



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 10:38 PM UTC

PDB ID : 2AXT / pdb_00002axt
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

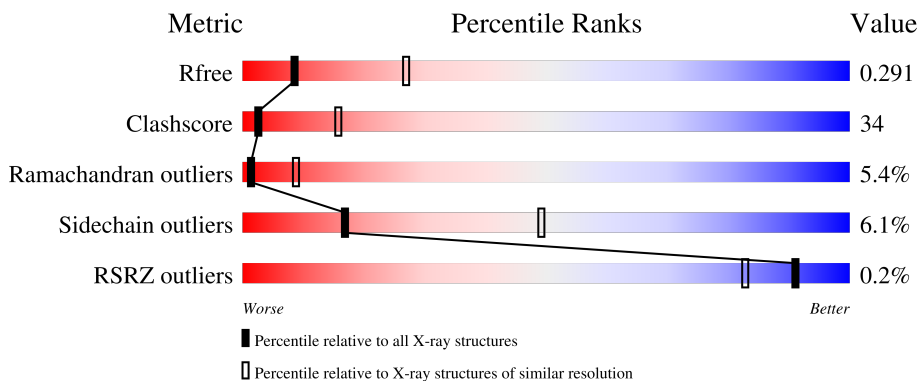
1 Overall quality at a glance

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.






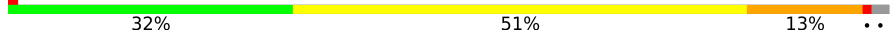
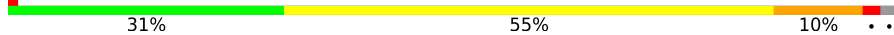
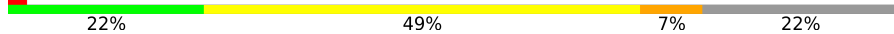
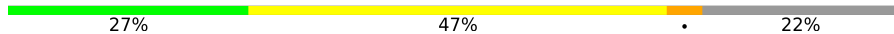
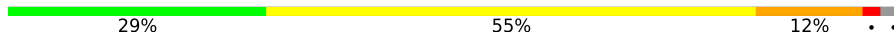
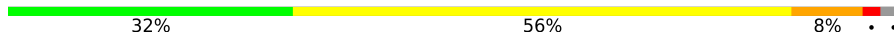
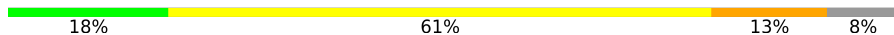
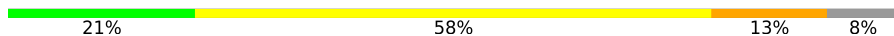
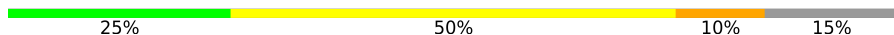
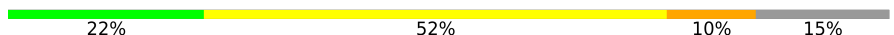
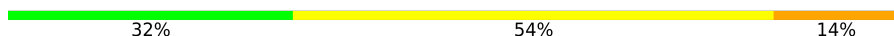











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	 39% 48% 9% . .
1	a	344	 37% 48% 11% . .
2	B	510	 50% 38% 7% . .
2	b	510	 48% 40% 7% . .
3	C	473	 37% 48% 9% . 5%

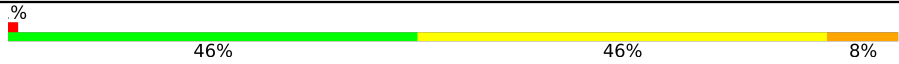
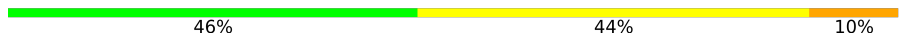


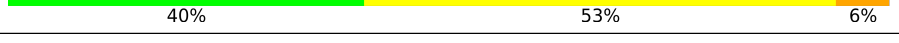
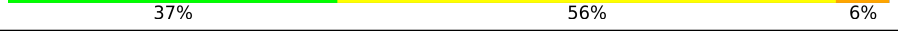
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Mol	Chain	Length	Quality of chain
3	c	473	 36% 48% 9% 5%
4	D	352	 40% 46% 10% ..
4	d	352	 40% 46% 9% ..
5	E	84	 32% 51% 13% ..
5	e	84	 31% 55% 10% ..
6	F	45	 22% 49% 7% 22%
6	f	45	 27% 47% 22%
7	H	66	 29% 55% 12% ..
7	h	66	 32% 56% 8% ..
8	I	38	 18% 61% 13% 8%
8	i	38	 21% 58% 13% 8%
9	J	40	 25% 50% 10% 15%
9	j	40	 22% 52% 10% 15%
10	K	37	 32% 54% 14%
10	k	37	 32% 54% 11% .
11	L	37	 57% 30% 14%
11	l	37	 54% 32% 11% .
12	M	36	 58% 36% 6%
12	m	36	 56% 39% 6%
13	O	247	 37% 49% 11% ..
13	o	247	 37% 50% 10% ..
14	T	32	 41% 44% 9% 6%
14	t	32	 44% 41% 9% 6%
15	U	104	 36% 50% 9% 6%
15	u	104	 39% 47% 8% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	-
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	X	-	-	-
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 [i](#)

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
			Total	C	N	O	S			
1	A	335	2623	1718	432	458	15	0	0	0
1	a	335	2623	1718	432	458	15	0	0	0

- Molecule 2 is a protein called CP47 protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

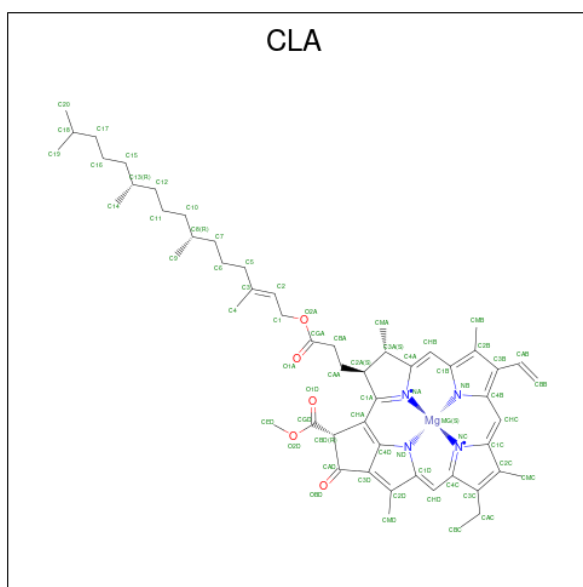
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

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 (CCD ID: 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 (CCD ID: 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		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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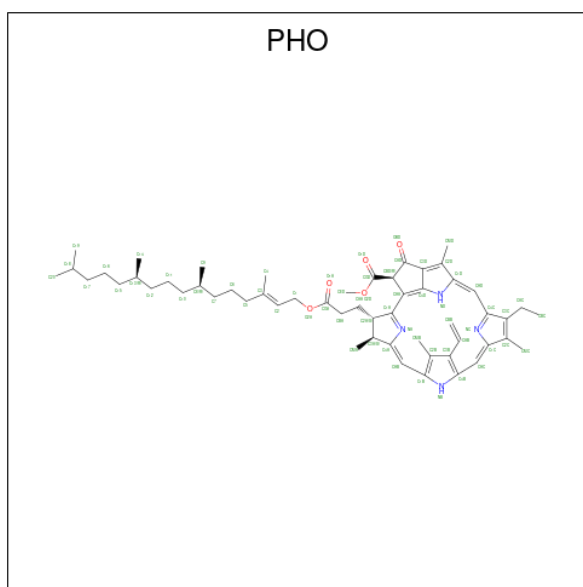
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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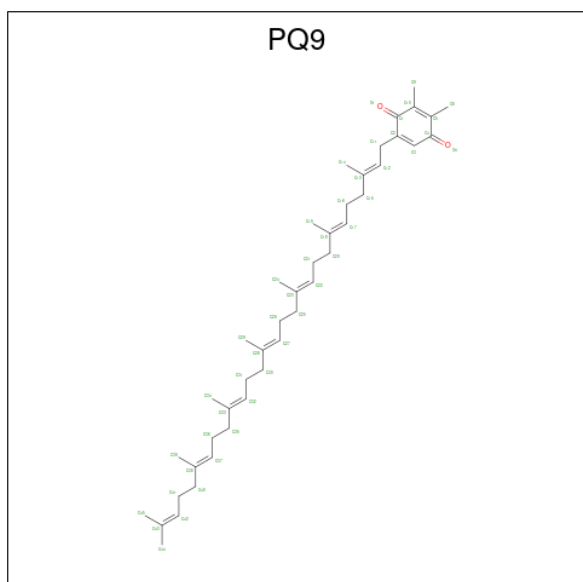
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



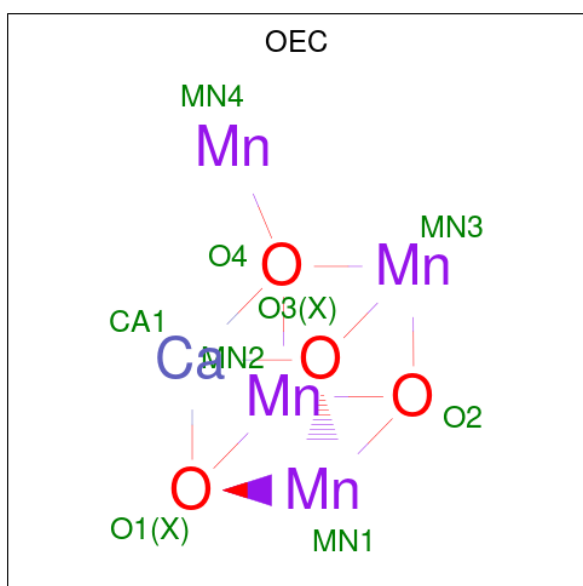
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
21	A	1	64	55	4	5	0	0
21	A	1	64	55	4	5	0	0
21	a	1	64	55	4	5	0	0
21	a	1	64	55	4	5	0	0

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACO SA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂).



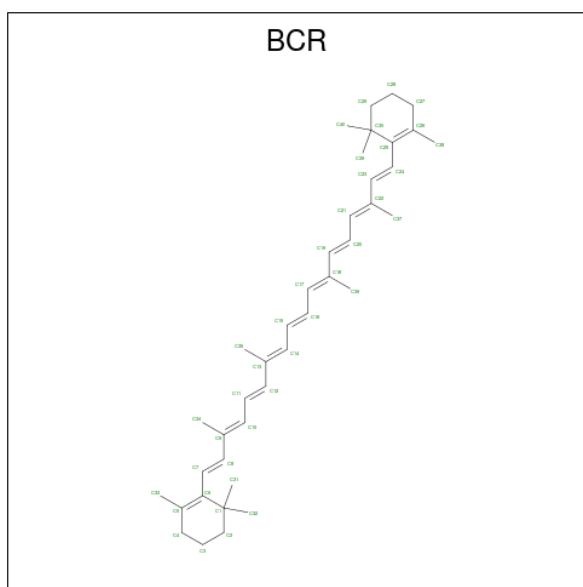
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (CCD ID: 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 (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



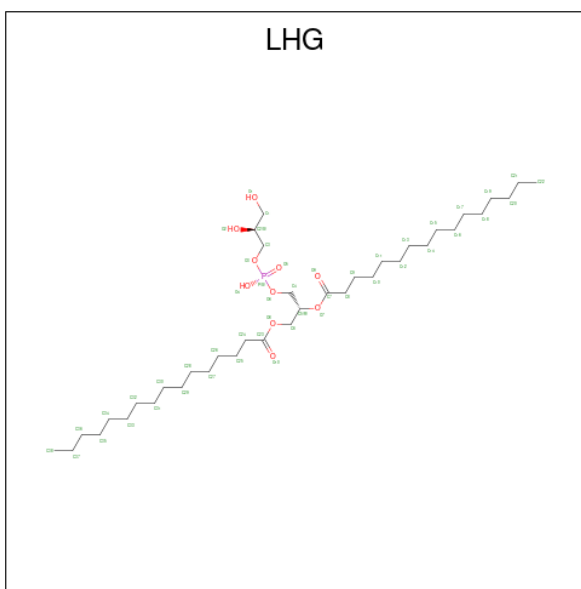
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total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

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

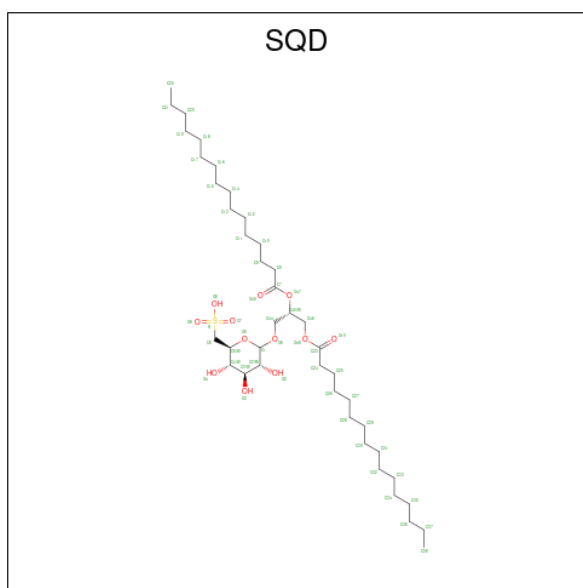
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

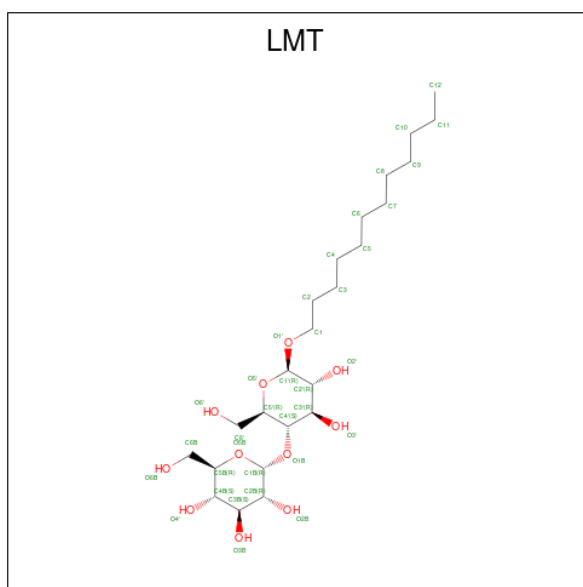
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



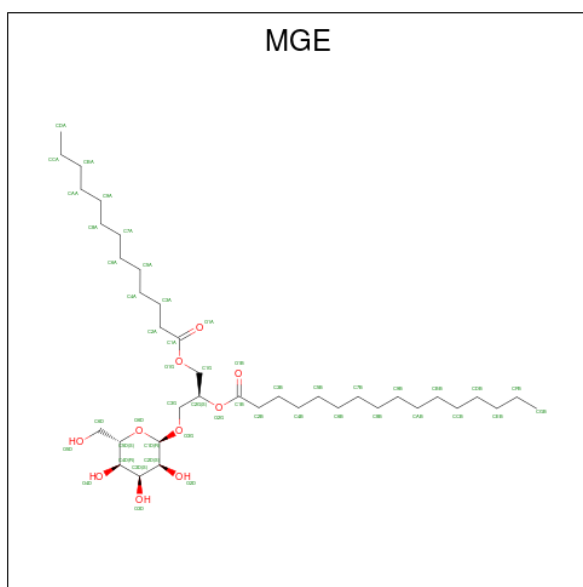
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀).

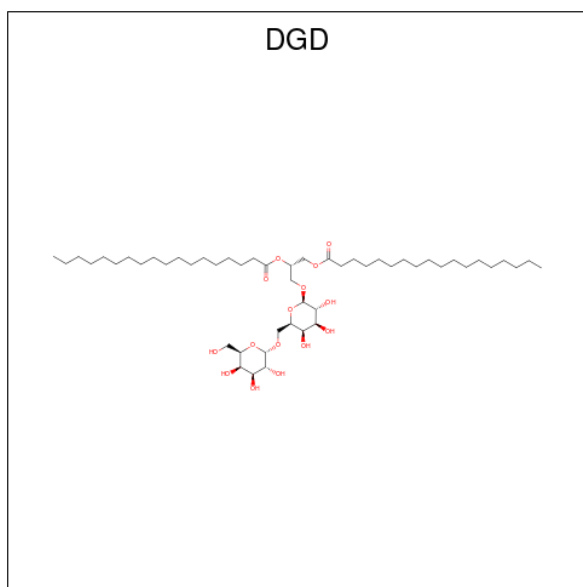


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total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

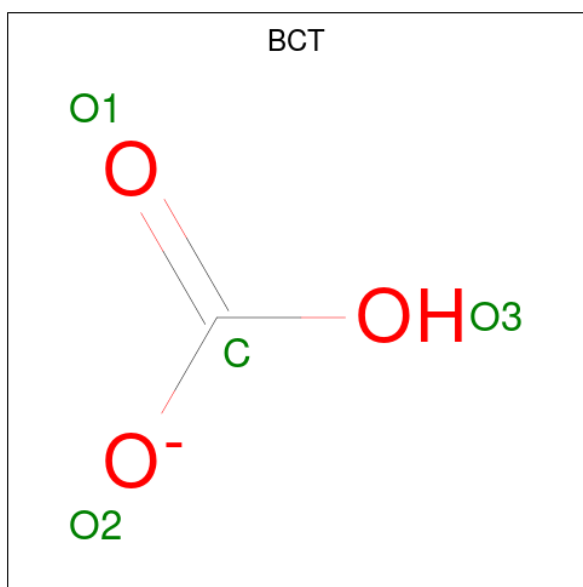
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

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



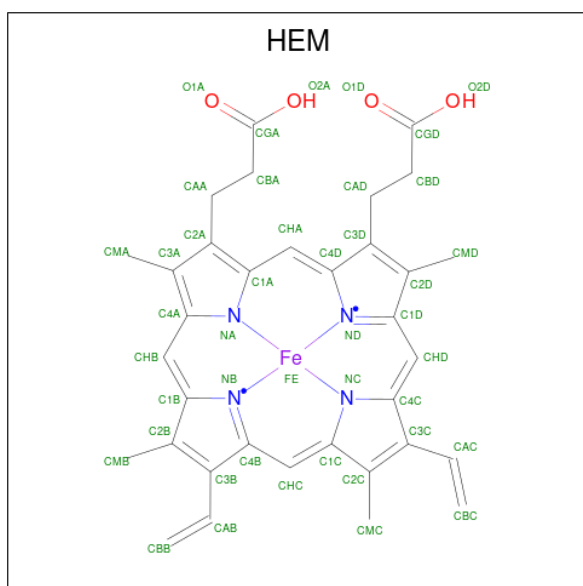
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total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

- Molecule 31 is BICARBONATE ION (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

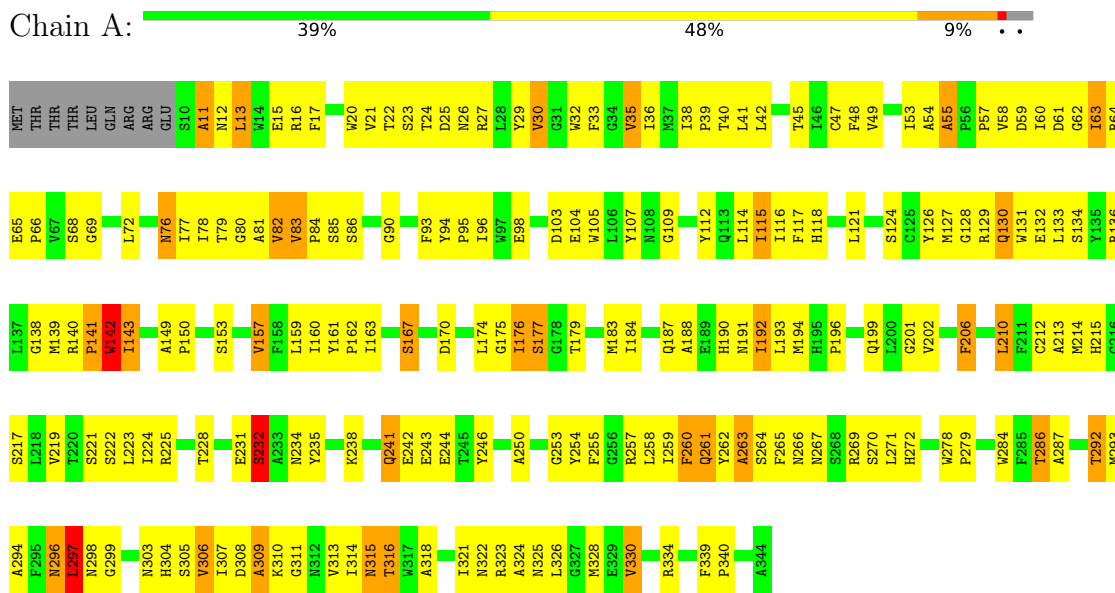
- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

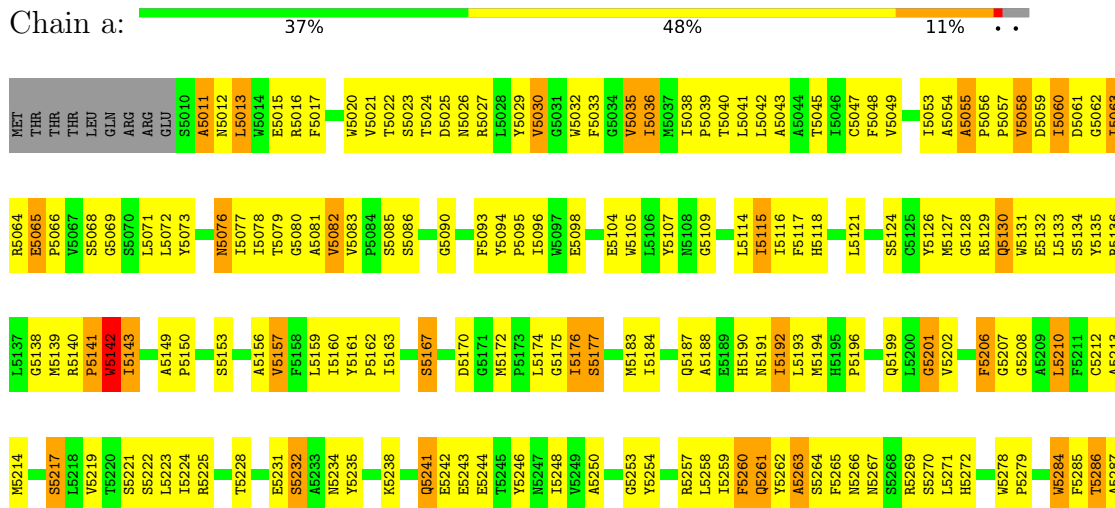
3 Residue-property plots

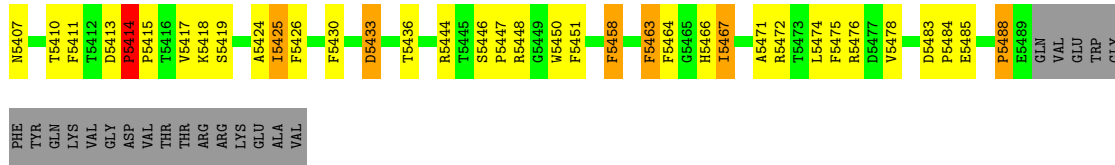
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

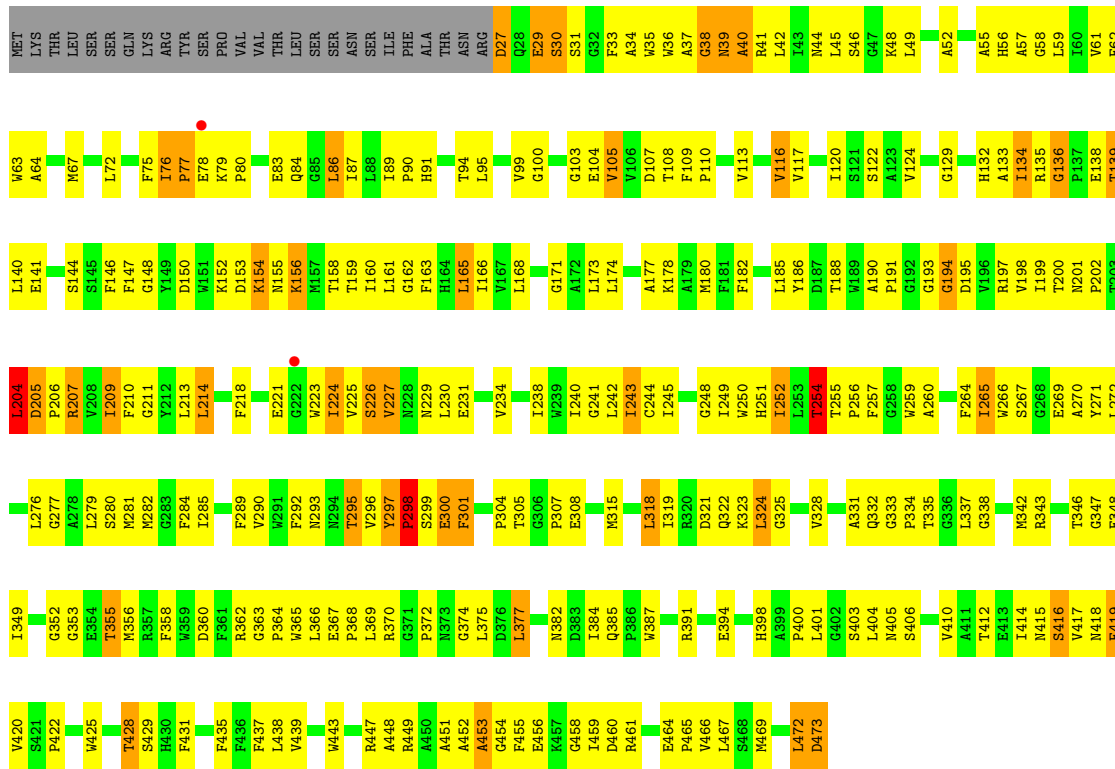
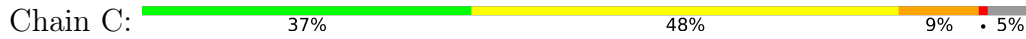


- Molecule 1: Photosystem Q(B) protein

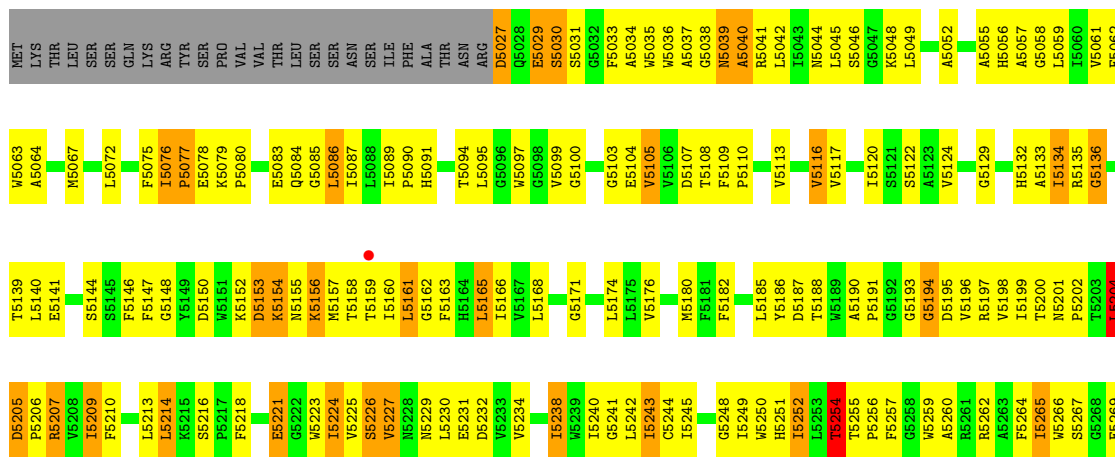
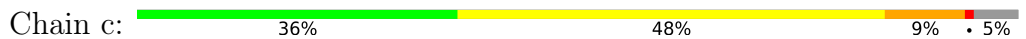


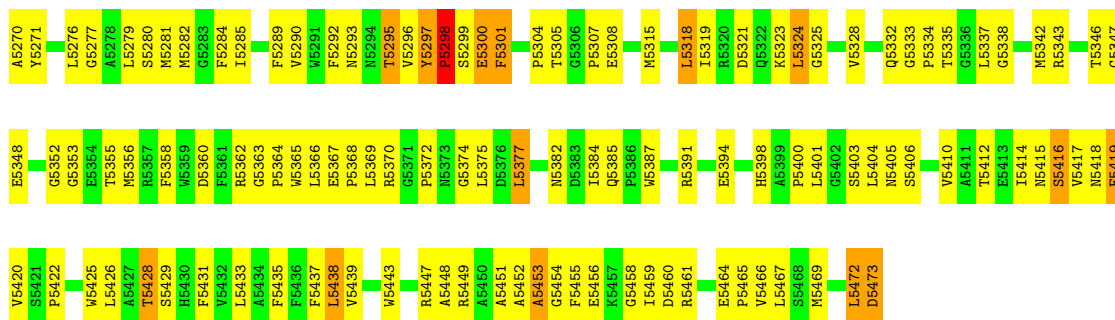


● Molecule 3: photosystem II CP43 protein

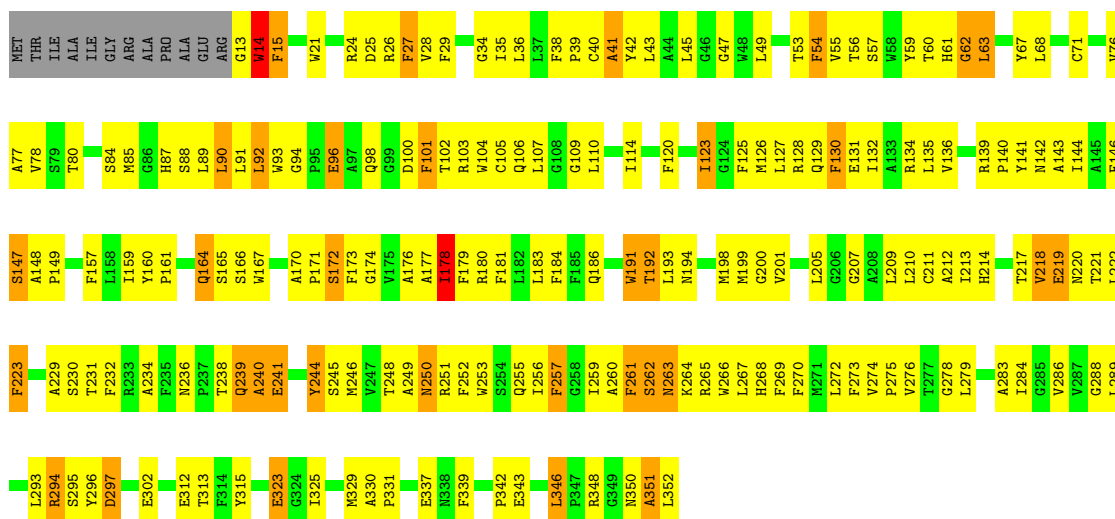


● Molecule 3: photosystem II CP43 protein

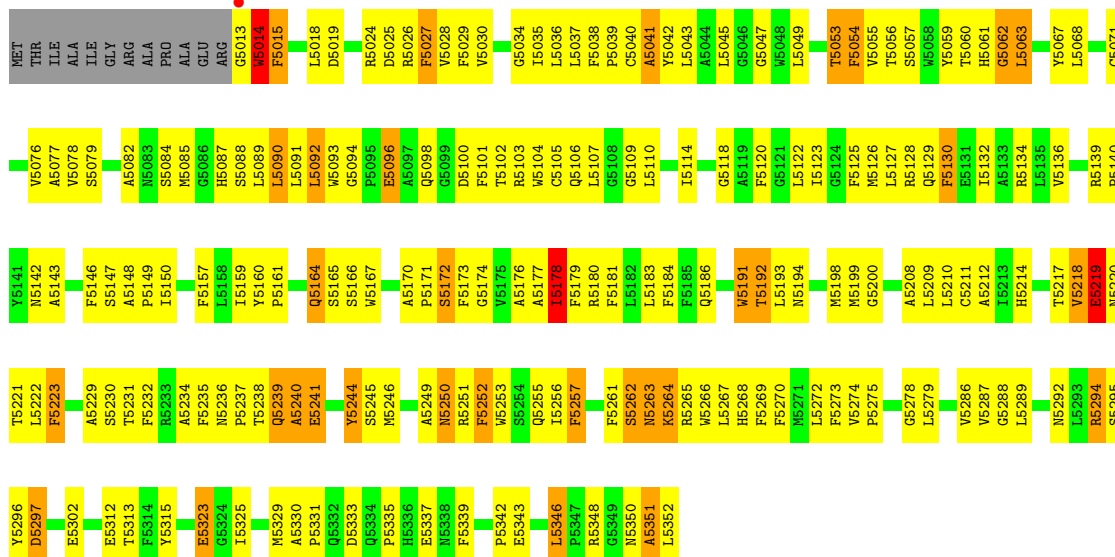




• Molecule 4: photosystem II reaction center D2 protein



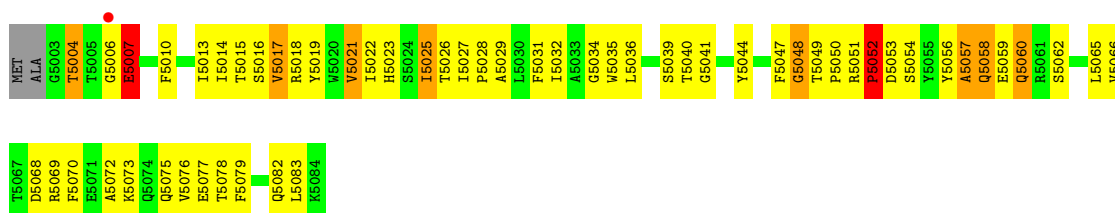
• Molecule 4: photosystem II reaction center D2 protein



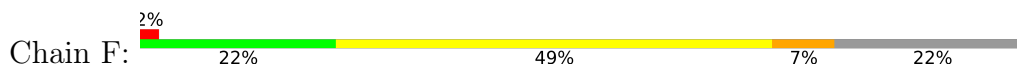
- Molecule 5: Cytochrome b559 alpha subunit



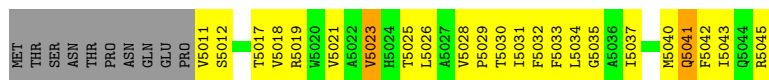
- Molecule 5: Cytochrome b559 alpha subunit



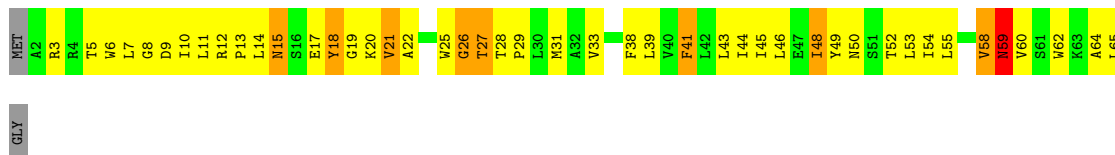
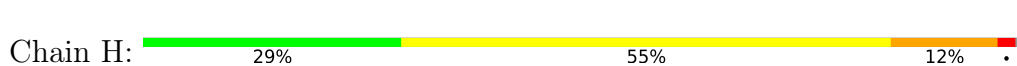
- Molecule 6: Cytochrome b559 beta subunit



- Molecule 6: Cytochrome b559 beta subunit



- Molecule 7: Photosystem II reaction center H protein

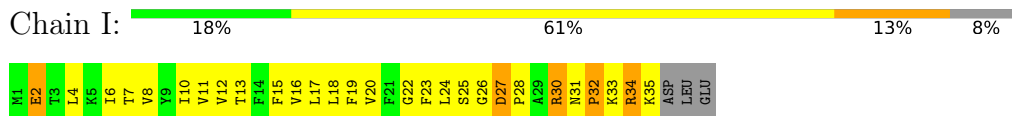


- Molecule 7: Photosystem II reaction center H protein

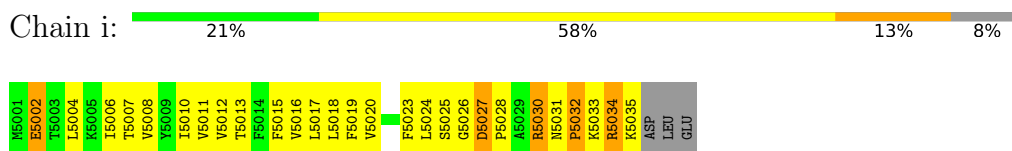




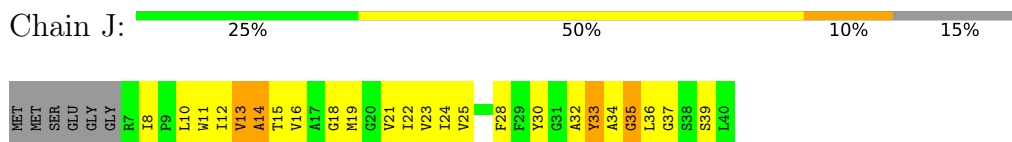
- Molecule 8: Photosystem II reaction center I protein



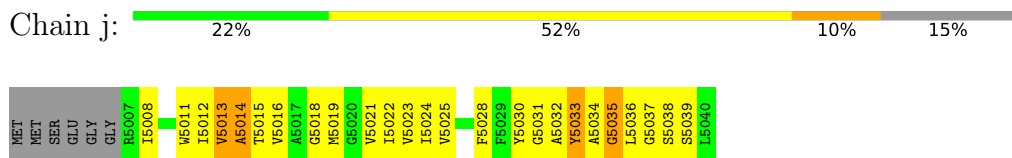
- Molecule 8: Photosystem II reaction center I protein



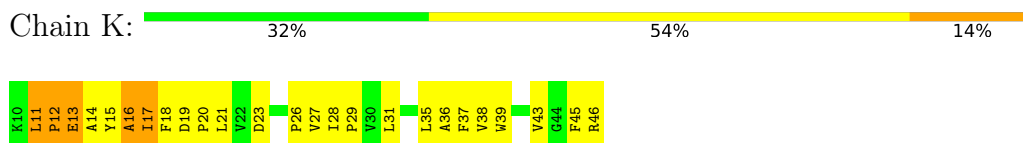
- Molecule 9: Photosystem II reaction center J protein



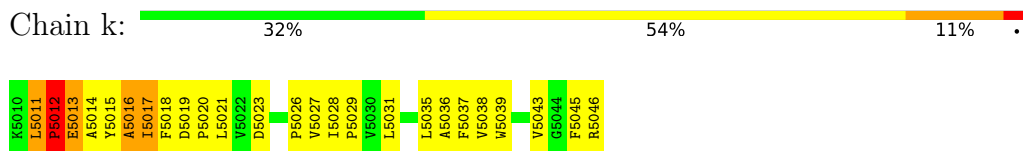
- Molecule 9: Photosystem II reaction center J protein



- Molecule 10: Photosystem II reaction center protein K

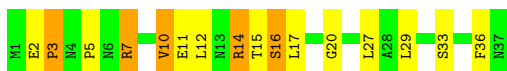


- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center L protein





- Molecule 11: Photosystem II reaction center L protein



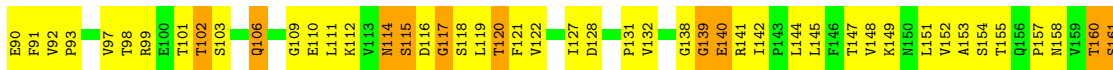
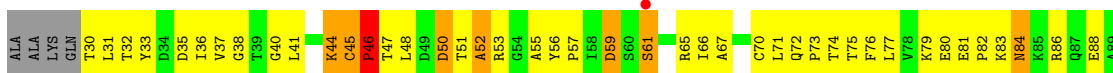
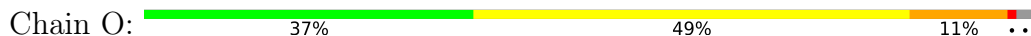
- Molecule 12: Photosystem II reaction center M protein



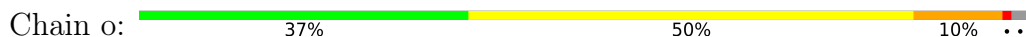
- Molecule 12: Photosystem II reaction center M protein

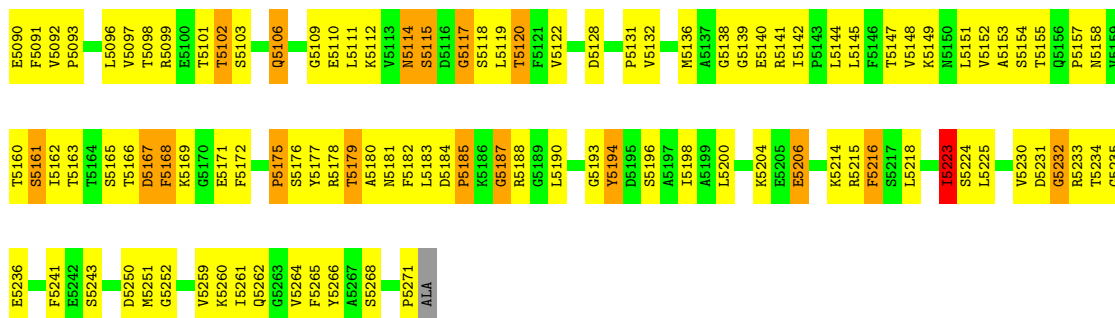


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





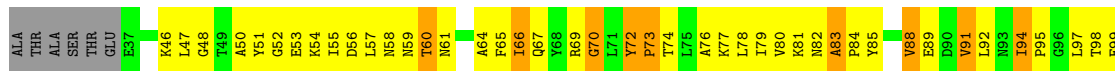
• Molecule 14: Photosystem II reaction center T protein



• Molecule 14: Photosystem II reaction center T protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

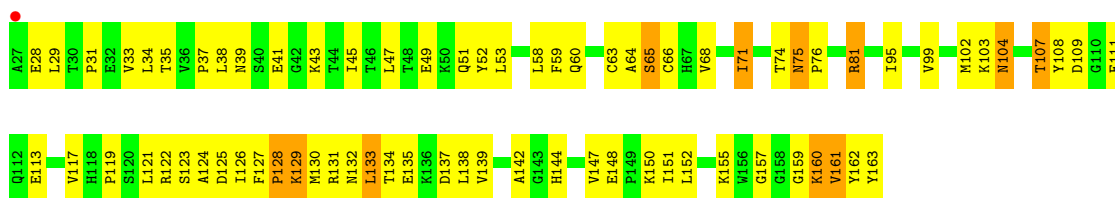


• Molecule 15: Photosystem II 12 kDa extrinsic protein

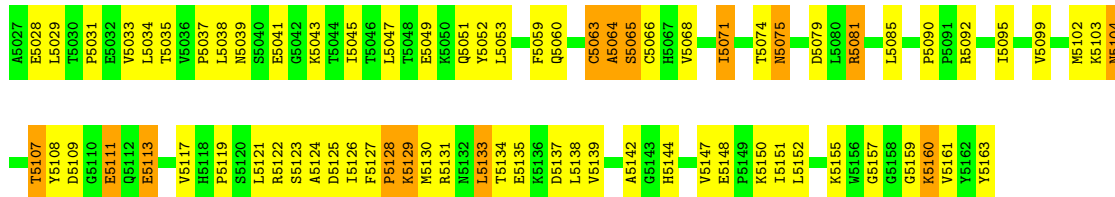


• Molecule 16: Cytochrome c-550

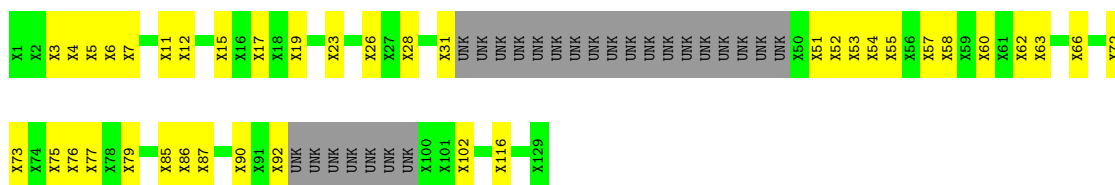




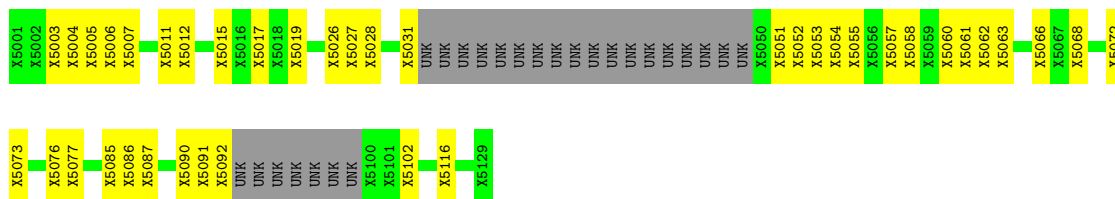
● Molecule 16: Cytochrome c-550



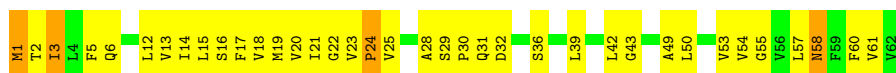
● Molecule 17: Unassigned subunits



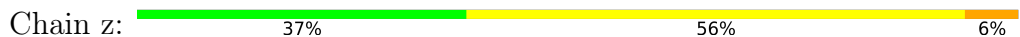
● Molecule 17: Unassigned subunits



● Molecule 18: Photosystem II reaction center Z protein



● Molecule 18: Photosystem II reaction center Z protein



M5001	L5012	V5053
L5002	V5013	V5054
L5003	L5014	G5055
L5004	L5015	L5057
F5005	S5016	N5058
Q5006	F5017	F5059
	V5018	V5060
	M5019	V5061
	V5020	V5062
	L5021	
	G5022	
	V5023	
	F5024	
	V5025	
	A5026	
	Y5027	
	A5028	
	S5029	
	F5030	
	Q5031	
	D5032	
	S5036	
	L5039	
	L5042	
	G5043	
	H5047	
	L5048	
	A5049	
	L5050	
	V5053	
	V5054	
	G5055	
	L5057	
	N5058	
	F5059	
	V5060	
	V5061	
	V5062	

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)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.241 , 0.291	Depositor DCC
R_{free} test set	1908 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtrriage
Anisotropy	0.468	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: SQD, OEC, MGE, HEM, PQ9, FE2, DGD, BCR, CA, PHO, BCT, LHG, CLA, UNL, LMT

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	0.80	0/2708	1.15	24/3694 (0.6%)
1	a	0.76	0/2708	1.16	29/3694 (0.8%)
2	B	0.74	0/3935	1.06	21/5366 (0.4%)
2	b	0.74	0/3935	1.07	23/5366 (0.4%)
3	C	0.66	0/3533	1.11	26/4815 (0.5%)
3	c	0.67	0/3533	1.13	27/4815 (0.6%)
4	D	0.81	1/2791 (0.0%)	1.08	19/3806 (0.5%)
4	d	0.75	1/2791 (0.0%)	1.08	15/3806 (0.4%)
5	E	0.75	0/665	1.24	7/911 (0.8%)
5	e	0.73	0/665	1.21	4/911 (0.4%)
6	F	0.77	0/287	0.98	0/392
6	f	0.75	0/287	0.93	0/392
7	H	0.72	0/505	1.07	3/692 (0.4%)
7	h	0.69	0/505	1.07	3/692 (0.4%)
8	I	0.77	0/293	1.06	1/395 (0.3%)
8	i	0.70	0/293	1.08	1/395 (0.3%)
9	J	0.75	0/246	1.22	4/335 (1.2%)
9	j	0.69	0/246	1.24	4/335 (1.2%)
10	K	0.78	0/299	1.11	1/412 (0.2%)
10	k	0.88	0/299	1.08	2/412 (0.5%)
11	L	0.78	0/308	1.07	1/419 (0.2%)
11	l	0.85	0/308	1.05	2/419 (0.5%)
12	M	0.90	0/279	1.04	0/379
12	m	0.92	0/279	1.06	0/379
13	O	0.78	1/1803 (0.1%)	1.10	13/2461 (0.5%)
13	o	0.76	1/1803 (0.1%)	1.10	14/2461 (0.6%)
14	T	0.93	0/263	1.08	2/356 (0.6%)
14	t	0.90	0/263	1.07	2/356 (0.6%)
15	U	0.79	0/786	1.13	7/1066 (0.7%)
15	u	0.74	0/786	1.12	5/1066 (0.5%)
16	V	0.74	0/1085	1.03	3/1473 (0.2%)
16	v	0.71	0/1085	1.00	4/1473 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Z	0.82	1/451 (0.2%)	1.08	0/620
18	z	0.90	1/451 (0.2%)	1.11	0/620
All	All	0.75	6/40474 (0.0%)	1.10	267/55184 (0.5%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	z	5001	MET	SD-CE	6.21	1.95	1.79
18	Z	1	MET	SD-CE	5.99	1.94	1.79
4	d	5013	GLY	N-CA	5.40	1.54	1.45
13	O	213	VAL	CA-CB	-5.32	1.47	1.53
4	D	13	GLY	N-CA	5.12	1.53	1.45

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	5090	PHE	N-CA-C	-9.53	100.42	112.90
4	D	143	ALA	N-CA-C	-9.33	102.03	113.50
4	d	5143	ALA	N-CA-C	-8.99	102.44	113.41
8	i	5002	GLU	N-CA-C	-8.92	101.97	113.12
4	D	14	TRP	N-CA-C	-8.88	102.60	113.97

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 [i](#)

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	233	0
1	a	2623	0	2517	251	0
2	B	3800	0	3637	285	0
2	b	3800	0	3637	288	0
3	C	3421	0	3326	310	0
3	c	3421	0	3326	320	0
4	D	2696	0	2591	251	0
4	d	2696	0	2591	257	0
5	E	646	0	616	56	0
5	e	646	0	616	63	0
6	F	278	0	279	31	0
6	f	278	0	279	30	0
7	H	492	0	495	56	0
7	h	492	0	495	51	0
8	I	286	0	308	33	0
8	i	286	0	305	31	0
9	J	240	0	242	27	0
9	j	240	0	242	29	0
10	K	289	0	294	51	0
10	k	289	0	294	47	0
11	L	301	0	309	25	0
11	l	301	0	306	25	0
12	M	276	0	288	23	0
12	m	276	0	285	21	0
13	O	1772	0	1664	166	0
13	o	1772	0	1664	162	0
14	T	254	0	257	27	0
14	t	254	0	254	29	0
15	U	775	0	771	61	0
15	u	775	0	771	64	0
16	V	1064	0	1072	73	0
16	v	1064	0	1072	76	0
17	X	687	0	268	44	0
17	x	687	0	268	45	0
18	Z	442	0	460	40	0
18	z	442	0	457	44	0
19	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	1	0	0	0	0
20	A	250	0	265	13	0
20	B	1007	0	1088	62	0
20	C	774	0	783	44	0
20	D	115	0	111	9	0
20	a	250	0	265	15	0
20	b	1007	0	1088	61	0
20	c	774	0	783	42	0
20	d	115	0	111	10	0
21	A	128	0	148	12	0
21	a	128	0	148	12	0
22	A	30	0	37	1	0
22	D	30	0	37	5	0
22	a	30	0	37	0	0
22	d	30	0	37	5	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	7	0
24	C	120	0	168	19	0
24	D	40	0	56	4	0
24	H	40	0	56	2	0
24	T	40	0	56	8	0
24	X	40	0	56	9	0
24	a	40	0	56	3	0
24	b	120	0	168	6	0
24	c	120	0	168	21	0
24	d	40	0	56	6	0
24	h	40	0	56	3	0
24	t	40	0	56	9	0
24	x	40	0	56	10	0
25	A	39	0	51	4	0
25	a	39	0	51	4	0
26	A	80	0	92	0	0
26	L	47	0	60	1	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	1	0
27	A	35	0	46	3	0
27	M	35	0	46	0	0
27	T	35	0	46	6	0
27	a	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	m	35	0	46	0	0
27	t	35	0	46	5	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	1	0
28	d	136	0	194	11	0
28	i	48	0	72	2	0
28	l	48	0	72	4	0
29	C	152	0	0	1	0
29	c	152	0	0	1	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	18	0
30	h	54	0	66	3	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	3	0
32	v	43	0	30	1	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47073	3260	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 34.

The worst 5 of 3260 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
17:x:5026:UNK:NE2	17:x:5026:UNK:CD	1.34	1.41
17:x:5006:UNK:NE2	17:x:5006:UNK:CD	1.33	1.40
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	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	19
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	3	19
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

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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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	252 (94%)	17 (6%)	16	48
1	a	269/280 (96%)	253 (94%)	16 (6%)	18	50
2	B	378/407 (93%)	356 (94%)	22 (6%)	18	51
2	b	378/407 (93%)	353 (93%)	25 (7%)	15	46
3	C	341/374 (91%)	322 (94%)	19 (6%)	19	52
3	c	341/374 (91%)	320 (94%)	21 (6%)	16	49
4	D	273/283 (96%)	258 (94%)	15 (6%)	19	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	273/283 (96%)	255 (93%)	18 (7%)	15	46
5	E	68/73 (93%)	65 (96%)	3 (4%)	25	60
5	e	68/73 (93%)	65 (96%)	3 (4%)	25	60
6	F	27/39 (69%)	26 (96%)	1 (4%)	30	64
6	f	27/39 (69%)	26 (96%)	1 (4%)	30	64
7	H	50/55 (91%)	44 (88%)	6 (12%)	5	22
7	h	50/55 (91%)	44 (88%)	6 (12%)	5	22
8	I	32/35 (91%)	27 (84%)	5 (16%)	2	13
8	i	32/35 (91%)	27 (84%)	5 (16%)	2	13
9	J	22/28 (79%)	22 (100%)	0	100	100
9	j	22/28 (79%)	22 (100%)	0	100	100
10	K	29/30 (97%)	27 (93%)	2 (7%)	14	45
10	k	29/30 (97%)	27 (93%)	2 (7%)	14	45
11	L	34/35 (97%)	30 (88%)	4 (12%)	5	22
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	22
12	M	32/33 (97%)	31 (97%)	1 (3%)	35	68
12	m	32/33 (97%)	31 (97%)	1 (3%)	35	68
13	O	181/208 (87%)	169 (93%)	12 (7%)	15	46
13	o	181/208 (87%)	170 (94%)	11 (6%)	17	49
14	T	26/29 (90%)	24 (92%)	2 (8%)	12	40
14	t	26/29 (90%)	24 (92%)	2 (8%)	12	40
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	73
15	u	83/89 (93%)	81 (98%)	2 (2%)	43	73
16	V	117/117 (100%)	110 (94%)	7 (6%)	17	50
16	v	117/117 (100%)	109 (93%)	8 (7%)	14	45
18	Z	43/52 (83%)	42 (98%)	1 (2%)	44	74
18	z	43/52 (83%)	42 (98%)	1 (2%)	44	74
All	All	4010/4334 (92%)	3765 (94%)	245 (6%)	17	49

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	107	THR

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Mol	Chain	Res	Type
13	o	5046	PRO
2	b	5222	PRO
11	l	5016	SER
16	v	5035	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	108	ASN
13	o	5114	ASN
1	a	5272	HIS
13	o	5108	GLN
4	d	5250	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.47	7 (10%)
24	BCR	H	107	-	41,41,41	2.11	6 (14%)	56,56,56	2.29	24 (42%)
20	CLA	c	5499	-	51,55,73	1.45	7 (13%)	60,91,113	1.90	7 (11%)
20	CLA	B	525	-	69,73,73	1.25	9 (13%)	82,113,113	1.75	9 (10%)
20	CLA	B	523	-	69,73,73	1.36	8 (11%)	82,113,113	1.76	9 (10%)
24	BCR	C	506	-	41,41,41	1.74	8 (19%)	56,56,56	2.23	21 (37%)
20	CLA	b	5512	2	69,73,73	1.23	6 (8%)	82,113,113	1.60	9 (10%)
27	LMT	M	5216	-	36,36,36	1.45	8 (22%)	47,47,47	0.92	2 (4%)
20	CLA	A	559	-	69,73,73	1.14	5 (7%)	82,113,113	1.63	8 (9%)
20	CLA	c	5492	3	64,68,73	1.29	8 (12%)	76,107,113	1.84	9 (11%)
20	CLA	C	496	3	69,73,73	1.43	10 (14%)	82,113,113	1.78	13 (15%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	4 (8%)
20	CLA	b	5516	-	69,73,73	1.49	5 (7%)	82,113,113	1.85	8 (9%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.06	2 (3%)
20	CLA	D	354	4	69,73,73	1.24	7 (10%)	82,113,113	1.61	10 (12%)
20	CLA	C	503	3	54,58,73	1.72	8 (14%)	64,95,113	1.95	9 (14%)
26	SQD	a	212	-	24,26,54	3.09	13 (54%)	34,37,65	2.73	13 (38%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.56	9 (13%)
20	CLA	C	499	-	51,55,73	1.53	8 (15%)	60,91,113	1.95	8 (13%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.67	11 (17%)
28	MGE	L	210	-	48,48,48	0.99	3 (6%)	56,56,56	1.15	5 (8%)
24	BCR	h	5107	-	41,41,41	2.04	7 (17%)	56,56,56	2.30	25 (44%)
28	MGE	i	5201	-	48,48,48	1.24	7 (14%)	56,56,56	1.08	4 (7%)
20	CLA	b	5518	2	69,73,73	1.41	6 (8%)	82,113,113	1.79	11 (13%)
24	BCR	B	527	-	41,41,41	1.74	8 (19%)	56,56,56	2.08	16 (28%)
20	CLA	b	5523	-	69,73,73	1.29	9 (13%)	82,113,113	1.78	9 (10%)
21	PHO	a	5561	-	58,69,69	1.60	11 (18%)	55,99,99	1.98	15 (27%)
32	HEM	v	5552	16	50,50,50	2.09	22 (44%)	67,82,82	1.98	14 (20%)
20	CLA	a	5559	-	69,73,73	1.13	4 (5%)	82,113,113	1.66	9 (10%)
22	PQ9	d	5356	-	30,30,45	0.82	0	38,39,57	1.66	6 (15%)
20	CLA	b	5517	-	69,73,73	1.44	8 (11%)	82,113,113	1.77	9 (10%)
20	CLA	a	5563	-	59,63,73	1.48	9 (15%)	70,101,113	1.69	10 (14%)
25	LHG	a	5567	-	38,38,48	2.02	5 (13%)	41,44,54	1.46	4 (9%)
20	CLA	C	498	3	69,73,73	1.31	7 (10%)	82,113,113	1.76	10 (12%)
20	CLA	B	513	2	69,73,73	1.44	11 (15%)	82,113,113	1.69	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.96	3 (5%)
20	CLA	C	493	3	69,73,73	1.30	7 (10%)	82,113,113	1.82	13 (15%)
20	CLA	d	5355	-	54,58,73	1.65	11 (20%)	64,95,113	1.93	9 (14%)
28	MGE	l	5210	-	48,48,48	0.90	4 (8%)	56,56,56	1.12	5 (8%)
20	CLA	b	5511	-	45,49,73	1.66	10 (22%)	54,84,113	2.02	8 (14%)
20	CLA	B	520	-	69,73,73	1.25	8 (11%)	82,113,113	1.66	11 (13%)
30	DGD	c	5509	-	58,58,67	1.35	7 (12%)	72,72,81	1.39	6 (8%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.46	6 (8%)
20	CLA	b	5513	2	69,73,73	1.30	8 (11%)	82,113,113	1.64	13 (15%)
28	MGE	d	5360	-	41,41,48	1.19	6 (14%)	49,49,56	1.05	4 (8%)
24	BCR	T	5104	-	41,41,41	1.55	9 (21%)	56,56,56	2.31	25 (44%)
24	BCR	D	357	-	41,41,41	1.96	8 (19%)	56,56,56	2.27	20 (35%)
20	CLA	d	5354	4	69,73,73	1.26	11 (15%)	82,113,113	1.68	11 (13%)
24	BCR	t	104	-	41,41,41	1.67	10 (24%)	56,56,56	2.28	23 (41%)
20	CLA	C	497	-	69,73,73	1.31	10 (14%)	82,113,113	1.87	11 (13%)
20	CLA	C	501	3	69,73,73	1.47	9 (13%)	82,113,113	1.86	11 (13%)
20	CLA	B	524	2	60,64,73	1.50	7 (11%)	71,102,113	1.93	9 (12%)
20	CLA	C	491	3	69,73,73	1.24	5 (7%)	82,113,113	1.62	9 (10%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	1.00	3 (6%)
32	HEM	F	51	5,6	50,50,50	2.08	16 (32%)	67,82,82	1.98	16 (23%)
20	CLA	C	500	-	69,73,73	1.29	8 (11%)	82,113,113	1.70	12 (14%)
20	CLA	c	5496	-	69,73,73	1.36	8 (11%)	82,113,113	1.73	11 (13%)
26	SQD	t	213	-	45,47,54	2.81	23 (51%)	55,58,65	2.49	14 (25%)
27	LMT	a	5568	-	36,36,36	1.46	6 (16%)	47,47,47	1.09	1 (2%)
26	SQD	d	5358	-	52,54,54	2.58	29 (55%)	62,65,65	2.53	18 (29%)
24	BCR	c	5506	-	41,41,41	1.95	7 (17%)	56,56,56	2.16	20 (35%)
24	BCR	B	529	-	41,41,41	1.79	6 (14%)	56,56,56	2.22	21 (37%)
20	CLA	b	5521	2	69,73,73	1.17	5 (7%)	82,113,113	1.76	12 (14%)
22	PQ9	D	356	-	30,30,45	0.91	1 (3%)	38,39,57	1.68	9 (23%)
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	B	521	2	69,73,73	1.31	9 (13%)	82,113,113	1.81	11 (13%)
20	CLA	c	5503	3	54,58,73	1.73	9 (16%)	64,95,113	1.96	6 (9%)
20	CLA	C	495	-	69,73,73	1.50	11 (15%)	82,113,113	1.82	11 (13%)
24	BCR	c	5505	-	41,41,41	2.01	8 (19%)	56,56,56	2.14	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	X	130	-	41,41,41	1.93	8 (19%)	56,56,56	2.54	23 (41%)
32	HEM	f	5051	5,6	50,50,50	2.16	17 (34%)	67,82,82	2.05	13 (19%)
20	CLA	D	355	-	54,58,73	1.65	11 (20%)	64,95,113	1.94	11 (17%)
24	BCR	b	5528	-	41,41,41	1.74	6 (14%)	56,56,56	2.06	17 (30%)
26	SQD	L	5213	-	45,47,54	2.81	24 (53%)	55,58,65	2.42	12 (21%)
20	CLA	B	522	-	69,73,73	1.29	10 (14%)	82,113,113	1.67	9 (10%)
20	CLA	B	512	2	69,73,73	1.31	8 (11%)	82,113,113	1.63	11 (13%)
20	CLA	b	5519	-	69,73,73	1.37	7 (10%)	82,113,113	1.73	12 (14%)
20	CLA	c	5500	-	69,73,73	1.24	6 (8%)	82,113,113	1.70	12 (14%)
20	CLA	b	5526	-	69,73,73	1.49	11 (15%)	82,113,113	1.77	11 (13%)
20	CLA	b	5525	-	69,73,73	1.22	7 (10%)	82,113,113	1.78	9 (10%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.11	6 (10%)
20	CLA	b	5520	-	69,73,73	1.25	9 (13%)	82,113,113	1.66	10 (12%)
24	BCR	b	5529	-	41,41,41	1.66	6 (14%)	56,56,56	2.15	21 (37%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.16	6 (10%)
20	CLA	c	5495	-	69,73,73	1.59	8 (11%)	82,113,113	1.85	12 (14%)
20	CLA	c	5493	3	69,73,73	1.35	7 (10%)	82,113,113	1.81	13 (15%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.07	4 (7%)
31	BCT	D	353	19	3,3,3	2.28	1 (33%)	2,3,3	0.32	0
20	CLA	B	518	2	69,73,73	1.41	6 (8%)	82,113,113	1.82	9 (10%)
20	CLA	c	5497	-	69,73,73	1.31	10 (14%)	82,113,113	1.76	11 (13%)
20	CLA	c	5501	3	69,73,73	1.45	9 (13%)	82,113,113	1.84	9 (10%)
20	CLA	B	517	-	69,73,73	1.53	7 (10%)	82,113,113	1.87	12 (14%)
20	CLA	B	519	-	69,73,73	1.46	6 (8%)	82,113,113	1.73	11 (13%)
27	LMT	A	569	-	36,36,36	1.54	6 (16%)	47,47,47	1.07	1 (2%)
20	CLA	b	5524	2	60,64,73	1.43	7 (11%)	71,102,113	1.82	8 (11%)
20	CLA	C	502	-	55,59,73	1.66	13 (23%)	64,96,113	2.00	11 (17%)
24	BCR	c	5504	-	41,41,41	2.18	5 (12%)	56,56,56	2.18	23 (41%)
24	BCR	b	5527	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
22	PQ9	A	564	-	30,30,45	0.85	0	38,39,57	1.50	8 (21%)
27	LMT	T	217	-	36,36,36	1.40	5 (13%)	47,47,47	1.03	4 (8%)
20	CLA	B	515	-	69,73,73	1.29	9 (13%)	82,113,113	1.77	14 (17%)
24	BCR	x	5130	-	41,41,41	1.95	9 (21%)	56,56,56	2.52	24 (42%)
20	CLA	b	5514	2	69,73,73	1.45	10 (14%)	82,113,113	1.84	10 (12%)
20	CLA	C	492	3	64,68,73	1.29	7 (10%)	76,107,113	1.82	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	528	-	41,41,41	1.93	6 (14%)	56,56,56	2.02	17 (30%)
21	PHO	a	5562	-	58,69,69	1.75	7 (12%)	55,99,99	2.06	13 (23%)
27	LMT	m	216	-	36,36,36	1.45	7 (19%)	47,47,47	0.98	3 (6%)
21	PHO	A	562	-	58,69,69	1.73	8 (13%)	55,99,99	2.11	12 (21%)
24	BCR	d	5357	-	41,41,41	2.02	8 (19%)	56,56,56	2.33	21 (37%)
30	DGD	c	5508	-	48,48,67	1.48	8 (16%)	62,62,81	1.71	10 (16%)
22	PQ9	a	5564	-	30,30,45	0.86	1 (3%)	38,39,57	1.46	6 (15%)
20	CLA	A	563	-	59,63,73	1.46	10 (16%)	70,101,113	1.75	11 (15%)
20	CLA	c	5498	3	69,73,73	1.50	9 (13%)	82,113,113	1.80	12 (14%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.12	4 (7%)
32	HEM	V	552	16	50,50,50	1.97	17 (34%)	67,82,82	1.98	13 (19%)
20	CLA	c	5491	3	69,73,73	1.42	6 (8%)	82,113,113	1.84	11 (13%)
20	CLA	b	5515	-	69,73,73	1.28	10 (14%)	82,113,113	1.74	15 (18%)
20	CLA	A	560	-	69,73,73	1.34	9 (13%)	82,113,113	1.72	10 (12%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
21	PHO	A	561	-	58,69,69	1.61	9 (15%)	55,99,99	2.06	16 (29%)
24	BCR	A	566	-	41,41,41	1.63	8 (19%)	56,56,56	2.14	22 (39%)
20	CLA	a	5560	-	69,73,73	1.37	8 (11%)	82,113,113	1.75	10 (12%)
24	BCR	C	504	-	41,41,41	1.87	6 (14%)	56,56,56	2.21	22 (39%)
25	LHG	A	567	-	38,38,48	1.98	5 (13%)	41,44,54	1.51	4 (9%)
20	CLA	B	514	2	69,73,73	1.43	8 (11%)	82,113,113	1.81	10 (12%)
20	CLA	B	516	-	69,73,73	1.39	4 (5%)	82,113,113	1.81	7 (8%)
20	CLA	C	494	-	50,54,73	1.45	7 (14%)	59,90,113	2.05	7 (11%)
26	SQD	A	568	-	52,54,54	2.59	31 (59%)	62,65,65	2.55	18 (29%)
20	CLA	c	5502	-	55,59,73	1.71	12 (21%)	64,96,113	2.03	11 (17%)
31	BCT	d	5353	19	3,3,3	2.70	1 (33%)	2,3,3	0.35	0
20	CLA	c	5494	-	50,54,73	1.39	6 (12%)	59,90,113	1.89	8 (13%)
20	CLA	B	511	-	45,49,73	1.61	10 (22%)	54,84,113	1.94	8 (14%)
20	CLA	a	5558	1	69,73,73	1.31	11 (15%)	82,113,113	1.58	11 (13%)
20	CLA	b	5522	-	69,73,73	1.40	10 (14%)	82,113,113	1.68	7 (8%)
24	BCR	a	5566	-	41,41,41	1.68	7 (17%)	56,56,56	2.14	23 (41%)
30	DGD	C	509	-	58,58,67	1.12	7 (12%)	72,72,81	1.40	5 (6%)
20	CLA	B	526	-	69,73,73	1.49	12 (17%)	82,113,113	1.76	10 (12%)
24	BCR	C	505	-	41,41,41	1.98	9 (21%)	56,56,56	2.13	18 (32%)
20	CLA	A	558	1	69,73,73	1.29	8 (11%)	82,113,113	1.64	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5499	-	1/1/11/20	8/18/94/115	-
20	CLA	B	525	-	1/1/15/20	14/39/115/115	-
20	CLA	B	523	-	1/1/15/20	15/39/115/115	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5512	2	1/1/15/20	12/39/115/115	-
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
20	CLA	A	559	-	1/1/15/20	14/39/115/115	-
20	CLA	c	5492	3	1/1/14/20	11/33/109/115	-
20	CLA	C	496	3	1/1/15/20	13/39/115/115	-
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
20	CLA	b	5516	-	1/1/15/20	15/39/115/115	-
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	D	354	4	1/1/15/20	10/39/115/115	-
20	CLA	C	503	3	1/1/12/20	7/21/97/115	-
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	C	499	-	1/1/11/20	8/18/94/115	-
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
28	MGE	L	210	-	-	23/43/63/63	0/1/1/1
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
20	CLA	b	5518	2	1/1/15/20	16/39/115/115	-
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	b	5523	-	1/1/15/20	15/39/115/115	-
21	PHO	a	5561	-	-	13/37/103/103	0/5/6/6
32	HEM	v	5552	16	-	6/14/54/54	-
20	CLA	a	5559	-	1/1/15/20	14/39/115/115	-
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
20	CLA	b	5517	-	1/1/15/20	14/39/115/115	-
20	CLA	a	5563	-	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	a	5567	-	-	14/43/43/53	-
20	CLA	C	498	3	1/1/15/20	18/39/115/115	-
20	CLA	B	513	2	1/1/15/20	14/39/115/115	-
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
20	CLA	C	493	3	1/1/15/20	12/39/115/115	-
20	CLA	d	5355	-	1/1/12/20	11/21/97/115	-
28	MGE	l	5210	-	-	23/43/63/63	0/1/1/1
20	CLA	b	5511	-	1/1/10/20	4/10/86/115	-
20	CLA	B	520	-	1/1/15/20	15/39/115/115	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
20	CLA	b	5513	2	1/1/15/20	12/39/115/115	-
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
20	CLA	d	5354	4	1/1/15/20	8/39/115/115	-
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
20	CLA	C	497	-	1/1/15/20	9/39/115/115	-
20	CLA	C	501	3	1/1/15/20	15/39/115/115	-
20	CLA	B	524	2	1/1/13/20	9/29/105/115	-
20	CLA	C	491	3	1/1/15/20	9/39/115/115	-
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
32	HEM	F	51	5,6	-	2/14/54/54	-
20	CLA	C	500	-	1/1/15/20	13/39/115/115	-
20	CLA	c	5496	-	1/1/15/20	13/39/115/115	-
26	SQD	t	213	-	-	20/42/62/69	0/1/1/1
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
24	BCR	B	529	-	-	3/29/63/63	0/2/2/2
20	CLA	b	5521	2	1/1/15/20	9/39/115/115	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
26	SQD	A	5212	-	-	5/19/39/69	0/1/1/1
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	521	2	1/1/15/20	9/39/115/115	-
20	CLA	c	5503	3	1/1/12/20	7/21/97/115	-
20	CLA	C	495	-	1/1/15/20	18/39/115/115	-
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
24	BCR	X	130	-	-	5/29/63/63	0/2/2/2
32	HEM	f	5051	5,6	-	2/14/54/54	-
20	CLA	D	355	-	1/1/12/20	11/21/97/115	-
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
26	SQD	L	5213	-	-	21/42/62/69	0/1/1/1
20	CLA	B	522	-	1/1/15/20	12/39/115/115	-
20	CLA	B	512	2	1/1/15/20	12/39/115/115	-
20	CLA	b	5519	-	1/1/15/20	13/39/115/115	-
20	CLA	c	5500	-	1/1/15/20	13/39/115/115	-
20	CLA	b	5526	-	1/1/15/20	12/39/115/115	-
20	CLA	b	5525	-	1/1/15/20	14/39/115/115	-
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
20	CLA	b	5520	-	1/1/15/20	13/39/115/115	-
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
20	CLA	c	5495	-	1/1/15/20	18/39/115/115	-
20	CLA	c	5493	3	1/1/15/20	12/39/115/115	-
28	MGE	I	201	-	-	24/43/63/63	0/1/1/1
20	CLA	B	518	2	1/1/15/20	16/39/115/115	-
20	CLA	c	5497	-	1/1/15/20	10/39/115/115	-
20	CLA	c	5501	3	1/1/15/20	13/39/115/115	-
20	CLA	B	517	-	1/1/15/20	14/39/115/115	-
20	CLA	B	519	-	1/1/15/20	13/39/115/115	-
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
20	CLA	b	5524	2	1/1/13/20	9/29/105/115	-
20	CLA	C	502	-	1/1/12/20	9/23/99/115	-
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
20	CLA	B	515	-	1/1/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5514	2	1/1/15/20	14/39/115/115	-
20	CLA	C	492	3	1/1/14/20	11/33/109/115	-
24	BCR	B	528	-	-	1/29/63/63	0/2/2/2
21	PHO	a	5562	-	-	9/37/103/103	0/5/6/6
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
21	PHO	A	562	-	-	9/37/103/103	0/5/6/6
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
20	CLA	A	563	-	1/1/13/20	7/27/103/115	-
20	CLA	c	5498	3	1/1/15/20	18/39/115/115	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
32	HEM	V	552	16	-	6/14/54/54	-
20	CLA	c	5491	3	1/1/15/20	11/39/115/115	-
20	CLA	b	5515	-	1/1/15/20	19/39/115/115	-
20	CLA	A	560	-	1/1/15/20	9/39/115/115	-
28	MGE	d	5359	-	-	13/42/62/63	0/1/1/1
21	PHO	A	561	-	-	13/37/103/103	0/5/6/6
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
20	CLA	a	5560	-	1/1/15/20	9/39/115/115	-
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
25	LHG	A	567	-	-	16/43/43/53	-
20	CLA	B	514	2	1/1/15/20	13/39/115/115	-
20	CLA	B	516	-	1/1/15/20	15/39/115/115	-
20	CLA	C	494	-	1/1/11/20	9/17/93/115	-
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
20	CLA	c	5502	-	1/1/12/20	8/23/99/115	-
20	CLA	c	5494	-	1/1/11/20	9/17/93/115	-
20	CLA	B	511	-	1/1/10/20	4/10/86/115	-
20	CLA	a	5558	1	1/1/15/20	11/39/115/115	-
20	CLA	b	5522	-	1/1/15/20	12/39/115/115	-
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	526	-	1/1/15/20	12/39/115/115	-
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
20	CLA	A	558	1	1/1/15/20	10/39/115/115	-

The worst 5 of 1162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5495	CLA	MG-NA	8.38	2.26	2.06
25	A	567	LHG	P-O5	8.23	1.79	1.50
24	c	5504	BCR	C1-C6	8.20	1.64	1.53
20	B	517	CLA	MG-NA	8.14	2.25	2.06
25	a	5567	LHG	P-O5	8.13	1.79	1.50

The worst 5 of 1531 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 1538 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	558	CLA	C2B-C3B-CAB-CBB
20	A	558	CLA	C4B-C3B-CAB-CBB
20	A	559	CLA	C2B-C3B-CAB-CBB
20	A	559	CLA	C4B-C3B-CAB-CBB
20	A	560	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

126 monomers are involved in 476 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	507	DGD	6	0
24	H	107	BCR	2	0
20	c	5499	CLA	1	0
20	B	525	CLA	2	0
24	C	506	BCR	6	0
20	b	5512	CLA	3	0
20	A	559	CLA	4	0
20	c	5492	CLA	1	0
20	C	496	CLA	2	0
28	D	359	MGE	1	0
20	b	5516	CLA	1	0
28	d	5361	MGE	7	0
20	D	354	CLA	6	0
20	C	503	CLA	1	0
30	h	5208	DGD	3	0
20	C	499	CLA	2	0
30	C	508	DGD	2	0
28	L	210	MGE	2	0
24	h	5107	BCR	3	0
28	i	5201	MGE	2	0
20	b	5518	CLA	9	0
24	B	527	BCR	3	0
20	b	5523	CLA	1	0
21	a	5561	PHO	5	0
32	v	5552	HEM	1	0
20	a	5559	CLA	5	0
22	d	5356	PQ9	5	0
20	b	5517	CLA	9	0
25	a	5567	LHG	4	0
20	C	498	CLA	6	0
20	B	513	CLA	8	0
28	D	358	MGE	2	0
20	C	493	CLA	7	0
20	d	5355	CLA	4	0
28	l	5210	MGE	4	0
20	b	5511	CLA	1	0
20	B	520	CLA	7	0
30	c	5509	DGD	9	0
30	c	5507	DGD	5	0
20	b	5513	CLA	8	0
28	d	5360	MGE	2	0
24	T	5104	BCR	8	0

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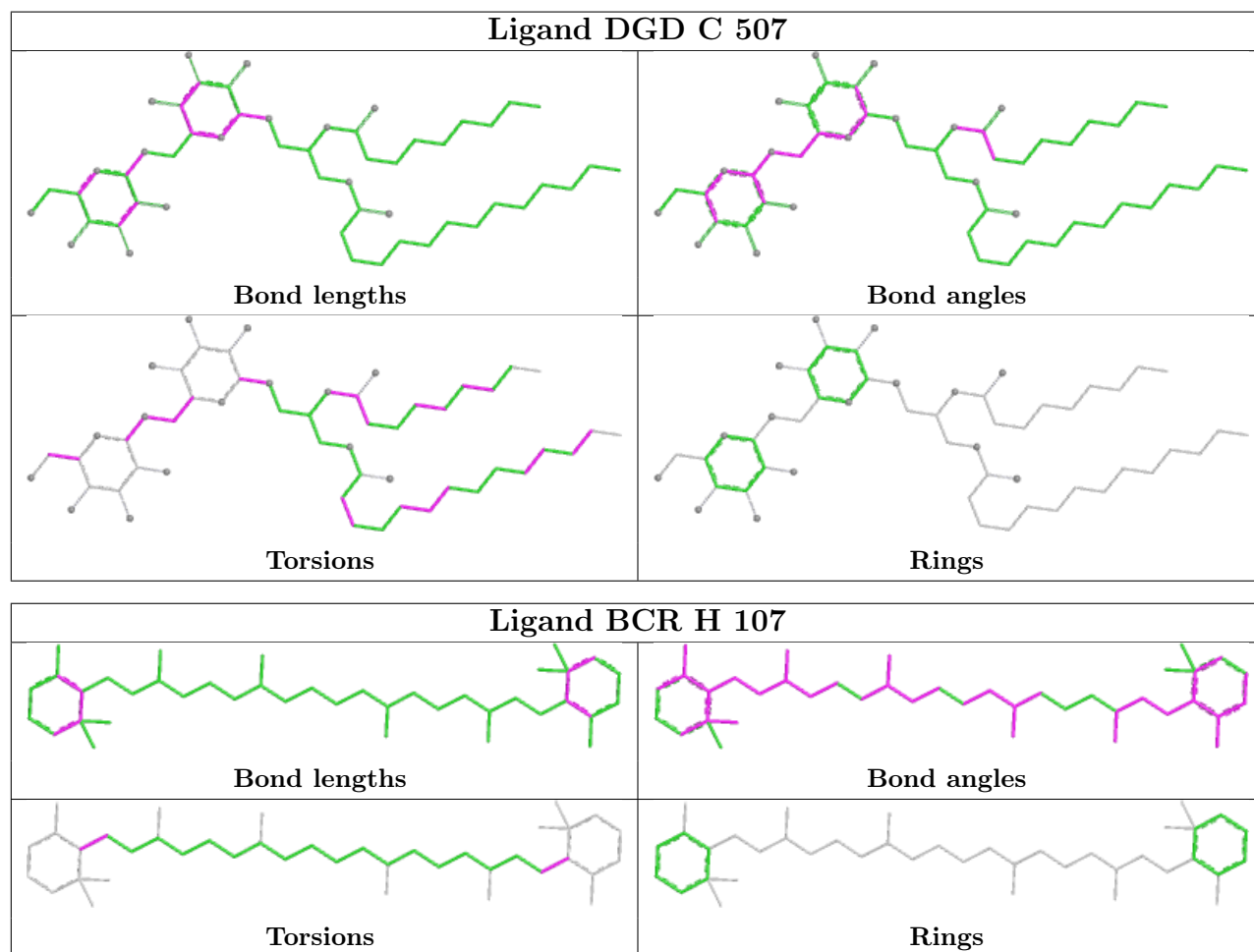
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	357	BCR	4	0
20	d	5354	CLA	6	0
24	t	104	BCR	9	0
20	C	497	CLA	5	0
20	C	501	CLA	9	0
20	B	524	CLA	4	0
20	C	491	CLA	2	0
27	t	5217	LMT	5	0
32	F	51	HEM	3	0
20	C	500	CLA	2	0
20	c	5496	CLA	2	0
26	t	213	SQD	1	0
27	a	5568	LMT	1	0
24	c	5506	BCR	6	0
24	B	529	BCR	2	0
20	b	5521	CLA	1	0
22	D	356	PQ9	5	0
30	H	208	DGD	3	0
20	B	521	CLA	3	0
20	c	5503	CLA	1	0
20	C	495	CLA	9	0
24	c	5505	BCR	6	0
24	X	130	BCR	9	0
32	f	5051	HEM	3	0
20	D	355	CLA	3	0
24	b	5528	BCR	2	0
26	L	5213	SQD	1	0
20	B	522	CLA	3	0
20	B	512	CLA	2	0
20	b	5519	CLA	3	0
20	b	5526	CLA	1	0
20	b	5525	CLA	2	0
28	b	5530	MGE	1	0
20	b	5520	CLA	6	0
24	b	5529	BCR	1	0
28	B	530	MGE	1	0
20	c	5495	CLA	10	0
20	c	5493	CLA	6	0
28	I	201	MGE	1	0
20	B	518	CLA	9	0
20	c	5497	CLA	5	0
20	c	5501	CLA	9	0

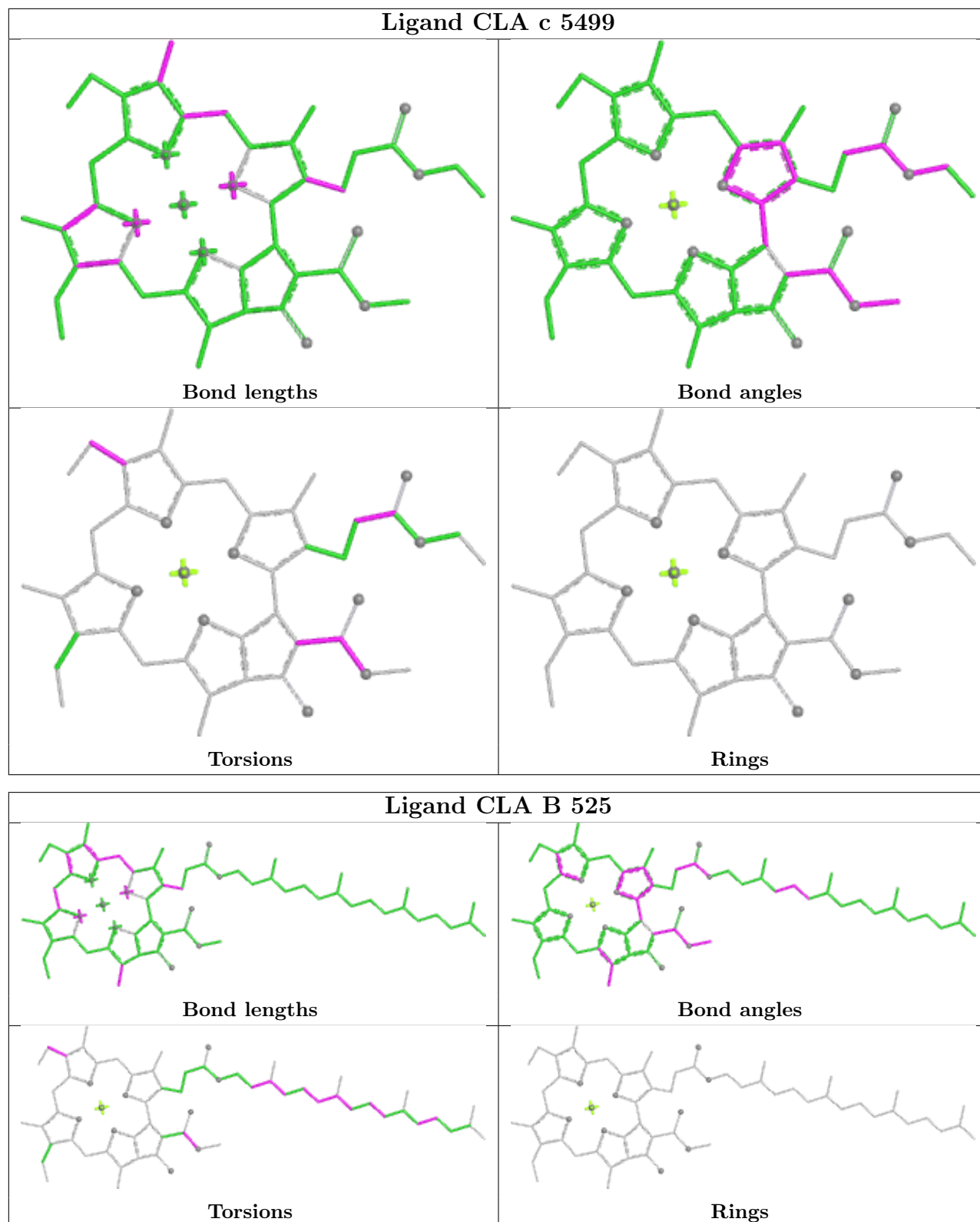
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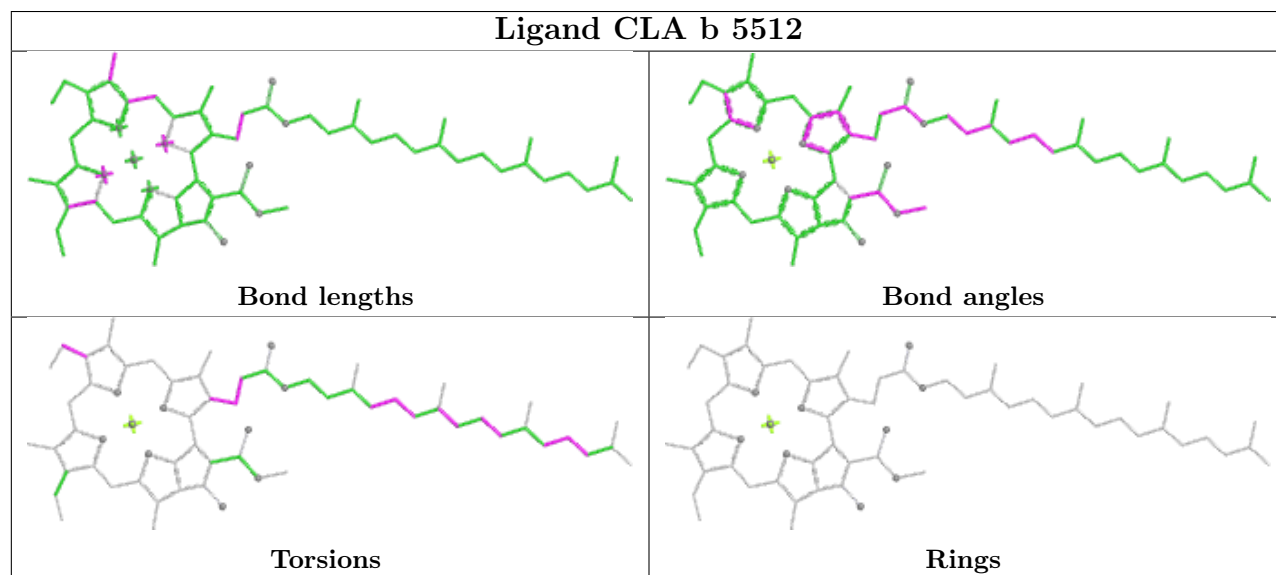
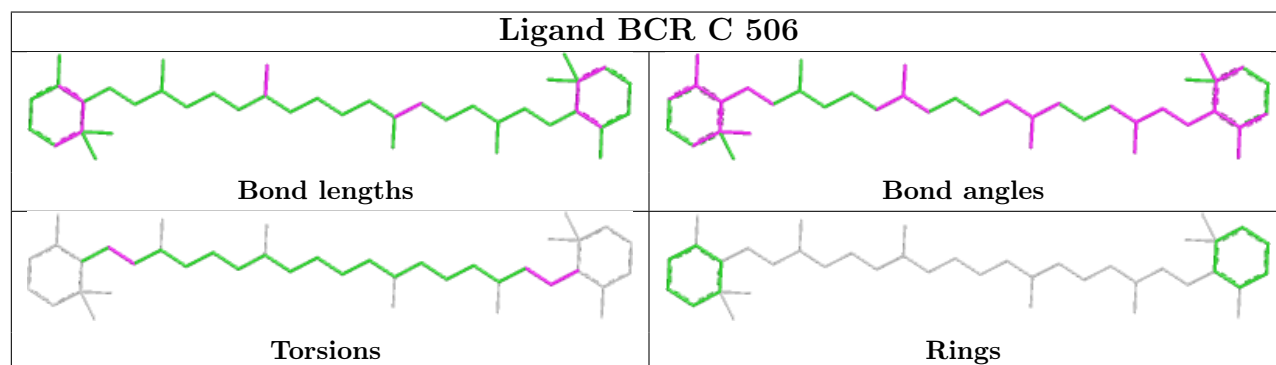
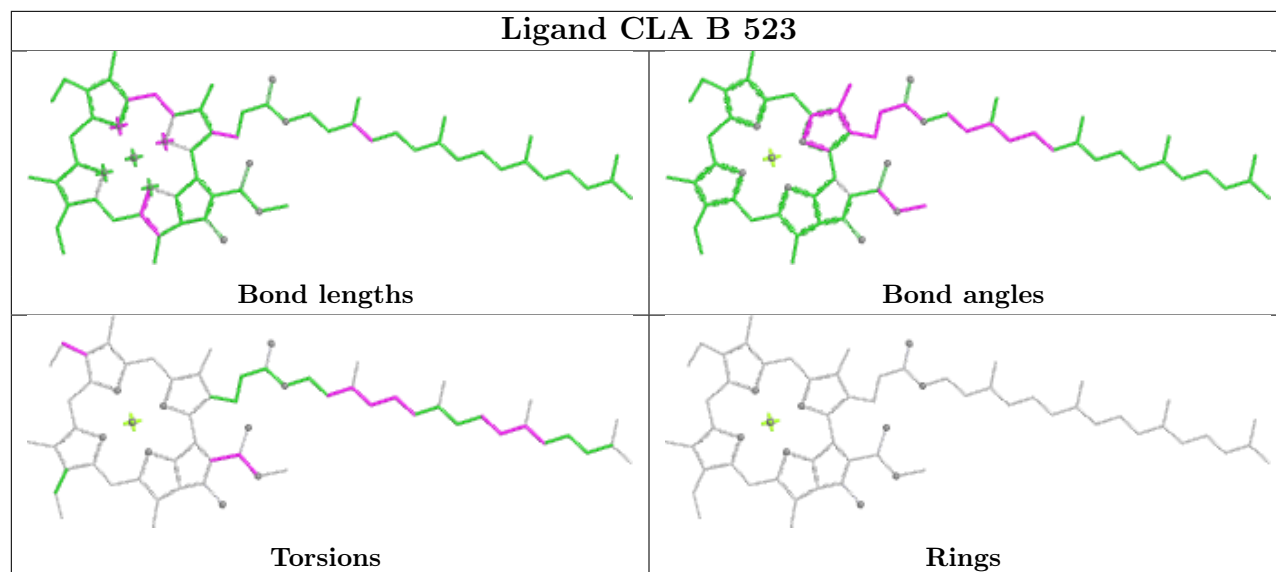
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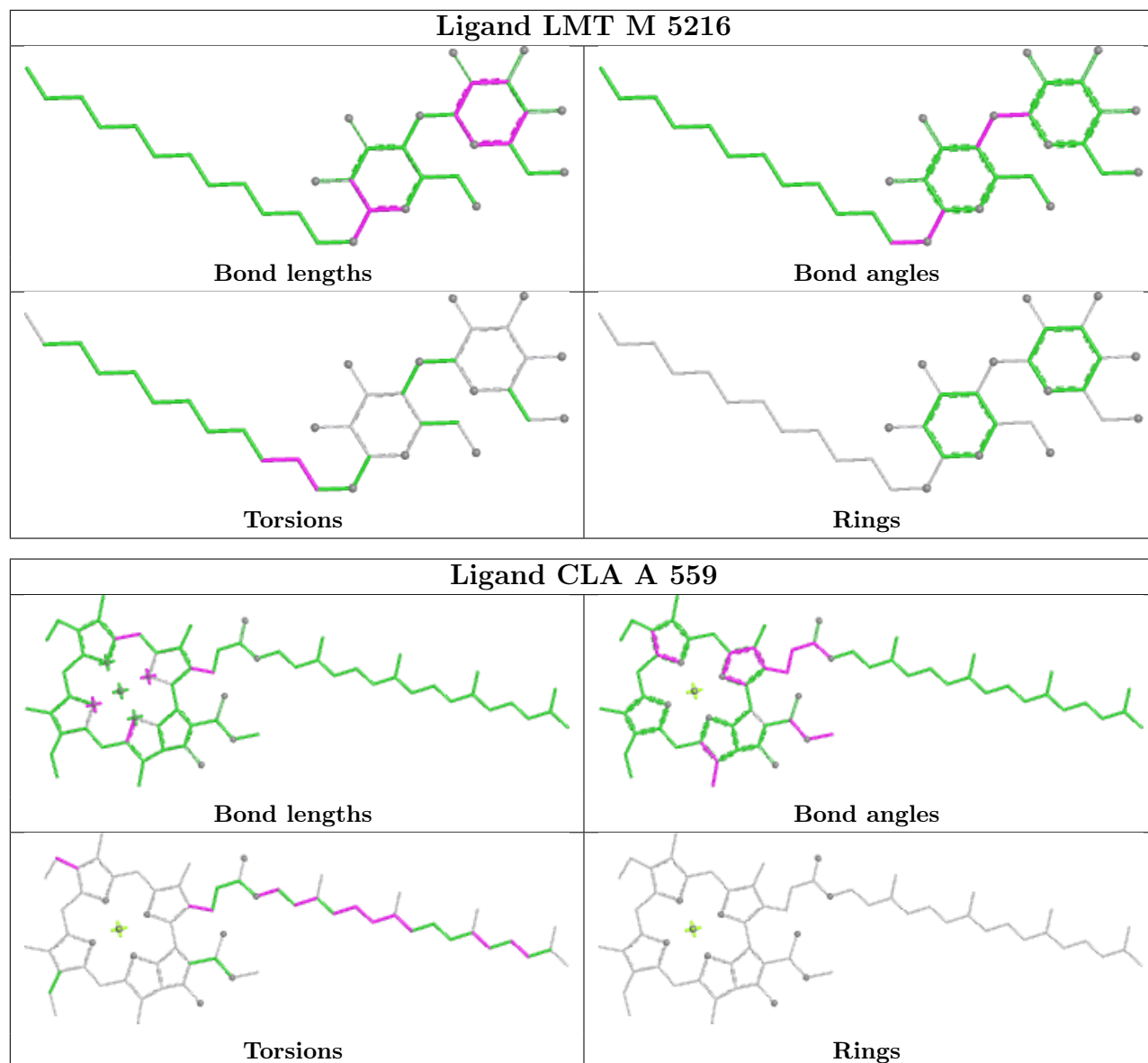
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	517	CLA	9	0
20	B	519	CLA	3	0
27	A	569	LMT	3	0
20	b	5524	CLA	2	0
20	C	502	CLA	2	0
24	c	5504	BCR	9	0
24	b	5527	BCR	3	0
22	A	564	PQ9	1	0
27	T	217	LMT	6	0
20	B	515	CLA	11	0
24	x	5130	BCR	10	0
20	b	5514	CLA	6	0
24	B	528	BCR	2	0
21	a	5562	PHO	7	0
21	A	562	PHO	6	0
24	d	5357	BCR	6	0
30	c	5508	DGD	4	0
20	c	5498	CLA	5	0
28	D	360	MGE	7	0
32	V	552	HEM	2	0
20	c	5491	CLA	2	0
20	b	5515	CLA	10	0
20	A	560	CLA	1	0
28	d	5359	MGE	2	0
21	A	561	PHO	6	0
24	A	566	BCR	1	0
20	a	5560	CLA	1	0
24	C	504	BCR	7	0
25	A	567	LHG	4	0
20	B	514	CLA	5	0
20	B	516	CLA	3	0
20	C	494	CLA	2	0
20	c	5502	CLA	1	0
20	c	5494	CLA	2	0
20	B	511	CLA	1	0
20	a	5558	CLA	10	0
20	b	5522	CLA	4	0
24	a	5566	BCR	3	0
30	C	509	DGD	10	0
20	B	526	CLA	1	0
24	C	505	BCR	6	0
20	A	558	CLA	9	0

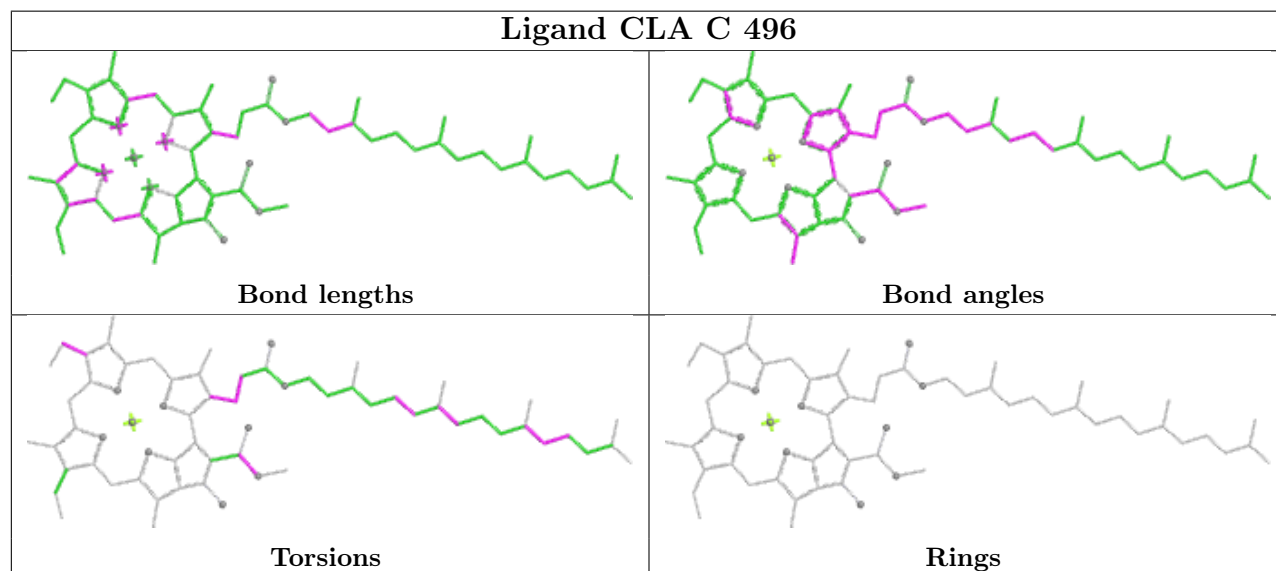
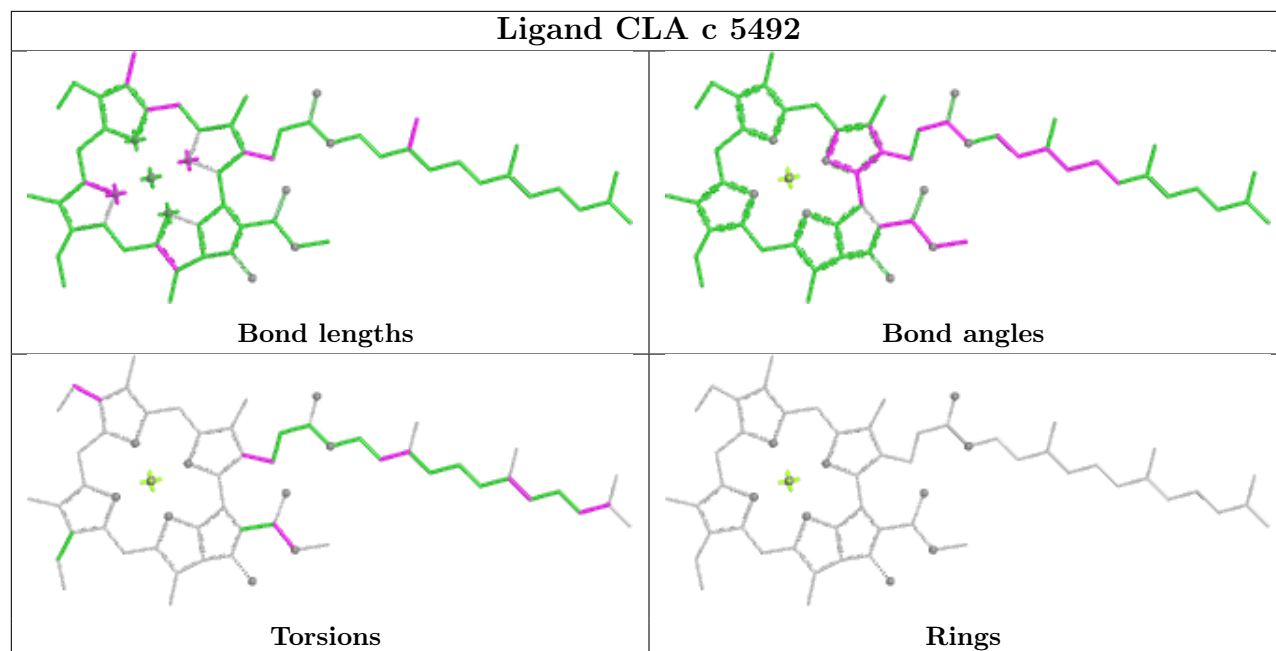
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

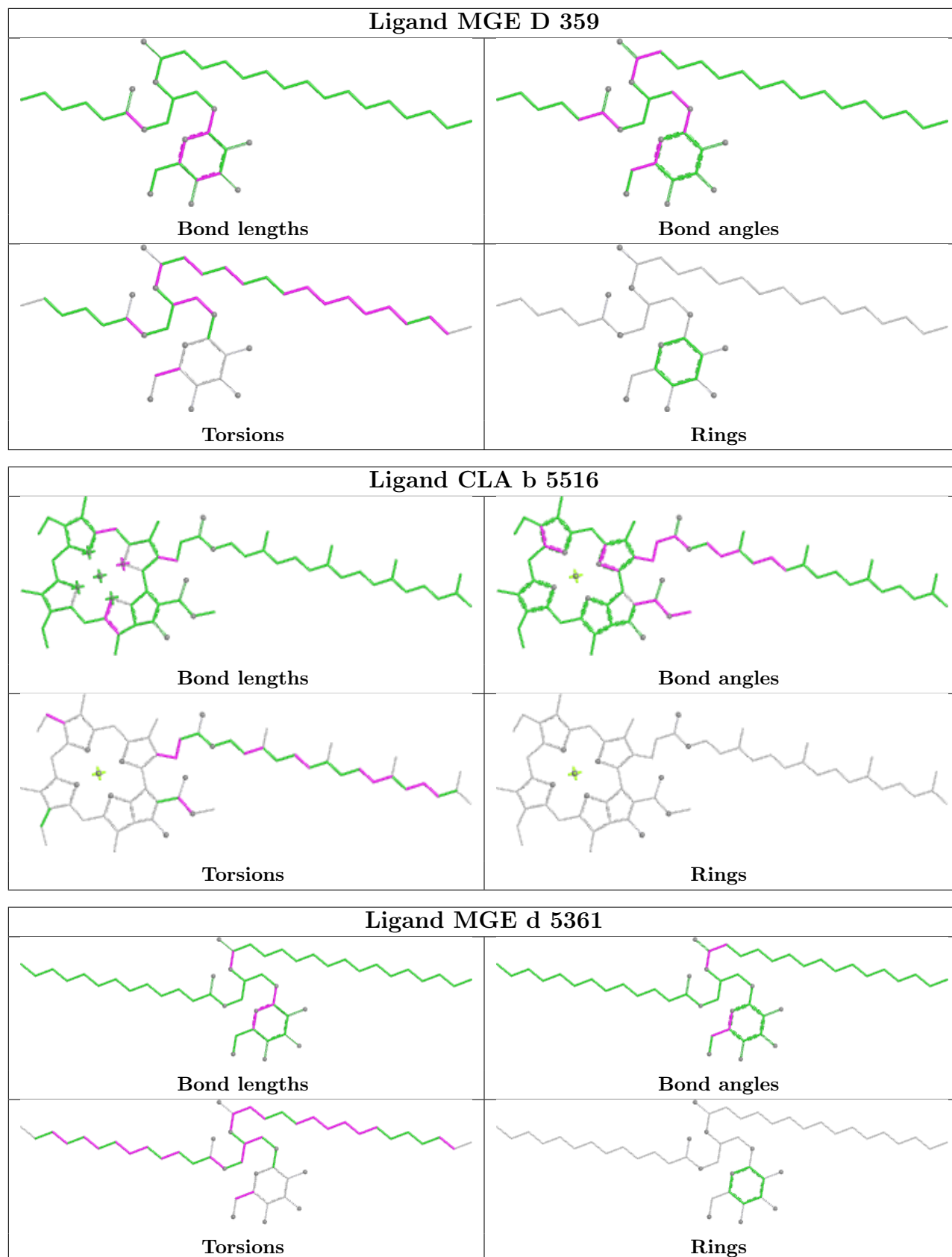


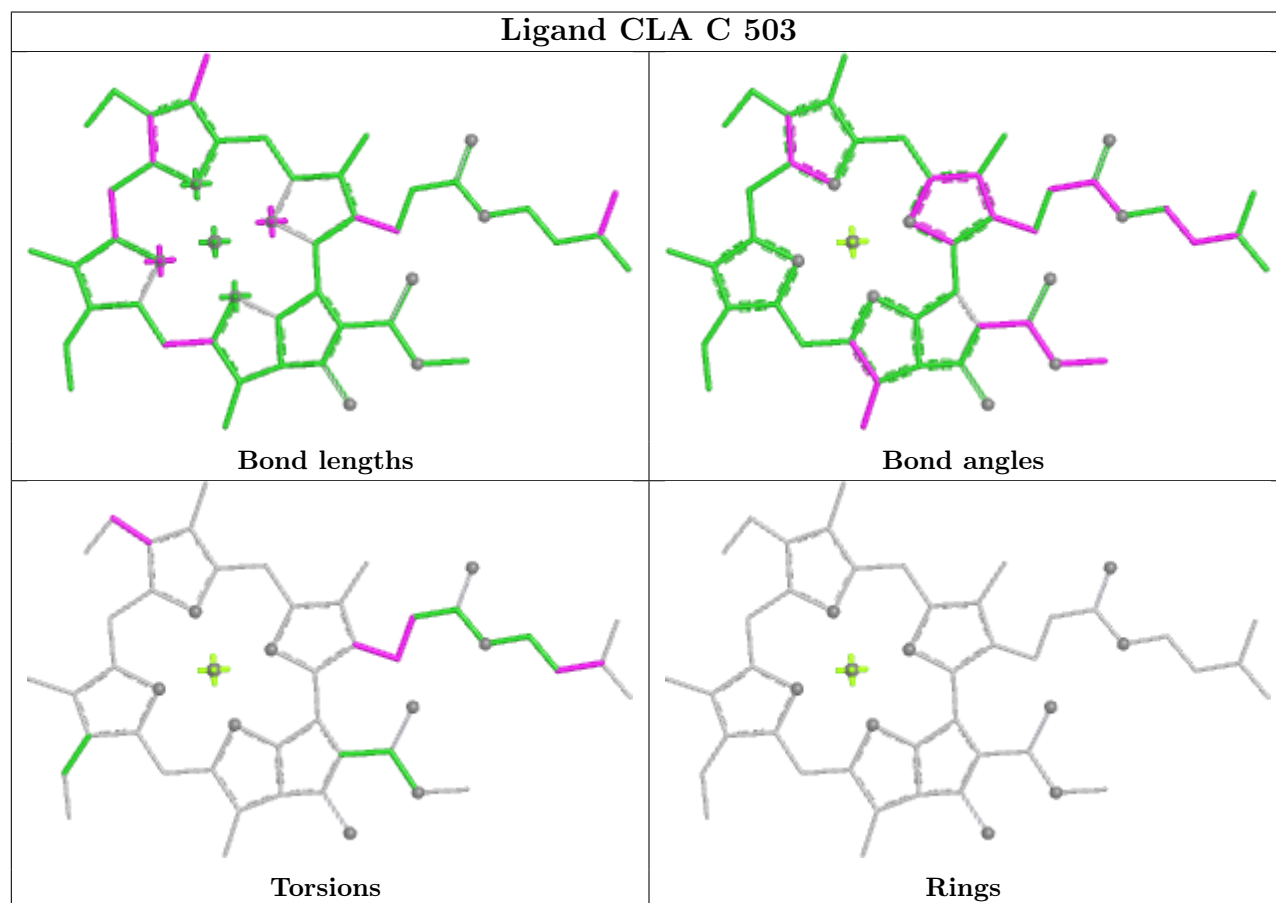
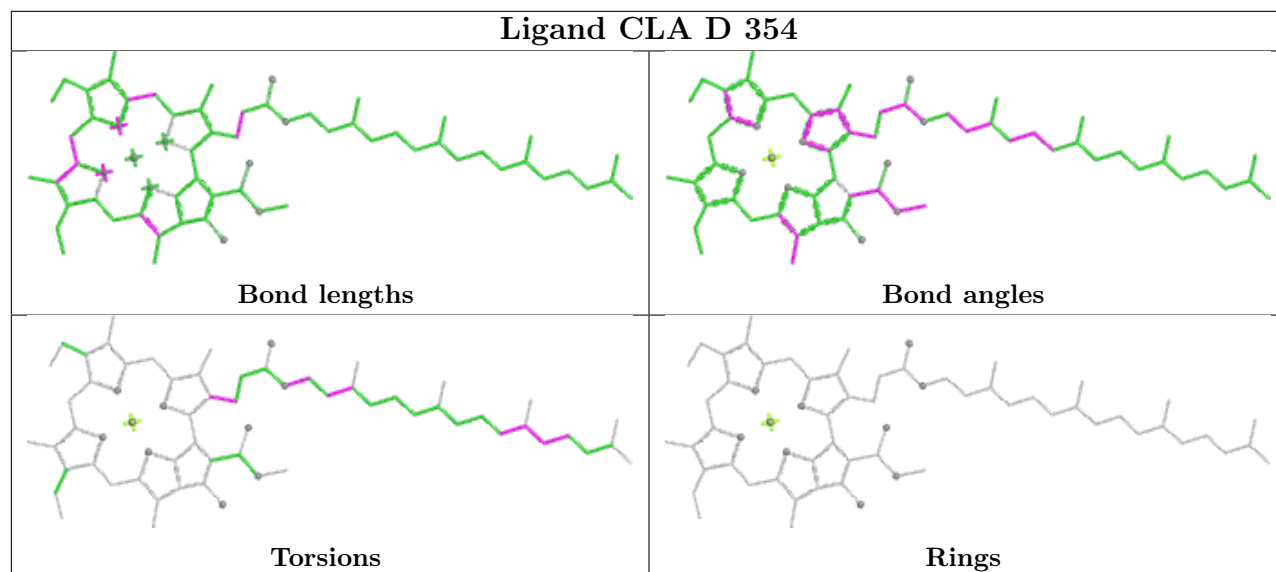


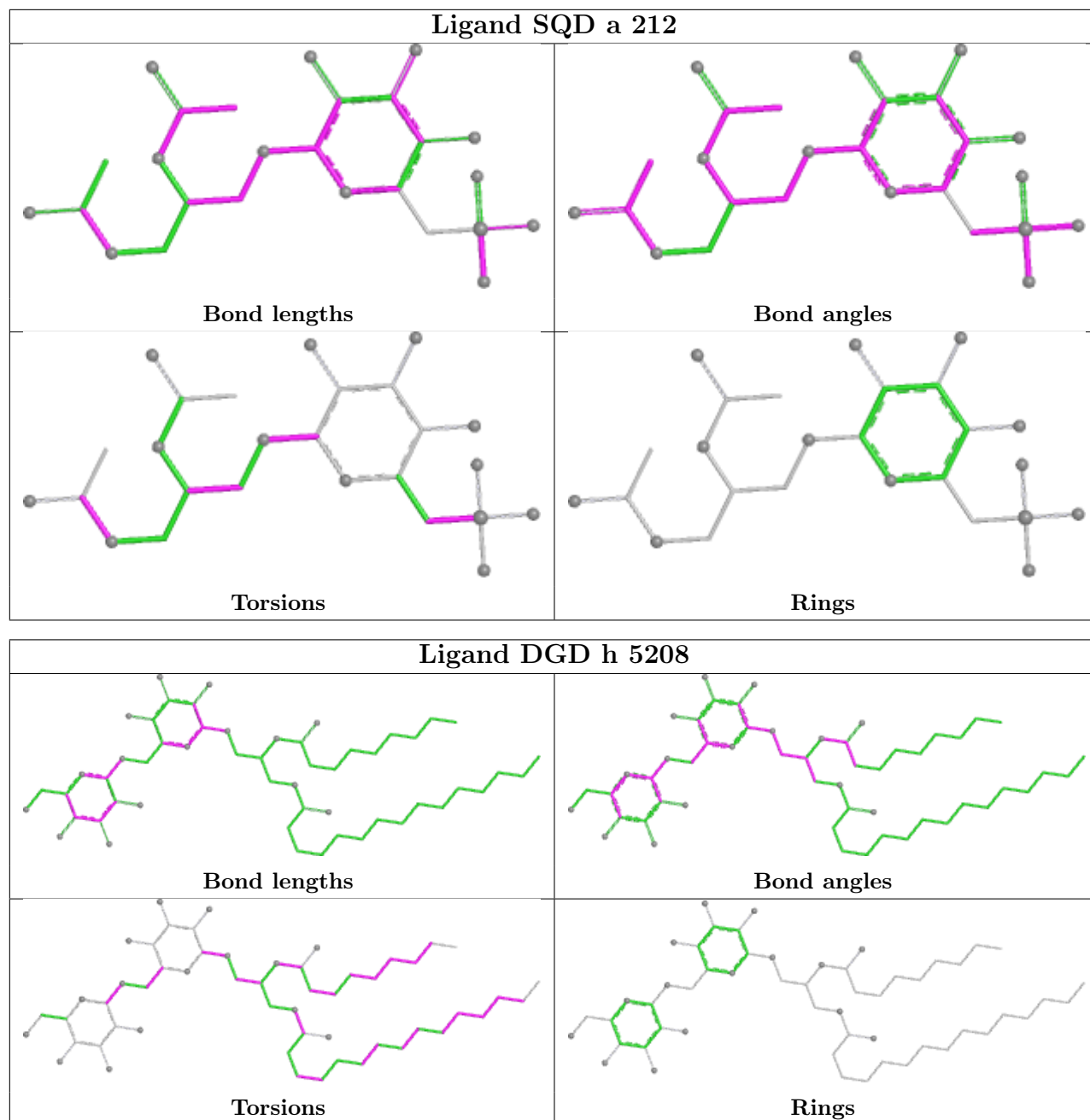


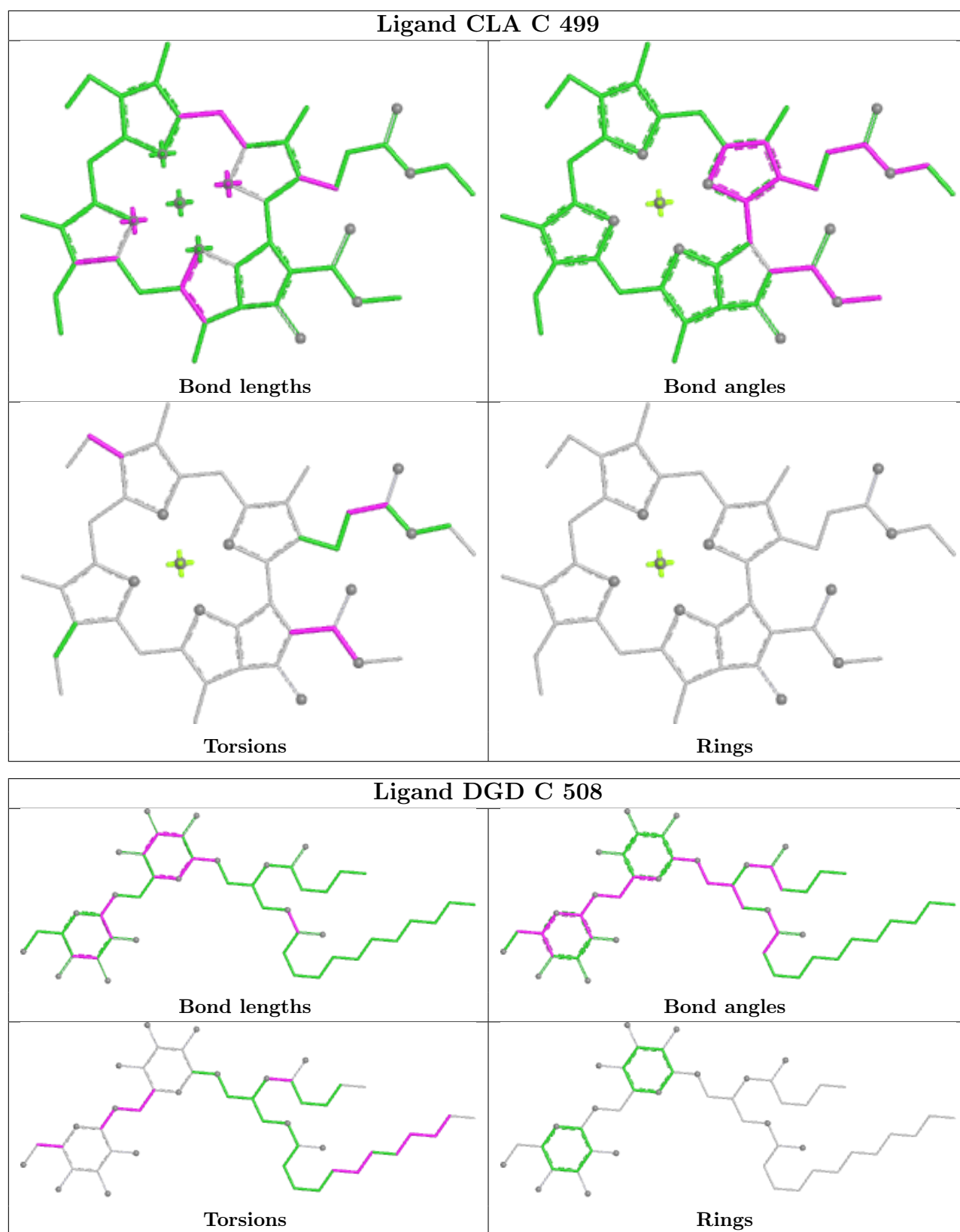


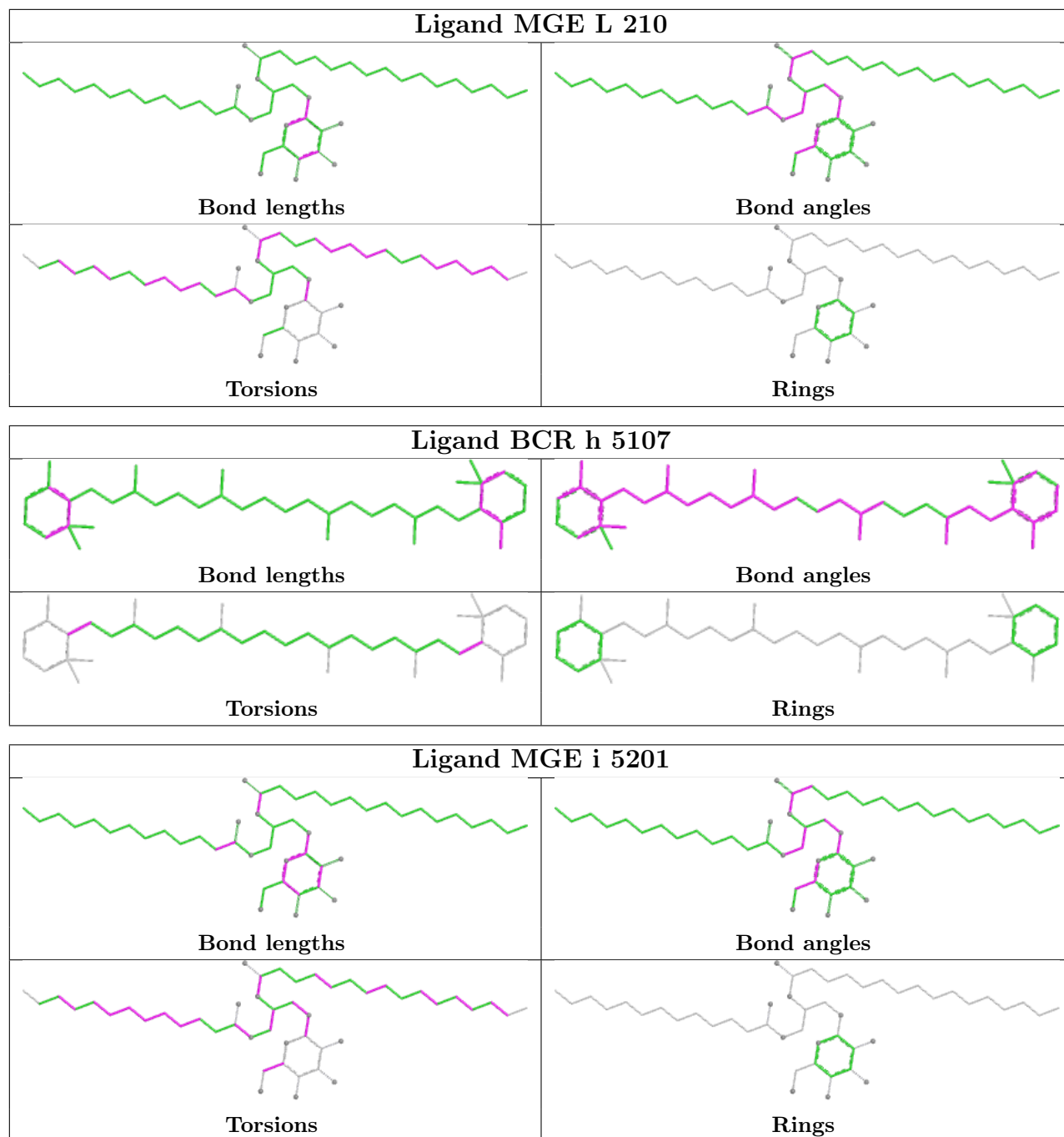


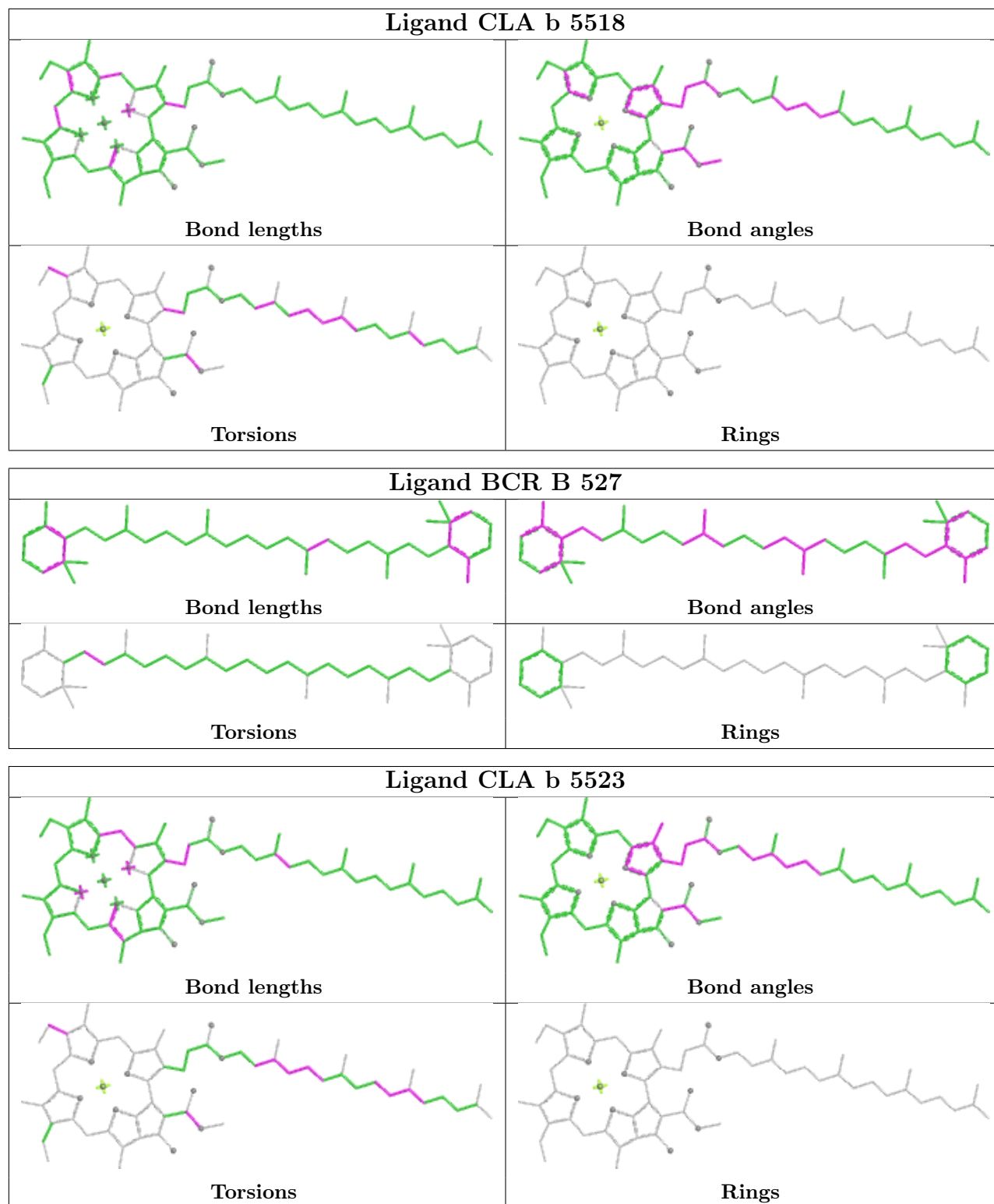


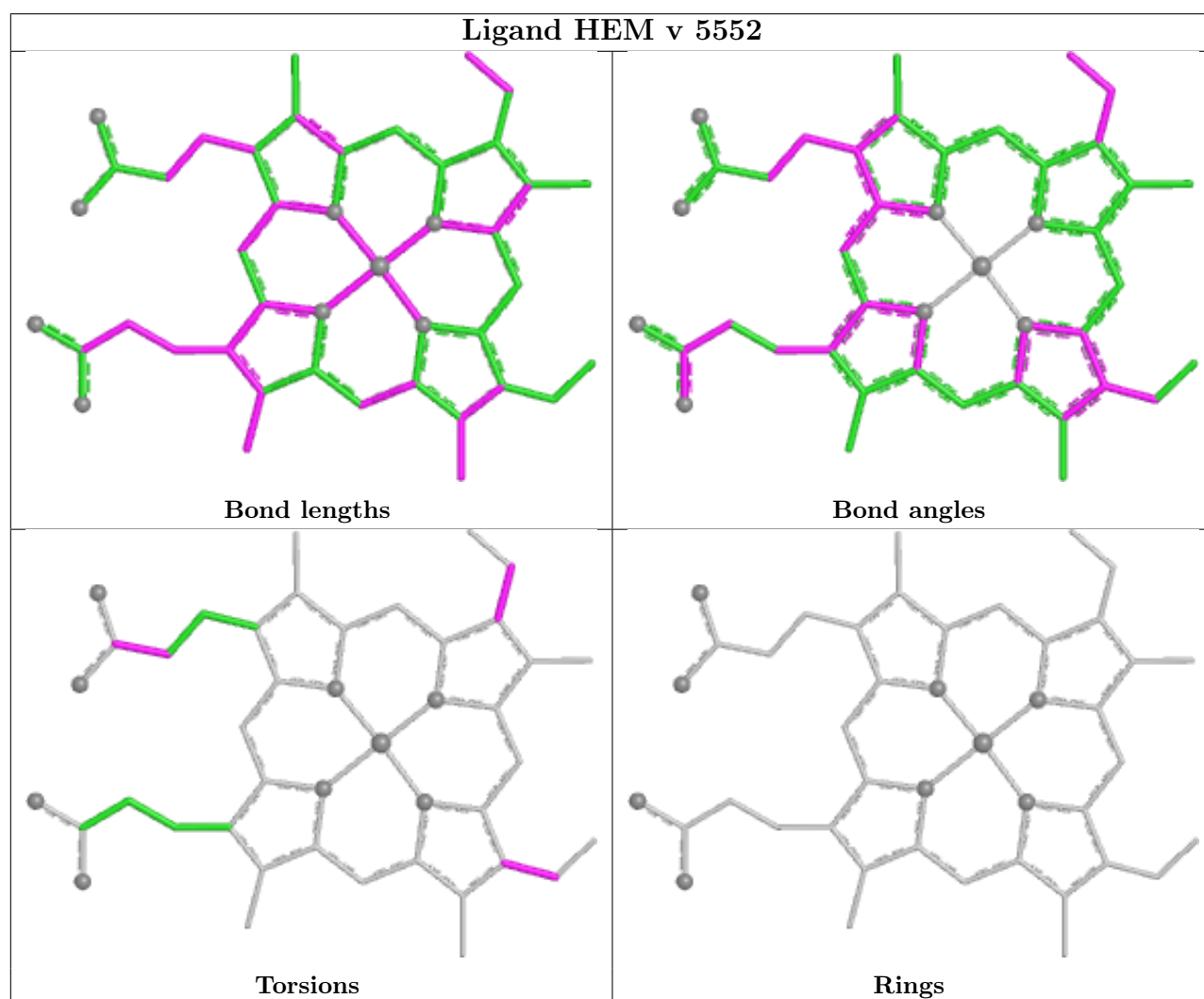
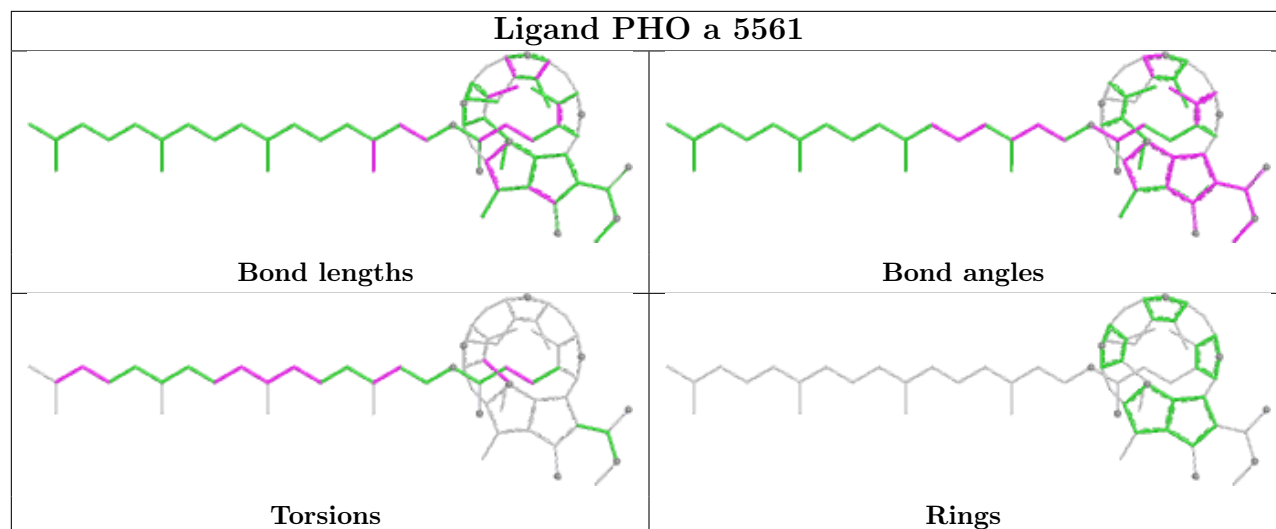


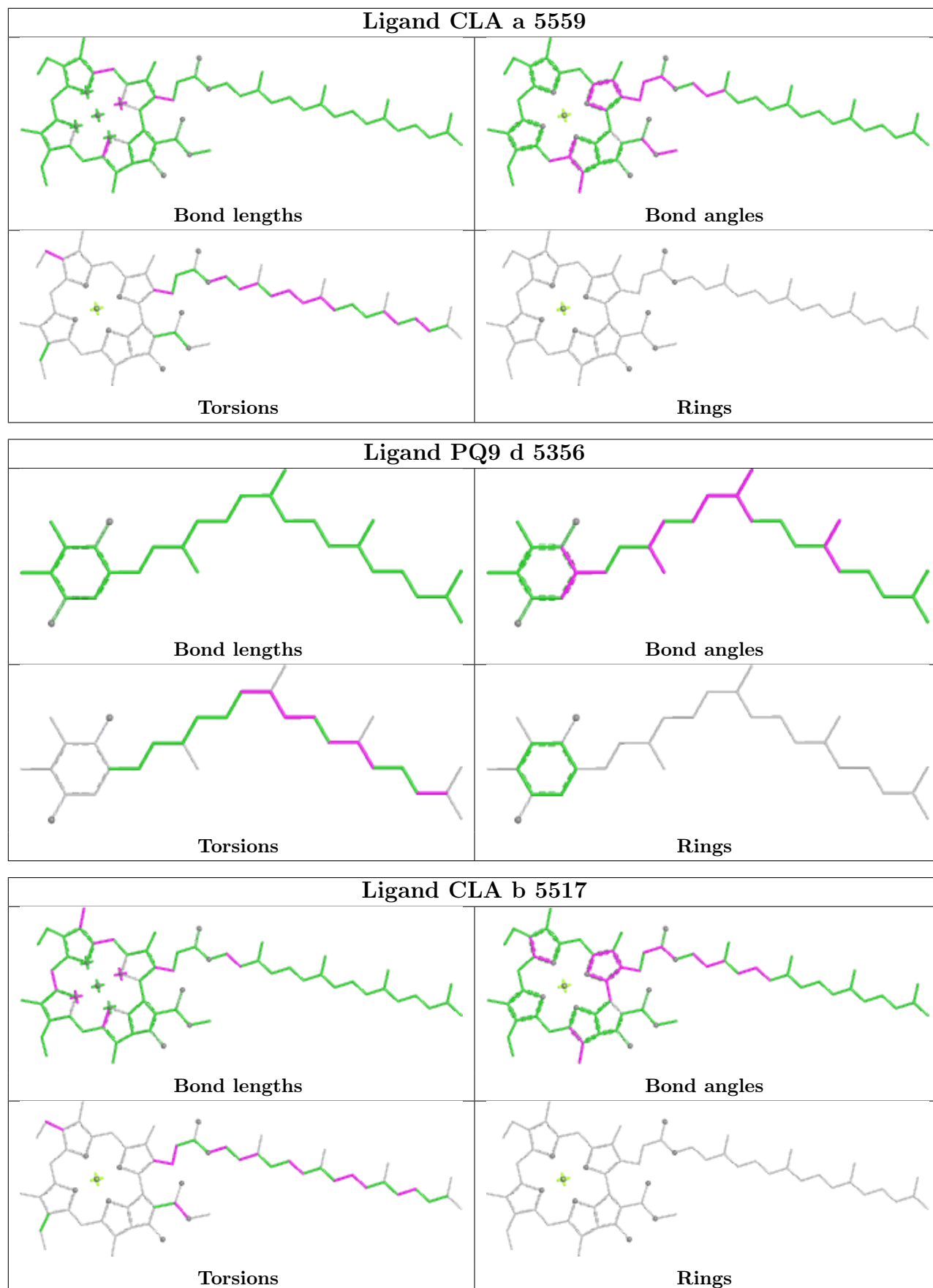


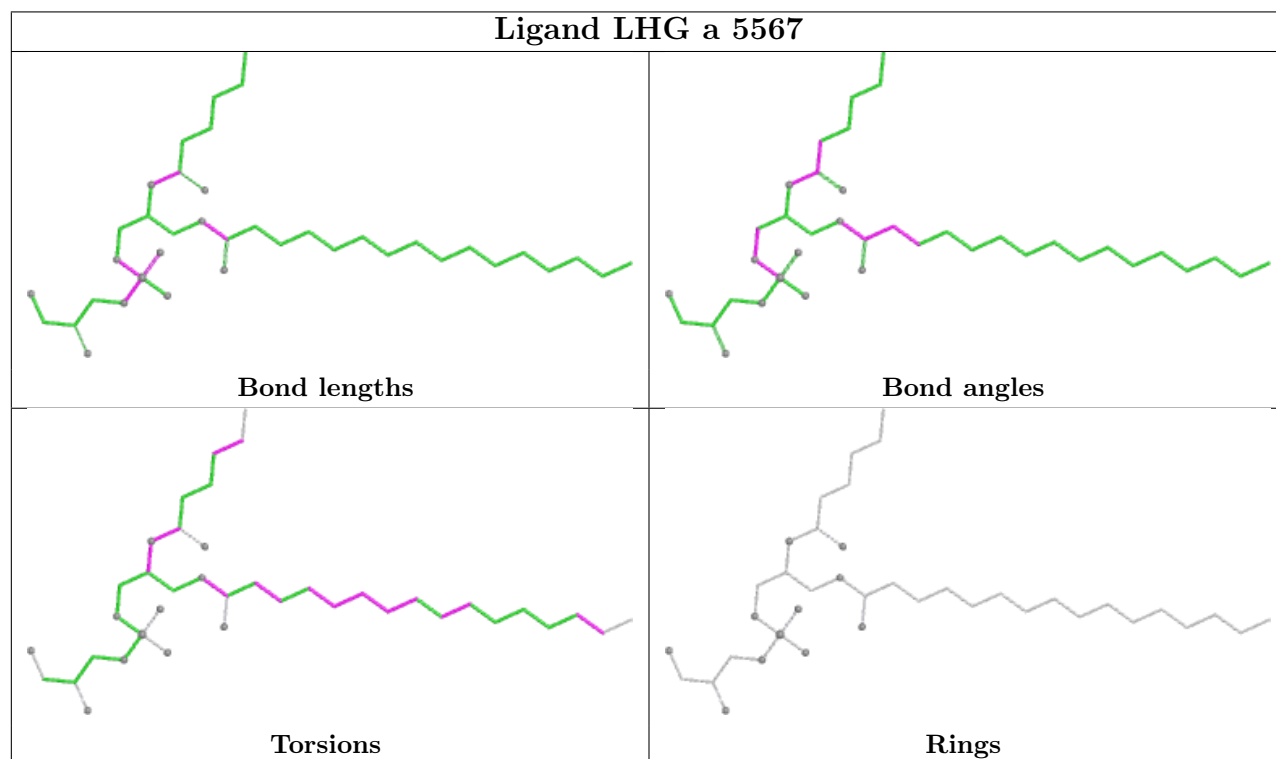
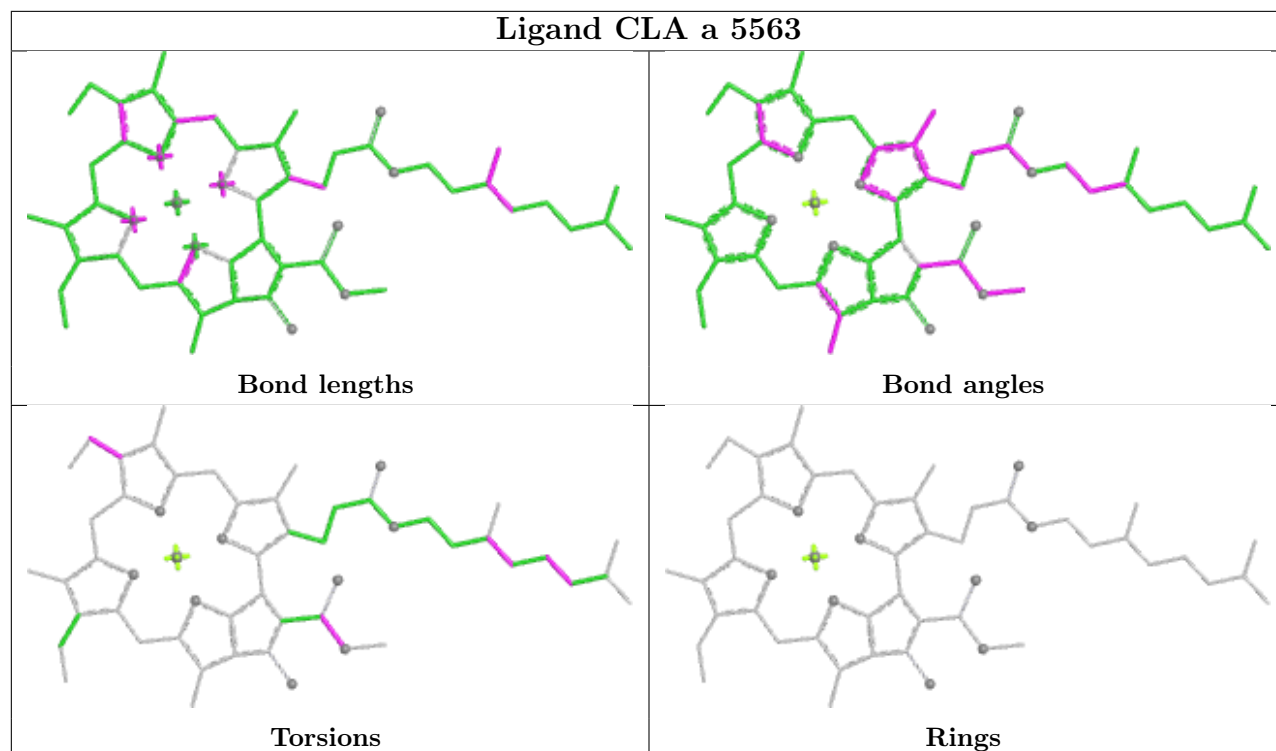


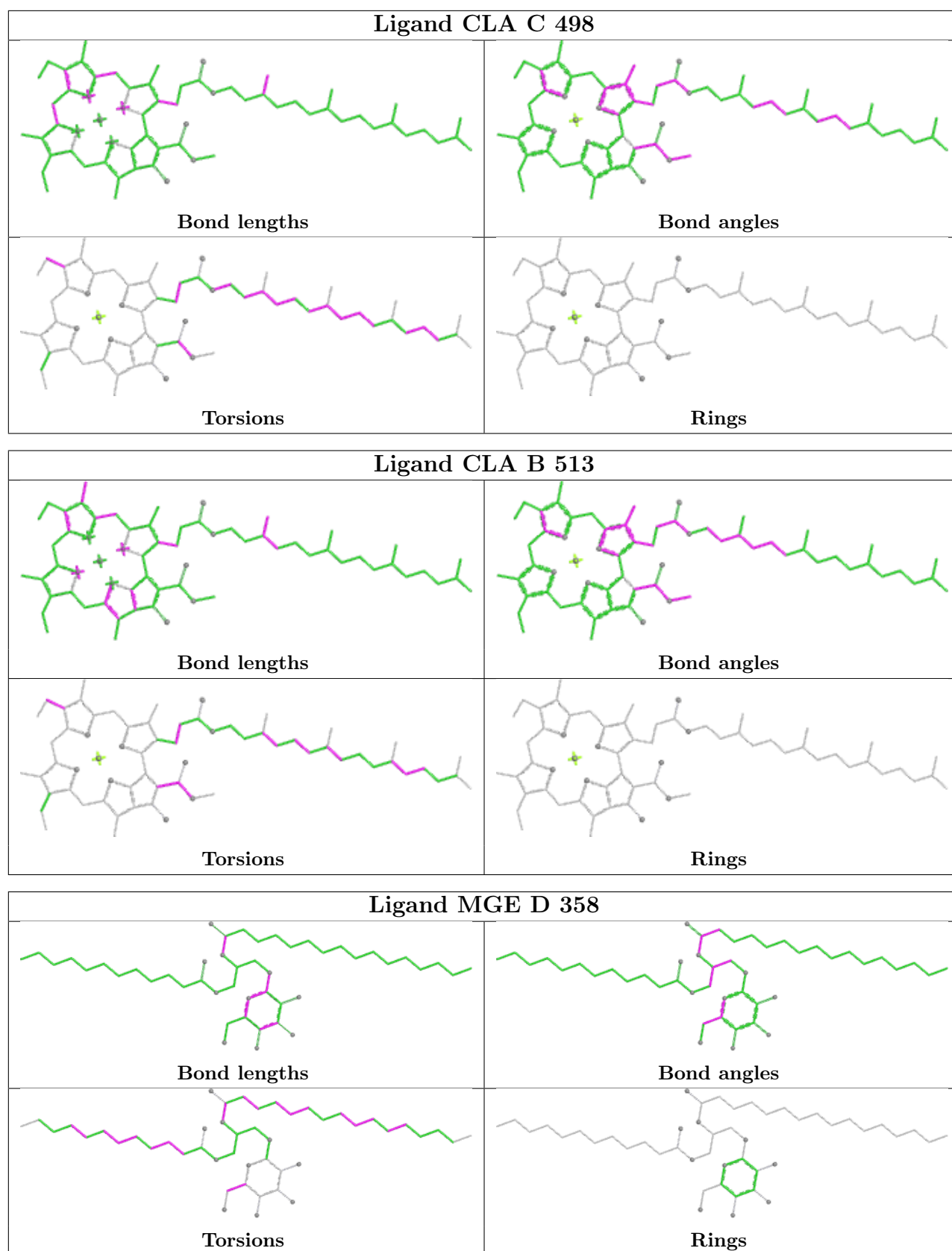


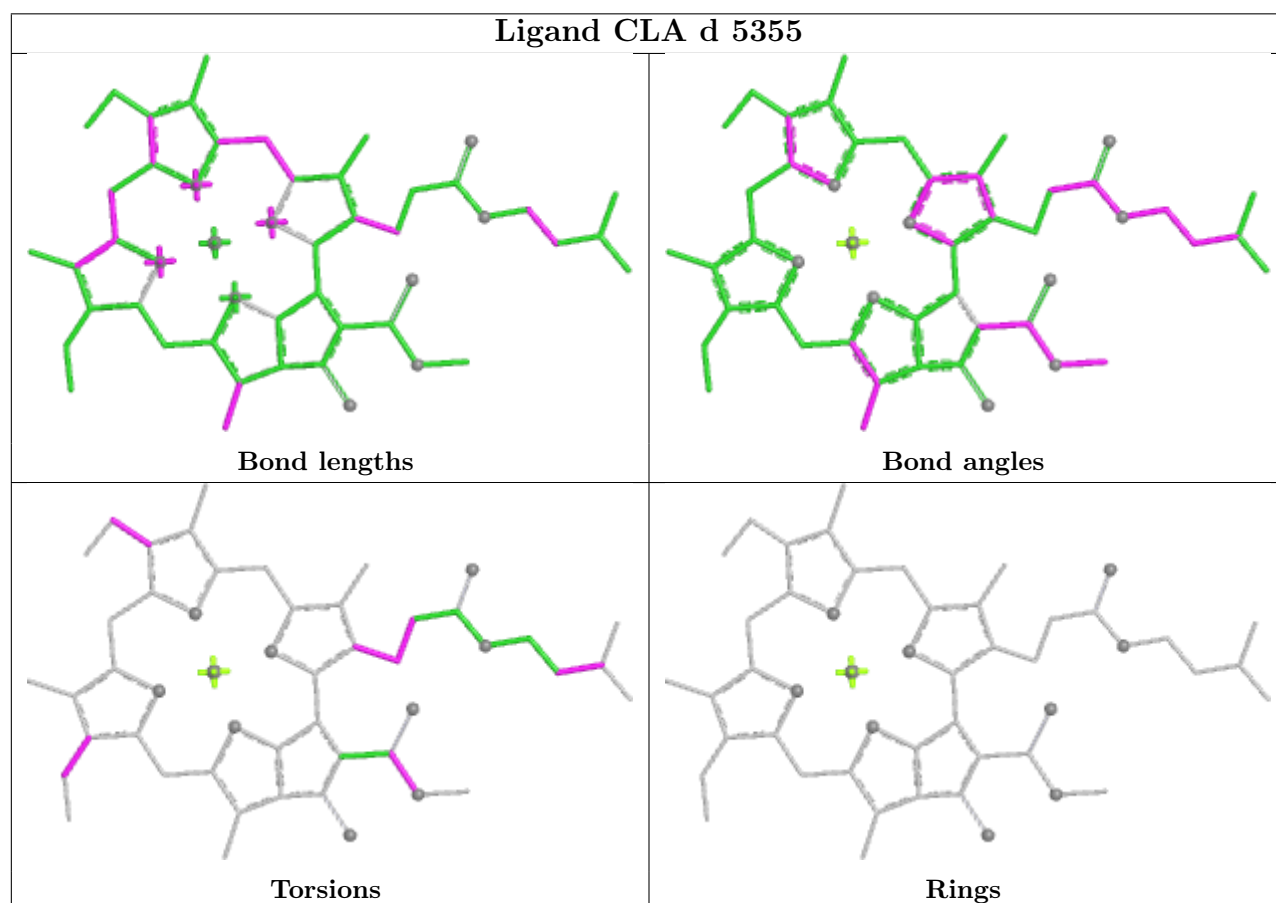
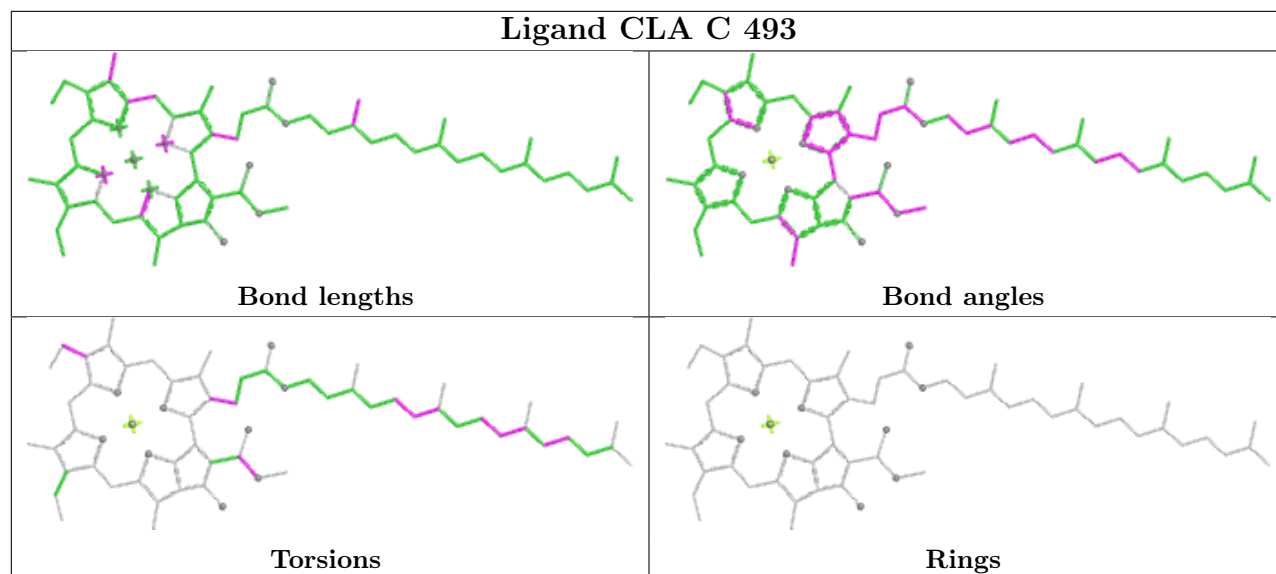


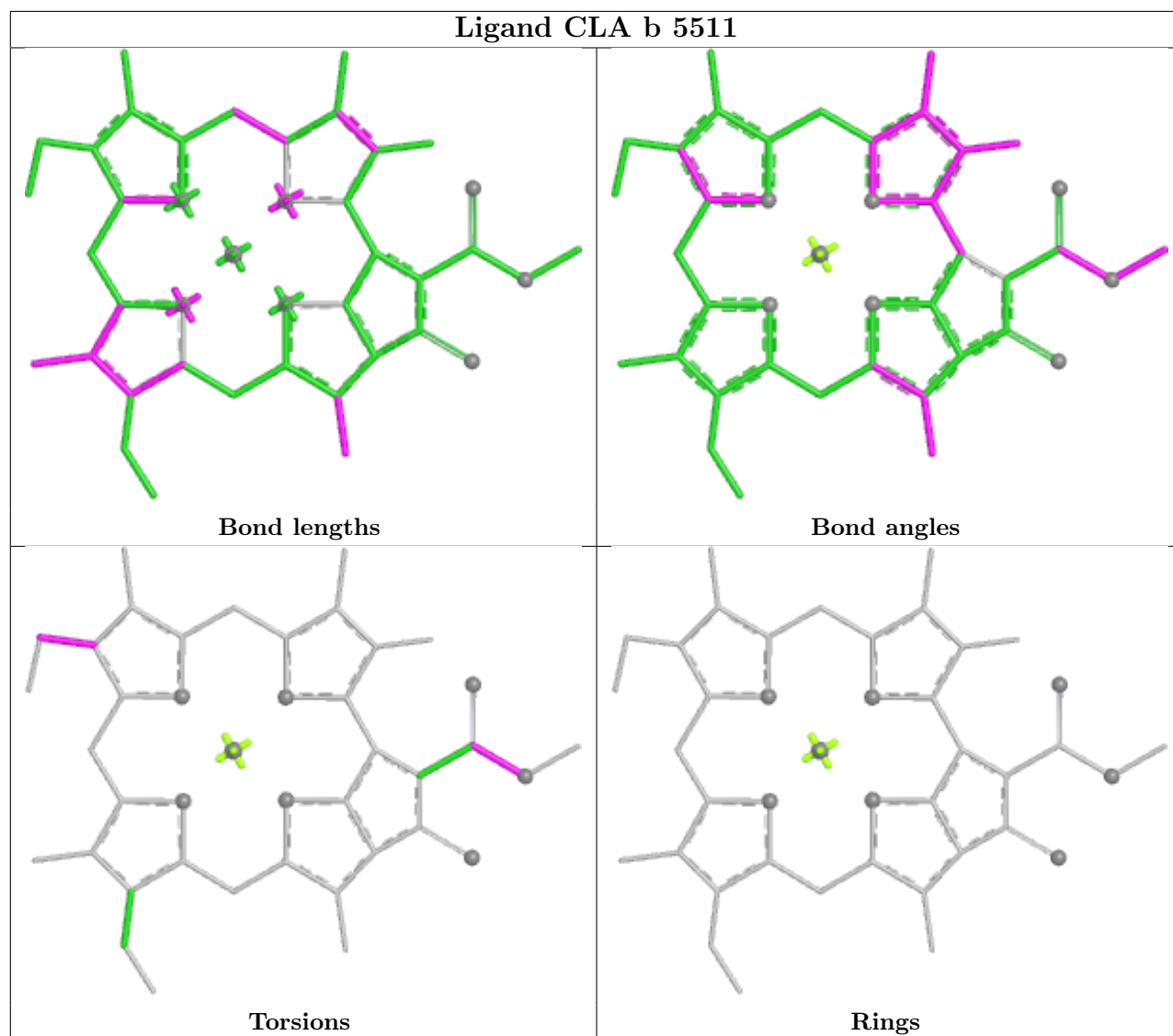
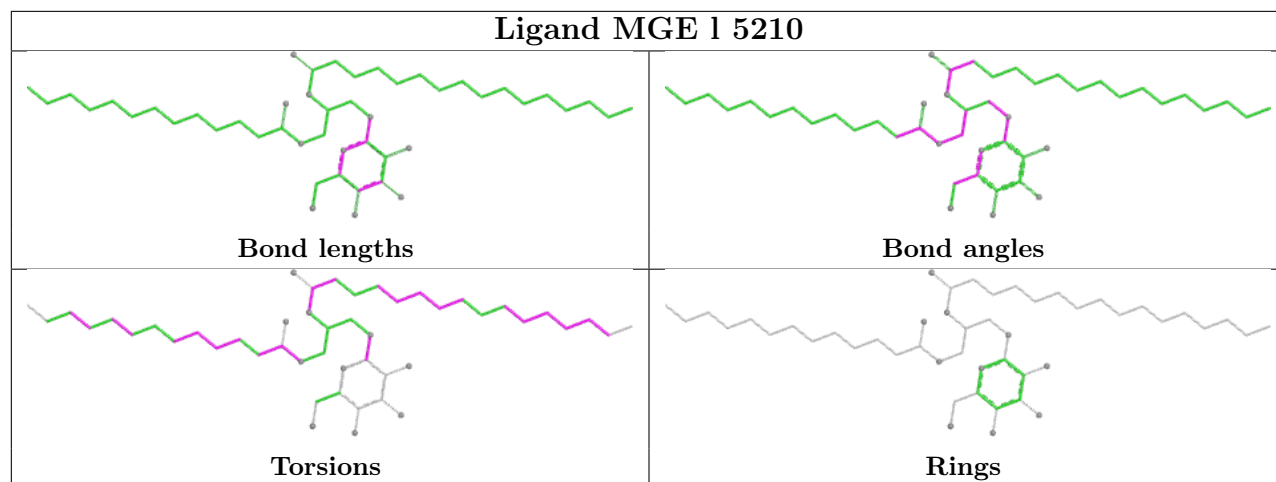


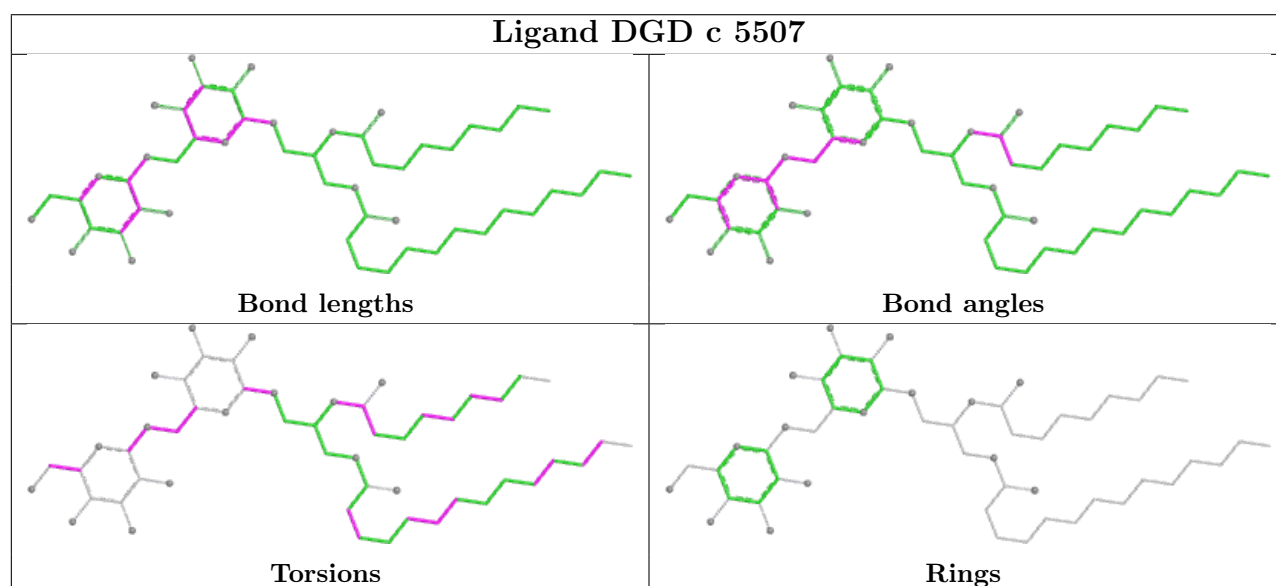
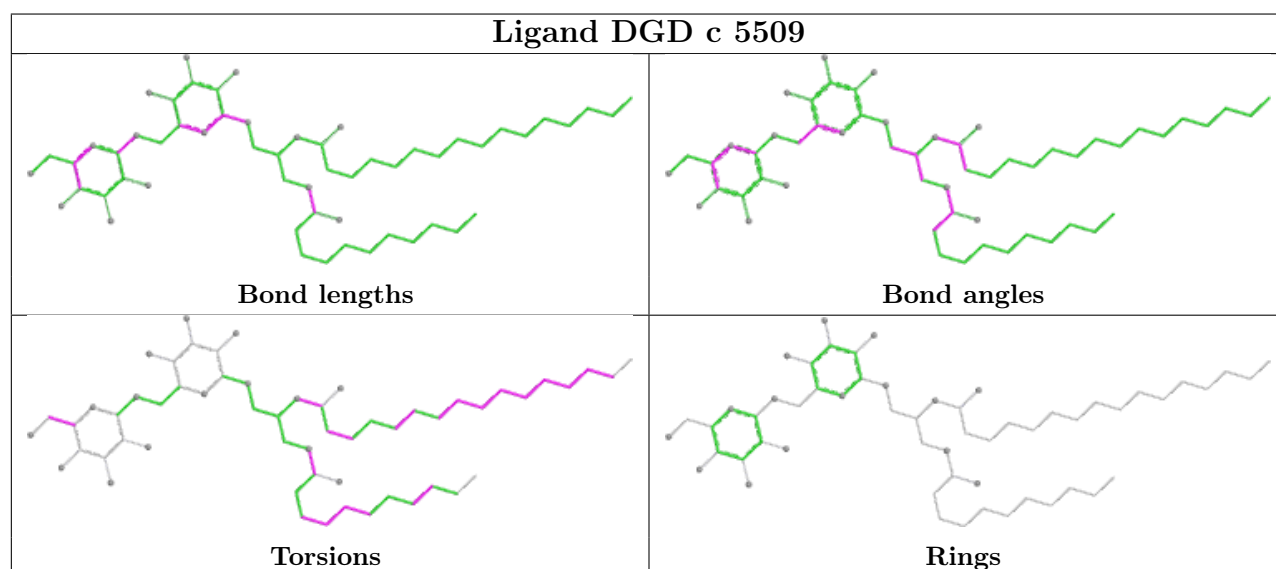
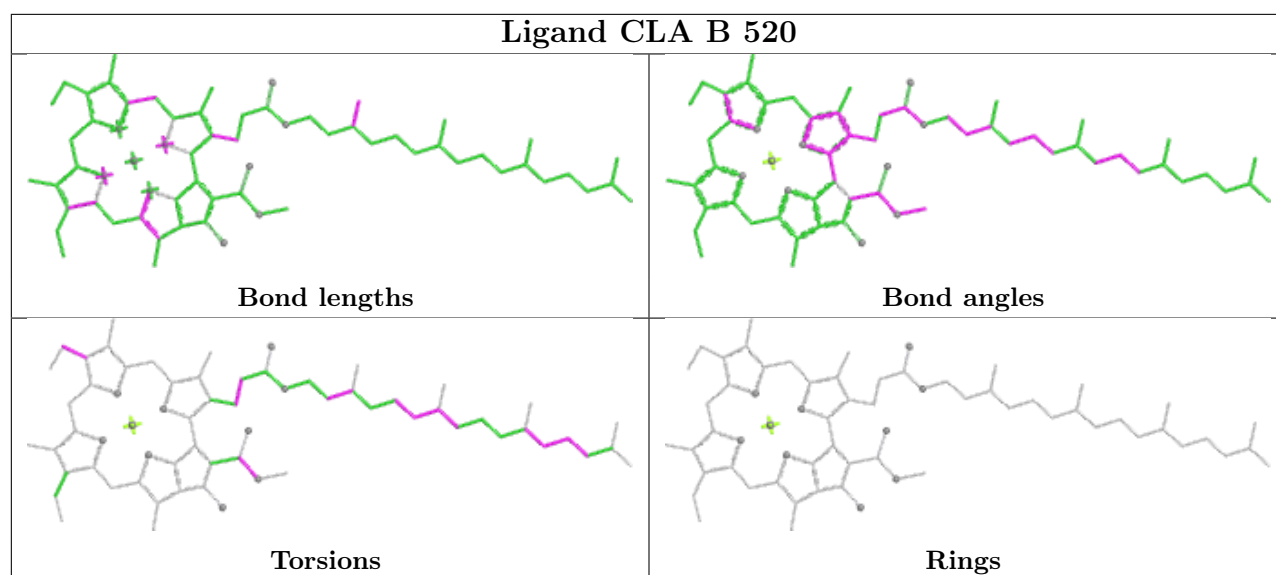


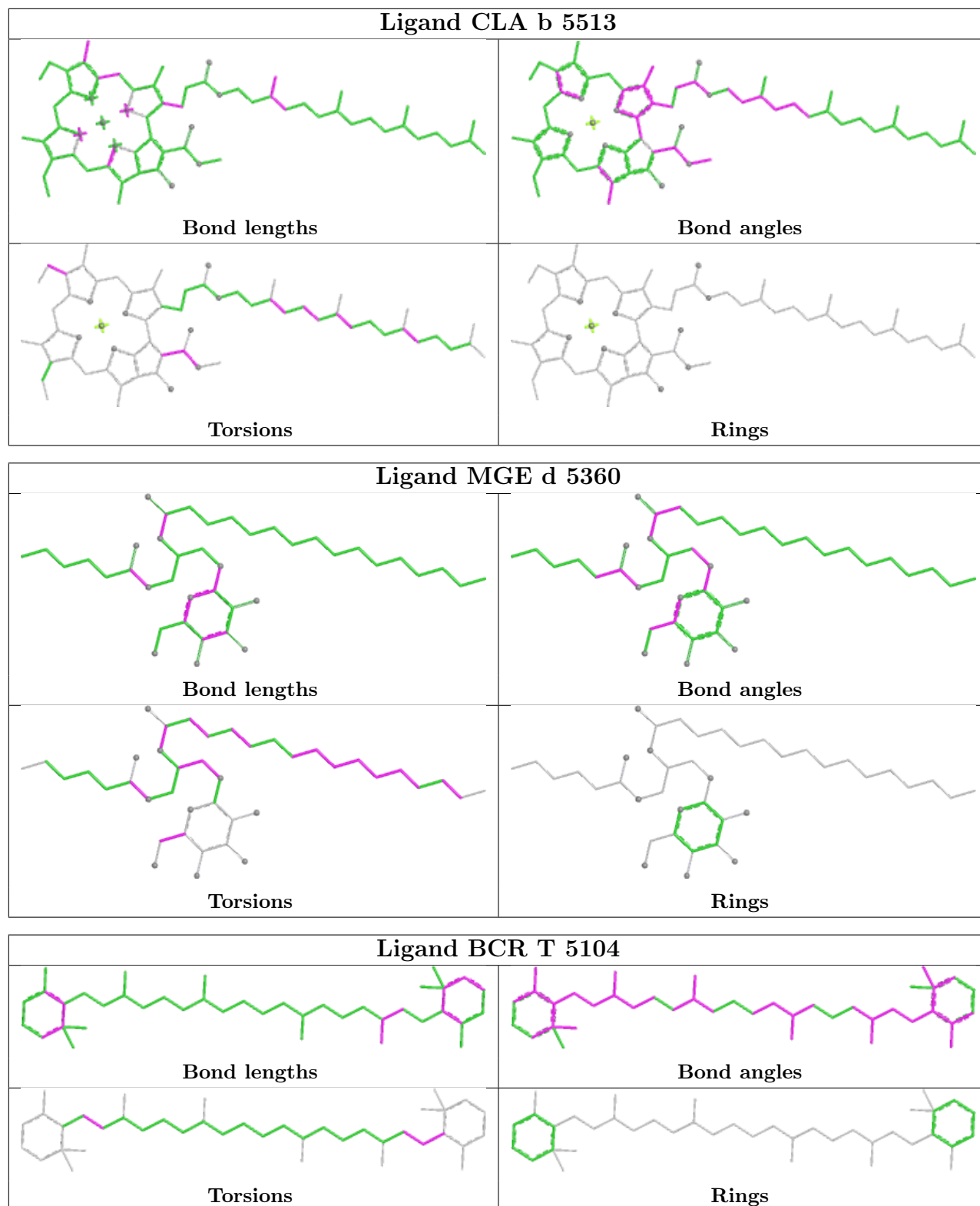


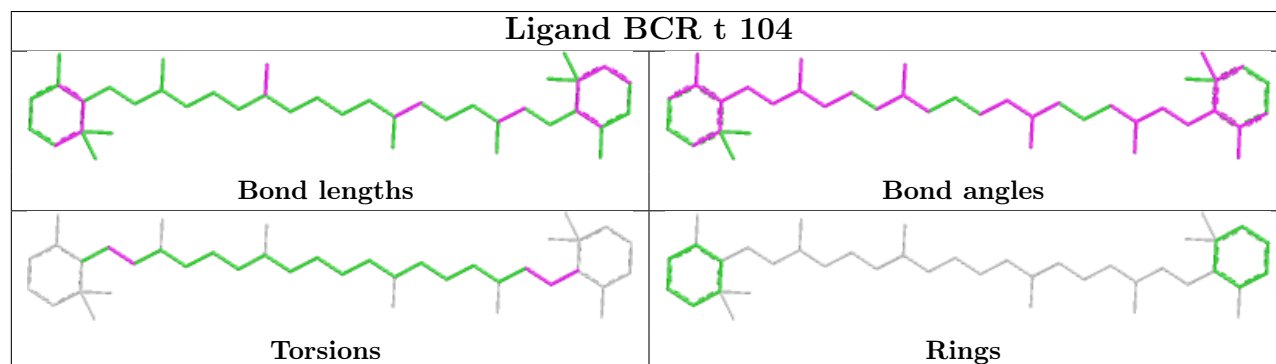
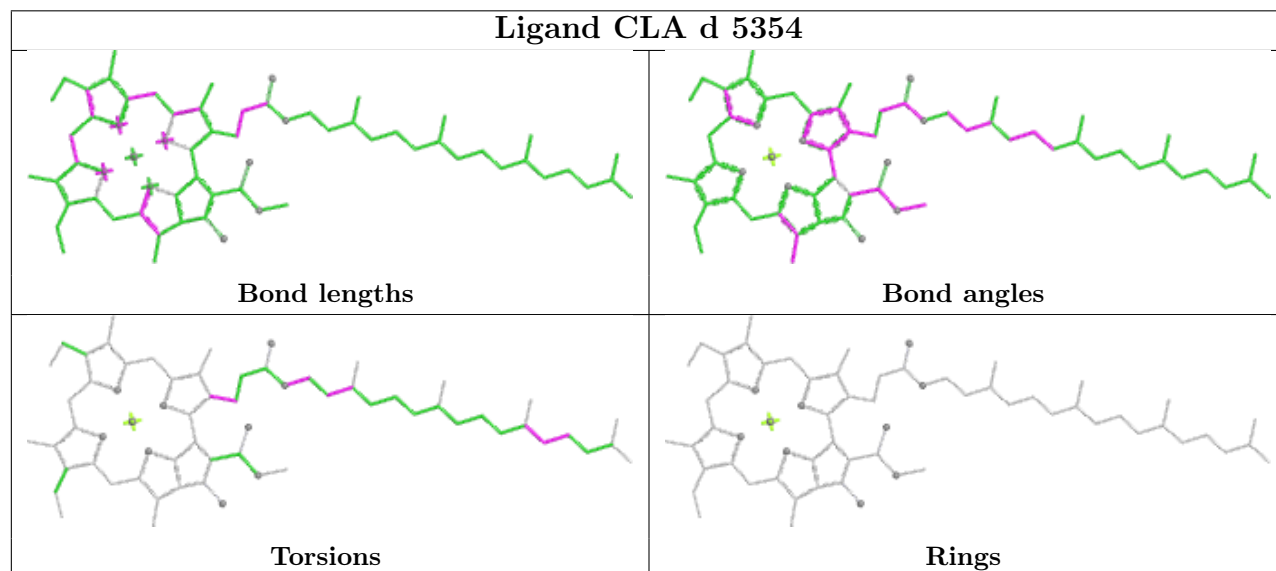
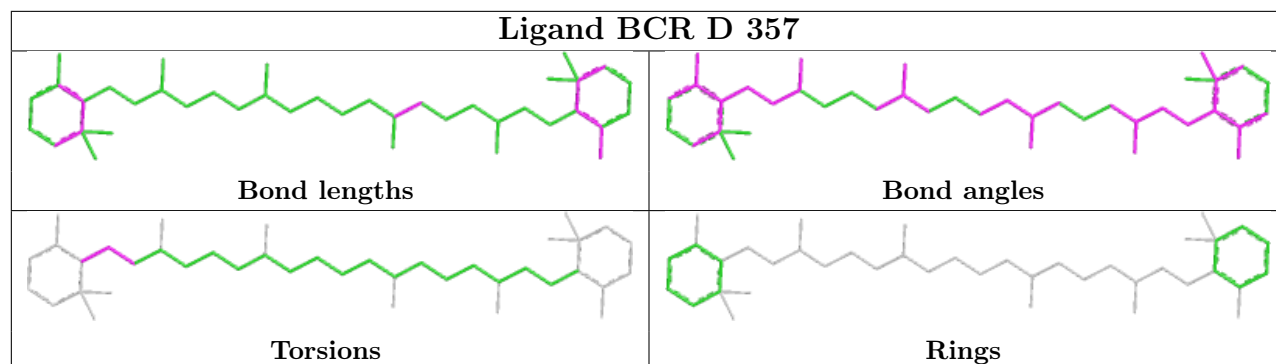


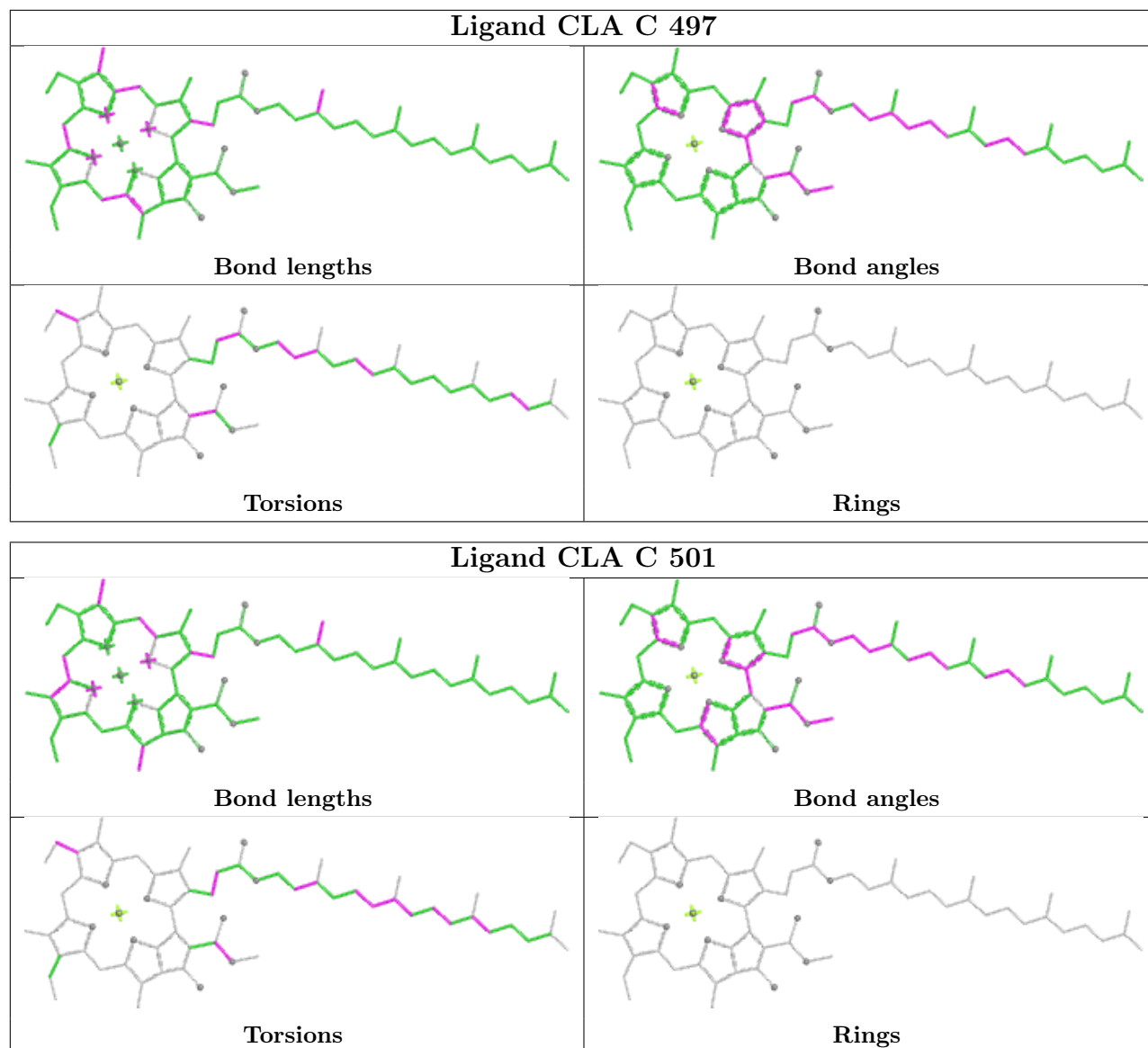


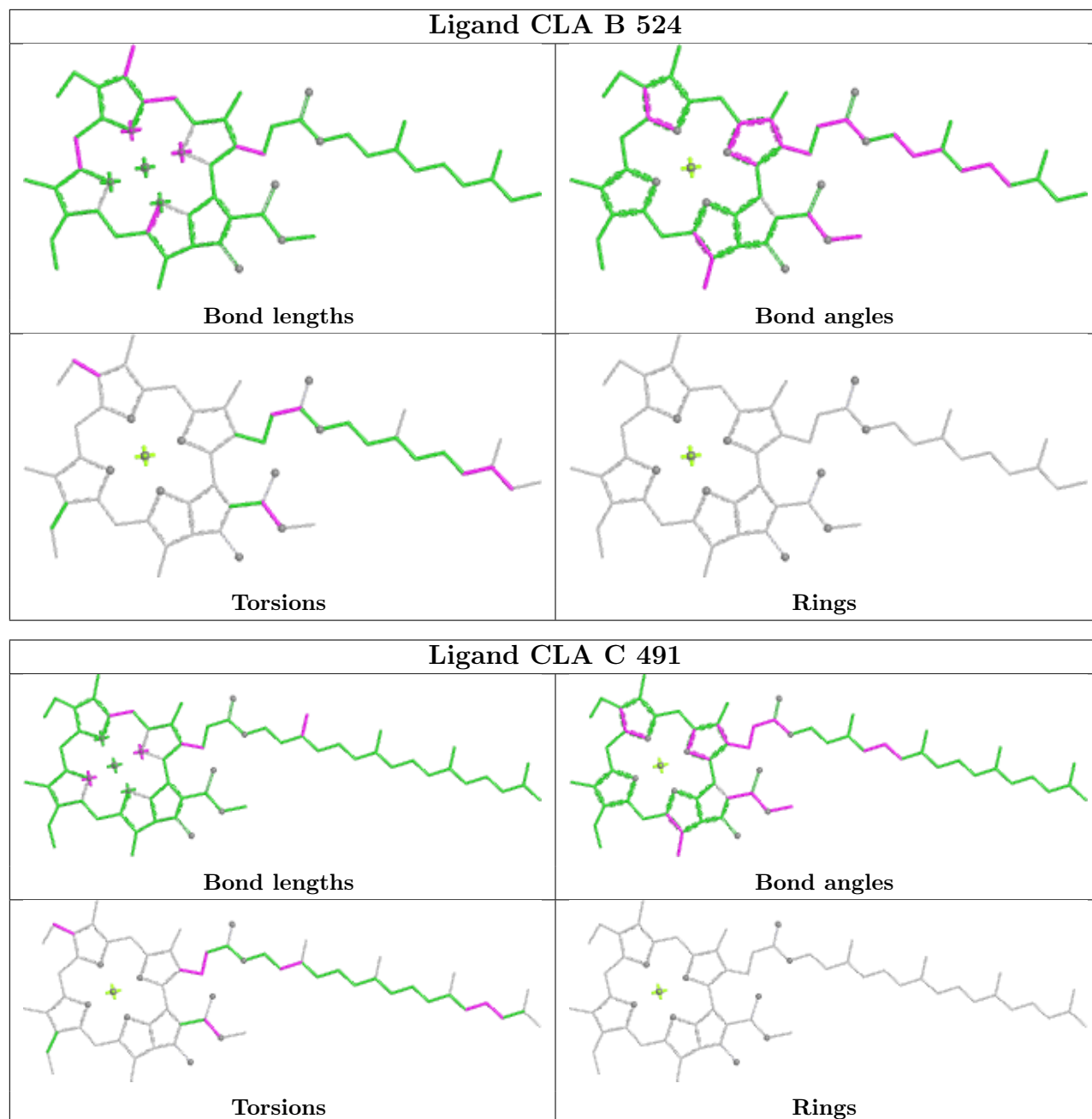


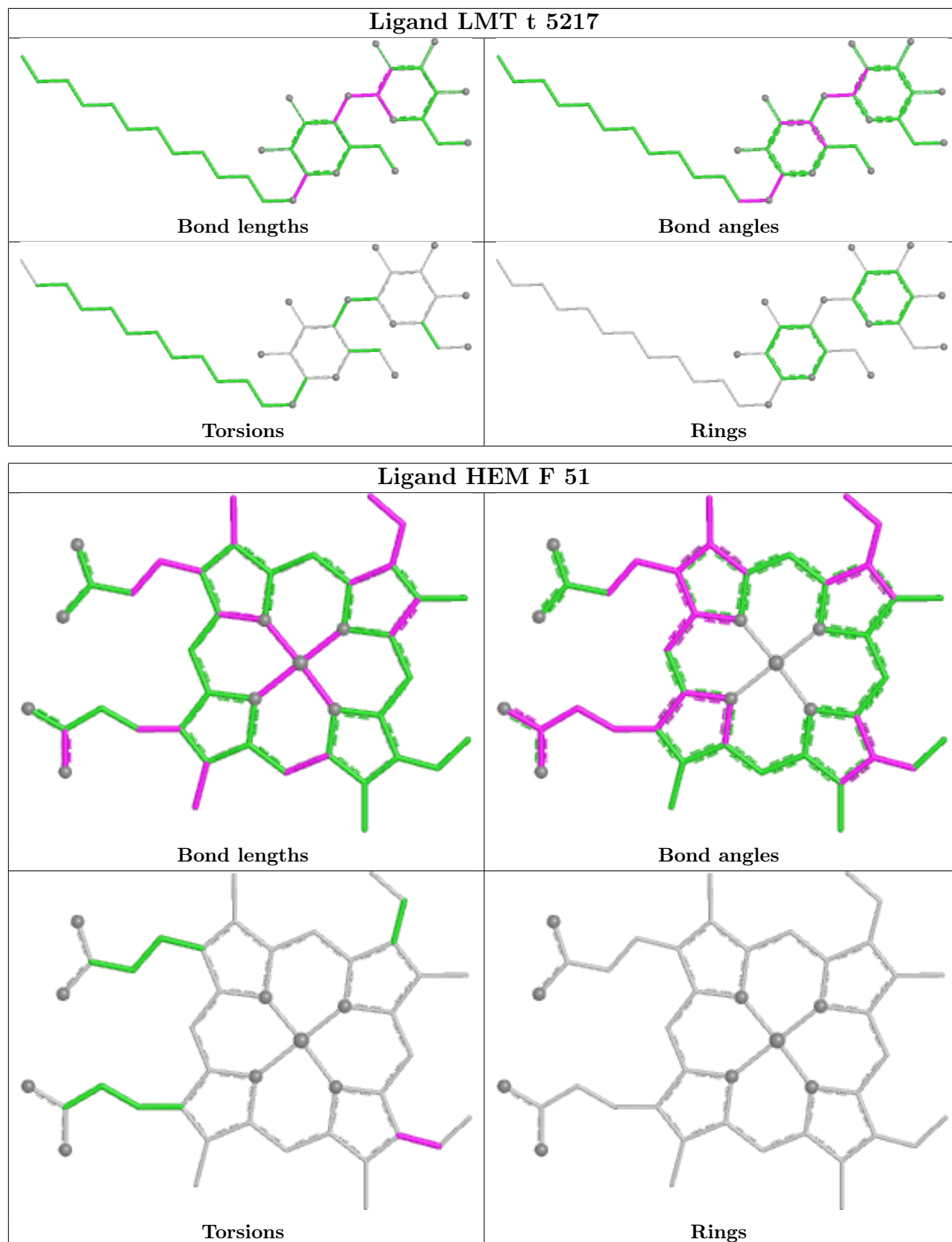


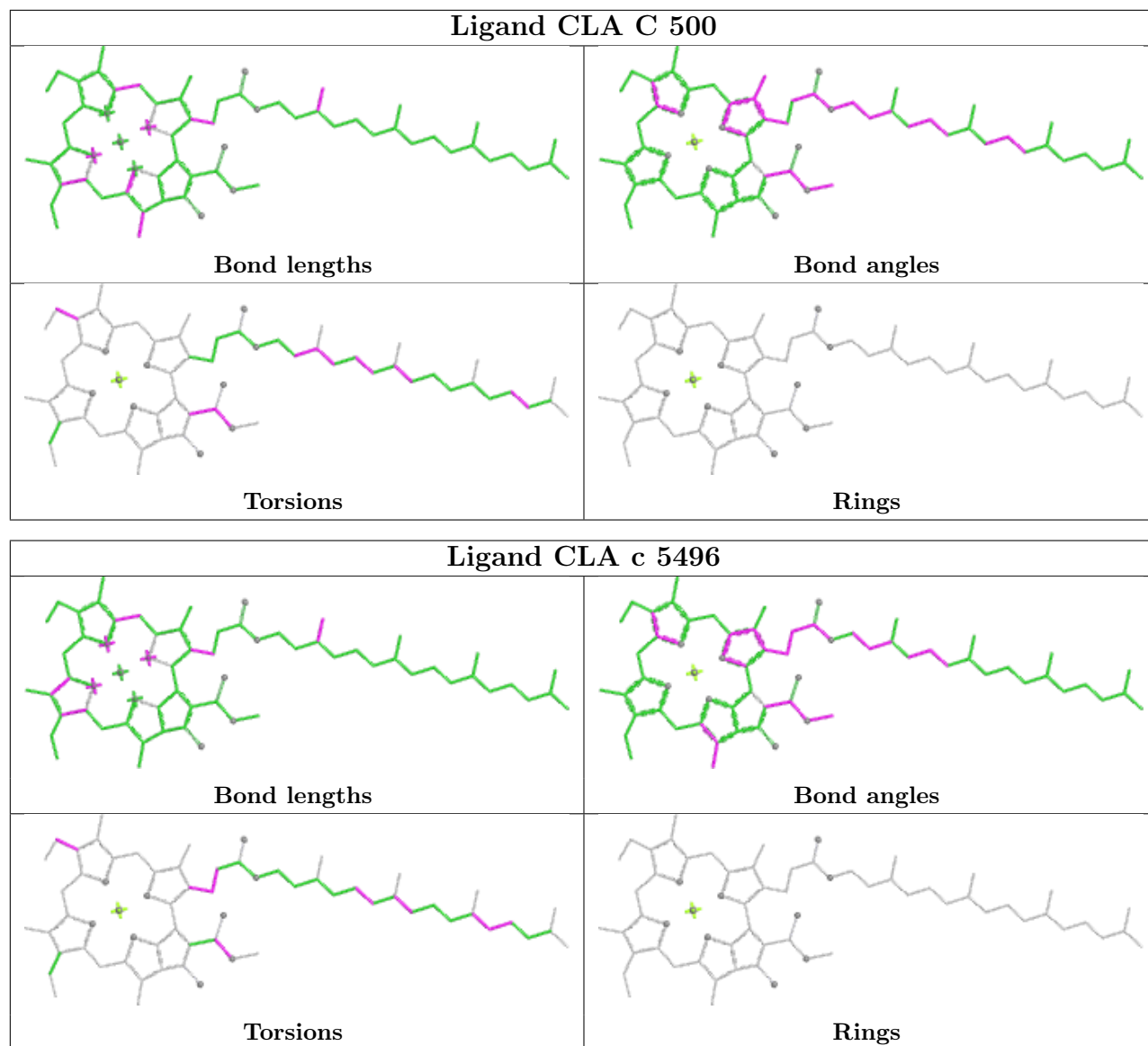


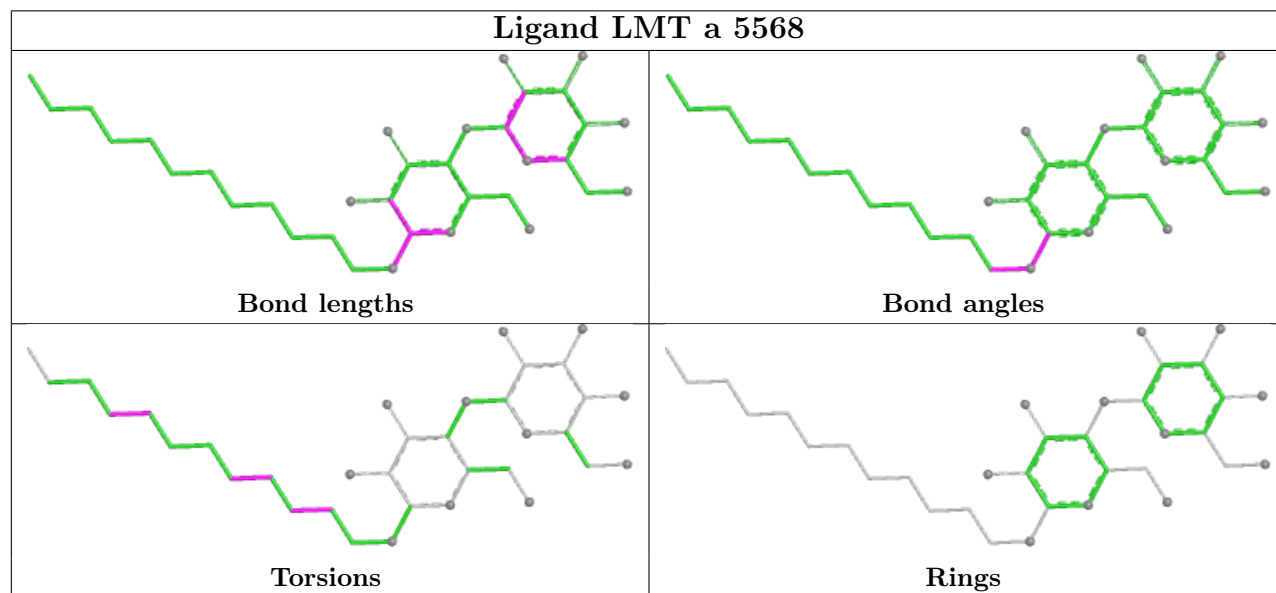
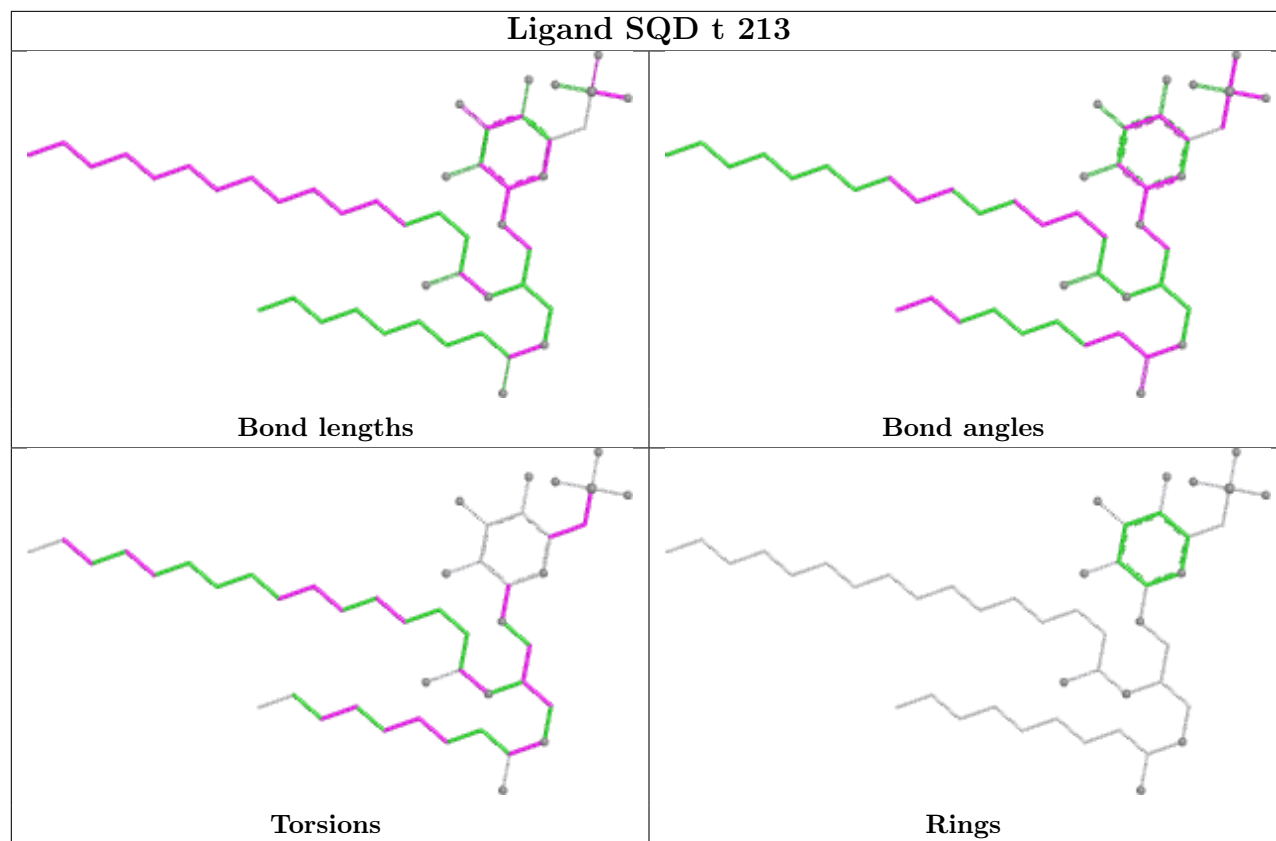


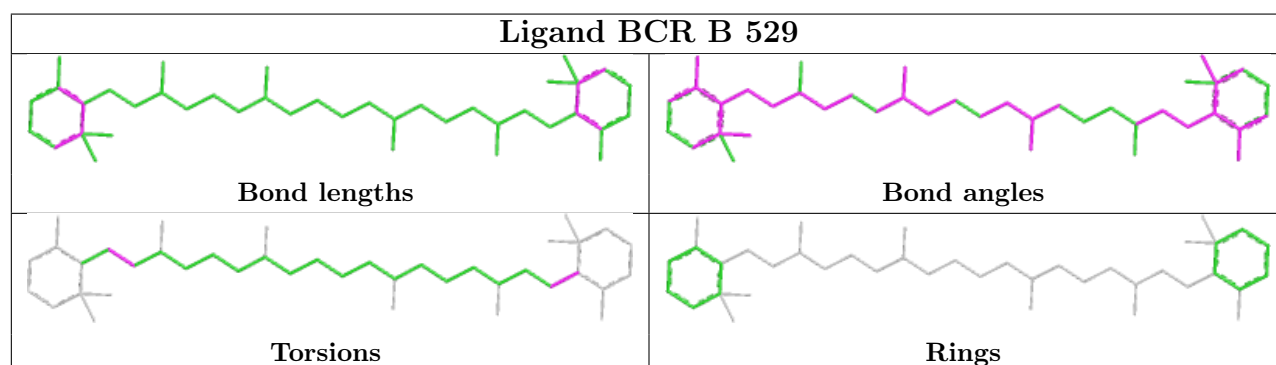
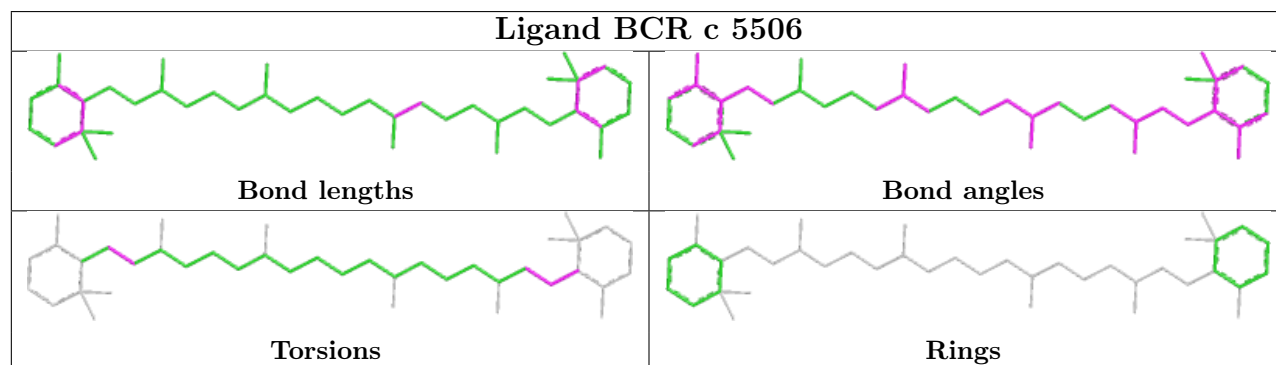
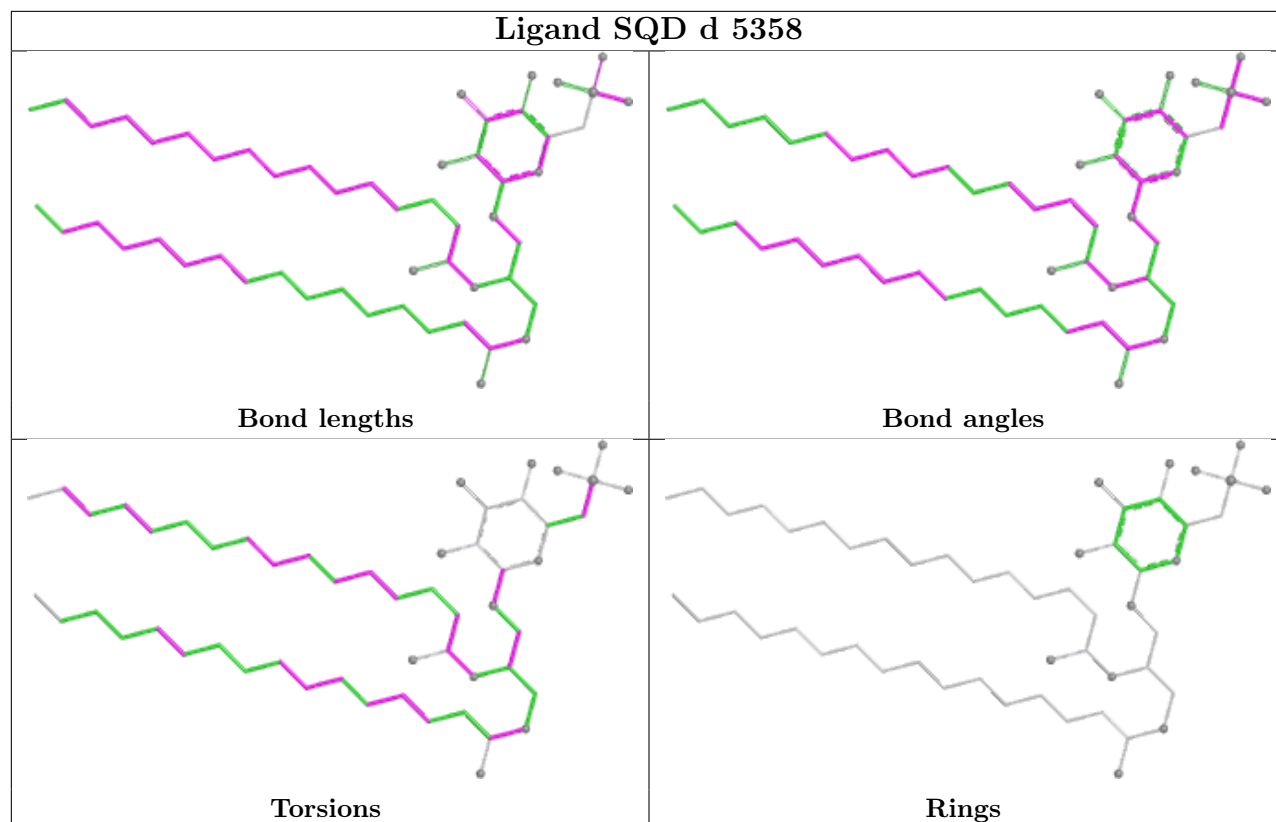


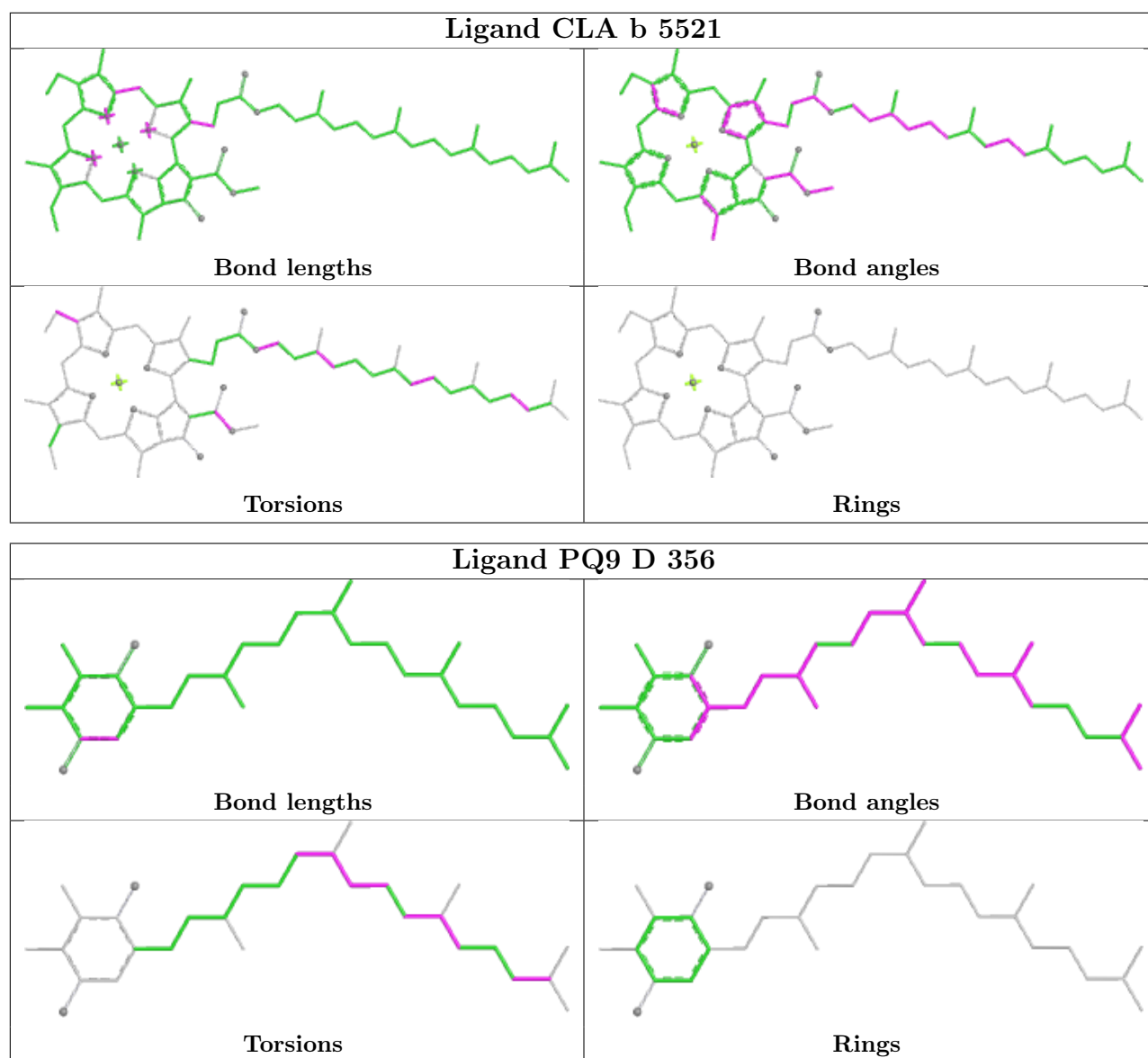


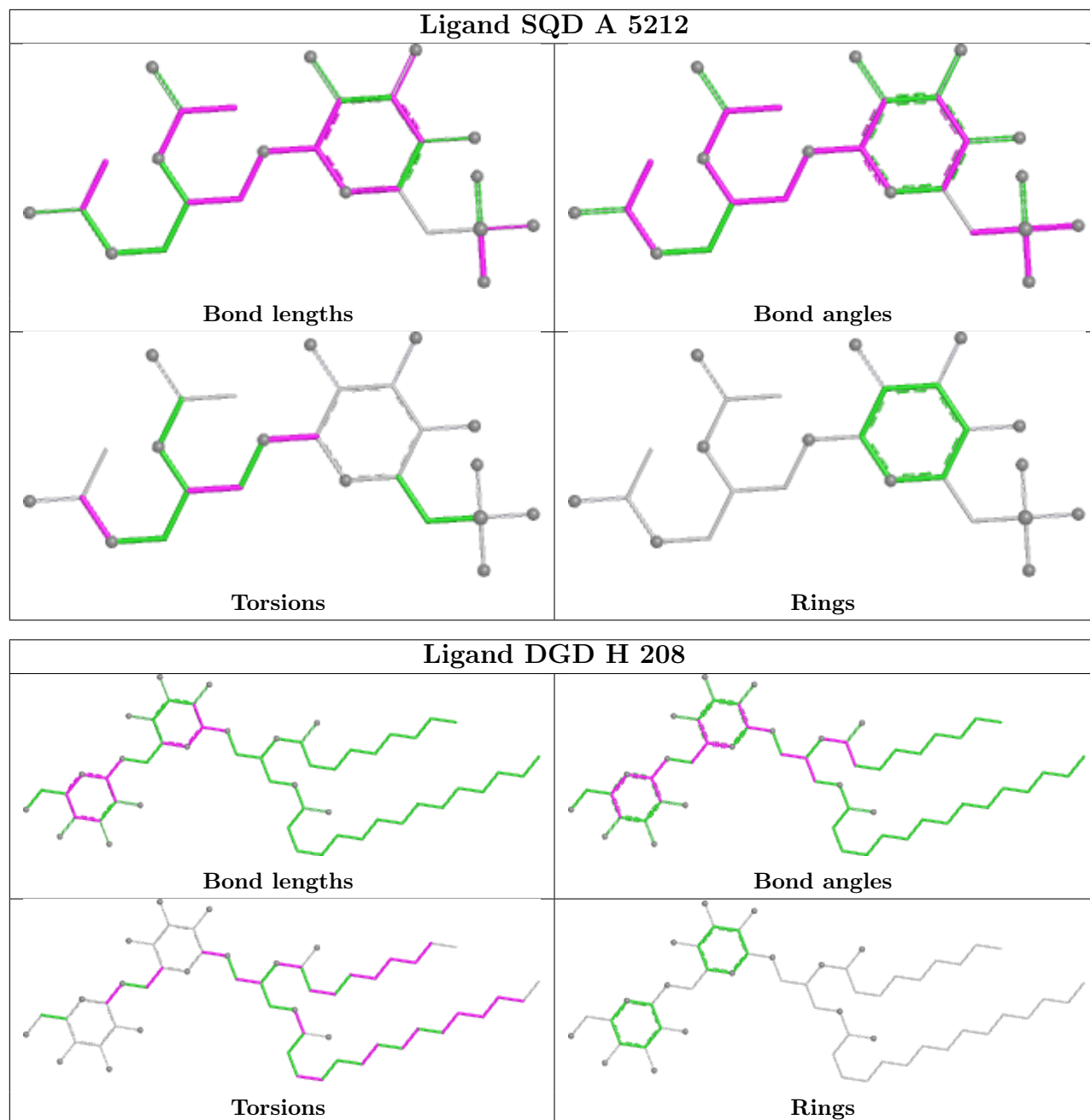


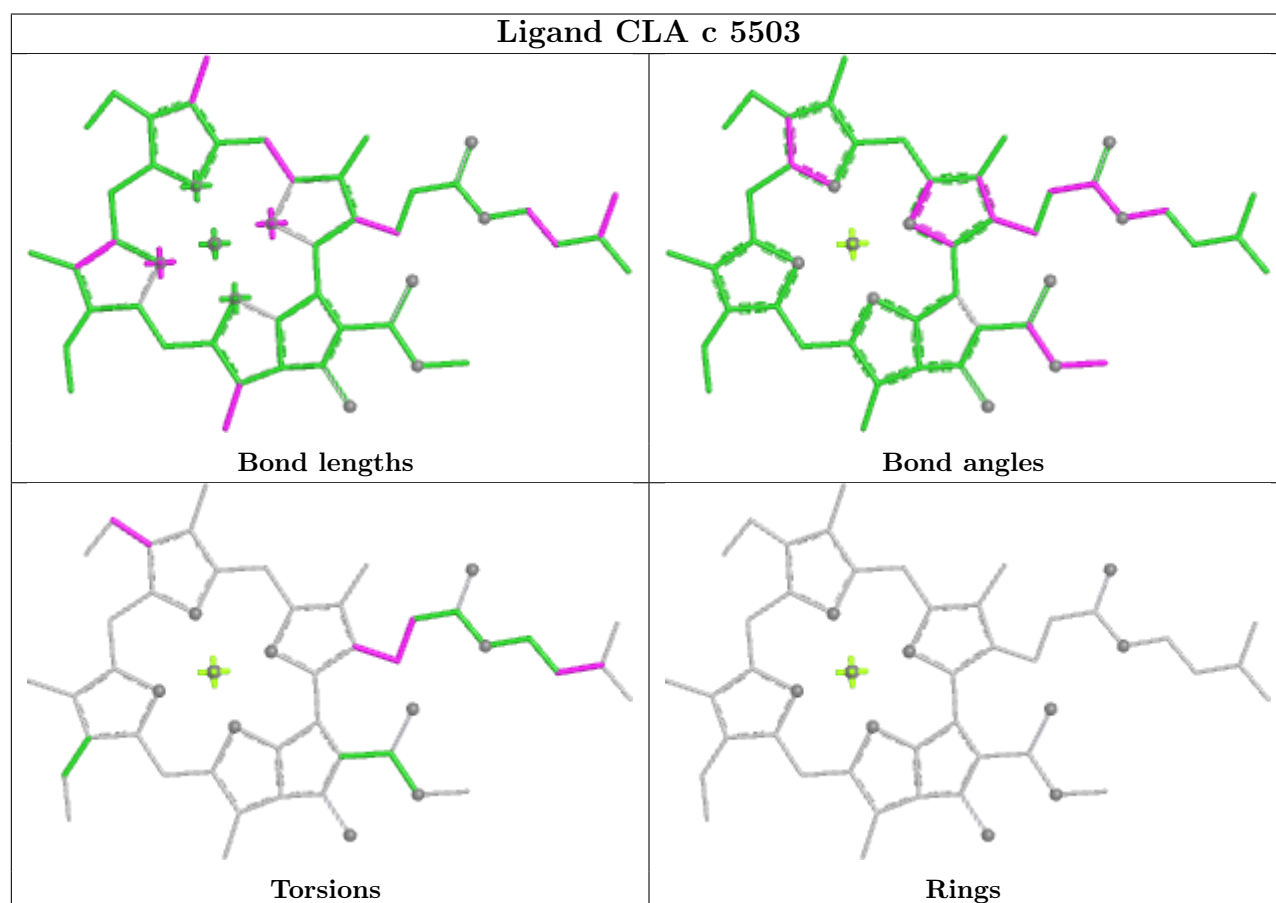
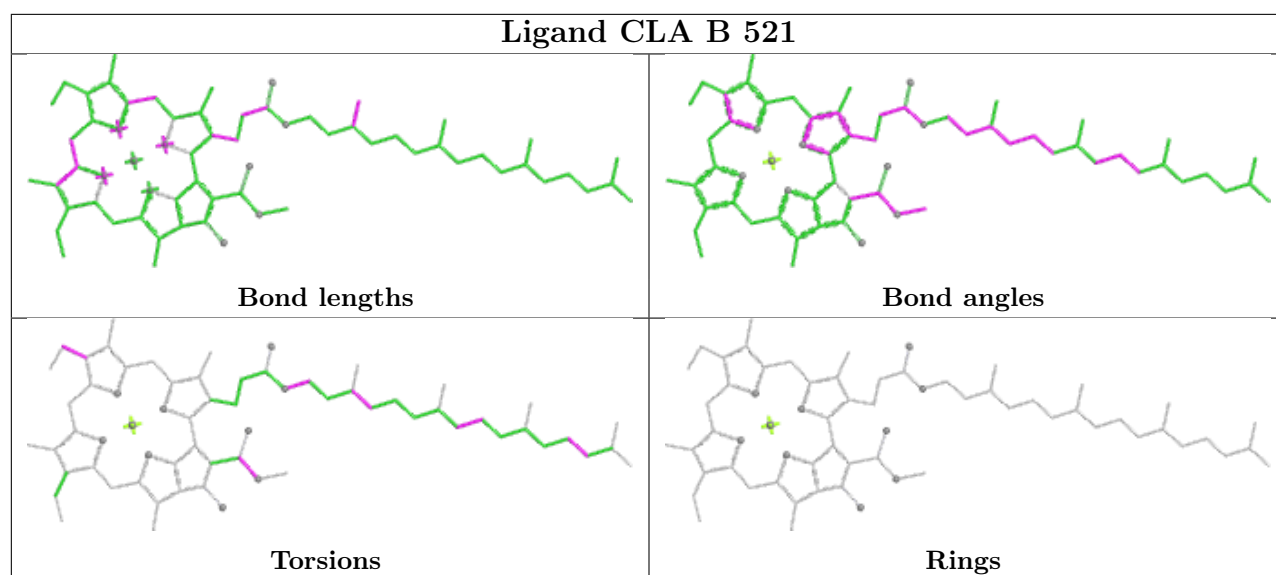


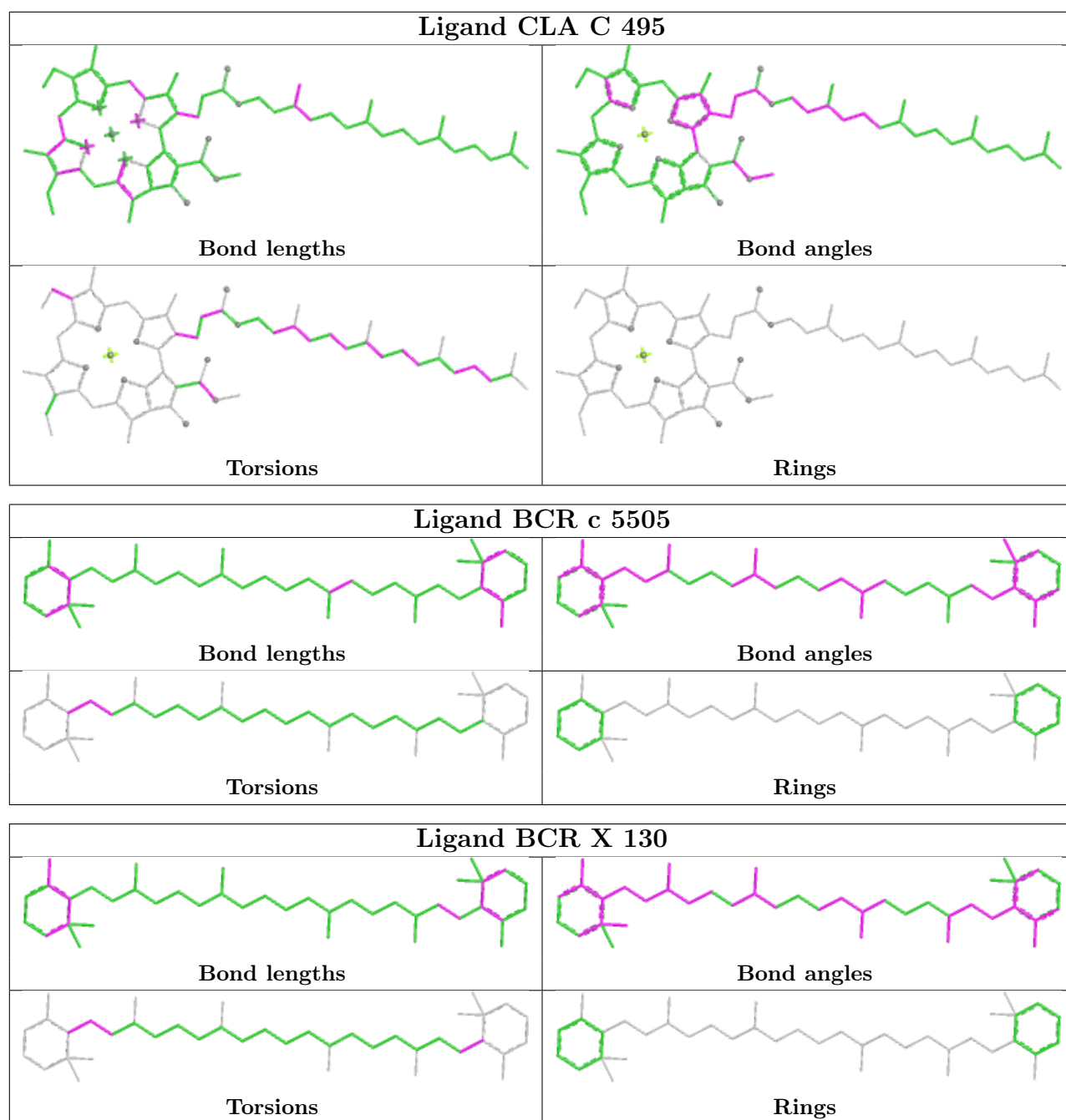


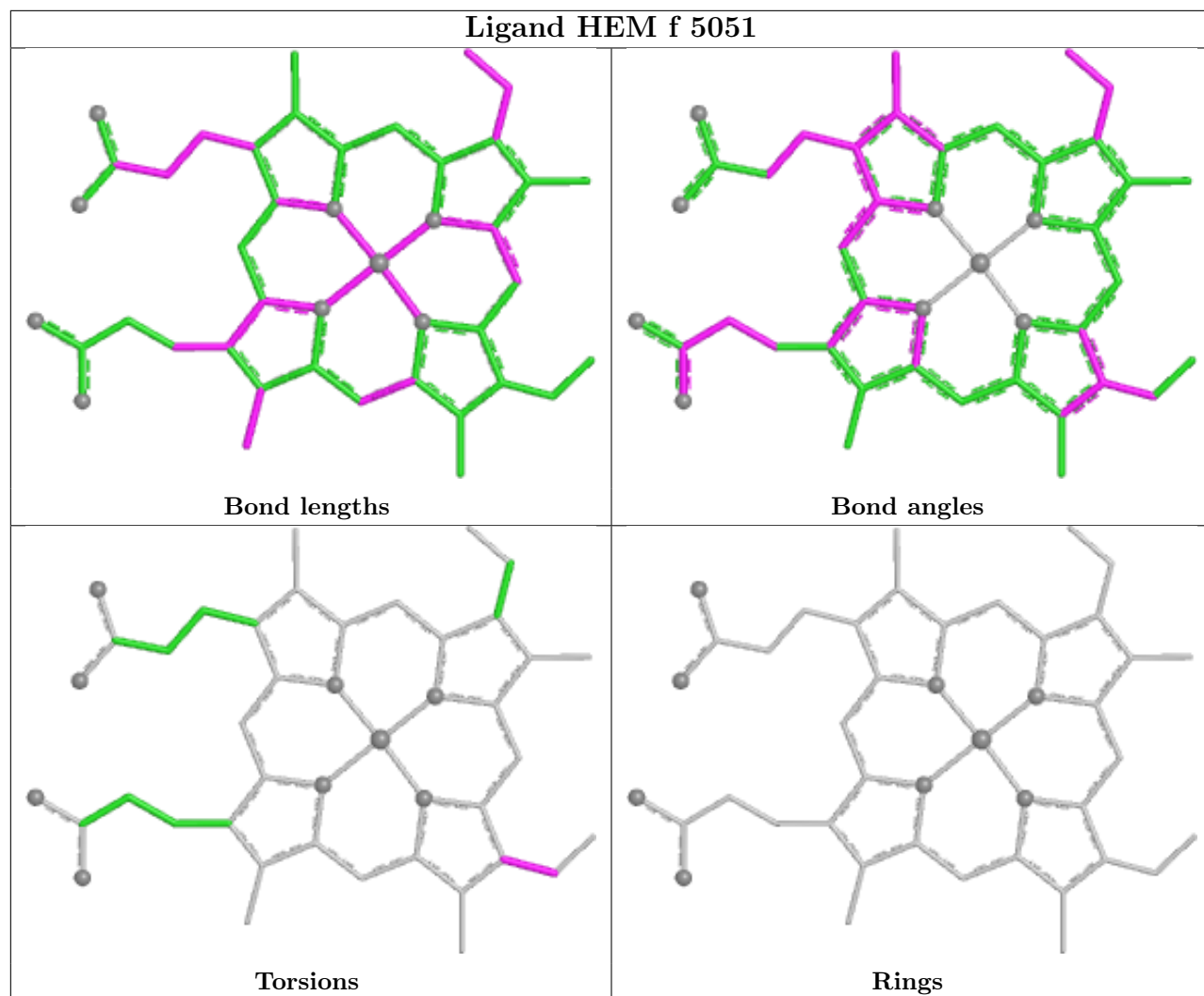


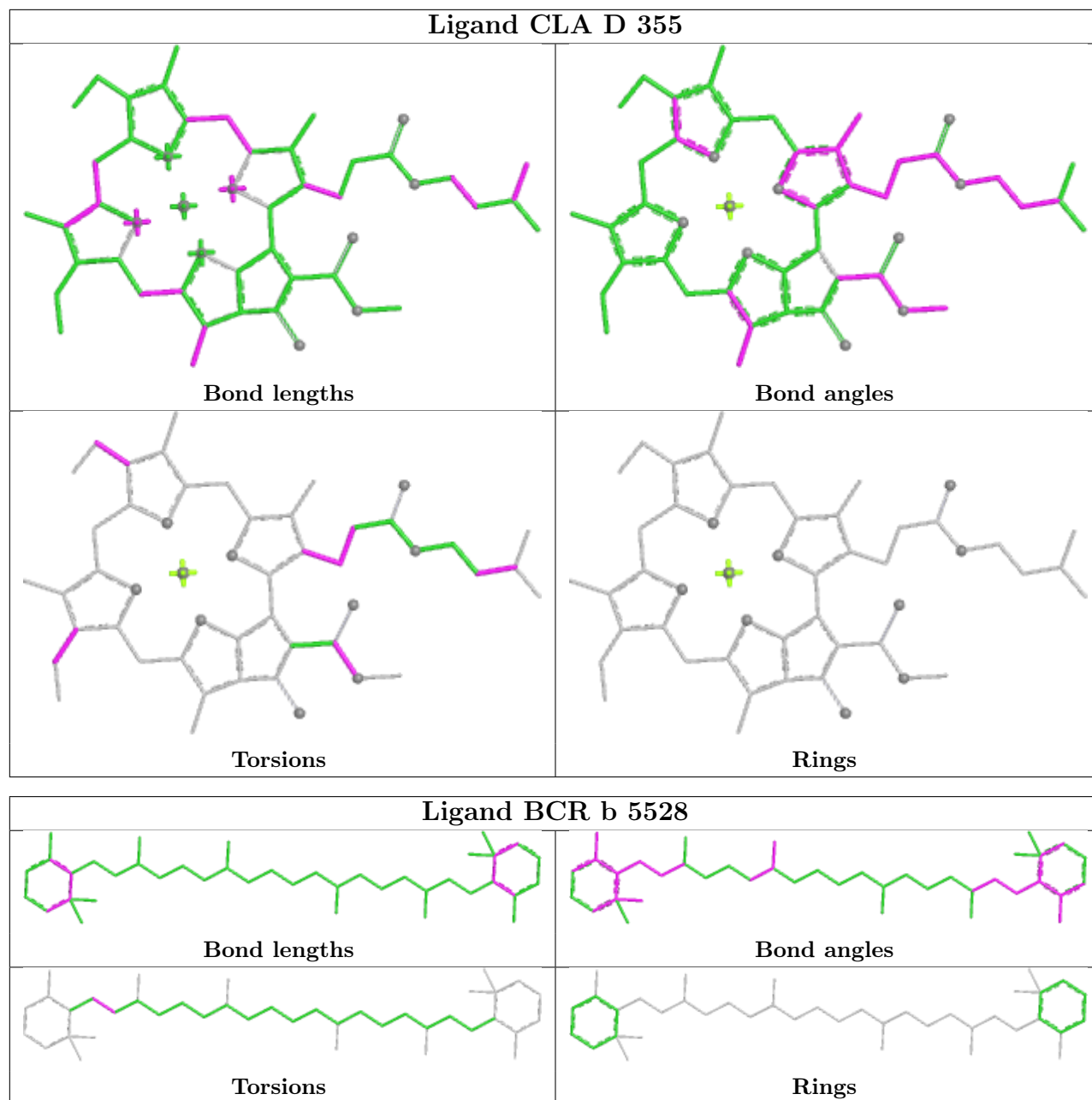


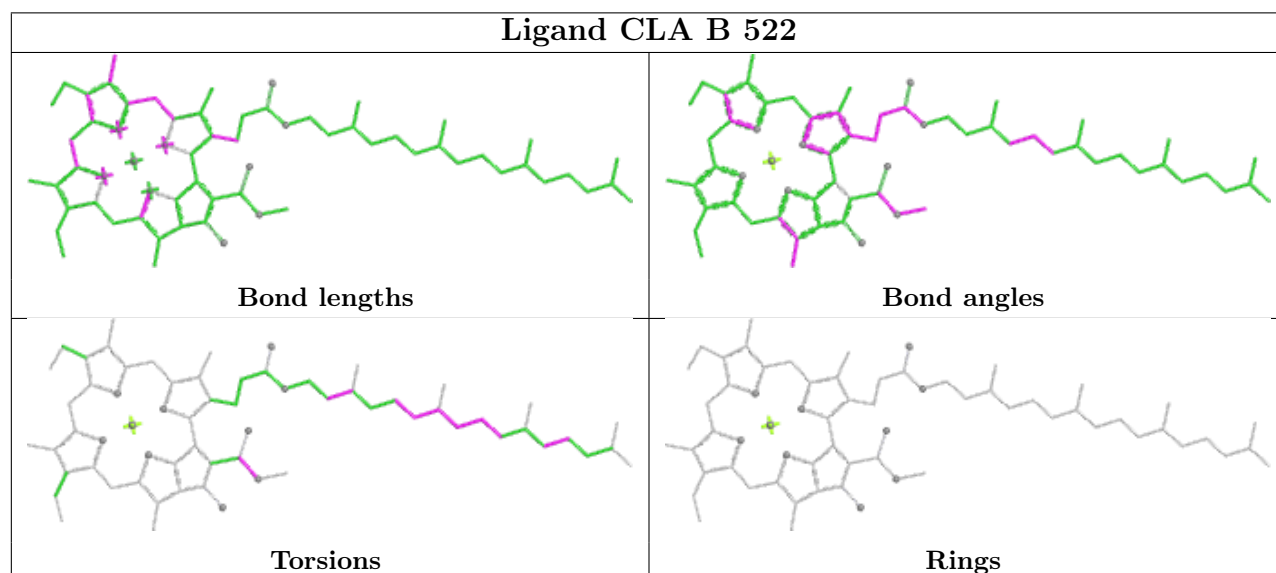
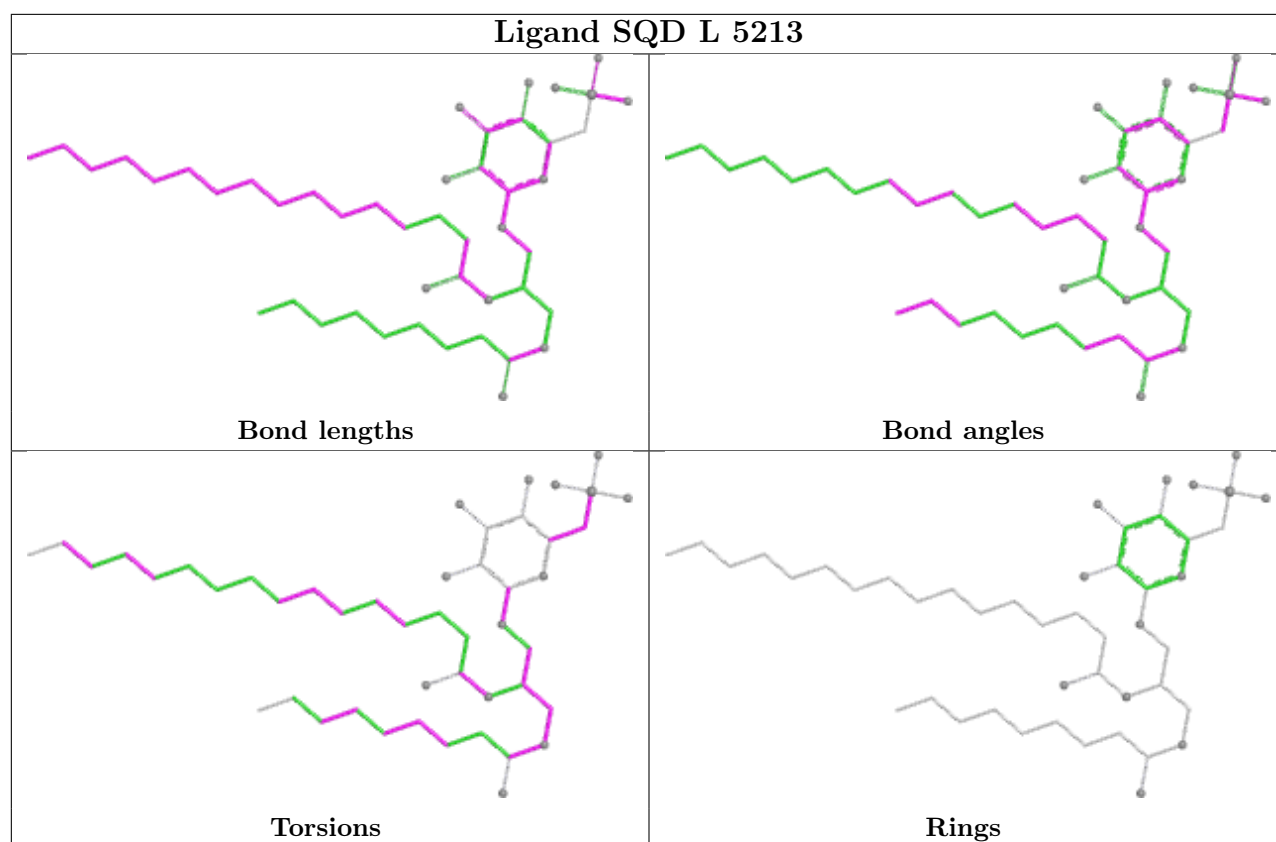


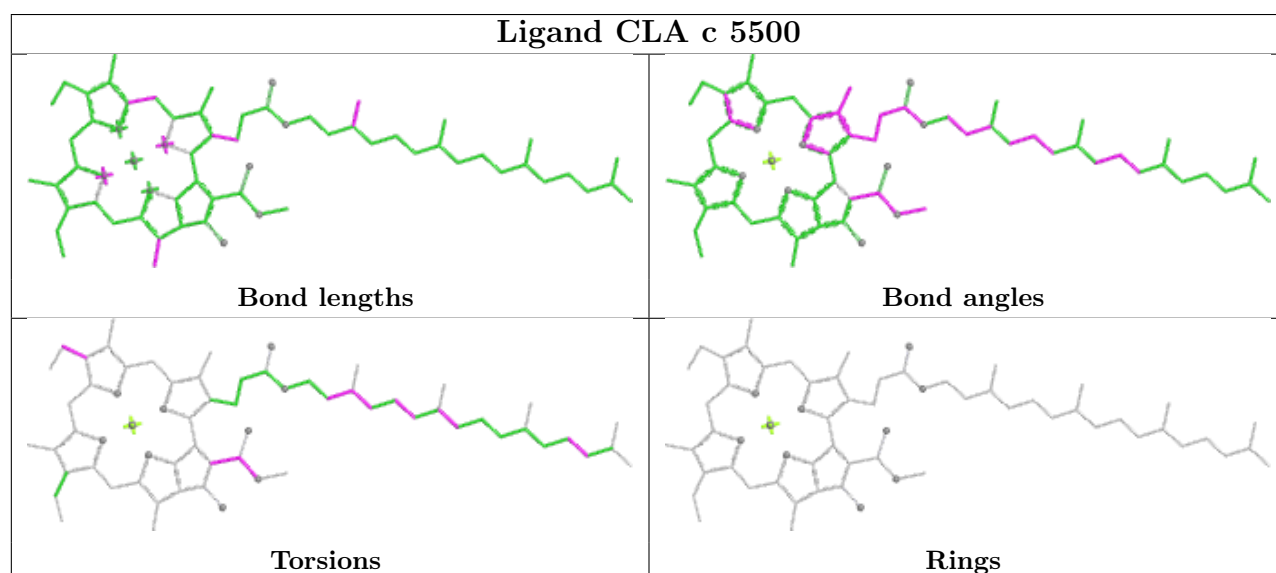
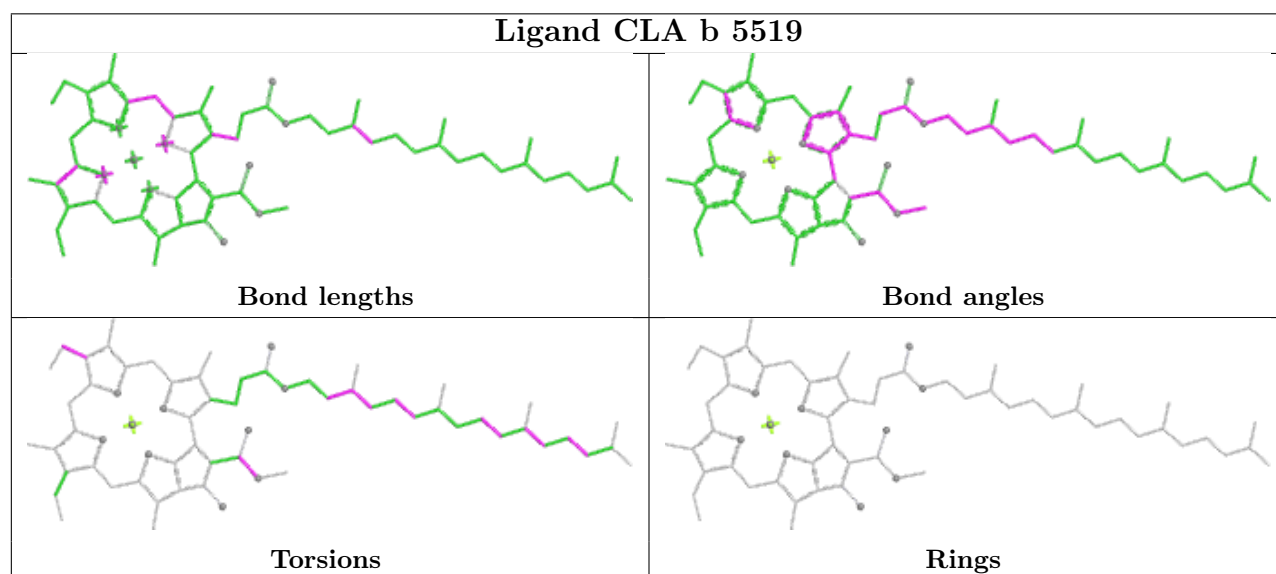
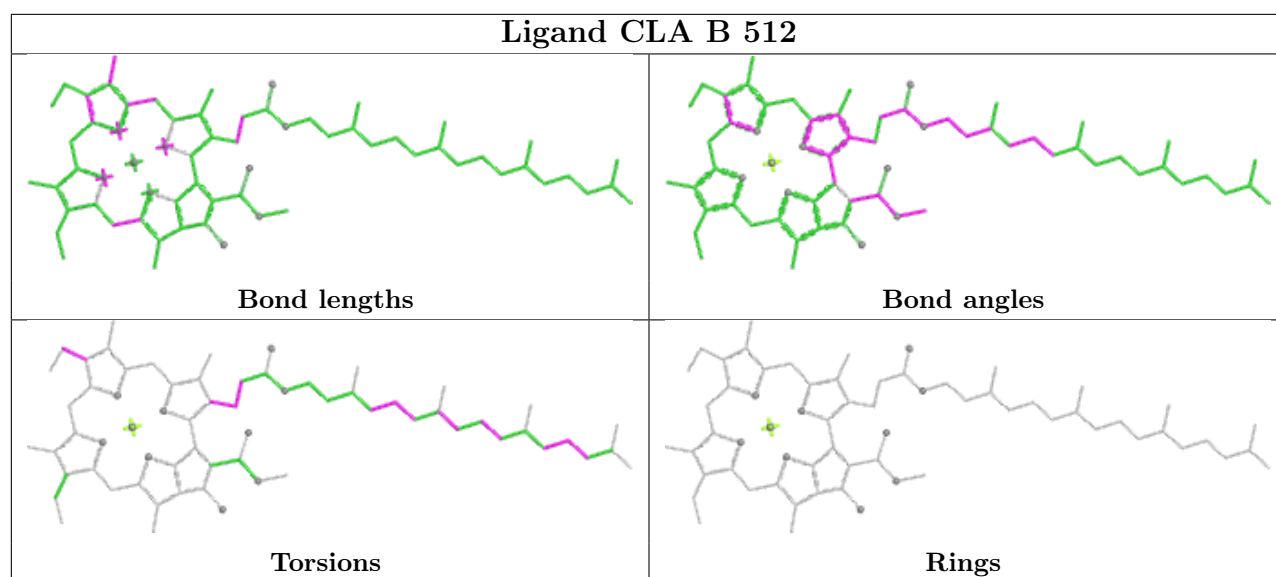


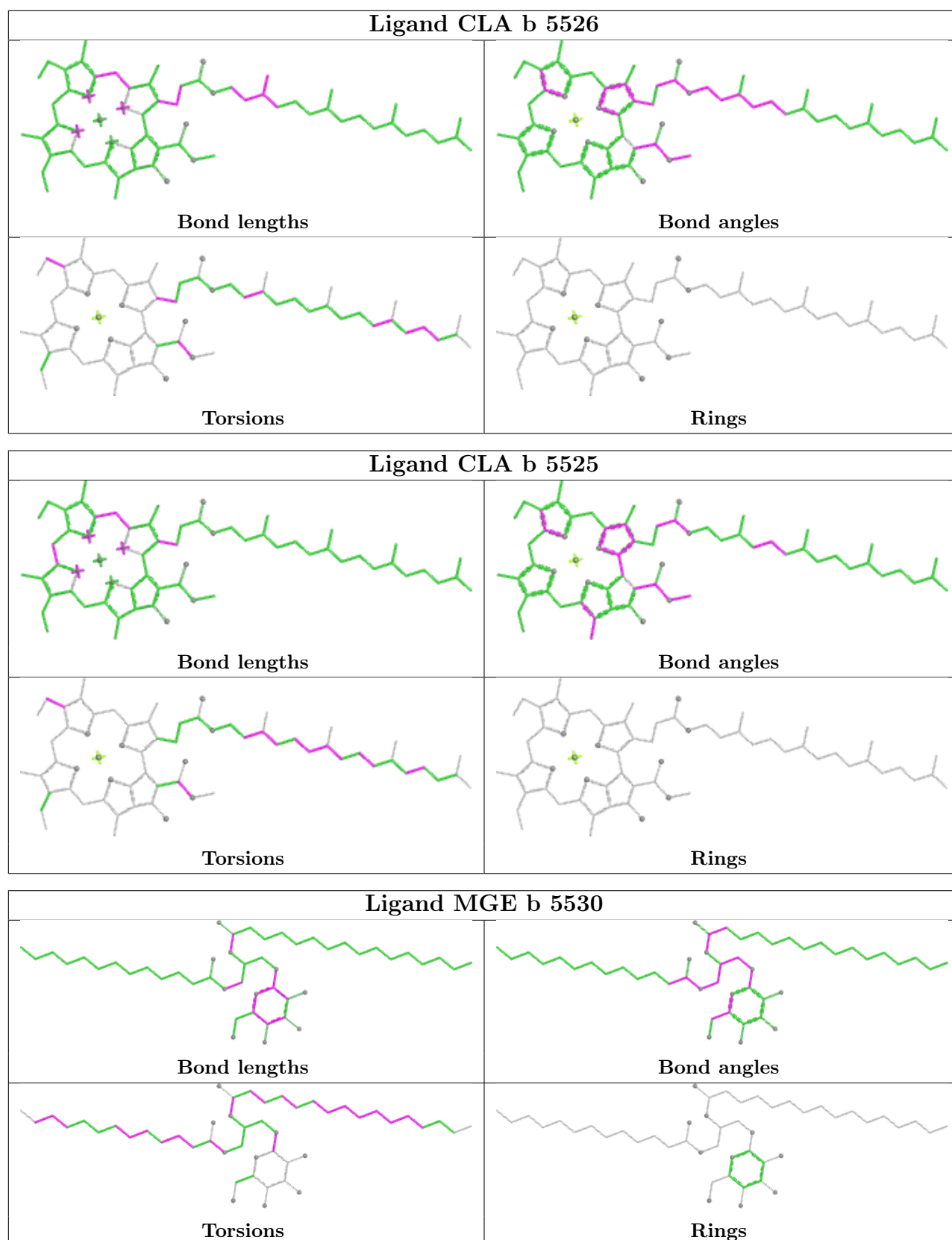


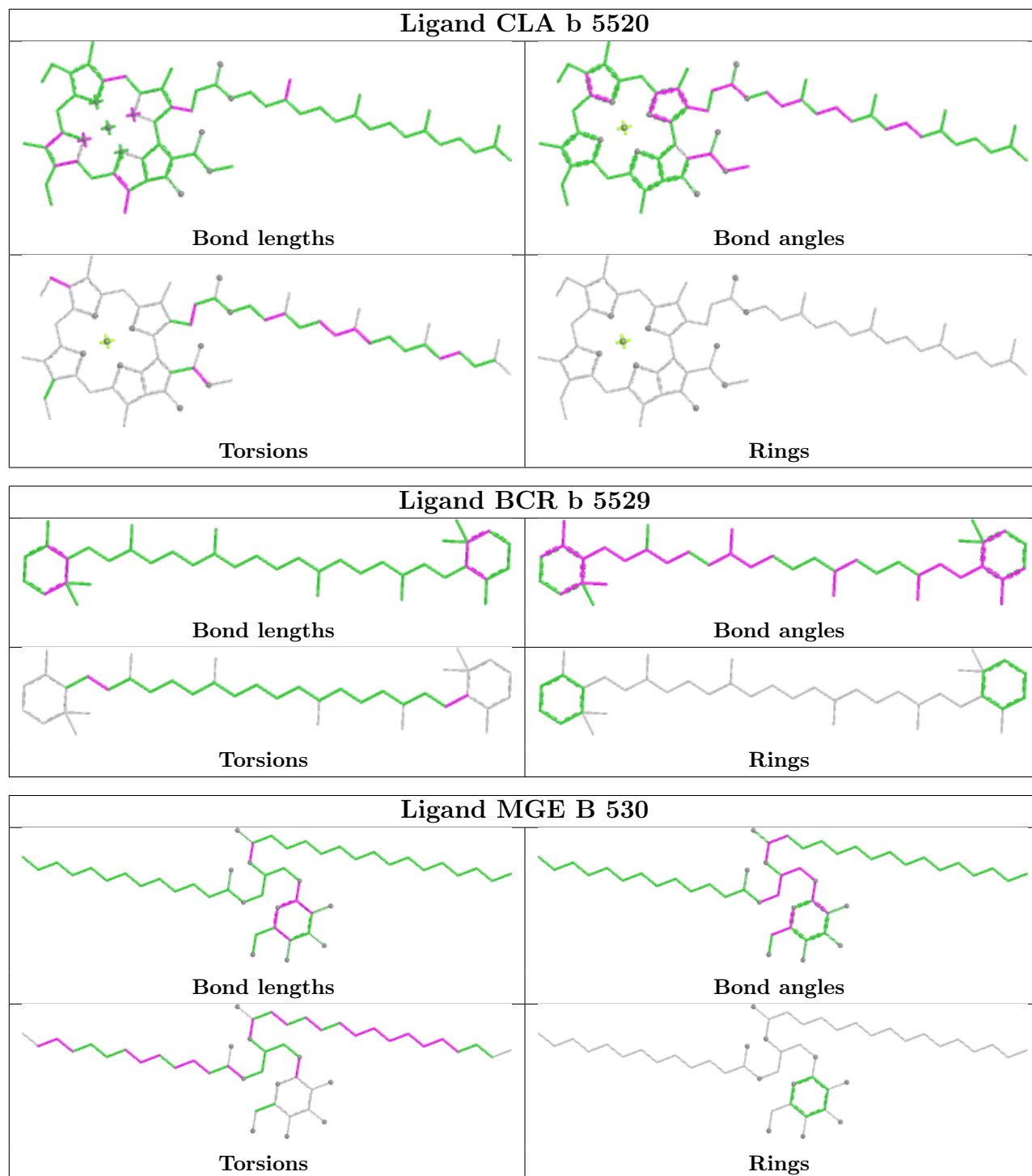


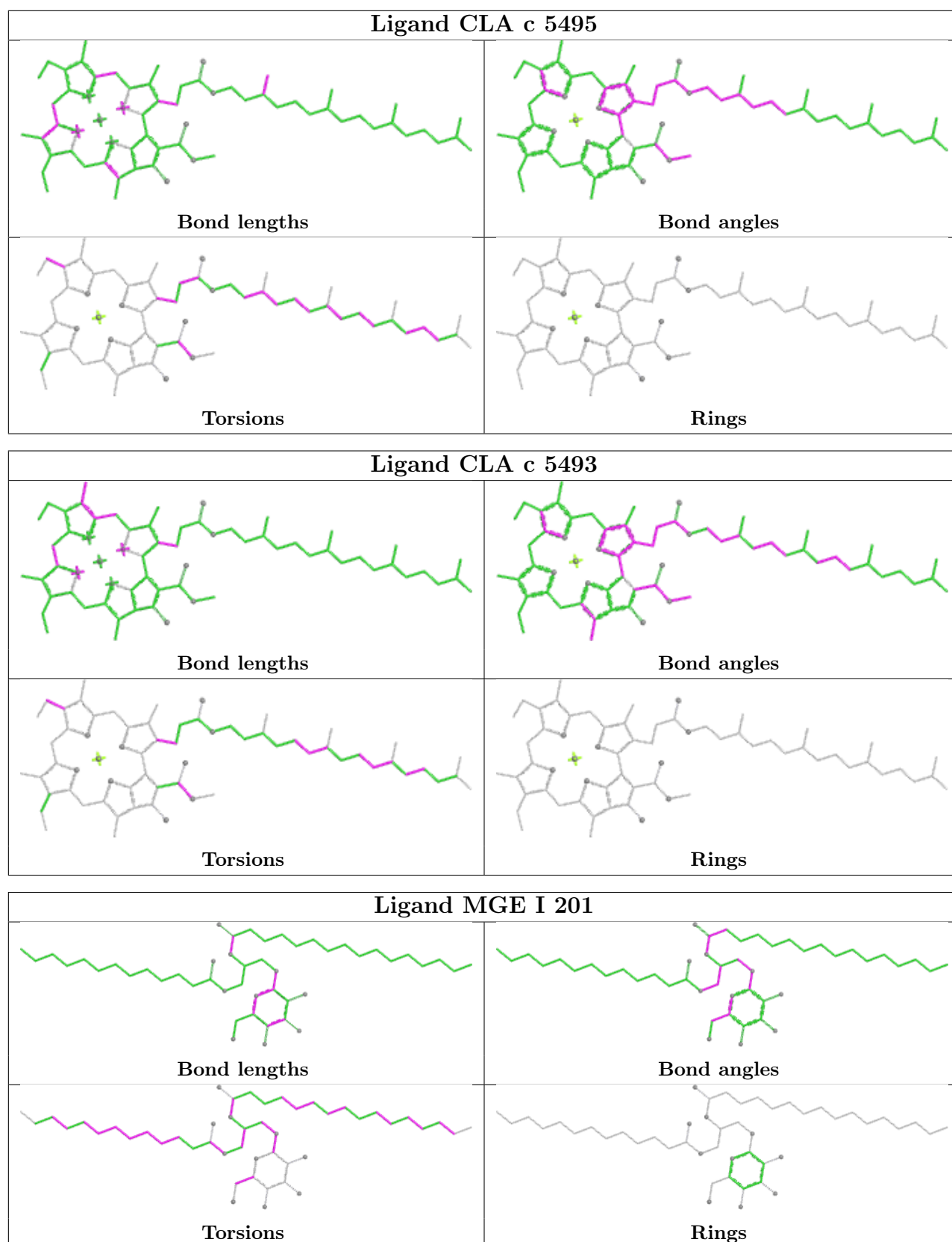


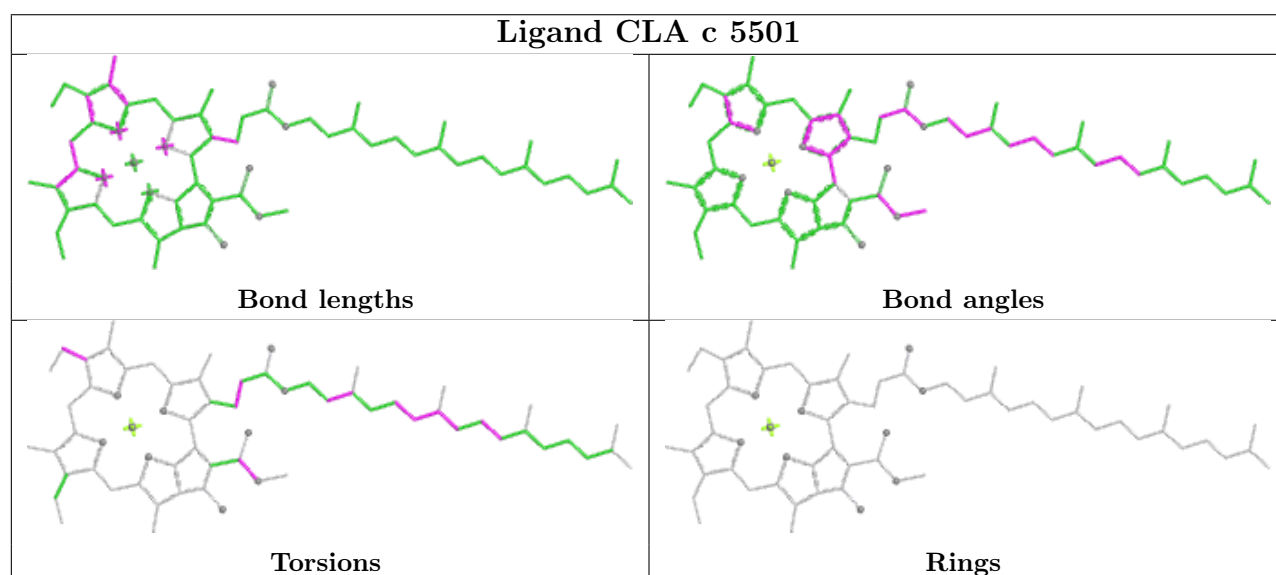
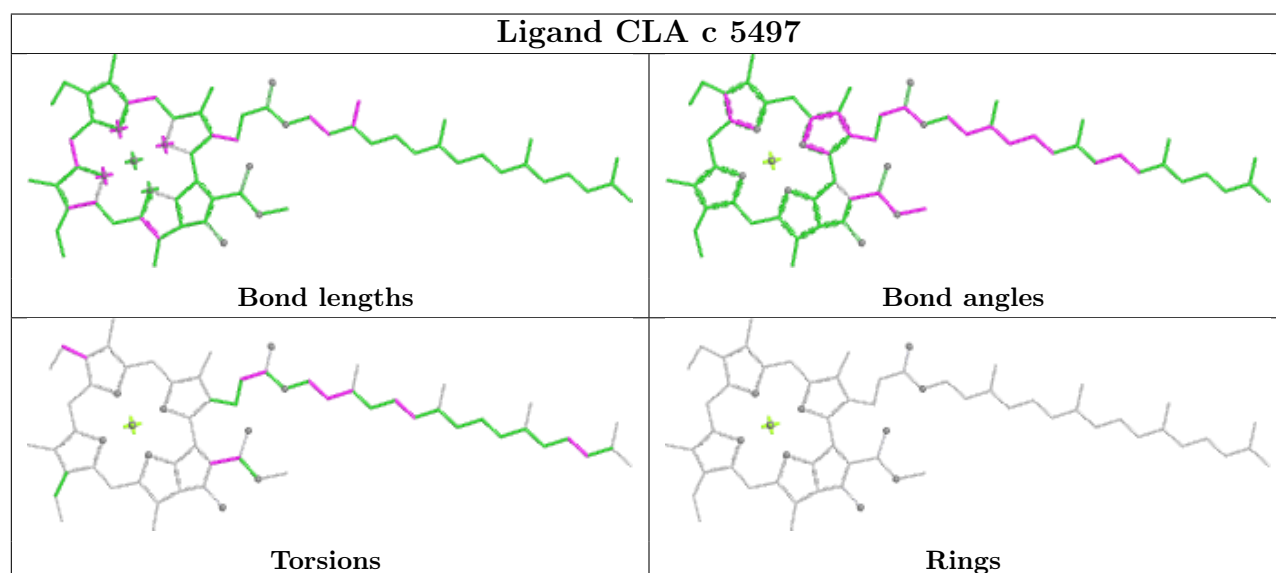
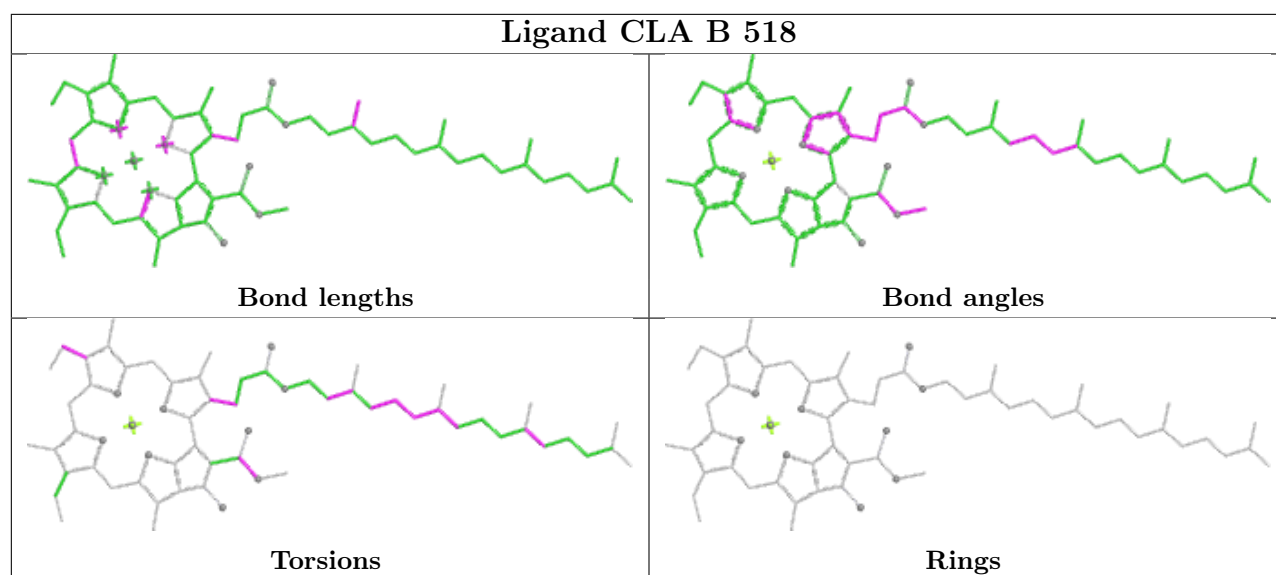


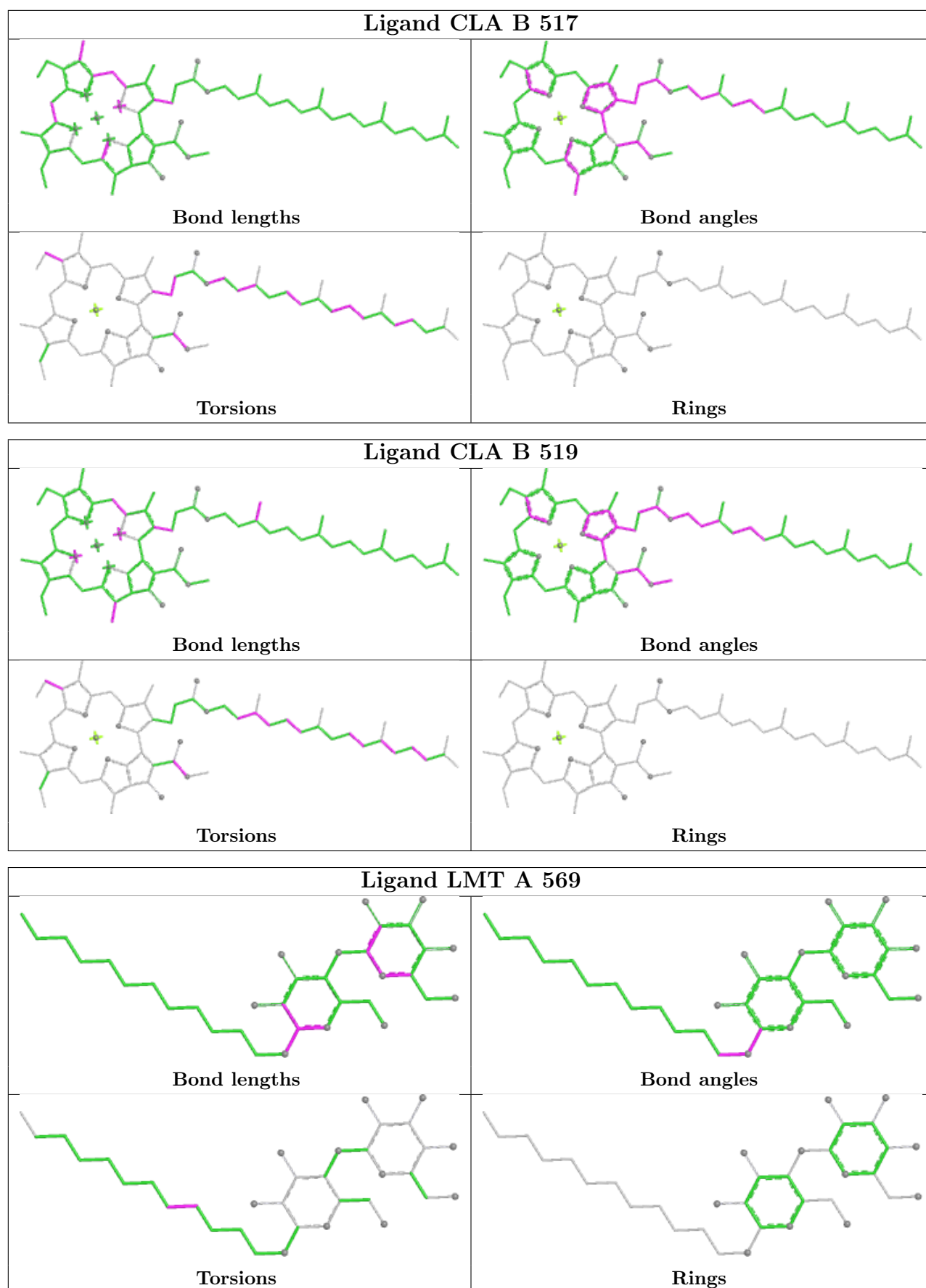


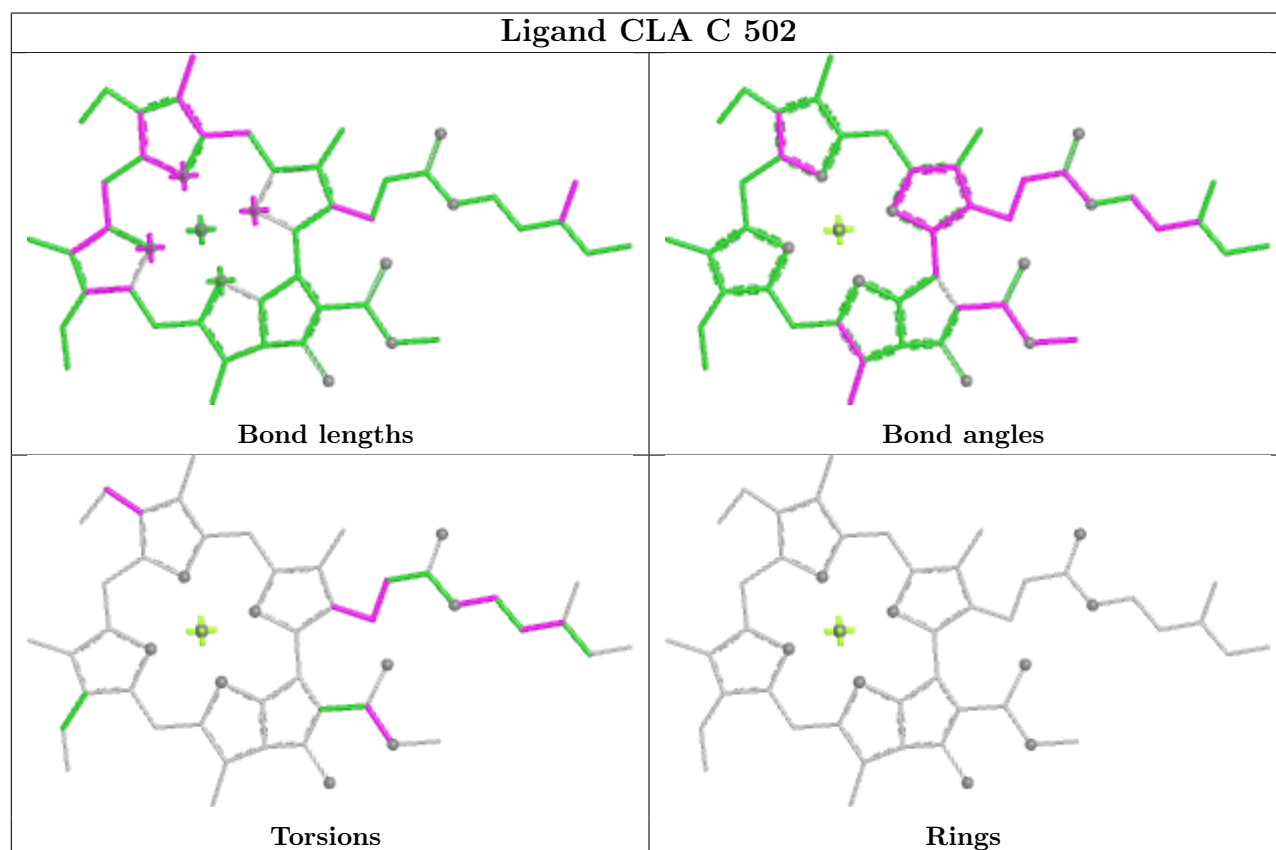
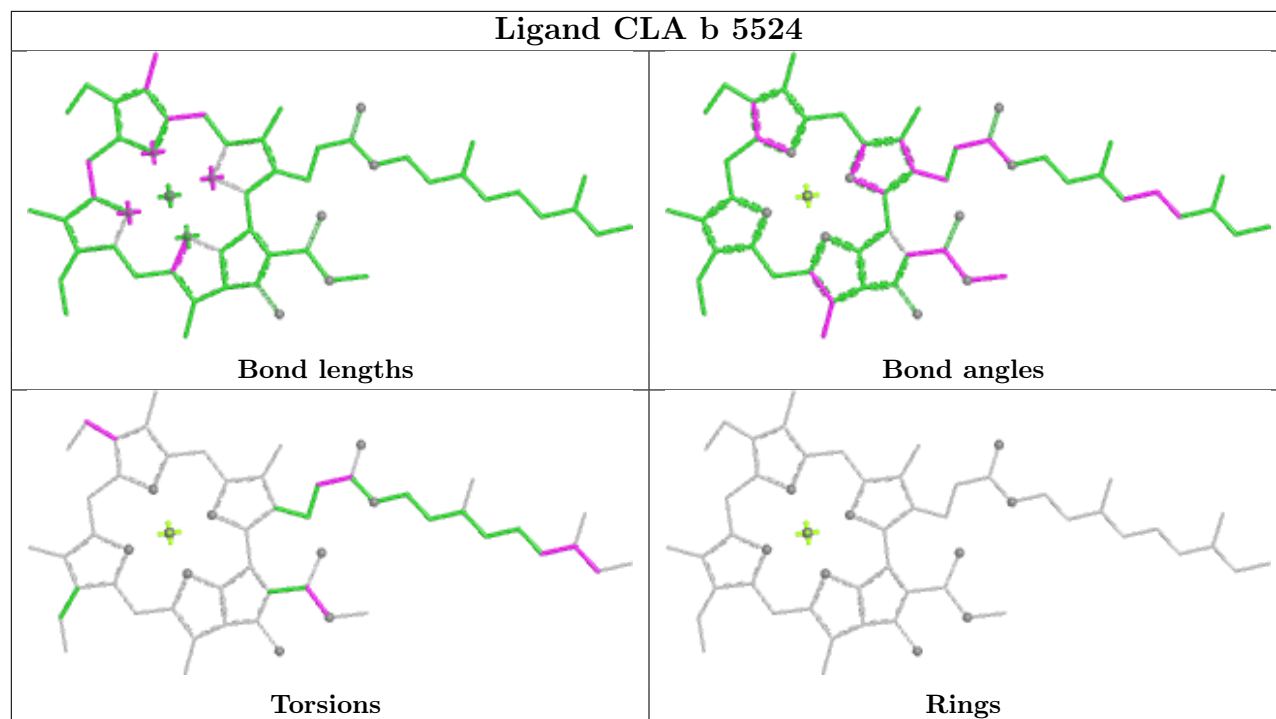


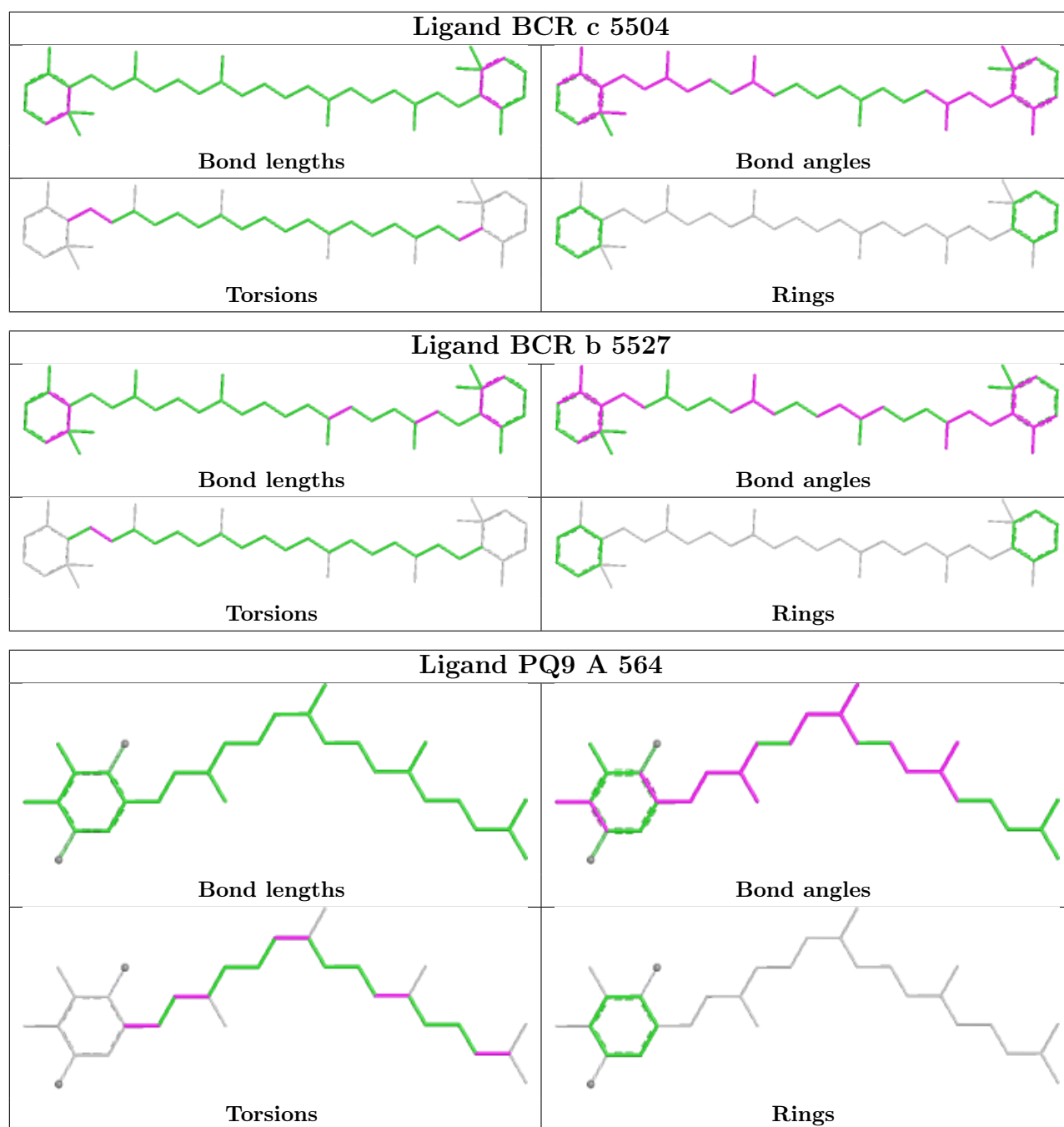


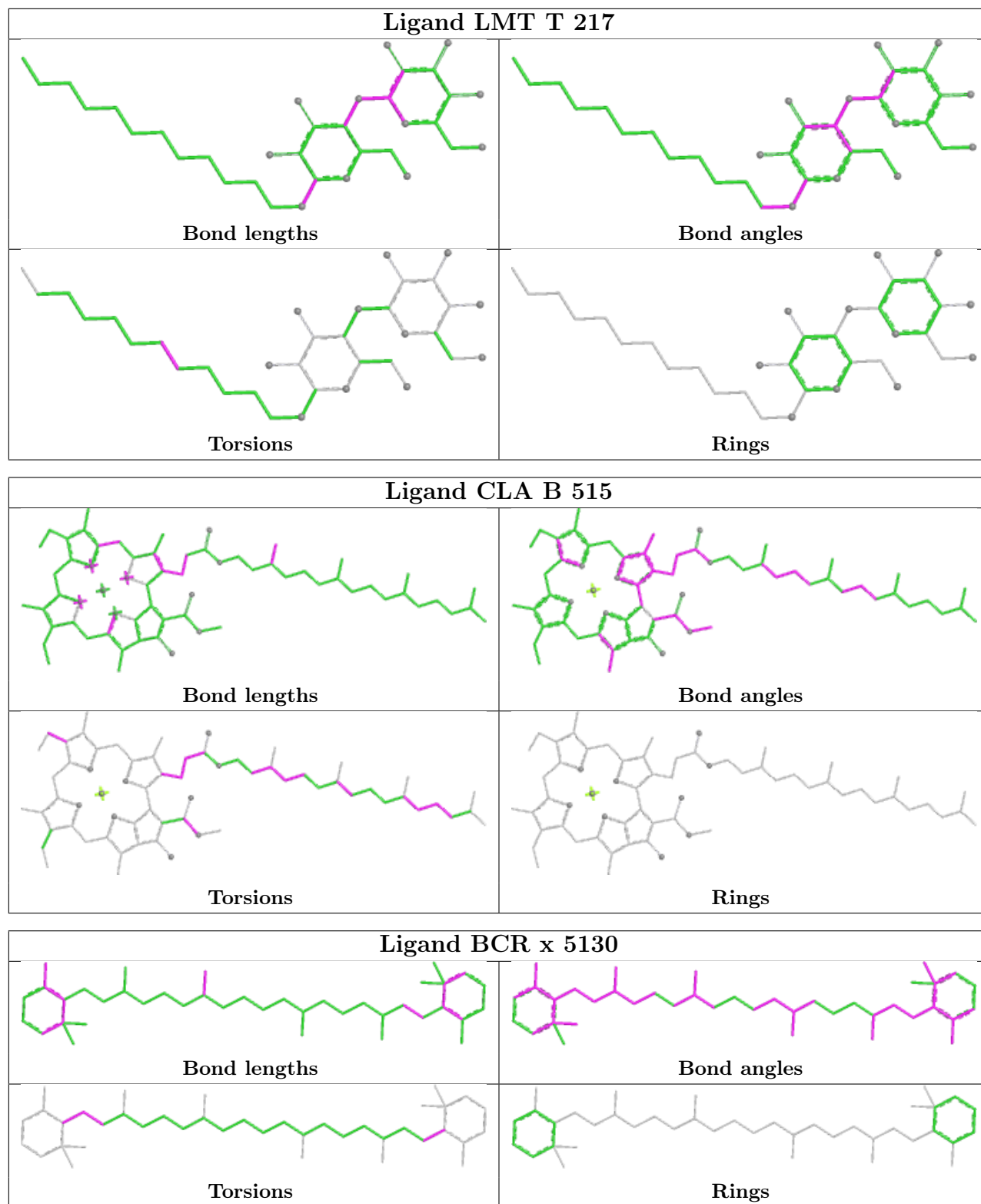


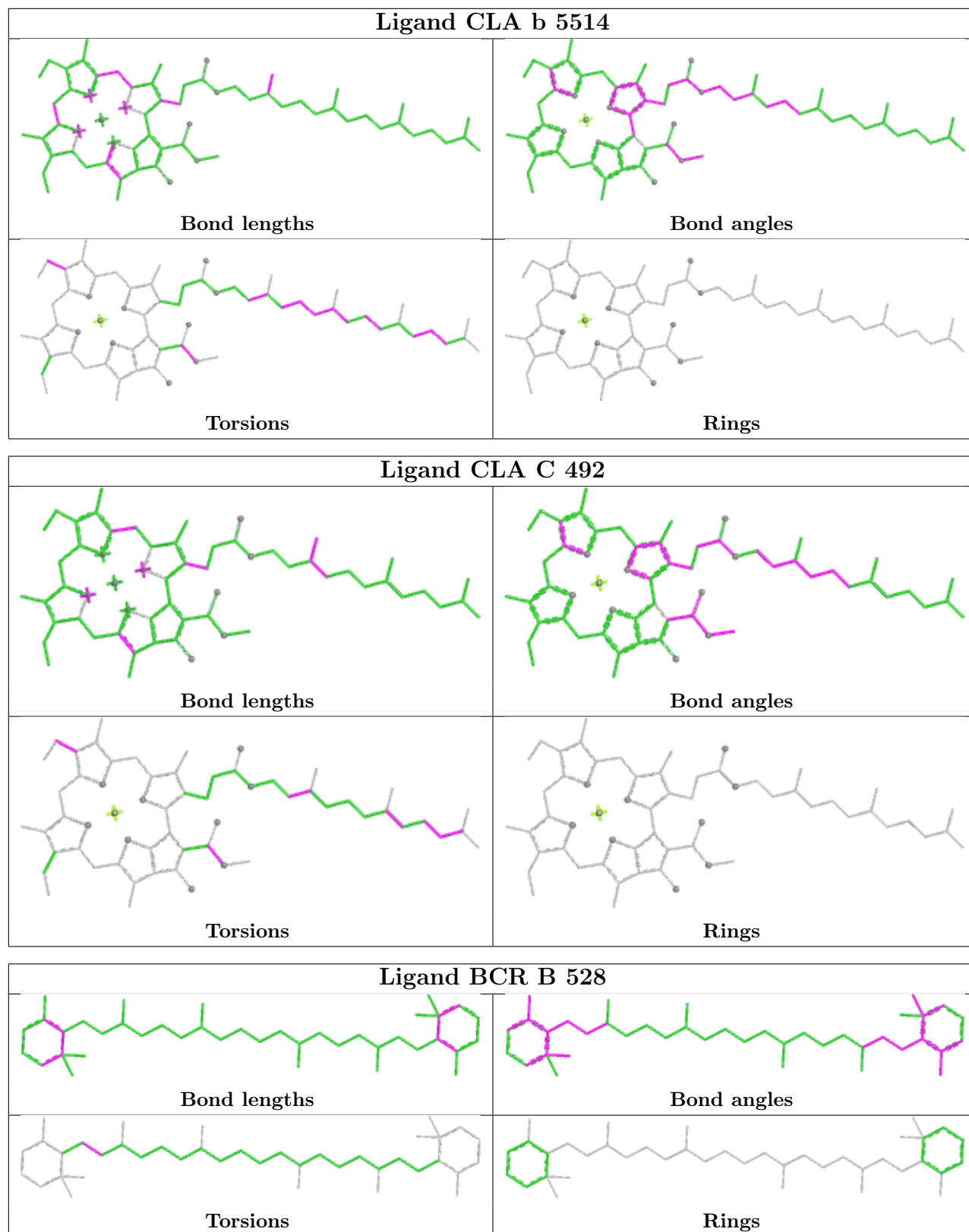


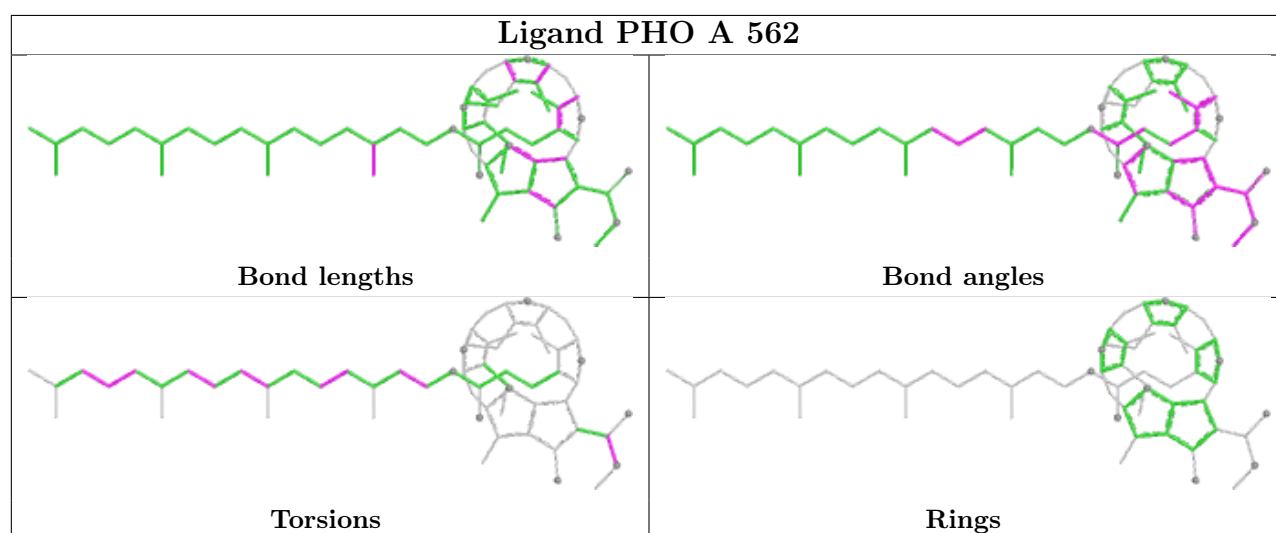
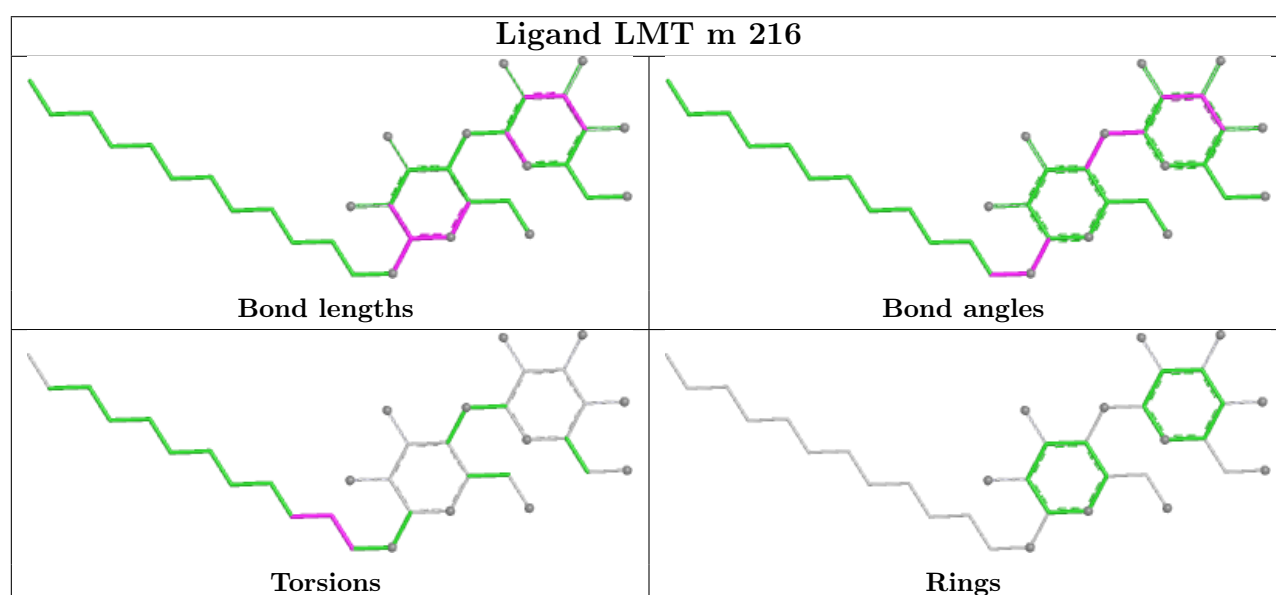
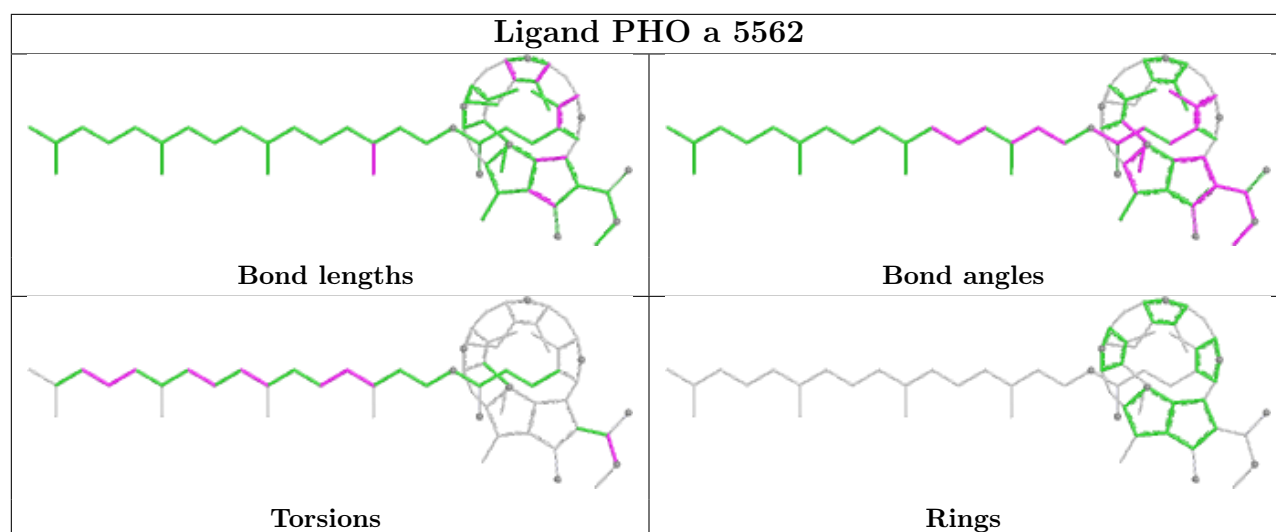


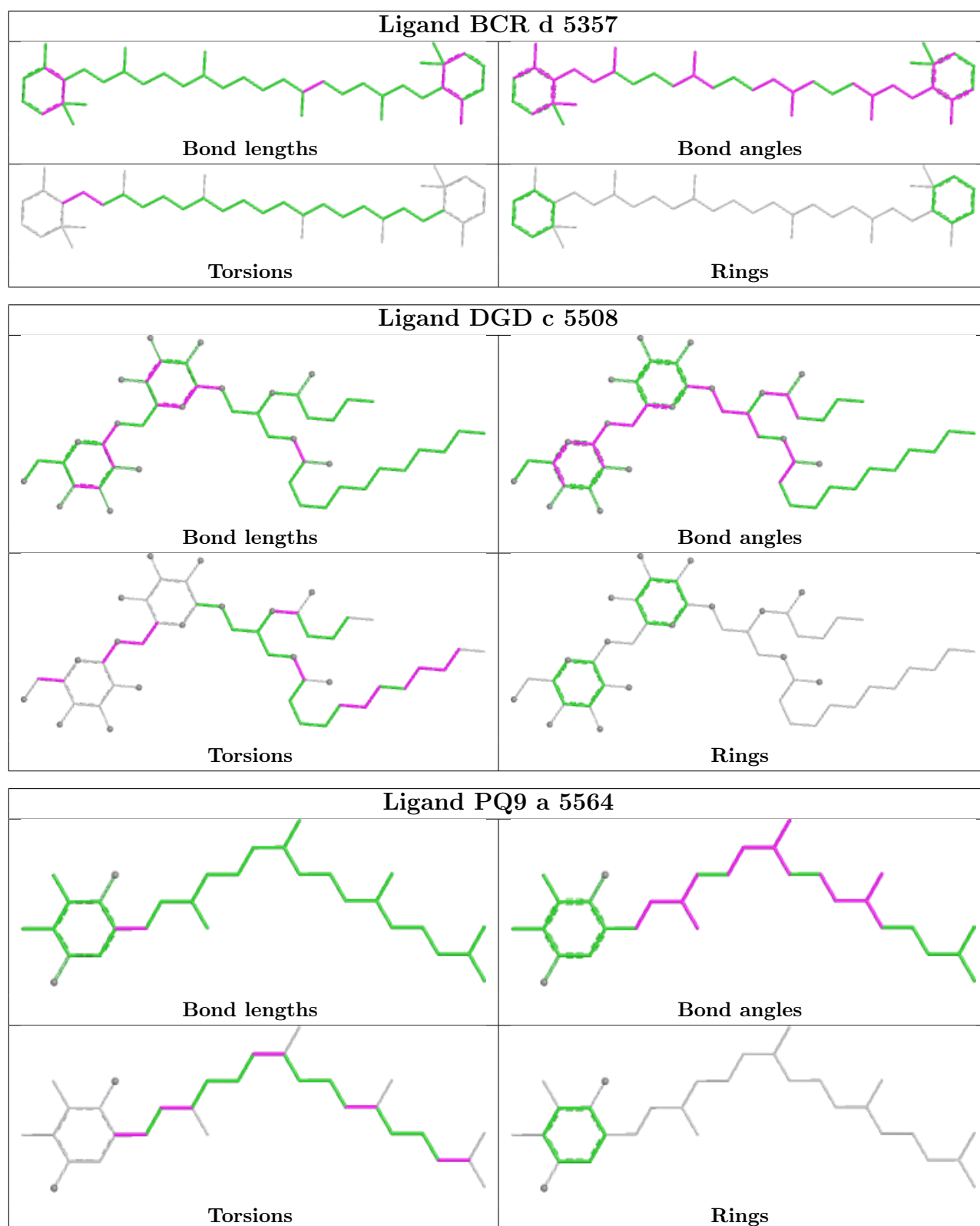


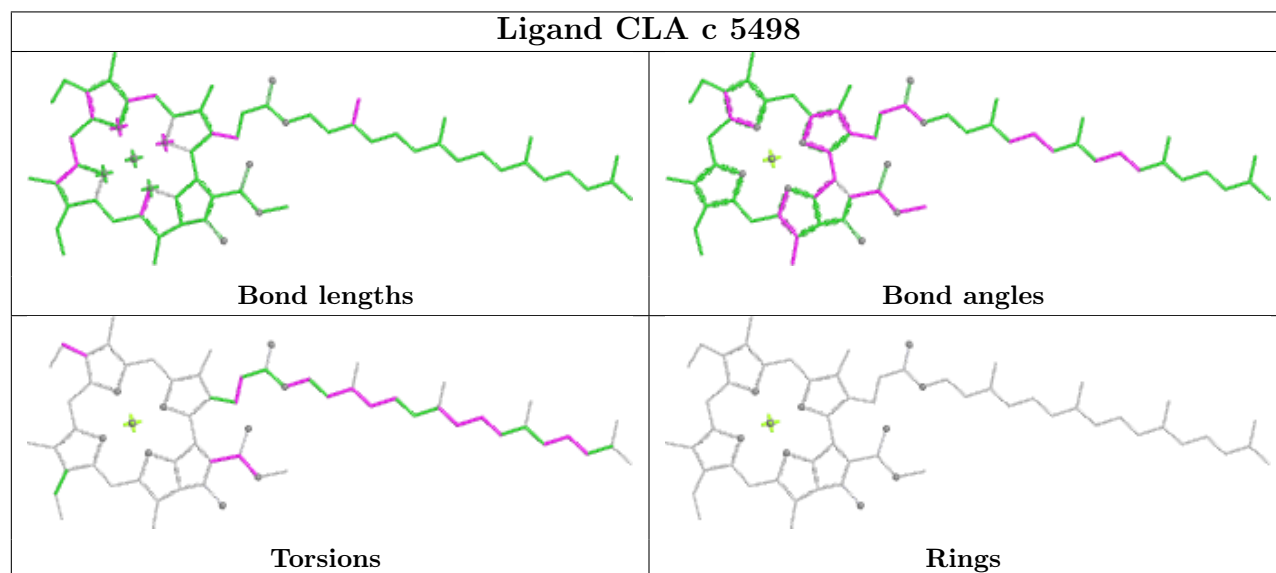
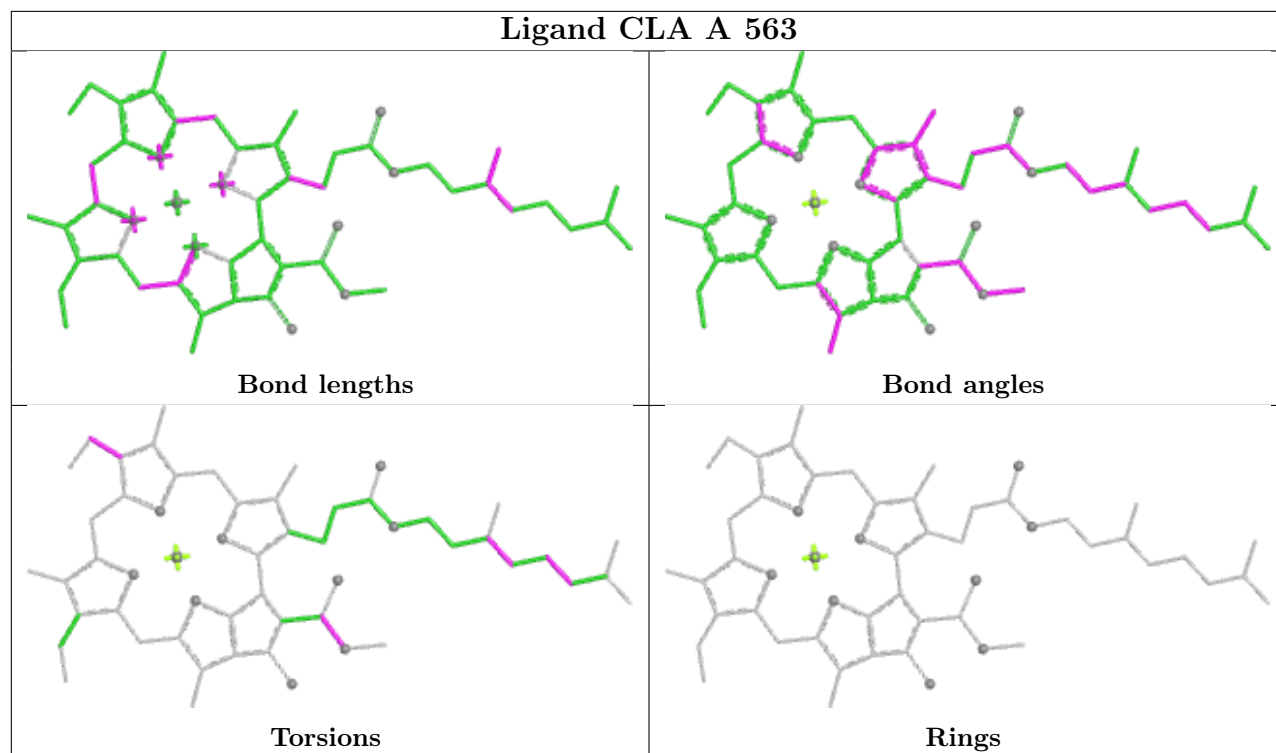


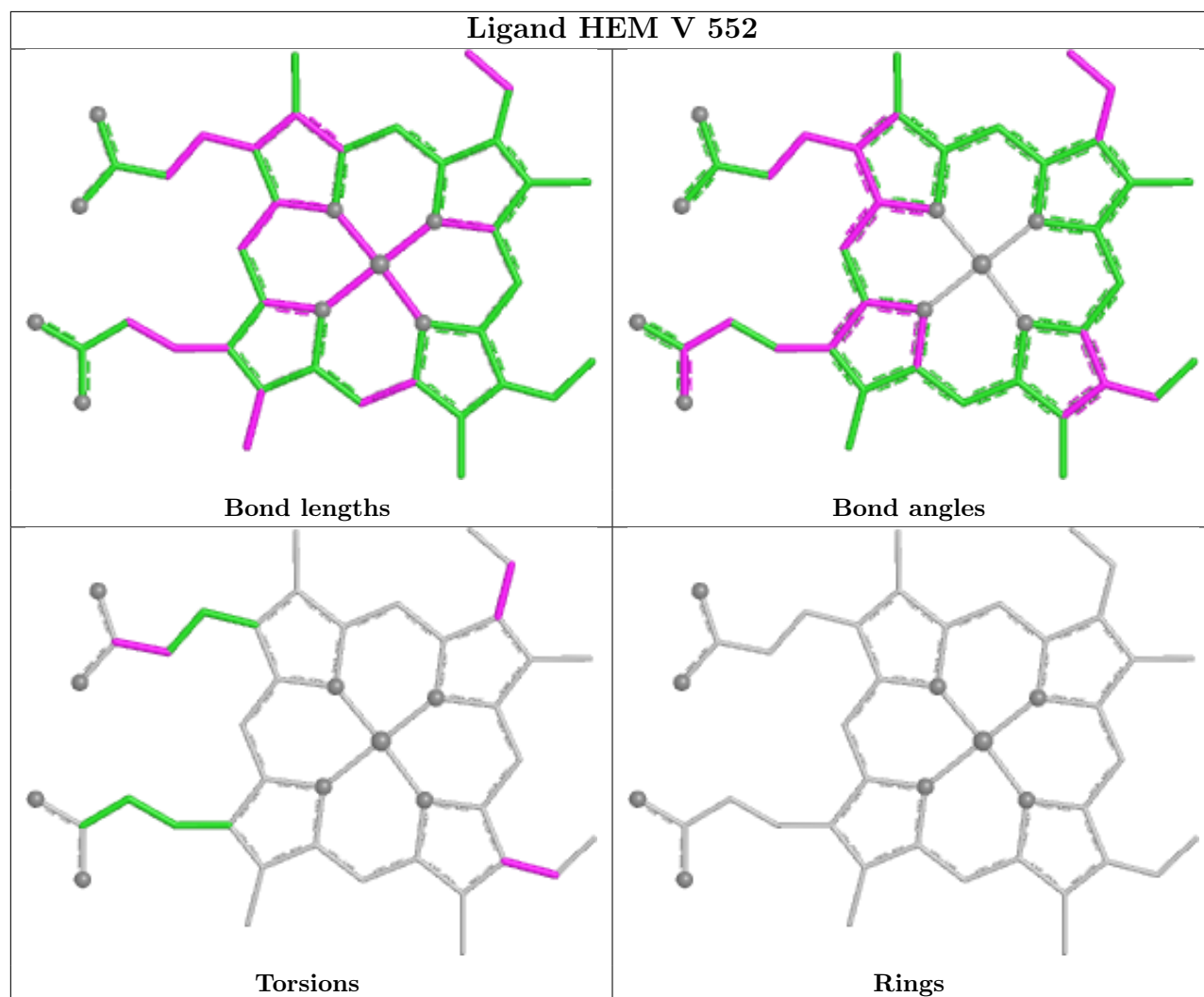
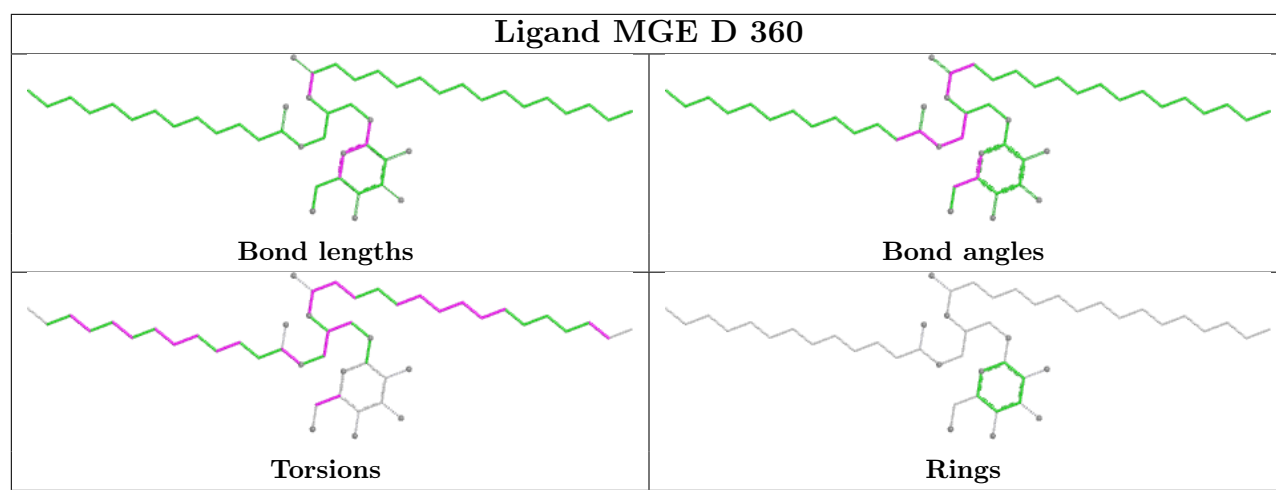


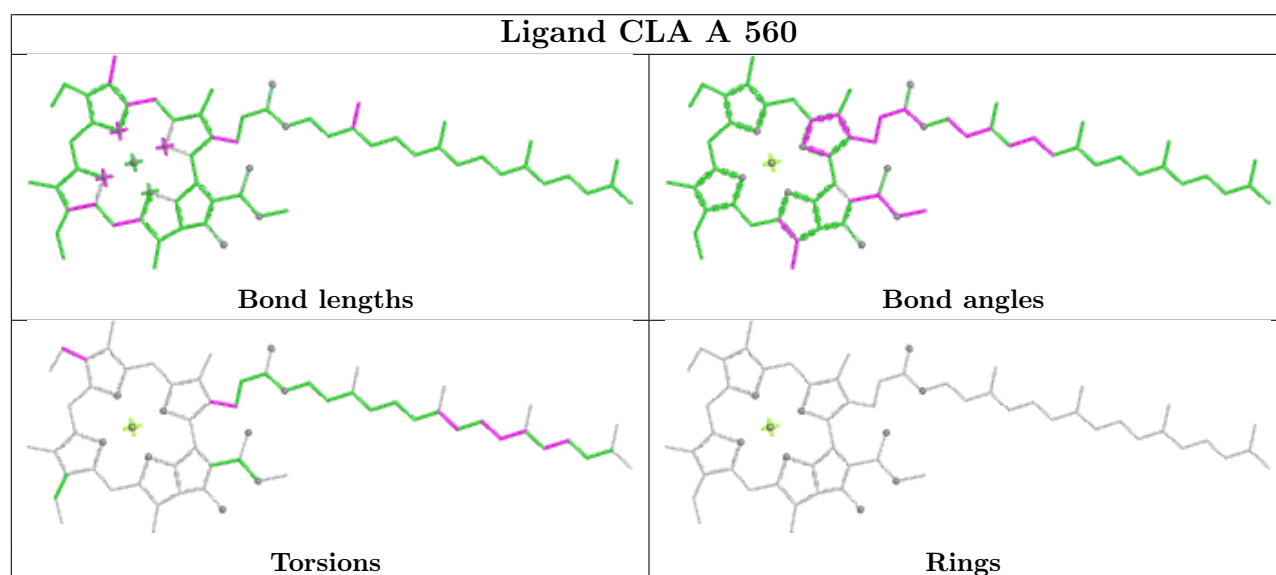
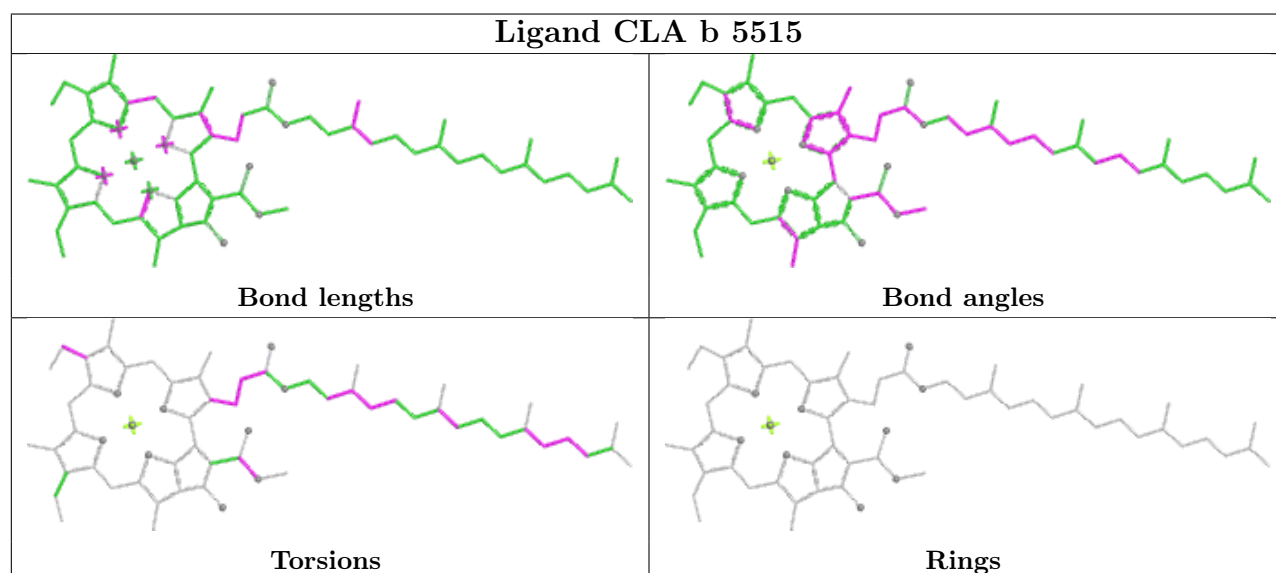
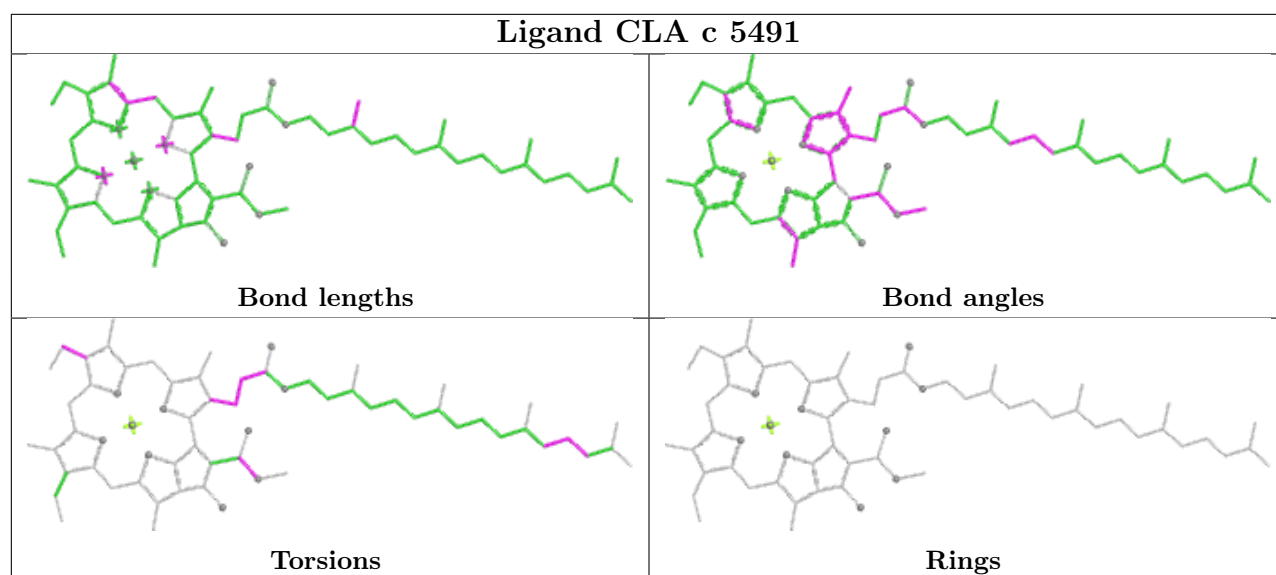


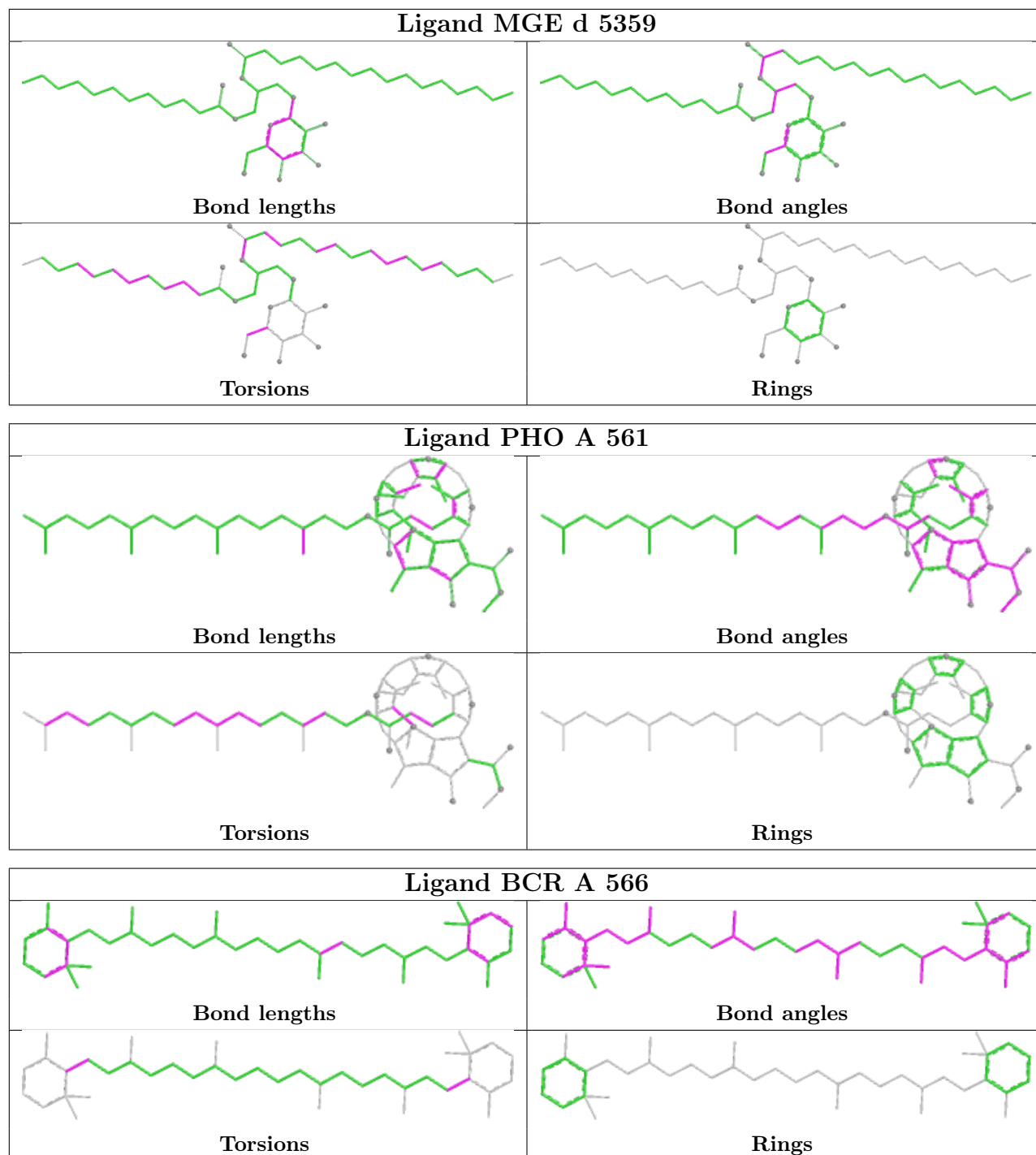


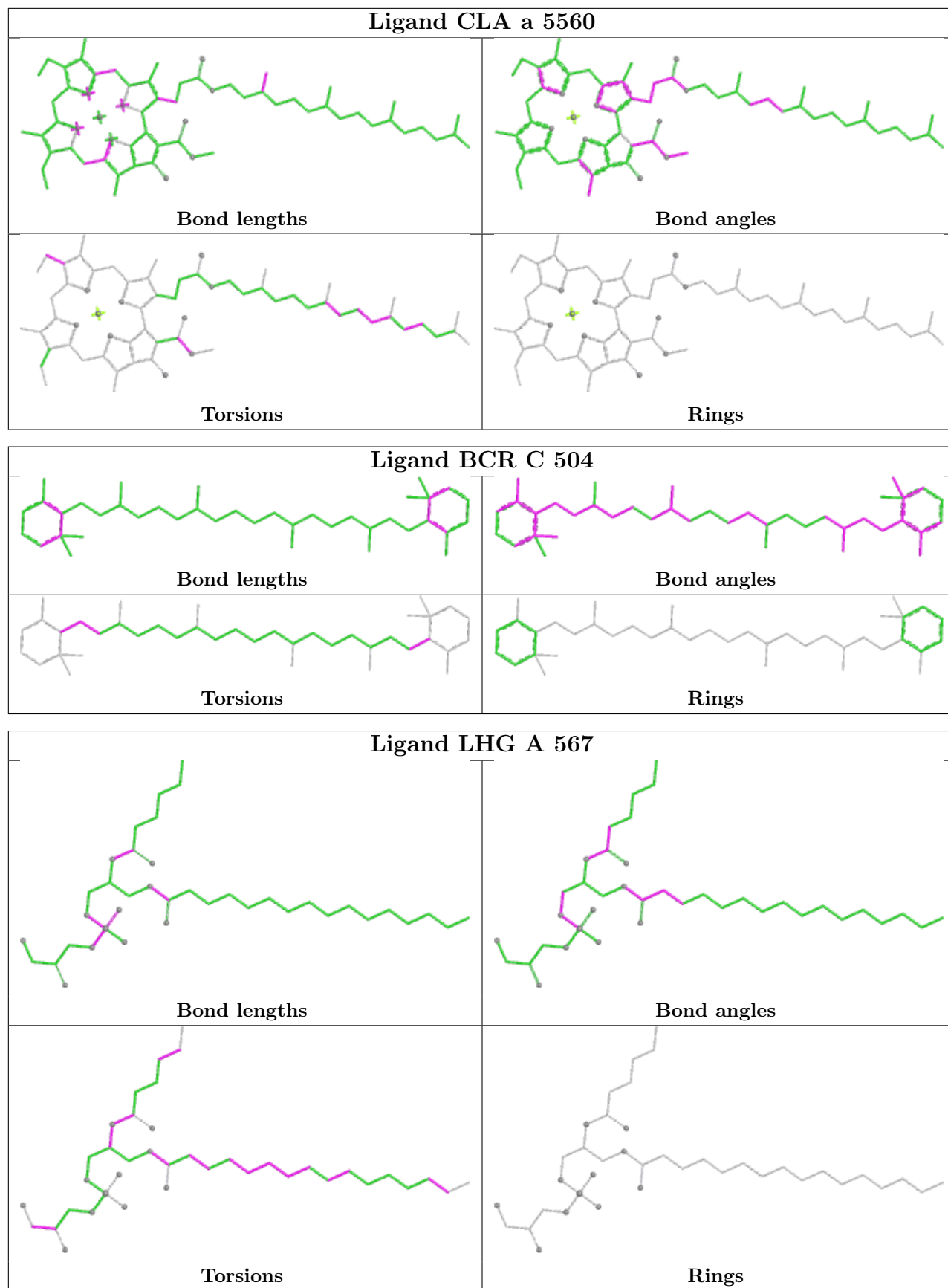


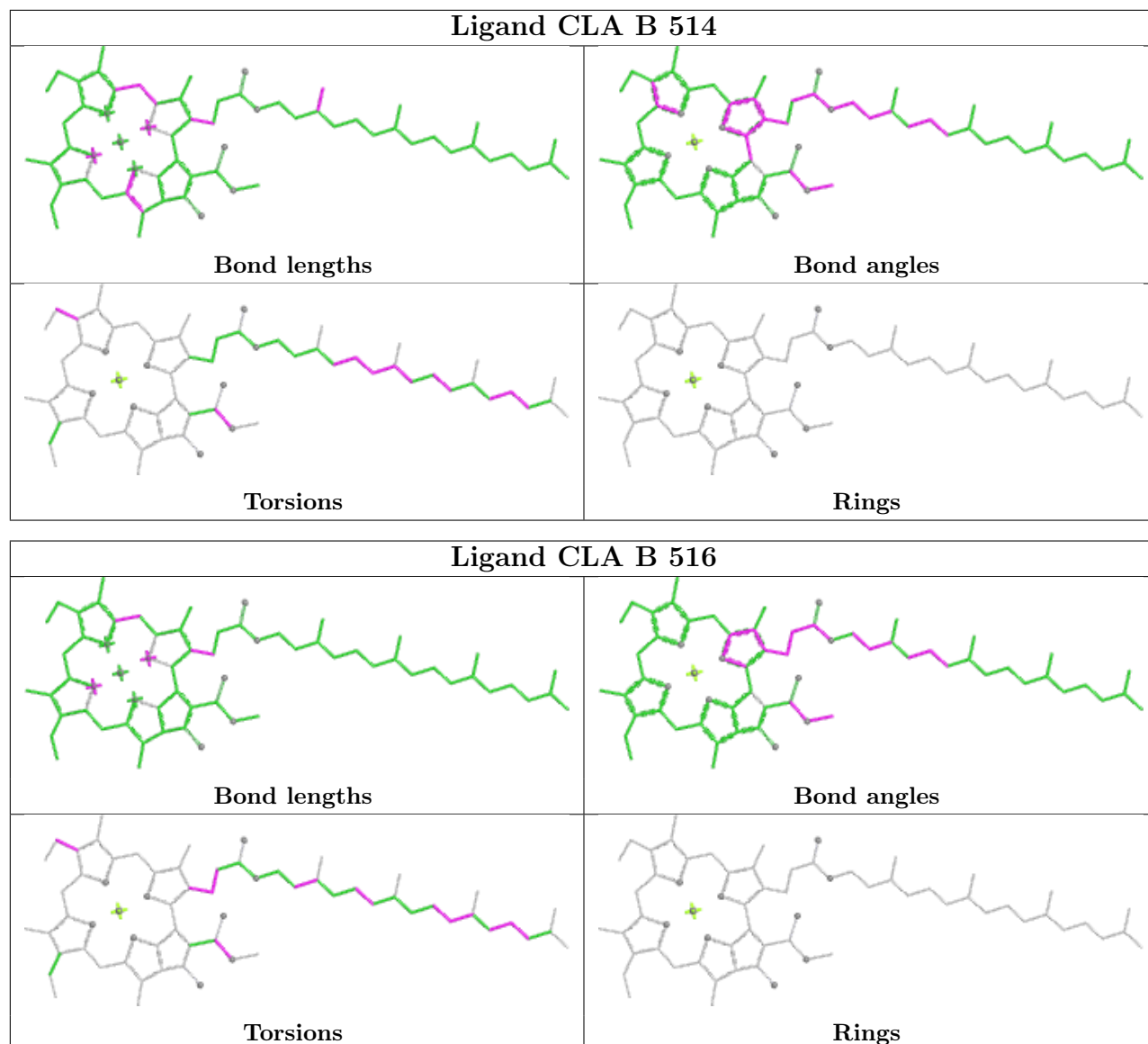


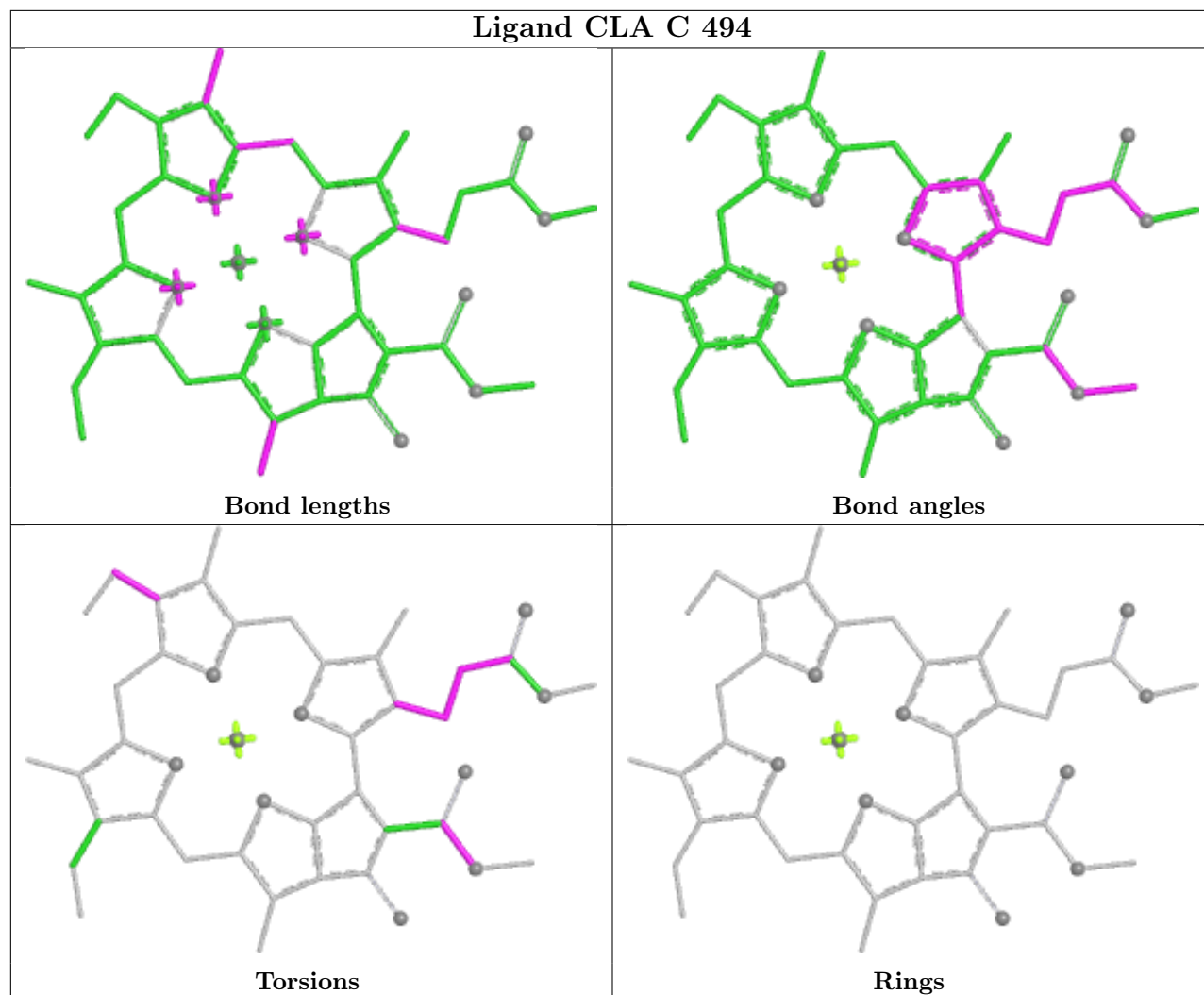


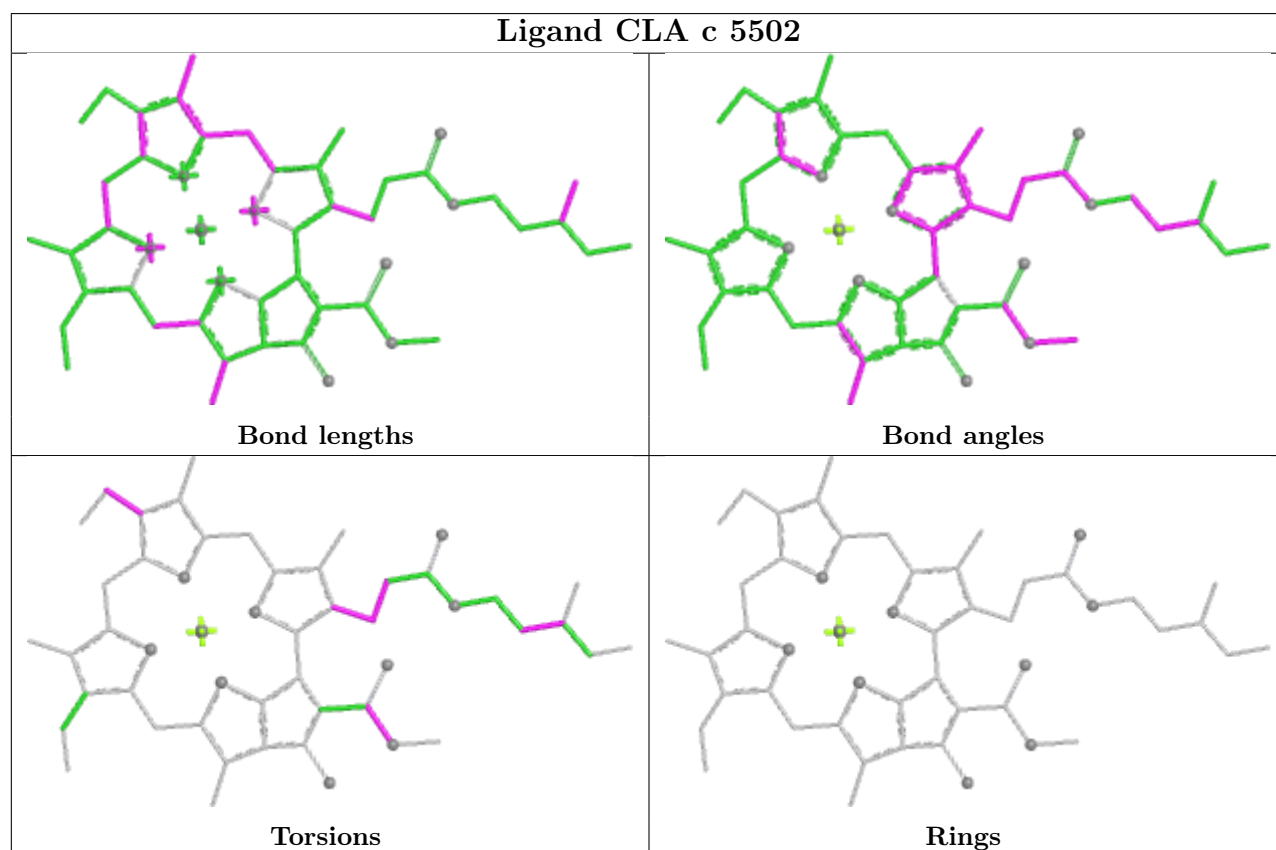
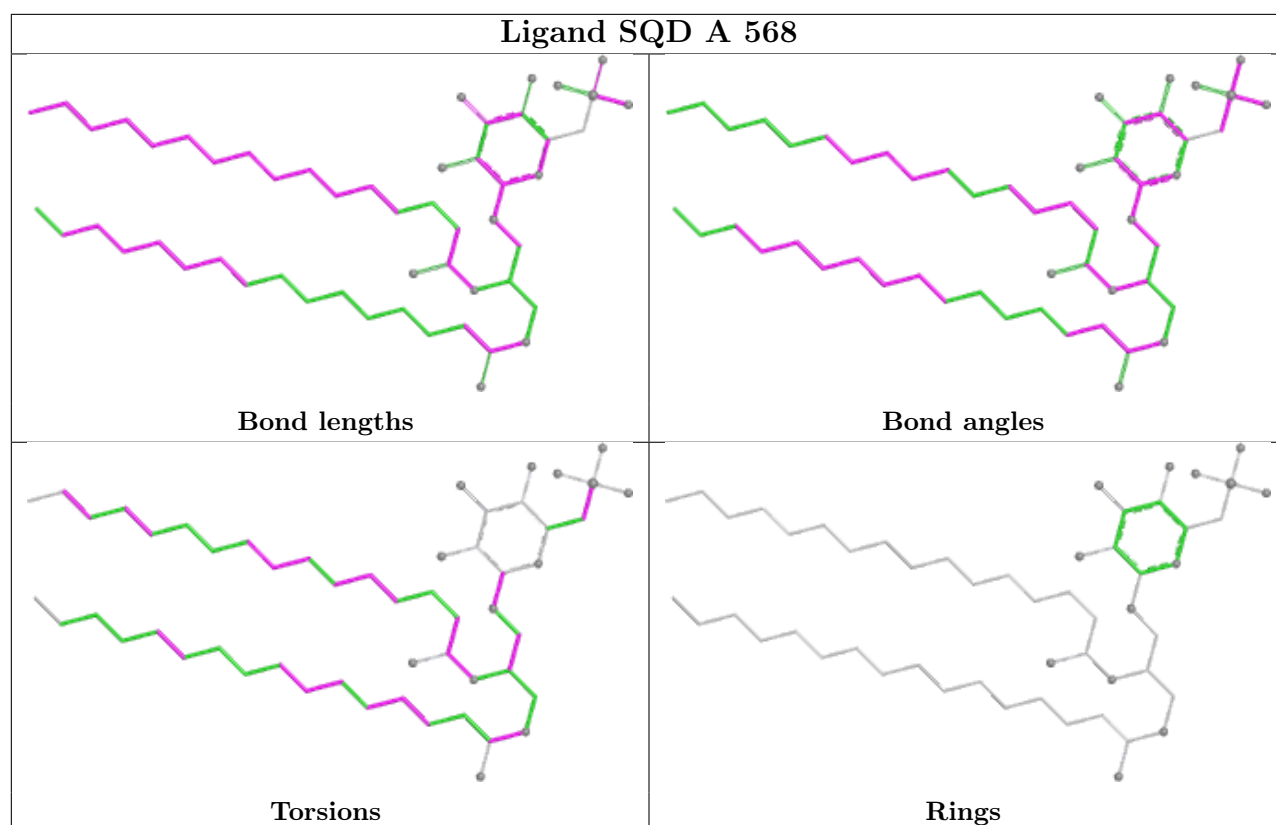


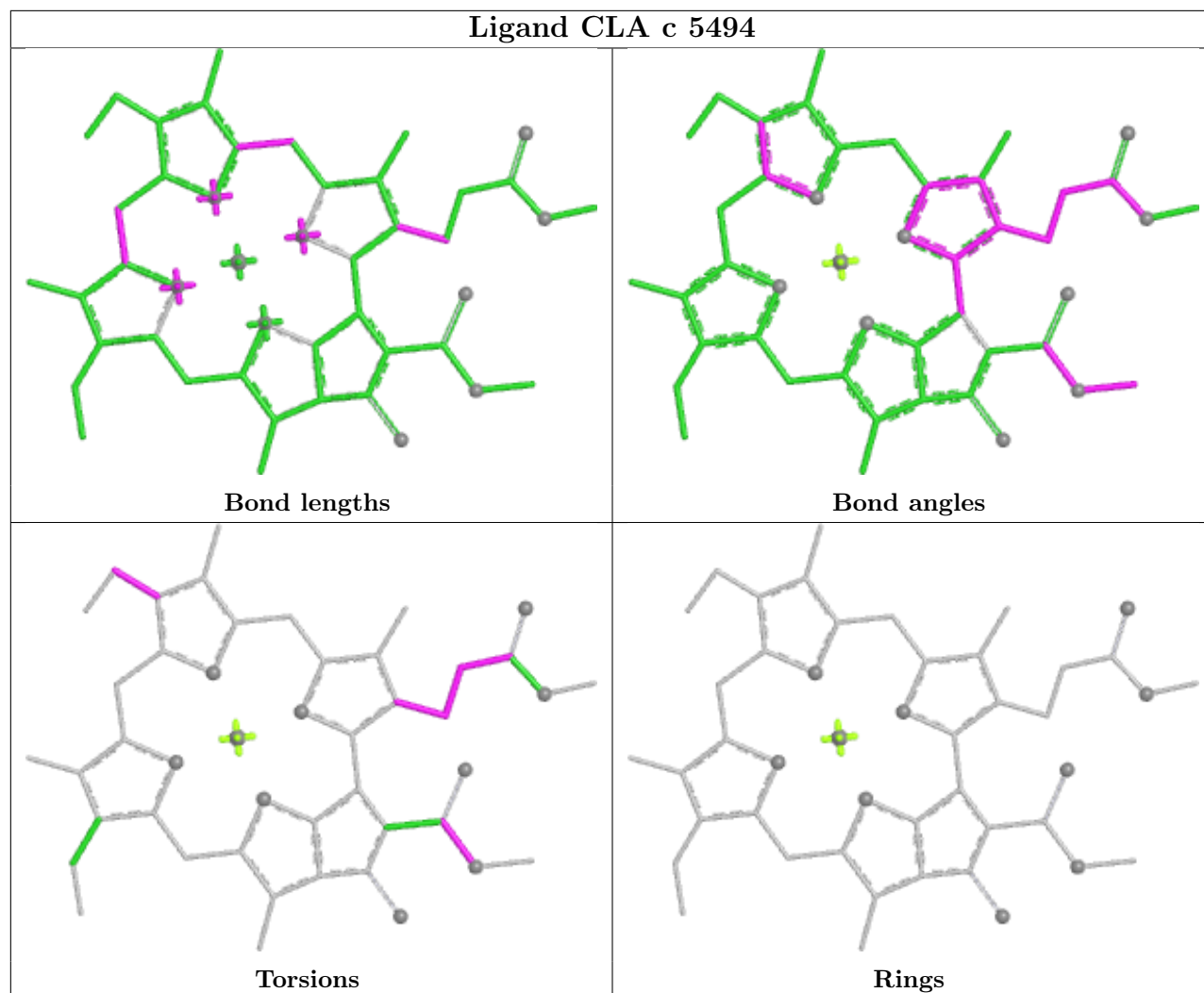


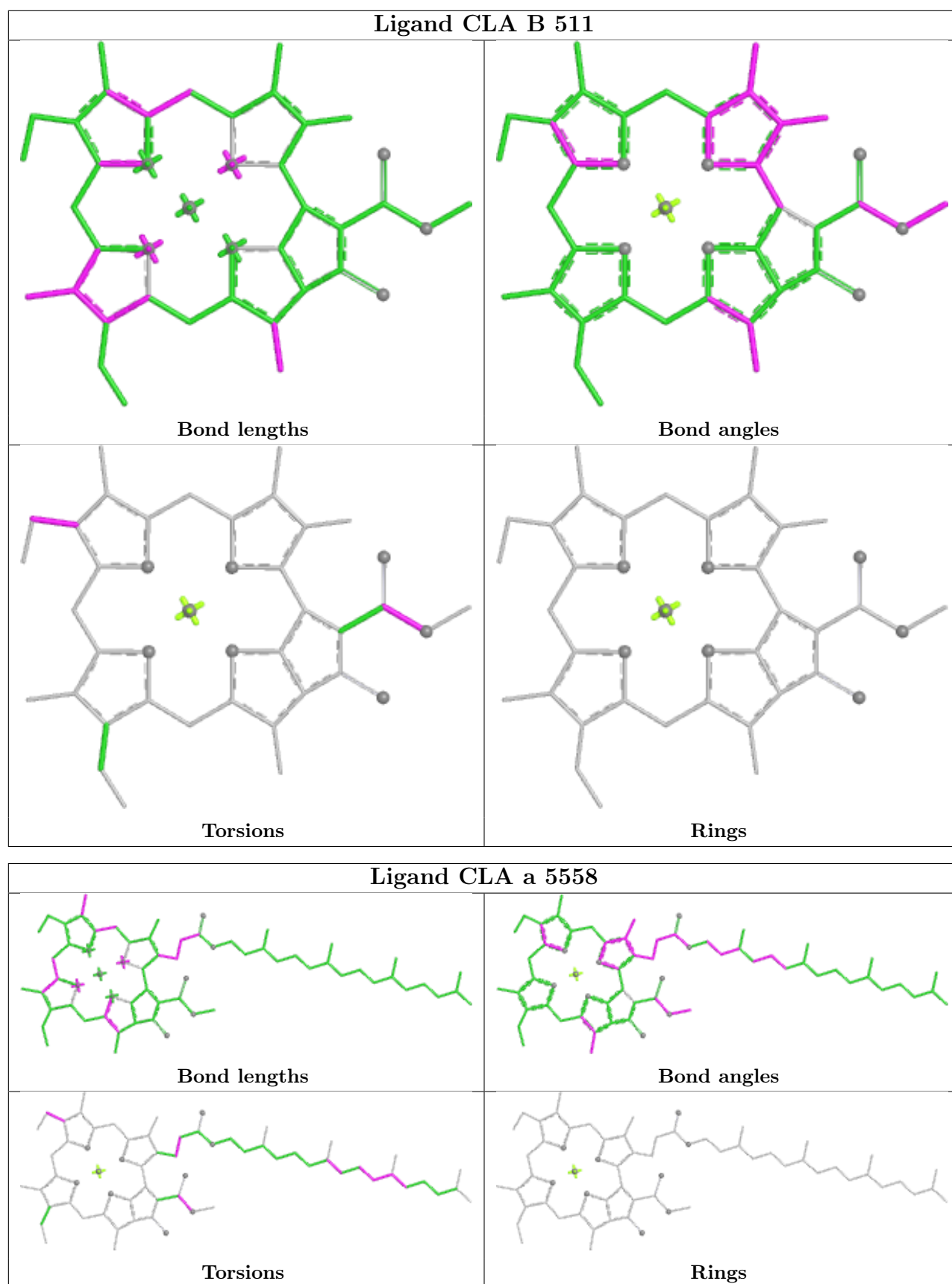


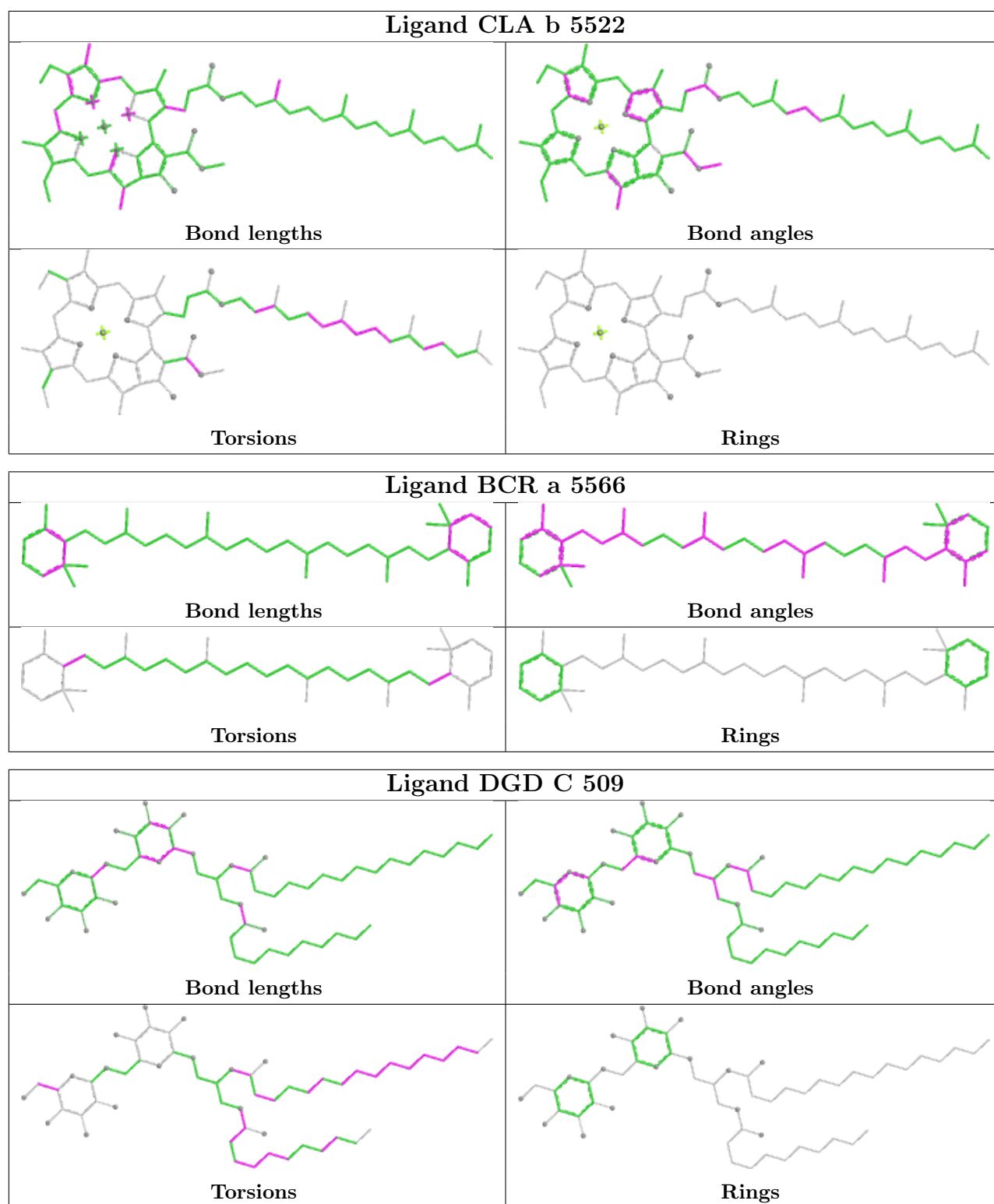


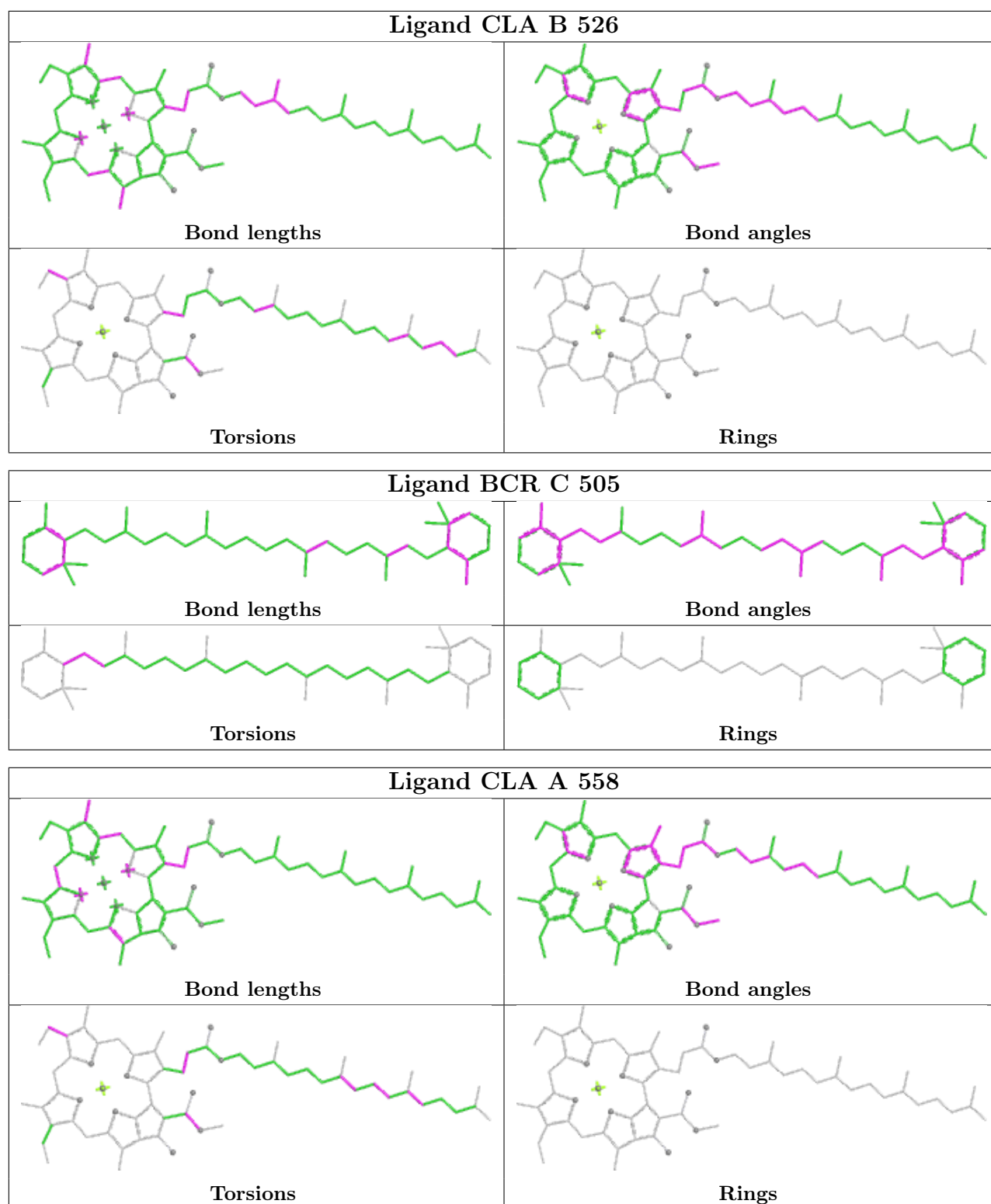












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.62	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.58	0 100 100	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.63	0 100 100	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.63	0 100 100	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.57	2 (0%) 88 76	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.43	1 (0%) 91 83	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.75	0 100 100	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.65	1 (0%) 90 79	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.32	1 (1%) 76 55	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.21	1 (1%) 76 55	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.34	1 (2%) 53 31	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.31	0 100 100	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.40	0 100 100	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.47	0 100 100	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	0 100 100	57, 66, 80, 88	0
8	i	35/38 (92%)	-0.46	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.28	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.30	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.62	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.33	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.39	0 100 100	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.51	0 100 100	45, 56, 86, 91	0
12	M	36/36 (100%)	-0.43	0 100 100	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.49	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.47	1 (0%) 88 76	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.43	0 100 100	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.38	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.43	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.58	0 100 100	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.56	0 100 100	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.60	1 (0%) 84 66	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.42	0 100 100	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.28	0 100 100	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.04	0 100 100	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.54	9 (0%) 91 83	35, 66, 85, 101	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	222	GLY	3.6
16	V	27	ALA	3.0
5	E	4	THR	2.5
5	e	5006	GLY	2.3
4	d	5013	GLY	2.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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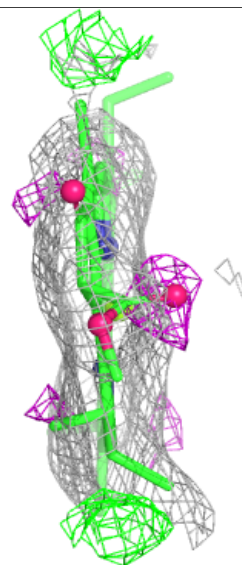
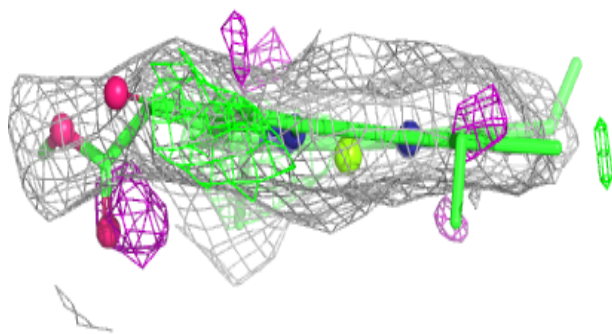
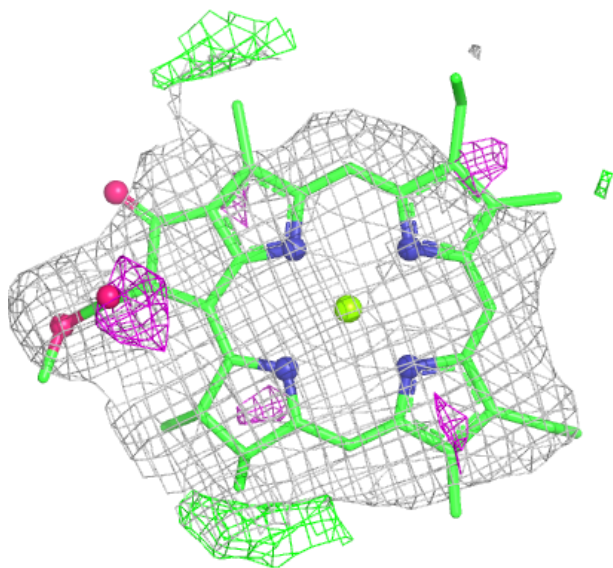
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	a	5558	65/65	0.95	0.07	41,50,55,61	0
32	HEM	F	51	43/43	0.95	0.10	78,84,92,95	0
20	CLA	b	5514	65/65	0.95	0.06	41,51,74,75	0
32	HEM	v	5552	43/43	0.95	0.08	65,67,70,70	0
33	CA	K	56	1/1	0.95	0.13	119,119,119,119	0
20	CLA	A	558	65/65	0.96	0.07	41,46,50,51	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.

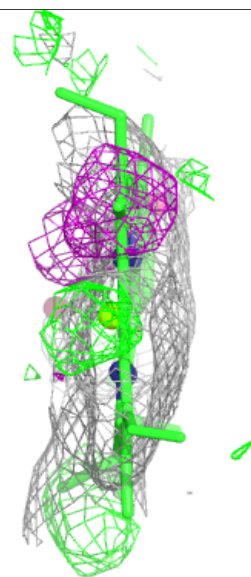
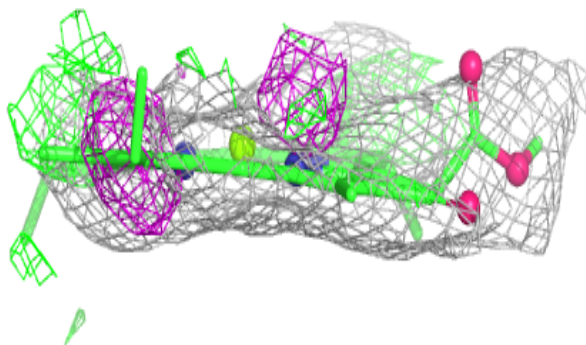
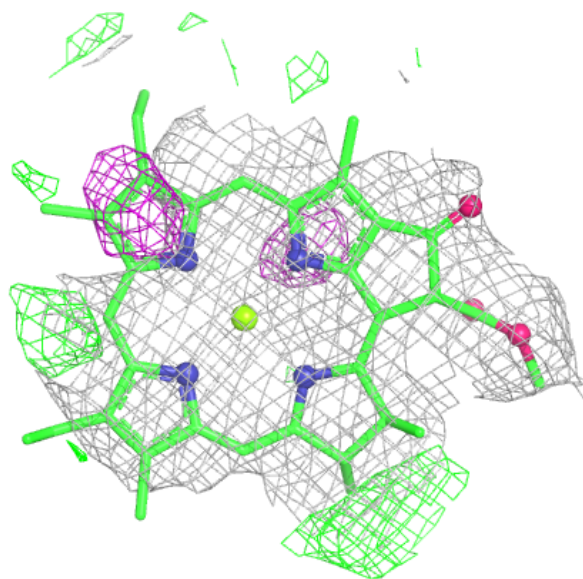
Electron density around CLA B 511:

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



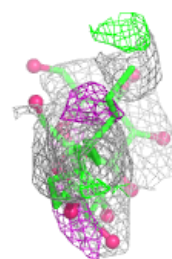
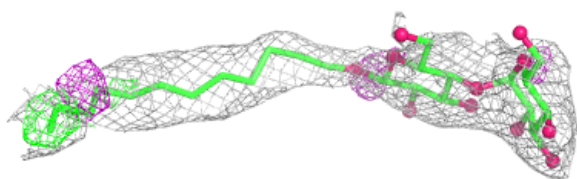
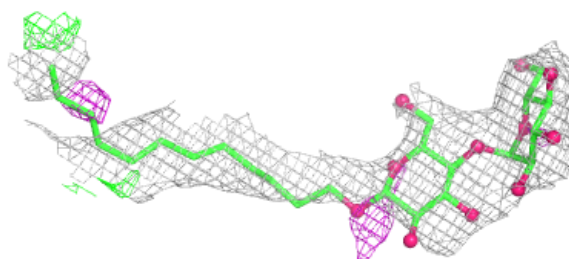
Electron density around CLA b 5511:

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



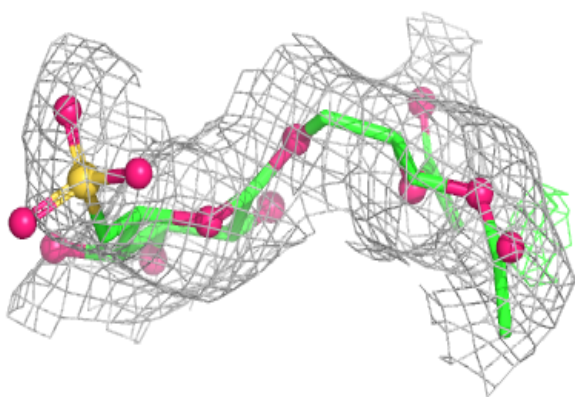
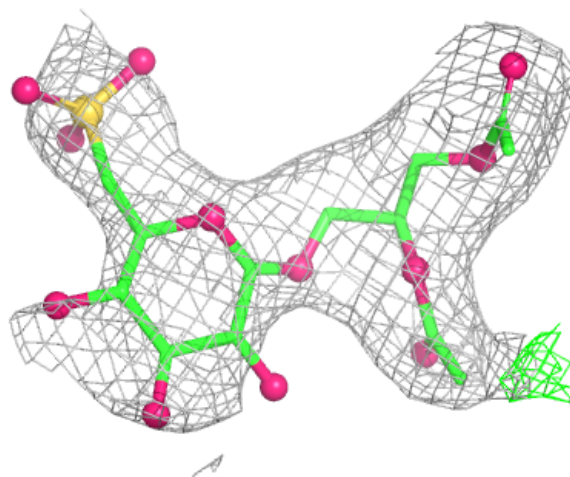
Electron density around LMT A 569:

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



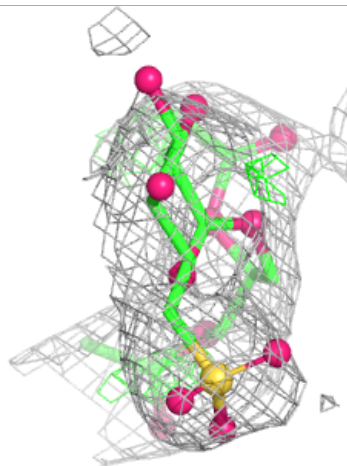
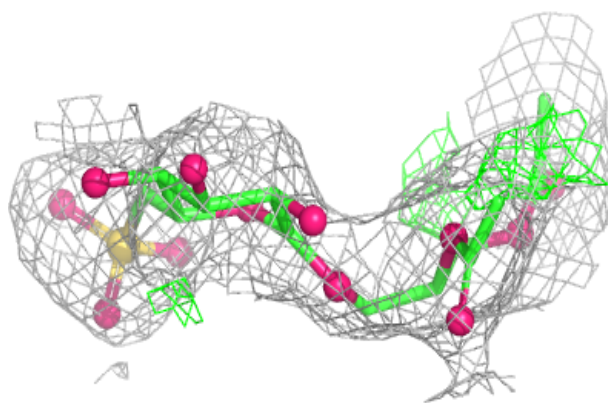
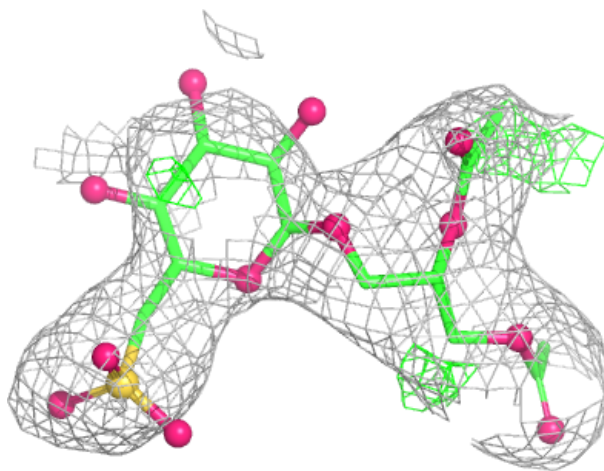
Electron density around SQD a 212:

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



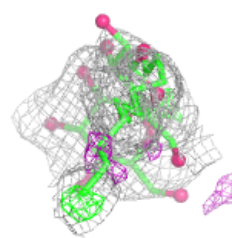
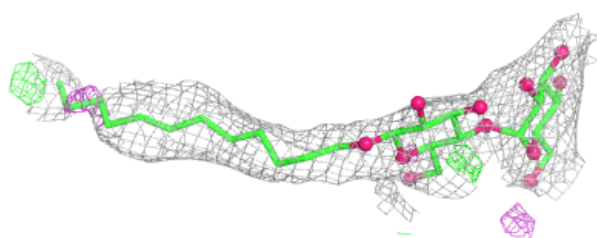
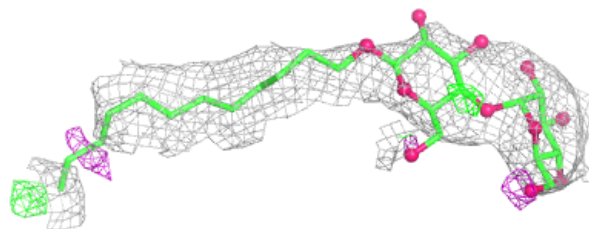
Electron density around SQD A 5212:

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

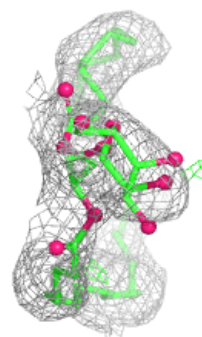
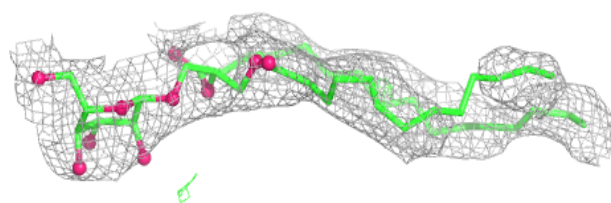
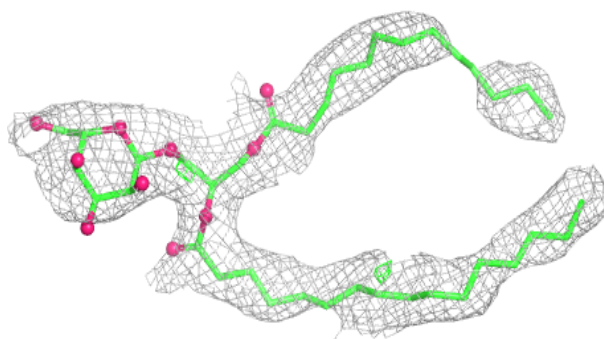


Electron density around LMT a 5568:

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

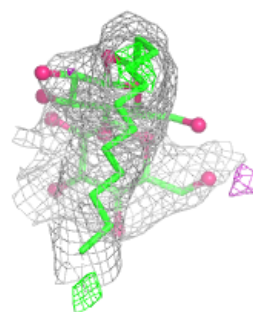
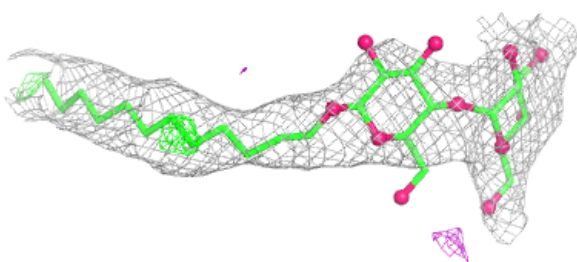
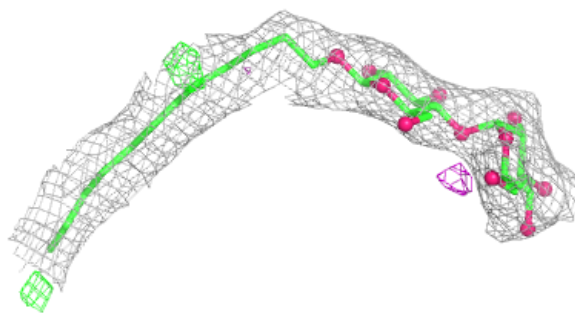
**Electron density around MGE i 5201:**

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

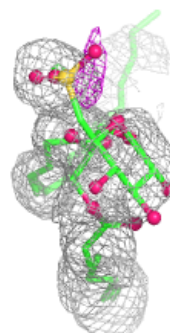
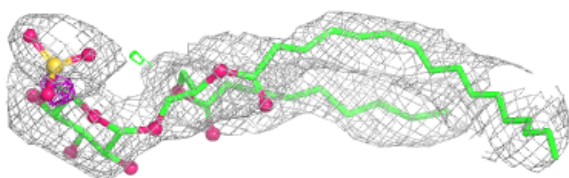
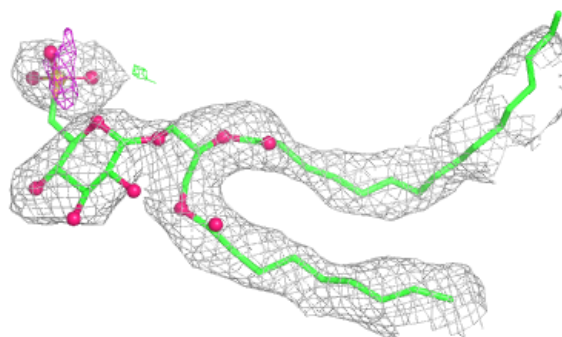


Electron density around LMT m 216:

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

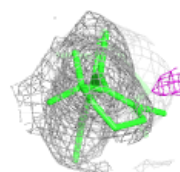
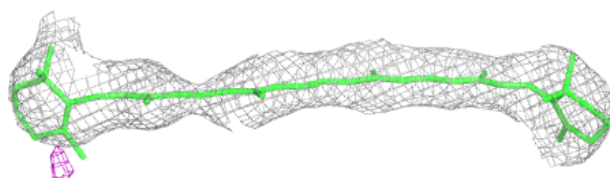
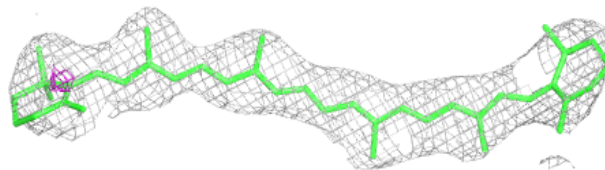
**Electron density around SQD L 5213:**

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

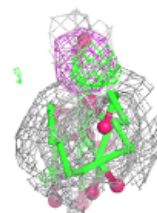
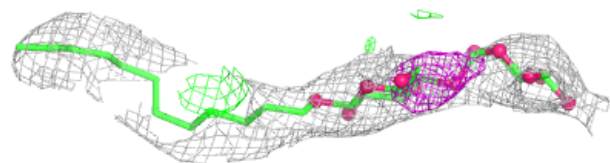
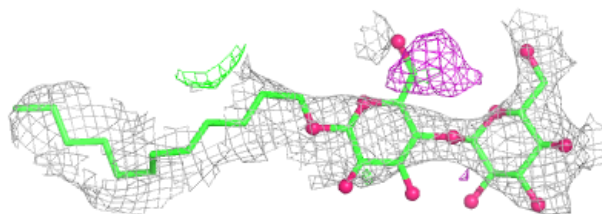


Electron density around BCR c 5506:

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and green (positive)

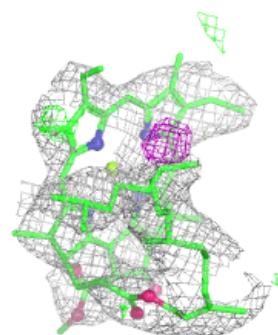
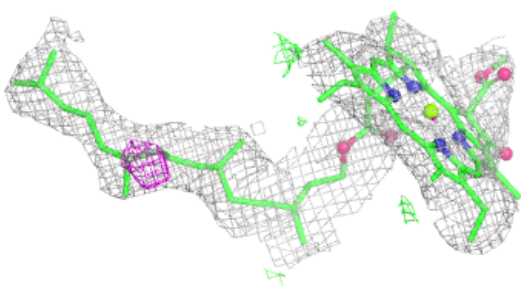
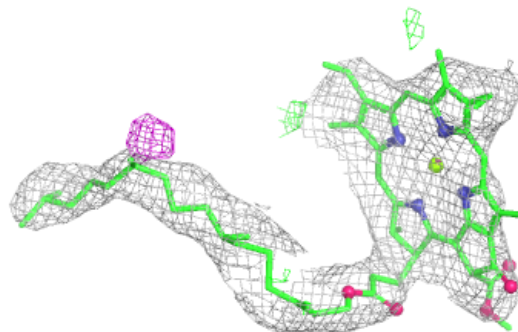
**Electron density around LMT t 5217:**

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

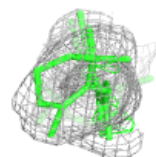
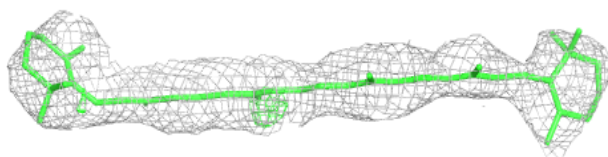
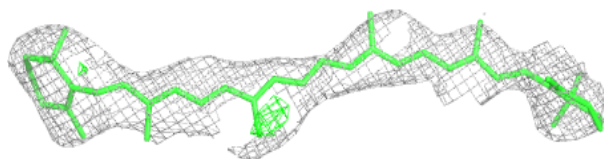


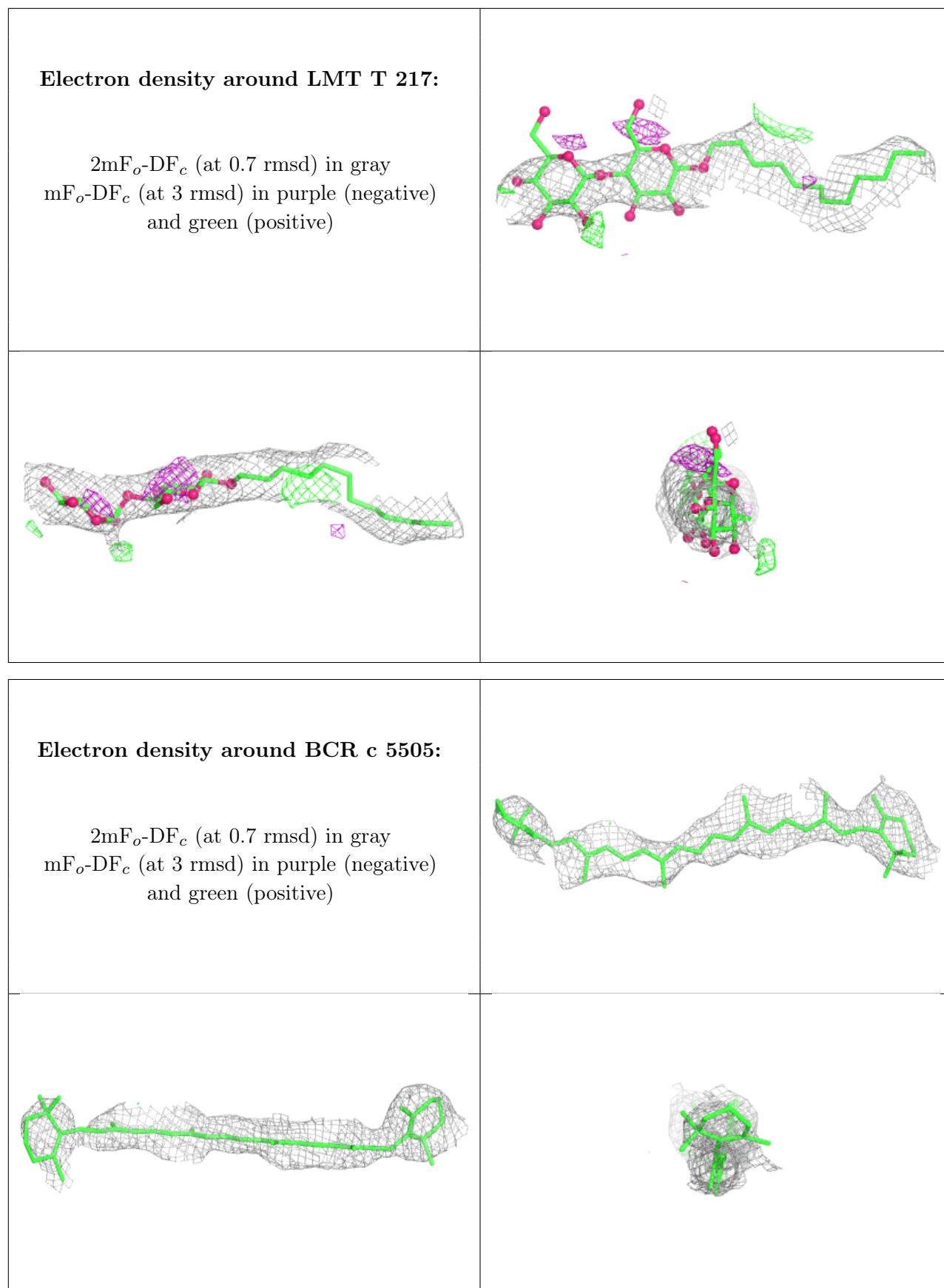
Electron density around CLA c 5501:

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and green (positive)

**Electron density around BCR C 505:**

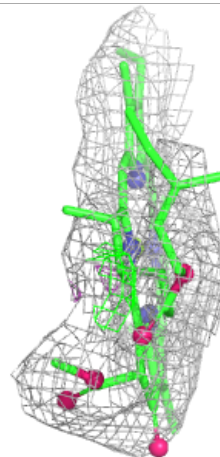
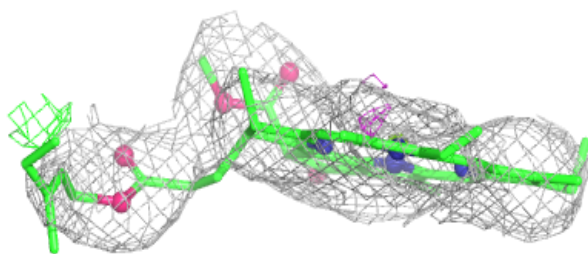
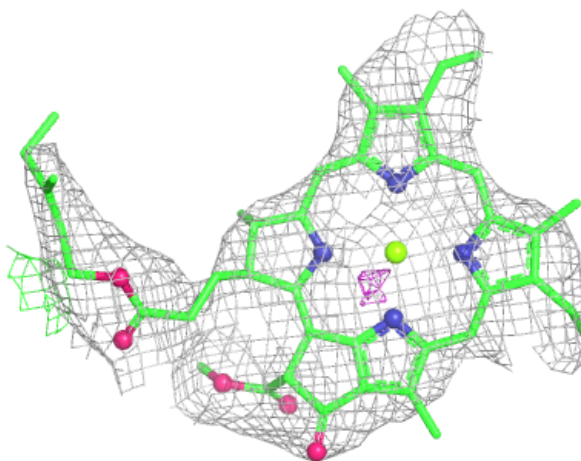
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





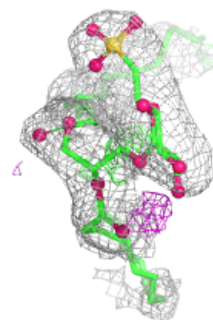
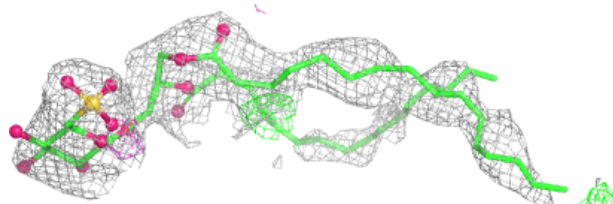
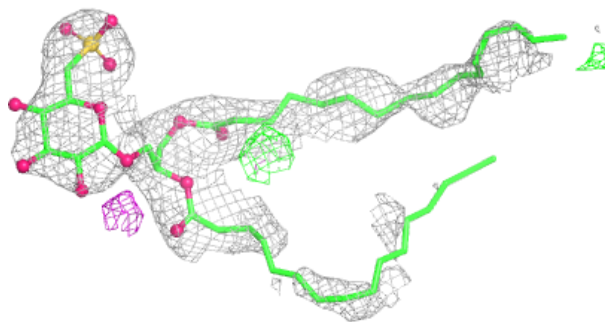
Electron density around CLA c 5502:

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

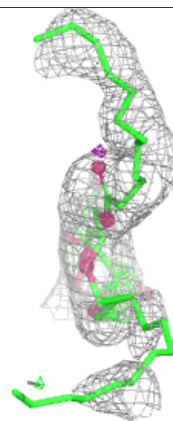
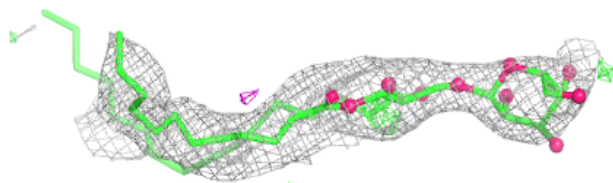
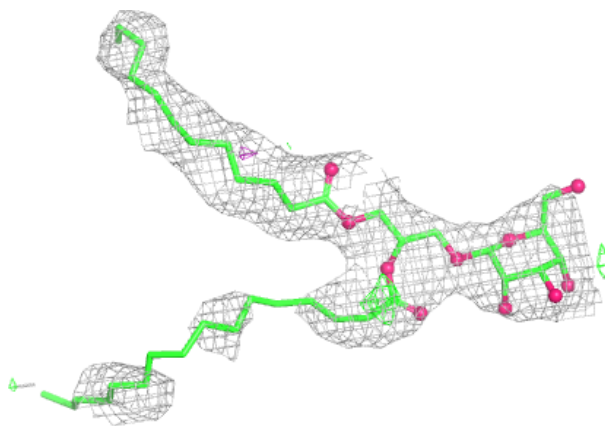


Electron density around SQD d 5358:

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

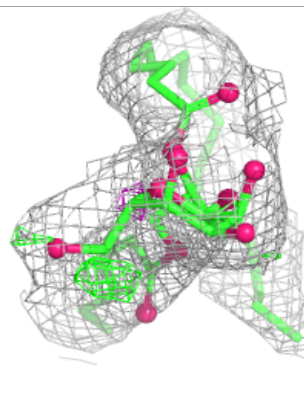
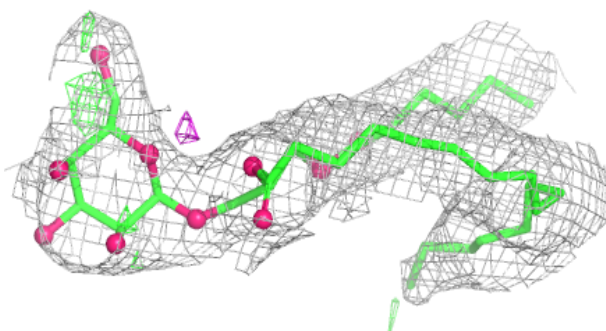
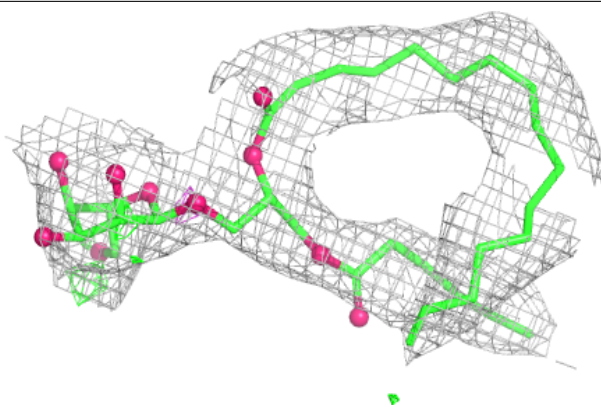
**Electron density around MGE d 5359:**

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

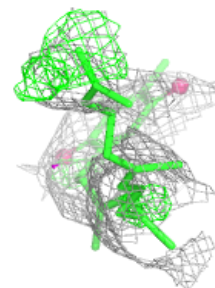
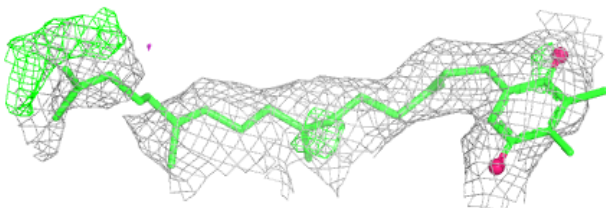
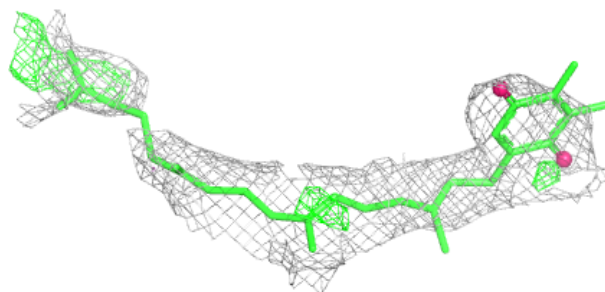


Electron density around MGE d 5360:

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

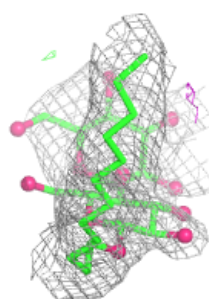
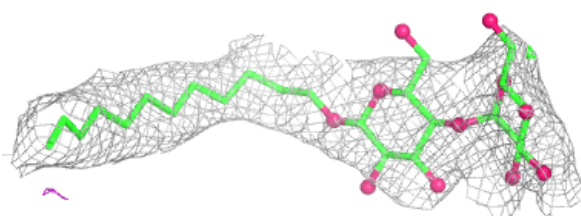
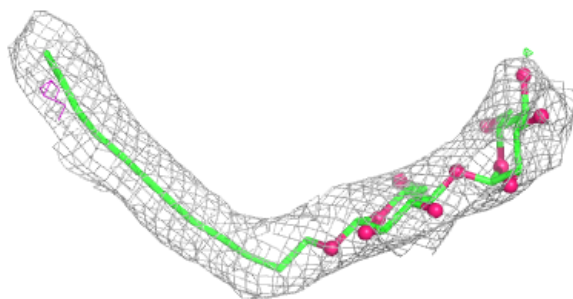
**Electron density around PQ9 A 564:**

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

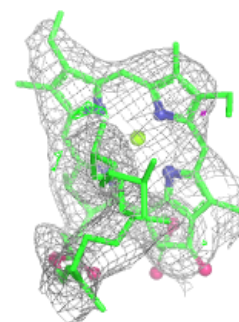
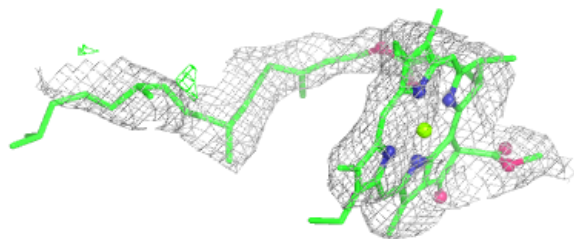
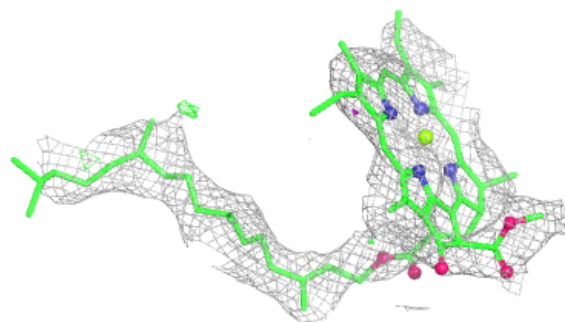


Electron density around LMT M 5216:

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

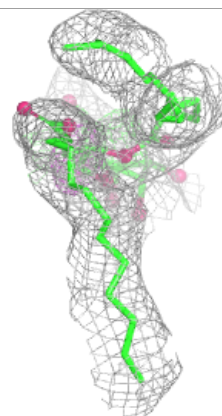
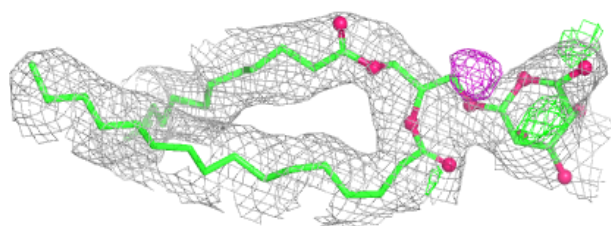
**Electron density around CLA c 5498:**

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

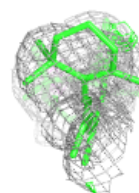
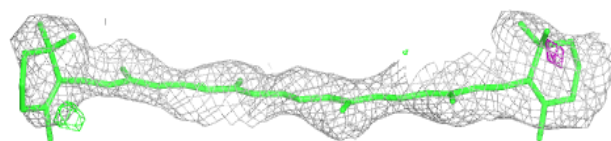
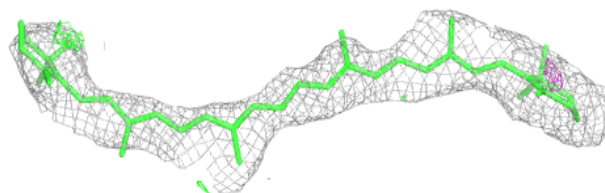


Electron density around MGE d 5361:

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

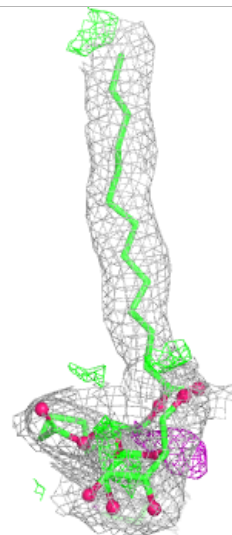
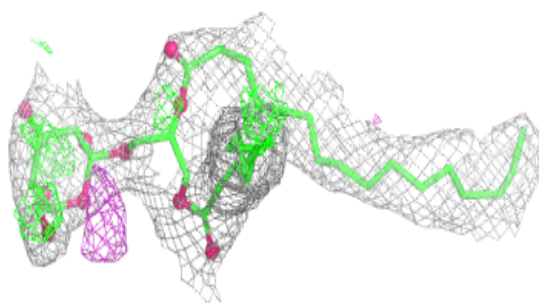
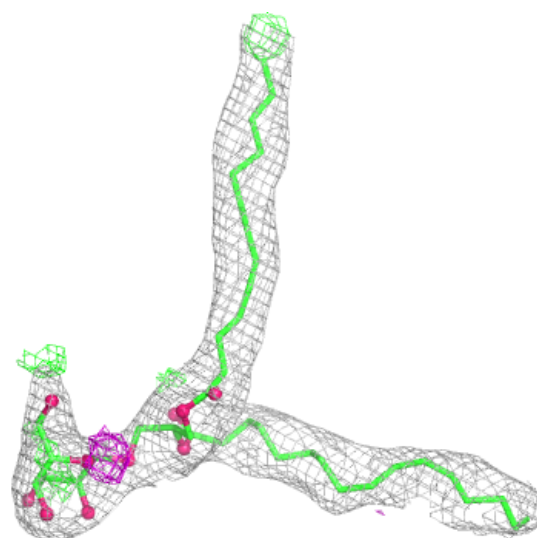
**Electron density around BCR H 107:**

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



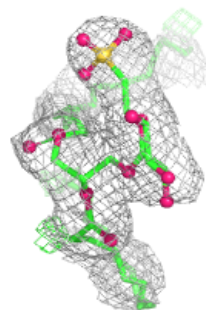
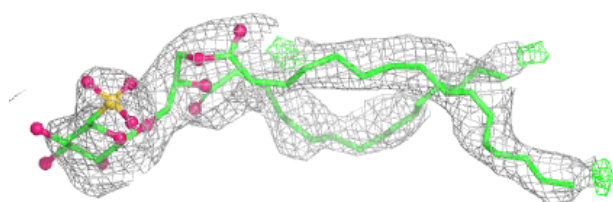
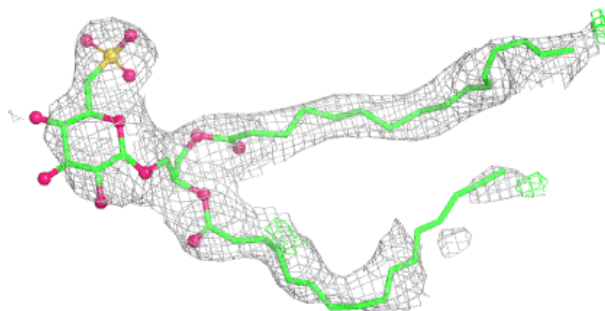
Electron density around MGE 1 5210:

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

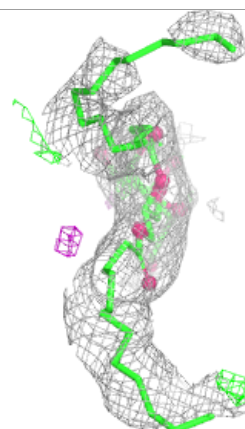
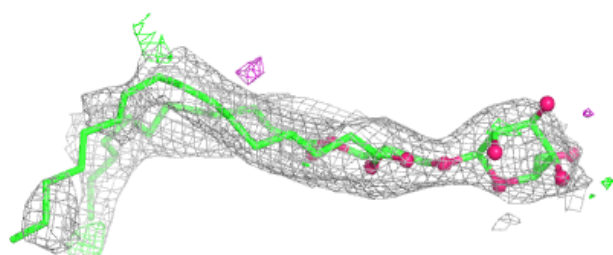
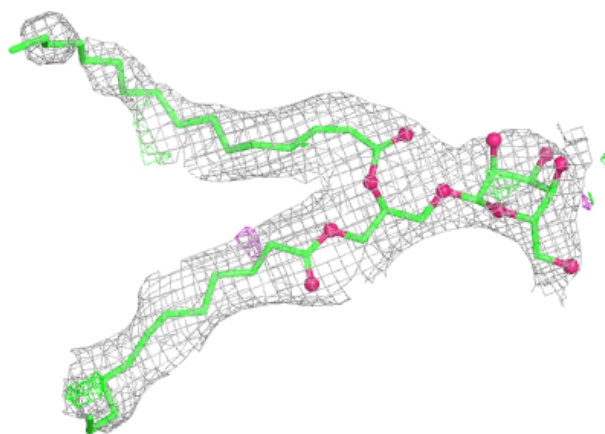


Electron density around SQD A 568:

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

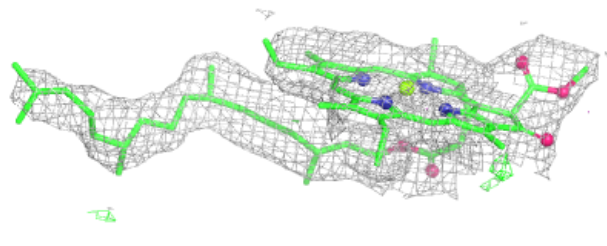
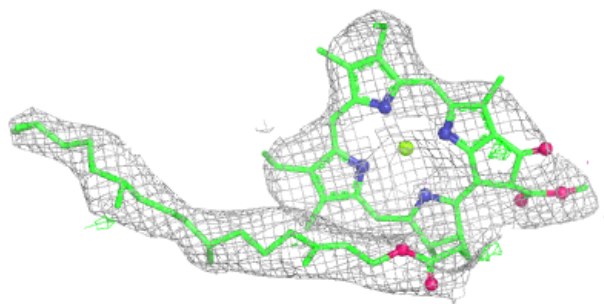
**Electron density around MGE D 358:**

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

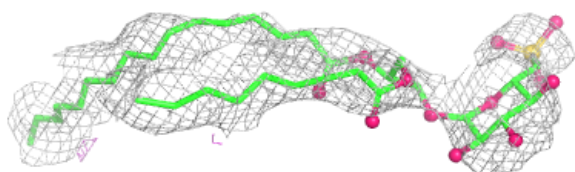
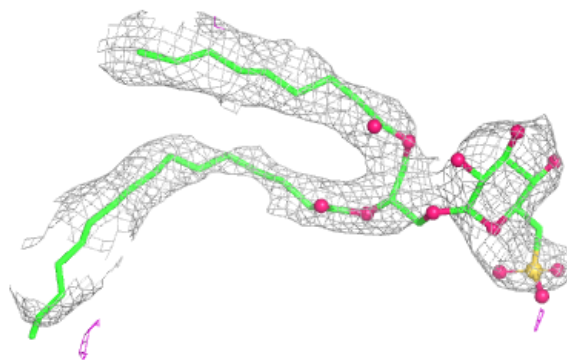


Electron density around CLA c 5491:

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

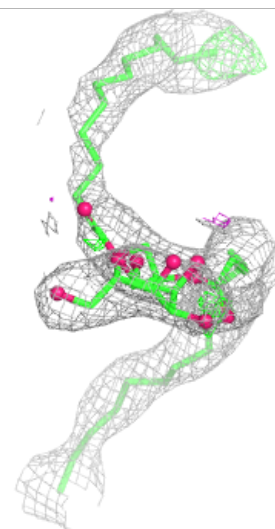
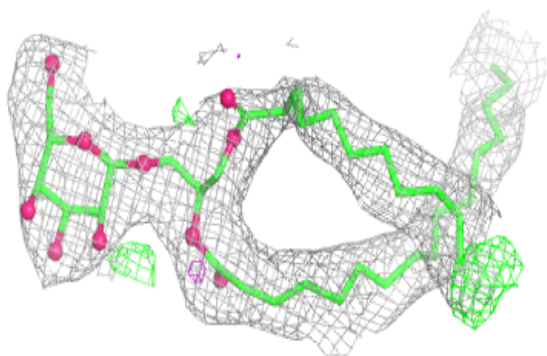
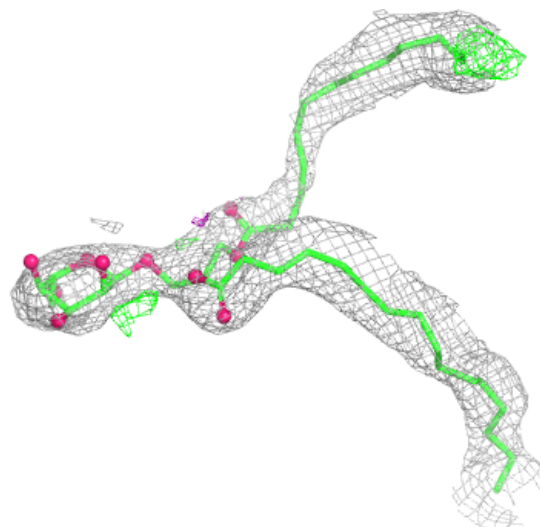
**Electron density around SQD t 213:**

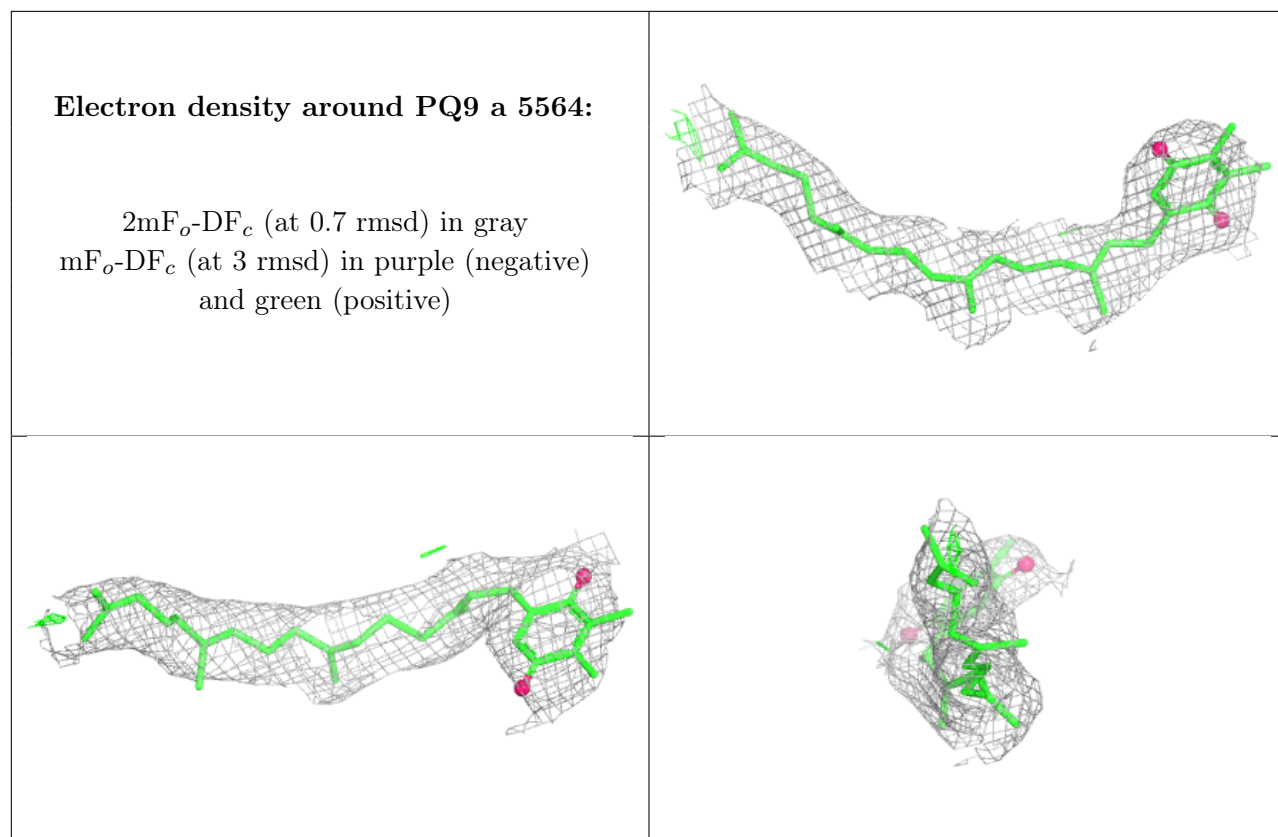
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE b 5530:

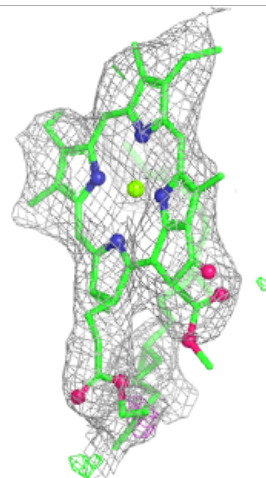
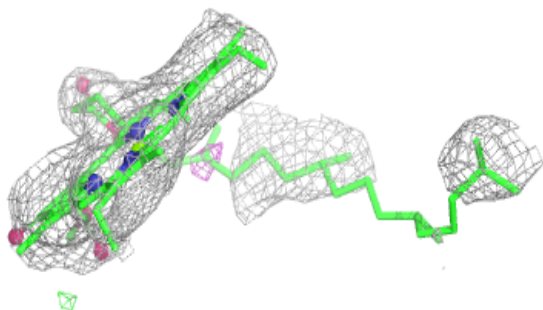
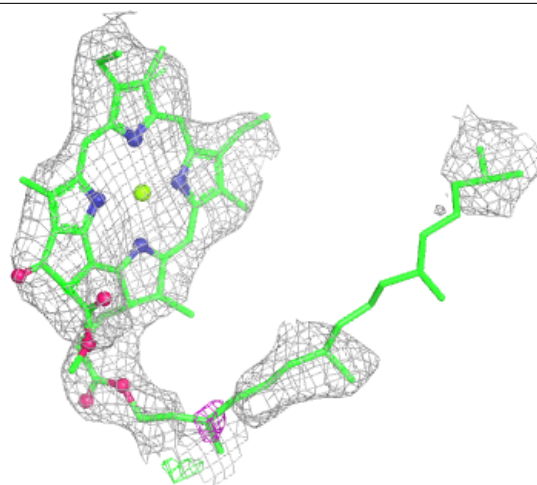
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





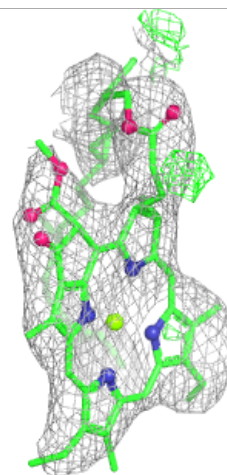
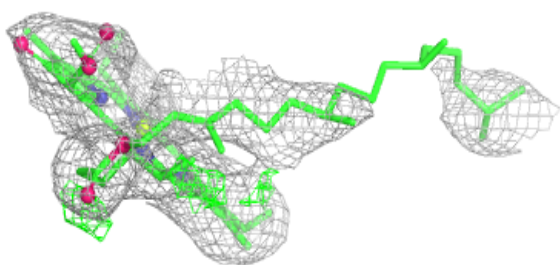
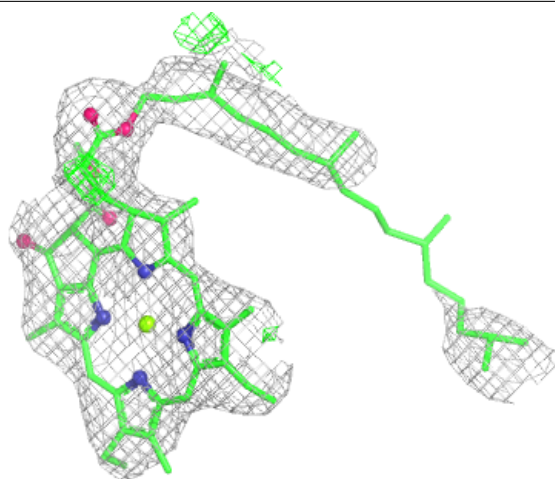
Electron density around CLA B 526:

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



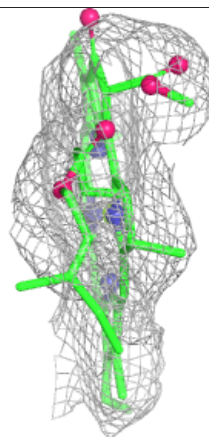
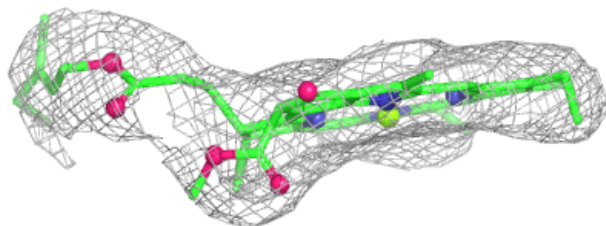
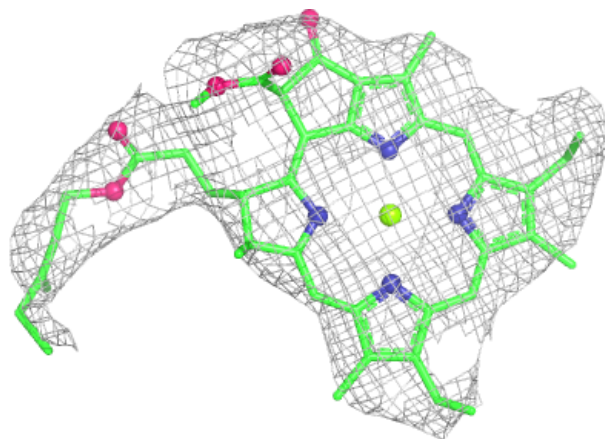
Electron density around CLA b 5526:

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



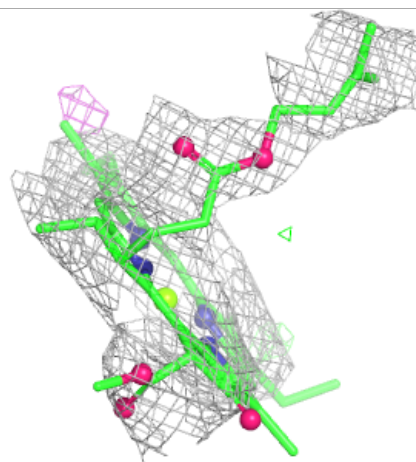
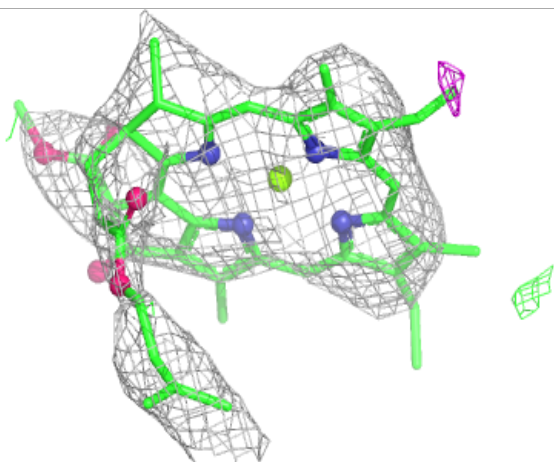
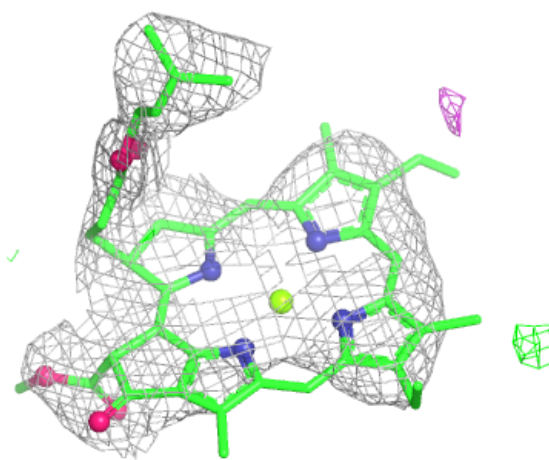
Electron density around CLA C 502:

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



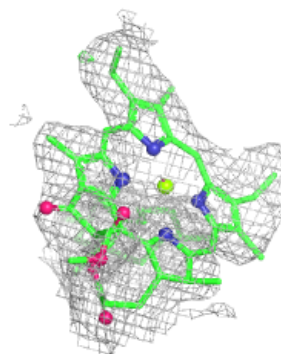
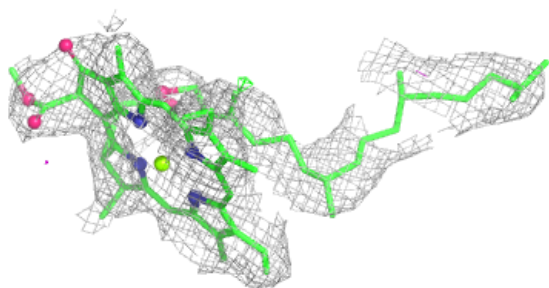
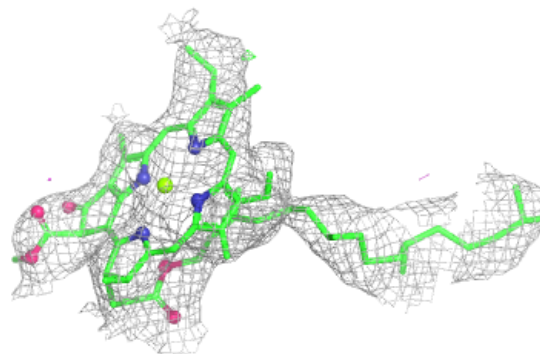
Electron density around CLA c 5503:

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

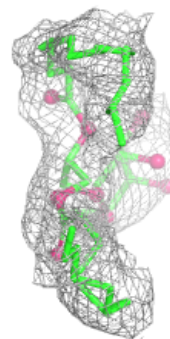
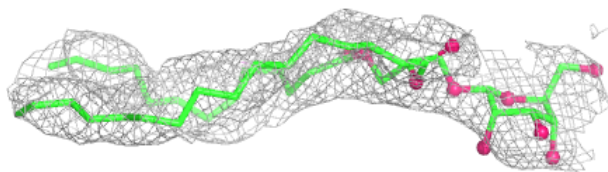
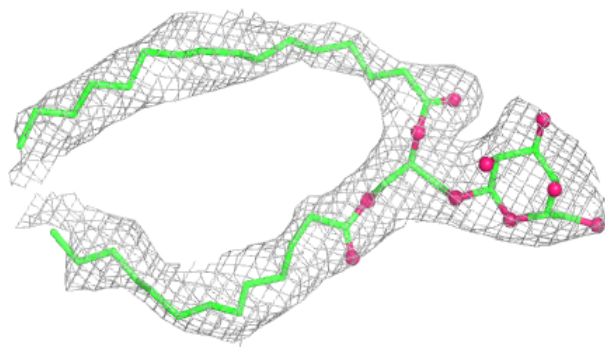


Electron density around CLA c 5495:

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

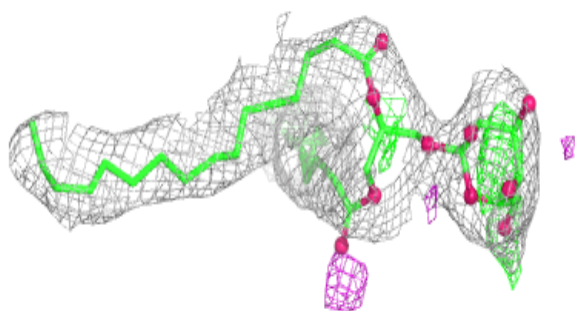
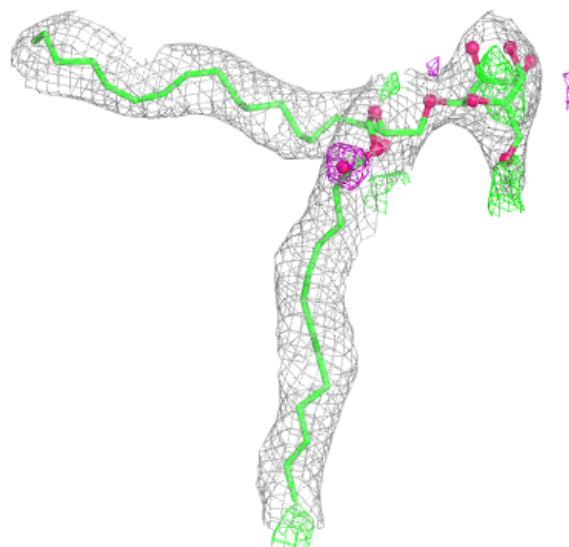
**Electron density around MGE I 201:**

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



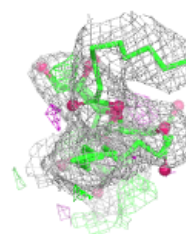
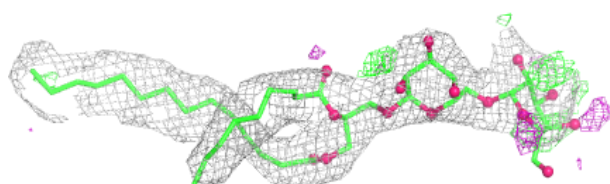
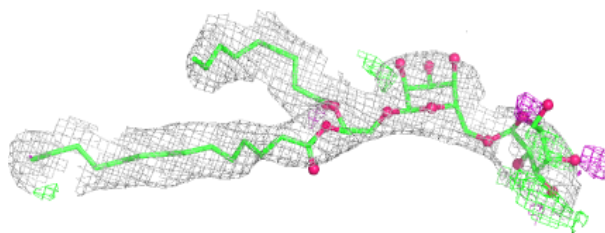
Electron density around MGE L 210:

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

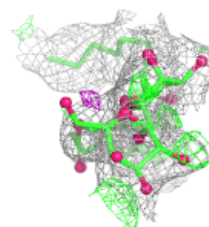
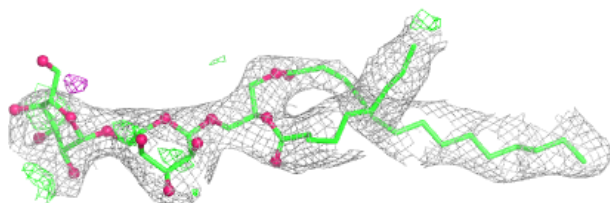
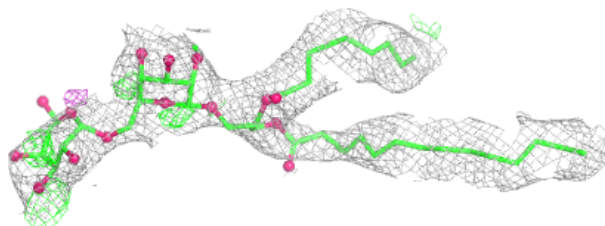


Electron density around DGD C 507:

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

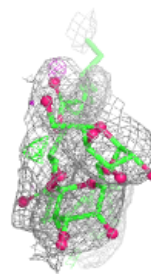
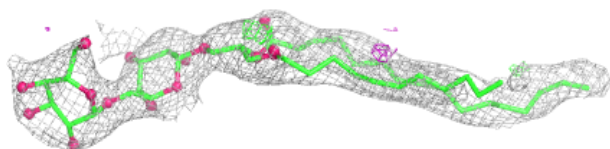
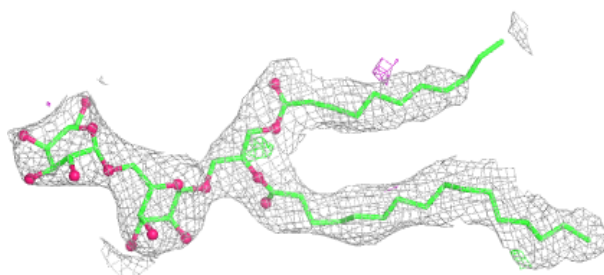
**Electron density around DGD c 5507:**

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

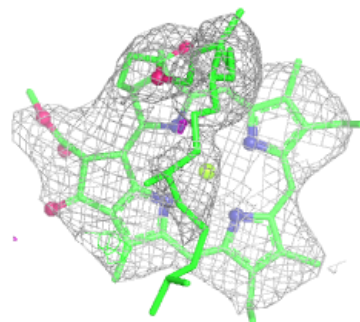
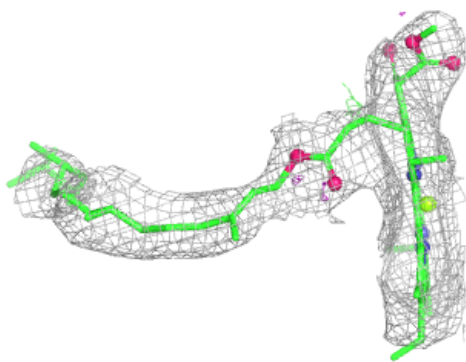
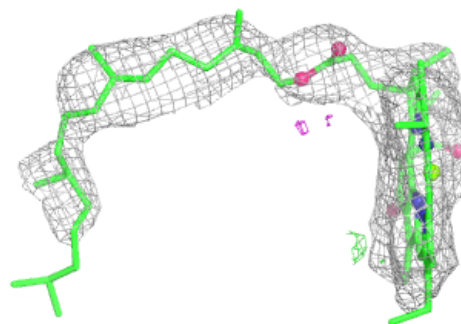


Electron density around DGD c 5509:

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

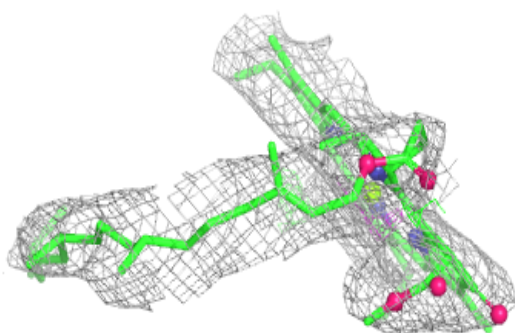
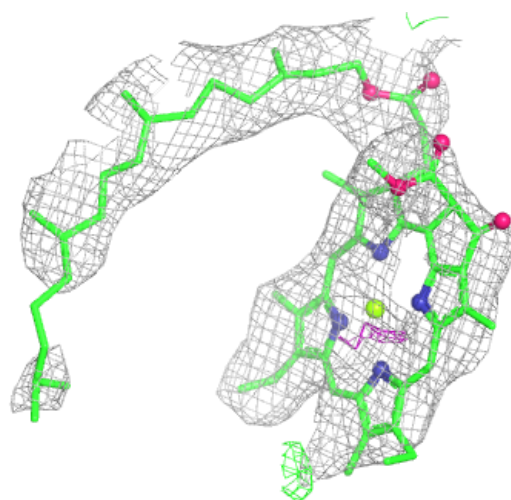
**Electron density around CLA B 516:**

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



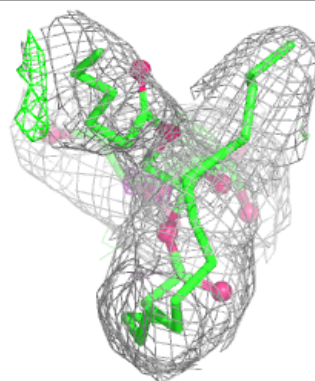
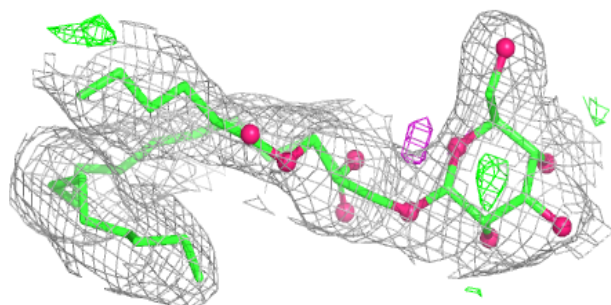
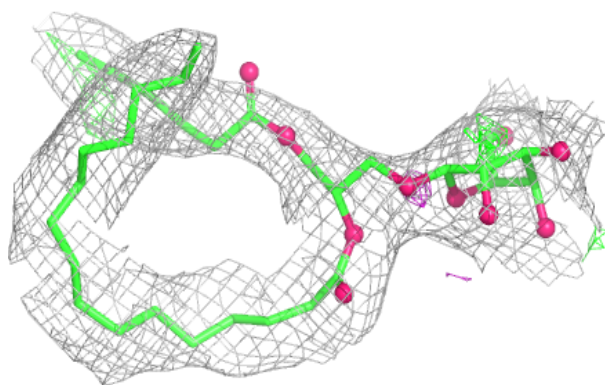
Electron density around CLA c 5497:

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

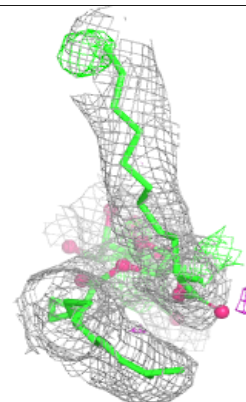
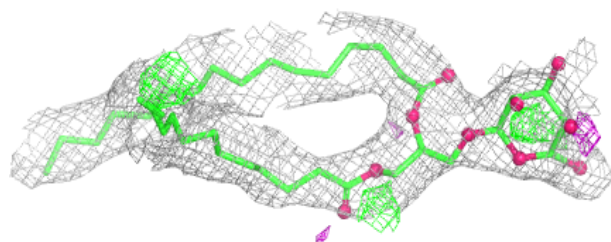
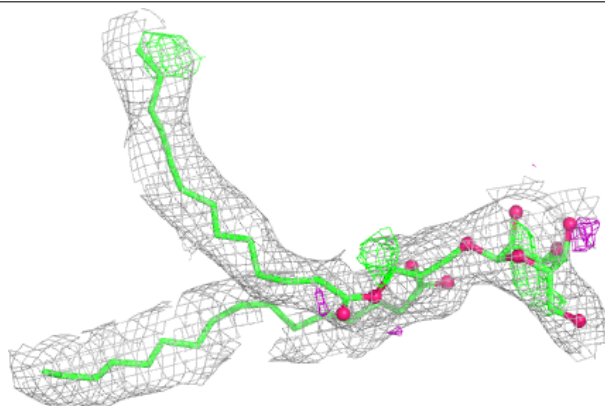


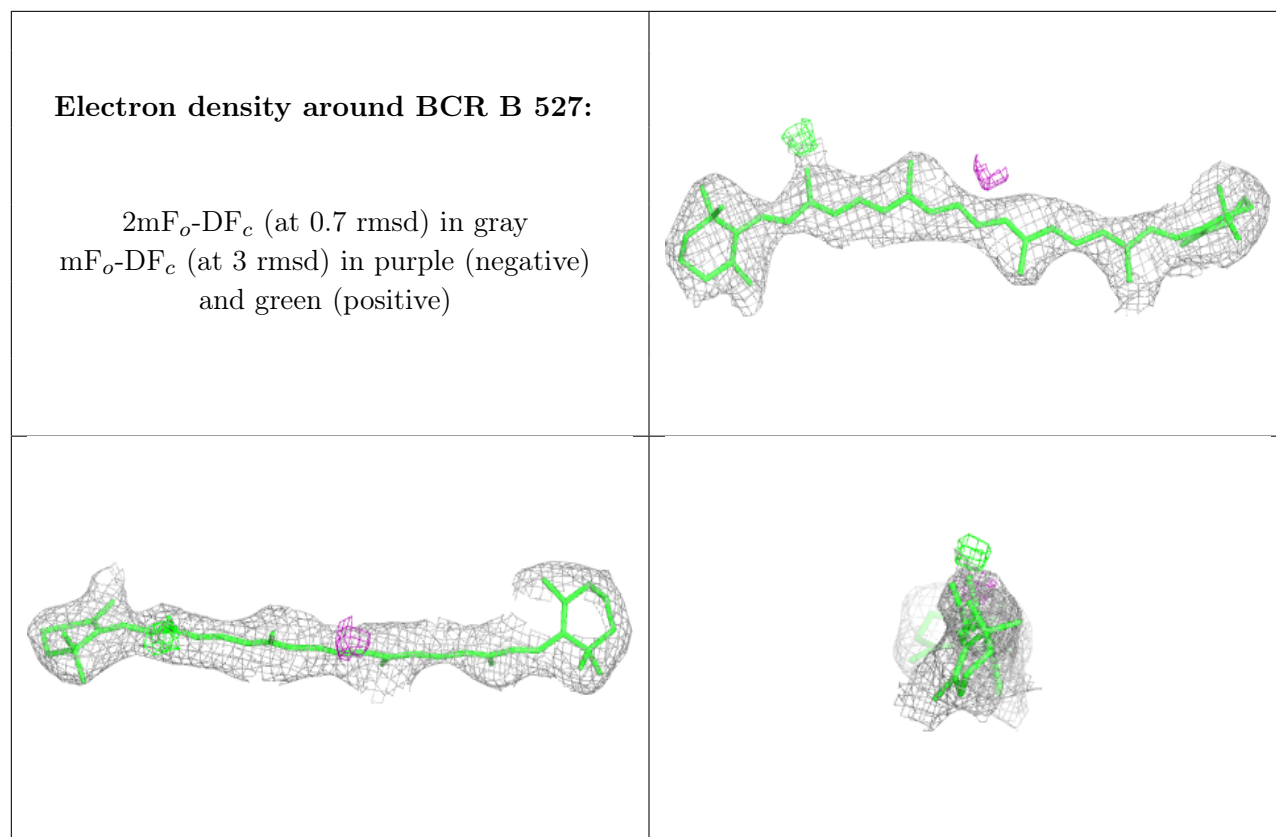
Electron density around MGE D 359:

$2mF_o-DF_c$ (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:**

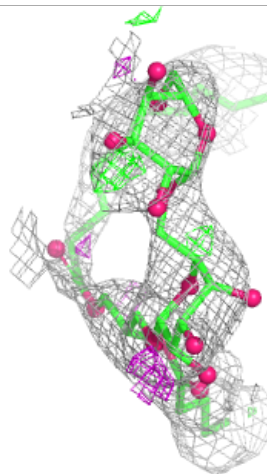
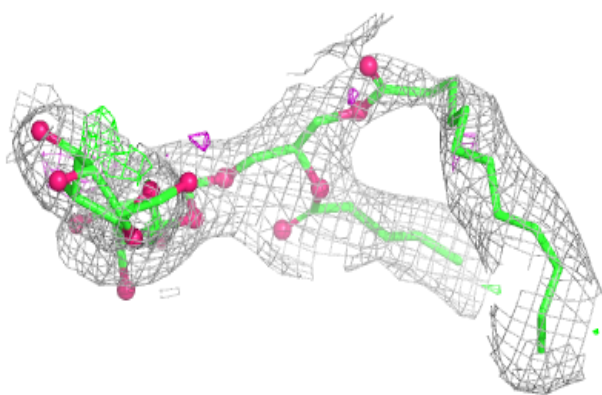
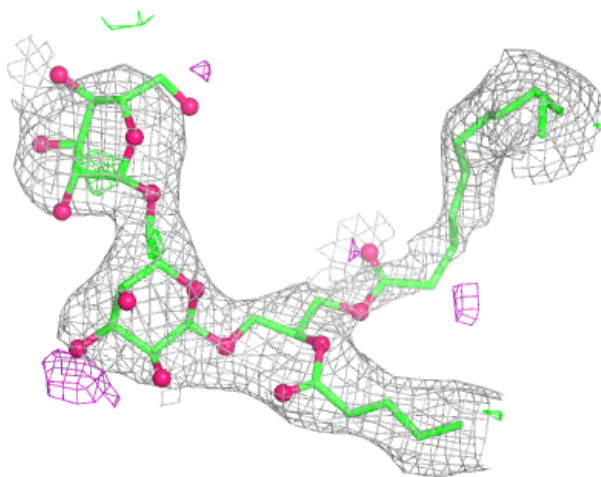
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





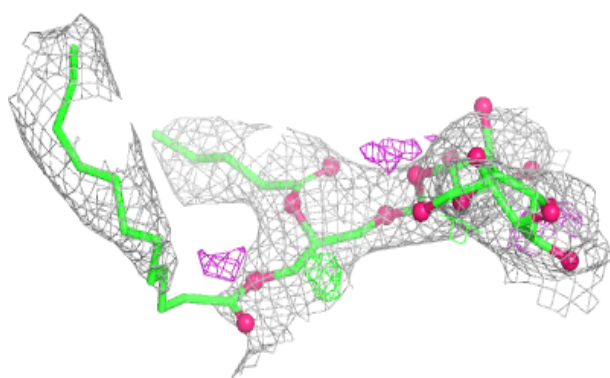
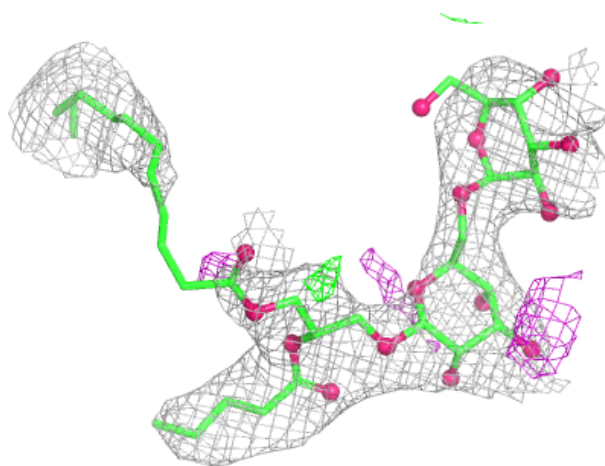
Electron density around DGD C 508:

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



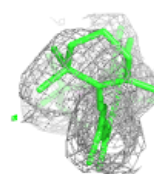
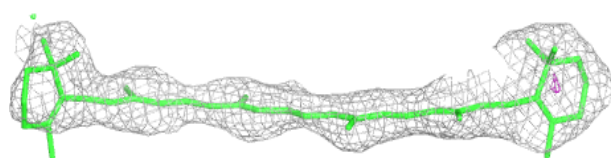
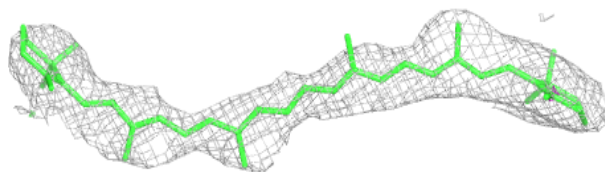
Electron density around DGD c 5508:

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

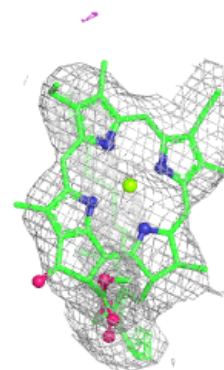
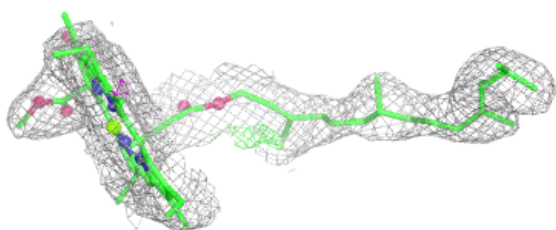
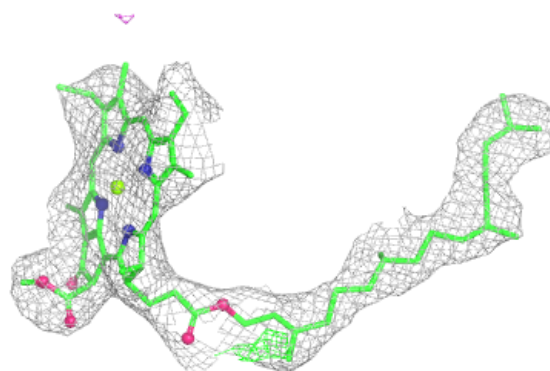


Electron density around BCR h 5107:

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

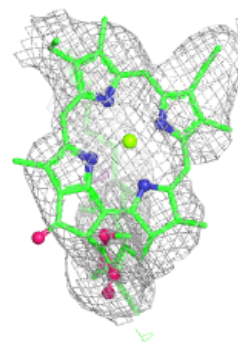
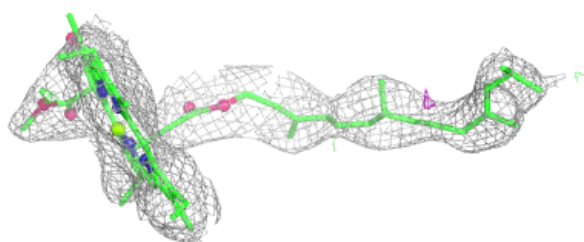
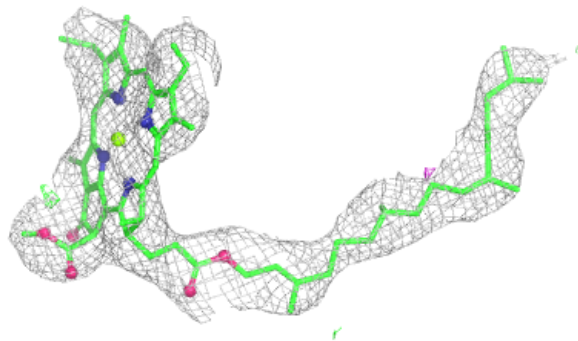
**Electron density around CLA b 5519:**

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



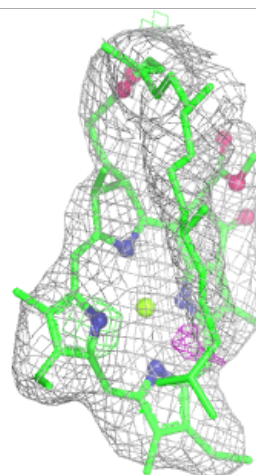
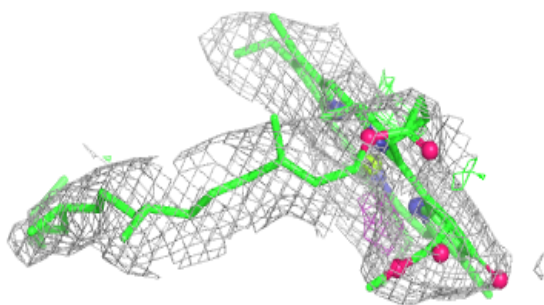
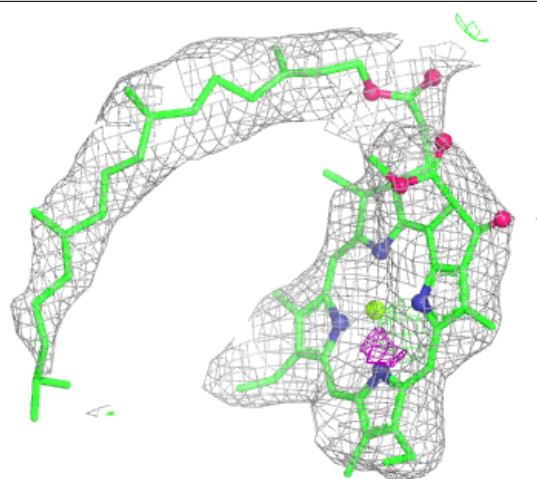
Electron density around CLA B 519:

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



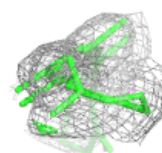
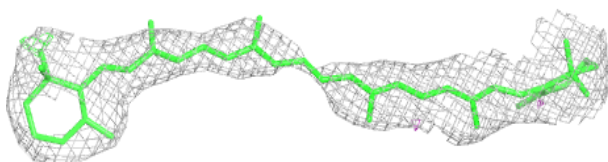
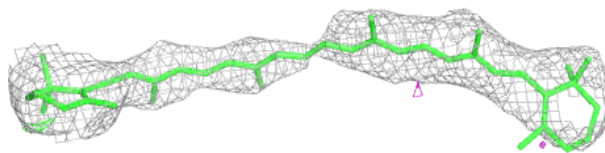
Electron density around CLA C 497:

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

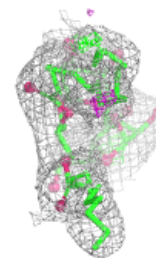
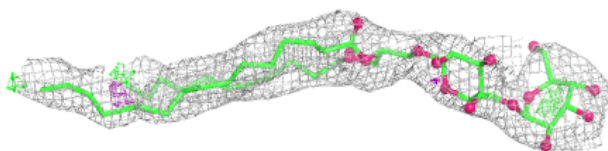


Electron density around BCR d 5357:

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

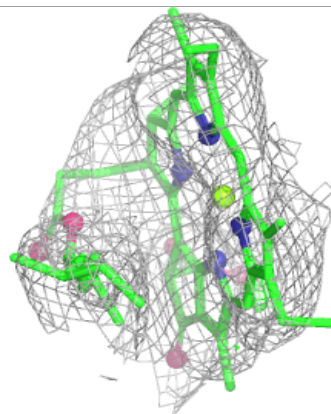
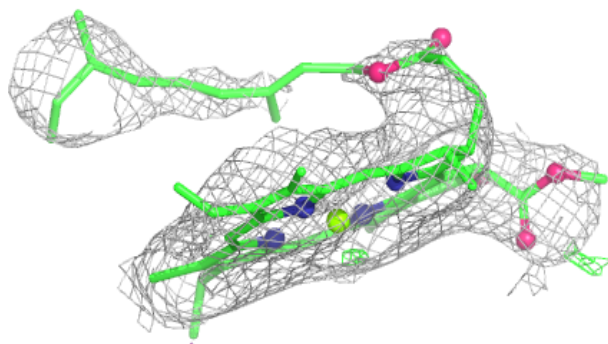
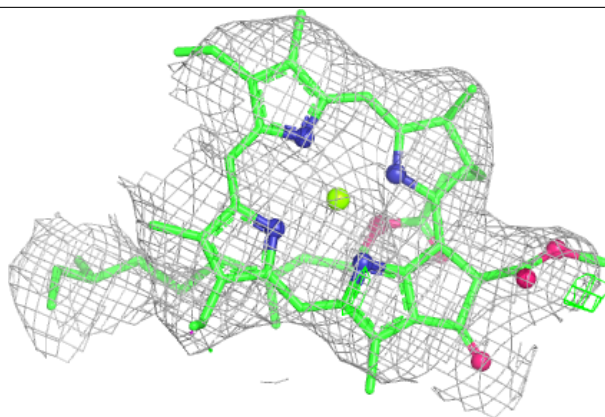
**Electron density around DGD C 509:**

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

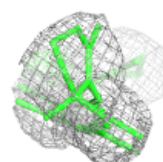
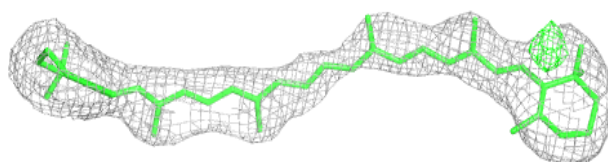


Electron density around CLA b 5524:

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

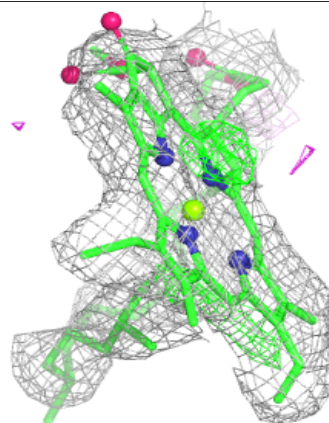
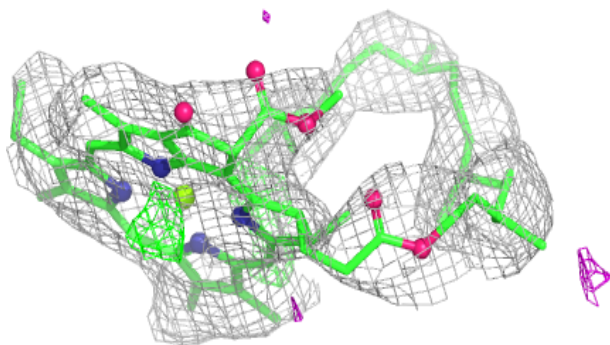
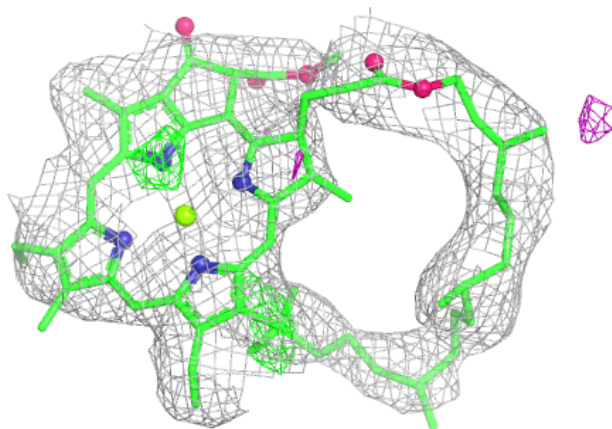
**Electron density around BCR D 357:**

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



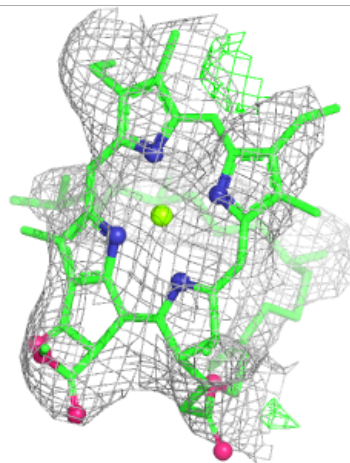
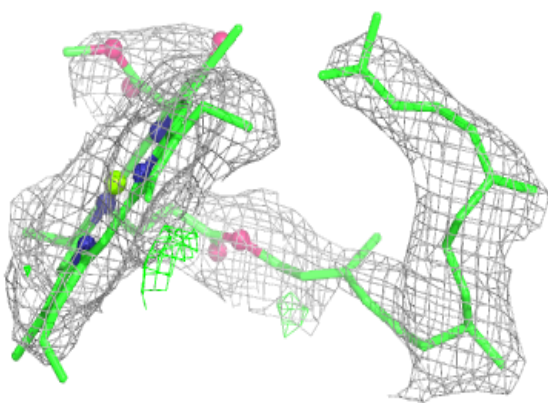
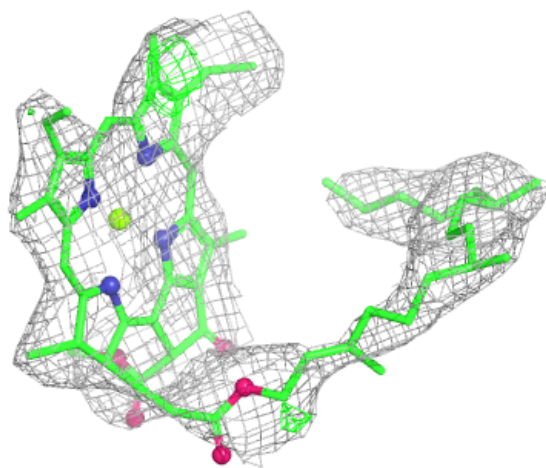
Electron density around CLA B 525:

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



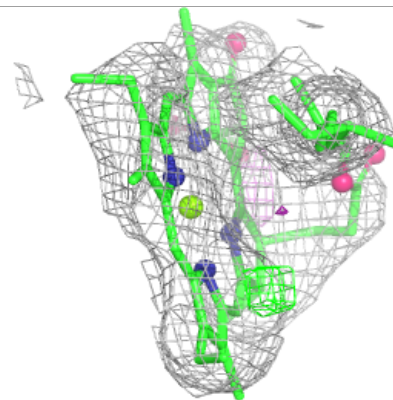
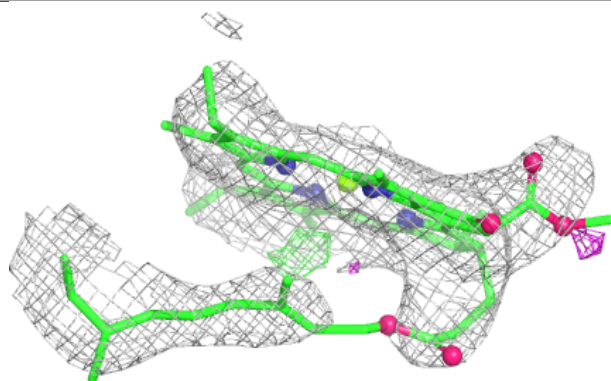
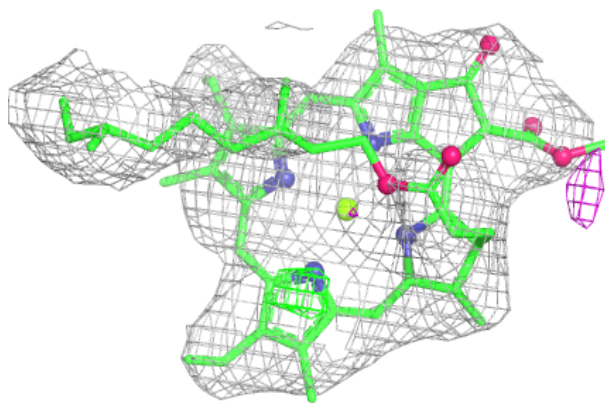
Electron density around CLA c 5493:

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

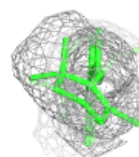
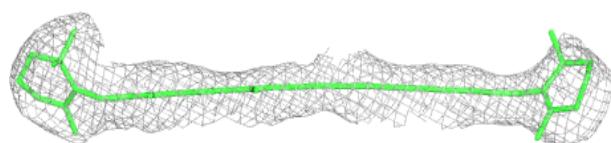
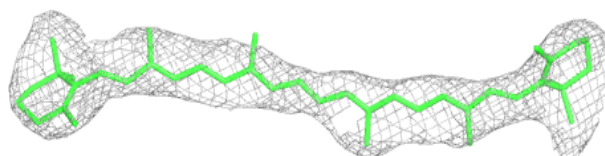


Electron density around CLA B 524:

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

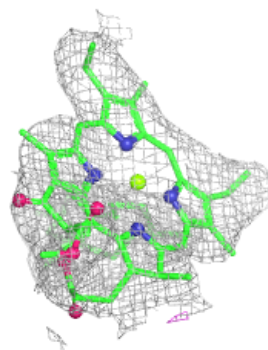
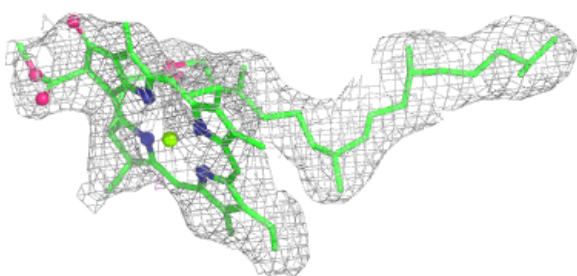
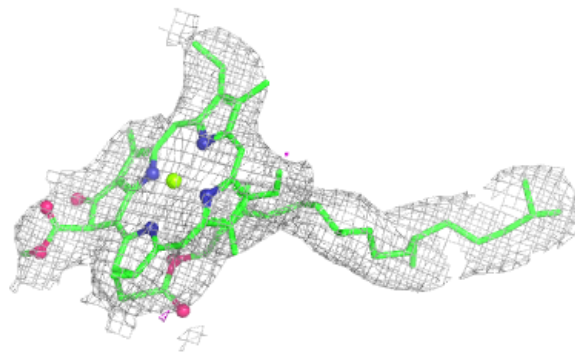
**Electron density around BCR B 528:**

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



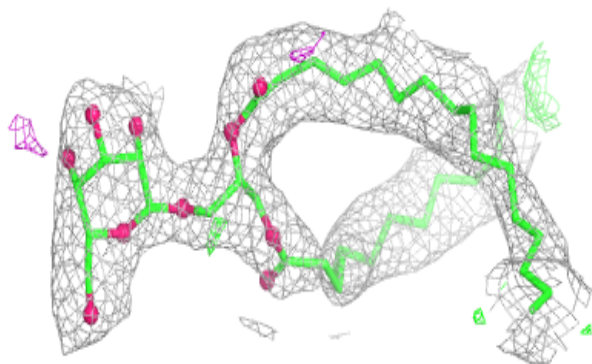
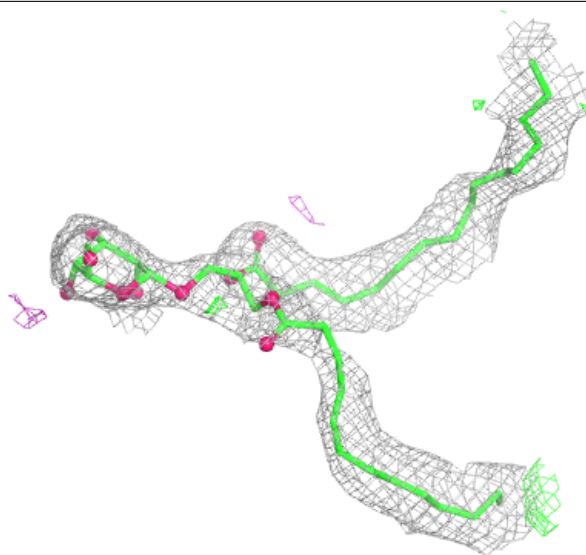
Electron density around CLA C 495:

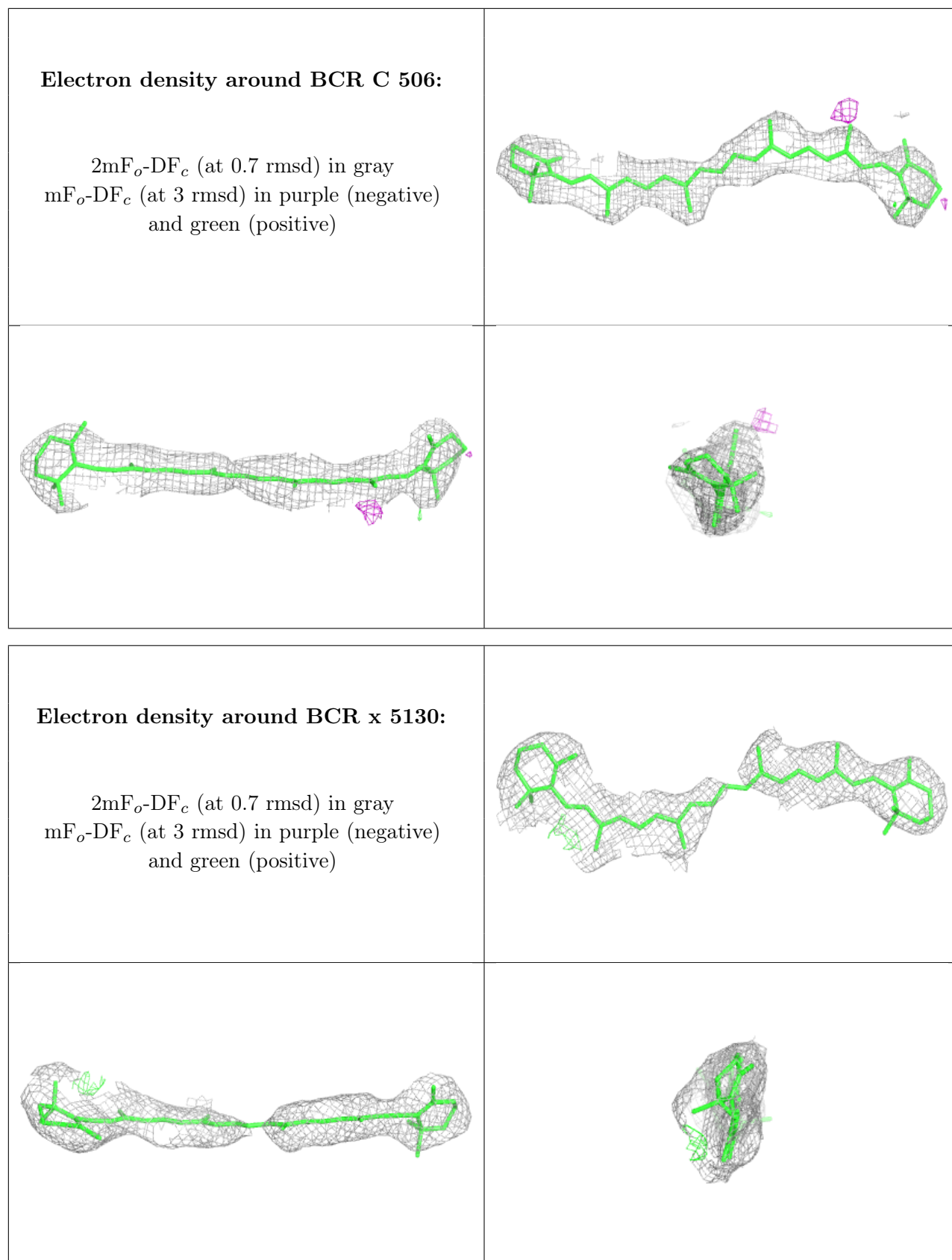
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGE B 530:

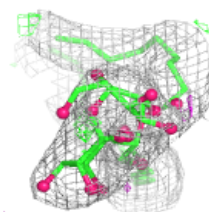
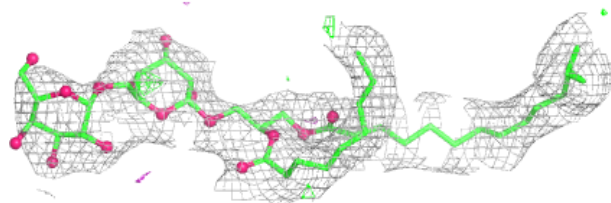
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



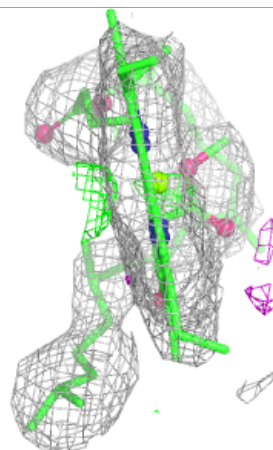
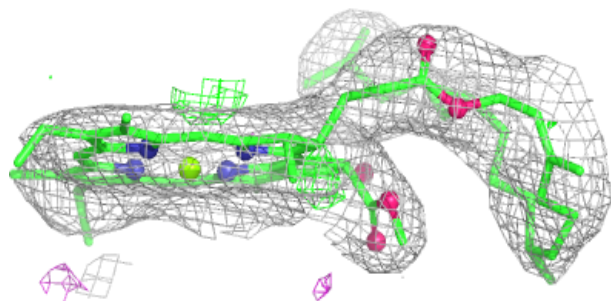
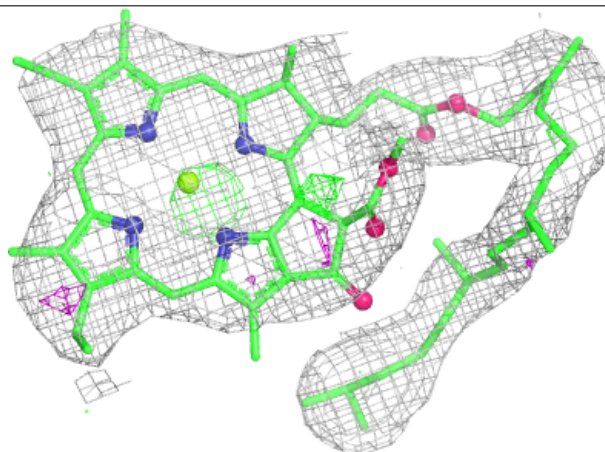


Electron density around DGD h 5208:

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

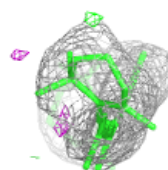
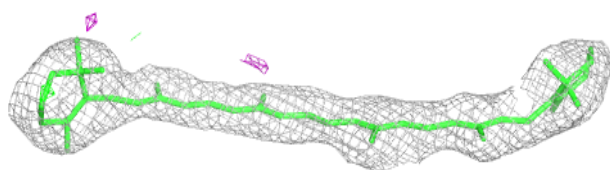
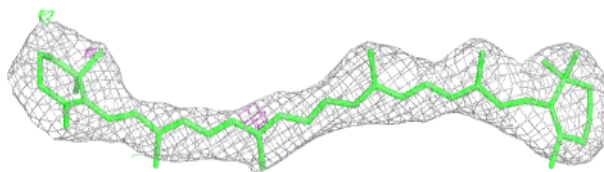
**Electron density around CLA b 5520:**

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

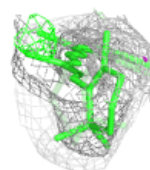
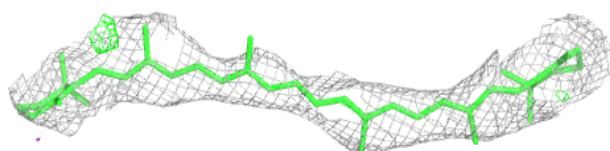


Electron density around BCR b 5529:

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

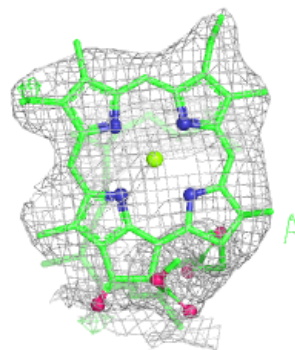
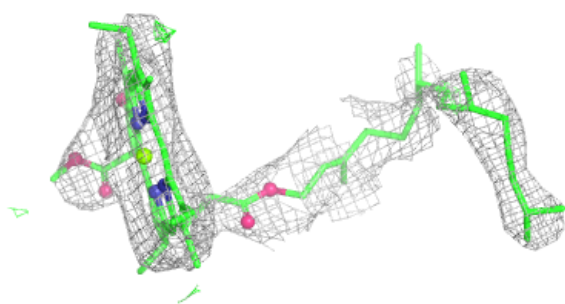
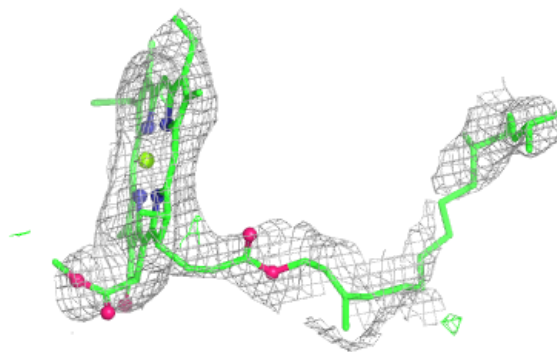
**Electron density around BCR c 5504:**

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



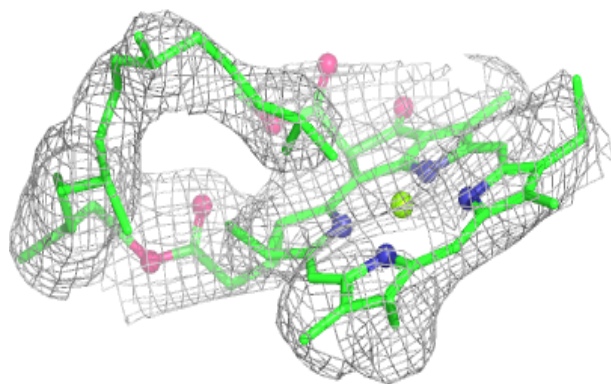
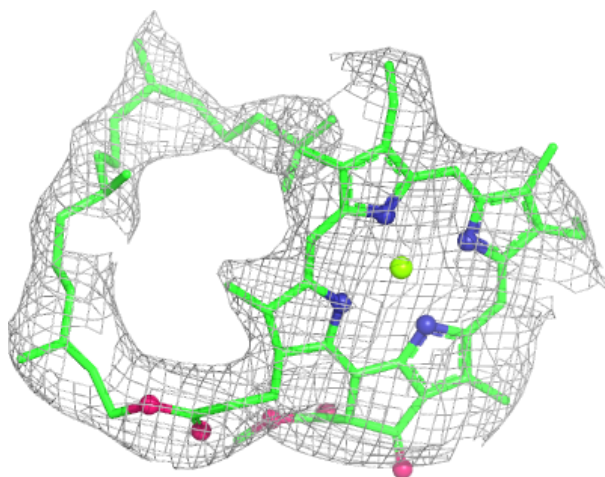
Electron density around CLA c 5496:

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



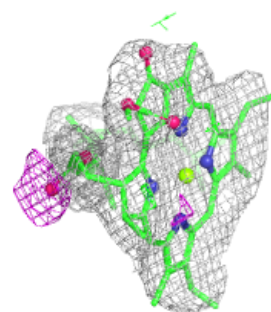
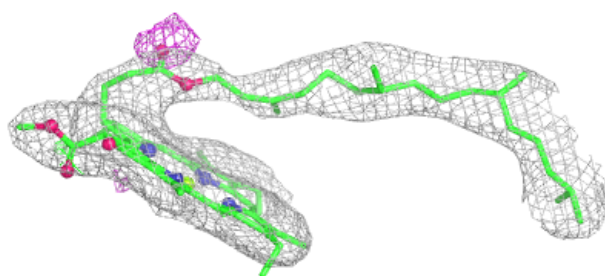
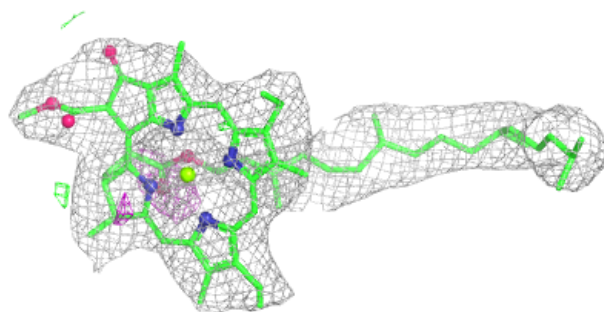
Electron density around CLA b 5525:

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

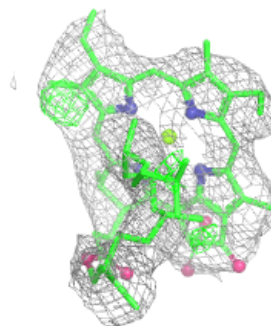
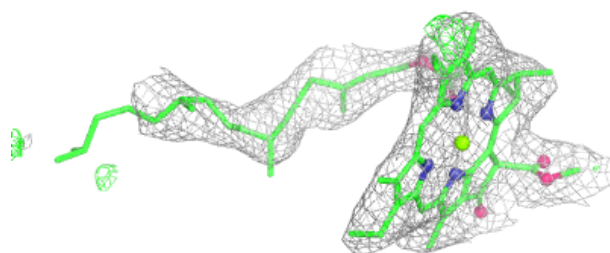
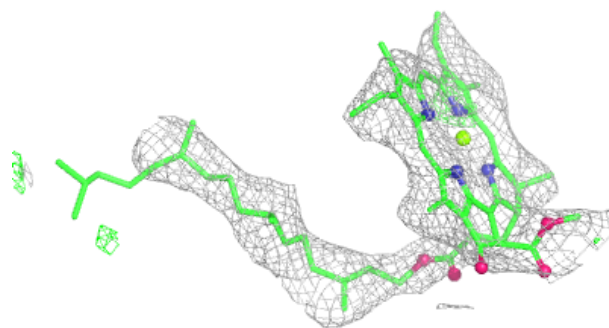


Electron density around CLA b 5518:

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

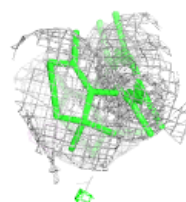
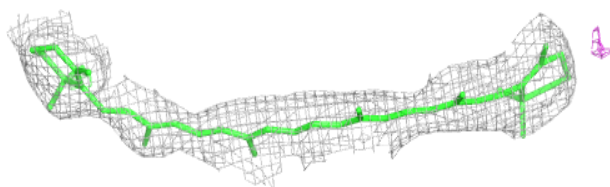
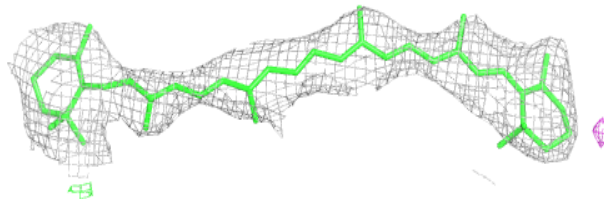
**Electron density around CLA C 498:**

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

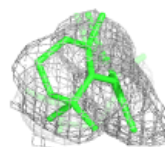
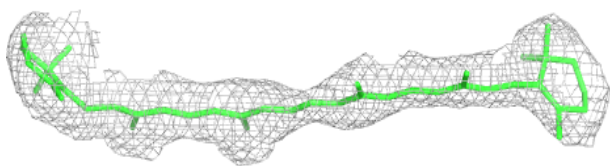
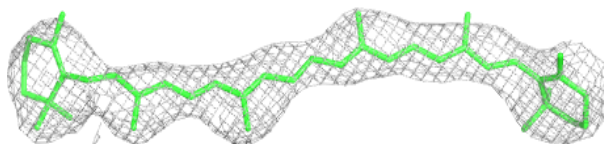


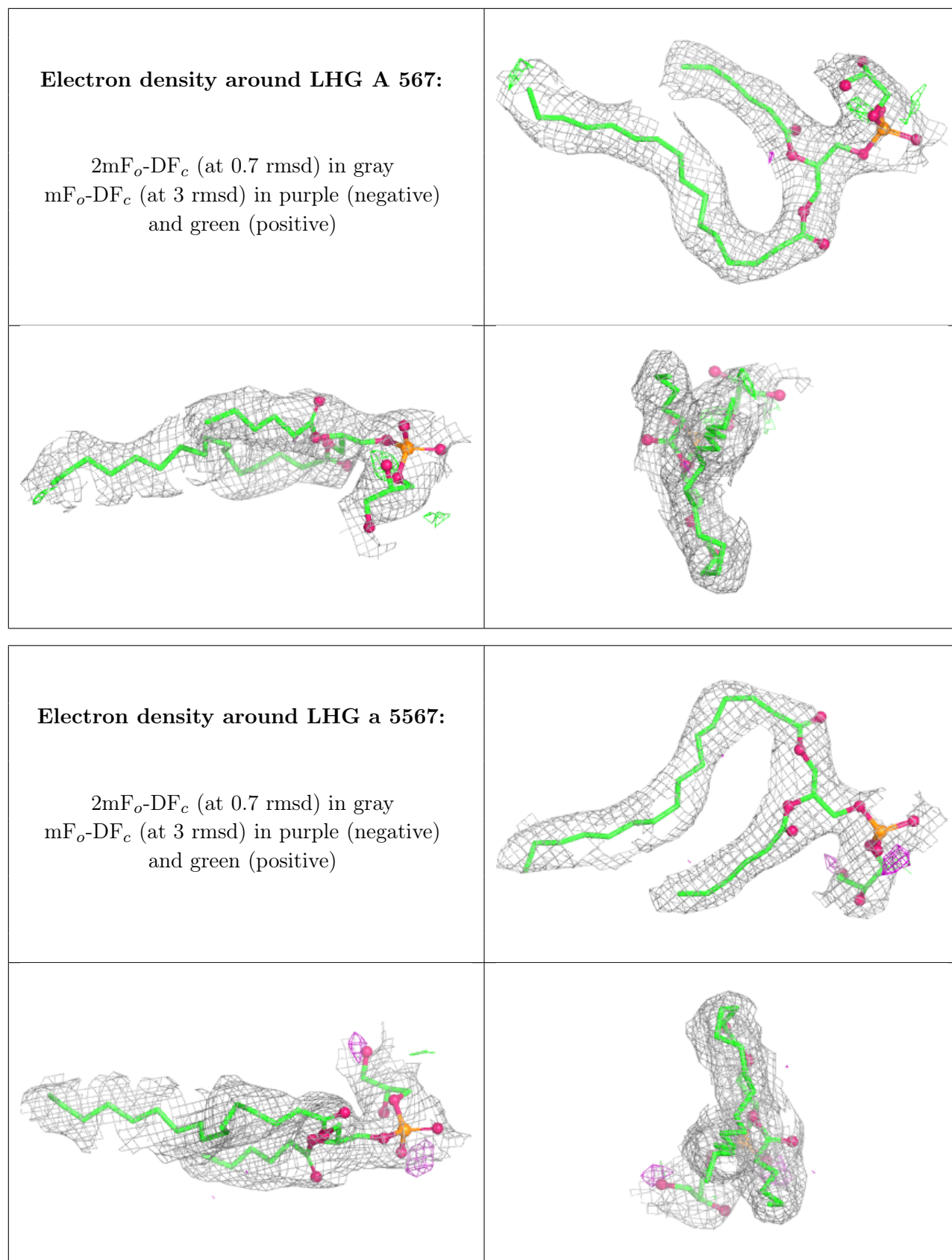
Electron density around BCR t 104:

$2mF_o-DF_c$ (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:**

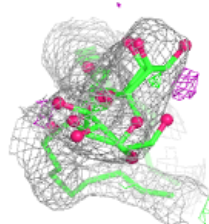
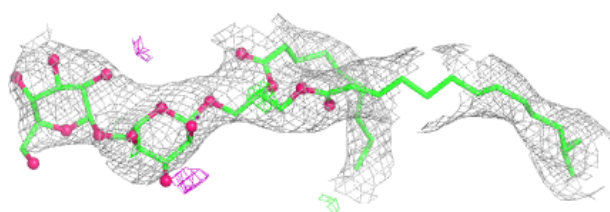
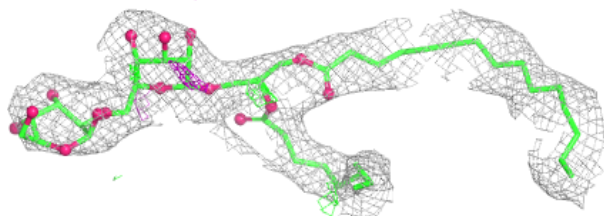
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



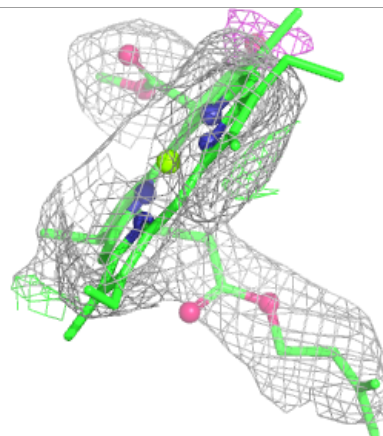
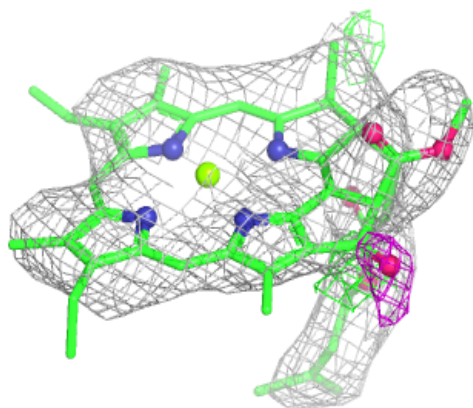
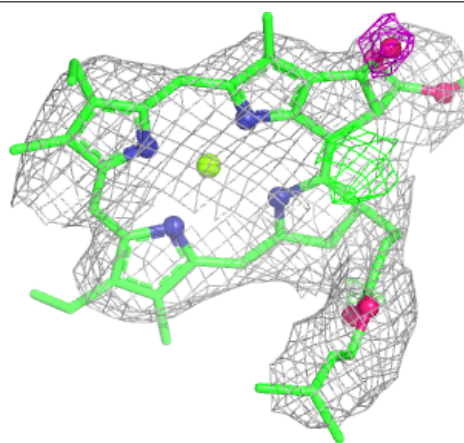


Electron density around DGD H 208:

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

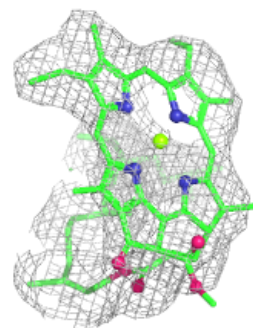
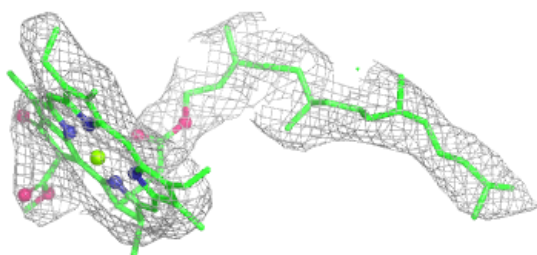
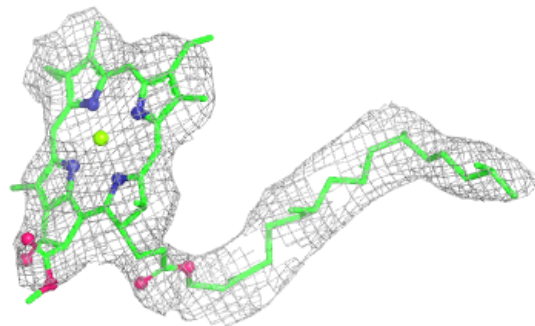
**Electron density around CLA C 503:**

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



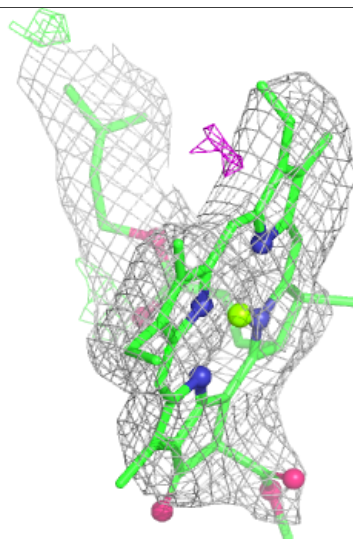
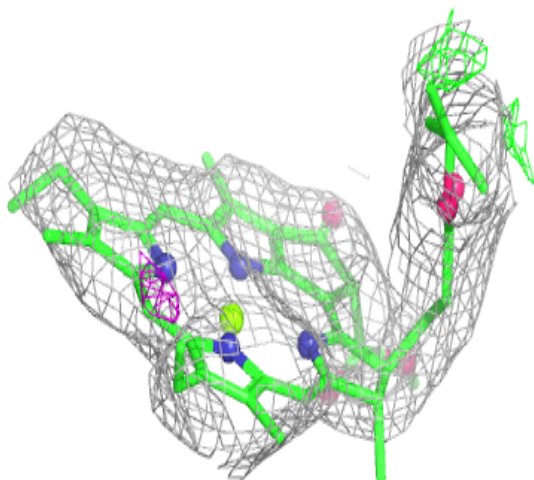
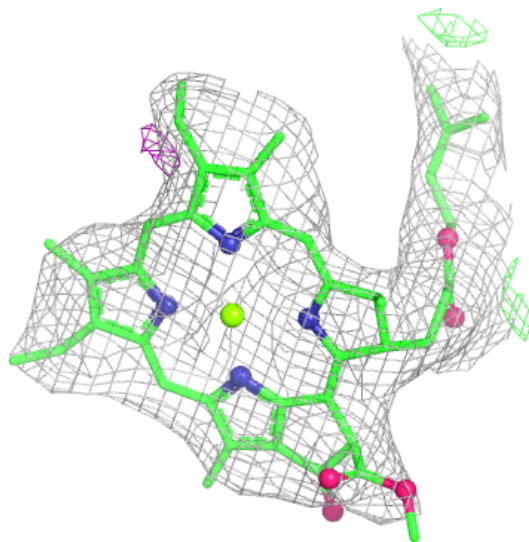
Electron density around CLA C 501:

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



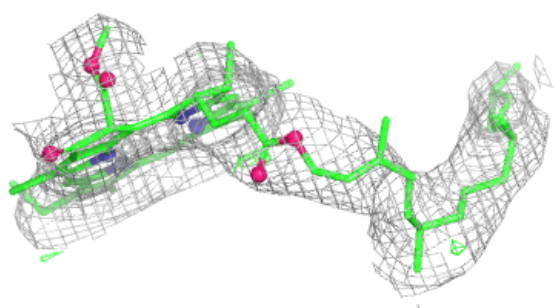
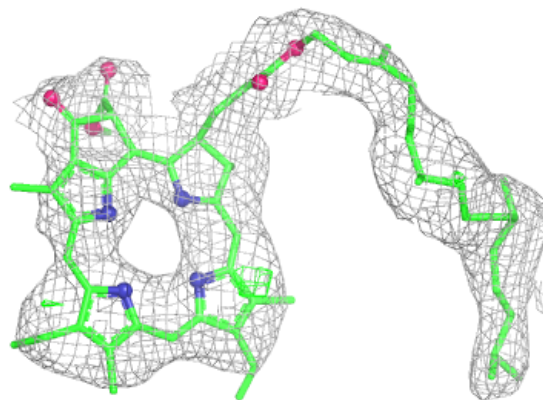
Electron density around CLA d 5355:

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

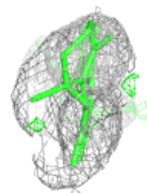
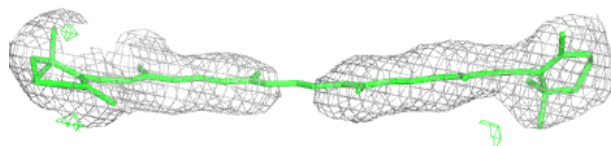
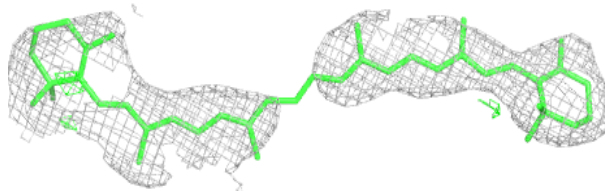


Electron density around PHO a 5562:

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

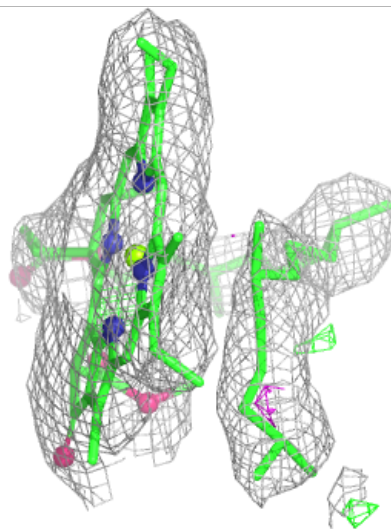
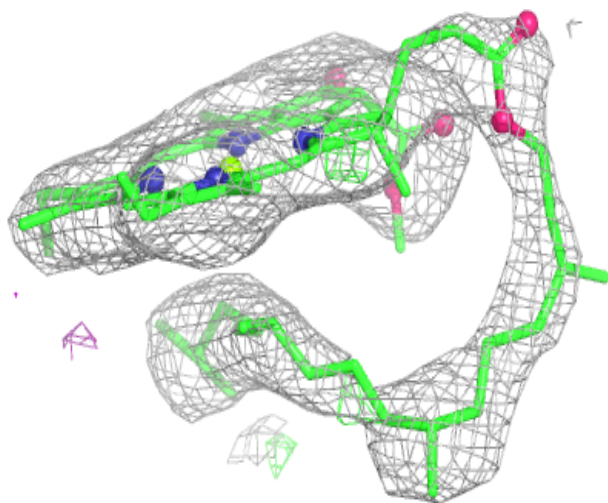
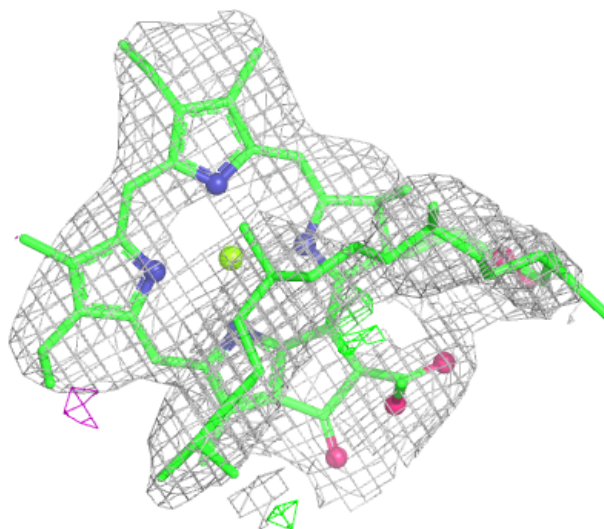
**Electron density around BCR X 130:**

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



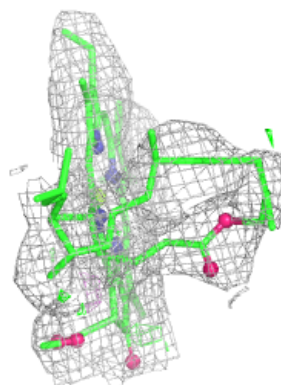
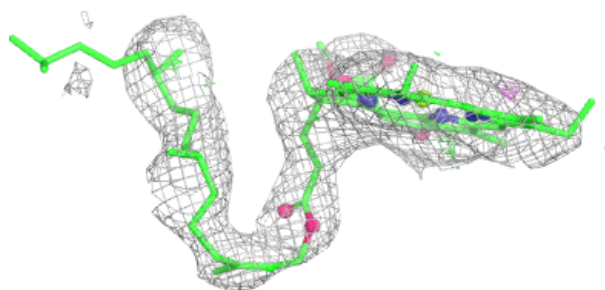
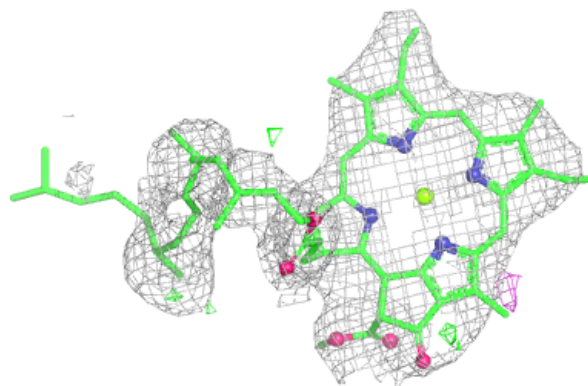
Electron density around CLA c 5500:

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

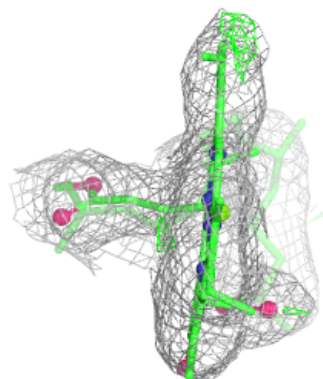
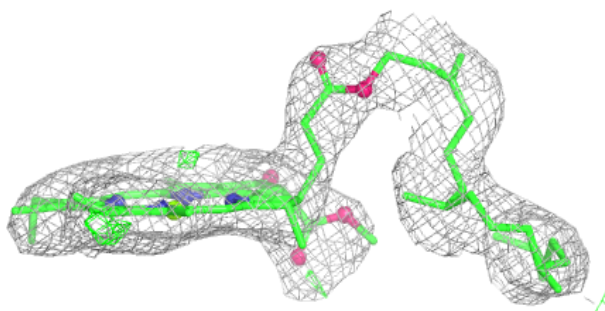
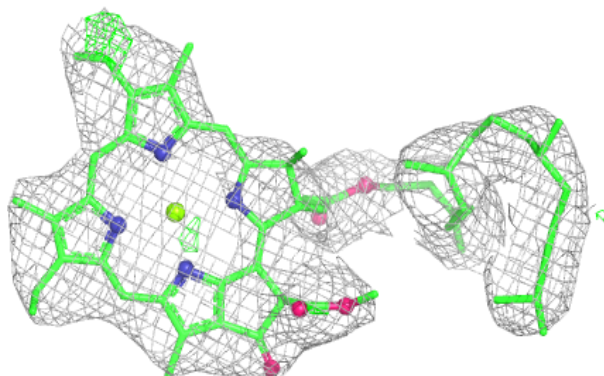


Electron density around CLA a 5560:

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

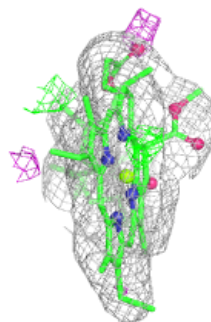
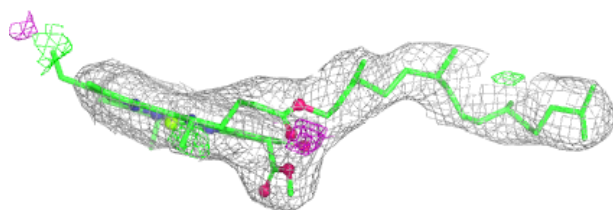
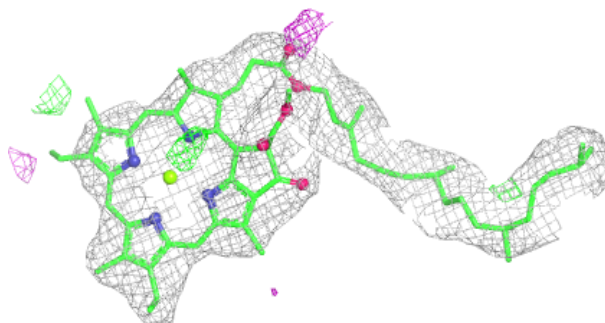
**Electron density around CLA B 522:**

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

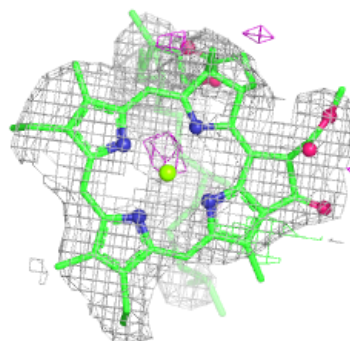
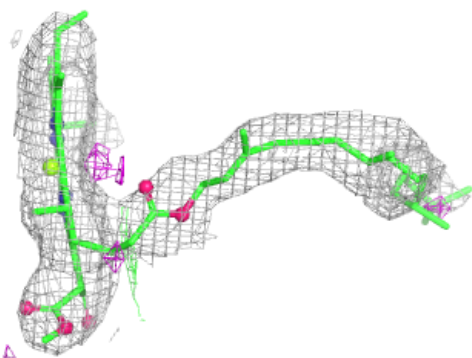
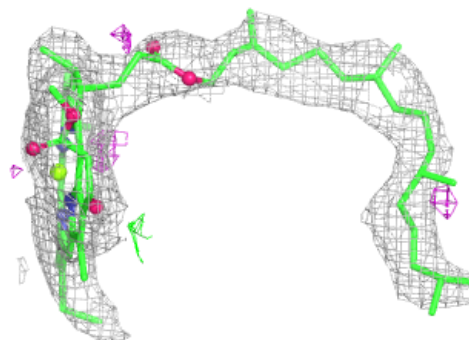


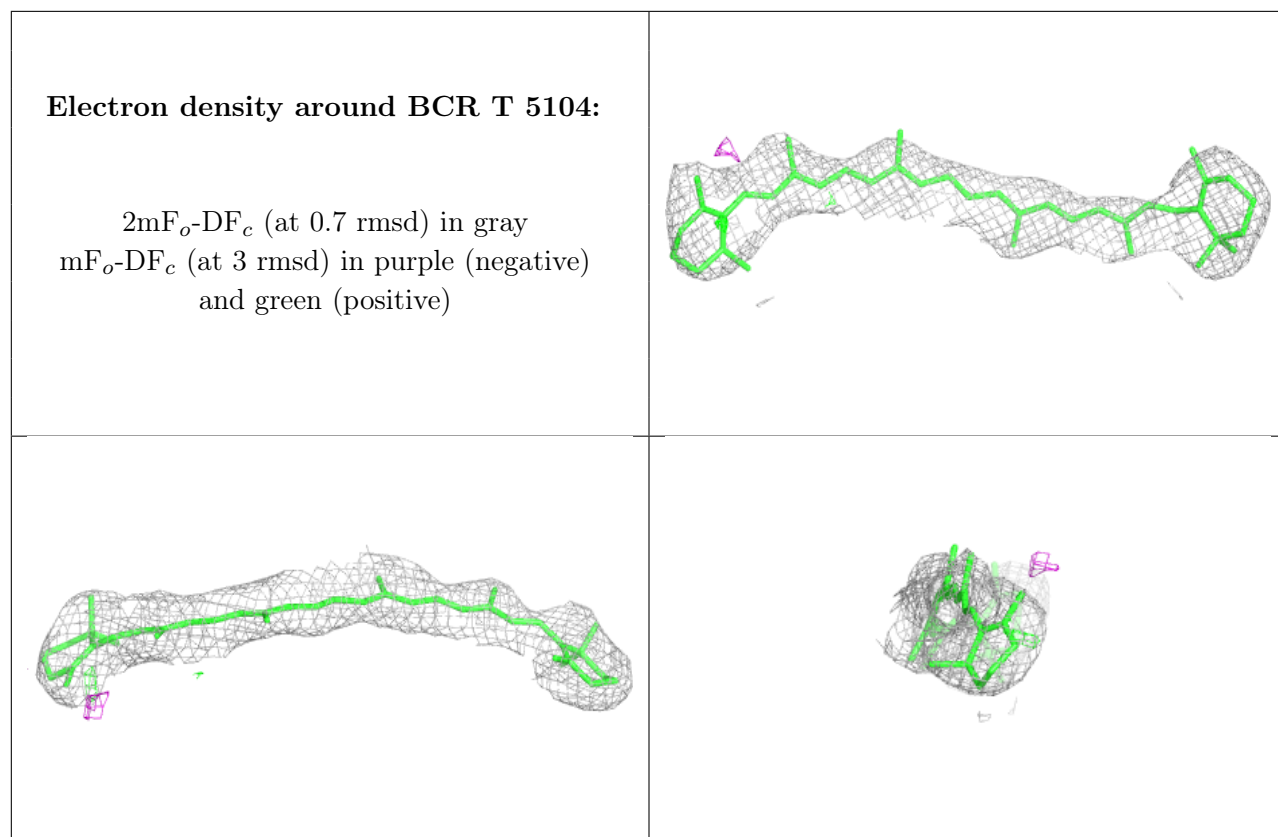
Electron density around CLA b 5512:

$2mF_o-DF_c$ (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:**

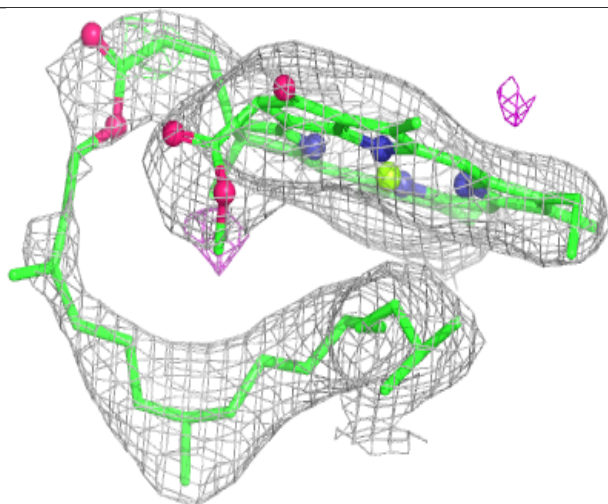
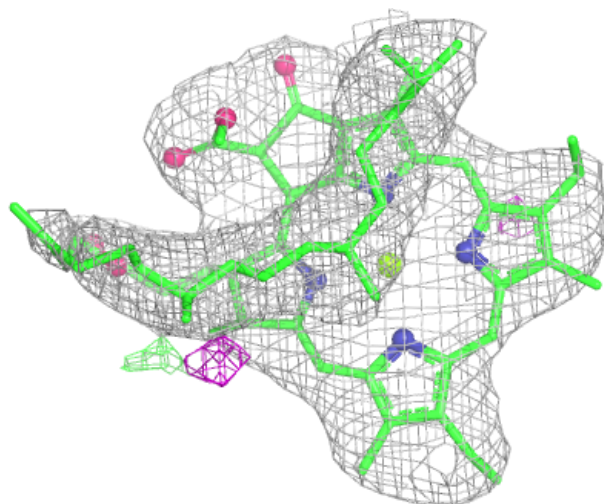
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





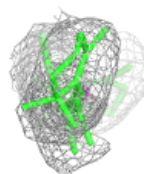
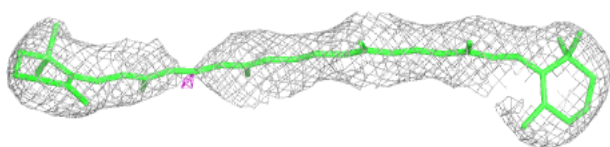
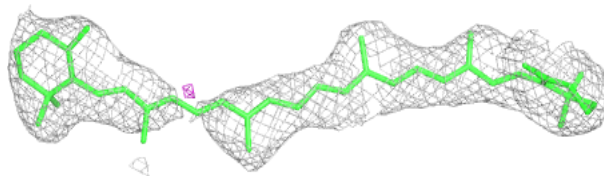
Electron density around CLA C 500:

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

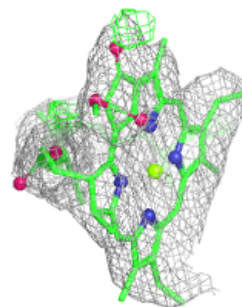
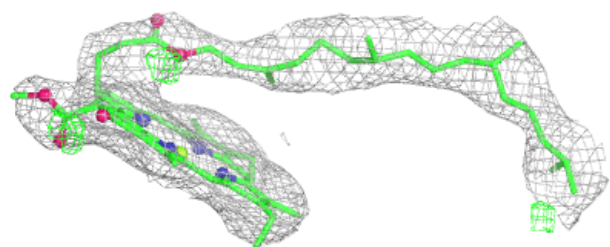
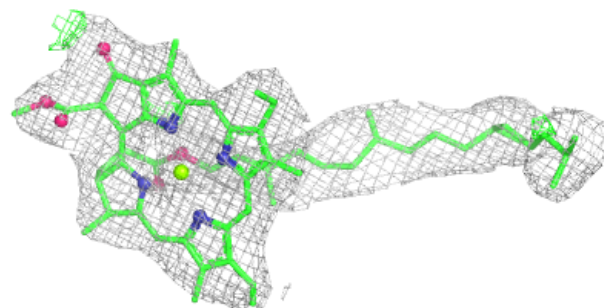


Electron density around BCR b 5527:

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

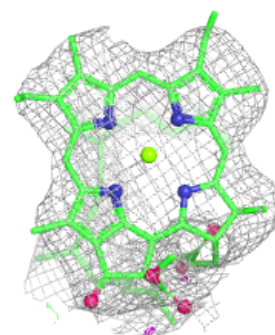
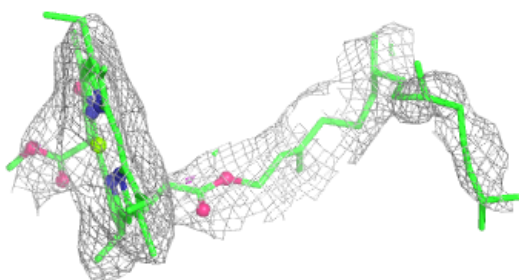
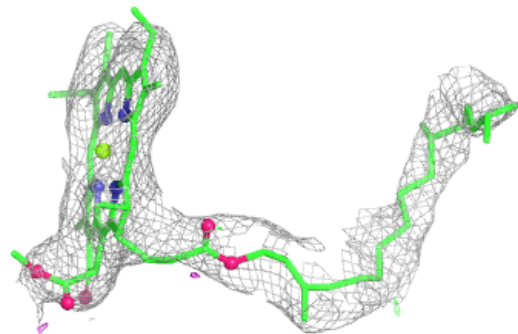
**Electron density around CLA B 518:**

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



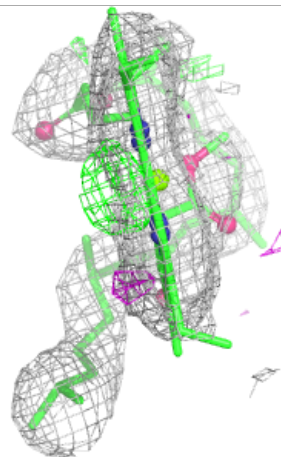
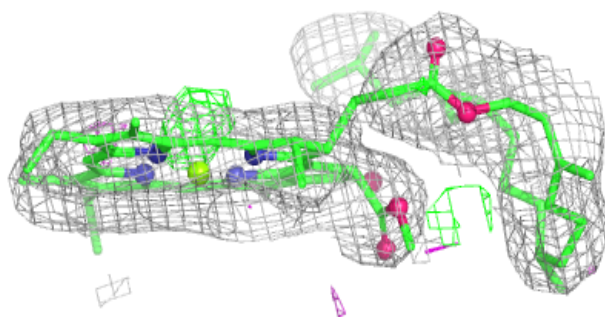
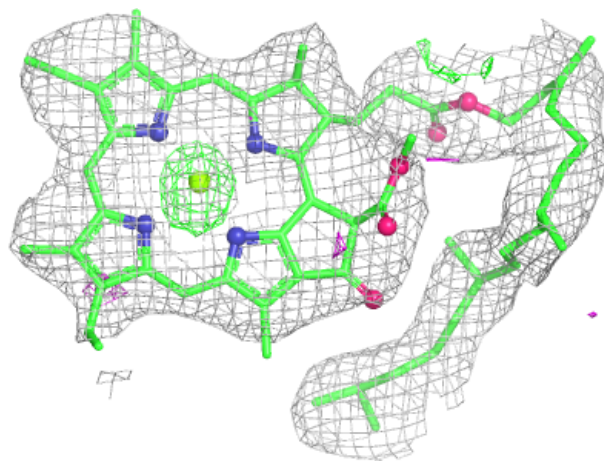
Electron density around CLA C 496:

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



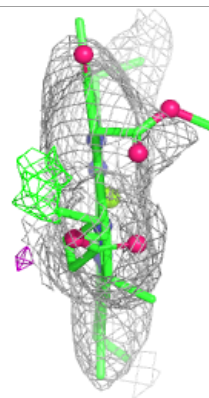
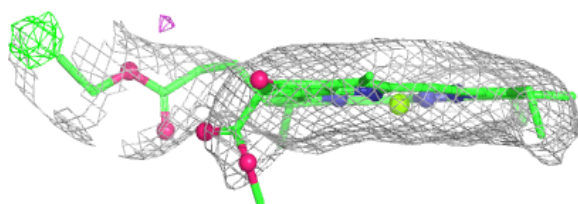
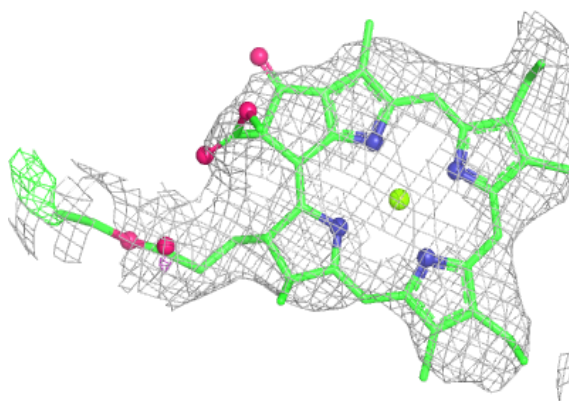
Electron density around CLA B 520:

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

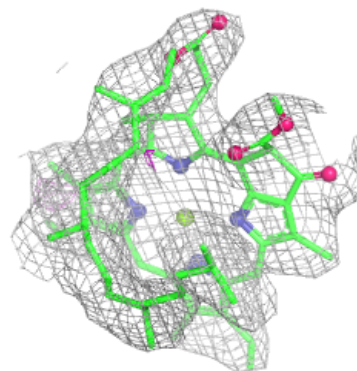
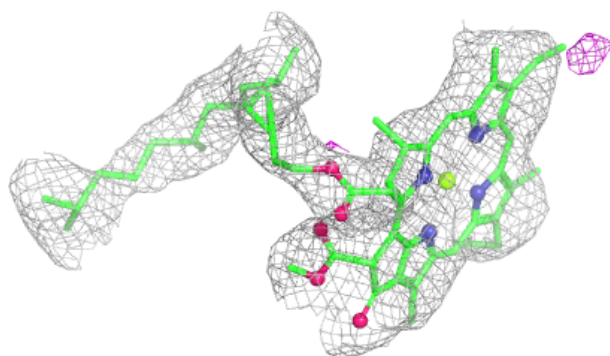
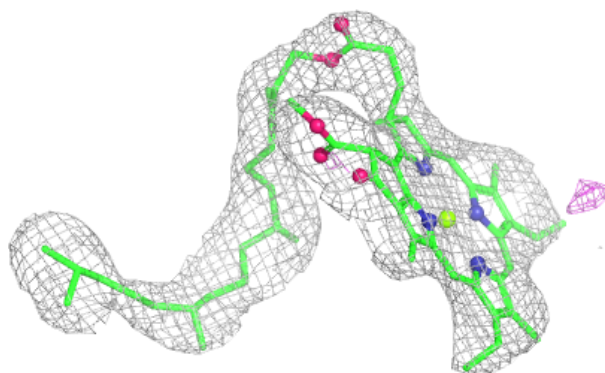


Electron density around CLA c 5499:

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

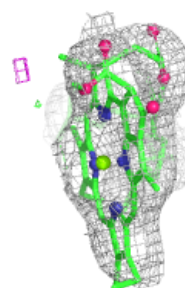
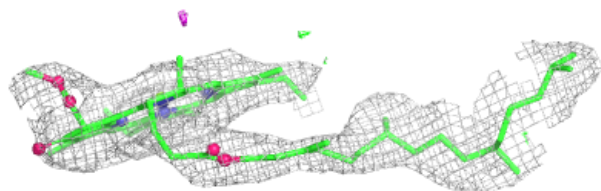
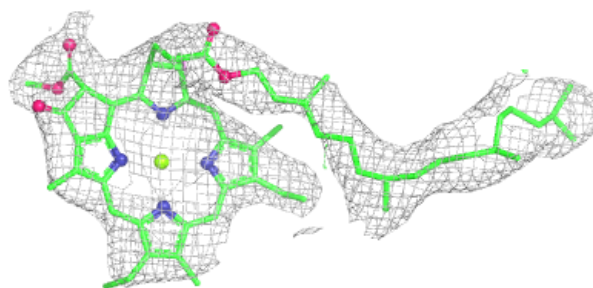
**Electron density around CLA b 5523:**

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

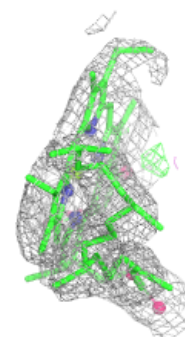
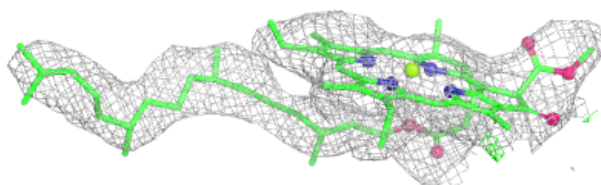
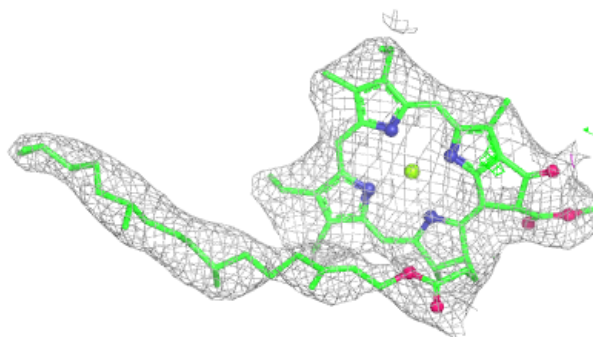


Electron density around CLA B 513:

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

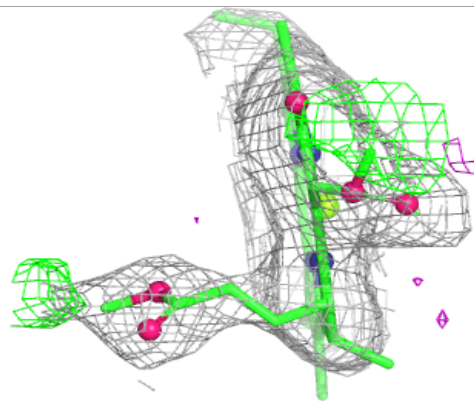
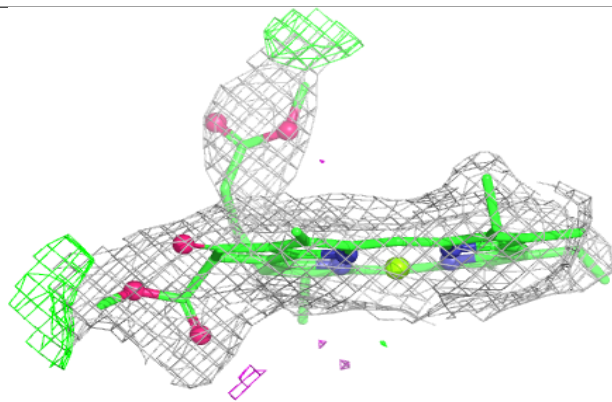
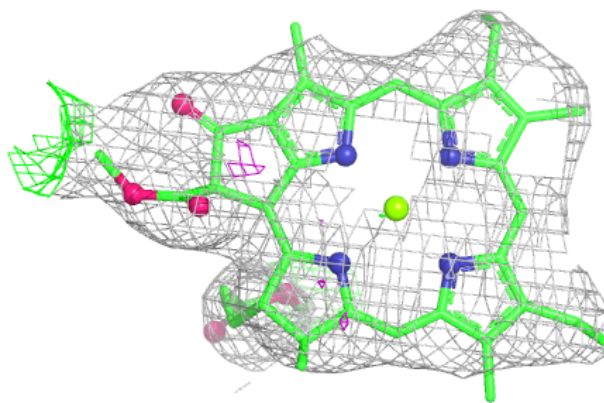
**Electron density around CLA C 491:**

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

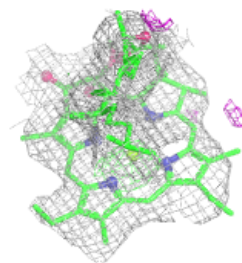
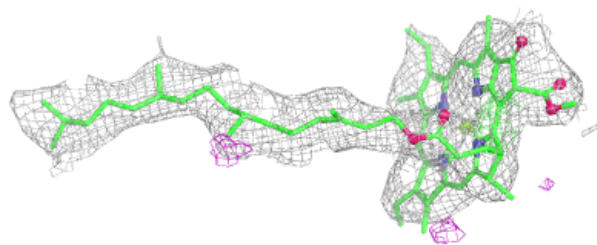
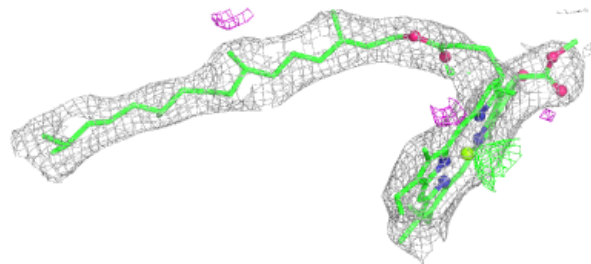


Electron density around CLA C 494:

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

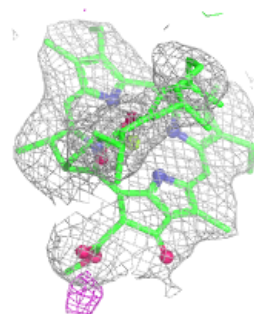
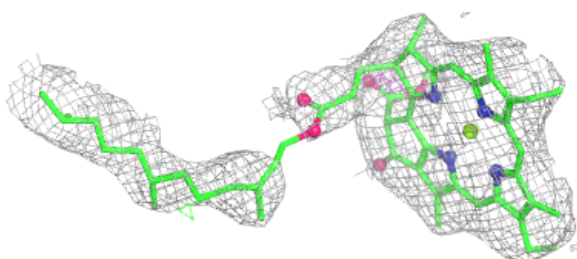
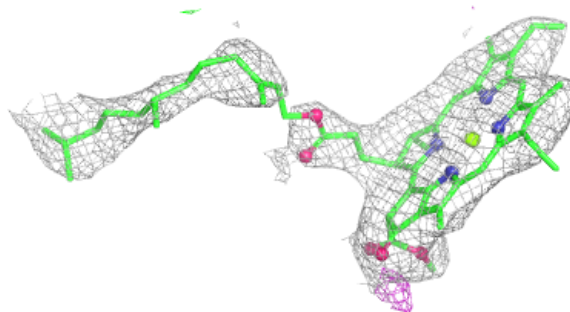
**Electron density around CLA b 5517:**

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

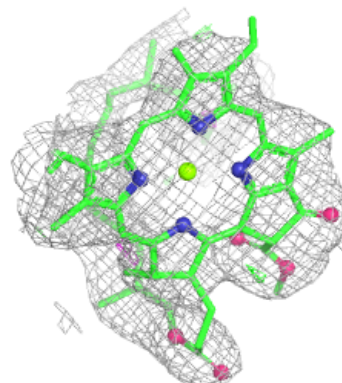
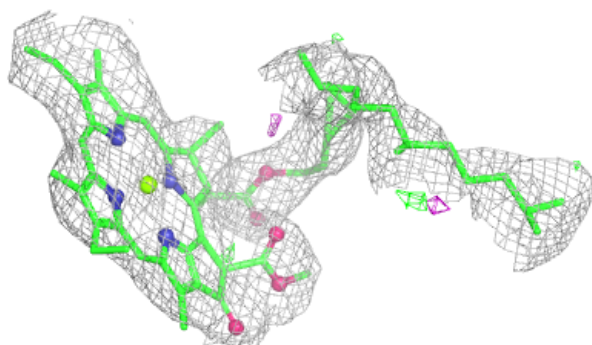
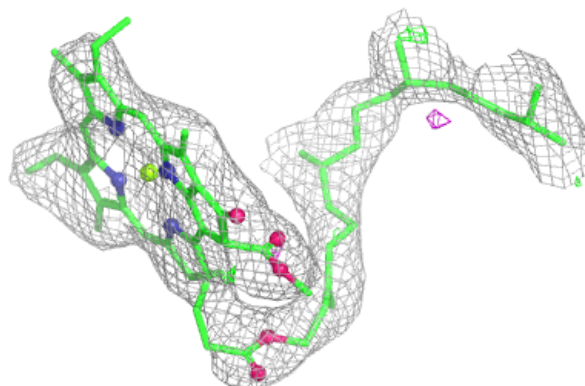


Electron density around CLA c 5492:

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

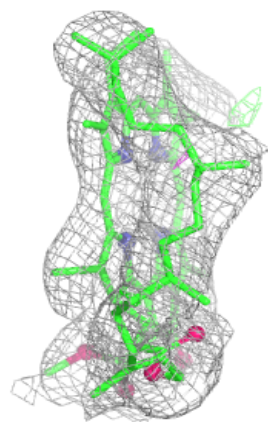
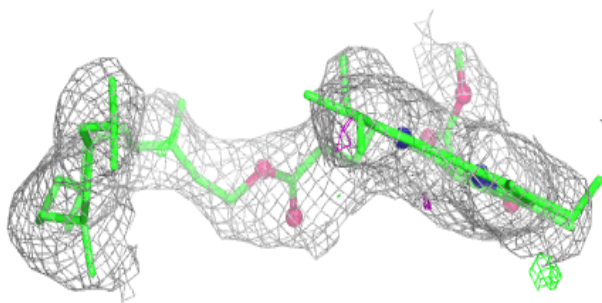
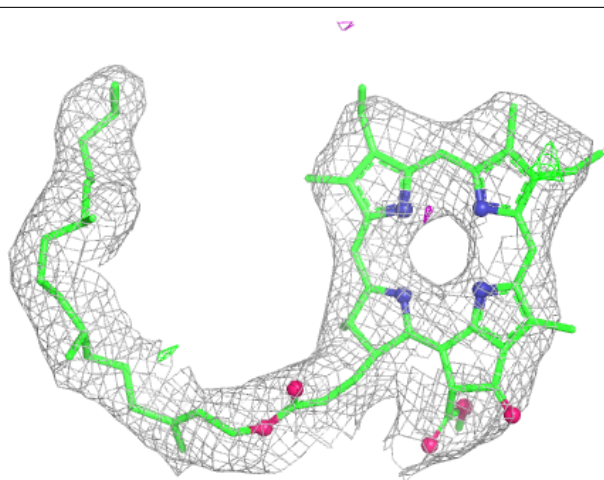
**Electron density around CLA B 523:**

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



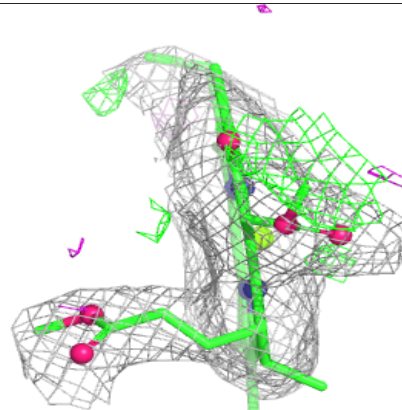
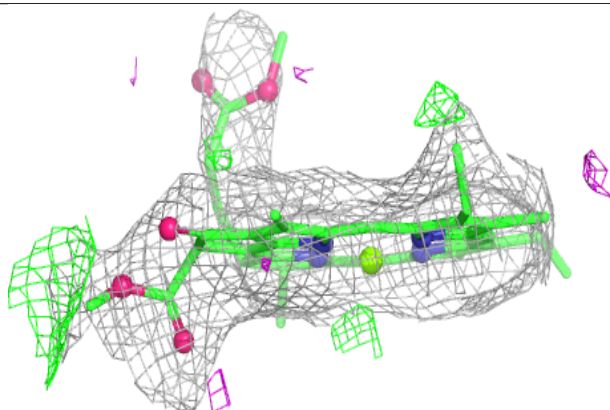
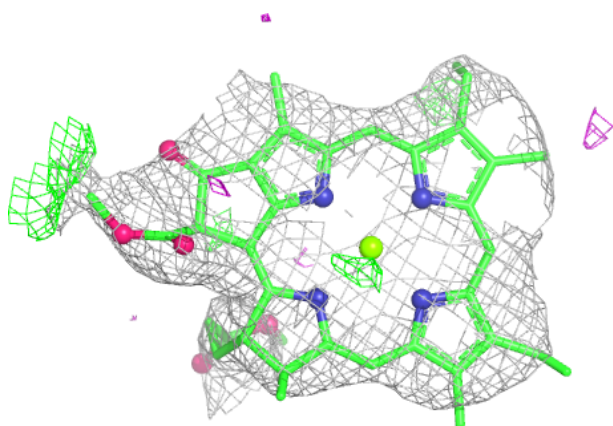
Electron density around PHO a 5561:

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

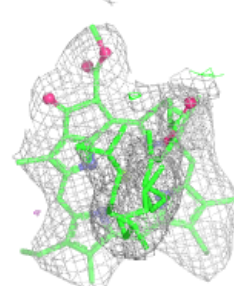
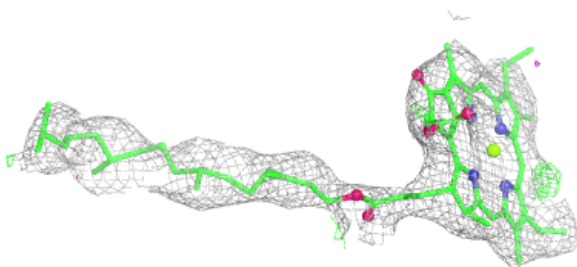
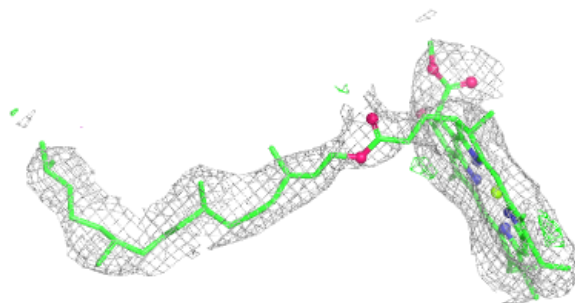


Electron density around CLA c 5494:

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

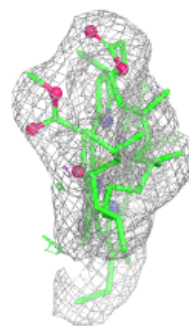
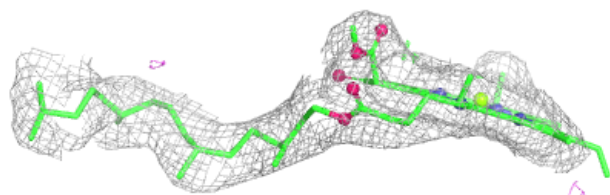
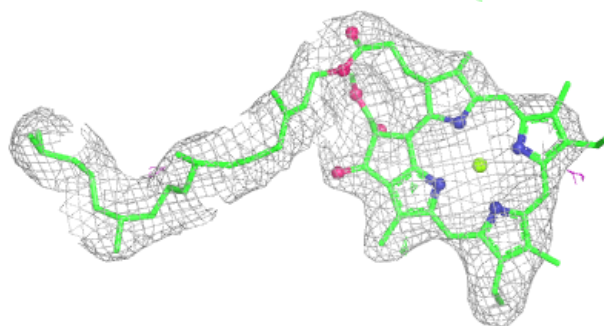
**Electron density around CLA B 514:**

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

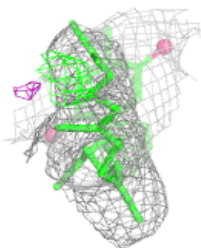
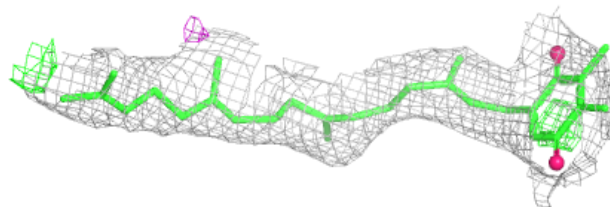
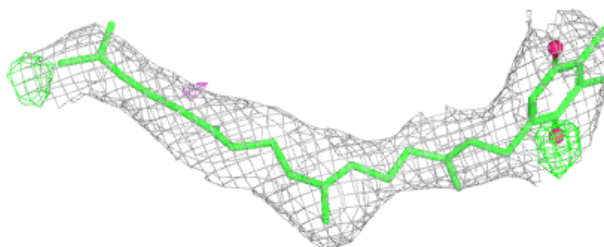


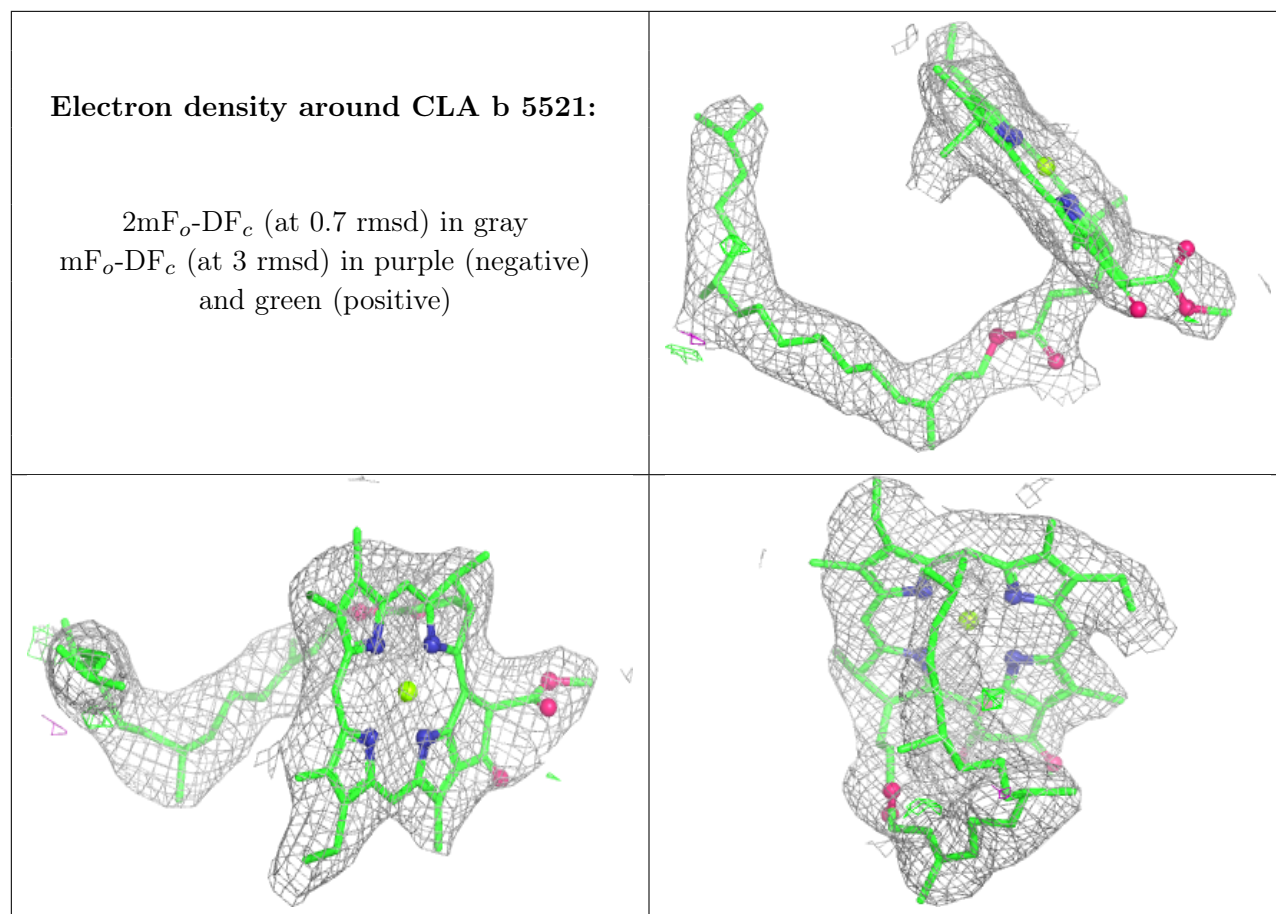
Electron density around CLA B 512:

$2mF_o-DF_c$ (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:**

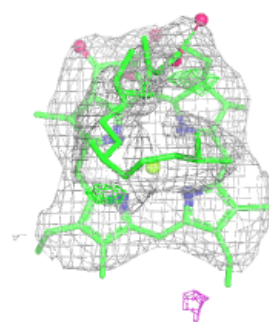
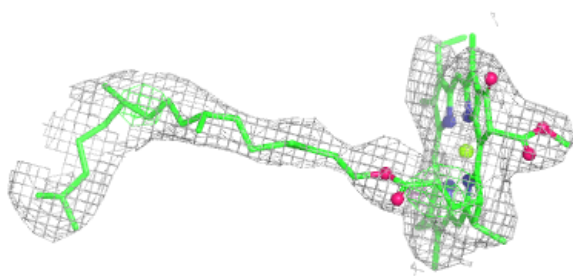
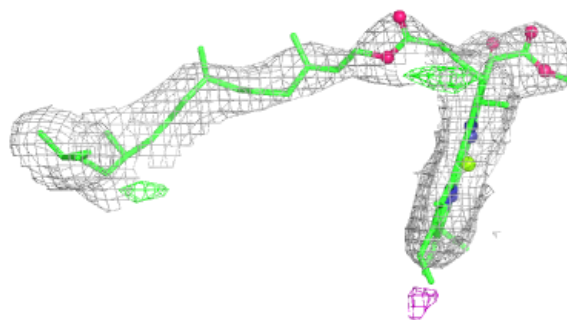
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

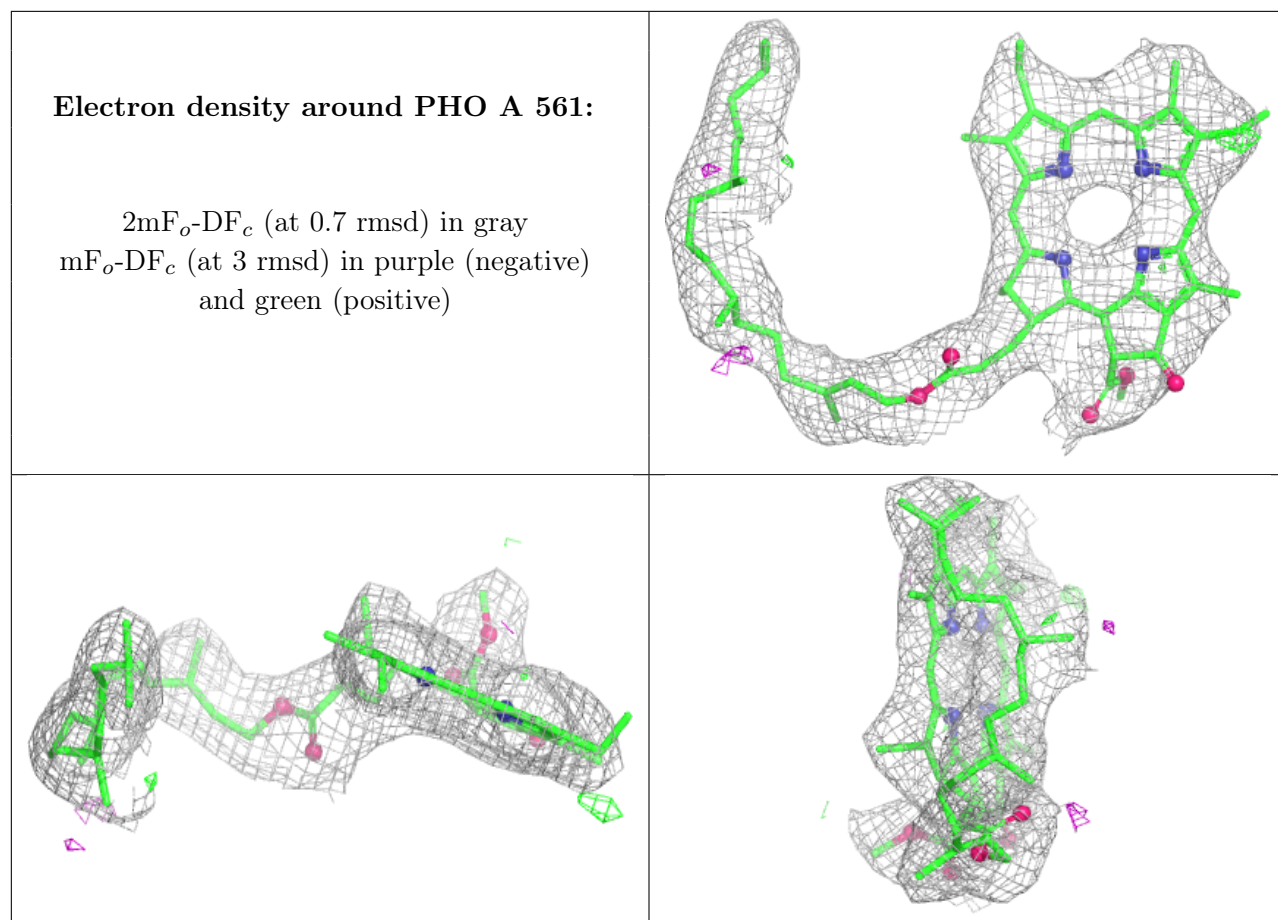




Electron density around CLA B 515:

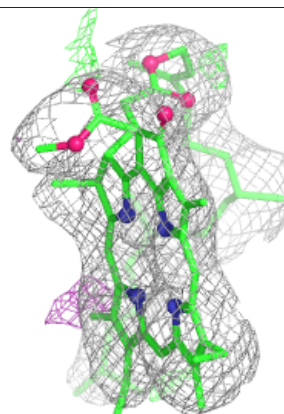
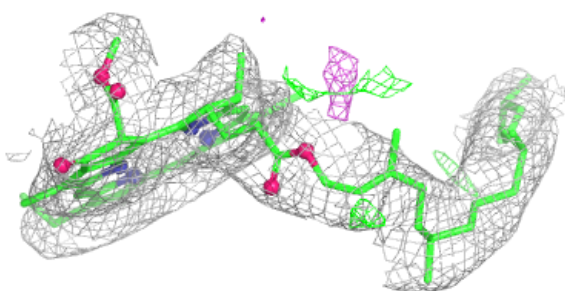
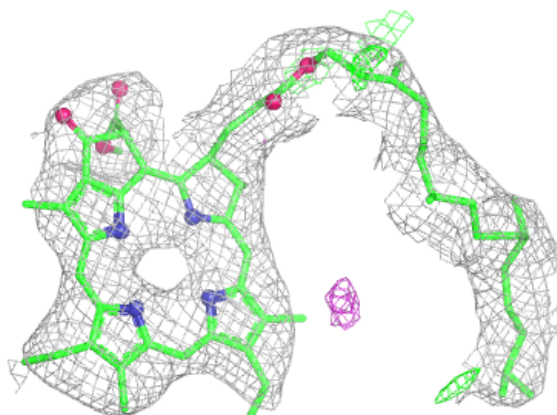
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



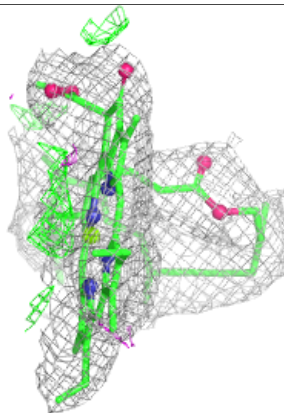
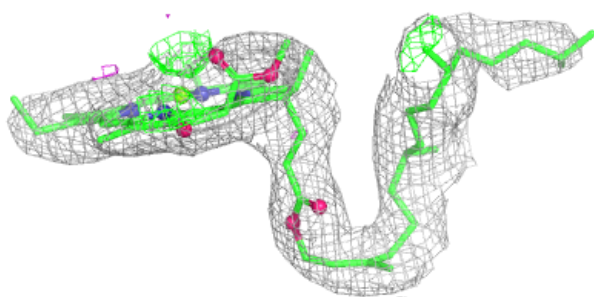
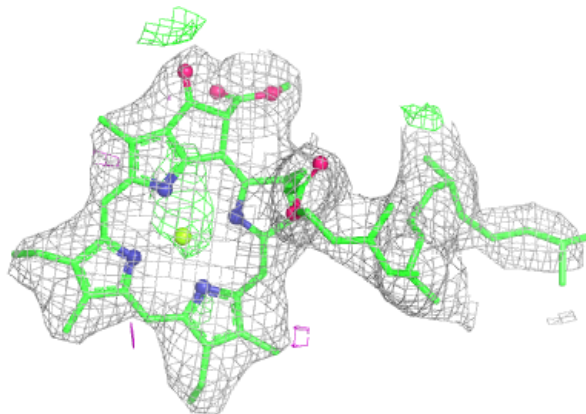


Electron density around PHO A 562:

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

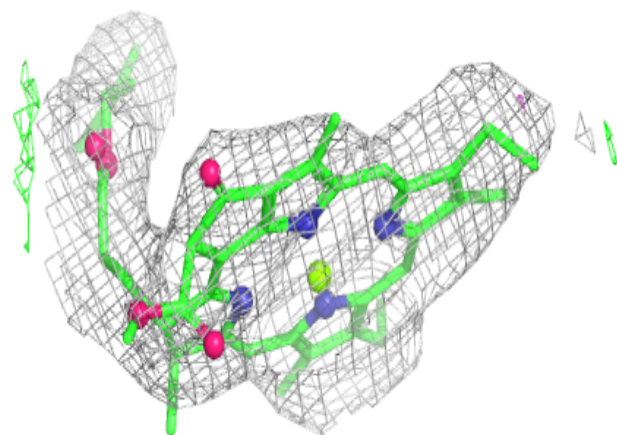
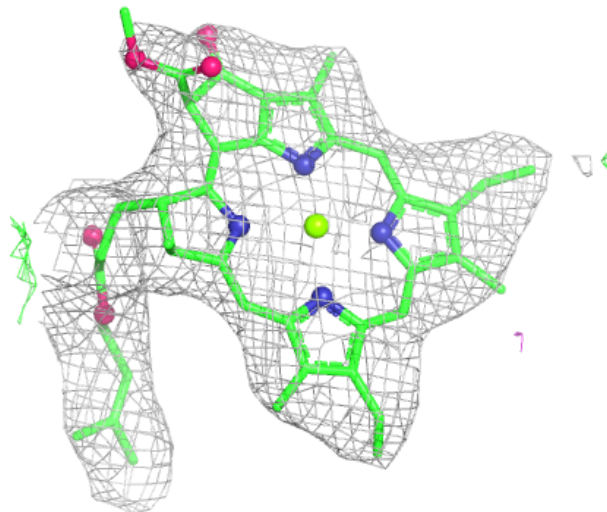
**Electron density around CLA A 560:**

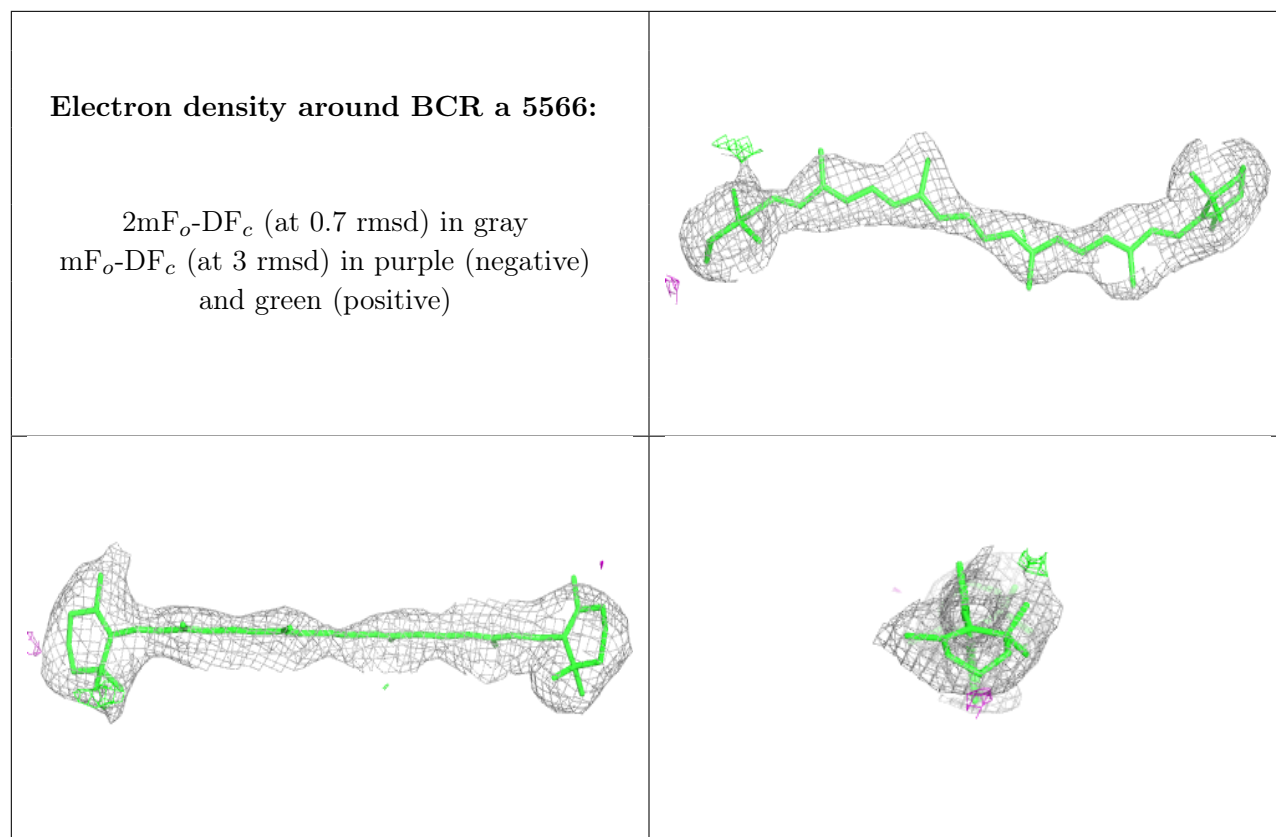
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



Electron density around CLA D 355:

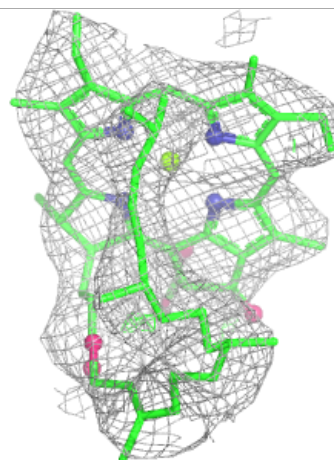
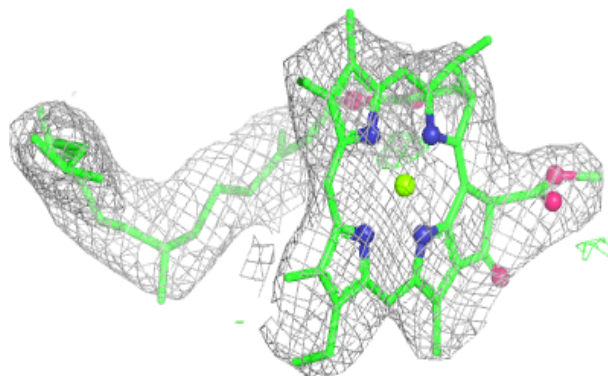
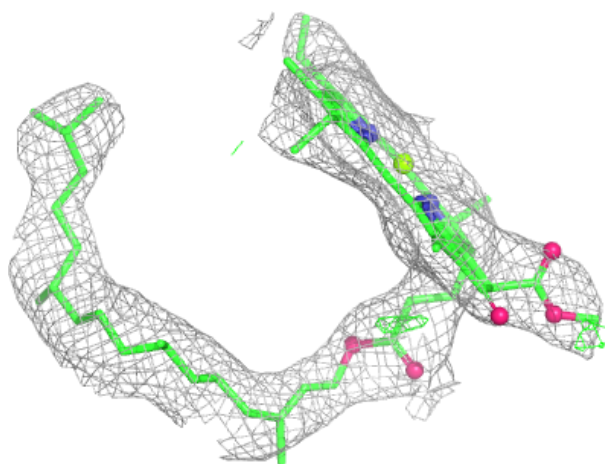
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

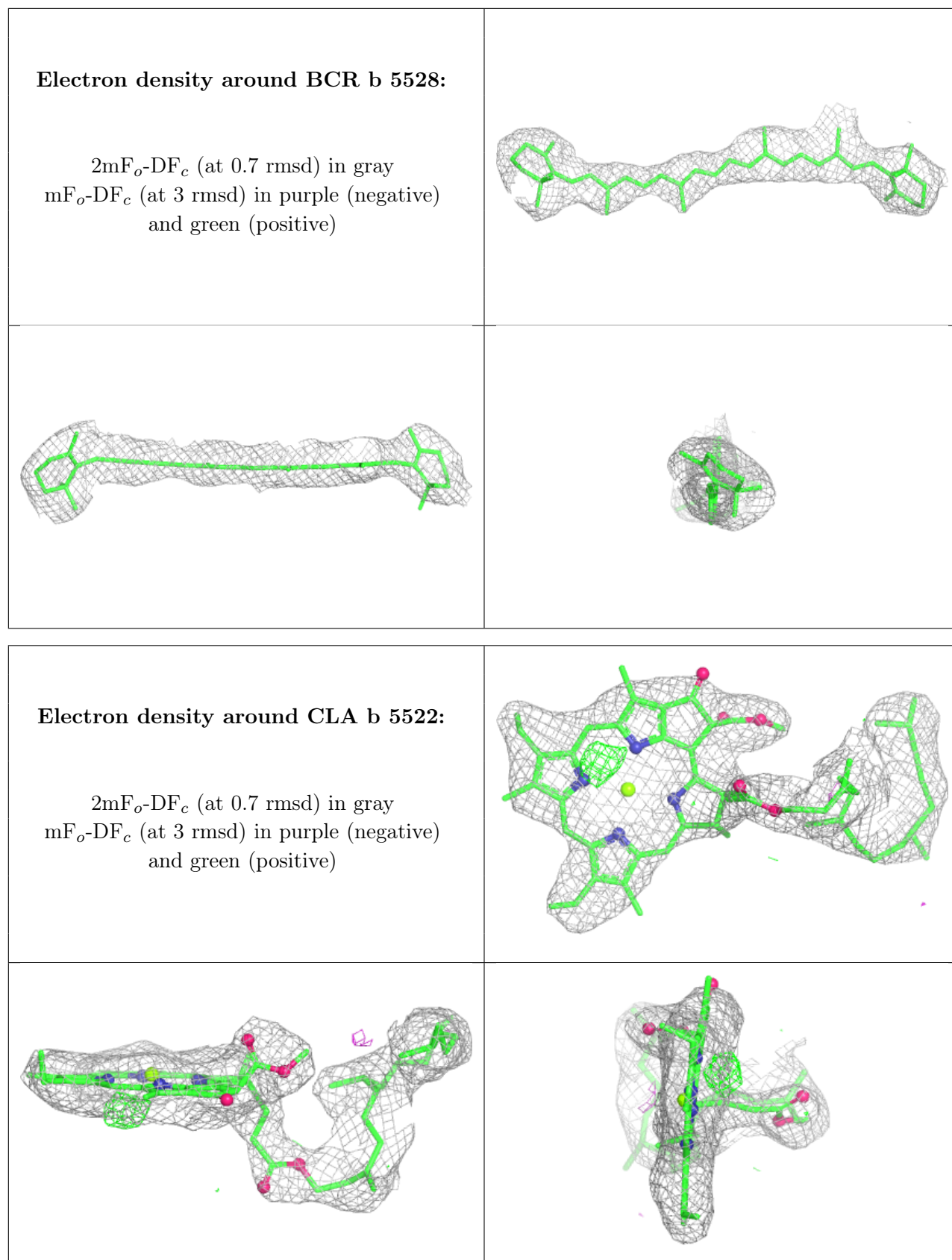




Electron density around CLA B 521:

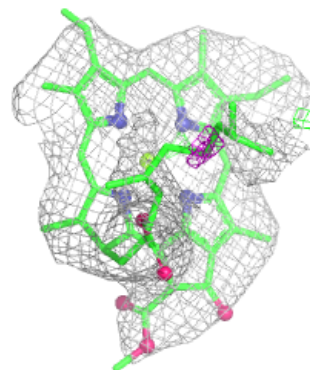
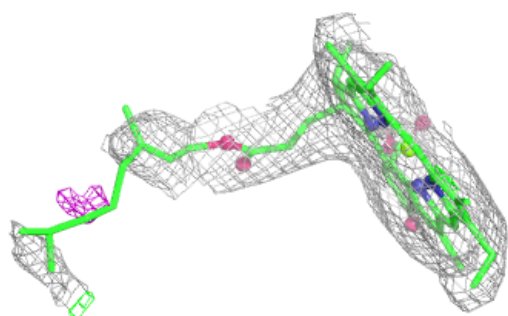
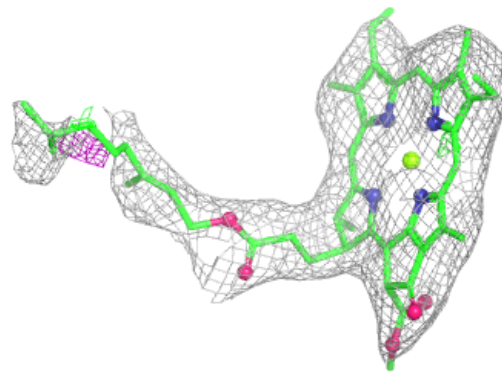
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



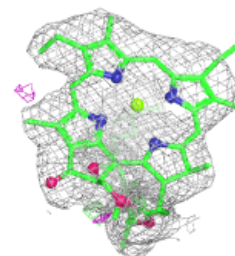
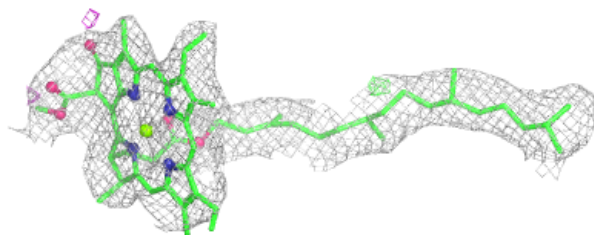
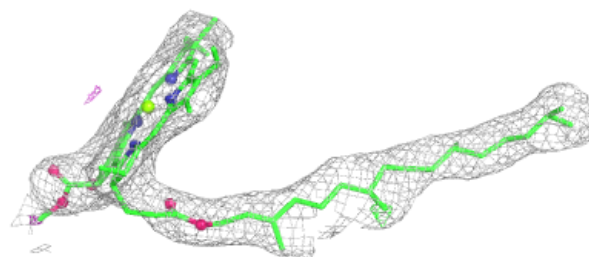


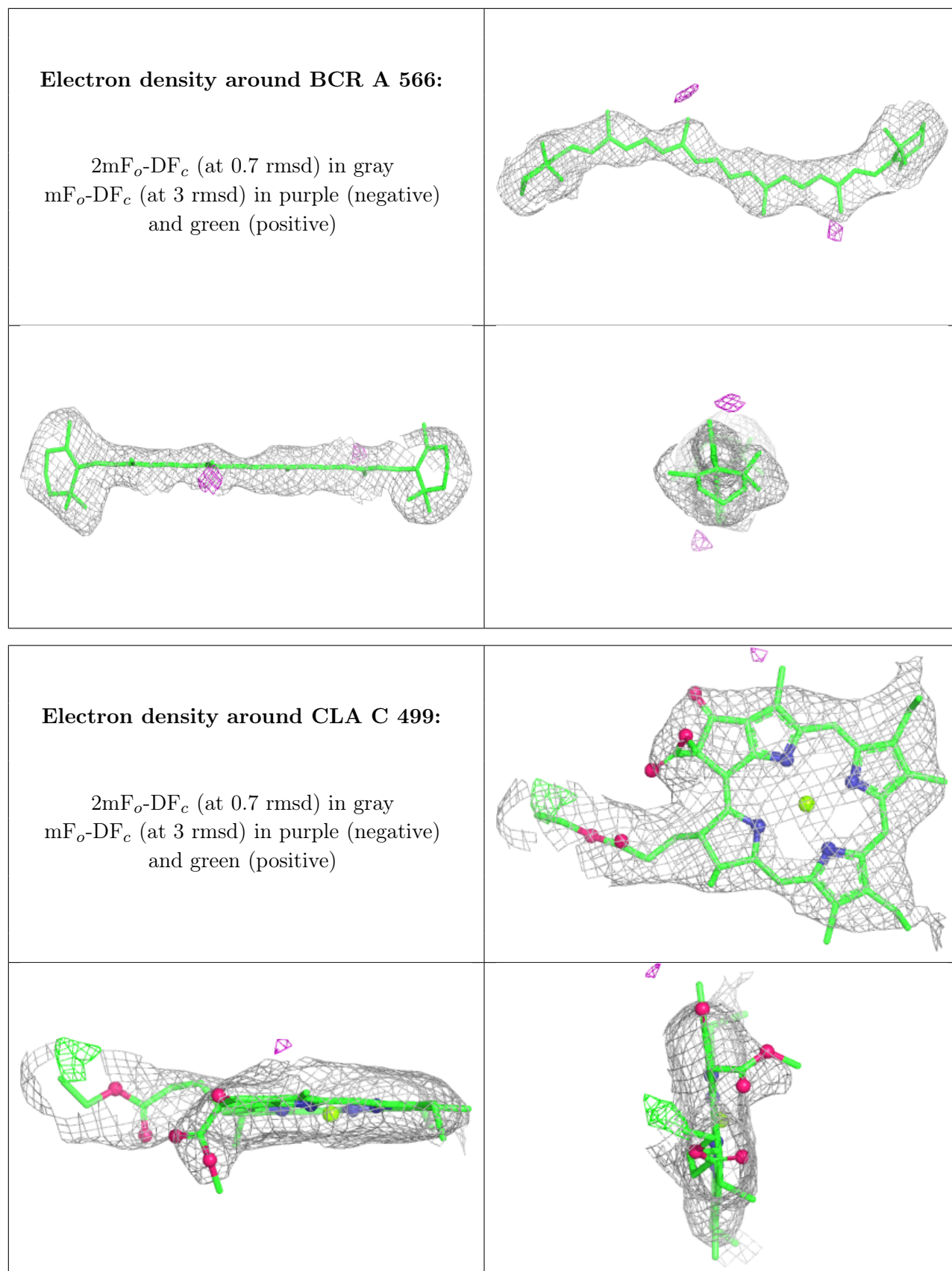
Electron density around CLA a 5563:

$2mF_o-DF_c$ (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:**

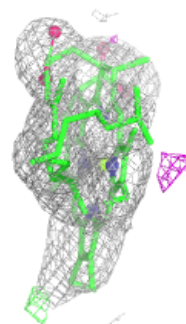
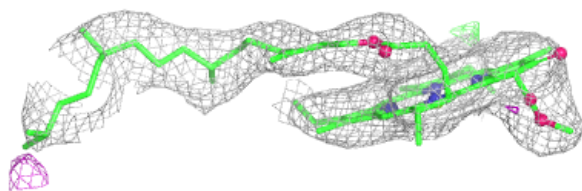
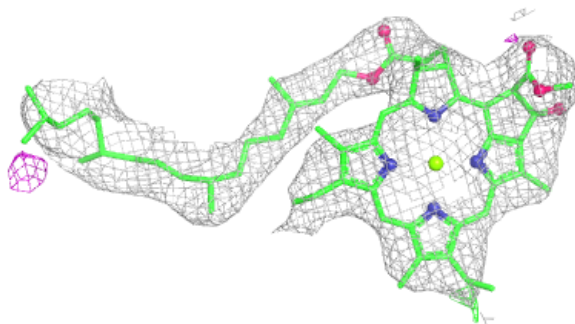
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





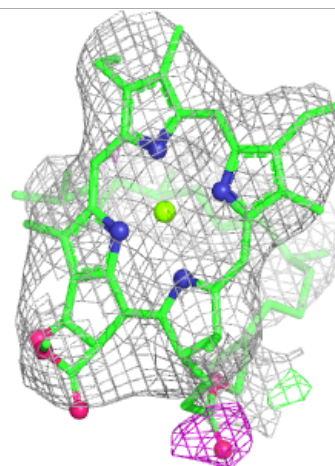
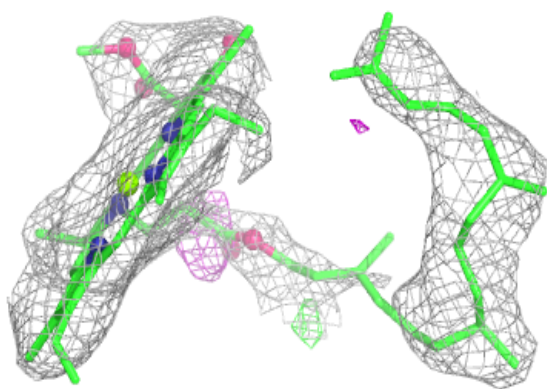
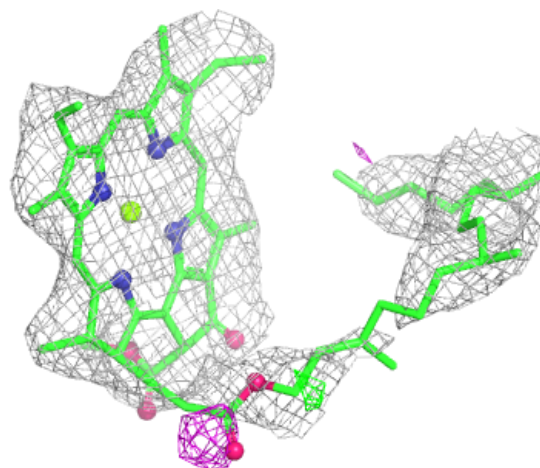
Electron density around CLA b 5513:

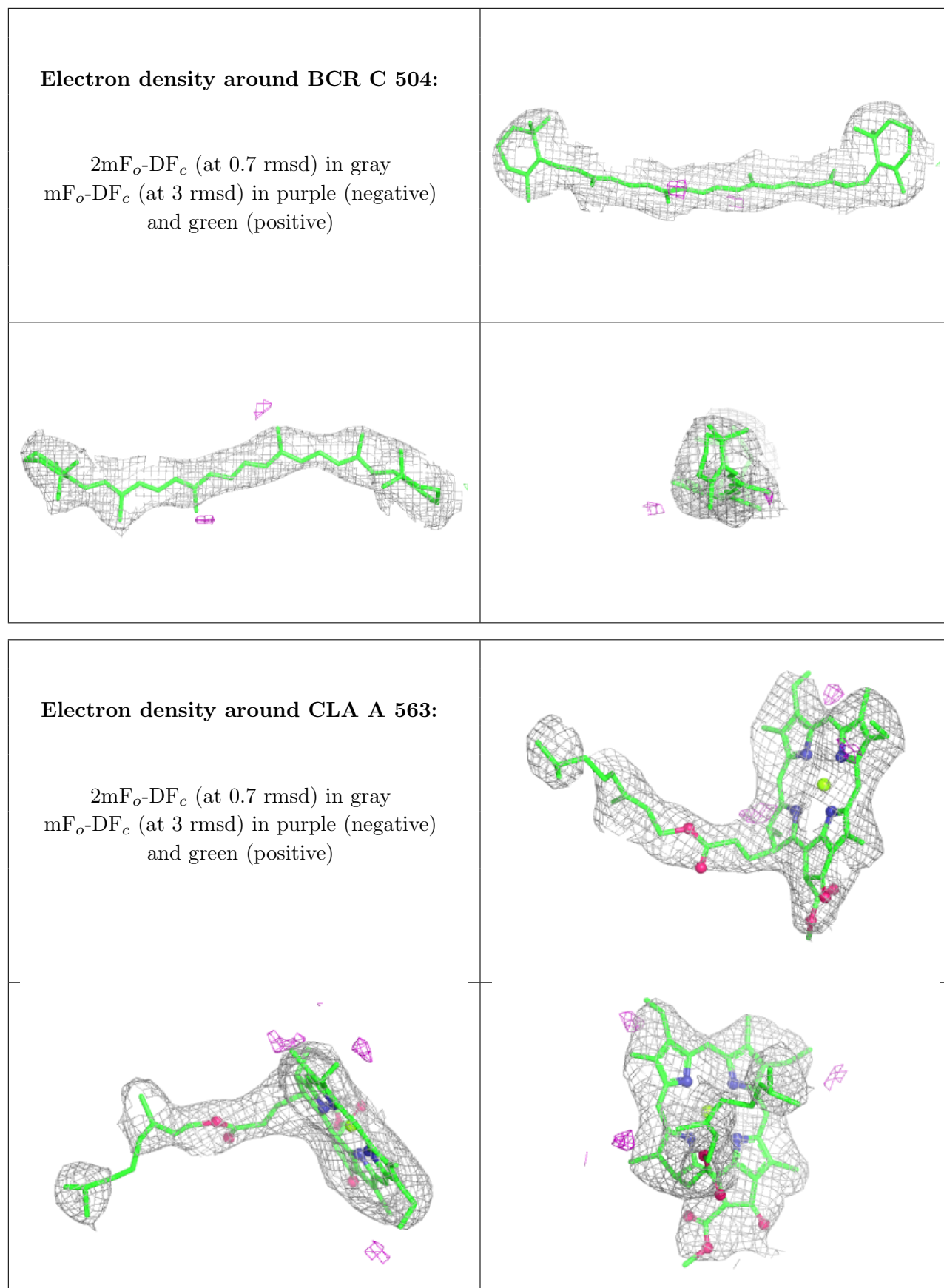
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 493:

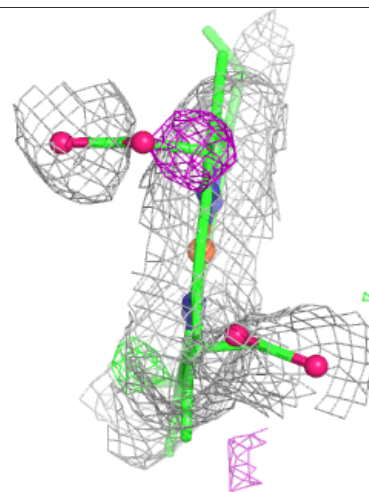
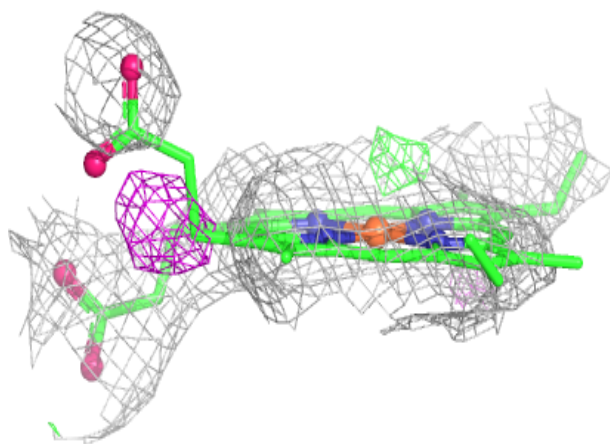
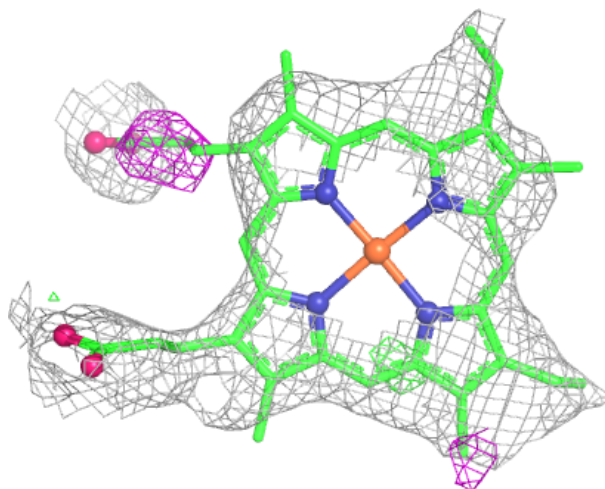
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





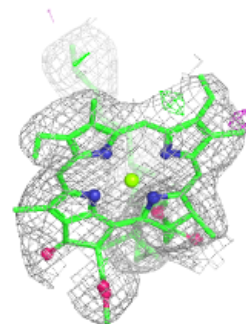
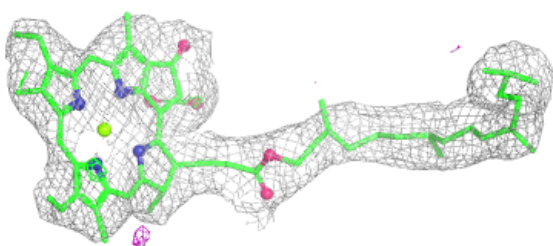
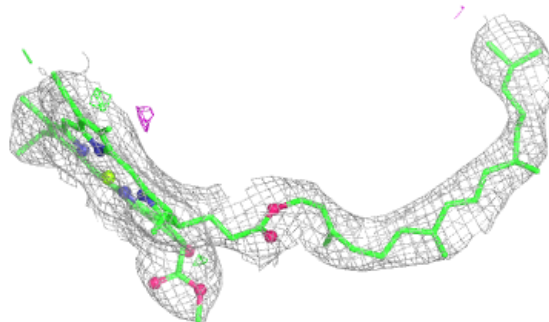
Electron density around HEM f 5051:

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

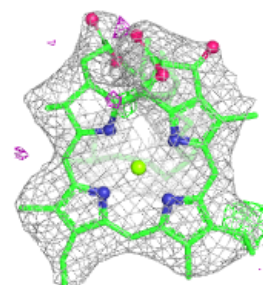
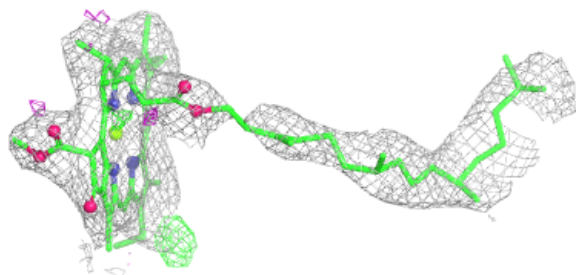
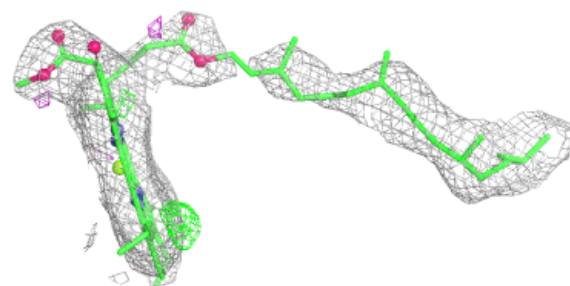


Electron density around CLA D 354:

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

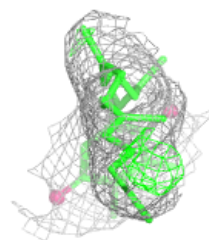
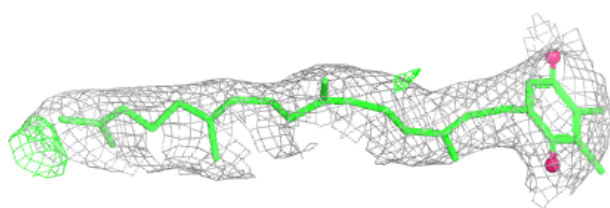
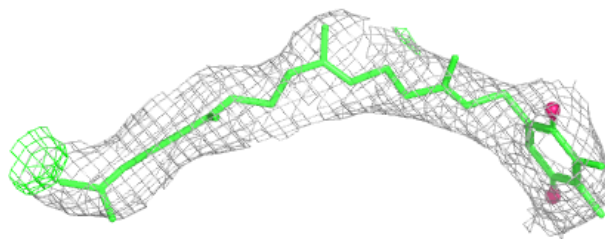
**Electron density around CLA b 5515:**

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

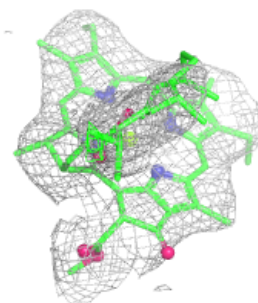
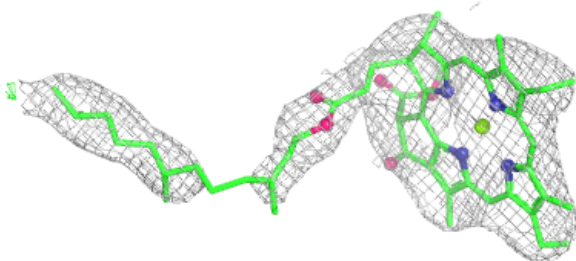
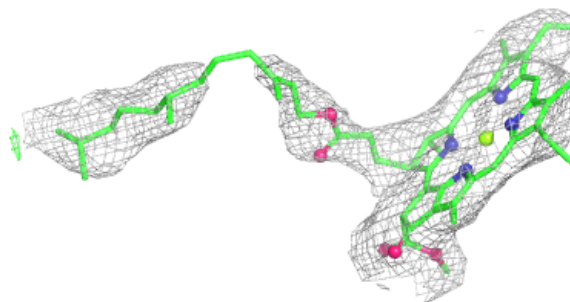


Electron density around PQ9 D 356:

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

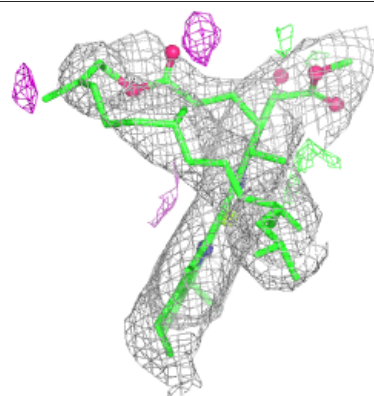
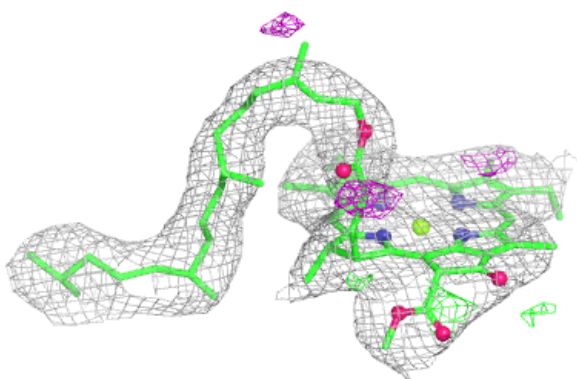
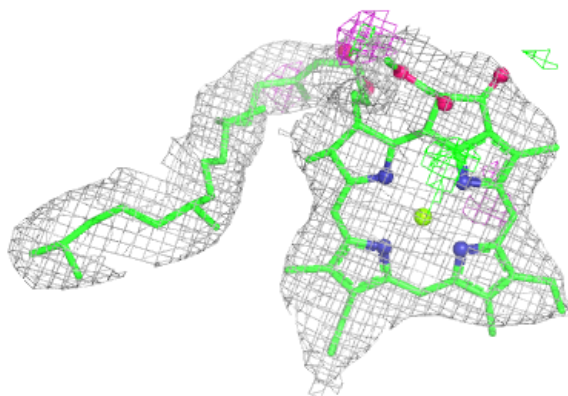
**Electron density around CLA C 492:**

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

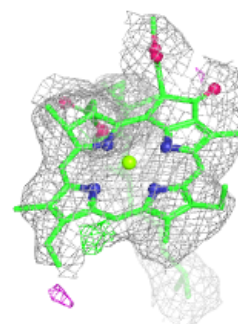
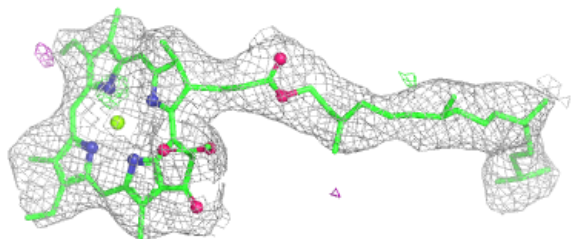
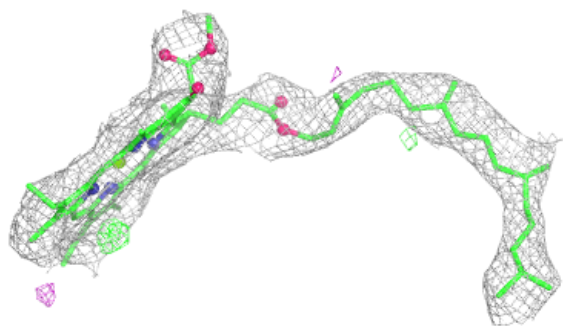


Electron density around CLA a 5559:

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

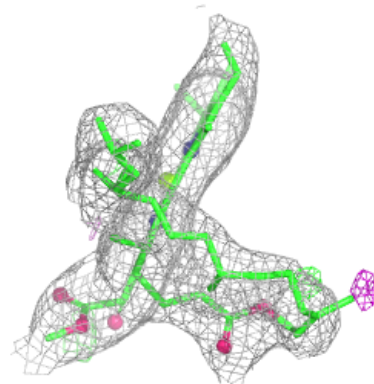
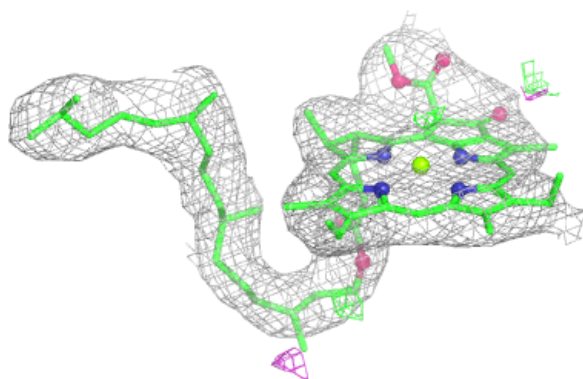
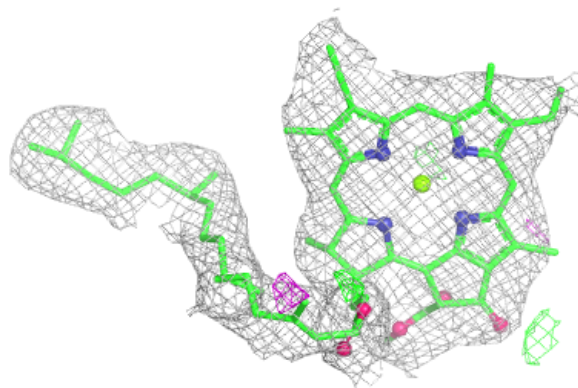
**Electron density around CLA d 5354:**

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

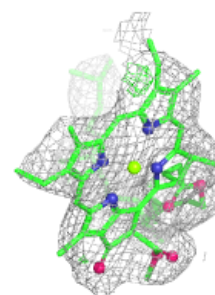
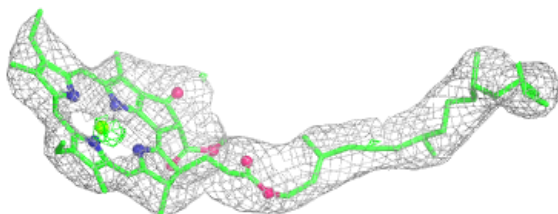
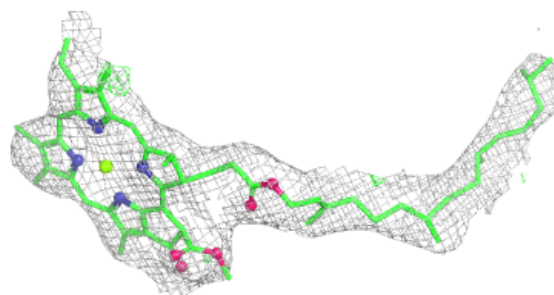


Electron density around CLA A 559:

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

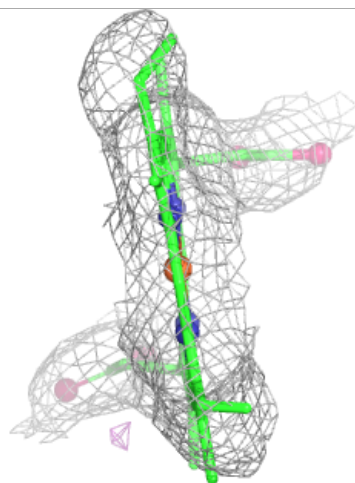
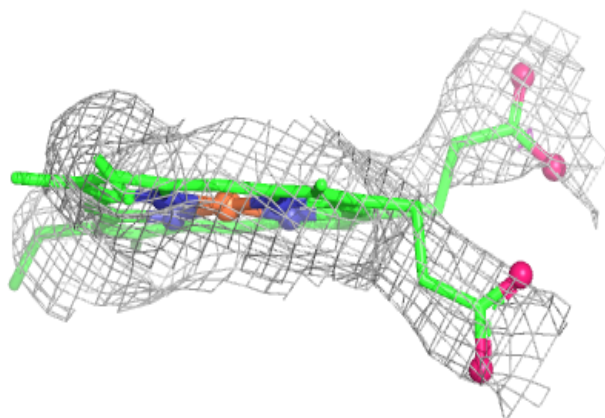
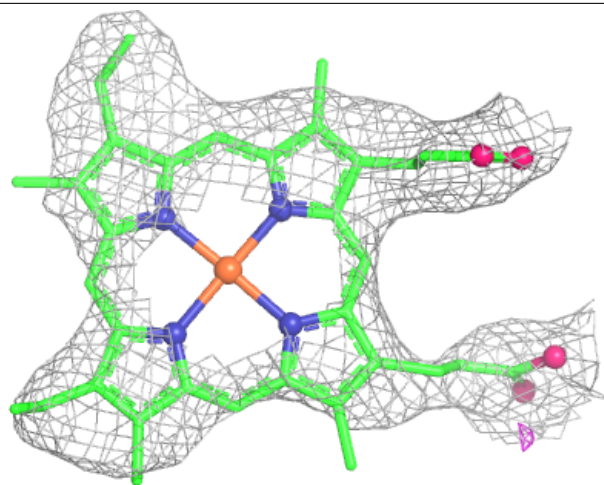
**Electron density around CLA a 5558:**

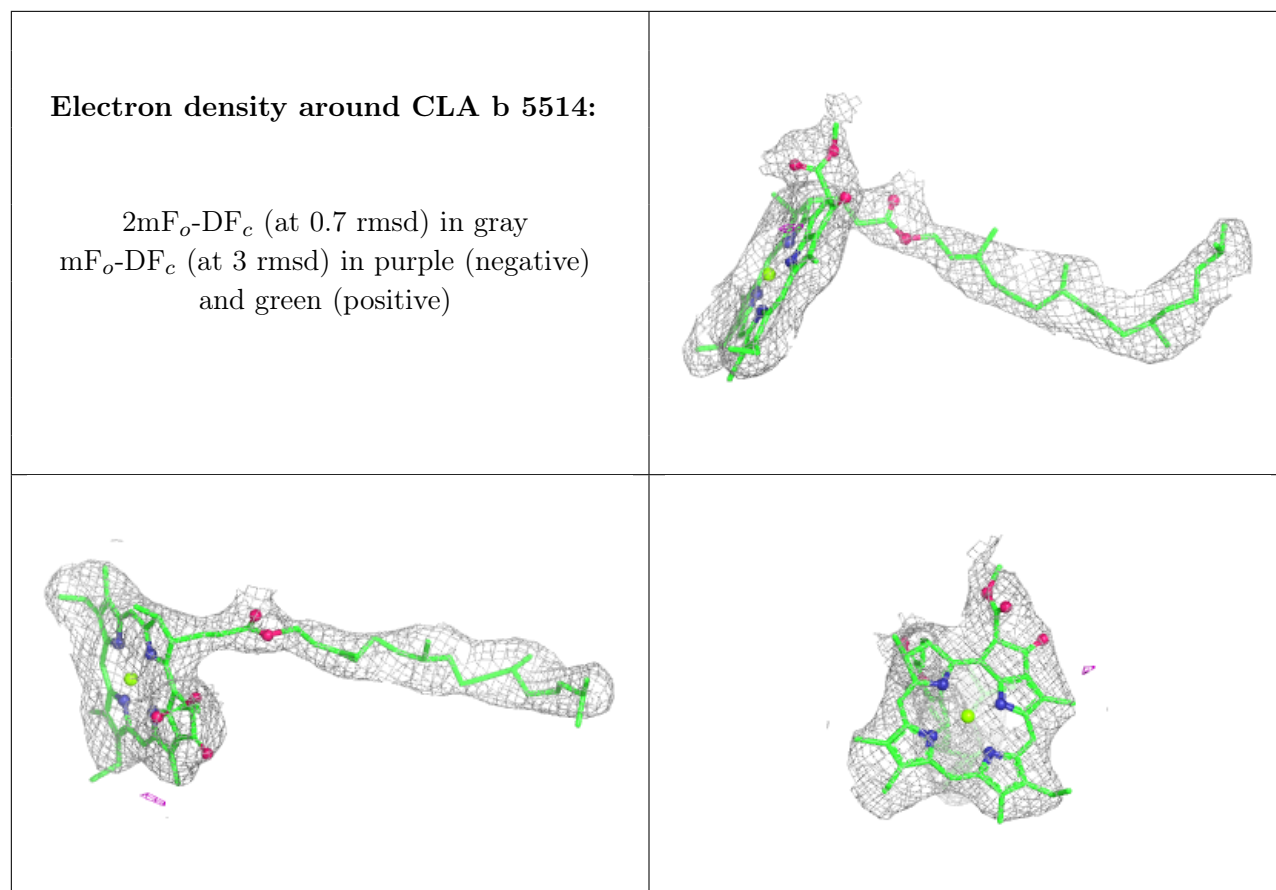
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM F 51:

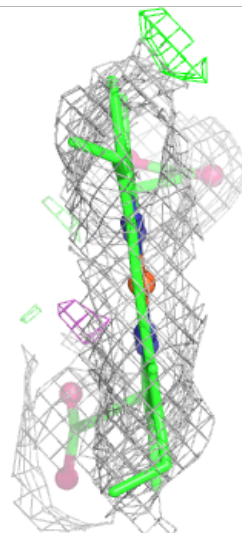
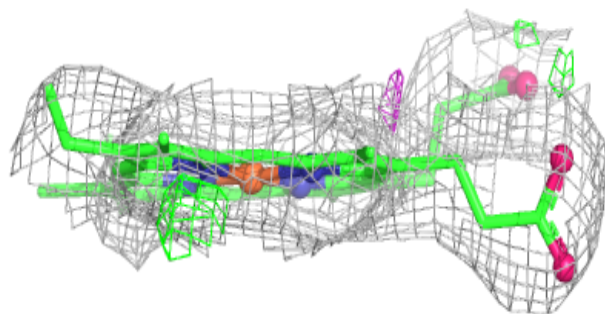
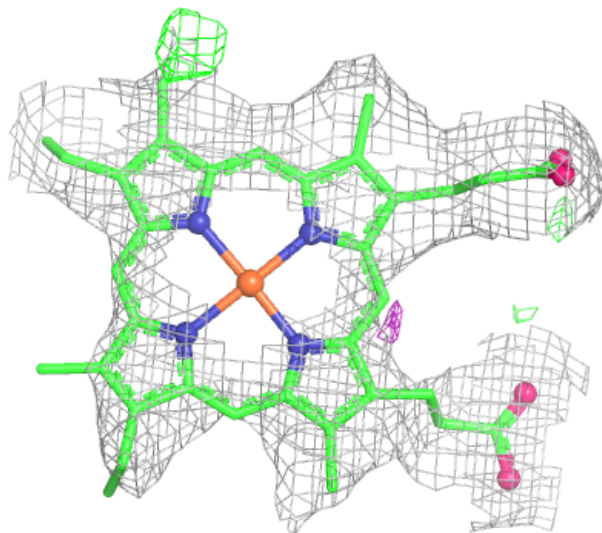
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

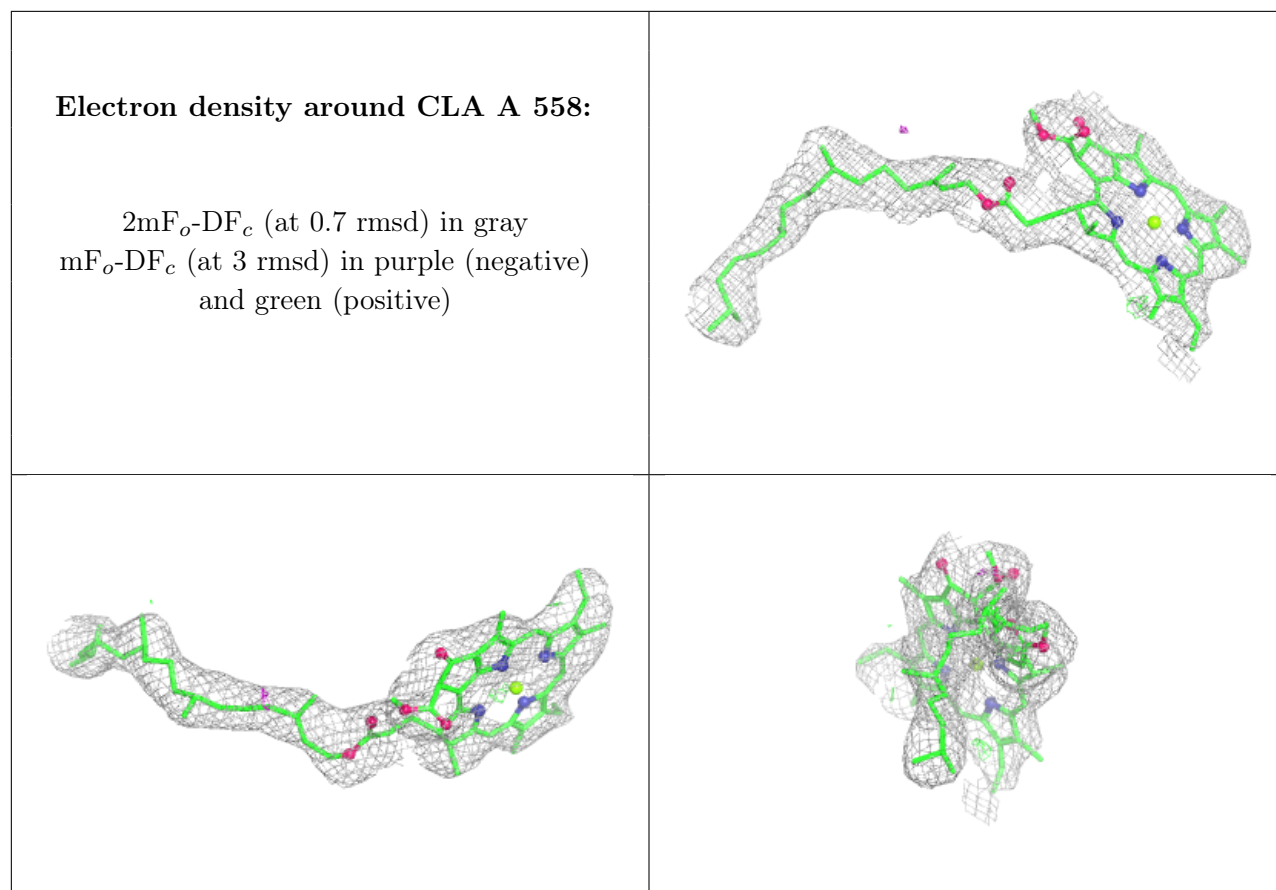


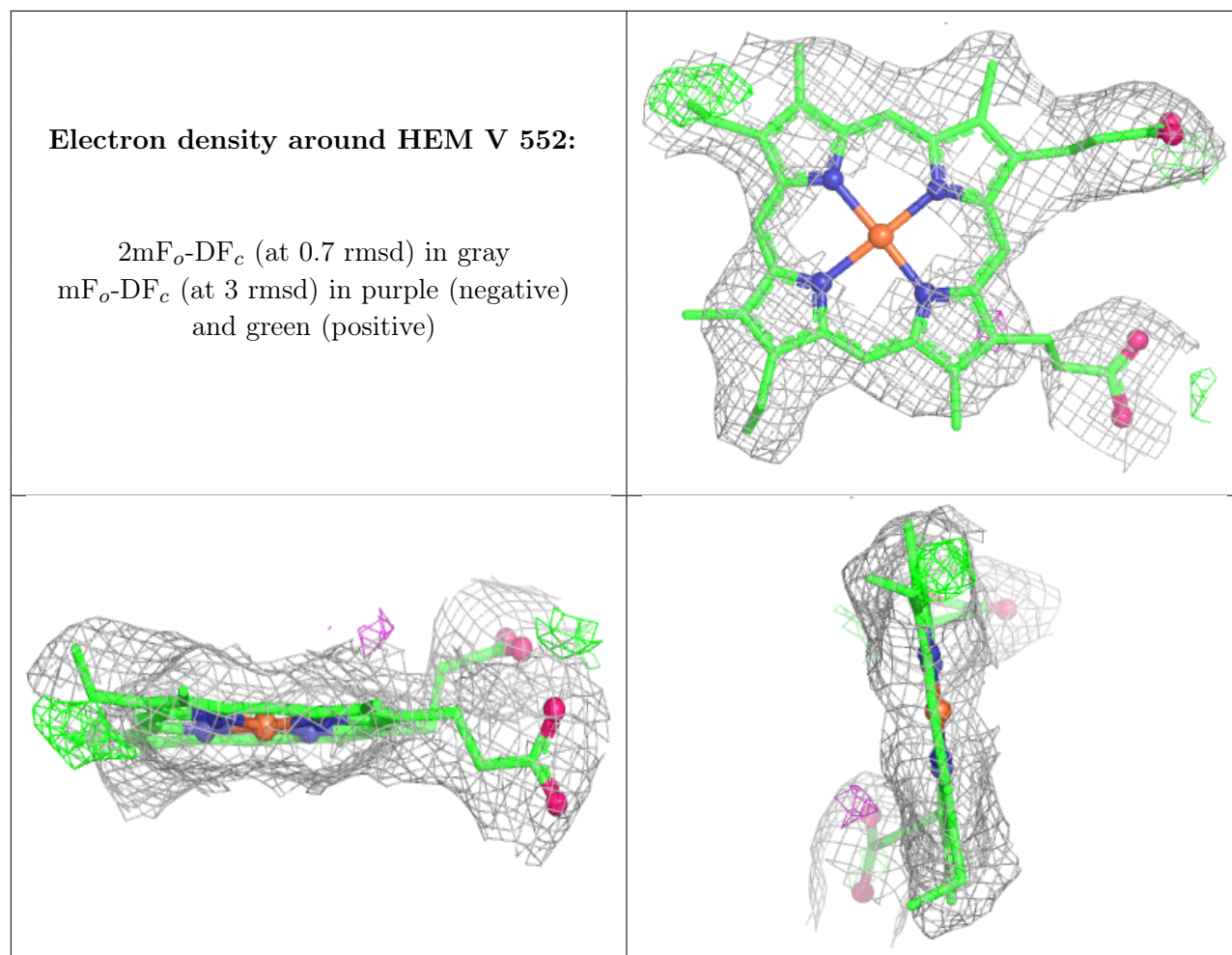


Electron density around HEM v 5552:

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







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

There are no such residues in this entry.