



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:16 PM UTC

PDB ID : 7RF6 / pdb\_00007rf6  
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 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 : 2.01 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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)

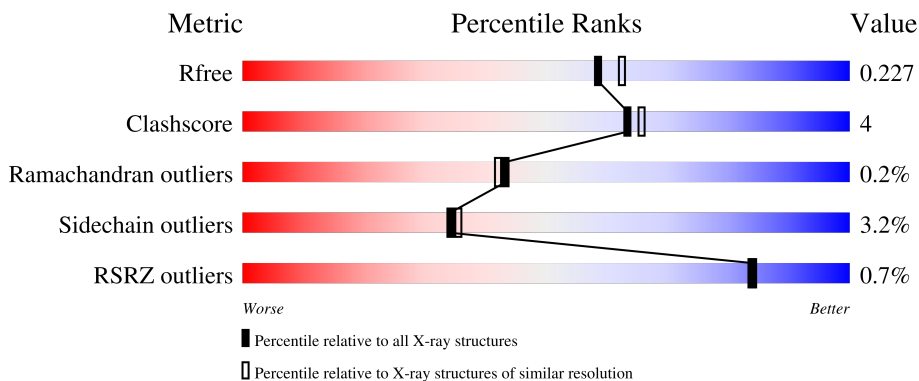
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	 89% 8% .
1	a	344	 85% 11% .

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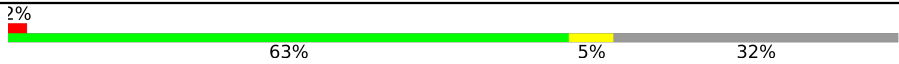
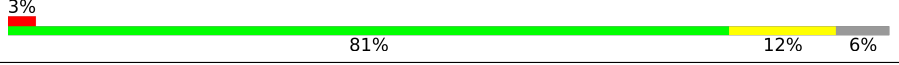
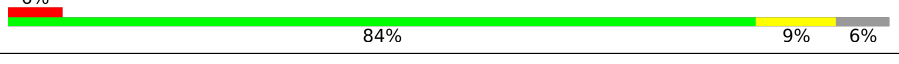


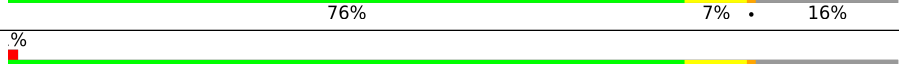
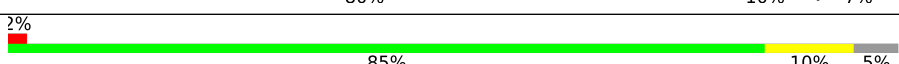

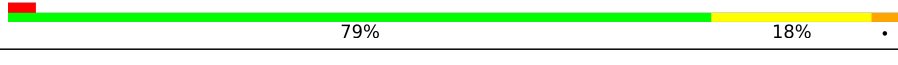
Density-Fitness : 1.0.12  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	510	90% 9%
2	b	510	89% 9%
3	C	461	87% 8%
3	c	461	90% 8%
4	D	352	90% 7%
4	d	352	84% 13%
5	E	84	82% 15%
5	e	84	76% 21%
6	F	45	60% 13% 24%
6	f	45	60% 13% 24%
7	H	66	95%
7	h	66	91% 5% 5%
8	I	38	79% 16% 5%
8	i	38	82% 13% 5%
9	J	40	72% 15% 10%
9	j	40	70% 20% 10%
10	K	46	70% 9% 20%
10	k	46	57% 22% 20%
11	L	37	89% 11%
11	l	37	89% 5%
12	M	36	75% 17% 8%
12	m	36	78% 11% 11%
13	O	272	78% 10% 10%
13	o	272	81% 8% 10%
14	R	41	54% 15% 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	608	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	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	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	402	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	612	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	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	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	403	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
24	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106128 atoms, of which 52762 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			

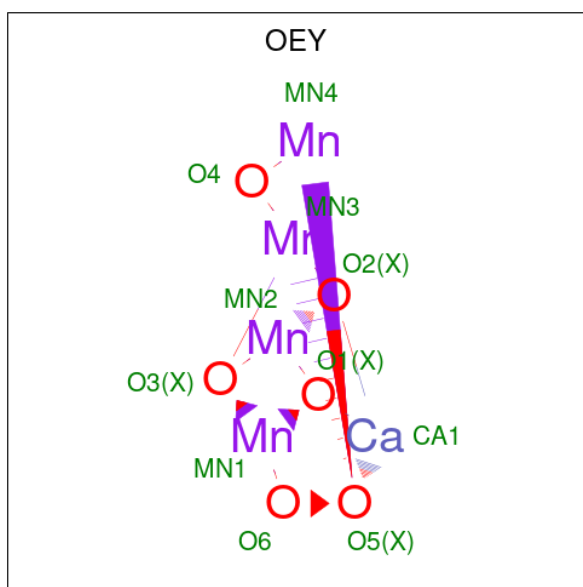
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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.

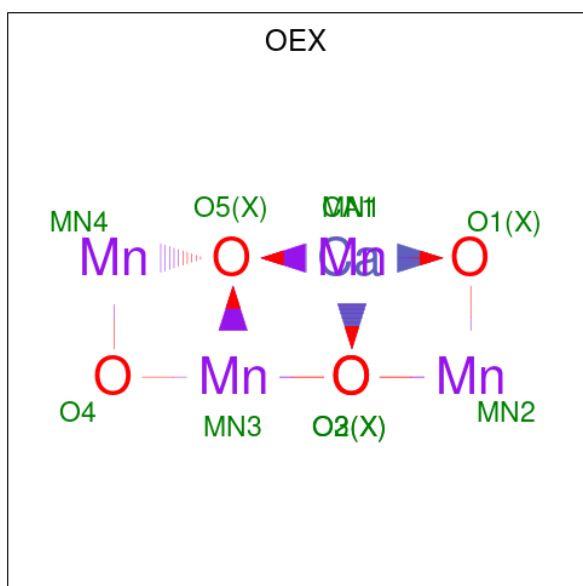
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (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:  $\text{CaMn}_4\text{O}_5$ ) (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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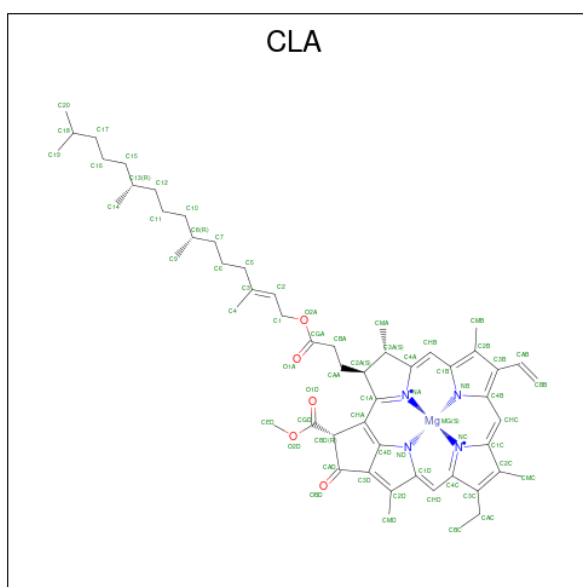
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
22	a	1	10	1	4	5	0	1

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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
			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
			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		

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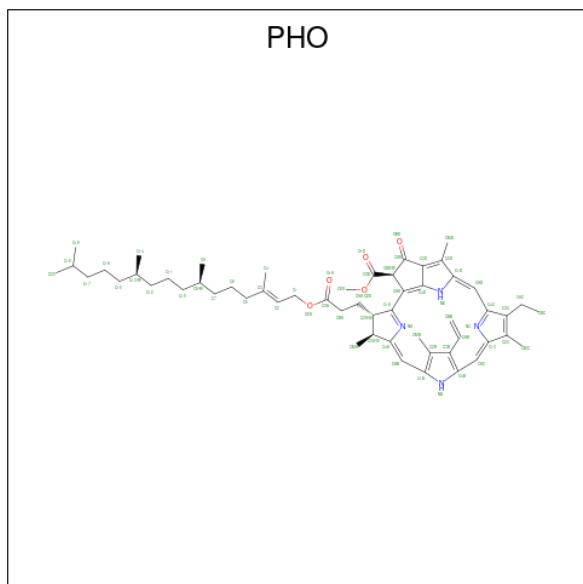
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
24	c	1	Total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

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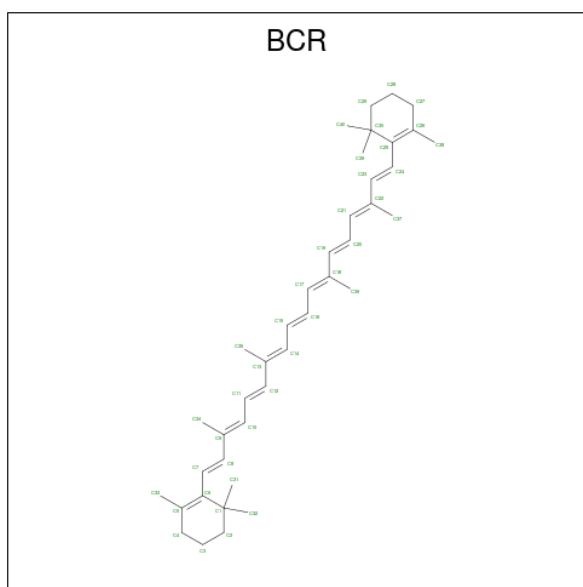
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
24	d	1	137	55	72	1	4	5	0	0

- 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	A	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	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	T	1	Total	C	H	0	0
			96	40	56		
26	Y	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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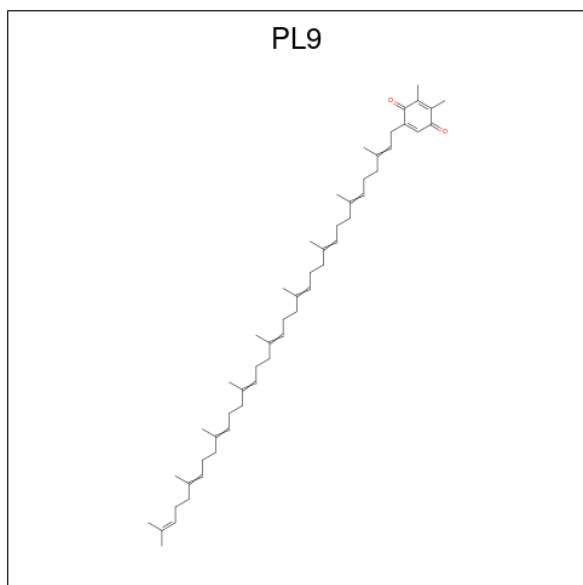
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		
26	x	1	Total	C	H	0	0
			96	40	56		

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

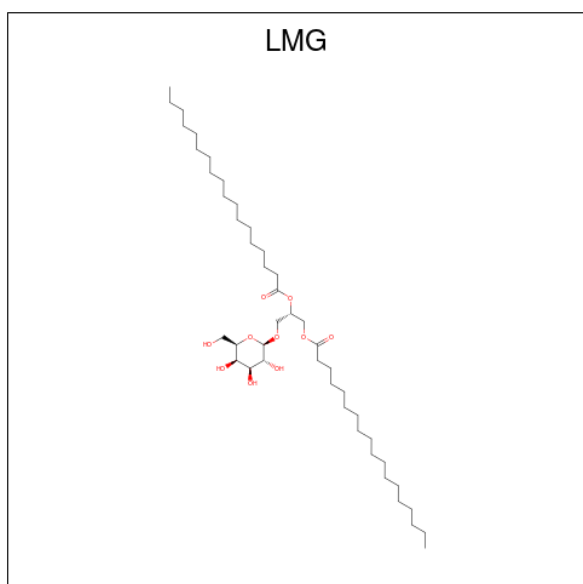
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- 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: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



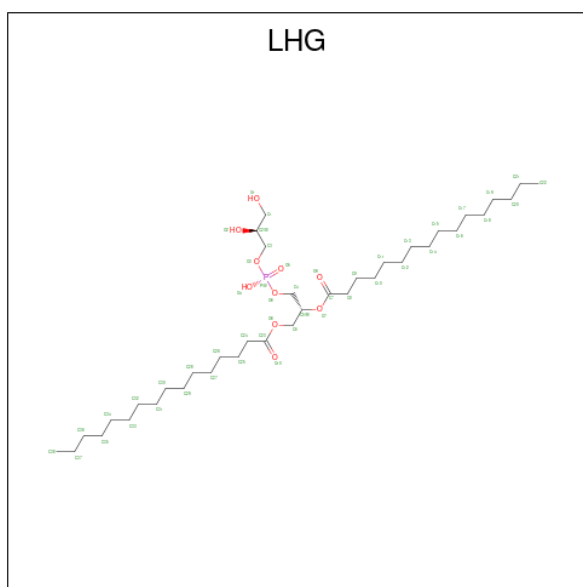
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
28	A	1	135	53	80	2	0	0
28	D	1	135	53	80	2	0	0
28	a	1	135	53	80	2	0	0
28	d	1	135	53	80	2	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



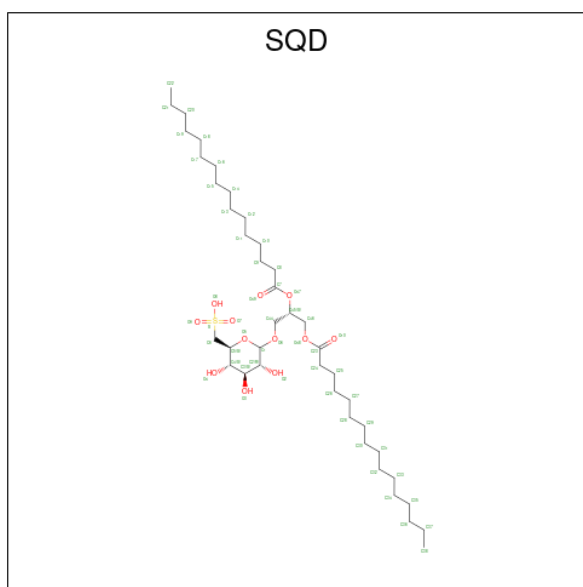
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			123	41	72	10		
29	D	1	Total	C	H	O	0	0
			78	27	45	6		
29	D	1	Total	C	H	O	0	0
			68	24	40	4		
29	M	1	Total	C	H	O	0	0
			123	41	72	10		
29	a	1	Total	C	H	O	0	0
			141	45	86	10		
29	b	1	Total	C	H	O	0	0
			123	41	72	10		
29	b	1	Total	C	H	O	0	0
			141	45	86	10		
29	c	1	Total	C	H	O	0	0
			81	27	44	10		
29	c	1	Total	C	H	O	0	0
			117	38	69	10		
29	c	1	Total	C	H	O	0	0
			117	39	68	10		
29	d	1	Total	C	H	O	0	0
			102	34	58	10		

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



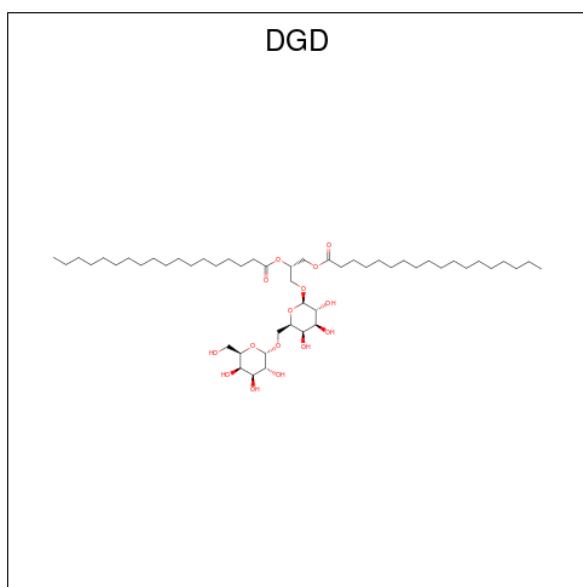
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
30	A	1	114	36	67	10	1	0	0
30	B	1	123	38	74	10	1	0	0
30	B	1	123	38	74	10	1	0	0
30	D	1	123	38	74	10	1	0	0
30	E	1	123	38	74	10	1	0	0
30	d	1	123	38	74	10	1	0	0
30	d	1	123	38	74	10	1	0	0
30	d	1	90	28	51	10	1	0	0
30	e	1	99	31	57	10	1	0	0
30	l	1	123	38	74	10	1	0	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



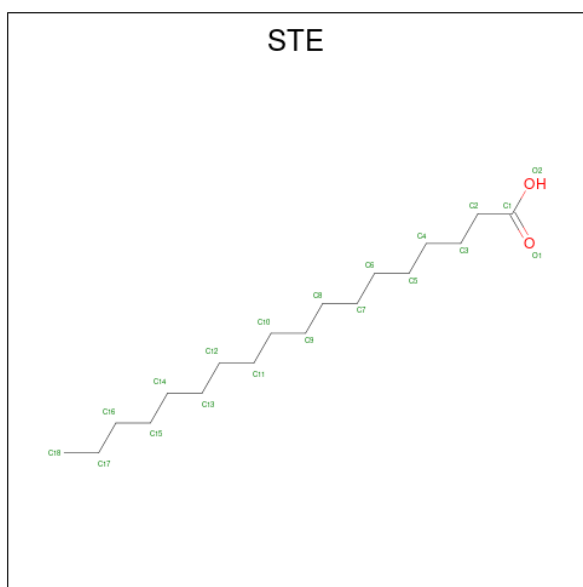
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
31	A	1	123	39	71	12	1	0	0
31	A	1	104	35	65	4		0	0
31	B	1	132	41	78	12	1	0	0
31	D	1	82	25	46	10	1	0	0
31	a	1	132	41	78	12	1	0	0
31	a	1	92	31	56	5		0	0
31	b	1	114	36	65	12	1	0	0
31	f	1	89	28	48	12	1	0	0

- Molecule 32 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		
32	A	1	Total	C	H	O	0	0
			162	51	96	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	H	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula:  $C_{18}H_{36}O_2$ ).



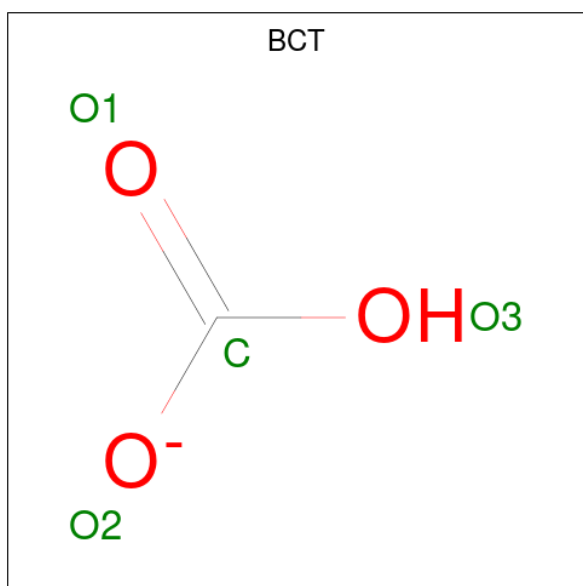
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	D	1	Total	C	H	O	0	0
			55	18	35	2		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		

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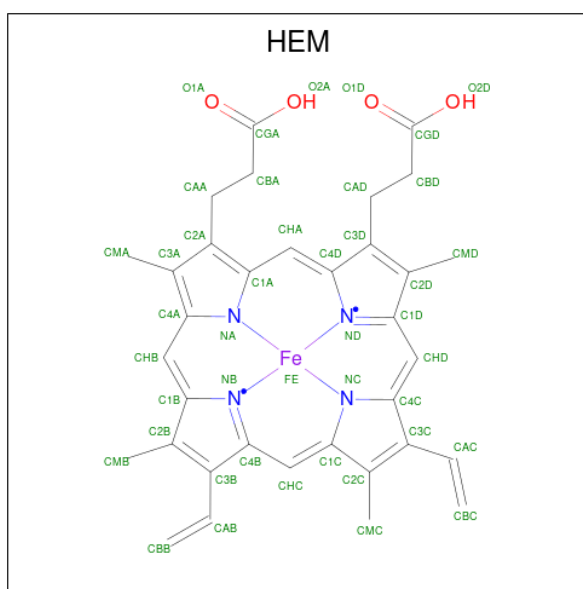
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	M	1	Total C H 26 10 16	0	0
33	T	1	Total C H 47 16 31	0	0
33	T	1	Total C H 44 15 29	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	a	1	Total C H 41 15 26	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H O 40 14 24 2	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H 26 10 16	0	0
33	b	1	Total C H 41 14 27	0	0
33	c	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	j	1	Total C H O 28 10 16 2	0	0
33	k	1	Total C H O 28 10 16 2	0	0
33	l	1	Total C H 53 18 35	0	0
33	m	1	Total C H O 28 10 16 2	0	0
33	t	1	Total C H O 46 16 28 2	0	0
33	x	1	Total C H O 55 18 35 2	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



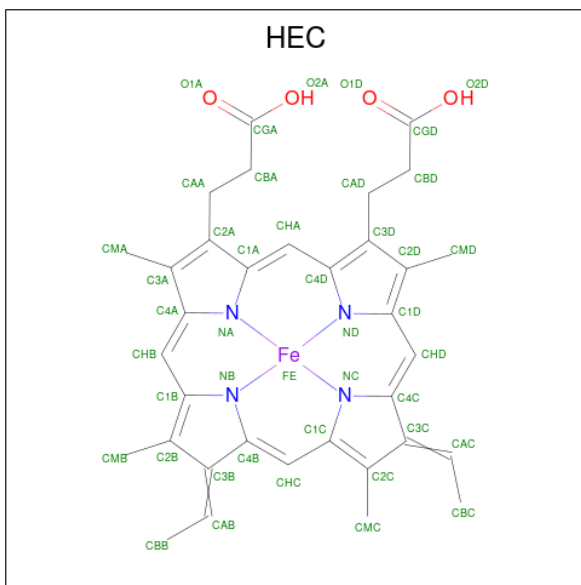
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	149	Total	O	0	0
			149	149		
37	B	200	Total	O	0	0
			200	200		
37	C	166	Total	O	0	0
			166	166		
37	D	124	Total	O	0	0
			124	124		
37	E	24	Total	O	0	0
			24	24		
37	F	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	28	Total O 28 28	0	0
37	I	6	Total O 6 6	0	0
37	J	13	Total O 13 13	0	0
37	K	4	Total O 4 4	0	0
37	L	12	Total O 12 12	0	0
37	M	8	Total O 8 8	0	0
37	O	96	Total O 96 96	0	0
37	R	5	Total O 5 5	0	0
37	T	12	Total O 12 12	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	11	Total O 11 11	0	0
37	Y	2	Total O 2 2	0	0
37	Z	7	Total O 7 7	0	0
37	a	131	Total O 131 131	0	0
37	b	207	Total O 207 207	0	0
37	c	162	Total O 162 162	0	0
37	d	123	Total O 123 123	0	0
37	e	29	Total O 29 29	0	0
37	f	7	Total O 7 7	0	0
37	h	22	Total O 22 22	0	0

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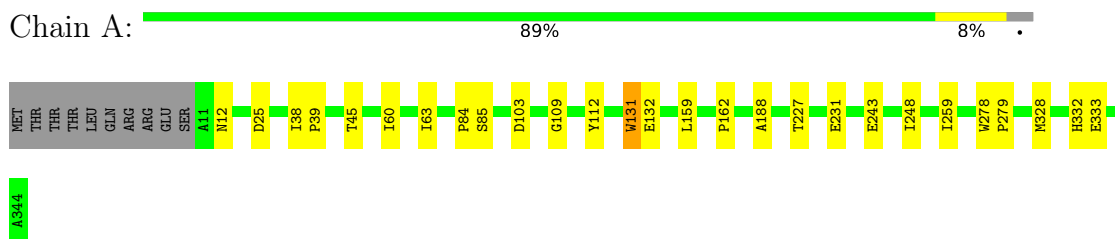
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	i	7	Total O 7 7	0	0
37	j	8	Total O 8 8	0	0
37	k	11	Total O 11 11	0	0
37	l	8	Total O 8 8	0	0
37	m	9	Total O 9 9	0	0
37	o	104	Total O 104 104	0	0
37	r	5	Total O 5 5	0	0
37	t	9	Total O 9 9	0	0
37	u	68	Total O 68 68	0	0
37	v	59	Total O 59 59	0	0
37	x	8	Total O 8 8	0	0
37	y	3	Total O 3 3	0	0
37	z	7	Total O 7 7	0	0

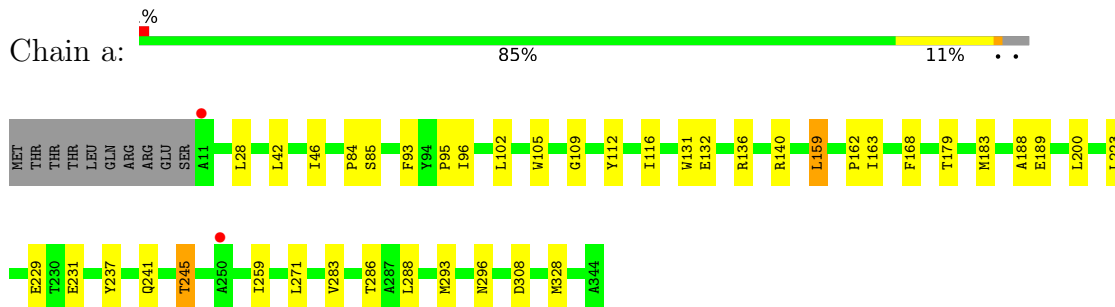
### 3 Residue-property plots [i](#)

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.

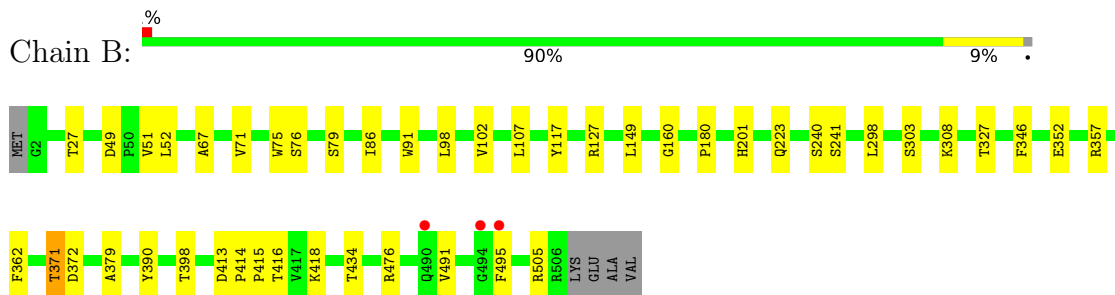
- Molecule 1: Photosystem II protein D1 1



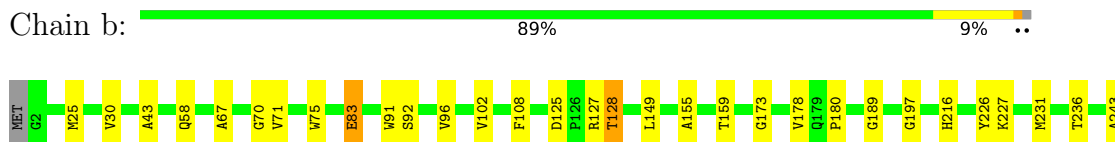
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



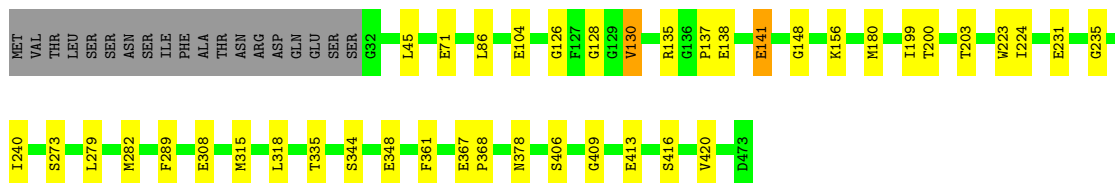
- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8%



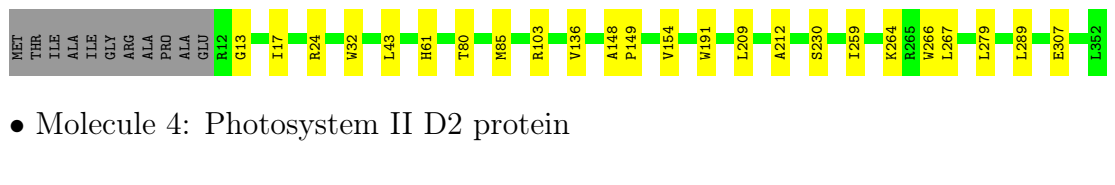
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 8%



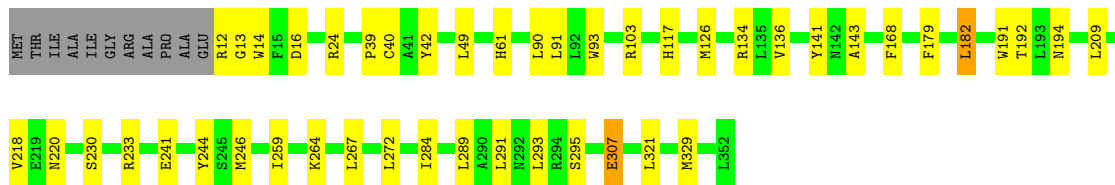
- Molecule 4: Photosystem II D2 protein

Chain D: 90% 7%



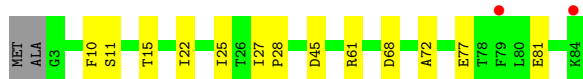
- Molecule 4: Photosystem II D2 protein

Chain d: 84% 13%

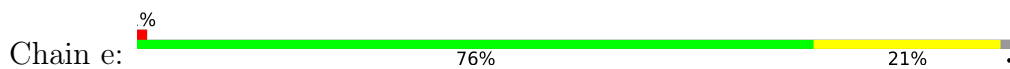


- Molecule 5: Cytochrome b559 subunit alpha

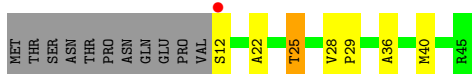
Chain E: 2% 82% 15%



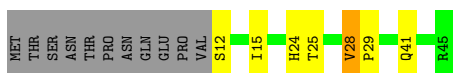
- Molecule 5: Cytochrome b559 subunit alpha



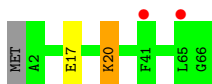
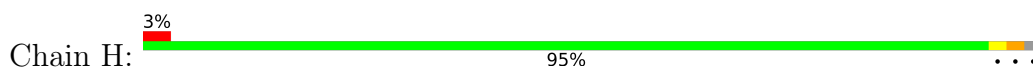
- Molecule 6: Cytochrome b559 subunit beta



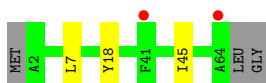
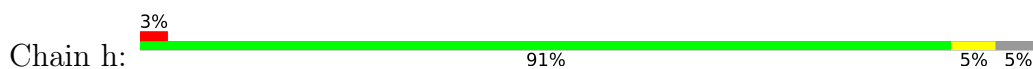
- Molecule 6: Cytochrome b559 subunit beta



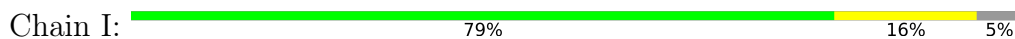
- Molecule 7: Photosystem II reaction center protein H



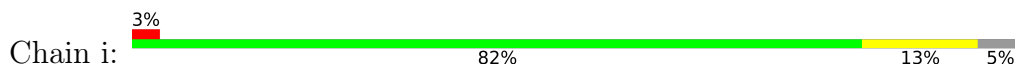
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



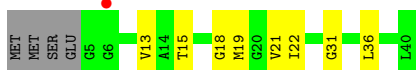
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



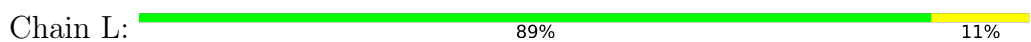
- Molecule 10: Photosystem II reaction center protein K



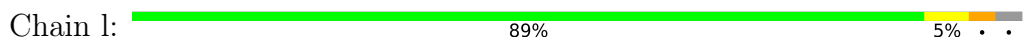
- Molecule 10: Photosystem II reaction center protein K



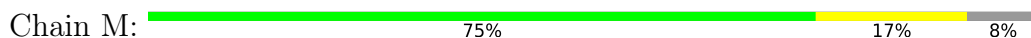
- Molecule 11: Photosystem II reaction center protein L




- Molecule 11: Photosystem II reaction center protein L

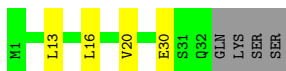


- Molecule 12: Photosystem II reaction center protein M




- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%




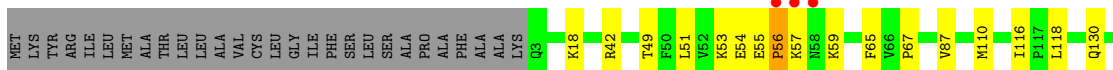
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  78% 10% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 8% 10%



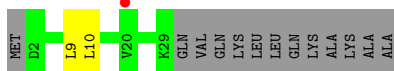
- Molecule 14: Photosystem II protein Y

Chain R:  54% 15% 32%




- Molecule 14: Photosystem II protein Y

Chain r:  2% 63% 5% 32%

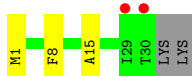
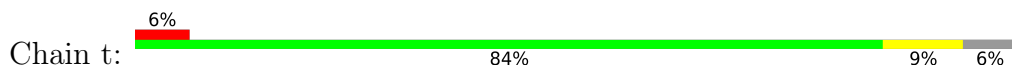


- Molecule 15: Photosystem II reaction center protein T

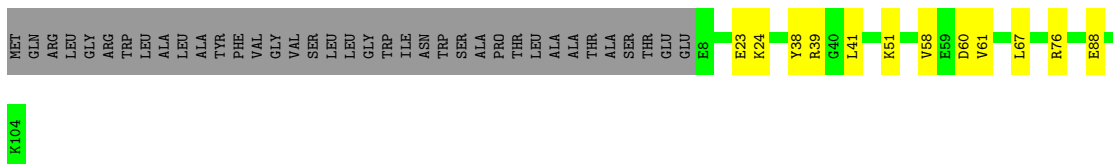
Chain T:  3% 81% 12% 6%



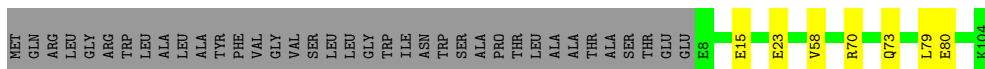
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein



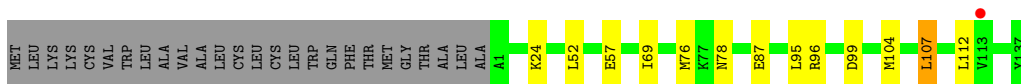
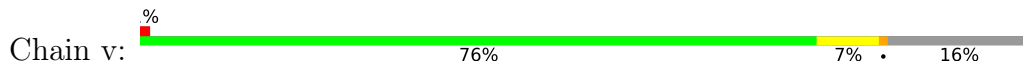
- Molecule 16: Photosystem II 12 kDa extrinsic protein



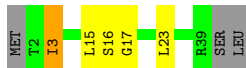
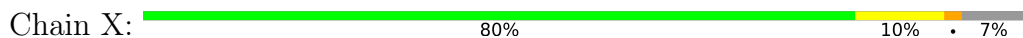
- Molecule 17: Cytochrome c-550



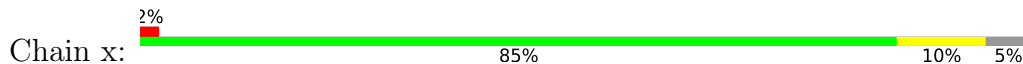
- Molecule 17: Cytochrome c-550

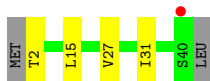


- Molecule 18: Photosystem II reaction center X protein

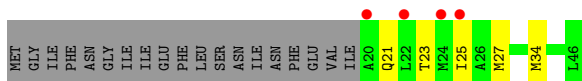


- Molecule 18: Photosystem II reaction center X protein

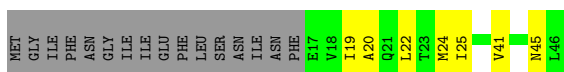




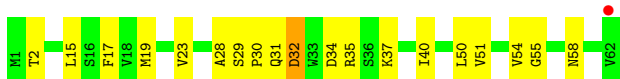
- Molecule 19: Photosystem II reaction center protein Ycf12



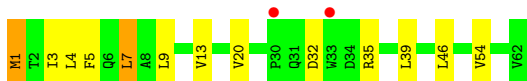
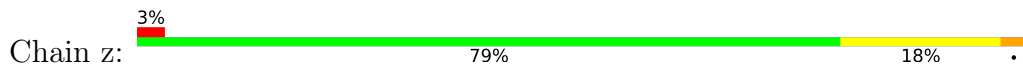
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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, $\alpha$ , $\beta$ , $\gamma$	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.9 (33.59-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.180 , 0.227 0.180 , 0.227	Depositor DCC
$R_{free}$ test set	4767 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	106128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.52	0/3227	0.60	1/4397 (0.0%)
1	a	0.48	0/3224	0.59	1/4393 (0.0%)
2	B	0.55	0/4161	0.62	0/5669
2	b	0.52	0/4118	0.60	0/5611
3	C	0.53	0/3647	0.60	0/4965
3	c	0.49	0/3719	0.59	0/5061
4	D	0.59	0/2825	0.65	0/3847
4	d	0.54	0/2834	0.63	0/3859
5	E	0.46	0/688	0.53	0/940
5	e	0.40	0/683	0.52	0/932
6	F	0.45	0/284	0.55	0/387
6	f	0.44	0/284	0.62	0/387
7	H	0.56	0/523	0.58	0/713
7	h	0.48	0/511	0.59	0/697
8	I	0.51	0/293	0.58	0/396
8	i	0.52	0/293	0.57	0/396
9	J	0.39	0/263	0.55	0/356
9	j	0.39	0/263	0.51	0/356
10	K	0.39	0/303	0.54	0/416
10	k	0.39	0/303	0.50	0/416
11	L	0.56	0/311	0.59	0/422
11	l	0.57	0/303	0.60	0/412
12	M	0.58	0/249	0.64	0/341
12	m	0.57	0/244	0.67	0/334
13	O	0.52	0/1904	0.61	0/2585
13	o	0.53	0/1905	0.60	0/2583
14	R	0.33	0/227	0.42	0/313
14	r	0.28	0/227	0.38	0/313
15	T	0.59	0/257	0.64	0/349
15	t	0.61	0/255	0.55	0/346
16	U	0.46	0/785	0.56	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.49	0/785	0.59	0/1064
17	V	0.51	0/1085	0.62	0/1473
17	v	0.48	0/1085	0.55	0/1473
18	X	0.41	0/284	0.48	0/384
18	x	0.38	0/289	0.47	0/391
19	Y	0.38	0/197	0.45	0/264
19	y	0.35	0/219	0.47	0/294
20	Z	0.35	0/490	0.49	0/669
20	z	0.27	0/488	0.39	0/666
All	All	0.51	0/44035	0.59	2/59934 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	131	TRP	CA-CB-CG	-5.19	103.73	113.60
1	A	131	TRP	CA-CB-CG	-5.02	104.06	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

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	15	0
1	a	3110	2976	2954	22	0
2	B	4005	3873	3867	31	0
2	b	3978	3836	3836	32	0
3	C	3509	3432	3409	22	0
3	c	3583	3503	3492	27	0
4	D	2731	2637	2637	17	0
4	d	2737	2643	2643	36	0
5	E	666	651	651	8	0
5	e	664	648	648	10	0
6	F	275	282	282	5	0
6	f	275	282	282	7	0
7	H	510	532	532	1	0
7	h	498	518	518	2	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	5	0
9	j	257	268	268	4	0
10	K	293	305	305	3	0
10	k	293	305	305	6	0
11	L	304	316	316	3	0
11	l	296	304	304	1	0
12	M	256	269	269	5	0
12	m	251	267	267	3	0
13	O	1870	1830	1830	22	0
13	o	1874	1846	1846	16	0
14	R	221	238	238	2	0
14	r	221	238	238	0	0
15	T	258	261	261	2	0
15	t	256	256	256	4	0
16	U	774	773	773	8	0
16	u	774	773	773	3	0
17	V	1064	1071	1073	5	0
17	v	1064	1071	1073	8	0
18	X	281	312	312	4	0
18	x	286	316	314	2	0
19	Y	196	217	217	3	0
19	y	218	241	241	2	0
20	Z	479	516	516	8	0
20	z	477	509	509	7	0
21	A	11	0	0	1	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	5	0
24	B	1035	1139	1139	19	0
24	C	839	922	922	6	0
24	D	130	144	144	3	0
24	a	195	216	216	0	0
24	b	1035	1139	1139	13	0
24	c	839	919	919	12	0
24	d	195	216	216	1	0
25	A	128	148	148	1	0
25	a	64	74	74	0	0
25	d	64	74	74	1	0
26	A	40	56	56	0	0
26	B	120	168	168	4	0
26	C	80	112	112	0	0
26	D	40	56	56	1	0
26	H	40	56	56	1	0
26	K	40	56	56	0	0
26	T	40	56	56	1	0
26	Y	40	56	56	1	0
26	a	40	56	56	1	0
26	b	120	168	168	2	0
26	c	80	112	112	1	0
26	d	40	56	56	2	0
26	k	80	112	112	0	0
26	t	40	56	56	3	0
26	x	40	56	56	0	0
27	A	2	0	0	0	0
27	a	2	0	0	0	0
28	A	55	80	80	2	0
28	D	55	80	80	0	0
28	a	55	80	80	2	0
28	d	55	80	80	0	0
29	A	48	66	66	0	0
29	C	48	66	66	0	0
29	D	112	157	157	2	0
29	M	51	72	72	1	0
29	a	55	86	86	5	0
29	b	106	158	158	1	0
29	c	134	181	181	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	d	44	58	58	0	0
30	A	47	67	67	1	0
30	B	98	148	148	1	0
30	D	49	74	74	3	0
30	E	49	74	74	1	0
30	d	137	199	199	5	0
30	e	42	57	57	0	0
30	l	49	74	74	1	0
31	A	91	136	134	2	0
31	B	54	78	76	2	0
31	D	36	46	45	1	0
31	a	90	134	132	0	0
31	b	49	65	64	1	0
31	f	41	48	47	1	0
32	A	66	96	96	3	0
32	C	186	246	245	0	0
32	H	62	82	81	0	0
32	c	186	246	244	2	0
32	h	62	82	79	0	0
33	B	71	109	109	3	0
33	C	40	63	63	0	0
33	D	20	35	35	6	0
33	E	12	16	16	1	0
33	H	18	35	35	1	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	M	25	38	38	1	0
33	T	31	60	60	1	0
33	Z	8	12	12	0	0
33	a	37	58	58	1	0
33	b	80	137	137	4	0
33	c	20	35	35	1	0
33	d	37	61	61	1	0
33	j	12	16	16	0	0
33	k	12	16	16	0	0
33	l	18	35	35	1	0
33	m	12	16	16	1	0
33	t	18	28	28	2	0
33	x	20	35	35	0	0
34	D	4	1	1	1	0
34	a	4	1	1	0	0
35	F	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	e	43	30	30	4	0
36	V	43	30	30	1	0
36	v	43	30	30	1	0
37	A	149	0	0	3	0
37	B	200	0	0	9	0
37	C	166	0	0	4	0
37	D	124	0	0	2	0
37	E	24	0	0	1	0
37	F	10	0	0	1	0
37	H	28	0	0	0	0
37	I	6	0	0	0	0
37	J	13	0	0	2	0
37	K	4	0	0	0	0
37	L	12	0	0	1	0
37	M	8	0	0	3	0
37	O	96	0	0	7	0
37	R	5	0	0	0	0
37	T	12	0	0	1	0
37	U	47	0	0	4	0
37	V	78	0	0	2	0
37	X	11	0	0	0	0
37	Y	2	0	0	0	0
37	Z	7	0	0	0	0
37	a	131	0	0	0	0
37	b	207	0	0	4	0
37	c	162	0	0	6	0
37	d	123	0	0	10	0
37	e	29	0	0	0	0
37	f	7	0	0	1	0
37	h	22	0	0	0	0
37	i	7	0	0	0	0
37	j	8	0	0	1	0
37	k	11	0	0	1	0
37	l	8	0	0	0	0
37	m	9	0	0	1	0
37	o	104	0	0	6	0
37	r	5	0	0	0	0
37	t	9	0	0	0	0
37	u	68	0	0	1	0
37	v	59	0	0	1	0
37	x	8	0	0	0	0
37	y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	z	7	0	0	1	0
All	All	53366	52762	52664	415	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 4.

The worst 5 of 415 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)
3:c:315:MET:SD	37:c:746:HOH:O	2.15	1.04
13:o:54:GLU:HA	37:o:302:HOH:O	1.61	0.98
4:d:307:GLU:OE1	37:d:501:HOH:O	1.83	0.94
12:M:5:GLN:O	37:M:201:HOH:O	1.84	0.94
3:C:231:GLU:OE1	37:C:601:HOH:O	1.86	0.93

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%)	392 (99%)	4 (1%)	1 (0%)	36	35
1	a	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	36	35
2	B	508/510 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	442 (97%)	11 (2%)	1 (0%)	43	42
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	43	42
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
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%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	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%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	230 (95%)	11 (4%)	2 (1%)	16	11
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	30	27
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (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	
20	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
All	All	5387/5700 (94%)	5245 (97%)	134 (2%)	8 (0%)	43	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	58	ASN
13	O	62	GLU

### 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%)	319 (98%)	5 (2%)	57	64
1	a	323/280 (115%)	313 (97%)	10 (3%)	35	37
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	50
2	b	402/407 (99%)	394 (98%)	8 (2%)	48	54
3	C	356/362 (98%)	348 (98%)	8 (2%)	45	50
3	c	364/362 (101%)	355 (98%)	9 (2%)	42	45
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	73
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	11
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	41
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	31
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	11
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	201 (98%)	5 (2%)	43	47
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	40
14	R	22/33 (67%)	18 (82%)	4 (18%)	2	1
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	29
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	82 (98%)	2 (2%)	43	47
16	u	84/112 (75%)	82 (98%)	2 (2%)	43	47
17	V	117/138 (85%)	112 (96%)	5 (4%)	26	25
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	20	18
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	45 (88%)	6 (12%)	5	3
All	All	4451/4654 (96%)	4308 (97%)	143 (3%)	34	35

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	l	30	LEU
13	o	49	THR
17	v	69	ILE

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Mol	Chain	Res	Type
16	U	51	LYS
15	T	25	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	h	59	ASN
13	o	80	GLN
14	R	22	ASN
13	O	155	ASN
13	o	155	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.73	0
8	FME	i	1	8	8,9,10	1.07	1 (12%)	8,9,11	0.84	0
12	FME	M	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.97	0
15	FME	t	1	15	8,9,10	1.46	1 (12%)	8,9,11	1.03	1 (12%)
8	FME	I	1	8	8,9,10	1.01	1 (12%)	8,9,11	0.94	0
15	FME	T	1	15	8,9,10	0.97	1 (12%)	8,9,11	1.37	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
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.55	1.41	1.46
8	i	1	FME	CA-N	-2.27	1.43	1.46
8	I	1	FME	CA-N	-2.14	1.43	1.46
15	T	1	FME	CA-N	-2.05	1.43	1.46
12	M	1	FME	CA-N	-2.01	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.44	119.02	125.32
15	t	1	FME	CB-CA-N	2.22	114.56	110.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
15	T	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$
24	CLA	C	501	-	69,73,73	1.40	8 (11%)	82,113,113	1.54	7 (8%)
24	CLA	C	509	-	69,73,73	1.23	7 (10%)	82,113,113	1.46	8 (9%)
26	BCR	c	514	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	8 (14%)
33	STE	a	616	-	11,11,19	0.86	0	11,11,19	1.28	2 (18%)
24	CLA	B	613	-	69,73,73	1.24	8 (11%)	82,113,113	1.12	7 (8%)
29	LMG	a	618	-	55,55,55	1.06	5 (9%)	63,63,63	1.45	8 (12%)
24	CLA	C	504	37	63,67,73	1.17	6 (9%)	74,105,113	1.35	7 (9%)
29	LMG	c	522	-	49,49,55	0.88	2 (4%)	57,57,63	1.30	6 (10%)
25	PHO	A	606	-	58,69,69	1.78	14 (24%)	55,99,99	1.73	10 (18%)
32	DGD	c	516	-	63,63,67	1.17	8 (12%)	77,77,81	1.38	11 (14%)
21	OEY	a	601[B]	3,1,37	0,16,16	-	-	-	-	-
33	STE	B	624	-	13,13,19	0.70	0	13,13,19	1.12	1 (7%)
24	CLA	d	404	-	69,73,73	1.44	10 (14%)	82,113,113	1.18	8 (9%)
29	LMG	c	521	-	48,48,55	1.09	6 (12%)	56,56,63	1.27	3 (5%)
31	SQD	a	614	-	35,35,54	1.04	2 (5%)	37,37,65	1.52	6 (16%)
26	BCR	B	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.17	4 (7%)
33	STE	b	625	-	19,19,19	0.66	0	19,19,19	1.00	1 (5%)
24	CLA	b	615	-	69,73,73	1.55	10 (14%)	82,113,113	1.60	13 (15%)
26	BCR	A	609	-	41,41,41	1.22	5 (12%)	56,56,56	1.42	9 (16%)
24	CLA	B	615	-	69,73,73	1.33	8 (11%)	82,113,113	1.27	7 (8%)
24	CLA	b	612	-	69,73,73	1.58	10 (14%)	82,113,113	1.27	10 (12%)
33	STE	B	625	-	11,11,19	0.80	0	11,11,19	1.09	0
33	STE	a	617	-	14,14,19	0.43	0	13,13,19	0.80	0
30	LHG	d	408	-	48,48,48	0.86	1 (2%)	51,54,54	1.23	4 (7%)
24	CLA	C	502	-	69,73,73	1.22	7 (10%)	82,113,113	1.36	7 (8%)
24	CLA	b	605	-	69,73,73	1.19	8 (11%)	82,113,113	1.49	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	603	-	69,73,73	1.33	8 (11%)	82,113,113	1.60	11 (13%)
33	STE	b	627	-	13,13,19	0.49	0	12,12,19	0.54	0
24	CLA	b	608	-	69,73,73	1.28	10 (14%)	82,113,113	1.30	12 (14%)
31	SQD	b	620	-	47,49,54	0.99	3 (6%)	57,60,65	1.87	14 (24%)
24	CLA	b	607	37	69,73,73	1.26	8 (11%)	82,113,113	1.23	8 (9%)
33	STE	c	520	-	19,19,19	0.63	0	19,19,19	0.98	0
25	PHO	d	402	-	58,69,69	2.11	8 (13%)	55,99,99	1.53	7 (12%)
33	STE	b	626	-	9,9,19	0.46	0	8,8,19	0.64	0
24	CLA	b	602	-	69,73,73	1.19	8 (11%)	82,113,113	1.56	11 (13%)
24	CLA	B	610	37	69,73,73	1.40	10 (14%)	82,113,113	1.43	8 (9%)
24	CLA	c	508	-	68,72,73	1.41	7 (10%)	80,111,113	1.45	10 (12%)
25	PHO	A	607	-	58,69,69	2.01	9 (15%)	55,99,99	1.46	9 (16%)
32	DGD	h	101	-	63,63,67	1.16	7 (11%)	77,77,81	1.38	12 (15%)
24	CLA	c	503	-	69,73,73	1.25	8 (11%)	82,113,113	1.17	5 (6%)
30	LHG	B	621	-	48,48,48	0.85	1 (2%)	51,54,54	1.19	6 (11%)
24	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.38	11 (13%)
24	CLA	B	604	-	69,73,73	1.19	7 (10%)	82,113,113	1.48	7 (8%)
24	CLA	c	502	-	69,73,73	1.19	9 (13%)	82,113,113	1.34	8 (9%)
24	CLA	b	613	-	69,73,73	1.22	8 (11%)	82,113,113	1.31	8 (9%)
33	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.83	0
29	LMG	D	409	-	31,31,55	0.98	2 (6%)	33,33,63	1.11	1 (3%)
29	LMG	D	410	-	26,26,55	0.60	0	26,26,63	1.25	1 (3%)
24	CLA	A	613	37	69,73,73	1.30	11 (15%)	82,113,113	1.40	7 (8%)
24	CLA	B	605	-	69,73,73	1.19	5 (7%)	82,113,113	1.31	9 (10%)
33	STE	C	522	-	11,11,19	0.70	0	11,11,19	1.36	2 (18%)
31	SQD	A	617	-	38,38,54	0.97	3 (7%)	40,40,65	1.46	4 (10%)
24	CLA	b	609	-	69,73,73	1.47	8 (11%)	82,113,113	1.60	12 (14%)
24	CLA	C	505	-	69,73,73	1.33	7 (10%)	82,113,113	1.40	8 (9%)
30	LHG	D	408	-	48,48,48	1.14	4 (8%)	51,54,54	1.27	5 (9%)
30	LHG	E	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.28	5 (9%)
31	SQD	D	407	-	34,36,54	1.01	3 (8%)	42,45,65	2.09	10 (23%)
24	CLA	c	512	-	69,73,73	1.12	7 (10%)	82,113,113	1.34	6 (7%)
24	CLA	B	601	37	69,73,73	1.27	6 (8%)	82,113,113	1.38	9 (10%)
33	STE	b	624	-	15,15,19	0.83	1 (6%)	15,15,19	0.78	0
33	STE	t	102	-	17,17,19	0.57	0	17,17,19	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	d	403	-	69,73,73	1.33	11 (15%)	82,113,113	1.45	7 (8%)
26	BCR	T	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	6 (10%)
29	LMG	b	623	-	55,55,55	0.87	3 (5%)	63,63,63	1.40	8 (12%)
24	CLA	b	610	37	69,73,73	1.33	7 (10%)	82,113,113	1.46	11 (13%)
24	CLA	c	501	-	69,73,73	1.09	3 (4%)	82,113,113	1.39	9 (10%)
26	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
24	CLA	b	606	-	69,73,73	1.73	8 (11%)	82,113,113	1.61	9 (10%)
24	CLA	B	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.66	11 (13%)
28	PL9	a	611	-	55,55,55	1.13	6 (10%)	68,69,69	1.67	14 (20%)
26	BCR	C	514	-	41,41,41	1.24	3 (7%)	56,56,56	1.36	8 (14%)
26	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
34	BCT	a	610	23	3,3,3	0.97	0	2,3,3	3.21	1 (50%)
24	CLA	C	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.50	11 (13%)
29	LMG	d	410	-	44,44,55	1.02	3 (6%)	52,52,63	1.26	6 (11%)
29	LMG	M	101	-	51,51,55	1.08	4 (7%)	59,59,63	1.50	7 (11%)
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.90	0
24	CLA	A	605	37	69,73,73	1.29	7 (10%)	82,113,113	1.46	11 (13%)
33	STE	k	103	-	11,11,19	0.82	0	11,11,19	0.94	0
26	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.18	4 (7%)
33	STE	d	411	-	16,16,19	0.60	0	16,16,19	1.43	1 (6%)
29	LMG	b	621	-	51,51,55	0.95	3 (5%)	59,59,63	1.49	10 (16%)
33	STE	a	615	-	9,9,19	0.57	0	8,8,19	0.48	0
36	HEC	V	201	17	46,50,50	1.80	5 (10%)	58,82,82	1.94	8 (13%)
31	SQD	A	616	-	50,52,54	1.12	6 (12%)	60,63,65	2.05	11 (18%)
33	STE	m	101	-	11,11,19	0.66	0	11,11,19	1.35	1 (9%)
32	DGD	A	618	-	67,67,67	1.22	7 (10%)	81,81,81	1.38	9 (11%)
24	CLA	B	607	37	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
24	CLA	c	509	-	69,73,73	1.30	5 (7%)	82,113,113	1.48	8 (9%)
31	SQD	a	613	-	52,54,54	1.05	5 (9%)	62,65,65	1.87	11 (17%)
26	BCR	C	515	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
26	BCR	a	607	-	41,41,41	1.08	4 (9%)	56,56,56	1.23	6 (10%)
33	STE	b	622	-	19,19,19	0.59	0	19,19,19	1.04	1 (5%)
26	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
35	HEM	F	101	5,6	50,50,50	1.35	4 (8%)	67,82,82	1.20	6 (8%)
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.05	4 (7%)
24	CLA	a	606	-	69,73,73	1.57	11 (15%)	82,113,113	1.30	8 (9%)
30	LHG	l	101	-	48,48,48	0.88	1 (2%)	51,54,54	1.29	8 (15%)
28	PL9	D	405	-	55,55,55	1.51	9 (16%)	68,69,69	1.66	16 (23%)
32	DGD	c	518	-	63,63,67	1.10	6 (9%)	77,77,81	1.42	14 (18%)
26	BCR	K	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.18	4 (7%)
24	CLA	c	504	37	64,68,73	1.23	7 (10%)	76,107,113	1.24	9 (11%)
29	LMG	C	519	-	48,48,55	0.90	3 (6%)	56,56,63	1.38	7 (12%)
32	DGD	C	517	-	63,63,67	1.19	6 (9%)	77,77,81	1.35	8 (10%)
33	STE	T	103	-	14,14,19	0.45	0	13,13,19	0.79	0
30	LHG	d	407	-	48,48,48	0.88	4 (8%)	51,54,54	1.46	7 (13%)
28	PL9	d	406	-	55,55,55	1.54	7 (12%)	68,69,69	1.75	14 (20%)
24	CLA	b	611	-	69,73,73	1.29	8 (11%)	82,113,113	1.40	8 (9%)
31	SQD	B	623	-	52,54,54	0.97	3 (5%)	62,65,65	1.96	14 (22%)
24	CLA	b	614	-	69,73,73	1.43	9 (13%)	82,113,113	1.48	12 (14%)
26	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
28	PL9	A	612	-	55,55,55	1.13	4 (7%)	68,69,69	1.57	11 (16%)
24	CLA	B	616	-	64,68,73	1.36	8 (12%)	76,107,113	1.56	8 (10%)
24	CLA	c	507	37	69,73,73	1.19	5 (7%)	82,113,113	1.39	10 (12%)
24	CLA	c	513	-	69,73,73	1.26	9 (13%)	82,113,113	1.23	9 (10%)
26	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.40	8 (14%)
24	CLA	B	606	-	69,73,73	1.31	12 (17%)	82,113,113	1.42	12 (14%)
24	CLA	B	608	-	69,73,73	1.07	5 (7%)	82,113,113	1.27	10 (12%)
24	CLA	B	602	-	69,73,73	1.42	9 (13%)	82,113,113	1.27	10 (12%)
33	STE	B	620	-	16,16,19	0.74	0	16,16,19	1.08	0
24	CLA	C	512	-	69,73,73	1.15	6 (8%)	82,113,113	1.35	9 (10%)
30	LHG	d	409	-	38,38,48	0.93	1 (2%)	41,44,54	1.19	2 (4%)
33	STE	x	102	-	19,19,19	0.77	1 (5%)	19,19,19	1.09	1 (5%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-	-	-
29	LMG	c	519	-	37,37,55	1.23	6 (16%)	45,45,63	1.35	6 (13%)
24	CLA	D	402	-	69,73,73	1.21	10 (14%)	82,113,113	1.34	8 (9%)
33	STE	I	101	-	14,14,19	0.45	0	13,13,19	0.64	0
24	CLA	C	506	-	69,73,73	1.72	10 (14%)	82,113,113	1.22	7 (8%)
32	DGD	c	517	-	63,63,67	1.22	8 (12%)	77,77,81	1.40	15 (19%)
24	CLA	d	401	37	69,73,73	1.32	12 (17%)	82,113,113	1.37	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	STE	D	411	-	19,19,19	0.57	0	19,19,19	1.24	1 (5%)
26	BCR	c	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.35	8 (14%)
24	CLA	a	604	-	69,73,73	1.25	8 (11%)	82,113,113	1.28	6 (7%)
33	STE	B	627	-	11,11,19	0.83	0	11,11,19	1.06	1 (9%)
24	CLA	C	513	-	69,73,73	1.14	5 (7%)	82,113,113	1.43	10 (12%)
33	STE	M	103	-	9,9,19	0.41	0	8,8,19	0.88	0
34	BCT	D	401	23	3,3,3	0.99	0	2,3,3	3.31	1 (50%)
29	LMG	D	406	-	51,51,55	0.96	3 (5%)	59,59,63	1.27	3 (5%)
24	CLA	A	604	-	69,73,73	1.26	7 (10%)	82,113,113	1.24	10 (12%)
33	STE	E	102	-	11,11,19	0.88	0	11,11,19	1.18	1 (9%)
24	CLA	C	511	3	69,73,73	1.54	9 (13%)	82,113,113	1.32	7 (8%)
26	BCR	B	619	-	41,41,41	1.27	5 (12%)	56,56,56	1.28	4 (7%)
30	LHG	A	615	-	46,46,48	1.14	4 (8%)	49,52,54	1.39	5 (10%)
33	STE	Z	101	-	7,7,19	0.48	0	6,6,19	0.46	0
24	CLA	C	510	-	69,73,73	1.23	10 (14%)	82,113,113	1.47	10 (12%)
26	BCR	B	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.33	9 (16%)
24	CLA	A	608	-	58,62,73	1.37	8 (13%)	68,99,113	1.30	6 (8%)
26	BCR	d	405	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	6 (10%)
25	PHO	a	605	-	58,69,69	1.90	12 (20%)	55,99,99	1.62	10 (18%)
32	DGD	C	518	-	63,63,67	1.12	5 (7%)	77,77,81	1.34	8 (10%)
33	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.34	1 (9%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-	-	-
24	CLA	B	609	-	69,73,73	1.46	9 (13%)	82,113,113	1.41	12 (14%)
26	BCR	b	618	-	41,41,41	1.28	4 (9%)	56,56,56	1.18	7 (12%)
30	LHG	B	622	-	48,48,48	0.92	3 (6%)	51,54,54	1.35	8 (15%)
33	STE	C	520	-	11,11,19	0.92	0	11,11,19	1.03	0
35	HEM	e	101	5,6	50,50,50	1.39	8 (16%)	67,82,82	1.23	6 (8%)
24	CLA	a	612	37	69,73,73	1.76	11 (15%)	82,113,113	1.48	8 (9%)
24	CLA	b	616	-	64,68,73	1.18	9 (14%)	76,107,113	1.41	8 (10%)
24	CLA	D	403	-	69,73,73	1.56	10 (14%)	82,113,113	1.31	6 (7%)
32	DGD	H	102	-	63,63,67	1.35	13 (20%)	77,77,81	1.38	8 (10%)
30	LHG	e	102	-	41,41,48	0.89	2 (4%)	44,47,54	1.33	5 (11%)
24	CLA	c	510	-	69,73,73	1.54	10 (14%)	82,113,113	1.47	11 (13%)
24	CLA	C	503	-	69,73,73	1.31	7 (10%)	82,113,113	1.69	11 (13%)
24	CLA	c	506	-	69,73,73	1.43	11 (15%)	82,113,113	1.39	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.43	12 (14%)
26	BCR	D	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	4 (7%)
24	CLA	b	601	37	69,73,73	1.27	8 (11%)	82,113,113	1.40	6 (7%)
24	CLA	c	505	-	69,73,73	1.19	10 (14%)	82,113,113	1.31	7 (8%)
33	STE	j	101	-	11,11,19	0.85	0	11,11,19	0.99	1 (9%)
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.69	0
33	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.67	0
33	STE	d	412	-	19,19,19	0.55	0	19,19,19	1.14	0
33	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.14	1 (7%)
24	CLA	B	612	-	69,73,73	1.32	8 (11%)	82,113,113	1.49	11 (13%)
24	CLA	b	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	15 (18%)
32	DGD	C	516	-	63,63,67	1.29	9 (14%)	77,77,81	1.39	9 (11%)
24	CLA	C	508	-	69,73,73	1.51	10 (14%)	82,113,113	1.47	11 (13%)
24	CLA	c	511	3	69,73,73	1.49	9 (13%)	82,113,113	1.29	4 (4%)
26	BCR	t	101	-	41,41,41	1.15	5 (12%)	56,56,56	1.39	8 (14%)
33	STE	C	521	-	15,15,19	0.37	0	14,14,19	0.86	0
29	LMG	A	614	-	48,48,55	1.04	4 (8%)	56,56,63	1.41	6 (10%)
31	SQD	f	101	-	39,41,54	1.12	4 (10%)	49,52,65	1.94	11 (22%)
36	HEC	v	201	17	46,50,50	1.90	5 (10%)	58,82,82	1.95	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	501	-	1/1/20/20	3/39/115/115	-
24	CLA	C	509	-	1/1/20/20	16/39/115/115	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
33	STE	a	616	-	-	3/9/9/17	-
24	CLA	B	613	-	1/1/20/20	14/39/115/115	-
29	LMG	a	618	-	-	30/50/70/70	0/1/1/1
24	CLA	C	504	37	1/1/18/20	7/32/108/115	-
29	LMG	c	522	-	-	20/44/64/70	0/1/1/1
25	PHO	A	606	-	-	1/37/103/103	0/5/6/6
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
33	STE	B	624	-	-	3/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	404	-	1/1/20/20	11/39/115/115	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
31	SQD	a	614	-	-	18/37/37/69	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	STE	b	625	-	-	12/17/17/17	-
24	CLA	b	615	-	1/1/20/20	8/39/115/115	-
26	BCR	A	609	-	-	8/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/20/20	12/39/115/115	-
24	CLA	b	612	-	1/1/20/20	6/39/115/115	-
33	STE	B	625	-	-	5/9/9/17	-
33	STE	a	617	-	-	8/12/12/17	-
30	LHG	d	408	-	-	18/53/53/53	-
24	CLA	C	502	-	-	5/39/115/115	-
24	CLA	b	605	-	1/1/20/20	7/39/115/115	-
24	CLA	B	603	-	1/1/20/20	7/39/115/115	-
33	STE	b	627	-	-	6/11/11/17	-
24	CLA	b	608	-	-	1/39/115/115	-
31	SQD	b	620	-	-	20/44/64/69	0/1/1/1
24	CLA	b	607	37	1/1/20/20	12/39/115/115	-
33	STE	c	520	-	-	10/17/17/17	-
25	PHO	d	402	-	-	1/37/103/103	0/5/6/6
33	STE	b	626	-	-	5/7/7/17	-
24	CLA	b	602	-	-	4/39/115/115	-
24	CLA	B	610	37	1/1/20/20	5/39/115/115	-
24	CLA	c	508	-	-	7/38/114/115	-
25	PHO	A	607	-	-	1/37/103/103	0/5/6/6
32	DGD	h	101	-	-	15/51/91/95	0/2/2/2
24	CLA	c	503	-	1/1/20/20	6/39/115/115	-
30	LHG	B	621	-	-	25/53/53/53	-
24	CLA	B	614	-	1/1/20/20	15/39/115/115	-
24	CLA	B	604	-	1/1/20/20	8/39/115/115	-
24	CLA	c	502	-	-	3/39/115/115	-
24	CLA	b	613	-	1/1/20/20	7/39/115/115	-
33	STE	T	102	-	-	8/13/13/17	-
29	LMG	D	409	-	-	16/33/33/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	D	410	-	-	14/22/22/70	-
24	CLA	A	613	37	-	4/39/115/115	-
24	CLA	B	605	-	1/1/20/20	9/39/115/115	-
33	STE	C	522	-	-	3/9/9/17	-
31	SQD	A	617	-	-	13/39/39/69	-
24	CLA	b	609	-	-	9/39/115/115	-
24	CLA	C	505	-	1/1/20/20	7/39/115/115	-
30	LHG	D	408	-	-	23/53/53/53	-
30	LHG	E	101	-	-	22/53/53/53	-
31	SQD	D	407	-	-	14/28/48/69	0/1/1/1
24	CLA	c	512	-	1/1/20/20	20/39/115/115	-
24	CLA	B	601	37	1/1/20/20	15/39/115/115	-
33	STE	b	624	-	-	10/13/13/17	-
33	STE	t	102	-	-	9/15/15/17	-
24	CLA	d	403	-	1/1/20/20	5/39/115/115	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
29	LMG	b	623	-	-	25/50/70/70	0/1/1/1
24	CLA	b	610	37	1/1/20/20	4/39/115/115	-
24	CLA	c	501	-	1/1/20/20	1/39/115/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/20/20	9/39/115/115	-
24	CLA	B	611	-	1/1/20/20	6/39/115/115	-
28	PL9	a	611	-	-	22/53/73/73	0/1/1/1
26	BCR	C	514	-	-	8/29/63/63	0/2/2/2
26	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	CLA	C	507	37	1/1/20/20	11/39/115/115	-
29	LMG	d	410	-	-	11/39/59/70	0/1/1/1
29	LMG	M	101	-	-	24/46/66/70	0/1/1/1
33	STE	l	102	-	-	9/15/15/17	-
24	CLA	A	605	37	1/1/20/20	11/39/115/115	-
33	STE	k	103	-	-	4/9/9/17	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
33	STE	d	411	-	-	8/14/14/17	-
29	LMG	b	621	-	-	24/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	a	615	-	-	4/7/7/17	-
36	HEC	V	201	17	-	6/14/54/54	-
31	SQD	A	616	-	-	15/47/67/69	0/1/1/1
33	STE	m	101	-	-	3/9/9/17	-
32	DGD	A	618	-	-	27/55/95/95	0/2/2/2
24	CLA	B	607	37	1/1/20/20	4/39/115/115	-
24	CLA	c	509	-	1/1/20/20	11/39/115/115	-
31	SQD	a	613	-	-	22/49/69/69	0/1/1/1
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
26	BCR	a	607	-	-	1/29/63/63	0/2/2/2
33	STE	b	622	-	-	10/17/17/17	-
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2
35	HEM	F	101	5,6	-	2/14/54/54	-
26	BCR	k	101	-	-	12/29/63/63	0/2/2/2
24	CLA	a	606	-	1/1/20/20	8/39/115/115	-
30	LHG	l	101	-	-	15/53/53/53	-
28	PL9	D	405	-	-	10/53/73/73	0/1/1/1
32	DGD	c	518	-	-	12/51/91/95	0/2/2/2
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
24	CLA	c	504	37	1/1/19/20	7/33/109/115	-
29	LMG	C	519	-	-	17/43/63/70	0/1/1/1
32	DGD	C	517	-	-	23/51/91/95	0/2/2/2
33	STE	T	103	-	-	11/12/12/17	-
30	LHG	d	407	-	-	21/53/53/53	-
28	PL9	d	406	-	-	11/53/73/73	0/1/1/1
24	CLA	b	611	-	1/1/20/20	5/39/115/115	-
31	SQD	B	623	-	-	22/49/69/69	0/1/1/1
24	CLA	b	614	-	1/1/20/20	12/39/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
28	PL9	A	612	-	-	24/53/73/73	0/1/1/1
24	CLA	B	616	-	1/1/19/20	8/33/109/115	-
24	CLA	c	507	37	1/1/20/20	10/39/115/115	-
24	CLA	c	513	-	1/1/20/20	6/39/115/115	-
26	BCR	b	617	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	606	-	1/1/20/20	11/39/115/115	-
24	CLA	B	608	-	-	2/39/115/115	-
24	CLA	B	602	-	1/1/20/20	6/39/115/115	-
33	STE	B	620	-	-	5/14/14/17	-
24	CLA	C	512	-	1/1/20/20	12/39/115/115	-
30	LHG	d	409	-	-	14/43/43/53	-
33	STE	x	102	-	-	6/17/17/17	-
33	STE	I	101	-	-	4/12/12/17	-
29	LMG	c	519	-	-	11/31/51/70	0/1/1/1
24	CLA	D	402	-	1/1/20/20	5/39/115/115	-
24	CLA	C	506	-	1/1/20/20	9/39/115/115	-
32	DGD	c	517	-	-	18/51/91/95	0/2/2/2
24	CLA	d	401	37	-	12/39/115/115	-
33	STE	D	411	-	-	11/17/17/17	-
26	BCR	c	515	-	-	3/29/63/63	0/2/2/2
24	CLA	a	604	-	1/1/20/20	4/39/115/115	-
33	STE	B	627	-	-	5/9/9/17	-
24	CLA	C	513	-	1/1/20/20	5/39/115/115	-
33	STE	M	103	-	-	1/7/7/17	-
29	LMG	D	406	-	-	14/46/66/70	0/1/1/1
24	CLA	A	604	-	1/1/20/20	4/39/115/115	-
33	STE	E	102	-	-	4/9/9/17	-
24	CLA	C	511	3	1/1/20/20	3/39/115/115	-
26	BCR	B	619	-	-	5/29/63/63	0/2/2/2
30	LHG	A	615	-	-	20/51/51/53	-
33	STE	Z	101	-	-	2/5/5/17	-
24	CLA	C	510	-	1/1/20/20	9/39/115/115	-
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	CLA	A	608	-	1/1/17/20	2/26/102/115	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
25	PHO	a	605	-	-	1/37/103/103	0/5/6/6
32	DGD	C	518	-	-	18/51/91/95	0/2/2/2
33	STE	J	101	-	-	7/9/9/17	-
24	CLA	B	609	-	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	618	-	-	4/29/63/63	0/2/2/2
30	LHG	B	622	-	-	14/53/53/53	-
33	STE	C	520	-	-	6/9/9/17	-
35	HEM	e	101	5,6	-	3/14/54/54	-
24	CLA	a	612	37	1/1/20/20	4/39/115/115	-
24	CLA	b	616	-	1/1/19/20	10/33/109/115	-
24	CLA	D	403	-	-	9/39/115/115	-
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
30	LHG	e	102	-	-	26/46/46/53	-
24	CLA	c	510	-	1/1/20/20	7/39/115/115	-
24	CLA	C	503	-	1/1/20/20	2/39/115/115	-
24	CLA	c	506	-	1/1/20/20	13/39/115/115	-
24	CLA	b	603	-	1/1/20/20	8/39/115/115	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CLA	b	601	37	1/1/20/20	16/39/115/115	-
24	CLA	c	505	-	1/1/20/20	11/39/115/115	-
33	STE	j	101	-	-	4/9/9/17	-
33	STE	H	103	-	-	9/15/15/17	-
33	STE	B	626	-	-	8/13/13/17	-
33	STE	d	412	-	-	11/17/17/17	-
33	STE	M	102	-	-	5/12/12/17	-
24	CLA	B	612	-	1/1/20/20	8/39/115/115	-
24	CLA	b	604	-	1/1/20/20	7/39/115/115	-
32	DGD	C	516	-	-	19/51/91/95	0/2/2/2
24	CLA	C	508	-	-	7/39/115/115	-
24	CLA	c	511	3	1/1/20/20	11/39/115/115	-
26	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	STE	C	521	-	-	7/13/13/17	-
29	LMG	A	614	-	-	21/43/63/70	0/1/1/1
31	SQD	f	101	-	-	13/36/56/69	0/1/1/1
36	HEC	v	201	17	-	6/14/54/54	-

The worst 5 of 900 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	MG-NA	9.48	2.28	2.06
25	d	402	PHO	C1B-C2B	9.37	1.49	1.39
25	A	607	PHO	C3B-C4B	9.23	1.50	1.41
25	d	402	PHO	C3B-C4B	9.22	1.50	1.41
24	a	606	CLA	MG-ND	-8.26	1.89	2.05

The worst 5 of 1203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4A-NA-C1A	9.98	111.23	106.68
24	b	615	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	a	613	SQD	O6-C1-C2	9.24	122.30	108.27
24	B	611	CLA	C4A-NA-C1A	9.16	110.86	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.93	109.58	127.43

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	608	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

5 of 1751 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	C4-C3-C5-C6
24	B	606	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

105 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	501	CLA	1	0
24	C	509	CLA	1	0
24	B	613	CLA	3	0
29	a	618	LMG	5	0
24	C	504	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	522	LMG	1	0
21	a	601[B]	OEY	1	0
33	B	624	STE	1	0
29	c	521	LMG	2	0
26	B	618	BCR	3	0
33	b	625	STE	2	0
24	b	615	CLA	3	0
24	B	615	CLA	1	0
33	B	625	STE	1	0
33	a	617	STE	1	0
24	b	605	CLA	3	0
31	b	620	SQD	1	0
24	b	607	CLA	1	0
33	c	520	STE	1	0
25	d	402	PHO	1	0
24	b	602	CLA	1	0
24	B	610	CLA	2	0
24	c	508	CLA	4	0
25	A	607	PHO	1	0
24	c	503	CLA	1	0
30	B	621	LHG	1	0
24	B	614	CLA	3	0
24	B	604	CLA	1	0
24	b	613	CLA	1	0
29	D	409	LMG	1	0
24	A	613	CLA	4	0
31	A	617	SQD	1	0
24	b	609	CLA	1	0
30	D	408	LHG	3	0
30	E	101	LHG	1	0
31	D	407	SQD	1	0
24	c	512	CLA	1	0
24	B	601	CLA	3	0
33	t	102	STE	2	0
24	d	403	CLA	1	0
26	T	101	BCR	1	0
29	b	623	LMG	1	0
24	c	501	CLA	2	0
26	Y	101	BCR	1	0
24	b	606	CLA	1	0
24	B	611	CLA	1	0
28	a	611	PL9	2	0

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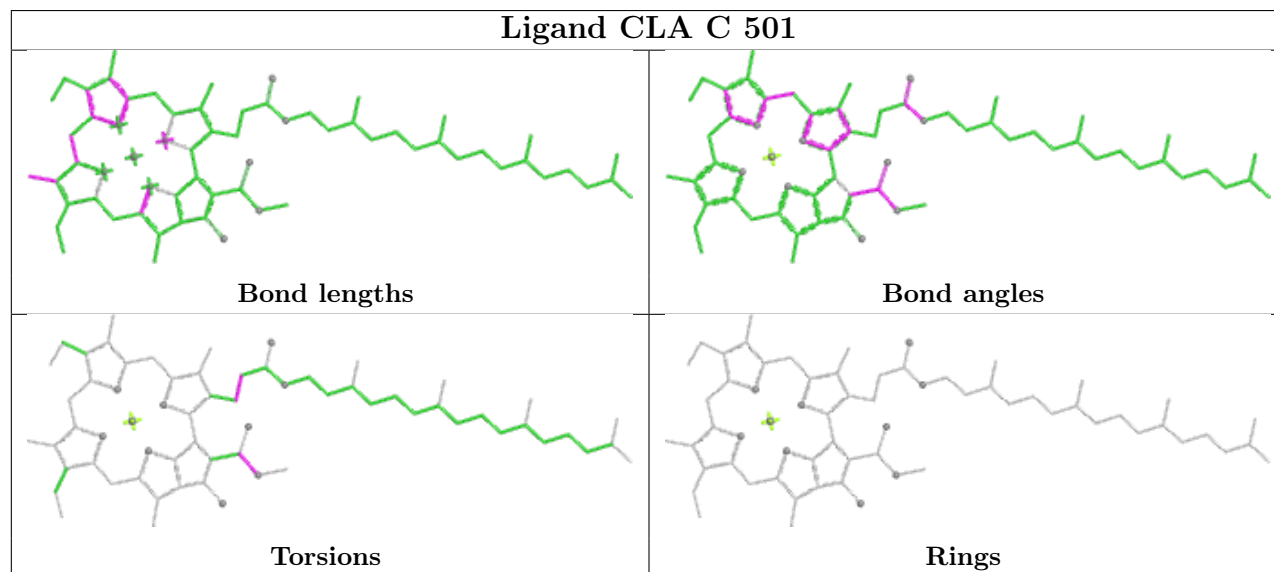
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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29	M	101	LMG	1	0
33	l	102	STE	1	0
33	d	411	STE	1	0
36	V	201	HEC	1	0
31	A	616	SQD	1	0
33	m	101	STE	1	0
32	A	618	DGD	3	0
24	B	607	CLA	1	0
24	c	509	CLA	1	0
26	a	607	BCR	1	0
33	b	622	STE	2	0
26	H	101	BCR	1	0
35	F	101	HEM	2	0
30	l	101	LHG	1	0
24	c	504	CLA	3	0
33	T	103	STE	1	0
30	d	407	LHG	4	0
31	B	623	SQD	2	0
24	b	614	CLA	1	0
26	b	619	BCR	1	0
28	A	612	PL9	2	0
24	B	616	CLA	1	0
24	c	507	CLA	1	0
24	c	513	CLA	1	0
24	B	606	CLA	3	0
24	B	602	CLA	1	0
33	B	620	STE	1	0
30	d	409	LHG	1	0
29	c	519	LMG	1	0
32	c	517	DGD	2	0
33	D	411	STE	6	0
26	c	515	BCR	1	0
24	C	513	CLA	2	0
34	D	401	BCT	1	0
29	D	406	LMG	1	0
24	A	604	CLA	1	0
33	E	102	STE	1	0
26	B	619	BCR	1	0
30	A	615	LHG	1	0
26	d	405	BCR	2	0
21	A	601[B]	OEY	1	0

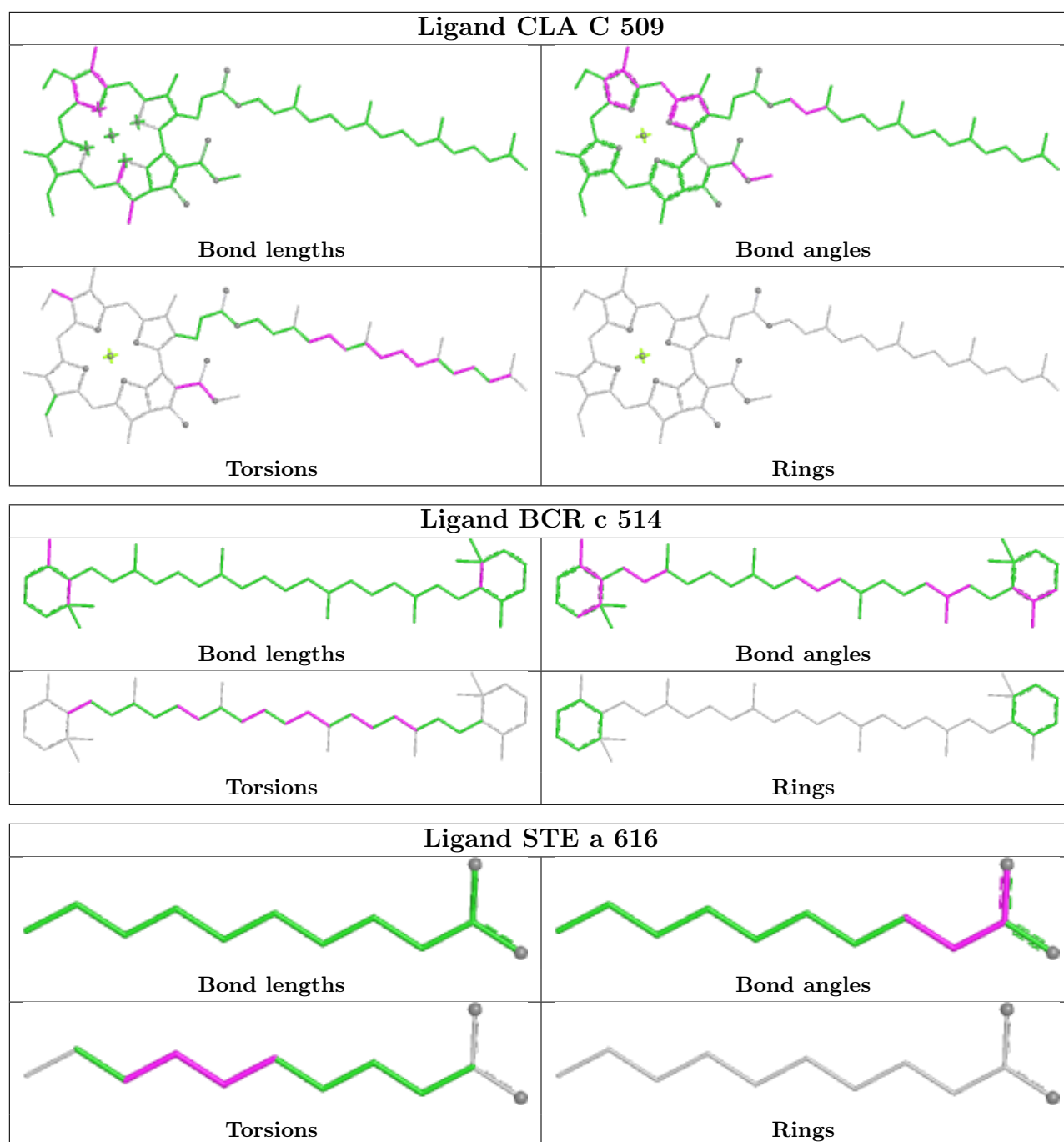
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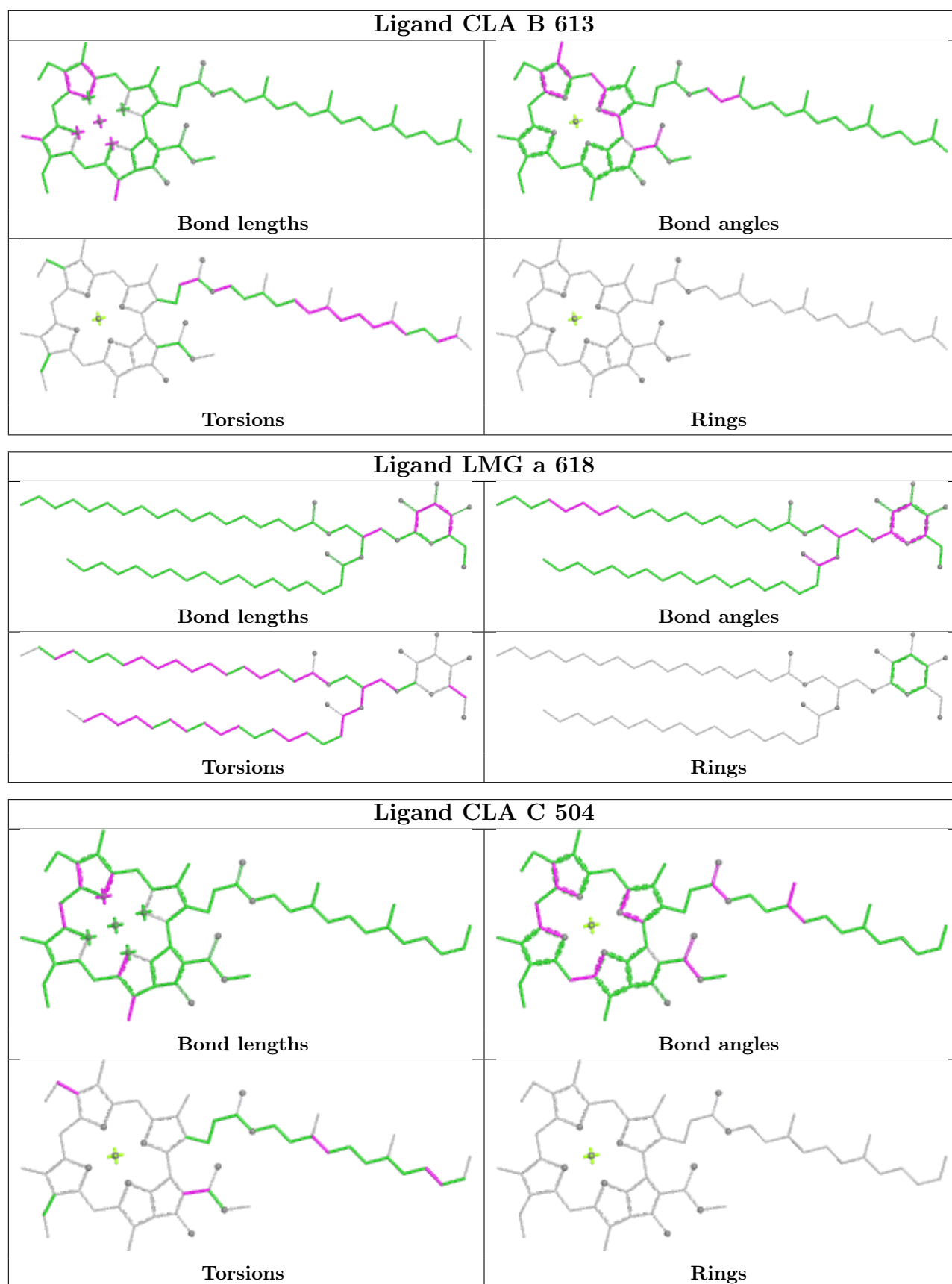
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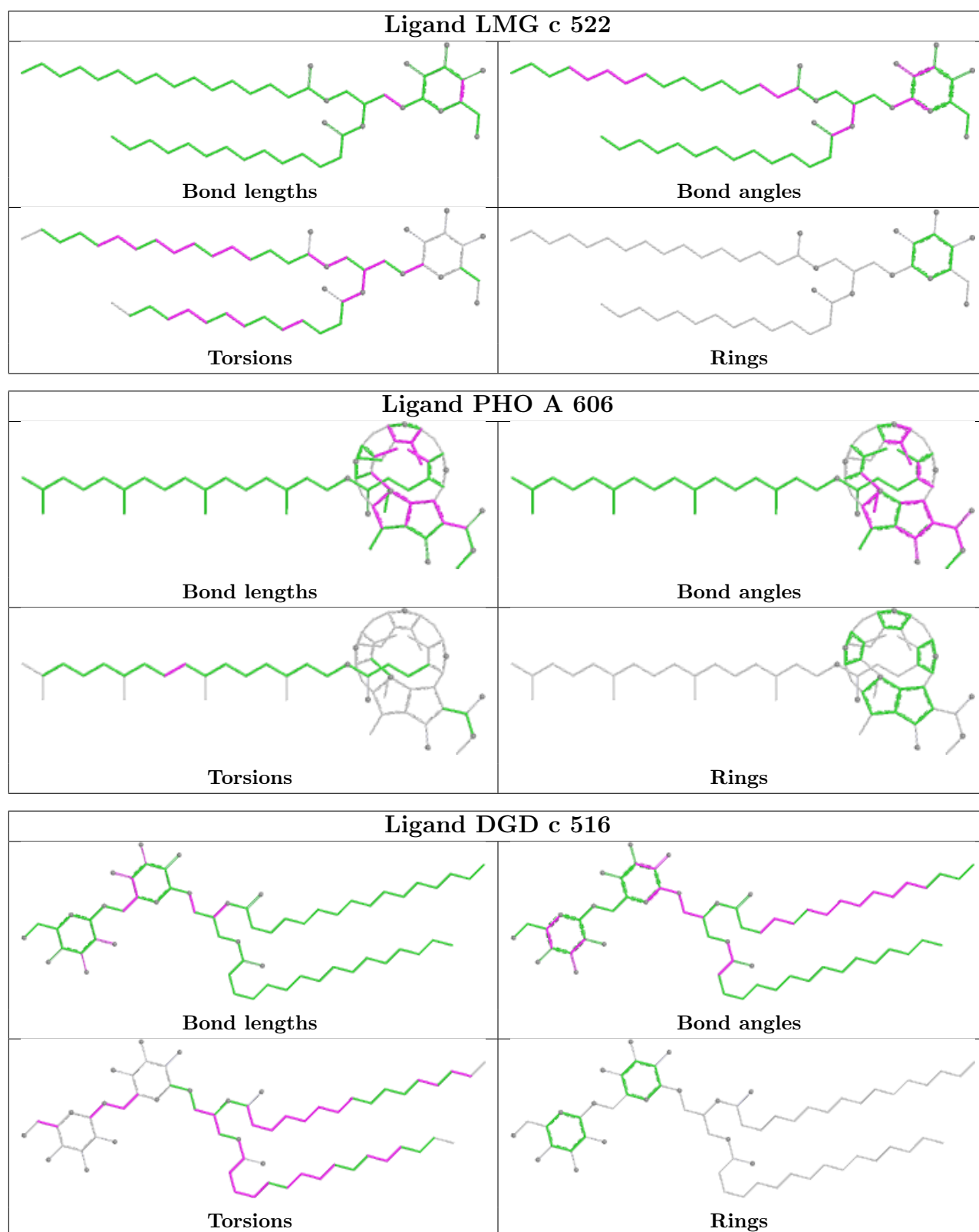
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	618	BCR	1	0
30	B	622	LHG	1	0
35	e	101	HEM	4	0
24	b	616	CLA	1	0
24	D	403	CLA	3	0
24	C	503	CLA	1	0
26	D	404	BCR	1	0
24	b	601	CLA	1	0
33	H	103	STE	1	0
33	M	102	STE	1	0
24	B	612	CLA	1	0
24	b	604	CLA	1	0
24	c	511	CLA	2	0
26	t	101	BCR	3	0
31	f	101	SQD	1	0
36	v	201	HEC	1	0

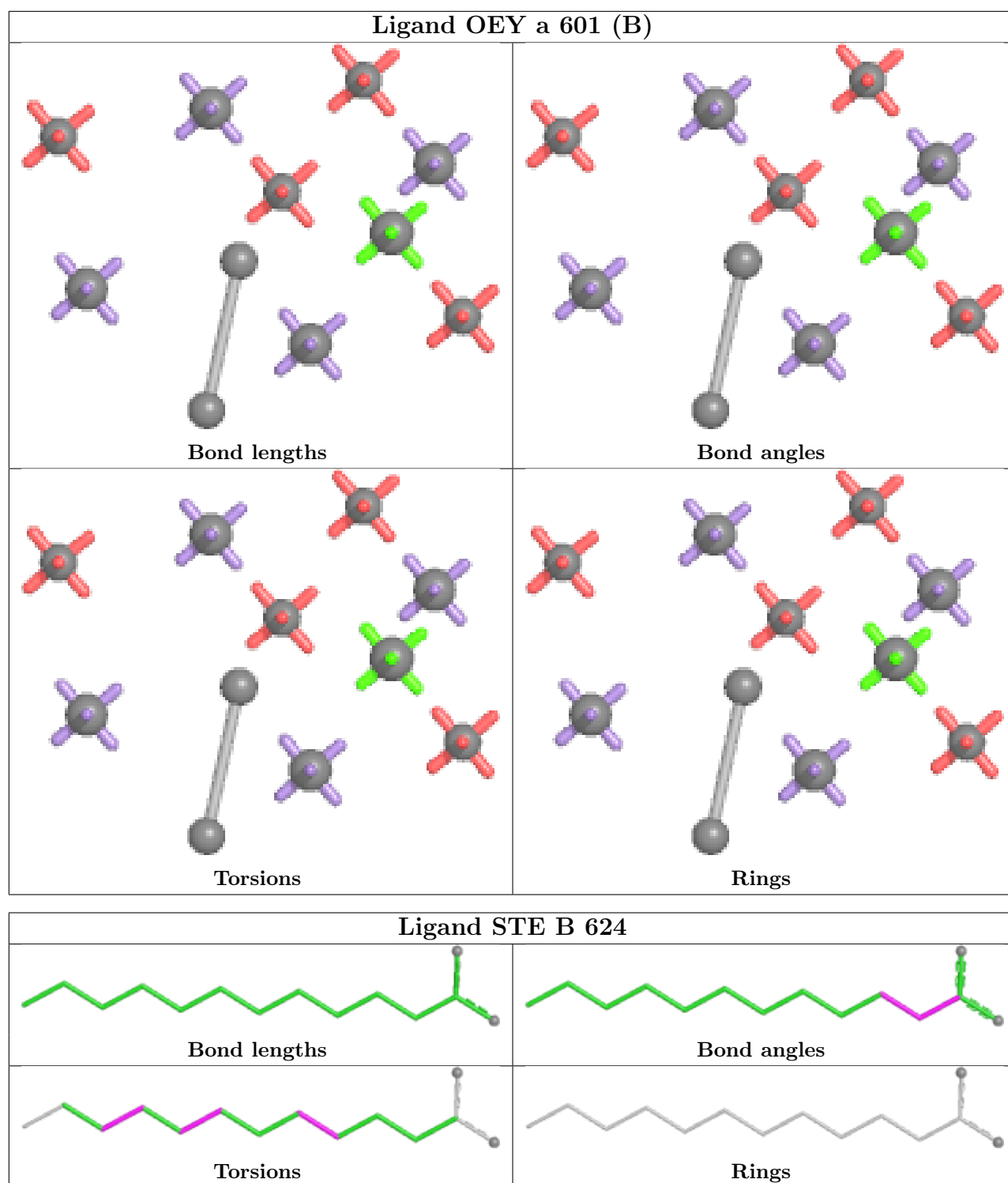
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

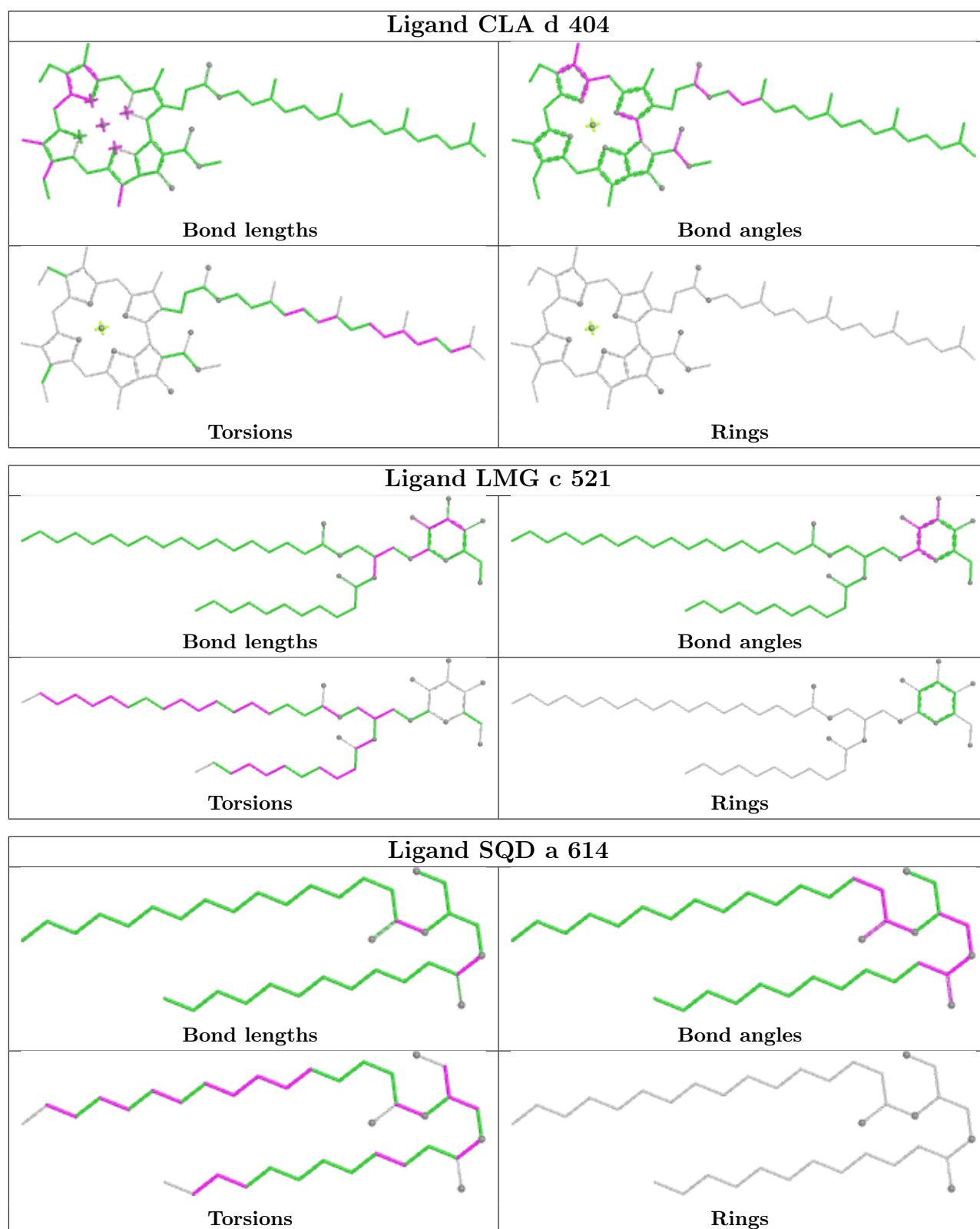


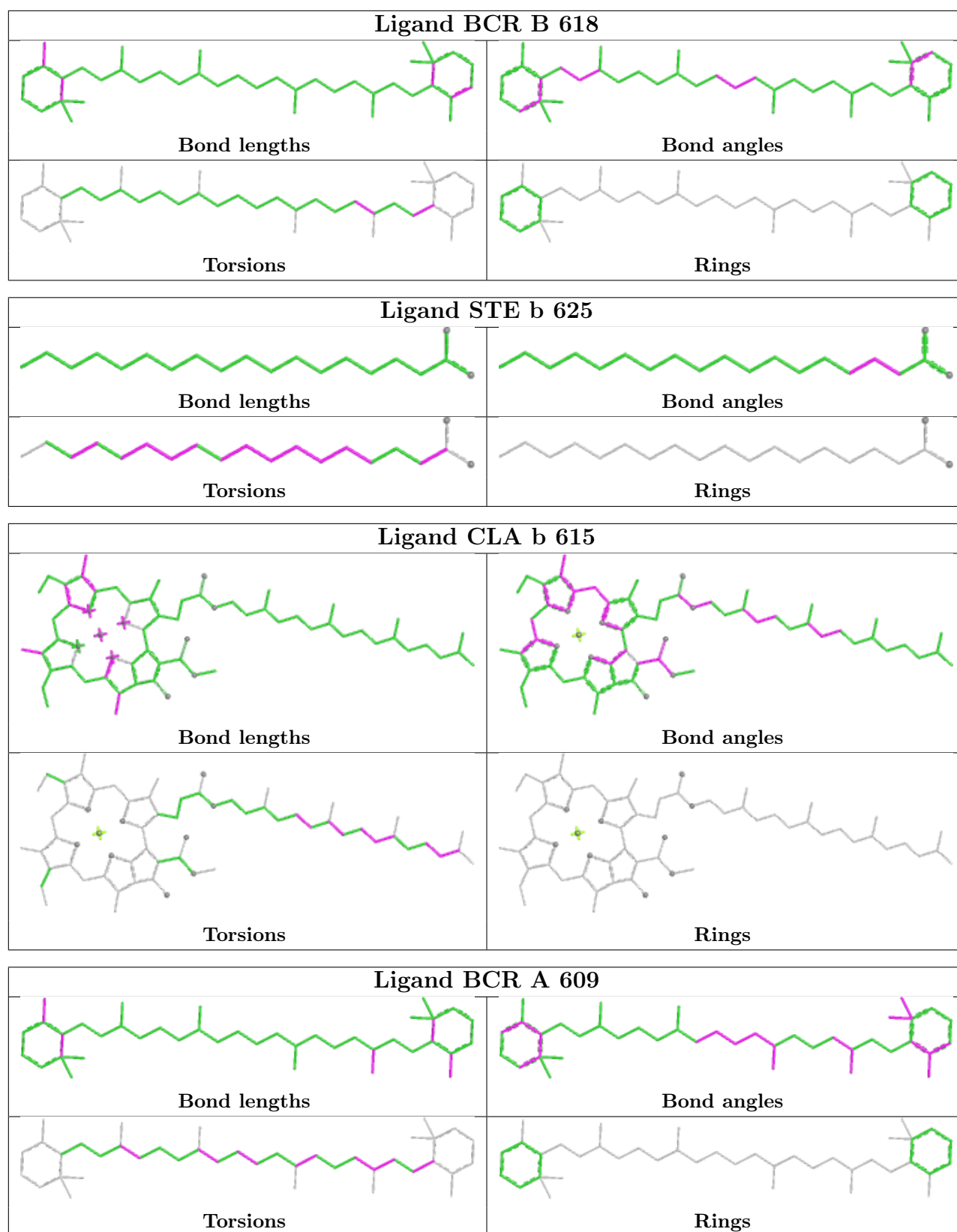


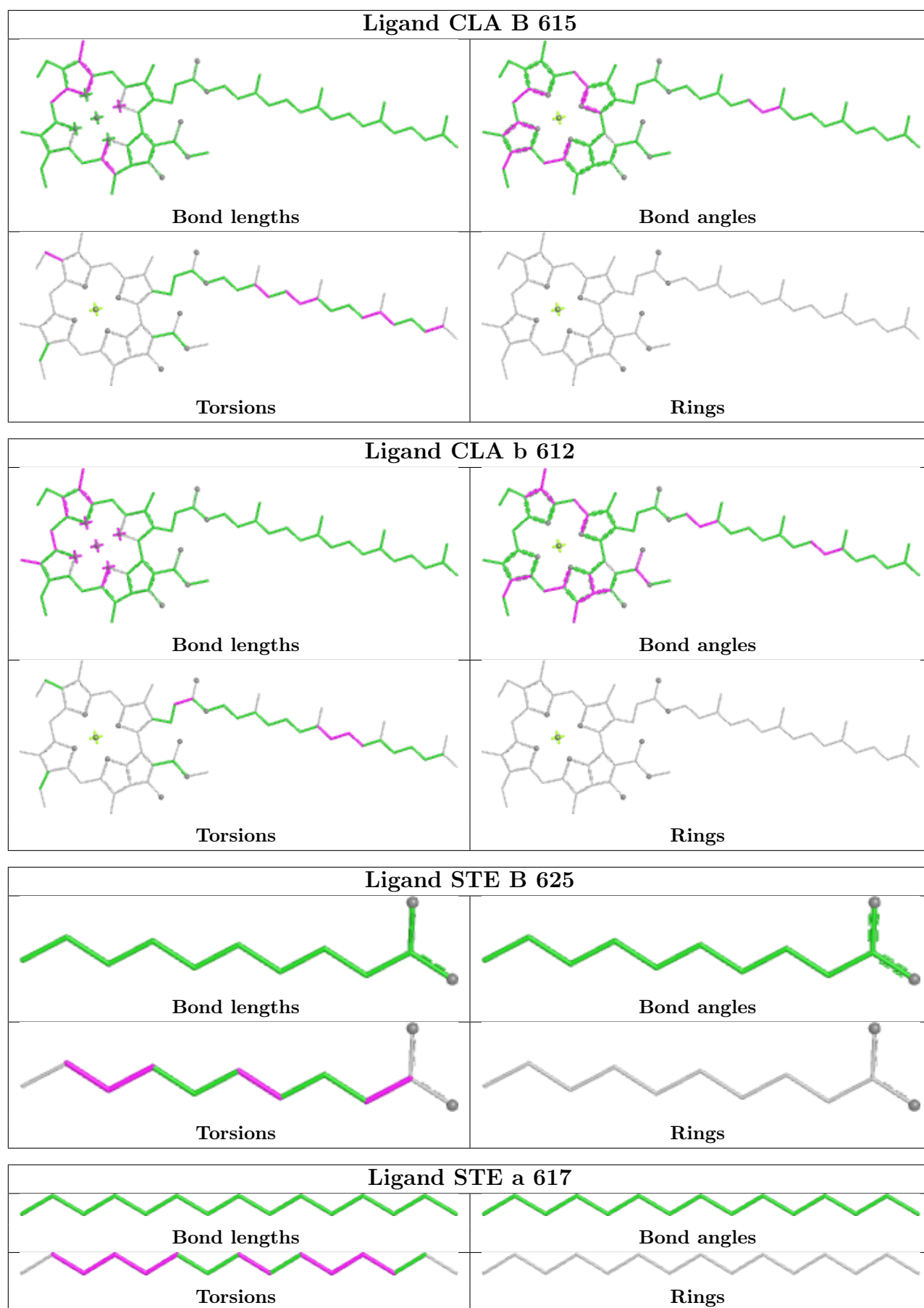


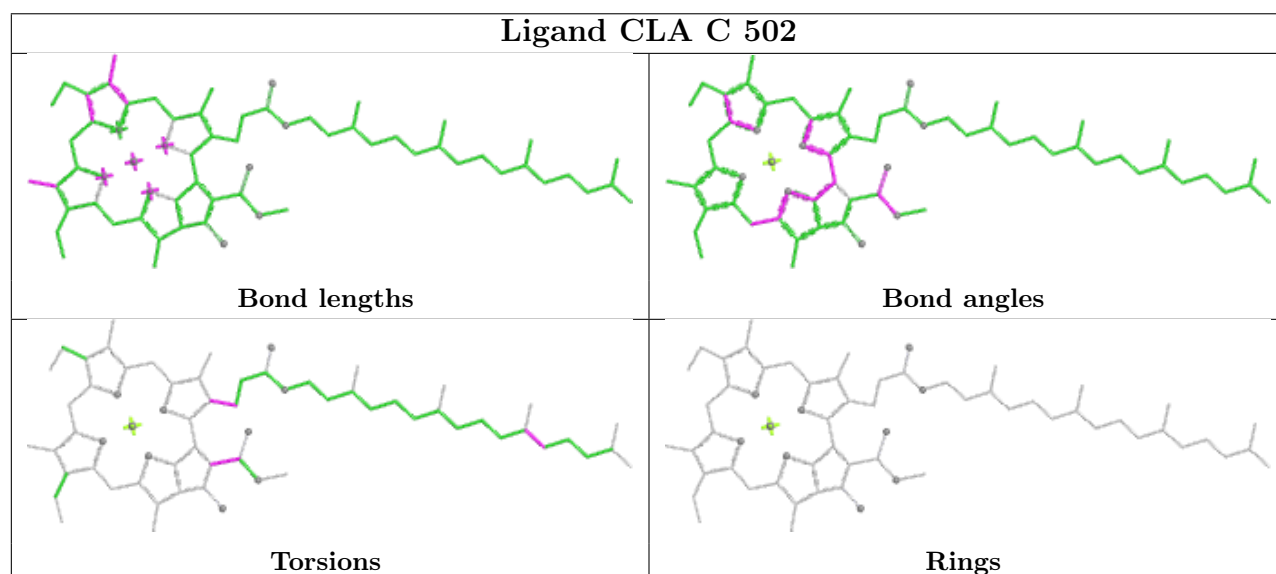
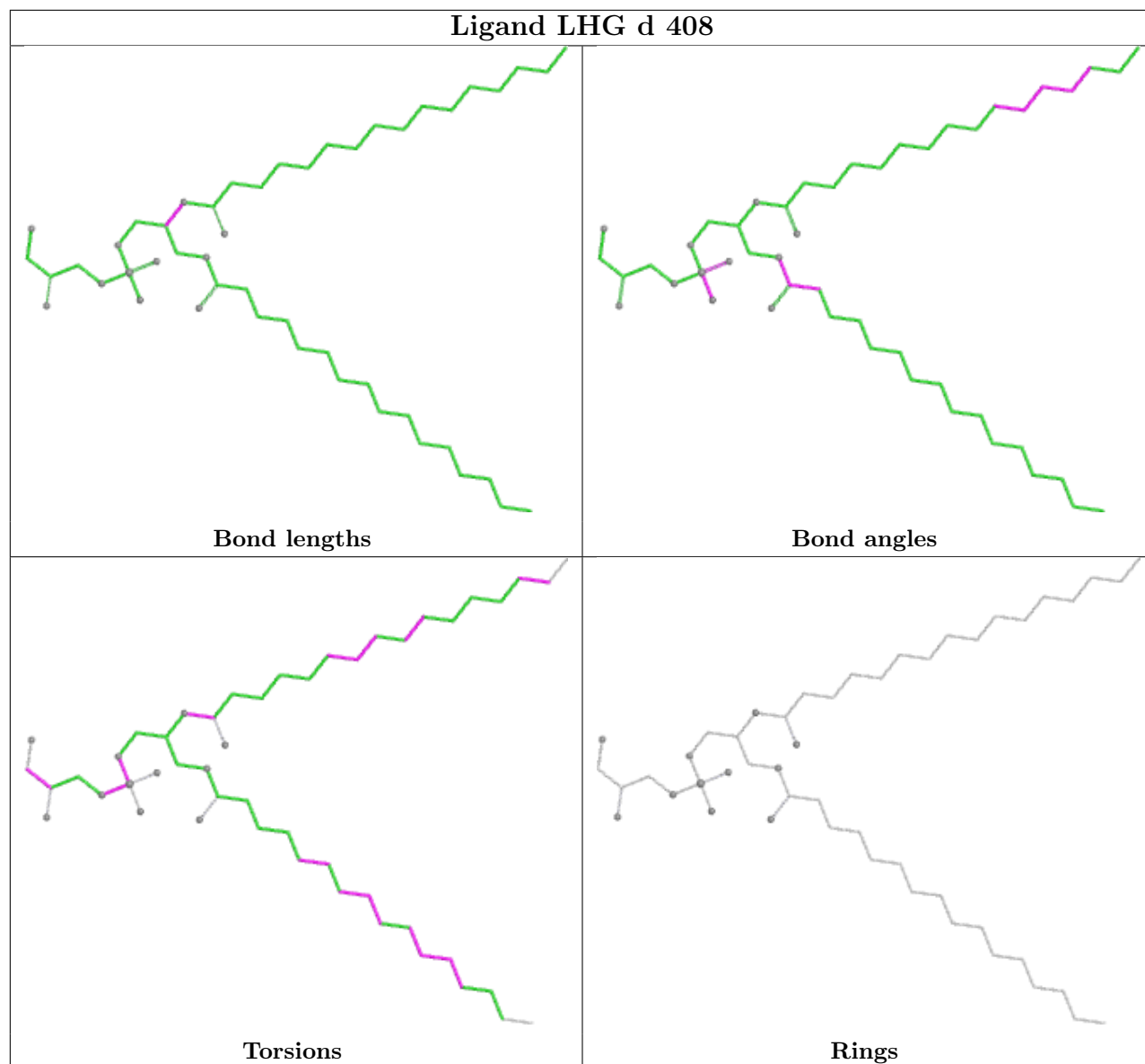


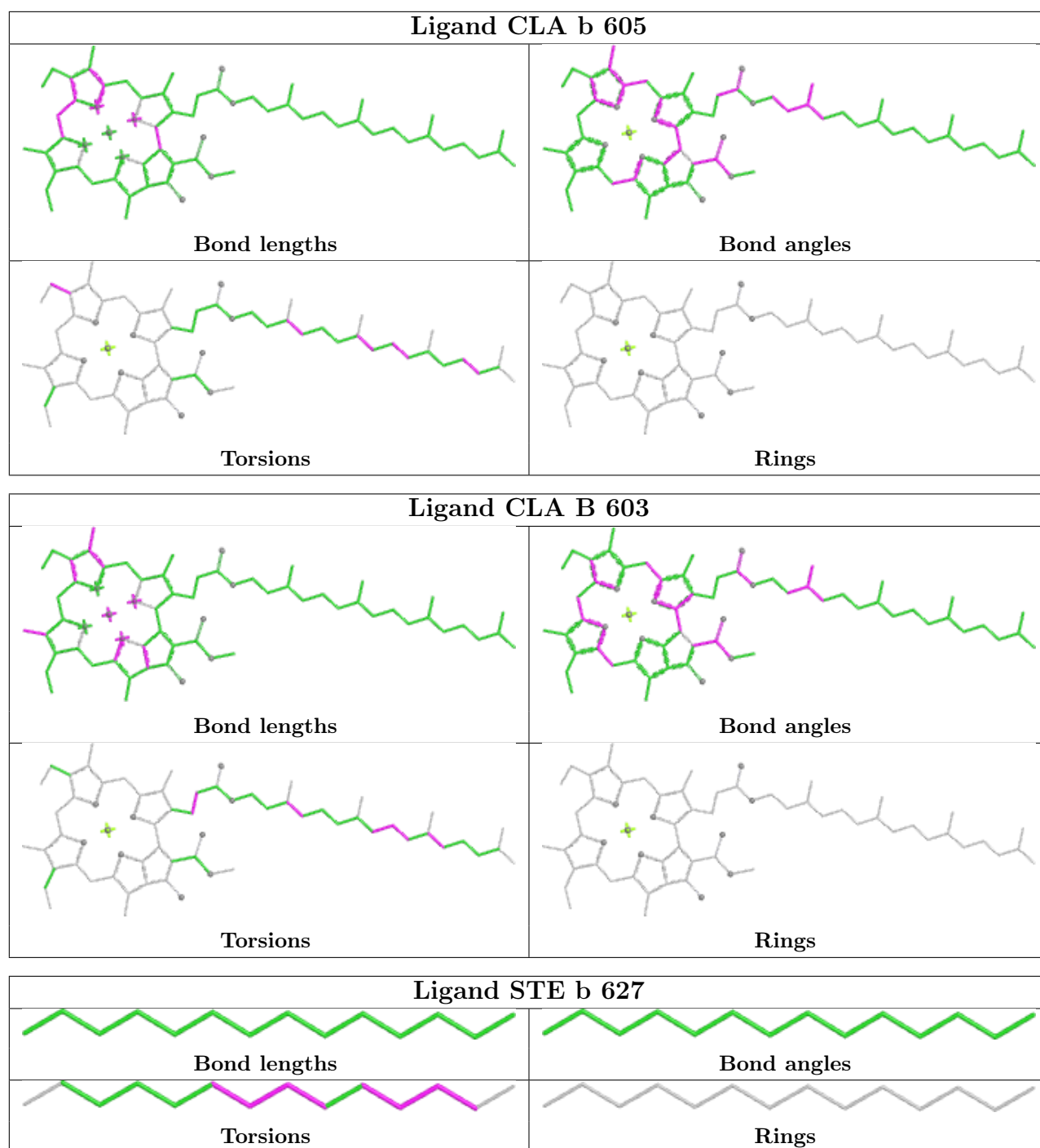


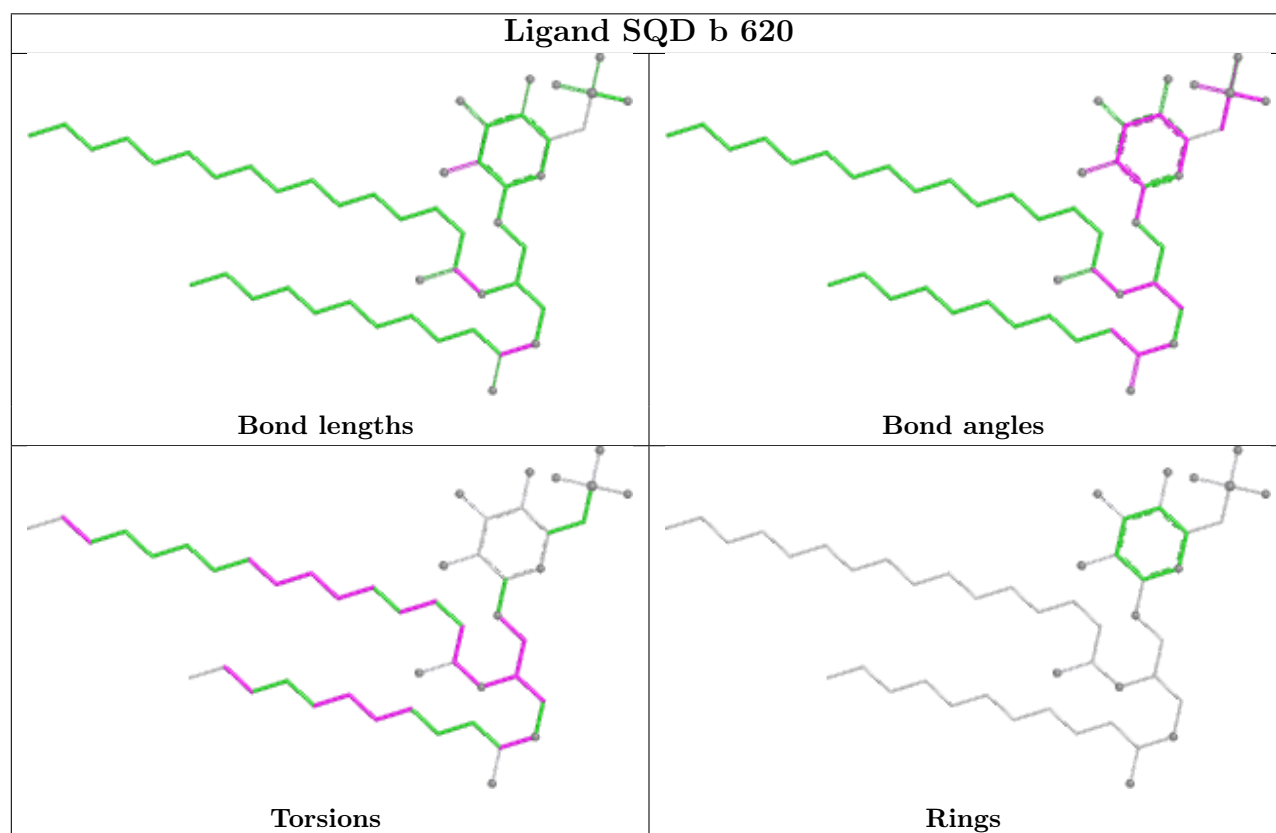
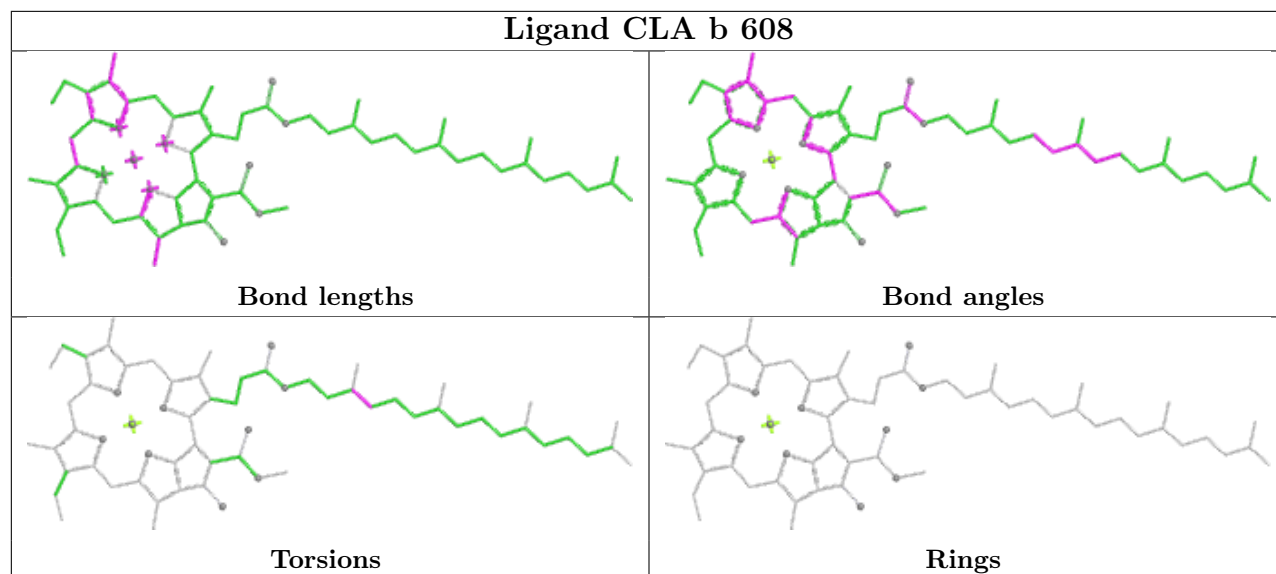


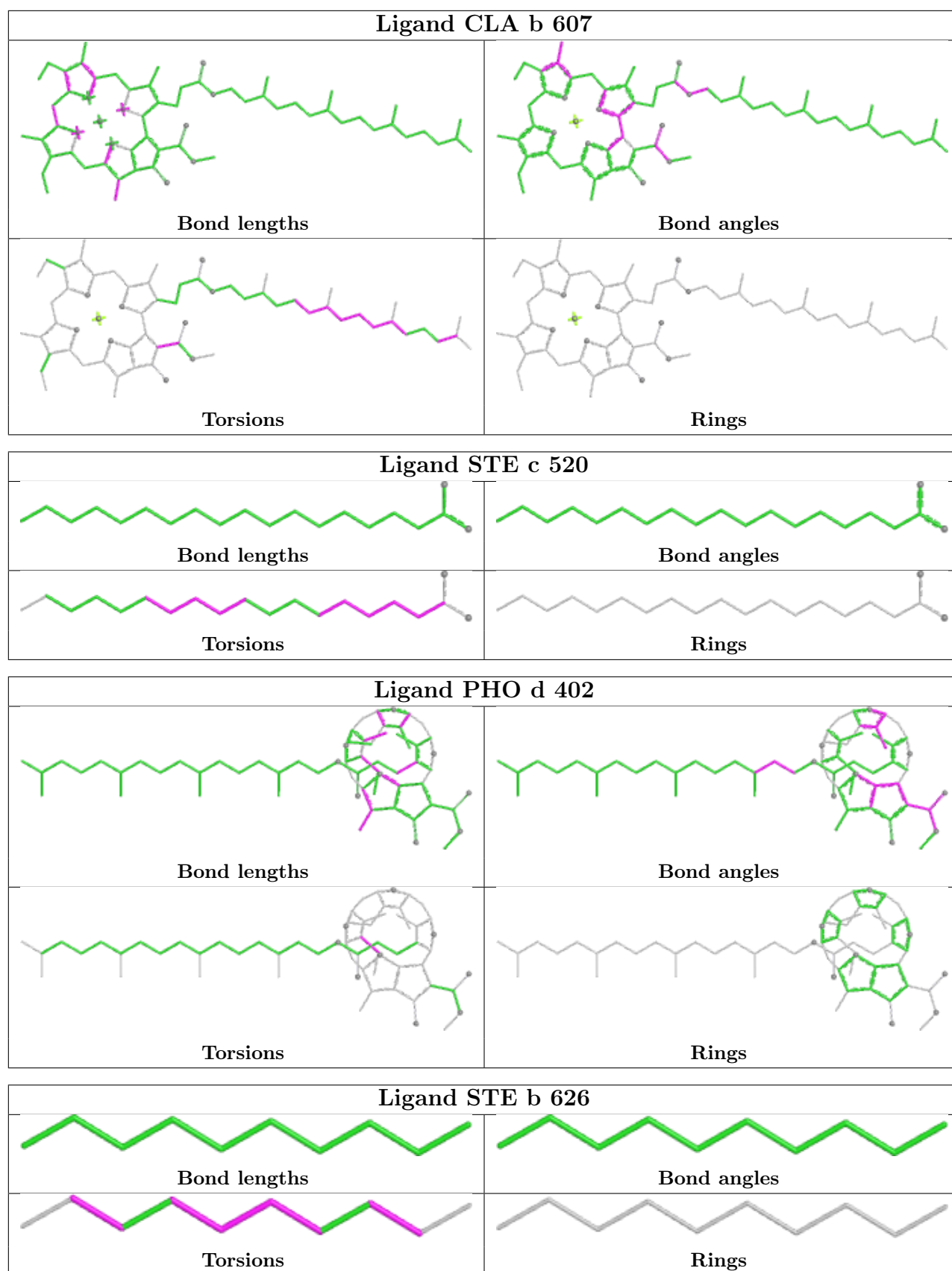


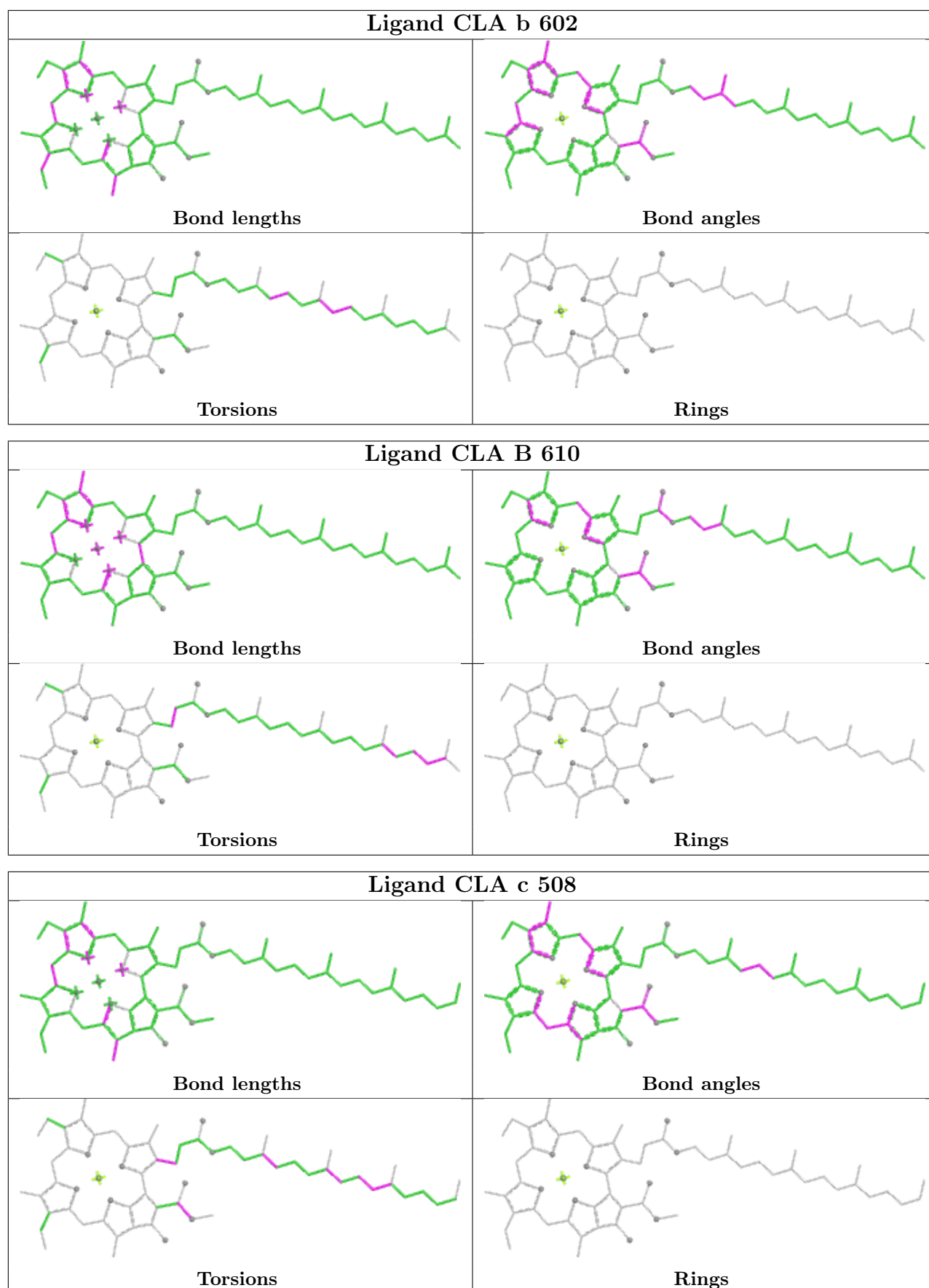


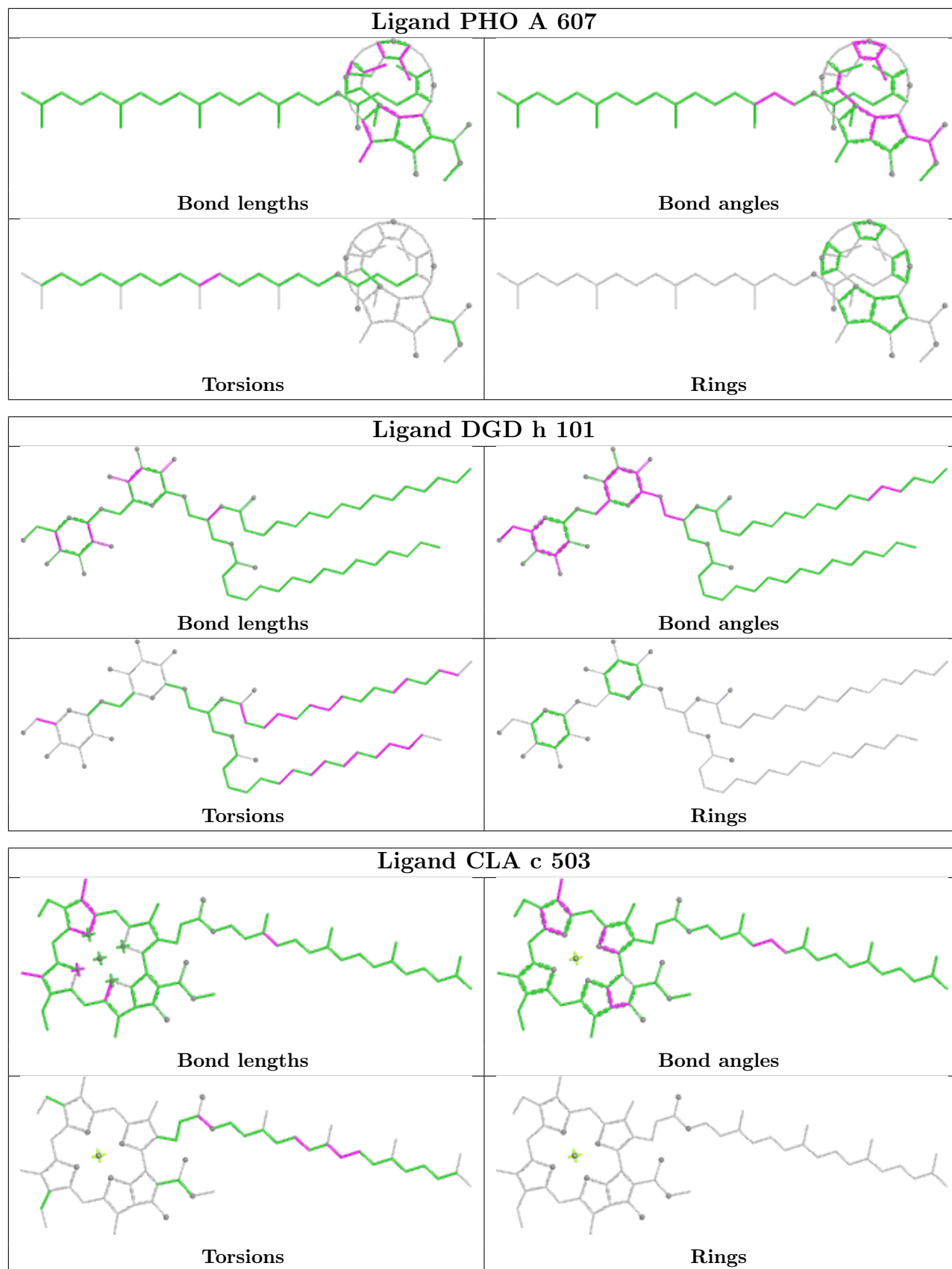


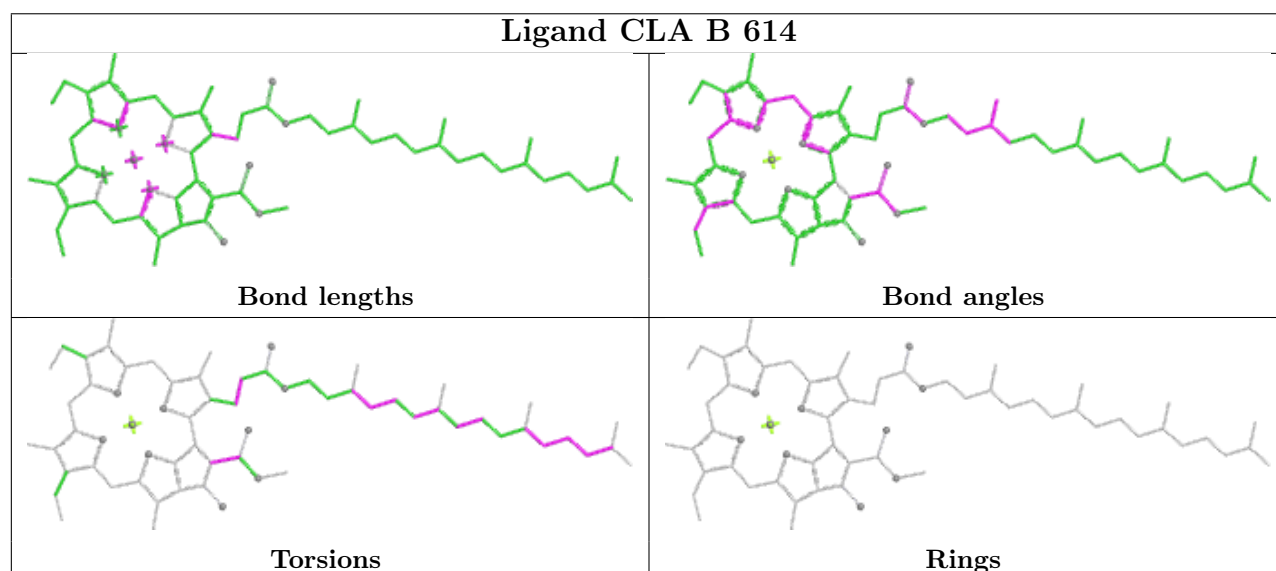
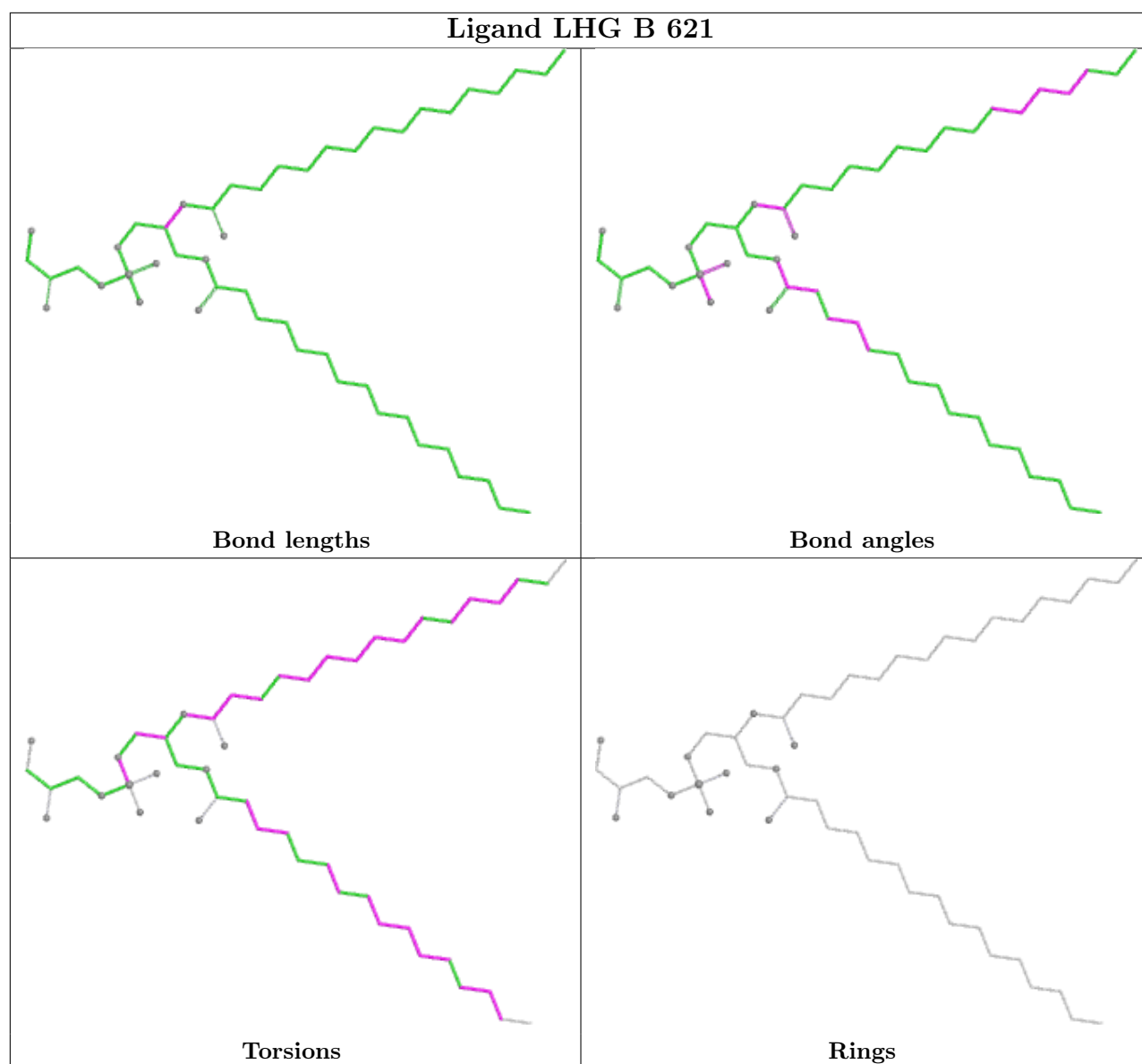


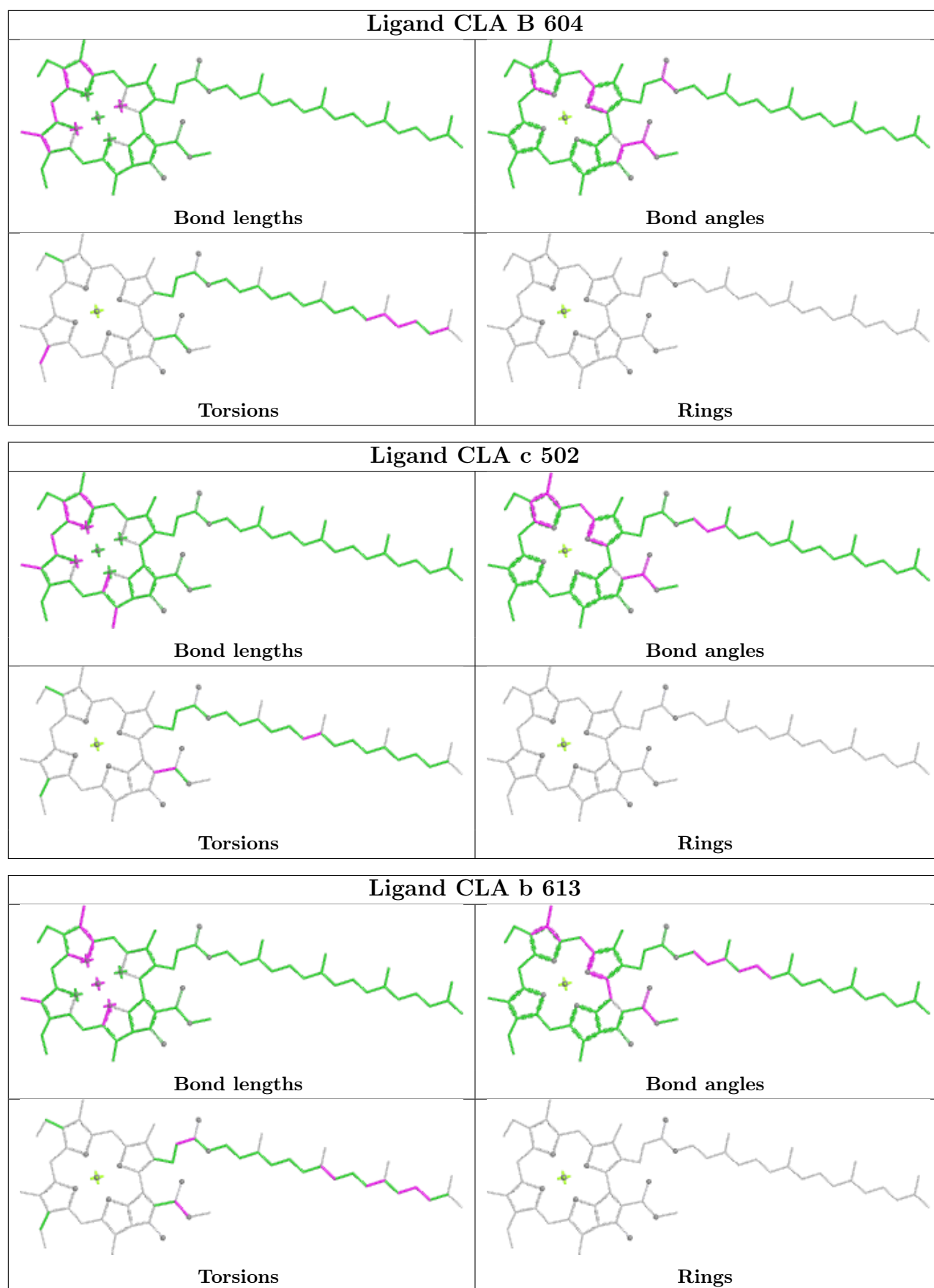


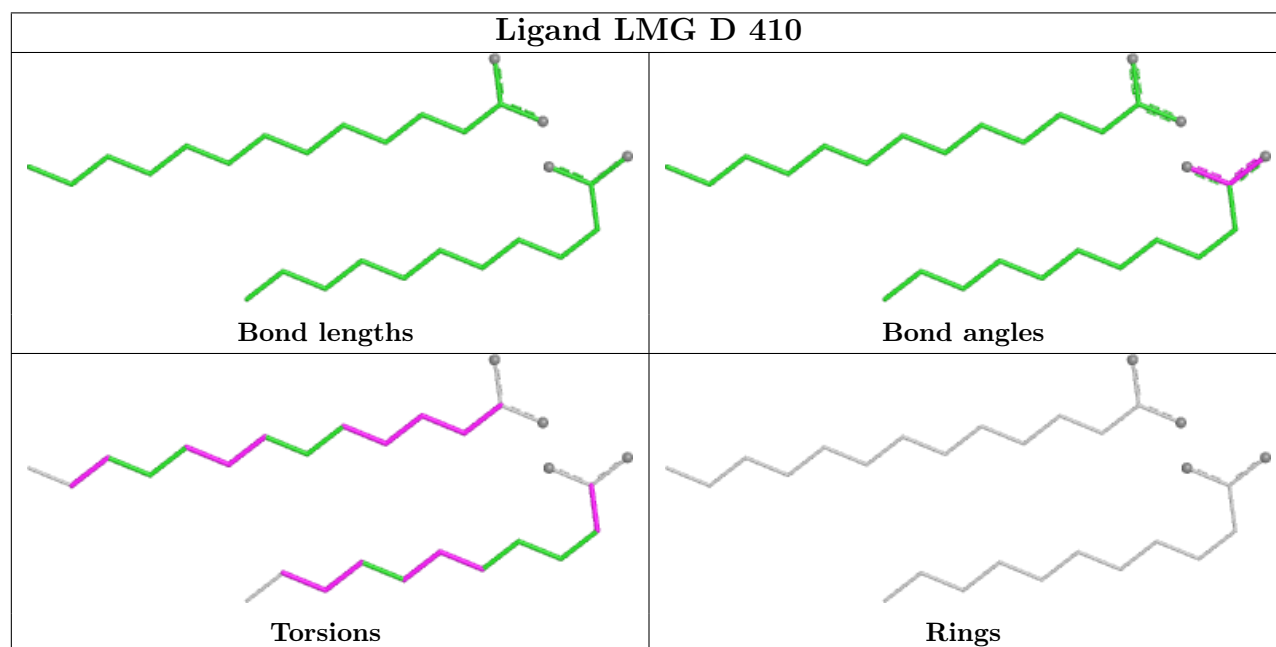
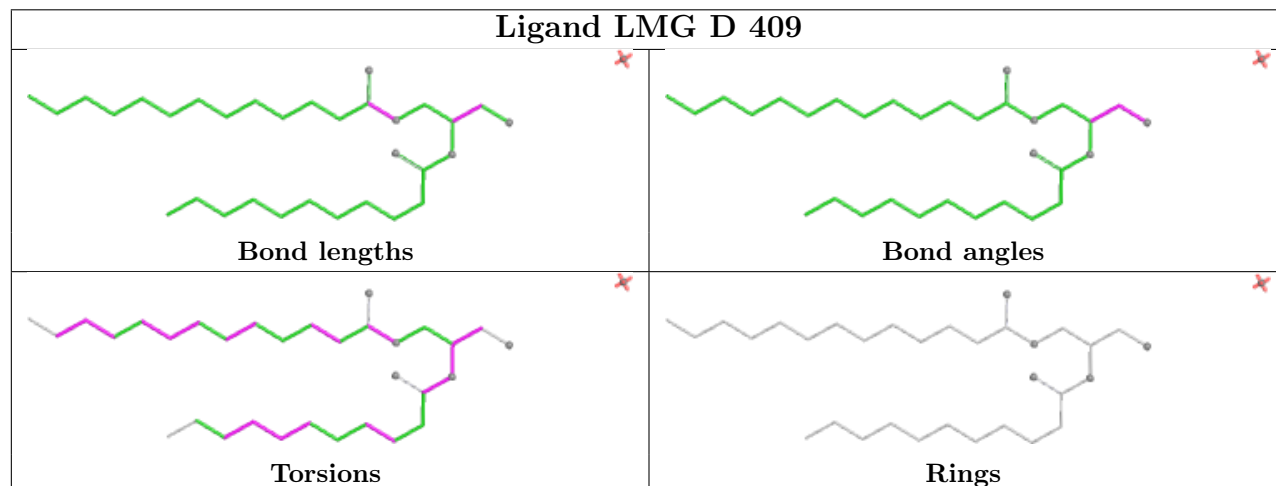
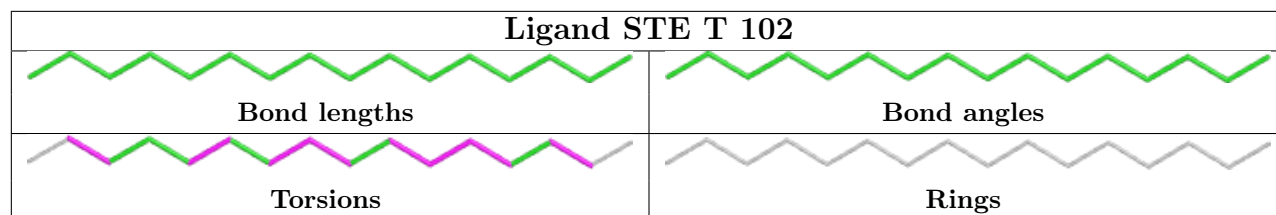


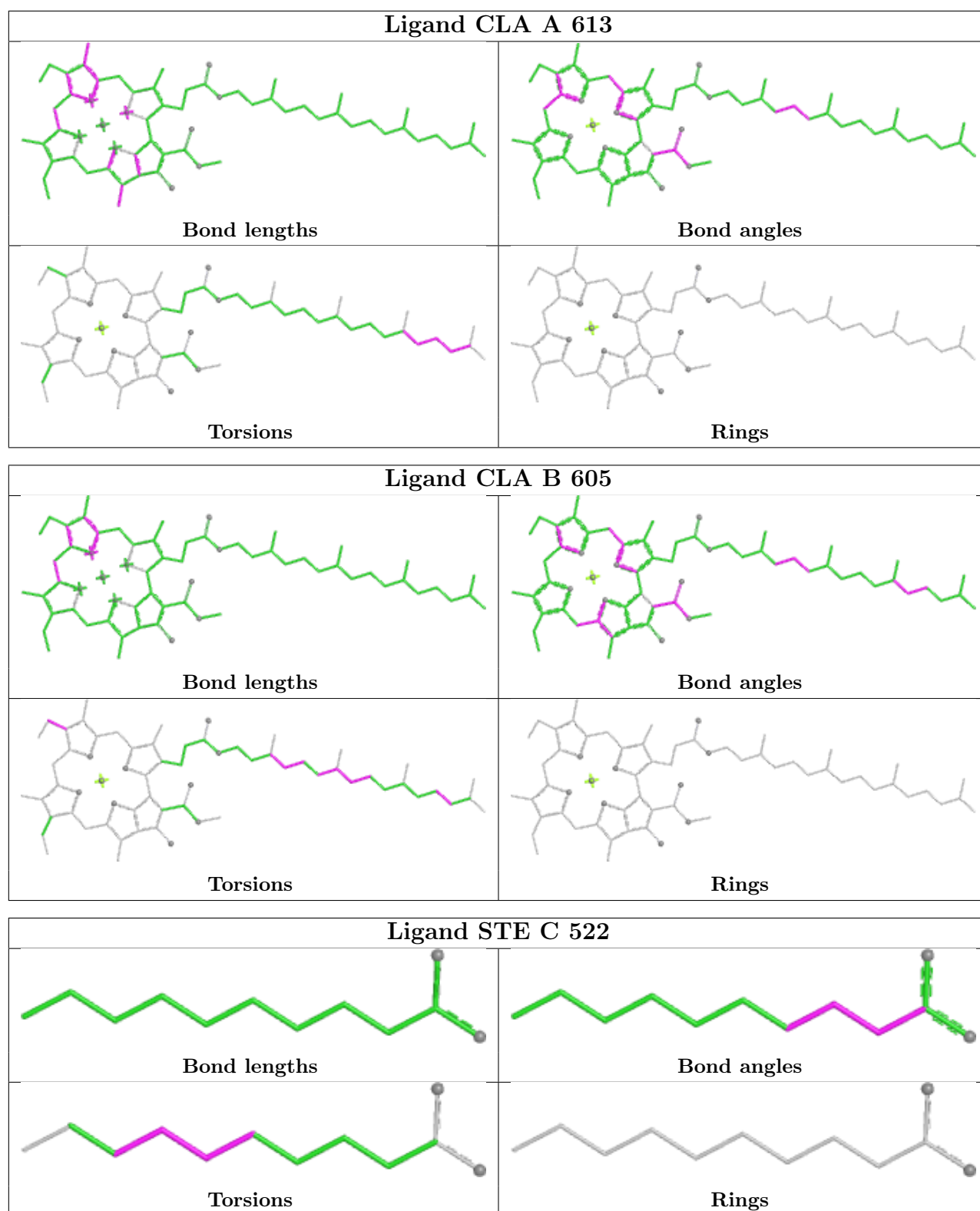


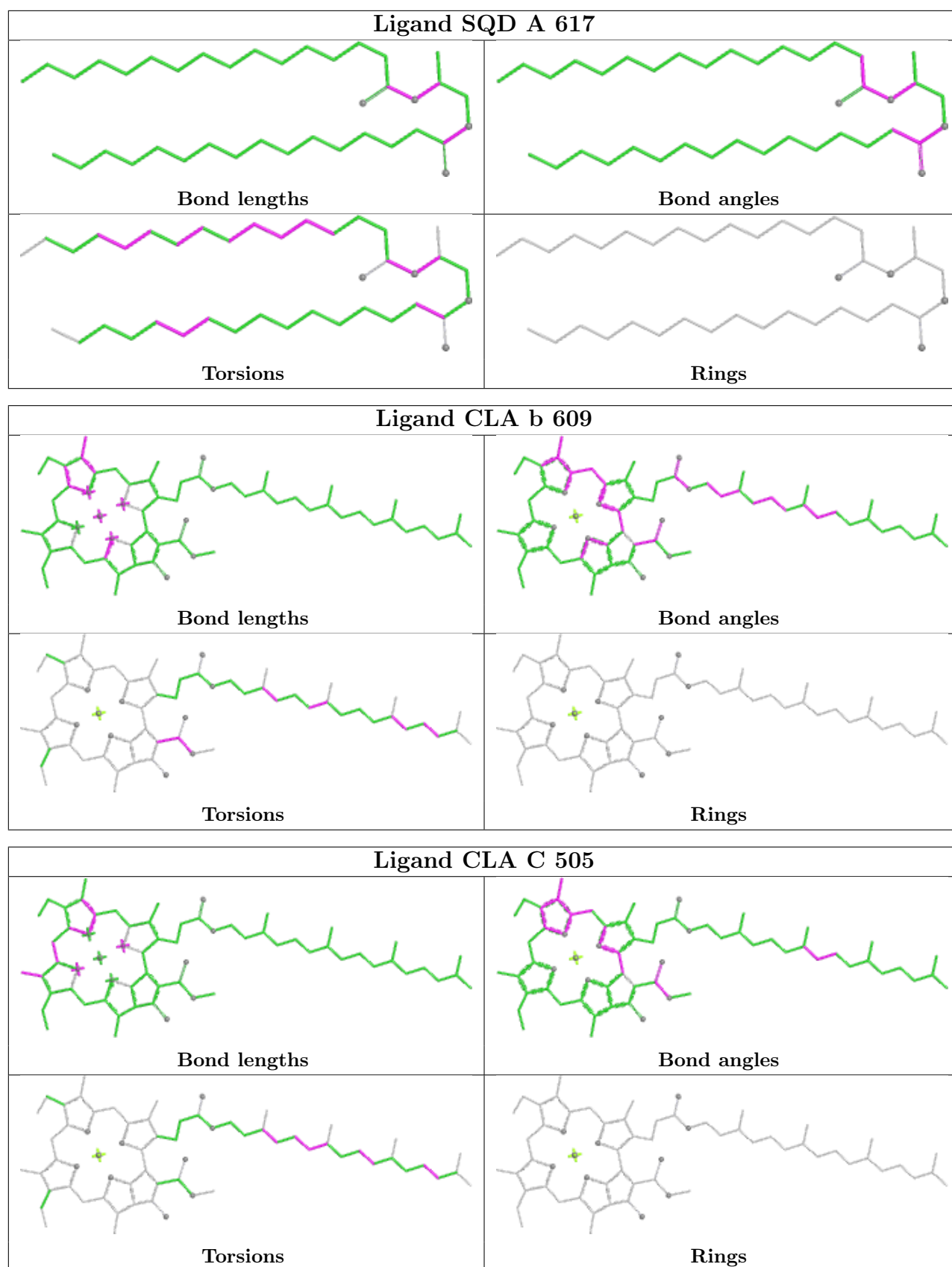


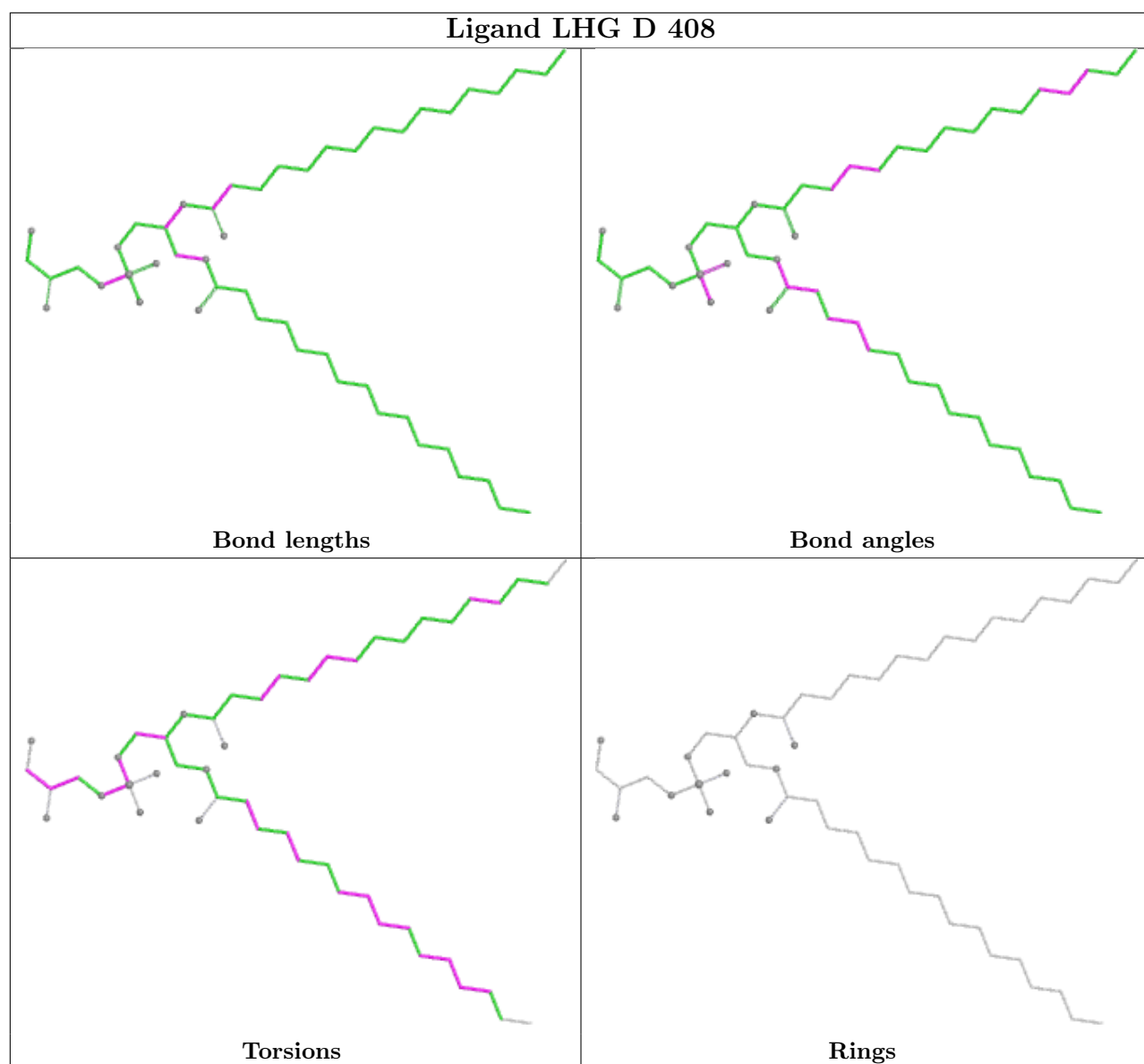


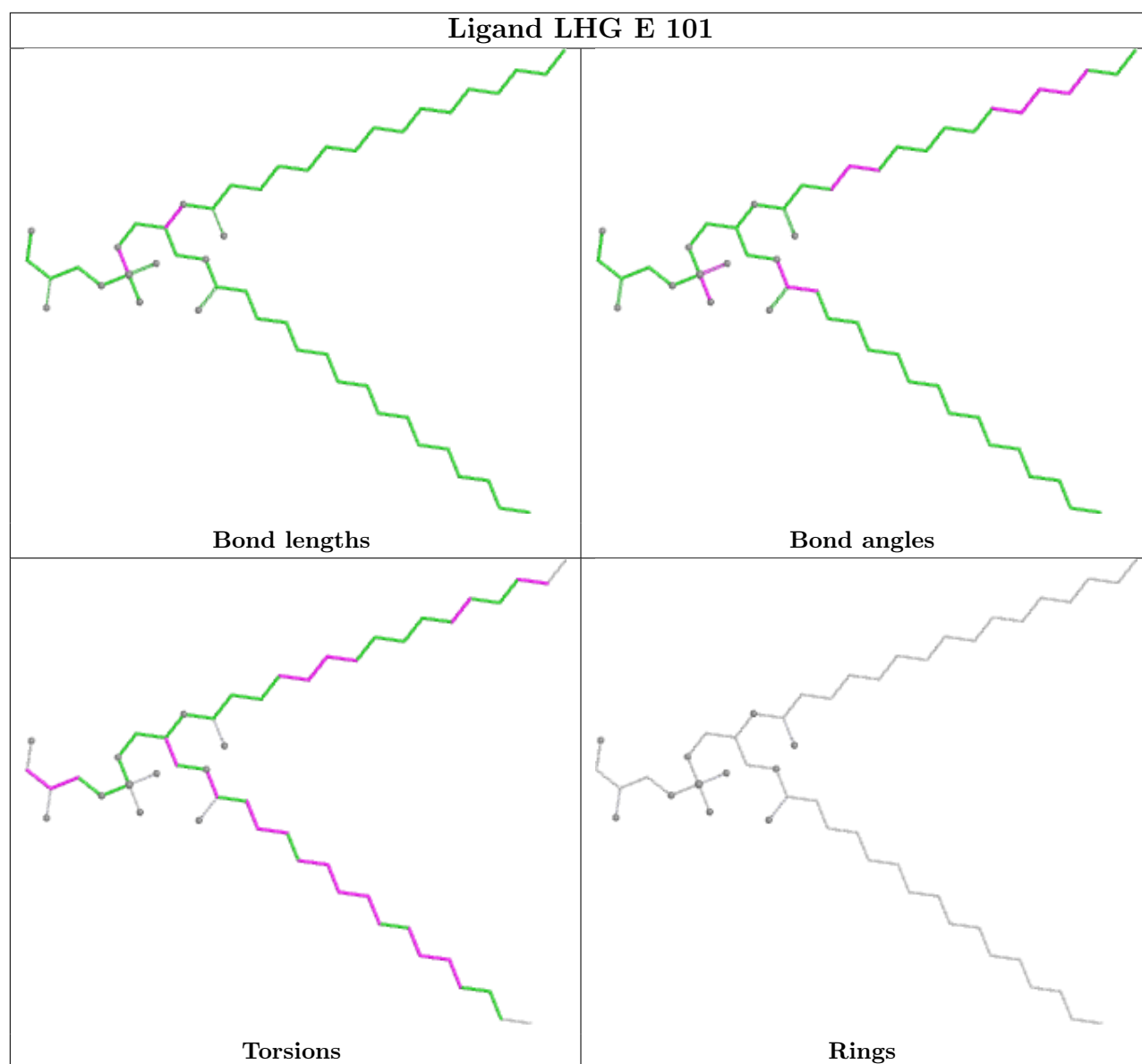


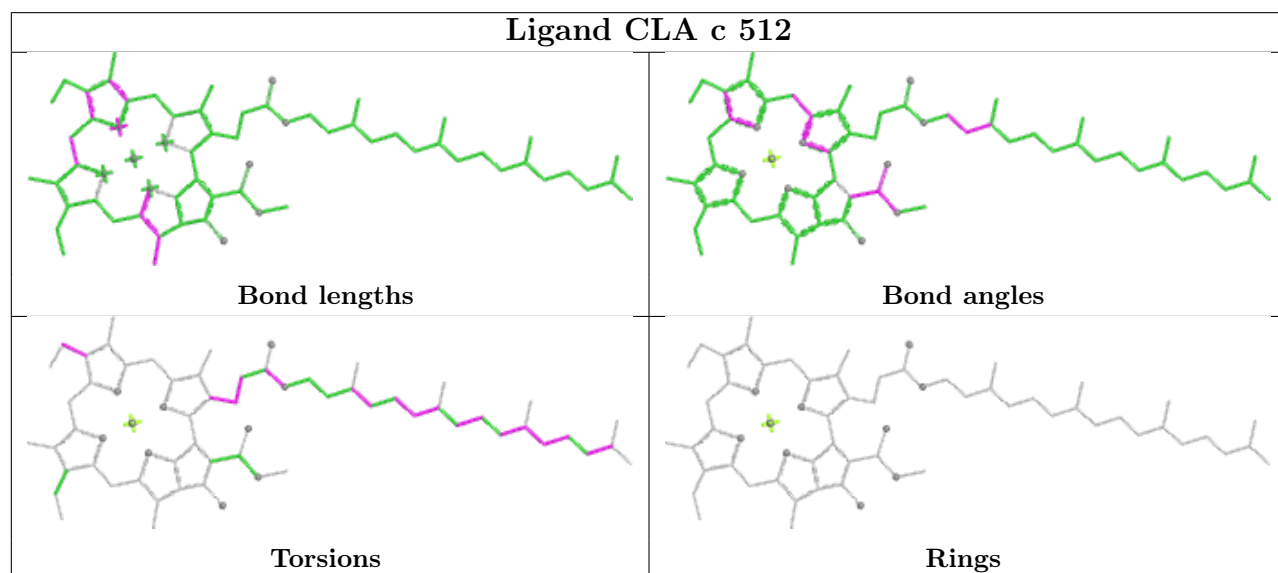
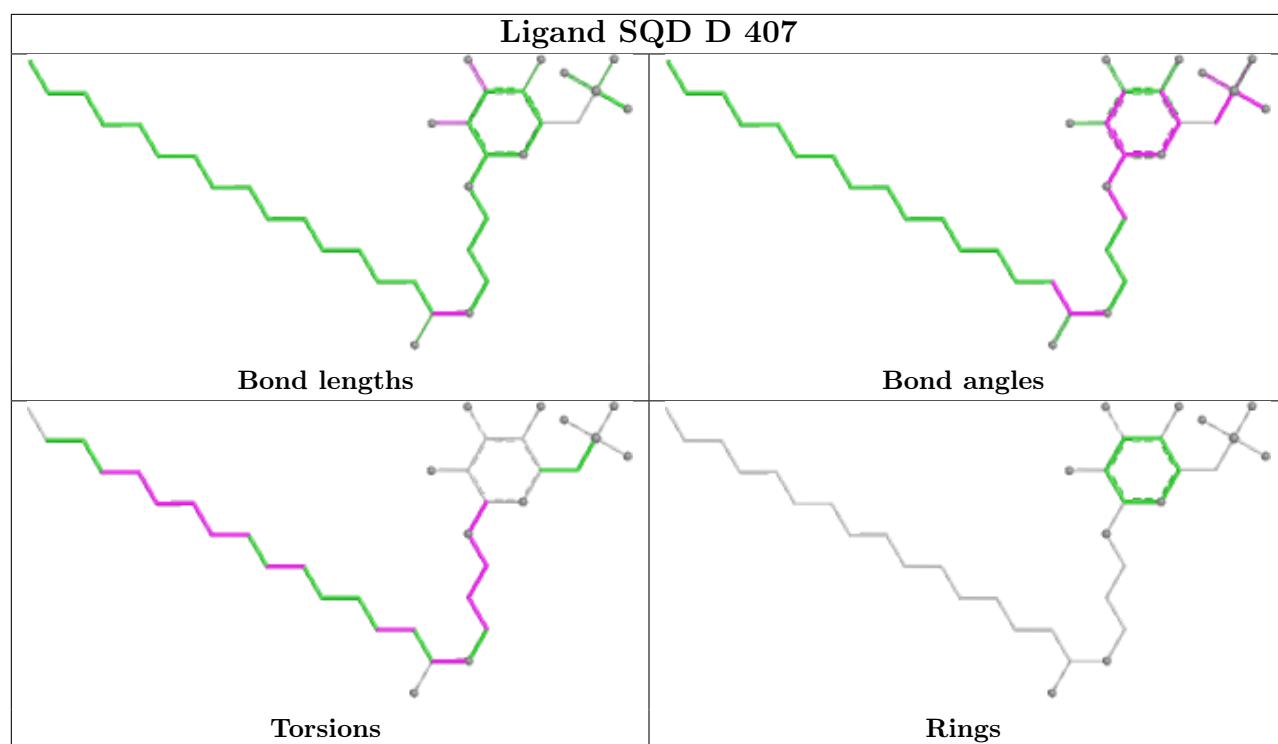


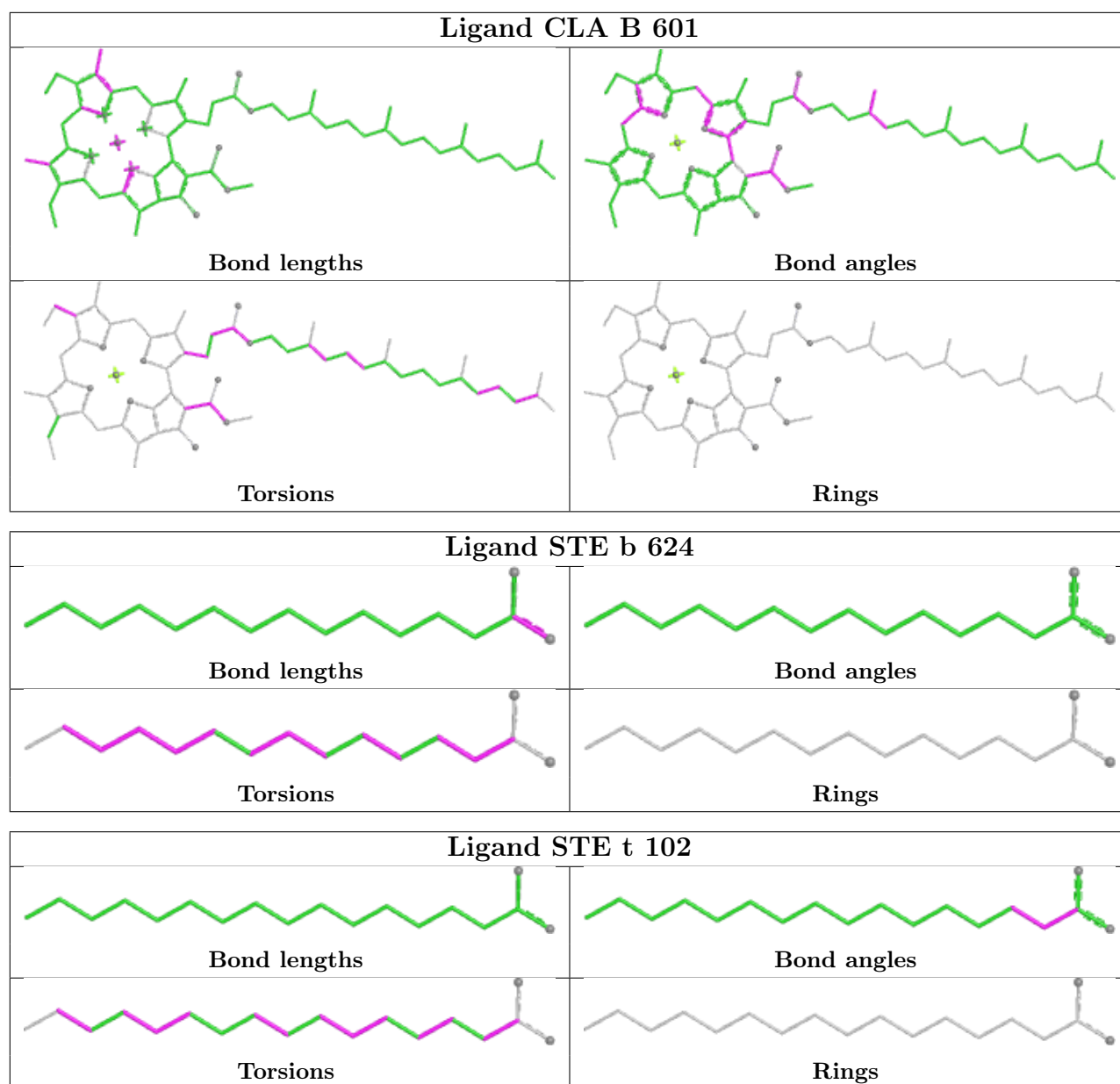


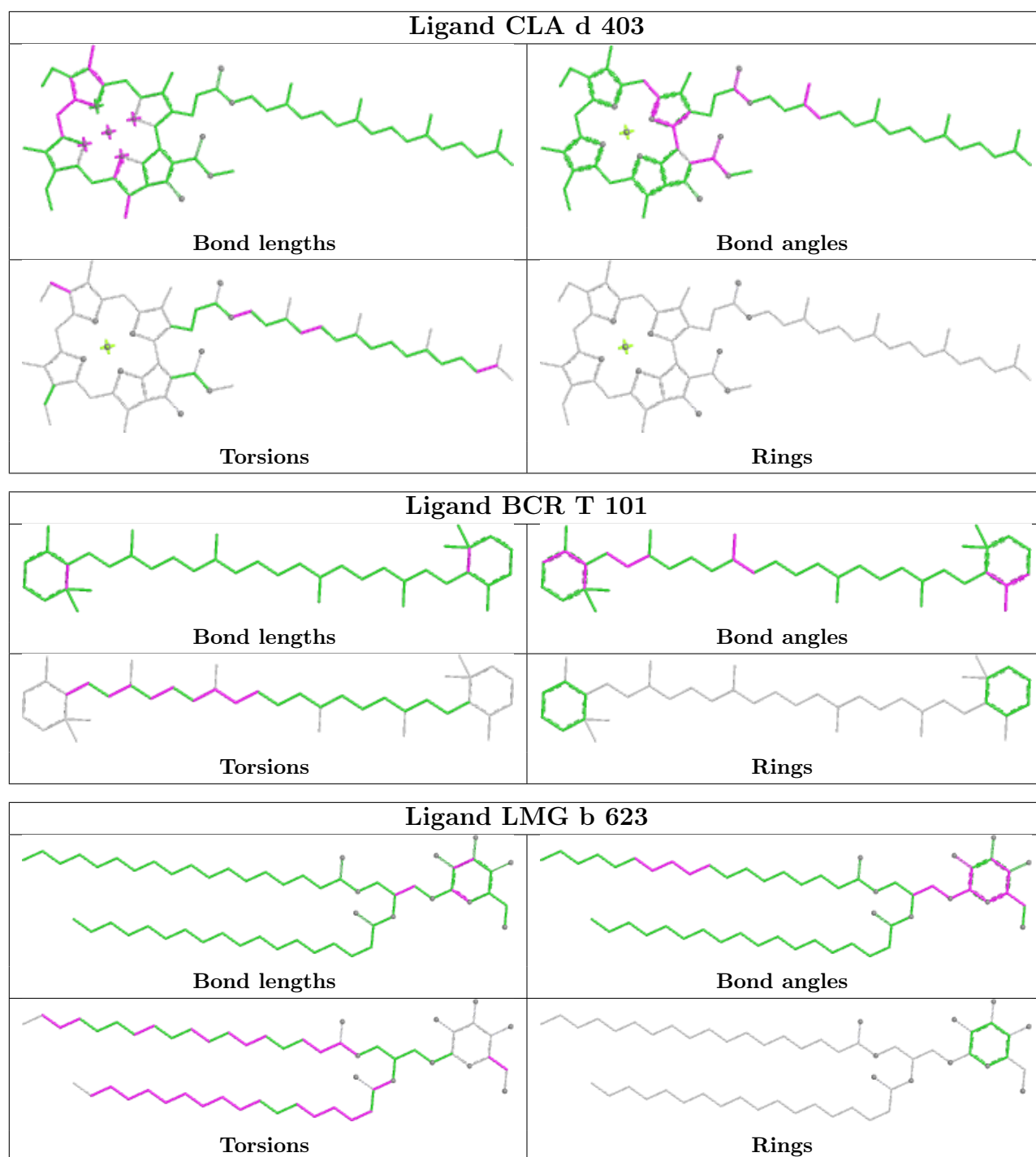


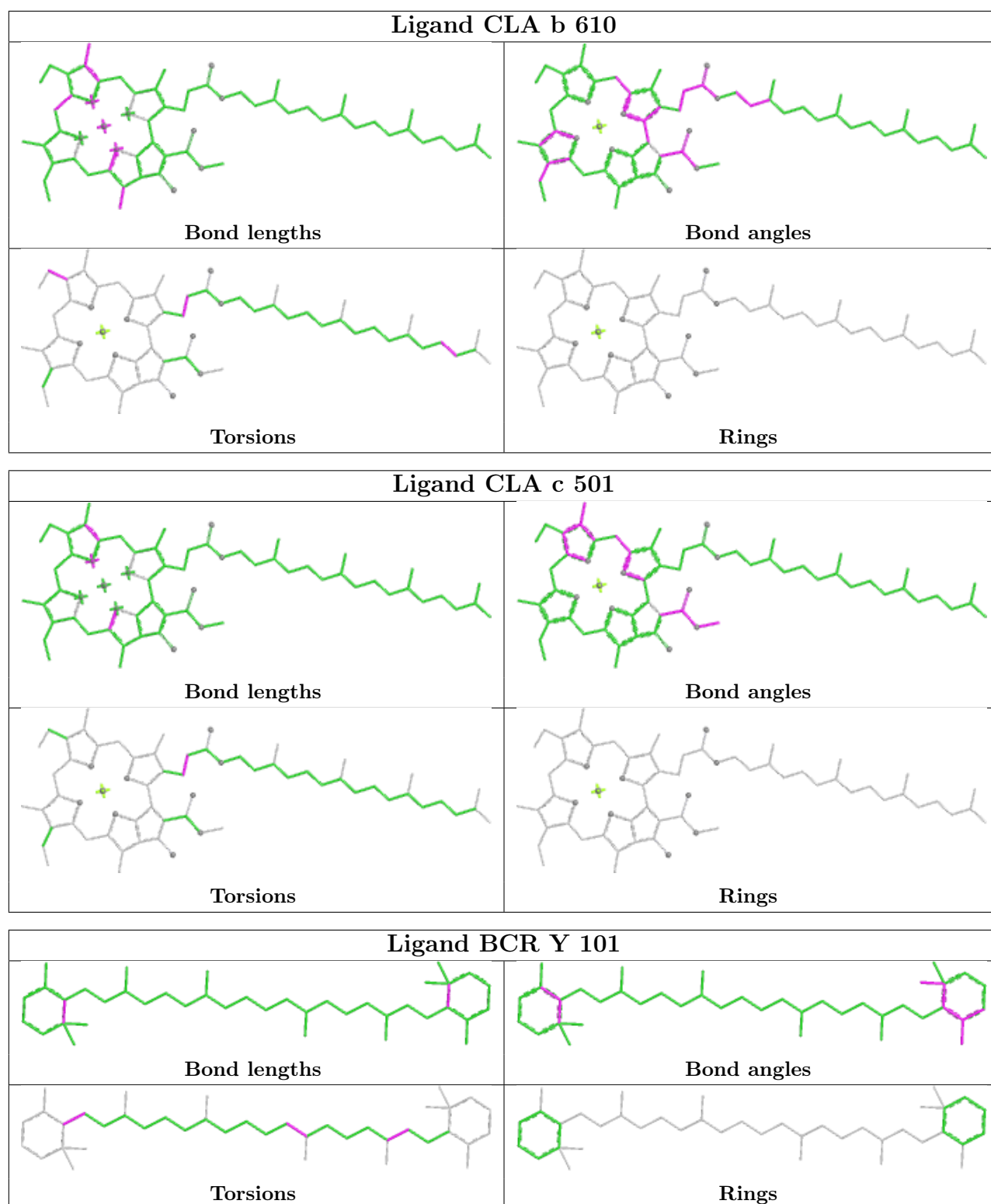


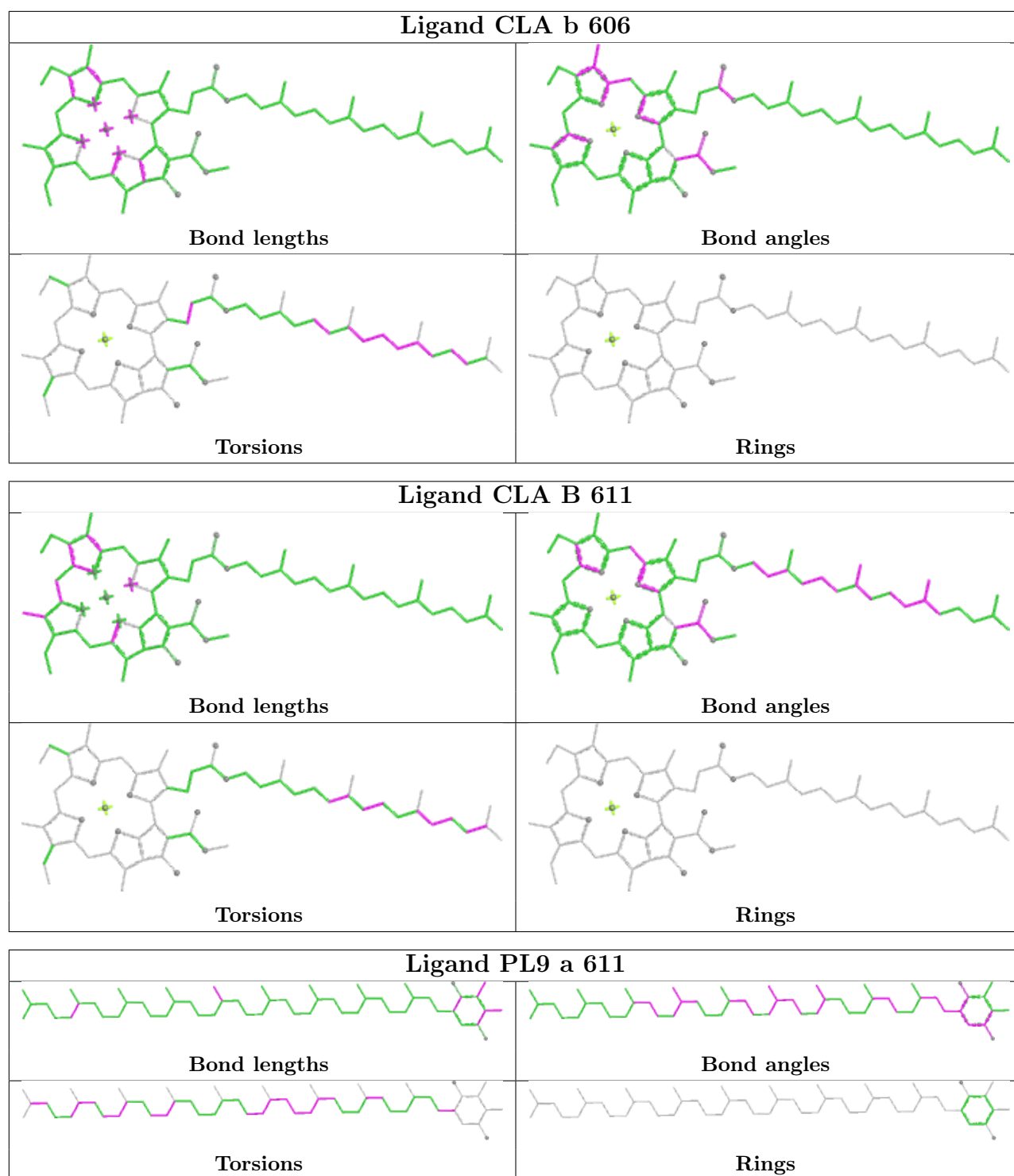


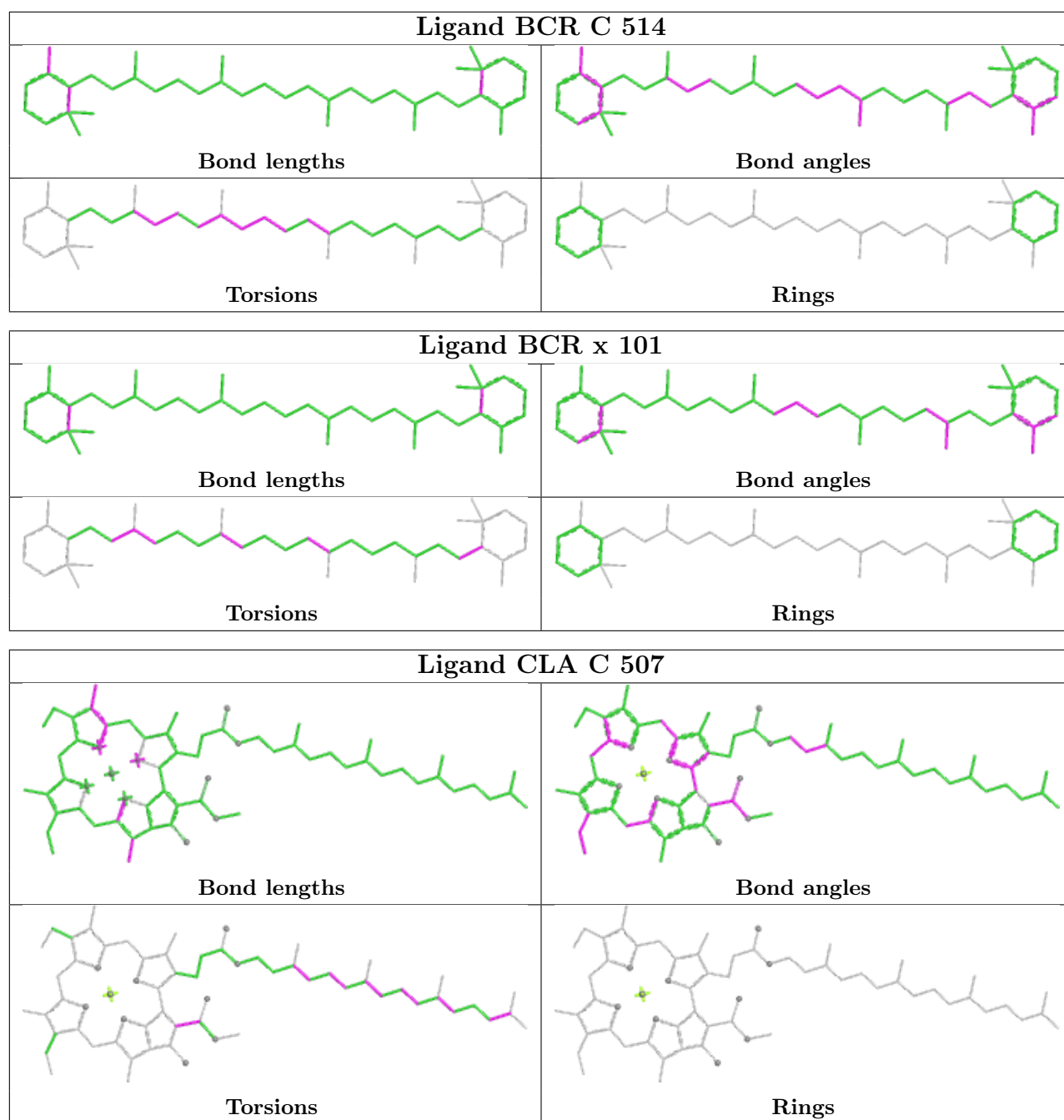


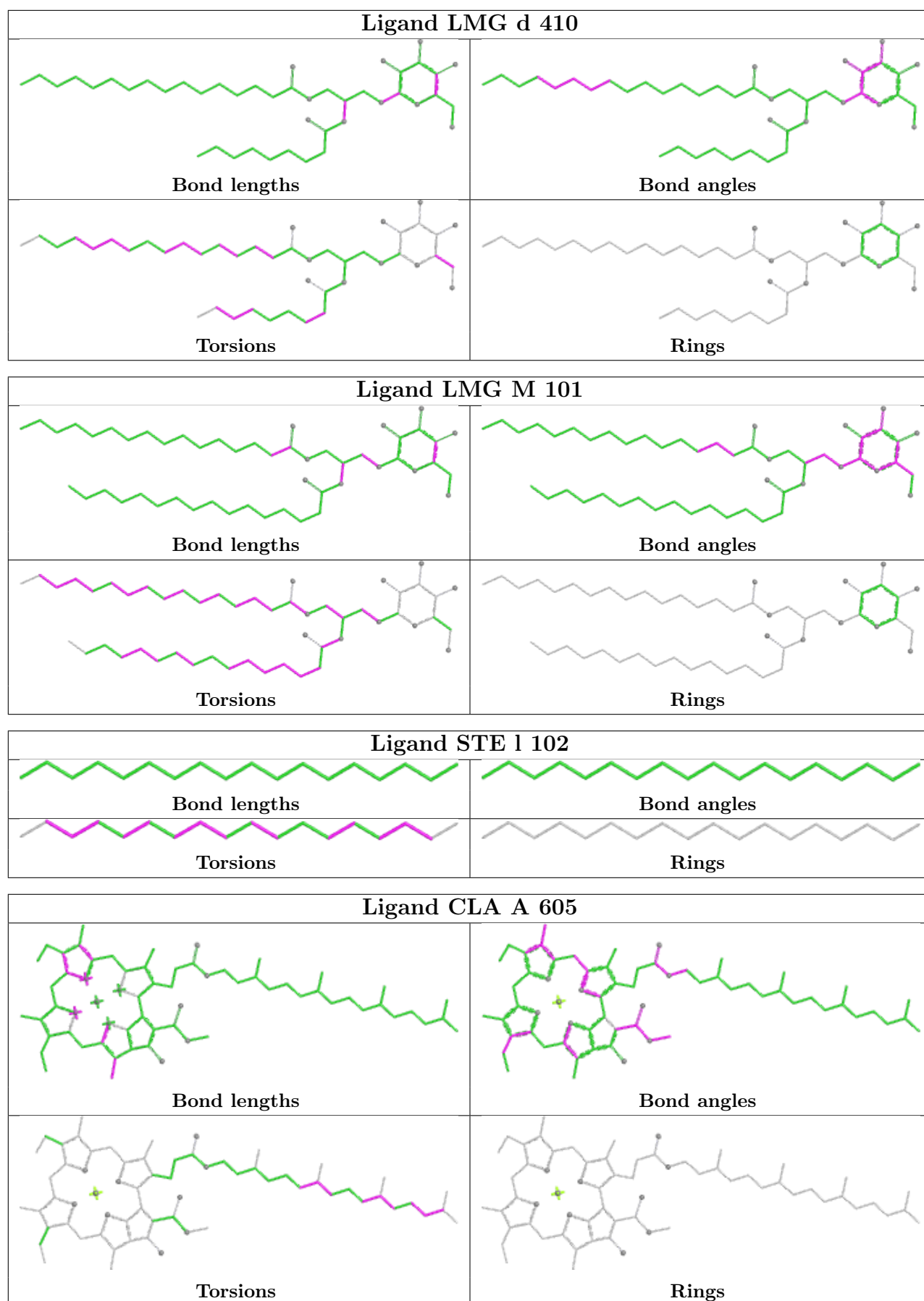


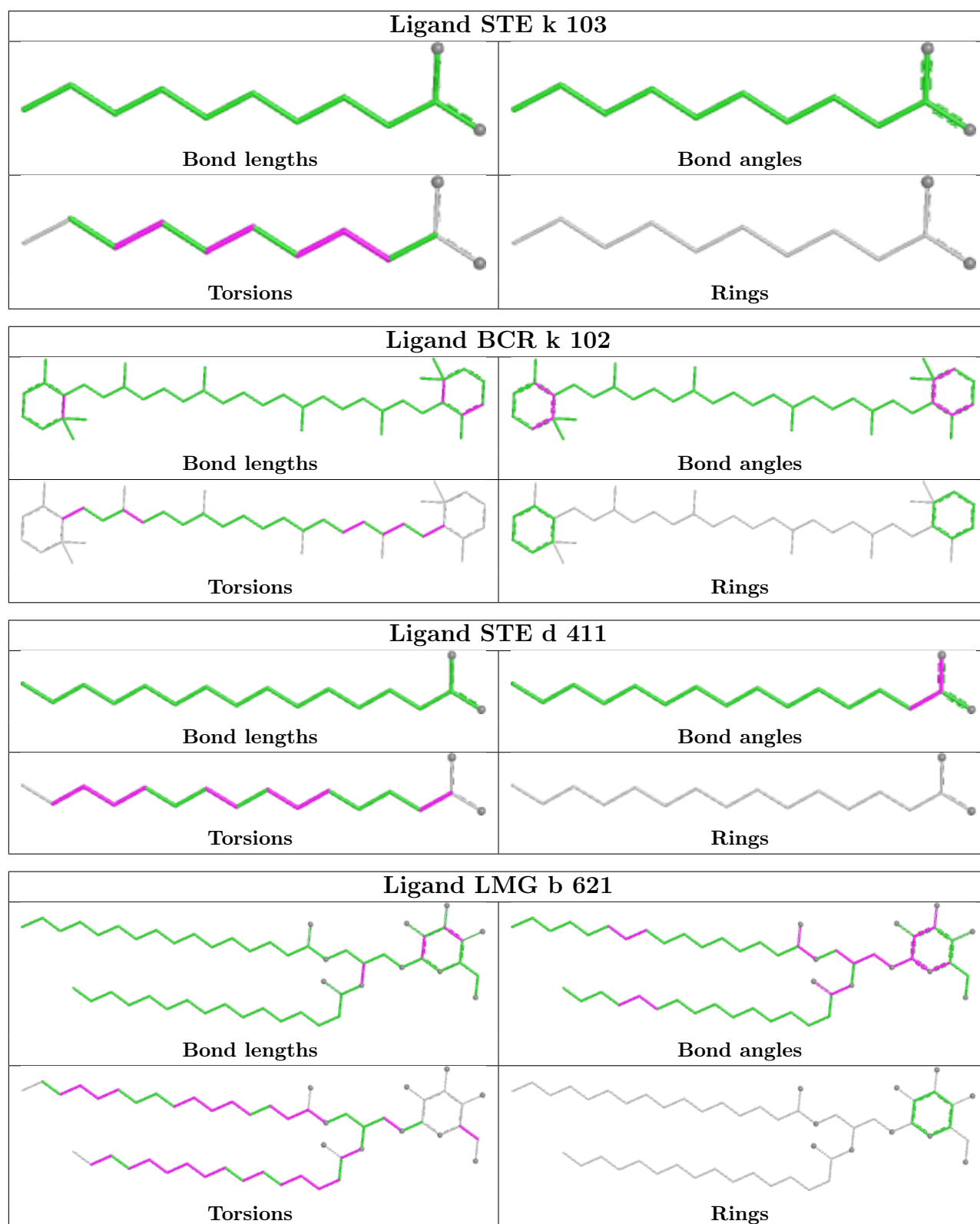


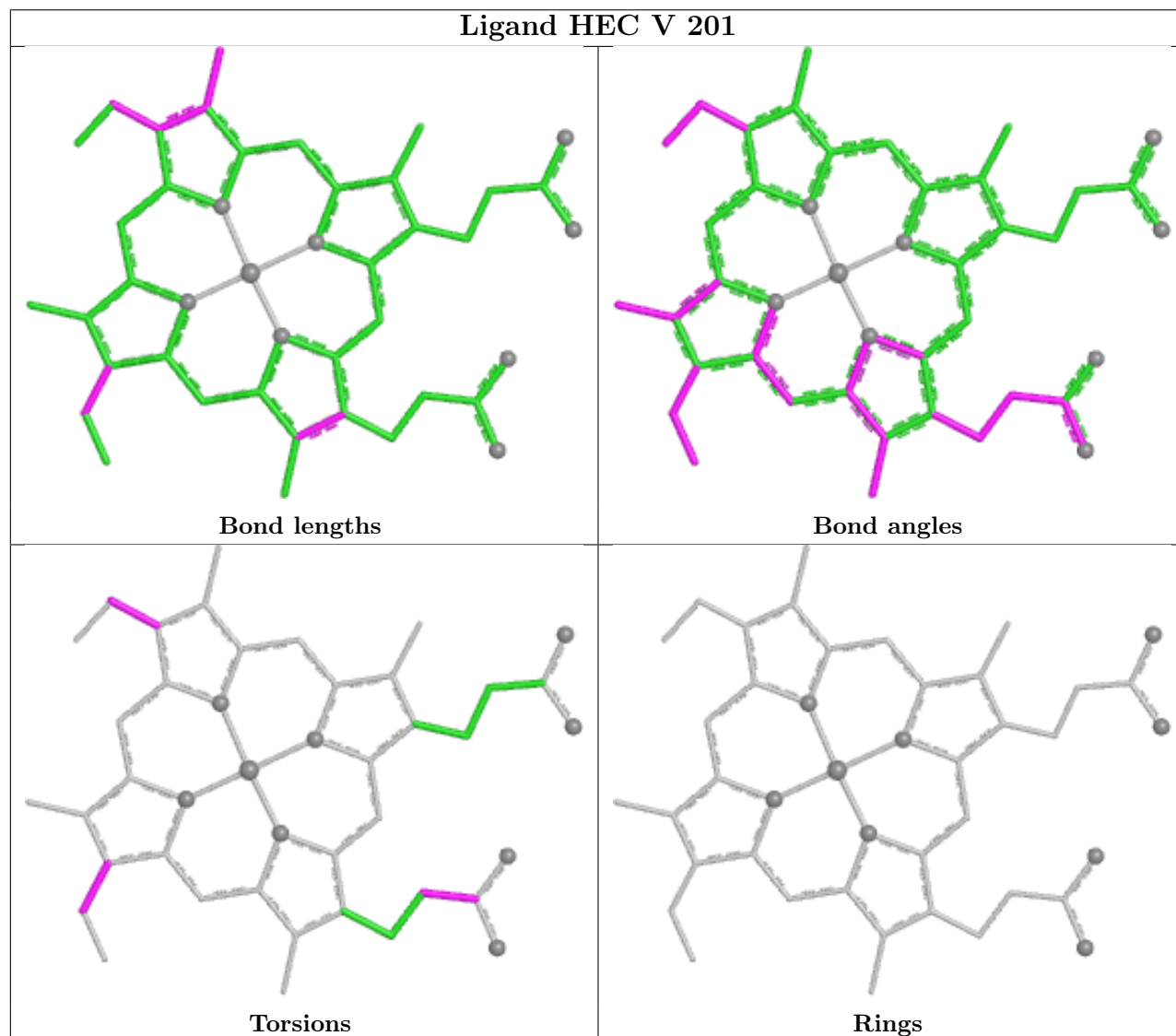
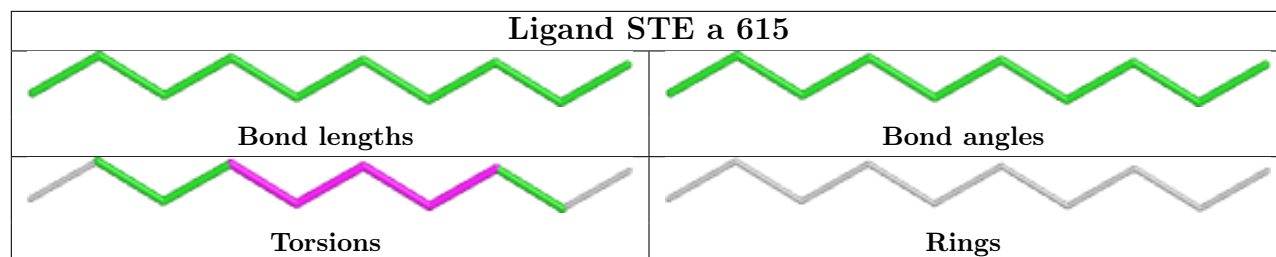


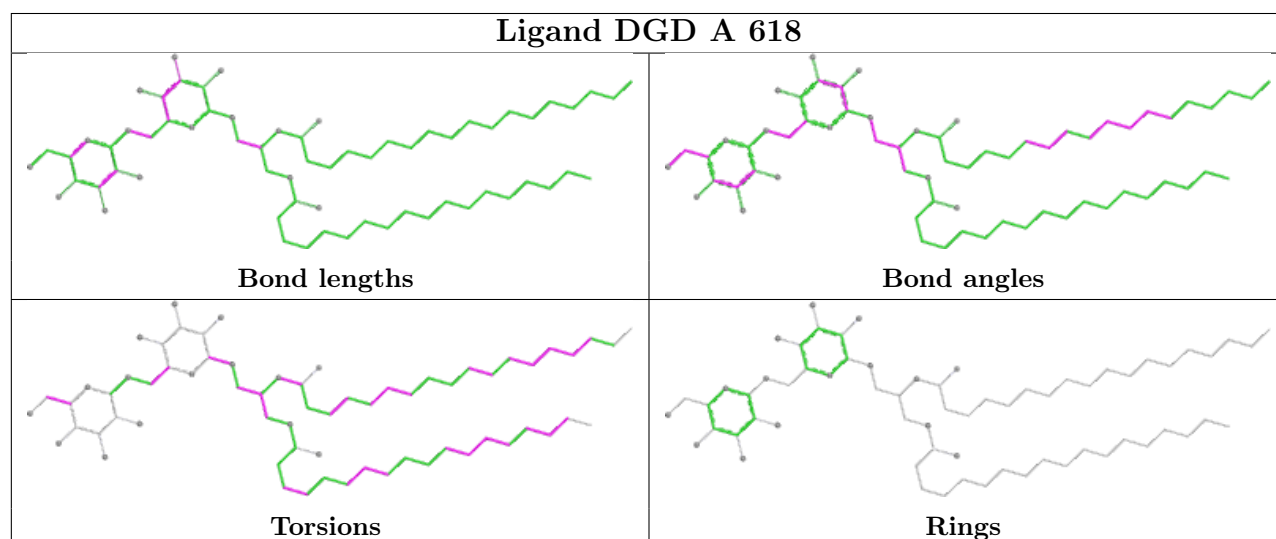
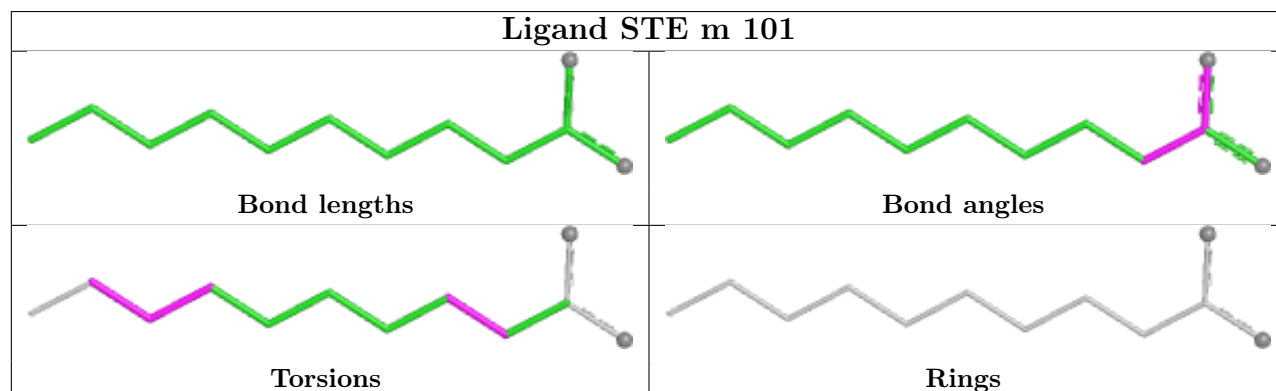
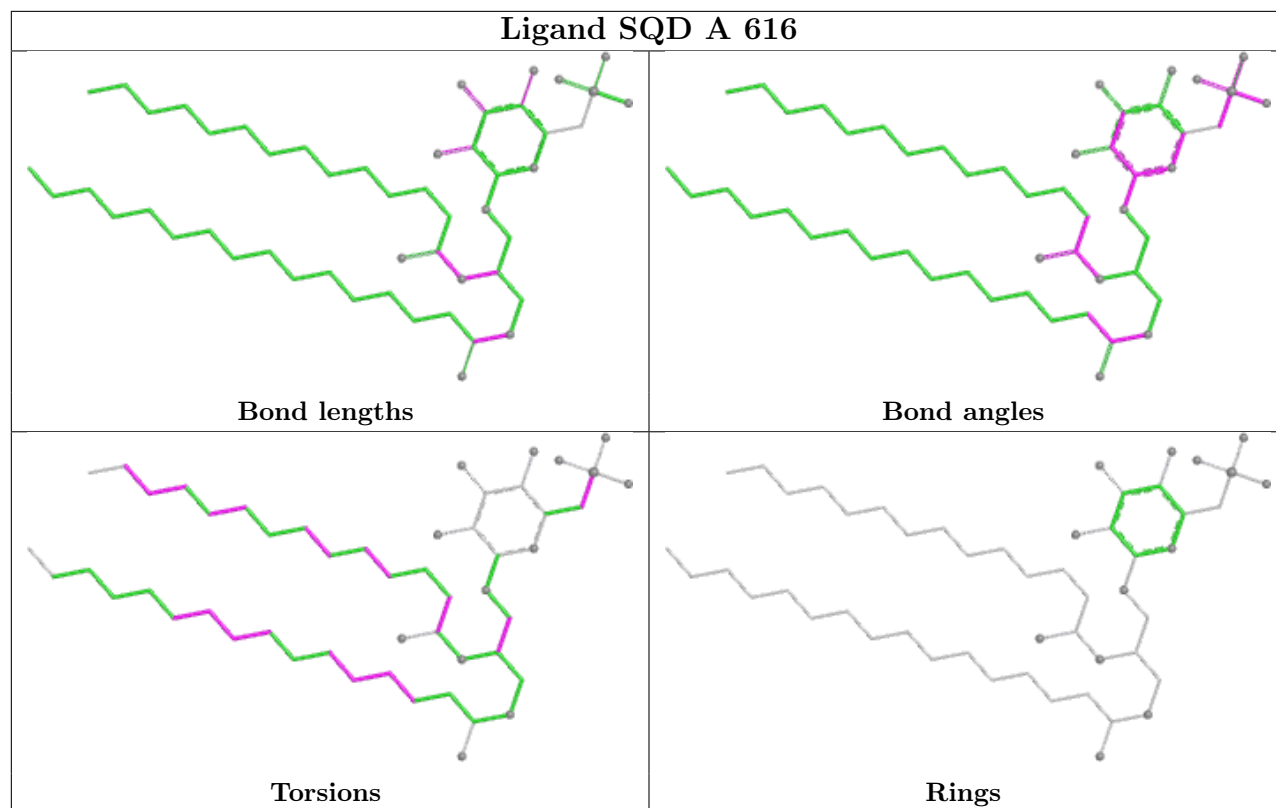


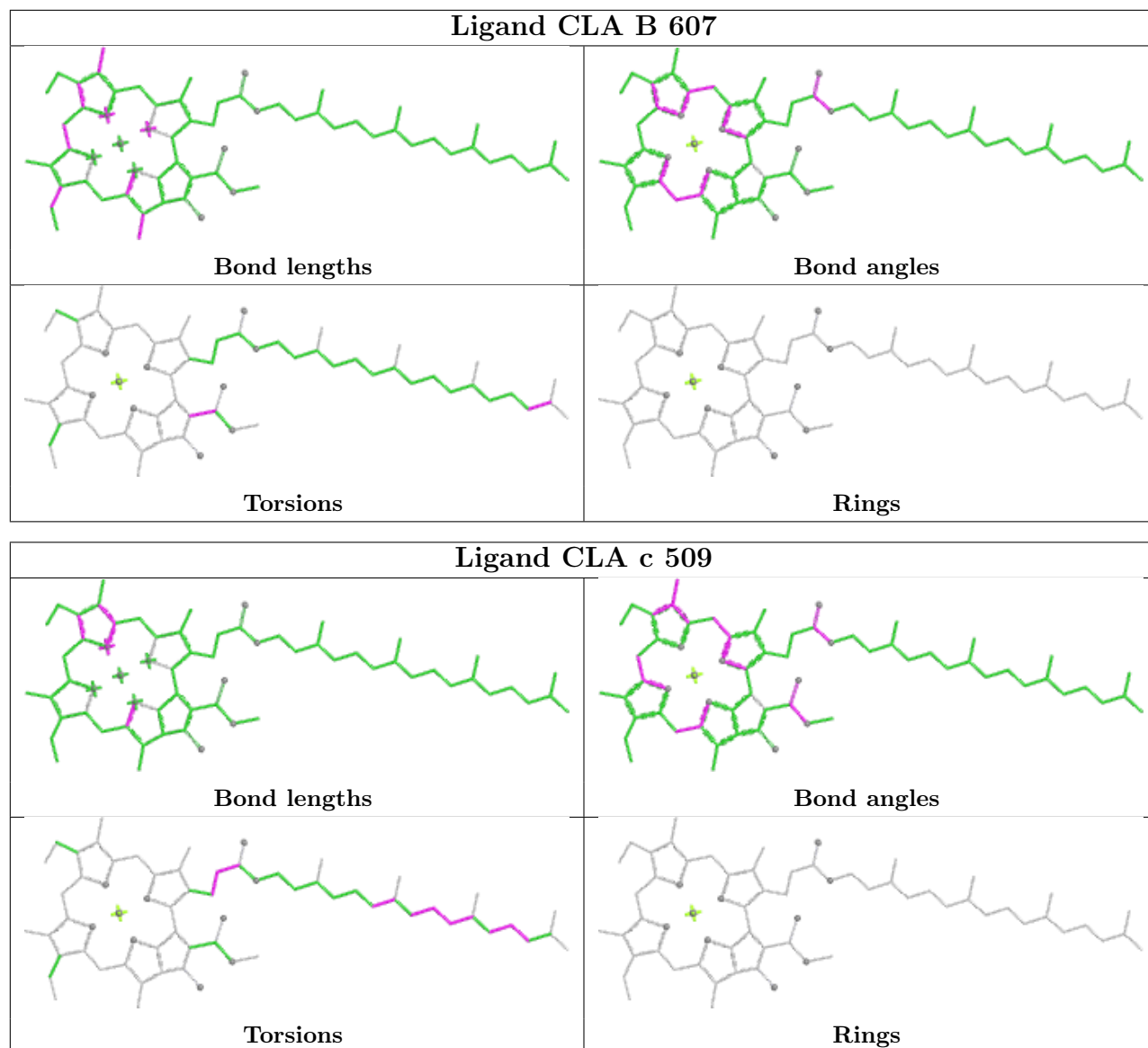


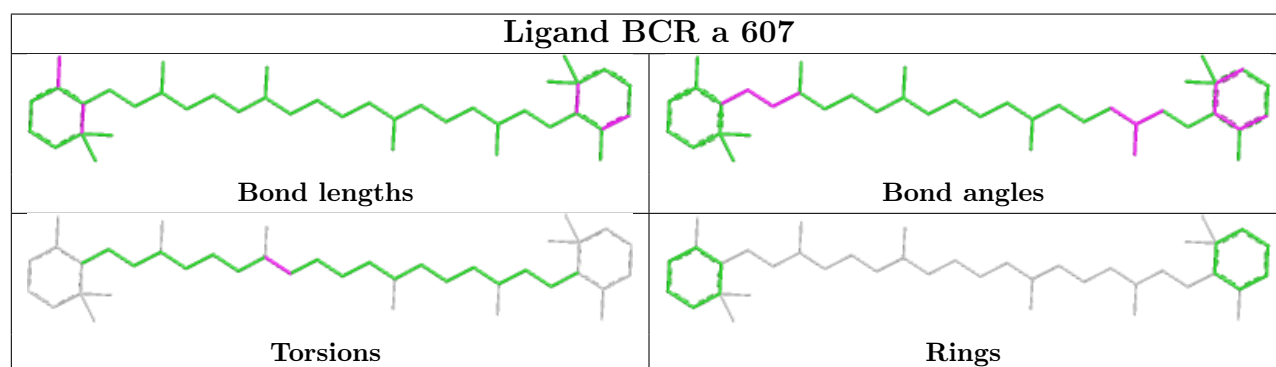
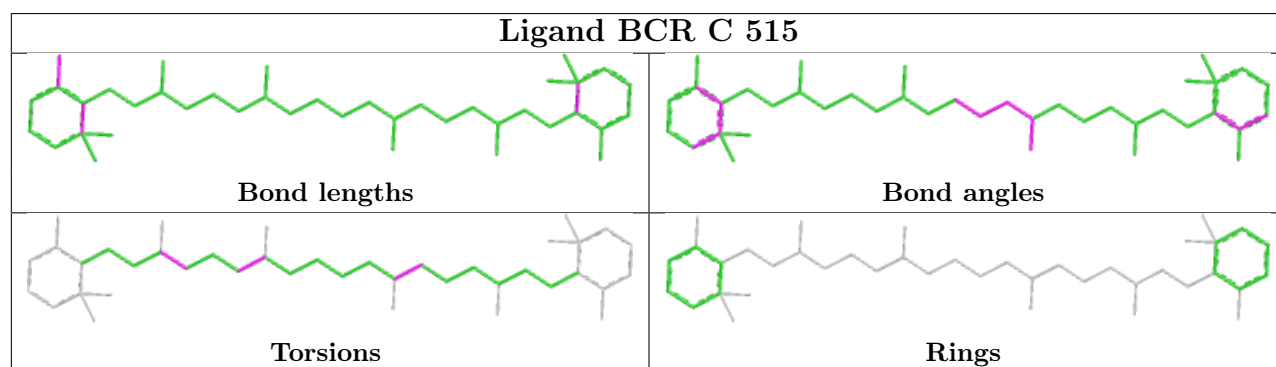
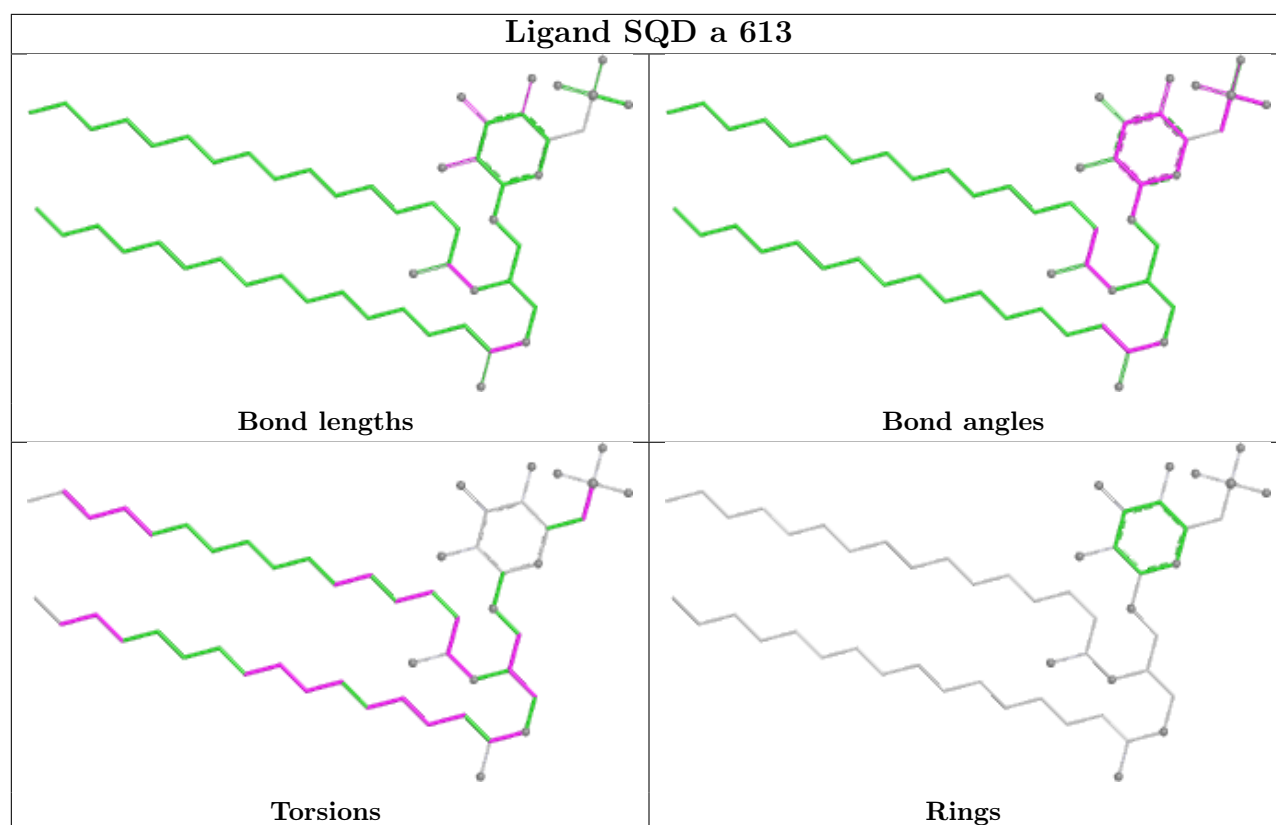


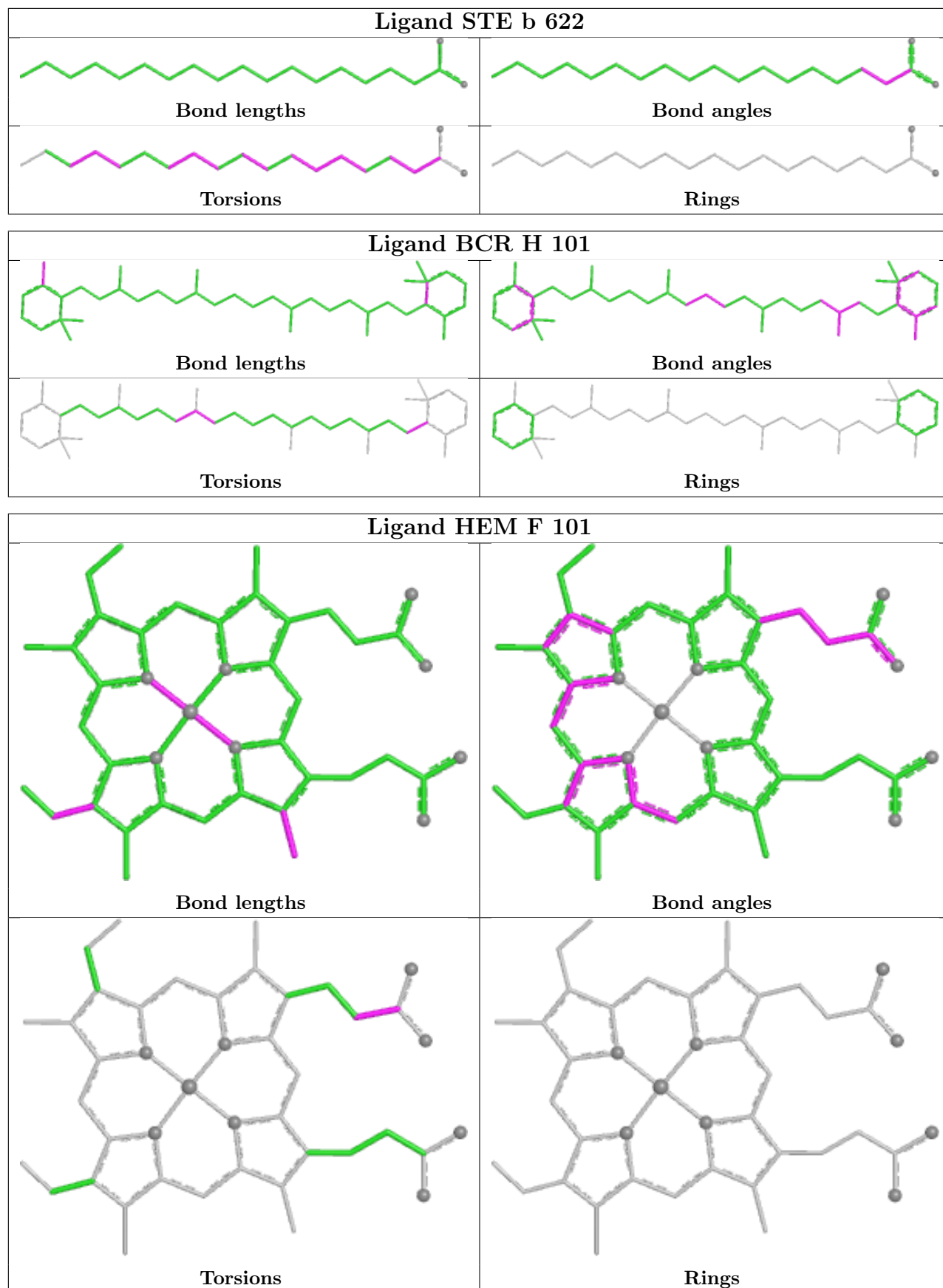


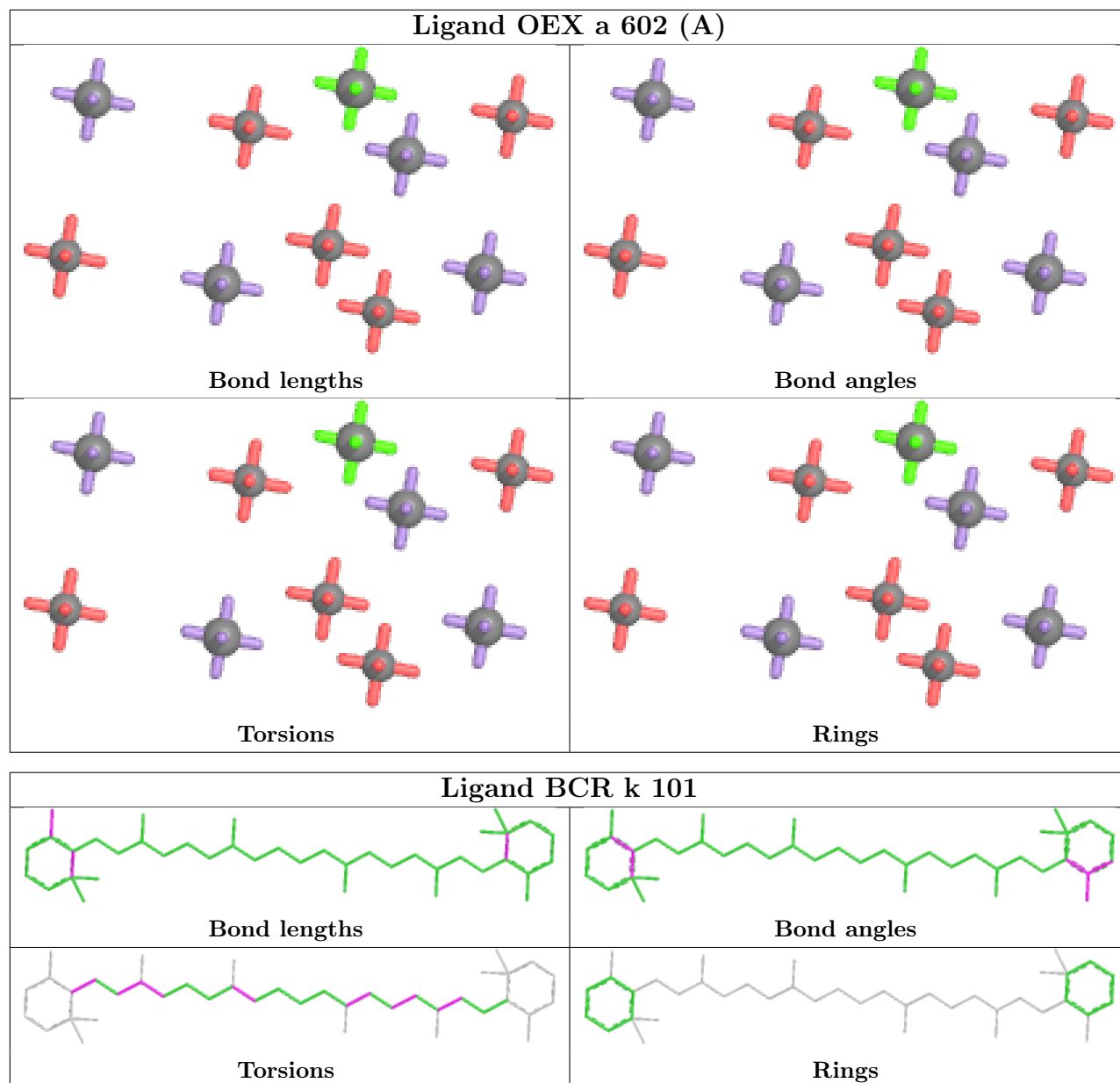


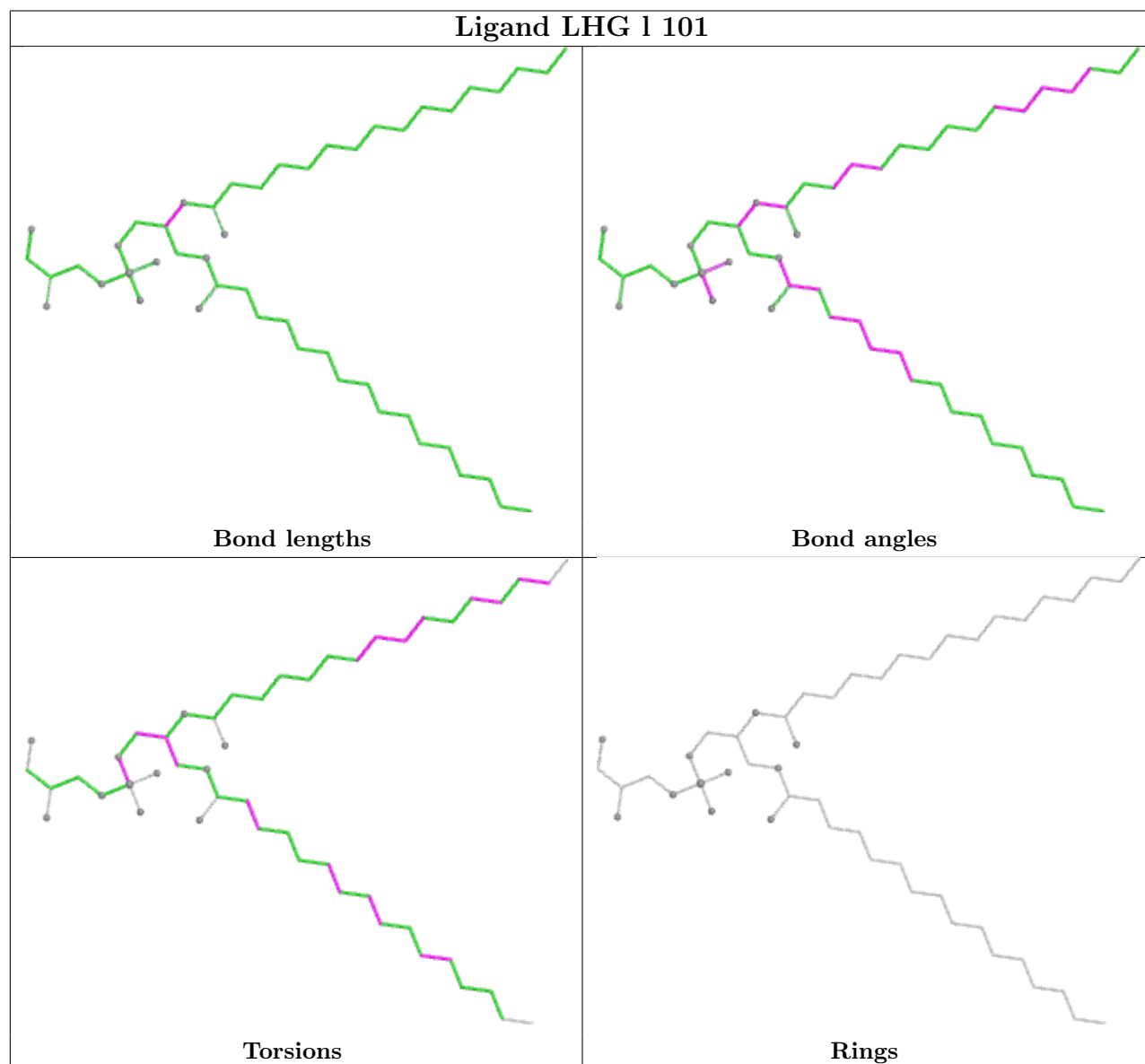
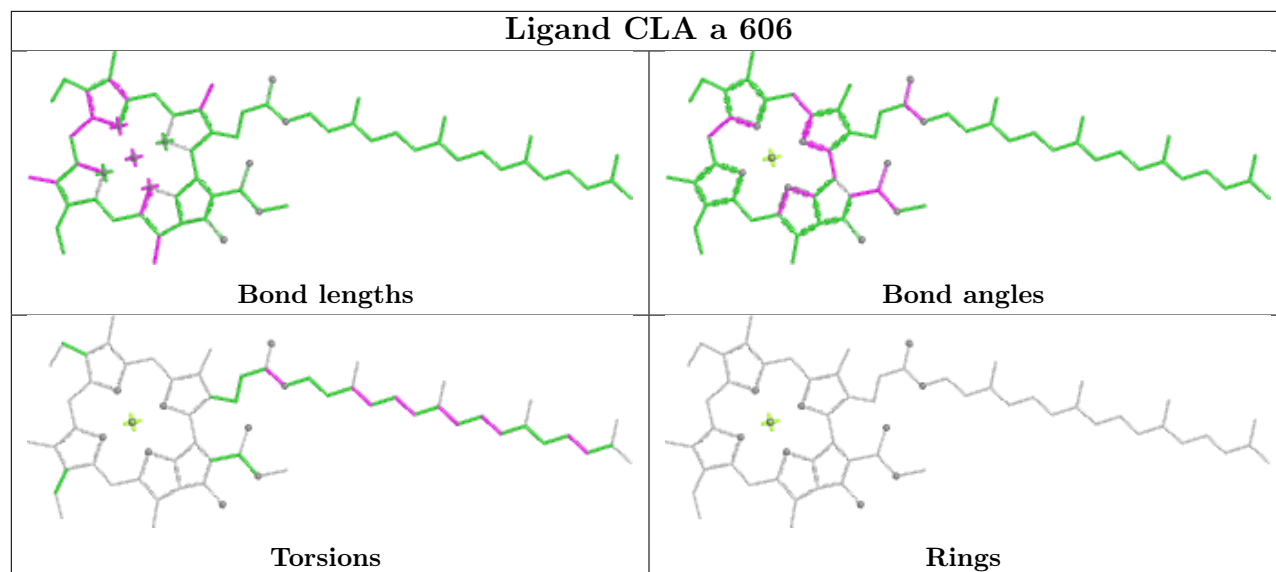


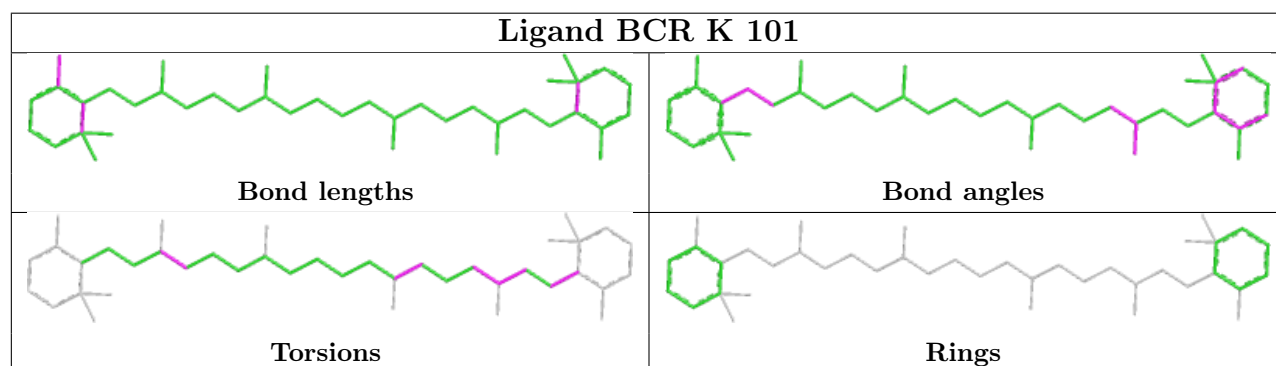
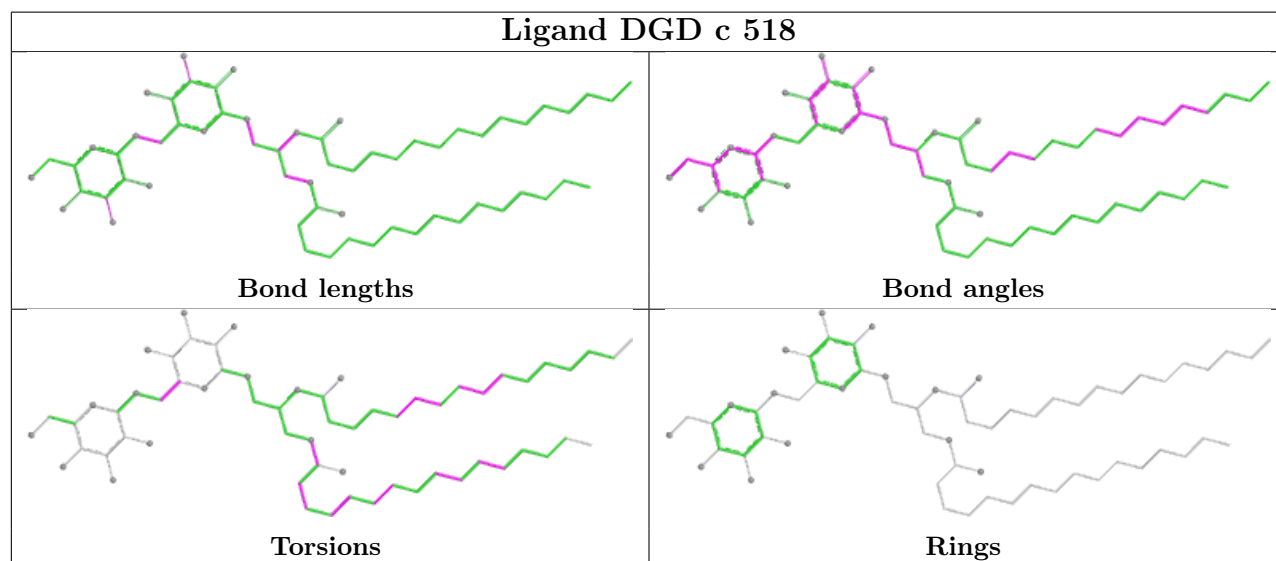
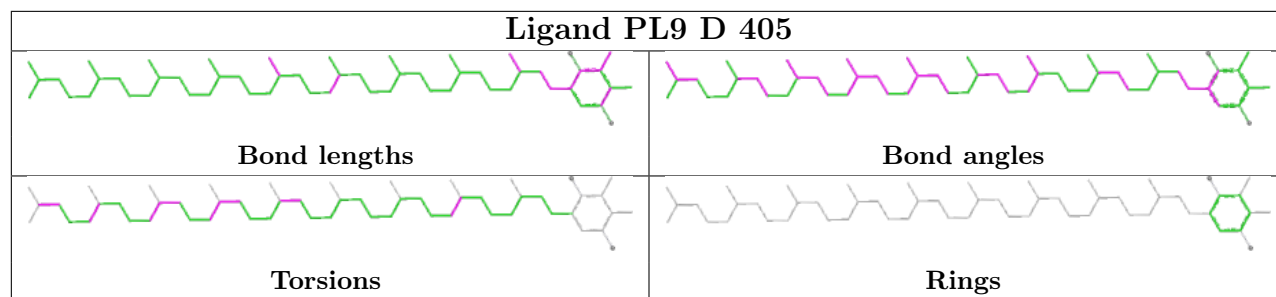


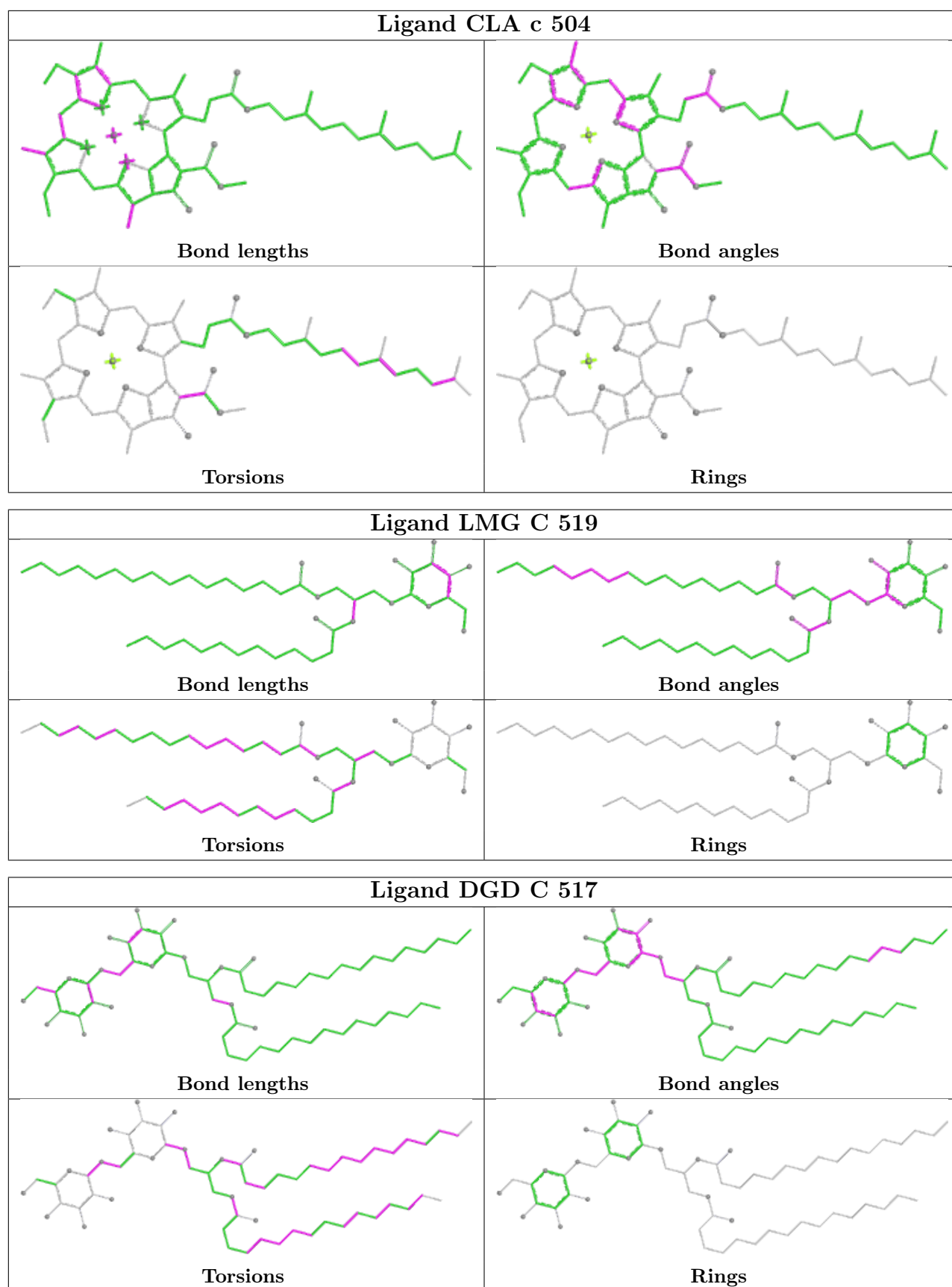


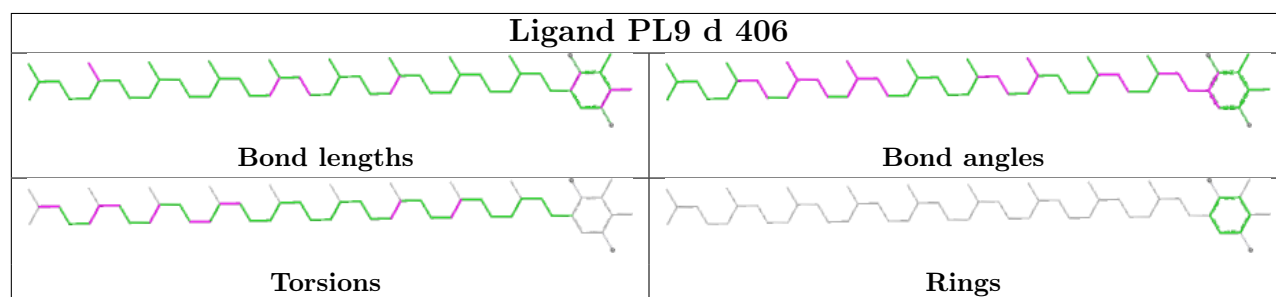
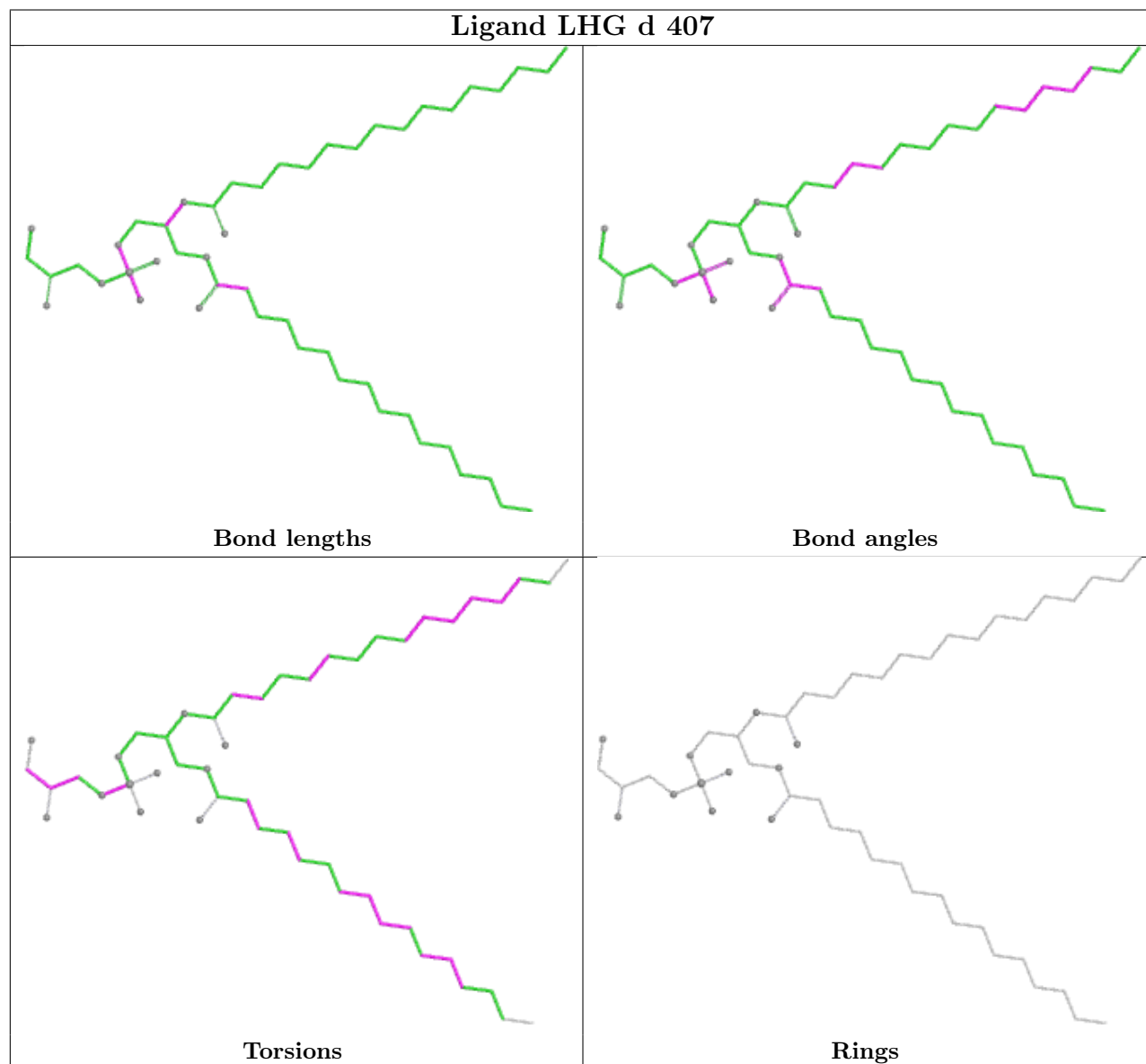
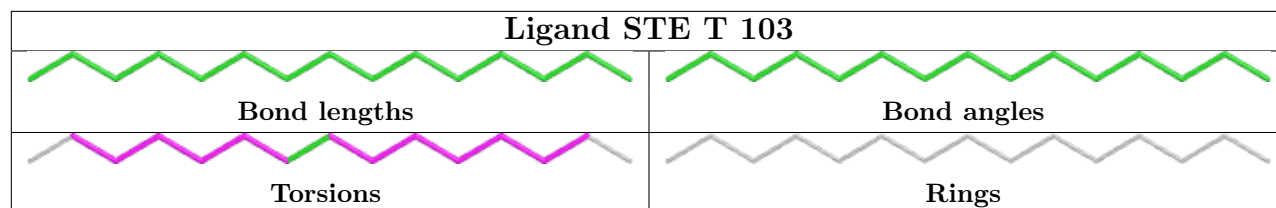


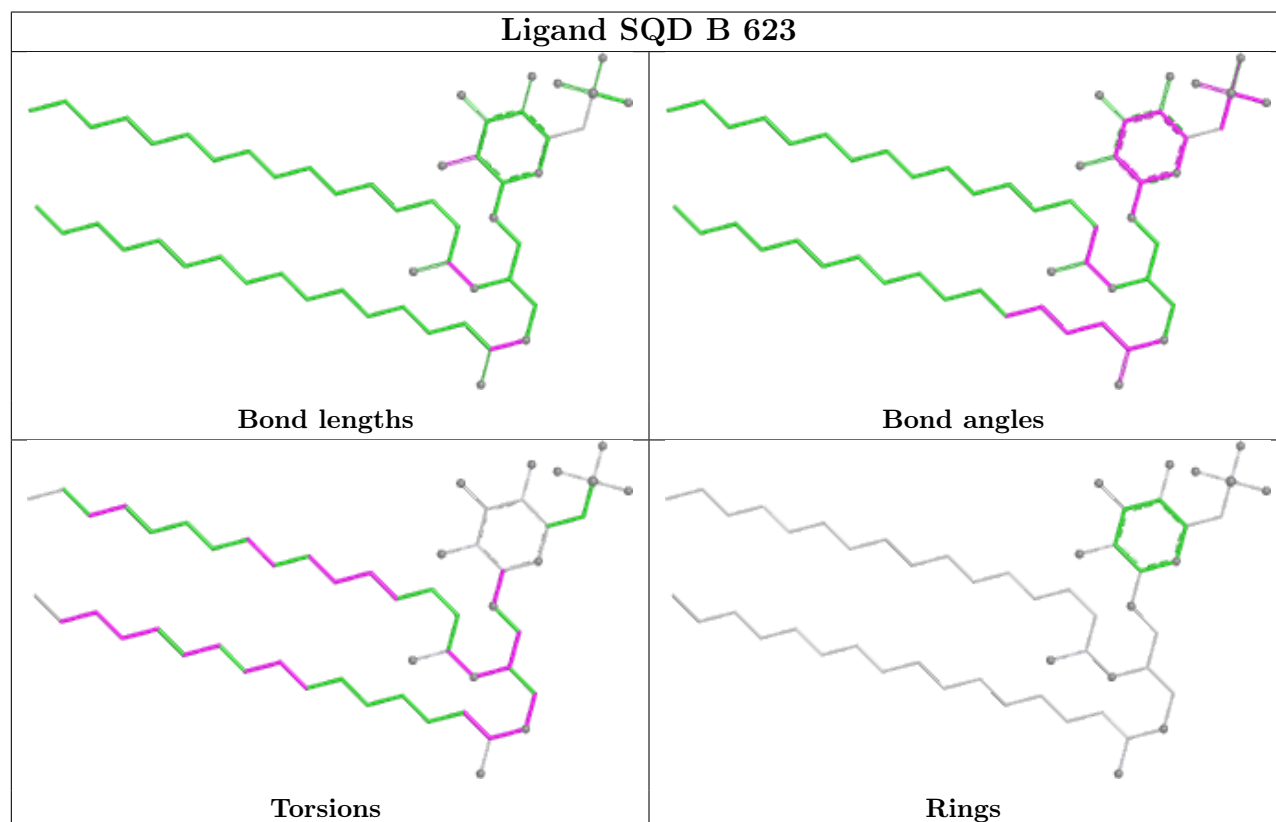
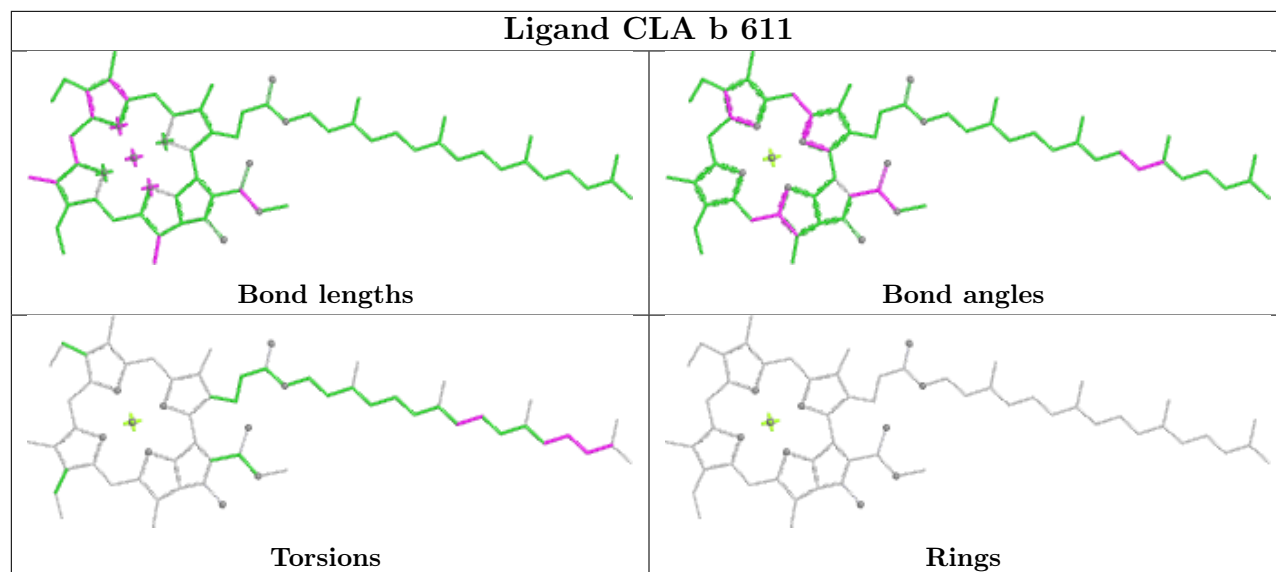


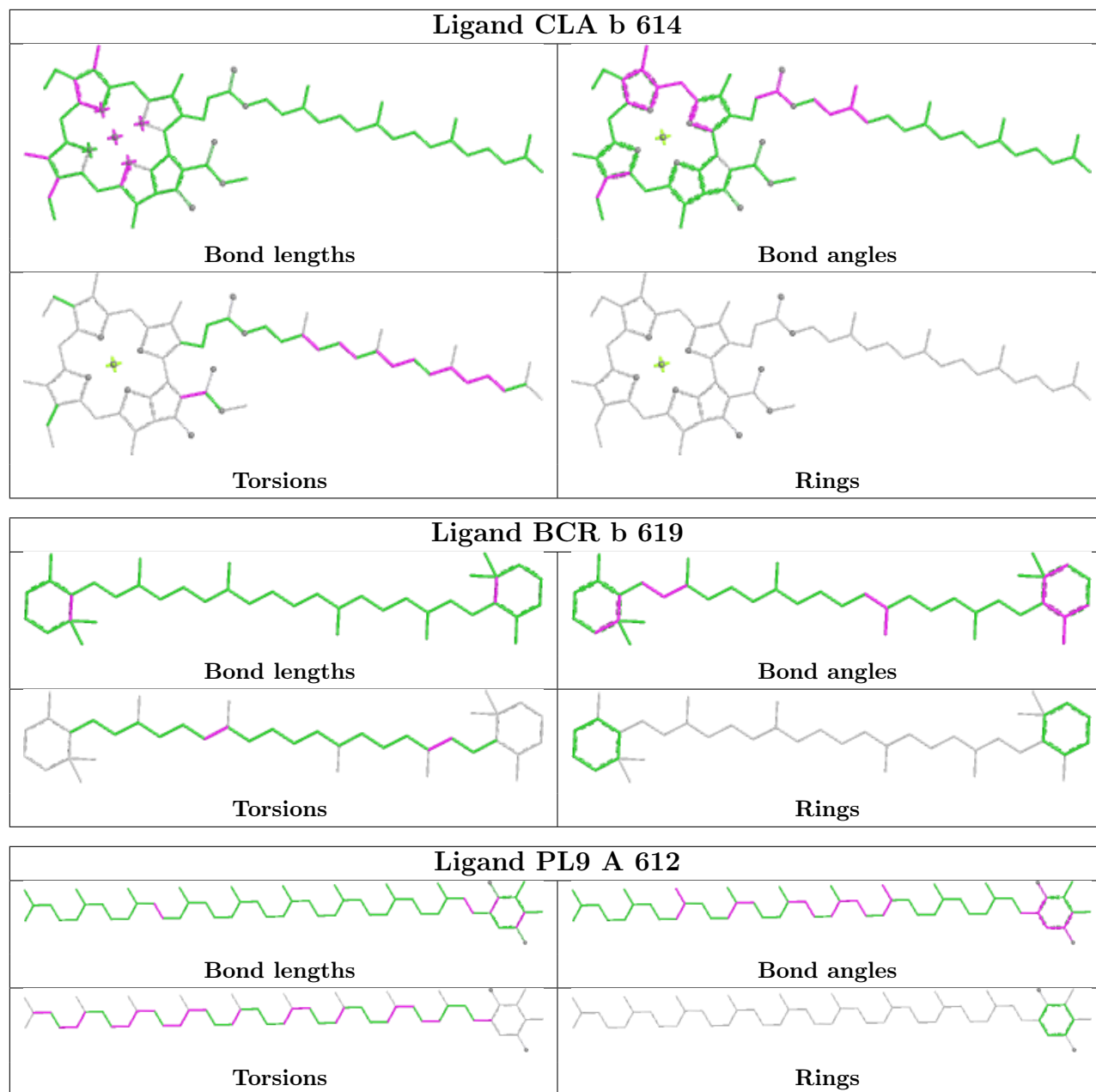


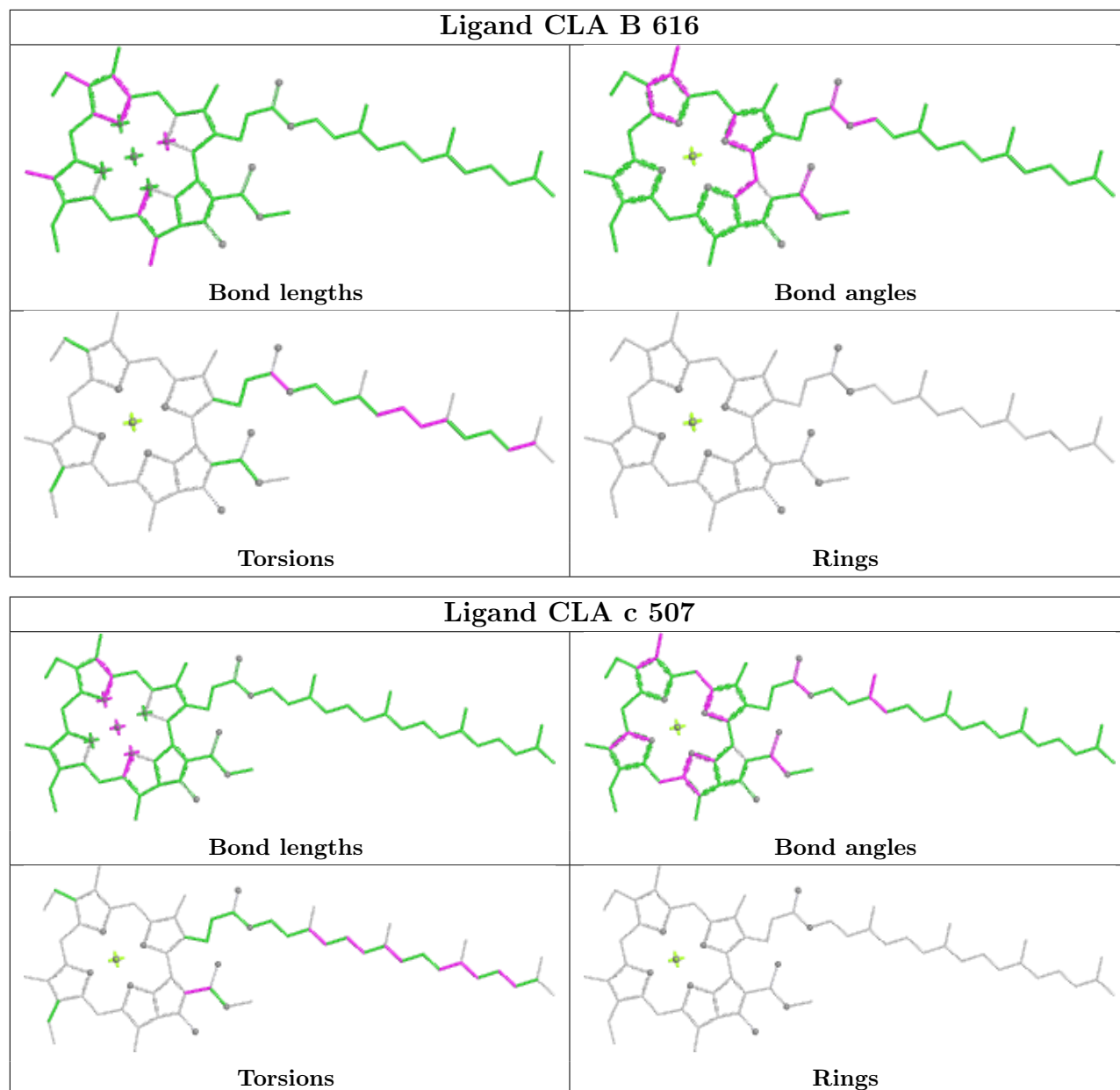


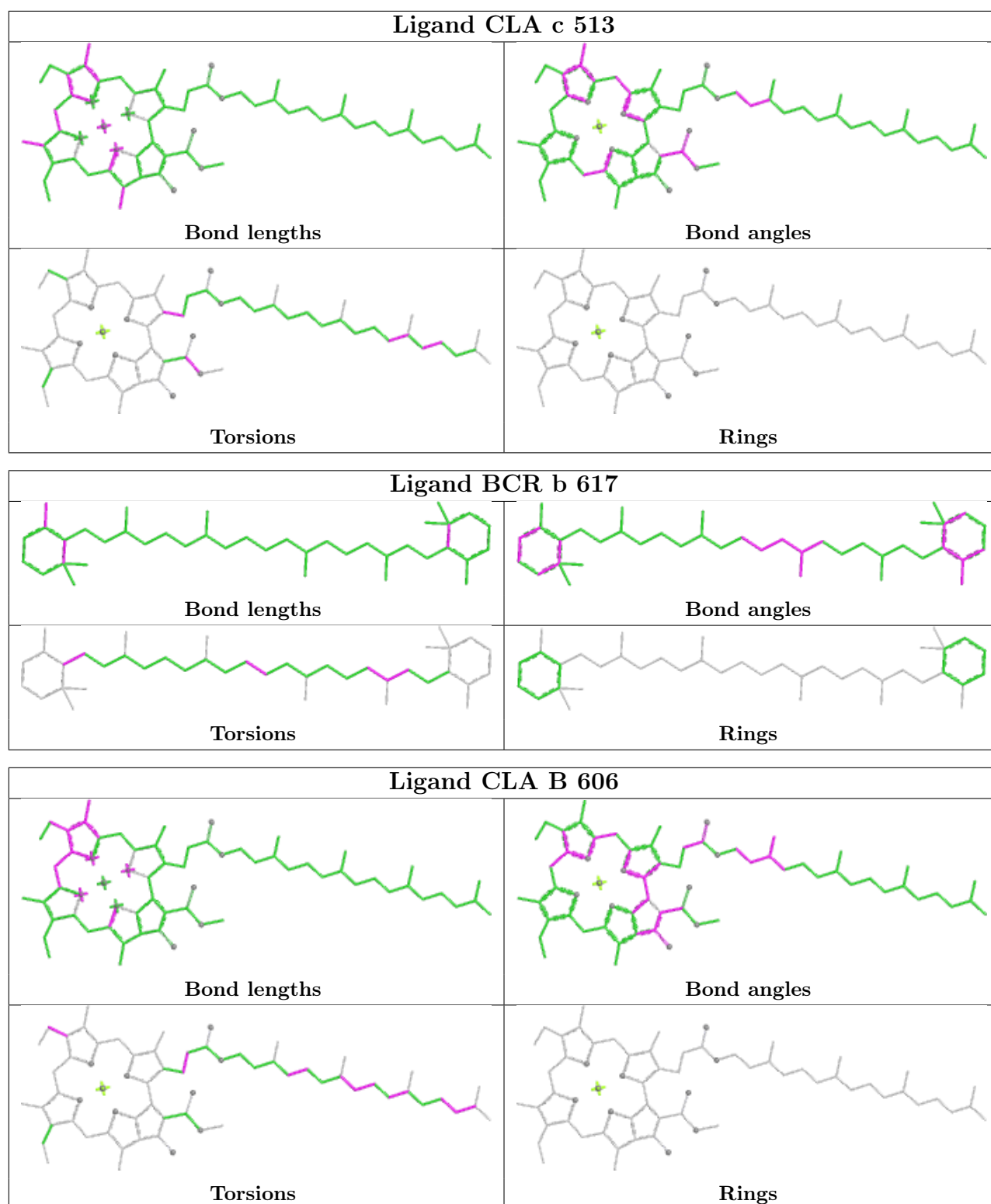


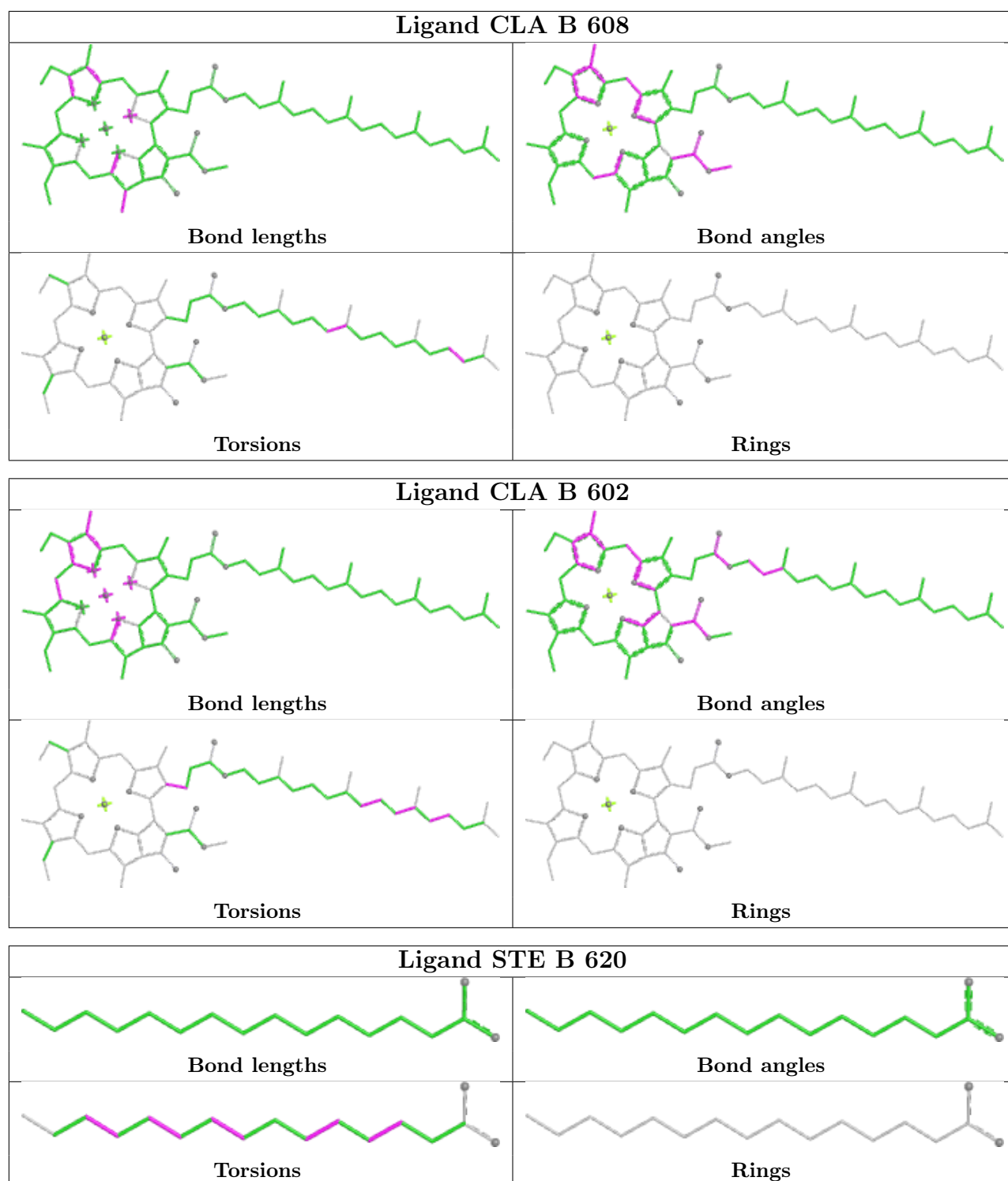


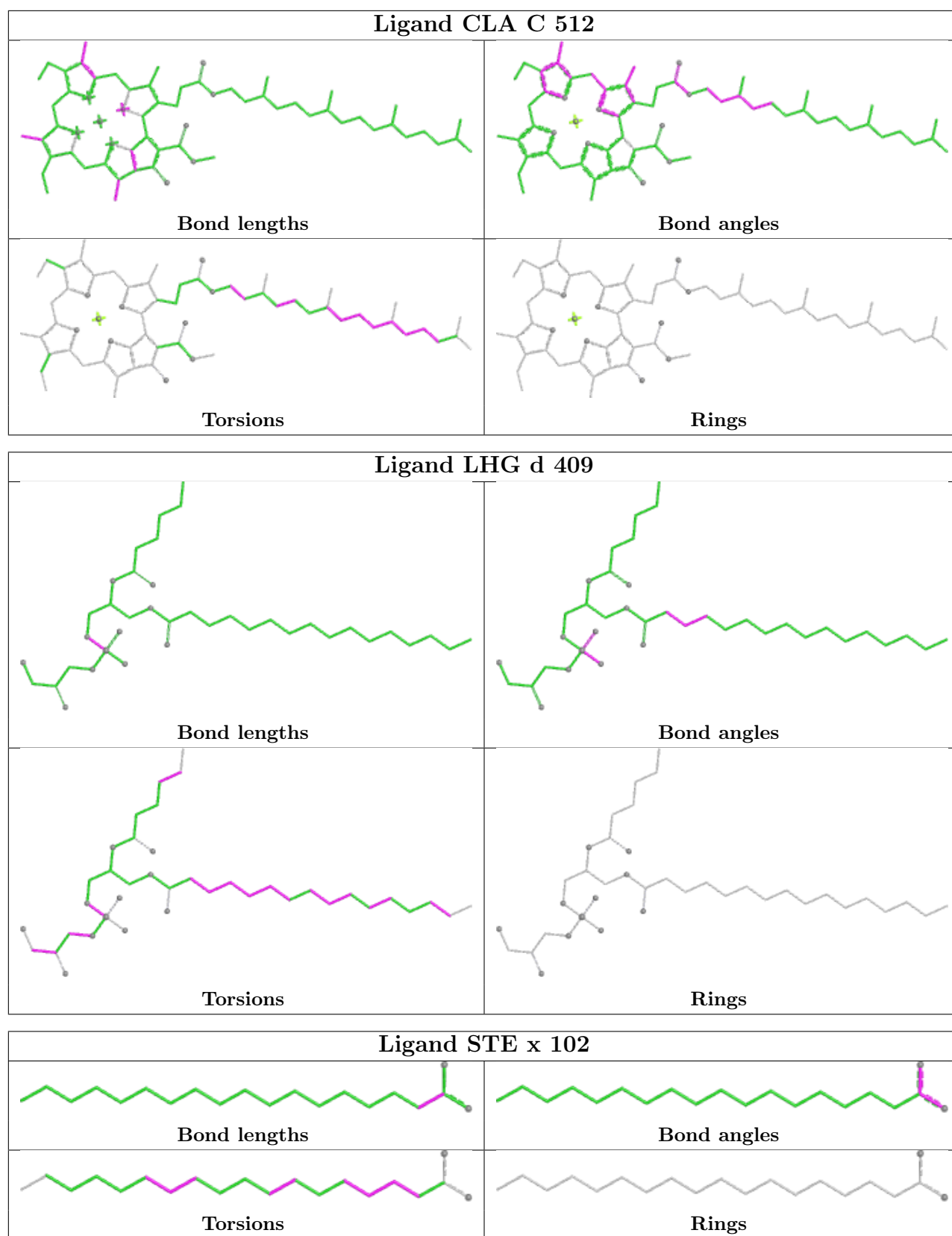


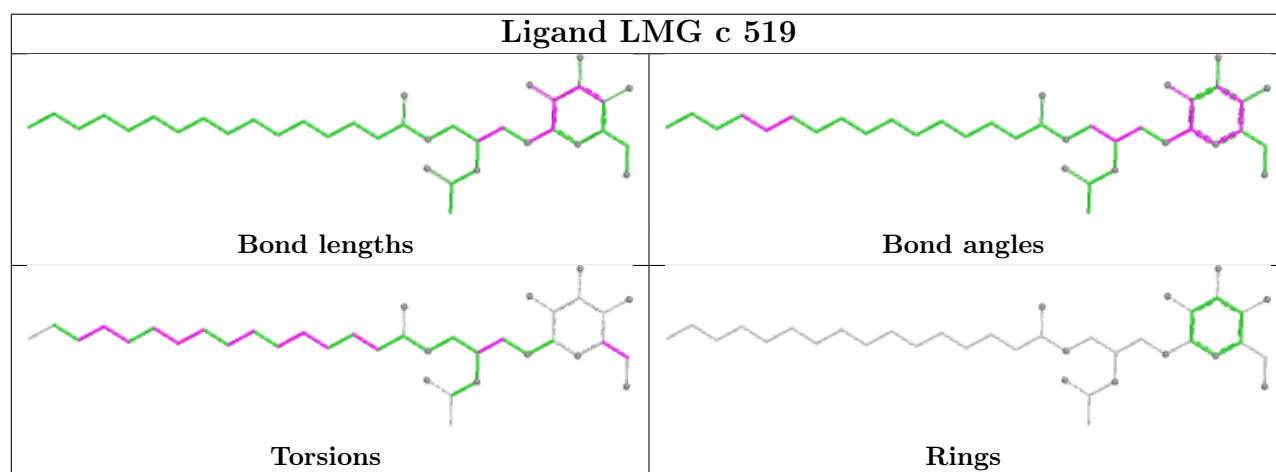
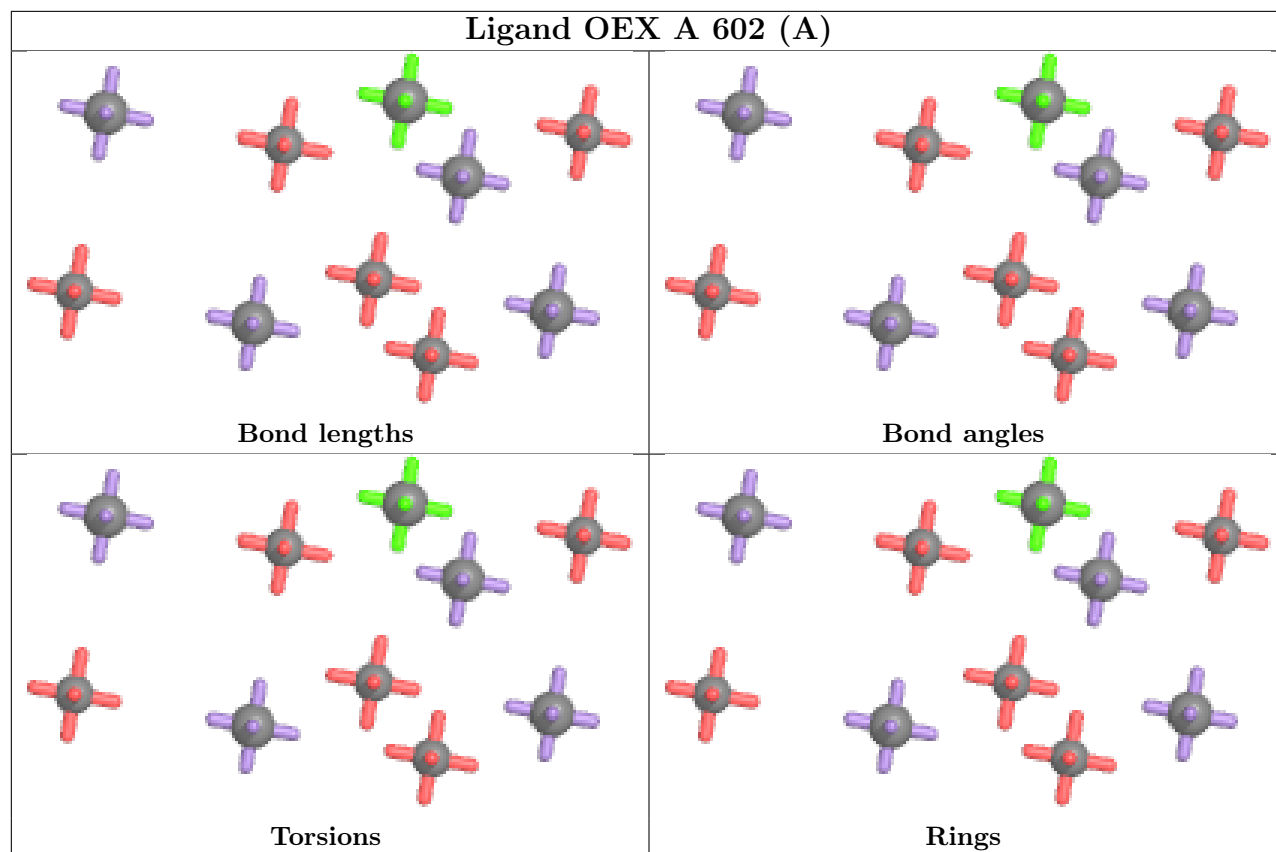


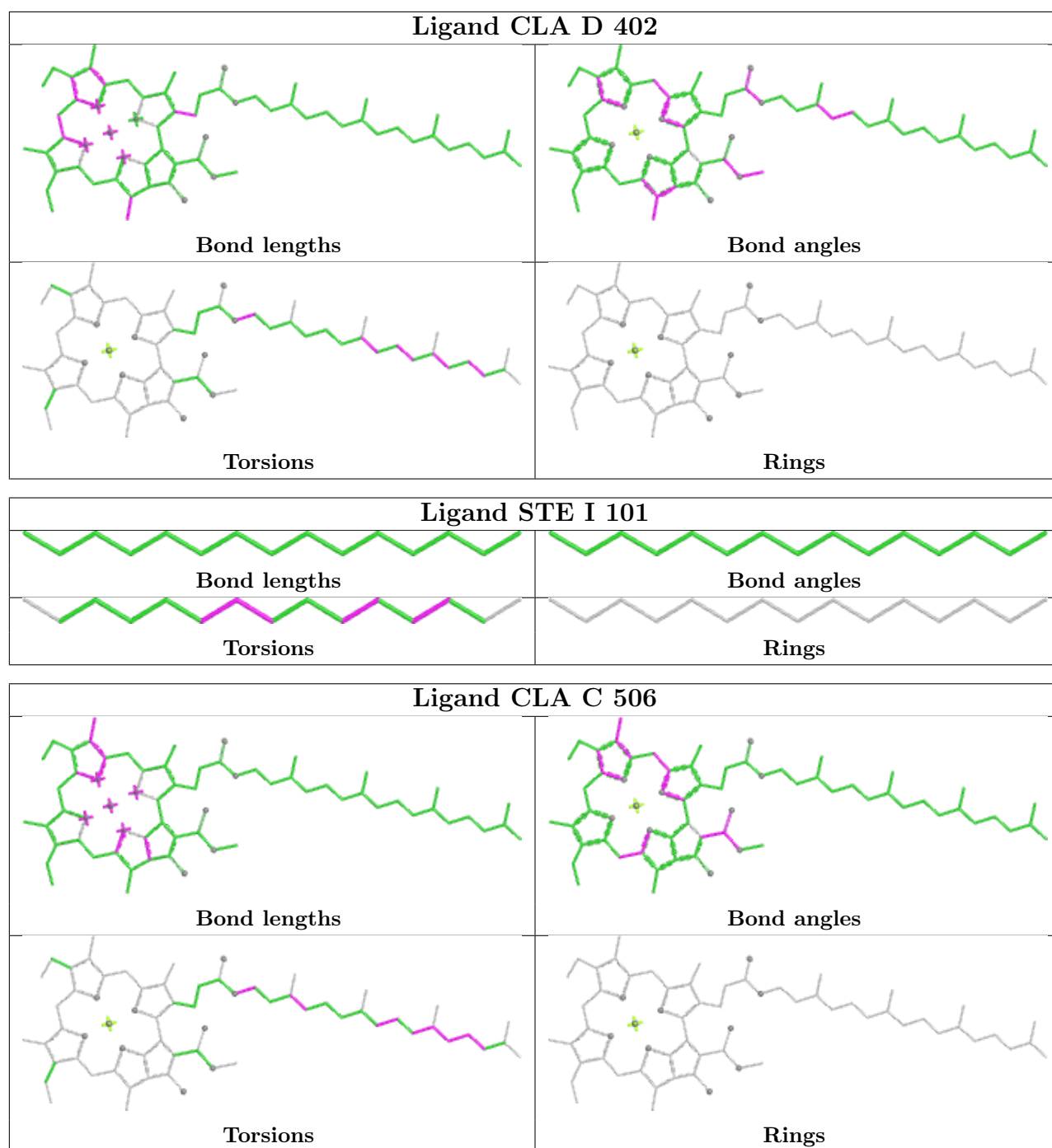


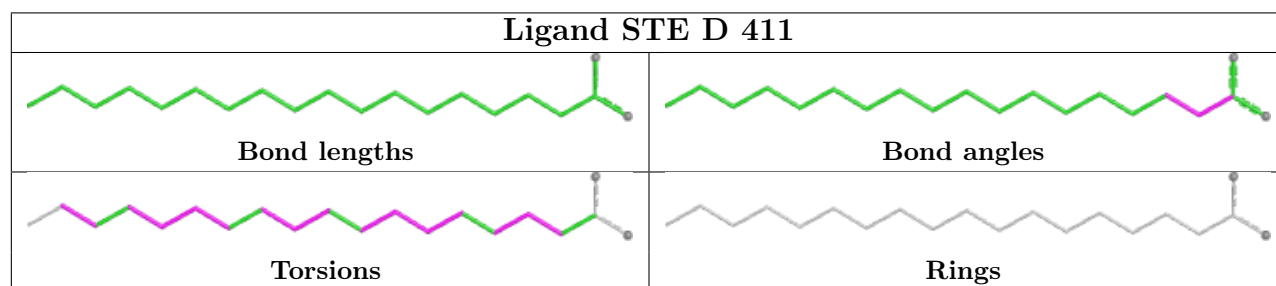
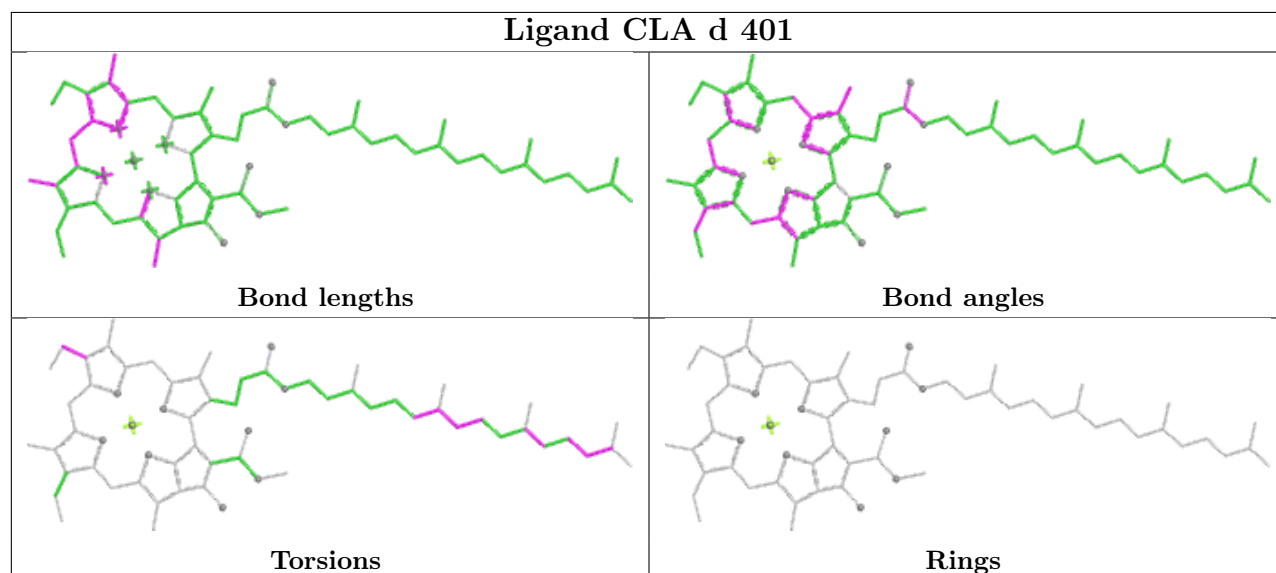
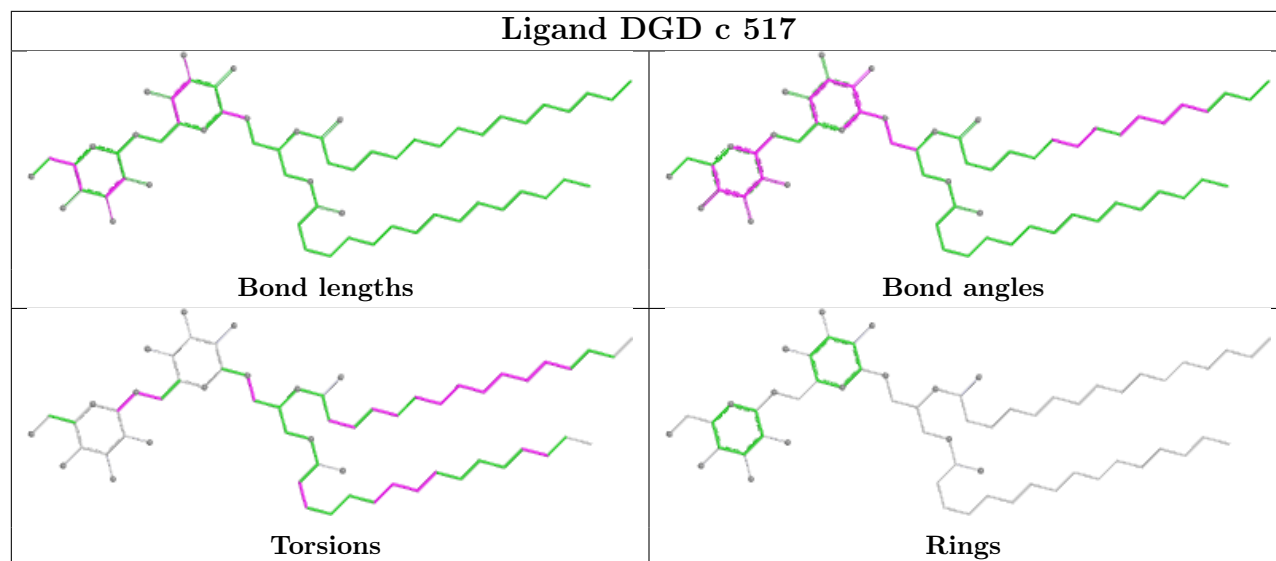


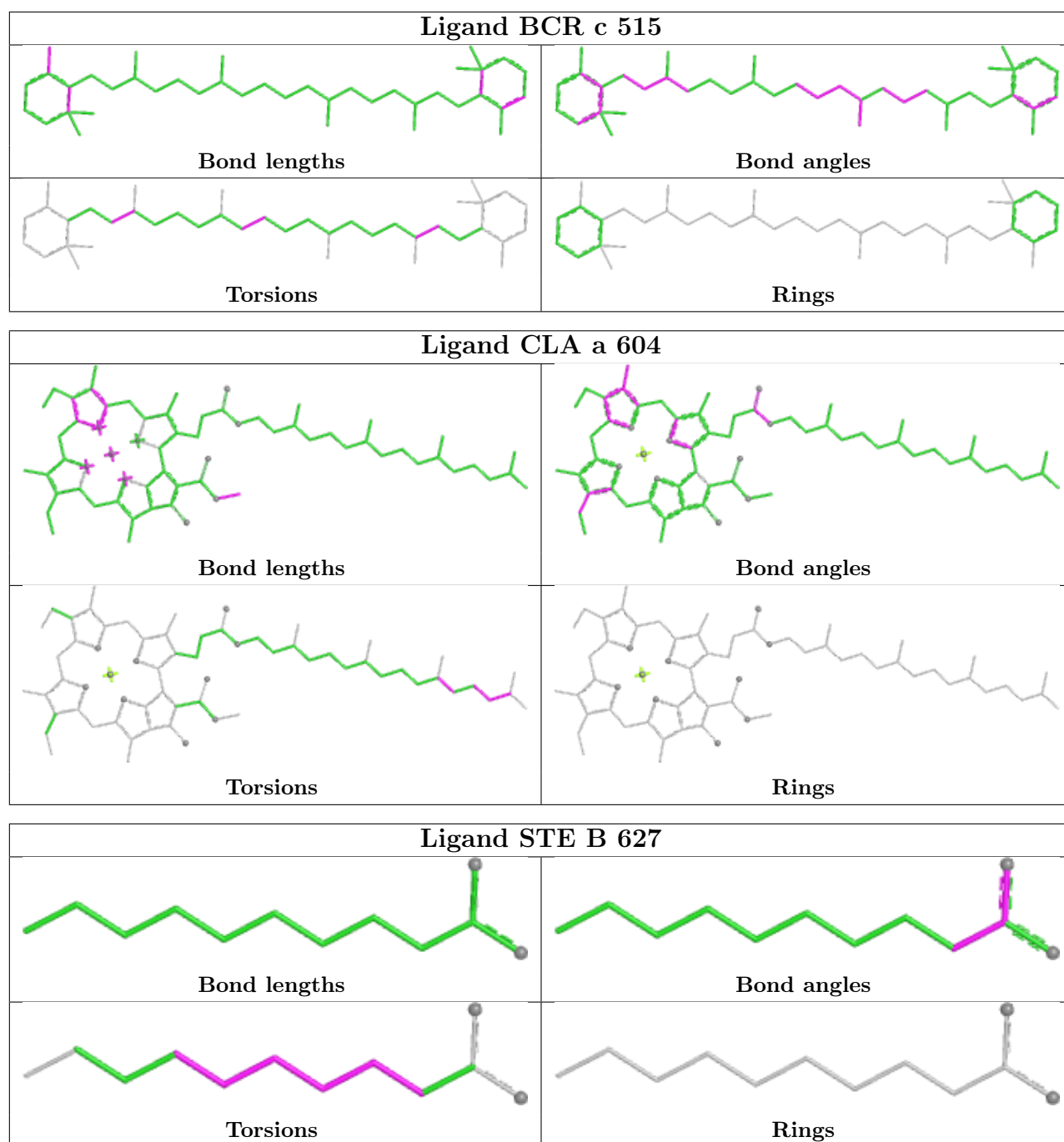


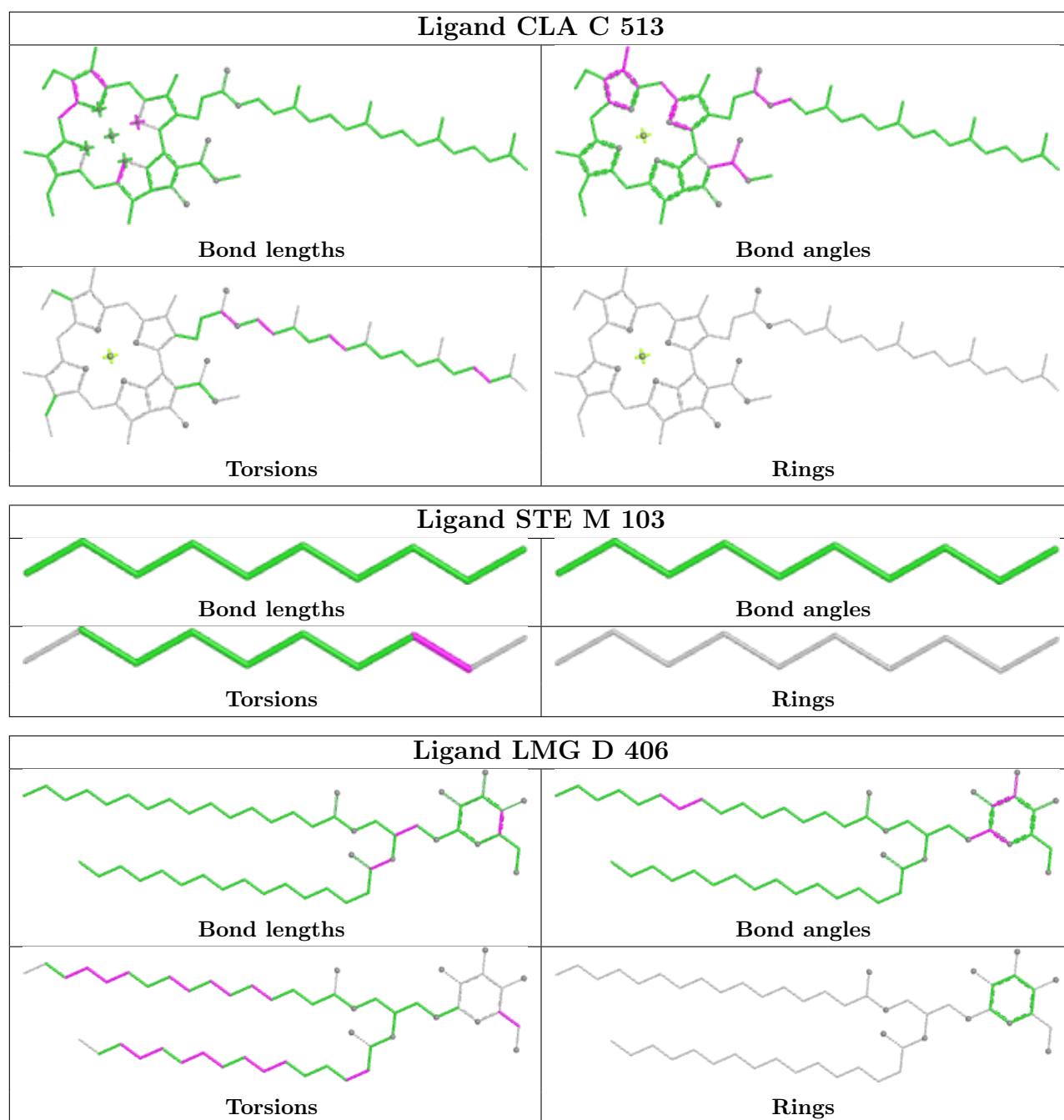


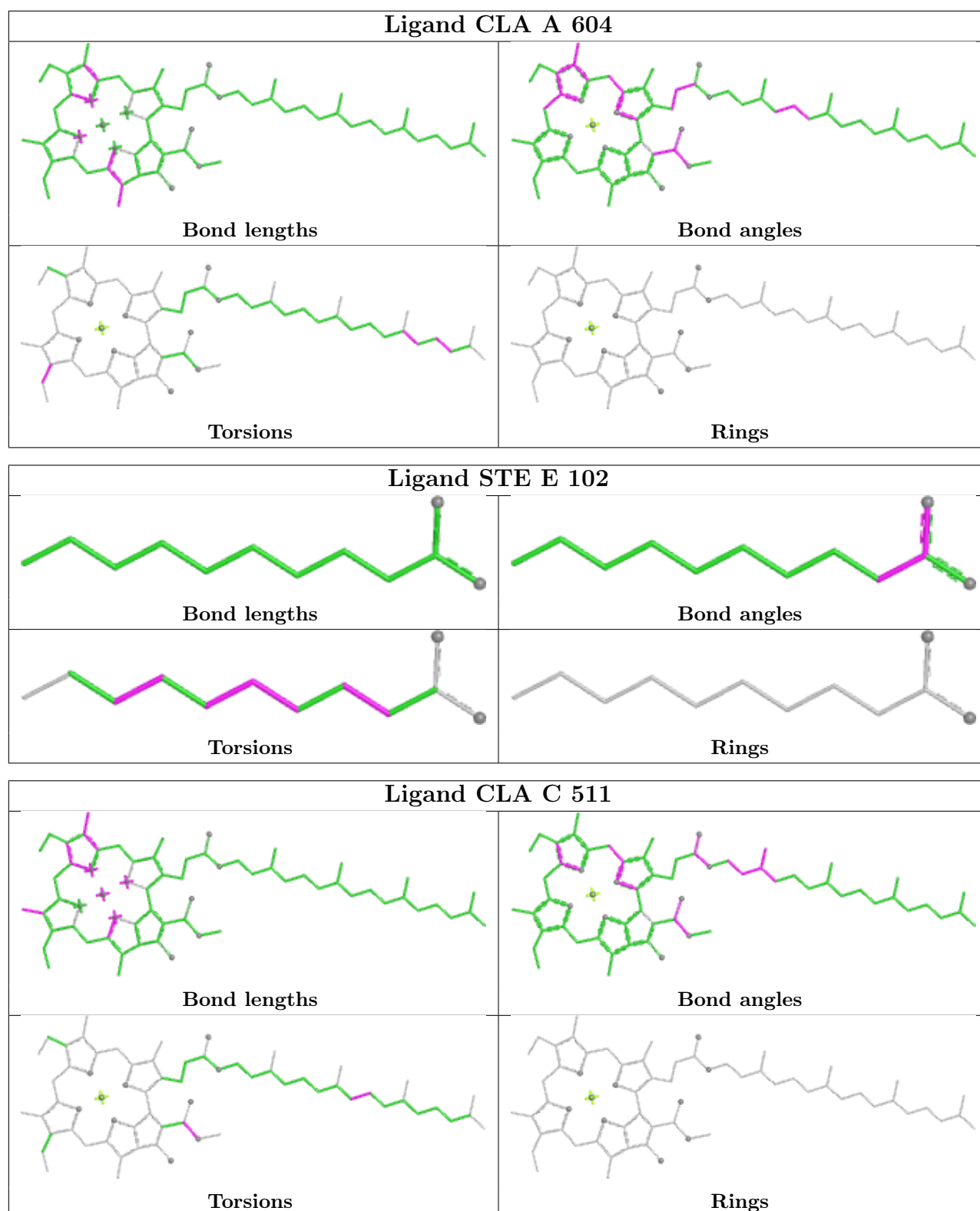


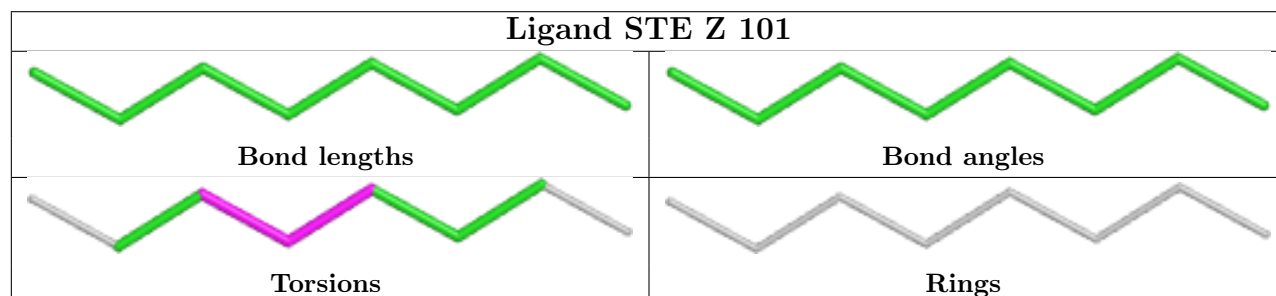
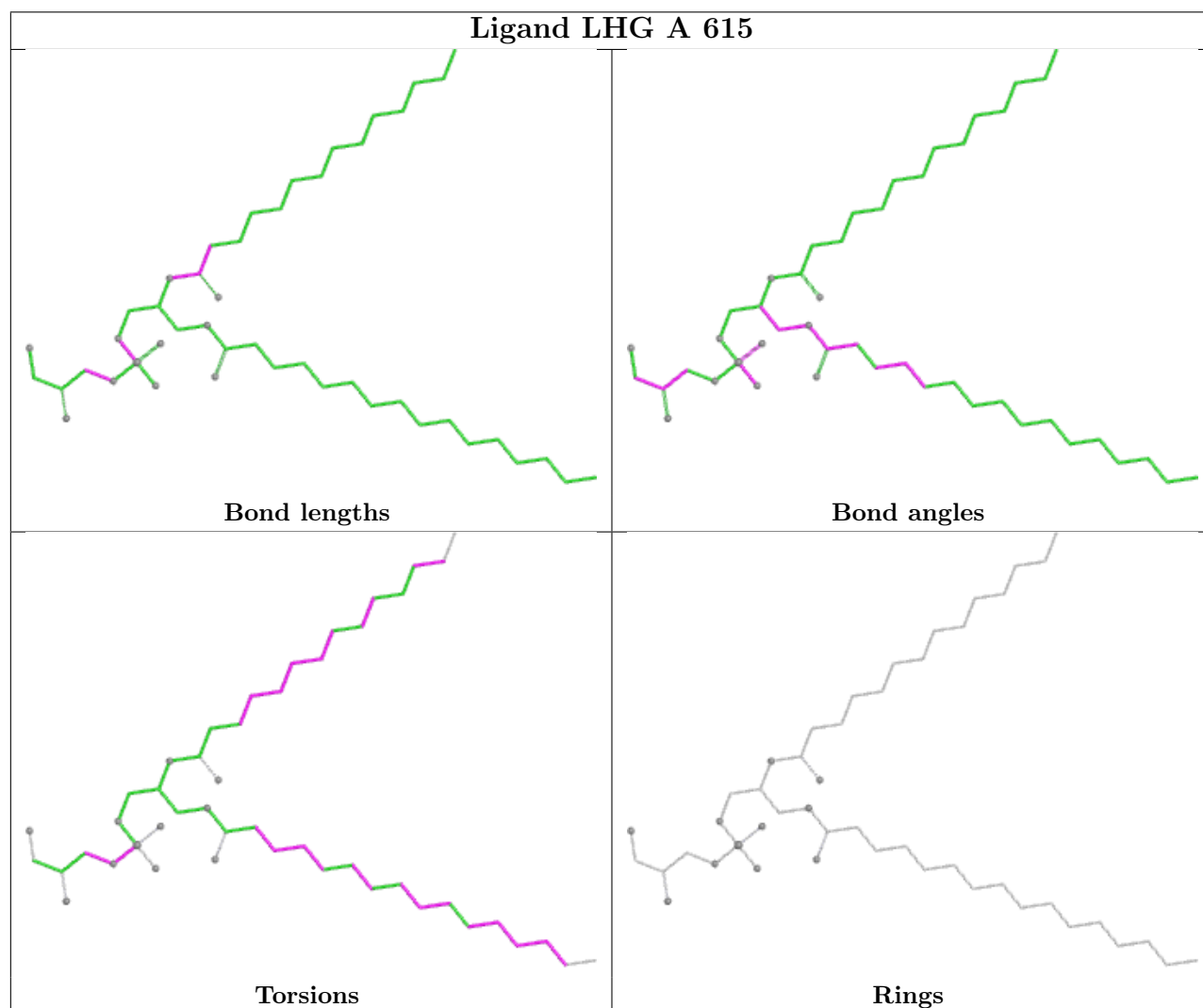
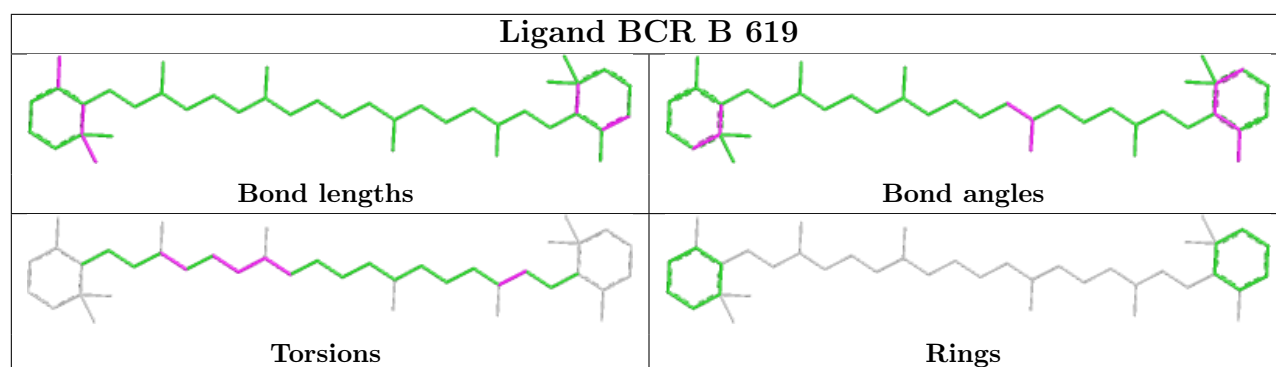


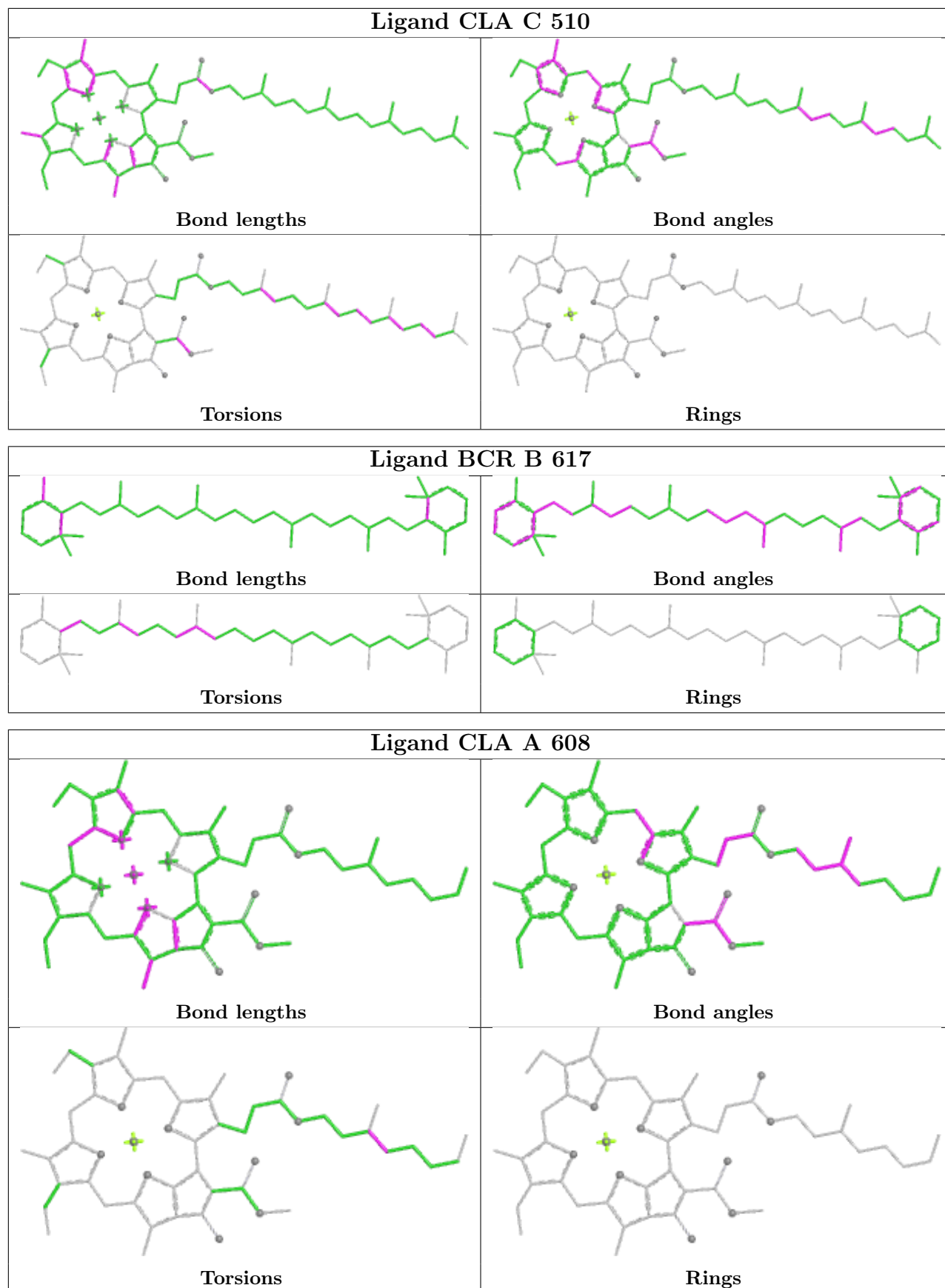


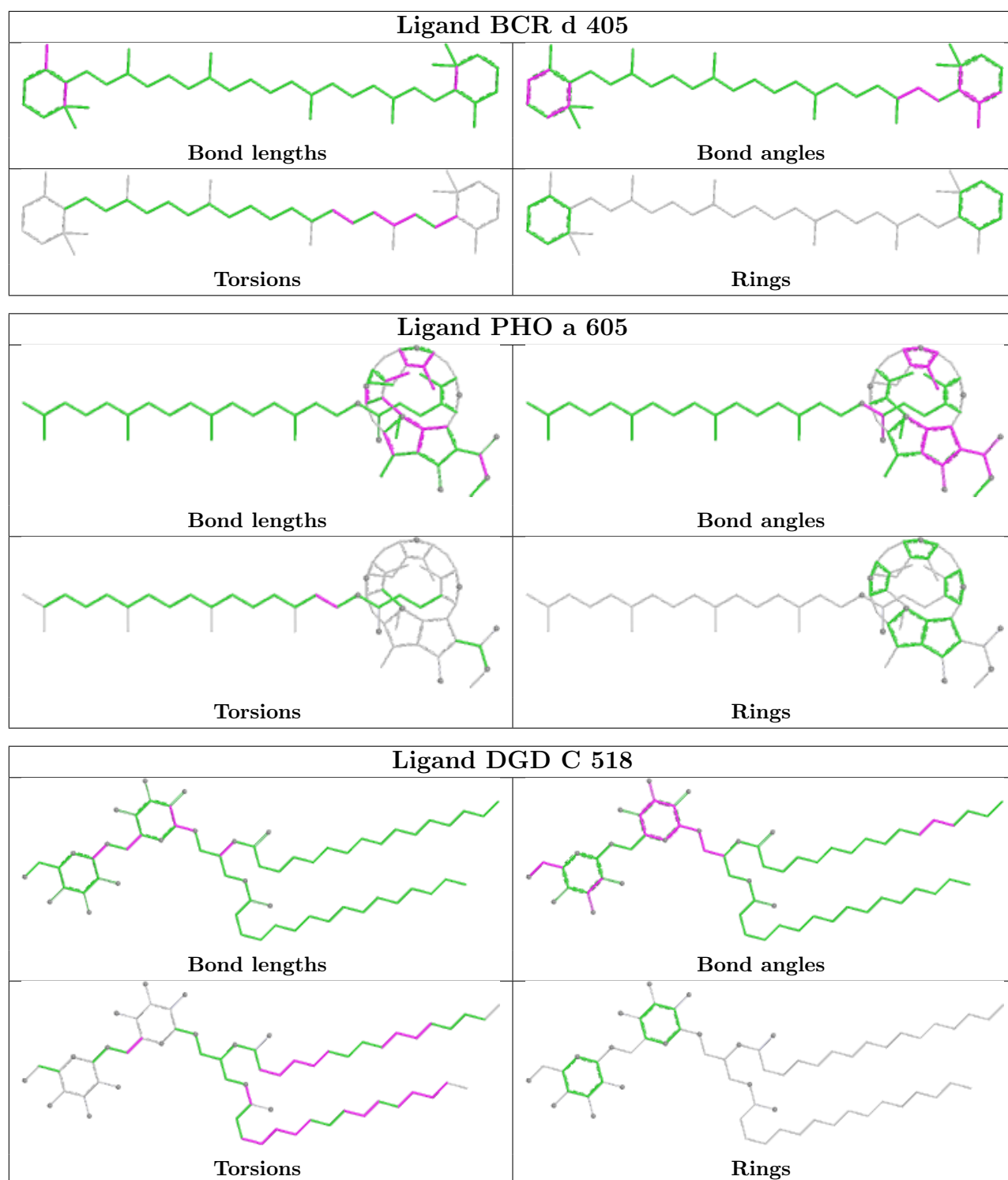


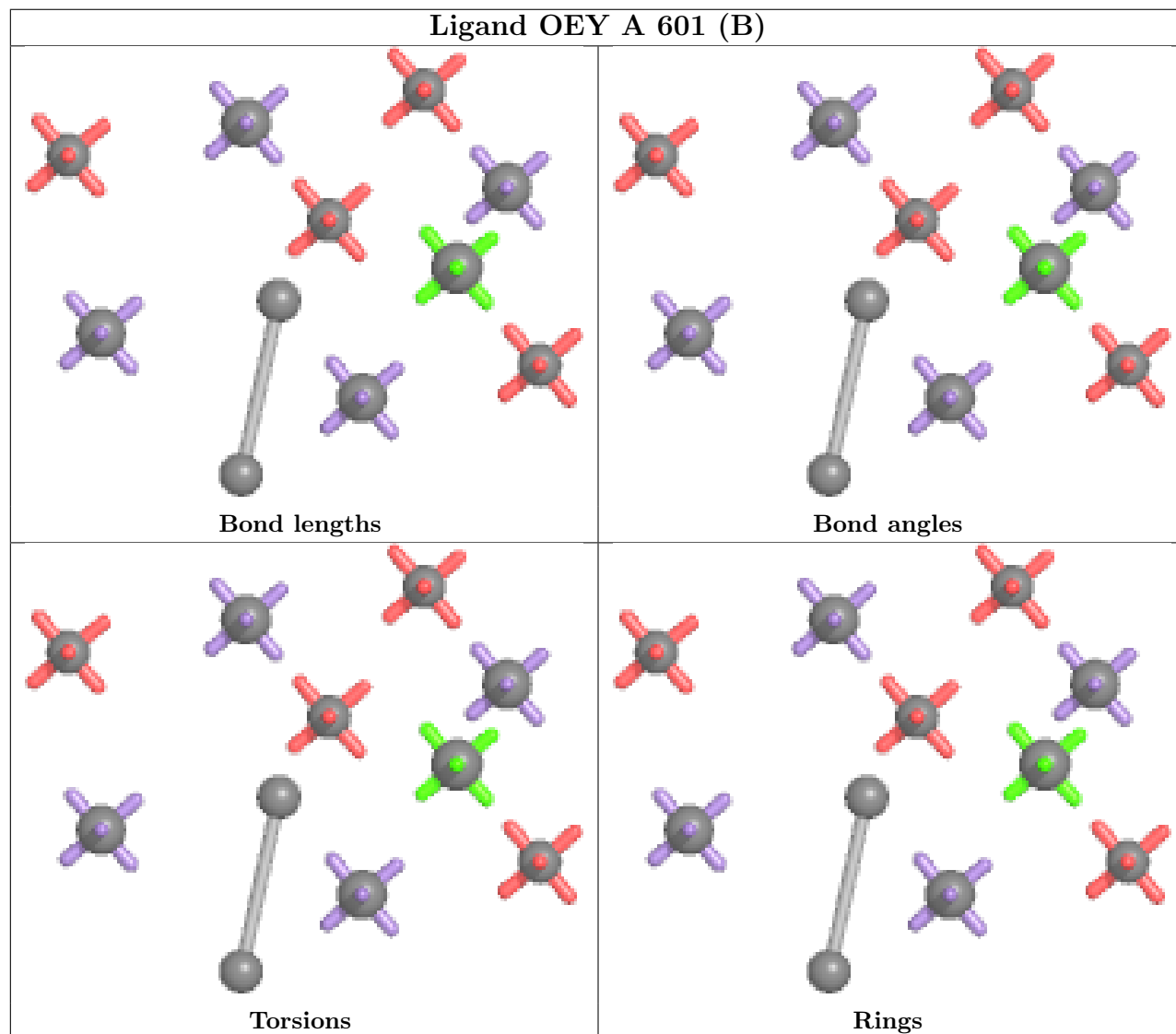
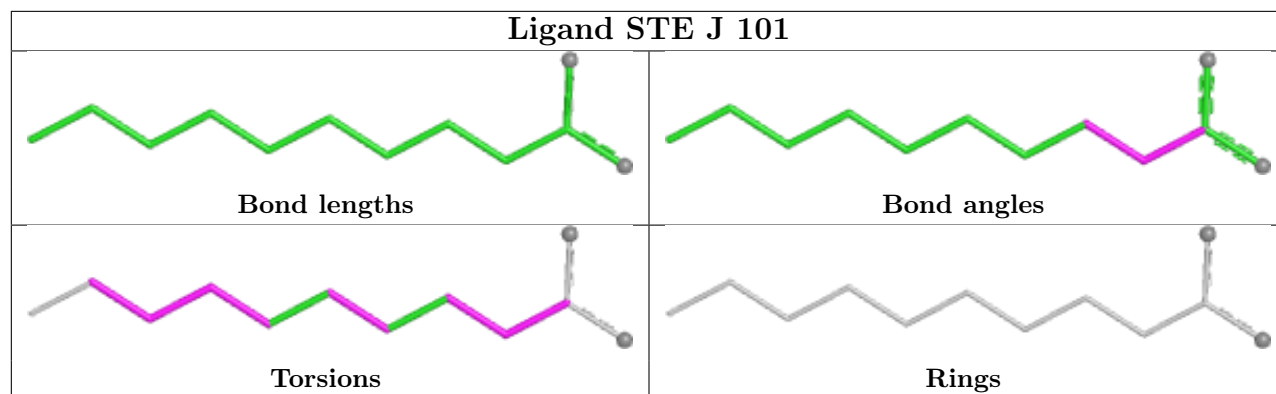


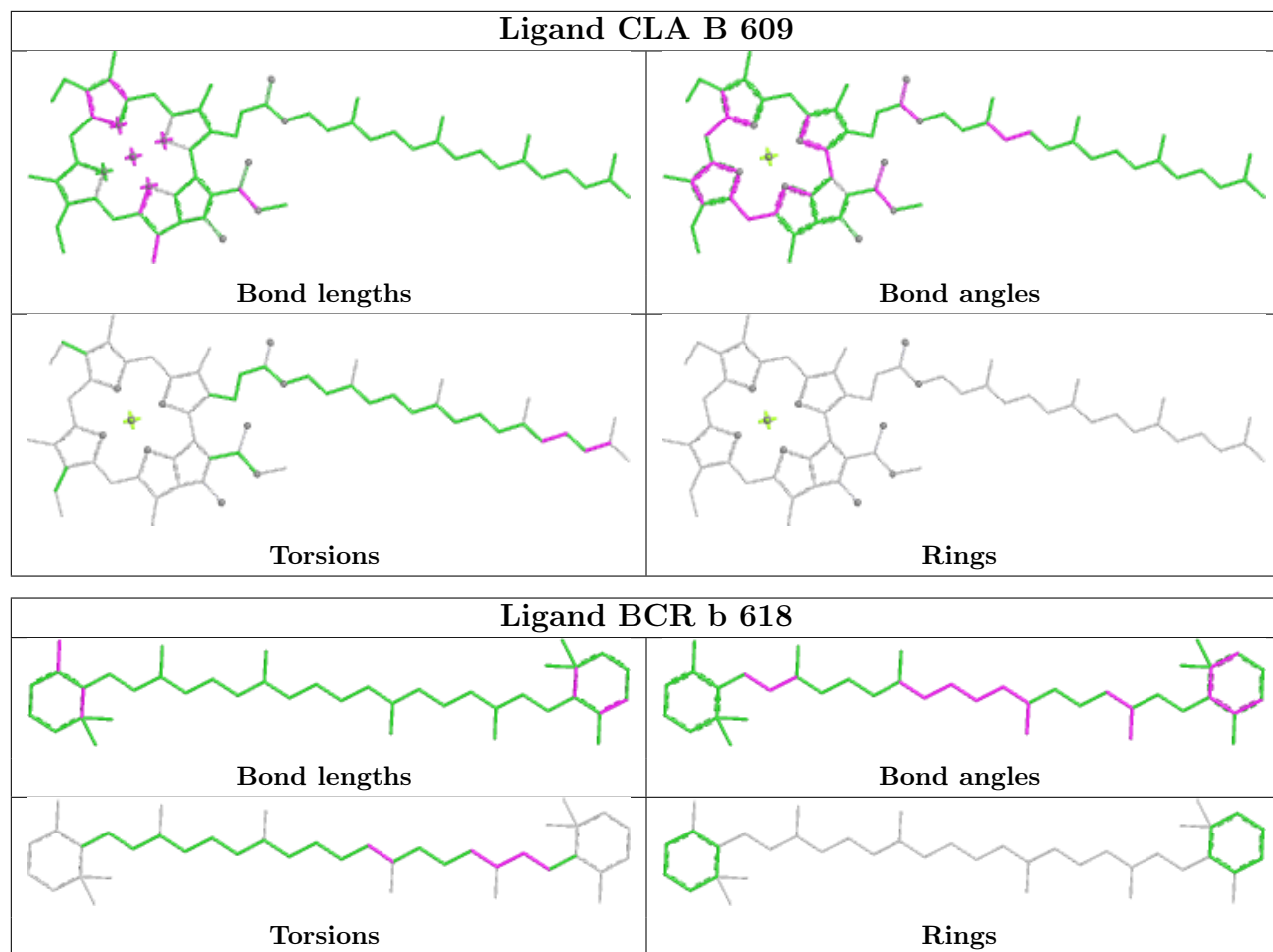


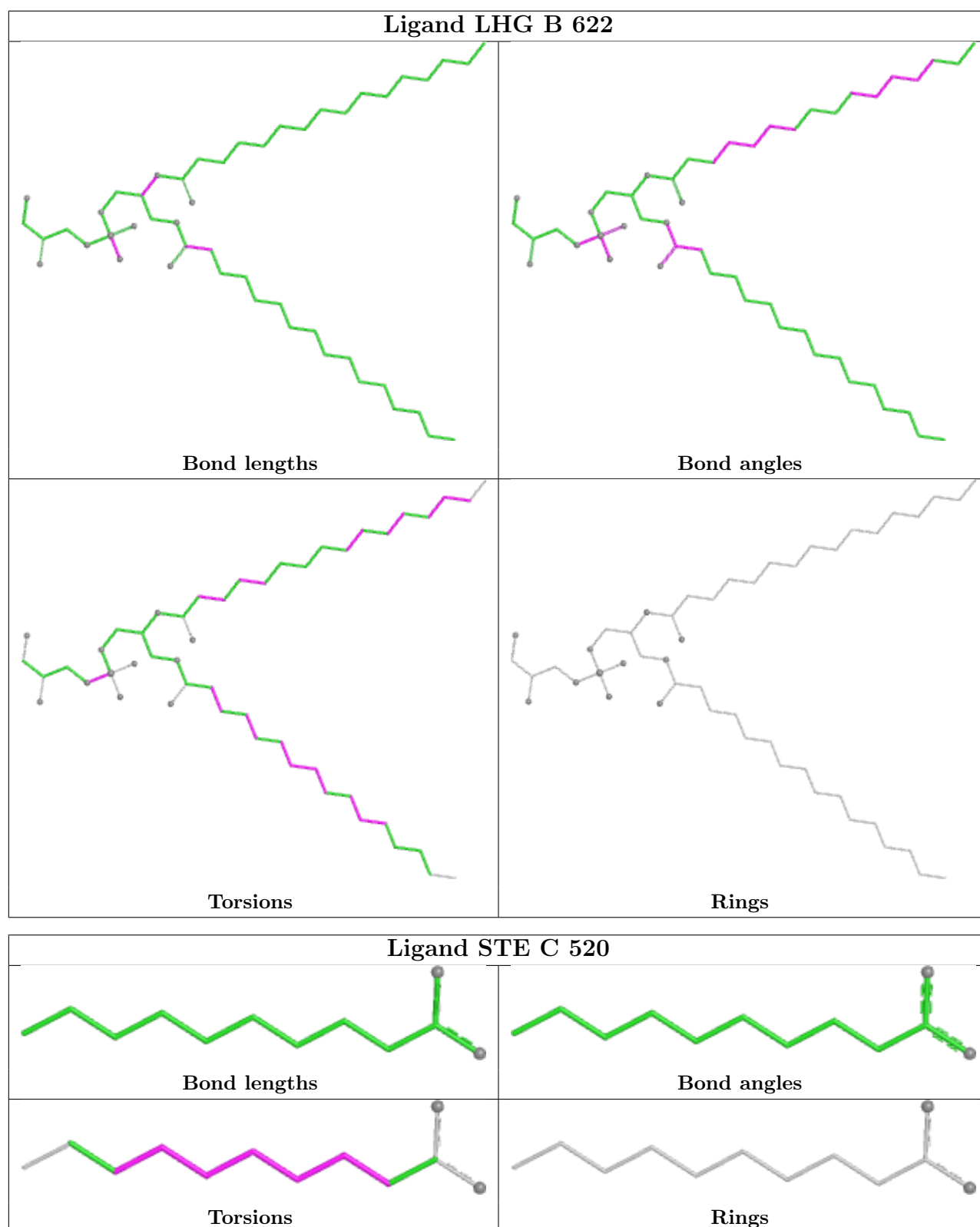


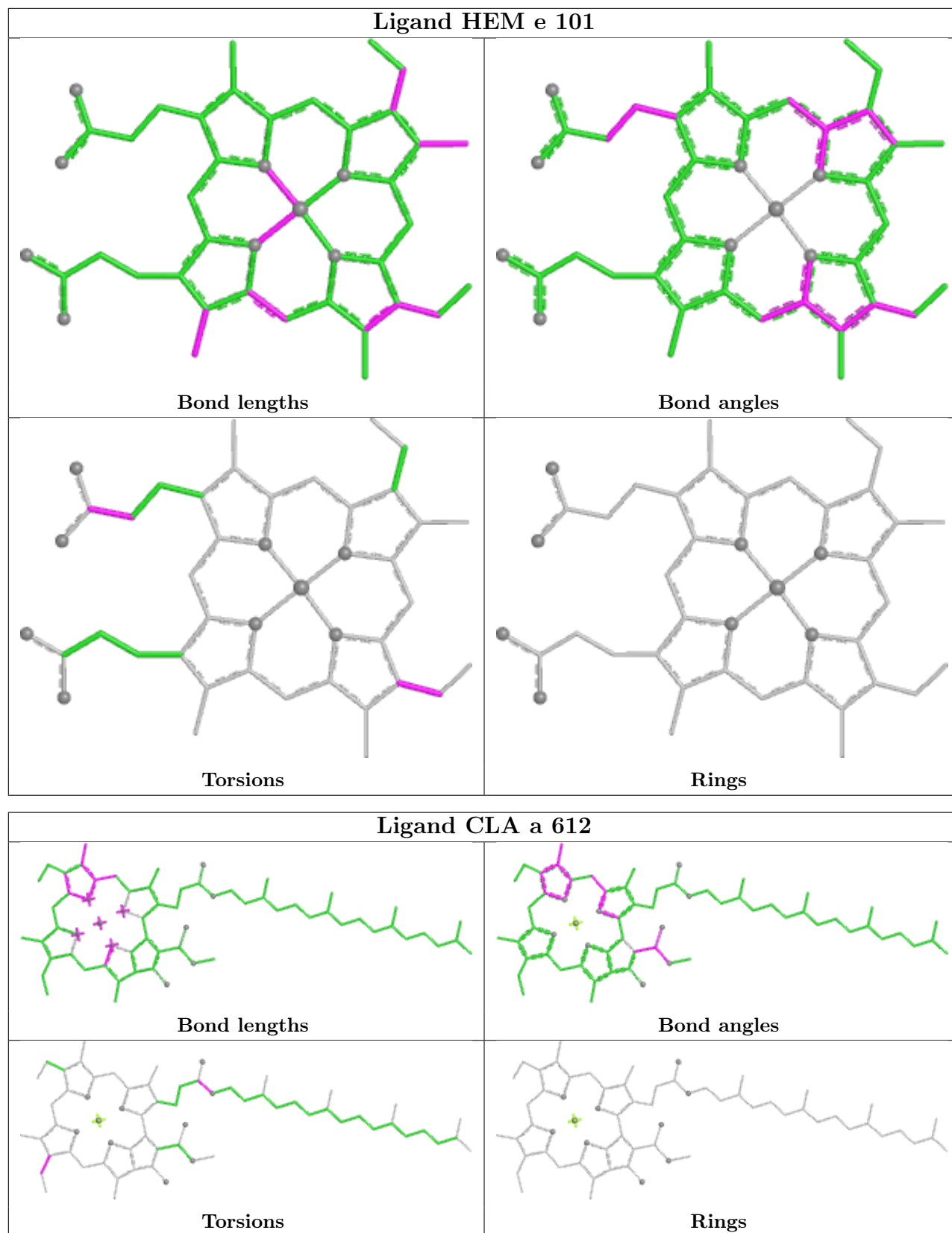


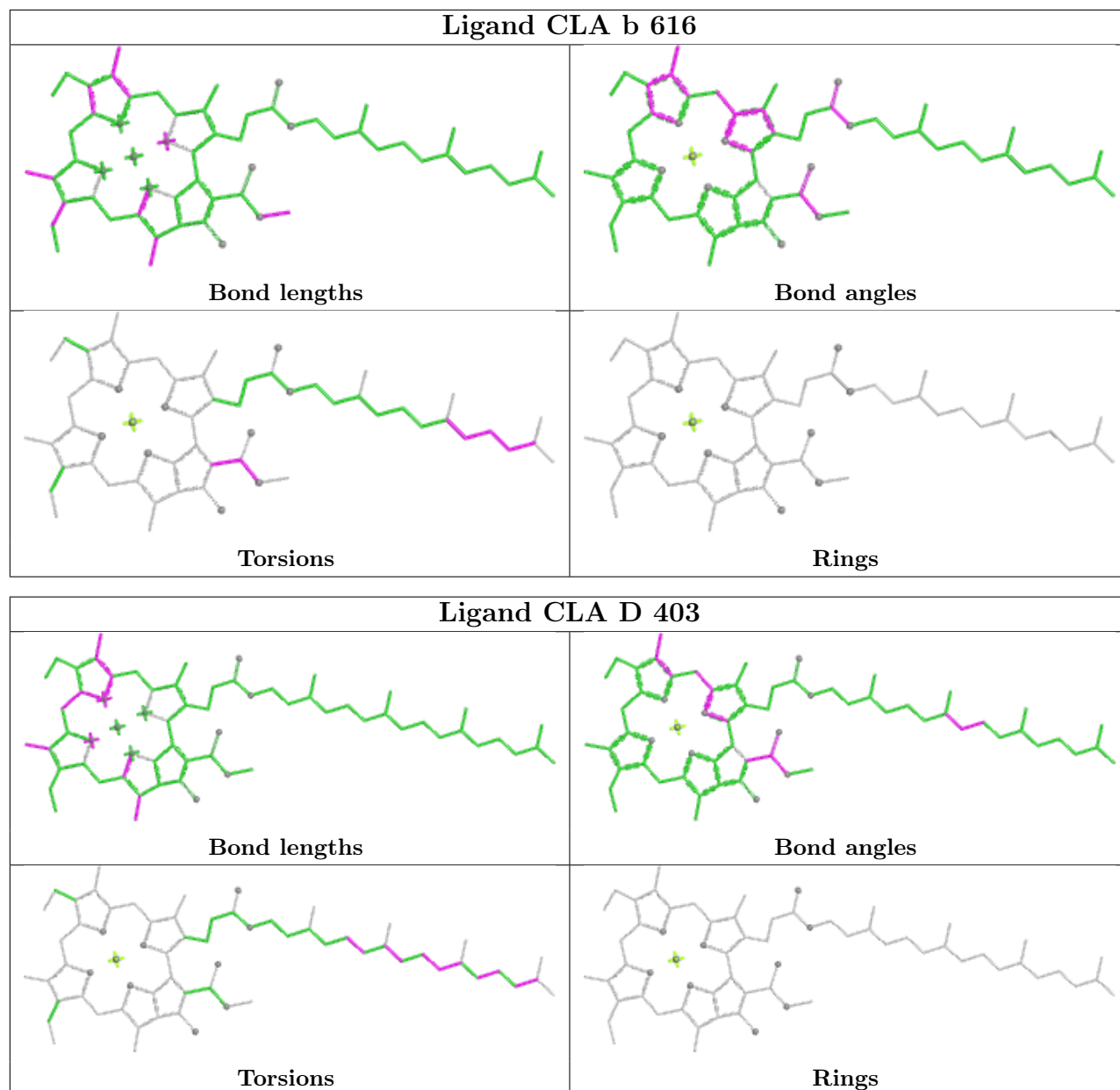


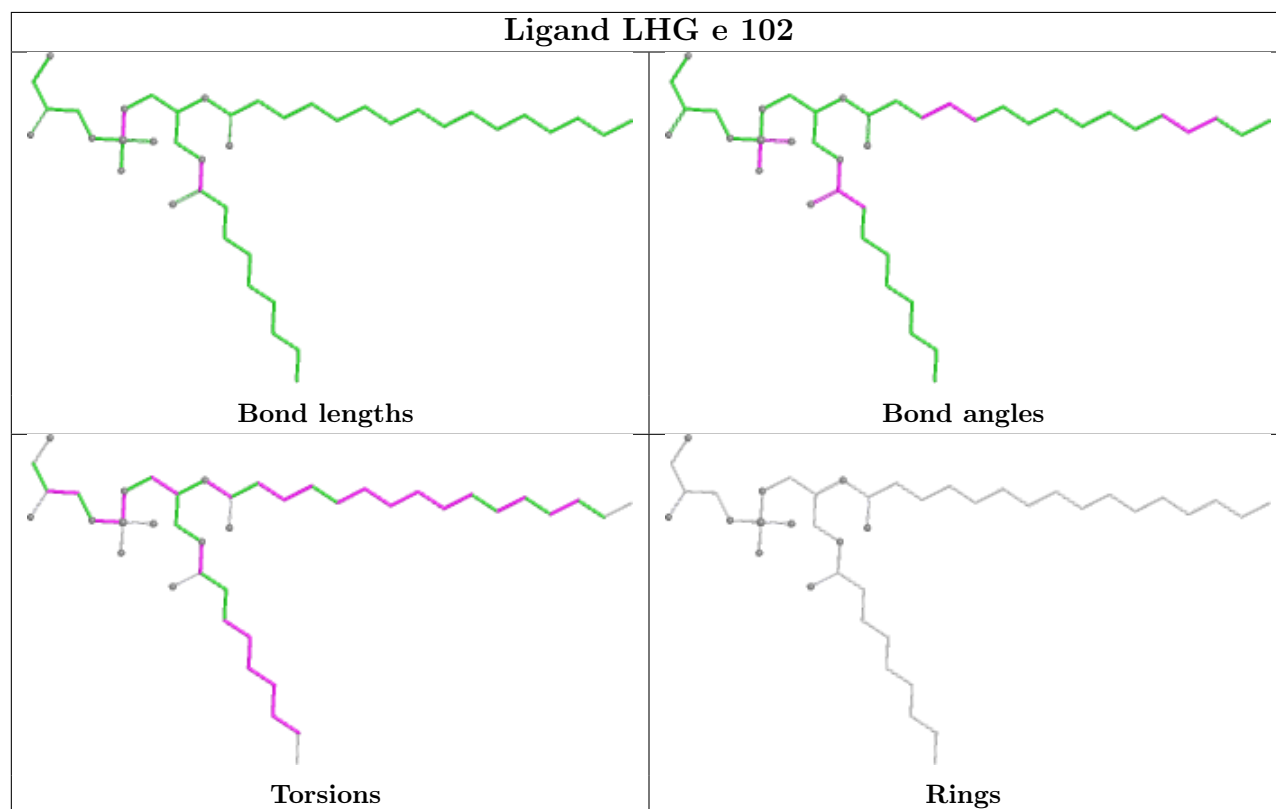
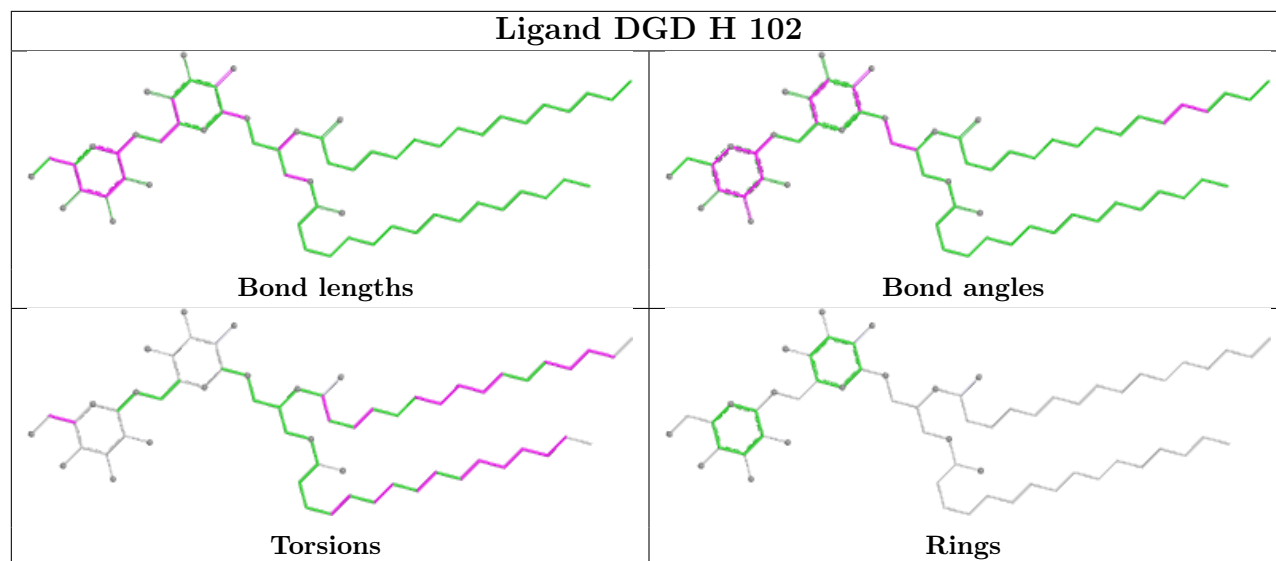


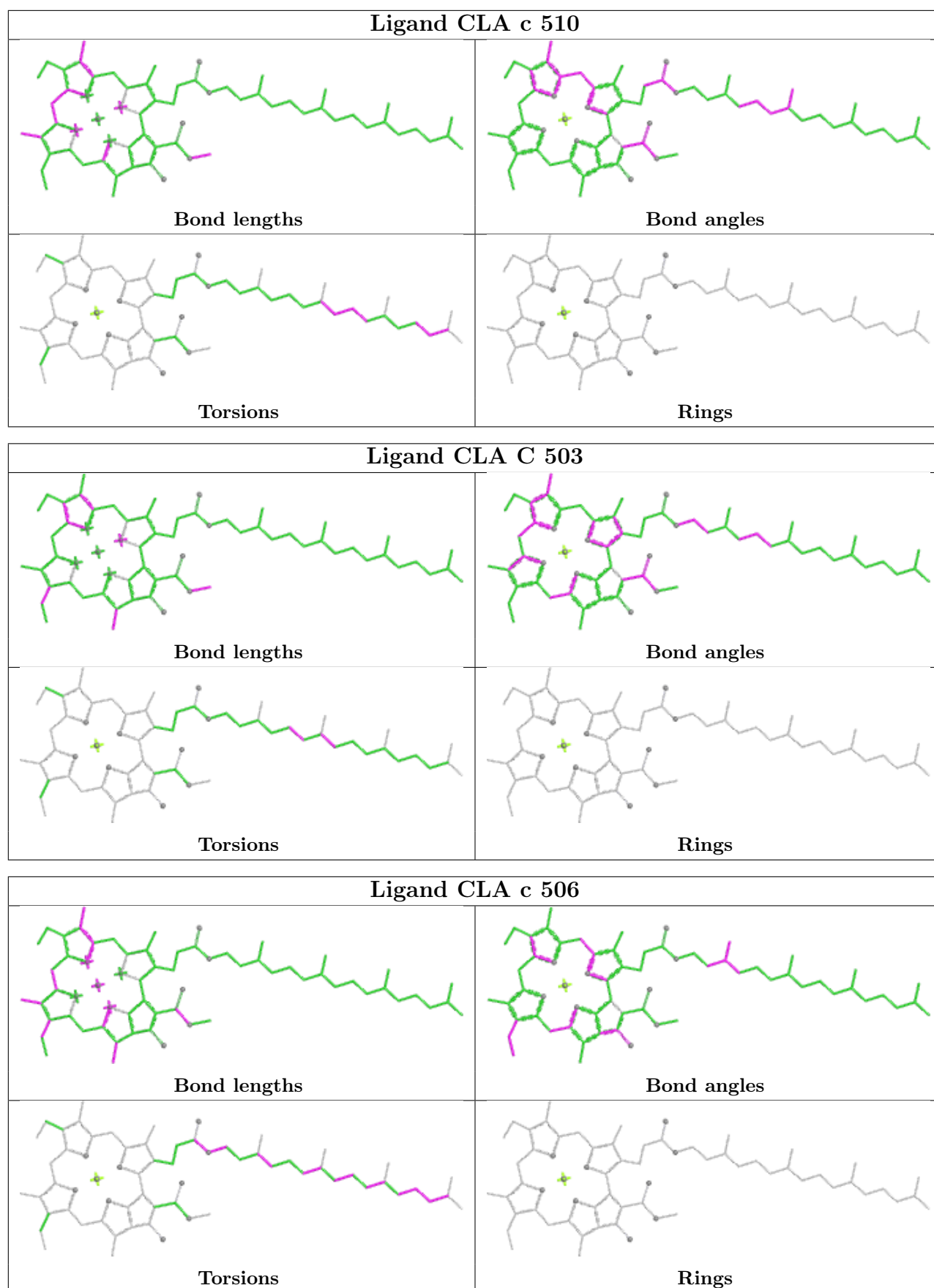


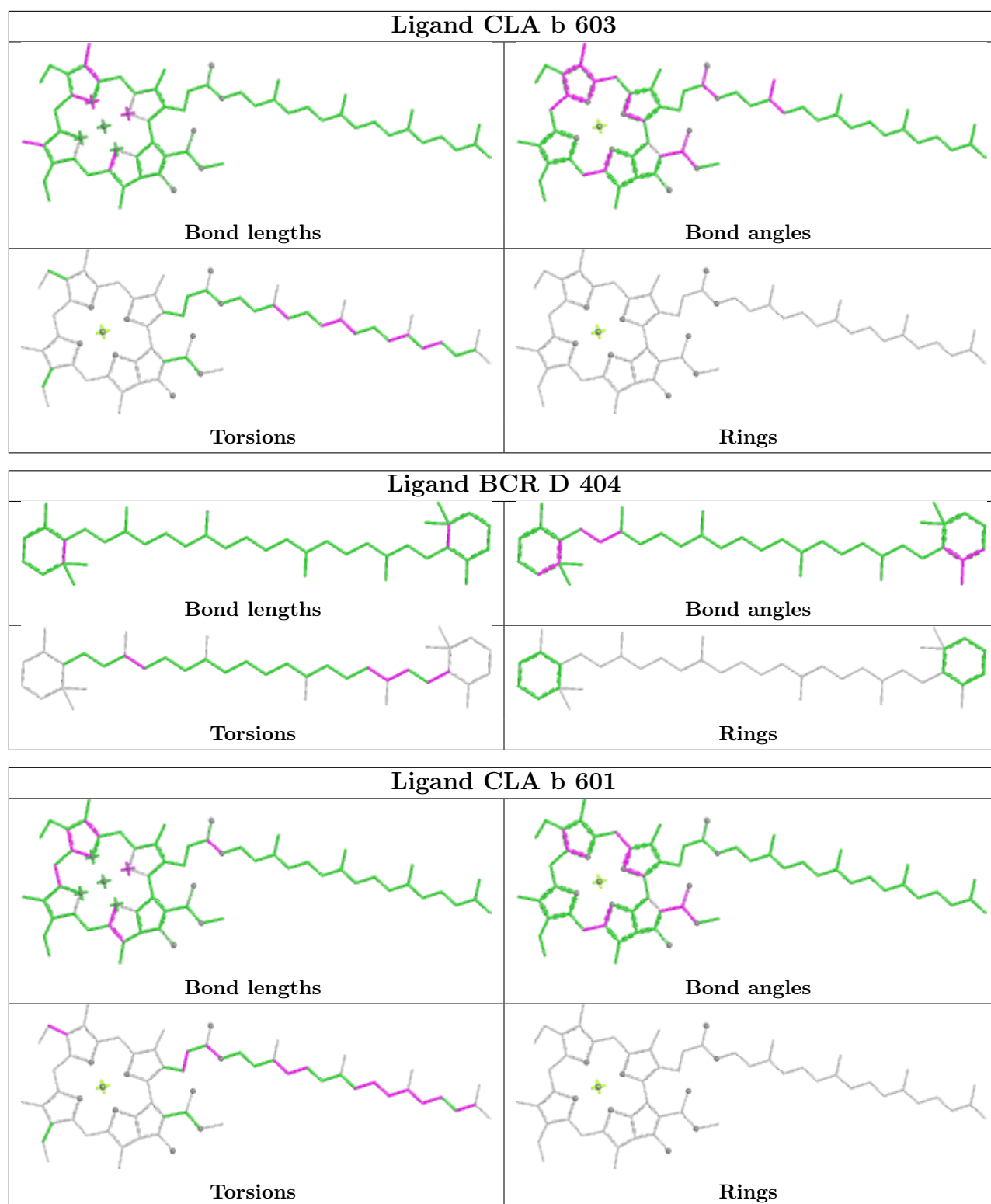


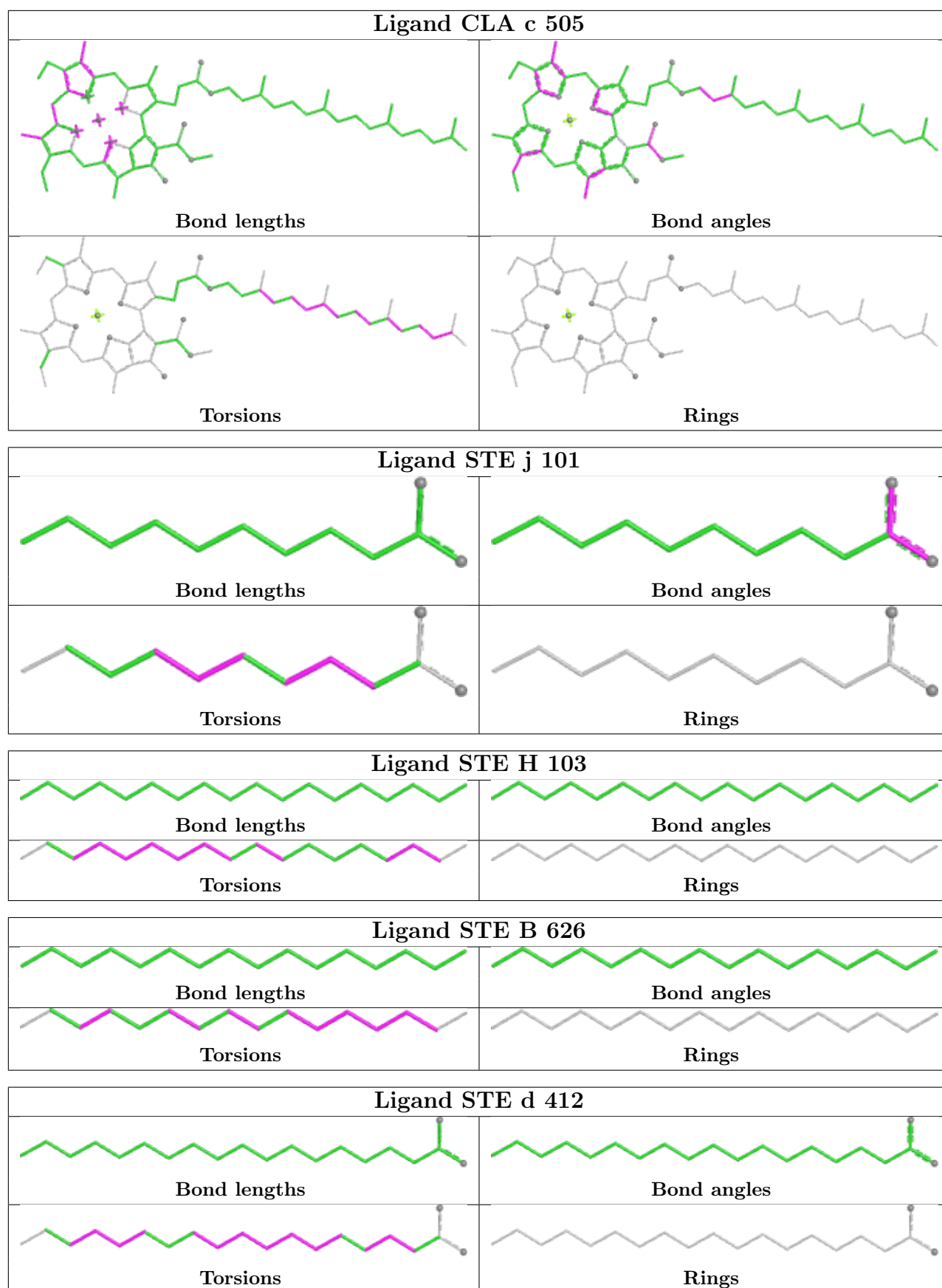


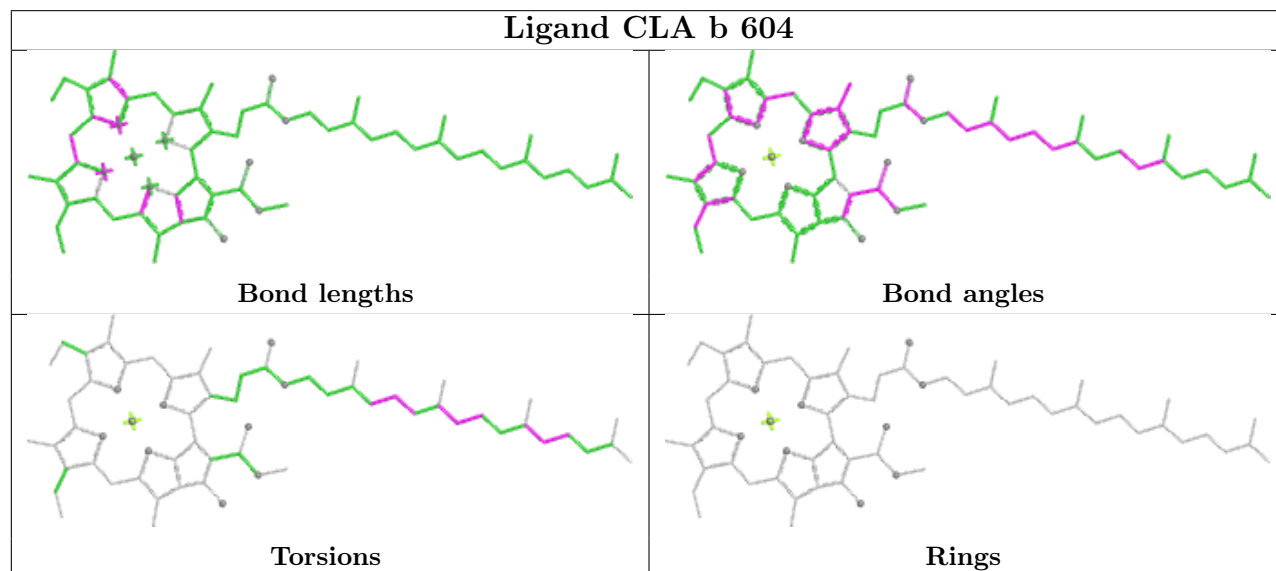
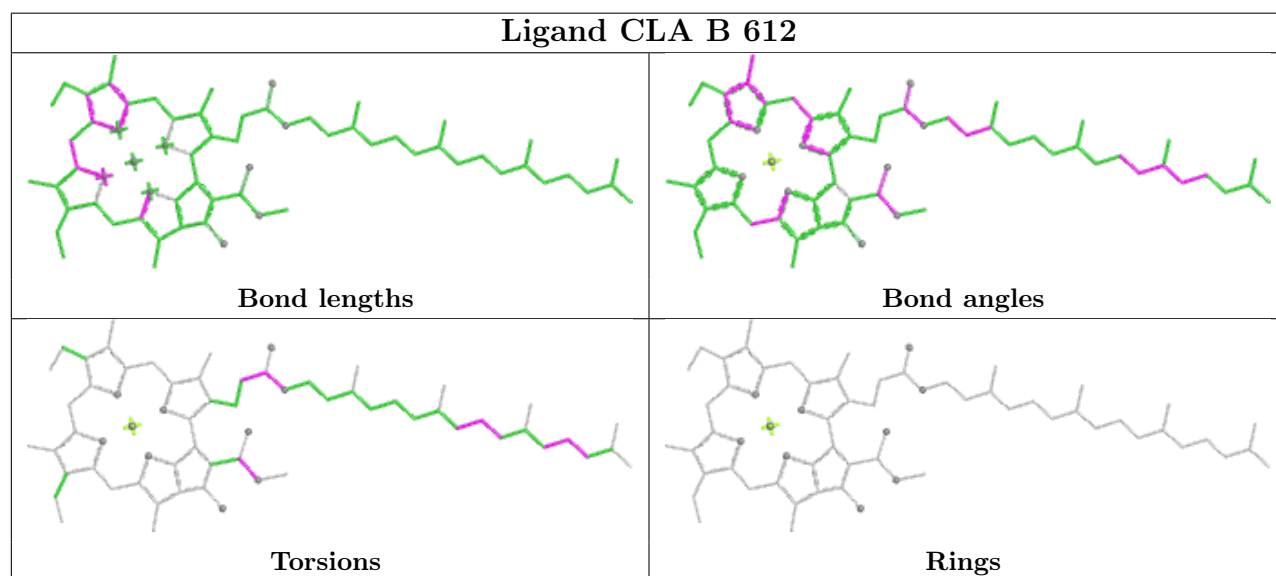
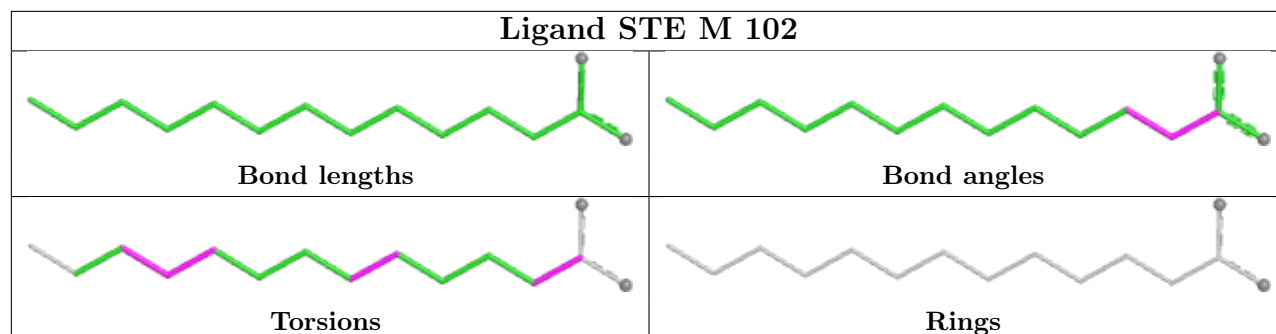


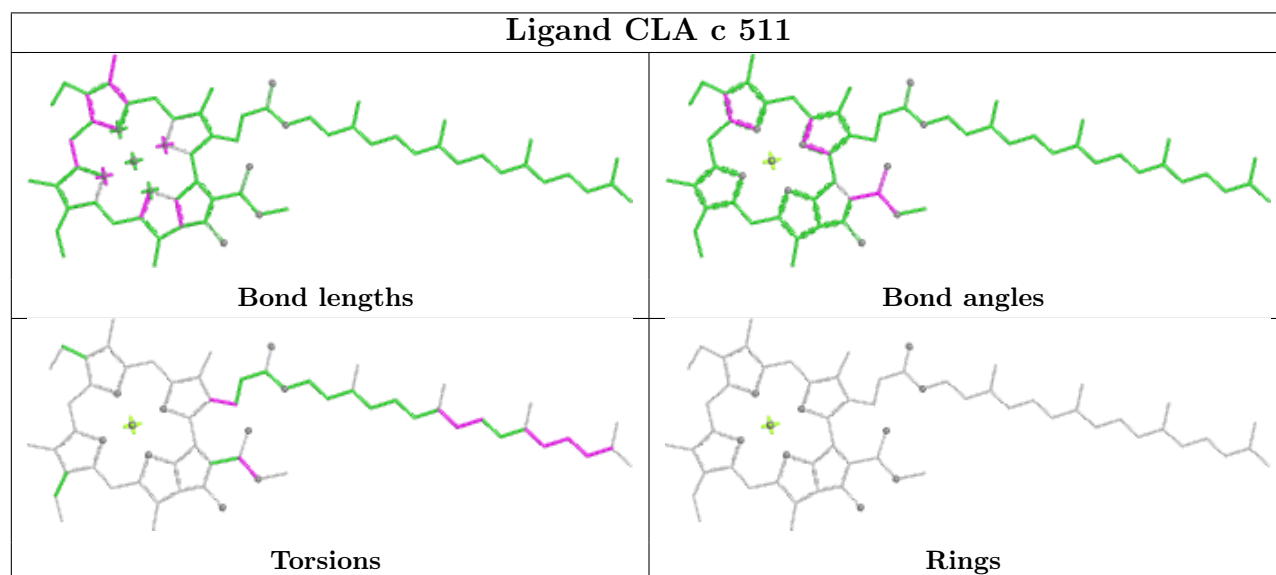
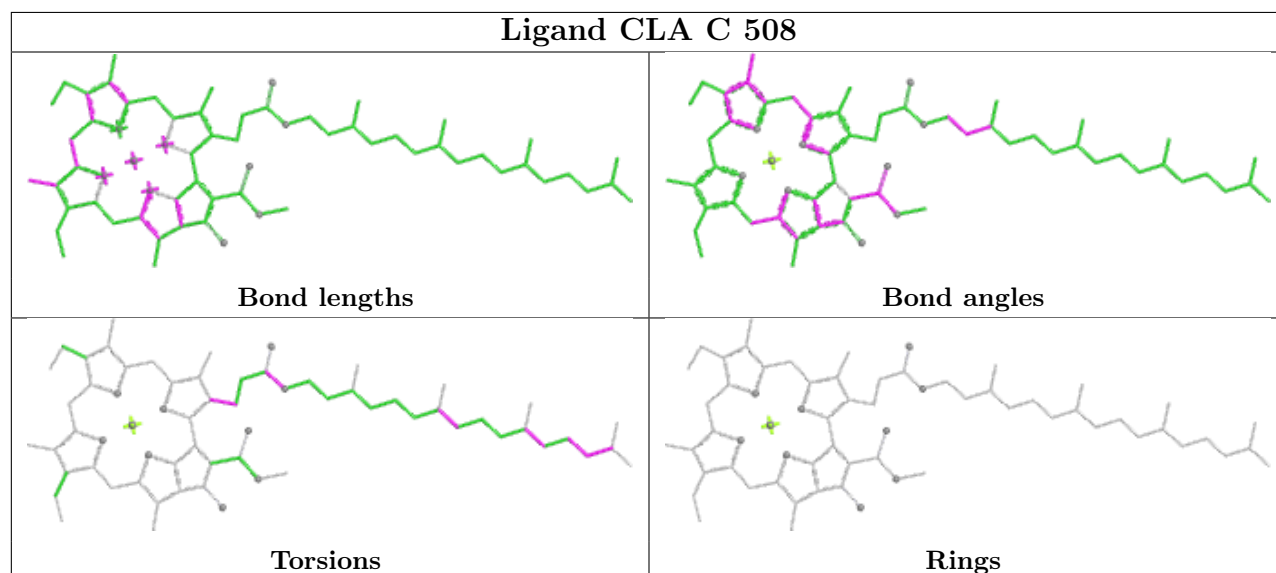
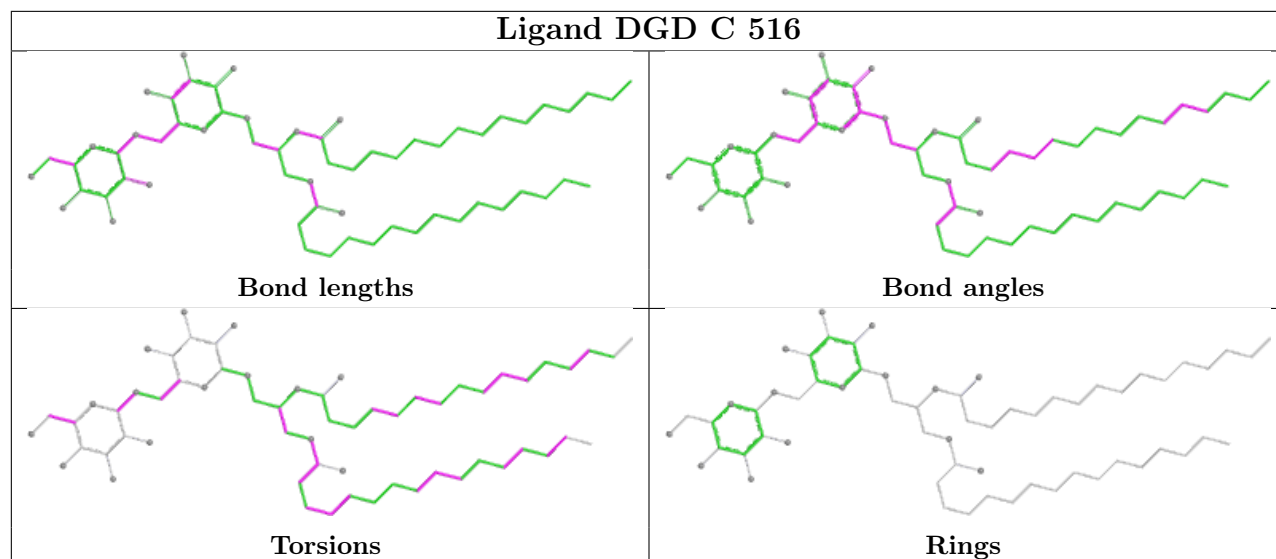


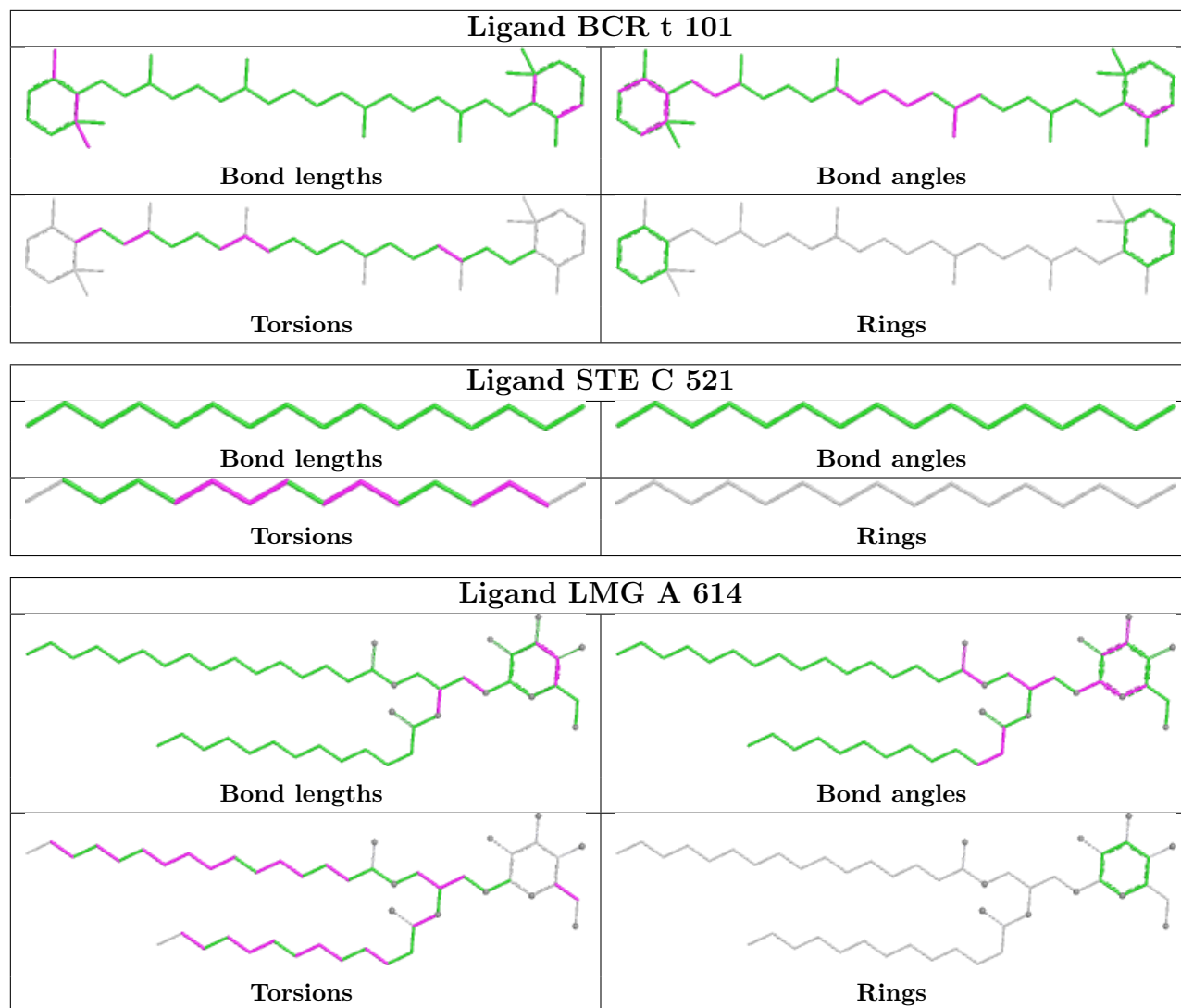


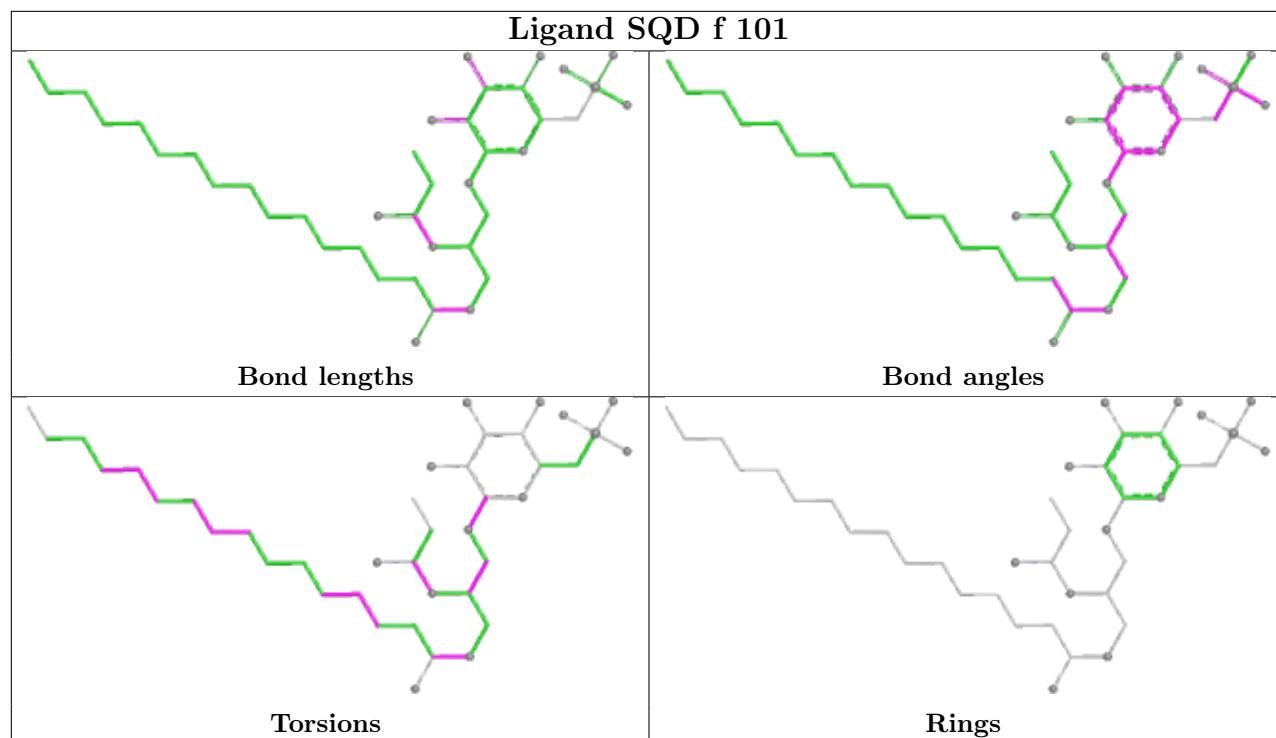


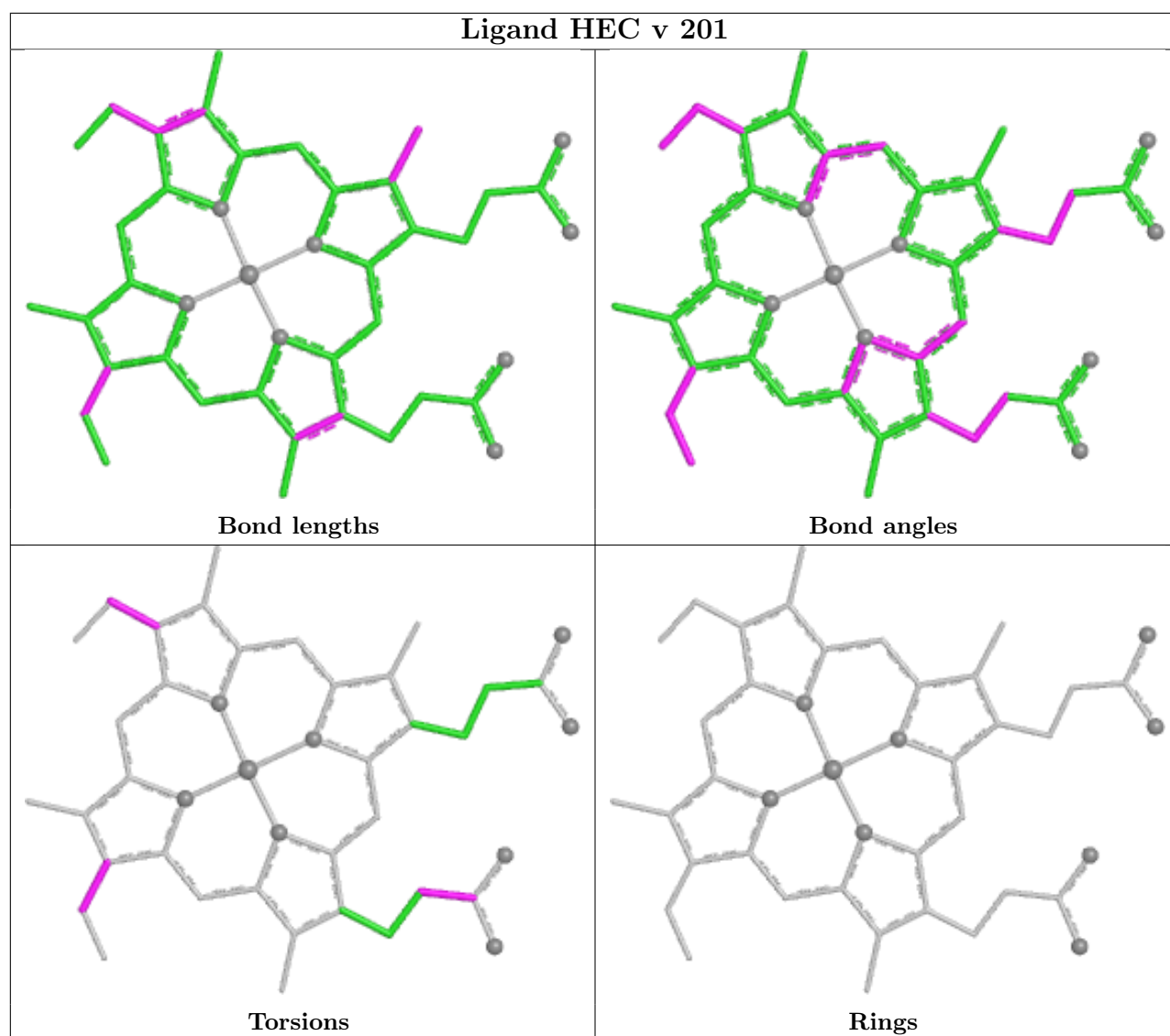












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.58	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	13, 29, 48, 83	64 (19%)
1	a	334/344 (97%)	-0.47	2 (0%) <span style="border: 1px solid black; padding: 2px;">85</span> <span style="border: 1px solid black; padding: 2px;">85</span>	12, 31, 57, 84	64 (19%)
2	B	505/510 (99%)	-0.46	3 (0%) <span style="border: 1px solid black; padding: 2px;">85</span> <span style="border: 1px solid black; padding: 2px;">85</span>	16, 34, 61, 87	4 (0%)
2	b	505/510 (99%)	-0.30	2 (0%) <span style="border: 1px solid black; padding: 2px;">88</span> <span style="border: 1px solid black; padding: 2px;">88</span>	25, 38, 69, 107	0
3	C	442/461 (95%)	-0.43	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	14, 37, 53, 80	11 (2%)
3	c	451/461 (97%)	-0.29	1 (0%) <span style="border: 1px solid black; padding: 2px;">91</span> <span style="border: 1px solid black; padding: 2px;">90</span>	14, 41, 62, 101	12 (2%)
4	D	341/352 (96%)	-0.65	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	15, 31, 47, 84	2 (0%)
4	d	341/352 (96%)	-0.46	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	16, 34, 56, 81	3 (0%)
5	E	82/84 (97%)	0.19	2 (2%) <span style="border: 1px solid black; padding: 2px;">59</span> <span style="border: 1px solid black; padding: 2px;">59</span>	30, 51, 69, 85	1 (1%)
5	e	82/84 (97%)	0.36	1 (1%) <span style="border: 1px solid black; padding: 2px;">76</span> <span style="border: 1px solid black; padding: 2px;">76</span>	39, 60, 76, 92	0
6	F	34/45 (75%)	-0.17	1 (2%) <span style="border: 1px solid black; padding: 2px;">53</span> <span style="border: 1px solid black; padding: 2px;">52</span>	37, 43, 62, 83	0
6	f	34/45 (75%)	0.03	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	41, 49, 77, 91	0
7	H	65/66 (98%)	-0.29	2 (3%) <span style="border: 1px solid black; padding: 2px;">51</span> <span style="border: 1px solid black; padding: 2px;">50</span>	32, 42, 58, 72	0
7	h	63/66 (95%)	0.06	2 (3%) <span style="border: 1px solid black; padding: 2px;">50</span> <span style="border: 1px solid black; padding: 2px;">49</span>	39, 51, 65, 73	0
8	I	35/38 (92%)	-0.39	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	32, 40, 68, 84	0
8	i	35/38 (92%)	-0.18	1 (2%) <span style="border: 1px solid black; padding: 2px;">53</span> <span style="border: 1px solid black; padding: 2px;">52</span>	31, 42, 75, 91	0
9	J	36/40 (90%)	-0.08	1 (2%) <span style="border: 1px solid black; padding: 2px;">55</span> <span style="border: 1px solid black; padding: 2px;">54</span>	34, 51, 72, 91	0
9	j	36/40 (90%)	0.10	1 (2%) <span style="border: 1px solid black; padding: 2px;">55</span> <span style="border: 1px solid black; padding: 2px;">54</span>	38, 53, 91, 107	0
10	K	37/46 (80%)	-0.02	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	41, 52, 73, 77	0
10	k	37/46 (80%)	0.19	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	47, 57, 71, 80	0
11	L	37/37 (100%)	-0.57	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	25, 32, 61, 68	0
11	l	36/37 (97%)	-0.49	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	26, 32, 74, 90	0
12	M	32/36 (88%)	-0.50	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	25, 36, 56, 68	0
12	m	31/36 (86%)	-0.47	0 <span style="border: 1px solid black; padding: 2px;">100</span> <span style="border: 1px solid black; padding: 2px;">100</span>	27, 36, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.14	4 (1%) 70 70	25, 44, 82, 136	1 (0%)
13	o	244/272 (89%)	-0.17	3 (1%) 76 76	26, 42, 78, 135	0
14	R	28/41 (68%)	0.72	0 100 100	61, 71, 87, 91	0
14	r	28/41 (68%)	1.14	1 (3%) 46 45	69, 87, 104, 114	0
15	T	29/32 (90%)	-0.53	1 (3%) 48 47	27, 32, 61, 75	0
15	t	29/32 (90%)	-0.36	2 (6%) 23 21	29, 33, 78, 85	0
16	U	97/134 (72%)	-0.21	0 100 100	33, 44, 72, 88	0
16	u	97/134 (72%)	-0.28	0 100 100	30, 41, 56, 86	0
17	V	137/163 (84%)	-0.36	0 100 100	30, 41, 57, 77	0
17	v	137/163 (84%)	-0.11	1 (0%) 84 84	34, 48, 69, 86	0
18	X	38/41 (92%)	-0.05	0 100 100	37, 50, 67, 77	0
18	x	39/41 (95%)	0.26	1 (2%) 57 56	48, 58, 86, 100	0
19	Y	27/46 (58%)	1.11	4 (14%) 5 5	52, 70, 96, 99	0
19	y	30/46 (65%)	0.84	0 100 100	60, 72, 91, 100	0
20	Z	62/62 (100%)	0.76	1 (1%) 70 70	53, 68, 119, 126	0
20	z	62/62 (100%)	0.76	2 (3%) 50 49	59, 73, 111, 121	0
All	All	5293/5700 (92%)	-0.28	39 (0%) 84 84	12, 39, 74, 136	162 (3%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.0
13	O	59	LYS	4.1
5	e	79	PHE	3.7
20	Z	62	VAL	3.7
15	t	30	THR	3.7

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.94	0.09	37,48,67,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	FME	t	1	10/11	0.94	0.08	31,44,66,66	0
8	FME	I	1	10/11	0.95	0.09	35,46,65,66	0
12	FME	m	1	10/11	0.96	0.09	34,42,59,71	0
8	FME	i	1	10/11	0.96	0.08	33,48,59,64	0
15	FME	T	1	10/11	0.97	0.06	28,45,61,61	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	STE	a	616	12/20	0.74	0.15	45,61,68,71	0
33	STE	H	103	18/20	0.75	0.17	49,67,78,81	0
33	STE	b	626	10/20	0.76	0.17	42,54,62,63	0
33	STE	d	412	20/20	0.76	0.16	41,65,84,85	0
33	STE	b	625	20/20	0.78	0.14	47,62,72,76	0
29	LMG	a	618	55/55	0.79	0.14	38,58,72,83	0
33	STE	a	615	10/20	0.79	0.16	40,60,68,69	0
29	LMG	b	623	55/55	0.79	0.16	51,68,87,91	0
33	STE	a	617	15/20	0.80	0.18	38,57,69,77	0
33	STE	m	101	12/20	0.80	0.15	45,61,75,76	0
29	LMG	c	521	48/55	0.81	0.14	50,71,93,96	0
33	STE	b	627	14/20	0.81	0.15	50,65,77,78	0
33	STE	I	101	15/20	0.81	0.15	40,55,75,80	0
30	LHG	e	102	42/49	0.81	0.13	52,77,103,111	0
33	STE	B	627	12/20	0.82	0.15	47,60,73,74	0
33	STE	k	103	12/20	0.82	0.12	49,67,78,80	0
33	STE	E	102	12/20	0.82	0.16	56,72,77,83	0
30	LHG	E	101	49/49	0.83	0.13	46,71,102,108	0
33	STE	B	626	16/20	0.83	0.14	45,58,70,74	0
33	STE	T	103	15/20	0.83	0.14	43,55,68,71	0
31	SQD	a	614	36/54	0.84	0.13	33,61,81,83	0
33	STE	j	101	12/20	0.84	0.12	45,58,67,70	0
33	STE	C	520	12/20	0.84	0.12	44,56,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	b	601	65/65	0.84	0.12	47,65,83,96	0
33	STE	T	102	16/20	0.85	0.12	30,48,62,65	0
33	STE	b	624	16/20	0.85	0.13	45,61,70,73	0
33	STE	B	620	17/20	0.85	0.12	36,51,64,65	0
33	STE	x	102	20/20	0.85	0.11	38,55,68,71	0
33	STE	C	522	12/20	0.86	0.12	39,49,57,58	0
33	STE	Z	101	8/20	0.86	0.17	41,57,64,64	0
29	LMG	A	614	48/55	0.86	0.11	37,55,74,84	0
31	SQD	A	617	39/54	0.86	0.13	40,59,87,92	0
29	LMG	D	409	33/55	0.86	0.13	37,56,77,84	0
33	STE	J	101	12/20	0.86	0.12	45,55,63,65	0
33	STE	t	102	18/20	0.86	0.12	42,55,72,77	0
32	DGD	A	618	66/66	0.86	0.11	43,61,74,82	0
33	STE	b	622	20/20	0.87	0.11	38,53,67,67	0
29	LMG	c	522	49/55	0.87	0.11	37,56,81,96	0
33	STE	B	624	14/20	0.87	0.11	36,51,61,63	0
33	STE	l	102	18/20	0.87	0.12	36,49,76,78	0
29	LMG	c	519	37/55	0.87	0.12	44,63,80,85	0
28	PL9	A	612	55/55	0.87	0.13	33,62,82,85	0
33	STE	c	520	20/20	0.87	0.11	36,55,71,76	0
28	PL9	a	611	55/55	0.88	0.13	32,65,80,88	0
31	SQD	B	623	54/54	0.88	0.10	39,57,81,90	0
29	LMG	C	519	48/55	0.88	0.12	39,67,85,89	0
33	STE	M	103	10/20	0.89	0.13	33,43,52,58	0
33	STE	C	521	16/20	0.89	0.11	37,51,64,71	0
33	STE	B	625	12/20	0.89	0.10	37,51,59,66	0
26	BCR	C	514	40/40	0.89	0.12	38,55,68,71	0
33	STE	d	411	17/20	0.90	0.11	41,52,64,65	0
29	LMG	D	410	28/55	0.90	0.11	36,50,61,63	0
24	CLA	B	601	65/65	0.90	0.11	32,58,84,95	0
31	SQD	D	407	36/54	0.90	0.11	41,65,80,82	0
33	STE	D	411	20/20	0.90	0.10	35,49,68,72	0
29	LMG	b	621	51/55	0.90	0.10	35,51,70,76	0
31	SQD	b	620	49/54	0.90	0.09	38,54,87,97	0
31	SQD	f	101	41/54	0.90	0.12	54,77,98,101	0
26	BCR	d	405	40/40	0.91	0.10	37,52,87,93	0
31	SQD	a	613	54/54	0.91	0.10	38,60,79,84	0
29	LMG	M	101	51/55	0.91	0.09	31,47,64,73	0
24	CLA	C	513	65/65	0.91	0.10	41,62,84,92	0
26	BCR	D	404	40/40	0.91	0.10	28,43,79,87	0
26	BCR	H	101	40/40	0.92	0.08	30,46,59,63	0
32	DGD	H	102	62/66	0.92	0.08	25,43,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
26	BCR	k	101	40/40	0.92	0.09	39,56,68,69	0
26	BCR	x	101	40/40	0.92	0.09	37,52,71,75	0
26	BCR	Y	101	40/40	0.92	0.09	32,50,62,69	0
26	BCR	c	514	40/40	0.92	0.09	46,59,68,70	0
32	DGD	c	517	62/66	0.93	0.08	31,51,87,90	0
32	DGD	h	101	62/66	0.93	0.08	31,45,57,64	0
24	CLA	c	512	65/65	0.93	0.10	41,56,88,94	0
24	CLA	c	513	65/65	0.93	0.11	44,65,100,105	0
29	LMG	D	406	51/55	0.93	0.10	26,52,75,84	0
24	CLA	C	512	65/65	0.93	0.10	33,51,81,86	0
26	BCR	b	617	40/40	0.93	0.07	29,40,51,54	0
29	LMG	d	410	44/55	0.93	0.10	33,51,79,86	0
26	BCR	b	618	40/40	0.93	0.07	26,39,51,54	0
30	LHG	d	407	49/49	0.93	0.11	34,47,70,74	0
32	DGD	C	517	62/66	0.93	0.09	27,47,92,108	0
26	BCR	b	619	40/40	0.93	0.08	26,47,61,69	0
26	BCR	B	618	40/40	0.94	0.07	23,38,49,49	0
24	CLA	c	509	65/65	0.94	0.09	32,46,61,69	0
33	STE	M	102	15/20	0.94	0.08	36,47,59,62	0
26	BCR	C	515	40/40	0.94	0.08	27,40,50,61	0
24	CLA	C	511	65/65	0.94	0.09	30,48,65,70	0
24	CLA	b	606	65/65	0.94	0.08	25,39,70,73	0
26	BCR	k	102	40/40	0.94	0.10	39,51,63,68	0
32	DGD	C	516	62/66	0.94	0.09	21,40,77,80	0
26	BCR	T	101	40/40	0.94	0.07	25,37,50,52	0
31	SQD	A	616	52/54	0.94	0.10	34,54,90,95	0
26	BCR	A	609	40/40	0.94	0.07	21,34,42,44	0
26	BCR	B	617	40/40	0.94	0.07	26,38,56,60	0
30	LHG	d	409	39/49	0.95	0.08	30,44,67,68	0
26	BCR	t	101	40/40	0.95	0.06	27,37,50,54	0
24	CLA	C	507	65/65	0.95	0.07	25,38,53,57	0
26	BCR	B	619	40/40	0.95	0.07	25,41,54,62	0
28	PL9	D	405	55/55	0.95	0.06	19,31,46,47	0
24	CLA	b	608	65/65	0.95	0.08	25,42,61,66	0
28	PL9	d	406	55/55	0.95	0.06	20,34,42,44	0
24	CLA	b	609	65/65	0.95	0.08	29,43,62,68	0
24	CLA	c	504	60/65	0.95	0.08	31,43,78,85	0
24	CLA	c	506	65/65	0.95	0.09	31,48,89,90	0
26	BCR	K	101	40/40	0.95	0.08	34,49,65,65	0
24	CLA	c	508	64/65	0.95	0.09	29,43,83,98	0
24	CLA	C	510	65/65	0.95	0.07	26,41,61,62	0
32	DGD	C	518	62/66	0.95	0.08	24,46,75,85	0

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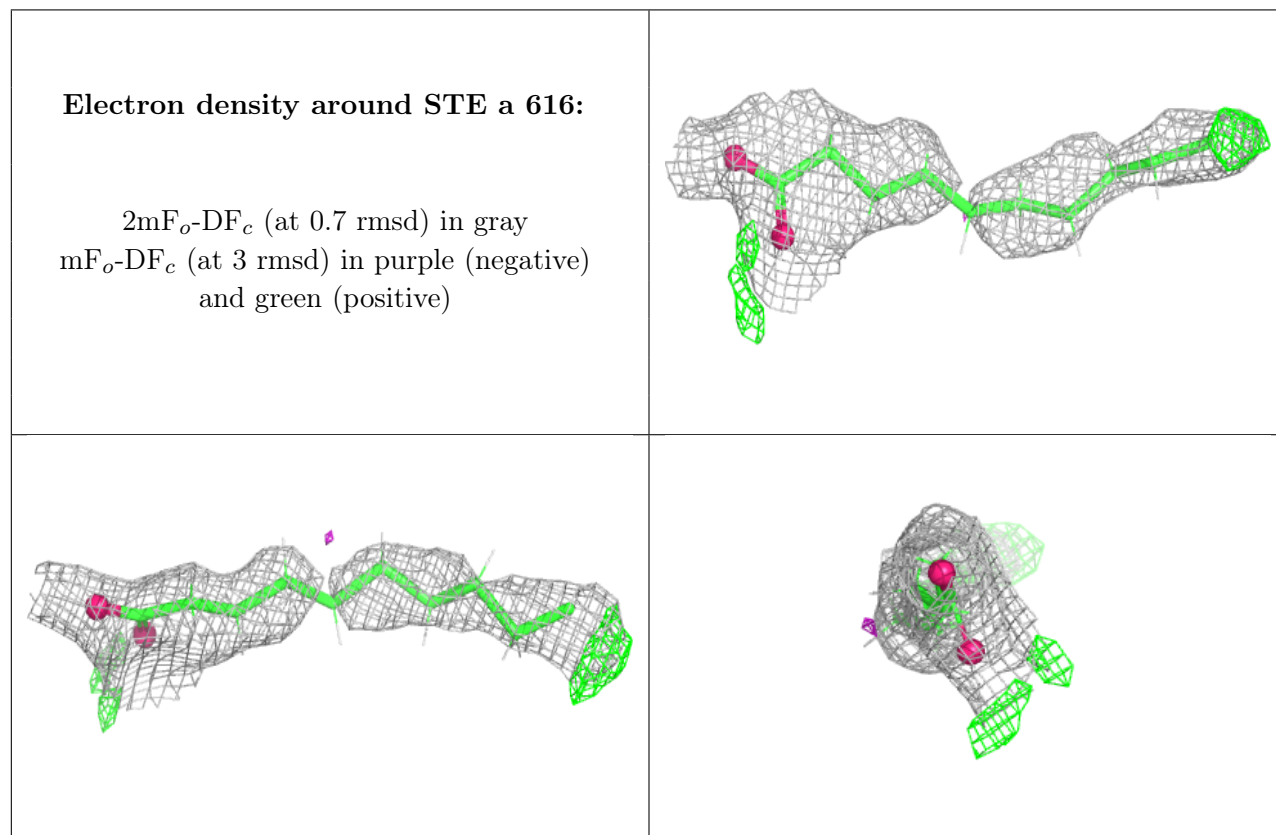
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	a	607	40/40	0.95	0.06	23,33,43,49	0
32	DGD	c	516	62/66	0.95	0.08	21,41,67,74	0
24	CLA	c	511	65/65	0.95	0.09	33,50,70,75	0
32	DGD	c	518	62/66	0.95	0.09	25,49,80,86	0
24	CLA	B	610	65/65	0.95	0.07	20,32,42,45	0
24	CLA	C	503	65/65	0.95	0.06	27,39,48,51	0
24	CLA	d	404	65/65	0.95	0.09	28,47,81,87	0
26	BCR	c	515	40/40	0.95	0.07	27,42,58,61	0
25	PHO	d	402	64/64	0.95	0.06	26,35,45,49	0
30	LHG	A	615	47/49	0.95	0.10	27,48,77,88	0
30	LHG	B	622	49/49	0.95	0.08	29,43,64,69	0
24	CLA	C	504	59/65	0.95	0.08	28,40,79,80	0
24	CLA	C	506	65/65	0.95	0.09	26,42,78,84	0
34	BCT	a	610	4/4	0.95	0.09	28,33,39,47	0
24	CLA	B	605	65/65	0.96	0.07	20,31,47,50	0
24	CLA	c	505	65/65	0.96	0.08	25,38,66,72	0
24	CLA	C	505	65/65	0.96	0.08	23,39,65,81	0
24	CLA	c	507	65/65	0.96	0.07	26,43,58,64	0
24	CLA	B	606	65/65	0.96	0.07	23,34,65,71	0
24	CLA	B	609	65/65	0.96	0.07	24,36,58,66	0
24	CLA	c	510	65/65	0.96	0.07	28,45,58,71	0
24	CLA	C	508	65/65	0.96	0.07	26,38,98,109	0
24	CLA	C	509	65/65	0.96	0.08	26,42,60,64	0
24	CLA	A	604	65/65	0.96	0.06	15,26,44,54	0
24	CLA	d	401	65/65	0.96	0.08	24,37,86,90	0
24	CLA	B	613	65/65	0.96	0.07	17,31,65,70	0
25	PHO	A	606	64/64	0.96	0.05	17,27,35,41	0
25	PHO	A	607	64/64	0.96	0.05	22,31,40,42	0
24	CLA	B	614	65/65	0.96	0.08	20,35,70,80	0
24	CLA	B	615	65/65	0.96	0.07	22,36,59,63	0
24	CLA	a	604	65/65	0.96	0.05	18,28,45,55	0
24	CLA	a	606	65/65	0.96	0.08	19,36,78,84	0
30	LHG	B	621	49/49	0.96	0.07	26,40,54,61	0
24	CLA	a	612	65/65	0.96	0.06	20,29,46,51	0
24	CLA	B	616	60/65	0.96	0.08	23,37,88,95	0
24	CLA	b	602	65/65	0.96	0.07	27,41,57,62	0
24	CLA	b	603	65/65	0.96	0.07	23,36,60,68	0
24	CLA	b	605	65/65	0.96	0.06	21,34,49,54	0
30	LHG	l	101	49/49	0.96	0.06	30,42,51,57	0
24	CLA	C	501	65/65	0.96	0.06	21,35,48,51	0
24	CLA	b	607	65/65	0.96	0.07	20,35,62,68	0
24	CLA	C	502	65/65	0.96	0.06	25,39,52,59	0

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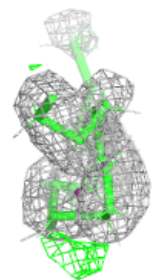
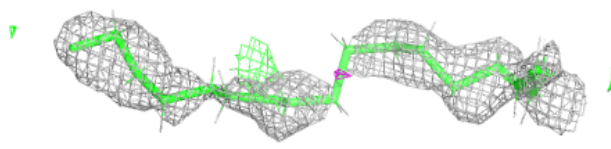
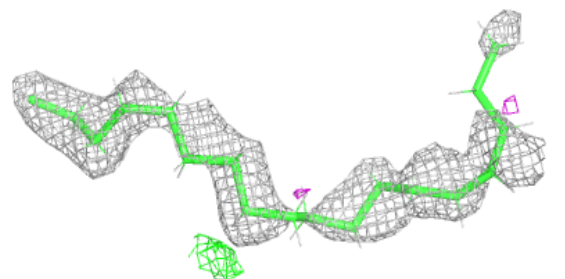
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	CLA	B	602	65/65	0.96	0.06	23,35,54,61	0
24	CLA	b	610	65/65	0.96	0.07	22,37,50,54	0
24	CLA	b	611	65/65	0.96	0.06	22,33,52,62	0
24	CLA	b	612	65/65	0.96	0.07	21,34,47,56	0
24	CLA	b	613	65/65	0.96	0.07	17,33,66,74	0
24	CLA	b	614	65/65	0.96	0.07	24,38,68,76	0
24	CLA	b	615	65/65	0.96	0.07	26,39,57,63	0
24	CLA	b	616	60/65	0.96	0.08	26,41,81,83	0
24	CLA	c	501	65/65	0.96	0.06	28,39,51,55	0
24	CLA	c	502	65/65	0.96	0.06	29,40,55,62	0
24	CLA	c	503	65/65	0.96	0.07	28,42,53,61	0
30	LHG	D	408	49/49	0.97	0.07	21,40,52,57	0
24	CLA	B	612	65/65	0.97	0.06	19,32,49,53	0
24	CLA	A	605	65/65	0.97	0.08	23,33,83,91	0
30	LHG	d	408	49/49	0.97	0.07	24,41,51,60	0
24	CLA	D	402	65/65	0.97	0.06	17,28,54,56	0
24	CLA	D	403	65/65	0.97	0.08	22,42,105,112	0
24	CLA	d	403	65/65	0.97	0.06	20,32,54,64	0
24	CLA	A	613	65/65	0.97	0.06	18,28,47,53	0
24	CLA	B	607	65/65	0.97	0.07	17,32,57,67	0
24	CLA	B	608	65/65	0.97	0.06	18,33,54,56	0
25	PHO	a	605	64/64	0.97	0.05	18,29,37,46	0
24	CLA	B	603	65/65	0.97	0.06	20,32,61,63	0
24	CLA	B	604	65/65	0.97	0.07	21,32,68,71	0
24	CLA	B	611	65/65	0.97	0.06	19,31,49,52	0
34	BCT	D	401	4/4	0.97	0.06	27,28,31,38	0
24	CLA	b	604	65/65	0.97	0.07	19,35,79,89	0
35	HEM	F	101	43/43	0.97	0.08	34,46,60,62	0
35	HEM	e	101	43/43	0.97	0.09	41,53,73,73	0
27	CL	A	611	1/1	0.98	0.05	27,27,27,27	0
24	CLA	A	608	54/65	0.98	0.06	17,32,67,69	0
36	HEC	V	201	43/43	0.98	0.05	23,31,40,40	0
36	HEC	v	201	43/43	0.98	0.06	26,36,46,46	0
22	OEX	a	602[A]	10/10	0.99	0.03	27,32,35,35	10
23	FE2	a	603	1/1	0.99	0.03	29,29,29,29	0
27	CL	A	610	1/1	0.99	0.03	28,28,28,28	0
21	OEY	a	601[B]	11/11	0.99	0.03	15,21,24,26	11
27	CL	a	608	1/1	0.99	0.04	25,25,25,25	0
27	CL	a	609	1/1	0.99	0.06	25,25,25,25	0
22	OEX	A	602[A]	10/10	0.99	0.03	29,31,35,35	10
21	OEY	A	601[B]	11/11	1.00	0.03	15,20,23,26	11
23	FE2	A	603	1/1	1.00	0.01	24,24,24,24	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.

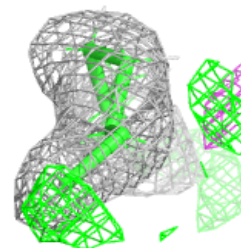
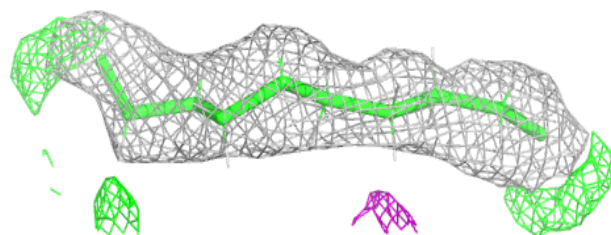
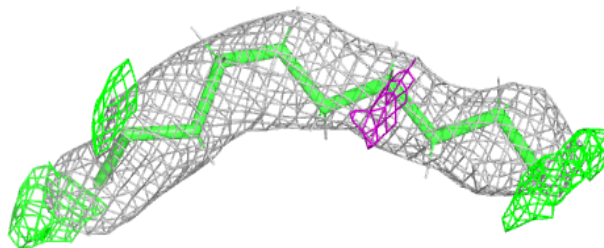


**Electron density around STE H 103:**

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

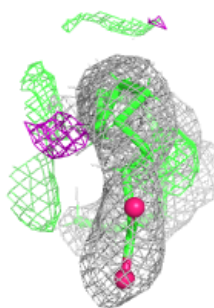
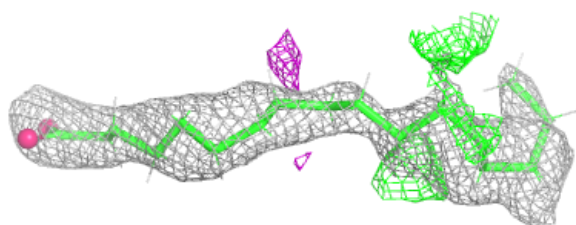
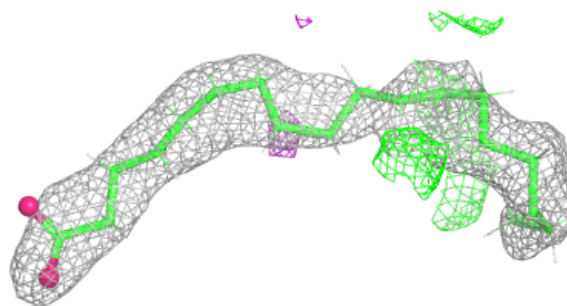
**Electron density around STE b 626:**

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

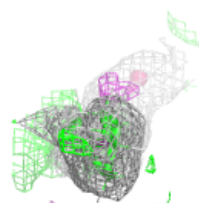
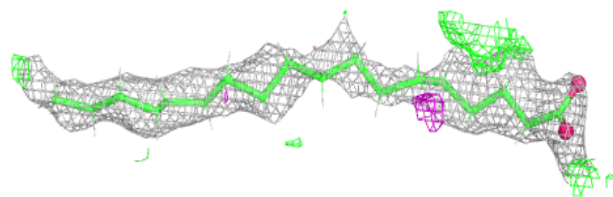
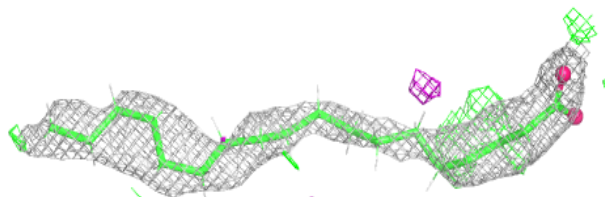


**Electron density around STE d 412:**

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

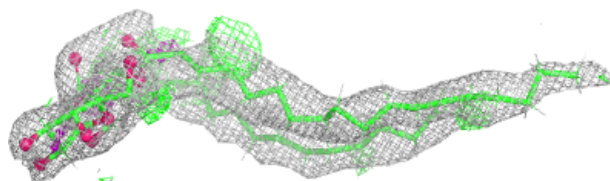
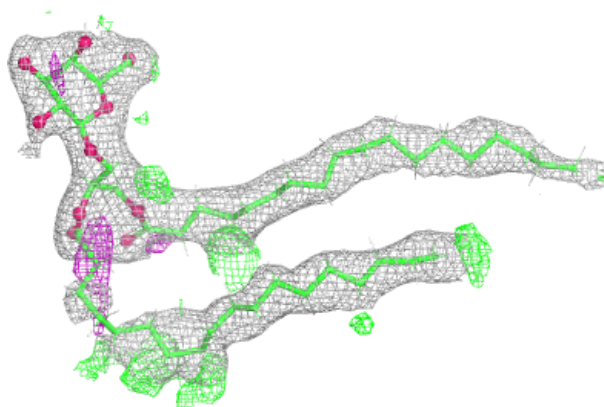
**Electron density around STE b 625:**

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

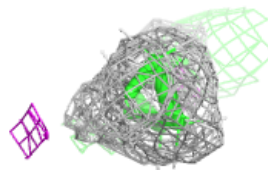
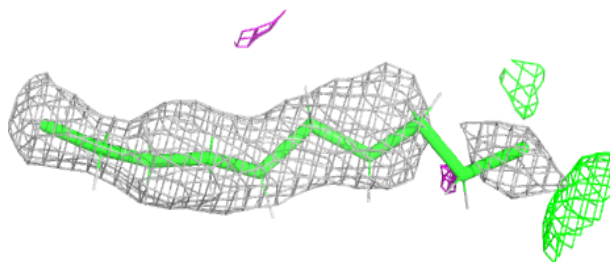
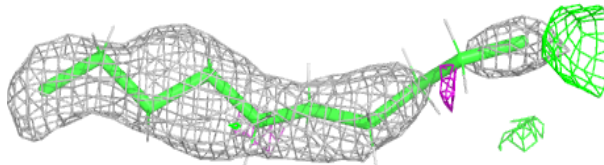


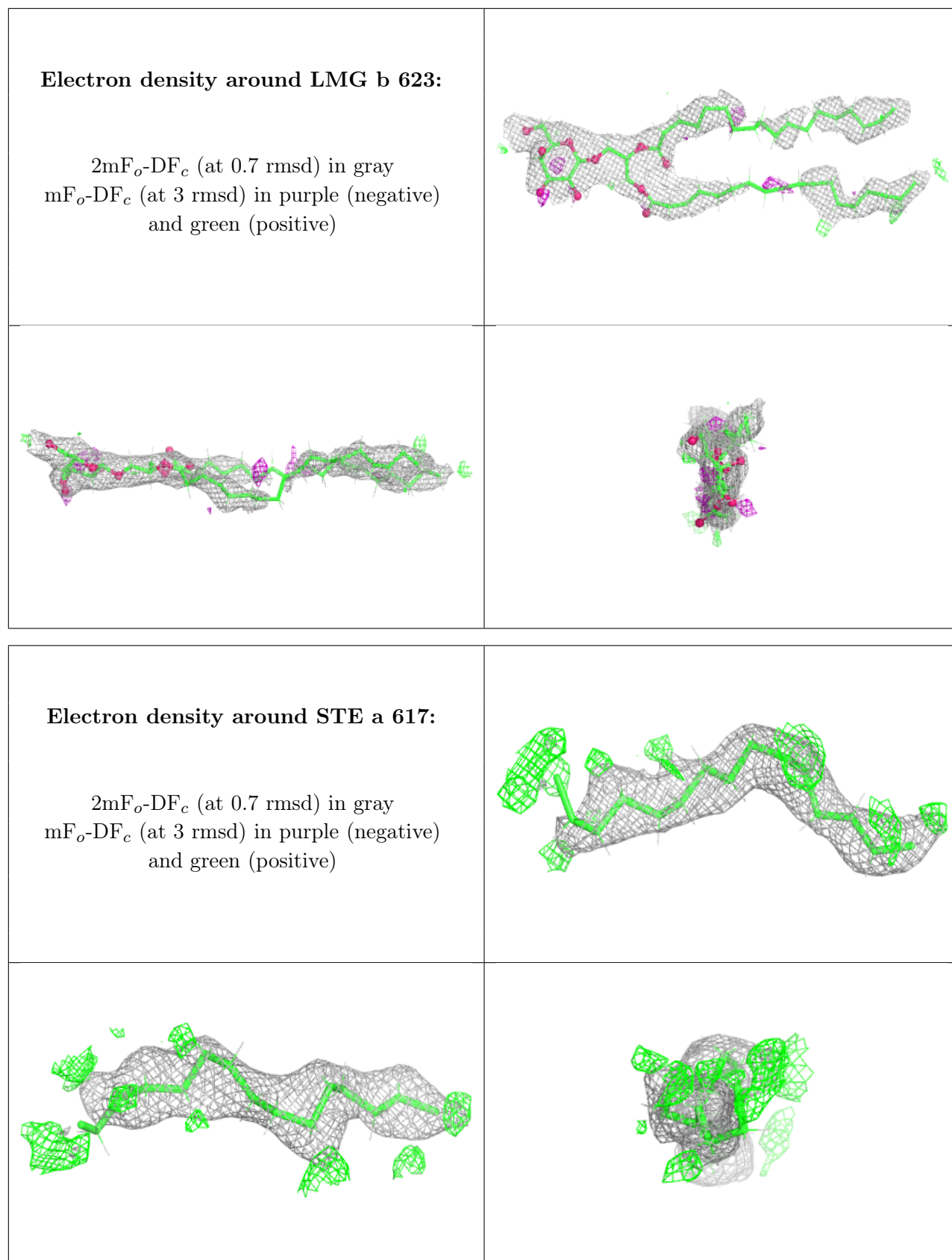
**Electron density around LMG a 618:**

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

**Electron density around STE a 615:**

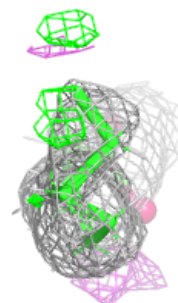
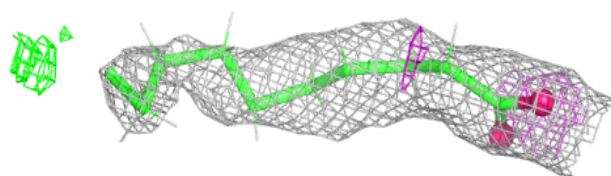
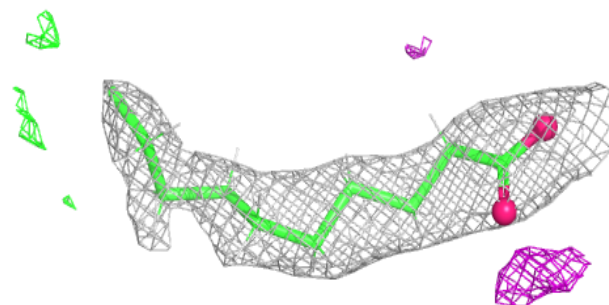
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



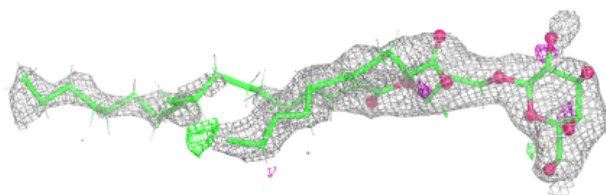
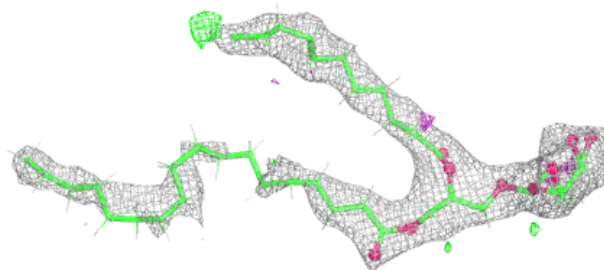


**Electron density around STE m 101:**

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

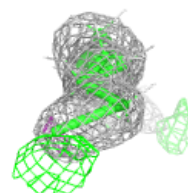
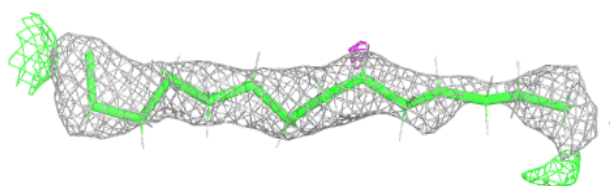
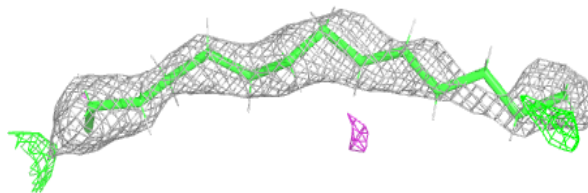
**Electron density around LMG c 521:**

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

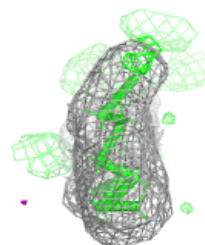
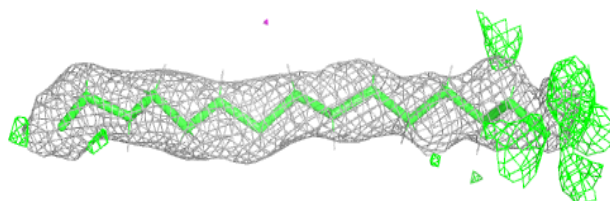
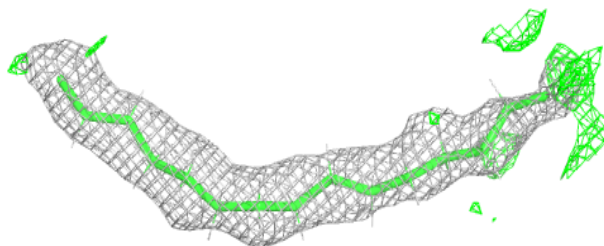


**Electron density around STE b 627:**

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

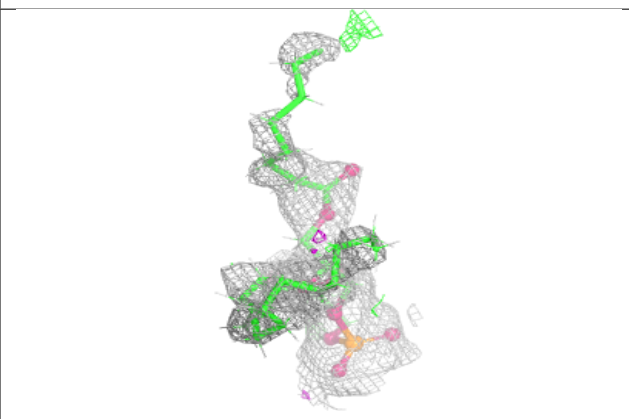
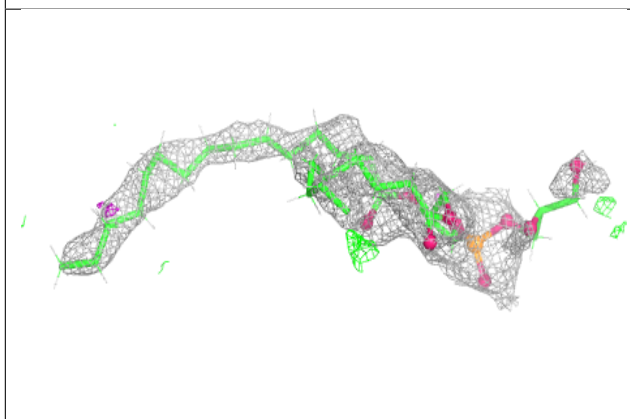
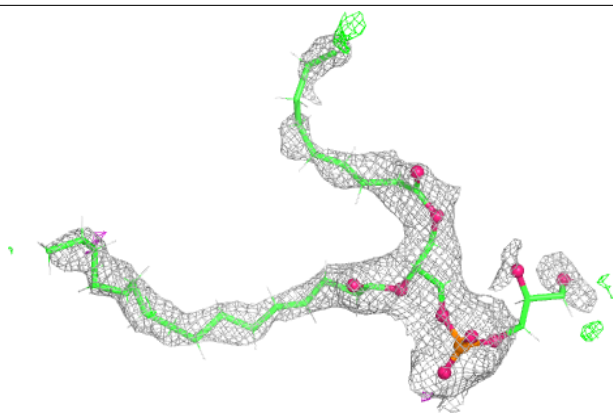
**Electron density around STE I 101:**

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

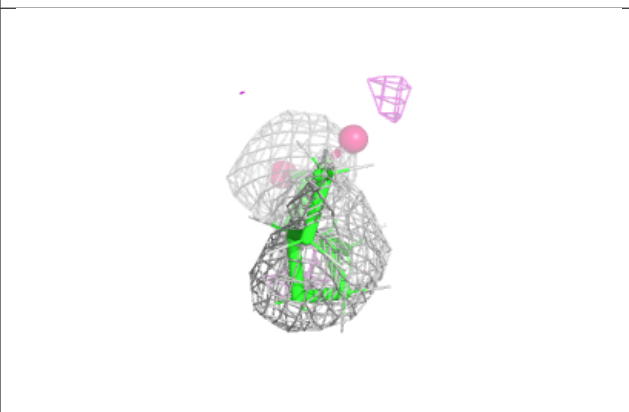
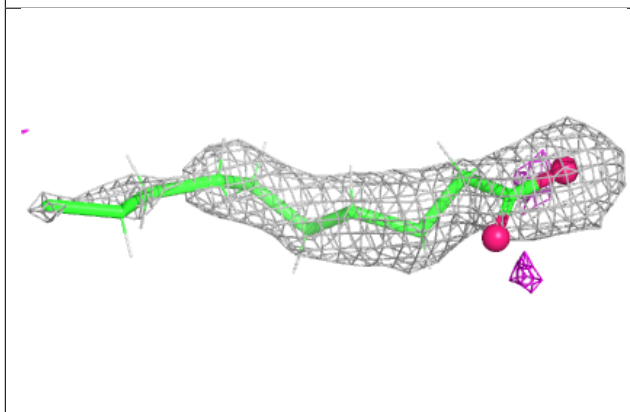
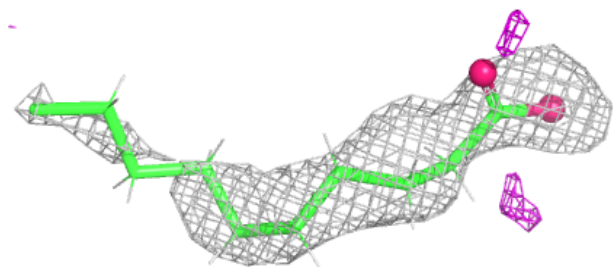


**Electron density around LHG e 102:**

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

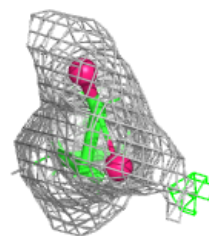
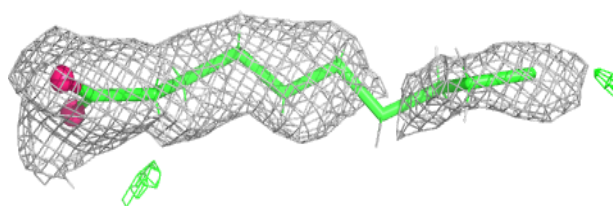
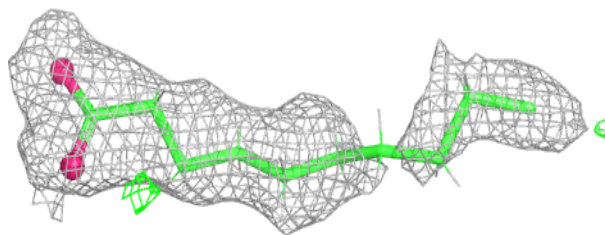
**Electron density around STE B 627:**

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

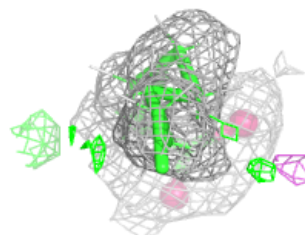
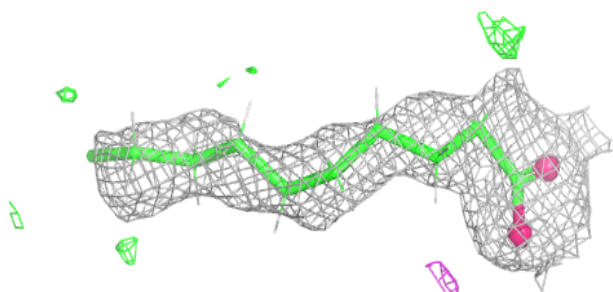
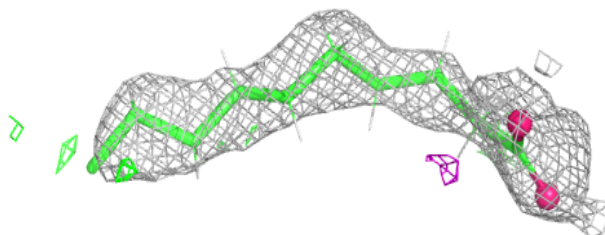


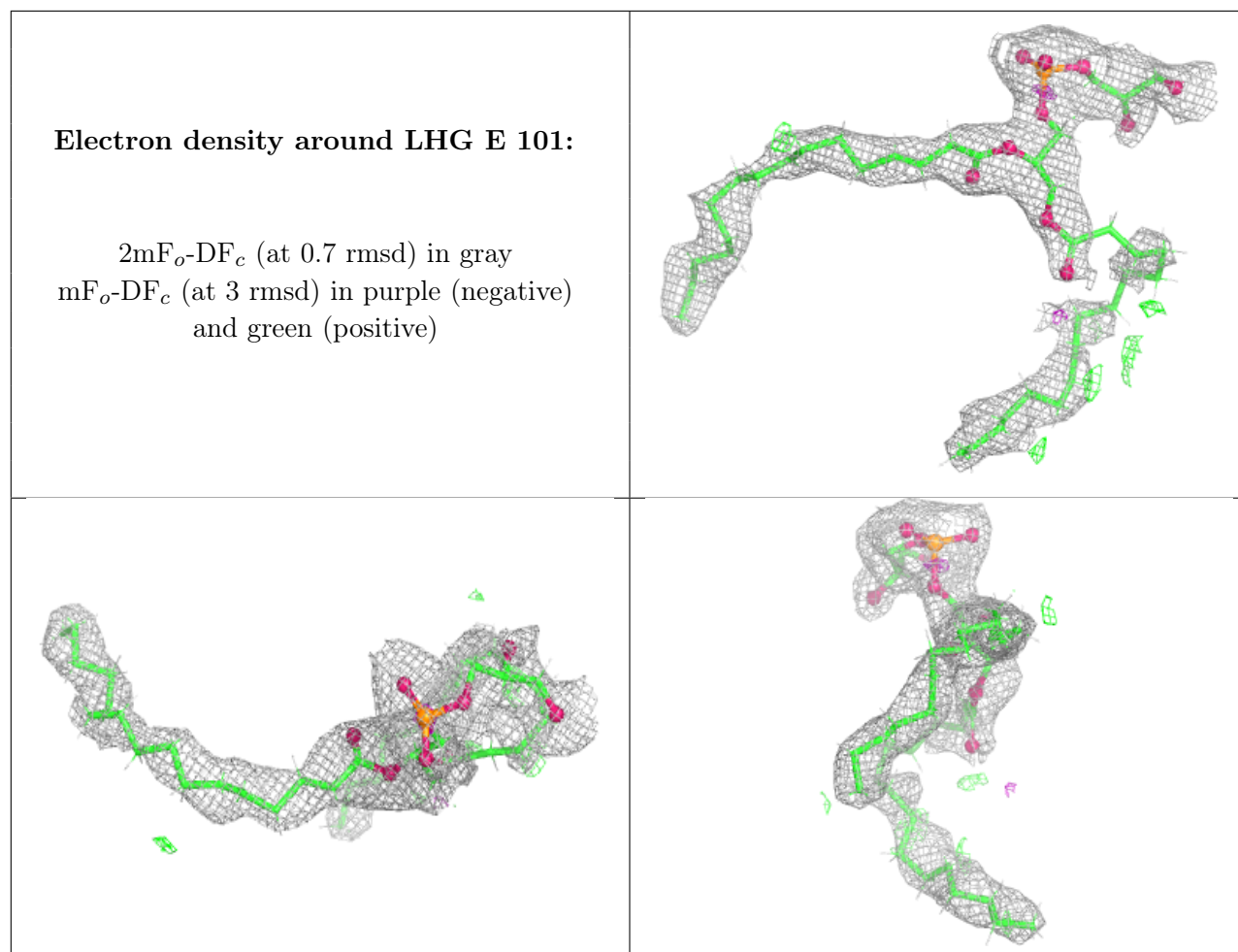
**Electron density around STE k 103:**

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

**Electron density around STE E 102:**

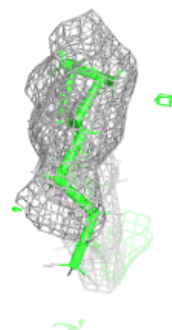
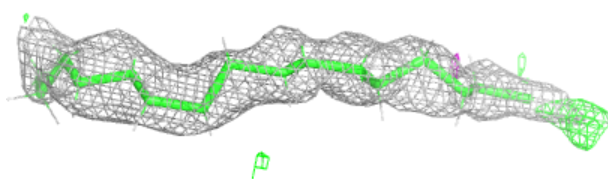
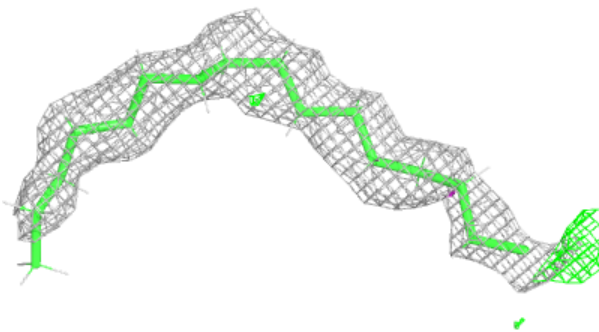
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



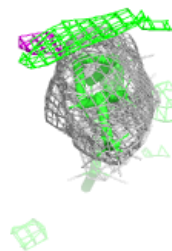
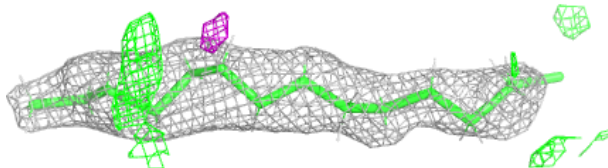
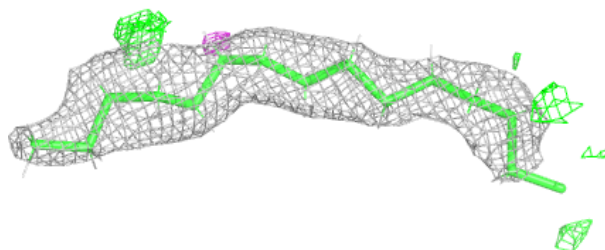


**Electron density around STE B 626:**

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

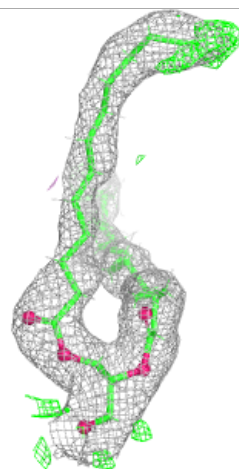
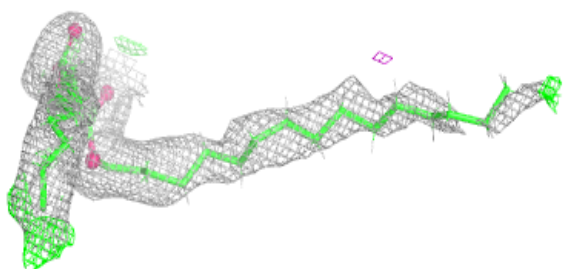
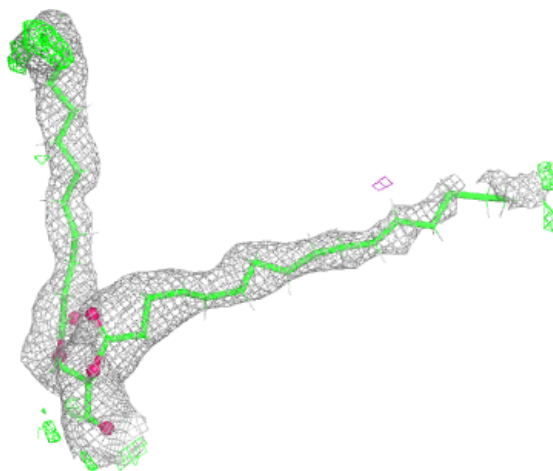
**Electron density around STE T 103:**

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



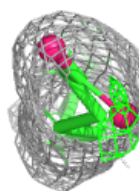
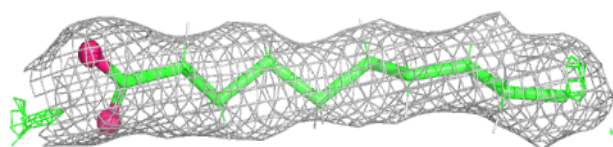
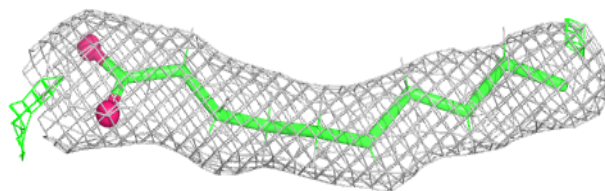
**Electron density around SQD a 614:**

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

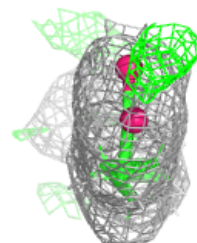
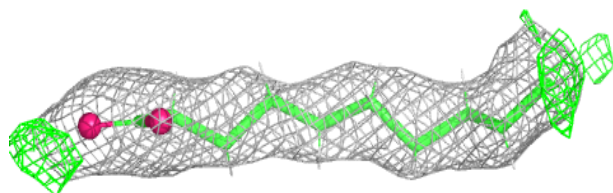
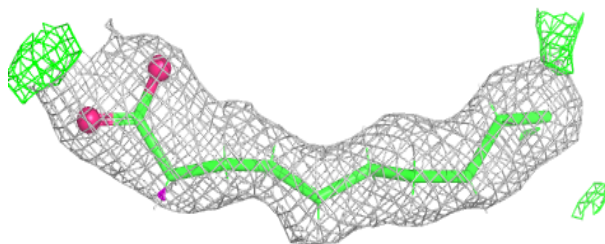


**Electron density around STE j 101:**

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

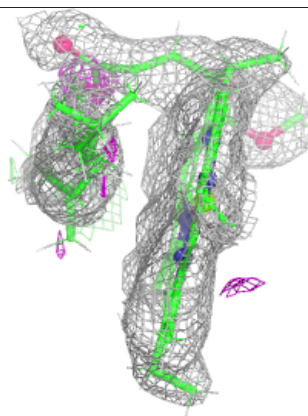
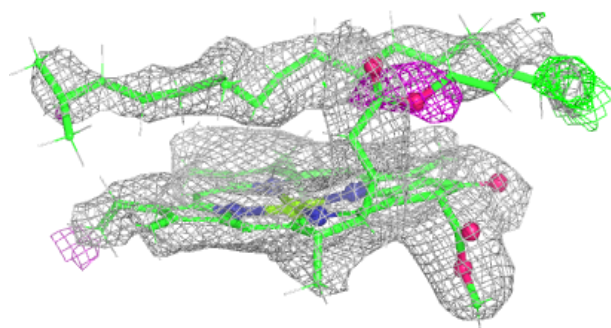
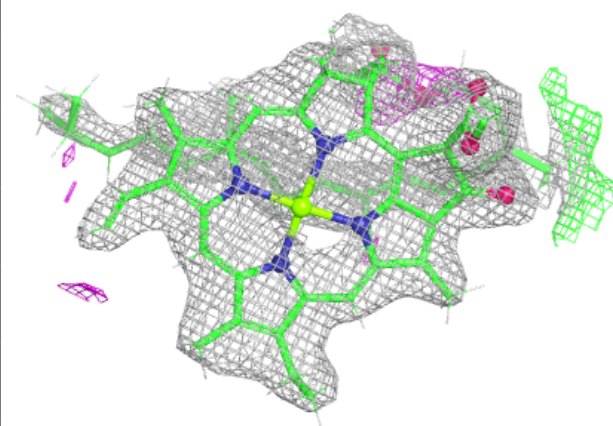
**Electron density around STE C 520:**

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

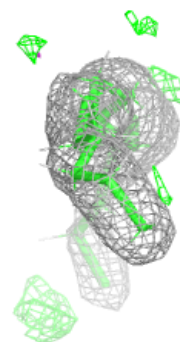
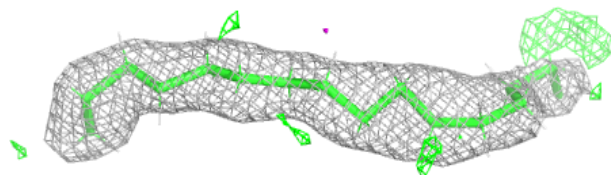
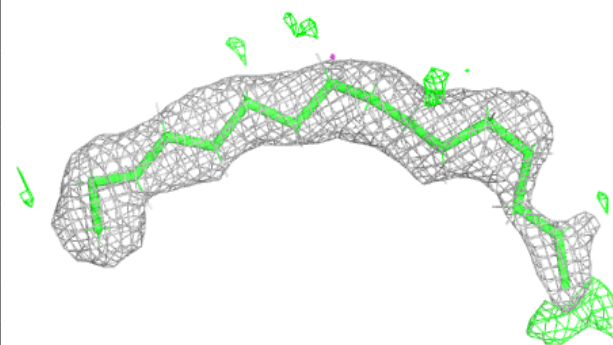


**Electron density around CLA b 601:**

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

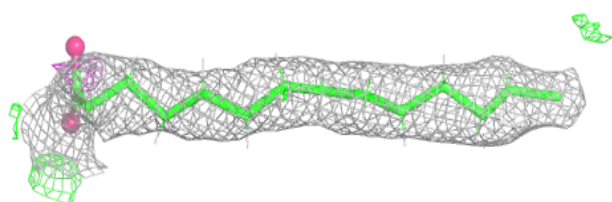
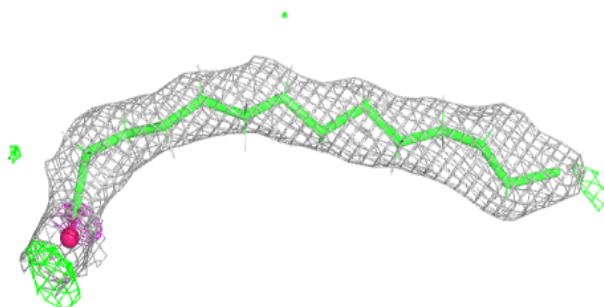
**Electron density around STE T 102:**

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

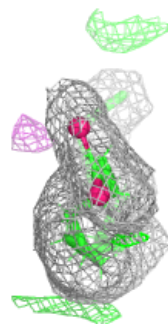
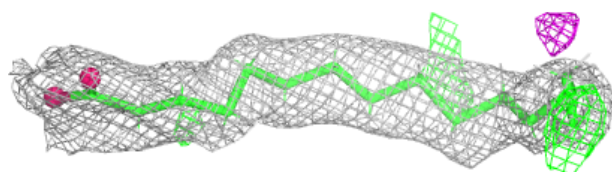
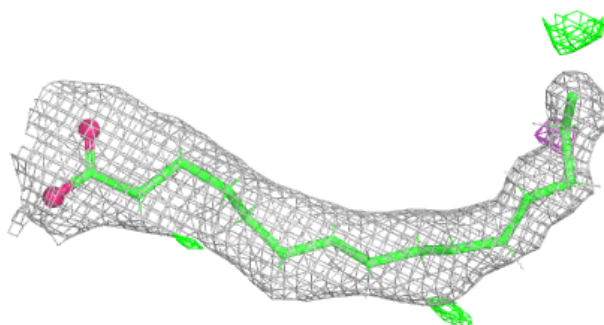


**Electron density around STE b 624:**

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

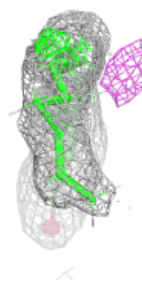
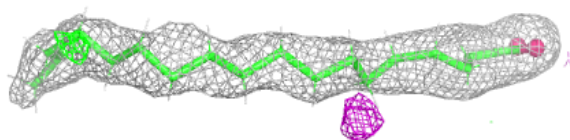
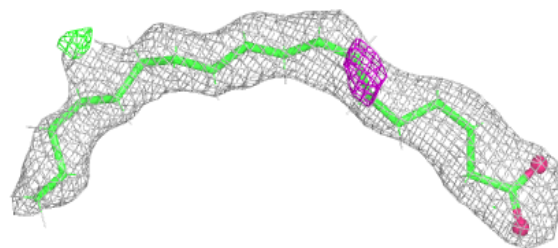
**Electron density around STE B 620:**

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

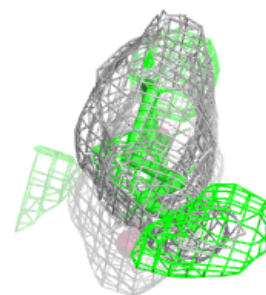
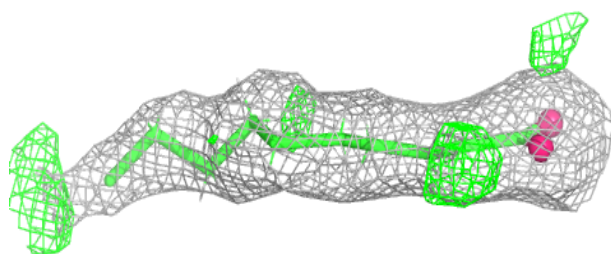
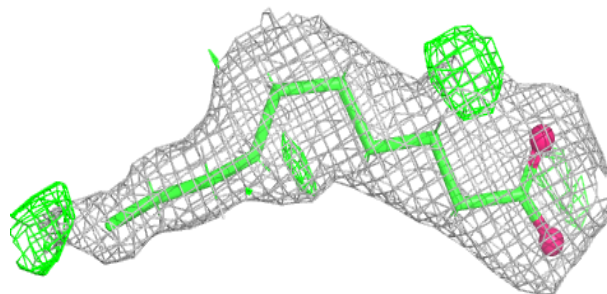


**Electron density around STE x 102:**

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

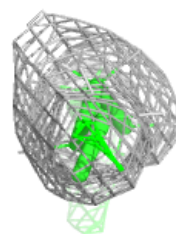
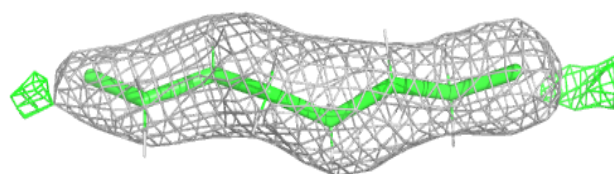
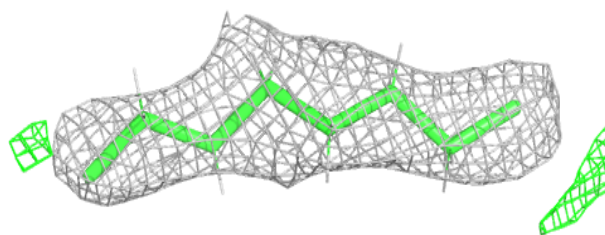
**Electron density around STE C 522:**

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

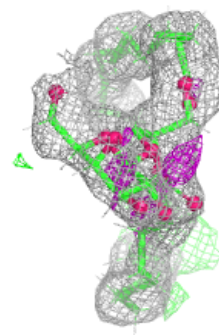
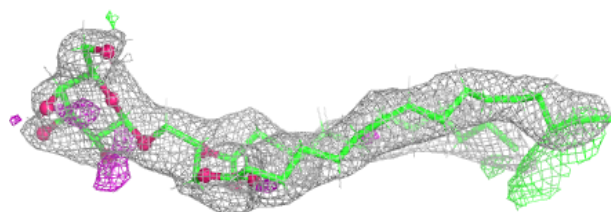
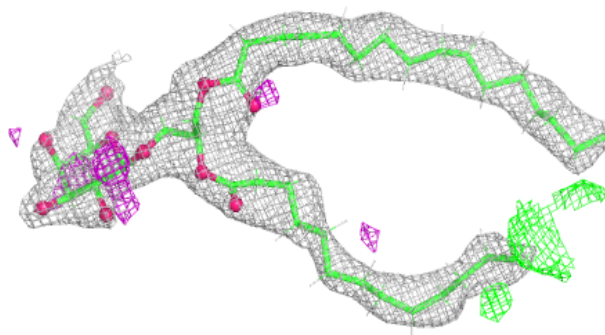


**Electron density around STE Z 101:**

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

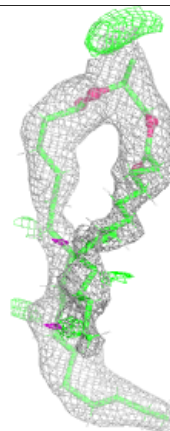
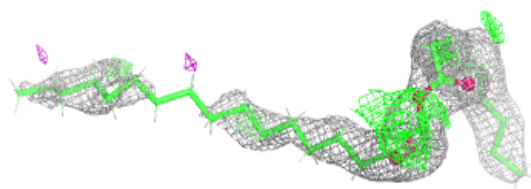
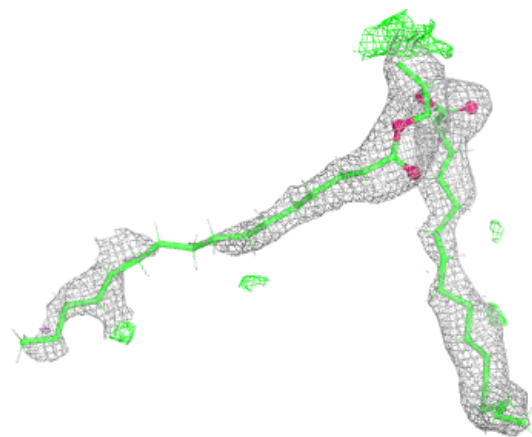
**Electron density around LMG A 614:**

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

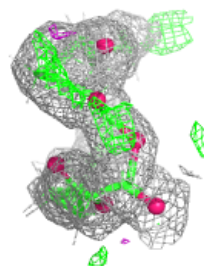
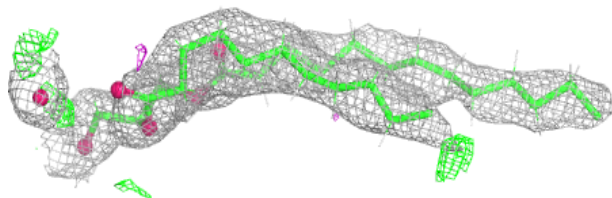
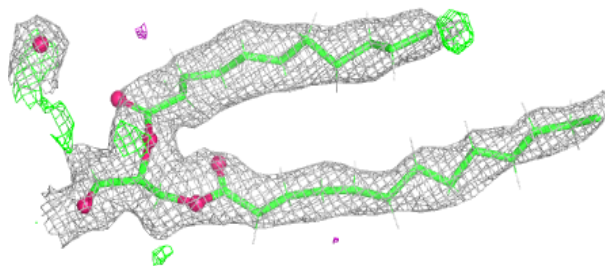


**Electron density around SQD A 617:**

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

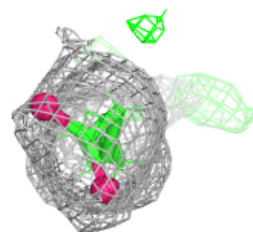
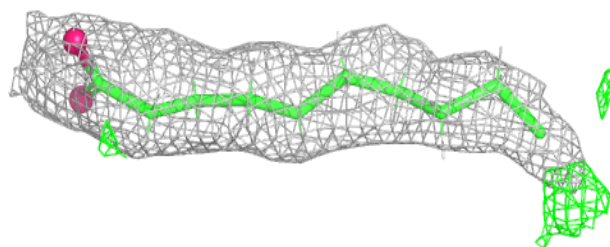
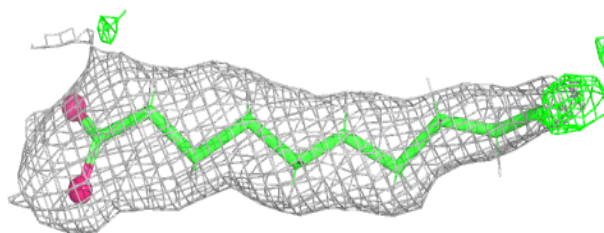
**Electron density around LMG D 409:**

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

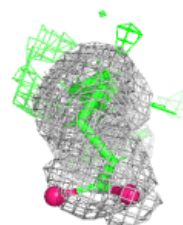
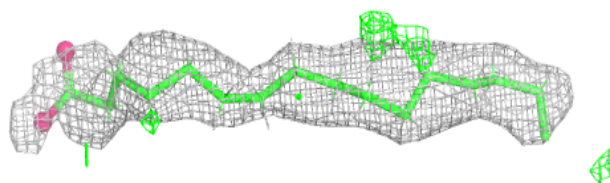
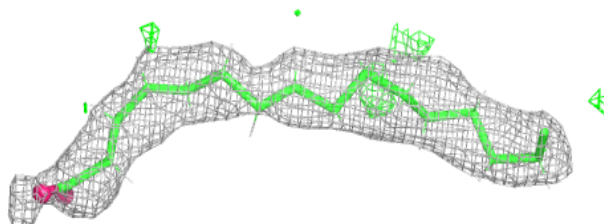


**Electron density around STE J 101:**

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

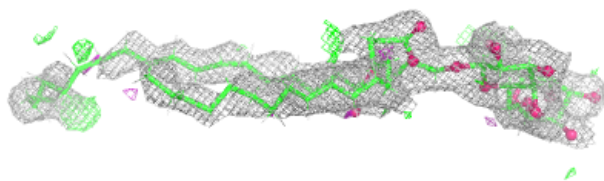
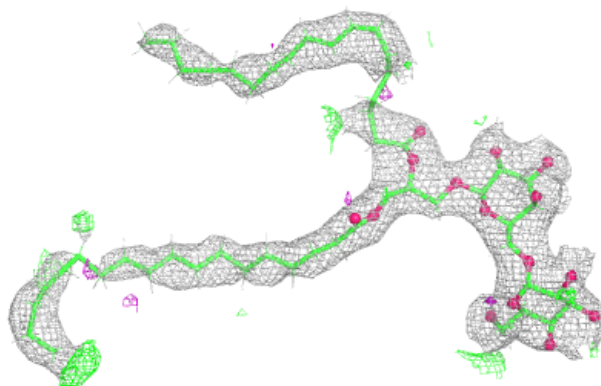
**Electron density around STE t 102:**

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

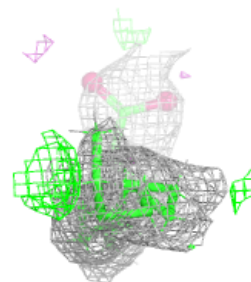
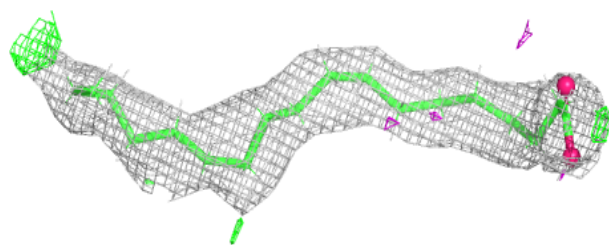
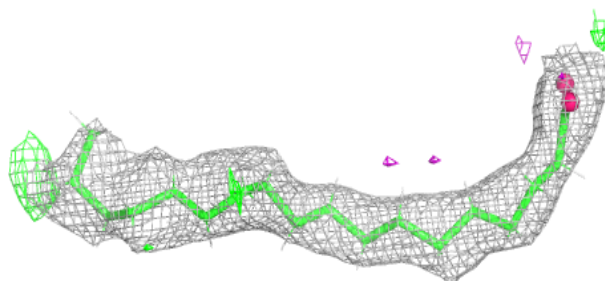


**Electron density around DGD A 618:**

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

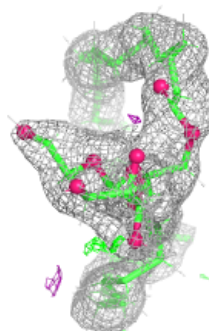
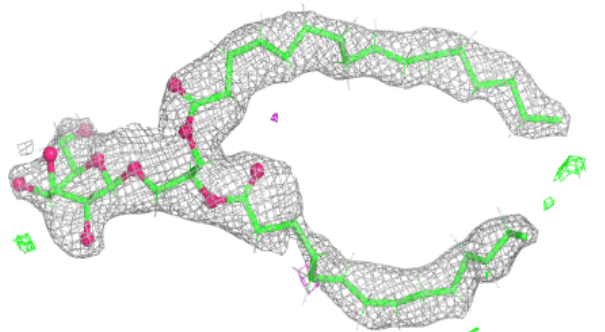
**Electron density around STE b 622:**

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

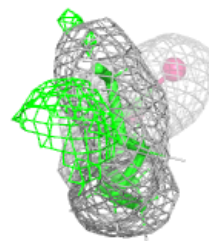
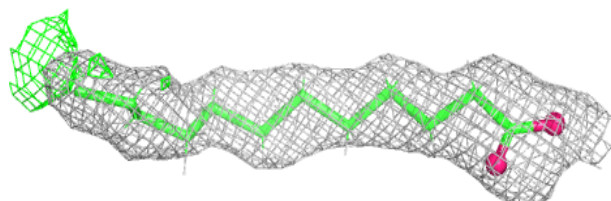
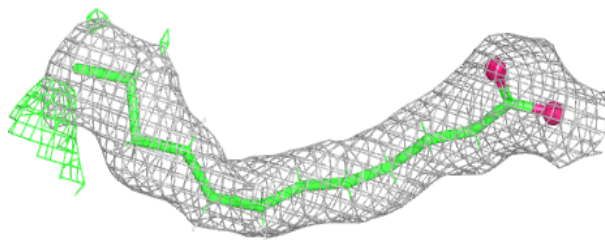


**Electron density around LMG c 522:**

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

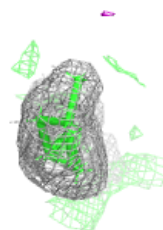
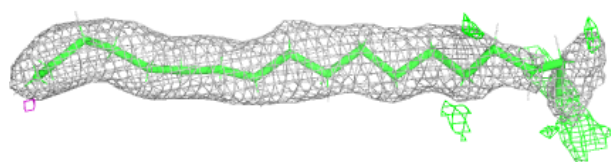
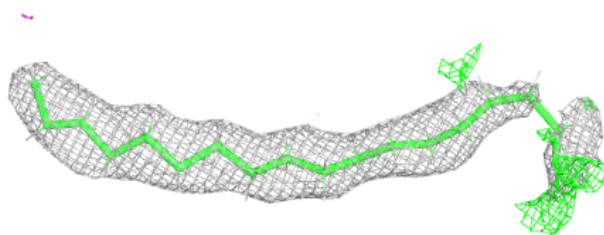
**Electron density around STE B 624:**

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

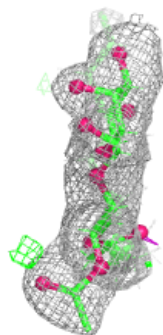
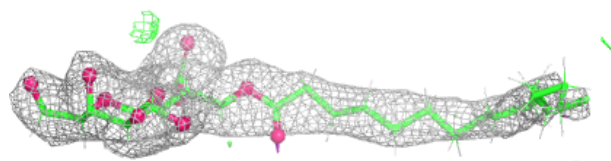
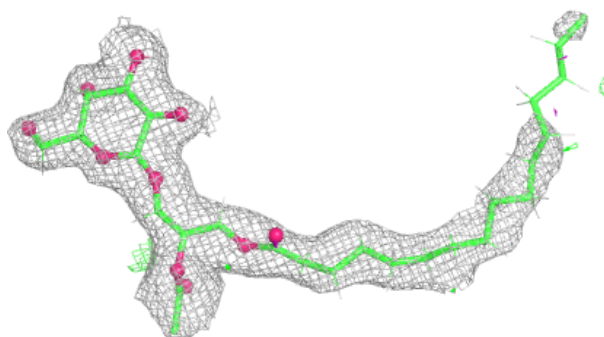


**Electron density around STE 1 102:**

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

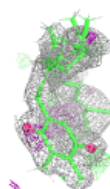
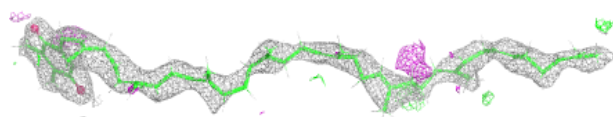
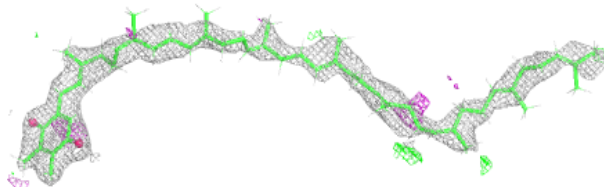
**Electron density around LMG c 519:**

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

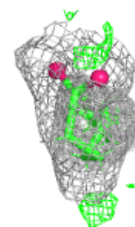
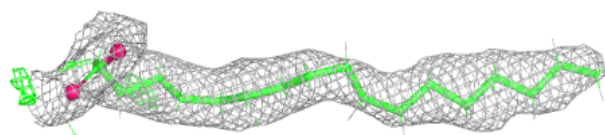
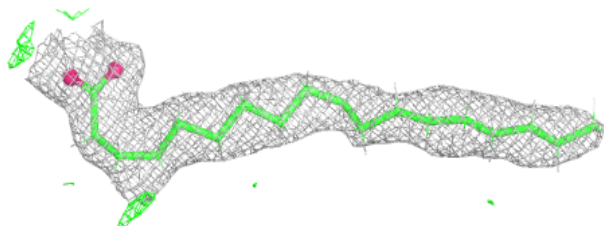


**Electron density around PL9 A 612:**

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

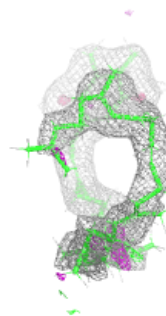
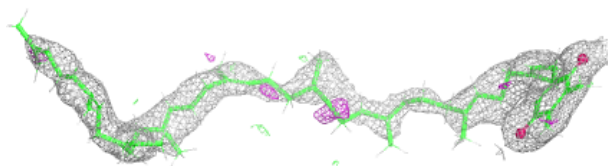
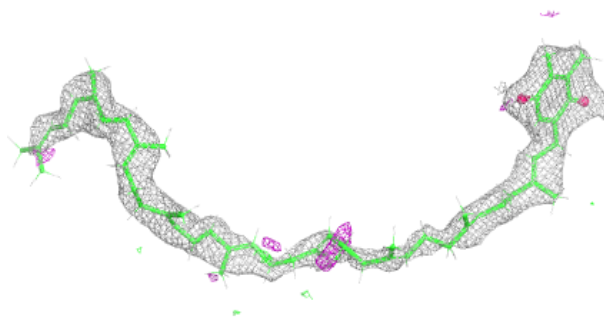
**Electron density around STE c 520:**

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

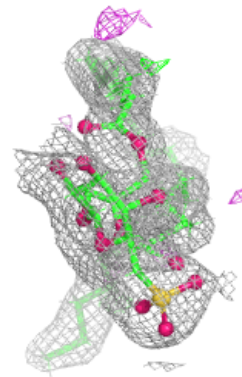
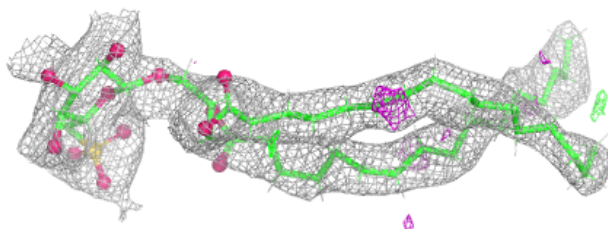
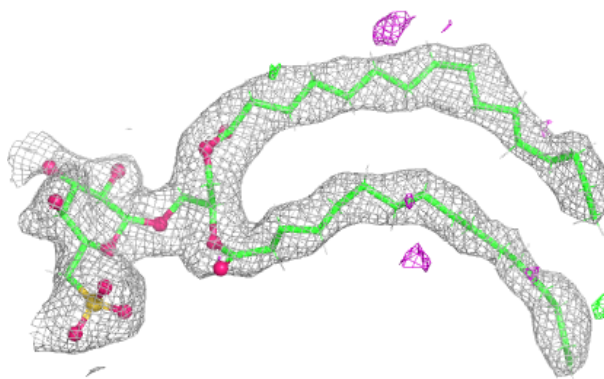


**Electron density around PL9 a 611:**

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

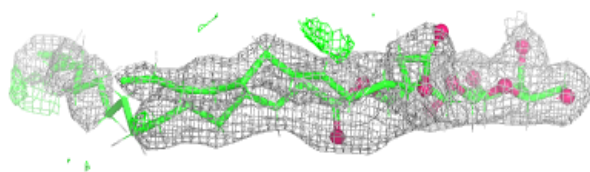
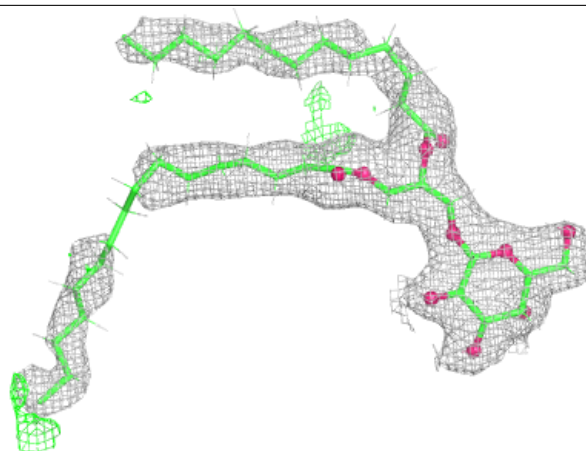
**Electron density around SQD B 623:**

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

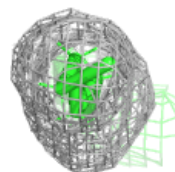
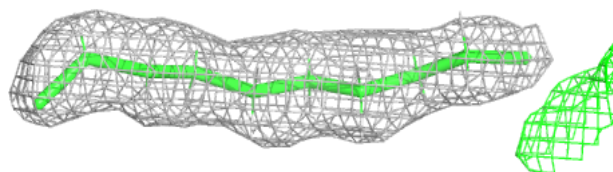
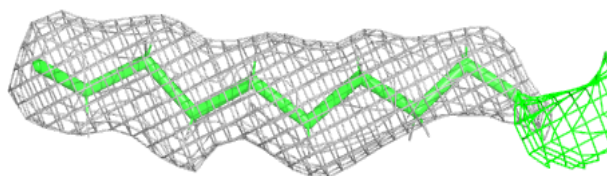


**Electron density around LMG C 519:**

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

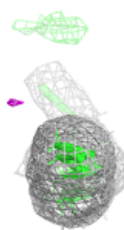
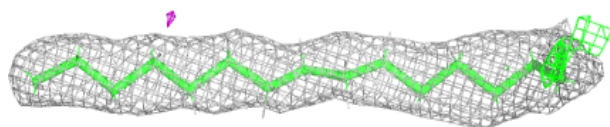
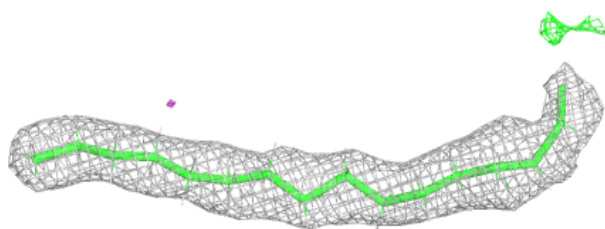
**Electron density around STE M 103:**

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

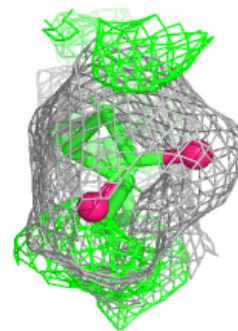
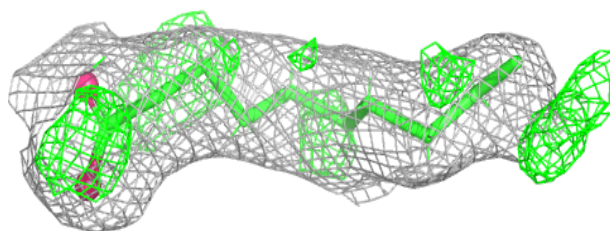
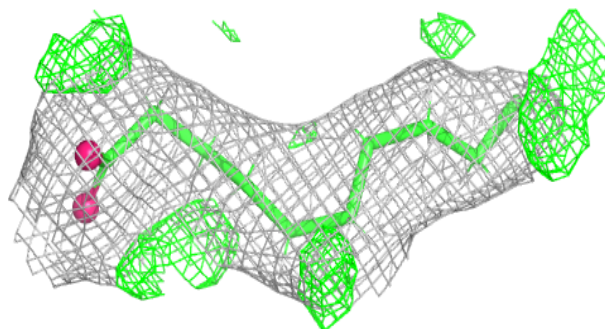


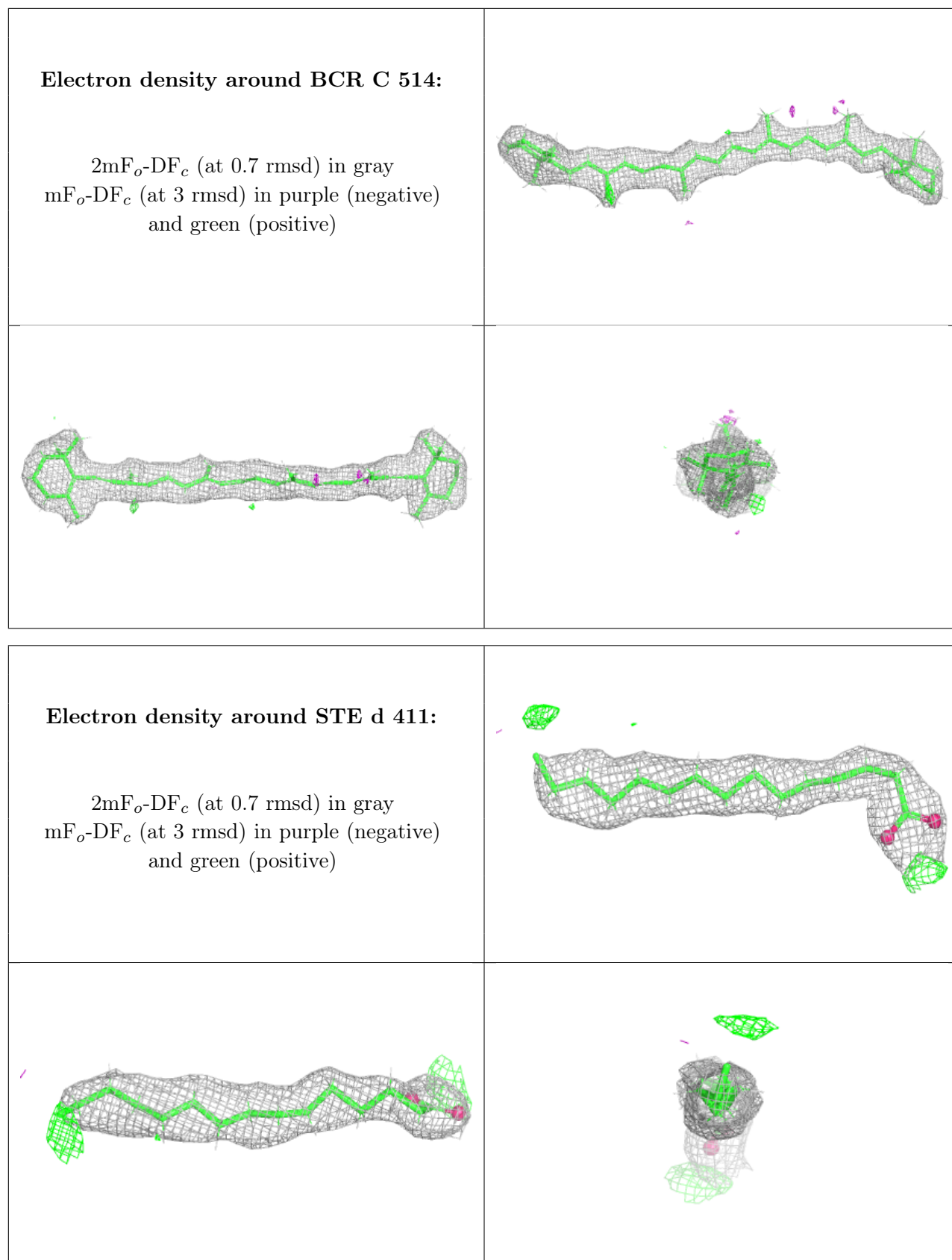
**Electron density around STE C 521:**

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

**Electron density around STE B 625:**

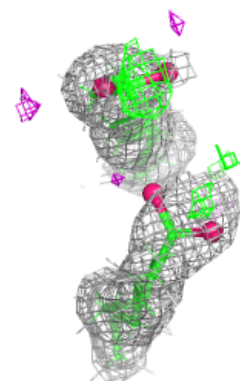
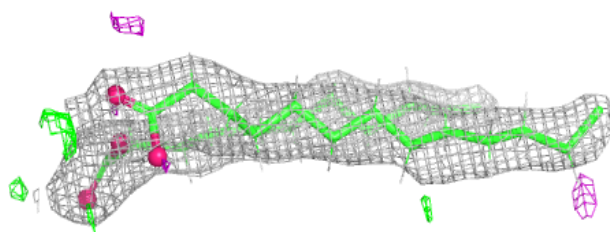
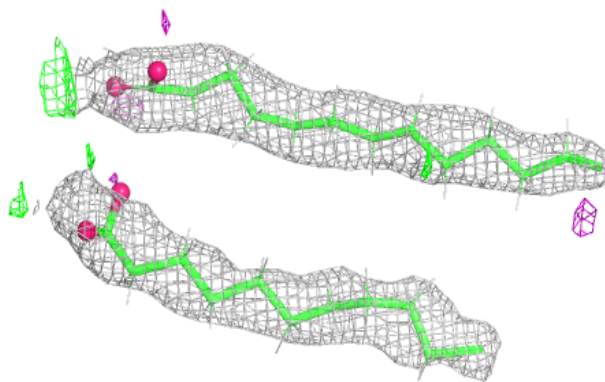
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



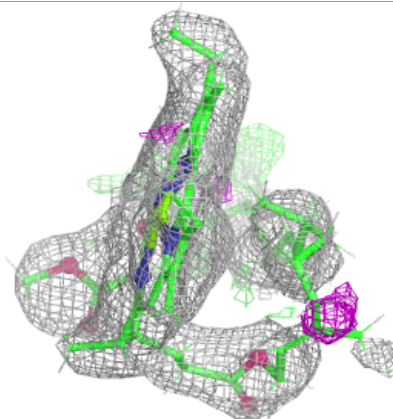
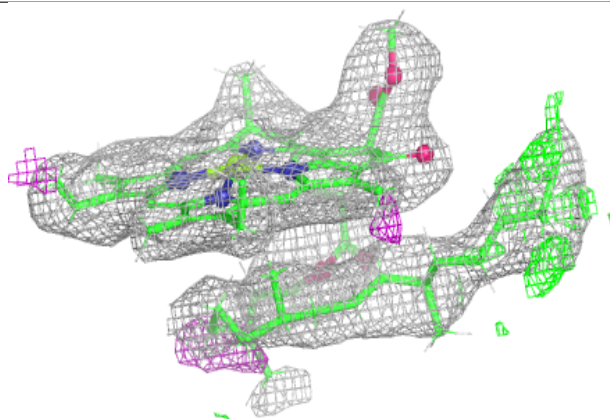
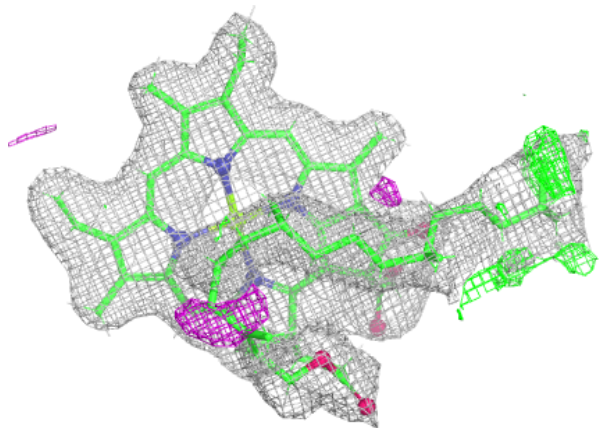


**Electron density around LMG D 410:**

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

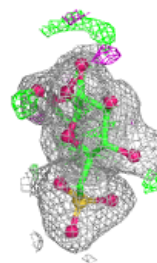
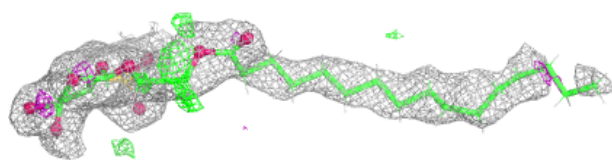
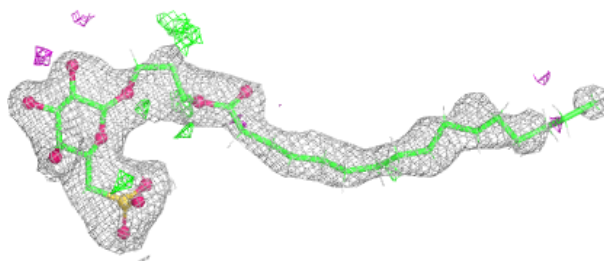
**Electron density around CLA B 601:**

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

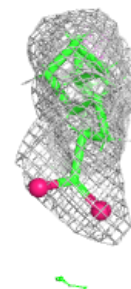
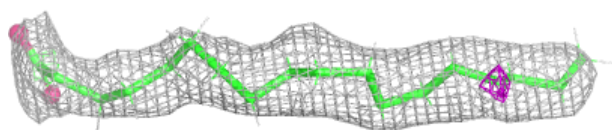
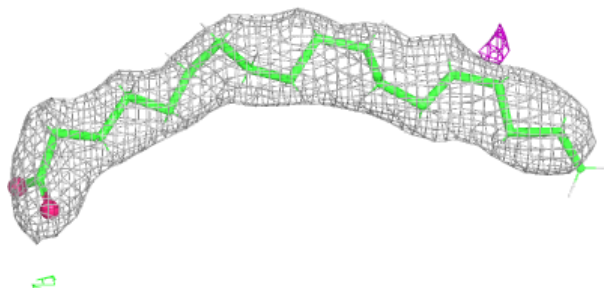


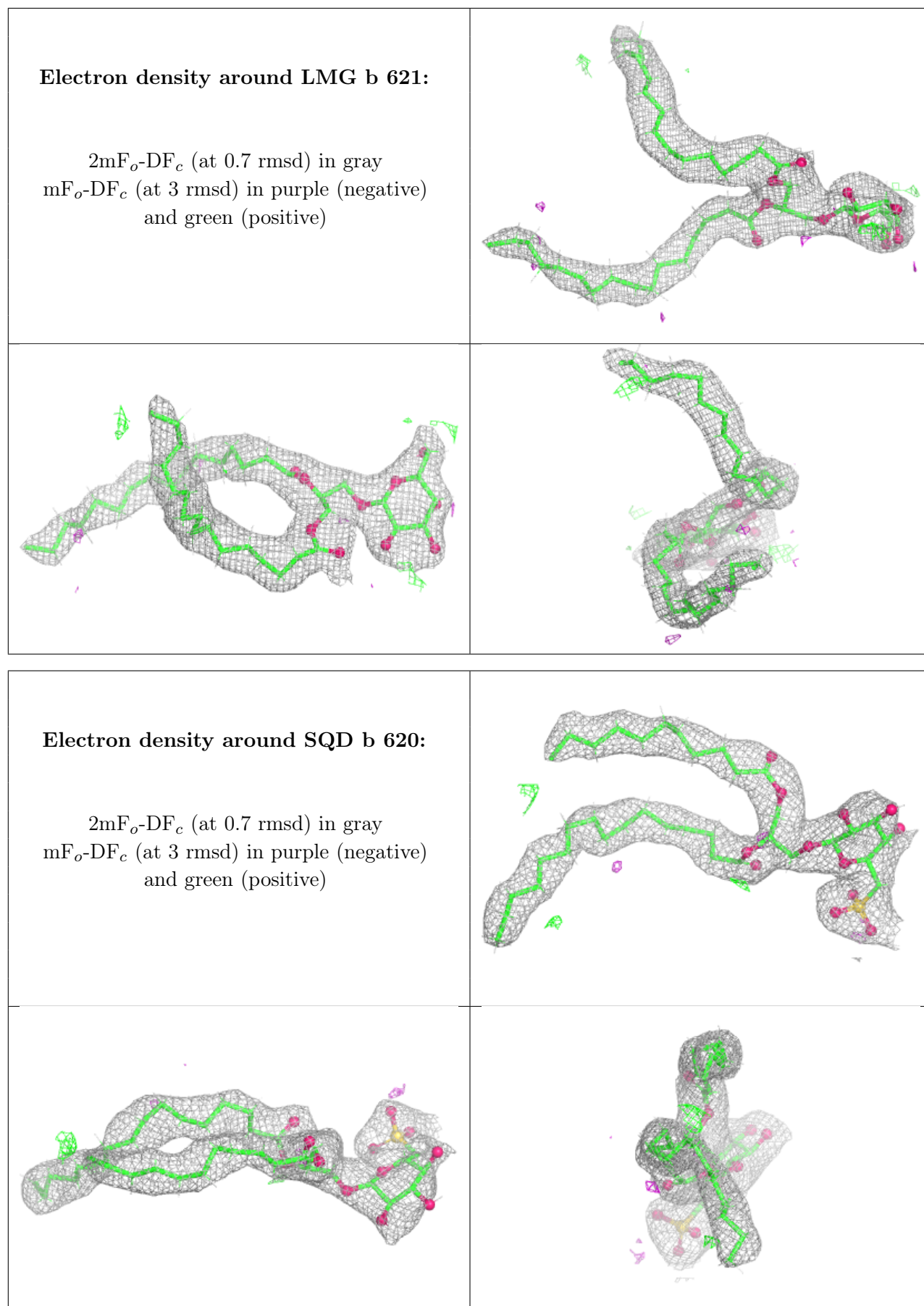
**Electron density around SQD D 407:**

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

**Electron density around STE D 411:**

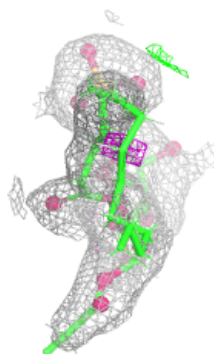
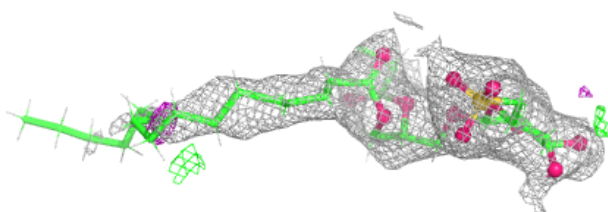
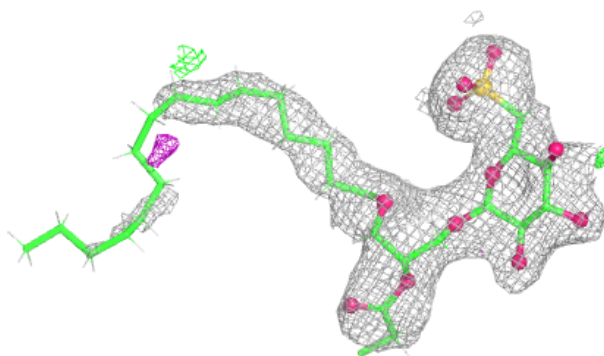
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



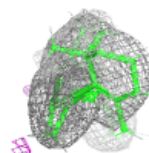
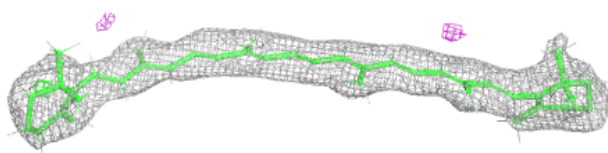


**Electron density around SQD f 101:**

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

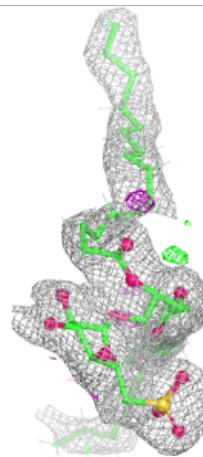
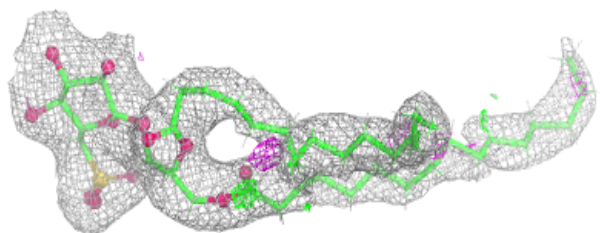
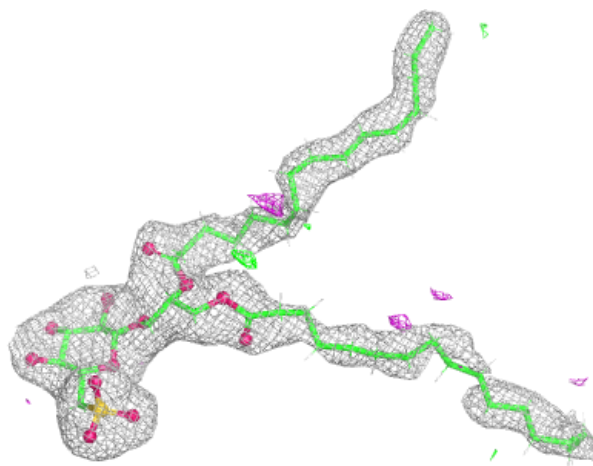
**Electron density around BCR d 405:**

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



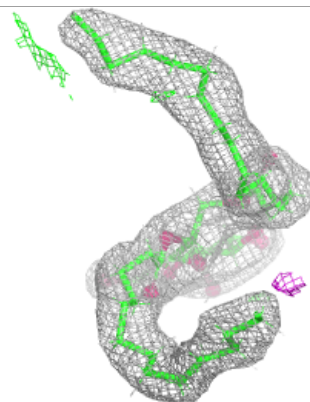
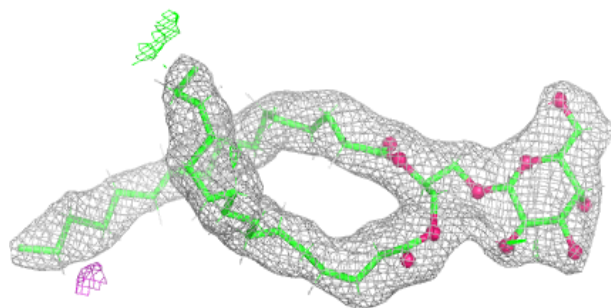
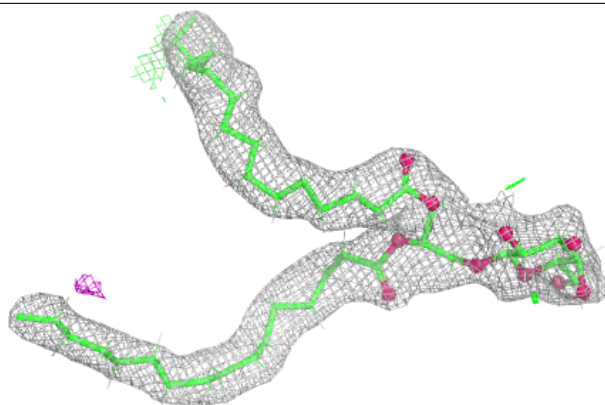
**Electron density around SQD a 613:**

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

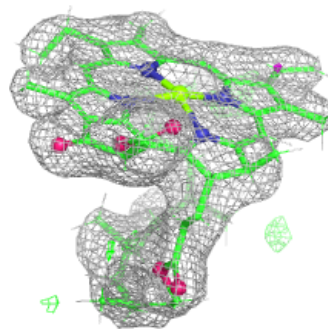
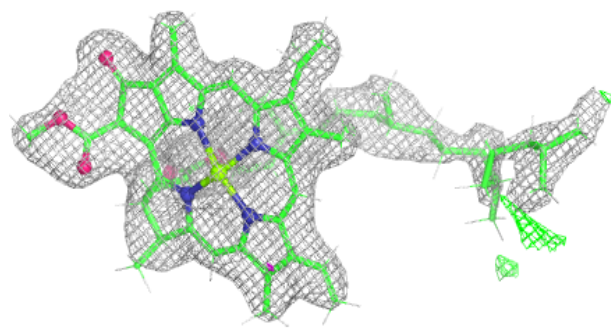
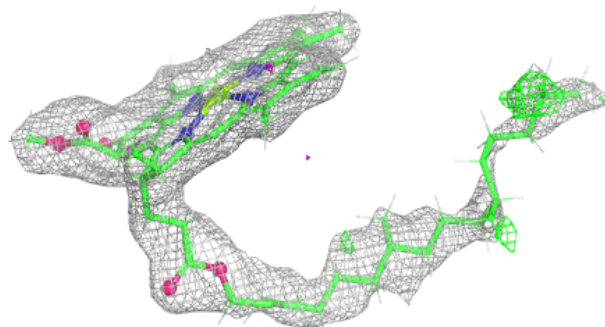


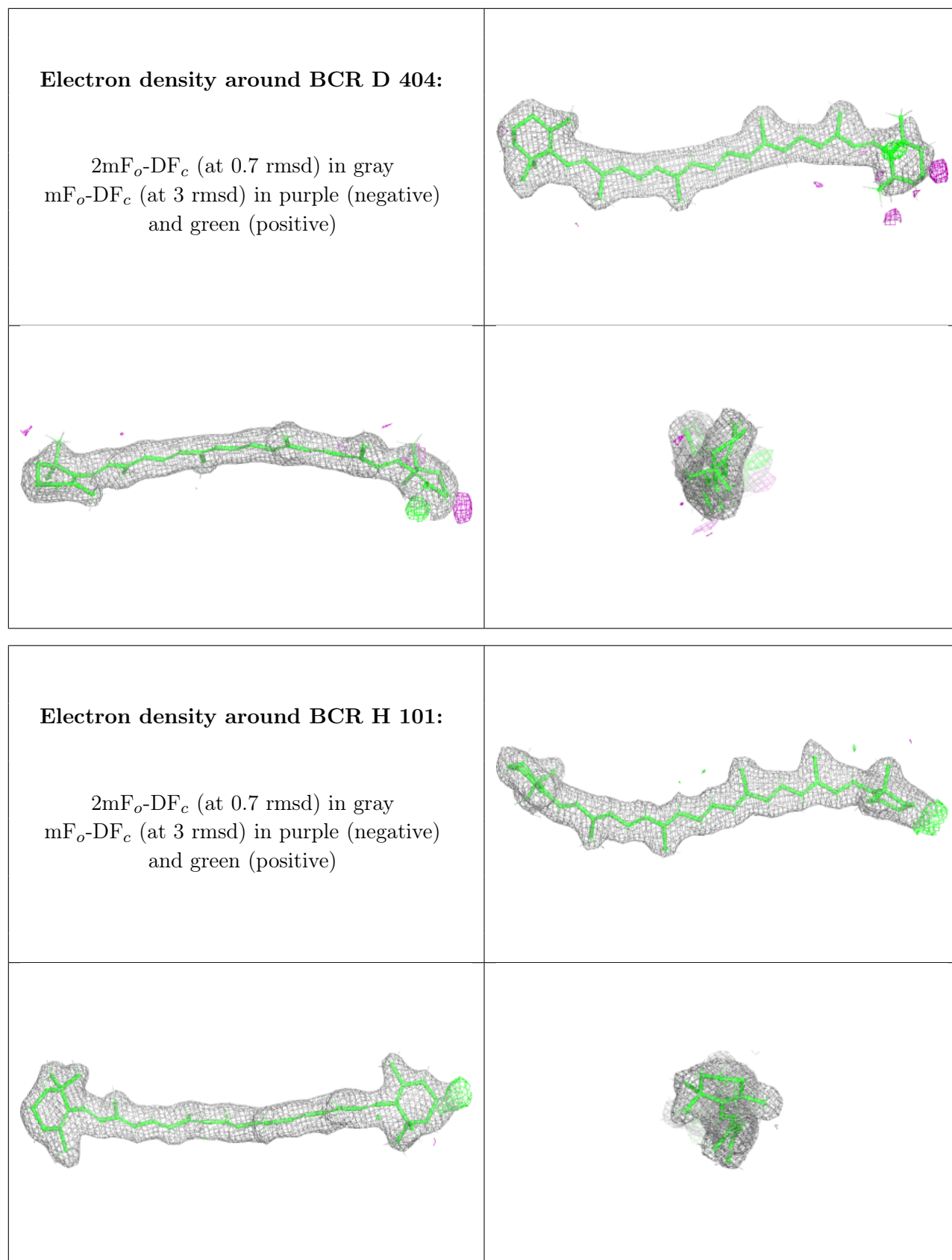
**Electron density around LMG M 101:**

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

**Electron density around CLA C 513:**

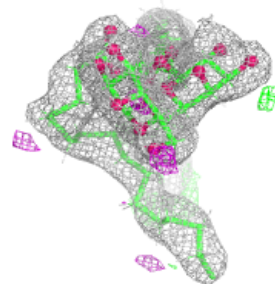
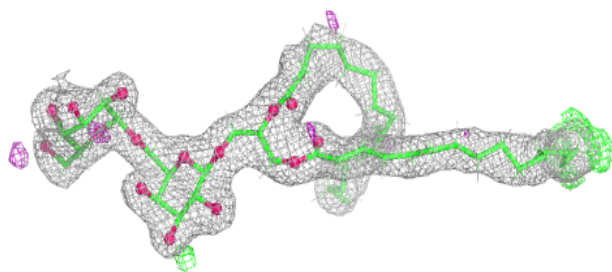
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



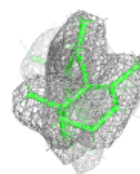
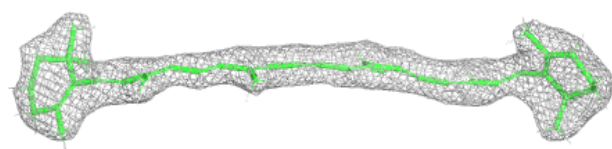


**Electron density around DGD H 102:**

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

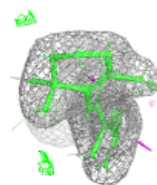
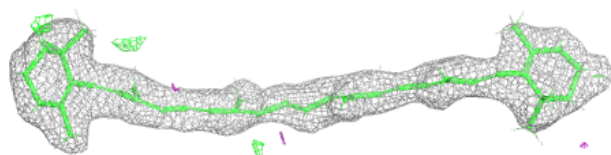
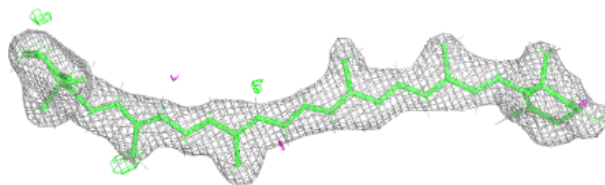
**Electron density around BCR k 101:**

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

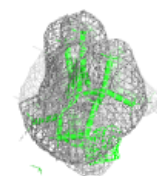
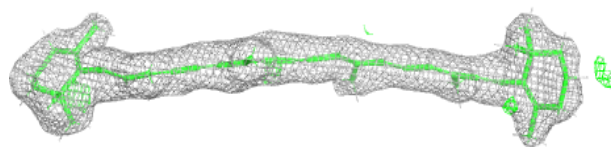


**Electron density around BCR x 101:**

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

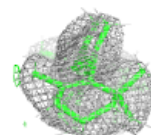
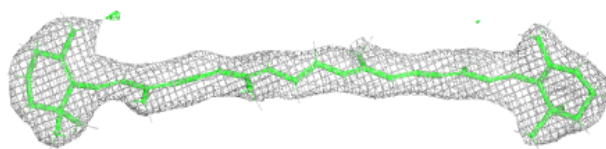
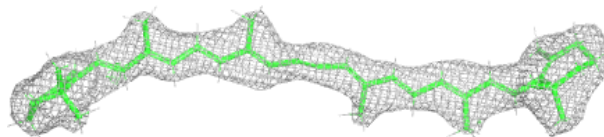
**Electron density around BCR Y 101:**

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

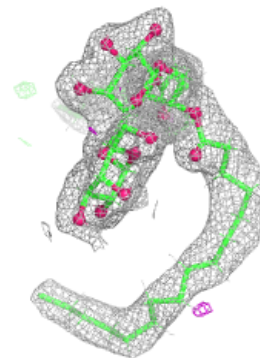
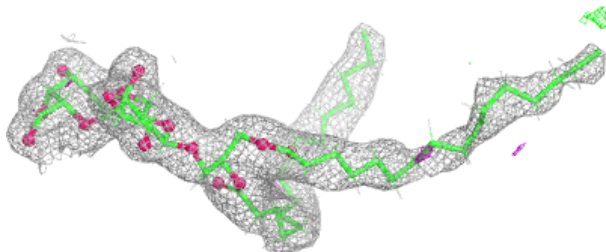
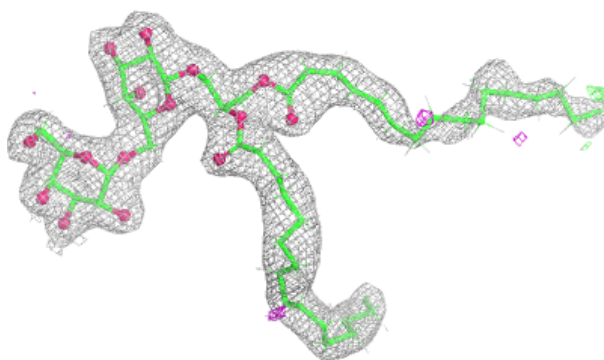


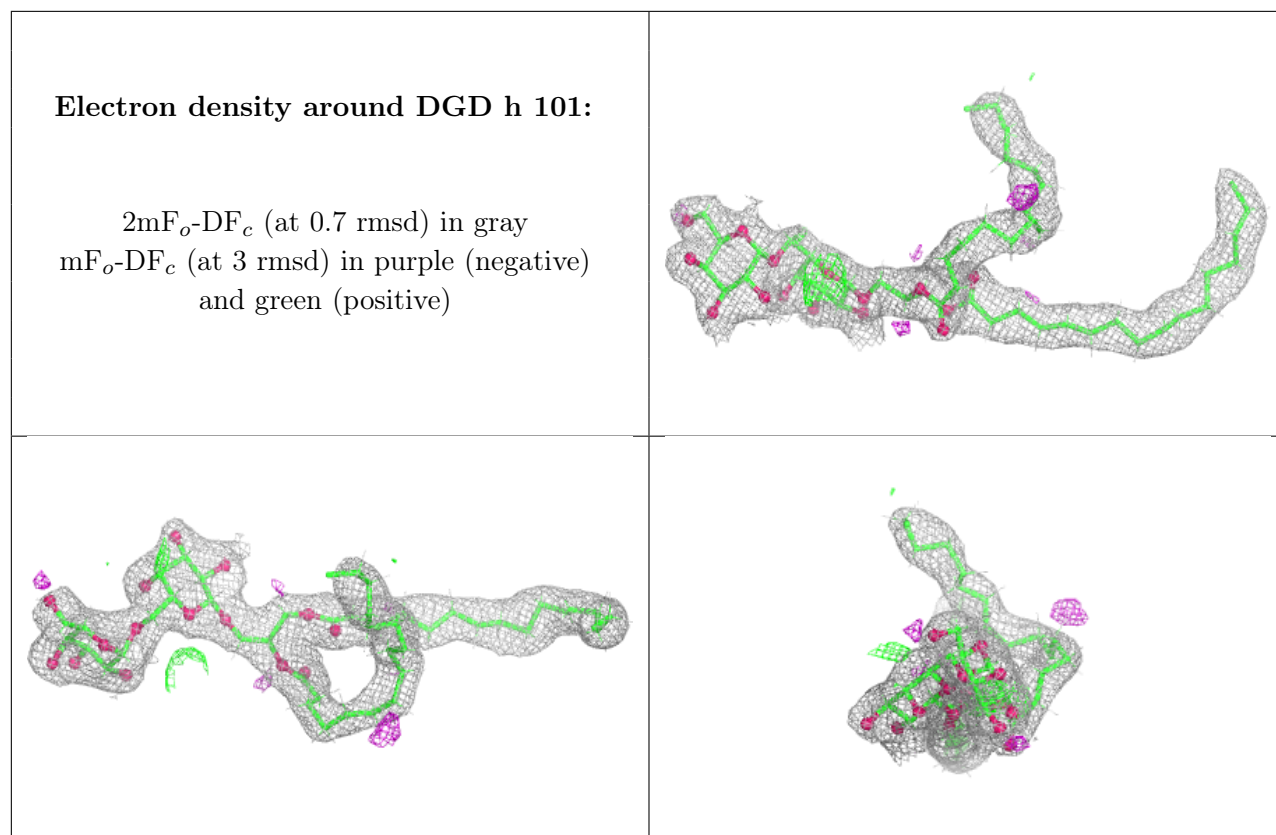
**Electron density around BCR c 514:**

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

**Electron density around DGD c 517:**

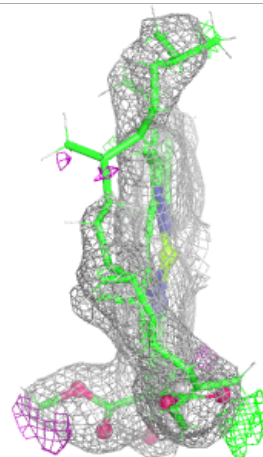
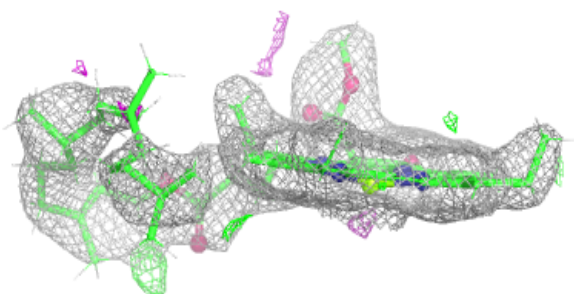
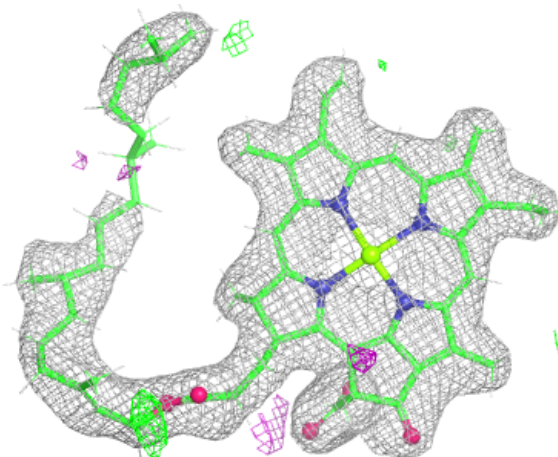
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





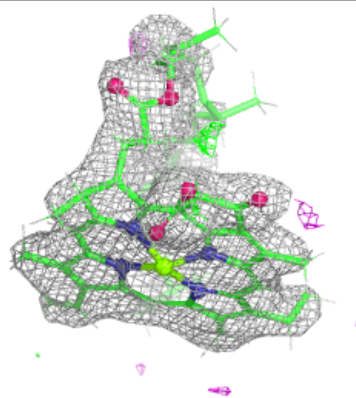
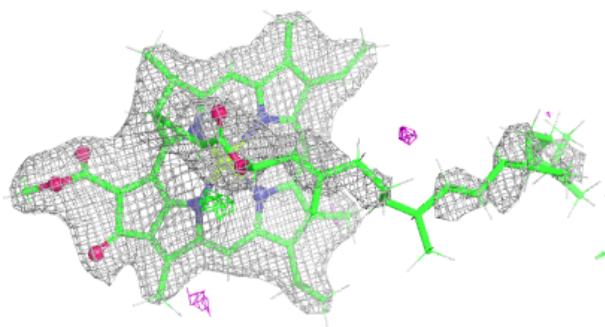
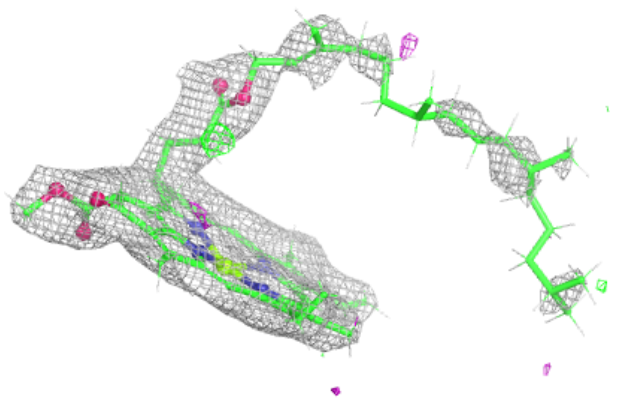
**Electron density around CLA c 512:**

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

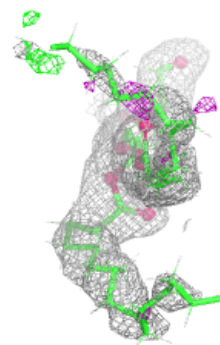
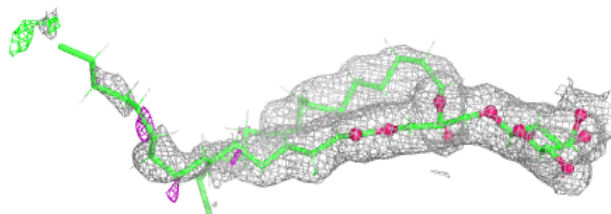
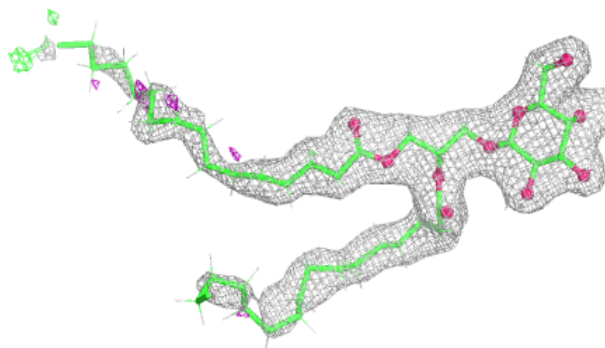


**Electron density around CLA c 513:**

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

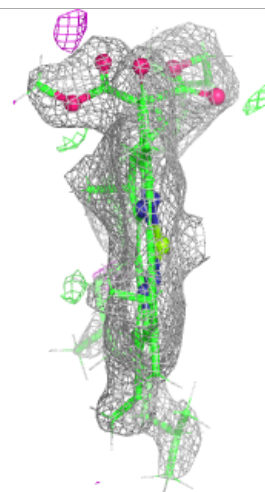
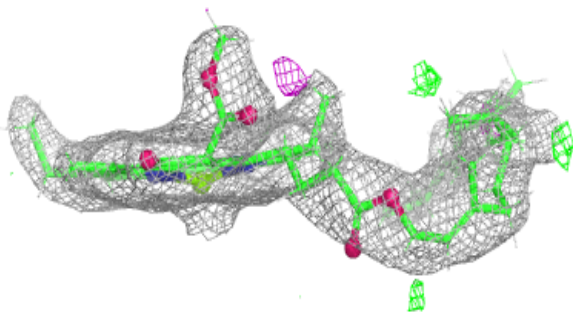
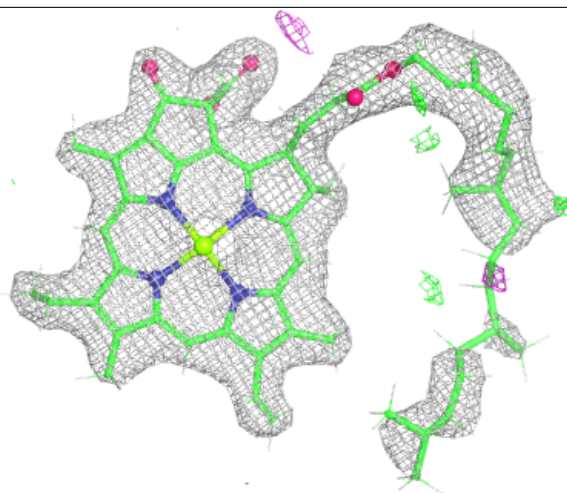
**Electron density around LMG D 406:**

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



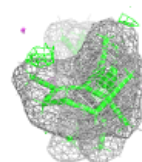
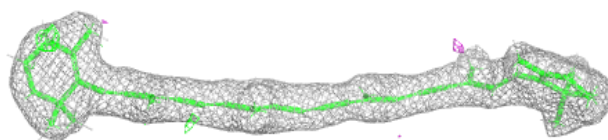
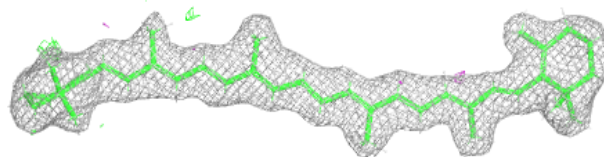
**Electron density around CLA C 512:**

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

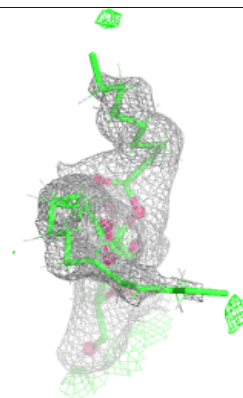
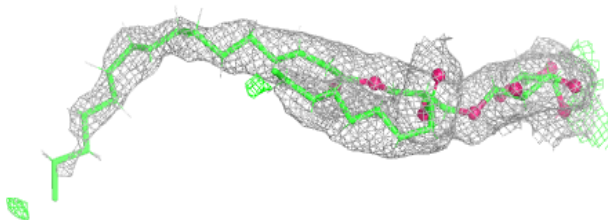
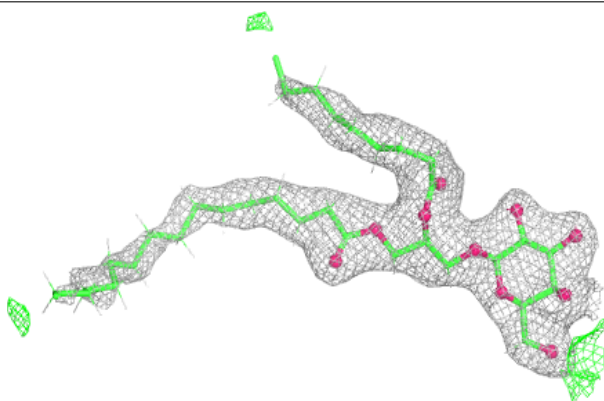


**Electron density around BCR b 617:**

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

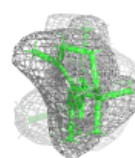
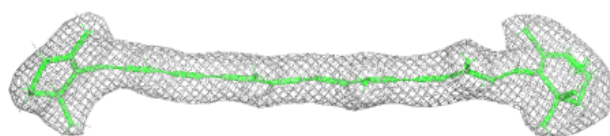
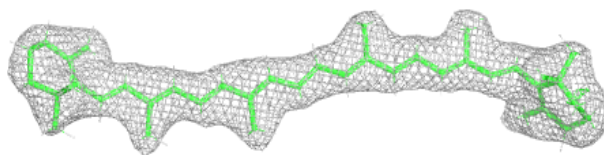
**Electron density around LMG d 410:**

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

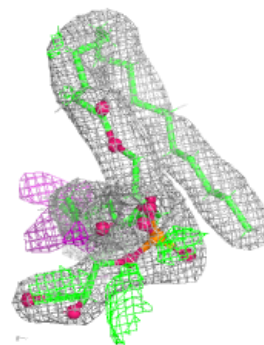
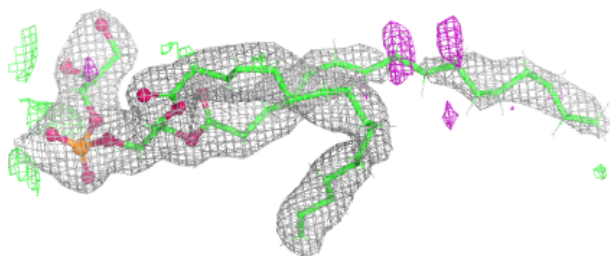
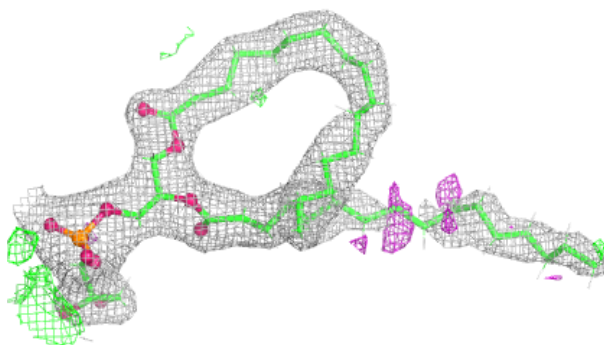


**Electron density around BCR b 618:**

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

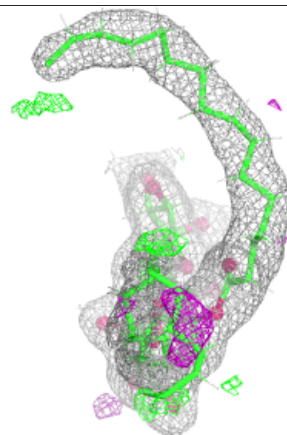
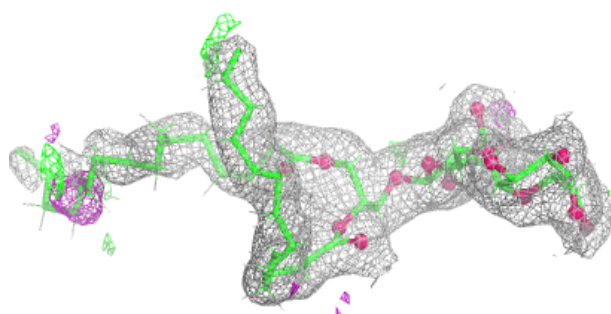
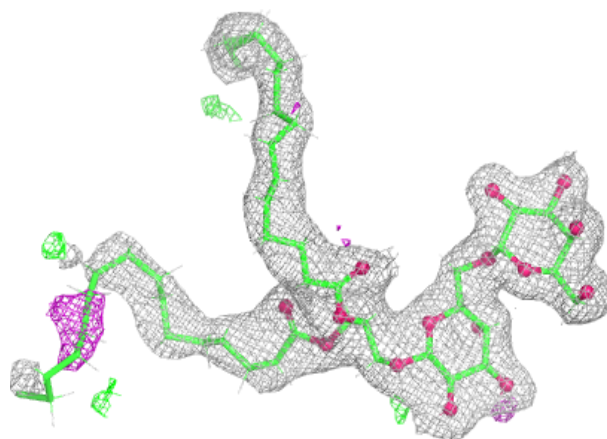
**Electron density around LHG d 407:**

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

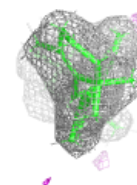
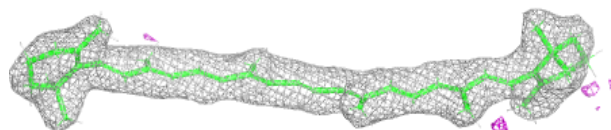
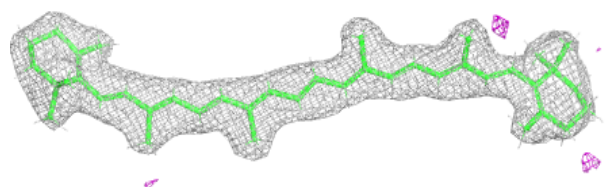


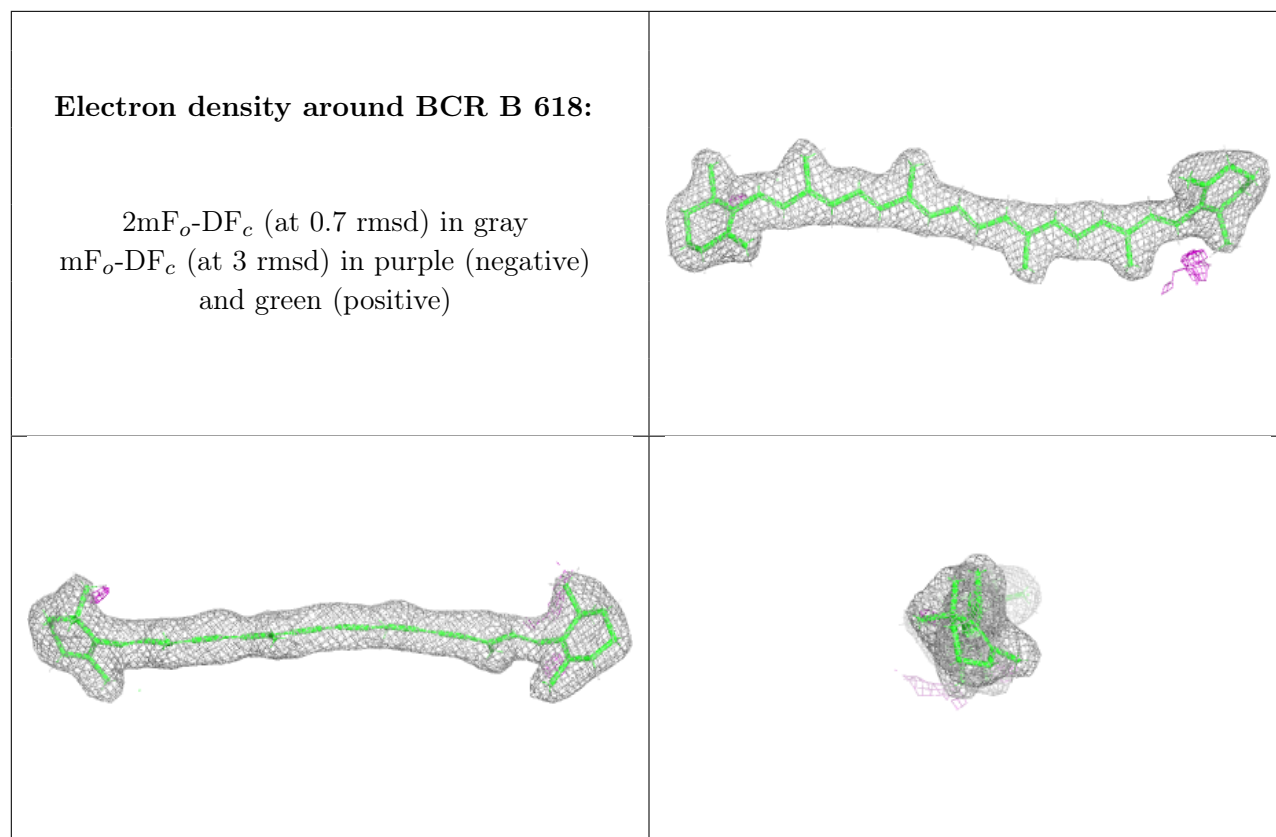
**Electron density around DGD C 517:**

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

**Electron density around BCR b 619:**

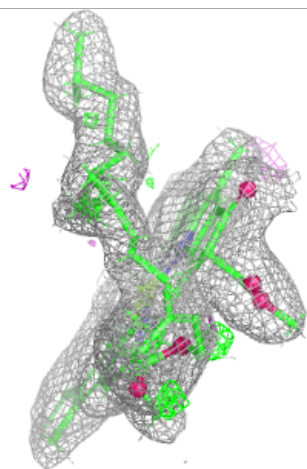
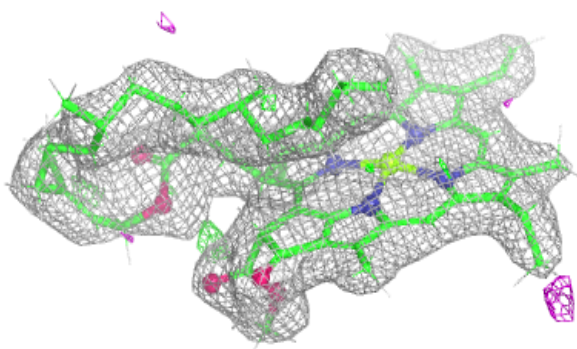
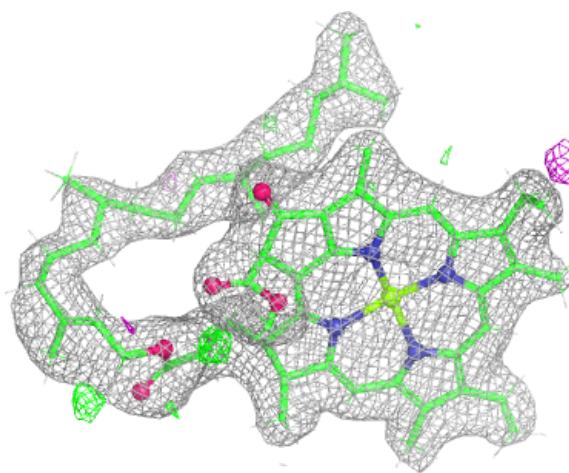
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

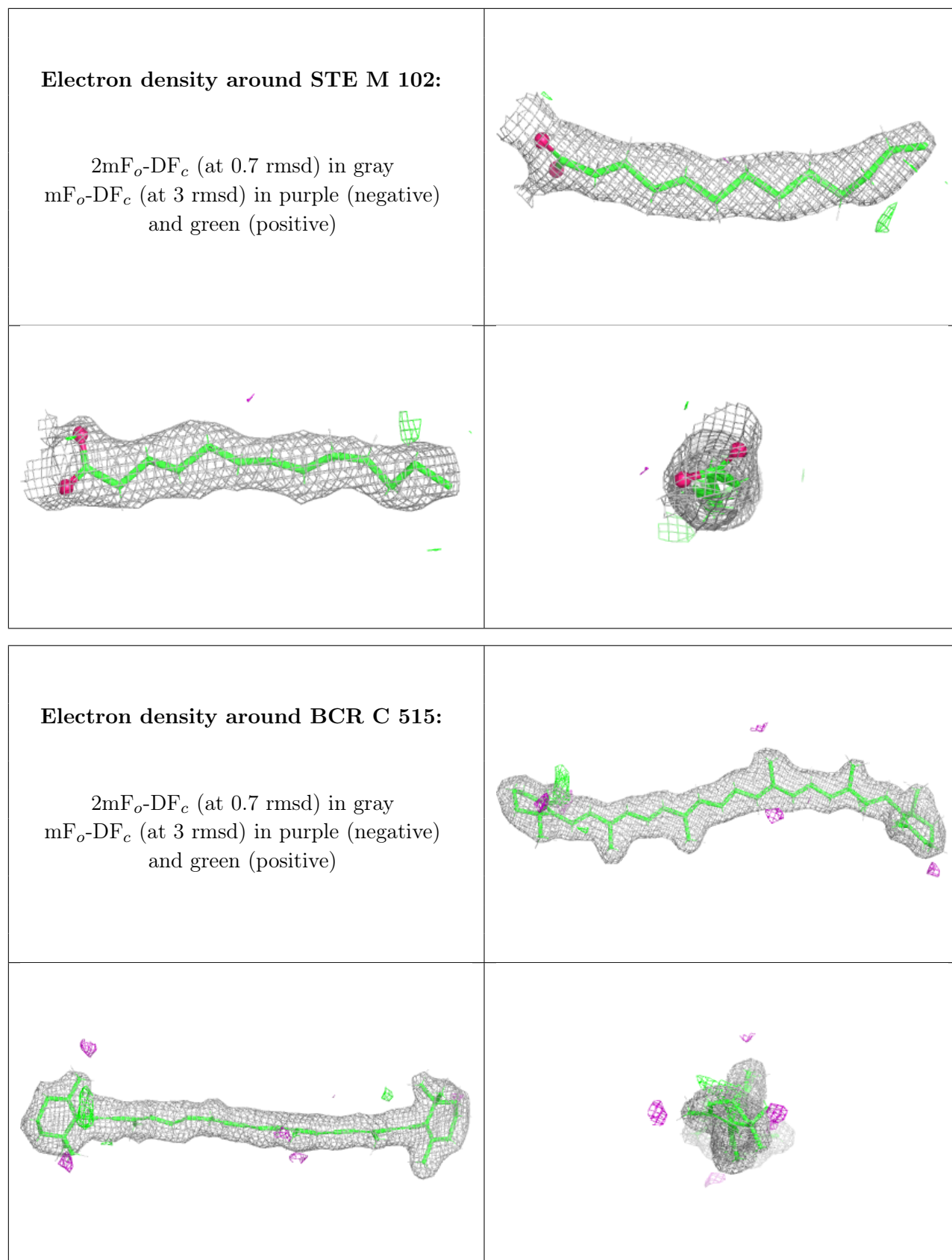




**Electron density around CLA c 509:**

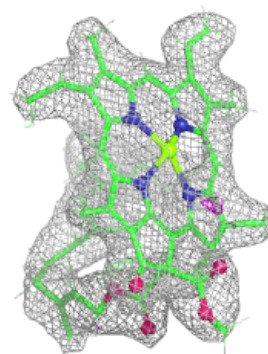
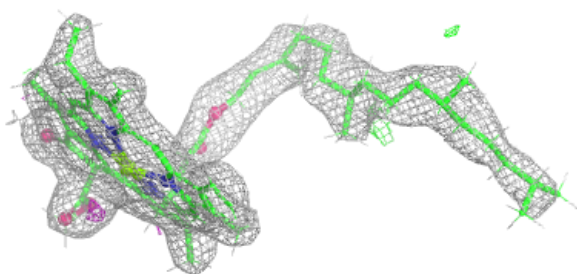
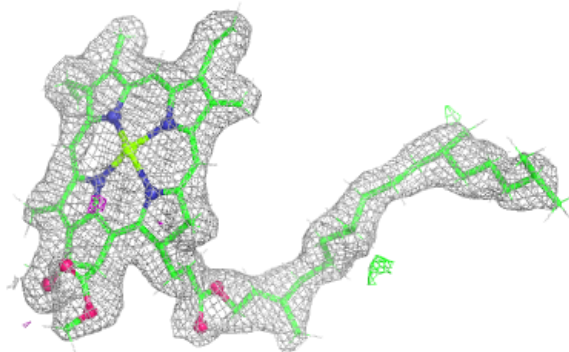
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



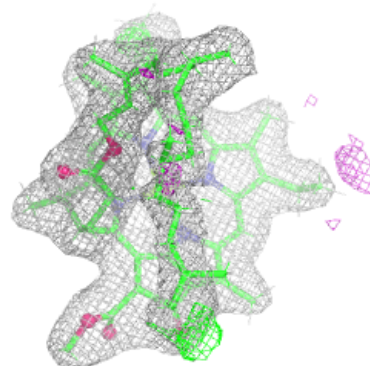
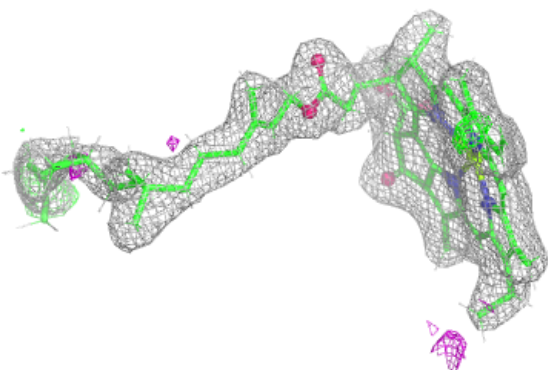
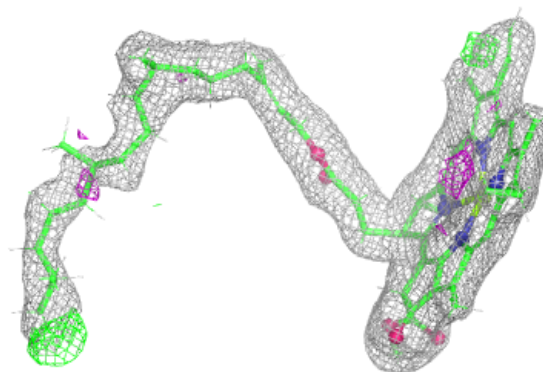


**Electron density around CLA C 511:**

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

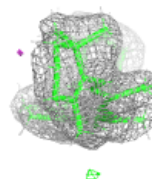
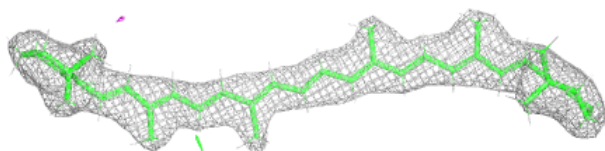
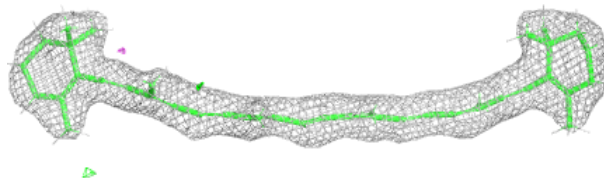
**Electron density around CLA b 606:**

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

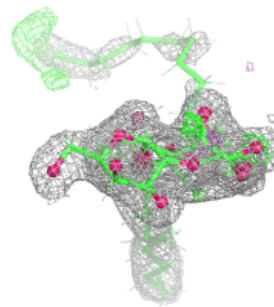
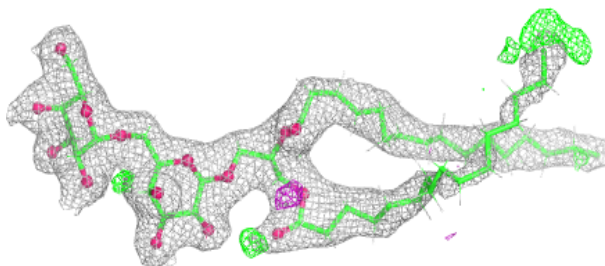
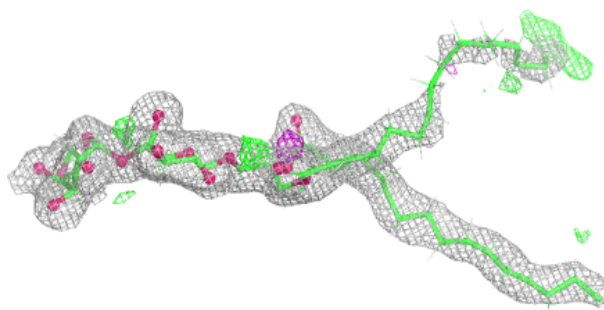


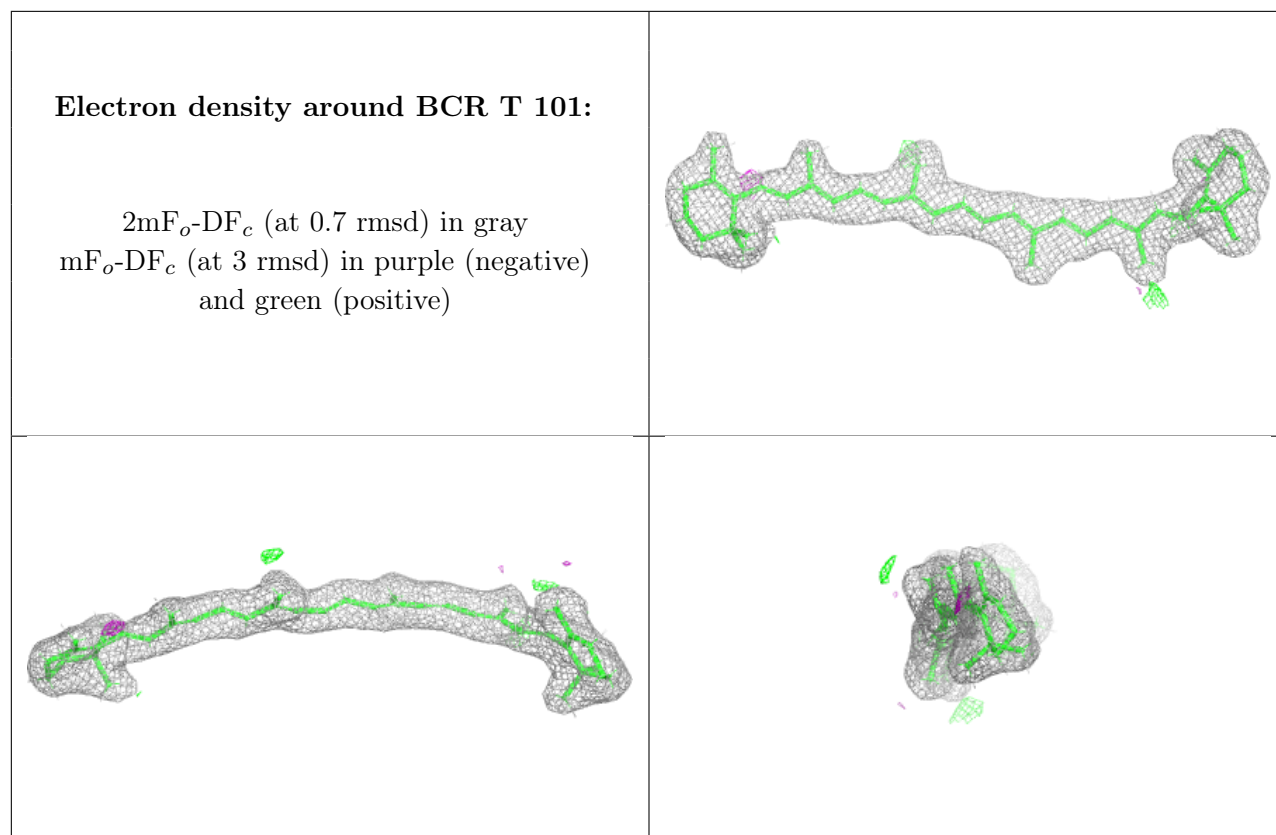
**Electron density around BCR k 102:**

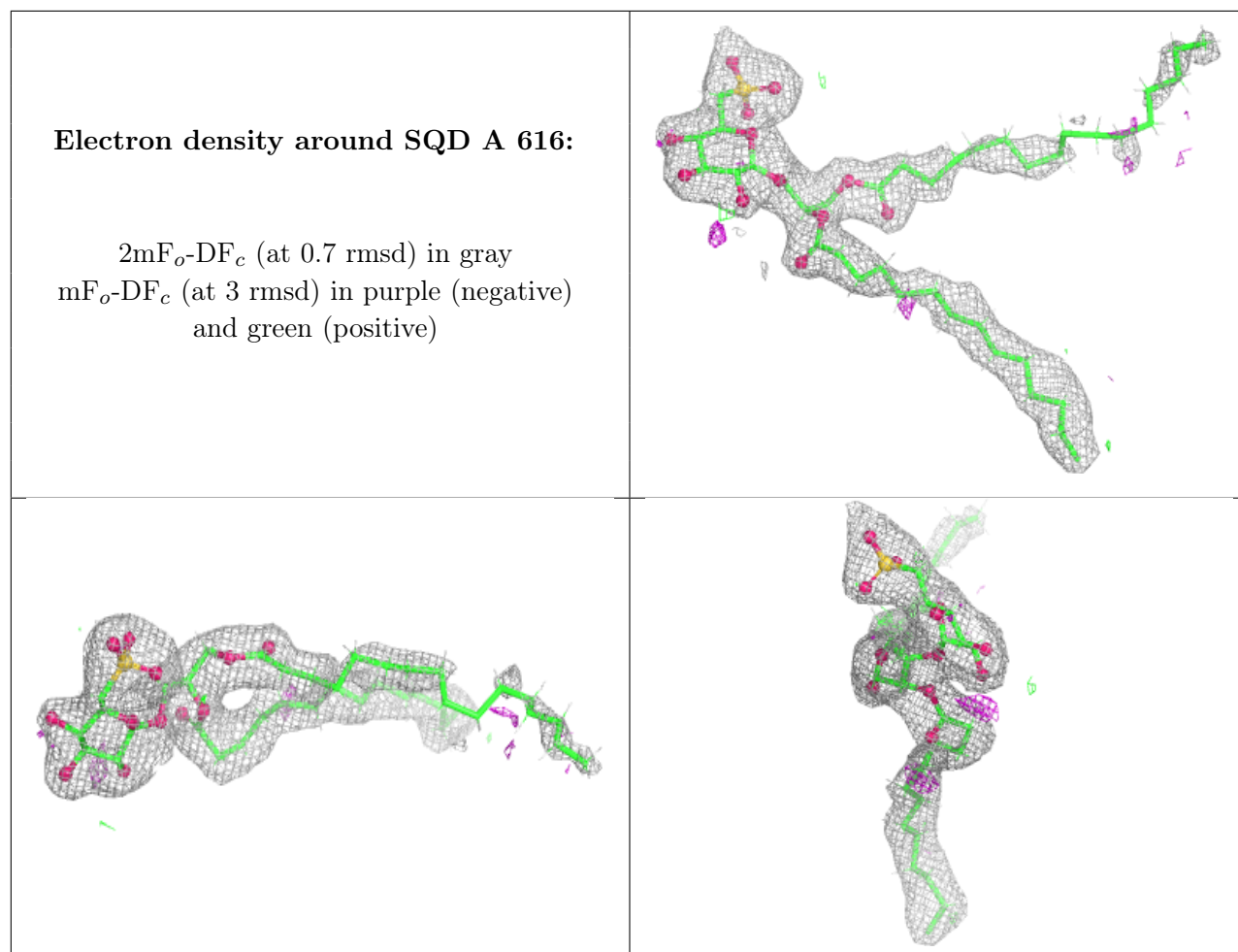
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

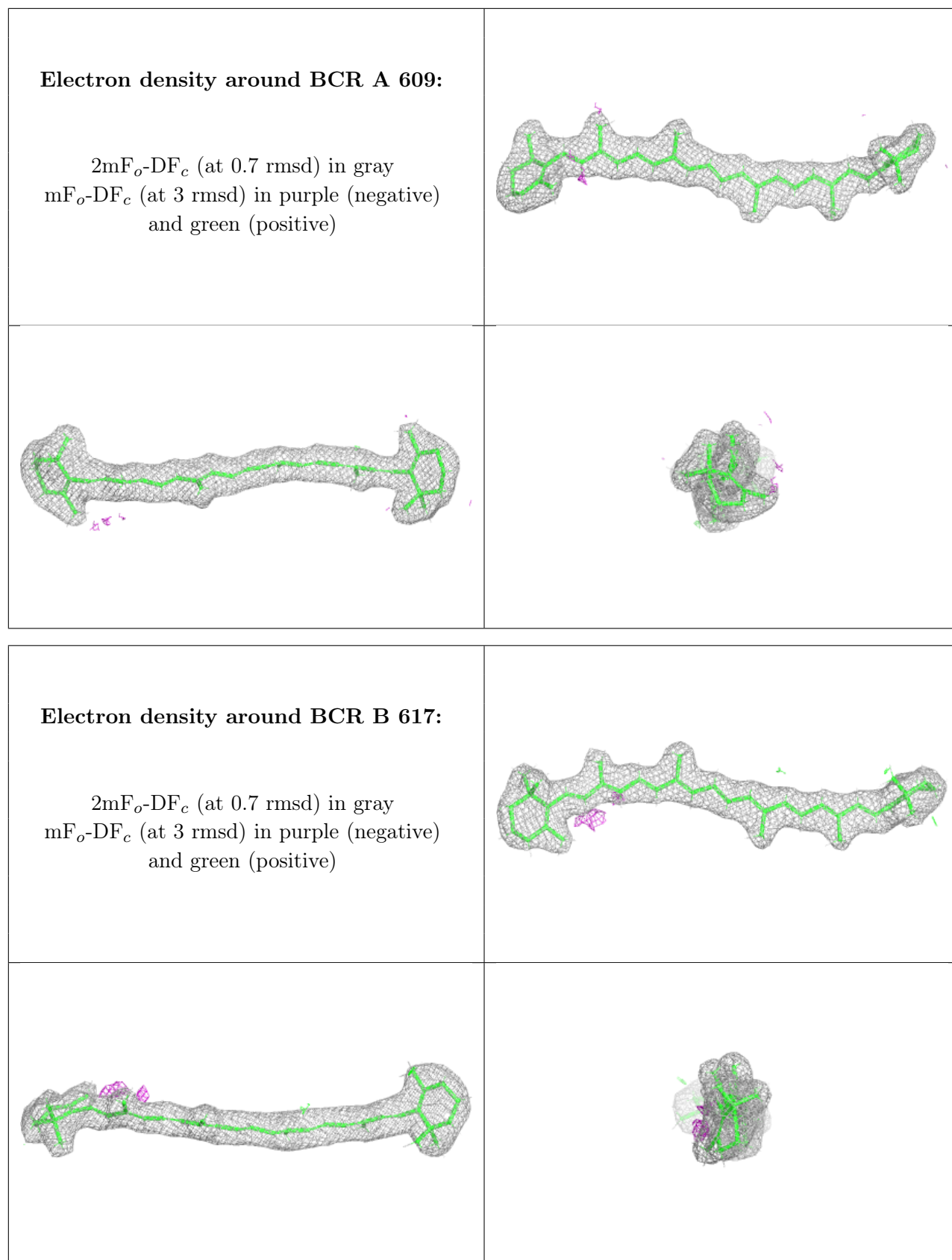
**Electron density around DGD C 516:**

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



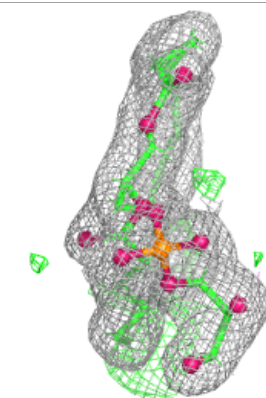
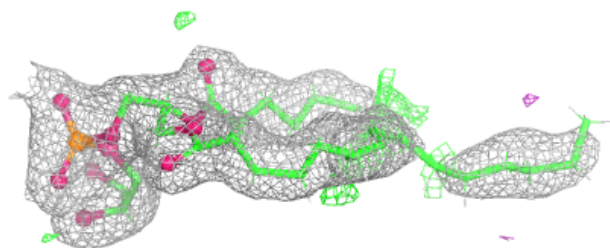
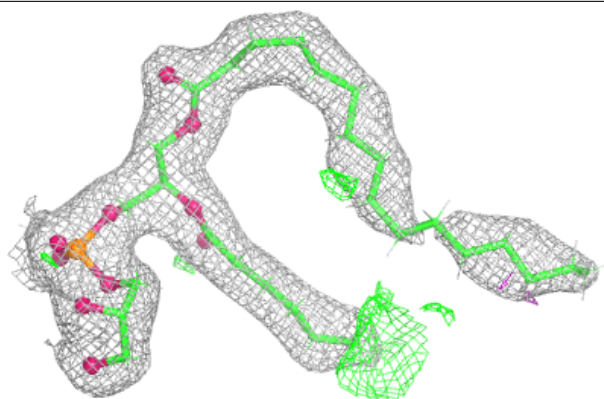




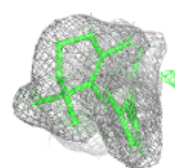
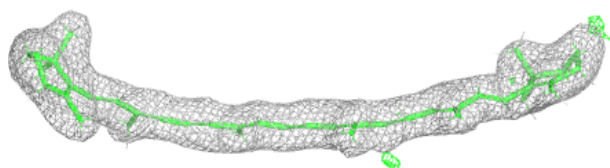
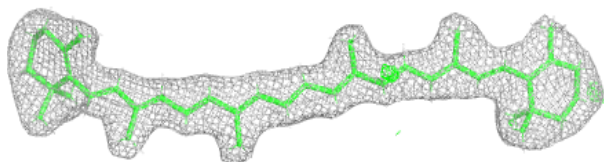


**Electron density around LHG d 409:**

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

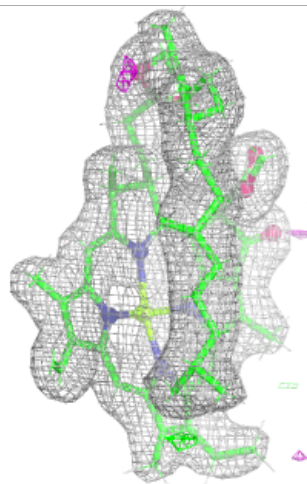
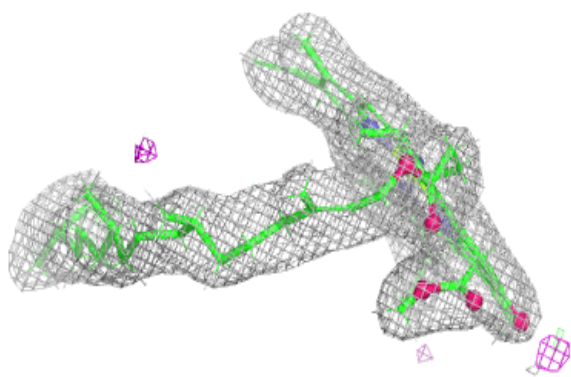
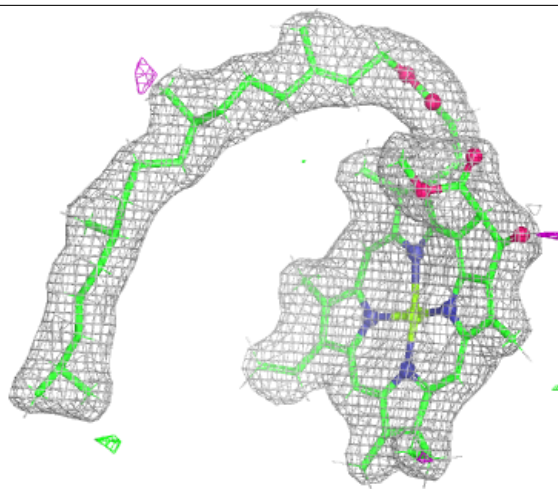
**Electron density around BCR t 101:**

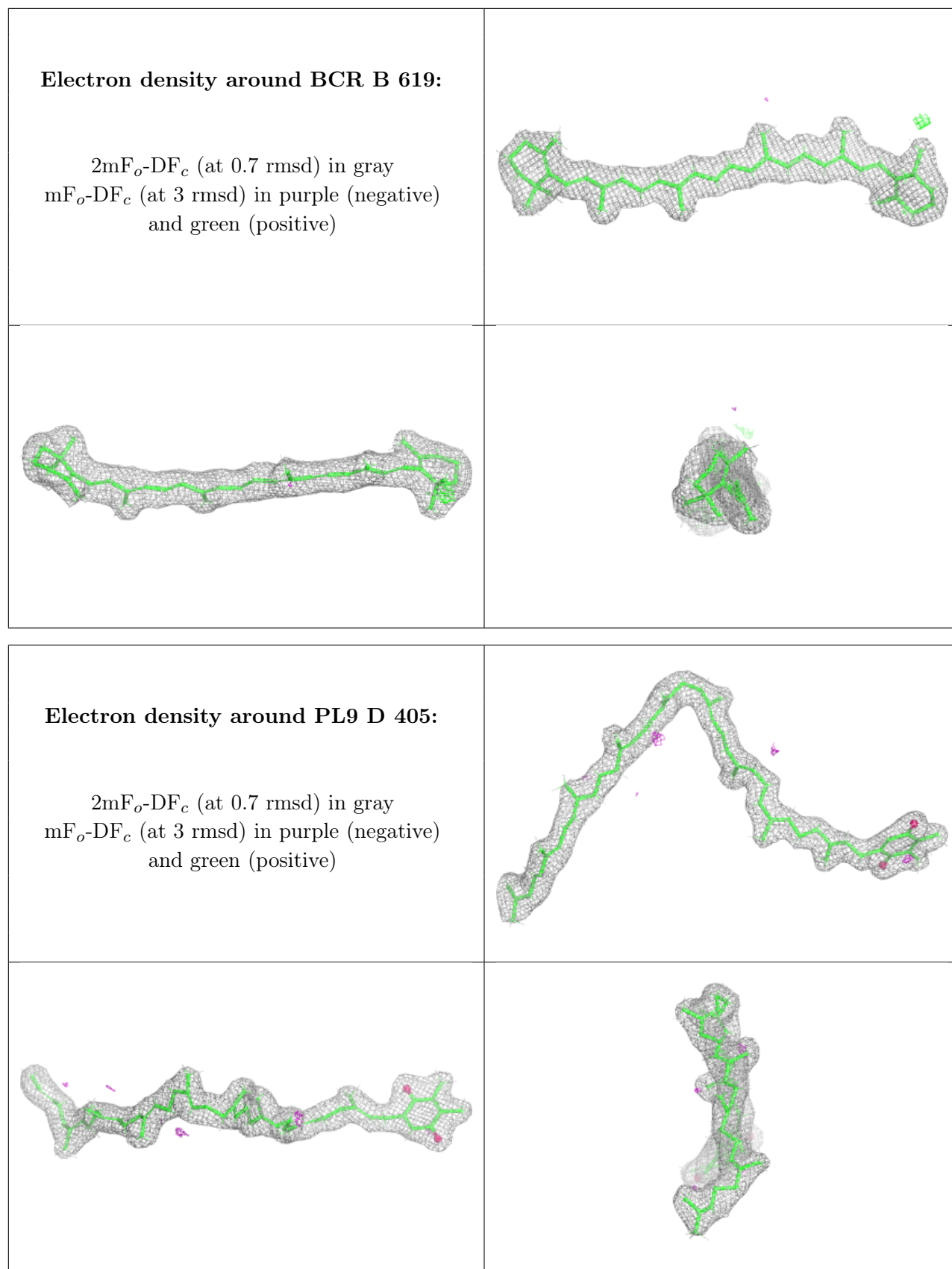
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 507:**

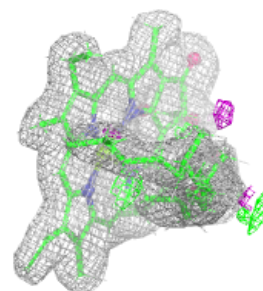
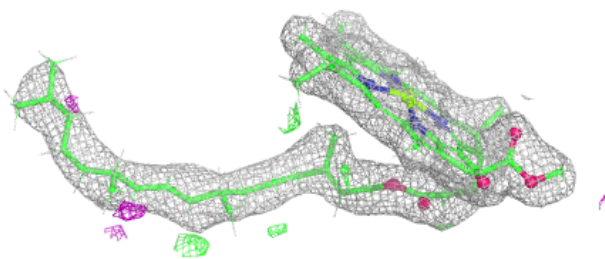
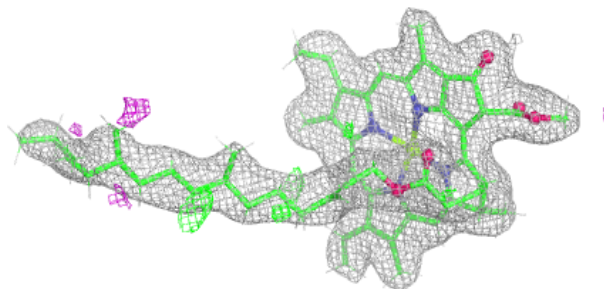
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



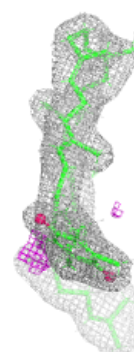
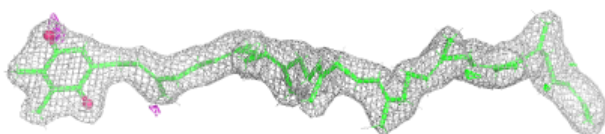
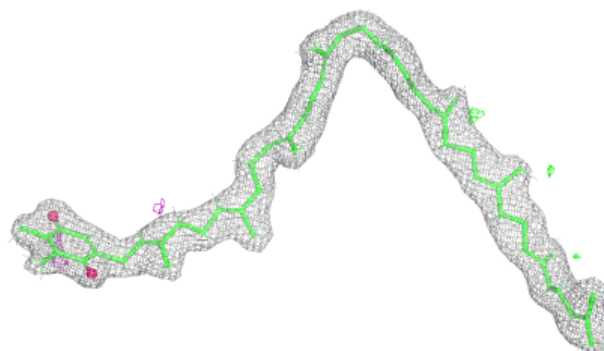


**Electron density around CLA b 608:**

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

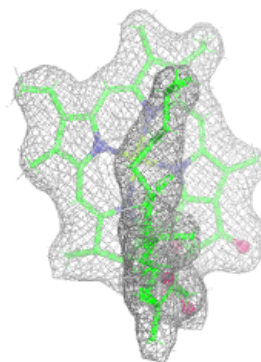
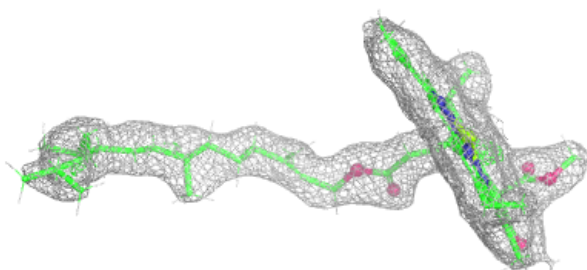
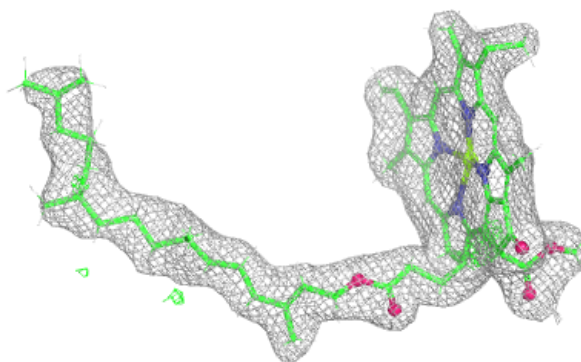
**Electron density around PL9 d 406:**

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

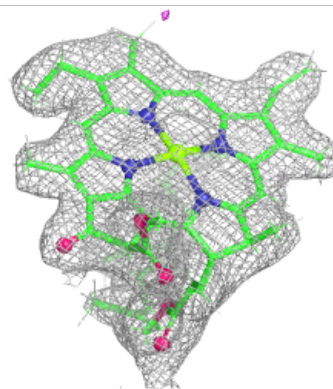
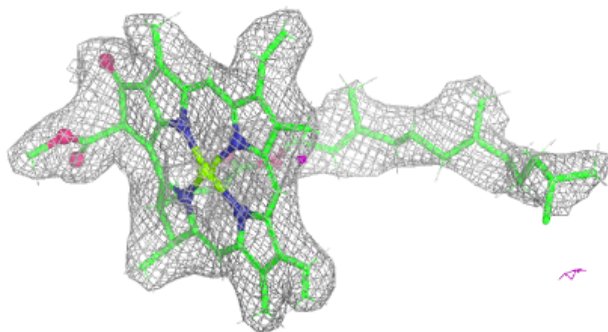
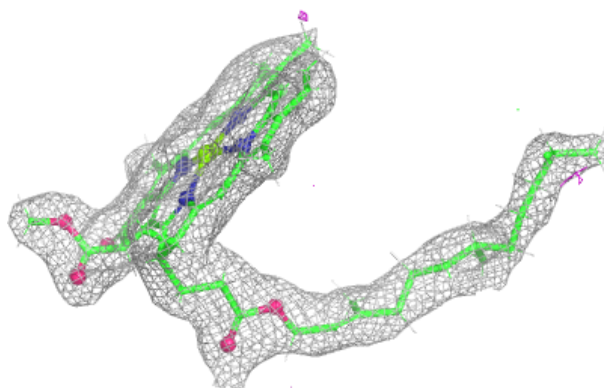


**Electron density around CLA b 609:**

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

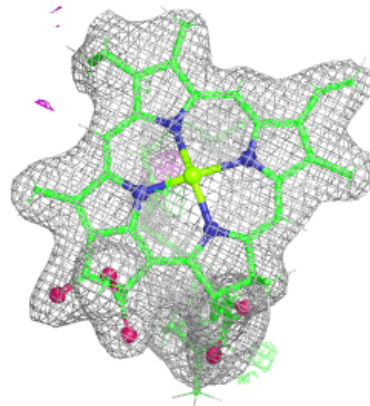
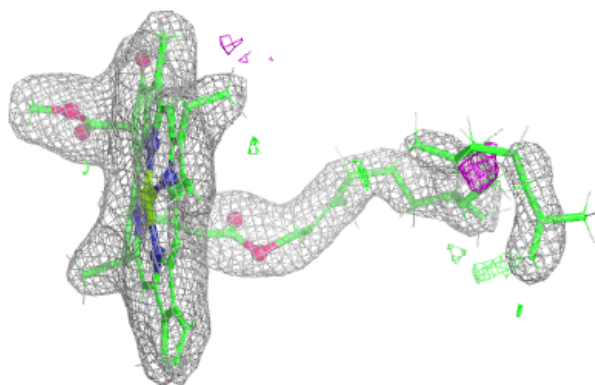
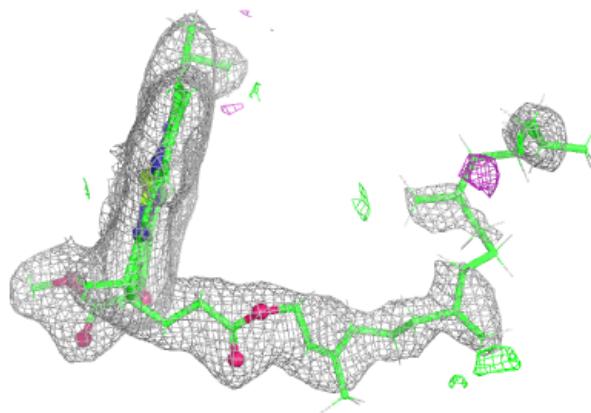
**Electron density around CLA c 504:**

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

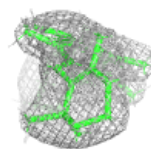
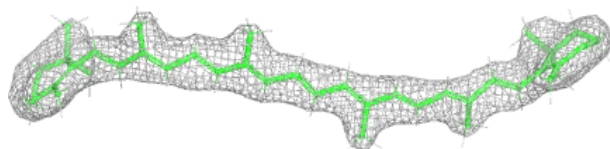
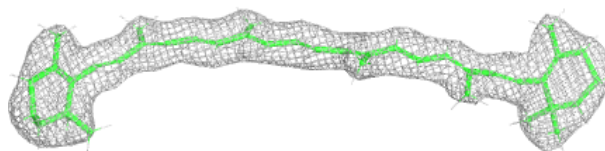


**Electron density around CLA c 506:**

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

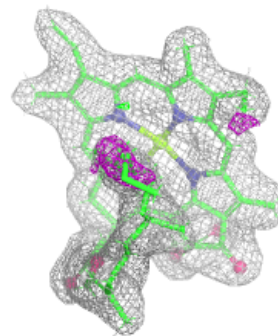
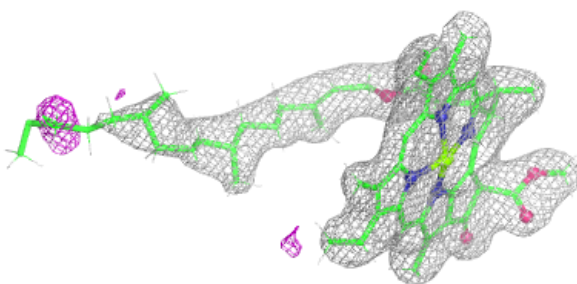
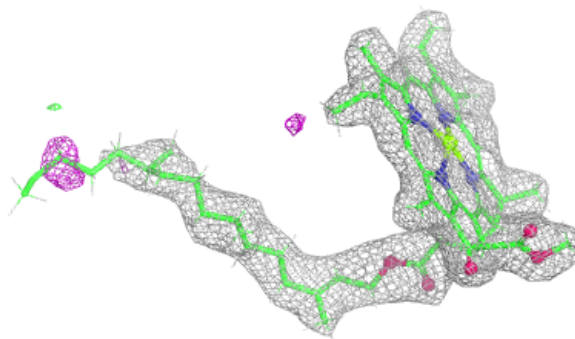
**Electron density around BCR K 101:**

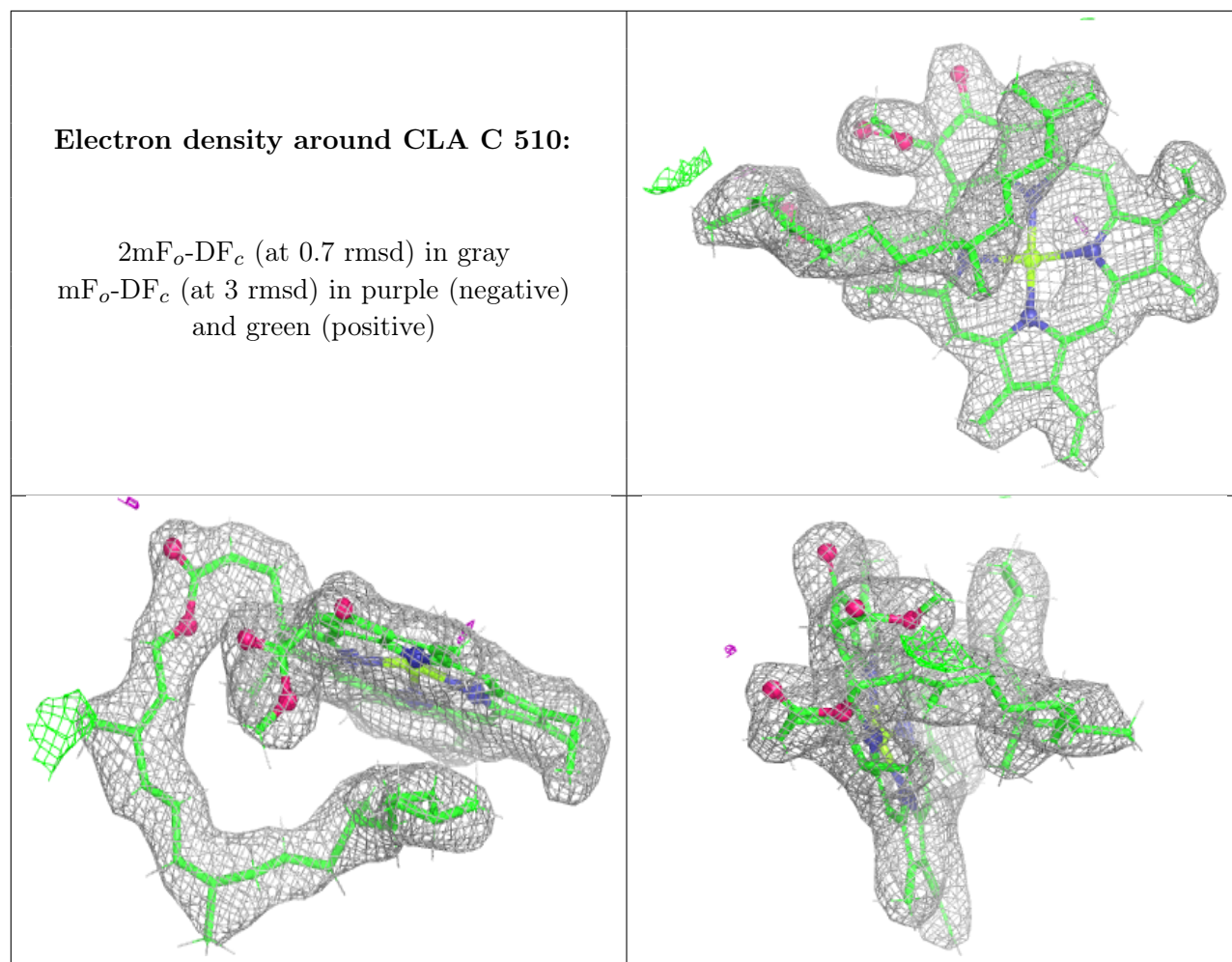
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 508:**

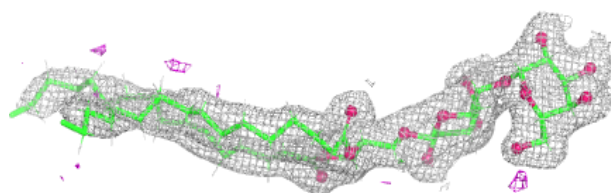
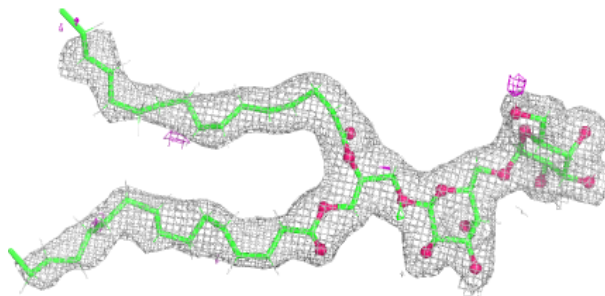
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



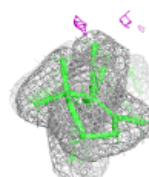
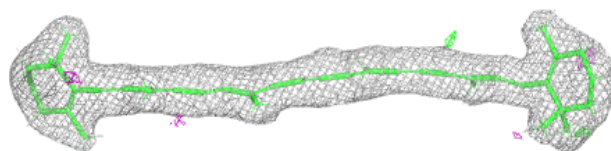
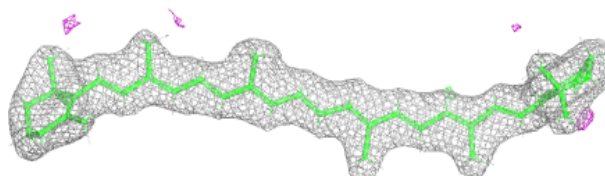


**Electron density around DGD C 518:**

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

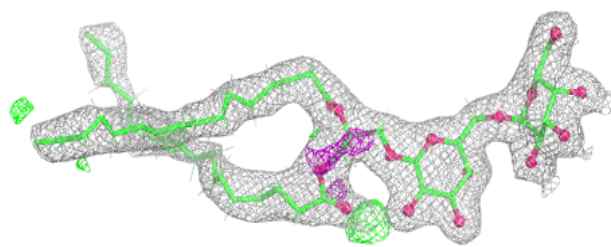
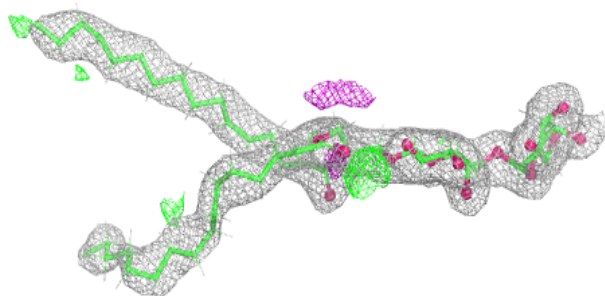
**Electron density around BCR a 607:**

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

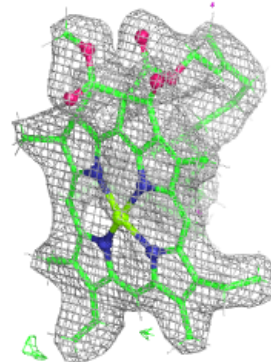
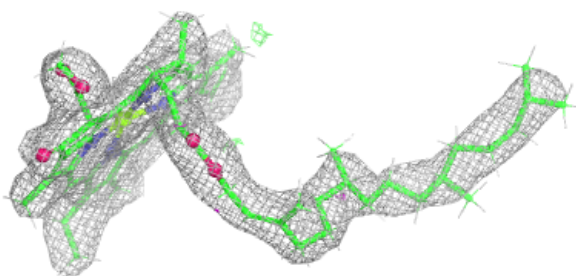
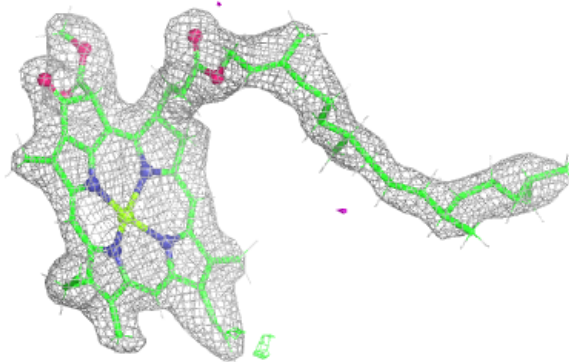


**Electron density around DGD c 516:**

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

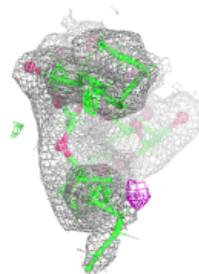
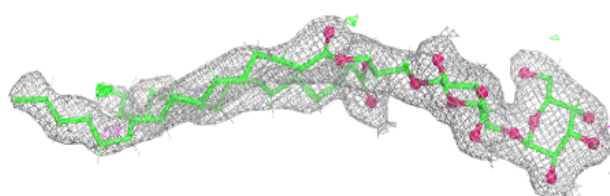
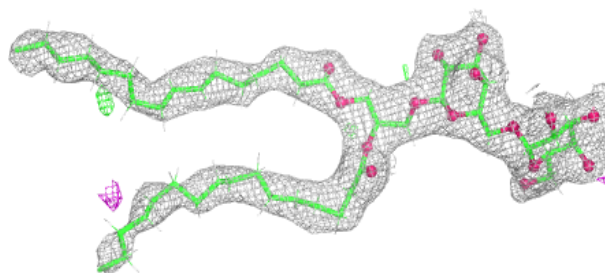
**Electron density around CLA c 511:**

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

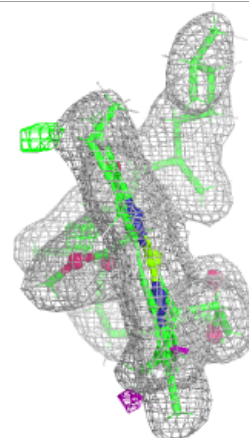
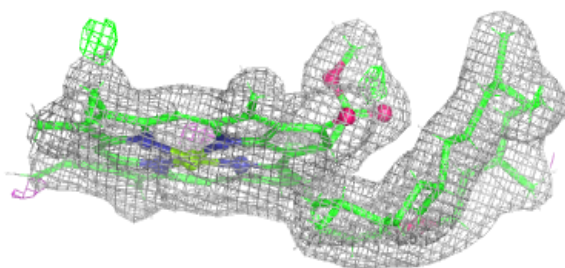
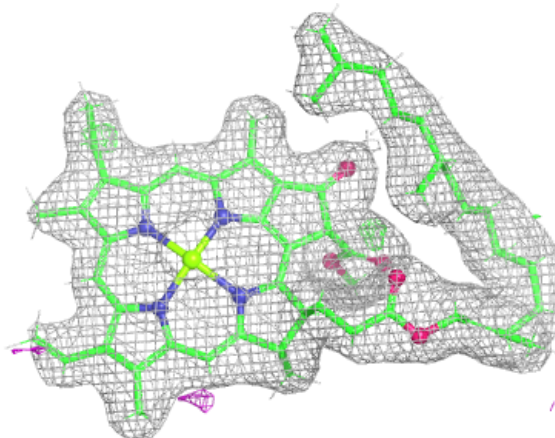


**Electron density around DGD c 518:**

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

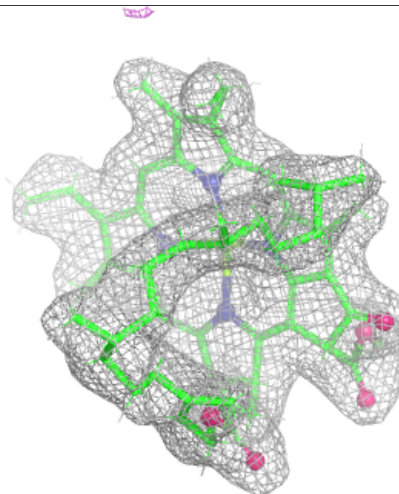
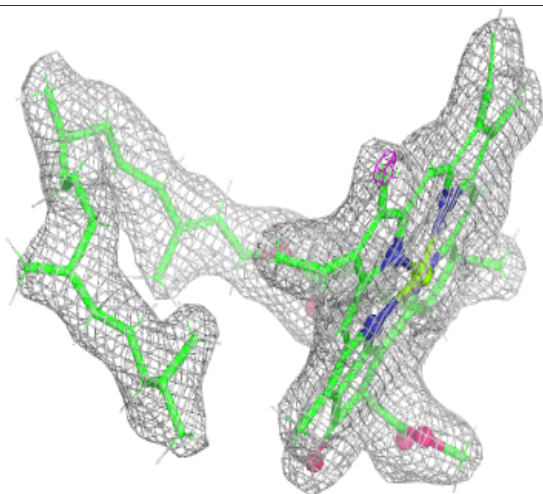
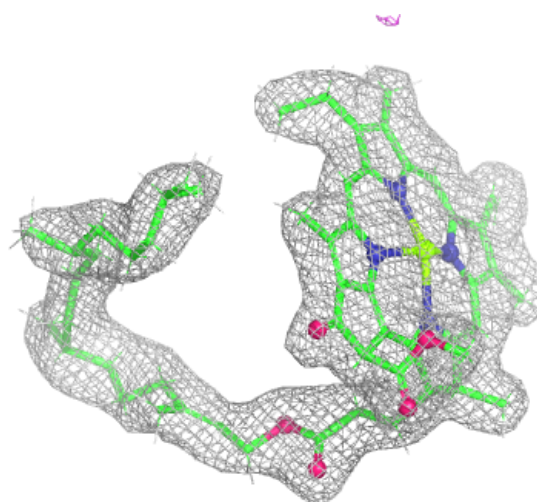
**Electron density around CLA B 610:**

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



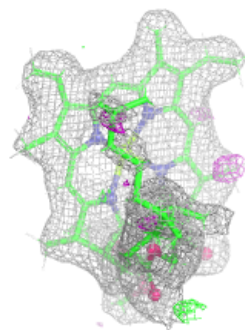
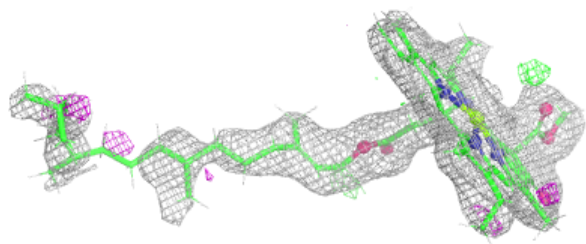
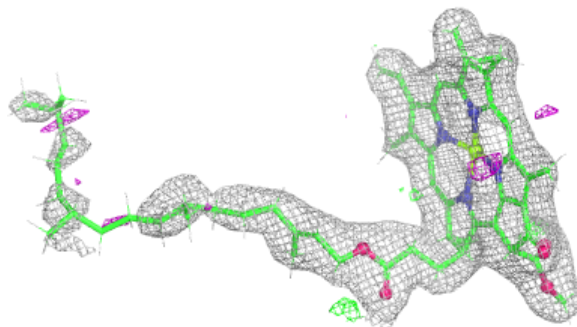
**Electron density around CLA C 503:**

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

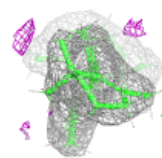
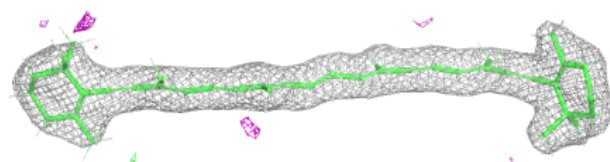


**Electron density around CLA d 404:**

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

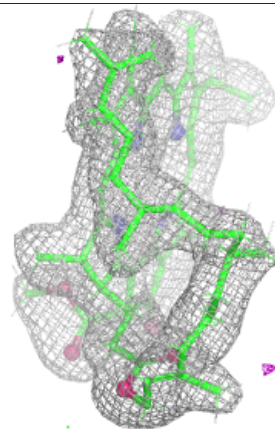
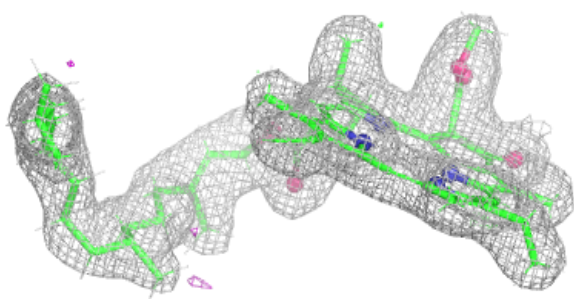
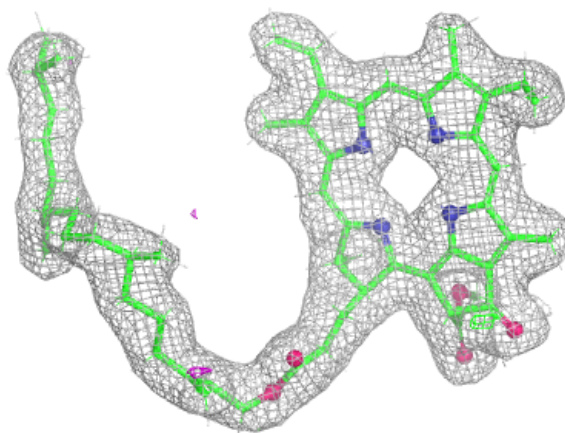
**Electron density around BCR c 515:**

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

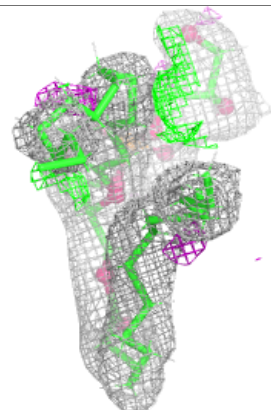
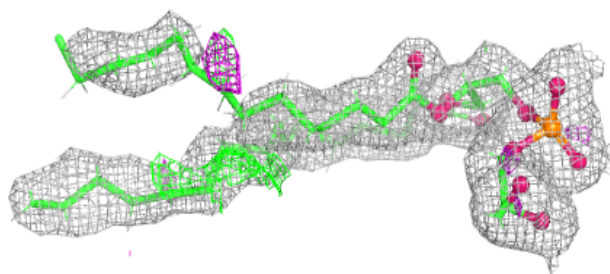
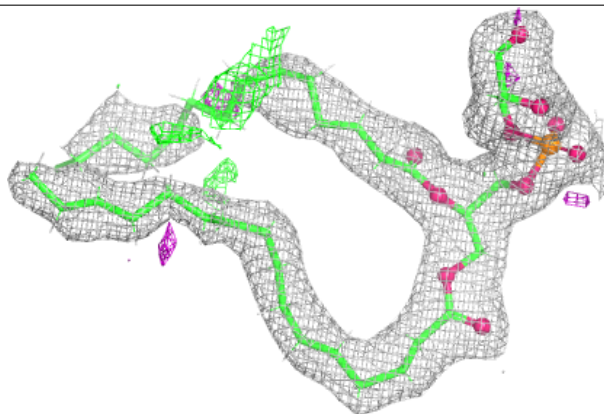


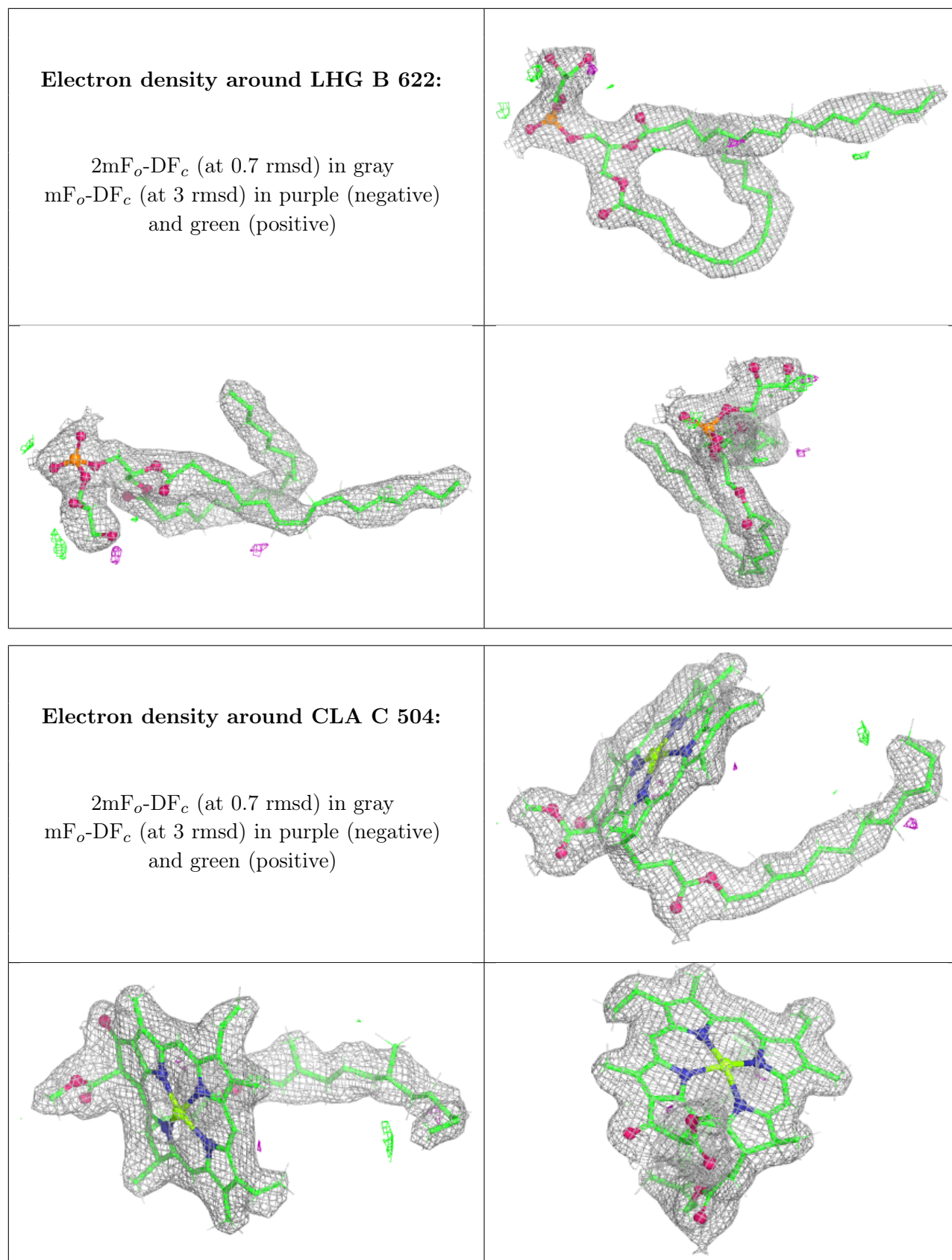
**Electron density around PHO d 402:**

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

**Electron density around LHG A 615:**

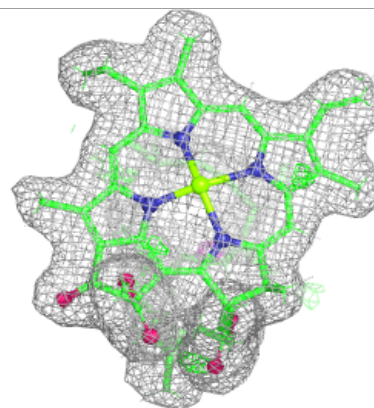
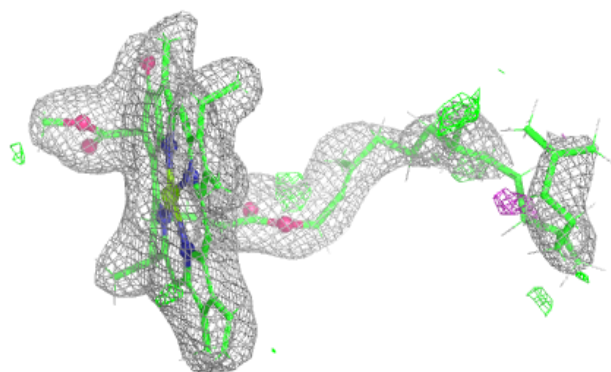
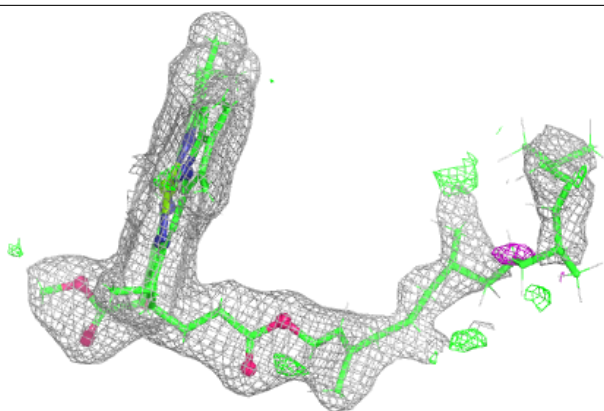
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



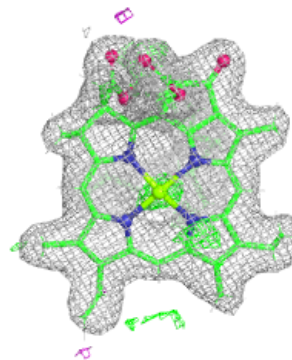
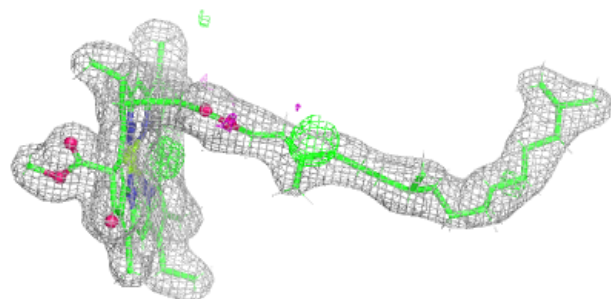
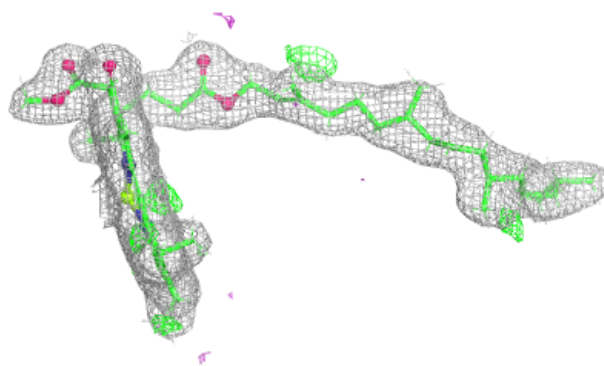


**Electron density around CLA C 506:**

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

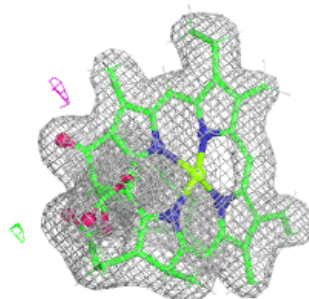
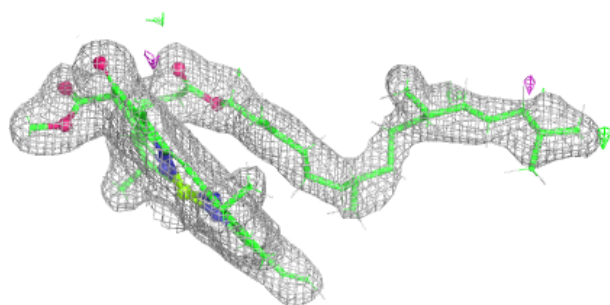
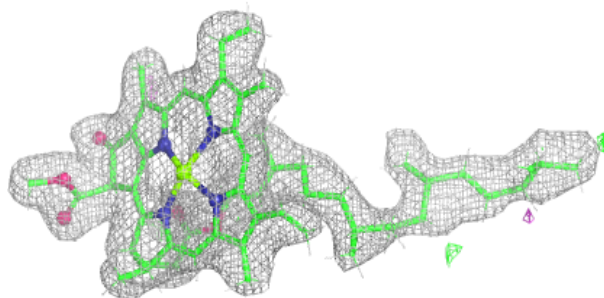
**Electron density around CLA B 605:**

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

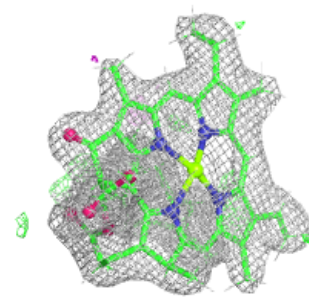
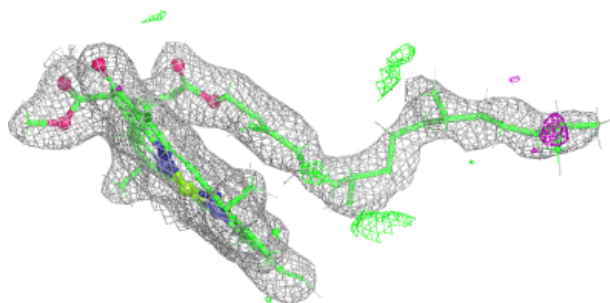
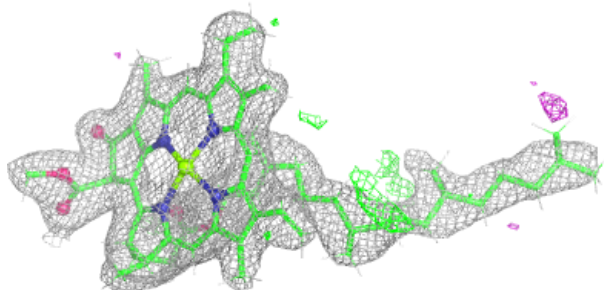


**Electron density around CLA c 505:**

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

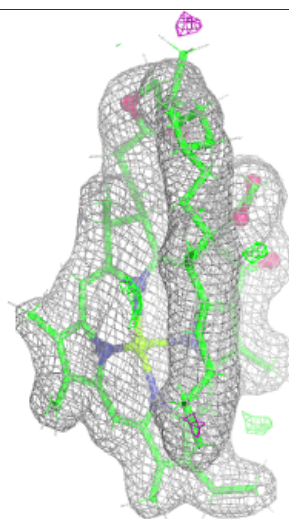
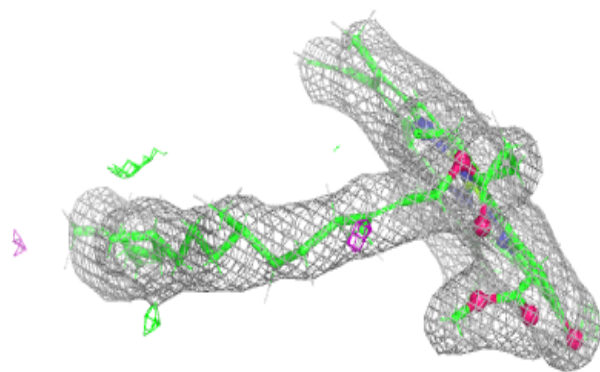
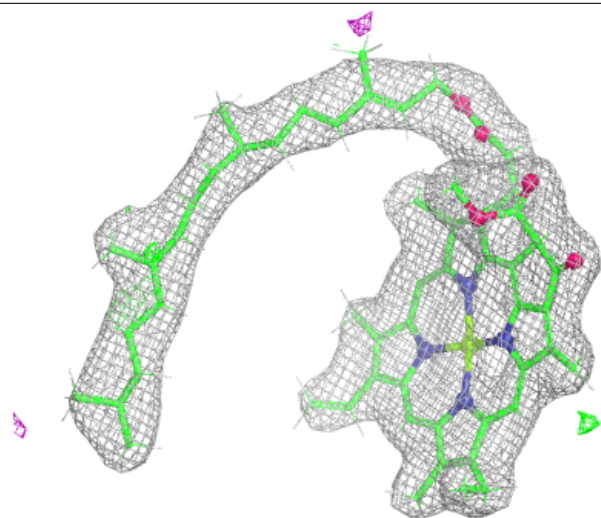
**Electron density around CLA C 505:**

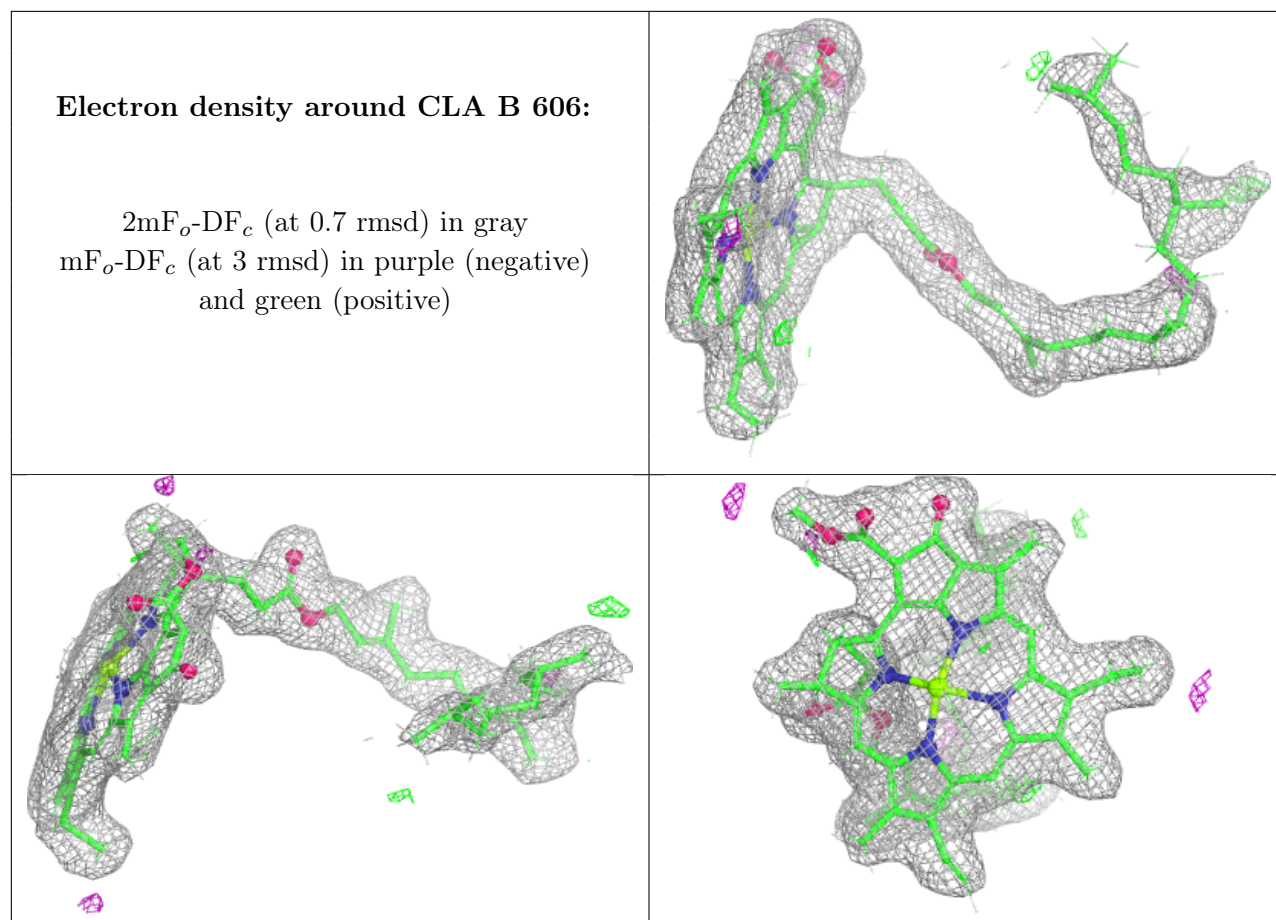
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

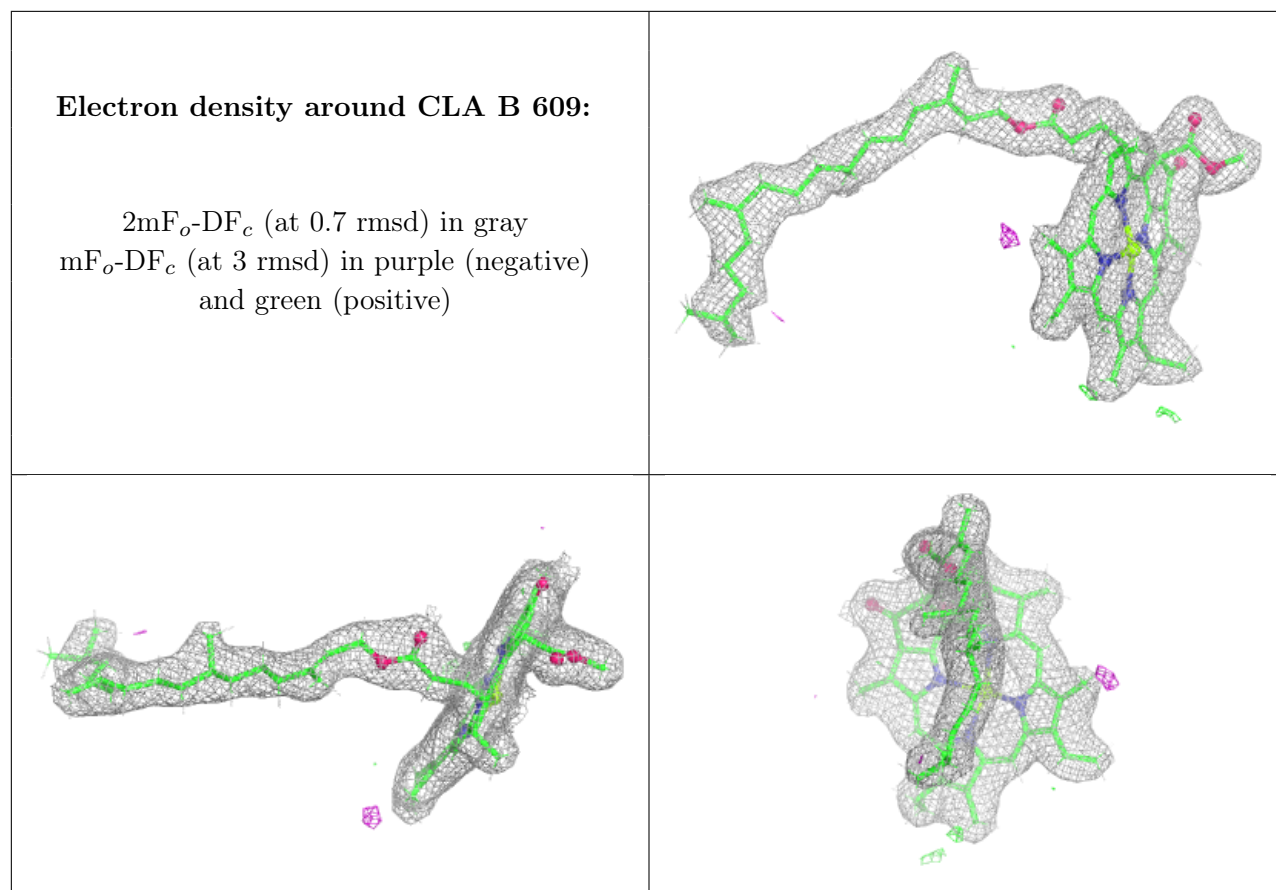


**Electron density around CLA c 507:**

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

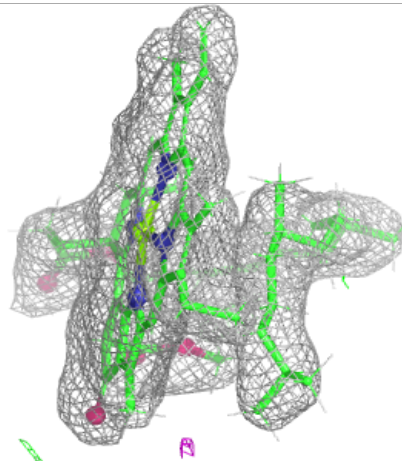
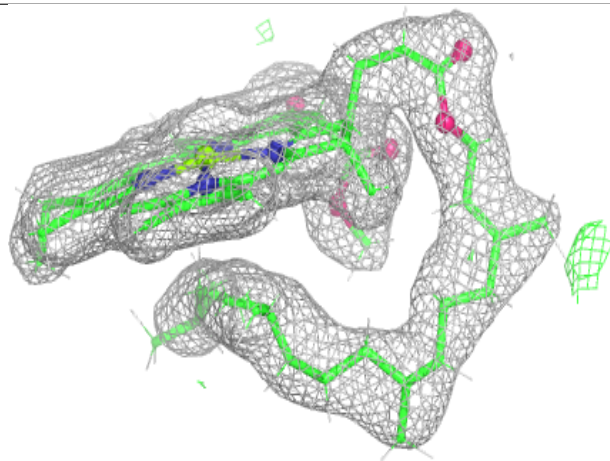
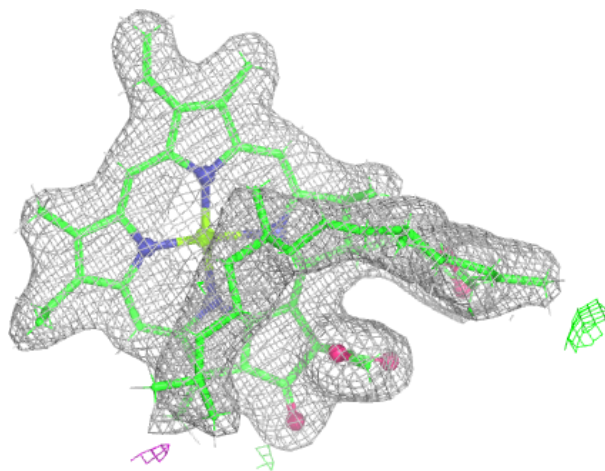






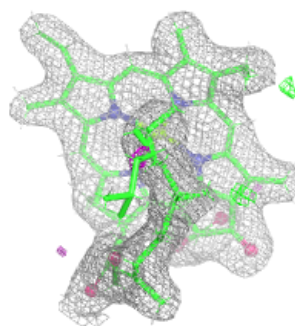
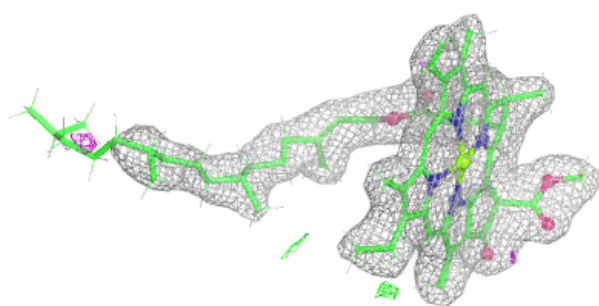
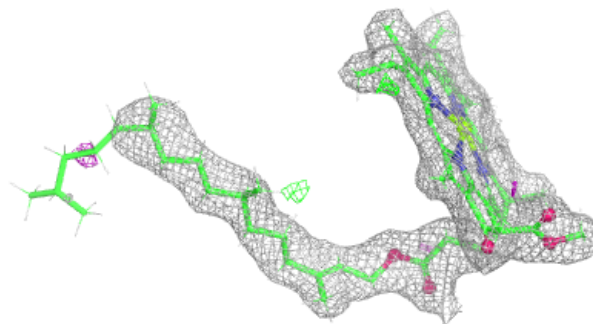
**Electron density around CLA c 510:**

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



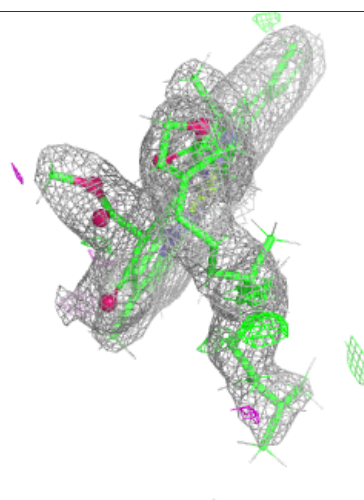
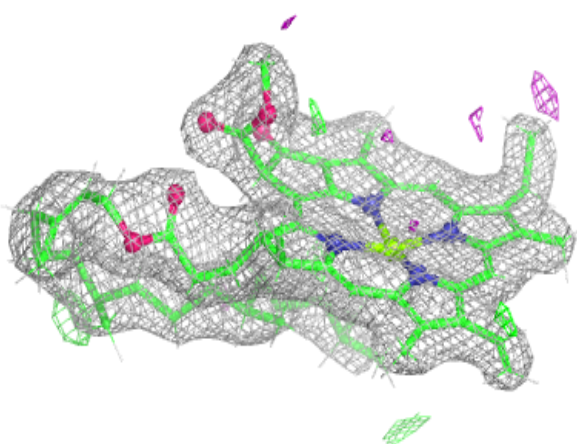
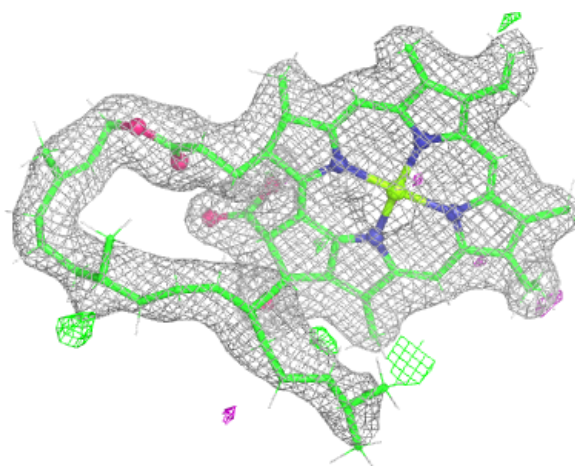
**Electron density around CLA C 508:**

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



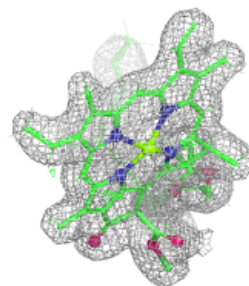
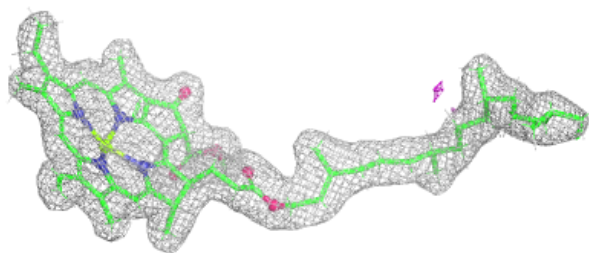
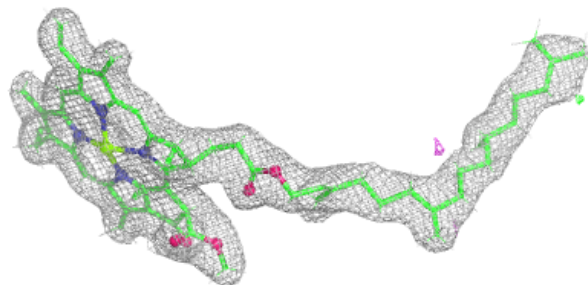
**Electron density around CLA C 509:**

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

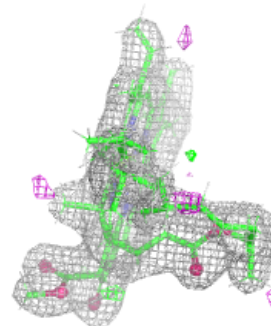
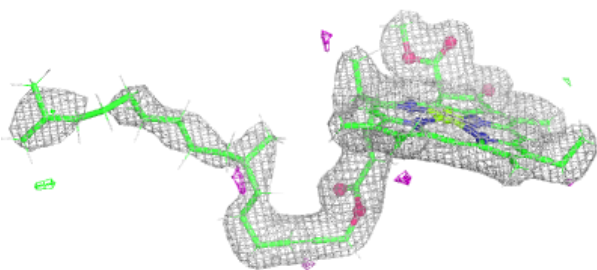
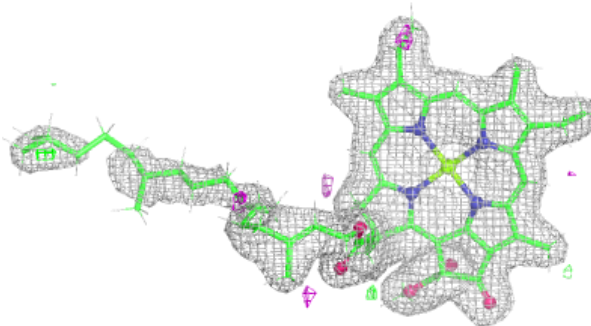


**Electron density around CLA A 604:**

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

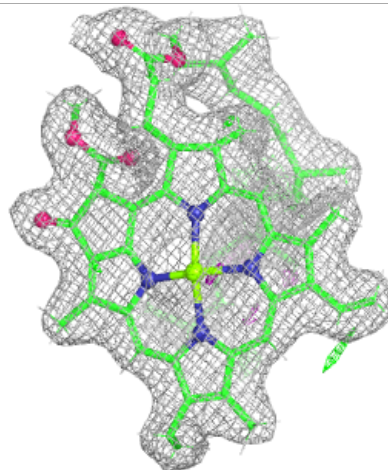
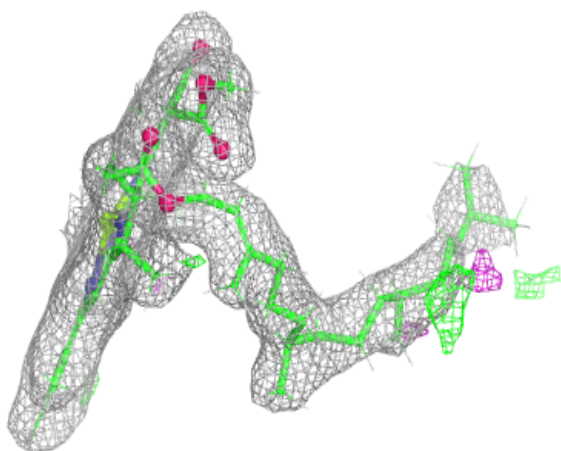
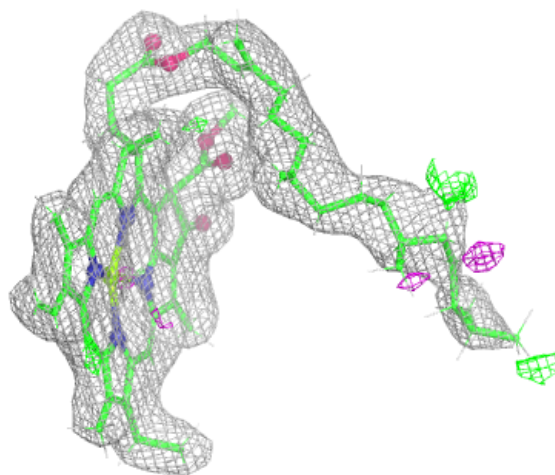
**Electron density around CLA d 401:**

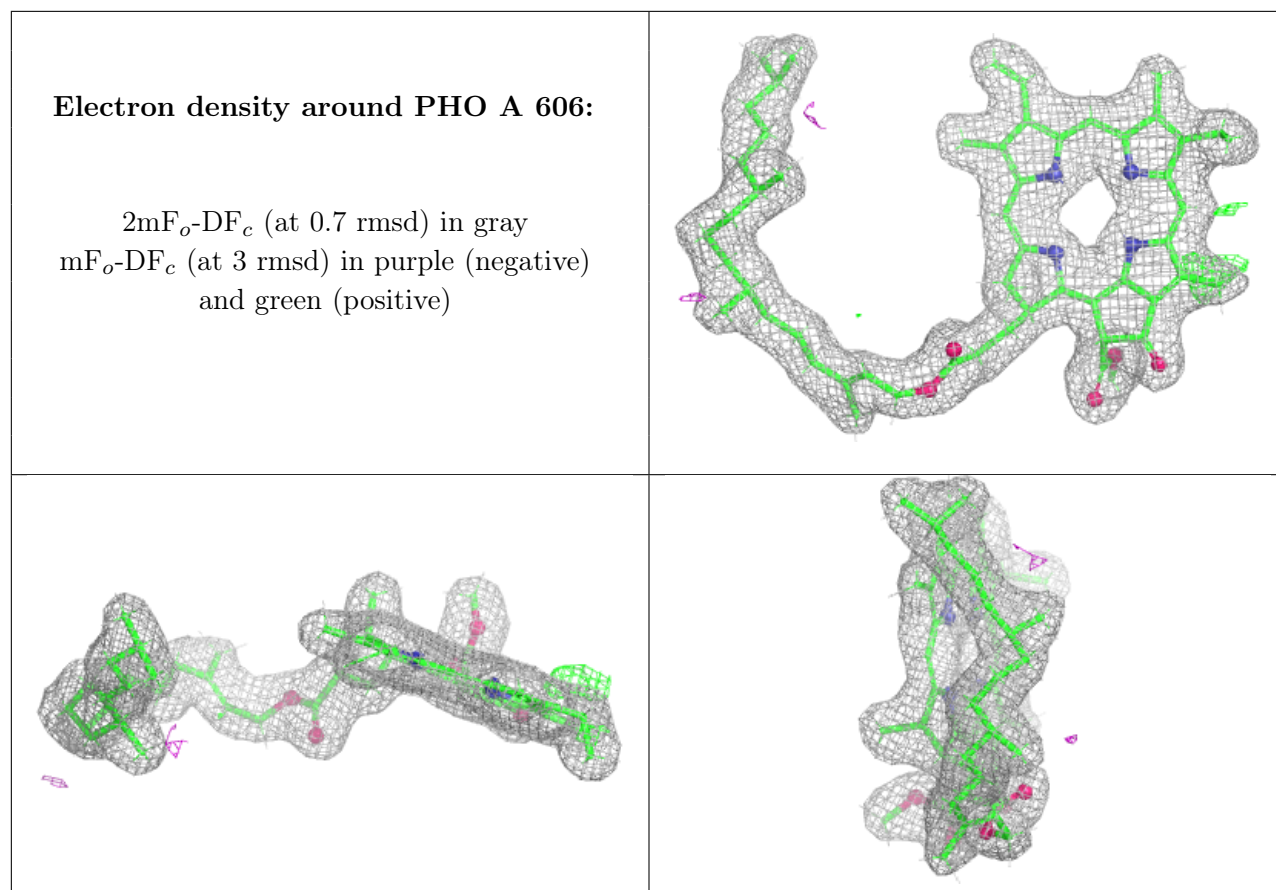
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 613:**

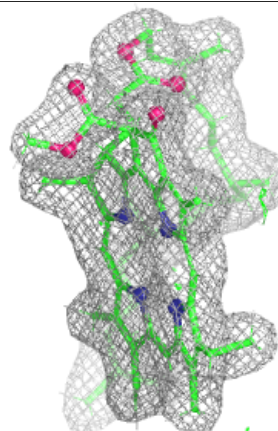
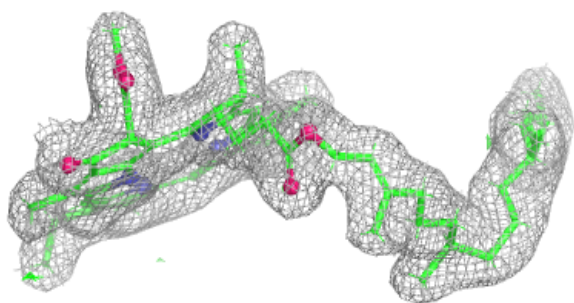
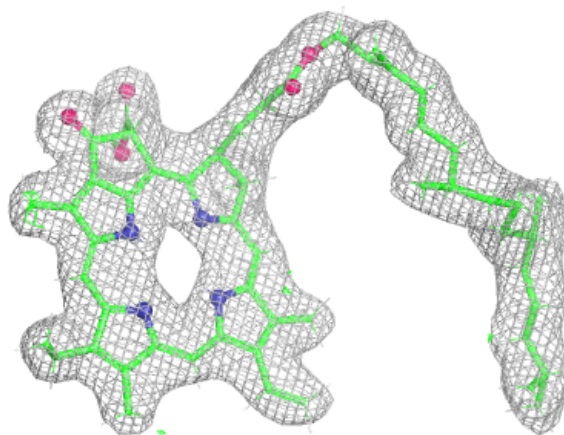
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



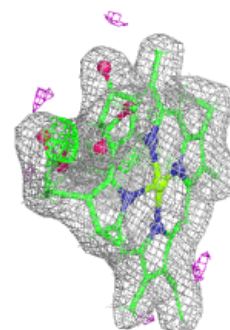
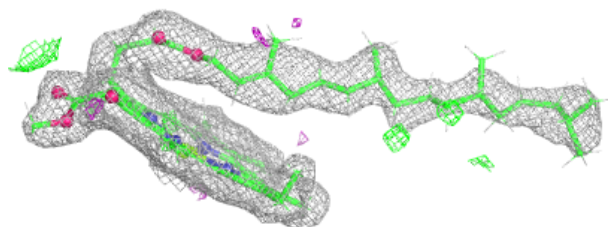
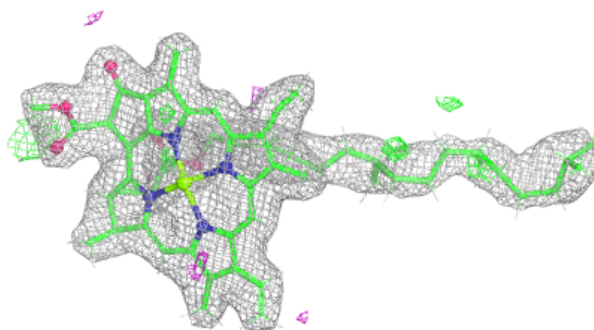


**Electron density around PHO A 607:**

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

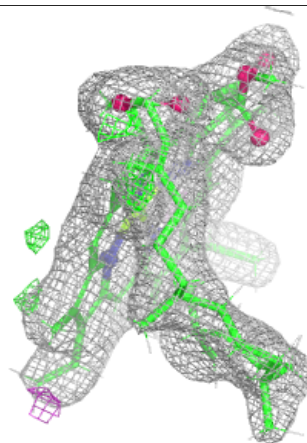
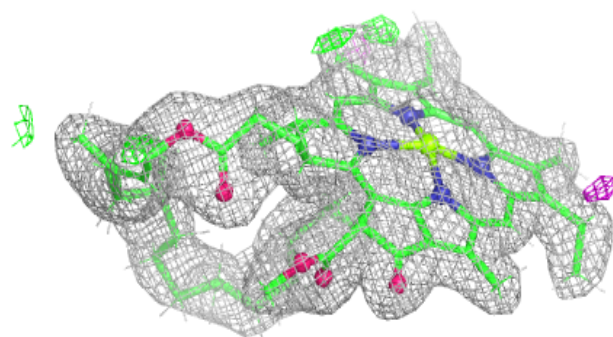
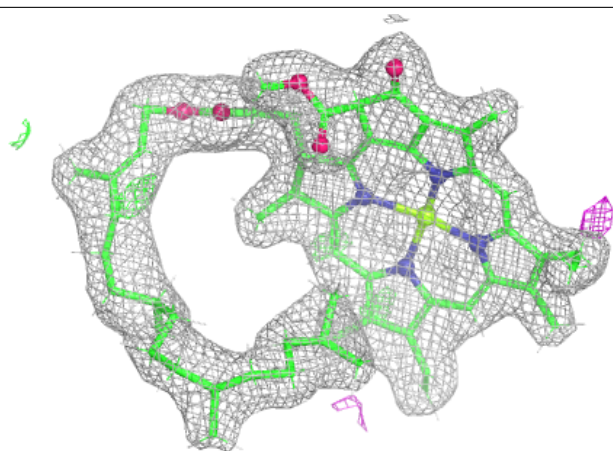
**Electron density around CLA B 614:**

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



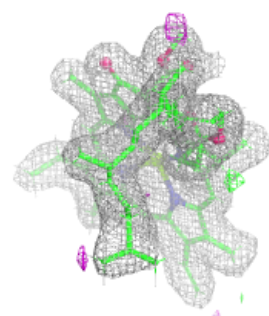
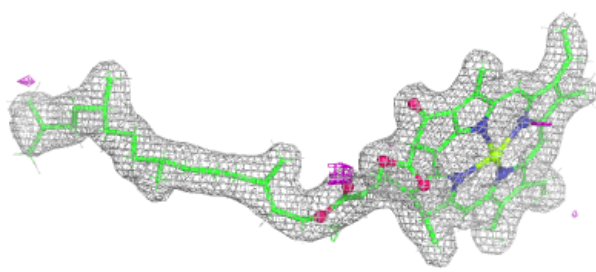
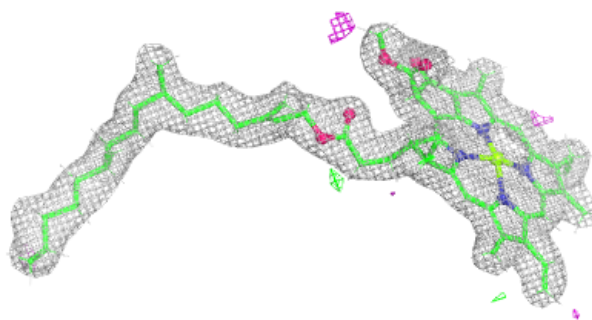
**Electron density around CLA B 615:**

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



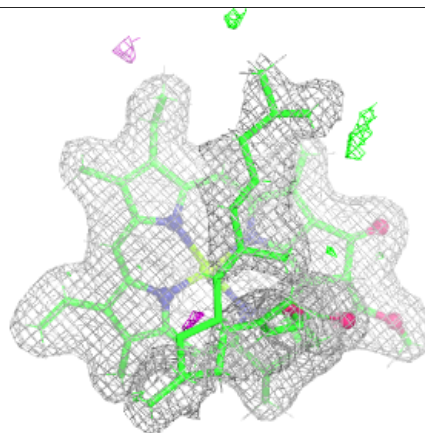
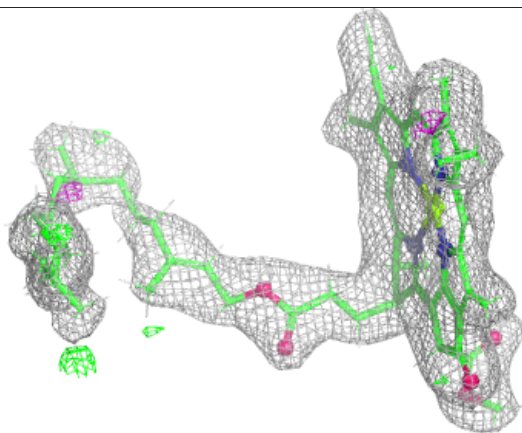
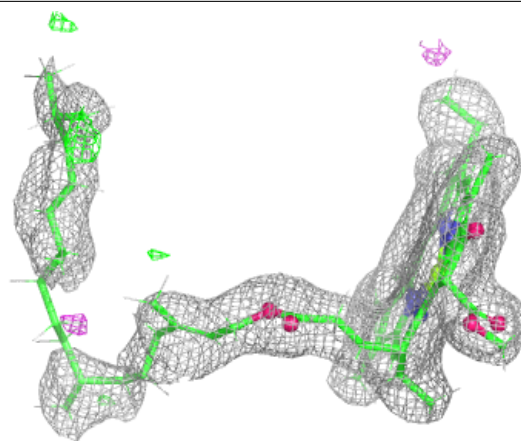
**Electron density around CLA a 604:**

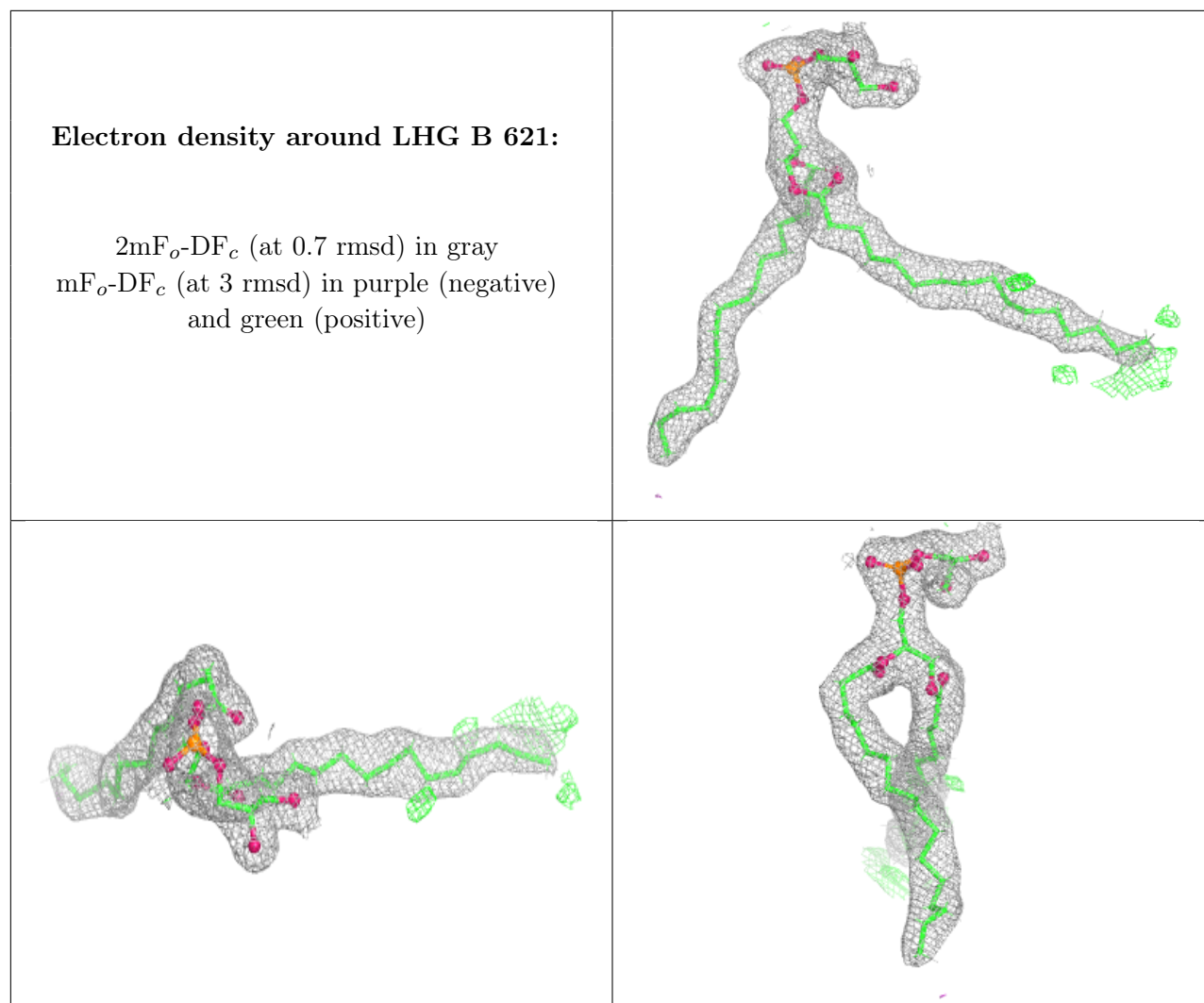
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA a 606:**

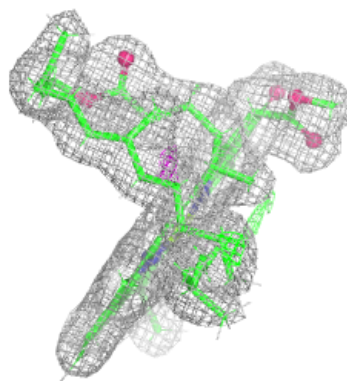
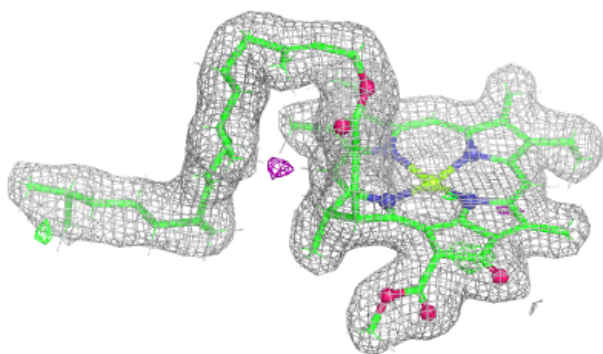
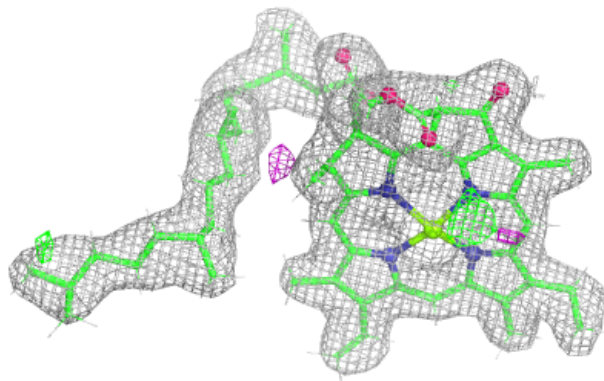
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





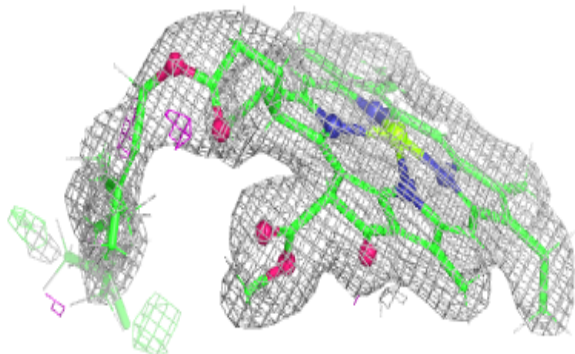
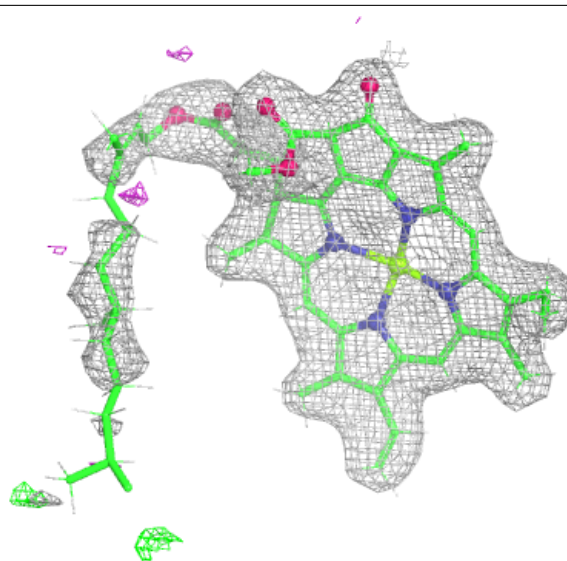
**Electron density around CLA a 612:**

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



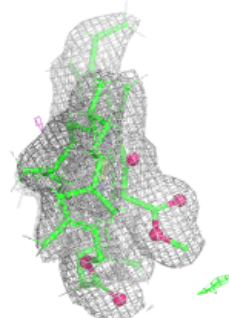
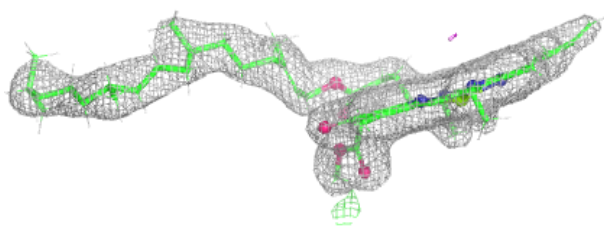
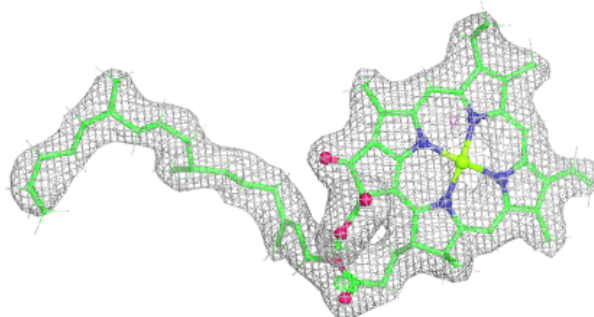
**Electron density around CLA B 616:**

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

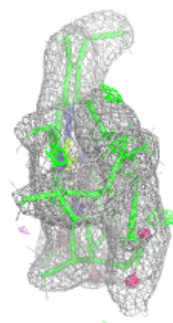
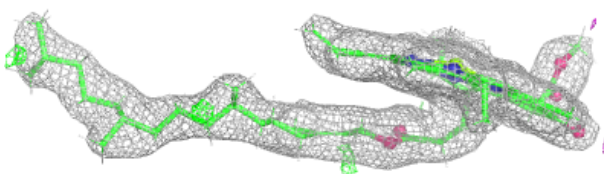
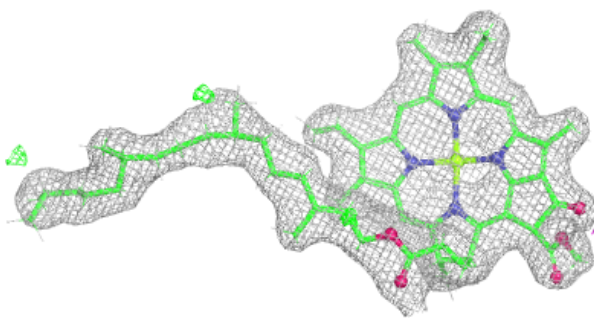


**Electron density around CLA b 602:**

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

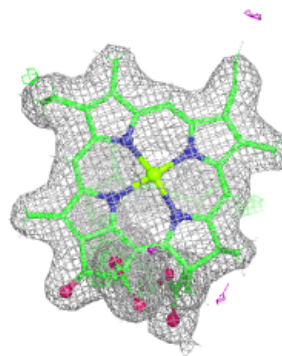
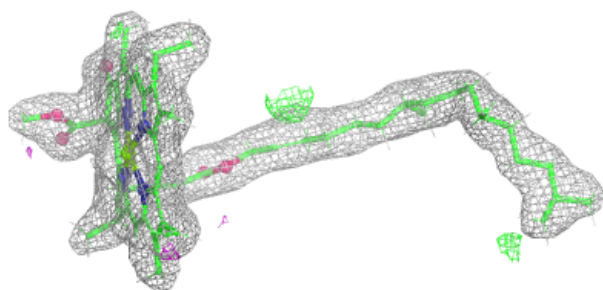
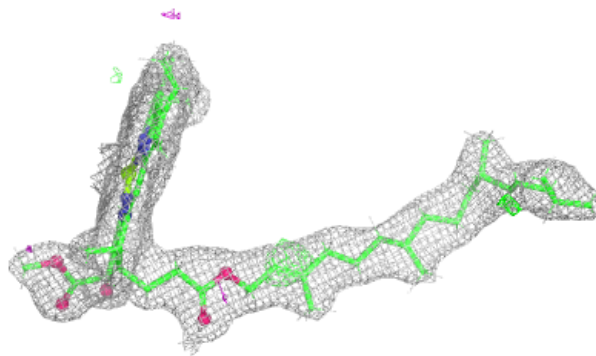
**Electron density around CLA b 603:**

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



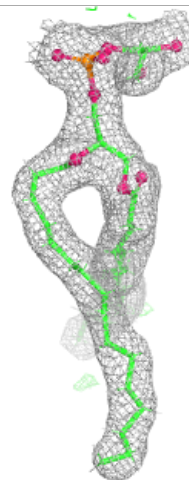
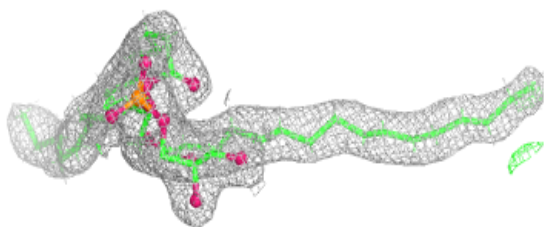
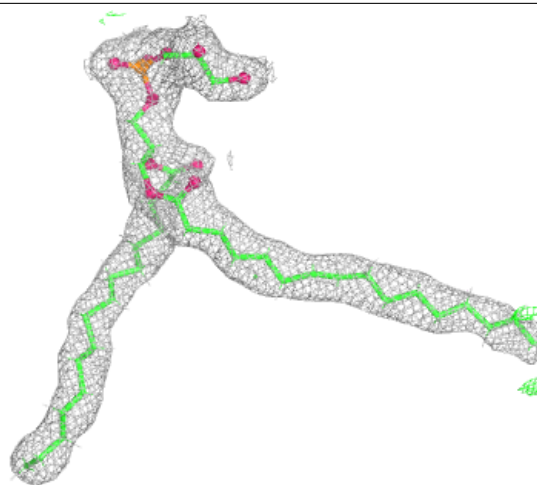
**Electron density around CLA b 605:**

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



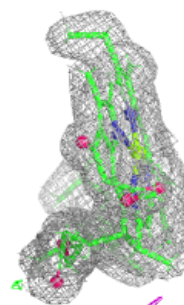
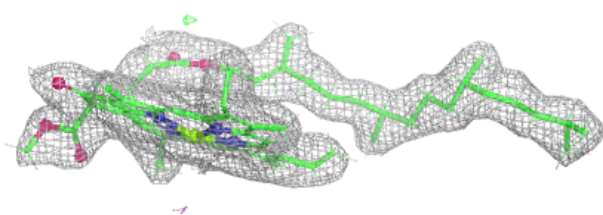
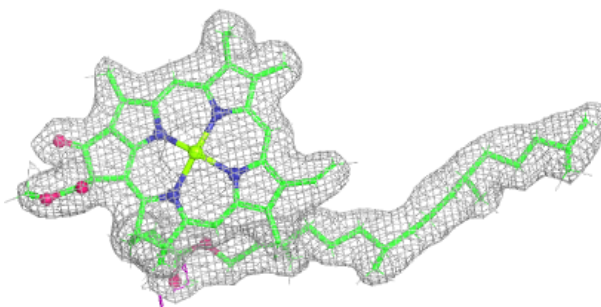
**Electron density around LHG 1 101:**

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

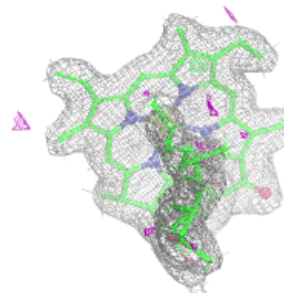
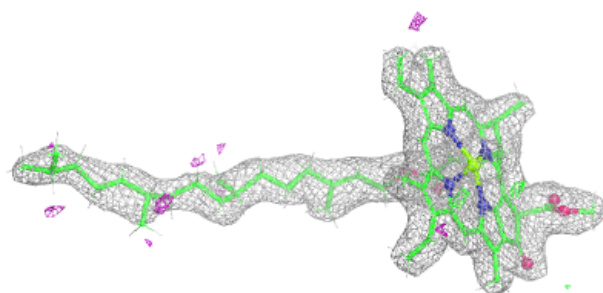
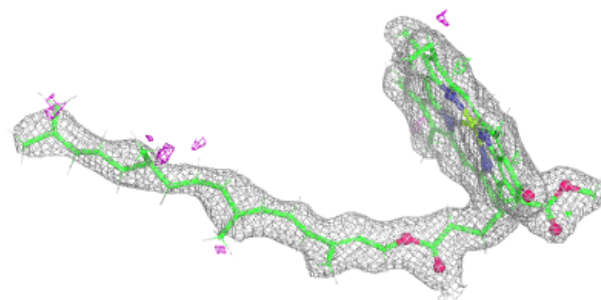


**Electron density around CLA C 501:**

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

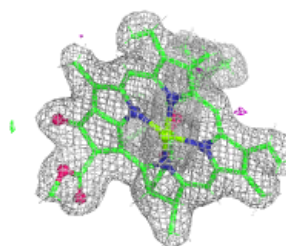
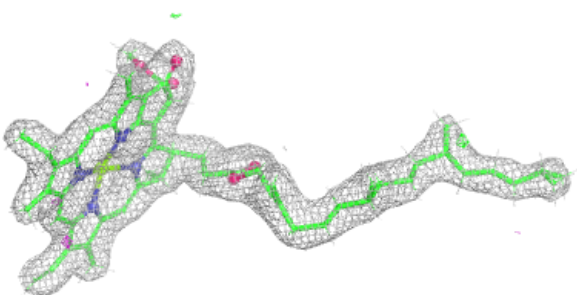
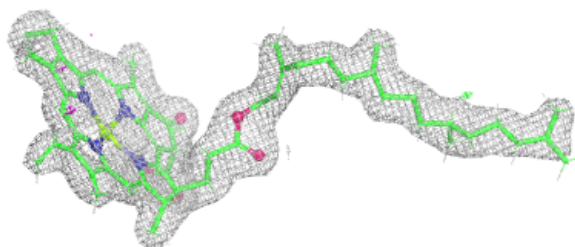
**Electron density around CLA b 607:**

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

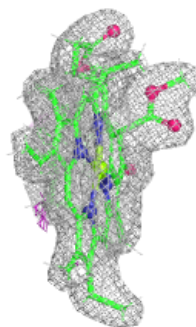
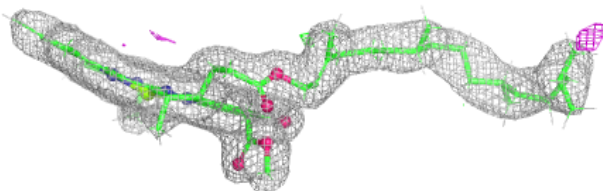
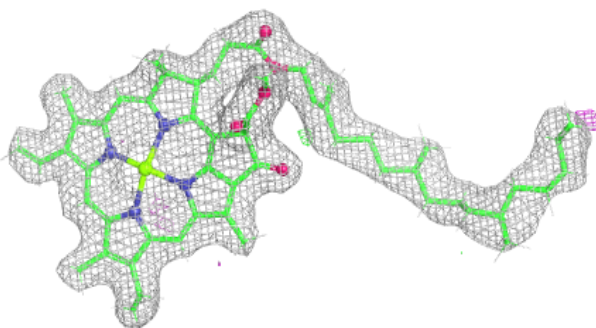


**Electron density around CLA C 502:**

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

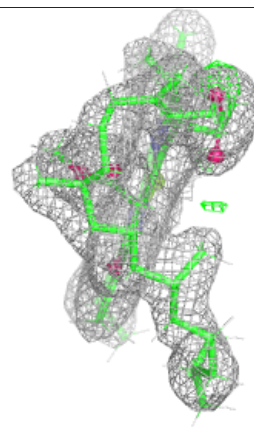
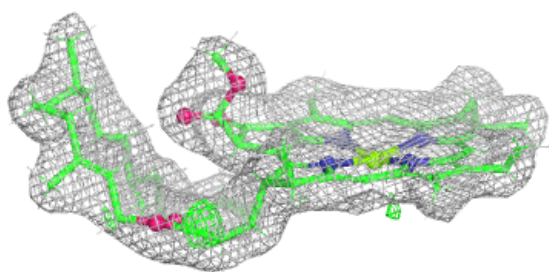
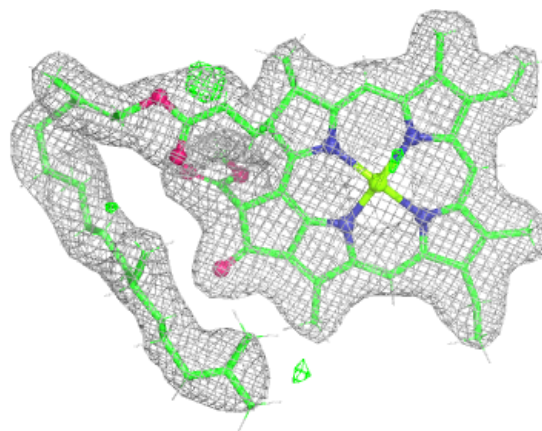
**Electron density around CLA B 602:**

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



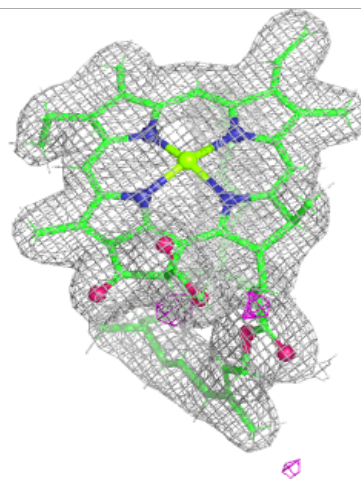
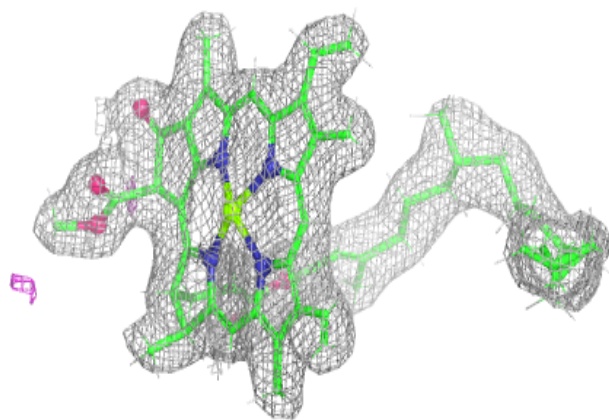
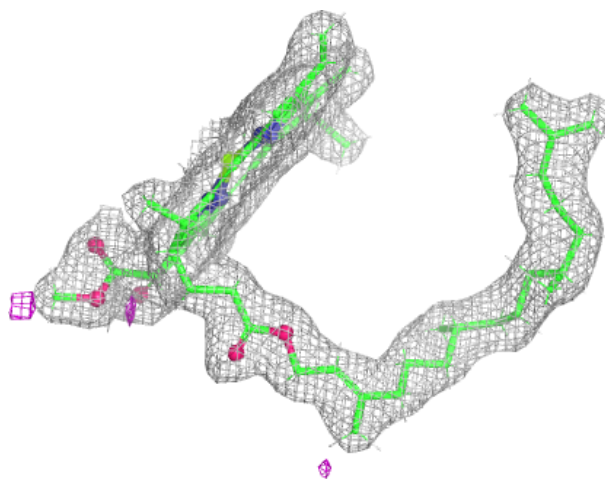
**Electron density around CLA b 610:**

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



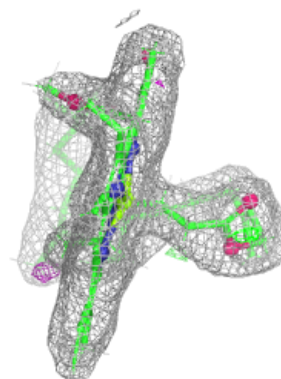
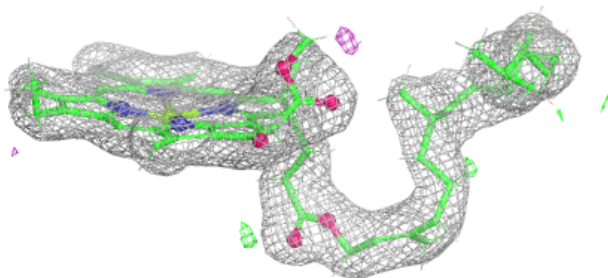
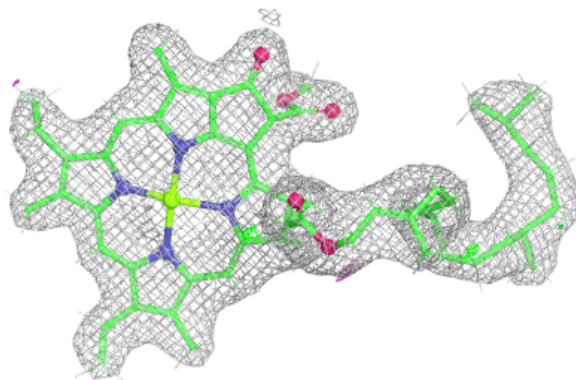
**Electron density around CLA b 611:**

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



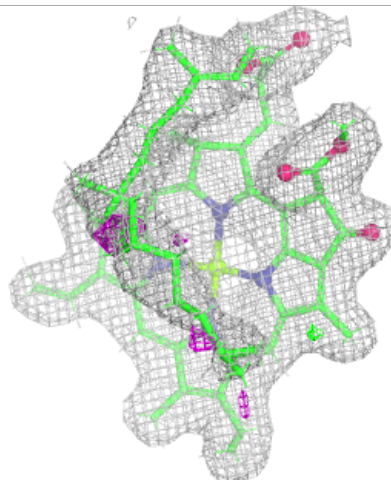
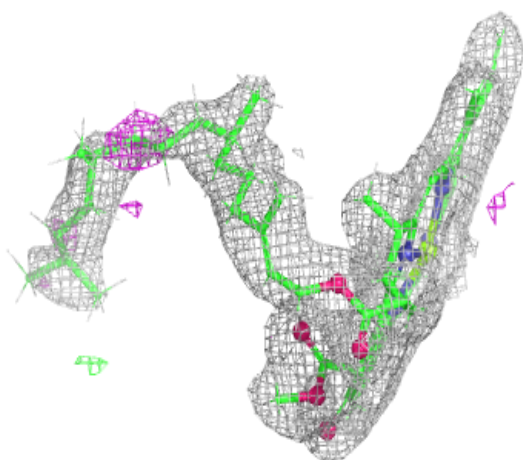
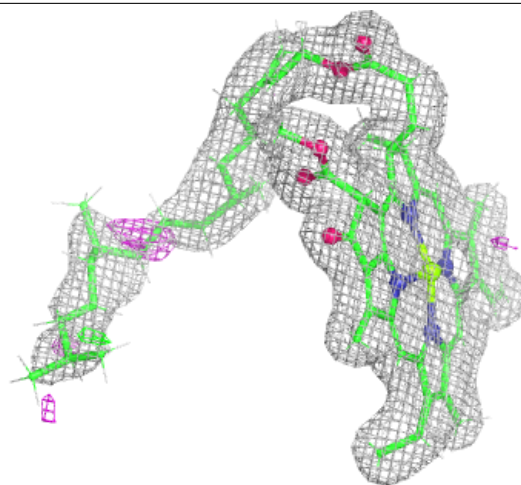
**Electron density around CLA b 612:**

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



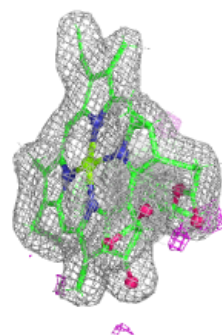
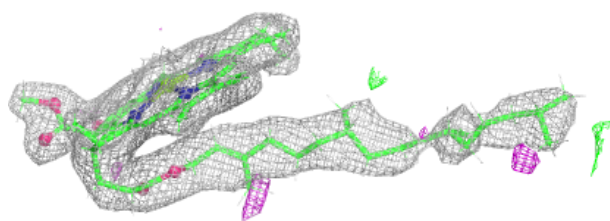
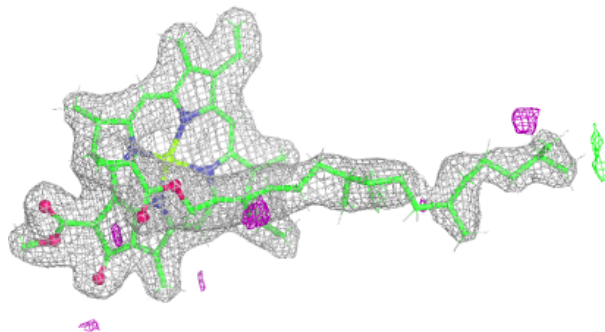
**Electron density around CLA b 613:**

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



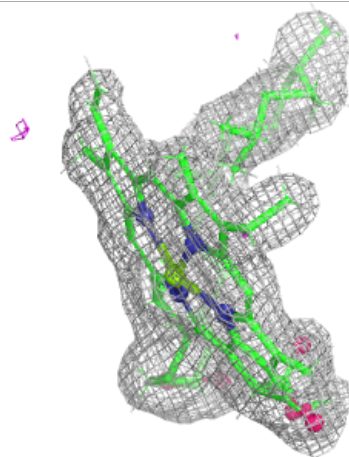
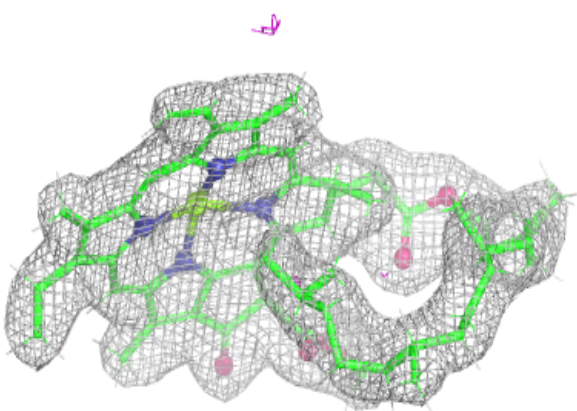
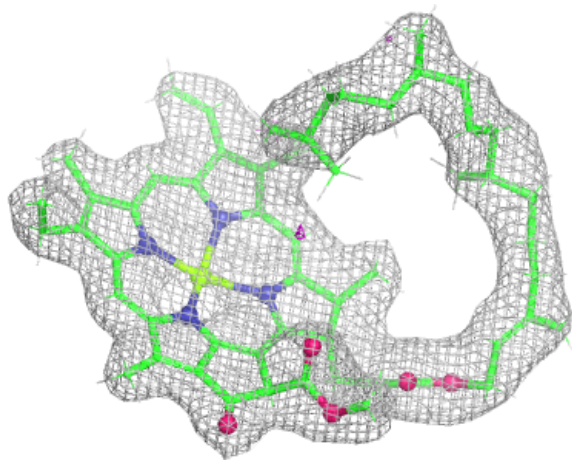
**Electron density around CLA b 614:**

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



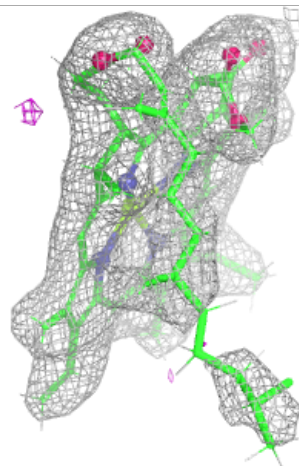
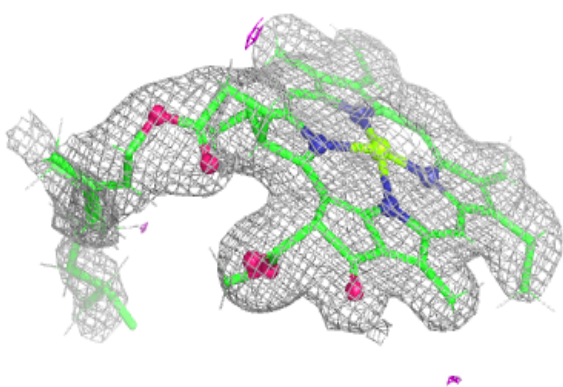
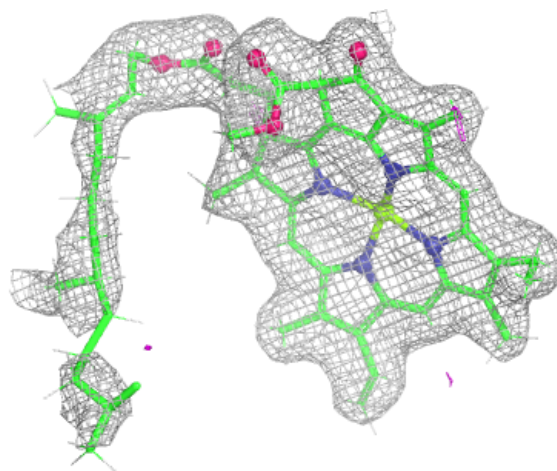
**Electron density around CLA b 615:**

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



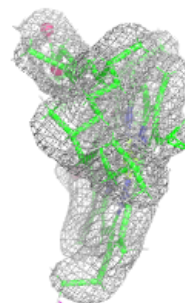
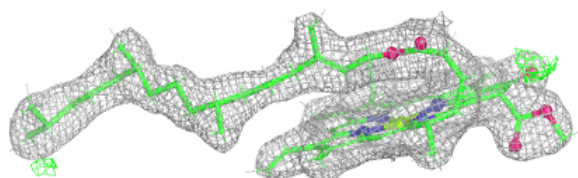
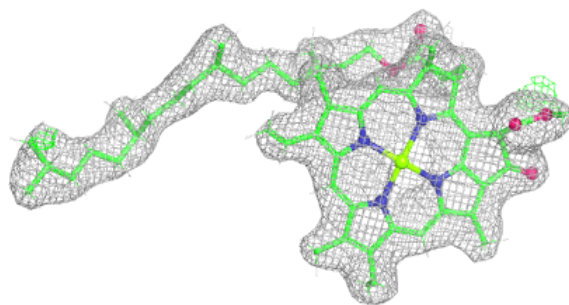
**Electron density around CLA b 616:**

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

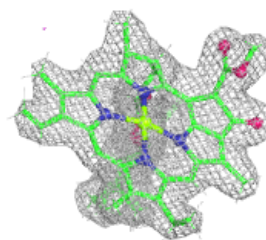
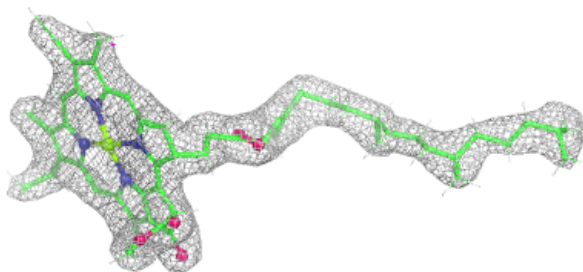
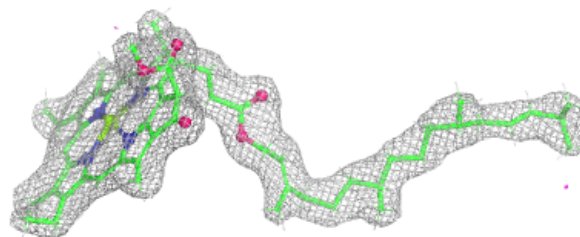


**Electron density around CLA c 501:**

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

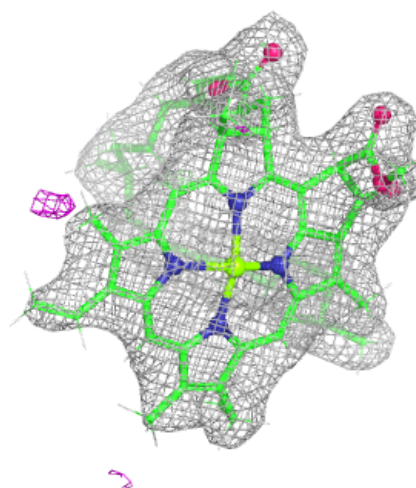
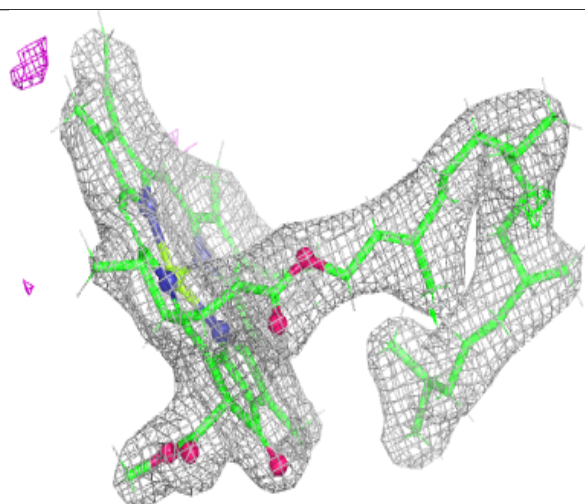
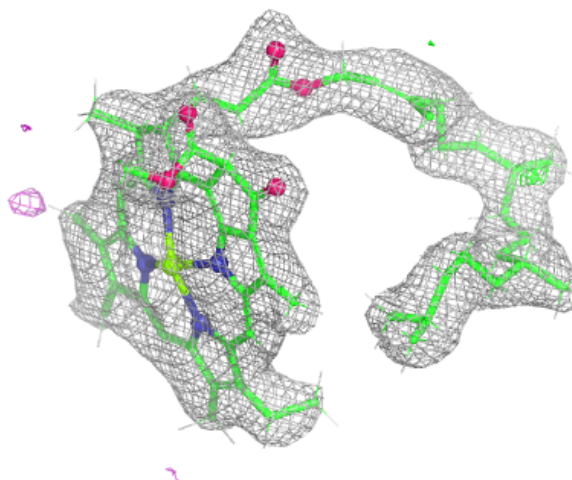
**Electron density around CLA c 502:**

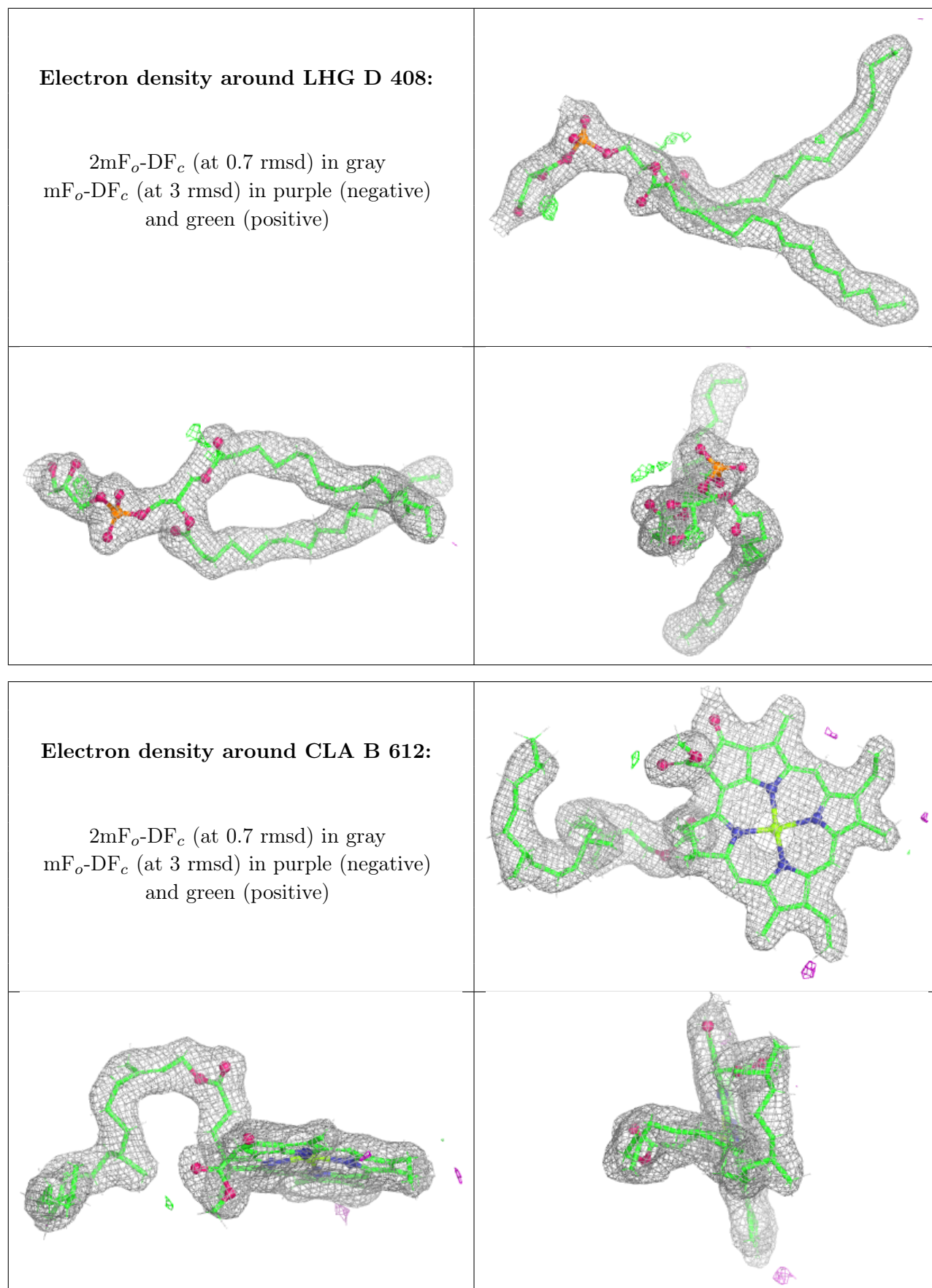
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 503:**

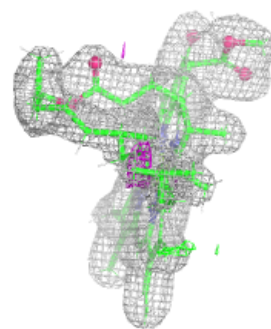
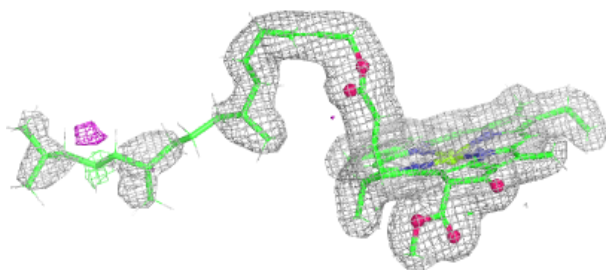
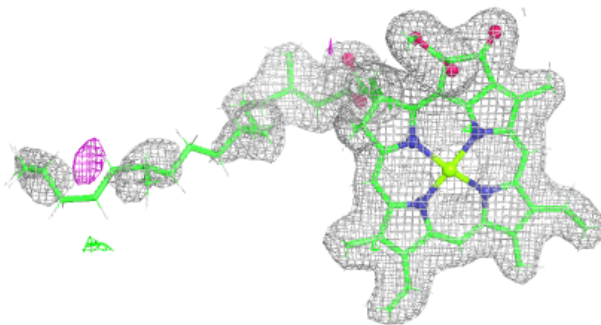
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



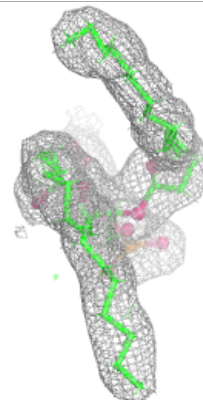
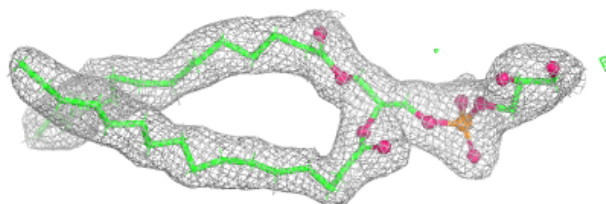
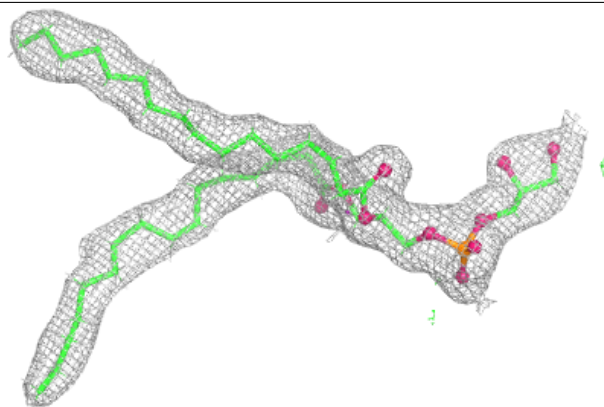


**Electron density around CLA A 605:**

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

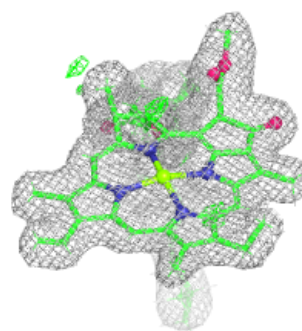
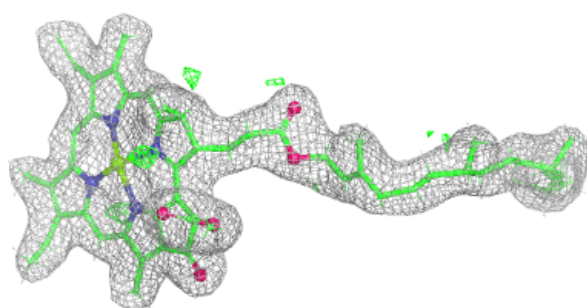
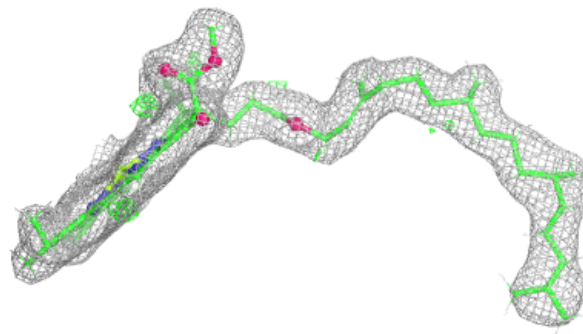
**Electron density around LHG d 408:**

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

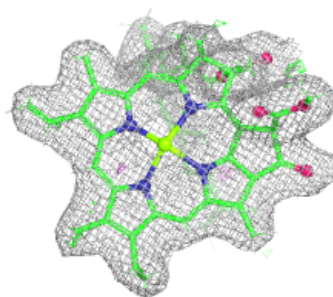
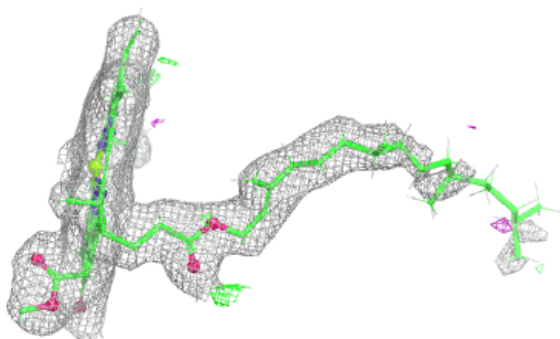
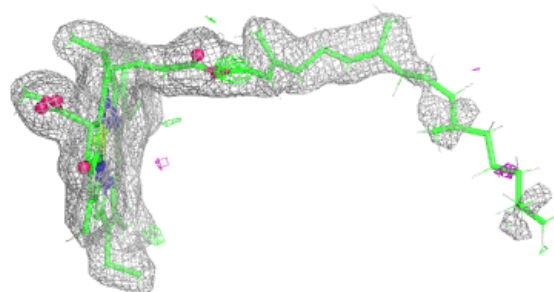


**Electron density around CLA D 402:**

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

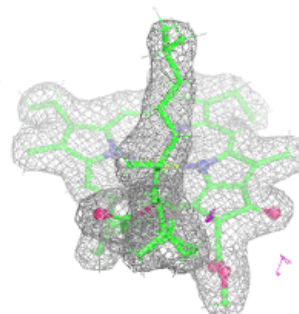
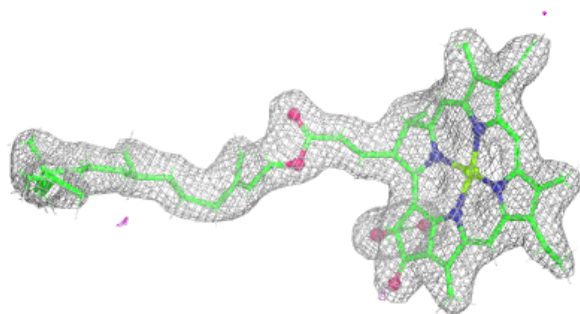
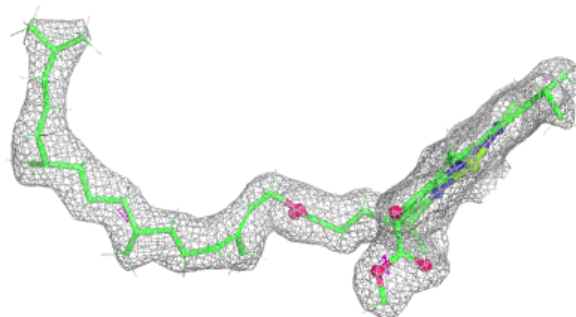
**Electron density around CLA D 403:**

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

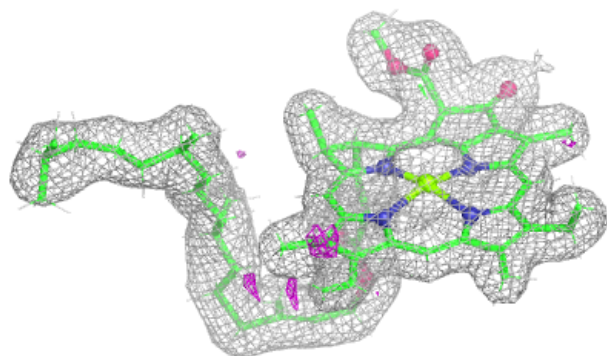
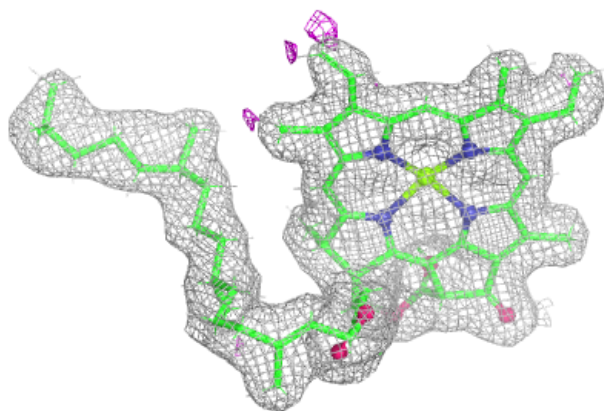


**Electron density around CLA d 403:**

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

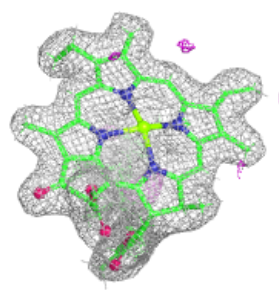
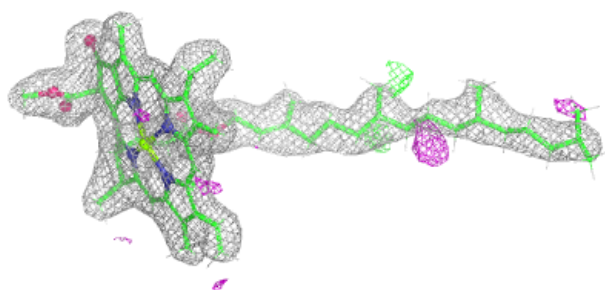
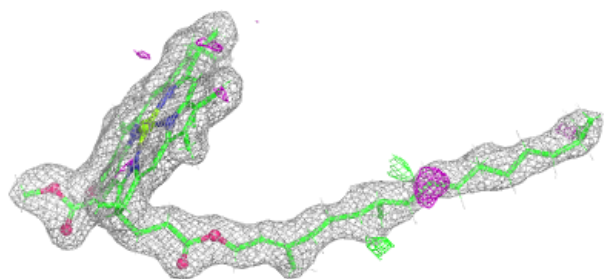
**Electron density around CLA A 613:**

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

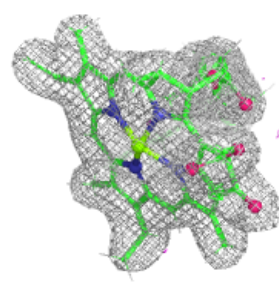
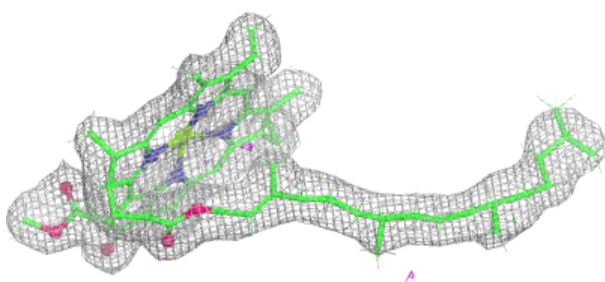
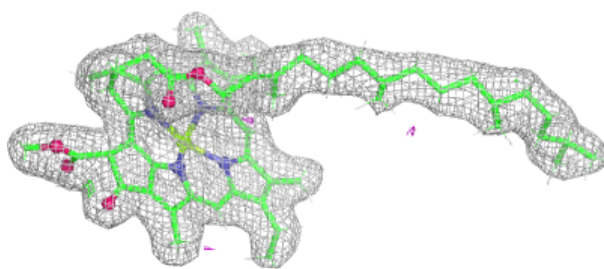


**Electron density around CLA B 607:**

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

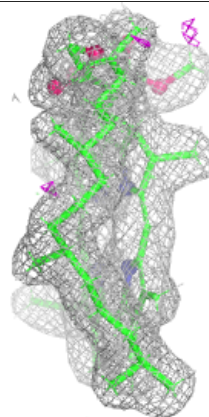
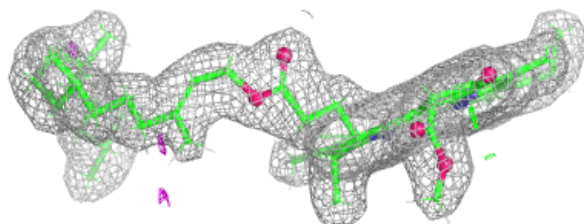
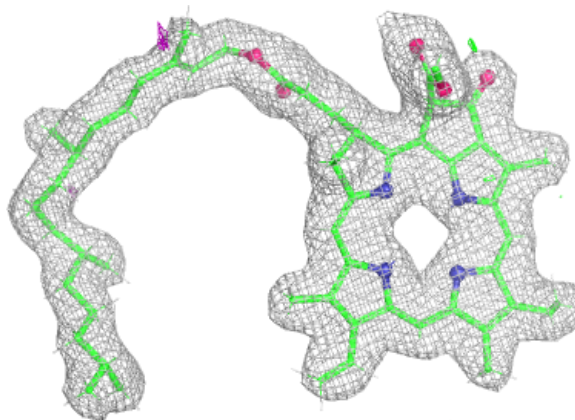
**Electron density around CLA B 608:**

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

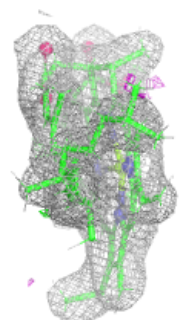
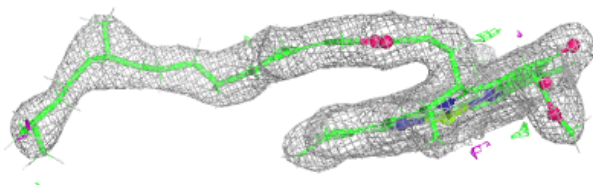
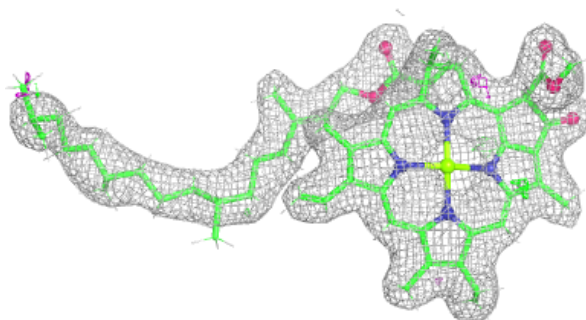


**Electron density around PHO a 605:**

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

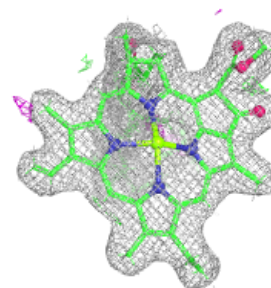
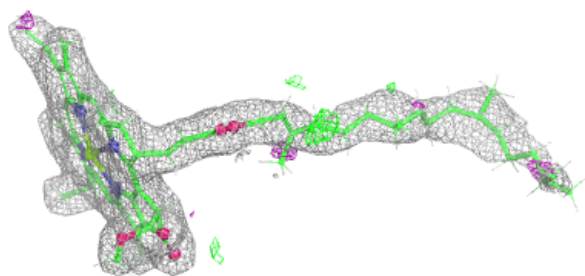
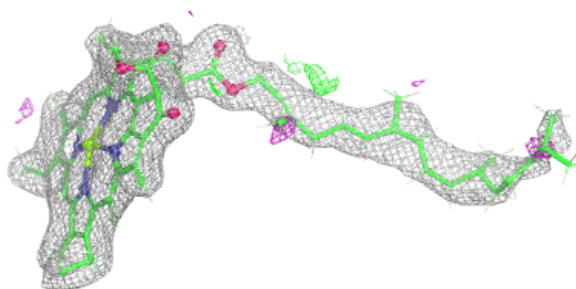
**Electron density around CLA B 603:**

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



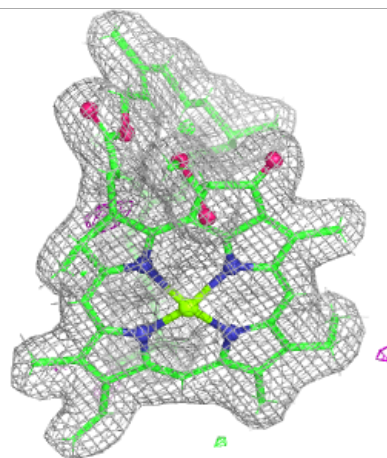
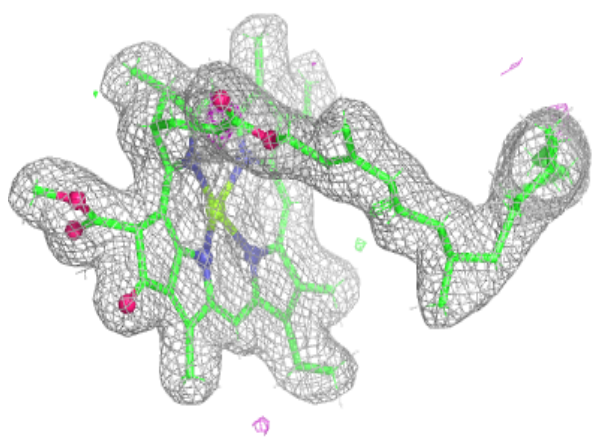
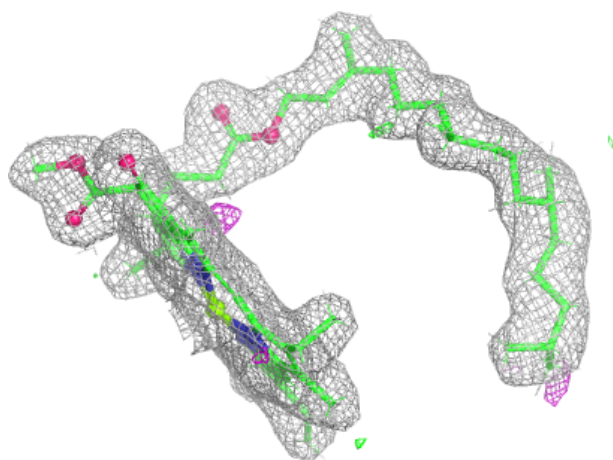
**Electron density around CLA B 604:**

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



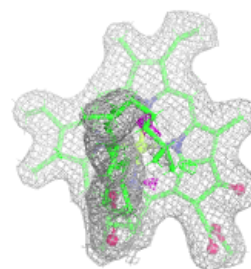
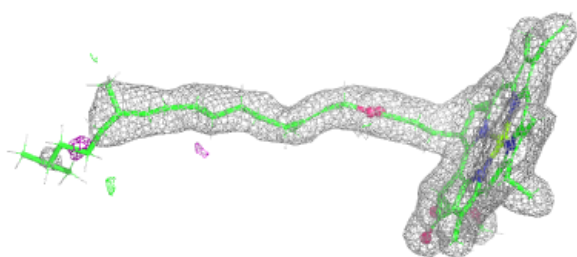
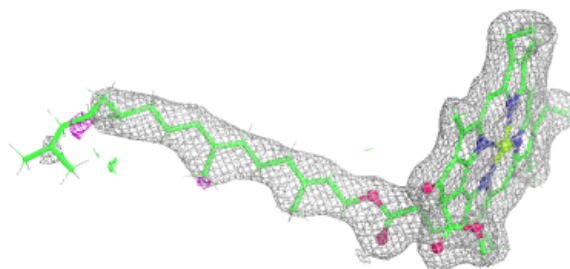
**Electron density around CLA B 611:**

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



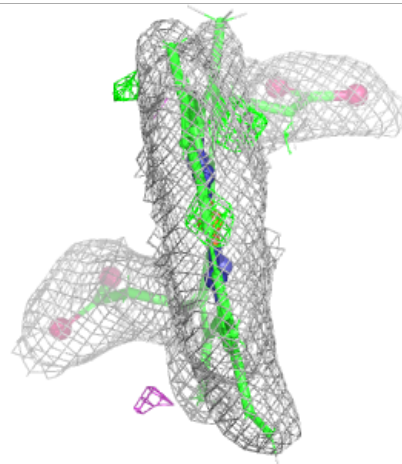
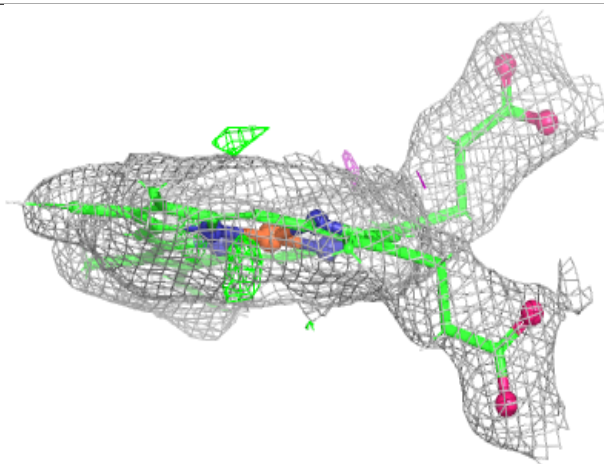
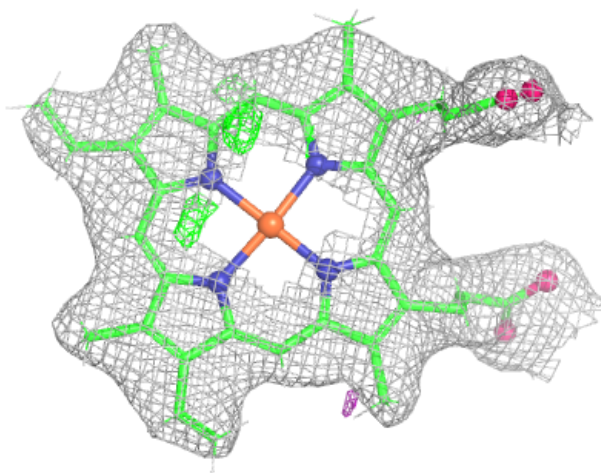
**Electron density around CLA b 604:**

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



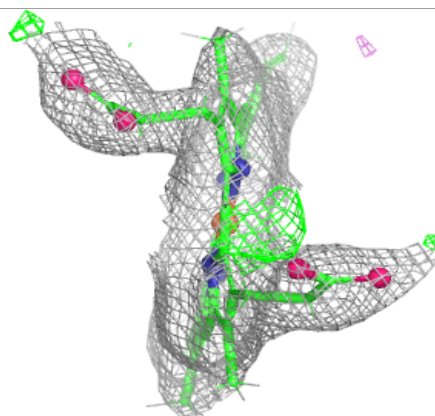
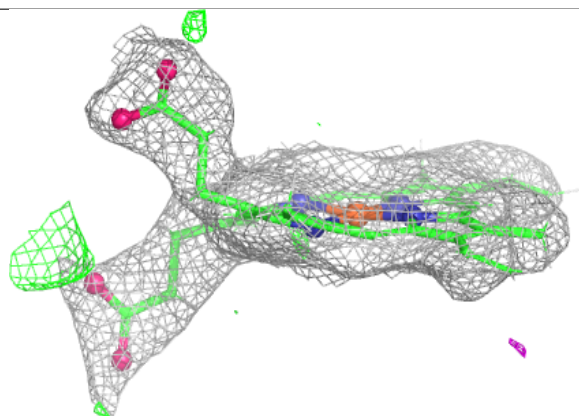
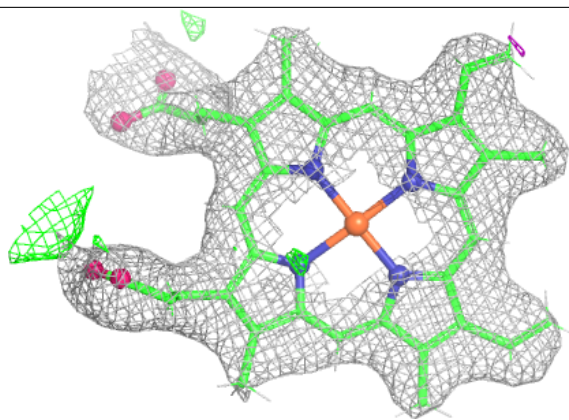
**Electron density around HEM F 101:**

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

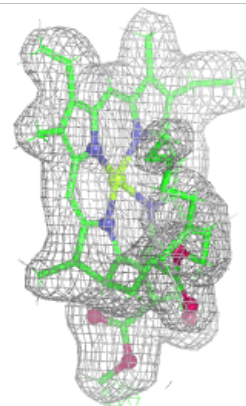
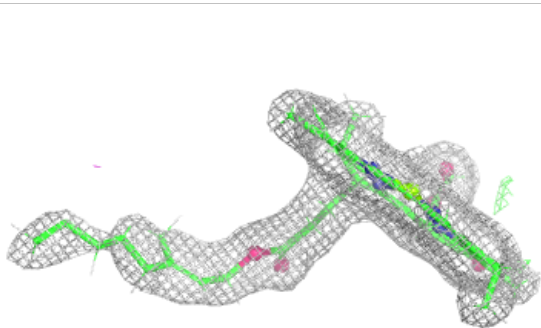
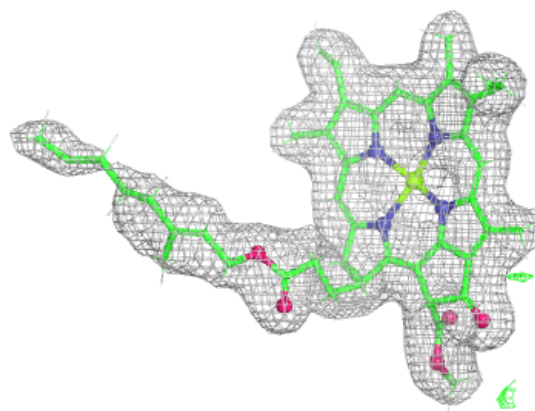


**Electron density around HEM e 101:**

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

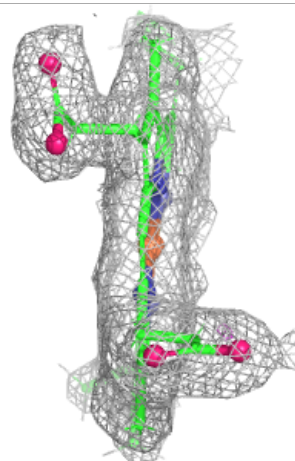
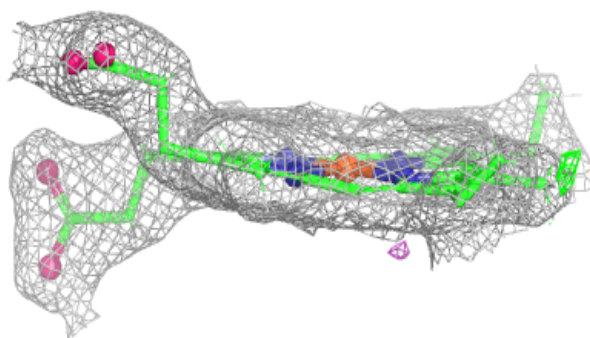
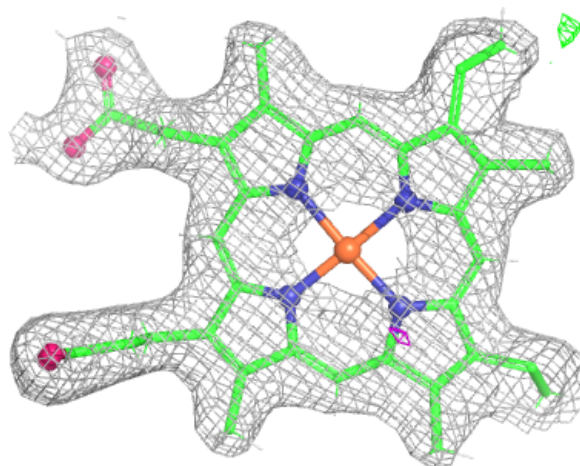
**Electron density around CLA A 608:**

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



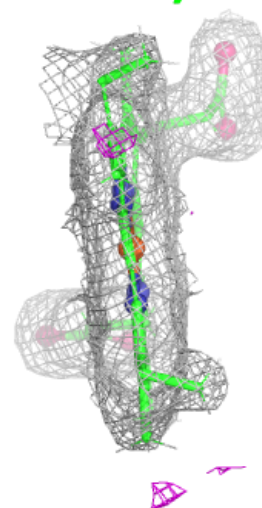
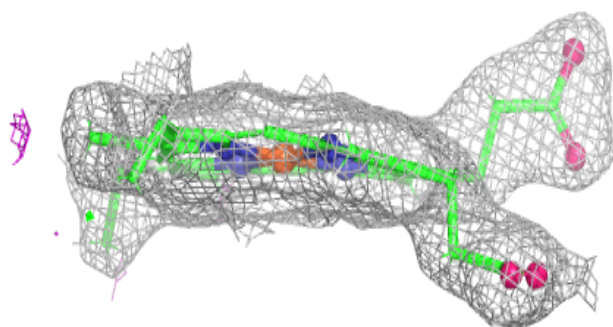
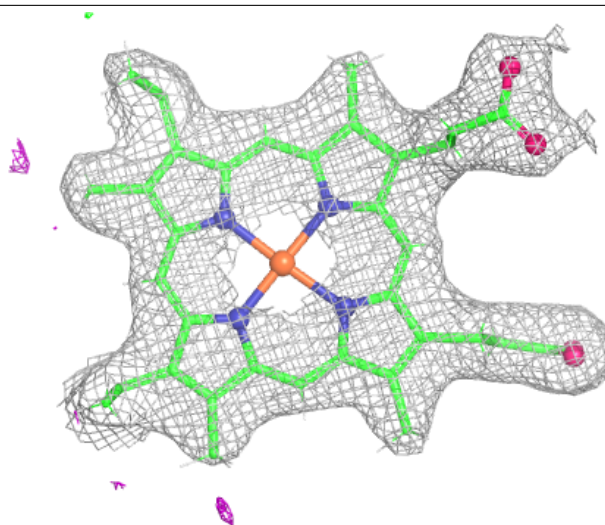
**Electron density around HEC V 201:**

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



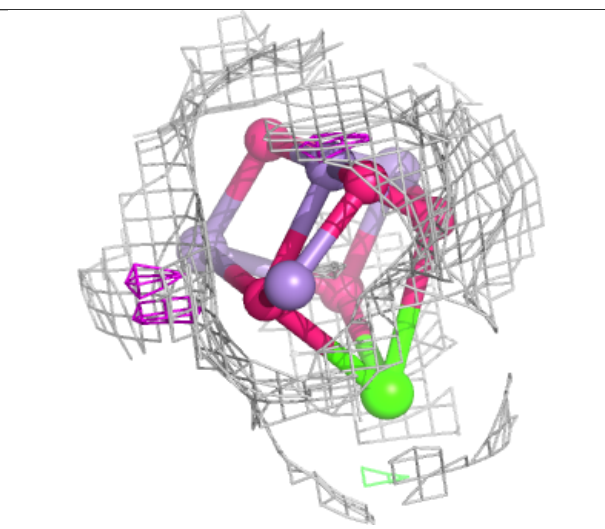
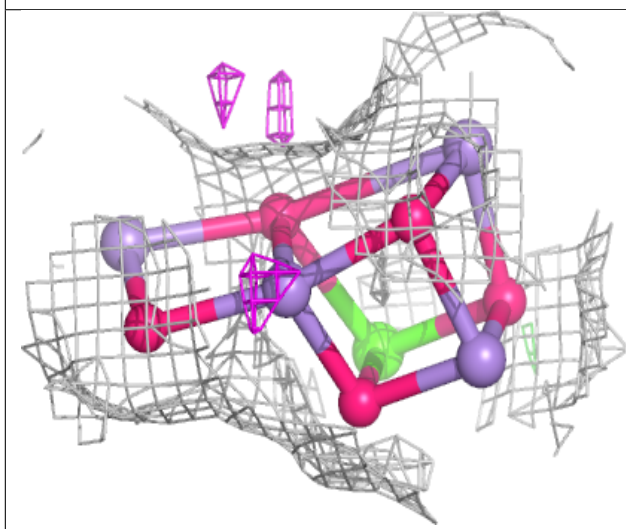
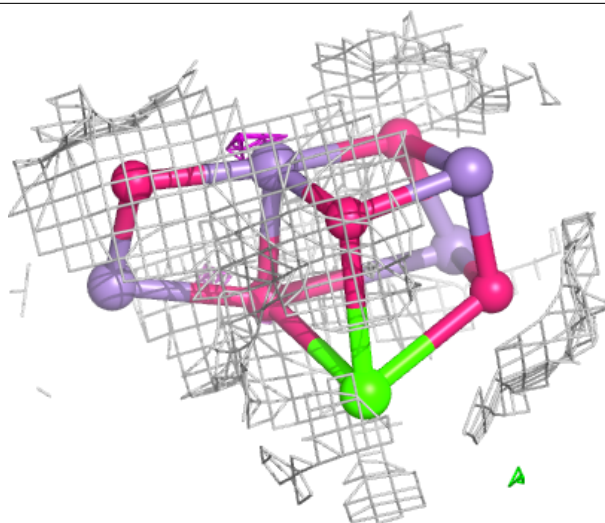
**Electron density around HEC v 201:**

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



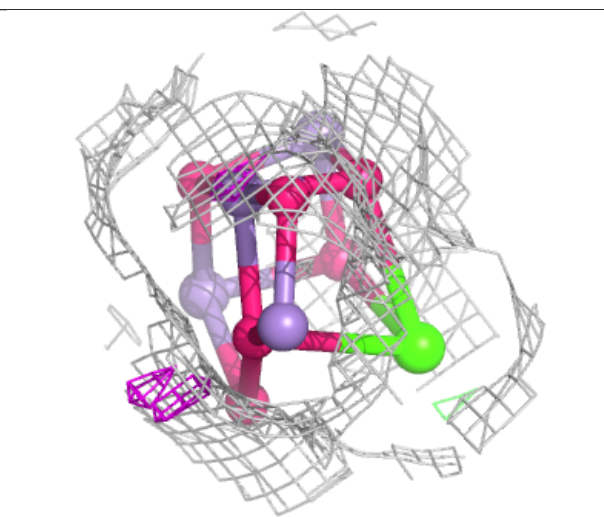
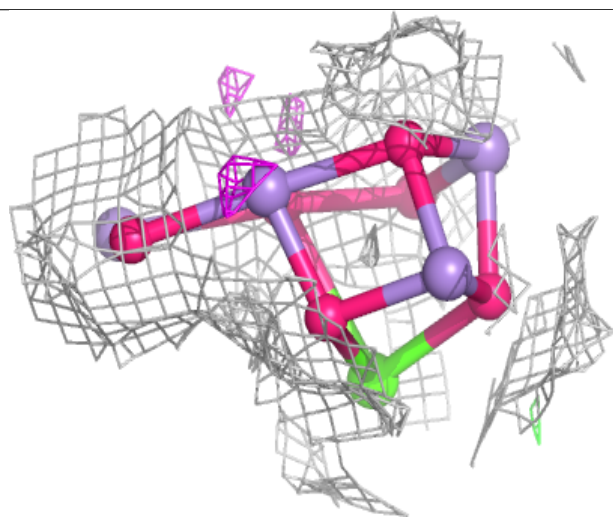
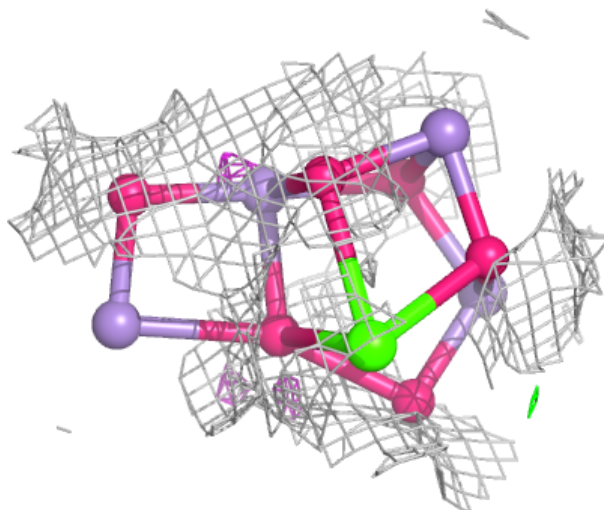
**Electron density around OEX a 602 (A):**

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



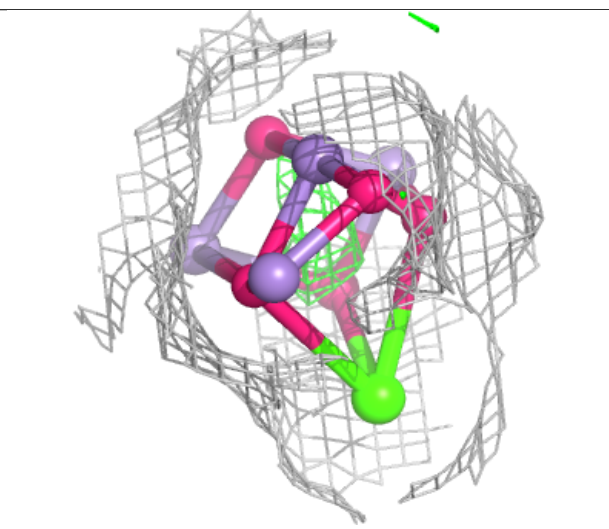
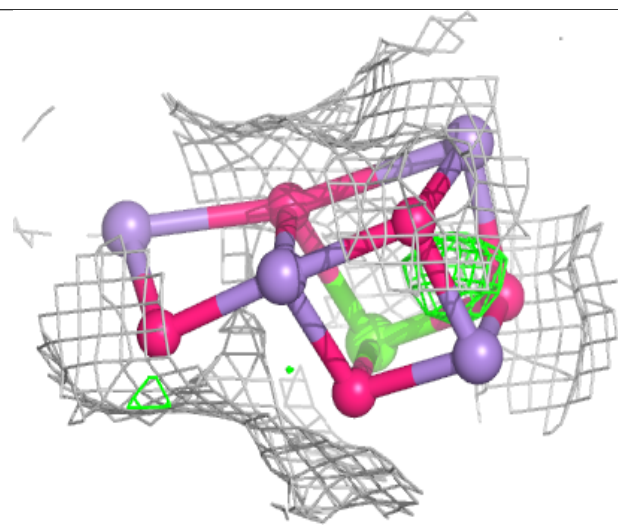
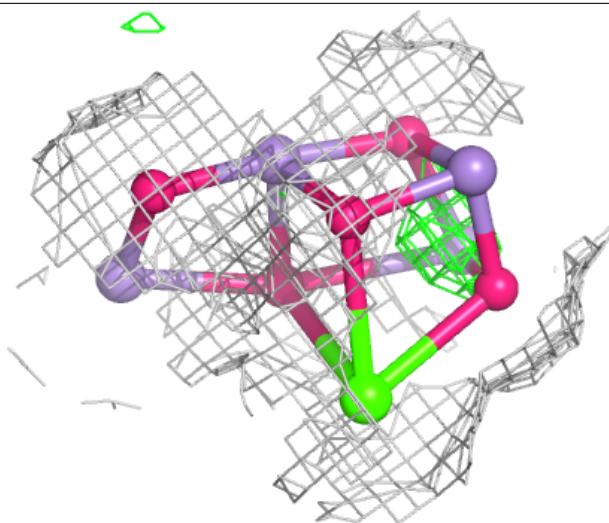
**Electron density around OEY a 601 (B):**

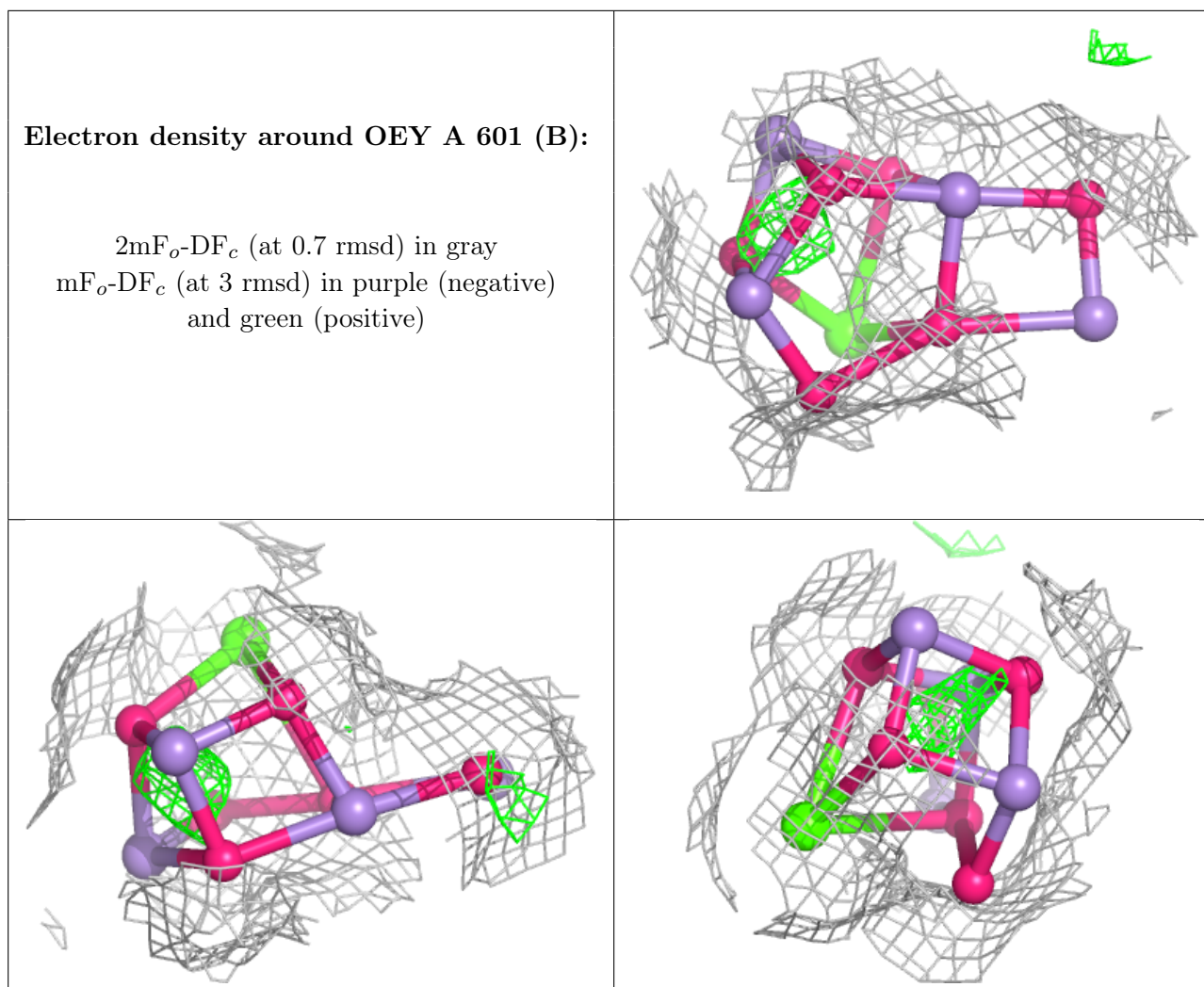
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.