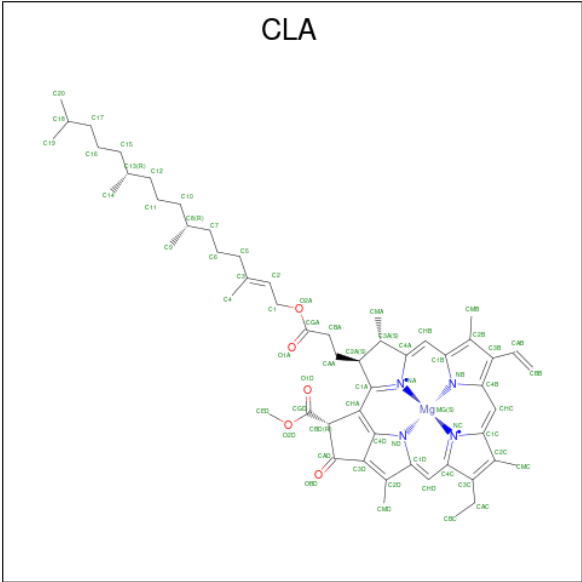
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

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: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

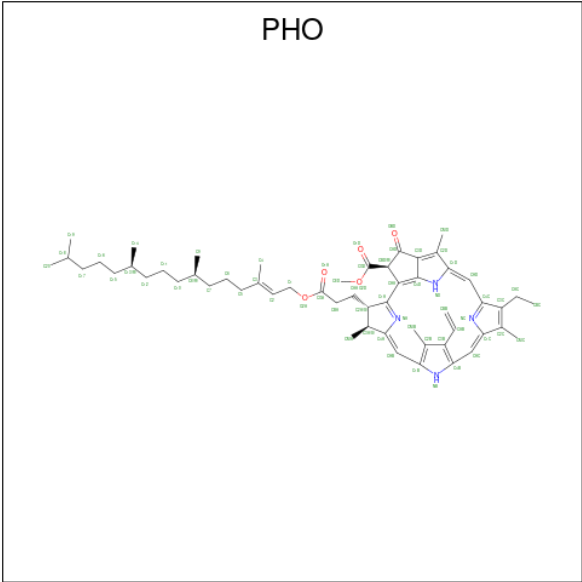
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	b	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

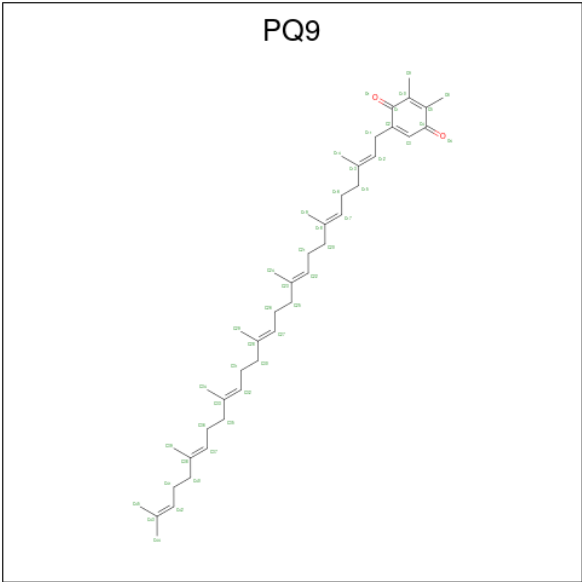
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C₅₅H₇₄N₄O₅).



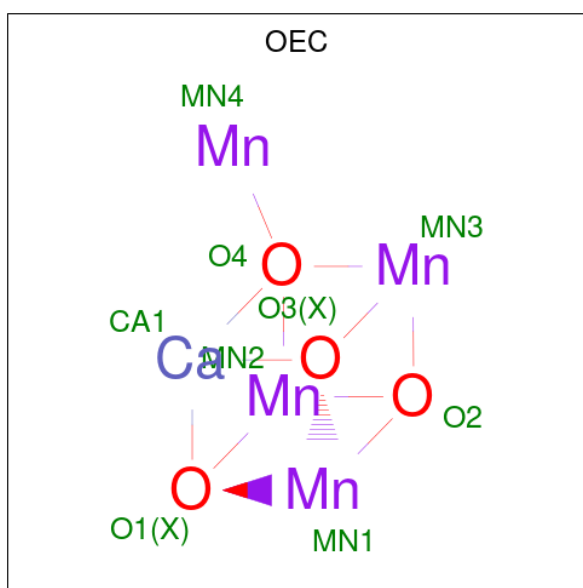
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- 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: C₄₃H₆₄O₂).



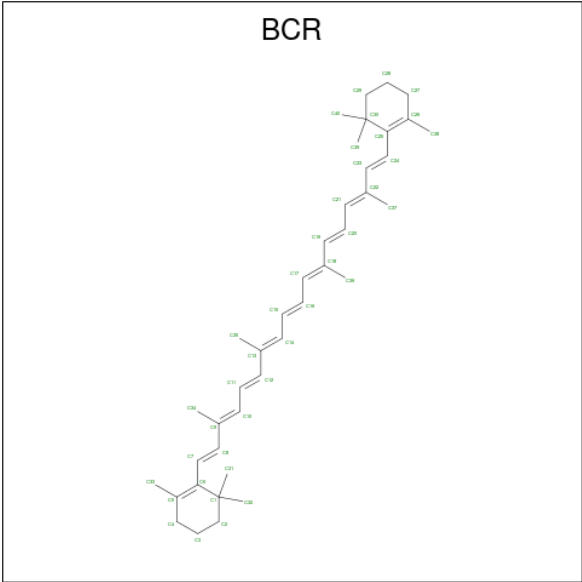
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_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: $\text{C}_{40}\text{H}_{56}$).



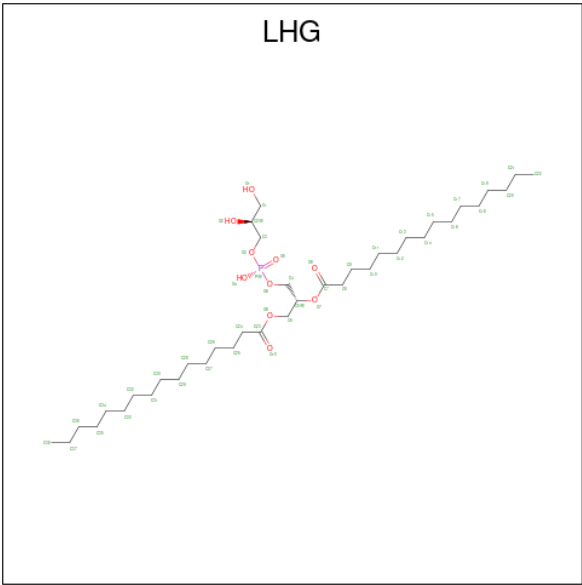
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total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

Continued on next page...

Continued from previous page...

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

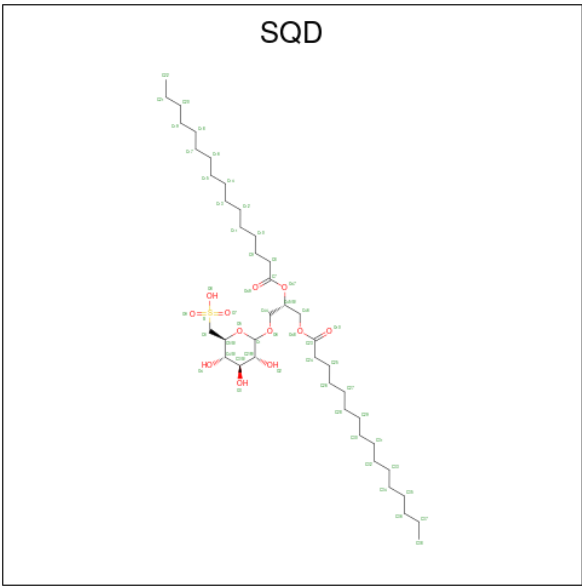
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

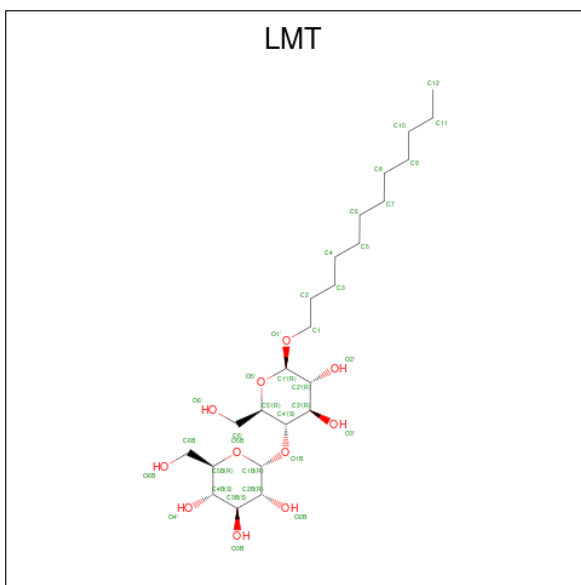
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



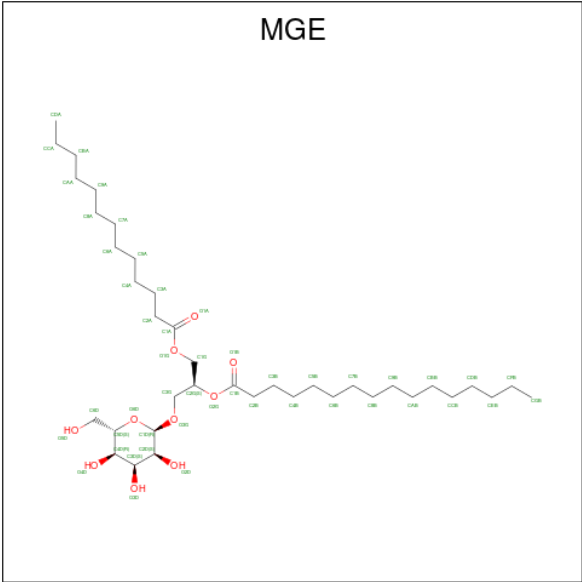
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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: $C_{38}H_{72}O_{10}$).

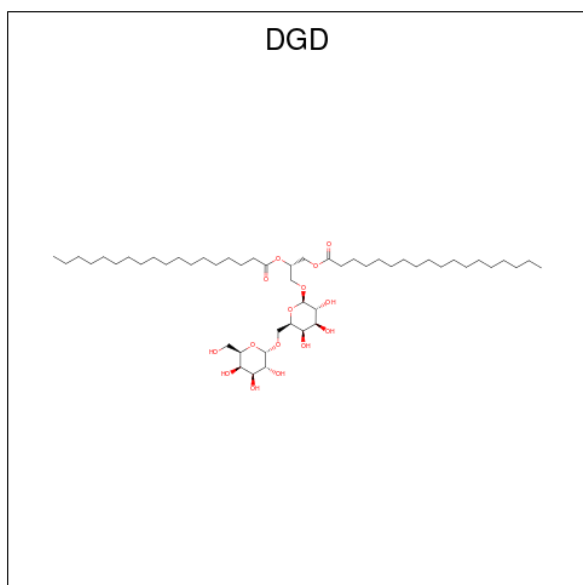


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	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 LIGAND (three-letter code: UNL) (formula:).

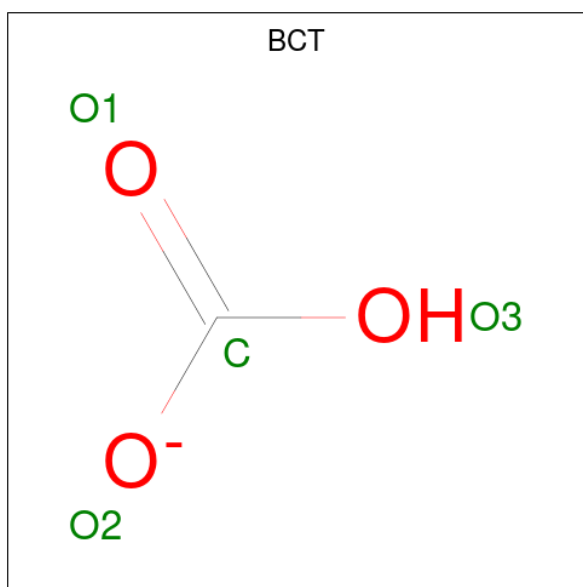
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

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



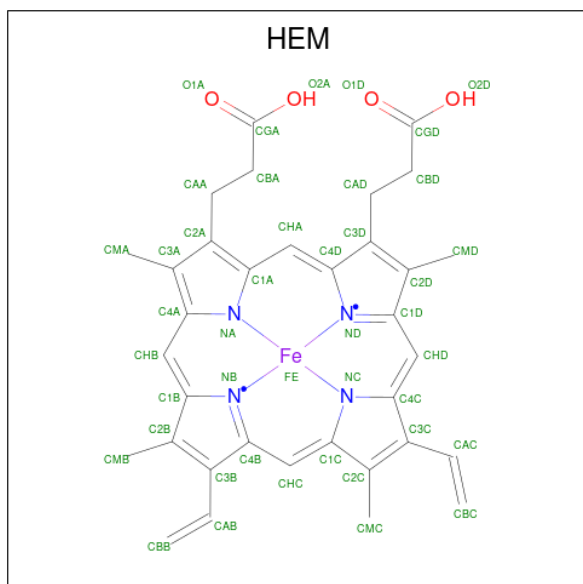
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total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

Continued on next page...

Continued from previous page...

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

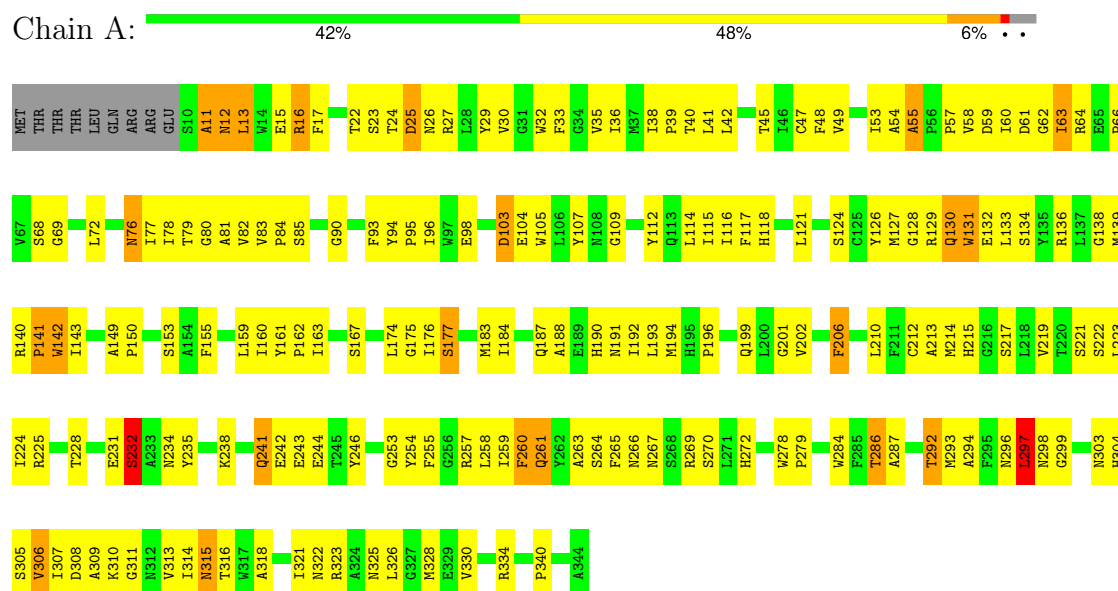
- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

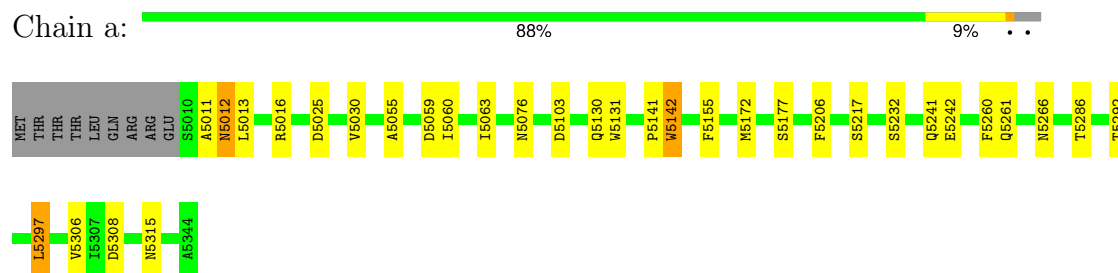
3 Residue-property plots

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.

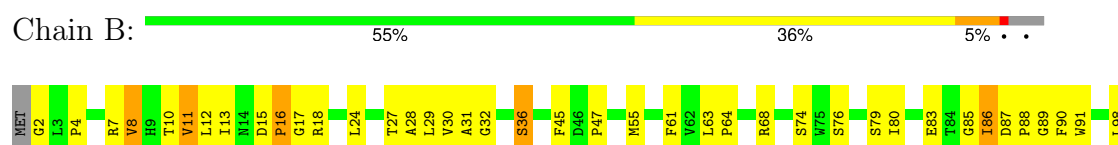
• Molecule 1: Photosystem Q(B) protein



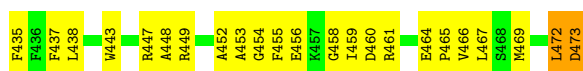
• Molecule 1: Photosystem Q(B) protein



• Molecule 2: CP47 protein

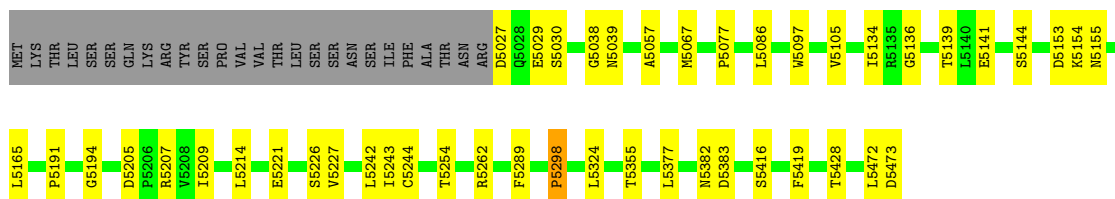






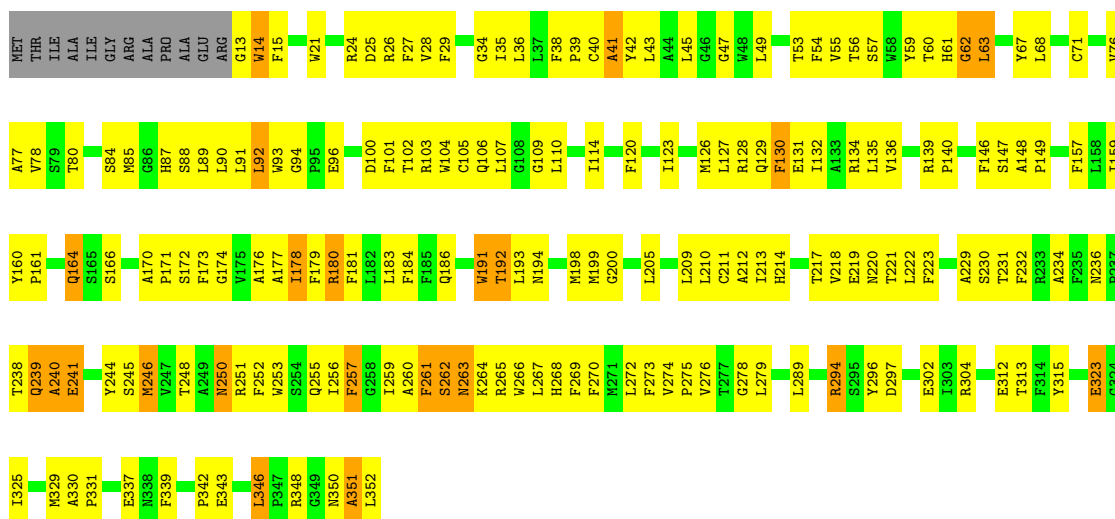
• Molecule 3: photosystem II CP43 protein

Chain c: 85% 10% 5%



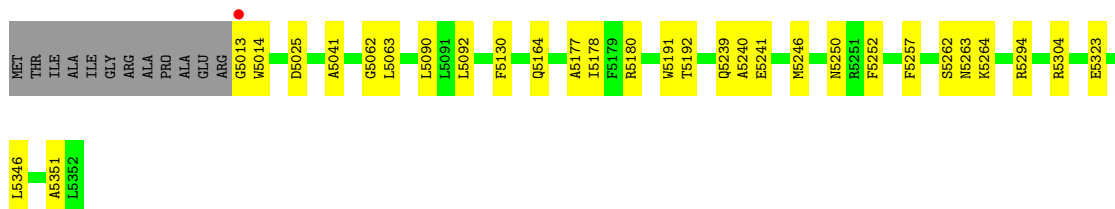
• Molecule 4: photosystem II reaction center D2 protein

Chain D: 45% 45% 7%



• Molecule 4: photosystem II reaction center D2 protein

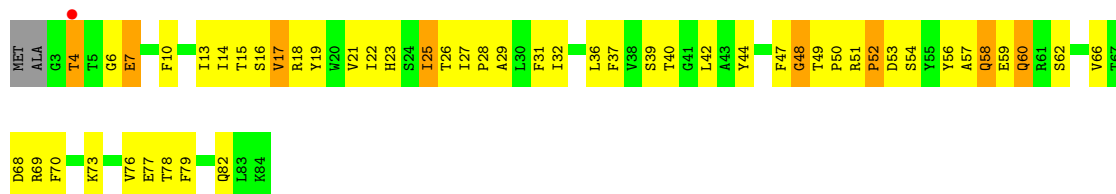
Chain d: 88% 9% 3%



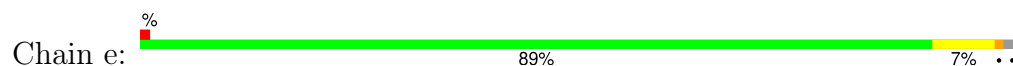
• Molecule 5: Cytochrome b559 alpha subunit

Chain E: 37% 51% 10%

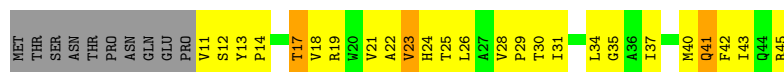




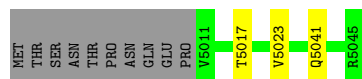
- Molecule 5: Cytochrome b559 alpha subunit



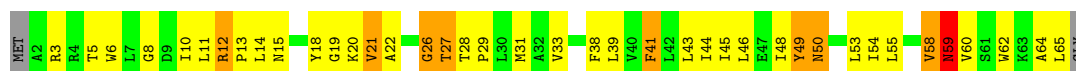
- Molecule 6: Cytochrome b559 beta subunit



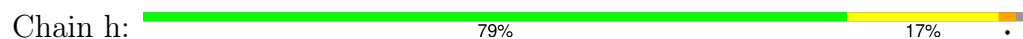
- Molecule 6: Cytochrome b559 beta subunit



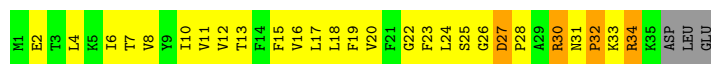
- Molecule 7: Photosystem II reaction center H protein



- Molecule 7: Photosystem II reaction center H protein

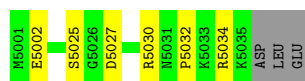


- Molecule 8: Photosystem II reaction center I protein




- 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%



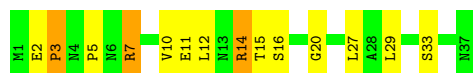
- Molecule 10: Photosystem II reaction center protein K

Chain k:  89% 11%




- Molecule 11: Photosystem II reaction center L protein

Chain L:  62% 30% 8%



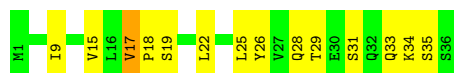
- Molecule 11: Photosystem II reaction center L protein

Chain l:  84% 16%



- Molecule 12: Photosystem II reaction center M protein

Chain M:  61% 36% .



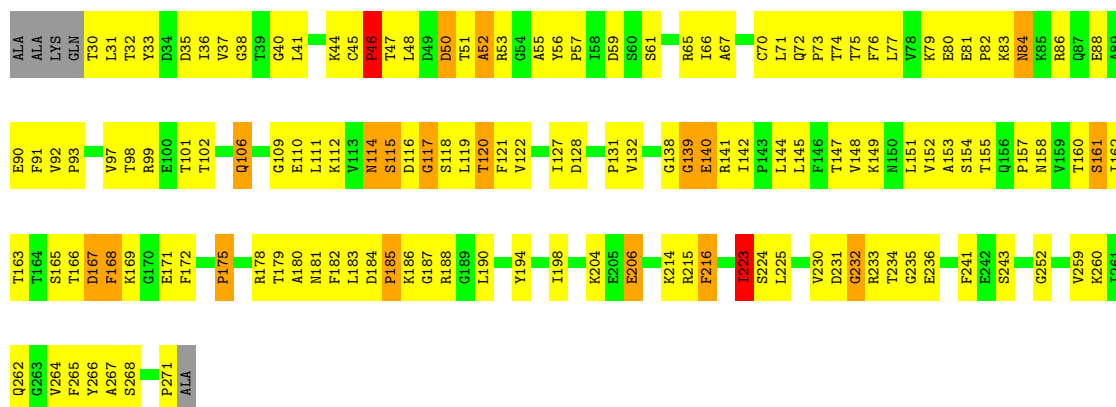
- Molecule 12: Photosystem II reaction center M protein

Chain m:  94% 6%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  41% 49% 7% ..



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  88% 9% ..




- Molecule 14: Photosystem II reaction center T protein

Chain T:  50% 41% 6%

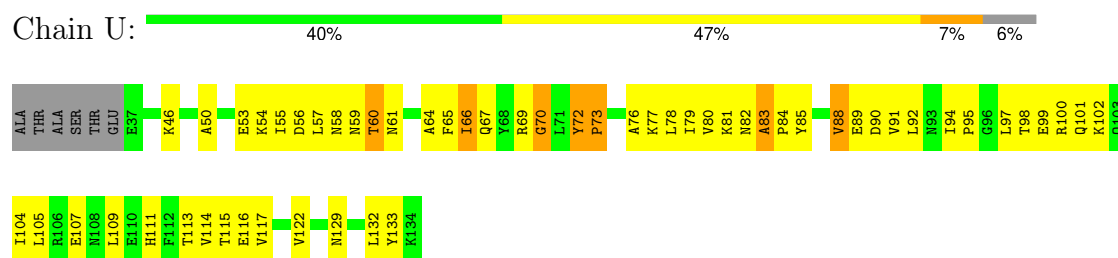


- Molecule 14: Photosystem II reaction center T protein

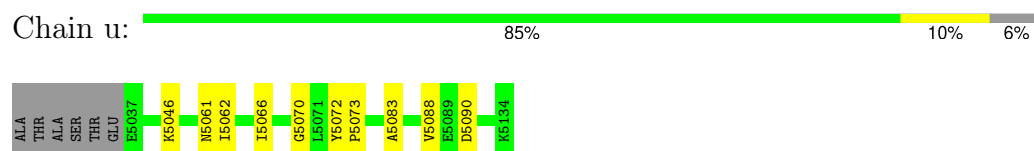
Chain t:  91% 6%



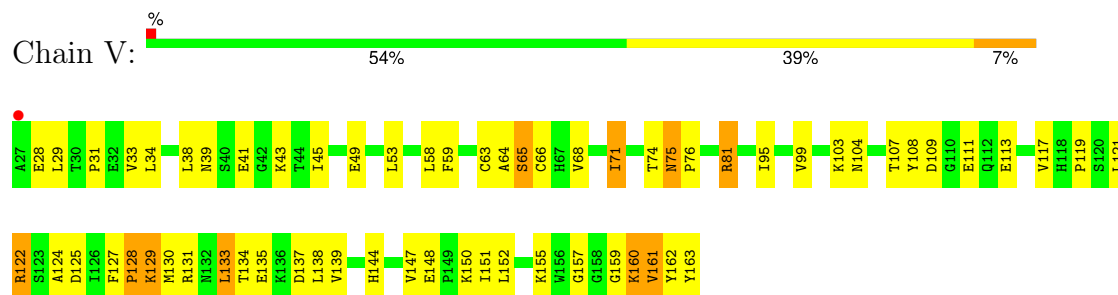
- Molecule 15: Photosystem II 12 kDa extrinsic protein



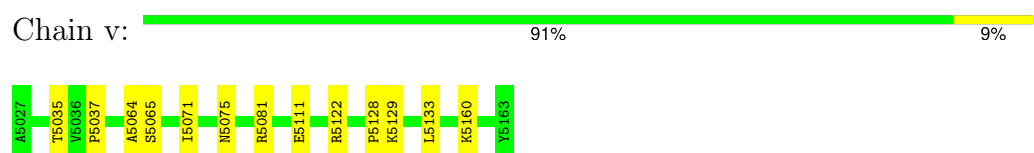
- Molecule 15: Photosystem II 12 kDa extrinsic protein



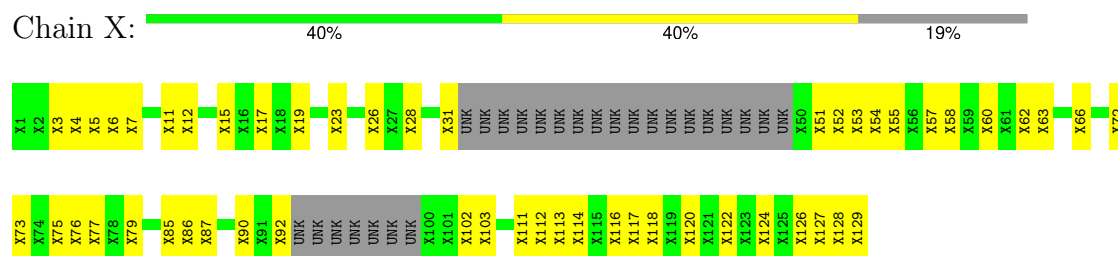
- Molecule 16: Cytochrome c-550



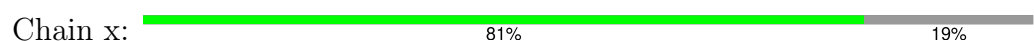
- Molecule 16: Cytochrome c-550



- Molecule 17: Unassigned subunits



- Molecule 17: Unassigned subunits





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 79.0 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1860 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	0	1	0
29	c	152	0	0	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	47073	1537	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 1537 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	12
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	1	10
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	2	14
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	3	16
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	1	8
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	1	8
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	2	11
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	2	13
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	4
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	4
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	7
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	7
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%)	3	20
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	3	20
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	0	2
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	0	2
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	8
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	0	3
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	8
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	0	3
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	7
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	1	7
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	4
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	4
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1	4
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	1	9
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	1	9
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	5
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	5
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	1	9

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%)	13	43
1	a	269/280 (96%)	252 (94%)	17 (6%)	15	45
2	B	378/407 (93%)	361 (96%)	17 (4%)	23	57
2	b	378/407 (93%)	360 (95%)	18 (5%)	21	55
3	C	341/374 (91%)	320 (94%)	21 (6%)	15	45
3	c	341/374 (91%)	320 (94%)	21 (6%)	15	45
4	D	273/283 (96%)	259 (95%)	14 (5%)	20	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	273/283 (96%)	258 (94%)	15 (6%)	18	50
5	E	68/73 (93%)	65 (96%)	3 (4%)	24	58
5	e	68/73 (93%)	66 (97%)	2 (3%)	37	70
6	F	27/39 (69%)	26 (96%)	1 (4%)	29	63
6	f	27/39 (69%)	26 (96%)	1 (4%)	29	63
7	H	50/55 (91%)	42 (84%)	8 (16%)	2	10
7	h	50/55 (91%)	43 (86%)	7 (14%)	3	13
8	I	32/35 (91%)	27 (84%)	5 (16%)	2	11
8	i	32/35 (91%)	27 (84%)	5 (16%)	2	11
9	J	22/28 (79%)	21 (96%)	1 (4%)	23	57
9	j	22/28 (79%)	21 (96%)	1 (4%)	23	57
10	K	29/30 (97%)	28 (97%)	1 (3%)	32	66
10	k	29/30 (97%)	28 (97%)	1 (3%)	32	66
11	L	34/35 (97%)	31 (91%)	3 (9%)	8	31
11	l	34/35 (97%)	31 (91%)	3 (9%)	8	31
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%)	18	50
13	o	181/208 (87%)	172 (95%)	9 (5%)	20	53
14	T	26/29 (90%)	25 (96%)	1 (4%)	28	62
14	t	26/29 (90%)	25 (96%)	1 (4%)	28	62
15	U	83/89 (93%)	80 (96%)	3 (4%)	30	64
15	u	83/89 (93%)	80 (96%)	3 (4%)	30	64
16	V	117/117 (100%)	113 (97%)	4 (3%)	32	66
16	v	117/117 (100%)	111 (95%)	6 (5%)	20	53
18	Z	43/52 (83%)	42 (98%)	1 (2%)	45	75
18	z	43/52 (83%)	42 (98%)	1 (2%)	45	75
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	18	50

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

Mol	Chain	Res	Type
1	a	5030	VAL

Continued on next page...

Continued from previous page...

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	4 (8%)
32	HEM	V	552	16	42,50,50	2.00	14 (33%)	46,82,82	2.34	13 (28%)
20	CLA	c	5501	3	63,73,73	1.89	7 (11%)	74,113,113	1.91	8 (10%)
20	CLA	C	495	-	63,73,73	2.08	11 (17%)	74,113,113	1.92	12 (16%)
30	DGD	c	5508	-	48,48,67	1.48	8 (16%)	62,62,81	1.71	10 (16%)
20	CLA	B	518	2	63,73,73	1.91	6 (9%)	74,113,113	1.91	9 (12%)
24	BCR	X	130	-	41,41,41	1.93	8 (19%)	56,56,56	2.54	23 (41%)
28	MGE	i	5201	-	48,48,48	1.24	7 (14%)	56,56,56	1.08	4 (7%)
20	CLA	c	5503	3	48,58,73	2.38	9 (18%)	56,95,113	2.08	6 (10%)
24	BCR	B	529	-	41,41,41	1.79	6 (14%)	56,56,56	2.22	21 (37%)
20	CLA	b	5513	2	63,73,73	1.70	9 (14%)	74,113,113	1.73	14 (18%)
24	BCR	c	5506	-	41,41,41	1.95	7 (17%)	56,56,56	2.16	20 (35%)
20	CLA	A	560	-	63,73,73	1.74	9 (14%)	74,113,113	1.82	12 (16%)
24	BCR	H	107	-	41,41,41	2.11	6 (14%)	56,56,56	2.29	24 (42%)
26	SQD	L	5213	-	45,47,54	2.81	24 (53%)	55,58,65	2.42	12 (21%)
20	CLA	b	5516	-	63,73,73	1.94	7 (11%)	74,113,113	1.94	8 (10%)
25	LHG	A	567	-	38,38,48	1.98	5 (13%)	41,44,54	1.51	4 (9%)
31	BCT	d	5353	19	3,3,3	2.70	1 (33%)	2,3,3	0.35	0
20	CLA	C	503	3	48,58,73	2.28	8 (16%)	56,95,113	2.08	10 (17%)
24	BCR	T	5104	-	41,41,41	1.55	9 (21%)	56,56,56	2.31	25 (44%)
27	LMT	T	217	-	36,36,36	1.40	5 (13%)	47,47,47	1.03	4 (8%)
20	CLA	B	511	-	39,49,73	2.25	11 (28%)	46,84,113	2.11	9 (19%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.96	3 (5%)
24	BCR	c	5505	-	41,41,41	2.01	8 (19%)	56,56,56	2.14	19 (33%)
31	BCT	D	353	19	3,3,3	2.28	1 (33%)	2,3,3	0.32	0
26	SQD	A	568	-	52,54,54	2.59	31 (59%)	62,65,65	2.55	18 (29%)
24	BCR	C	505	-	41,41,41	1.98	9 (21%)	56,56,56	2.13	18 (32%)
20	CLA	b	5524	2	54,64,73	1.91	6 (11%)	63,102,113	1.93	8 (12%)
20	CLA	C	497	-	63,73,73	1.78	9 (14%)	74,113,113	1.95	11 (14%)
20	CLA	b	5512	2	63,73,73	1.67	7 (11%)	74,113,113	1.69	10 (13%)
20	CLA	b	5523	-	63,73,73	1.87	10 (15%)	74,113,113	1.89	11 (14%)
20	CLA	c	5495	-	63,73,73	2.06	9 (14%)	74,113,113	1.95	13 (17%)
20	CLA	B	522	-	63,73,73	1.83	7 (11%)	74,113,113	1.75	9 (12%)
20	CLA	B	520	-	63,73,73	1.71	10 (15%)	74,113,113	1.76	12 (16%)
20	CLA	b	5526	-	63,73,73	2.01	11 (17%)	74,113,113	1.86	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	513	2	63,73,73	1.87	11 (17%)	74,113,113	1.76	11 (14%)
20	CLA	B	521	2	63,73,73	1.85	9 (14%)	74,113,113	1.90	11 (14%)
20	CLA	b	5517	-	63,73,73	1.82	8 (12%)	74,113,113	1.86	9 (12%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.46	6 (8%)
24	BCR	A	566	-	41,41,41	1.63	8 (19%)	56,56,56	2.14	22 (39%)
20	CLA	A	563	-	53,63,73	1.82	10 (18%)	62,101,113	1.86	11 (17%)
20	CLA	B	514	2	63,73,73	1.98	9 (14%)	74,113,113	1.89	10 (13%)
24	BCR	h	5107	-	41,41,41	2.04	7 (17%)	56,56,56	2.30	25 (44%)
20	CLA	B	519	-	63,73,73	2.00	8 (12%)	74,113,113	1.82	11 (14%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	1.00	3 (6%)
24	BCR	x	5130	-	41,41,41	1.95	9 (21%)	56,56,56	2.52	24 (42%)
20	CLA	c	5500	-	63,73,73	1.76	8 (12%)	74,113,113	1.79	12 (16%)
26	SQD	t	213	-	45,47,54	2.81	23 (51%)	55,58,65	2.49	14 (25%)
24	BCR	c	5504	-	41,41,41	2.18	5 (12%)	56,56,56	2.18	23 (41%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.16	6 (10%)
28	MGE	d	5360	-	41,41,48	1.19	6 (14%)	49,49,56	1.05	4 (8%)
22	PQ9	D	356	-	30,30,45	0.91	1 (3%)	38,39,57	1.68	9 (23%)
32	HEM	v	5552	16	42,50,50	2.11	15 (35%)	46,82,82	2.34	15 (32%)
20	CLA	d	5355	-	48,58,73	2.30	9 (18%)	56,95,113	2.05	9 (16%)
20	CLA	C	499	-	45,55,73	2.28	9 (20%)	52,91,113	2.09	10 (19%)
24	BCR	D	357	-	41,41,41	1.96	8 (19%)	56,56,56	2.27	20 (35%)
20	CLA	c	5493	3	63,73,73	1.81	7 (11%)	74,113,113	1.90	13 (17%)
24	BCR	a	5566	-	41,41,41	1.68	7 (17%)	56,56,56	2.14	23 (41%)
20	CLA	C	492	3	58,68,73	1.75	9 (15%)	68,107,113	1.91	11 (16%)
20	CLA	A	559	-	63,73,73	1.73	7 (11%)	74,113,113	1.72	8 (10%)
20	CLA	b	5522	-	63,73,73	1.87	8 (12%)	74,113,113	1.76	7 (9%)
20	CLA	c	5502	-	49,59,73	2.29	10 (20%)	56,96,113	2.17	11 (19%)
21	PHO	A	561	-	50,69,69	1.12	3 (6%)	48,99,99	1.69	12 (25%)
30	DGD	C	509	-	58,58,67	1.12	7 (12%)	72,72,81	1.40	5 (6%)
20	CLA	B	517	-	63,73,73	2.03	7 (11%)	74,113,113	1.96	12 (16%)
20	CLA	A	558	1	63,73,73	1.70	8 (12%)	74,113,113	1.71	10 (13%)
20	CLA	b	5511	-	39,49,73	2.46	10 (25%)	46,84,113	2.18	9 (19%)
20	CLA	b	5525	-	63,73,73	1.85	6 (9%)	74,113,113	1.87	9 (12%)
20	CLA	d	5354	4	63,73,73	1.64	10 (15%)	74,113,113	1.75	11 (14%)
27	LMT	A	569	-	36,36,36	1.54	6 (16%)	47,47,47	1.07	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.06	2 (3%)
20	CLA	c	5499	-	45,55,73	2.04	8 (17%)	52,91,113	2.04	8 (15%)
20	CLA	b	5515	-	63,73,73	1.71	11 (17%)	74,113,113	1.83	15 (20%)
20	CLA	b	5518	2	63,73,73	1.91	6 (9%)	74,113,113	1.89	11 (14%)
20	CLA	a	5563	-	53,63,73	1.84	9 (16%)	62,101,113	1.80	11 (17%)
22	PQ9	A	564	-	30,30,45	0.85	0	38,39,57	1.50	8 (21%)
20	CLA	B	512	2	63,73,73	1.67	7 (11%)	74,113,113	1.73	12 (16%)
20	CLA	c	5498	3	63,73,73	1.86	8 (12%)	74,113,113	1.88	12 (16%)
20	CLA	C	496	3	63,73,73	1.89	11 (17%)	74,113,113	1.87	13 (17%)
20	CLA	B	525	-	63,73,73	1.82	7 (11%)	74,113,113	1.84	9 (12%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.11	6 (10%)
20	CLA	c	5491	3	63,73,73	1.90	7 (11%)	74,113,113	1.91	10 (13%)
27	LMT	M	5216	-	36,36,36	1.45	8 (22%)	47,47,47	0.92	2 (4%)
20	CLA	C	500	-	63,73,73	1.66	10 (15%)	74,113,113	1.78	12 (16%)
24	BCR	b	5529	-	41,41,41	1.66	6 (14%)	56,56,56	2.15	21 (37%)
24	BCR	C	504	-	41,41,41	1.87	6 (14%)	56,56,56	2.21	22 (39%)
21	PHO	a	5562	-	50,69,69	1.09	3 (6%)	48,99,99	1.64	11 (22%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.12	4 (7%)
24	BCR	t	104	-	41,41,41	1.67	10 (24%)	56,56,56	2.28	23 (41%)
20	CLA	B	524	2	54,64,73	2.01	6 (11%)	63,102,113	2.04	9 (14%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.67	11 (17%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.47	7 (10%)
22	PQ9	d	5356	-	30,30,45	0.82	0	38,39,57	1.66	6 (15%)
28	MGE	l	5210	-	48,48,48	0.90	4 (8%)	56,56,56	1.12	5 (8%)
21	PHO	a	5561	-	50,69,69	1.13	5 (10%)	48,99,99	1.57	11 (22%)
20	CLA	C	493	3	63,73,73	1.81	8 (12%)	74,113,113	1.91	13 (17%)
20	CLA	c	5492	3	58,68,73	1.76	9 (15%)	68,107,113	1.93	9 (13%)
24	BCR	b	5527	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
26	SQD	d	5358	-	52,54,54	2.58	29 (55%)	62,65,65	2.53	18 (29%)
24	BCR	B	527	-	41,41,41	1.74	8 (19%)	56,56,56	2.08	16 (28%)
28	MGE	L	210	-	48,48,48	0.99	3 (6%)	56,56,56	1.15	5 (8%)
20	CLA	a	5558	1	63,73,73	1.67	11 (17%)	74,113,113	1.66	12 (16%)
24	BCR	b	5528	-	41,41,41	1.74	6 (14%)	56,56,56	2.06	17 (30%)
32	HEM	f	5051	6,5	42,50,50	2.08	14 (33%)	46,82,82	2.49	14 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	5212	-	24,26,54	2.85	13 (54%)	34,37,65	2.65	11 (32%)
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.55	8 (11%)
20	CLA	C	494	-	44,54,73	1.97	7 (15%)	51,90,113	2.23	9 (17%)
20	CLA	C	502	-	49,59,73	2.16	10 (20%)	56,96,113	2.13	11 (19%)
20	CLA	b	5520	-	63,73,73	1.81	11 (17%)	74,113,113	1.75	11 (14%)
24	BCR	C	506	-	41,41,41	1.74	8 (19%)	56,56,56	2.23	21 (37%)
32	HEM	F	51	6,5	42,50,50	2.06	15 (35%)	46,82,82	2.41	15 (32%)
24	BCR	d	5357	-	41,41,41	2.02	8 (19%)	56,56,56	2.33	21 (37%)
20	CLA	c	5496	-	63,73,73	1.78	9 (14%)	74,113,113	1.81	11 (14%)
21	PHO	A	562	-	50,69,69	1.12	3 (6%)	48,99,99	1.66	10 (20%)
20	CLA	C	498	3	63,73,73	1.69	6 (9%)	74,113,113	1.84	10 (13%)
27	LMT	a	5568	-	36,36,36	1.46	6 (16%)	47,47,47	1.09	1 (2%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.07	4 (7%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.56	9 (13%)
20	CLA	c	5497	-	63,73,73	1.81	10 (15%)	74,113,113	1.85	11 (14%)
20	CLA	D	355	-	48,58,73	2.30	11 (22%)	56,95,113	2.07	11 (19%)
25	LHG	a	5567	-	38,38,48	2.02	5 (13%)	41,44,54	1.46	4 (9%)
20	CLA	b	5521	2	63,73,73	1.56	6 (9%)	74,113,113	1.84	12 (16%)
22	PQ9	a	5564	-	30,30,45	0.86	1 (3%)	38,39,57	1.46	6 (15%)
20	CLA	B	516	-	63,73,73	1.82	6 (9%)	74,113,113	1.90	8 (10%)
20	CLA	B	523	-	63,73,73	1.98	8 (12%)	74,113,113	1.86	11 (14%)
27	LMT	m	216	-	36,36,36	1.45	7 (19%)	47,47,47	0.98	3 (6%)
20	CLA	C	491	3	63,73,73	1.76	7 (11%)	74,113,113	1.70	8 (10%)
26	SQD	a	212	-	24,26,54	3.09	13 (54%)	34,37,65	2.73	13 (38%)
20	CLA	D	354	4	63,73,73	1.70	8 (12%)	74,113,113	1.68	10 (13%)
20	CLA	a	5559	-	63,73,73	1.61	6 (9%)	74,113,113	1.75	10 (13%)
30	DGD	c	5509	-	58,58,67	1.35	7 (12%)	72,72,81	1.39	6 (8%)
20	CLA	B	515	-	63,73,73	1.78	10 (15%)	74,113,113	1.86	14 (18%)
20	CLA	c	5494	-	44,54,73	2.00	6 (13%)	51,90,113	2.05	9 (17%)
20	CLA	a	5560	-	63,73,73	1.78	9 (14%)	74,113,113	1.84	11 (14%)
20	CLA	B	526	-	63,73,73	1.94	14 (22%)	74,113,113	1.84	10 (13%)
24	BCR	B	528	-	41,41,41	1.93	6 (14%)	56,56,56	2.02	17 (30%)
20	CLA	b	5514	2	63,73,73	1.99	9 (14%)	74,113,113	1.92	10 (13%)
20	CLA	b	5519	-	63,73,73	1.92	8 (12%)	74,113,113	1.81	12 (16%)
20	CLA	C	501	3	63,73,73	2.06	9 (14%)	74,113,113	1.94	11 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
32	HEM	V	552	16	-	4/12/54/54	-
20	CLA	c	5501	3	1/1/15/20	11/37/115/115	-
20	CLA	C	495	-	1/1/15/20	16/37/115/115	-
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
20	CLA	B	518	2	1/1/15/20	14/37/115/115	-
24	BCR	X	130	-	-	5/29/63/63	0/2/2/2
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
20	CLA	c	5503	3	1/1/12/20	5/19/97/115	-
24	BCR	B	529	-	-	3/29/63/63	0/2/2/2
20	CLA	b	5513	2	1/1/15/20	10/37/115/115	-
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
20	CLA	A	560	-	1/1/15/20	7/37/115/115	-
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
26	SQD	L	5213	-	-	21/42/62/69	0/1/1/1
20	CLA	b	5516	-	1/1/15/20	13/37/115/115	-
25	LHG	A	567	-	-	16/43/43/53	-
20	CLA	C	503	3	1/1/12/20	5/19/97/115	-
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
20	CLA	B	511	-	1/1/10/20	2/8/86/115	-
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
20	CLA	b	5524	2	1/1/13/20	7/27/105/115	-
20	CLA	C	497	-	1/1/15/20	7/37/115/115	-
20	CLA	b	5512	2	1/1/15/20	10/37/115/115	-
20	CLA	b	5523	-	1/1/15/20	13/37/115/115	-
20	CLA	c	5495	-	1/1/15/20	16/37/115/115	-
20	CLA	B	522	-	1/1/15/20	12/37/115/115	-
20	CLA	B	520	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5526	-	1/1/15/20	10/37/115/115	-
20	CLA	B	513	2	1/1/15/20	12/37/115/115	-
20	CLA	B	521	2	1/1/15/20	7/37/115/115	-
20	CLA	b	5517	-	1/1/15/20	12/37/115/115	-
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
20	CLA	A	563	-	1/1/13/20	5/25/103/115	-
20	CLA	B	514	2	1/1/15/20	11/37/115/115	-
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
20	CLA	B	519	-	1/1/15/20	11/37/115/115	-
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5500	-	1/1/15/20	11/37/115/115	-
26	SQD	t	213	-	-	20/42/62/69	0/1/1/1
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
32	HEM	v	5552	16	-	4/12/54/54	-
20	CLA	d	5355	-	1/1/12/20	9/19/97/115	-
20	CLA	C	499	-	1/1/11/20	6/16/94/115	-
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5493	3	1/1/15/20	10/37/115/115	-
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2
20	CLA	C	492	3	1/1/14/20	9/31/109/115	-
20	CLA	A	559	-	1/1/15/20	12/37/115/115	-
20	CLA	b	5522	-	1/1/15/20	12/37/115/115	-
20	CLA	c	5502	-	1/1/12/20	6/21/99/115	-
21	PHO	A	561	-	-	12/37/103/103	0/5/6/6
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
20	CLA	B	517	-	1/1/15/20	12/37/115/115	-
20	CLA	A	558	1	1/1/15/20	8/37/115/115	-
20	CLA	b	5511	-	1/1/10/20	2/8/86/115	-
20	CLA	b	5525	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	d	5354	4	1/1/15/20	8/37/115/115	-
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	c	5499	-	1/1/11/20	6/16/94/115	-
20	CLA	b	5515	-	1/1/15/20	17/37/115/115	-
20	CLA	b	5518	2	1/1/15/20	14/37/115/115	-
20	CLA	a	5563	-	1/1/13/20	5/25/103/115	-
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	512	2	1/1/15/20	10/37/115/115	-
20	CLA	c	5498	3	1/1/15/20	16/37/115/115	-
20	CLA	C	496	3	1/1/15/20	11/37/115/115	-
20	CLA	B	525	-	1/1/15/20	12/37/115/115	-
28	MGE	d	5359	-	-	13/42/62/63	0/1/1/1
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
20	CLA	c	5491	3	1/1/15/20	9/37/115/115	-
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
20	CLA	C	500	-	1/1/15/20	11/37/115/115	-
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
21	PHO	a	5562	-	-	9/37/103/103	0/5/6/6
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
20	CLA	B	524	2	1/1/13/20	7/27/105/115	-
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
28	MGE	l	5210	-	-	23/43/63/63	0/1/1/1
21	PHO	a	5561	-	-	12/37/103/103	0/5/6/6
20	CLA	C	493	3	1/1/15/20	10/37/115/115	-
20	CLA	c	5492	3	1/1/14/20	9/31/109/115	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
28	MGE	L	210	-	-	23/43/63/63	0/1/1/1
20	CLA	a	5558	1	1/1/15/20	9/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
32	HEM	f	5051	6,5	-	2/12/54/54	-
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
26	SQD	A	5212	-	-	5/19/39/69	0/1/1/1
20	CLA	C	494	-	1/1/11/20	7/15/93/115	-
20	CLA	C	502	-	1/1/12/20	7/21/99/115	-
20	CLA	b	5520	-	1/1/15/20	11/37/115/115	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
32	HEM	F	51	6,5	-	2/12/54/54	-
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5496	-	1/1/15/20	11/37/115/115	-
21	PHO	A	562	-	-	9/37/103/103	0/5/6/6
20	CLA	C	498	3	1/1/15/20	16/37/115/115	-
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
28	MGE	I	201	-	-	24/43/63/63	0/1/1/1
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	c	5497	-	1/1/15/20	8/37/115/115	-
20	CLA	D	355	-	1/1/12/20	9/19/97/115	-
25	LHG	a	5567	-	-	14/43/43/53	-
20	CLA	b	5521	2	1/1/15/20	7/37/115/115	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
20	CLA	B	516	-	1/1/15/20	13/37/115/115	-
20	CLA	B	523	-	1/1/15/20	13/37/115/115	-
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	C	491	3	1/1/15/20	7/37/115/115	-
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
20	CLA	D	354	4	1/1/15/20	10/37/115/115	-
20	CLA	a	5559	-	1/1/15/20	12/37/115/115	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
20	CLA	B	515	-	1/1/15/20	17/37/115/115	-
20	CLA	c	5494	-	1/1/11/20	7/15/93/115	-
20	CLA	a	5560	-	1/1/15/20	7/37/115/115	-
20	CLA	B	526	-	1/1/15/20	10/37/115/115	-
24	BCR	B	528	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5514	2	1/1/15/20	12/37/115/115	-
20	CLA	b	5519	-	1/1/15/20	11/37/115/115	-
20	CLA	C	501	3	1/1/15/20	13/37/115/115	-

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:

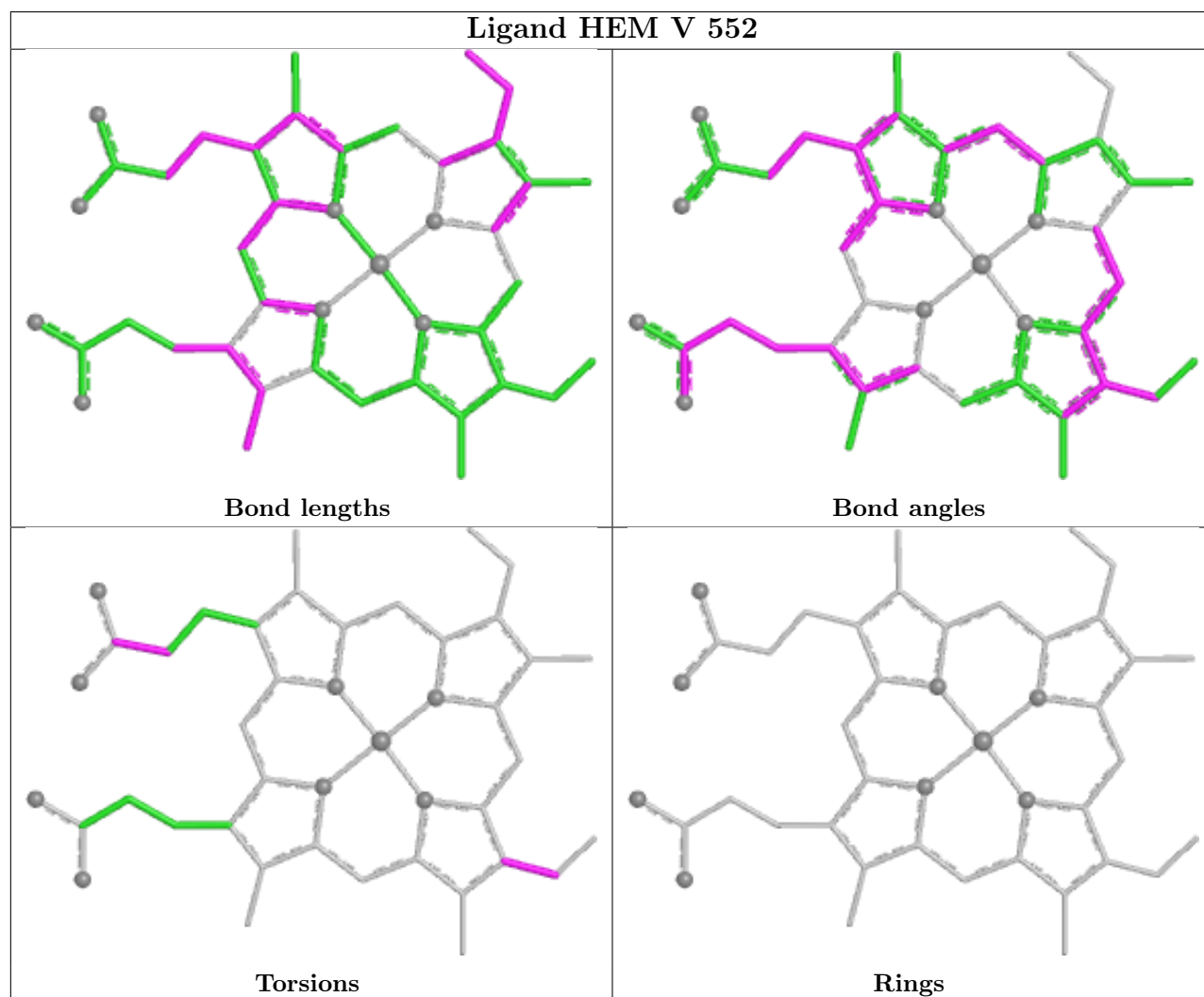
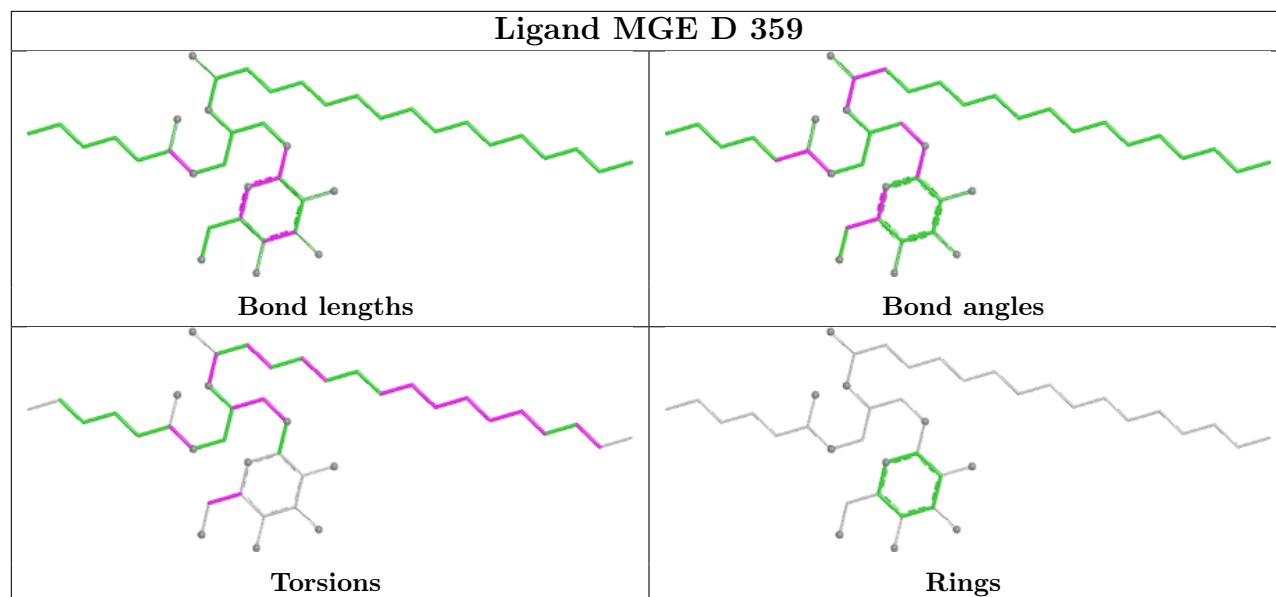
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	D	359	MGE	1	0
32	V	552	HEM	2	0
20	C	495	CLA	9	0
20	B	518	CLA	11	0
24	X	130	BCR	9	0
24	B	529	BCR	2	0
20	A	560	CLA	1	0
24	H	107	BCR	3	0
25	A	567	LHG	4	0
20	C	503	CLA	1	0
24	T	5104	BCR	5	0
27	T	217	LMT	3	0
20	B	511	CLA	1	0
28	D	358	MGE	2	0
24	C	505	BCR	6	0
20	C	497	CLA	5	0
20	B	522	CLA	4	0
20	B	520	CLA	6	0
20	B	513	CLA	8	0
20	B	521	CLA	2	0
24	A	566	BCR	1	0
20	B	514	CLA	5	0
20	B	519	CLA	5	0
28	B	530	MGE	1	0
22	D	356	PQ9	7	0
20	C	499	CLA	2	0
24	D	357	BCR	4	0
20	C	492	CLA	2	0
20	A	559	CLA	5	0
21	A	561	PHO	7	0
30	C	509	DGD	10	0
20	B	517	CLA	9	0
20	A	558	CLA	10	0
22	A	564	PQ9	2	0
20	B	512	CLA	2	0
20	C	496	CLA	2	0
20	B	525	CLA	4	0
20	C	500	CLA	3	0
24	C	504	BCR	7	0
28	D	360	MGE	7	0
20	B	524	CLA	4	0
30	C	508	DGD	2	0

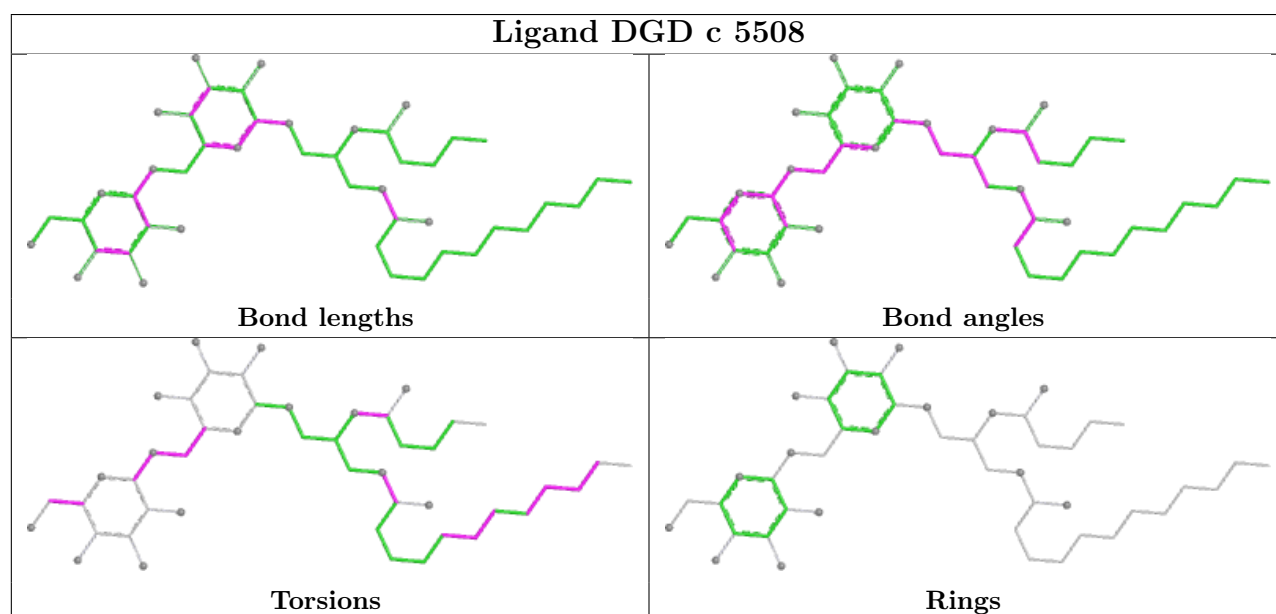
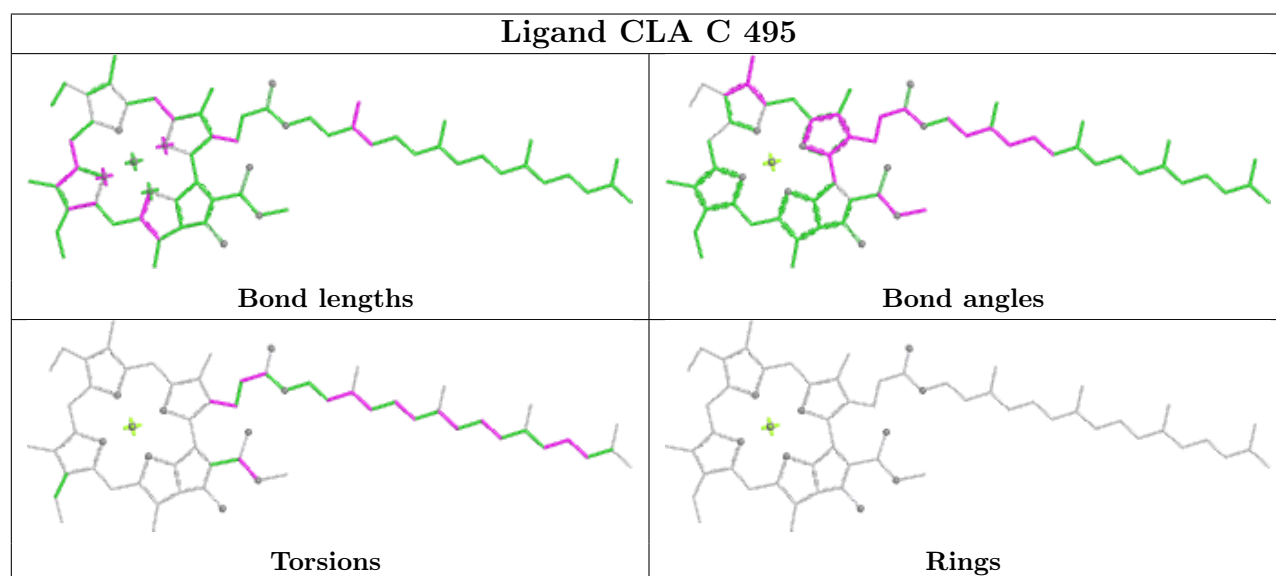
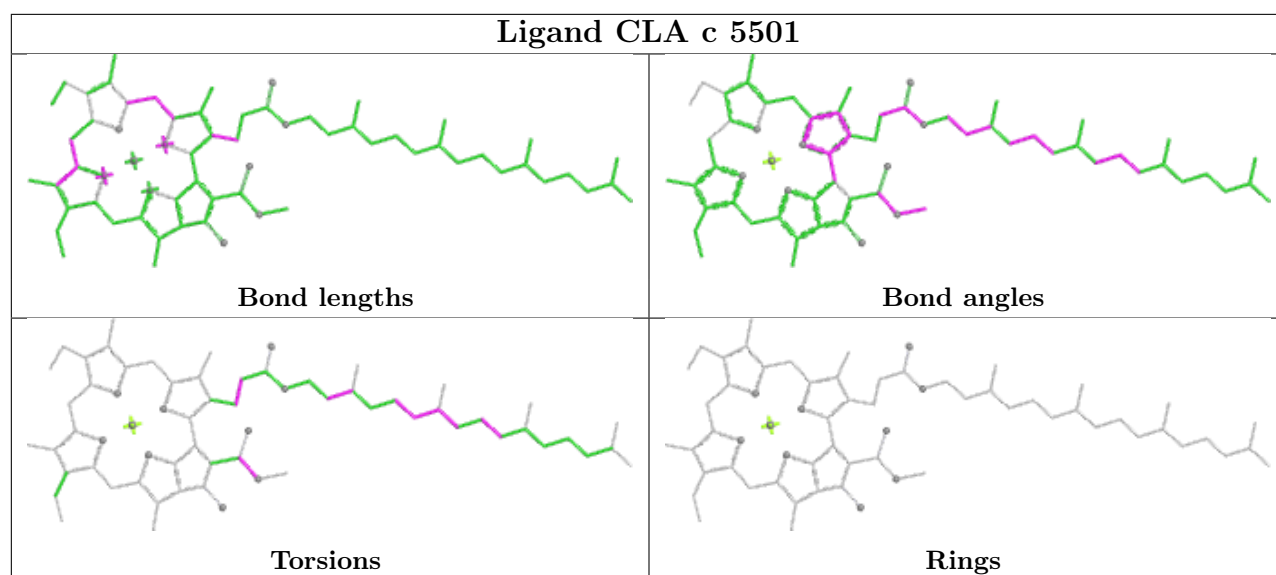
Continued on next page...

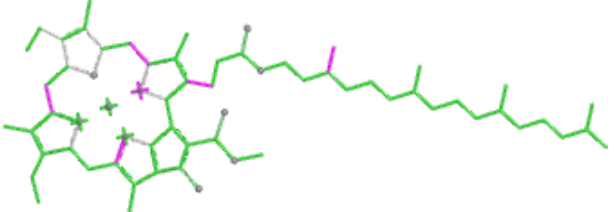
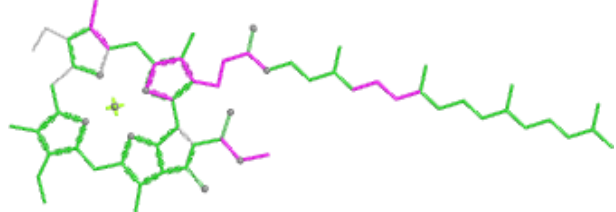
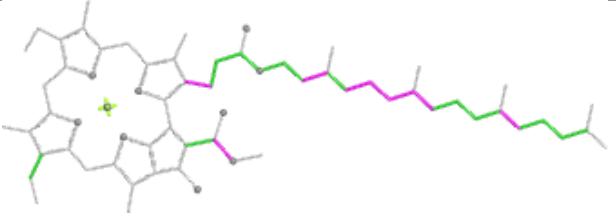
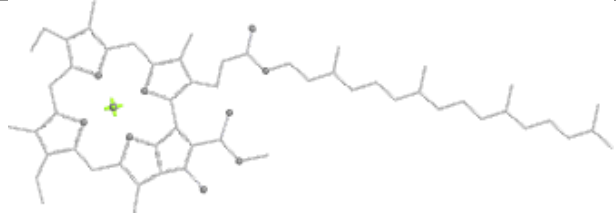
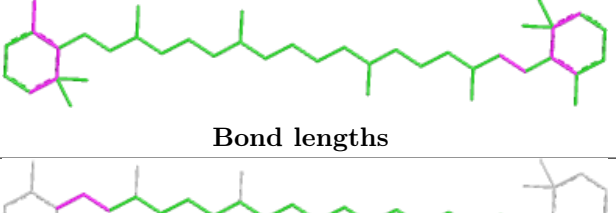
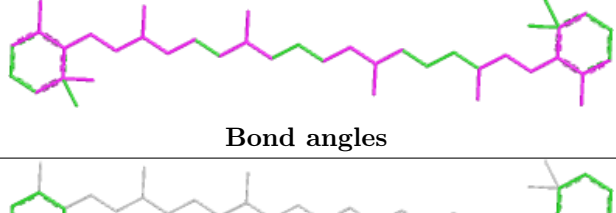
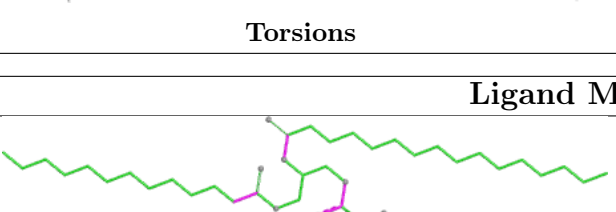
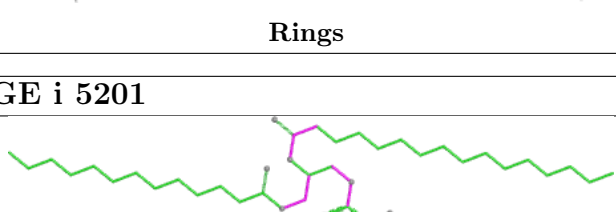
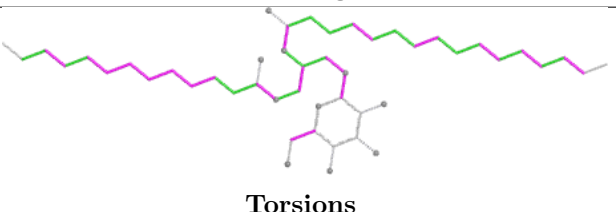
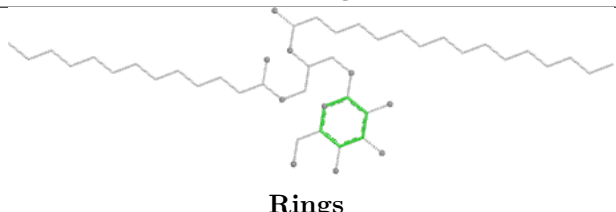


Continued from previous page...

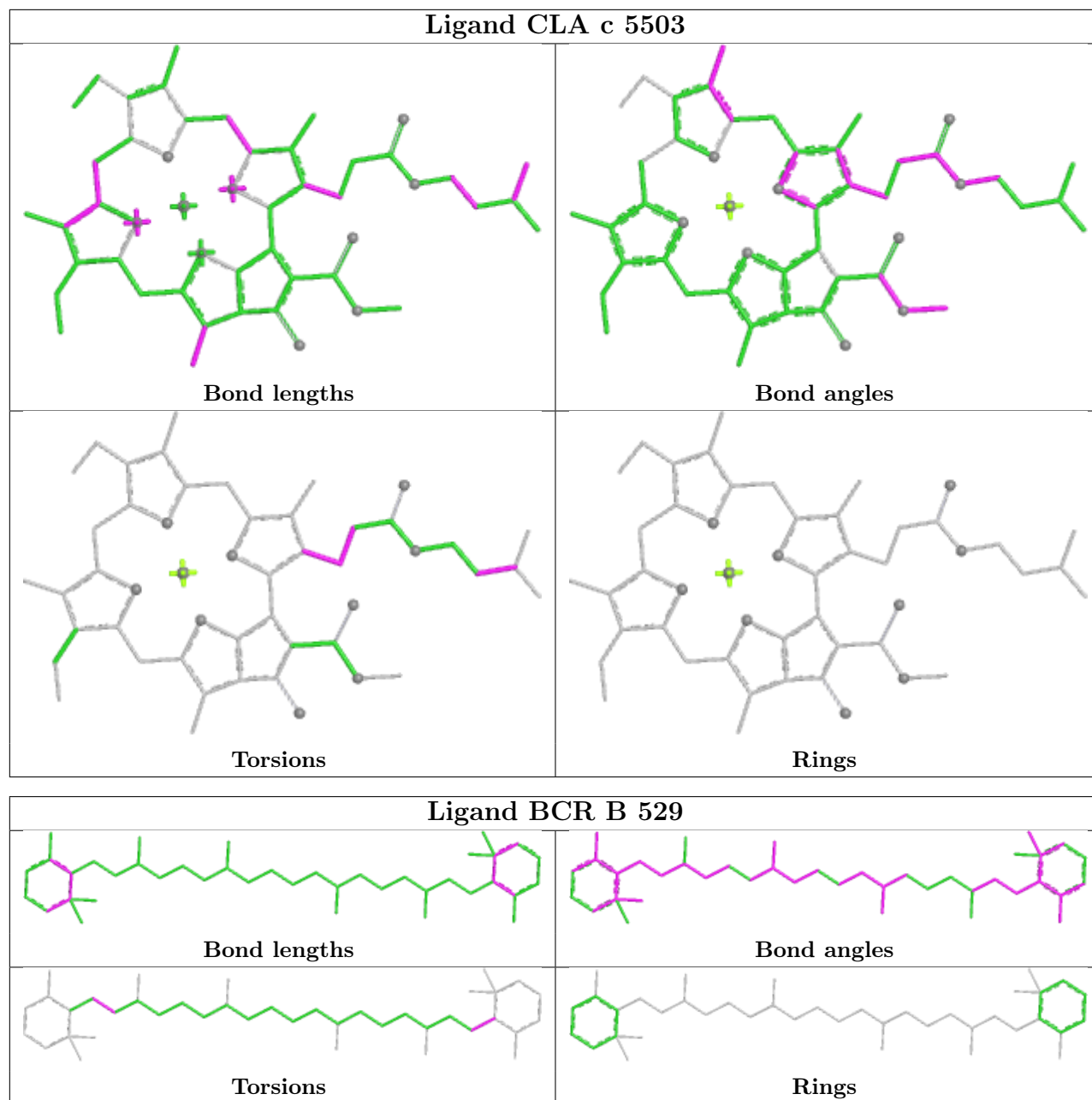
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	507	DGD	6	0
20	C	493	CLA	7	0
24	B	527	BCR	2	0
28	L	210	MGE	2	0
30	H	208	DGD	3	0
20	C	494	CLA	2	0
20	C	502	CLA	2	0
24	C	506	BCR	7	0
32	F	51	HEM	3	0
21	A	562	PHO	5	0
20	C	498	CLA	6	0
28	I	201	MGE	1	0
20	D	355	CLA	3	0
20	B	516	CLA	6	0
20	B	523	CLA	2	0
20	C	491	CLA	4	0
20	D	354	CLA	5	0
20	B	515	CLA	12	0
20	B	526	CLA	2	0
24	B	528	BCR	2	0
20	C	501	CLA	13	0

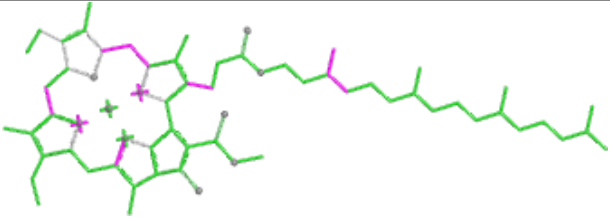
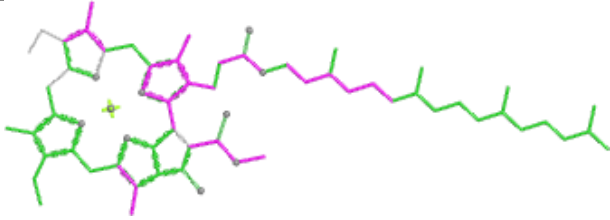
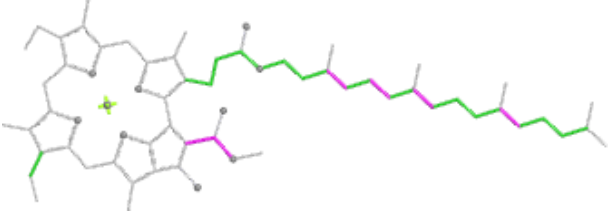
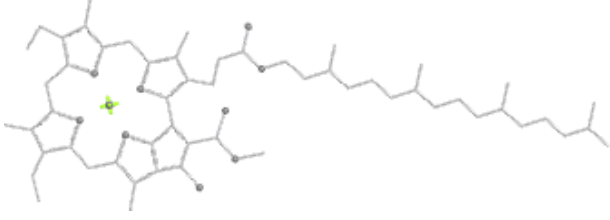
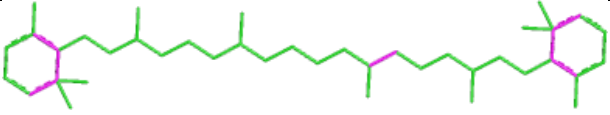

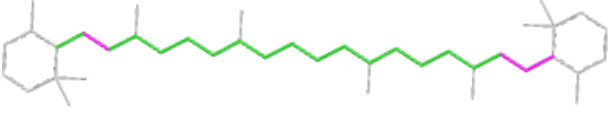
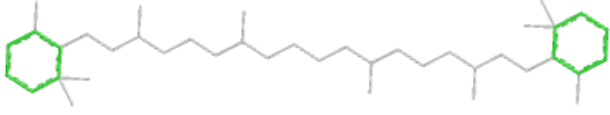
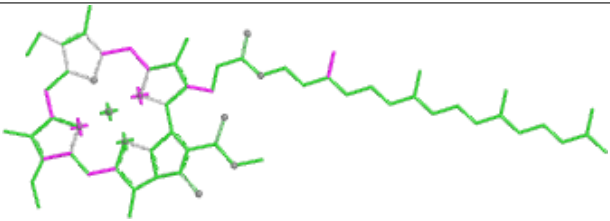
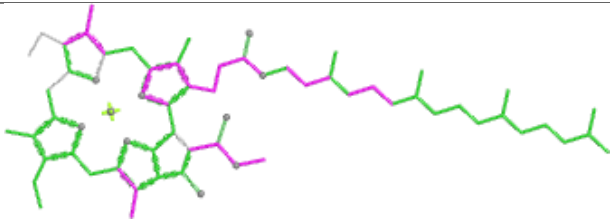
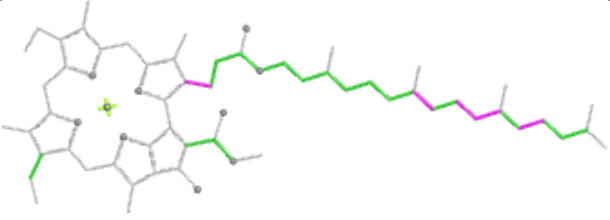
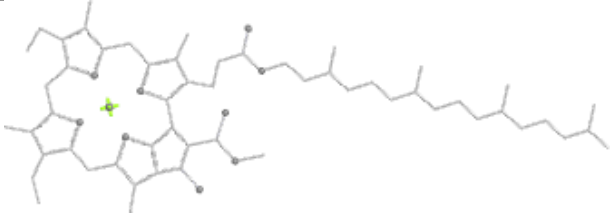
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

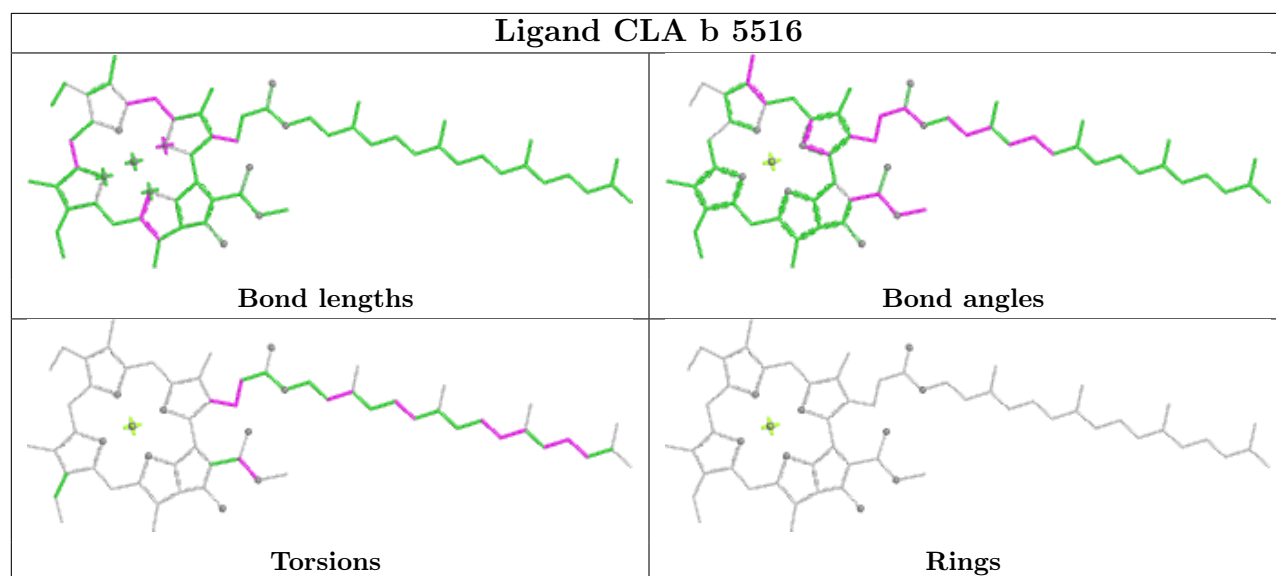
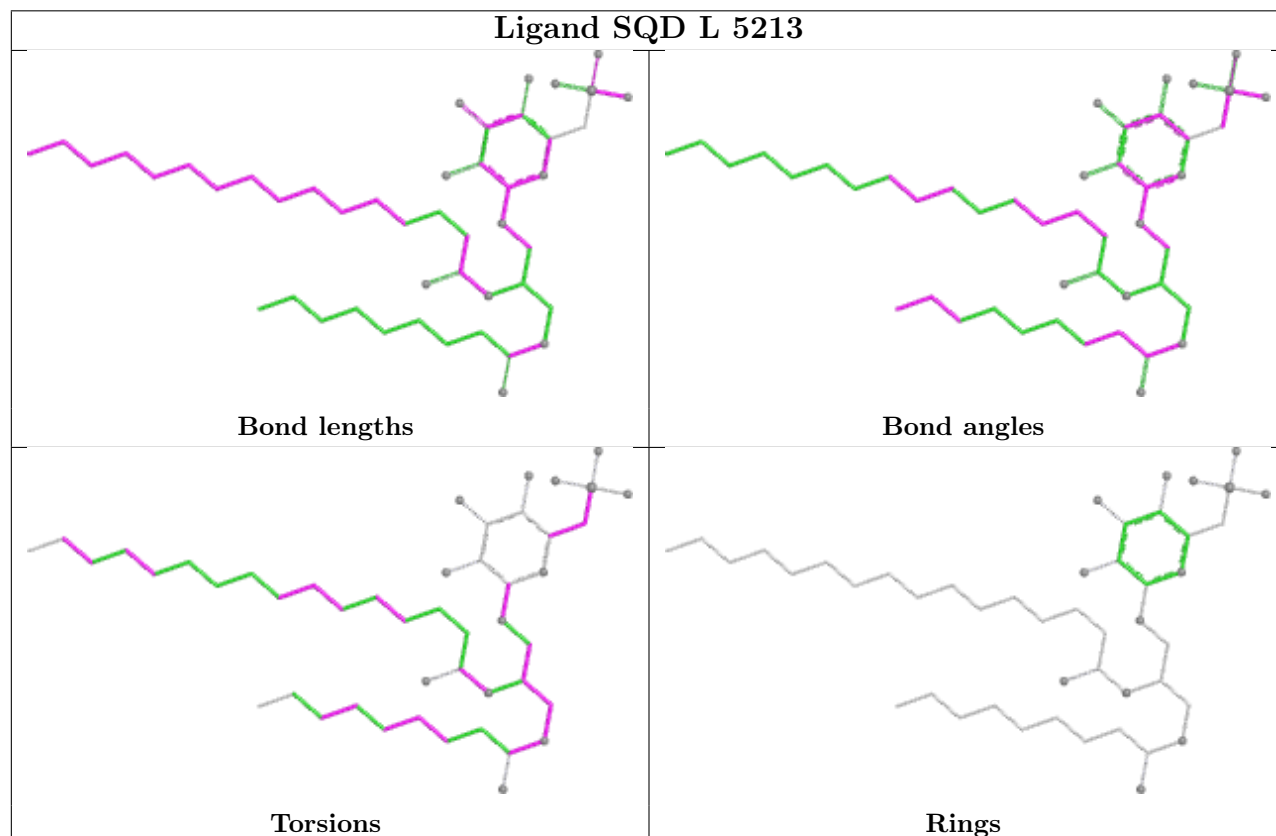
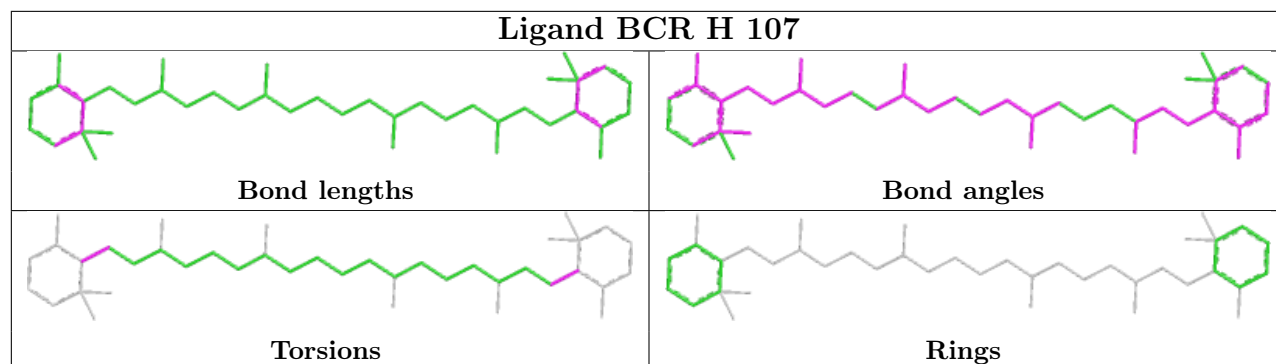


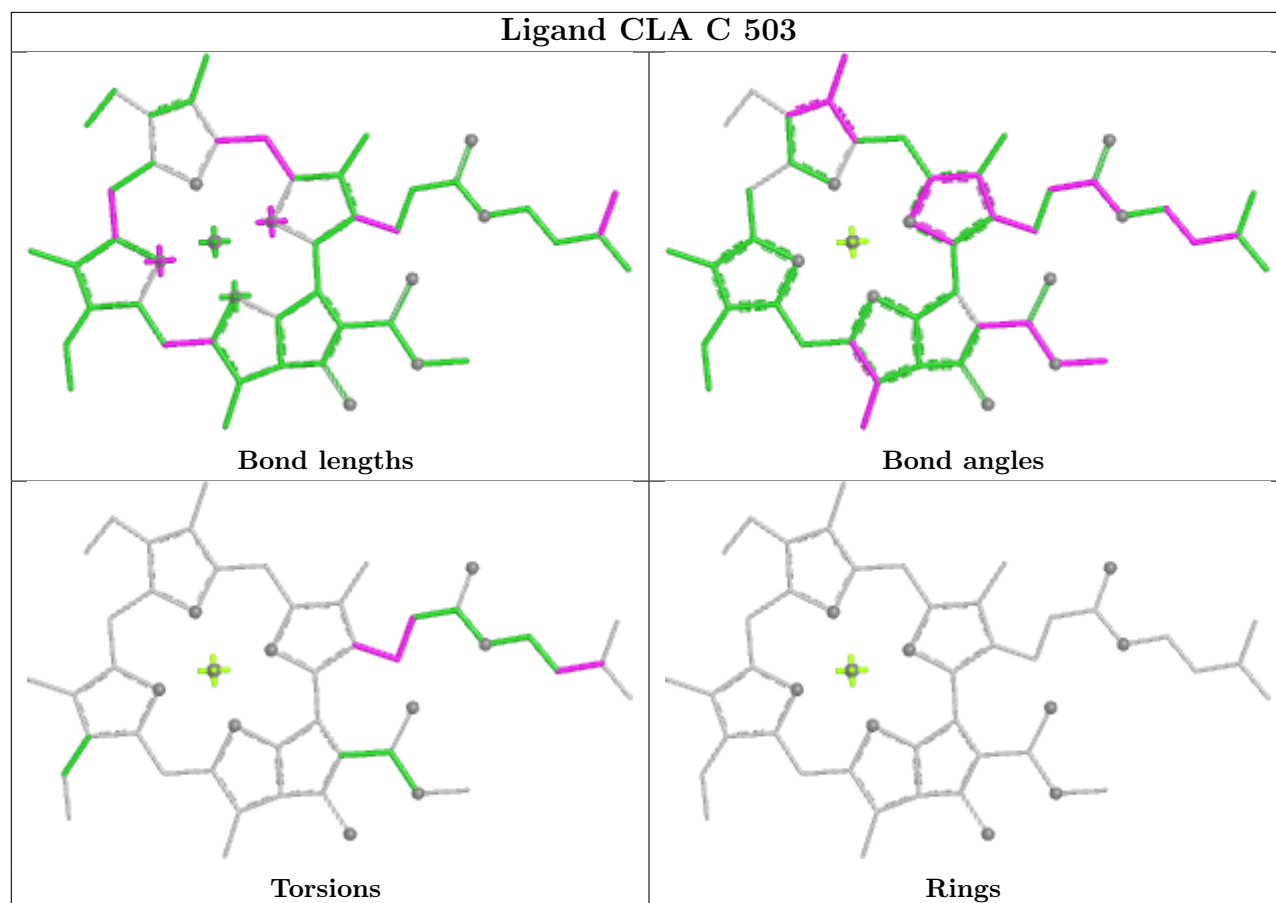
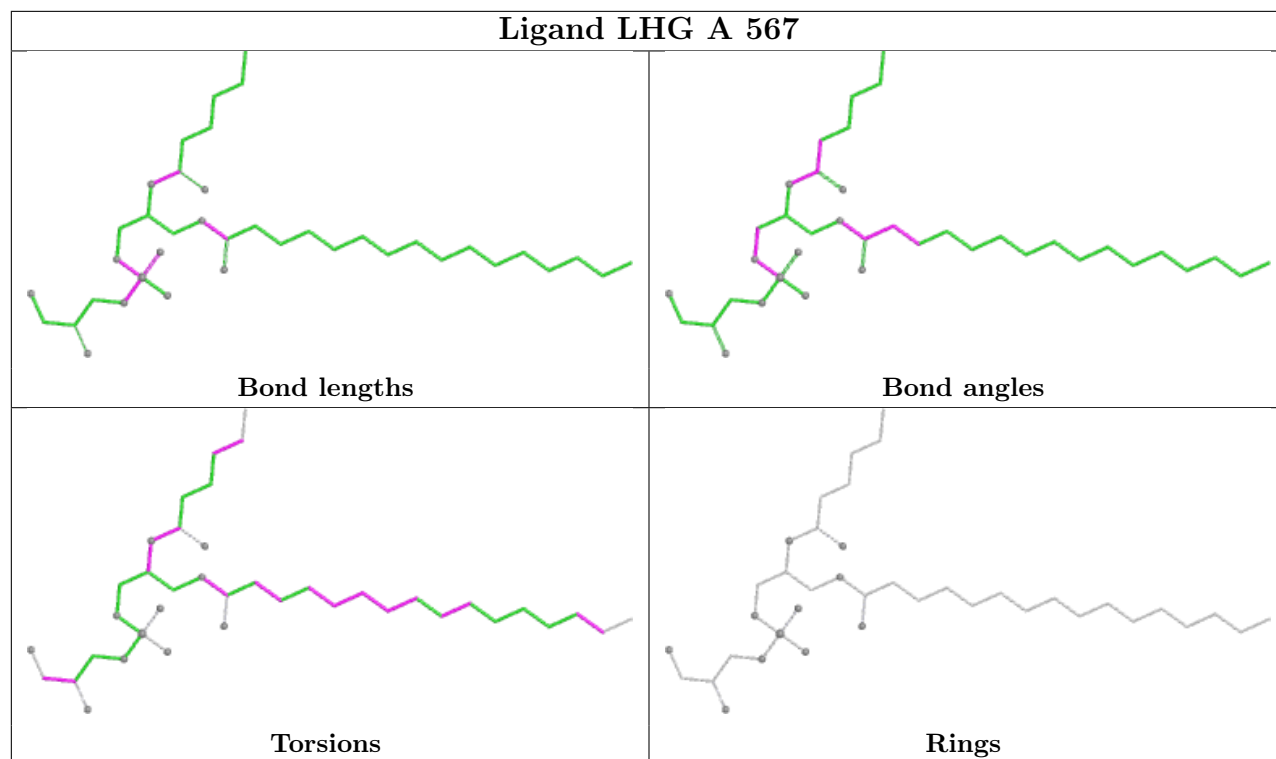


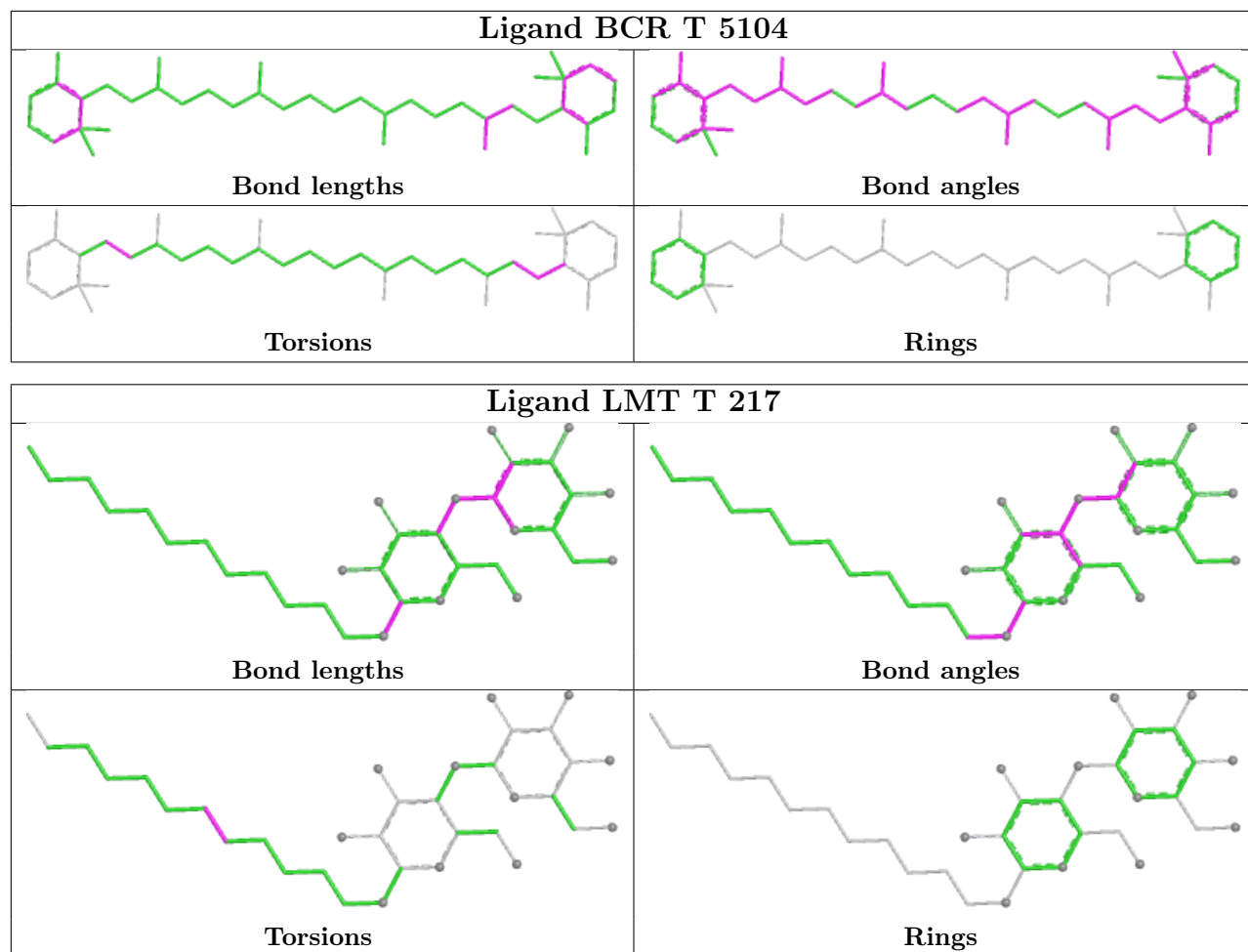
Ligand CLA B 518	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR X 130	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand MGE i 5201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



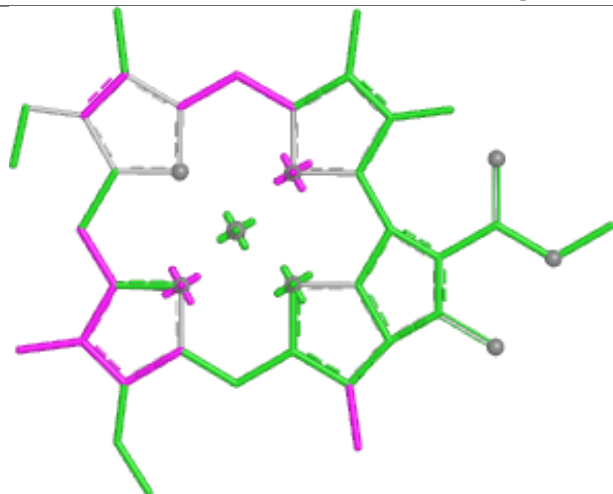
Ligand CLA b 5513	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 5506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 560	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



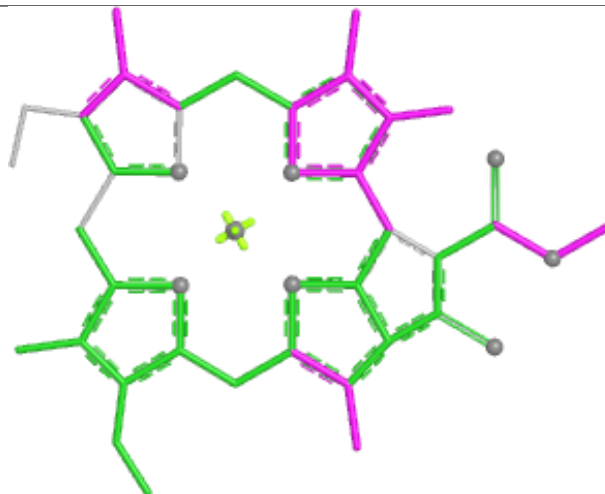




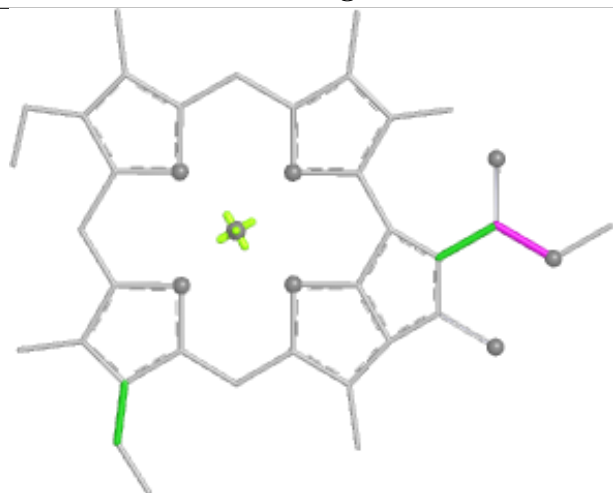
Ligand CLA B 511



Bond lengths



Bond angles

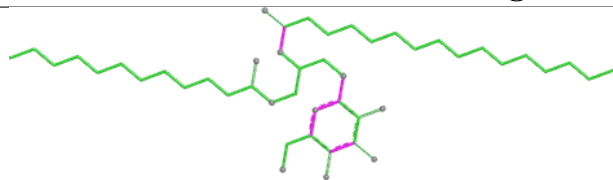


Torsions

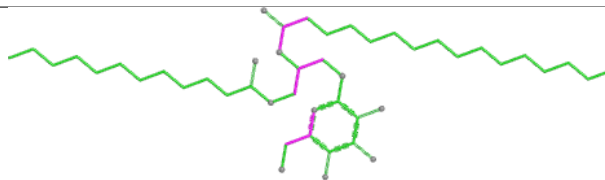


Rings

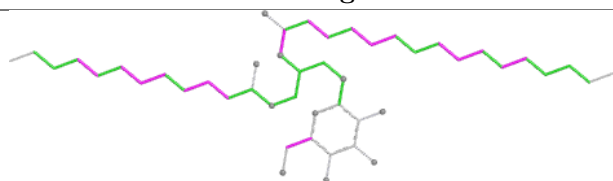
Ligand MGE D 358



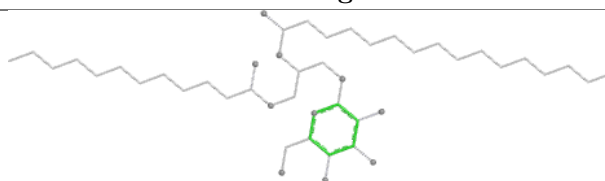
Bond lengths



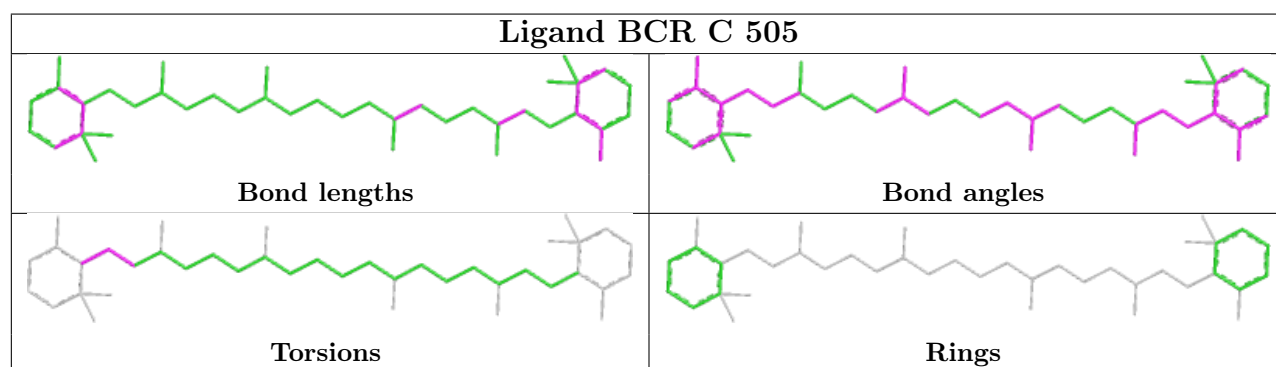
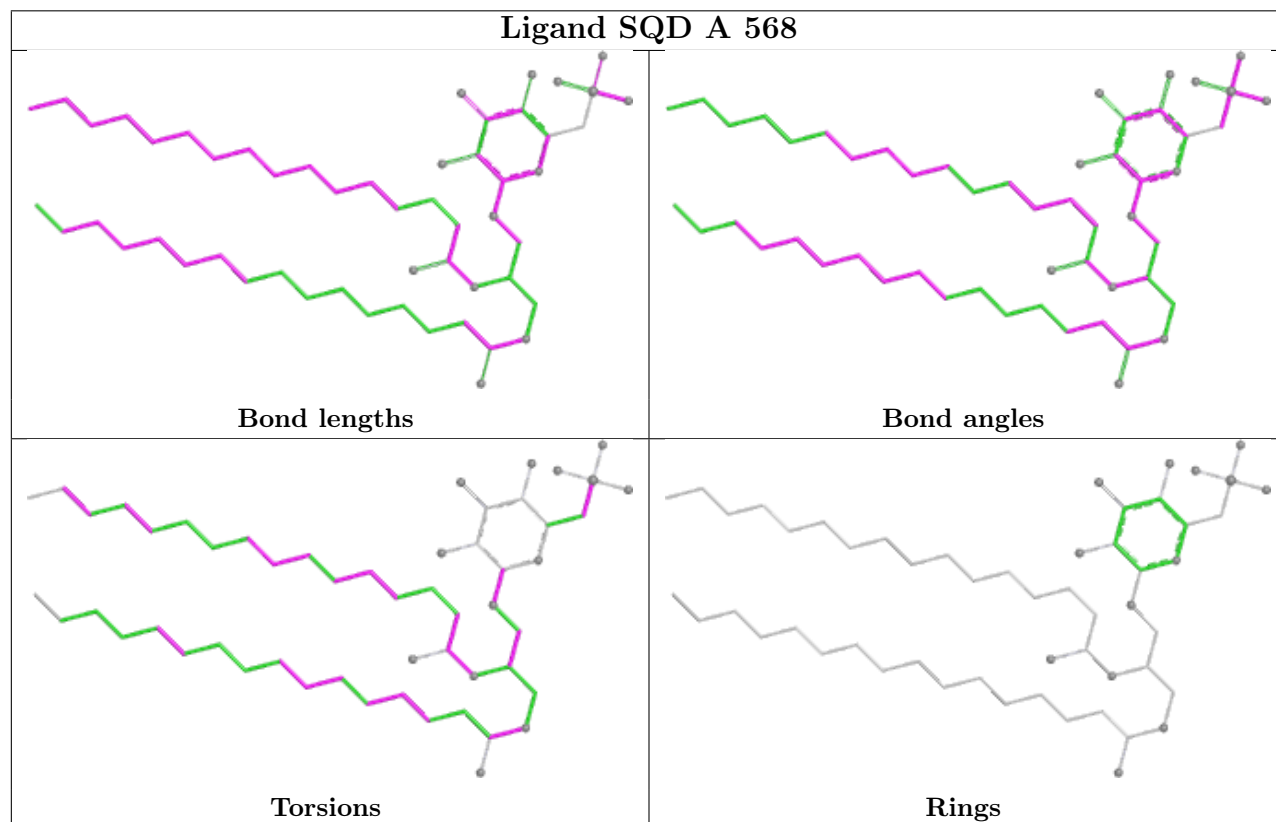
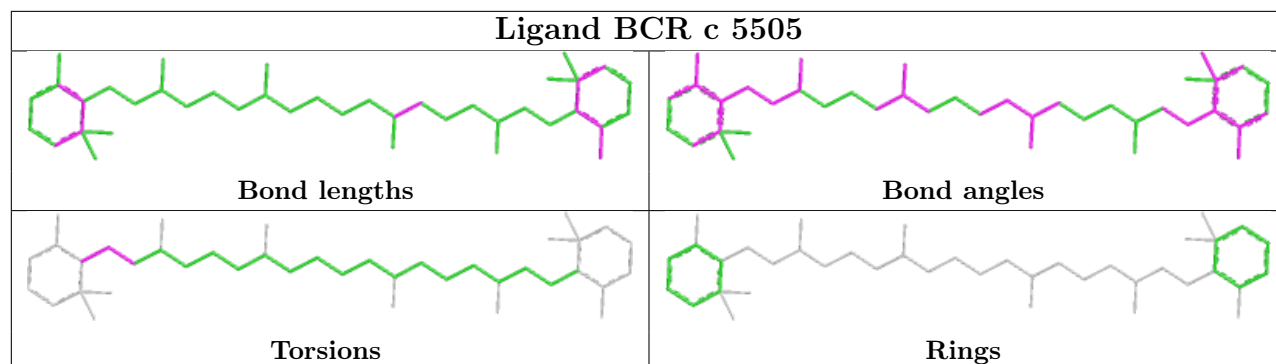
Bond angles

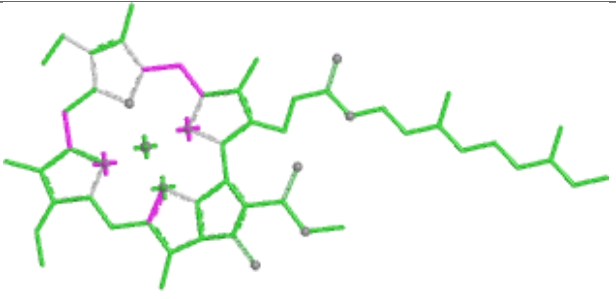
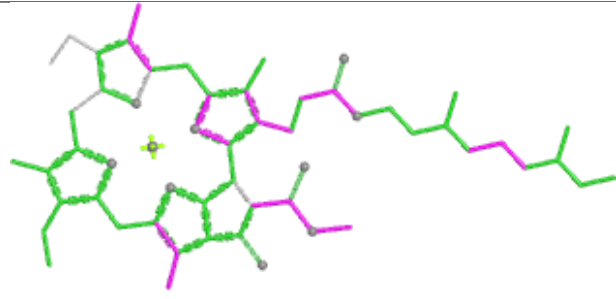
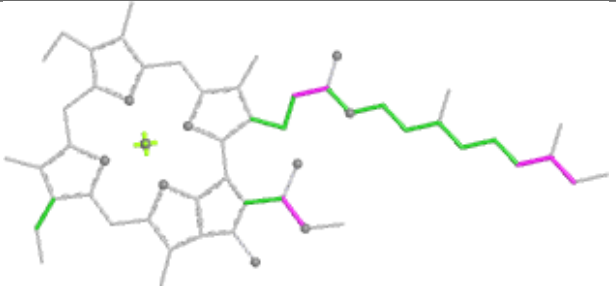
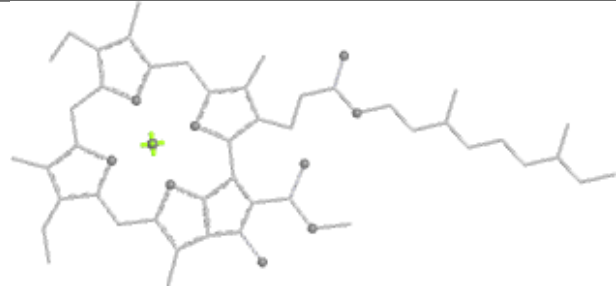


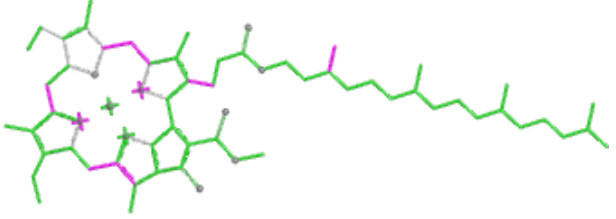
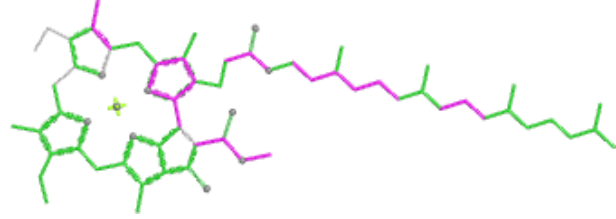
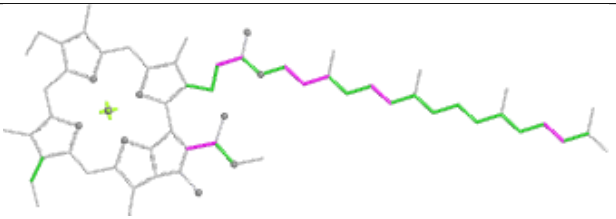
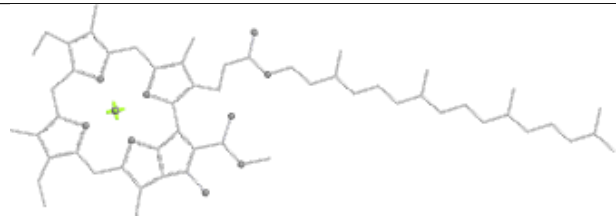
Torsions

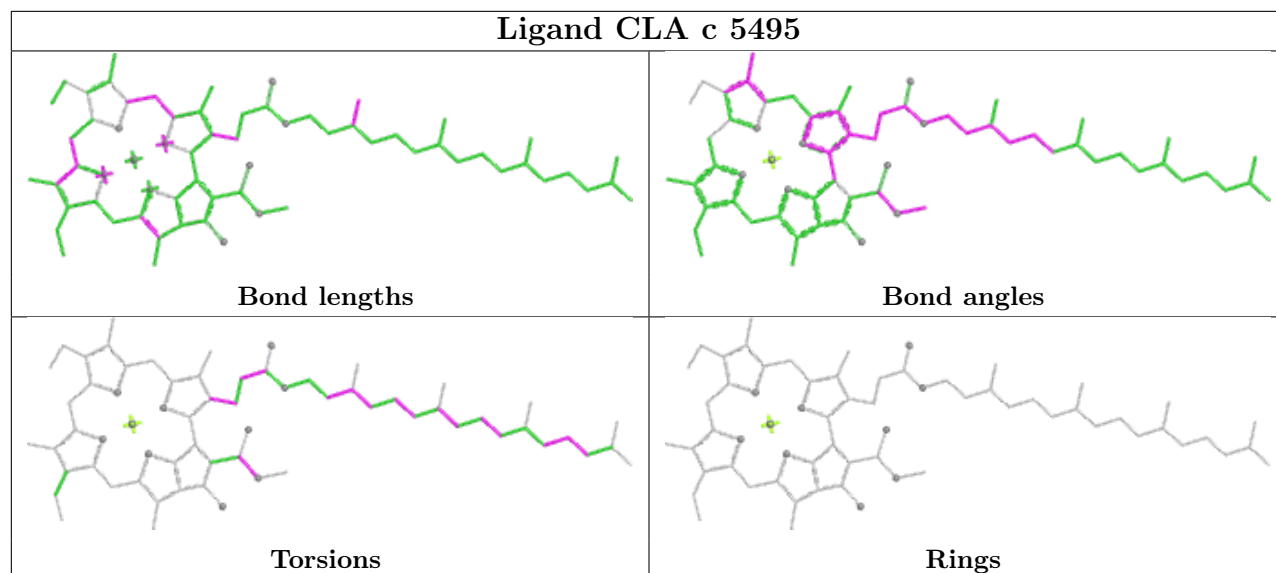
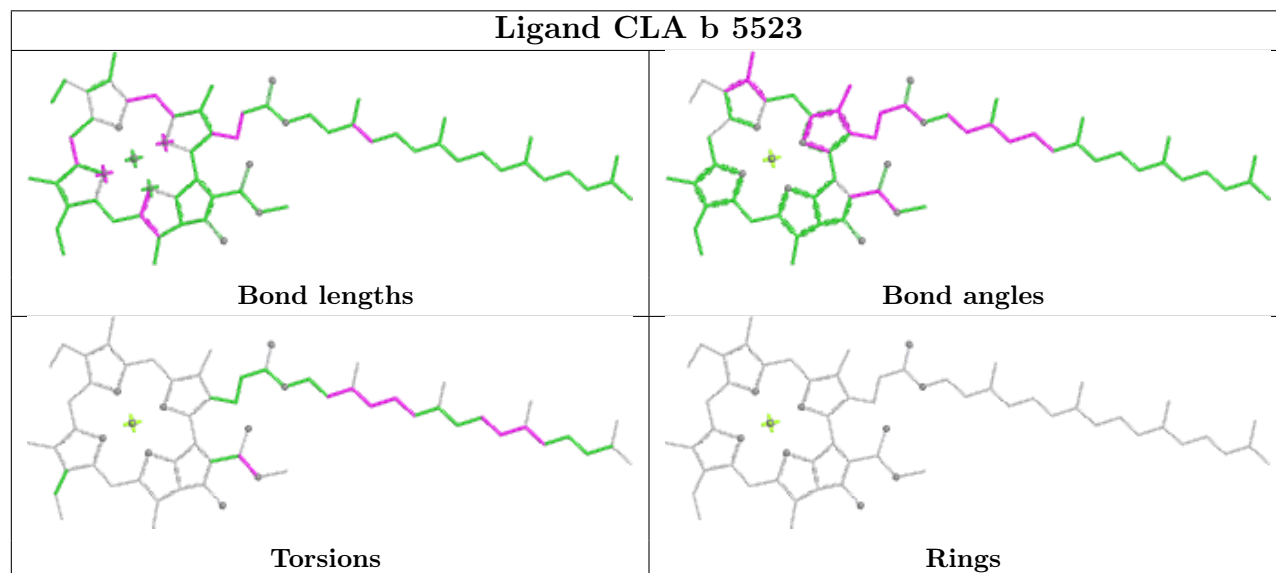
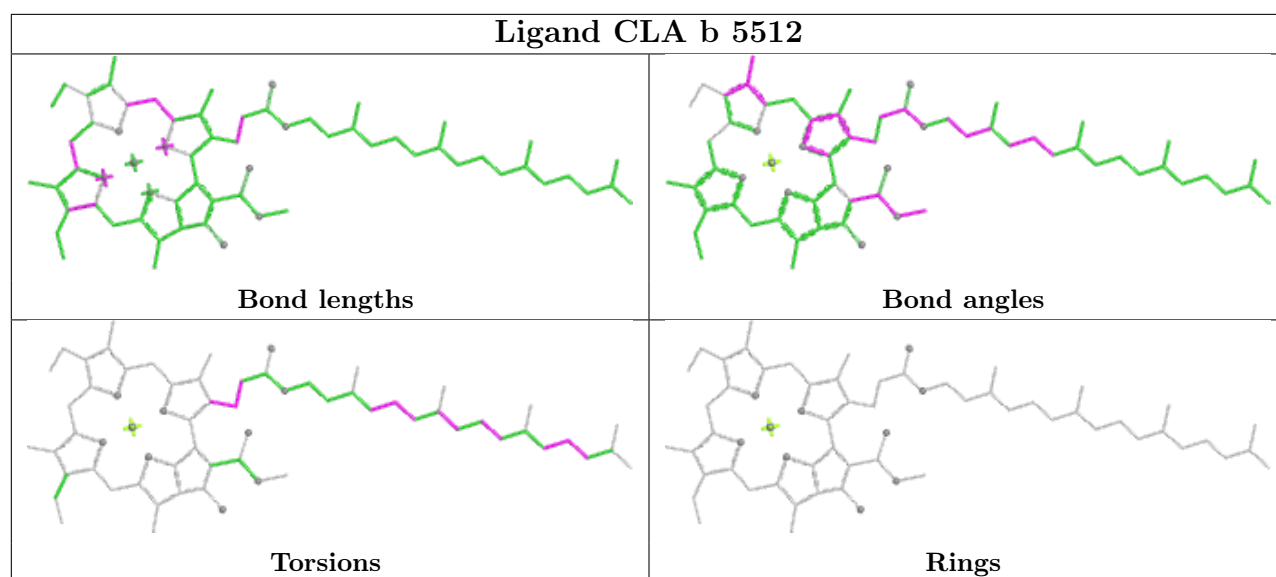


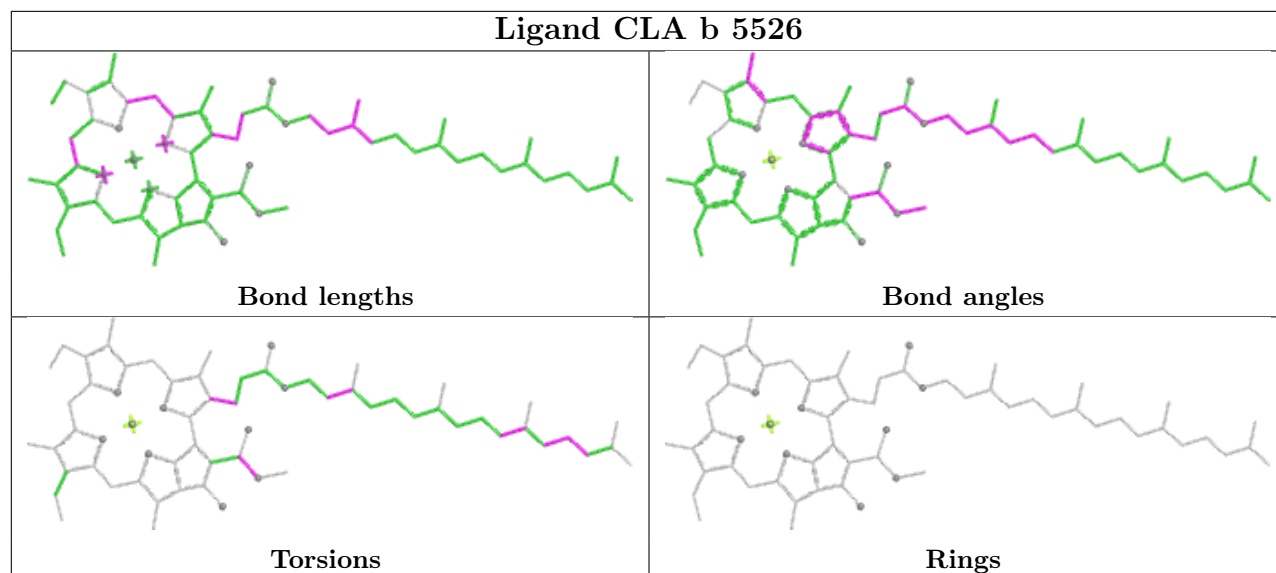
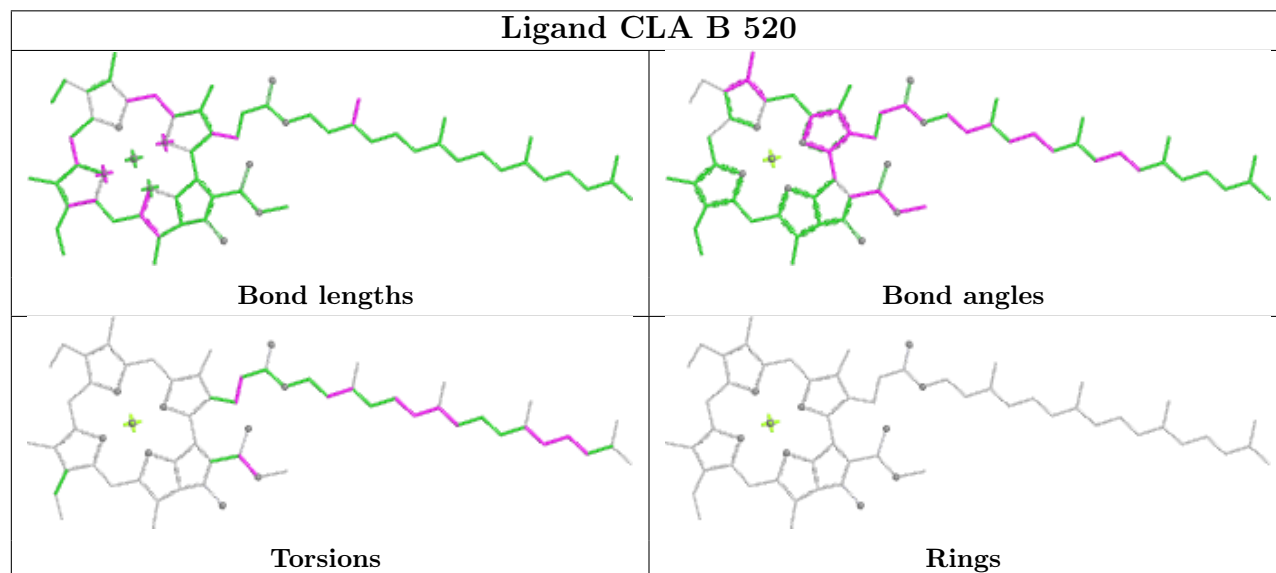
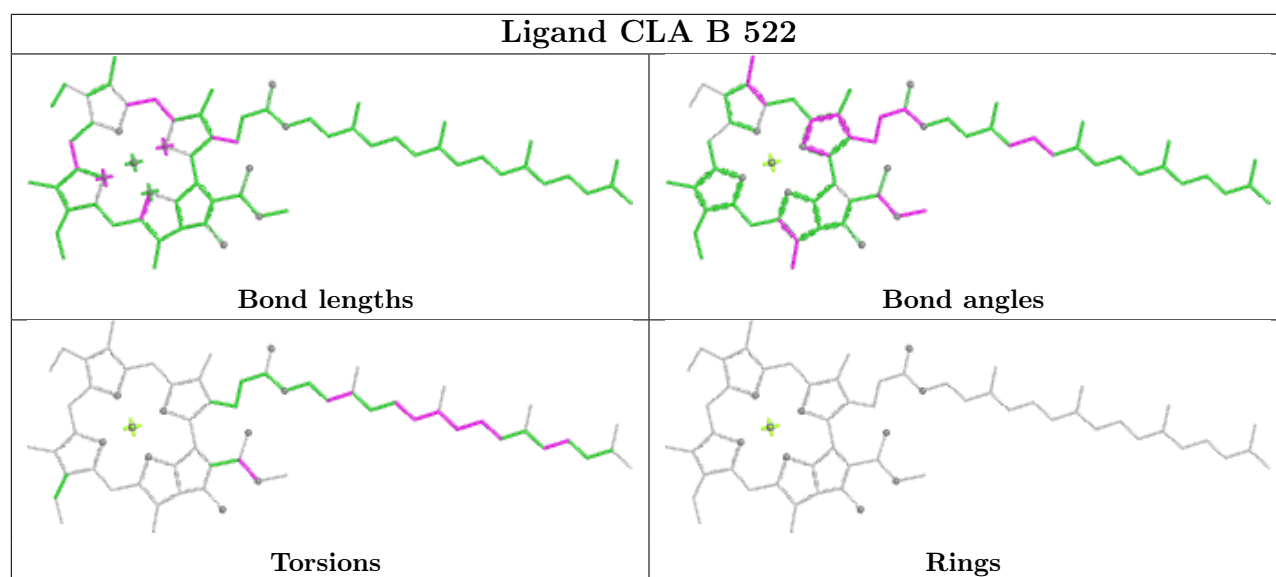
Rings

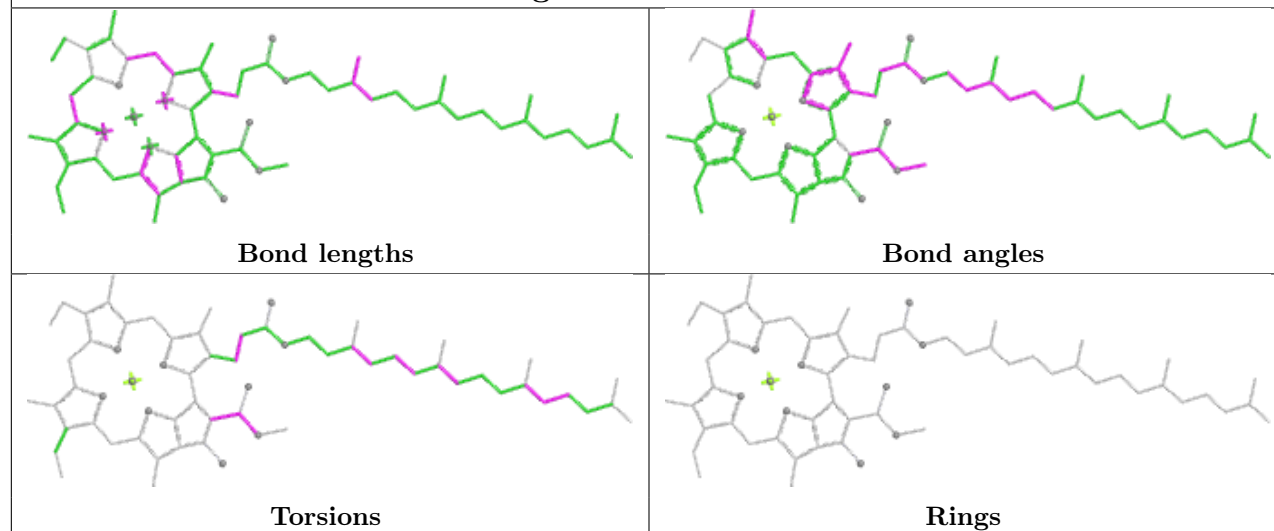
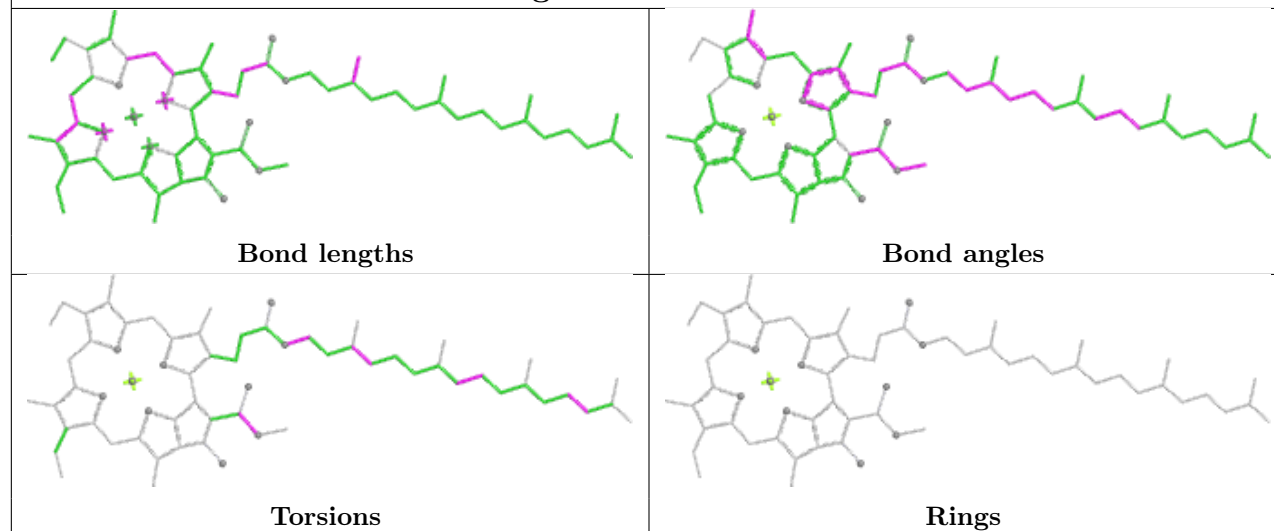
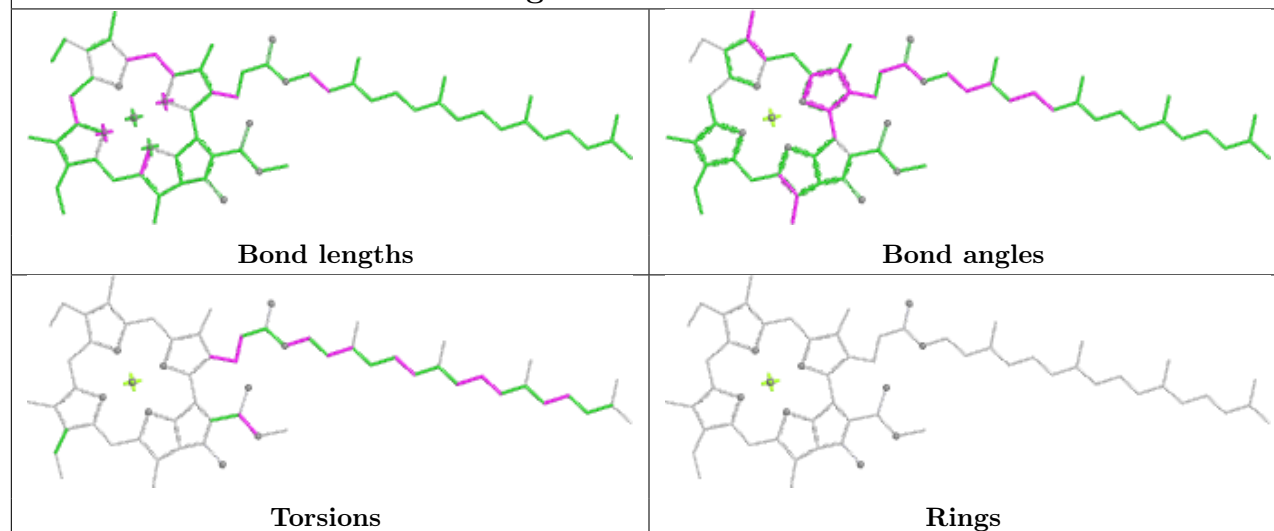


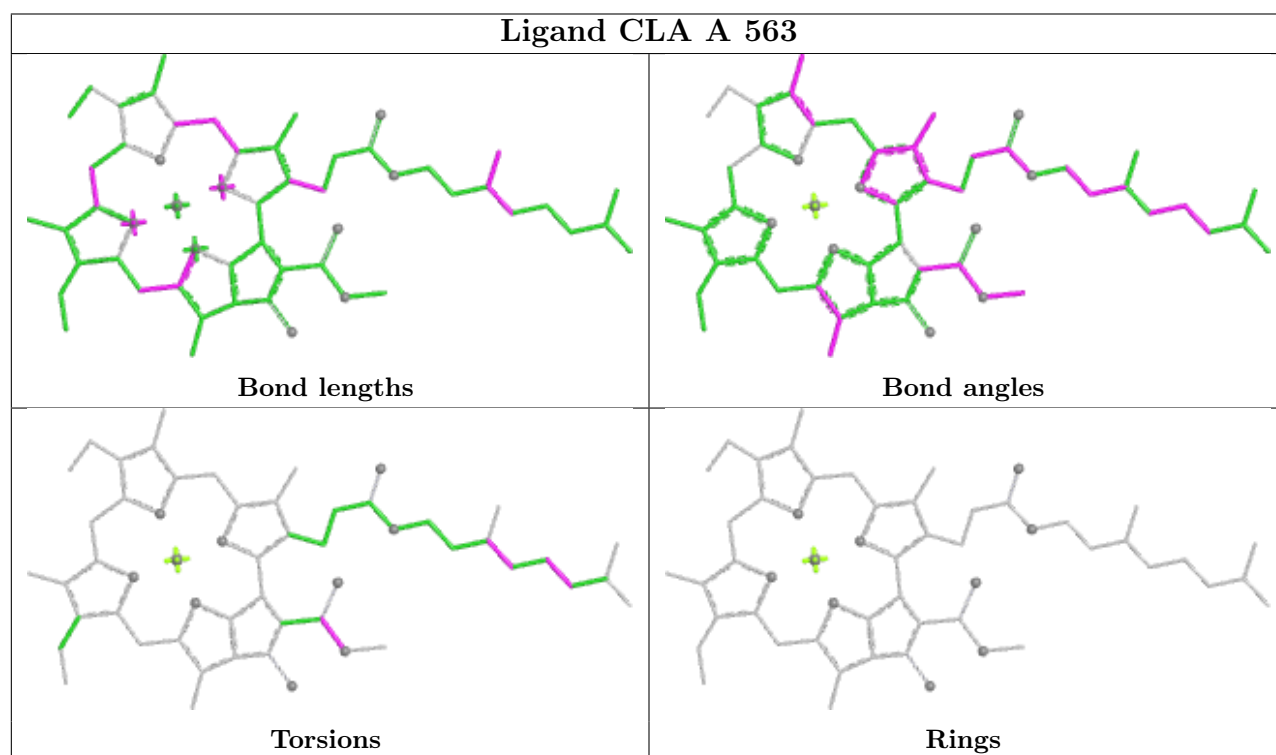
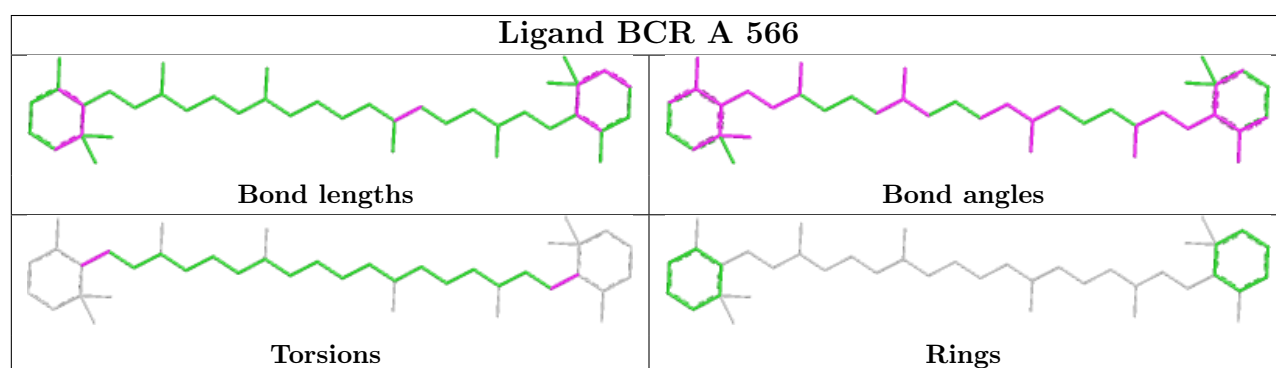
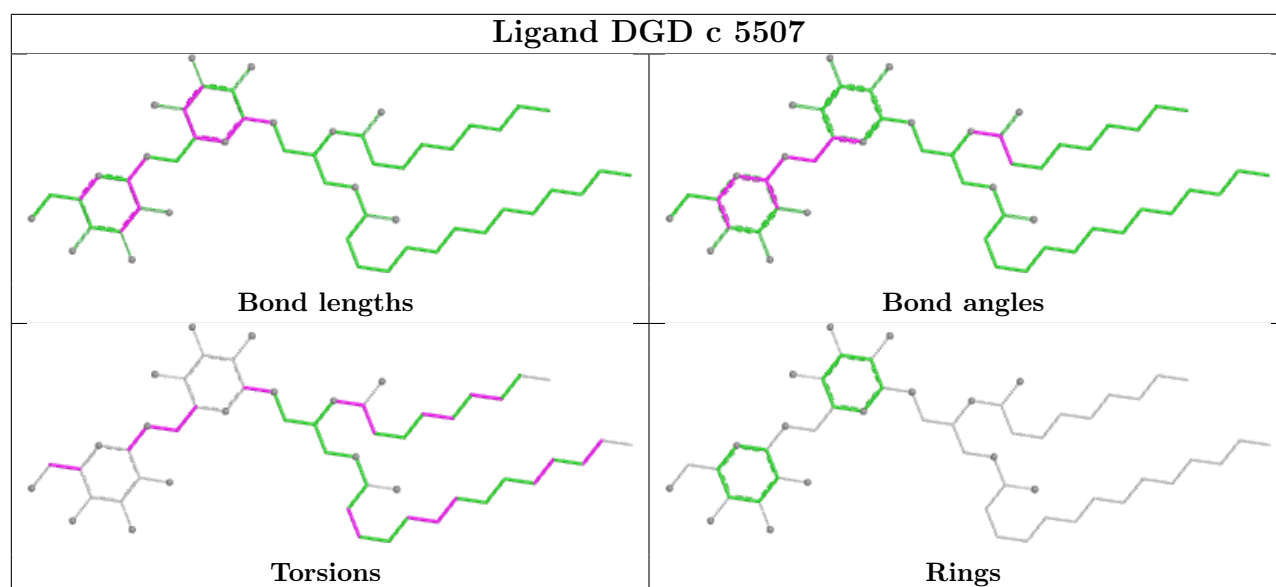
Ligand CLA b 5524	
	
Bond lengths	Bond angles
	
Torsions	Rings

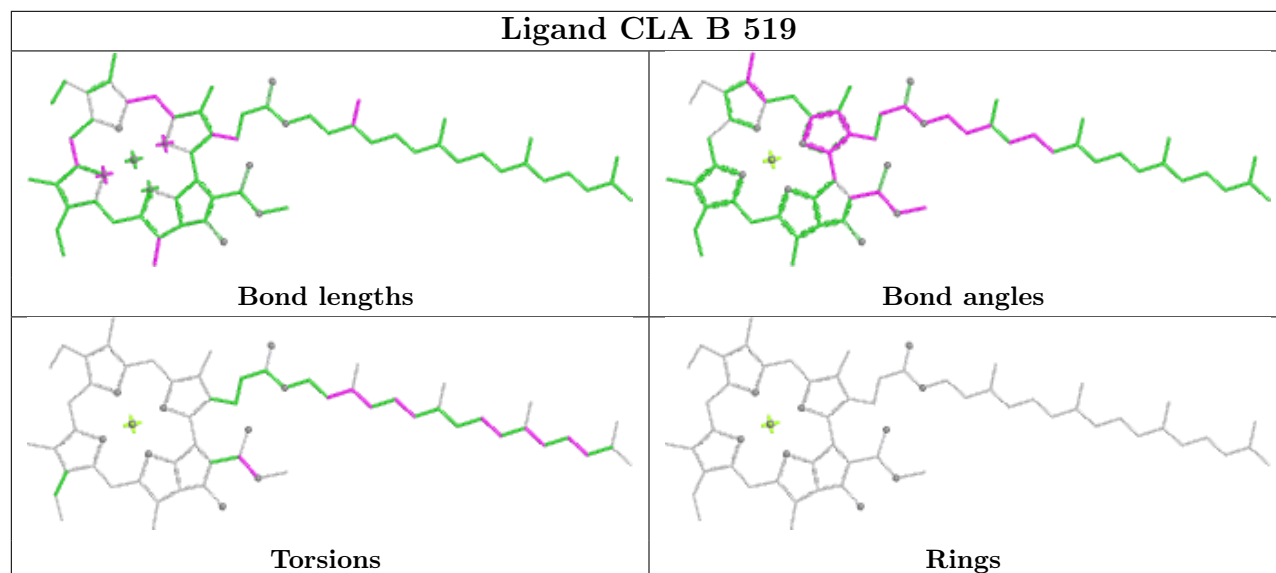
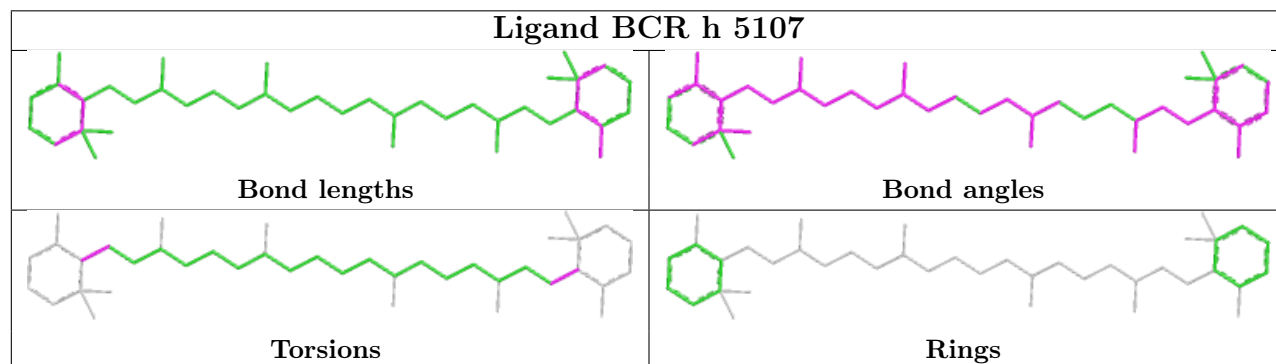
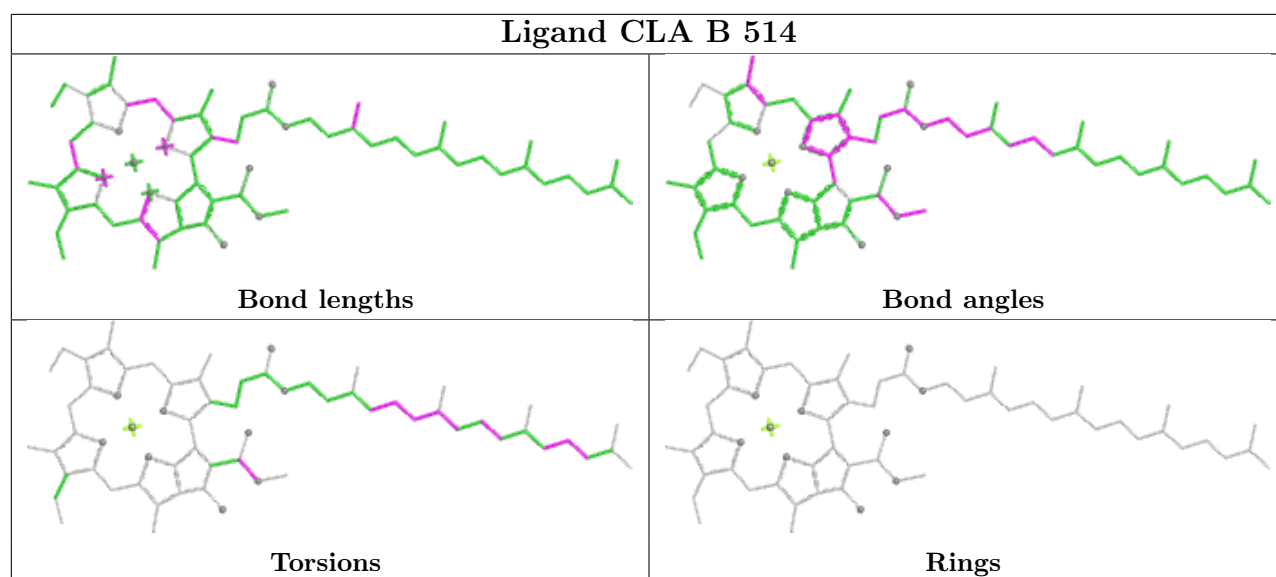
Ligand CLA C 497	
	
Bond lengths	Bond angles
	
Torsions	Rings

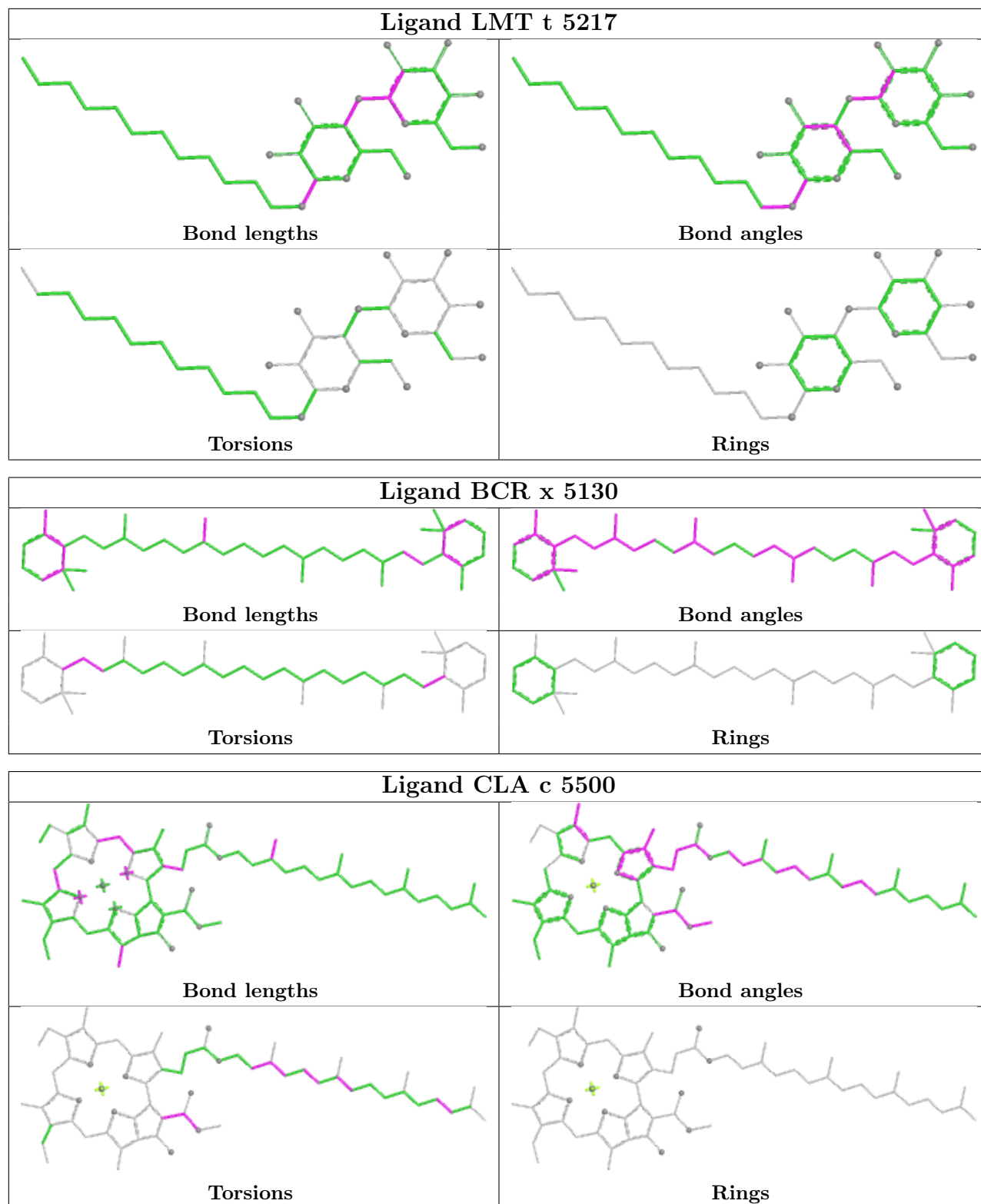


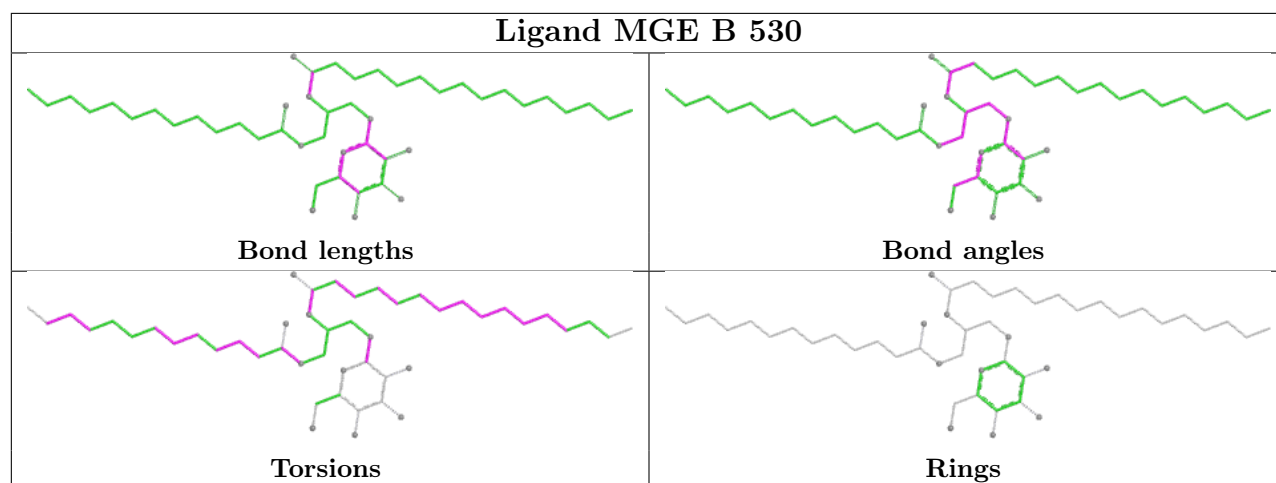
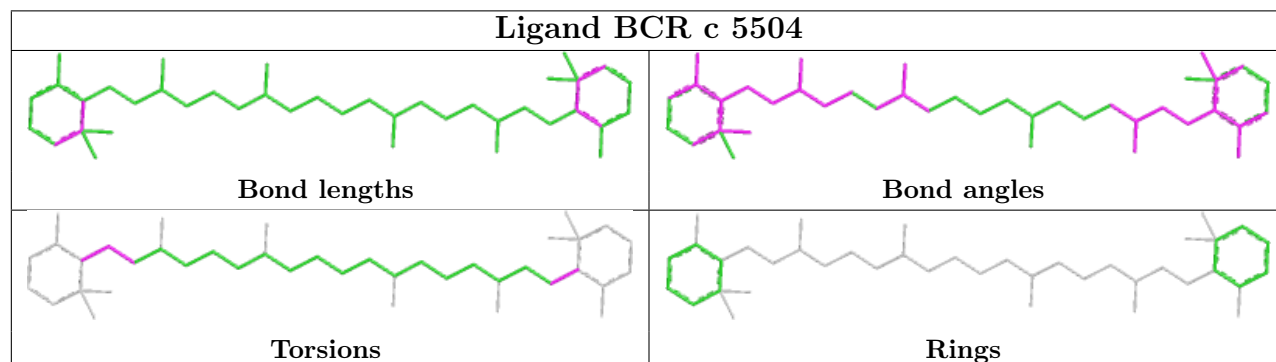
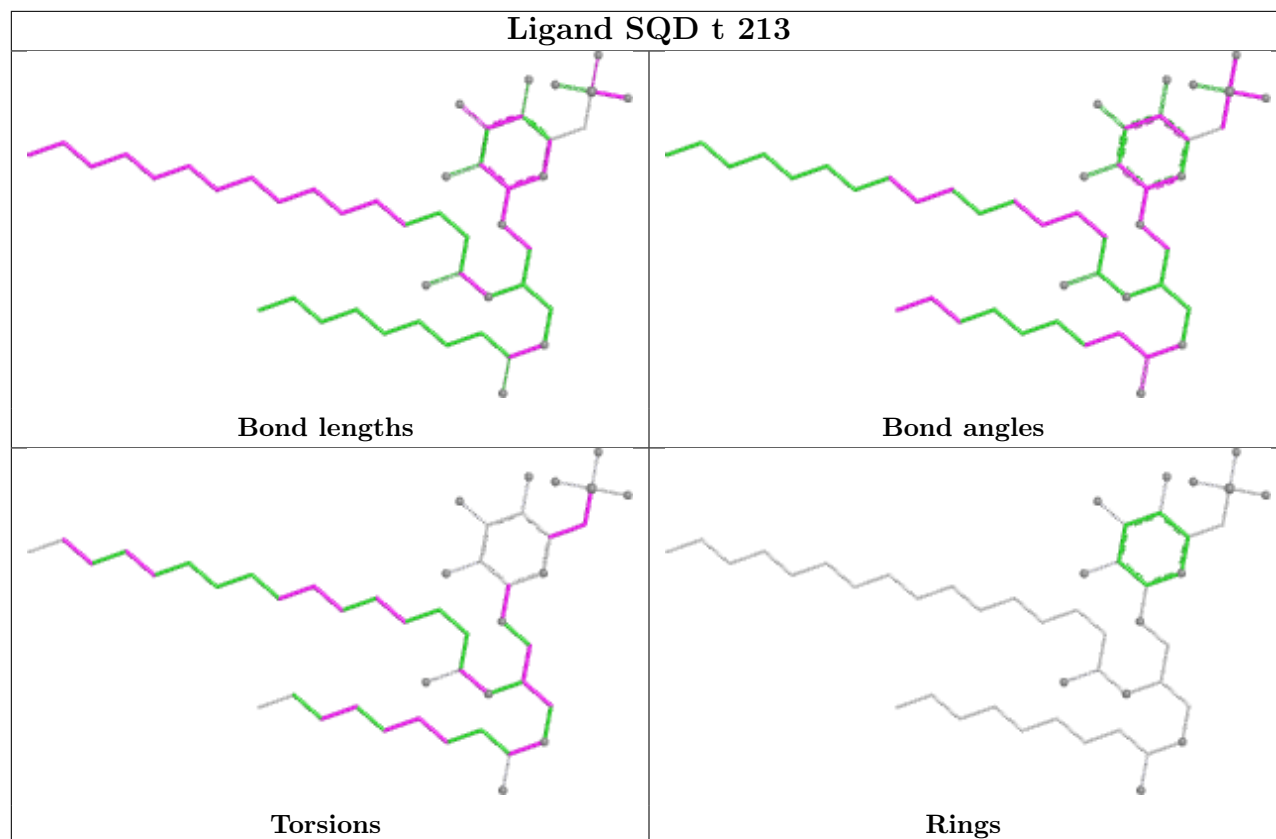


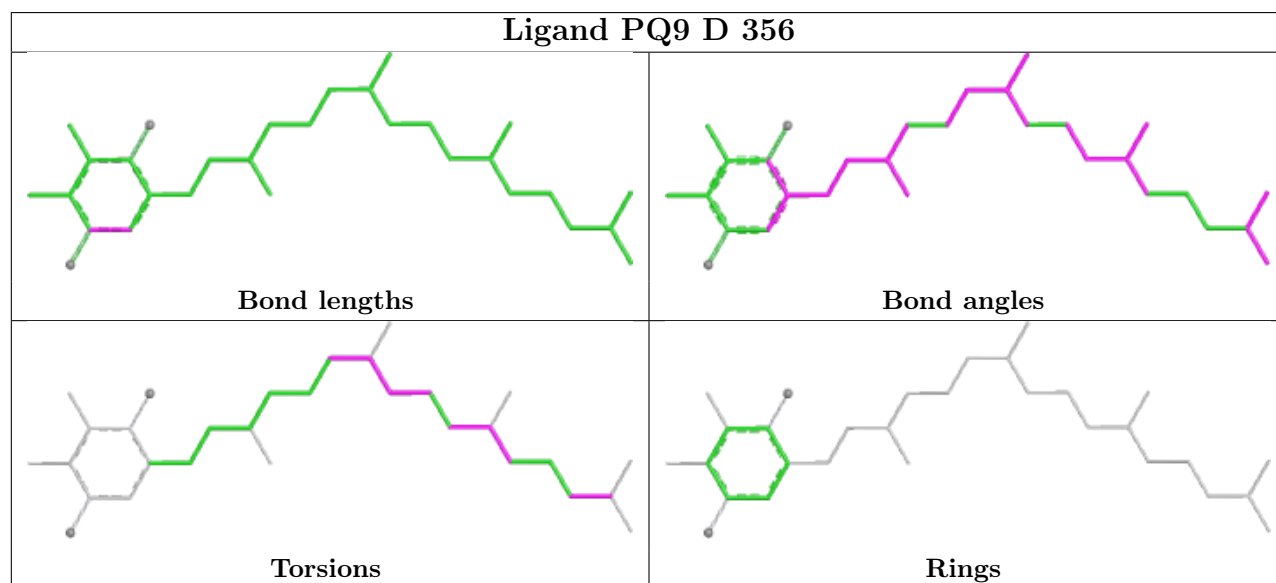
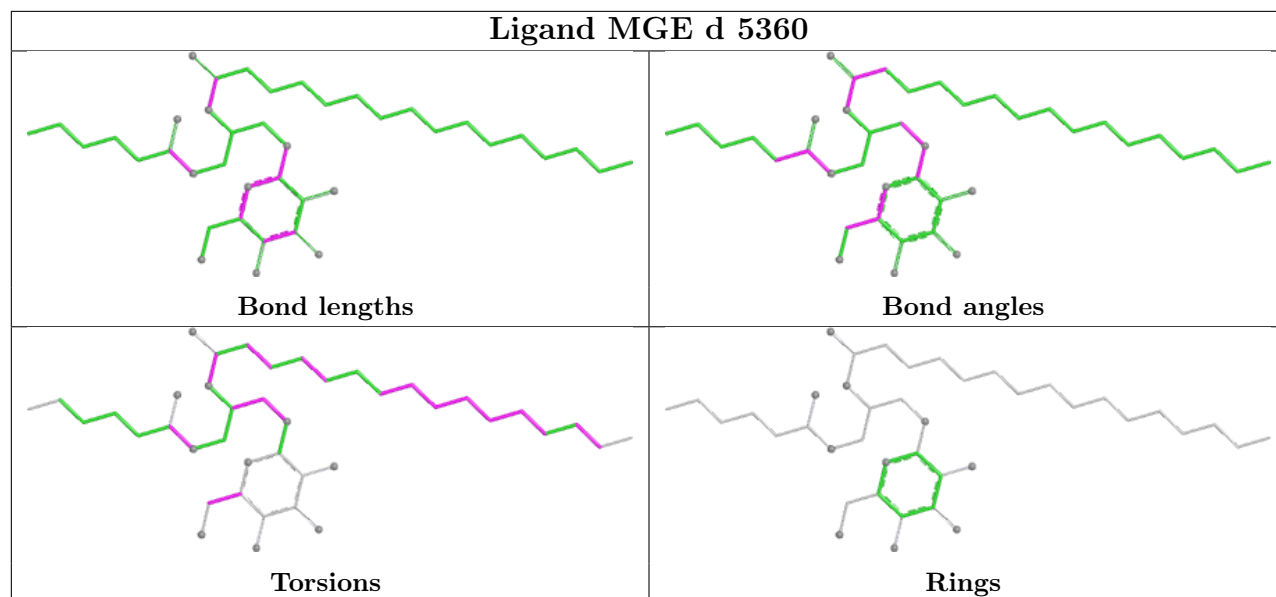
Ligand CLA B 513**Ligand CLA B 521****Ligand CLA b 5517**

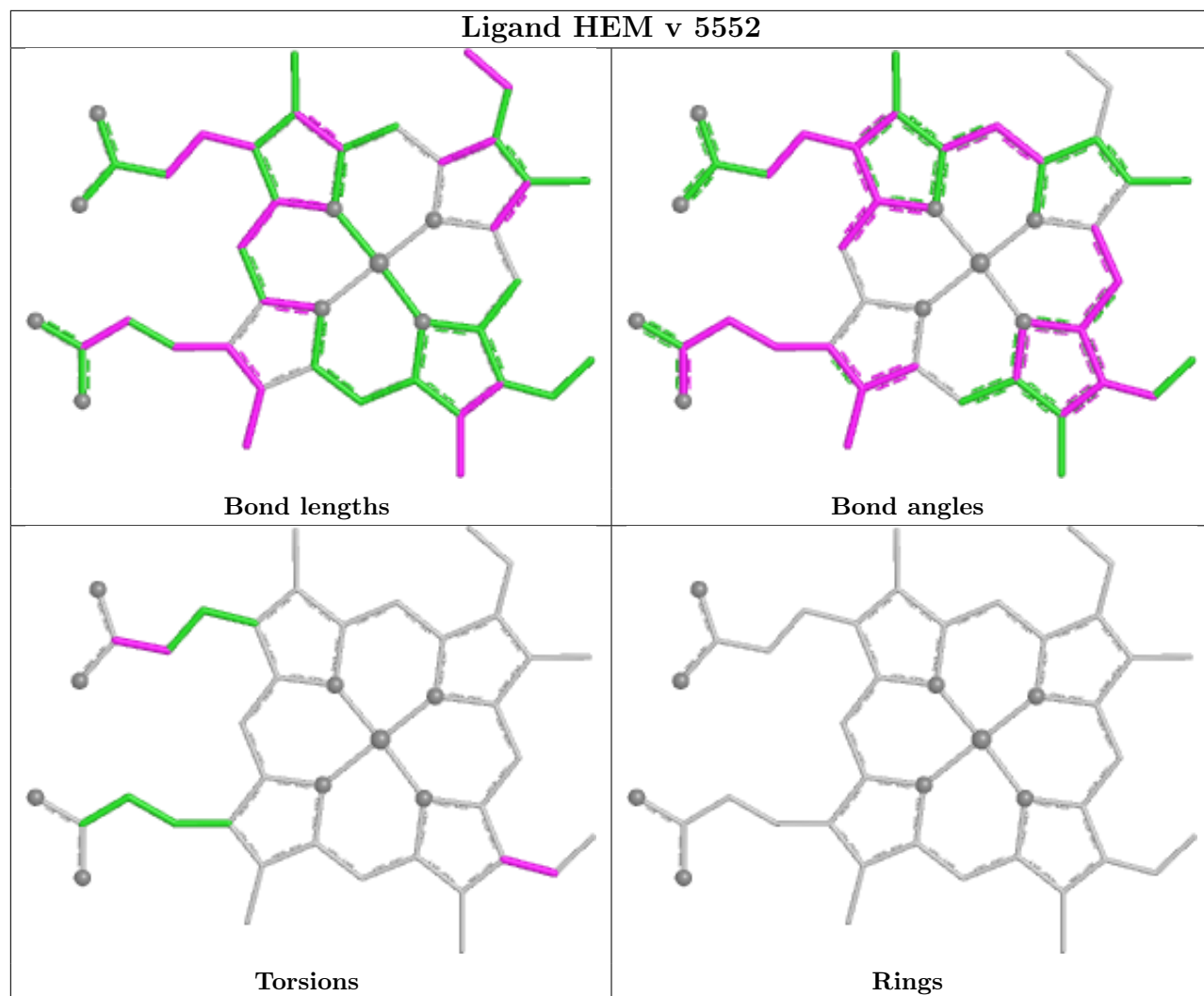


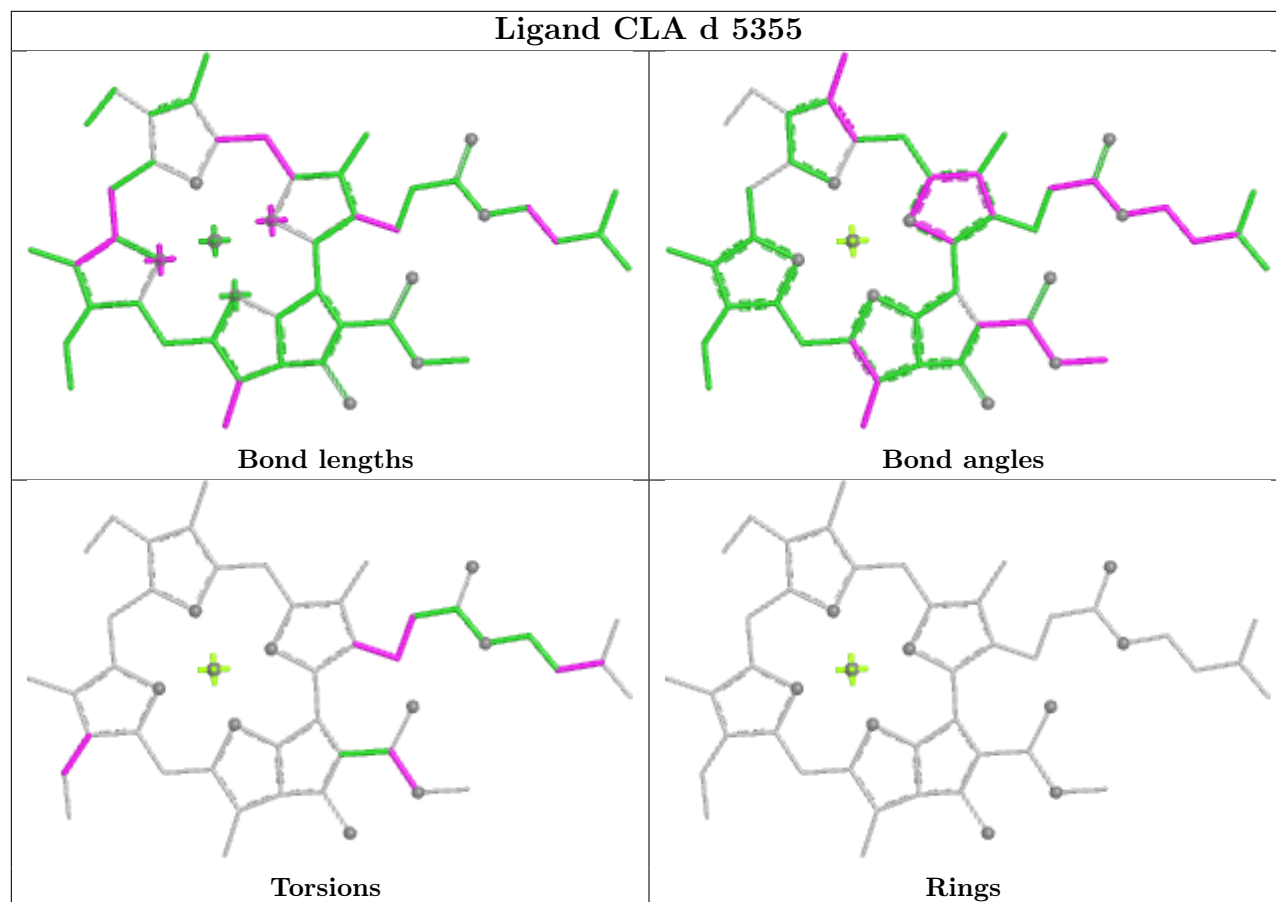




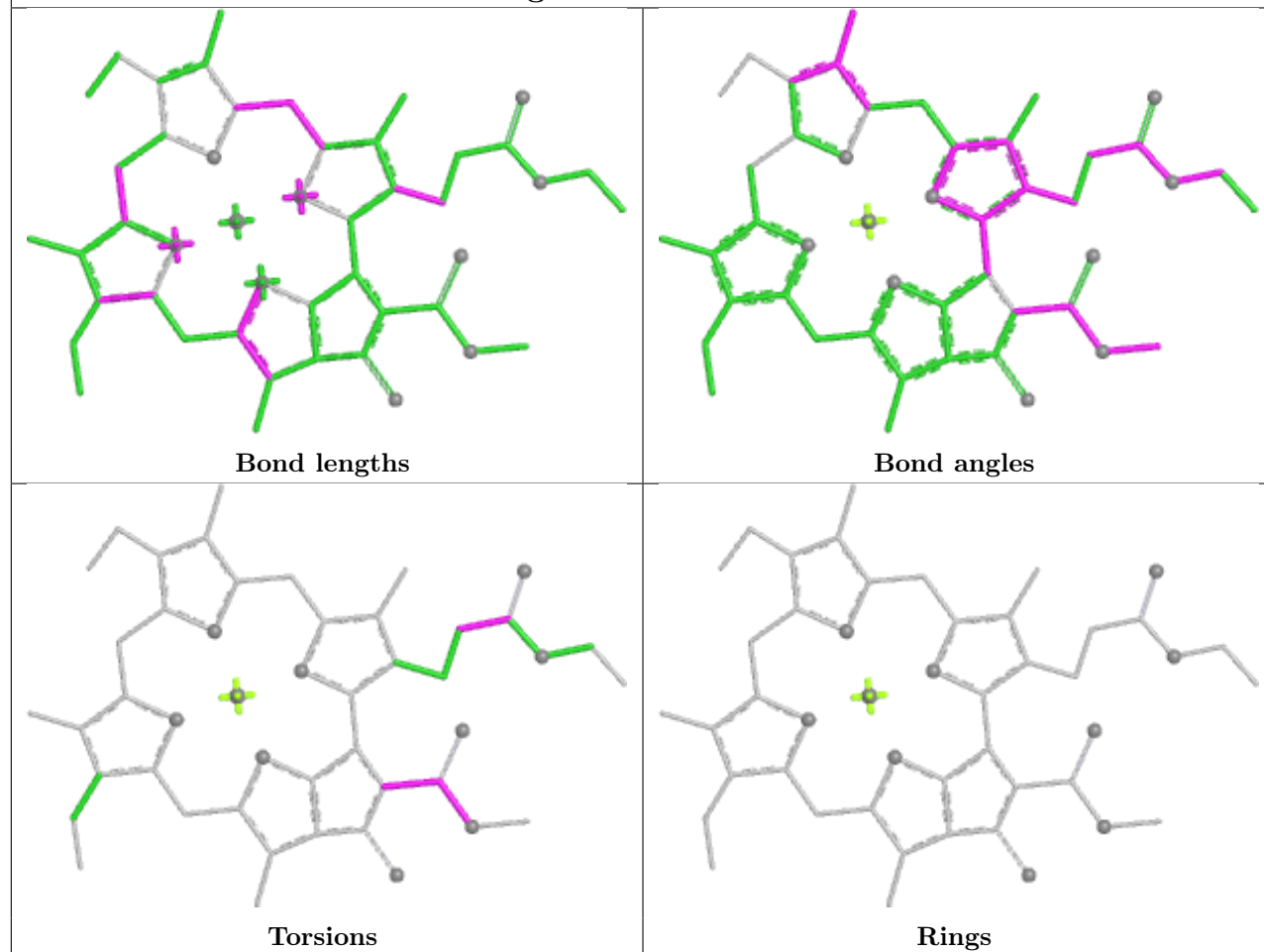




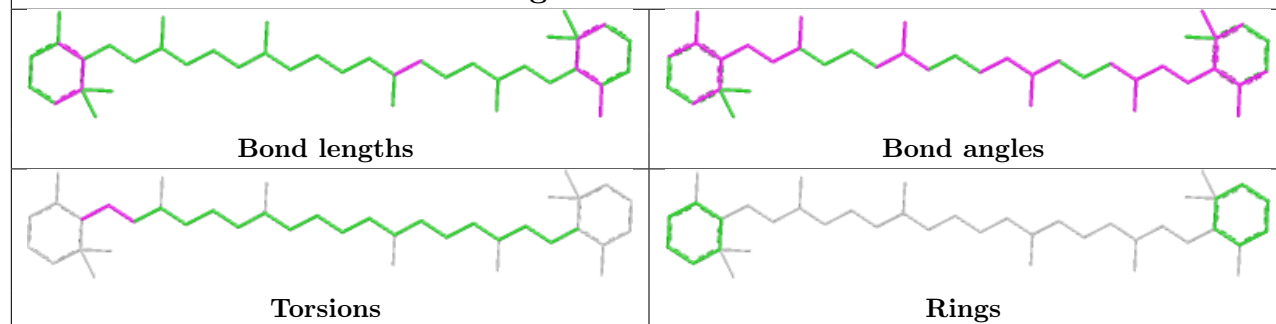


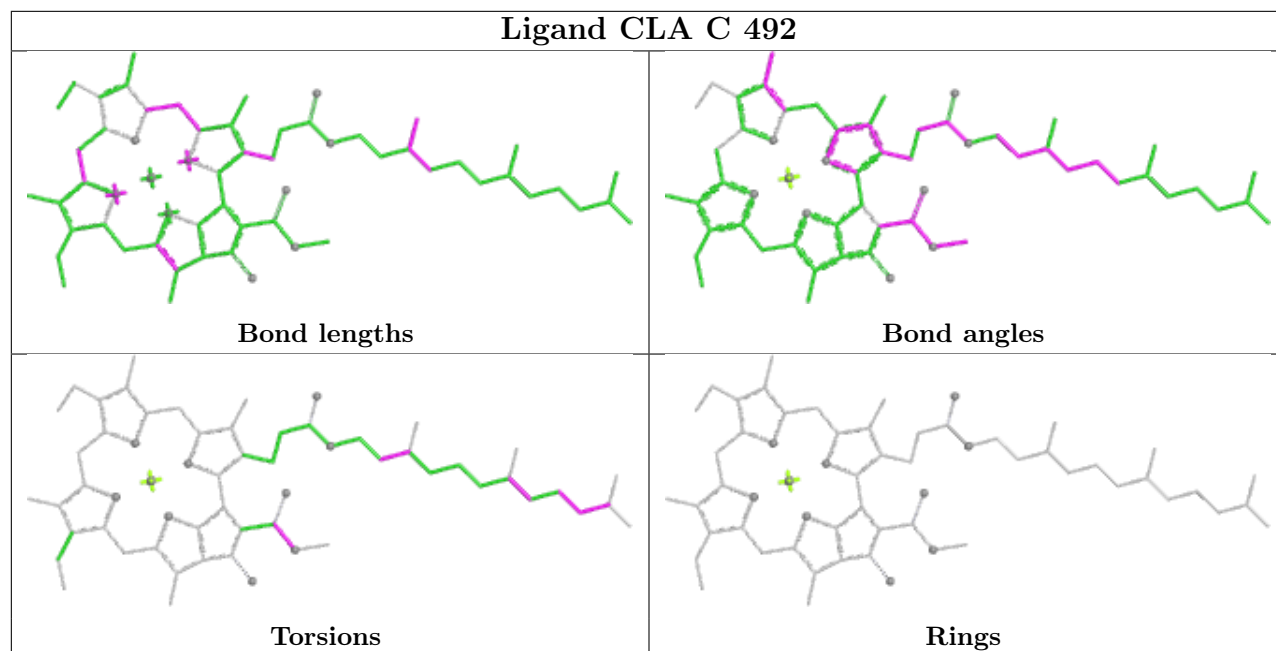
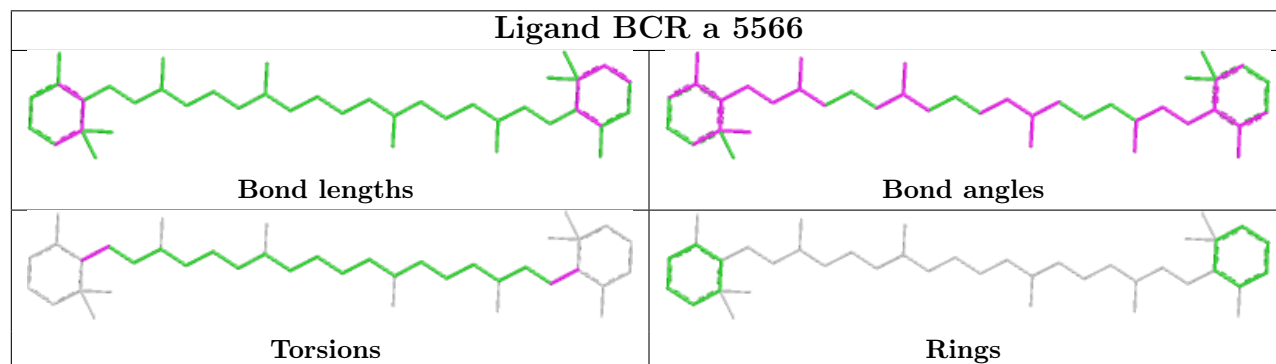
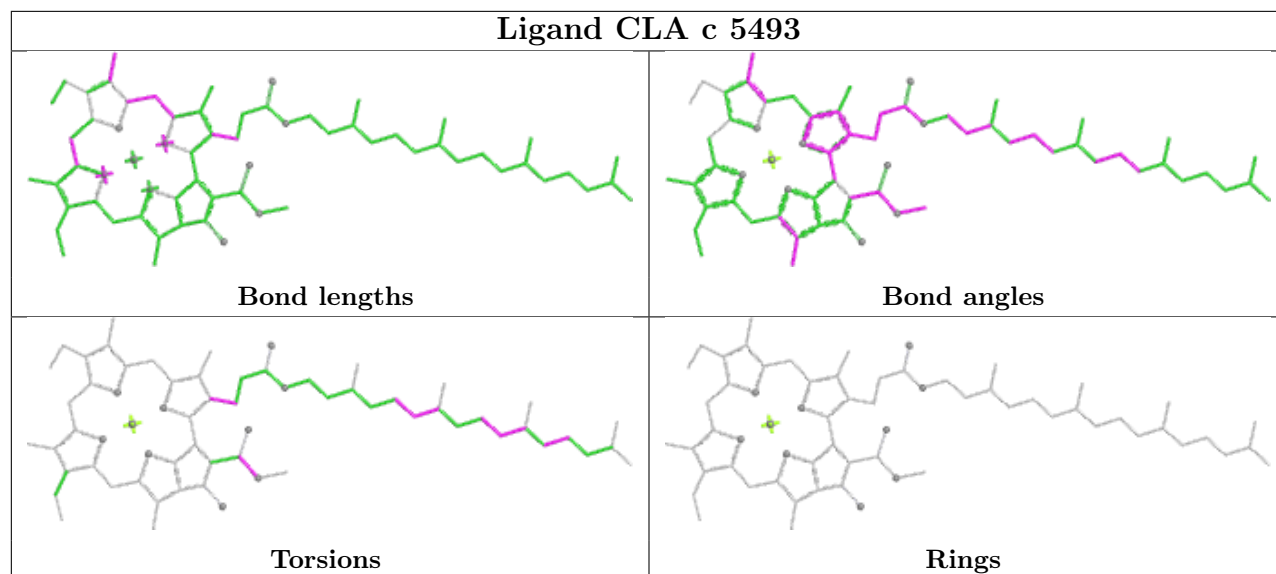


Ligand CLA C 499

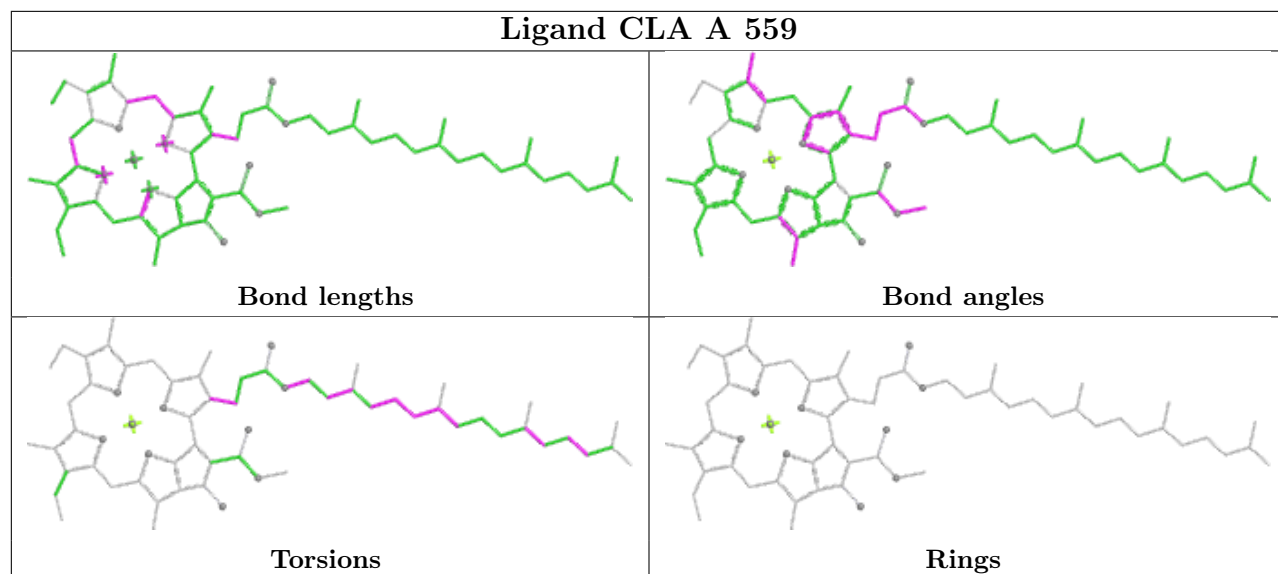


Ligand BCR D 357

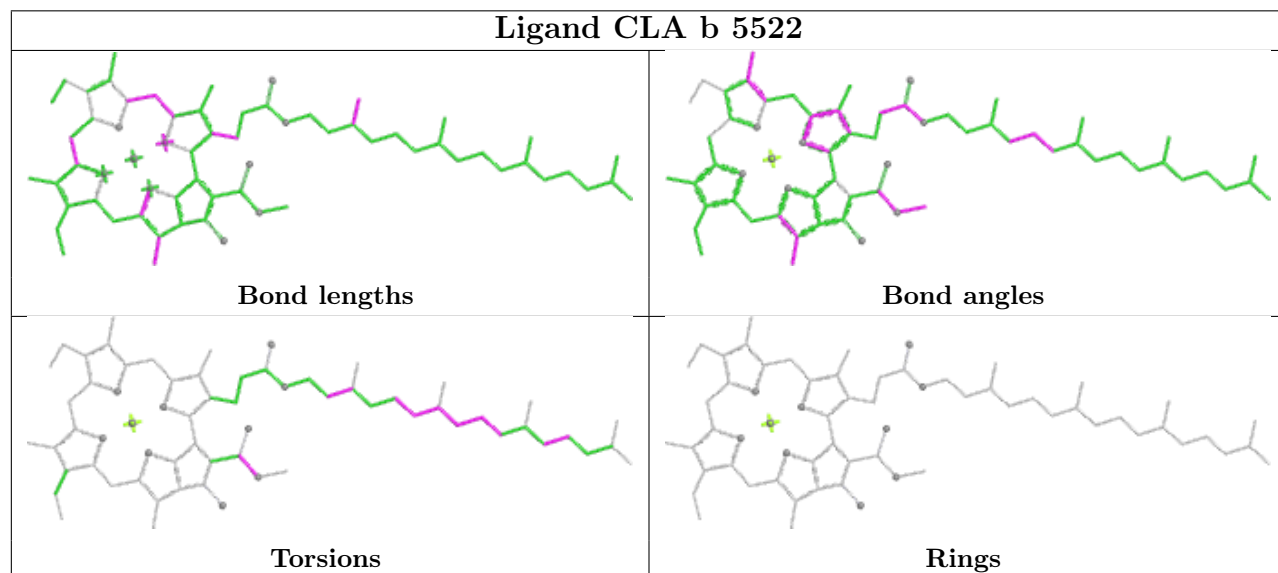


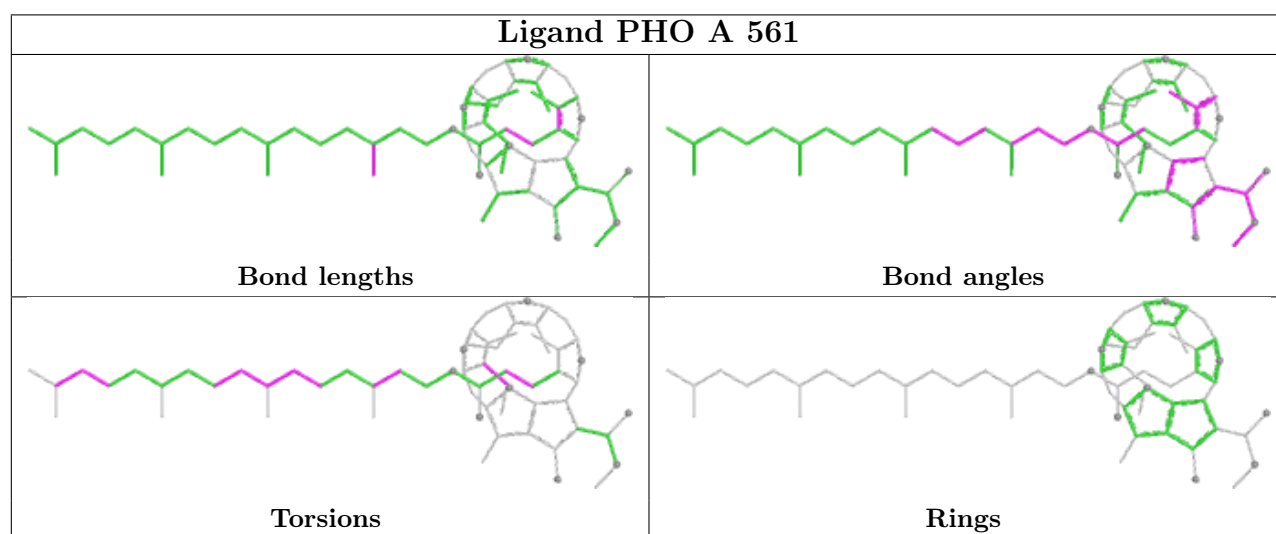
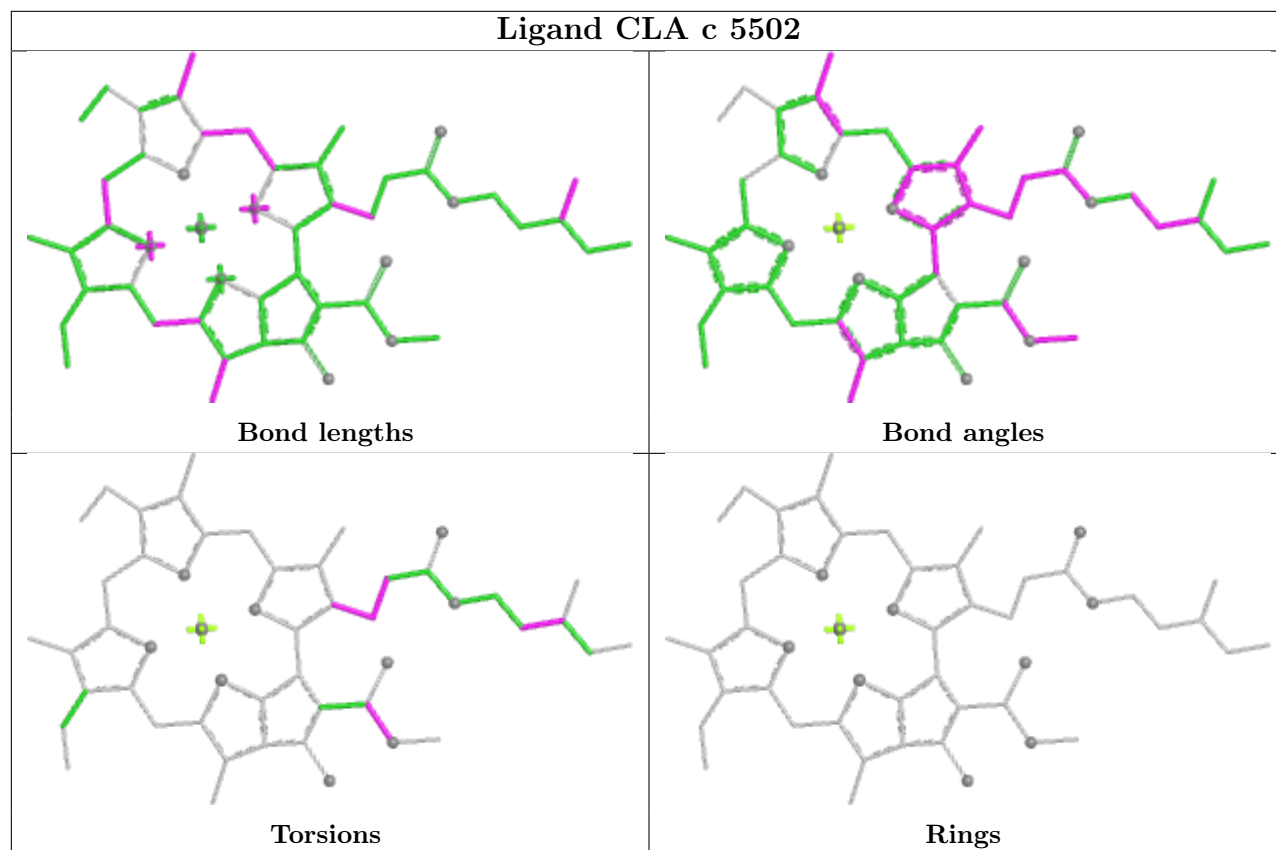


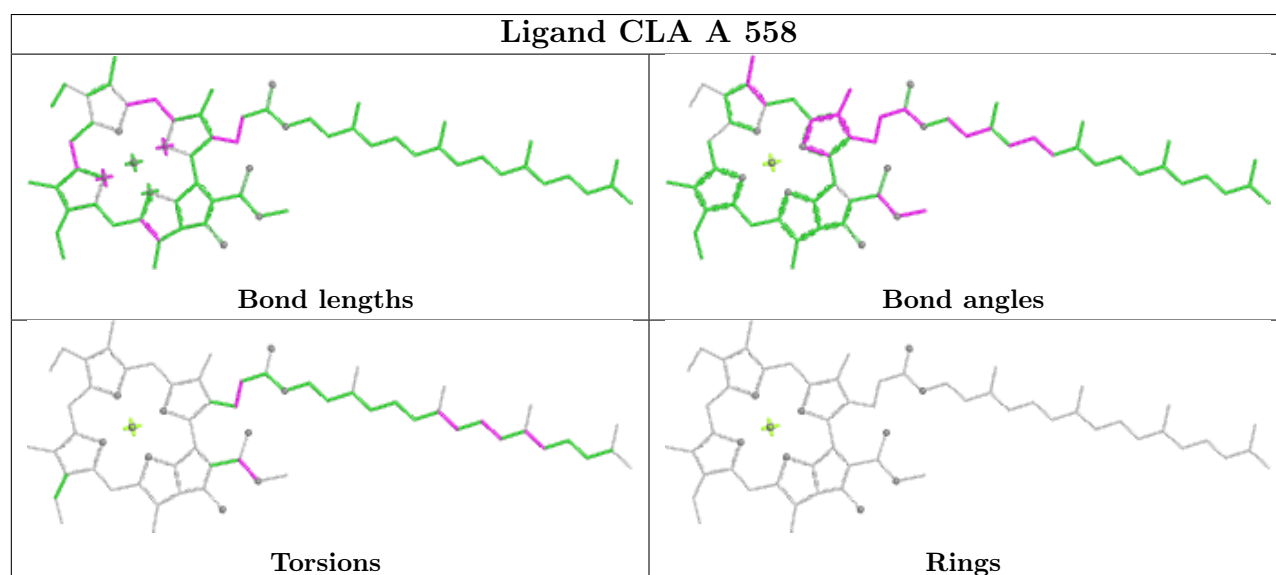
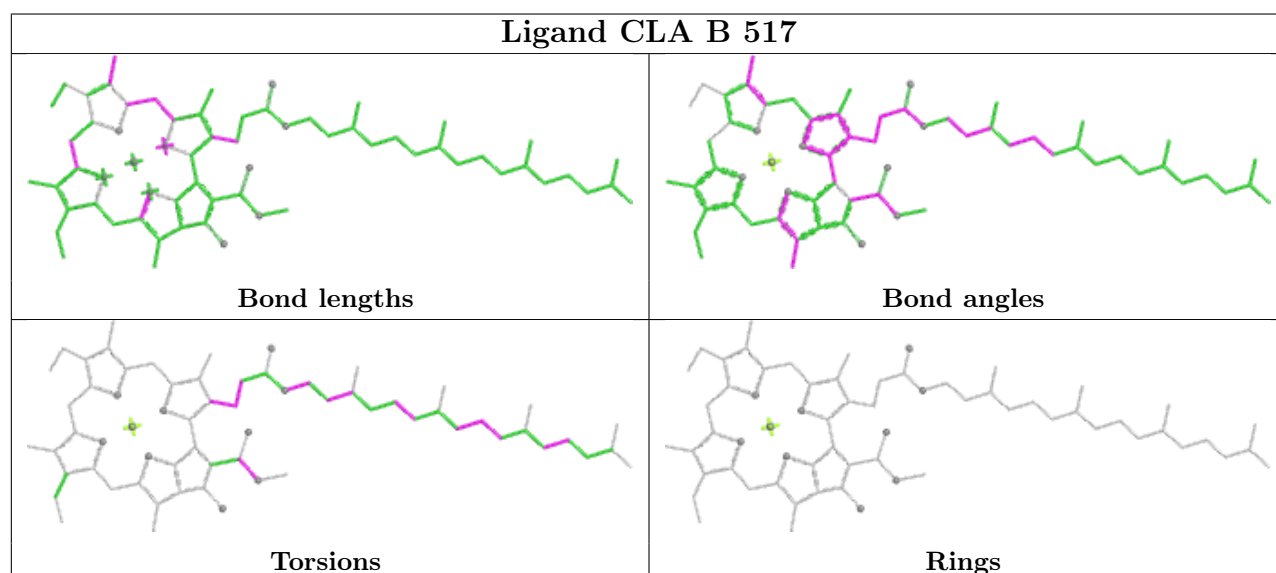
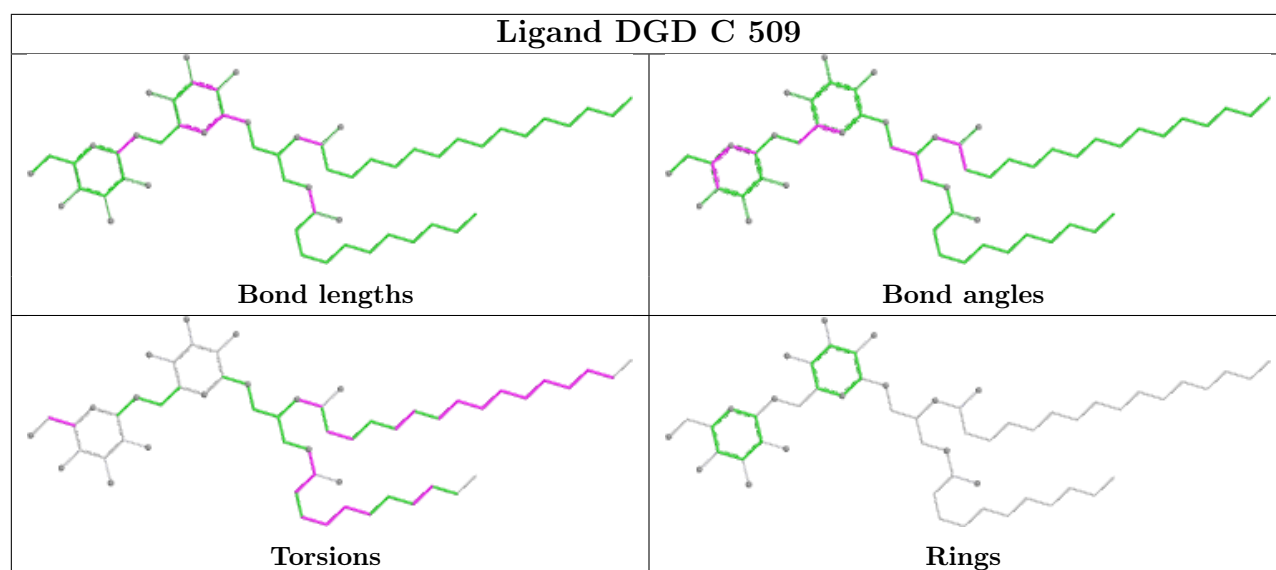
Ligand CLA A 559

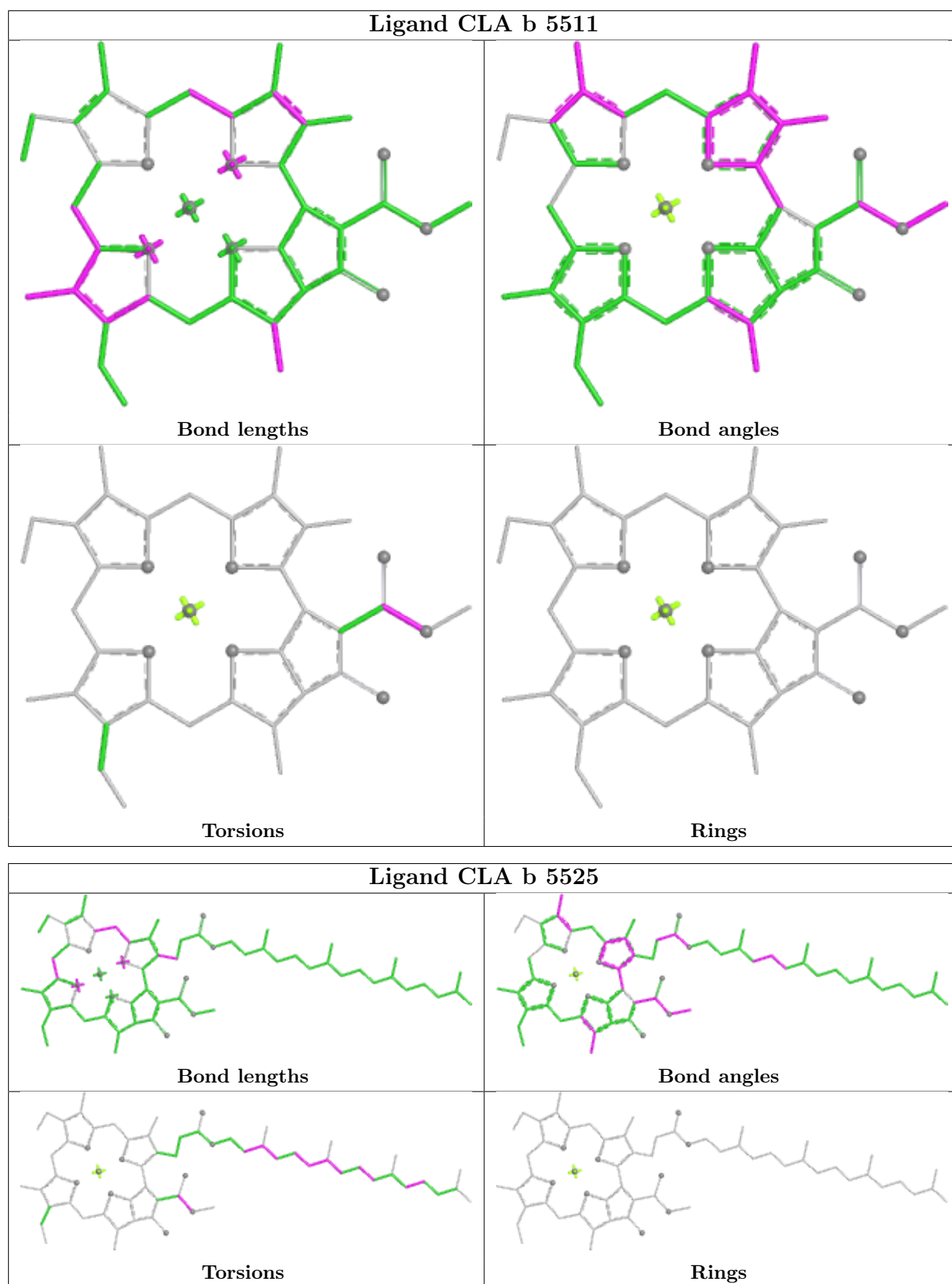


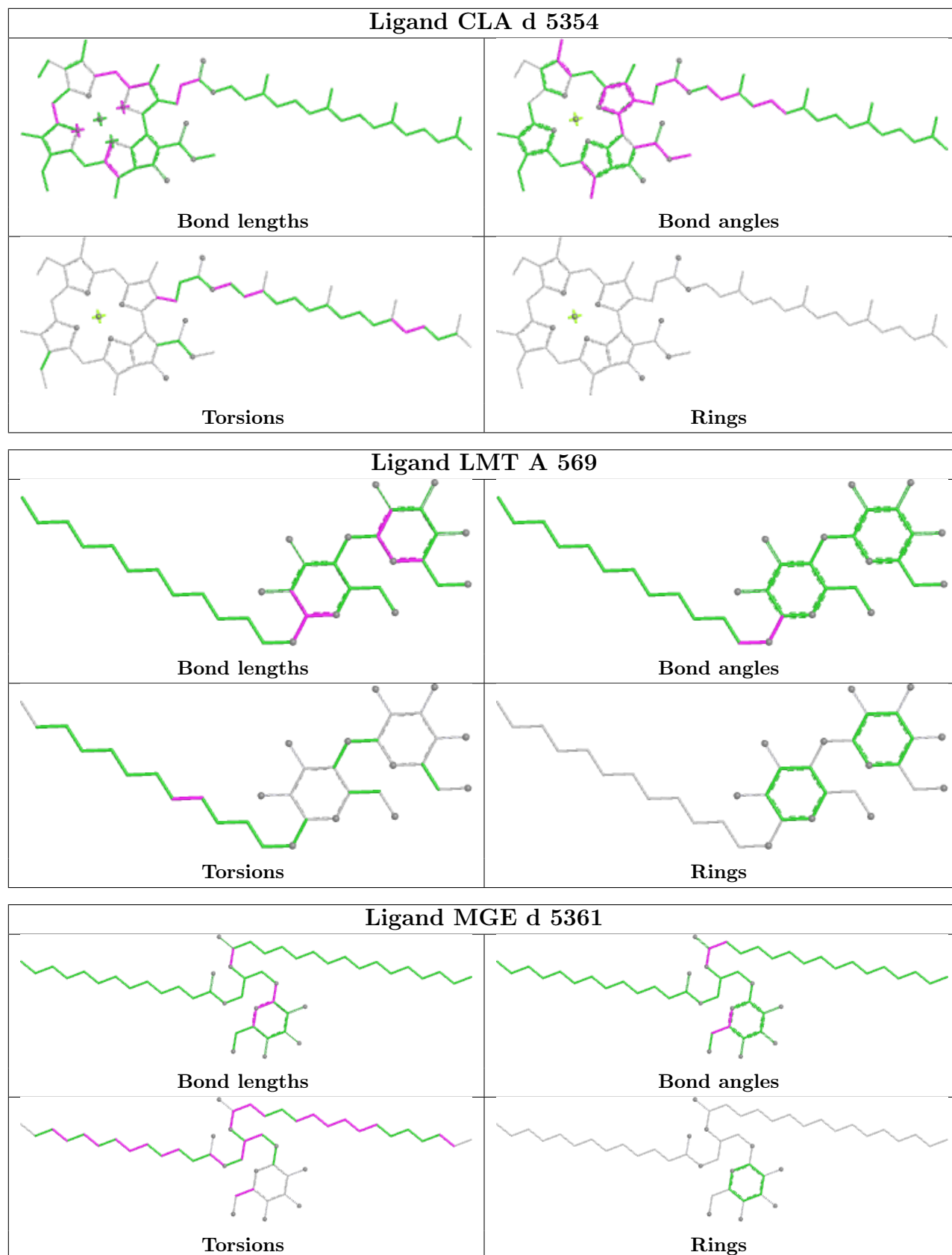
Ligand CLA b 5522

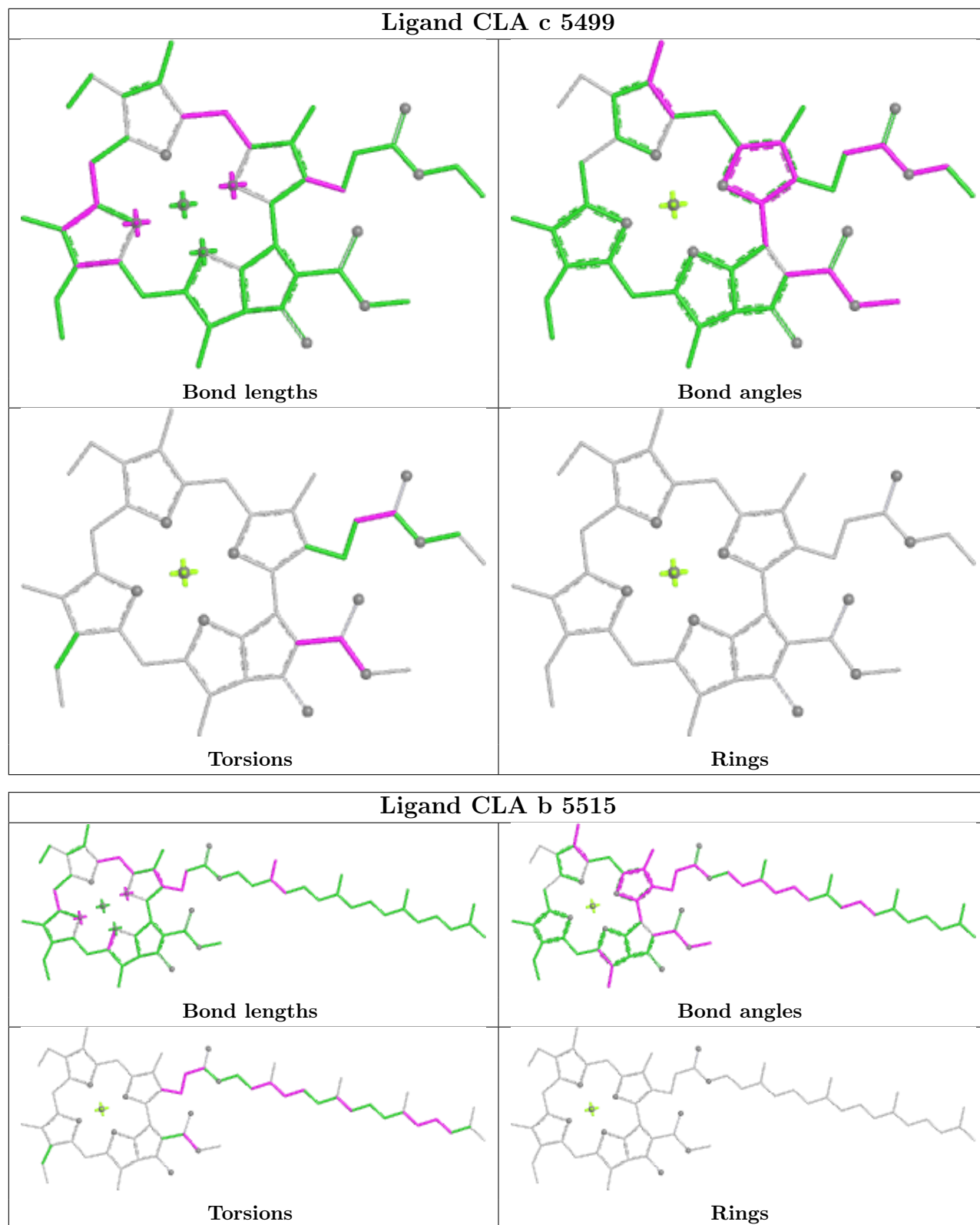


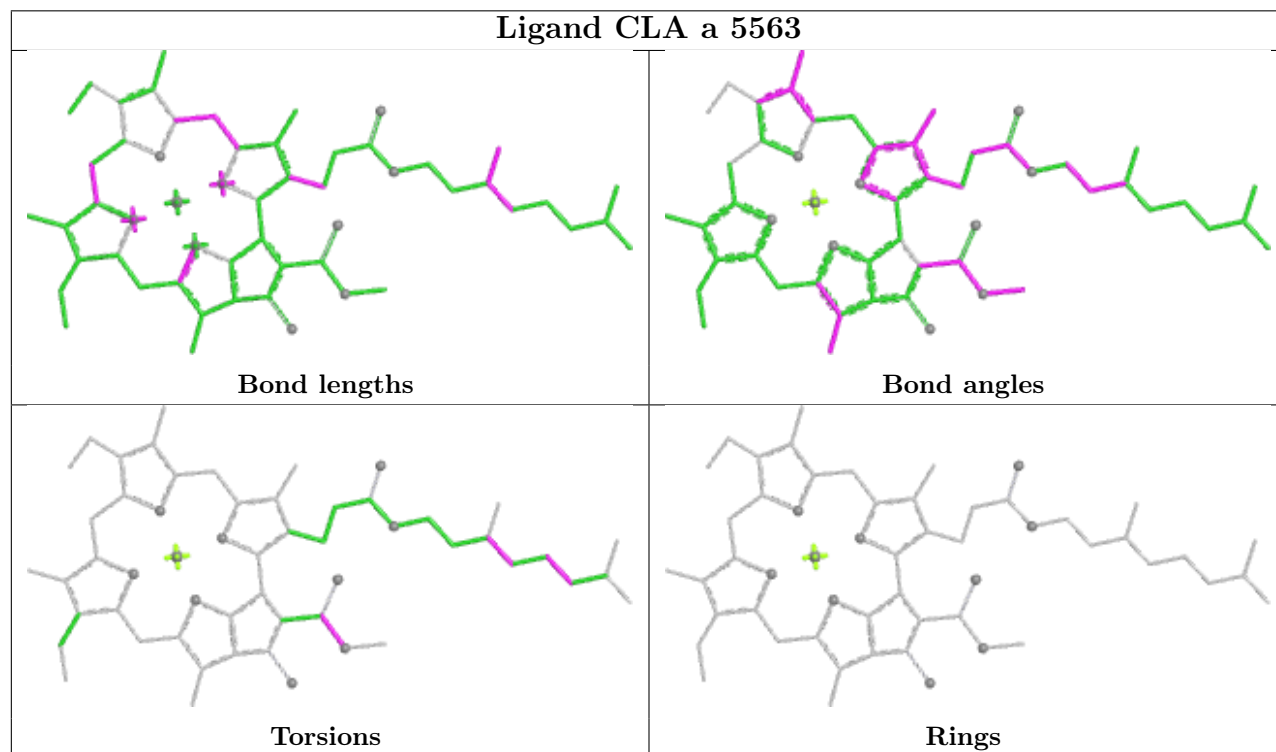
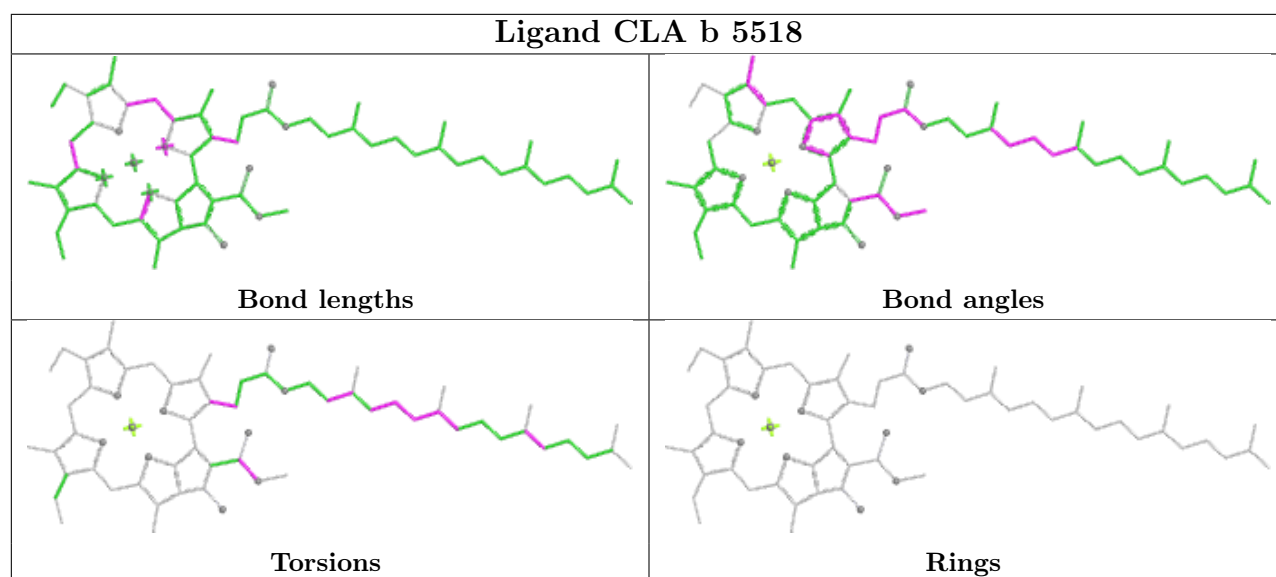


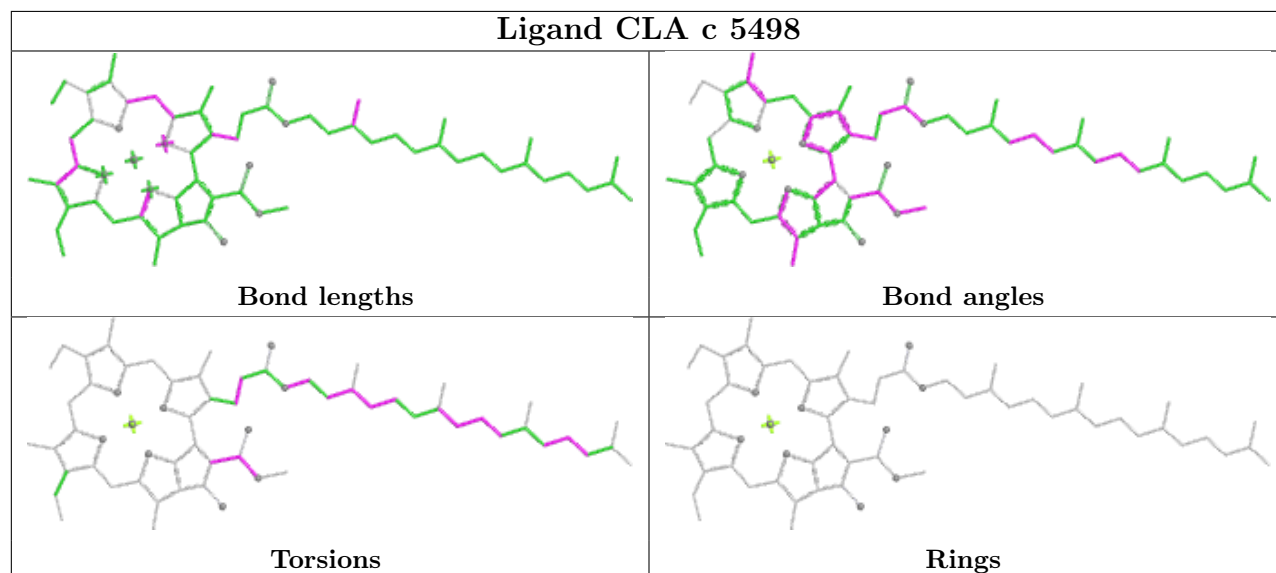
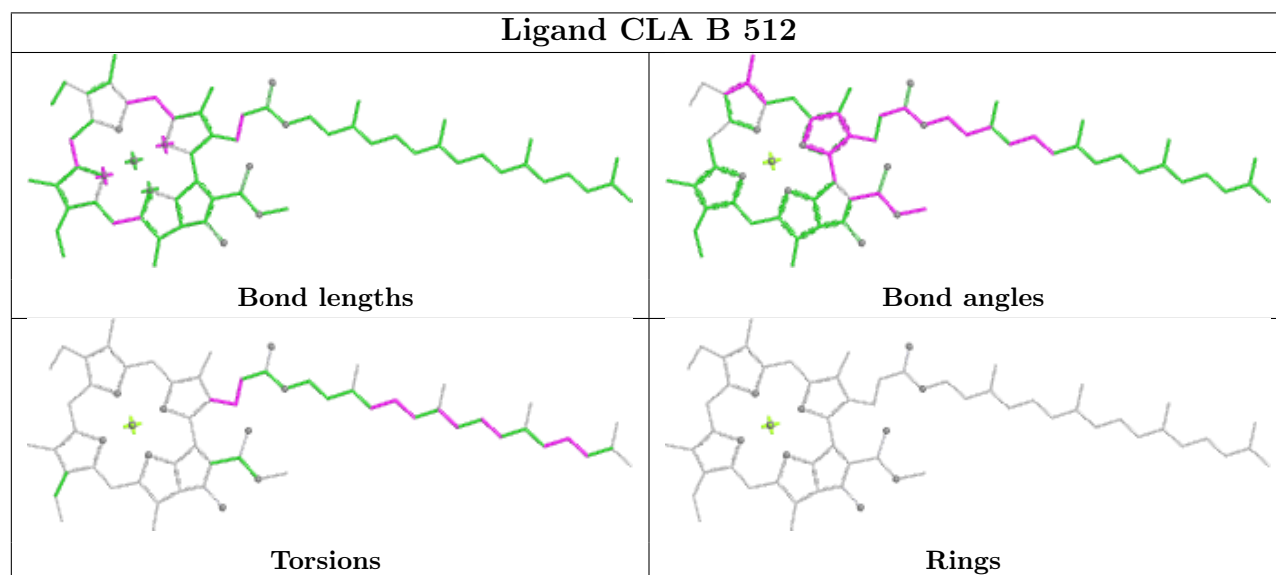
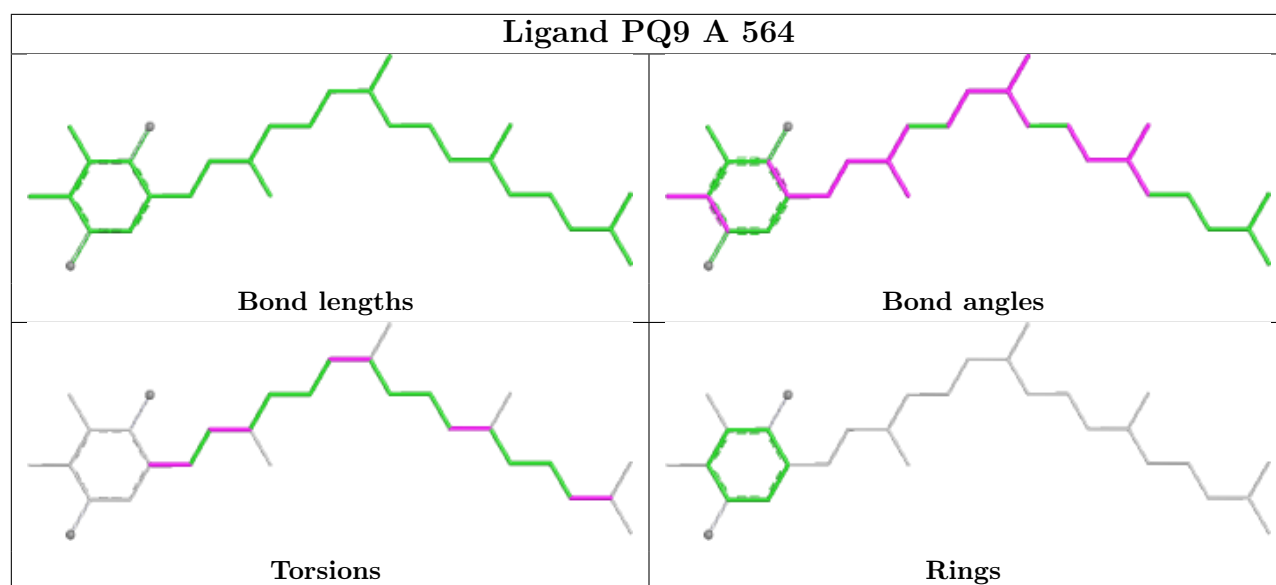


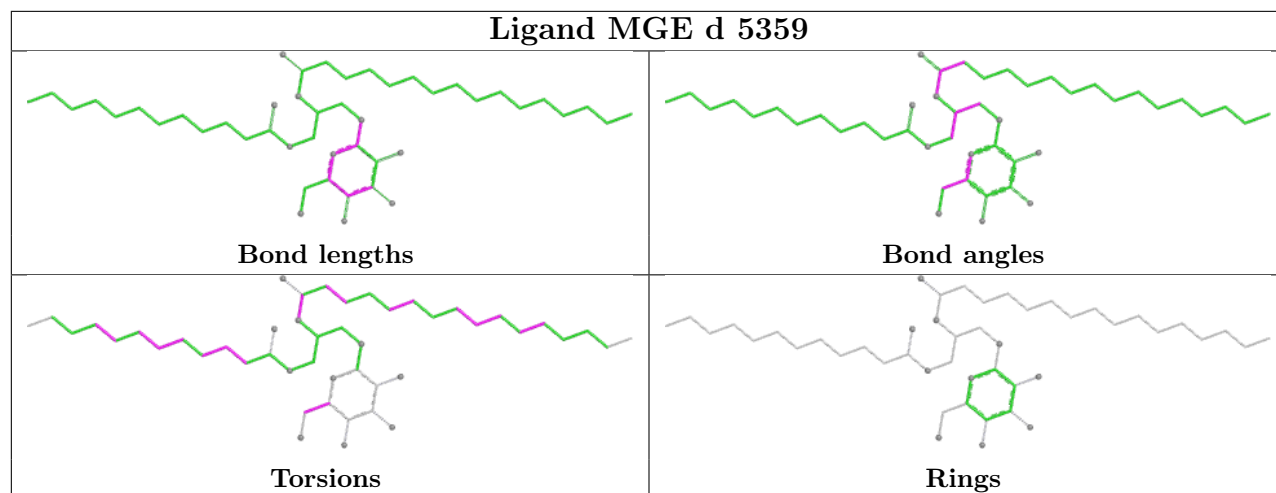
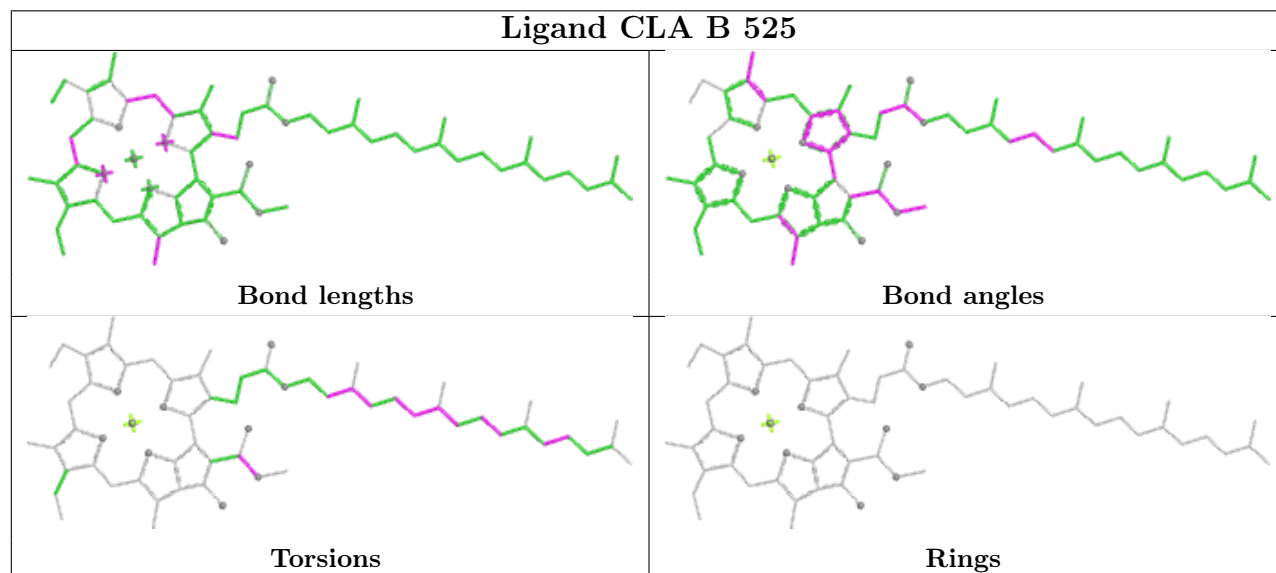
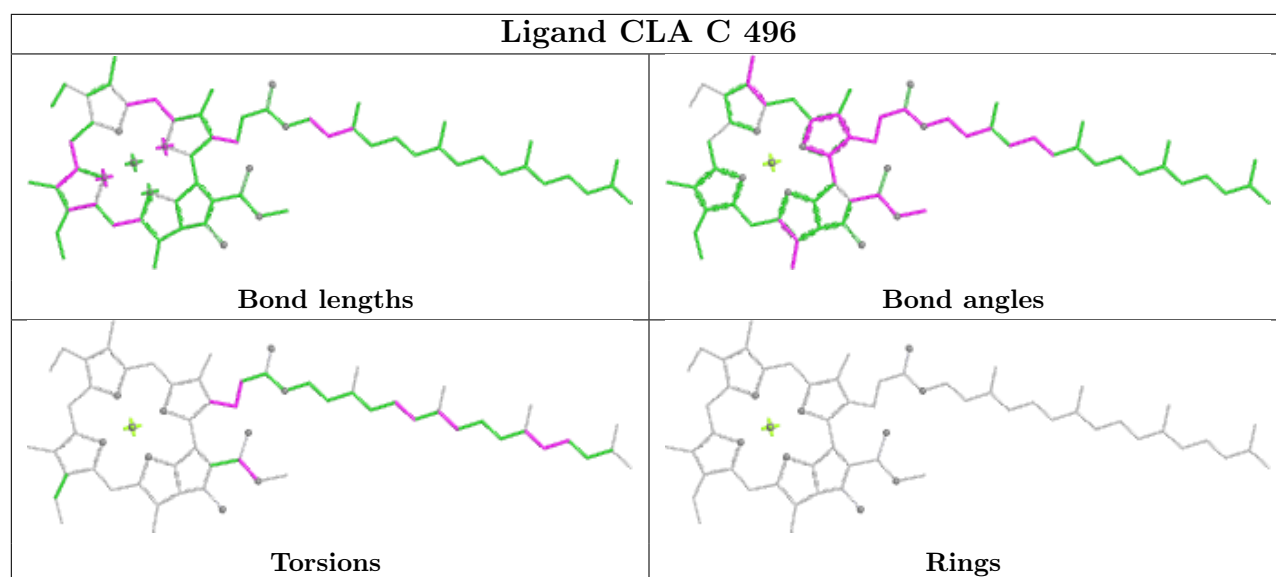


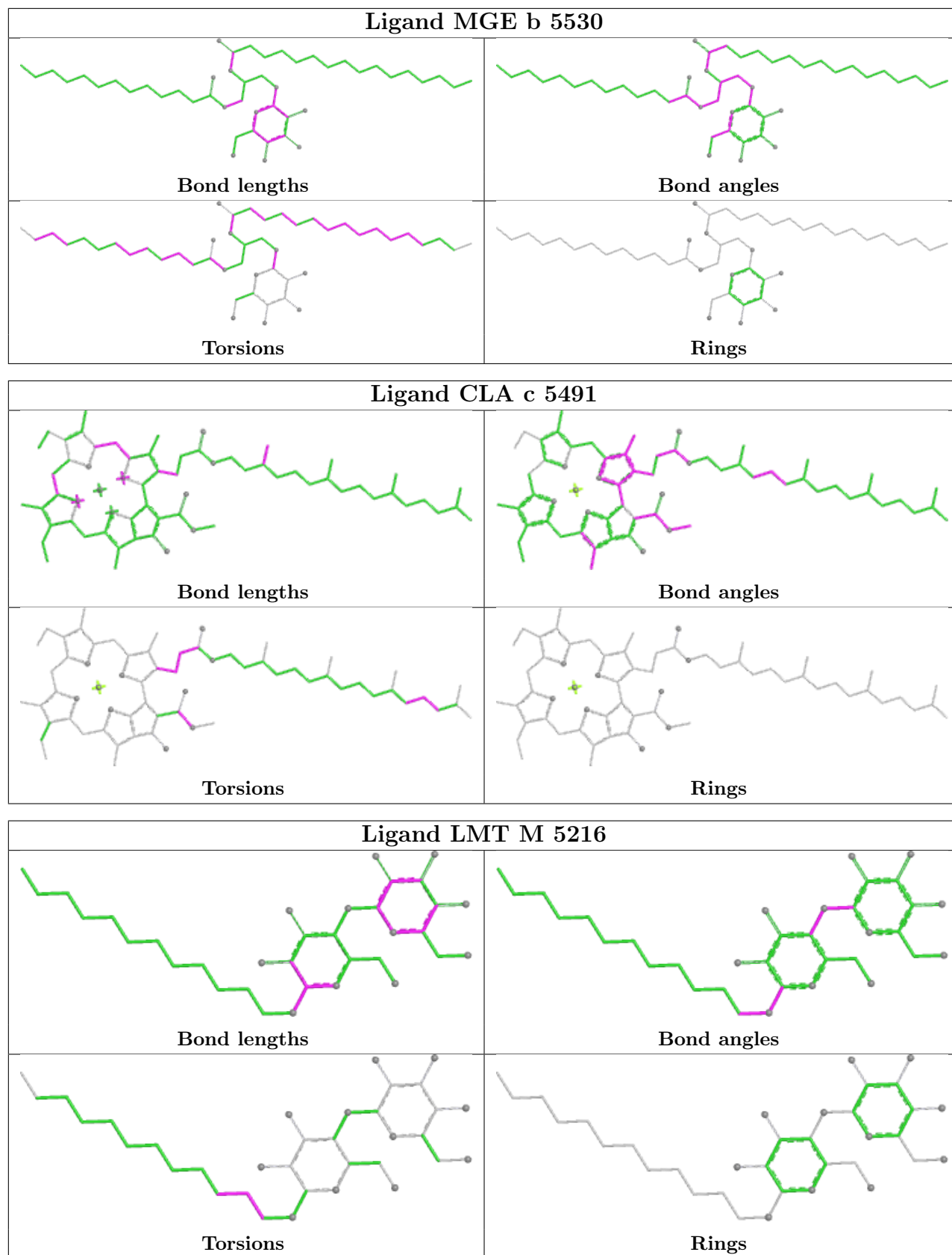


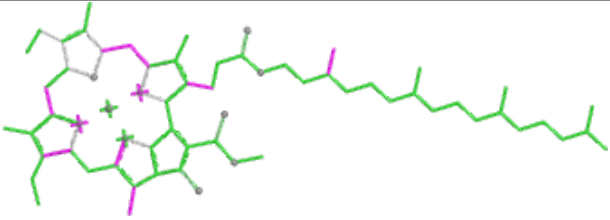
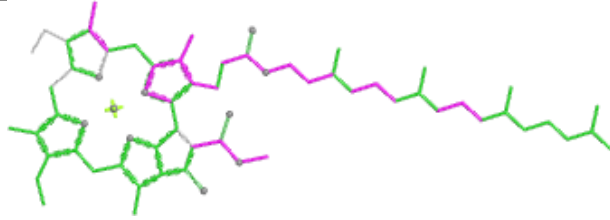
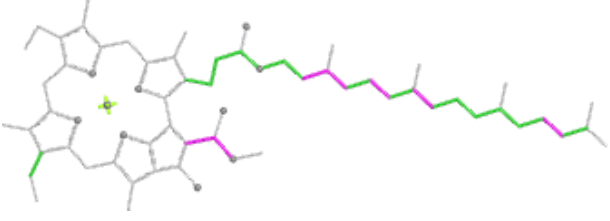
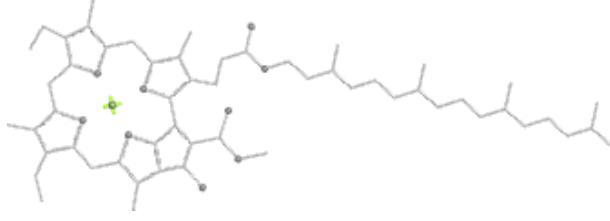
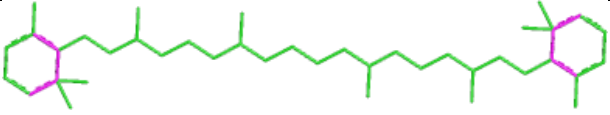
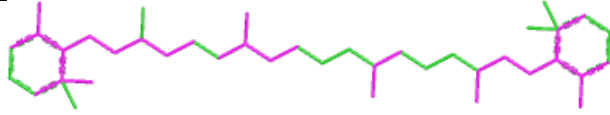
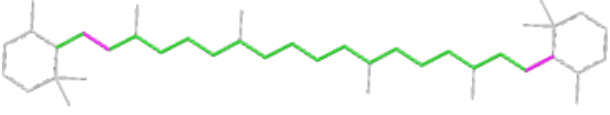
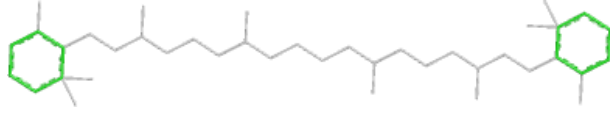
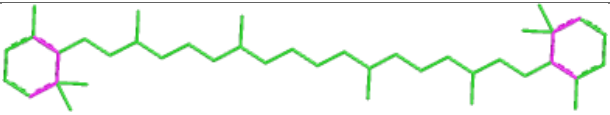
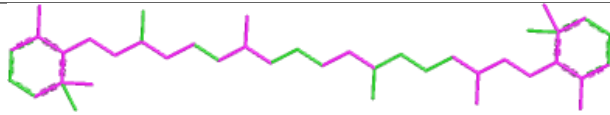
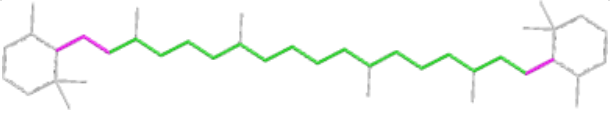
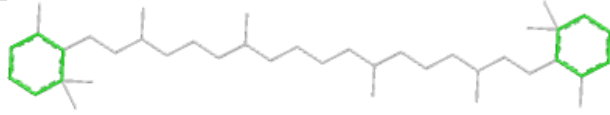


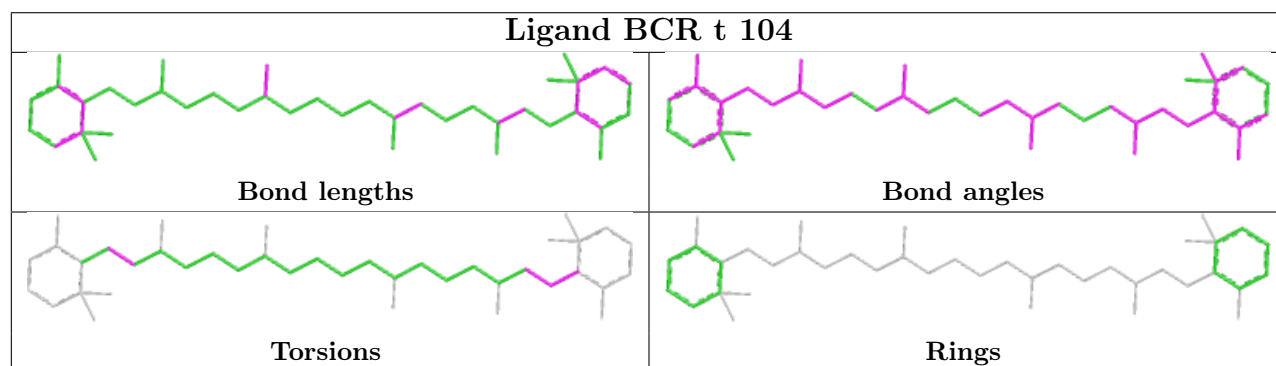
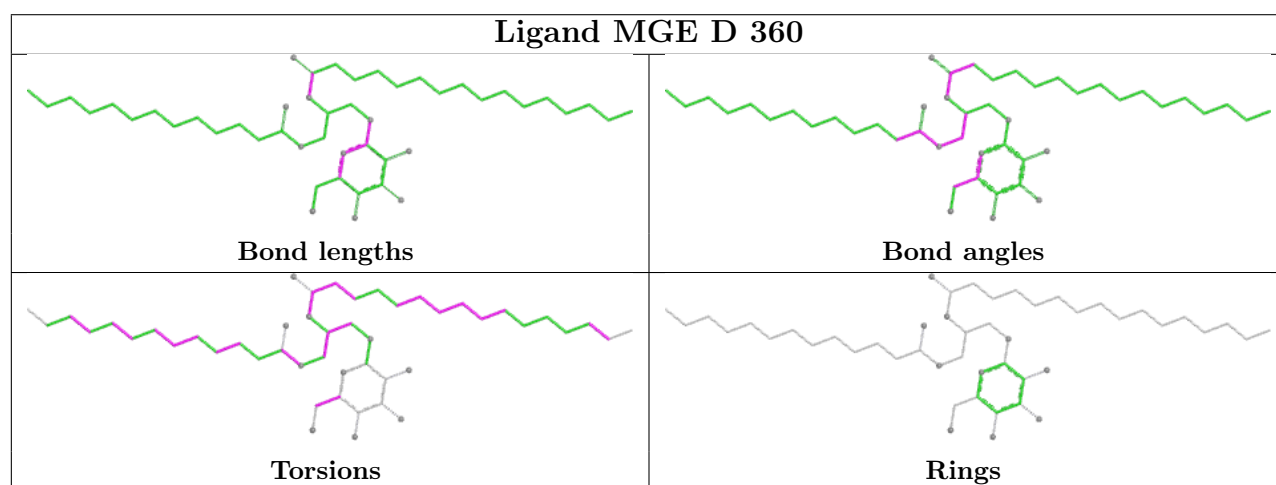
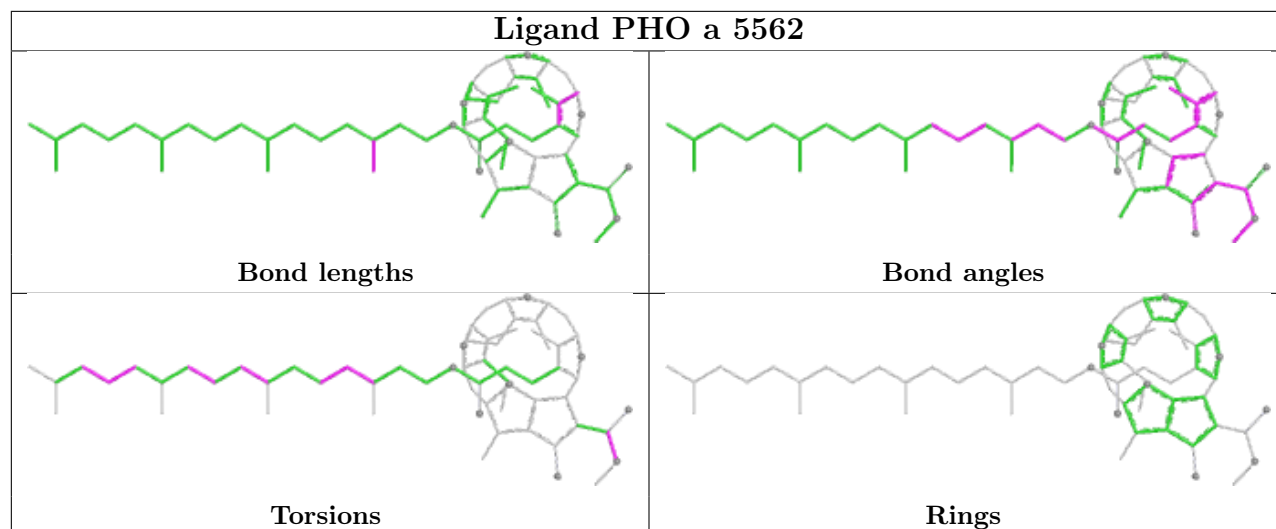




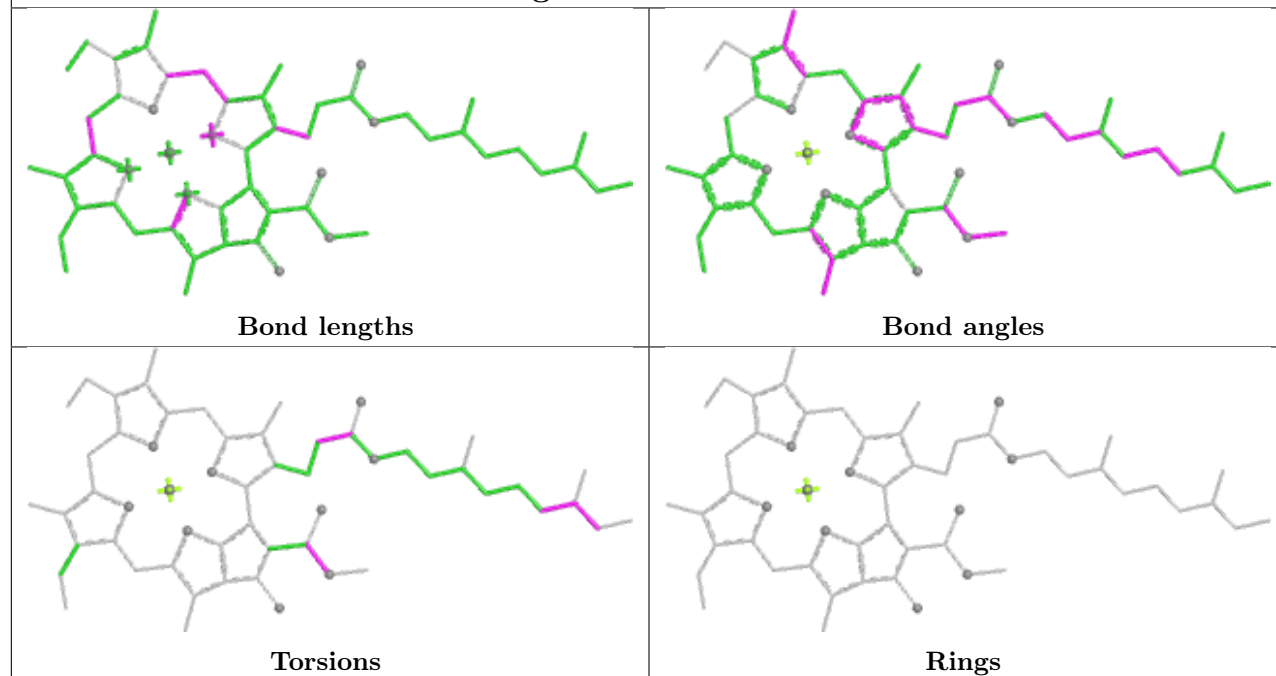




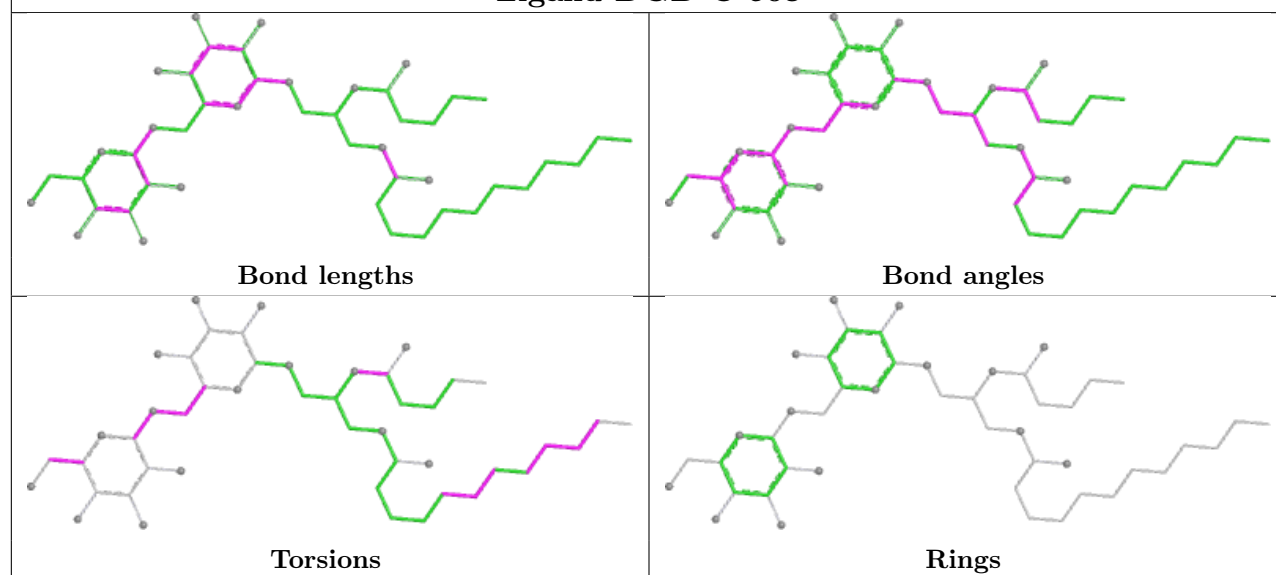
Ligand CLA C 500	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 5529	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

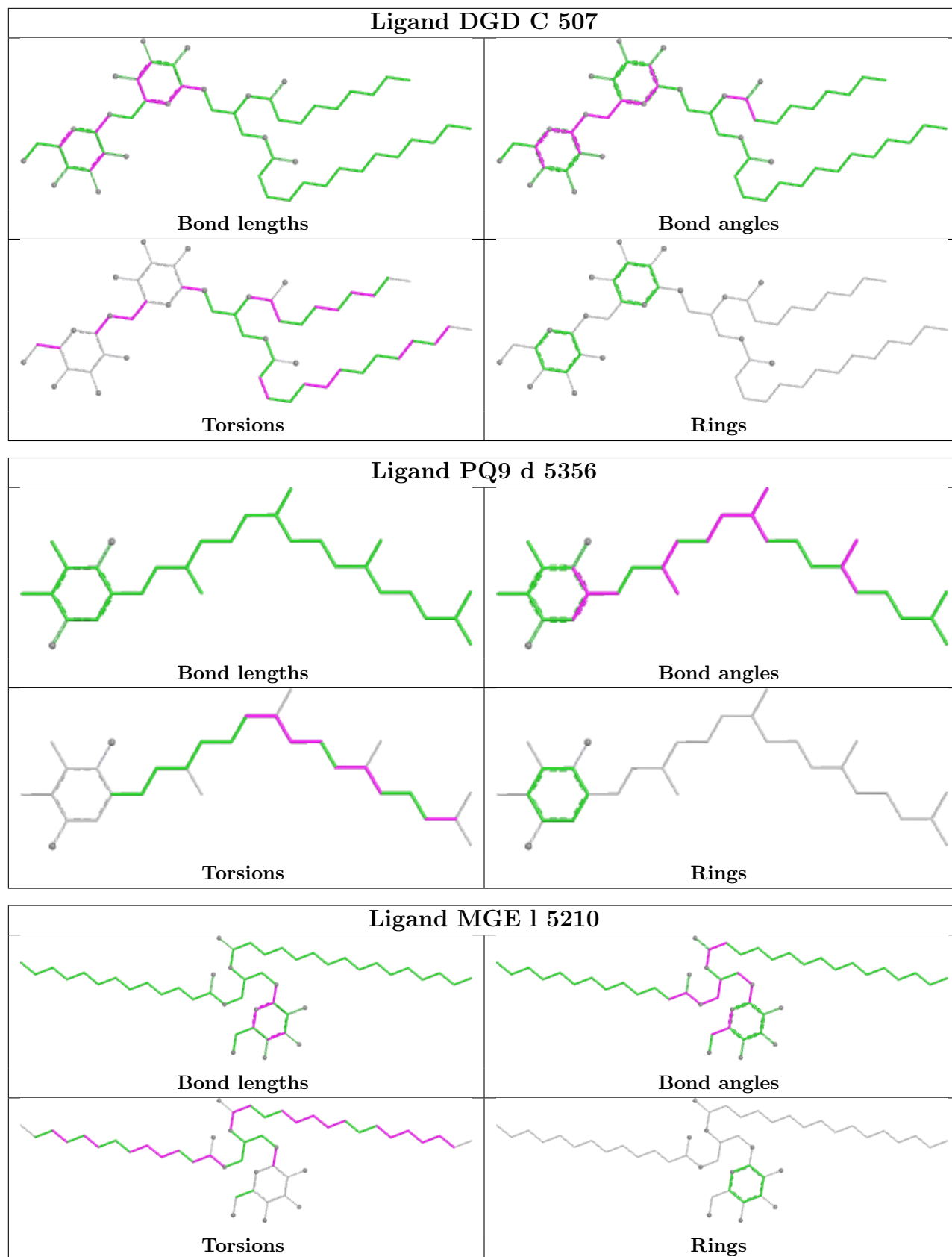


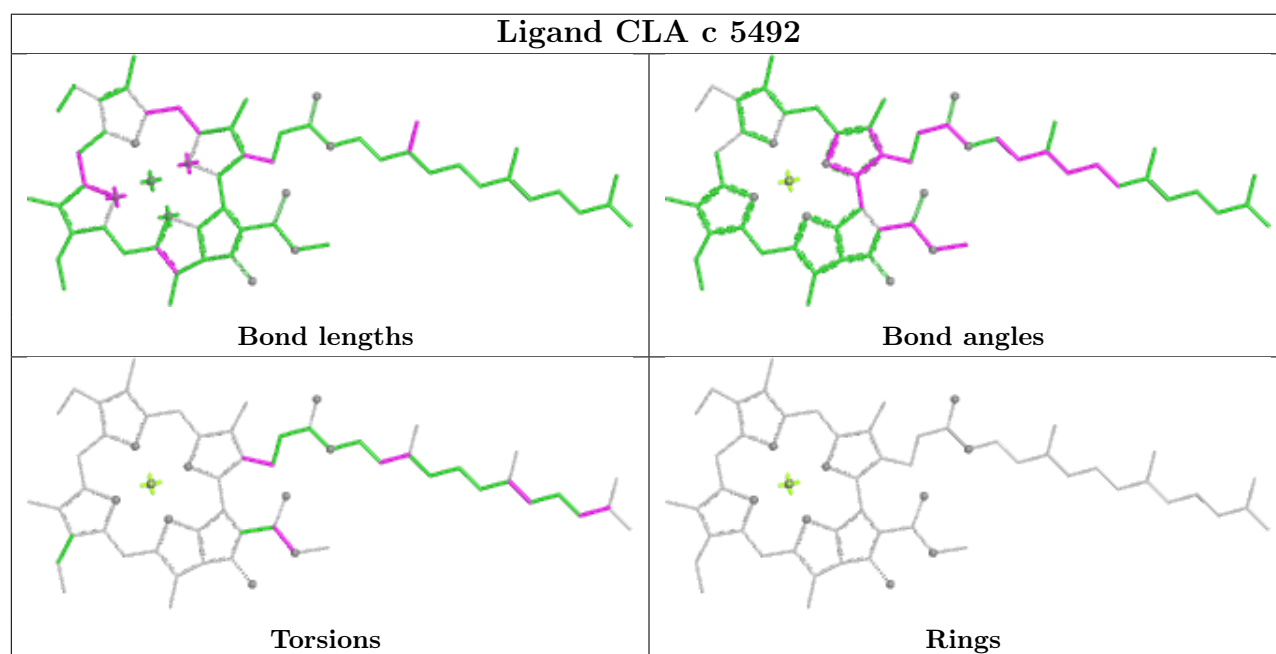
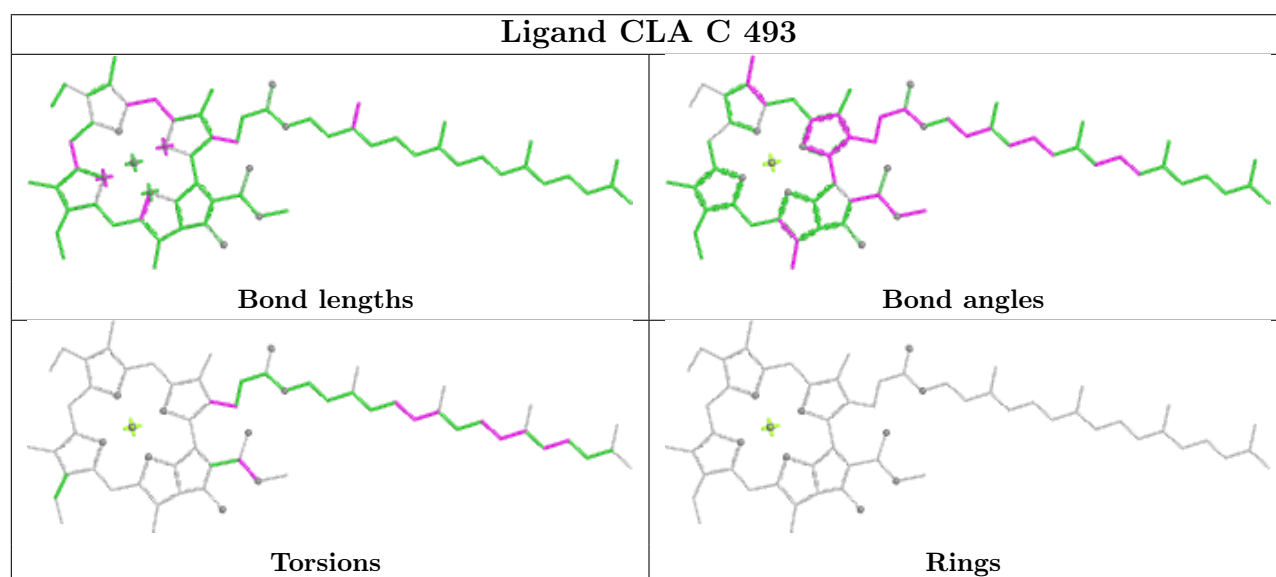
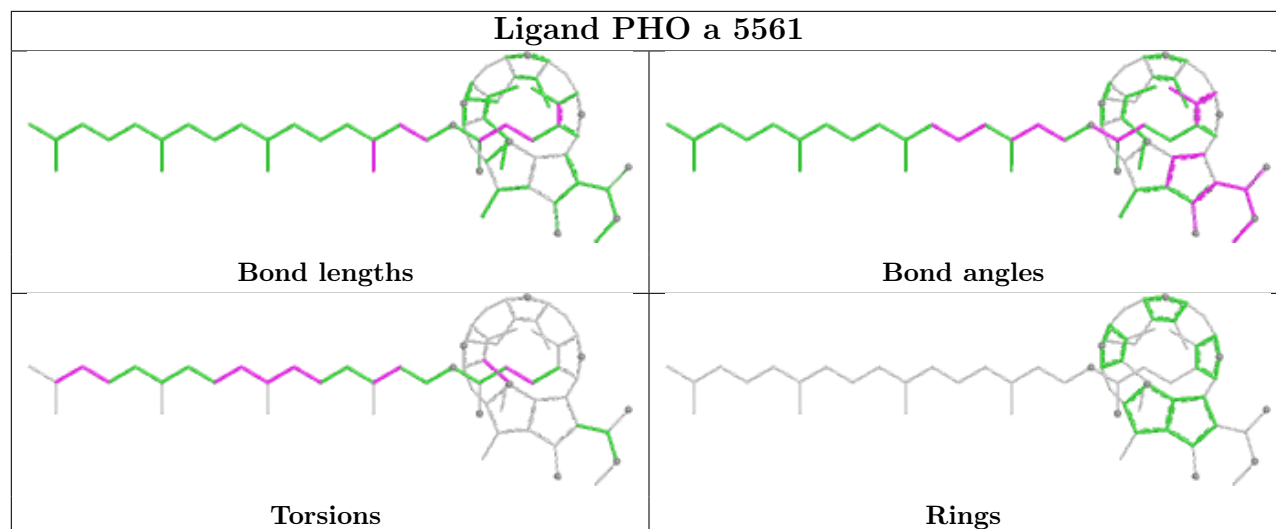
Ligand CLA B 524

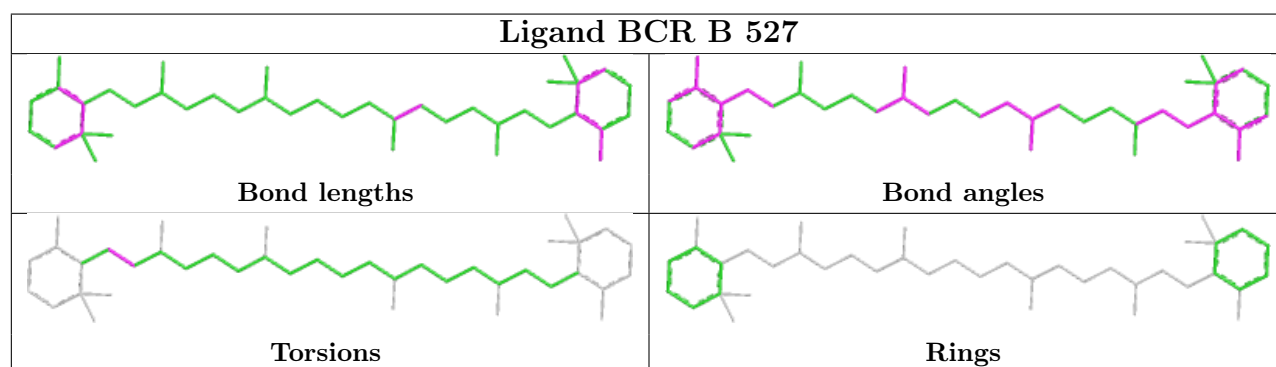
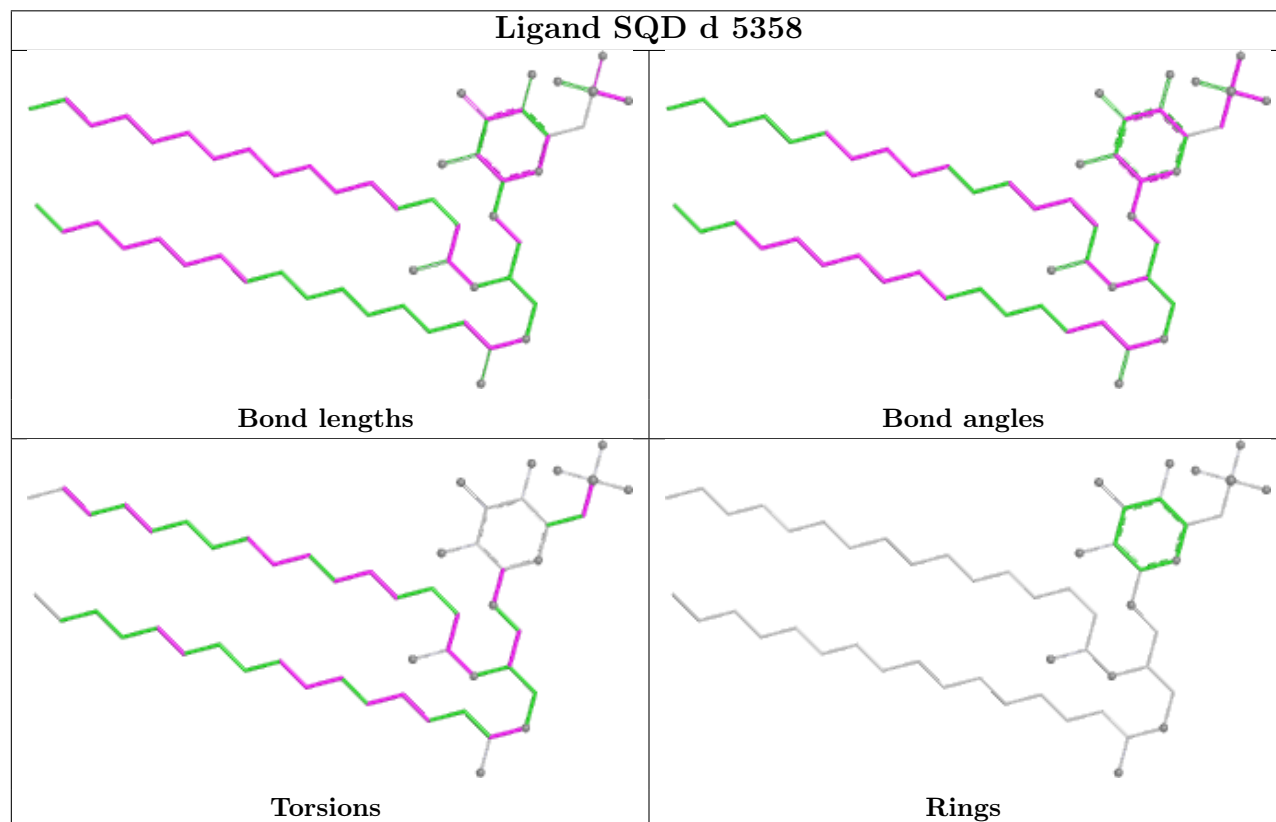
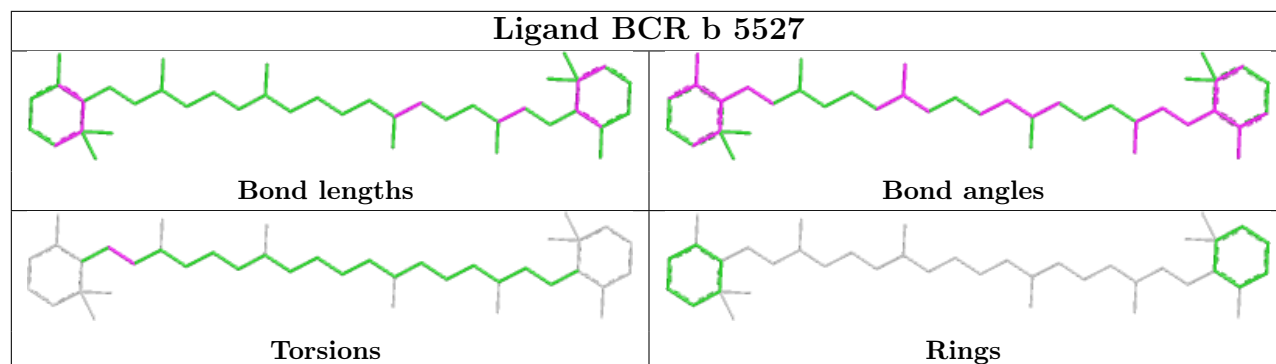


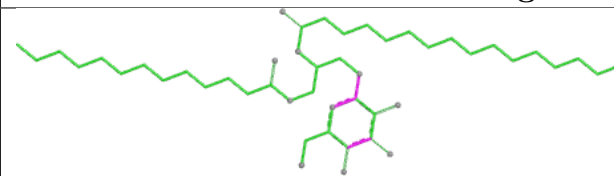
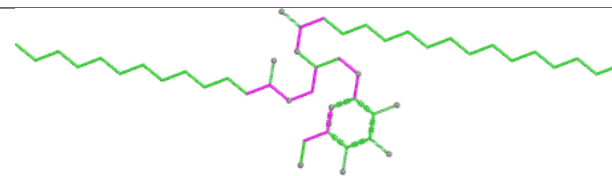
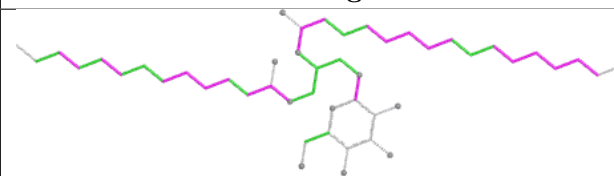
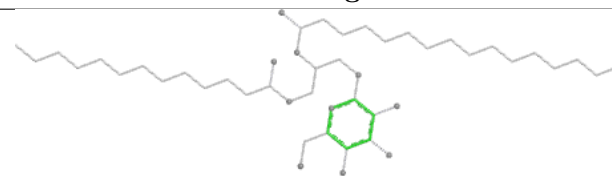
Ligand DGD C 508

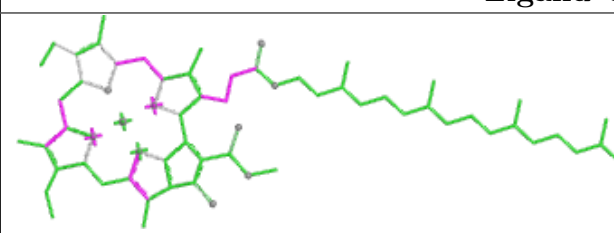
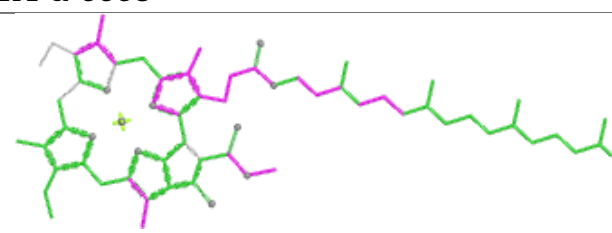
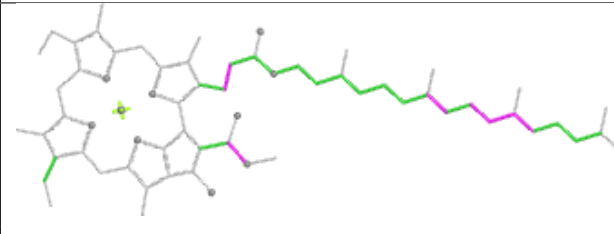
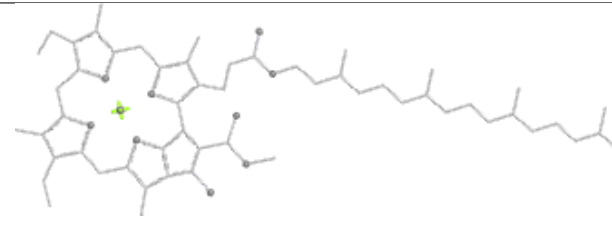


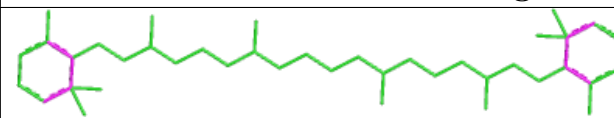
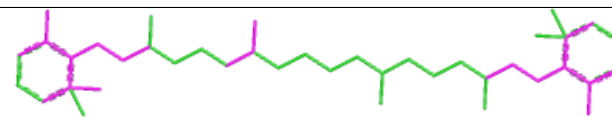
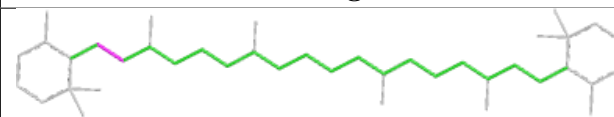
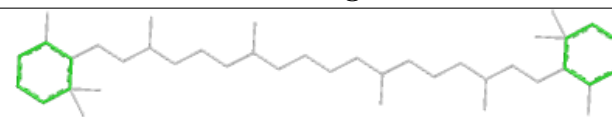


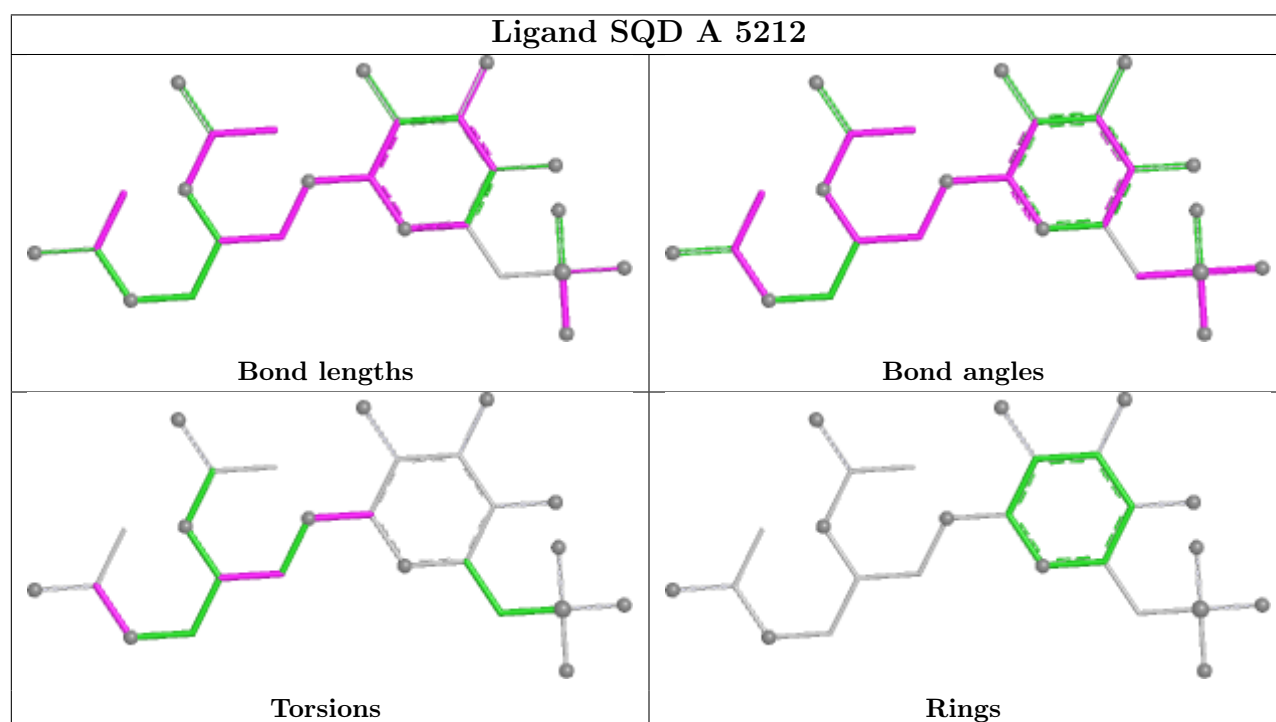
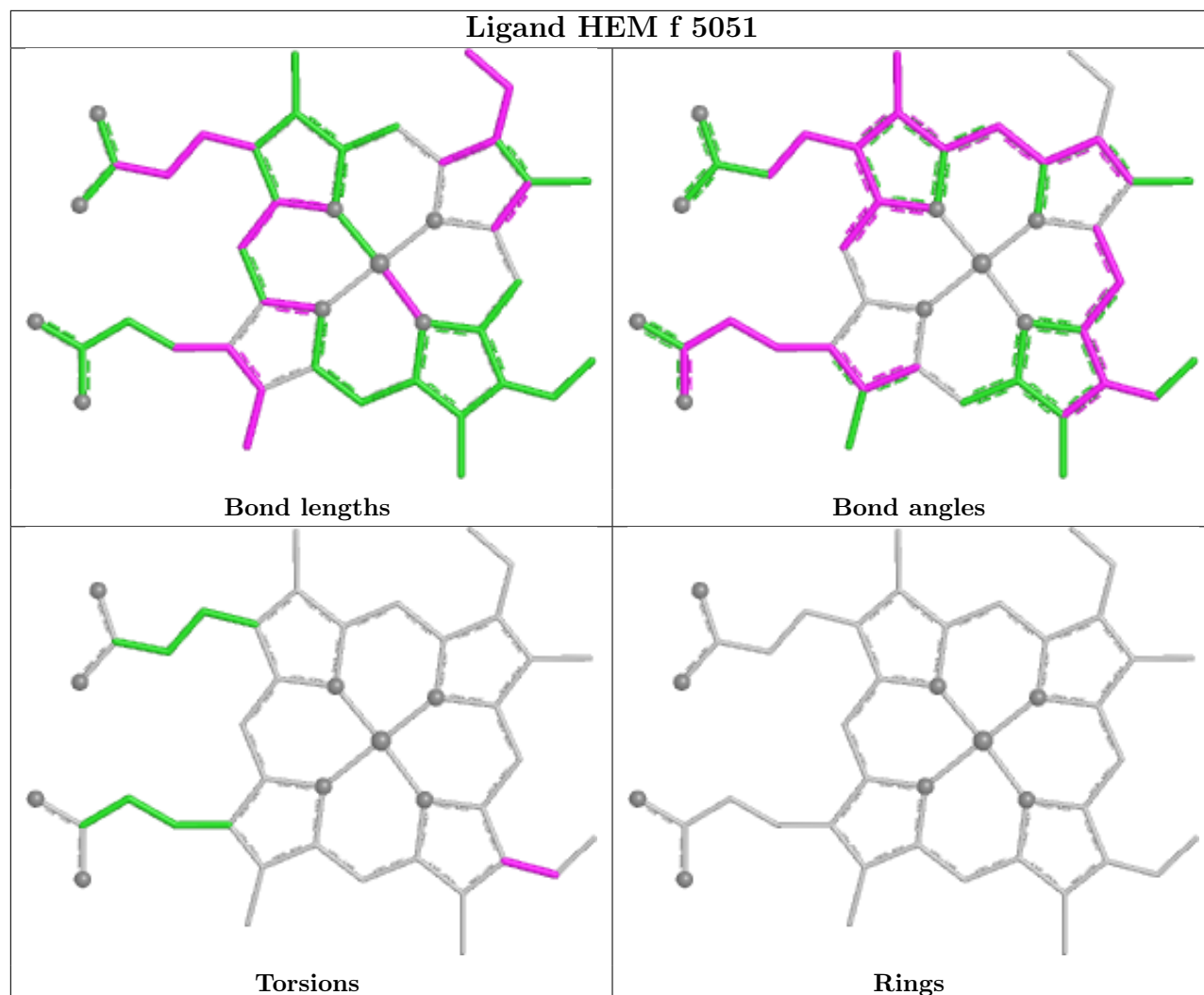


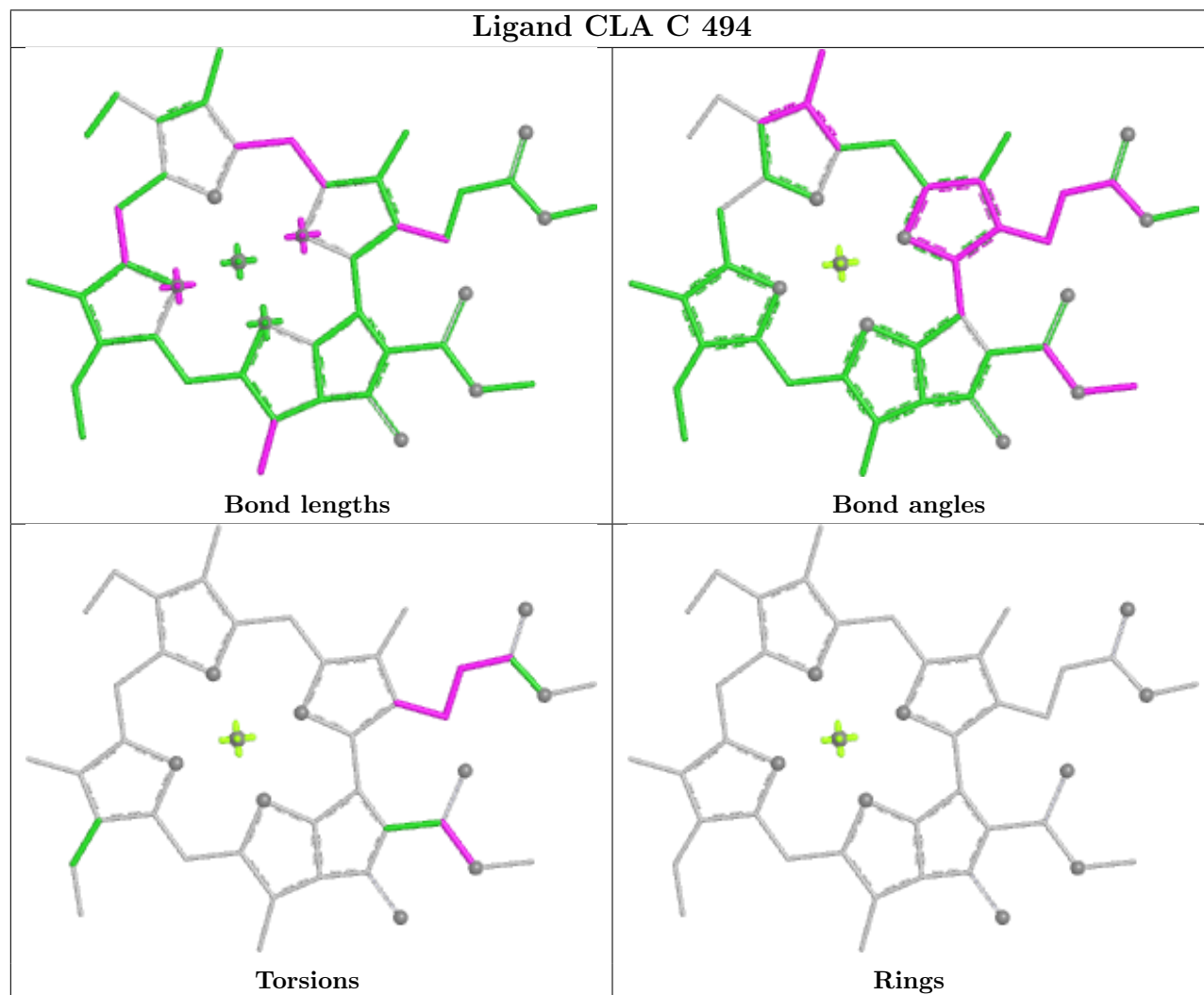
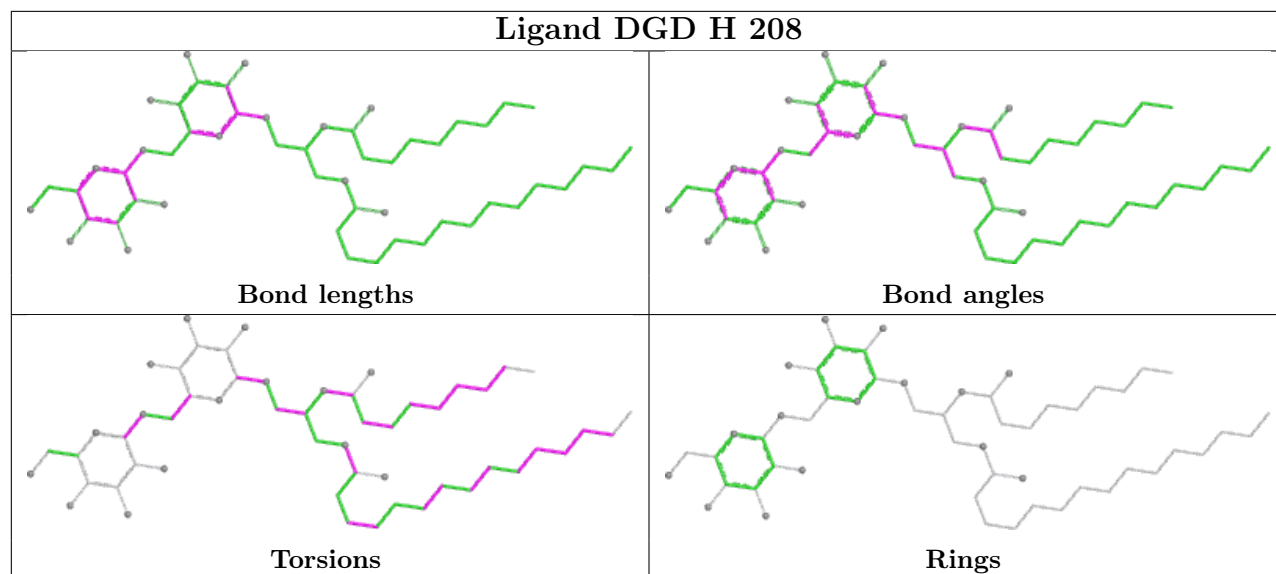


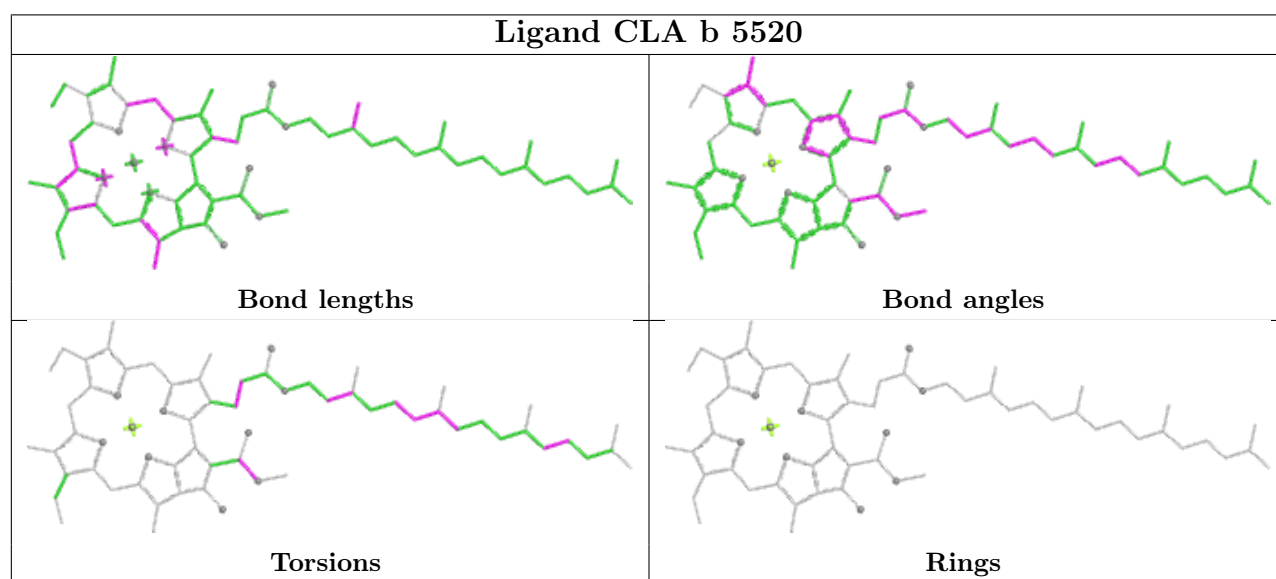
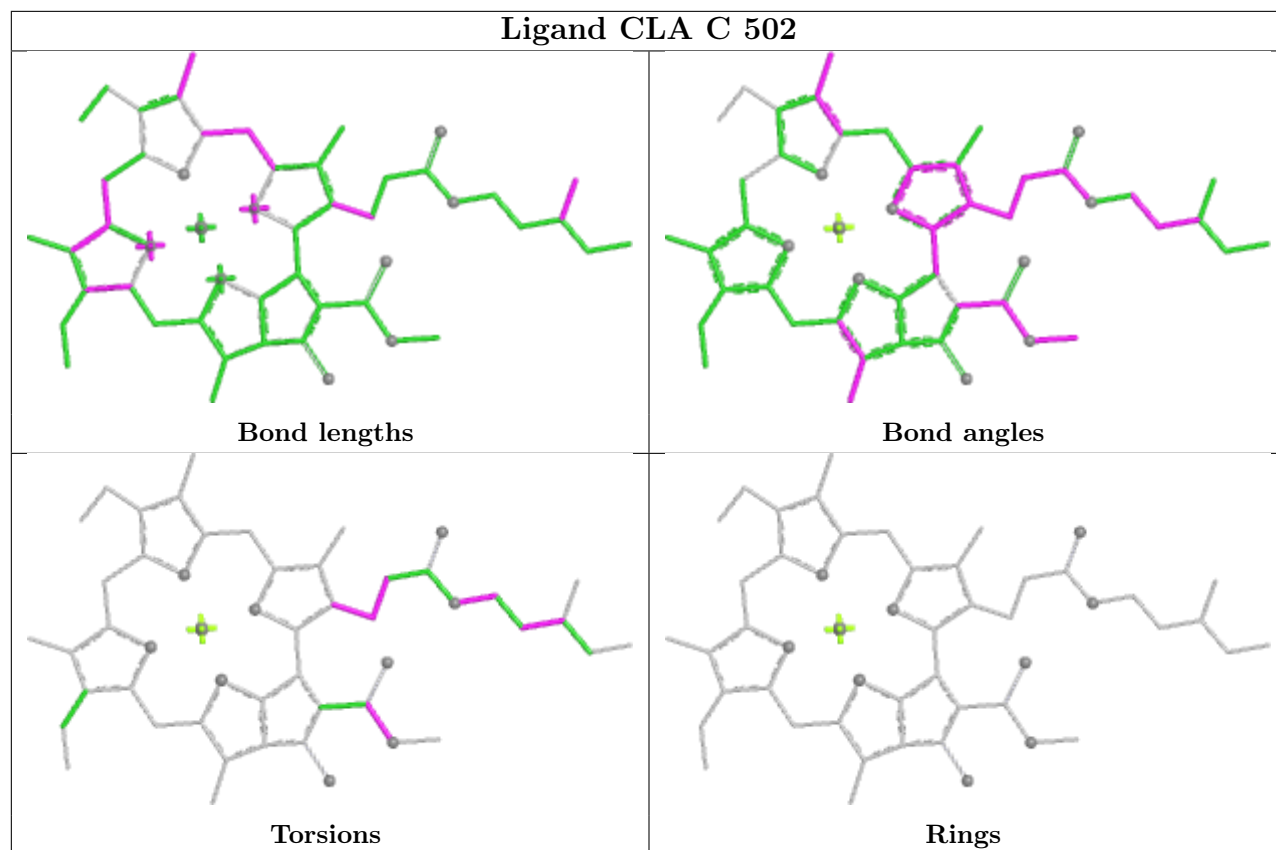
Ligand MGE L 210	
	
Bond lengths	Bond angles
	
Torsions	Rings

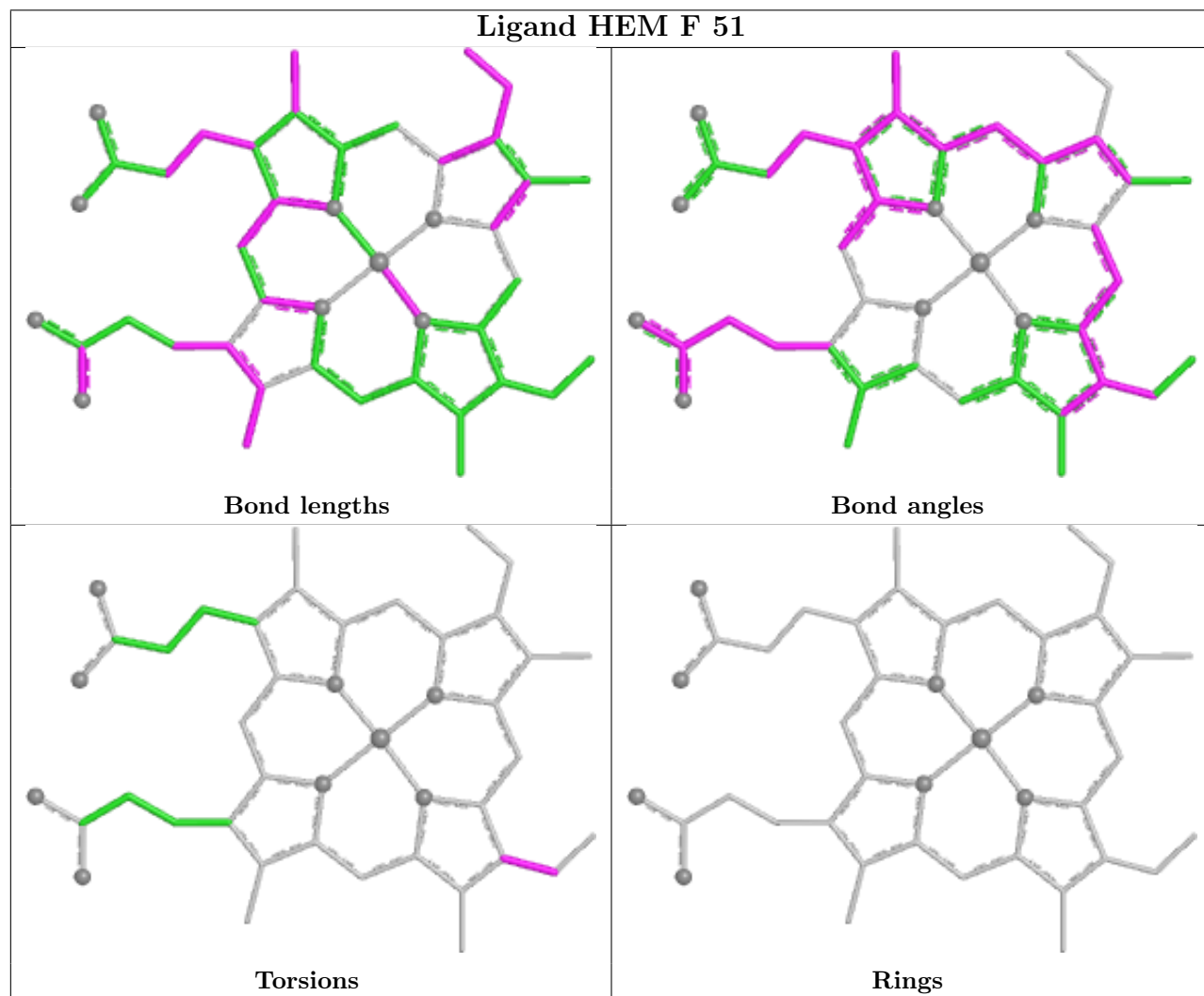
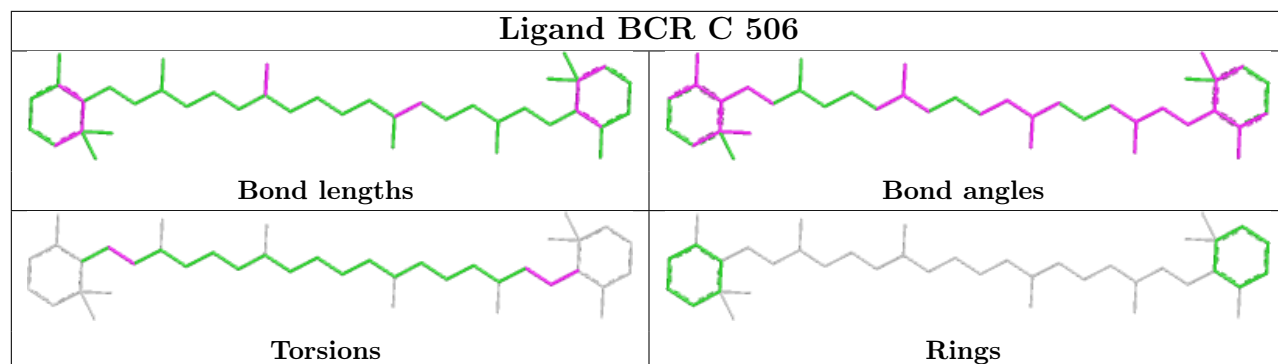
Ligand CLA a 5558	
	
Bond lengths	Bond angles
	
Torsions	Rings

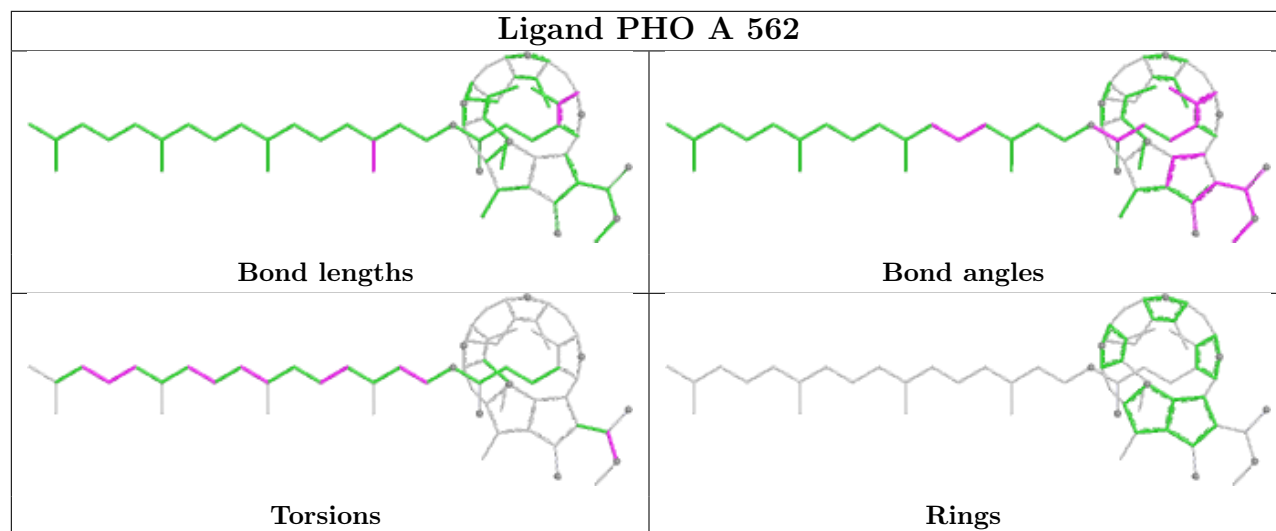
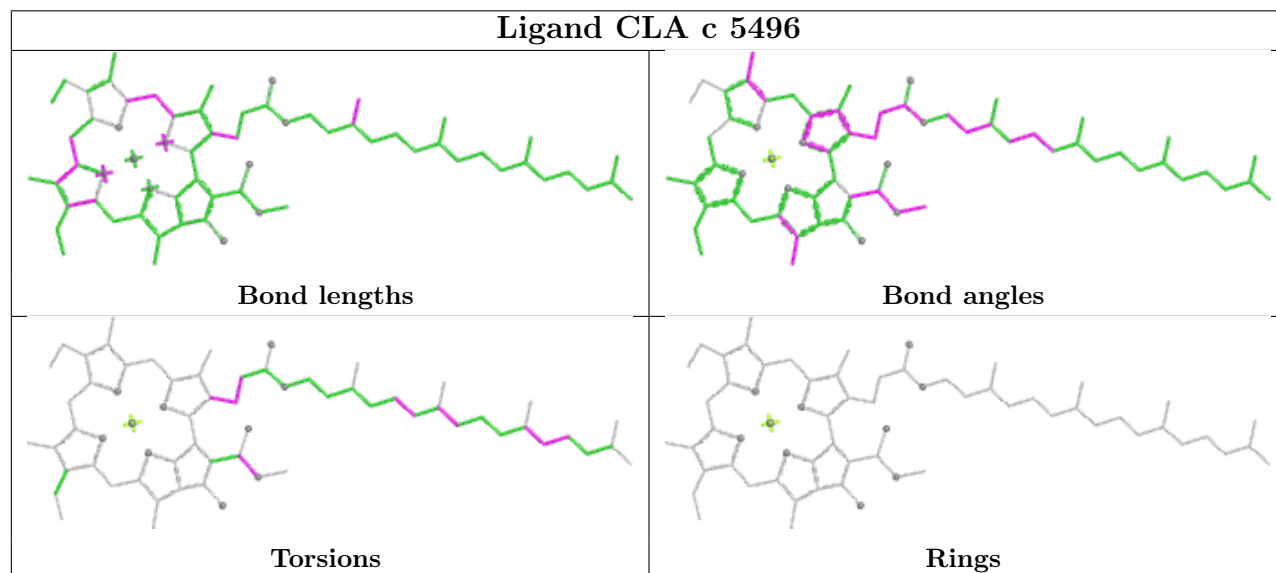
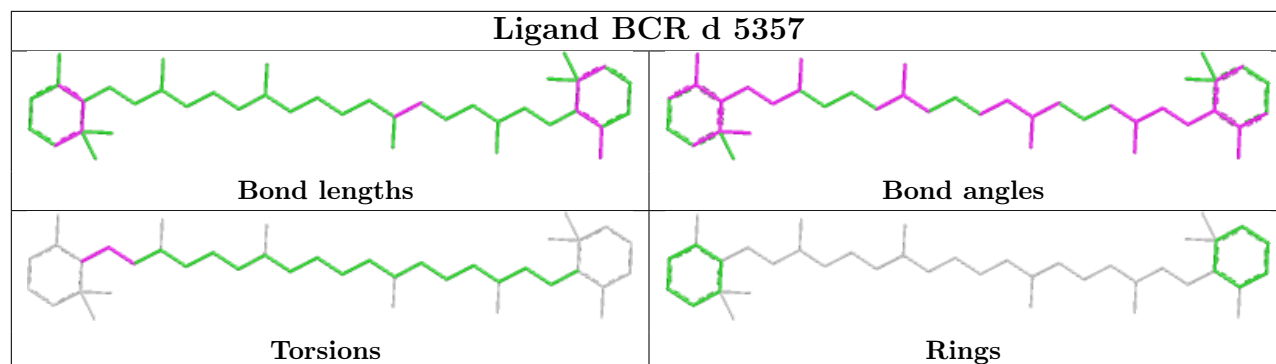
Ligand BCR b 5528	
	
Bond lengths	Bond angles
	
Torsions	Rings

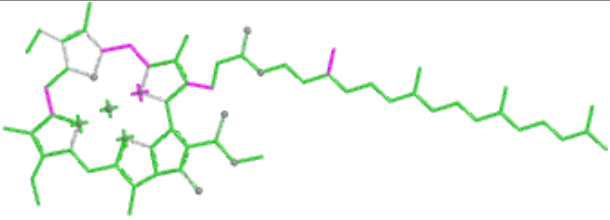
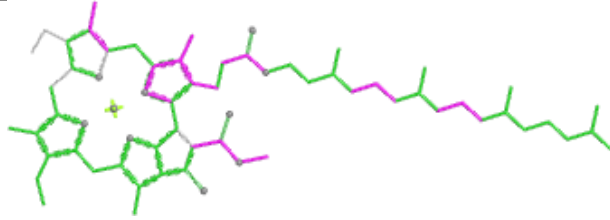
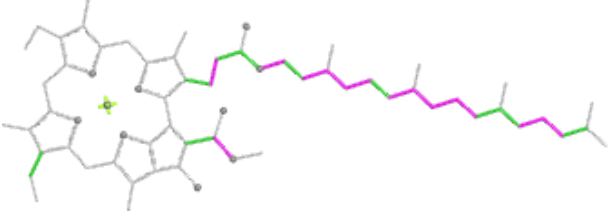
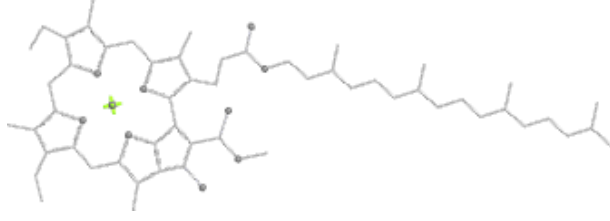
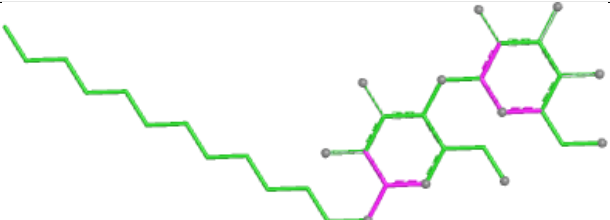

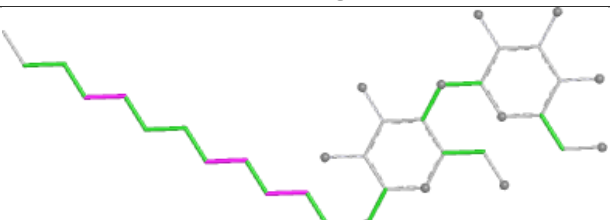
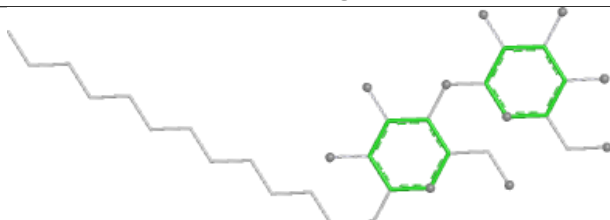
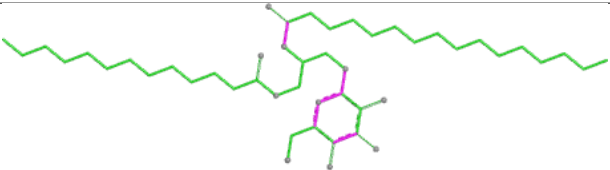
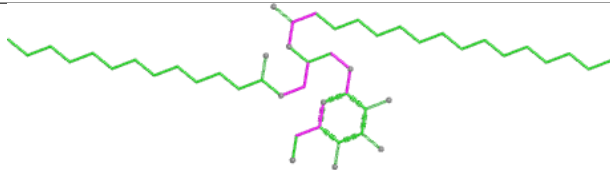
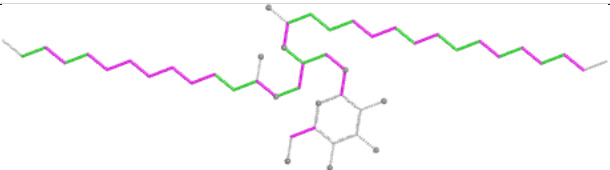
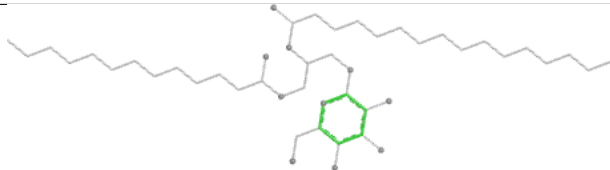


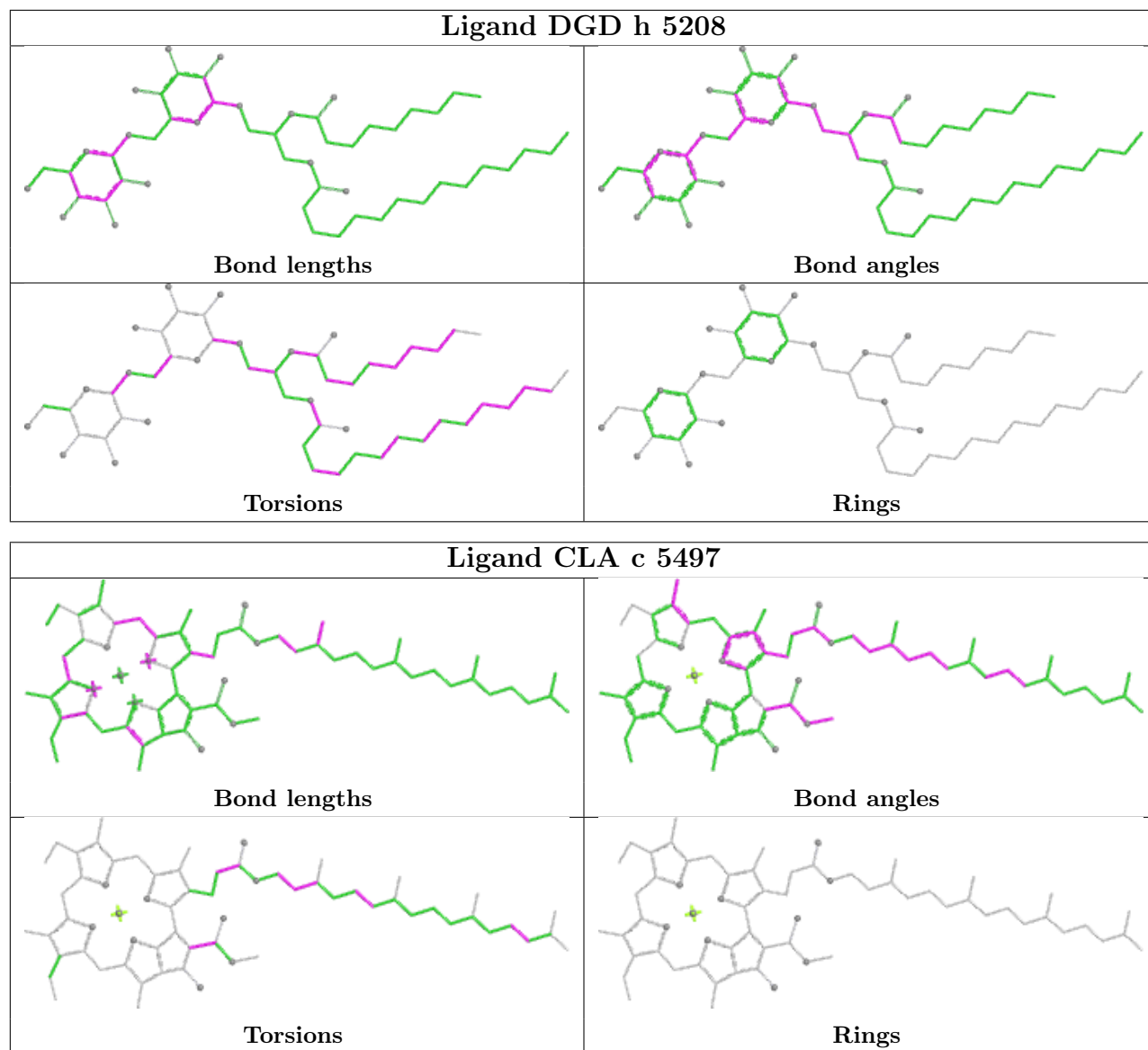




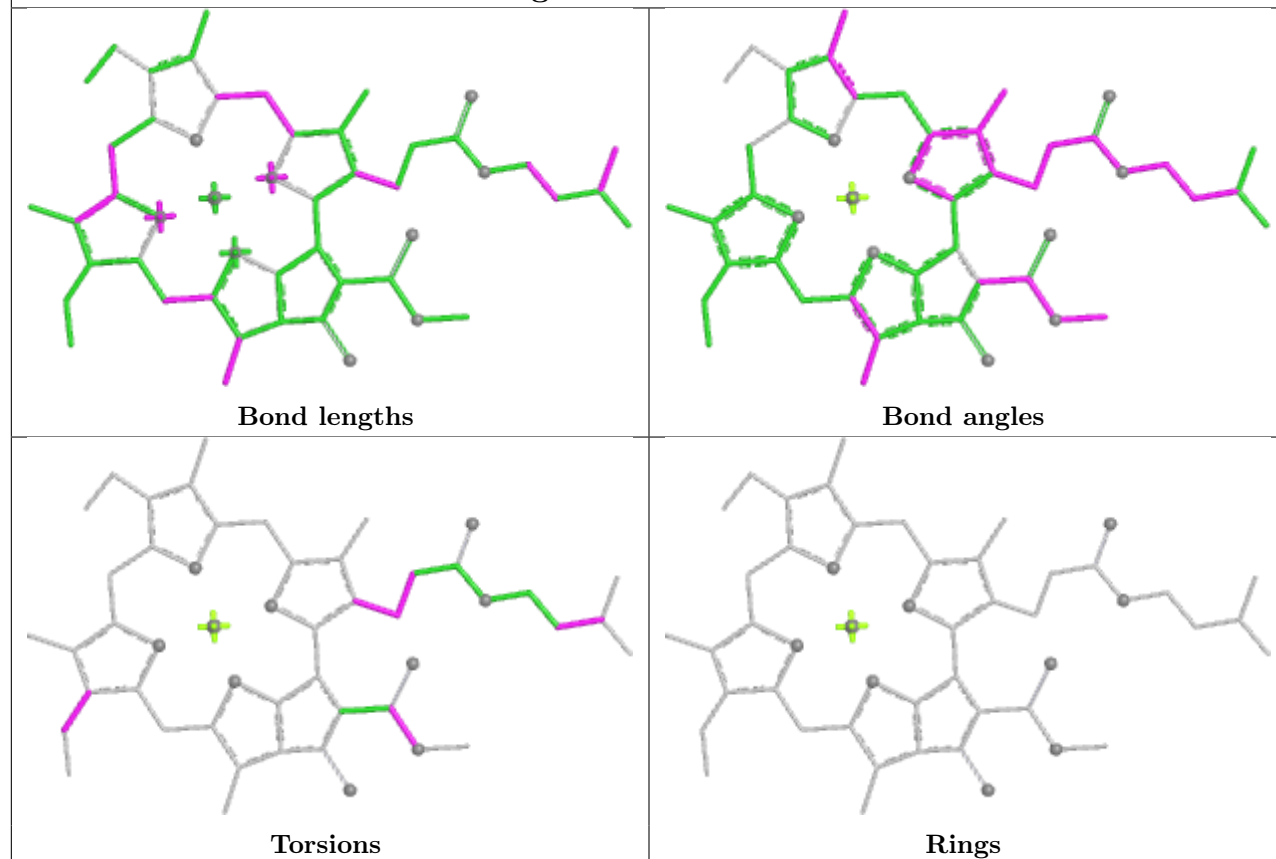




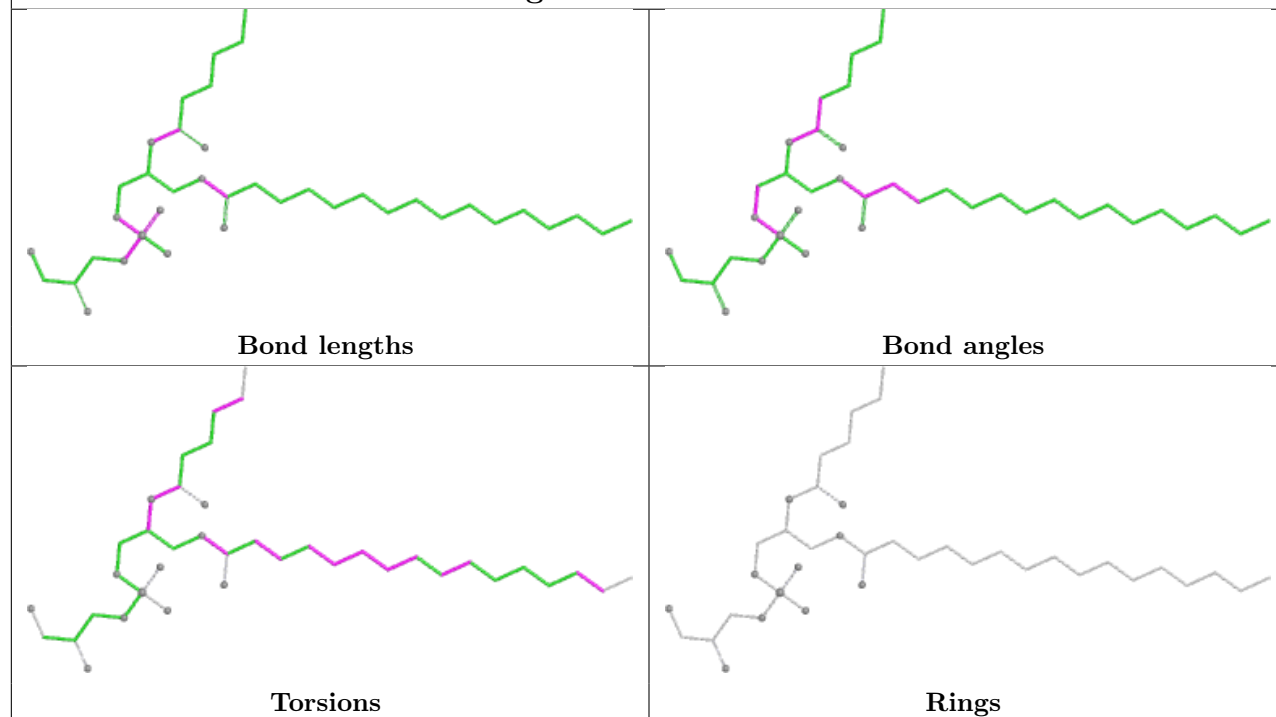
Ligand CLA C 498	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT a 5568	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand MGE I 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

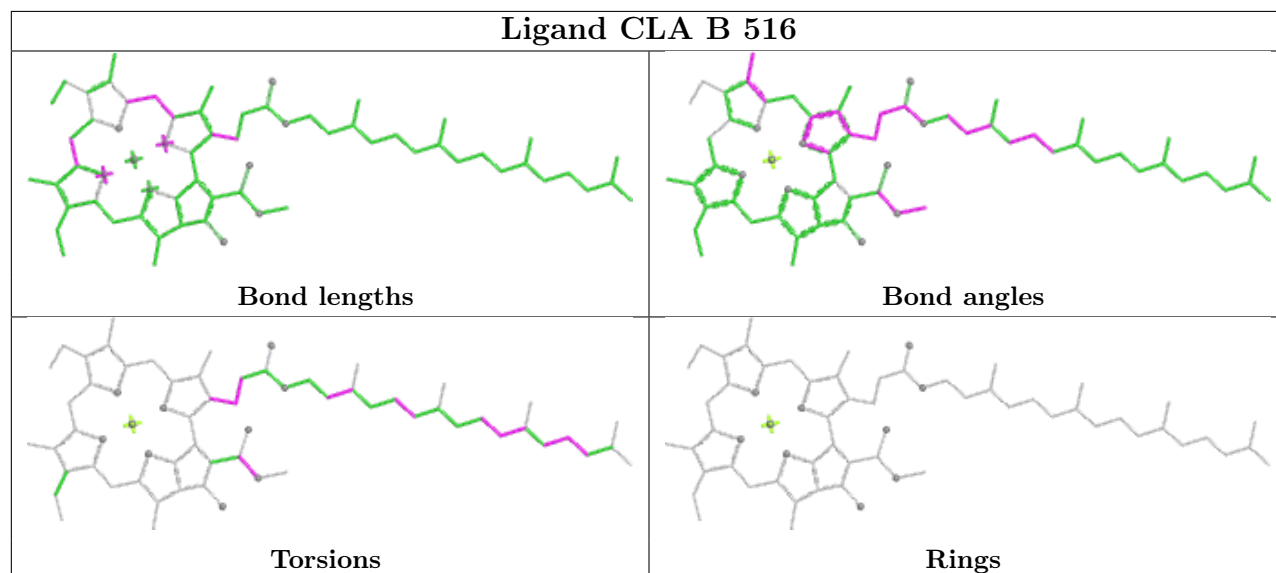
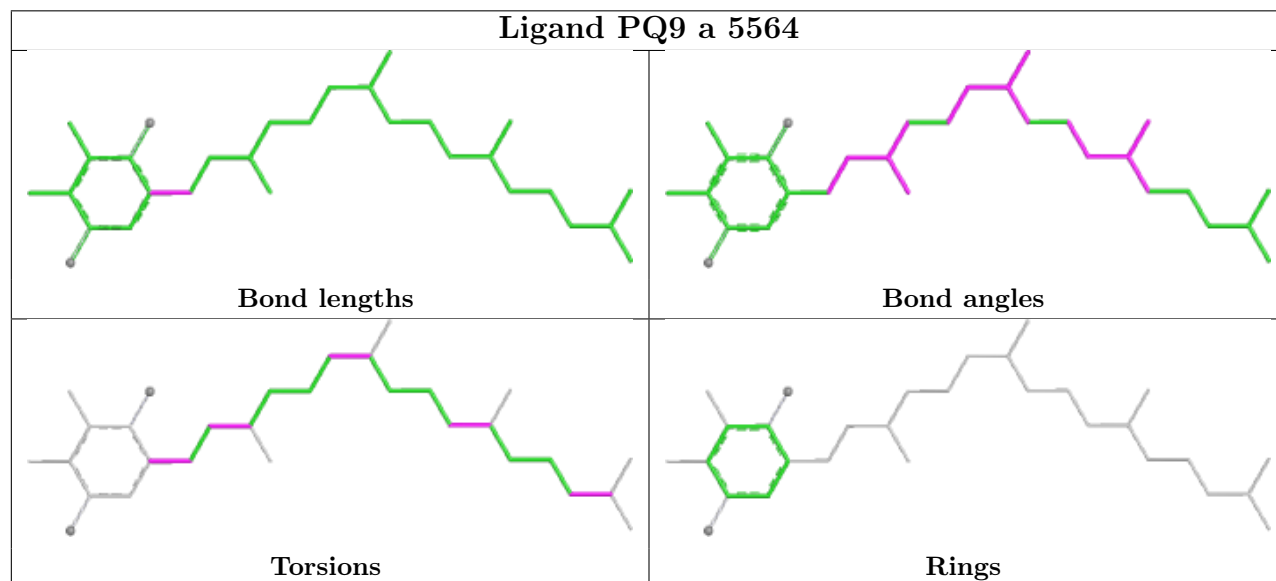
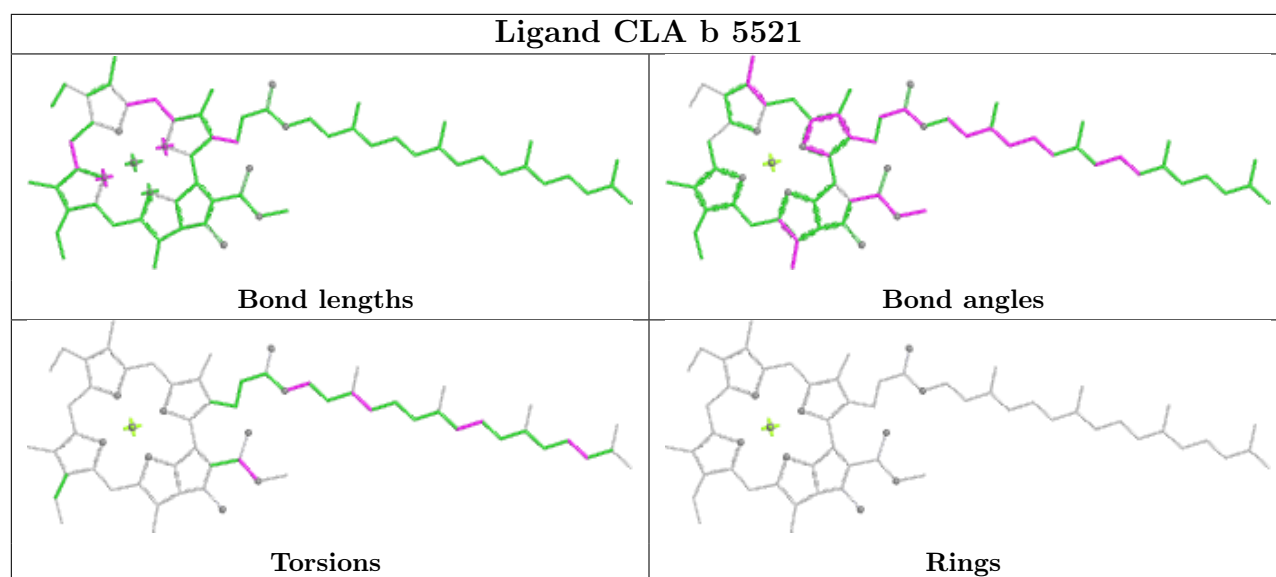


Ligand CLA D 355

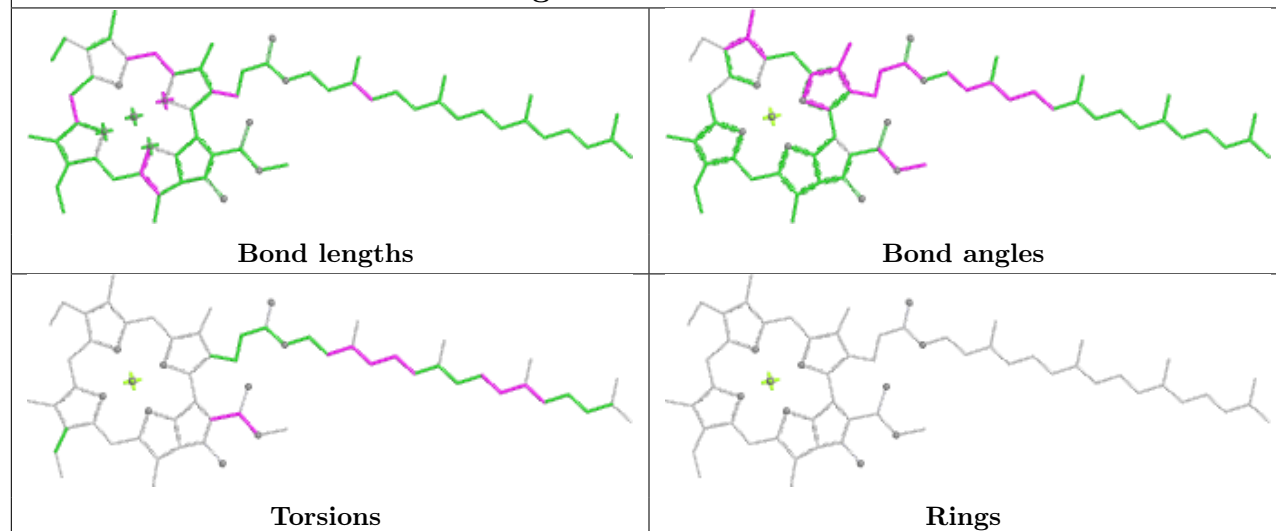


Ligand LHG a 5567

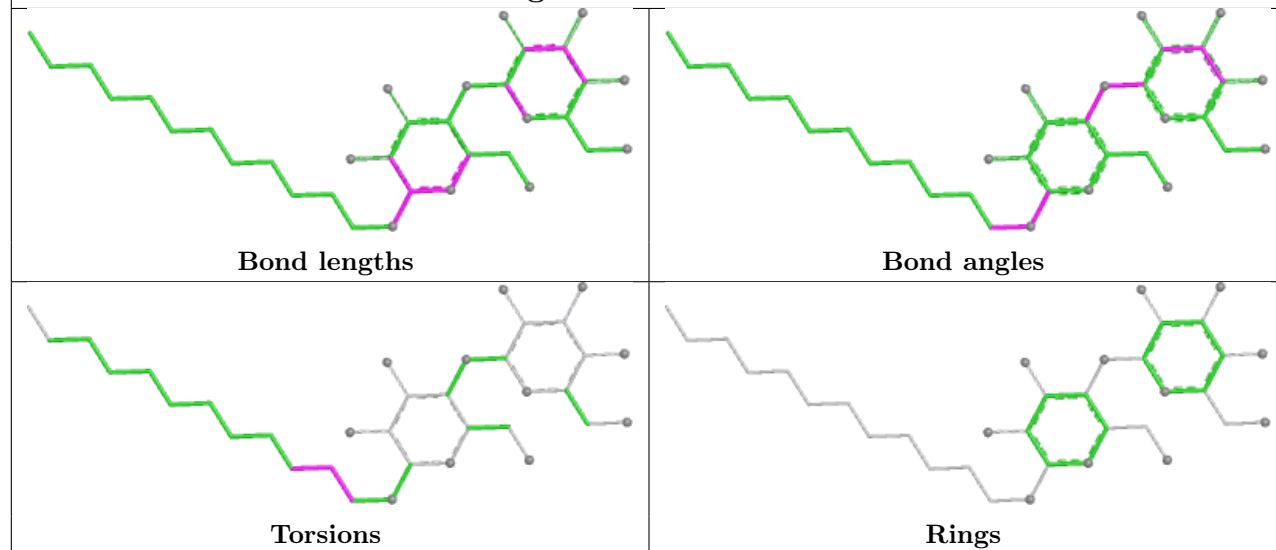




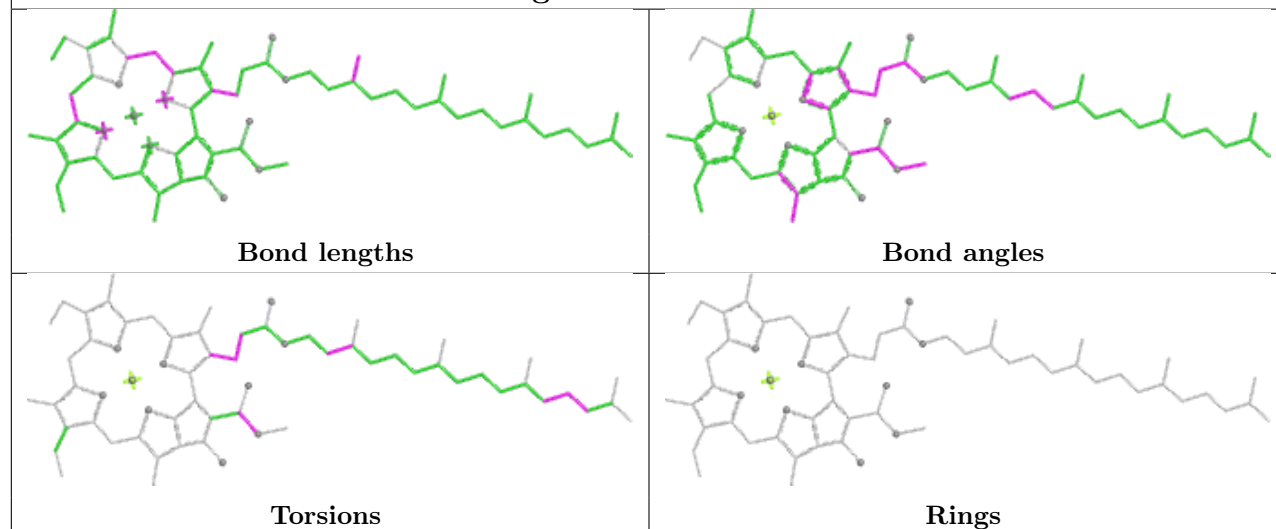
Ligand CLA B 523

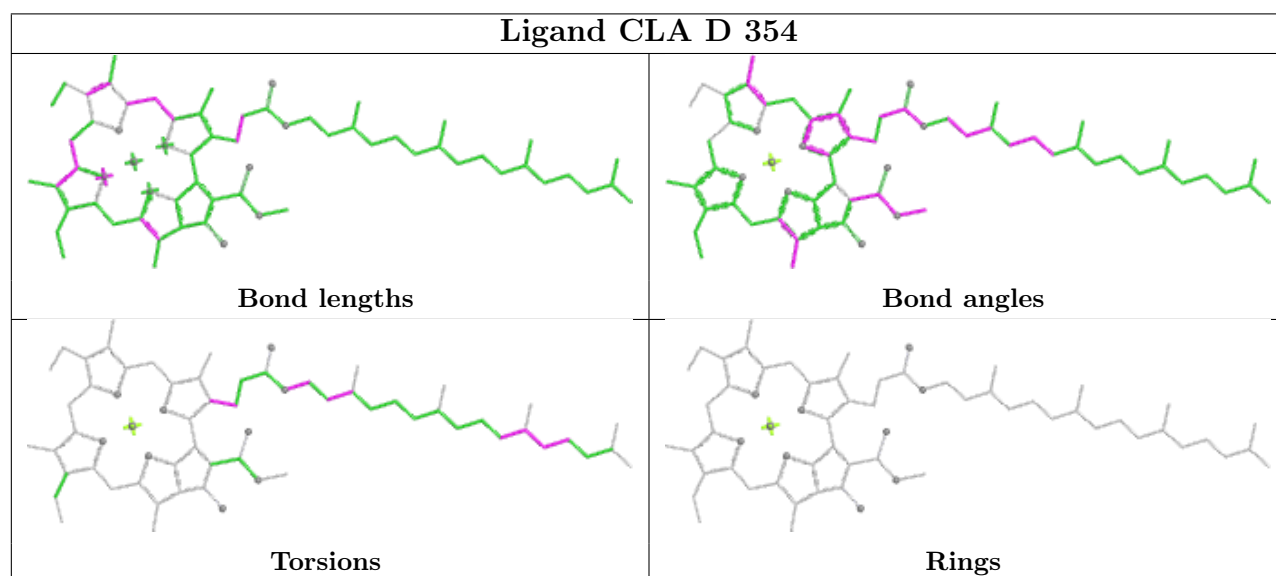
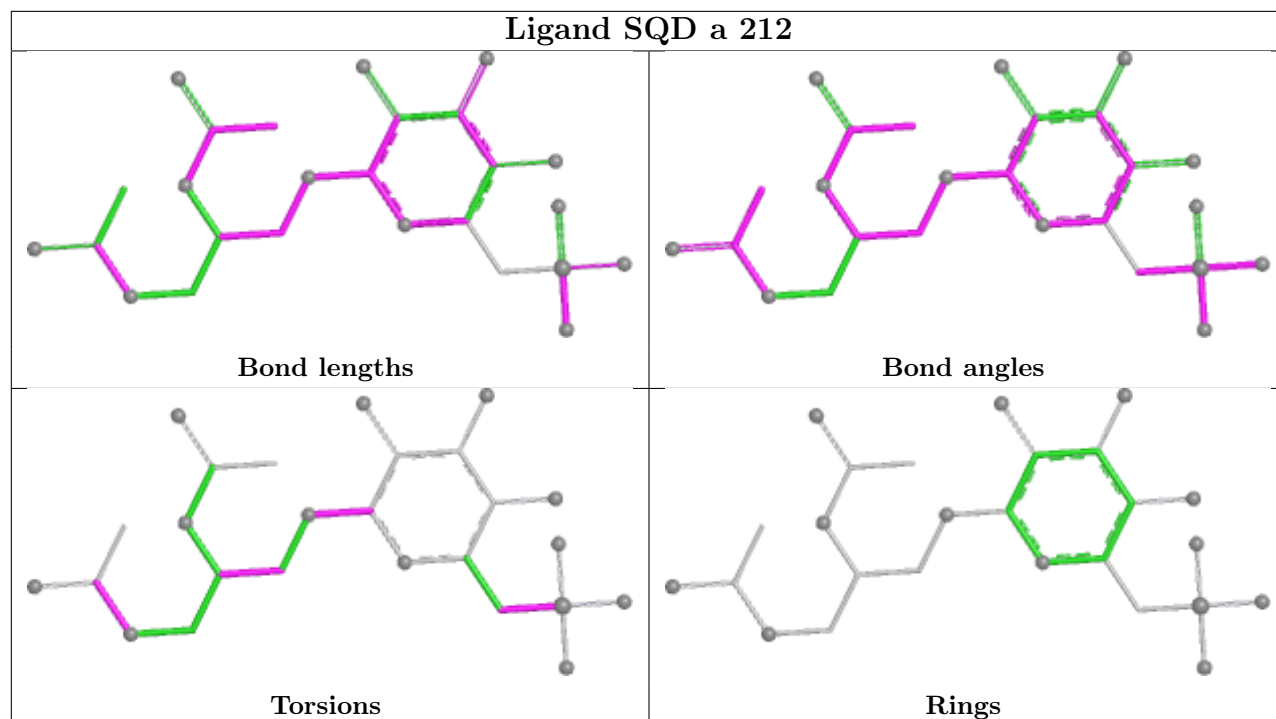


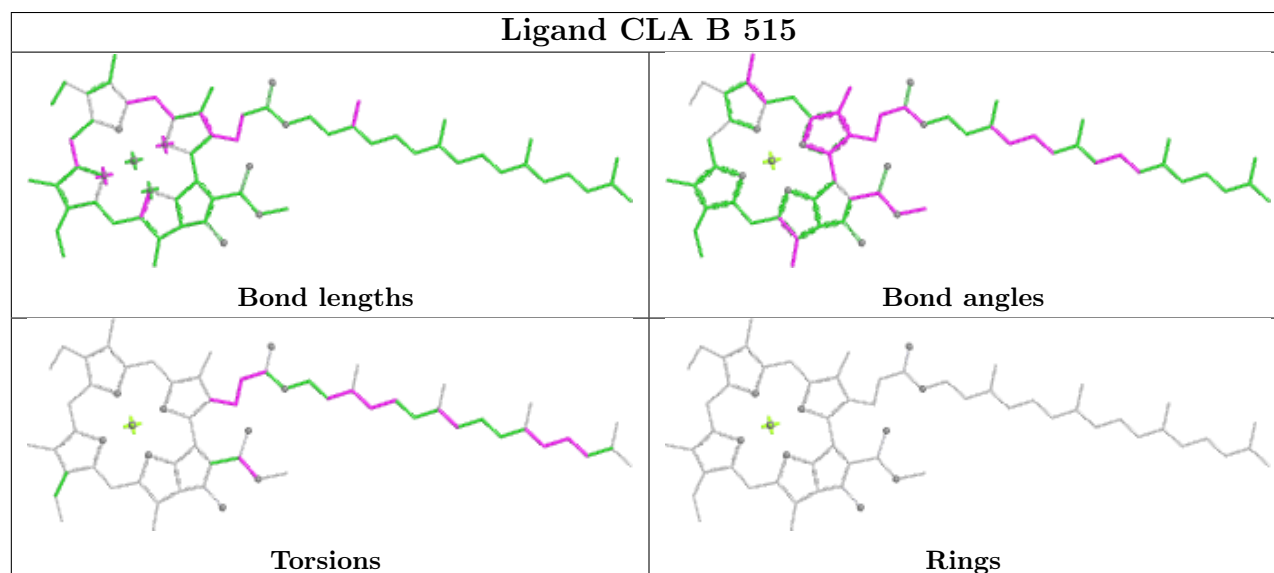
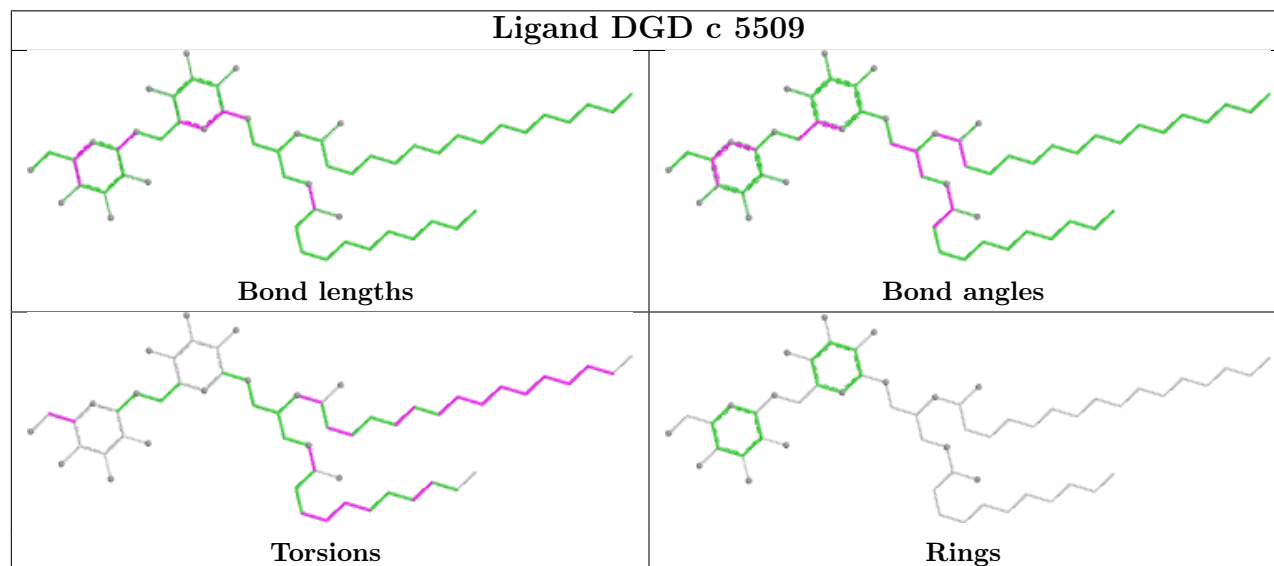
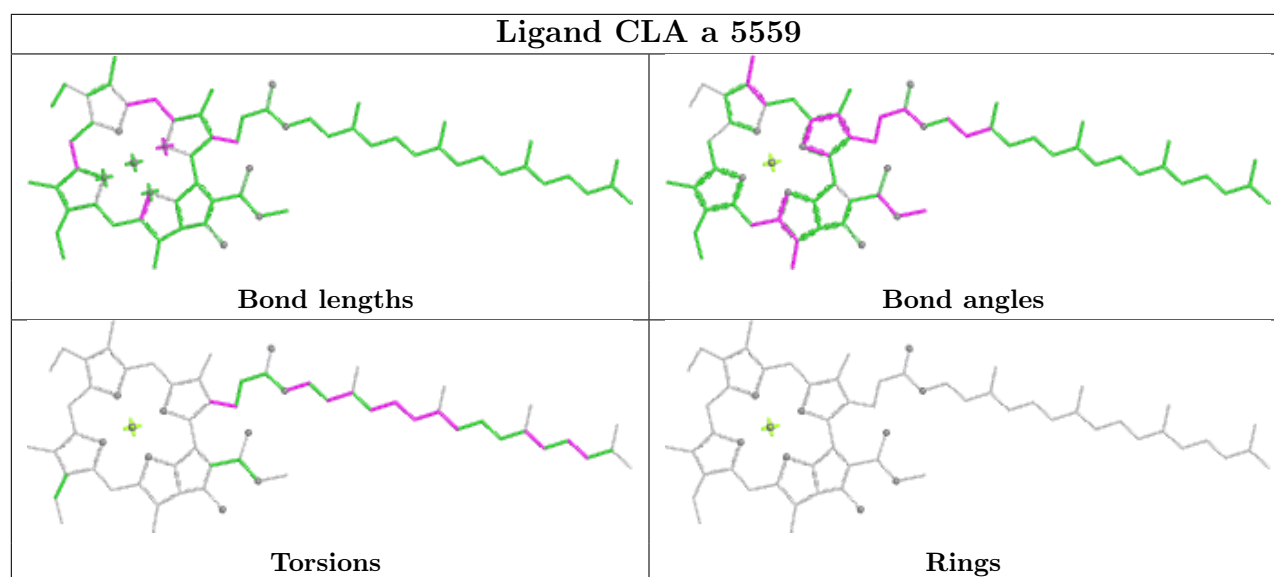
Ligand LMT m 216

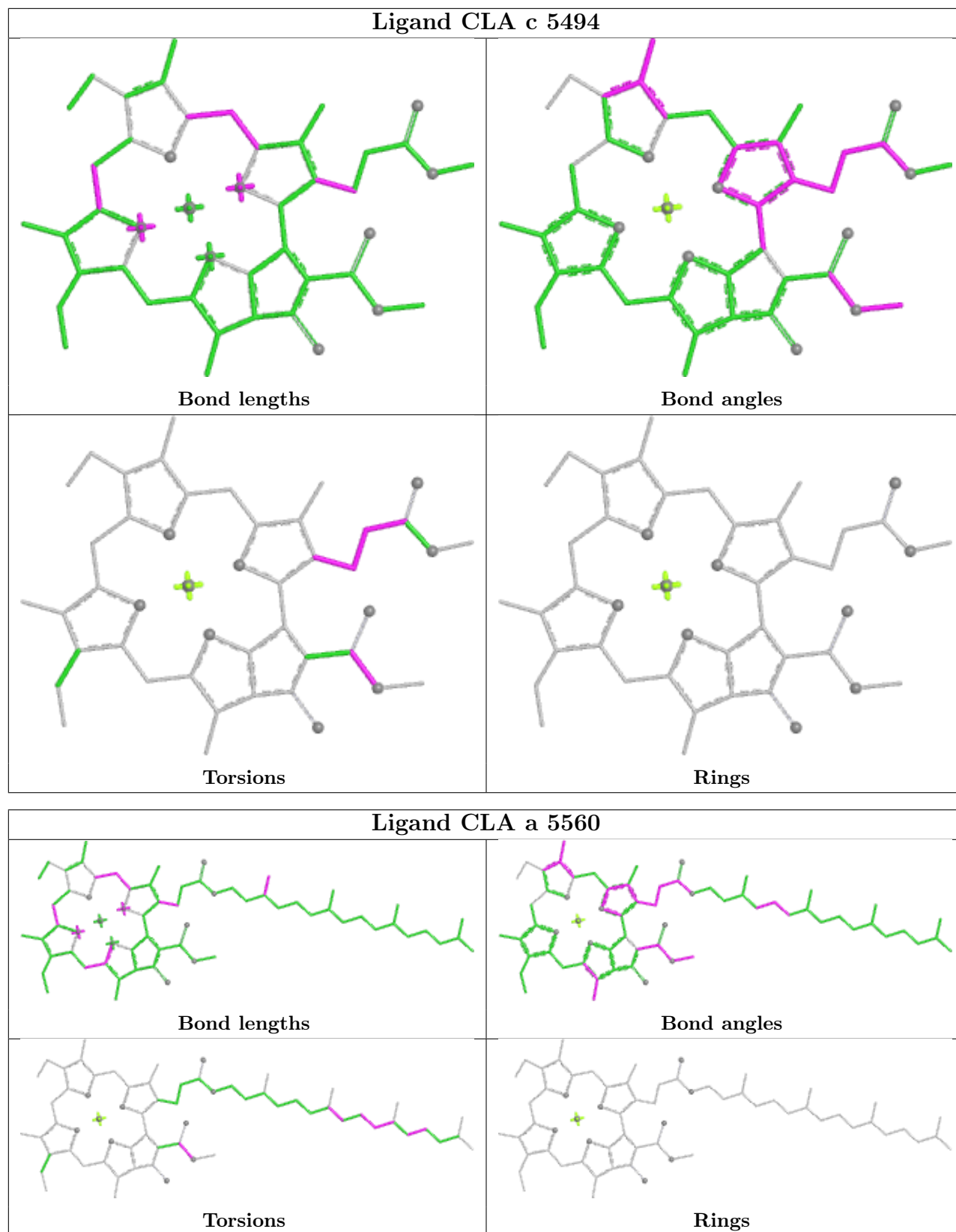


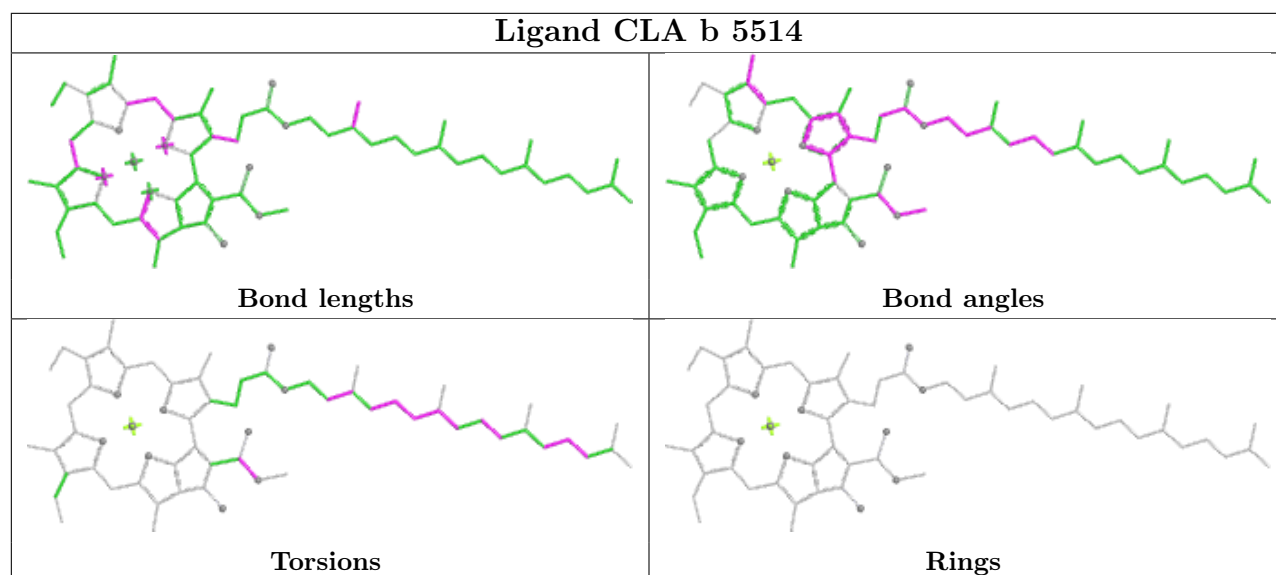
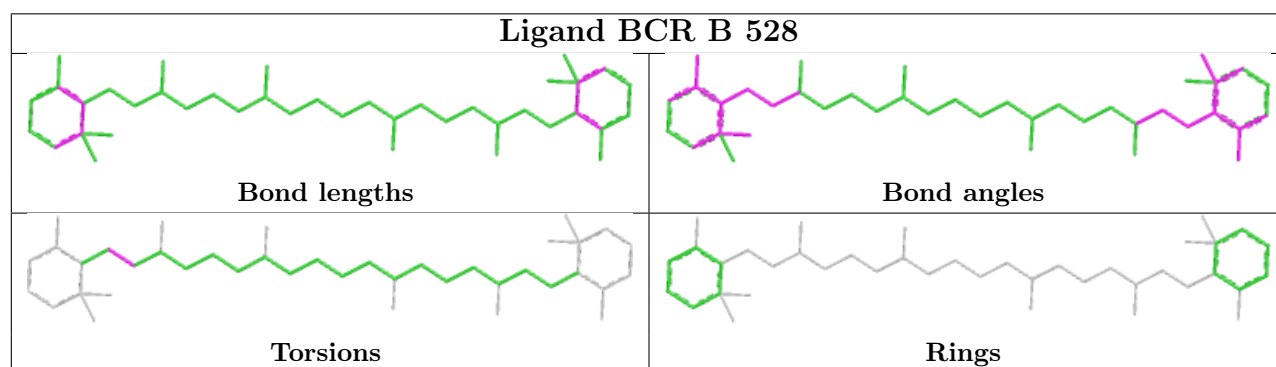
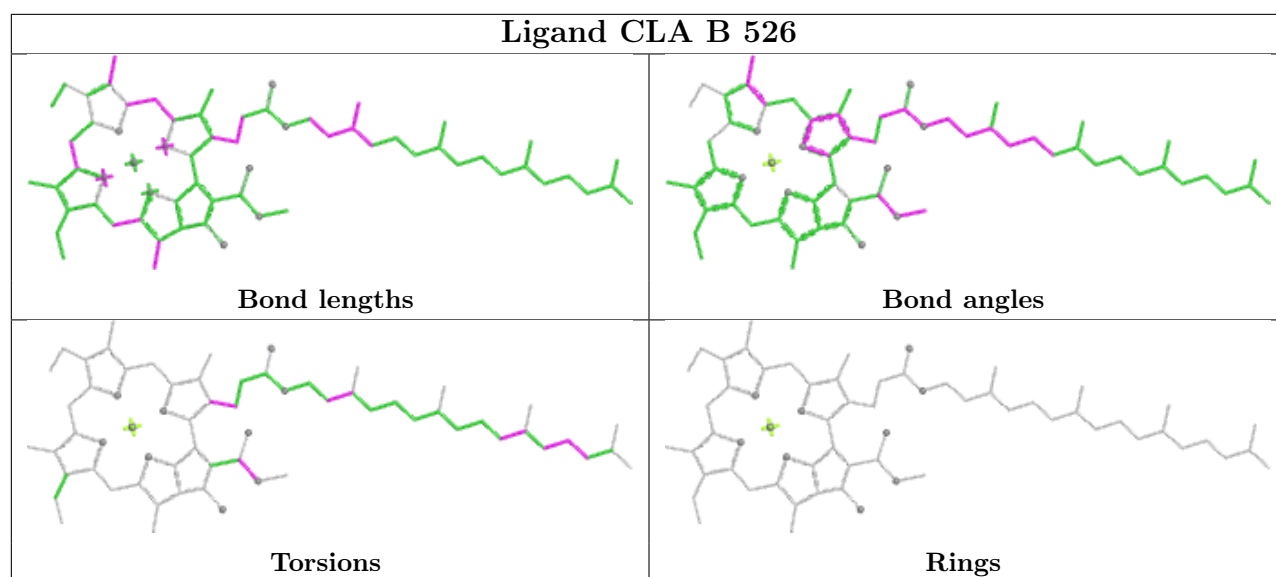
Ligand CLA C 491

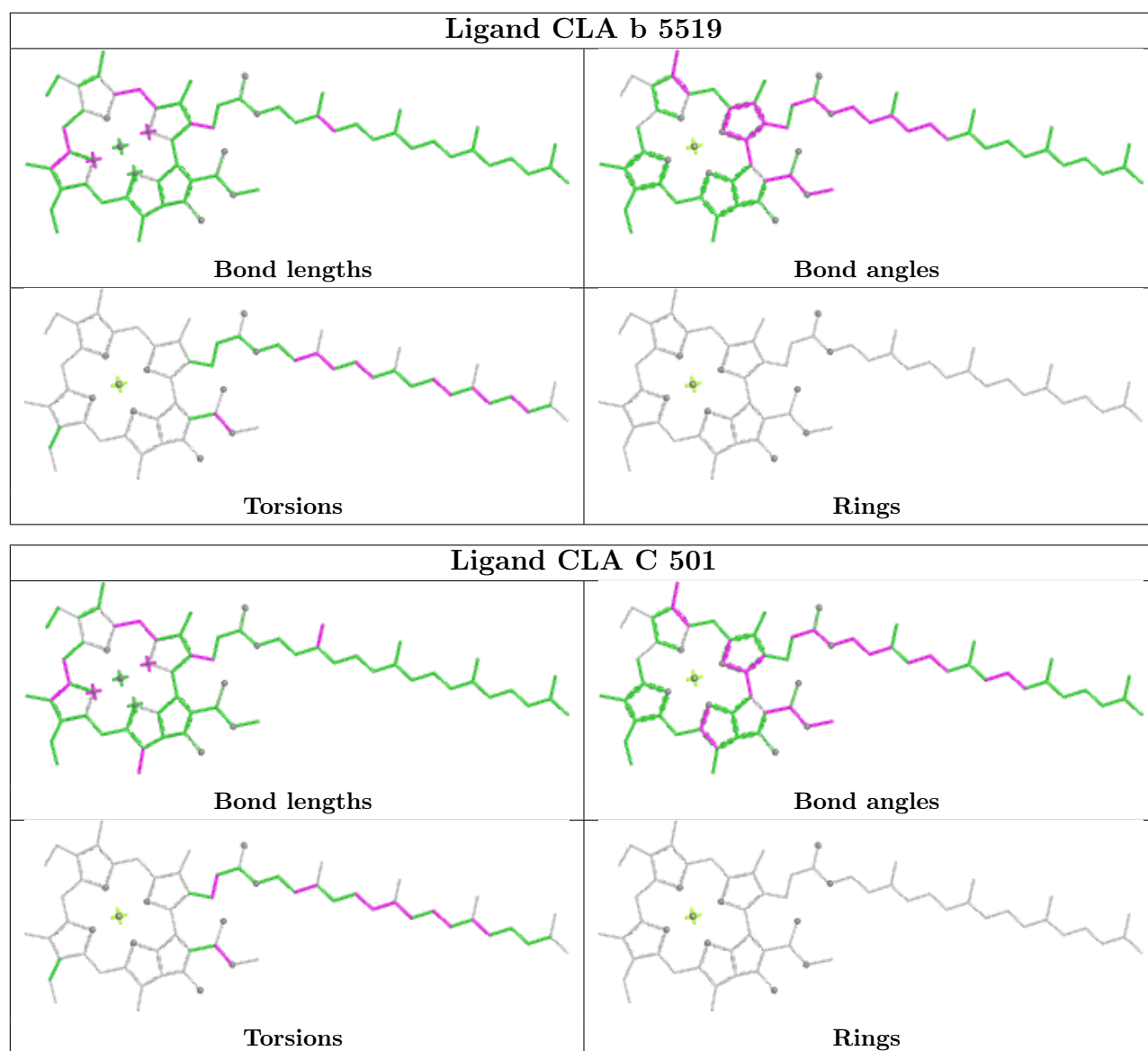












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.76	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.73	0 100 100	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.77	0 100 100	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.77	0 100 100	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.72	1 (0%) 92 84	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.58	0 100 100	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.89	0 100 100	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.80	1 (0%) 90 81	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.47	1 (1%) 76 56	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.36	1 (1%) 76 56	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.48	0 100 100	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.45	0 100 100	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.54	0 100 100	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.61	0 100 100	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.62	0 100 100	57, 66, 80, 88	0
8	i	35/38 (92%)	-0.60	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.42	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.44	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.76	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.47	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.53	0 100 100	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.66	0 100 100	45, 56, 86, 91	0
12	M	36/36 (100%)	-0.58	0 100 100	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.64	0 100 100	54, 60, 86, 91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	O	242/247 (97%)	-0.62	0	100	100	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.58	0	100	100	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.53	0	100	100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.58	0	100	100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.72	0	100	100	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.71	0	100	100	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.74	1 (0%)	84	68	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.57	0	100	100	54, 74, 87, 99	0
17	X	0/129	-	-		-	-	-
17	x	0/129	-	-		-	-	-
18	Z	62/62 (100%)	-0.42	0	100	100	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.19	0	100	100	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.68	5 (0%)	92	88	35, 66, 85, 101	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	222	GLY	3.4
16	V	27	ALA	2.9
5	E	4	THR	2.4
5	e	5006	GLY	2.2
4	d	5013	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	UNL	C	486	8/-	0.49	0.12	55,56,59,60	0
29	UNL	c	5490	4/-	0.63	0.10	91,92,92,92	0
20	CLA	B	511	41/65	0.64	0.13	88,90,92,98	0
20	CLA	b	5511	41/65	0.65	0.13	88,92,95,96	0
29	UNL	c	5485	5/-	0.67	0.08	68,69,69,70	0
29	UNL	C	485	5/-	0.67	0.11	57,59,61,61	0
29	UNL	C	477	7/-	0.71	0.12	47,49,51,51	0
29	UNL	C	481	13/-	0.71	0.10	61,64,68,69	0
27	LMT	A	569	35/35	0.71	0.12	80,89,92,93	0
29	UNL	c	5479	11/-	0.72	0.12	76,77,77,77	0
29	UNL	c	5481	13/-	0.72	0.09	60,62,66,66	0
29	UNL	C	484	5/-	0.75	0.10	47,51,52,53	0
29	UNL	C	479	11/-	0.75	0.10	58,64,67,67	0
29	UNL	C	482	13/-	0.75	0.09	64,66,67,67	0
29	UNL	c	5486	8/-	0.75	0.08	63,64,65,66	0
29	UNL	C	487	7/-	0.75	0.07	49,52,52,53	0
29	UNL	c	5483	13/-	0.76	0.10	71,75,80,82	0
26	SQD	a	212	26/54	0.77	0.10	82,94,101,103	0
29	UNL	C	476	9/-	0.77	0.06	61,62,63,64	0
29	UNL	c	5478	11/-	0.77	0.09	76,79,81,81	0
26	SQD	A	5212	26/54	0.78	0.11	75,100,107,107	0
29	UNL	c	5484	5/-	0.78	0.09	69,69,70,72	0
27	LMT	a	5568	35/35	0.78	0.10	79,92,94,96	0
29	UNL	c	5480	7/-	0.78	0.13	65,66,66,67	0
29	UNL	c	5489	7/-	0.78	0.09	73,73,74,74	0
28	MGE	i	5201	48/48	0.78	0.10	67,83,88,90	0
27	LMT	m	216	35/35	0.79	0.10	62,87,89,91	0
29	UNL	C	488	5/-	0.79	0.09	41,45,47,47	0
29	UNL	C	478	11/-	0.79	0.08	58,65,66,66	0
29	UNL	c	5488	5/-	0.81	0.07	59,59,59,60	0
29	UNL	C	483	13/-	0.81	0.10	61,68,78,78	0
29	UNL	C	475	12/-	0.81	0.08	68,69,72,73	0
26	SQD	L	5213	47/54	0.82	0.10	52,85,106,108	0
29	UNL	C	480	7/-	0.82	0.12	35,36,38,38	0
24	BCR	c	5506	40/40	0.82	0.09	75,81,86,86	0
27	LMT	t	5217	35/35	0.82	0.13	76,95,104,105	0
29	UNL	c	5482	13/-	0.82	0.08	60,61,71,72	0
20	CLA	c	5501	65/65	0.82	0.10	82,91,94,95	0
24	BCR	C	505	40/40	0.83	0.11	75,81,91,92	0
27	LMT	T	217	35/35	0.83	0.12	83,93,96,97	0
24	BCR	c	5505	40/40	0.83	0.10	84,87,91,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	c	5502	51/65	0.83	0.10	93,96,97,98	0
26	SQD	d	5358	54/54	0.83	0.10	74,85,106,107	0
29	UNL	c	5477	7/-	0.83	0.14	67,68,70,70	0
28	MGE	d	5359	47/48	0.84	0.10	72,81,96,98	0
28	MGE	d	5360	41/48	0.84	0.09	68,72,78,80	0
22	PQ9	A	564	30/45	0.84	0.14	54,57,63,64	30
27	LMT	M	5216	35/35	0.84	0.09	58,83,90,90	0
20	CLA	c	5498	65/65	0.84	0.10	81,90,93,93	0
28	MGE	d	5361	48/48	0.85	0.09	61,68,78,83	0
24	BCR	H	107	40/40	0.85	0.10	77,83,88,89	0
28	MGE	l	5210	48/48	0.85	0.09	59,69,78,81	0
29	UNL	c	5475	12/-	0.85	0.07	74,78,84,84	0
29	UNL	c	5476	9/-	0.85	0.05	58,60,62,62	0
26	SQD	A	568	54/54	0.85	0.09	76,82,90,90	0
29	UNL	c	5487	7/-	0.85	0.06	57,57,58,58	0
28	MGE	D	358	47/48	0.85	0.10	65,72,79,81	0
20	CLA	c	5491	65/65	0.85	0.09	70,78,81,86	0
26	SQD	t	213	47/54	0.85	0.10	61,95,116,117	0
28	MGE	b	5530	48/48	0.86	0.09	59,64,71,73	0
22	PQ9	a	5564	30/45	0.86	0.10	51,55,62,62	30
20	CLA	B	526	65/65	0.86	0.10	71,82,97,98	0
20	CLA	b	5526	65/65	0.86	0.09	66,71,92,95	0
20	CLA	C	502	51/65	0.86	0.09	74,80,83,84	0
20	CLA	c	5503	50/65	0.86	0.10	88,91,92,93	0
20	CLA	c	5495	65/65	0.86	0.09	74,81,86,88	0
28	MGE	I	201	48/48	0.86	0.09	73,81,89,90	0
28	MGE	L	210	48/48	0.86	0.09	59,68,73,75	0
30	DGD	C	507	53/66	0.86	0.10	55,66,86,88	0
30	DGD	c	5507	53/66	0.86	0.09	66,74,90,91	0
30	DGD	c	5509	57/66	0.86	0.08	67,72,77,78	0
31	BCT	d	5353	4/4	0.86	0.06	75,75,76,77	0
20	CLA	B	516	65/65	0.87	0.10	61,76,92,97	0
20	CLA	c	5497	65/65	0.87	0.10	66,82,84,87	0
28	MGE	D	359	41/48	0.87	0.09	60,67,76,79	0
28	MGE	D	360	48/48	0.87	0.09	52,60,63,68	0
24	BCR	B	527	40/40	0.87	0.09	58,65,68,69	0
29	UNL	C	489	7/-	0.87	0.12	75,76,77,78	0
30	DGD	C	508	47/66	0.87	0.12	61,71,80,83	0
29	UNL	c	5474	15/-	0.87	0.06	39,50,56,56	0
30	DGD	c	5508	47/66	0.87	0.11	66,76,82,84	0
24	BCR	h	5107	40/40	0.87	0.09	74,79,82,83	0
20	CLA	b	5519	65/65	0.87	0.08	70,75,80,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	B	519	65/65	0.88	0.08	73,82,85,87	0
20	CLA	C	497	65/65	0.88	0.09	74,78,80,82	0
24	BCR	d	5357	40/40	0.88	0.09	61,72,86,88	0
30	DGD	C	509	57/66	0.88	0.09	52,60,69,70	0
29	UNL	C	474	15/-	0.88	0.05	26,37,40,40	0
20	CLA	b	5524	56/65	0.88	0.10	63,68,89,91	0
24	BCR	D	357	40/40	0.88	0.08	61,66,78,80	0
20	CLA	B	525	65/65	0.88	0.09	67,84,91,92	0
20	CLA	c	5493	65/65	0.89	0.09	67,81,86,86	0
20	CLA	B	524	56/65	0.89	0.09	67,72,77,80	0
24	BCR	B	528	40/40	0.89	0.09	54,68,74,75	0
20	CLA	C	495	65/65	0.89	0.08	58,68,74,76	0
28	MGE	B	530	48/48	0.89	0.09	55,64,70,72	0
24	BCR	C	506	40/40	0.89	0.08	68,72,79,80	0
24	BCR	x	5130	40/40	0.89	0.08	77,81,85,86	0
30	DGD	h	5208	54/66	0.89	0.08	57,68,73,75	0
20	CLA	b	5520	65/65	0.89	0.09	63,72,74,76	0
24	BCR	b	5529	40/40	0.90	0.08	69,72,74,74	0
24	BCR	c	5504	40/40	0.90	0.09	73,80,88,89	0
20	CLA	c	5496	65/65	0.90	0.08	79,83,95,97	0
20	CLA	b	5525	65/65	0.90	0.09	71,77,80,82	0
20	CLA	b	5518	65/65	0.90	0.08	60,64,69,75	0
20	CLA	C	498	65/65	0.90	0.09	64,74,98,101	0
24	BCR	t	104	40/40	0.90	0.07	65,72,84,85	0
24	BCR	B	529	40/40	0.90	0.07	62,69,80,80	0
25	LHG	A	567	39/49	0.90	0.08	57,73,79,81	0
25	LHG	a	5567	39/49	0.90	0.07	65,68,74,80	0
30	DGD	H	208	54/66	0.90	0.09	61,69,75,76	0
20	CLA	C	503	50/65	0.90	0.10	83,86,88,94	0
20	CLA	C	501	65/65	0.90	0.08	70,78,83,85	0
20	CLA	d	5355	50/65	0.90	0.08	74,77,80,81	0
21	PHO	a	5562	64/64	0.90	0.09	70,75,81,82	0
24	BCR	X	130	40/40	0.90	0.08	68,71,80,81	0
20	CLA	c	5500	65/65	0.91	0.09	64,69,82,83	0
20	CLA	a	5560	65/65	0.91	0.09	62,68,100,101	0
20	CLA	B	522	65/65	0.91	0.09	54,65,75,77	0
20	CLA	b	5512	65/65	0.91	0.09	68,72,75,76	0
20	CLA	b	5516	65/65	0.91	0.09	62,66,84,86	0
24	BCR	T	5104	40/40	0.91	0.09	67,71,78,79	0
20	CLA	C	500	65/65	0.91	0.09	59,63,73,74	0
24	BCR	b	5527	40/40	0.91	0.09	58,63,72,72	0
20	CLA	B	518	65/65	0.91	0.07	53,64,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	C	496	65/65	0.91	0.08	71,78,88,89	0
20	CLA	B	520	65/65	0.91	0.09	62,67,76,79	0
20	CLA	c	5499	47/65	0.91	0.09	60,69,76,78	0
20	CLA	b	5523	65/65	0.92	0.08	45,52,74,75	0
20	CLA	B	513	65/65	0.92	0.09	56,61,67,67	0
20	CLA	C	491	65/65	0.92	0.07	63,70,77,79	0
29	UNL	C	490	4/-	0.92	0.04	67,67,68,68	0
20	CLA	C	494	46/65	0.92	0.08	59,66,68,72	0
20	CLA	b	5517	65/65	0.92	0.07	54,58,66,71	0
20	CLA	c	5492	60/65	0.92	0.08	57,61,83,84	0
20	CLA	B	523	65/65	0.92	0.08	47,56,73,74	0
21	PHO	a	5561	64/64	0.92	0.08	51,55,66,68	0
20	CLA	c	5494	46/65	0.92	0.09	72,77,86,88	0
20	CLA	B	514	65/65	0.92	0.08	59,64,82,83	0
20	CLA	B	512	65/65	0.92	0.07	68,75,78,79	0
22	PQ9	d	5356	30/45	0.92	0.07	51,57,66,66	0
23	OEC	A	565	5/9	0.92	0.07	62,63,65,66	0
20	CLA	b	5521	65/65	0.92	0.07	48,57,63,64	0
20	CLA	B	515	65/65	0.93	0.08	55,66,71,72	0
21	PHO	A	561	64/64	0.93	0.07	32,52,55,59	0
21	PHO	A	562	64/64	0.93	0.07	47,53,63,66	0
20	CLA	A	560	65/65	0.93	0.07	49,57,86,88	0
20	CLA	D	355	50/65	0.93	0.07	63,65,68,70	0
24	BCR	a	5566	40/40	0.93	0.07	59,75,78,79	0
20	CLA	B	521	65/65	0.93	0.08	58,63,66,68	0
24	BCR	b	5528	40/40	0.93	0.07	61,64,72,73	0
20	CLA	b	5522	65/65	0.93	0.09	60,66,75,76	0
20	CLA	a	5563	55/65	0.93	0.09	59,65,102,103	0
20	CLA	B	517	65/65	0.93	0.07	37,44,56,57	0
24	BCR	A	566	40/40	0.93	0.07	50,57,64,66	0
20	CLA	C	499	47/65	0.93	0.09	57,60,66,69	0
20	CLA	b	5513	65/65	0.93	0.07	54,61,84,90	0
20	CLA	C	493	65/65	0.93	0.09	67,71,77,79	0
24	BCR	C	504	40/40	0.93	0.07	57,64,70,70	0
20	CLA	A	563	55/65	0.93	0.08	43,49,75,78	0
32	HEM	f	5051	43/43	0.93	0.11	80,84,97,101	0
20	CLA	D	354	65/65	0.94	0.07	35,43,63,66	0
20	CLA	b	5515	65/65	0.94	0.08	46,51,74,76	0
23	OEC	a	5565	5/9	0.94	0.05	63,64,71,87	0
22	PQ9	D	356	30/45	0.94	0.07	49,67,80,83	0
20	CLA	C	492	60/65	0.94	0.08	53,58,76,77	0
20	CLA	a	5559	65/65	0.95	0.07	42,49,60,60	0

Continued on next page...

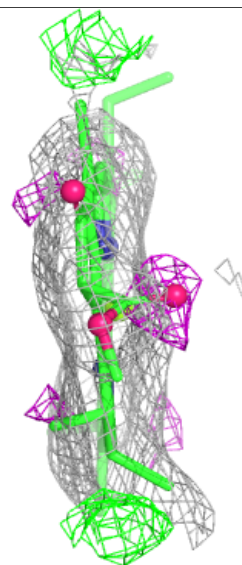
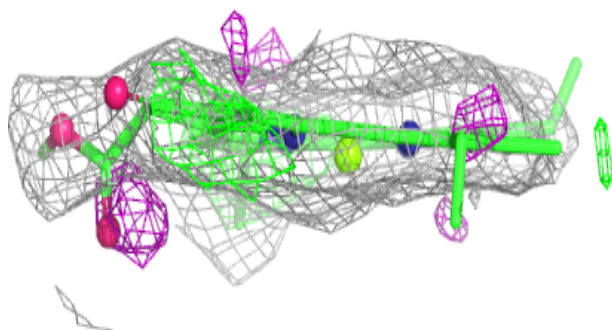
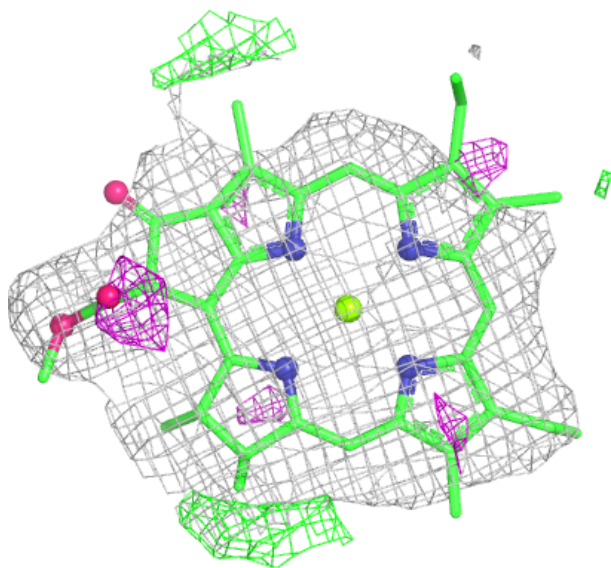
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	d	5354	65/65	0.95	0.06	39,47,64,65	0
20	CLA	A	559	65/65	0.95	0.06	39,43,49,52	0
20	CLA	a	5558	65/65	0.95	0.07	41,50,55,61	0
32	HEM	F	51	43/43	0.95	0.10	78,84,92,95	0
20	CLA	b	5514	65/65	0.95	0.06	41,51,74,75	0
32	HEM	v	5552	43/43	0.95	0.08	65,67,70,70	0
20	CLA	A	558	65/65	0.96	0.07	41,46,50,51	0
33	CA	K	56	1/1	0.96	0.13	119,119,119,119	0
33	CA	k	5056	1/1	0.96	0.08	119,119,119,119	0
31	BCT	D	353	4/4	0.97	0.05	72,73,73,74	0
32	HEM	V	552	43/43	0.97	0.07	37,54,58,59	0
19	FE2	A	557	1/1	0.98	0.01	60,60,60,60	0
19	FE2	a	5557	1/1	1.00	0.03	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.

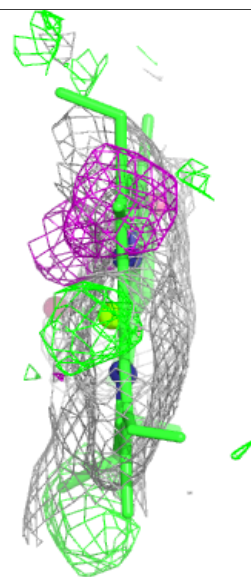
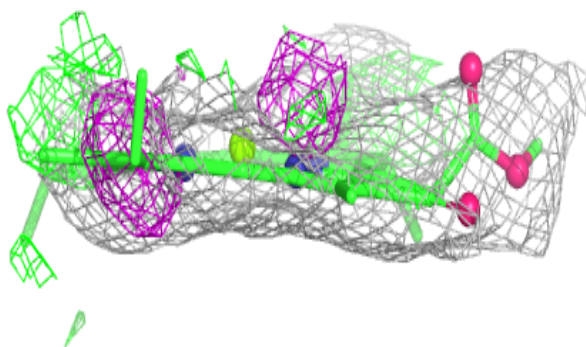
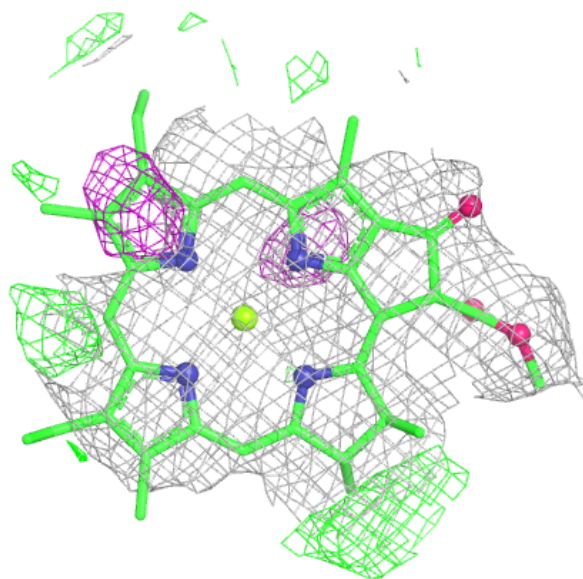
Electron density around CLA B 511:

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



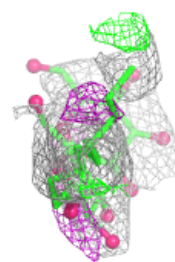
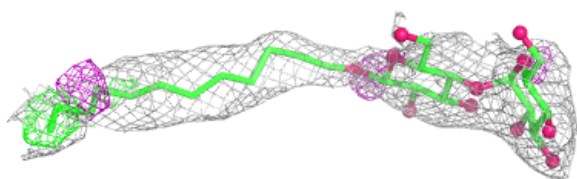
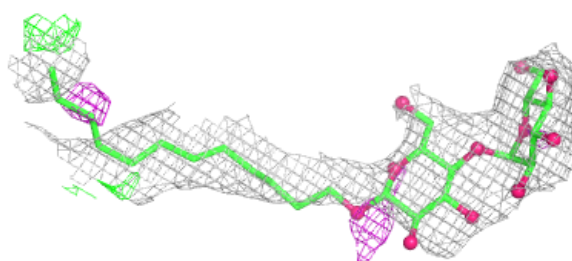
Electron density around CLA b 5511:

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



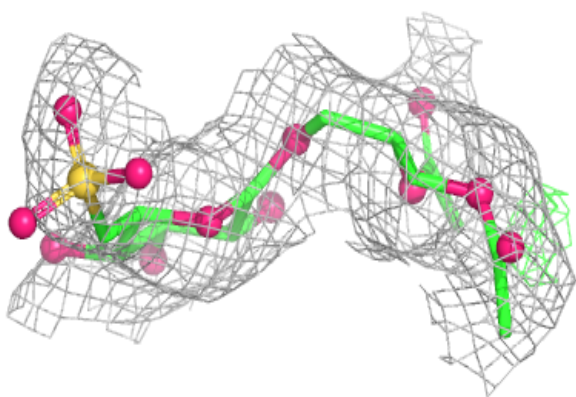
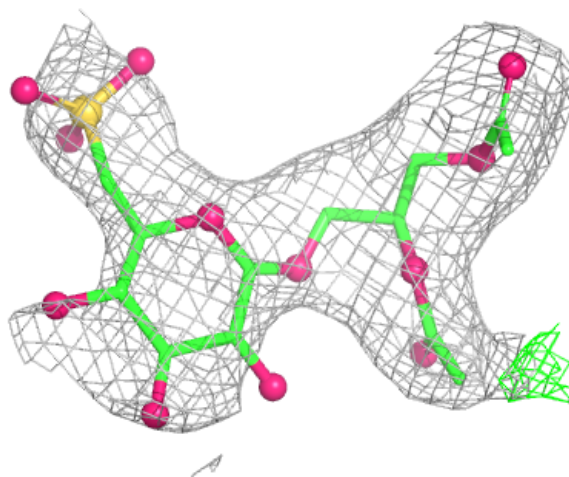
Electron density around LMT A 569:

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



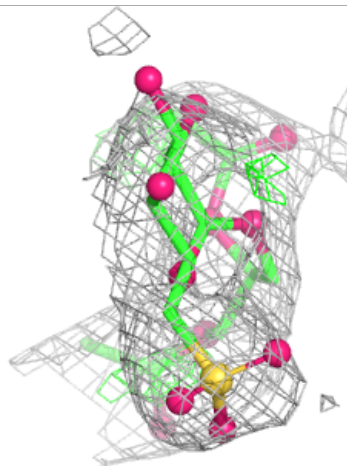
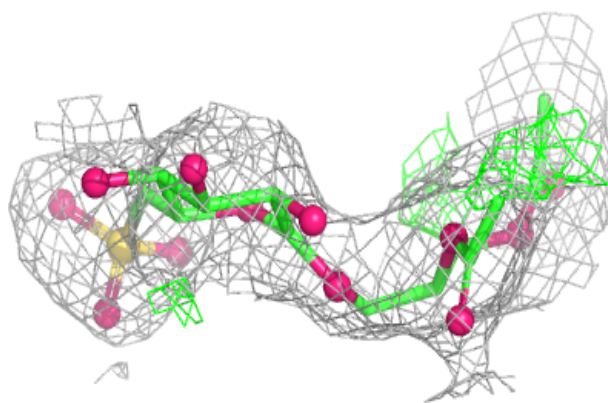
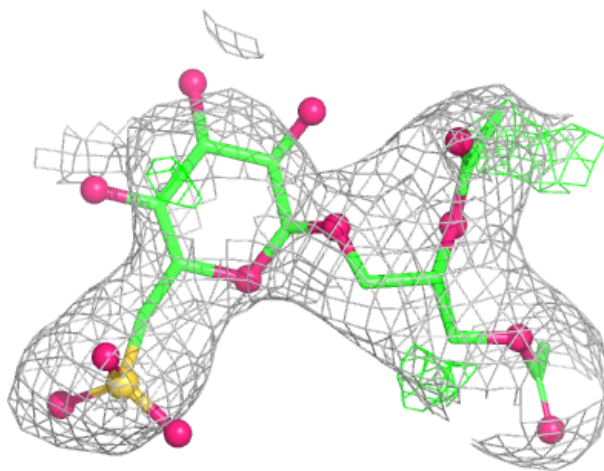
Electron density around SQD a 212:

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



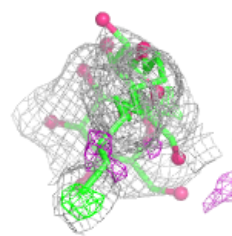
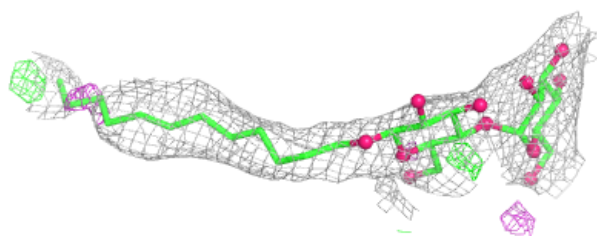
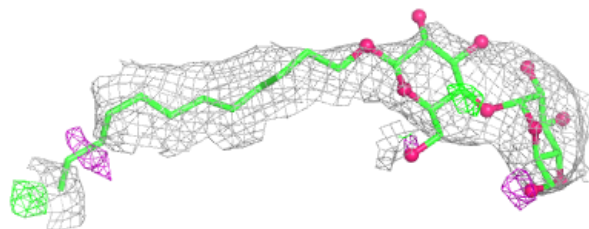
Electron density around SQD A 5212:

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

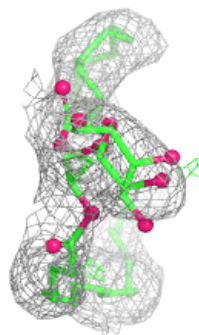
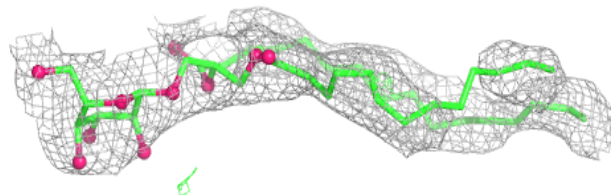
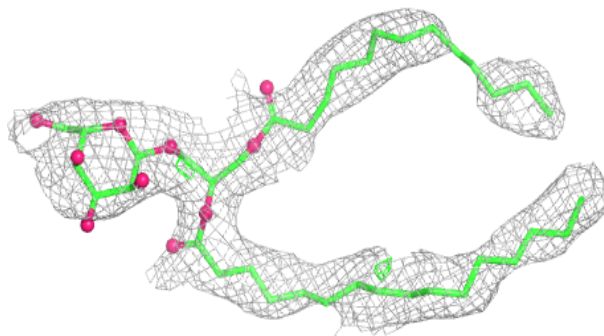


Electron density around LMT a 5568:

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

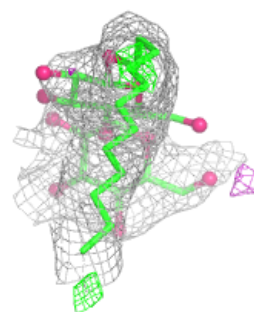
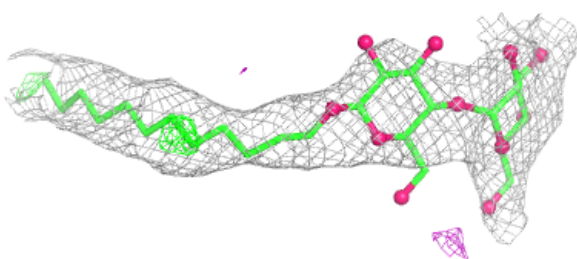
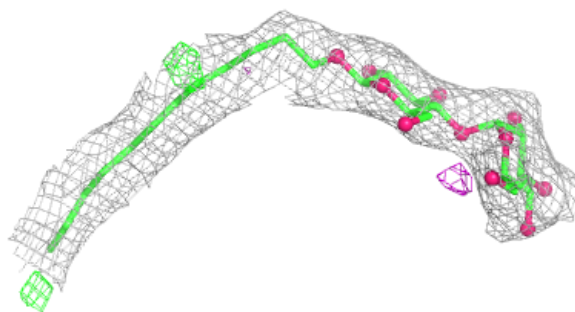
**Electron density around MGE i 5201:**

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

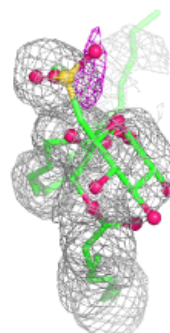
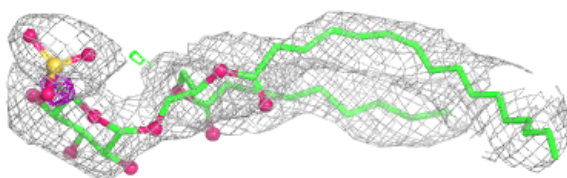
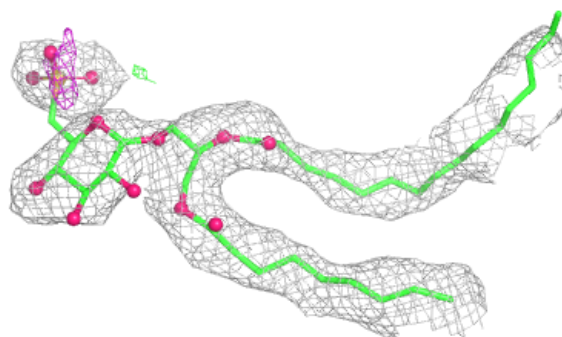


Electron density around LMT m 216:

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

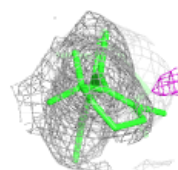
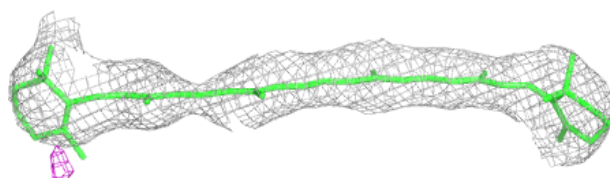
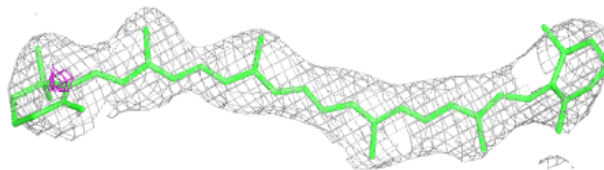
**Electron density around SQD L 5213:**

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

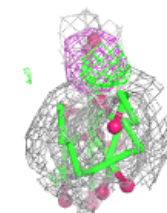
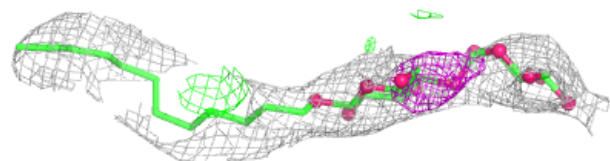
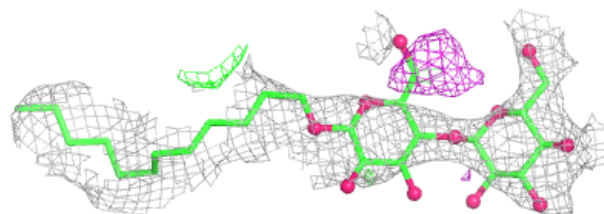


Electron density around BCR c 5506:

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

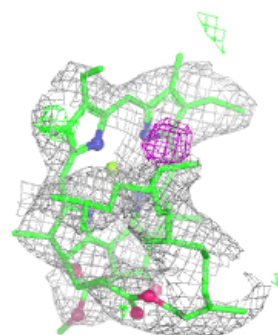
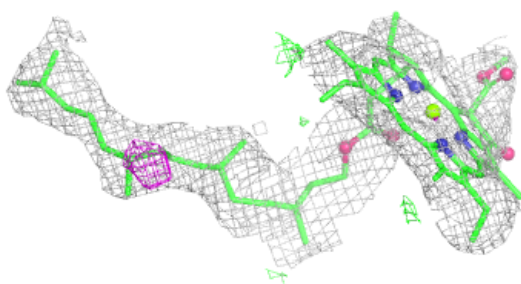
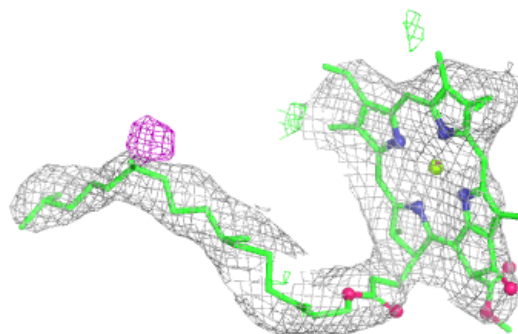
**Electron density around LMT t 5217:**

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

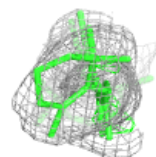
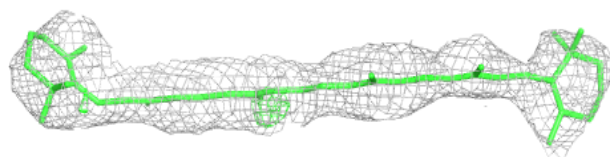
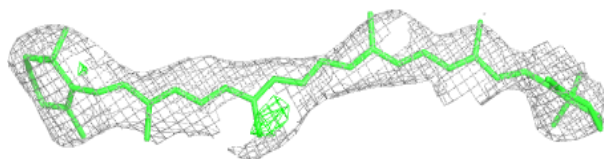


Electron density around CLA c 5501:

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

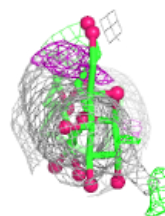
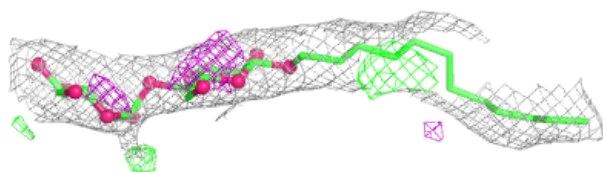
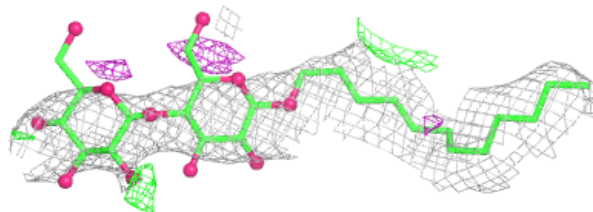
**Electron density around BCR C 505:**

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

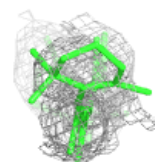
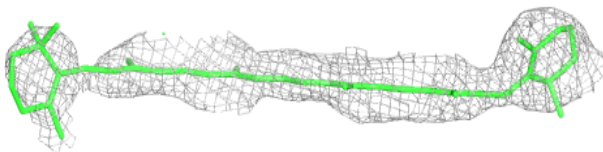
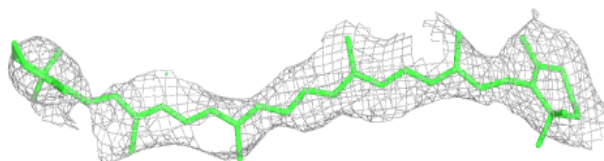


Electron density around LMT T 217:

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

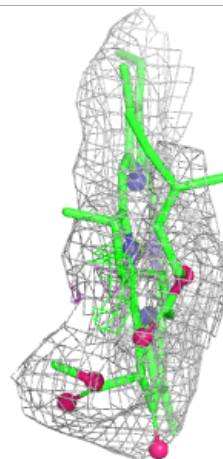
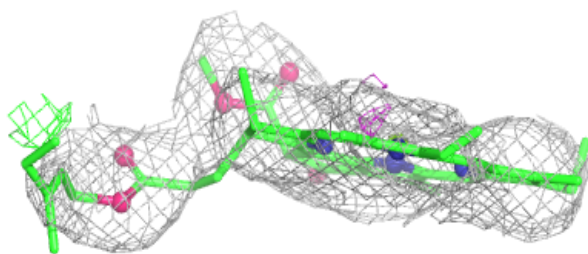
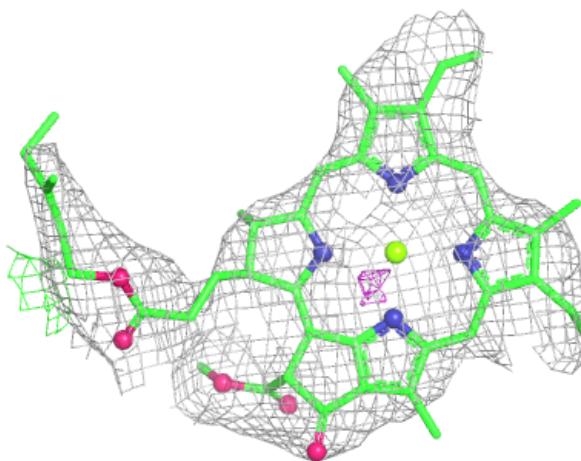
**Electron density around BCR c 5505:**

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



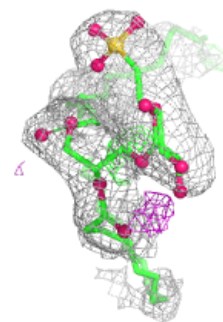
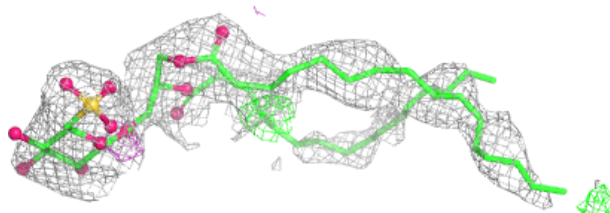
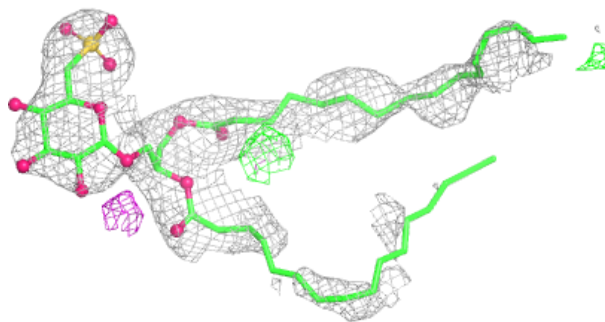
Electron density around CLA c 5502:

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

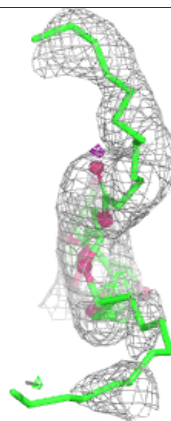
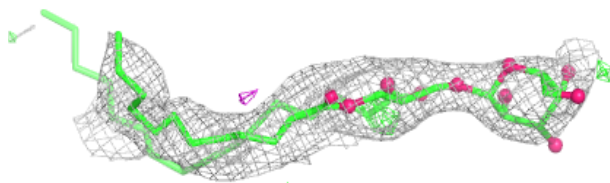
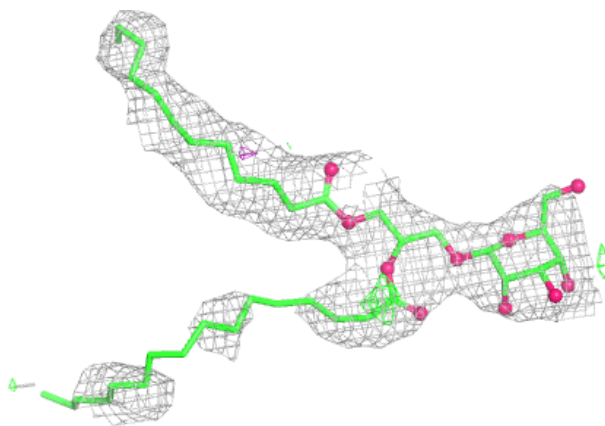


Electron density around SQD d 5358:

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

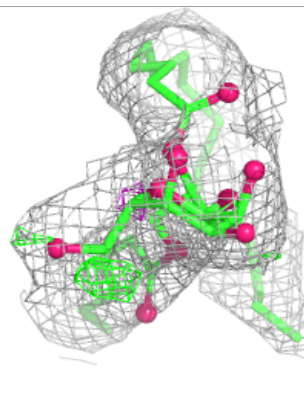
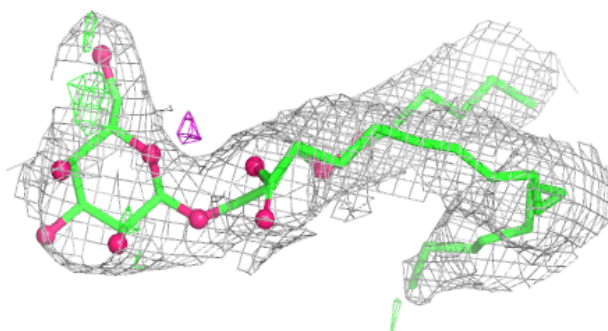
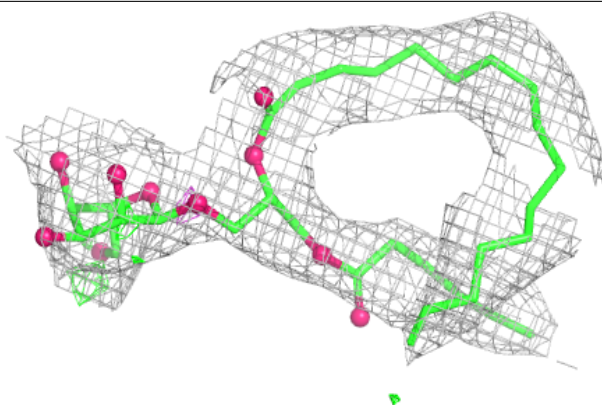
**Electron density around MGE d 5359:**

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

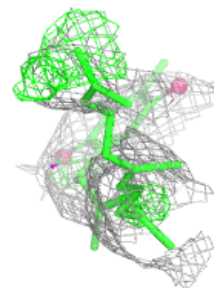
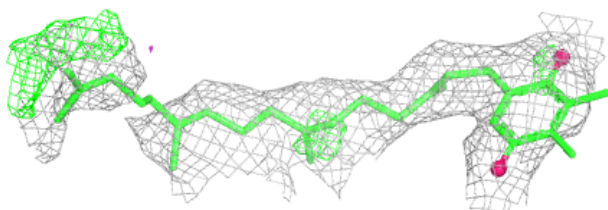
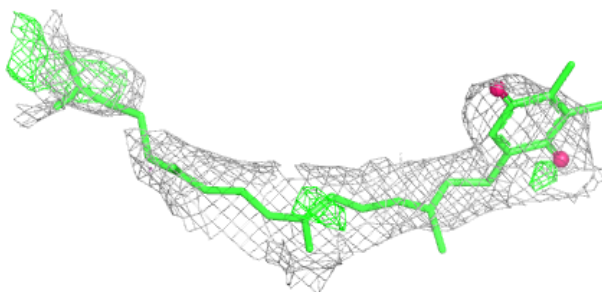


Electron density around MGE d 5360:

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

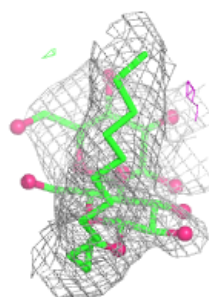
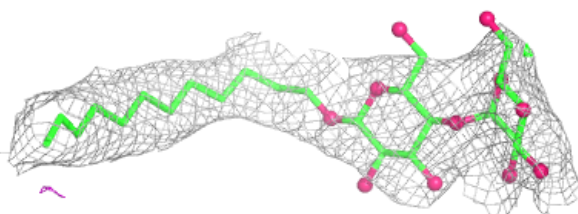
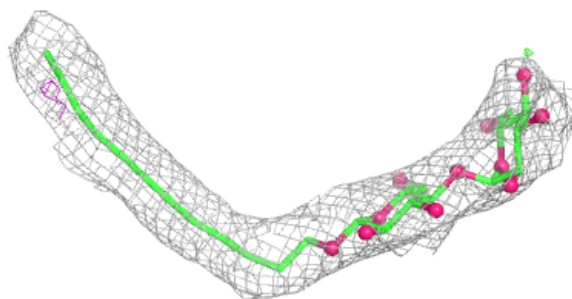
**Electron density around PQ9 A 564:**

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

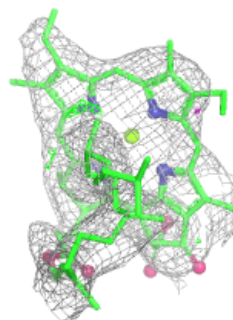
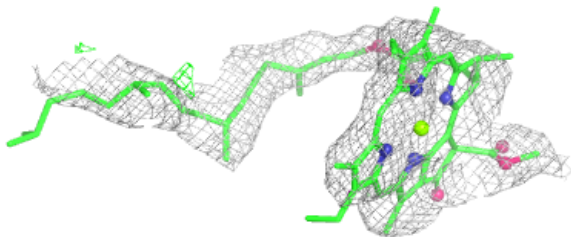
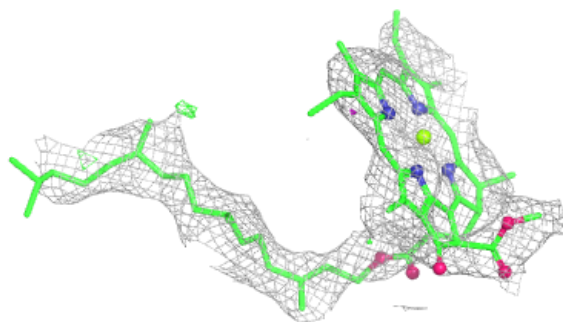


Electron density around LMT M 5216:

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

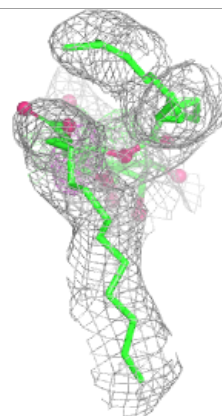
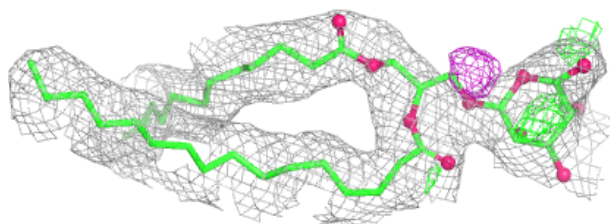
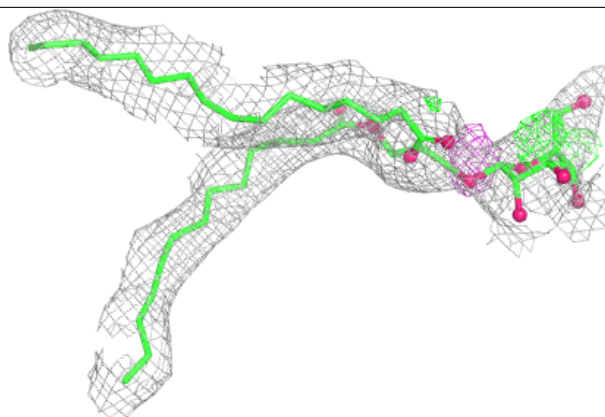
**Electron density around CLA c 5498:**

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

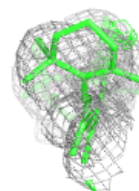
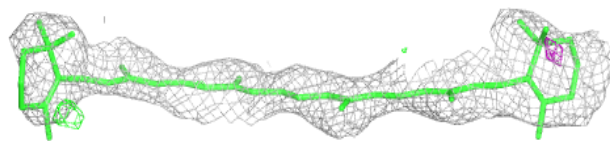
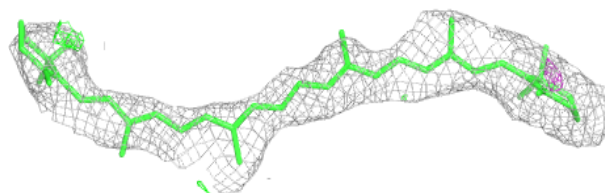


Electron density around MGE d 5361:

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

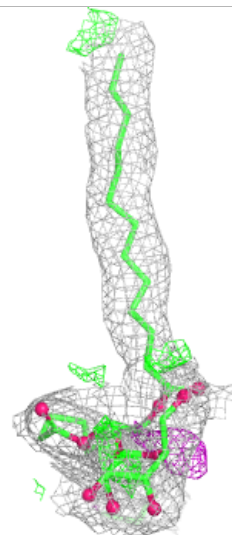
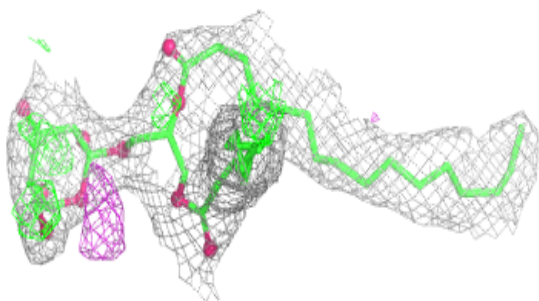
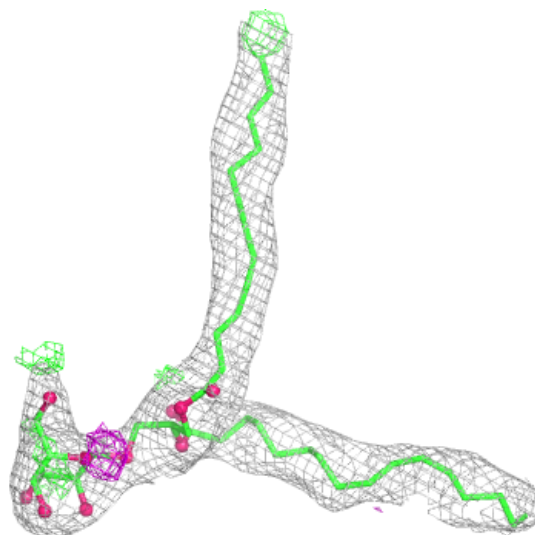
**Electron density around BCR H 107:**

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



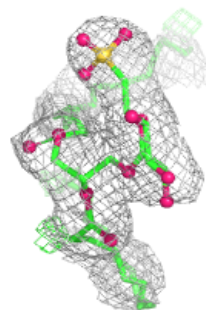
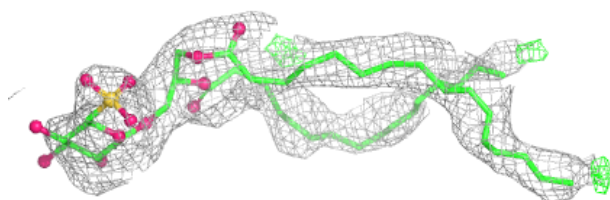
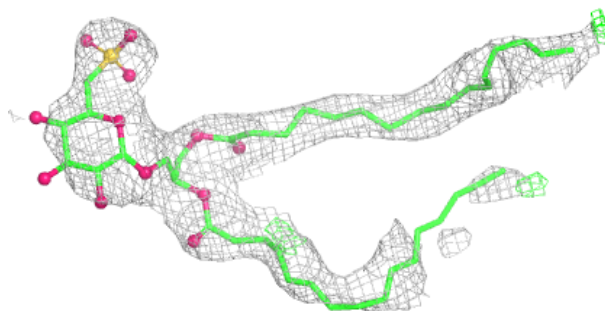
Electron density around MGE 1 5210:

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

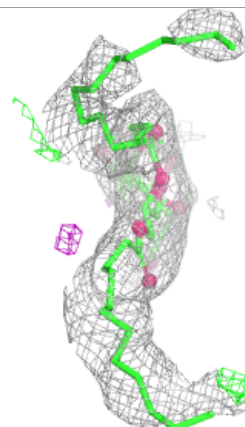
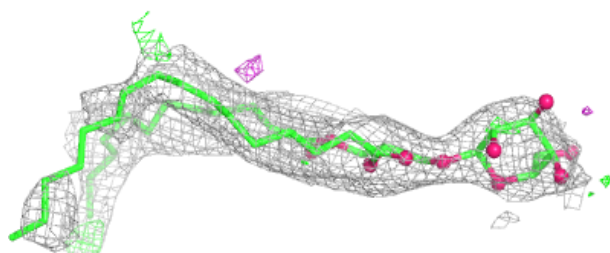
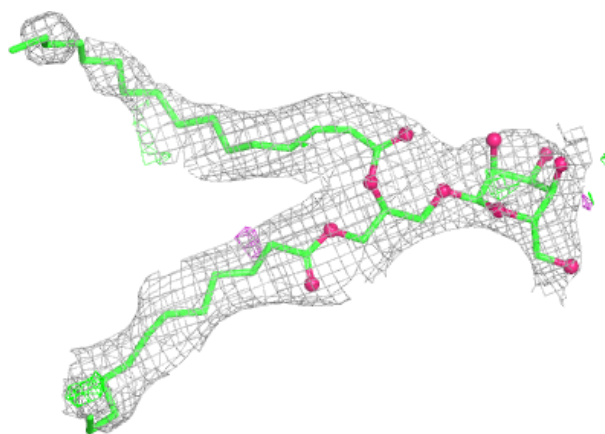


Electron density around SQD A 568:

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

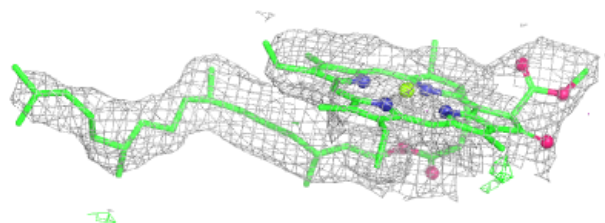
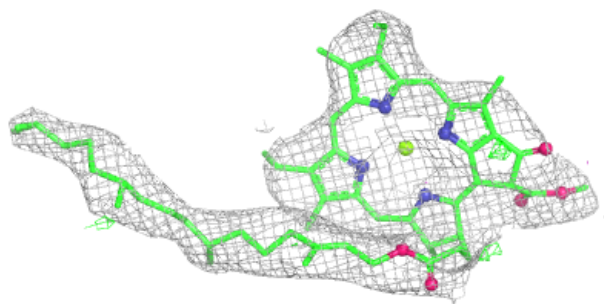
**Electron density around MGE D 358:**

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

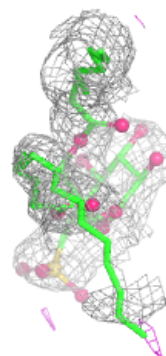
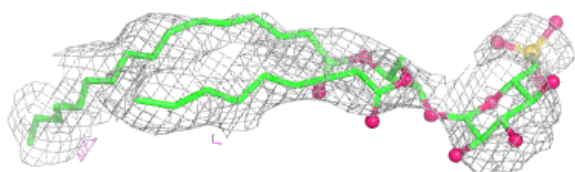
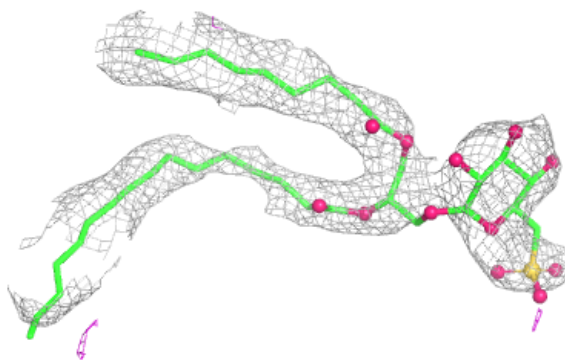


Electron density around CLA c 5491:

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

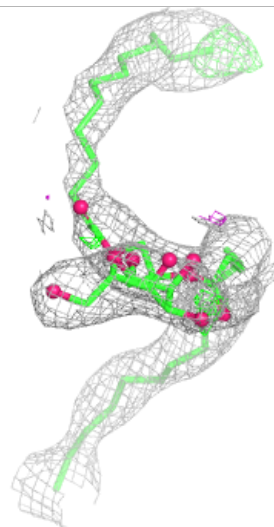
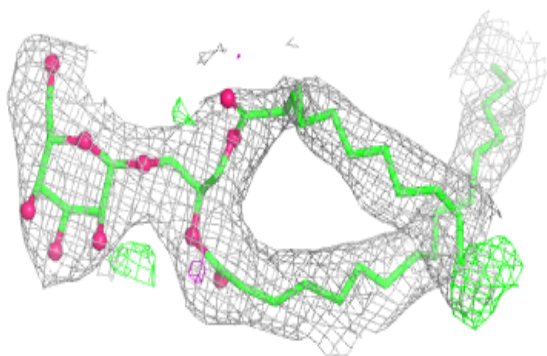
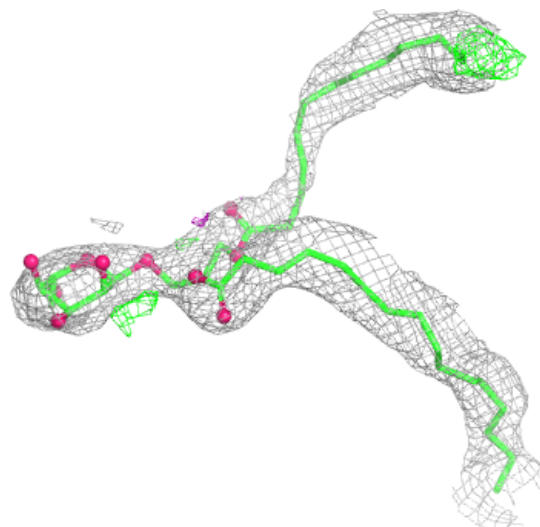
**Electron density around SQD t 213:**

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



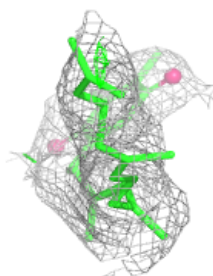
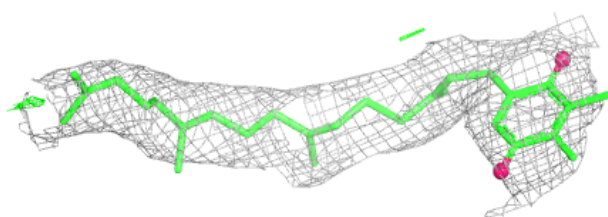
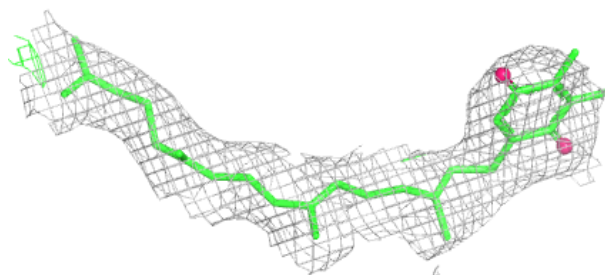
Electron density around MGE b 5530:

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



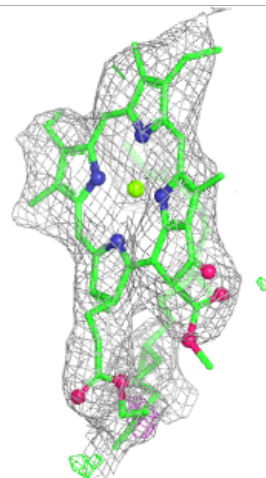
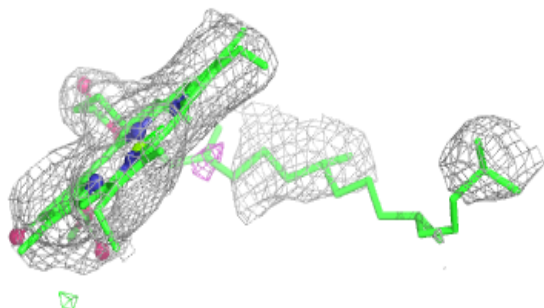
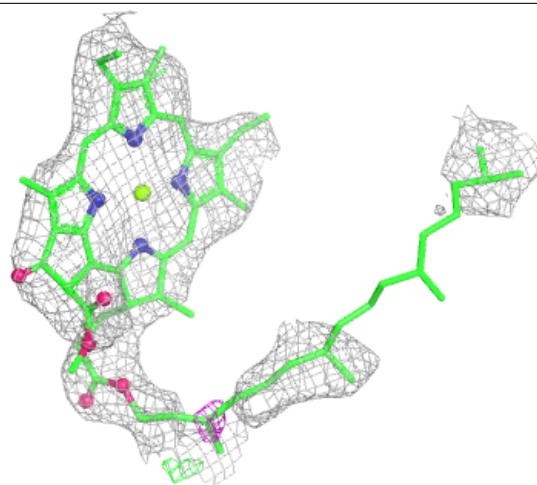
Electron density around PQ9 a 5564:

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



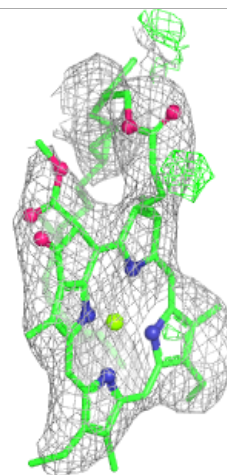
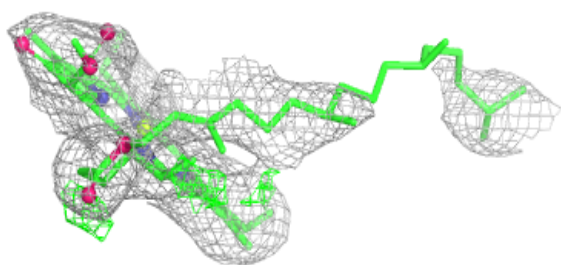
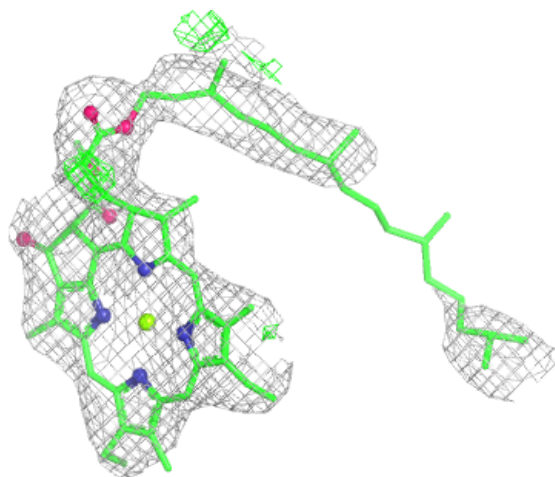
Electron density around CLA B 526:

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



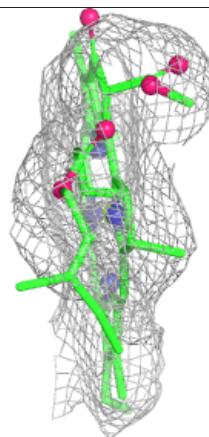
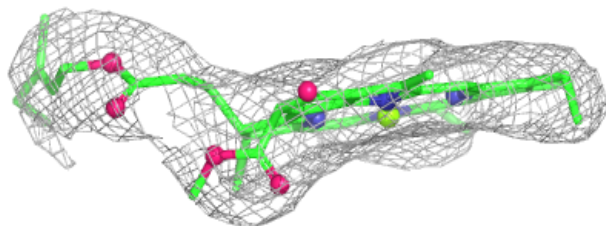
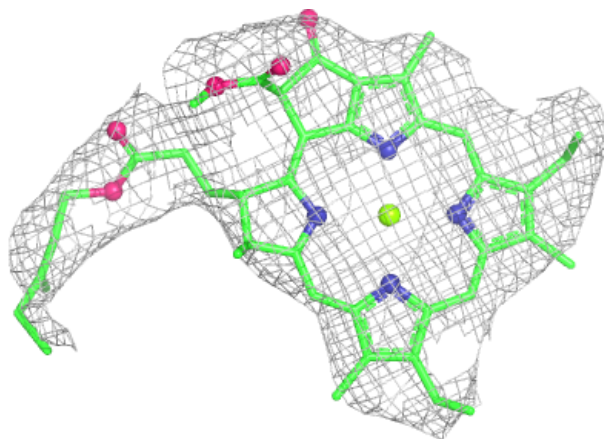
Electron density around CLA b 5526:

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



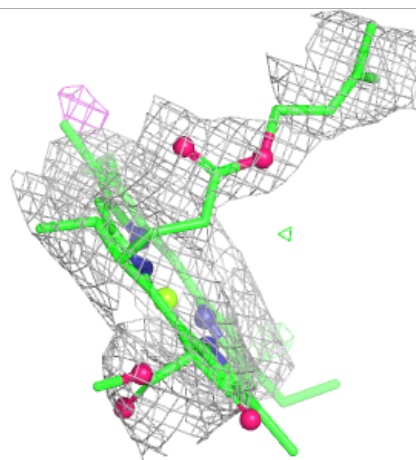
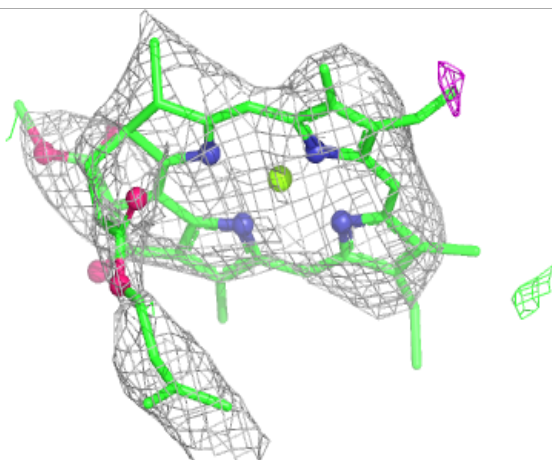
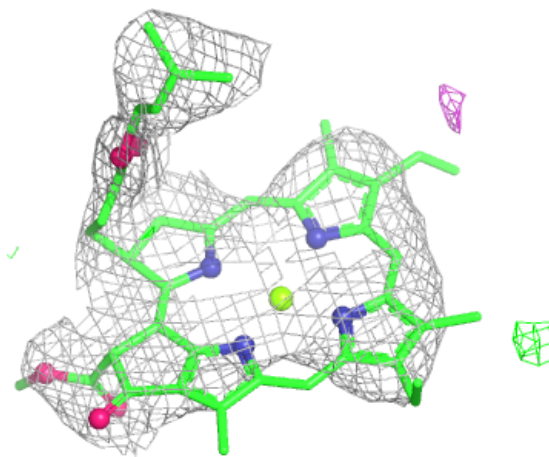
Electron density around CLA C 502:

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



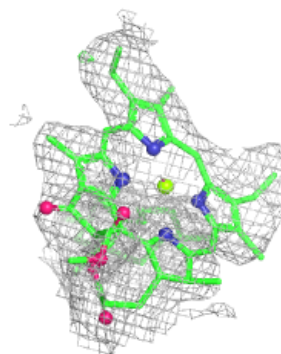
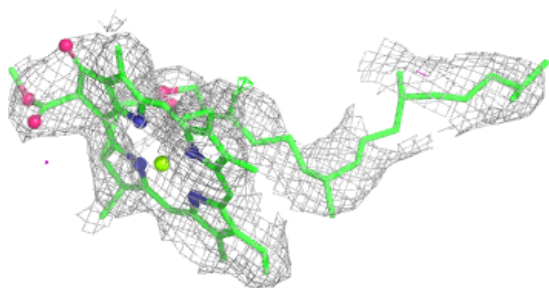
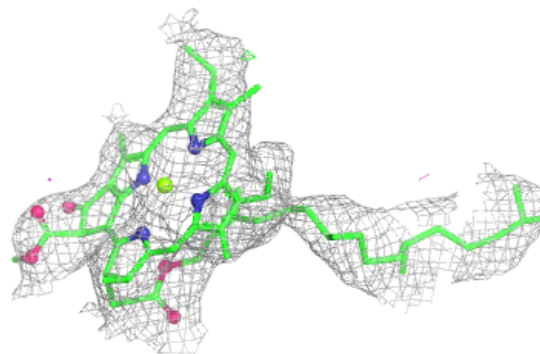
Electron density around CLA c 5503:

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

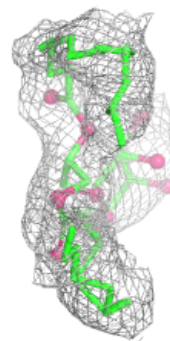
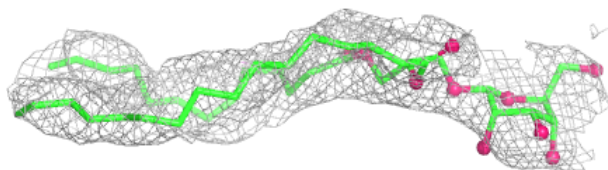
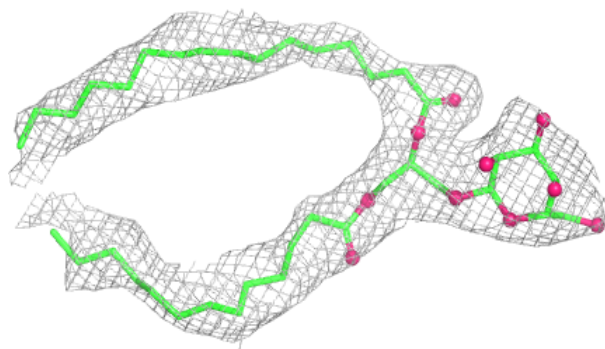


Electron density around CLA c 5495:

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

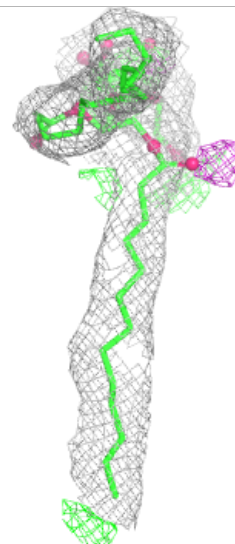
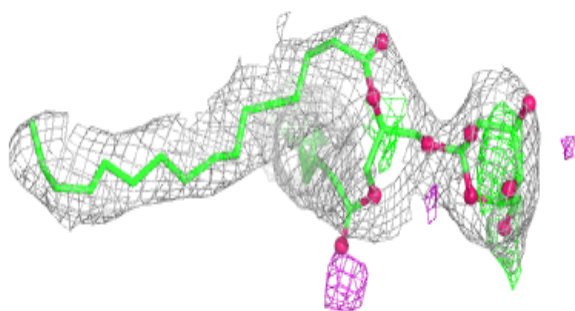
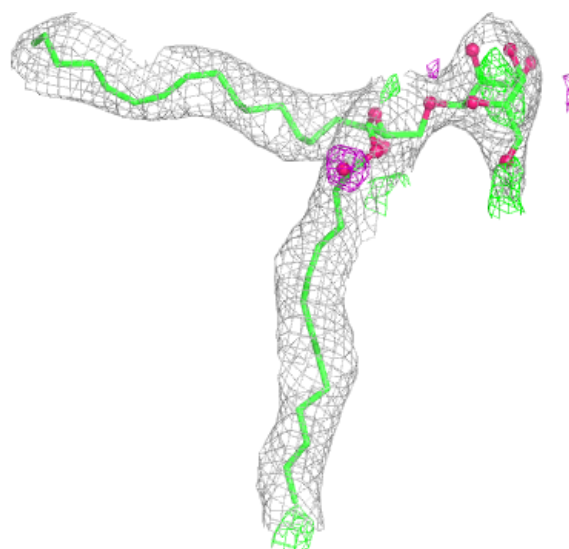
**Electron density around MGE I 201:**

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



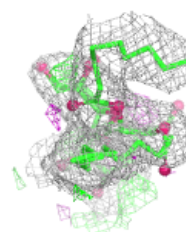
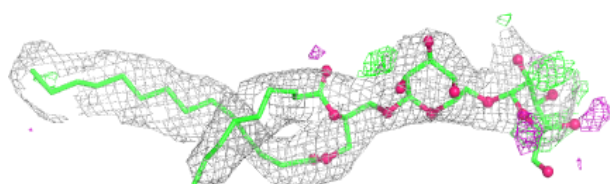
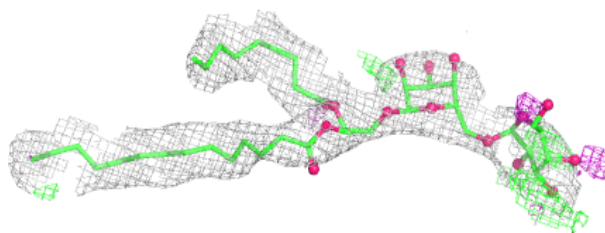
Electron density around MGE L 210:

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

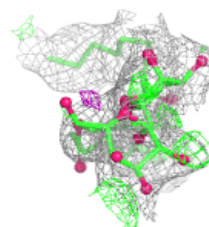
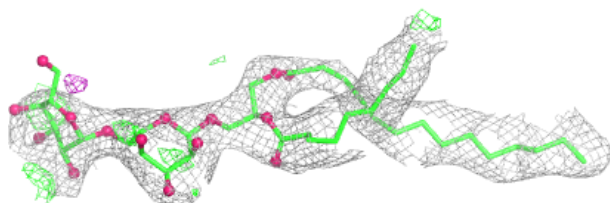
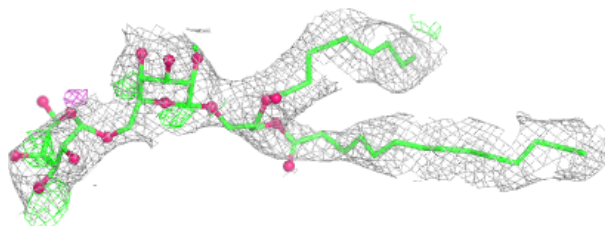


Electron density around DGD C 507:

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

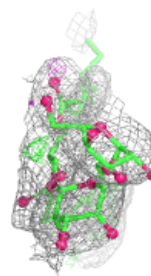
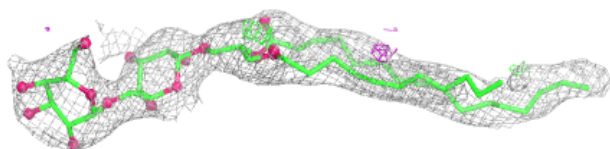
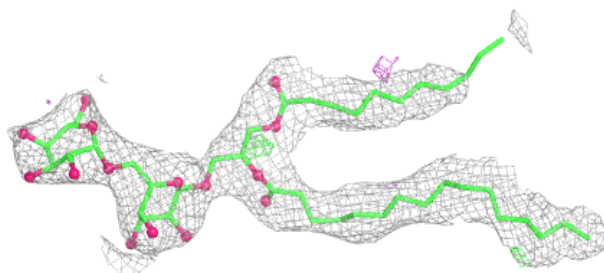
**Electron density around DGD c 5507:**

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

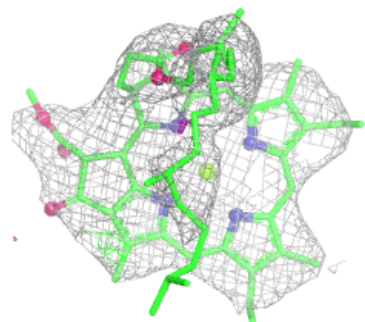
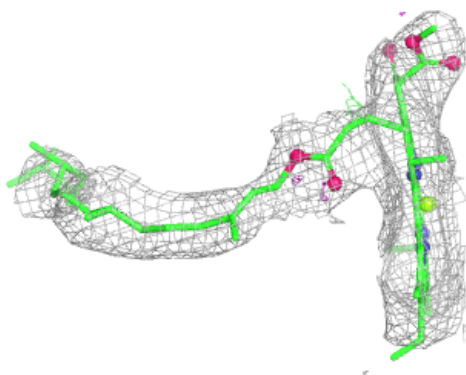
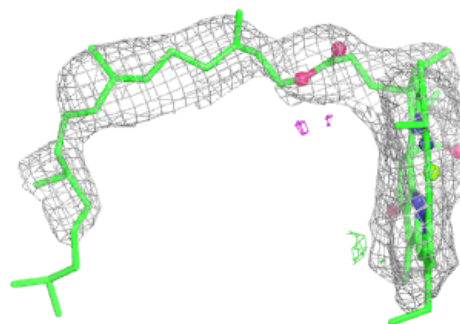


Electron density around DGD c 5509:

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

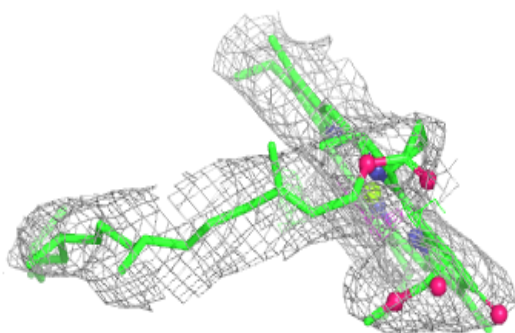
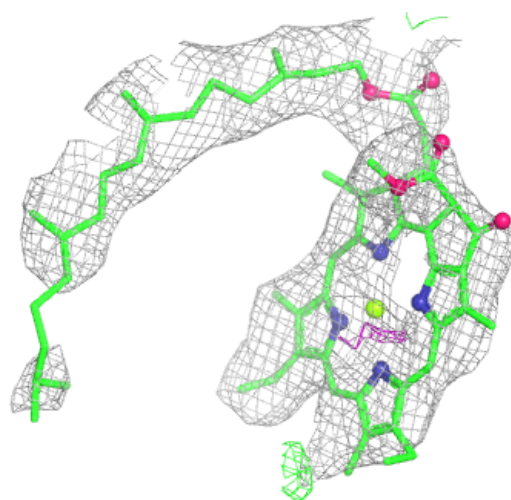
**Electron density around CLA B 516:**

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



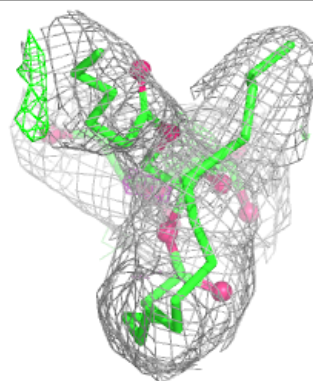
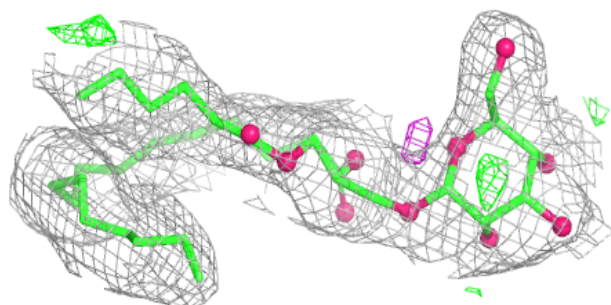
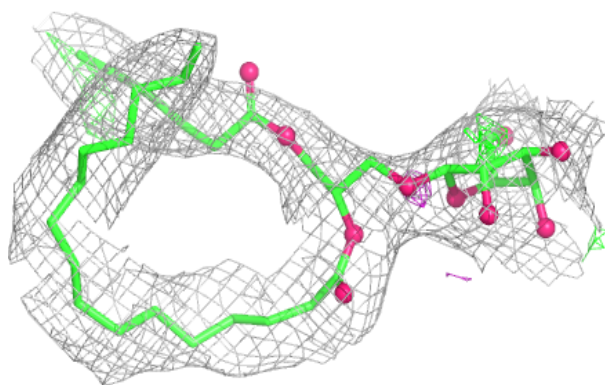
Electron density around CLA c 5497:

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

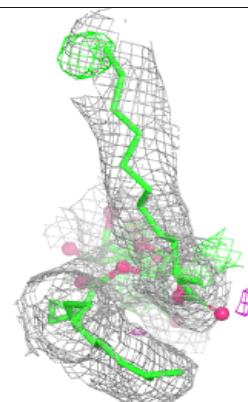
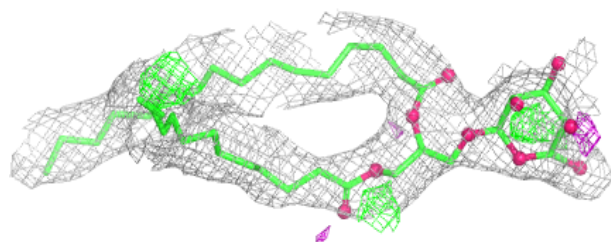
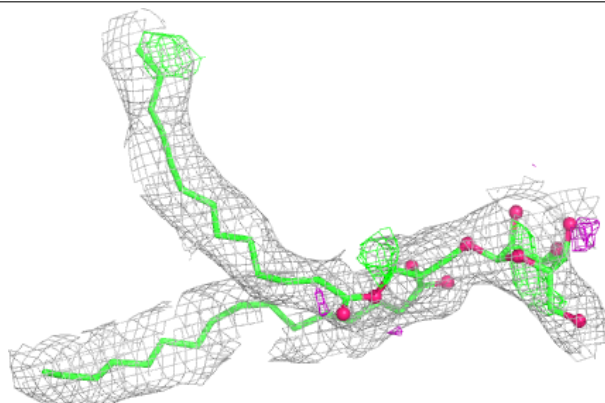


Electron density around MGE D 359:

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

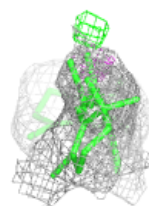
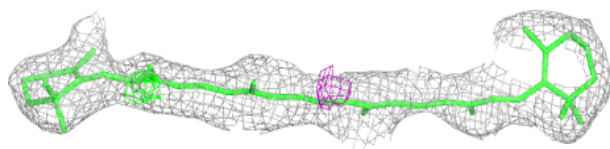
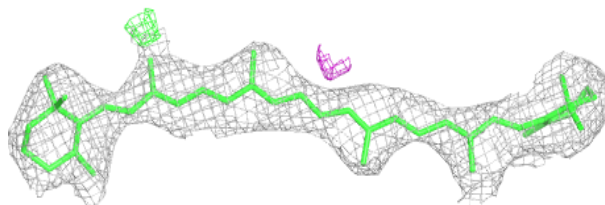
**Electron density around MGE D 360:**

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



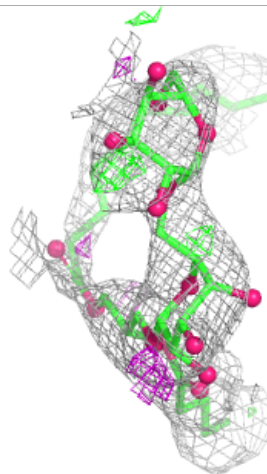
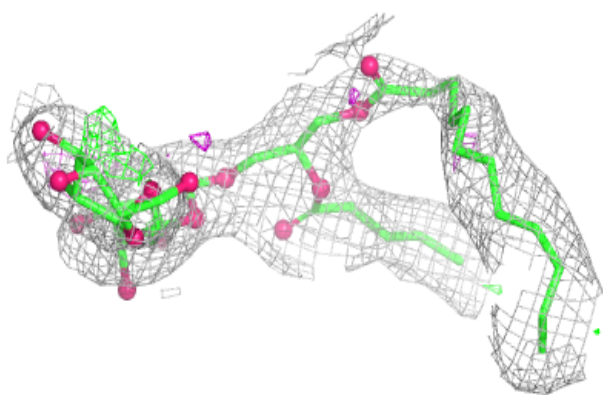
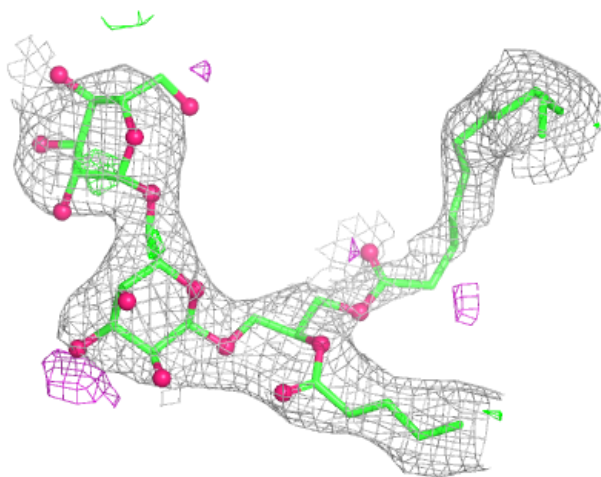
Electron density around BCR B 527:

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



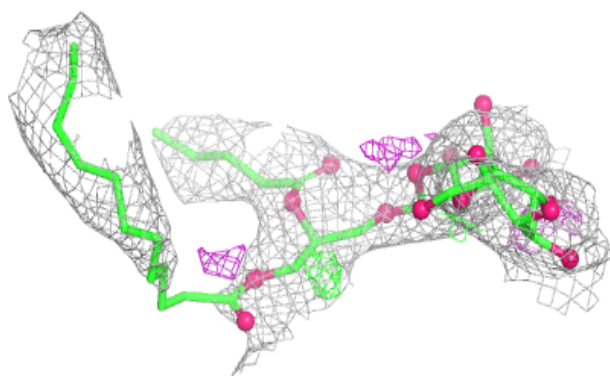
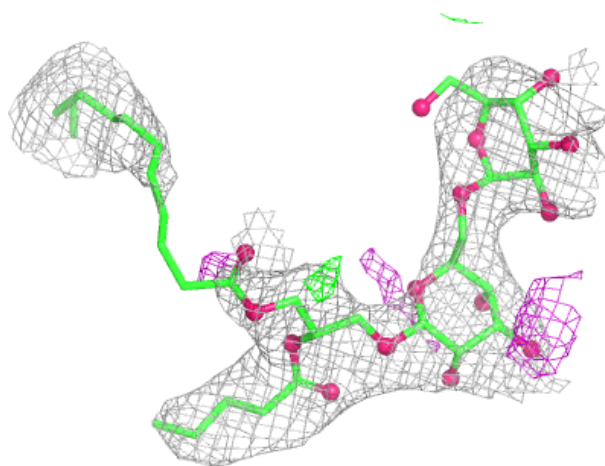
Electron density around DGD C 508:

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



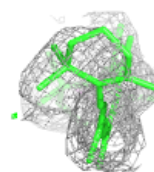
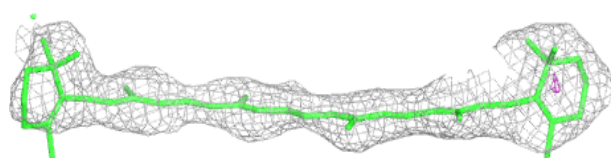
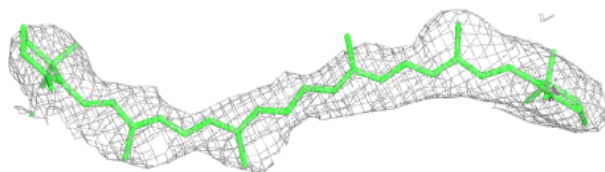
Electron density around DGD c 5508:

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

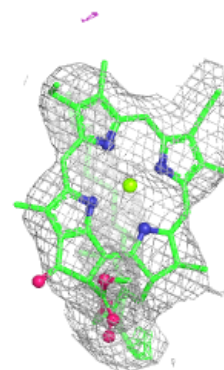
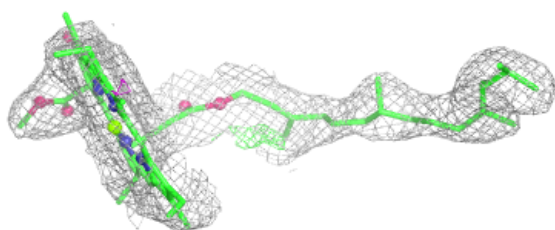
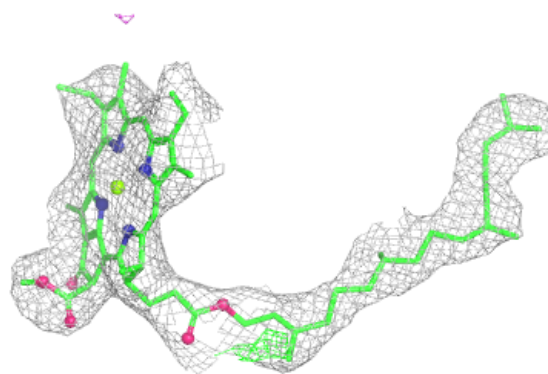


Electron density around BCR h 5107:

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

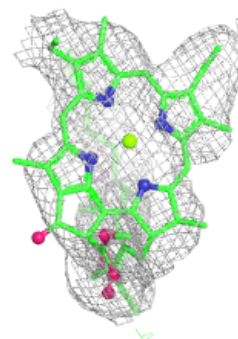
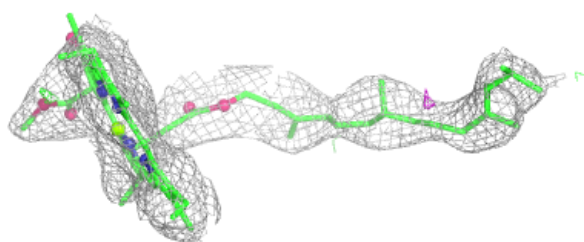
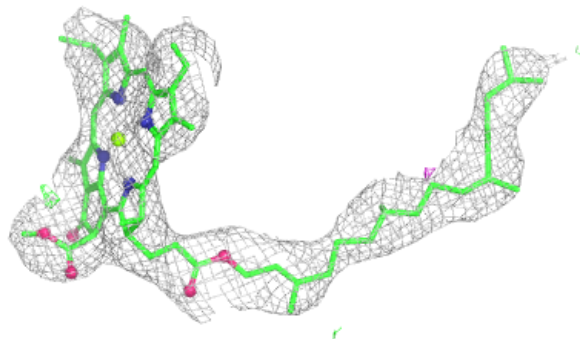
**Electron density around CLA b 5519:**

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



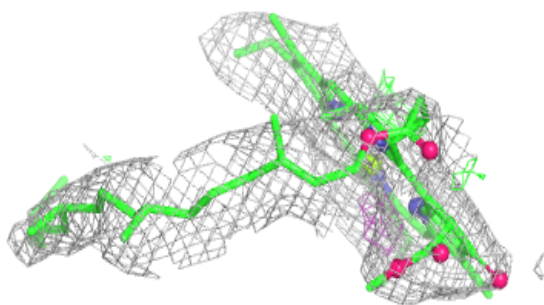
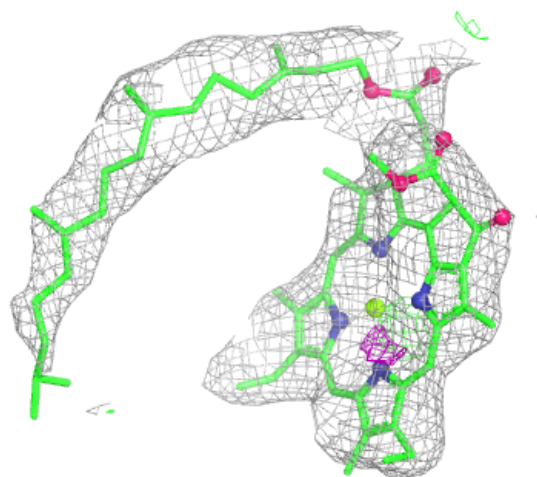
Electron density around CLA B 519:

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



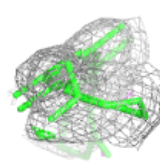
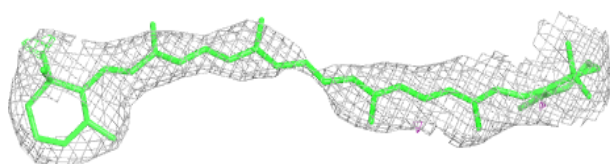
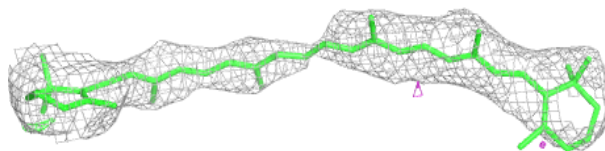
Electron density around CLA C 497:

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

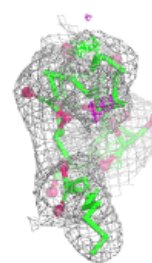
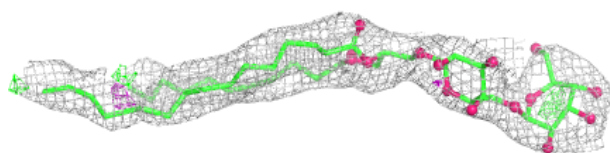


Electron density around BCR d 5357:

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

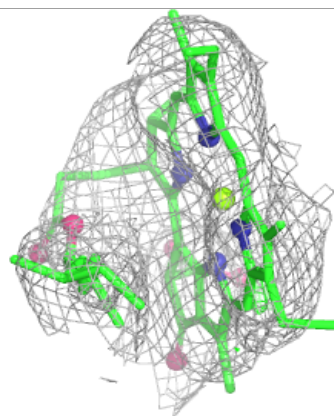
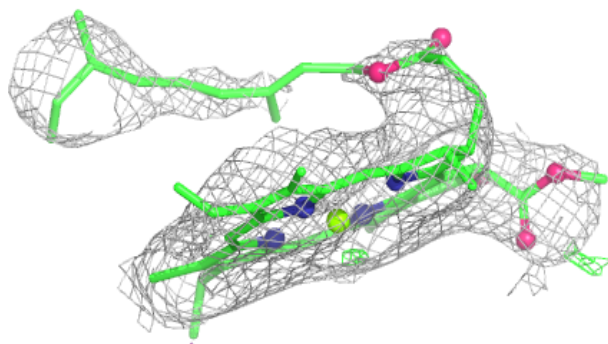
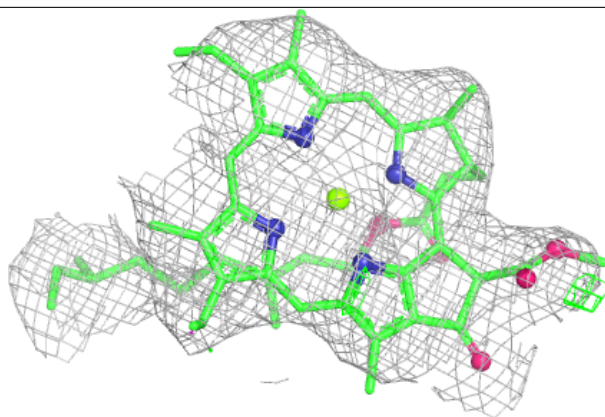
**Electron density around DGD C 509:**

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

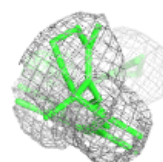
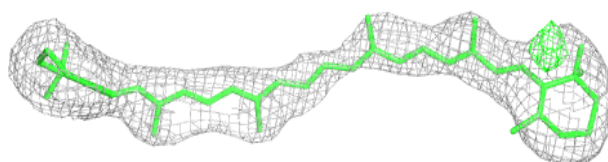


Electron density around CLA b 5524:

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

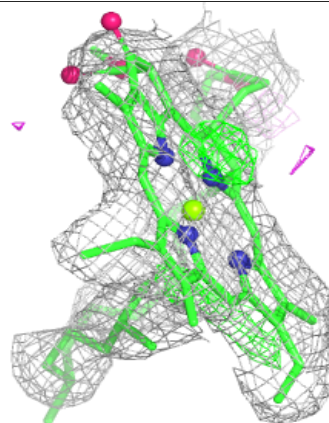
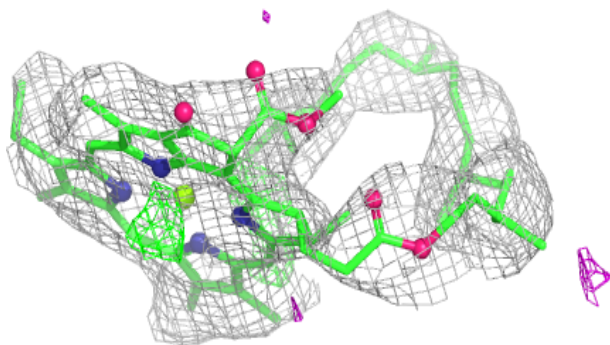
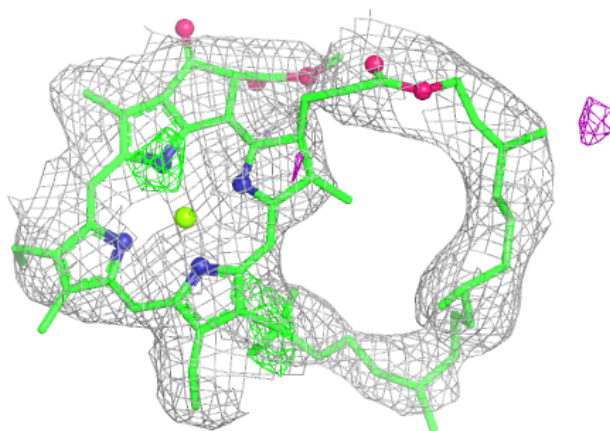
**Electron density around BCR D 357:**

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



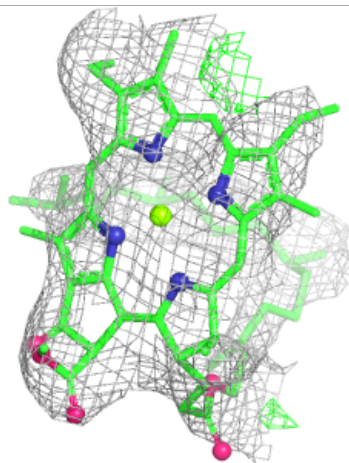
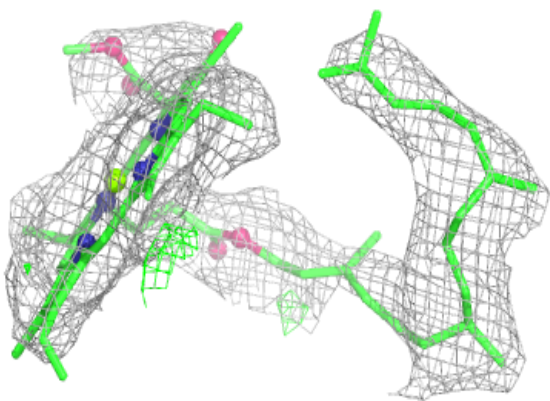
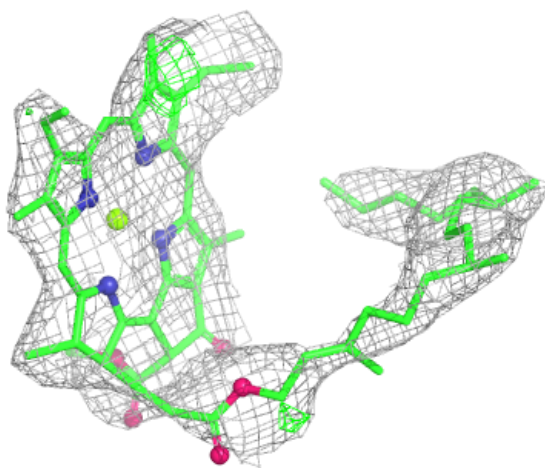
Electron density around CLA B 525:

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



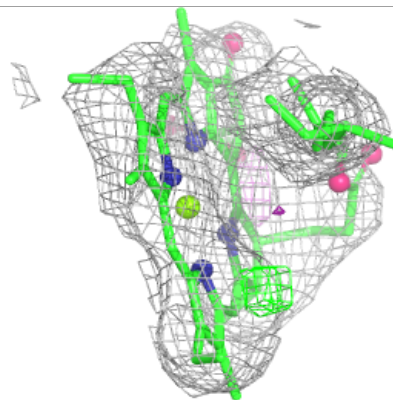
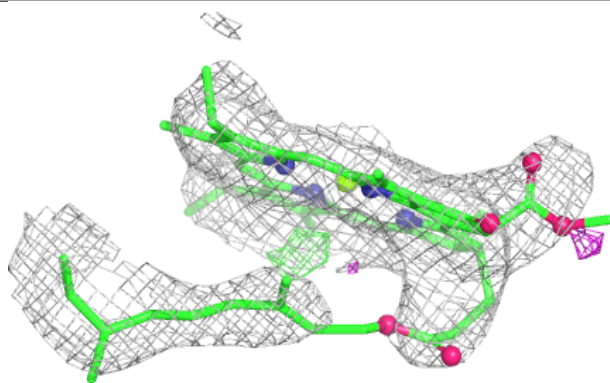
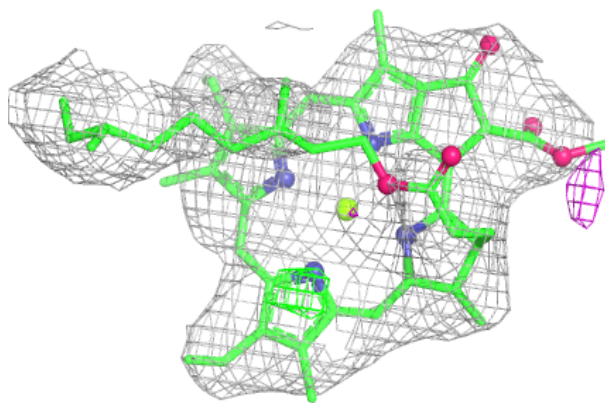
Electron density around CLA c 5493:

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

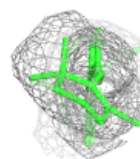
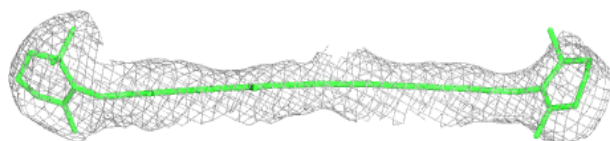
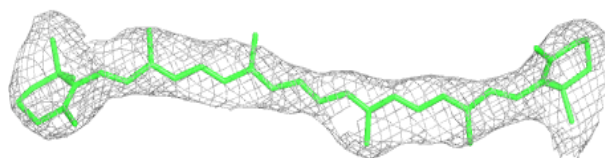


Electron density around CLA B 524:

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

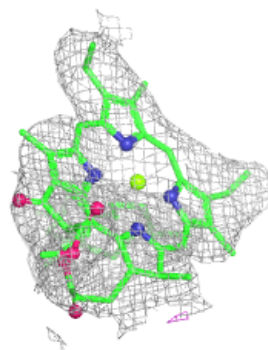
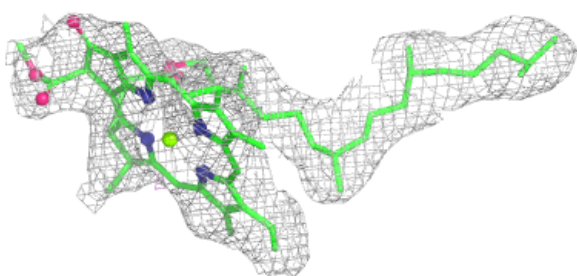
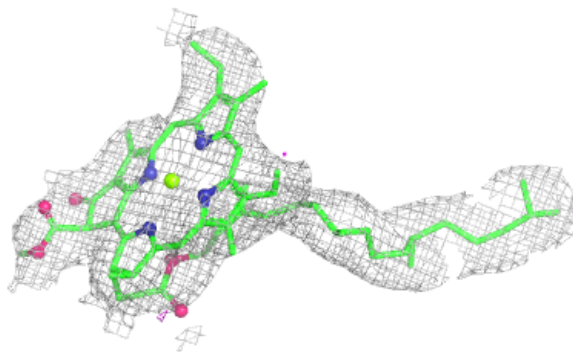
**Electron density around BCR B 528:**

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



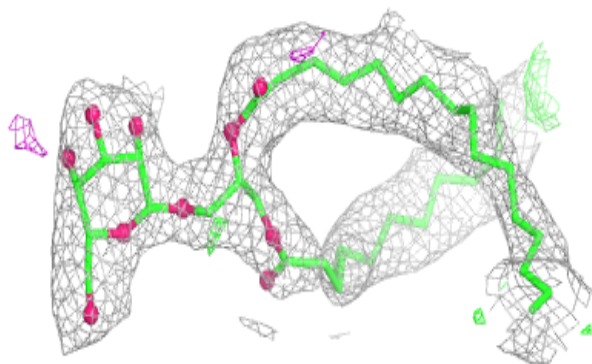
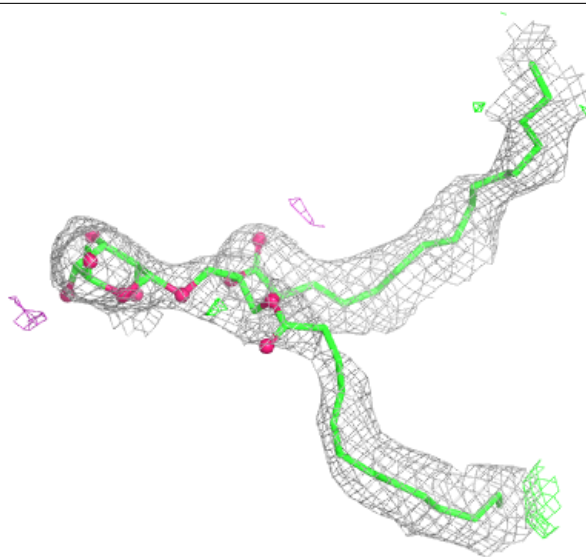
Electron density around CLA C 495:

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



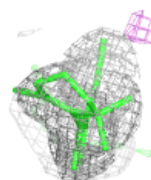
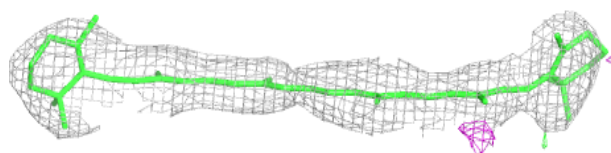
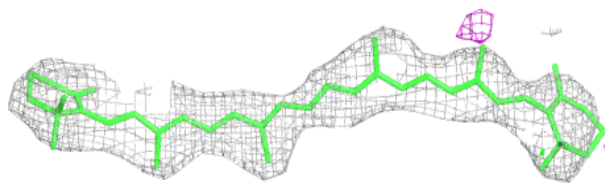
Electron density around MGE B 530:

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

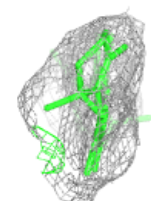
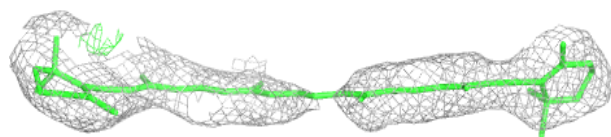
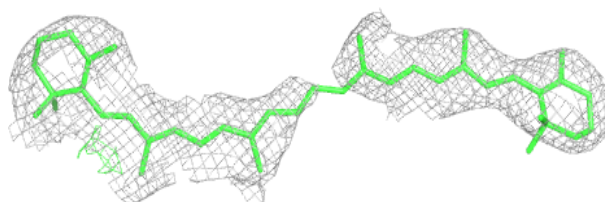


Electron density around BCR C 506:

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

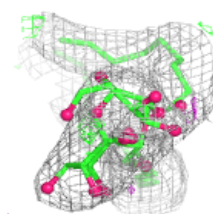
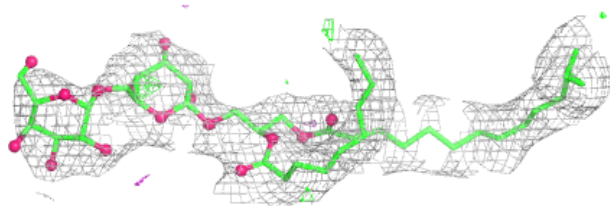
**Electron density around BCR x 5130:**

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

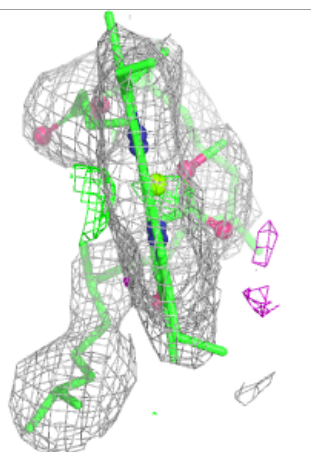
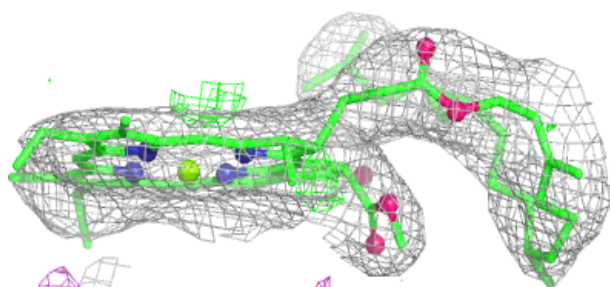
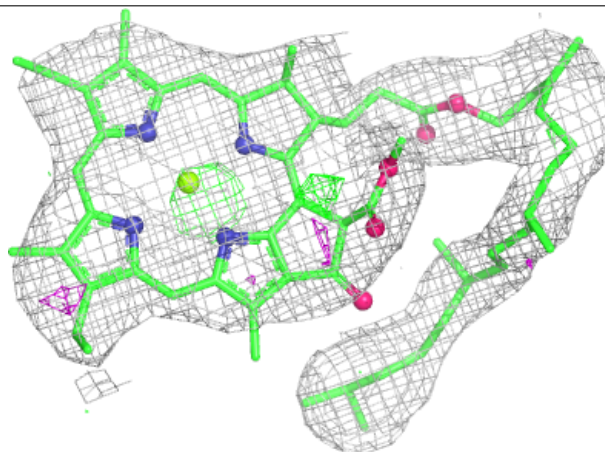


Electron density around DGD h 5208:

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

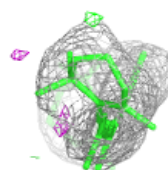
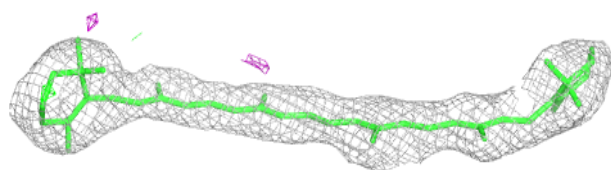
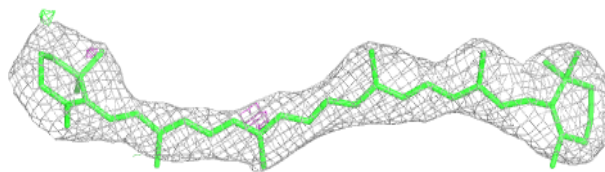
**Electron density around CLA b 5520:**

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

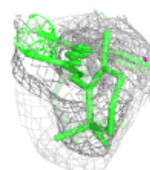
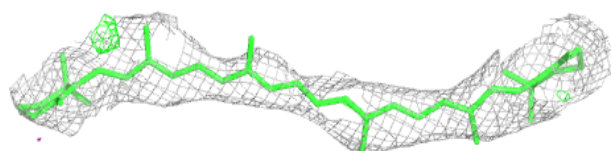


Electron density around BCR b 5529:

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

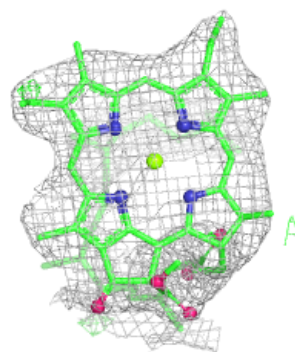
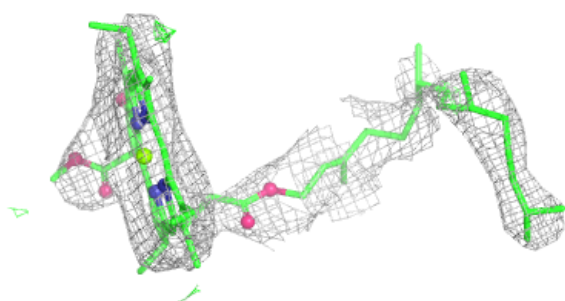
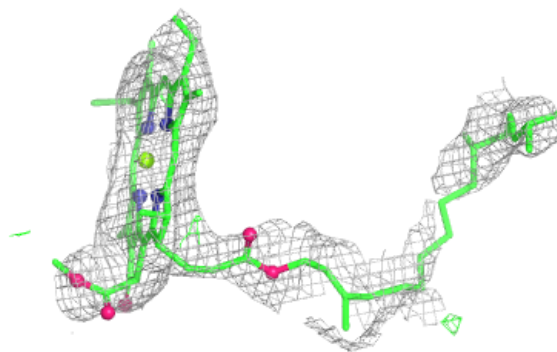
**Electron density around BCR c 5504:**

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



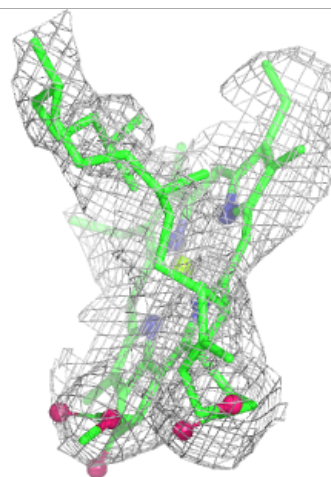
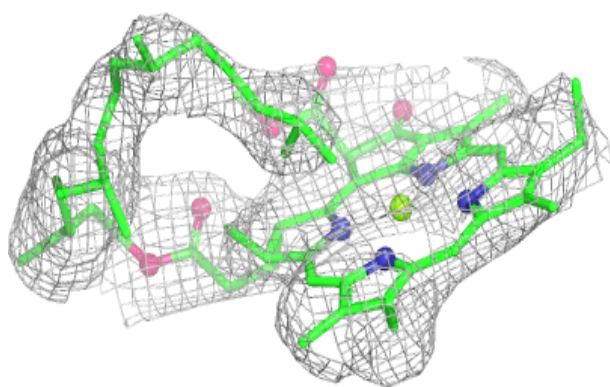
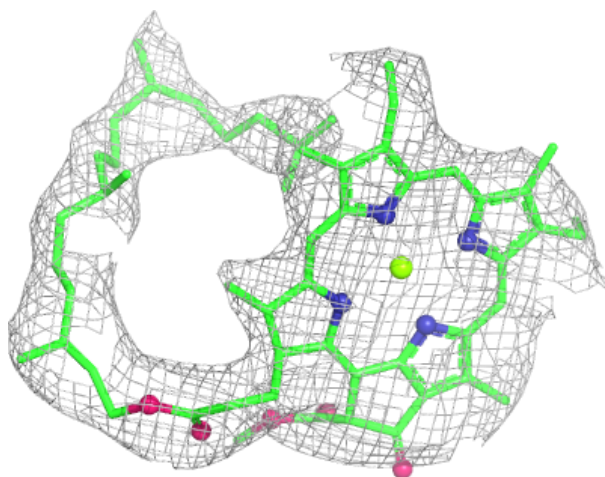
Electron density around CLA c 5496:

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



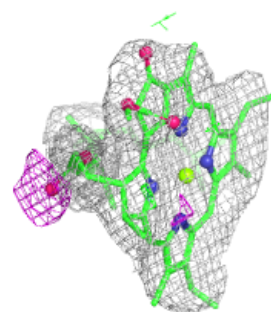
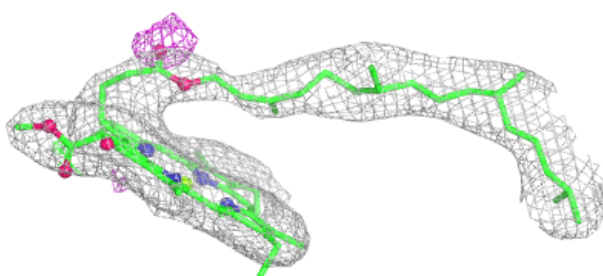
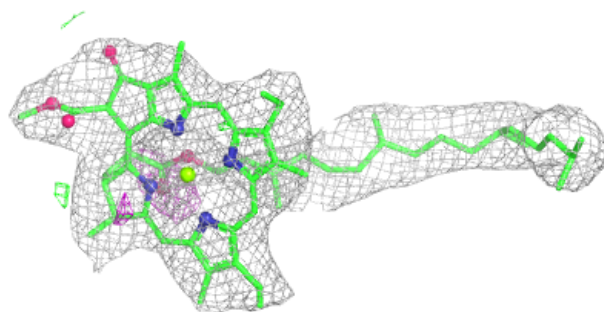
Electron density around CLA b 5525:

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

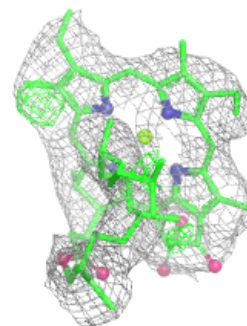
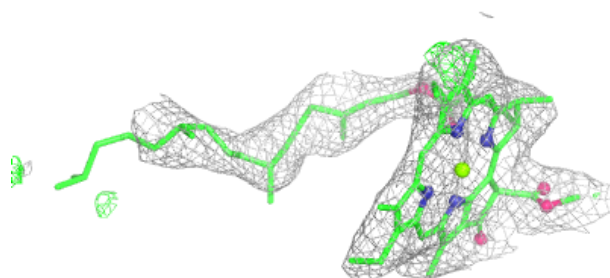
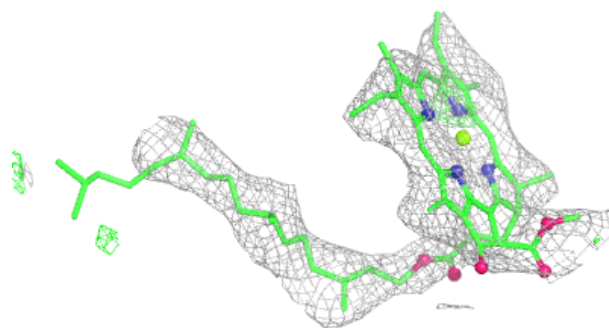


Electron density around CLA b 5518:

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

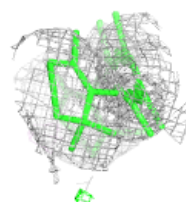
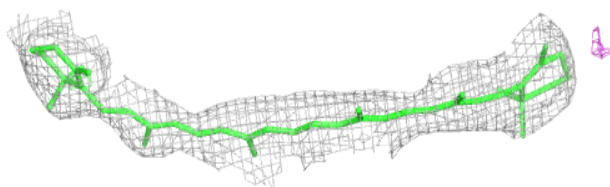
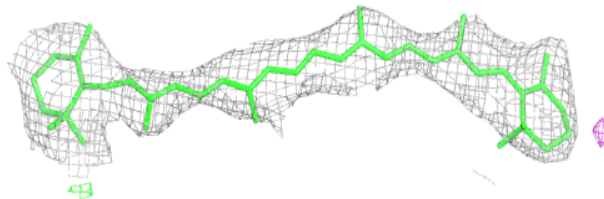
**Electron density around CLA C 498:**

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

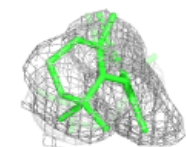
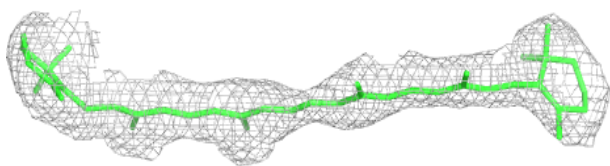
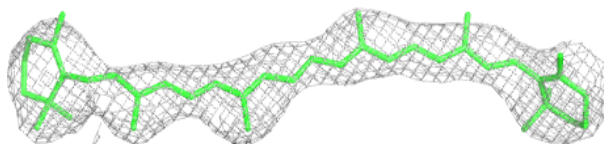


Electron density around BCR t 104:

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

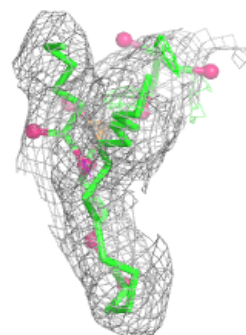
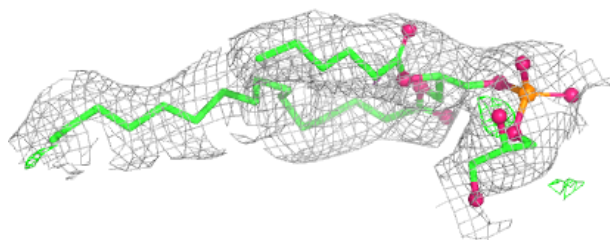
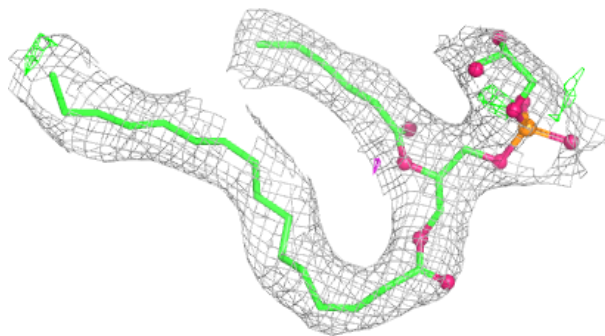
**Electron density around BCR B 529:**

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

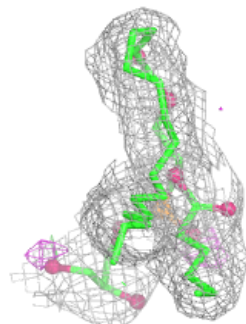
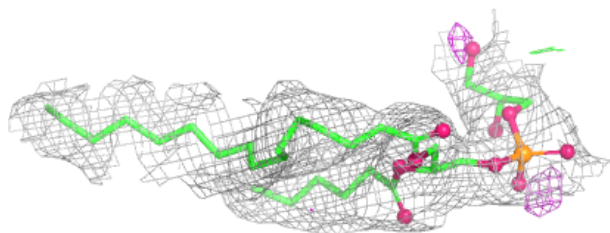
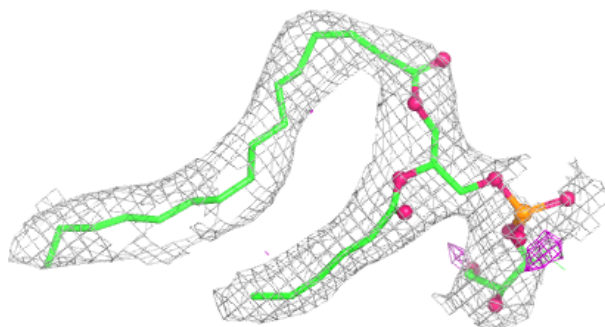


Electron density around LHG A 567:

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

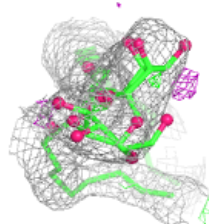
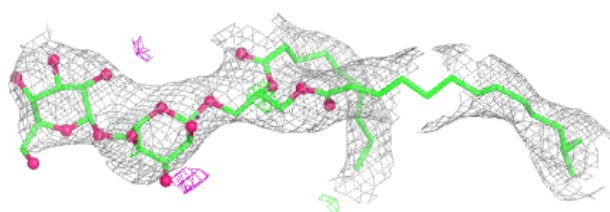
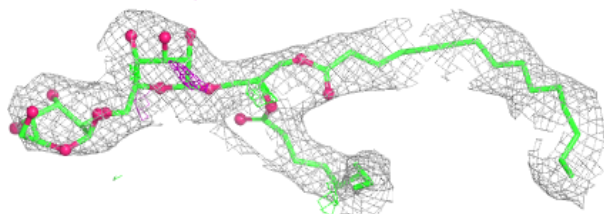
**Electron density around LHG a 5567:**

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

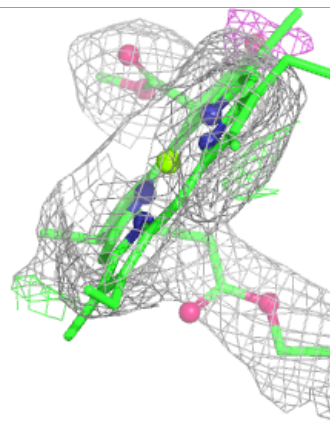
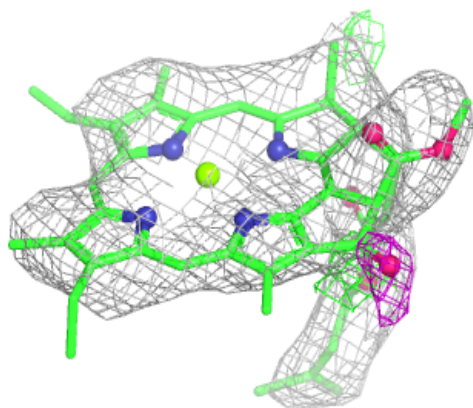
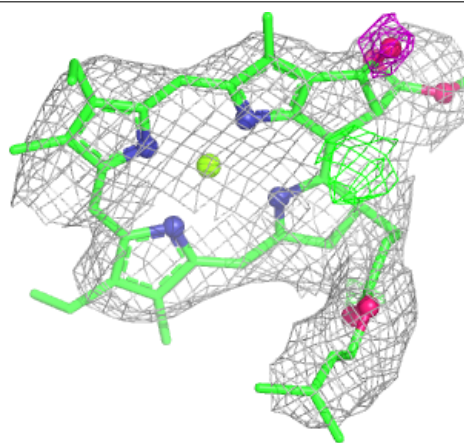


Electron density around DGD H 208:

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

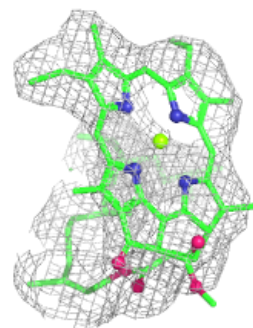
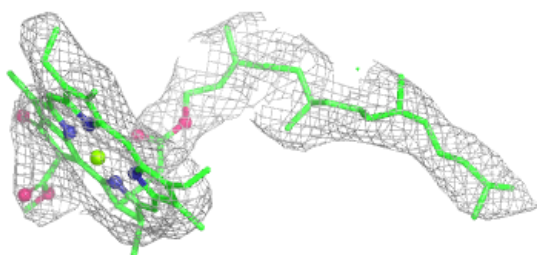
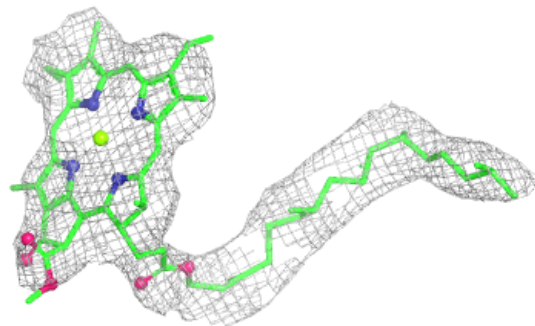
**Electron density around CLA C 503:**

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



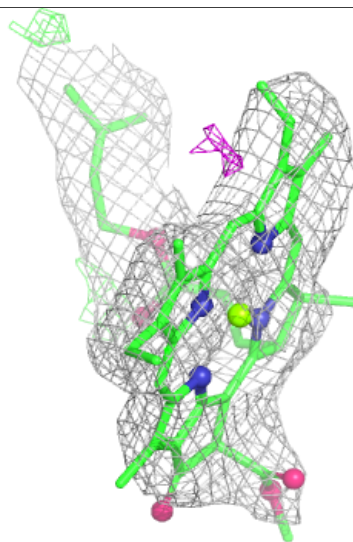
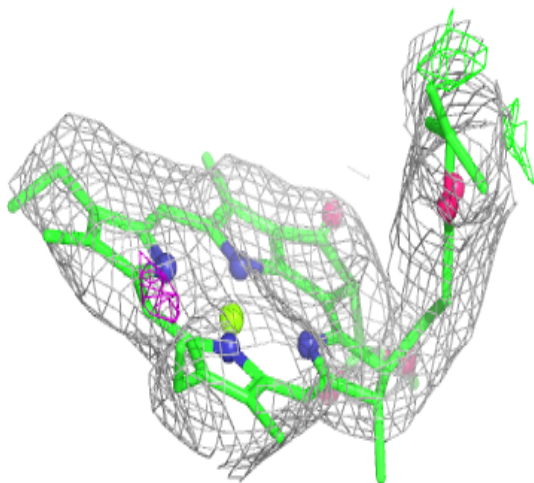
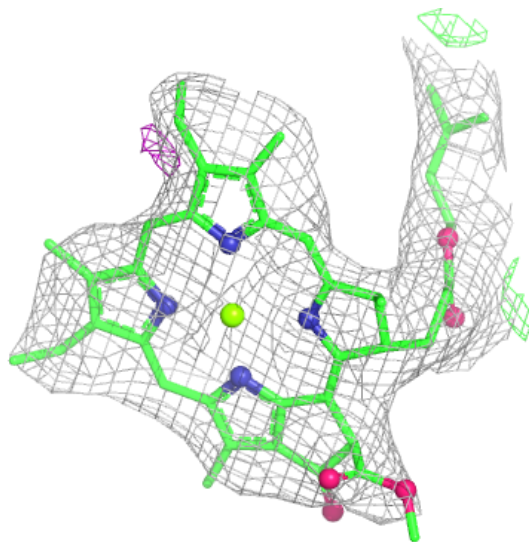
Electron density around CLA C 501:

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



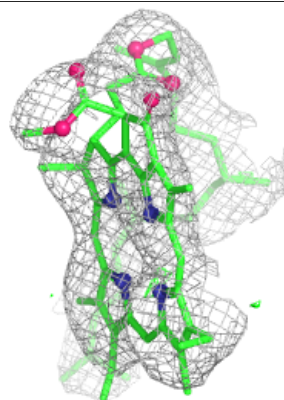
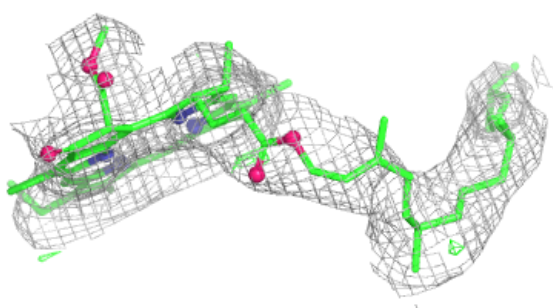
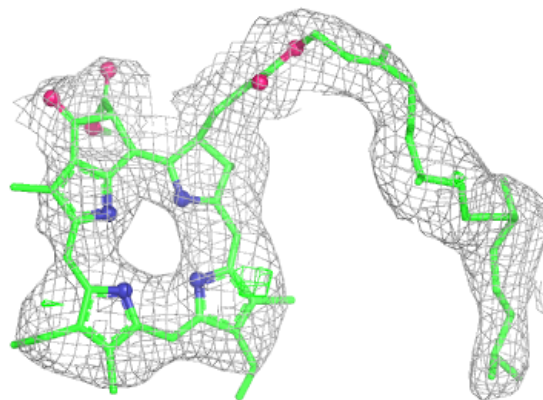
Electron density around CLA d 5355:

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

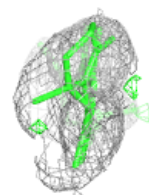
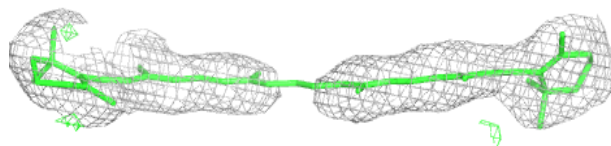
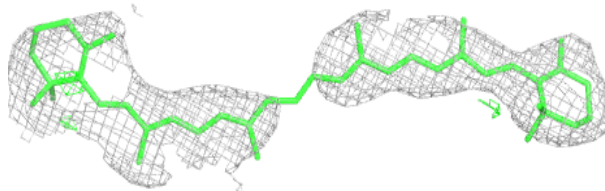


Electron density around PHO a 5562:

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

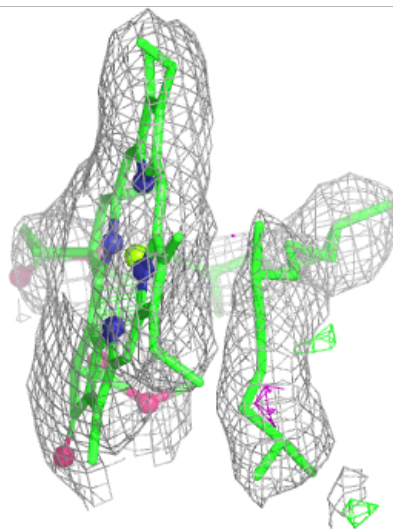
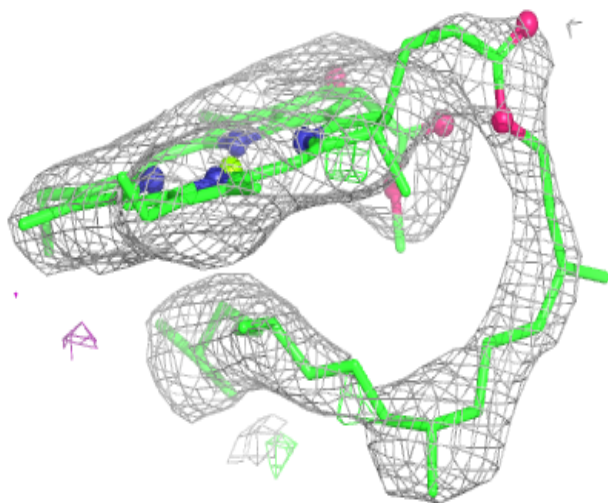
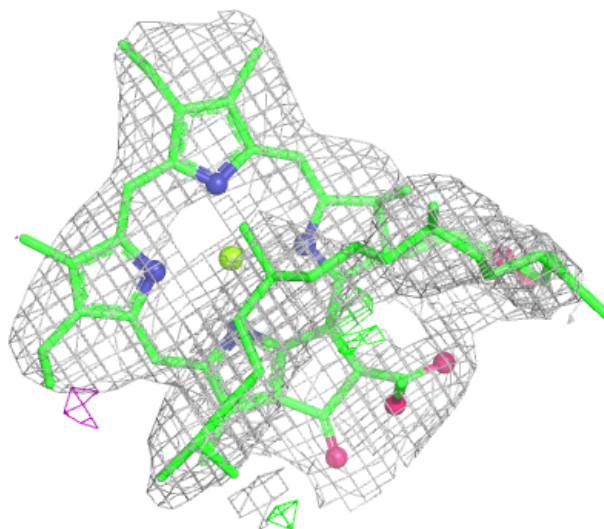
**Electron density around BCR X 130:**

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



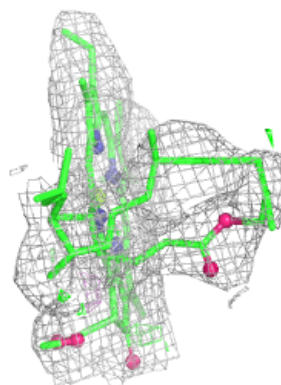
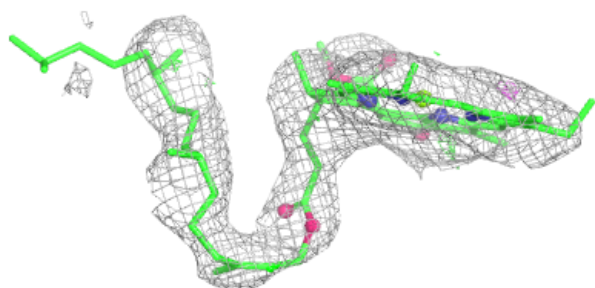
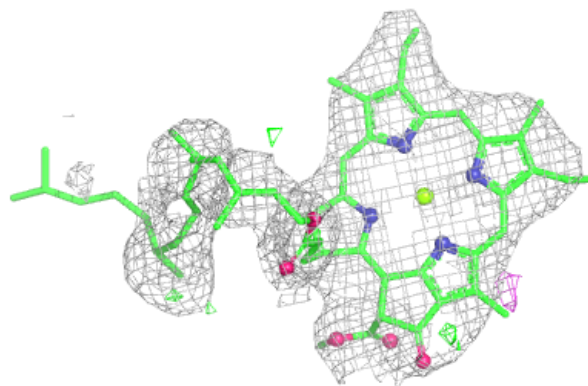
Electron density around CLA c 5500:

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

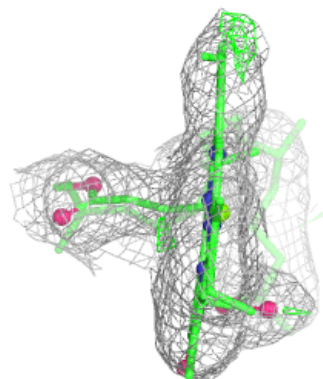
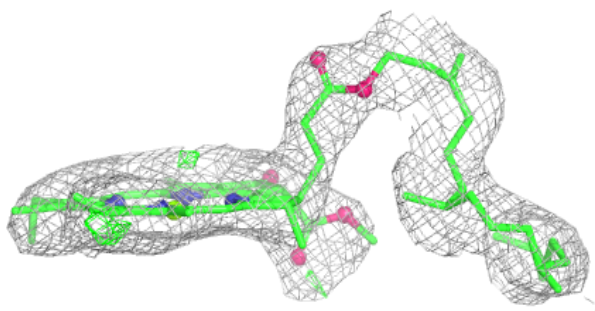
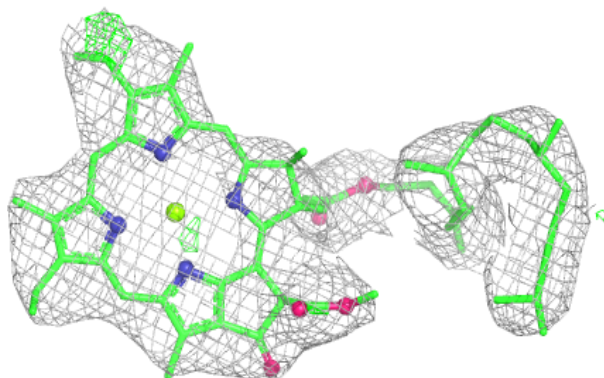


Electron density around CLA a 5560:

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

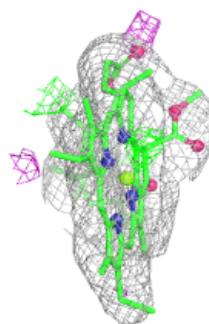
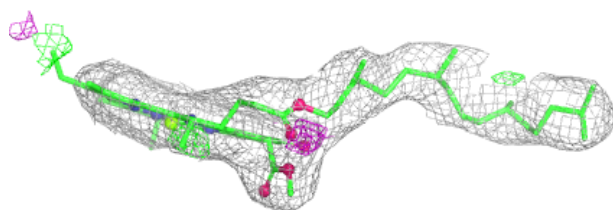
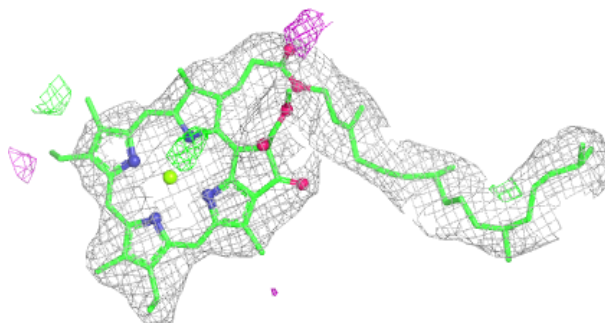
**Electron density around CLA B 522:**

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

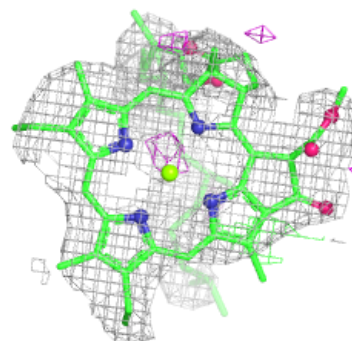
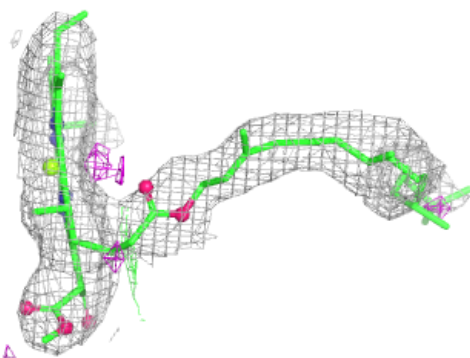
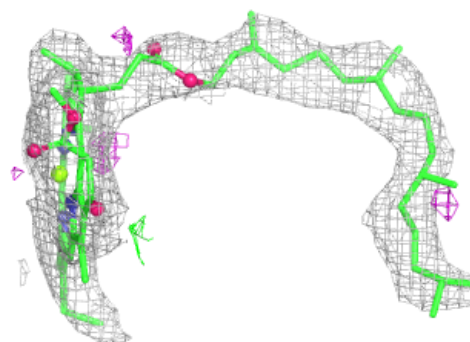


Electron density around CLA b 5512:

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

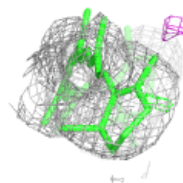
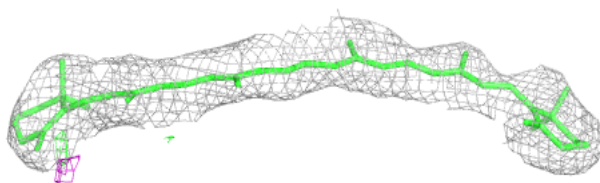
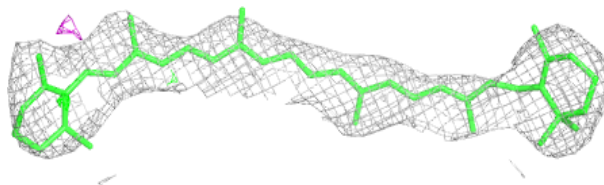
**Electron density around CLA b 5516:**

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



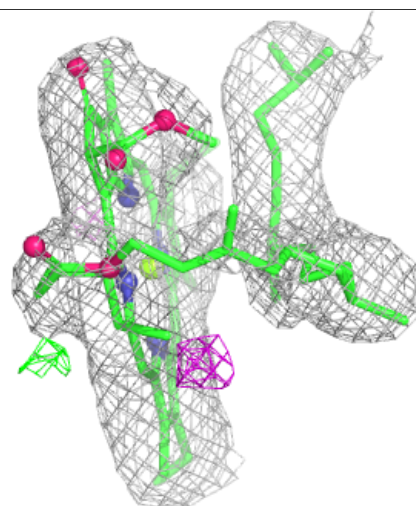
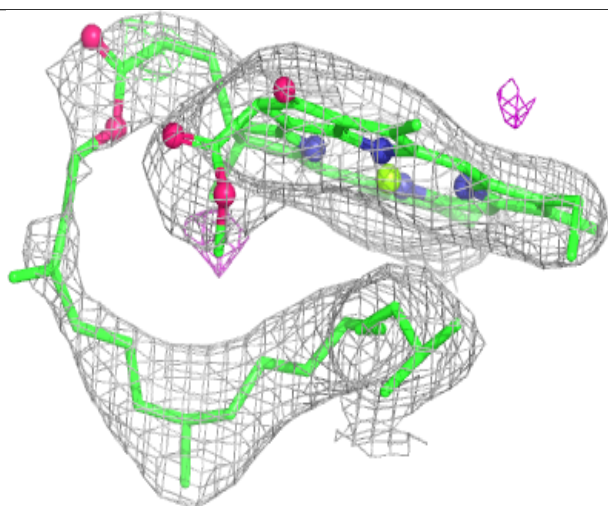
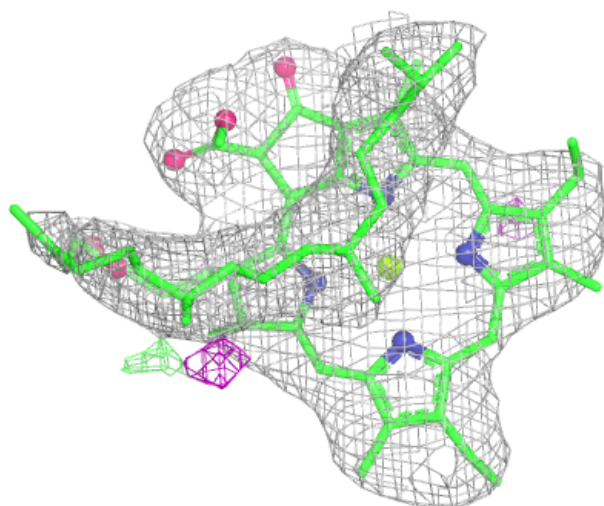
Electron density around BCR T 5104:

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



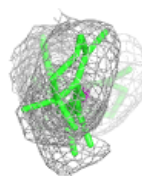
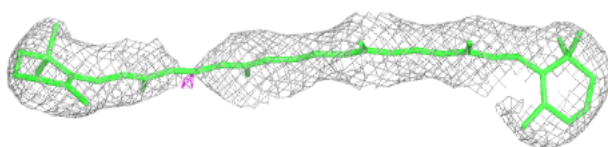
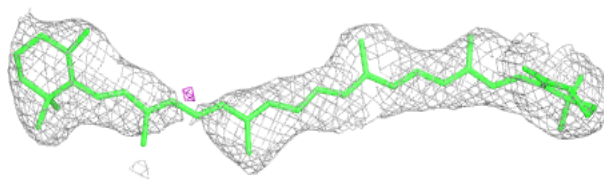
Electron density around CLA C 500:

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

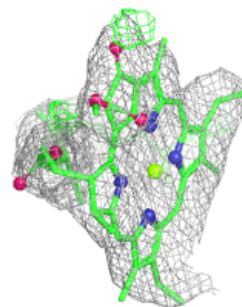
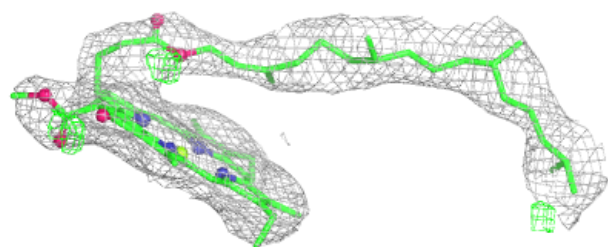
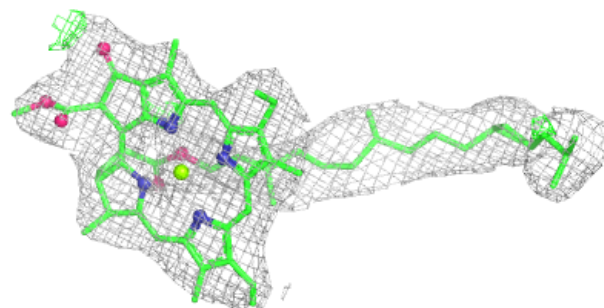


Electron density around BCR b 5527:

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

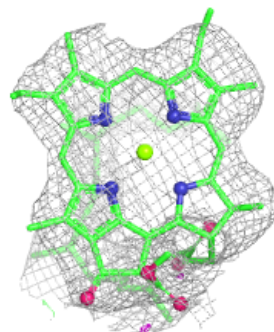
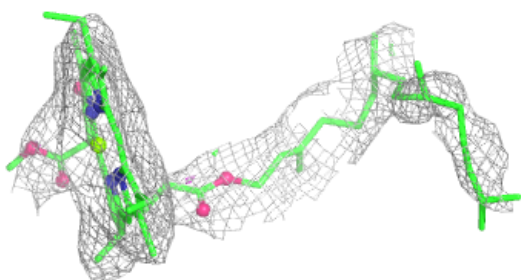
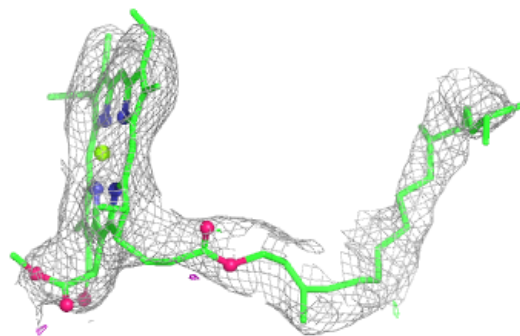
**Electron density around CLA B 518:**

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



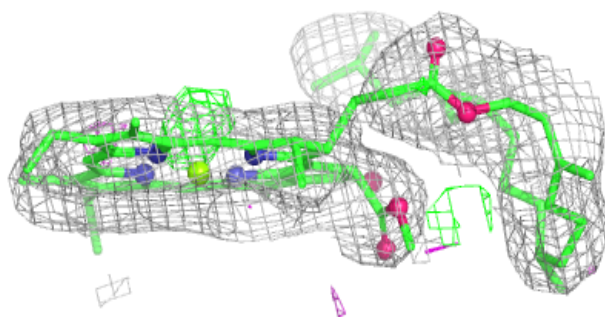
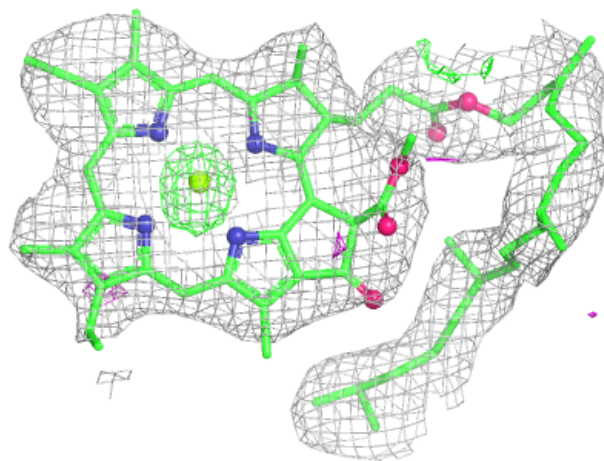
Electron density around CLA C 496:

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



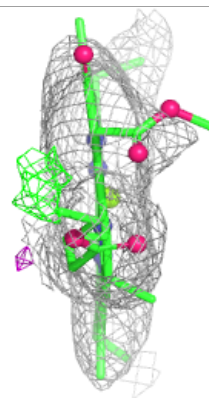
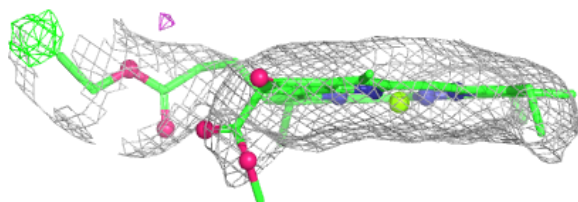
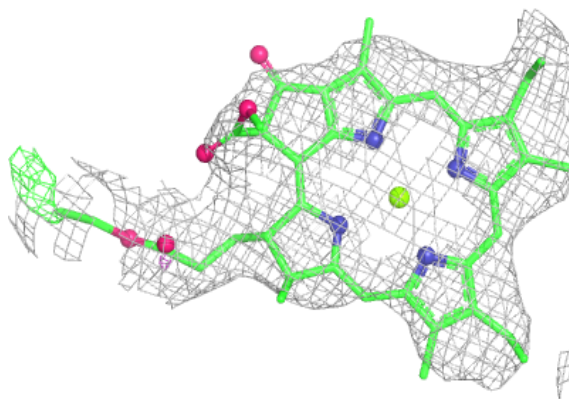
Electron density around CLA B 520:

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

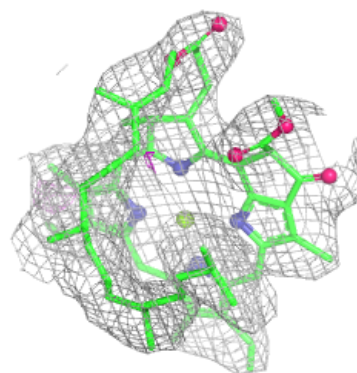
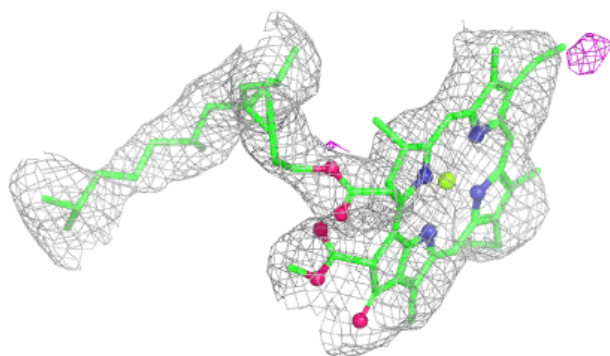
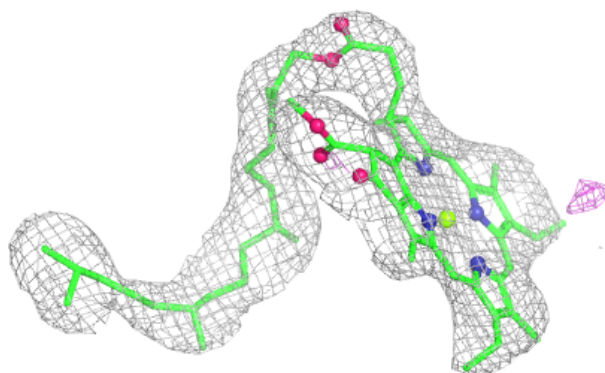


Electron density around CLA c 5499:

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

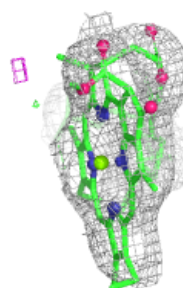
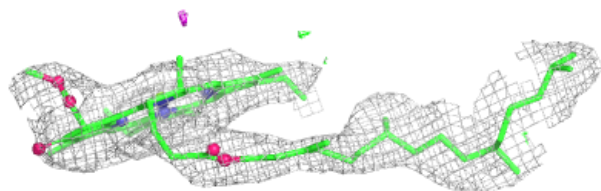
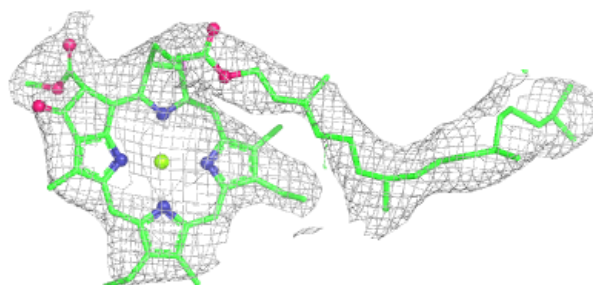
**Electron density around CLA b 5523:**

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

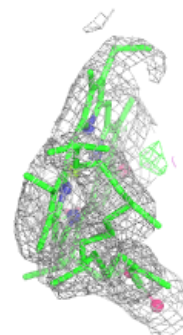
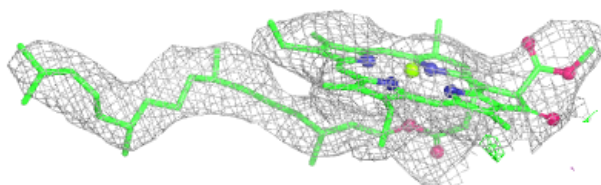
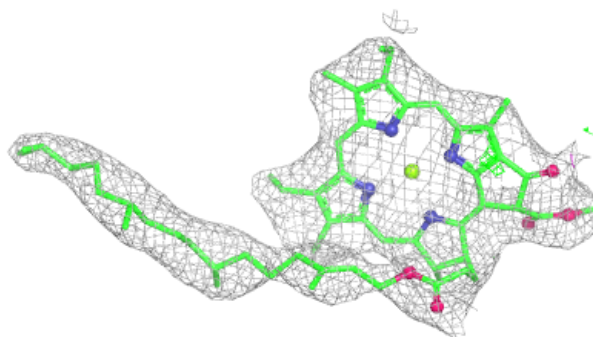


Electron density around CLA B 513:

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

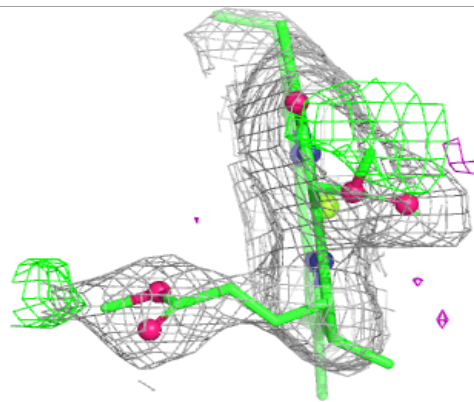
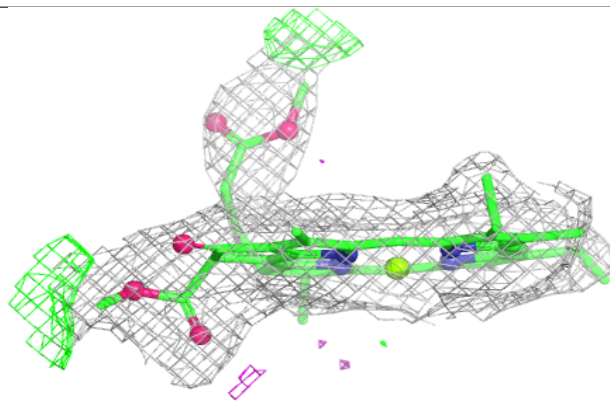
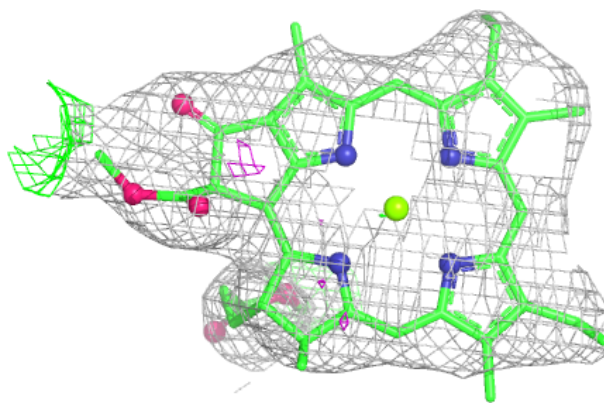
**Electron density around CLA C 491:**

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

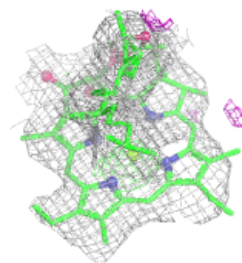
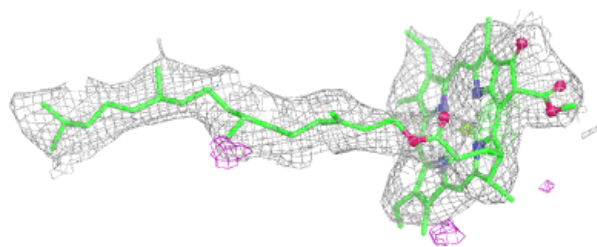
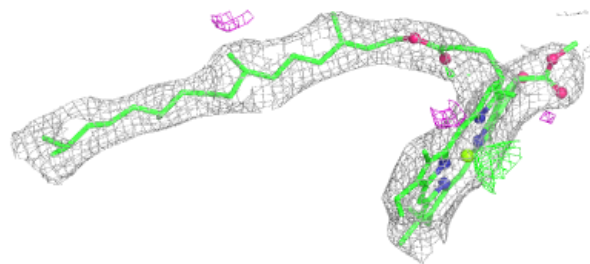


Electron density around CLA C 494:

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

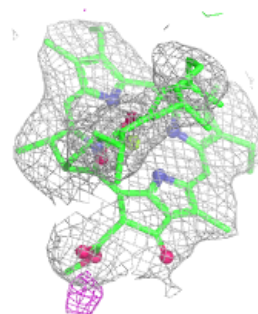
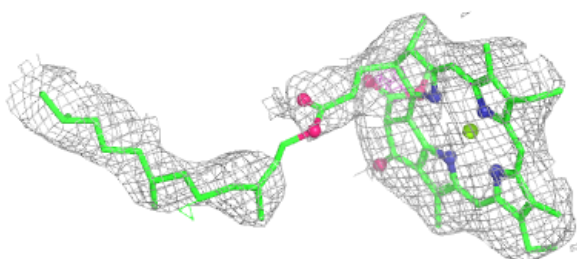
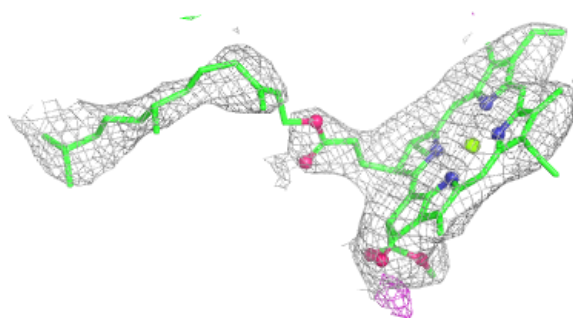
**Electron density around CLA b 5517:**

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

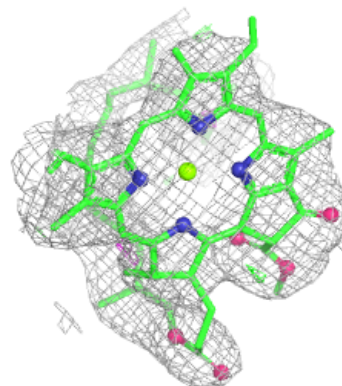
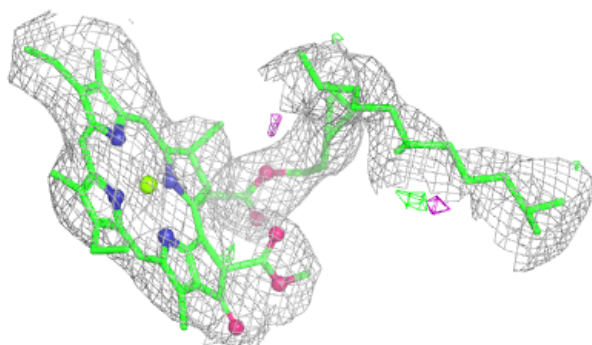
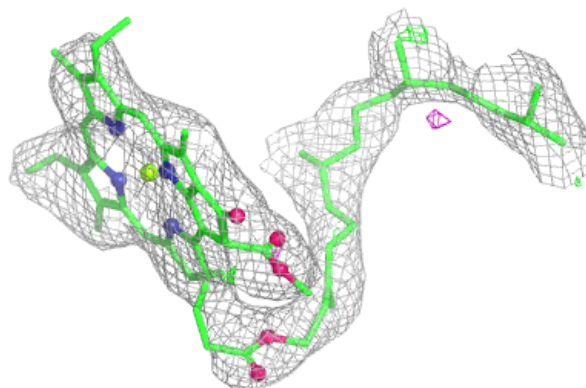


Electron density around CLA c 5492:

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

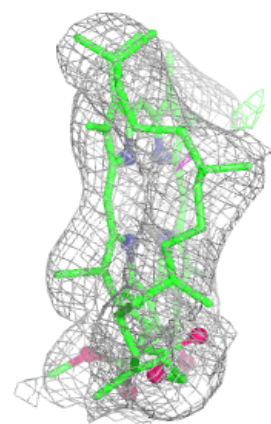
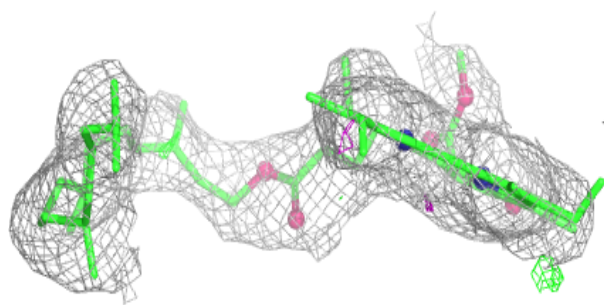
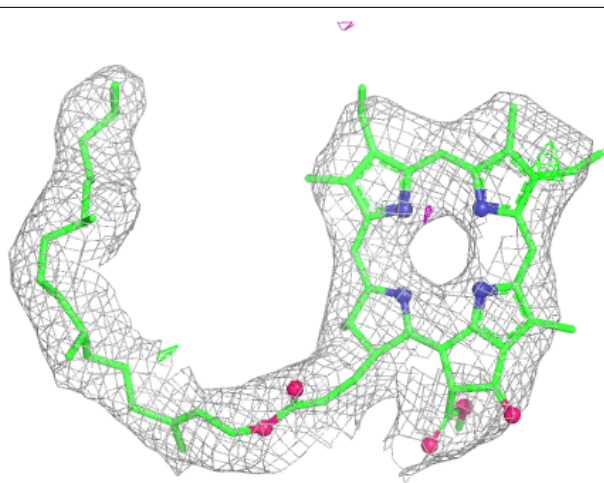
**Electron density around CLA B 523:**

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



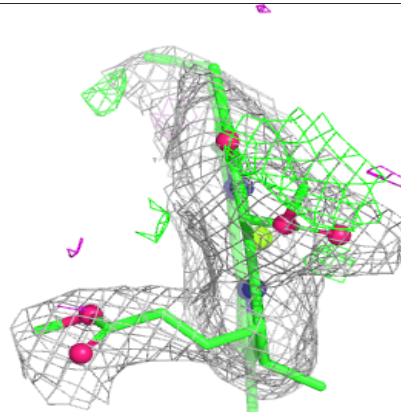
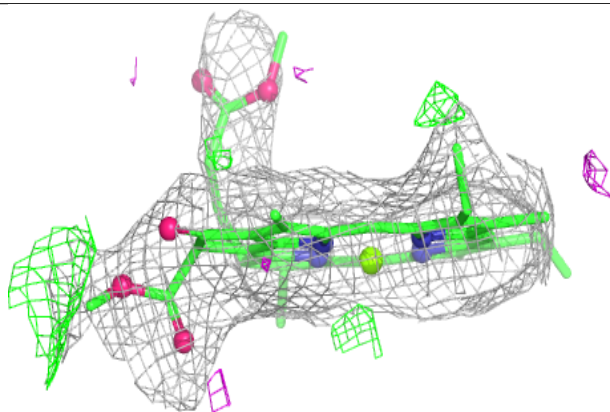
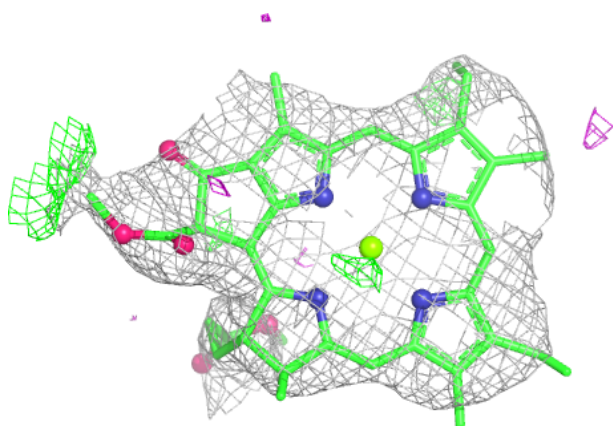
Electron density around PHO a 5561:

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

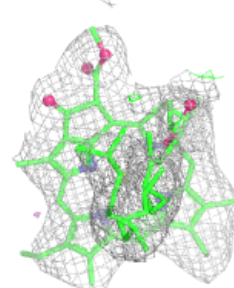
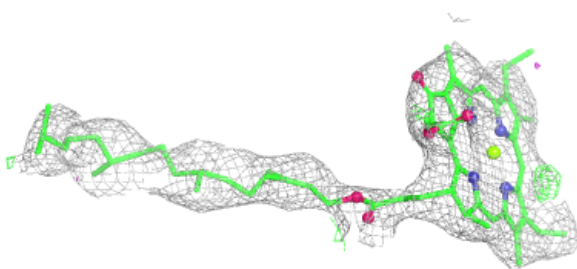
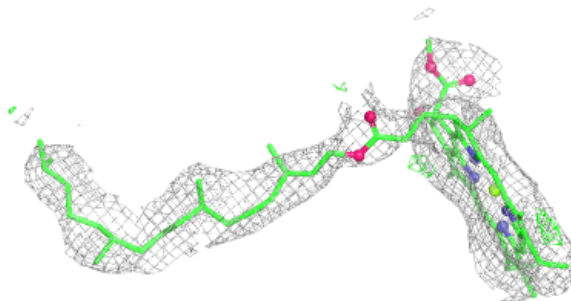


Electron density around CLA c 5494:

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

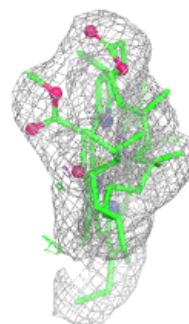
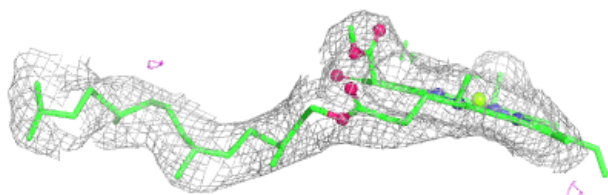
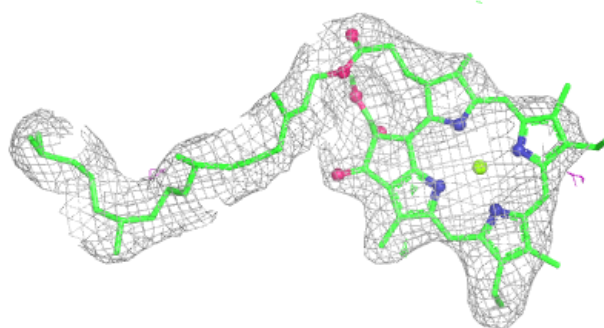
**Electron density around CLA B 514:**

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

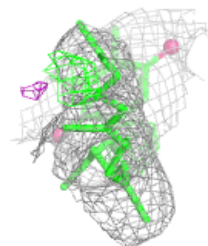
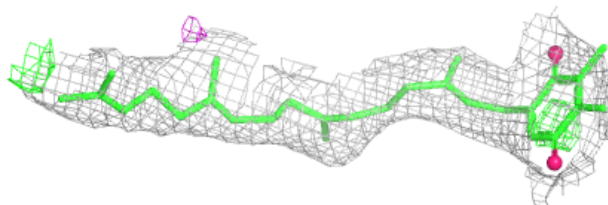
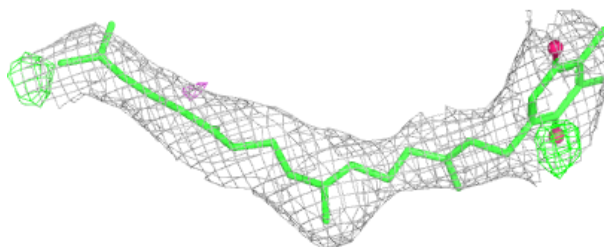


Electron density around CLA B 512:

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

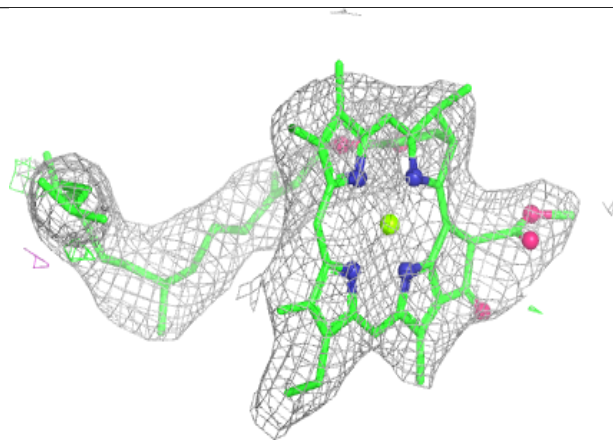
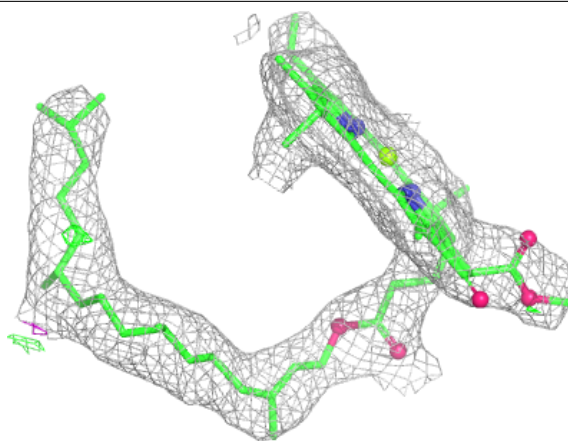
**Electron density around PQ9 d 5356:**

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



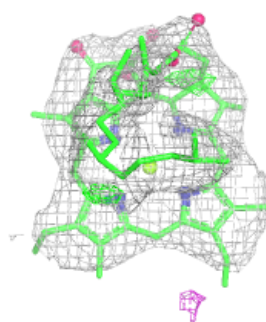
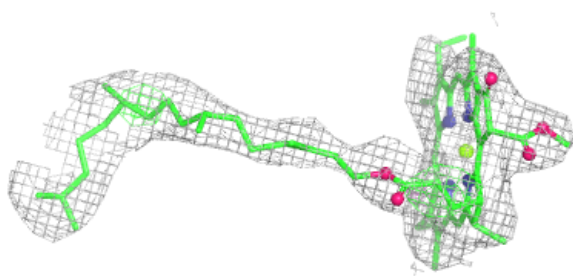
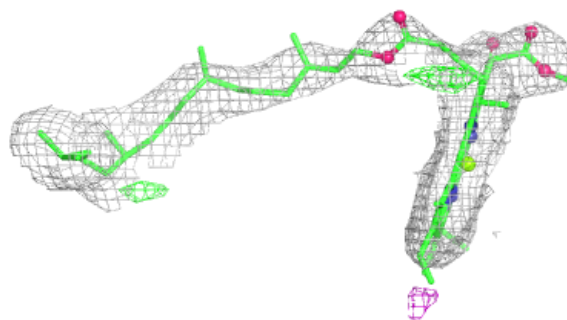
Electron density around CLA b 5521:

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



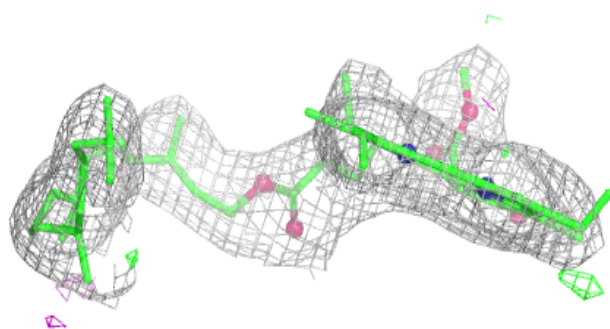
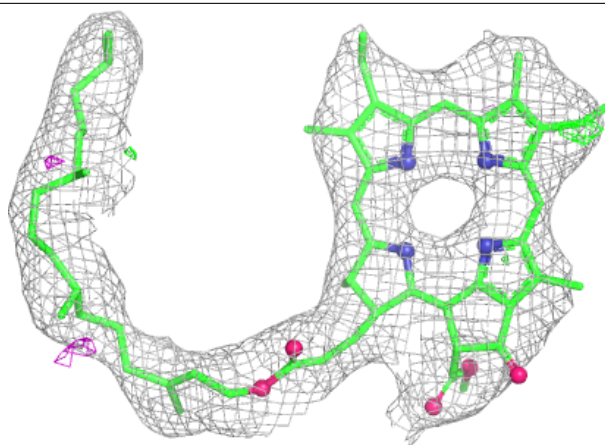
Electron density around CLA B 515:

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



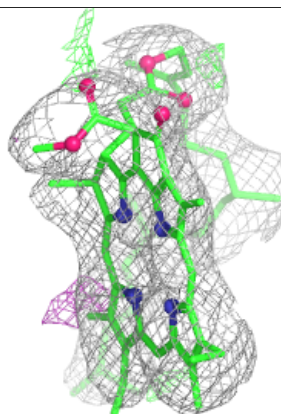
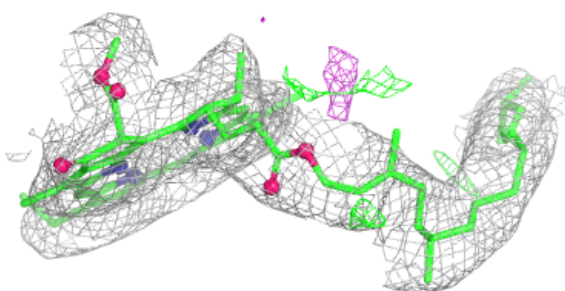
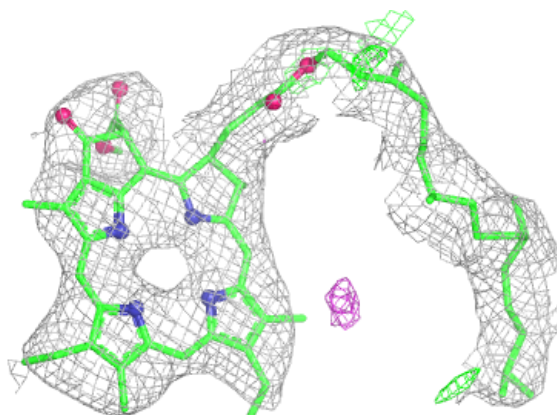
Electron density around PHO A 561:

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

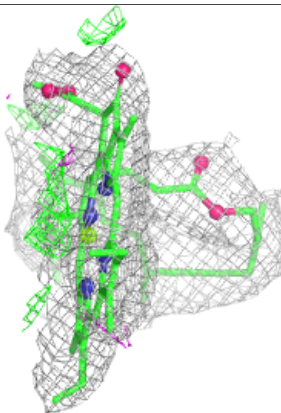
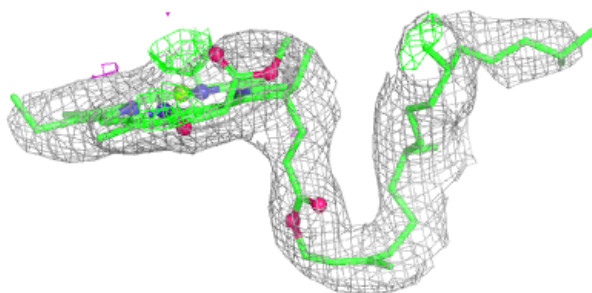
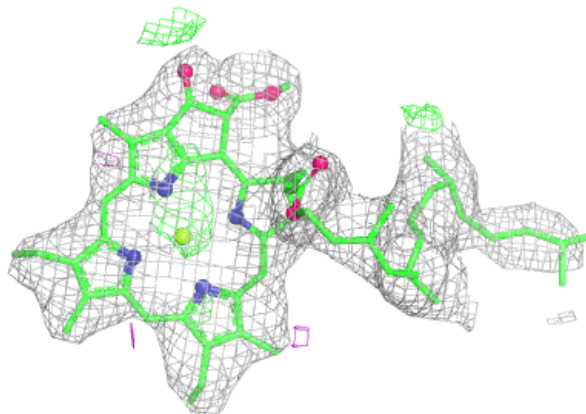


Electron density around PHO A 562:

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

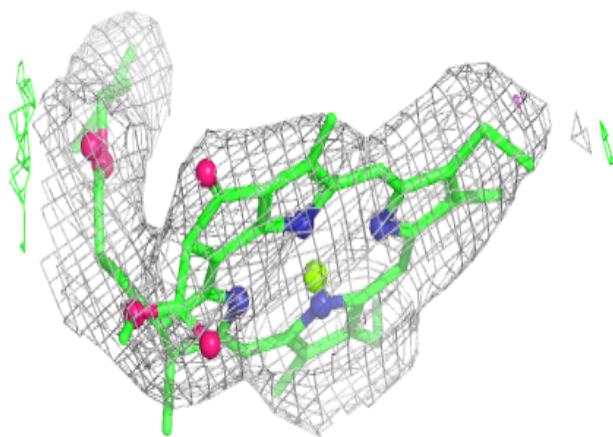
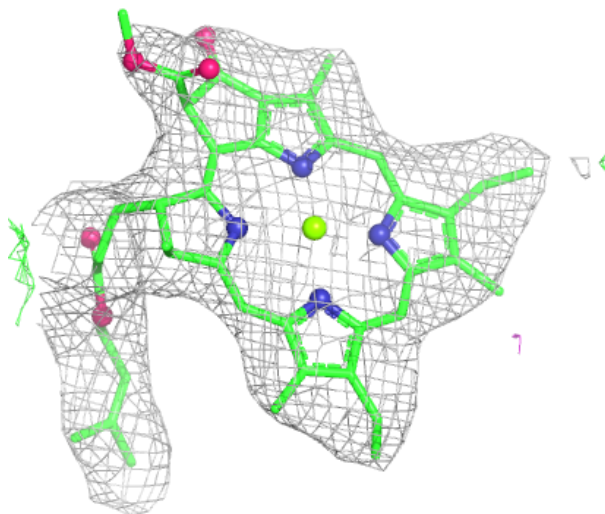
**Electron density around CLA A 560:**

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



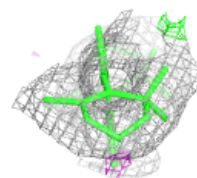
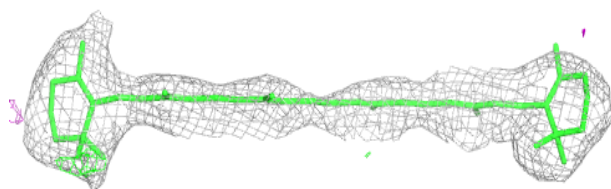
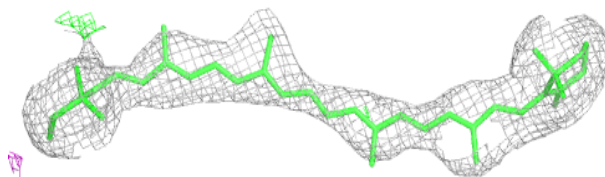
Electron density around CLA D 355:

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



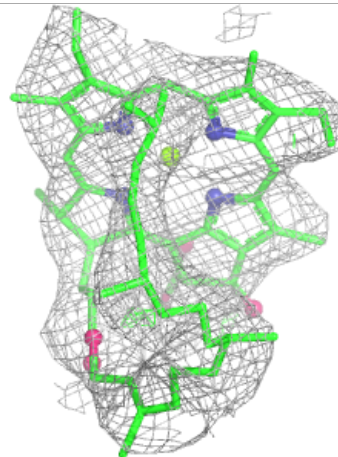
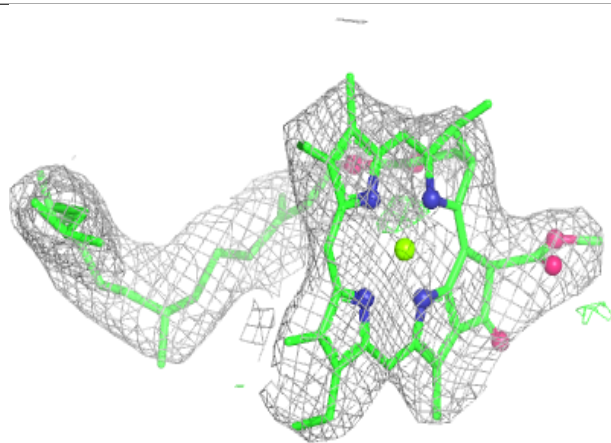
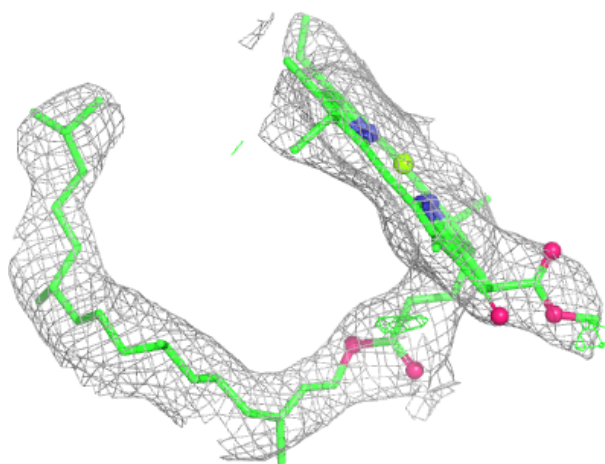
Electron density around BCR a 5566:

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



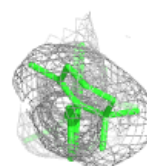
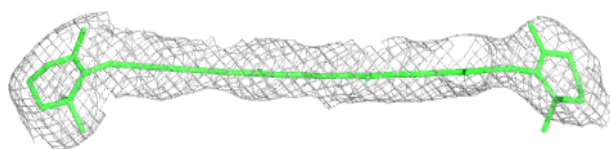
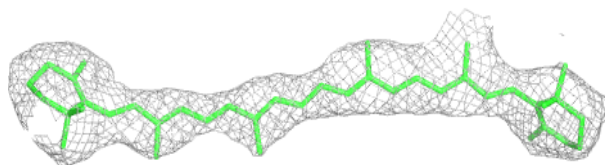
Electron density around CLA B 521:

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

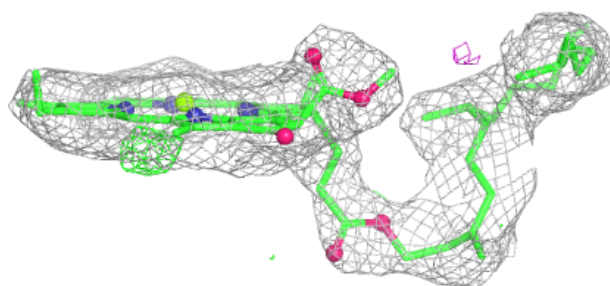
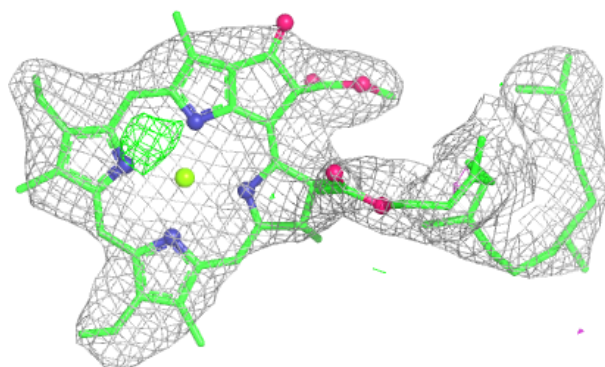


Electron density around BCR b 5528:

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

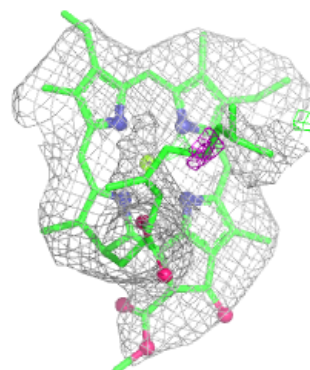
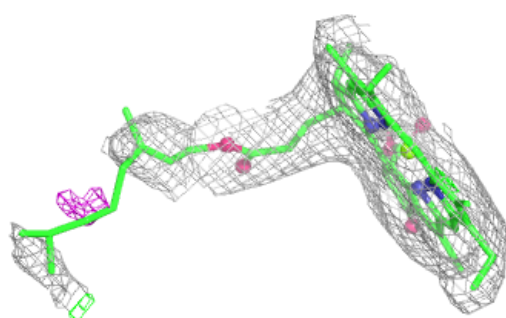
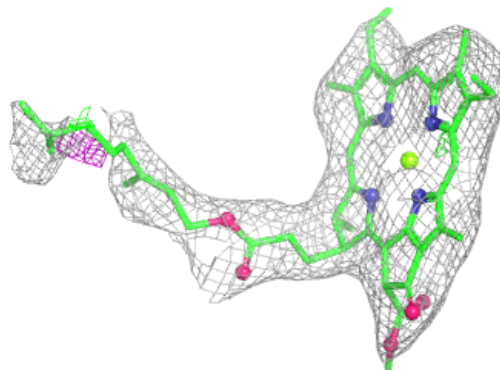
**Electron density around CLA b 5522:**

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

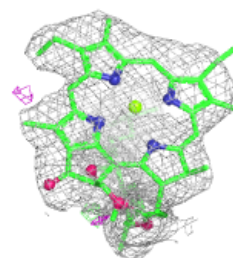
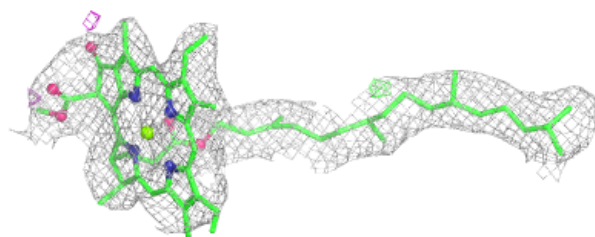
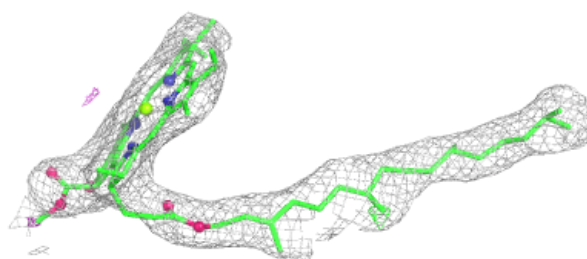


Electron density around CLA a 5563:

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

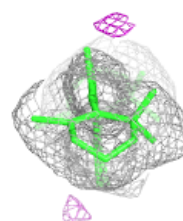
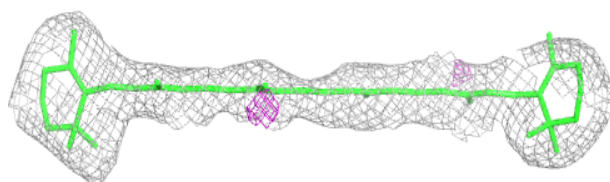
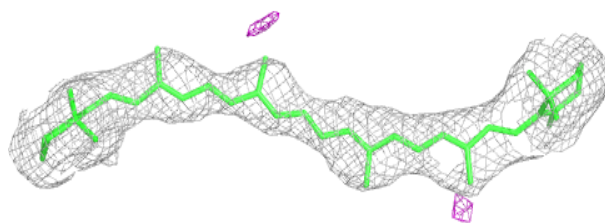
**Electron density around CLA B 517:**

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

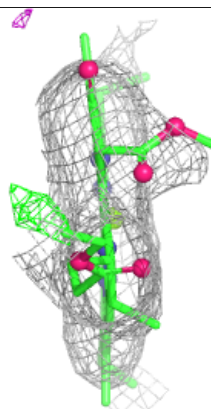
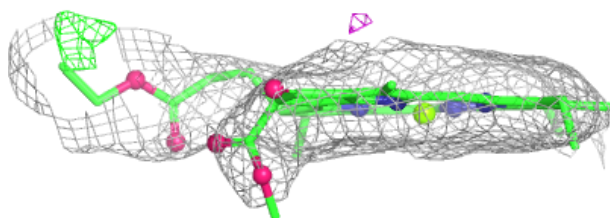
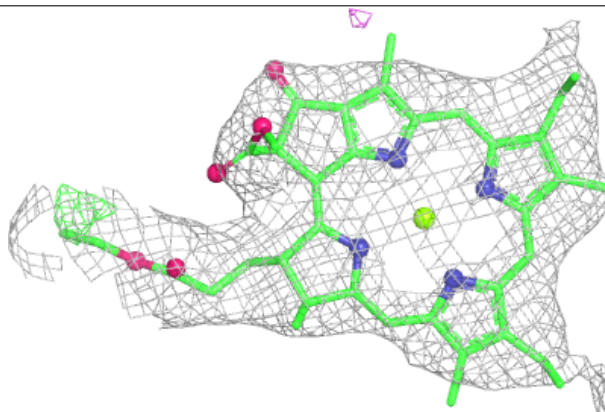


Electron density around BCR A 566:

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

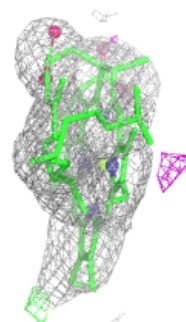
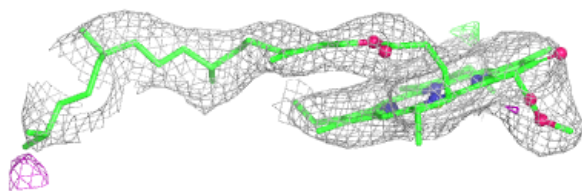
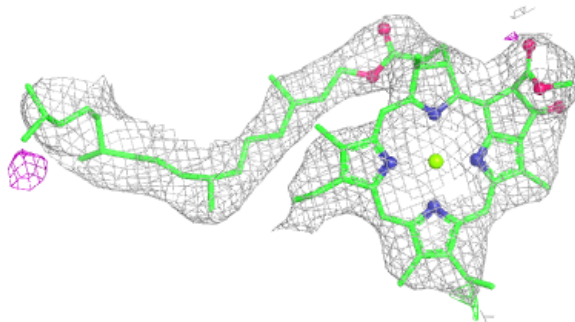
**Electron density around CLA C 499:**

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



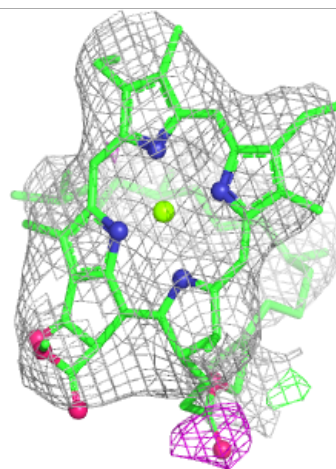
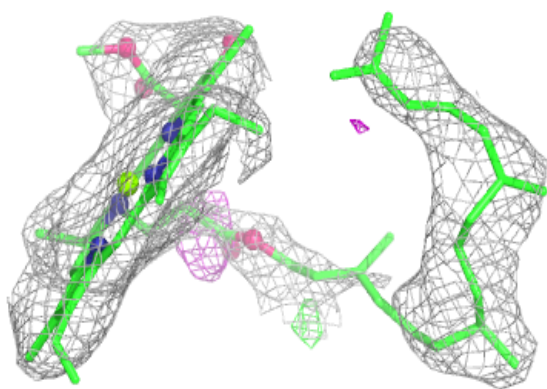
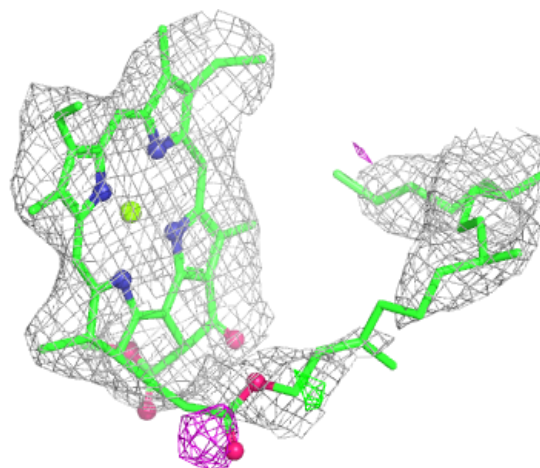
Electron density around CLA b 5513:

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



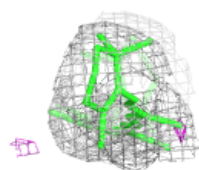
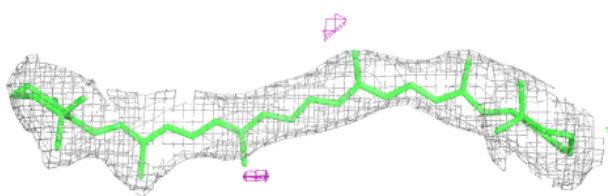
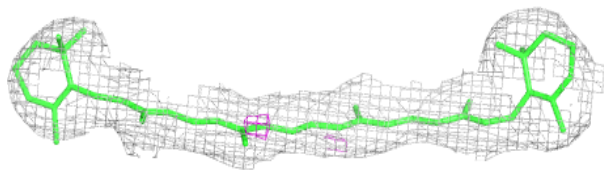
Electron density around CLA C 493:

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

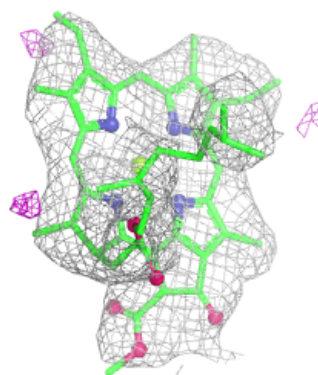
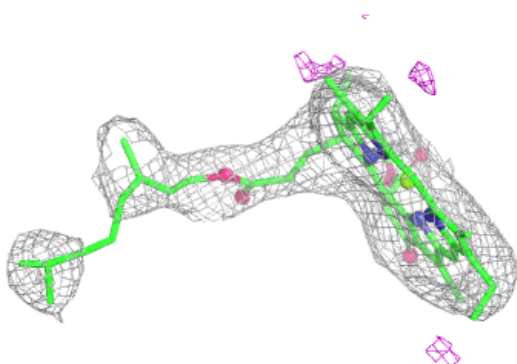
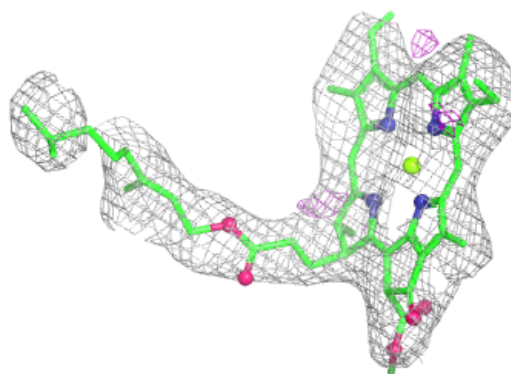


Electron density around BCR C 504:

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

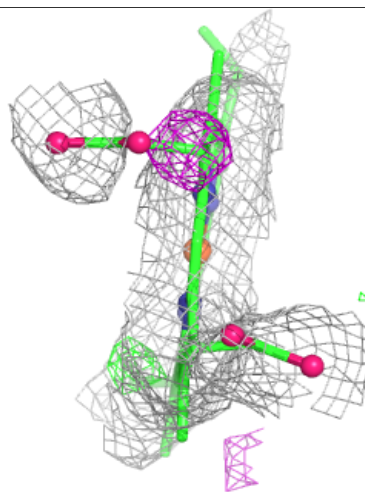
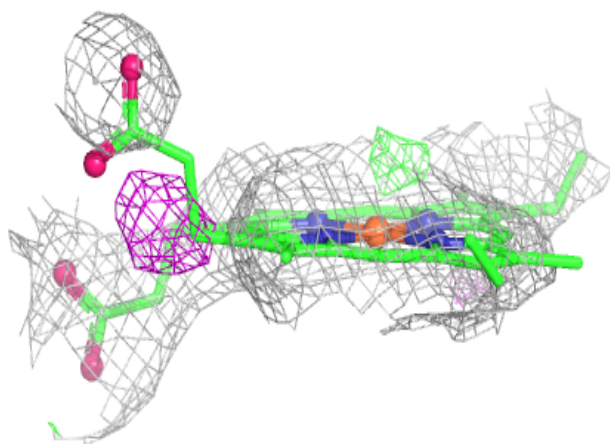
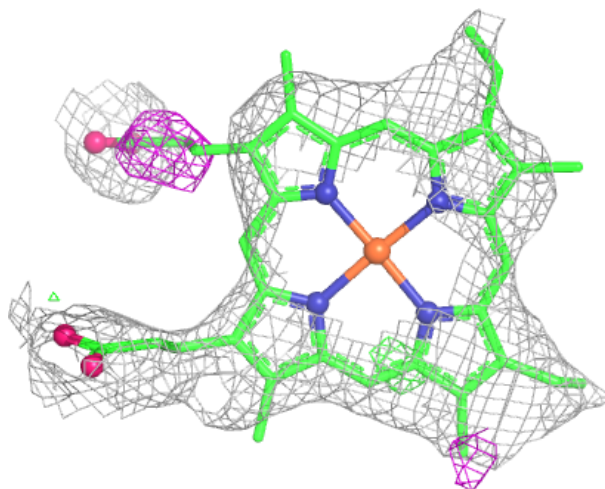
**Electron density around CLA A 563:**

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



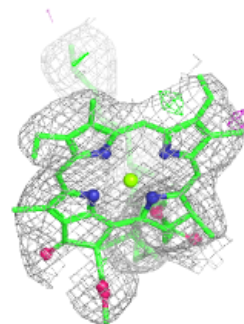
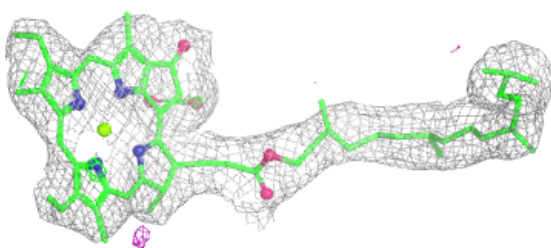
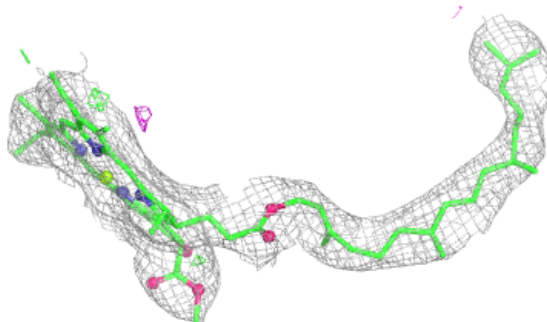
Electron density around HEM f 5051:

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

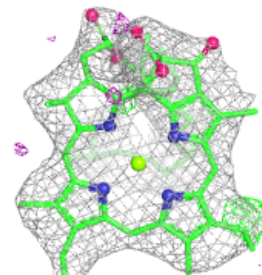
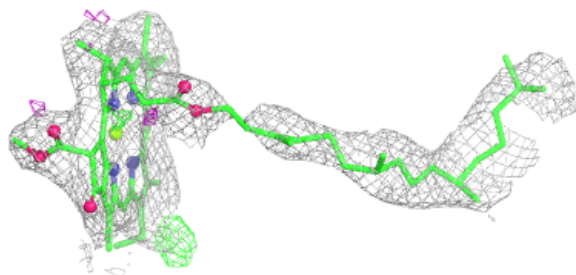
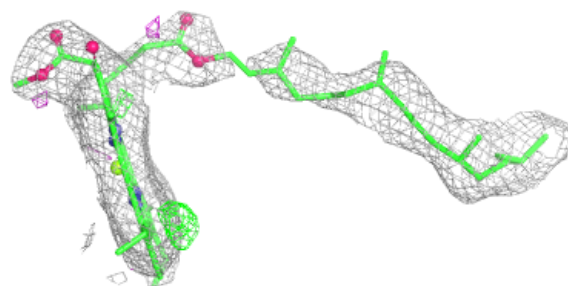


Electron density around CLA D 354:

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

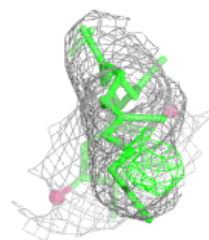
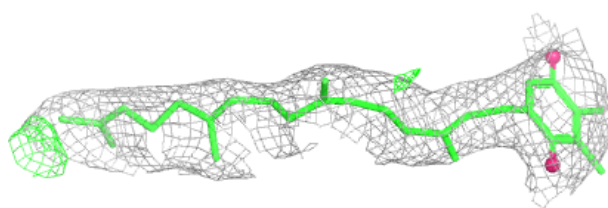
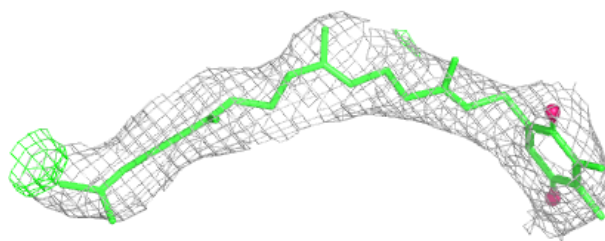
**Electron density around CLA b 5515:**

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

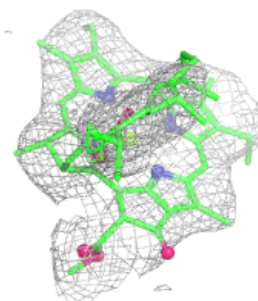
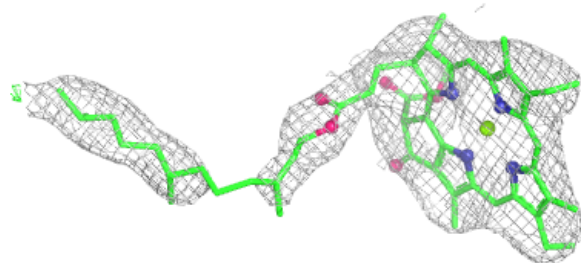
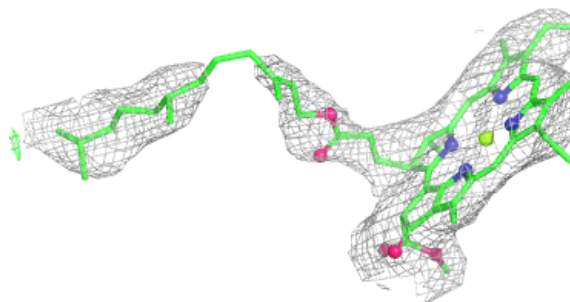


Electron density around PQ9 D 356:

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

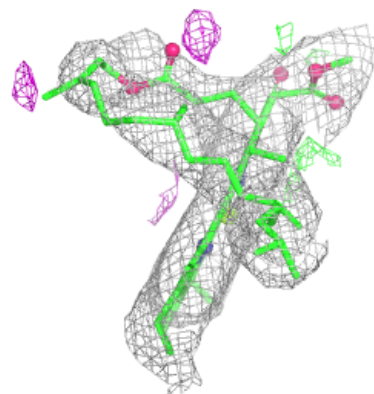
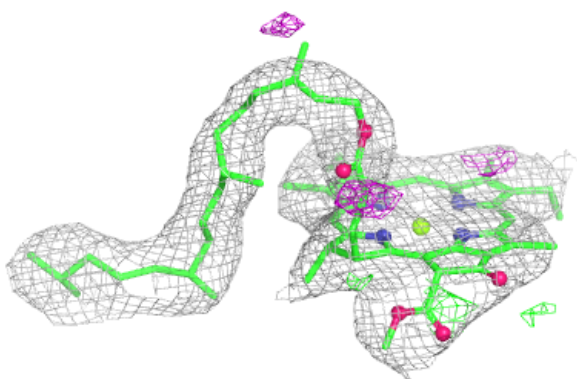
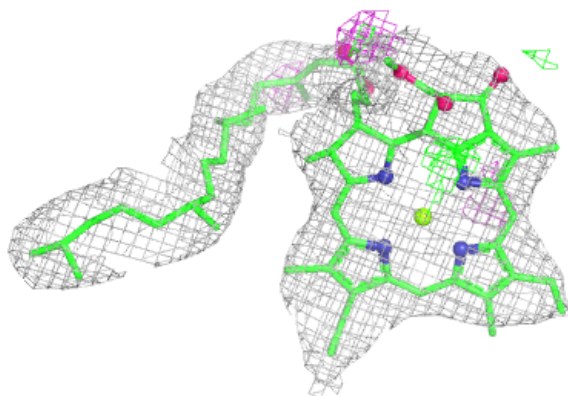
**Electron density around CLA C 492:**

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

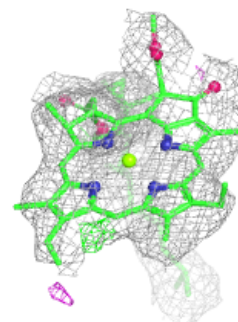
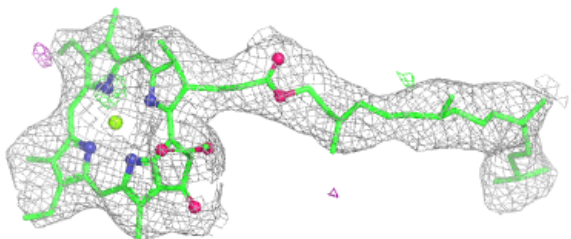
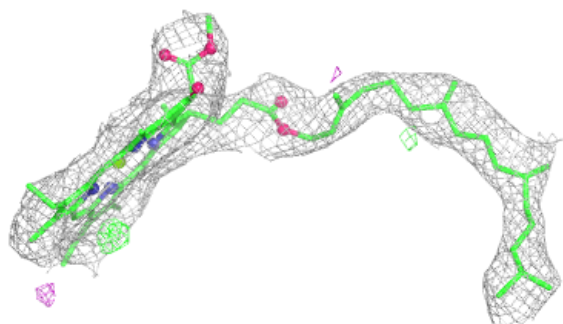


Electron density around CLA a 5559:

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

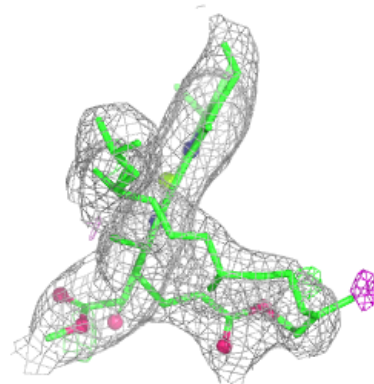
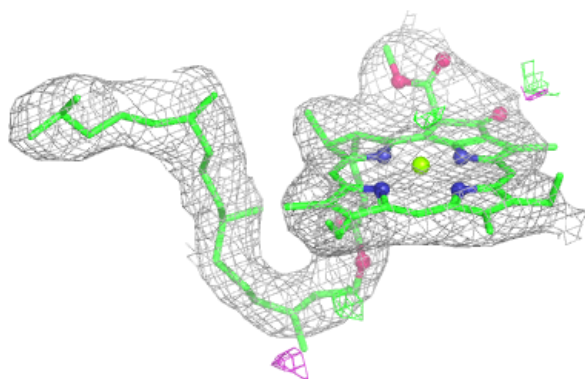
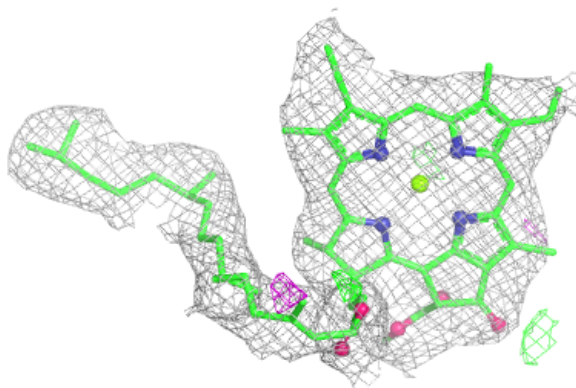
**Electron density around CLA d 5354:**

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

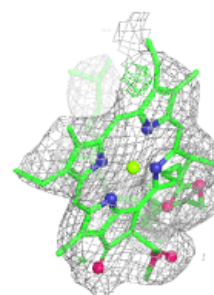
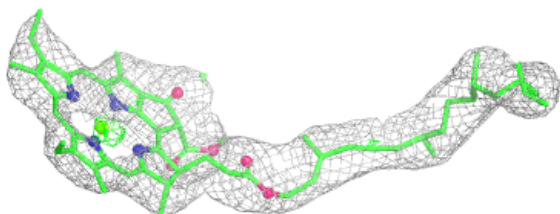
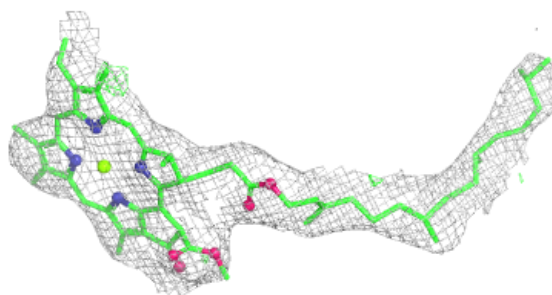


Electron density around CLA A 559:

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

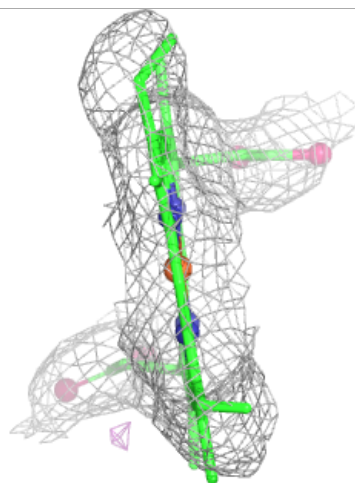
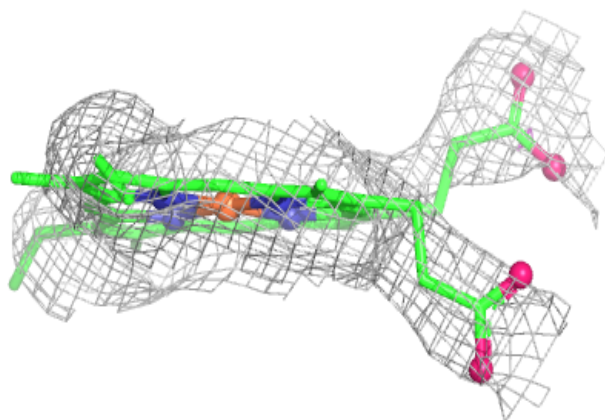
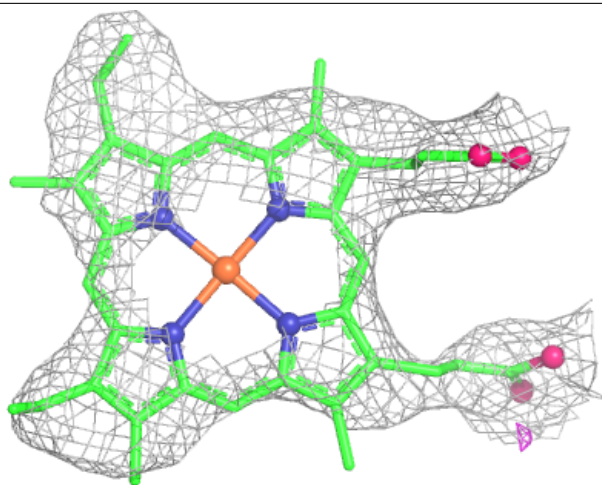
**Electron density around CLA a 5558:**

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



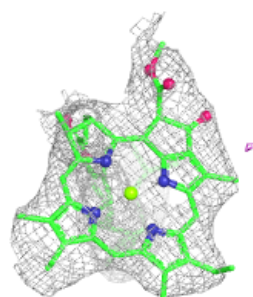
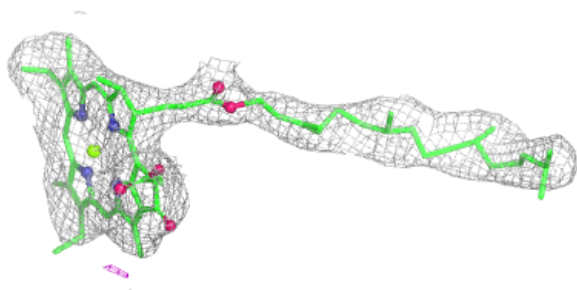
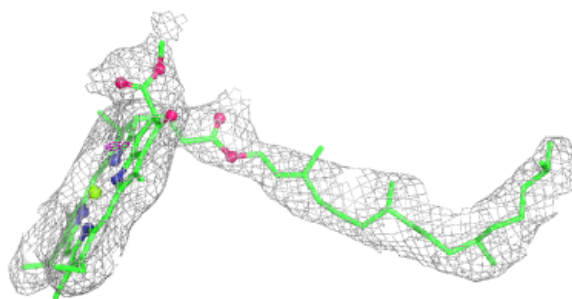
Electron density around HEM F 51:

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



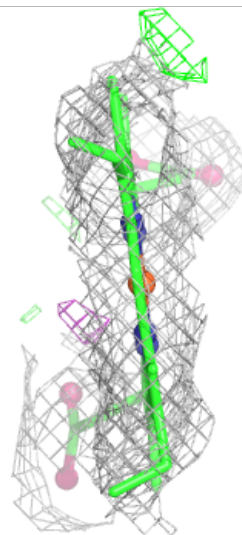
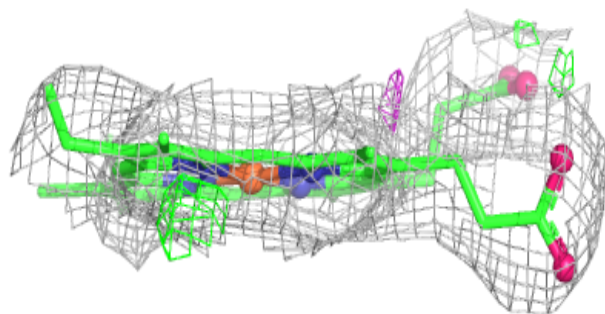
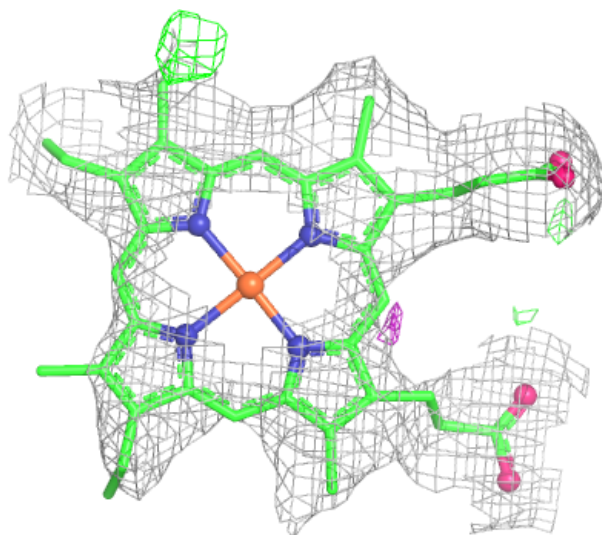
Electron density around CLA b 5514:

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



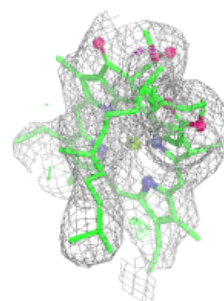
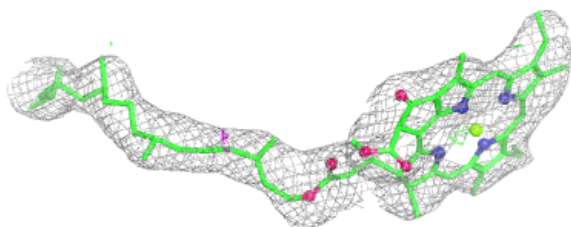
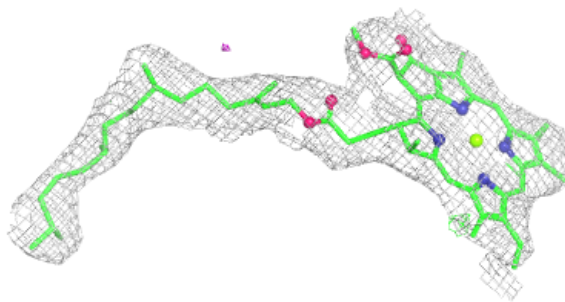
Electron density around HEM v 5552:

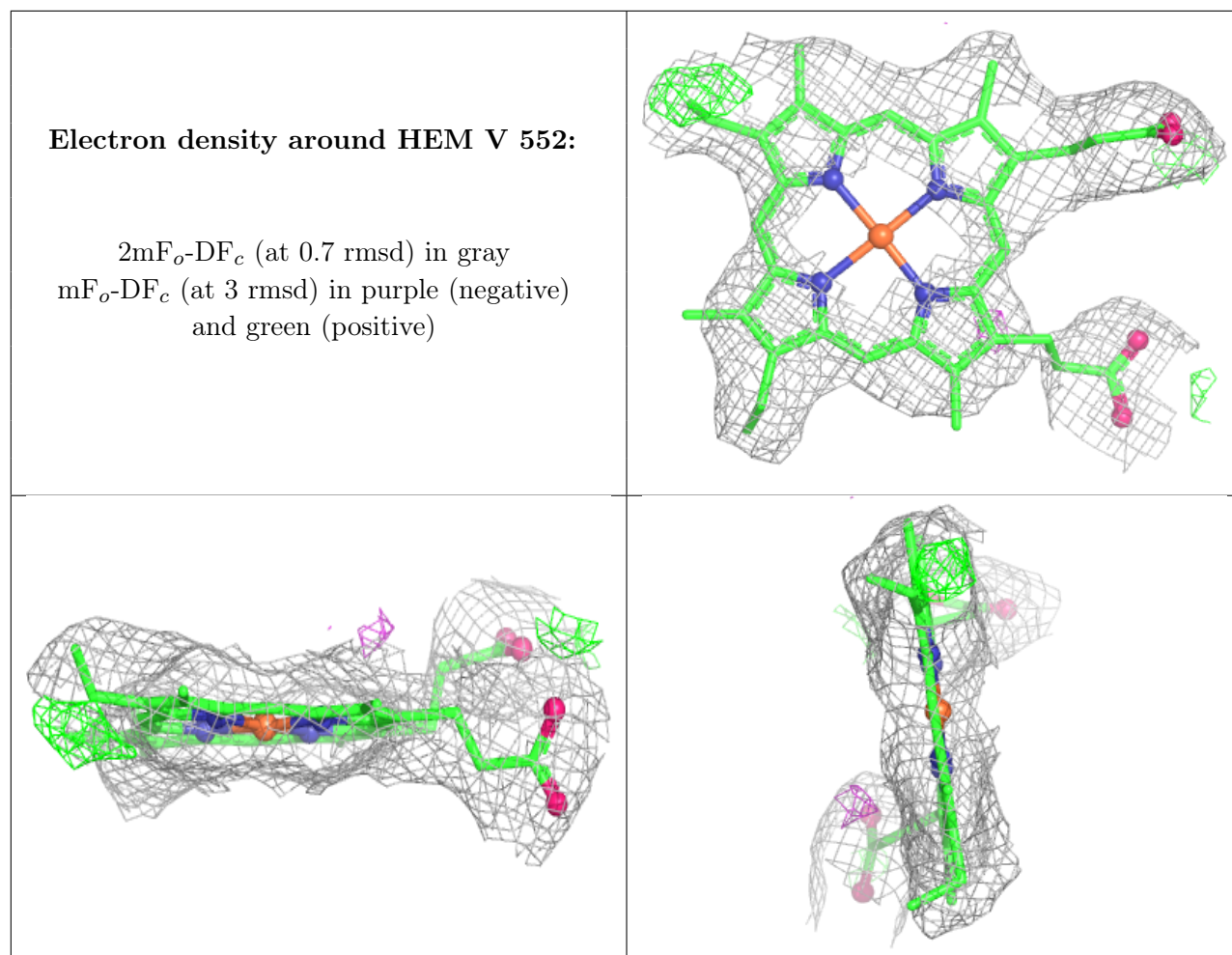
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.