



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 11:02 AM UTC

PDB ID : 7RF5 / pdb_00007rf5
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.23 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)

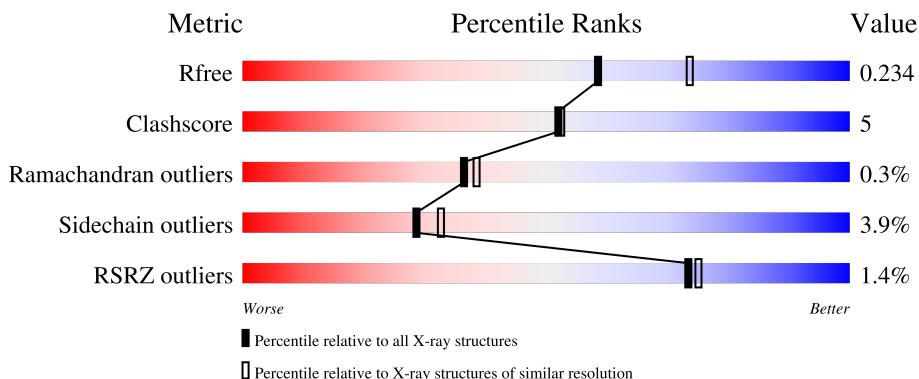
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

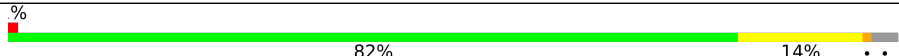
The reported resolution of this entry is 2.23 Å.

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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	 84% 12% .
1	a	344	 % 82% 14% ..

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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

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Mol	Chain	Length	Quality of chain
2	B	510	85% 13% ..
2	b	510	89% 9% ..
3	C	461	86% 10% .
3	c	461	83% 14% .
4	D	352	86% 10% ..
4	d	352	84% 13% ..
5	E	84	81% 17% .
5	e	84	79% 18% ..
6	F	45	64% 9% . 24%
6	f	45	56% 16% . 24%
7	H	66	91% 8% .
7	h	66	65% 30% 5%
8	I	38	84% 11% 5%
8	i	38	84% 11% 5%
9	J	40	75% 15% 10%
9	j	40	72% 18% 10%
10	K	46	61% 13% 7% 20%
10	k	46	52% 28% 20%
11	L	37	86% 14%
11	l	37	89% 5% . .
12	M	36	61% 25% 6% 8%
12	m	36	69% 19% 11%
13	O	272	78% 9% . 10%
13	o	272	77% 12% . 10%
14	R	41	51% 17% 32%

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Mol	Chain	Length	Quality of chain
14	r	41	
15	T	32	
15	t	32	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	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
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	612	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	H	101	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	613	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105562 atoms, of which 52760 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	334	6098	2030	2985	513	551	19	0	66	0
1	a	334	6086	2027	2976	513	551	19	0	66	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	505	7878	2631	3873	666	695	13	0	5	0
2	b	505	7814	2610	3836	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6941	2302	3432	586	607	14	0	14	0
3	c	451	7086	2343	3503	602	624	14	0	14	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	341	5368	1809	2637	446	464	12	0	2	0
4	d	341	5380	1813	2643	446	466	12	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O	0	0	0	
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

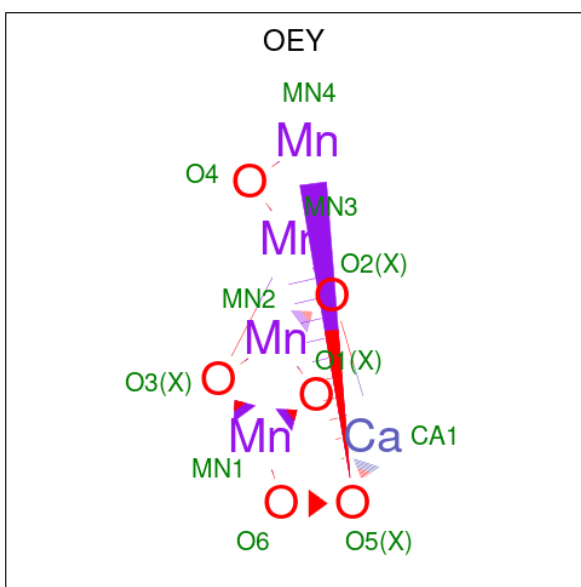
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

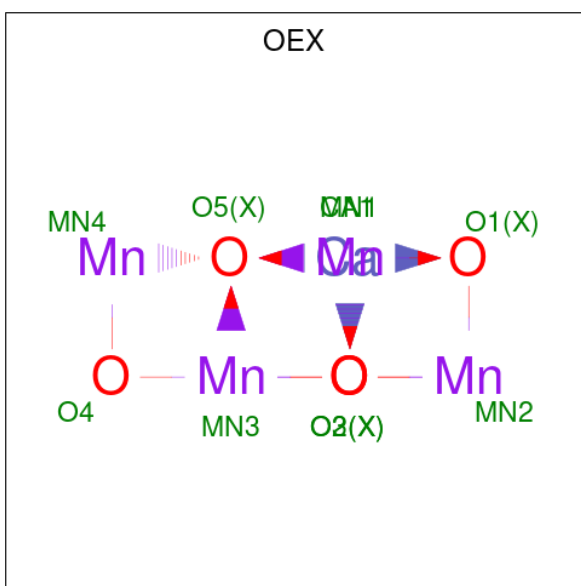
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
21	A	1	11	1	4	6	0	1
21	a	1	11	1	4	6	0	1

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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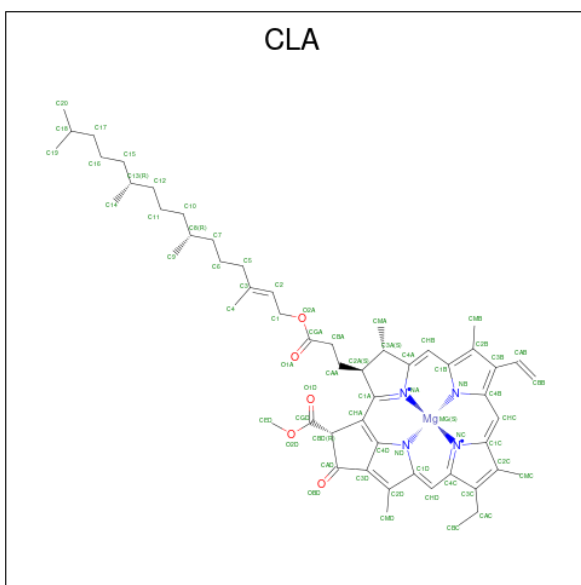
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
22	a	1	10	1	4	5	0	1

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
24	A	1	137	55	72	1	4	5	0	0
24	A	1	137	55	72	1	4	5	0	0
24	A	1	102	44	48	1	4	5	0	0
24	A	1	137	55	72	1	4	5	0	0
24	B	1	137	55	72	1	4	5	0	0
24	B	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	H	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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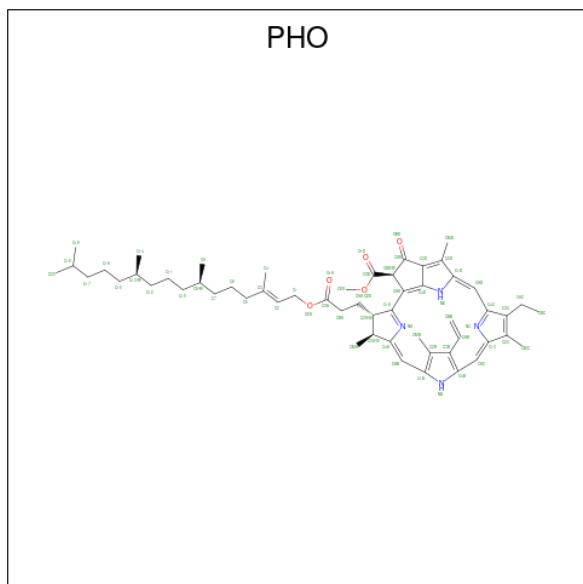
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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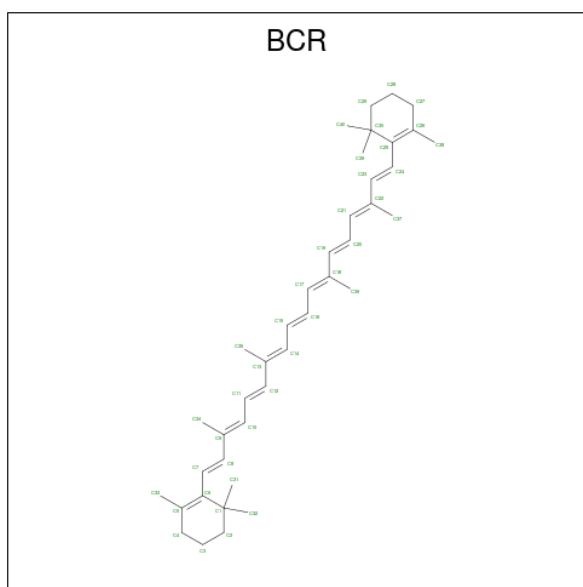
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
24	d	1	137	55	72	1	4	5	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
25	A	1	138	55	74	4	5	0	0
25	D	1	138	55	74	4	5	0	0
25	a	1	138	55	74	4	5	0	0
25	d	1	138	55	74	4	5	0	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	B	1	Total	C	H	0	0
			96	40	56		
26	C	1	Total	C	H	0	0
			96	40	56		
26	D	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	K	1	Total	C	H	0	0
			96	40	56		
26	T	1	Total	C	H	0	0
			96	40	56		
26	X	1	Total	C	H	0	0
			96	40	56		
26	a	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		
26	b	1	Total	C	H	0	0
			96	40	56		

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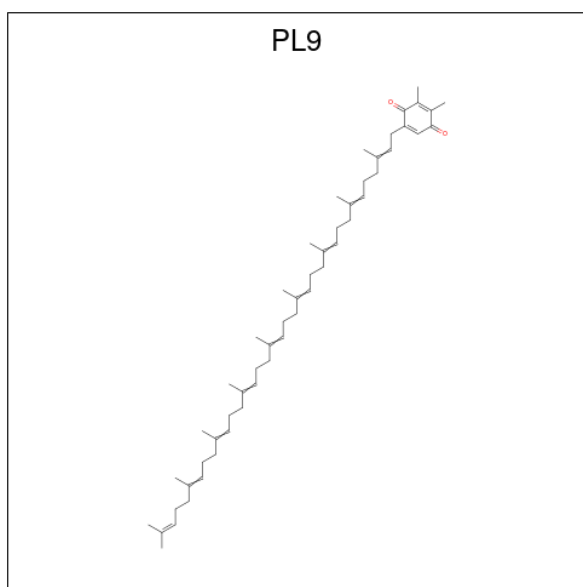
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

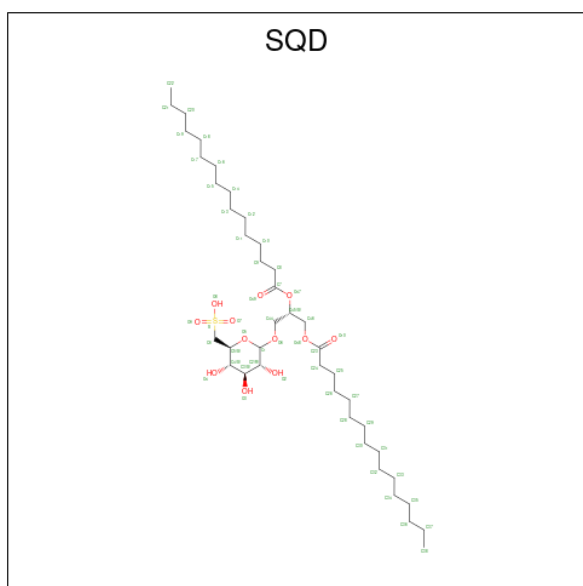
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



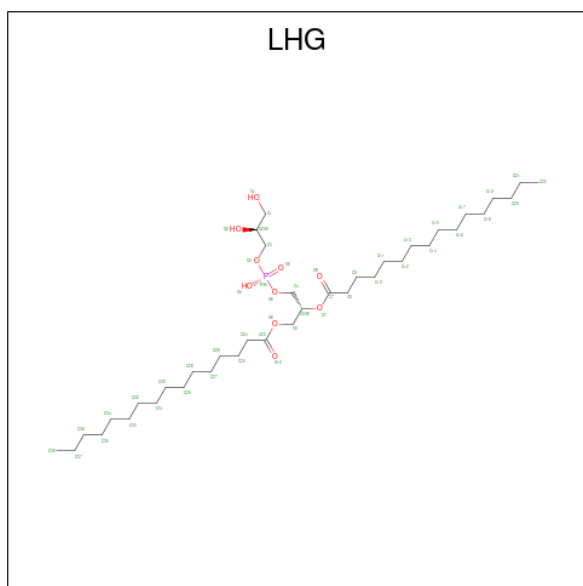
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
28	A	1	135	53	80	2	0	0
28	D	1	135	53	80	2	0	0
28	a	1	135	53	80	2	0	0
28	d	1	135	53	80	2	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



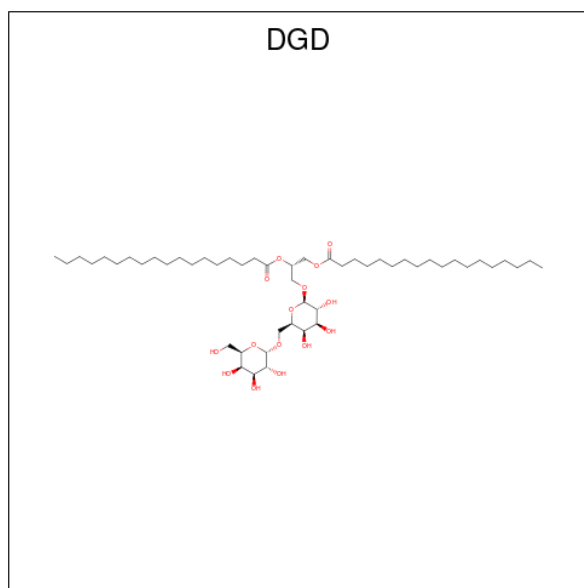
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	O			P
30	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
30	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
30	a	1	Total 123	C 38	H 74	O 10	P 1	0	0
30	d	1	Total 123	C 38	H 74	O 10	P 1	0	0
30	d	1	Total 90	C 28	H 51	O 10	P 1	0	0
30	e	1	Total 99	C 31	H 57	O 10	P 1	0	0
30	l	1	Total 123	C 38	H 74	O 10	P 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



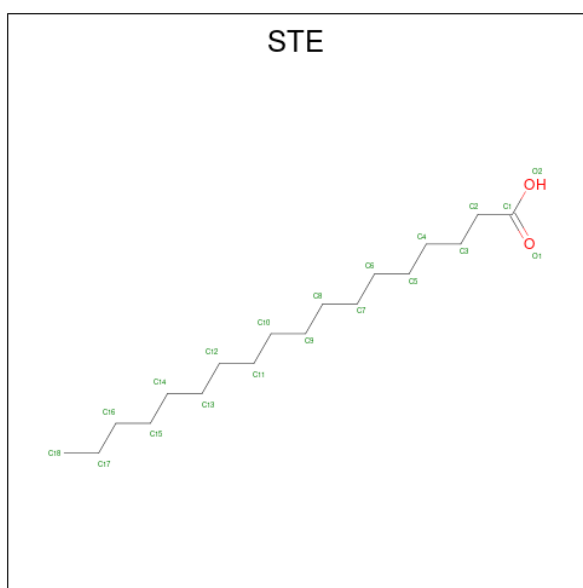
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
31	A	1	Total 162	C 51	H 96	O 15	0	0
31	C	1	Total 144	C 47	H 82	O 15	0	0
31	C	1	Total 144	C 47	H 82	O 15	0	0
31	C	1	Total 144	C 47	H 82	O 15	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			53	18	35			
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H		0	0
			41	15	26			

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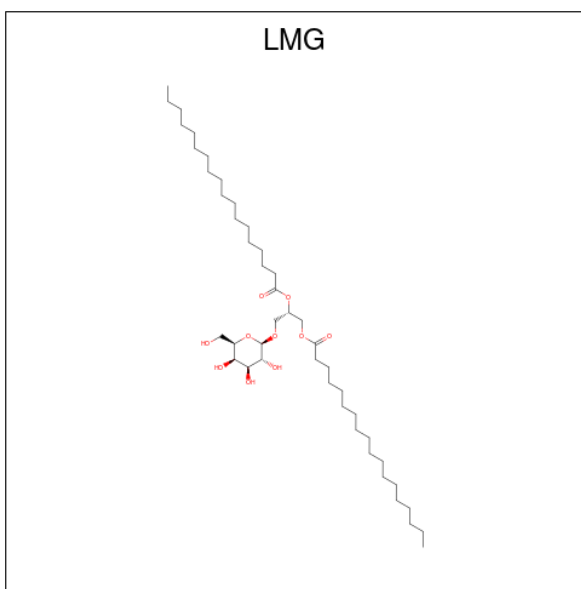
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	R	1	Total C H O 28 10 16 2	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			55	18	35	2		
32	c	1	Total	C	H	O	0	0
			28	10	16	2		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	h	1	Total	C	H		0	0
			41	14	27			
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



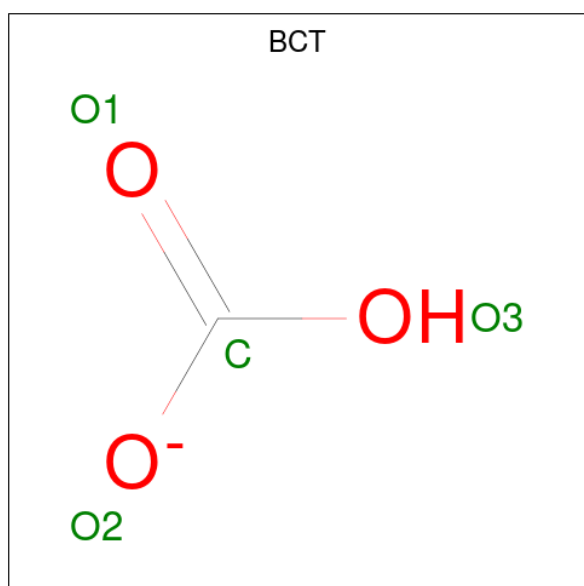
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			122	41	71	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
33	D	1	Total 68	C 24	H 40	O 4	0	0
33	M	1	Total 123	C 41	H 72	O 10	0	0
33	Y	1	Total 114	C 38	H 66	O 10	0	0
33	a	1	Total 141	C 45	H 86	O 10	0	0
33	b	1	Total 141	C 45	H 86	O 10	0	0
33	c	1	Total 81	C 27	H 44	O 10	0	0
33	c	1	Total 117	C 38	H 69	O 10	0	0
33	c	1	Total 117	C 39	H 68	O 10	0	0
33	d	1	Total 102	C 34	H 58	O 10	0	0
33	m	1	Total 123	C 41	H 72	O 10	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



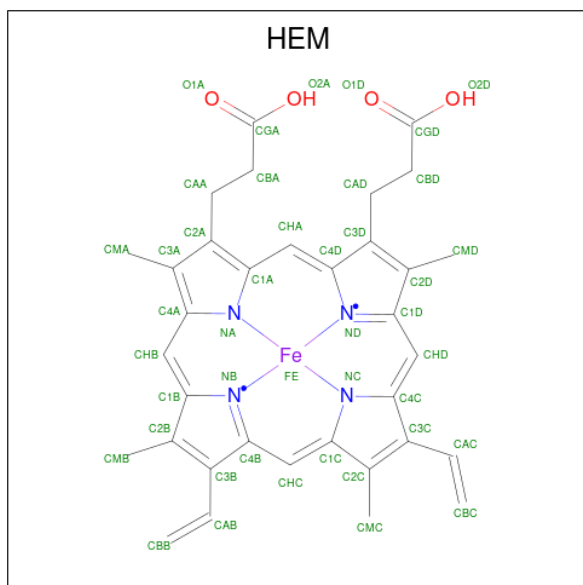
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
34	D	1	Total 5	C 1	H 1	O 3	0	0

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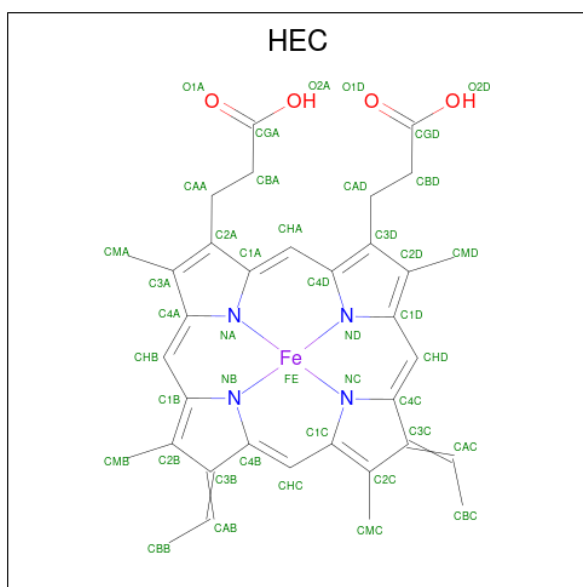
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
35	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
36	V	1	73	34	1	30	4	4	0	0
36	v	1	73	34	1	30	4	4	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	118	Total	O	0	0
			118	118		
37	B	141	Total	O	0	0
			141	141		
37	C	114	Total	O	0	0
			114	114		
37	D	100	Total	O	0	0
			100	100		
37	E	20	Total	O	0	0
			20	20		
37	F	3	Total	O	0	0
			3	3		
37	H	29	Total	O	0	0
			29	29		
37	I	7	Total	O	0	0
			7	7		
37	J	6	Total	O	0	0
			6	6		
37	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	10	Total O 10 10	0	0
37	M	5	Total O 5 5	0	0
37	O	71	Total O 71 71	0	0
37	R	1	Total O 1 1	0	0
37	T	5	Total O 5 5	0	0
37	U	33	Total O 33 33	0	0
37	V	49	Total O 49 49	0	0
37	X	7	Total O 7 7	0	0
37	Y	4	Total O 4 4	0	0
37	Z	2	Total O 2 2	0	0
37	a	117	Total O 117 117	0	0
37	b	131	Total O 131 131	0	0
37	c	118	Total O 118 118	0	0
37	d	100	Total O 100 100	0	0
37	e	10	Total O 10 10	0	0
37	f	2	Total O 2 2	0	0
37	h	19	Total O 19 19	0	0
37	i	8	Total O 8 8	0	0
37	j	11	Total O 11 11	0	0
37	k	4	Total O 4 4	0	0
37	l	10	Total O 10 10	0	0

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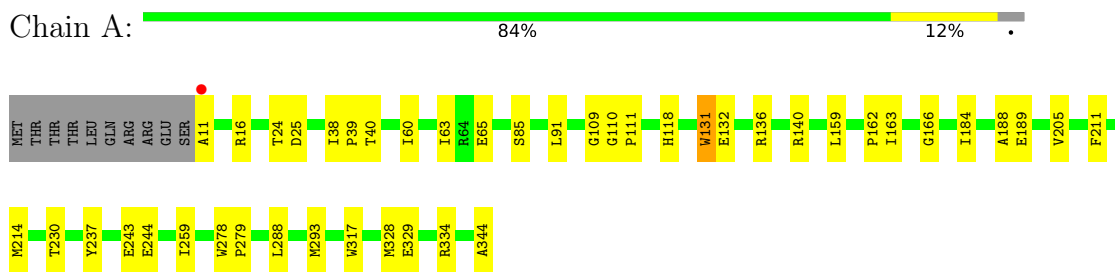
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	m	5	Total O 5 5	0	0
37	o	65	Total O 65 65	0	0
37	r	1	Total O 1 1	0	0
37	t	5	Total O 5 5	0	0
37	u	41	Total O 41 41	0	0
37	v	36	Total O 36 36	0	0
37	x	8	Total O 8 8	0	0
37	y	1	Total O 1 1	0	0
37	z	2	Total O 2 2	0	0

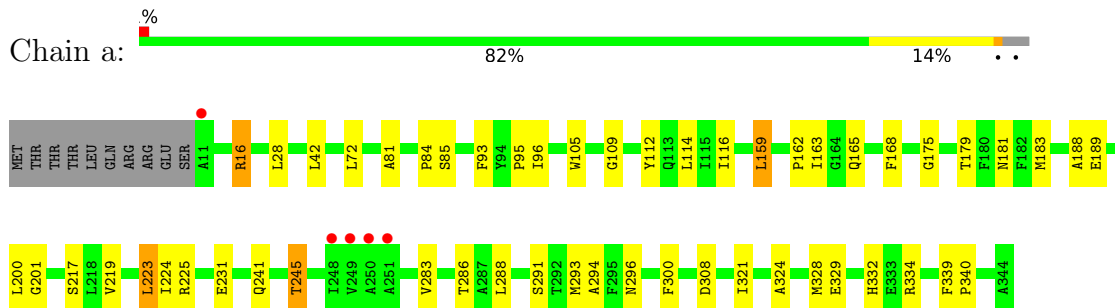
3 Residue-property plots [i](#)

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

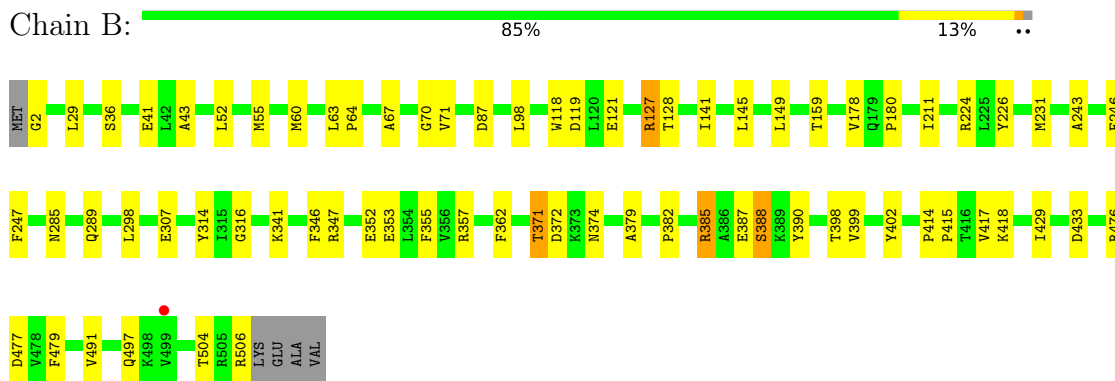
- Molecule 1: Photosystem II protein D1 1



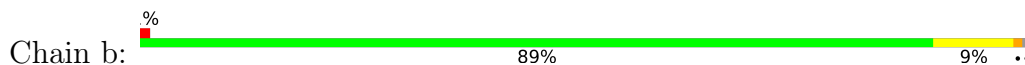
- Molecule 1: Photosystem II protein D1 1

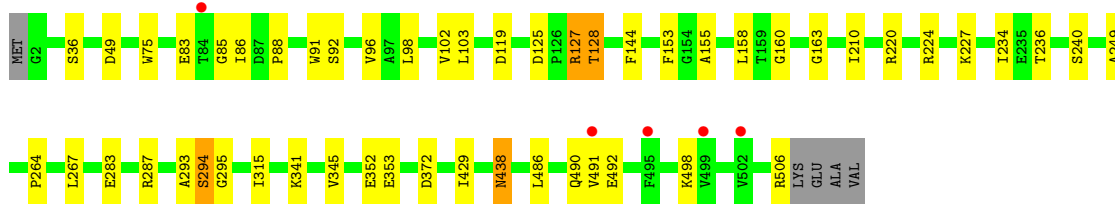


- Molecule 2: Photosystem II CP47 reaction center protein

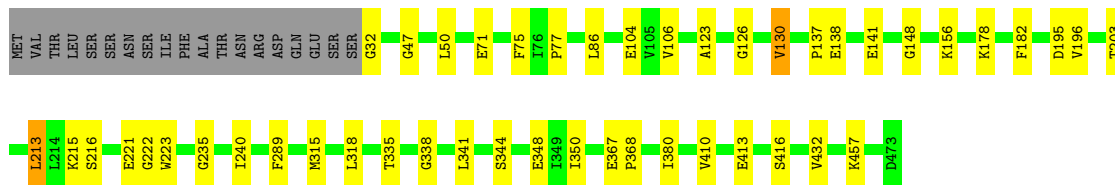
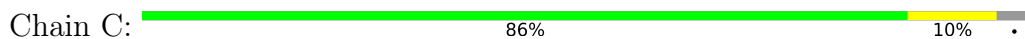


- Molecule 2: Photosystem II CP47 reaction center protein

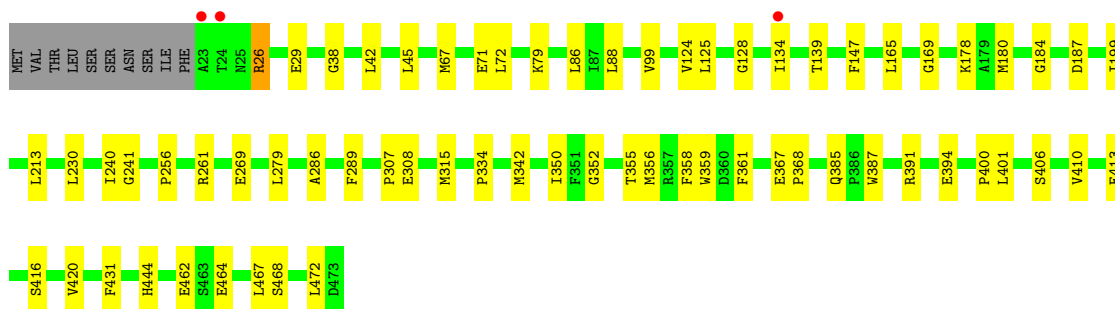
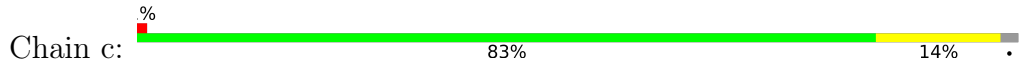




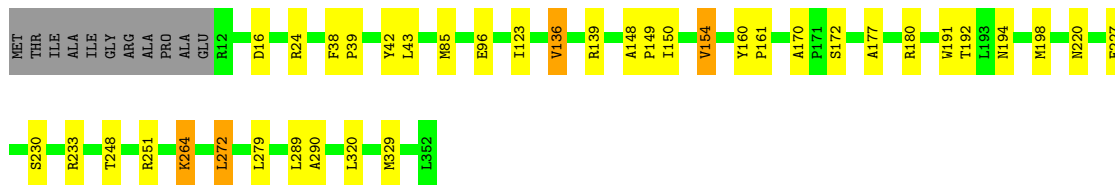
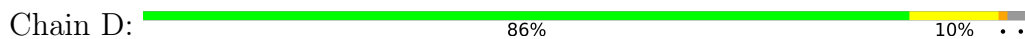
● Molecule 3: Photosystem II CP43 reaction center protein



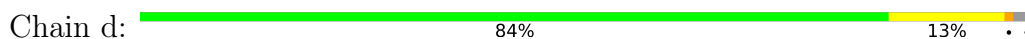
● Molecule 3: Photosystem II CP43 reaction center protein



● Molecule 4: Photosystem II D2 protein

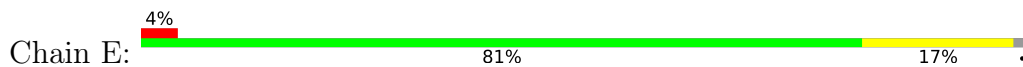


● Molecule 4: Photosystem II D2 protein

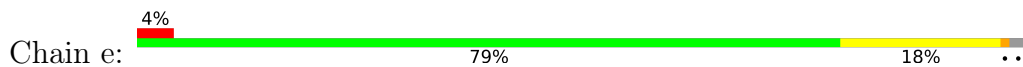




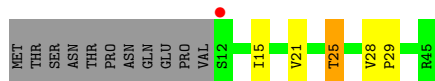
- Molecule 5: Cytochrome b559 subunit alpha



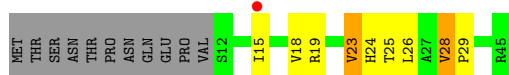
- Molecule 5: Cytochrome b559 subunit alpha



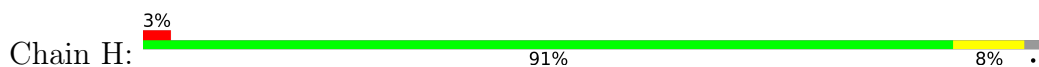
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



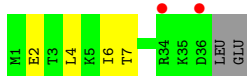
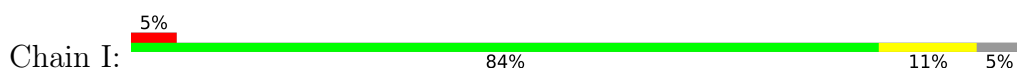
- Molecule 7: Photosystem II reaction center protein H



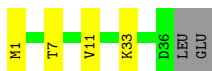
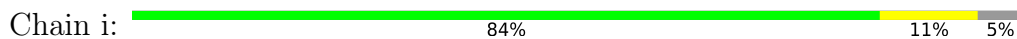
- Molecule 7: Photosystem II reaction center protein H



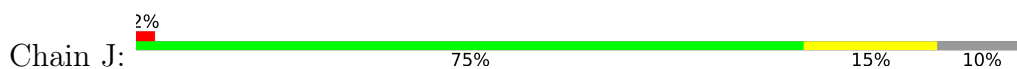
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



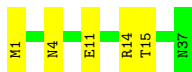
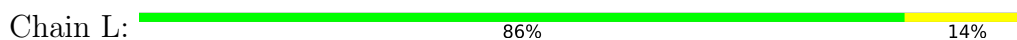
- Molecule 10: Photosystem II reaction center protein K



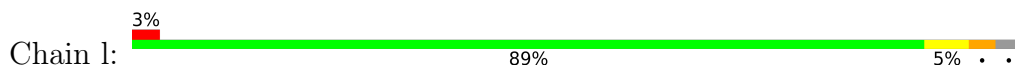
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



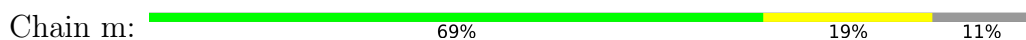
- Molecule 11: Photosystem II reaction center protein L



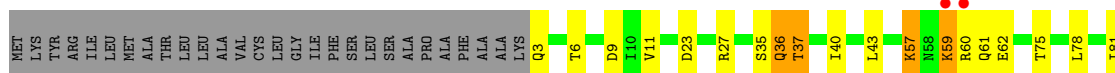
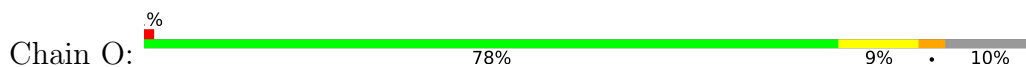
- Molecule 12: Photosystem II reaction center protein M



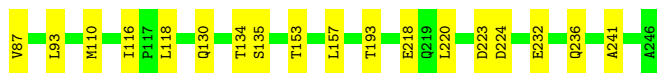
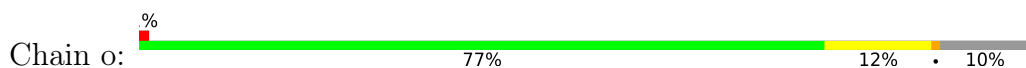
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



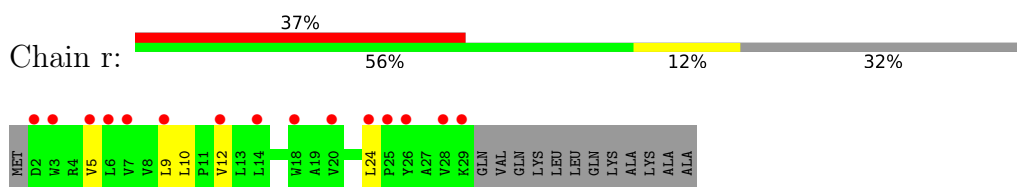
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



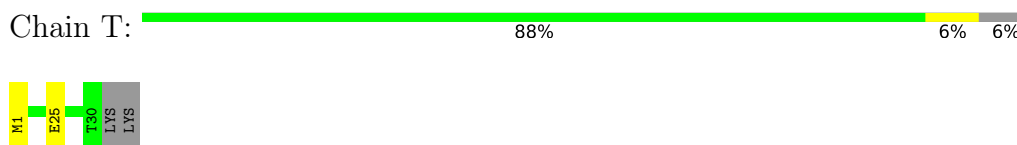
- Molecule 14: Photosystem II protein Y



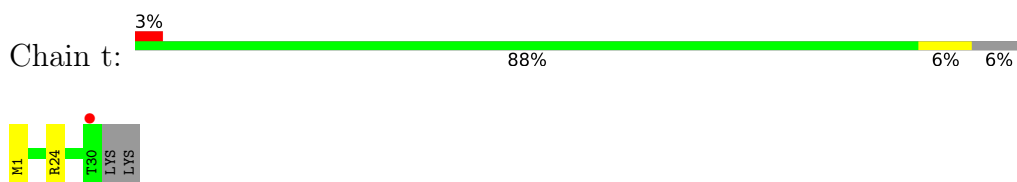
- Molecule 14: Photosystem II protein Y



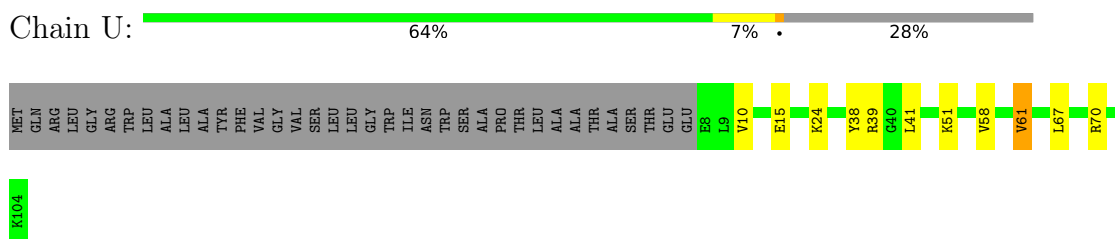
- Molecule 15: Photosystem II reaction center protein T



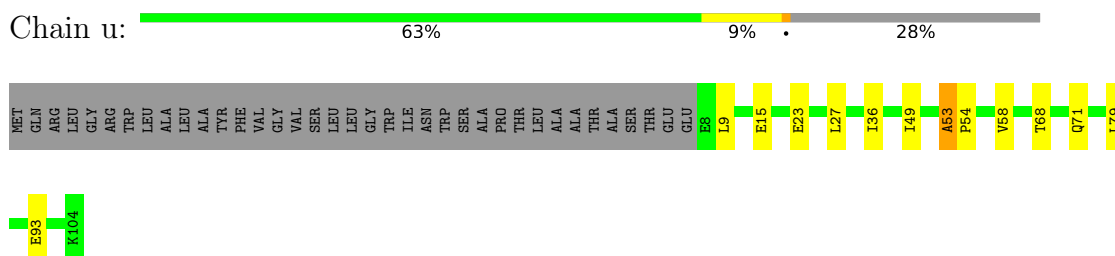
- Molecule 15: Photosystem II reaction center protein T



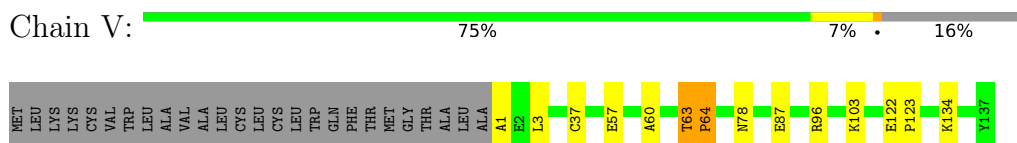
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 17: Cytochrome c-550

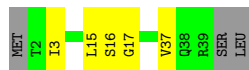
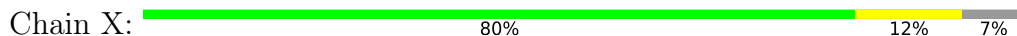


- Molecule 17: Cytochrome c-550

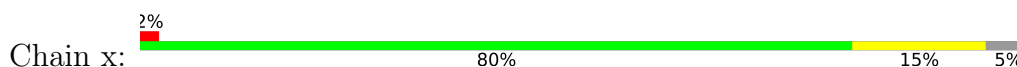




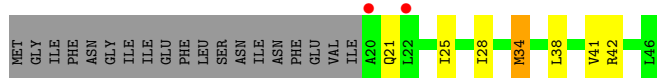
• Molecule 18: Photosystem II reaction center X protein



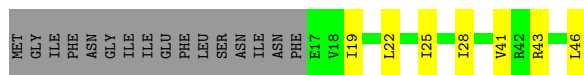
• Molecule 18: Photosystem II reaction center X protein



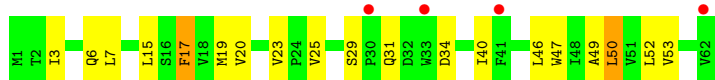
• Molecule 19: Photosystem II reaction center protein Ycf12



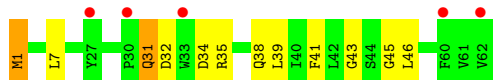
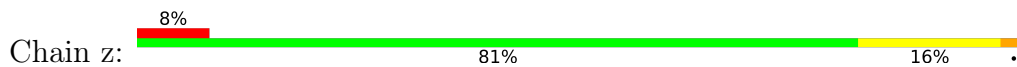
• Molecule 19: Photosystem II reaction center protein Ycf12



• Molecule 20: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.0 (33.70-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.22Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.233 0.177 , 0.234	Depositor DCC
R_{free} test set	3445 reflections (0.55%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105562	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LMG, LHG, STE, OEX, DGD, PHO, FME, FE2, SQD, CLA, CL, OEY, HEC, BCT, PL9, HEM

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	0.50	0/3227	0.60	1/4397 (0.0%)
1	a	0.49	0/3224	0.57	0/4393
2	B	0.57	0/4161	0.64	0/5669
2	b	0.53	0/4118	0.62	0/5611
3	C	0.55	0/3647	0.62	0/4965
3	c	0.51	0/3719	0.60	0/5061
4	D	0.60	0/2825	0.67	0/3847
4	d	0.55	0/2834	0.65	0/3859
5	E	0.46	0/688	0.56	0/940
5	e	0.42	0/683	0.56	0/932
6	F	0.40	0/284	0.56	0/387
6	f	0.47	0/284	0.63	0/387
7	H	0.54	0/523	0.60	0/713
7	h	0.49	0/511	0.58	0/697
8	I	0.53	0/293	0.66	0/396
8	i	0.55	0/293	0.57	0/396
9	J	0.41	0/263	0.55	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.42	0/303	0.51	0/416
10	k	0.48	0/303	0.53	0/416
11	L	0.63	0/311	0.63	0/422
11	l	0.61	0/303	0.57	0/412
12	M	0.60	0/249	0.67	0/341
12	m	0.62	0/244	0.73	0/334
13	O	0.55	0/1904	0.67	0/2585
13	o	0.56	0/1905	0.63	0/2583
14	R	0.34	0/227	0.44	0/313
14	r	0.32	0/227	0.42	0/313
15	T	0.64	0/257	0.68	0/349
15	t	0.61	0/255	0.64	0/346
16	U	0.48	0/785	0.58	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.56	0/785	0.63	0/1064
17	V	0.54	0/1085	0.65	0/1473
17	v	0.48	0/1085	0.59	0/1473
18	X	0.42	0/284	0.51	0/384
18	x	0.36	0/289	0.46	0/391
19	Y	0.43	0/197	0.47	0/264
19	y	0.36	0/219	0.48	0/294
20	Z	0.36	0/490	0.47	0/669
20	z	0.33	0/488	0.45	0/666
All	All	0.53	0/44035	0.61	1/59934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	TRP	CA-CB-CG	-5.16	103.80	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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	3113	2985	2963	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3110	2976	2954	41	0
2	B	4005	3873	3867	47	0
2	b	3978	3836	3836	33	0
3	C	3509	3432	3409	27	0
3	c	3583	3503	3492	37	0
4	D	2731	2637	2637	28	0
4	d	2737	2643	2643	32	0
5	E	666	651	651	11	0
5	e	664	648	648	12	0
6	F	275	282	282	4	0
6	f	275	282	282	7	0
7	H	510	532	532	4	0
7	h	498	518	518	11	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	3	0
9	j	257	268	268	4	0
10	K	293	305	305	6	0
10	k	293	305	305	8	0
11	L	304	316	316	6	0
11	l	296	304	304	1	0
12	M	256	269	269	8	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	19	0
13	o	1874	1846	1846	19	0
14	R	221	238	238	4	0
14	r	221	238	238	0	0
15	T	258	261	261	1	0
15	t	256	256	256	1	0
16	U	774	773	773	5	0
16	u	774	773	773	9	0
17	V	1064	1071	1073	9	0
17	v	1064	1071	1073	18	0
18	X	281	312	312	3	0
18	x	286	316	314	3	0
19	Y	196	217	217	5	0
19	y	218	241	241	3	0
20	Z	479	516	516	8	0
20	z	477	509	509	7	0
21	A	11	0	0	2	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	249	264	264	3	0
24	B	970	1067	1067	12	0
24	C	839	922	922	12	0
24	D	130	144	144	2	0
24	H	65	72	72	3	0
24	a	260	288	288	1	0
24	b	1035	1139	1139	12	0
24	c	839	919	919	17	0
24	d	130	144	144	2	0
25	A	64	74	74	3	0
25	D	64	74	74	0	0
25	a	64	74	74	1	0
25	d	64	74	74	2	0
26	A	40	56	56	0	0
26	B	120	168	168	6	0
26	C	40	56	56	3	0
26	D	40	56	56	2	0
26	K	120	168	168	3	0
26	T	40	56	56	1	0
26	X	40	56	56	1	0
26	a	40	56	56	0	0
26	b	120	168	168	2	0
26	c	80	112	112	3	0
26	d	40	56	56	1	0
26	h	40	56	56	0	0
26	k	80	112	112	1	0
26	t	40	56	56	1	0
27	A	2	0	0	0	0
27	a	2	0	0	0	0
28	A	55	80	80	5	0
28	D	55	80	80	1	0
28	a	55	80	80	1	0
28	d	55	80	80	1	0
29	A	91	135	135	4	0
29	B	54	78	77	3	0
29	D	36	46	45	1	0
29	a	90	134	133	0	0
29	b	49	65	64	0	0
29	f	41	48	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	49	74	74	0	0
30	D	145	215	215	4	0
30	L	49	74	74	3	0
30	a	49	74	74	3	0
30	d	88	125	125	0	0
30	e	42	57	57	1	0
30	l	49	74	74	2	0
31	A	66	96	96	3	0
31	C	186	246	245	2	0
31	H	62	82	82	1	0
31	c	186	246	245	2	0
31	h	62	82	81	1	0
32	B	108	178	178	6	0
32	C	40	63	63	1	0
32	I	15	26	26	1	0
32	J	12	16	16	1	0
32	L	12	16	16	0	0
32	M	43	73	73	2	0
32	R	12	16	16	0	0
32	T	31	60	60	2	0
32	X	20	35	35	2	0
32	Z	8	12	12	3	0
32	a	22	32	32	1	0
32	b	66	110	110	2	0
32	c	32	51	51	1	0
32	d	57	96	96	9	0
32	h	14	27	27	1	0
32	j	12	16	16	2	0
32	t	14	20	20	1	0
33	C	48	66	66	2	0
33	D	112	156	156	1	0
33	M	51	72	72	1	0
33	Y	48	66	66	1	0
33	a	55	86	86	1	0
33	b	55	86	86	1	0
33	c	134	181	181	2	0
33	d	44	58	57	0	0
33	m	51	72	72	3	0
34	D	4	1	1	1	0
34	a	4	1	1	0	0
35	F	43	30	30	4	0
35	f	43	30	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	30	30	0	0
36	v	43	30	30	0	0
37	A	118	0	0	6	0
37	B	141	0	0	4	0
37	C	114	0	0	1	0
37	D	100	0	0	2	0
37	E	20	0	0	4	0
37	F	3	0	0	0	0
37	H	29	0	0	1	0
37	I	7	0	0	0	0
37	J	6	0	0	0	0
37	K	6	0	0	0	0
37	L	10	0	0	0	0
37	M	5	0	0	1	0
37	O	71	0	0	3	0
37	R	1	0	0	0	0
37	T	5	0	0	0	0
37	U	33	0	0	1	0
37	V	49	0	0	2	0
37	X	7	0	0	0	0
37	Y	4	0	0	1	0
37	Z	2	0	0	0	0
37	a	117	0	0	5	0
37	b	131	0	0	7	0
37	c	118	0	0	3	0
37	d	100	0	0	5	0
37	e	10	0	0	1	0
37	f	2	0	0	0	0
37	h	19	0	0	2	0
37	i	8	0	0	0	0
37	j	11	0	0	3	0
37	k	4	0	0	1	0
37	l	10	0	0	3	0
37	m	5	0	0	1	0
37	o	65	0	0	5	0
37	r	1	0	0	0	0
37	t	5	0	0	1	0
37	u	41	0	0	4	0
37	v	36	0	0	6	0
37	x	8	0	0	0	0
37	y	1	0	0	0	0
37	z	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52802	52760	52670	526	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 5.

The worst 5 of 526 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)
11:l:7:ARG:NH1	37:l:201:HOH:O	1.85	0.96
16:u:23:GLU:O	37:u:201:HOH:O	1.84	0.94
13:o:224:ASP:OD2	37:o:301:HOH:O	1.87	0.93
1:A:25:ASP:OD1	37:A:701:HOH:O	1.89	0.89
10:k:46:ARG:O	37:k:201:HOH:O	1.90	0.89

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	397/344 (115%)	384 (97%)	12 (3%)	1 (0%)	36	38
1	a	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	488 (97%)	13 (3%)	2 (0%)	30	30
3	C	454/461 (98%)	441 (97%)	12 (3%)	1 (0%)	43	48
3	c	463/461 (100%)	453 (98%)	9 (2%)	1 (0%)	43	48
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	5
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	7	4
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	226 (93%)	12 (5%)	5 (2%)	5	2
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	30	30
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	7
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	16
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5387/5700 (94%)	5206 (97%)	164 (3%)	17 (0%)	36 38

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	V	64	PRO
3	c	416	SER
3	C	416	SER
13	O	36	GLN
13	O	59	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/280 (116%)	320 (99%)	4 (1%)	63 72
1	a	323/280 (115%)	312 (97%)	11 (3%)	32 38
2	B	408/407 (100%)	397 (97%)	11 (3%)	39 47
2	b	402/407 (99%)	392 (98%)	10 (2%)	42 50
3	C	356/362 (98%)	346 (97%)	10 (3%)	38 45
3	c	364/362 (101%)	351 (96%)	13 (4%)	31 36
4	D	277/283 (98%)	269 (97%)	8 (3%)	37 44
4	d	278/283 (98%)	267 (96%)	11 (4%)	28 32
5	E	72/73 (99%)	70 (97%)	2 (3%)	38 45
5	e	71/73 (97%)	68 (96%)	3 (4%)	26 29
6	F	28/39 (72%)	27 (96%)	1 (4%)	31 36
6	f	28/39 (72%)	25 (89%)	3 (11%)	6 3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50 59
7	h	53/55 (96%)	48 (91%)	5 (9%)	8 5
8	I	32/34 (94%)	31 (97%)	1 (3%)	35 41
8	i	32/34 (94%)	32 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	29
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	25 (83%)	5 (17%)	2	0
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	23
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23
14	R	22/33 (67%)	20 (91%)	2 (9%)	9	5
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	0
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
17	V	117/138 (85%)	115 (98%)	2 (2%)	53	63
17	v	117/138 (85%)	114 (97%)	3 (3%)	40	48
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	40
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	3
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	47 (92%)	4 (8%)	11	8
All	All	4451/4654 (96%)	4279 (96%)	172 (4%)	28	33

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	182	LEU
11	l	30	LEU
4	d	291	LEU
7	h	12	ARG
13	o	86	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
16	U	81	HIS
12	m	5	GLN
18	X	38	GLN
13	o	155	ASN
2	b	490	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.01	0
15	FME	T	1	15	8,9,10	1.11	1 (12%)	8,9,11	1.48	2 (25%)
12	FME	M	1	12	8,9,10	0.88	0	8,9,11	0.87	0
15	FME	t	1	15	8,9,10	1.26	1 (12%)	8,9,11	0.79	0
8	FME	i	1	8	8,9,10	1.14	1 (12%)	8,9,11	1.06	1 (12%)
12	FME	m	1	12	8,9,10	0.90	0	8,9,11	1.09	1 (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
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.96	1.42	1.46
8	i	1	FME	CA-N	-2.42	1.43	1.46
15	T	1	FME	CA-N	-2.03	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	3.03	127.49	122.82
15	T	1	FME	CB-CA-N	2.09	114.32	110.52
12	m	1	FME	CA-N-CN	-2.06	119.65	122.82
8	i	1	FME	CB-CA-N	2.01	114.18	110.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
12	m	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 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$
26	BCR	c	515	-	41,41,41	1.28	5 (12%)	56,56,56	1.48	10 (17%)
32	STE	t	102	-	13,13,19	0.70	0	13,13,19	1.33	2 (15%)
32	STE	B	622	-	17,17,19	0.71	0	17,17,19	0.97	1 (5%)
24	CLA	C	502	-	69,73,73	1.12	5 (7%)	82,113,113	1.24	7 (8%)
32	STE	M	104	-	17,17,19	0.37	0	16,16,19	0.86	0
33	LMG	C	515	-	48,48,55	1.21	5 (10%)	56,56,63	1.57	12 (21%)
26	BCR	T	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	4 (7%)
33	LMG	a	619	-	55,55,55	1.40	8 (14%)	63,63,63	1.49	10 (15%)
26	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.31	9 (16%)
33	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.33	6 (13%)
22	OEX	a	602[A]	3,37,1	0,15,15	-	-	-	-	-
26	BCR	d	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	4 (7%)
25	PHO	D	401	-	58,69,69	1.83	13 (22%)	55,99,99	1.50	9 (16%)
32	STE	d	409	-	16,16,19	0.67	0	16,16,19	1.30	2 (12%)
30	LHG	L	101	-	48,48,48	0.76	2 (4%)	51,54,54	1.18	3 (5%)
29	SQD	D	408	-	34,36,54	0.95	2 (5%)	42,45,65	1.75	8 (19%)
32	STE	b	621	-	19,19,19	0.79	1 (5%)	19,19,19	1.05	0
26	BCR	k	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.09	4 (7%)
24	CLA	A	605	37	69,73,73	1.39	8 (11%)	82,113,113	1.31	10 (12%)
34	BCT	a	611	23	3,3,3	1.03	0	2,3,3	3.16	1 (50%)
24	CLA	B	612	-	69,73,73	1.48	8 (11%)	82,113,113	1.51	11 (13%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
24	CLA	c	507	37	69,73,73	1.71	7 (10%)	82,113,113	1.42	9 (10%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
24	CLA	C	508	-	69,73,73	1.35	6 (8%)	82,113,113	1.29	9 (10%)
24	CLA	b	609	-	69,73,73	1.49	8 (11%)	82,113,113	1.39	7 (8%)
24	CLA	B	613	-	69,73,73	1.52	9 (13%)	82,113,113	1.29	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	510	-	69,73,73	1.26	7 (10%)	82,113,113	1.50	9 (10%)
26	BCR	B	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.38	10 (17%)
31	DGD	C	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.38	9 (11%)
30	LHG	D	409	-	48,48,48	1.19	5 (10%)	51,54,54	1.24	5 (9%)
32	STE	B	621	-	11,11,19	1.01	1 (9%)	11,11,19	1.11	0
24	CLA	b	615	-	69,73,73	1.45	11 (15%)	82,113,113	1.25	7 (8%)
24	CLA	B	602	-	69,73,73	1.23	11 (15%)	82,113,113	1.32	8 (9%)
36	HEC	v	201	17	46,50,50	1.87	6 (13%)	58,82,82	1.97	12 (20%)
30	LHG	a	614	-	48,48,48	1.09	4 (8%)	51,54,54	1.36	7 (13%)
24	CLA	B	606	37	69,73,73	1.34	9 (13%)	82,113,113	1.46	6 (7%)
33	LMG	Y	101	-	48,48,55	1.27	7 (14%)	56,56,63	1.29	5 (8%)
32	STE	d	410	-	19,19,19	0.62	0	19,19,19	1.02	1 (5%)
29	SQD	b	620	-	47,49,54	0.96	2 (4%)	57,60,65	2.50	15 (26%)
24	CLA	B	607	-	69,73,73	1.39	9 (13%)	82,113,113	1.54	11 (13%)
24	CLA	C	501	-	69,73,73	1.37	10 (14%)	82,113,113	1.31	10 (12%)
32	STE	a	618	-	11,11,19	0.92	0	11,11,19	0.98	0
32	STE	c	520	-	19,19,19	0.78	1 (5%)	19,19,19	1.00	1 (5%)
32	STE	C	521	-	11,11,19	0.84	0	11,11,19	1.02	1 (9%)
24	CLA	b	606	-	69,73,73	1.30	7 (10%)	82,113,113	1.63	12 (14%)
32	STE	C	520	-	15,15,19	0.46	0	14,14,19	0.63	0
24	CLA	C	511	3	69,73,73	1.51	11 (15%)	82,113,113	1.18	5 (6%)
24	CLA	b	613	-	69,73,73	1.26	8 (11%)	82,113,113	1.25	7 (8%)
33	LMG	c	522	-	49,49,55	0.99	4 (8%)	57,57,63	1.26	3 (5%)
26	BCR	K	103	-	41,41,41	1.29	4 (9%)	56,56,56	1.29	7 (12%)
32	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.82	0
33	LMG	d	408	-	44,44,55	1.00	3 (6%)	52,52,63	1.25	4 (7%)
33	LMG	D	407	-	51,51,55	1.00	4 (7%)	59,59,63	1.35	6 (10%)
32	STE	C	519	-	11,11,19	1.08	2 (18%)	11,11,19	0.75	0
32	STE	d	411	-	19,19,19	0.58	0	19,19,19	1.10	1 (5%)
34	BCT	D	402	23	3,3,3	1.05	0	2,3,3	2.99	1 (50%)
26	BCR	t	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.45	8 (14%)
24	CLA	C	505	-	69,73,73	1.44	10 (14%)	82,113,113	1.28	9 (10%)
29	SQD	a	615	-	52,54,54	0.96	6 (11%)	62,65,65	2.01	11 (17%)
33	LMG	D	411	-	31,31,55	1.02	3 (9%)	33,33,63	1.20	3 (9%)
32	STE	Z	101	-	7,7,19	0.50	0	6,6,19	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	a	608	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	9 (16%)
30	LHG	d	406	-	48,48,48	0.84	2 (4%)	51,54,54	1.21	4 (7%)
24	CLA	C	506	-	69,73,73	1.45	8 (11%)	82,113,113	1.36	7 (8%)
30	LHG	e	101	-	41,41,48	1.01	1 (2%)	44,47,54	1.31	6 (13%)
32	STE	R	101	-	11,11,19	0.88	0	11,11,19	1.18	1 (9%)
32	STE	c	523	-	11,11,19	0.80	0	11,11,19	1.08	1 (9%)
24	CLA	A	612	37	69,73,73	1.04	3 (4%)	82,113,113	1.40	10 (12%)
31	DGD	A	616	-	67,67,67	1.26	9 (13%)	81,81,81	1.45	14 (17%)
29	SQD	A	613	-	50,52,54	1.11	6 (12%)	60,63,65	2.02	13 (21%)
24	CLA	b	603	-	69,73,73	1.25	9 (13%)	82,113,113	1.39	6 (7%)
24	CLA	B	615	-	64,68,73	1.44	10 (15%)	76,107,113	1.52	5 (6%)
32	STE	b	624	-	19,19,19	0.64	0	19,19,19	1.05	1 (5%)
26	BCR	B	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	8 (14%)
24	CLA	B	603	-	69,73,73	1.51	9 (13%)	82,113,113	1.85	11 (13%)
24	CLA	C	509	-	69,73,73	1.30	9 (13%)	82,113,113	1.41	11 (13%)
24	CLA	B	614	-	69,73,73	1.48	10 (14%)	82,113,113	1.40	6 (7%)
28	PL9	d	405	-	55,55,55	1.50	5 (9%)	68,69,69	1.56	14 (20%)
26	BCR	B	616	-	41,41,41	1.15	3 (7%)	56,56,56	1.46	8 (14%)
32	STE	b	623	-	15,15,19	0.92	1 (6%)	15,15,19	1.02	2 (13%)
24	CLA	a	604	-	69,73,73	1.52	13 (18%)	82,113,113	1.21	6 (7%)
25	PHO	a	606	-	58,69,69	2.10	8 (13%)	55,99,99	1.39	11 (20%)
32	STE	T	103	-	14,14,19	0.42	0	13,13,19	0.83	0
26	BCR	D	405	-	41,41,41	1.25	2 (4%)	56,56,56	1.15	5 (8%)
31	DGD	H	102	-	63,63,67	1.32	7 (11%)	77,77,81	1.40	8 (10%)
26	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
32	STE	B	625	-	14,14,19	0.45	0	13,13,19	0.82	0
24	CLA	a	607	-	69,73,73	1.34	10 (14%)	82,113,113	1.18	6 (7%)
24	CLA	a	605	37	69,73,73	1.50	9 (13%)	82,113,113	1.23	6 (7%)
30	LHG	D	413	-	48,48,48	1.05	3 (6%)	51,54,54	1.34	7 (13%)
24	CLA	d	403	-	69,73,73	1.33	9 (13%)	82,113,113	1.08	5 (6%)
26	BCR	A	608	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
24	CLA	c	509	-	69,73,73	1.21	7 (10%)	82,113,113	1.46	7 (8%)
24	CLA	C	503	-	69,73,73	1.40	9 (13%)	82,113,113	1.45	10 (12%)
26	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	10 (17%)
32	STE	h	103	-	13,13,19	0.44	0	12,12,19	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	j	101	-	11,11,19	0.90	0	11,11,19	0.96	0
29	SQD	A	615	-	38,38,54	1.06	3 (7%)	40,40,65	1.42	4 (10%)
24	CLA	H	101	37	69,73,73	1.37	8 (11%)	82,113,113	1.32	6 (7%)
26	BCR	b	617	-	41,41,41	1.07	4 (9%)	56,56,56	1.27	6 (10%)
30	LHG	A	614	-	48,48,48	0.84	2 (4%)	51,54,54	1.24	6 (11%)
35	HEM	f	101	5,6	50,50,50	1.40	10 (20%)	67,82,82	1.20	6 (8%)
24	CLA	B	610	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	7 (8%)
24	CLA	b	608	-	69,73,73	1.58	12 (17%)	82,113,113	1.30	12 (14%)
24	CLA	B	609	37	69,73,73	1.54	12 (17%)	82,113,113	1.35	9 (10%)
24	CLA	c	502	-	69,73,73	1.50	9 (13%)	82,113,113	1.40	11 (13%)
24	CLA	C	504	37	63,67,73	1.53	10 (15%)	74,105,113	1.29	12 (16%)
30	LHG	d	407	-	38,38,48	0.97	2 (5%)	41,44,54	1.18	3 (7%)
35	HEM	F	101	5,6	50,50,50	1.67	7 (14%)	67,82,82	1.04	2 (2%)
32	STE	a	617	-	9,9,19	0.54	0	8,8,19	0.57	0
32	STE	B	624	-	15,15,19	0.53	0	14,14,19	0.57	0
32	STE	b	625	-	9,9,19	0.42	0	8,8,19	0.53	0
26	BCR	C	514	-	41,41,41	1.34	3 (7%)	56,56,56	1.19	3 (5%)
24	CLA	b	605	-	69,73,73	1.21	8 (11%)	82,113,113	1.40	8 (9%)
30	LHG	l	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.26	5 (9%)
31	DGD	c	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.31	7 (9%)
32	STE	M	102	-	14,14,19	0.81	0	14,14,19	0.99	0
24	CLA	b	616	-	64,68,73	1.20	9 (14%)	76,107,113	1.44	11 (14%)
24	CLA	B	604	-	69,73,73	1.44	11 (15%)	82,113,113	1.16	5 (6%)
31	DGD	c	516	-	63,63,67	1.28	7 (11%)	77,77,81	1.44	14 (18%)
26	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	4 (7%)
24	CLA	B	601	-	69,73,73	1.25	9 (13%)	82,113,113	1.33	11 (13%)
30	LHG	D	410	-	46,46,48	1.15	4 (8%)	49,52,54	1.19	2 (4%)
32	STE	J	101	-	11,11,19	0.77	0	11,11,19	1.31	2 (18%)
32	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.57	0
24	CLA	B	608	-	69,73,73	1.27	8 (11%)	82,113,113	1.41	6 (7%)
24	CLA	d	402	-	69,73,73	1.08	6 (8%)	82,113,113	1.18	6 (7%)
24	CLA	b	604	-	69,73,73	1.20	5 (7%)	82,113,113	1.84	13 (15%)
24	CLA	b	607	37	69,73,73	1.52	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	B	605	-	69,73,73	1.53	9 (13%)	82,113,113	1.25	10 (12%)
33	LMG	D	412	-	26,26,55	0.80	1 (3%)	26,26,63	1.26	1 (3%)
24	CLA	b	601	37	69,73,73	1.35	8 (11%)	82,113,113	1.50	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	d	401	-	58,69,69	2.18	11 (18%)	55,99,99	1.62	9 (16%)
31	DGD	c	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.39	12 (15%)
24	CLA	c	505	-	69,73,73	1.18	6 (8%)	82,113,113	1.59	11 (13%)
33	LMG	b	622	-	55,55,55	0.92	3 (5%)	63,63,63	1.51	11 (17%)
32	STE	B	623	-	17,17,19	0.45	0	16,16,19	0.77	0
25	PHO	A	606	-	58,69,69	1.92	9 (15%)	55,99,99	1.71	11 (20%)
26	BCR	b	618	-	41,41,41	1.39	3 (7%)	56,56,56	1.35	9 (16%)
24	CLA	c	512	-	69,73,73	1.14	8 (11%)	82,113,113	1.41	9 (10%)
22	OEX	A	602[A]	3,37,1	0,15,15	-	-	-	-	-
24	CLA	C	507	37	69,73,73	1.64	10 (14%)	82,113,113	1.54	9 (10%)
24	CLA	b	612	-	69,73,73	1.46	8 (11%)	82,113,113	1.38	13 (15%)
24	CLA	c	501	-	69,73,73	1.26	9 (13%)	82,113,113	1.32	6 (7%)
29	SQD	f	102	-	39,41,54	1.09	3 (7%)	49,52,65	1.76	10 (20%)
24	CLA	D	403	-	69,73,73	1.39	9 (13%)	82,113,113	1.33	9 (10%)
28	PL9	a	612	-	55,55,55	0.92	1 (1%)	68,69,69	1.52	11 (16%)
24	CLA	C	513	-	69,73,73	1.40	12 (17%)	82,113,113	1.49	13 (15%)
32	STE	B	619	-	16,16,19	0.76	1 (6%)	16,16,19	1.03	1 (6%)
24	CLA	b	614	-	69,73,73	1.21	8 (11%)	82,113,113	1.28	7 (8%)
32	STE	X	102	-	19,19,19	0.63	0	19,19,19	1.03	0
26	BCR	K	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.22	7 (12%)
26	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.13	4 (7%)
24	CLA	A	604	-	69,73,73	1.48	11 (15%)	82,113,113	1.42	11 (13%)
24	CLA	c	506	-	69,73,73	1.32	9 (13%)	82,113,113	1.29	7 (8%)
29	SQD	B	620	-	52,54,54	0.96	2 (3%)	62,65,65	2.16	13 (20%)
24	CLA	c	508	-	68,72,73	1.42	11 (16%)	80,111,113	1.38	9 (11%)
33	LMG	m	101	-	51,51,55	1.23	4 (7%)	59,59,63	1.57	8 (13%)
31	DGD	C	516	-	63,63,67	1.40	11 (17%)	77,77,81	1.33	12 (15%)
24	CLA	B	611	-	69,73,73	1.31	10 (14%)	82,113,113	1.53	10 (12%)
32	STE	L	102	-	11,11,19	0.77	0	11,11,19	1.36	2 (18%)
31	DGD	h	102	-	63,63,67	1.19	8 (12%)	77,77,81	1.35	9 (11%)
24	CLA	c	513	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	11 (13%)
24	CLA	c	511	3	69,73,73	1.50	10 (14%)	82,113,113	1.38	7 (8%)
24	CLA	a	613	37	69,73,73	1.45	9 (13%)	82,113,113	1.26	9 (10%)
24	CLA	b	610	37	69,73,73	1.09	6 (8%)	82,113,113	1.44	10 (12%)
24	CLA	b	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.36	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	B	626	-	11,11,19	0.74	0	11,11,19	0.99	0
24	CLA	c	504	37	64,68,73	1.24	5 (7%)	76,107,113	1.36	13 (17%)
24	CLA	b	602	-	69,73,73	1.18	9 (13%)	82,113,113	1.39	10 (12%)
24	CLA	A	607	-	58,62,73	1.35	11 (18%)	68,99,113	1.41	9 (13%)
26	BCR	X	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	7 (12%)
29	SQD	a	616	-	35,35,54	1.07	2 (5%)	37,37,65	1.18	3 (8%)
36	HEC	V	201	17	46,50,50	1.75	6 (13%)	58,82,82	1.83	6 (10%)
24	CLA	C	510	-	69,73,73	1.30	10 (14%)	82,113,113	1.27	5 (6%)
31	DGD	C	518	-	63,63,67	1.18	8 (12%)	77,77,81	1.39	8 (10%)
24	CLA	D	404	-	69,73,73	1.40	10 (14%)	82,113,113	1.28	10 (12%)
28	PL9	A	611	-	55,55,55	1.22	5 (9%)	68,69,69	1.70	15 (22%)
32	STE	I	101	-	14,14,19	0.53	0	13,13,19	0.61	0
33	LMG	M	101	-	51,51,55	1.03	5 (9%)	59,59,63	1.40	9 (15%)
28	PL9	D	406	-	55,55,55	1.27	5 (9%)	68,69,69	1.83	17 (25%)
24	CLA	c	503	-	69,73,73	1.18	5 (7%)	82,113,113	1.16	4 (4%)
33	LMG	c	521	-	48,48,55	1.20	5 (10%)	56,56,63	1.30	5 (8%)
24	CLA	C	512	-	69,73,73	1.57	9 (13%)	82,113,113	1.36	11 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	STE	t	102	-	-	2/11/11/17	-
32	STE	B	622	-	-	8/15/15/17	-
24	CLA	C	502	-	1/1/20/20	5/39/115/115	-
32	STE	M	104	-	-	10/15/15/17	-
33	LMG	C	515	-	-	16/43/63/70	0/1/1/1
26	BCR	T	101	-	-	11/29/63/63	0/2/2/2
33	LMG	a	619	-	-	36/50/70/70	0/1/1/1
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
33	LMG	c	519	-	-	9/31/51/70	0/1/1/1
26	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	d	409	-	-	12/14/14/17	-
30	LHG	L	101	-	-	19/53/53/53	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
32	STE	b	621	-	-	9/17/17/17	-
26	BCR	k	101	-	-	11/29/63/63	0/2/2/2
24	CLA	A	605	37	1/1/20/20	11/39/115/115	-
24	CLA	B	612	-	1/1/20/20	10/39/115/115	-
24	CLA	c	507	37	1/1/20/20	11/39/115/115	-
24	CLA	B	613	-	1/1/20/20	15/39/115/115	-
24	CLA	C	508	-	-	5/39/115/115	-
24	CLA	b	609	-	-	8/39/115/115	-
24	CLA	c	510	-	1/1/20/20	11/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
31	DGD	C	517	-	-	18/51/91/95	0/2/2/2
30	LHG	D	409	-	-	21/53/53/53	-
32	STE	B	621	-	-	6/9/9/17	-
24	CLA	b	615	-	1/1/20/20	4/39/115/115	-
24	CLA	B	602	-	1/1/20/20	12/39/115/115	-
36	HEC	v	201	17	-	6/14/54/54	-
30	LHG	a	614	-	-	24/53/53/53	-
24	CLA	B	606	37	1/1/20/20	13/39/115/115	-
33	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
32	STE	d	410	-	-	11/17/17/17	-
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
24	CLA	B	607	-	1/1/20/20	5/39/115/115	-
24	CLA	C	501	-	1/1/20/20	4/39/115/115	-
32	STE	a	618	-	-	4/9/9/17	-
32	STE	c	520	-	-	7/17/17/17	-
32	STE	C	521	-	-	2/9/9/17	-
24	CLA	b	606	-	1/1/20/20	4/39/115/115	-
32	STE	C	520	-	-	7/13/13/17	-
24	CLA	C	511	3	1/1/20/20	9/39/115/115	-
24	CLA	b	613	-	1/1/20/20	4/39/115/115	-
33	LMG	c	522	-	-	27/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	K	103	-	-	6/29/63/63	0/2/2/2
32	STE	T	102	-	-	9/13/13/17	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
33	LMG	D	407	-	-	14/46/66/70	0/1/1/1
32	STE	C	519	-	-	4/9/9/17	-
32	STE	d	411	-	-	11/17/17/17	-
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/20/20	11/39/115/115	-
29	SQD	a	615	-	-	25/49/69/69	0/1/1/1
33	LMG	D	411	-	-	14/33/33/70	-
32	STE	Z	101	-	-	2/5/5/17	-
26	BCR	a	608	-	-	5/29/63/63	0/2/2/2
30	LHG	d	406	-	-	26/53/53/53	-
24	CLA	C	506	-	1/1/20/20	13/39/115/115	-
30	LHG	e	101	-	-	21/46/46/53	-
32	STE	R	101	-	-	4/9/9/17	-
32	STE	c	523	-	-	7/9/9/17	-
24	CLA	A	612	37	1/1/20/20	4/39/115/115	-
31	DGD	A	616	-	-	29/55/95/95	0/2/2/2
29	SQD	A	613	-	-	22/47/67/69	0/1/1/1
24	CLA	b	603	-	1/1/20/20	4/39/115/115	-
24	CLA	B	615	-	1/1/19/20	7/33/109/115	-
32	STE	b	624	-	-	11/17/17/17	-
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/20/20	11/39/115/115	-
24	CLA	C	509	-	1/1/20/20	13/39/115/115	-
24	CLA	B	614	-	1/1/20/20	8/39/115/115	-
28	PL9	d	405	-	-	13/53/73/73	0/1/1/1
26	BCR	B	616	-	-	7/29/63/63	0/2/2/2
32	STE	b	623	-	-	8/13/13/17	-
24	CLA	a	604	-	1/1/20/20	4/39/115/115	-
25	PHO	a	606	-	-	2/37/103/103	0/5/6/6
32	STE	T	103	-	-	8/12/12/17	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	102	-	-	16/51/91/95	0/2/2/2
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
32	STE	B	625	-	-	8/12/12/17	-
24	CLA	a	607	-	1/1/20/20	10/39/115/115	-
24	CLA	a	605	37	-	7/39/115/115	-
30	LHG	D	413	-	-	15/53/53/53	-
24	CLA	d	403	-	1/1/20/20	9/39/115/115	-
26	BCR	A	608	-	-	6/29/63/63	0/2/2/2
24	CLA	c	509	-	1/1/20/20	13/39/115/115	-
24	CLA	C	503	-	1/1/20/20	6/39/115/115	-
26	BCR	h	101	-	-	5/29/63/63	0/2/2/2
32	STE	h	103	-	-	6/11/11/17	-
32	STE	j	101	-	-	5/9/9/17	-
29	SQD	A	615	-	-	17/39/39/69	-
24	CLA	H	101	37	1/1/20/20	18/39/115/115	-
26	BCR	b	617	-	-	5/29/63/63	0/2/2/2
30	LHG	A	614	-	-	30/53/53/53	-
35	HEM	f	101	5,6	-	4/14/54/54	-
24	CLA	B	610	-	1/1/20/20	6/39/115/115	-
24	CLA	b	608	-	1/1/20/20	6/39/115/115	-
24	CLA	B	609	37	1/1/20/20	6/39/115/115	-
24	CLA	c	502	-	1/1/20/20	9/39/115/115	-
24	CLA	C	504	37	1/1/18/20	8/32/108/115	-
30	LHG	d	407	-	-	16/43/43/53	-
35	HEM	F	101	5,6	-	4/14/54/54	-
32	STE	a	617	-	-	4/7/7/17	-
32	STE	B	624	-	-	11/13/13/17	-
32	STE	b	625	-	-	5/7/7/17	-
26	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/20/20	7/39/115/115	-
30	LHG	l	101	-	-	14/53/53/53	-
31	DGD	c	517	-	-	17/51/91/95	0/2/2/2
32	STE	M	102	-	-	6/12/12/17	-
24	CLA	b	616	-	1/1/19/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	604	-	1/1/20/20	14/39/115/115	-
31	DGD	c	516	-	-	21/51/91/95	0/2/2/2
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
24	CLA	B	601	-	1/1/20/20	8/39/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
32	STE	J	101	-	-	2/9/9/17	-
32	STE	M	103	-	-	2/7/7/17	-
24	CLA	B	608	-	-	1/39/115/115	-
24	CLA	d	402	-	-	8/39/115/115	-
24	CLA	b	604	-	1/1/20/20	10/39/115/115	-
24	CLA	b	607	37	1/1/20/20	13/39/115/115	-
24	CLA	B	605	-	1/1/20/20	13/39/115/115	-
33	LMG	D	412	-	-	9/22/22/70	-
24	CLA	b	601	37	1/1/20/20	20/39/115/115	-
25	PHO	d	401	-	-	9/37/103/103	0/5/6/6
31	DGD	c	518	-	-	14/51/91/95	0/2/2/2
24	CLA	c	505	-	1/1/20/20	11/39/115/115	-
33	LMG	b	622	-	-	25/50/70/70	0/1/1/1
32	STE	B	623	-	-	9/15/15/17	-
25	PHO	A	606	-	-	1/37/103/103	0/5/6/6
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	512	-	1/1/20/20	17/39/115/115	-
24	CLA	C	507	37	1/1/20/20	7/39/115/115	-
24	CLA	b	612	-	1/1/20/20	5/39/115/115	-
24	CLA	c	501	-	1/1/20/20	3/39/115/115	-
29	SQD	f	102	-	-	17/36/56/69	0/1/1/1
24	CLA	D	403	-	-	12/39/115/115	-
28	PL9	a	612	-	-	20/53/73/73	0/1/1/1
24	CLA	C	513	-	1/1/20/20	10/39/115/115	-
32	STE	B	619	-	-	9/14/14/17	-
24	CLA	b	614	-	1/1/20/20	12/39/115/115	-
32	STE	X	102	-	-	14/17/17/17	-
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
26	BCR	k	102	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	604	-	1/1/20/20	9/39/115/115	-
24	CLA	c	506	-	1/1/20/20	15/39/115/115	-
29	SQD	B	620	-	-	23/49/69/69	0/1/1/1
24	CLA	c	508	-	1/1/19/20	7/38/114/115	-
33	LMG	m	101	-	-	22/46/66/70	0/1/1/1
31	DGD	C	516	-	-	22/51/91/95	0/2/2/2
24	CLA	B	611	-	1/1/20/20	11/39/115/115	-
32	STE	L	102	-	-	3/9/9/17	-
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	c	513	-	1/1/20/20	7/39/115/115	-
24	CLA	c	511	3	1/1/20/20	6/39/115/115	-
24	CLA	a	613	37	1/1/20/20	2/39/115/115	-
24	CLA	b	610	37	1/1/20/20	10/39/115/115	-
24	CLA	b	611	-	1/1/20/20	4/39/115/115	-
32	STE	B	626	-	-	4/9/9/17	-
24	CLA	c	504	37	1/1/19/20	9/33/109/115	-
24	CLA	b	602	-	-	8/39/115/115	-
24	CLA	A	607	-	1/1/17/20	2/26/102/115	-
26	BCR	X	101	-	-	5/29/63/63	0/2/2/2
29	SQD	a	616	-	-	18/37/37/69	-
36	HEC	V	201	17	-	6/14/54/54	-
24	CLA	C	510	-	1/1/20/20	5/39/115/115	-
31	DGD	C	518	-	-	18/51/91/95	0/2/2/2
24	CLA	D	404	-	1/1/20/20	11/39/115/115	-
28	PL9	A	611	-	-	22/53/73/73	0/1/1/1
32	STE	I	101	-	-	7/12/12/17	-
33	LMG	M	101	-	-	24/46/66/70	0/1/1/1
28	PL9	D	406	-	-	11/53/73/73	0/1/1/1
24	CLA	c	503	-	1/1/20/20	6/39/115/115	-
33	LMG	c	521	-	-	26/43/63/70	0/1/1/1
24	CLA	C	512	-	1/1/20/20	11/39/115/115	-

The worst 5 of 939 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	606	PHO	C1B-C2B	10.15	1.50	1.39
25	d	401	PHO	C1B-C2B	9.46	1.49	1.39
25	d	401	PHO	C3B-C4B	8.85	1.50	1.41
24	c	507	CLA	MG-NB	-8.83	1.88	2.05
25	A	606	PHO	C1B-C2B	8.50	1.48	1.39

The worst 5 of 1202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O6-C1-C2	12.20	126.80	108.27
24	B	603	CLA	C4A-NA-C1A	11.81	112.07	106.68
24	b	604	CLA	C4A-NA-C1A	11.14	111.76	106.68
29	B	620	SQD	O6-C1-C2	9.38	122.52	108.27
24	b	606	CLA	C4A-NA-C1A	9.31	110.93	106.68

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	607	CLA	ND
24	A	612	CLA	ND
24	B	601	CLA	ND

5 of 1874 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	613	CLA	CAD-CBD-CGD-O1D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C11-C10-C8-C9
24	C	507	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

121 monomers are involved in 163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	515	BCR	3	0
32	t	102	STE	1	0
24	C	502	CLA	1	0
32	M	104	STE	2	0
33	C	515	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T	101	BCR	1	0
33	a	619	LMG	1	0
26	d	404	BCR	1	0
32	d	409	STE	2	0
30	L	101	LHG	3	0
29	D	408	SQD	1	0
32	b	621	STE	1	0
26	k	101	BCR	1	0
24	B	612	CLA	1	0
21	a	601[B]	OEY	1	0
24	c	507	CLA	1	0
21	A	601[B]	OEY	2	0
24	C	508	CLA	1	0
24	b	609	CLA	1	0
24	B	613	CLA	1	0
24	c	510	CLA	1	0
26	B	618	BCR	2	0
30	D	409	LHG	1	0
24	b	615	CLA	2	0
30	a	614	LHG	3	0
24	B	606	CLA	1	0
33	Y	101	LMG	1	0
32	d	410	STE	5	0
32	c	520	STE	1	0
24	b	606	CLA	2	0
32	C	520	STE	1	0
24	C	511	CLA	1	0
24	b	613	CLA	1	0
33	c	522	LMG	1	0
32	T	102	STE	1	0
33	D	407	LMG	1	0
32	d	411	STE	2	0
34	D	402	BCT	1	0
26	t	101	BCR	1	0
24	C	505	CLA	2	0
32	Z	101	STE	3	0
24	C	506	CLA	2	0
30	e	101	LHG	1	0
24	A	612	CLA	2	0
31	A	616	DGD	3	0
29	A	613	SQD	2	0
26	B	617	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	603	CLA	2	0
28	d	405	PL9	1	0
26	B	616	BCR	1	0
32	b	623	STE	1	0
25	a	606	PHO	1	0
32	T	103	STE	2	0
26	D	405	BCR	2	0
31	H	102	DGD	1	0
32	B	625	STE	2	0
30	D	413	LHG	1	0
24	d	403	CLA	1	0
24	c	509	CLA	1	0
24	C	503	CLA	1	0
32	h	103	STE	1	0
32	j	101	STE	2	0
29	A	615	SQD	2	0
24	H	101	CLA	3	0
26	b	617	BCR	1	0
35	f	101	HEM	3	0
24	B	610	CLA	2	0
24	c	502	CLA	1	0
35	F	101	HEM	4	0
32	a	617	STE	1	0
26	C	514	BCR	3	0
24	b	605	CLA	2	0
30	l	101	LHG	2	0
24	b	616	CLA	1	0
24	B	604	CLA	1	0
31	c	516	DGD	1	0
26	K	102	BCR	2	0
24	B	601	CLA	2	0
30	D	410	LHG	2	0
32	J	101	STE	1	0
24	B	608	CLA	1	0
24	d	402	CLA	1	0
24	b	604	CLA	3	0
24	B	605	CLA	3	0
24	b	601	CLA	1	0
25	d	401	PHO	2	0
31	c	518	DGD	1	0
33	b	622	LMG	1	0
32	B	623	STE	2	0

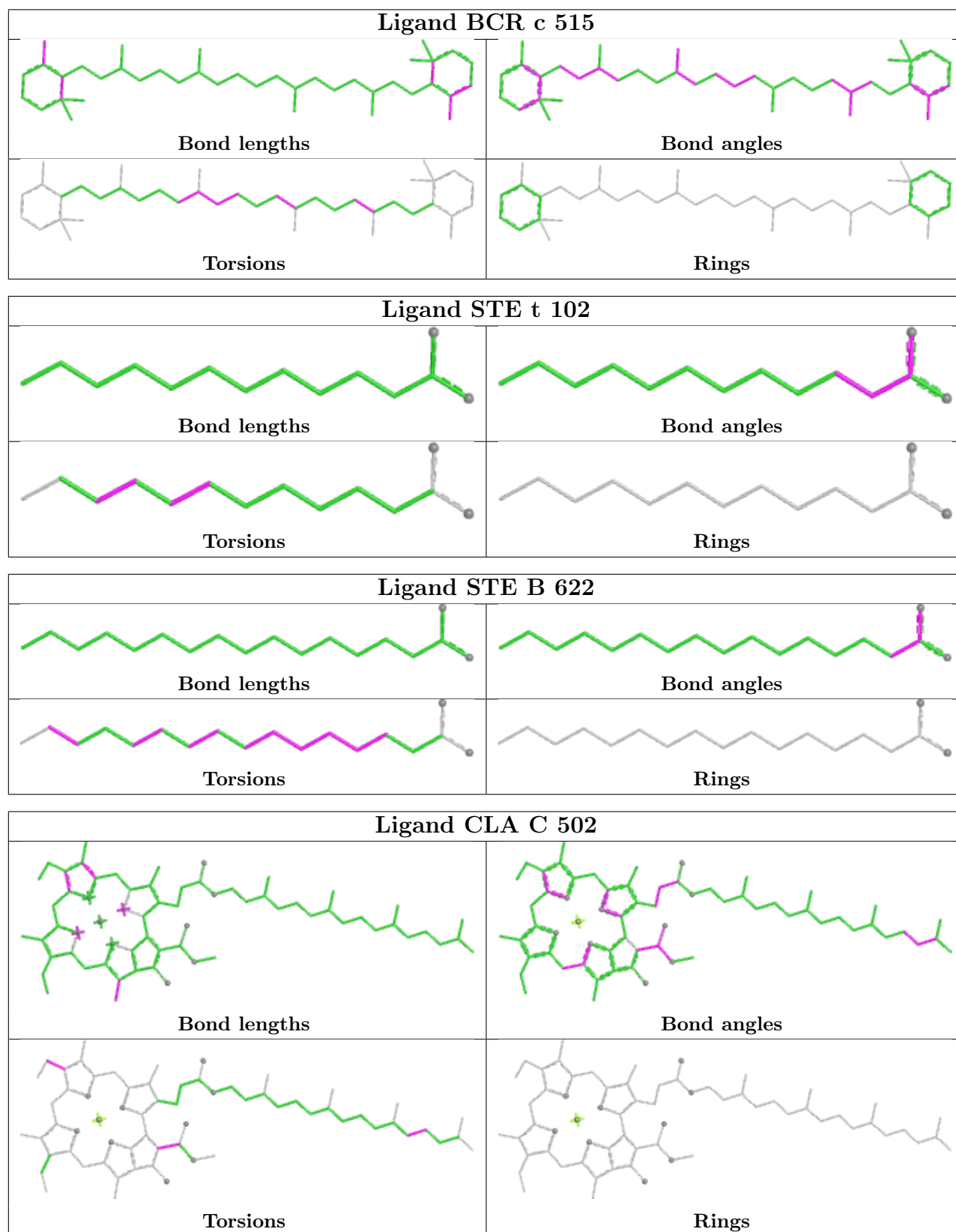
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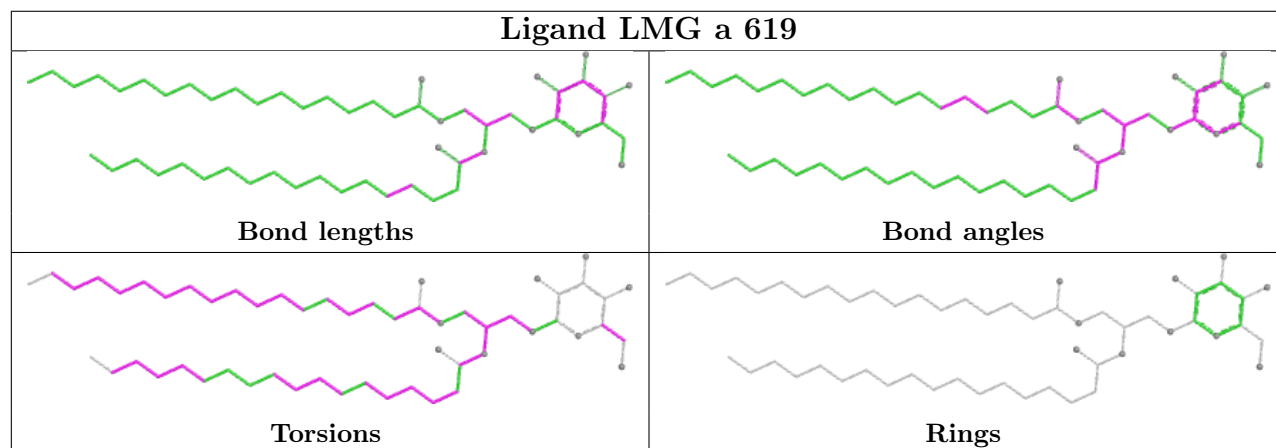
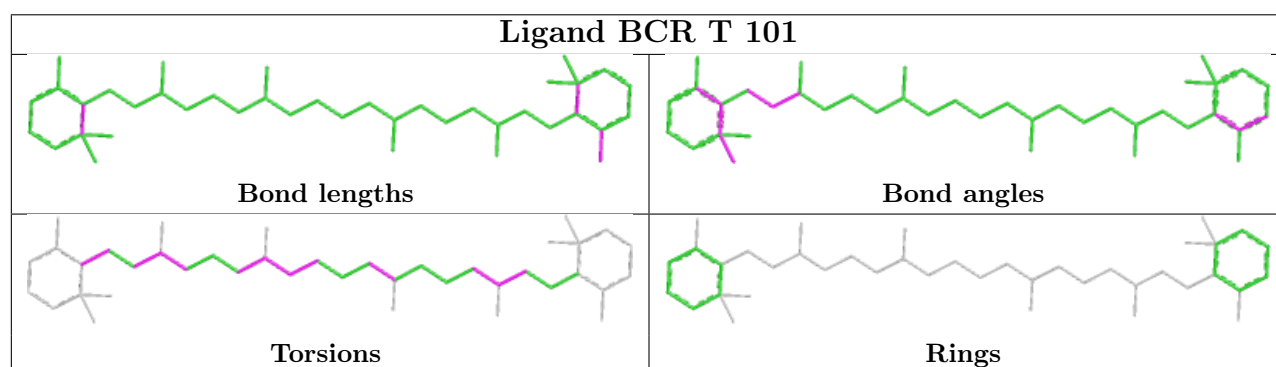
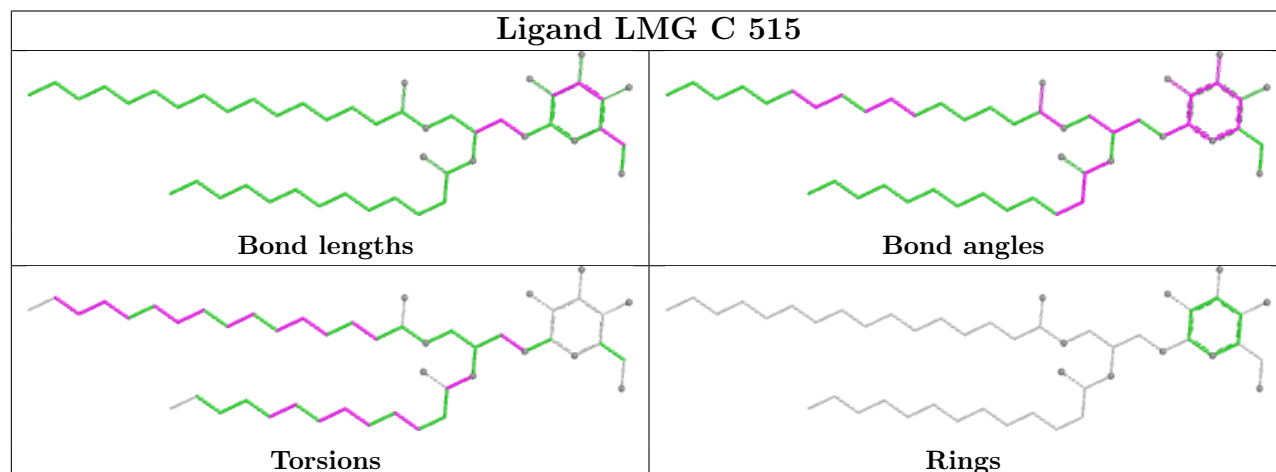
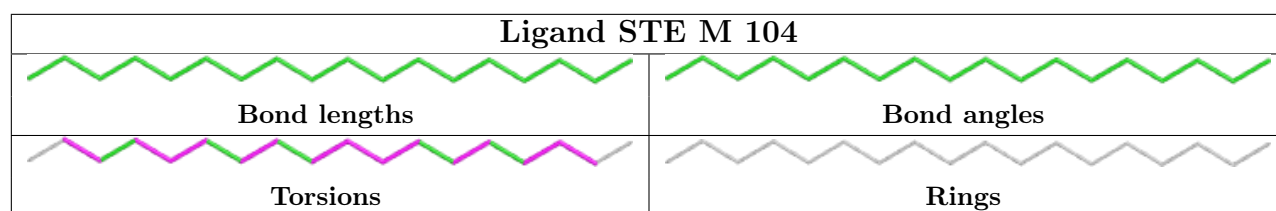
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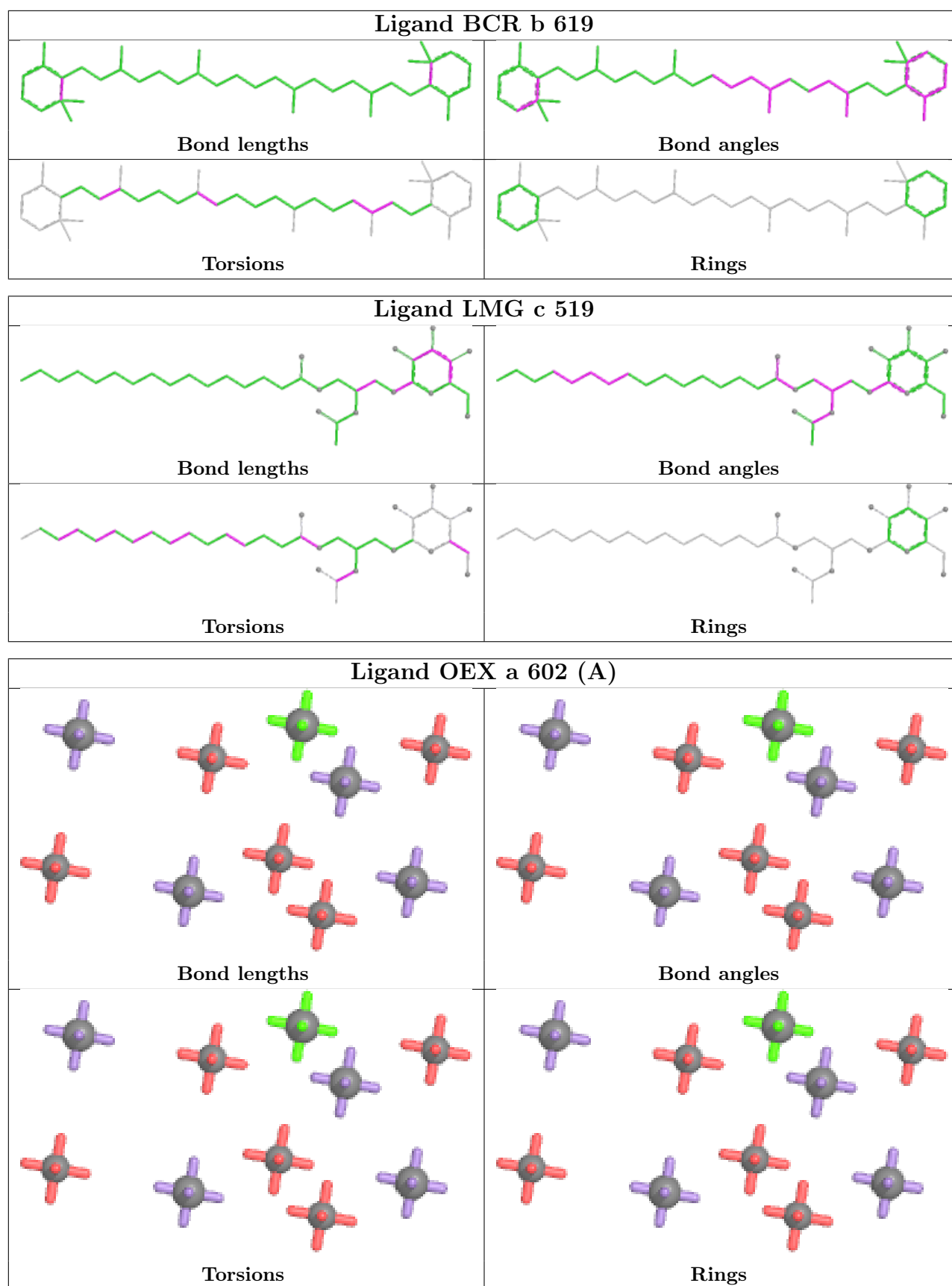
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	606	PHO	3	0
26	b	618	BCR	1	0
24	C	507	CLA	1	0
24	b	612	CLA	1	0
24	c	501	CLA	3	0
29	f	102	SQD	1	0
24	D	403	CLA	2	0
28	a	612	PL9	1	0
24	C	513	CLA	3	0
32	B	619	STE	1	0
32	X	102	STE	2	0
26	K	101	BCR	1	0
24	A	604	CLA	1	0
29	B	620	SQD	3	0
24	c	508	CLA	2	0
33	m	101	LMG	3	0
31	C	516	DGD	1	0
31	h	102	DGD	1	0
24	c	513	CLA	4	0
24	c	511	CLA	5	0
24	a	613	CLA	1	0
24	b	610	CLA	1	0
32	B	626	STE	1	0
24	b	602	CLA	2	0
26	X	101	BCR	1	0
31	C	518	DGD	1	0
28	A	611	PL9	5	0
32	I	101	STE	1	0
33	M	101	LMG	1	0
28	D	406	PL9	1	0
24	c	503	CLA	1	0
33	c	521	LMG	1	0

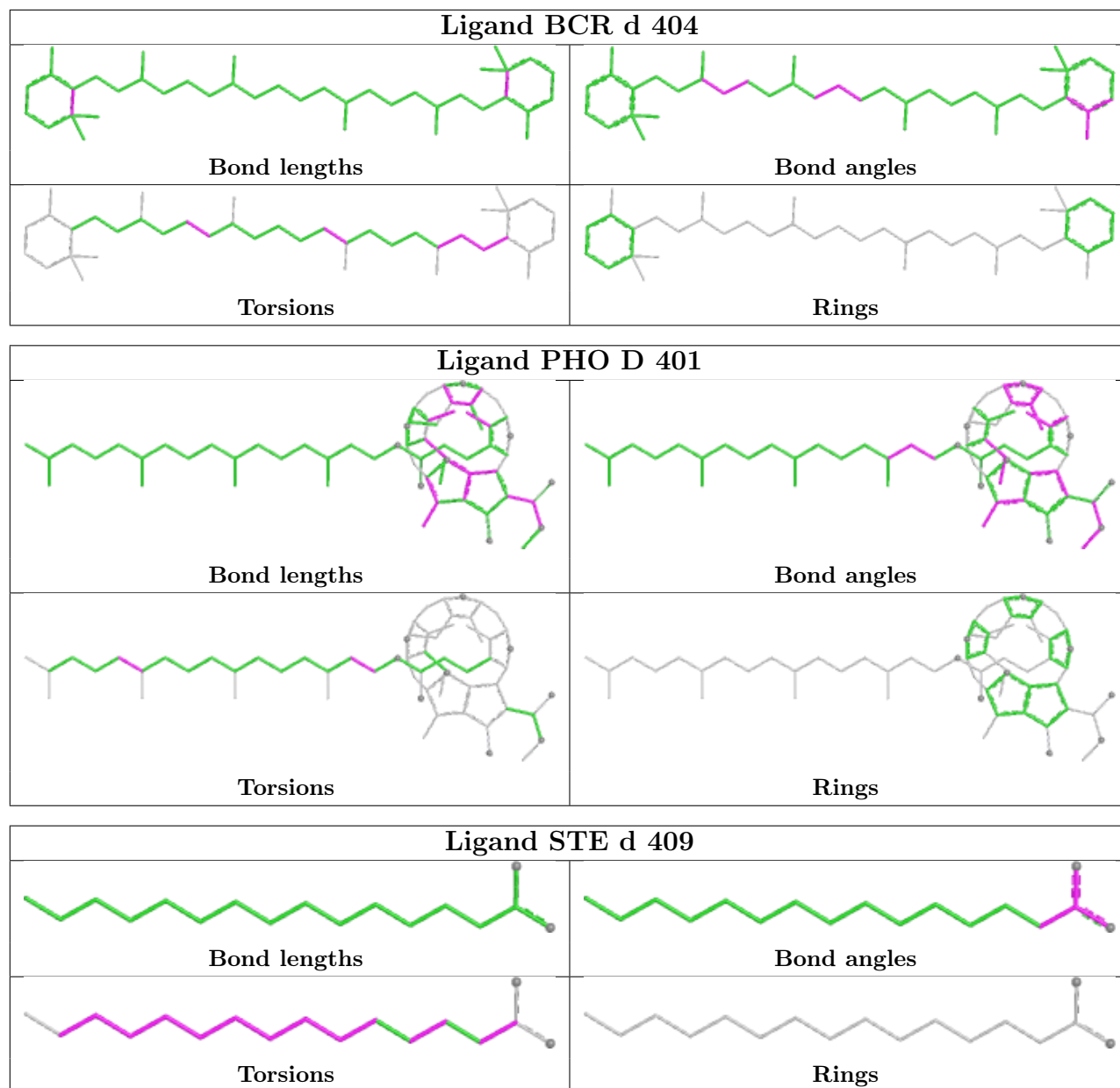
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

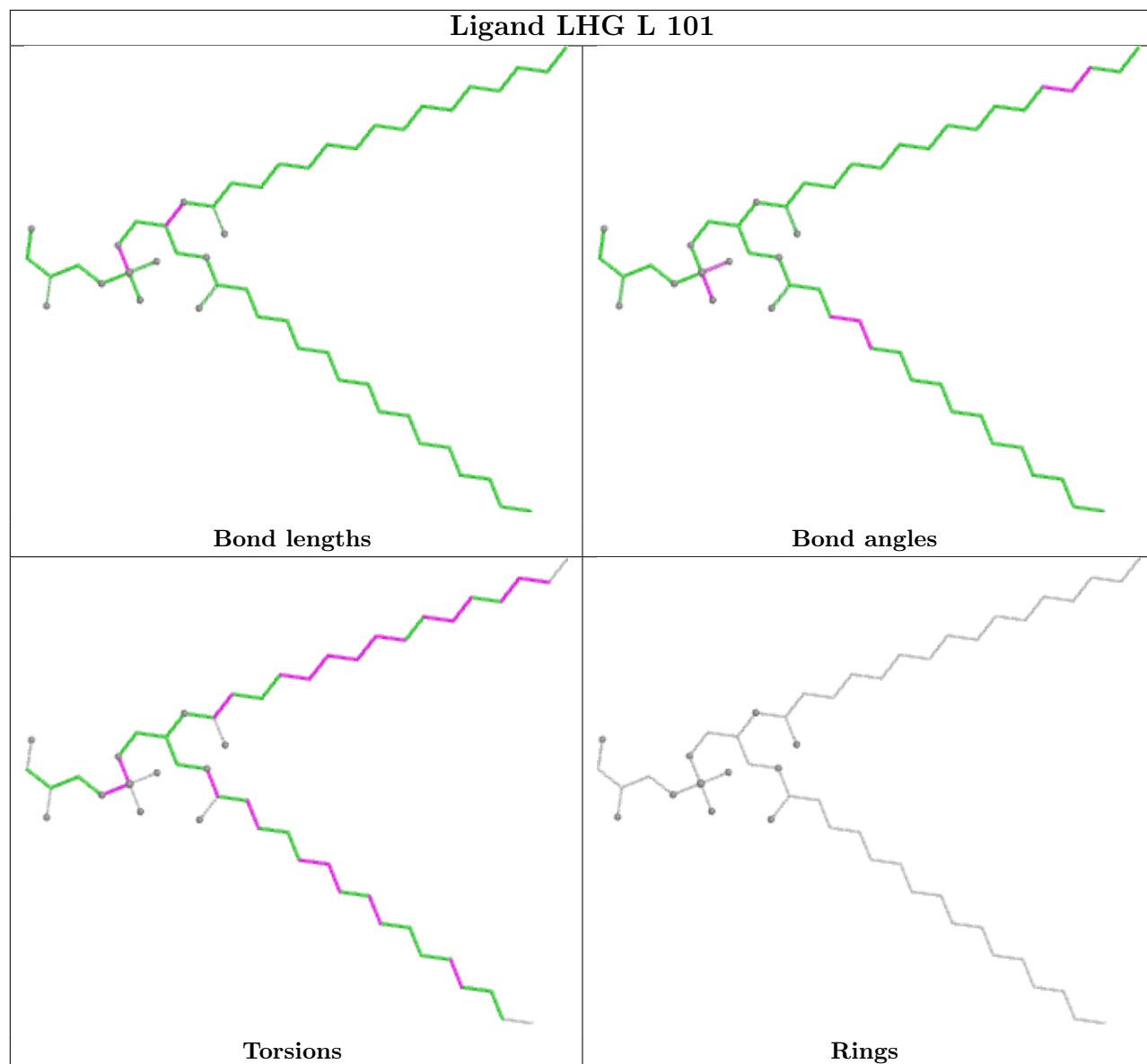
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

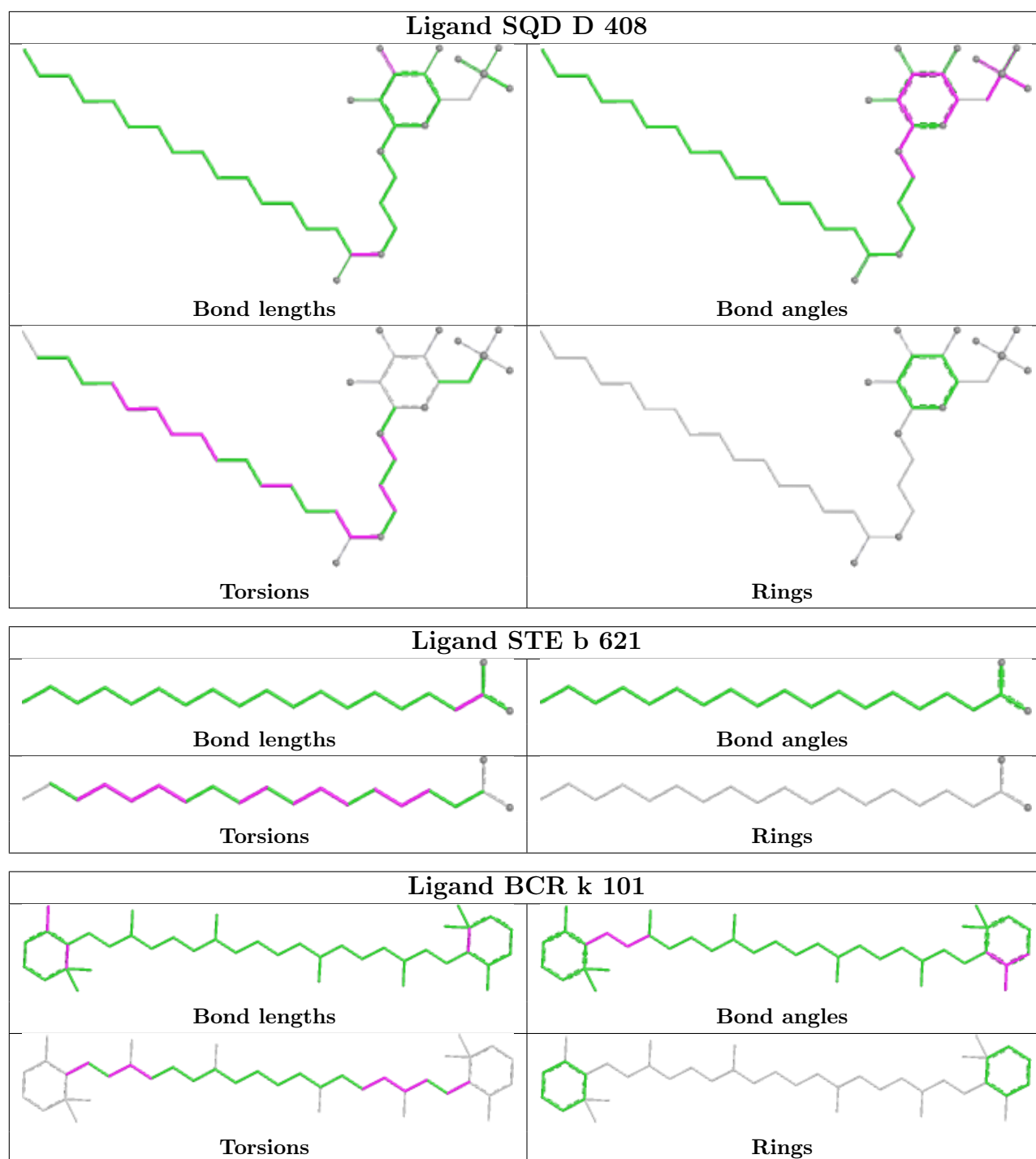


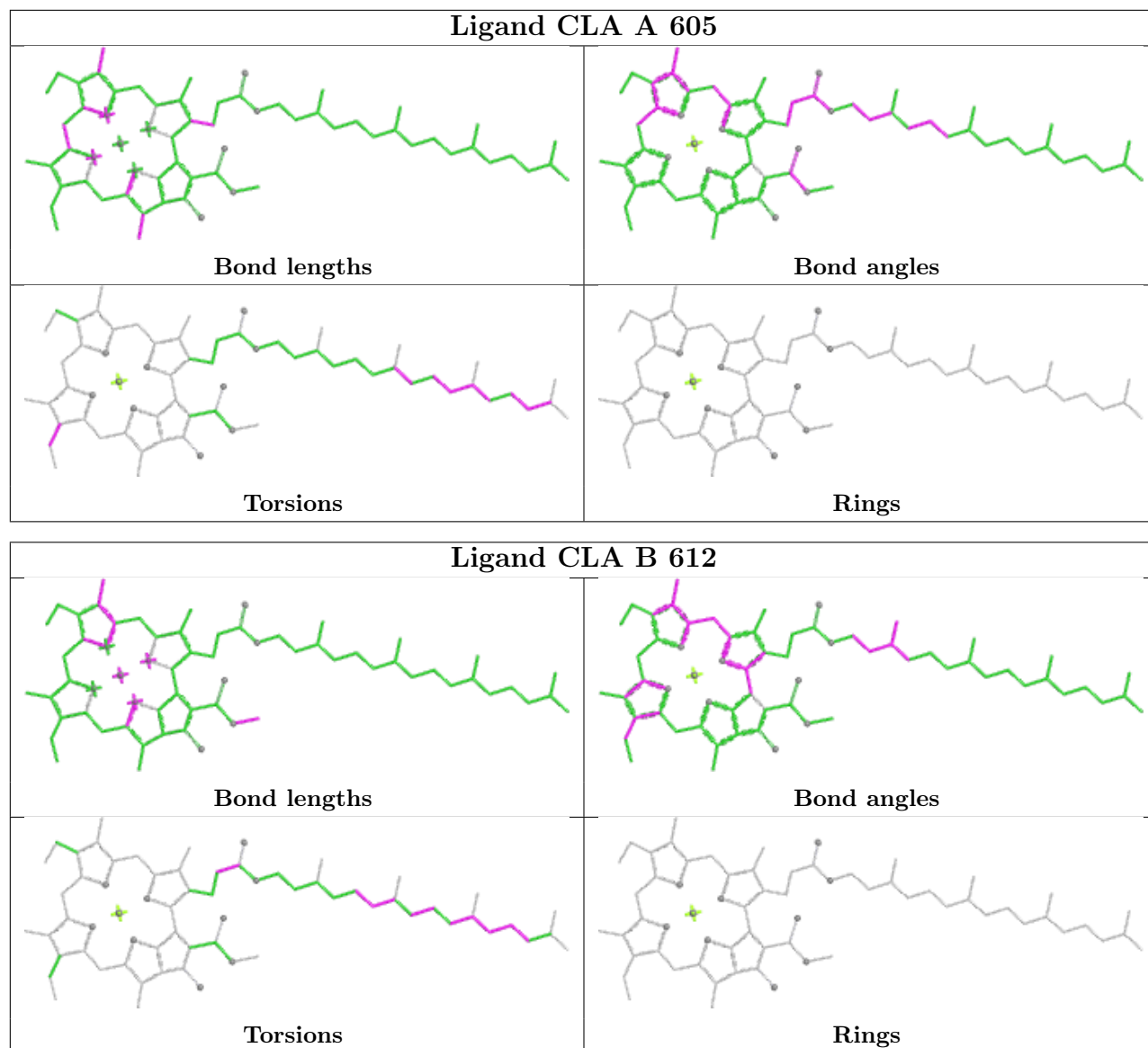


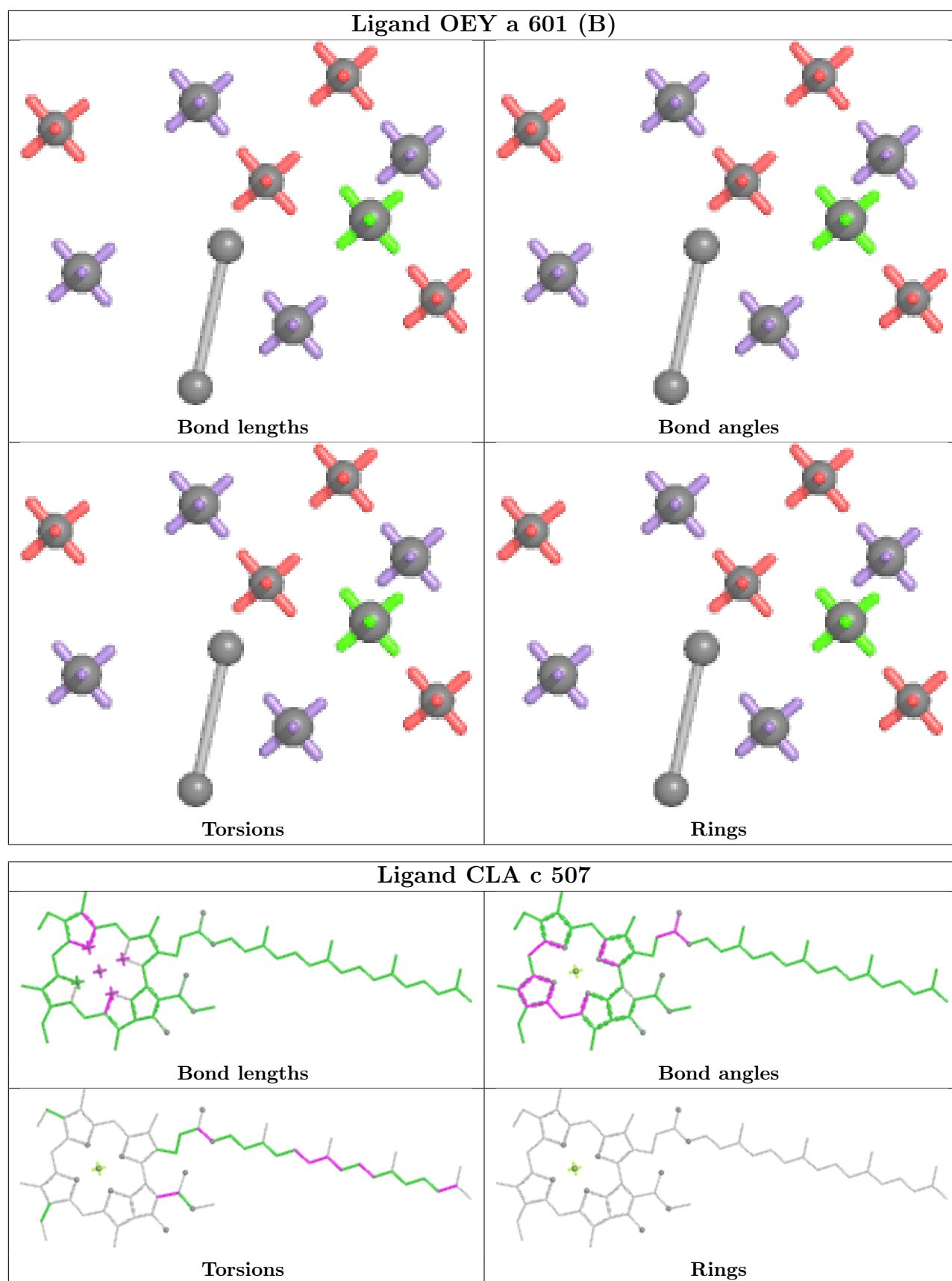


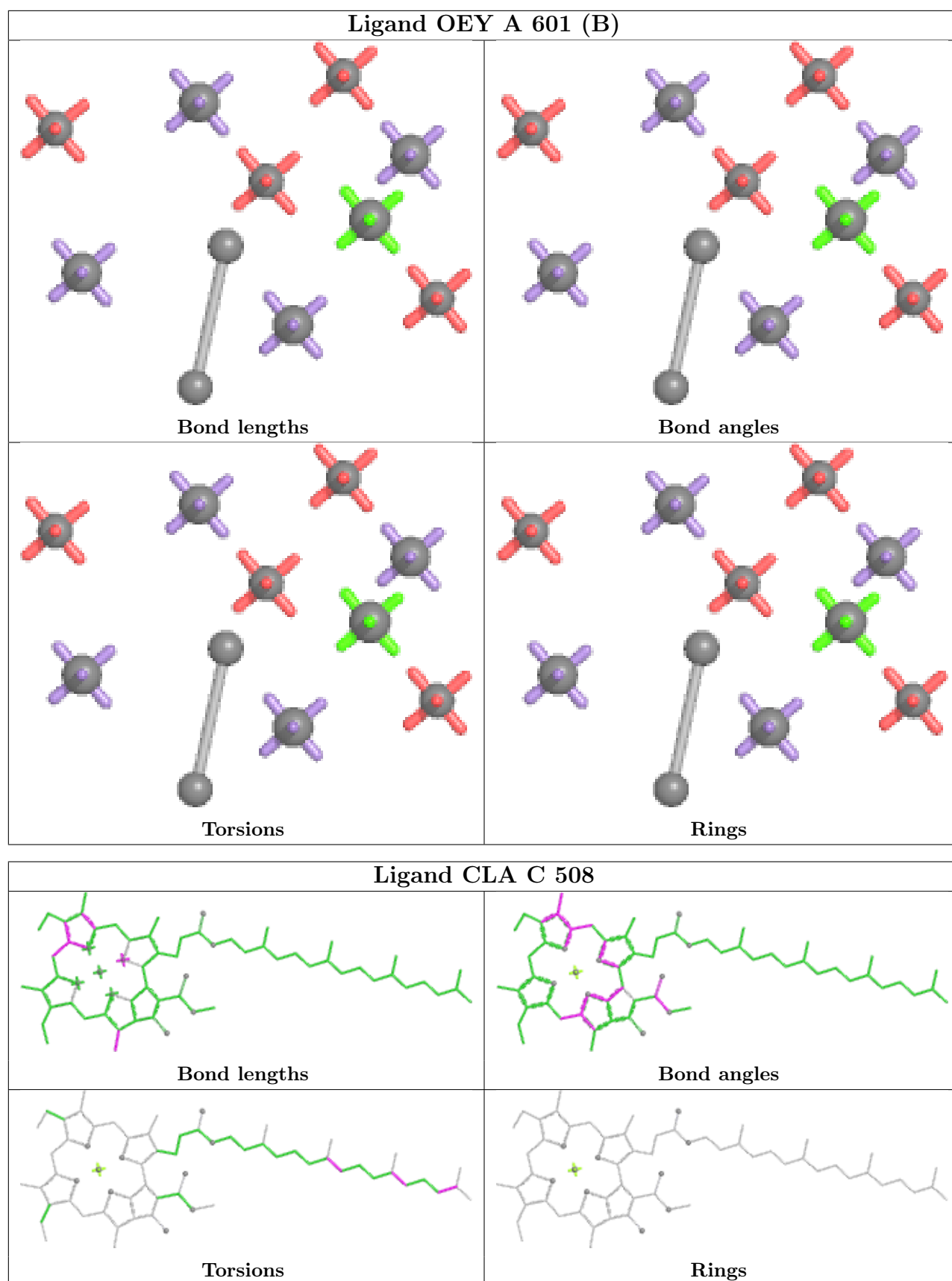


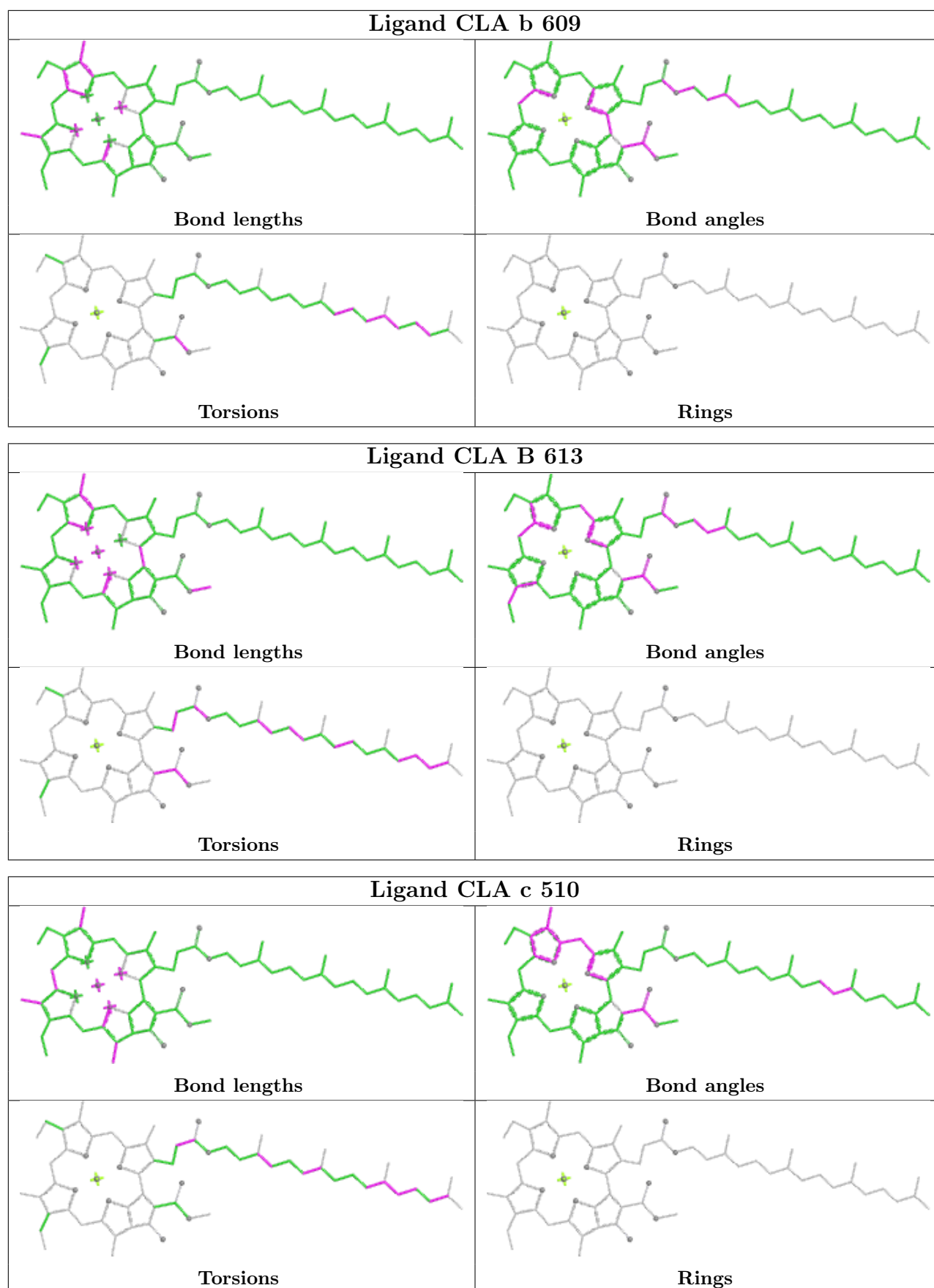


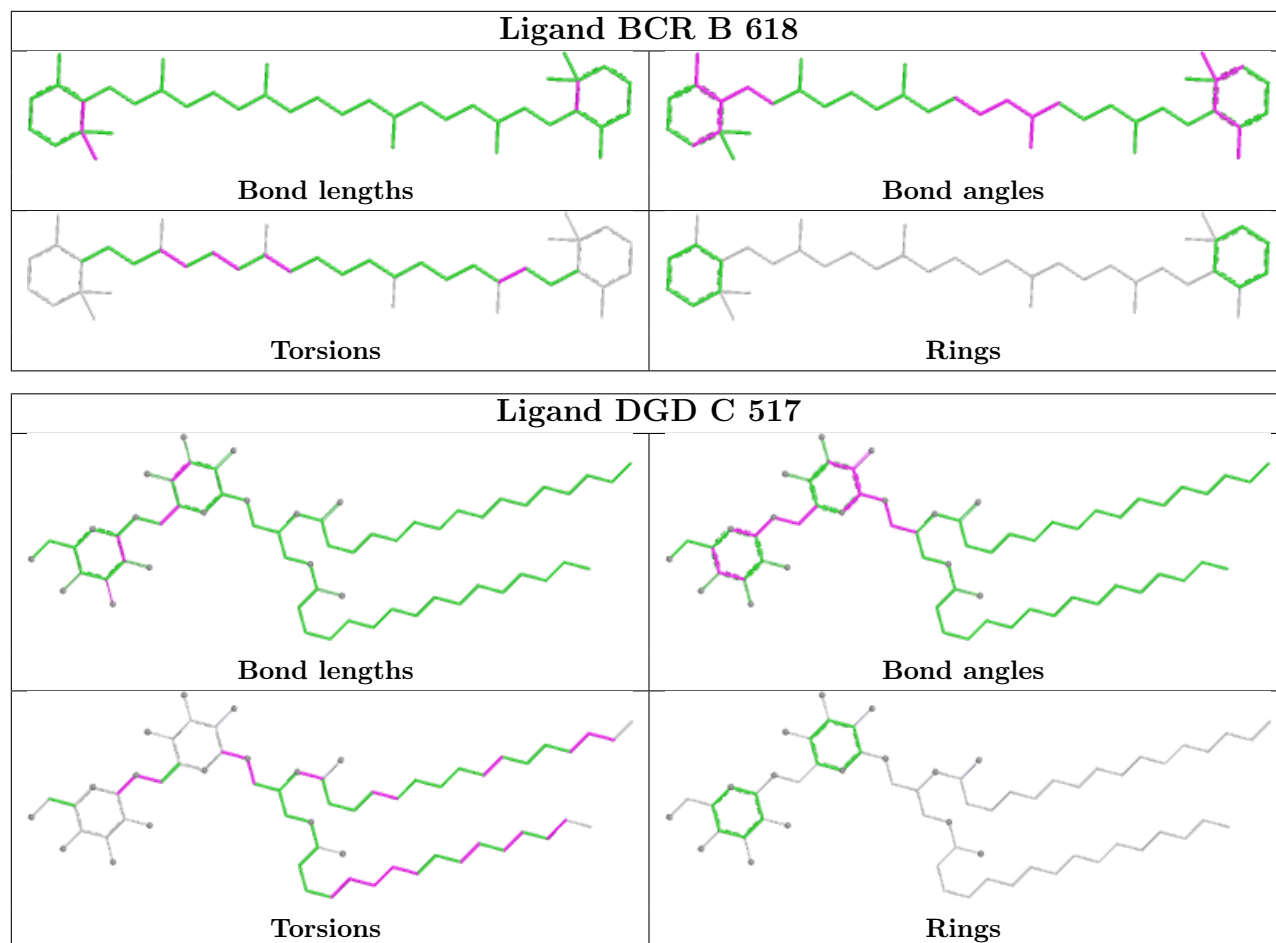


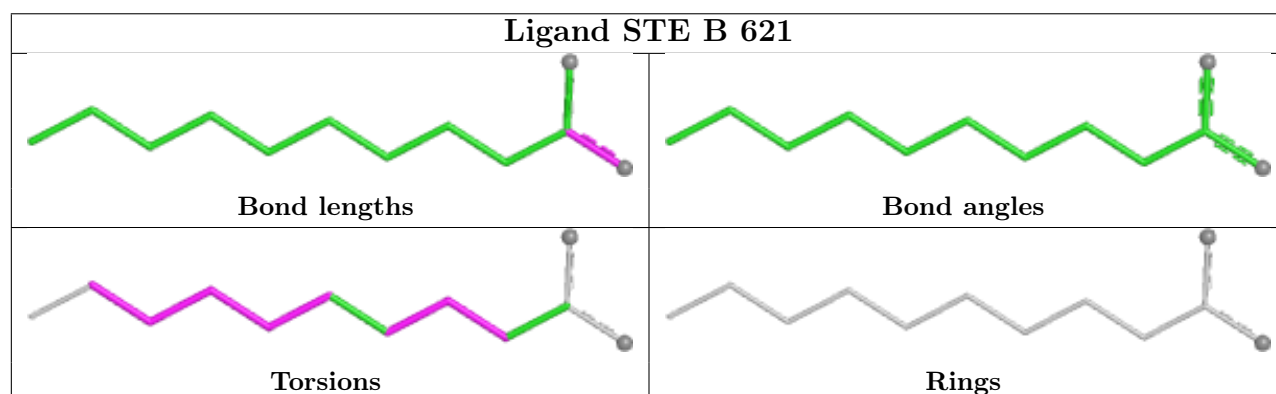
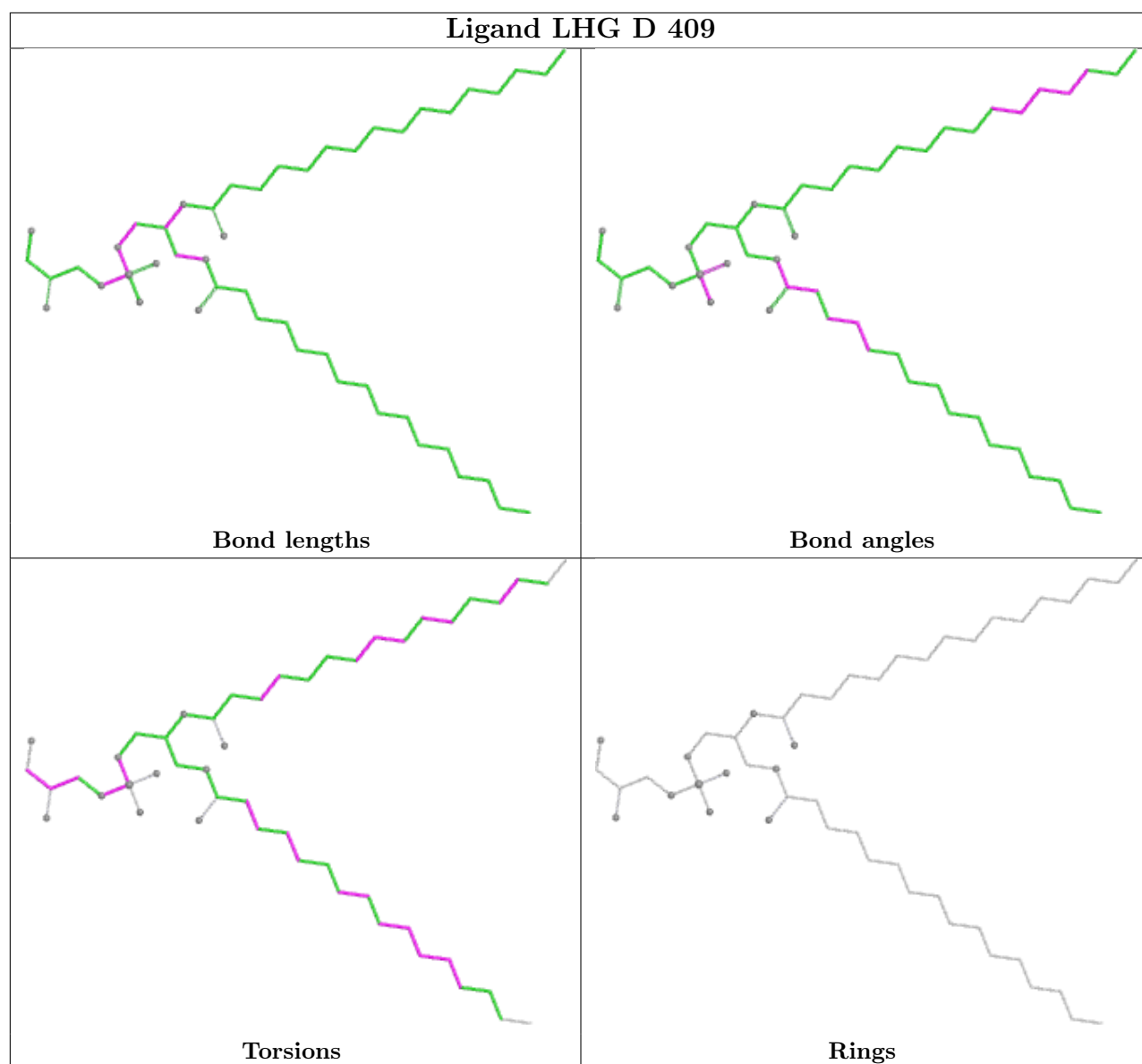


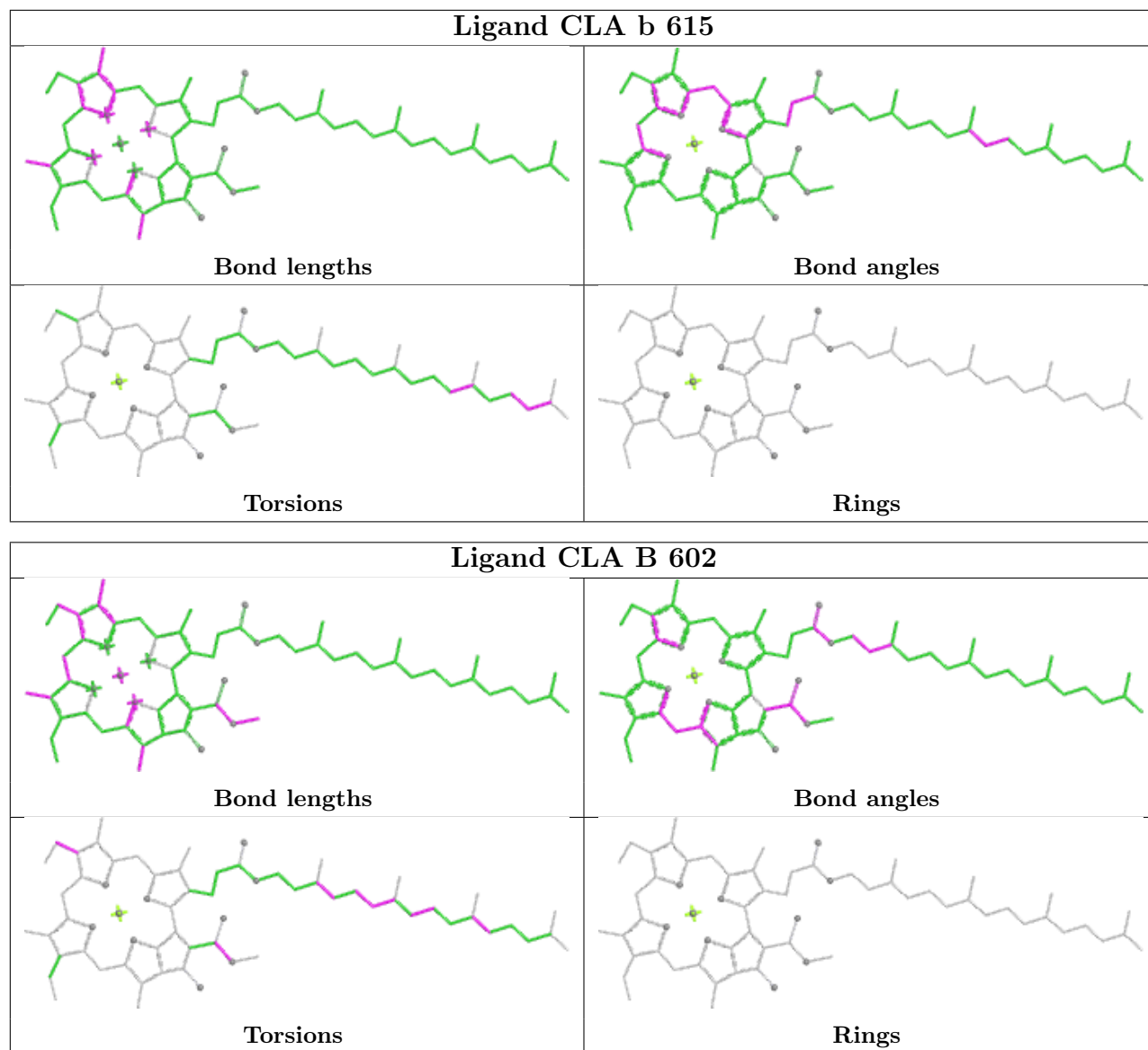


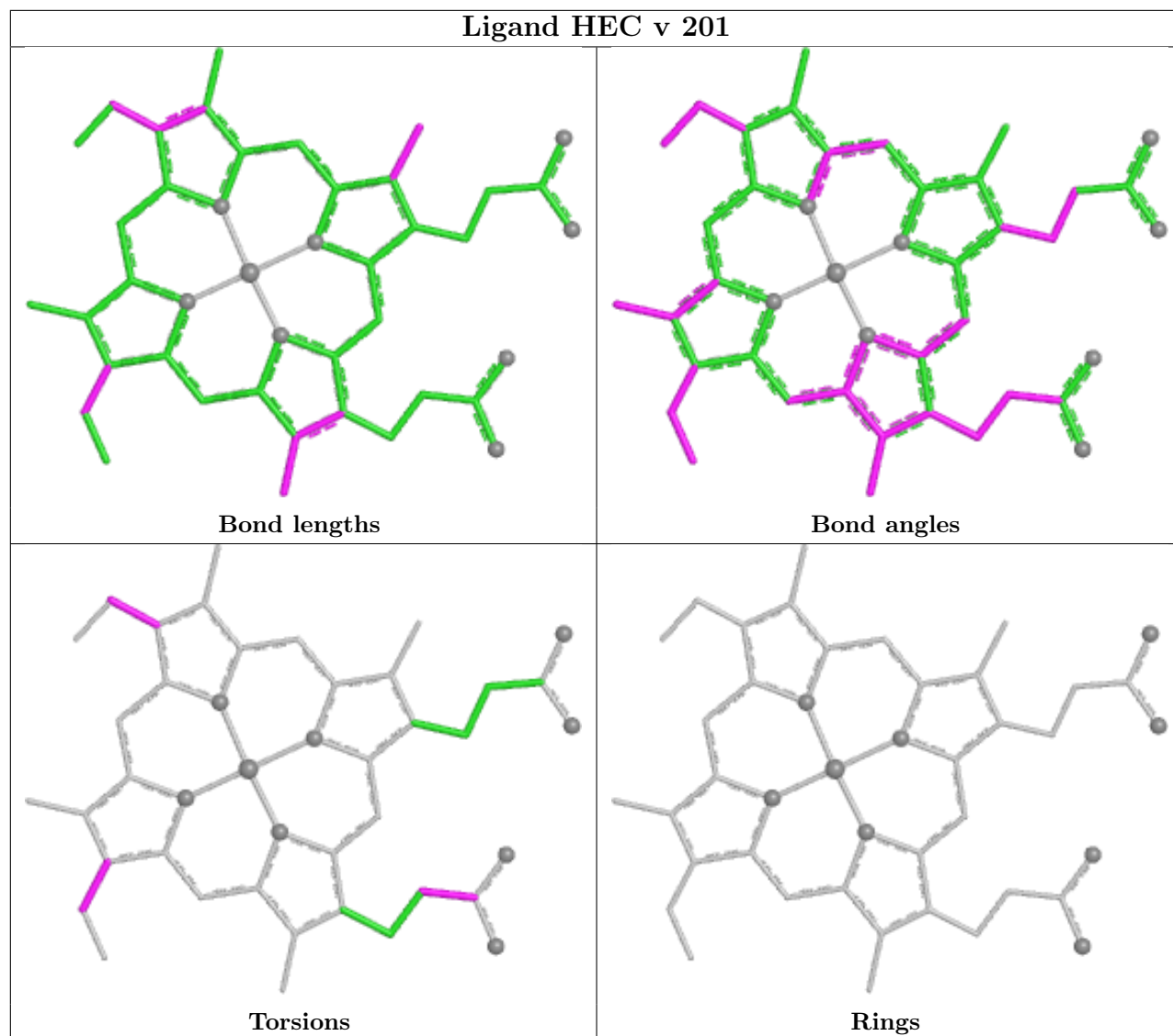


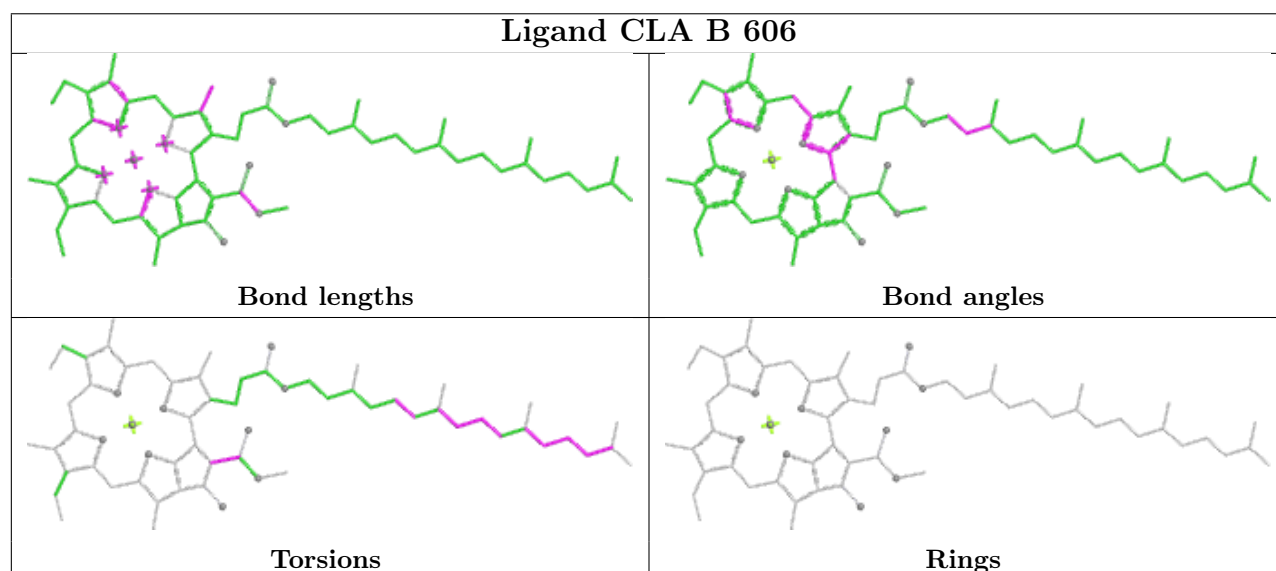
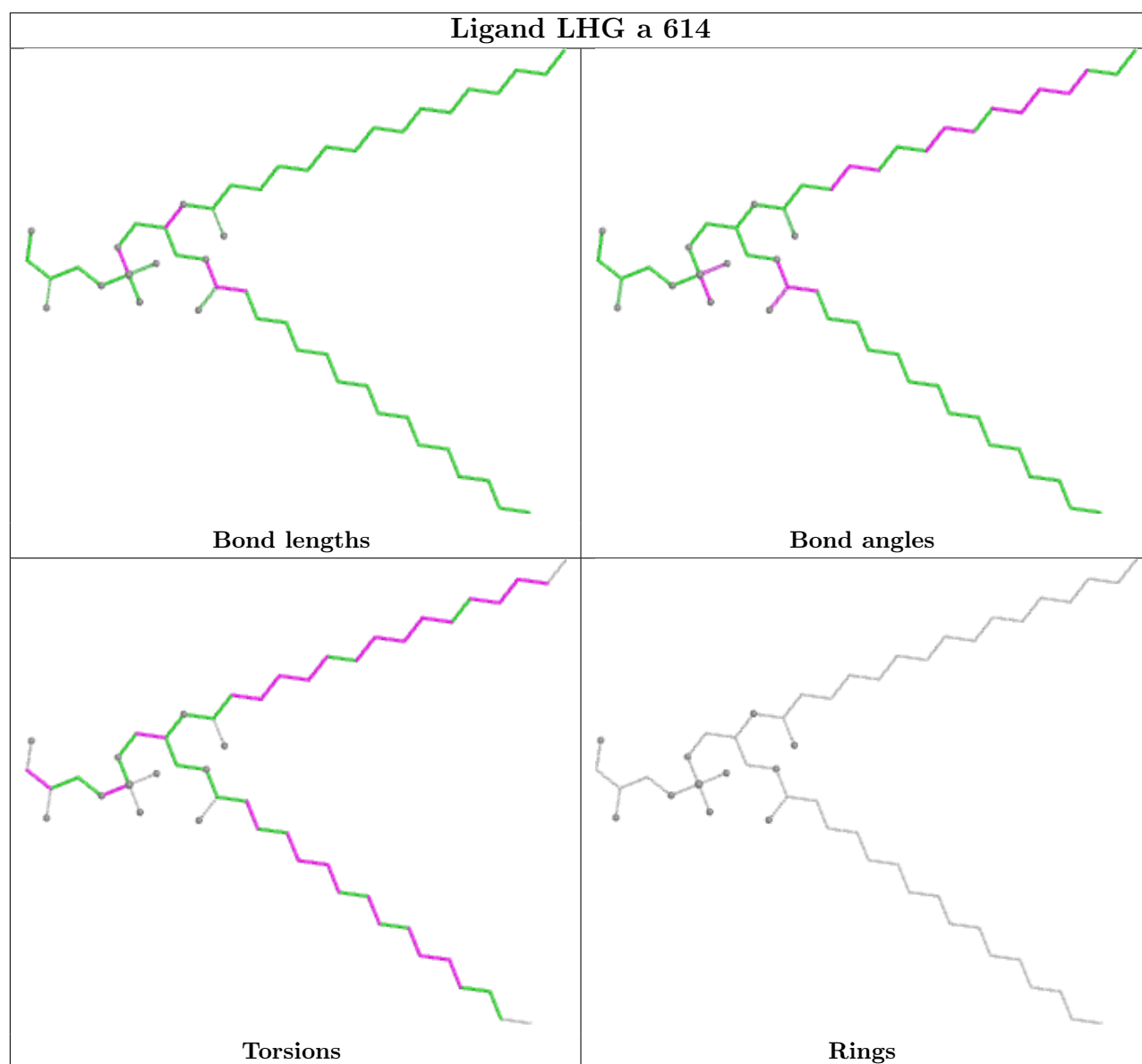


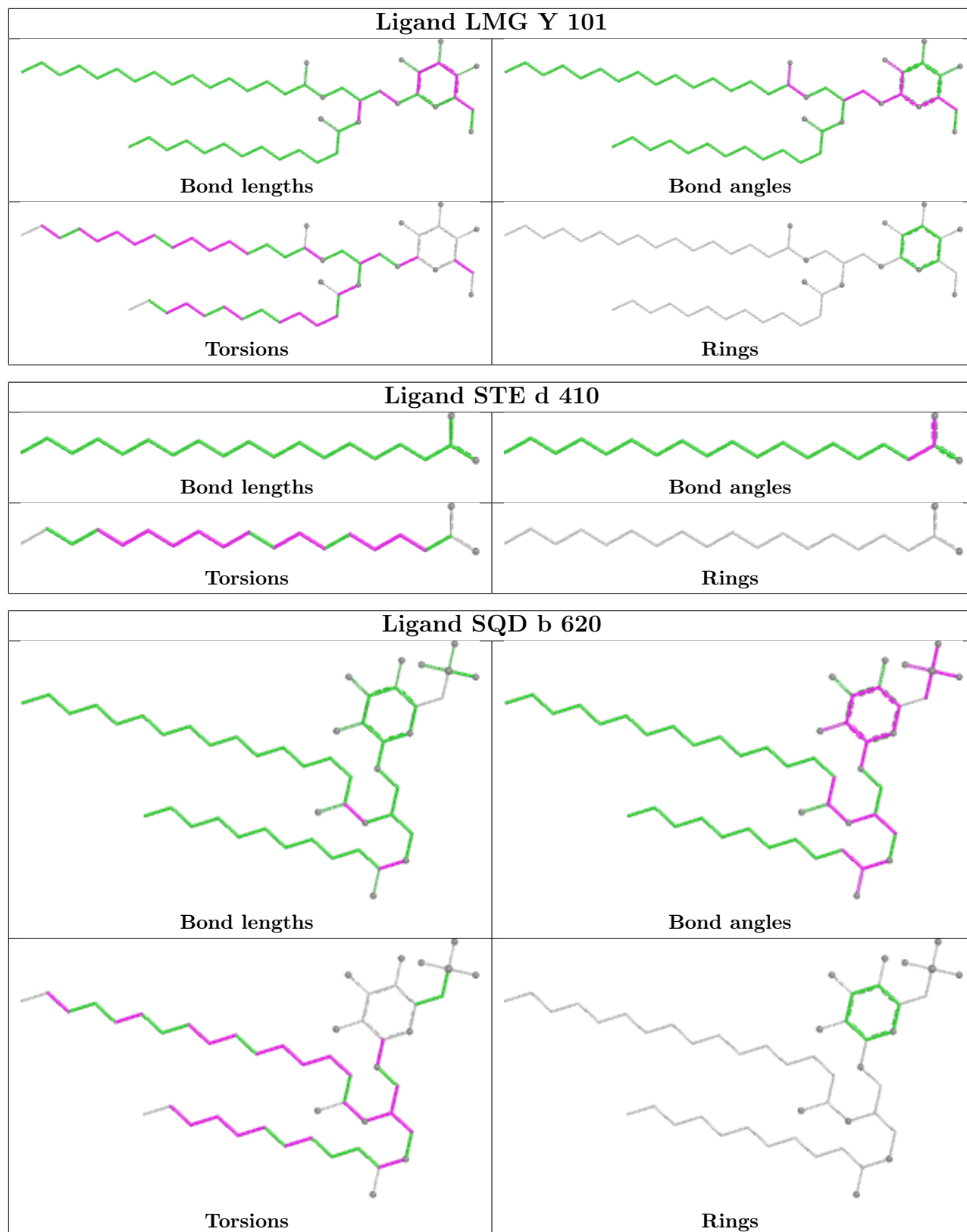


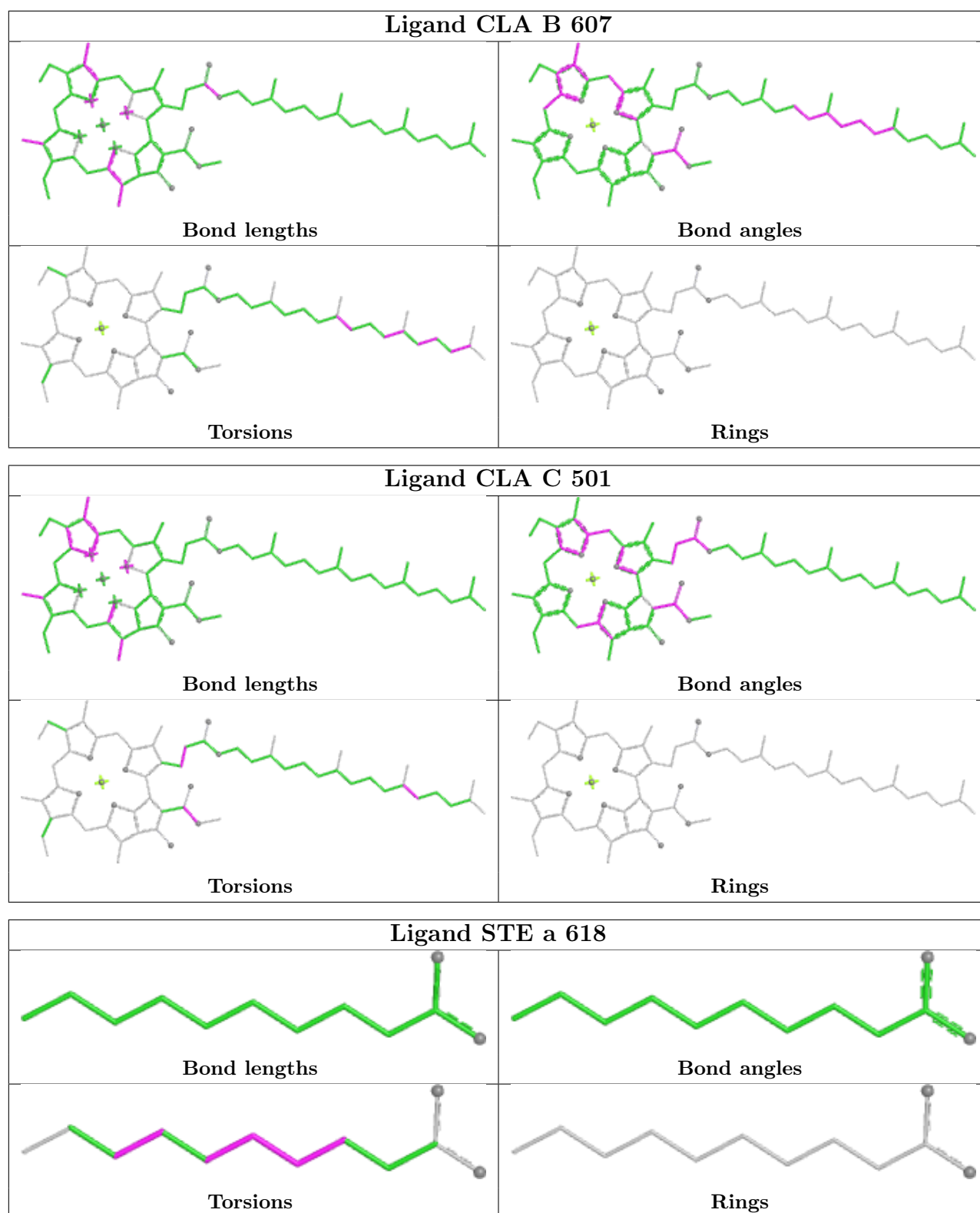


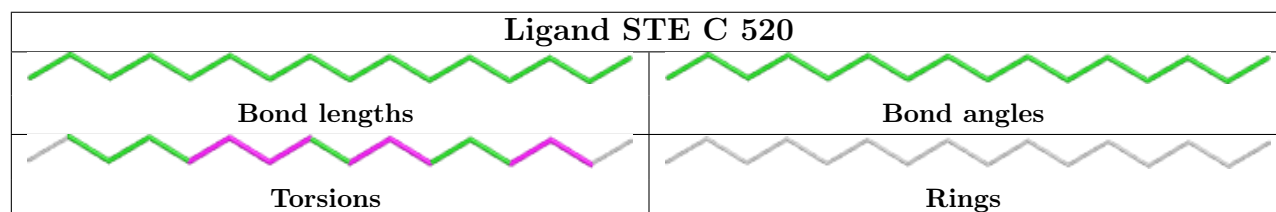
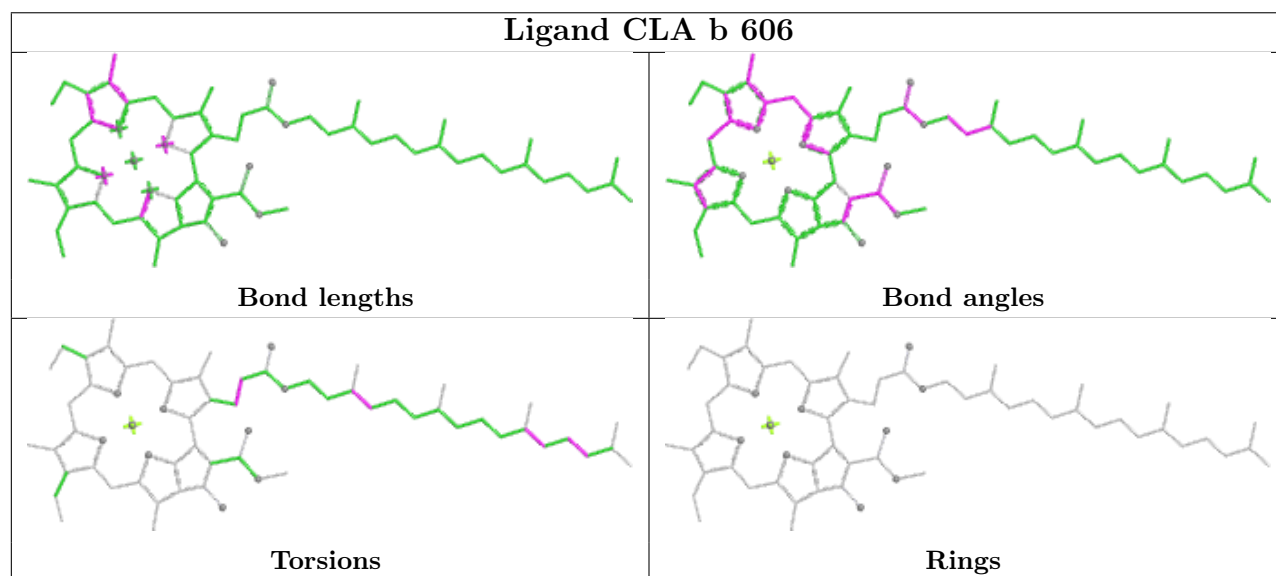
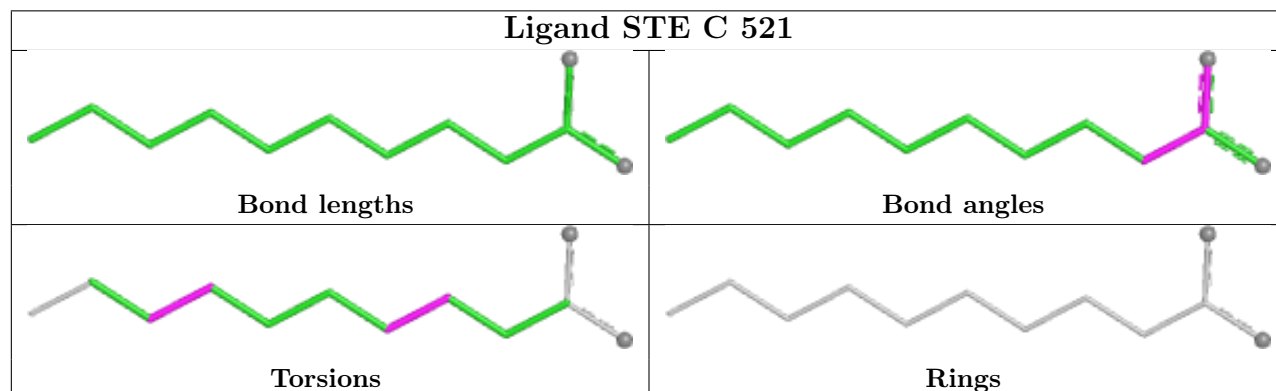
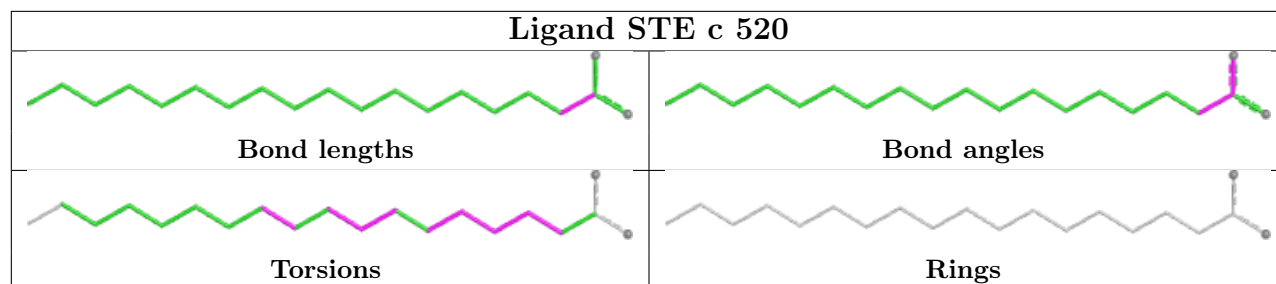


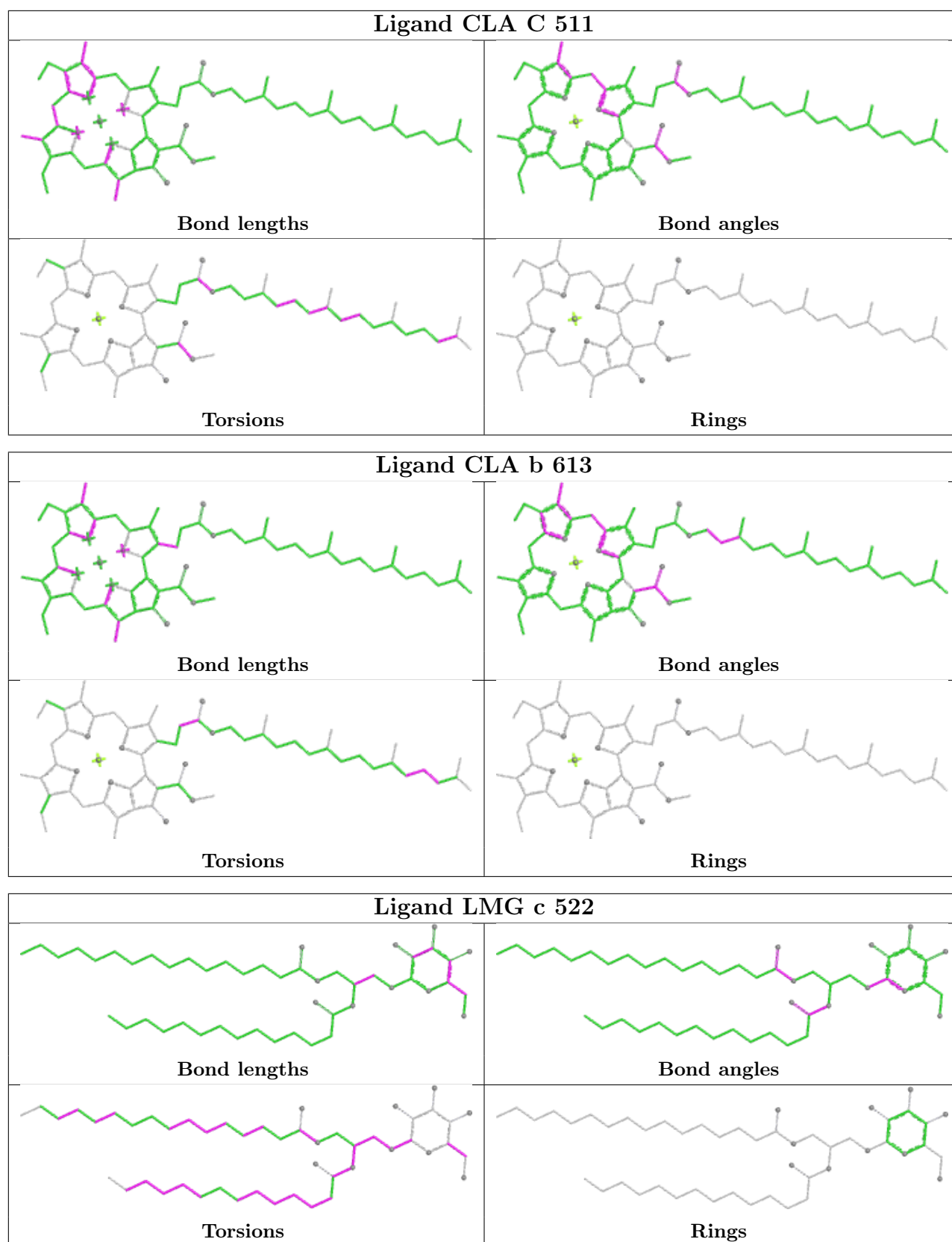


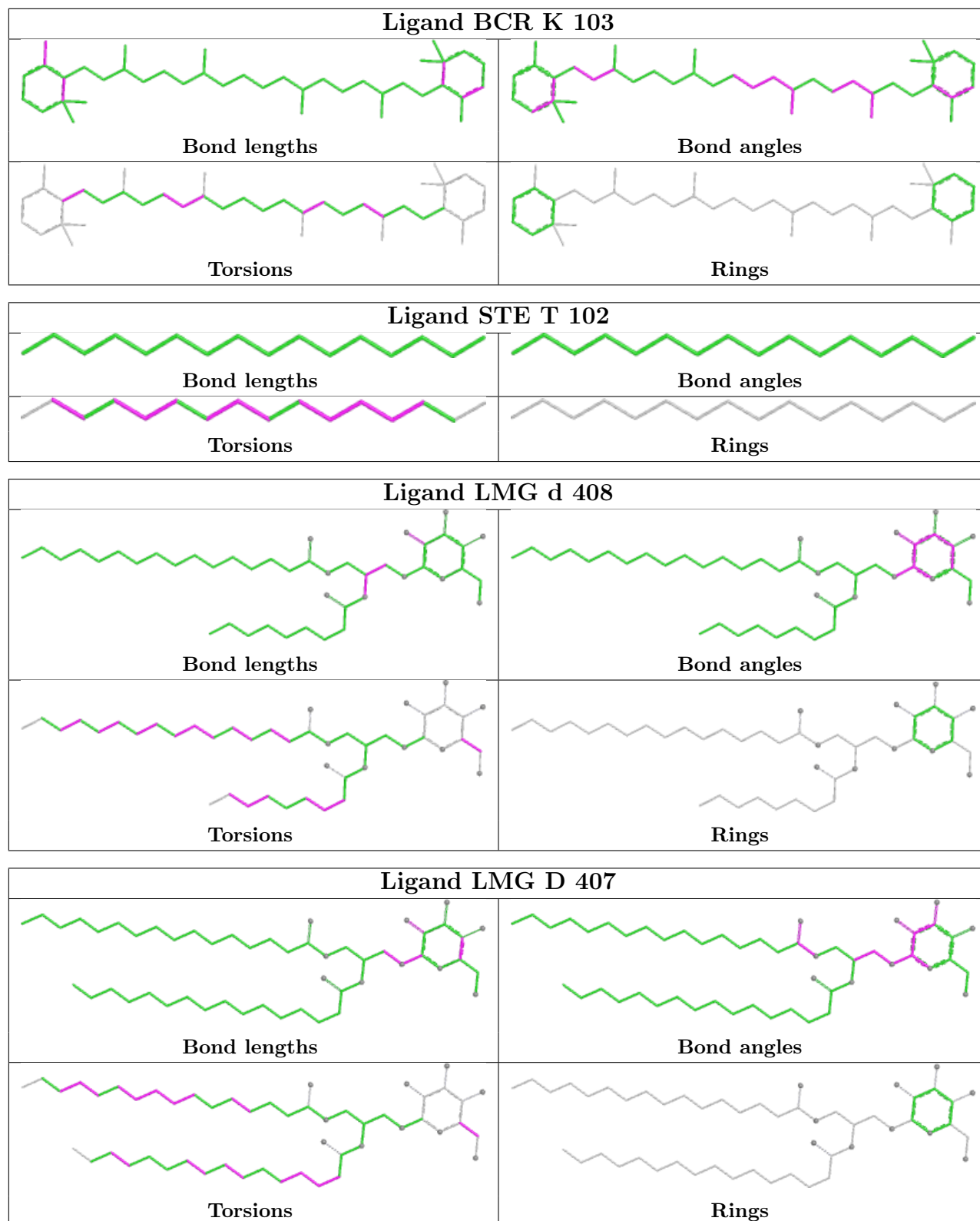


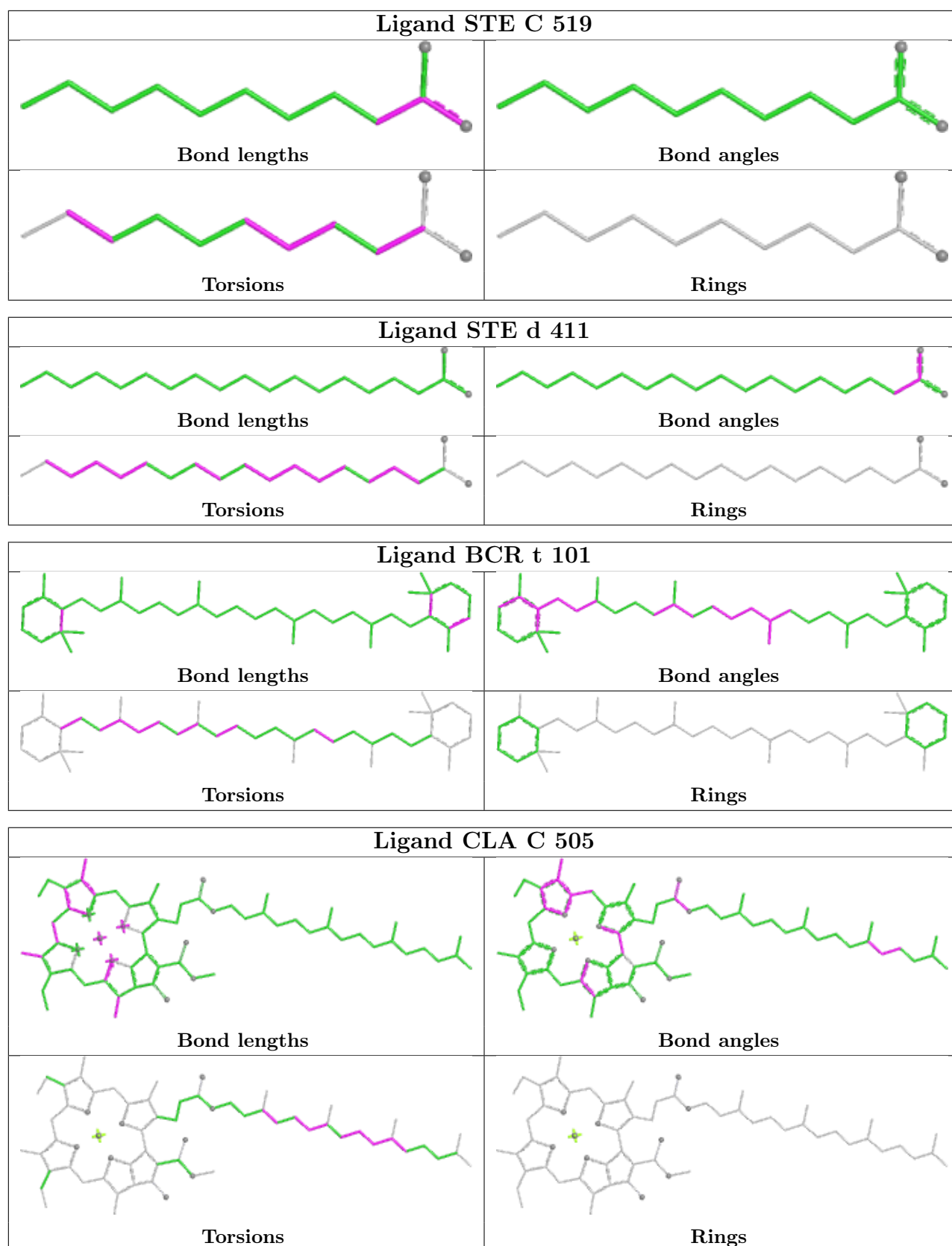


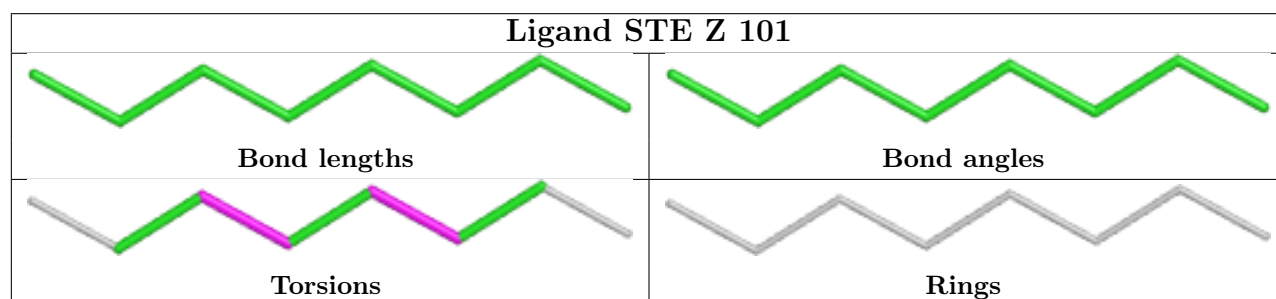
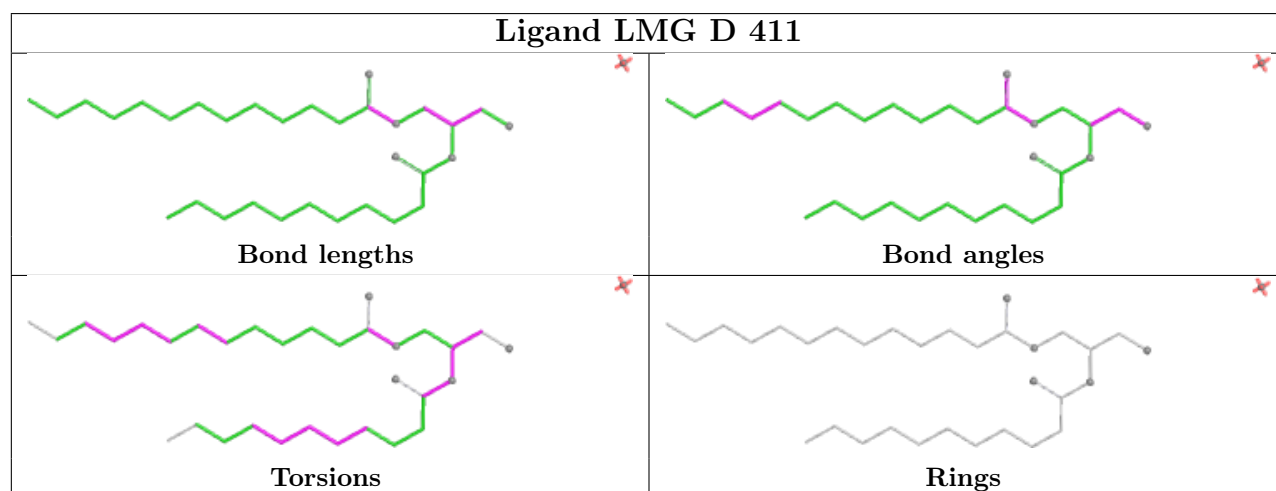
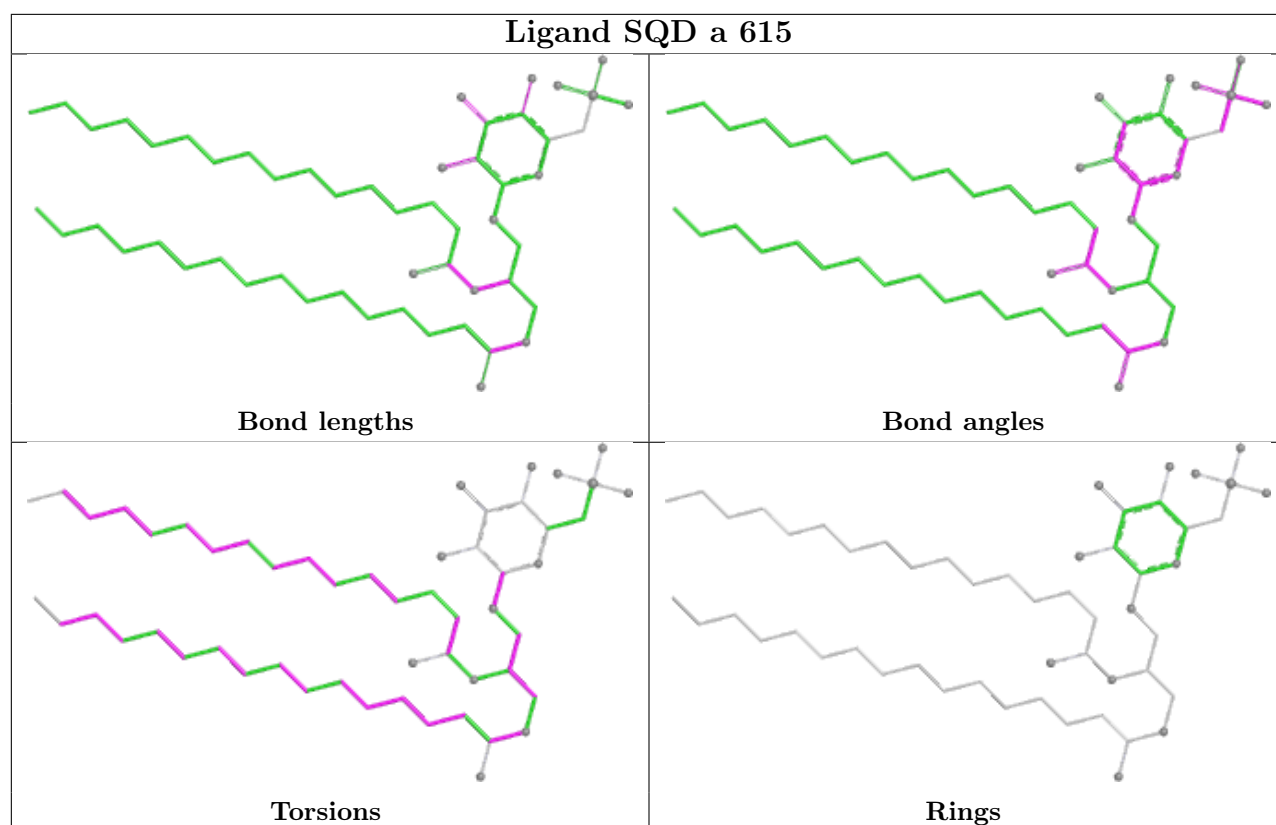


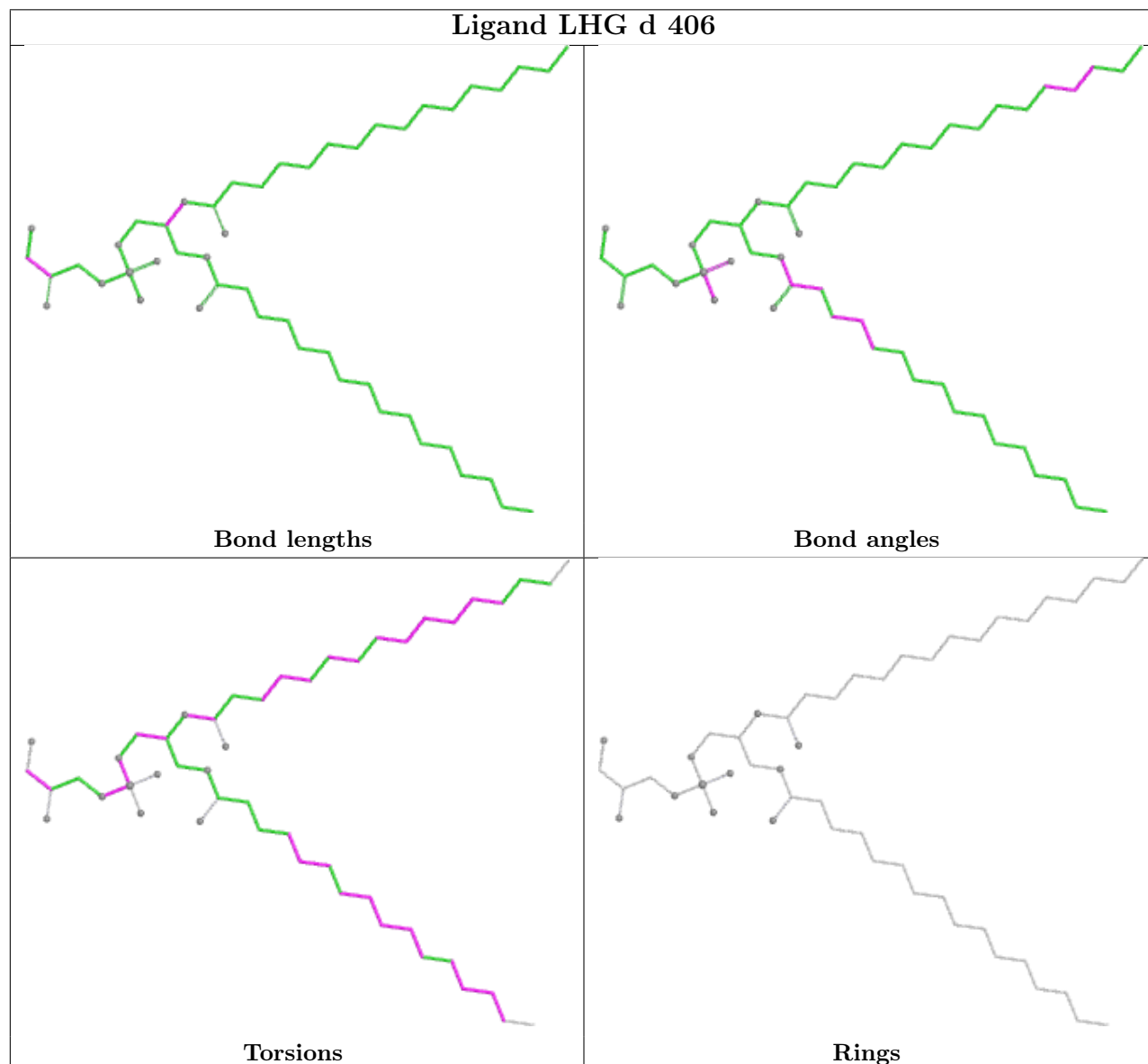
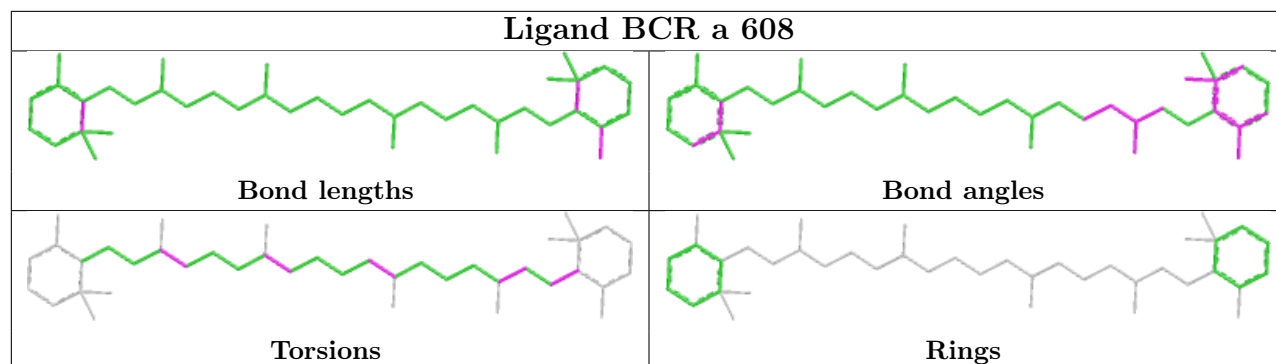


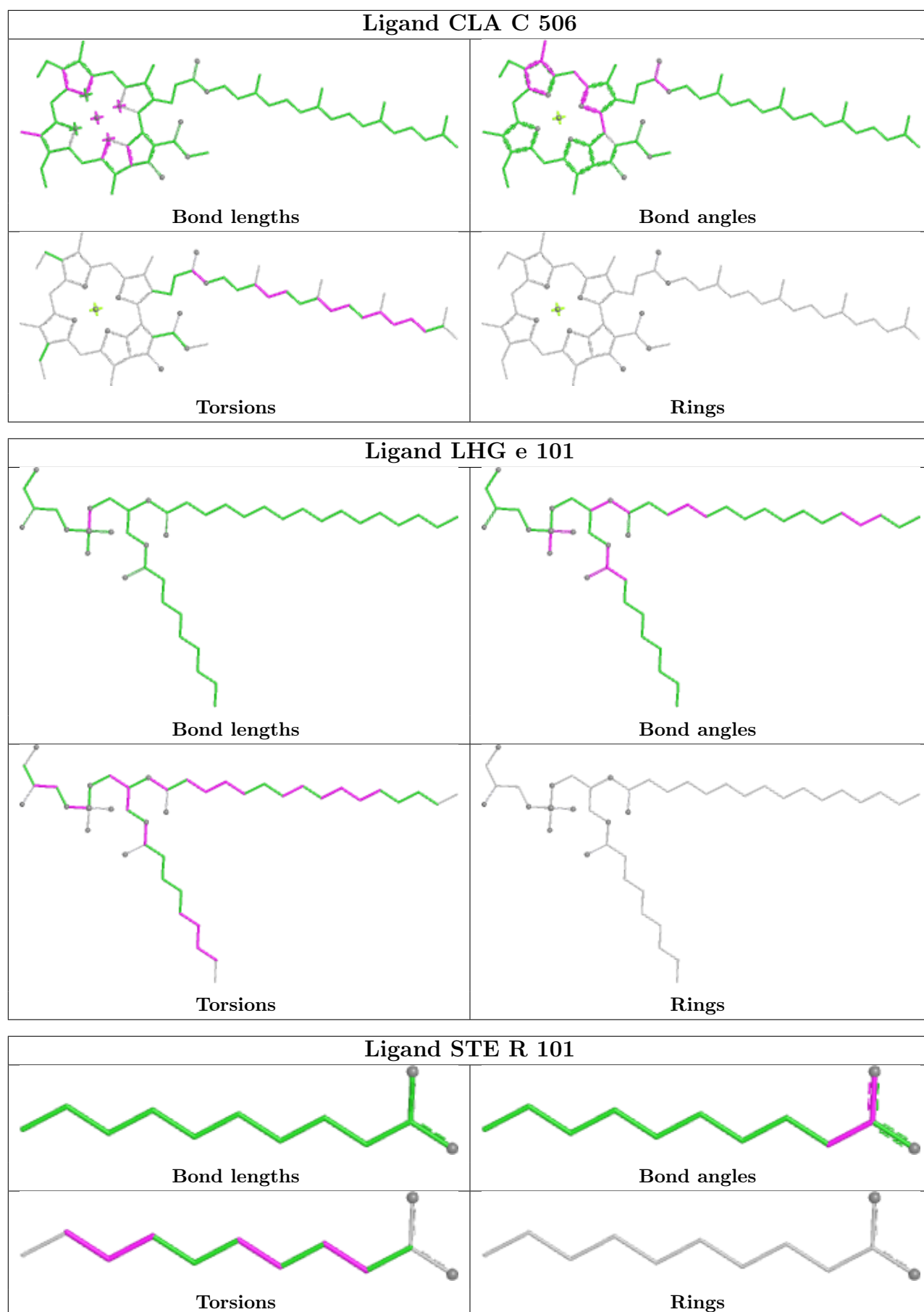


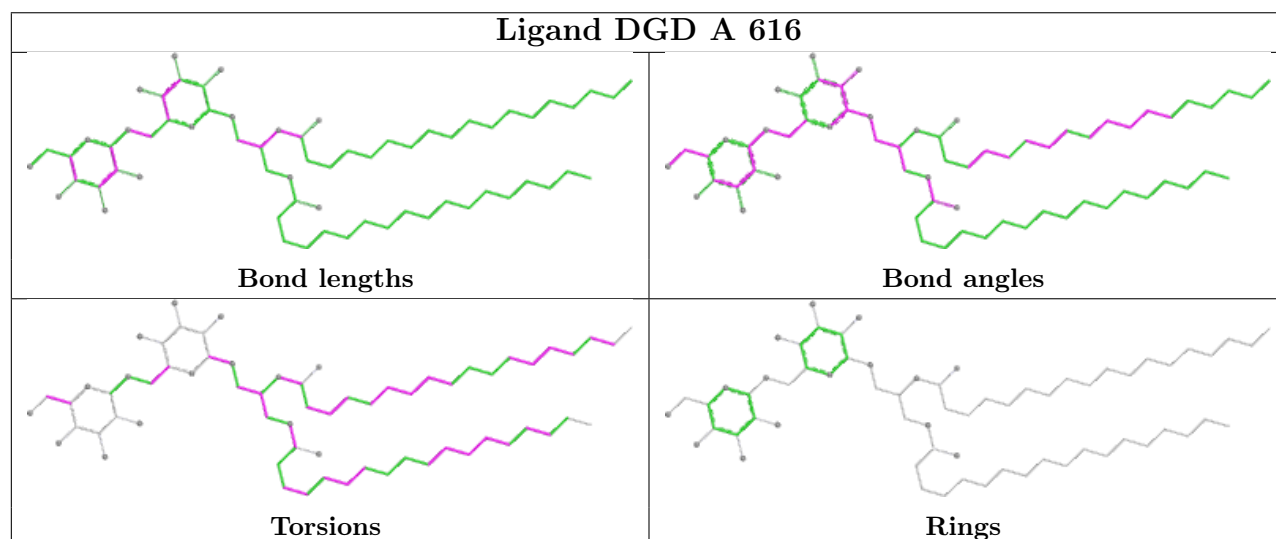
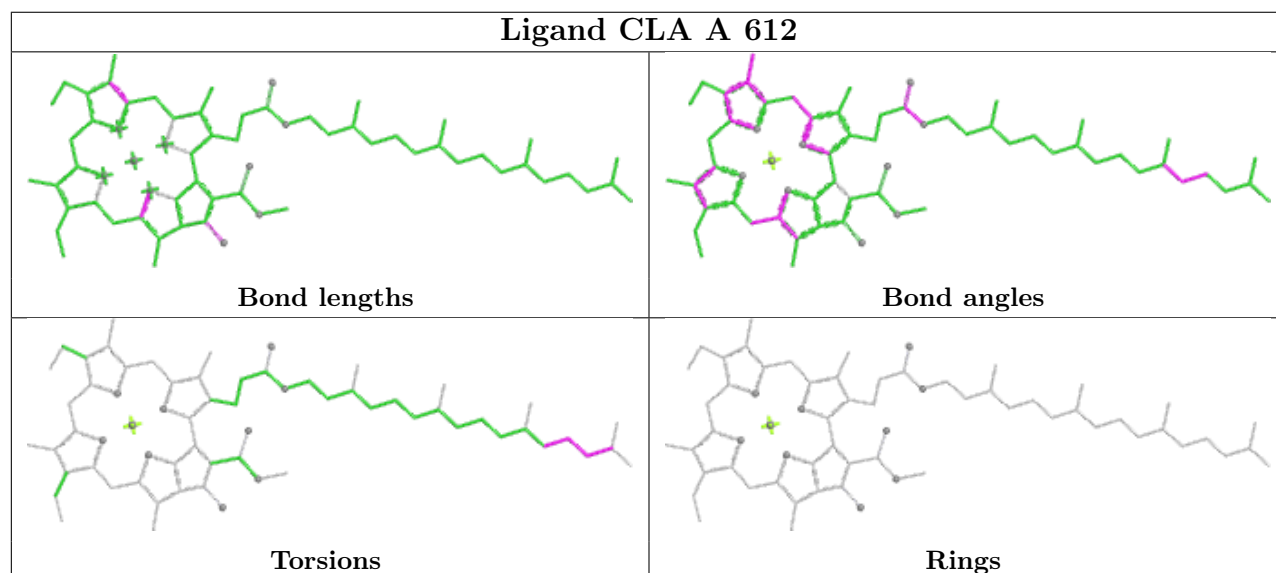
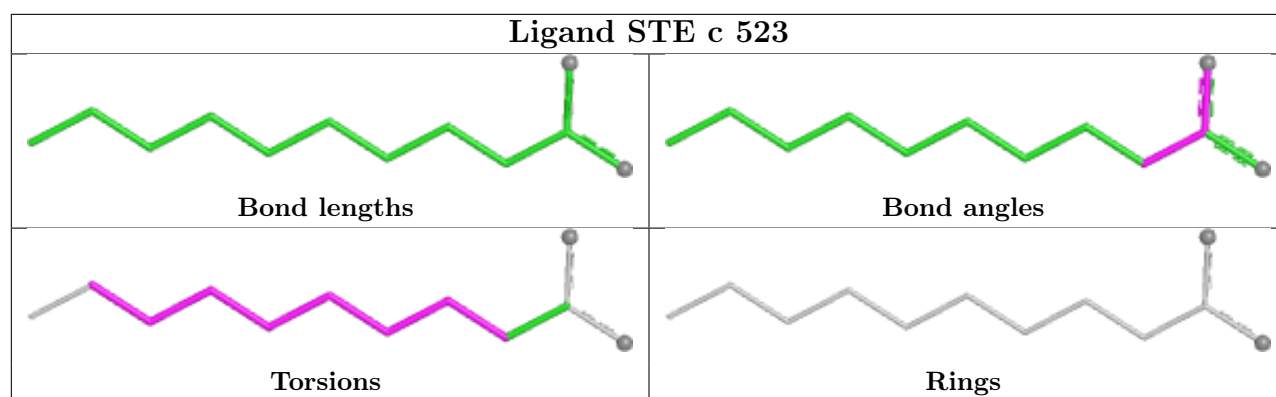


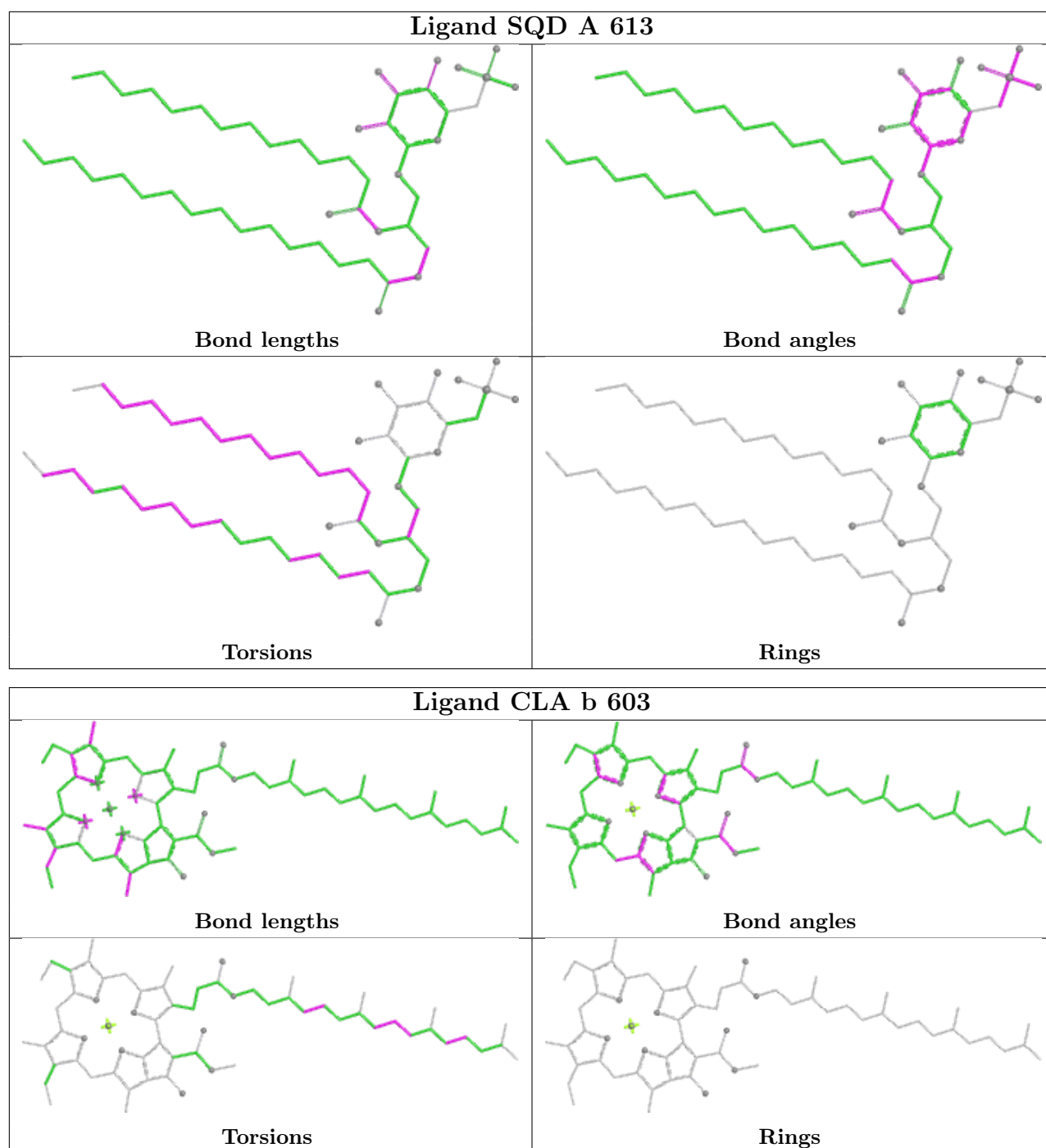


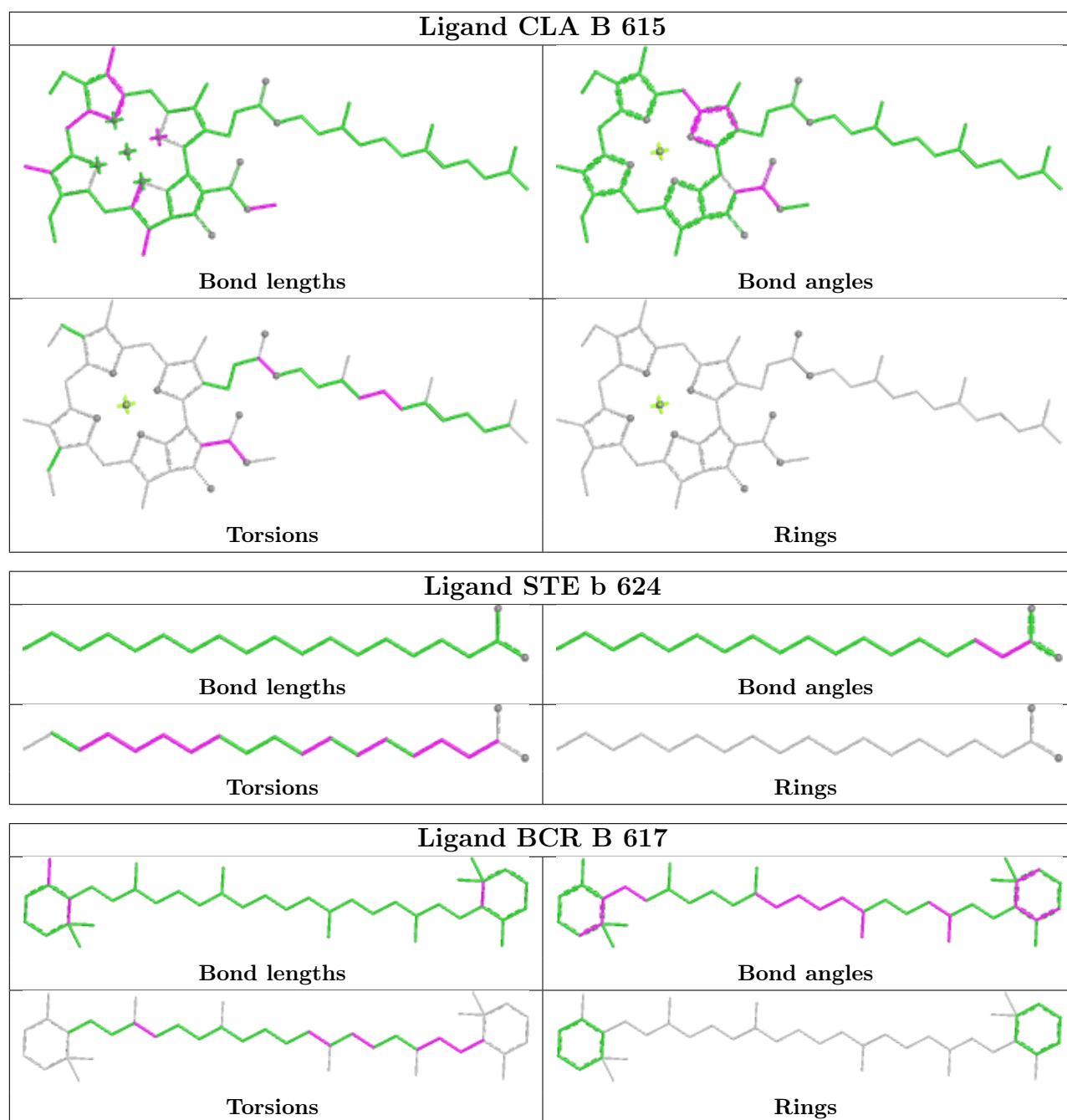


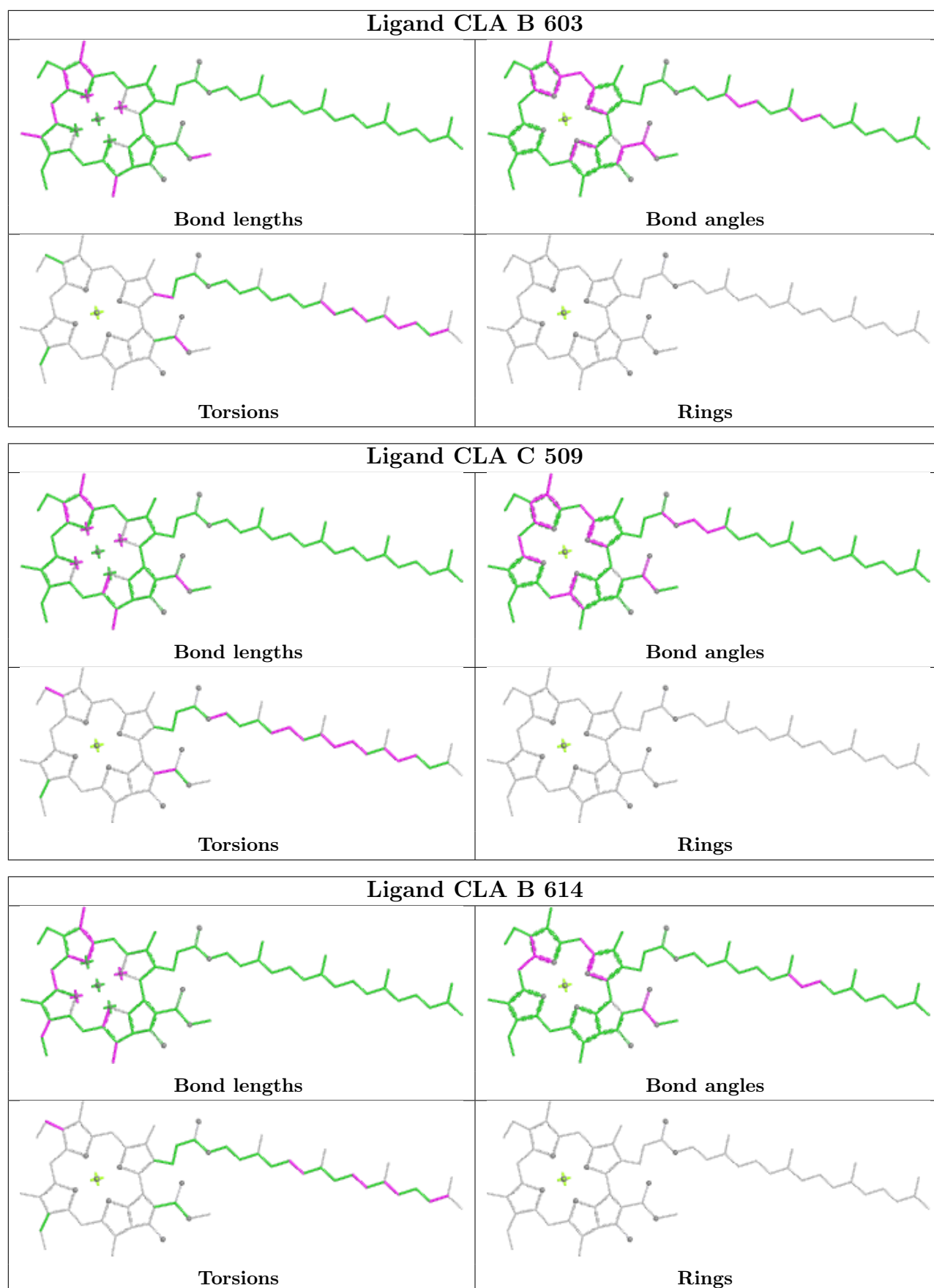


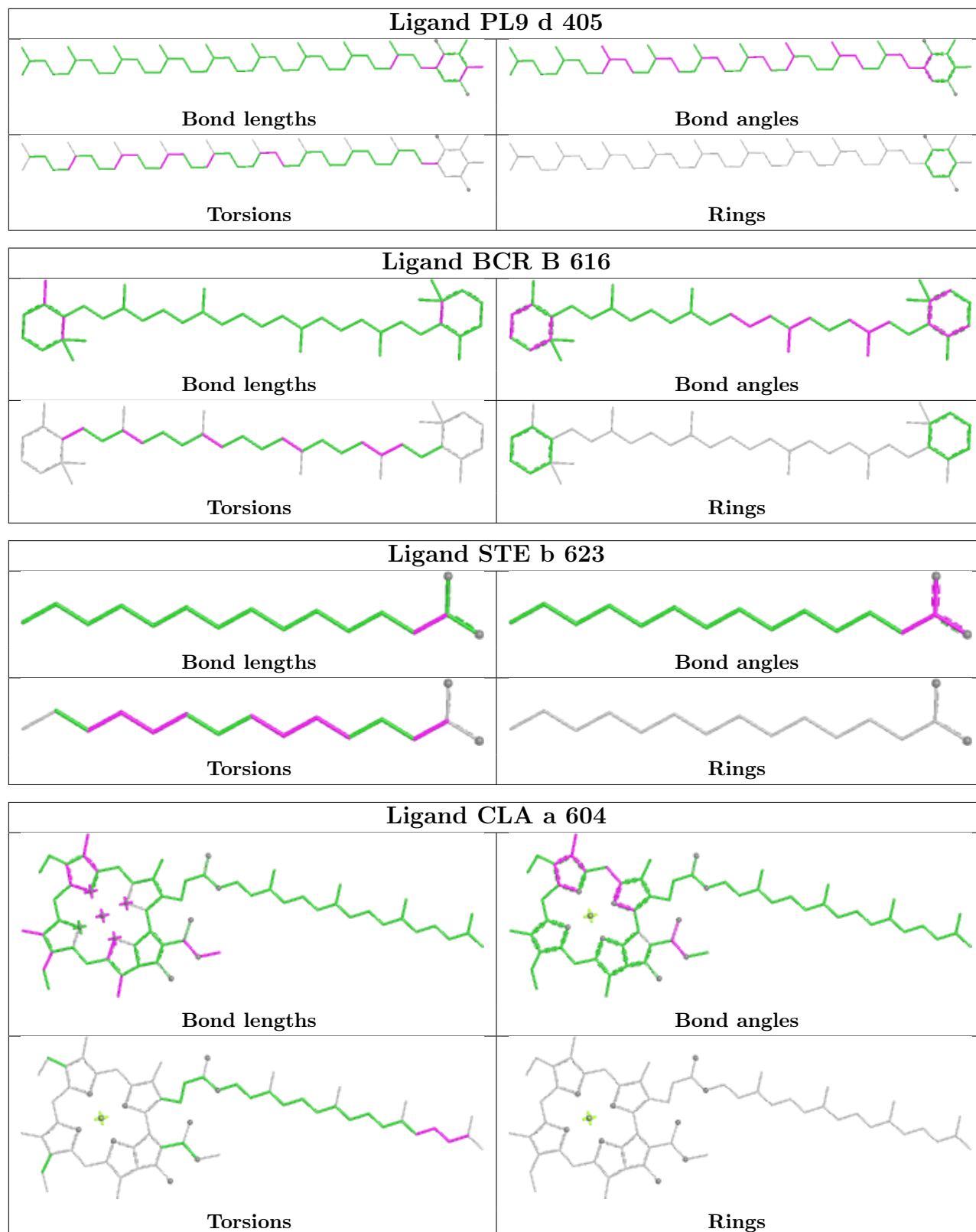


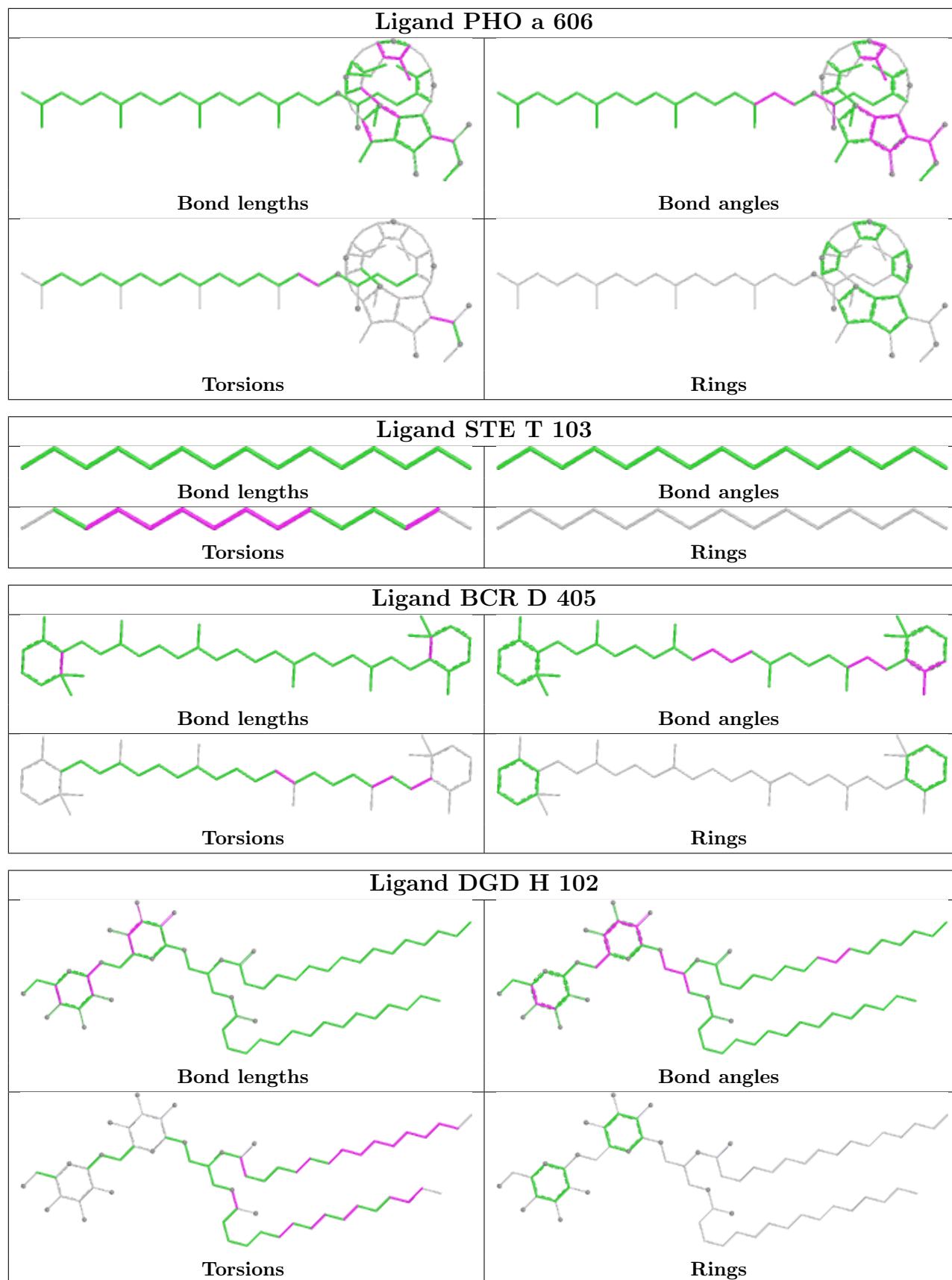


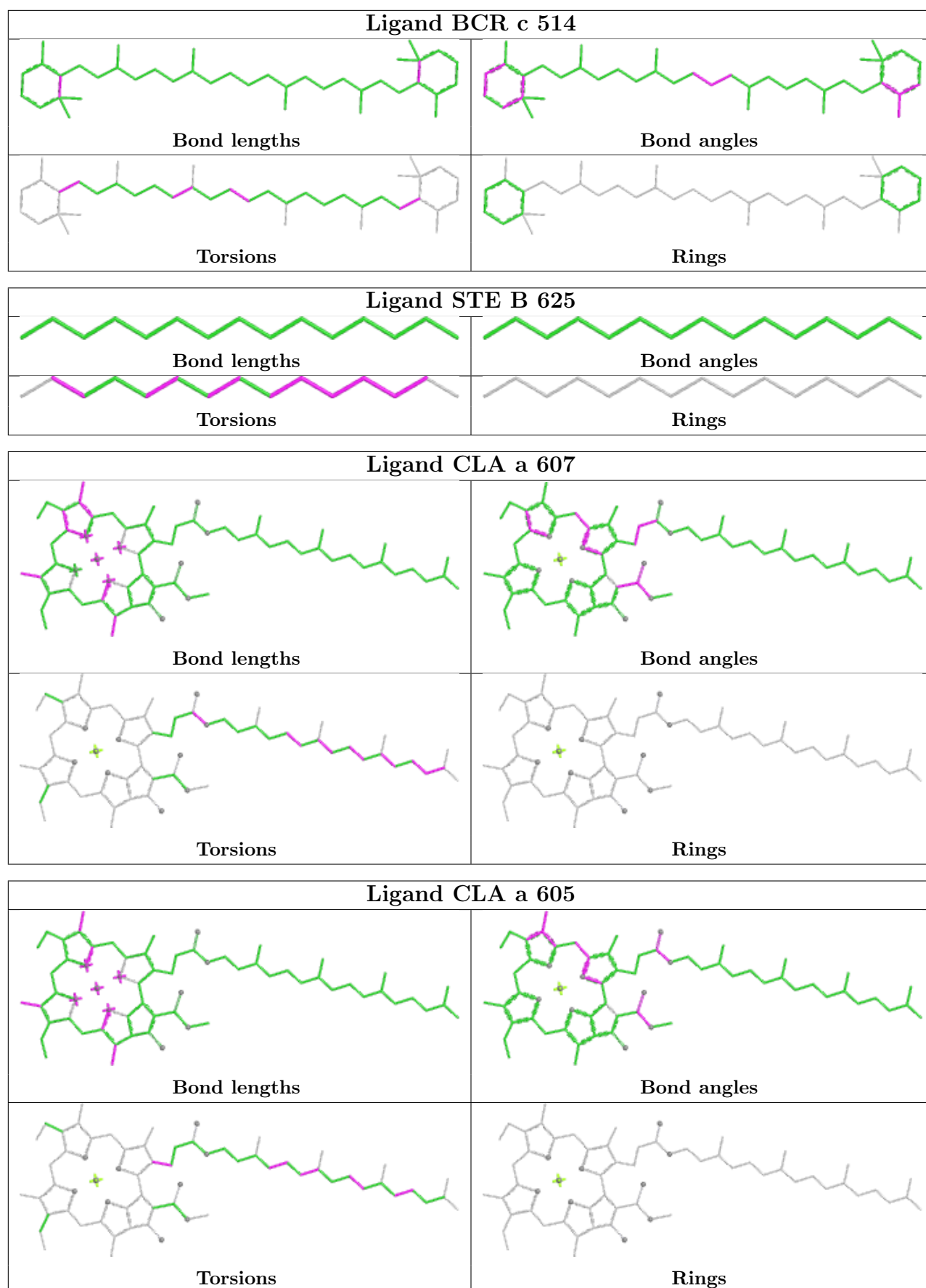


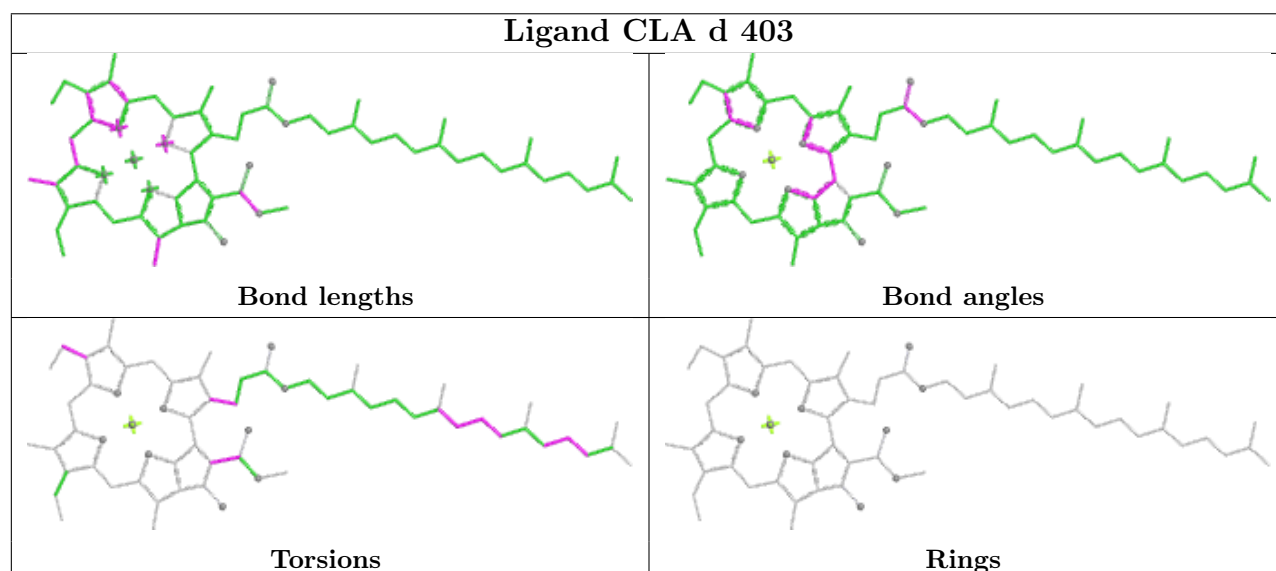
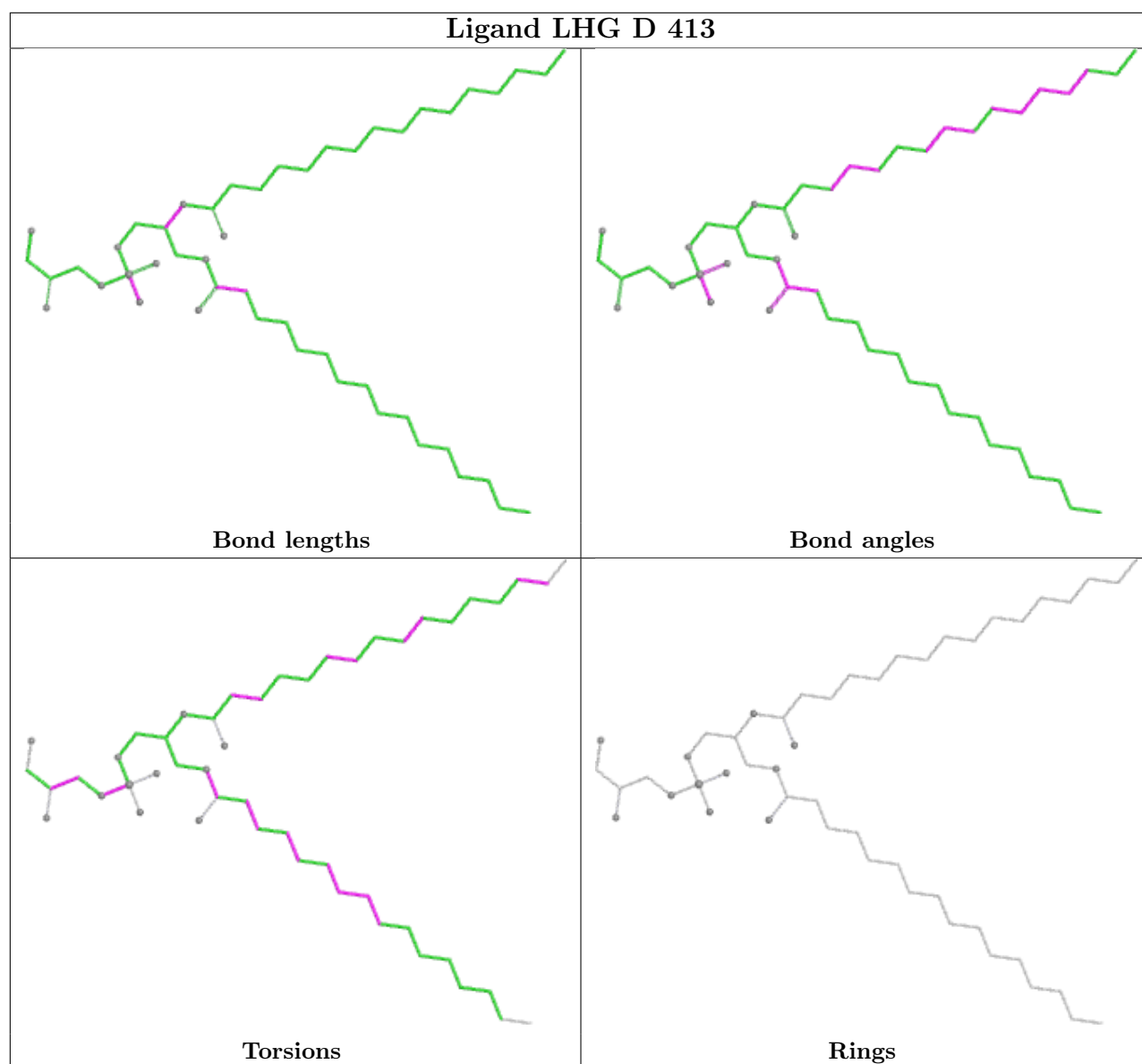


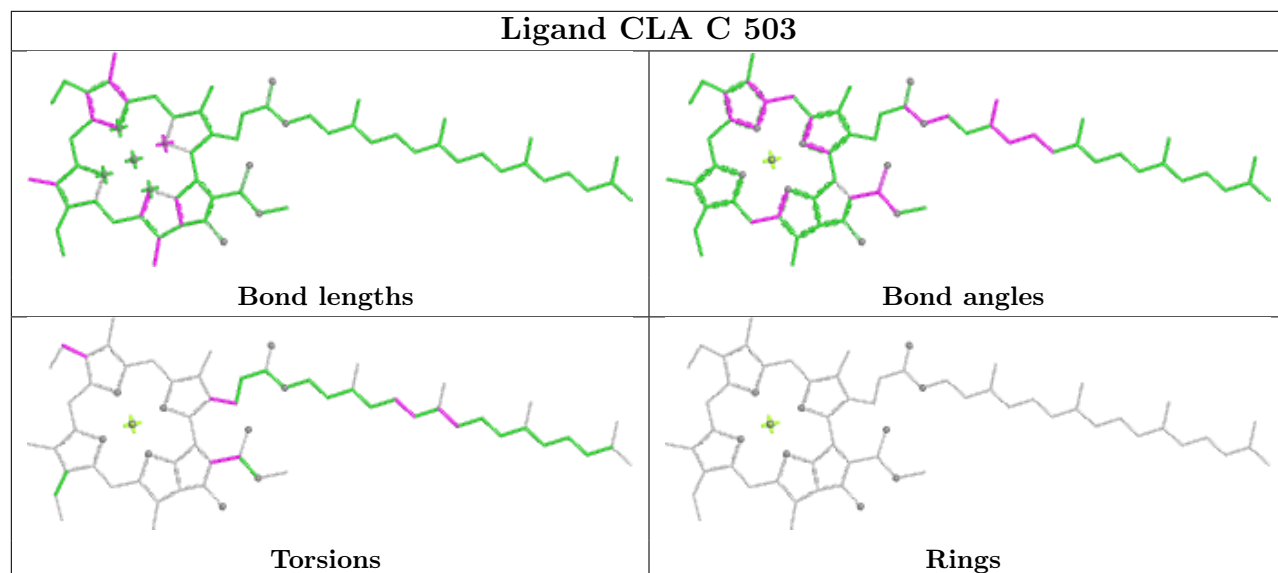
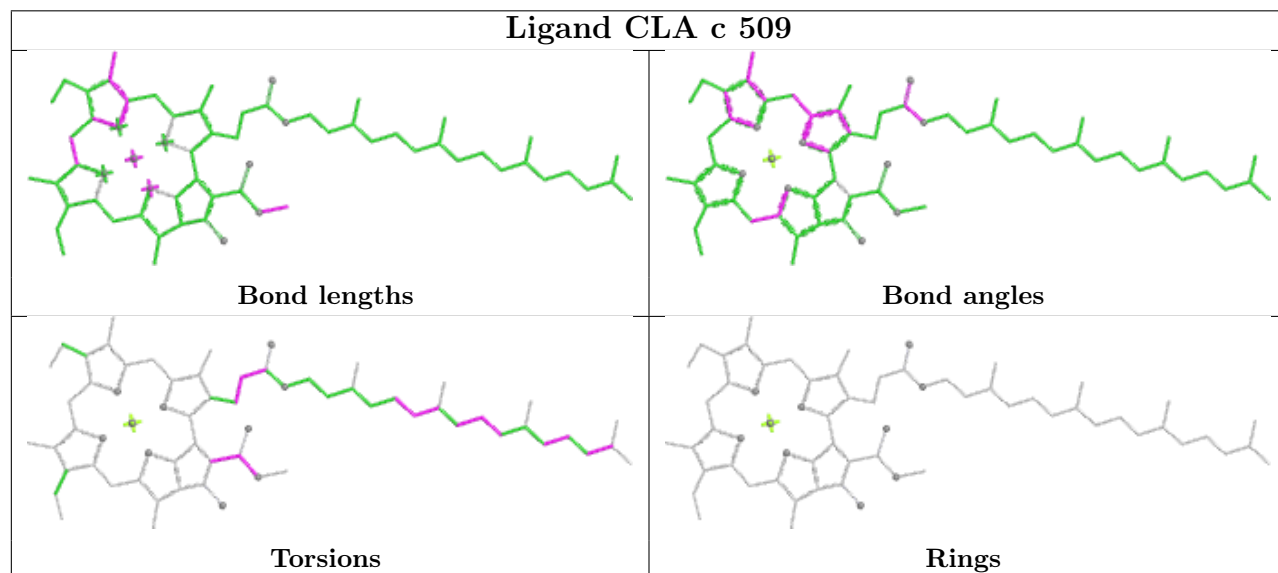
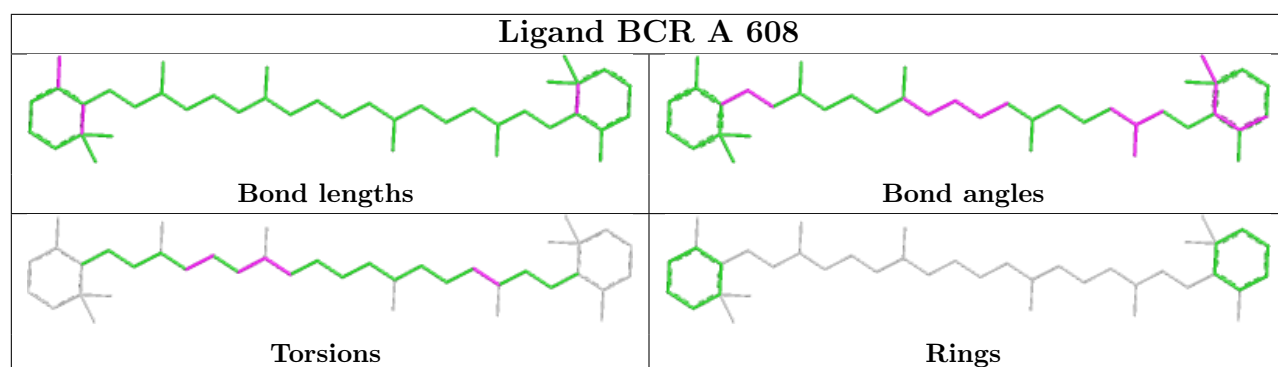


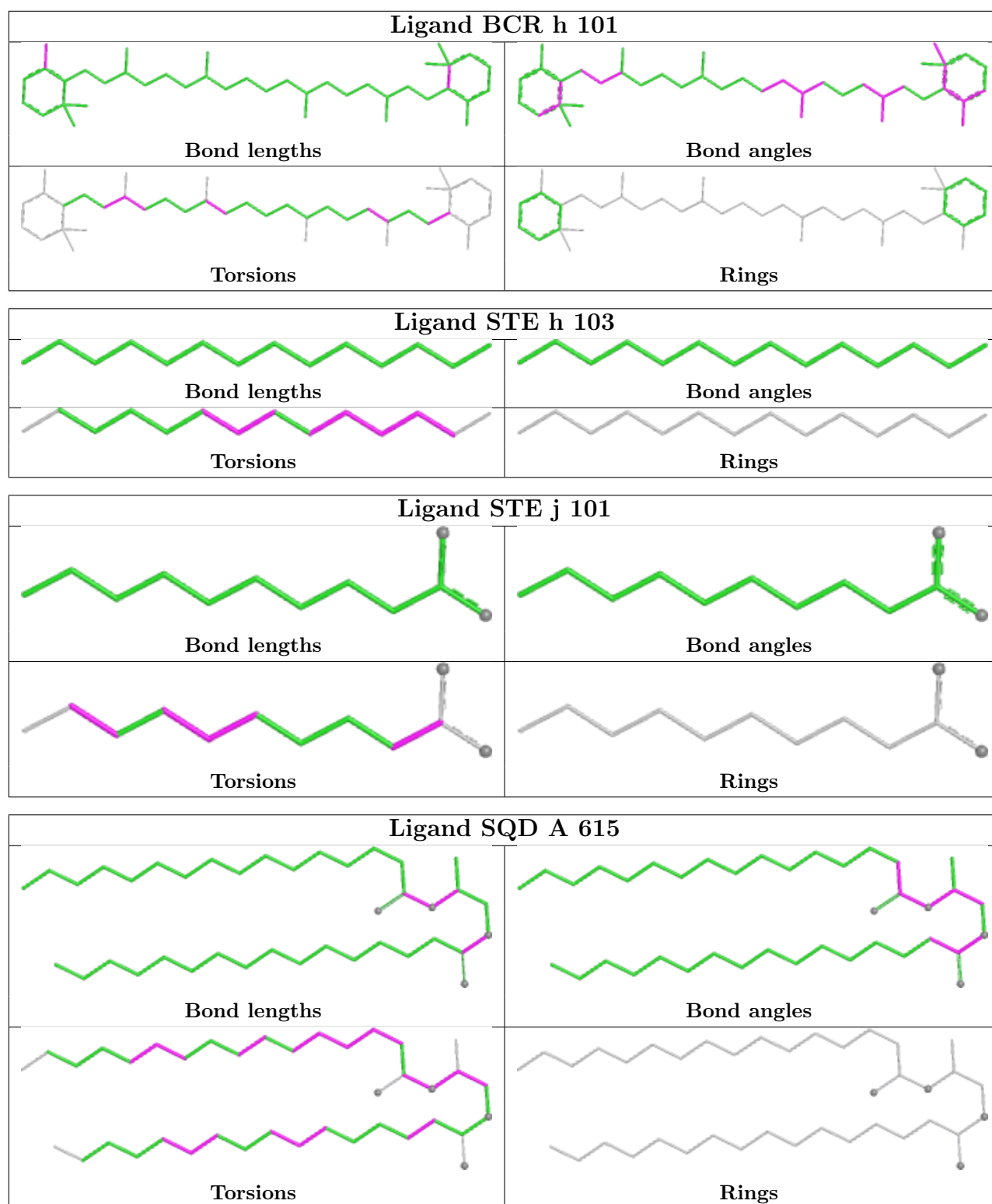


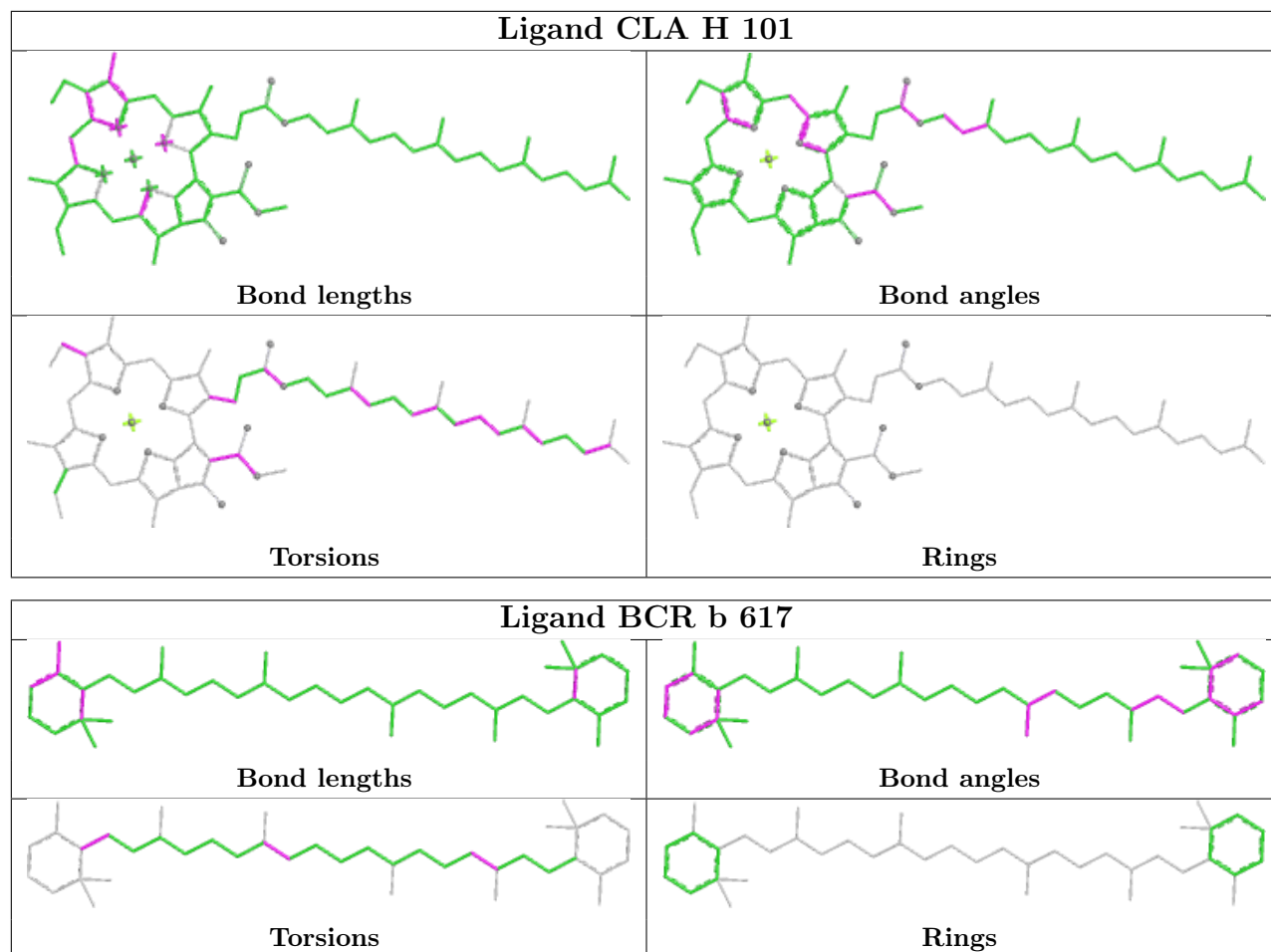


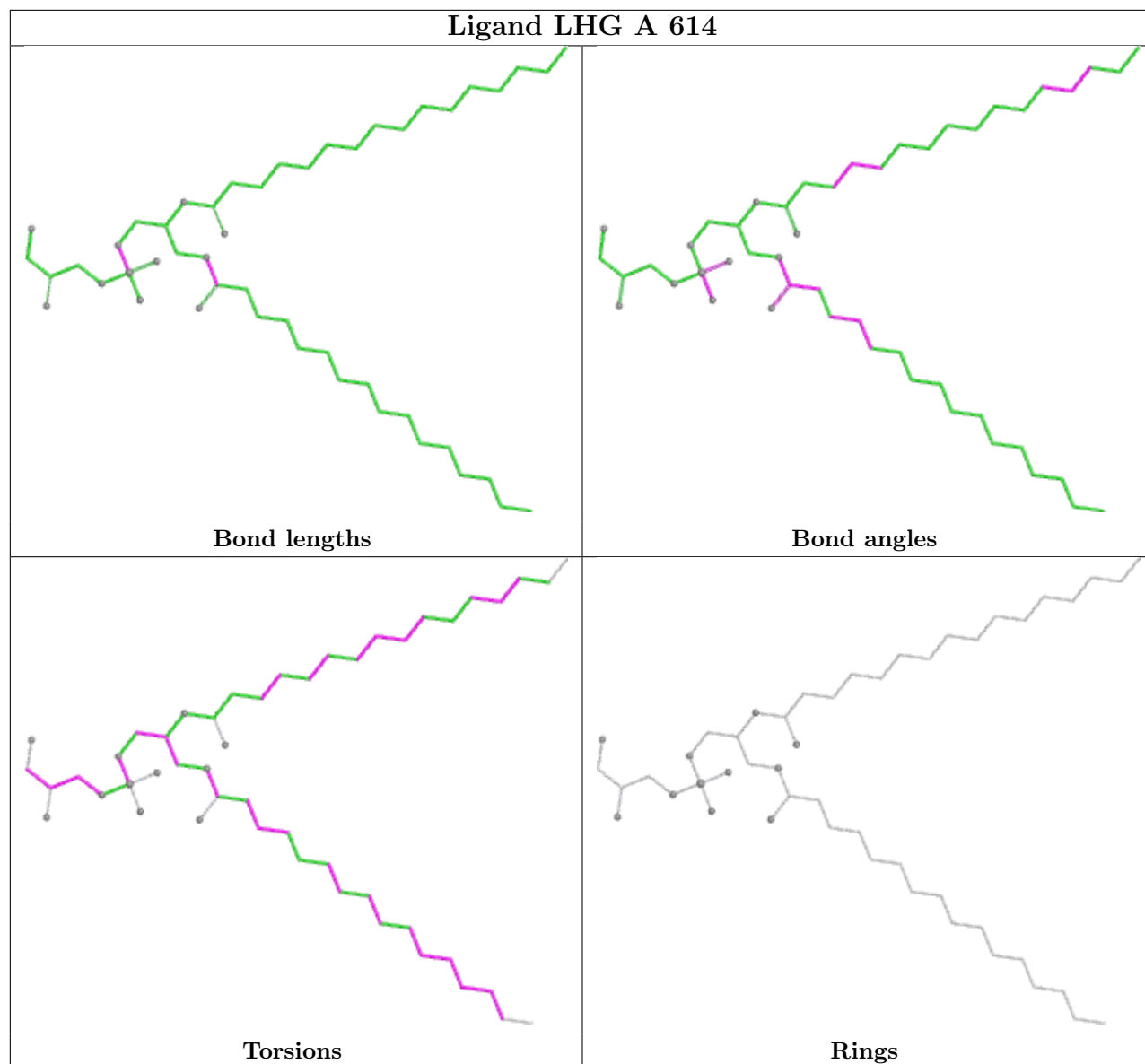


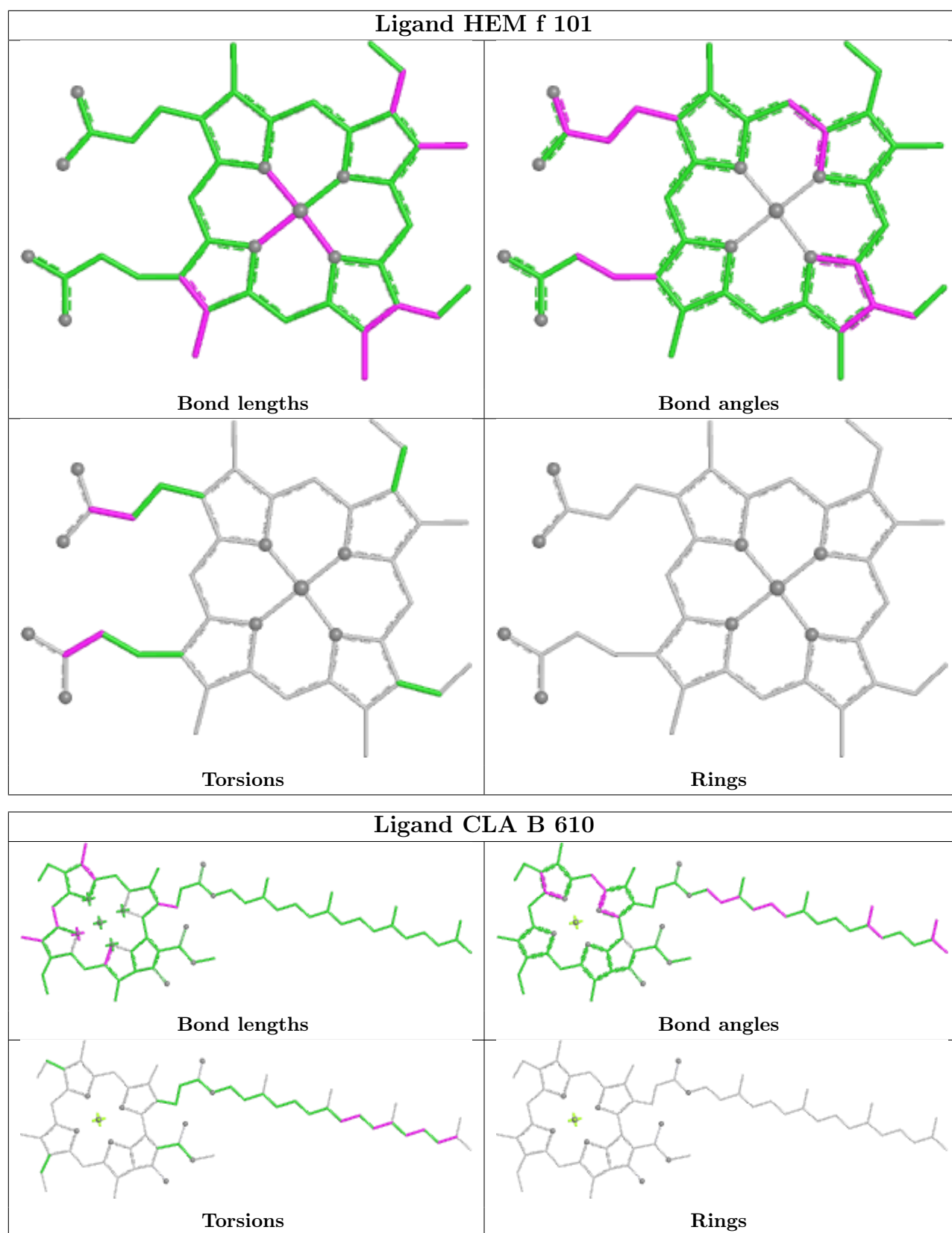


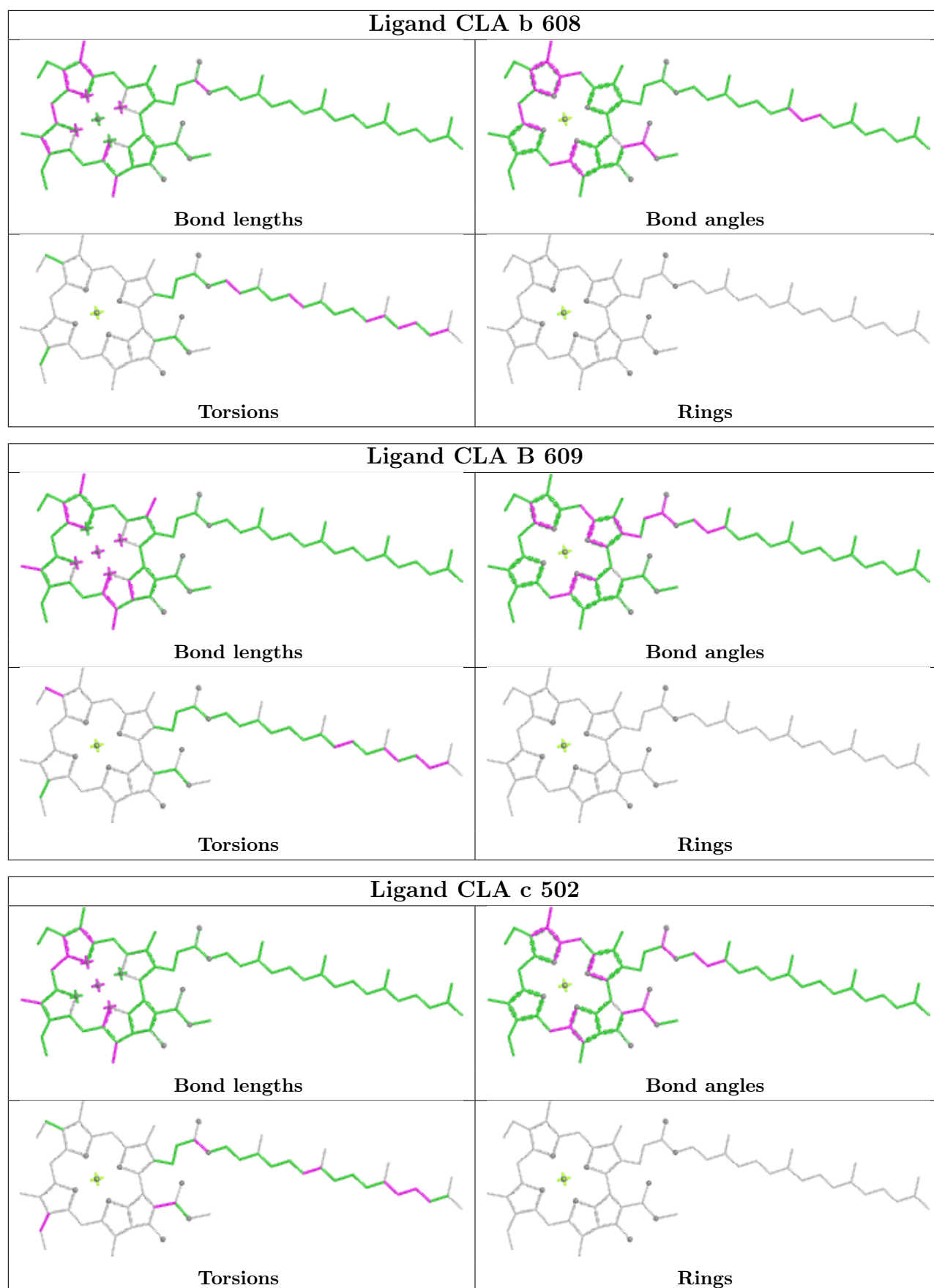


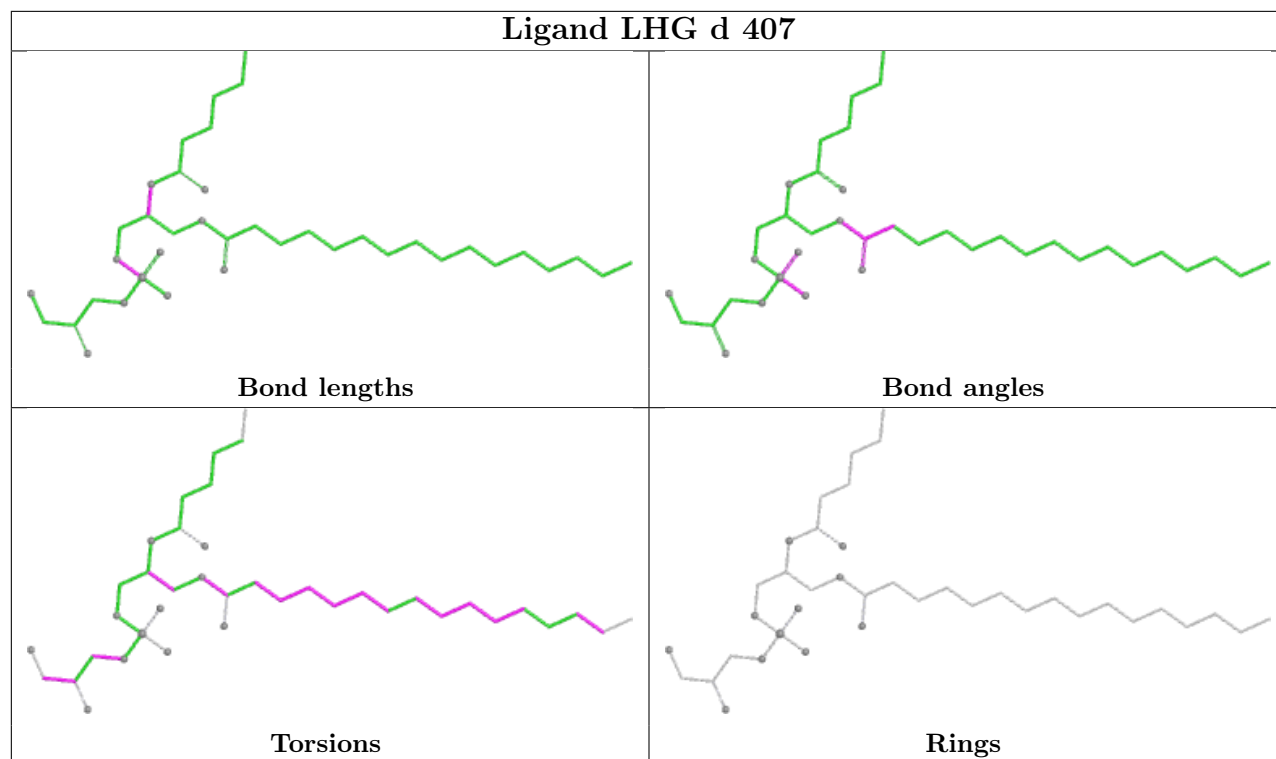
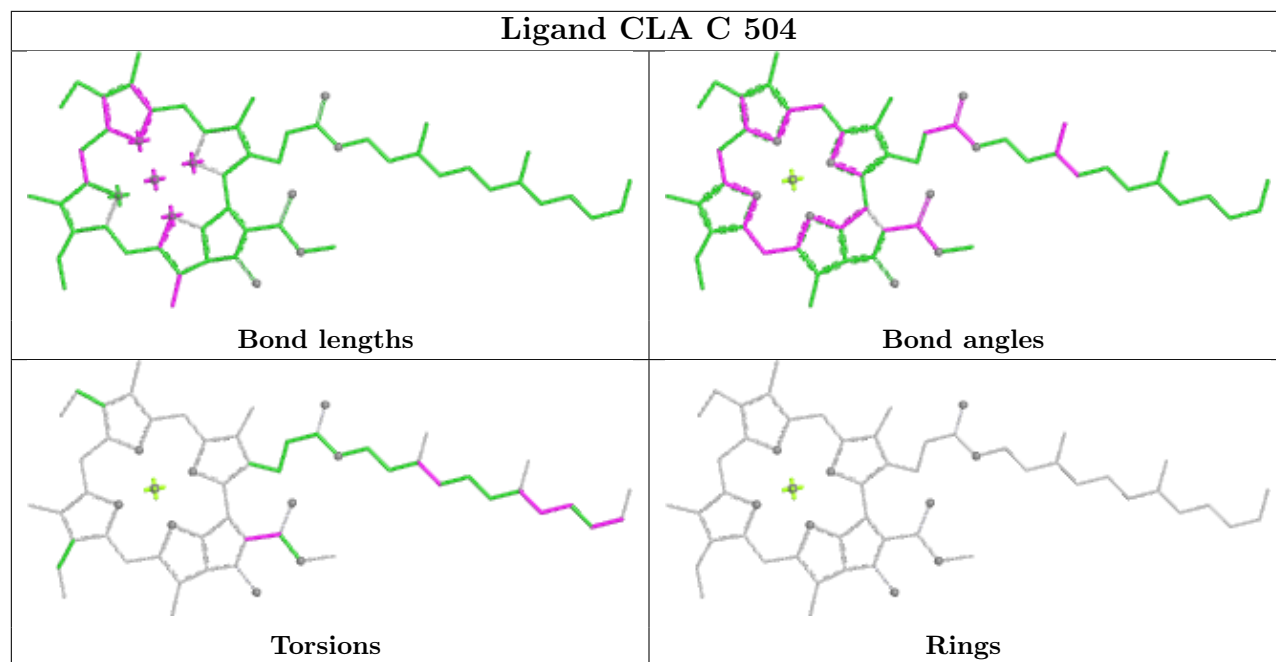


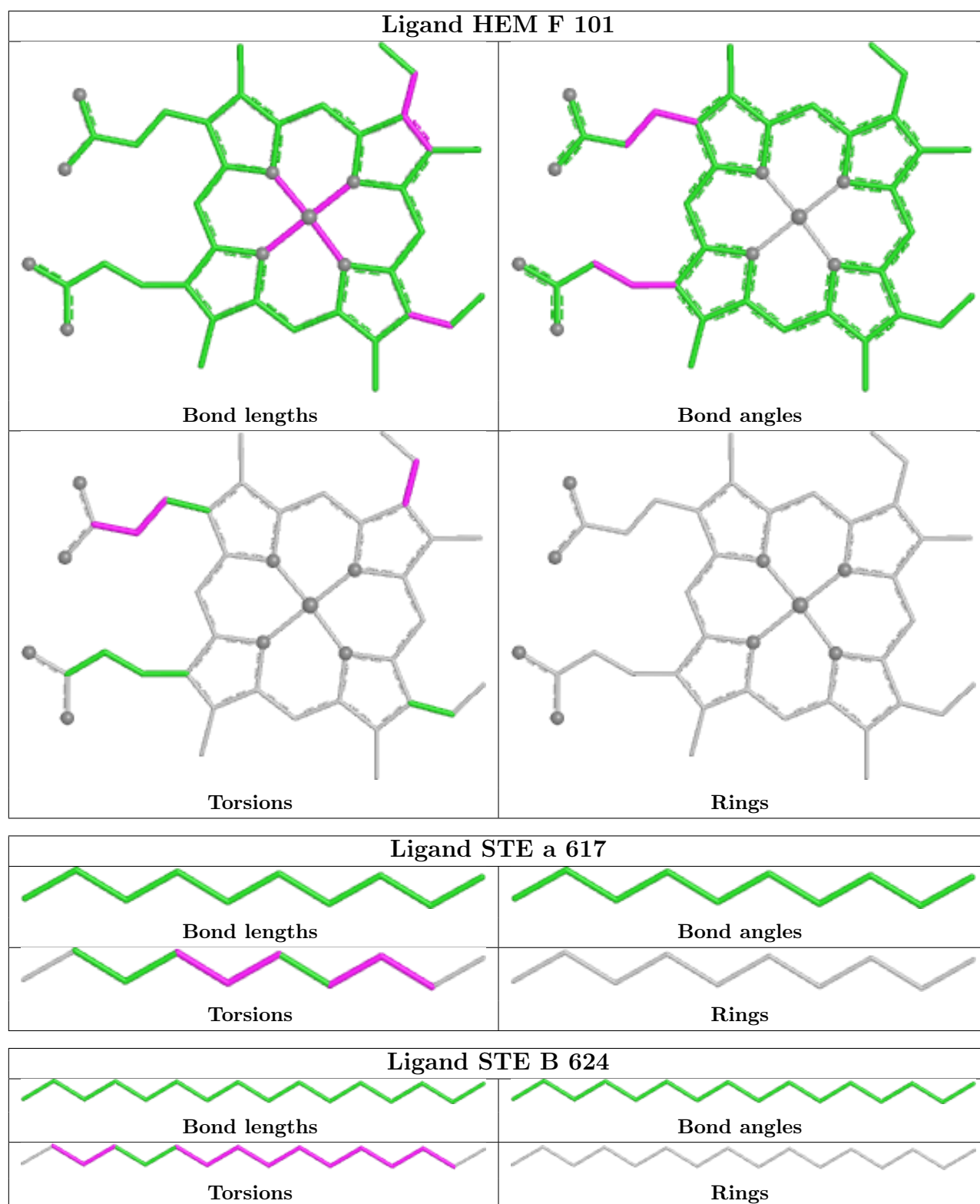


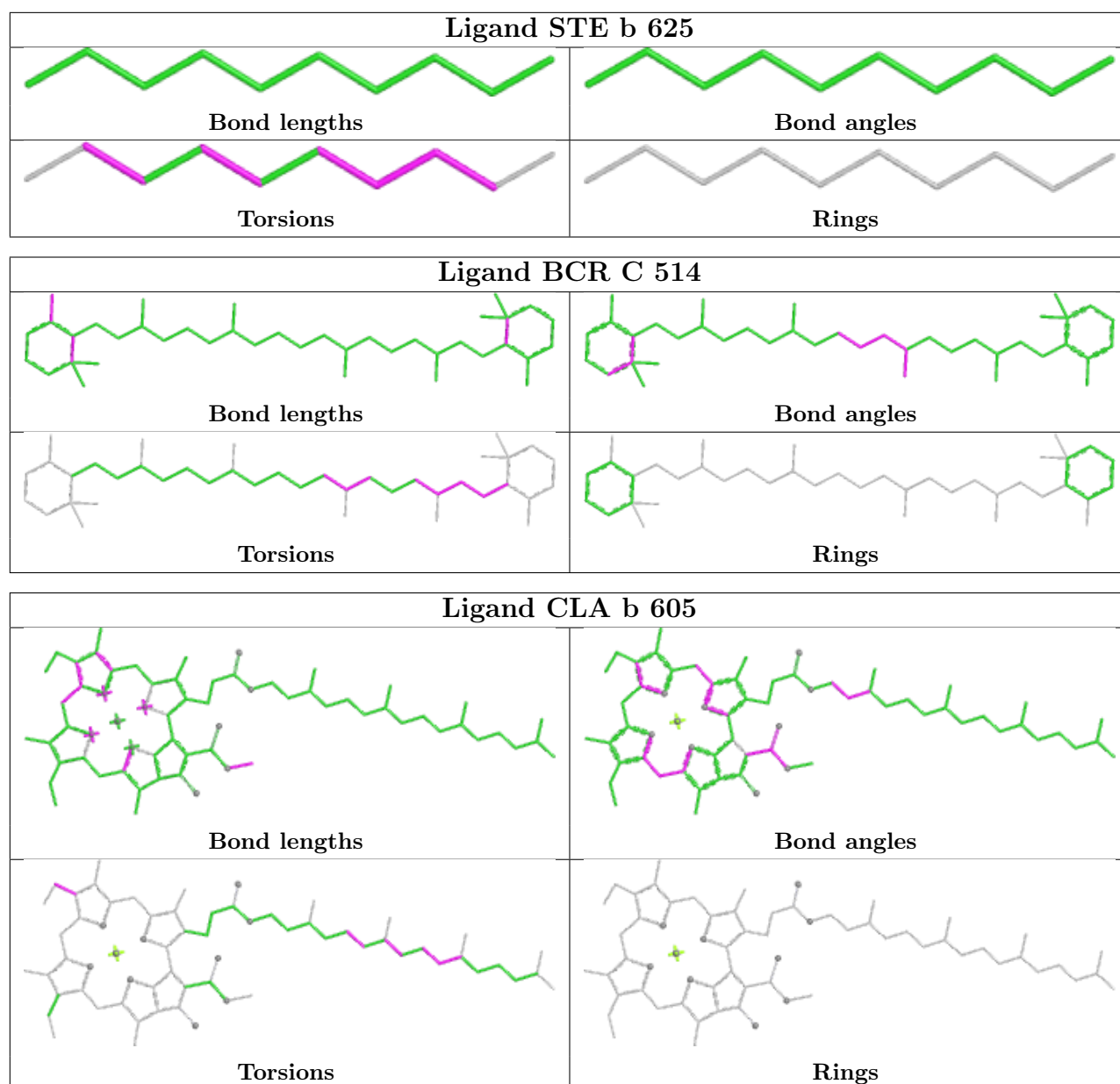


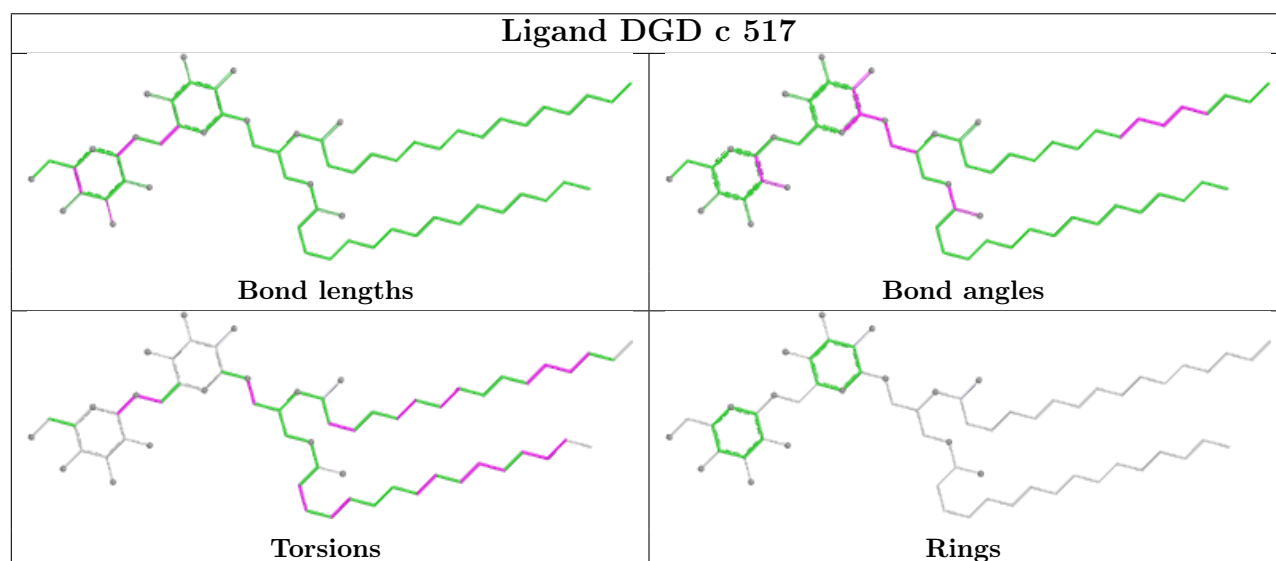
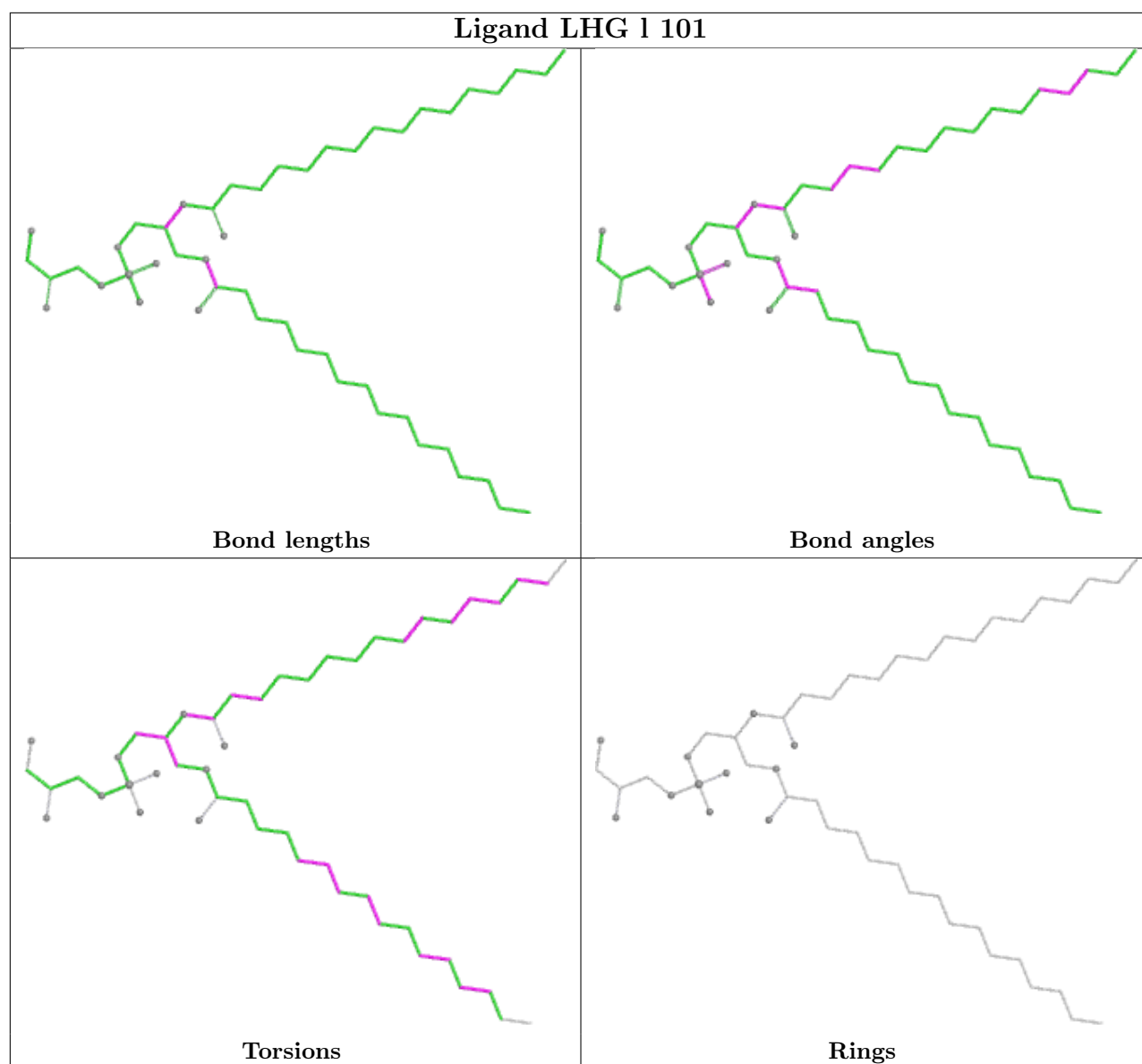


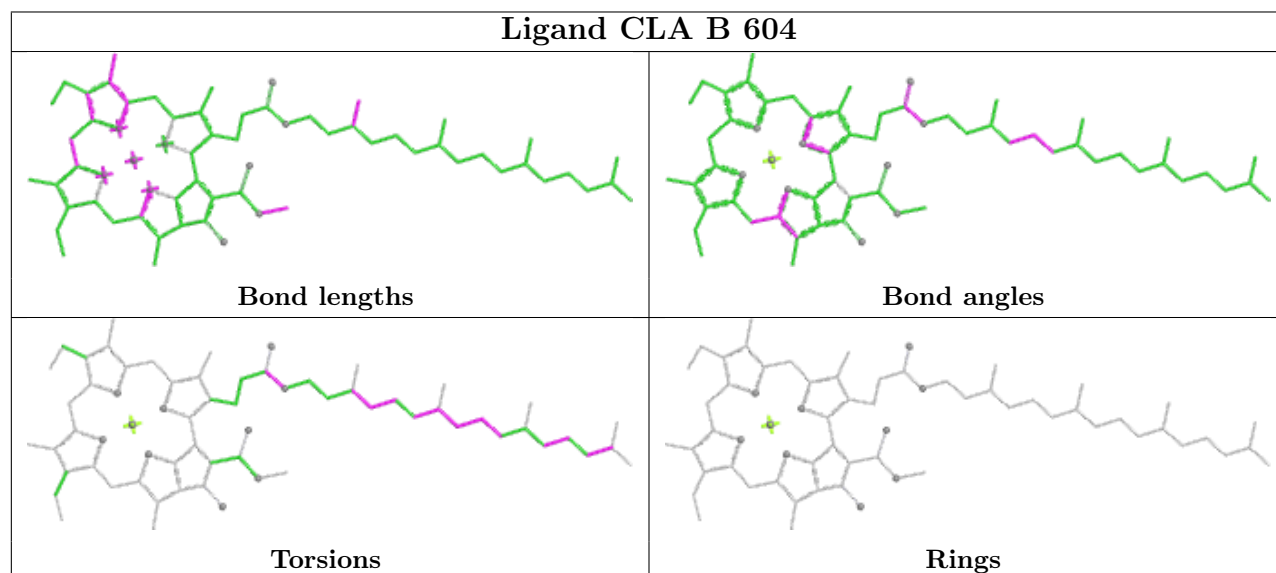
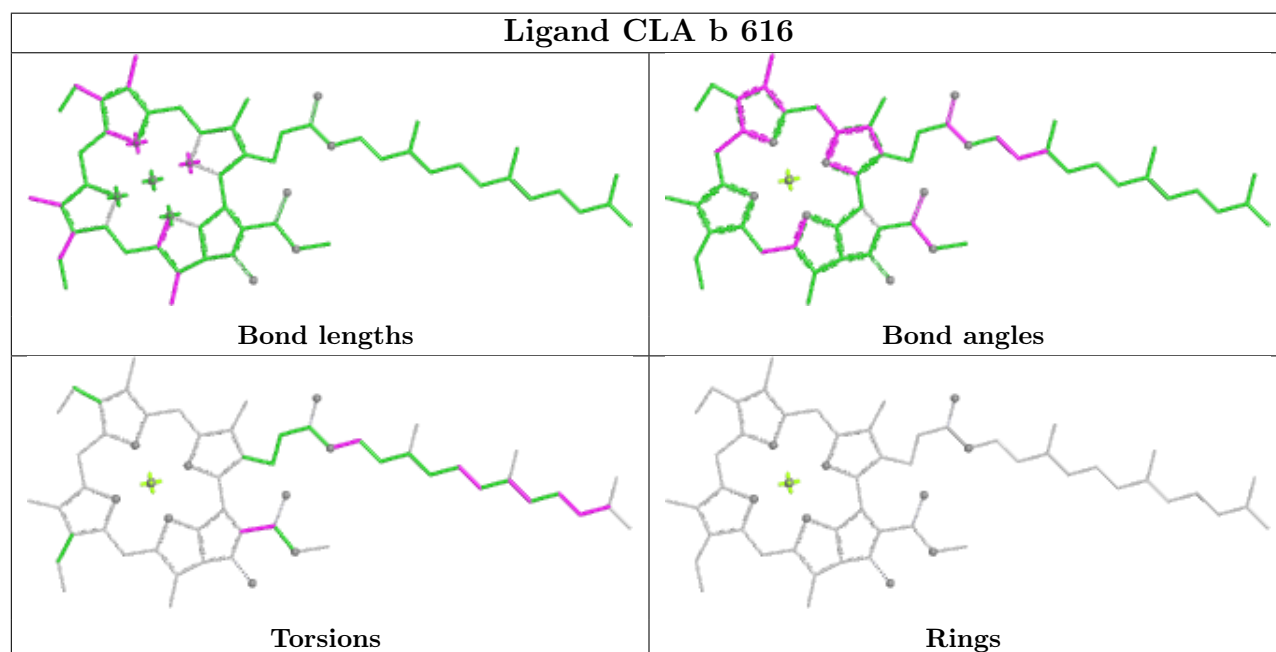
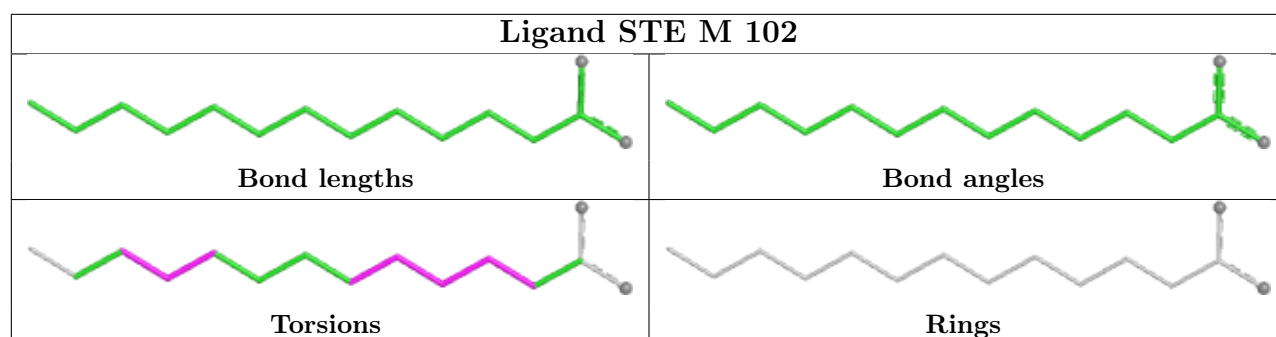


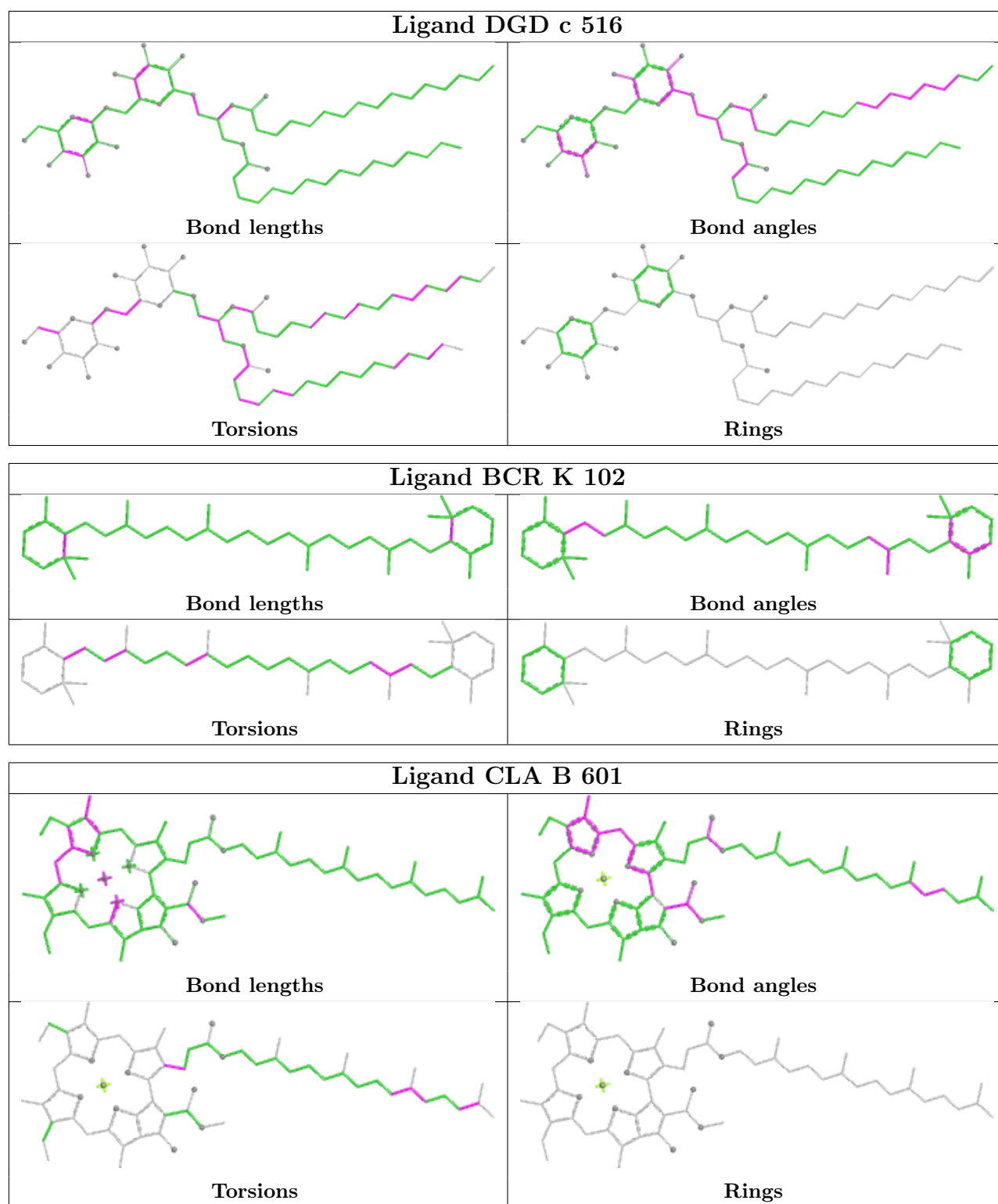


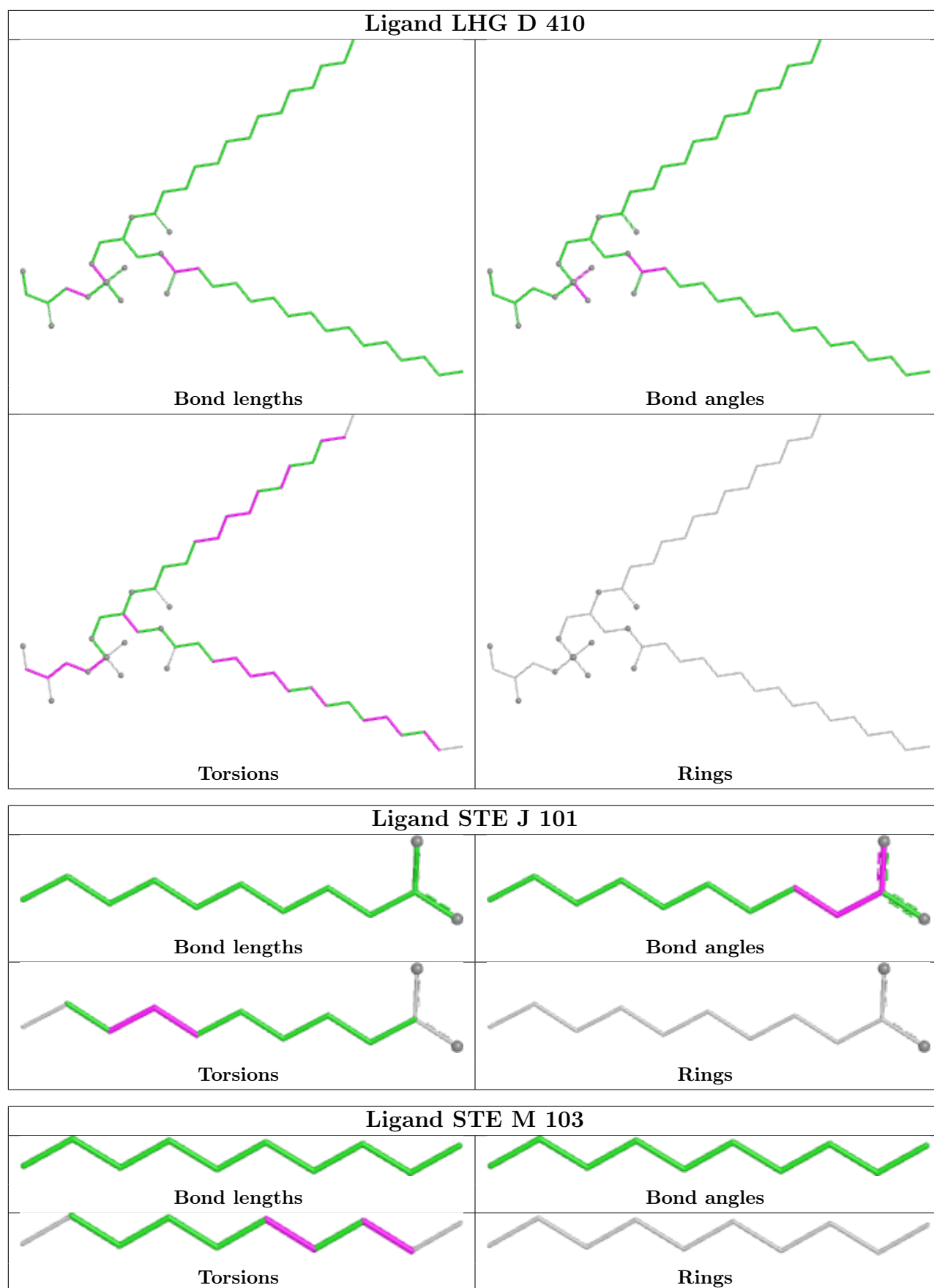


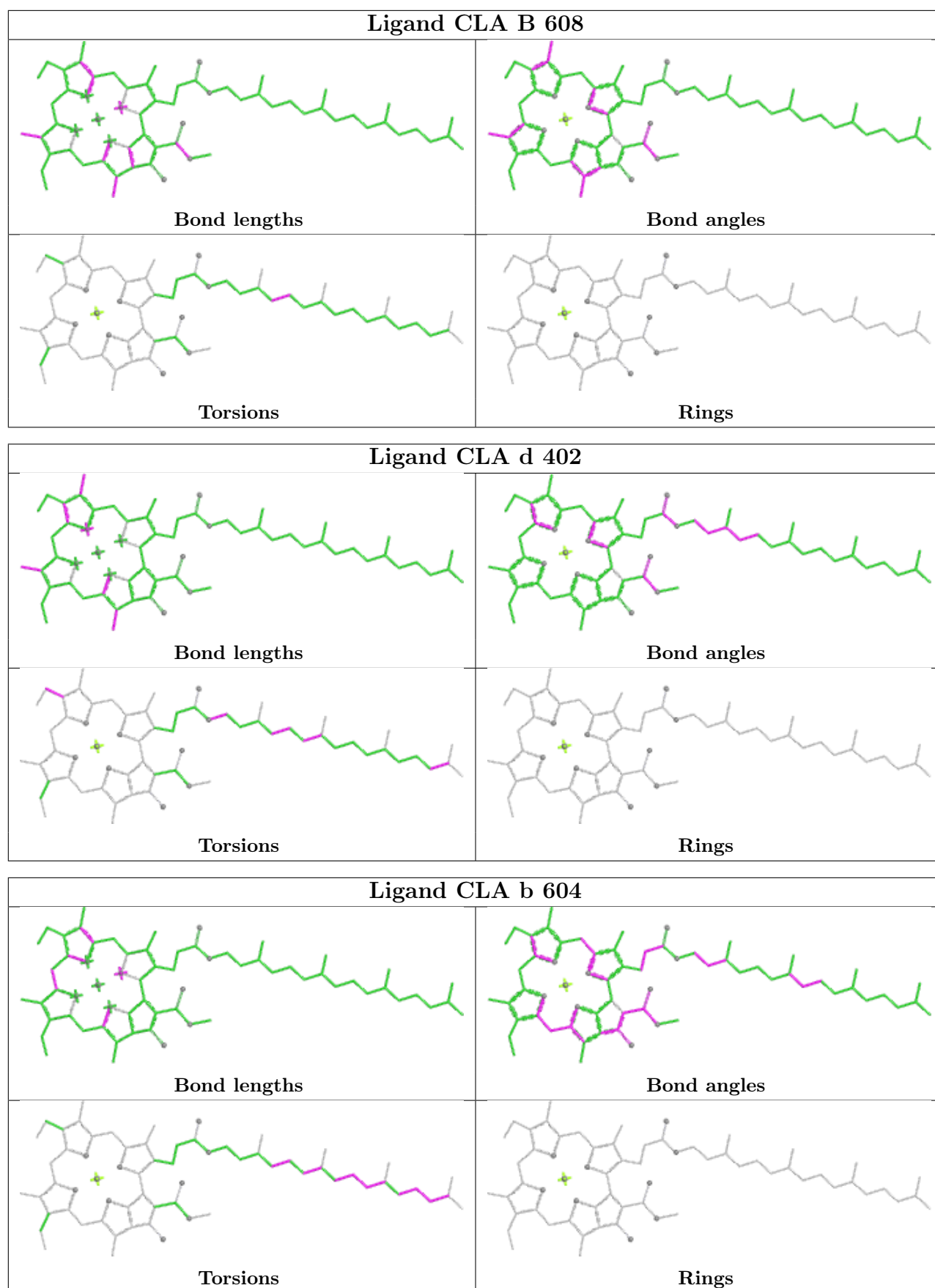


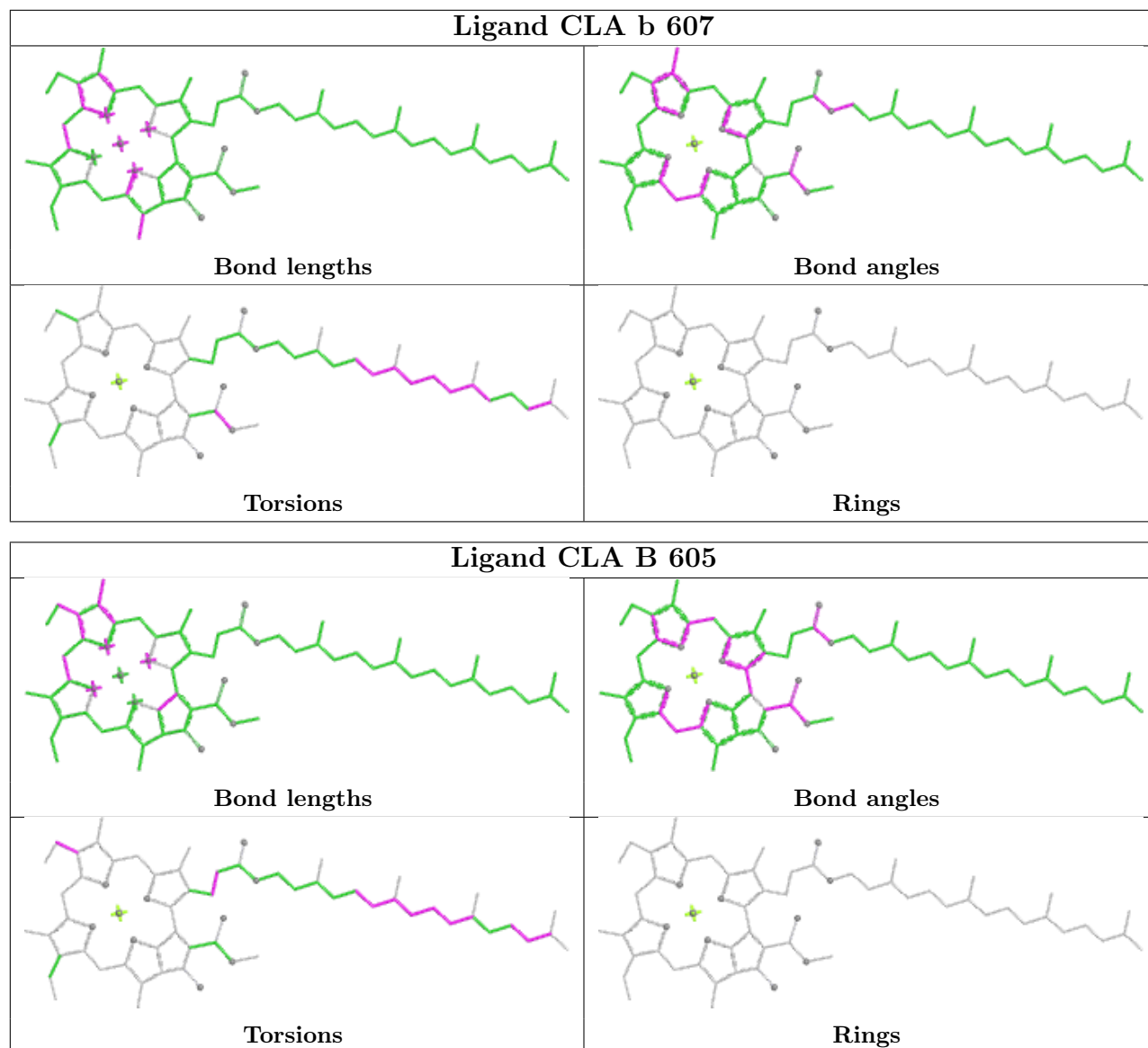


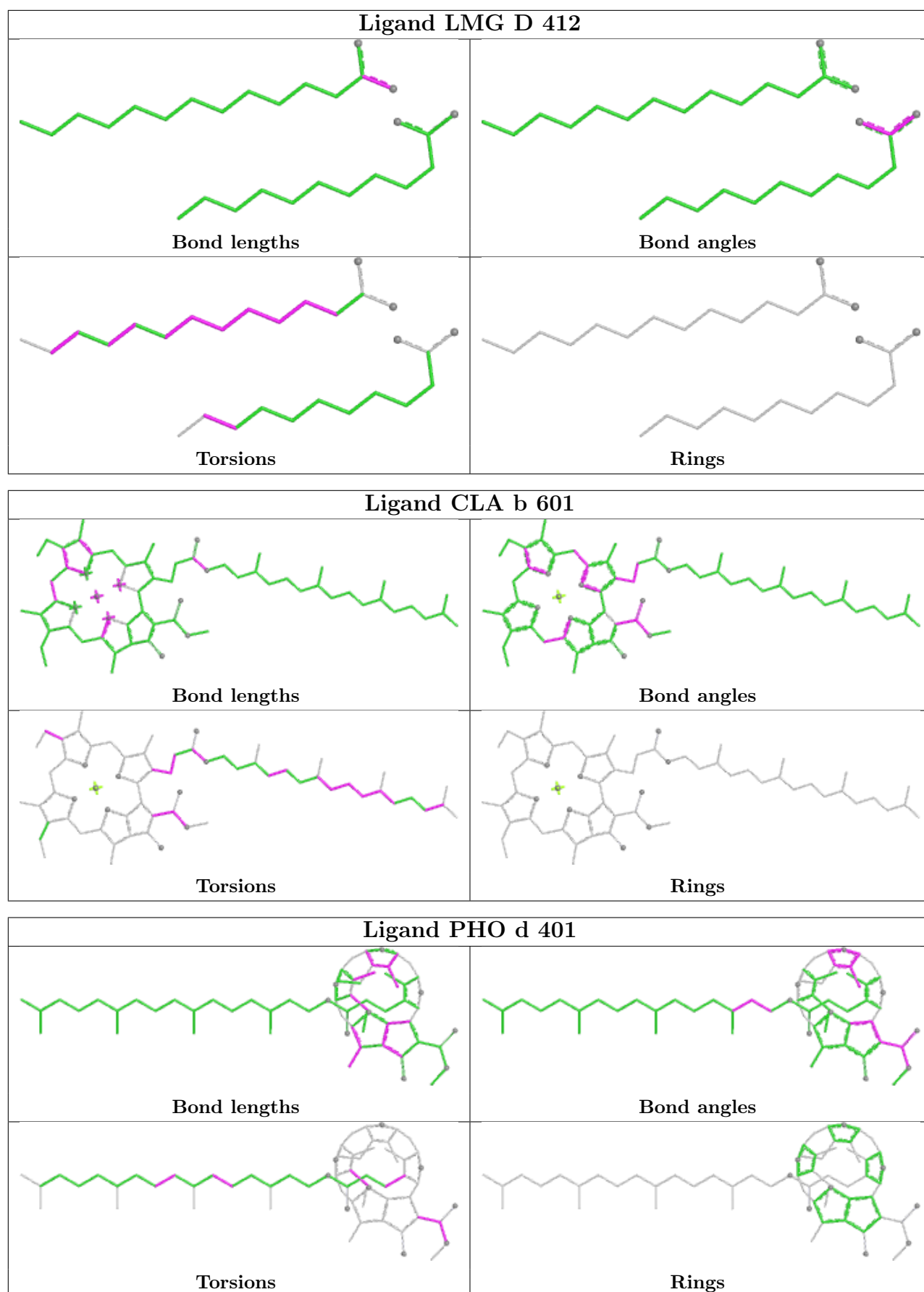


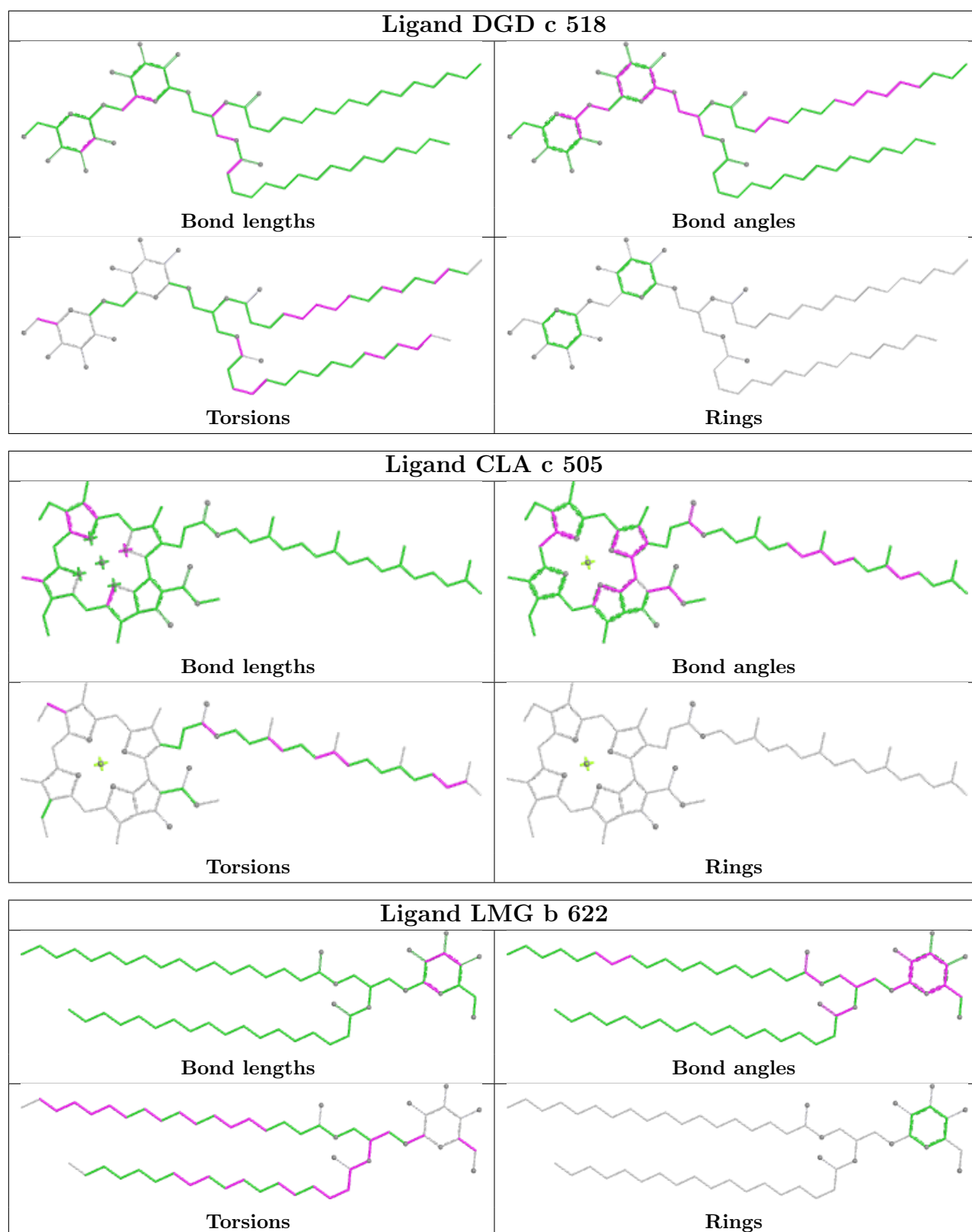


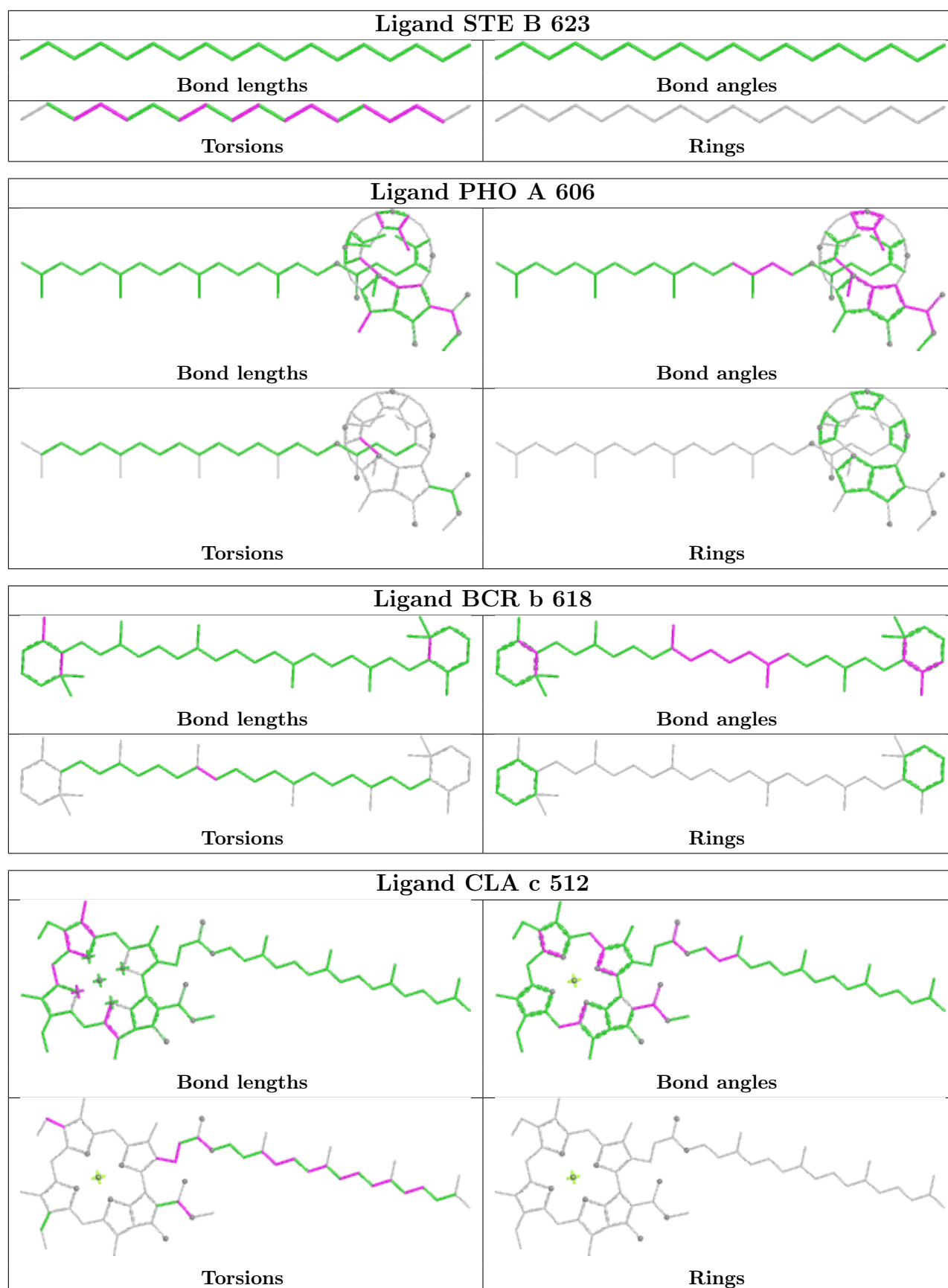


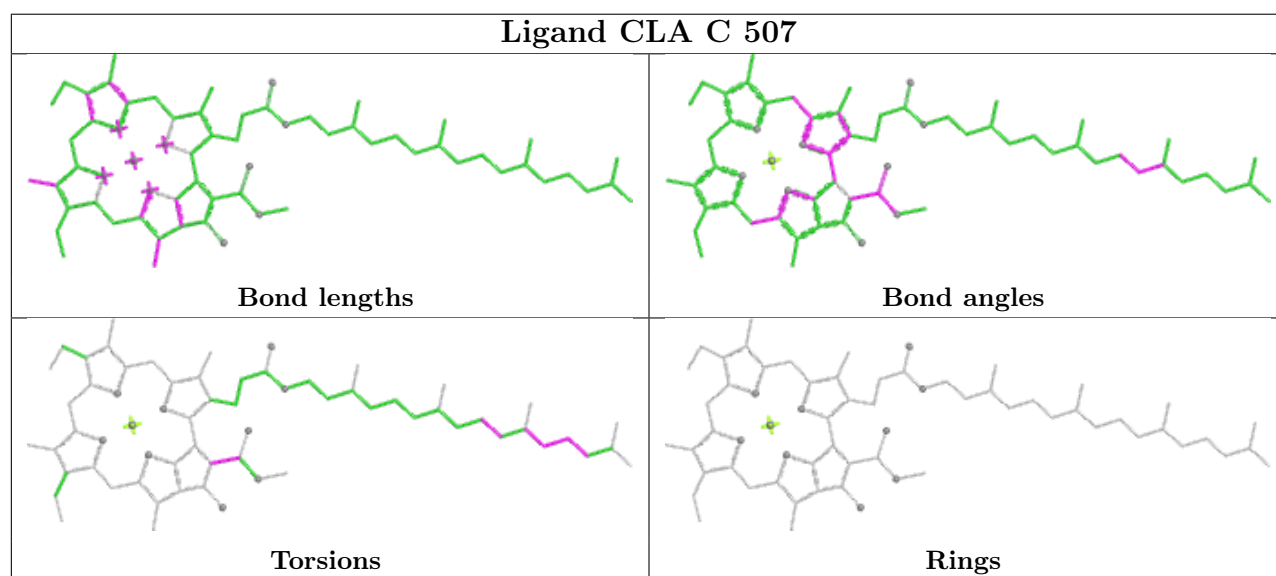
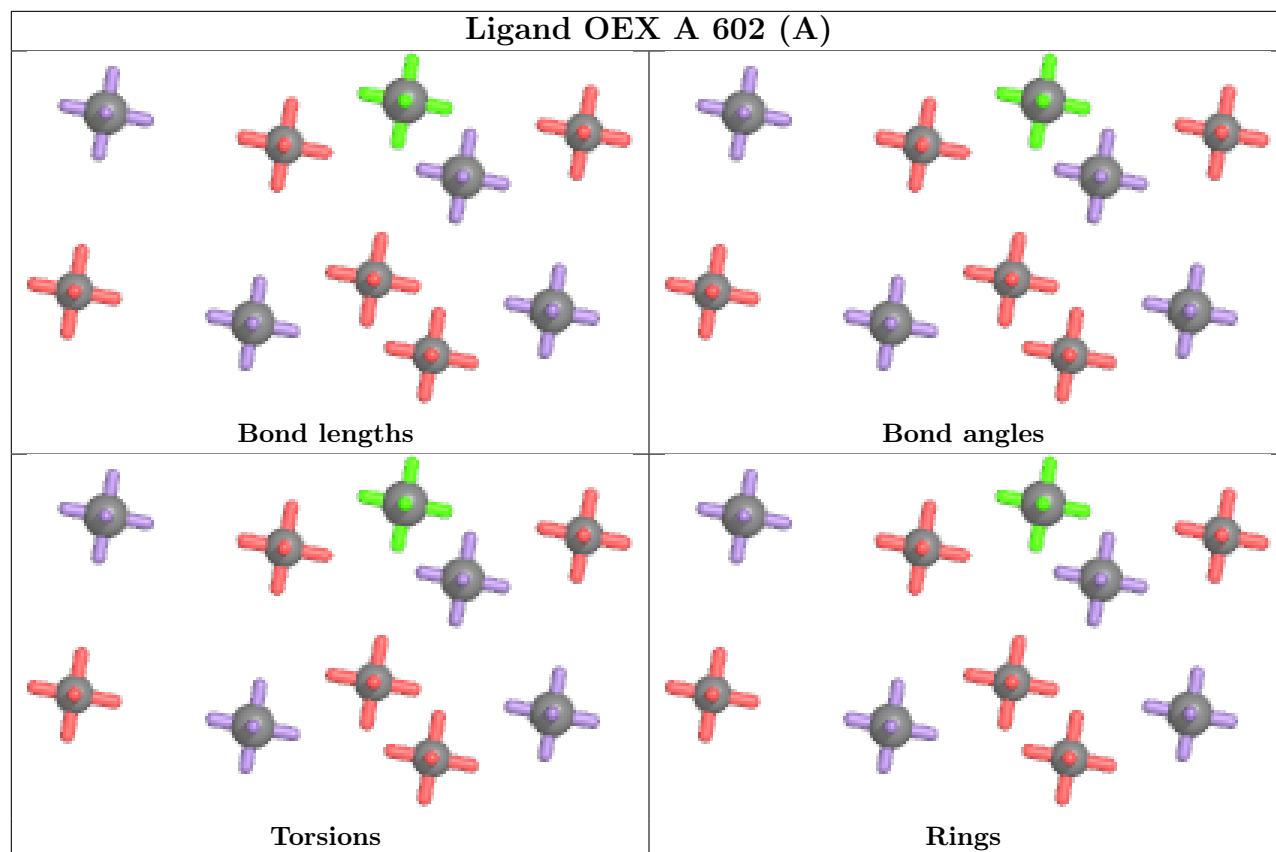


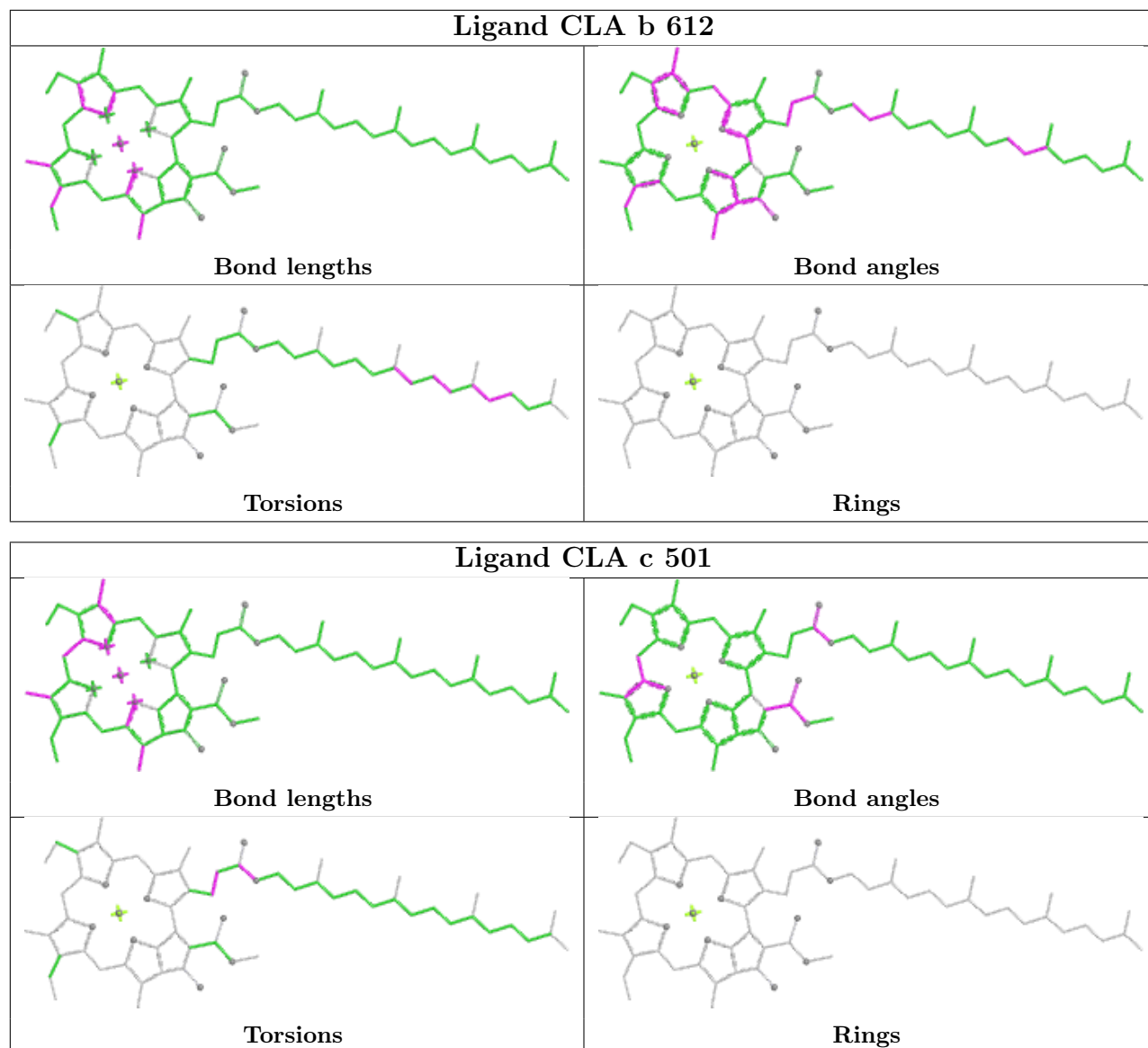


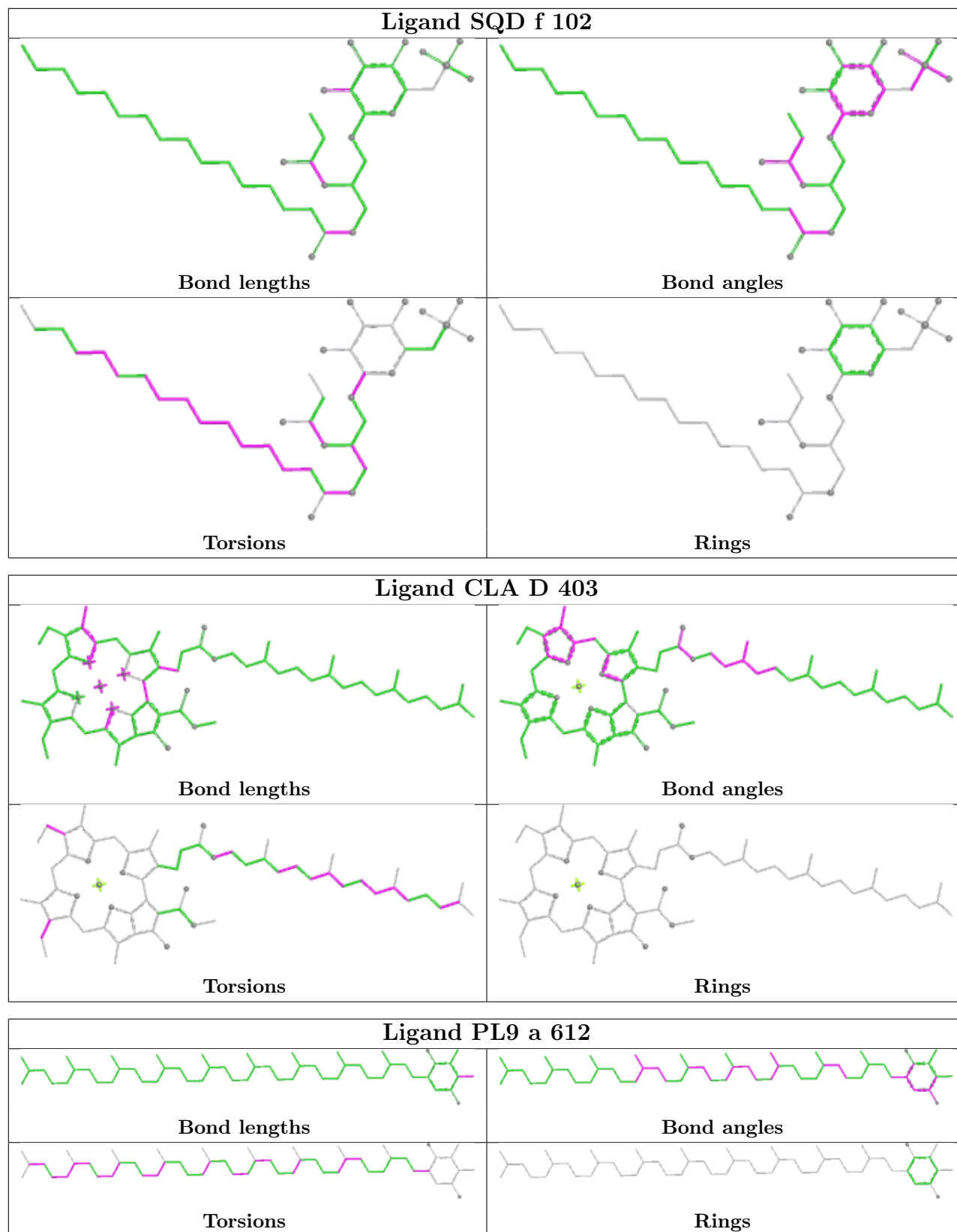


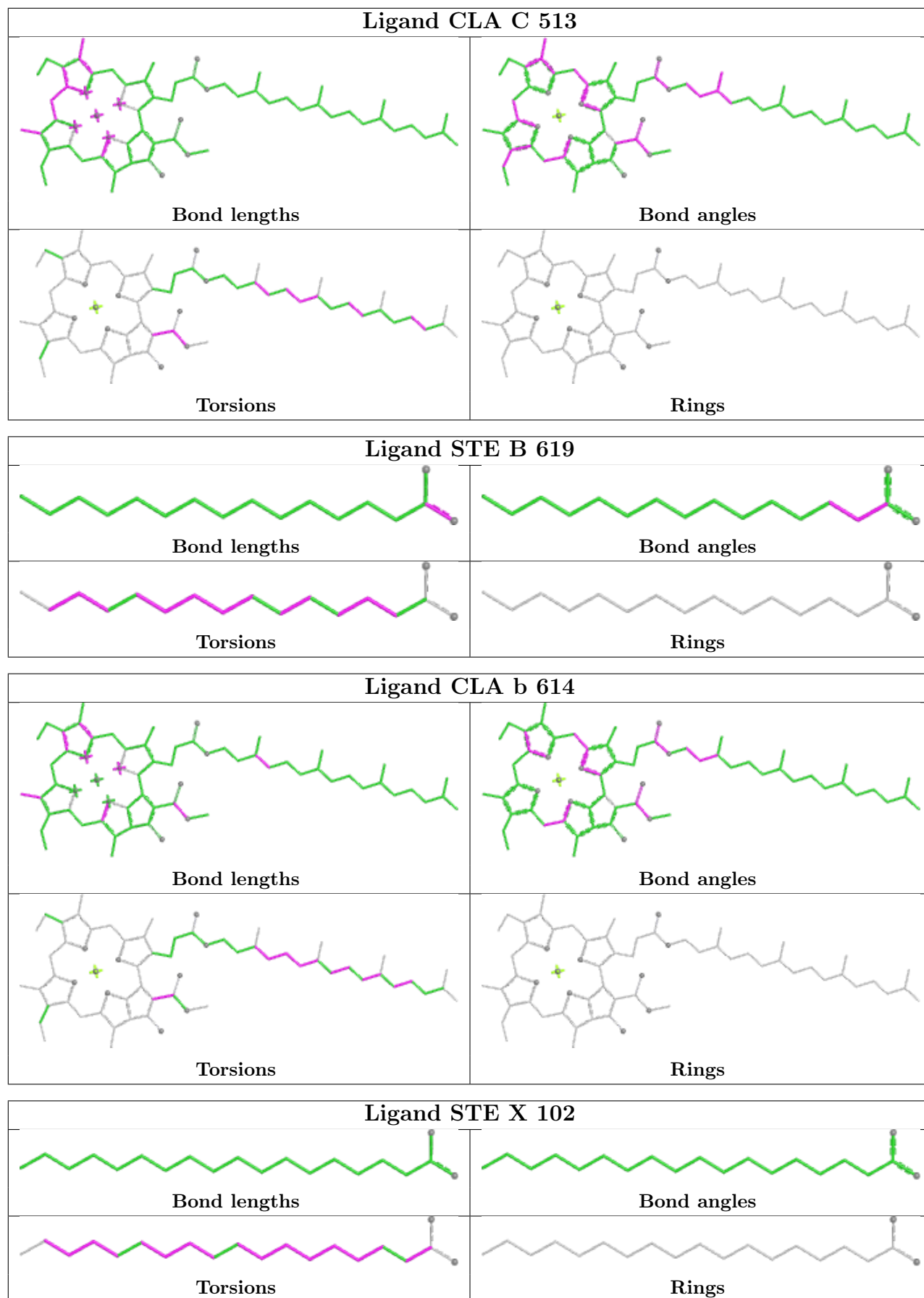


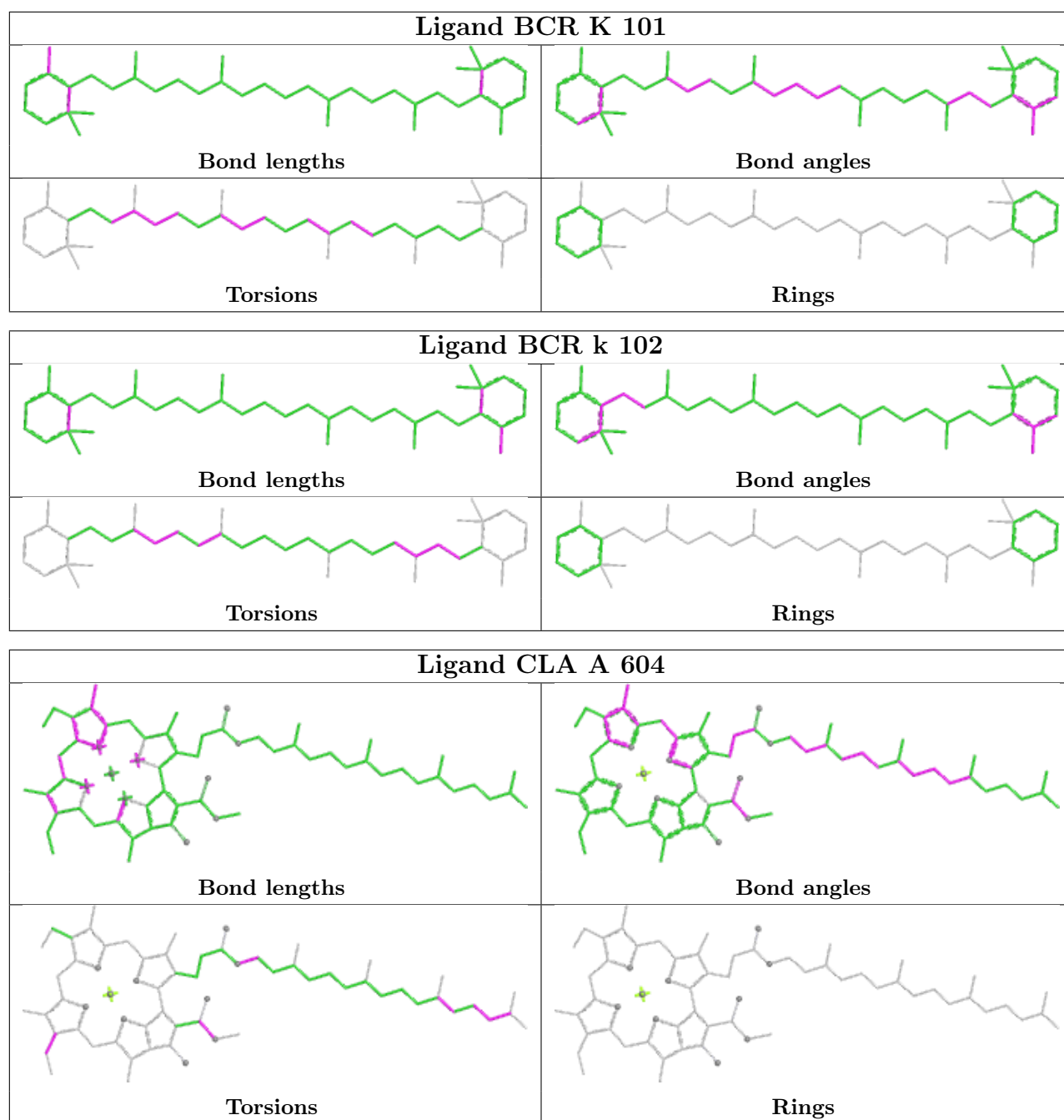


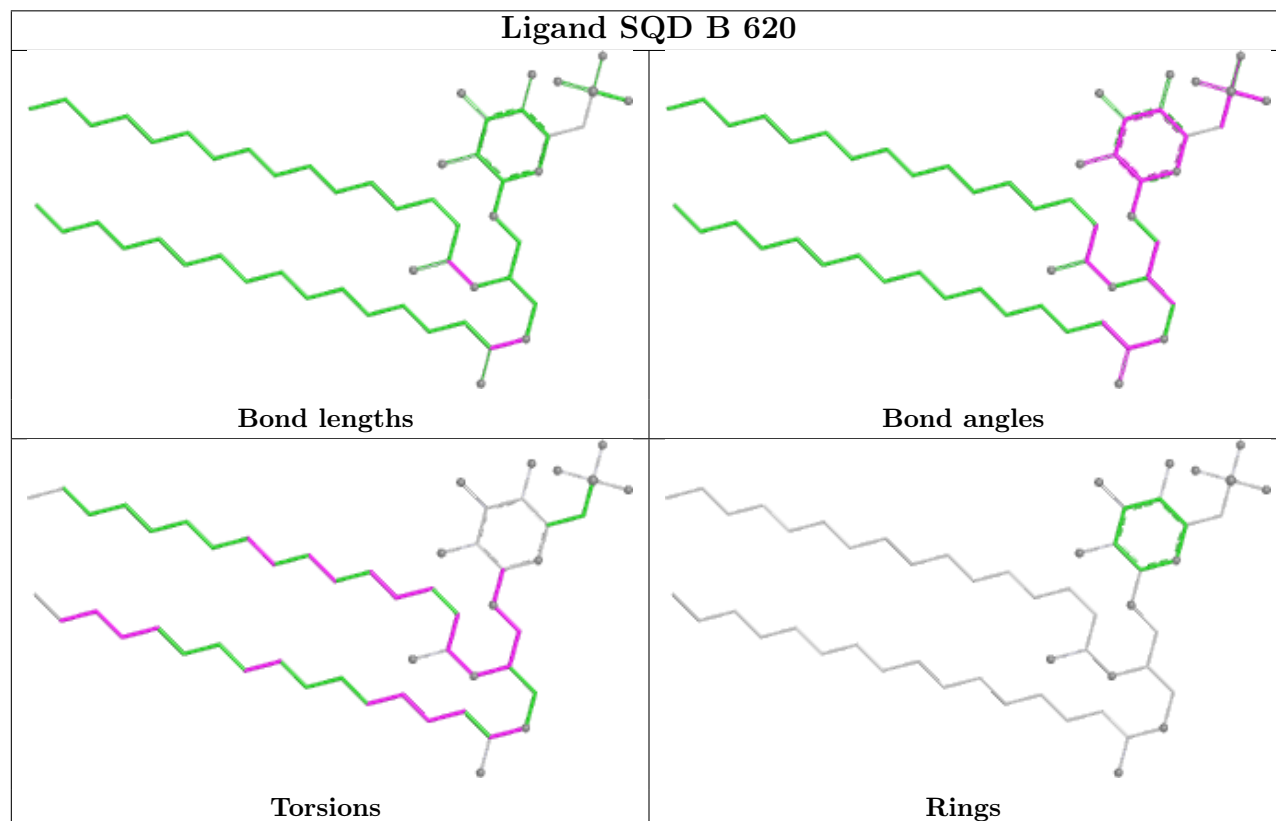
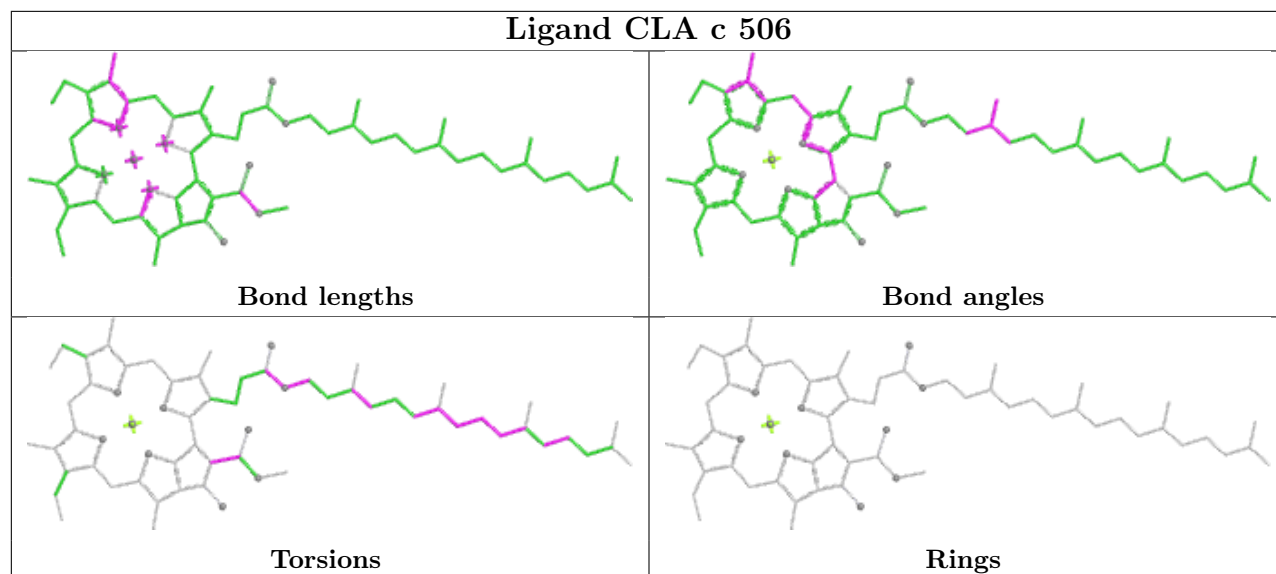


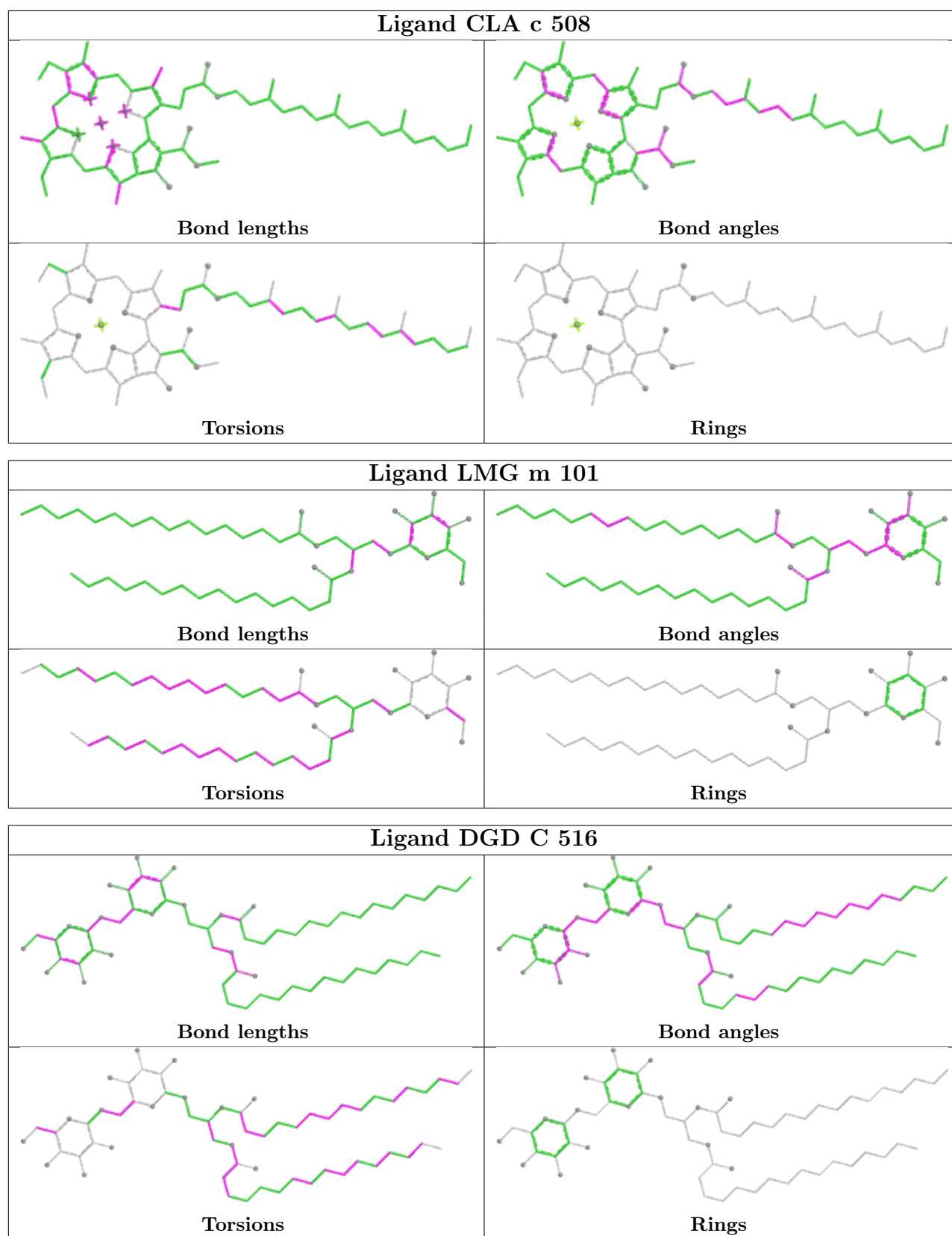


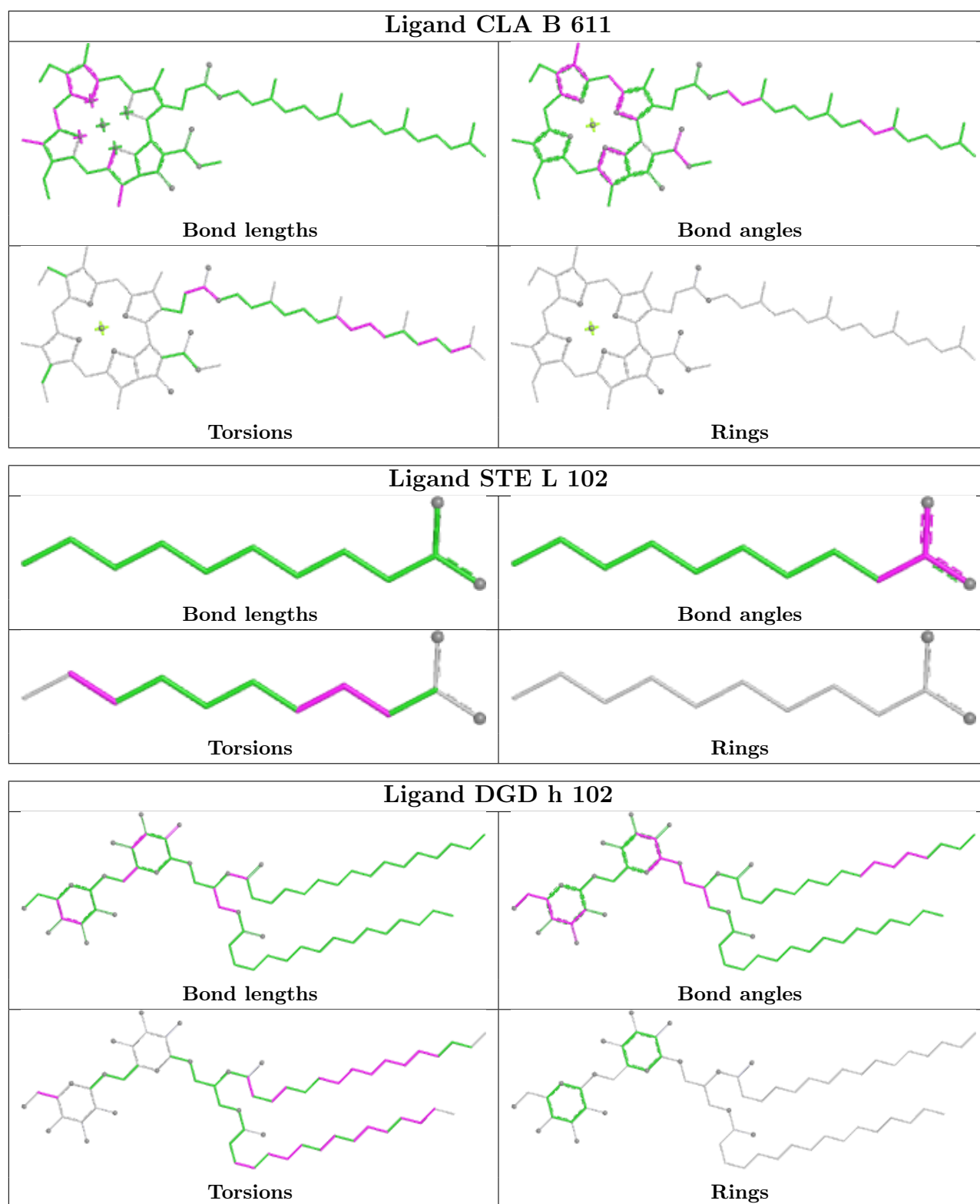


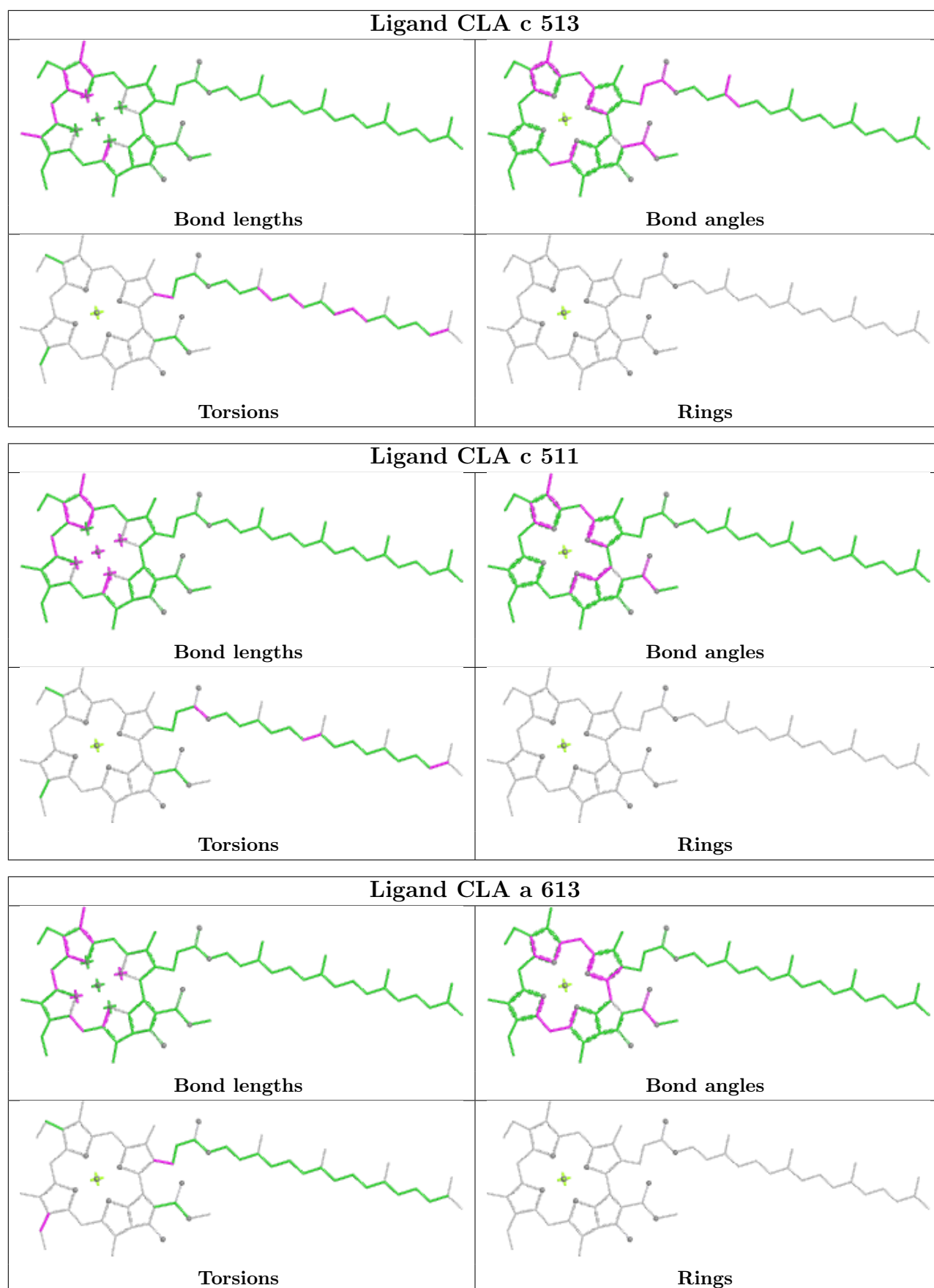


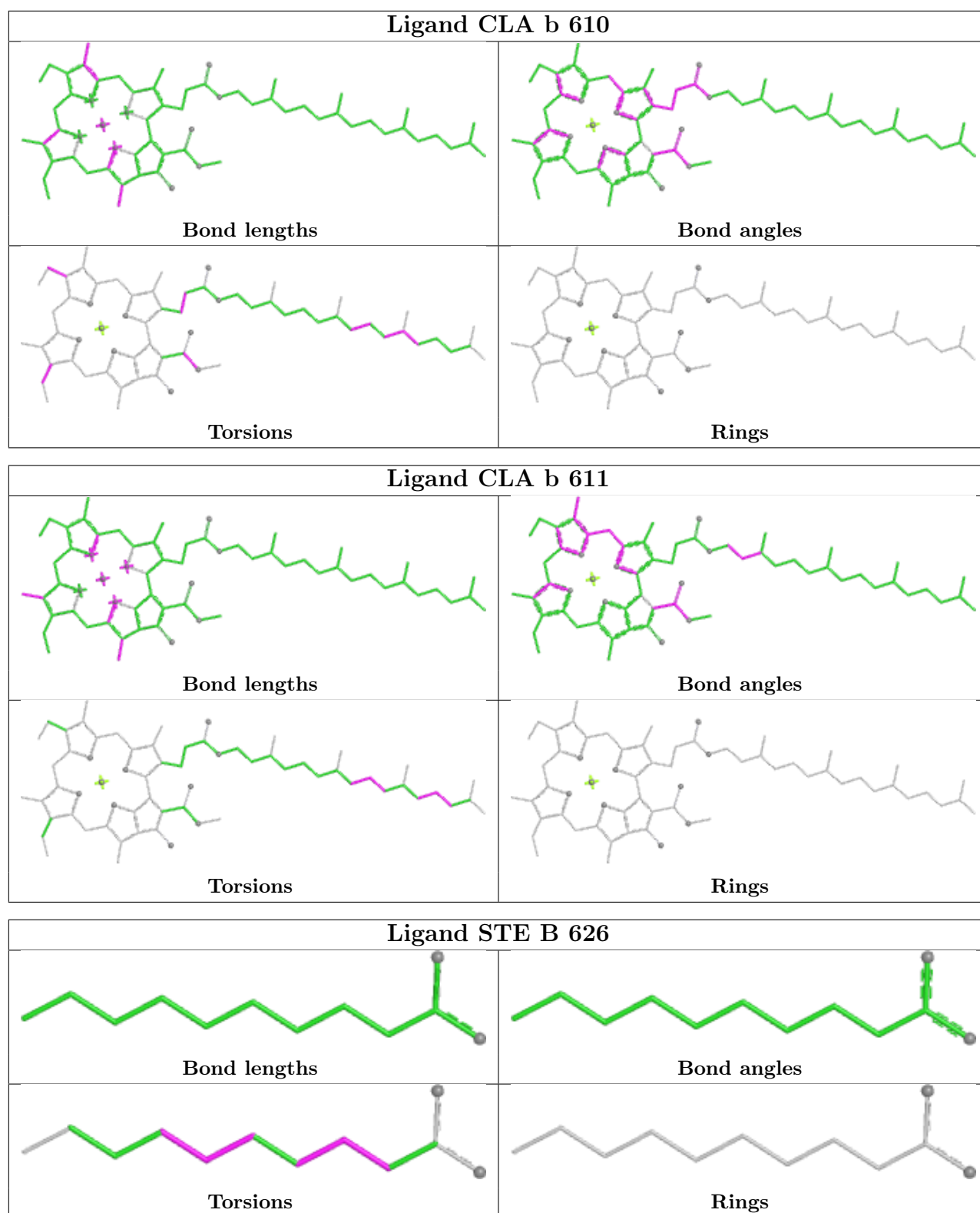


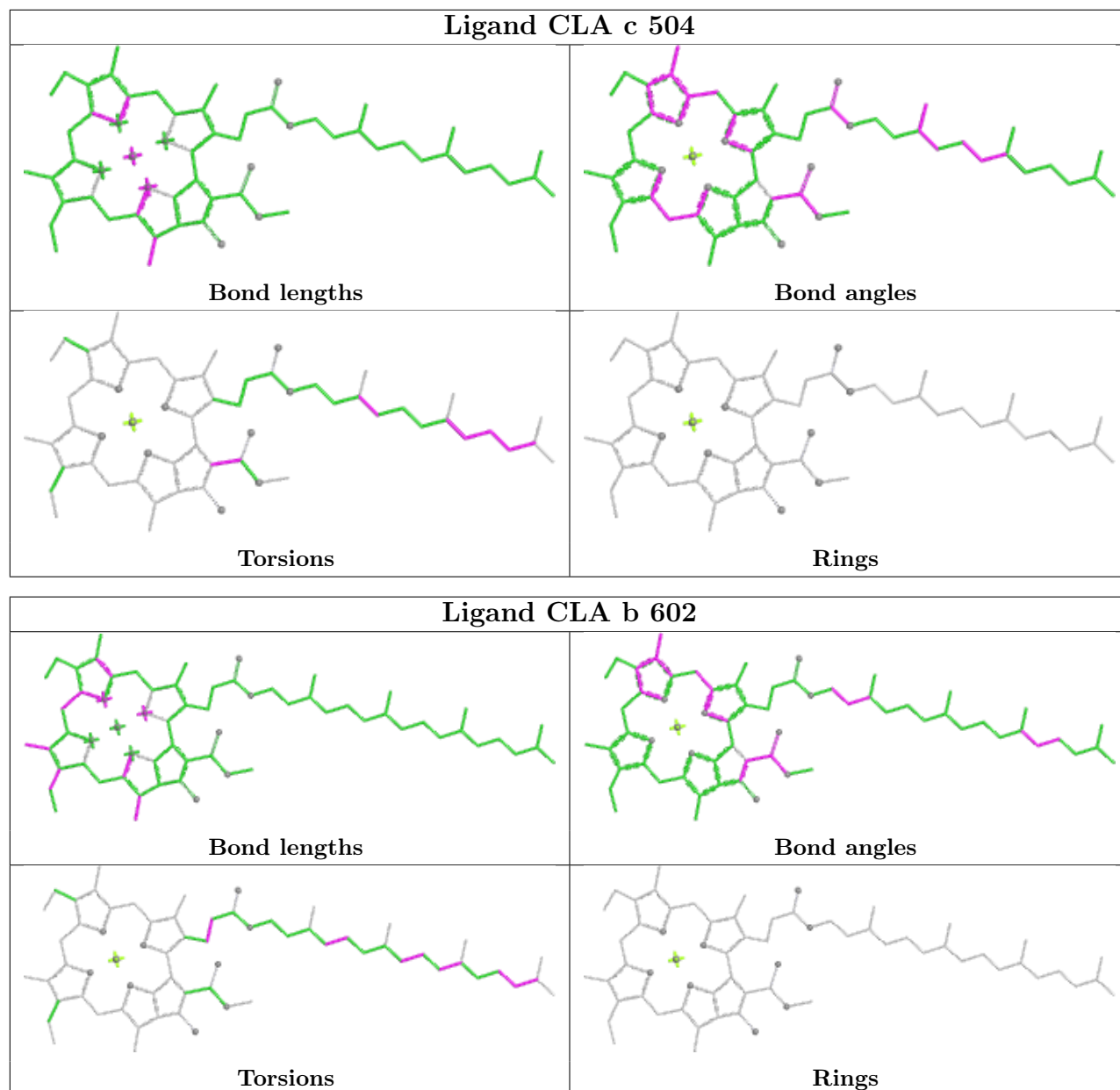


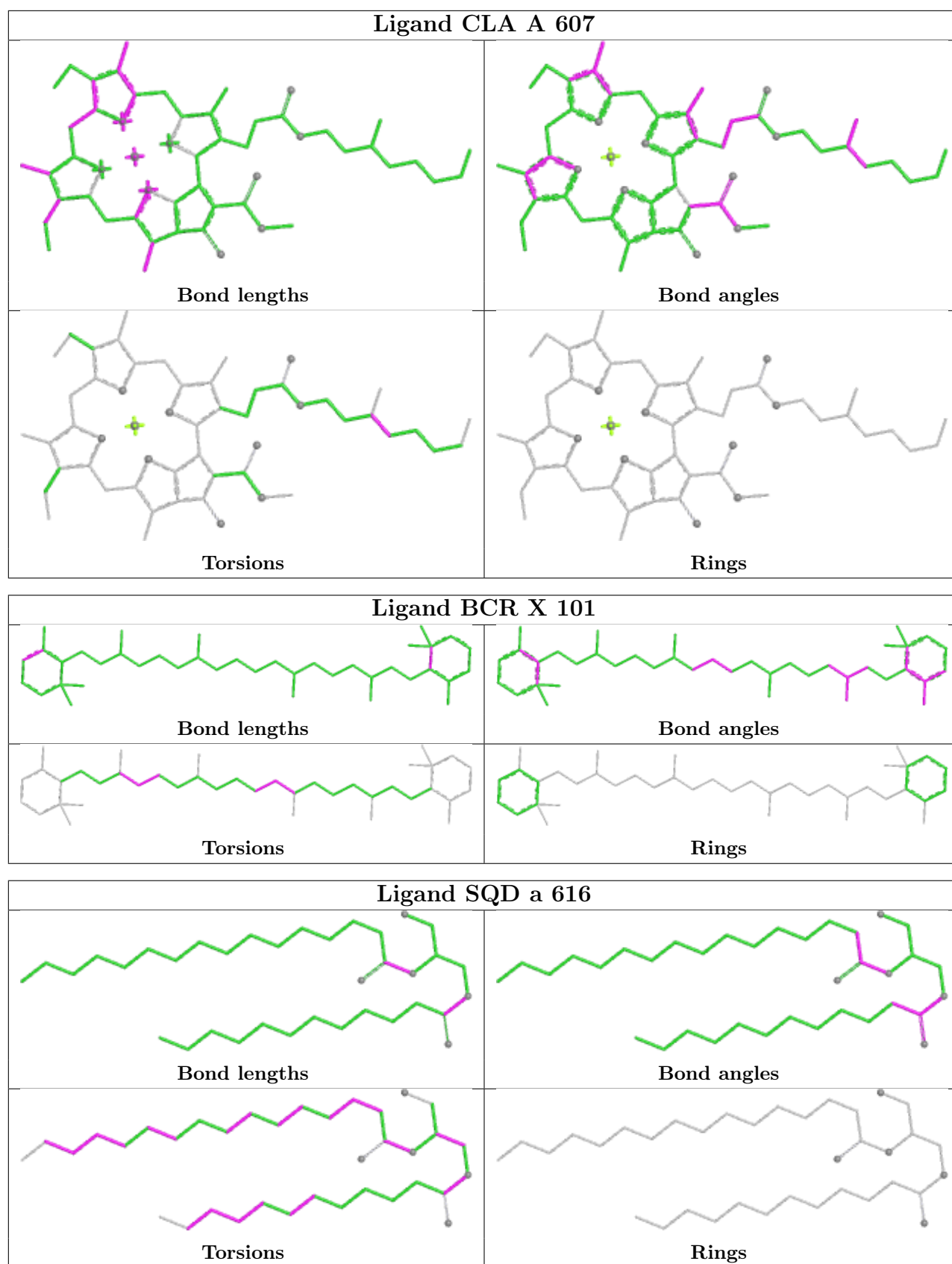


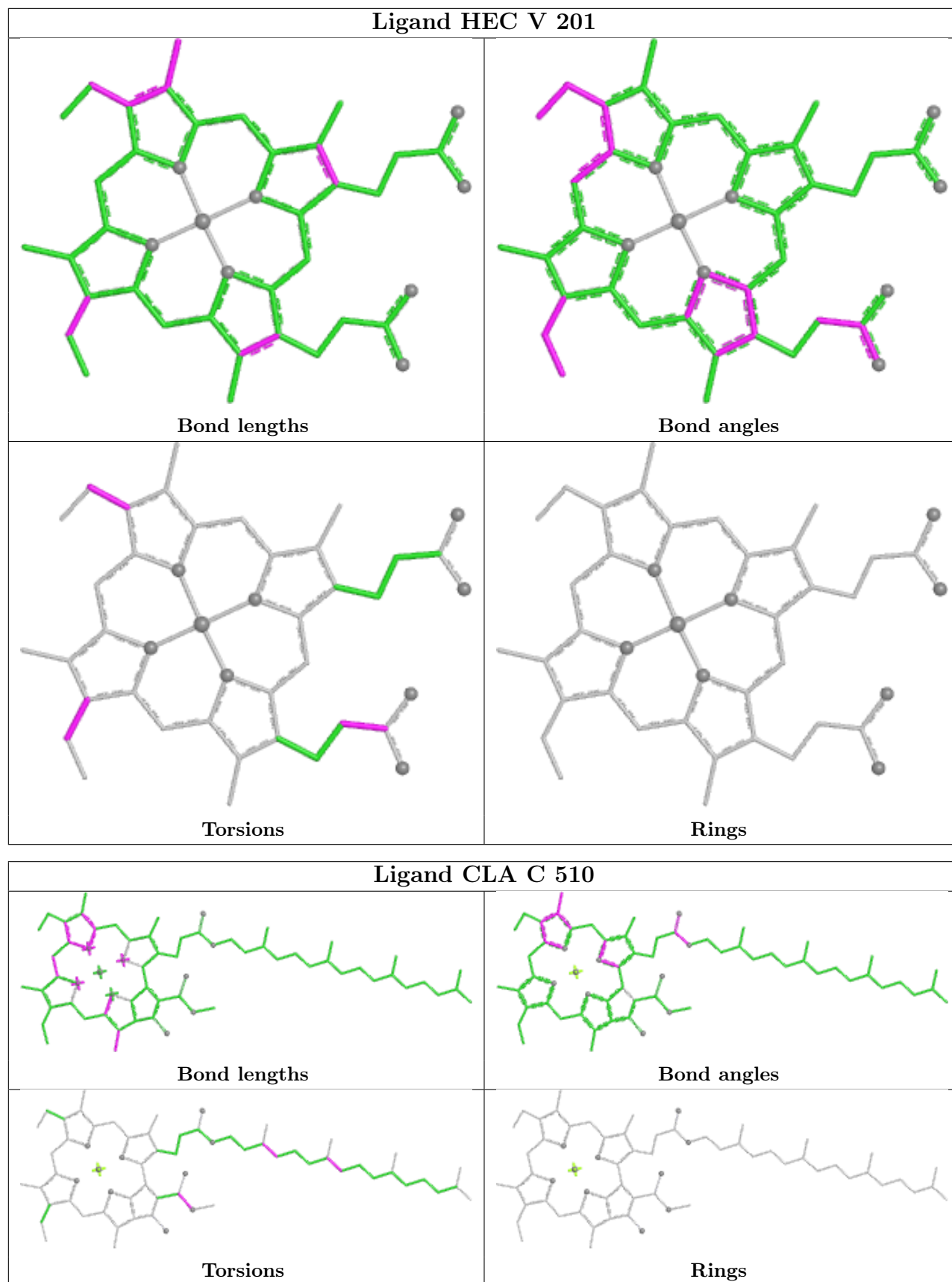


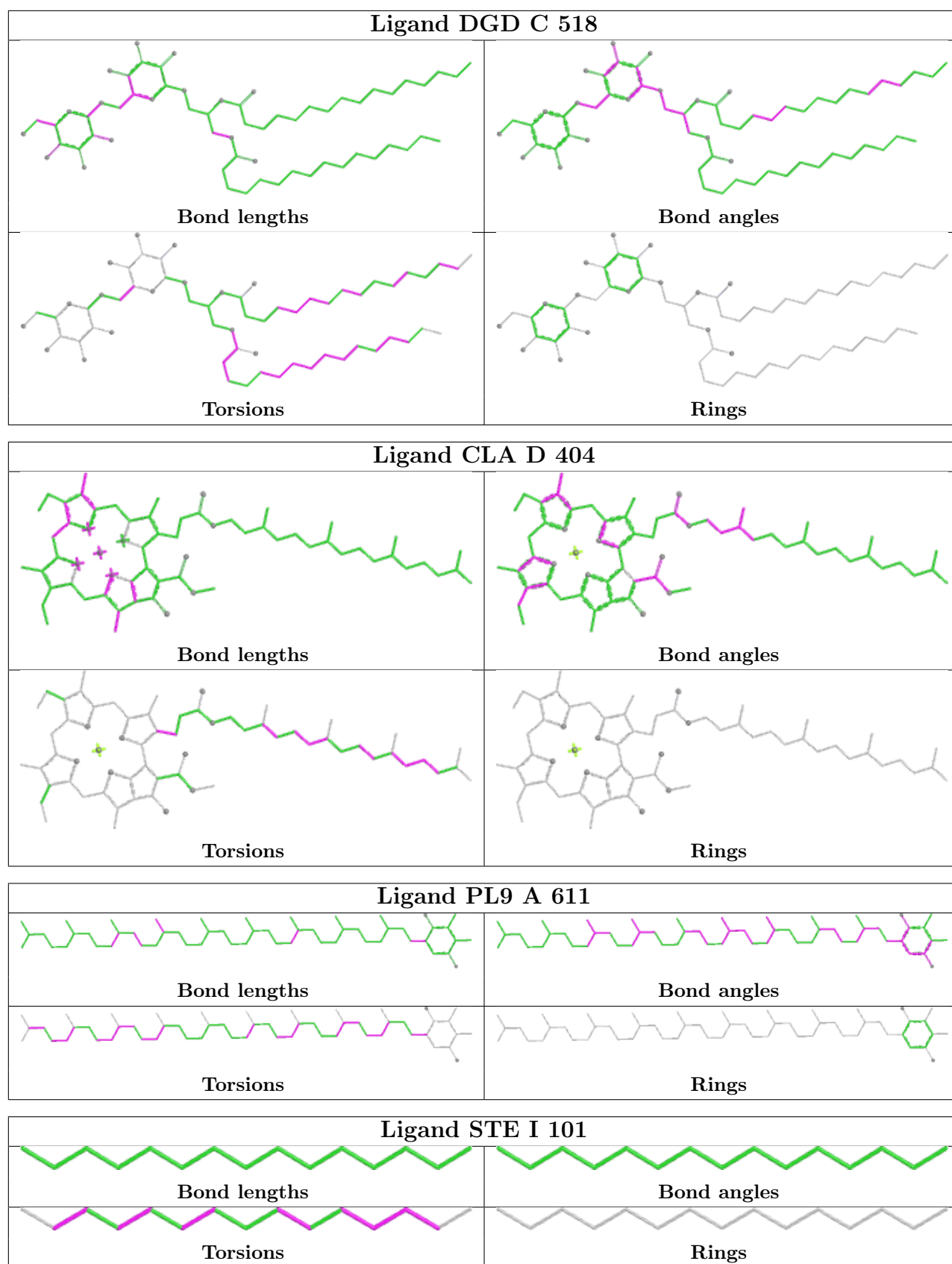


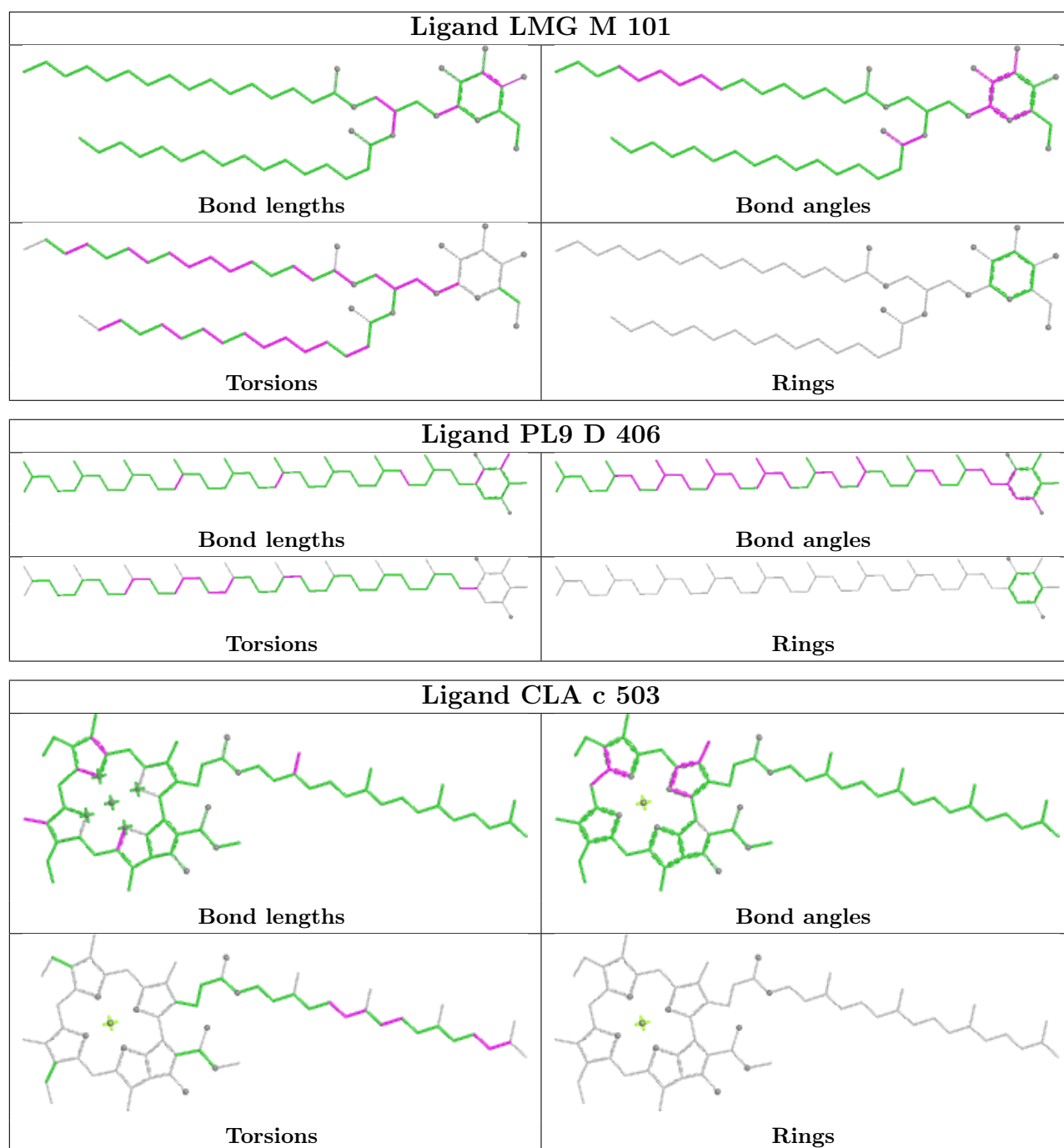


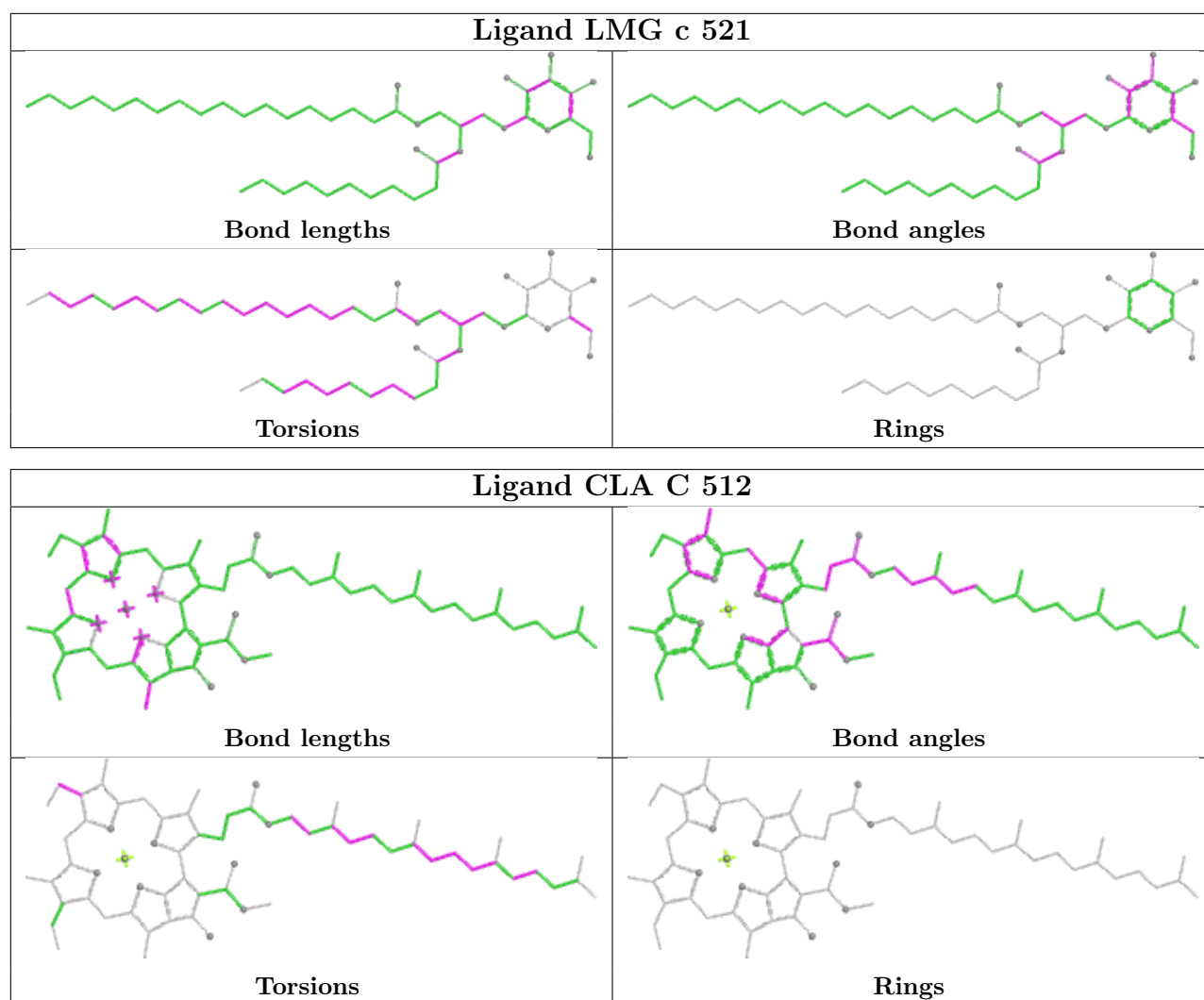












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.51	1 (0%) 90 91	16, 36, 59, 92	64 (19%)
1	a	334/344 (97%)	-0.41	5 (1%) 72 73	16, 38, 67, 90	64 (19%)
2	B	505/510 (99%)	-0.45	1 (0%) 91 92	22, 41, 69, 104	4 (0%)
2	b	505/510 (99%)	-0.35	5 (0%) 79 81	32, 44, 80, 119	0
3	C	442/461 (95%)	-0.41	0 100 100	18, 45, 62, 90	11 (2%)
3	c	451/461 (97%)	-0.31	3 (0%) 84 85	18, 48, 70, 106	12 (2%)
4	D	341/352 (96%)	-0.57	0 100 100	19, 38, 58, 92	2 (0%)
4	d	341/352 (96%)	-0.47	0 100 100	19, 41, 68, 94	3 (0%)
5	E	82/84 (97%)	0.10	3 (3%) 45 45	39, 60, 81, 94	1 (1%)
5	e	82/84 (97%)	0.28	3 (3%) 45 45	43, 71, 92, 101	0
6	F	34/45 (75%)	-0.09	1 (2%) 53 54	45, 53, 80, 106	0
6	f	34/45 (75%)	0.06	1 (2%) 53 54	49, 60, 100, 119	0
7	H	65/66 (98%)	-0.25	2 (3%) 51 51	39, 50, 67, 83	0
7	h	63/66 (95%)	0.01	1 (1%) 70 72	47, 61, 72, 79	0
8	I	35/38 (92%)	-0.37	2 (5%) 29 27	39, 47, 76, 95	0
8	i	35/38 (92%)	-0.23	0 100 100	39, 48, 80, 86	0
9	J	36/40 (90%)	-0.01	1 (2%) 55 55	44, 60, 92, 103	0
9	j	36/40 (90%)	0.00	1 (2%) 55 55	46, 63, 100, 114	0
10	K	37/46 (80%)	0.01	0 100 100	53, 63, 87, 92	0
10	k	37/46 (80%)	0.10	0 100 100	55, 66, 85, 92	0
11	L	37/37 (100%)	-0.63	0 100 100	33, 37, 70, 75	0
11	l	36/37 (97%)	-0.52	1 (2%) 55 55	29, 39, 73, 96	0
12	M	32/36 (88%)	-0.42	1 (3%) 51 51	32, 42, 65, 79	0
12	m	31/36 (86%)	-0.48	0 100 100	33, 42, 62, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.21	2 (0%) 82 84	32, 50, 89, 135	1 (0%)
13	o	244/272 (89%)	-0.26	2 (0%) 82 84	31, 48, 87, 133	0
14	R	28/41 (68%)	1.53	9 (32%) 1 1	81, 97, 111, 119	0
14	r	28/41 (68%)	2.22	15 (53%) 0 0	90, 127, 142, 149	0
15	T	29/32 (90%)	-0.52	0 100 100	33, 39, 66, 86	0
15	t	29/32 (90%)	-0.40	1 (3%) 48 48	35, 40, 76, 84	0
16	U	97/134 (72%)	-0.30	0 100 100	39, 52, 76, 96	0
16	u	97/134 (72%)	-0.37	0 100 100	37, 48, 63, 91	0
17	V	137/163 (84%)	-0.41	0 100 100	34, 48, 65, 79	0
17	v	137/163 (84%)	-0.17	0 100 100	40, 56, 78, 87	0
18	X	38/41 (92%)	-0.07	0 100 100	48, 61, 83, 86	0
18	x	39/41 (95%)	0.30	1 (2%) 57 58	54, 72, 99, 115	0
19	Y	27/46 (58%)	0.92	2 (7%) 20 18	64, 85, 99, 105	0
19	y	30/46 (65%)	0.65	0 100 100	68, 84, 103, 109	0
20	Z	62/62 (100%)	0.60	4 (6%) 25 23	65, 81, 128, 135	0
20	z	62/62 (100%)	0.67	5 (8%) 18 16	68, 79, 118, 135	0
All	All	5293/5700 (92%)	-0.28	73 (1%) 73 75	16, 46, 85, 149	162 (3%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	6.4
14	r	14	LEU	5.0
13	o	58	ASN	4.7
20	z	33	TRP	3.9
14	r	20	VAL	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	45,56,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.95	0.09	45,54,73,74	0
15	FME	T	1	10/11	0.95	0.08	37,46,65,67	0
8	FME	i	1	10/11	0.95	0.08	46,57,67,70	0
15	FME	t	1	10/11	0.95	0.08	34,48,77,77	0
12	FME	m	1	10/11	0.96	0.08	39,54,76,81	0

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(Å ²)	Q<0.9
32	STE	I	101	15/20	0.70	0.20	45,62,89,90	0
32	STE	d	411	20/20	0.72	0.18	54,78,96,100	0
32	STE	B	623	18/20	0.74	0.19	54,80,90,94	0
30	LHG	e	101	42/49	0.77	0.16	59,92,114,126	0
30	LHG	A	614	49/49	0.77	0.16	51,87,115,118	0
32	STE	a	618	12/20	0.78	0.14	40,72,79,81	0
32	STE	b	623	16/20	0.79	0.17	50,67,85,92	0
32	STE	L	102	12/20	0.79	0.18	54,70,85,93	0
32	STE	b	625	10/20	0.80	0.16	47,58,68,69	0
24	CLA	b	601	65/65	0.80	0.14	54,74,95,108	0
33	LMG	D	411	33/55	0.80	0.15	44,61,84,94	0
33	LMG	b	622	55/55	0.80	0.17	54,76,98,109	0
33	LMG	c	521	48/55	0.80	0.16	43,78,104,111	0
32	STE	h	103	14/20	0.81	0.18	60,77,87,92	0
32	STE	R	101	12/20	0.81	0.19	66,87,95,107	0
32	STE	B	624	16/20	0.82	0.15	38,69,90,91	0
32	STE	a	617	10/20	0.82	0.15	37,70,76,81	0
32	STE	b	624	20/20	0.83	0.14	42,67,87,89	0
28	PL9	A	611	55/55	0.83	0.16	38,69,87,92	0
33	LMG	a	619	55/55	0.83	0.13	39,61,83,85	0
32	STE	c	523	12/20	0.83	0.13	58,75,87,90	0
32	STE	B	625	15/20	0.83	0.20	46,67,82,96	0
32	STE	T	103	15/20	0.84	0.15	46,65,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	B	622	18/20	0.84	0.12	45,66,89,89	0
32	STE	B	626	12/20	0.84	0.15	57,71,88,88	0
32	STE	d	410	20/20	0.84	0.12	50,65,79,81	0
32	STE	C	521	12/20	0.84	0.14	36,54,66,68	0
32	STE	T	102	16/20	0.85	0.14	43,58,78,83	0
31	DGD	A	616	66/66	0.85	0.11	46,68,85,98	0
32	STE	Z	101	8/20	0.85	0.17	50,64,77,77	0
32	STE	C	519	12/20	0.85	0.13	43,63,75,76	0
32	STE	M	103	10/20	0.86	0.14	44,55,60,69	0
32	STE	j	101	12/20	0.86	0.11	49,65,78,78	0
32	STE	c	520	20/20	0.86	0.13	43,68,86,100	0
33	LMG	Y	101	48/55	0.86	0.13	47,75,101,104	0
32	STE	b	621	20/20	0.86	0.13	45,62,80,86	0
29	SQD	A	615	39/54	0.86	0.13	45,65,95,96	0
29	SQD	a	616	36/54	0.86	0.13	31,69,93,98	0
29	SQD	f	102	41/54	0.87	0.13	64,94,114,118	0
28	PL9	a	612	55/55	0.87	0.14	43,77,95,103	0
32	STE	t	102	14/20	0.87	0.12	42,54,65,66	0
33	LMG	c	519	37/55	0.87	0.11	48,69,83,87	0
32	STE	C	520	16/20	0.87	0.12	47,59,68,73	0
32	STE	B	619	17/20	0.88	0.11	35,53,73,77	0
33	LMG	C	515	48/55	0.88	0.11	31,61,83,93	0
33	LMG	c	522	49/55	0.88	0.11	36,61,90,107	0
32	STE	B	621	12/20	0.89	0.12	38,62,74,78	0
33	LMG	D	412	28/55	0.89	0.12	39,56,67,75	0
24	CLA	C	513	65/65	0.89	0.11	50,69,101,107	0
24	CLA	H	101	65/65	0.89	0.10	44,68,98,103	0
33	LMG	m	101	51/55	0.89	0.10	37,55,75,85	0
32	STE	d	409	17/20	0.90	0.11	43,58,66,77	0
32	STE	M	102	15/20	0.90	0.11	42,58,67,69	0
26	BCR	h	101	40/40	0.90	0.11	42,63,87,92	0
29	SQD	B	620	54/54	0.90	0.10	41,62,87,95	0
26	BCR	K	101	40/40	0.90	0.12	45,64,76,82	0
29	SQD	b	620	49/54	0.90	0.10	40,62,90,107	0
32	STE	J	101	12/20	0.90	0.10	50,62,78,78	0
26	BCR	c	514	40/40	0.90	0.11	45,65,82,84	0
33	LMG	M	101	51/55	0.91	0.09	34,53,80,85	0
32	STE	M	104	18/20	0.91	0.11	39,52,86,91	0
29	SQD	D	408	36/54	0.91	0.10	57,78,93,96	0
33	LMG	d	408	44/55	0.91	0.11	37,61,93,102	0
32	STE	X	102	20/20	0.91	0.10	38,57,80,83	0
31	DGD	h	102	62/66	0.92	0.09	35,53,66,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	c	513	65/65	0.92	0.11	47,75,105,109	0
26	BCR	k	101	40/40	0.92	0.09	40,67,79,81	0
26	BCR	X	101	40/40	0.92	0.09	34,52,70,73	0
29	SQD	a	615	54/54	0.92	0.10	45,70,92,96	0
26	BCR	D	405	40/40	0.92	0.09	35,51,89,97	0
31	DGD	C	517	62/66	0.92	0.09	38,58,106,117	0
31	DGD	c	517	62/66	0.92	0.09	36,56,97,103	0
26	BCR	b	617	40/40	0.93	0.08	33,49,64,65	0
26	BCR	b	618	40/40	0.93	0.07	28,46,61,65	0
29	SQD	A	613	52/54	0.93	0.10	36,63,92,97	0
26	BCR	B	616	40/40	0.93	0.08	31,44,61,67	0
26	BCR	d	404	40/40	0.93	0.10	40,59,99,107	0
26	BCR	K	102	40/40	0.93	0.09	44,62,77,85	0
33	LMG	D	407	51/55	0.93	0.11	31,64,87,89	0
24	CLA	c	512	65/65	0.93	0.10	47,65,93,98	0
31	DGD	H	102	62/66	0.93	0.09	32,49,62,71	0
34	BCT	a	611	4/4	0.93	0.10	35,36,48,53	0
31	DGD	c	518	62/66	0.94	0.09	32,59,84,90	0
26	BCR	A	608	40/40	0.94	0.07	29,40,48,49	0
24	CLA	c	506	65/65	0.94	0.09	35,55,90,101	0
26	BCR	B	617	40/40	0.94	0.07	29,44,58,59	0
26	BCR	b	619	40/40	0.94	0.08	33,54,68,72	0
26	BCR	B	618	40/40	0.94	0.07	29,46,61,71	0
26	BCR	C	514	40/40	0.94	0.09	27,47,60,72	0
24	CLA	c	509	65/65	0.94	0.10	34,55,70,75	0
24	CLA	C	512	65/65	0.94	0.10	41,62,97,102	0
30	LHG	D	410	47/49	0.94	0.10	33,53,93,98	0
30	LHG	a	614	49/49	0.94	0.09	33,54,72,75	0
30	LHG	d	407	39/49	0.94	0.09	38,54,74,77	0
26	BCR	k	102	40/40	0.94	0.10	45,61,74,77	0
26	BCR	t	101	40/40	0.94	0.06	29,44,55,58	0
24	CLA	C	511	65/65	0.94	0.08	38,55,72,78	0
26	BCR	K	103	40/40	0.94	0.09	42,59,74,83	0
26	BCR	T	101	40/40	0.94	0.07	26,47,62,63	0
24	CLA	b	616	60/65	0.95	0.09	33,50,93,101	0
30	LHG	l	101	49/49	0.95	0.08	34,51,61,71	0
26	BCR	a	608	40/40	0.95	0.06	26,39,47,55	0
31	DGD	C	516	62/66	0.95	0.09	27,43,82,94	0
24	CLA	c	502	65/65	0.95	0.07	33,48,67,71	0
31	DGD	C	518	62/66	0.95	0.08	28,53,75,87	0
24	CLA	c	503	65/65	0.95	0.08	36,50,65,65	0
31	DGD	c	516	62/66	0.95	0.09	28,45,75,84	0

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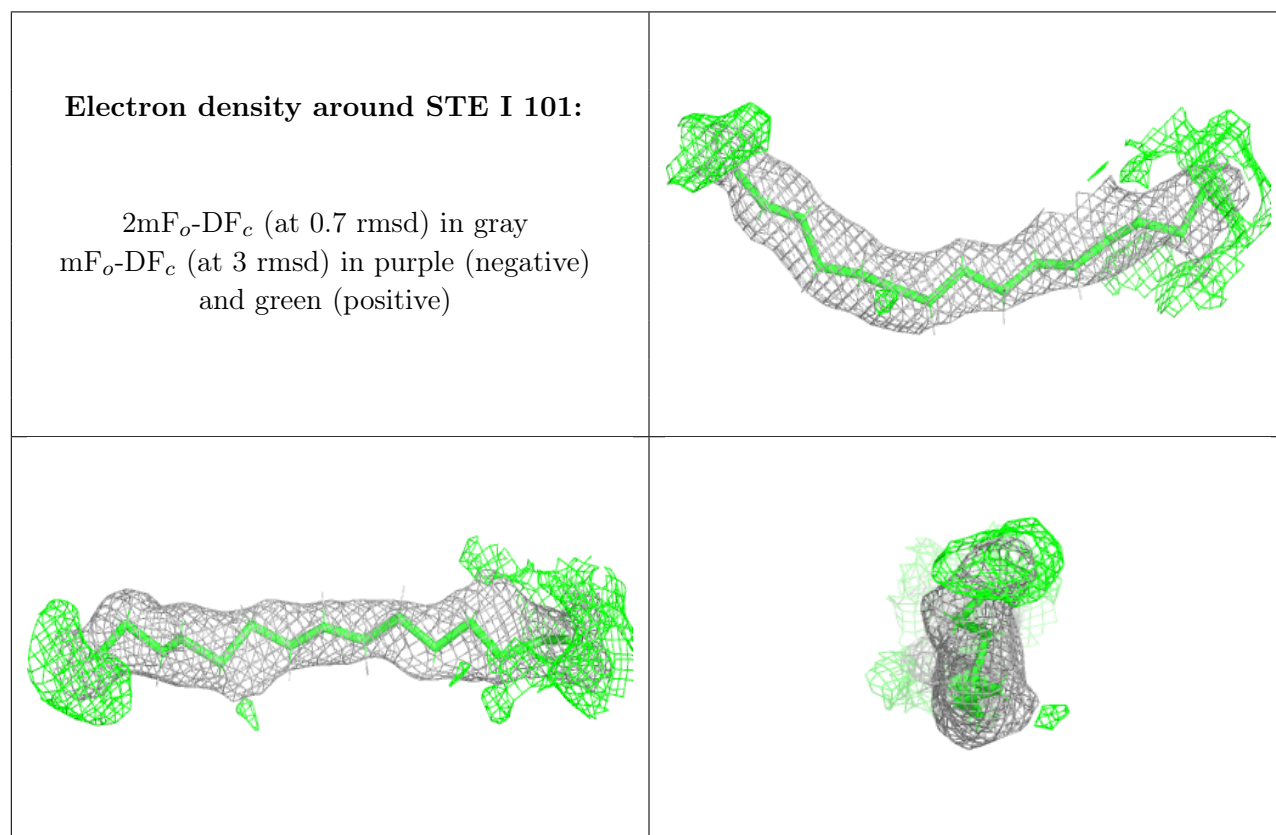
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	504	60/65	0.95	0.07	36,52,83,88	0
24	CLA	c	505	65/65	0.95	0.08	30,48,69,76	0
26	BCR	c	515	40/40	0.95	0.09	32,50,72,73	0
24	CLA	C	506	65/65	0.95	0.09	28,47,91,95	0
24	CLA	c	508	64/65	0.95	0.09	36,53,99,120	0
24	CLA	C	508	65/65	0.95	0.09	31,49,105,118	0
24	CLA	c	510	65/65	0.95	0.08	38,54,70,72	0
24	CLA	c	511	65/65	0.95	0.09	41,60,78,81	0
24	CLA	C	510	65/65	0.95	0.07	33,51,68,70	0
24	CLA	B	605	65/65	0.95	0.07	22,41,70,73	0
24	CLA	d	403	65/65	0.95	0.09	31,55,98,106	0
25	PHO	d	401	64/64	0.95	0.07	27,43,53,64	0
24	CLA	B	614	65/65	0.95	0.08	28,43,63,67	0
24	CLA	B	615	60/65	0.95	0.09	27,46,103,111	0
24	CLA	C	503	65/65	0.95	0.07	36,49,61,63	0
24	CLA	a	607	65/65	0.95	0.08	23,41,90,102	0
24	CLA	C	504	59/65	0.95	0.08	34,47,85,97	0
24	CLA	b	602	65/65	0.95	0.08	29,48,67,71	0
24	CLA	b	605	65/65	0.95	0.07	28,42,56,59	0
24	CLA	b	606	65/65	0.95	0.07	29,46,76,85	0
24	CLA	b	608	65/65	0.95	0.07	30,48,71,80	0
24	CLA	b	609	65/65	0.95	0.08	34,51,74,79	0
24	CLA	c	507	65/65	0.96	0.07	32,49,62,74	0
28	PL9	D	406	55/55	0.96	0.07	25,39,50,65	0
24	CLA	B	611	65/65	0.96	0.06	23,37,51,60	0
28	PL9	d	405	55/55	0.96	0.07	27,41,52,54	0
24	CLA	B	612	65/65	0.96	0.07	22,39,78,86	0
24	CLA	D	403	65/65	0.96	0.07	19,33,57,66	0
24	CLA	D	404	65/65	0.96	0.08	24,47,107,122	0
24	CLA	B	613	65/65	0.96	0.08	25,42,82,92	0
24	CLA	a	604	65/65	0.96	0.06	24,35,49,57	0
24	CLA	d	402	65/65	0.96	0.07	25,40,67,76	0
24	CLA	a	605	65/65	0.96	0.09	30,45,99,110	0
25	PHO	A	606	64/64	0.96	0.06	25,37,46,48	0
25	PHO	D	401	64/64	0.96	0.06	21,34,45,47	0
30	LHG	D	409	49/49	0.96	0.07	29,42,55,71	0
24	CLA	A	612	65/65	0.96	0.06	22,34,54,58	0
30	LHG	D	413	49/49	0.96	0.08	34,47,70,76	0
30	LHG	L	101	49/49	0.96	0.07	32,46,60,67	0
24	CLA	a	613	65/65	0.96	0.07	23,37,48,53	0
30	LHG	d	406	49/49	0.96	0.07	28,45,61,66	0
24	CLA	B	601	65/65	0.96	0.07	27,41,63,71	0

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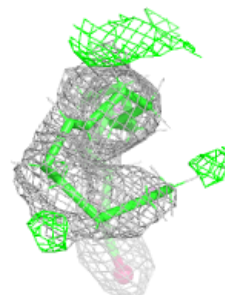
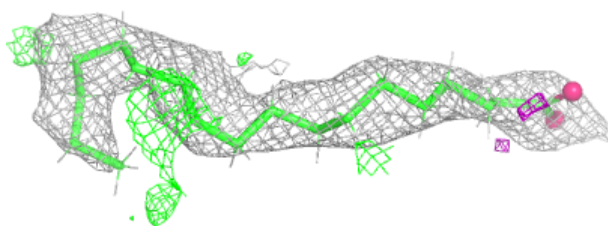
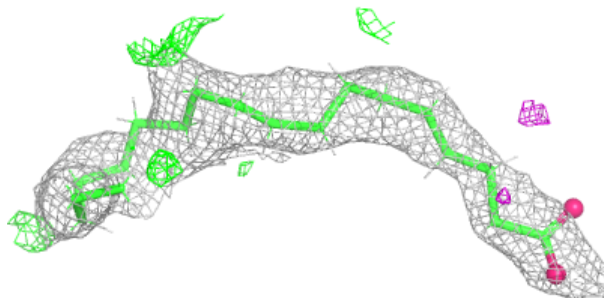
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	C	501	65/65	0.96	0.07	29,41,55,61	0
24	CLA	b	604	65/65	0.96	0.07	26,41,79,98	0
24	CLA	C	502	65/65	0.96	0.07	32,47,64,67	0
24	CLA	B	602	65/65	0.96	0.07	22,38,61,72	0
24	CLA	b	607	65/65	0.96	0.07	22,43,71,75	0
24	CLA	B	603	65/65	0.96	0.07	23,38,77,86	0
24	CLA	C	505	65/65	0.96	0.08	25,48,71,77	0
24	CLA	b	610	65/65	0.96	0.07	27,43,54,62	0
24	CLA	b	611	65/65	0.96	0.07	25,38,62,75	0
24	CLA	b	612	65/65	0.96	0.07	23,39,55,56	0
24	CLA	b	613	65/65	0.96	0.07	23,41,81,88	0
24	CLA	b	614	65/65	0.96	0.07	29,44,78,91	0
24	CLA	b	615	65/65	0.96	0.08	30,46,69,80	0
24	CLA	B	604	65/65	0.96	0.07	25,38,51,54	0
24	CLA	c	501	65/65	0.96	0.07	31,45,60,63	0
24	CLA	C	507	65/65	0.96	0.07	31,47,67,70	0
24	CLA	A	604	65/65	0.96	0.06	19,33,50,61	0
24	CLA	C	509	65/65	0.96	0.08	30,50,66,77	0
24	CLA	B	608	65/65	0.96	0.08	27,45,63,72	0
24	CLA	B	609	65/65	0.96	0.06	22,36,48,51	0
24	CLA	b	603	65/65	0.97	0.07	26,42,74,82	0
25	PHO	a	606	64/64	0.97	0.06	23,35,43,45	0
24	CLA	A	605	65/65	0.97	0.08	24,39,100,106	0
24	CLA	A	607	54/65	0.97	0.06	20,36,69,78	0
24	CLA	B	610	65/65	0.97	0.06	21,35,51,55	0
24	CLA	B	606	65/65	0.97	0.07	22,37,71,79	0
34	BCT	D	402	4/4	0.97	0.07	34,36,43,47	0
24	CLA	B	607	65/65	0.97	0.06	24,40,63,68	0
35	HEM	F	101	43/43	0.97	0.08	42,58,73,76	0
35	HEM	f	101	43/43	0.97	0.09	49,67,93,97	0
36	HEC	V	201	43/43	0.98	0.06	28,38,45,53	0
36	HEC	v	201	43/43	0.98	0.07	32,41,54,58	0
27	CL	A	610	1/1	0.99	0.06	37,37,37,37	0
27	CL	a	609	1/1	0.99	0.04	32,32,32,32	0
27	CL	a	610	1/1	0.99	0.08	35,35,35,35	0
21	OEY	A	601[B]	11/11	0.99	0.04	21,25,29,31	11
21	OEY	a	601[B]	11/11	0.99	0.03	21,26,32,32	11
22	OEX	A	602[A]	10/10	0.99	0.03	33,36,40,40	10
22	OEX	a	602[A]	10/10	0.99	0.03	31,36,39,40	10
27	CL	A	609	1/1	0.99	0.05	34,34,34,34	0
23	FE2	a	603	1/1	1.00	0.03	32,32,32,32	0
23	FE2	A	603	1/1	1.00	0.01	31,31,31,31	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.

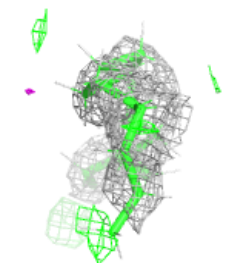
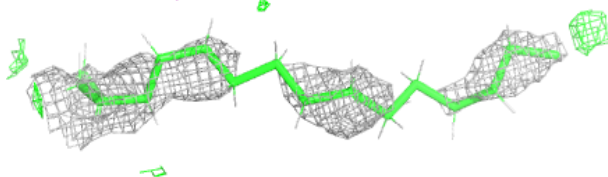
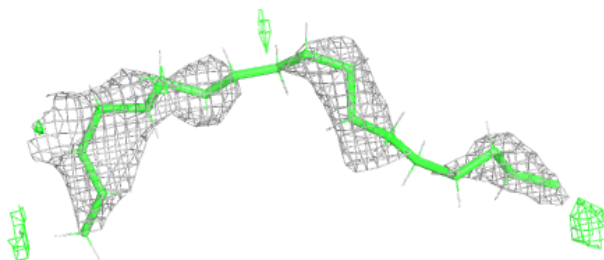


Electron density around STE d 411:

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

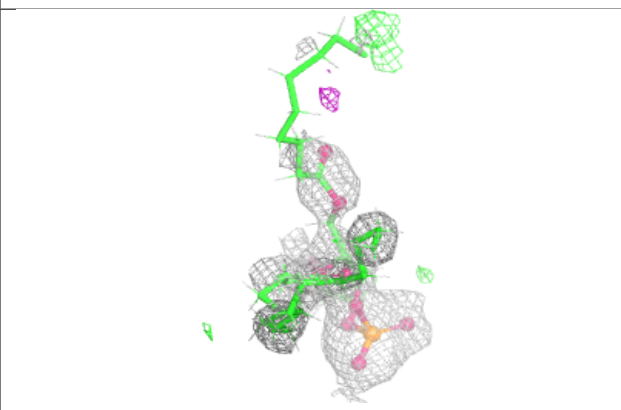
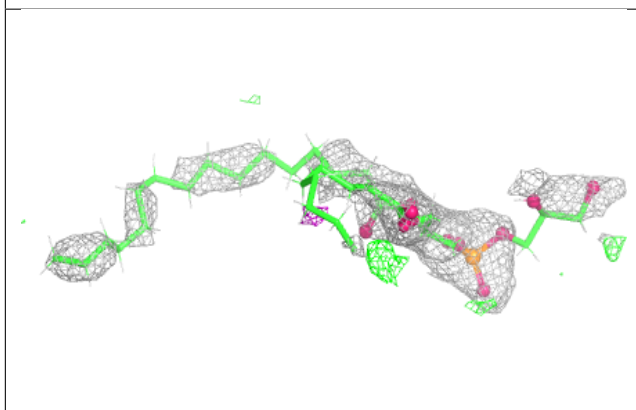
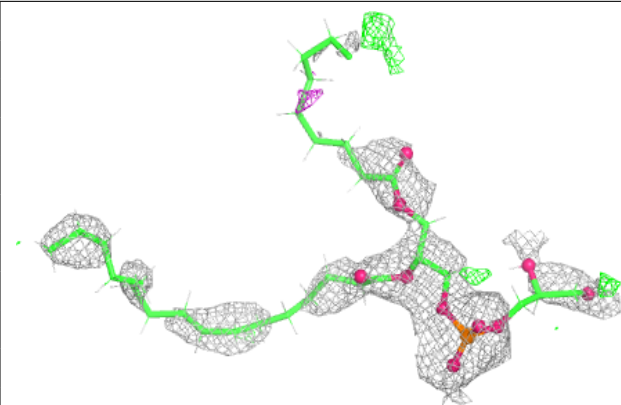
**Electron density around STE B 623:**

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



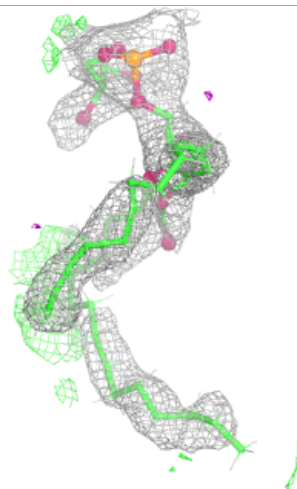
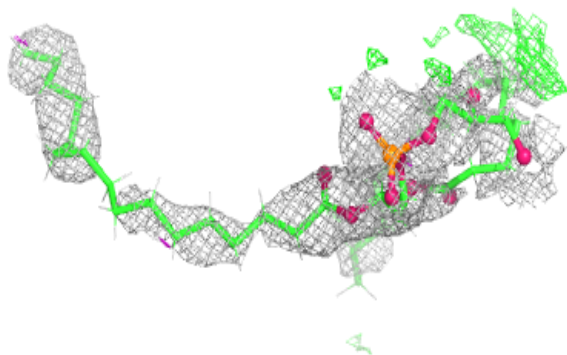
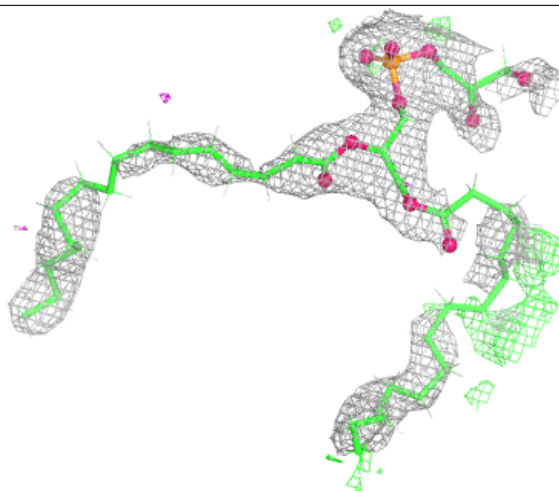
Electron density around LHG e 101:

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



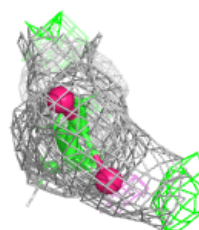
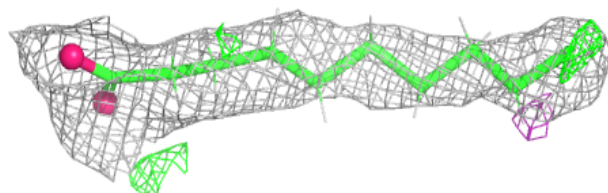
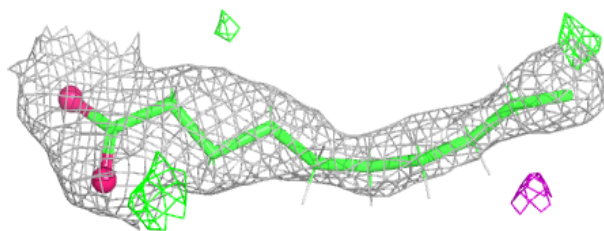
Electron density around LHG A 614:

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

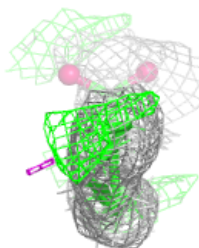
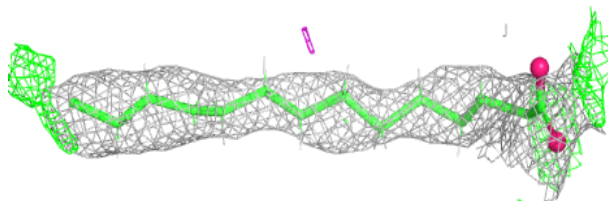


Electron density around STE a 618:

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

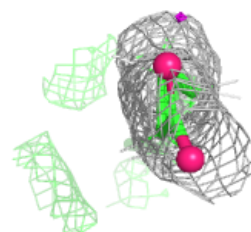
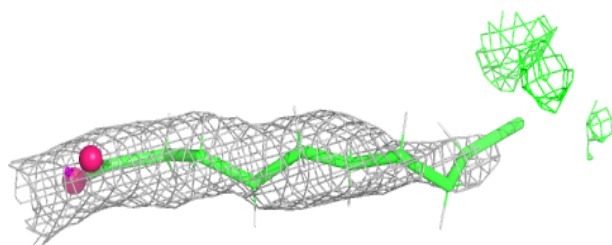
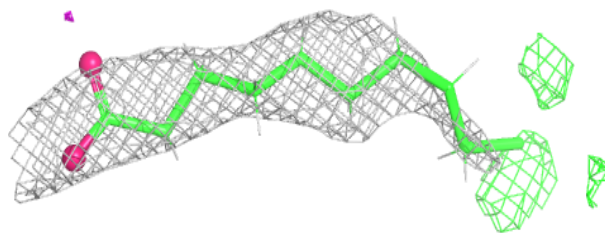
**Electron density around STE b 623:**

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

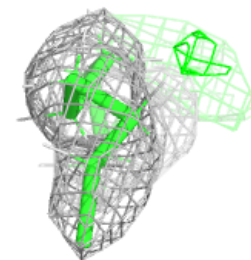
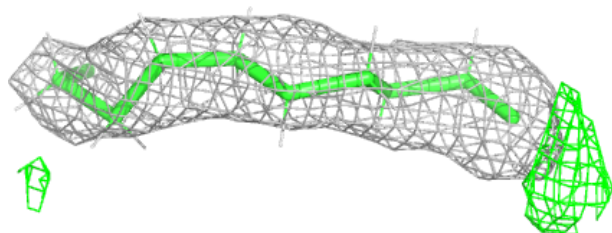
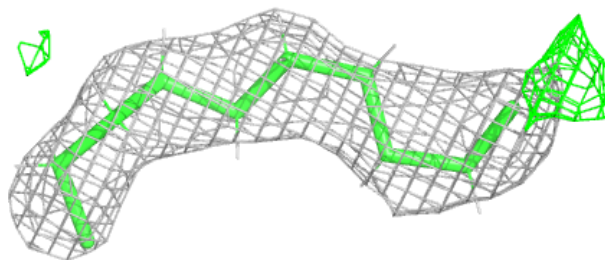


Electron density around STE L 102:

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

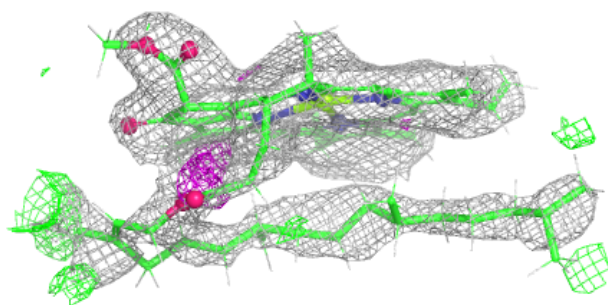
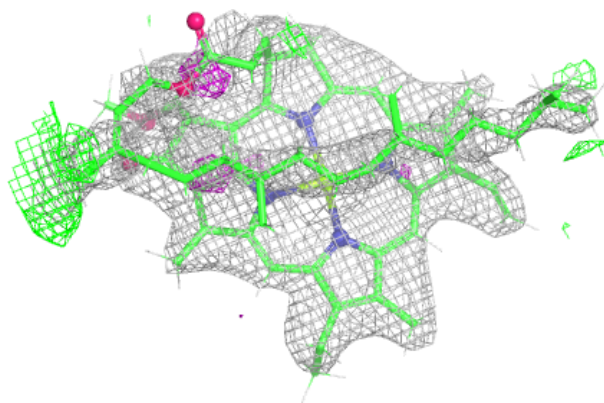
**Electron density around STE b 625:**

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and green (positive)

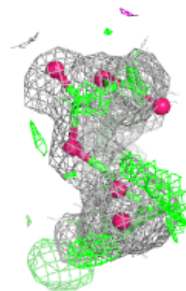
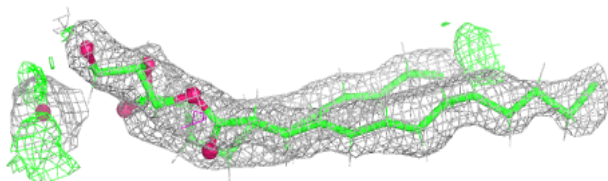
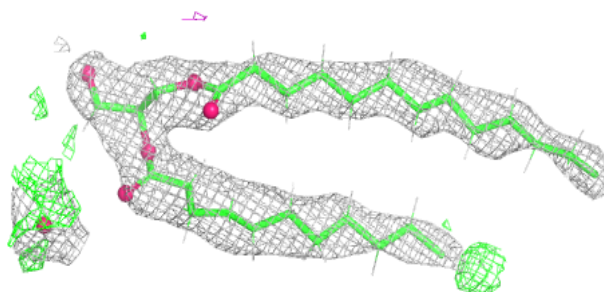


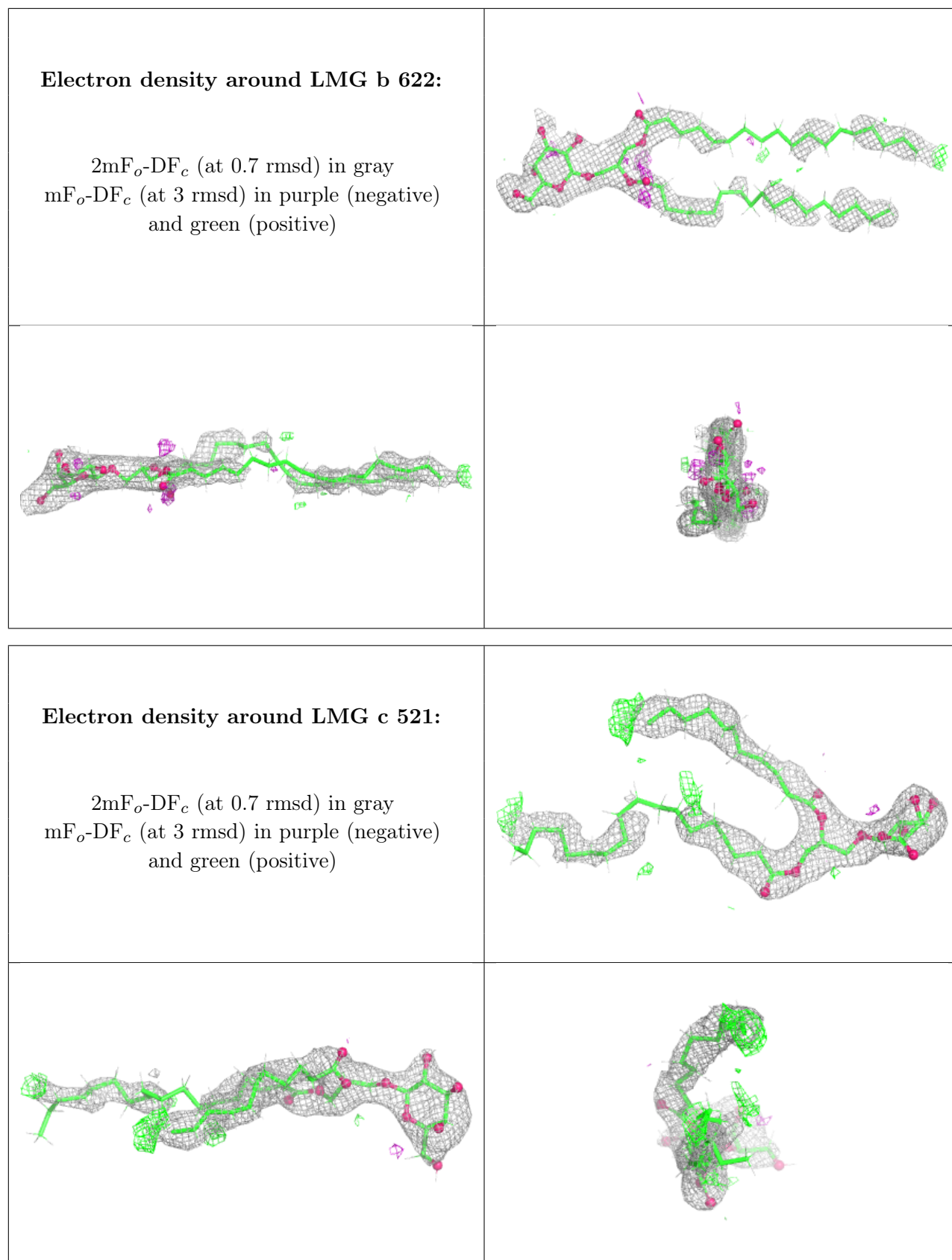
Electron density around CLA b 601:

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

**Electron density around LMG D 411:**

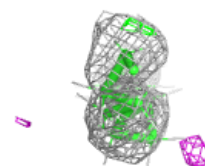
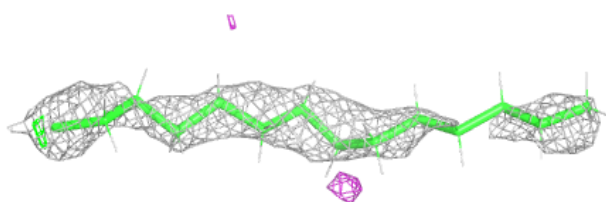
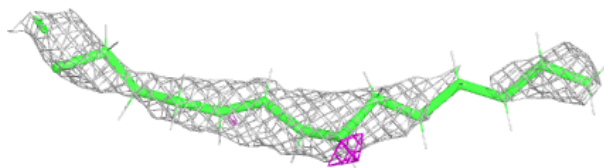
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



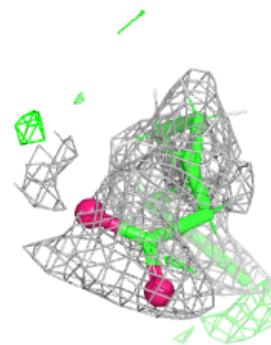
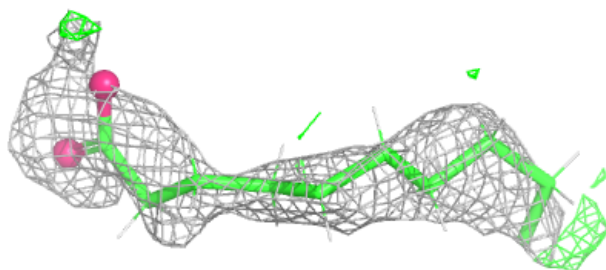
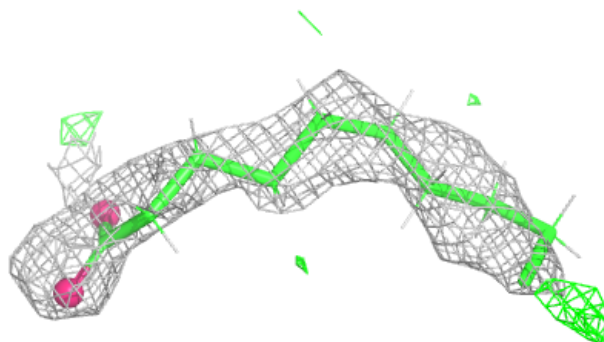


Electron density around STE h 103:

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

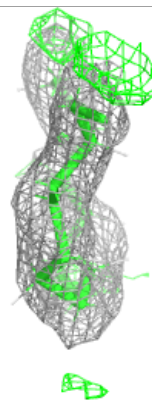
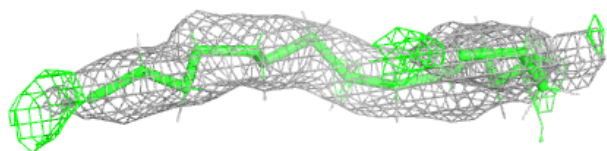
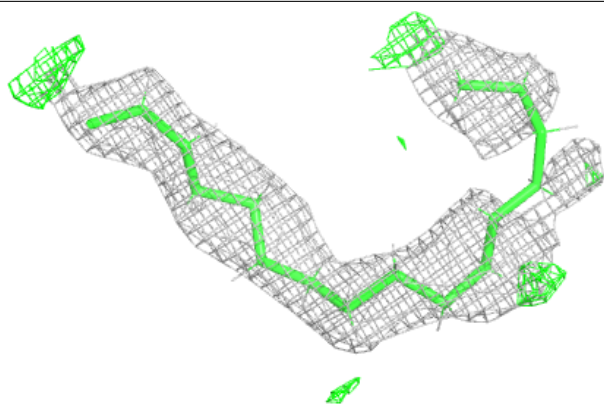
**Electron density around STE R 101:**

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and green (positive)

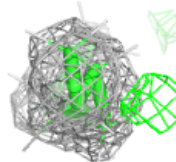
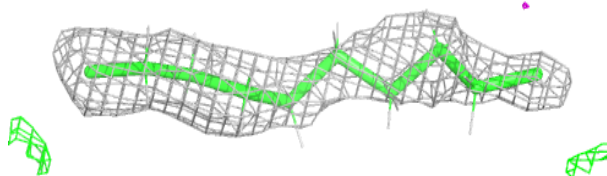
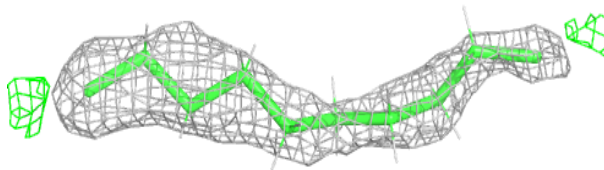


Electron density around STE B 624:

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and green (positive)

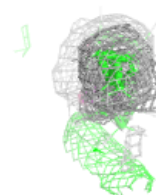
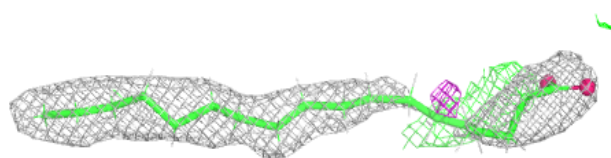
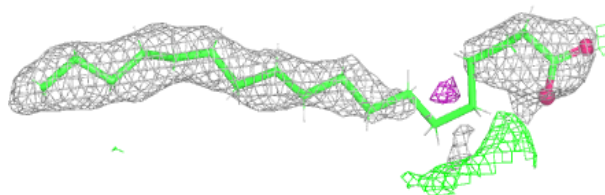
**Electron density around STE a 617:**

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

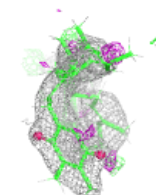
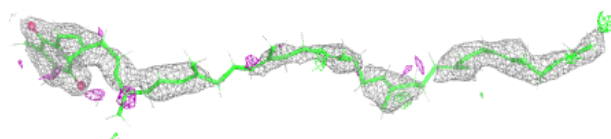
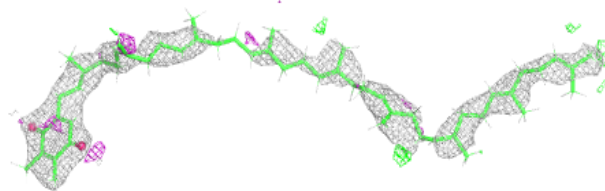


Electron density around STE b 624:

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

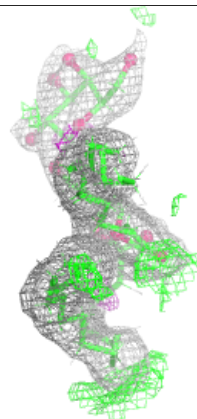
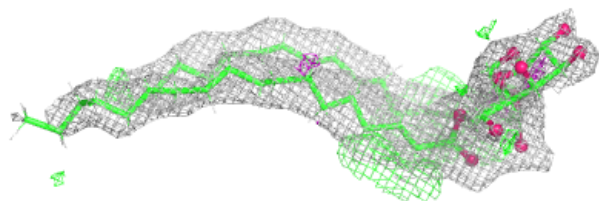
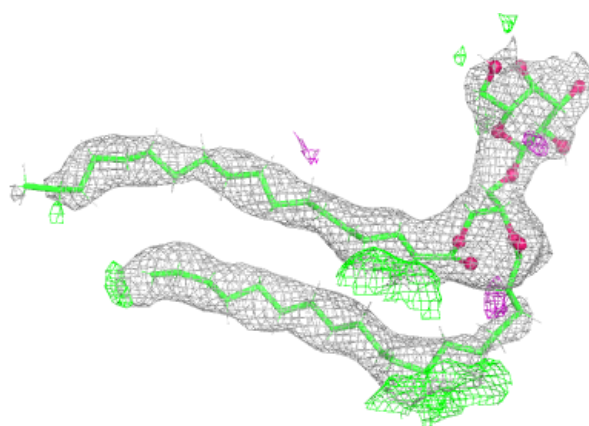
**Electron density around PL9 A 611:**

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

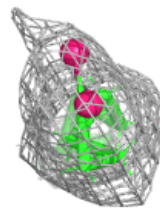
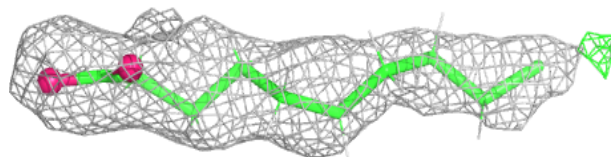
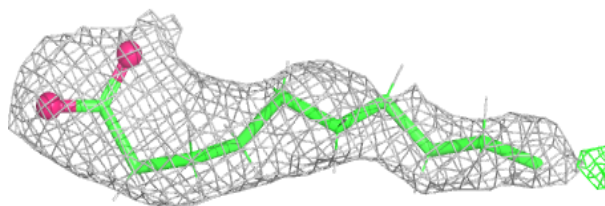


Electron density around LMG a 619:

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

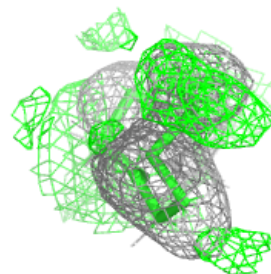
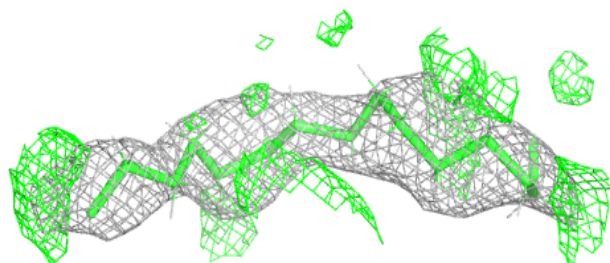
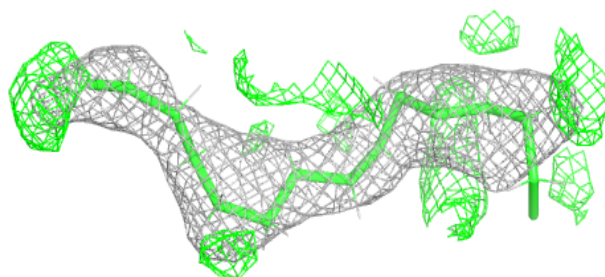
**Electron density around STE c 523:**

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

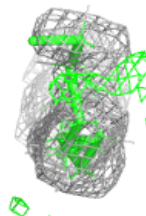
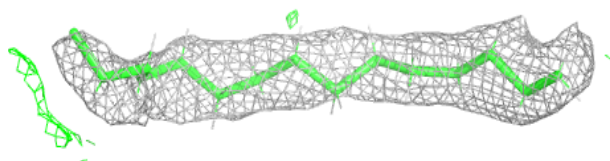
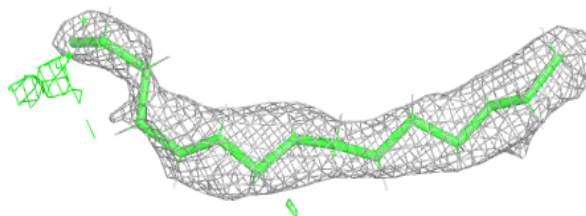


Electron density around STE B 625:

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

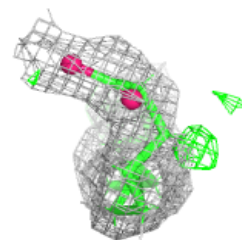
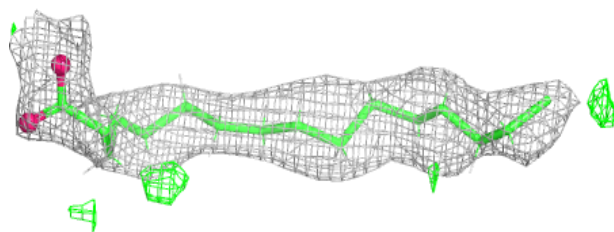
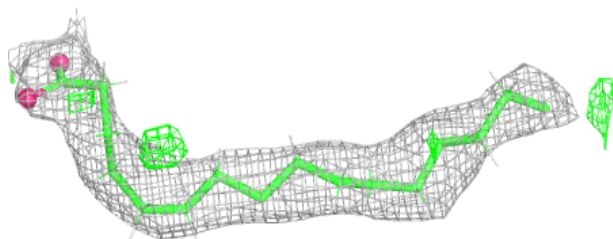
**Electron density around STE T 103:**

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

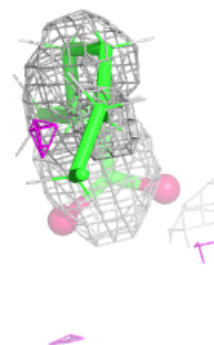
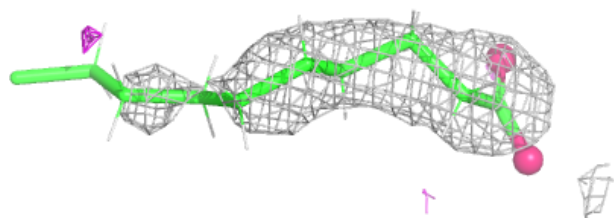
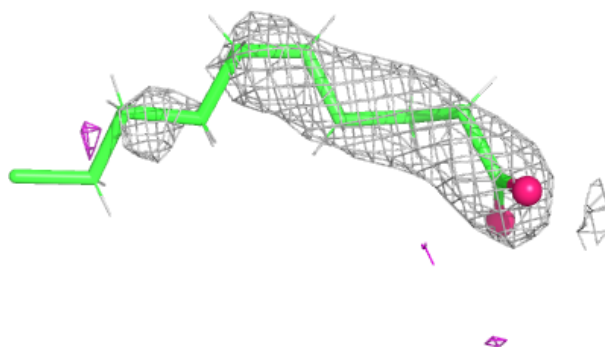


Electron density around STE B 622:

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

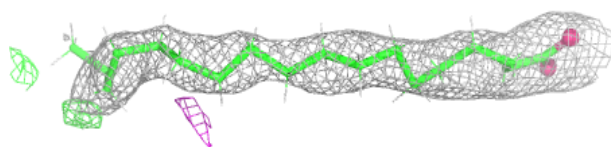
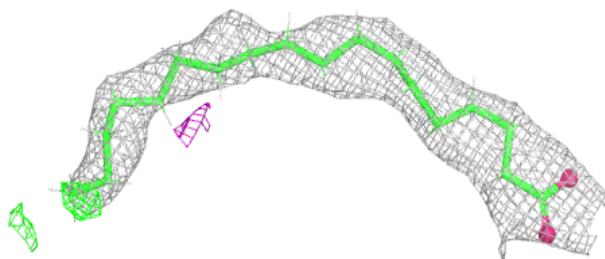
**Electron density around STE B 626:**

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

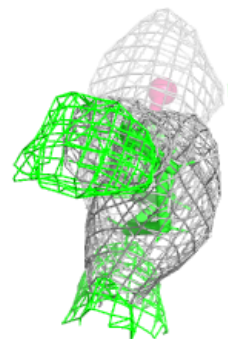
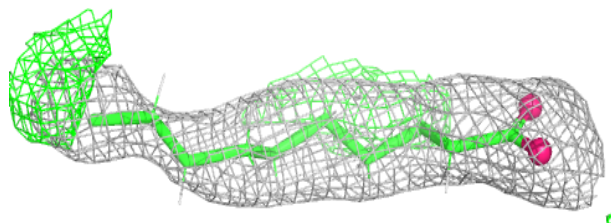
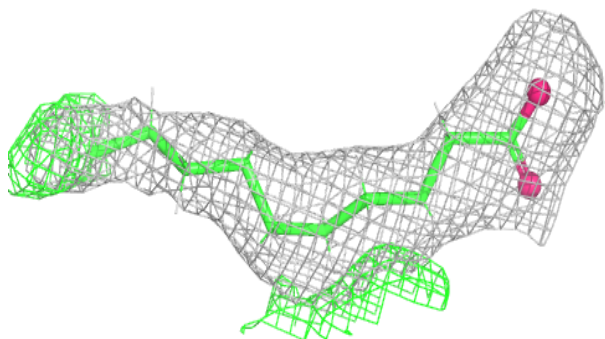


Electron density around STE d 410:

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

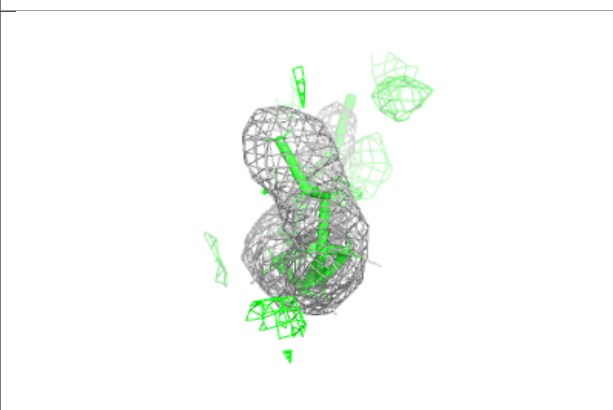
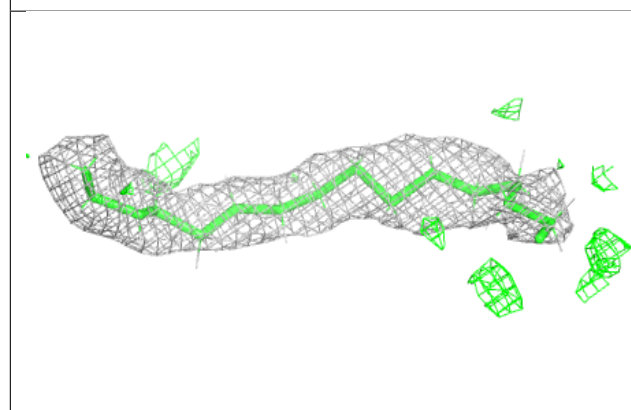
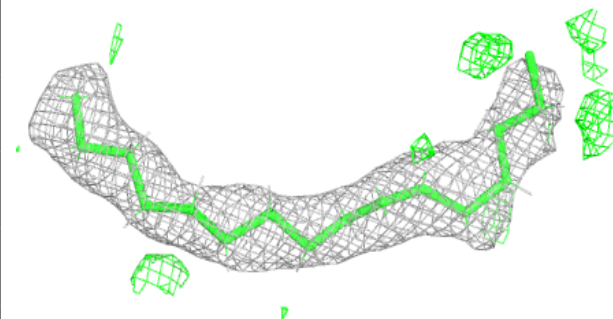
**Electron density around STE C 521:**

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

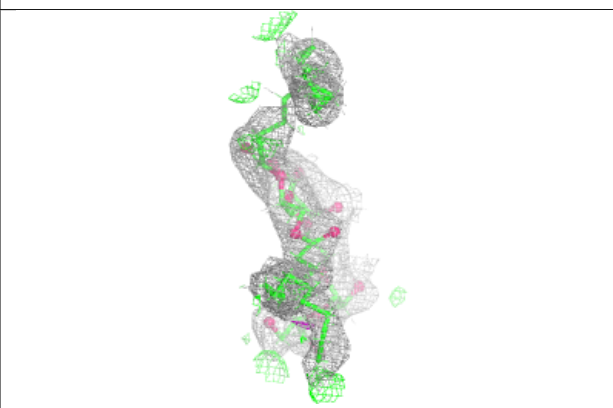
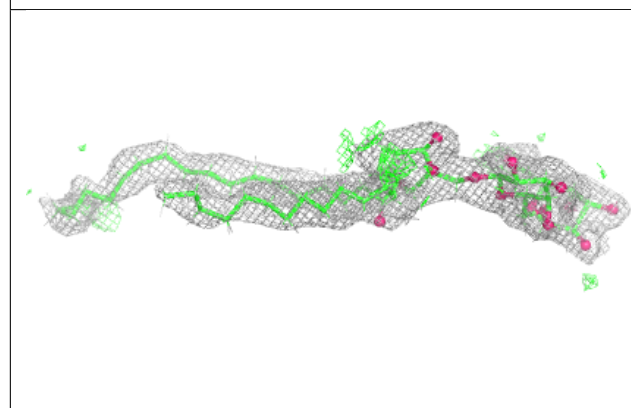
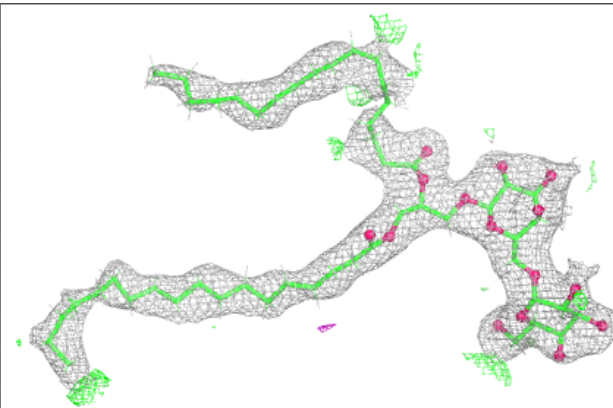


Electron density around STE T 102:

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

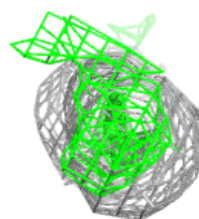
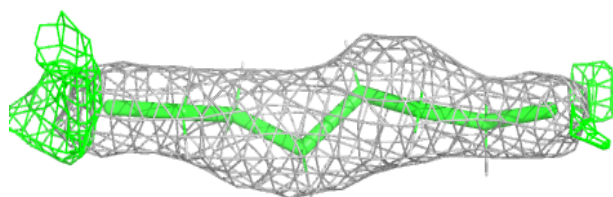
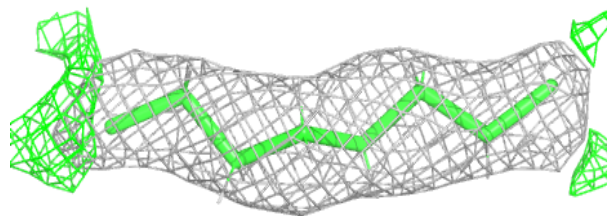
**Electron density around DGD A 616:**

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

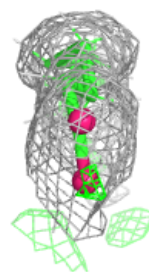
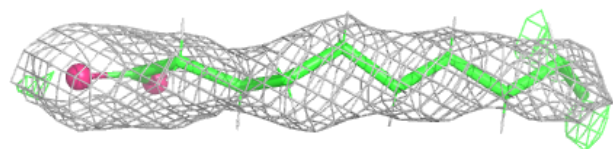
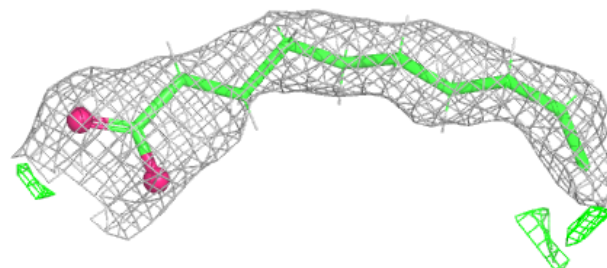


Electron density around STE Z 101:

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

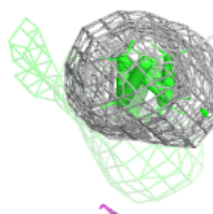
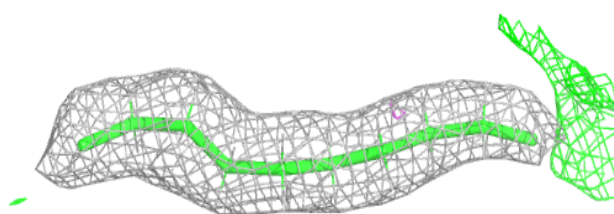
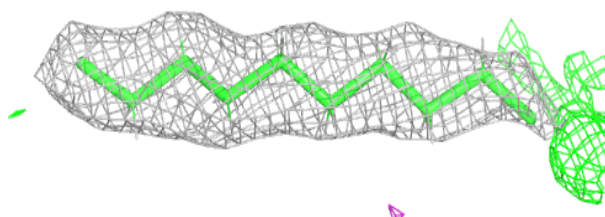
**Electron density around STE C 519:**

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

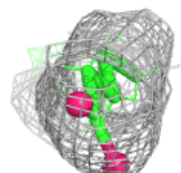
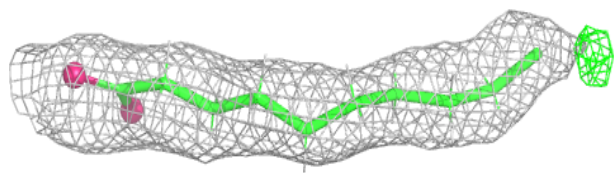
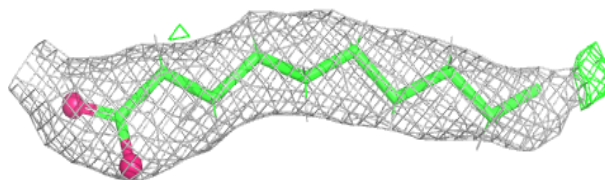


Electron density around STE M 103:

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

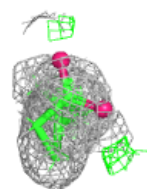
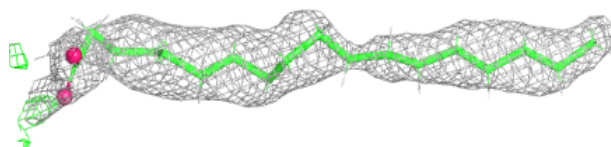
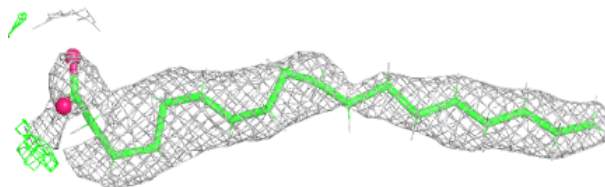
**Electron density around STE j 101:**

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



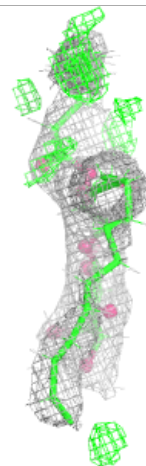
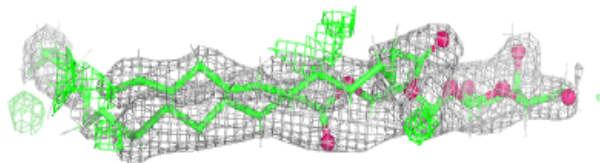
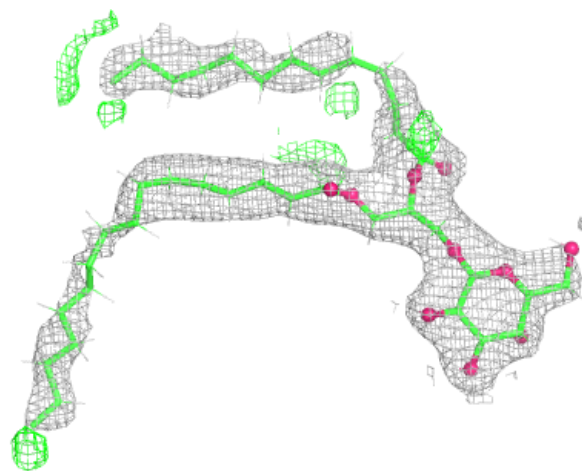
Electron density around STE c 520:

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



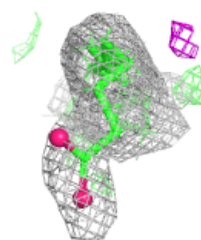
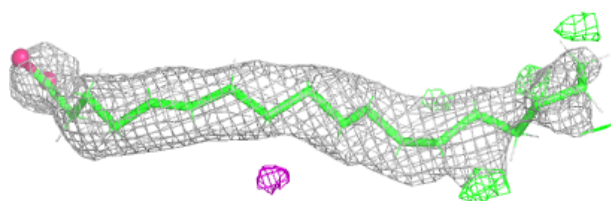
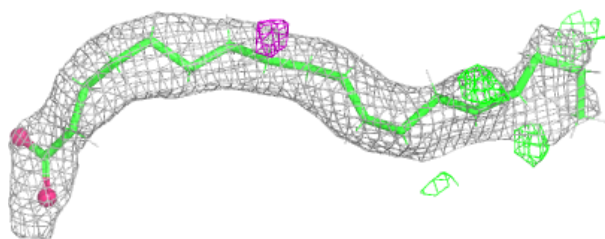
Electron density around LMG Y 101:

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

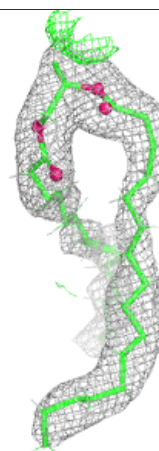
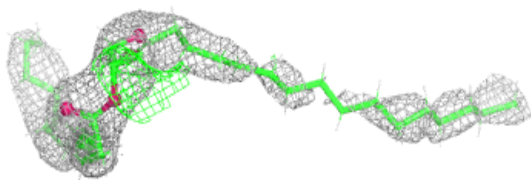
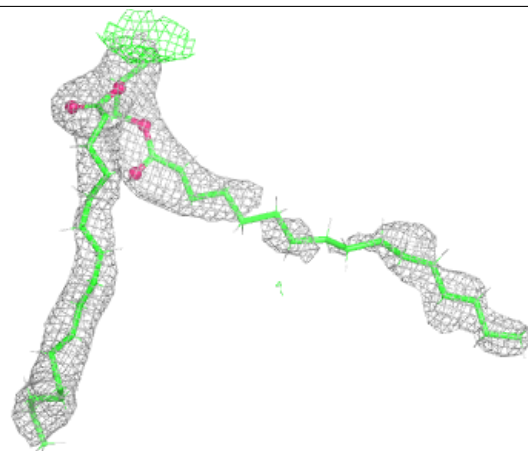


Electron density around STE b 621:

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

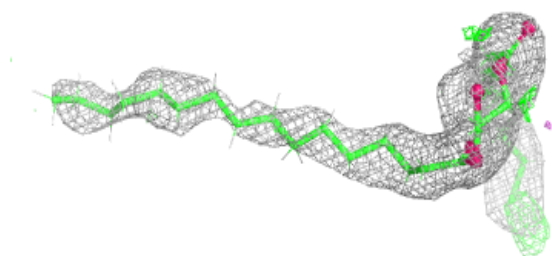
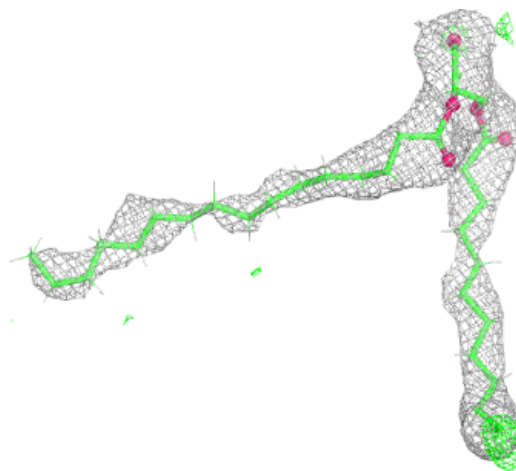
**Electron density around SQD A 615:**

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



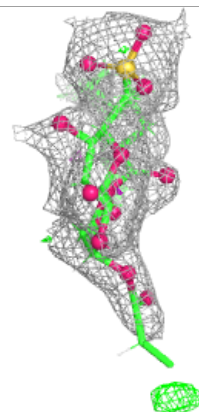
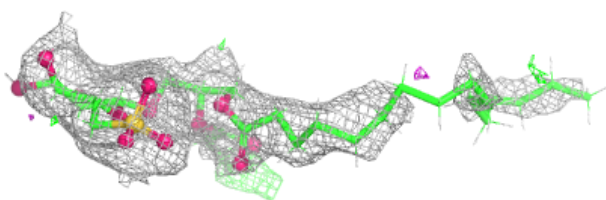
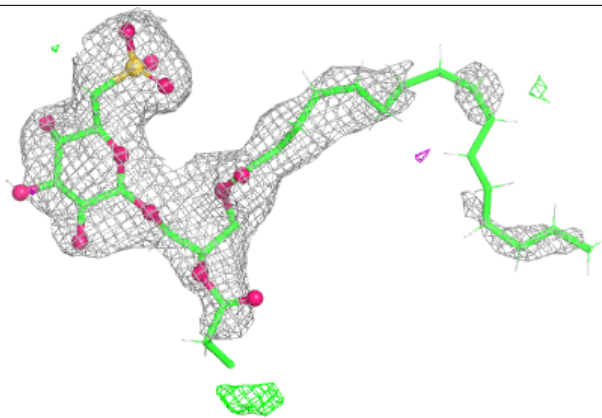
Electron density around SQD a 616:

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

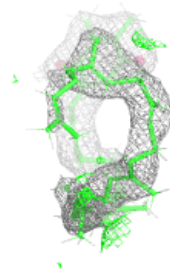
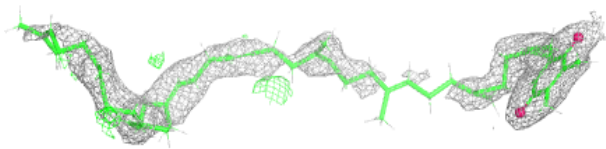
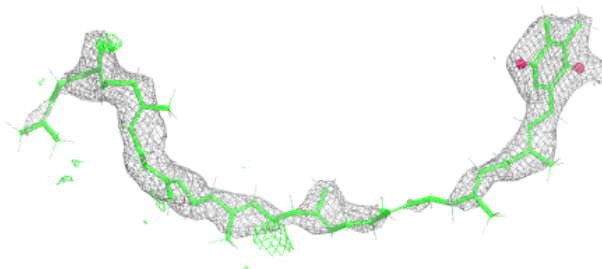


Electron density around SQD f 102:

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

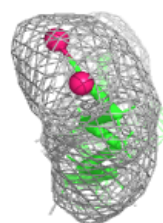
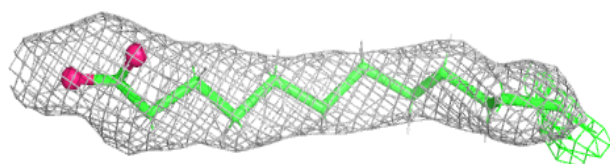
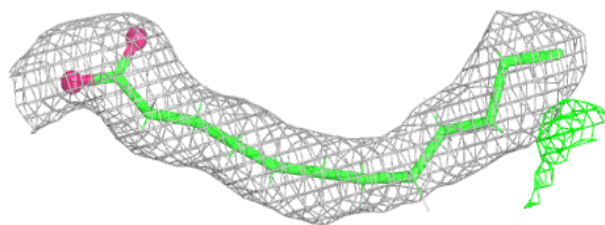
**Electron density around PL9 a 612:**

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

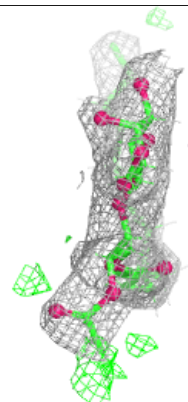
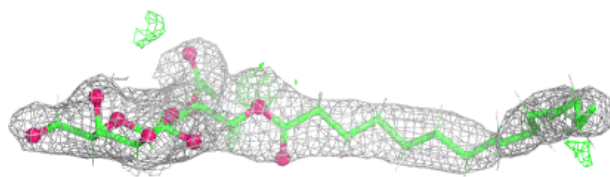
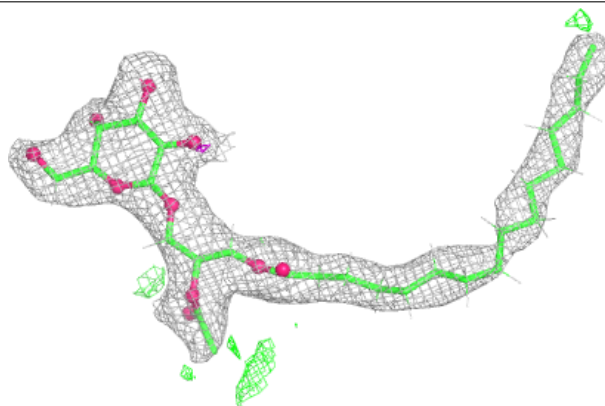


Electron density around STE t 102:

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

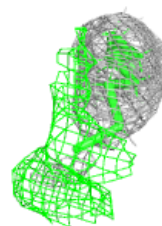
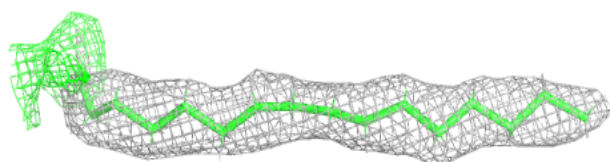
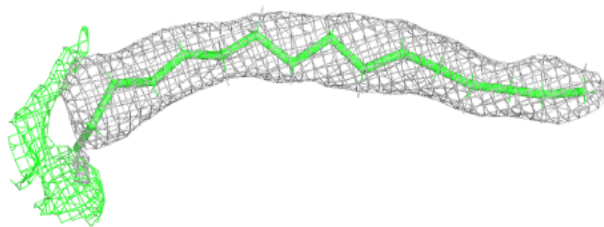
**Electron density around LMG c 519:**

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

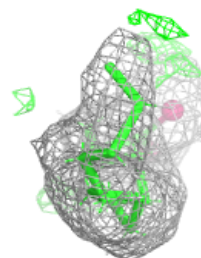
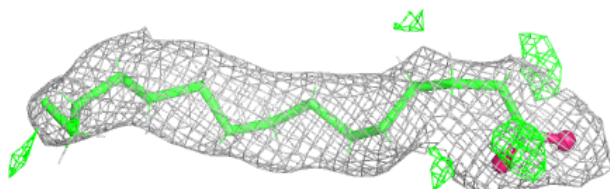
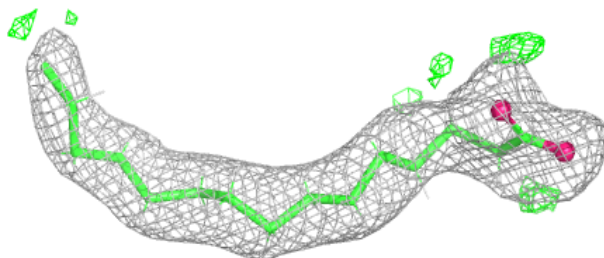


Electron density around STE C 520:

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

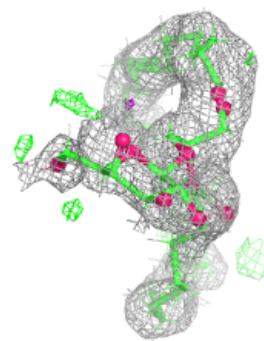
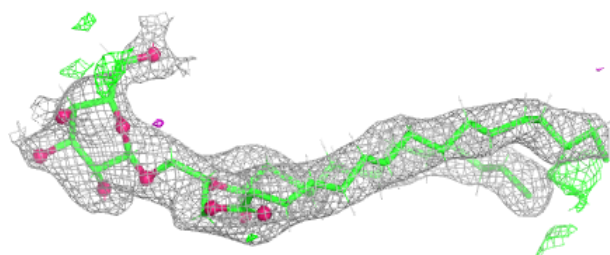
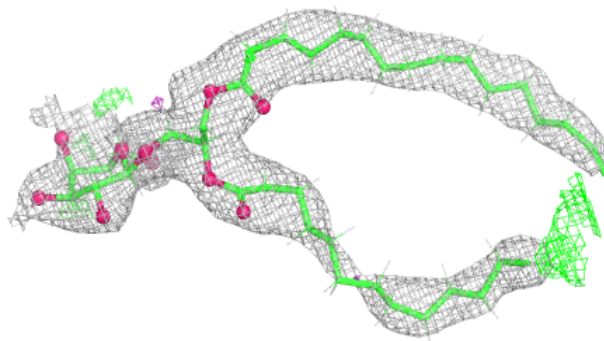
**Electron density around STE B 619:**

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

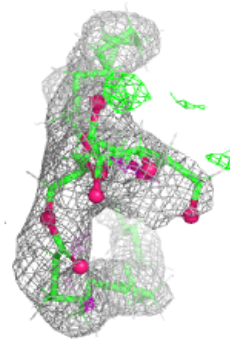
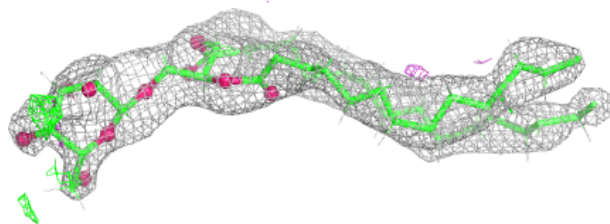
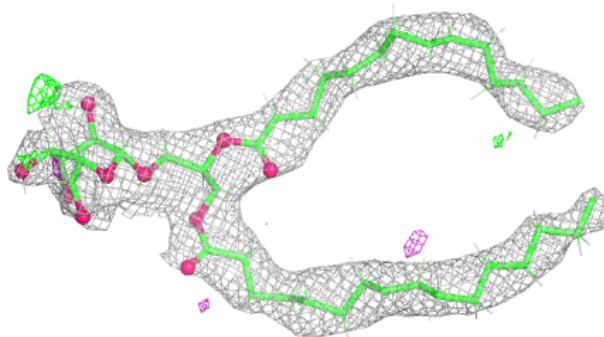


Electron density around LMG C 515:

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

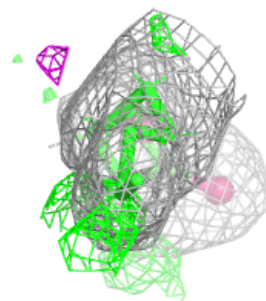
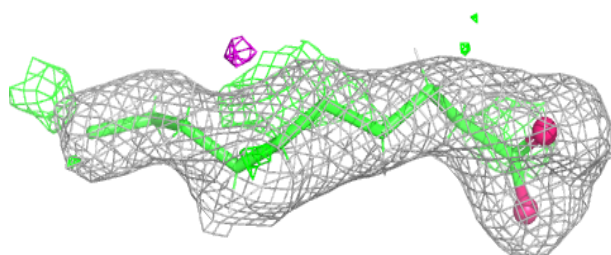
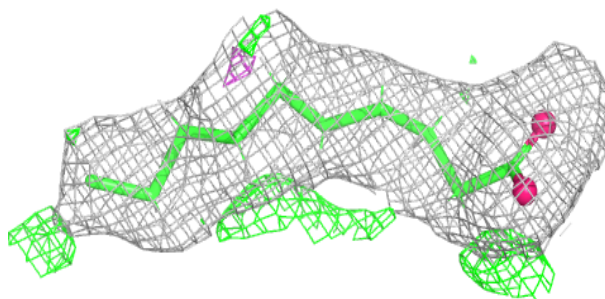
**Electron density around LMG c 522:**

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

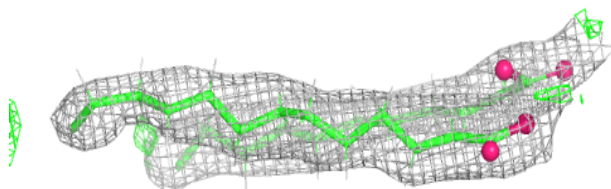
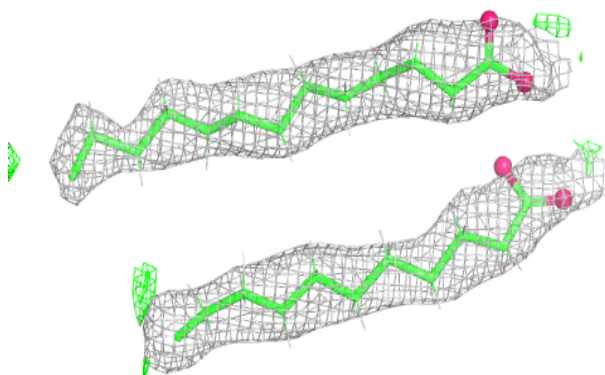


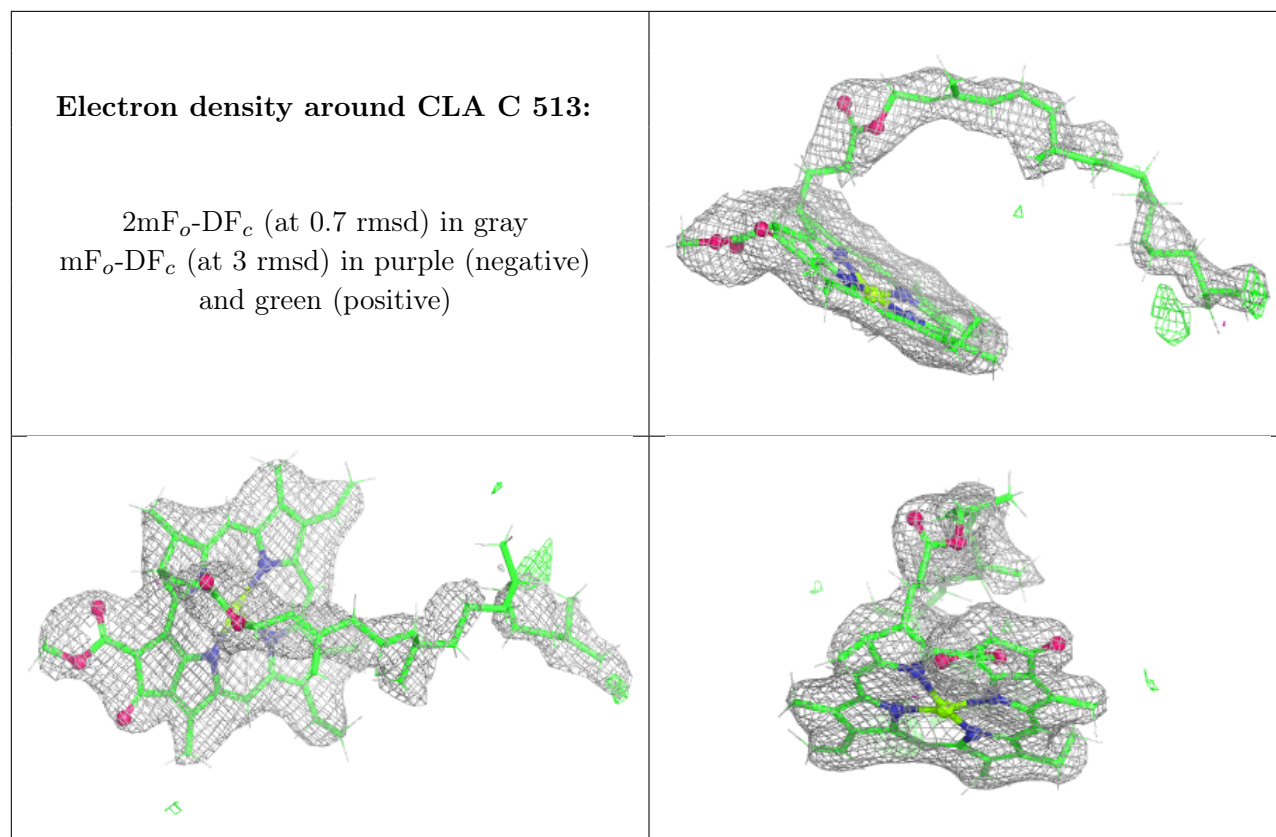
Electron density around STE B 621:

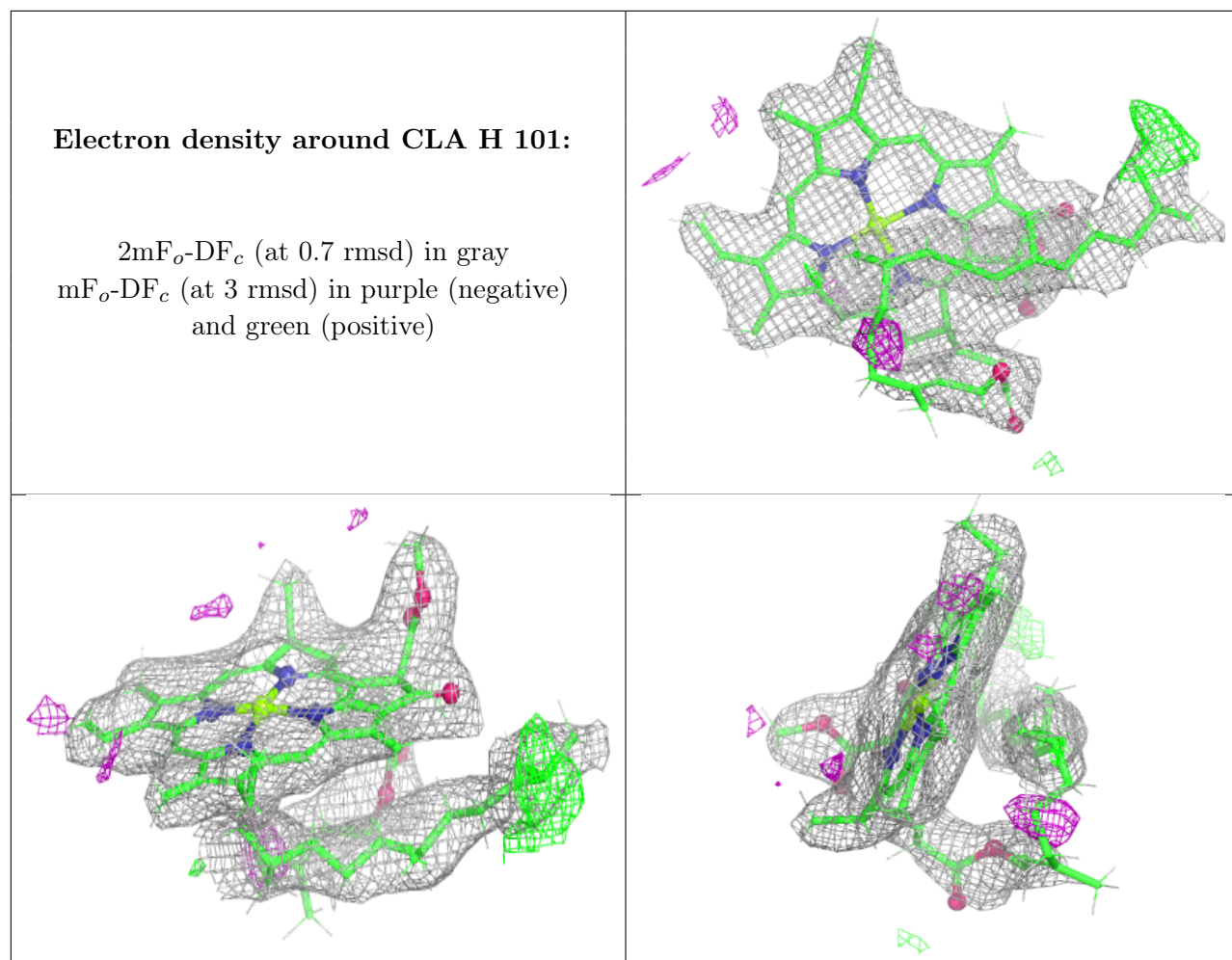
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG D 412:**

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

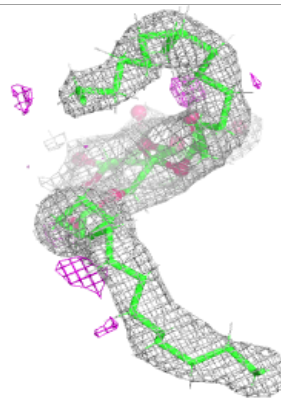
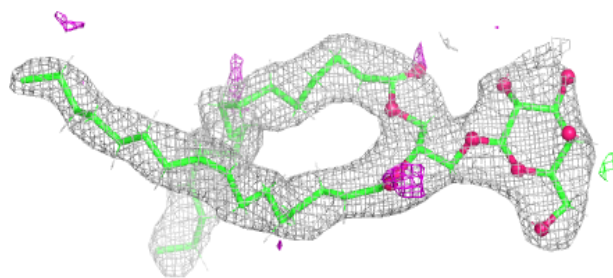
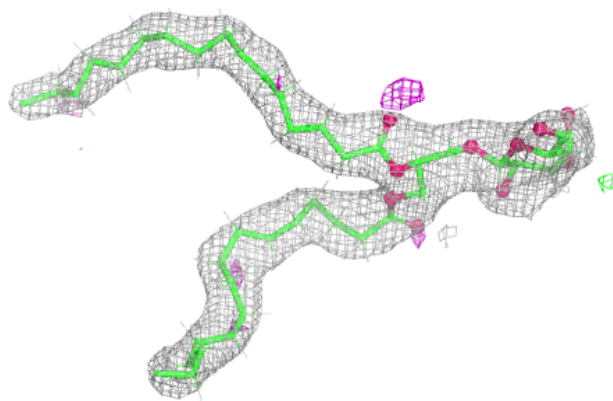




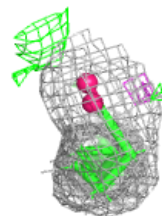
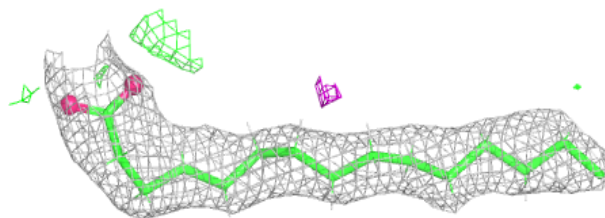


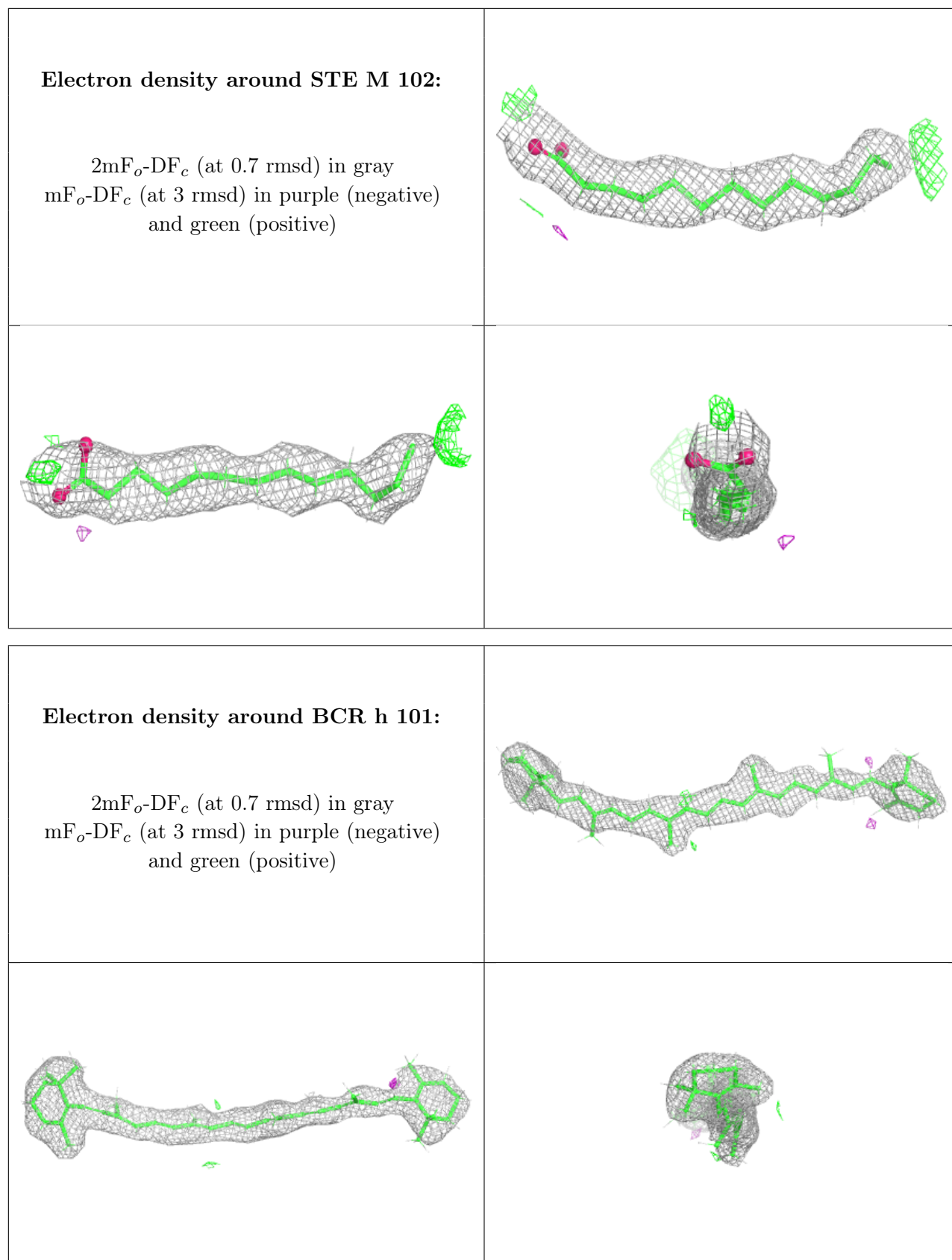
Electron density around LMG m 101:

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

**Electron density around STE d 409:**

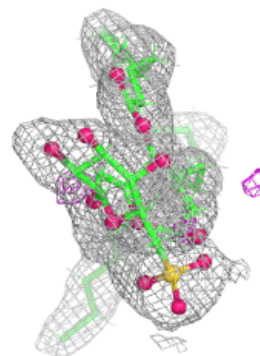
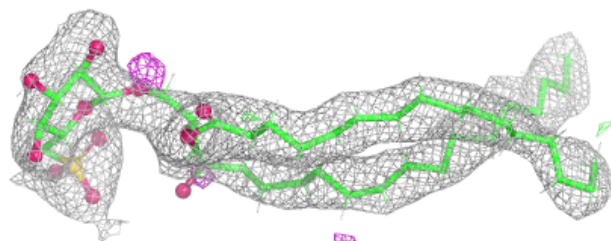
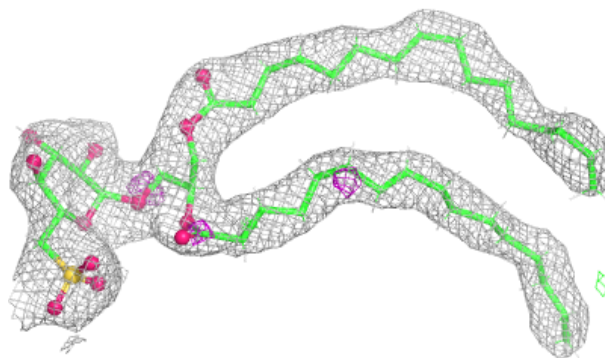
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around SQD B 620:

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

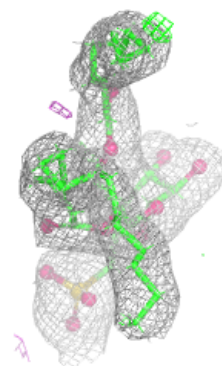
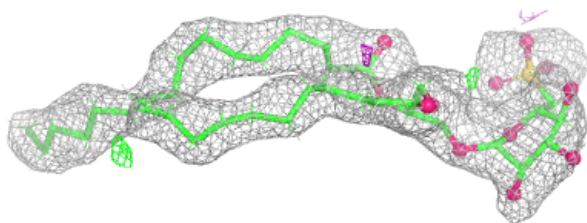
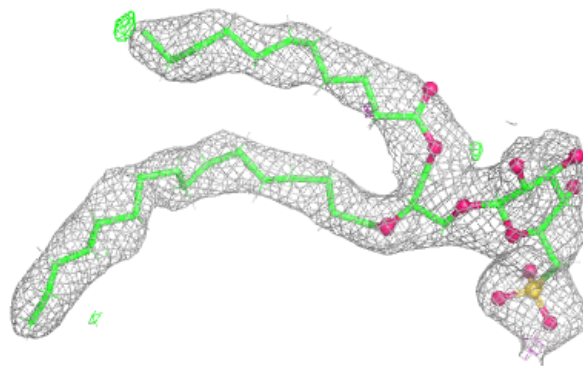
**Electron density around BCR K 101:**

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

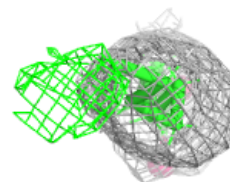
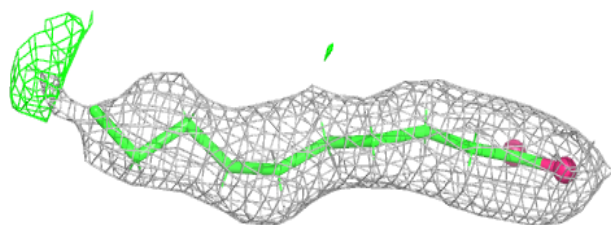
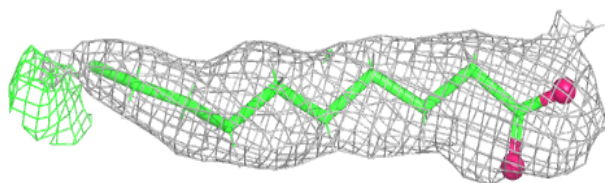


Electron density around SQD b 620:

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

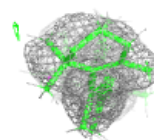
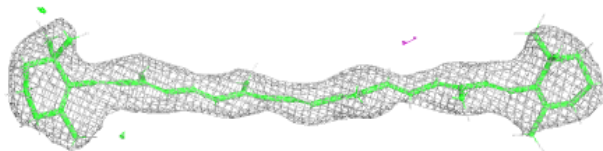
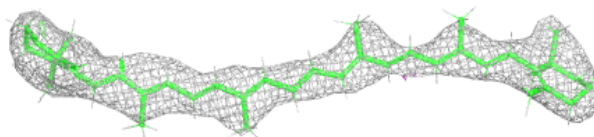
**Electron density around STE J 101:**

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

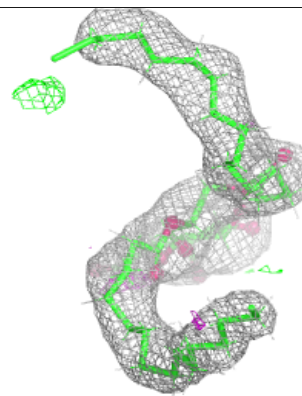
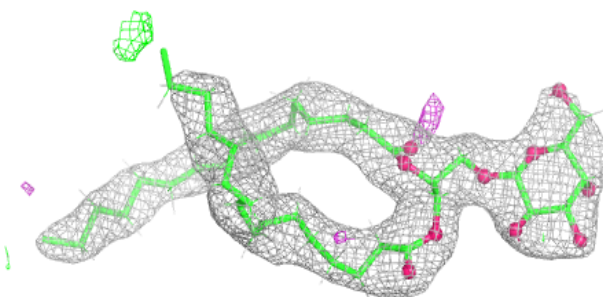
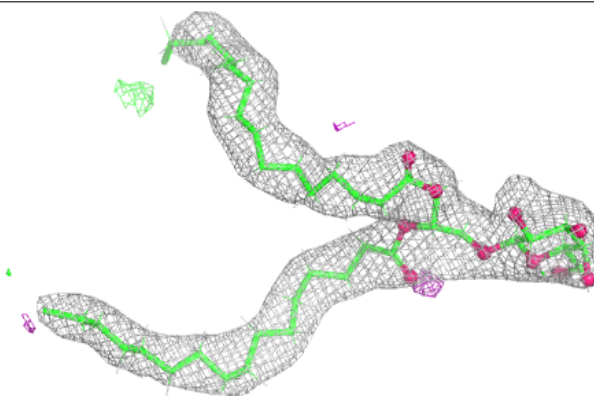


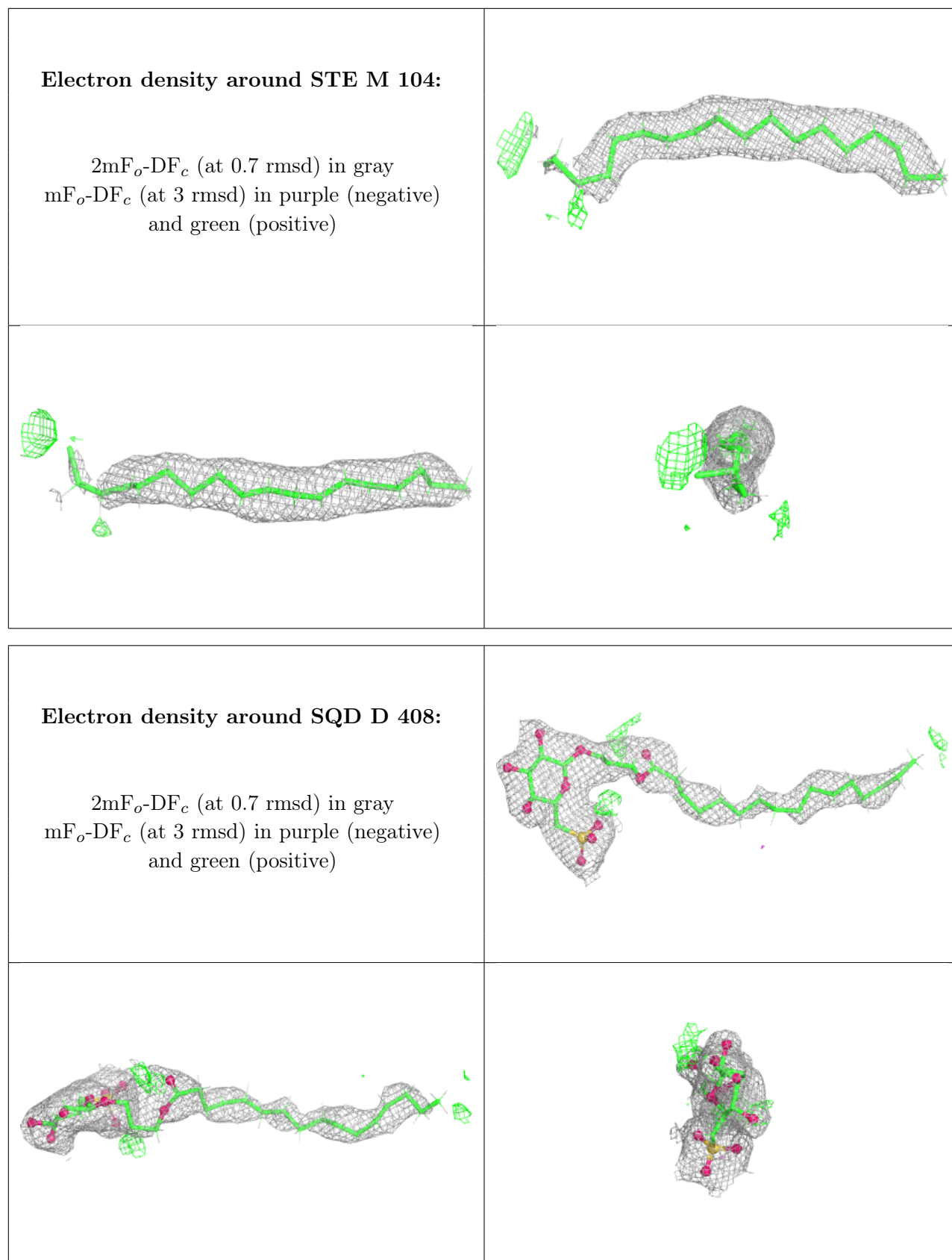
Electron density around BCR c 514:

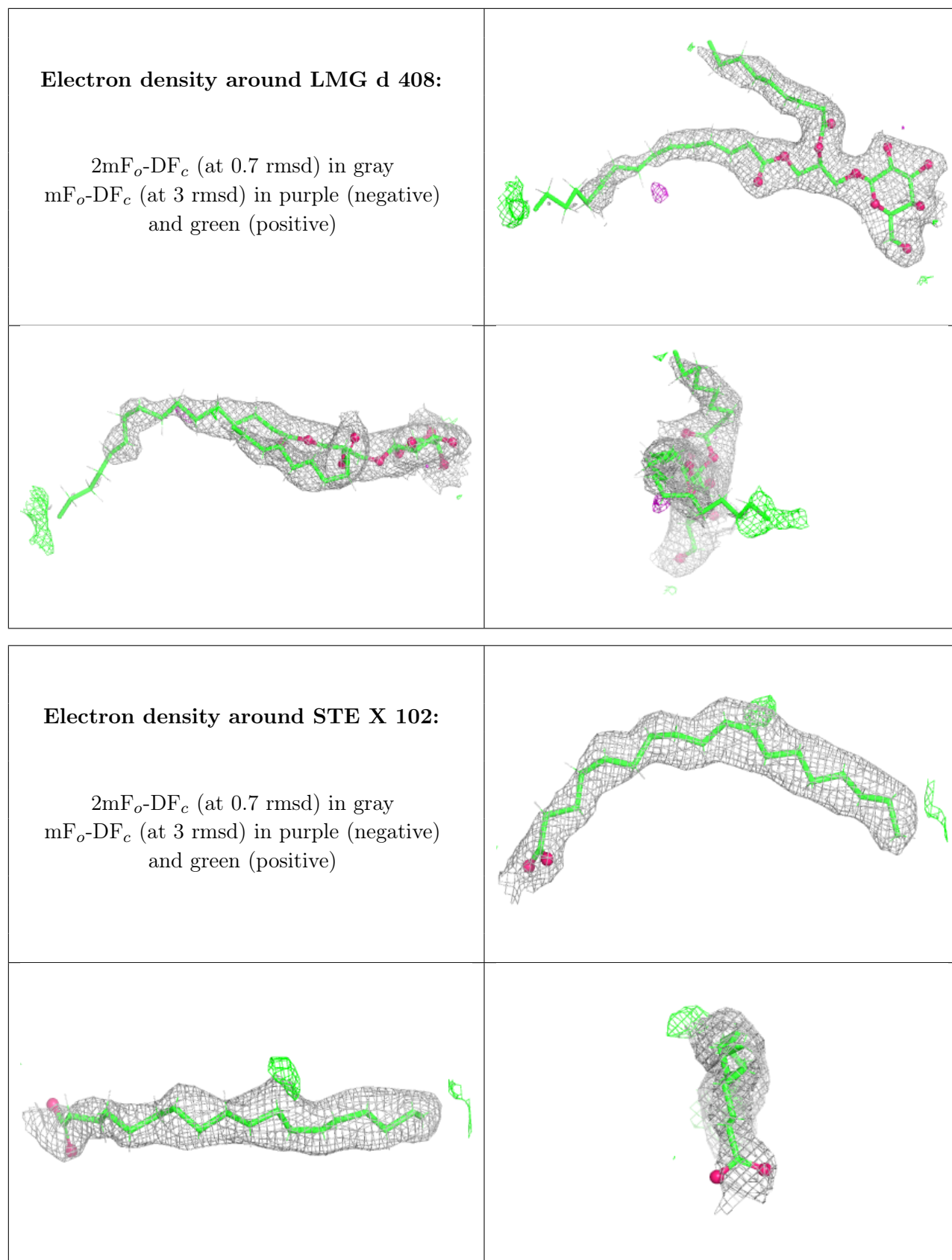
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

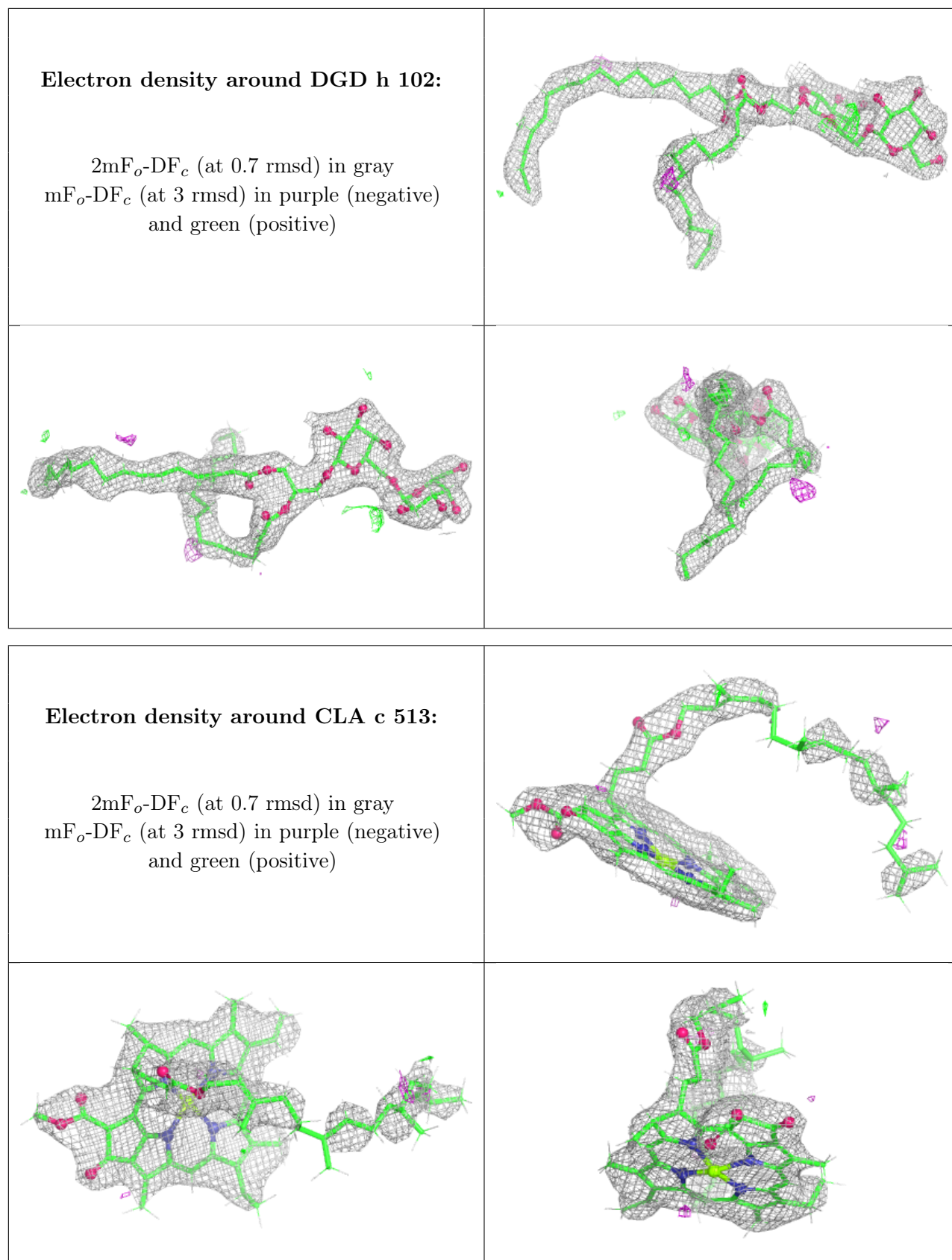
**Electron density around LMG M 101:**

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



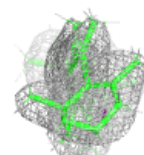
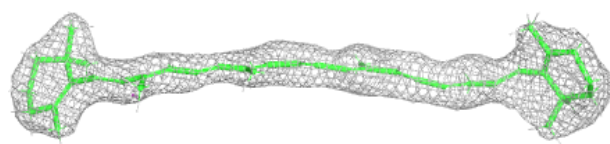
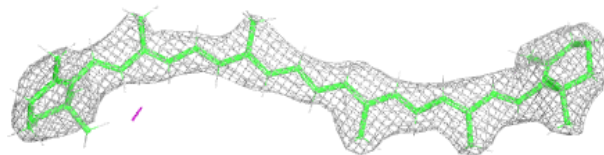




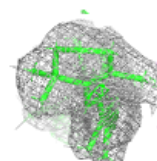
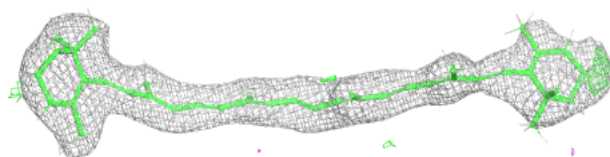
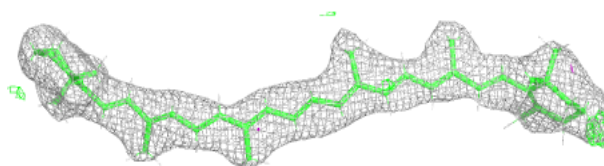


Electron density around BCR k 101:

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

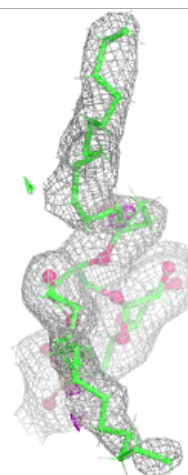
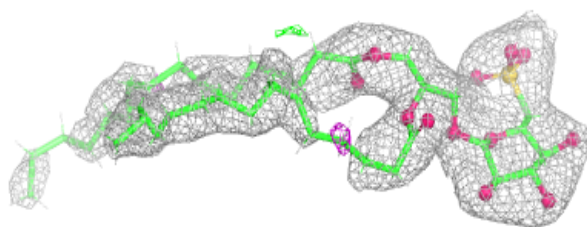
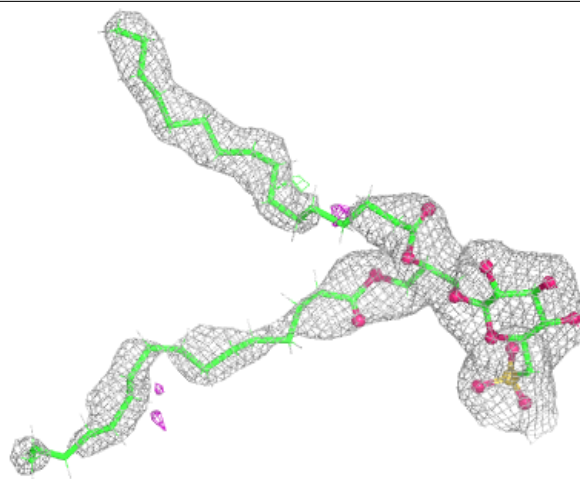
**Electron density around BCR X 101:**

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



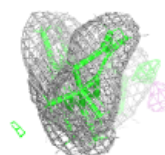
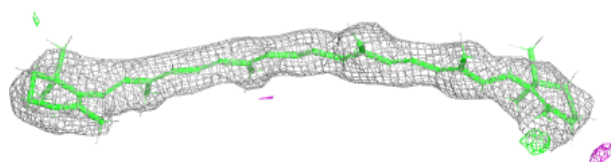
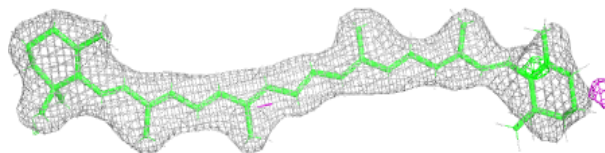
Electron density around SQD a 615:

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

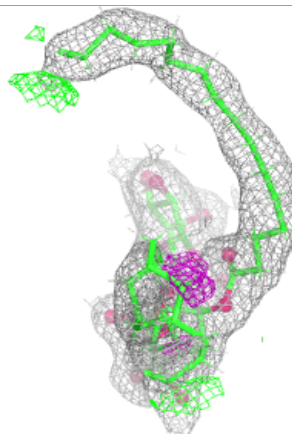
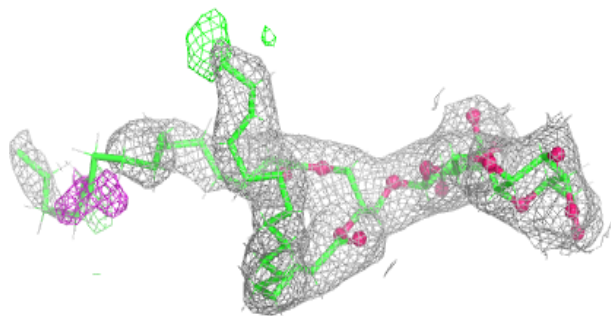
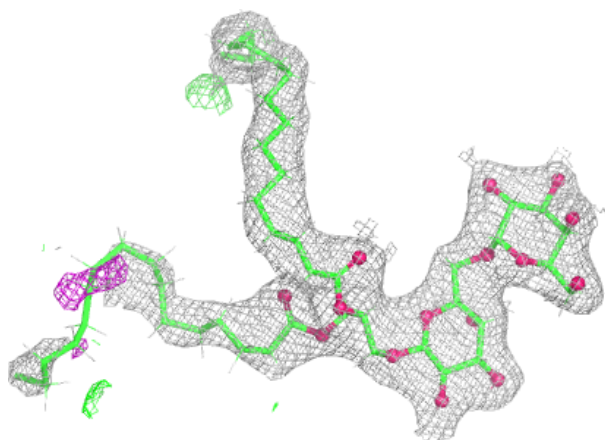


Electron density around BCR D 405:

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

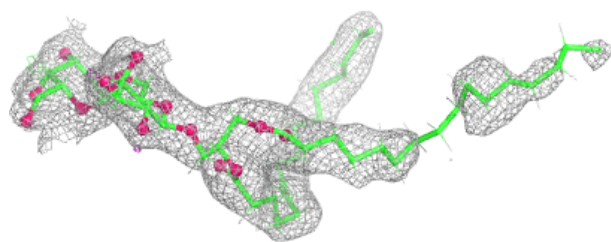
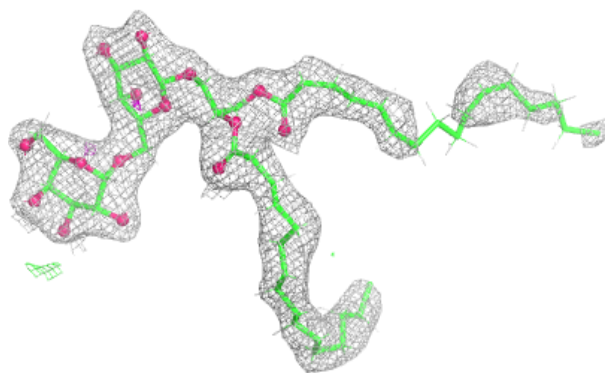
**Electron density around DGD C 517:**

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

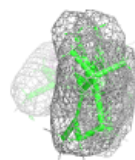
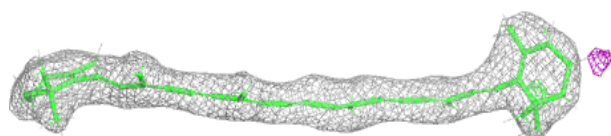
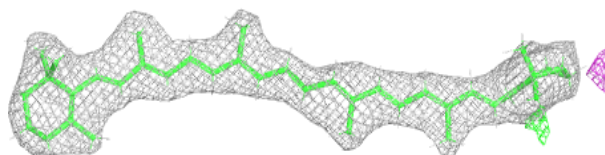


Electron density around DGD c 517:

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

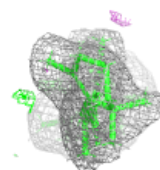
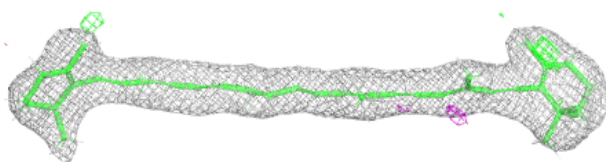
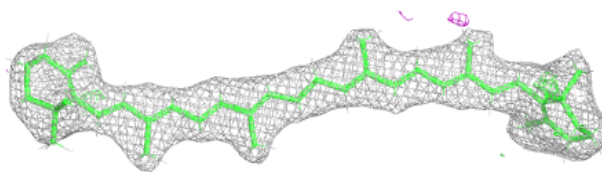
**Electron density around BCR b 617:**

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

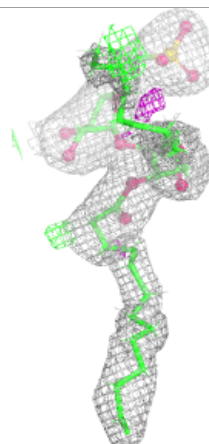
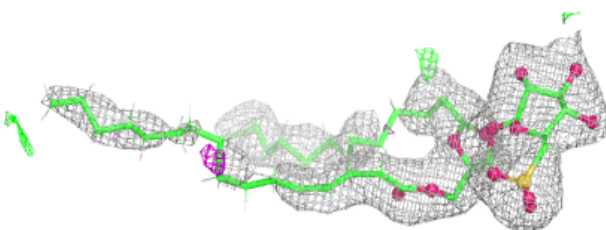
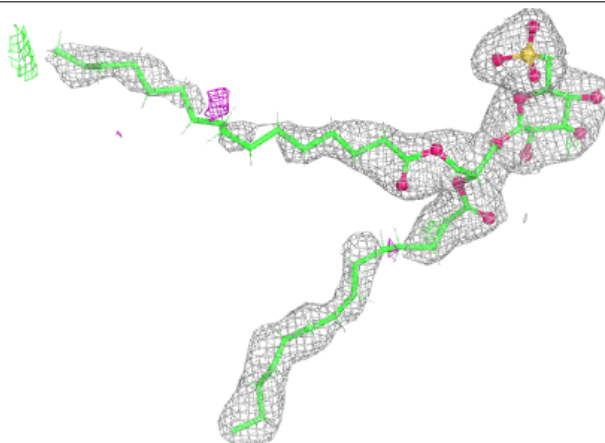


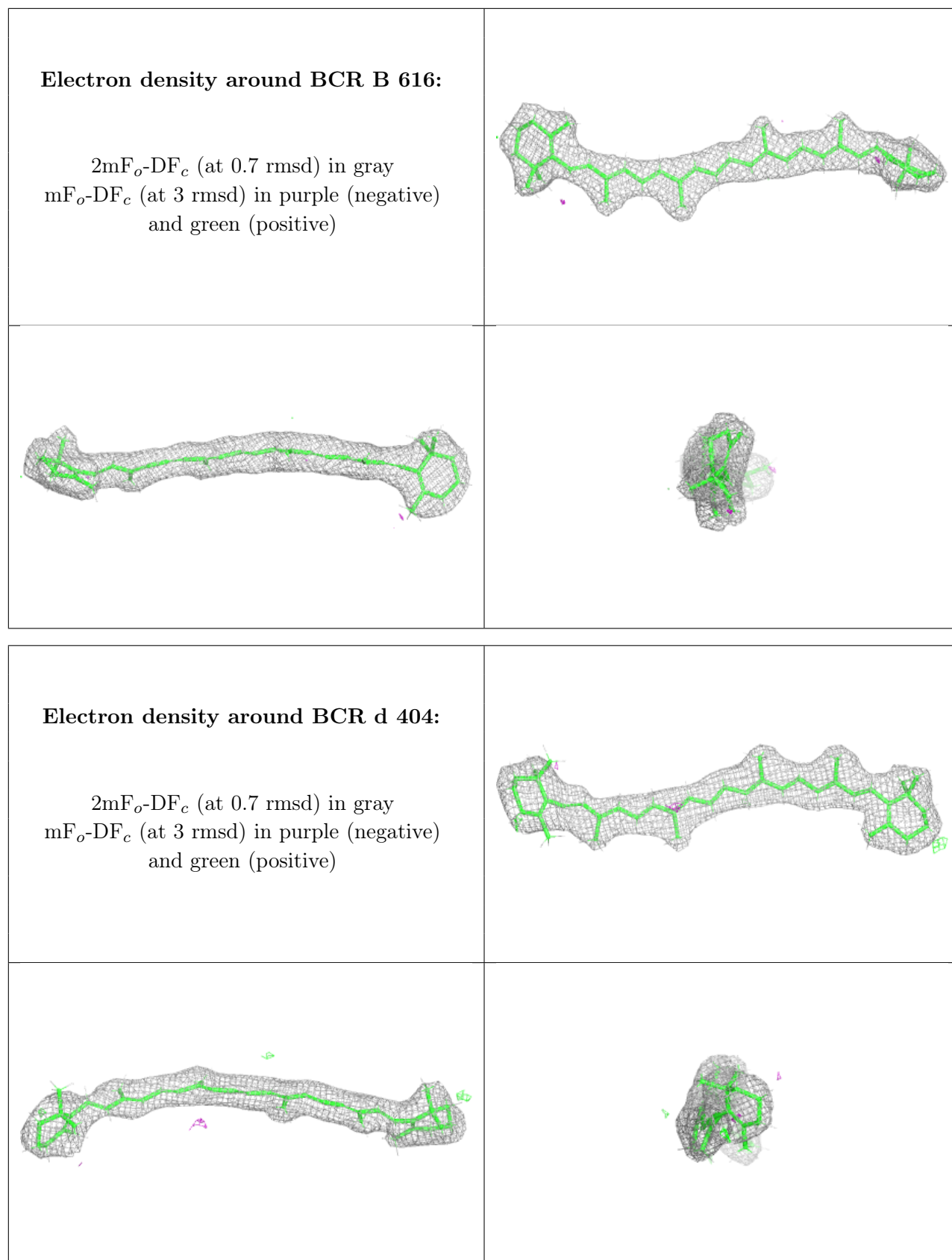
Electron density around BCR b 618:

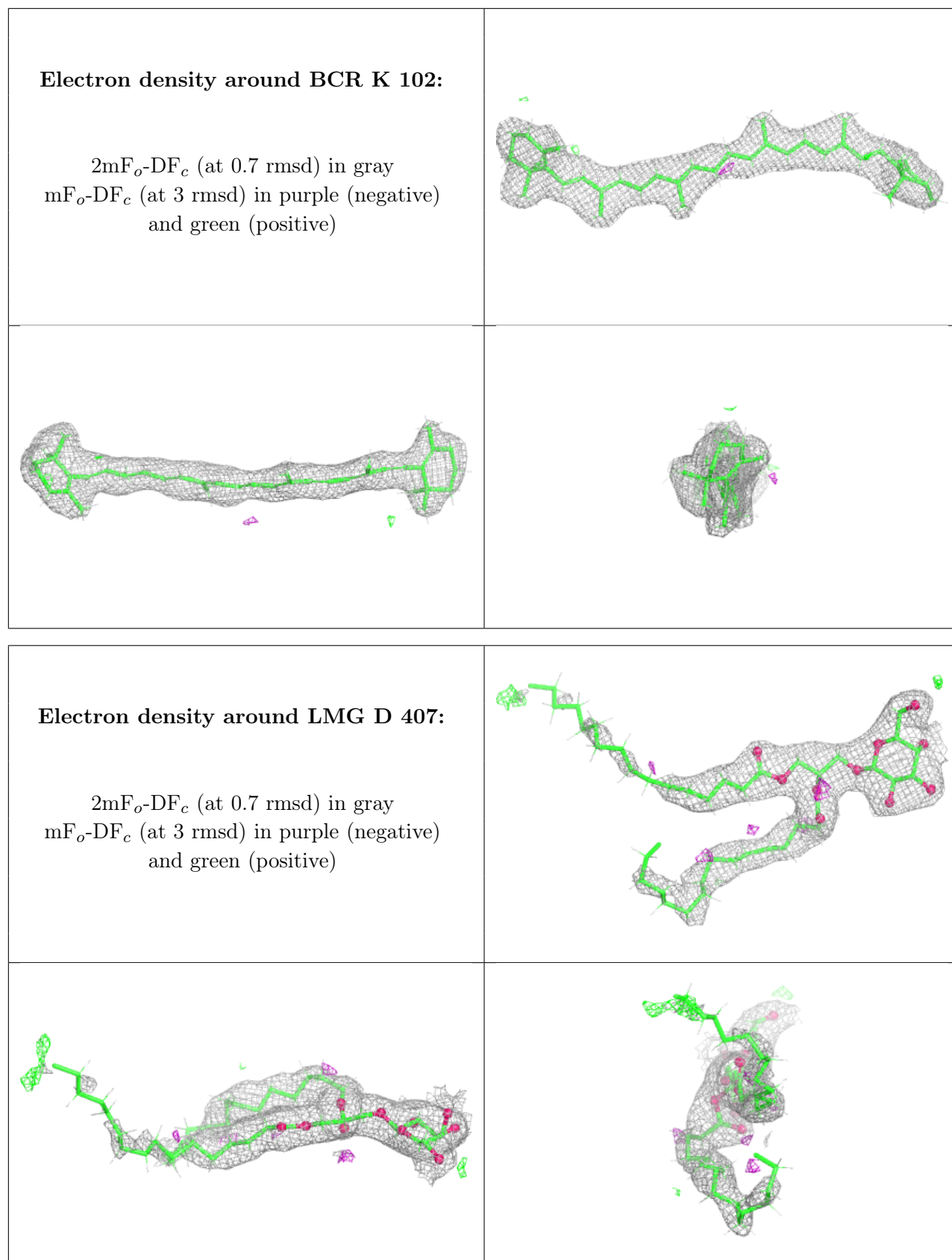
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SQD A 613:**

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

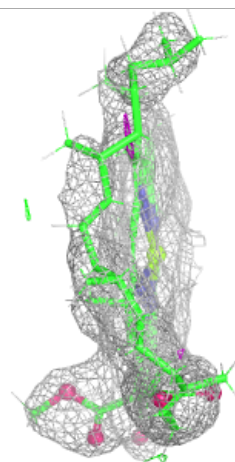
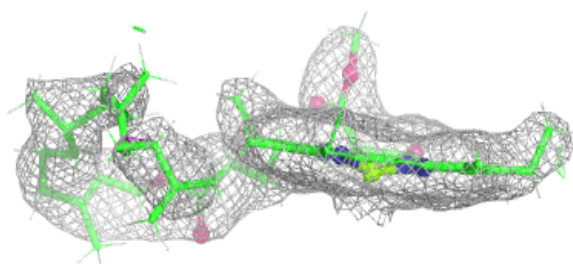
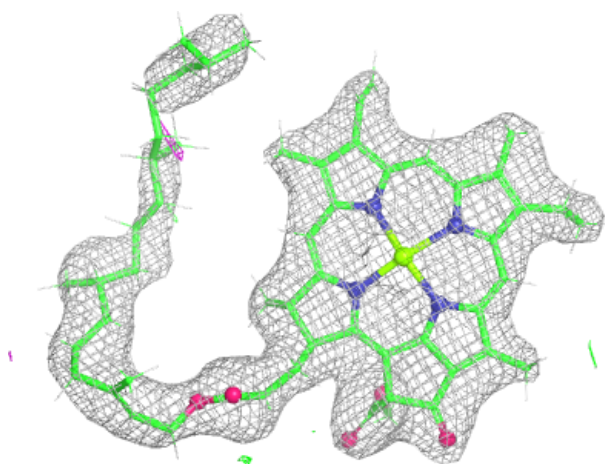






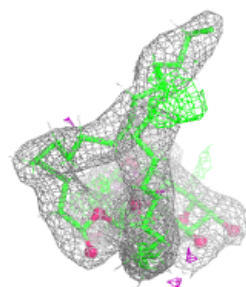
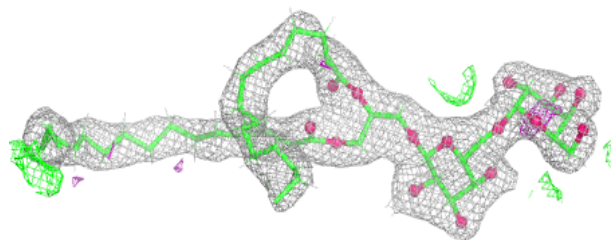
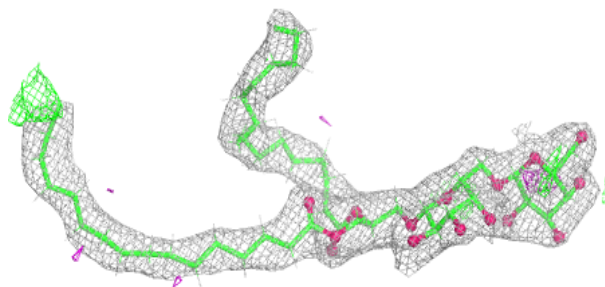
Electron density around CLA c 512:

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

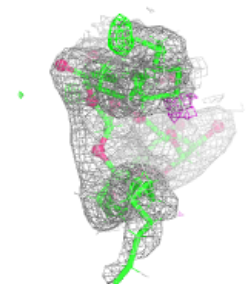
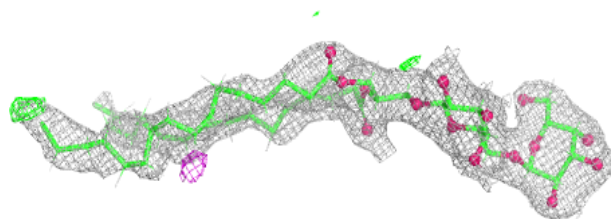
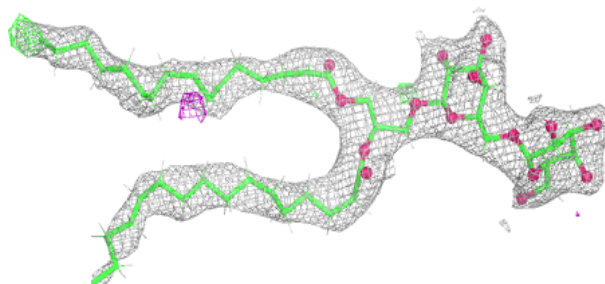


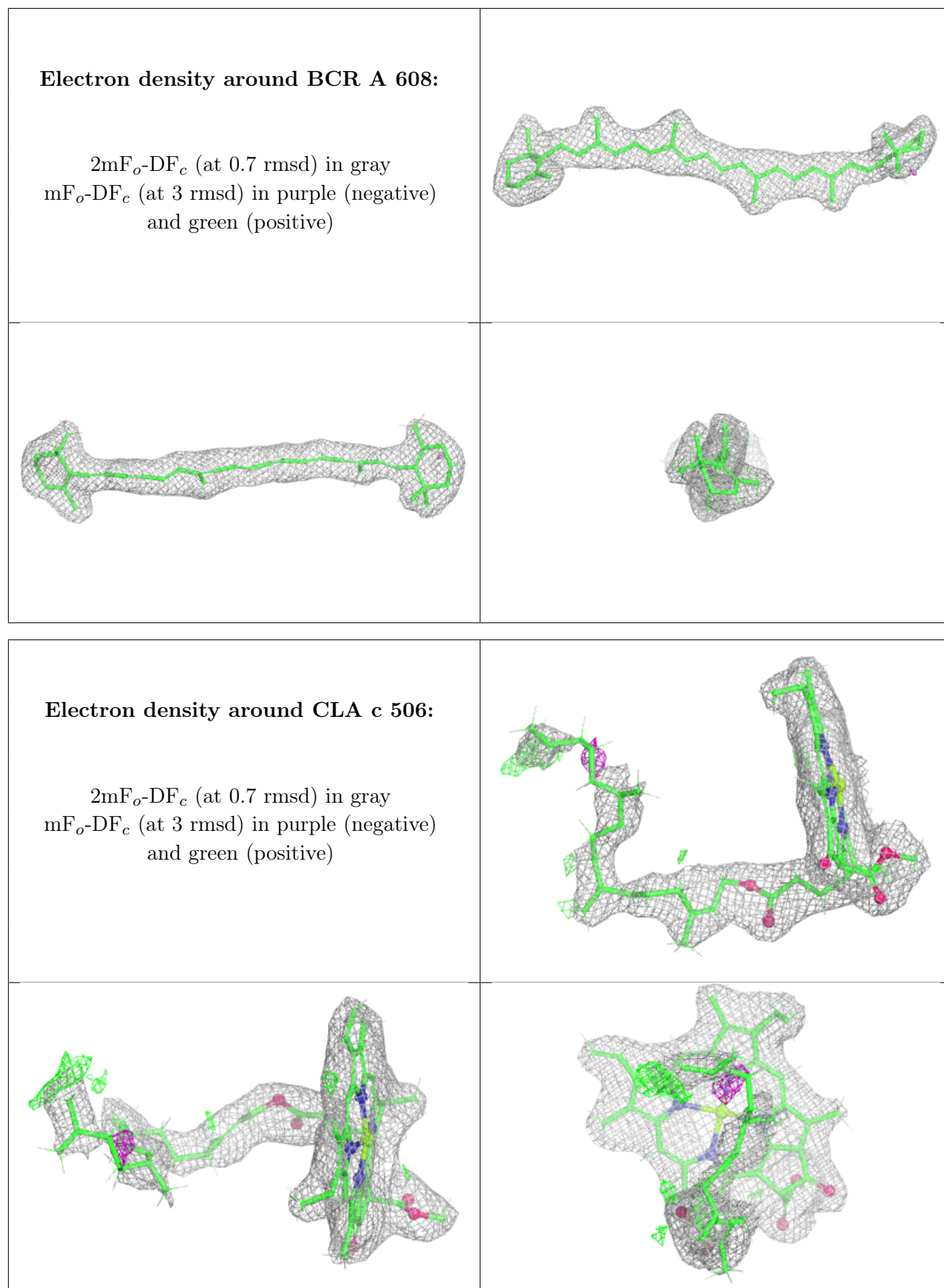
Electron density around DGD H 102:

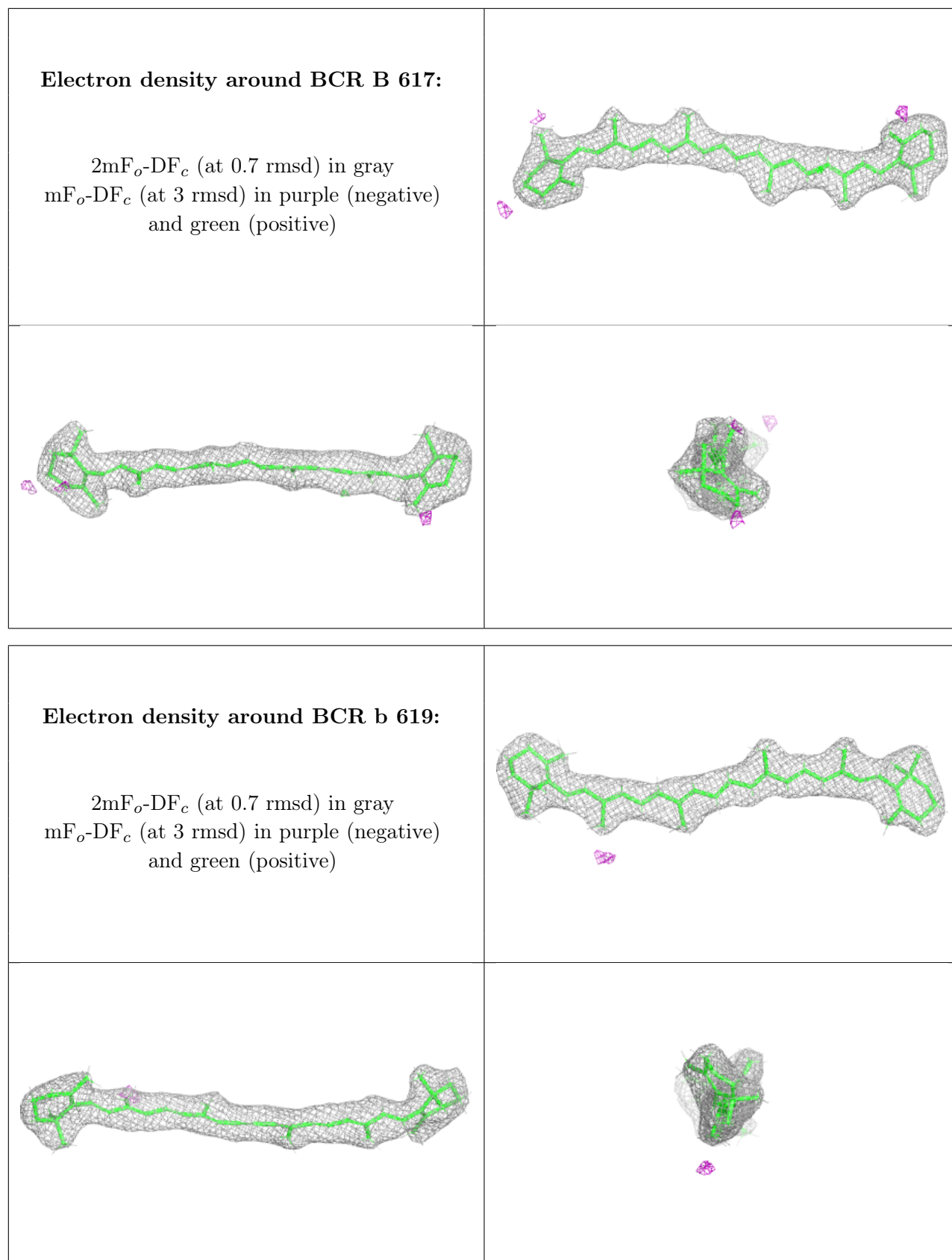
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

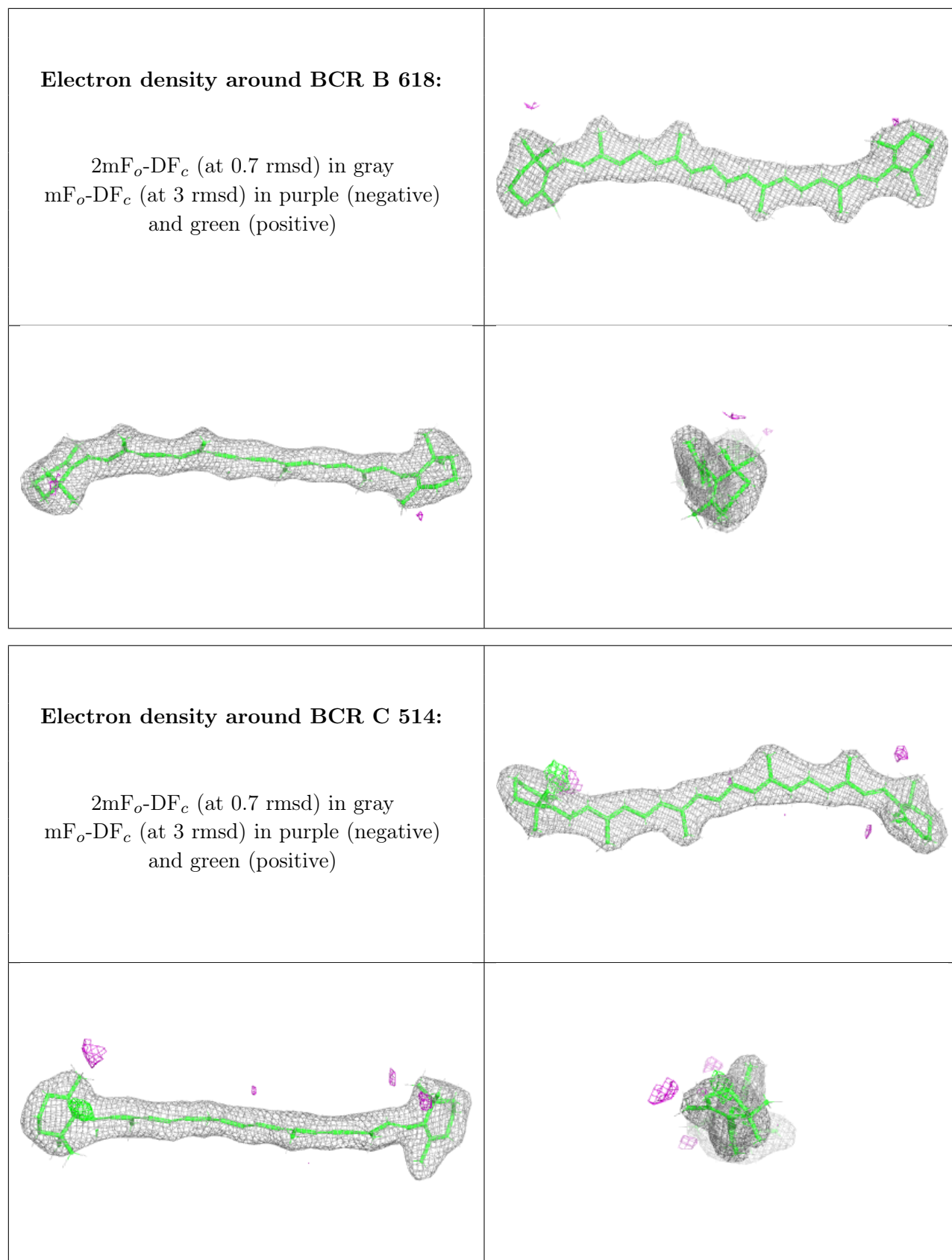
**Electron density around DGD c 518:**

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



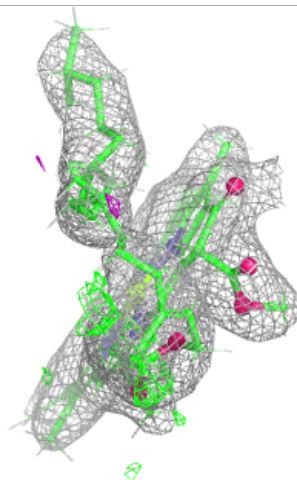
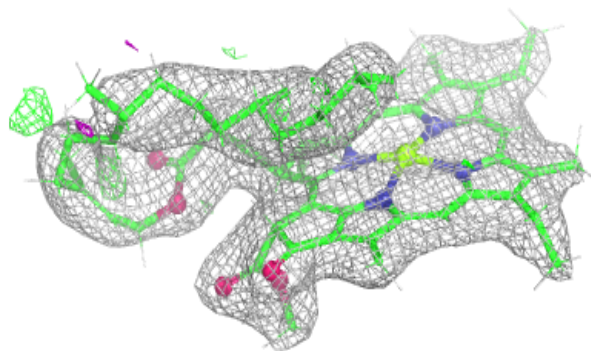
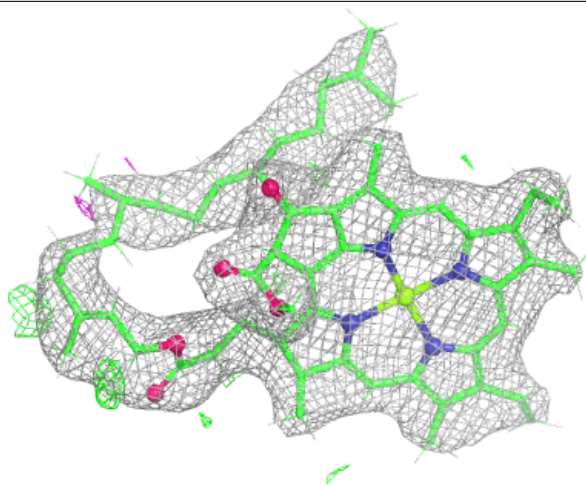






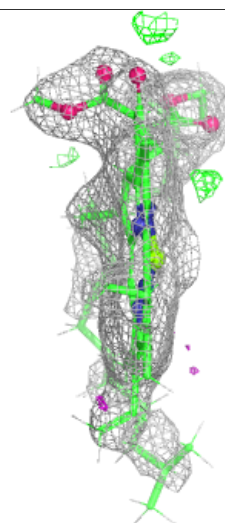
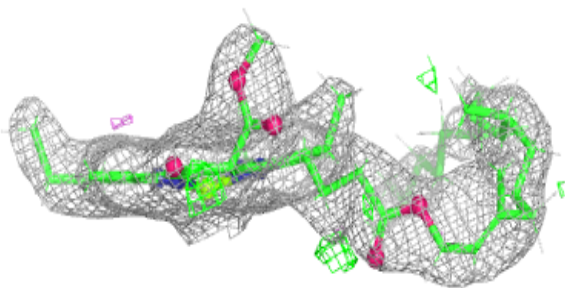
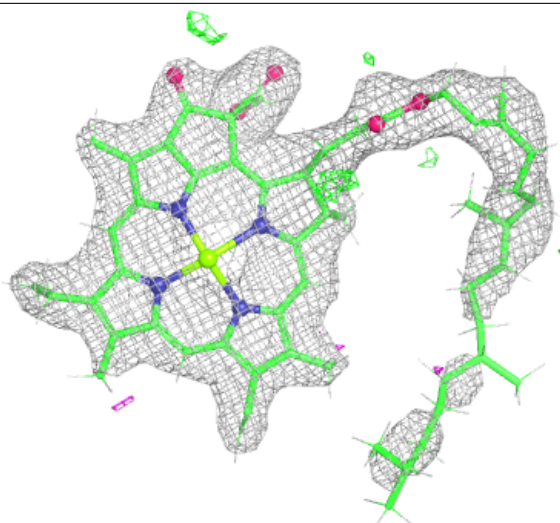
Electron density around CLA c 509:

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



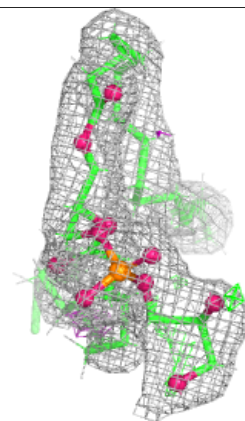
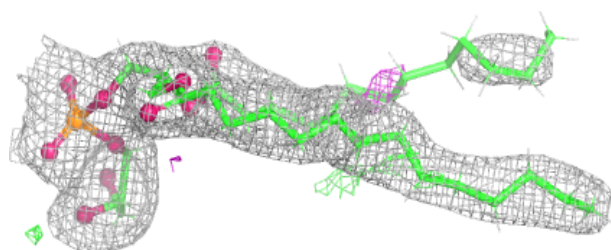
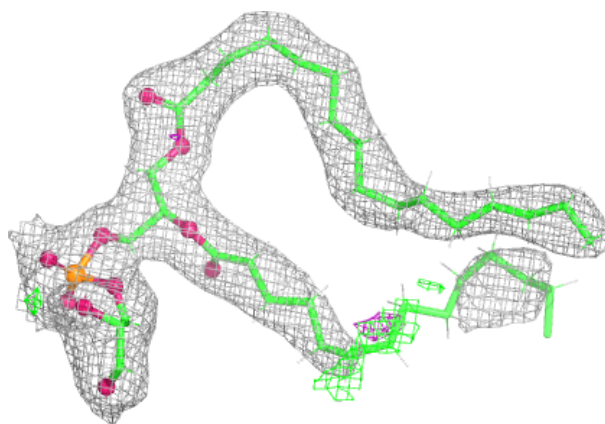
Electron density around CLA C 512:

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

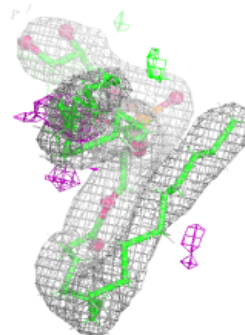
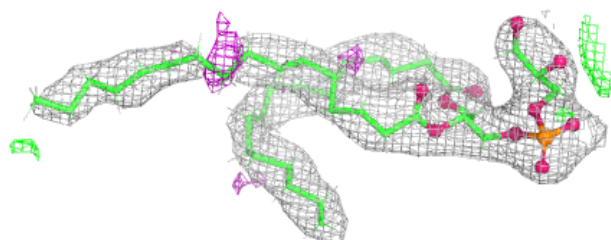
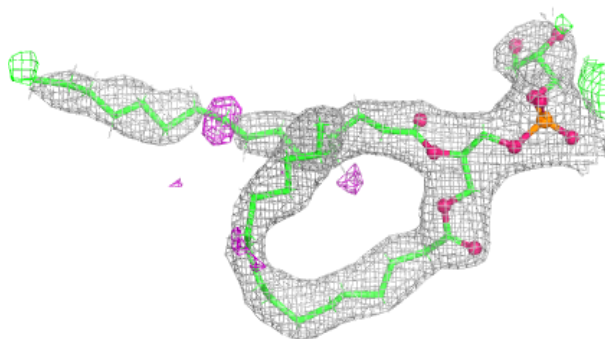


Electron density around LHG D 410:

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

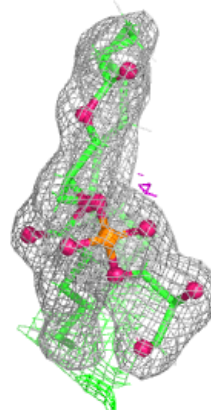
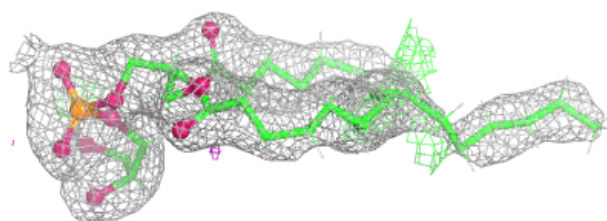
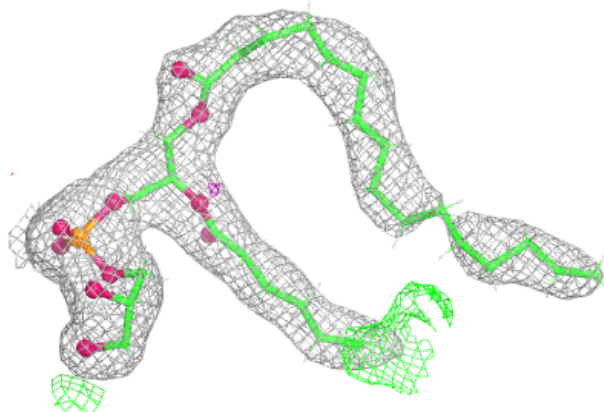
**Electron density around LHG a 614:**

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

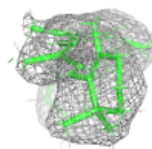
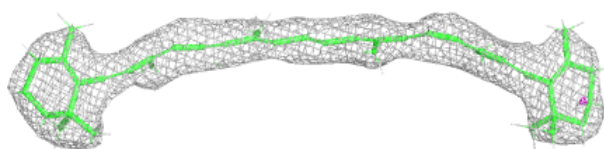


Electron density around LHG d 407:

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

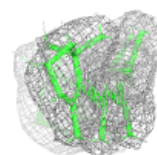
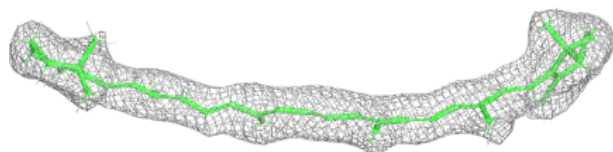
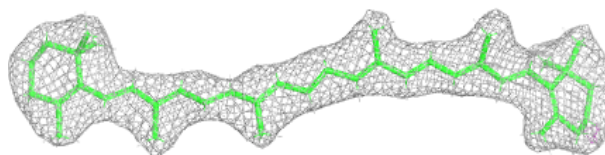
**Electron density around BCR k 102:**

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

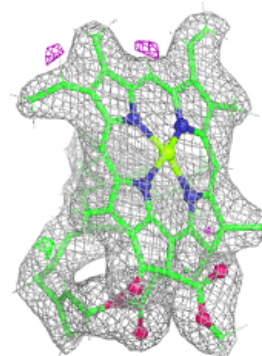
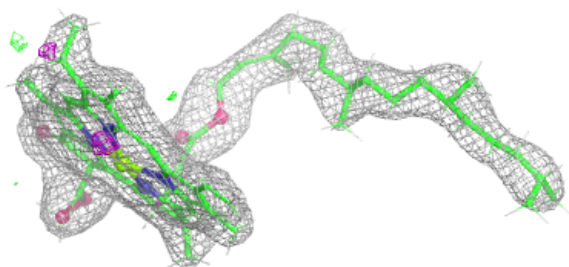
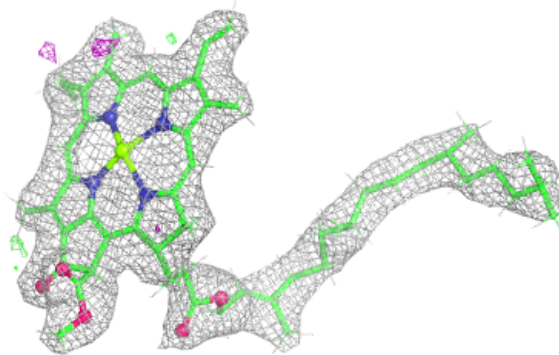


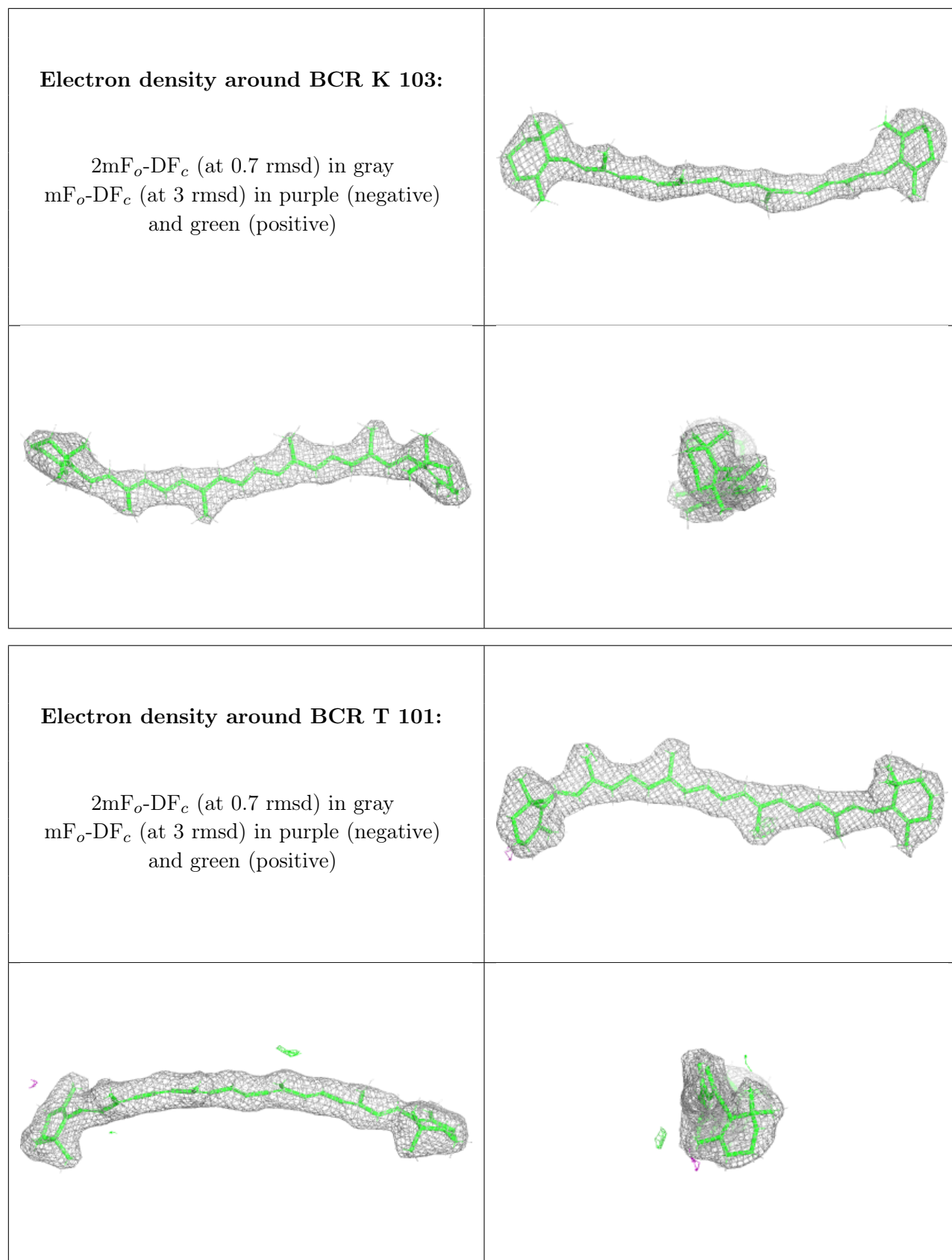
Electron density around BCR t 101:

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

**Electron density around CLA C 511:**

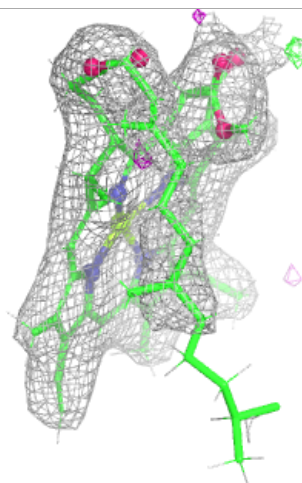
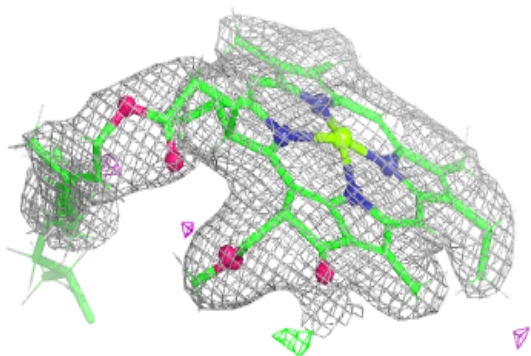
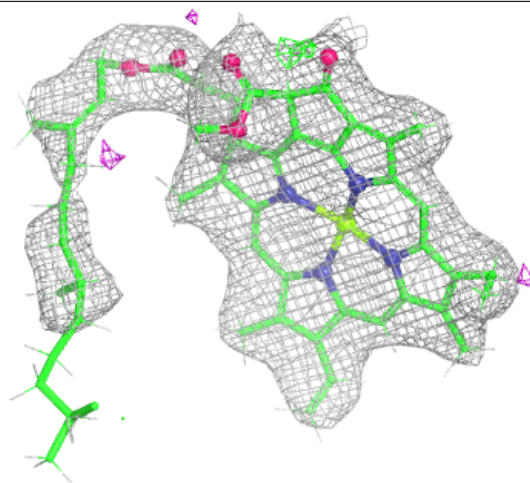
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





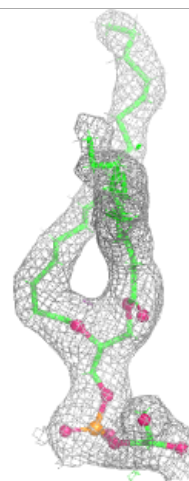
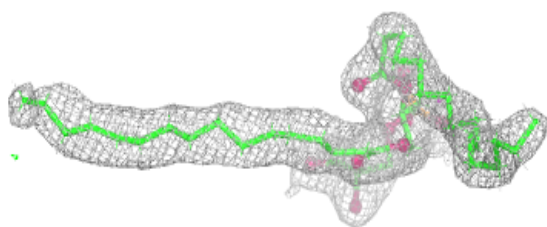
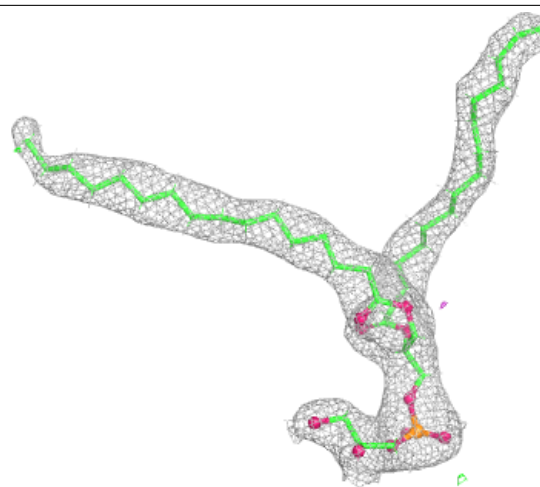
Electron density around CLA b 616:

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



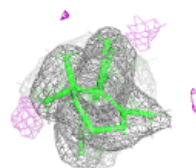
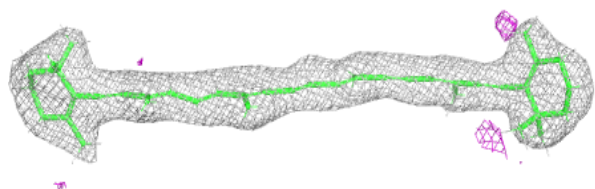
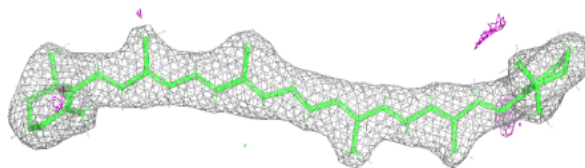
Electron density around LHG 1 101:

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

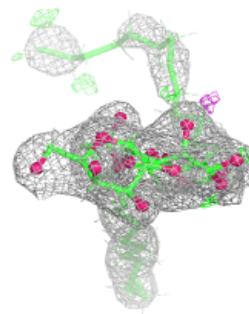
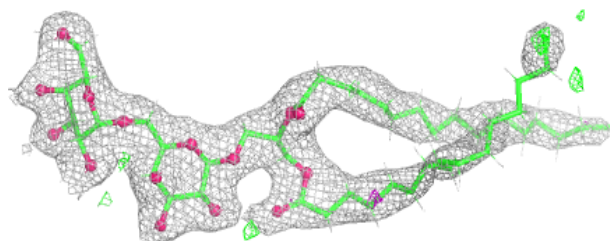
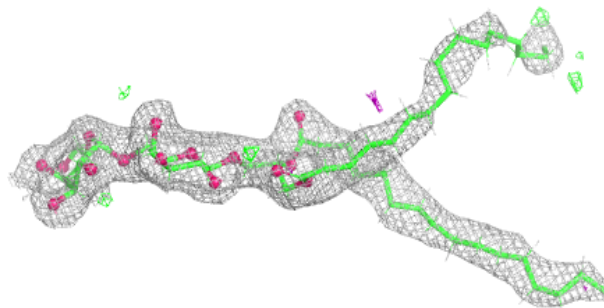


Electron density around BCR a 608:

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

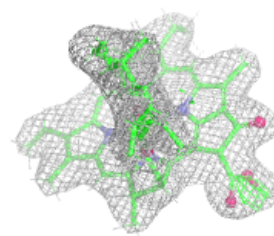
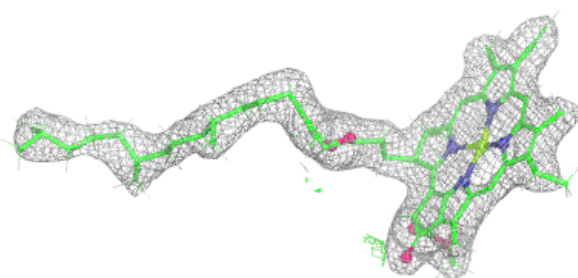
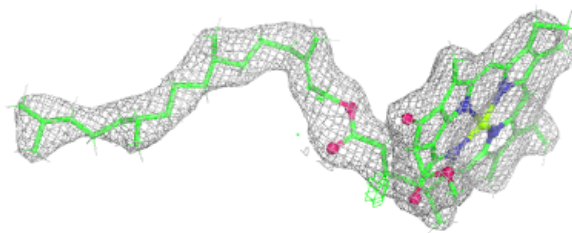
**Electron density around DGD C 516:**

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

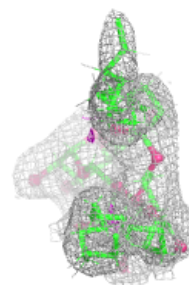
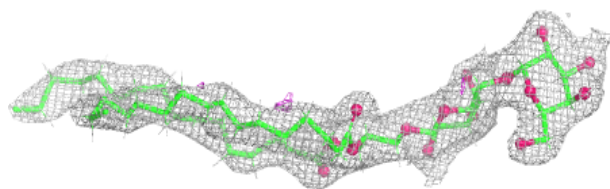
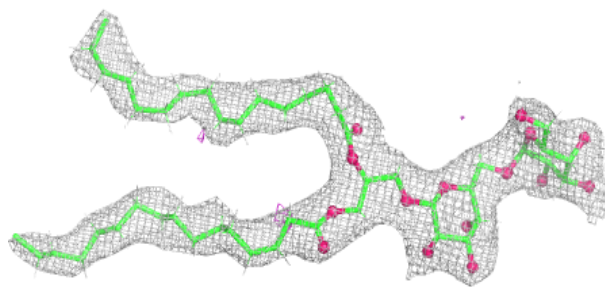


Electron density around CLA c 502:

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

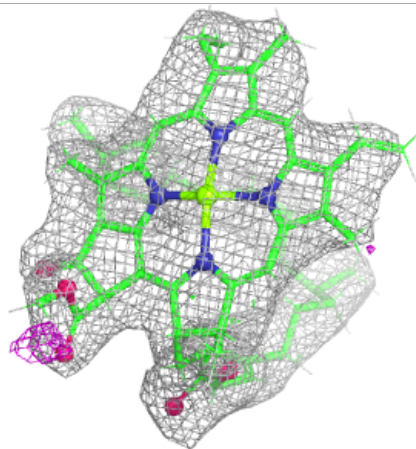
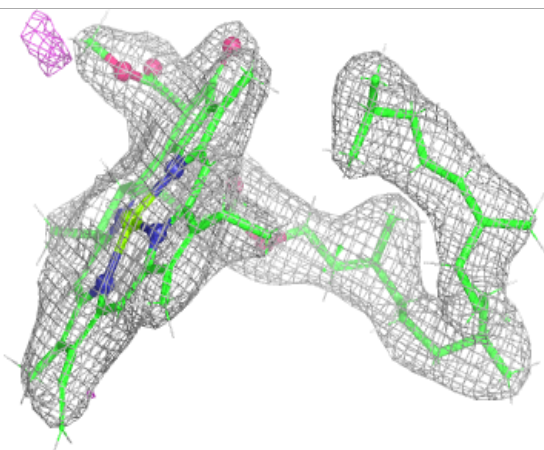
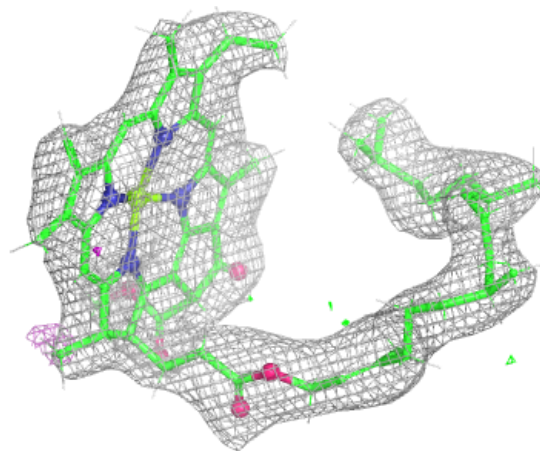
**Electron density around DGD C 518:**

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



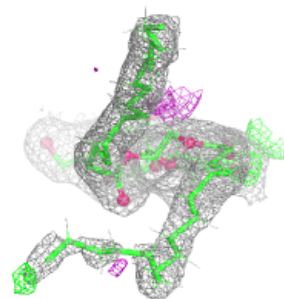
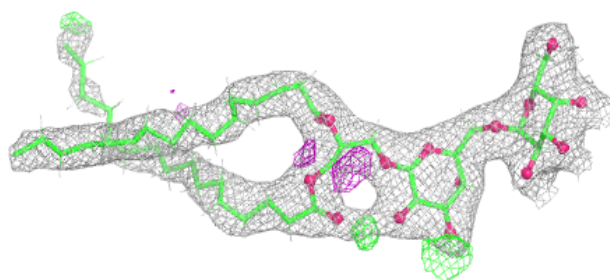
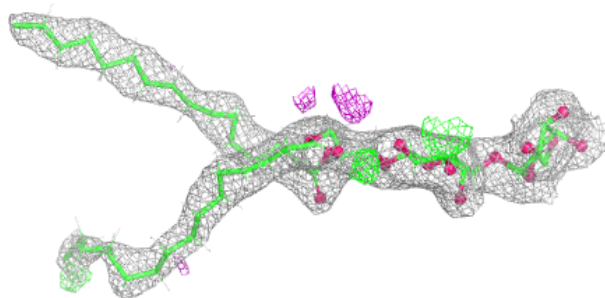
Electron density around CLA c 503:

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

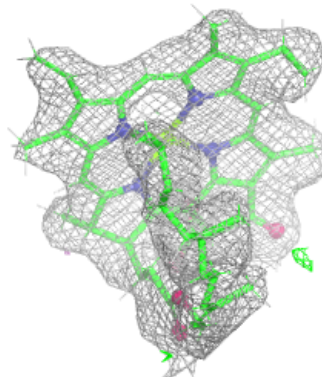
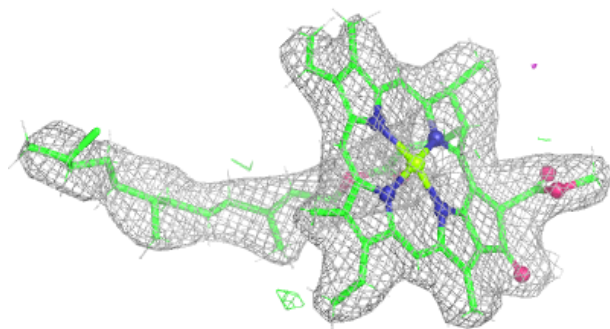
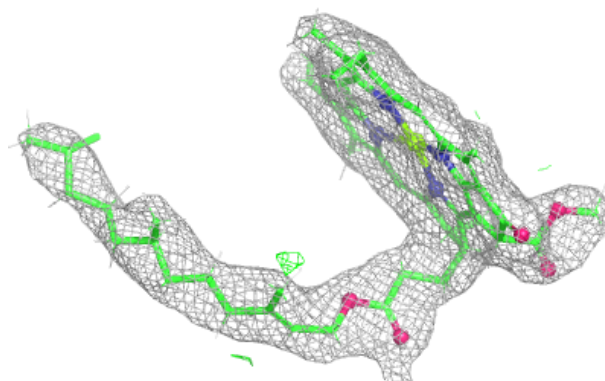


Electron density around DGD c 516:

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

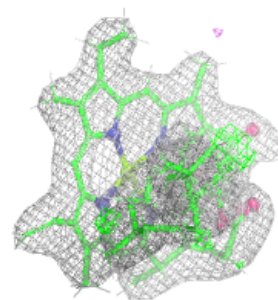
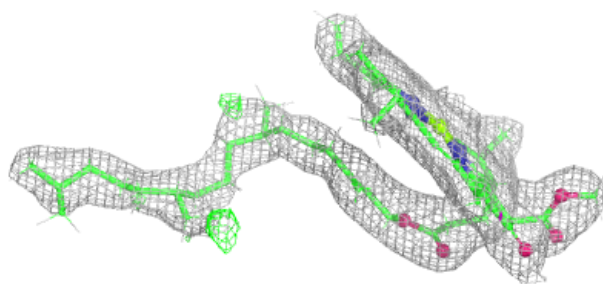
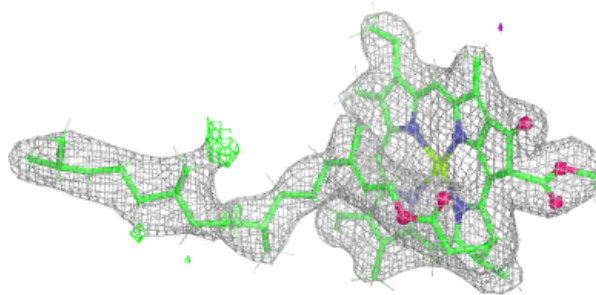
**Electron density around CLA c 504:**

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

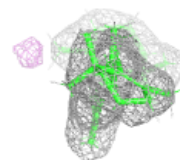
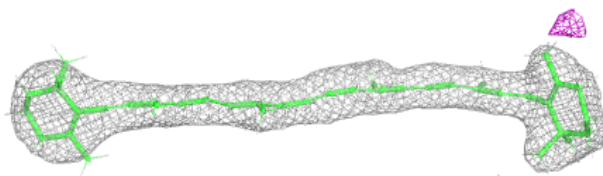
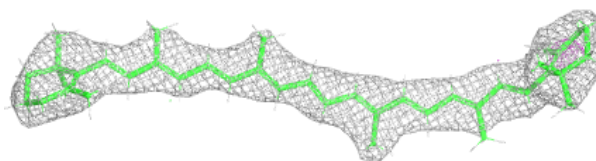


Electron density around CLA c 505:

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

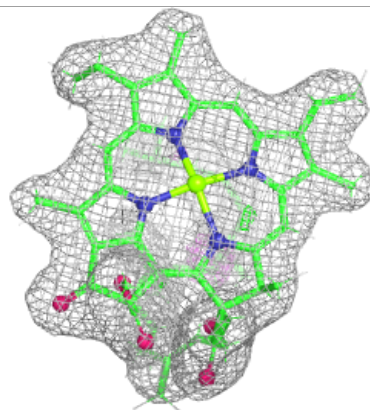
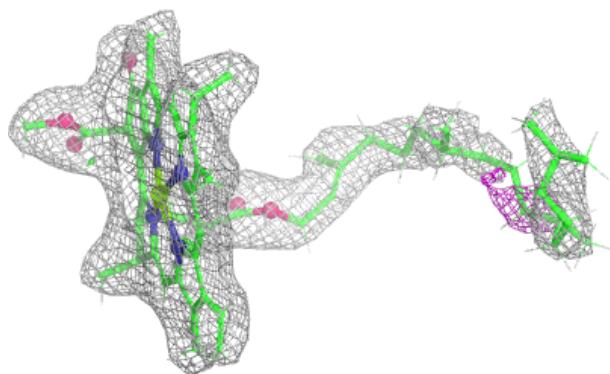
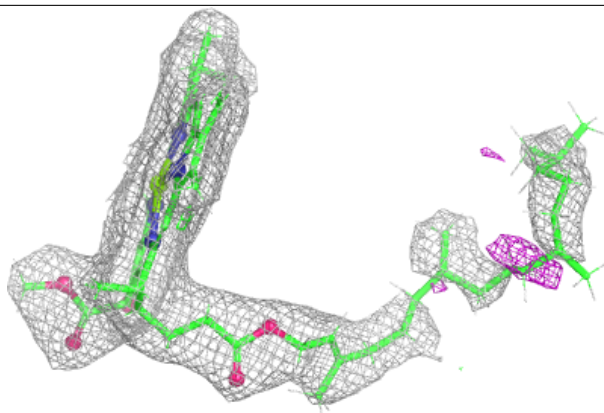
**Electron density around BCR c 515:**

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

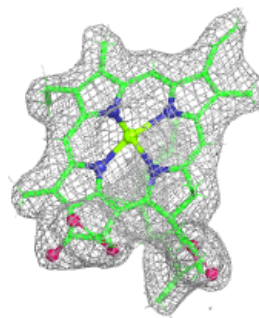
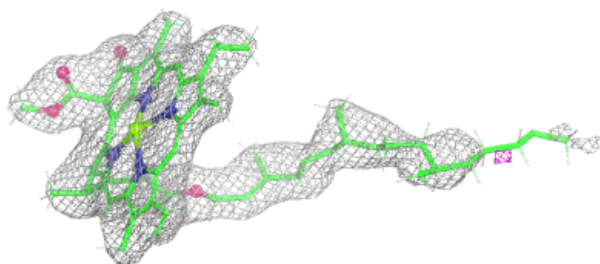
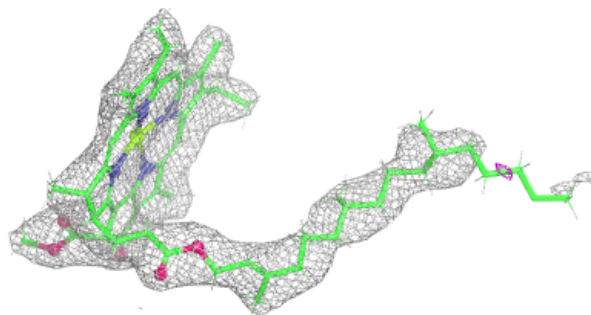


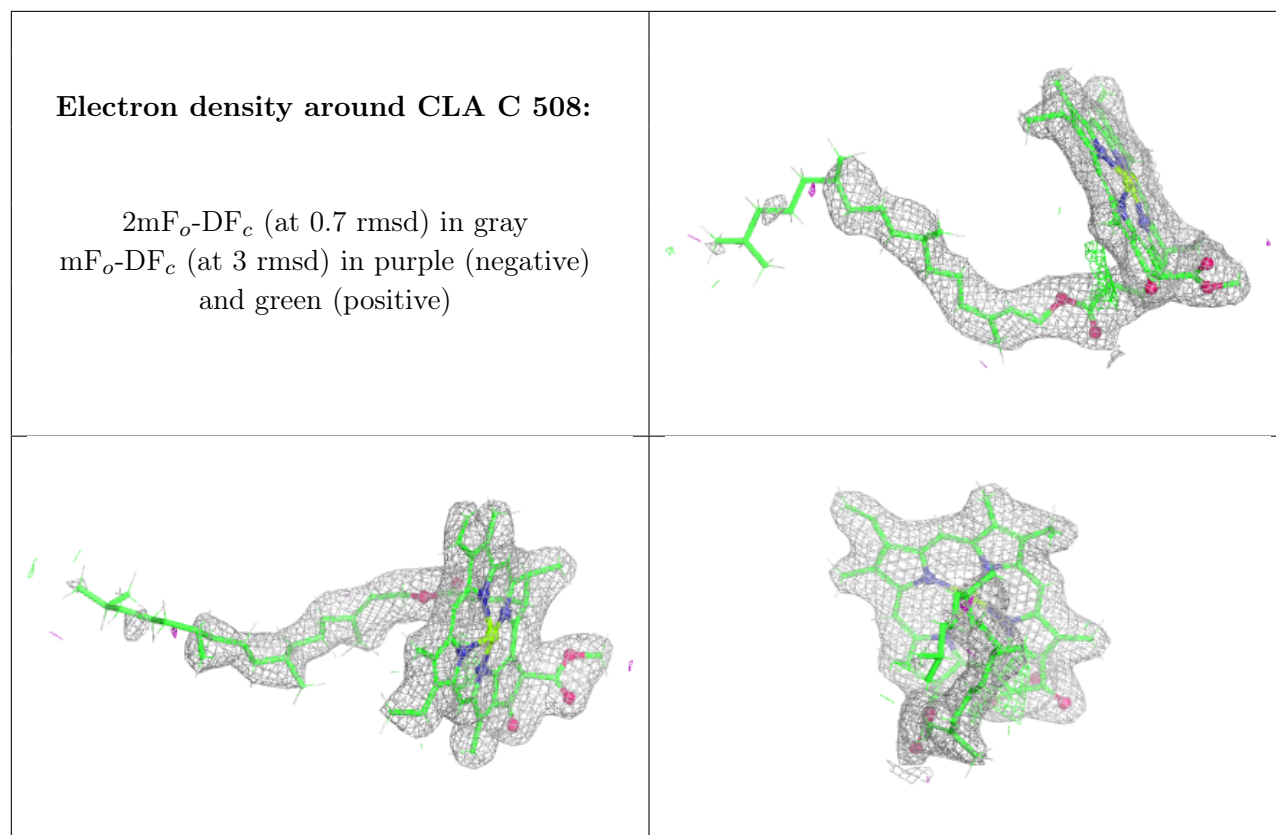
Electron density around CLA C 506:

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

**Electron density around CLA c 508:**

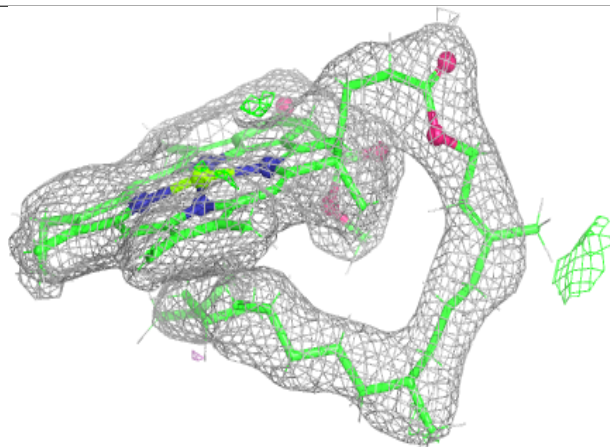
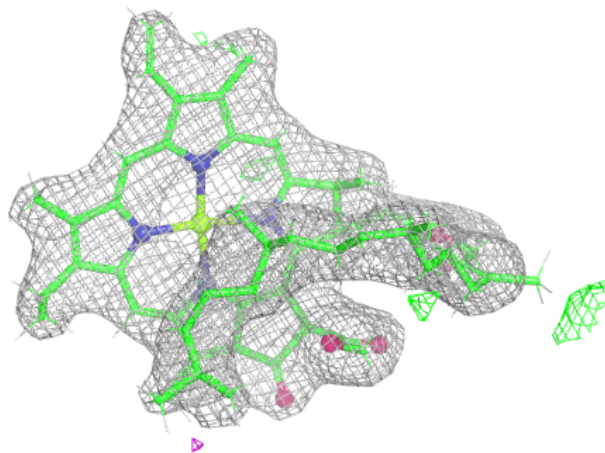
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





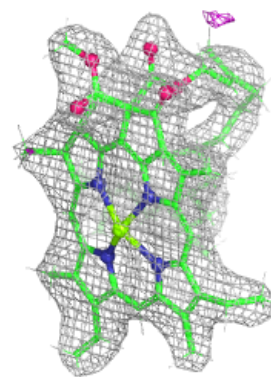
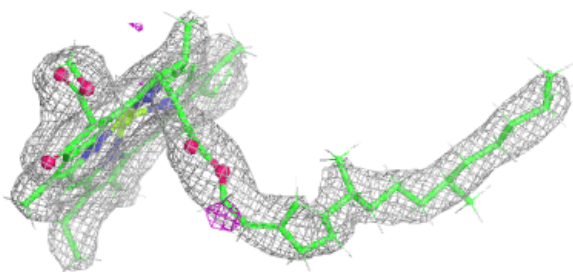
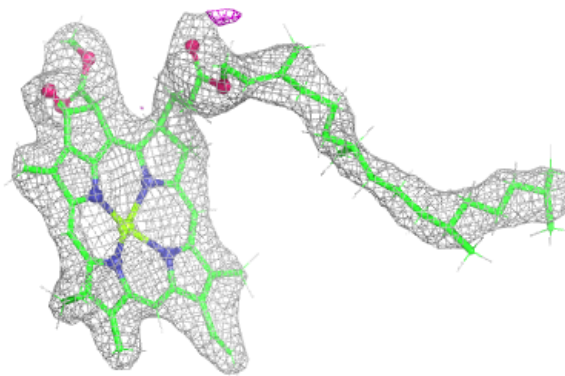
Electron density around CLA c 510:

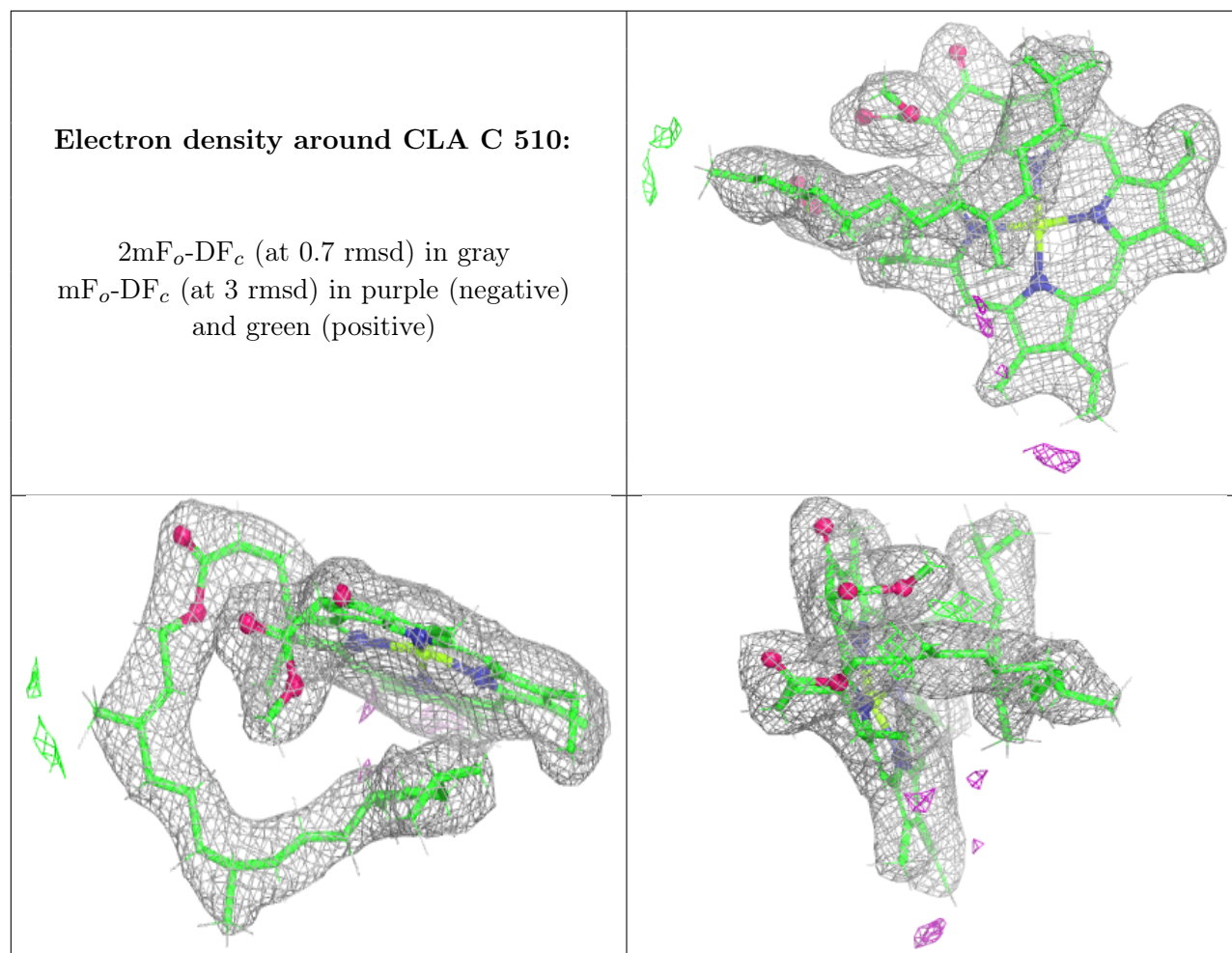
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 511:

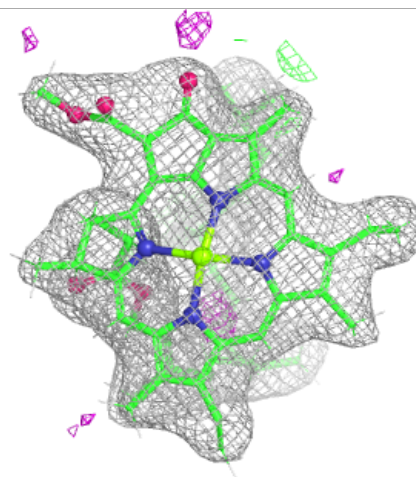
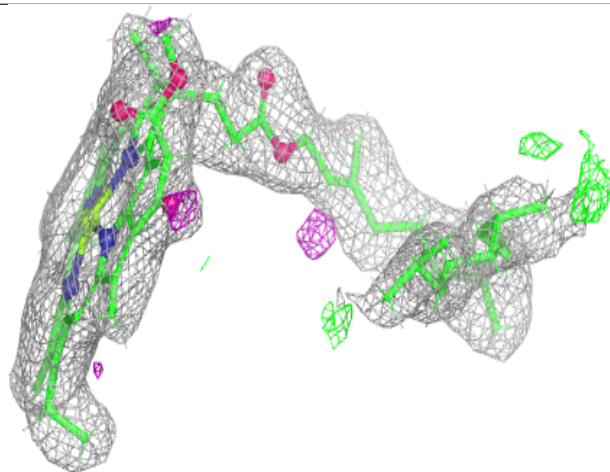
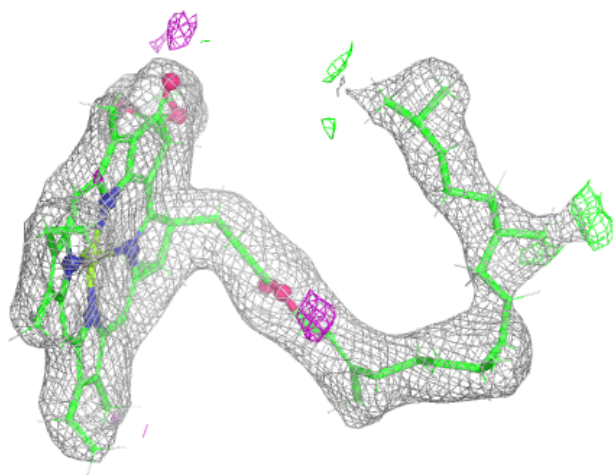
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





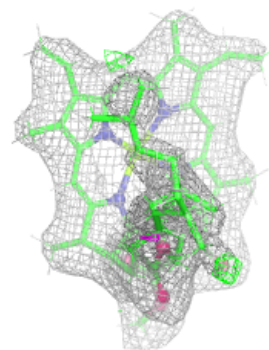
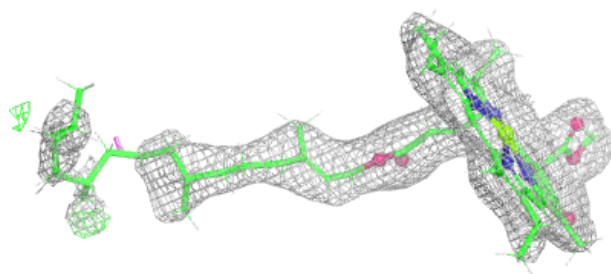
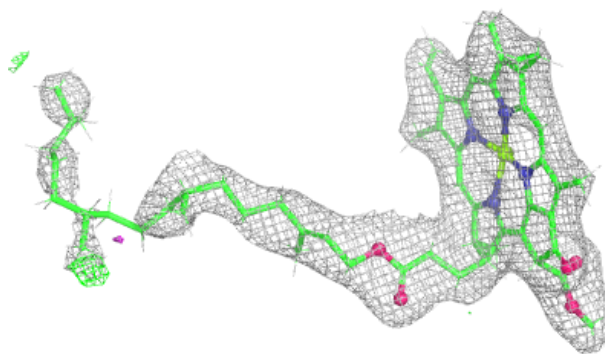
Electron density around CLA B 605:

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



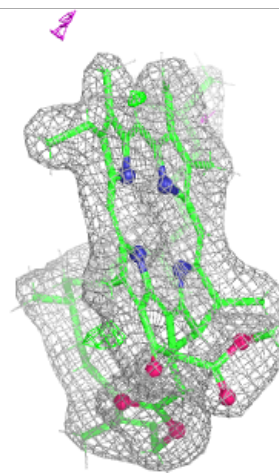
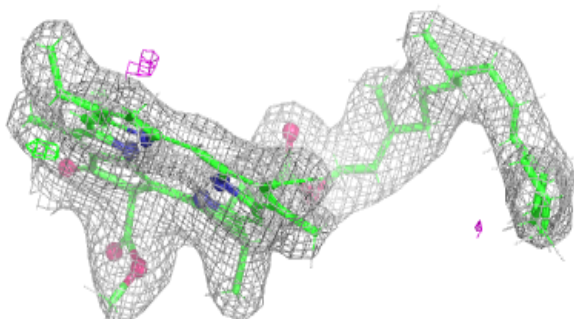
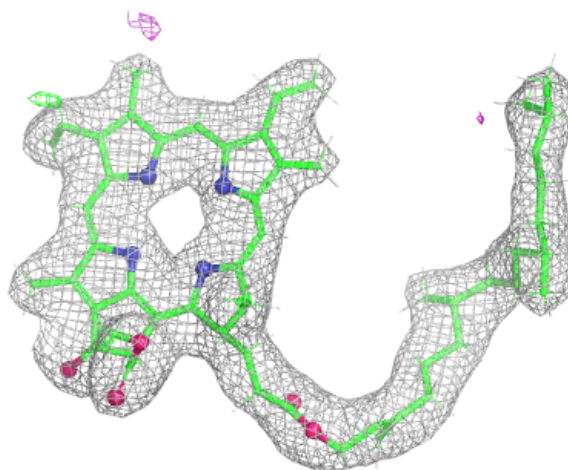
Electron density around CLA d 403:

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



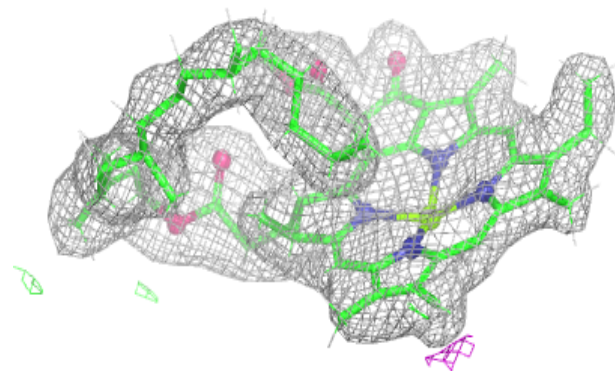
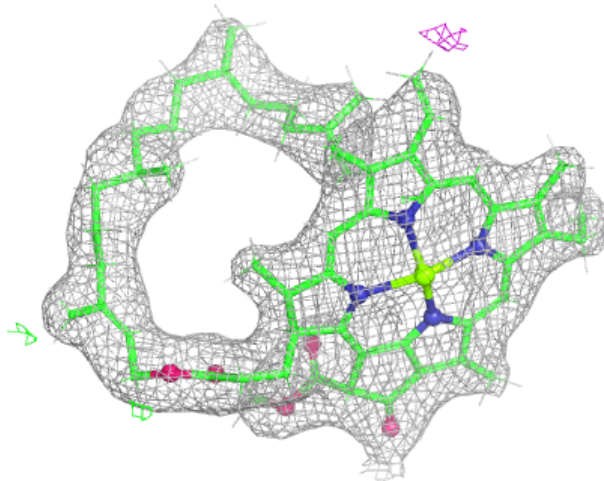
Electron density around PHO d 401:

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



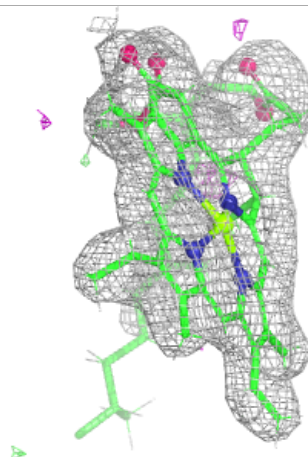
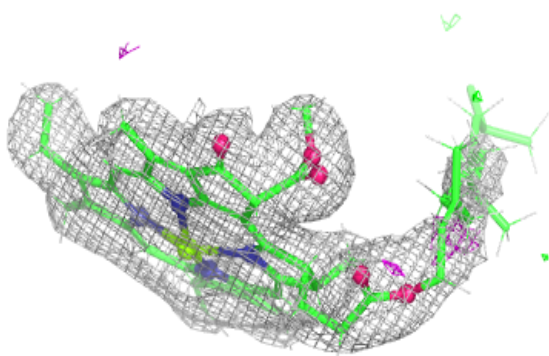
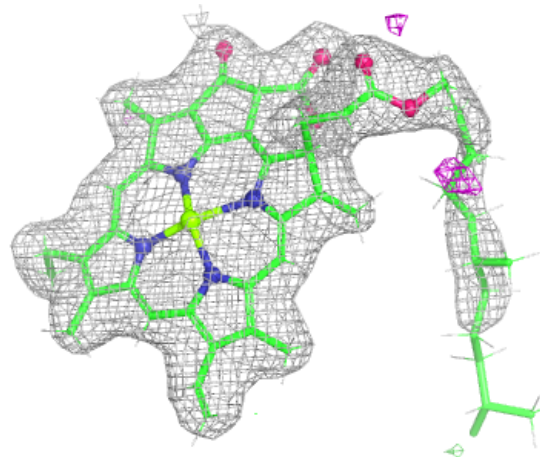
Electron density around CLA B 614:

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



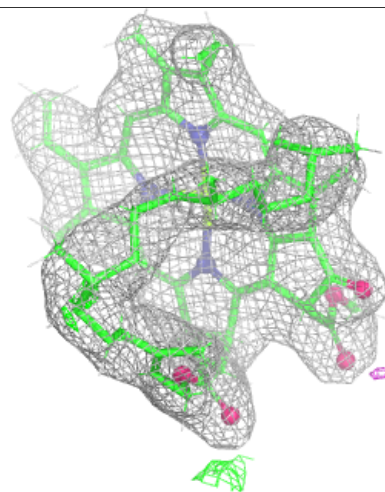
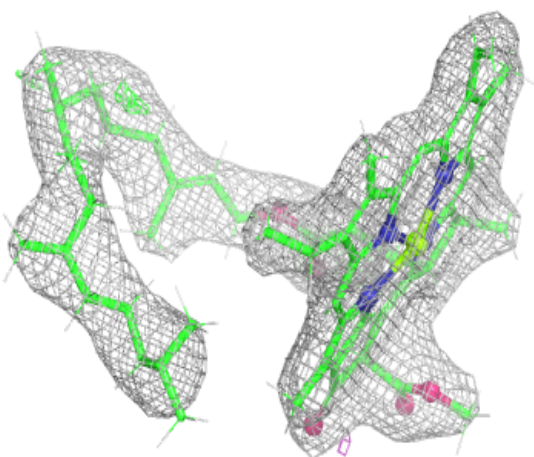
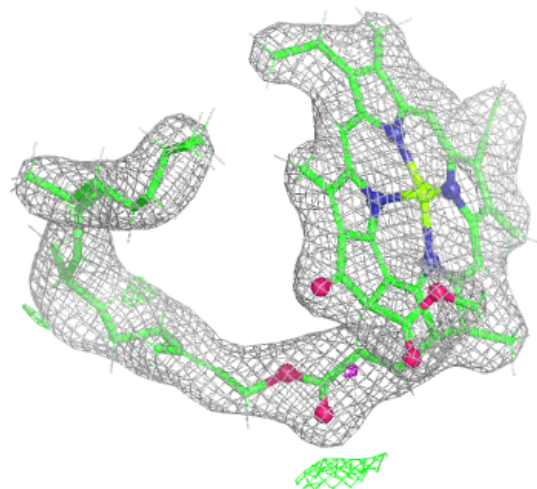
Electron density around CLA B 615:

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



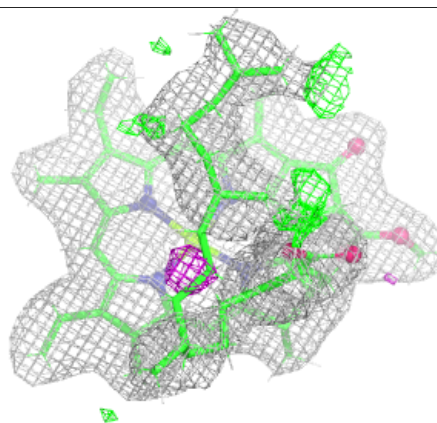
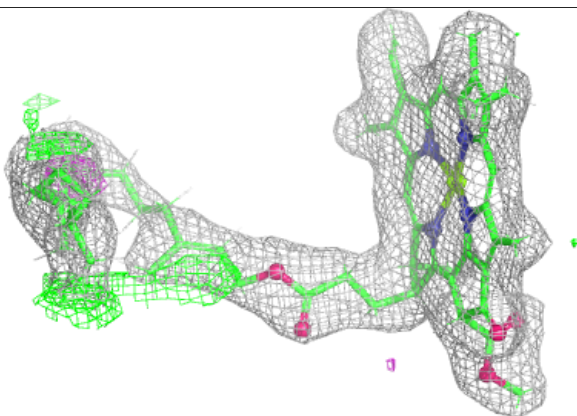
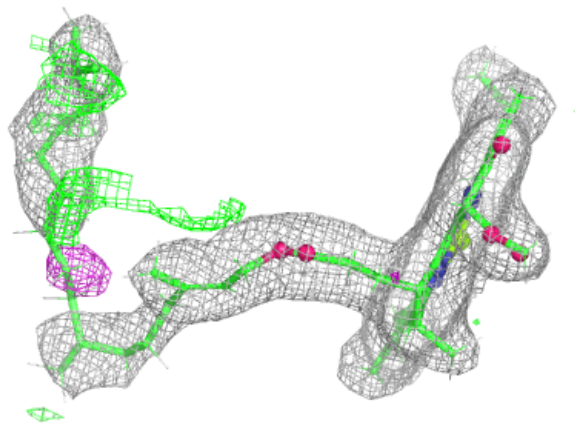
Electron density around CLA C 503:

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

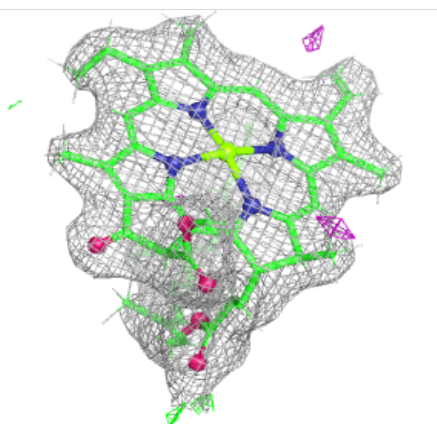
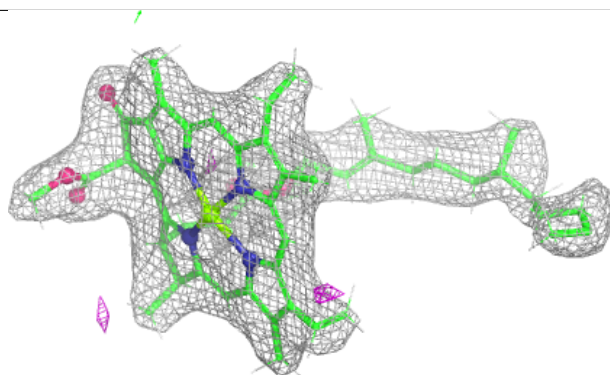
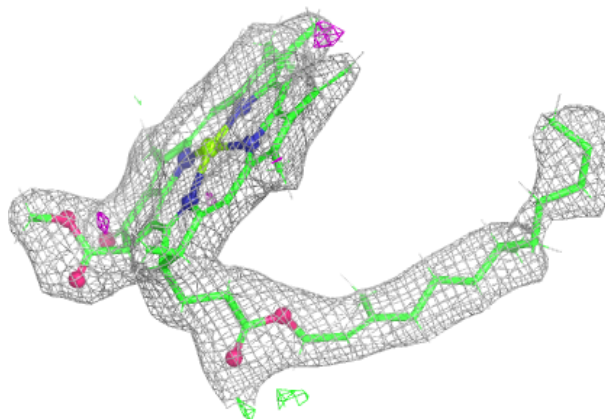


Electron density around CLA a 607:

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

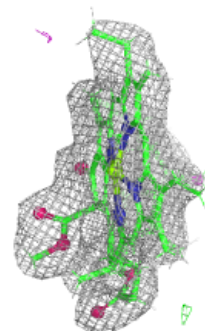
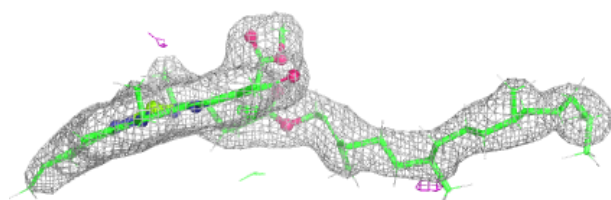
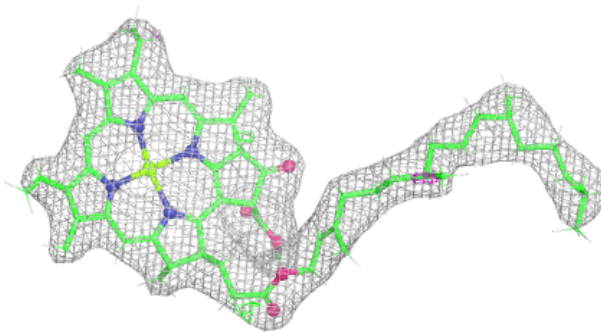
**Electron density around CLA C 504:**

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

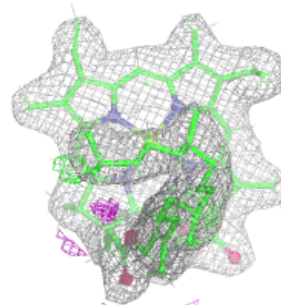
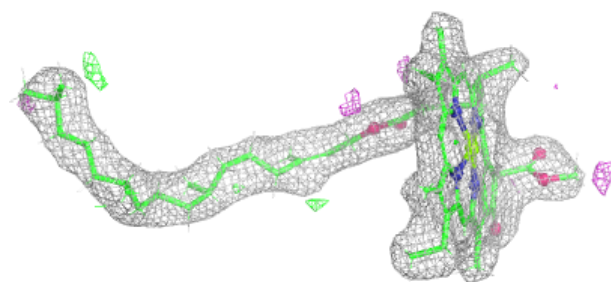
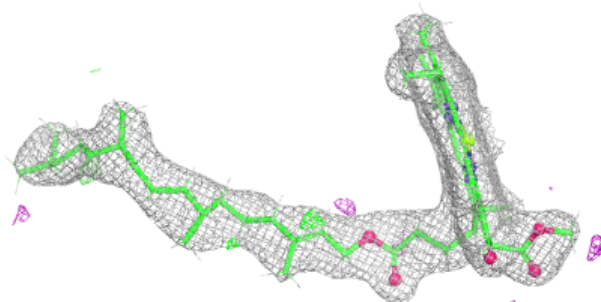


Electron density around CLA b 602:

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

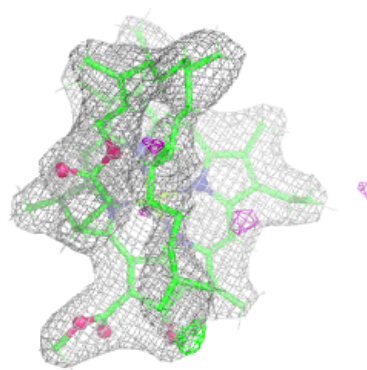
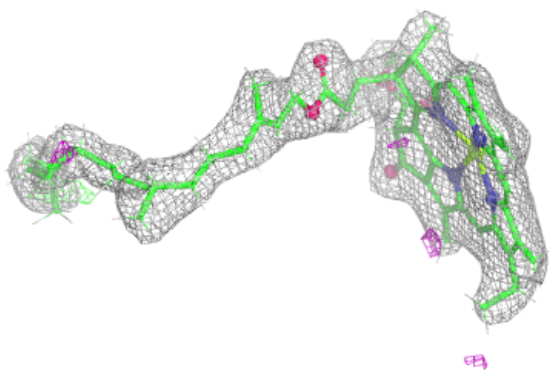
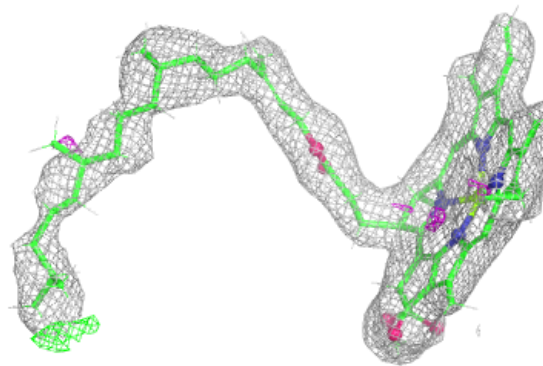
**Electron density around CLA b 605:**

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

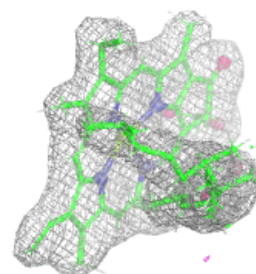
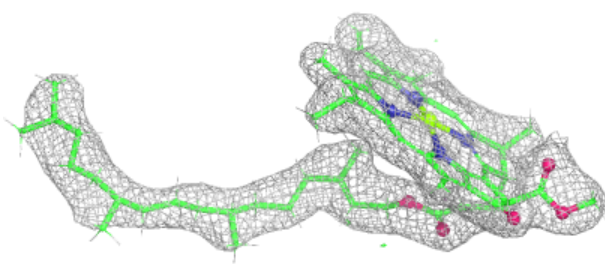
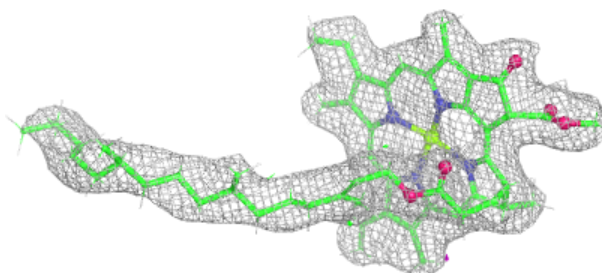


Electron density around CLA b 606:

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

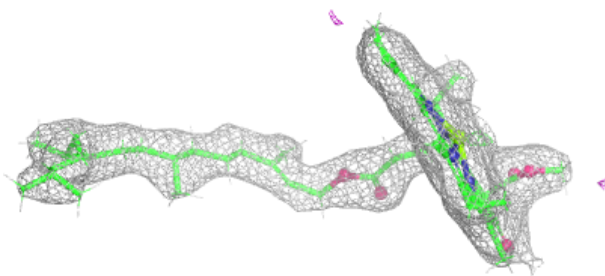
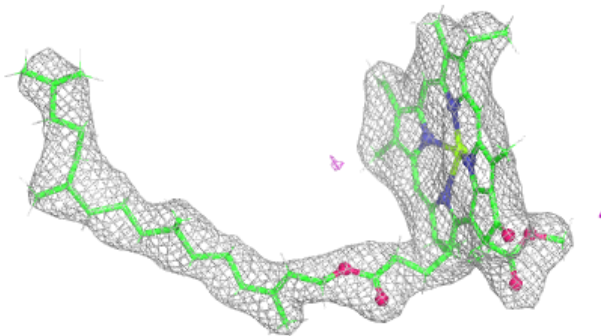
**Electron density around CLA b 608:**

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



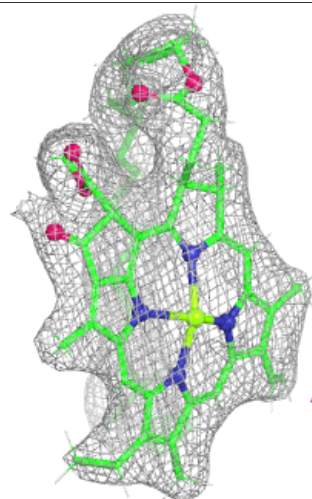
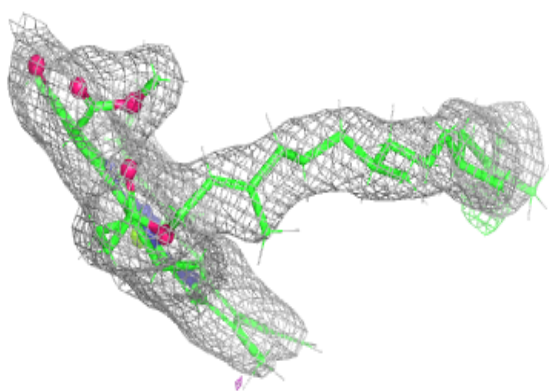
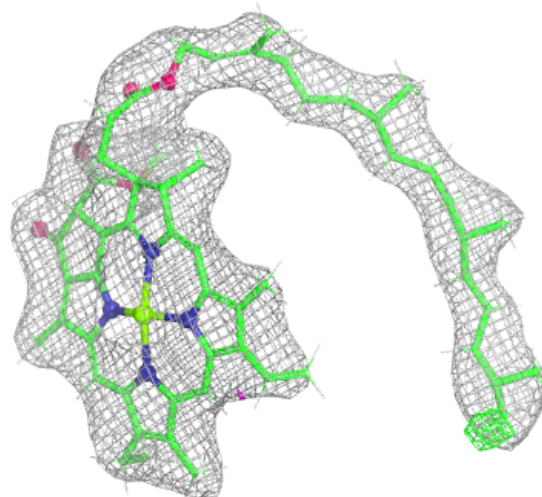
Electron density around CLA b 609:

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



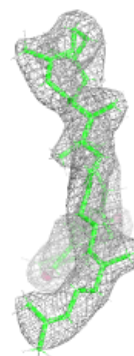
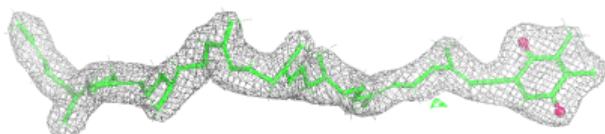
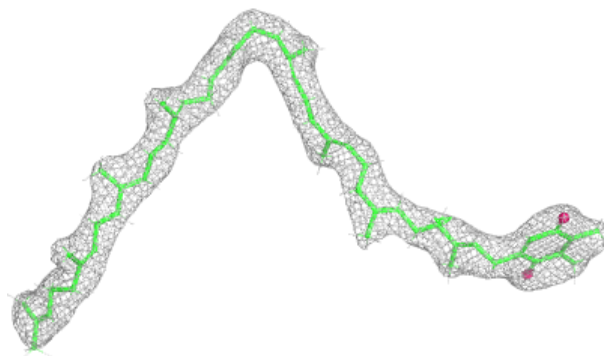
Electron density around CLA c 507:

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

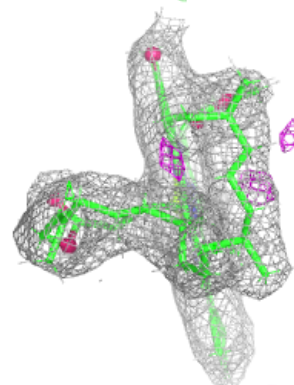
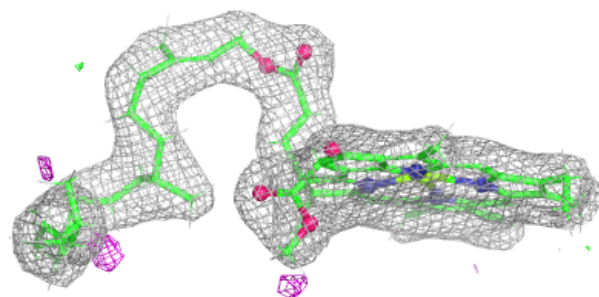
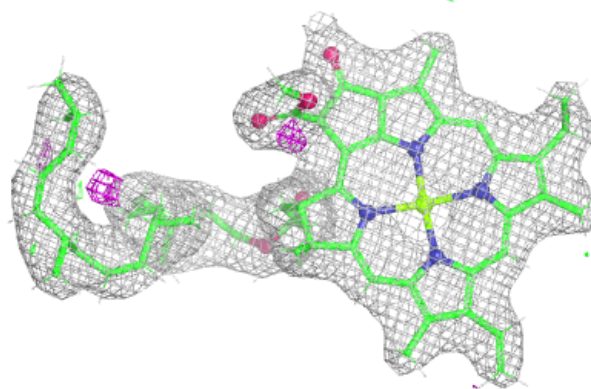


Electron density around PL9 D 406:

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

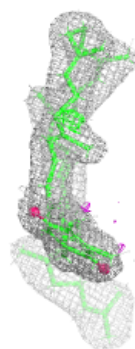
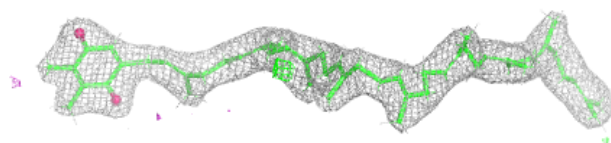
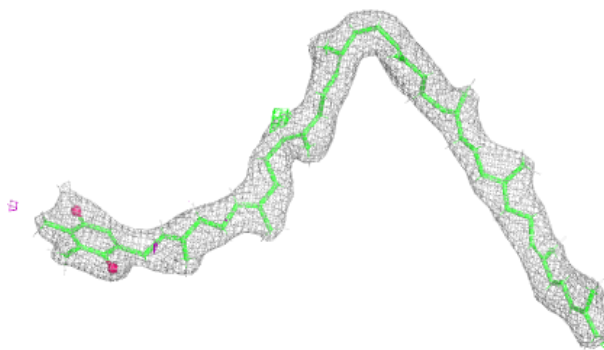
**Electron density around CLA B 611:**

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



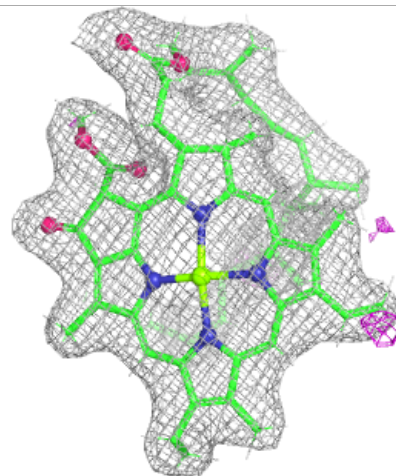
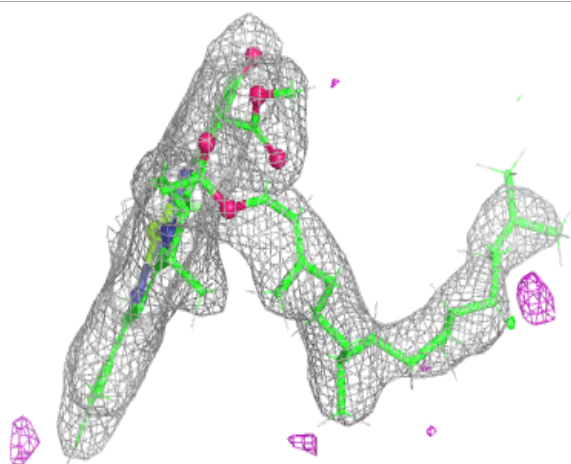
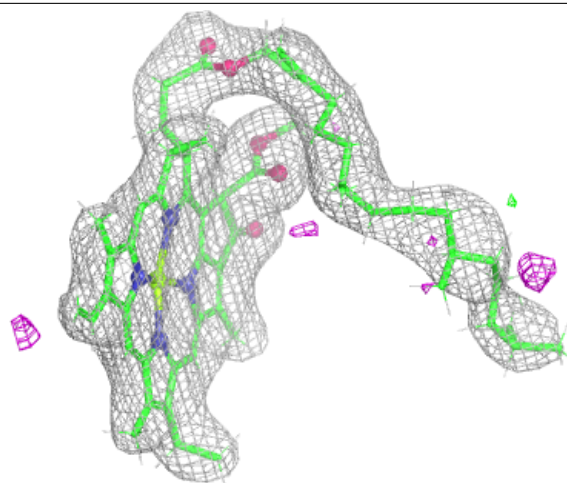
Electron density around PL9 d 405:

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



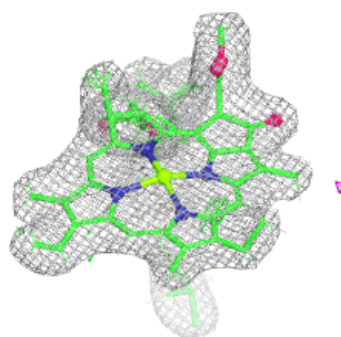
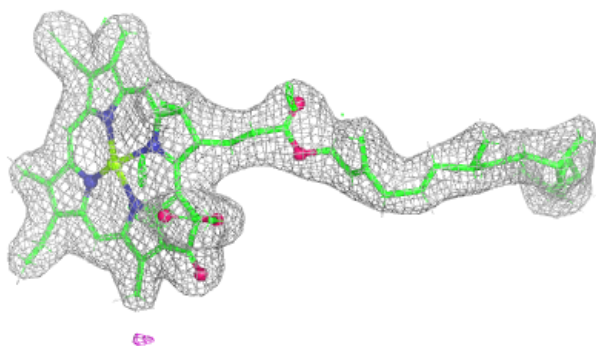
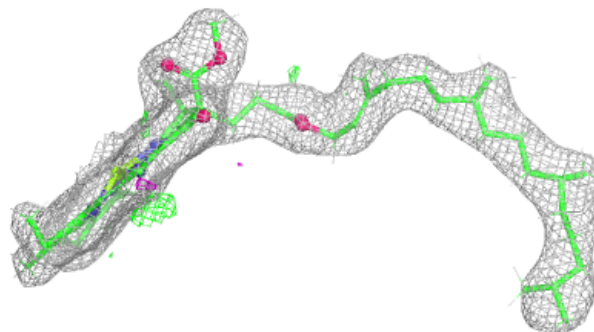
Electron density around CLA B 612:

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

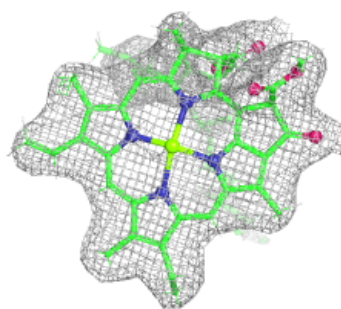
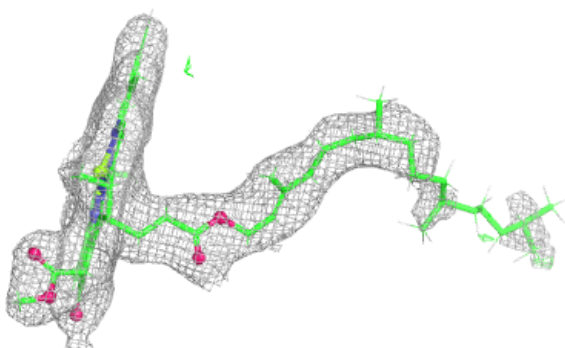
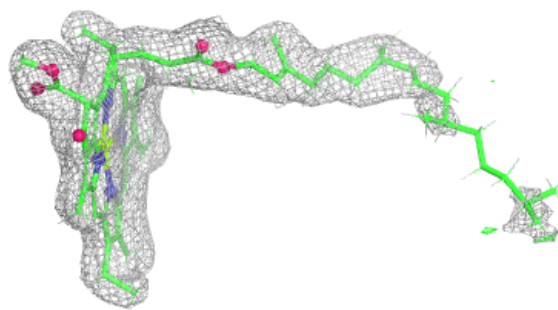


Electron density around CLA D 403:

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

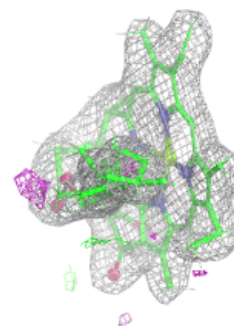
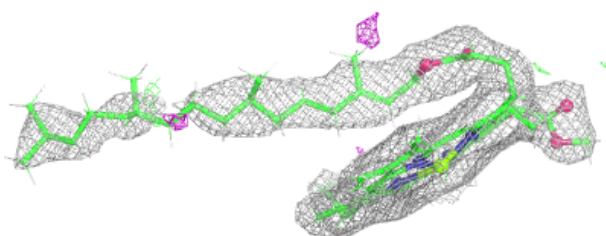
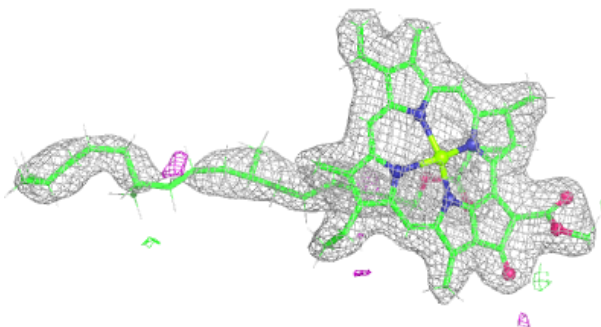
**Electron density around CLA D 404:**

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

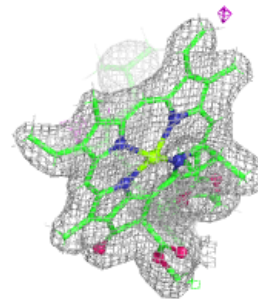
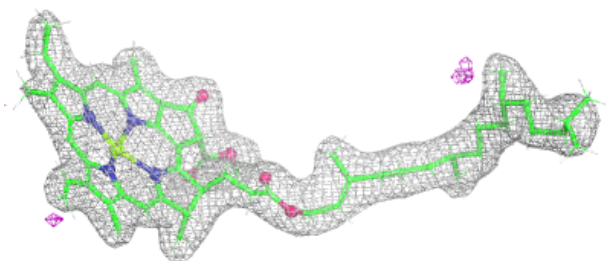
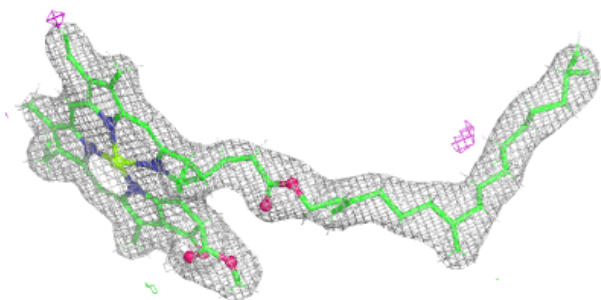


Electron density around CLA B 613:

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

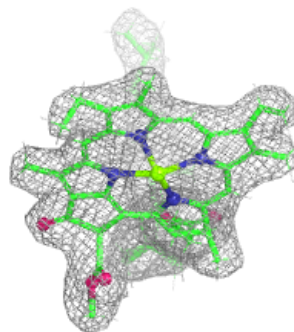
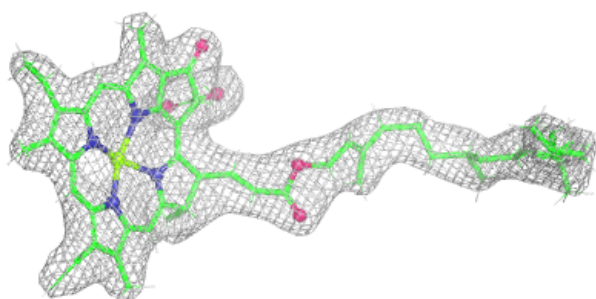
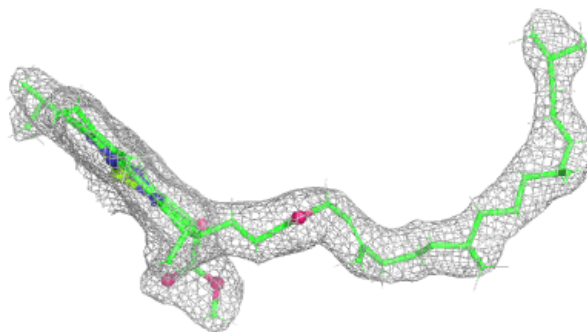
**Electron density around CLA a 604:**

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

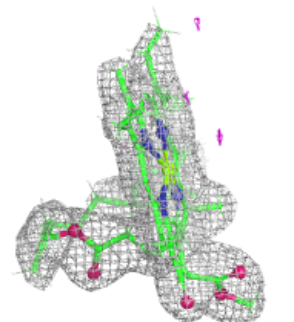
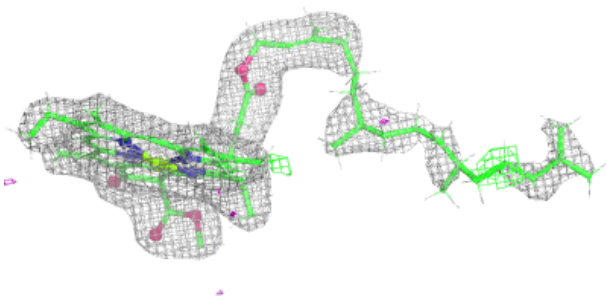
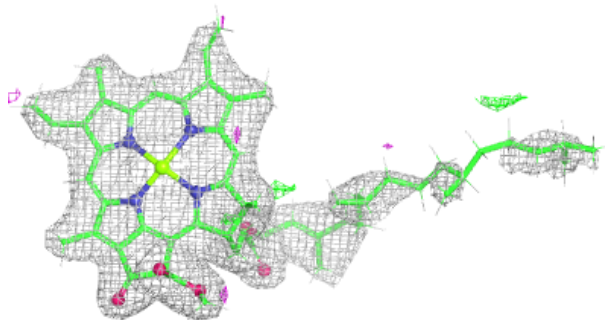


Electron density around CLA d 402:

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

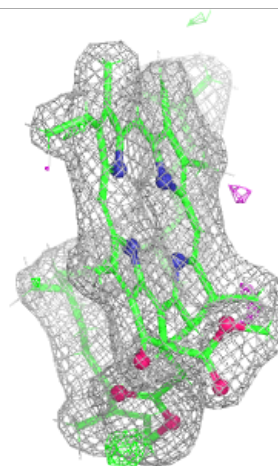
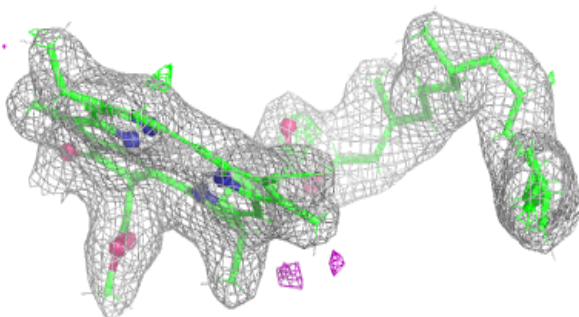
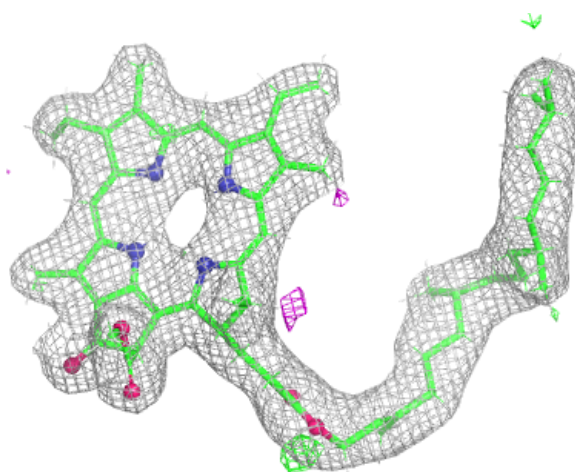
**Electron density around CLA a 605:**

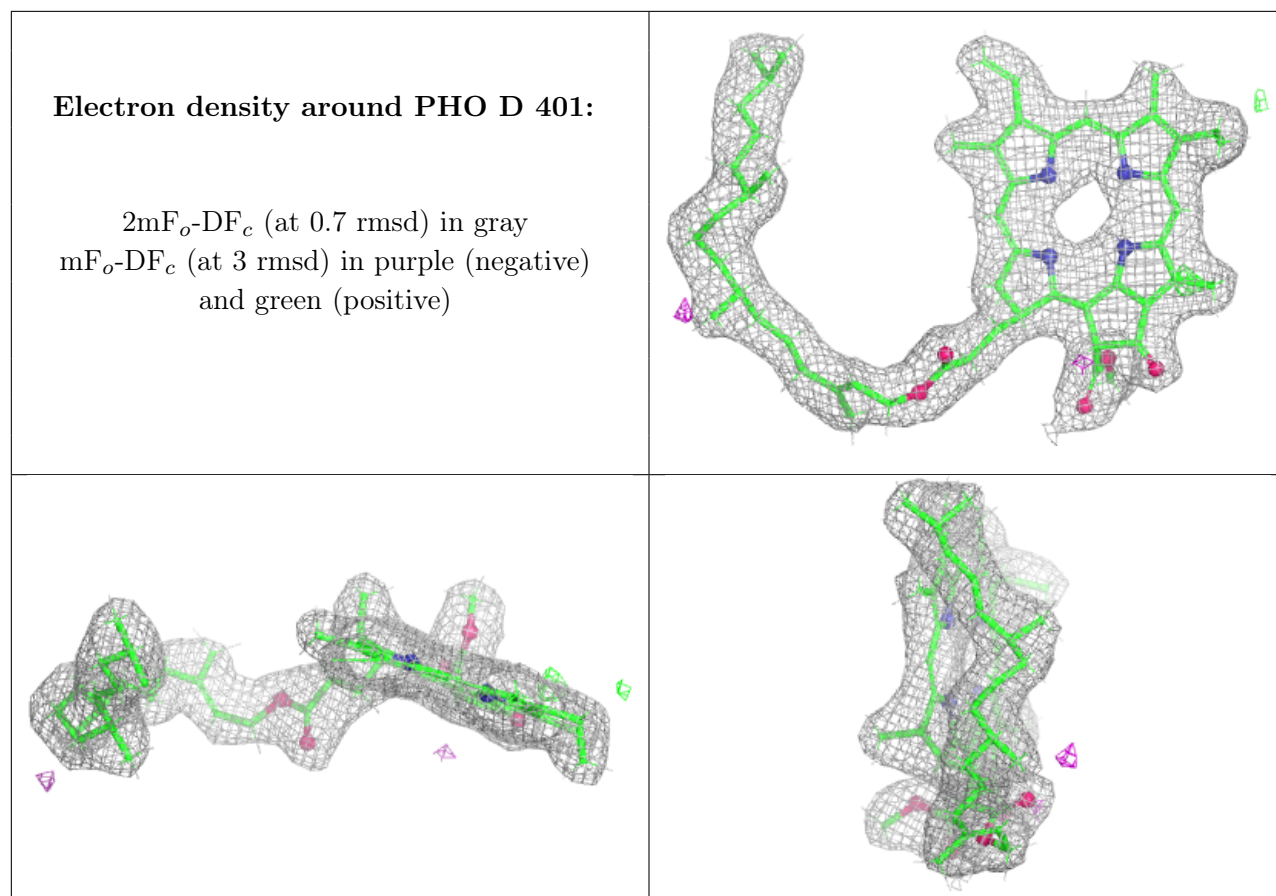
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO A 606:

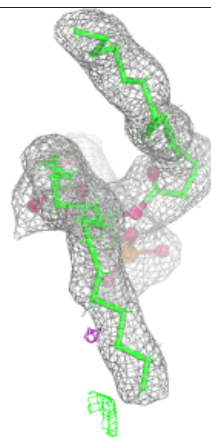
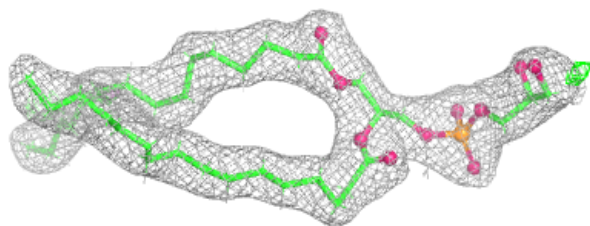
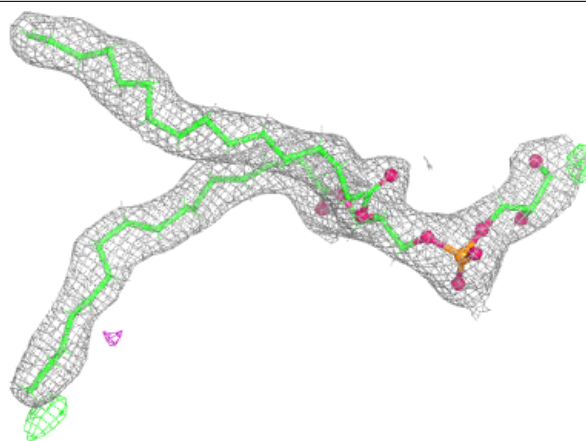
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



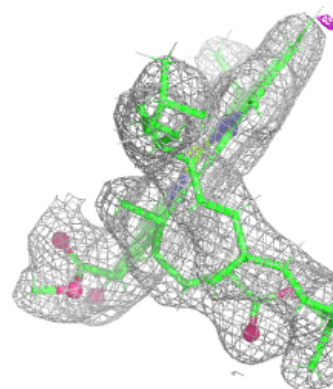
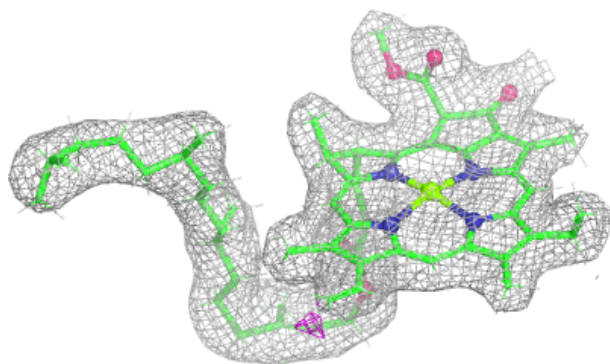
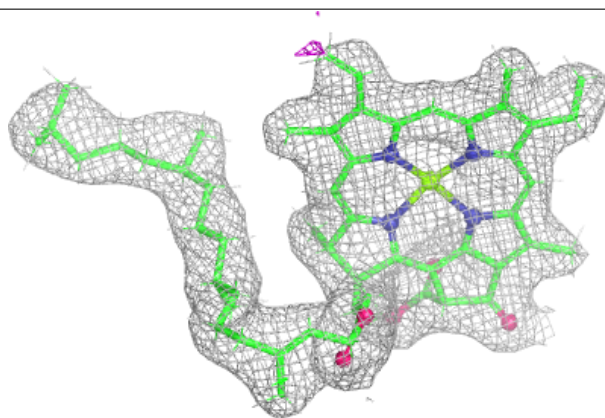


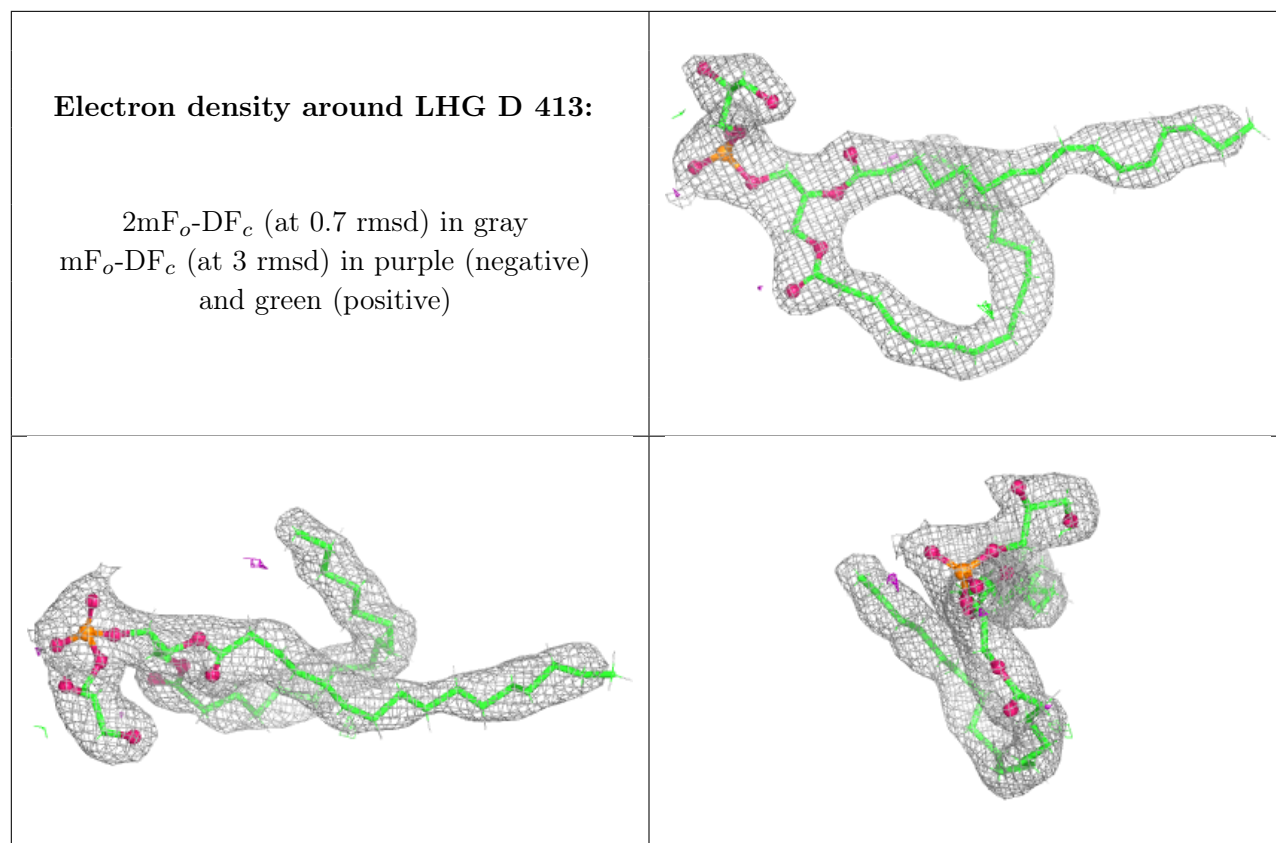
Electron density around LHG D 409:

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

**Electron density around CLA A 612:**

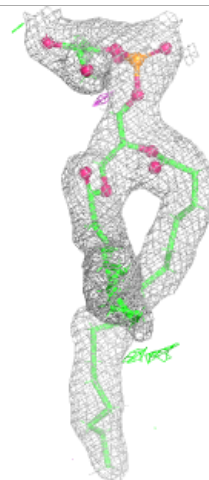
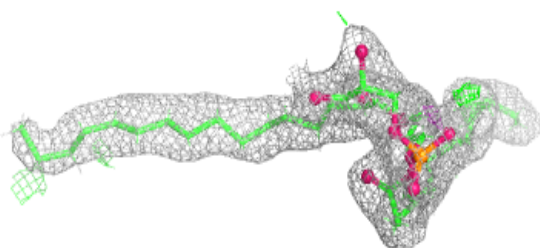
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





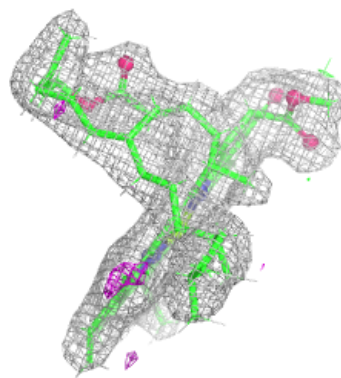
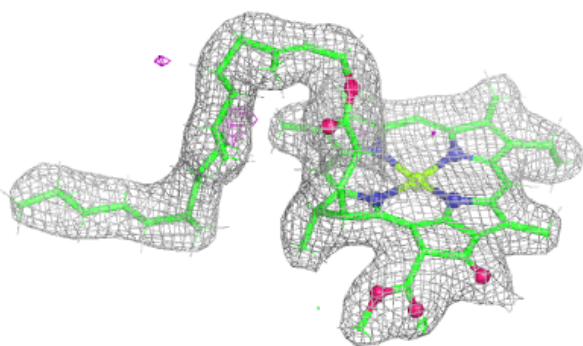
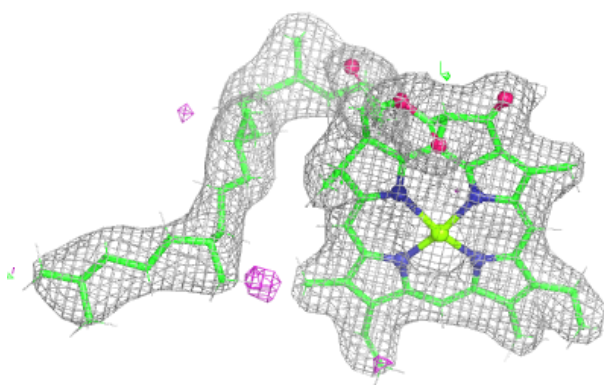
Electron density around LHG L 101:

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

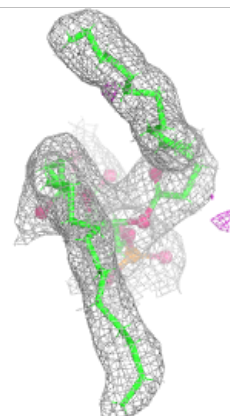
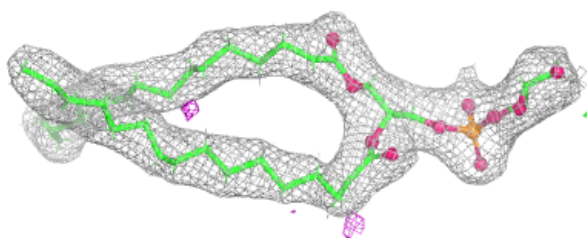
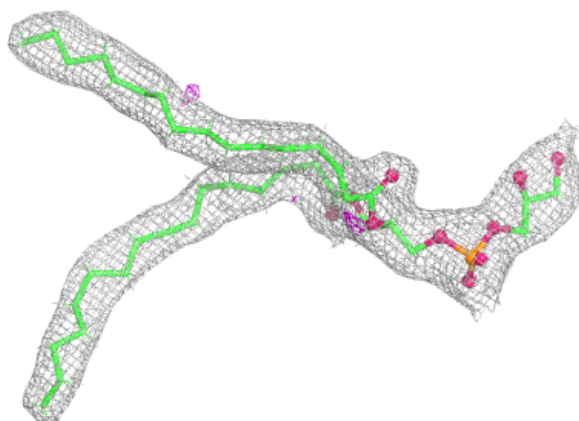


Electron density around CLA a 613:

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

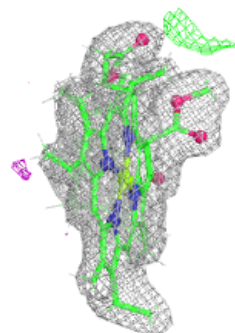
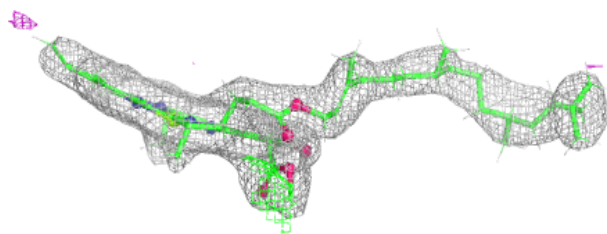
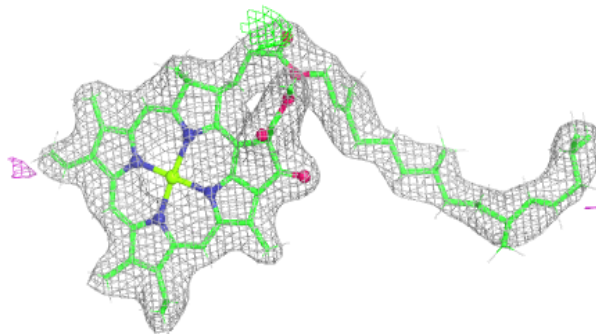
**Electron density around LHG d 406:**

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

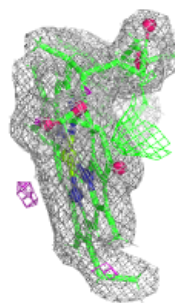
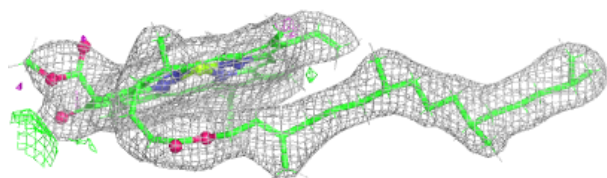
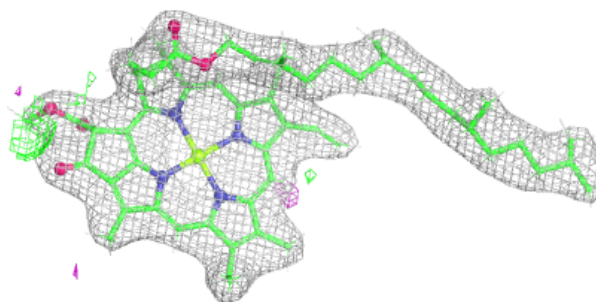


Electron density around CLA B 601:

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

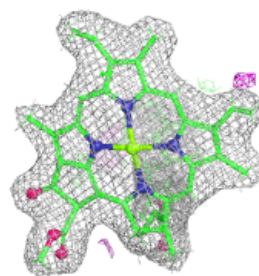
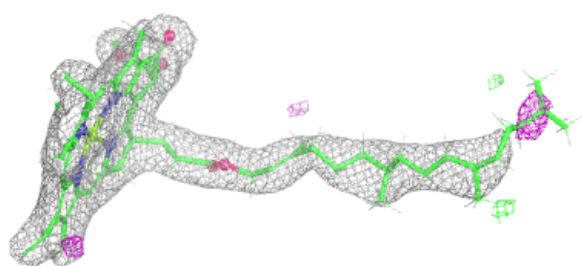
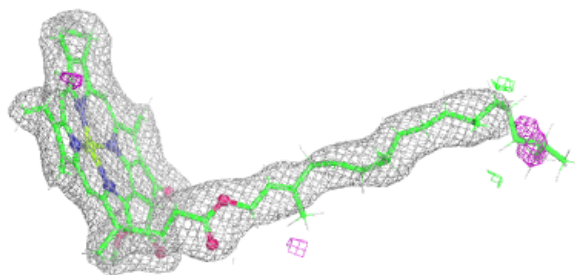
**Electron density around CLA C 501:**

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

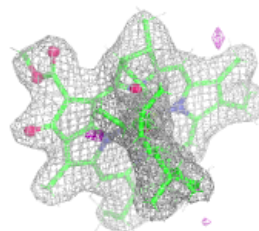
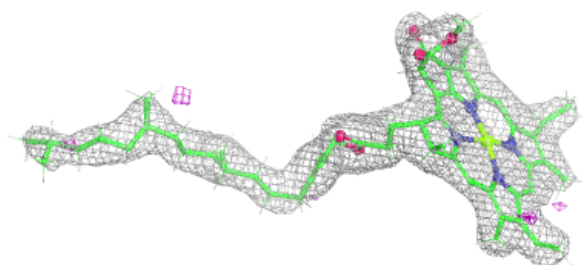
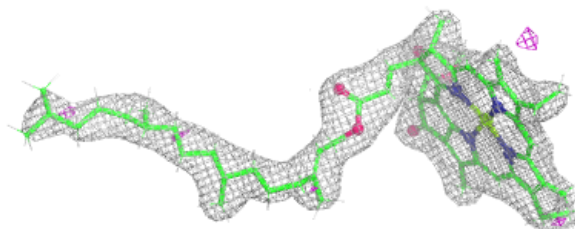


Electron density around CLA b 604:

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

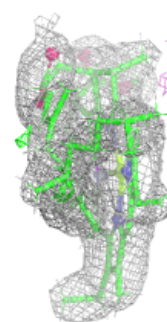
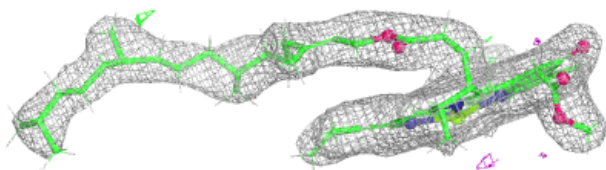
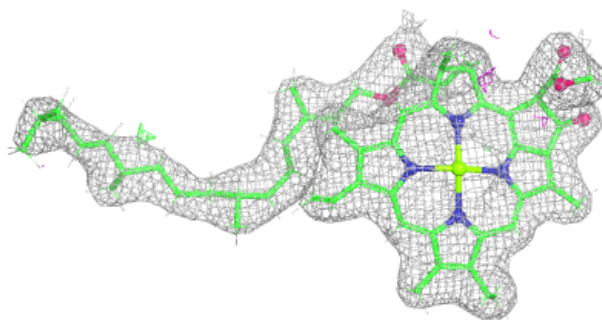
**Electron density around CLA C 502:**

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

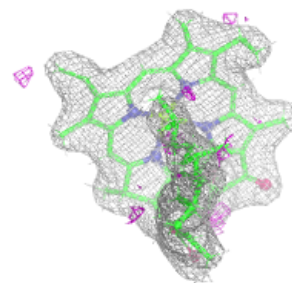
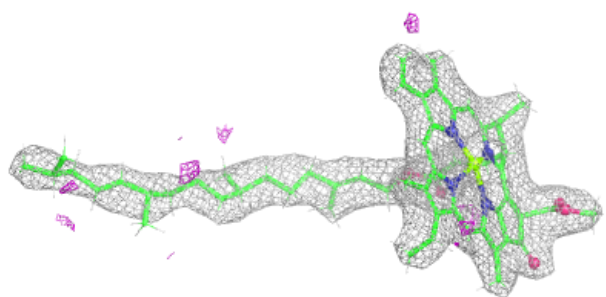
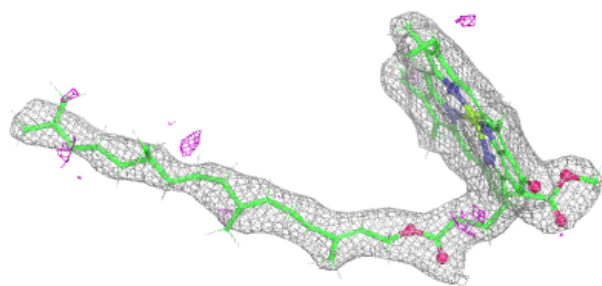


Electron density around CLA B 602:

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

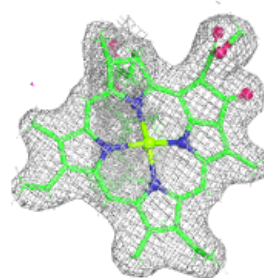
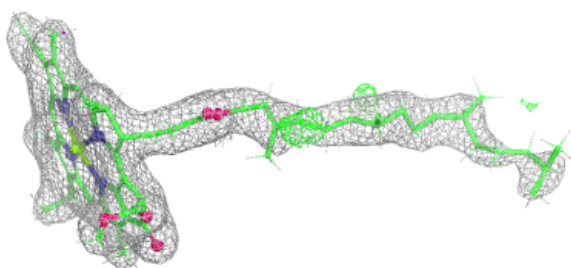
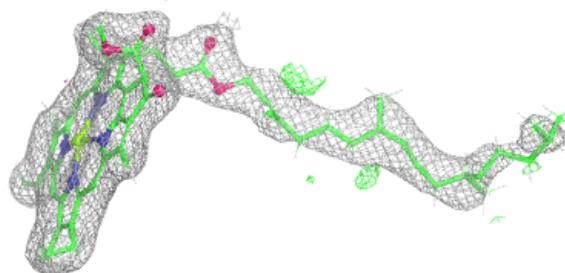
**Electron density around CLA b 607:**

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

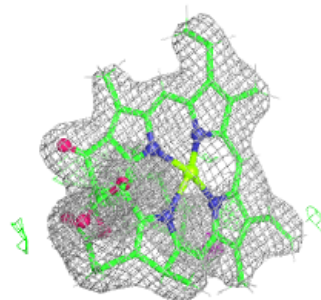
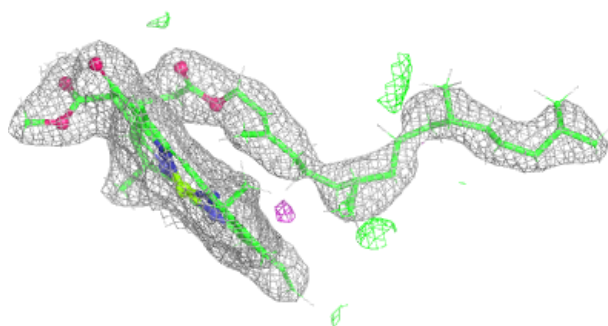
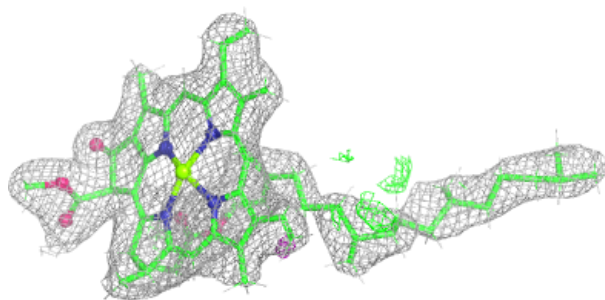


Electron density around CLA B 603:

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

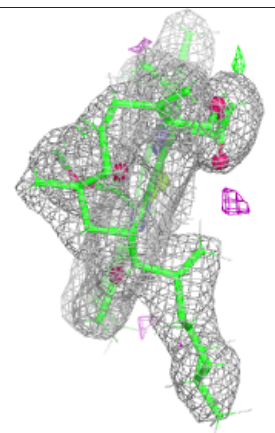
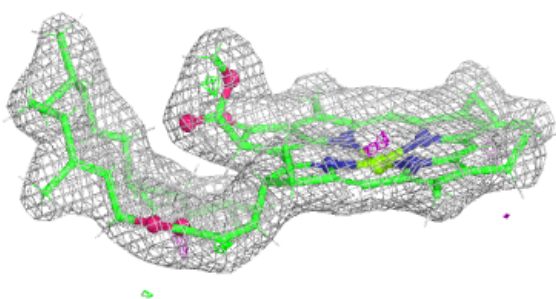
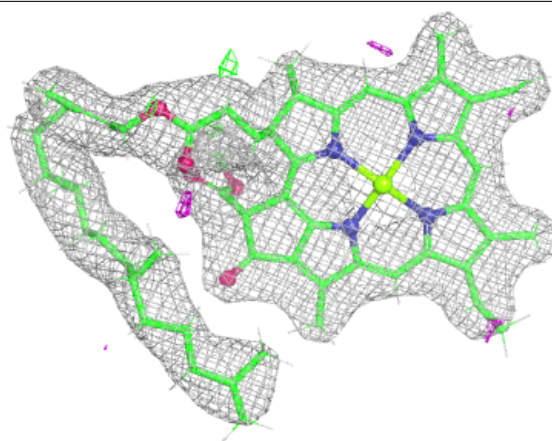
**Electron density around CLA C 505:**

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



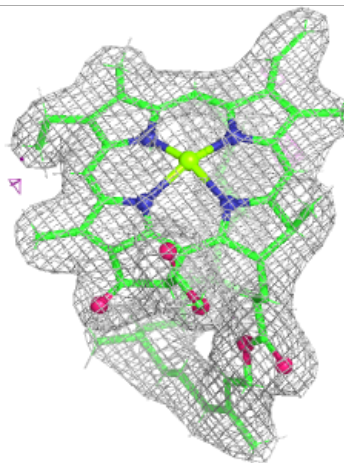
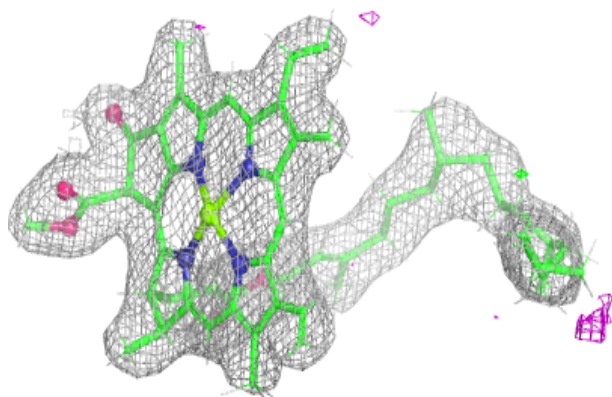
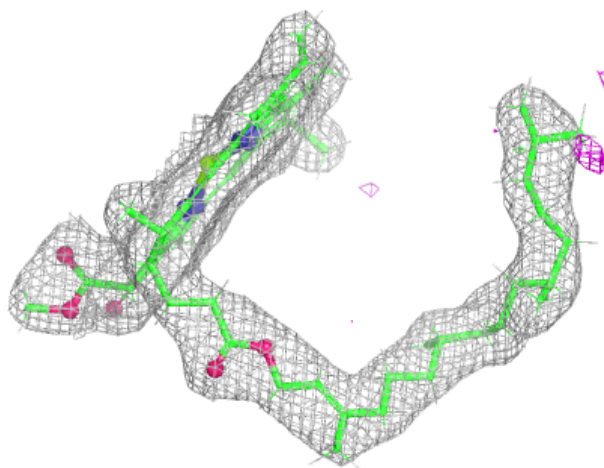
Electron density around CLA b 610:

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



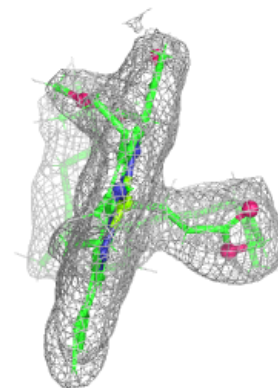
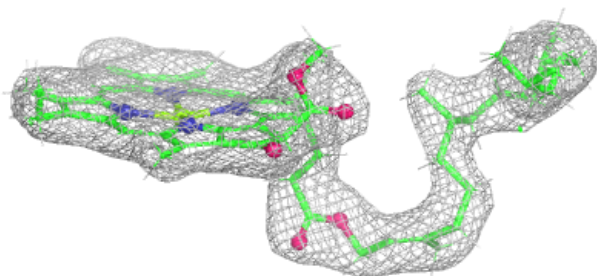
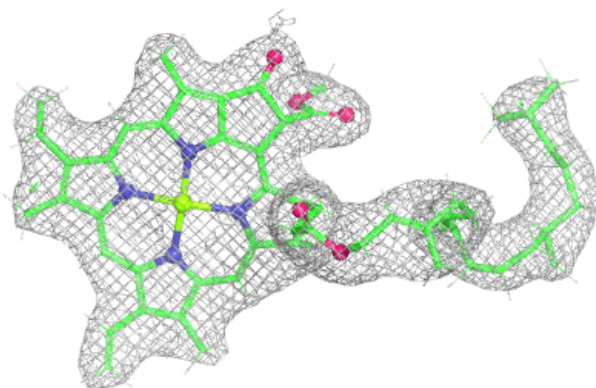
Electron density around CLA b 611:

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



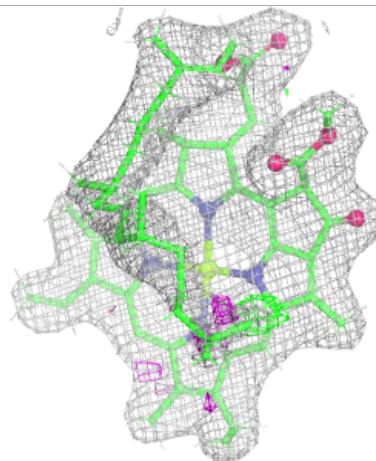
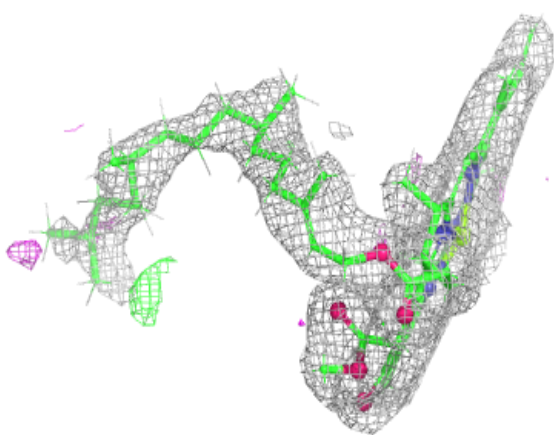
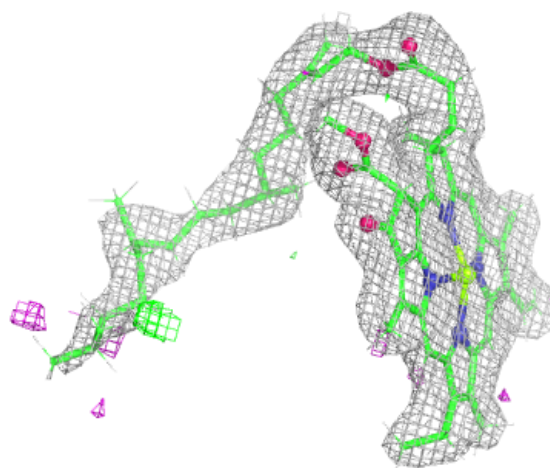
Electron density around CLA b 612:

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



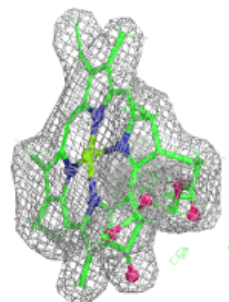
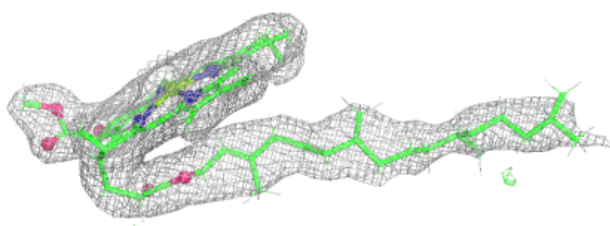
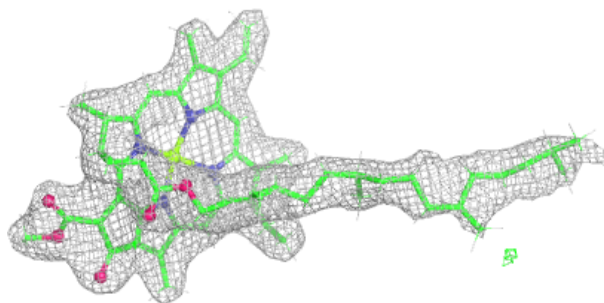
Electron density around CLA b 613:

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



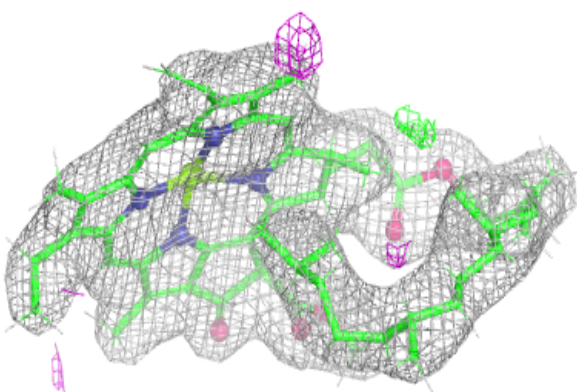
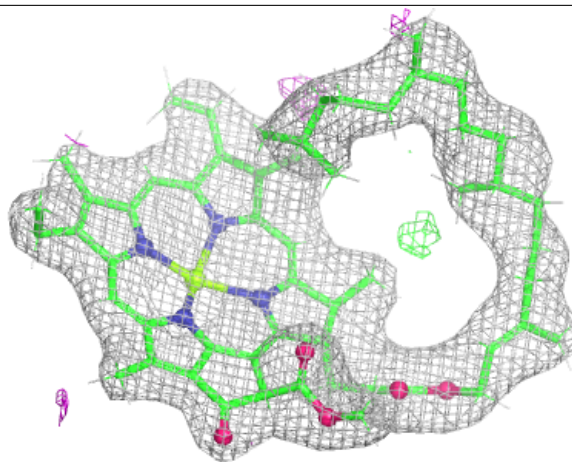
Electron density around CLA b 614:

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



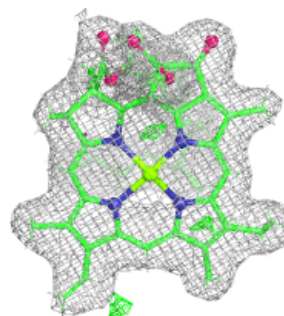
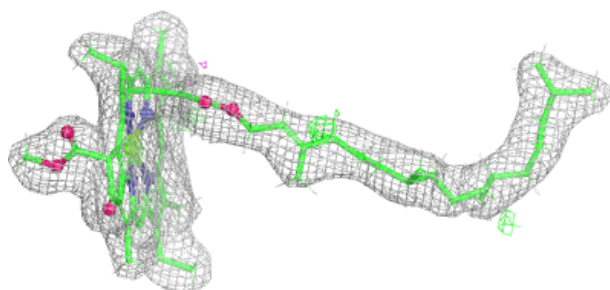
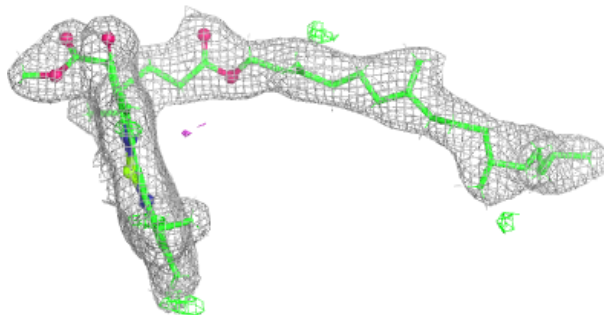
Electron density around CLA b 615:

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

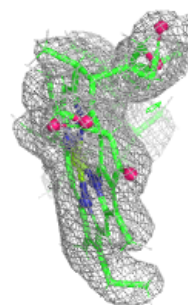
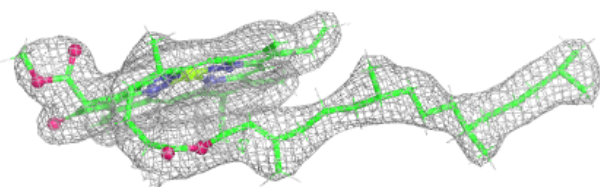
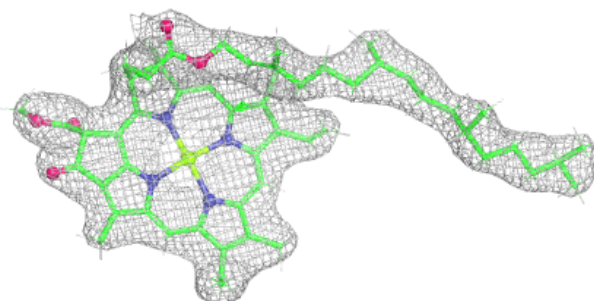


Electron density around CLA B 604:

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

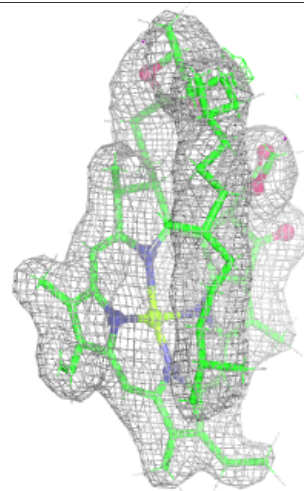
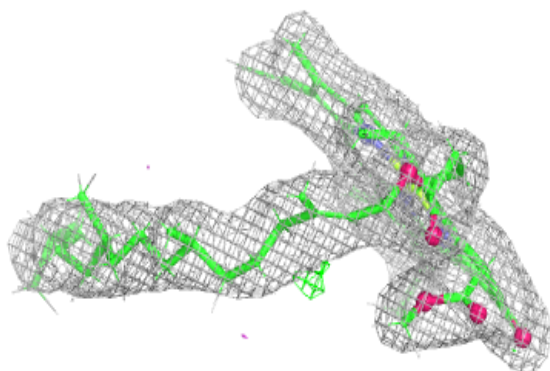
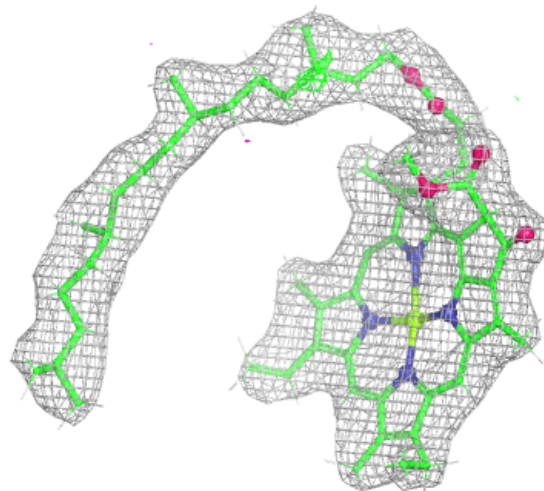
**Electron density around CLA c 501:**

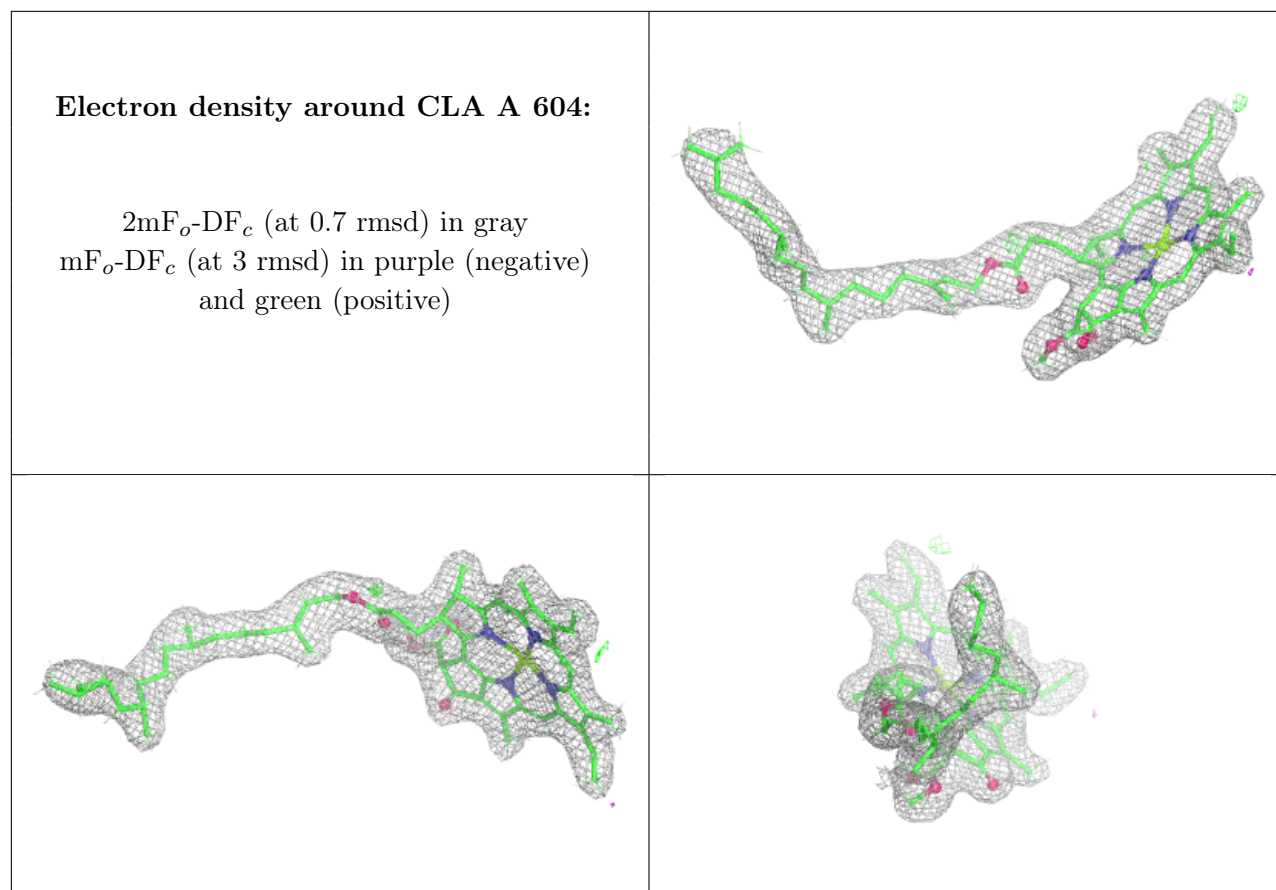
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 507:

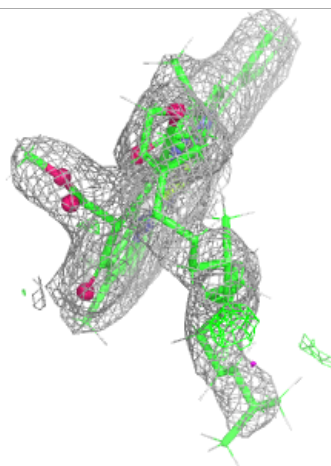
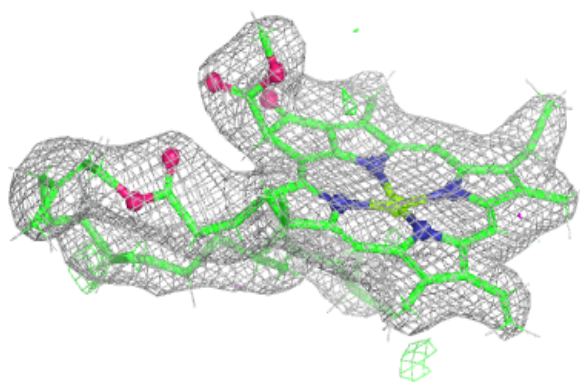
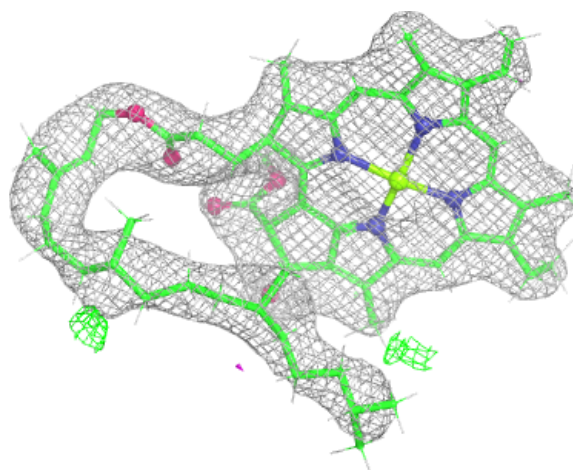
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





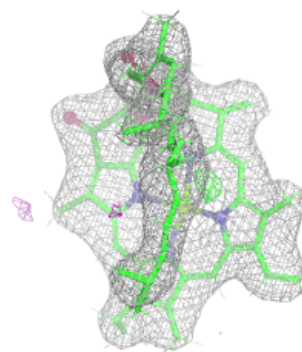
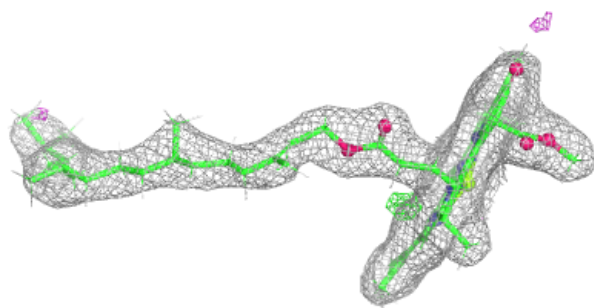
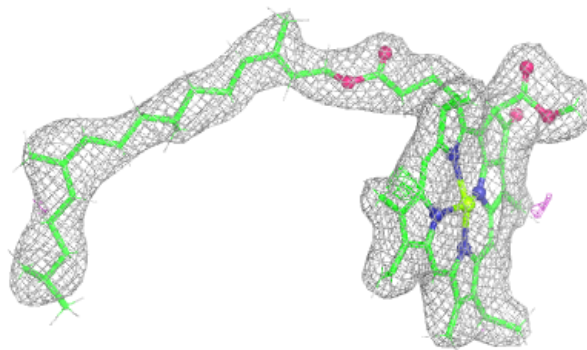
Electron density around CLA C 509:

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

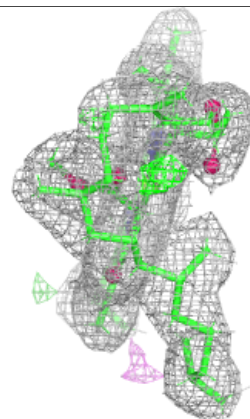
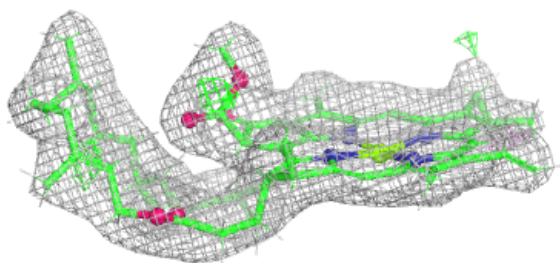
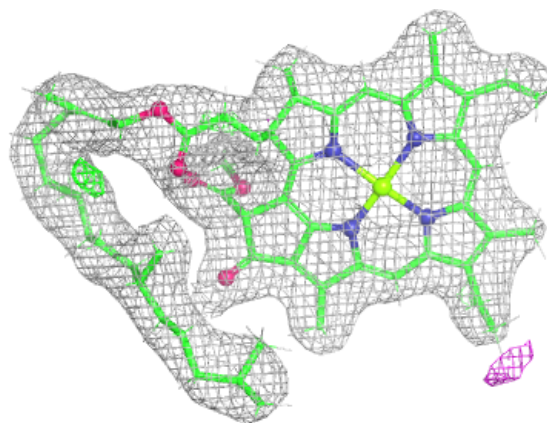


Electron density around CLA B 608:

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

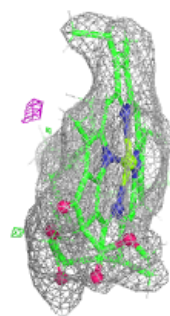
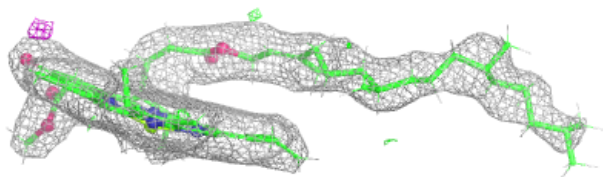
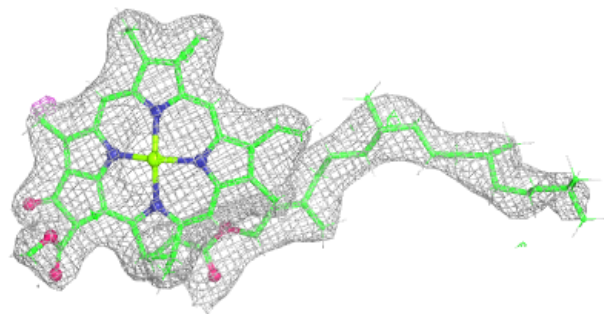
**Electron density around CLA B 609:**

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



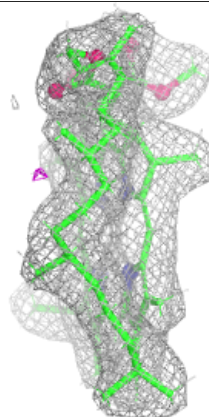
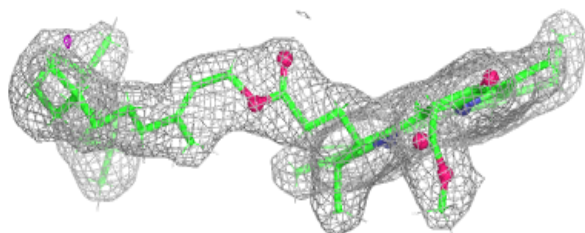
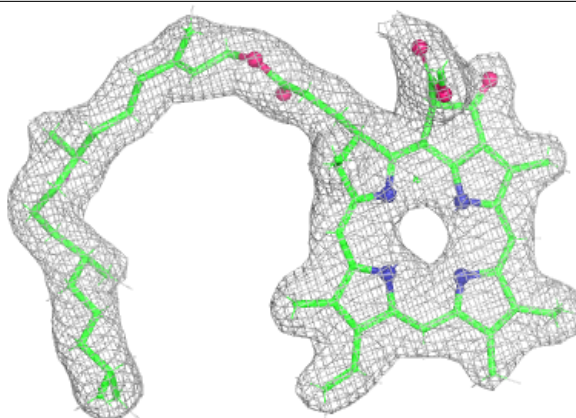
Electron density around CLA b 603:

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

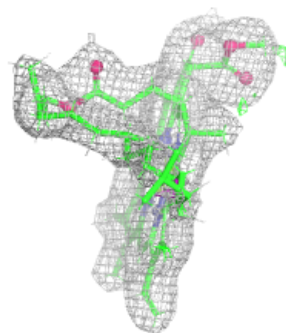
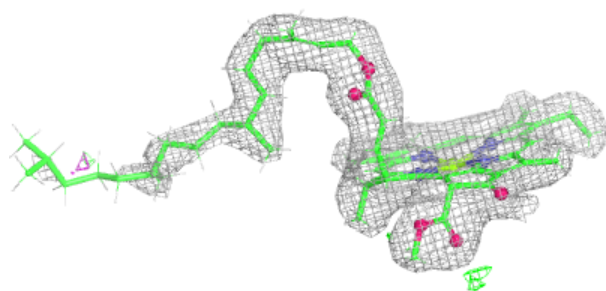
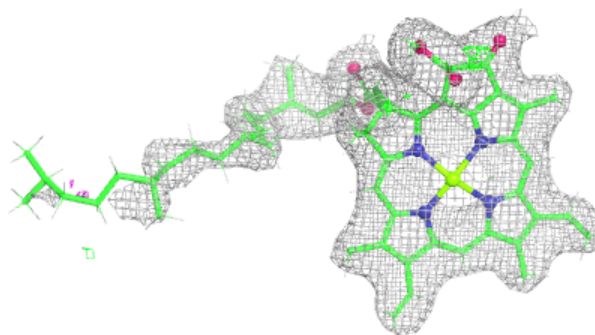


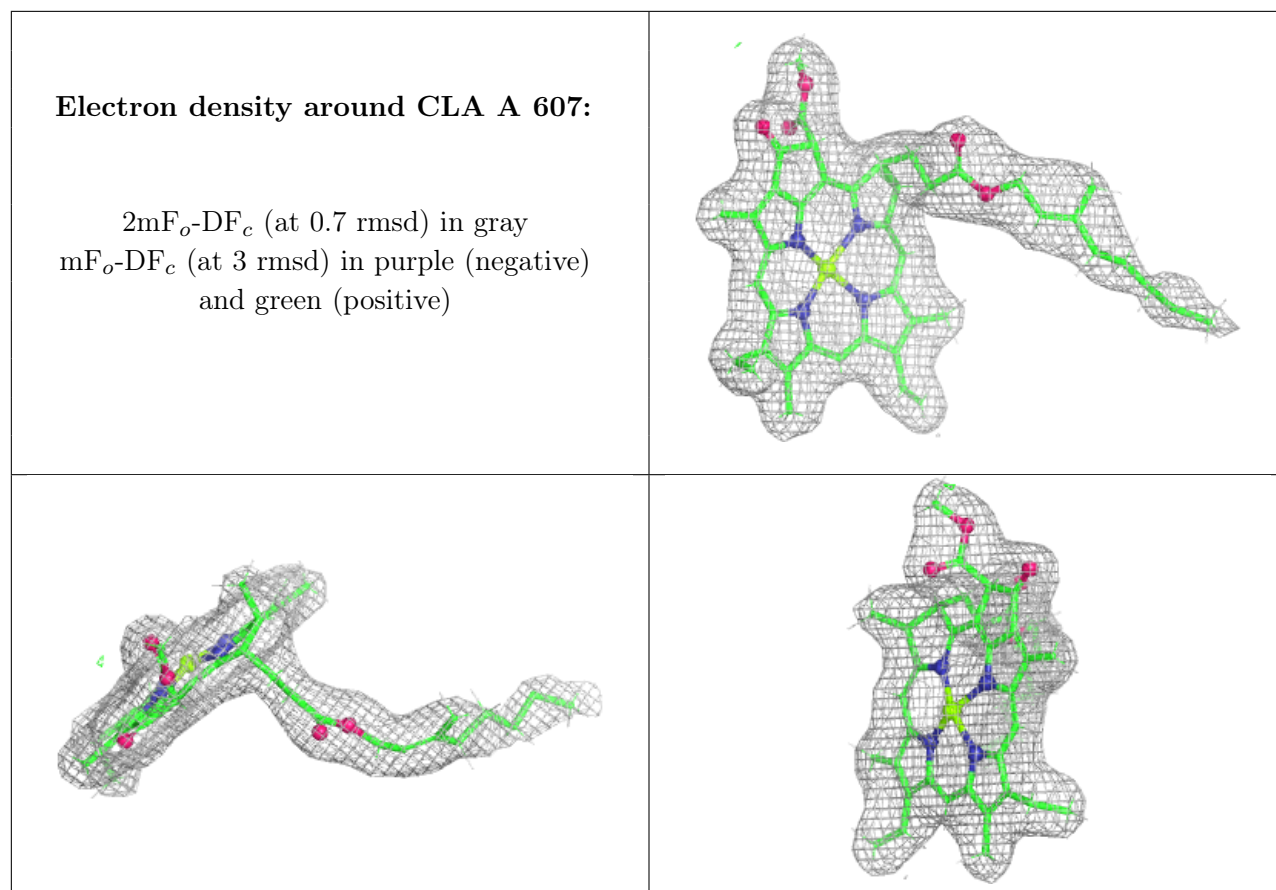
Electron density around PHO a 606:

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

**Electron density around CLA A 605:**

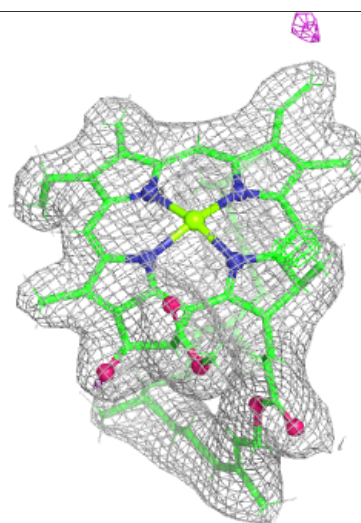
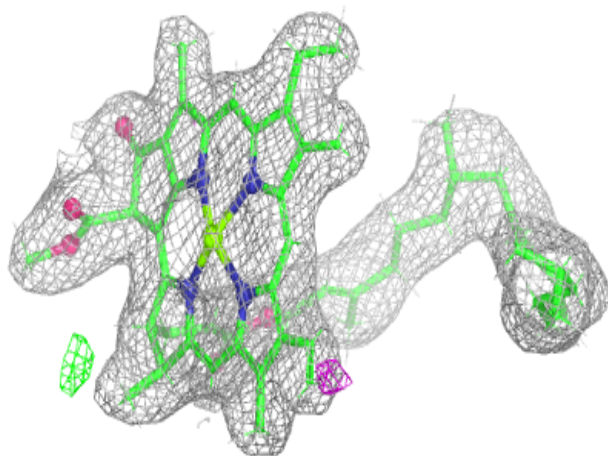
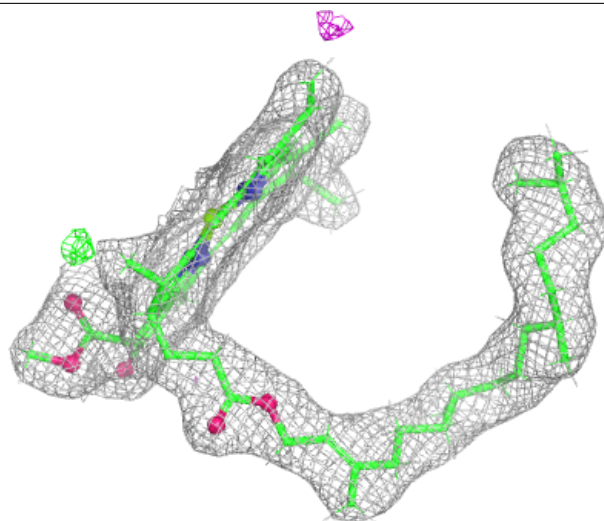
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





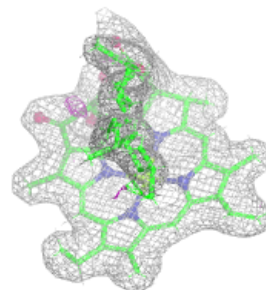
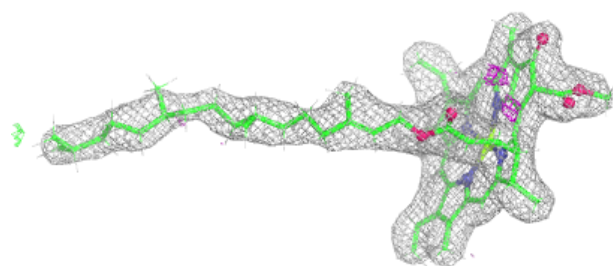
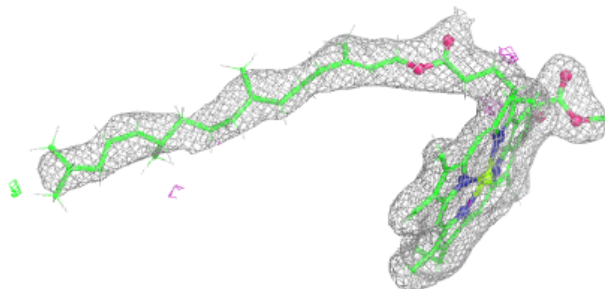
Electron density around CLA B 610:

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

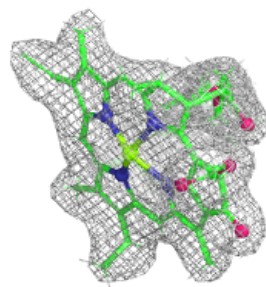
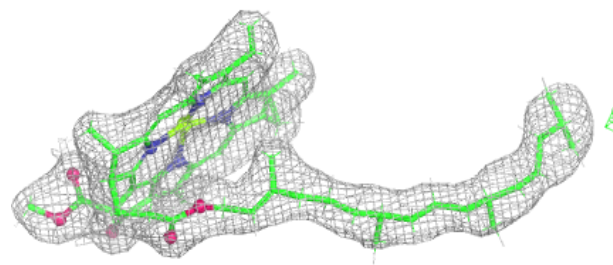
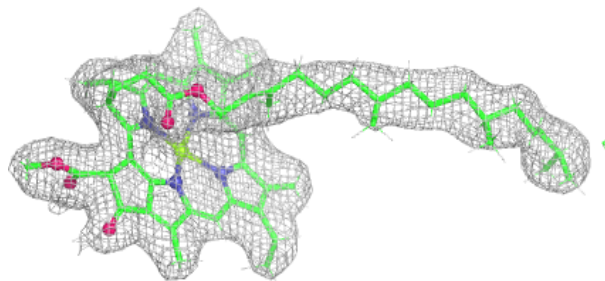


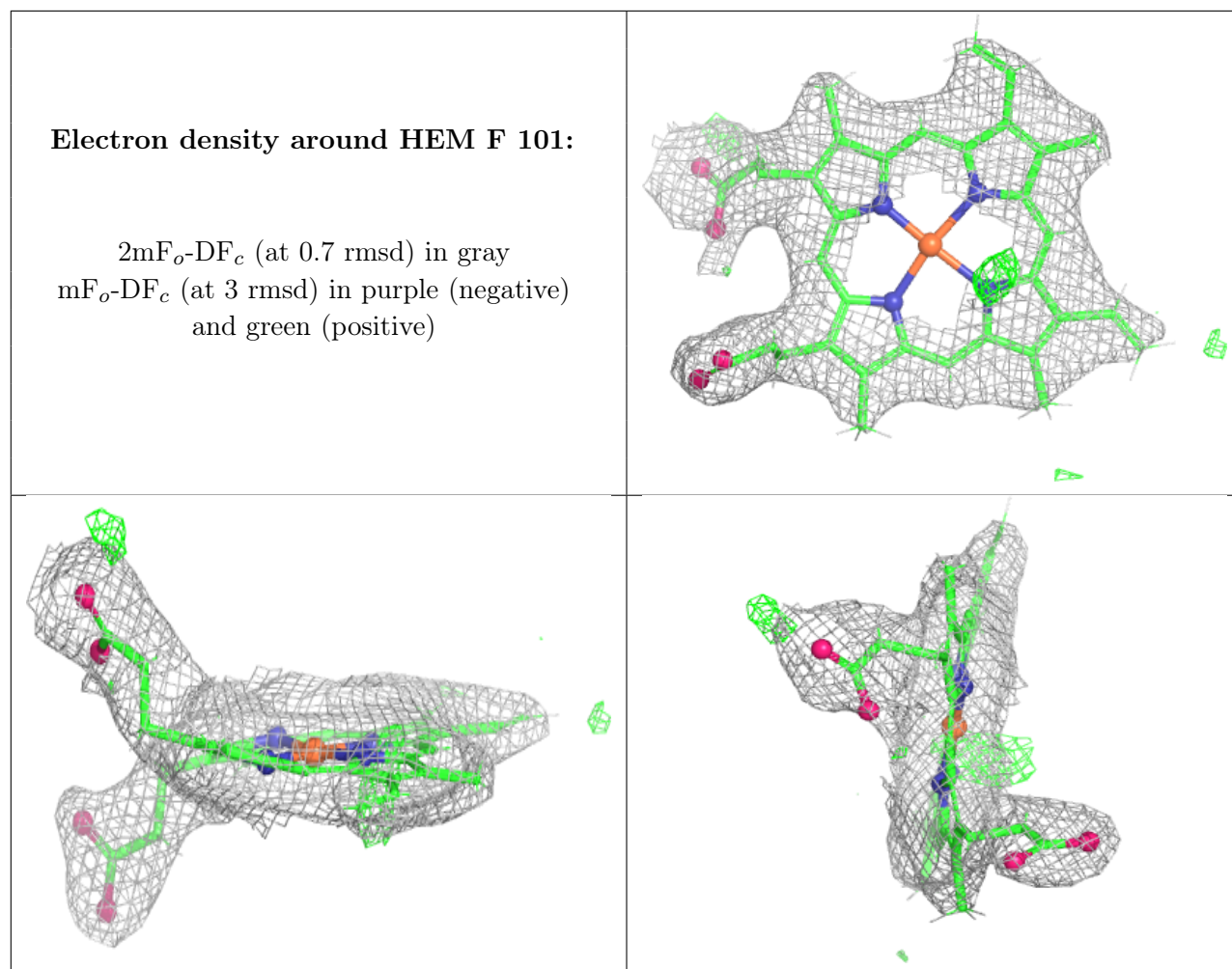
Electron density around CLA B 606:

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

**Electron density around CLA B 607:**

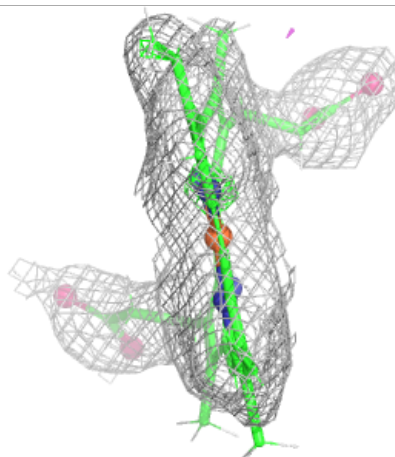
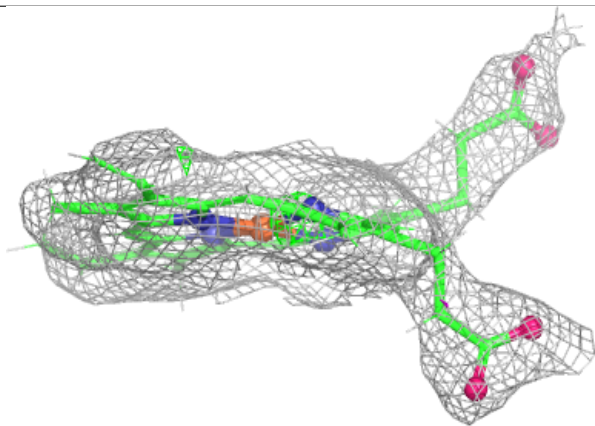
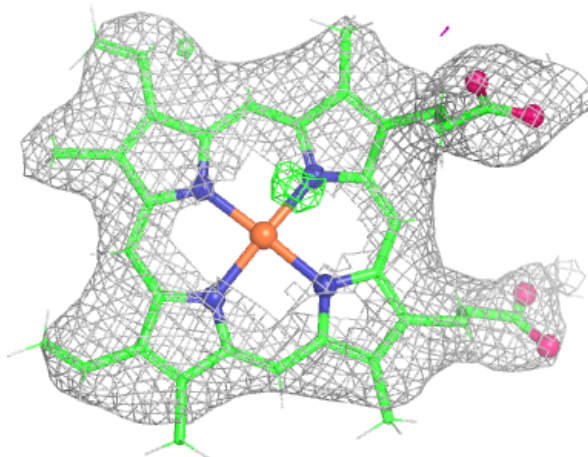
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





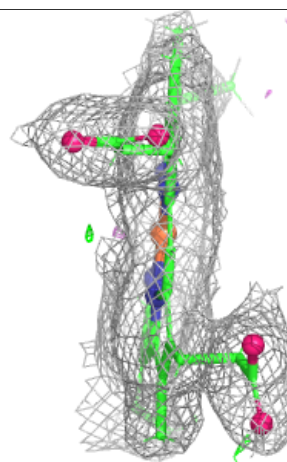
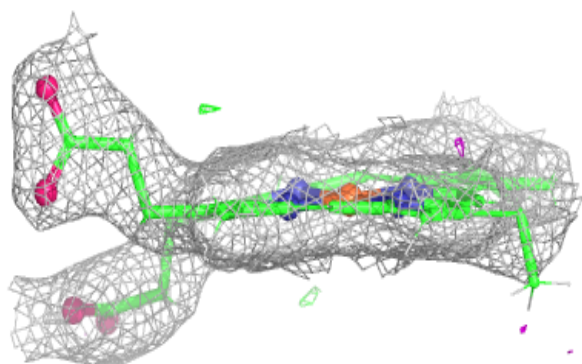
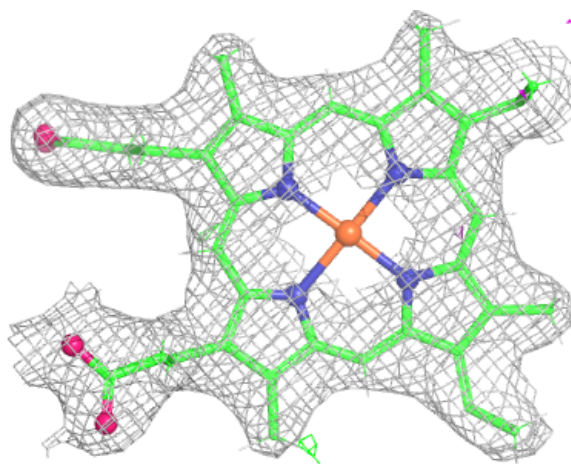
Electron density around HEM f 101:

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



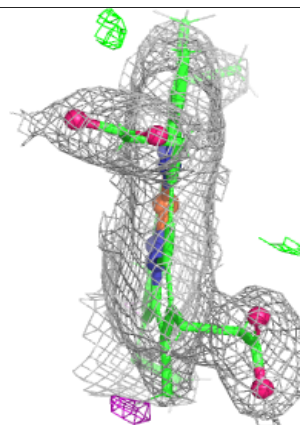
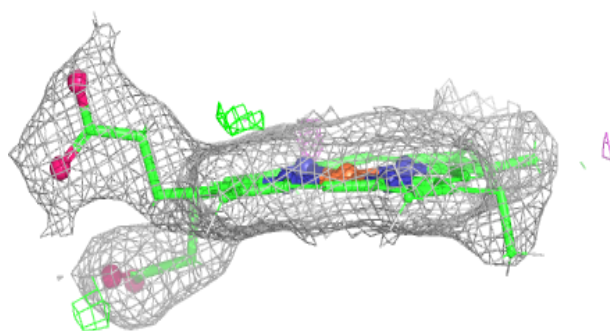
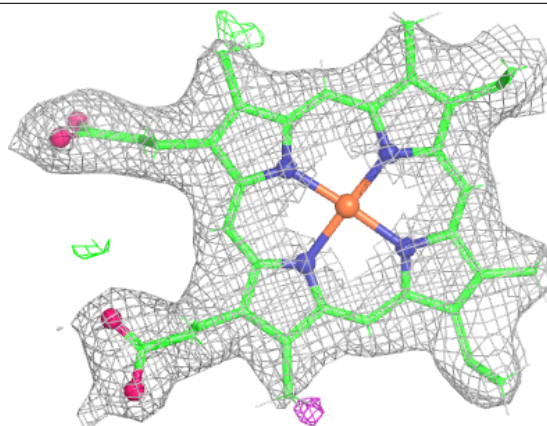
Electron density around HEC V 201:

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



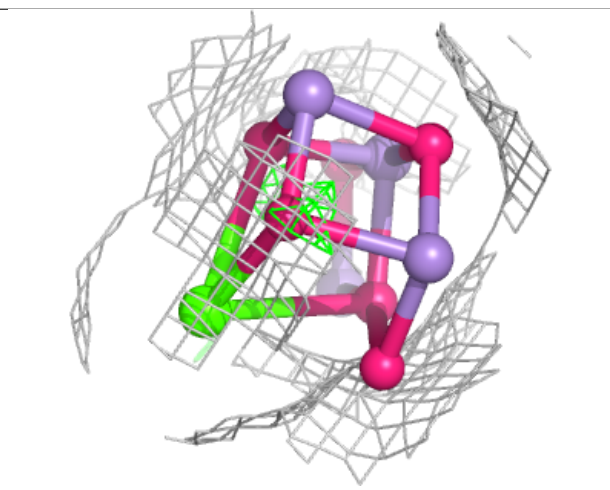
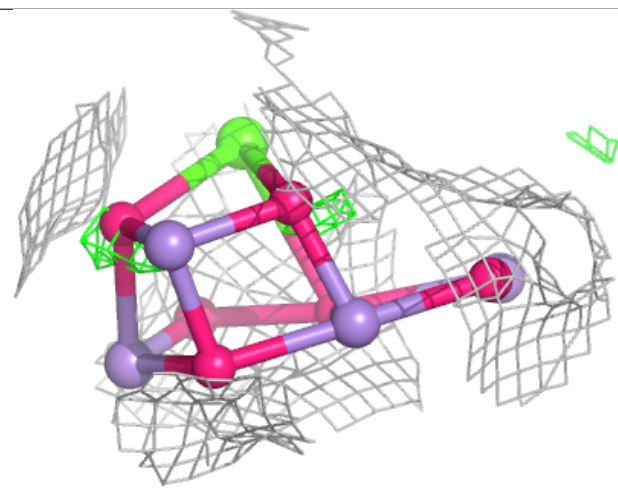
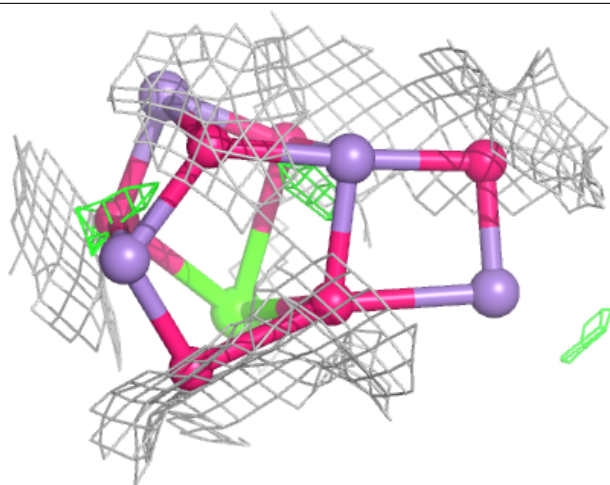
Electron density around HEC v 201:

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



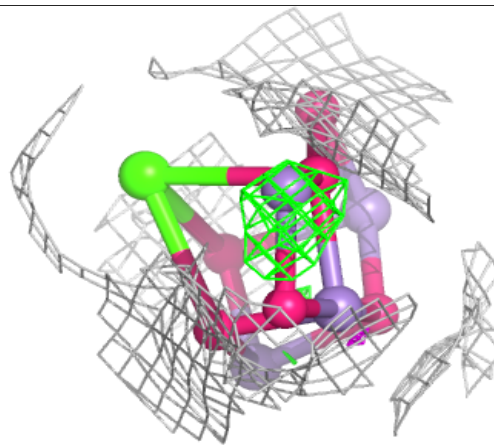
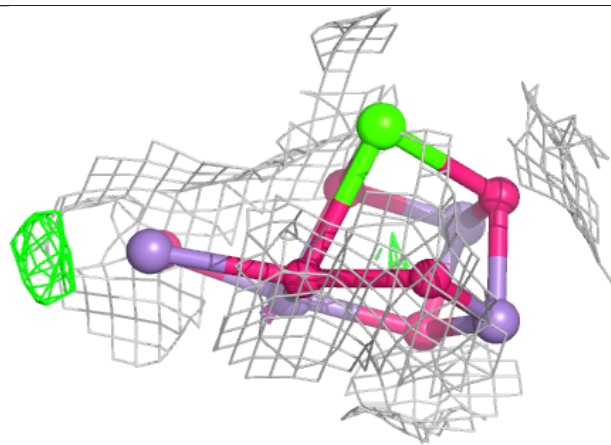
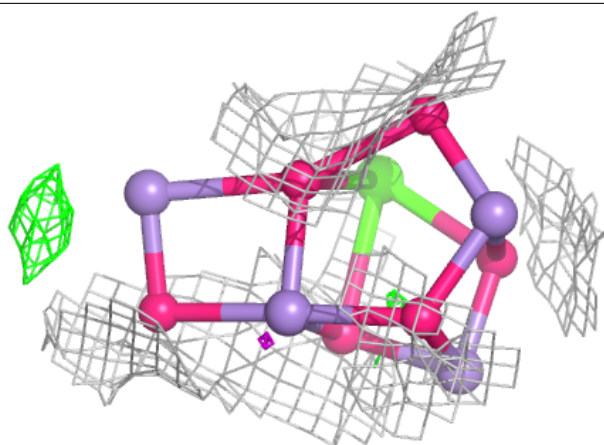
Electron density around OEY A 601 (B):

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



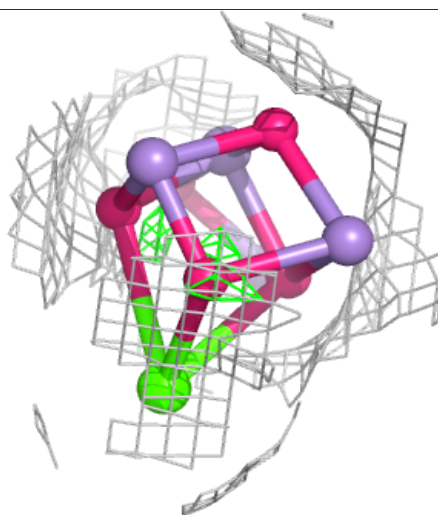
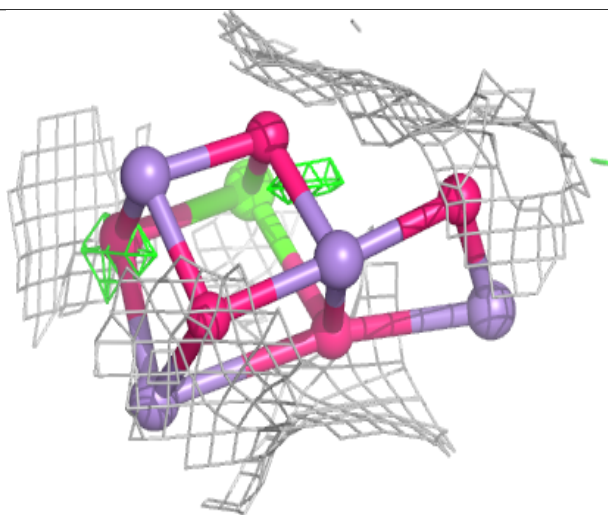
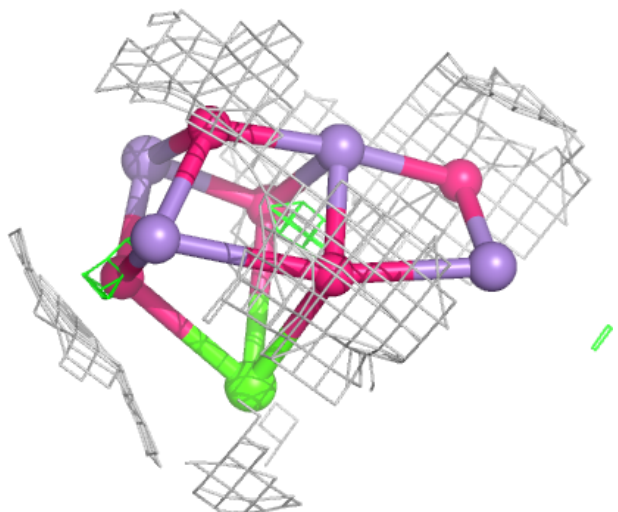
Electron density around OEY a 601 (B):

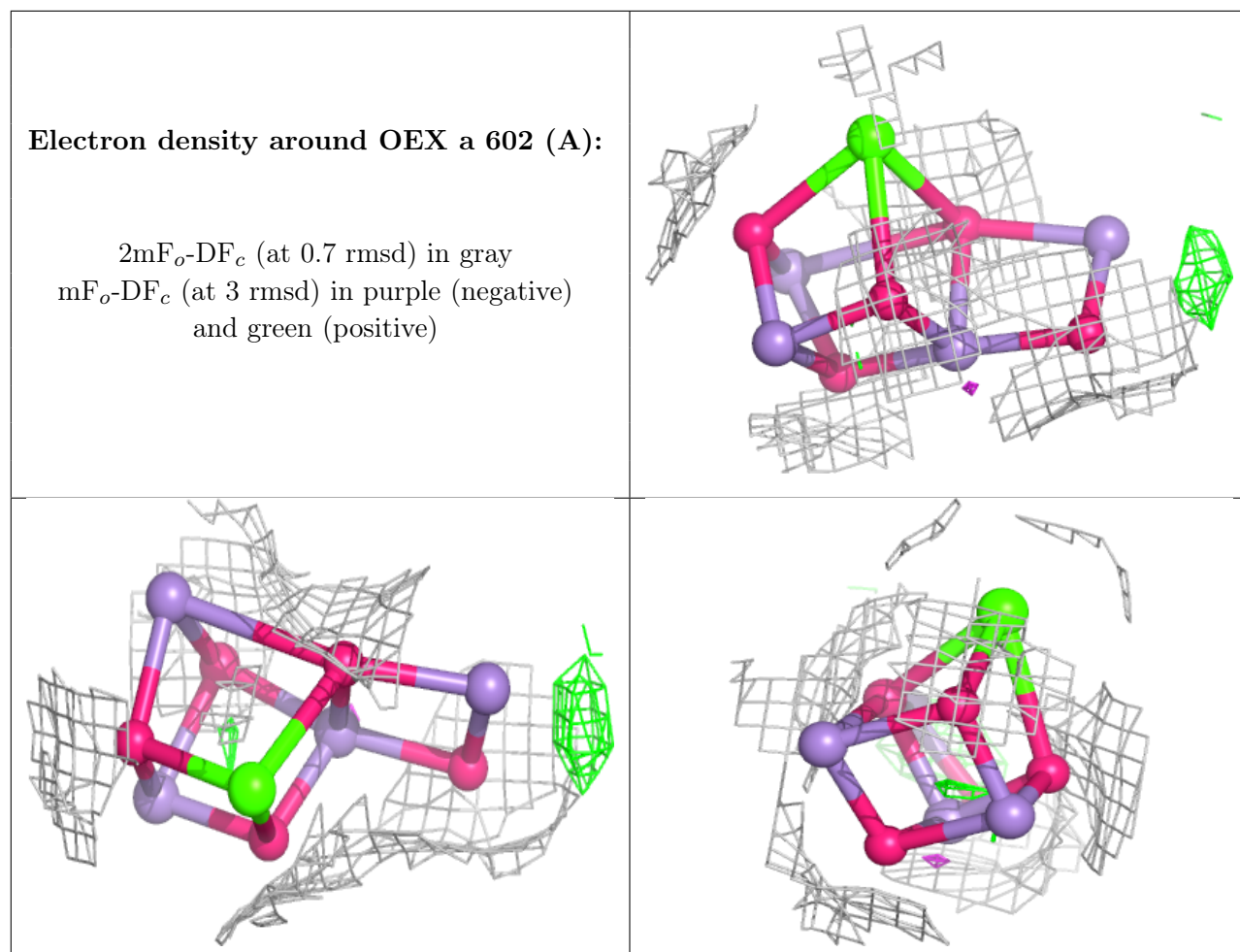
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX A 602 (A):

$2mF_o-DF_c$ (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.