



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2023 – 02:02 PM EDT

PDB ID : 8F4F  
Title : RT XFEL structure of Photosystem II 500 microseconds after the third illumination at 2.03 Angstrom resolution  
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.  
Deposited on : 2022-11-10  
Resolution : 2.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35

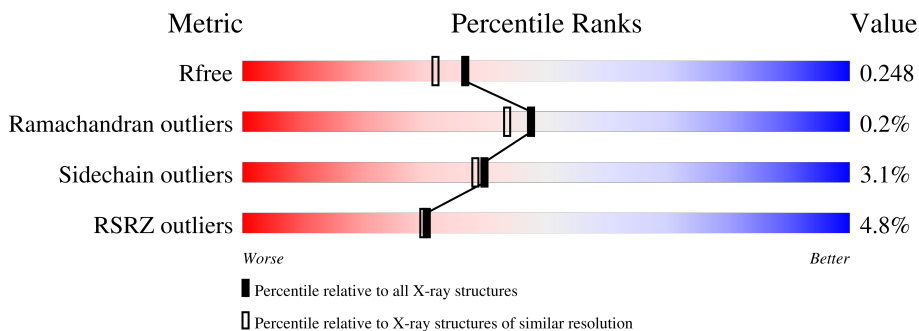
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	10434 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	96%
1	a	344	94%

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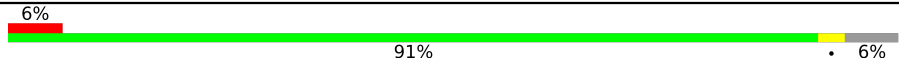
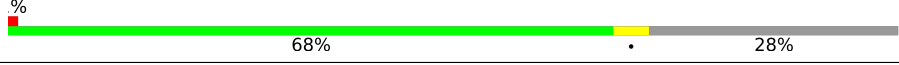
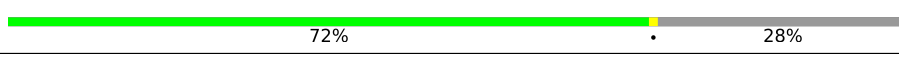


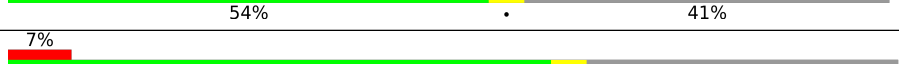
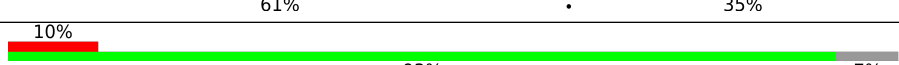
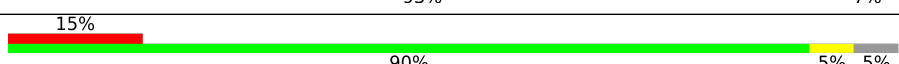
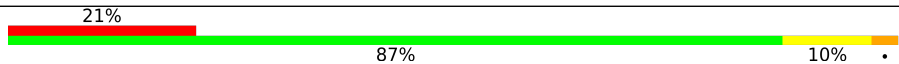
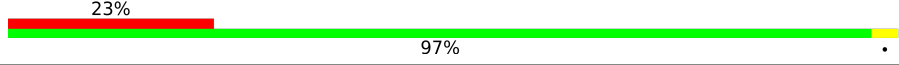

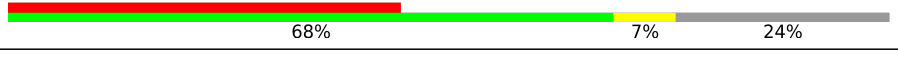

buster-report : 1.1.7 (2018)  
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
 Refmac : 5.8.0158  
 CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
2	B	510	3% 98%
2	b	510	3% 97%
3	C	461	% 95%
3	c	461	3% 95%
4	D	352	2% 96%
4	d	352	% 94%
5	E	84	10% 95%
5	e	84	14% 95%
6	F	45	7% 73% 24%
6	f	45	4% 73% 24%
7	H	66	9% 95%
7	h	66	11% 89% 6% 5%
8	I	38	3% 89% 5% 5%
8	i	38	3% 92% 5%
9	J	40	10% 88% 10%
9	j	40	18% 85% 5% 10%
10	K	46	2% 80% 20%
10	k	46	2% 76% 20%
11	L	37	3% 100%
11	l	37	5% 86% 11%
12	M	36	6% 89% 8%
12	m	36	89% 11%
13	O	272	6% 86% 10%
13	o	272	6% 85% 10%
14	T	32	6% 91% 6%

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	A	611	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	611	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	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>
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 53209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 3113	C 2030	N 513	O 551	S 19	0	64	0
1	a	334	Total 3110	C 2027	N 513	O 551	S 19	0	64	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	Total 4005	C 2631	N 666	O 695	S 13	0	4	0
2	b	505	Total 3978	C 2610	N 665	O 690	S 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	N	O	S			
3	C	442	Total 3509	C 2302	N 586	O 607	S 14	0	11	0
3	c	451	Total 3583	C 2343	N 602	O 624	S 14	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	Total 2731	C 1809	N 446	O 464	S 12	0	2	0
4	d	341	Total 2737	C 1813	N 446	O 466	S 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	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	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	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	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	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	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	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	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	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	293	204	43	46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
11	l	36	296	197	47	52		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	256	171	37	47	1	0	0	0
12	m	32	251	168	36	46	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1870	1168	313	385	4	0	1	0
13	o	244	1874	1170	317	383	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0
14	t	30	256	180	36	38	2	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
15	U	97	774	491	129	154	0	0	0
15	u	97	774	491	129	154	0	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O	S	0	0	0
			286	191	46	49				

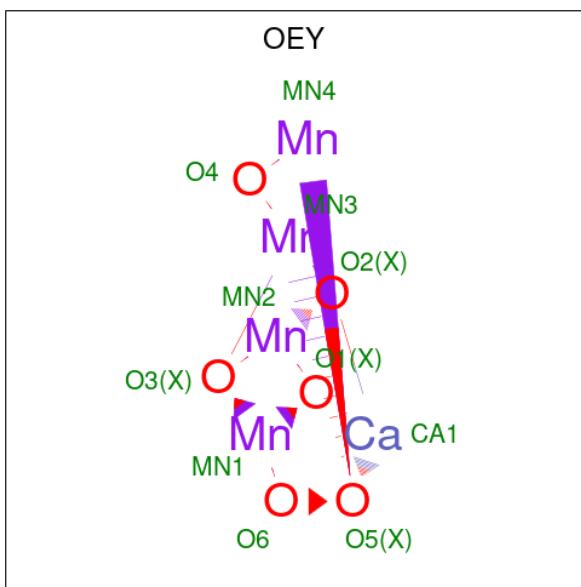
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O	S	0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: 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	22	2	8	12	0	1
21	a	1	22	2	8	12	0	1

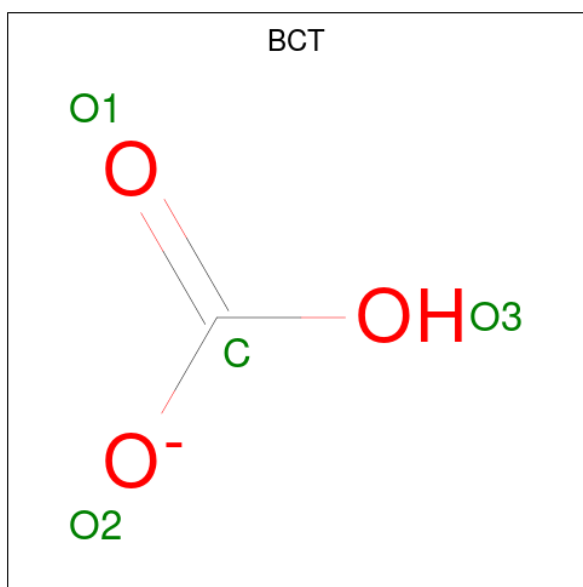
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

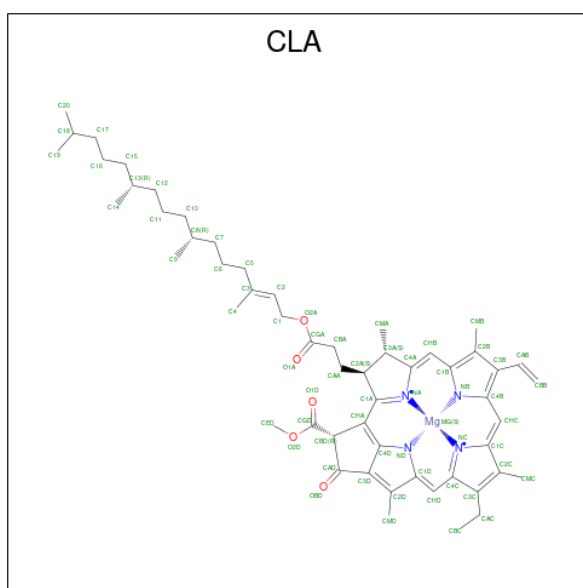
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
23	A	2	2	2	0	0
23	a	2	2	2	0	0

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	0	0	
			4	1	3			
24	d	1	Total	C	O	0	0	
			4	1	3			

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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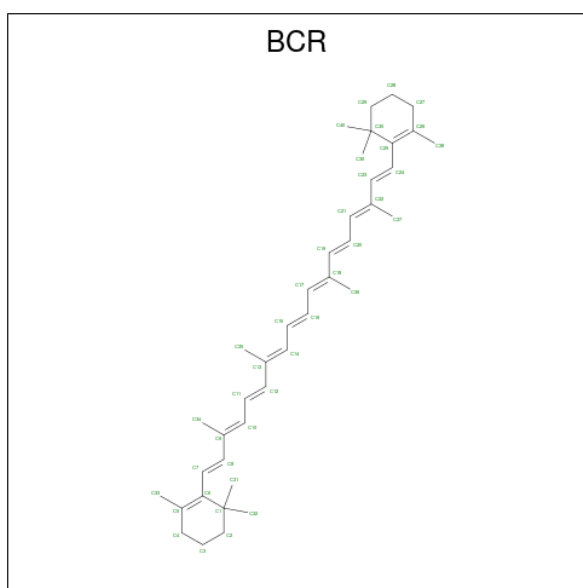
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		

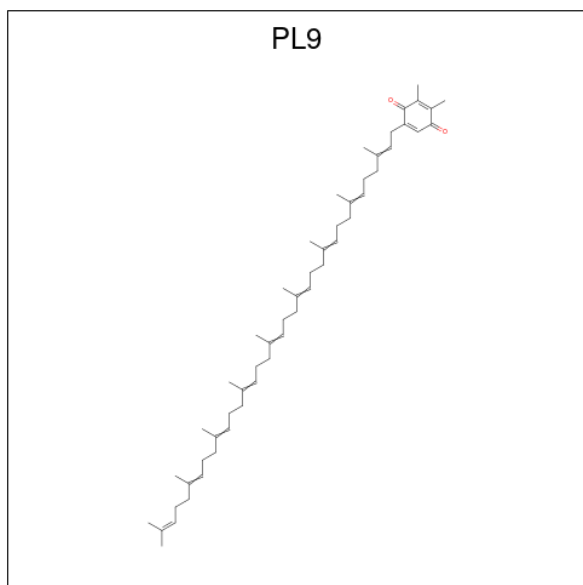
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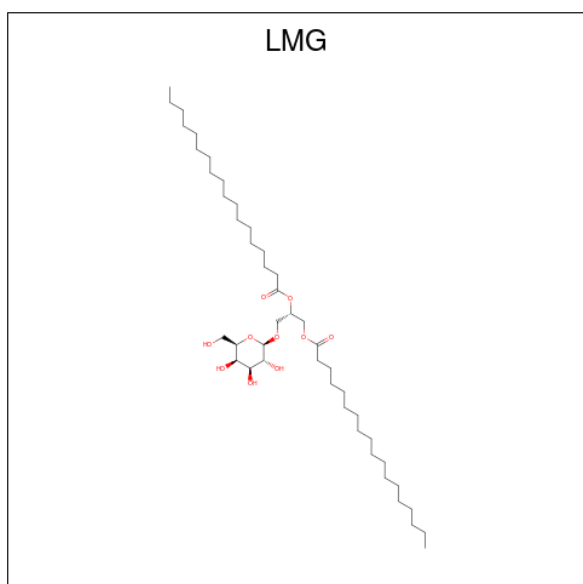
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 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 (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



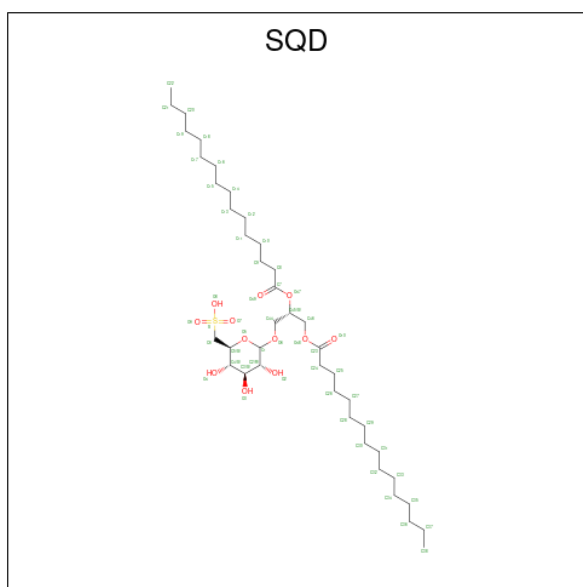
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



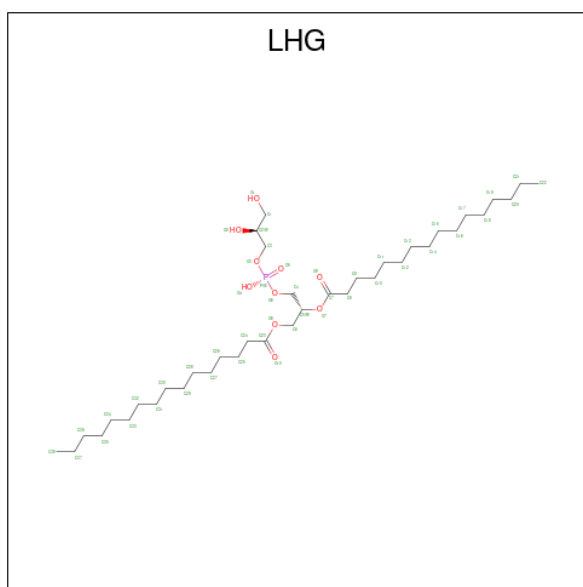
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	b	1	Total	C	O	0	0
			55	45	10		
28	c	1	Total	C	O	0	0
			37	27	10		
28	c	1	Total	C	O	0	0
			48	38	10		
28	c	1	Total	C	O	0	0
			49	39	10		
28	d	1	Total	C	O	0	0
			23	21	2		
28	d	1	Total	C	O	0	0
			44	34	10		
28	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



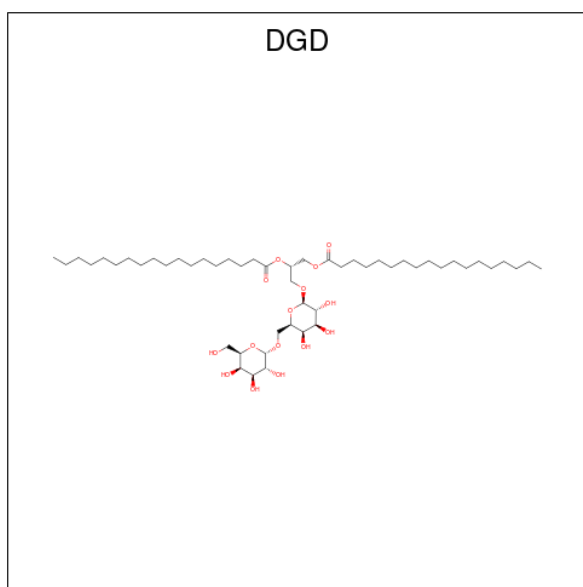
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			39	35	4			
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	b	1	Total	C	O	S	0	0
			49	36	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

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



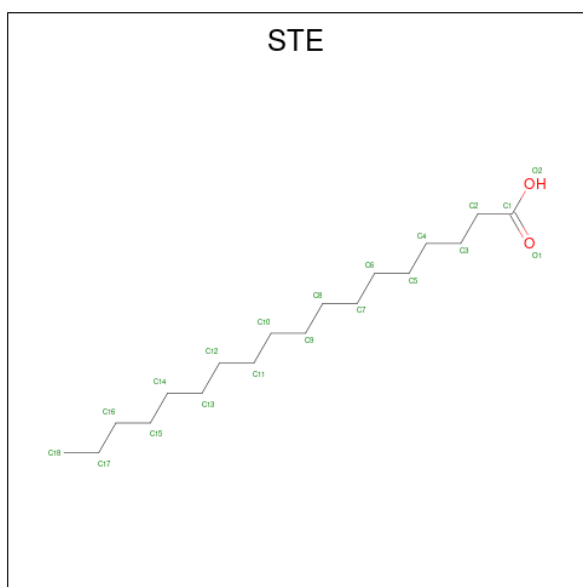
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
30	A	1	49	38	10	1	0	0
30	D	1	49	38	10	1	0	0
30	D	1	47	36	10	1	0	0
30	D	1	49	38	10	1	0	0
30	L	1	49	38	10	1	0	0
30	d	1	49	38	10	1	0	0
30	d	1	49	38	10	1	0	0
30	d	1	39	28	10	1	0	0
30	e	1	42	31	10	1	0	0
30	l	1	49	38	10	1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			66	51	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			62	47	15		
31	J	1	Total	C	O	0	0
			62	47	15		
31	a	1	Total	C	O	0	0
			44	39	5		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 20 18 2	0	0
32	B	1	Total C O 17 15 2	0	0
32	B	1	Total C O 12 10 2	0	0
32	B	1	Total C O 18 16 2	0	0
32	B	1	Total C O 12 10 2	0	0
32	B	1	Total C 16 16	0	0
32	C	1	Total C O 12 10 2	0	0
32	C	1	Total C O 12 10 2	0	0
32	C	1	Total C 16 16	0	0
32	D	1	Total C O 20 18 2	0	0
32	E	1	Total C O 12 10 2	0	0
32	H	1	Total C 18 18	0	0
32	I	1	Total C 15 15	0	0
32	J	1	Total C O 12 10 2	0	0

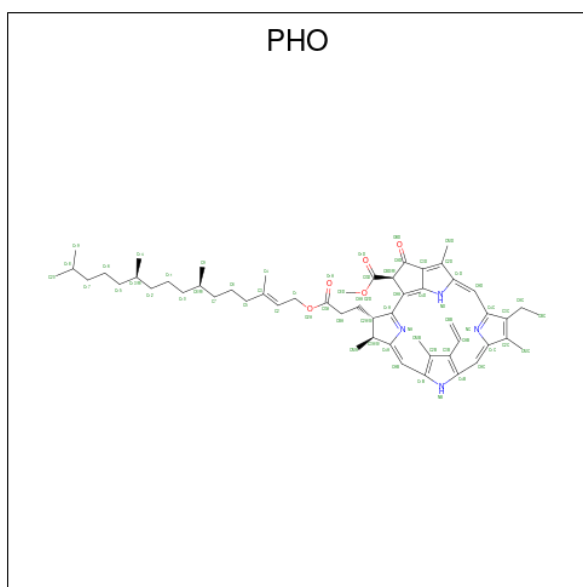
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	L	1	Total C O 12 10 2	0	0
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	k	1	Total C O 12 10 2	0	0
32	m	1	Total C 18 18	0	0
32	t	1	Total C O 14 12 2	0	0
32	t	1	Total C 10 10	0	0

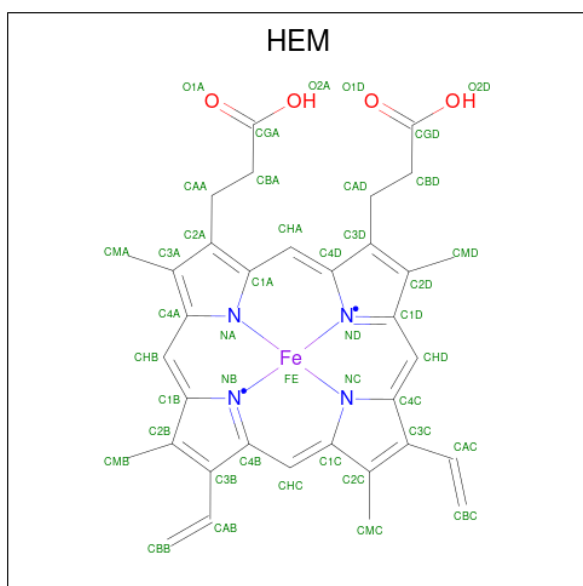
- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





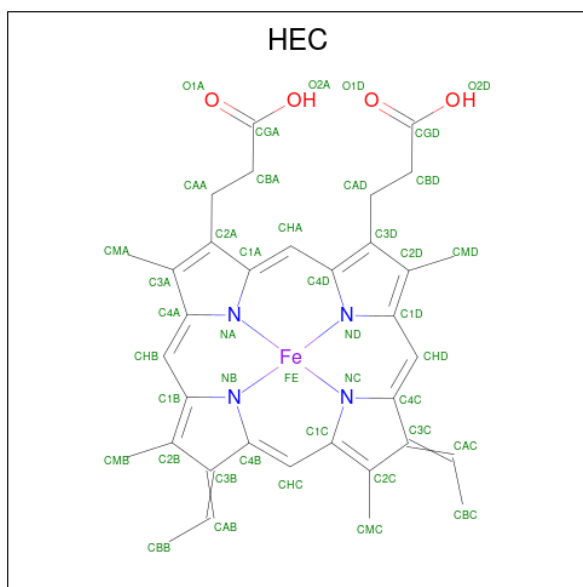
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	a	1	Total	C	N	O	0	0
			64	55	4	5		
33	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	124	Total	O	0	4
			128	128		
36	B	185	Total	O	0	0
			185	185		
36	C	160	Total	O	0	0
			160	160		
36	D	123	Total	O	0	0
			123	123		
36	E	17	Total	O	0	0
			17	17		
36	F	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	32	Total O 32 32	0	0
36	I	9	Total O 9 9	0	0
36	J	11	Total O 11 11	0	0
36	K	10	Total O 10 10	0	0
36	L	7	Total O 7 7	0	0
36	M	8	Total O 8 8	0	0
36	O	108	Total O 108 108	0	0
36	T	9	Total O 9 9	0	0
36	U	33	Total O 33 33	0	0
36	V	74	Total O 74 74	0	0
36	Y	10	Total O 10 10	0	0
36	X	11	Total O 11 11	0	0
36	Z	4	Total O 4 4	0	0
36	R	4	Total O 4 4	0	0
36	a	107	Total O 111 111	0	4
36	b	171	Total O 171 171	0	0
36	c	150	Total O 150 150	0	0
36	d	94	Total O 94 94	0	0
36	e	16	Total O 16 16	0	0
36	f	3	Total O 3 3	0	0
36	h	16	Total O 16 16	0	0

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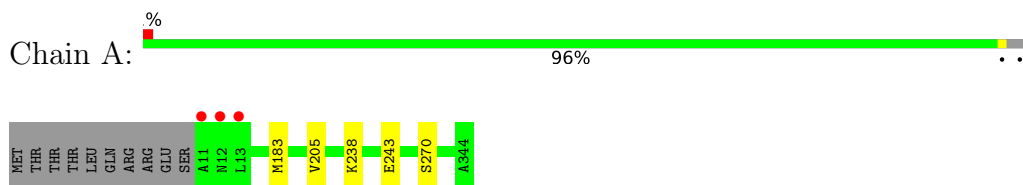
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
36	i	16	Total 16	O 16	0	0
36	j	11	Total 11	O 11	0	0
36	k	6	Total 6	O 6	0	0
36	l	14	Total 14	O 14	0	0
36	m	8	Total 8	O 8	0	0
36	o	96	Total 96	O 96	0	0
36	t	9	Total 9	O 9	0	0
36	u	58	Total 58	O 58	0	0
36	v	44	Total 44	O 44	0	0
36	y	11	Total 11	O 11	0	0
36	x	11	Total 11	O 11	0	0
36	r	10	Total 10	O 10	0	0

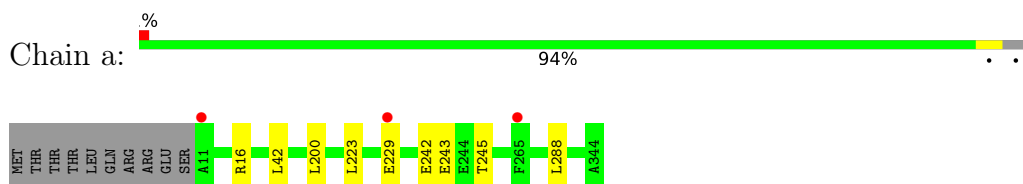
### 3 Residue-property plots [i](#)

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

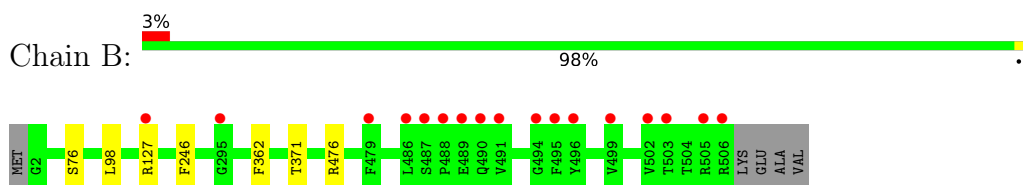
- Molecule 1: Photosystem II protein D1 1



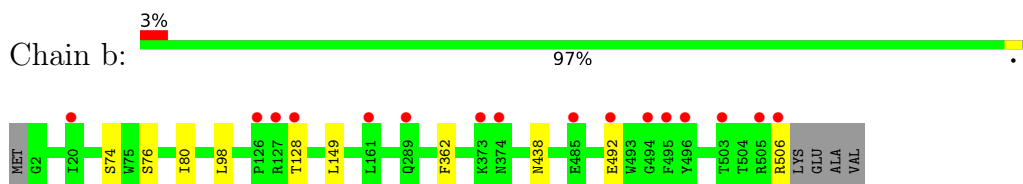
- Molecule 1: Photosystem II protein D1 1



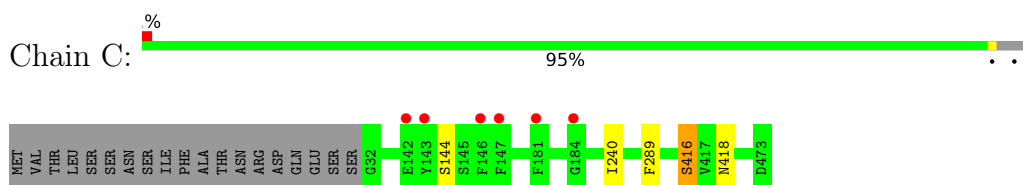
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



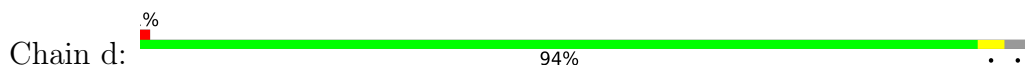
- Molecule 3: Photosystem II CP43 reaction center protein



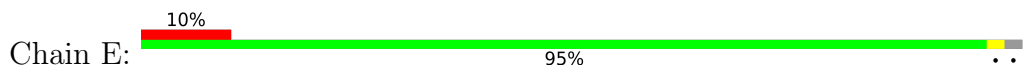
- Molecule 4: Photosystem II D2 protein



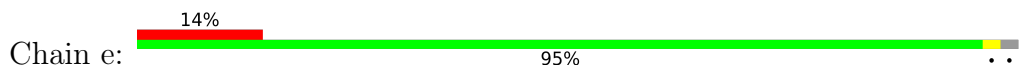
- Molecule 4: Photosystem II D2 protein



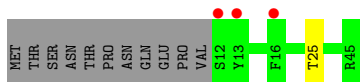
- Molecule 5: Cytochrome b559 subunit alpha



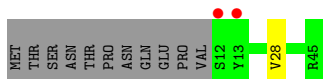
- Molecule 5: Cytochrome b559 subunit alpha



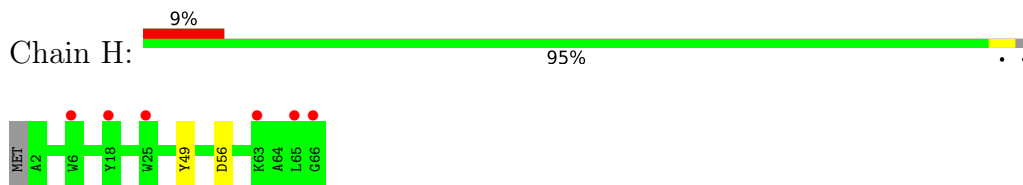
- Molecule 6: Cytochrome b559 subunit beta



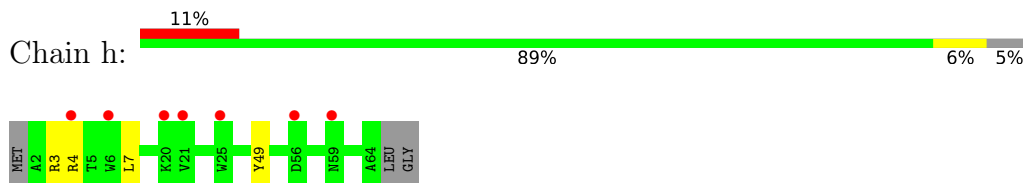
- Molecule 6: Cytochrome b559 subunit beta



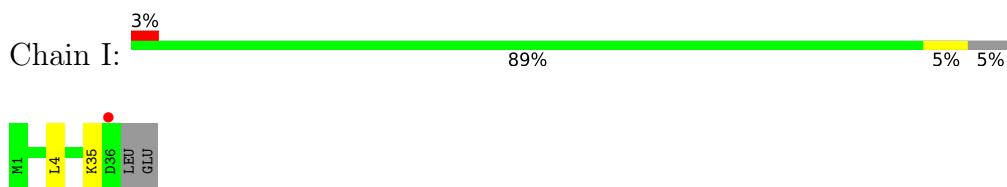
- Molecule 7: Photosystem II reaction center protein H



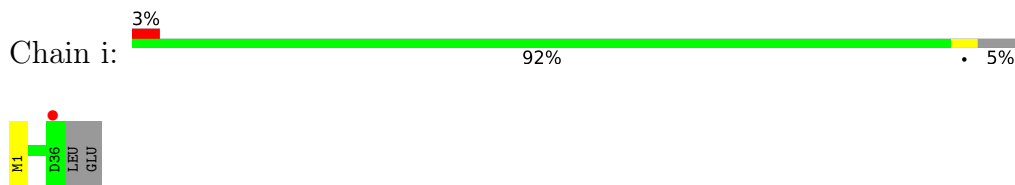
- Molecule 7: Photosystem II reaction center protein H



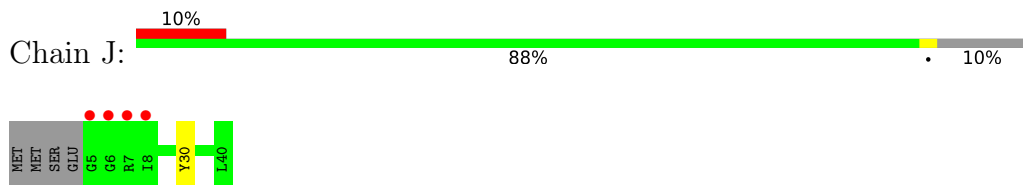
- Molecule 8: Photosystem II reaction center protein I



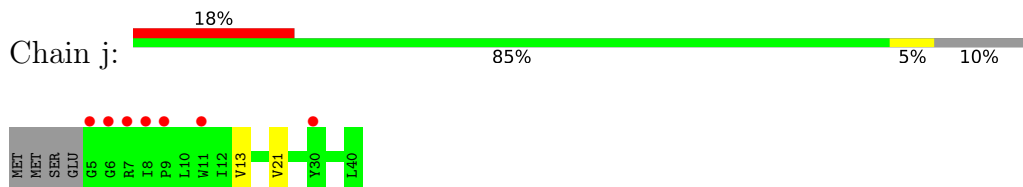
- Molecule 8: Photosystem II reaction center protein I



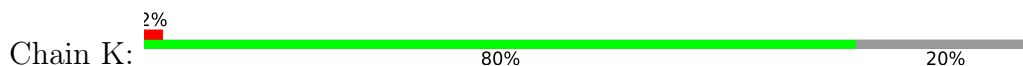
- Molecule 9: Photosystem II reaction center protein J

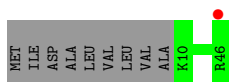


- Molecule 9: Photosystem II reaction center protein J

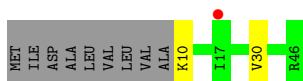
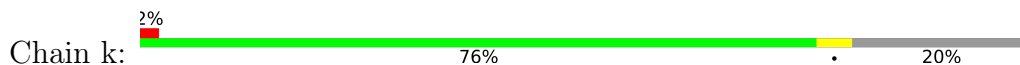


- Molecule 10: Photosystem II reaction center protein K





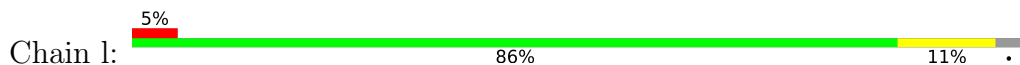
- Molecule 10: Photosystem II reaction center protein K



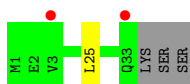
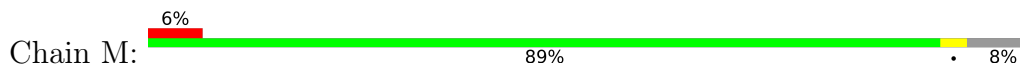
- Molecule 11: Photosystem II reaction center protein L



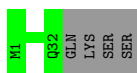
- Molecule 11: Photosystem II reaction center protein L



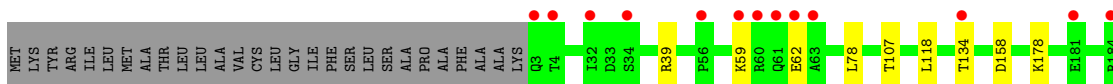
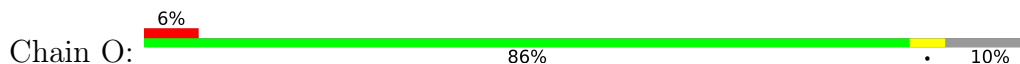
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

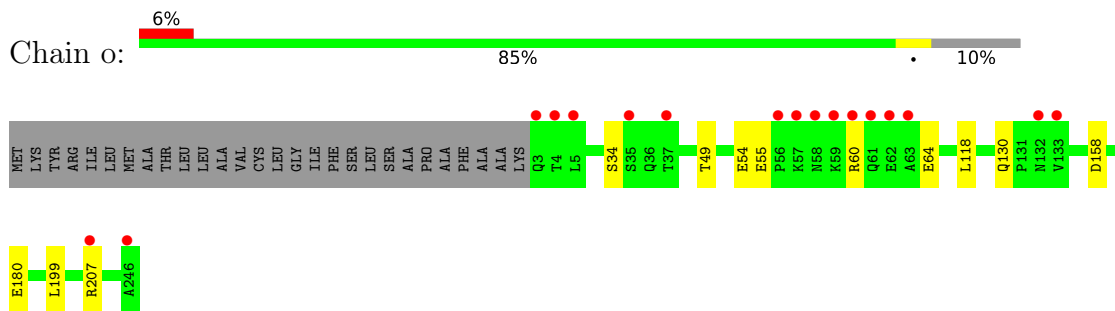


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

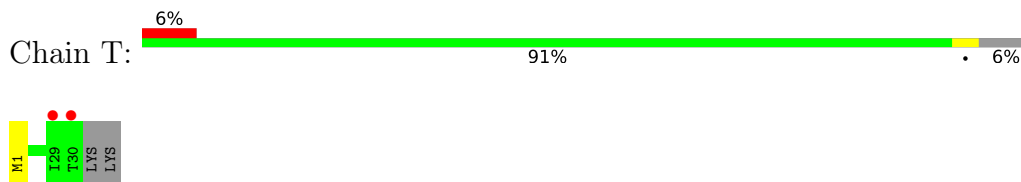




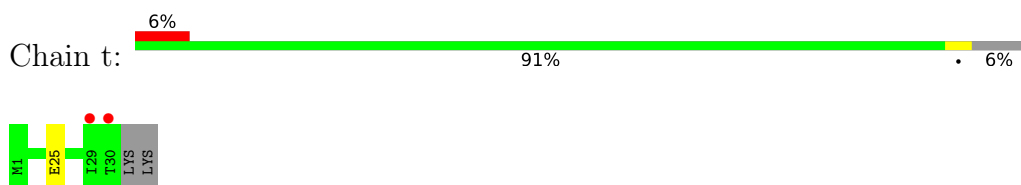
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



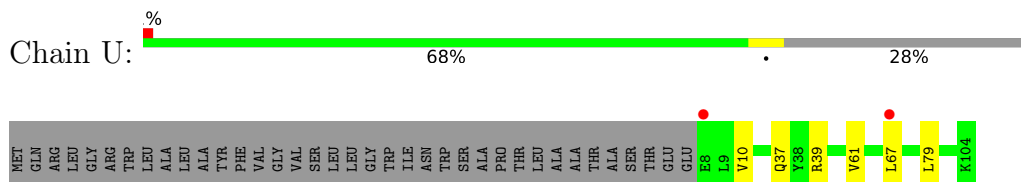
- Molecule 14: Photosystem II reaction center protein T



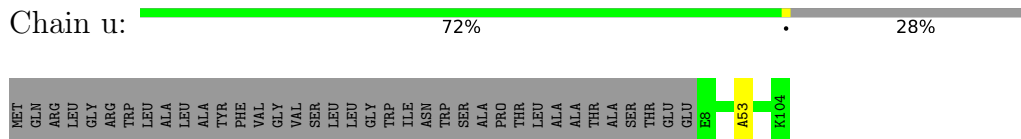
- Molecule 14: Photosystem II reaction center protein T



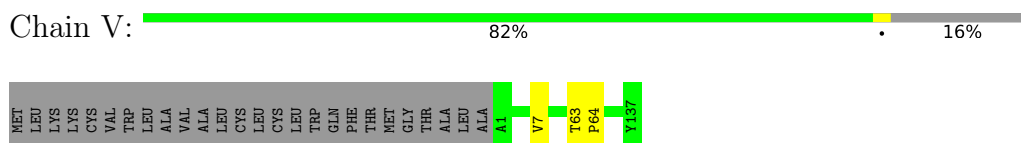
- Molecule 15: Photosystem II 12 kDa extrinsic protein



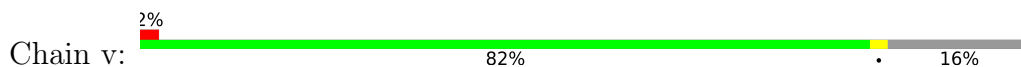
- Molecule 15: Photosystem II 12 kDa extrinsic protein

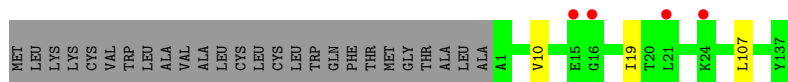


- Molecule 16: Cytochrome c-550

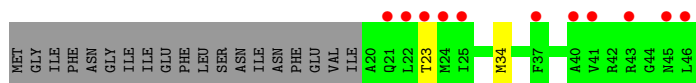


- Molecule 16: Cytochrome c-550

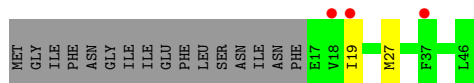




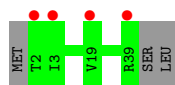
- Molecule 17: Photosystem II reaction center protein Ycf12



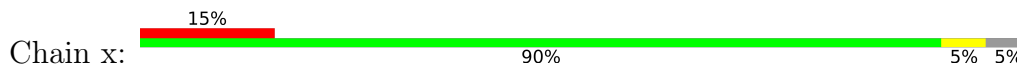
- Molecule 17: Photosystem II reaction center protein Ycf12



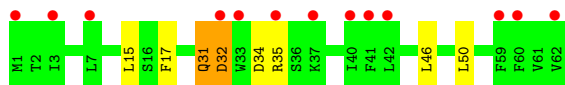
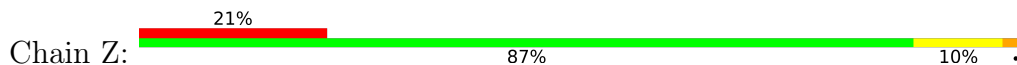
- Molecule 18: Photosystem II reaction center X protein



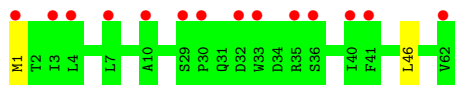
- Molecule 18: Photosystem II reaction center X protein



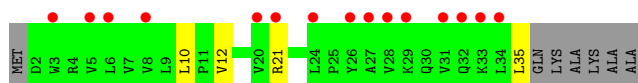
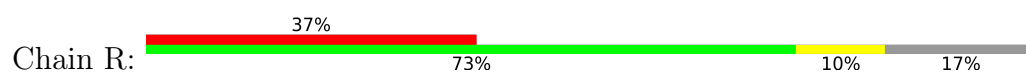
- Molecule 19: Photosystem II reaction center protein Z



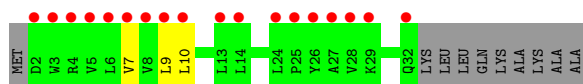
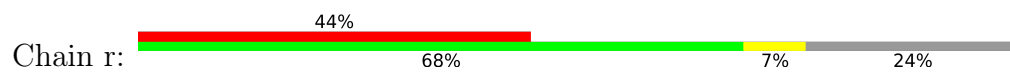
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.53Å 222.83Å 309.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.23 – 2.03 31.23 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.23-2.03) 85.3 (31.23-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.33 (at 2.03Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.199 , 0.248 0.200 , 0.248	Depositor DCC
$R_{free}$ test set	4617 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtrriage
Anisotropy	0.276	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	53209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

### 5.1 Standard geometry

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

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	0.42	0/3212	0.59	2/4376 (0.0%)
1	a	0.41	0/3209	0.57	0/4372
2	B	0.42	0/4155	0.57	0/5661
2	b	0.40	0/4118	0.57	1/5611 (0.0%)
3	C	0.39	0/3625	0.56	0/4935
3	c	0.37	0/3705	0.55	0/5042
4	D	0.43	0/2825	0.57	0/3847
4	d	0.41	0/2834	0.58	0/3859
5	E	0.36	0/688	0.50	0/940
5	e	0.31	0/683	0.51	0/932
6	F	0.36	0/284	0.47	0/387
6	f	0.33	0/284	0.52	0/387
7	H	0.38	0/523	0.56	0/713
7	h	0.38	0/511	0.55	0/697
8	I	0.39	0/293	0.56	0/396
8	i	0.41	0/293	0.55	0/396
9	J	0.37	0/263	0.56	0/356
9	j	0.33	0/263	0.49	0/356
10	K	0.34	0/303	0.53	0/416
10	k	0.33	0/303	0.54	0/416
11	L	0.40	0/311	0.57	0/422
11	l	0.41	0/303	0.61	0/412
12	M	0.38	0/249	0.49	0/341
12	m	0.40	0/244	0.51	0/334
13	O	0.37	0/1904	0.62	1/2585 (0.0%)
13	o	0.39	0/1905	0.63	1/2583 (0.0%)
14	T	0.43	0/257	0.55	0/349
14	t	0.40	0/255	0.52	0/346
15	U	0.34	0/785	0.55	0/1064
15	u	0.36	0/785	0.60	0/1064
16	V	0.36	0/1085	0.59	0/1473
16	v	0.32	0/1085	0.54	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.32	0/197	0.55	0/264
17	y	0.26	0/219	0.46	0/294
18	X	0.36	0/284	0.51	0/384
18	x	0.31	0/289	0.44	0/391
19	Z	0.32	0/490	0.48	0/669
19	z	0.30	0/488	0.41	0/666
20	R	0.32	0/277	0.52	0/380
20	r	0.28	0/252	0.50	0/347
All	All	0.39	0/44038	0.56	5/59936 (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
16	V	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
13	o	158	ASP	CB-CG-OD1	6.79	124.41	118.30
13	O	158	ASP	CB-CG-OD1	5.90	123.61	118.30
2	b	98	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	183[A]	MET	CA-CB-CG	5.17	122.10	113.30
1	A	183[B]	MET	CA-CB-CG	5.17	122.10	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	395/344 (115%)	391 (99%)	4 (1%)	0	100	100
1	a	395/344 (115%)	390 (99%)	5 (1%)	0	100	100
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	8 (2%)	0	100	100
3	C	451/461 (98%)	439 (97%)	11 (2%)	1 (0%)	47	43
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	47	43
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	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%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	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%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	13	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14	7
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	15
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4	1
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5252 (98%)	125 (2%)	9 (0%)	47	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
19	Z	31	GLN
3	c	416	SER
13	O	59	LYS
15	u	53	ALA
13	O	62	GLU
19	Z	32	ASP
13	O	134	THR

### 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	322/280 (115%)	318 (99%)	4 (1%)	71	75
1	a	321/280 (115%)	312 (97%)	9 (3%)	43	43
2	B	407/407 (100%)	400 (98%)	7 (2%)	60	63
2	b	402/407 (99%)	393 (98%)	9 (2%)	52	53
3	C	353/362 (98%)	348 (99%)	5 (1%)	67	70
3	c	362/362 (100%)	349 (96%)	13 (4%)	35	32
4	D	277/283 (98%)	275 (99%)	2 (1%)	84	87
4	d	278/283 (98%)	268 (96%)	10 (4%)	35	32
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	26
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	43
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	32
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	32
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	31
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	8
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	12
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	26
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	6
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	28 (93%)	2 (7%)	16	11
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	32
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	199 (97%)	7 (3%)	37	35
13	o	207/228 (91%)	196 (95%)	11 (5%)	22	17
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	31	28
15	U	84/112 (75%)	78 (93%)	6 (7%)	14	9
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	116 (99%)	1 (1%)	78	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	114 (97%)	3 (3%)	46	46
17	Y	19/37 (51%)	17 (90%)	2 (10%)	7	3
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	11
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
19	z	51/52 (98%)	49 (96%)	2 (4%)	32	29
20	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
20	r	25/33 (76%)	22 (88%)	3 (12%)	5	2
All	All	4450/4654 (96%)	4314 (97%)	136 (3%)	40	38

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	238	LYS
1	A	243	GLU
1	A	270	SER
2	B	76	SER
2	B	98	LEU
2	B	127	ARG
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	144	SER
3	C	240	ILE
3	C	289	PHE
3	C	416	SER
3	C	418	ASN
4	D	180	ARG
4	D	264	LYS
5	E	4	THR
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	I	35	LYS
9	J	30	TYR
12	M	25	LEU
13	O	39	ARG
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	178	LYS
13	O	199	LEU
13	O	214	THR
15	U	10	VAL
15	U	37	GLN
15	U	39	ARG
15	U	61	VAL
15	U	67	LEU
15	U	79	LEU
16	V	7	VAL
17	Y	23	THR
17	Y	34	MET
19	Z	15	LEU
19	Z	17	PHE
19	Z	31	GLN
19	Z	32	ASP
19	Z	34	ASP
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
20	R	10	LEU
20	R	12	VAL
20	R	21	ARG
20	R	35	LEU
1	a	16	ARG
1	a	42	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	242	GLU
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	74	SER
2	b	76	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	80	ILE
2	b	128	THR
2	b	149	LEU
2	b	362	PHE
2	b	438	ASN
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	355[A]	THR
3	c	355[B]	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416	SER
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	238	THR
4	d	259	ILE
4	d	264	LYS
4	d	291	LEU
4	d	321	LEU
5	e	83	LEU
5	e	84	LYS
6	f	28	VAL
7	h	3	ARG
7	h	4	ARG
7	h	7	LEU
7	h	49	TYR
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	30	VAL
11	l	2	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
13	o	34	SER
13	o	49	THR
13	o	54	GLU
13	o	55	GLU
13	o	60	ARG
13	o	64	GLU
13	o	118	LEU
13	o	130	GLN
13	o	180	GLU
13	o	199	LEU
13	o	207	ARG
14	t	25	GLU
16	v	10	VAL
16	v	19	ILE
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
18	x	2	THR
18	x	15	LEU
19	z	1	MET
19	z	46	LEU
20	r	7	VAL
20	r	9	LEU
20	r	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	H	59	ASN
13	O	88	ASN
16	V	86	GLN
17	Y	45	ASN
18	X	38	GLN
19	Z	31	GLN
1	a	234	ASN
2	b	179	GLN
2	b	409	GLN
4	d	61	HIS
5	e	60	GLN

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Mol	Chain	Res	Type
5	e	82	GLN
19	z	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	FME	T	1	14	8,9,10	1.26	1 (12%)	7,9,11	1.22	1 (14%)
14	FME	t	1	14	8,9,10	1.11	0	7,9,11	0.81	0
12	FME	M	1	12	8,9,10	0.96	0	7,9,11	0.96	0
8	FME	I	1	8	8,9,10	1.03	0	7,9,11	0.57	0
12	FME	m	1	12	8,9,10	1.01	0	7,9,11	0.69	0
8	FME	i	1	8	8,9,10	0.98	0	7,9,11	0.96	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.78	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.63	114.48	109.73
8	i	1	FME	CA-N-CN	-2.01	119.73	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O-C-CA-CB
14	t	1	FME	C-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-CA-CB-CG
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	N-CA-CB-CG
12	m	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	b	619	-	41,41,41	0.94	2 (4%)	56,56,56	1.14	3 (5%)
25	CLA	c	509	-	65,73,73	1.48	8 (12%)	76,113,113	1.63	8 (10%)
25	CLA	b	615	-	65,73,73	1.68	7 (10%)	76,113,113	1.33	7 (9%)
28	LMG	d	411	-	44,44,55	0.90	3 (6%)	52,52,63	1.33	5 (9%)
31	DGD	A	616	-	67,67,67	1.09	9 (13%)	81,81,81	1.33	10 (12%)
25	CLA	A	606	-	65,73,73	1.55	6 (9%)	76,113,113	1.44	10 (13%)
25	CLA	b	604	-	65,73,73	1.59	9 (13%)	76,113,113	1.57	14 (18%)
28	LMG	B	620	-	51,51,55	0.84	2 (3%)	59,59,63	1.36	6 (10%)
25	CLA	B	608	-	65,73,73	1.51	10 (15%)	76,113,113	1.45	8 (10%)
32	STE	M	102	-	9,9,19	0.36	0	8,8,19	0.82	0
26	BCR	k	103	-	41,41,41	0.99	2 (4%)	56,56,56	1.07	2 (3%)
26	BCR	b	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	6 (10%)
27	PL9	a	610	-	55,55,55	0.73	0	68,69,69	1.48	11 (16%)
30	LHG	A	614	-	48,48,48	0.78	2 (4%)	51,54,54	1.18	5 (9%)
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.16	2 (15%)
30	LHG	d	407	-	48,48,48	0.81	3 (6%)	51,54,54	1.28	5 (9%)
33	PHO	D	401	-	51,69,69	0.97	3 (5%)	47,99,99	1.08	1 (2%)
25	CLA	B	616	-	60,68,73	1.55	8 (13%)	70,107,113	1.52	10 (14%)
26	BCR	a	609	-	41,41,41	0.93	2 (4%)	56,56,56	1.16	4 (7%)
32	STE	J	102	-	11,11,19	0.70	0	11,11,19	1.17	0
21	OEY	a	601[B]	3,36,1	0,16,16	-	-	-	-	-
25	CLA	B	601	36	65,73,73	1.65	6 (9%)	76,113,113	1.59	8 (10%)
29	SQD	f	102	-	40,41,54	1.64	7 (17%)	49,52,65	1.78	10 (20%)
32	STE	B	624	-	11,11,19	0.73	0	11,11,19	1.41	2 (18%)
25	CLA	C	512	-	65,73,73	1.61	7 (10%)	76,113,113	1.48	11 (14%)
26	BCR	k	102	-	41,41,41	1.03	3 (7%)	56,56,56	1.07	2 (3%)
26	BCR	B	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	5 (8%)
26	BCR	B	617	-	41,41,41	0.96	2 (4%)	56,56,56	1.22	3 (5%)
33	PHO	d	402	-	51,69,69	1.00	2 (3%)	47,99,99	1.39	7 (14%)
26	BCR	T	101	-	41,41,41	0.96	2 (4%)	56,56,56	1.25	5 (8%)
24	BCT	A	605	22	2,3,3	1.27	0	2,3,3	2.82	1 (50%)
33	PHO	a	607	-	51,69,69	1.01	3 (5%)	47,99,99	1.05	4 (8%)
29	SQD	b	620	-	48,49,54	1.63	10 (20%)	57,60,65	1.93	11 (19%)
30	LHG	D	412	-	48,48,48	0.79	1 (2%)	51,54,54	1.36	7 (13%)
24	BCT	d	401	22	2,3,3	1.32	0	2,3,3	2.95	1 (50%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	HEM	E	101	5,6	41,50,50	1.51	4 (9%)	45,82,82	1.33	7 (15%)
32	STE	T	102	-	15,15,19	0.37	0	14,14,19	0.75	0
30	LHG	e	101	-	41,41,48	0.78	1 (2%)	44,47,54	1.28	6 (13%)
35	HEC	v	201	16	32,50,50	2.16	4 (12%)	24,82,82	1.69	4 (16%)
25	CLA	c	502	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	9 (11%)
26	BCR	K	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
30	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	4 (7%)
25	CLA	c	501	-	65,73,73	1.56	9 (13%)	76,113,113	1.52	10 (13%)
26	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
25	CLA	b	609	-	65,73,73	1.60	7 (10%)	76,113,113	1.50	9 (11%)
25	CLA	b	610	36	65,73,73	1.41	7 (10%)	76,113,113	1.28	11 (14%)
32	STE	b	624	-	14,14,19	0.30	0	13,13,19	0.97	0
31	DGD	c	517	-	63,63,67	0.92	3 (4%)	77,77,81	1.39	10 (12%)
26	BCR	h	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.25	7 (12%)
32	STE	C	519	-	11,11,19	0.70	0	11,11,19	1.11	0
32	STE	B	626	-	11,11,19	0.65	0	11,11,19	1.56	2 (18%)
29	SQD	A	613	-	51,52,54	1.55	7 (13%)	60,63,65	2.01	12 (20%)
25	CLA	C	507	36	65,73,73	1.43	5 (7%)	76,113,113	1.60	11 (14%)
31	DGD	C	515	-	63,63,67	1.03	6 (9%)	77,77,81	1.31	11 (14%)
25	CLA	c	508	-	64,72,73	1.61	8 (12%)	74,111,113	1.42	9 (12%)
32	STE	B	621	-	16,16,19	0.68	0	16,16,19	1.04	0
28	LMG	c	518	-	37,37,55	0.96	2 (5%)	45,45,63	1.31	5 (11%)
25	CLA	A	611	36	65,73,73	1.40	6 (9%)	76,113,113	1.51	10 (13%)
34	HEM	f	101	5,6	41,50,50	1.51	6 (14%)	45,82,82	1.75	9 (20%)
25	CLA	C	511	3	65,73,73	1.61	7 (10%)	76,113,113	1.56	7 (9%)
25	CLA	b	603	-	65,73,73	1.58	8 (12%)	76,113,113	1.42	8 (10%)
29	SQD	B	623	-	53,54,54	1.55	11 (20%)	62,65,65	1.61	9 (14%)
26	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	c	511	3	65,73,73	1.72	6 (9%)	76,113,113	1.54	8 (10%)
28	LMG	C	517	-	48,48,55	0.82	2 (4%)	56,56,63	1.33	6 (10%)
28	LMG	d	410	-	21,21,55	0.51	0	20,20,63	1.19	3 (15%)
32	STE	C	518	-	11,11,19	0.70	0	11,11,19	1.39	2 (18%)
25	CLA	C	503	-	65,73,73	1.65	9 (13%)	76,113,113	1.64	12 (15%)
25	CLA	B	606	-	65,73,73	1.73	10 (15%)	76,113,113	1.59	11 (14%)
25	CLA	C	504	36	59,67,73	1.77	7 (11%)	68,105,113	1.48	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	d	404	-	65,73,73	1.55	8 (12%)	76,113,113	1.46	10 (13%)
28	LMG	B	622	-	26,26,55	0.75	2 (7%)	26,26,63	1.21	1 (3%)
26	BCR	C	514	-	41,41,41	1.01	2 (4%)	56,56,56	1.21	6 (10%)
32	STE	I	101	-	14,14,19	0.34	0	13,13,19	0.87	0
25	CLA	a	606	36	65,73,73	1.53	5 (7%)	76,113,113	1.49	11 (14%)
25	CLA	C	508	-	65,73,73	1.54	8 (12%)	76,113,113	1.65	11 (14%)
25	CLA	C	509	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
25	CLA	A	608	-	54,62,73	1.64	6 (11%)	62,99,113	1.61	12 (19%)
25	CLA	B	603	-	65,73,73	1.60	7 (10%)	76,113,113	1.49	13 (17%)
26	BCR	t	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.26	5 (8%)
25	CLA	c	506	-	65,73,73	1.64	7 (10%)	76,113,113	1.33	6 (7%)
25	CLA	c	507	36	65,73,73	1.52	9 (13%)	76,113,113	1.47	8 (10%)
25	CLA	B	613	-	65,73,73	1.62	8 (12%)	76,113,113	1.54	9 (11%)
28	LMG	D	407	-	51,51,55	0.95	3 (5%)	59,59,63	1.36	9 (15%)
25	CLA	B	611	-	65,73,73	1.40	6 (9%)	76,113,113	1.48	11 (14%)
32	STE	B	625	-	17,17,19	0.66	0	17,17,19	1.01	0
25	CLA	B	605	-	65,73,73	1.44	5 (7%)	76,113,113	1.44	12 (15%)
25	CLA	b	605	-	65,73,73	1.57	6 (9%)	76,113,113	1.43	11 (14%)
31	DGD	J	101	-	63,63,67	0.84	3 (4%)	77,77,81	1.41	11 (14%)
32	STE	M	101	-	14,14,19	0.65	0	14,14,19	1.27	1 (7%)
31	DGD	C	516	-	63,63,67	1.05	5 (7%)	77,77,81	1.37	10 (12%)
31	DGD	h	102	-	63,63,67	0.97	4 (6%)	77,77,81	1.45	12 (15%)
25	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	1.31	9 (11%)
25	CLA	b	616	-	60,68,73	1.60	8 (13%)	70,107,113	1.69	8 (11%)
32	STE	B	627	-	15,15,19	0.33	0	14,14,19	0.87	0
25	CLA	C	505	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
25	CLA	b	613	-	65,73,73	1.53	7 (10%)	76,113,113	1.45	9 (11%)
25	CLA	c	503	-	65,73,73	1.57	8 (12%)	76,113,113	1.61	11 (14%)
32	STE	b	621	-	19,19,19	0.58	0	19,19,19	1.14	1 (5%)
26	BCR	H	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	d	403	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	8 (10%)
31	DGD	H	102	-	63,63,67	1.10	7 (11%)	77,77,81	1.44	9 (11%)
25	CLA	b	608	-	65,73,73	1.57	8 (12%)	76,113,113	1.44	10 (13%)
26	BCR	b	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.32	7 (12%)
28	LMG	c	521	-	49,49,55	0.89	3 (6%)	57,57,63	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	607	36	65,73,73	1.40	7 (10%)	76,113,113	1.37	8 (10%)
25	CLA	b	606	-	65,73,73	1.56	8 (12%)	76,113,113	1.55	9 (11%)
28	LMG	b	622	-	55,55,55	0.89	4 (7%)	63,63,63	1.42	11 (17%)
26	BCR	d	405	-	41,41,41	1.01	3 (7%)	56,56,56	1.15	5 (8%)
29	SQD	a	612	-	53,54,54	1.58	7 (13%)	62,65,65	1.81	9 (14%)
32	STE	d	413	-	19,19,19	0.55	0	19,19,19	1.20	1 (5%)
25	CLA	B	612	-	65,73,73	1.53	9 (13%)	76,113,113	1.48	9 (11%)
21	OEY	A	601[B]	3,36,1	0,16,16	-	-	-		
30	LHG	D	409	-	48,48,48	0.73	2 (4%)	51,54,54	1.23	7 (13%)
25	CLA	c	504	36	60,68,73	1.68	7 (11%)	70,107,113	1.47	9 (12%)
25	CLA	a	605	-	65,73,73	1.65	8 (12%)	76,113,113	1.53	9 (11%)
25	CLA	C	513	-	65,73,73	1.68	8 (12%)	76,113,113	1.42	10 (13%)
26	BCR	K	103	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	2 (3%)
25	CLA	B	610	36	65,73,73	1.50	7 (10%)	76,113,113	1.49	11 (14%)
25	CLA	b	611	-	65,73,73	1.63	7 (10%)	76,113,113	1.43	10 (13%)
21	OEY	a	601[A]	3,36,1	0,16,16	-	-	-		
25	CLA	B	615	-	65,73,73	1.64	7 (10%)	76,113,113	1.50	8 (10%)
25	CLA	A	607	36	65,73,73	1.66	6 (9%)	76,113,113	1.54	14 (18%)
25	CLA	B	609	-	65,73,73	1.52	9 (13%)	76,113,113	1.46	6 (7%)
27	PL9	A	610	-	55,55,55	0.71	1 (1%)	68,69,69	1.52	9 (13%)
32	STE	b	623	-	15,15,19	0.66	0	15,15,19	1.12	0
28	LMG	A	612	-	48,48,55	0.70	0	56,56,63	1.36	6 (10%)
25	CLA	a	608	-	65,73,73	1.55	7 (10%)	76,113,113	1.31	7 (9%)
32	STE	A	617	-	19,19,19	0.61	0	19,19,19	0.96	0
32	STE	D	413	-	19,19,19	0.58	0	19,19,19	1.14	0
25	CLA	b	602	-	65,73,73	1.50	6 (9%)	76,113,113	1.48	11 (14%)
29	SQD	a	613	-	35,35,54	1.68	5 (14%)	37,37,65	1.36	2 (5%)
32	STE	H	103	-	17,17,19	0.35	0	16,16,19	0.80	0
33	PHO	D	402	-	51,69,69	0.94	1 (1%)	47,99,99	1.48	6 (12%)
26	BCR	B	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.36	6 (10%)
25	CLA	c	513	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	6 (7%)
25	CLA	C	501	-	65,73,73	1.77	9 (13%)	76,113,113	1.51	9 (11%)
25	CLA	b	601	36	65,73,73	1.69	7 (10%)	76,113,113	1.51	12 (15%)
27	PL9	d	406	-	55,55,55	0.87	1 (1%)	68,69,69	1.62	16 (23%)
25	CLA	C	502	-	65,73,73	1.40	6 (9%)	76,113,113	1.38	7 (9%)
32	STE	L	102	-	11,11,19	0.66	0	11,11,19	1.19	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	K	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	9 (16%)
30	LHG	d	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.12	3 (7%)
31	DGD	c	516	-	63,63,67	1.03	7 (11%)	77,77,81	1.46	15 (19%)
32	STE	t	103	-	9,9,19	0.32	0	8,8,19	0.83	0
30	LHG	l	101	-	48,48,48	0.81	2 (4%)	51,54,54	1.22	4 (7%)
25	CLA	a	611	36	65,73,73	1.53	7 (10%)	76,113,113	1.56	12 (15%)
28	LMG	D	411	-	31,31,55	0.69	1 (3%)	33,33,63	1.23	2 (6%)
29	SQD	D	408	-	35,36,54	1.51	6 (17%)	42,45,65	1.90	11 (26%)
30	LHG	d	408	-	48,48,48	0.67	0	51,54,54	1.24	6 (11%)
32	STE	a	615	-	11,11,19	0.78	0	11,11,19	1.01	0
32	STE	c	519	-	19,19,19	0.63	0	19,19,19	0.90	0
25	CLA	D	404	-	65,73,73	1.56	8 (12%)	76,113,113	1.33	8 (10%)
21	OEY	A	601[A]	3,36,1	0,16,16	-	-	-	-	-
32	STE	E	102	-	11,11,19	0.75	0	11,11,19	1.13	1 (9%)
32	STE	b	625	-	9,9,19	0.39	0	8,8,19	0.63	0
31	DGD	c	515	-	63,63,67	0.99	5 (7%)	77,77,81	1.41	11 (14%)
32	STE	k	104	-	11,11,19	0.74	0	11,11,19	1.08	0
25	CLA	C	510	-	65,73,73	1.48	8 (12%)	76,113,113	1.63	10 (13%)
31	DGD	a	614	-	43,43,67	0.68	2 (4%)	45,45,81	1.40	6 (13%)
25	CLA	B	604	-	65,73,73	1.70	6 (9%)	76,113,113	1.64	8 (10%)
25	CLA	b	614	-	65,73,73	1.70	7 (10%)	76,113,113	1.44	14 (18%)
26	BCR	A	609	-	41,41,41	0.91	1 (2%)	56,56,56	1.20	5 (8%)
29	SQD	A	615	-	38,38,54	1.71	5 (13%)	40,40,65	1.13	2 (5%)
32	STE	C	520	-	15,15,19	0.37	0	14,14,19	0.80	0
25	CLA	c	510	-	65,73,73	1.60	6 (9%)	76,113,113	1.39	7 (9%)
32	STE	j	101	-	11,11,19	0.72	0	11,11,19	1.19	1 (9%)
25	CLA	c	505	-	65,73,73	1.59	8 (12%)	76,113,113	1.40	10 (13%)
25	CLA	B	602	-	65,73,73	1.52	6 (9%)	76,113,113	1.53	10 (13%)
28	LMG	m	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.39	9 (15%)
35	HEC	V	201	16	32,50,50	2.04	3 (9%)	24,82,82	1.95	7 (29%)
32	STE	d	412	-	16,16,19	0.64	0	16,16,19	1.11	0
25	CLA	c	512	-	65,73,73	1.62	9 (13%)	76,113,113	1.43	8 (10%)
25	CLA	b	607	36	65,73,73	1.39	6 (9%)	76,113,113	1.42	9 (11%)
28	LMG	c	520	-	48,48,55	0.82	1 (2%)	56,56,63	1.39	9 (16%)
26	BCR	D	405	-	41,41,41	0.97	2 (4%)	56,56,56	1.23	5 (8%)
25	CLA	D	403	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C	506	-	65,73,73	1.57	7 (10%)	76,113,113	1.43	6 (7%)
32	STE	m	102	-	17,17,19	0.35	0	16,16,19	0.90	0
25	CLA	b	612	-	65,73,73	1.36	6 (9%)	76,113,113	1.53	12 (15%)
30	LHG	D	410	-	46,46,48	0.81	3 (6%)	49,52,54	1.25	6 (12%)
27	PL9	D	406	-	55,55,55	0.95	3 (5%)	68,69,69	1.52	15 (22%)

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
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
25	CLA	b	615	-	1/1/15/20	10/37/115/115	-
28	LMG	d	411	-	-	15/39/59/70	0/1/1/1
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
25	CLA	A	606	-	1/1/15/20	5/37/115/115	-
25	CLA	b	604	-	1/1/15/20	8/37/115/115	-
28	LMG	B	620	-	-	13/46/66/70	0/1/1/1
25	CLA	B	608	-	1/1/15/20	1/37/115/115	-
32	STE	M	102	-	-	2/7/7/17	-
26	BCR	k	103	-	-	5/29/63/63	0/2/2/2
26	BCR	b	618	-	-	6/29/63/63	0/2/2/2
27	PL9	a	610	-	-	17/53/73/73	0/1/1/1
30	LHG	A	614	-	-	26/53/53/53	-
32	STE	t	102	-	-	7/11/11/17	-
30	LHG	d	407	-	-	15/53/53/53	-
33	PHO	D	401	-	-	6/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/14/20	12/31/109/115	-
26	BCR	a	609	-	-	1/29/63/63	0/2/2/2
32	STE	J	102	-	-	3/9/9/17	-
25	CLA	B	601	36	1/1/15/20	21/37/115/115	-
29	SQD	f	102	-	-	14/36/56/69	0/1/1/1
32	STE	B	624	-	-	5/9/9/17	-
25	CLA	C	512	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	102	-	-	8/29/63/63	0/2/2/2
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
33	PHO	d	402	-	-	11/37/103/103	0/5/6/6
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
33	PHO	a	607	-	-	4/37/103/103	0/5/6/6
29	SQD	b	620	-	-	22/44/64/69	0/1/1/1
30	LHG	D	412	-	-	14/53/53/53	-
34	HEM	E	101	5,6	-	1/12/54/54	-
32	STE	T	102	-	-	8/13/13/17	-
30	LHG	e	101	-	-	22/46/46/53	-
35	HEC	v	201	16	-	2/10/54/54	-
25	CLA	c	502	-	1/1/15/20	9/37/115/115	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
30	LHG	L	101	-	-	16/53/53/53	-
25	CLA	c	501	-	1/1/15/20	4/37/115/115	-
26	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	b	609	-	-	12/37/115/115	-
25	CLA	b	610	36	1/1/15/20	8/37/115/115	-
32	STE	b	624	-	-	10/12/12/17	-
31	DGD	c	517	-	-	22/51/91/95	0/2/2/2
26	BCR	h	101	-	-	8/29/63/63	0/2/2/2
32	STE	C	519	-	-	5/9/9/17	-
32	STE	B	626	-	-	3/9/9/17	-
29	SQD	A	613	-	-	20/47/67/69	0/1/1/1
25	CLA	C	507	36	1/1/15/20	9/37/115/115	-
31	DGD	C	515	-	-	18/51/91/95	0/2/2/2
25	CLA	c	508	-	-	10/36/114/115	-
32	STE	B	621	-	-	6/14/14/17	-
28	LMG	c	518	-	-	13/31/51/70	0/1/1/1
25	CLA	A	611	36	1/1/15/20	6/37/115/115	-
34	HEM	f	101	5,6	-	2/12/54/54	-
25	CLA	C	511	3	1/1/15/20	7/37/115/115	-
25	CLA	b	603	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	B	623	-	-	25/49/69/69	0/1/1/1
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	511	3	1/1/15/20	6/37/115/115	-
28	LMG	C	517	-	-	19/43/63/70	0/1/1/1
28	LMG	d	410	-	-	11/17/17/70	-
32	STE	C	518	-	-	5/9/9/17	-
25	CLA	C	503	-	-	8/37/115/115	-
25	CLA	B	606	-	1/1/15/20	14/37/115/115	-
25	CLA	C	504	36	1/1/13/20	7/30/108/115	-
25	CLA	d	404	-	1/1/15/20	8/37/115/115	-
28	LMG	B	622	-	-	12/22/22/70	-
26	BCR	C	514	-	-	3/29/63/63	0/2/2/2
32	STE	I	101	-	-	4/12/12/17	-
25	CLA	a	606	36	1/1/15/20	10/37/115/115	-
25	CLA	C	508	-	-	8/37/115/115	-
25	CLA	C	509	-	1/1/15/20	11/37/115/115	-
25	CLA	A	608	-	1/1/12/20	5/24/102/115	-
25	CLA	B	603	-	1/1/15/20	10/37/115/115	-
26	BCR	t	101	-	-	5/29/63/63	0/2/2/2
25	CLA	c	506	-	1/1/15/20	12/37/115/115	-
25	CLA	c	507	36	1/1/15/20	8/37/115/115	-
25	CLA	B	613	-	1/1/15/20	13/37/115/115	-
28	LMG	D	407	-	-	20/46/66/70	0/1/1/1
25	CLA	B	611	-	1/1/15/20	2/37/115/115	-
32	STE	B	625	-	-	5/15/15/17	-
25	CLA	B	605	-	1/1/15/20	11/37/115/115	-
25	CLA	b	605	-	1/1/15/20	8/37/115/115	-
31	DGD	J	101	-	-	14/51/91/95	0/2/2/2
32	STE	M	101	-	-	4/12/12/17	-
31	DGD	C	516	-	-	17/51/91/95	0/2/2/2
31	DGD	h	102	-	-	16/51/91/95	0/2/2/2
25	CLA	B	614	-	1/1/15/20	18/37/115/115	-
25	CLA	b	616	-	1/1/14/20	5/31/109/115	-
32	STE	B	627	-	-	7/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	505	-	1/1/15/20	6/37/115/115	-
25	CLA	b	613	-	1/1/15/20	8/37/115/115	-
25	CLA	c	503	-	1/1/15/20	13/37/115/115	-
32	STE	b	621	-	-	11/17/17/17	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	CLA	d	403	-	1/1/15/20	10/37/115/115	-
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	CLA	b	608	-	1/1/15/20	5/37/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2
28	LMG	c	521	-	-	27/44/64/70	0/1/1/1
25	CLA	B	607	36	1/1/15/20	11/37/115/115	-
25	CLA	b	606	-	1/1/15/20	12/37/115/115	-
28	LMG	b	622	-	-	26/50/70/70	0/1/1/1
26	BCR	d	405	-	-	7/29/63/63	0/2/2/2
29	SQD	a	612	-	-	29/49/69/69	0/1/1/1
32	STE	d	413	-	-	11/17/17/17	-
25	CLA	B	612	-	1/1/15/20	12/37/115/115	-
30	LHG	D	409	-	-	23/53/53/53	-
25	CLA	a	605	-	1/1/15/20	2/37/115/115	-
25	CLA	C	513	-	1/1/15/20	13/37/115/115	-
25	CLA	c	504	36	1/1/14/20	10/31/109/115	-
26	BCR	K	103	-	-	9/29/63/63	0/2/2/2
25	CLA	B	610	36	1/1/15/20	8/37/115/115	-
25	CLA	b	611	-	1/1/15/20	9/37/115/115	-
25	CLA	B	615	-	1/1/15/20	7/37/115/115	-
25	CLA	A	607	36	1/1/15/20	10/37/115/115	-
25	CLA	B	609	-	-	6/37/115/115	-
27	PL9	A	610	-	-	20/53/73/73	0/1/1/1
32	STE	b	623	-	-	9/13/13/17	-
28	LMG	A	612	-	-	20/43/63/70	0/1/1/1
25	CLA	a	608	-	1/1/15/20	11/37/115/115	-
32	STE	A	617	-	-	10/17/17/17	-
32	STE	D	413	-	-	12/17/17/17	-
25	CLA	b	602	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	613	-	-	22/37/37/69	-
32	STE	H	103	-	-	11/15/15/17	-
33	PHO	D	402	-	-	2/37/103/103	0/5/6/6
26	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	CLA	c	513	-	1/1/15/20	12/37/115/115	-
25	CLA	C	501	-	1/1/15/20	3/37/115/115	-
25	CLA	b	601	36	1/1/15/20	15/37/115/115	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	C	502	-	1/1/15/20	7/37/115/115	-
32	STE	L	102	-	-	4/9/9/17	-
26	BCR	K	101	-	-	12/29/63/63	0/2/2/2
30	LHG	d	409	-	-	13/43/43/53	-
31	DGD	c	516	-	-	24/51/91/95	0/2/2/2
32	STE	t	103	-	-	5/7/7/17	-
30	LHG	l	101	-	-	16/53/53/53	-
25	CLA	a	611	36	1/1/15/20	5/37/115/115	-
28	LMG	D	411	-	-	13/33/33/70	-
29	SQD	D	408	-	-	16/28/48/69	0/1/1/1
30	LHG	d	408	-	-	20/53/53/53	-
32	STE	a	615	-	-	5/9/9/17	-
32	STE	c	519	-	-	11/17/17/17	-
25	CLA	D	404	-	1/1/15/20	10/37/115/115	-
32	STE	E	102	-	-	5/9/9/17	-
32	STE	b	625	-	-	4/7/7/17	-
31	DGD	c	515	-	-	27/51/91/95	0/2/2/2
32	STE	k	104	-	-	4/9/9/17	-
25	CLA	C	510	-	1/1/15/20	8/37/115/115	-
31	DGD	a	614	-	-	27/45/45/95	-
25	CLA	B	604	-	1/1/15/20	14/37/115/115	-
25	CLA	b	614	-	1/1/15/20	15/37/115/115	-
26	BCR	A	609	-	-	4/29/63/63	0/2/2/2
29	SQD	A	615	-	-	15/39/39/69	-
32	STE	C	520	-	-	5/13/13/17	-
25	CLA	c	510	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	c	505	-	1/1/15/20	9/37/115/115	-
25	CLA	B	602	-	1/1/15/20	10/37/115/115	-
28	LMG	m	101	-	-	24/46/66/70	0/1/1/1
35	HEC	V	201	16	-	2/10/54/54	-
32	STE	d	412	-	-	8/14/14/17	-
25	CLA	c	512	-	1/1/15/20	16/37/115/115	-
25	CLA	b	607	36	1/1/15/20	13/37/115/115	-
28	LMG	c	520	-	-	20/43/63/70	0/1/1/1
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
25	CLA	D	403	-	-	7/37/115/115	-
25	CLA	C	506	-	1/1/15/20	14/37/115/115	-
32	STE	m	102	-	-	8/15/15/17	-
25	CLA	b	612	-	1/1/15/20	13/37/115/115	-
30	LHG	D	410	-	-	22/51/51/53	-
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1

All (733) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	C4B-NB	8.46	1.42	1.35
25	B	614	CLA	C4B-NB	8.39	1.42	1.35
25	B	610	CLA	C4B-NB	8.35	1.42	1.35
25	B	601	CLA	C4B-NB	8.28	1.42	1.35
25	b	605	CLA	C4B-NB	8.10	1.42	1.35
25	b	614	CLA	C4B-NB	8.09	1.42	1.35
25	B	602	CLA	C4B-NB	8.08	1.42	1.35
25	A	607	CLA	C4B-NB	8.06	1.42	1.35
25	B	615	CLA	C4B-NB	8.05	1.42	1.35
25	B	606	CLA	C4B-NB	8.05	1.42	1.35
25	c	504	CLA	C4B-NB	7.97	1.42	1.35
25	c	512	CLA	C4B-NB	7.92	1.42	1.35
25	b	601	CLA	C4B-NB	7.91	1.42	1.35
25	c	505	CLA	C4B-NB	7.84	1.42	1.35
25	b	609	CLA	C4B-NB	7.77	1.42	1.35
25	C	506	CLA	C4B-NB	7.73	1.42	1.35
25	C	501	CLA	C4B-NB	7.67	1.42	1.35
25	D	404	CLA	C4B-NB	7.54	1.41	1.35
25	c	508	CLA	C4B-NB	7.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C4B-NB	7.51	1.41	1.35
25	a	606	CLA	C4B-NB	7.48	1.41	1.35
25	a	608	CLA	C4B-NB	7.47	1.41	1.35
25	d	404	CLA	C4B-NB	7.46	1.41	1.35
25	c	511	CLA	C4B-NB	7.41	1.41	1.35
25	b	615	CLA	C4B-NB	7.39	1.41	1.35
25	A	608	CLA	C4B-NB	7.34	1.41	1.35
25	b	608	CLA	C4B-NB	7.31	1.41	1.35
25	A	606	CLA	C4B-NB	7.29	1.41	1.35
25	c	503	CLA	C4B-NB	7.27	1.41	1.35
25	b	603	CLA	C4B-NB	7.25	1.41	1.35
25	C	509	CLA	C4B-NB	7.24	1.41	1.35
25	D	403	CLA	C4B-NB	7.24	1.41	1.35
25	B	608	CLA	C4B-NB	7.13	1.41	1.35
25	b	602	CLA	C4B-NB	7.12	1.41	1.35
25	B	612	CLA	C4B-NB	7.11	1.41	1.35
25	C	511	CLA	C4B-NB	7.10	1.41	1.35
25	c	513	CLA	C4B-NB	7.09	1.41	1.35
25	d	403	CLA	C4B-NB	7.08	1.41	1.35
25	C	513	CLA	C4B-NB	7.08	1.41	1.35
25	c	509	CLA	C4B-NB	7.05	1.41	1.35
25	C	508	CLA	C4B-NB	7.05	1.41	1.35
25	c	511	CLA	MG-NA	7.01	2.22	2.06
25	c	507	CLA	C4B-NB	7.01	1.41	1.35
25	C	512	CLA	C4B-NB	6.99	1.41	1.35
25	c	510	CLA	C4B-NB	6.95	1.41	1.35
25	C	501	CLA	MG-NA	6.92	2.22	2.06
25	B	605	CLA	C4B-NB	6.92	1.41	1.35
25	b	613	CLA	C4B-NB	6.91	1.41	1.35
25	C	503	CLA	C4B-NB	6.90	1.41	1.35
25	c	501	CLA	C4B-NB	6.89	1.41	1.35
25	b	615	CLA	MG-NA	6.89	2.22	2.06
25	C	505	CLA	C4B-NB	6.88	1.41	1.35
25	a	605	CLA	C4B-NB	6.87	1.41	1.35
25	b	611	CLA	C4B-NB	6.82	1.41	1.35
25	B	603	CLA	C4B-NB	6.81	1.41	1.35
25	b	616	CLA	C4B-NB	6.76	1.41	1.35
25	B	616	CLA	C4B-NB	6.72	1.41	1.35
25	b	607	CLA	C4B-NB	6.65	1.41	1.35
25	b	606	CLA	C4B-NB	6.61	1.41	1.35
25	B	613	CLA	C4B-NB	6.60	1.41	1.35
25	c	502	CLA	C4B-NB	6.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	MG-NA	6.48	2.21	2.06
25	B	604	CLA	C4B-NB	6.45	1.41	1.35
25	C	510	CLA	C4B-NB	6.33	1.40	1.35
25	a	611	CLA	MG-NA	6.31	2.21	2.06
25	B	606	CLA	MG-NA	6.30	2.21	2.06
25	B	611	CLA	C4B-NB	6.28	1.40	1.35
25	C	502	CLA	C4B-NB	6.28	1.40	1.35
25	B	609	CLA	C4B-NB	6.27	1.40	1.35
25	b	604	CLA	C4B-NB	6.26	1.40	1.35
25	B	604	CLA	MG-NA	6.17	2.20	2.06
25	C	507	CLA	C4B-NB	6.17	1.40	1.35
25	B	603	CLA	MG-NA	6.15	2.20	2.06
25	b	610	CLA	C4B-NB	6.10	1.40	1.35
35	v	201	HEC	C2B-C3B	-6.06	1.34	1.40
25	b	612	CLA	C4B-NB	5.84	1.40	1.35
35	V	201	HEC	C2B-C3B	-5.83	1.34	1.40
35	v	201	HEC	C3C-C2C	-5.81	1.34	1.40
25	b	614	CLA	MG-NA	5.81	2.20	2.06
25	c	510	CLA	MG-NA	5.64	2.19	2.06
25	b	601	CLA	MG-NA	5.56	2.19	2.06
25	B	613	CLA	MG-NC	5.56	2.19	2.06
25	C	513	CLA	MG-NA	5.55	2.19	2.06
25	A	611	CLA	C4B-NB	5.51	1.40	1.35
25	B	607	CLA	C4B-NB	5.43	1.40	1.35
25	a	611	CLA	C4B-NB	5.41	1.40	1.35
35	v	201	HEC	C3D-C2D	5.40	1.53	1.37
25	b	606	CLA	MG-NA	5.38	2.19	2.06
29	A	615	SQD	O47-C45	-5.32	1.37	1.47
25	C	512	CLA	MG-NA	5.32	2.18	2.06
25	A	607	CLA	MG-NA	5.31	2.18	2.06
35	V	201	HEC	C3C-C2C	-5.25	1.35	1.40
25	C	511	CLA	MG-NA	5.21	2.18	2.06
29	a	612	SQD	O48-C23	5.03	1.48	1.33
35	V	201	HEC	C3D-C2D	4.96	1.52	1.37
29	b	620	SQD	O48-C23	4.91	1.47	1.33
25	C	507	CLA	MG-NA	4.82	2.17	2.06
25	a	605	CLA	MG-NA	4.77	2.17	2.06
34	E	101	HEM	C3C-C2C	-4.76	1.33	1.40
29	D	408	SQD	O48-C23	4.75	1.47	1.33
25	b	604	CLA	C1D-ND	4.73	1.43	1.37
29	A	615	SQD	O48-C23	4.71	1.47	1.33
25	c	506	CLA	MG-ND	-4.70	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	MG-ND	-4.70	1.96	2.05
29	B	623	SQD	O48-C23	4.69	1.47	1.33
25	b	609	CLA	MG-NA	4.67	2.17	2.06
29	a	613	SQD	O48-C23	4.66	1.47	1.33
25	B	604	CLA	C1D-ND	4.66	1.43	1.37
29	f	102	SQD	O48-C23	4.60	1.46	1.33
25	b	603	CLA	MG-NA	4.56	2.17	2.06
25	B	601	CLA	MG-NA	4.51	2.17	2.06
25	B	615	CLA	MG-NA	4.47	2.16	2.06
29	A	613	SQD	O48-C23	4.43	1.46	1.33
25	a	605	CLA	C1D-ND	4.43	1.43	1.37
25	C	501	CLA	C1D-ND	4.41	1.43	1.37
25	C	504	CLA	MG-ND	-4.33	1.97	2.05
25	C	503	CLA	MG-NA	4.32	2.16	2.06
25	B	601	CLA	C1D-ND	4.31	1.43	1.37
25	A	606	CLA	MG-NA	4.30	2.16	2.06
25	A	607	CLA	C1D-ND	4.28	1.43	1.37
25	b	608	CLA	MG-NA	4.27	2.16	2.06
25	a	608	CLA	C1D-ND	4.26	1.43	1.37
25	B	613	CLA	C1D-ND	4.25	1.43	1.37
25	D	404	CLA	C1D-ND	4.23	1.43	1.37
25	b	613	CLA	MG-NA	4.21	2.16	2.06
25	B	609	CLA	MG-NC	4.21	2.16	2.06
25	B	614	CLA	C1D-ND	4.21	1.43	1.37
25	B	616	CLA	C1D-ND	4.20	1.42	1.37
25	B	614	CLA	MG-ND	-4.17	1.97	2.05
25	c	507	CLA	MG-NA	4.15	2.16	2.06
25	b	612	CLA	C1D-ND	4.15	1.42	1.37
25	B	609	CLA	C1D-ND	4.12	1.42	1.37
25	A	606	CLA	C1D-ND	4.11	1.42	1.37
25	b	614	CLA	C1D-ND	4.06	1.42	1.37
25	B	613	CLA	MG-ND	-4.06	1.97	2.05
25	c	511	CLA	C1D-ND	4.06	1.42	1.37
25	A	611	CLA	C1D-ND	4.05	1.42	1.37
25	c	512	CLA	C1D-ND	4.04	1.42	1.37
25	B	604	CLA	MG-NC	4.01	2.15	2.06
25	b	610	CLA	C1D-ND	4.01	1.42	1.37
25	B	612	CLA	MG-ND	-3.98	1.97	2.05
25	C	511	CLA	C1D-ND	3.98	1.42	1.37
25	c	506	CLA	MG-NC	3.98	2.15	2.06
25	B	605	CLA	C1D-ND	3.98	1.42	1.37
25	B	614	CLA	MG-NC	3.97	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	605	CLA	CHC-C1C	3.95	1.45	1.35
25	D	403	CLA	MG-NC	3.95	2.15	2.06
25	c	501	CLA	C1D-ND	3.95	1.42	1.37
25	c	504	CLA	MG-ND	-3.92	1.98	2.05
34	f	101	HEM	C3C-CAC	3.92	1.55	1.47
25	b	605	CLA	CHC-C1C	3.91	1.45	1.35
25	b	604	CLA	MG-ND	-3.90	1.98	2.05
25	C	513	CLA	MG-ND	3.90	2.13	2.05
25	c	503	CLA	C1D-ND	3.90	1.42	1.37
25	B	602	CLA	C1D-ND	3.89	1.42	1.37
25	c	508	CLA	MG-NA	3.88	2.15	2.06
25	b	602	CLA	C1D-ND	3.87	1.42	1.37
25	b	613	CLA	C1D-ND	3.86	1.42	1.37
25	c	504	CLA	MG-NC	3.85	2.15	2.06
25	c	509	CLA	C1D-ND	3.84	1.42	1.37
25	C	505	CLA	C1D-ND	3.83	1.42	1.37
25	C	508	CLA	MG-NA	3.81	2.15	2.06
25	C	503	CLA	MG-ND	3.79	2.13	2.05
25	c	507	CLA	C1D-ND	3.79	1.42	1.37
25	c	505	CLA	C4D-ND	-3.78	1.32	1.37
25	B	606	CLA	C1D-ND	3.77	1.42	1.37
25	C	506	CLA	C1D-ND	3.76	1.42	1.37
25	a	606	CLA	C1D-ND	3.76	1.42	1.37
25	b	605	CLA	C4D-ND	-3.75	1.32	1.37
25	b	606	CLA	C1D-ND	3.75	1.42	1.37
34	E	101	HEM	C3C-CAC	3.74	1.55	1.47
25	b	601	CLA	C1D-ND	3.73	1.42	1.37
25	a	608	CLA	MG-ND	-3.73	1.98	2.05
25	B	611	CLA	MG-NA	3.72	2.15	2.06
25	c	513	CLA	C1D-ND	3.72	1.42	1.37
25	d	404	CLA	C1D-ND	3.72	1.42	1.37
25	B	615	CLA	C1D-ND	3.71	1.42	1.37
25	C	513	CLA	C1D-ND	3.71	1.42	1.37
25	B	603	CLA	C1D-ND	3.71	1.42	1.37
25	c	508	CLA	CHC-C1C	3.70	1.44	1.35
25	a	611	CLA	C1D-ND	3.69	1.42	1.37
25	b	614	CLA	CHC-C1C	3.68	1.44	1.35
25	a	605	CLA	MG-NC	3.68	2.15	2.06
25	B	608	CLA	MG-NA	3.68	2.15	2.06
29	A	613	SQD	O47-C45	-3.67	1.37	1.46
25	C	504	CLA	C1D-ND	3.67	1.42	1.37
25	b	615	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	503	CLA	MG-NC	3.65	2.14	2.06
25	C	512	CLA	C1D-ND	3.65	1.42	1.37
25	B	605	CLA	CHC-C1C	3.64	1.44	1.35
25	b	616	CLA	C1D-ND	3.64	1.42	1.37
25	d	403	CLA	C1D-ND	3.63	1.42	1.37
25	b	616	CLA	MG-ND	3.63	2.13	2.05
25	c	510	CLA	C1D-ND	3.62	1.42	1.37
25	C	508	CLA	C1D-ND	3.61	1.42	1.37
25	b	609	CLA	C1D-ND	3.61	1.42	1.37
25	C	510	CLA	MG-NA	3.60	2.14	2.06
25	b	616	CLA	C4D-ND	-3.58	1.32	1.37
25	A	608	CLA	C4D-ND	-3.57	1.32	1.37
29	b	620	SQD	O47-C7	3.57	1.44	1.34
25	C	505	CLA	CHC-C1C	3.57	1.44	1.35
30	D	412	LHG	O7-C5	-3.57	1.37	1.46
25	A	611	CLA	MG-NA	3.56	2.14	2.06
29	A	615	SQD	O47-C7	3.56	1.44	1.34
25	b	603	CLA	C1D-ND	3.55	1.42	1.37
25	c	502	CLA	C4D-ND	-3.55	1.32	1.37
25	c	505	CLA	CHC-C1C	3.54	1.44	1.35
29	B	623	SQD	O47-C7	3.54	1.44	1.34
25	a	606	CLA	C4D-ND	-3.53	1.32	1.37
25	C	509	CLA	C1D-ND	3.52	1.42	1.37
26	B	618	BCR	C30-C25	-3.52	1.48	1.53
25	C	502	CLA	C4D-ND	-3.51	1.32	1.37
25	c	510	CLA	CHC-C1C	3.51	1.44	1.35
25	C	510	CLA	C4D-ND	-3.51	1.32	1.37
25	B	615	CLA	C4D-ND	-3.51	1.32	1.37
25	C	501	CLA	CHC-C1C	3.51	1.44	1.35
25	C	506	CLA	CHC-C1C	3.50	1.43	1.35
29	f	102	SQD	O47-C7	3.49	1.44	1.34
25	c	502	CLA	C1D-ND	3.49	1.42	1.37
25	c	503	CLA	MG-NA	3.48	2.14	2.06
34	f	101	HEM	C3C-C2C	-3.48	1.35	1.40
25	c	513	CLA	CHC-C1C	3.45	1.43	1.35
26	k	101	BCR	C30-C25	-3.45	1.49	1.53
25	B	607	CLA	C1D-ND	3.45	1.42	1.37
25	c	506	CLA	C1D-ND	3.44	1.42	1.37
25	b	604	CLA	C4D-ND	-3.44	1.33	1.37
25	b	602	CLA	MG-NC	3.44	2.14	2.06
25	c	506	CLA	CHC-C1C	3.43	1.43	1.35
25	a	606	CLA	CHC-C1C	3.43	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	CHC-C1C	3.42	1.43	1.35
25	c	511	CLA	CHC-C1C	3.42	1.43	1.35
25	b	601	CLA	CHC-C1C	3.41	1.43	1.35
25	c	512	CLA	MG-NC	3.41	2.14	2.06
25	B	614	CLA	CHC-C1C	3.41	1.43	1.35
25	c	508	CLA	C1D-ND	3.40	1.42	1.37
29	D	408	SQD	C24-C23	3.40	1.60	1.50
29	a	612	SQD	O47-C7	3.39	1.43	1.34
25	d	403	CLA	MG-NC	3.39	2.14	2.06
29	a	612	SQD	O47-C45	-3.39	1.38	1.46
25	b	611	CLA	C1D-ND	3.39	1.41	1.37
25	C	512	CLA	CHC-C1C	3.38	1.43	1.35
25	C	504	CLA	CHC-C1C	3.37	1.43	1.35
26	K	102	BCR	C1-C6	-3.37	1.49	1.53
30	D	410	LHG	P-O6	3.36	1.72	1.59
25	B	611	CLA	C1D-ND	3.36	1.41	1.37
25	A	606	CLA	CHC-C1C	3.35	1.43	1.35
26	c	514	BCR	C1-C6	-3.35	1.49	1.53
25	c	504	CLA	C4D-ND	-3.35	1.33	1.37
26	C	514	BCR	C1-C6	-3.35	1.49	1.53
25	A	608	CLA	CHC-C1C	3.33	1.43	1.35
25	B	612	CLA	C1D-ND	3.31	1.41	1.37
31	H	102	DGD	O5D-C1E	3.31	1.45	1.40
29	b	620	SQD	O5-C1	3.31	1.50	1.41
29	a	613	SQD	O47-C7	3.31	1.43	1.34
25	b	608	CLA	C1D-ND	3.30	1.41	1.37
25	B	608	CLA	C1D-ND	3.30	1.41	1.37
25	C	503	CLA	CHC-C1C	3.29	1.43	1.35
25	C	504	CLA	MG-NA	3.29	2.14	2.06
29	a	613	SQD	O47-C45	-3.29	1.38	1.46
25	c	512	CLA	CHC-C1C	3.29	1.43	1.35
26	b	618	BCR	C30-C25	-3.29	1.49	1.53
25	b	612	CLA	CHC-C1C	3.28	1.43	1.35
25	A	611	CLA	CHC-C1C	3.26	1.43	1.35
25	c	505	CLA	MG-NC	3.24	2.14	2.06
25	B	604	CLA	CHC-C1C	3.23	1.43	1.35
25	B	607	CLA	C4D-ND	-3.23	1.33	1.37
25	b	602	CLA	C4D-ND	-3.23	1.33	1.37
25	C	507	CLA	CHC-C1C	3.22	1.43	1.35
25	c	508	CLA	C4D-ND	-3.21	1.33	1.37
25	B	605	CLA	C4D-ND	-3.21	1.33	1.37
25	c	503	CLA	CHC-C1C	3.21	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	C1D-ND	3.21	1.41	1.37
25	B	606	CLA	CHC-C1C	3.20	1.43	1.35
25	B	601	CLA	CHC-C1C	3.20	1.43	1.35
25	C	503	CLA	C1D-ND	3.20	1.41	1.37
27	D	406	PL9	C6-C1	-3.20	1.42	1.48
25	C	502	CLA	C1D-ND	3.20	1.41	1.37
25	C	511	CLA	CHC-C1C	3.19	1.43	1.35
26	K	103	BCR	C1-C6	-3.19	1.49	1.53
25	a	611	CLA	CHC-C1C	3.18	1.43	1.35
29	a	612	SQD	C24-C23	3.18	1.60	1.50
29	A	613	SQD	O47-C7	3.18	1.43	1.34
25	C	508	CLA	CHC-C1C	3.17	1.43	1.35
25	B	615	CLA	CHC-C1C	3.17	1.43	1.35
25	C	505	CLA	C4D-ND	-3.17	1.33	1.37
25	c	504	CLA	C1D-ND	3.16	1.41	1.37
25	b	604	CLA	MG-NA	3.16	2.13	2.06
25	B	608	CLA	C4D-ND	-3.16	1.33	1.37
25	d	403	CLA	CHC-C1C	3.16	1.43	1.35
25	D	403	CLA	CHC-C1C	3.15	1.43	1.35
29	f	102	SQD	O47-C45	-3.15	1.38	1.46
26	b	617	BCR	C1-C6	-3.14	1.49	1.53
25	B	607	CLA	MG-ND	-3.14	1.99	2.05
25	b	607	CLA	C1D-ND	3.14	1.41	1.37
29	a	613	SQD	C24-C23	3.14	1.59	1.50
25	a	608	CLA	C4D-ND	-3.14	1.33	1.37
29	A	615	SQD	C24-C23	3.14	1.59	1.50
25	b	613	CLA	CHC-C1C	3.14	1.43	1.35
29	B	623	SQD	O47-C45	-3.13	1.38	1.46
25	C	513	CLA	C4D-ND	-3.13	1.33	1.37
26	k	103	BCR	C1-C6	-3.12	1.49	1.53
25	c	505	CLA	C1D-ND	3.12	1.41	1.37
25	b	609	CLA	CHC-C1C	3.12	1.43	1.35
25	D	404	CLA	C4D-ND	-3.12	1.33	1.37
25	c	502	CLA	MG-NA	3.12	2.13	2.06
25	C	513	CLA	CHC-C1C	3.11	1.42	1.35
25	C	510	CLA	C1D-ND	3.11	1.41	1.37
25	b	607	CLA	C4D-ND	-3.11	1.33	1.37
25	b	602	CLA	CHC-C1C	3.10	1.42	1.35
25	C	505	CLA	MG-NA	3.10	2.13	2.06
25	d	404	CLA	MG-NC	3.10	2.13	2.06
25	c	503	CLA	MG-NC	3.09	2.13	2.06
25	B	612	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	CHC-C1C	3.08	1.42	1.35
25	B	613	CLA	C4D-ND	-3.08	1.33	1.37
25	B	610	CLA	CHC-C1C	3.08	1.42	1.35
29	A	613	SQD	O5-C1	3.07	1.49	1.41
25	c	509	CLA	CHC-C1C	3.07	1.42	1.35
31	c	517	DGD	C4D-C5D	3.07	1.59	1.53
25	B	611	CLA	CHC-C1C	3.06	1.42	1.35
25	b	609	CLA	C4D-ND	-3.06	1.33	1.37
25	b	610	CLA	C4D-ND	-3.06	1.33	1.37
29	A	613	SQD	C24-C23	3.06	1.59	1.50
25	D	403	CLA	C1D-ND	3.05	1.41	1.37
25	B	609	CLA	C4D-ND	-3.05	1.33	1.37
25	b	611	CLA	CHC-C1C	3.05	1.42	1.35
25	C	507	CLA	C1D-ND	3.05	1.41	1.37
25	D	403	CLA	C4D-ND	-3.05	1.33	1.37
25	c	504	CLA	CHC-C1C	3.04	1.42	1.35
25	A	606	CLA	C4D-ND	-3.04	1.33	1.37
26	d	405	BCR	C30-C25	-3.03	1.49	1.53
25	c	509	CLA	MG-NA	3.03	2.13	2.06
31	C	516	DGD	C1E-C2E	3.03	1.61	1.52
26	k	102	BCR	C1-C6	-3.03	1.49	1.53
25	C	509	CLA	C4D-ND	-3.02	1.33	1.37
25	C	503	CLA	C4D-ND	-3.00	1.33	1.37
25	B	602	CLA	CHC-C1C	3.00	1.42	1.35
25	B	616	CLA	C4D-ND	-3.00	1.33	1.37
29	B	623	SQD	O5-C1	3.00	1.49	1.41
25	b	611	CLA	C4D-ND	-3.00	1.33	1.37
25	C	510	CLA	CHC-C1C	2.99	1.42	1.35
25	c	507	CLA	CHC-C1C	2.99	1.42	1.35
25	A	607	CLA	CHC-C1C	2.99	1.42	1.35
25	C	502	CLA	CHC-C1C	2.98	1.42	1.35
25	B	607	CLA	CHC-C1C	2.98	1.42	1.35
25	d	404	CLA	MG-ND	-2.97	1.99	2.05
25	C	511	CLA	C4D-ND	-2.97	1.33	1.37
29	a	612	SQD	O5-C1	2.97	1.49	1.41
26	B	618	BCR	C1-C6	-2.96	1.49	1.53
28	b	622	LMG	C4-C3	2.96	1.59	1.52
26	b	617	BCR	C30-C25	-2.96	1.49	1.53
25	b	603	CLA	CHC-C1C	2.96	1.42	1.35
25	B	608	CLA	CHC-C1C	2.96	1.42	1.35
31	A	616	DGD	C4D-C5D	2.95	1.59	1.53
25	C	512	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	102	SQD	C24-C23	2.94	1.59	1.50
30	A	614	LHG	P-O6	2.94	1.71	1.59
25	b	608	CLA	C4D-ND	-2.93	1.33	1.37
33	a	607	PHO	CAC-C3C	-2.93	1.47	1.52
25	b	604	CLA	CHC-C1C	2.93	1.42	1.35
26	H	101	BCR	C30-C25	-2.93	1.49	1.53
25	C	506	CLA	MG-NC	2.92	2.13	2.06
25	c	513	CLA	C4D-ND	-2.92	1.33	1.37
26	B	617	BCR	C1-C6	-2.92	1.49	1.53
25	b	616	CLA	CHC-C1C	2.92	1.42	1.35
25	A	608	CLA	MG-ND	2.91	2.11	2.05
25	C	508	CLA	C4D-ND	-2.91	1.33	1.37
25	a	605	CLA	C4D-ND	-2.91	1.33	1.37
25	B	616	CLA	MG-NA	2.90	2.13	2.06
28	d	411	LMG	O7-C8	-2.90	1.39	1.46
25	C	509	CLA	CHC-C1C	2.89	1.42	1.35
25	b	607	CLA	CHC-C1C	2.89	1.42	1.35
31	h	102	DGD	C4D-C5D	2.89	1.59	1.53
25	B	612	CLA	C4D-ND	-2.88	1.33	1.37
26	h	101	BCR	C30-C25	-2.88	1.49	1.53
26	K	102	BCR	C30-C25	-2.87	1.49	1.53
25	c	507	CLA	C4D-ND	-2.87	1.33	1.37
25	d	403	CLA	CMB-C2B	-2.87	1.45	1.51
31	c	515	DGD	O2G-C2G	-2.87	1.39	1.46
25	B	616	CLA	CHC-C1C	2.86	1.42	1.35
25	b	601	CLA	MG-ND	2.86	2.11	2.05
29	B	623	SQD	C24-C23	2.85	1.59	1.50
29	b	620	SQD	C24-C23	2.84	1.59	1.50
29	f	102	SQD	O5-C1	2.84	1.49	1.41
25	b	616	CLA	MG-NA	2.83	2.13	2.06
31	C	515	DGD	C4E-C3E	2.83	1.59	1.52
25	A	611	CLA	C4D-ND	-2.83	1.33	1.37
25	b	612	CLA	C4D-ND	-2.83	1.33	1.37
25	b	604	CLA	MG-NC	2.83	2.13	2.06
34	E	101	HEM	CAB-C3B	2.83	1.55	1.47
31	c	515	DGD	O1G-C1G	-2.83	1.38	1.45
25	C	506	CLA	C4D-ND	-2.83	1.33	1.37
25	c	501	CLA	CHC-C1C	2.82	1.42	1.35
30	d	407	LHG	C24-C23	2.82	1.59	1.50
25	b	610	CLA	CHC-C1C	2.81	1.42	1.35
26	K	103	BCR	C30-C25	-2.81	1.49	1.53
25	d	404	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	501	CLA	MG-ND	-2.80	2.00	2.05
25	B	604	CLA	C4D-ND	-2.80	1.33	1.37
25	c	503	CLA	C4D-ND	-2.80	1.33	1.37
26	K	101	BCR	C1-C6	-2.80	1.49	1.53
25	b	606	CLA	CHC-C1C	2.80	1.42	1.35
25	C	507	CLA	C4D-ND	-2.79	1.33	1.37
25	c	502	CLA	CHC-C1C	2.78	1.42	1.35
25	B	603	CLA	CHC-C1C	2.78	1.42	1.35
25	D	404	CLA	MG-NA	2.77	2.12	2.06
25	b	606	CLA	C4D-ND	-2.76	1.33	1.37
26	b	618	BCR	C1-C6	-2.76	1.50	1.53
25	B	614	CLA	C4D-ND	-2.76	1.33	1.37
28	D	407	LMG	C4-C5	2.76	1.58	1.53
25	B	613	CLA	CHC-C1C	2.76	1.42	1.35
26	K	101	BCR	C30-C25	-2.75	1.50	1.53
25	B	603	CLA	C4D-ND	-2.75	1.33	1.37
30	l	101	LHG	O7-C5	-2.75	1.39	1.46
25	c	513	CLA	MG-NA	2.75	2.12	2.06
28	D	407	LMG	O2-C2	-2.75	1.36	1.43
26	k	102	BCR	C30-C25	-2.75	1.50	1.53
25	c	509	CLA	C4D-ND	-2.74	1.33	1.37
25	a	608	CLA	CHC-C1C	2.74	1.42	1.35
25	b	605	CLA	MG-ND	2.74	2.11	2.05
25	c	512	CLA	C4D-ND	-2.74	1.33	1.37
25	B	606	CLA	C3B-C2B	-2.73	1.36	1.40
25	b	603	CLA	C4D-ND	-2.72	1.33	1.37
25	b	605	CLA	C1D-ND	2.72	1.41	1.37
26	A	609	BCR	C1-C6	-2.72	1.50	1.53
29	b	620	SQD	O47-C45	-2.72	1.39	1.46
26	t	101	BCR	C30-C25	-2.72	1.50	1.53
25	c	506	CLA	C4D-ND	-2.71	1.34	1.37
30	l	101	LHG	O8-C23	2.71	1.41	1.33
28	B	620	LMG	C4-C5	2.70	1.58	1.53
26	k	101	BCR	C1-C6	-2.70	1.50	1.53
25	b	613	CLA	C4D-ND	-2.69	1.34	1.37
25	b	608	CLA	CMB-C2B	-2.69	1.46	1.51
25	c	501	CLA	C4D-ND	-2.68	1.34	1.37
25	B	607	CLA	CMB-C2B	-2.68	1.46	1.51
25	B	609	CLA	CHC-C1C	2.68	1.41	1.35
25	c	510	CLA	C4D-ND	-2.68	1.34	1.37
31	C	516	DGD	C1G-C2G	2.67	1.58	1.50
26	D	405	BCR	C30-C25	-2.66	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	MG-NA	2.66	2.12	2.06
31	H	102	DGD	C6D-C5D	2.66	1.59	1.51
28	m	101	LMG	C4-C5	2.65	1.58	1.53
30	d	409	LHG	P-O6	2.65	1.70	1.59
28	c	518	LMG	C4-C5	2.64	1.58	1.53
25	b	614	CLA	C4D-ND	-2.64	1.34	1.37
25	C	506	CLA	MG-NA	2.64	2.12	2.06
25	C	501	CLA	C4D-ND	-2.62	1.34	1.37
34	f	101	HEM	CAB-C3B	2.62	1.54	1.47
26	B	619	BCR	C1-C6	-2.62	1.50	1.53
25	B	615	CLA	CMB-C2B	-2.61	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.61	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.61	1.46	1.51
25	d	403	CLA	C4D-ND	-2.61	1.34	1.37
25	b	610	CLA	C3B-C2B	-2.59	1.36	1.40
25	d	404	CLA	C4D-ND	-2.59	1.34	1.37
25	c	511	CLA	C4D-ND	-2.59	1.34	1.37
25	D	404	CLA	CHC-C1C	2.59	1.41	1.35
26	d	405	BCR	C1-C6	-2.58	1.50	1.53
25	A	607	CLA	C4D-ND	-2.58	1.34	1.37
29	D	408	SQD	O5-C1	2.57	1.48	1.41
33	d	402	PHO	CAC-C3C	-2.57	1.47	1.52
31	h	102	DGD	O2E-C2E	-2.56	1.36	1.43
25	B	601	CLA	CMB-C2B	-2.56	1.46	1.51
31	A	616	DGD	C4D-C3D	2.56	1.58	1.52
25	a	611	CLA	C4D-ND	-2.56	1.34	1.37
25	B	611	CLA	C4D-ND	-2.55	1.34	1.37
31	C	516	DGD	O2G-C2G	-2.55	1.40	1.46
25	c	507	CLA	CMB-C2B	-2.54	1.46	1.51
31	c	517	DGD	C6D-C5D	2.54	1.59	1.51
28	c	520	LMG	C4-C3	2.53	1.58	1.52
26	a	609	BCR	C1-C6	-2.53	1.50	1.53
28	b	622	LMG	C3-C2	2.53	1.58	1.52
26	T	101	BCR	C1-C6	-2.52	1.50	1.53
34	E	101	HEM	FE-NB	2.52	2.09	1.96
25	c	509	CLA	CMB-C2B	-2.52	1.46	1.51
26	T	101	BCR	C30-C25	-2.51	1.50	1.53
28	B	622	LMG	O8-C28	2.51	1.39	1.30
25	B	606	CLA	C4D-ND	-2.51	1.34	1.37
26	b	619	BCR	C1-C6	-2.49	1.50	1.53
26	a	609	BCR	C30-C25	-2.49	1.50	1.53
30	e	101	LHG	P-O6	2.48	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	CMB-C2B	-2.48	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.47	1.46	1.51
33	D	401	PHO	O2D-CGD	2.47	1.39	1.33
25	c	510	CLA	CMB-C2B	-2.47	1.46	1.51
28	b	622	LMG	C9-C8	2.47	1.58	1.50
29	A	615	SQD	C46-C45	2.47	1.56	1.50
25	c	501	CLA	CMB-C2B	-2.47	1.46	1.51
28	B	622	LMG	O7-C10	2.47	1.39	1.30
25	c	508	CLA	MG-NC	2.47	2.12	2.06
25	D	404	CLA	CMB-C2B	-2.46	1.46	1.51
25	C	508	CLA	MG-NC	2.46	2.12	2.06
31	a	614	DGD	O1G-C1A	2.46	1.40	1.33
25	C	508	CLA	C1D-C2D	2.45	1.50	1.45
25	d	404	CLA	CMB-C2B	-2.45	1.46	1.51
28	D	407	LMG	C4-C3	2.45	1.58	1.52
31	A	616	DGD	C3E-C2E	2.44	1.58	1.52
25	C	502	CLA	MG-NA	2.44	2.12	2.06
25	b	615	CLA	C4D-ND	-2.43	1.34	1.37
25	b	616	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.42	1.46	1.51
31	A	616	DGD	C1E-C2E	2.42	1.59	1.52
28	d	411	LMG	C4-C5	2.42	1.58	1.53
25	C	513	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	614	CLA	MG-NA	2.41	2.12	2.06
25	B	603	CLA	C3B-CAB	-2.40	1.43	1.47
25	C	510	CLA	MG-ND	-2.40	2.01	2.05
25	C	511	CLA	MG-NC	2.40	2.12	2.06
34	f	101	HEM	C3B-C2B	-2.40	1.32	1.37
31	A	616	DGD	C3G-C2G	2.40	1.58	1.50
25	B	607	CLA	MG-NA	2.40	2.12	2.06
25	c	501	CLA	MG-NA	2.39	2.12	2.06
25	C	509	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	608	CLA	C1D-ND	2.39	1.40	1.37
25	B	614	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.36	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.36	1.46	1.51
30	D	409	LHG	P-O3	2.36	1.68	1.59
25	b	609	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.36	1.46	1.51
26	c	514	BCR	C30-C25	-2.35	1.50	1.53
25	a	606	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	CMC-C2C	-2.34	1.45	1.50
25	C	512	CLA	MG-ND	-2.34	2.01	2.05
25	D	404	CLA	CMD-C2D	-2.34	1.45	1.50
31	c	515	DGD	C3G-C2G	2.33	1.57	1.50
25	c	512	CLA	MG-NA	2.33	2.11	2.06
25	C	504	CLA	C4D-ND	-2.33	1.34	1.37
26	b	619	BCR	C30-C25	-2.33	1.50	1.53
29	f	102	SQD	O7-S	2.33	1.51	1.45
28	m	101	LMG	C4-C3	2.32	1.58	1.52
25	B	610	CLA	C1D-C2D	2.32	1.49	1.45
25	b	610	CLA	MG-NC	2.32	2.11	2.06
25	a	611	CLA	CMB-C2B	-2.32	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.32	1.46	1.51
31	a	614	DGD	C3G-C2G	2.32	1.56	1.51
25	B	606	CLA	C1B-NB	2.31	1.37	1.35
31	c	516	DGD	C1E-C2E	2.31	1.59	1.52
31	c	516	DGD	C3E-C2E	2.31	1.58	1.52
25	B	605	CLA	MG-NA	2.30	2.11	2.06
29	a	612	SQD	C6-S	2.30	1.85	1.77
25	A	607	CLA	CMB-C2B	-2.30	1.46	1.51
25	b	603	CLA	CMD-C2D	-2.29	1.45	1.50
31	J	101	DGD	C1G-C2G	2.29	1.57	1.50
25	c	505	CLA	CMB-C2B	-2.28	1.46	1.51
25	B	611	CLA	CMD-C2D	-2.28	1.46	1.50
31	H	102	DGD	C1E-C2E	2.28	1.59	1.52
33	D	402	PHO	CAC-C3C	-2.28	1.48	1.52
25	b	613	CLA	CMD-C2D	-2.28	1.46	1.50
25	C	503	CLA	C1D-C2D	2.28	1.49	1.45
25	C	509	CLA	CMD-C2D	-2.28	1.46	1.50
25	C	505	CLA	MG-NC	2.27	2.11	2.06
25	B	602	CLA	MG-NC	2.27	2.11	2.06
34	f	101	HEM	FE-NB	2.27	2.08	1.96
25	B	609	CLA	MG-NA	2.27	2.11	2.06
29	f	102	SQD	O9-S	2.27	1.51	1.45
25	C	511	CLA	CMB-C2B	-2.27	1.46	1.51
31	A	616	DGD	C6E-C5E	2.27	1.59	1.51
25	B	606	CLA	C3B-CAB	-2.26	1.43	1.47
25	d	403	CLA	CMC-C2C	-2.26	1.46	1.50
28	c	518	LMG	C7-C8	2.26	1.57	1.50
25	C	506	CLA	CMB-C2B	-2.25	1.47	1.51
29	B	623	SQD	O9-S	2.25	1.51	1.45
25	b	604	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	CMB-C2B	-2.25	1.47	1.51
31	H	102	DGD	C1G-C2G	2.24	1.57	1.50
25	b	601	CLA	C4D-ND	-2.24	1.34	1.37
25	b	607	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	612	CLA	CMC-C2C	-2.24	1.46	1.50
29	b	620	SQD	C6-S	2.23	1.85	1.77
29	b	620	SQD	O9-S	2.23	1.51	1.45
29	a	613	SQD	C44-C45	2.23	1.56	1.51
29	b	620	SQD	C46-C45	2.22	1.57	1.50
33	d	402	PHO	CMD-C2D	-2.22	1.46	1.51
31	h	102	DGD	C6D-C5D	2.22	1.58	1.51
28	C	517	LMG	O7-C8	-2.22	1.41	1.46
25	b	615	CLA	CMB-C2B	-2.22	1.47	1.51
25	B	608	CLA	C1D-C2D	2.21	1.49	1.45
26	D	405	BCR	C1-C6	-2.21	1.50	1.53
31	c	516	DGD	O3D-C3D	-2.21	1.37	1.43
25	B	601	CLA	C4D-ND	-2.21	1.34	1.37
31	C	516	DGD	C4D-C3D	2.21	1.57	1.52
26	B	617	BCR	C33-C5	-2.21	1.47	1.50
25	C	505	CLA	CMB-C2B	-2.20	1.47	1.51
35	v	201	HEC	CAA-C2A	2.20	1.56	1.52
34	f	101	HEM	FE-ND	2.20	2.07	1.96
25	B	602	CLA	C4D-ND	-2.20	1.34	1.37
29	b	620	SQD	O5-C5	2.20	1.49	1.44
25	b	612	CLA	CMB-C2B	-2.20	1.47	1.51
31	c	516	DGD	O2G-C2G	-2.20	1.41	1.46
33	a	607	PHO	CMC-C2C	-2.19	1.46	1.51
25	C	509	CLA	MG-NA	2.19	2.11	2.06
30	A	614	LHG	O8-C23	2.19	1.39	1.33
31	C	515	DGD	C3D-C2D	2.19	1.57	1.52
26	k	103	BCR	C30-C25	-2.19	1.50	1.53
25	b	607	CLA	CMB-C2B	-2.19	1.47	1.51
28	D	411	LMG	C9-C8	2.18	1.57	1.50
29	A	613	SQD	C8-C7	2.18	1.57	1.50
25	D	404	CLA	C3D-C4D	2.18	1.49	1.44
25	b	613	CLA	CMB-C2B	-2.18	1.47	1.51
25	B	603	CLA	CMD-C2D	-2.18	1.46	1.50
25	A	608	CLA	C1D-C2D	2.18	1.49	1.45
25	C	503	CLA	CMB-C2B	-2.18	1.47	1.51
28	c	521	LMG	C1-C2	2.17	1.58	1.52
30	D	410	LHG	O7-C7	2.17	1.40	1.34
29	a	612	SQD	O7-S	2.17	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	408	SQD	C6-S	2.16	1.85	1.77
33	D	401	PHO	CAC-C3C	-2.16	1.48	1.52
25	C	513	CLA	C1D-C2D	2.16	1.49	1.45
25	c	504	CLA	CMB-C2B	-2.16	1.47	1.51
31	A	616	DGD	O1G-C1G	-2.16	1.40	1.45
31	c	516	DGD	C4D-C5D	2.15	1.57	1.53
25	a	605	CLA	C3D-C4D	2.15	1.49	1.44
25	B	612	CLA	C3D-C4D	2.15	1.49	1.44
25	B	610	CLA	C4D-ND	-2.15	1.34	1.37
29	B	623	SQD	C8-C7	2.15	1.57	1.50
25	b	611	CLA	CMB-C2B	-2.15	1.47	1.51
25	c	507	CLA	CMC-C2C	-2.15	1.46	1.50
25	b	608	CLA	MG-ND	2.15	2.10	2.05
31	J	101	DGD	O2G-C2G	-2.15	1.41	1.46
27	D	406	PL9	C11-C9	-2.14	1.46	1.51
25	a	608	CLA	C4B-CHC	-2.14	1.35	1.41
25	C	502	CLA	CMB-C2B	-2.14	1.47	1.51
25	B	602	CLA	CMB-C2B	-2.14	1.47	1.51
25	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	616	CLA	CMB-C2B	-2.13	1.47	1.51
33	a	607	PHO	O2D-CGD	2.13	1.38	1.33
25	a	611	CLA	C1D-C2D	2.13	1.49	1.45
29	D	408	SQD	O9-S	2.13	1.51	1.45
25	c	513	CLA	CMD-C2D	-2.13	1.46	1.50
30	d	407	LHG	O7-C5	-2.12	1.41	1.46
31	C	515	DGD	C3G-C2G	2.12	1.57	1.50
25	B	609	CLA	CMB-C2B	-2.12	1.47	1.51
25	a	605	CLA	CMB-C2B	-2.12	1.47	1.51
31	c	516	DGD	C3D-C2D	2.12	1.57	1.52
25	b	614	CLA	C1D-C2D	2.12	1.49	1.45
31	c	515	DGD	C4D-C3D	2.12	1.57	1.52
25	B	608	CLA	CMD-C2D	-2.11	1.46	1.50
25	b	606	CLA	C1B-NB	2.11	1.37	1.35
26	B	619	BCR	C30-C25	-2.11	1.50	1.53
25	C	501	CLA	CMD-C2D	-2.11	1.46	1.50
25	b	601	CLA	CMB-C2B	-2.11	1.47	1.51
25	c	505	CLA	C3B-C2B	-2.11	1.37	1.40
25	B	614	CLA	C3B-CAB	-2.11	1.43	1.47
31	C	515	DGD	C1D-C2D	2.11	1.58	1.52
28	b	622	LMG	C7-C8	2.11	1.57	1.50
25	c	505	CLA	MG-ND	-2.11	2.01	2.05
25	b	602	CLA	CMB-C2B	-2.11	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	CMB-C2B	-2.11	1.47	1.51
25	c	507	CLA	C3D-C4D	2.11	1.48	1.44
25	b	615	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	501	CLA	CMD-C2D	-2.10	1.46	1.50
31	A	616	DGD	O3G-C1D	2.10	1.43	1.40
31	A	616	DGD	O2G-C1B	2.10	1.40	1.34
25	c	502	CLA	C3B-CAB	-2.10	1.43	1.47
25	c	511	CLA	CMB-C2B	-2.10	1.47	1.51
30	D	409	LHG	P-O6	2.10	1.67	1.59
31	H	102	DGD	C4D-C3D	2.09	1.57	1.52
28	B	620	LMG	C9-C8	2.09	1.57	1.50
25	c	507	CLA	C3B-CAB	-2.09	1.43	1.47
25	b	609	CLA	CMC-C2C	-2.09	1.46	1.50
25	c	509	CLA	C1B-NB	2.09	1.37	1.35
26	H	101	BCR	C1-C6	-2.09	1.50	1.53
27	d	406	PL9	C3-C4	-2.09	1.46	1.49
25	b	614	CLA	CMB-C2B	-2.09	1.47	1.51
25	C	501	CLA	C3D-C4D	2.09	1.48	1.44
25	B	612	CLA	CMC-C2C	-2.09	1.46	1.50
25	c	509	CLA	C3C-C2C	2.08	1.41	1.36
29	D	408	SQD	O7-S	2.08	1.51	1.45
30	D	410	LHG	O3-C3	-2.08	1.36	1.44
25	B	613	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	604	CLA	CMB-C2B	-2.08	1.47	1.51
31	h	102	DGD	C4D-C3D	2.08	1.57	1.52
30	d	407	LHG	O8-C23	2.08	1.39	1.33
25	B	610	CLA	C3B-C2B	-2.08	1.37	1.40
31	C	516	DGD	C6D-C5D	2.08	1.58	1.51
31	J	101	DGD	C4D-C5D	2.08	1.57	1.53
25	B	608	CLA	C3C-C2C	2.08	1.41	1.36
25	A	611	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	606	CLA	MG-ND	2.07	2.09	2.05
25	c	501	CLA	MG-NC	2.07	2.11	2.06
25	b	605	CLA	CMB-C2B	-2.07	1.47	1.51
25	B	609	CLA	C3D-C4D	2.07	1.48	1.44
25	b	616	CLA	CMC-C2C	-2.07	1.46	1.50
29	A	613	SQD	O9-S	2.07	1.51	1.45
25	c	503	CLA	C1D-C2D	2.06	1.49	1.45
25	B	615	CLA	C3B-CAB	-2.06	1.43	1.47
25	d	404	CLA	CMD-C2D	-2.06	1.46	1.50
27	D	406	PL9	C3-C4	-2.06	1.46	1.49
25	a	608	CLA	C3B-C2B	-2.06	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	CMB-C2B	-2.06	1.47	1.51
31	C	515	DGD	C6D-C5D	2.06	1.58	1.51
28	c	521	LMG	C3-C2	2.06	1.57	1.52
25	b	611	CLA	C1B-NB	2.06	1.37	1.35
25	b	603	CLA	CMC-C2C	-2.06	1.46	1.50
28	d	411	LMG	C9-C8	2.06	1.57	1.50
28	c	521	LMG	O1-C7	-2.06	1.40	1.43
25	C	501	CLA	C1B-NB	2.05	1.37	1.35
25	c	506	CLA	CMC-C2C	-2.05	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	512	CLA	C3D-C4D	2.05	1.48	1.44
25	c	502	CLA	CMC-C2C	-2.05	1.46	1.50
25	b	608	CLA	C3B-CAB	-2.05	1.43	1.47
25	B	616	CLA	O2D-CGD	2.04	1.38	1.33
29	B	623	SQD	C46-C45	2.04	1.57	1.50
33	D	401	PHO	CMC-C2C	-2.04	1.46	1.51
25	C	510	CLA	O2D-CGD	2.04	1.38	1.33
29	B	623	SQD	C44-C45	2.04	1.57	1.50
25	b	606	CLA	CMD-C2D	-2.04	1.46	1.50
25	c	502	CLA	C4B-CHC	-2.03	1.35	1.41
25	C	508	CLA	CMB-C2B	-2.03	1.47	1.51
30	L	101	LHG	P-O6	2.03	1.67	1.59
25	B	609	CLA	CMD-C2D	-2.03	1.46	1.50
29	b	620	SQD	C44-C45	2.03	1.56	1.50
27	A	610	PL9	C7-C3	-2.03	1.49	1.51
29	B	623	SQD	O7-S	2.03	1.51	1.45
26	b	617	BCR	C33-C5	-2.03	1.47	1.50
25	A	606	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	608	CLA	C3B-C2B	-2.02	1.37	1.40
25	B	612	CLA	CMB-C2B	-2.02	1.47	1.51
29	B	623	SQD	C6-S	2.02	1.84	1.77
28	C	517	LMG	C4-C5	2.02	1.57	1.53
31	c	515	DGD	O3E-C3E	-2.02	1.38	1.43
26	d	405	BCR	C33-C5	-2.01	1.47	1.50
26	C	514	BCR	C30-C25	-2.01	1.51	1.53
25	B	606	CLA	CMC-C2C	-2.01	1.46	1.50
31	H	102	DGD	O2G-C2G	-2.01	1.41	1.46
31	c	516	DGD	O6D-C5D	-2.01	1.39	1.44
31	H	102	DGD	O1G-C1G	-2.01	1.40	1.45
31	C	515	DGD	C1G-C2G	2.00	1.56	1.50
26	k	102	BCR	C33-C5	-2.00	1.47	1.50
31	c	517	DGD	O2G-C2G	-2.00	1.41	1.46

All (1184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	9.72	111.08	106.71
25	b	616	CLA	C4A-NA-C1A	9.18	110.83	106.71
25	B	601	CLA	C4A-NA-C1A	9.11	110.80	106.71
25	c	511	CLA	C4A-NA-C1A	8.76	110.64	106.71
25	C	503	CLA	C4A-NA-C1A	8.55	110.55	106.71
25	C	510	CLA	C4A-NA-C1A	8.54	110.55	106.71
25	b	606	CLA	C4A-NA-C1A	8.29	110.43	106.71
25	a	605	CLA	C4A-NA-C1A	8.16	110.37	106.71
25	C	508	CLA	C4A-NA-C1A	8.13	110.36	106.71
25	c	503	CLA	C4A-NA-C1A	8.06	110.33	106.71
25	C	511	CLA	C4A-NA-C1A	8.04	110.32	106.71
25	c	509	CLA	C4A-NA-C1A	7.91	110.26	106.71
25	C	507	CLA	C4A-NA-C1A	7.87	110.24	106.71
25	B	606	CLA	C4A-NA-C1A	7.79	110.21	106.71
25	c	507	CLA	C4A-NA-C1A	7.76	110.19	106.71
25	b	601	CLA	C4A-NA-C1A	7.53	110.09	106.71
25	B	615	CLA	C4A-NA-C1A	7.48	110.07	106.71
25	C	501	CLA	C4A-NA-C1A	7.44	110.05	106.71
25	C	506	CLA	C4A-NA-C1A	7.36	110.01	106.71
25	b	615	CLA	C4A-NA-C1A	7.10	109.90	106.71
25	A	606	CLA	C4A-NA-C1A	6.93	109.82	106.71
25	A	611	CLA	C4A-NA-C1A	6.85	109.78	106.71
25	B	609	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	b	609	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	a	606	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	B	607	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	c	512	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	B	612	CLA	C4A-NA-C1A	6.59	109.67	106.71
25	c	502	CLA	C4A-NA-C1A	6.55	109.65	106.71
29	A	613	SQD	O6-C1-C2	6.55	118.53	108.30
25	b	611	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	B	613	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	c	501	CLA	C4A-NA-C1A	6.26	109.52	106.71
27	A	610	PL9	C7-C3-C4	6.23	121.94	116.88
25	b	602	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	d	403	CLA	C4A-NA-C1A	6.19	109.49	106.71
29	A	613	SQD	O7-S-C6	6.16	114.27	106.94
25	D	403	CLA	C4A-NA-C1A	6.03	109.42	106.71
25	C	513	CLA	C4A-NA-C1A	5.98	109.39	106.71
25	C	509	CLA	C4A-NA-C1A	5.98	109.39	106.71
25	c	506	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	c	513	CLA	C4A-NA-C1A	5.92	109.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	c	505	CLA	C4A-NA-C1A	5.84	109.33	106.71
29	A	613	SQD	C1-O5-C5	-5.82	102.26	113.69
29	a	612	SQD	C1-O5-C5	-5.70	102.50	113.69
25	B	616	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	c	510	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	C	512	CLA	C4A-NA-C1A	5.56	109.20	106.71
25	B	611	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	B	602	CLA	C4A-NA-C1A	5.50	109.18	106.71
25	C	502	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	C	505	CLA	C4A-NA-C1A	5.44	109.15	106.71
25	c	508	CLA	C4A-NA-C1A	5.43	109.15	106.71
34	f	101	HEM	CBA-CAA-C2A	-5.42	103.37	112.62
29	b	620	SQD	O6-C1-C2	5.38	116.70	108.30
25	b	613	CLA	C4A-NA-C1A	5.38	109.12	106.71
25	b	604	CLA	C4A-NA-C1A	5.36	109.12	106.71
25	c	504	CLA	C4A-NA-C1A	5.36	109.11	106.71
25	d	404	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	a	610	PL9	C7-C3-C4	5.32	121.20	116.88
25	B	605	CLA	C4A-NA-C1A	5.32	109.10	106.71
29	a	612	SQD	O6-C1-C2	5.31	116.59	108.30
29	a	613	SQD	O47-C7-C8	5.31	122.94	111.50
25	A	607	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	C	504	CLA	C4A-NA-C1A	5.12	109.01	106.71
25	c	504	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
25	b	605	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	b	603	CLA	C4A-NA-C1A	5.07	108.99	106.71
25	B	603	CLA	C4A-NA-C1A	5.05	108.98	106.71
25	a	611	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	b	608	CLA	C4A-NA-C1A	5.04	108.97	106.71
29	a	612	SQD	O7-S-C6	5.04	112.92	106.94
25	D	404	CLA	C4A-NA-C1A	4.94	108.93	106.71
29	D	408	SQD	O6-C1-C2	4.89	115.93	108.30
25	C	504	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
25	B	610	CLA	O2D-CGD-O1D	-4.83	114.40	123.84
25	c	501	CLA	O2D-CGD-O1D	-4.80	114.46	123.84
29	B	623	SQD	O7-S-C6	4.74	112.58	106.94
25	b	613	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
25	B	613	CLA	C1-C2-C3	-4.71	117.89	126.04
29	b	620	SQD	O7-S-C6	4.65	112.47	106.94
25	B	602	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
25	b	607	CLA	C4A-NA-C1A	4.61	108.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C1-C2-C3	-4.60	118.09	126.04
25	C	508	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
25	A	607	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
29	f	102	SQD	O7-S-C6	4.55	112.35	106.94
25	C	505	CLA	CMB-C2B-C1B	-4.55	121.46	128.46
25	B	606	CLA	O2D-CGD-O1D	-4.49	115.05	123.84
25	a	611	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
25	c	510	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
29	b	620	SQD	O9-S-O7	-4.47	98.49	113.95
29	b	620	SQD	O5-C5-C4	4.46	117.79	109.69
25	b	607	CLA	CMB-C2B-C1B	-4.46	121.62	128.46
25	a	608	CLA	C4A-NA-C1A	4.46	108.71	106.71
31	H	102	DGD	O3G-C3G-C2G	-4.44	100.18	110.90
25	b	610	CLA	C4A-NA-C1A	4.41	108.69	106.71
35	v	201	HEC	CBD-CAD-C3D	-4.41	105.09	112.62
25	A	608	CLA	C4A-NA-C1A	4.38	108.68	106.71
25	C	509	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
25	b	612	CLA	C4A-NA-C1A	4.35	108.66	106.71
25	c	509	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
25	B	608	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	B	610	CLA	C4A-NA-C1A	4.32	108.65	106.71
29	A	613	SQD	O9-S-O7	-4.30	99.07	113.95
25	b	603	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
30	D	410	LHG	O4-P-O5	4.28	133.40	112.24
29	f	102	SQD	O9-S-C6	4.28	112.02	106.94
25	b	612	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
25	b	609	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
25	B	605	CLA	CHD-C1D-ND	-4.24	120.55	124.45
25	B	614	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
29	B	623	SQD	O47-C7-C8	4.22	120.59	111.50
29	a	612	SQD	O9-S-O7	-4.21	99.36	113.95
29	D	408	SQD	O8-S-C6	4.20	112.44	105.74
35	V	201	HEC	CMB-C2B-C1B	-4.19	122.02	128.46
25	B	607	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	b	614	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	B	611	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
30	e	101	LHG	O4-P-O5	4.14	132.72	112.24
29	A	613	SQD	C1-C2-C3	-4.14	101.37	110.00
25	C	512	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	A	608	CLA	CHD-C1D-ND	-4.13	120.66	124.45
29	B	623	SQD	O6-C1-C2	4.11	114.72	108.30
27	d	406	PL9	C7-C3-C4	4.11	120.21	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
30	d	408	LHG	O4-P-O5	4.10	132.49	112.24
25	b	614	CLA	C4A-NA-C1A	4.09	108.55	106.71
25	c	513	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
25	c	508	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
29	f	102	SQD	O9-S-O7	-4.07	99.87	113.95
25	c	504	CLA	CMB-C2B-C3B	4.06	132.27	124.68
29	f	102	SQD	O6-C1-C2	4.06	114.64	108.30
30	D	412	LHG	O4-P-O5	4.05	132.28	112.24
25	b	603	CLA	O2D-CGD-O1D	-4.05	115.91	123.84
25	C	506	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
25	b	612	CLA	CMB-C2B-C3B	4.02	132.20	124.68
25	B	612	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
30	A	614	LHG	O4-P-O5	4.00	132.03	112.24
30	L	101	LHG	O4-P-O5	4.00	132.01	112.24
30	d	407	LHG	O4-P-O5	3.99	131.97	112.24
25	B	602	CLA	CMB-C2B-C3B	3.99	132.14	124.68
30	D	409	LHG	O4-P-O5	3.98	131.89	112.24
31	c	516	DGD	O3G-C3G-C2G	-3.97	101.31	110.90
25	c	501	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	d	404	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
29	A	613	SQD	O47-C7-C8	3.96	120.05	111.50
33	D	402	PHO	O1D-CGD-CBD	3.96	131.33	124.74
30	d	409	LHG	O4-P-O5	3.96	131.80	112.24
24	d	401	BCT	O2-C-O1	3.94	129.77	119.55
31	c	515	DGD	O3G-C3G-C2G	-3.94	101.39	110.90
25	C	513	CLA	CHD-C1D-ND	-3.94	120.83	124.45
29	D	408	SQD	C1-O5-C5	-3.93	105.97	113.69
25	b	601	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	b	608	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
25	B	614	CLA	C4A-NA-C1A	3.91	108.46	106.71
31	c	517	DGD	O3G-C3G-C2G	-3.90	101.48	110.90
25	b	613	CLA	CMB-C2B-C3B	3.88	131.93	124.68
25	b	604	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
26	T	101	BCR	C7-C8-C9	-3.86	120.40	126.23
25	A	607	CLA	CMB-C2B-C3B	3.86	131.90	124.68
25	b	606	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
33	D	401	PHO	CMB-C2B-C3B	3.86	131.90	124.68
25	A	611	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
24	A	605	BCT	O2-C-O1	3.85	129.53	119.55
25	D	404	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	C	508	CLA	O2D-CGD-O1D	-3.84	116.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	608	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	B	603	CLA	O2D-CGD-O1D	-3.84	116.34	123.84
29	b	620	SQD	C3-C4-C5	3.83	117.06	110.24
25	C	511	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
26	b	617	BCR	C2-C1-C6	3.80	116.33	110.48
25	C	510	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
25	c	503	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	C	505	CLA	CMB-C2B-C3B	3.78	131.74	124.68
29	D	408	SQD	O9-S-C6	3.77	111.42	106.94
30	l	101	LHG	O4-P-O5	3.77	130.88	112.24
33	D	402	PHO	C1-C2-C3	-3.77	119.52	126.04
25	B	606	CLA	O2D-CGD-CBD	3.77	117.96	111.27
25	C	503	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
25	c	509	CLA	CMB-C2B-C3B	3.76	131.71	124.68
29	b	620	SQD	O9-S-C6	3.75	111.39	106.94
25	C	502	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	a	611	CLA	CMB-C2B-C3B	3.74	131.67	124.68
25	b	607	CLA	CHD-C1D-ND	-3.74	121.02	124.45
25	a	611	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
25	A	608	CLA	CMB-C2B-C3B	3.73	131.66	124.68
31	C	516	DGD	O3G-C3G-C2G	-3.73	101.90	110.90
25	a	605	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
31	h	102	DGD	O3G-C3G-C2G	-3.72	101.92	110.90
25	B	613	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	b	610	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
25	A	607	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
25	b	608	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	b	602	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
25	C	509	CLA	CMB-C2B-C3B	3.70	131.61	124.68
25	C	508	CLA	CMB-C2B-C3B	3.70	131.61	124.68
25	b	612	CLA	CHB-C4A-NA	3.70	129.63	124.51
27	d	406	PL9	C40-C39-C41	3.69	121.48	115.27
25	B	608	CLA	CMB-C2B-C3B	3.69	131.58	124.68
26	B	617	BCR	C2-C1-C6	3.68	116.15	110.48
25	B	615	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	C	507	CLA	CHB-C4A-NA	3.66	129.57	124.51
25	B	603	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
25	b	607	CLA	CMB-C2B-C3B	3.65	131.51	124.68
25	B	614	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
25	B	609	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
35	V	201	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
25	c	506	CLA	CMB-C2B-C1B	-3.62	122.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	O2A-CGA-O1A	-3.62	114.46	123.59
35	v	201	HEC	CMC-C2C-C1C	-3.62	122.90	128.46
25	B	608	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
25	B	603	CLA	CMB-C2B-C3B	3.62	131.45	124.68
27	d	406	PL9	C7-C8-C9	-3.62	120.77	126.79
25	b	603	CLA	CMB-C2B-C3B	3.61	131.43	124.68
25	d	404	CLA	CMB-C2B-C3B	3.61	131.43	124.68
25	d	403	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
27	A	610	PL9	C7-C3-C2	-3.60	118.56	123.30
25	B	612	CLA	CMB-C2B-C3B	3.60	131.41	124.68
33	D	402	PHO	O2D-CGD-O1D	-3.60	116.80	123.84
29	a	612	SQD	O47-C7-C8	3.59	119.23	111.50
25	C	501	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
25	b	605	CLA	CHD-C1D-ND	-3.58	121.16	124.45
25	B	614	CLA	CMB-C2B-C3B	3.57	131.36	124.68
27	D	406	PL9	C7-C3-C4	3.57	119.78	116.88
25	c	510	CLA	CMB-C2B-C3B	3.57	131.36	124.68
29	B	623	SQD	O9-S-O7	-3.55	101.68	113.95
25	c	501	CLA	O2D-CGD-CBD	3.54	117.56	111.27
33	D	402	PHO	CMB-C2B-C3B	3.53	131.28	124.68
25	b	605	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
35	V	201	HEC	CMC-C2C-C1C	-3.52	123.05	128.46
29	b	620	SQD	O47-C7-C8	3.51	119.07	111.50
31	J	101	DGD	O3G-C3G-C2G	-3.51	102.44	110.90
25	b	604	CLA	CMB-C2B-C3B	3.51	131.24	124.68
25	c	508	CLA	CMB-C2B-C3B	3.48	131.18	124.68
25	b	601	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
25	a	606	CLA	CHD-C1D-ND	-3.46	121.28	124.45
25	b	612	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
25	C	507	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
31	a	614	DGD	O3G-C3G-C2G	-3.46	102.62	111.78
25	B	607	CLA	CMB-C2B-C3B	3.45	131.14	124.68
25	c	501	CLA	CMB-C2B-C3B	3.44	131.12	124.68
25	B	613	CLA	CMB-C2B-C3B	3.44	131.12	124.68
25	C	510	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	a	606	CLA	CHB-C4A-NA	3.44	129.27	124.51
25	C	512	CLA	CMB-C2B-C3B	3.44	131.10	124.68
25	b	611	CLA	O2D-CGD-CBD	3.44	117.37	111.27
28	b	622	LMG	O1-C1-C2	-3.43	102.94	108.30
25	B	604	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	a	610	PL9	C7-C3-C2	-3.43	118.79	123.30
25	A	608	CLA	CHB-C4A-NA	3.43	129.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	505	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
33	d	402	PHO	CMB-C2B-C3B	3.43	131.09	124.68
31	H	102	DGD	C1D-C2D-C3D	-3.42	102.87	110.00
25	c	502	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	a	611	CLA	O2D-CGD-CBD	3.41	117.33	111.27
25	C	504	CLA	CMB-C2B-C3B	3.41	131.05	124.68
25	C	513	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
26	D	405	BCR	C2-C1-C6	3.40	115.72	110.48
25	C	512	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
25	B	611	CLA	O2D-CGD-CBD	3.38	117.28	111.27
25	c	513	CLA	CMB-C2B-C3B	3.38	131.01	124.68
25	C	501	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
25	b	602	CLA	CMB-C2B-C3B	3.37	130.99	124.68
25	b	608	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	B	610	CLA	O2A-CGA-O1A	-3.36	115.11	123.59
25	B	610	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	A	611	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
25	d	403	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
29	f	102	SQD	O47-C7-C8	3.35	120.15	110.80
25	C	502	CLA	CHD-C1D-ND	-3.35	121.37	124.45
29	A	615	SQD	O47-C7-C8	3.35	118.73	111.50
29	a	612	SQD	O8-S-C6	3.35	111.08	105.74
25	B	610	CLA	C1-C2-C3	-3.35	120.25	126.04
30	D	412	LHG	O8-C23-C24	3.34	122.40	111.91
26	b	618	BCR	C15-C14-C13	-3.34	122.54	127.31
25	A	608	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
25	b	614	CLA	CMB-C2B-C3B	3.34	130.92	124.68
25	B	602	CLA	O2D-CGD-CBD	3.34	117.20	111.27
29	D	408	SQD	C1-C2-C3	-3.34	103.05	110.00
25	A	606	CLA	CHB-C4A-NA	3.34	129.12	124.51
25	b	609	CLA	CMB-C2B-C3B	3.33	130.92	124.68
29	b	620	SQD	C1-C2-C3	-3.33	103.05	110.00
25	b	616	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
25	b	616	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
25	d	404	CLA	CHB-C4A-NA	3.31	129.10	124.51
25	b	606	CLA	O2D-CGD-CBD	3.31	117.14	111.27
31	A	616	DGD	C3G-C2G-C1G	-3.30	103.99	111.79
25	C	502	CLA	CMB-C2B-C3B	3.29	130.84	124.68
25	b	602	CLA	CHB-C4A-NA	3.29	129.06	124.51
33	d	402	PHO	O1D-CGD-CBD	3.29	130.22	124.74
25	B	613	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
25	C	508	CLA	CHD-C1D-ND	-3.28	121.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	CMB-C2B-C3B	3.28	130.81	124.68
25	C	510	CLA	CHB-C4A-NA	3.28	129.04	124.51
25	B	616	CLA	CMB-C2B-C3B	3.27	130.81	124.68
28	d	411	LMG	O6-C1-O1	-3.27	102.22	109.97
32	M	101	STE	C3-C2-C1	-3.27	106.22	114.47
26	h	101	BCR	C2-C1-C6	3.27	115.51	110.48
34	E	101	HEM	CBA-CAA-C2A	-3.26	107.05	112.62
25	C	502	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
25	b	603	CLA	O2D-CGD-CBD	3.26	117.06	111.27
25	C	503	CLA	CMB-C2B-C3B	3.25	130.76	124.68
25	b	608	CLA	CHB-C4A-NA	3.25	129.00	124.51
29	f	102	SQD	O5-C5-C4	3.24	115.58	109.69
25	B	602	CLA	CHB-C4A-NA	3.23	128.98	124.51
31	C	515	DGD	O6D-C1D-O3G	-3.22	102.34	109.97
25	A	611	CLA	CMB-C2B-C3B	3.22	130.70	124.68
25	B	602	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
29	a	612	SQD	C3-C4-C5	3.21	115.97	110.24
25	D	403	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
26	B	619	BCR	C2-C1-C6	3.20	115.41	110.48
25	C	512	CLA	C1-C2-C3	-3.20	120.51	126.04
25	D	404	CLA	CMB-C2B-C3B	3.20	130.66	124.68
35	V	201	HEC	CMB-C2B-C3B	3.20	129.58	125.82
25	a	608	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
29	b	620	SQD	O8-S-C6	3.18	110.81	105.74
25	B	615	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
25	B	616	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
25	c	512	CLA	C1-C2-C3	-3.18	120.54	126.04
29	A	613	SQD	O9-S-C6	3.18	110.72	106.94
25	a	605	CLA	CMB-C2B-C3B	3.18	130.62	124.68
25	B	601	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
25	c	511	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
29	B	623	SQD	O9-S-C6	3.17	110.71	106.94
25	C	507	CLA	CMB-C2B-C3B	3.17	130.61	124.68
25	C	507	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	C	513	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
28	m	101	LMG	O1-C7-C8	-3.16	103.28	110.90
25	b	602	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
25	c	506	CLA	CMB-C2B-C3B	3.16	130.58	124.68
31	J	101	DGD	O6D-C1D-O3G	-3.16	102.50	109.97
25	B	609	CLA	CMB-C2B-C3B	3.15	130.58	124.68
25	c	507	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	b	614	CLA	O2D-CGD-O1D	-3.14	117.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
25	c	513	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
29	D	408	SQD	O9-S-O7	-3.13	103.11	113.95
28	c	521	LMG	O6-C1-O1	-3.13	102.57	109.97
26	T	101	BCR	C33-C5-C6	-3.12	121.02	124.53
25	c	505	CLA	O2D-CGD-CBD	3.12	116.81	111.27
25	A	606	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
29	a	612	SQD	O48-C23-C24	3.11	121.66	111.91
25	a	608	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	C	506	CLA	CMB-C2B-C3B	3.10	130.48	124.68
31	C	516	DGD	O6D-C1D-O3G	-3.10	102.64	109.97
25	c	512	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	B	611	CLA	C1-C2-C3	-3.08	120.71	126.04
32	B	626	STE	C3-C2-C1	-3.08	106.71	114.47
29	b	620	SQD	O48-C23-C24	3.08	121.56	111.91
25	b	611	CLA	CHD-C1D-ND	-3.08	121.63	124.45
25	b	616	CLA	CHD-C1D-ND	-3.06	121.64	124.45
25	c	503	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	c	507	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
25	c	503	CLA	CMB-C2B-C3B	3.06	130.40	124.68
35	V	201	HEC	CAD-CBD-CGD	-3.06	105.19	113.76
25	c	507	CLA	CHB-C4A-NA	3.05	128.74	124.51
25	B	615	CLA	CHB-C4A-NA	3.05	128.73	124.51
25	B	610	CLA	O2D-CGD-CBD	3.05	116.69	111.27
25	B	610	CLA	CHB-C4A-NA	3.05	128.73	124.51
25	a	606	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
25	A	611	CLA	O2D-CGD-CBD	3.05	116.68	111.27
25	b	605	CLA	C1-C2-C3	-3.05	120.78	126.04
25	b	612	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
25	b	606	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
27	d	406	PL9	C22-C23-C24	-3.03	120.36	127.66
25	C	511	CLA	CAC-C3C-C4C	3.03	128.74	124.81
25	c	512	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
25	B	606	CLA	C1-C2-C3	-3.02	120.82	126.04
25	B	616	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
25	C	510	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	503	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
26	b	617	BCR	C11-C10-C9	-3.01	123.02	127.31
27	D	406	PL9	C37-C38-C39	-3.01	120.42	127.66
25	B	612	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
25	A	607	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
25	b	601	CLA	CMB-C2B-C3B	2.99	130.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C11-C10-C9	-2.99	123.04	127.31
25	b	613	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	B	605	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
31	c	517	DGD	O6D-C1D-O3G	-2.98	102.91	109.97
26	K	101	BCR	C15-C14-C13	-2.98	123.05	127.31
25	B	610	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	b	612	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
25	b	612	CLA	CAC-C3C-C4C	2.98	128.68	124.81
28	b	622	LMG	C1-O6-C5	-2.98	107.84	113.69
31	C	515	DGD	CDB-CCB-CBB	-2.97	99.32	114.42
25	B	604	CLA	CMB-C2B-C3B	2.97	130.23	124.68
33	a	607	PHO	CMB-C2B-C3B	2.97	130.23	124.68
25	C	511	CLA	CMB-C2B-C3B	2.97	130.23	124.68
27	D	406	PL9	C22-C23-C24	-2.96	120.54	127.66
27	d	406	PL9	C7-C3-C2	-2.96	119.41	123.30
25	C	505	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	a	611	CLA	CHD-C1D-ND	-2.95	121.74	124.45
33	d	402	PHO	CMC-C2C-C3C	2.95	130.51	124.94
25	b	601	CLA	CHD-C1D-ND	-2.95	121.74	124.45
28	b	622	LMG	O3-C3-C2	-2.95	103.53	110.35
29	B	623	SQD	C1-O5-C5	-2.95	107.90	113.69
25	b	605	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
31	C	515	DGD	O3G-C3G-C2G	-2.94	103.80	110.90
25	B	605	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
25	c	502	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	d	404	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
25	B	616	CLA	O2D-CGD-CBD	2.94	116.49	111.27
31	h	102	DGD	C4E-C3E-C2E	-2.94	105.70	110.82
25	c	509	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
28	c	520	LMG	O1-C1-C2	-2.93	103.73	108.30
27	A	610	PL9	C36-C34-C33	-2.93	115.19	121.12
25	A	611	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	d	403	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
25	D	403	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
25	b	616	CLA	CHB-C4A-NA	2.91	128.53	124.51
29	a	613	SQD	O48-C23-C24	2.91	121.03	111.91
25	b	604	CLA	CHB-C4A-NA	2.90	128.53	124.51
25	c	512	CLA	O2A-CGA-O1A	-2.90	116.26	123.59
25	b	611	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	C	501	CLA	O2D-CGD-CBD	2.89	116.41	111.27
25	a	608	CLA	CMB-C2B-C3B	2.89	130.08	124.68
28	D	407	LMG	O1-C7-C8	-2.89	103.93	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	C	503	CLA	O1D-CGD-CBD	2.88	130.38	124.48
25	b	606	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	b	602	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	k	101	BCR	C7-C8-C9	-2.88	121.89	126.23
25	D	403	CLA	C4-C3-C5	2.88	120.11	115.27
25	A	606	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
27	D	406	PL9	C27-C28-C29	-2.87	120.75	127.66
25	b	616	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	b	612	CLA	C1-C2-C3	-2.86	121.09	126.04
25	C	511	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	a	614	DGD	CDB-CCB-CBB	-2.86	99.89	114.42
25	C	504	CLA	CHD-C1D-ND	-2.86	121.83	124.45
34	f	101	HEM	CHC-C4B-C3B	2.86	128.94	124.57
26	A	609	BCR	C2-C1-C6	2.86	114.88	110.48
26	B	617	BCR	C3-C4-C5	-2.85	108.98	114.08
25	b	604	CLA	C2D-C1D-ND	-2.85	108.00	110.10
27	d	406	PL9	C20-C19-C21	2.85	120.07	115.27
25	b	611	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
30	l	101	LHG	O8-C23-C24	2.84	120.83	111.91
25	B	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
31	h	102	DGD	CDB-CCB-CBB	-2.84	100.00	114.42
26	c	514	BCR	C27-C26-C25	2.84	126.85	122.73
33	d	402	PHO	O2D-CGD-O1D	-2.83	118.30	123.84
26	A	609	BCR	C27-C26-C25	2.83	126.84	122.73
27	a	610	PL9	C7-C8-C9	-2.83	122.08	126.79
25	B	615	CLA	CMB-C2B-C3B	2.83	129.97	124.68
25	B	615	CLA	C6-C7-C8	-2.83	106.78	115.92
31	c	516	DGD	O6D-C1D-O3G	-2.83	103.28	109.97
30	L	101	LHG	C5-O7-C7	-2.82	110.84	117.79
29	f	102	SQD	C1-O5-C5	-2.82	108.15	113.69
25	C	509	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	c	508	CLA	C7-C6-C5	-2.81	105.71	113.36
27	D	406	PL9	C42-C43-C44	-2.81	120.89	127.66
26	B	619	BCR	C29-C30-C25	2.81	114.81	110.48
31	H	102	DGD	C3E-C4E-C5E	-2.80	105.24	110.24
25	b	603	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	B	602	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
29	B	623	SQD	O48-C23-C24	2.80	120.68	111.91
25	C	512	CLA	CHB-C4A-NA	2.79	128.38	124.51
25	C	508	CLA	O2D-CGD-CBD	2.79	116.23	111.27
28	m	101	LMG	C1-C2-C3	-2.79	104.18	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
25	C	506	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	K	101	BCR	C15-C16-C17	-2.79	117.77	123.47
25	d	403	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	b	612	CLA	O1D-CGD-CBD	2.78	130.18	124.48
25	C	503	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	C	507	CLA	CHD-C1D-ND	-2.78	121.90	124.45
27	D	406	PL9	C36-C34-C33	-2.78	115.49	121.12
25	c	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	c	504	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	B	601	CLA	CMB-C2B-C1B	-2.78	124.20	128.46
26	a	609	BCR	C2-C1-C6	2.77	114.75	110.48
25	C	509	CLA	C1-C2-C3	-2.77	121.25	126.04
31	C	516	DGD	CDB-CCB-CBB	-2.77	100.38	114.42
34	f	101	HEM	C4B-CHC-C1C	2.76	126.21	122.56
28	C	517	LMG	O1-C7-C8	-2.76	104.23	110.90
26	a	609	BCR	C27-C26-C25	2.76	126.74	122.73
25	A	606	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	K	101	BCR	C27-C26-C25	2.76	126.74	122.73
30	d	407	LHG	O8-C23-C24	2.76	120.56	111.91
25	c	510	CLA	CHD-C1D-ND	-2.76	121.92	124.45
31	H	102	DGD	CDB-CCB-CBB	-2.75	100.45	114.42
25	b	608	CLA	CHD-C1D-ND	-2.75	121.92	124.45
26	T	101	BCR	C27-C26-C25	2.75	126.72	122.73
28	D	407	LMG	O6-C1-O1	-2.75	103.46	109.97
26	b	618	BCR	C8-C7-C6	-2.75	119.48	127.20
27	D	406	PL9	C12-C13-C14	-2.75	121.04	127.66
25	b	614	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
26	k	102	BCR	C33-C5-C6	-2.74	121.45	124.53
30	A	614	LHG	O8-C23-C24	2.74	120.51	111.91
25	B	610	CLA	CMB-C2B-C3B	2.74	129.81	124.68
25	B	611	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
25	c	511	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
26	b	617	BCR	C27-C26-C25	2.74	126.70	122.73
25	C	513	CLA	CMB-C2B-C3B	2.74	129.80	124.68
25	b	602	CLA	O2D-CGD-CBD	2.74	116.13	111.27
30	D	409	LHG	O8-C23-C24	2.74	120.49	111.91
26	k	101	BCR	C2-C1-C6	2.73	114.69	110.48
26	t	101	BCR	C33-C5-C6	-2.73	121.46	124.53
25	a	611	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	b	609	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
28	C	517	LMG	O6-C1-O1	-2.72	103.52	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	405	BCR	C27-C26-C25	2.72	126.69	122.73
25	B	604	CLA	C2D-C1D-ND	-2.72	108.10	110.10
25	A	606	CLA	CMB-C2B-C3B	2.72	129.76	124.68
29	D	408	SQD	O48-C23-C24	2.71	120.42	111.91
25	c	511	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	a	608	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	c	503	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	e	101	LHG	O8-C23-C24	2.70	120.39	111.91
26	k	101	BCR	C24-C23-C22	-2.70	122.15	126.23
25	B	606	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
25	A	607	CLA	O2D-CGD-CBD	2.70	116.06	111.27
26	b	619	BCR	C29-C30-C25	2.70	114.63	110.48
25	c	504	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
29	D	408	SQD	O7-S-C6	2.69	110.14	106.94
31	C	515	DGD	C6D-O5D-C1E	2.69	119.00	113.74
25	b	614	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	B	611	CLA	CHD-C1D-ND	-2.69	121.98	124.45
32	d	413	STE	C3-C2-C1	-2.69	107.69	114.47
31	h	102	DGD	O6D-C1D-O3G	-2.68	103.62	109.97
25	B	604	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
30	d	407	LHG	O8-C23-O10	-2.68	116.83	123.59
31	J	101	DGD	CDB-CCB-CBB	-2.68	100.83	114.42
25	B	601	CLA	CHB-C4A-NA	2.68	128.22	124.51
31	h	102	DGD	C6D-C5D-C4D	2.68	117.68	112.09
25	C	504	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
25	c	512	CLA	CHB-C4A-NA	2.68	128.21	124.51
31	c	517	DGD	CDB-CCB-CBB	-2.67	100.86	114.42
25	B	603	CLA	O2D-CGD-CBD	2.67	116.01	111.27
25	B	603	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	c	513	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	c	507	CLA	CMB-C2B-C3B	2.67	129.67	124.68
25	B	602	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
26	D	405	BCR	C27-C26-C25	2.67	126.60	122.73
26	B	618	BCR	C27-C26-C25	2.66	126.60	122.73
25	c	513	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
25	c	510	CLA	C16-C15-C13	-2.66	107.31	115.92
25	a	611	CLA	C2D-C1D-ND	-2.66	108.14	110.10
26	b	619	BCR	C7-C8-C9	-2.66	122.22	126.23
25	b	609	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
26	k	101	BCR	C27-C26-C25	2.66	126.59	122.73
34	f	101	HEM	CAB-C3B-C2B	-2.66	119.86	128.60
33	d	402	PHO	C1-C2-C3	-2.65	121.45	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	C1-C2-C3	-2.65	121.45	126.04
25	c	504	CLA	CHD-C1D-ND	-2.65	122.02	124.45
26	B	619	BCR	C38-C26-C25	-2.65	121.56	124.53
29	f	102	SQD	O5-C1-C2	-2.65	104.75	110.35
26	K	102	BCR	C33-C5-C6	-2.64	121.56	124.53
25	c	502	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
25	D	404	CLA	CHB-C4A-NA	2.64	128.17	124.51
25	B	613	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
26	C	514	BCR	C15-C16-C17	-2.64	118.06	123.47
25	b	609	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
25	A	607	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
35	V	201	HEC	CMC-C2C-C3C	2.64	128.92	125.82
25	c	501	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	c	501	CLA	C2D-C1D-ND	-2.63	108.16	110.10
30	D	412	LHG	C11-C10-C9	-2.63	101.07	114.42
29	A	613	SQD	O8-S-C6	2.63	109.93	105.74
25	b	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
34	E	101	HEM	C4D-ND-C1D	2.63	107.79	105.07
25	c	505	CLA	C1-C2-C3	-2.63	121.50	126.04
26	B	618	BCR	C7-C8-C9	-2.62	122.27	126.23
25	b	607	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	c	507	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
30	d	407	LHG	C11-C10-C9	-2.62	101.13	114.42
25	a	611	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
25	c	511	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	b	622	LMG	C8-O7-C10	2.61	124.23	117.79
25	a	611	CLA	C1D-ND-C4D	2.61	108.19	106.33
29	D	408	SQD	C44-O6-C1	-2.61	109.51	113.84
31	h	102	DGD	C1E-O6E-C5E	2.61	118.81	113.69
31	c	516	DGD	O3D-C3D-C4D	-2.61	104.33	110.35
25	B	611	CLA	CMB-C2B-C3B	2.60	129.55	124.68
25	C	501	CLA	CHD-C1D-ND	-2.60	122.06	124.45
25	c	508	CLA	CHD-C1D-ND	-2.60	122.06	124.45
30	d	408	LHG	O8-C23-C24	2.60	120.07	111.91
27	A	610	PL9	C22-C23-C24	-2.60	121.40	127.66
26	t	101	BCR	C35-C13-C14	-2.60	119.28	122.92
25	a	605	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	B	607	CLA	CED-O2D-CGD	2.60	121.81	115.94
31	c	516	DGD	CDB-CCB-CBB	-2.60	101.25	114.42
34	f	101	HEM	C4D-ND-C1D	2.60	107.75	105.07
25	c	505	CLA	CHB-C4A-NA	2.59	128.10	124.51
32	B	624	STE	C3-C2-C1	-2.59	107.94	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	CHD-C1D-ND	-2.59	122.07	124.45
31	c	515	DGD	C3G-C2G-C1G	-2.59	105.67	111.79
27	A	610	PL9	C7-C8-C9	-2.59	122.49	126.79
25	D	403	CLA	CMB-C2B-C3B	2.58	129.51	124.68
25	B	605	CLA	CMB-C2B-C3B	2.58	129.51	124.68
27	D	406	PL9	C40-C39-C41	2.58	119.61	115.27
25	b	604	CLA	C6-C7-C8	-2.58	107.59	115.92
26	b	617	BCR	C3-C4-C5	-2.58	109.47	114.08
25	a	608	CLA	O2D-CGD-CBD	2.57	115.84	111.27
26	C	514	BCR	C15-C14-C13	-2.57	123.64	127.31
26	K	103	BCR	C27-C26-C25	2.57	126.47	122.73
25	C	510	CLA	O2D-CGD-CBD	2.57	115.84	111.27
25	c	504	CLA	C1-C2-C3	-2.57	121.60	126.04
25	a	608	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
25	C	501	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
25	b	608	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
34	f	101	HEM	C3B-C2B-C1B	2.57	108.39	106.49
25	b	613	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
29	D	408	SQD	C3-C4-C5	2.56	114.81	110.24
25	C	503	CLA	C2D-C1D-ND	-2.56	108.22	110.10
25	a	606	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
28	m	101	LMG	C38-C37-C36	-2.56	101.45	114.42
25	B	614	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
25	a	606	CLA	CMB-C2B-C3B	2.56	129.46	124.68
25	b	611	CLA	CMB-C2B-C3B	2.55	129.45	124.68
26	H	101	BCR	C2-C1-C6	2.55	114.41	110.48
25	D	403	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
25	C	511	CLA	C2D-C1D-ND	-2.55	108.23	110.10
26	K	101	BCR	C2-C1-C6	2.55	114.40	110.48
25	c	509	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
34	f	101	HEM	C1B-NB-C4B	2.55	107.70	105.07
27	A	610	PL9	C40-C39-C41	2.54	119.55	115.27
26	H	101	BCR	C27-C26-C25	2.54	126.42	122.73
25	c	505	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	C	513	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	d	404	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
27	D	406	PL9	C7-C8-C9	-2.53	122.57	126.79
31	C	516	DGD	C3E-C4E-C5E	-2.53	105.72	110.24
27	a	610	PL9	C40-C39-C41	2.53	119.53	115.27
31	c	515	DGD	O5D-C6D-C5D	-2.53	104.36	109.05
34	E	101	HEM	CBD-CAD-C3D	-2.53	105.59	112.63
25	D	403	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C27-C26-C25	2.53	126.40	122.73
25	B	611	CLA	C2D-C1D-ND	-2.53	108.24	110.10
30	D	412	LHG	O8-C23-O10	-2.53	117.22	123.59
27	D	406	PL9	C20-C19-C21	2.53	119.52	115.27
25	b	607	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
25	c	506	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
25	b	610	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
25	B	602	CLA	C2D-C1D-ND	-2.52	108.25	110.10
29	A	613	SQD	O5-C1-C2	-2.52	105.02	110.35
28	m	101	LMG	C40-C39-C38	-2.52	101.65	114.42
25	B	606	CLA	CHB-C4A-NA	2.51	127.99	124.51
31	h	102	DGD	O6E-C5E-C4E	2.51	114.26	109.69
25	A	611	CLA	C11-C12-C13	-2.51	107.80	115.92
31	c	515	DGD	O3E-C3E-C2E	-2.51	104.55	110.35
25	B	609	CLA	C7-C6-C5	-2.51	106.55	113.36
25	B	609	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
25	a	605	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
25	d	404	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
25	c	512	CLA	CMB-C2B-C3B	2.50	129.36	124.68
27	a	610	PL9	O1-C4-C3	-2.50	117.96	120.72
26	a	609	BCR	C3-C4-C5	-2.50	109.61	114.08
27	A	610	PL9	O2-C1-C2	-2.50	116.05	121.78
27	A	610	PL9	C20-C19-C21	2.50	119.48	115.27
25	c	508	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
26	H	101	BCR	C16-C15-C14	-2.50	118.35	123.47
31	A	616	DGD	CDB-CCB-CBB	-2.50	101.73	114.42
26	B	619	BCR	C15-C16-C17	-2.50	118.35	123.47
31	c	516	DGD	O6E-C1E-O5D	-2.50	104.06	109.97
34	f	101	HEM	CBD-CAD-C3D	-2.49	105.69	112.63
25	B	606	CLA	CGD-CBD-CAD	-2.49	102.66	110.73
28	D	407	LMG	O3-C3-C2	-2.49	104.59	110.35
25	b	611	CLA	C2D-C1D-ND	-2.49	108.27	110.10
28	c	520	LMG	O3-C3-C2	-2.49	104.59	110.35
25	a	606	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	A	614	LHG	C11-C10-C9	-2.48	101.83	114.42
25	b	607	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	b	613	CLA	CED-O2D-CGD	2.47	121.53	115.94
31	C	516	DGD	C4E-C3E-C2E	-2.47	106.51	110.82
33	D	402	PHO	OBD-CAD-CBD	-2.47	122.20	125.82
28	d	411	LMG	C40-C39-C38	-2.47	101.89	114.42
25	A	611	CLA	C2D-C1D-ND	-2.47	108.28	110.10
30	D	410	LHG	C11-C10-C9	-2.47	101.90	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	515	DGD	CDB-CCB-CBB	-2.47	101.91	114.42
25	A	608	CLA	CHD-C4C-NC	2.47	128.09	124.20
25	b	601	CLA	CHB-C4A-NA	2.46	127.92	124.51
31	c	516	DGD	O2D-C2D-C1D	-2.46	104.06	110.05
25	B	611	CLA	CHB-C4A-NA	2.46	127.92	124.51
28	c	520	LMG	C38-C37-C36	-2.46	101.93	114.42
30	d	408	LHG	C11-C10-C9	-2.46	101.93	114.42
29	b	620	SQD	O2-C2-C1	2.46	116.02	110.05
25	b	608	CLA	O2D-CGD-CBD	2.46	115.64	111.27
25	b	614	CLA	C1-C2-C3	-2.46	121.79	126.04
25	b	604	CLA	CAC-C3C-C4C	2.46	128.00	124.81
26	t	101	BCR	C27-C26-C25	2.46	126.30	122.73
26	A	609	BCR	C7-C8-C9	-2.46	122.52	126.23
26	a	609	BCR	C7-C8-C9	-2.46	122.52	126.23
28	D	407	LMG	O8-C28-O10	-2.46	117.39	123.59
32	B	626	STE	O2-C1-C2	2.46	121.92	114.03
26	C	514	BCR	C35-C13-C14	-2.46	119.48	122.92
28	c	518	LMG	O6-C1-O1	-2.45	104.16	109.97
28	A	612	LMG	C40-C39-C38	-2.45	101.99	114.42
26	B	619	BCR	C15-C14-C13	-2.45	123.81	127.31
28	c	521	LMG	O7-C10-O9	-2.45	117.78	123.70
25	A	608	CLA	O2D-CGD-CBD	2.45	115.62	111.27
26	k	102	BCR	C27-C26-C25	2.44	126.28	122.73
31	A	616	DGD	O5D-C6D-C5D	-2.44	104.52	109.05
30	L	101	LHG	C20-C19-C18	-2.44	102.02	114.42
25	C	501	CLA	CMB-C2B-C3B	2.44	129.24	124.68
31	h	102	DGD	O5E-C6E-C5E	-2.44	102.93	111.29
25	d	404	CLA	CHD-C1D-ND	-2.44	122.21	124.45
26	k	103	BCR	C27-C26-C25	2.44	126.27	122.73
25	C	510	CLA	C11-C10-C8	-2.43	108.05	115.92
28	D	411	LMG	O1-C7-C8	-2.43	105.33	111.78
25	C	512	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	B	607	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
26	b	618	BCR	C27-C26-C25	2.43	126.25	122.73
25	b	612	CLA	C11-C12-C13	-2.42	108.09	115.92
33	d	402	PHO	OBD-CAD-CBD	-2.42	122.27	125.82
25	A	607	CLA	C2D-C1D-ND	-2.42	108.32	110.10
27	d	406	PL9	C37-C38-C39	-2.42	121.83	127.66
25	B	612	CLA	C11-C12-C13	-2.42	108.11	115.92
25	C	513	CLA	CHB-C4A-NA	2.42	127.85	124.51
25	C	508	CLA	C2D-C1D-ND	-2.42	108.32	110.10
27	a	610	PL9	C37-C38-C39	-2.41	121.84	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C38-C26-C27	-2.41	108.98	113.62
25	b	610	CLA	CAA-CBA-CGA	-2.41	106.20	113.25
25	C	508	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	B	608	CLA	O2D-CGD-CBD	2.41	115.54	111.27
30	D	412	LHG	C18-C17-C16	-2.41	102.21	114.42
32	L	102	STE	O2-C1-C2	2.40	121.76	114.03
28	d	411	LMG	O1-C7-C8	-2.40	105.10	110.90
31	h	102	DGD	CBB-CAB-C9B	-2.40	102.22	114.42
25	B	601	CLA	C2A-C1A-CHA	2.40	128.06	123.86
30	l	101	LHG	C11-C10-C9	-2.40	102.23	114.42
25	C	506	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	f	102	SQD	C3-C4-C5	2.40	114.52	110.24
25	A	607	CLA	C1-C2-C3	-2.40	121.89	126.04
26	b	619	BCR	C2-C1-C6	2.40	114.17	110.48
25	B	603	CLA	C4-C3-C5	2.40	119.31	115.27
30	A	614	LHG	C20-C19-C18	-2.40	102.25	114.42
25	D	404	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
31	c	516	DGD	O5D-C6D-C5D	-2.40	104.61	109.05
25	b	605	CLA	CMB-C2B-C3B	2.40	129.16	124.68
31	c	517	DGD	CAB-C9B-C8B	-2.39	102.27	114.42
25	B	603	CLA	C5-C3-C2	-2.39	116.27	121.12
31	C	515	DGD	O5D-C6D-C5D	-2.39	104.62	109.05
25	b	615	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	C	501	CLA	C1-C2-C3	-2.39	121.91	126.04
25	C	504	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
28	C	517	LMG	C40-C39-C38	-2.39	102.30	114.42
30	l	101	LHG	C20-C19-C18	-2.39	102.30	114.42
25	A	607	CLA	C2A-C1A-CHA	2.39	128.03	123.86
25	b	606	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	B	601	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
25	B	611	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
30	D	409	LHG	C20-C19-C18	-2.38	102.32	114.42
25	c	506	CLA	CHB-C4A-NA	2.38	127.81	124.51
28	A	612	LMG	C38-C37-C36	-2.38	102.33	114.42
25	C	505	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	B	615	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	B	605	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
25	b	610	CLA	C1-C2-C3	-2.38	121.93	126.04
27	d	406	PL9	C27-C28-C29	-2.38	121.94	127.66
25	b	605	CLA	CHB-C4A-NA	2.38	127.80	124.51
28	b	622	LMG	C40-C39-C38	-2.38	102.37	114.42
25	c	502	CLA	C1-C2-C3	-2.37	121.94	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
31	a	614	DGD	CBB-CAB-C9B	-2.37	102.39	114.42
31	c	515	DGD	O6D-C1D-O3G	-2.37	104.36	109.97
29	B	623	SQD	O8-S-C6	2.37	109.51	105.74
31	c	516	DGD	CBB-CAB-C9B	-2.37	102.41	114.42
31	h	102	DGD	O3E-C3E-C2E	-2.37	104.88	110.35
25	B	616	CLA	CHB-C4A-NA	2.37	127.78	124.51
25	b	607	CLA	CHD-C4C-NC	2.36	127.93	124.20
25	D	404	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	H	102	DGD	C3G-C2G-C1G	-2.36	106.20	111.79
25	B	605	CLA	CHD-C1D-C2D	2.36	130.44	125.48
27	a	610	PL9	C12-C13-C14	-2.36	121.97	127.66
25	b	615	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
35	v	201	HEC	CBA-CAA-C2A	-2.36	108.63	112.60
25	A	607	CLA	C1D-ND-C4D	2.36	108.01	106.33
25	B	603	CLA	CHB-C4A-NA	2.36	127.77	124.51
28	A	612	LMG	O1-C7-C8	-2.35	105.22	110.90
25	B	612	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
28	d	411	LMG	O3-C3-C2	-2.35	104.91	110.35
25	c	502	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	b	606	CLA	C1-C2-C3	-2.35	121.98	126.04
26	D	405	BCR	C24-C23-C22	-2.35	122.68	126.23
25	C	510	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	C	509	CLA	CED-O2D-CGD	2.35	121.25	115.94
25	B	603	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
30	D	410	LHG	O8-C6-C5	-2.35	101.60	108.43
25	c	507	CLA	C4-C3-C5	2.35	119.22	115.27
25	b	601	CLA	O2D-CGD-CBD	2.34	115.44	111.27
31	A	616	DGD	CAB-C9B-C8B	-2.34	102.52	114.42
25	C	510	CLA	CHD-C1D-ND	-2.34	122.30	124.45
26	C	514	BCR	C2-C1-C6	2.34	114.09	110.48
27	D	406	PL9	C8-C7-C3	2.34	118.60	111.98
28	C	517	LMG	C38-C37-C36	-2.34	102.54	114.42
25	A	611	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	A	606	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	b	606	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	B	609	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
28	B	620	LMG	O1-C7-C8	-2.34	105.26	110.90
25	b	605	CLA	O1D-CGD-CBD	2.34	129.26	124.48
28	B	620	LMG	O7-C10-O9	-2.33	118.06	123.70
25	B	614	CLA	C1-C2-C3	-2.33	122.01	126.04
31	C	516	DGD	CBB-CAB-C9B	-2.33	102.59	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	502	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
25	b	613	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	d	409	LHG	C27-C26-C25	-2.33	102.60	114.42
30	e	101	LHG	C11-C10-C9	-2.33	102.60	114.42
25	b	601	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
25	B	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	c	510	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
28	c	520	LMG	O2-C2-C1	-2.32	104.40	110.05
25	A	608	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
31	H	102	DGD	CAB-C9B-C8B	-2.32	102.64	114.42
28	c	520	LMG	C40-C39-C38	-2.32	102.64	114.42
29	A	613	SQD	C44-O6-C1	-2.32	109.21	113.74
31	C	516	DGD	C1D-C2D-C3D	-2.32	105.17	110.00
31	c	516	DGD	C3G-C2G-C1G	-2.32	106.30	111.79
25	B	613	CLA	C2D-C1D-ND	-2.32	108.40	110.10
25	B	602	CLA	C16-C15-C13	-2.31	108.44	115.92
25	c	503	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
25	C	502	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
25	C	513	CLA	CHD-C1D-C2D	2.31	130.33	125.48
31	C	515	DGD	O3E-C3E-C2E	-2.31	105.00	110.35
25	C	507	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
30	d	408	LHG	C20-C19-C18	-2.31	102.69	114.42
32	j	101	STE	O2-C1-C2	2.31	121.45	114.03
25	b	614	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	b	615	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	D	404	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	B	618	BCR	C15-C14-C13	-2.31	124.02	127.31
31	c	516	DGD	O3G-C1D-C2D	-2.31	104.70	108.30
25	A	608	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
25	B	613	CLA	CED-O2D-CGD	2.31	121.15	115.94
27	a	610	PL9	O2-C1-C2	-2.30	116.50	121.78
25	D	403	CLA	C1-C2-C3	-2.30	122.06	126.04
28	d	411	LMG	C38-C37-C36	-2.30	102.73	114.42
25	C	508	CLA	C1-C2-C3	-2.30	122.06	126.04
25	D	403	CLA	O2D-CGD-CBD	2.30	115.36	111.27
27	D	406	PL9	O1-C4-C3	-2.30	118.19	120.72
26	D	405	BCR	C7-C8-C9	-2.30	122.77	126.23
27	d	406	PL9	C8-C7-C3	2.30	118.47	111.98
25	c	508	CLA	C2D-C1D-ND	-2.29	108.41	110.10
25	a	605	CLA	C4-C3-C5	2.29	119.13	115.27
25	b	602	CLA	C1-C2-C3	-2.29	122.08	126.04
31	a	614	DGD	C1G-C2G-C3G	-2.29	106.45	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CMB-C2B-C1B	-2.29	124.95	128.46
25	B	608	CLA	C2D-C1D-ND	-2.29	108.42	110.10
31	c	517	DGD	C6D-C5D-C4D	2.28	116.86	112.09
25	b	604	CLA	O2D-CGD-CBD	2.28	115.33	111.27
28	c	518	LMG	C40-C39-C38	-2.28	102.84	114.42
25	b	605	CLA	CHD-C4C-NC	2.28	127.80	124.20
27	A	610	PL9	O2-C1-C6	2.28	124.54	120.59
28	c	520	LMG	O7-C10-O9	-2.28	118.19	123.70
25	B	615	CLA	O2D-CGD-CBD	2.28	115.32	111.27
31	h	102	DGD	C3G-C2G-C1G	-2.28	106.40	111.79
25	c	507	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	B	612	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
25	B	605	CLA	CHB-C4A-NA	2.28	127.66	124.51
28	c	520	LMG	O6-C1-O1	-2.27	104.59	109.97
30	D	409	LHG	C11-C10-C9	-2.27	102.89	114.42
30	e	101	LHG	C20-C19-C18	-2.27	102.91	114.42
25	b	614	CLA	C2D-C1D-ND	-2.27	108.43	110.10
25	a	611	CLA	C3C-C4C-NC	-2.27	108.03	110.57
26	B	618	BCR	C33-C5-C6	-2.27	121.98	124.53
25	C	503	CLA	C16-C15-C13	-2.27	108.59	115.92
28	c	521	LMG	C38-C37-C36	-2.27	102.92	114.42
25	c	505	CLA	C1D-ND-C4D	2.27	107.94	106.33
28	b	622	LMG	O6-C1-O1	-2.27	104.61	109.97
25	A	606	CLA	O1D-CGD-CBD	2.27	129.12	124.48
27	d	406	PL9	O1-C4-C3	-2.26	118.23	120.72
25	c	503	CLA	C2D-C1D-ND	-2.26	108.44	110.10
25	C	510	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
25	C	503	CLA	CHB-C4A-NA	2.26	127.64	124.51
33	D	402	PHO	CMC-C2C-C3C	2.26	129.20	124.94
28	D	407	LMG	O2-C2-C1	-2.26	104.56	110.05
25	B	616	CLA	C1-O2A-CGA	2.26	122.37	116.44
25	C	508	CLA	CHD-C1D-C2D	2.26	130.22	125.48
28	B	620	LMG	C40-C39-C38	-2.26	102.96	114.42
25	b	613	CLA	C7-C6-C5	-2.26	107.23	113.36
25	C	506	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	D	405	BCR	C35-C13-C14	-2.26	119.76	122.92
30	d	409	LHG	O8-C23-C24	2.26	118.99	111.91
25	C	507	CLA	O2D-CGD-CBD	2.26	115.28	111.27
31	J	101	DGD	O5E-C6E-C5E	-2.25	103.56	111.29
25	c	511	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
28	c	518	LMG	C38-C37-C36	-2.25	102.99	114.42
25	B	614	CLA	O2A-CGA-O1A	-2.25	117.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	410	LHG	C27-C26-C25	-2.25	102.99	114.42
31	C	516	DGD	O5D-C1E-C2E	2.25	111.82	108.30
25	c	502	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
31	A	616	DGD	C8B-C7B-C6B	-2.25	103.01	114.42
28	m	101	LMG	C1-O6-C5	-2.25	109.27	113.69
31	c	517	DGD	C3G-C2G-C1G	-2.25	106.47	111.79
25	b	615	CLA	C1-C2-C3	-2.25	122.16	126.04
28	D	411	LMG	C38-C37-C36	-2.25	103.02	114.42
25	B	616	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	a	606	CLA	CHD-C1D-C2D	2.24	130.19	125.48
30	D	409	LHG	O8-C23-O10	-2.24	117.93	123.59
31	C	515	DGD	O1G-C1A-C2A	-2.24	104.87	111.91
27	a	610	PL9	C27-C28-C29	-2.24	122.26	127.66
31	C	515	DGD	C3D-C4D-C5D	-2.24	106.24	110.24
25	B	608	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	b	610	CLA	CMB-C2B-C3B	2.24	128.87	124.68
26	b	617	BCR	C15-C14-C13	-2.24	124.12	127.31
27	d	406	PL9	C42-C43-C44	-2.24	122.27	127.66
25	b	610	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
25	C	505	CLA	O2D-CGD-CBD	2.23	115.24	111.27
25	b	609	CLA	C7-C6-C5	-2.23	107.30	113.36
26	h	101	BCR	C35-C13-C14	-2.23	119.80	122.92
26	K	103	BCR	C24-C23-C22	-2.23	122.86	126.23
25	b	615	CLA	CMB-C2B-C3B	2.23	128.85	124.68
30	D	409	LHG	C27-C26-C25	-2.23	103.10	114.42
25	A	608	CLA	CHD-C1D-C2D	2.23	130.16	125.48
25	d	404	CLA	C2D-C1D-ND	-2.23	108.46	110.10
28	b	622	LMG	C42-C41-C40	-2.23	103.11	114.42
26	k	103	BCR	C33-C5-C6	-2.23	122.03	124.53
25	b	616	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
25	a	605	CLA	O1D-CGD-CBD	2.23	129.04	124.48
25	A	606	CLA	CHD-C1D-ND	-2.22	122.41	124.45
30	D	412	LHG	C20-C19-C18	-2.22	103.14	114.42
25	b	604	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
26	H	101	BCR	C35-C13-C14	-2.22	119.81	122.92
28	D	407	LMG	O1-C1-C2	-2.22	104.84	108.30
25	B	605	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
31	H	102	DGD	C8B-C7B-C6B	-2.22	103.16	114.42
32	t	102	STE	O2-C1-C2	2.22	121.15	114.03
28	D	407	LMG	C38-C37-C36	-2.22	103.18	114.42
25	c	508	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
31	A	616	DGD	O6D-C1D-O3G	-2.21	104.74	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	CHD-C1D-ND	-2.21	122.42	124.45
27	d	406	PL9	C11-C12-C13	-2.21	104.62	111.88
25	a	611	CLA	CHD-C1D-C2D	2.21	130.11	125.48
25	b	610	CLA	CHB-C4A-NA	2.21	127.56	124.51
29	A	613	SQD	O47-C7-O49	-2.21	118.37	123.70
25	d	404	CLA	C1-C2-C3	-2.21	122.23	126.04
25	b	611	CLA	CHD-C1D-C2D	2.20	130.10	125.48
29	f	102	SQD	O48-C23-C24	2.20	118.82	111.91
31	c	516	DGD	C7B-C6B-C5B	-2.20	103.25	114.42
25	c	503	CLA	C11-C12-C13	-2.20	108.81	115.92
25	c	503	CLA	CHD-C1D-ND	-2.20	122.43	124.45
27	D	406	PL9	C50-C49-C48	-2.20	116.29	122.65
25	c	503	CLA	O1D-CGD-CBD	2.20	128.98	124.48
32	C	518	STE	C3-C2-C1	-2.20	108.93	114.47
25	b	601	CLA	C3C-C4C-NC	-2.20	108.11	110.57
28	b	622	LMG	C38-C37-C36	-2.20	103.27	114.42
26	h	101	BCR	C7-C8-C9	-2.20	122.92	126.23
28	c	518	LMG	O1-C7-C8	-2.20	105.60	110.90
25	c	511	CLA	CHD-C1D-ND	-2.20	122.44	124.45
25	a	605	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
31	J	101	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
25	B	606	CLA	CHD-C4C-NC	2.20	127.66	124.20
28	c	521	LMG	C40-C39-C38	-2.19	103.29	114.42
25	b	603	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	d	405	BCR	C7-C8-C9	-2.19	122.93	126.23
25	b	613	CLA	C16-C15-C13	-2.19	108.85	115.92
25	b	610	CLA	O1D-CGD-CBD	2.18	128.95	124.48
31	c	517	DGD	C7A-C6A-C5A	-2.18	103.34	114.42
25	B	614	CLA	O2D-CGD-CBD	2.18	115.15	111.27
27	a	610	PL9	C22-C23-C24	-2.18	122.40	127.66
26	c	514	BCR	C11-C10-C9	-2.18	124.20	127.31
32	E	102	STE	O2-C1-C2	2.18	121.04	114.03
25	d	403	CLA	CHB-C4A-NA	2.18	127.53	124.51
32	t	102	STE	O2-C1-O1	-2.18	117.86	123.30
25	C	511	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	A	607	CLA	CHB-C4A-NA	2.18	127.52	124.51
31	a	614	DGD	C5B-C4B-C3B	-2.18	103.37	114.42
27	d	406	PL9	O2-C1-C6	2.18	124.36	120.59
26	K	102	BCR	C27-C26-C25	2.18	125.89	122.73
29	B	623	SQD	C45-O47-C7	-2.18	112.43	117.79
30	D	410	LHG	C18-C17-C16	-2.17	103.39	114.42
25	B	603	CLA	O2A-C1-C2	-2.17	102.92	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
25	b	610	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
25	B	614	CLA	C3B-C4B-NB	-2.17	106.40	109.21
31	c	515	DGD	CBB-CAB-C9B	-2.17	103.40	114.42
31	C	515	DGD	CBB-CAB-C9B	-2.17	103.41	114.42
31	c	517	DGD	C5B-C4B-C3B	-2.17	103.41	114.42
31	J	101	DGD	O3G-C1D-C2D	-2.17	104.92	108.30
25	b	606	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	a	606	CLA	C2D-C1D-ND	-2.17	108.51	110.10
25	B	613	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	c	510	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	k	101	BCR	C33-C5-C6	-2.16	122.10	124.53
31	H	102	DGD	O6D-C1D-O3G	-2.16	104.85	109.97
26	b	618	BCR	C35-C13-C14	-2.16	119.89	122.92
25	C	512	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	K	101	BCR	C24-C23-C22	-2.16	122.97	126.23
25	c	503	CLA	C4-C3-C5	2.16	118.91	115.27
30	D	412	LHG	C15-C14-C13	-2.16	103.45	114.42
26	c	514	BCR	C33-C5-C6	-2.16	122.10	124.53
26	B	617	BCR	C27-C26-C25	2.16	125.86	122.73
28	b	622	LMG	C4-C3-C2	2.16	114.59	110.82
30	e	101	LHG	C27-C26-C25	-2.16	103.47	114.42
31	J	101	DGD	C7B-C6B-C5B	-2.16	103.48	114.42
25	b	604	CLA	C11-C10-C8	-2.16	108.95	115.92
27	D	406	PL9	C35-C34-C36	2.16	118.90	115.27
29	A	615	SQD	O48-C23-C24	2.16	118.67	111.91
25	b	601	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	B	610	CLA	O1D-CGD-CBD	2.15	128.89	124.48
28	B	622	LMG	C38-C37-C36	-2.15	103.49	114.42
25	b	614	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
26	A	609	BCR	C15-C16-C17	-2.15	119.06	123.47
25	C	509	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	D	403	CLA	C6-C5-C3	2.15	119.09	113.45
34	E	101	HEM	C4C-CHD-C1D	2.15	125.40	122.56
25	C	501	CLA	C3B-C4B-NB	-2.15	106.43	109.21
25	C	507	CLA	C2A-C1A-CHA	2.15	127.61	123.86
26	C	514	BCR	C33-C5-C6	-2.15	122.12	124.53
31	A	616	DGD	O3G-C3G-C2G	-2.15	105.72	110.90
33	d	402	PHO	CMD-C2D-C3D	2.14	128.69	124.68
25	B	608	CLA	CHD-C1D-ND	-2.14	122.48	124.45
35	V	201	HEC	CBD-CAD-C3D	-2.14	108.96	112.62
34	f	101	HEM	CMC-C2C-C3C	2.14	128.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	C2D-C1D-ND	-2.14	108.53	110.10
28	B	620	LMG	C38-C37-C36	-2.14	103.58	114.42
25	B	601	CLA	O2D-CGD-CBD	2.13	115.06	111.27
31	c	515	DGD	C7A-C6A-C5A	-2.13	103.59	114.42
26	b	617	BCR	C33-C5-C6	-2.13	122.13	124.53
25	b	609	CLA	CHB-C4A-NA	2.13	127.46	124.51
28	C	517	LMG	O8-C28-O10	-2.13	118.21	123.59
30	D	410	LHG	O8-C23-C24	2.13	118.59	111.91
26	B	619	BCR	C3-C4-C5	-2.13	110.28	114.08
25	C	507	CLA	C1-C2-C3	-2.12	122.37	126.04
25	A	611	CLA	C1-C2-C3	-2.12	122.37	126.04
27	d	406	PL9	C32-C33-C34	-2.12	122.55	127.66
25	B	604	CLA	CAA-CBA-CGA	-2.12	107.07	113.25
34	E	101	HEM	C4B-CHC-C1C	2.12	125.35	122.56
27	d	406	PL9	C31-C32-C33	-2.12	104.93	111.88
30	D	409	LHG	C18-C17-C16	-2.12	103.69	114.42
26	d	405	BCR	C38-C26-C25	-2.11	122.15	124.53
25	B	605	CLA	CHD-C4C-NC	2.11	127.53	124.20
25	b	607	CLA	C16-C15-C13	-2.11	109.09	115.92
29	A	613	SQD	O48-C23-C24	2.11	118.53	111.91
25	c	512	CLA	CHA-C1A-NA	-2.11	121.56	126.40
25	A	606	CLA	CHC-C1C-NC	2.11	127.41	124.20
26	k	101	BCR	C15-C14-C13	-2.11	124.30	127.31
26	C	514	BCR	C27-C26-C25	2.11	125.79	122.73
31	c	517	DGD	O3E-C3E-C2E	-2.11	105.47	110.35
25	C	509	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	B	607	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
28	A	612	LMG	O8-C28-O10	-2.11	118.27	123.59
25	b	614	CLA	O2A-C1-C2	-2.11	103.10	108.64
25	c	505	CLA	C3B-C4B-NB	-2.11	106.49	109.21
25	b	602	CLA	C16-C15-C13	-2.11	109.11	115.92
31	H	102	DGD	O1G-C1A-O1A	-2.11	118.28	123.59
33	a	607	PHO	O2A-CGA-O1A	-2.11	118.28	123.59
31	h	102	DGD	O5D-C1E-C2E	2.10	111.59	108.30
25	C	513	CLA	CHD-C4C-NC	2.10	127.52	124.20
25	B	606	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	b	602	CLA	C6-C7-C8	-2.10	109.12	115.92
31	J	101	DGD	O6E-C5E-C4E	2.10	113.51	109.69
25	b	602	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	b	618	BCR	C30-C25-C26	-2.10	119.65	122.61
25	b	614	CLA	O1D-CGD-CBD	2.10	128.78	124.48
25	C	503	CLA	CHD-C1D-C2D	2.10	129.88	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	509	CLA	C2D-C1D-ND	-2.10	108.56	110.10
26	h	101	BCR	C24-C23-C22	-2.10	123.06	126.23
25	b	611	CLA	C11-C10-C8	-2.10	109.14	115.92
31	A	616	DGD	O2D-C2D-C1D	-2.10	104.95	110.05
28	m	101	LMG	O6-C1-O1	-2.10	105.01	109.97
26	d	405	BCR	C30-C25-C26	-2.10	119.66	122.61
30	d	408	LHG	C18-C17-C16	-2.10	103.78	114.42
31	C	515	DGD	CAB-C9B-C8B	-2.10	103.78	114.42
26	H	101	BCR	C3-C4-C5	-2.10	110.33	114.08
25	d	403	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	c	516	DGD	CAB-C9B-C8B	-2.09	103.79	114.42
25	a	605	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
25	c	505	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
25	C	503	CLA	C1-O2A-CGA	2.09	121.93	116.44
31	a	614	DGD	CFB-CEB-CDB	-2.09	103.81	114.42
27	d	406	PL9	C35-C34-C36	2.09	118.79	115.27
30	d	407	LHG	C20-C19-C18	-2.09	103.81	114.42
33	a	607	PHO	CMC-C2C-C3C	2.09	128.88	124.94
31	c	516	DGD	C1D-O6D-C5D	-2.09	109.58	113.69
26	t	101	BCR	C7-C8-C9	-2.09	123.08	126.23
25	c	508	CLA	C1-C2-C3	-2.09	122.43	126.04
26	T	101	BCR	C30-C25-C26	-2.09	119.67	122.61
28	c	521	LMG	O1-C7-C8	-2.09	105.86	110.90
28	d	410	LMG	C38-C37-C36	-2.09	103.83	114.42
25	C	505	CLA	CHB-C4A-NA	2.09	127.40	124.51
26	d	405	BCR	C1-C6-C5	-2.09	119.67	122.61
34	E	101	HEM	C3C-C4C-NC	-2.09	107.01	110.94
31	J	101	DGD	C5B-C4B-C3B	-2.09	103.84	114.42
25	c	501	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	A	607	CLA	CHA-C4D-ND	2.08	136.86	132.50
31	J	101	DGD	O3E-C3E-C2E	-2.08	105.53	110.35
28	C	517	LMG	O7-C10-O9	-2.08	118.67	123.70
25	b	609	CLA	O1D-CGD-CBD	2.08	128.75	124.48
25	B	603	CLA	C2D-C1D-ND	-2.08	108.57	110.10
28	c	521	LMG	O8-C28-O10	-2.08	118.34	123.59
26	b	618	BCR	C15-C16-C17	-2.08	119.21	123.47
28	A	612	LMG	O6-C1-O1	-2.08	105.05	109.97
26	h	101	BCR	C11-C10-C9	-2.08	124.34	127.31
31	A	616	DGD	CBB-CAB-C9B	-2.08	103.88	114.42
26	K	101	BCR	C3-C4-C5	-2.08	110.37	114.08
25	b	608	CLA	CHD-C4C-NC	2.07	127.47	124.20
25	b	603	CLA	O2A-CGA-O1A	-2.07	118.36	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	DGD	C5B-C4B-C3B	-2.07	103.91	114.42
26	b	617	BCR	C38-C26-C25	-2.07	122.20	124.53
25	B	606	CLA	CMB-C2B-C3B	2.07	128.55	124.68
25	b	612	CLA	CHD-C1D-ND	-2.07	122.56	124.45
25	b	601	CLA	C16-C15-C13	-2.07	109.24	115.92
25	B	605	CLA	O1D-CGD-CBD	2.06	128.71	124.48
28	c	521	LMG	C20-C19-C18	-2.06	103.94	114.42
25	A	608	CLA	CHC-C1C-NC	2.06	127.33	124.20
29	a	612	SQD	O5-C1-C2	-2.06	105.98	110.35
30	e	101	LHG	C5-O7-C7	-2.06	112.72	117.79
25	C	505	CLA	C2D-C1D-ND	-2.06	108.58	110.10
26	t	101	BCR	C1-C6-C5	-2.06	119.71	122.61
25	B	612	CLA	C1-C2-C3	-2.06	122.48	126.04
25	b	605	CLA	CHD-C1D-C2D	2.06	129.79	125.48
25	a	606	CLA	CHC-C1C-NC	2.06	127.32	124.20
25	c	502	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	C	504	CLA	CHB-C4A-NA	2.06	127.35	124.51
32	b	621	STE	C3-C2-C1	-2.06	109.29	114.47
25	C	512	CLA	O2D-CGD-CBD	2.05	114.91	111.27
31	c	517	DGD	C8B-C7B-C6B	-2.05	104.01	114.42
28	d	410	LMG	C40-C39-C38	-2.05	104.04	114.42
25	c	501	CLA	CHD-C1D-ND	-2.05	122.57	124.45
28	c	520	LMG	C42-C41-C40	-2.05	104.04	114.42
25	B	607	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	c	516	DGD	C9B-C8B-C7B	-2.04	104.06	114.42
29	D	408	SQD	C46-C45-C44	-2.04	106.91	113.70
25	B	611	CLA	CHD-C1D-C2D	2.04	129.76	125.48
27	a	610	PL9	O2-C1-C6	2.04	124.12	120.59
31	C	516	DGD	O2D-C2D-C1D	-2.04	105.09	110.05
26	h	101	BCR	C3-C4-C5	-2.04	110.44	114.08
33	a	607	PHO	C1B-NB-C4B	2.04	111.28	107.09
32	C	518	STE	C4-C3-C2	-2.04	105.87	113.19
25	c	504	CLA	O2D-CGD-CBD	2.04	114.89	111.27
31	A	616	DGD	C5B-C4B-C3B	-2.04	104.09	114.42
25	D	403	CLA	CED-O2D-CGD	2.04	120.54	115.94
25	c	505	CLA	C11-C10-C8	-2.03	109.34	115.92
25	B	604	CLA	CHA-C4D-ND	2.03	136.75	132.50
25	A	607	CLA	CHA-C1A-NA	-2.03	121.74	126.40
31	c	515	DGD	O3D-C3D-C4D	-2.03	105.65	110.35
31	c	515	DGD	C1D-C2D-C3D	-2.03	105.76	110.00
25	b	601	CLA	CHD-C1D-C2D	2.03	129.74	125.48
25	b	611	CLA	CHB-C4A-NA	2.03	127.32	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	609	BCR	C38-C26-C25	-2.03	122.25	124.53
25	b	616	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	c	511	CLA	C2A-C1A-CHA	2.03	127.40	123.86
30	A	614	LHG	C27-C26-C25	-2.03	104.14	114.42
26	K	101	BCR	C35-C13-C14	-2.03	120.09	122.92
26	K	101	BCR	C7-C8-C9	-2.03	123.17	126.23
25	B	607	CLA	C4-C3-C5	2.02	118.68	115.27
25	c	501	CLA	CHA-C4D-ND	2.02	136.73	132.50
25	C	508	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
28	c	518	LMG	O8-C28-O10	-2.02	118.49	123.59
28	m	101	LMG	O2-C2-C1	-2.02	105.14	110.05
28	b	622	LMG	O7-C10-O9	-2.02	118.82	123.70
28	m	101	LMG	O3-C3-C2	-2.02	105.68	110.35
31	C	516	DGD	CAB-C9B-C8B	-2.02	104.18	114.42
25	C	512	CLA	C11-C12-C13	-2.02	109.39	115.92
28	B	620	LMG	C6-C5-C4	-2.02	108.28	113.00
25	B	601	CLA	CAA-C2A-C1A	2.02	118.59	111.97
30	L	101	LHG	C27-C26-C25	-2.02	104.19	114.42
25	b	610	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	b	608	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	K	102	BCR	C1-C6-C5	-2.02	119.78	122.61
28	D	407	LMG	C3-C4-C5	-2.01	106.64	110.24
28	D	407	LMG	C40-C39-C38	-2.01	104.20	114.42
25	b	605	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	b	614	CLA	C16-C15-C13	-2.01	109.41	115.92
25	C	504	CLA	C2D-C1D-ND	-2.01	108.62	110.10
25	C	504	CLA	CHD-C4C-NC	2.01	127.38	124.20
25	c	504	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
25	B	605	CLA	C16-C15-C13	-2.01	109.42	115.92
32	B	624	STE	C6-C5-C4	-2.01	104.22	114.42
30	d	408	LHG	O8-C23-O10	-2.01	118.52	123.59
28	c	520	LMG	C6-C5-C4	-2.01	108.30	113.00
31	J	101	DGD	C7A-C6A-C5A	-2.01	104.23	114.42
34	E	101	HEM	C2D-C1D-ND	-2.01	107.48	109.88
25	b	604	CLA	C11-C12-C13	-2.01	109.43	115.92
27	D	406	PL9	C11-C12-C13	-2.01	105.28	111.88
28	b	622	LMG	O2-C2-C1	-2.01	105.17	110.05
28	A	612	LMG	O3-C3-C2	-2.01	105.71	110.35
25	C	512	CLA	CHA-C1A-NA	-2.01	121.81	126.40
25	d	403	CLA	O1D-CGD-CBD	2.01	128.59	124.48
31	c	515	DGD	O2D-C2D-C1D	-2.01	105.17	110.05
28	d	410	LMG	O7-C10-O9	-2.00	118.30	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C35-C13-C14	-2.00	120.12	122.92
28	m	101	LMG	C31-C30-C29	-2.00	105.99	113.19
31	C	515	DGD	C7B-C6B-C5B	-2.00	104.26	114.42
25	C	503	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
25	C	513	CLA	C3C-C4C-NC	-2.00	108.33	110.57
28	B	620	LMG	C1-O6-C5	-2.00	109.76	113.69
25	D	404	CLA	C3C-C4C-NC	-2.00	108.33	110.57
25	b	614	CLA	C3C-C4C-NC	-2.00	108.33	110.57

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	A	611	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND

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Mol	Chain	Res	Type	Atom
25	D	404	CLA	ND
25	a	605	CLA	ND
25	a	606	CLA	ND
25	a	608	CLA	ND
25	a	611	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND

All (1870) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	C2-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	B	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C2-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	a	606	CLA	CHA-CBD-CGD-O1D
25	a	606	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	C11-C10-C8-C9
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C2-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	b	616	CLA	C11-C10-C8-C9
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	513	CLA	CBD-CGD-O2D-CED
26	A	609	BCR	C20-C21-C22-C37
26	B	617	BCR	C1-C6-C7-C8
26	B	618	BCR	C37-C22-C23-C24
26	B	618	BCR	C23-C24-C25-C30
26	B	619	BCR	C11-C12-C13-C35
26	B	619	BCR	C37-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	K	101	BCR	C7-C8-C9-C34
26	K	101	BCR	C11-C10-C9-C8
26	K	102	BCR	C5-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C7-C8-C9-C34
26	b	617	BCR	C1-C6-C7-C8
26	b	618	BCR	C7-C8-C9-C34
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C34
26	d	405	BCR	C7-C8-C9-C34
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C22-C23-C24-C25
26	d	405	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
26	h	101	BCR	C11-C12-C13-C35
26	h	101	BCR	C22-C23-C24-C25
26	k	101	BCR	C6-C7-C8-C9
26	k	102	BCR	C20-C21-C22-C37
26	k	102	BCR	C37-C22-C23-C24
26	k	103	BCR	C17-C18-C19-C20
26	k	103	BCR	C36-C18-C19-C20
27	A	610	PL9	C9-C11-C12-C13
27	A	610	PL9	C18-C19-C21-C22
27	A	610	PL9	C20-C19-C21-C22
27	A	610	PL9	C35-C34-C36-C37
27	A	610	PL9	C37-C38-C39-C40
27	A	610	PL9	C37-C38-C39-C41
27	A	610	PL9	C40-C39-C41-C42
27	D	406	PL9	C35-C34-C36-C37
27	a	610	PL9	C12-C13-C14-C16
27	a	610	PL9	C32-C33-C34-C35
27	a	610	PL9	C47-C48-C49-C50
27	d	406	PL9	C32-C33-C34-C35
27	d	406	PL9	C35-C34-C36-C37
27	d	406	PL9	C40-C39-C41-C42
28	A	612	LMG	O6-C1-O1-C7
28	A	612	LMG	O9-C10-O7-C8
28	A	612	LMG	C11-C10-O7-C8
28	C	517	LMG	O9-C10-O7-C8
28	C	517	LMG	C11-C10-O7-C8
28	D	411	LMG	C11-C10-O7-C8
28	b	622	LMG	C2-C1-O1-C7
28	b	622	LMG	O6-C1-O1-C7
28	b	622	LMG	O7-C8-C9-O8
28	c	521	LMG	O6-C1-O1-C7
29	B	623	SQD	C2-C1-O6-C44
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	a	613	SQD	O6-C44-C45-C46
29	a	613	SQD	O6-C44-C45-O47
29	a	613	SQD	C8-C7-O47-C45
29	b	620	SQD	O5-C1-O6-C44
29	b	620	SQD	C8-C7-O47-C45
29	b	620	SQD	C24-C23-O48-C46
29	b	620	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C5-C6-S-O8
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
29	f	102	SQD	O10-C23-O48-C46
30	A	614	LHG	C4-O6-P-O4
30	D	409	LHG	C3-O3-P-O6
30	D	409	LHG	C4-O6-P-O4
30	L	101	LHG	C3-O3-P-O4
30	d	407	LHG	C4-O6-P-O5
30	d	408	LHG	C4-O6-P-O4
30	d	409	LHG	O1-C1-C2-C3
30	e	101	LHG	O1-C1-C2-O2
30	e	101	LHG	O1-C1-C2-C3
30	e	101	LHG	C3-O3-P-O4
30	e	101	LHG	C4-O6-P-O5
30	e	101	LHG	O10-C23-O8-C6
30	e	101	LHG	C24-C23-O8-C6
31	A	616	DGD	O1B-C1B-O2G-C2G
31	A	616	DGD	O2G-C2G-C3G-O3G
31	a	614	DGD	C2B-C1B-O2G-C2G
33	d	402	PHO	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CBD-CGD-O2D-CED
28	m	101	LMG	O10-C28-O8-C9
29	b	620	SQD	O10-C23-O48-C46
25	b	601	CLA	O1D-CGD-O2D-CED
31	a	614	DGD	C2G-C1G-O1G-C1A
33	d	402	PHO	O1D-CGD-O2D-CED
28	m	101	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
27	a	610	PL9	C47-C48-C49-C51
25	B	606	CLA	CBD-CGD-O2D-CED
28	c	520	LMG	O10-C28-O8-C9
29	a	613	SQD	O10-C23-O48-C46
31	H	102	DGD	O6E-C5E-C6E-O5E
25	c	513	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
28	D	411	LMG	O9-C10-O7-C8
28	c	520	LMG	O9-C10-O7-C8
29	a	613	SQD	O49-C7-O47-C45
31	a	614	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	A	608	CLA	C3-C5-C6-C7
25	B	604	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
29	a	613	SQD	C24-C23-O48-C46
28	c	520	LMG	C11-C10-O7-C8
29	B	623	SQD	C8-C7-O47-C45
31	A	616	DGD	C2B-C1B-O2G-C2G
27	A	610	PL9	C23-C24-C26-C27
25	b	607	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
28	c	520	LMG	C29-C28-O8-C9
25	C	511	CLA	O1D-CGD-O2D-CED
27	D	406	PL9	C32-C33-C34-C35
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
29	b	620	SQD	O49-C7-O47-C45
28	c	521	LMG	O10-C28-O8-C9
25	C	509	CLA	CBD-CGD-O2D-CED
30	d	408	LHG	O2-C2-C3-O3
25	B	605	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
28	c	521	LMG	C29-C28-O8-C9
29	D	408	SQD	C24-C23-O48-C46
31	H	102	DGD	C4E-C5E-C6E-O5E
25	C	503	CLA	CBD-CGD-O2D-CED
28	B	620	LMG	O10-C28-O8-C9
30	A	614	LHG	C32-C33-C34-C35
29	A	613	SQD	C30-C31-C32-C33
25	B	614	CLA	C15-C16-C17-C18
28	b	622	LMG	O6-C5-C6-O5
28	c	518	LMG	O6-C5-C6-O5
29	D	408	SQD	O10-C23-O48-C46
31	a	614	DGD	O1A-C1A-O1G-C1G
27	D	406	PL9	C47-C48-C49-C51
27	d	406	PL9	C47-C48-C49-C51
25	C	513	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	C4-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
27	A	610	PL9	C33-C34-C36-C37
27	A	610	PL9	C43-C44-C46-C47
27	d	406	PL9	C38-C39-C41-C42
25	B	606	CLA	C2A-CAA-CBA-CGA
29	A	613	SQD	C32-C33-C34-C35
28	b	622	LMG	O10-C28-O8-C9
28	A	612	LMG	C4-C5-C6-O5
28	m	101	LMG	O6-C1-O1-C7
27	A	610	PL9	C29-C31-C32-C33
27	a	610	PL9	C24-C26-C27-C28
27	a	610	PL9	C39-C41-C42-C43
31	h	102	DGD	O6E-C5E-C6E-O5E
28	d	411	LMG	C10-C11-C12-C13
25	B	606	CLA	O1D-CGD-O2D-CED
28	C	517	LMG	C4-C5-C6-O5
27	a	610	PL9	C22-C23-C24-C25
25	b	602	CLA	CBD-CGD-O2D-CED
29	a	612	SQD	C7-C8-C9-C10
27	a	610	PL9	C22-C23-C24-C26
27	a	610	PL9	C42-C43-C44-C46
28	B	620	LMG	C29-C28-O8-C9
28	b	622	LMG	C29-C28-O8-C9
25	b	606	CLA	C15-C16-C17-C18
31	A	616	DGD	O6E-C5E-C6E-O5E
29	B	623	SQD	C10-C11-C12-C13
25	B	613	CLA	C8-C10-C11-C12
25	a	611	CLA	C15-C16-C17-C18
25	b	607	CLA	C8-C10-C11-C12
32	B	624	STE	C1-C2-C3-C4
31	A	616	DGD	C4E-C5E-C6E-O5E
27	D	406	PL9	C33-C34-C36-C37
25	A	607	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	501	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C12-C13-C14
25	a	611	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	610	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	b	615	CLA	C6-C7-C8-C9
25	c	513	CLA	C6-C7-C8-C9
26	K	102	BCR	C7-C8-C9-C34
26	b	617	BCR	C36-C18-C19-C20
28	c	521	LMG	C4-C5-C6-O5
28	B	622	LMG	C28-C29-C30-C31
28	c	520	LMG	C10-C11-C12-C13
29	a	612	SQD	C23-C24-C25-C26
31	c	517	DGD	O1A-C1A-O1G-C1G
25	B	607	CLA	C13-C15-C16-C17
29	B	623	SQD	C29-C30-C31-C32
28	A	612	LMG	O6-C5-C6-O5
31	a	614	DGD	C2A-C1A-O1G-C1G
25	C	507	CLA	C15-C16-C17-C18
25	D	404	CLA	C10-C11-C12-C13
25	b	605	CLA	C15-C16-C17-C18
25	b	607	CLA	C5-C6-C7-C8
25	b	608	CLA	C13-C15-C16-C17
25	c	503	CLA	C5-C6-C7-C8
30	e	101	LHG	C23-C24-C25-C26
32	A	617	STE	C1-C2-C3-C4
25	A	606	CLA	C15-C16-C17-C18
25	B	601	CLA	C5-C6-C7-C8
25	B	601	CLA	C15-C16-C17-C18
25	B	607	CLA	C5-C6-C7-C8
25	b	602	CLA	C15-C16-C17-C18
25	b	605	CLA	C5-C6-C7-C8
25	b	615	CLA	C15-C16-C17-C18
25	c	509	CLA	C10-C11-C12-C13
25	c	510	CLA	C5-C6-C7-C8
25	c	511	CLA	C13-C15-C16-C17
25	c	513	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	c	521	LMG	C10-C11-C12-C13
28	d	411	LMG	C28-C29-C30-C31
28	m	101	LMG	C28-C29-C30-C31
29	A	615	SQD	C23-C24-C25-C26
30	d	407	LHG	C23-C24-C25-C26
30	e	101	LHG	C7-C8-C9-C10
31	c	516	DGD	C1A-C2A-C3A-C4A
32	C	519	STE	C1-C2-C3-C4
32	t	102	STE	C1-C2-C3-C4
28	C	517	LMG	O6-C5-C6-O5
29	b	620	SQD	C12-C13-C14-C15
25	B	603	CLA	C13-C15-C16-C17
25	C	509	CLA	C10-C11-C12-C13
25	b	614	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
25	c	512	CLA	O1D-CGD-O2D-CED
27	D	406	PL9	C32-C33-C34-C36
25	C	502	CLA	C13-C15-C16-C17
25	C	507	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	c	507	CLA	C5-C6-C7-C8
28	C	517	LMG	C28-C29-C30-C31
29	f	102	SQD	C23-C24-C25-C26
30	d	407	LHG	C7-C8-C9-C10
31	c	517	DGD	C1B-C2B-C3B-C4B
32	B	626	STE	C1-C2-C3-C4
25	b	601	CLA	C8-C10-C11-C12
25	C	501	CLA	C12-C13-C15-C16
25	C	506	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	C	512	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C10-C8-C7
26	K	101	BCR	C15-C16-C17-C18
25	c	512	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	C15-C16-C17-C18
25	C	509	CLA	C13-C15-C16-C17
25	C	510	CLA	C15-C16-C17-C18
25	c	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	c	518	LMG	C4-C5-C6-O5
29	b	620	SQD	C10-C11-C12-C13
27	A	610	PL9	C44-C46-C47-C48
26	d	405	BCR	C18-C19-C20-C21
26	k	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C18-C19-C20-C21
31	C	515	DGD	O6E-C5E-C6E-O5E
30	e	101	LHG	O2-C2-C3-O3
25	b	608	CLA	C8-C10-C11-C12
25	b	613	CLA	C13-C15-C16-C17
25	c	507	CLA	C8-C10-C11-C12
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8
25	C	504	CLA	C8-C10-C11-C12
25	C	506	CLA	C8-C10-C11-C12
25	a	608	CLA	C5-C6-C7-C8
25	c	511	CLA	C15-C16-C17-C18
25	B	601	CLA	CBD-CGD-O2D-CED
25	A	607	CLA	C15-C16-C17-C18
25	C	512	CLA	C8-C10-C11-C12
25	a	606	CLA	C8-C10-C11-C12
25	b	613	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
30	D	409	LHG	C4-O6-P-O3
30	D	410	LHG	C3-O3-P-O6
30	d	408	LHG	C4-O6-P-O3
30	e	101	LHG	C3-O3-P-O6
30	e	101	LHG	C4-O6-P-O3
31	c	517	DGD	C2A-C1A-O1G-C1G
25	C	513	CLA	CBD-CGD-O2D-CED
25	B	603	CLA	C8-C10-C11-C12
25	b	615	CLA	C10-C11-C12-C13
25	c	508	CLA	C10-C11-C12-C13
31	c	515	DGD	C1A-C2A-C3A-C4A
32	d	412	STE	C1-C2-C3-C4
25	c	503	CLA	O1D-CGD-O2D-CED
30	d	408	LHG	C1-C2-C3-O3
30	e	101	LHG	C1-C2-C3-O3
25	c	503	CLA	C8-C10-C11-C12
25	c	509	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	C4E-C5E-C6E-O5E
25	b	604	CLA	C15-C16-C17-C18
28	b	622	LMG	C4-C5-C6-O5
30	D	410	LHG	C7-C8-C9-C10
28	d	410	LMG	C33-C34-C35-C36
29	A	615	SQD	C14-C15-C16-C17
31	J	101	DGD	C5B-C6B-C7B-C8B
32	a	615	STE	C3-C4-C5-C6
32	d	412	STE	C10-C11-C12-C13
25	b	607	CLA	O1D-CGD-O2D-CED
26	D	405	BCR	C20-C21-C22-C37
26	K	101	BCR	C20-C21-C22-C37
26	K	102	BCR	C20-C21-C22-C37
26	T	101	BCR	C35-C13-C14-C15
26	T	101	BCR	C16-C17-C18-C36
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C16-C17-C18-C36
26	b	619	BCR	C20-C21-C22-C37
26	h	101	BCR	C11-C10-C9-C34
26	h	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C20-C21-C22-C37
28	D	407	LMG	C17-C18-C19-C20
29	D	408	SQD	C33-C34-C35-C36
29	a	612	SQD	C12-C13-C14-C15
29	a	612	SQD	C13-C14-C15-C16
29	a	613	SQD	C10-C11-C12-C13
30	D	410	LHG	C34-C35-C36-C37
31	C	515	DGD	C4B-C5B-C6B-C7B
31	H	102	DGD	CAB-CBB-CCB-CDB
32	B	621	STE	C6-C7-C8-C9
32	B	621	STE	C9-C10-C11-C12
32	B	624	STE	C2-C3-C4-C5
32	B	627	STE	C7-C8-C9-C10
32	C	518	STE	C2-C3-C4-C5
32	H	103	STE	C6-C7-C8-C9
32	I	101	STE	C11-C10-C9-C8
32	b	621	STE	C10-C11-C12-C13
25	B	602	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
33	d	402	PHO	C16-C17-C18-C19
28	c	518	LMG	C35-C36-C37-C38
28	d	410	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	d	410	LMG	C37-C38-C39-C40
28	m	101	LMG	C17-C18-C19-C20
29	B	623	SQD	C12-C13-C14-C15
30	A	614	LHG	C15-C16-C17-C18
30	A	614	LHG	C24-C25-C26-C27
30	D	409	LHG	C10-C11-C12-C13
30	L	101	LHG	C28-C29-C30-C31
30	d	407	LHG	C15-C16-C17-C18
30	d	408	LHG	C29-C30-C31-C32
30	l	101	LHG	C31-C32-C33-C34
31	A	616	DGD	C2B-C3B-C4B-C5B
31	A	616	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C7A-C8A-C9A-CAA
31	H	102	DGD	C9A-CAA-CBA-CCA
31	J	101	DGD	CBB-CCB-CDB-CEB
31	c	517	DGD	C9B-CAB-CBB-CCB
31	h	102	DGD	C3B-C4B-C5B-C6B
32	D	413	STE	C4-C5-C6-C7
32	D	413	STE	C7-C8-C9-C10
32	b	623	STE	C11-C10-C9-C8
28	D	411	LMG	C9-C8-O7-C10
29	b	620	SQD	C46-C45-O47-C7
30	e	101	LHG	O9-C7-O7-C5
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
28	D	407	LMG	C16-C17-C18-C19
30	D	410	LHG	C9-C10-C11-C12
30	d	407	LHG	C30-C31-C32-C33
31	h	102	DGD	C5B-C6B-C7B-C8B
32	D	413	STE	C5-C6-C7-C8
32	D	413	STE	C9-C10-C11-C12
32	b	624	STE	C11-C10-C9-C8
28	m	101	LMG	C32-C33-C34-C35
29	D	408	SQD	C29-C30-C31-C32
30	l	101	LHG	C9-C10-C11-C12
31	c	515	DGD	C3B-C4B-C5B-C6B
31	c	516	DGD	CBA-CCA-CDA-CEA
32	H	103	STE	C14-C15-C16-C17
30	A	614	LHG	O2-C2-C3-O3
30	D	409	LHG	O2-C2-C3-O3
30	D	410	LHG	O2-C2-C3-O3
29	B	623	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	L	101	LHG	C17-C18-C19-C20
32	H	103	STE	C9-C10-C11-C12
32	T	102	STE	C7-C8-C9-C10
26	A	609	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C20-C21-C22-C23
26	T	101	BCR	C12-C13-C14-C15
26	h	101	BCR	C11-C10-C9-C8
26	h	101	BCR	C20-C21-C22-C23
28	A	612	LMG	C2-C1-O1-C7
28	m	101	LMG	C2-C1-O1-C7
31	C	516	DGD	C2E-C1E-O5D-C6D
31	c	516	DGD	C2E-C1E-O5D-C6D
28	A	612	LMG	O1-C7-C8-O7
28	B	620	LMG	C37-C38-C39-C40
28	c	518	LMG	O9-C10-O7-C8
29	a	612	SQD	C34-C35-C36-C37
29	b	620	SQD	C28-C29-C30-C31
30	A	614	LHG	C27-C28-C29-C30
30	d	409	LHG	C26-C27-C28-C29
31	A	616	DGD	CEB-CFB-CGB-CHB
31	c	515	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C6A-C7A-C8A-C9A
25	b	615	CLA	C8-C10-C11-C12
25	c	503	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	C	509	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	C4-C3-C5-C6
28	C	517	LMG	C31-C32-C33-C34
31	A	616	DGD	C4B-C5B-C6B-C7B
31	J	101	DGD	C5A-C6A-C7A-C8A
31	a	614	DGD	C2B-C3B-C4B-C5B
32	T	102	STE	C11-C10-C9-C8
32	T	102	STE	C14-C15-C16-C17
32	c	519	STE	C9-C10-C11-C12
32	m	102	STE	C3-C4-C5-C6
33	d	402	PHO	C14-C13-C15-C16
28	A	612	LMG	C35-C36-C37-C38
28	B	620	LMG	C12-C13-C14-C15
28	C	517	LMG	C17-C18-C19-C20
28	D	407	LMG	C13-C14-C15-C16
28	D	411	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	622	LMG	C19-C20-C21-C22
28	b	622	LMG	C30-C31-C32-C33
29	a	612	SQD	C30-C31-C32-C33
30	L	101	LHG	C27-C28-C29-C30
30	d	407	LHG	C16-C17-C18-C19
30	l	101	LHG	C32-C33-C34-C35
31	c	517	DGD	C3B-C4B-C5B-C6B
32	A	617	STE	C4-C5-C6-C7
32	A	617	STE	C14-C15-C16-C17
25	B	614	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
29	f	102	SQD	C25-C26-C27-C28
30	d	408	LHG	C17-C18-C19-C20
31	a	614	DGD	C5A-C6A-C7A-C8A
31	c	515	DGD	C9B-CAB-CBB-CCB
32	J	102	STE	C5-C6-C7-C8
30	D	410	LHG	O1-C1-C2-C3
30	D	412	LHG	O1-C1-C2-C3
25	B	606	CLA	C13-C15-C16-C17
25	B	607	CLA	C15-C16-C17-C18
25	c	504	CLA	C8-C10-C11-C12
28	A	612	LMG	C16-C17-C18-C19
28	D	407	LMG	C36-C37-C38-C39
31	a	614	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	C9A-CAA-CBA-CCA
32	A	617	STE	C9-C10-C11-C12
31	c	517	DGD	C1A-C2A-C3A-C4A
28	b	622	LMG	C32-C33-C34-C35
28	c	521	LMG	C32-C33-C34-C35
28	d	410	LMG	C31-C32-C33-C34
28	d	410	LMG	C32-C33-C34-C35
28	m	101	LMG	C14-C15-C16-C17
28	m	101	LMG	C19-C20-C21-C22
29	A	615	SQD	C10-C11-C12-C13
29	A	615	SQD	C18-C19-C20-C21
29	A	615	SQD	C30-C31-C32-C33
29	a	613	SQD	C11-C12-C13-C14
30	L	101	LHG	C24-C25-C26-C27
30	L	101	LHG	C32-C33-C34-C35
30	e	101	LHG	C11-C10-C9-C8
31	C	515	DGD	C5A-C6A-C7A-C8A
31	J	101	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
31	c	515	DGD	C2A-C3A-C4A-C5A
31	c	515	DGD	C5B-C6B-C7B-C8B
32	b	623	STE	C6-C7-C8-C9
32	b	624	STE	C10-C11-C12-C13
32	b	624	STE	C13-C14-C15-C16
32	b	625	STE	C5-C6-C7-C8
25	B	612	CLA	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	B	615	CLA	C16-C17-C18-C20
25	D	403	CLA	C16-C17-C18-C20
25	b	601	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
31	c	516	DGD	O6E-C1E-O5D-C6D
25	B	604	CLA	C10-C11-C12-C13
29	a	612	SQD	C32-C33-C34-C35
29	b	620	SQD	C26-C27-C28-C29
30	D	410	LHG	C29-C30-C31-C32
30	l	101	LHG	C16-C17-C18-C19
30	l	101	LHG	C25-C26-C27-C28
31	C	515	DGD	C5B-C6B-C7B-C8B
31	J	101	DGD	CCB-CDB-CEB-CFB
32	C	519	STE	C5-C6-C7-C8
32	L	102	STE	C6-C7-C8-C9
28	B	620	LMG	C38-C39-C40-C41
28	D	407	LMG	C18-C19-C20-C21
28	c	518	LMG	C36-C37-C38-C39
28	c	521	LMG	C33-C34-C35-C36
30	d	407	LHG	C25-C26-C27-C28
30	d	409	LHG	C27-C28-C29-C30
31	A	616	DGD	CEA-CFA-CGA-CHA
31	A	616	DGD	C6B-C7B-C8B-C9B
31	H	102	DGD	C3A-C4A-C5A-C6A
31	H	102	DGD	CBB-CCB-CDB-CEB
31	J	101	DGD	C6A-C7A-C8A-C9A
31	J	101	DGD	C4B-C5B-C6B-C7B
31	c	515	DGD	C8B-C9B-CAB-CBB
32	B	625	STE	C10-C11-C12-C13
31	J	101	DGD	C1B-C2B-C3B-C4B
25	b	601	CLA	C10-C11-C12-C13
28	B	620	LMG	C13-C14-C15-C16
29	a	612	SQD	C14-C15-C16-C17
29	b	620	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	d	409	LHG	C29-C30-C31-C32
32	D	413	STE	C2-C3-C4-C5
31	c	516	DGD	O6E-C5E-C6E-O5E
28	B	622	LMG	C36-C37-C38-C39
28	D	407	LMG	C20-C21-C22-C23
28	D	407	LMG	C38-C39-C40-C41
29	B	623	SQD	C15-C16-C17-C18
29	b	620	SQD	C25-C26-C27-C28
30	D	410	LHG	C16-C17-C18-C19
30	d	407	LHG	C17-C18-C19-C20
32	T	102	STE	C5-C6-C7-C8
32	b	624	STE	C12-C13-C14-C15
25	c	512	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	C15-C16-C17-C18
28	c	520	LMG	C40-C41-C42-C43
30	D	409	LHG	C12-C13-C14-C15
30	D	410	LHG	C10-C11-C12-C13
31	A	616	DGD	C8A-C9A-CAA-CBA
31	a	614	DGD	C3B-C4B-C5B-C6B
31	a	614	DGD	C5B-C6B-C7B-C8B
31	c	515	DGD	CBB-CCB-CDB-CEB
32	H	103	STE	C5-C6-C7-C8
30	l	101	LHG	C23-C24-C25-C26
25	B	602	CLA	C16-C17-C18-C20
25	B	612	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
28	c	520	LMG	C30-C31-C32-C33
29	A	613	SQD	C11-C12-C13-C14
29	a	612	SQD	C25-C26-C27-C28
30	A	614	LHG	C16-C17-C18-C19
30	D	412	LHG	C27-C28-C29-C30
30	L	101	LHG	C12-C13-C14-C15
31	A	616	DGD	CBB-CCB-CDB-CEB
31	a	614	DGD	CEB-CFB-CGB-CHB
31	c	515	DGD	CCB-CDB-CEB-CFB
31	h	102	DGD	C6B-C7B-C8B-C9B
32	b	625	STE	C6-C7-C8-C9
25	b	612	CLA	C13-C15-C16-C17
28	d	411	LMG	C37-C38-C39-C40
30	D	412	LHG	C11-C12-C13-C14
30	d	408	LHG	C12-C13-C14-C15
32	j	101	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	O2A-C1-C2-C3
28	c	521	LMG	O6-C5-C6-O5
32	L	102	STE	C1-C2-C3-C4
28	d	411	LMG	C38-C39-C40-C41
28	m	101	LMG	C15-C16-C17-C18
30	D	410	LHG	C24-C25-C26-C27
31	H	102	DGD	C6B-C7B-C8B-C9B
31	c	515	DGD	C7A-C8A-C9A-CAA
32	a	615	STE	C5-C6-C7-C8
25	c	512	CLA	O1A-CGA-O2A-C1
25	B	606	CLA	C8-C10-C11-C12
25	C	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
27	a	610	PL9	C13-C14-C16-C17
27	d	406	PL9	C13-C14-C16-C17
27	d	406	PL9	C43-C44-C46-C47
28	c	520	LMG	C36-C37-C38-C39
30	D	412	LHG	C28-C29-C30-C31
30	L	101	LHG	C13-C14-C15-C16
31	A	616	DGD	CCA-CDA-CEA-CFA
31	H	102	DGD	C7B-C8B-C9B-CAB
32	t	103	STE	C3-C4-C5-C6
28	c	520	LMG	C15-C16-C17-C18
28	c	520	LMG	C35-C36-C37-C38
29	D	408	SQD	C25-C26-C27-C28
30	D	409	LHG	C15-C16-C17-C18
30	d	408	LHG	C11-C12-C13-C14
31	C	516	DGD	C9B-CAB-CBB-CCB
32	b	623	STE	C7-C8-C9-C10
25	a	606	CLA	C13-C15-C16-C17
28	c	520	LMG	C31-C32-C33-C34
29	B	623	SQD	C33-C34-C35-C36
29	D	408	SQD	C32-C33-C34-C35
30	A	614	LHG	C11-C12-C13-C14
30	A	614	LHG	C30-C31-C32-C33
28	B	622	LMG	C15-C16-C17-C18
30	D	410	LHG	C32-C33-C34-C35
31	c	516	DGD	C5A-C6A-C7A-C8A
32	c	519	STE	C3-C4-C5-C6
32	c	519	STE	C14-C15-C16-C17
28	B	620	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	c	521	LMG	C38-C39-C40-C41
30	A	614	LHG	C11-C10-C9-C8
32	T	102	STE	C13-C14-C15-C16
32	b	621	STE	C5-C6-C7-C8
32	b	623	STE	C3-C4-C5-C6
25	c	505	CLA	C10-C11-C12-C13
31	H	102	DGD	C5A-C6A-C7A-C8A
31	a	614	DGD	C4A-C5A-C6A-C7A
31	c	516	DGD	CCB-CDB-CEB-CFB
25	b	602	CLA	C16-C17-C18-C20
25	C	509	CLA	C3-C5-C6-C7
26	B	617	BCR	C5-C6-C7-C8
26	D	405	BCR	C23-C24-C25-C26
26	D	405	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
28	C	517	LMG	C37-C38-C39-C40
28	c	521	LMG	C39-C40-C41-C42
29	a	612	SQD	C16-C17-C18-C19
29	a	612	SQD	C26-C27-C28-C29
29	b	620	SQD	C11-C12-C13-C14
32	d	412	STE	C9-C10-C11-C12
25	B	605	CLA	C15-C16-C17-C18
25	c	508	CLA	C13-C15-C16-C17
29	f	102	SQD	C8-C7-O47-C45
29	a	612	SQD	C11-C10-C9-C8
29	b	620	SQD	C29-C30-C31-C32
28	D	407	LMG	C28-C29-C30-C31
31	H	102	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	C9B-CAB-CBB-CCB
32	H	103	STE	C7-C8-C9-C10
25	C	512	CLA	C13-C15-C16-C17
25	c	502	CLA	C15-C16-C17-C18
28	c	518	LMG	C11-C10-O7-C8
29	A	613	SQD	C34-C35-C36-C37
29	f	102	SQD	C27-C28-C29-C30
32	t	102	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
27	d	406	PL9	C15-C14-C16-C17
25	B	601	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	C	506	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C12-C13-C15
25	b	609	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
27	d	406	PL9	C28-C29-C31-C32
31	a	614	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	C4A-C5A-C6A-C7A
32	D	413	STE	C3-C4-C5-C6
26	K	103	BCR	C19-C20-C21-C22
25	b	613	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
28	C	517	LMG	C10-C11-C12-C13
31	c	516	DGD	C1B-C2B-C3B-C4B
32	c	519	STE	C2-C3-C4-C5
32	B	627	STE	C13-C14-C15-C16
32	c	519	STE	C4-C5-C6-C7
31	C	516	DGD	C6B-C7B-C8B-C9B
31	h	102	DGD	C2B-C3B-C4B-C5B
32	b	621	STE	C4-C5-C6-C7
28	C	517	LMG	C32-C33-C34-C35
29	f	102	SQD	C24-C25-C26-C27
29	f	102	SQD	C29-C30-C31-C32
32	d	412	STE	C11-C12-C13-C14
28	c	520	LMG	O6-C5-C6-O5
31	C	516	DGD	O6E-C1E-O5D-C6D
27	A	610	PL9	C39-C41-C42-C43
28	D	407	LMG	C15-C16-C17-C18
31	C	516	DGD	C8B-C9B-CAB-CBB
31	J	101	DGD	C3A-C4A-C5A-C6A
32	d	413	STE	C10-C11-C12-C13
29	A	613	SQD	C23-C24-C25-C26
30	e	101	LHG	C8-C7-O7-C5
30	e	101	LHG	O6-C4-C5-O7
26	b	617	BCR	C18-C19-C20-C21
28	c	521	LMG	C31-C32-C33-C34
29	A	615	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	C5A-C6A-C7A-C8A
32	d	412	STE	C12-C13-C14-C15
25	B	614	CLA	CBD-CGD-O2D-CED
28	c	521	LMG	C13-C14-C15-C16
30	L	101	LHG	C18-C19-C20-C21
29	f	102	SQD	O49-C7-O47-C45
30	d	408	LHG	O9-C7-O7-C5
31	c	515	DGD	O1B-C1B-O2G-C2G
28	c	518	LMG	C39-C40-C41-C42
28	d	411	LMG	C34-C35-C36-C37
30	d	408	LHG	C16-C17-C18-C19
31	C	516	DGD	C3B-C4B-C5B-C6B
32	L	102	STE	C5-C6-C7-C8
32	m	102	STE	C7-C8-C9-C10
29	a	612	SQD	O47-C45-C46-O48
32	t	102	STE	C5-C6-C7-C8
25	b	601	CLA	C16-C17-C18-C19
30	D	409	LHG	C25-C26-C27-C28
30	D	410	LHG	C25-C26-C27-C28
30	D	412	LHG	C29-C30-C31-C32
32	A	617	STE	C3-C4-C5-C6
25	B	615	CLA	C15-C16-C17-C18
25	C	505	CLA	C5-C6-C7-C8
27	A	610	PL9	C25-C24-C26-C27
27	A	610	PL9	C38-C39-C41-C42
27	d	406	PL9	C4-C3-C7-C8
30	d	407	LHG	C10-C11-C12-C13
25	B	615	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C10-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C9
25	c	508	CLA	C14-C13-C15-C16
25	c	510	CLA	C14-C13-C15-C16
30	L	101	LHG	C11-C12-C13-C14
31	C	516	DGD	CCB-CDB-CEB-CFB
32	b	624	STE	C14-C15-C16-C17
30	d	408	LHG	C33-C34-C35-C36
30	d	409	LHG	C30-C31-C32-C33
31	c	515	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
32	A	617	STE	C2-C3-C4-C5
26	K	102	BCR	C37-C22-C23-C24
26	k	102	BCR	C7-C8-C9-C34
29	A	613	SQD	C31-C32-C33-C34
31	A	616	DGD	CBA-CCA-CDA-CEA
32	H	103	STE	C2-C3-C4-C5
25	B	601	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C16-C17-C18-C19
33	d	402	PHO	C16-C17-C18-C20
30	l	101	LHG	O9-C7-O7-C5
29	A	613	SQD	C9-C10-C11-C12
29	B	623	SQD	C34-C35-C36-C37
29	D	408	SQD	C28-C29-C30-C31
30	D	410	LHG	C27-C28-C29-C30
31	C	515	DGD	C7A-C8A-C9A-CAA
31	c	516	DGD	C8A-C9A-CAA-CBA
32	b	621	STE	C9-C10-C11-C12
25	B	605	CLA	C8-C10-C11-C12
25	C	510	CLA	C10-C11-C12-C13
25	b	611	CLA	C15-C16-C17-C18
30	A	614	LHG	C4-O6-P-O3
28	b	622	LMG	C35-C36-C37-C38
31	c	516	DGD	CBB-CCB-CDB-CEB
30	A	614	LHG	O6-C4-C5-C6
28	b	622	LMG	C40-C41-C42-C43
28	m	101	LMG	C18-C19-C20-C21
32	B	624	STE	C4-C5-C6-C7
32	B	625	STE	C11-C10-C9-C8
31	c	515	DGD	O6E-C5E-C6E-O5E
25	c	503	CLA	C16-C17-C18-C19
25	c	504	CLA	C11-C12-C13-C15
29	f	102	SQD	C32-C33-C34-C35
28	A	612	LMG	C37-C38-C39-C40
31	A	616	DGD	C4A-C5A-C6A-C7A
32	d	412	STE	C2-C3-C4-C5
28	c	521	LMG	C15-C16-C17-C18
29	A	615	SQD	C12-C13-C14-C15
30	A	614	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C4-C3-C5-C6
28	d	410	LMG	C36-C37-C38-C39
32	I	101	STE	C1-C2-C3-C4
25	B	608	CLA	C15-C16-C17-C18
25	A	608	CLA	C5-C6-C7-C8
29	f	102	SQD	C30-C31-C32-C33
30	A	614	LHG	C12-C13-C14-C15
30	D	409	LHG	C11-C12-C13-C14
31	C	516	DGD	C4A-C5A-C6A-C7A
32	C	520	STE	C11-C10-C9-C8
32	d	413	STE	C13-C14-C15-C16
25	B	609	CLA	C16-C17-C18-C19
28	B	620	LMG	C7-C8-C9-O8
28	D	411	LMG	C7-C8-C9-O8
28	b	622	LMG	C7-C8-C9-O8
28	c	520	LMG	C7-C8-C9-O8
28	c	521	LMG	C7-C8-C9-O8
29	A	613	SQD	O6-C44-C45-C46
29	B	623	SQD	O6-C44-C45-C46
29	a	612	SQD	O6-C44-C45-C46
29	a	613	SQD	C44-C45-C46-O48
31	A	616	DGD	C1G-C2G-C3G-O3G
31	a	614	DGD	CFA-CGA-CHA-CIA
32	d	413	STE	C11-C10-C9-C8
32	m	102	STE	C12-C13-C14-C15
31	C	516	DGD	C2G-C3G-O3G-C1D
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C2G-C3G-O3G-C1D
29	B	623	SQD	C13-C14-C15-C16
31	c	517	DGD	C6A-C7A-C8A-C9A
32	A	617	STE	C11-C12-C13-C14
32	b	625	STE	C2-C3-C4-C5
25	C	513	CLA	C13-C15-C16-C17
28	B	622	LMG	C31-C32-C33-C34
32	B	624	STE	C6-C7-C8-C9
32	D	413	STE	C14-C15-C16-C17
28	D	407	LMG	O6-C5-C6-O5
28	m	101	LMG	C38-C39-C40-C41
31	A	616	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C2A-C3A-C4A-C5A
32	b	623	STE	C11-C12-C13-C14
32	J	102	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C24-C23-O48-C46
31	J	101	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	CBB-CCB-CDB-CEB
32	B	621	STE	C2-C3-C4-C5
28	B	622	LMG	C37-C38-C39-C40
30	d	407	LHG	C18-C19-C20-C21
31	c	517	DGD	C2B-C3B-C4B-C5B
25	b	602	CLA	O1D-CGD-O2D-CED
26	K	101	BCR	C11-C10-C9-C34
27	d	406	PL9	C45-C44-C46-C47
31	A	616	DGD	CDA-CEA-CFA-CGA
32	B	621	STE	C11-C10-C9-C8
25	A	608	CLA	CBA-CGA-O2A-C1
30	d	409	LHG	C25-C26-C27-C28
32	c	519	STE	C10-C11-C12-C13
25	c	506	CLA	C13-C15-C16-C17
29	A	615	SQD	C19-C20-C21-C22
32	b	621	STE	C3-C4-C5-C6
32	b	621	STE	C7-C8-C9-C10
28	A	612	LMG	C9-C8-O7-C10
28	d	411	LMG	O6-C5-C6-O5
25	c	501	CLA	C2A-CAA-CBA-CGA
32	B	627	STE	C11-C10-C9-C8
28	m	101	LMG	C12-C13-C14-C15
29	B	623	SQD	C27-C28-C29-C30
29	B	623	SQD	C28-C29-C30-C31
30	A	614	LHG	C29-C30-C31-C32
30	D	409	LHG	C18-C19-C20-C21
31	C	516	DGD	CDA-CEA-CFA-CGA
31	c	517	DGD	C4B-C5B-C6B-C7B
32	m	102	STE	C4-C5-C6-C7
25	b	609	CLA	CBA-CGA-O2A-C1
28	c	518	LMG	C29-C28-O8-C9
28	A	612	LMG	C17-C18-C19-C20
29	a	612	SQD	C27-C28-C29-C30
30	l	101	LHG	C26-C27-C28-C29
32	B	625	STE	C12-C13-C14-C15
32	E	102	STE	C6-C7-C8-C9
25	C	508	CLA	C10-C11-C12-C13
28	c	521	LMG	C40-C41-C42-C43
25	B	601	CLA	O1D-CGD-O2D-CED
28	D	407	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	D	409	LHG	C16-C17-C18-C19
32	D	413	STE	C11-C12-C13-C14
25	b	602	CLA	C5-C6-C7-C8
25	b	610	CLA	C15-C16-C17-C18
26	A	609	BCR	C20-C21-C22-C23
26	K	103	BCR	C11-C10-C9-C8
26	k	102	BCR	C20-C21-C22-C23
28	c	521	LMG	C2-C1-O1-C7
28	m	101	LMG	O7-C8-C9-O8
29	A	613	SQD	O6-C44-C45-O47
29	a	612	SQD	O6-C44-C45-O47
28	d	411	LMG	C12-C13-C14-C15
30	A	614	LHG	C10-C11-C12-C13
30	l	101	LHG	C28-C29-C30-C31
31	h	102	DGD	C7A-C8A-C9A-CAA
29	A	615	SQD	C28-C29-C30-C31
29	a	612	SQD	C28-C29-C30-C31
29	a	613	SQD	C31-C32-C33-C34
30	D	410	LHG	C11-C10-C9-C8
32	b	624	STE	C7-C8-C9-C10
32	d	412	STE	C5-C6-C7-C8
31	J	101	DGD	C1A-C2A-C3A-C4A
29	A	615	SQD	C11-C10-C9-C8
25	A	607	CLA	C12-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C7
25	C	503	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	506	CLA	C6-C7-C8-C10
25	C	511	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C10-C8-C7
25	a	606	CLA	C11-C10-C8-C7
25	b	603	CLA	C11-C10-C8-C7
25	b	606	CLA	C6-C7-C8-C10
25	b	606	CLA	C12-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C10
25	b	610	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C12-C13-C15-C16
25	c	513	CLA	C6-C7-C8-C10
33	d	402	PHO	C12-C13-C15-C16
25	C	506	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	a	608	CLA	C6-C7-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	605	CLA	C11-C12-C13-C14
25	b	606	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	c	506	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C10-C8-C9
29	a	613	SQD	C29-C30-C31-C32
30	e	101	LHG	C16-C17-C18-C19
32	a	615	STE	C4-C5-C6-C7
25	b	614	CLA	CBA-CGA-O2A-C1
32	M	102	STE	C5-C6-C7-C8
26	K	101	BCR	C37-C22-C23-C24
25	B	603	CLA	C16-C17-C18-C20
25	D	404	CLA	C16-C17-C18-C20
26	K	103	BCR	C21-C22-C23-C24
26	c	514	BCR	C7-C8-C9-C10
29	a	613	SQD	C15-C16-C17-C18
30	d	407	LHG	C28-C29-C30-C31
31	C	516	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	CCA-CDA-CEA-CFA
25	B	603	CLA	C10-C11-C12-C13
28	B	622	LMG	C17-C18-C19-C20
30	e	101	LHG	C11-C12-C13-C14
25	b	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	b	622	LMG	C15-C16-C17-C18
28	d	411	LMG	C35-C36-C37-C38
32	B	621	STE	C12-C13-C14-C15
32	t	102	STE	C3-C4-C5-C6
28	D	411	LMG	C31-C32-C33-C34
30	L	101	LHG	C30-C31-C32-C33
27	A	610	PL9	C24-C26-C27-C28
28	c	521	LMG	C16-C17-C18-C19
25	B	604	CLA	CBA-CGA-O2A-C1
26	D	405	BCR	C18-C19-C20-C21
30	D	409	LHG	C23-C24-C25-C26
31	C	515	DGD	C3A-C4A-C5A-C6A
32	B	621	STE	C11-C12-C13-C14
29	B	623	SQD	O10-C23-O48-C46
31	c	515	DGD	CBA-CCA-CDA-CEA
32	b	624	STE	C9-C10-C11-C12
31	C	515	DGD	C8B-C9B-CAB-CBB
31	J	101	DGD	C3B-C4B-C5B-C6B
31	c	516	DGD	CDA-CEA-CFA-CGA
25	B	602	CLA	C8-C10-C11-C12
25	c	502	CLA	CBA-CGA-O2A-C1
31	h	102	DGD	O2G-C1B-C2B-C3B
29	B	623	SQD	C26-C27-C28-C29
30	L	101	LHG	C31-C32-C33-C34
31	A	616	DGD	CCB-CDB-CEB-CFB
28	C	517	LMG	C30-C31-C32-C33
28	c	520	LMG	C41-C42-C43-C44
30	l	101	LHG	C34-C35-C36-C37
27	A	610	PL9	C47-C48-C49-C50
28	D	407	LMG	C33-C34-C35-C36
28	m	101	LMG	C11-C12-C13-C14
31	c	517	DGD	CDA-CEA-CFA-CGA
25	d	404	CLA	C5-C6-C7-C8
31	c	515	DGD	CDB-CEB-CFB-CGB
25	B	616	CLA	C11-C12-C13-C14
25	B	606	CLA	C5-C6-C7-C8
25	B	612	CLA	C10-C11-C12-C13
25	C	506	CLA	C15-C16-C17-C18
25	a	605	CLA	C15-C16-C17-C18
25	b	606	CLA	C8-C10-C11-C12
28	A	612	LMG	O1-C7-C8-C9
28	b	622	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	m	101	LMG	O1-C7-C8-C9
28	m	101	LMG	C7-C8-C9-O8
29	a	612	SQD	C44-C45-C46-O48
31	C	515	DGD	O1G-C1G-C2G-C3G
31	a	614	DGD	O1G-C1G-C2G-C3G
31	a	614	DGD	CAA-CBA-CCA-CDA
32	D	413	STE	C10-C11-C12-C13
32	m	102	STE	C9-C10-C11-C12
29	a	613	SQD	C9-C10-C11-C12
31	c	516	DGD	CAA-CBA-CCA-CDA
32	M	101	STE	C10-C11-C12-C13
29	a	612	SQD	C9-C10-C11-C12
30	D	412	LHG	C19-C20-C21-C22
28	b	622	LMG	C18-C19-C20-C21
32	m	102	STE	C2-C3-C4-C5
25	B	616	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
27	D	406	PL9	C15-C14-C16-C17
33	D	401	PHO	C4-C3-C5-C6
29	A	613	SQD	C13-C14-C15-C16
32	j	101	STE	C3-C4-C5-C6
25	A	608	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
30	D	412	LHG	O1-C1-C2-O2
28	A	612	LMG	C36-C37-C38-C39
31	h	102	DGD	C6A-C7A-C8A-C9A
32	b	623	STE	C5-C6-C7-C8
28	c	518	LMG	C40-C41-C42-C43
28	c	521	LMG	C35-C36-C37-C38
32	C	518	STE	C5-C6-C7-C8
32	H	103	STE	C11-C12-C13-C14
25	B	603	CLA	C16-C17-C18-C19
25	c	509	CLA	C16-C17-C18-C19
30	d	408	LHG	C32-C33-C34-C35
31	c	516	DGD	C8B-C9B-CAB-CBB
32	H	103	STE	C1-C2-C3-C4
32	H	103	STE	C15-C16-C17-C18
25	b	609	CLA	O1A-CGA-O2A-C1
30	D	412	LHG	C18-C19-C20-C21
28	A	612	LMG	C32-C33-C34-C35
29	D	408	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
28	m	101	LMG	O1-C7-C8-O7
29	a	613	SQD	O47-C45-C46-O48
28	c	518	LMG	C38-C39-C40-C41
29	A	613	SQD	C17-C18-C19-C20
30	A	614	LHG	C9-C10-C11-C12
31	a	614	DGD	C1B-C2B-C3B-C4B
25	b	610	CLA	C16-C17-C18-C20
28	c	520	LMG	C14-C15-C16-C17
28	c	518	LMG	O6-C1-O1-C7
25	C	507	CLA	C5-C6-C7-C8
27	A	610	PL9	C34-C36-C37-C38
30	D	409	LHG	C1-C2-C3-O3
32	C	520	STE	C10-C11-C12-C13
25	D	403	CLA	C2-C1-O2A-CGA
25	b	611	CLA	C2-C3-C5-C6
25	B	604	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	C	508	CLA	C6-C7-C8-C9
25	a	606	CLA	C11-C10-C8-C9
25	b	609	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	c	502	CLA	C6-C7-C8-C9
25	c	512	CLA	C6-C7-C8-C9
28	c	518	LMG	C31-C32-C33-C34
30	d	409	LHG	C9-C10-C11-C12
32	C	520	STE	C12-C13-C14-C15
32	d	413	STE	C9-C10-C11-C12
25	c	505	CLA	C13-C15-C16-C17
28	b	622	LMG	C13-C14-C15-C16
29	a	612	SQD	C31-C32-C33-C34
32	B	625	STE	C13-C14-C15-C16
25	b	602	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C20
25	b	604	CLA	C3-C5-C6-C7
26	B	618	BCR	C23-C24-C25-C26
26	B	619	BCR	C23-C24-C25-C30
26	H	101	BCR	C23-C24-C25-C26
26	K	103	BCR	C23-C24-C25-C26
26	K	103	BCR	C23-C24-C25-C30
26	k	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C23-C24-C25-C30
26	k	103	BCR	C5-C6-C7-C8
25	B	607	CLA	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
32	t	103	STE	C4-C5-C6-C7
29	a	612	SQD	C29-C30-C31-C32
30	l	101	LHG	C14-C15-C16-C17
26	A	609	BCR	C14-C15-C16-C17
28	B	620	LMG	C15-C16-C17-C18
28	c	521	LMG	C12-C13-C14-C15
30	A	614	LHG	C31-C32-C33-C34
28	D	407	LMG	C37-C38-C39-C40
29	D	408	SQD	C27-C28-C29-C30
25	A	611	CLA	C16-C17-C18-C19
25	b	607	CLA	C10-C11-C12-C13
29	a	612	SQD	C17-C18-C19-C20
30	D	412	LHG	C24-C25-C26-C27
31	C	515	DGD	C3B-C4B-C5B-C6B
32	B	626	STE	C6-C7-C8-C9
32	m	102	STE	C13-C14-C15-C16
29	B	623	SQD	C24-C25-C26-C27
29	a	612	SQD	C10-C11-C12-C13
31	C	516	DGD	C9A-CAA-CBA-CCA
30	e	101	LHG	O6-C4-C5-C6
25	C	513	CLA	O1D-CGD-O2D-CED
25	A	607	CLA	C11-C12-C13-C15
25	B	601	CLA	C11-C10-C8-C7
25	B	603	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C7
25	B	606	CLA	C11-C10-C8-C7
25	B	607	CLA	C11-C10-C8-C7
25	B	613	CLA	C12-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	513	CLA	C11-C10-C8-C7
25	D	404	CLA	C6-C7-C8-C10
25	a	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	a	608	CLA	C12-C13-C15-C16
25	b	601	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C12-C13-C15
25	b	607	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C15
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
28	d	411	LMG	C15-C16-C17-C18
32	t	103	STE	C5-C6-C7-C8
25	B	610	CLA	C15-C16-C17-C18
25	c	509	CLA	C16-C17-C18-C20
32	C	518	STE	C3-C4-C5-C6
27	d	406	PL9	C27-C28-C29-C31
28	d	411	LMG	C40-C41-C42-C43
32	d	412	STE	C3-C4-C5-C6
25	a	608	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
25	c	505	CLA	C5-C6-C7-C8
25	b	601	CLA	C2A-CAA-CBA-CGA
31	c	517	DGD	C7A-C8A-C9A-CAA
25	b	604	CLA	C5-C6-C7-C8
26	B	617	BCR	C35-C13-C14-C15
26	C	514	BCR	C20-C21-C22-C37
26	H	101	BCR	C20-C21-C22-C37
26	K	103	BCR	C35-C13-C14-C15
26	T	101	BCR	C11-C10-C9-C34
26	b	618	BCR	C16-C17-C18-C36
31	C	516	DGD	CBB-CCB-CDB-CEB
31	A	616	DGD	C1A-C2A-C3A-C4A
25	A	608	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C12-C13-C15
25	b	612	CLA	C16-C17-C18-C19
25	B	616	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
32	T	102	STE	C10-C11-C12-C13
32	b	621	STE	C2-C3-C4-C5
29	D	408	SQD	C23-C24-C25-C26
28	D	407	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	C6B-C7B-C8B-C9B
25	C	512	CLA	C10-C11-C12-C13
25	b	607	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
33	a	607	PHO	CAD-CBD-CGD-O2D
29	A	615	SQD	C15-C16-C17-C18
26	b	618	BCR	C22-C23-C24-C25
25	B	610	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	C16-C17-C18-C19
28	D	407	LMG	C32-C33-C34-C35
32	b	621	STE	C11-C12-C13-C14
29	A	613	SQD	C7-C8-C9-C10
28	c	520	LMG	O1-C7-C8-C9
25	c	502	CLA	O1A-CGA-O2A-C1
30	d	409	LHG	O10-C23-O8-C6
31	c	515	DGD	CAA-CBA-CCA-CDA
30	D	410	LHG	O6-C4-C5-O7
25	c	510	CLA	C15-C16-C17-C18
29	D	408	SQD	O48-C23-C24-C25
31	H	102	DGD	O2G-C1B-C2B-C3B
25	A	611	CLA	C13-C15-C16-C17
28	c	521	LMG	C20-C21-C22-C23
25	b	612	CLA	C16-C17-C18-C20
25	d	404	CLA	C16-C17-C18-C19
25	B	601	CLA	CHA-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
28	D	411	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	616	CLA	O1A-CGA-O2A-C1
32	b	623	STE	C9-C10-C11-C12
26	k	103	BCR	C11-C10-C9-C8
31	A	616	DGD	CFB-CGB-CHB-CIB
28	B	620	LMG	O7-C8-C9-O8
28	C	517	LMG	O1-C7-C8-O7
28	b	622	LMG	O1-C7-C8-O7
28	c	518	LMG	O1-C7-C8-O7
28	c	521	LMG	O7-C8-C9-O8
31	C	515	DGD	O1G-C1G-C2G-O2G
31	a	614	DGD	O1G-C1G-C2G-O2G
29	A	613	SQD	C16-C17-C18-C19
25	b	613	CLA	O1D-CGD-O2D-CED
29	a	613	SQD	C14-C15-C16-C17
32	B	627	STE	C9-C10-C11-C12
32	a	615	STE	C2-C3-C4-C5
32	t	102	STE	C11-C10-C9-C8
30	d	408	LHG	O1-C1-C2-O2
28	d	411	LMG	C32-C33-C34-C35
25	D	403	CLA	C3-C5-C6-C7
25	B	609	CLA	C4-C3-C5-C6
25	C	510	CLA	C4-C3-C5-C6
28	d	411	LMG	C39-C40-C41-C42
32	C	520	STE	C7-C8-C9-C10
27	A	610	PL9	C4-C3-C7-C8
27	a	610	PL9	C4-C3-C7-C8
30	D	409	LHG	O9-C7-O7-C5
25	B	601	CLA	C11-C10-C8-C9
25	B	604	CLA	C6-C7-C8-C9
25	B	607	CLA	C11-C10-C8-C9
25	B	613	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
25	c	510	CLA	C6-C7-C8-C9
32	J	102	STE	C6-C7-C8-C9
32	c	519	STE	C12-C13-C14-C15
25	c	504	CLA	O1A-CGA-O2A-C1
32	b	623	STE	C1-C2-C3-C4
30	e	101	LHG	C25-C26-C27-C28
25	B	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	d	410	LMG	C40-C41-C42-C43
25	B	614	CLA	O1D-CGD-O2D-CED
29	b	620	SQD	C14-C15-C16-C17
26	K	101	BCR	C21-C22-C23-C24
26	K	102	BCR	C7-C8-C9-C10
30	d	409	LHG	C31-C32-C33-C34
31	a	614	DGD	C7B-C8B-C9B-CAB
25	a	608	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	CBA-CGA-O2A-C1
30	d	408	LHG	C3-O3-P-O6
30	d	408	LHG	C18-C19-C20-C21
31	h	102	DGD	C4A-C5A-C6A-C7A
30	D	409	LHG	C31-C32-C33-C34
30	A	614	LHG	C3-O3-P-O4
30	D	409	LHG	C3-O3-P-O4
30	D	409	LHG	C4-O6-P-O5
30	D	410	LHG	C3-O3-P-O5
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O5
30	e	101	LHG	C4-O6-P-O4
28	c	521	LMG	C37-C38-C39-C40
31	C	515	DGD	CAB-CBB-CCB-CDB
32	a	615	STE	C7-C8-C9-C10
30	D	410	LHG	O6-C4-C5-C6
31	c	516	DGD	C7A-C8A-C9A-CAA
29	D	408	SQD	C34-C35-C36-C37
25	B	613	CLA	C16-C17-C18-C19
28	A	612	LMG	C12-C13-C14-C15
30	D	409	LHG	C35-C36-C37-C38
32	C	518	STE	C6-C7-C8-C9
32	c	519	STE	C11-C12-C13-C14
25	B	601	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
29	b	620	SQD	C5-C6-S-O9
25	C	512	CLA	C15-C16-C17-C18
30	D	412	LHG	C33-C34-C35-C36
25	a	608	CLA	C10-C11-C12-C13
32	B	627	STE	C15-C16-C17-C18
28	D	411	LMG	C28-C29-C30-C31
28	m	101	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	a	613	SQD	C13-C14-C15-C16
25	c	512	CLA	C4-C3-C5-C6
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	602	CLA	C12-C13-C15-C16
25	B	604	CLA	C6-C7-C8-C10
25	B	605	CLA	C12-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C10-C8-C7
25	C	507	CLA	C12-C13-C15-C16
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	a	608	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C10-C8-C7
25	c	501	CLA	C11-C12-C13-C15
25	c	504	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
30	A	614	LHG	O6-C4-C5-O7
31	a	614	DGD	CCB-CDB-CEB-CFB
25	c	503	CLA	O1A-CGA-O2A-C1
31	c	515	DGD	O6D-C5D-C6D-O5D
28	d	410	LMG	C34-C35-C36-C37
29	f	102	SQD	C28-C29-C30-C31
31	H	102	DGD	CCB-CDB-CEB-CFB
25	B	610	CLA	CBD-CGD-O2D-CED
25	A	611	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
28	C	517	LMG	O1-C7-C8-C9
28	D	411	LMG	O7-C8-C9-O8
28	c	520	LMG	O7-C8-C9-O8
32	b	621	STE	C14-C15-C16-C17
32	t	102	STE	C4-C5-C6-C7
28	A	612	LMG	C14-C15-C16-C17
30	D	412	LHG	C32-C33-C34-C35
32	k	104	STE	C2-C3-C4-C5
26	h	101	BCR	C14-C15-C16-C17
31	c	516	DGD	C5D-C6D-O5D-C1E
25	b	602	CLA	C10-C11-C12-C13
33	d	402	PHO	C13-C15-C16-C17
28	d	411	LMG	C36-C37-C38-C39
31	a	614	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
28	A	612	LMG	C31-C32-C33-C34
32	d	413	STE	C4-C5-C6-C7
25	c	513	CLA	CBA-CGA-O2A-C1
29	a	612	SQD	C24-C23-O48-C46
28	m	101	LMG	C4-C5-C6-O5
25	B	609	CLA	C2-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
33	D	401	PHO	C2-C3-C5-C6
28	b	622	LMG	C34-C35-C36-C37
29	B	623	SQD	C14-C15-C16-C17
25	B	603	CLA	C14-C13-C15-C16
25	B	606	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	502	CLA	C6-C7-C8-C9
25	C	505	CLA	C11-C12-C13-C14
25	C	508	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	609	CLA	C11-C10-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C14
33	D	401	PHO	C14-C13-C15-C16
33	a	607	PHO	C14-C13-C15-C16
29	a	612	SQD	O10-C23-O48-C46
25	B	613	CLA	C16-C17-C18-C20
31	c	517	DGD	C8A-C9A-CAA-CBA
30	e	101	LHG	C14-C15-C16-C17
31	c	516	DGD	C2A-C3A-C4A-C5A
32	I	101	STE	C12-C13-C14-C15
28	B	620	LMG	C39-C40-C41-C42
26	K	103	BCR	C37-C22-C23-C24
28	B	622	LMG	C14-C15-C16-C17
30	D	410	LHG	C14-C15-C16-C17
31	a	614	DGD	C9A-CAA-CBA-CCA
31	h	102	DGD	CDA-CEA-CFA-CGA
25	b	610	CLA	C16-C17-C18-C19
32	C	519	STE	C3-C4-C5-C6
26	t	101	BCR	C21-C22-C23-C24
30	d	408	LHG	C35-C36-C37-C38
25	B	601	CLA	CAA-CBA-CGA-O2A
25	c	509	CLA	CAA-CBA-CGA-O2A
28	d	411	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C16-C17-C18-C20
28	D	407	LMG	C31-C32-C33-C34
28	b	622	LMG	C16-C17-C18-C19
28	b	622	LMG	C42-C43-C44-C45
30	D	412	LHG	C25-C26-C27-C28
31	A	616	DGD	C7B-C8B-C9B-CAB
25	C	506	CLA	C13-C15-C16-C17
31	C	515	DGD	O6D-C5D-C6D-O5D
28	D	411	LMG	C33-C34-C35-C36
32	B	626	STE	C7-C8-C9-C10
28	b	622	LMG	C7-C8-O7-C10
25	A	606	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C1-O2A-CGA
25	B	613	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
30	d	407	LHG	C32-C33-C34-C35
32	B	627	STE	C5-C6-C7-C8
28	B	620	LMG	C28-C29-C30-C31
29	A	615	SQD	C7-C8-C9-C10
25	d	404	CLA	C8-C10-C11-C12
25	c	513	CLA	O1A-CGA-O2A-C1
31	C	515	DGD	O1G-C1A-C2A-C3A
31	h	102	DGD	C9A-CAA-CBA-CCA
26	B	619	BCR	C23-C24-C25-C26
26	C	514	BCR	C23-C24-C25-C30
26	H	101	BCR	C23-C24-C25-C30
26	b	618	BCR	C23-C24-C25-C30
26	k	103	BCR	C1-C6-C7-C8
25	C	504	CLA	C2-C3-C5-C6
28	B	622	LMG	C34-C35-C36-C37
28	m	101	LMG	C31-C32-C33-C34
25	b	615	CLA	C13-C15-C16-C17
30	l	101	LHG	C24-C25-C26-C27
30	D	412	LHG	C23-C24-C25-C26
25	b	611	CLA	C10-C11-C12-C13
28	C	517	LMG	C18-C19-C20-C21
32	b	624	STE	C4-C5-C6-C7
25	B	610	CLA	C16-C17-C18-C20
29	a	613	SQD	C11-C10-C9-C8
25	B	602	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	K	102	BCR	C20-C21-C22-C23
26	k	101	BCR	C20-C21-C22-C23
30	l	101	LHG	C4-O6-P-O3
30	l	101	LHG	C13-C14-C15-C16
32	T	102	STE	C12-C13-C14-C15
25	B	612	CLA	C13-C15-C16-C17
33	d	402	PHO	CHA-CBD-CGD-O1D
33	d	402	PHO	CHA-CBD-CGD-O2D
25	b	609	CLA	O1D-CGD-O2D-CED
32	T	102	STE	C11-C12-C13-C14
32	A	617	STE	C13-C14-C15-C16
32	m	102	STE	C10-C11-C12-C13
25	B	613	CLA	C10-C11-C12-C13
25	a	606	CLA	C6-C7-C8-C10
25	b	609	CLA	C6-C7-C8-C10
25	b	612	CLA	C6-C7-C8-C10
25	b	615	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C12-C13-C15-C16
27	d	406	PL9	C33-C34-C36-C37
25	B	609	CLA	C3-C5-C6-C7
31	c	517	DGD	CBB-CCB-CDB-CEB
25	A	607	CLA	C11-C12-C13-C14
25	B	601	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C10-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	C	509	CLA	C14-C13-C15-C16
25	D	404	CLA	C6-C7-C8-C9
25	a	606	CLA	C14-C13-C15-C16
25	a	608	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	608	CLA	C11-C10-C8-C9
25	c	501	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
26	K	101	BCR	C9-C10-C11-C12
30	D	410	LHG	C12-C13-C14-C15
29	A	615	SQD	C32-C33-C34-C35
30	A	614	LHG	C28-C29-C30-C31
31	c	517	DGD	CCB-CDB-CEB-CFB
31	C	515	DGD	C4D-C5D-C6D-O5D
28	D	411	LMG	C34-C35-C36-C37
32	c	519	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	CBA-CGA-O2A-C1
30	A	614	LHG	C2-C3-O3-P
30	d	409	LHG	C2-C3-O3-P
28	m	101	LMG	C34-C35-C36-C37
27	D	406	PL9	C30-C29-C31-C32
25	c	512	CLA	C2-C3-C5-C6
25	C	511	CLA	CBA-CGA-O2A-C1
31	A	616	DGD	C2A-C1A-O1G-C1G
32	t	103	STE	C7-C8-C9-C10
32	b	621	STE	O2-C1-C2-C3
30	d	407	LHG	C14-C15-C16-C17
25	c	502	CLA	C13-C15-C16-C17
25	C	511	CLA	O1A-CGA-O2A-C1
31	H	102	DGD	C6A-C7A-C8A-C9A
31	C	516	DGD	O6D-C1D-O3G-C3G
32	t	103	STE	C6-C7-C8-C9
27	D	406	PL9	C39-C41-C42-C43
27	a	610	PL9	C19-C21-C22-C23
25	c	513	CLA	C15-C16-C17-C18
26	B	617	BCR	C10-C11-C12-C13
32	b	624	STE	C11-C12-C13-C14
27	A	610	PL9	C45-C44-C46-C47
32	k	104	STE	O2-C1-C2-C3
25	B	612	CLA	C8-C10-C11-C12
29	D	408	SQD	C24-C25-C26-C27
28	c	521	LMG	C18-C19-C20-C21
28	c	521	LMG	C30-C31-C32-C33
25	b	613	CLA	C2-C1-O2A-CGA
25	C	513	CLA	C16-C17-C18-C20
32	b	624	STE	C6-C7-C8-C9
30	d	409	LHG	C32-C33-C34-C35
25	C	501	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
33	d	402	PHO	C3A-C2A-CAA-CBA
28	A	612	LMG	C38-C39-C40-C41
25	C	508	CLA	C13-C15-C16-C17
30	d	407	LHG	C29-C30-C31-C32
25	C	506	CLA	C4-C3-C5-C6
28	b	622	LMG	C14-C15-C16-C17
30	A	614	LHG	C17-C18-C19-C20
31	h	102	DGD	CCA-CDA-CEA-CFA
27	D	406	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C19-C20-C21-C22
25	A	611	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	a	606	CLA	C6-C7-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
31	c	515	DGD	C8A-C9A-CAA-CBA
32	d	413	STE	C2-C3-C4-C5
32	C	519	STE	O2-C1-C2-C3
25	B	607	CLA	CBA-CGA-O2A-C1
32	I	101	STE	C5-C6-C7-C8
32	b	623	STE	C2-C3-C4-C5
25	b	610	CLA	C13-C15-C16-C17
28	c	521	LMG	O1-C7-C8-C9
30	d	408	LHG	C19-C20-C21-C22
34	f	101	HEM	CAD-CBD-CGD-O1D
25	b	612	CLA	C8-C10-C11-C12
29	A	615	SQD	C24-C25-C26-C27
32	k	104	STE	C6-C7-C8-C9
33	a	607	PHO	O2A-C1-C2-C3
31	c	516	DGD	O6D-C1D-O3G-C3G
28	C	517	LMG	C16-C17-C18-C19
32	E	102	STE	C4-C5-C6-C7
32	M	102	STE	C1-C2-C3-C4
32	C	519	STE	O1-C1-C2-C3
31	a	614	DGD	C6B-C7B-C8B-C9B
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	515	DGD	C4D-C5D-C6D-O5D
28	D	411	LMG	C16-C17-C18-C19
32	B	627	STE	C4-C5-C6-C7
25	D	403	CLA	C2C-C3C-CAC-CBC
32	D	413	STE	C6-C7-C8-C9
28	B	622	LMG	O9-C10-C11-C12
29	B	623	SQD	C44-C45-O47-C7
29	B	623	SQD	C46-C45-O47-C7
29	a	613	SQD	C46-C45-O47-C7
31	a	614	DGD	C1G-C2G-O2G-C1B
25	B	602	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
29	a	613	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C10-C8-C7
25	c	509	CLA	C11-C12-C13-C15
25	B	612	CLA	O1A-CGA-O2A-C1
31	c	515	DGD	O1A-C1A-O1G-C1G
35	V	201	HEC	CAD-CBD-CGD-O2D
31	C	516	DGD	C2B-C3B-C4B-C5B
25	D	403	CLA	C13-C15-C16-C17
25	C	502	CLA	C16-C17-C18-C20
25	B	614	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C2A-CAA-CBA-CGA
32	D	413	STE	O1-C1-C2-C3
32	D	413	STE	O2-C1-C2-C3
32	c	519	STE	O2-C1-C2-C3
32	k	104	STE	O1-C1-C2-C3
31	H	102	DGD	C9B-CAB-CBB-CCB
32	t	102	STE	C6-C7-C8-C9
25	C	509	CLA	C5-C6-C7-C8
25	b	612	CLA	C2C-C3C-CAC-CBC
30	D	409	LHG	C30-C31-C32-C33
28	d	410	LMG	O7-C10-C11-C12
25	B	601	CLA	C13-C15-C16-C17
25	c	508	CLA	O1A-CGA-O2A-C1
29	b	620	SQD	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
32	c	519	STE	O1-C1-C2-C3
29	A	613	SQD	C26-C27-C28-C29
32	E	102	STE	C7-C8-C9-C10
28	c	520	LMG	O1-C7-C8-O7
31	c	515	DGD	O1G-C1G-C2G-O2G
31	c	515	DGD	C3A-C4A-C5A-C6A
29	A	613	SQD	C35-C36-C37-C38
26	k	102	BCR	C19-C20-C21-C22
32	b	621	STE	O1-C1-C2-C3
28	B	622	LMG	C29-C30-C31-C32
31	J	101	DGD	C9A-CAA-CBA-CCA
30	D	410	LHG	C1-C2-C3-O3
32	E	102	STE	O2-C1-C2-C3
25	C	511	CLA	C2C-C3C-CAC-CBC
28	c	520	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	616	CLA	C10-C11-C12-C13
25	B	601	CLA	C2-C1-O2A-CGA
25	a	605	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C3-C5-C6
25	B	607	CLA	O1A-CGA-O2A-C1
25	A	606	CLA	C14-C13-C15-C16
25	B	601	CLA	C11-C12-C13-C14
25	B	602	CLA	C14-C13-C15-C16
25	B	603	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C10-C8-C9
28	D	407	LMG	C34-C35-C36-C37
32	B	624	STE	C5-C6-C7-C8
28	C	517	LMG	C40-C41-C42-C43
30	L	101	LHG	C25-C26-C27-C28
31	c	516	DGD	C4A-C5A-C6A-C7A
26	B	619	BCR	C1-C6-C7-C8
26	K	103	BCR	C1-C6-C7-C8
26	a	609	BCR	C23-C24-C25-C30
26	b	618	BCR	C23-C24-C25-C26
26	c	514	BCR	C1-C6-C7-C8
26	c	514	BCR	C23-C24-C25-C30
26	k	102	BCR	C23-C24-C25-C30
25	d	403	CLA	C4-C3-C5-C6
28	c	521	LMG	C34-C35-C36-C37
30	D	409	LHG	C11-C10-C9-C8
26	K	101	BCR	C14-C15-C16-C17
31	c	515	DGD	C5D-C6D-O5D-C1E
29	A	615	SQD	C17-C18-C19-C20
25	B	614	CLA	C16-C17-C18-C20
31	H	102	DGD	C2A-C3A-C4A-C5A
35	V	201	HEC	CAD-CBD-CGD-O1D
25	c	508	CLA	CBA-CGA-O2A-C1
32	j	101	STE	C4-C5-C6-C7
25	d	404	CLA	C3-C5-C6-C7
25	C	504	CLA	C11-C12-C13-C14
30	l	101	LHG	O6-C4-C5-C6
31	c	517	DGD	C3A-C4A-C5A-C6A
25	B	616	CLA	C2-C3-C5-C6
25	a	608	CLA	C11-C10-C8-C7
25	b	603	CLA	C2-C3-C5-C6
25	c	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C11-C10-C8-C7
25	d	403	CLA	C6-C7-C8-C10
32	E	102	STE	O1-C1-C2-C3
31	c	516	DGD	CAB-CBB-CCB-CDB
30	D	410	LHG	C31-C32-C33-C34
29	B	623	SQD	C32-C33-C34-C35
25	C	510	CLA	C13-C15-C16-C17
25	C	513	CLA	C5-C6-C7-C8
25	c	503	CLA	C10-C11-C12-C13
28	D	411	LMG	O10-C28-O8-C9
29	a	613	SQD	C24-C25-C26-C27
32	A	617	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O2D
33	D	402	PHO	C4C-C3C-CAC-CBC
31	h	102	DGD	C1A-C2A-C3A-C4A
25	b	613	CLA	CAA-CBA-CGA-O2A
25	B	601	CLA	C4-C3-C5-C6
25	b	616	CLA	C5-C6-C7-C8
29	A	613	SQD	C25-C26-C27-C28
31	C	515	DGD	CCB-CDB-CEB-CFB
35	v	201	HEC	CAD-CBD-CGD-O1D
30	A	614	LHG	C3-O3-P-O6
29	B	623	SQD	C23-C24-C25-C26
28	D	407	LMG	C39-C40-C41-C42
32	H	103	STE	C11-C10-C9-C8
25	B	611	CLA	C11-C12-C13-C14
25	B	613	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C10-C8-C9
25	B	615	CLA	C11-C10-C8-C9
25	a	608	CLA	C11-C12-C13-C14
25	b	612	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
25	d	403	CLA	C14-C13-C15-C16
25	d	404	CLA	C6-C7-C8-C9
29	b	620	SQD	C27-C28-C29-C30
32	j	101	STE	C5-C6-C7-C8
31	C	516	DGD	C1A-C2A-C3A-C4A
25	B	602	CLA	C3A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
31	J	101	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	CAA-CBA-CGA-O2A
28	b	622	LMG	O7-C10-C11-C12
31	A	616	DGD	C6A-C7A-C8A-C9A
32	C	520	STE	C3-C4-C5-C6
34	f	101	HEM	CAD-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
33	D	401	PHO	CAD-CBD-CGD-O2D
30	D	409	LHG	C33-C34-C35-C36
29	a	612	SQD	O49-C7-O47-C45
27	a	610	PL9	C27-C28-C29-C31
28	B	622	LMG	O7-C10-C11-C12
25	B	613	CLA	CAA-CBA-CGA-O2A
31	a	614	DGD	O1G-C1A-C2A-C3A
25	b	605	CLA	C4-C3-C5-C6
27	a	610	PL9	C35-C34-C36-C37
30	d	409	LHG	C34-C35-C36-C37
25	B	601	CLA	C2-C3-C5-C6
28	b	622	LMG	C38-C39-C40-C41
28	A	612	LMG	C7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-C3G
31	c	515	DGD	C1G-C2G-C3G-O3G
33	D	402	PHO	C2C-C3C-CAC-CBC
33	d	402	PHO	C2C-C3C-CAC-CBC
29	D	408	SQD	C30-C31-C32-C33
30	l	101	LHG	O6-C4-C5-O7
32	b	625	STE	C1-C2-C3-C4
25	C	512	CLA	O2A-C1-C2-C3
25	D	404	CLA	O2A-C1-C2-C3
33	D	401	PHO	O2A-C1-C2-C3
30	D	412	LHG	C24-C23-O8-C6
29	a	612	SQD	O47-C7-C8-C9
32	d	413	STE	C6-C7-C8-C9
25	A	607	CLA	CHA-CBD-CGD-O1D
25	A	607	CLA	CHA-CBD-CGD-O2D
25	A	611	CLA	CHA-CBD-CGD-O1D
25	A	611	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	612	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	a	611	CLA	CHA-CBD-CGD-O1D
25	a	611	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O2D
32	A	617	STE	O1-C1-C2-C3
28	c	520	LMG	C16-C17-C18-C19
26	b	618	BCR	C11-C10-C9-C8
28	b	622	LMG	C33-C34-C35-C36
29	A	613	SQD	C29-C30-C31-C32
28	d	411	LMG	O7-C10-C11-C12
30	d	409	LHG	O8-C23-C24-C25
31	A	616	DGD	O1G-C1G-C2G-O2G
32	M	101	STE	C4-C5-C6-C7
25	c	506	CLA	C10-C11-C12-C13
28	d	410	LMG	O9-C10-C11-C12
25	c	510	CLA	CAA-CBA-CGA-O2A
28	m	101	LMG	O8-C28-C29-C30
32	H	103	STE	C13-C14-C15-C16
33	D	401	PHO	CHA-CBD-CGD-O1D
33	a	607	PHO	CHA-CBD-CGD-O1D
31	C	515	DGD	O2G-C1B-C2B-C3B
27	a	610	PL9	C40-C39-C41-C42
30	d	408	LHG	C28-C29-C30-C31
25	A	606	CLA	C12-C13-C15-C16
25	B	601	CLA	C11-C12-C13-C15
25	C	502	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C12-C13-C15
25	a	611	CLA	C12-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C7
32	M	101	STE	O1-C1-C2-C3
25	C	502	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C10-C8-C9
25	a	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C6-C7-C8-C9
25	b	612	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	d	403	CLA	C6-C7-C8-C9
27	a	610	PL9	C14-C16-C17-C18
26	k	101	BCR	C9-C10-C11-C12
32	C	518	STE	C4-C5-C6-C7
28	B	622	LMG	O8-C28-C29-C30
29	A	613	SQD	O47-C7-C8-C9
25	A	607	CLA	C16-C17-C18-C20
25	b	608	CLA	C2C-C3C-CAC-CBC
29	a	612	SQD	C8-C7-O47-C45
28	c	521	LMG	C28-C29-C30-C31
28	C	517	LMG	O7-C10-C11-C12
32	d	413	STE	O1-C1-C2-C3
31	c	515	DGD	C9A-CAA-CBA-CCA
30	d	407	LHG	O1-C1-C2-C3
31	H	102	DGD	CDA-CEA-CFA-CGA
31	a	614	DGD	CCA-CDA-CEA-CFA
32	j	101	STE	C1-C2-C3-C4
30	D	409	LHG	C34-C35-C36-C37
31	c	517	DGD	C7B-C8B-C9B-CAB
25	A	607	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
31	c	516	DGD	O1B-C1B-C2B-C3B
25	C	513	CLA	C2-C1-O2A-CGA
30	D	409	LHG	C9-C10-C11-C12
28	C	517	LMG	C12-C13-C14-C15
29	a	613	SQD	C27-C28-C29-C30
32	B	625	STE	C3-C4-C5-C6
25	b	612	CLA	CAA-CBA-CGA-O2A
25	A	606	CLA	C5-C6-C7-C8
25	c	513	CLA	C13-C15-C16-C17
32	L	102	STE	C3-C4-C5-C6
30	A	614	LHG	C3-O3-P-O5
30	A	614	LHG	C4-O6-P-O5
25	b	613	CLA	CAA-CBA-CGA-O1A
30	L	101	LHG	O10-C23-O8-C6
26	C	514	BCR	C23-C24-C25-C26
26	K	103	BCR	C5-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C5-C6-C7-C8
25	B	612	CLA	CAA-CBA-CGA-O1A
25	B	613	CLA	CAA-CBA-CGA-O1A
28	m	101	LMG	O10-C28-C29-C30
25	c	501	CLA	CAA-CBA-CGA-O2A
34	E	101	HEM	CAD-CBD-CGD-O2D
25	c	506	CLA	C16-C17-C18-C20
26	t	101	BCR	C18-C19-C20-C21
29	a	612	SQD	O49-C7-C8-C9
31	c	516	DGD	CCA-CDA-CEA-CFA
28	D	407	LMG	O7-C10-C11-C12
31	c	515	DGD	O1B-C1B-C2B-C3B
25	A	607	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
29	A	613	SQD	C5-C6-S-O7
29	a	613	SQD	C44-C45-O47-C7
29	A	613	SQD	O49-C7-C8-C9
31	C	515	DGD	O1B-C1B-C2B-C3B
32	d	413	STE	C12-C13-C14-C15
25	b	612	CLA	C15-C16-C17-C18
25	C	506	CLA	C11-C10-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C10-C8-C9
29	b	620	SQD	C11-C10-C9-C8
25	C	509	CLA	C8-C10-C11-C12
25	B	611	CLA	C13-C15-C16-C17
31	c	515	DGD	O2G-C1B-C2B-C3B
28	d	410	LMG	C38-C39-C40-C41
29	D	408	SQD	C31-C32-C33-C34
27	D	406	PL9	C42-C43-C44-C46
25	B	605	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C12-C13-C15
25	B	610	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10

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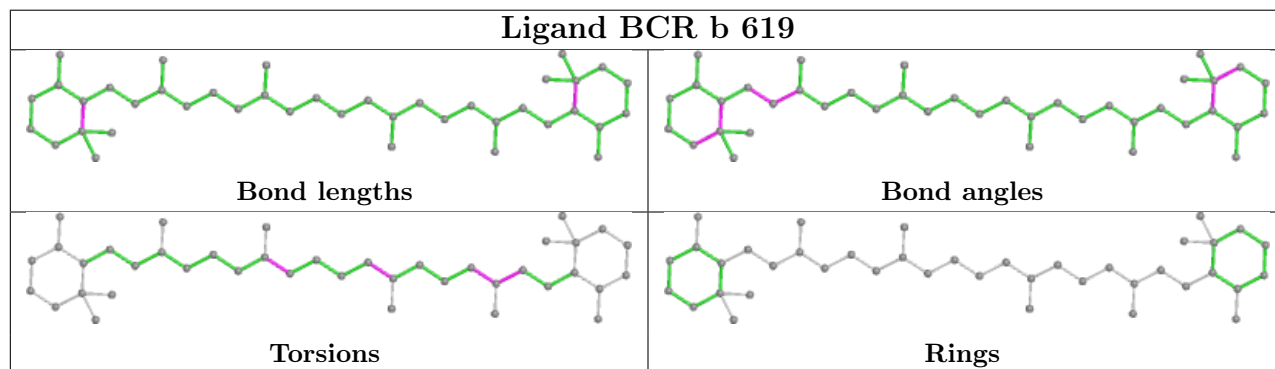
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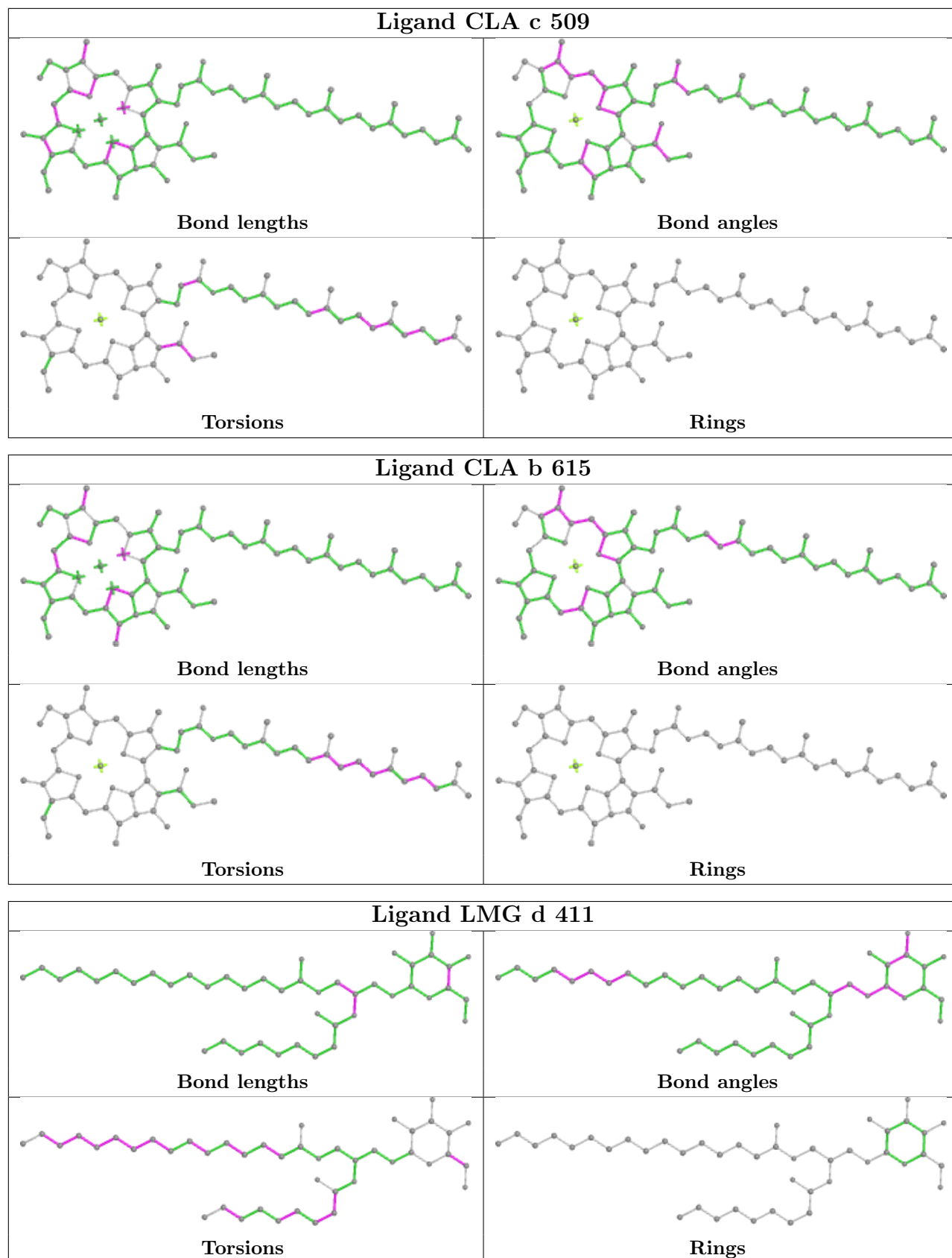
Mol	Chain	Res	Type	Atoms
30	L	101	LHG	O7-C7-C8-C9
28	B	620	LMG	C18-C19-C20-C21
32	d	413	STE	C14-C15-C16-C17
26	K	101	BCR	C11-C12-C13-C14
26	h	101	BCR	C11-C12-C13-C14
28	C	517	LMG	O10-C28-C29-C30
32	M	101	STE	O2-C1-C2-C3
32	d	413	STE	O2-C1-C2-C3
29	D	408	SQD	C45-C44-O6-C1
31	C	515	DGD	O6E-C1E-O5D-C6D
30	L	101	LHG	C34-C35-C36-C37
25	c	510	CLA	CAA-CBA-CGA-O1A
30	D	410	LHG	O10-C23-C24-C25
27	a	610	PL9	C44-C46-C47-C48
31	a	614	DGD	O1B-C1B-C2B-C3B
25	B	605	CLA	C10-C11-C12-C13
25	b	612	CLA	CAA-CBA-CGA-O1A
28	D	407	LMG	O9-C10-C11-C12

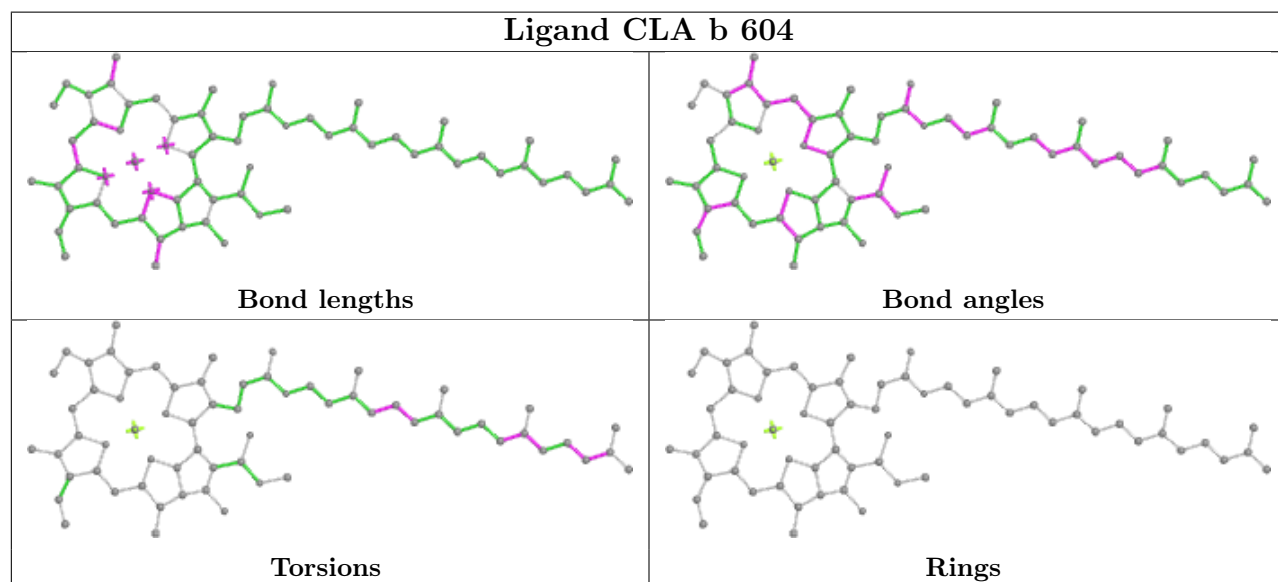
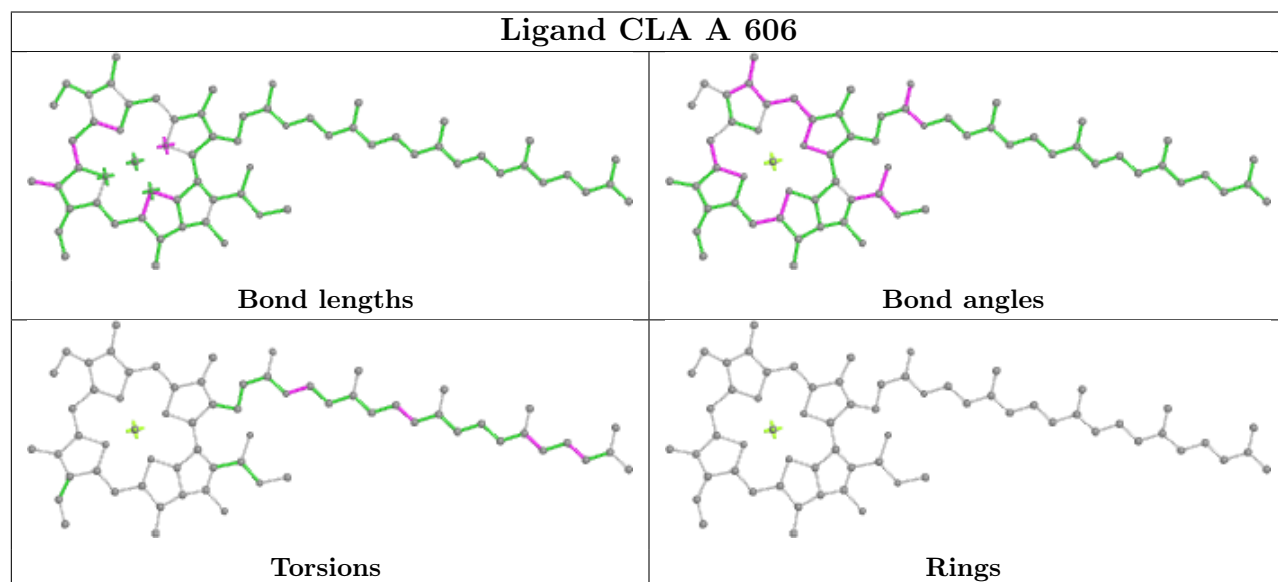
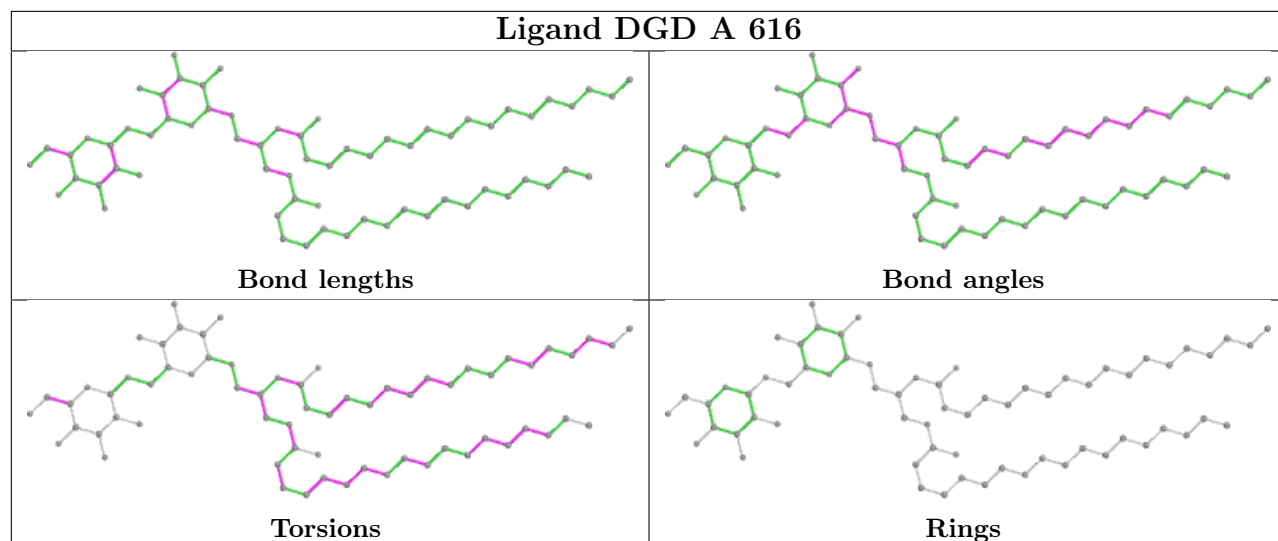
There are no ring outliers.

No monomer is involved in short contacts.

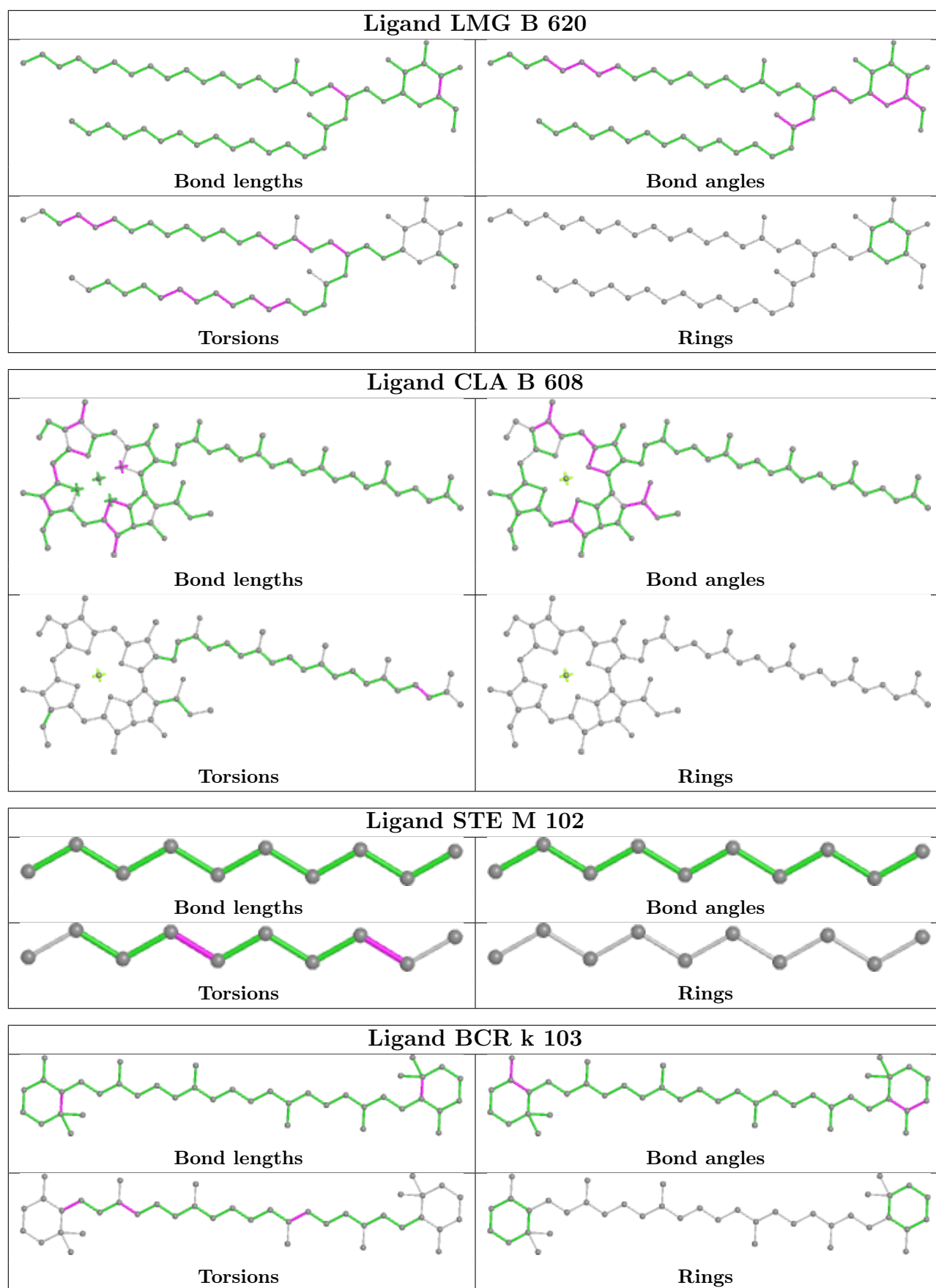
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

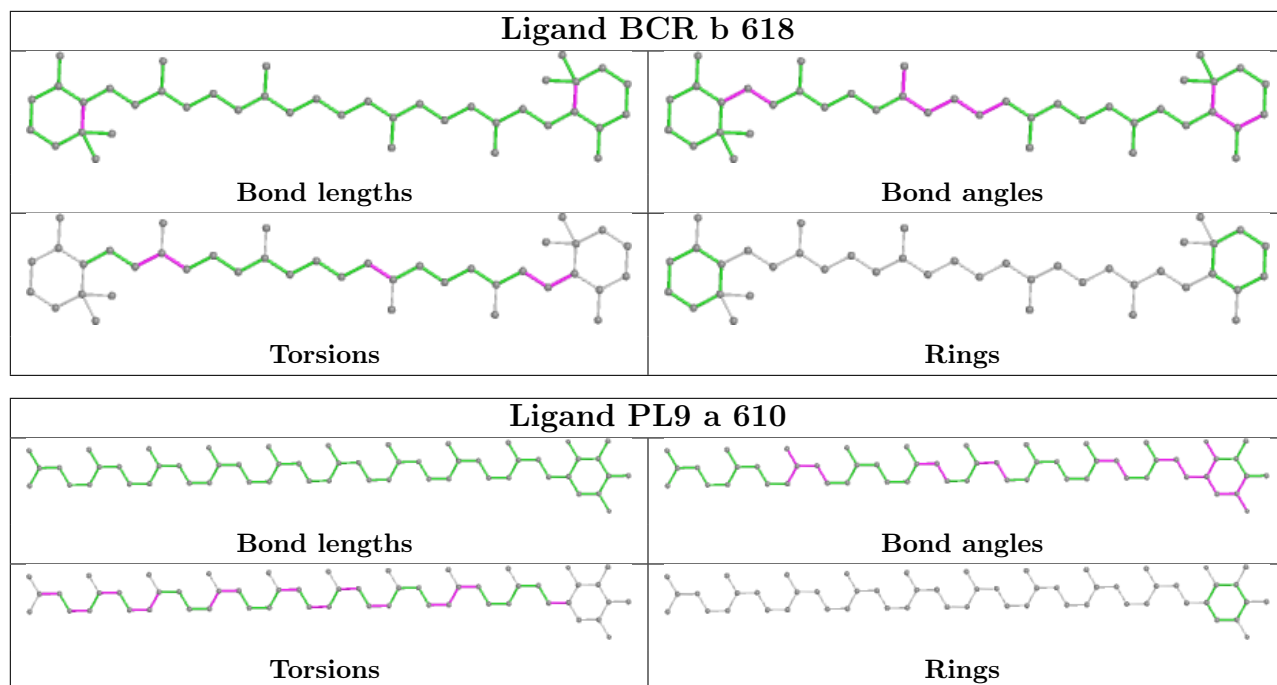


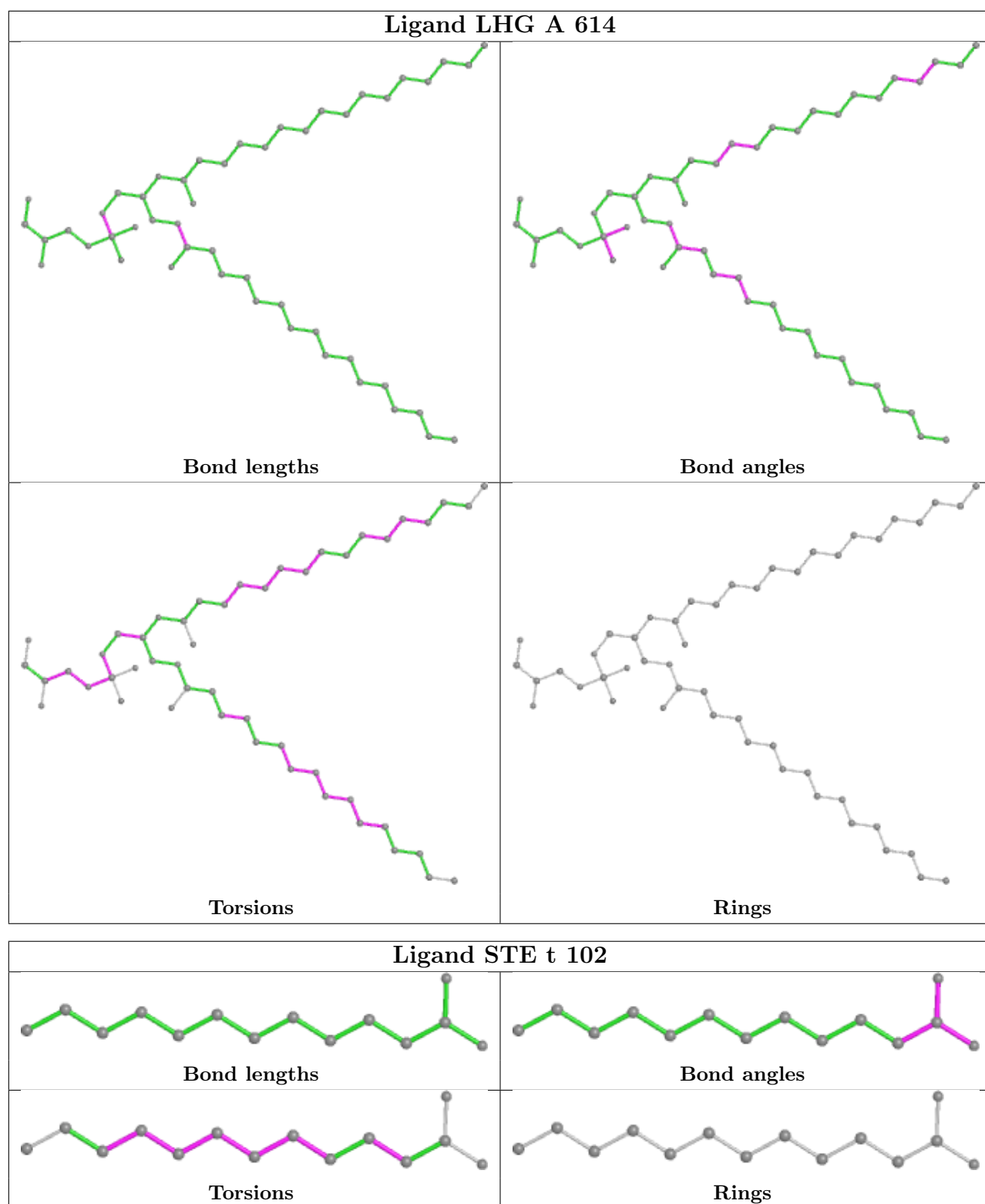


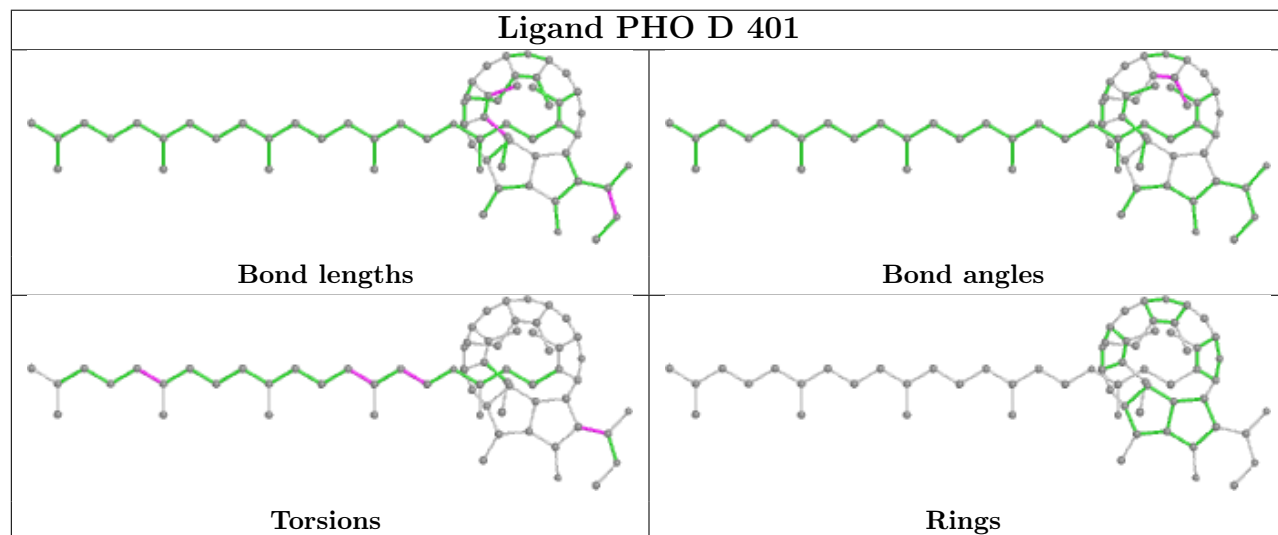
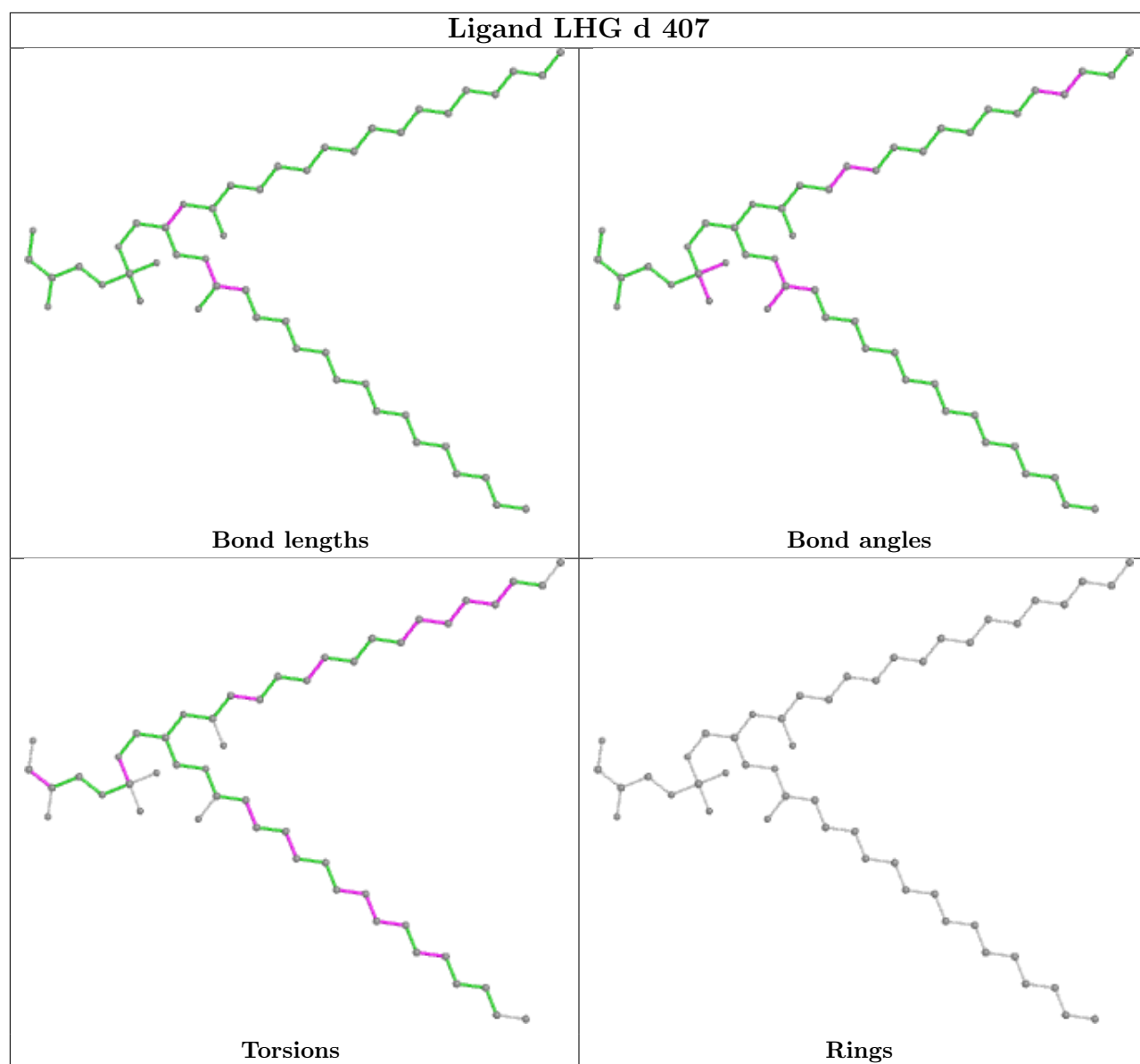


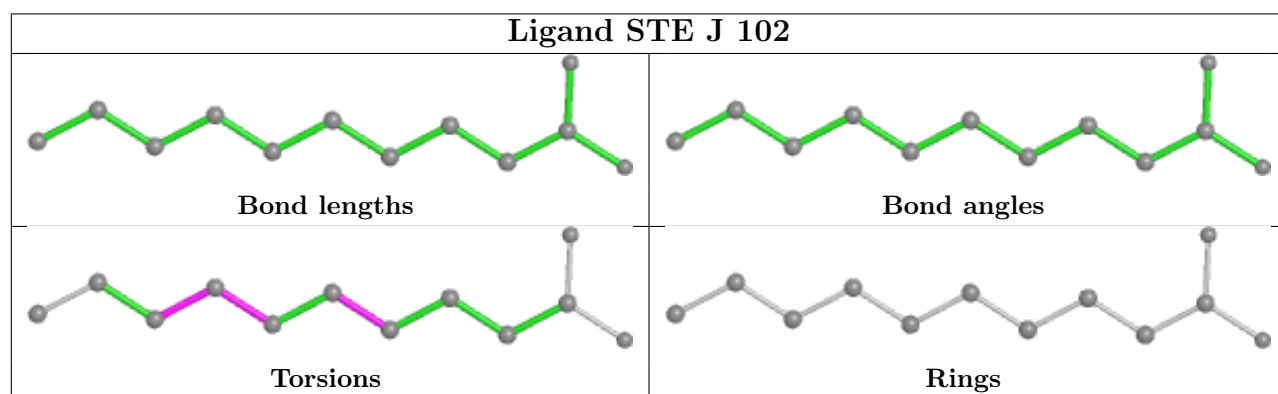
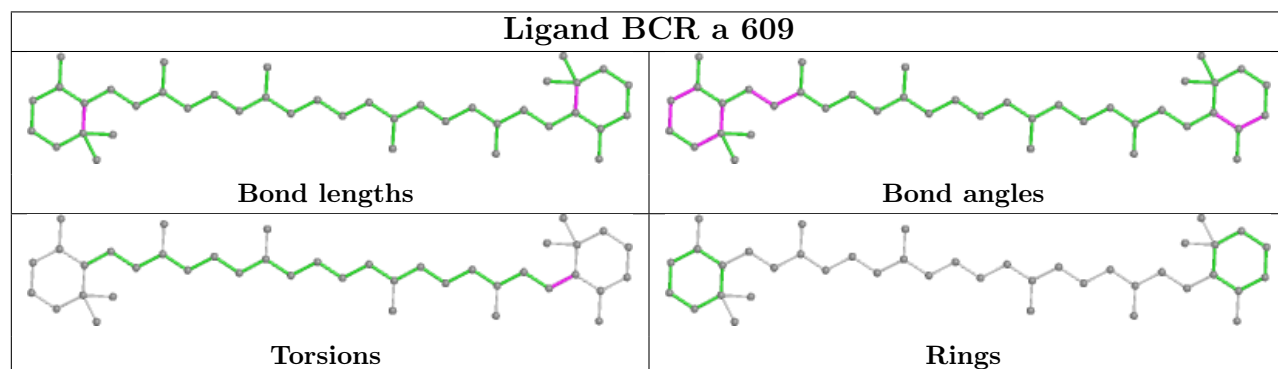
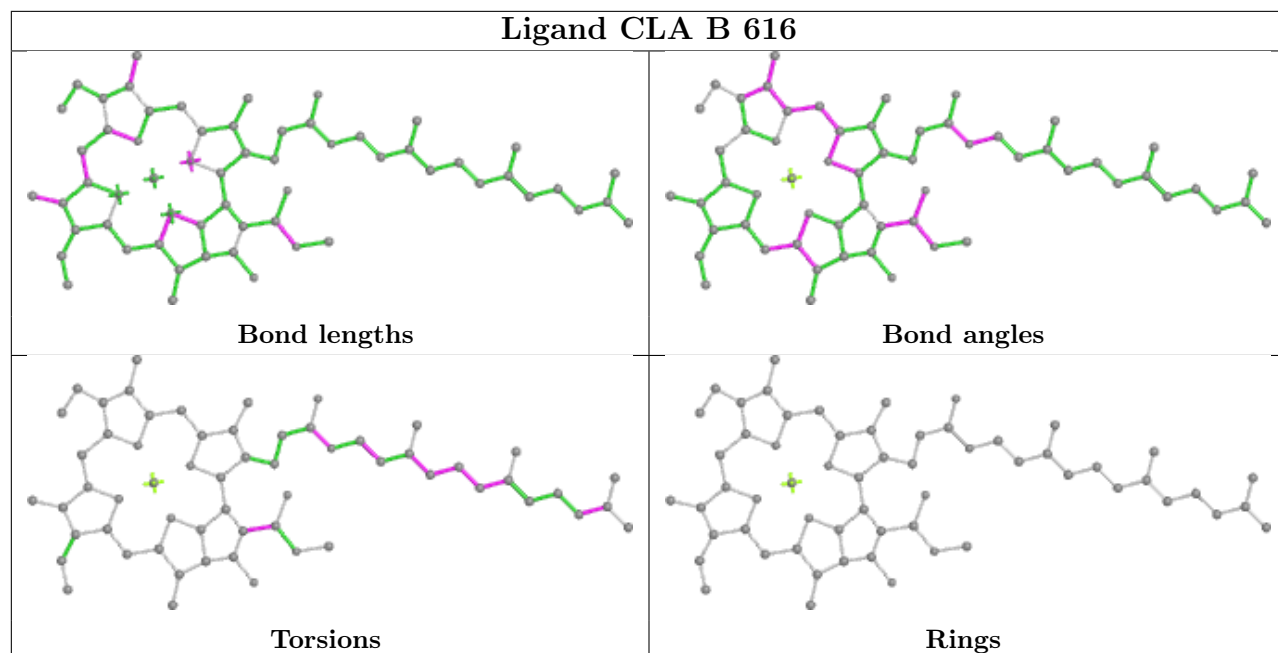


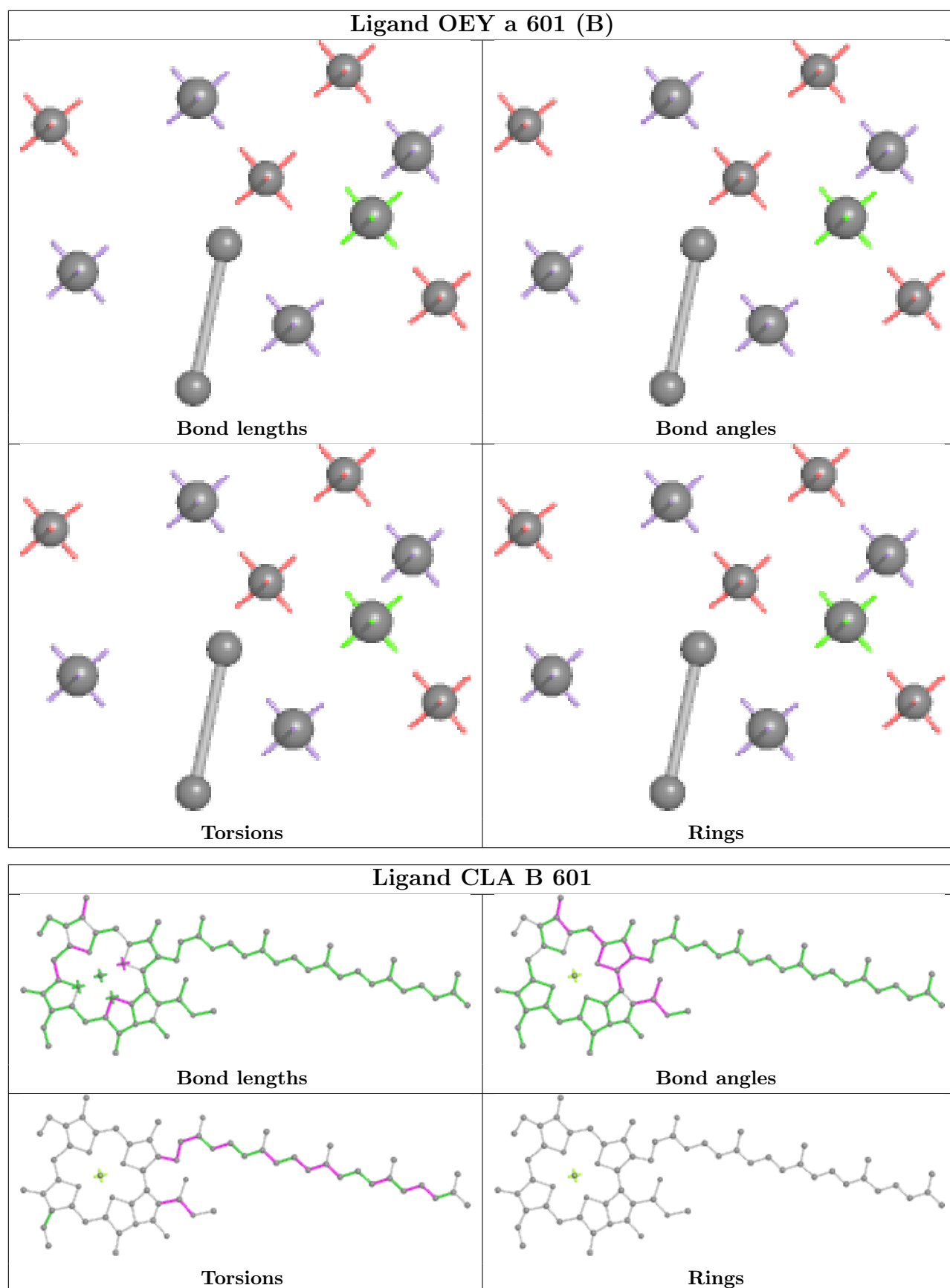


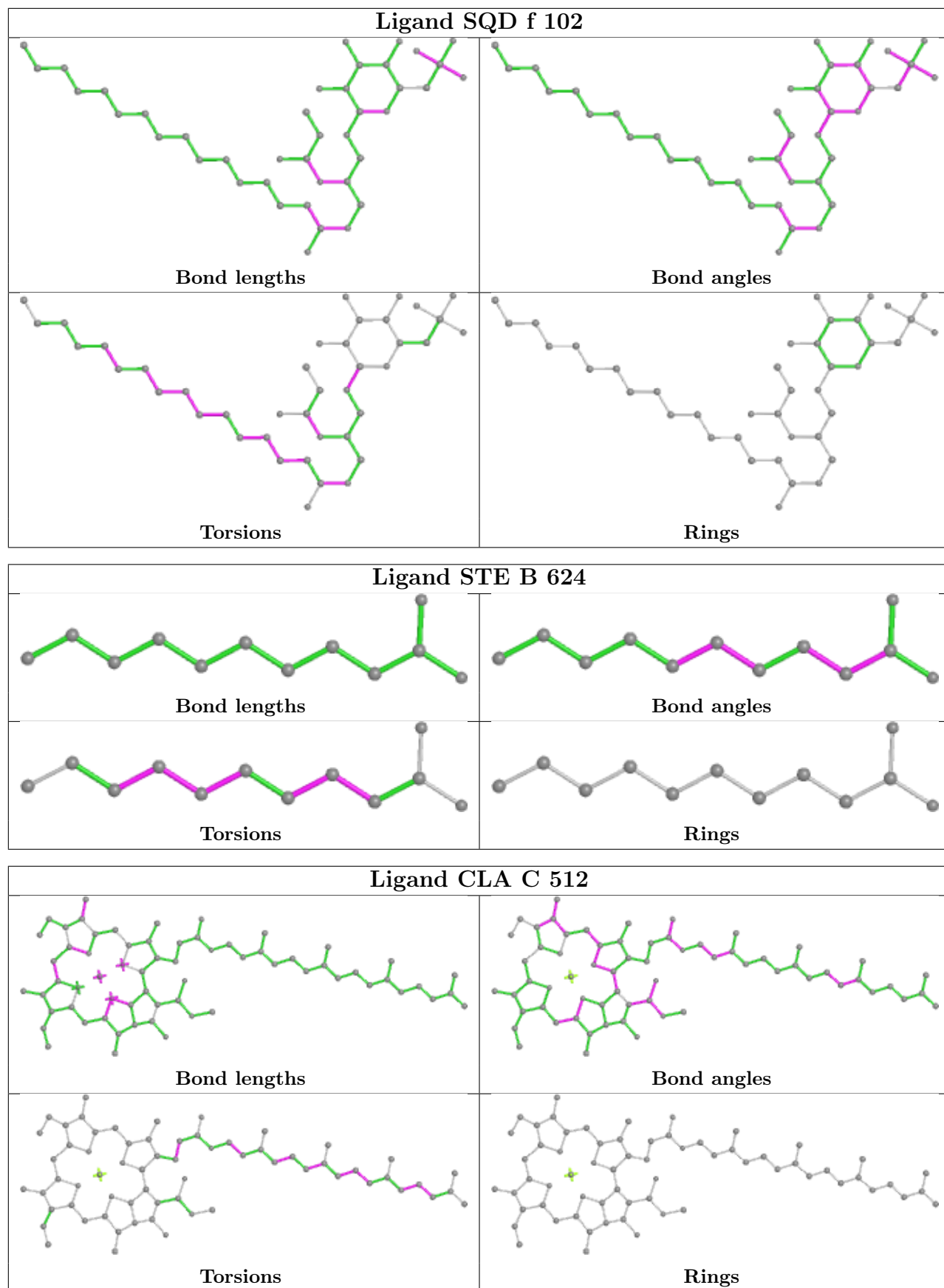


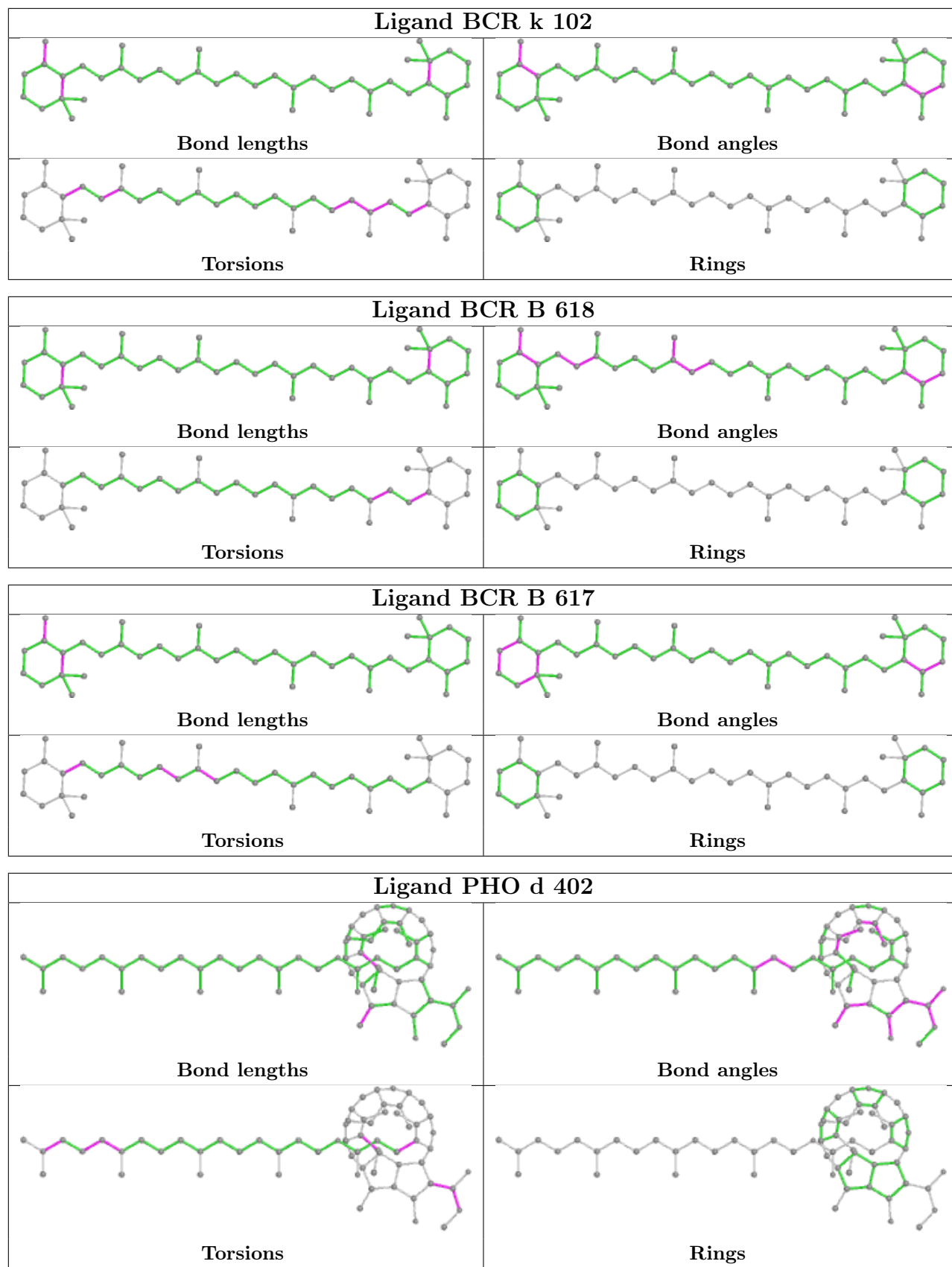




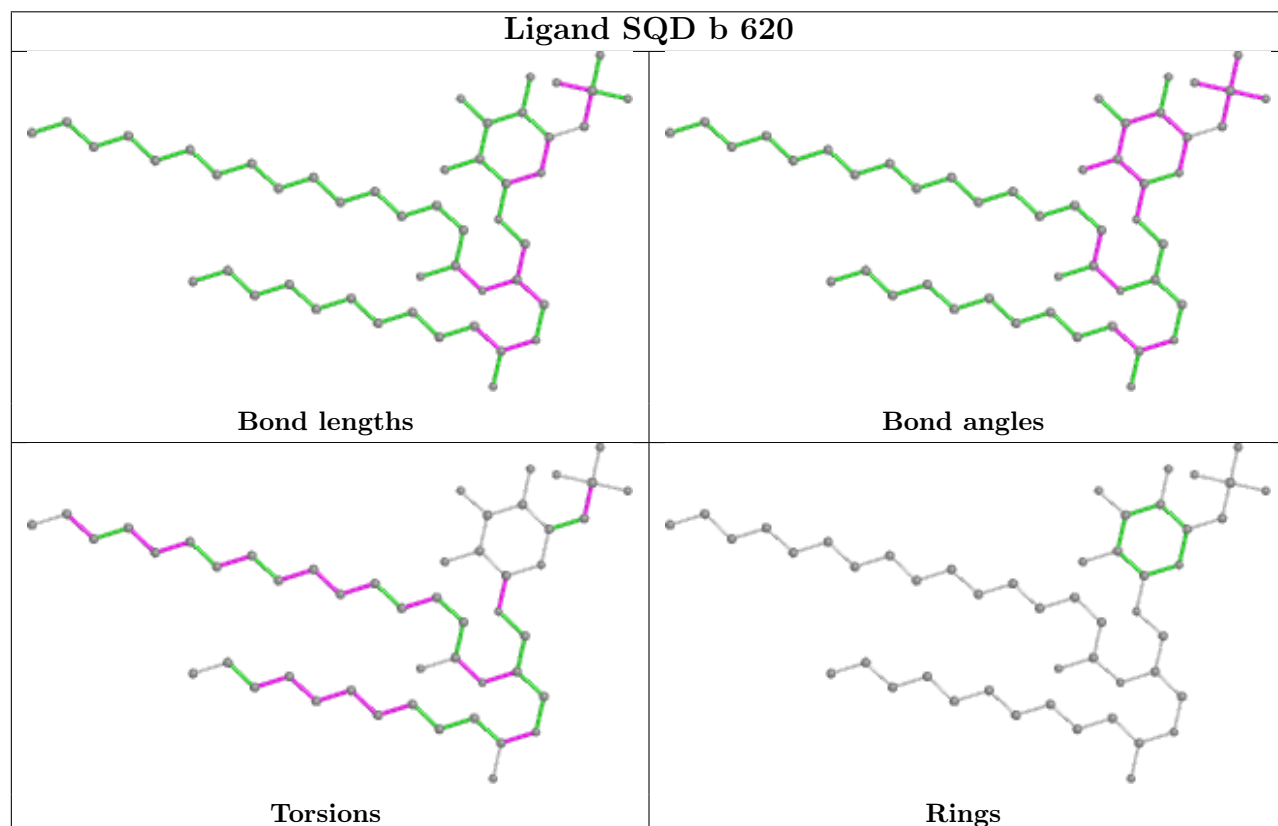
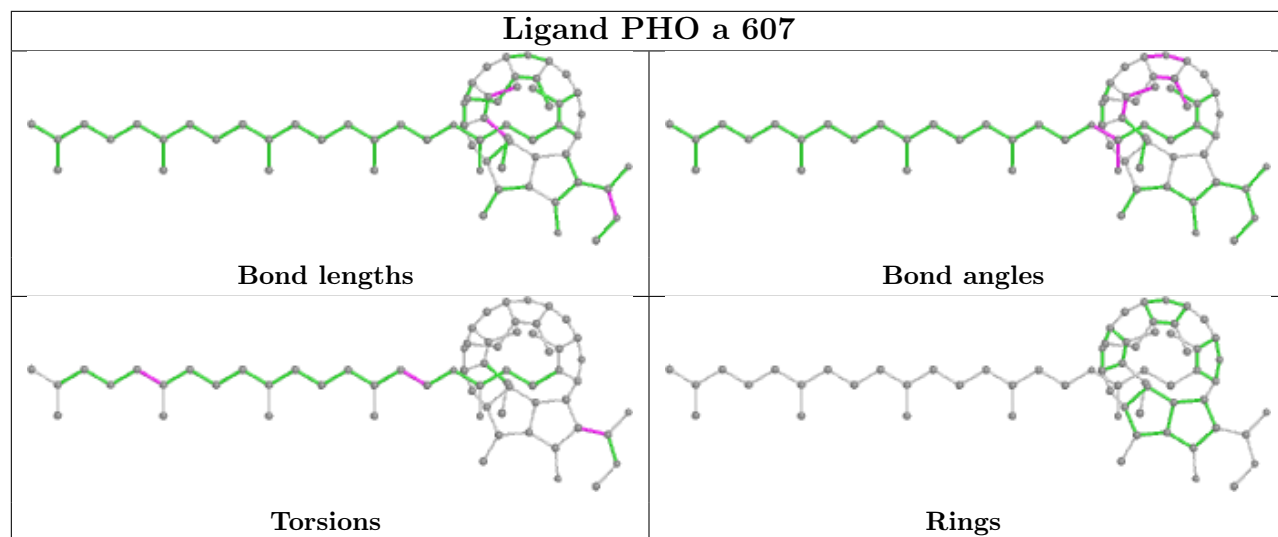
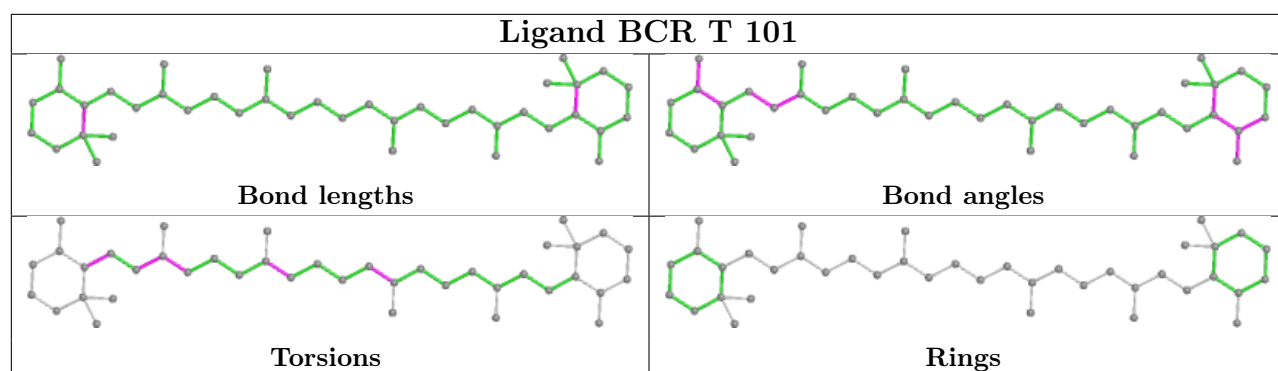


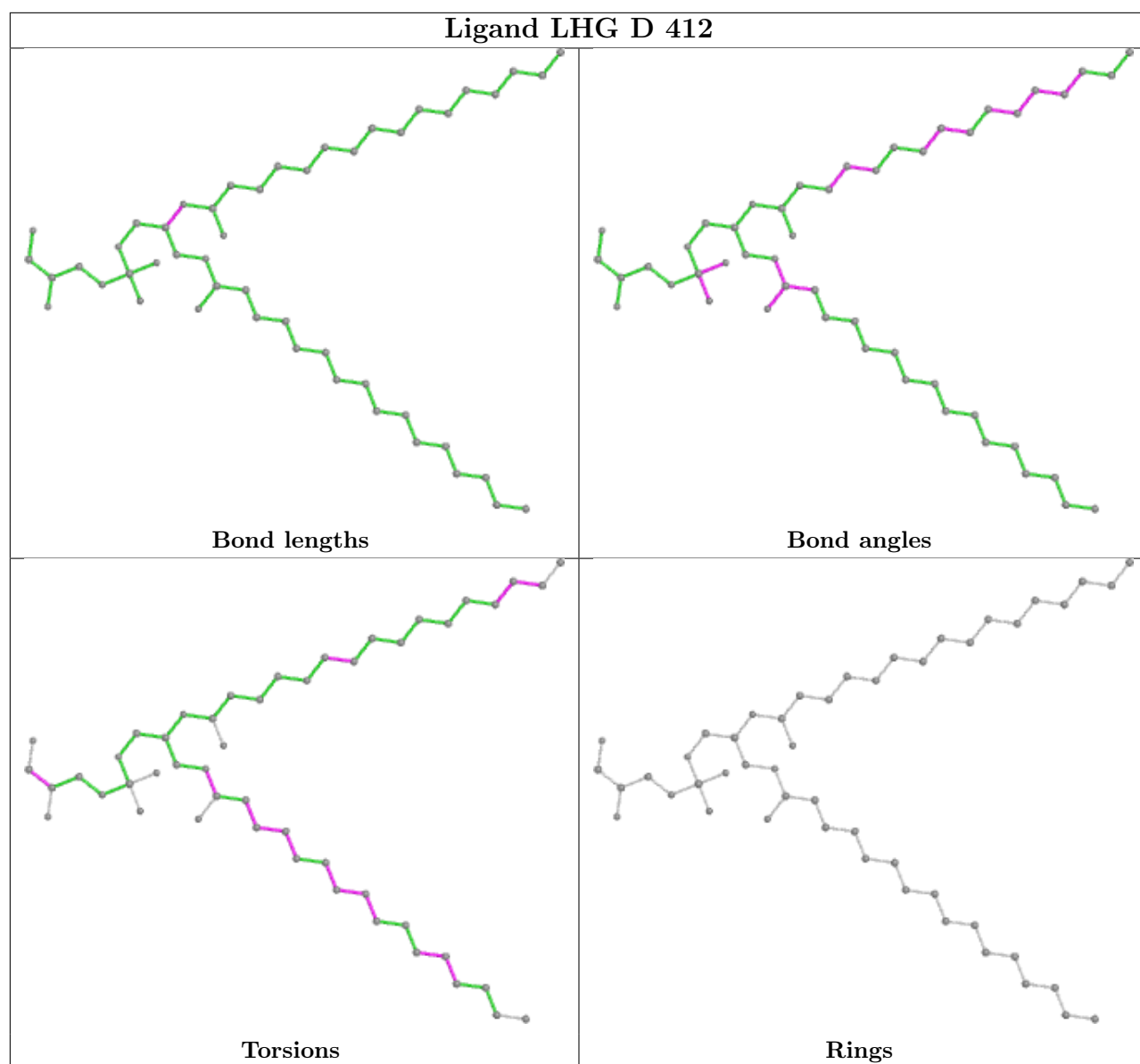


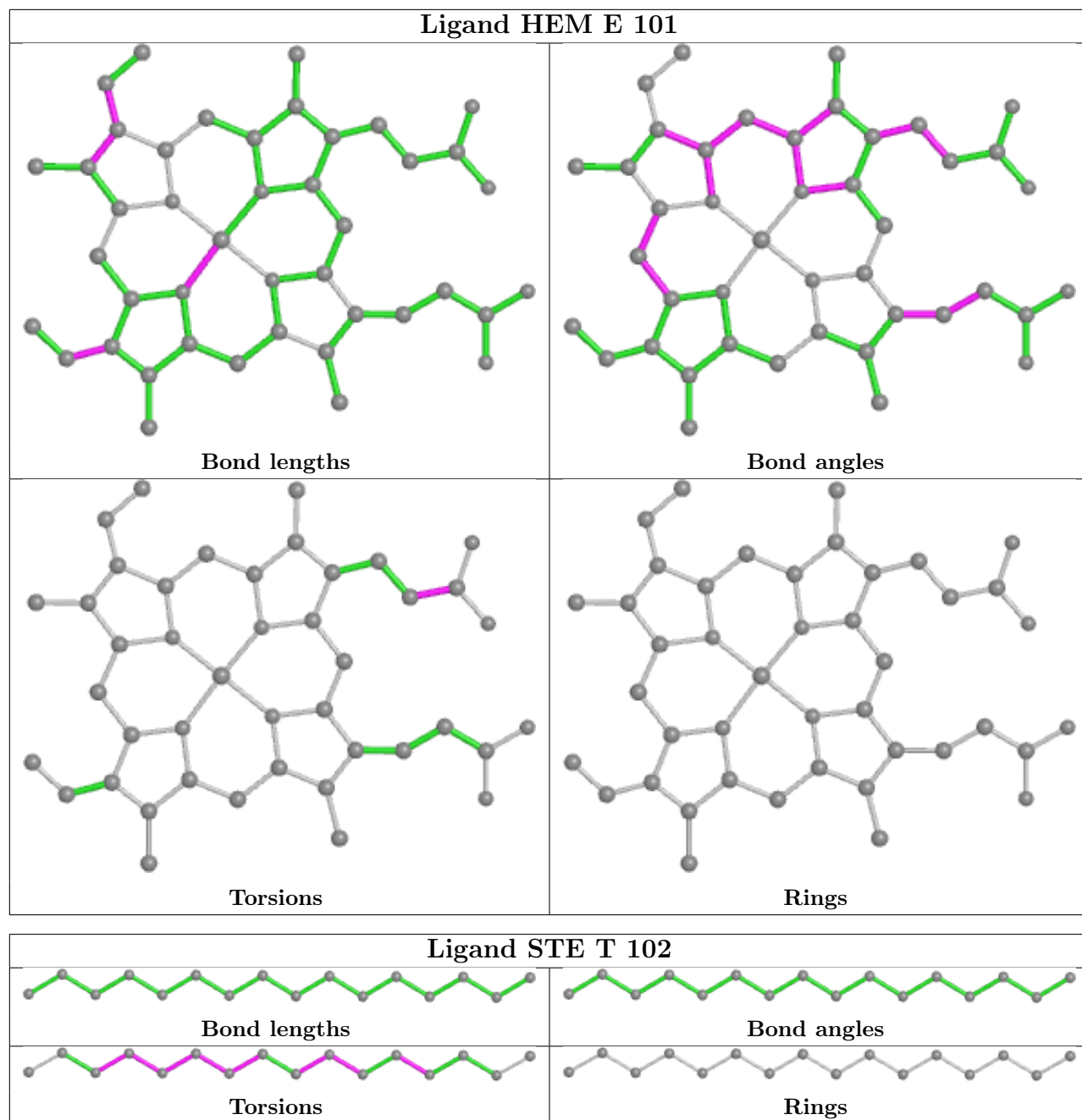


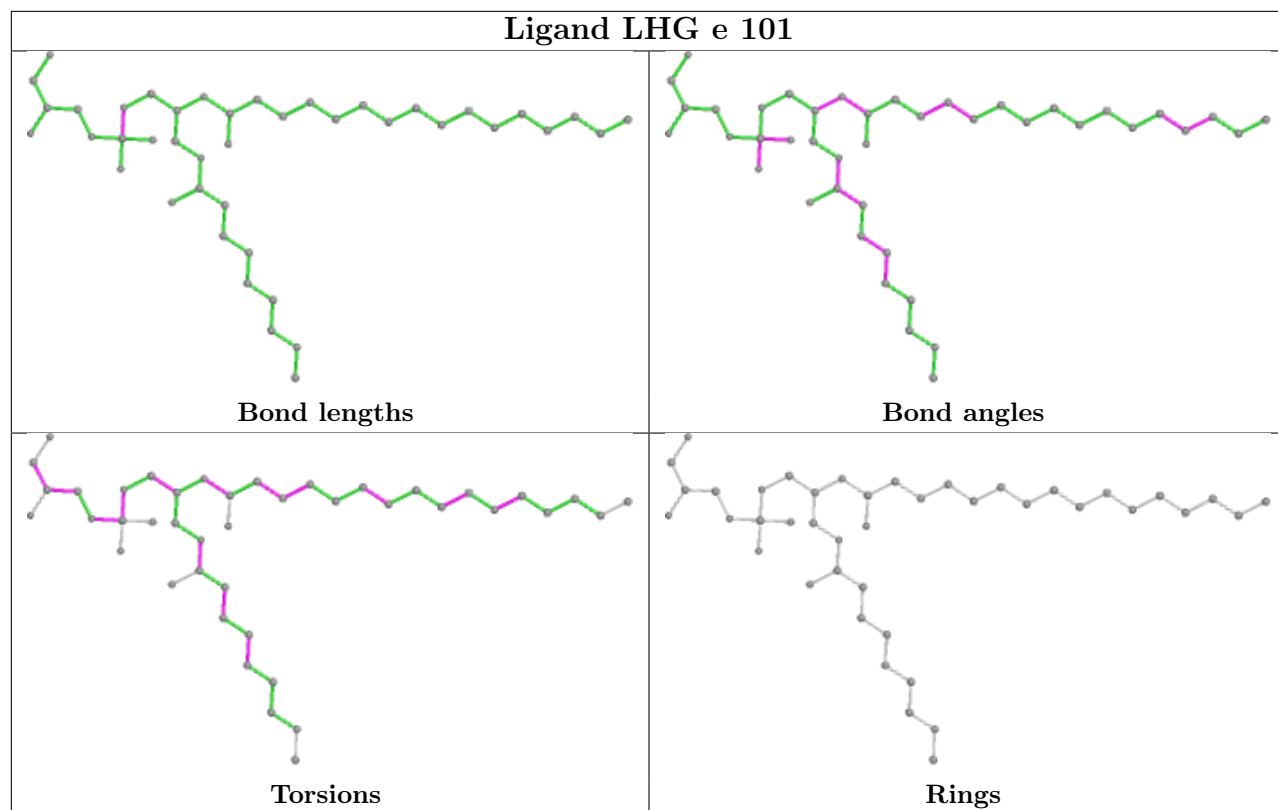


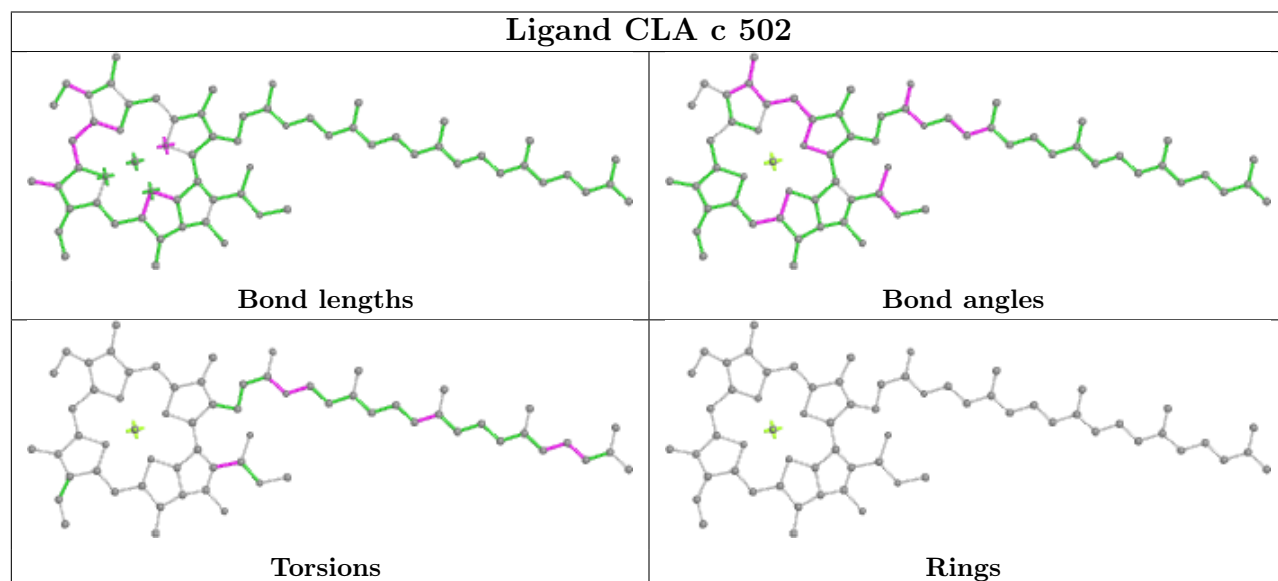
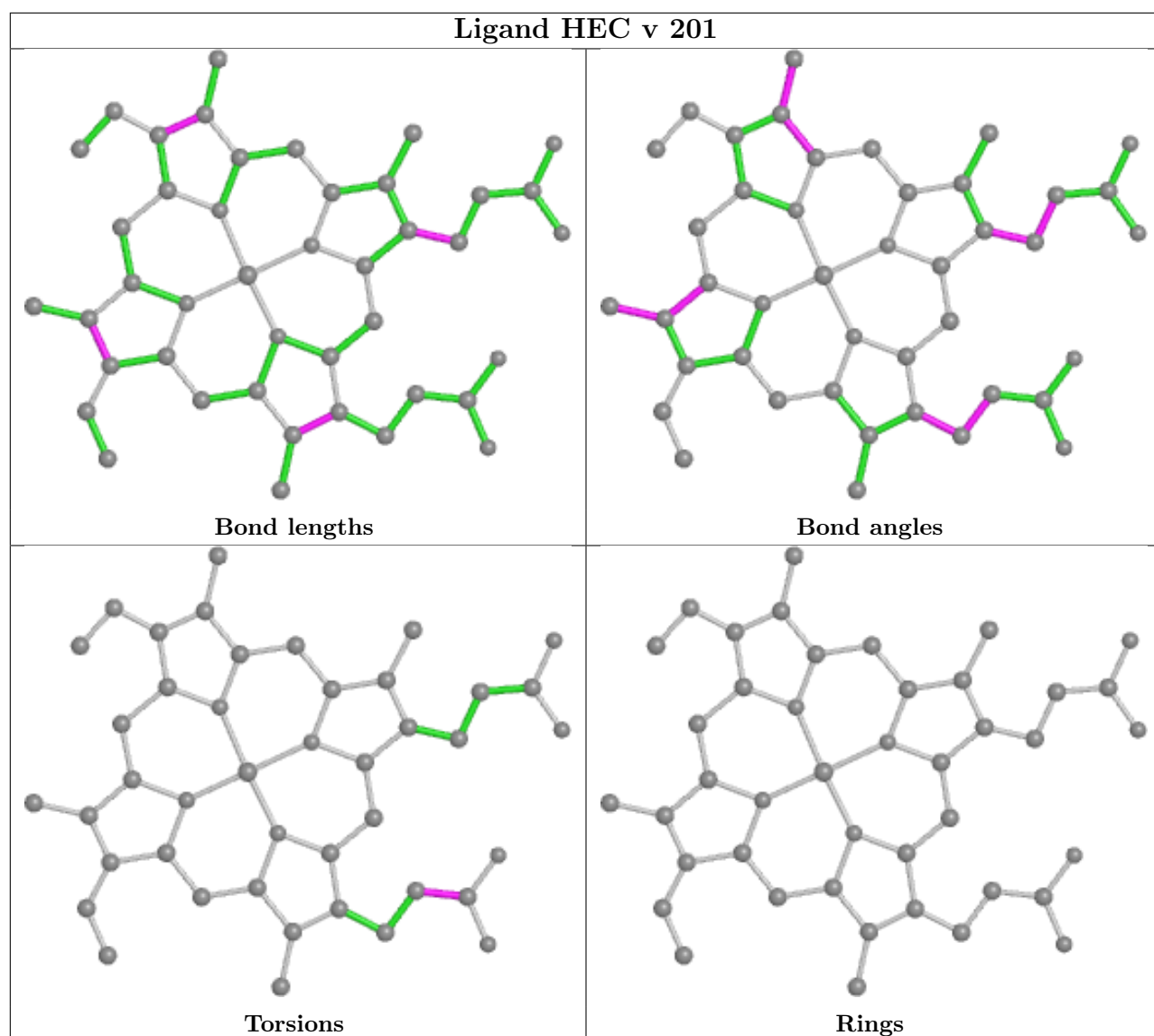


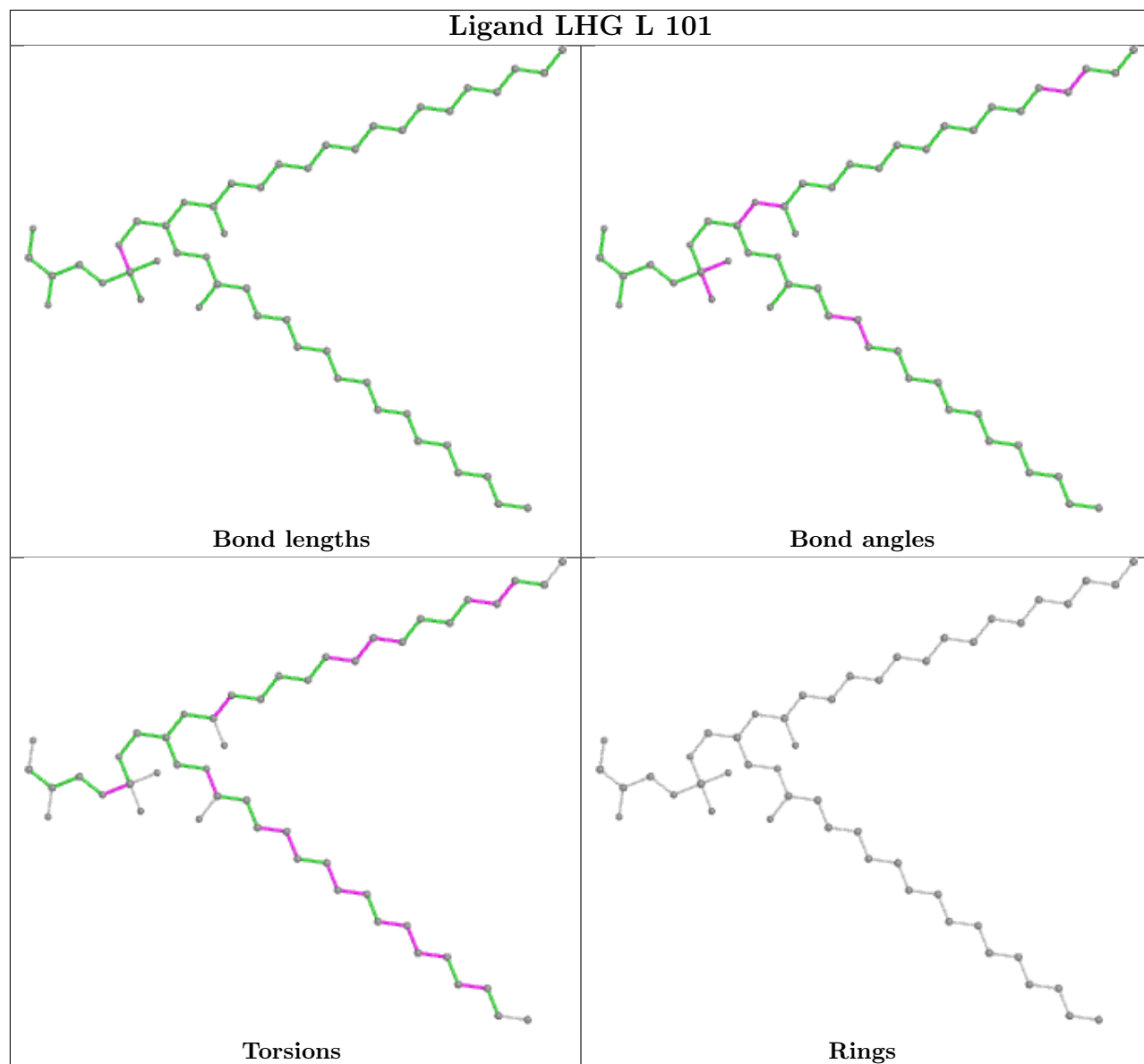
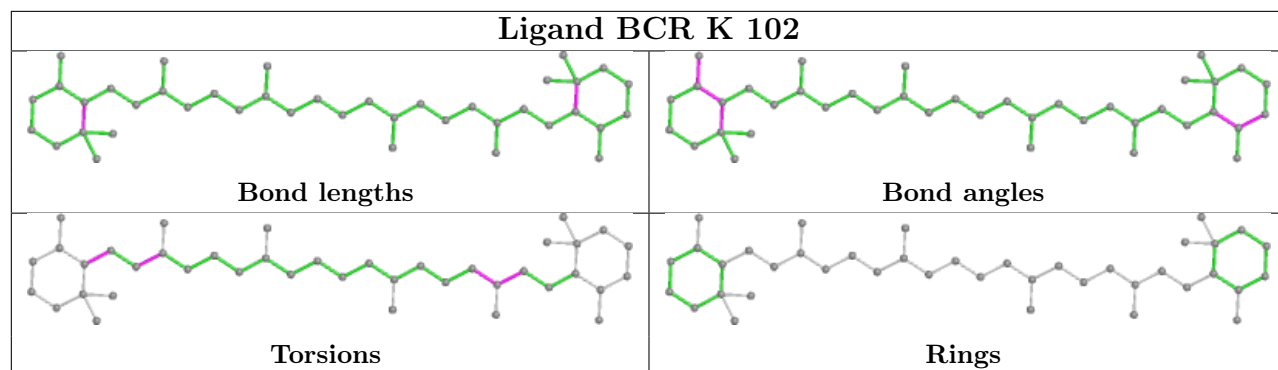


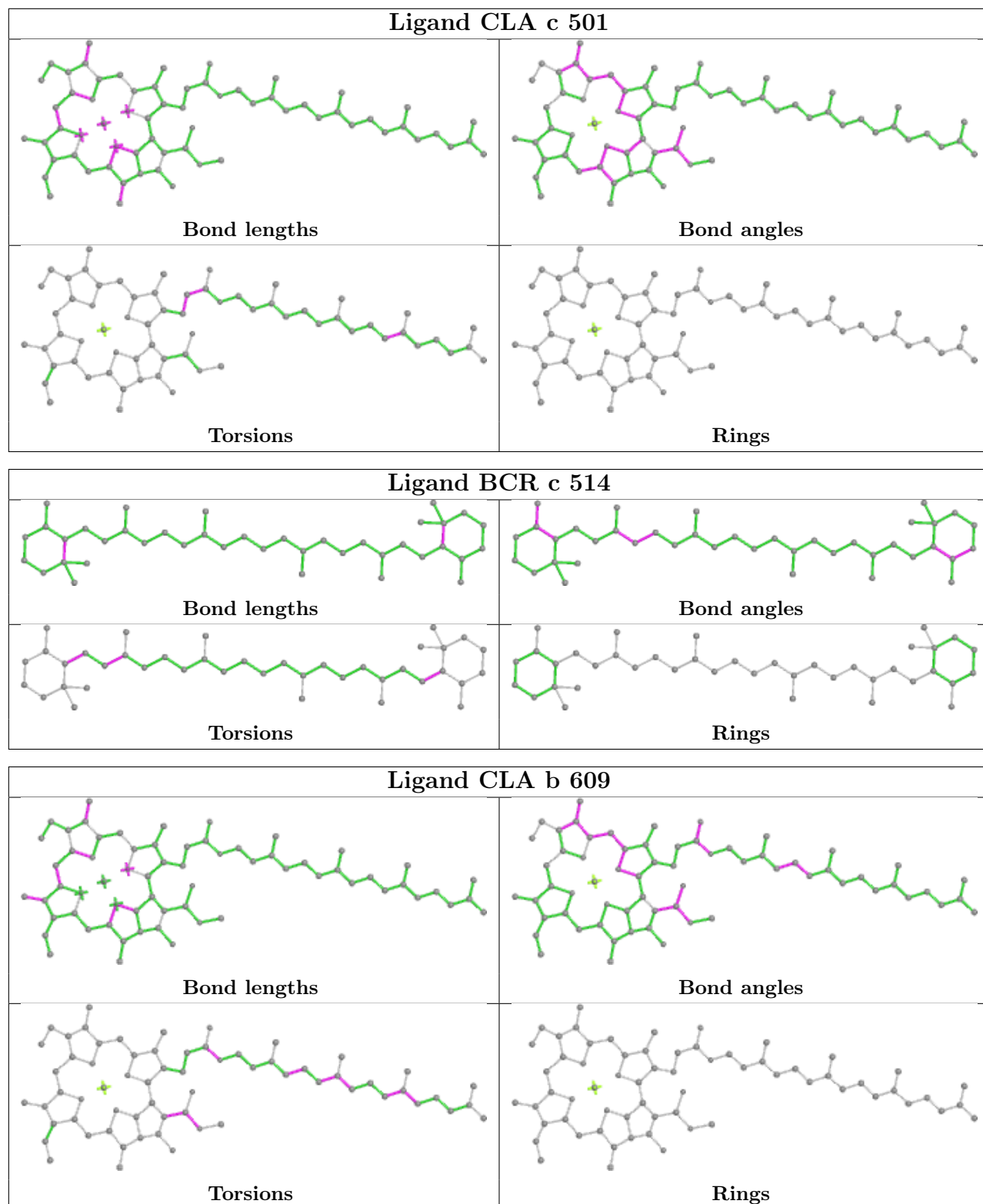


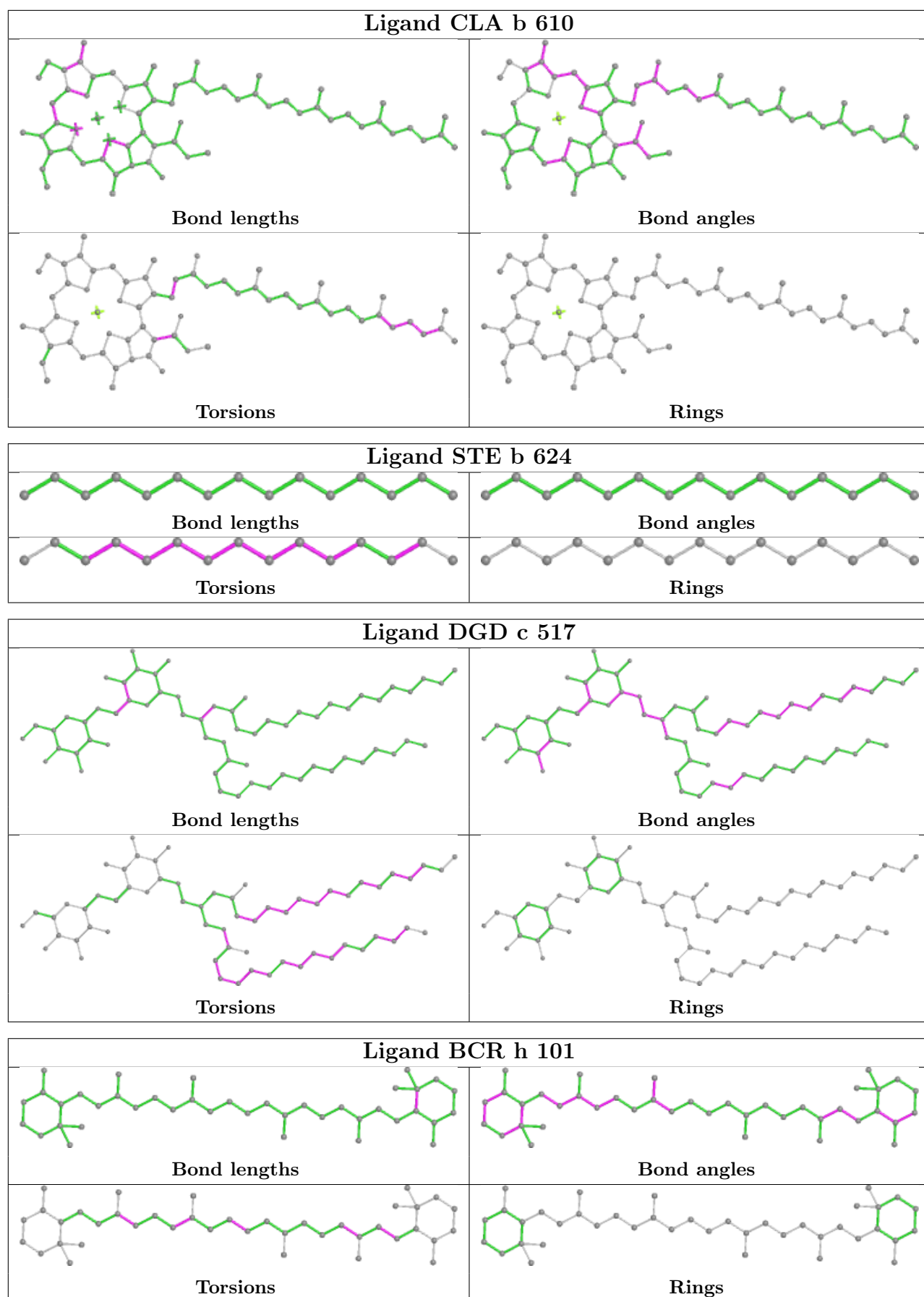




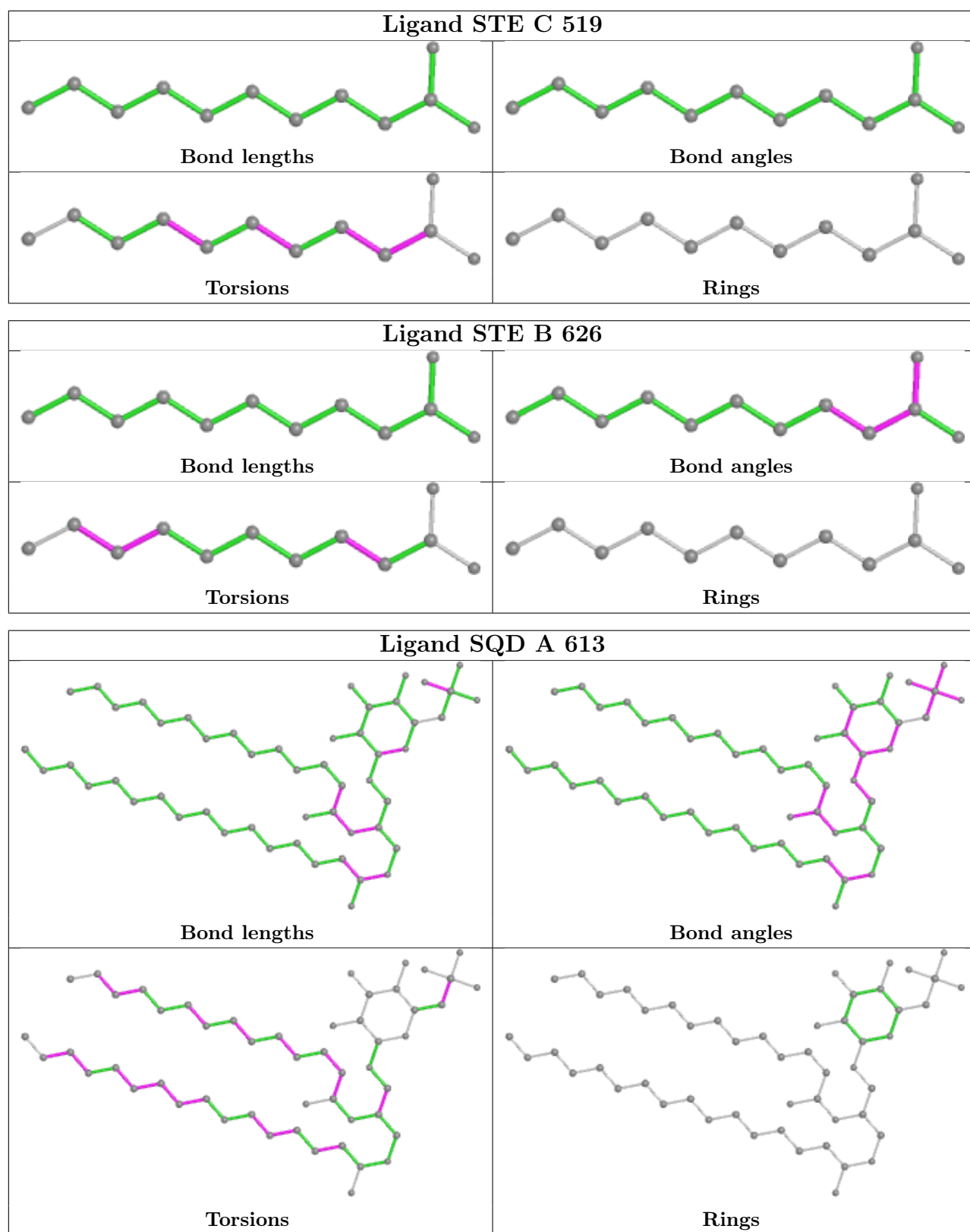


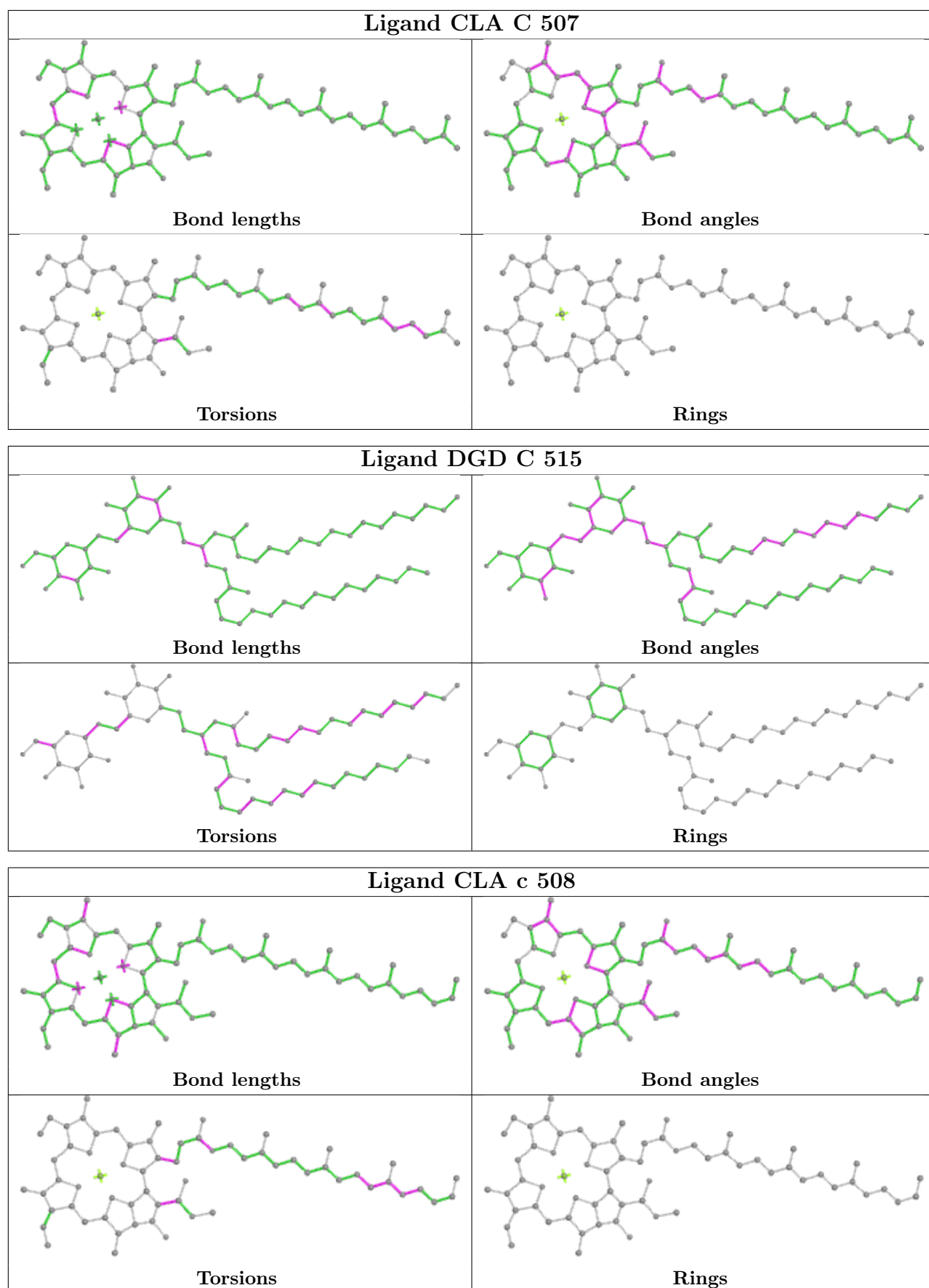


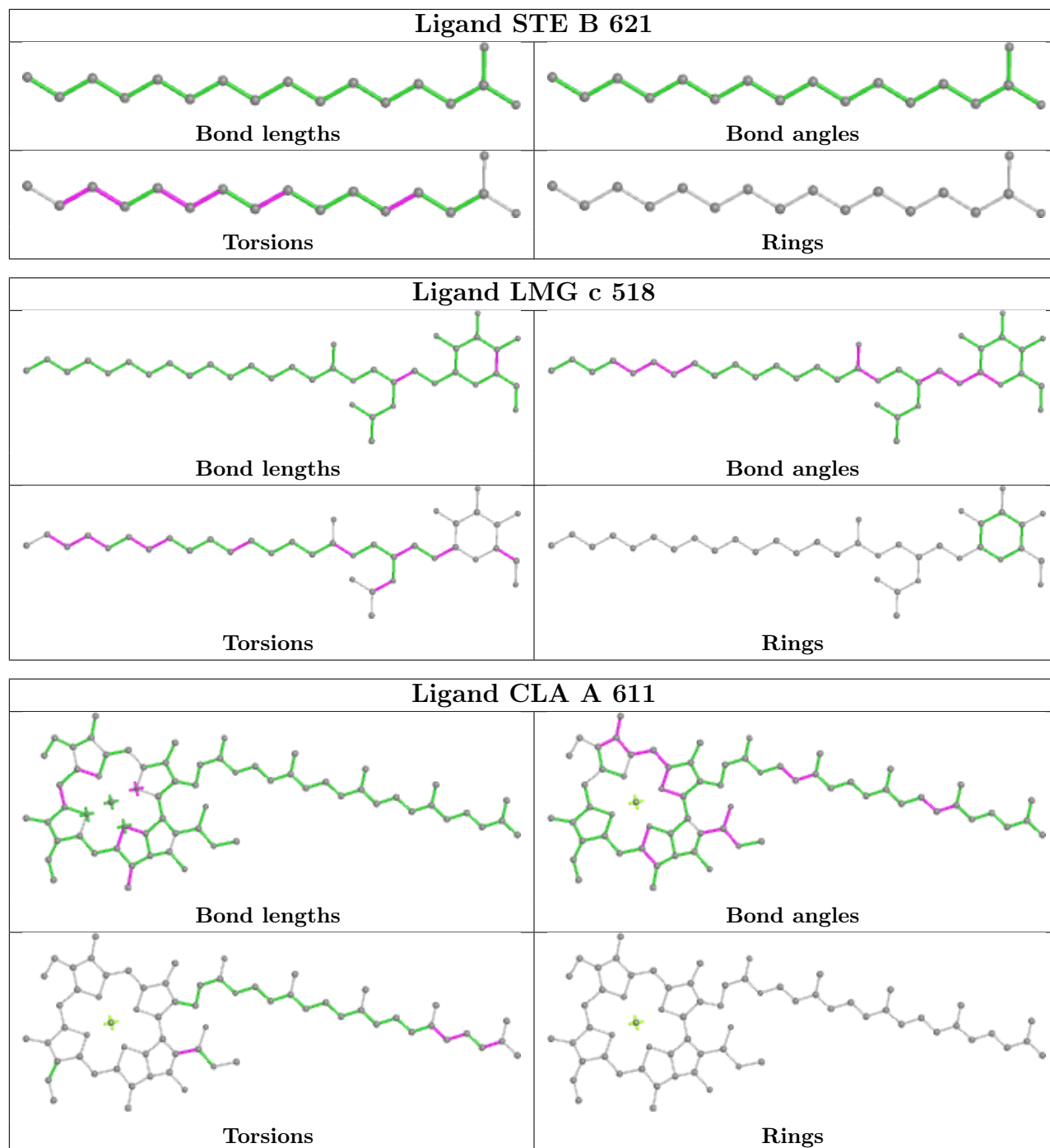


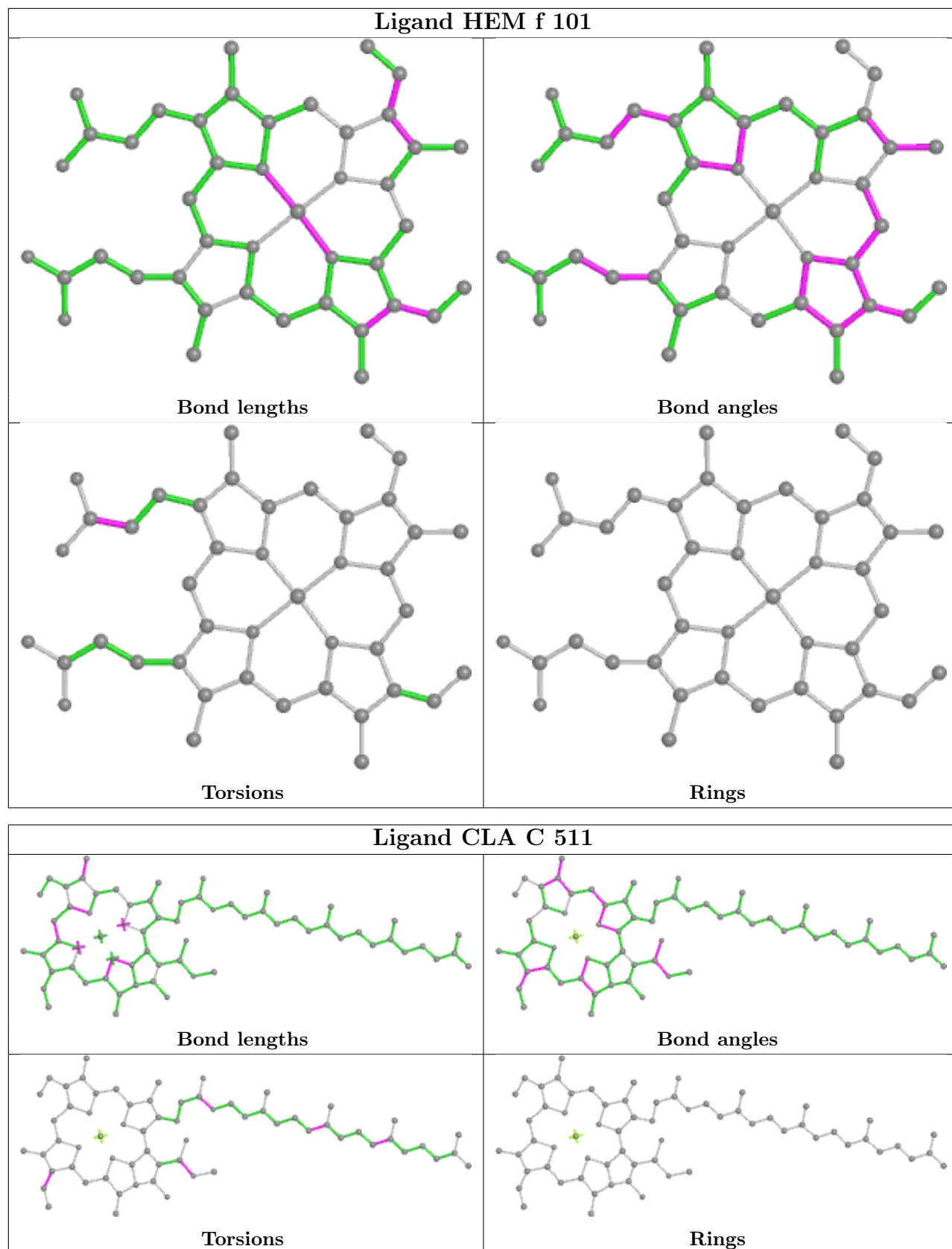


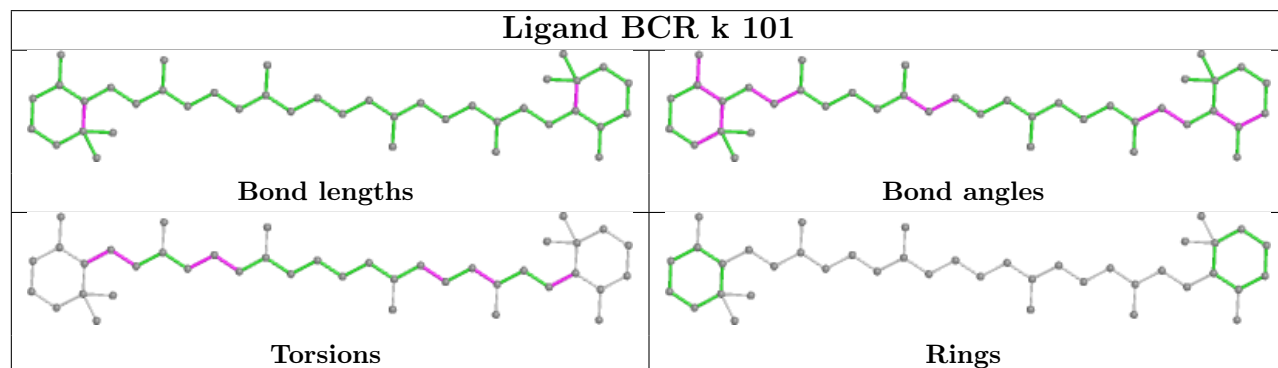
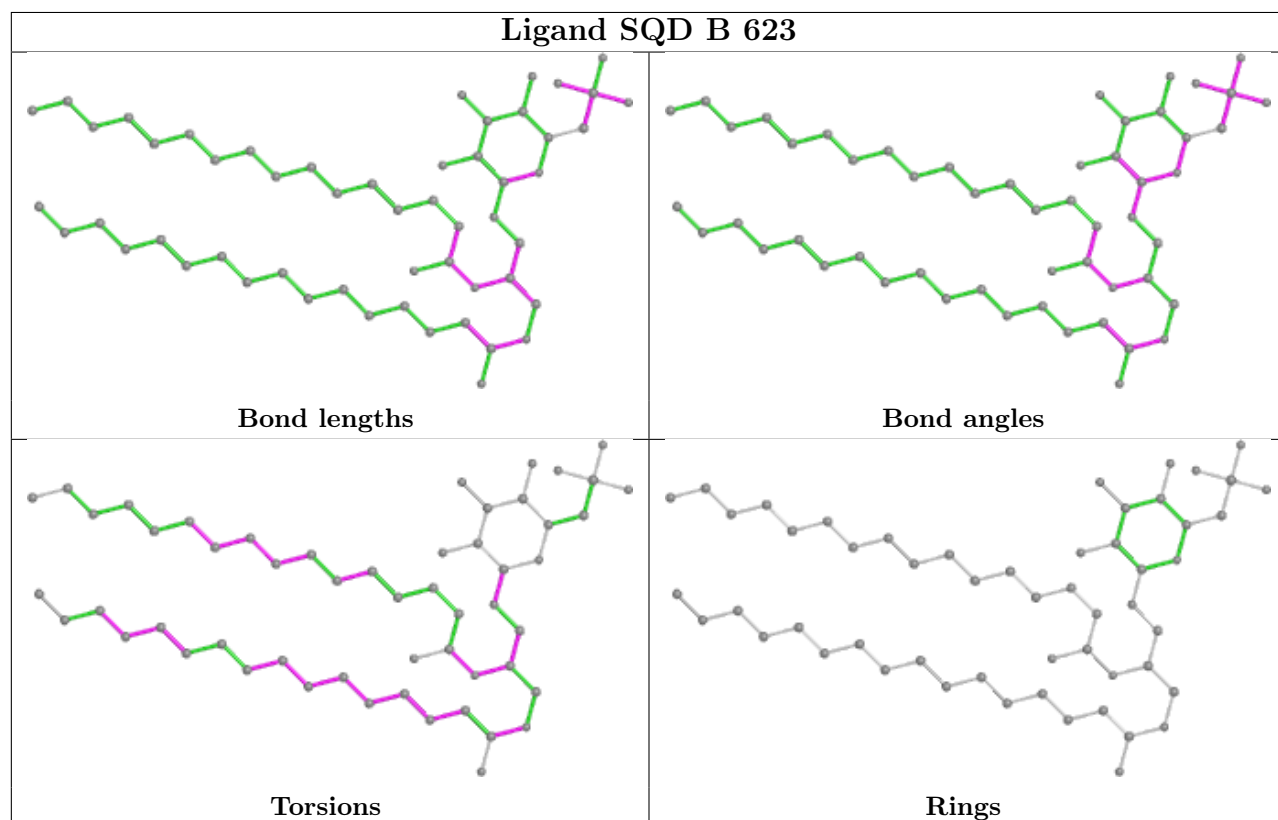
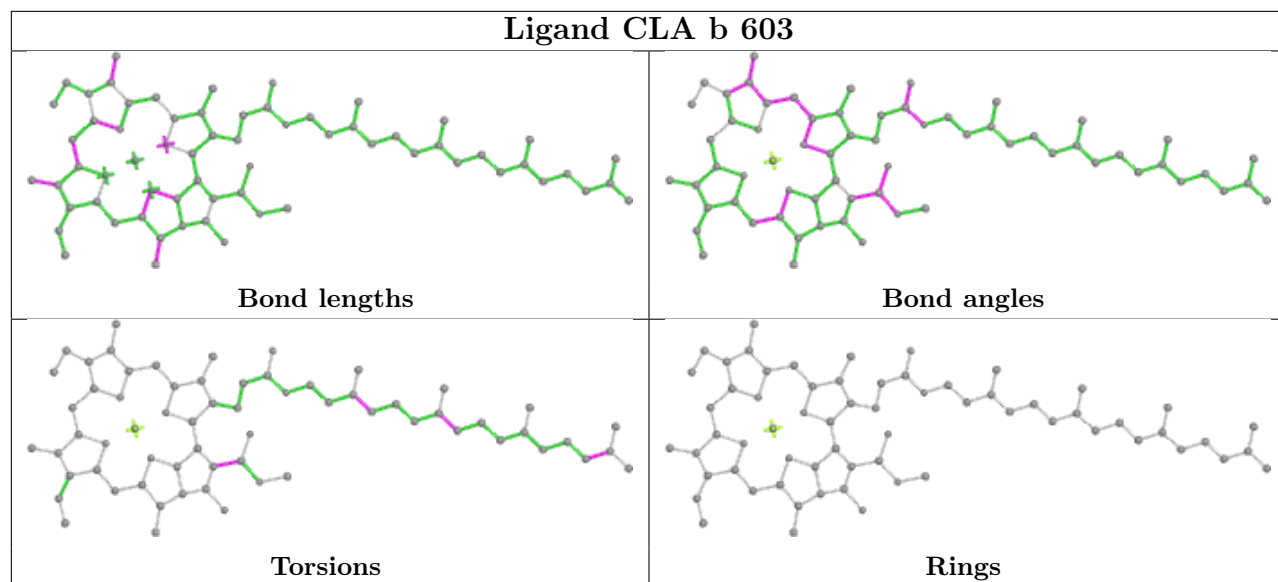


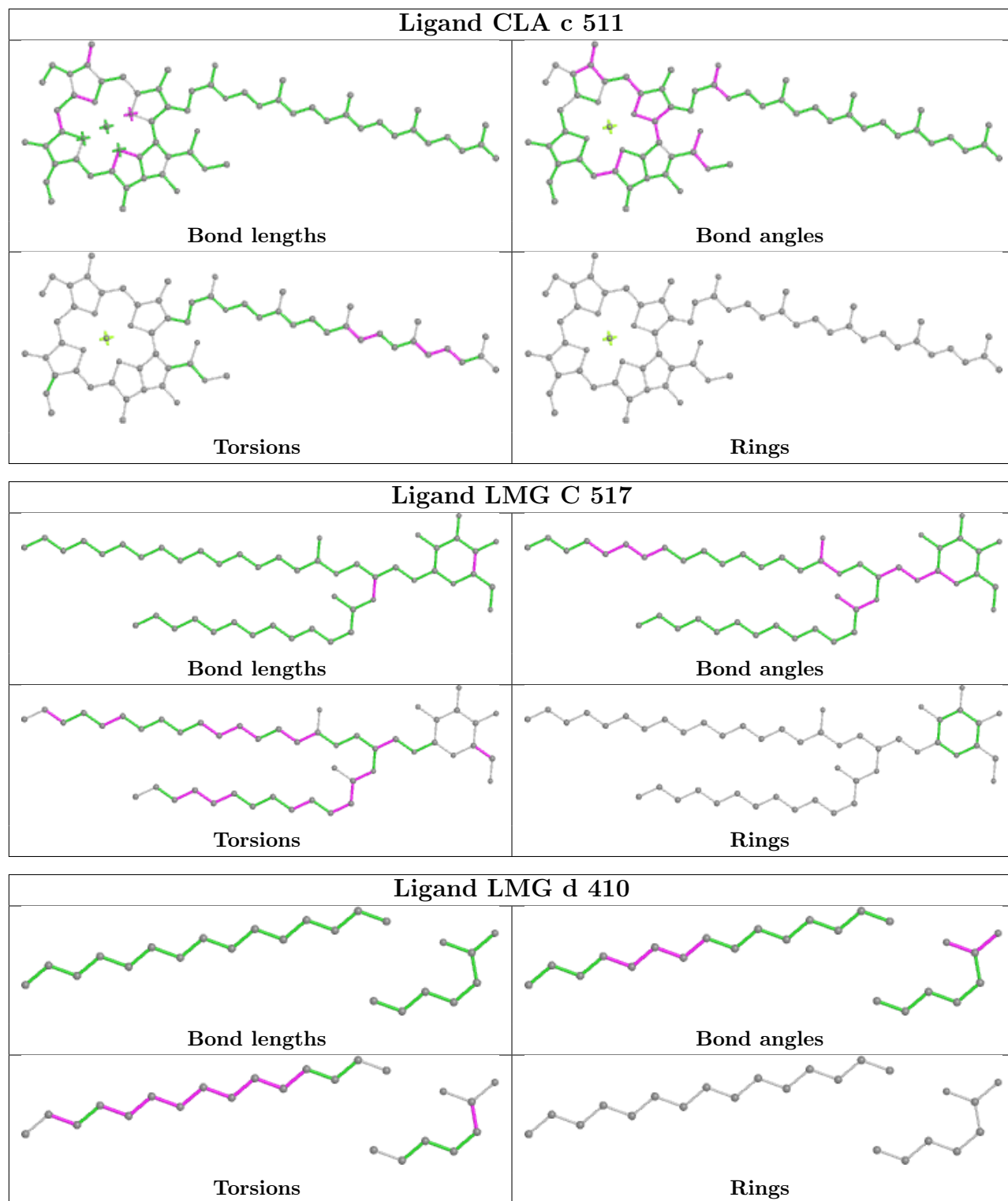


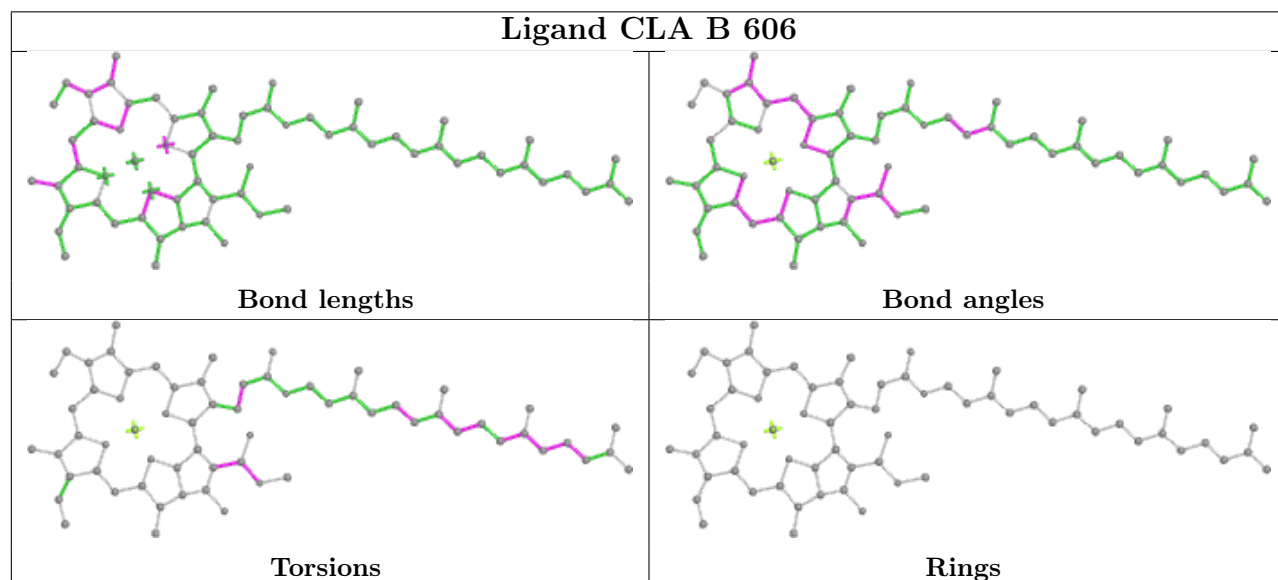
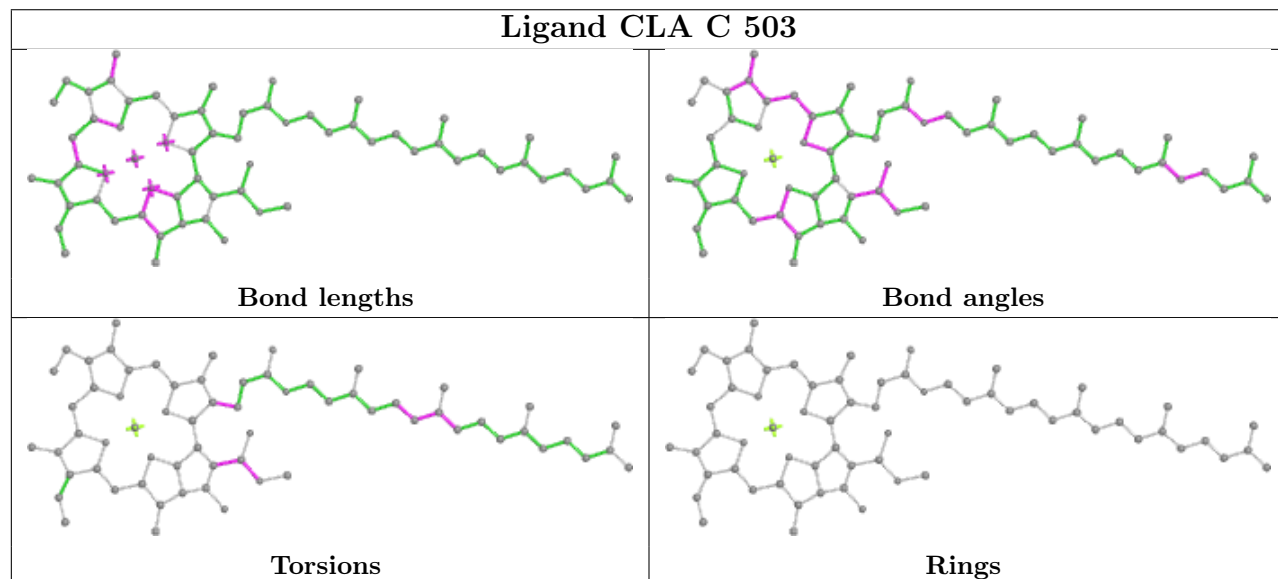
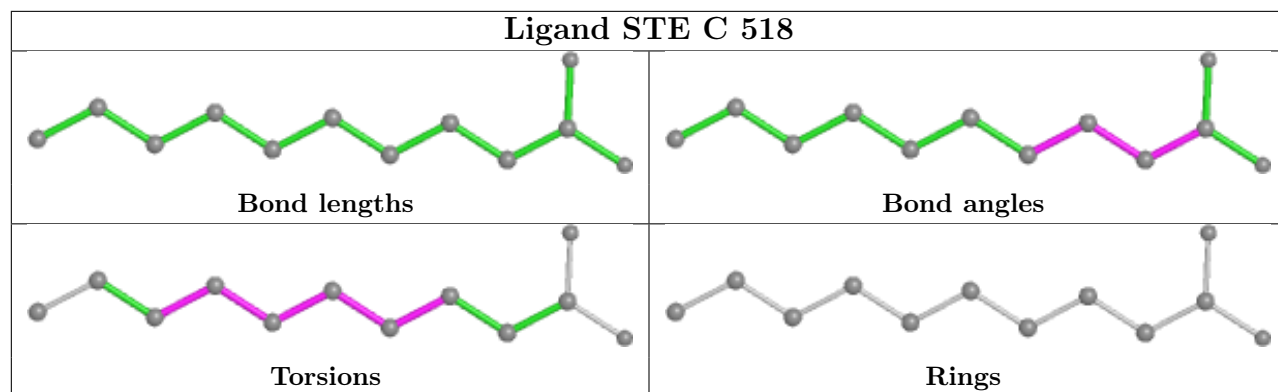


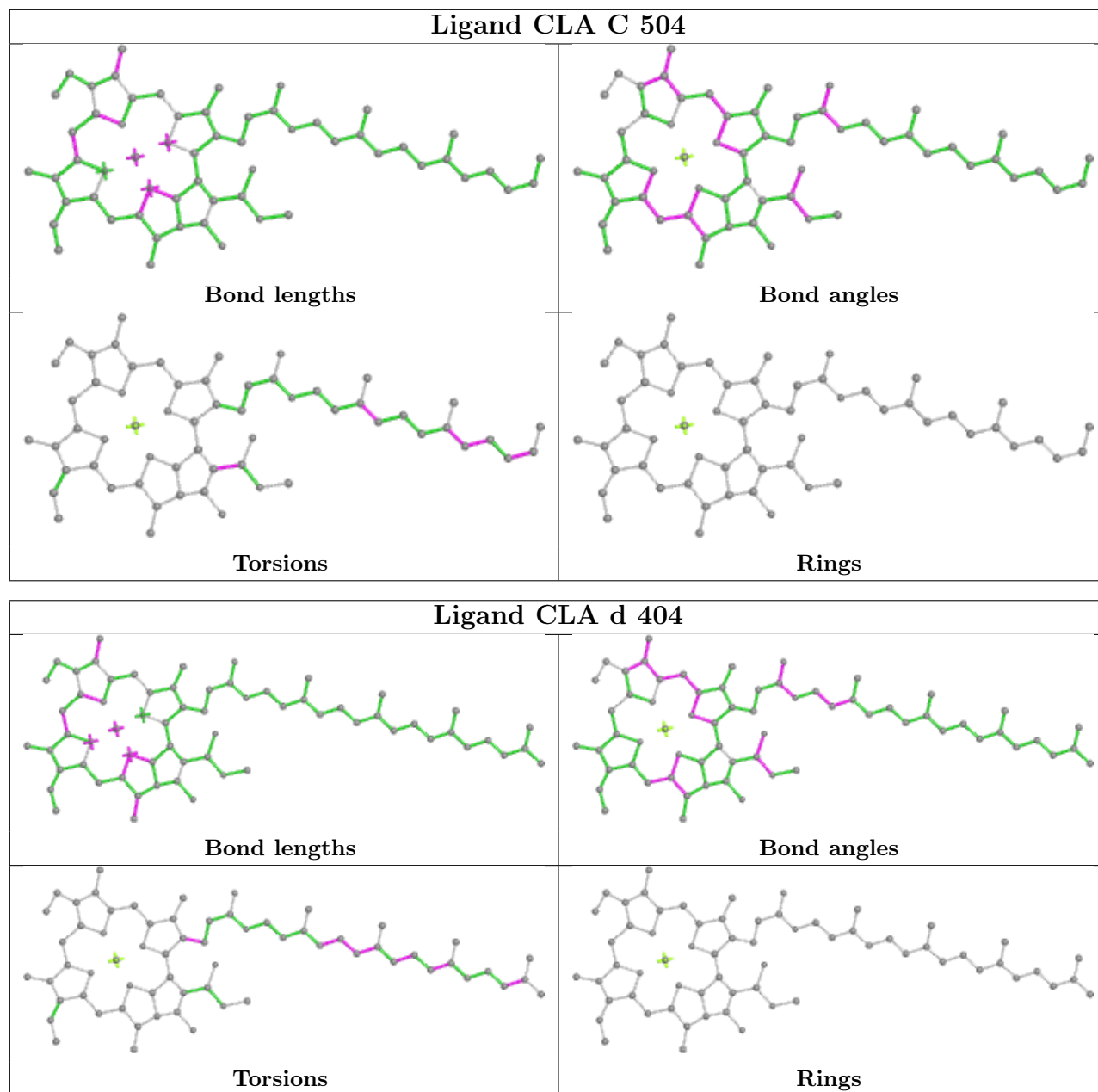




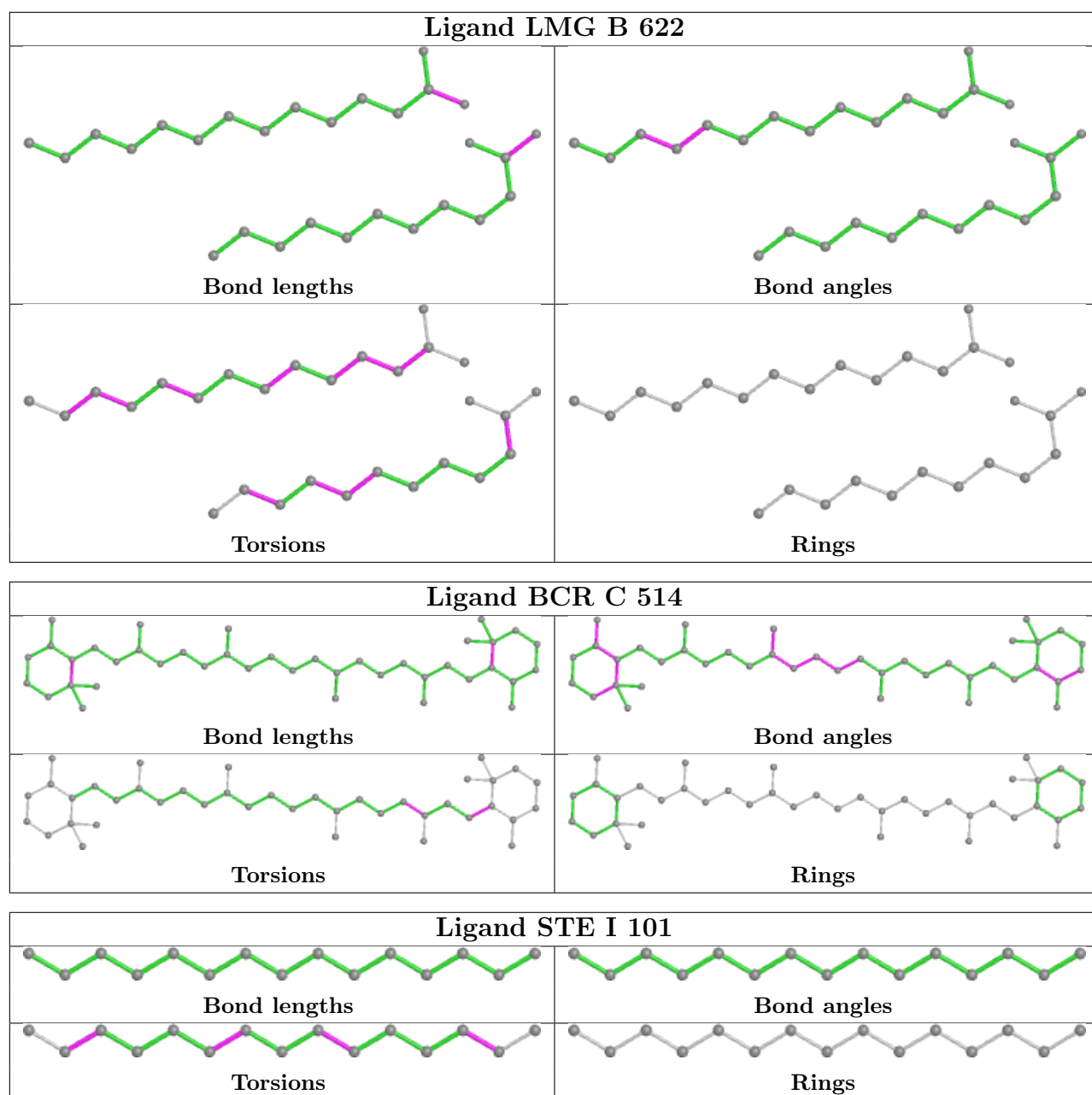


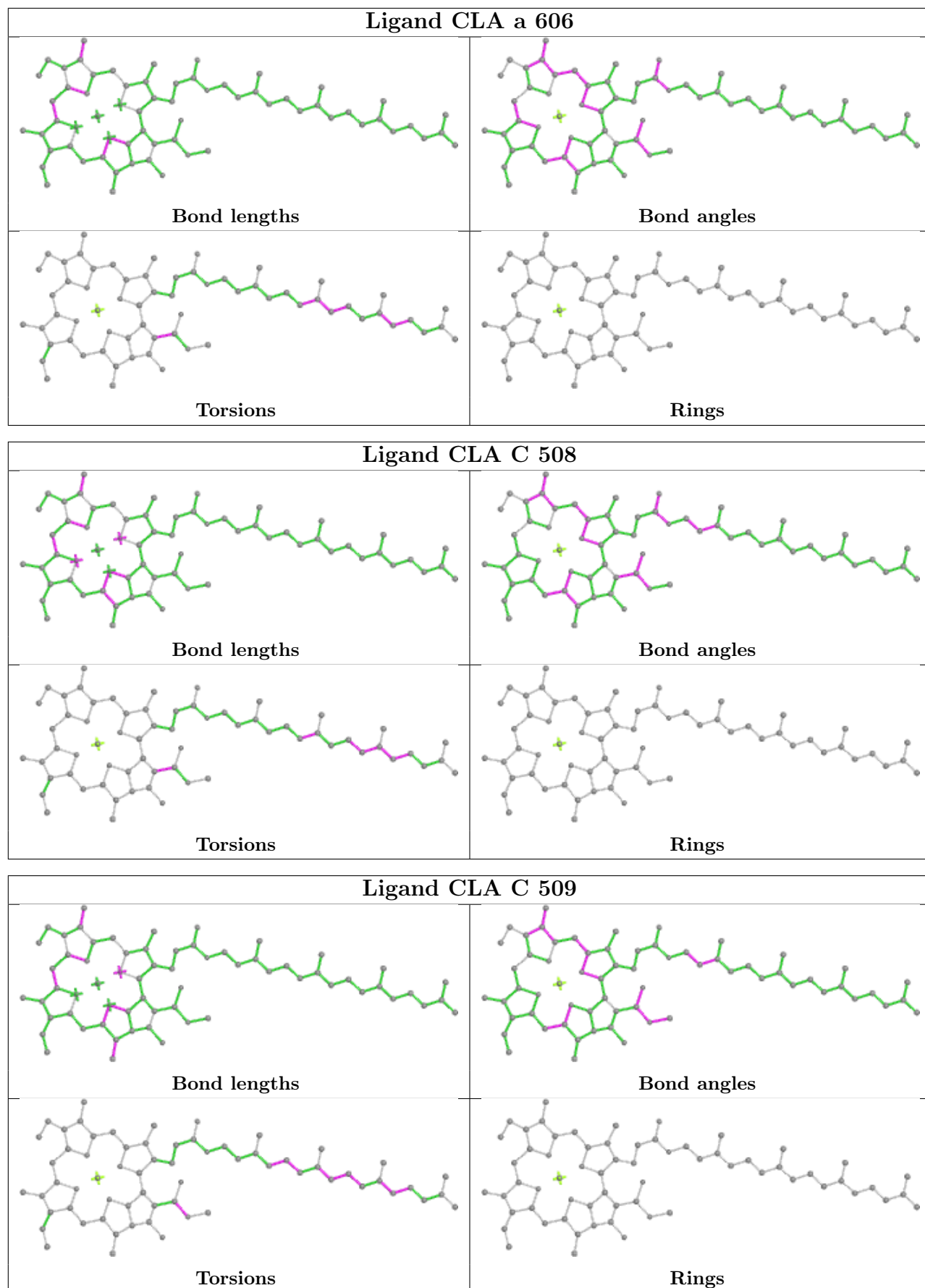


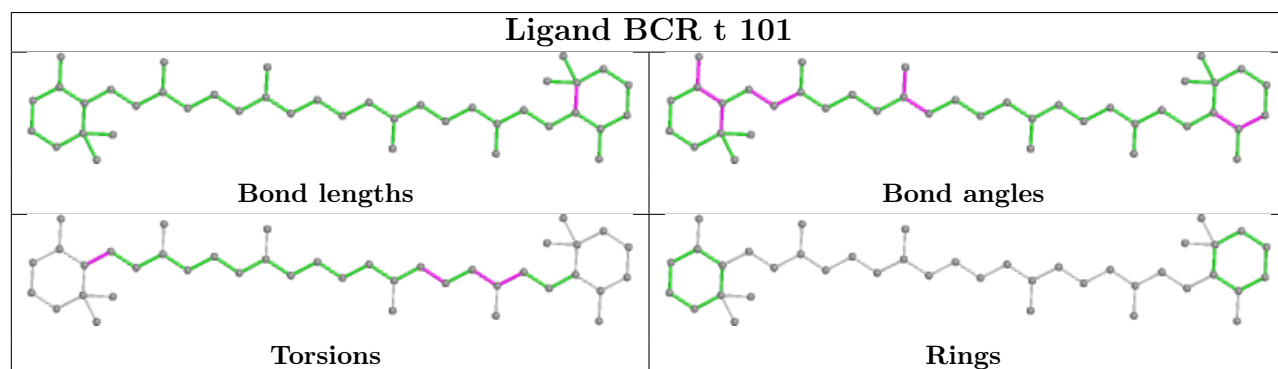
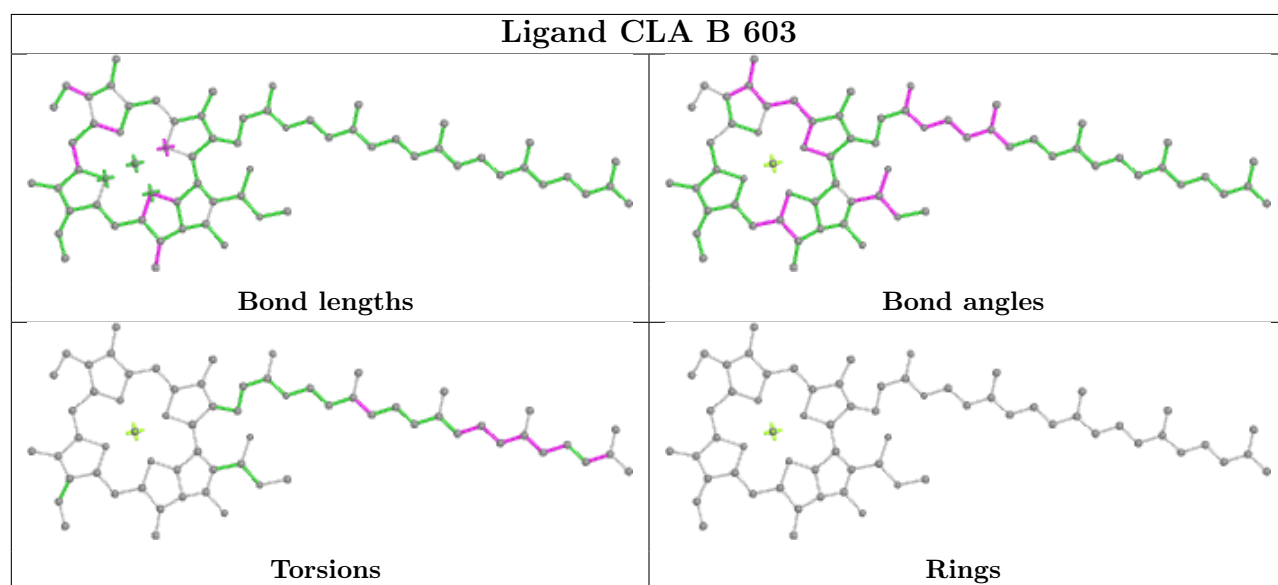
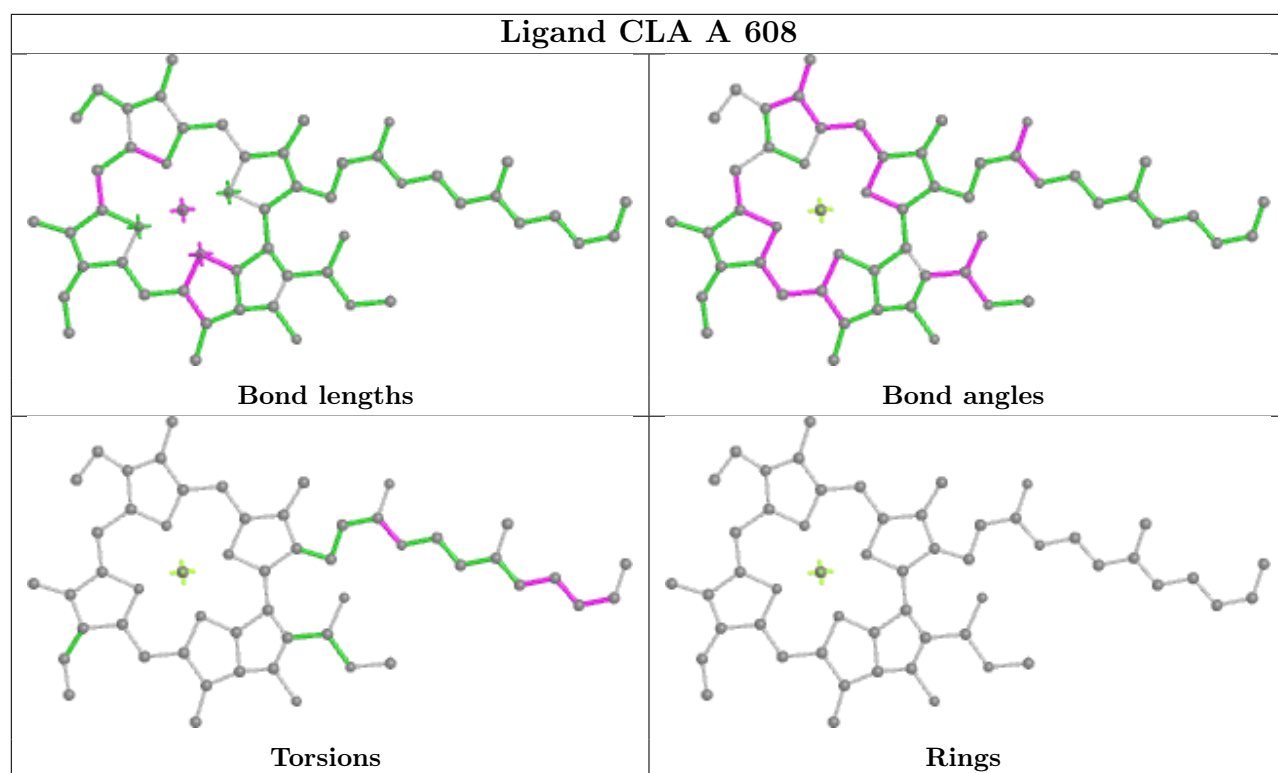


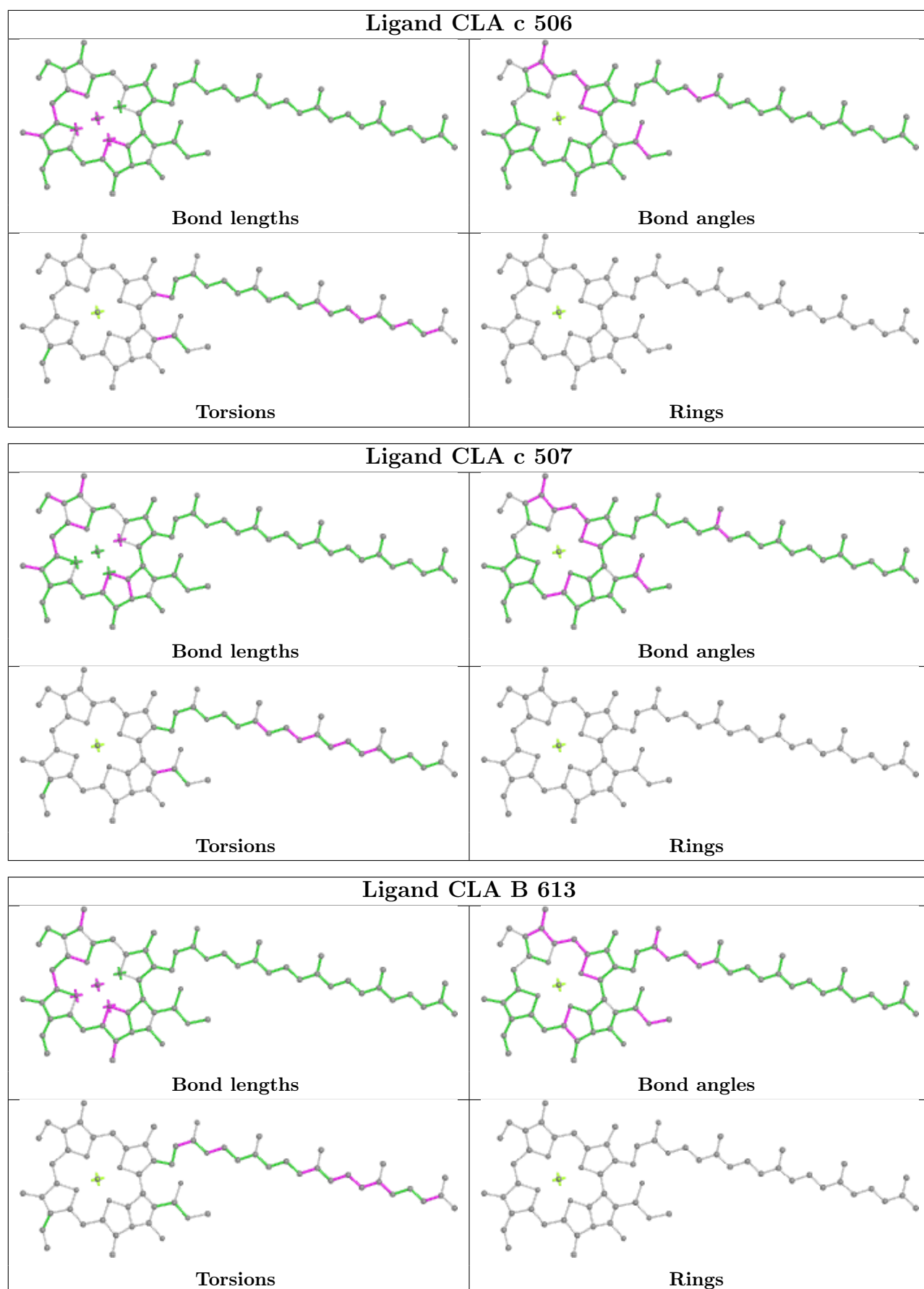


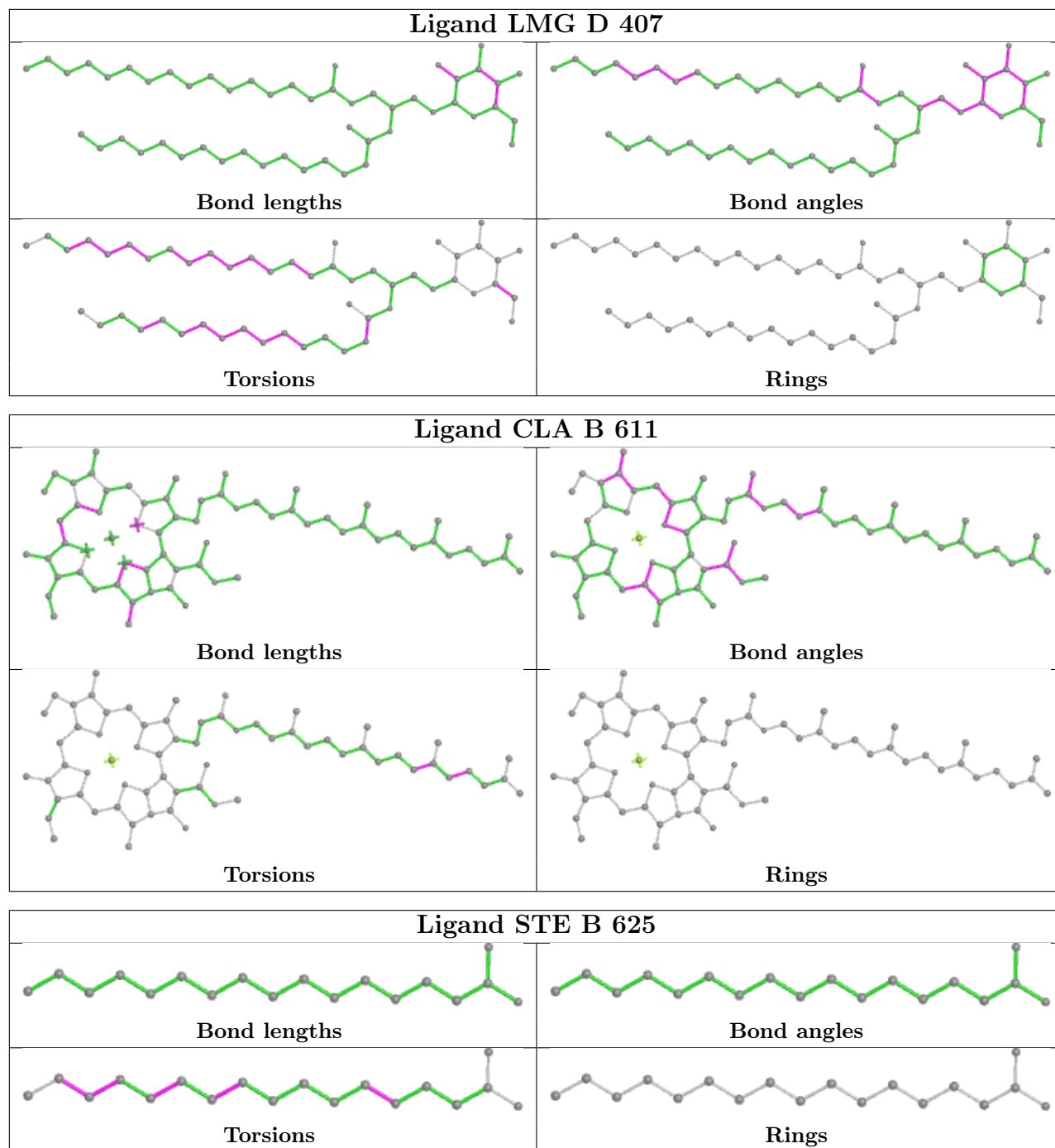


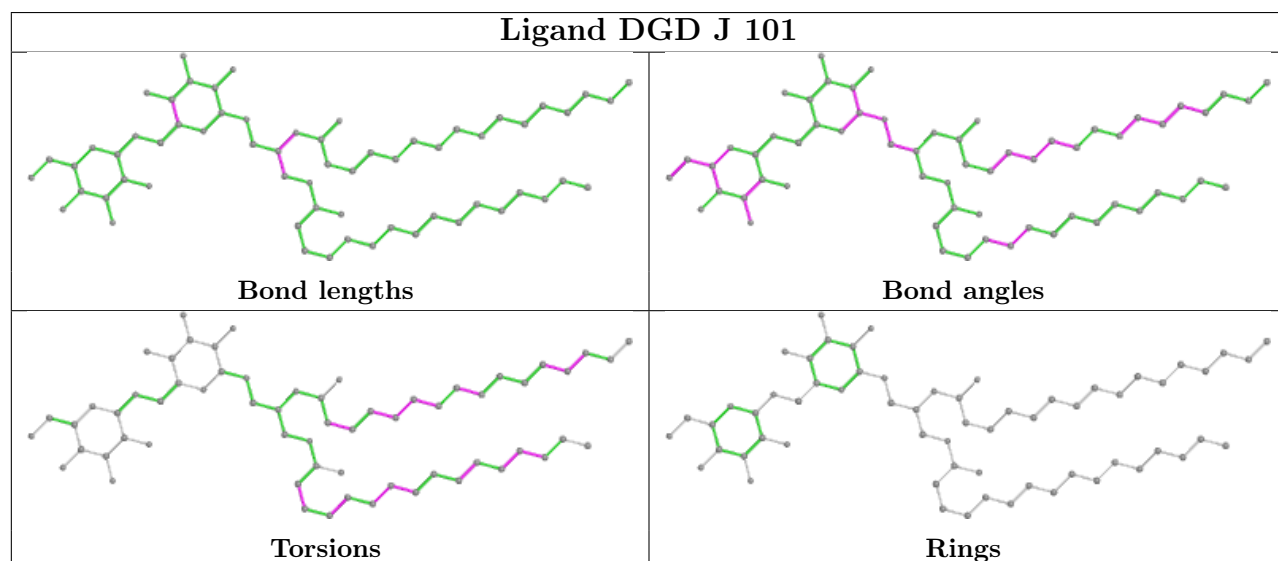
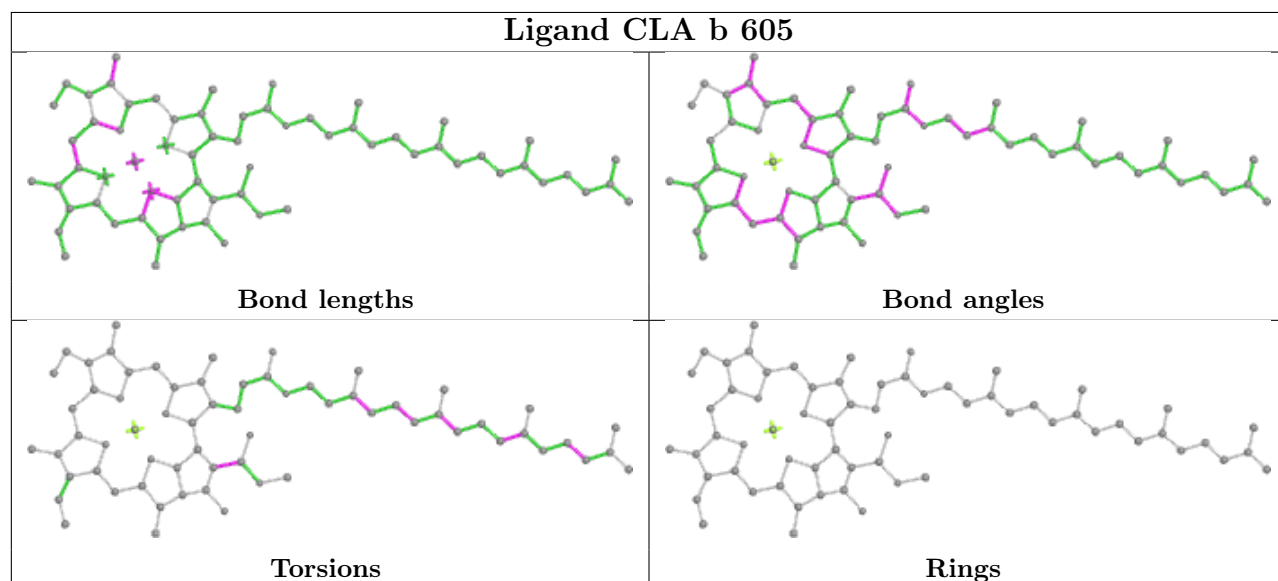
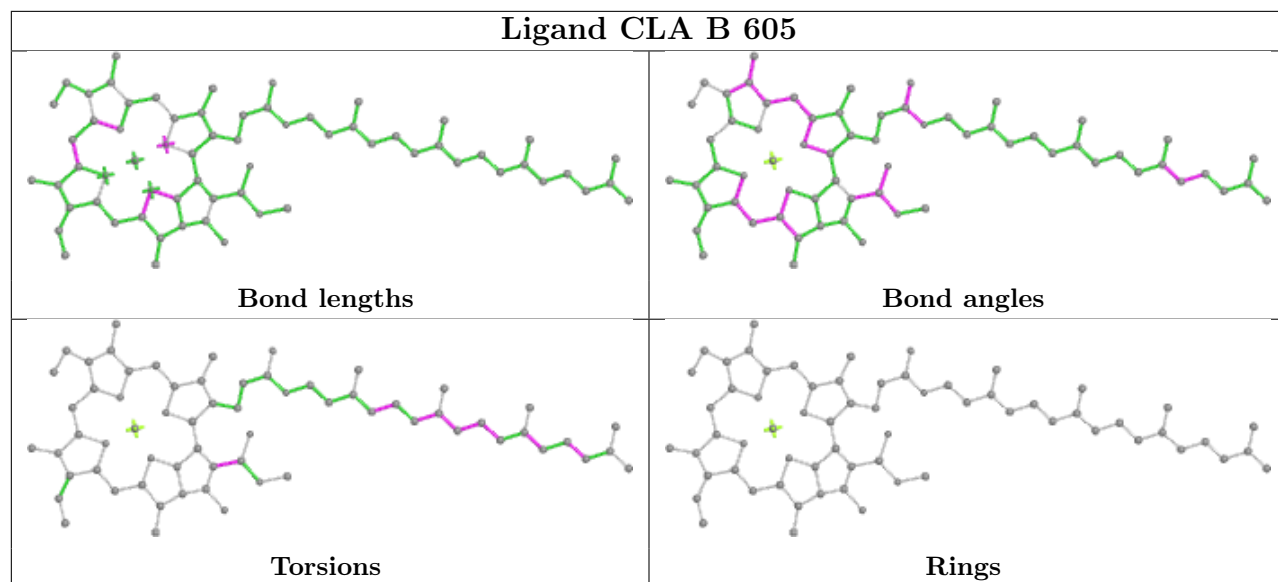


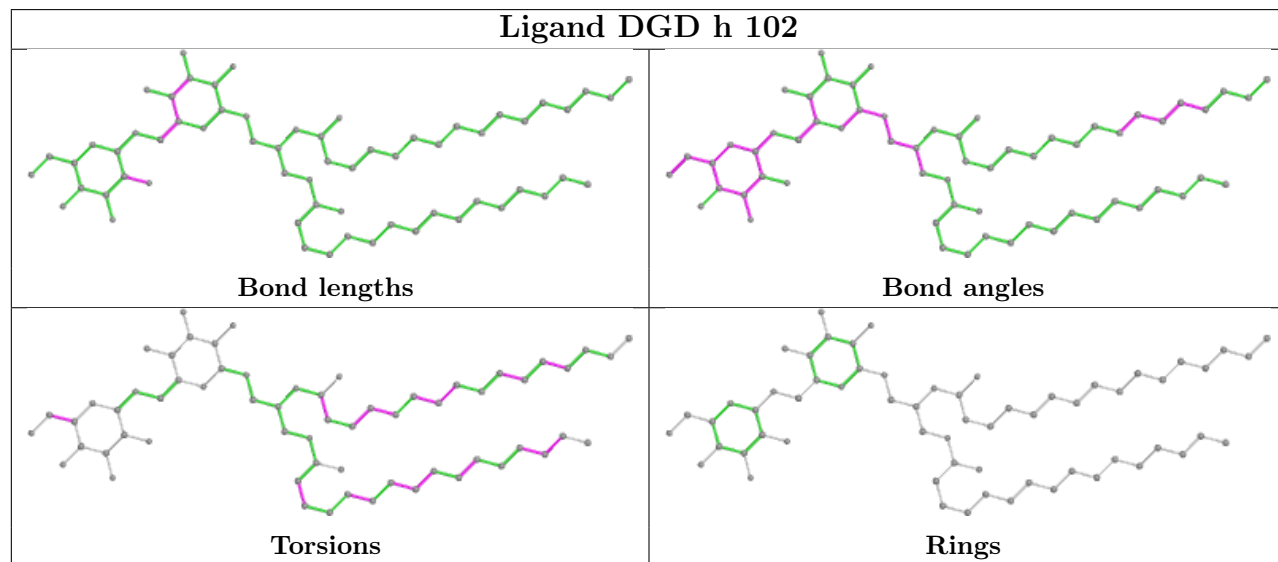
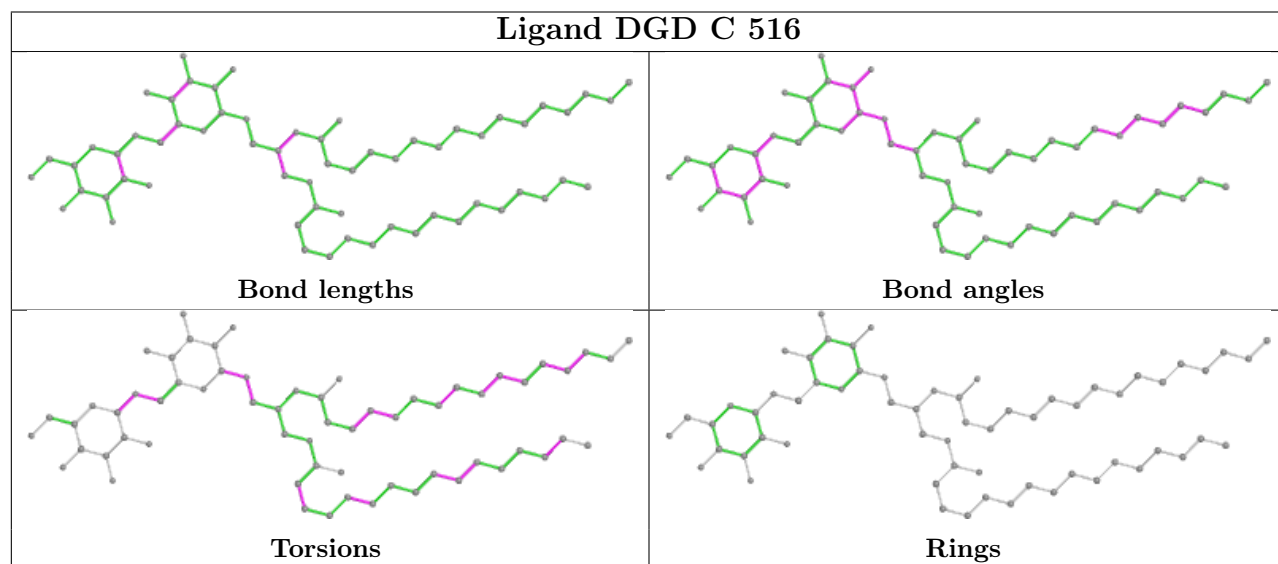
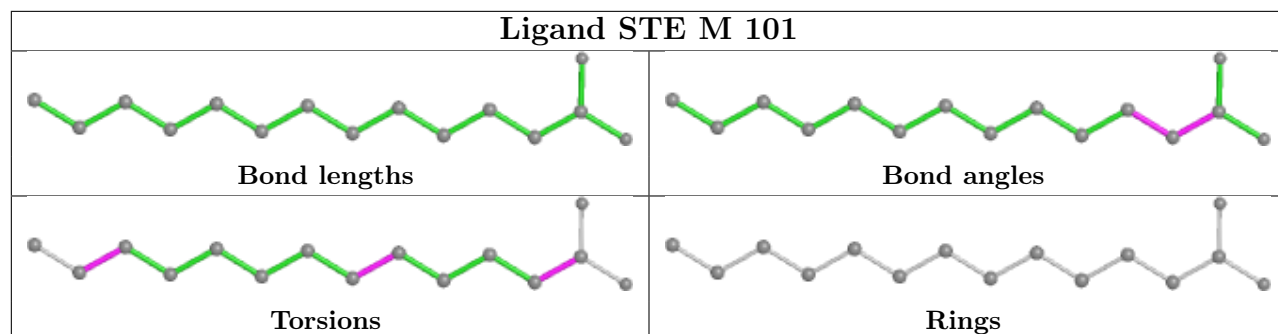


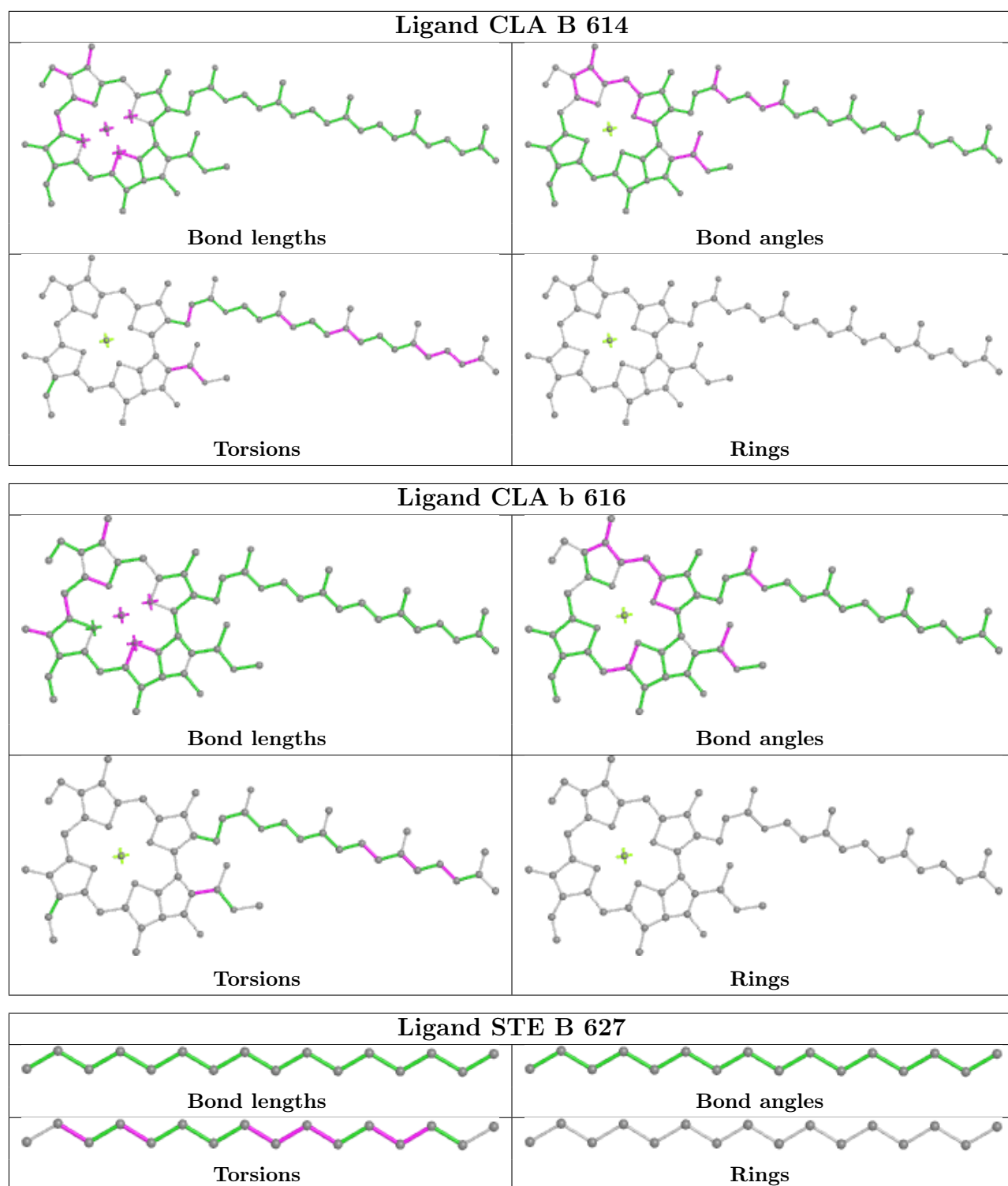




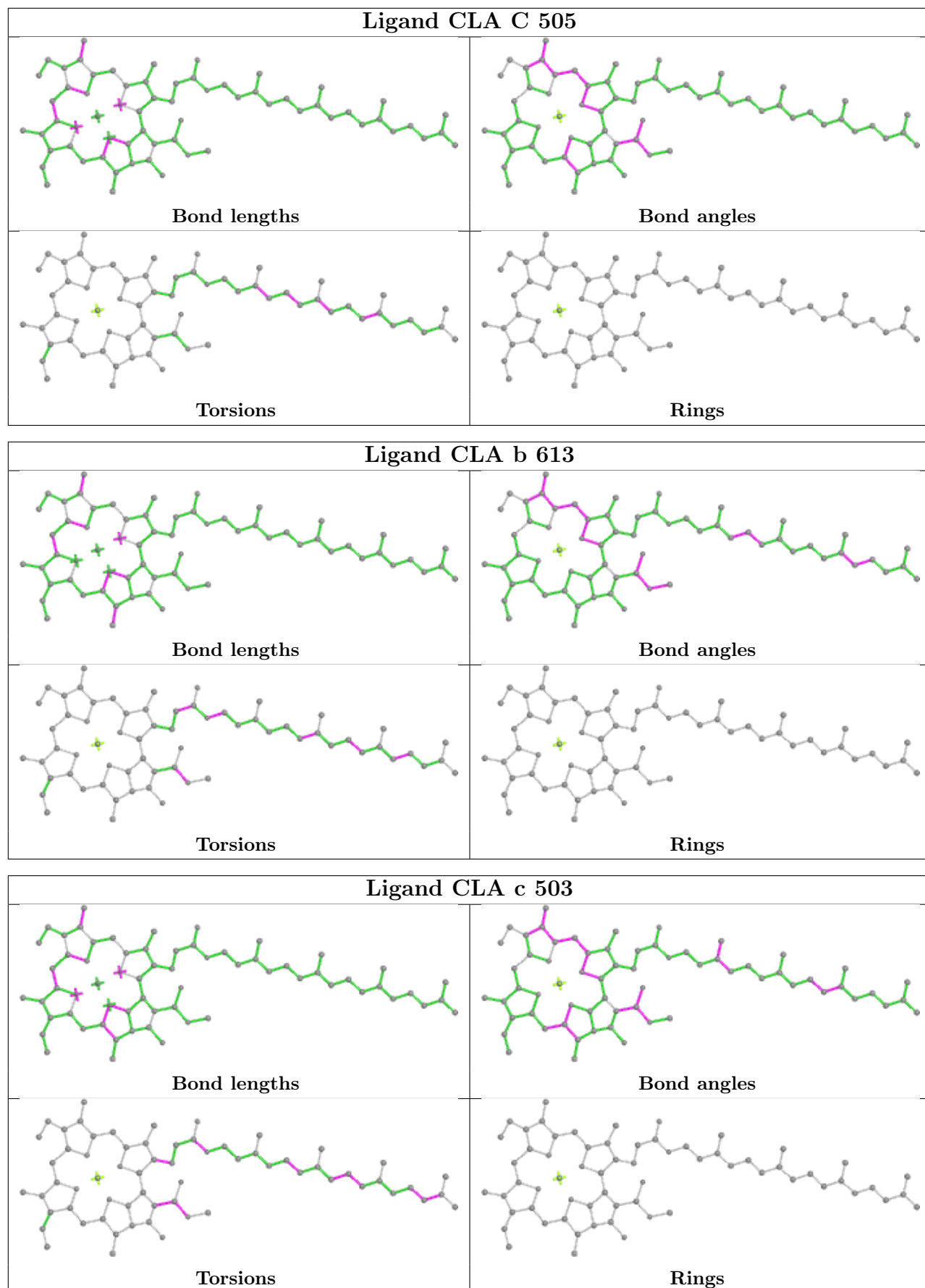


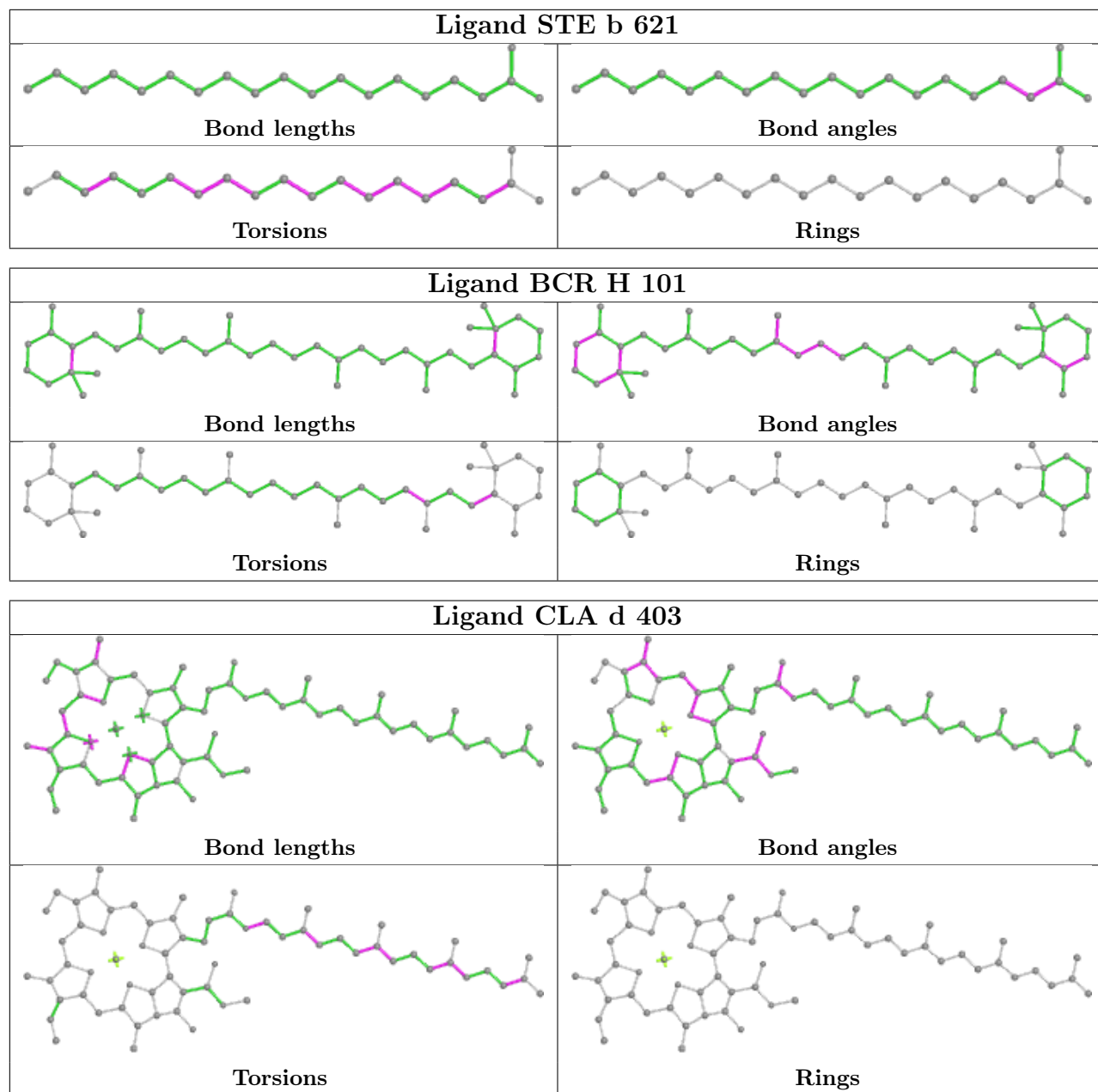


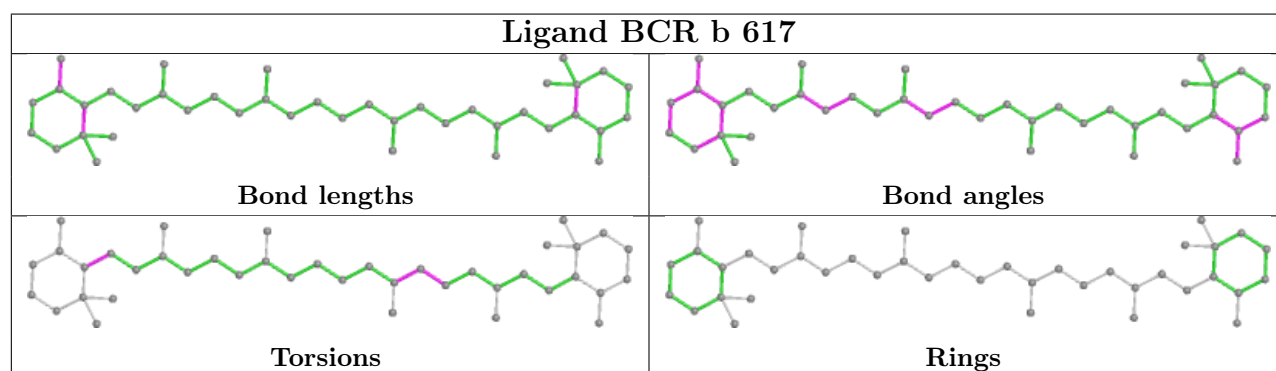
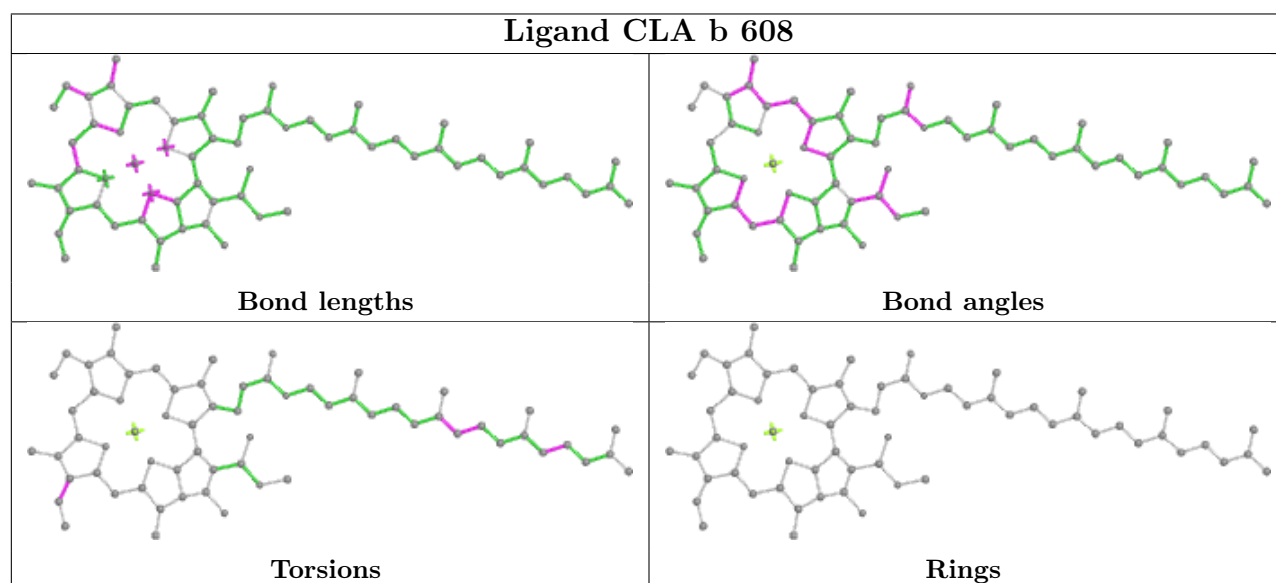
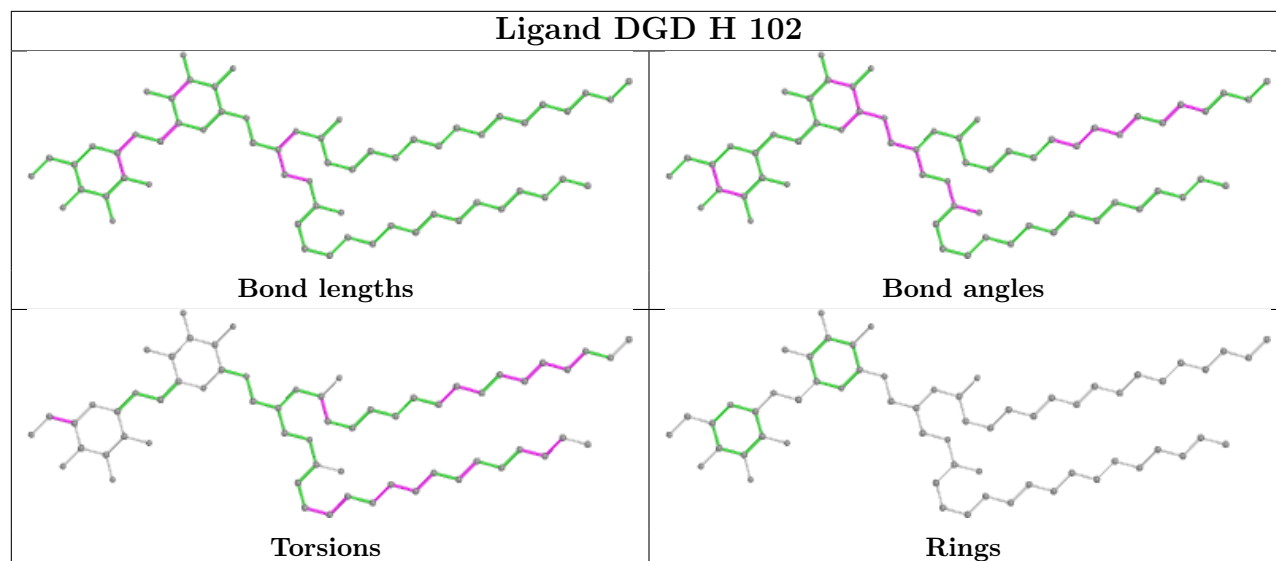


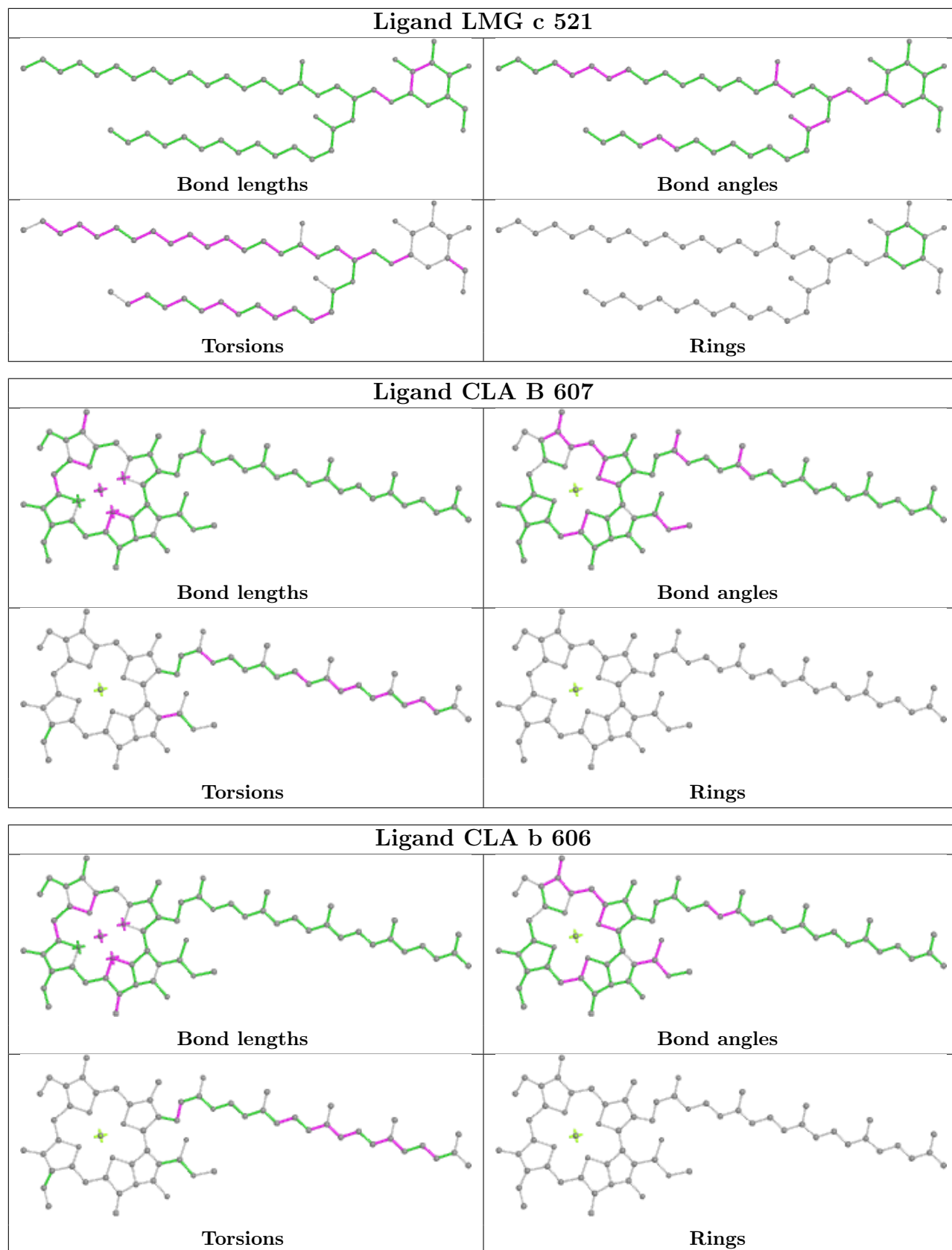


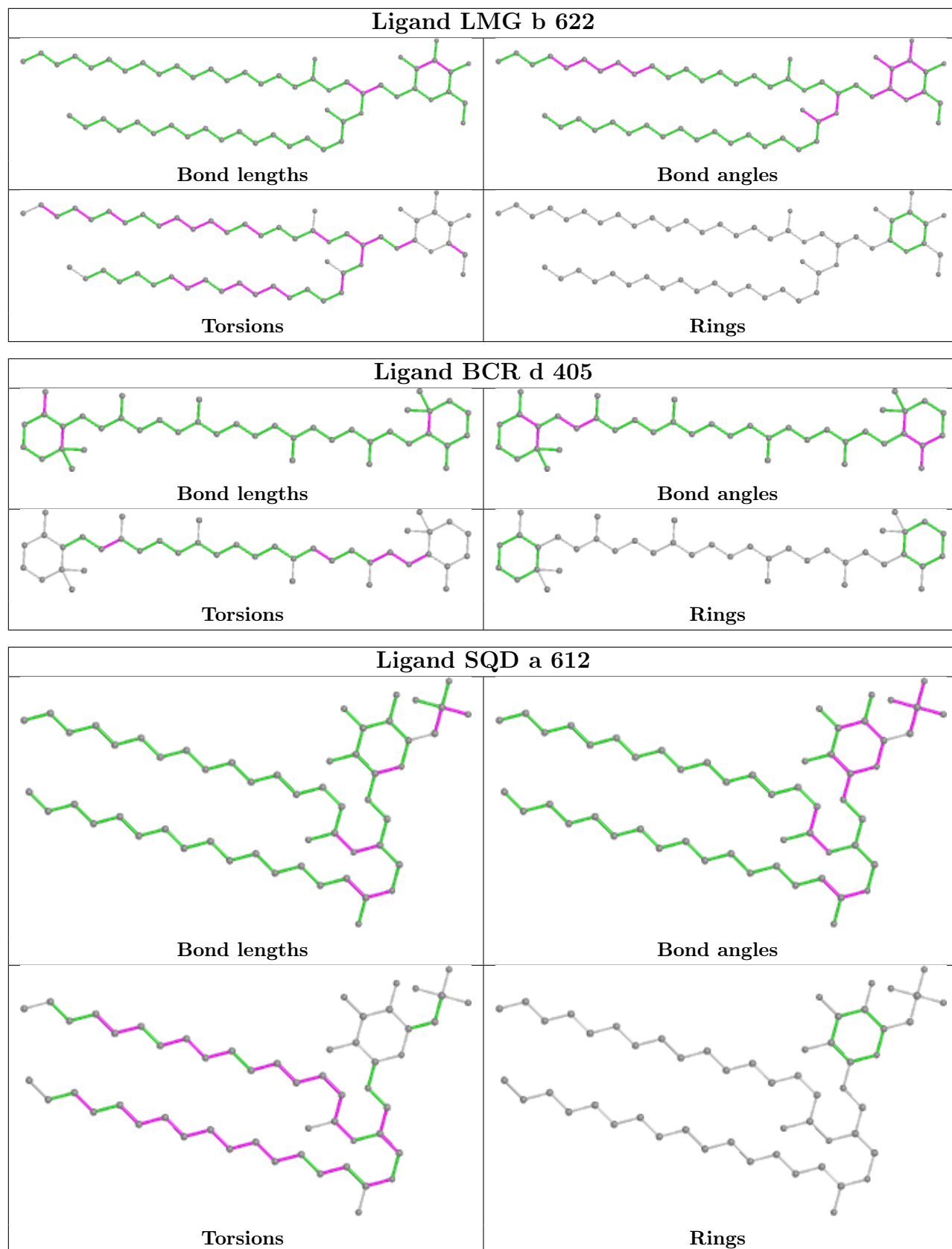


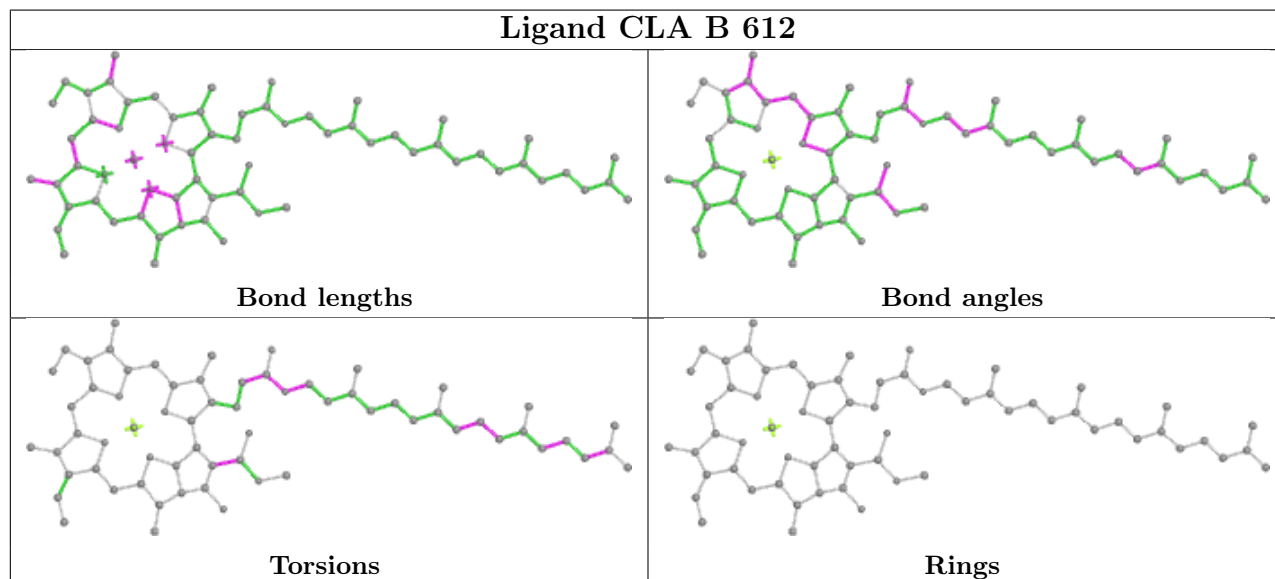
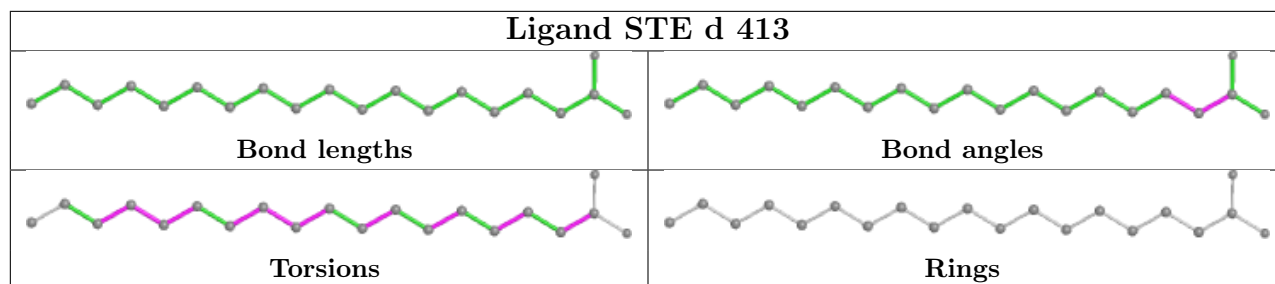


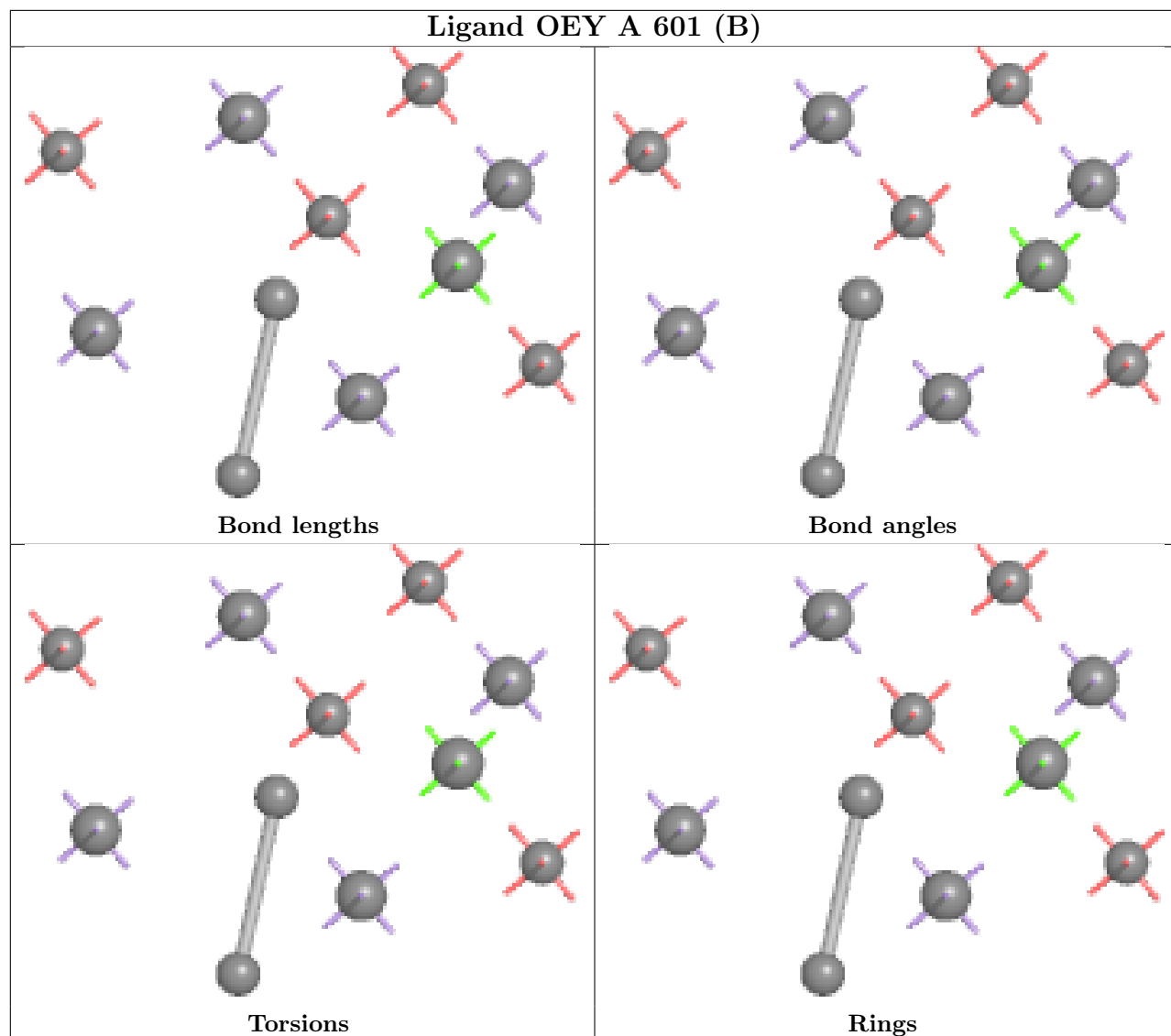


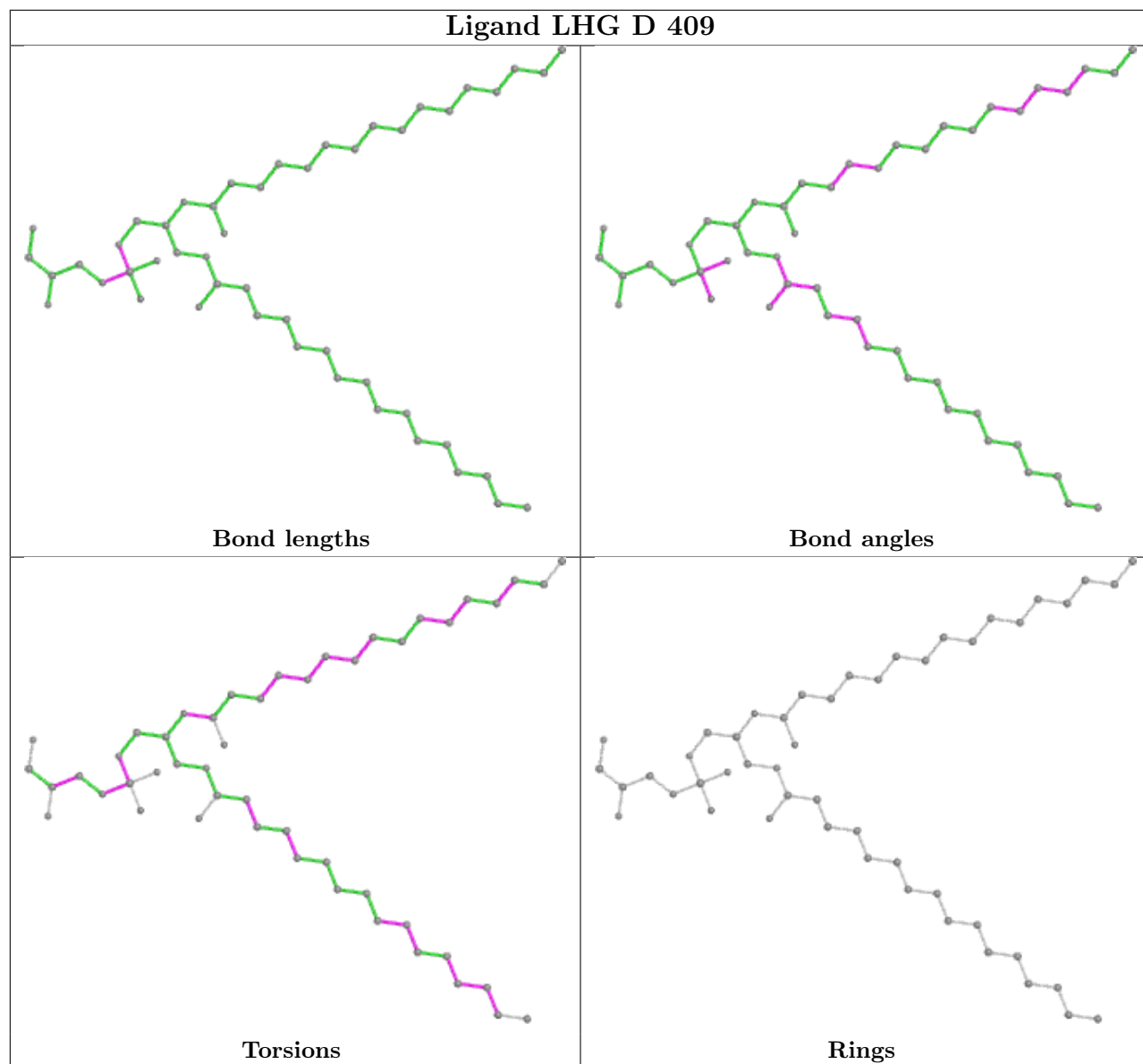




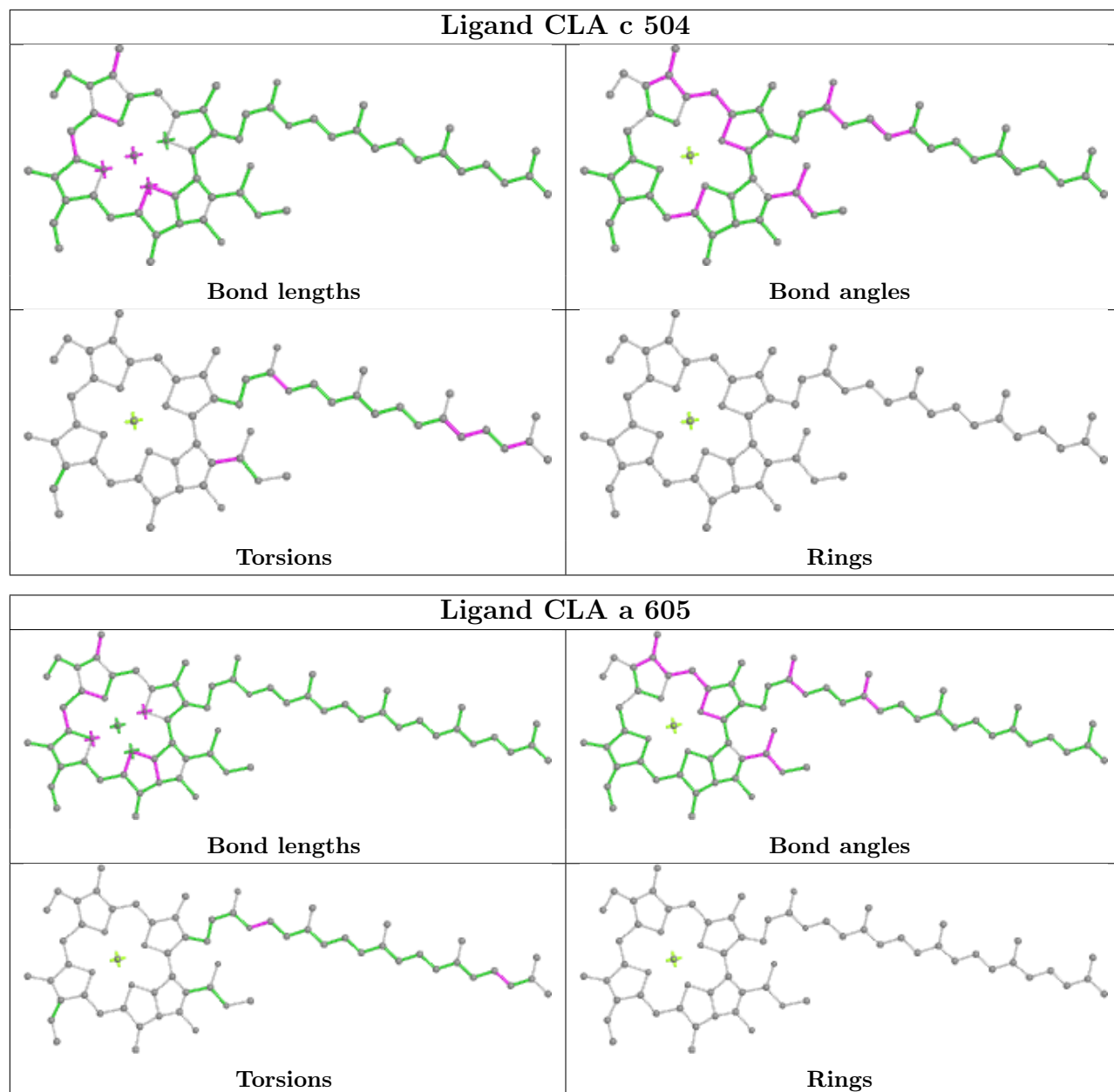


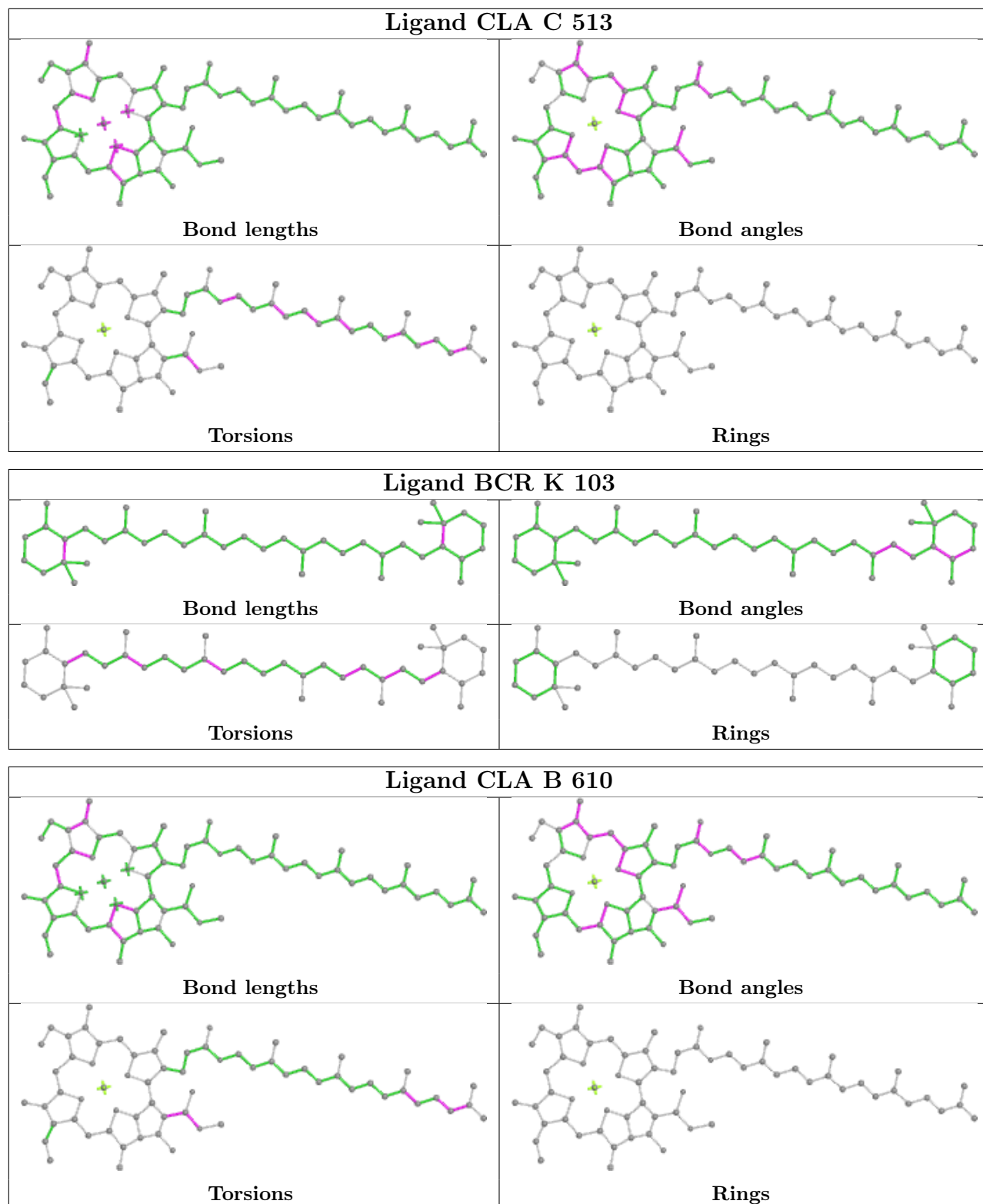


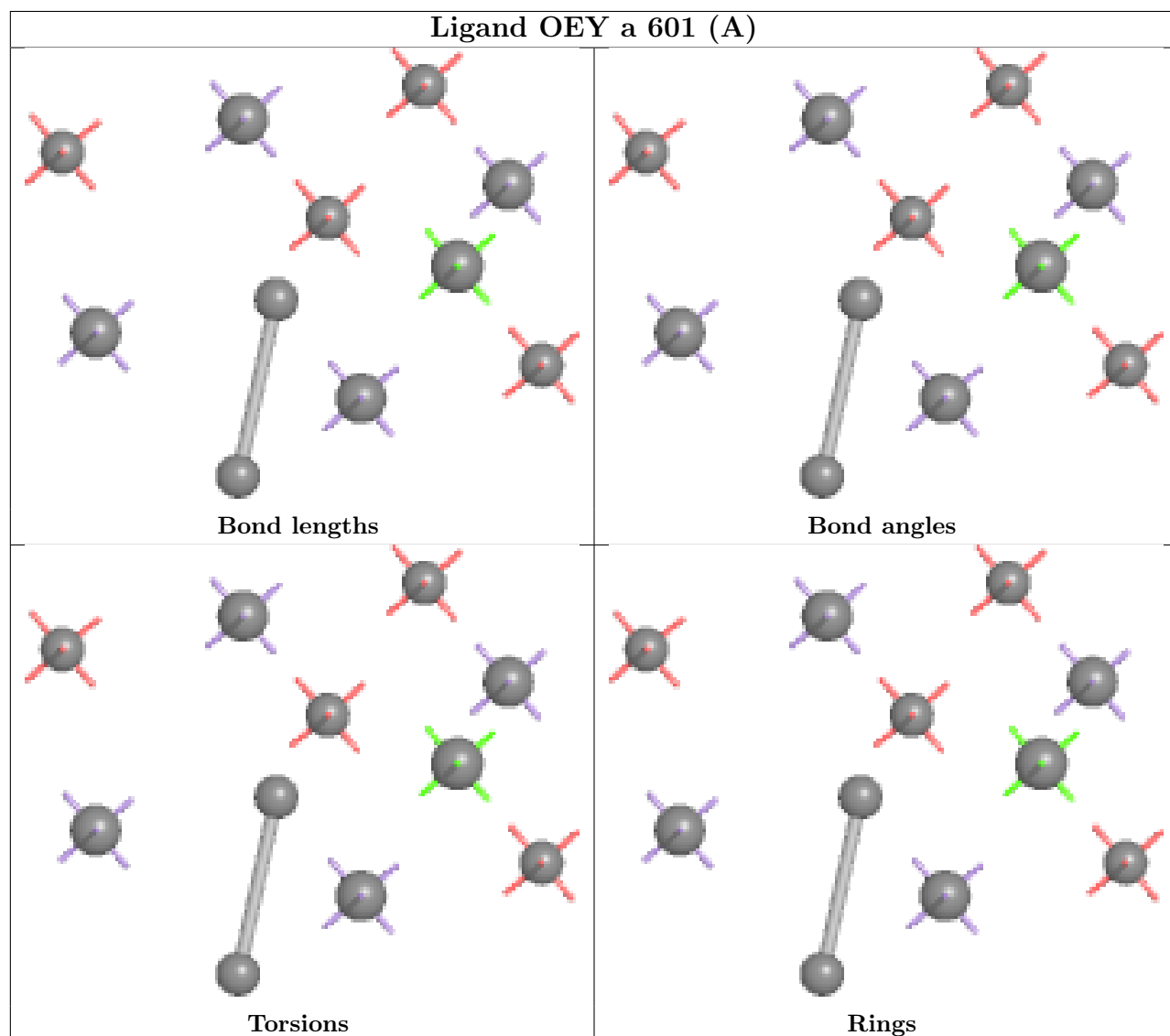
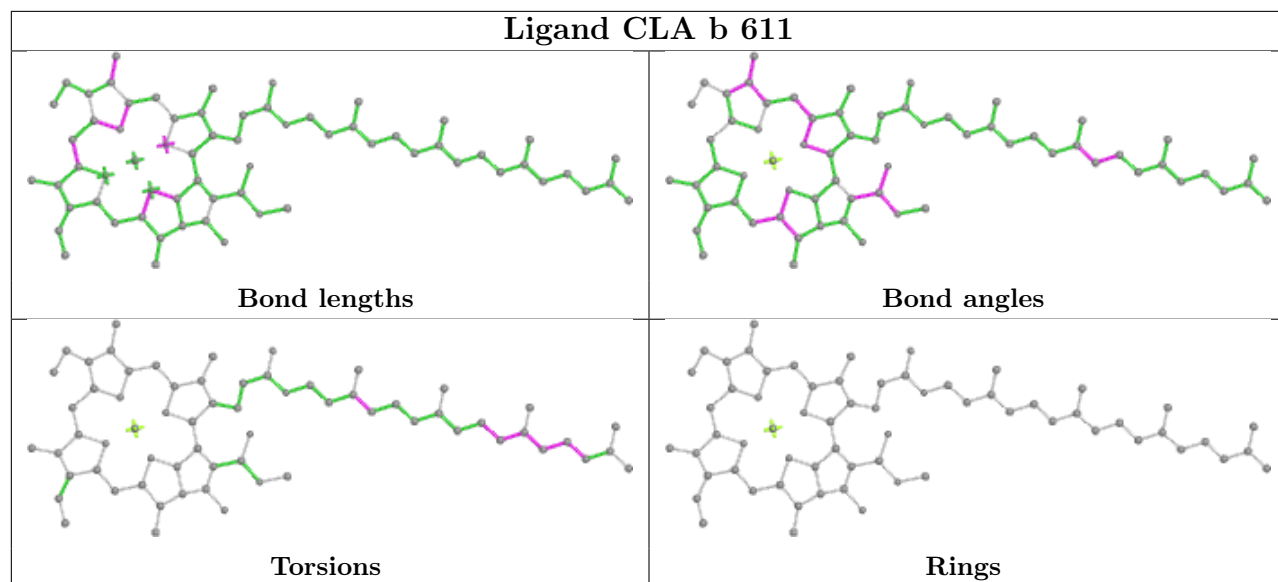


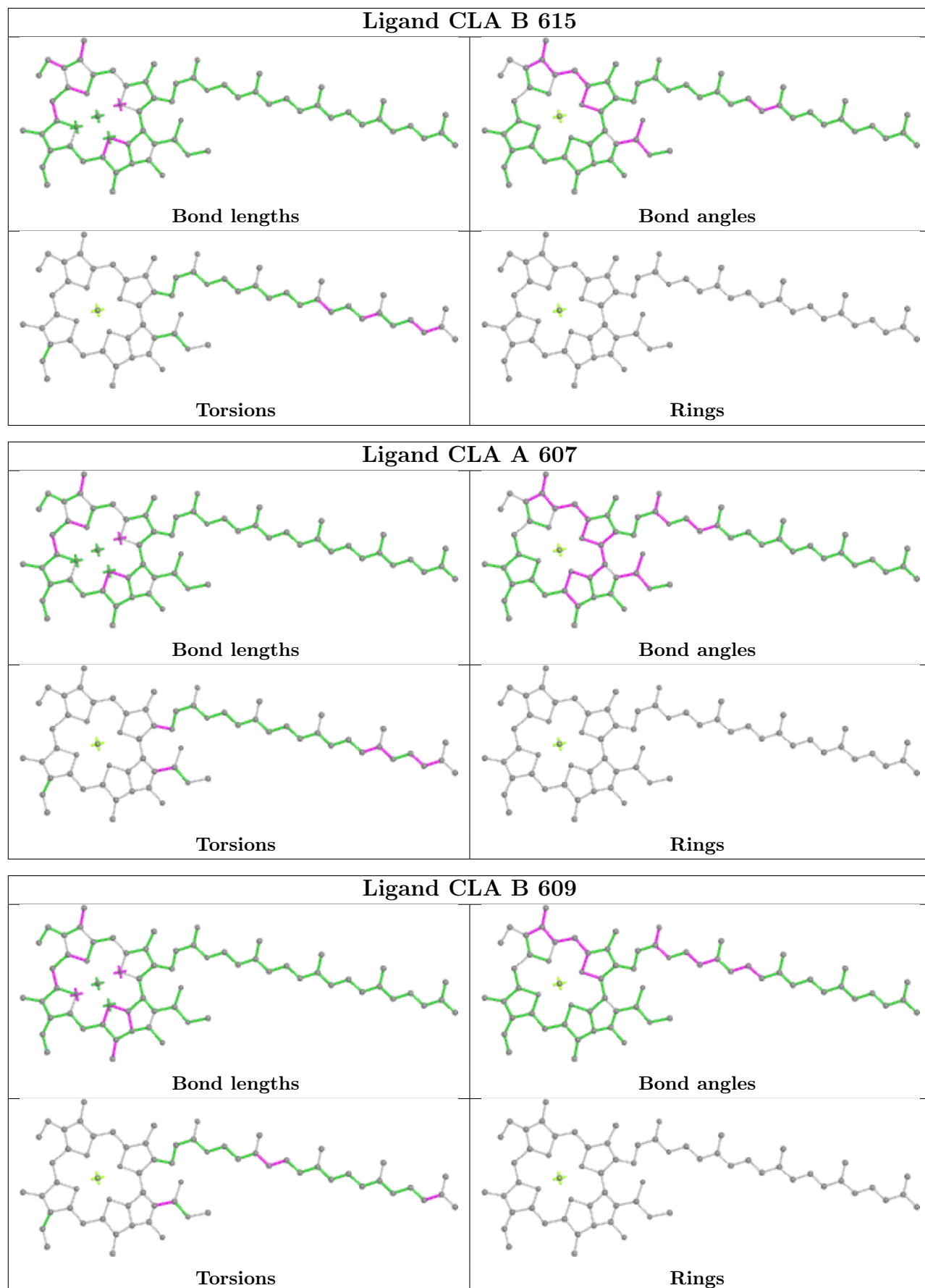


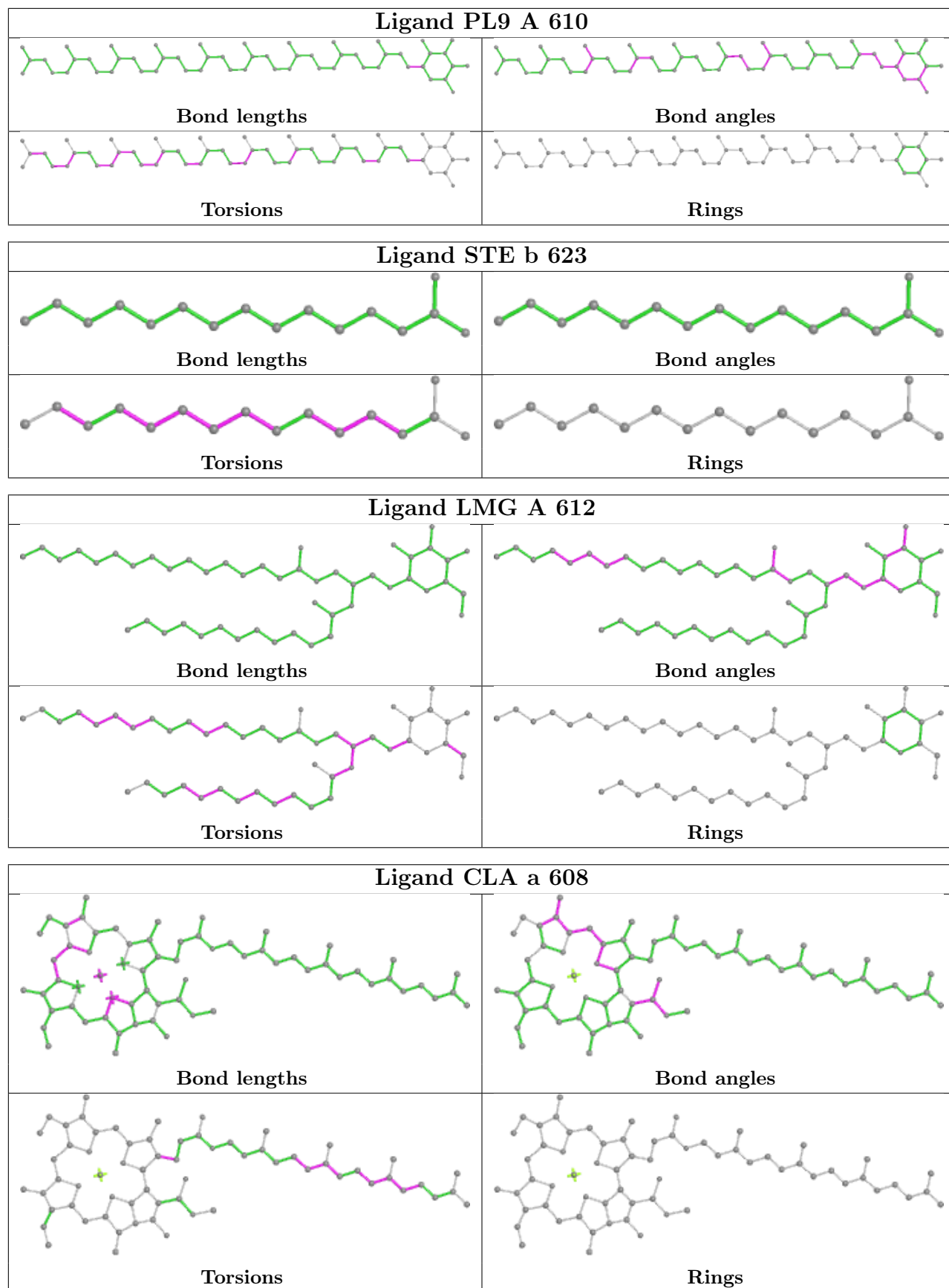


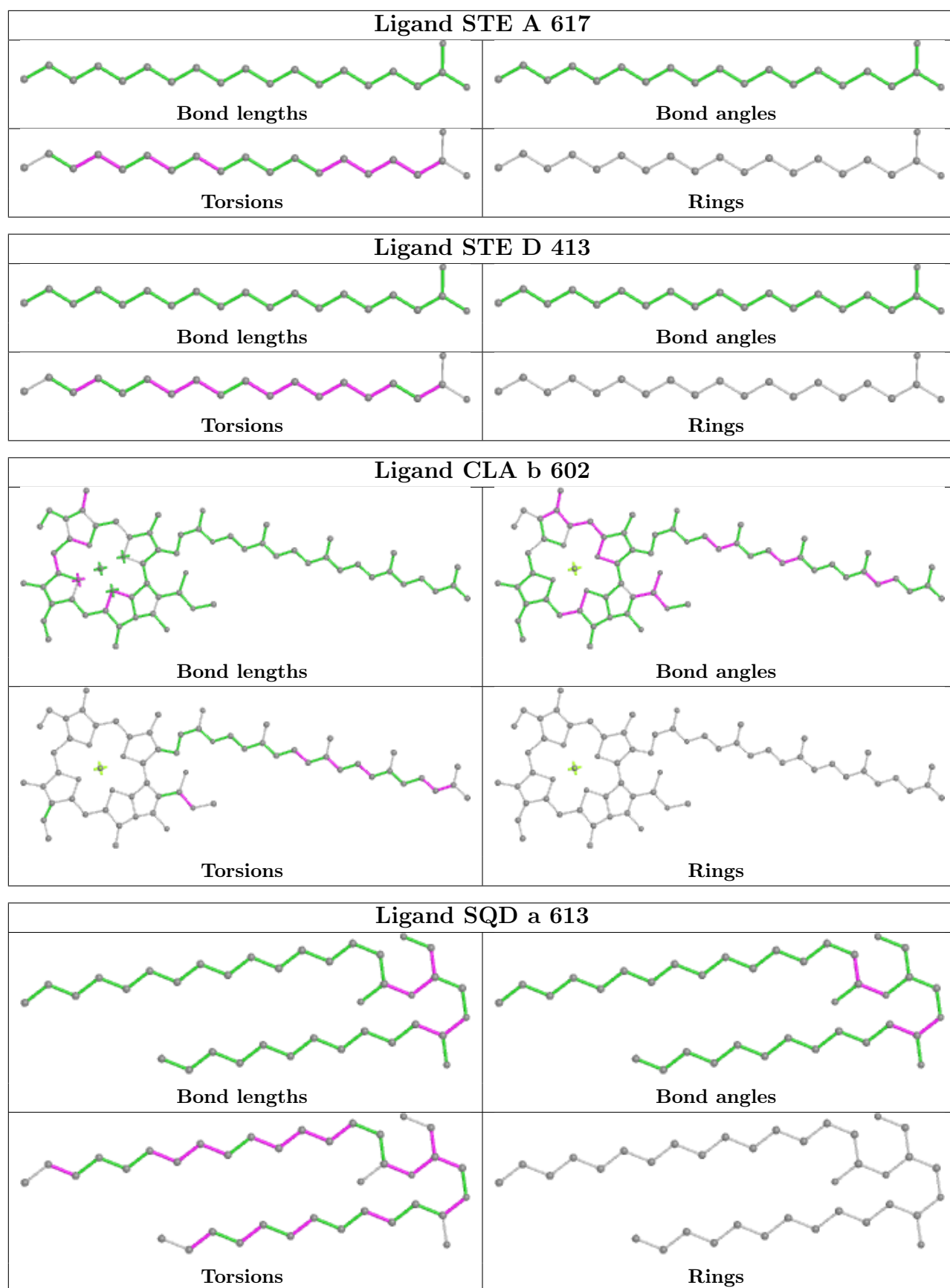


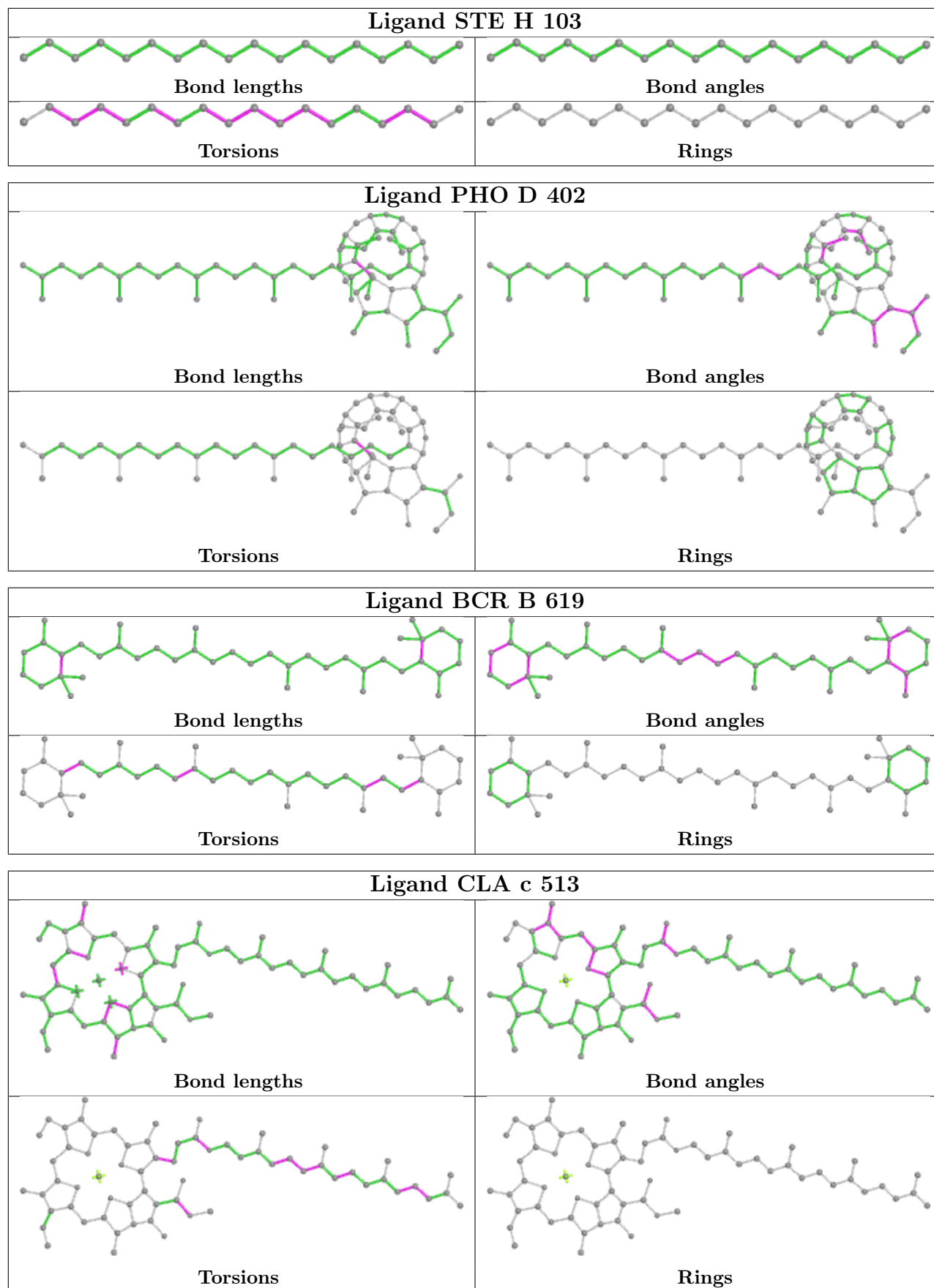


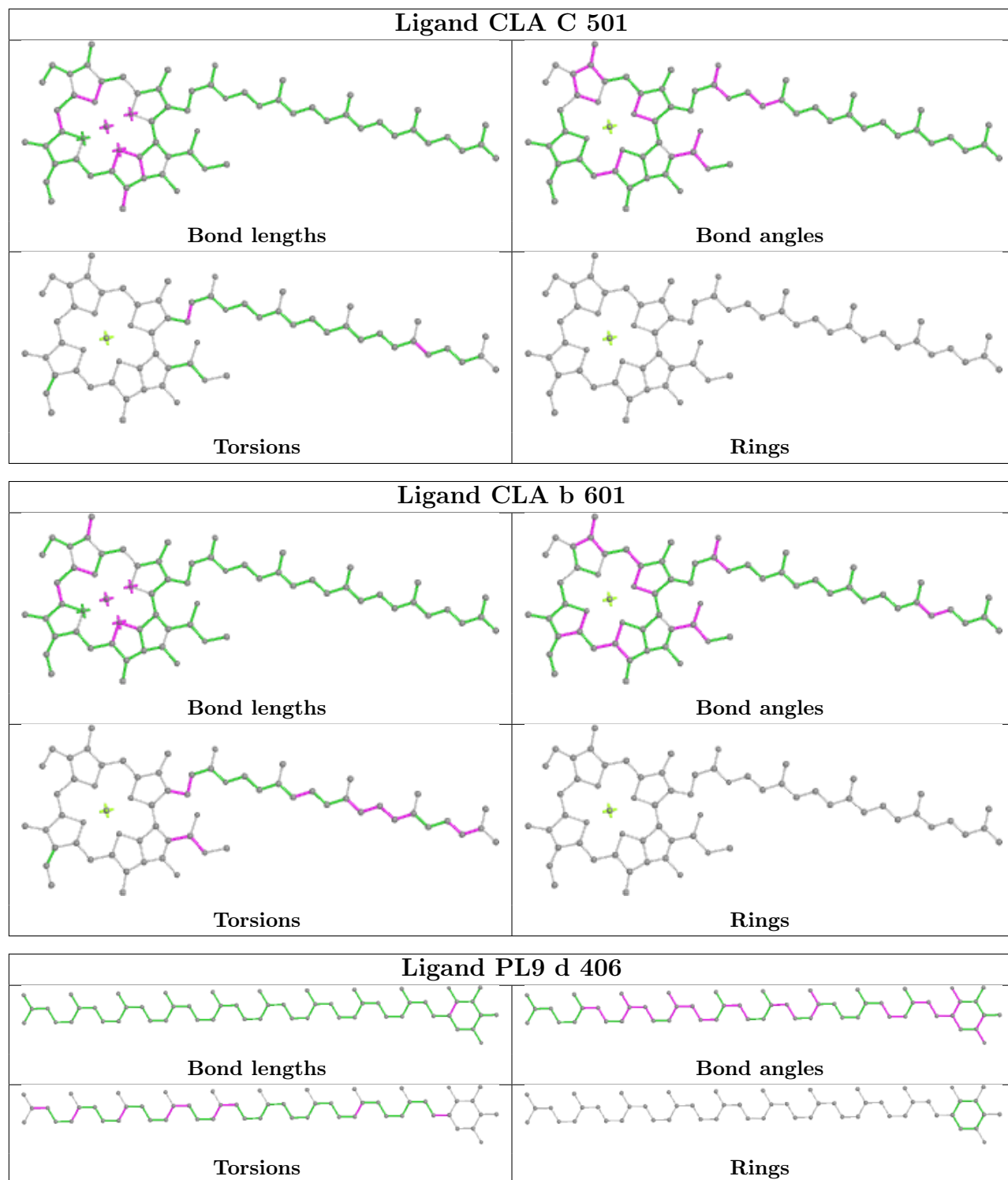




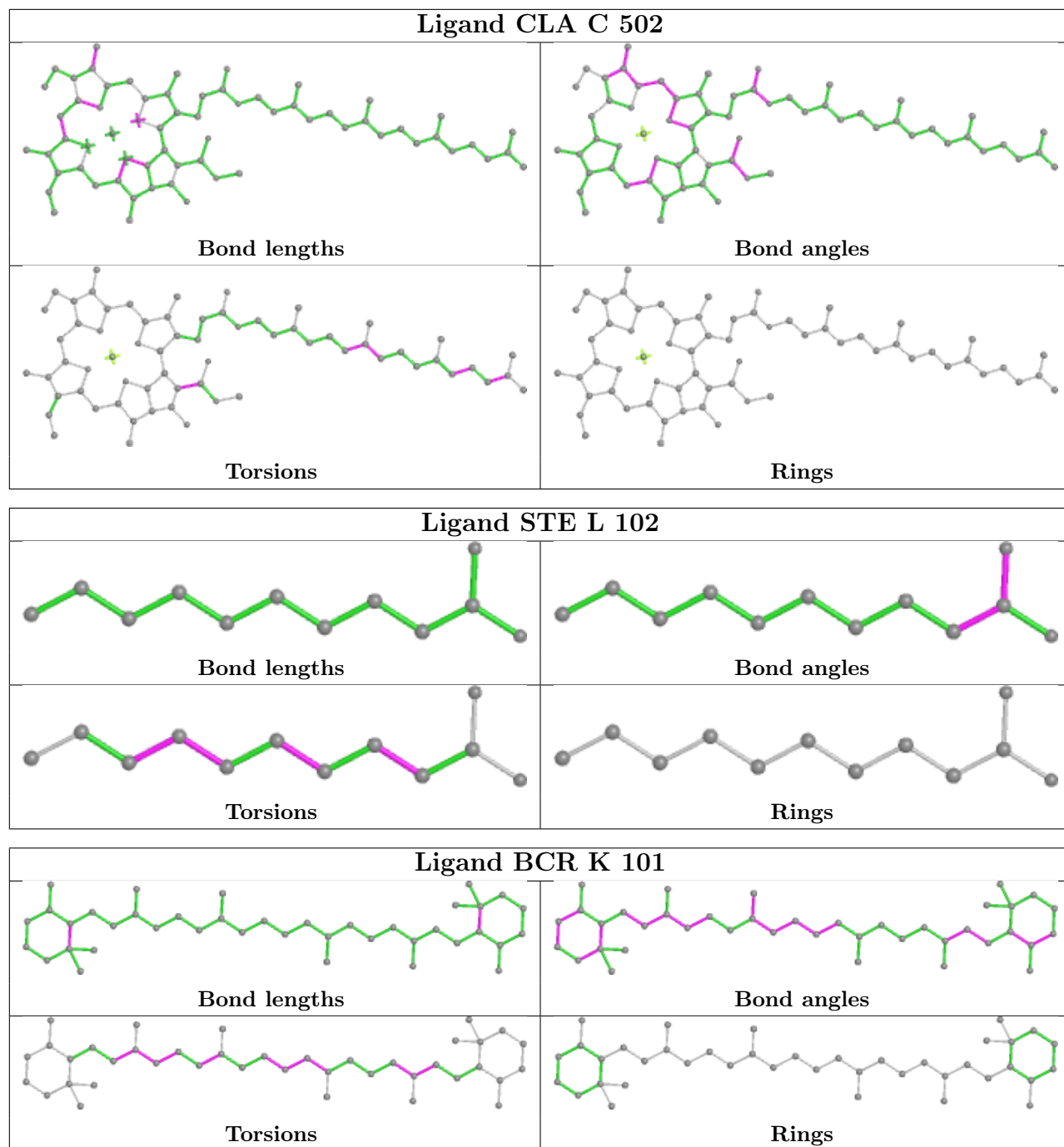


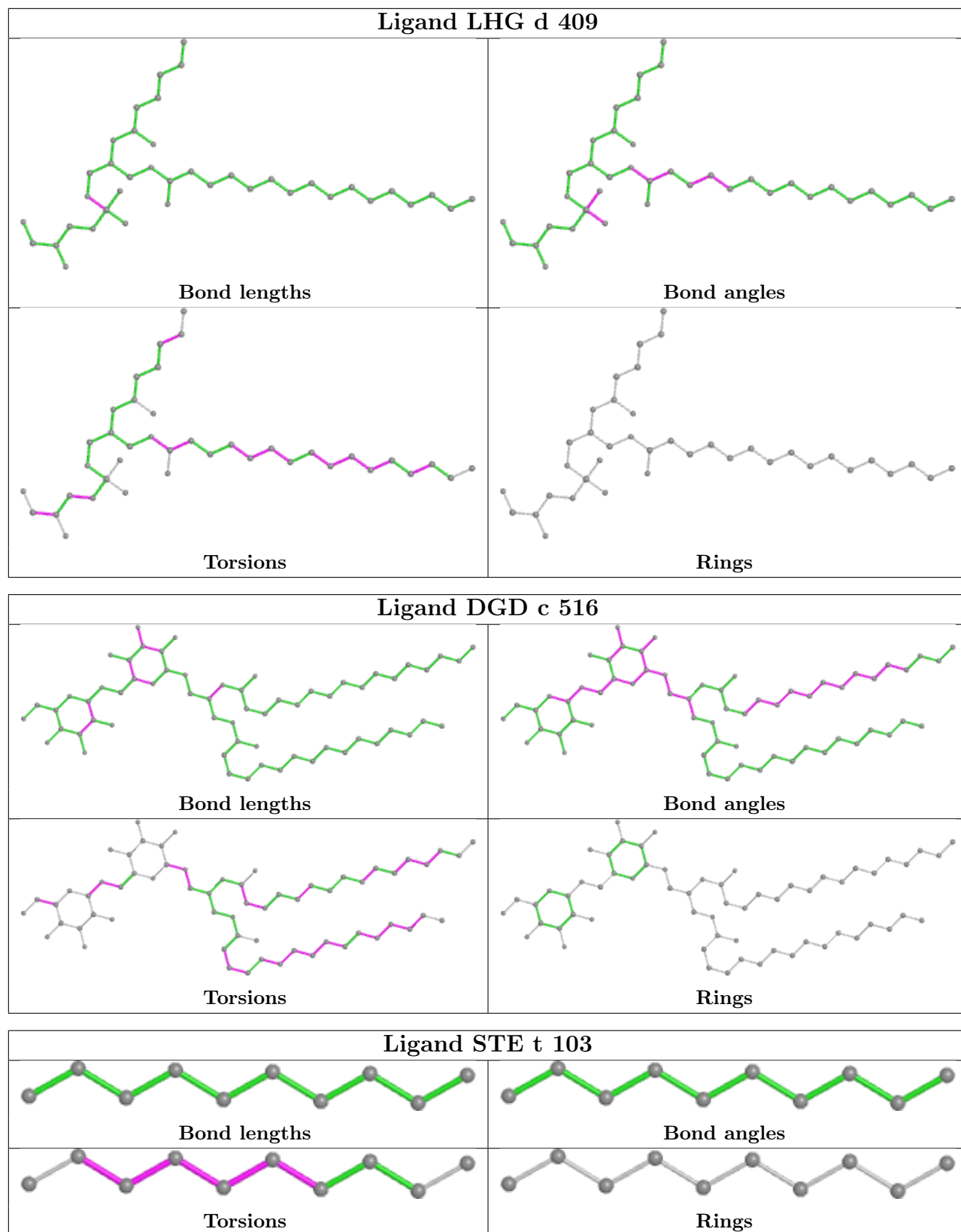


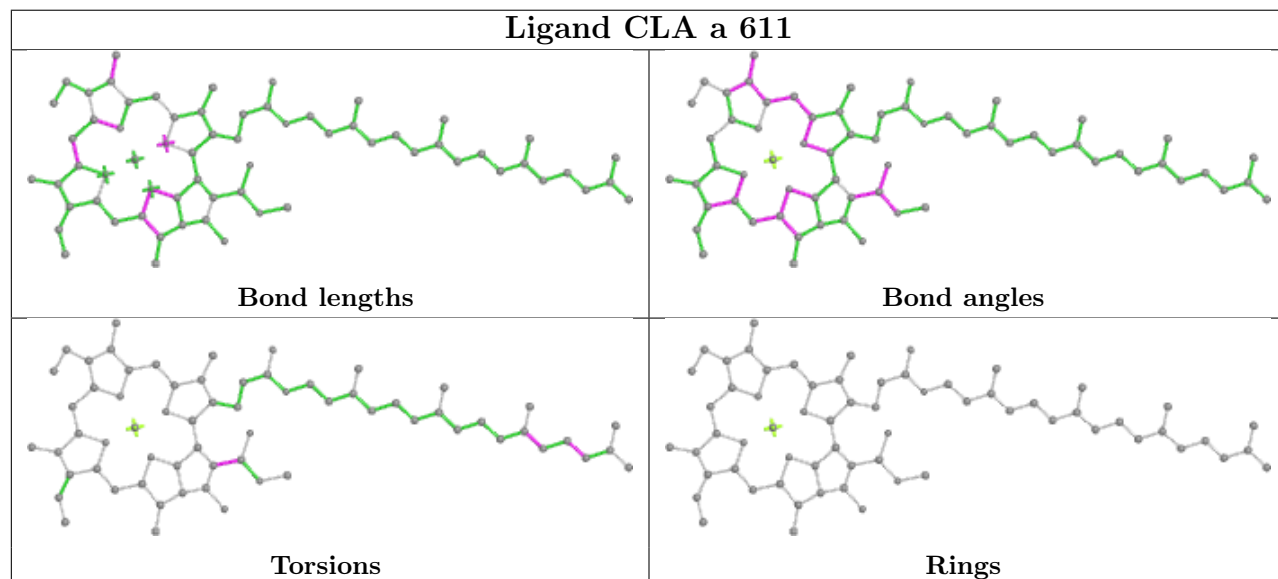
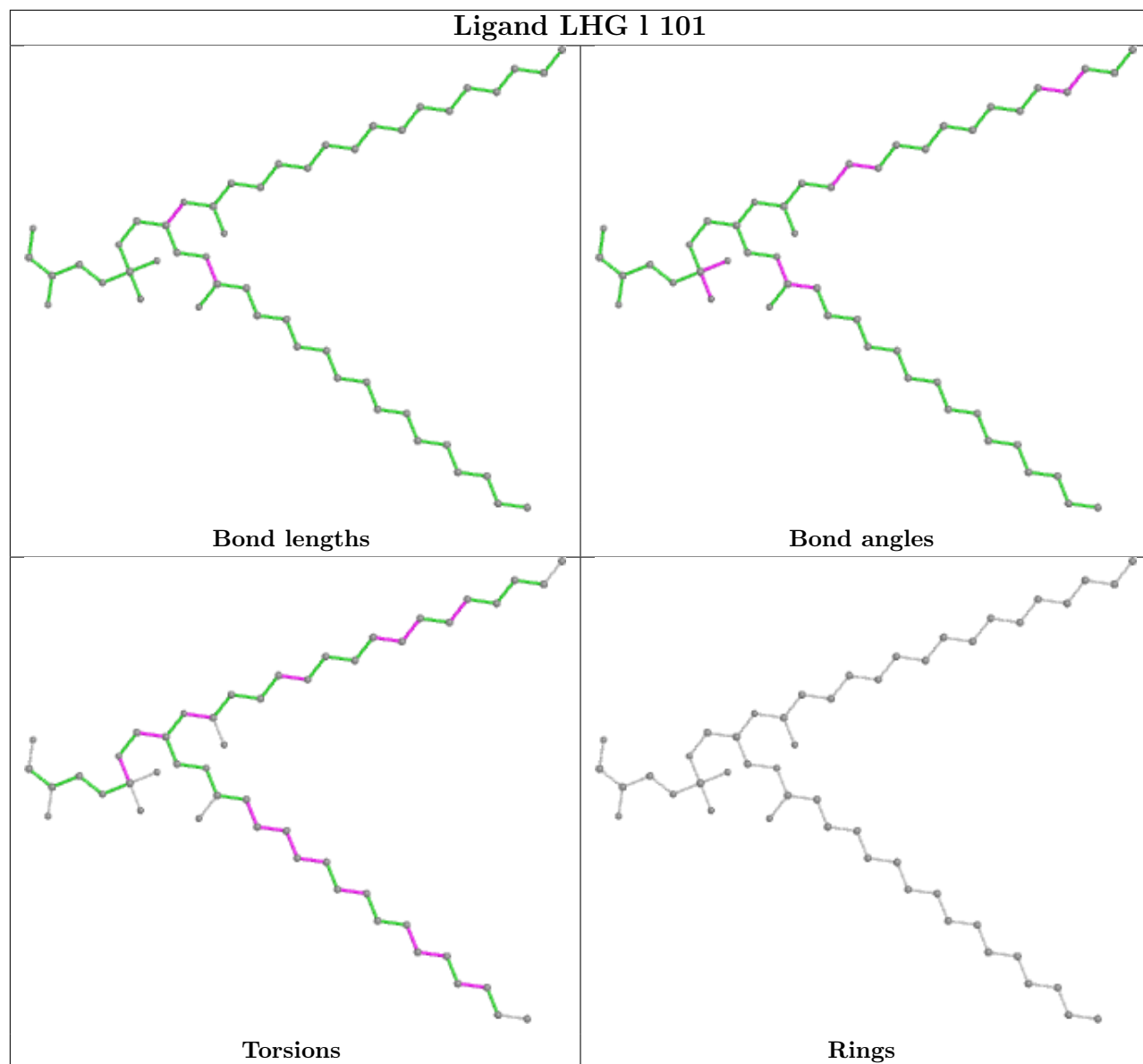


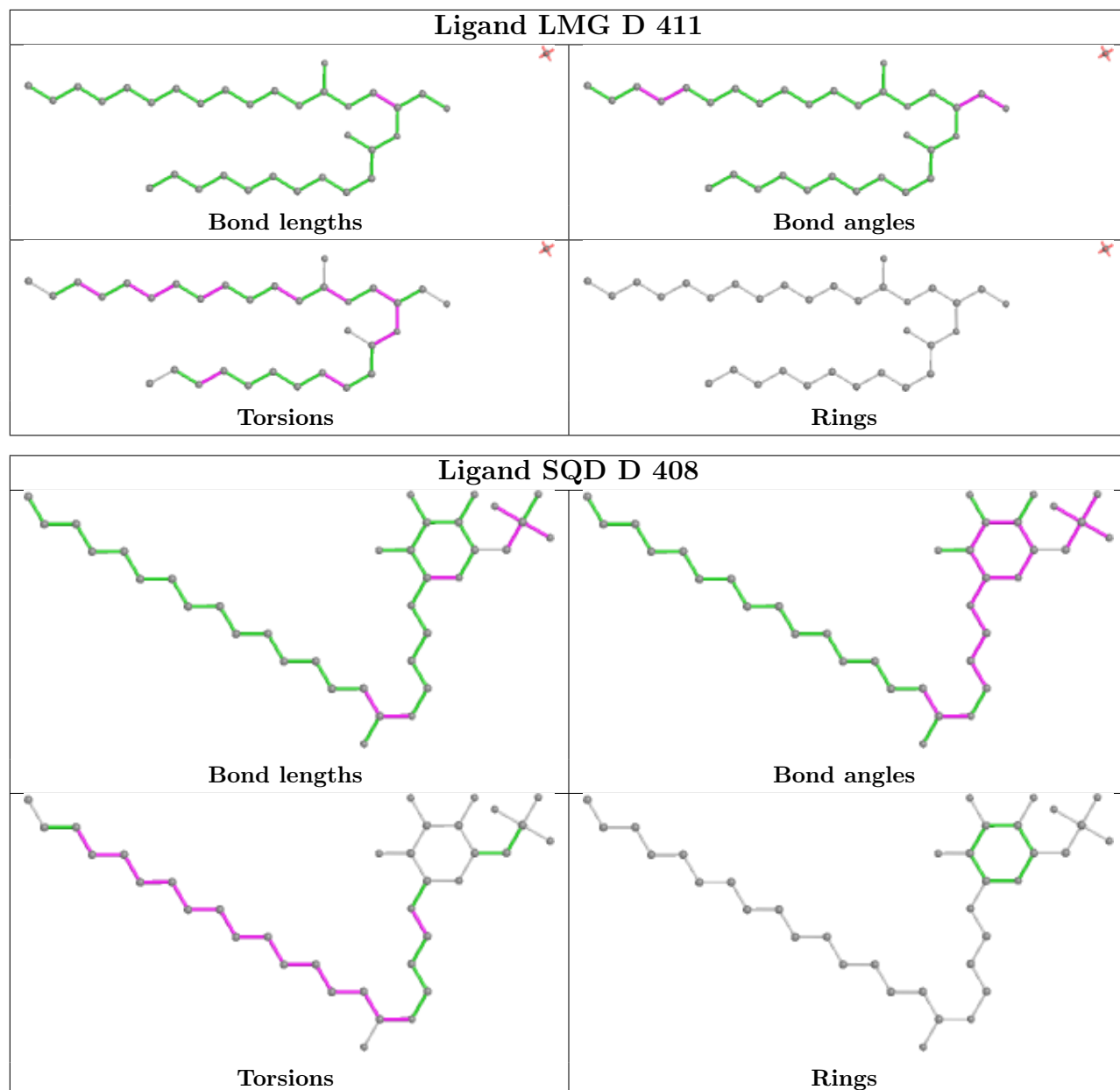


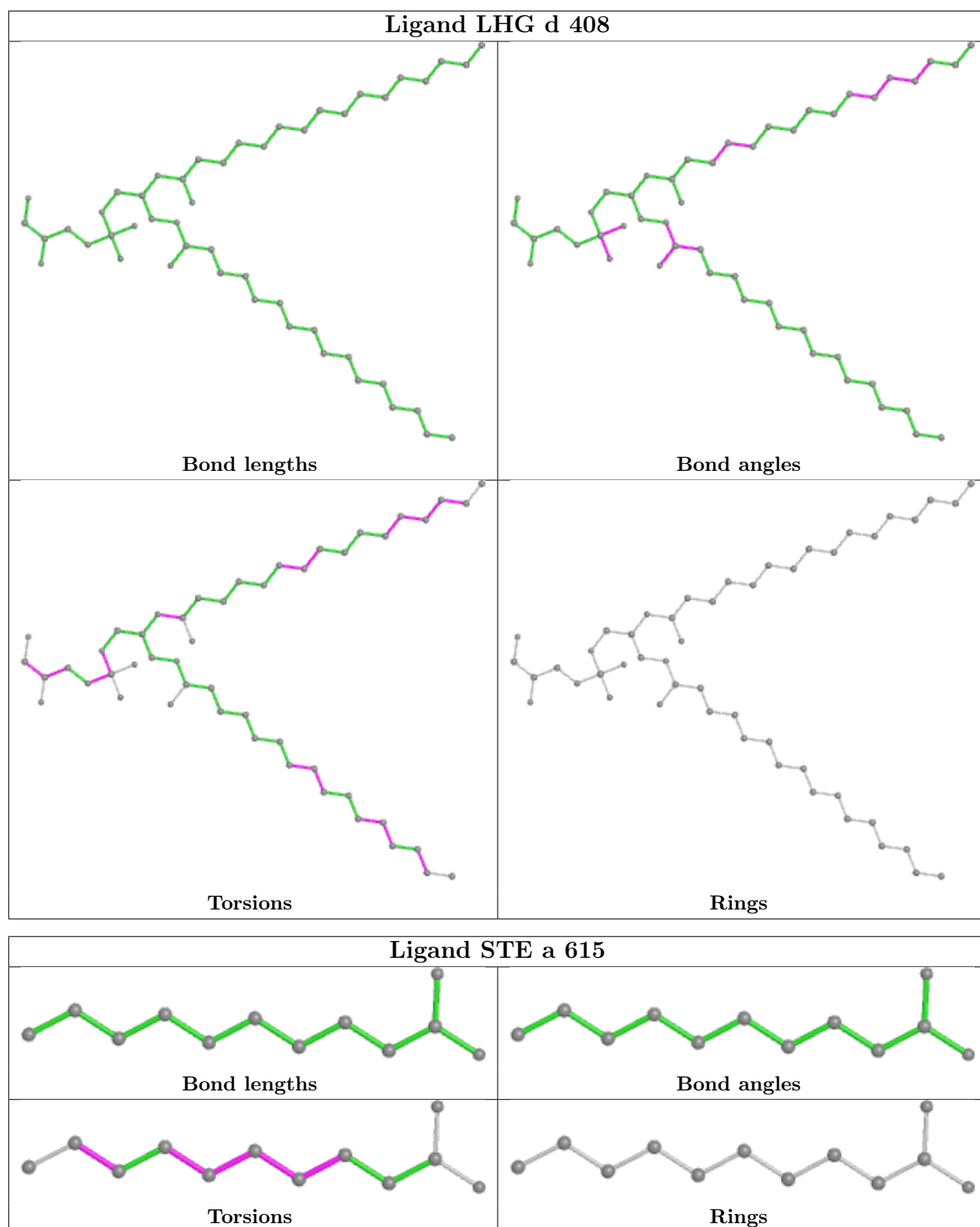


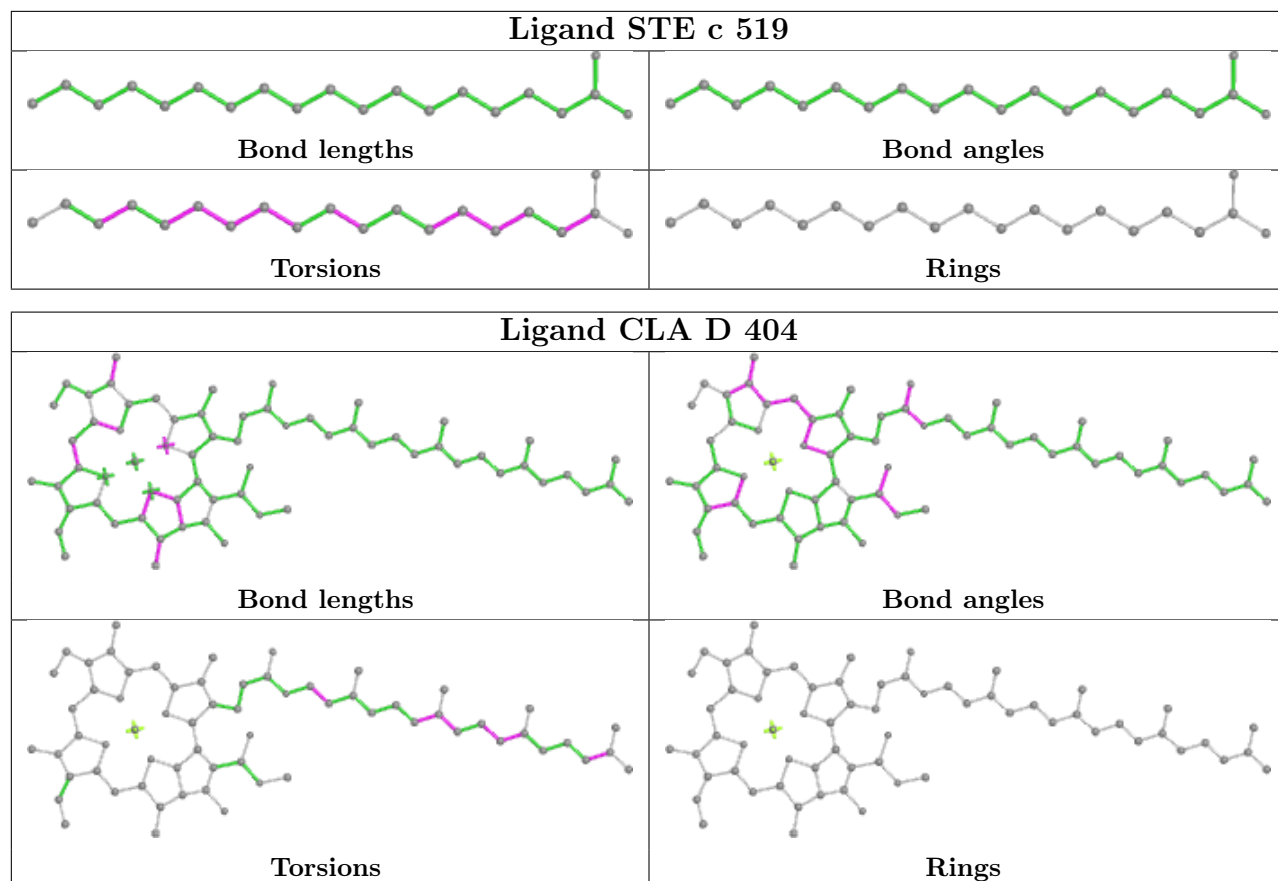


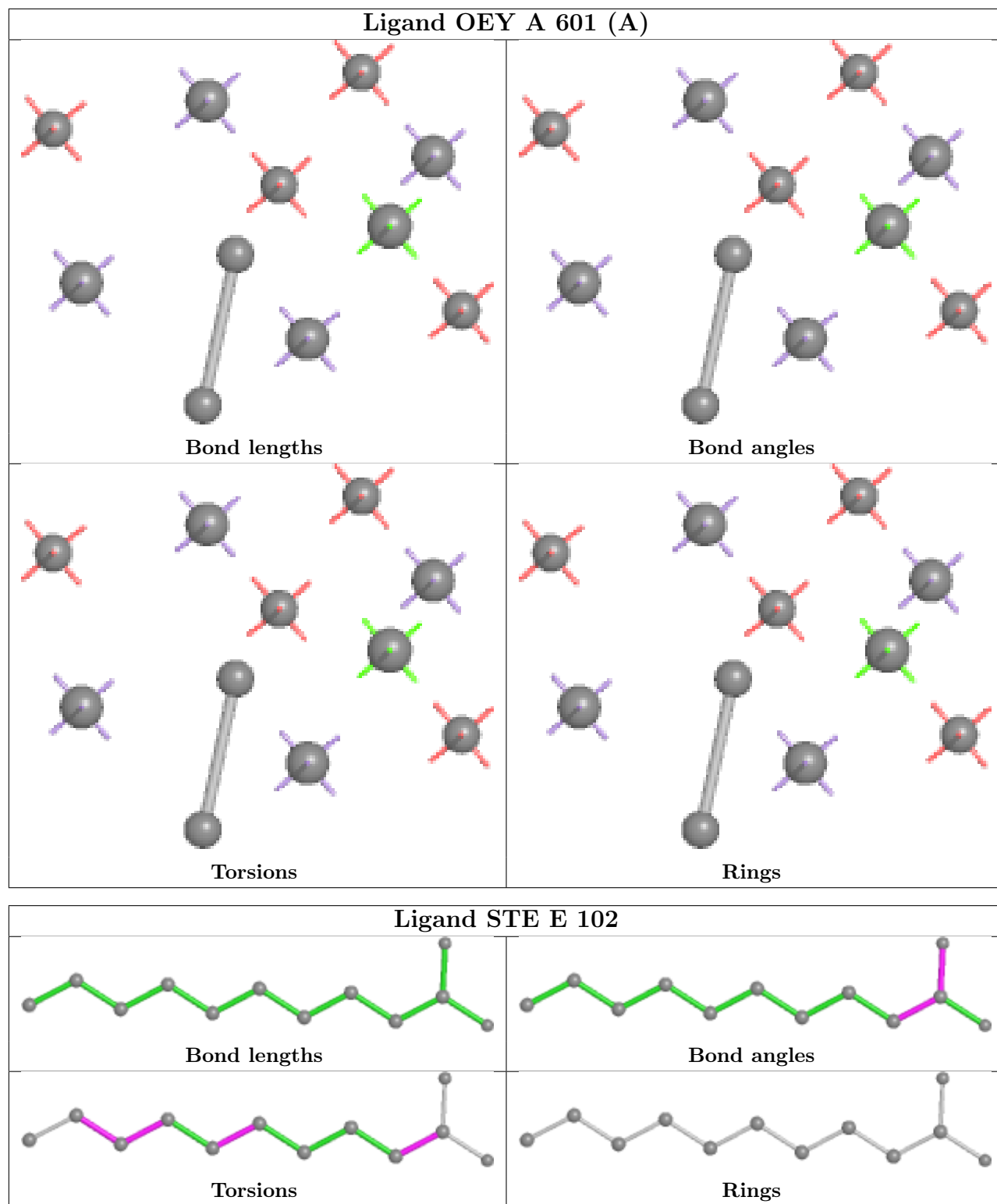


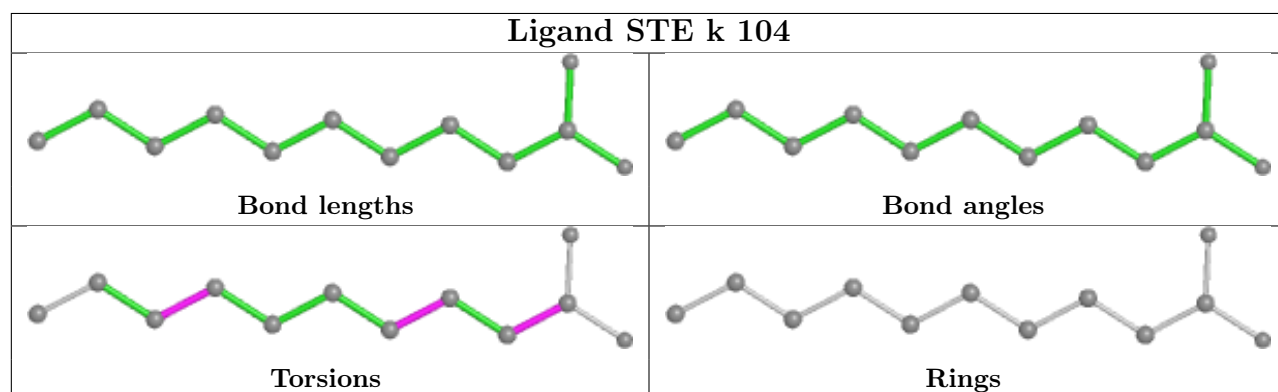
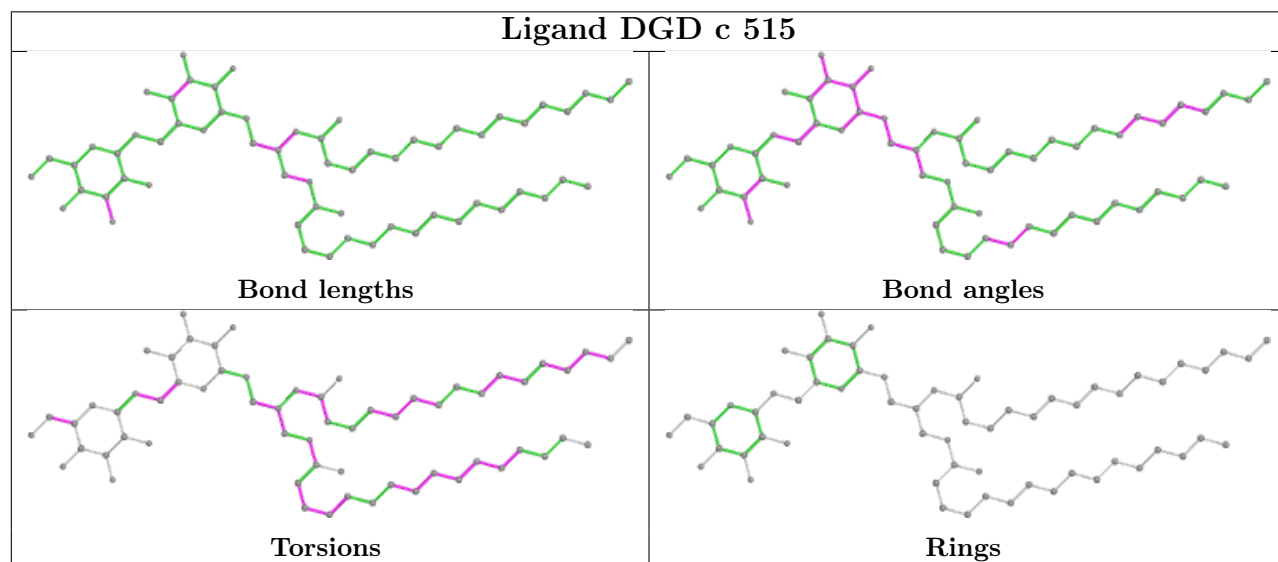
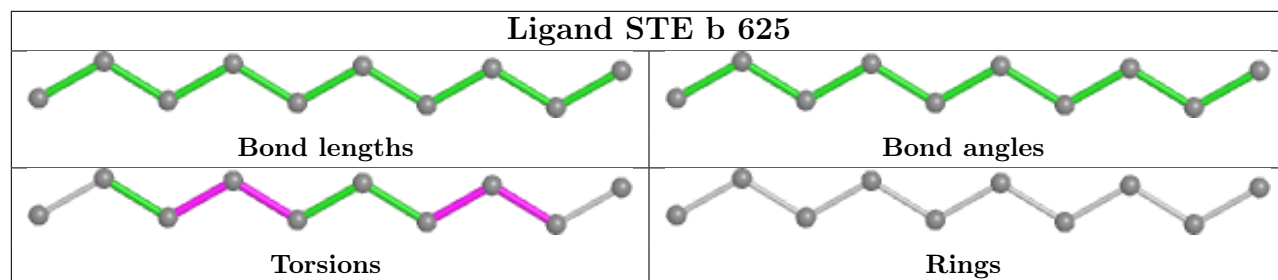




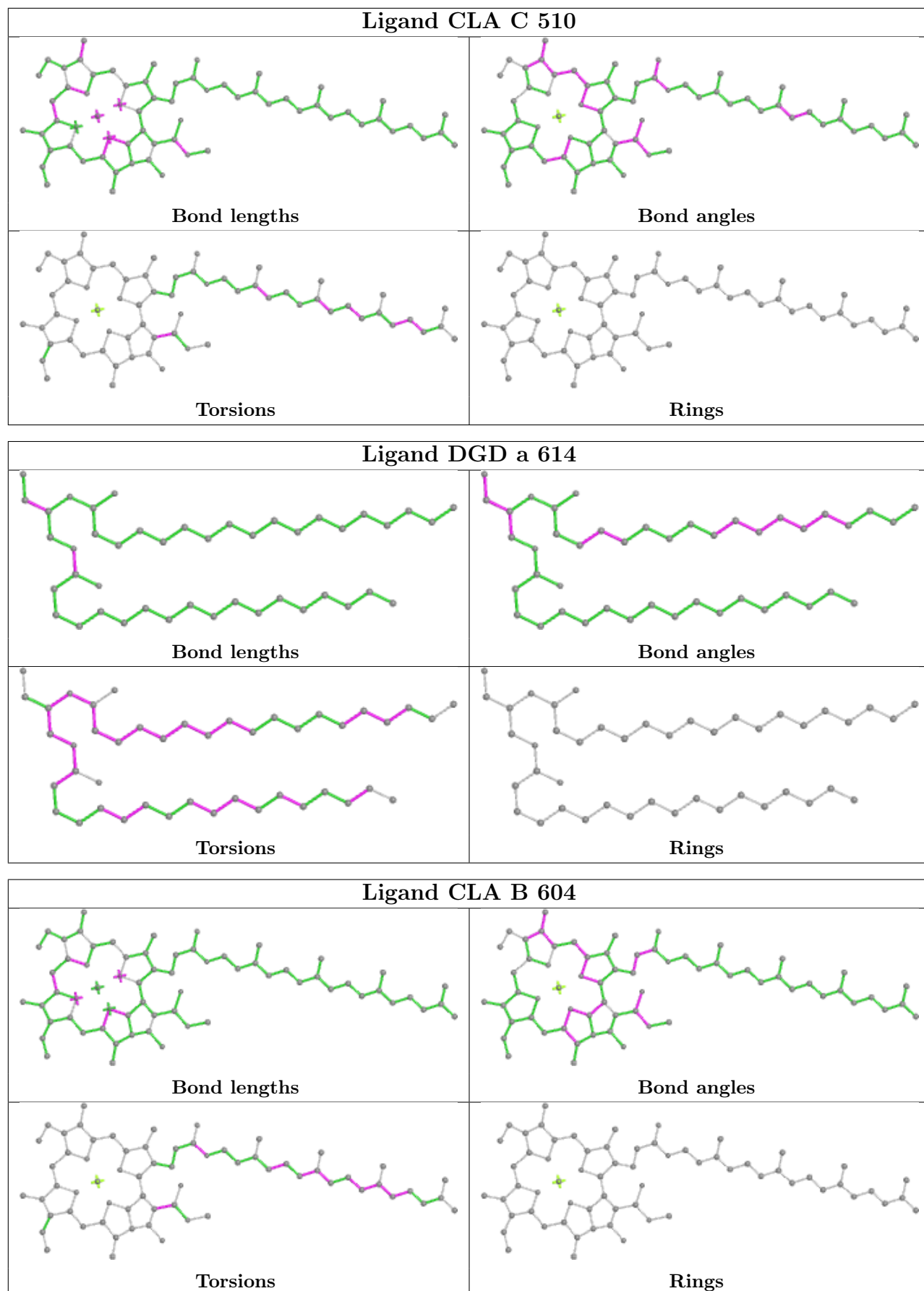


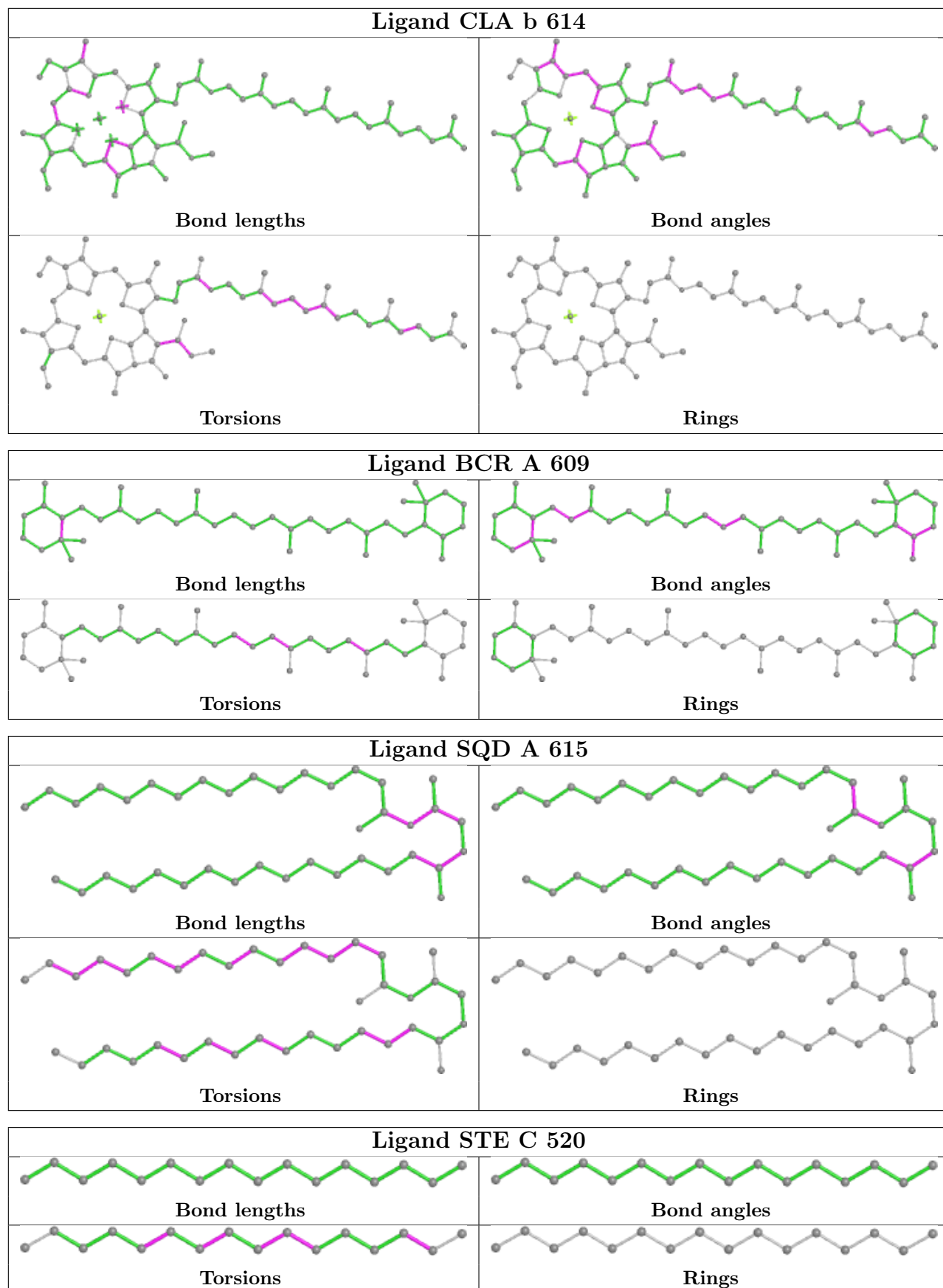


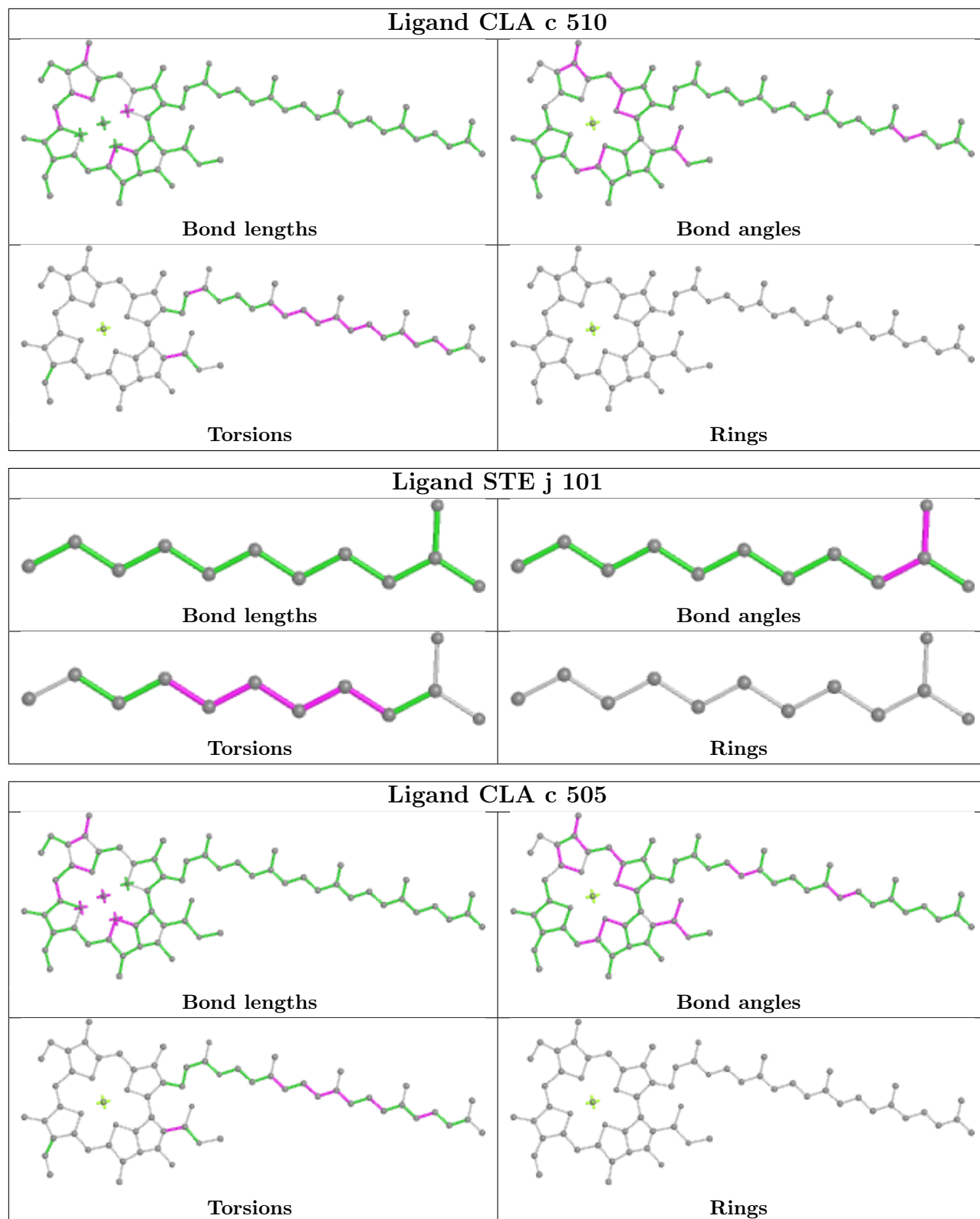


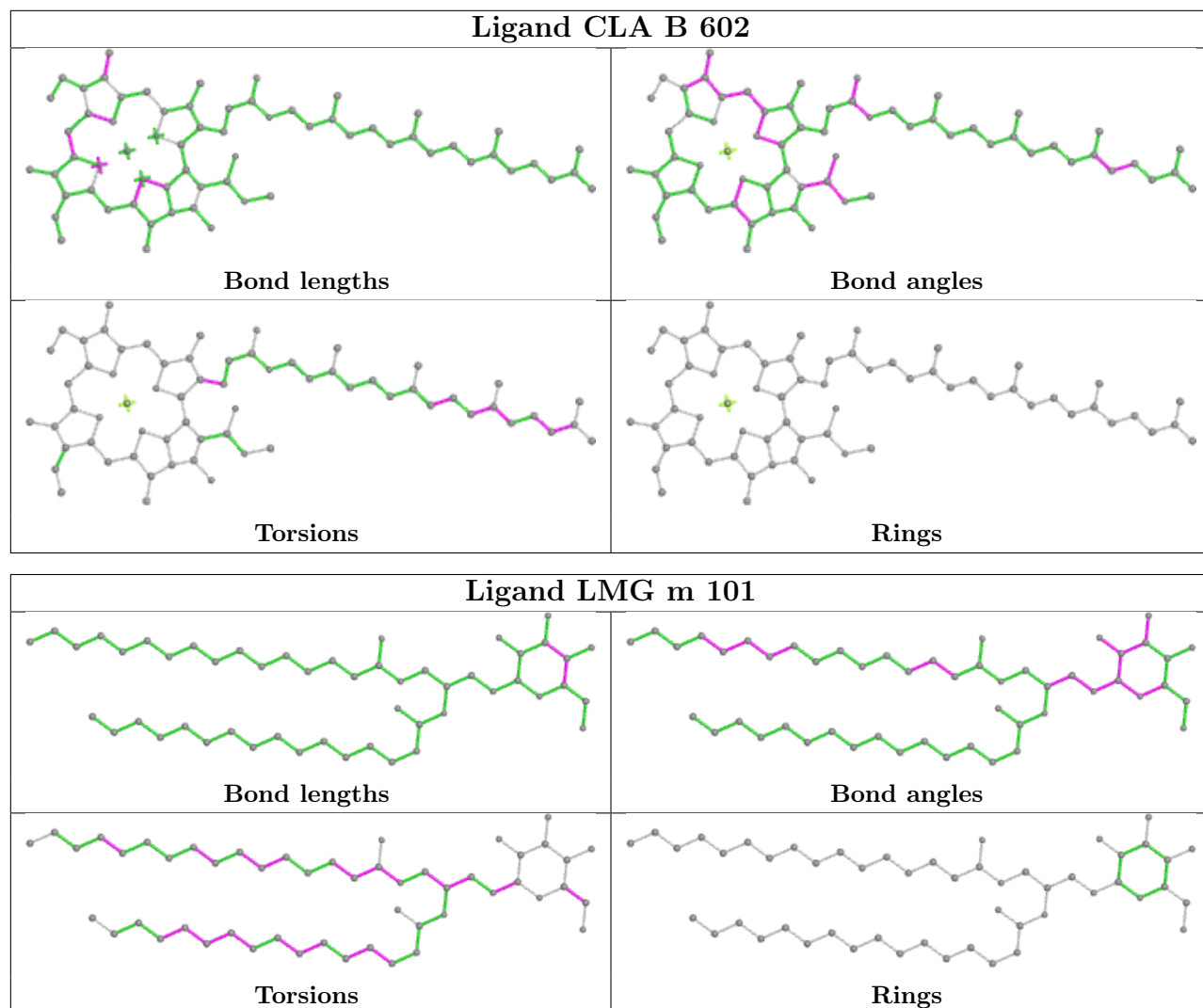


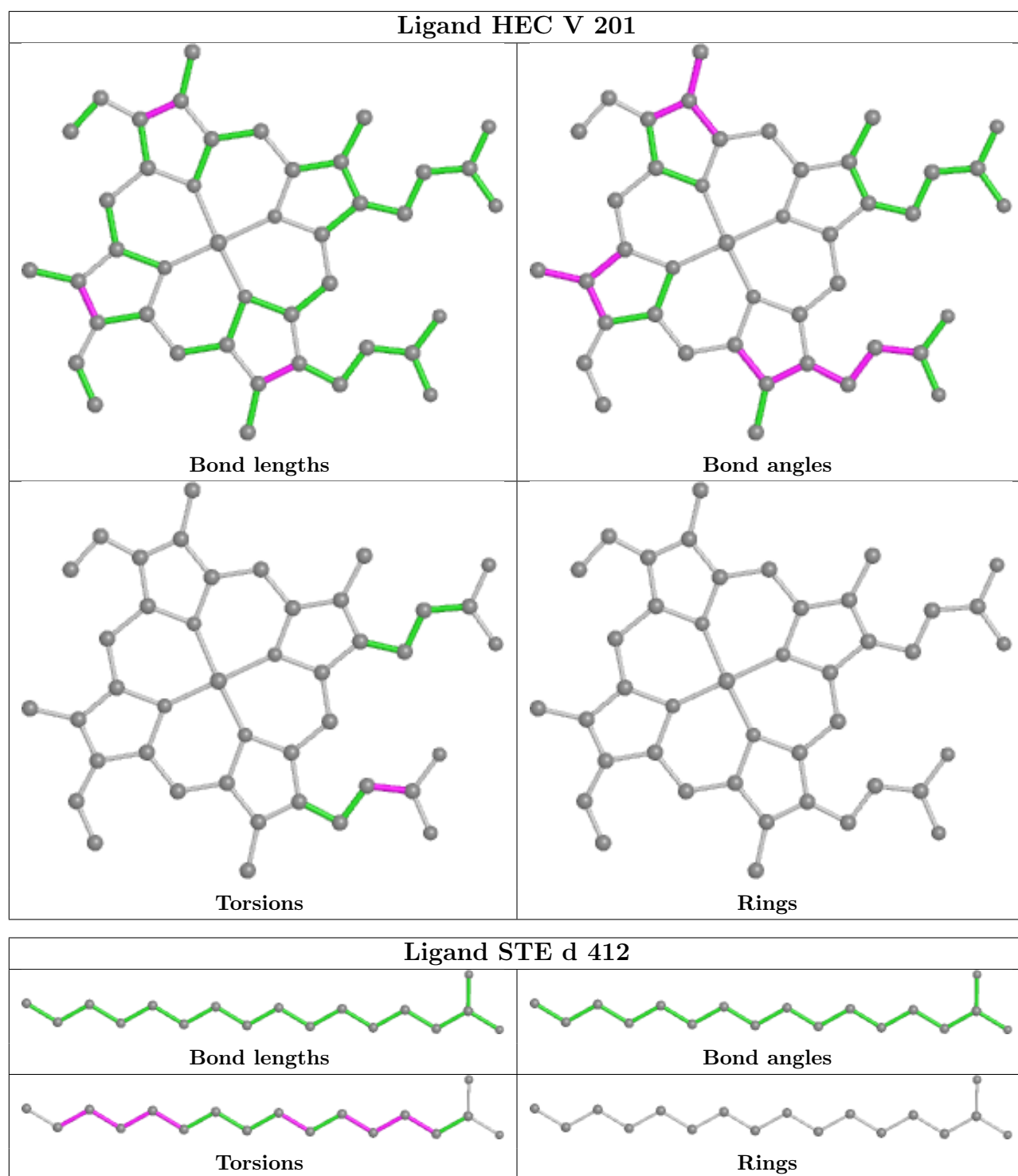


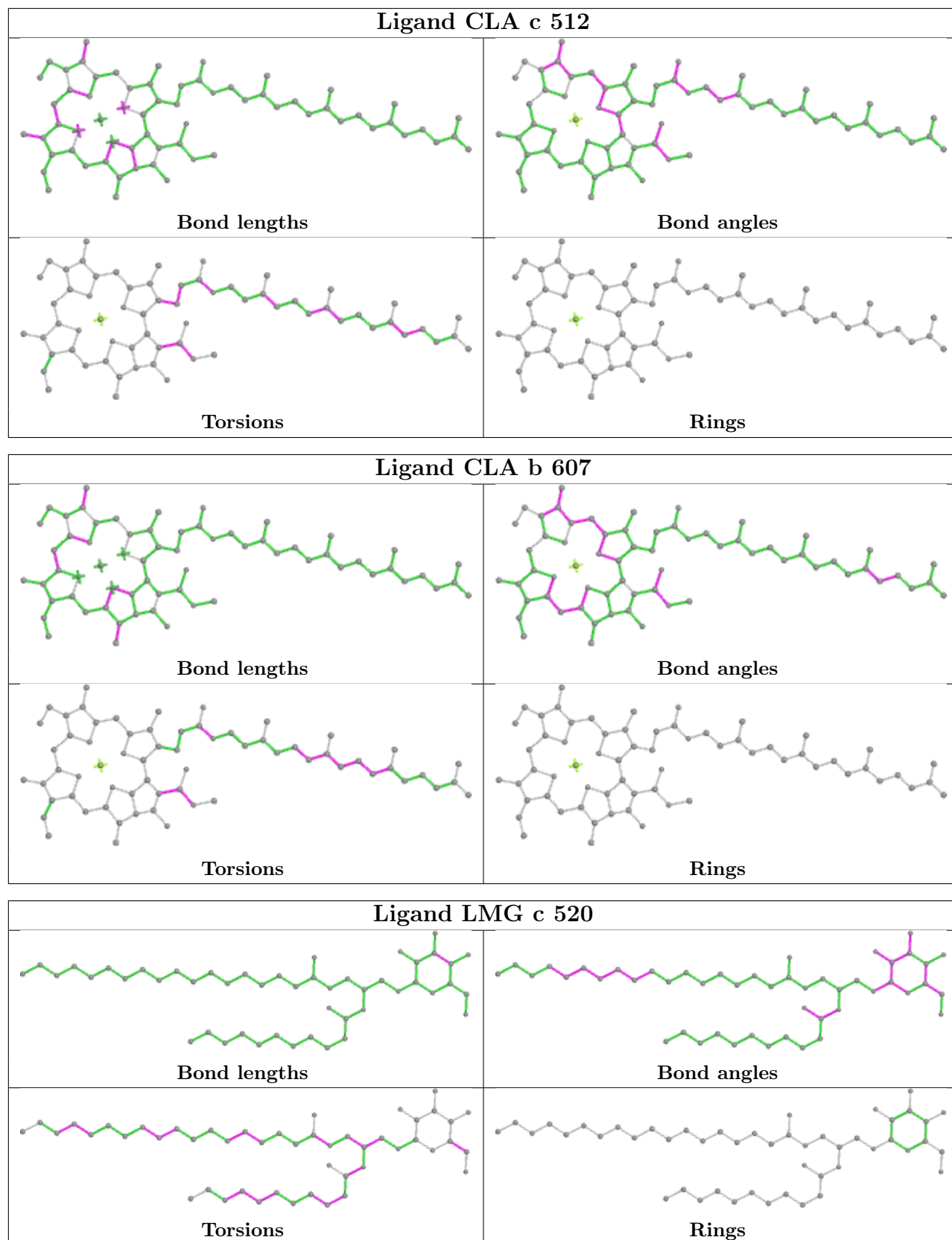


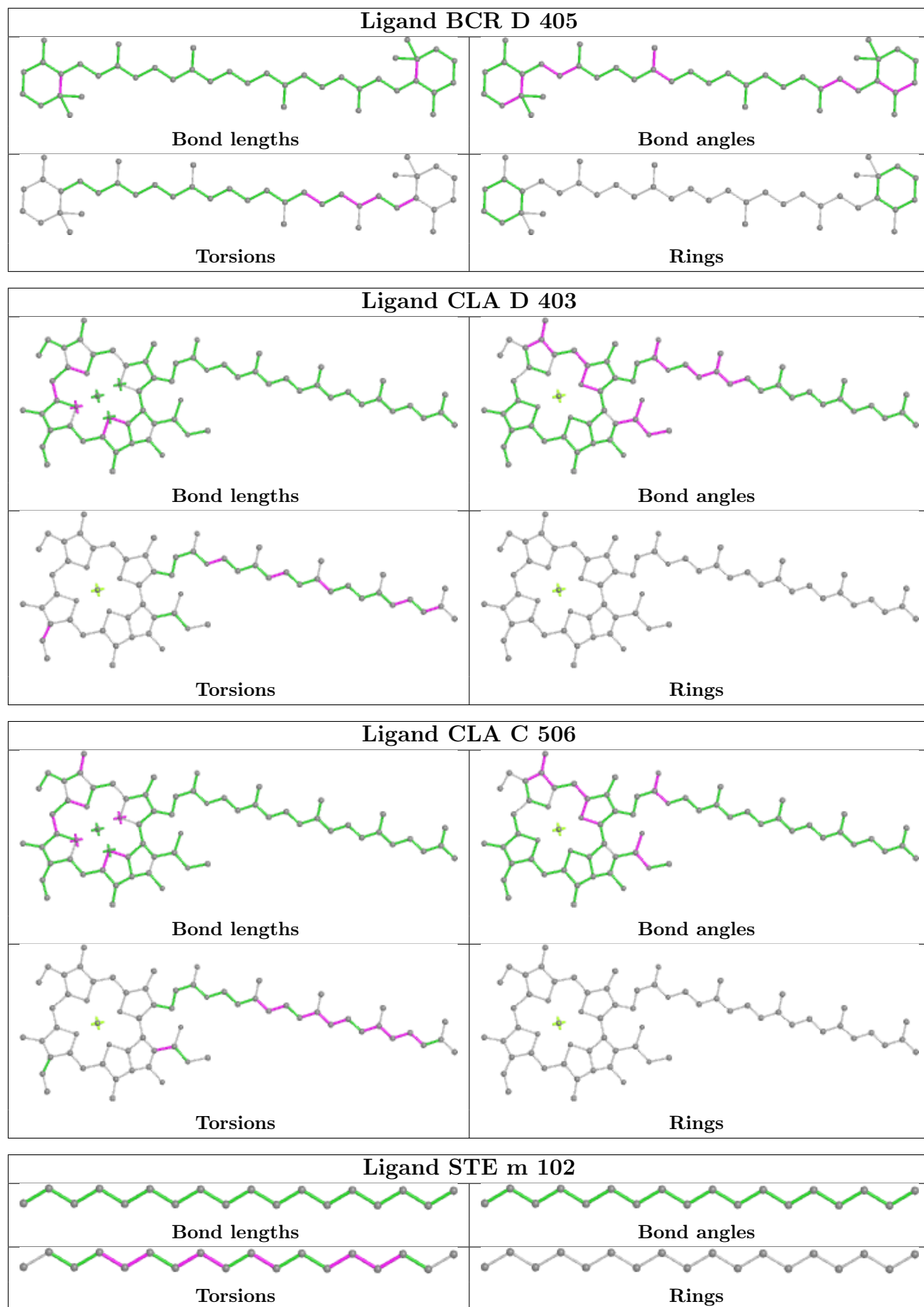


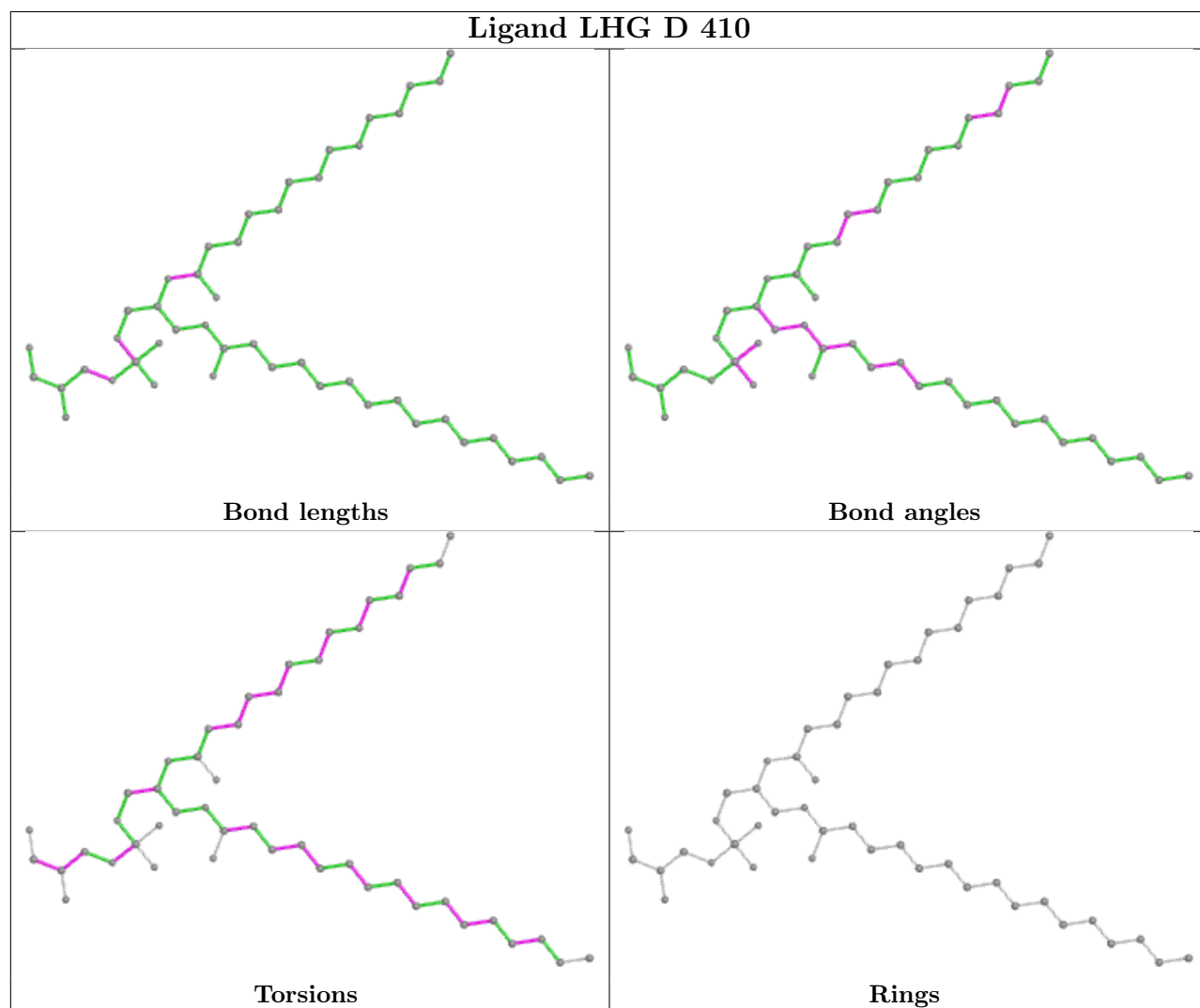
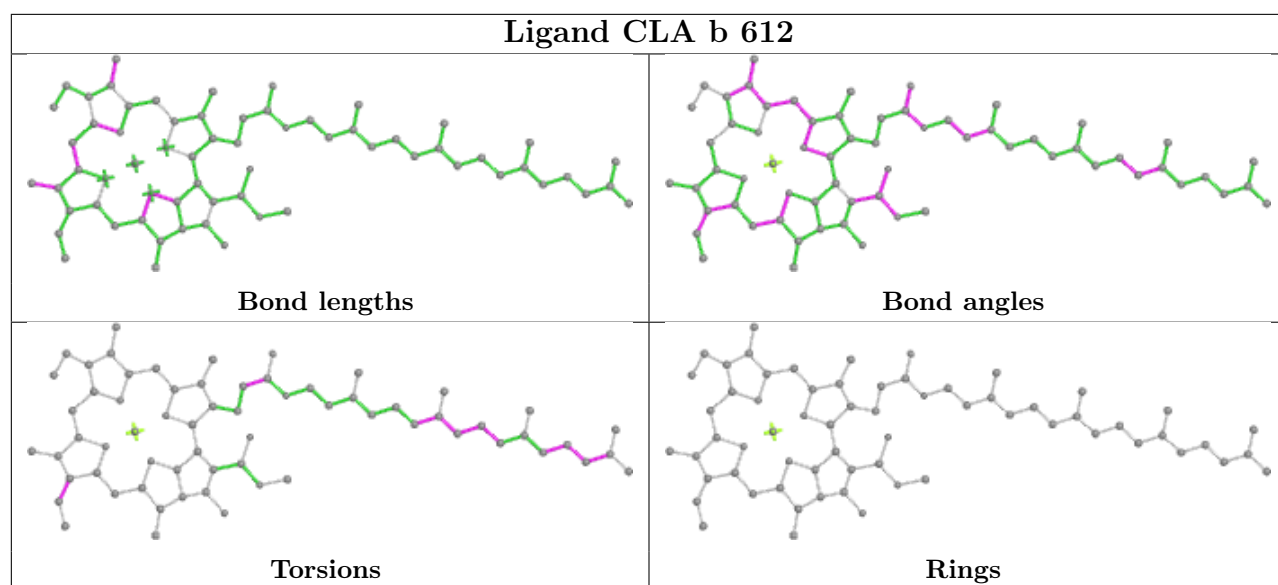




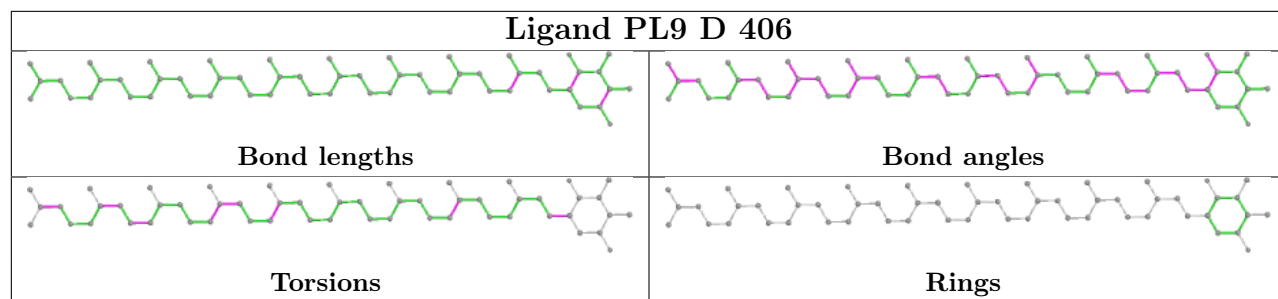












## 5.7 Other polymers [i](#)

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%)	-0.22	3 (0%) 84 83	22, 28, 49, 77	0
1	a	334/344 (97%)	-0.18	3 (0%) 84 83	22, 31, 57, 73	0
2	B	505/510 (99%)	-0.13	17 (3%) 45 45	24, 32, 60, 86	0
2	b	505/510 (99%)	-0.04	16 (3%) 47 47	26, 36, 69, 98	0
3	C	442/461 (95%)	-0.05	6 (1%) 75 74	23, 35, 50, 72	0
3	c	451/461 (97%)	0.03	14 (3%) 49 48	26, 40, 61, 86	0
4	D	341/352 (96%)	-0.14	7 (2%) 63 63	23, 30, 47, 77	0
4	d	341/352 (96%)	-0.09	4 (1%) 79 78	23, 34, 59, 75	0
5	E	82/84 (97%)	0.36	8 (9%) 7 7	33, 51, 68, 82	0
5	e	82/84 (97%)	0.87	12 (14%) 2 2	42, 61, 76, 84	0
6	F	34/45 (75%)	-0.10	3 (8%) 10 9	35, 42, 61, 80	0
6	f	34/45 (75%)	0.11	2 (5%) 22 21	43, 50, 77, 96	0
7	H	65/66 (98%)	0.25	6 (9%) 9 8	32, 41, 53, 68	0
7	h	63/66 (95%)	0.41	7 (11%) 5 5	40, 52, 60, 65	0
8	I	35/38 (92%)	-0.05	1 (2%) 51 51	31, 38, 60, 73	0
8	i	35/38 (92%)	-0.08	1 (2%) 51 51	30, 40, 64, 78	0
9	J	36/40 (90%)	0.40	4 (11%) 5 5	34, 49, 72, 83	0
9	j	36/40 (90%)	0.82	7 (19%) 1 0	39, 55, 88, 88	0
10	K	37/46 (80%)	0.12	1 (2%) 54 54	41, 51, 65, 70	0
10	k	37/46 (80%)	0.19	1 (2%) 54 54	49, 57, 75, 84	0
11	L	37/37 (100%)	-0.03	1 (2%) 54 54	25, 29, 58, 66	0
11	l	36/37 (97%)	-0.10	2 (5%) 24 23	27, 30, 58, 73	0
12	M	32/36 (88%)	0.11	2 (6%) 20 19	26, 33, 56, 69	0
12	m	31/36 (86%)	0.13	0 100 100	29, 33, 52, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	0.19	15 (6%) 21 20	26, 41, 74, 127	0
13	o	244/272 (89%)	0.07	17 (6%) 16 15	26, 40, 73, 103	0
14	T	29/32 (90%)	-0.28	2 (6%) 16 16	26, 31, 52, 67	0
14	t	29/32 (90%)	-0.19	2 (6%) 16 16	26, 32, 65, 78	0
15	U	97/134 (72%)	-0.04	2 (2%) 63 63	33, 42, 69, 83	0
15	u	97/134 (72%)	-0.16	0 100 100	30, 40, 54, 78	0
16	V	137/163 (84%)	-0.27	0 100 100	29, 40, 53, 69	0
16	v	137/163 (84%)	0.06	4 (2%) 51 51	34, 47, 69, 90	0
17	Y	27/46 (58%)	1.81	11 (40%) 0 0	51, 72, 91, 99	0
17	y	30/46 (65%)	0.73	3 (10%) 7 6	64, 74, 87, 93	0
18	X	38/41 (92%)	0.48	4 (10%) 6 5	41, 51, 74, 75	0
18	x	39/41 (95%)	0.74	6 (15%) 2 1	50, 60, 82, 95	0
19	Z	62/62 (100%)	0.79	13 (20%) 1 0	51, 64, 102, 110	0
19	z	62/62 (100%)	1.19	14 (22%) 0 0	62, 74, 108, 118	0
20	R	34/41 (82%)	1.88	15 (44%) 0 0	56, 67, 76, 80	0
20	r	31/41 (75%)	2.37	18 (58%) 0 0	65, 78, 95, 98	0
All	All	5302/5700 (93%)	0.05	254 (4%) 30 30	22, 38, 72, 127	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	j	5	GLY	8.8
19	z	33	TRP	7.0
13	O	59	LYS	6.9
9	j	6	GLY	6.9
20	r	3	TRP	6.7
13	O	56	PRO	6.3
13	o	58	ASN	6.2
19	Z	33	TRP	6.2
13	O	60	ARG	6.1
1	A	13	LEU	6.1
2	b	495	PHE	6.1
19	Z	62	VAL	6.1
2	b	127	ARG	6.0
17	Y	22	LEU	6.0
18	X	2	THR	5.8

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Mol	Chain	Res	Type	RSRZ
18	X	3	ILE	5.8
18	x	38	GLN	5.7
17	Y	25	ILE	5.7
5	e	79	PHE	5.6
13	o	4	THR	5.5
20	r	28	VAL	5.5
2	B	487	SER	5.5
13	o	3	GLN	5.4
19	z	35	ARG	5.3
2	B	494	GLY	5.2
17	Y	40	ALA	5.2
20	r	6	LEU	4.9
13	O	61	GLN	4.9
13	O	3	GLN	4.6
19	z	3	ILE	4.6
20	R	28	VAL	4.5
20	r	29	LYS	4.5
13	o	62	GLU	4.4
9	j	7	ARG	4.4
13	o	63	ALA	4.4
2	B	490	GLN	4.3
2	b	496	TYR	4.2
20	r	2	ASP	4.2
2	b	506	ARG	4.2
20	R	3	TRP	4.1
20	R	6	LEU	4.1
2	b	126	PRO	4.0
2	b	128	THR	4.0
19	z	29	SER	4.0
20	R	31	VAL	4.0
2	B	495	PHE	3.9
8	i	36	ASP	3.9
4	d	14	TRP	3.9
5	E	79	PHE	3.9
13	o	246	ALA	3.8
4	d	227[A]	GLU	3.8
20	r	24	LEU	3.8
13	O	4	THR	3.8
19	Z	7	LEU	3.8
19	Z	41	PHE	3.8
20	R	32	GLN	3.8
6	F	12	SER	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	r	10	LEU	3.7
8	I	36	ASP	3.6
9	J	7	ARG	3.6
4	D	237	PRO	3.6
3	c	24	THR	3.6
13	o	60	ARG	3.5
2	b	494	GLY	3.5
14	T	29	ILE	3.5
17	Y	24	MET	3.5
20	R	26	TYR	3.5
17	Y	21	GLN	3.5
5	E	17	VAL	3.4
6	f	12	SER	3.4
2	B	505	ARG	3.4
20	r	7	VAL	3.4
14	t	30	THR	3.4
4	D	12	ARG	3.4
20	R	34	LEU	3.4
3	C	143	TYR	3.4
2	B	295	GLY	3.4
18	X	39	ARG	3.4
20	R	27	ALA	3.3
19	z	7	LEU	3.3
17	y	19	ILE	3.3
13	o	57	LYS	3.3
9	j	8	ILE	3.3
20	R	21	ARG	3.2
20	r	26	TYR	3.2
3	c	191	PRO	3.2
20	r	4	ARG	3.2
13	o	5	LEU	3.2
19	Z	1	MET	3.2
19	Z	3	ILE	3.2
5	e	61	ARG	3.2
6	F	13	TYR	3.1
2	B	503	THR	3.1
2	b	503	THR	3.1
12	M	33	GLN	3.1
7	H	66	GLY	3.1
3	c	143	TYR	3.1
9	J	8	ILE	3.1
3	c	106	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	l	2	GLU	3.1
17	Y	41	VAL	3.1
3	c	193	GLY	3.1
16	v	16	GLY	3.1
13	o	56	PRO	3.1
3	c	147	PHE	3.1
10	k	17	ILE	3.1
19	z	30	PRO	3.0
3	c	146	PHE	3.0
5	e	13	ILE	3.0
5	e	72	ALA	3.0
13	O	62	GLU	3.0
15	U	8	GLU	3.0
2	B	496	TYR	3.0
7	h	56	ASP	3.0
9	j	9	PRO	2.9
20	r	14	LEU	2.9
5	e	8	ARG	2.9
17	Y	23	THR	2.9
17	y	18	VAL	2.9
17	Y	46	LEU	2.9
20	r	9	LEU	2.9
20	r	25	PRO	2.9
1	A	11	ALA	2.8
19	z	36	SER	2.8
9	j	11	TRP	2.8
9	J	6	GLY	2.8
3	c	262	ARG	2.8
20	r	32	GLN	2.8
2	b	485	GLU	2.8
5	E	84	LYS	2.8
4	d	17	ILE	2.8
19	Z	32	ASP	2.8
13	o	133	VAL	2.7
11	l	3	PRO	2.7
17	y	37	PHE	2.7
19	Z	59	PHE	2.7
13	o	132	ASN	2.7
7	h	21	VAL	2.7
5	E	4	THR	2.7
9	J	5	GLY	2.7
20	R	29	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
16	v	21	LEU	2.7
9	j	30	TYR	2.7
5	e	4	THR	2.7
5	e	42	LEU	2.7
7	H	65	LEU	2.7
13	o	61	GLN	2.7
14	T	30	THR	2.7
13	O	229[A]	GLU	2.6
20	r	8	VAL	2.6
3	C	142	GLU	2.6
14	t	29	ILE	2.6
11	L	1	MET	2.6
20	R	24	LEU	2.6
17	Y	43	ARG	2.6
2	B	502	VAL	2.6
7	h	6	TRP	2.6
5	E	61	ARG	2.6
18	x	23	LEU	2.6
2	B	488	PRO	2.6
3	c	23	ALA	2.6
19	Z	42	LEU	2.6
7	H	25	TRP	2.6
20	r	13	LEU	2.6
20	R	8	VAL	2.5
1	a	11	ALA	2.5
2	b	505	ARG	2.5
3	c	142	GLU	2.5
18	x	40	SER	2.5
16	v	15	GLU	2.5
3	c	261	ARG	2.5
19	Z	35	ARG	2.5
17	Y	37	PHE	2.5
4	D	240	ALA	2.5
2	B	127	ARG	2.4
19	z	1	MET	2.4
2	b	289	GLN	2.4
4	d	12	ARG	2.4
20	R	20	VAL	2.4
16	v	24	LYS	2.4
19	z	32	ASP	2.4
13	O	34	SER	2.4
2	B	486	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	b	374	ASN	2.4
3	C	184	GLY	2.4
2	b	373	LYS	2.4
3	C	181	PHE	2.4
17	Y	45	ASN	2.4
18	x	19	VAL	2.4
2	B	506	ARG	2.4
13	O	134	THR	2.4
19	z	41	PHE	2.3
5	e	15	THR	2.3
18	x	2	THR	2.3
3	C	146	PHE	2.3
6	F	16	PHE	2.3
3	c	30	SER	2.3
5	e	71	GLU	2.3
6	f	13	TYR	2.3
5	E	6	GLY	2.3
2	B	491	VAL	2.3
20	r	5	VAL	2.3
20	R	33	LYS	2.2
20	R	5	VAL	2.2
7	h	20	LYS	2.2
19	z	40	ILE	2.2
12	M	3	VAL	2.2
4	D	238	THR	2.2
5	E	5	THR	2.2
1	A	12	ASN	2.2
13	o	207	ARG	2.2
2	B	499	VAL	2.2
5	E	74	GLN	2.2
19	z	10	ALA	2.2
13	O	184	ARG	2.2
5	e	14	ILE	2.1
7	h	25	TRP	2.1
19	Z	60	PHE	2.1
13	o	35	SER	2.1
13	O	32	ILE	2.1
15	U	67	LEU	2.1
2	B	489	GLU	2.1
3	c	138	GLU	2.1
5	e	77	GLU	2.1
7	H	63	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	h	4	ARG	2.1
1	a	265	PHE	2.1
20	r	27	ALA	2.1
19	Z	37	LYS	2.1
18	X	19	VAL	2.1
7	h	59	ASN	2.1
7	H	6	TRP	2.1
18	x	3	ILE	2.1
19	z	4	LEU	2.1
4	D	227	GLU	2.1
13	O	207	ARG	2.1
2	B	479[A]	PHE	2.1
3	C	147	PHE	2.1
13	o	59	LYS	2.1
1	a	229	GLU	2.0
13	O	181	GLU	2.0
2	b	20	ILE	2.0
19	Z	40	ILE	2.0
13	o	37	THR	2.0
3	c	29	GLU	2.0
4	D	228	GLY	2.0
7	H	18	TYR	2.0
5	e	35	TRP	2.0
10	K	46	ARG	2.0
2	b	161	LEU	2.0
13	O	63	ALA	2.0
2	b	492	GLU	2.0
19	z	62	VAL	2.0
4	D	236	ASN	2.0

## 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
14	FME	t	1	10/11	0.89	0.15	32,34,49,55	0
12	FME	M	1	10/11	0.93	0.13	39,45,59,60	0
14	FME	T	1	10/11	0.94	0.15	28,32,52,66	0
8	FME	I	1	10/11	0.94	0.15	38,43,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	FME	i	1	10/11	0.95	0.12	36,44,49,52	0
12	FME	m	1	10/11	0.96	0.11	34,47,55,64	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
32	STE	a	615	12/20	0.70	0.31	52,57,68,69	0
32	STE	k	104	12/20	0.71	0.23	61,66,72,82	0
32	STE	b	623	16/20	0.72	0.24	48,59,75,76	0
28	LMG	d	410	23/55	0.72	0.28	48,57,66,67	0
28	LMG	D	411	33/55	0.74	0.22	37,53,72,74	0
32	STE	E	102	12/20	0.75	0.20	51,63,72,74	0
32	STE	H	103	18/20	0.77	0.36	48,62,67,71	0
32	STE	B	625	18/20	0.77	0.21	39,52,69,76	0
29	SQD	a	613	36/54	0.78	0.20	41,53,65,70	0
32	STE	c	519	20/20	0.78	0.19	41,49,76,82	0
32	STE	d	412	17/20	0.78	0.24	46,51,67,67	0
30	LHG	A	614	49/49	0.78	0.27	50,74,90,93	0
32	STE	B	624	12/20	0.79	0.18	40,51,59,60	0
32	STE	B	627	16/20	0.80	0.28	42,49,60,61	0
31	DGD	a	614	44/66	0.80	0.18	37,49,60,70	0
28	LMG	b	622	55/55	0.80	0.28	46,59,69,72	0
27	PL9	a	610	55/55	0.80	0.30	42,61,72,74	0
32	STE	b	621	20/20	0.81	0.21	40,48,67,73	0
28	LMG	c	520	48/55	0.81	0.24	45,66,74,78	0
32	STE	b	625	10/20	0.81	0.20	44,53,65,68	0
32	STE	m	102	18/20	0.81	0.21	32,42,61,63	0
32	STE	B	621	17/20	0.82	0.15	36,47,63,65	0
32	STE	D	413	20/20	0.82	0.24	37,45,67,73	0
32	STE	d	413	20/20	0.82	0.25	42,50,63,64	0
25	CLA	b	601	65/65	0.82	0.19	47,66,83,86	0
32	STE	A	617	20/20	0.82	0.24	41,50,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	STE	L	102	12/20	0.83	0.22	50,55,63,64	0
32	STE	C	518	12/20	0.83	0.14	36,44,54,57	0
32	STE	T	102	16/20	0.84	0.20	39,47,55,57	0
32	STE	b	624	15/20	0.84	0.24	45,48,60,69	0
28	LMG	c	521	49/55	0.84	0.19	37,50,74,82	0
32	STE	B	626	12/20	0.84	0.35	47,54,63,63	0
28	LMG	A	612	48/55	0.85	0.19	37,50,62,73	0
28	LMG	B	622	28/55	0.85	0.18	38,45,55,60	0
27	PL9	A	610	55/55	0.85	0.29	35,58,68,70	0
26	BCR	h	101	40/40	0.85	0.16	40,53,63,65	0
29	SQD	b	620	49/54	0.85	0.18	38,50,70,73	0
29	SQD	f	102	41/54	0.85	0.19	55,72,85,88	0
28	LMG	m	101	51/55	0.86	0.15	33,47,59,61	0
28	LMG	c	518	37/55	0.86	0.21	49,62,78,80	0
30	LHG	e	101	42/49	0.86	0.31	58,74,88,99	0
31	DGD	H	102	62/66	0.86	0.17	34,42,51,57	0
26	BCR	d	405	40/40	0.86	0.15	39,49,75,79	0
32	STE	I	101	15/20	0.86	0.17	46,50,59,60	0
32	STE	t	102	14/20	0.86	0.20	37,43,50,53	0
31	DGD	A	616	66/66	0.87	0.17	42,54,64,66	0
29	SQD	A	615	39/54	0.87	0.21	36,51,71,75	0
32	STE	j	101	12/20	0.87	0.16	47,53,58,58	0
32	STE	C	519	12/20	0.87	0.18	46,54,59,62	0
25	CLA	c	513	65/65	0.87	0.21	43,60,78,84	0
28	LMG	B	620	51/55	0.87	0.16	31,46,58,63	0
32	STE	M	101	15/20	0.88	0.17	38,45,56,65	0
32	STE	C	520	16/20	0.88	0.14	39,46,51,52	0
28	LMG	C	517	48/55	0.88	0.19	44,61,67,69	0
25	CLA	B	601	65/65	0.88	0.15	41,53,69,75	0
25	CLA	c	512	65/65	0.88	0.15	47,53,65,72	0
26	BCR	k	102	40/40	0.88	0.15	51,61,68,73	0
25	CLA	B	616	60/65	0.88	0.18	26,34,63,70	0
32	STE	t	103	10/20	0.88	0.23	46,54,55,57	0
25	CLA	b	616	60/65	0.89	0.14	31,39,71,75	0
32	STE	M	102	10/20	0.89	0.28	41,44,53,54	0
26	BCR	D	405	40/40	0.90	0.14	34,42,66,71	0
28	LMG	D	407	51/55	0.90	0.21	32,44,66,69	0
26	BCR	H	101	40/40	0.90	0.11	31,40,52,53	0
32	STE	J	102	12/20	0.90	0.12	48,53,60,61	0
26	BCR	k	103	40/40	0.90	0.18	45,51,62,64	0
25	CLA	C	513	65/65	0.90	0.18	41,52,73,76	0
29	SQD	B	623	54/54	0.90	0.16	39,52,71,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DGD	c	516	62/66	0.91	0.12	36,45,70,78	0
26	BCR	b	619	40/40	0.91	0.13	29,43,57,60	0
25	CLA	a	608	65/65	0.91	0.15	22,30,63,67	0
25	CLA	C	512	65/65	0.91	0.15	35,46,70,72	0
26	BCR	k	101	40/40	0.91	0.16	45,56,63,66	0
31	DGD	C	516	62/66	0.91	0.13	30,43,72,87	0
25	CLA	D	404	65/65	0.91	0.15	27,33,73,82	0
25	CLA	c	508	64/65	0.91	0.14	32,40,73,83	0
28	LMG	d	411	44/55	0.92	0.14	37,47,70,72	0
31	DGD	c	517	62/66	0.92	0.14	32,45,62,72	0
31	DGD	h	102	62/66	0.92	0.15	35,44,54,56	0
25	CLA	C	506	65/65	0.92	0.13	29,37,64,72	0
25	CLA	c	502	65/65	0.92	0.14	31,36,48,52	0
26	BCR	K	101	40/40	0.92	0.15	44,50,59,62	0
29	SQD	D	408	36/54	0.92	0.17	44,60,68,70	0
29	SQD	a	612	54/54	0.92	0.14	38,57,66,72	0
26	BCR	K	102	40/40	0.92	0.12	41,47,59,62	0
26	BCR	K	103	40/40	0.92	0.18	37,47,58,59	0
25	CLA	c	503	65/65	0.92	0.16	34,41,47,52	0
25	CLA	B	615	65/65	0.92	0.14	27,33,50,55	0
25	CLA	B	606	65/65	0.92	0.12	25,33,54,60	0
25	CLA	b	614	65/65	0.92	0.15	28,35,59,64	0
25	CLA	d	404	65/65	0.92	0.14	28,38,73,79	0
26	BCR	B	619	40/40	0.92	0.12	28,37,51,56	0
26	BCR	C	514	40/40	0.92	0.14	26,35,47,48	0
25	CLA	b	604	65/65	0.93	0.15	22,30,56,61	0
25	CLA	b	606	65/65	0.93	0.11	26,37,56,69	0
30	LHG	d	407	49/49	0.93	0.14	34,43,59,64	0
25	CLA	C	507	65/65	0.93	0.16	26,34,46,52	0
26	BCR	B	618	40/40	0.93	0.11	24,37,45,45	0
31	DGD	C	515	62/66	0.93	0.13	23,33,60,66	0
26	BCR	b	618	40/40	0.93	0.09	26,35,44,49	0
25	CLA	c	504	60/65	0.93	0.14	31,40,63,68	0
31	DGD	J	101	62/66	0.93	0.13	28,39,66,75	0
25	CLA	b	615	65/65	0.93	0.13	29,37,49,52	0
25	CLA	c	510	65/65	0.93	0.13	33,42,51,55	0
25	CLA	B	607	65/65	0.94	0.12	20,27,51,56	0
25	CLA	C	503	65/65	0.94	0.12	29,36,42,53	0
25	CLA	C	505	65/65	0.94	0.16	26,34,53,59	0
25	CLA	a	606	65/65	0.94	0.12	25,35,74,77	0
26	BCR	T	101	40/40	0.94	0.12	29,36,47,50	0
26	BCR	a	609	40/40	0.94	0.10	22,30,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	SQD	A	613	52/54	0.94	0.17	34,50,68,75	0
26	BCR	b	617	40/40	0.94	0.12	28,40,45,48	0
25	CLA	c	505	65/65	0.94	0.13	27,36,50,52	0
25	CLA	c	506	65/65	0.94	0.12	35,42,67,73	0
26	BCR	c	514	40/40	0.94	0.13	31,44,51,55	0
25	CLA	c	507	65/65	0.94	0.12	32,39,48,51	0
25	CLA	B	614	65/65	0.94	0.15	23,34,58,63	0
25	CLA	c	509	65/65	0.94	0.15	33,43,54,58	0
25	CLA	B	604	65/65	0.94	0.13	21,27,59,65	0
25	CLA	c	511	65/65	0.94	0.12	42,52,60,67	0
30	LHG	d	409	39/49	0.94	0.12	35,40,54,55	0
26	BCR	t	101	40/40	0.94	0.10	29,35,45,49	0
30	LHG	l	101	49/49	0.94	0.13	33,40,48,54	0
25	CLA	b	602	65/65	0.94	0.15	29,38,49,55	0
27	PL9	D	406	55/55	0.94	0.12	20,29,37,39	0
25	CLA	C	508	65/65	0.94	0.12	25,35,67,76	0
25	CLA	C	509	65/65	0.94	0.15	27,35,52,54	0
26	BCR	A	609	40/40	0.94	0.10	22,31,36,37	0
26	BCR	B	617	40/40	0.94	0.12	28,37,45,46	0
31	DGD	c	515	62/66	0.94	0.13	24,37,60,72	0
25	CLA	b	609	65/65	0.94	0.13	34,42,56,64	0
25	CLA	b	613	65/65	0.94	0.14	23,30,58,67	0
25	CLA	C	510	65/65	0.94	0.11	28,37,47,57	0
25	CLA	C	511	65/65	0.94	0.13	34,45,57,63	0
27	PL9	d	406	55/55	0.95	0.13	25,32,39,40	0
30	LHG	D	412	49/49	0.95	0.13	28,38,53,55	0
25	CLA	C	501	65/65	0.95	0.11	24,32,43,44	0
30	LHG	d	408	49/49	0.95	0.12	27,37,44,50	0
25	CLA	D	403	65/65	0.95	0.11	19,25,41,56	0
25	CLA	c	501	65/65	0.95	0.13	29,36,47,53	0
25	CLA	C	502	65/65	0.95	0.11	25,33,46,55	0
25	CLA	B	605	65/65	0.95	0.14	20,28,40,44	0
25	CLA	A	611	65/65	0.95	0.11	17,25,34,37	0
25	CLA	A	607	65/65	0.95	0.12	22,29,77,81	0
25	CLA	B	609	65/65	0.95	0.11	23,34,52,58	0
25	CLA	b	603	65/65	0.95	0.13	21,31,53,59	0
25	CLA	B	610	65/65	0.95	0.14	22,28,37,39	0
25	CLA	b	605	65/65	0.95	0.13	23,31,39,43	0
25	CLA	B	611	65/65	0.95	0.12	23,28,38,44	0
25	CLA	b	607	65/65	0.95	0.12	22,30,52,58	0
25	CLA	b	608	65/65	0.95	0.12	29,39,54,57	0
25	CLA	B	602	65/65	0.95	0.12	23,32,51,55	0

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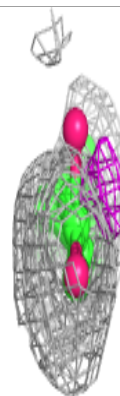
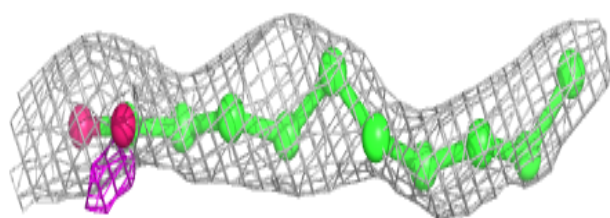
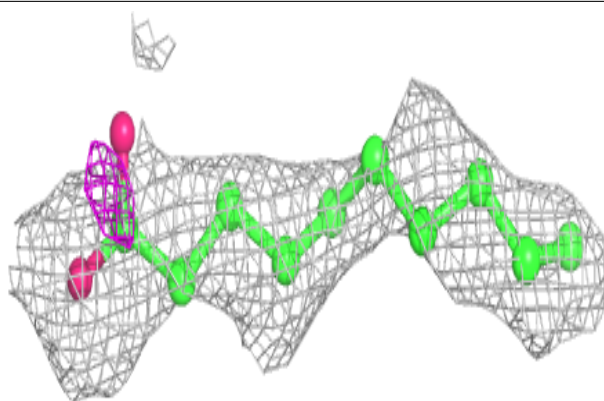
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	CLA	d	403	65/65	0.95	0.11	22,28,48,53	0
25	CLA	b	610	65/65	0.95	0.13	29,35,43,46	0
25	CLA	b	611	65/65	0.95	0.12	24,30,42,49	0
25	CLA	b	612	65/65	0.95	0.16	24,32,40,46	0
25	CLA	B	603	65/65	0.95	0.14	20,27,49,55	0
25	CLA	A	608	54/65	0.95	0.12	19,26,50,54	0
33	PHO	a	607	64/64	0.95	0.12	21,28,34,37	0
24	BCT	d	401	4/4	0.96	0.18	33,34,43,43	0
25	CLA	a	605	65/65	0.96	0.10	22,28,36,43	0
25	CLA	C	504	59/65	0.96	0.11	28,37,67,70	0
25	CLA	A	606	65/65	0.96	0.10	19,26,36,44	0
30	LHG	D	409	49/49	0.96	0.12	24,35,44,49	0
30	LHG	D	410	47/49	0.96	0.13	28,39,59,63	0
25	CLA	a	611	65/65	0.96	0.11	19,28,39,46	0
30	LHG	L	101	49/49	0.96	0.12	28,36,43,55	0
25	CLA	B	608	65/65	0.96	0.11	25,31,49,59	0
25	CLA	B	612	65/65	0.96	0.14	21,27,38,41	0
33	PHO	D	401	64/64	0.96	0.12	19,26,33,38	0
33	PHO	D	402	64/64	0.96	0.09	24,31,35,37	0
25	CLA	B	613	65/65	0.96	0.11	20,26,54,58	0
33	PHO	d	402	64/64	0.96	0.11	28,37,43,45	0
34	HEM	E	101	43/43	0.96	0.12	38,45,55,63	0
34	HEM	f	101	43/43	0.96	0.12	47,56,67,76	0
35	HEC	V	201	43/43	0.97	0.12	24,30,38,43	0
35	HEC	v	201	43/43	0.97	0.12	29,35,42,46	0
21	OEY	A	601[B]	11/11	0.98	0.11	23,28,31,31	11
21	OEY	A	601[A]	11/11	0.98	0.11	29,32,36,36	11
22	FE2	a	602	1/1	0.99	0.07	32,32,32,32	0
23	CL	A	603	1/1	0.99	0.03	27,27,27,27	0
23	CL	a	603	1/1	0.99	0.04	31,31,31,31	0
23	CL	a	604	1/1	0.99	0.06	32,32,32,32	0
24	BCT	A	605	4/4	0.99	0.18	28,32,34,34	0
21	OEY	a	601[A]	11/11	0.99	0.11	28,31,33,35	11
21	OEY	a	601[B]	11/11	0.99	0.11	24,29,29,31	11
22	FE2	A	602	1/1	1.00	0.06	29,29,29,29	0
23	CL	A	604	1/1	1.00	0.06	29,29,29,29	0

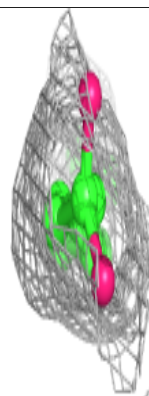
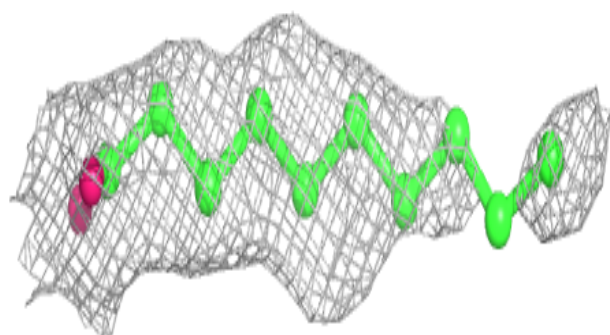
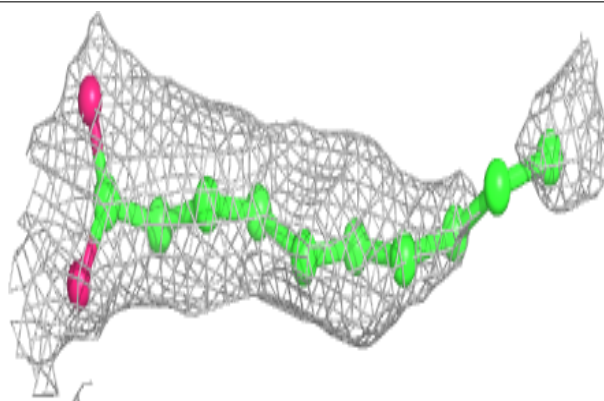
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around STE 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)

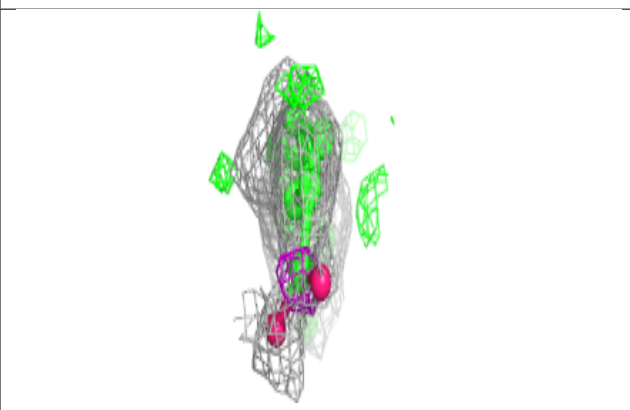
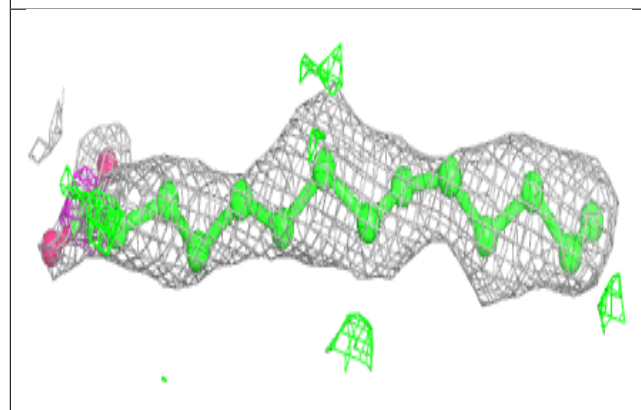
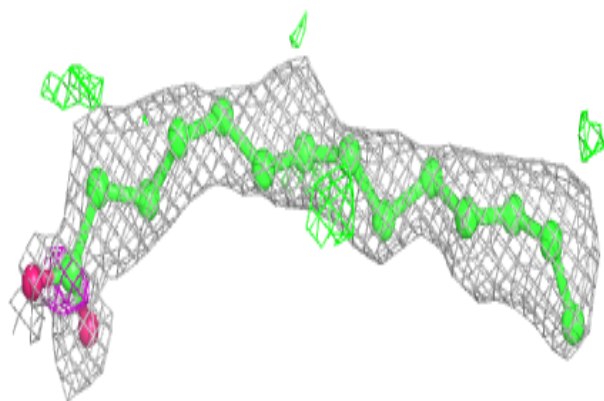
**Electron density around STE k 104:**

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

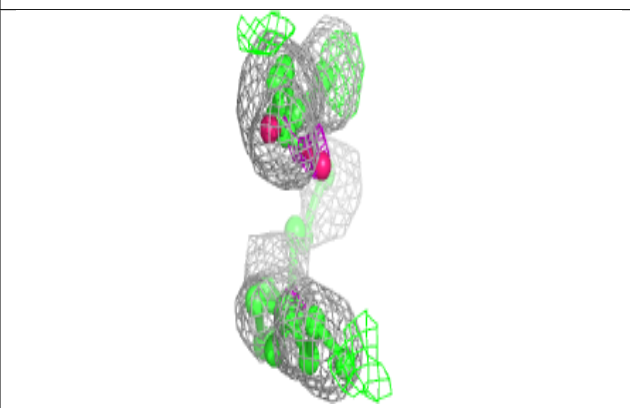
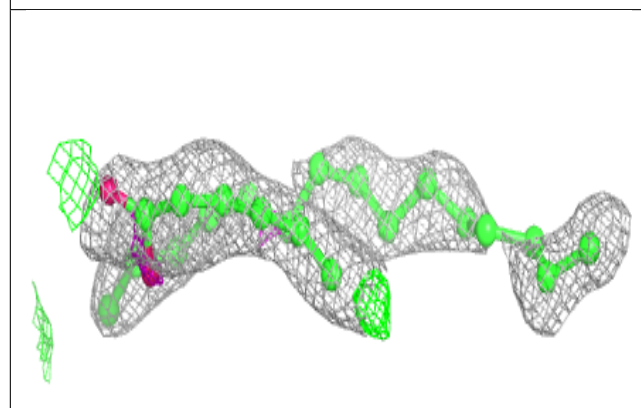
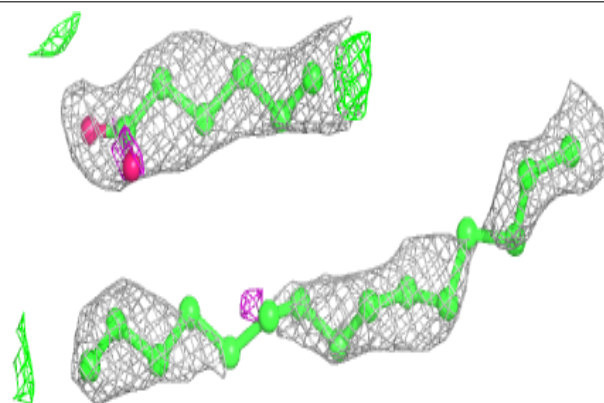


**Electron density around STE b 623:**

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

**Electron density around LMG d 410:**

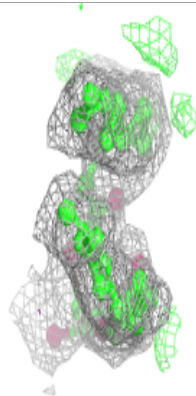
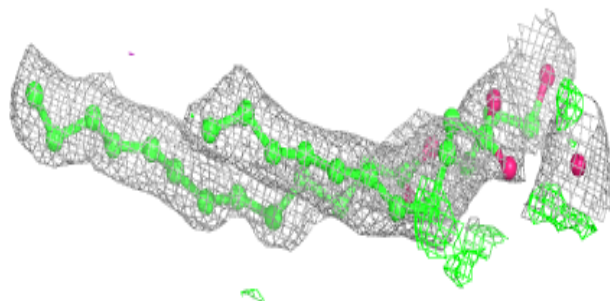
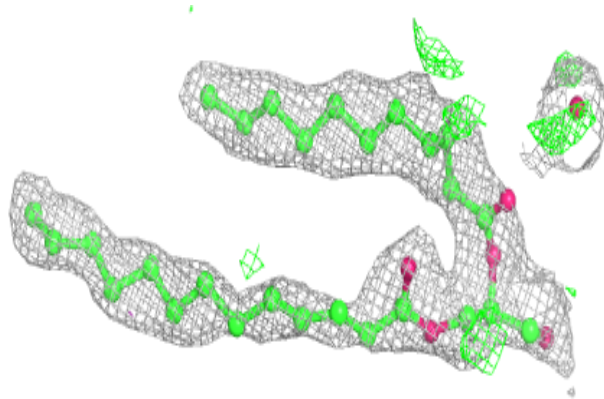
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



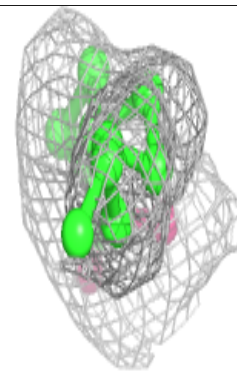
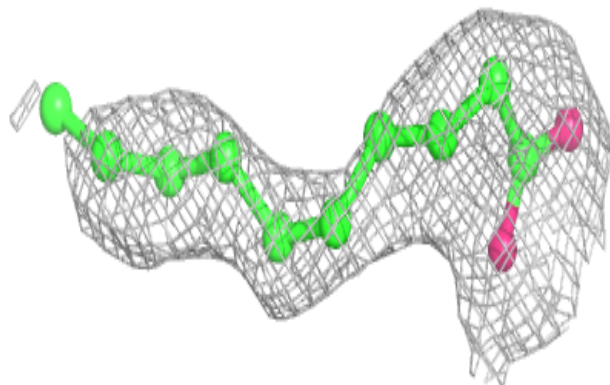
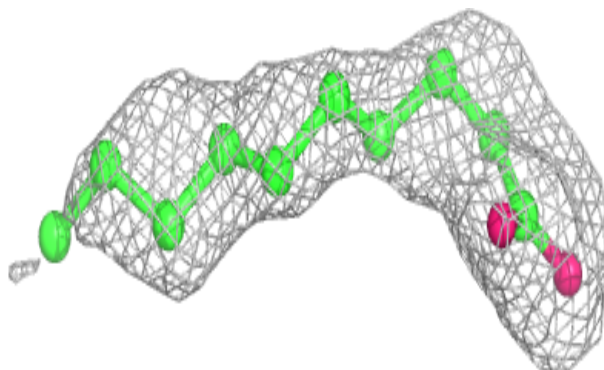


**Electron density around LMG D 411:**

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

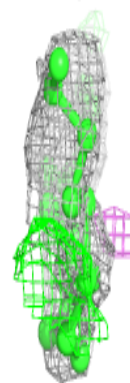
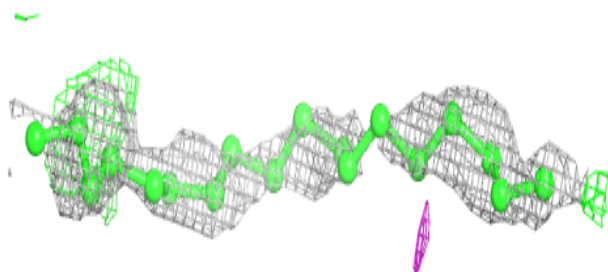
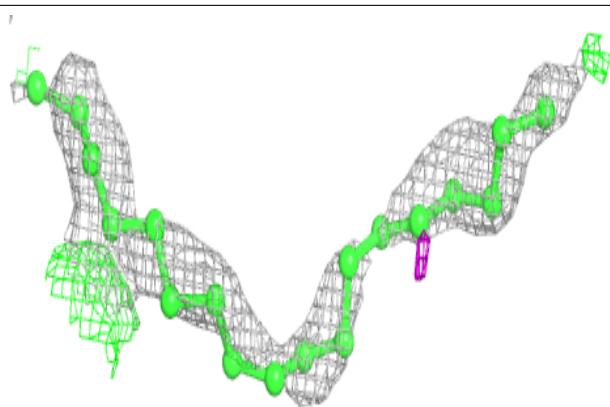
**Electron density around STE E 102:**

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

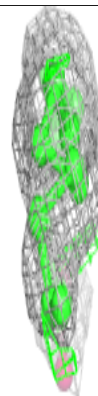
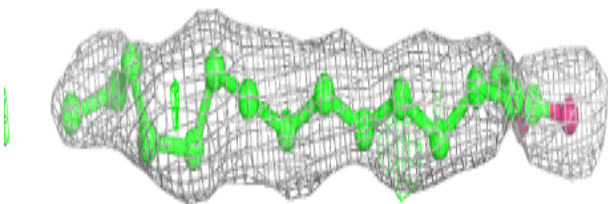
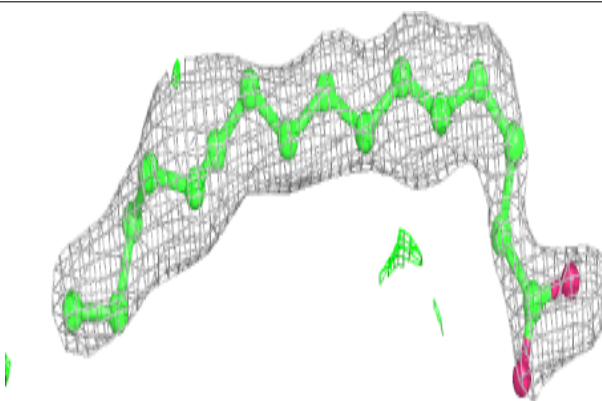


**Electron density around STE H 103:**

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

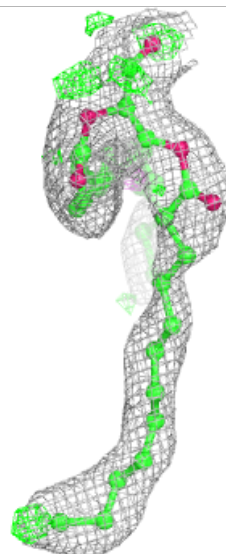
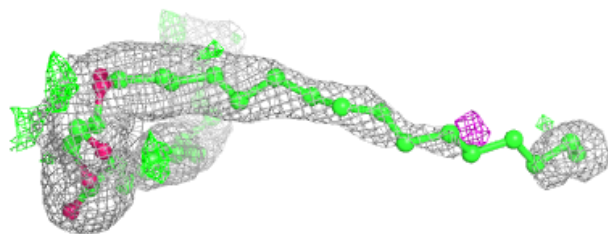
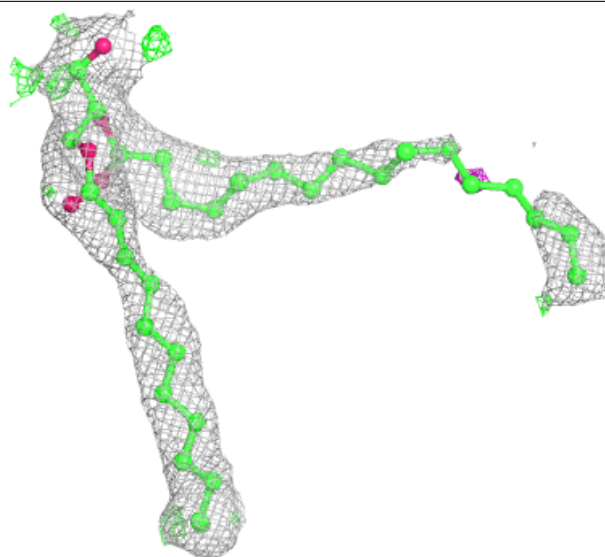
**Electron density around STE B 625:**

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



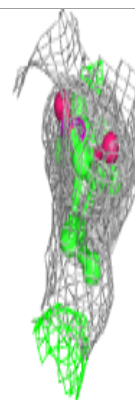
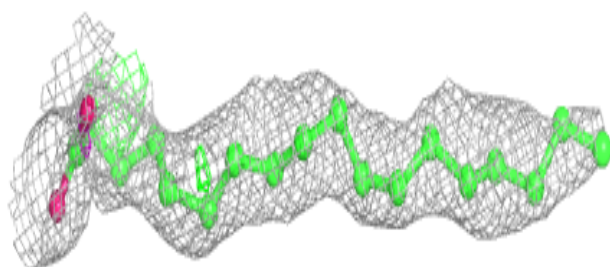
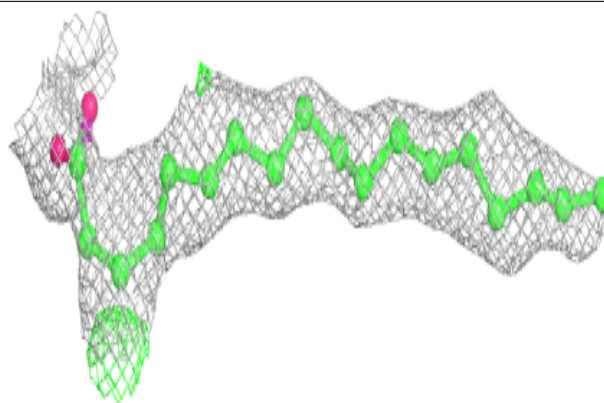
**Electron density around SQD a 613:**

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

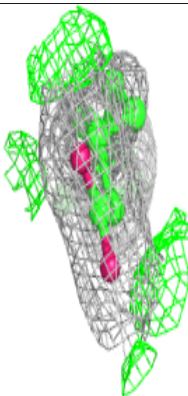
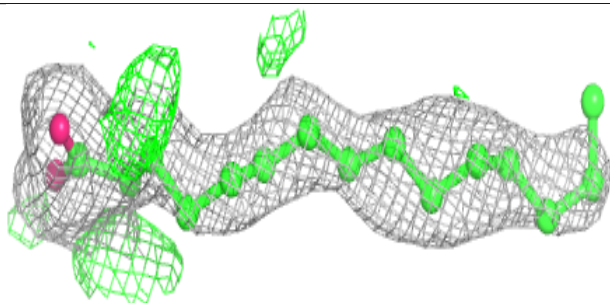
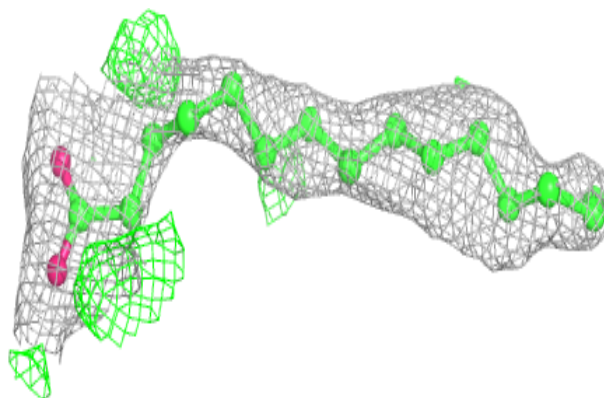


**Electron density around STE c 519:**

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

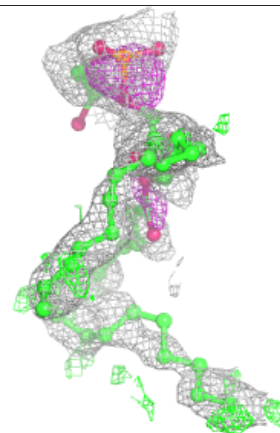
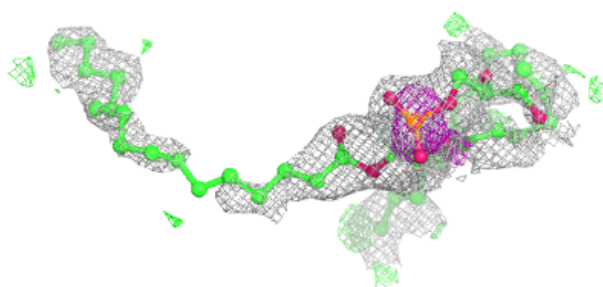
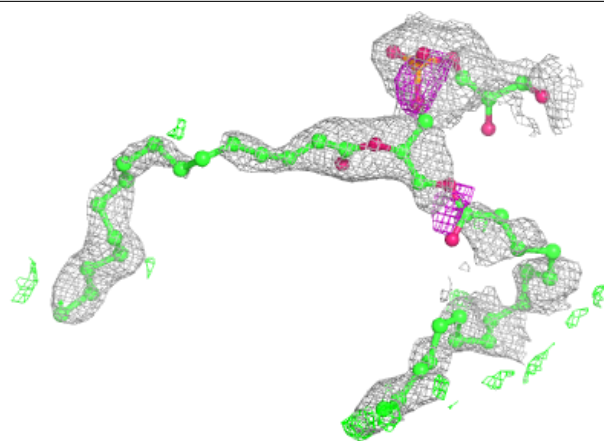
**Electron density around STE d 412:**

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

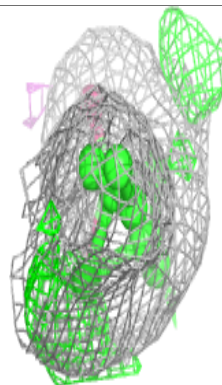
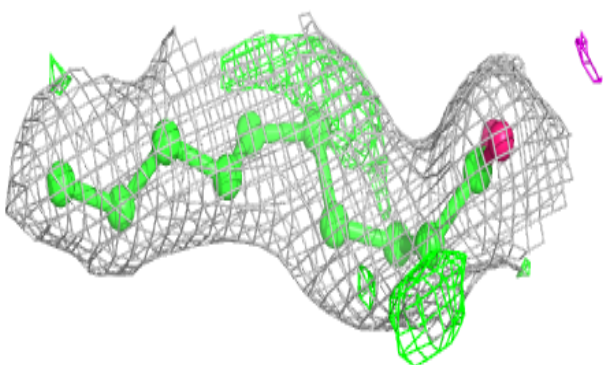
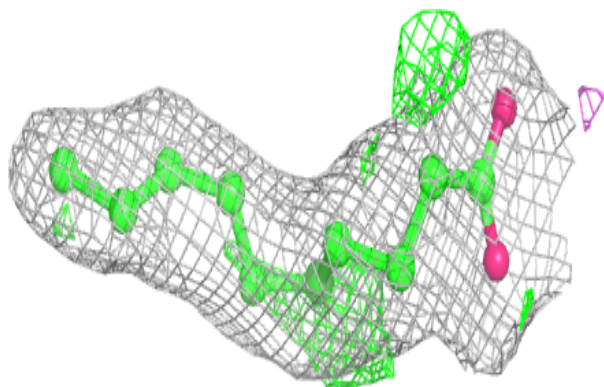


**Electron density around LHG A 614:**

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

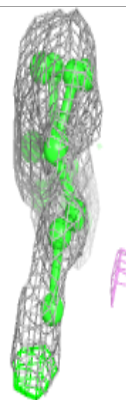
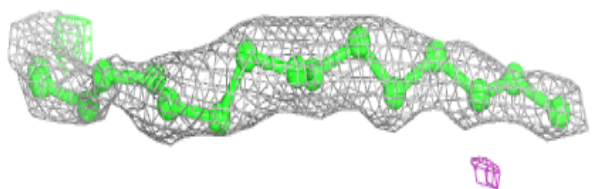
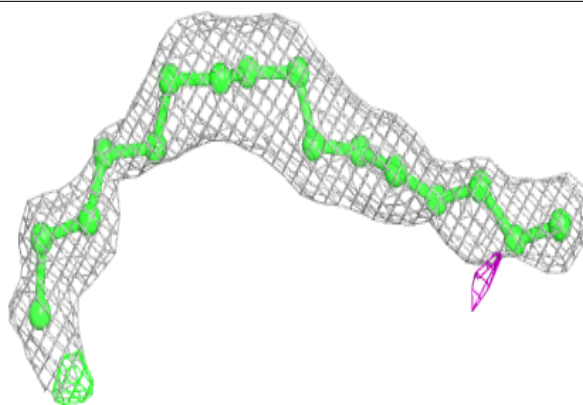
**Electron density around STE B 624:**

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

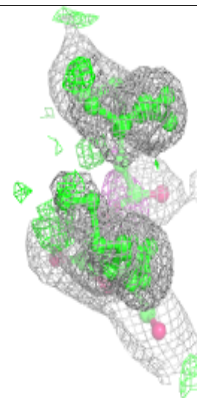
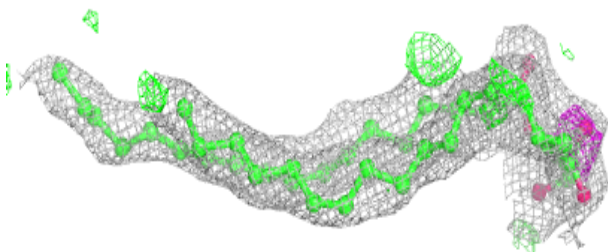
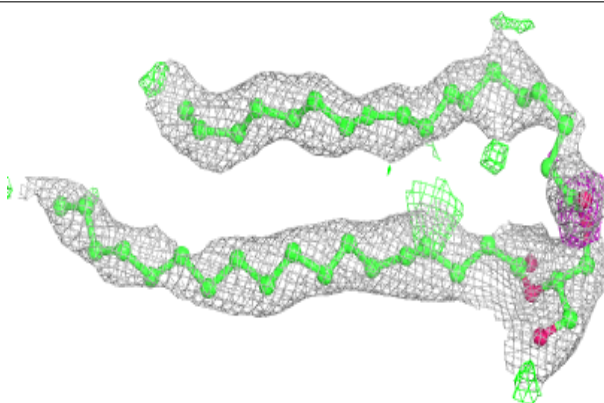


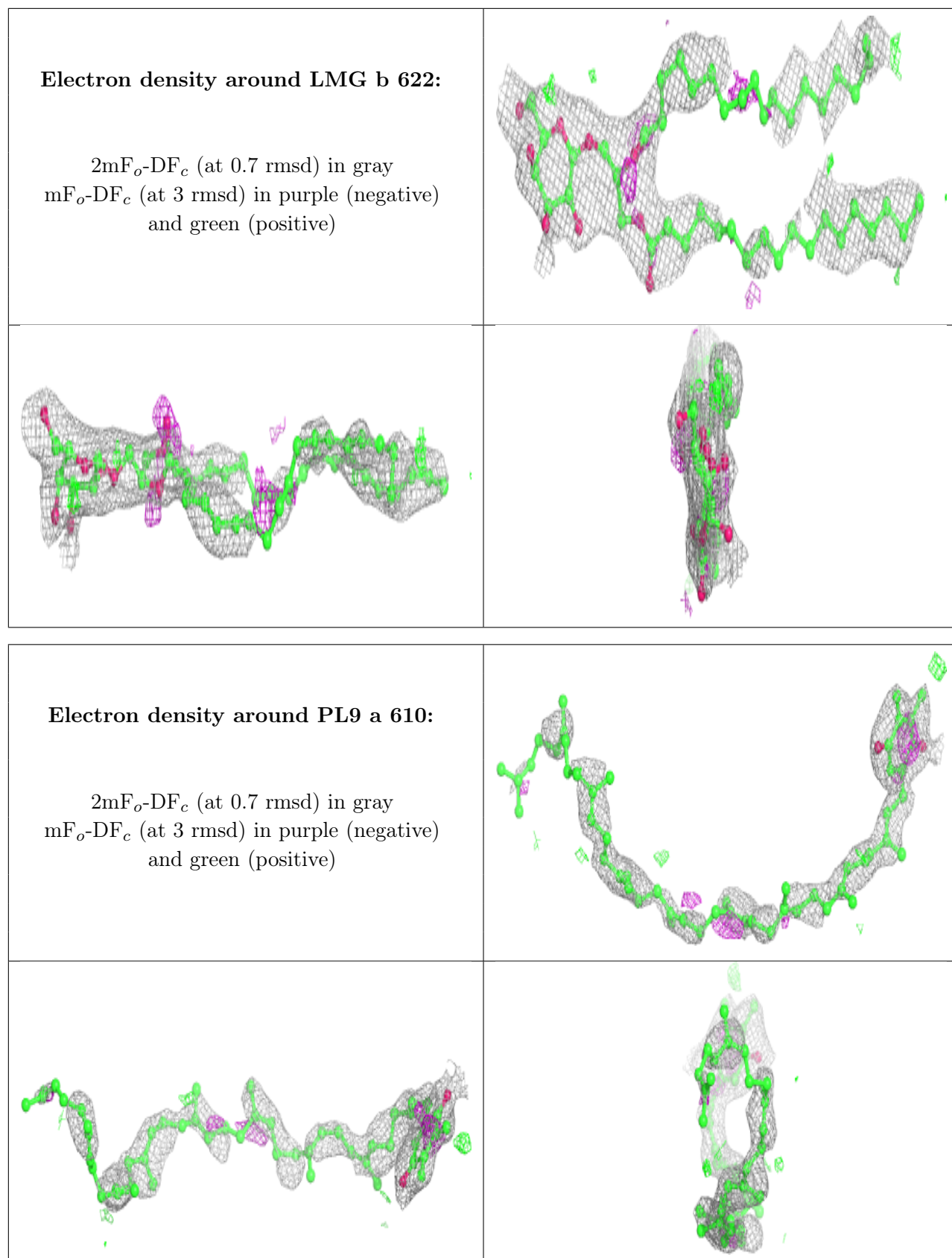
**Electron density around STE B 627:**

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

**Electron density around DGD a 614:**

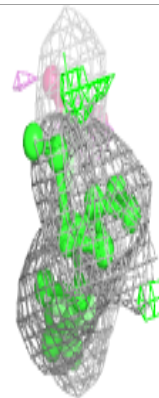
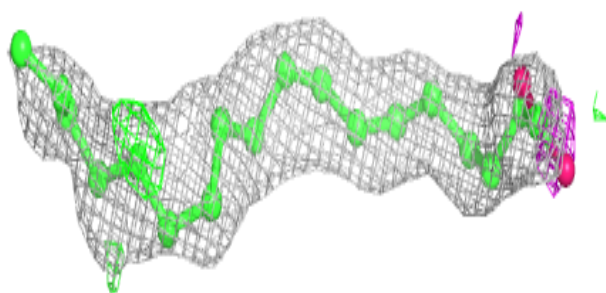
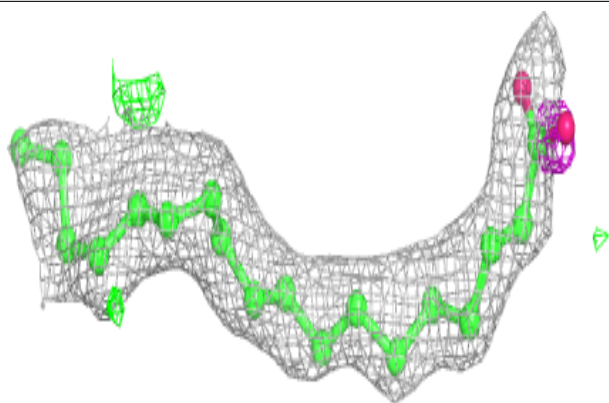
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



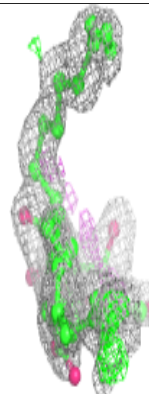
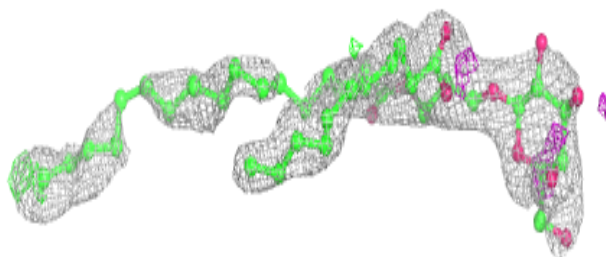
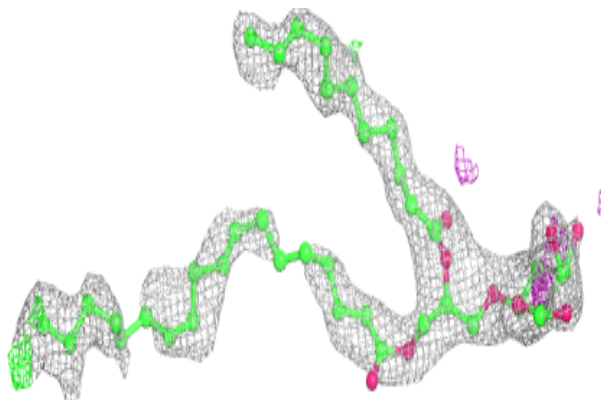


**Electron density around STE b 621:**

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

**Electron density around LMG c 520:**

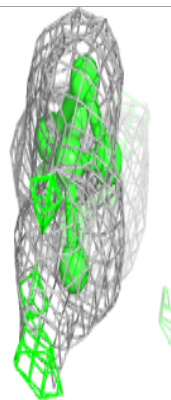
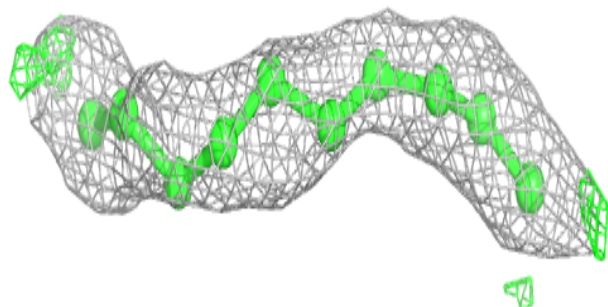
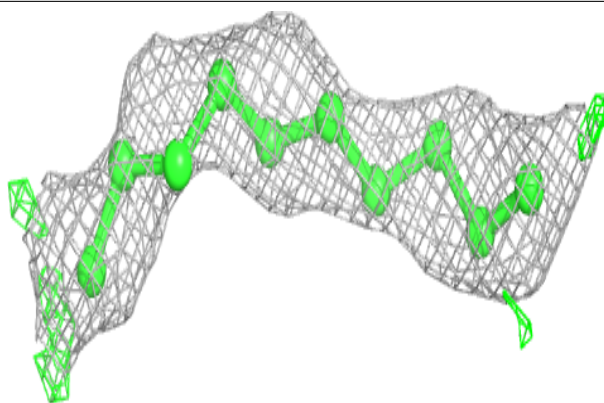
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



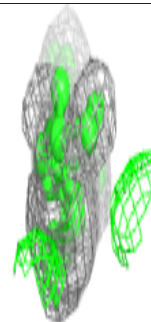
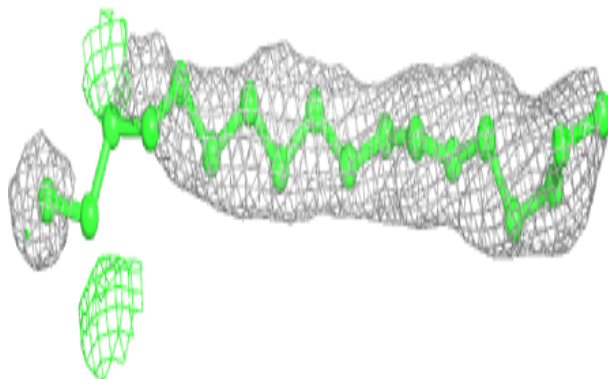
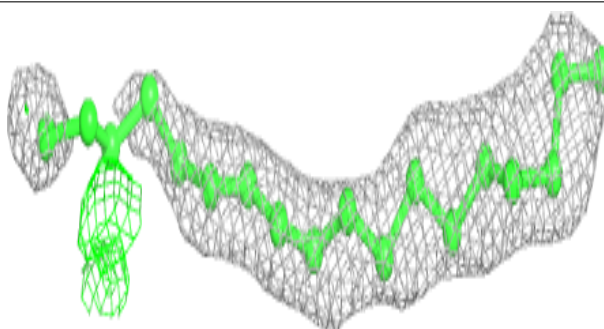


**Electron density around STE b 625:**

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

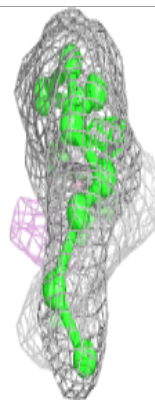
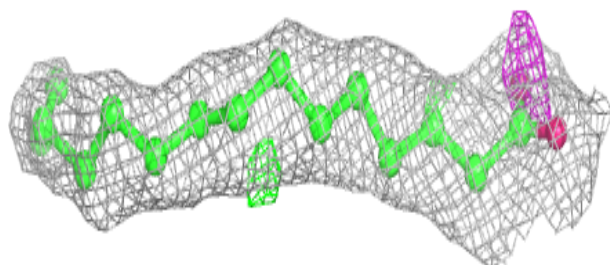
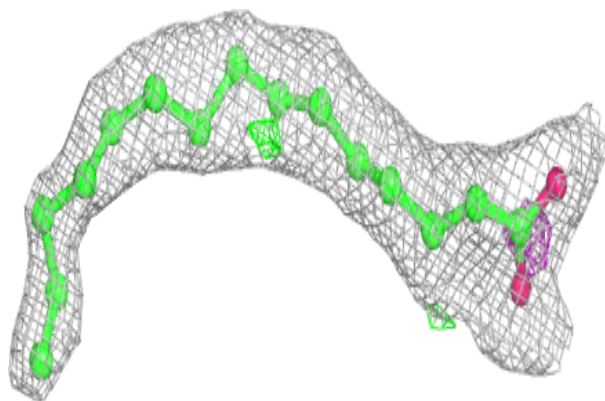
**Electron density around STE m 102:**

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

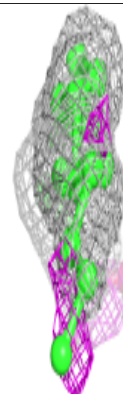
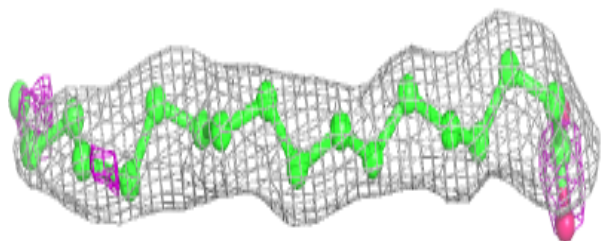
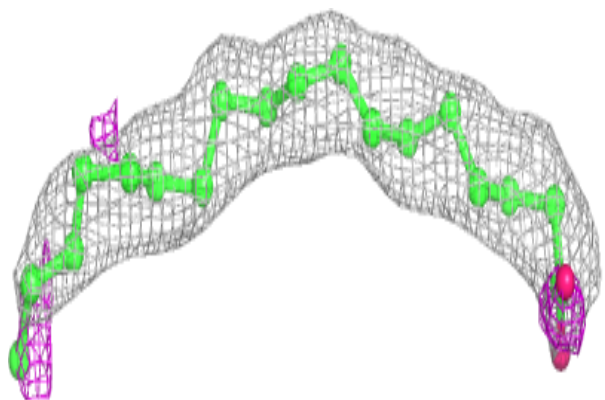


**Electron density around STE B 621:**

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

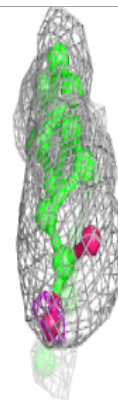
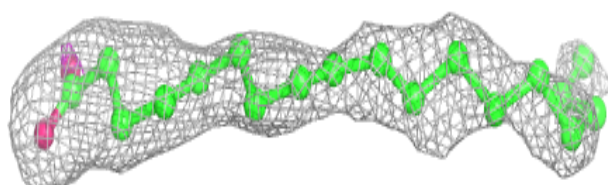
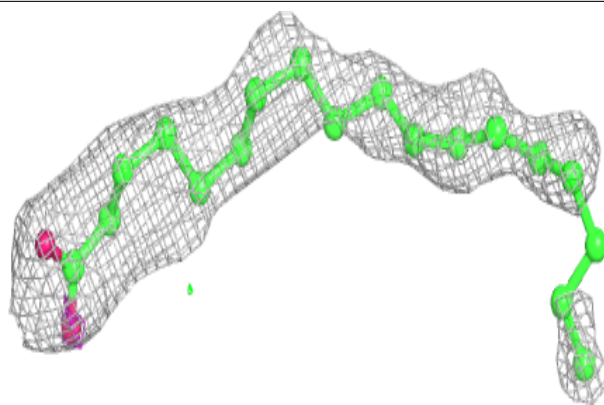
**Electron density around STE D 413:**

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

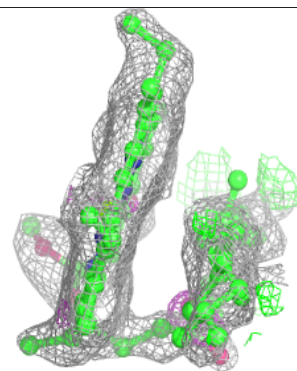
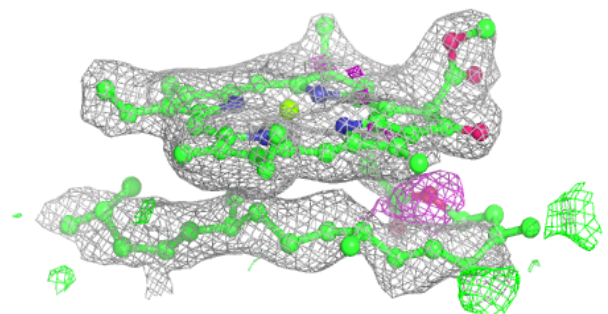
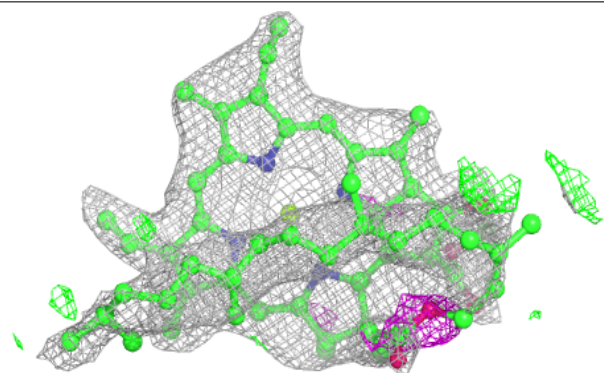


**Electron density around STE d 413:**

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

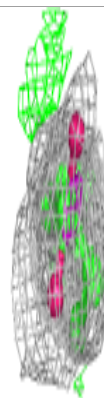
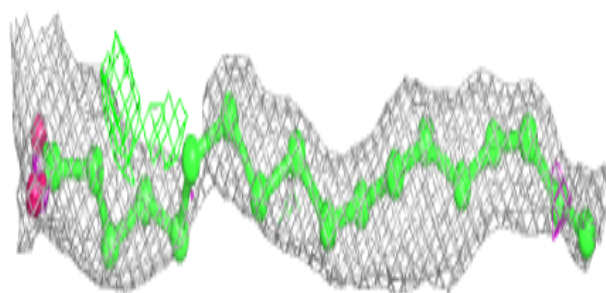
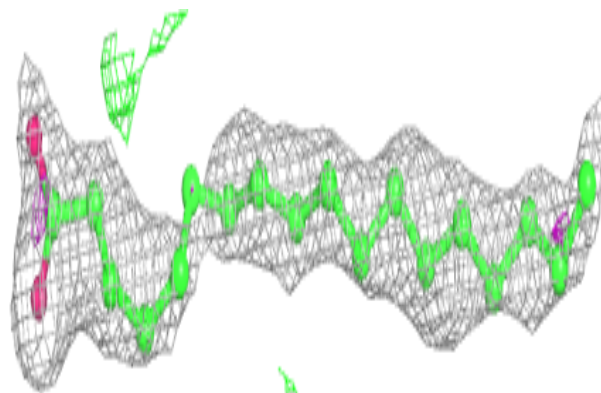
**Electron density around CLA b 601:**

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

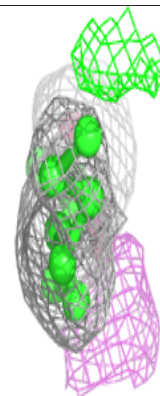
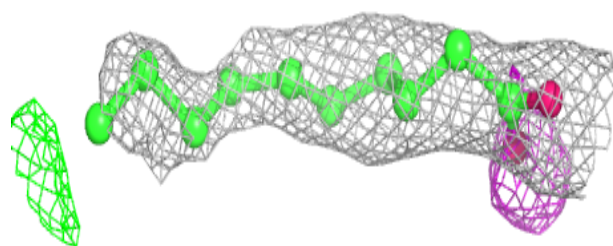
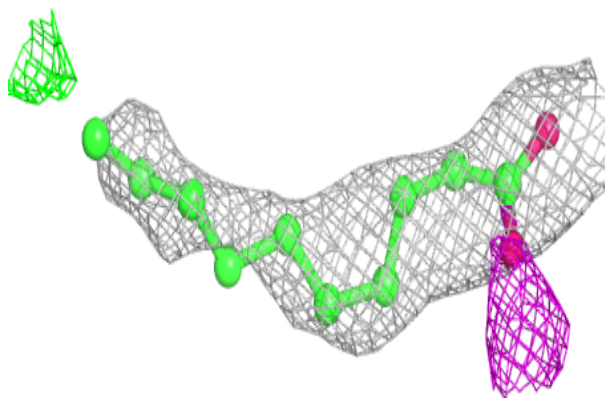


**Electron density around STE A 617:**

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

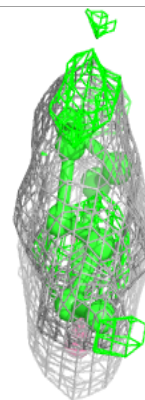
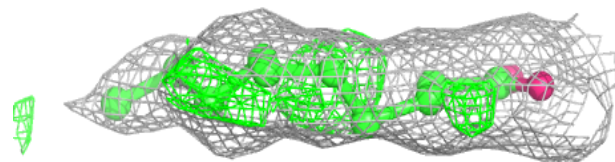
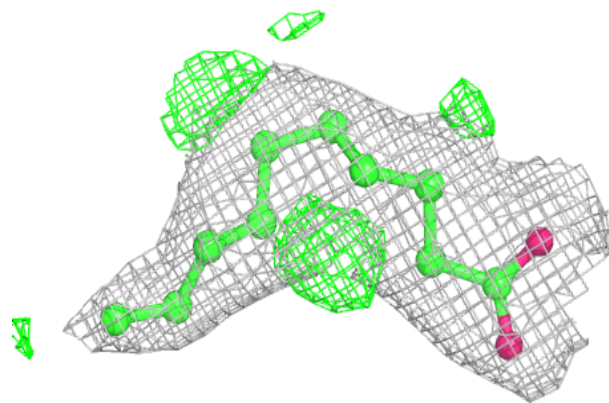
**Electron density around STE L 102:**

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

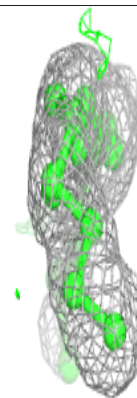
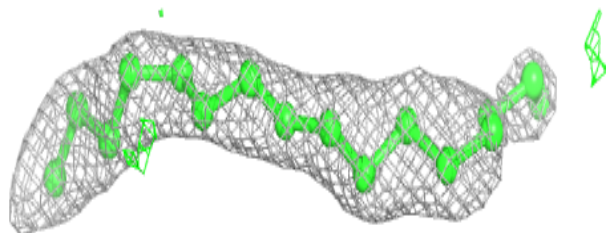
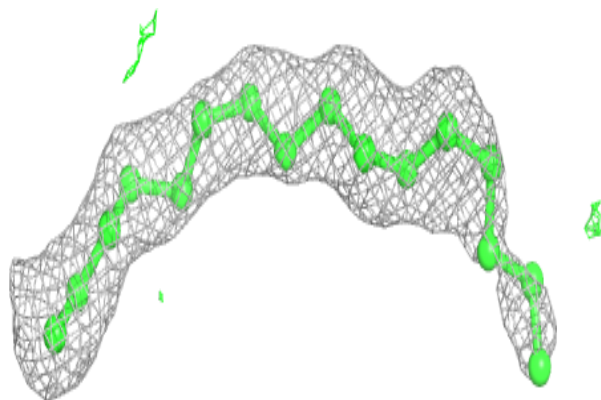


**Electron density around STE C 518:**

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

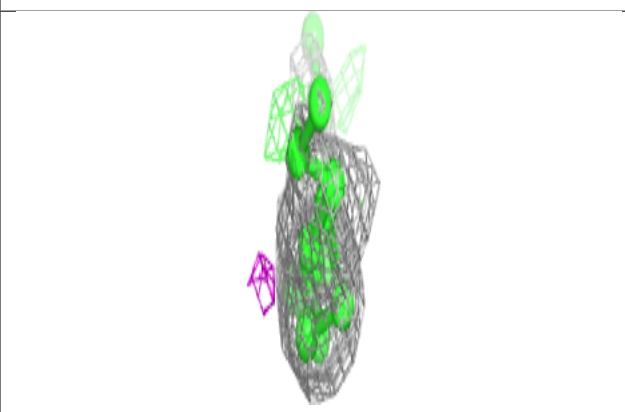
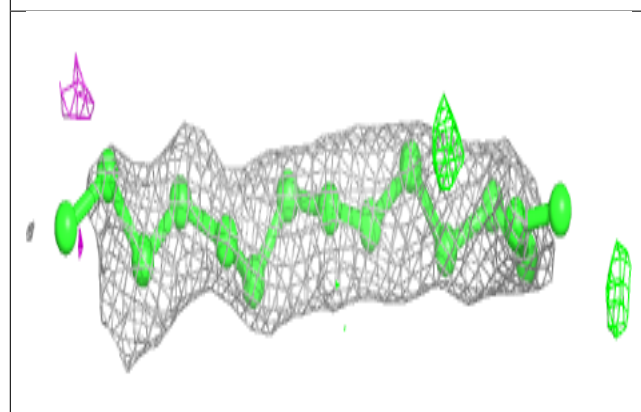
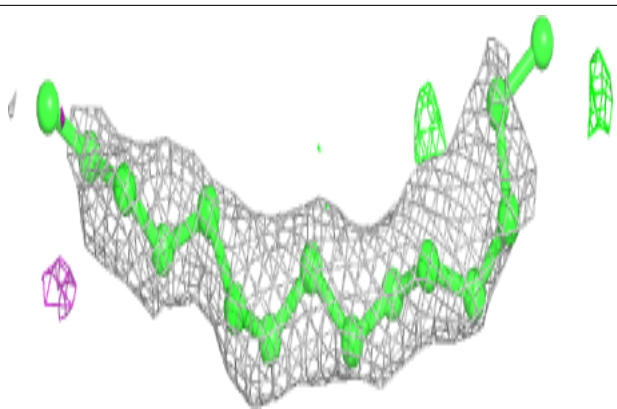
**Electron density around STE T 102:**

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

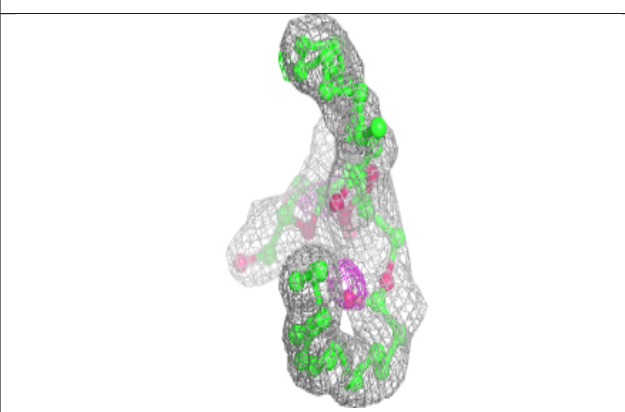
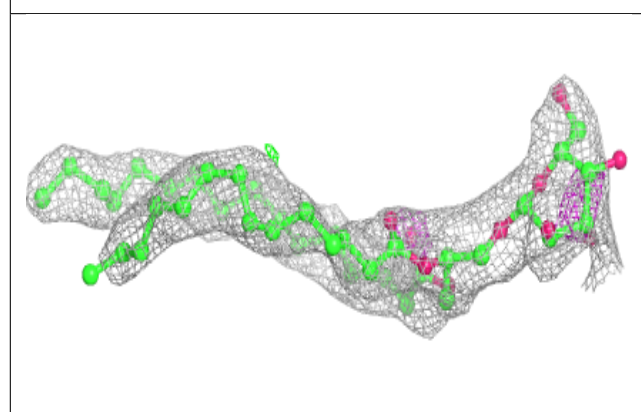
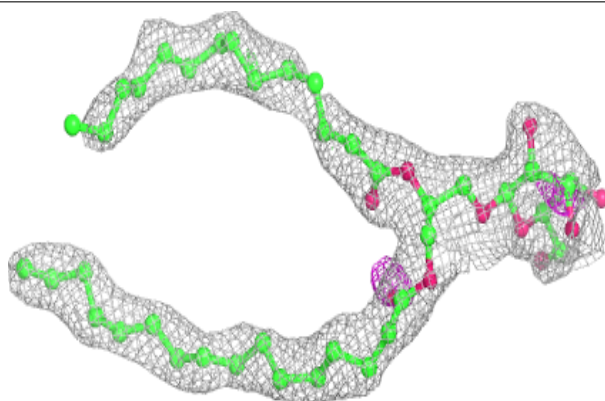


**Electron density around STE b 624:**

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

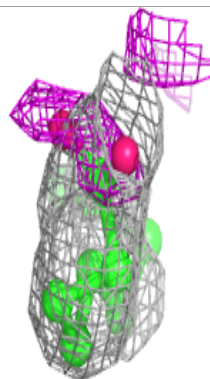
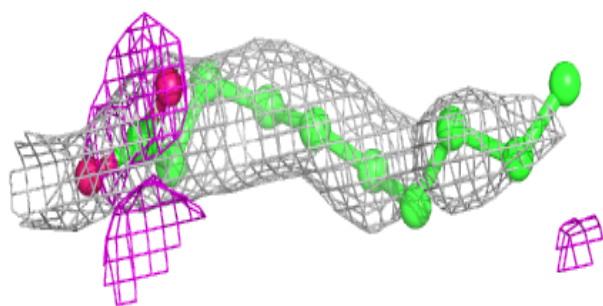
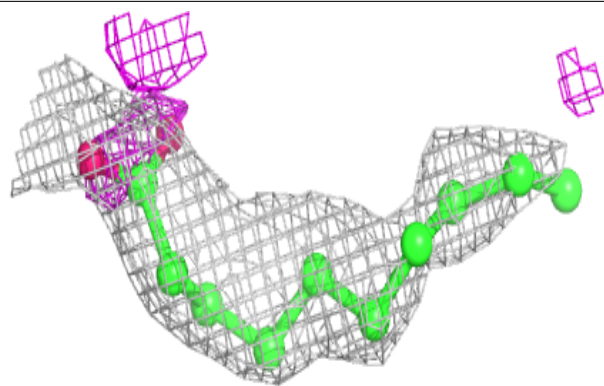
**Electron density around LMG c 521:**

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

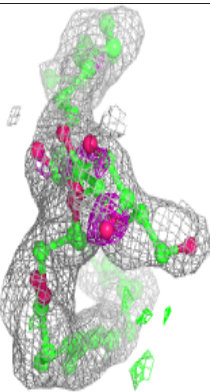
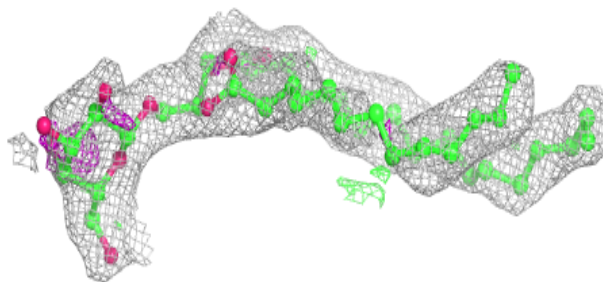
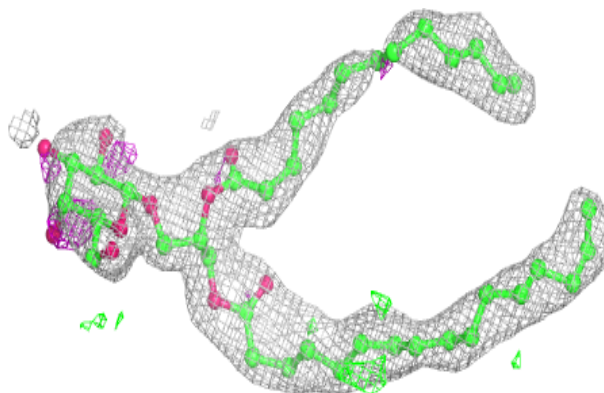


**Electron density around STE B 626:**

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

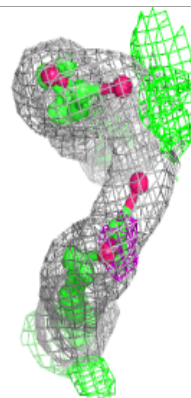
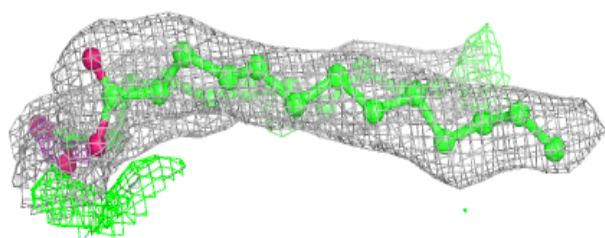
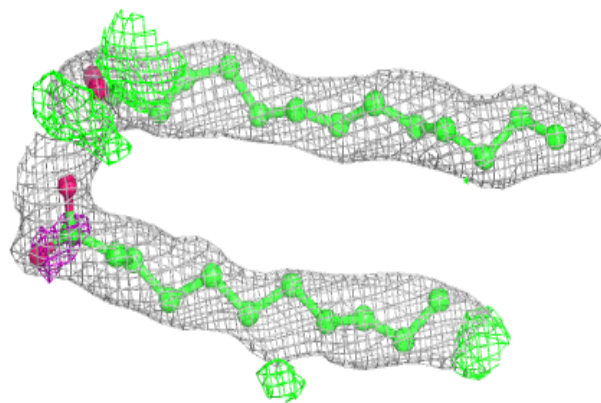
**Electron density around LMG A 612:**

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

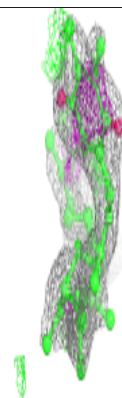
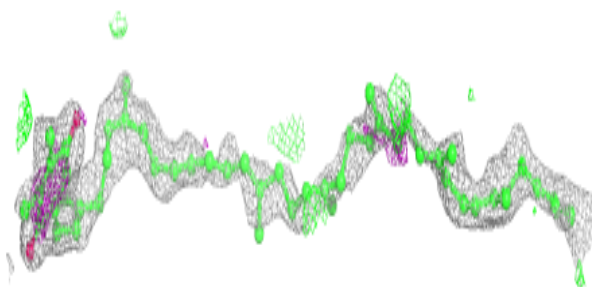
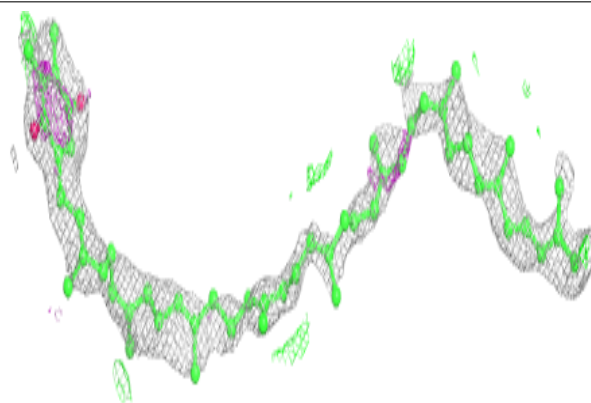


**Electron density around LMG B 622:**

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

**Electron density around PL9 A 610:**

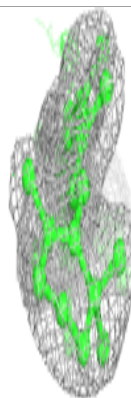
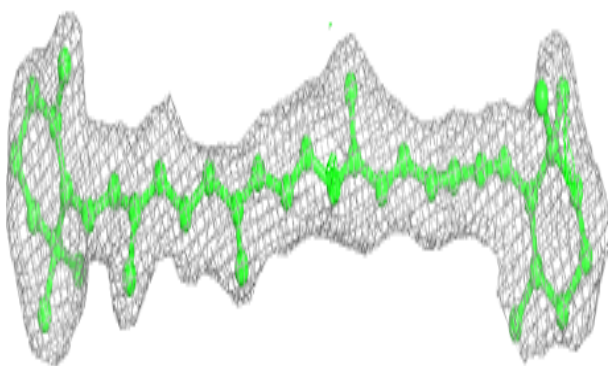
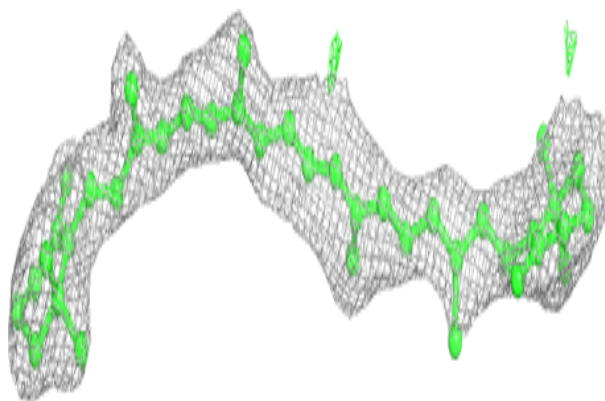
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



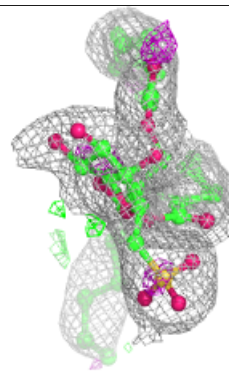
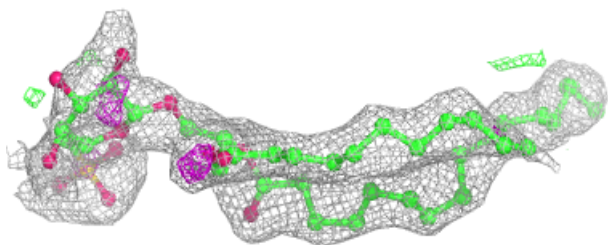
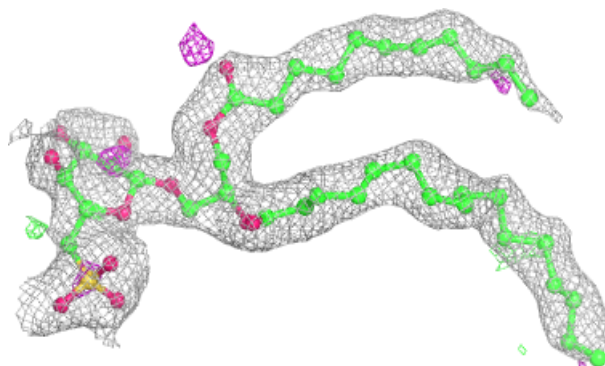


**Electron density around BCR h 101:**

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

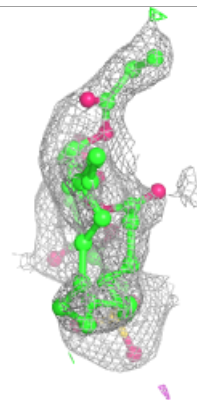
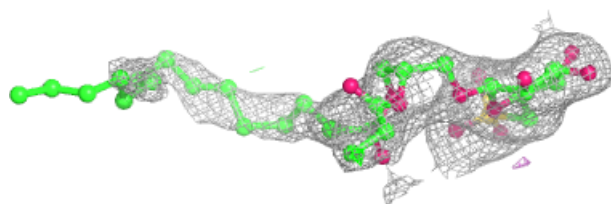
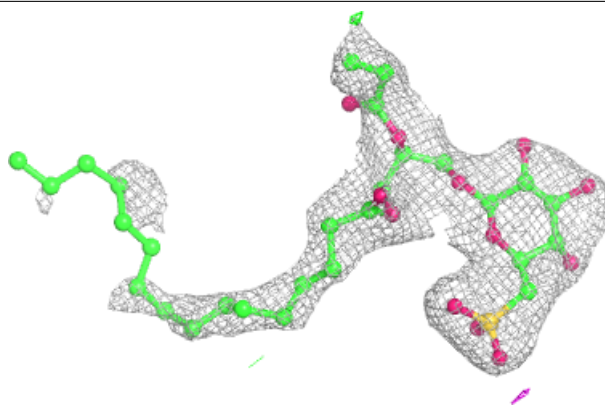
**Electron density around SQD b 620:**

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

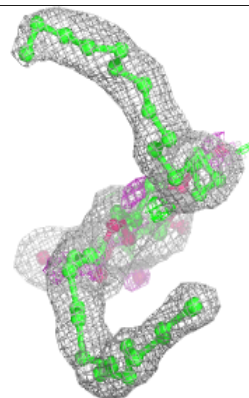
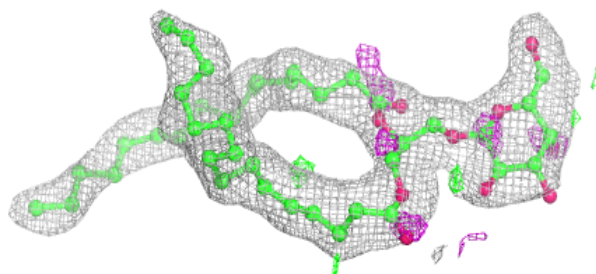
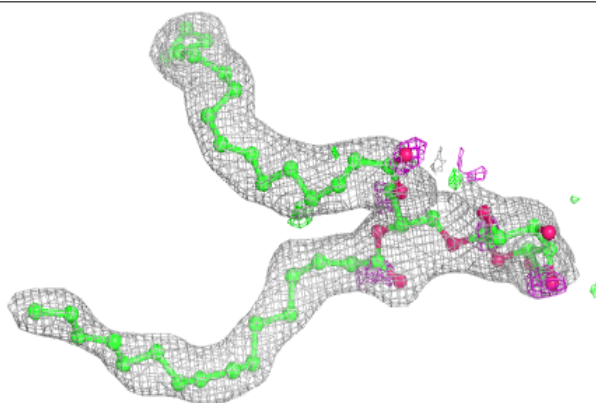


**Electron density around SQD f 102:**

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

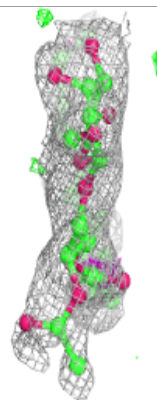
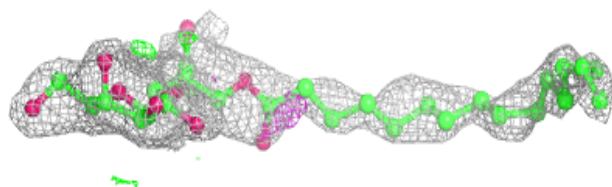
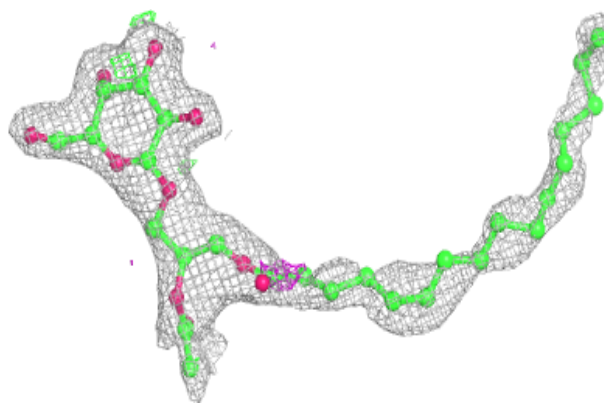
**Electron density around LMG m 101:**

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

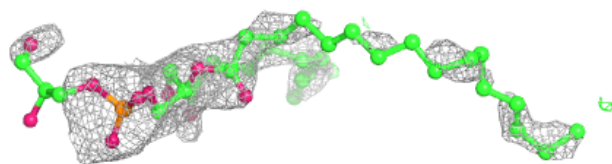
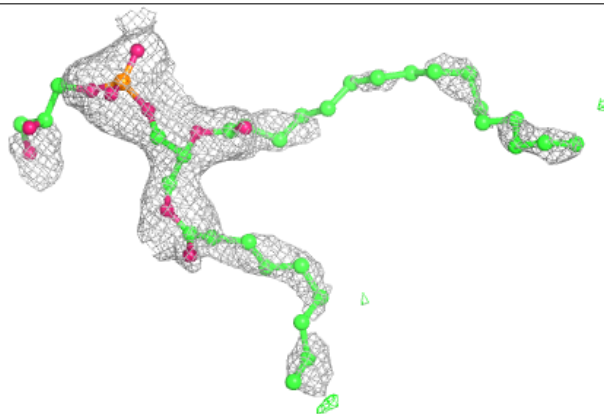


**Electron density around LMG c 518:**

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

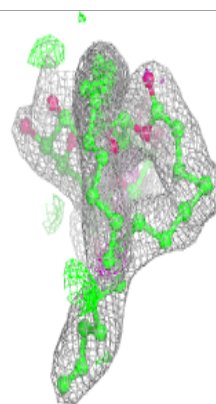
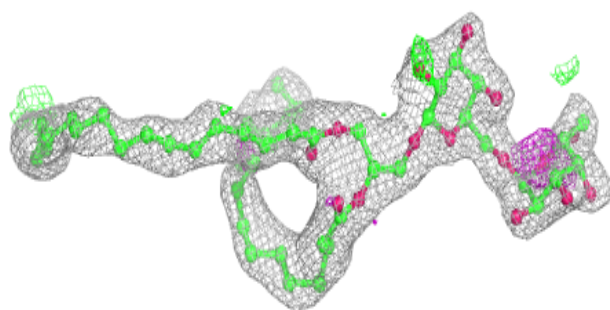
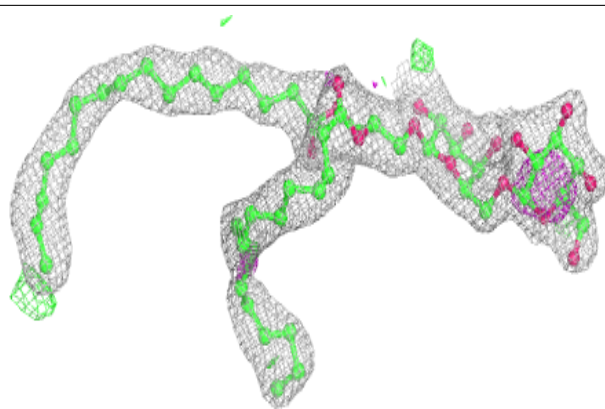
**Electron density around LHG e 101:**

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

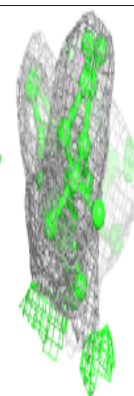
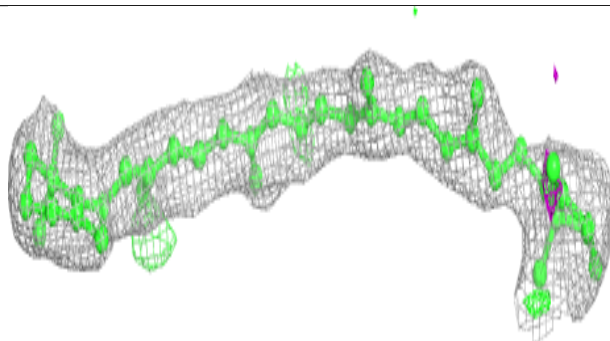
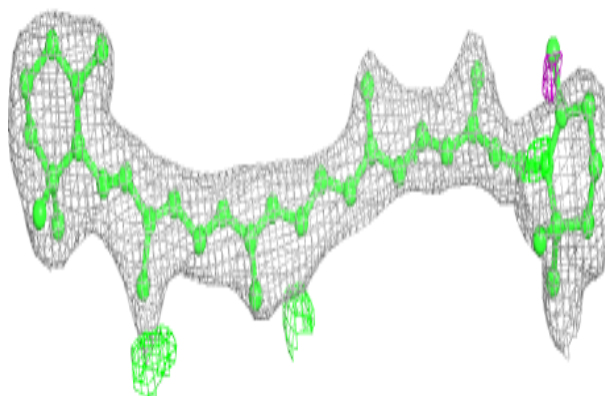


**Electron density around DGD H 102:**

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

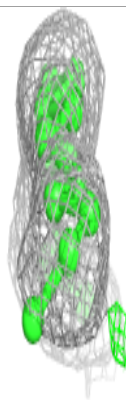
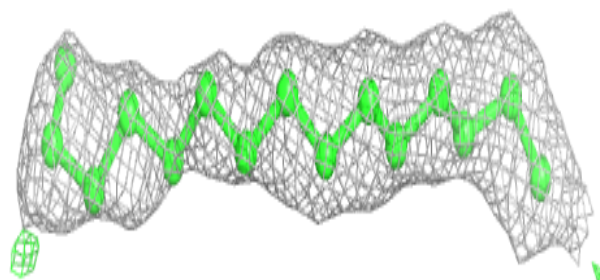
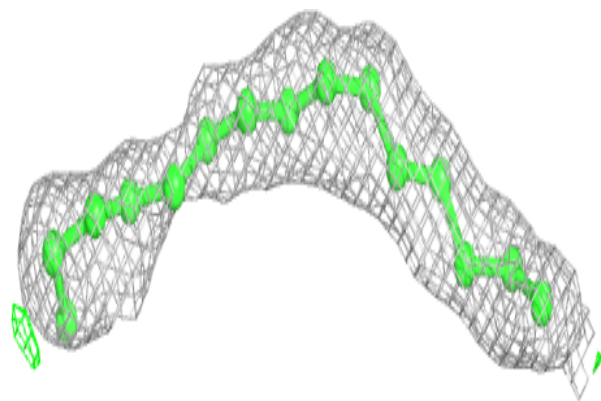
**Electron density around BCR d 405:**

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

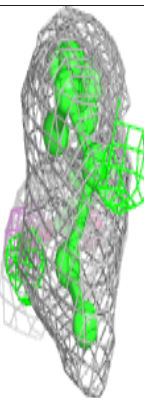
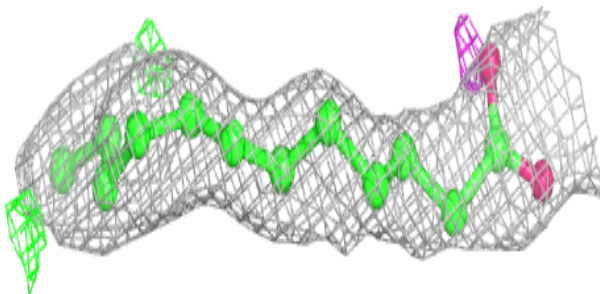
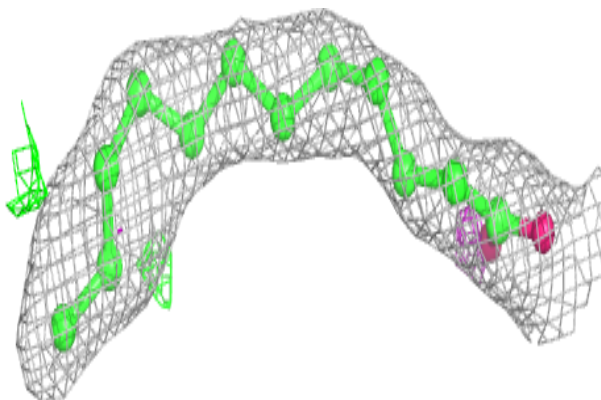


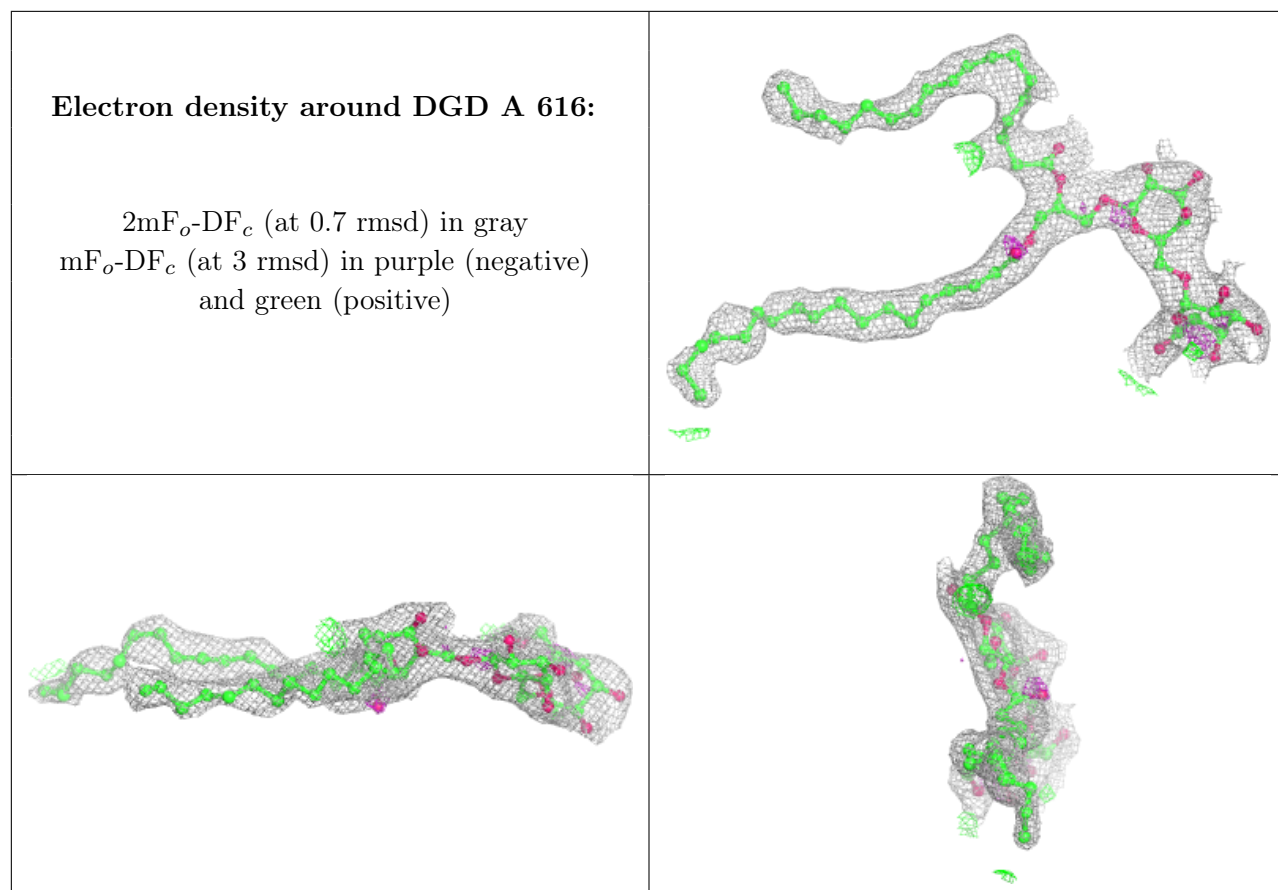
**Electron density around STE I 101:**

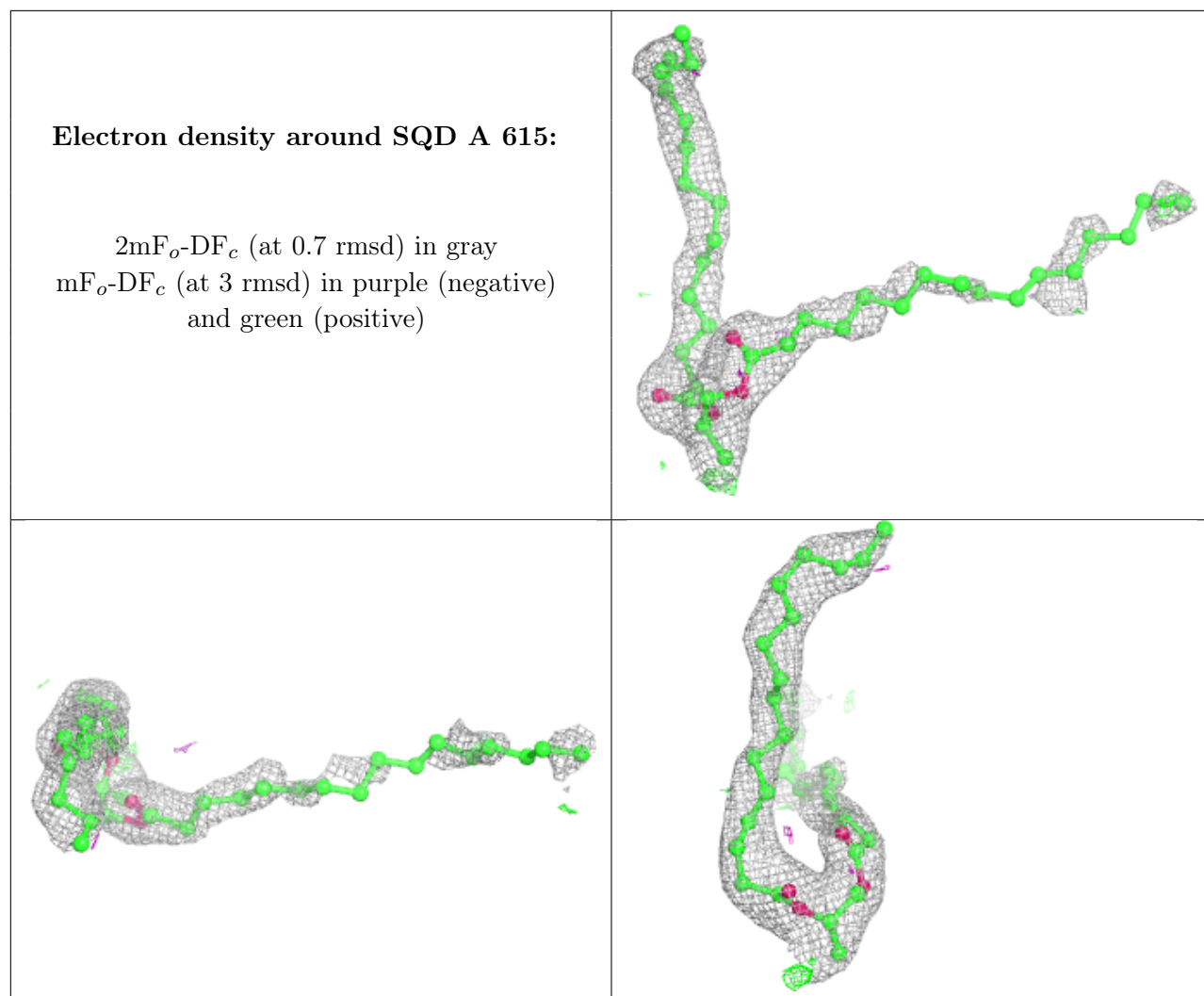
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

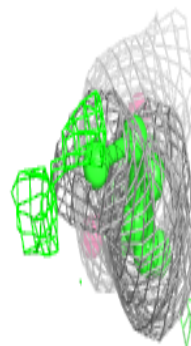
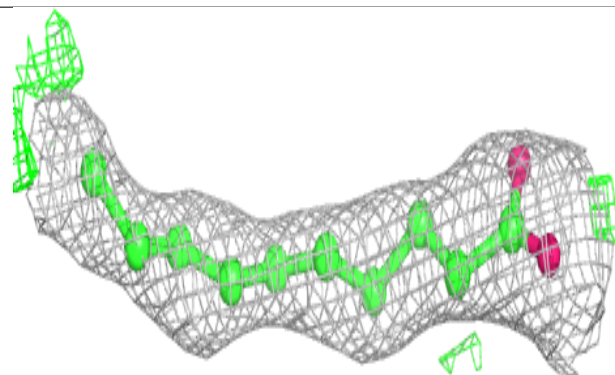
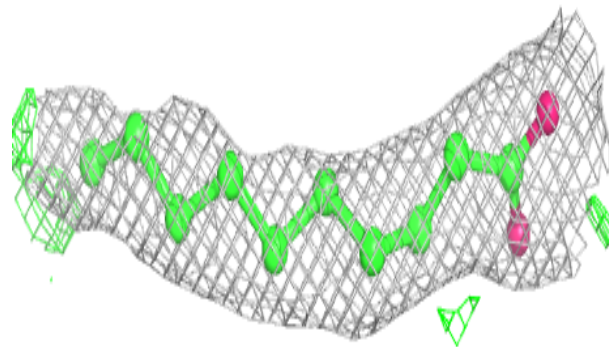




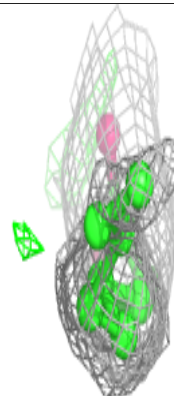
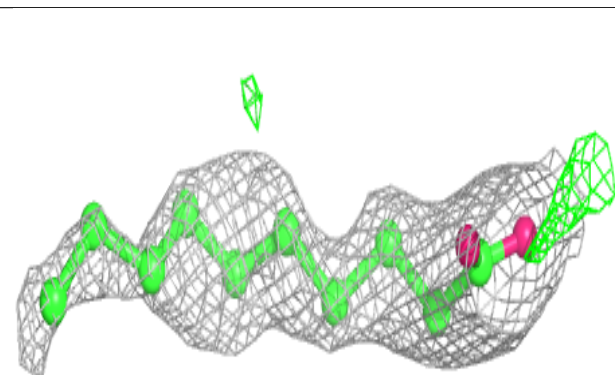
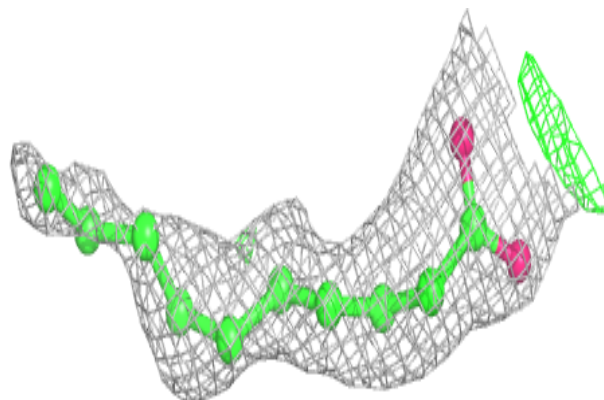


**Electron density around STE j 101:**

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

**Electron density around STE C 519:**

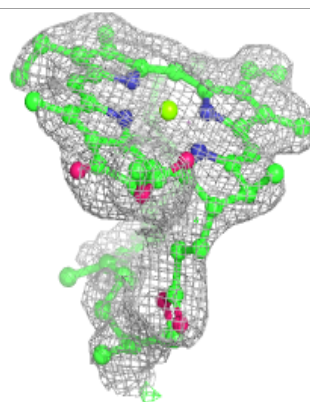
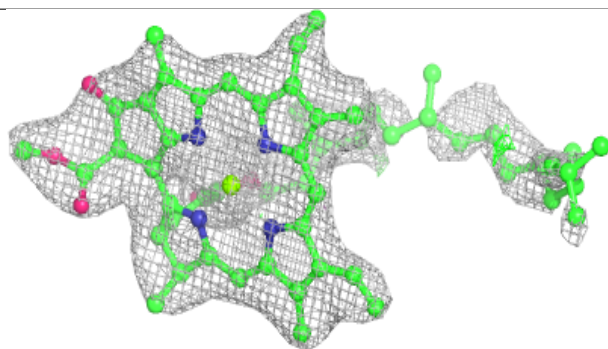
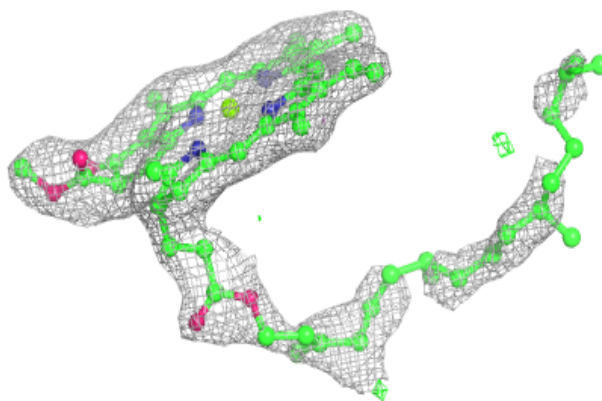
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



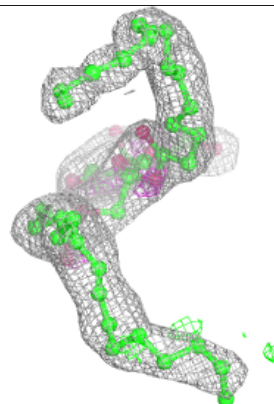
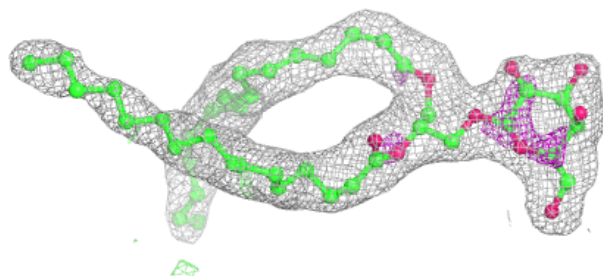
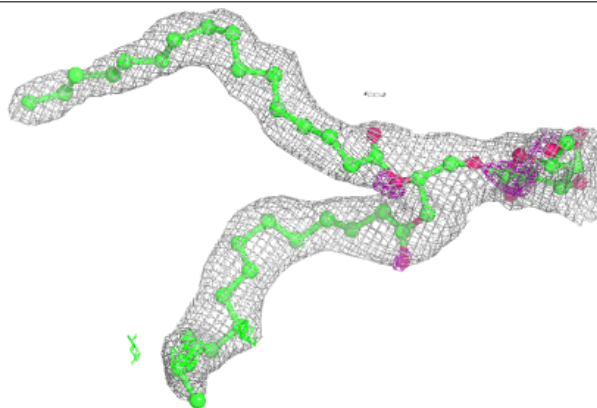


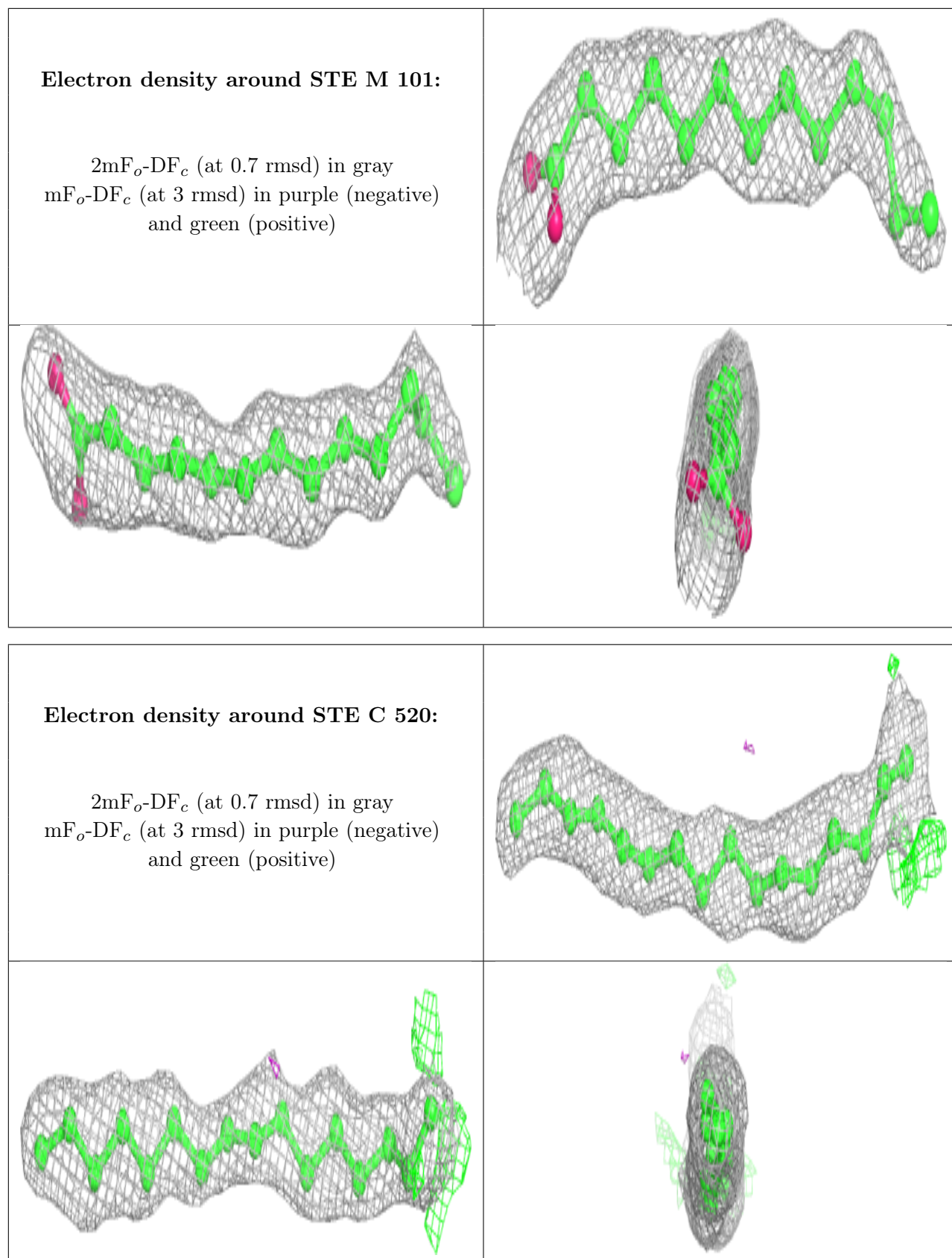
**Electron density around CLA c 513:**

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

**Electron density around LMG B 620:**

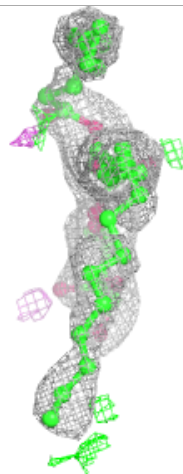
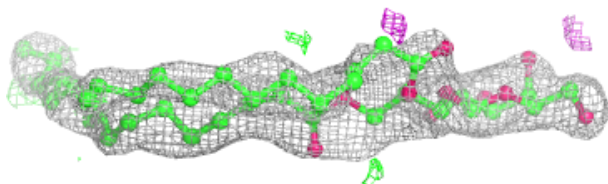
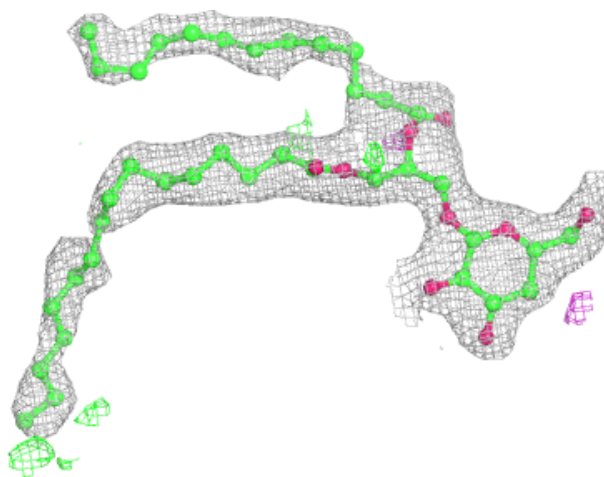
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





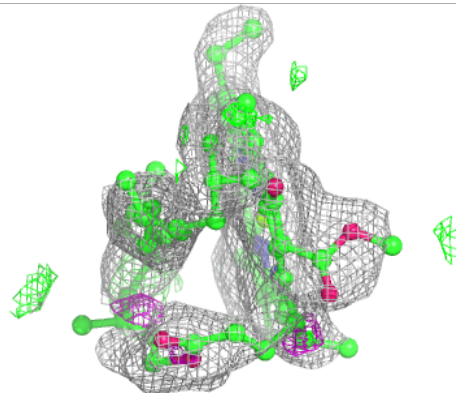
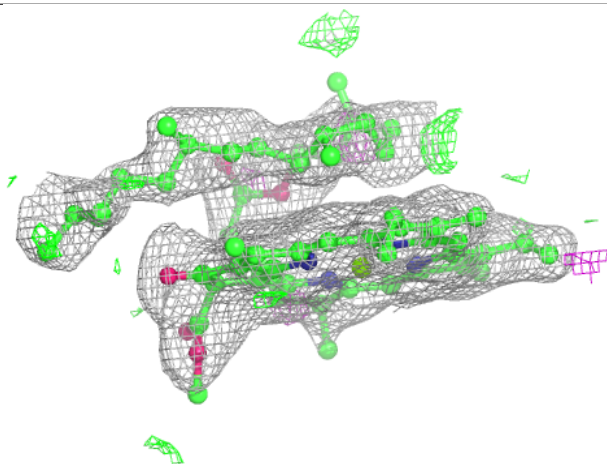
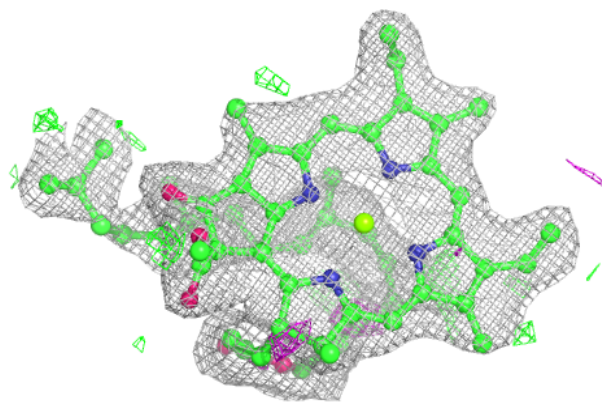
**Electron density around LMG C 517:**

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



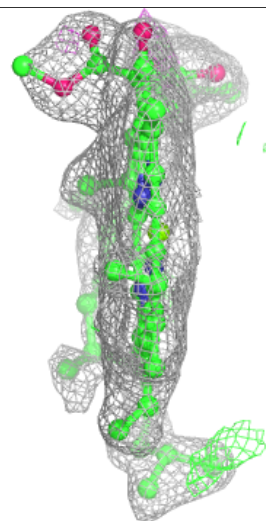
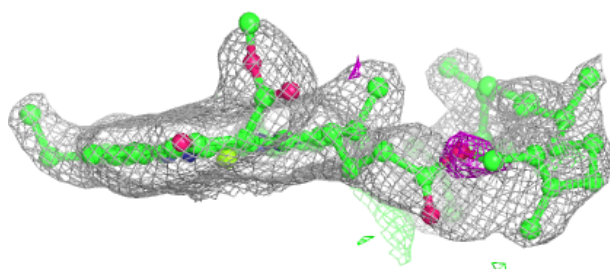
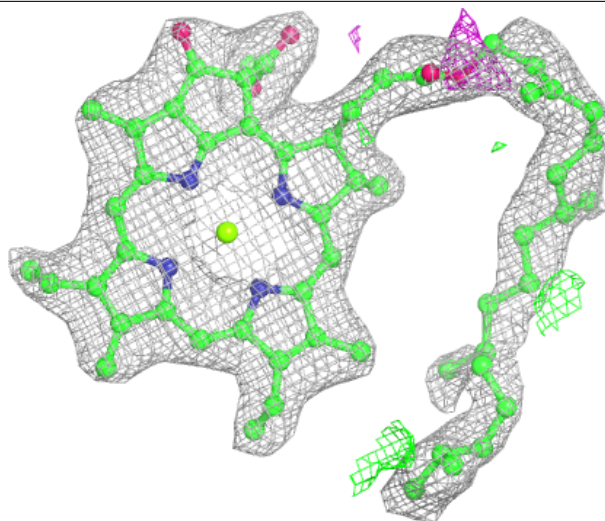
**Electron density around CLA B 601:**

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



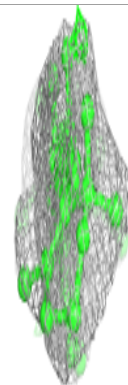
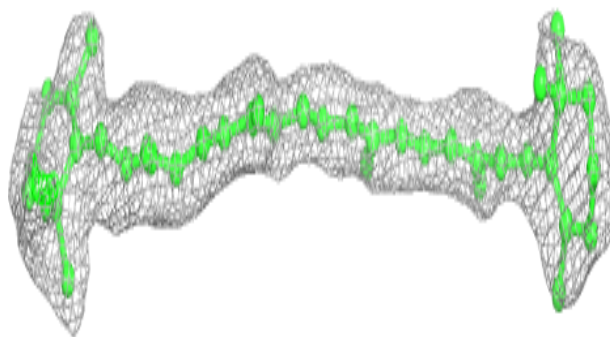
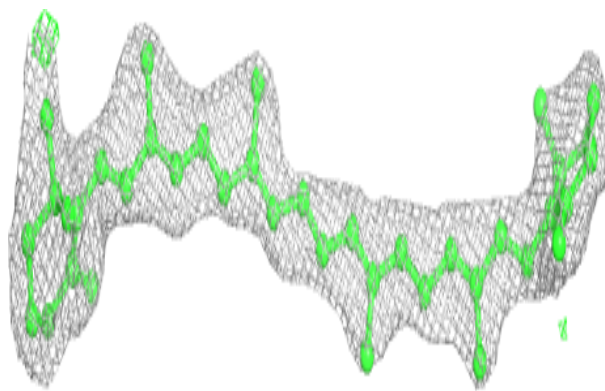
**Electron density around CLA c 512:**

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



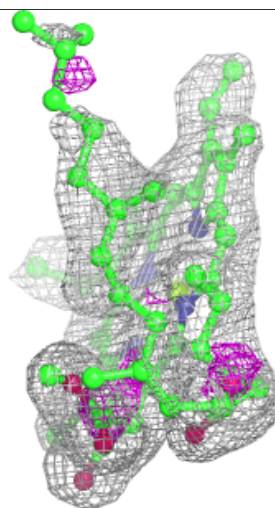
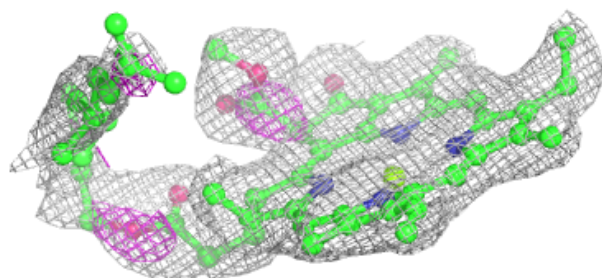
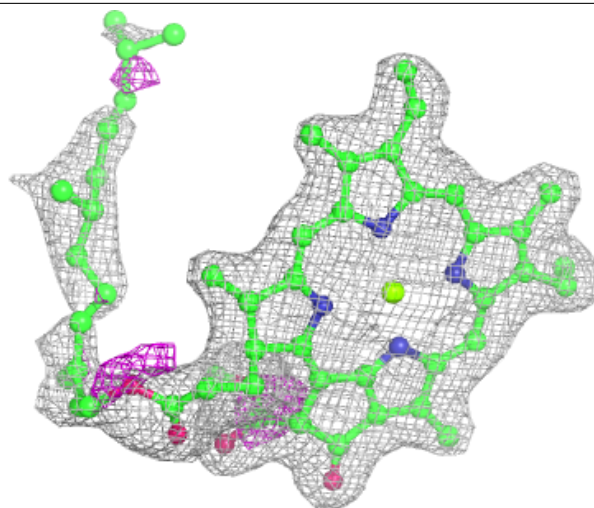
**Electron density around BCR k 102:**

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



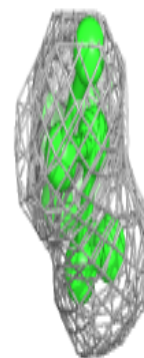
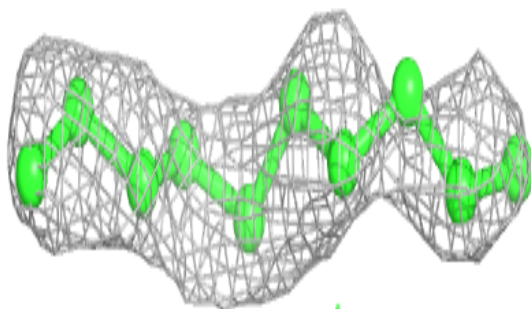
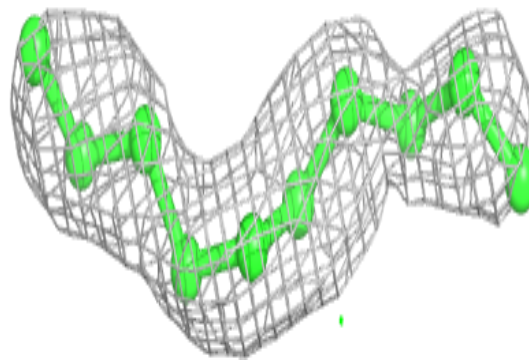
**Electron density around CLA B 616:**

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



**Electron density around STE t 103:**

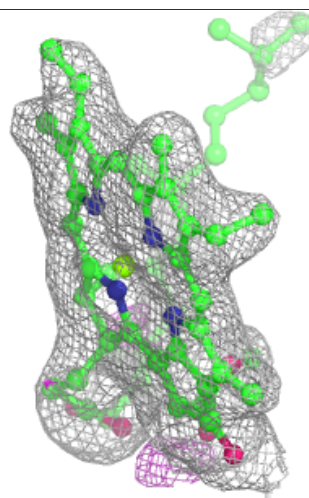
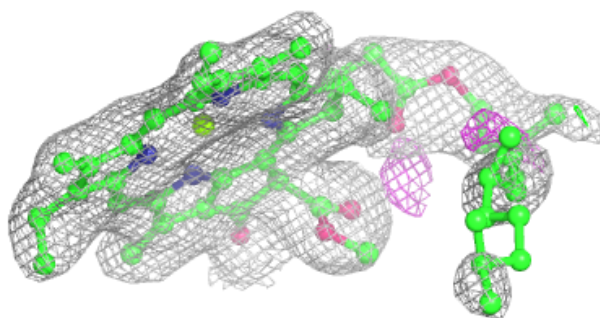
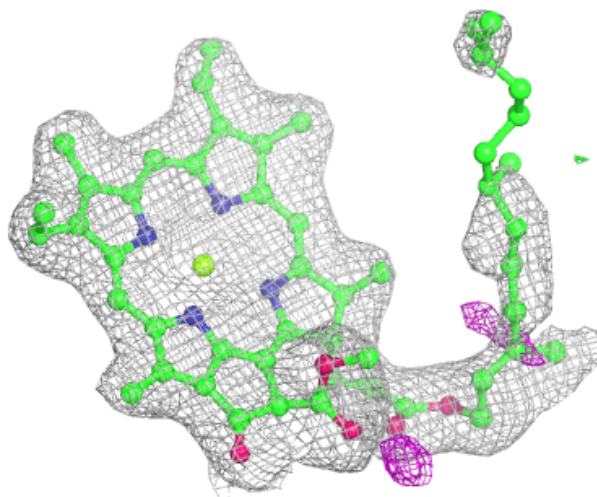
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





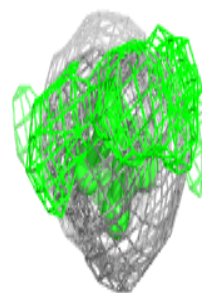
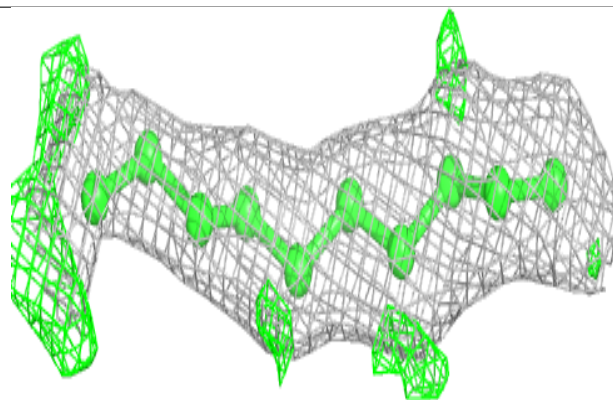
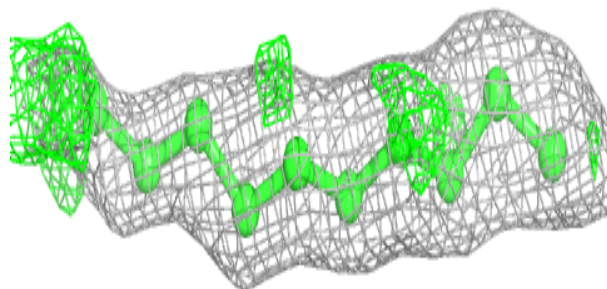
**Electron density around CLA b 616:**

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

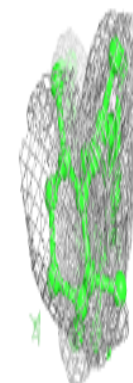
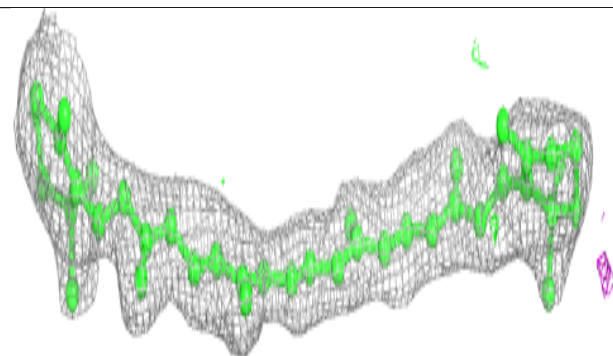
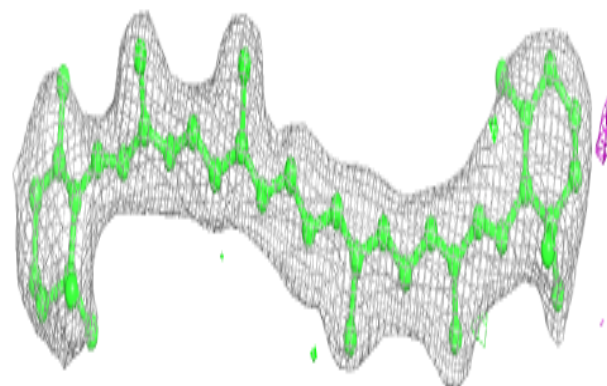


**Electron density around STE M 102:**

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

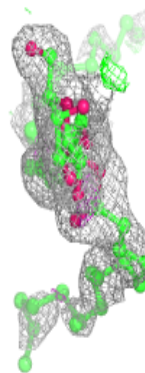
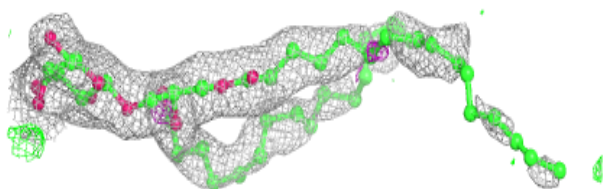
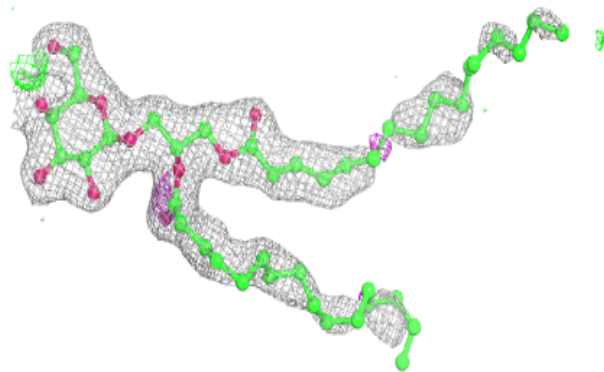
**Electron density around BCR D 405:**

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

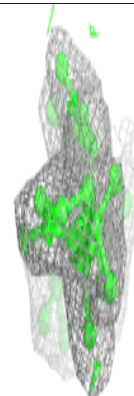
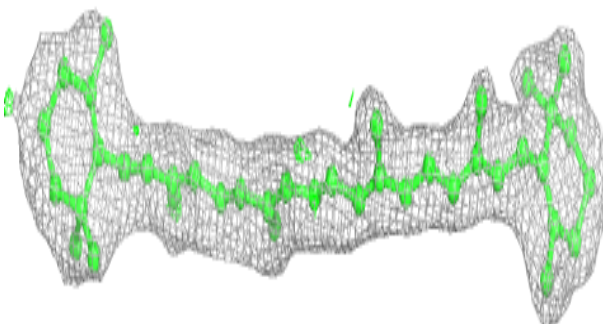
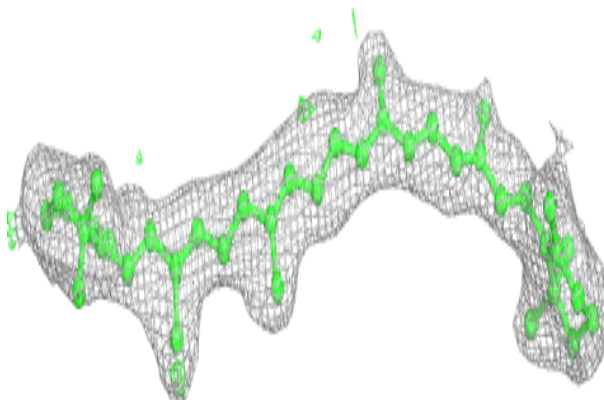


**Electron density around LMG D 407:**

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

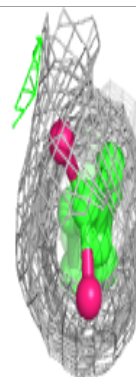
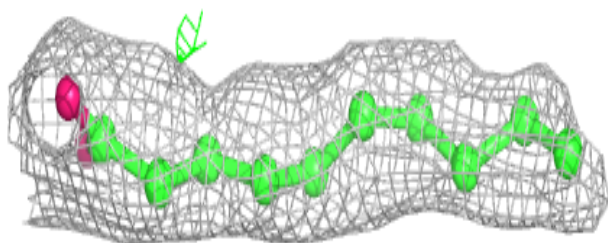
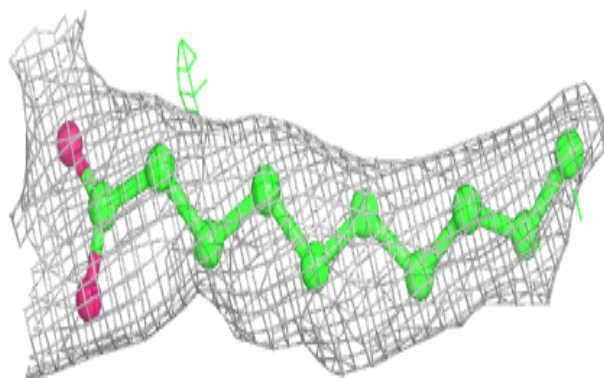
**Electron density around BCR H 101:**

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

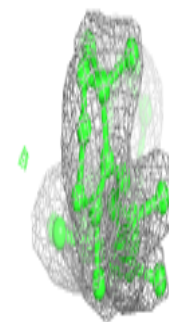
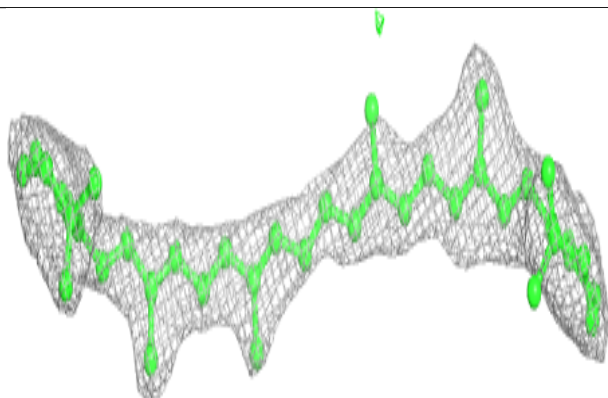
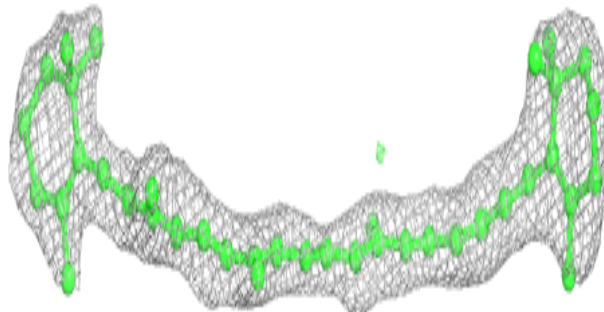


**Electron density around STE J 102:**

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

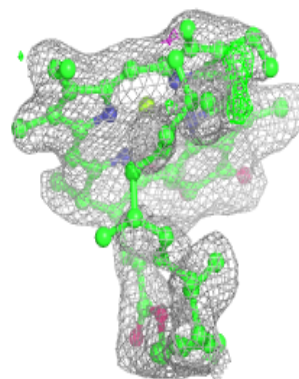
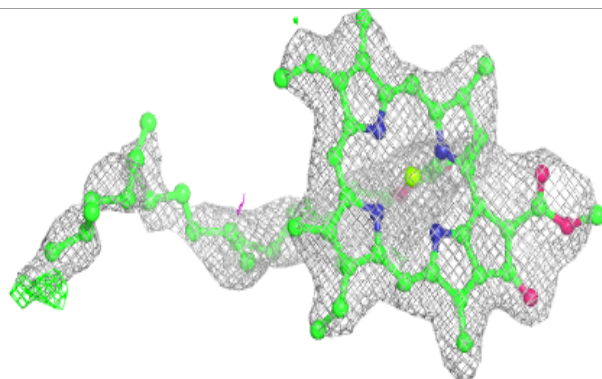
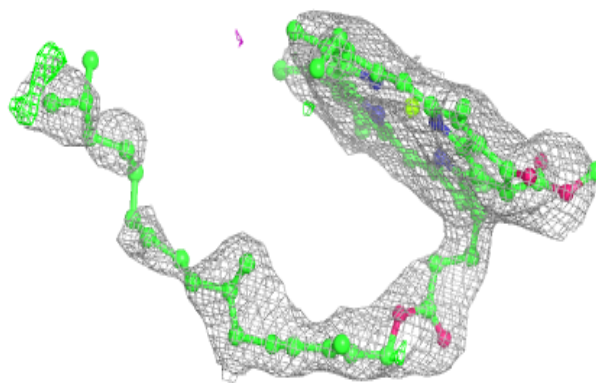
**Electron density around BCR k 103:**

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

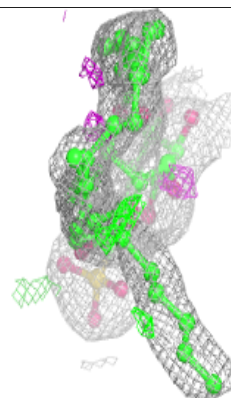
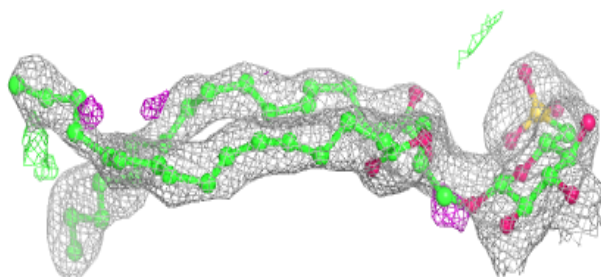
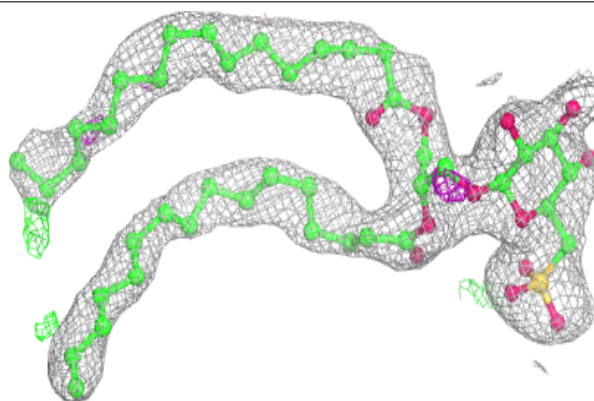


**Electron density around CLA C 513:**

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

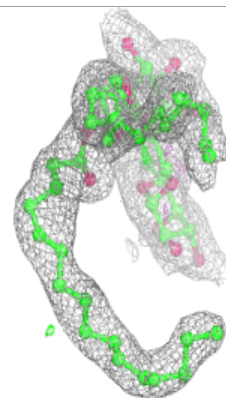
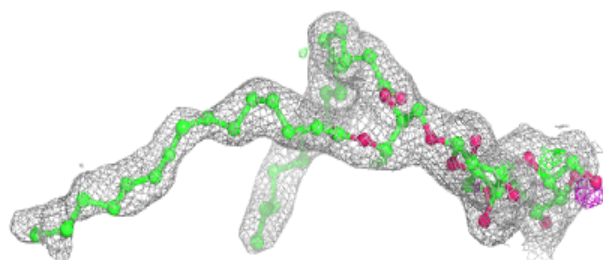
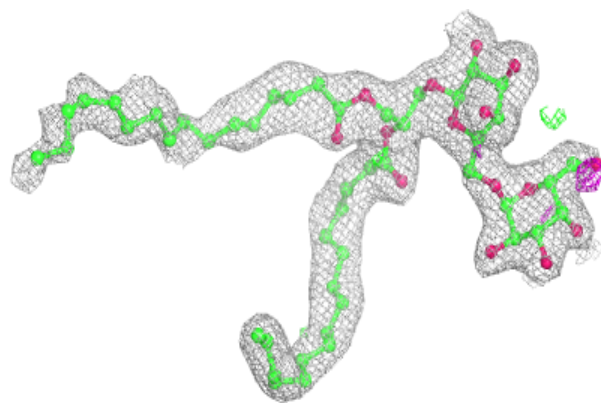
**Electron density around SQD B 623:**

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

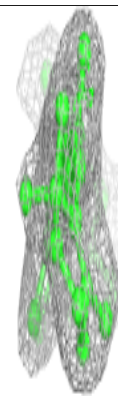
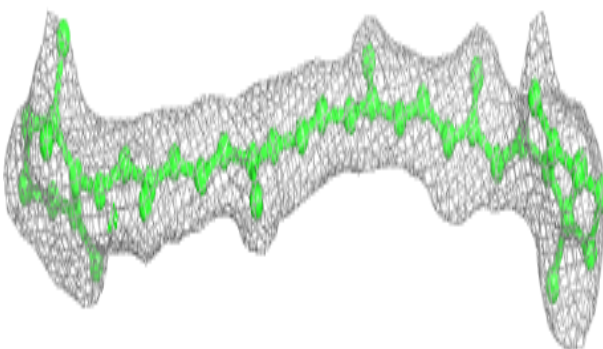
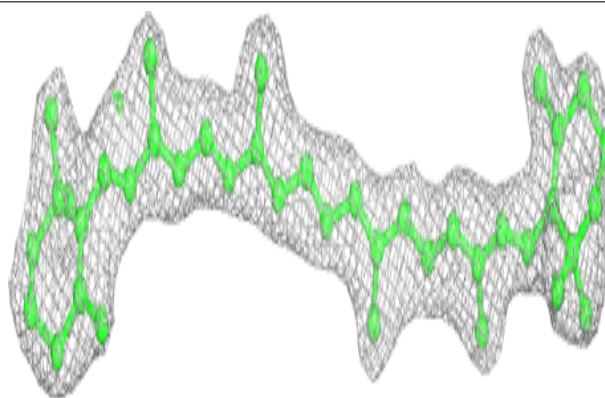


**Electron density around DGD c 516:**

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

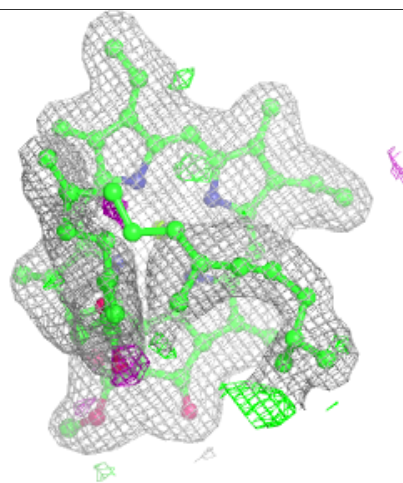
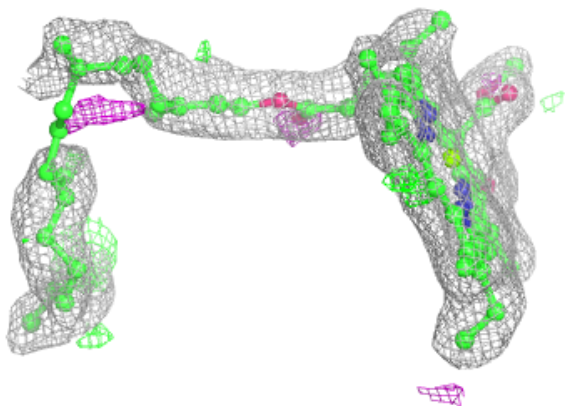
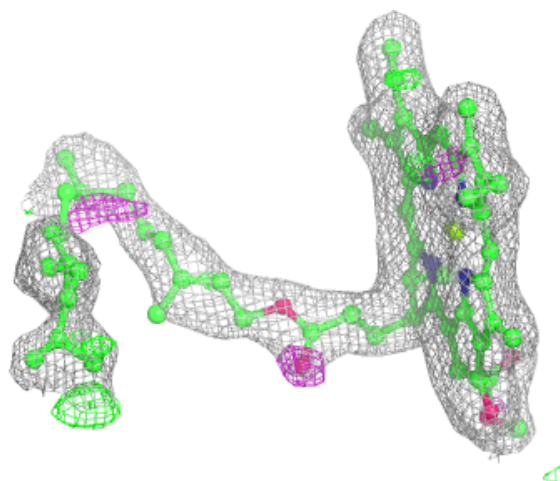
**Electron density around BCR b 619:**

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



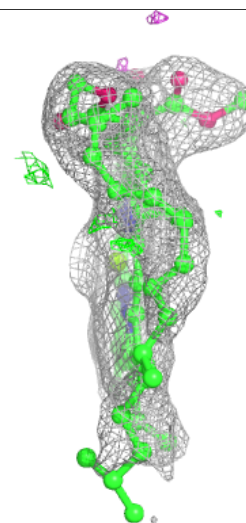
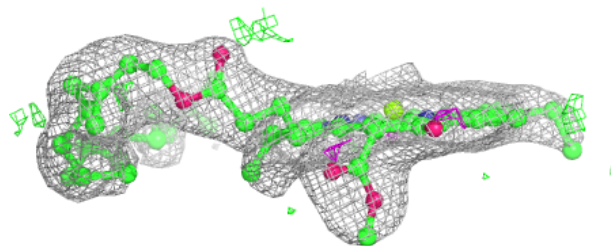
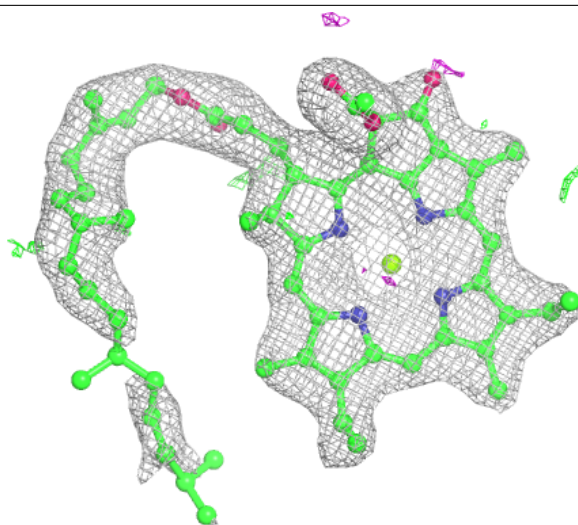
**Electron density around CLA a 608:**

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



**Electron density around CLA C 512:**

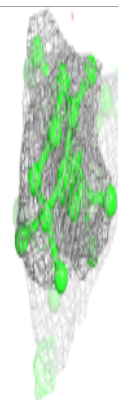
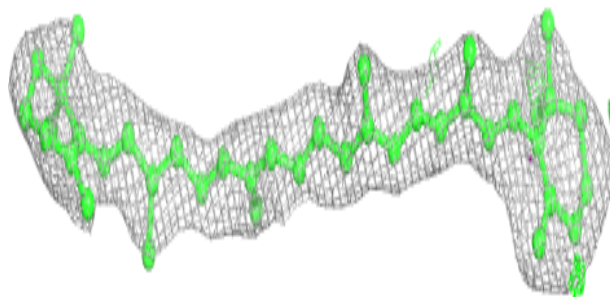
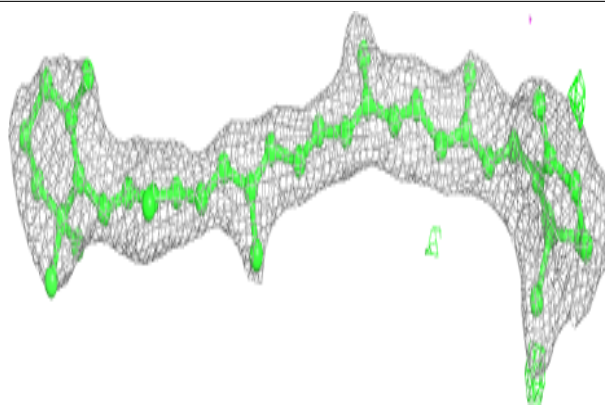
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



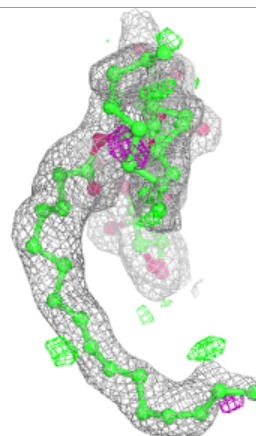
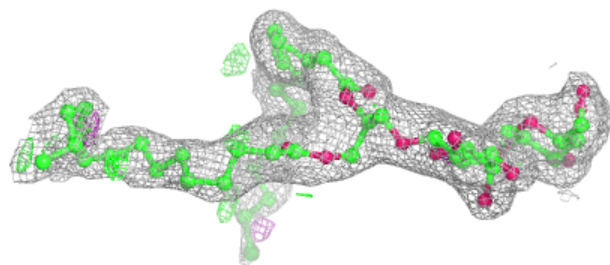
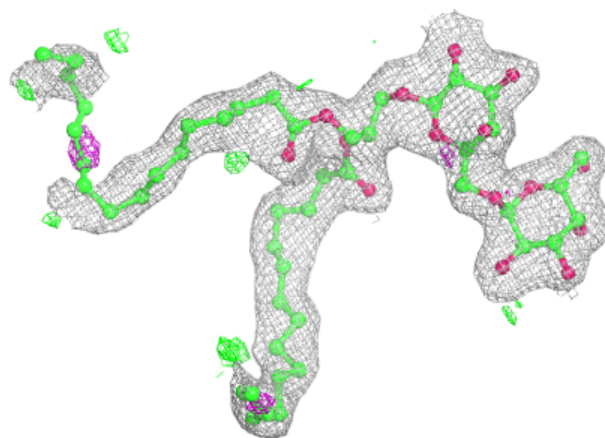


**Electron density around BCR k 101:**

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

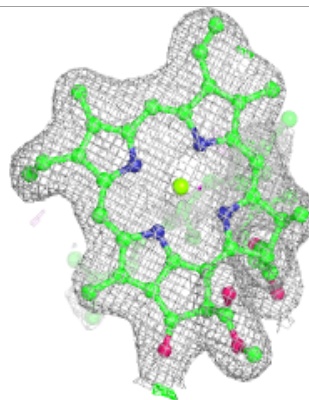
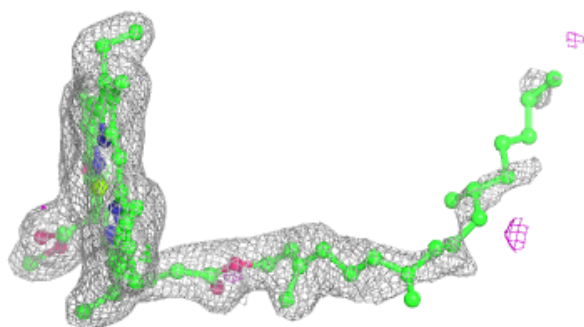
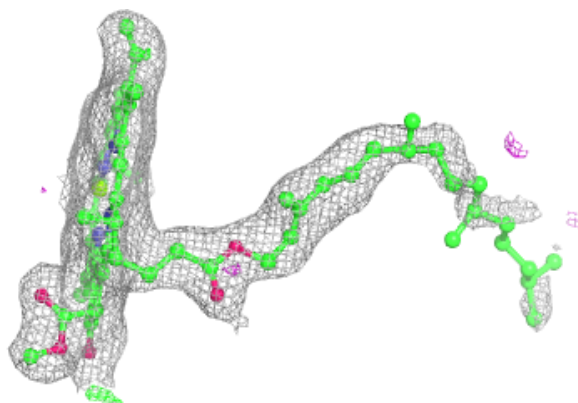
**Electron density around DGD C 516:**

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

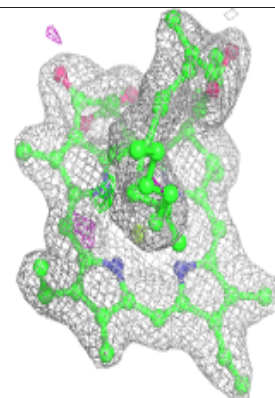
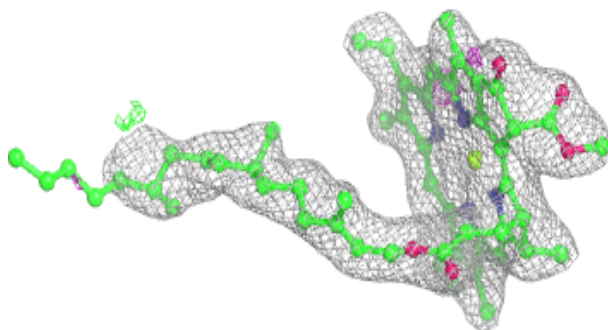
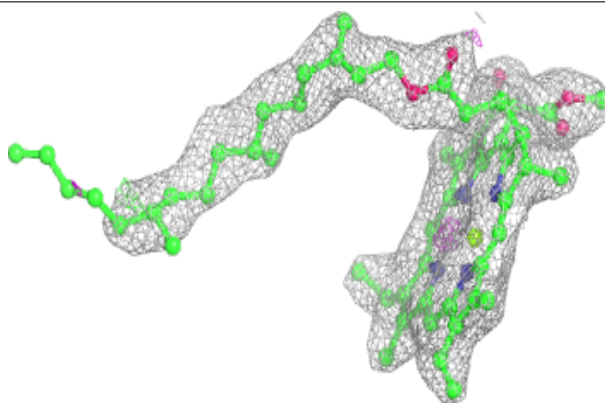


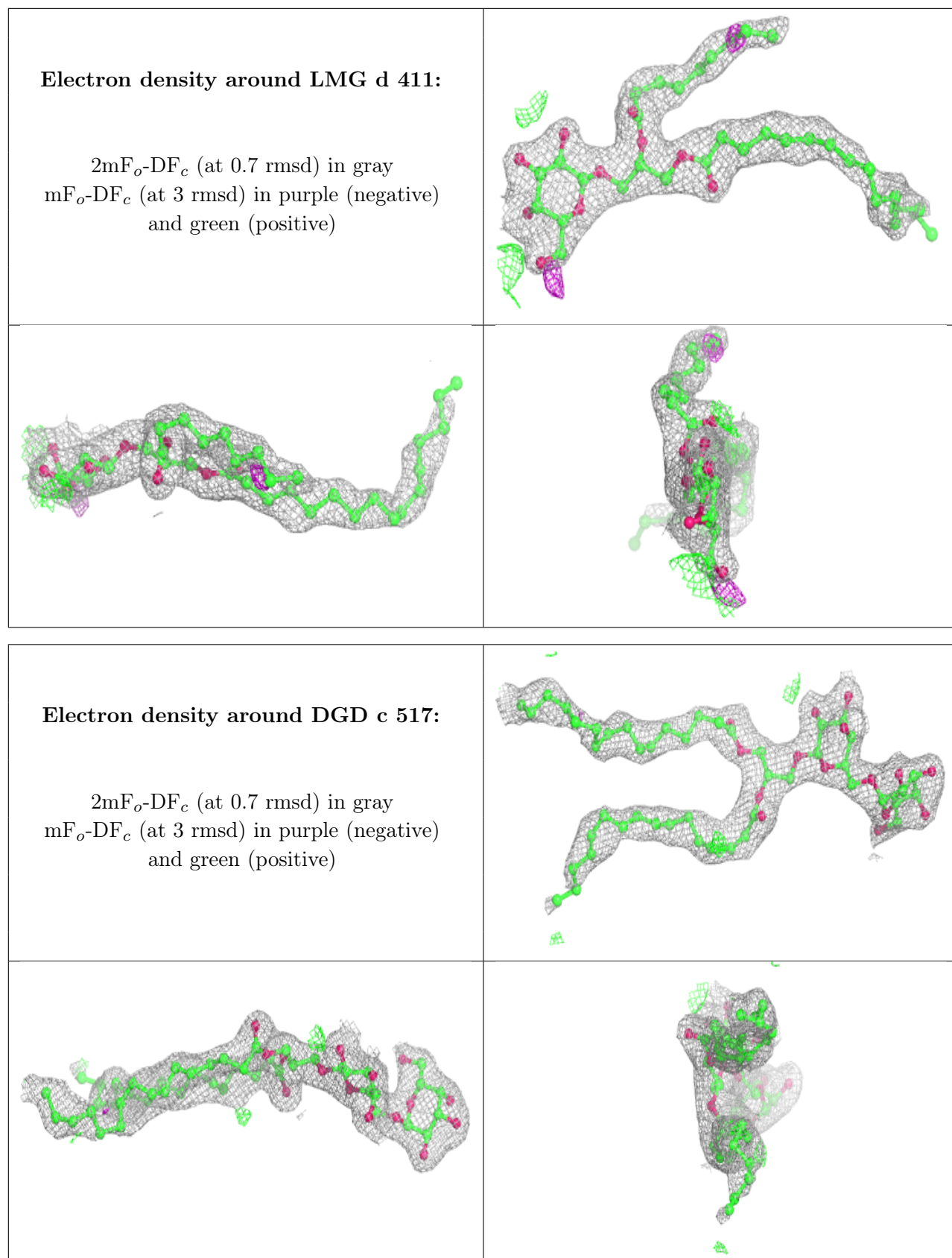
**Electron density around CLA D 404:**

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

**Electron density around CLA c 508:**

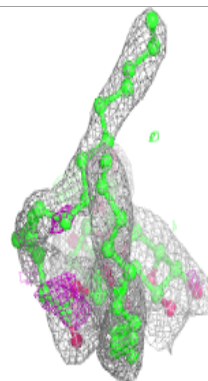
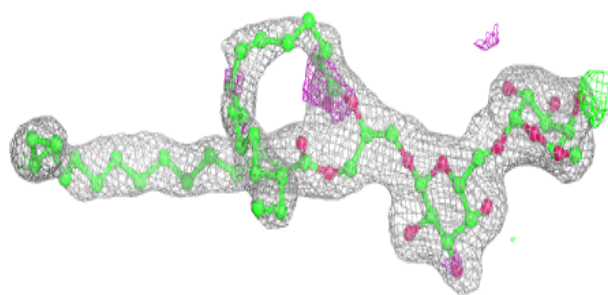
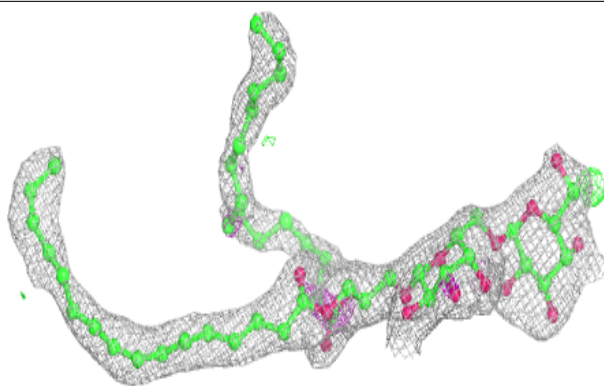
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



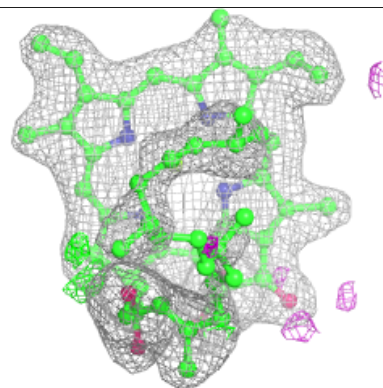
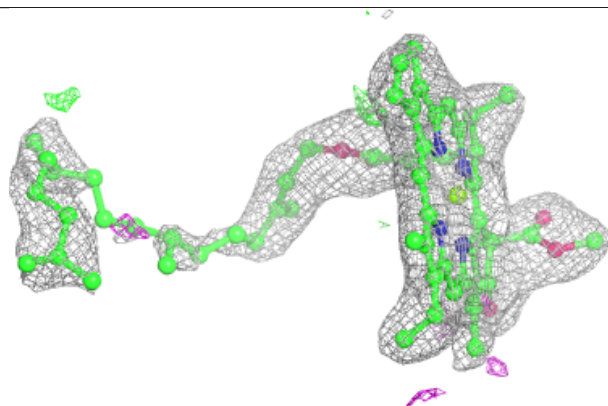
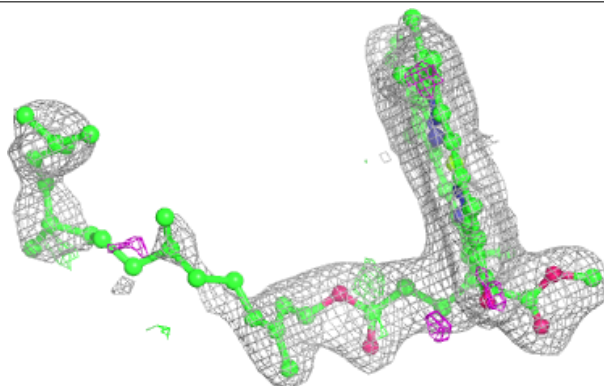


**Electron density around DGD h 102:**

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

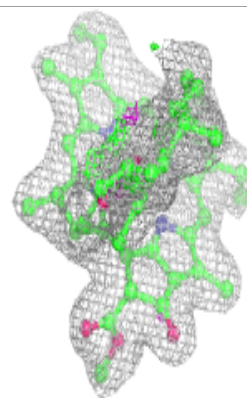
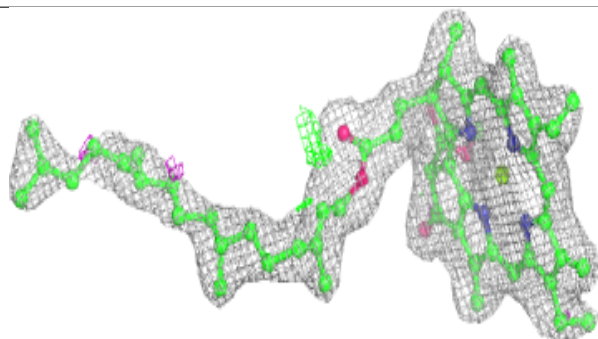
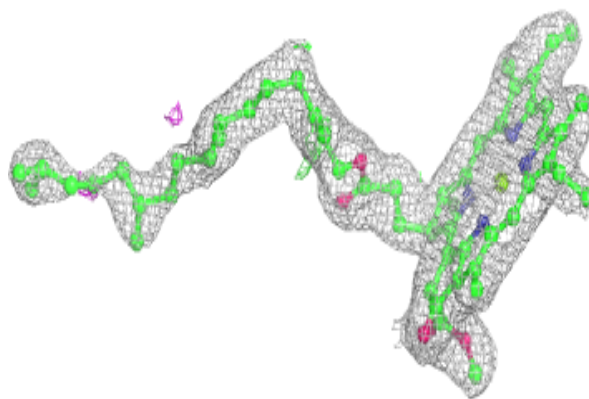
**Electron density around CLA C 506:**

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

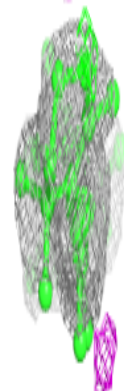
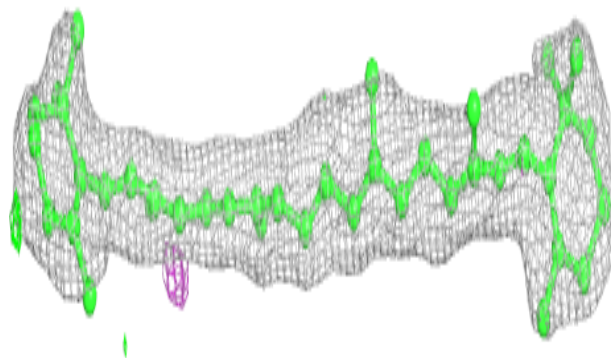
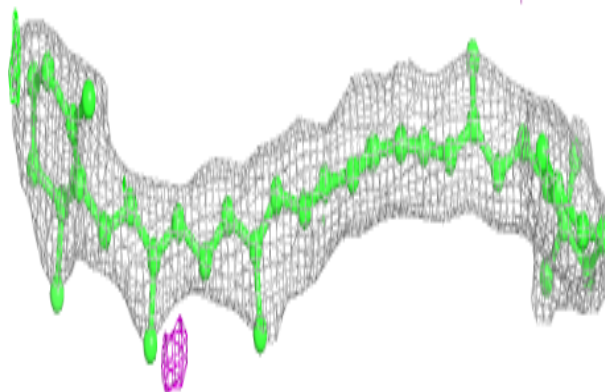


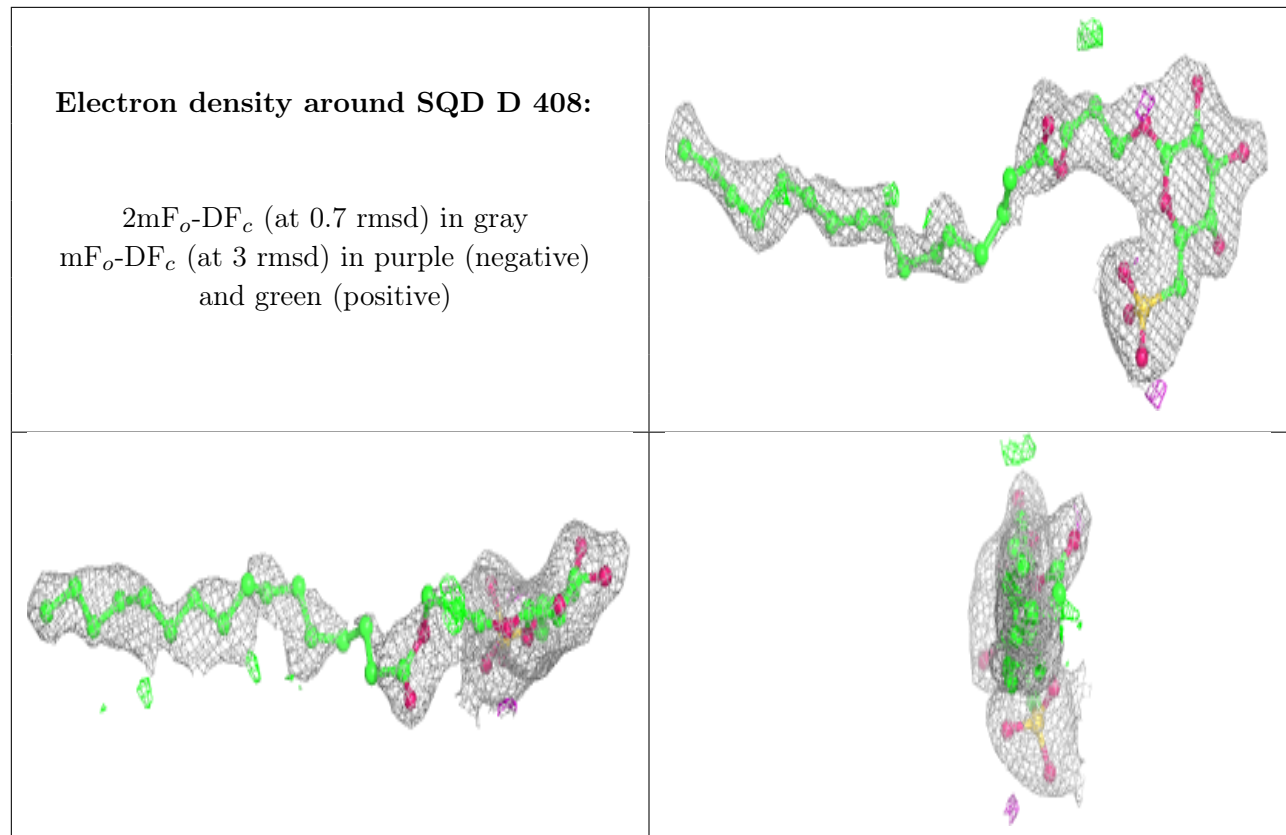
**Electron density around CLA c 502:**

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

**Electron density around BCR K 101:**

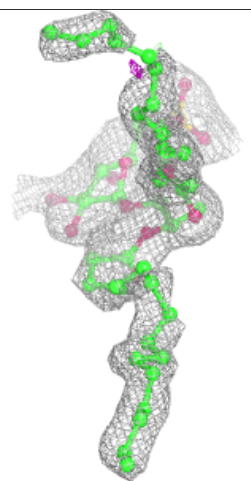
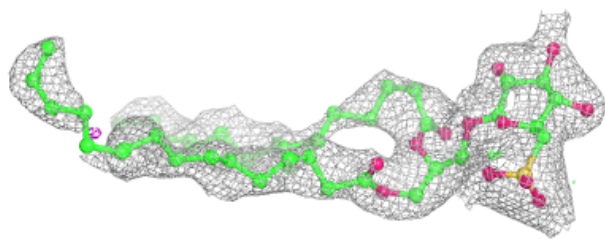
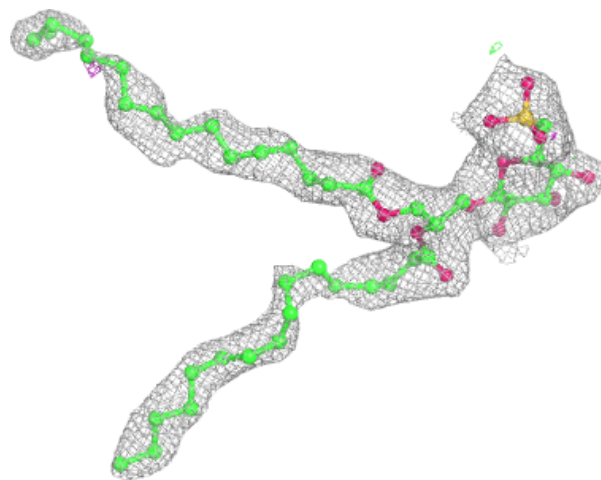
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)

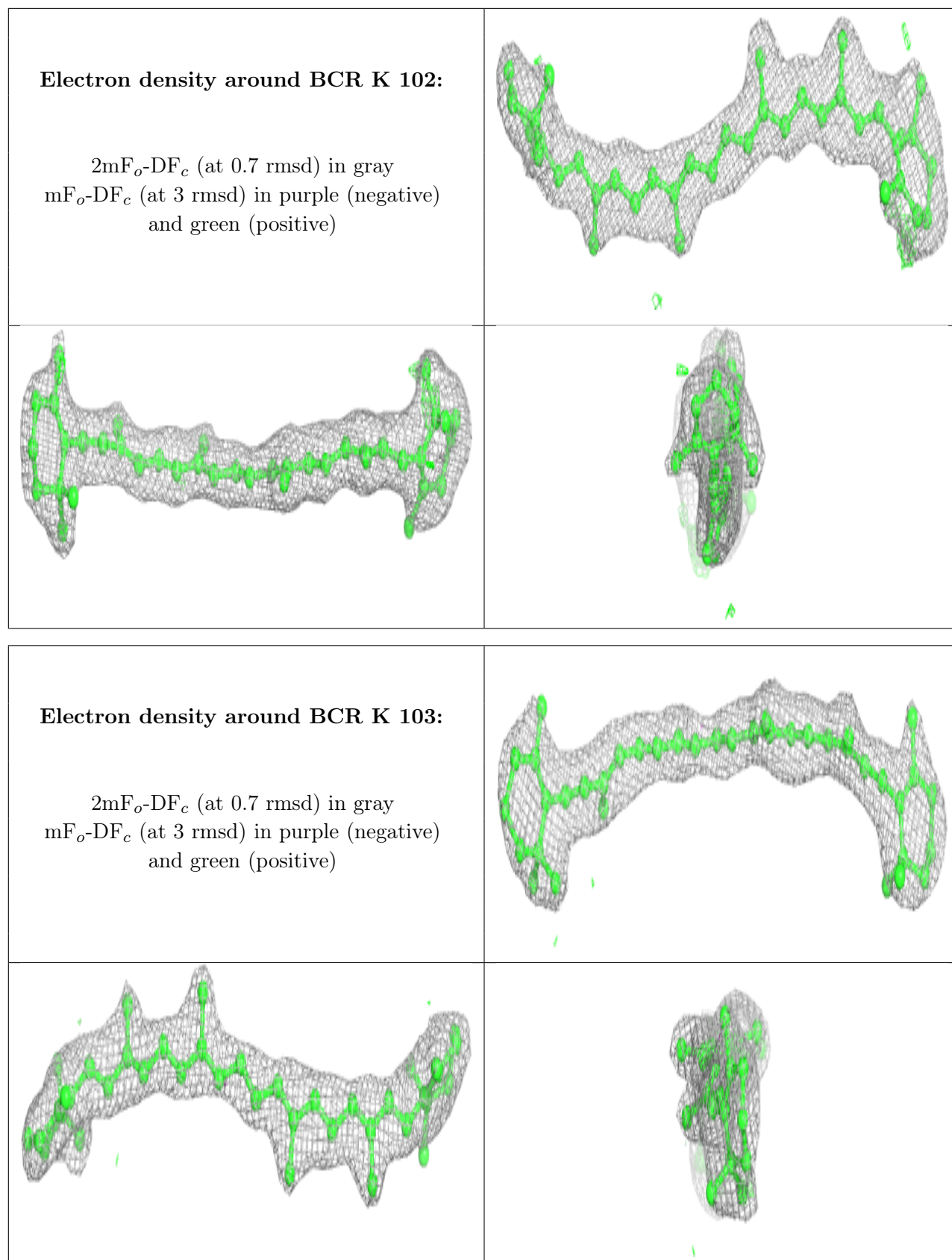




**Electron density around SQD a 612:**

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

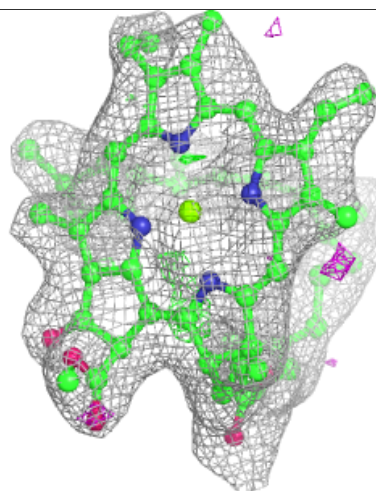
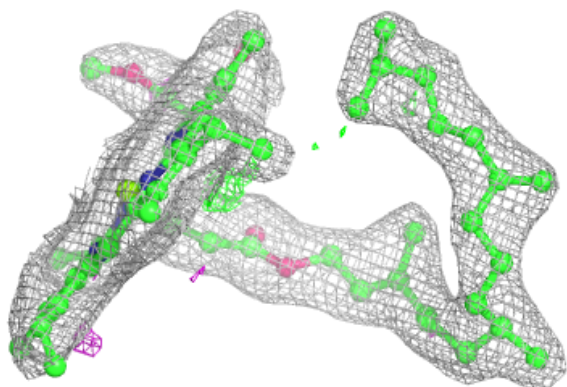
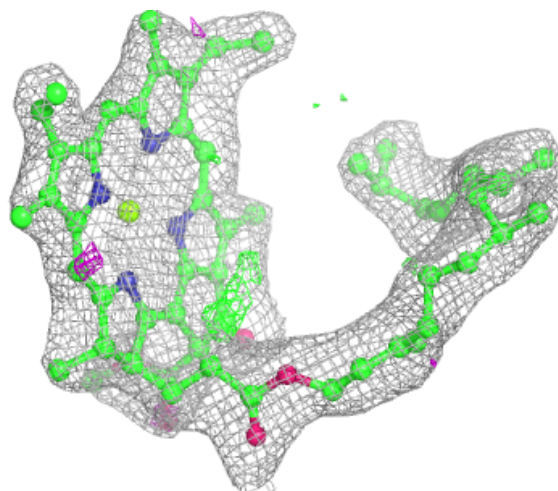






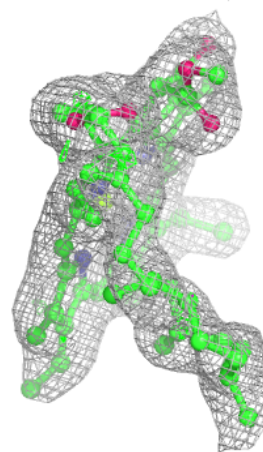
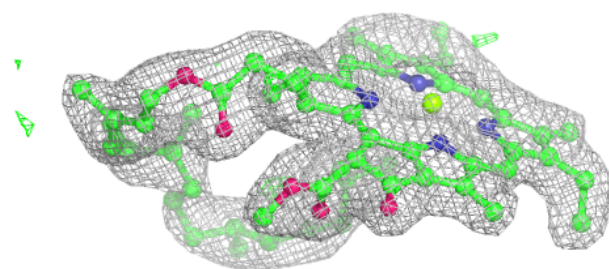
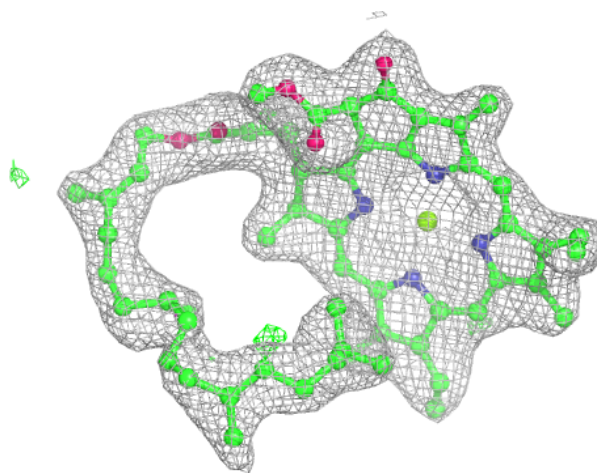
**Electron density around CLA c 503:**

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



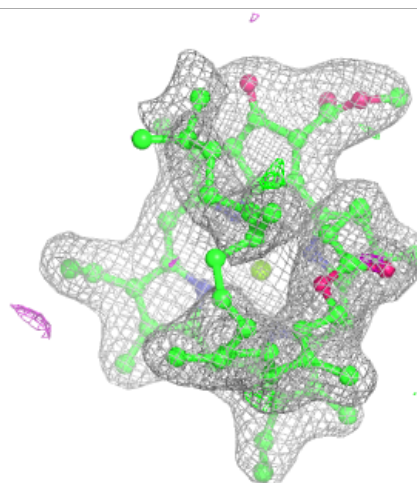
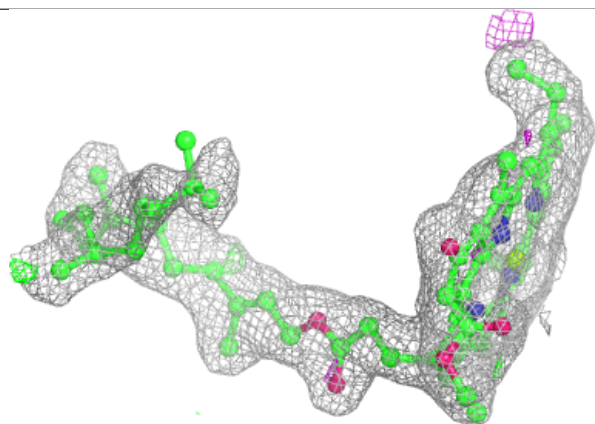
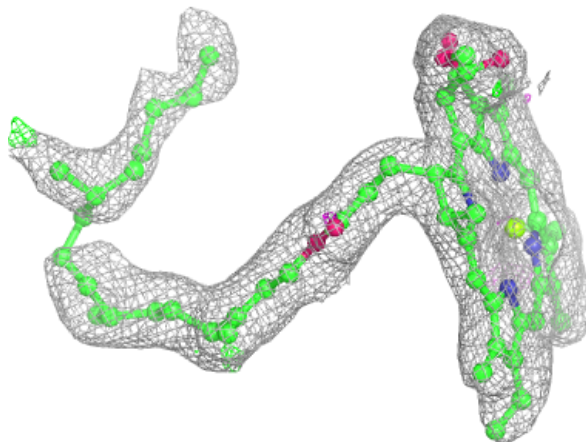
**Electron density around CLA B 615:**

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



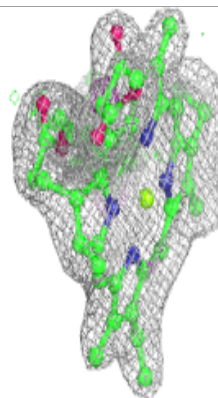
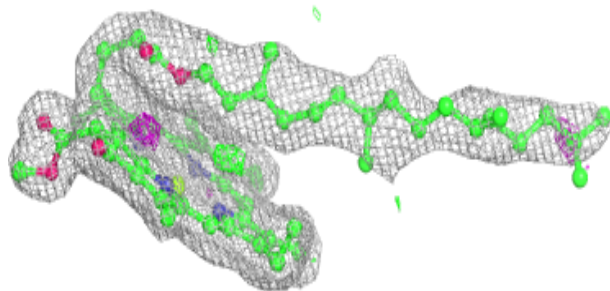
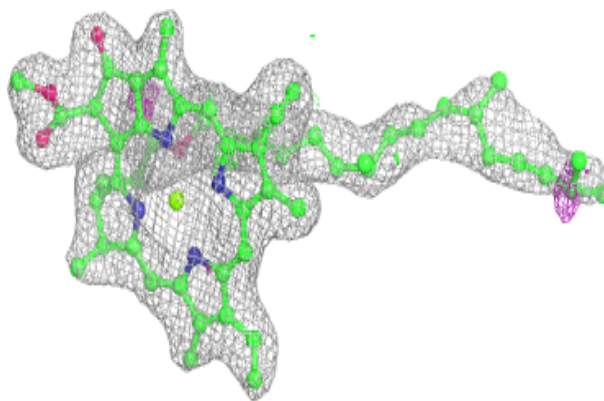
**Electron density around CLA B 606:**

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

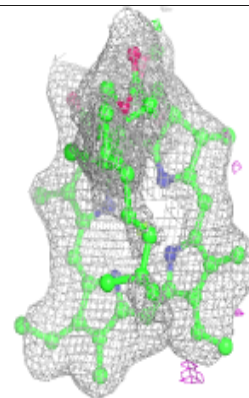
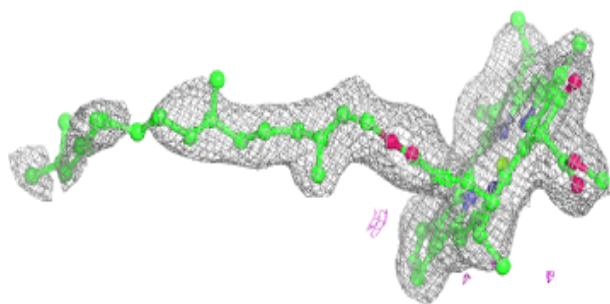
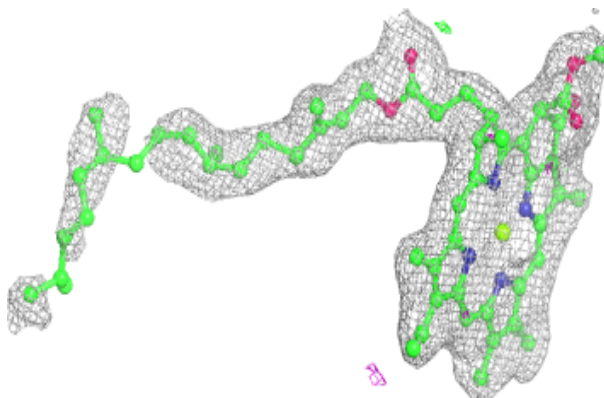


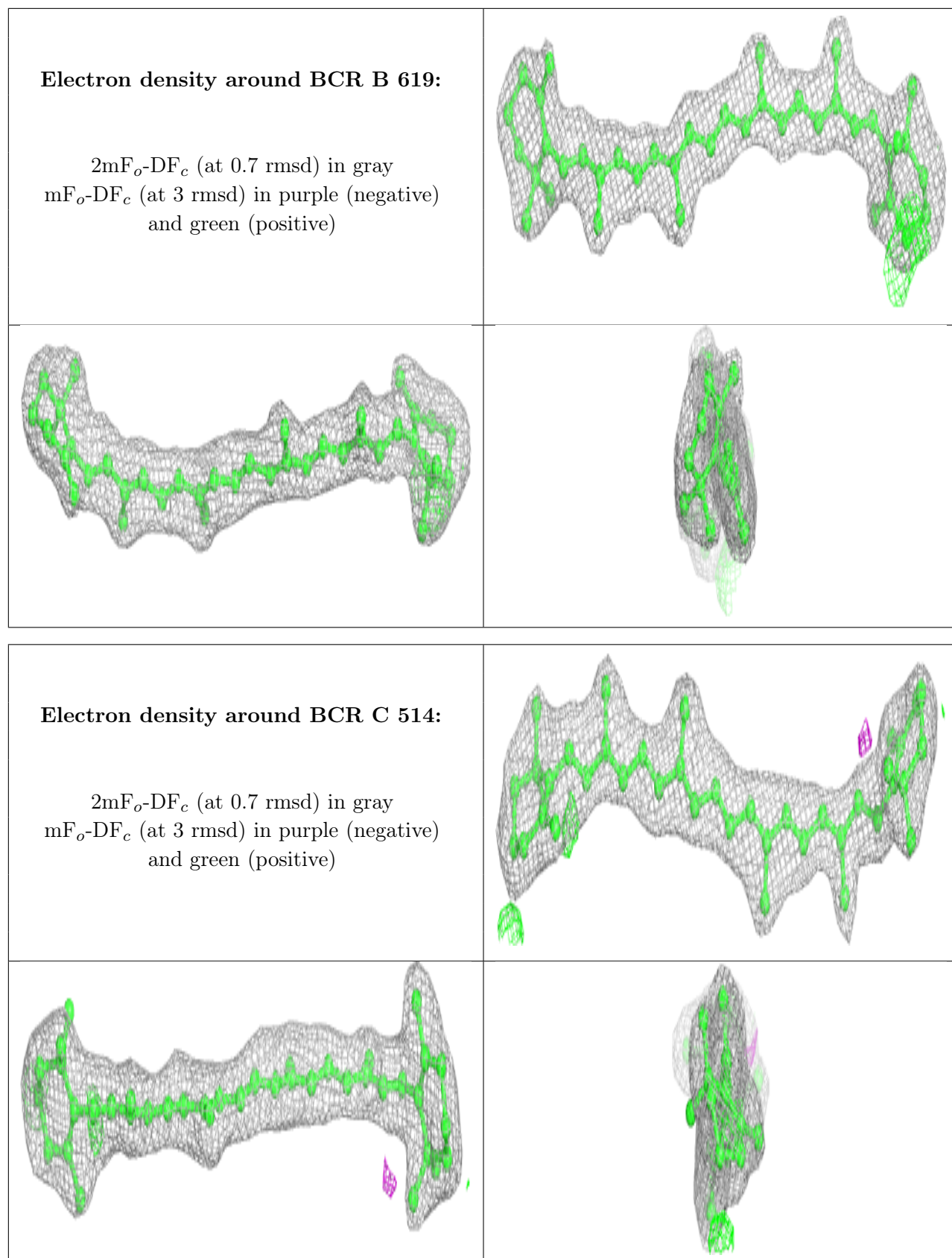
**Electron density around CLA b 614:**

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

**Electron density around CLA d 404:**

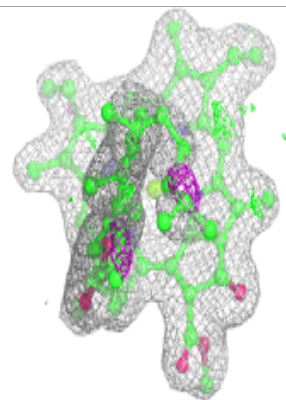
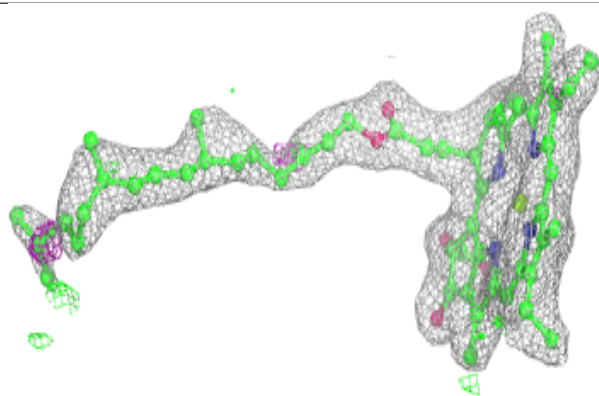
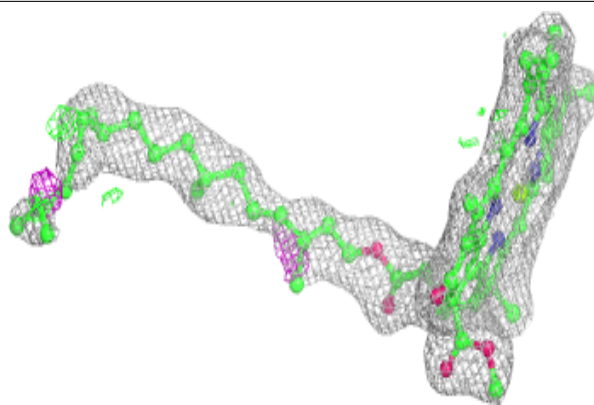
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



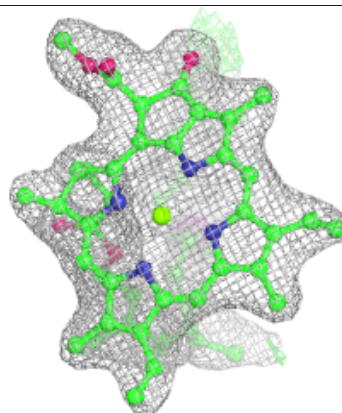
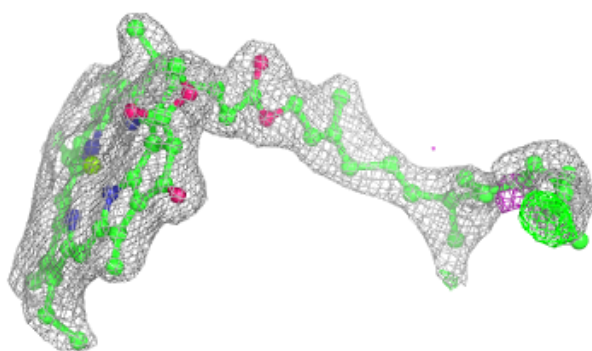
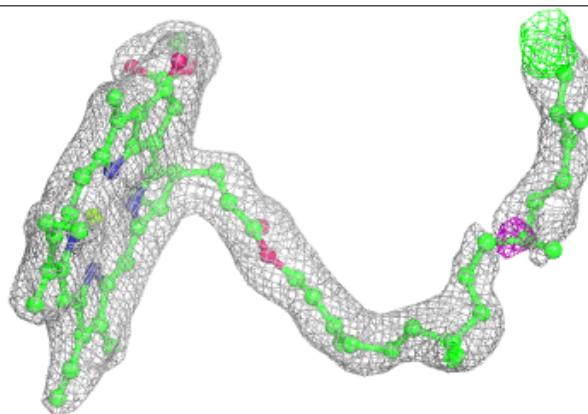


**Electron density around CLA b 604:**

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

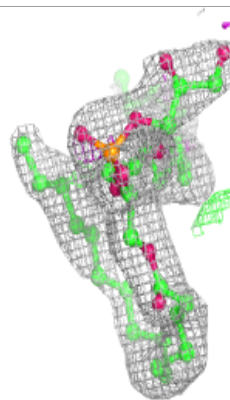
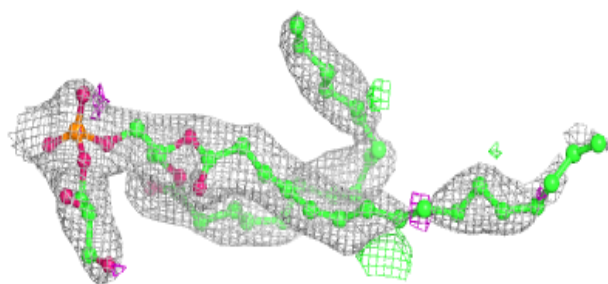
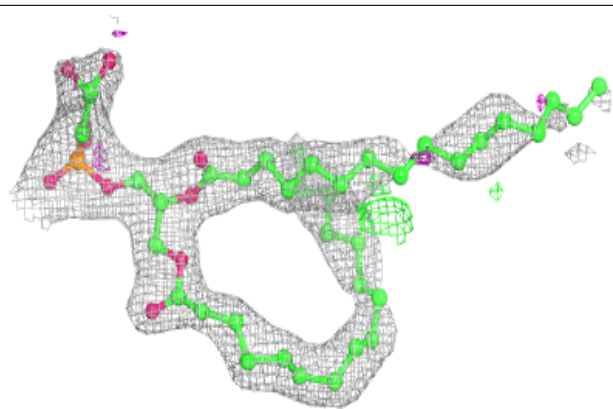
**Electron density around CLA b 606:**

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



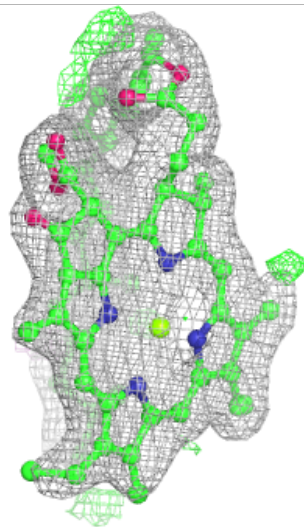
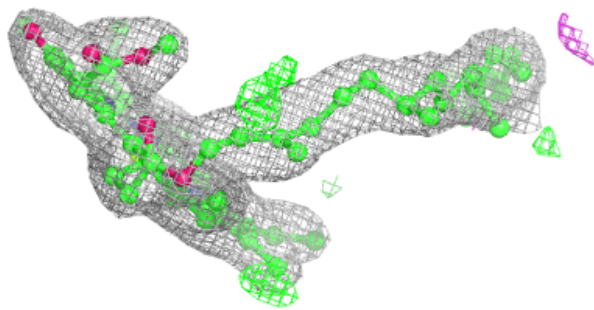
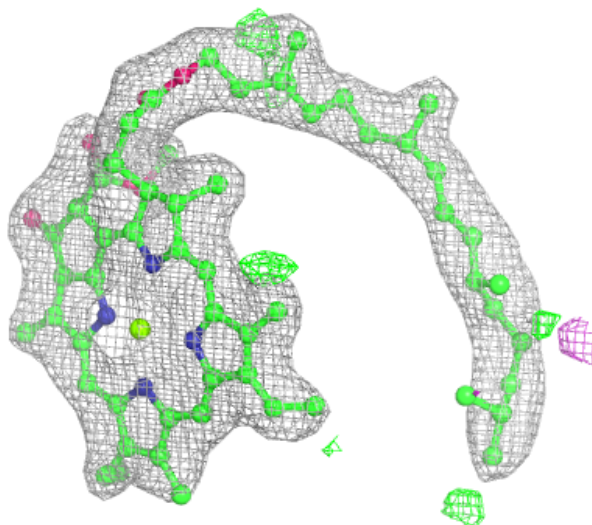
**Electron density around LHG d 407:**

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

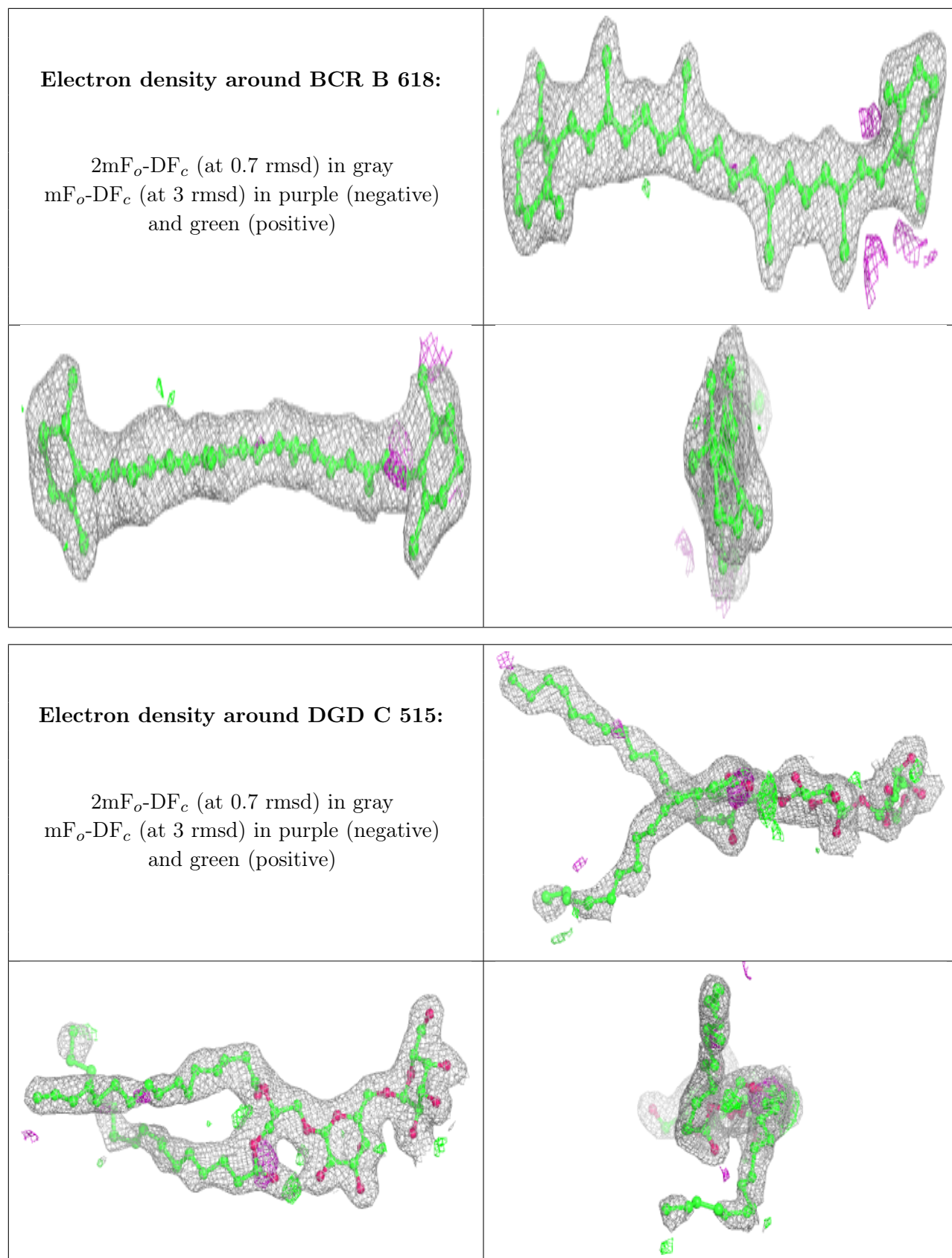


**Electron density around CLA C 507:**

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

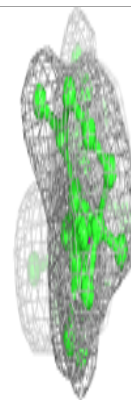
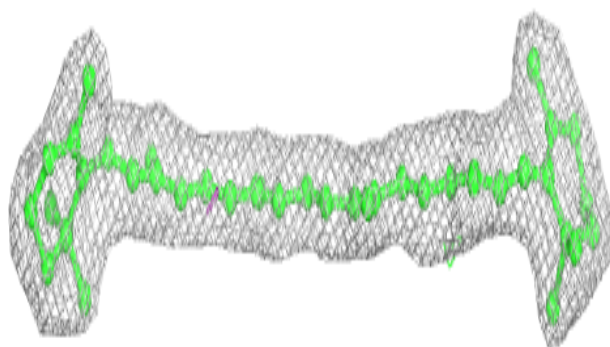
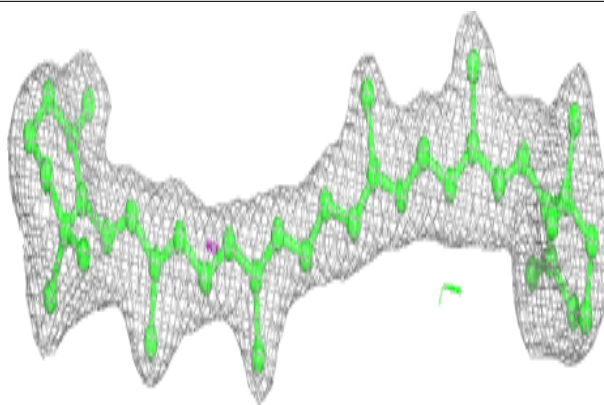




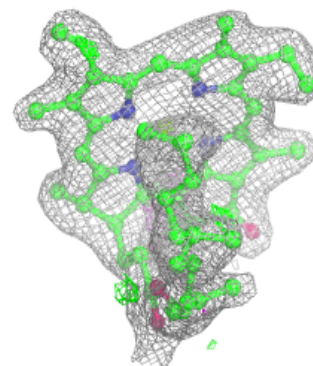
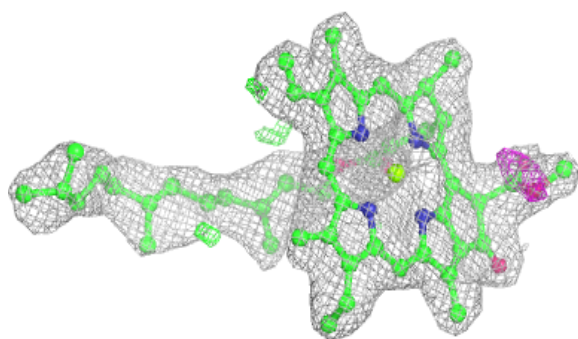
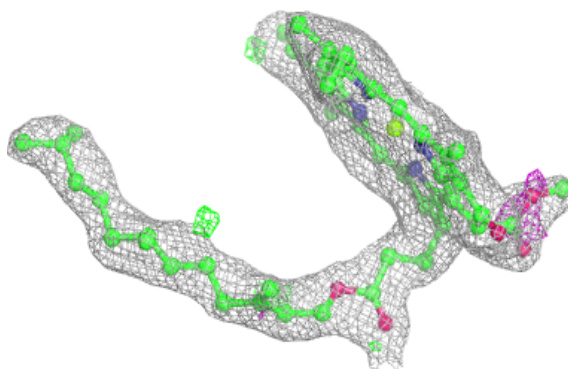


**Electron density around BCR b 618:**

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

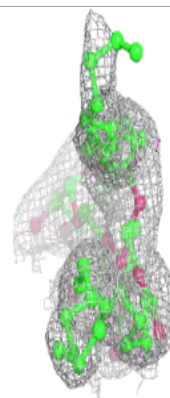
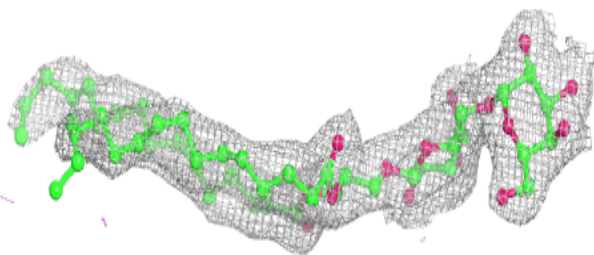
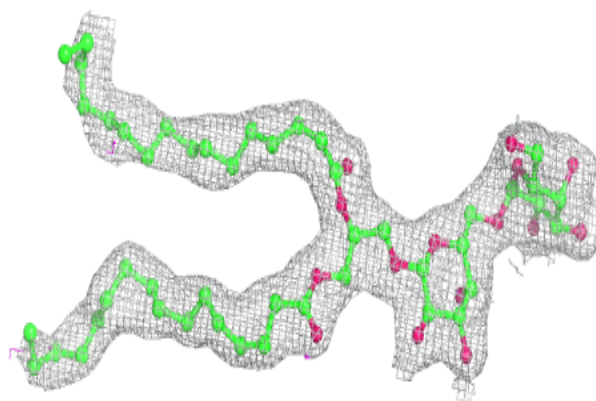
**Electron density around CLA c 504:**

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

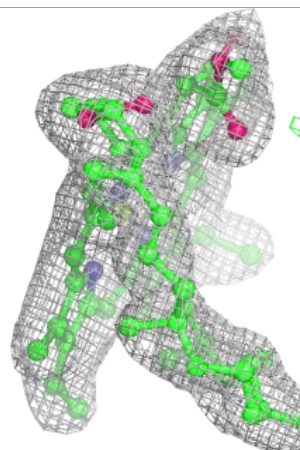
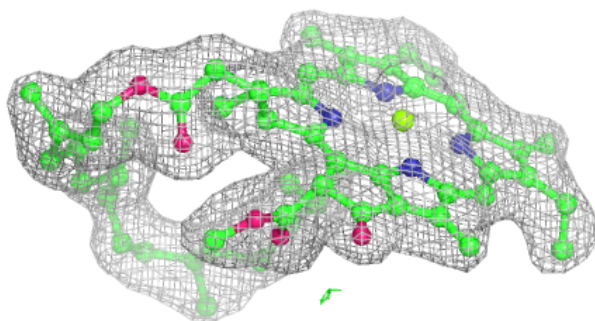
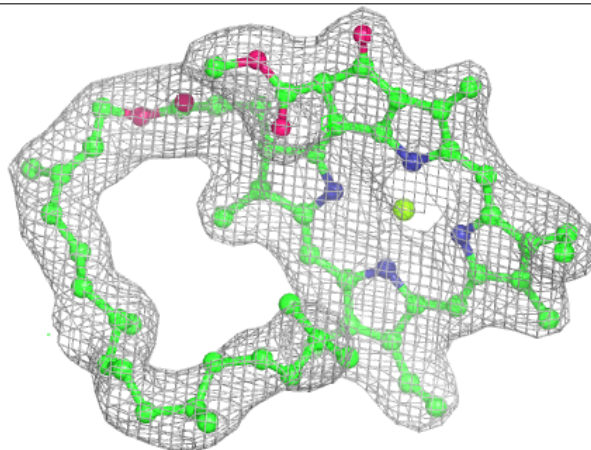


**Electron density around DGD J 101:**

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

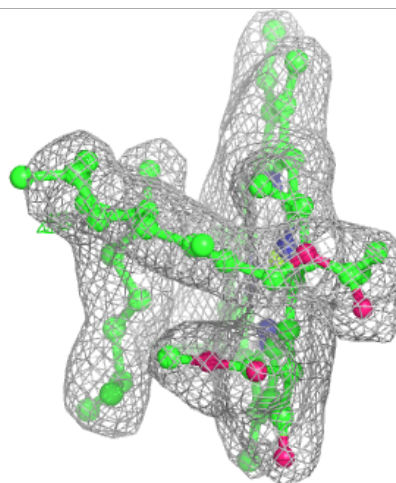
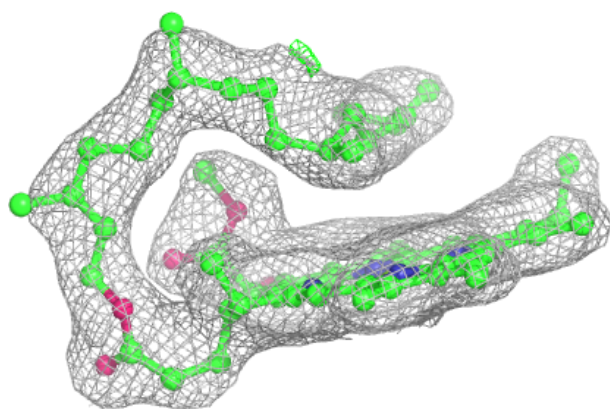
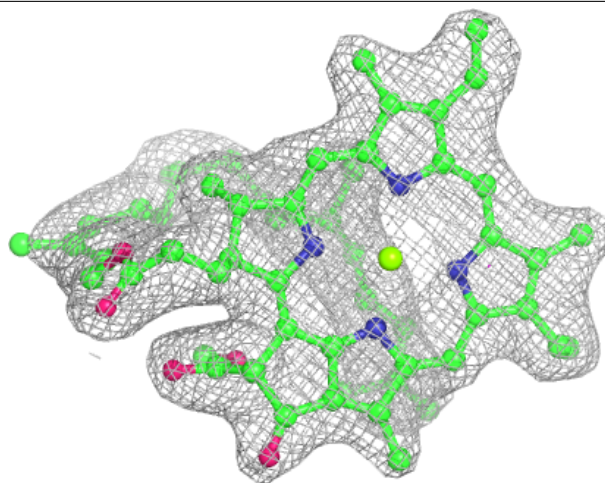
**Electron density around CLA b 615:**

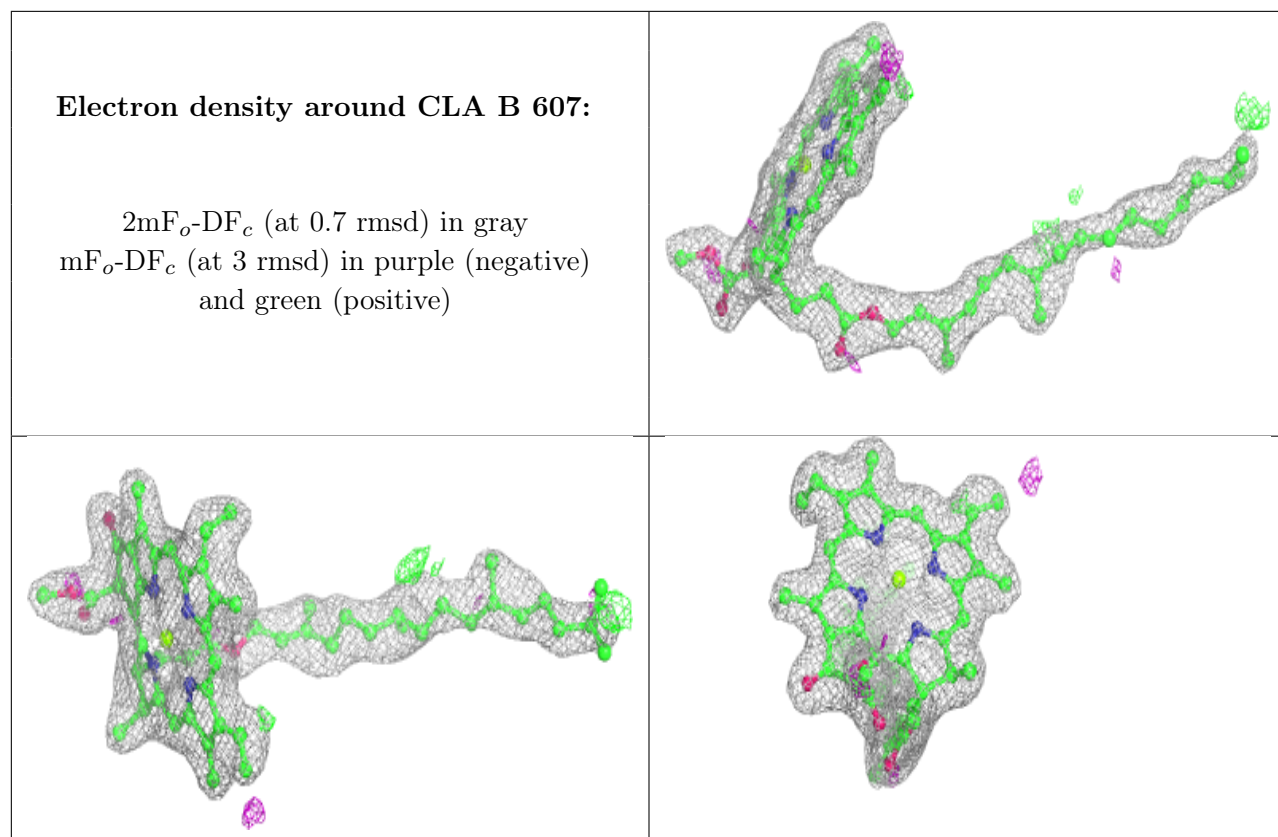
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 510:**

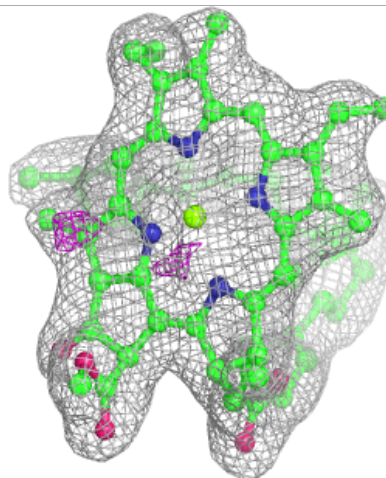
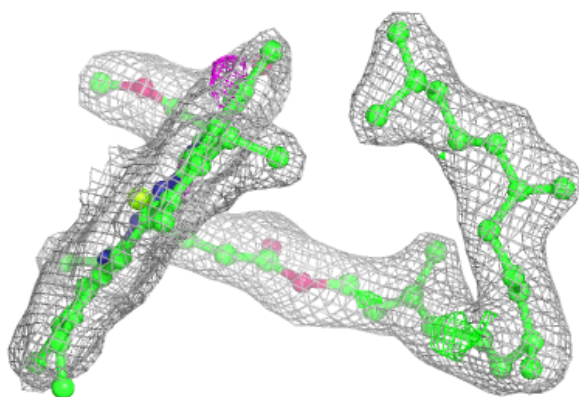
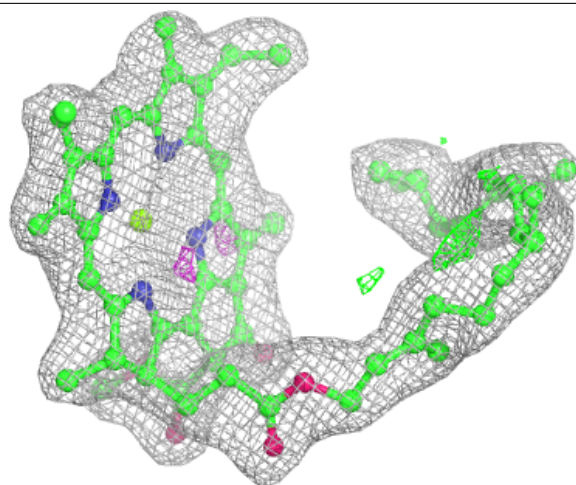
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





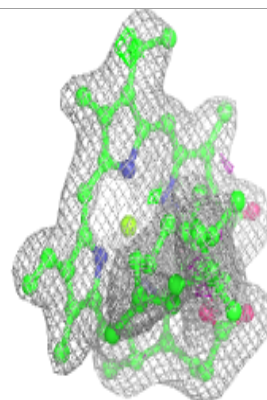
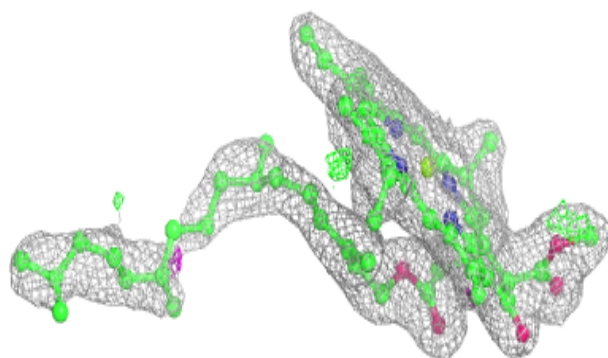
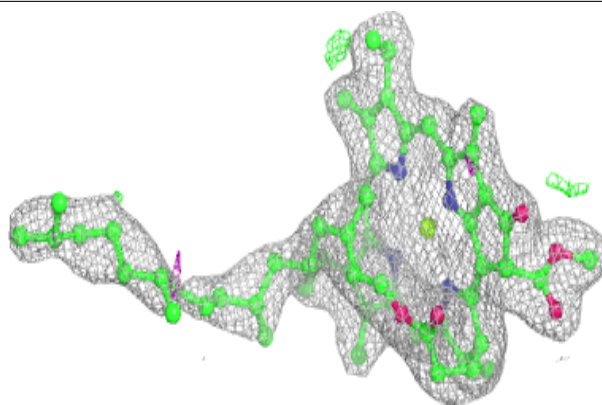
**Electron density around CLA C 503:**

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

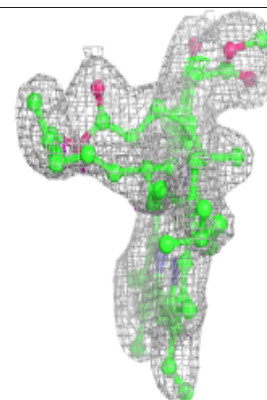
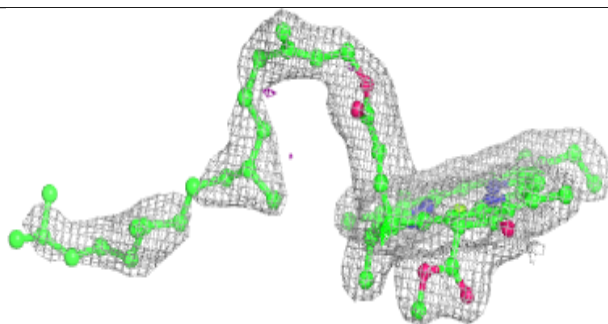
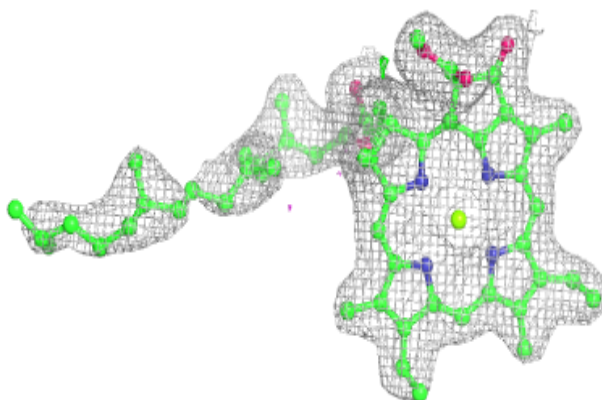


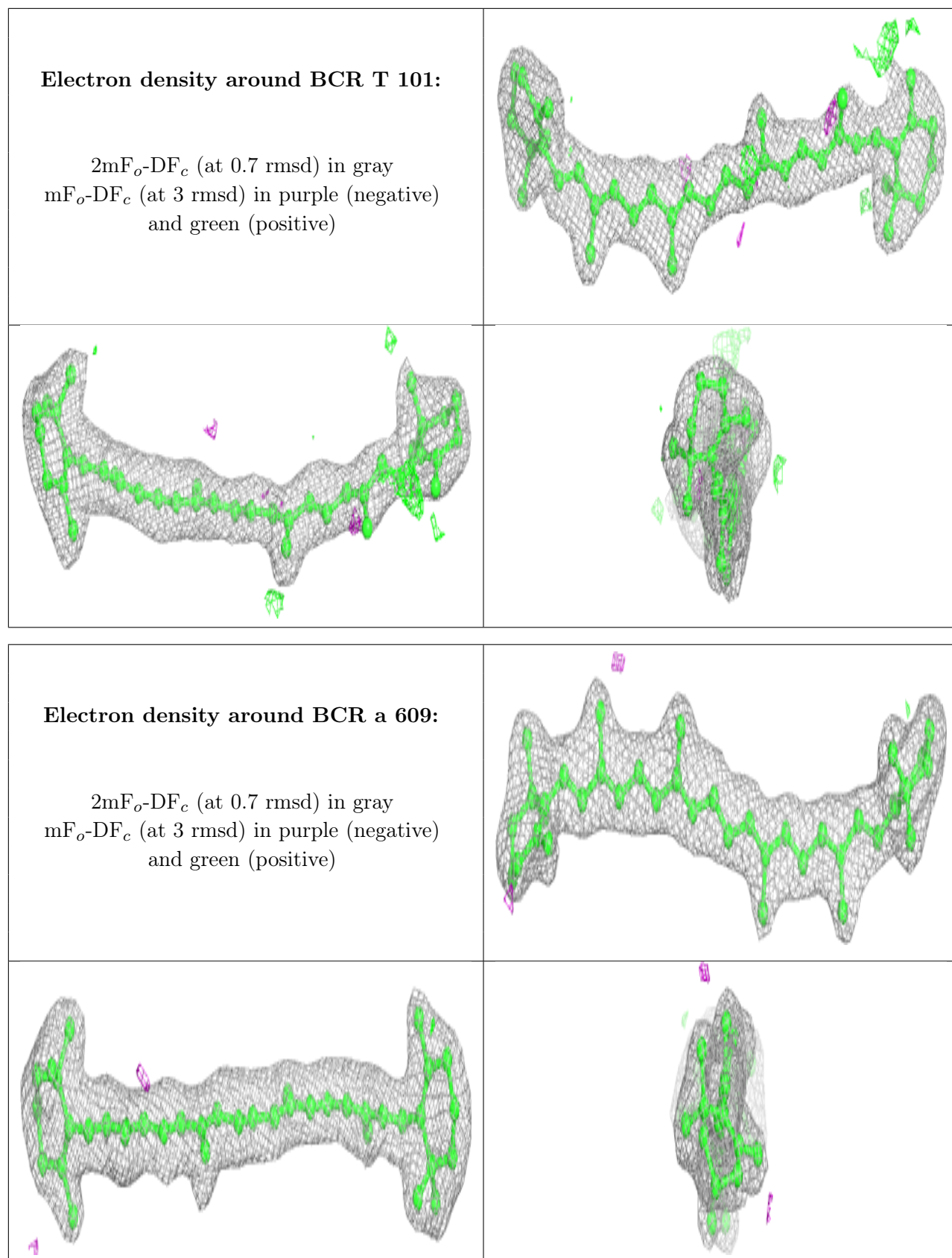
**Electron density around CLA C 505:**

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

**Electron density around CLA 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)

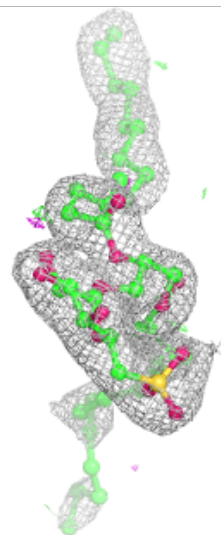
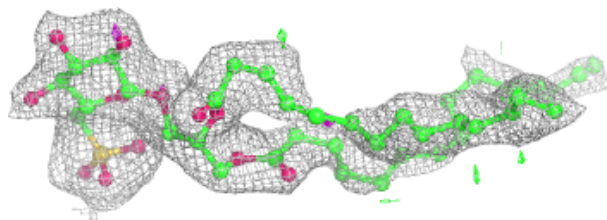
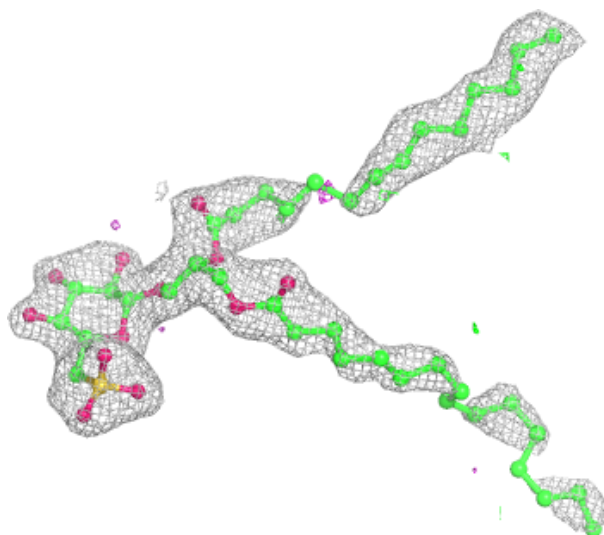






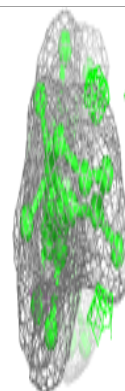
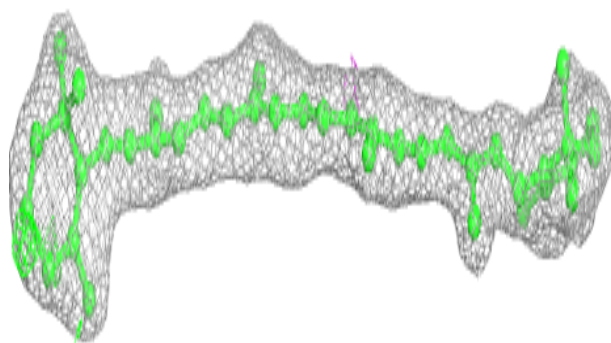
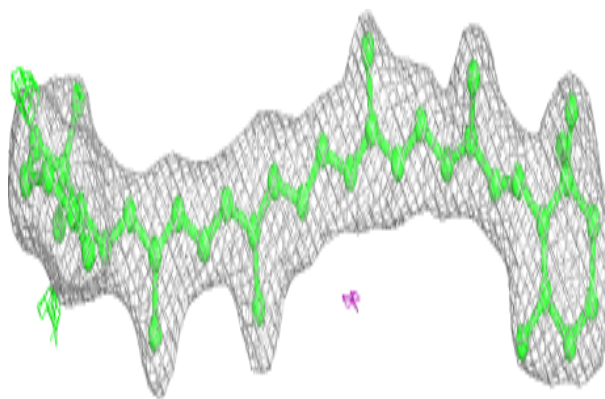
**Electron density around SQD A 613:**

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

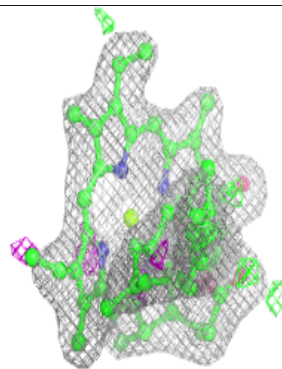
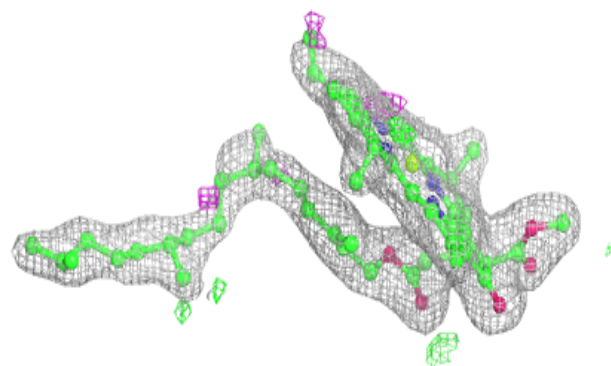
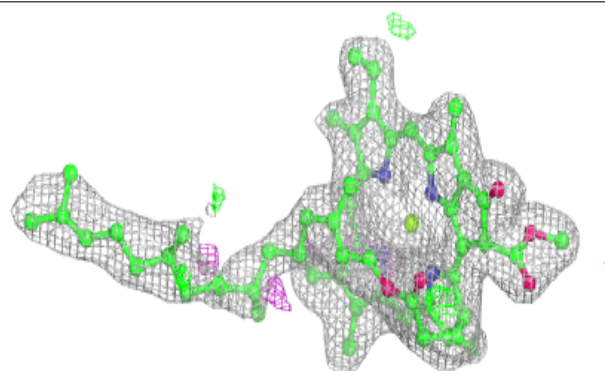


**Electron density around BCR b 617:**

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

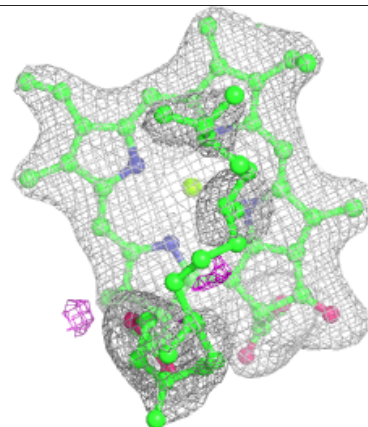
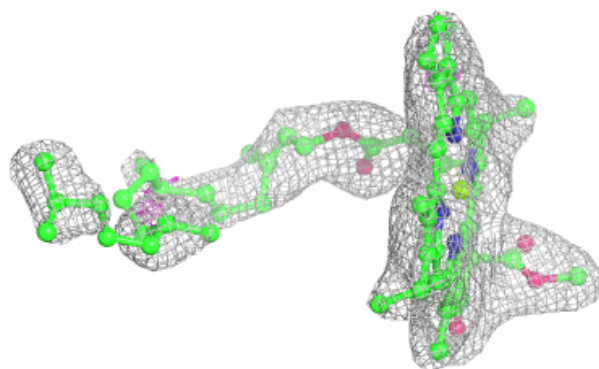
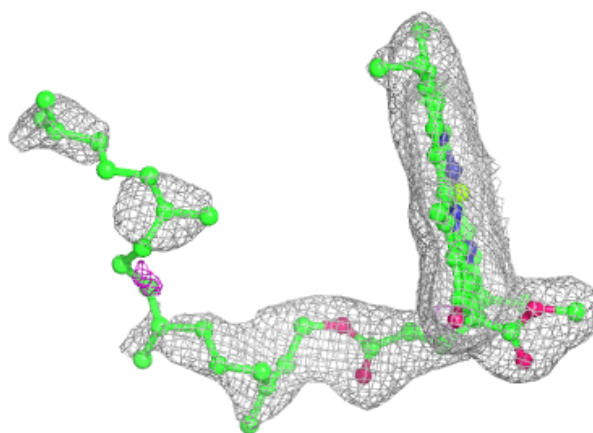
**Electron density around CLA c 505:**

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

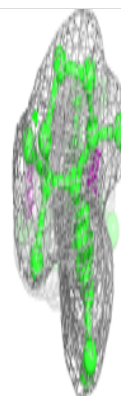
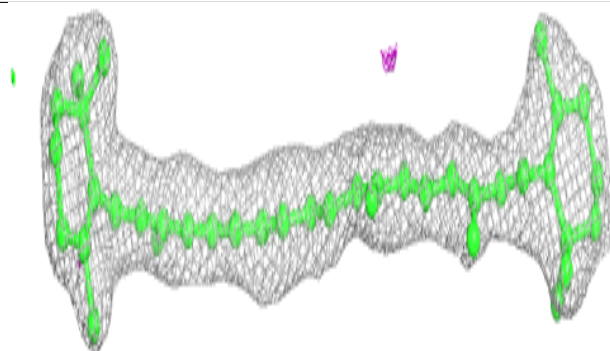
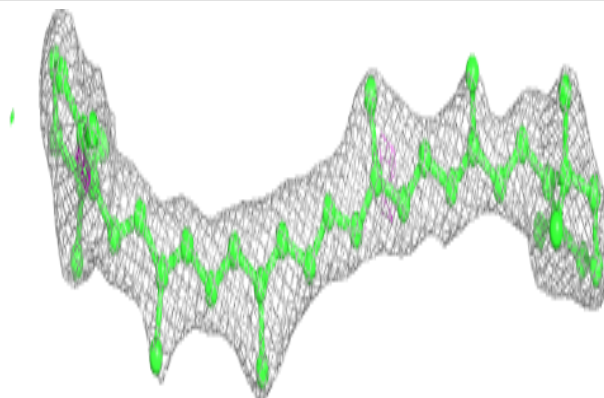


**Electron density around CLA c 506:**

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

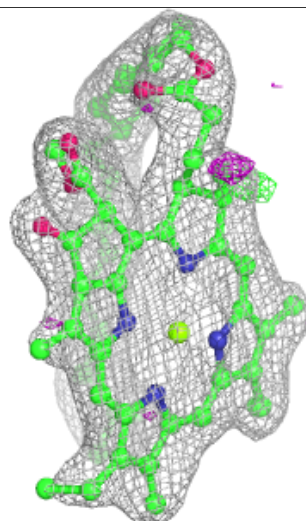
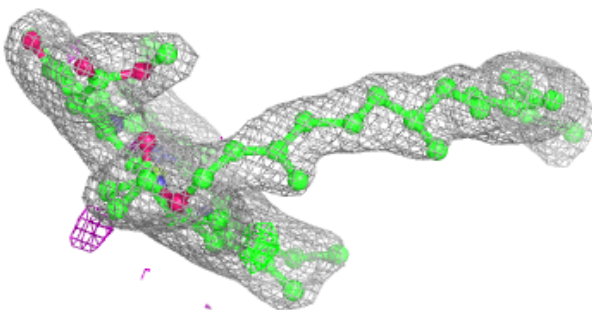
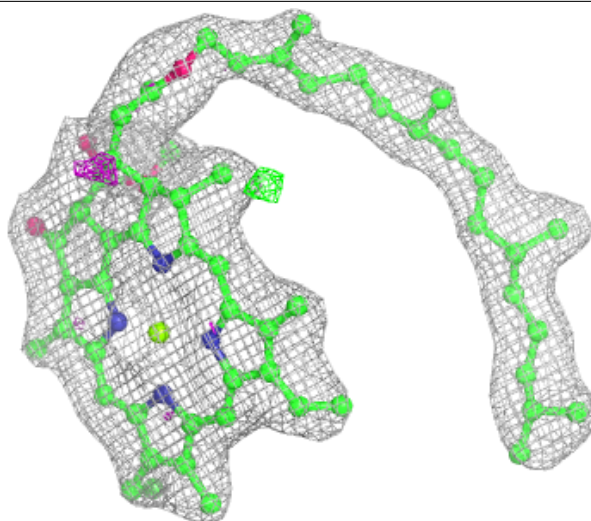
**Electron density around BCR c 514:**

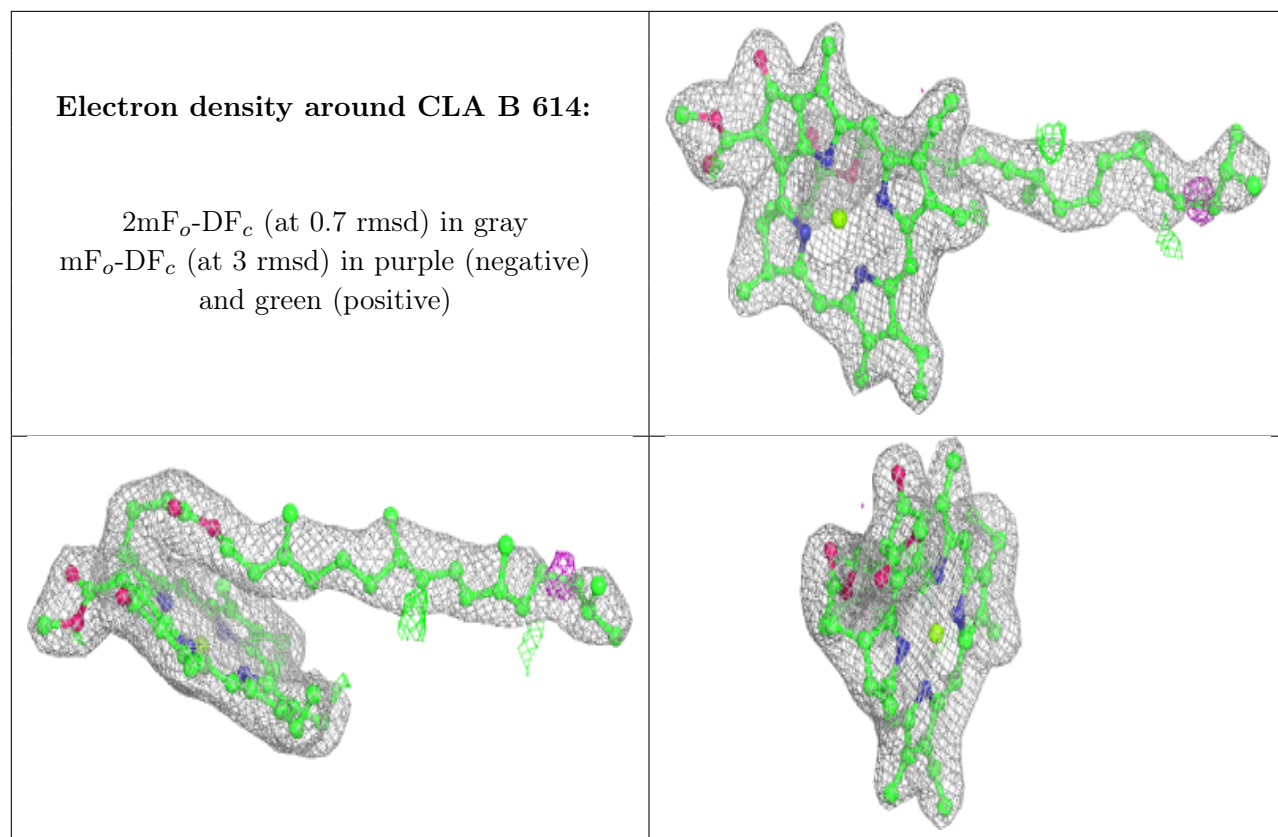
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 507:**

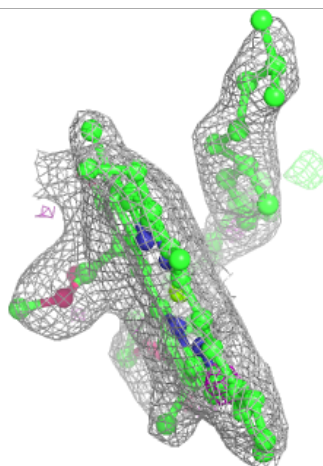
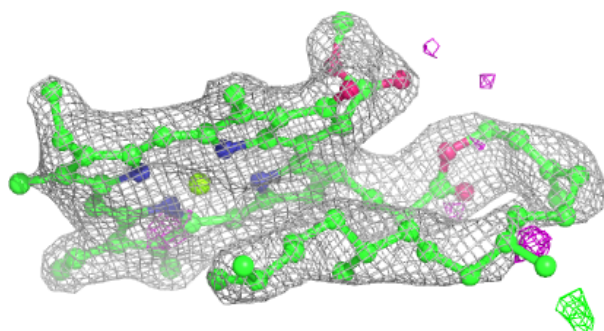
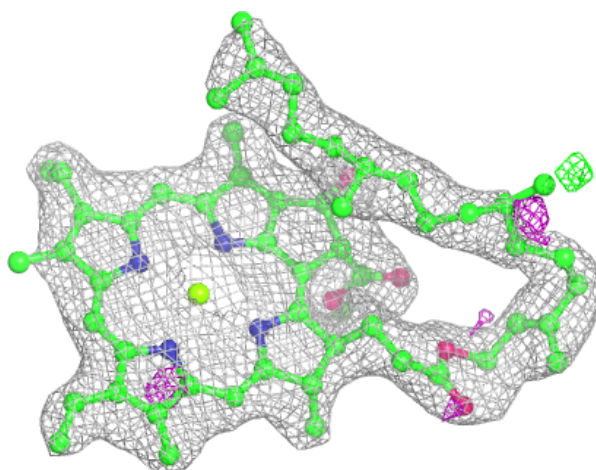
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





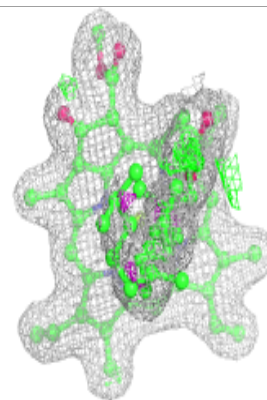
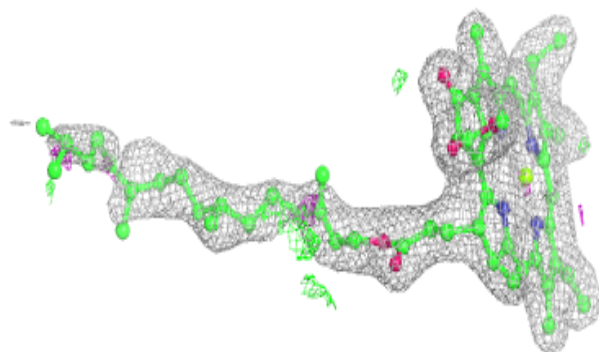
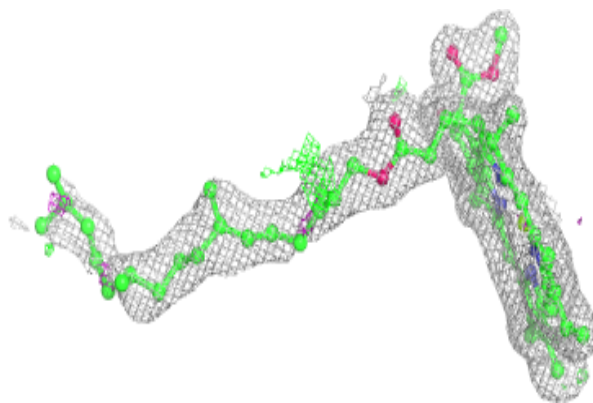
**Electron density around CLA c 509:**

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

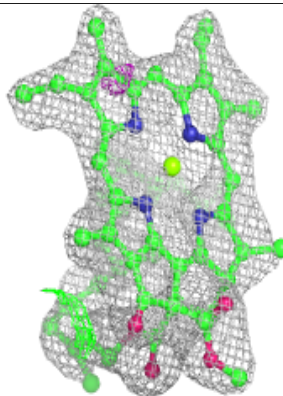
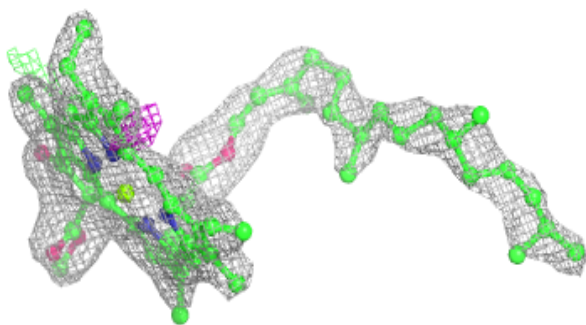
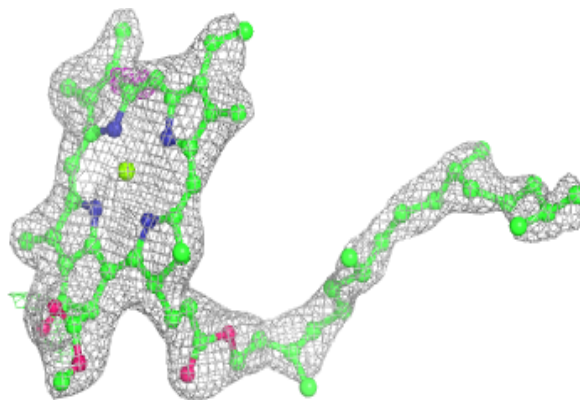


**Electron density around CLA B 604:**

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

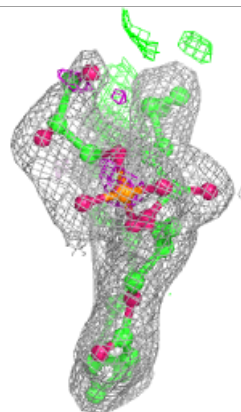
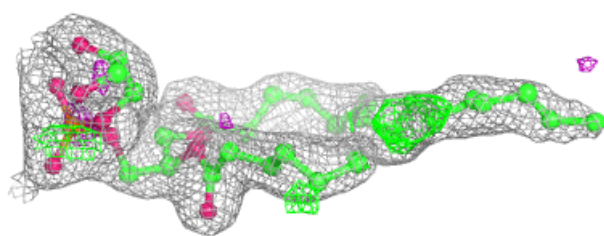
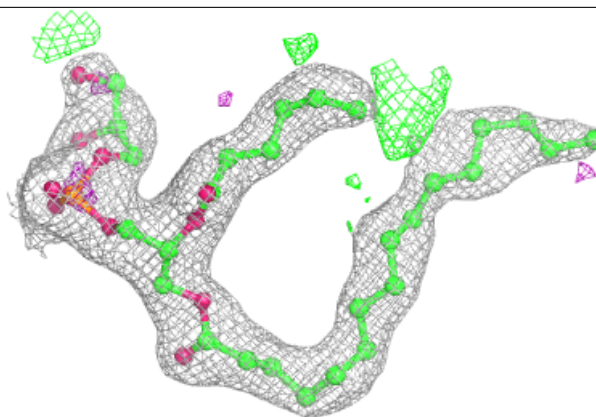
**Electron density around CLA c 511:**

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

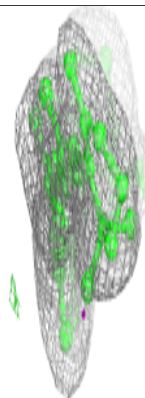
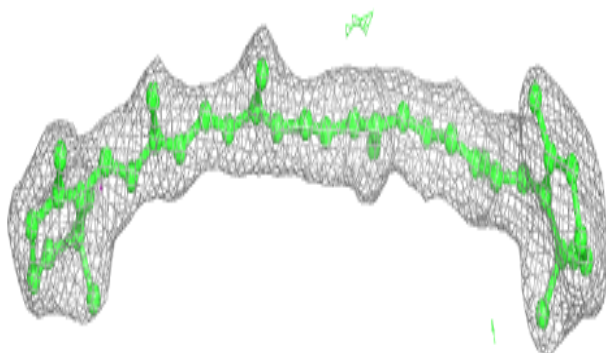
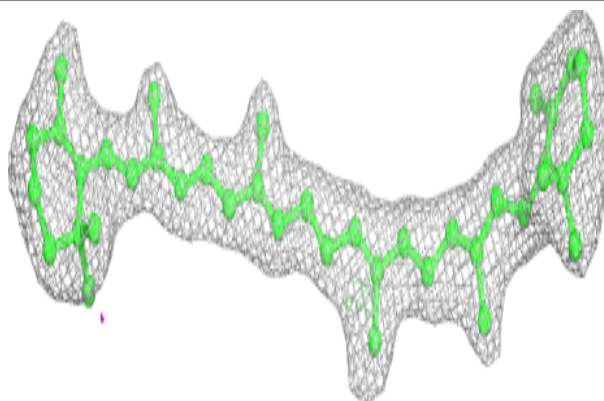


**Electron density around LHG d 409:**

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

**Electron density around BCR t 101:**

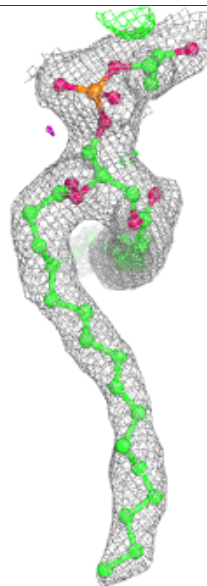
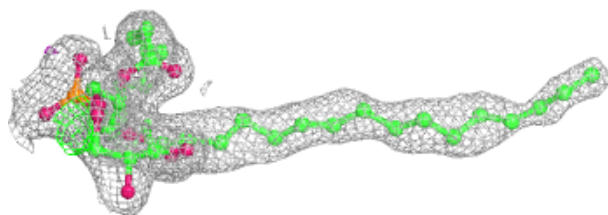
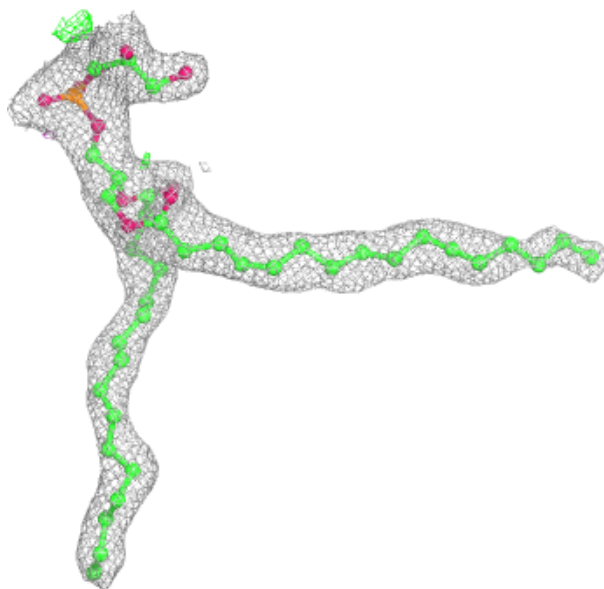
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





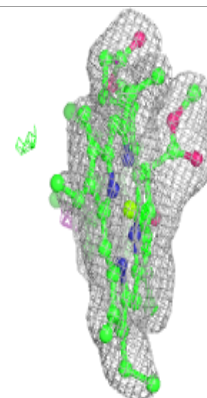
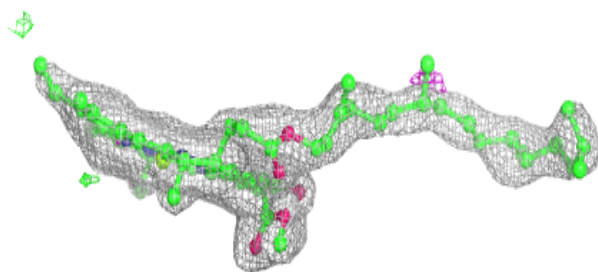
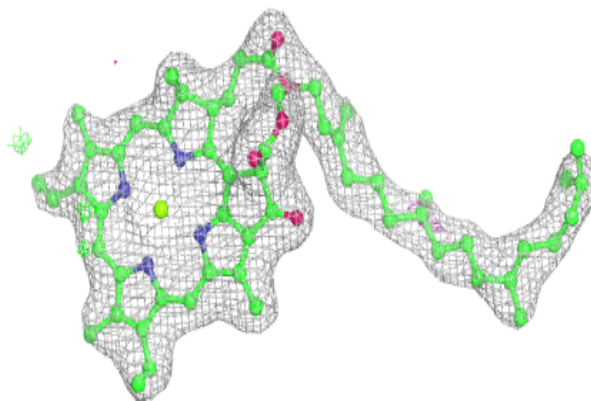
**Electron density around LHG 1 101:**

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

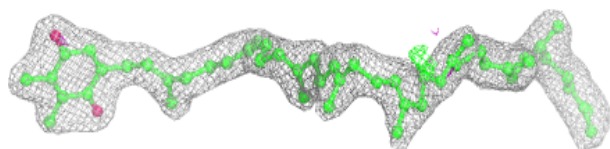
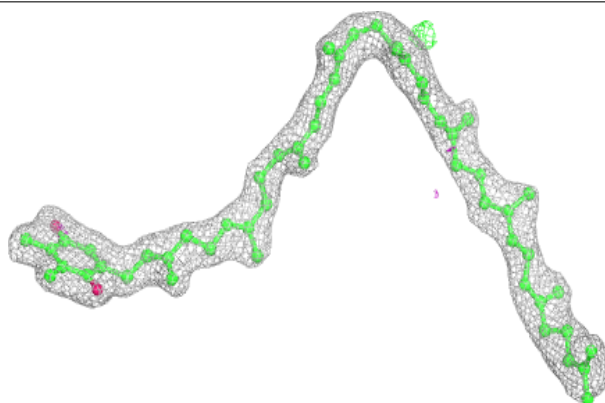


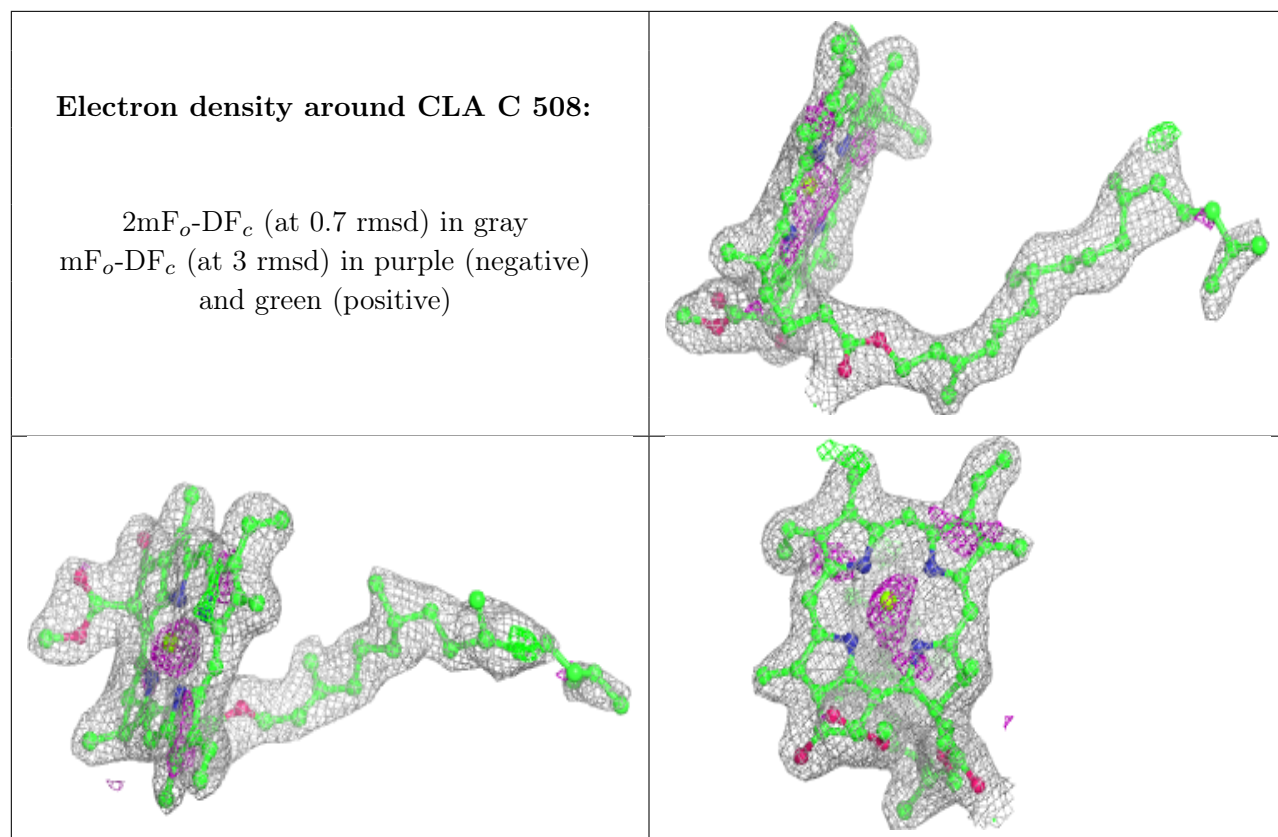
**Electron density around CLA b 602:**

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

**Electron density around PL9 D 406:**

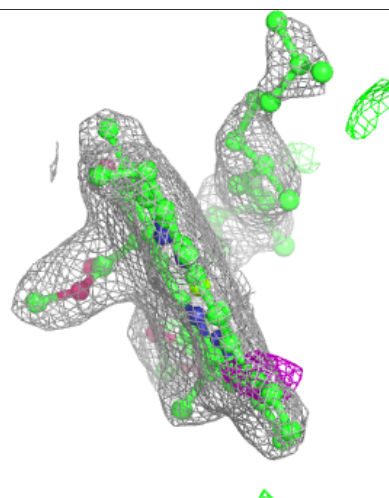
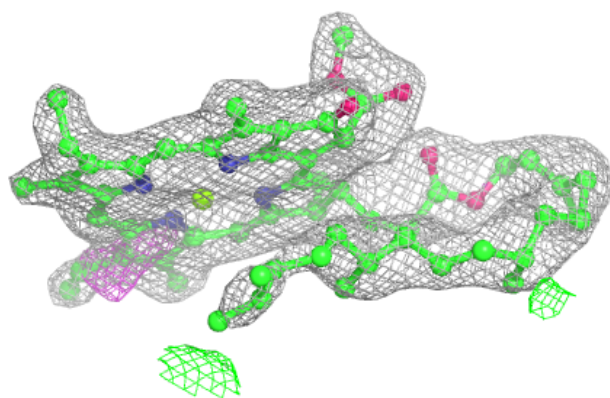
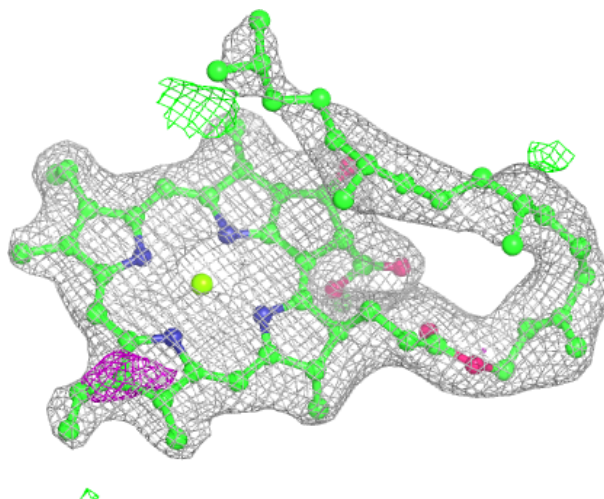
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

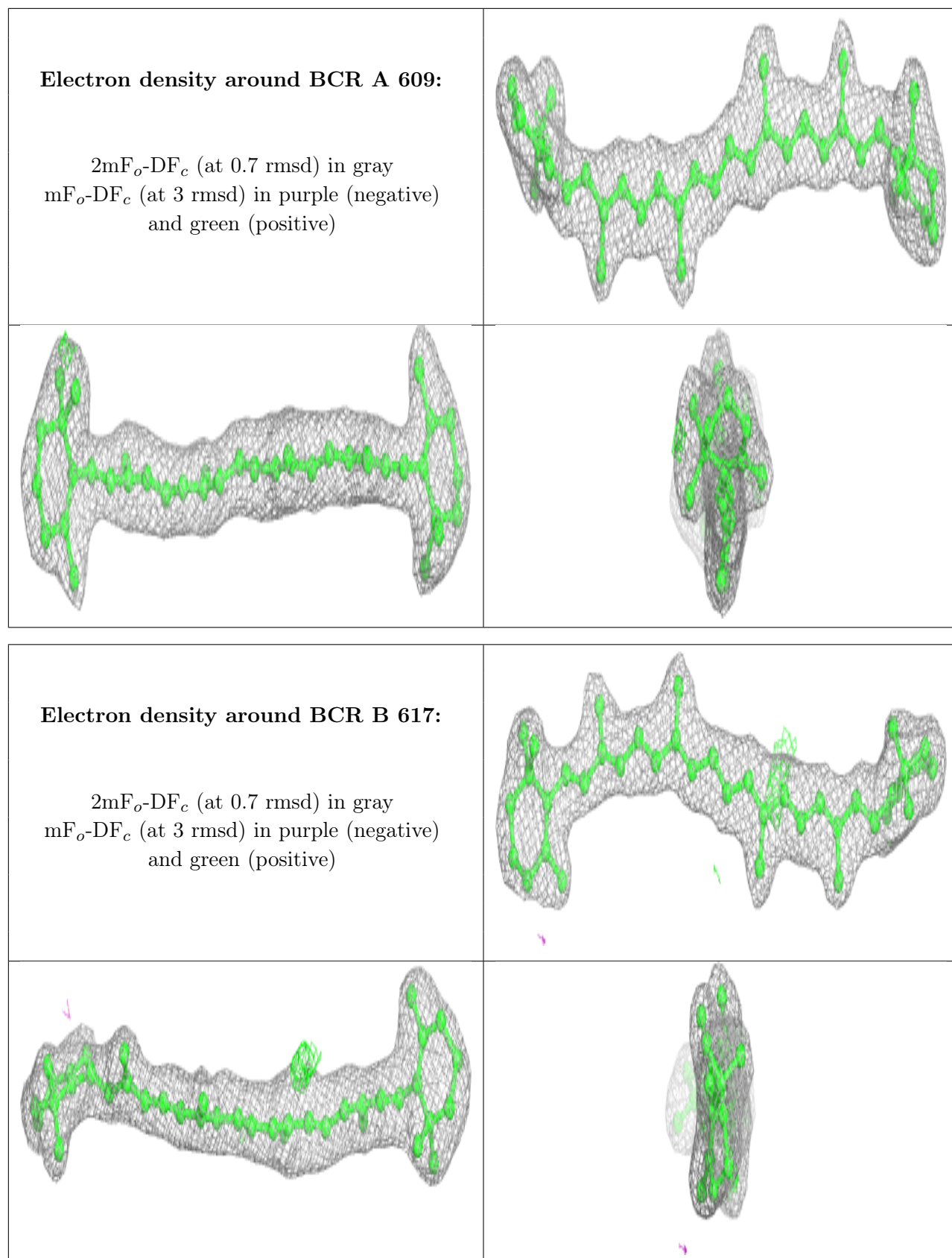




**Electron density around CLA C 509:**

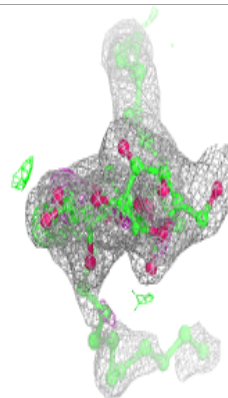
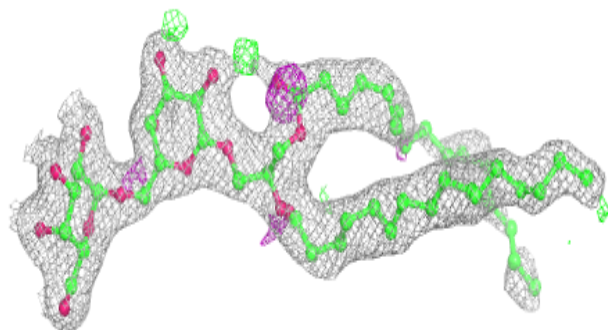
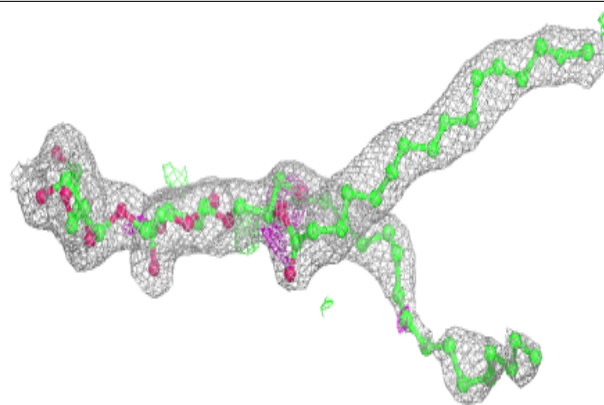
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



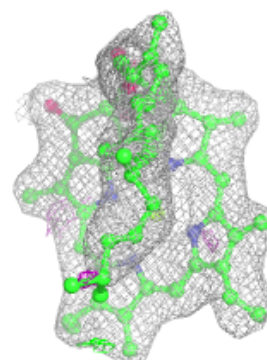
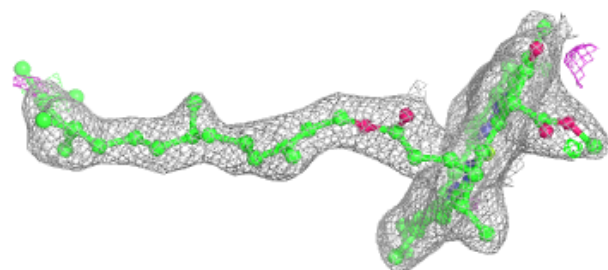
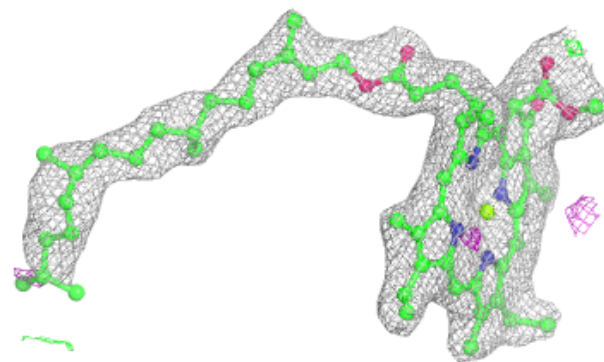


**Electron density around DGD c 515:**

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

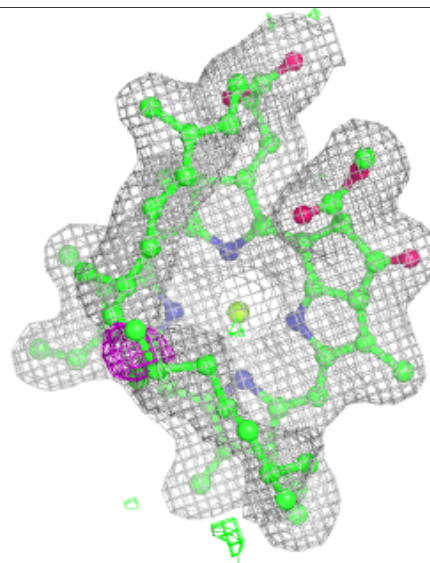
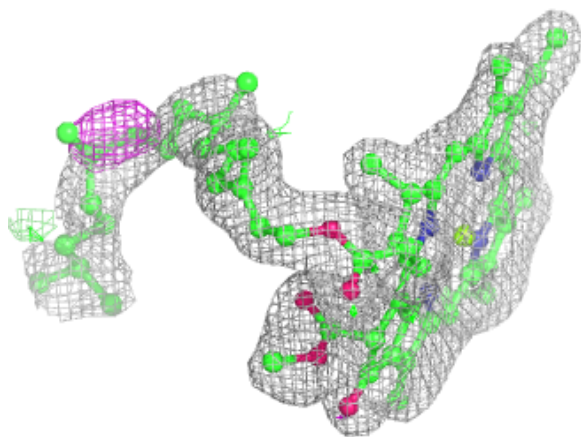
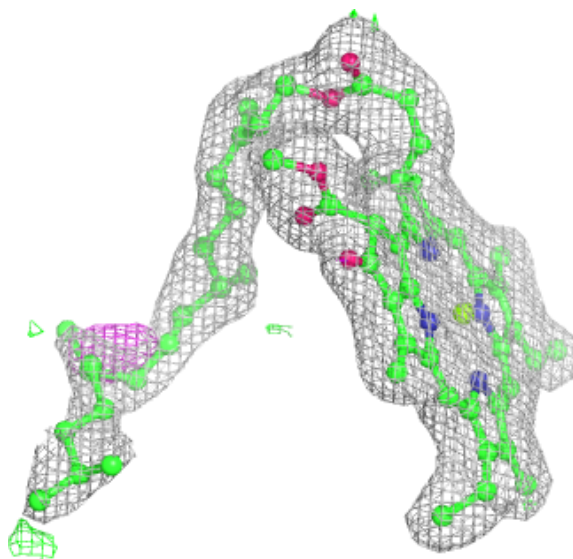
**Electron density around CLA b 609:**

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



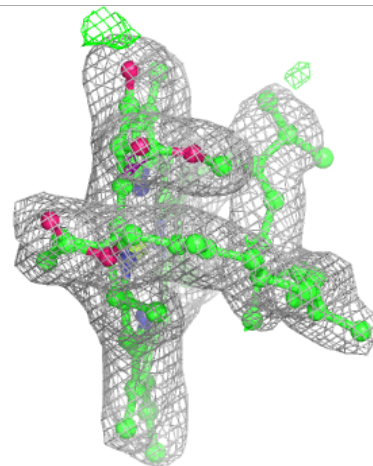
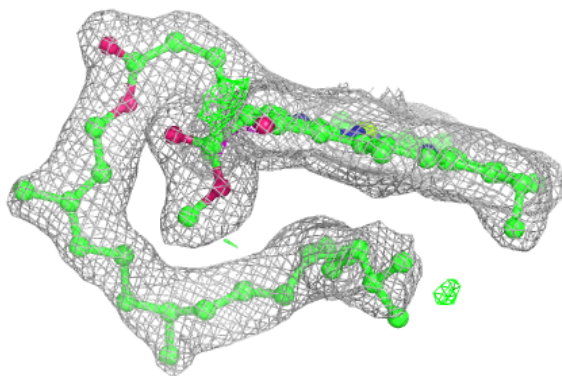
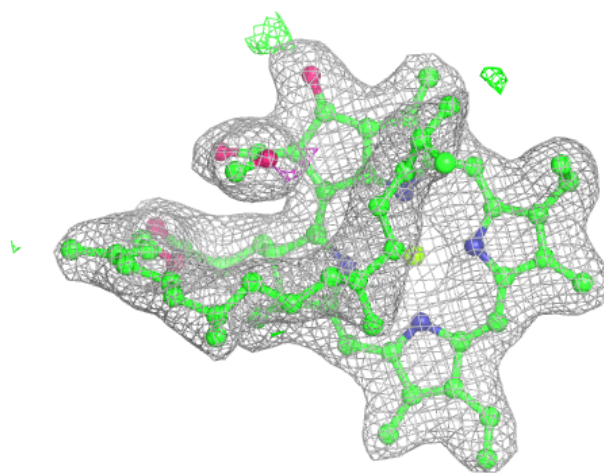
**Electron density around CLA b 613:**

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



**Electron density around CLA C 510:**

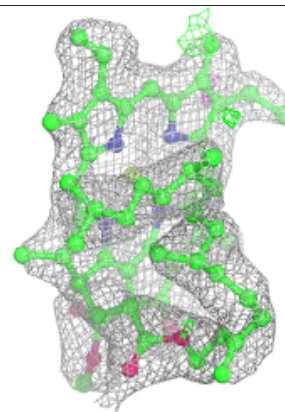
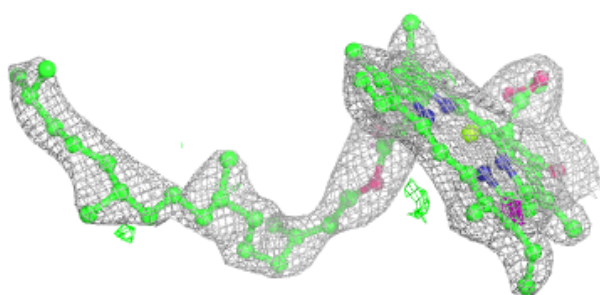
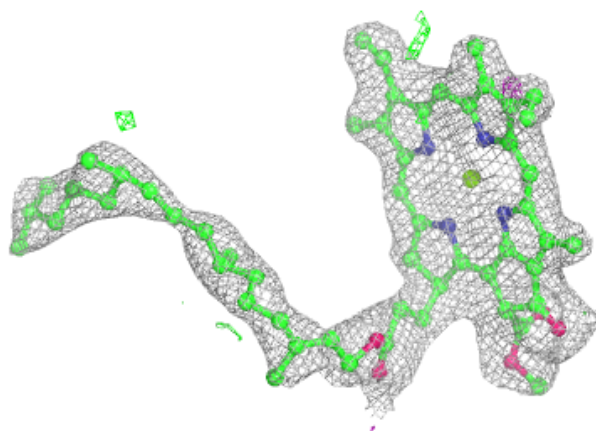
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



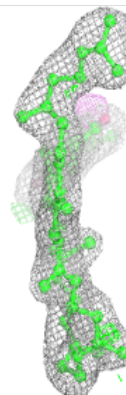
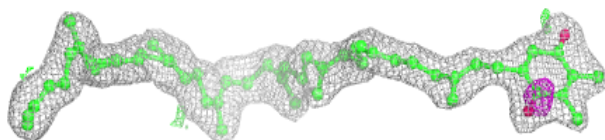
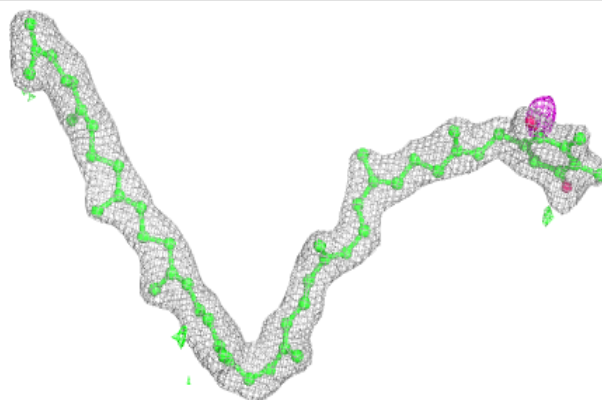


**Electron density around CLA C 511:**

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

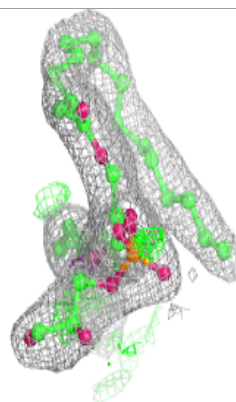
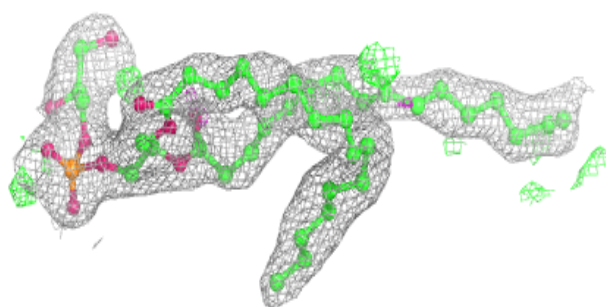
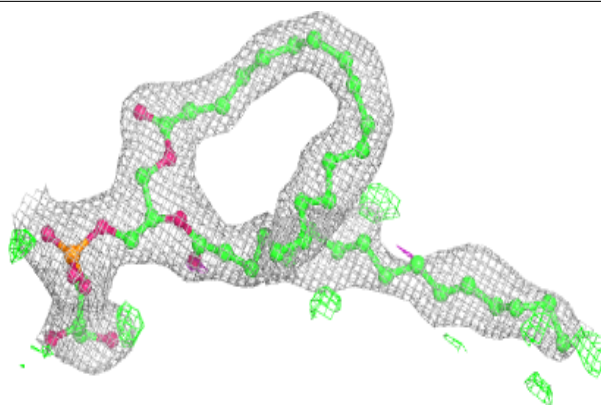
**Electron density around PL9 d 406:**

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

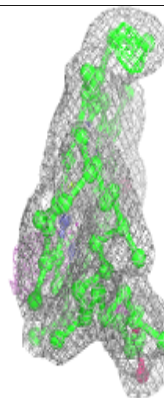
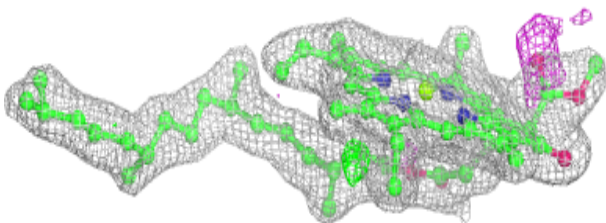
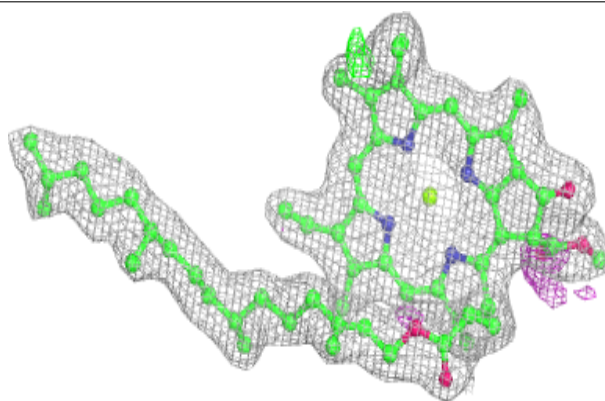


**Electron density around LHG D 412:**

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

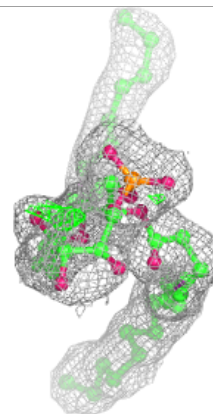
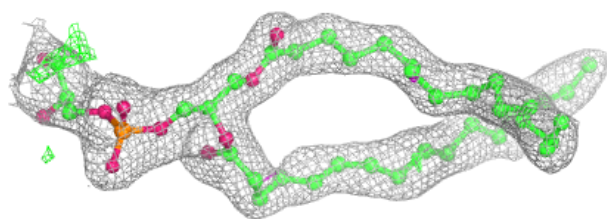
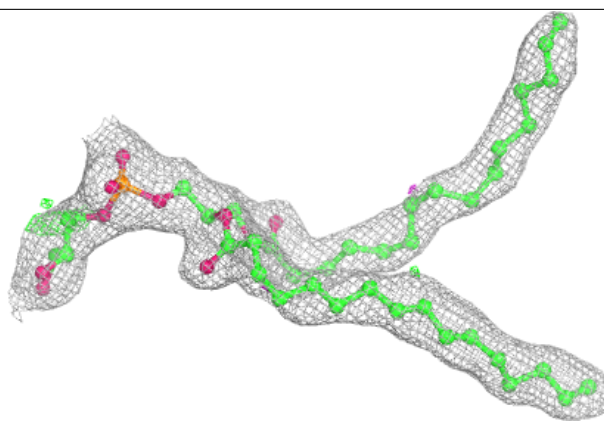
**Electron density around CLA C 501:**

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

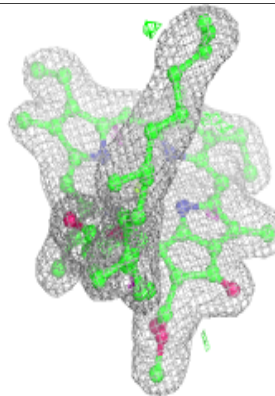
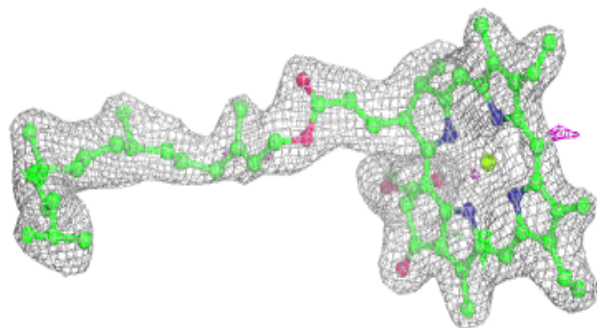
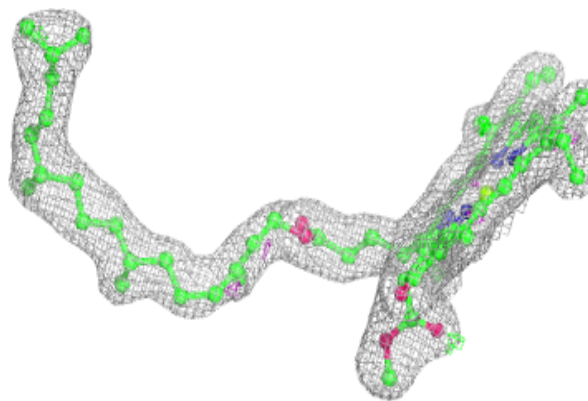


**Electron density around LHG d 408:**

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

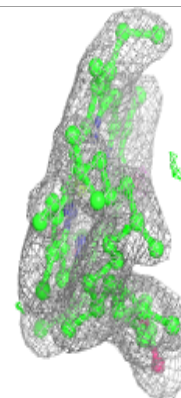
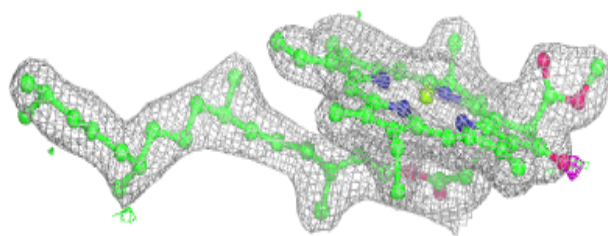
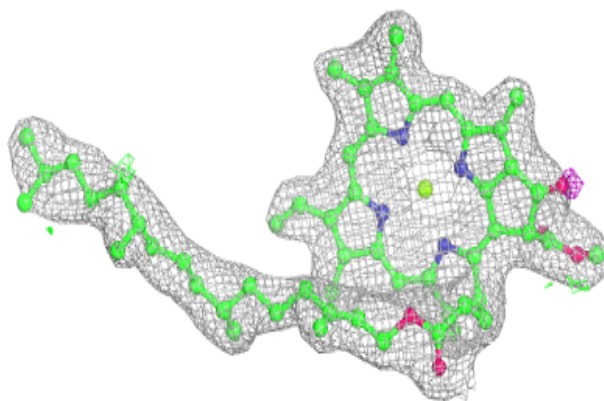
**Electron density around CLA D 403:**

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

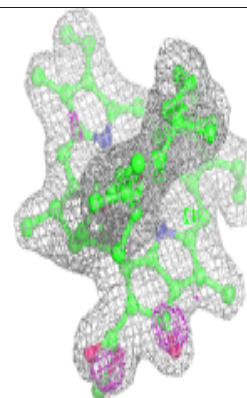
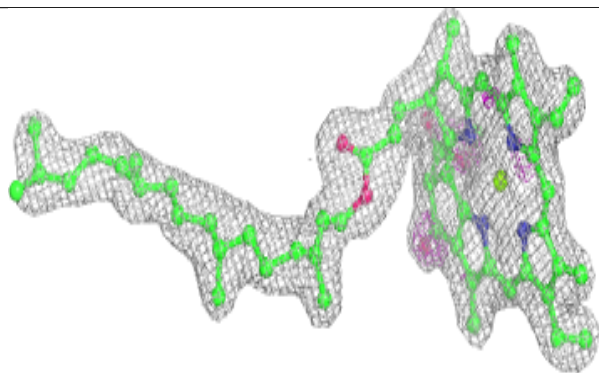
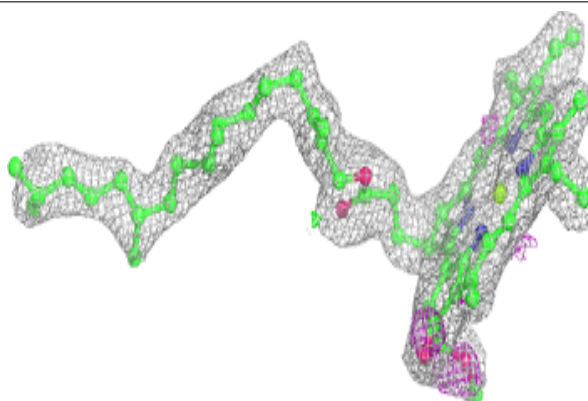


**Electron density around CLA c 501:**

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

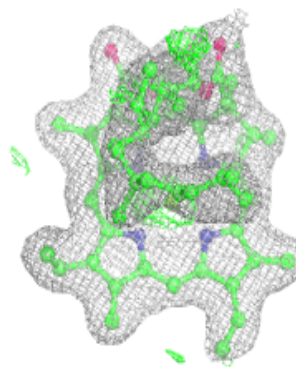
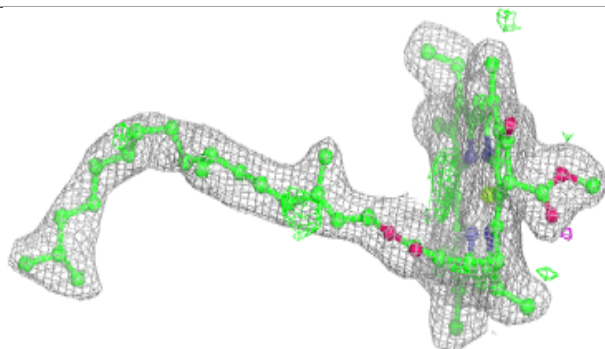
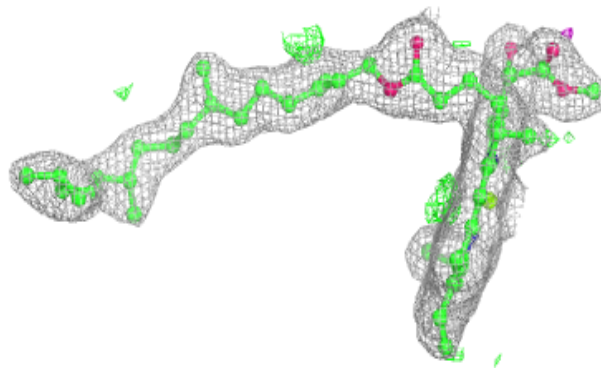
**Electron density around CLA C 502:**

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

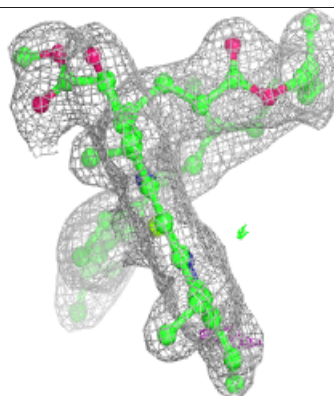
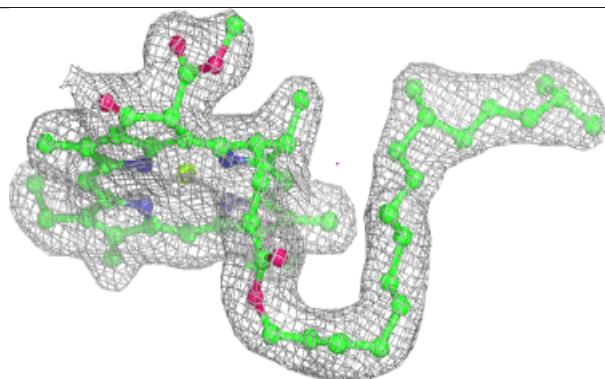
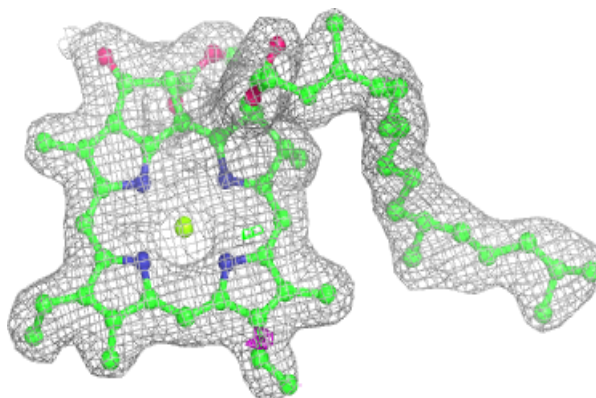


**Electron density around CLA B 605:**

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

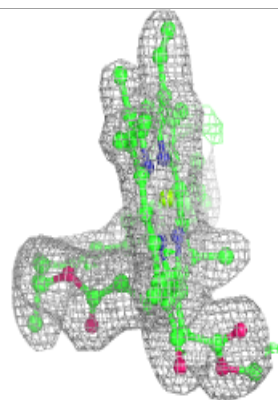
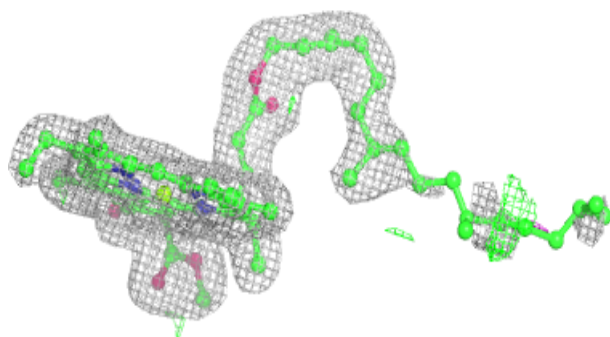
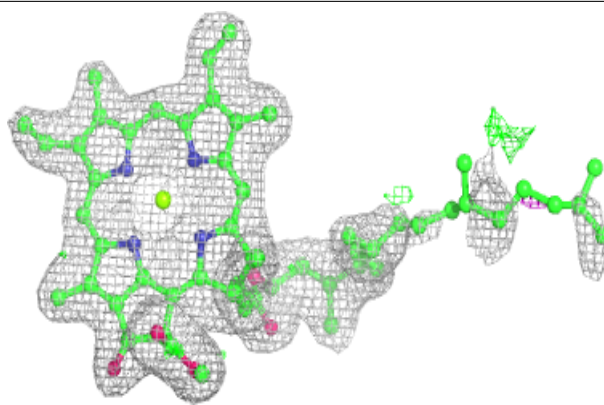
**Electron density around CLA A 611:**

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

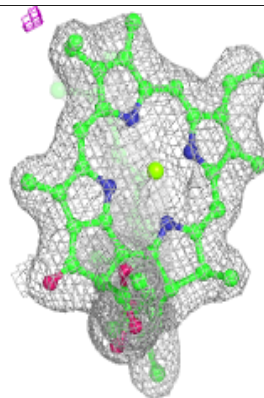
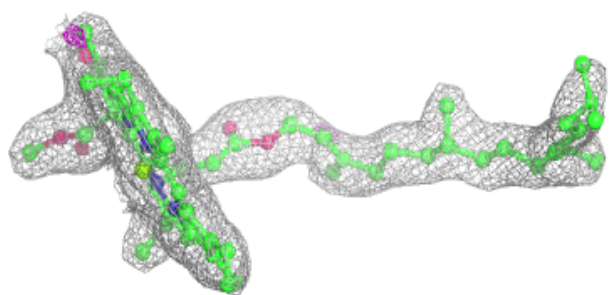
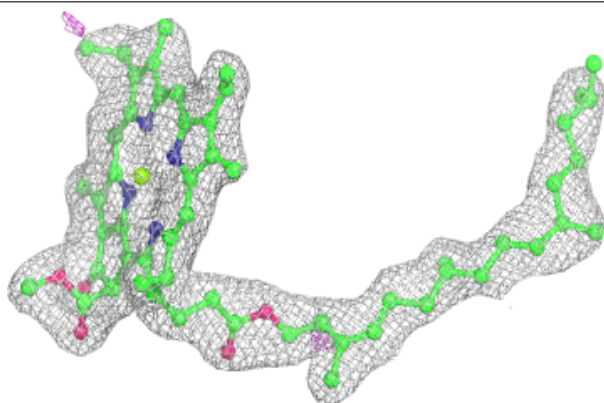


**Electron density around CLA A 607:**

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

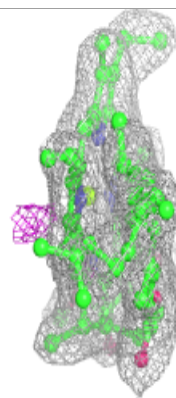
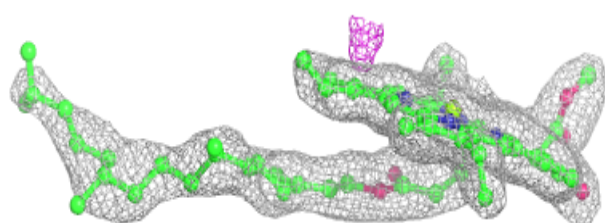
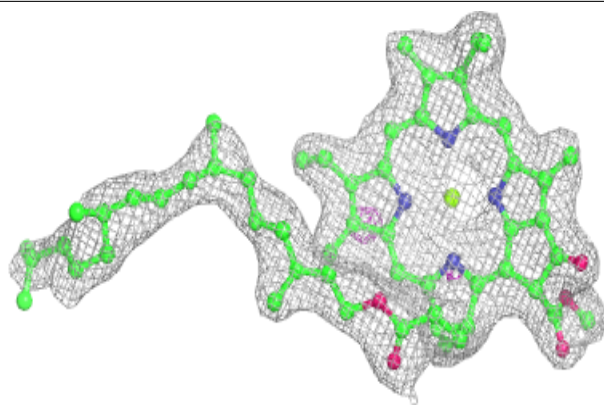
**Electron density around CLA B 609:**

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

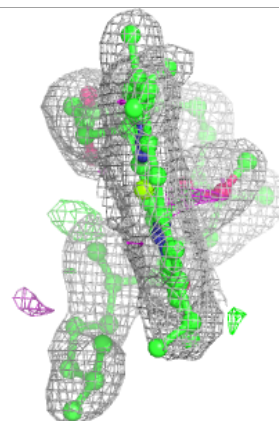
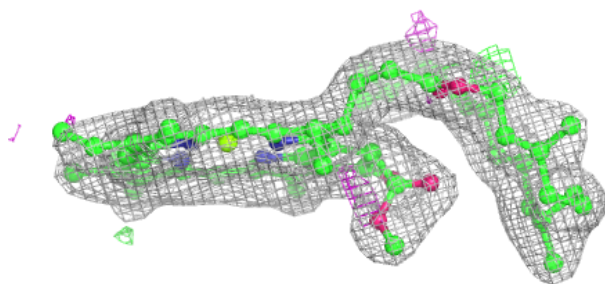
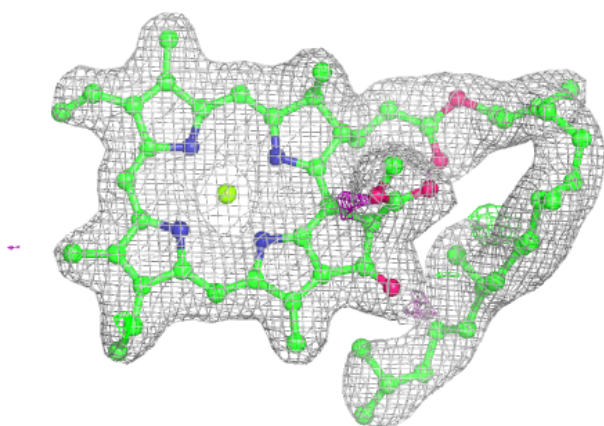


**Electron density around CLA b 603:**

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

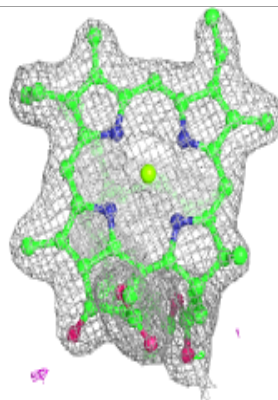
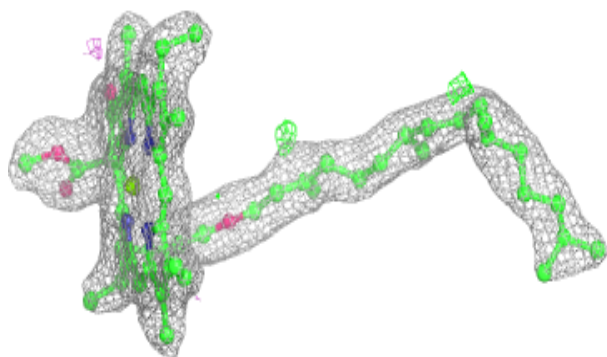
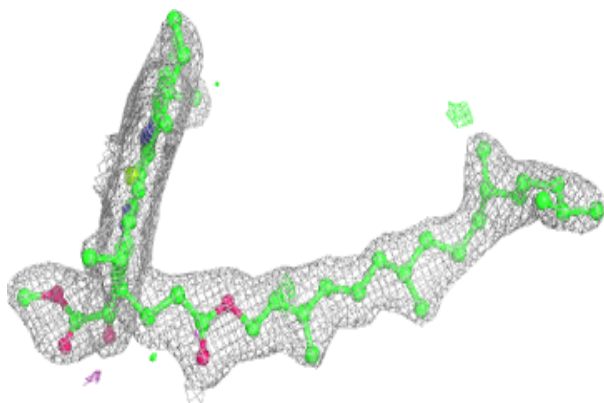
**Electron density around CLA B 610:**

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

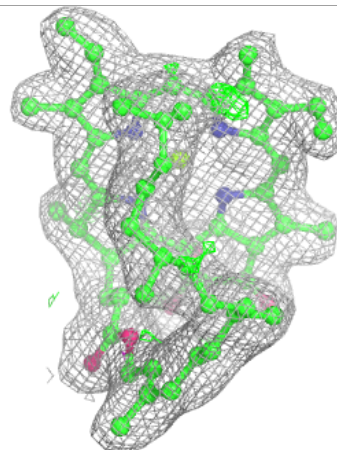
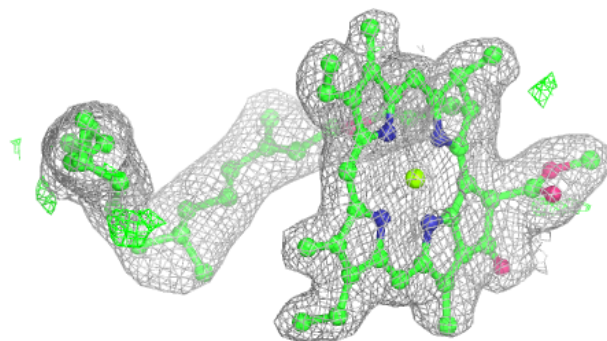
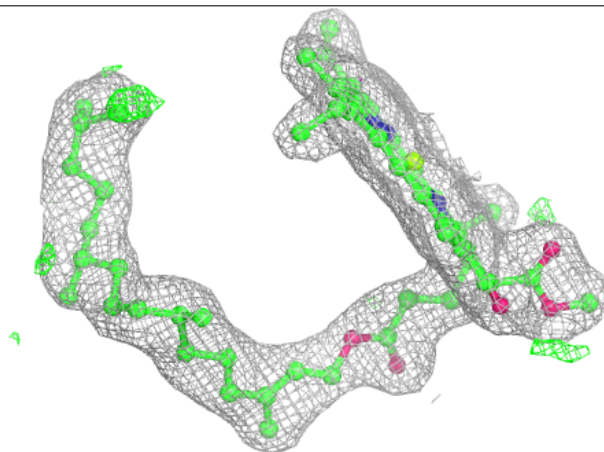


**Electron density around CLA b 605:**

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

**Electron density around CLA B 611:**

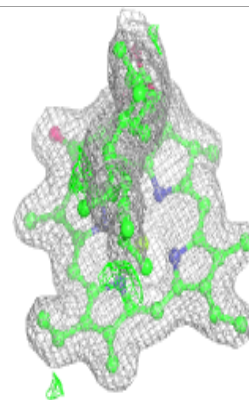
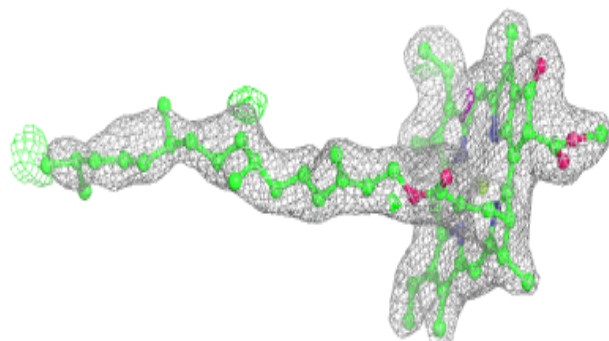
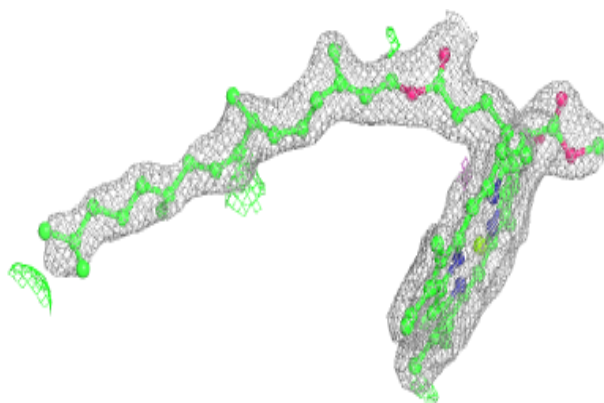
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



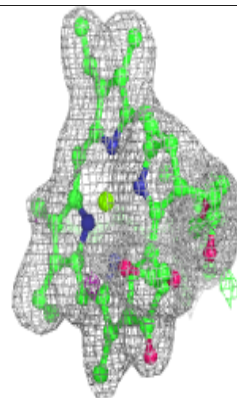
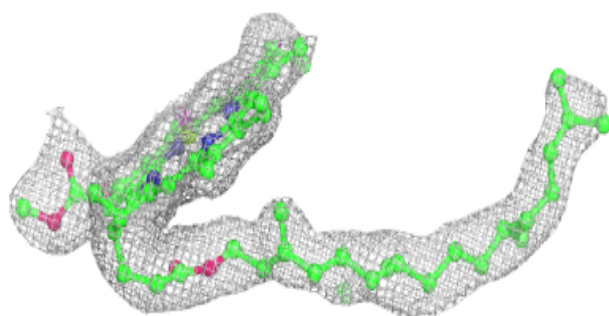
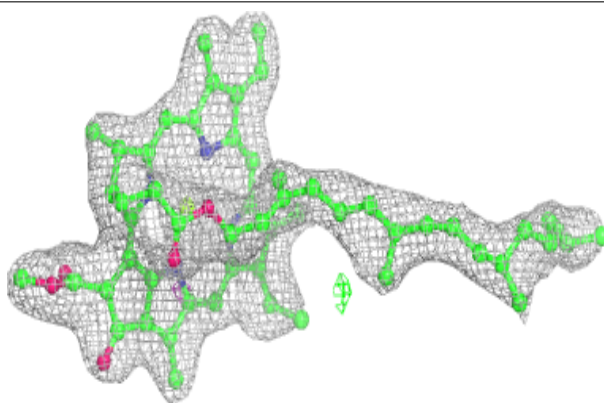


**Electron density around CLA b 607:**

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

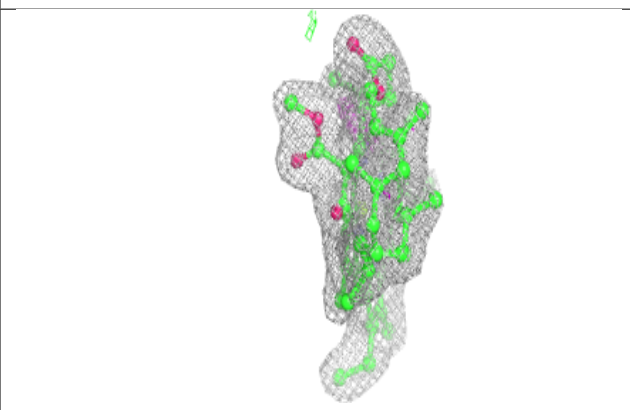
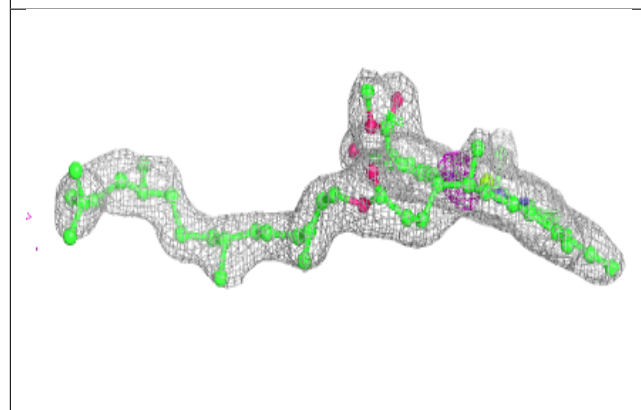
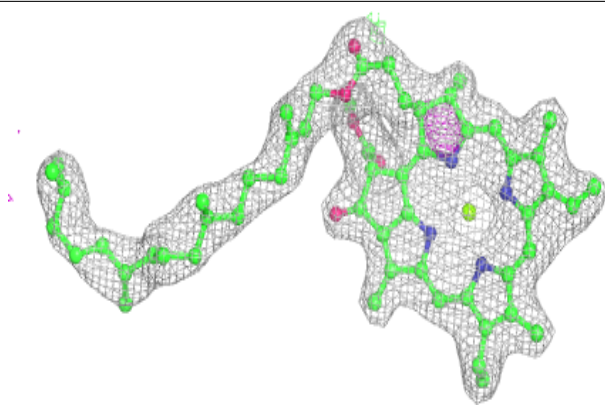
**Electron density around CLA b 608:**

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

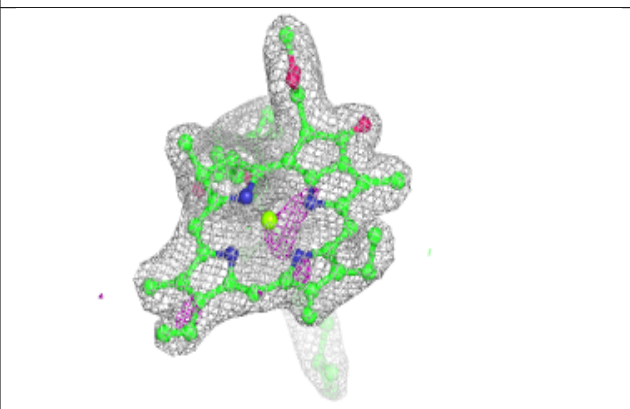
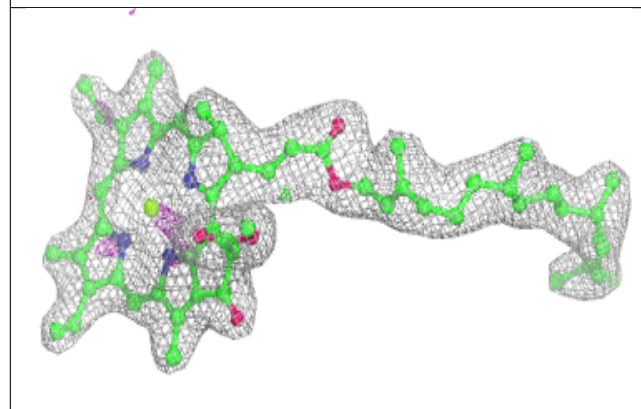
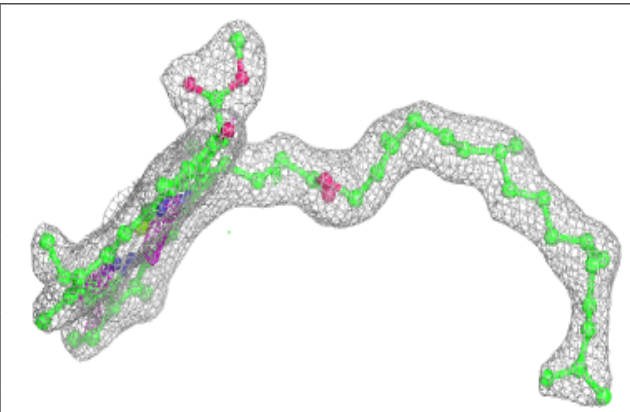


**Electron density around CLA B 602:**

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

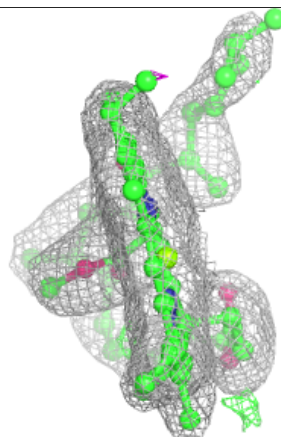
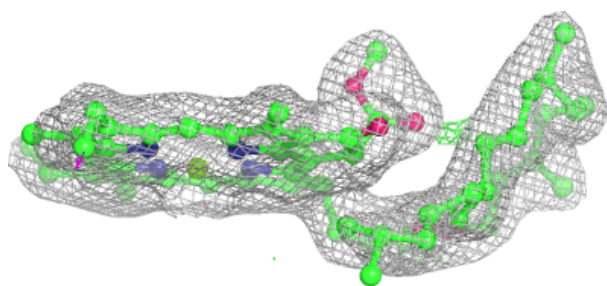
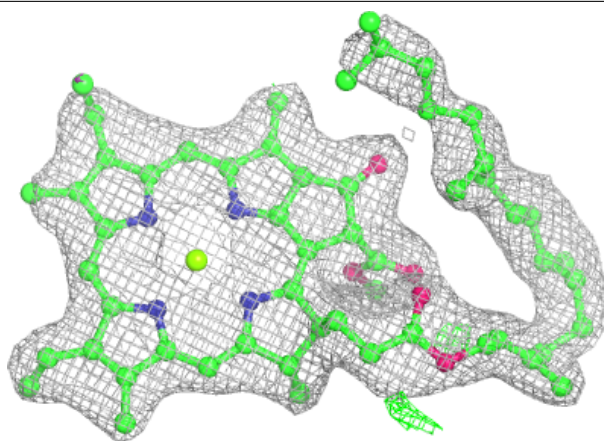
**Electron density around CLA d 403:**

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



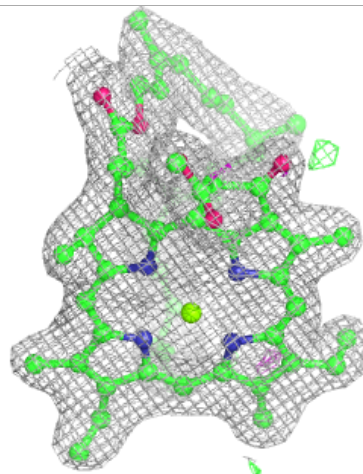
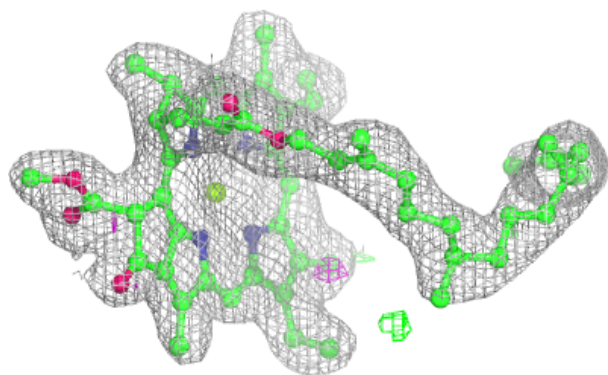
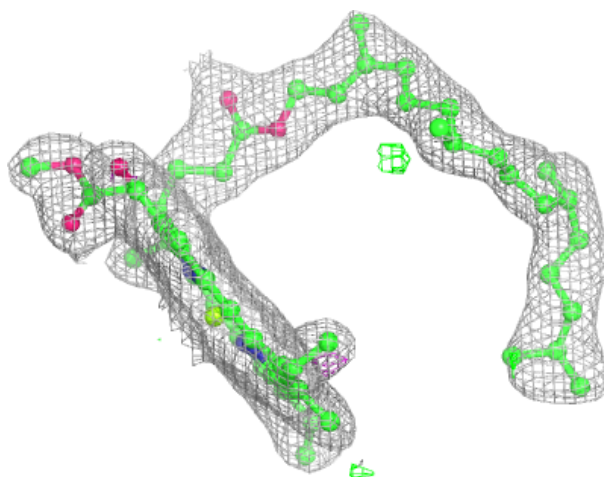
**Electron density around CLA b 610:**

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



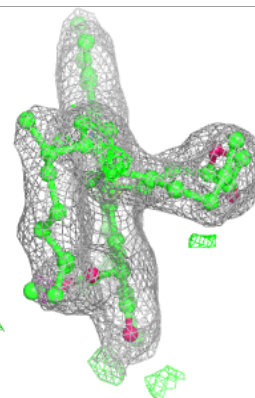
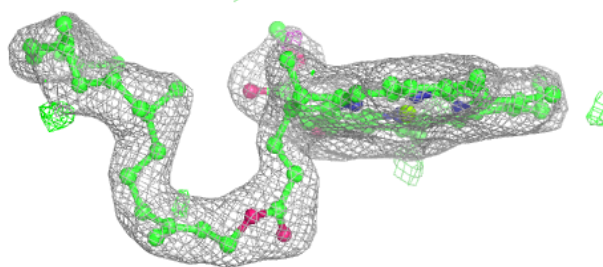
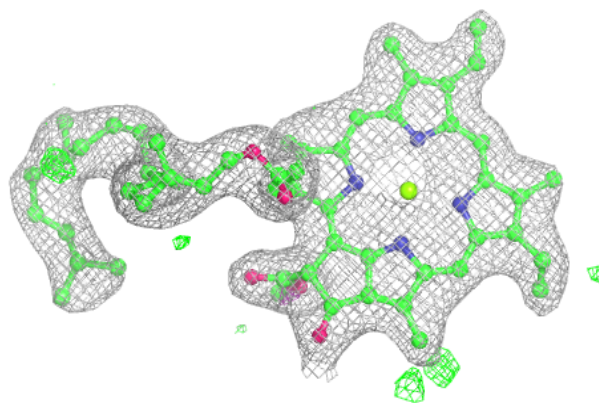
**Electron density around CLA b 611:**

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

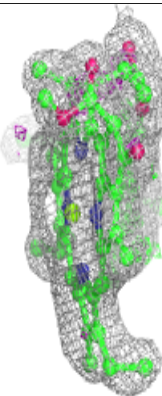
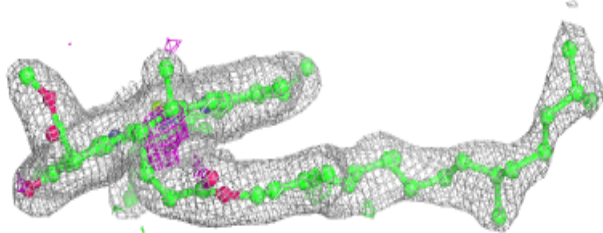
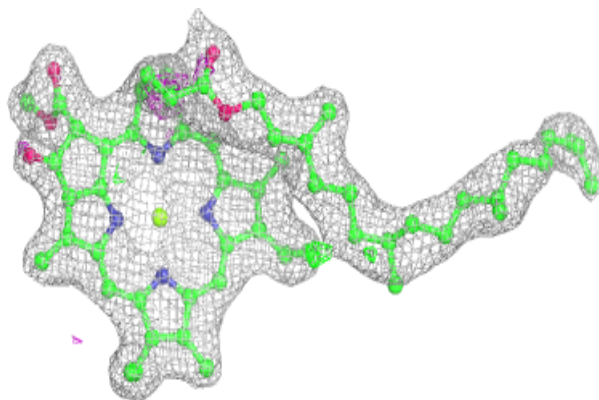


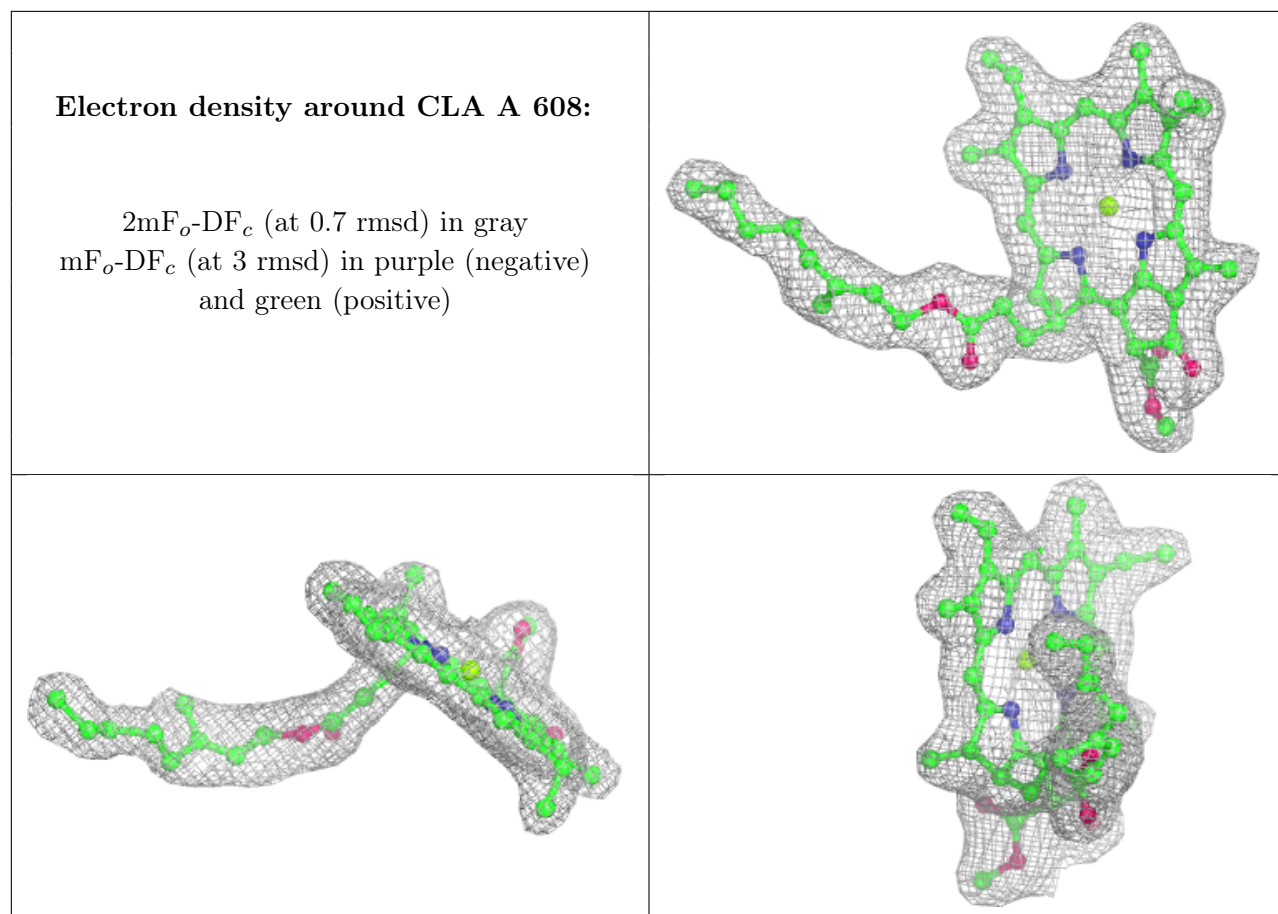
**Electron density around CLA b 612:**

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

**Electron density around CLA B 603:**

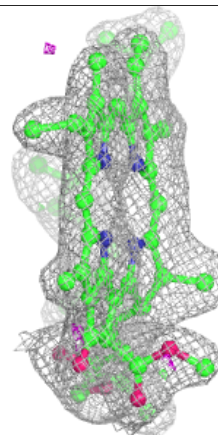
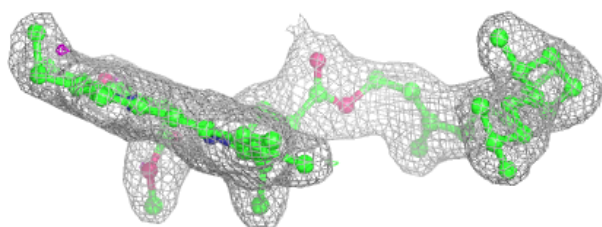
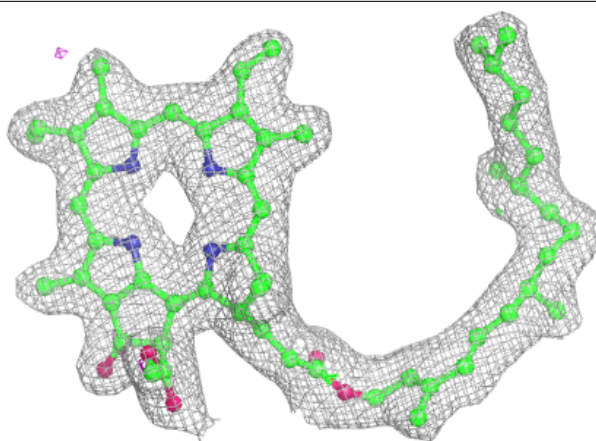
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



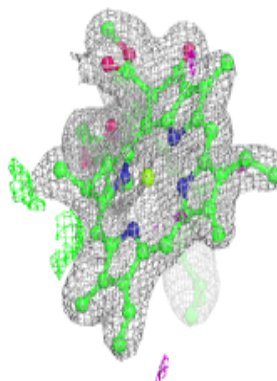
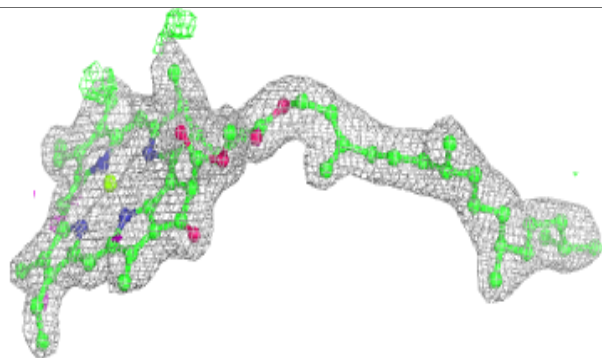
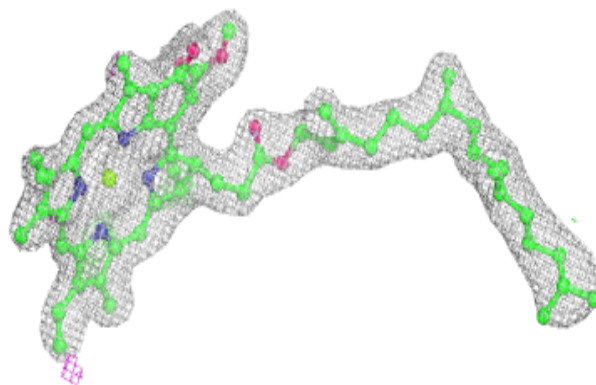


**Electron density around PHO a 607:**

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

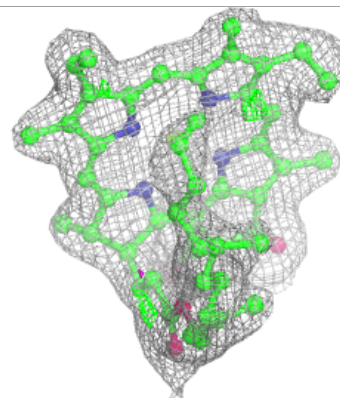
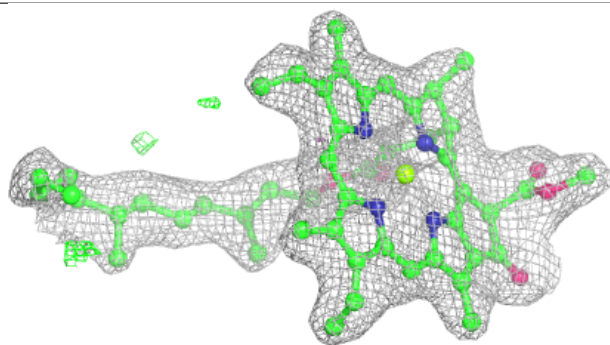
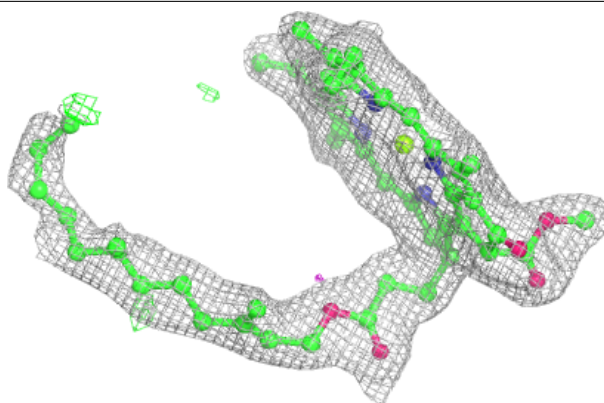
**Electron density around CLA a 605:**

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

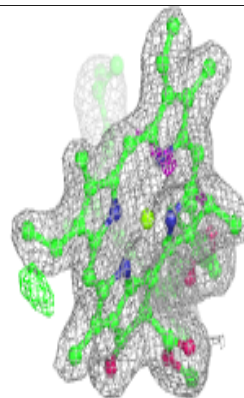
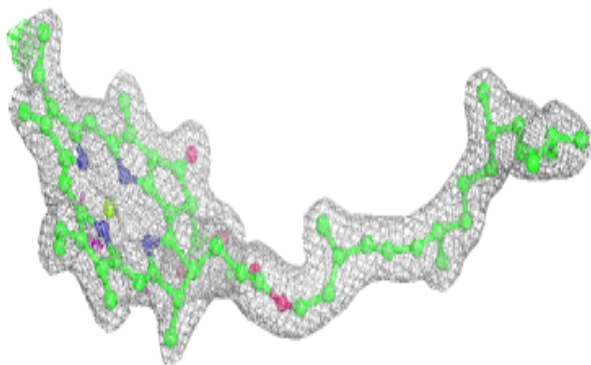
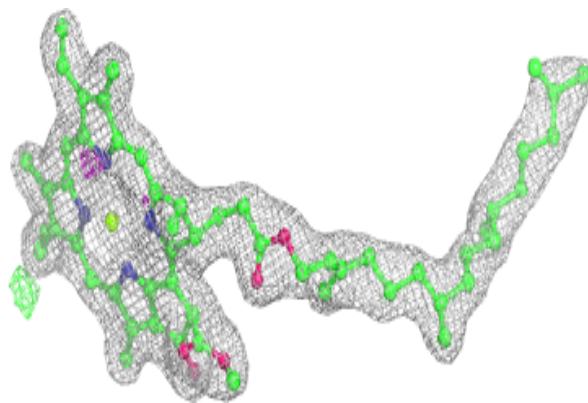


**Electron density around CLA C 504:**

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

**Electron density around CLA A 606:**

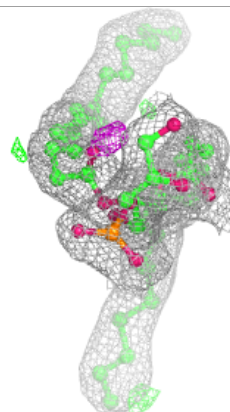
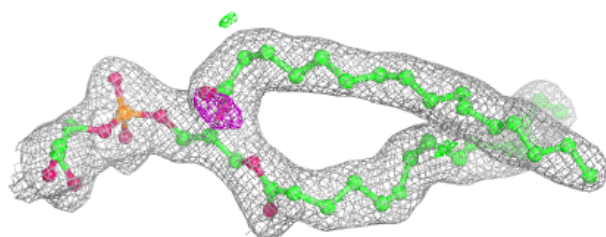
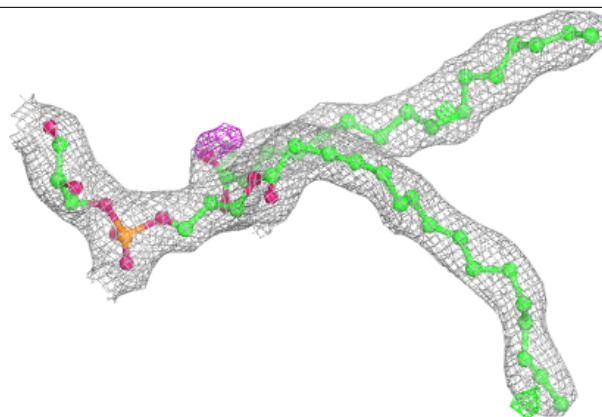
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



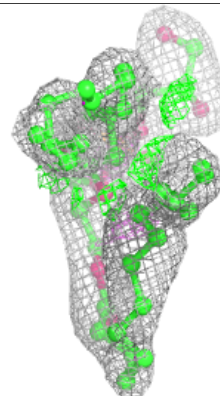
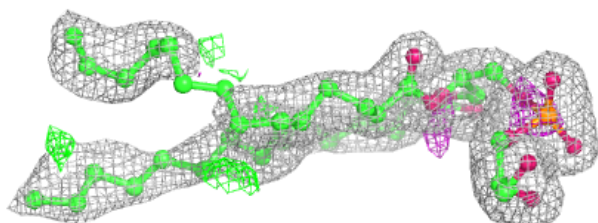
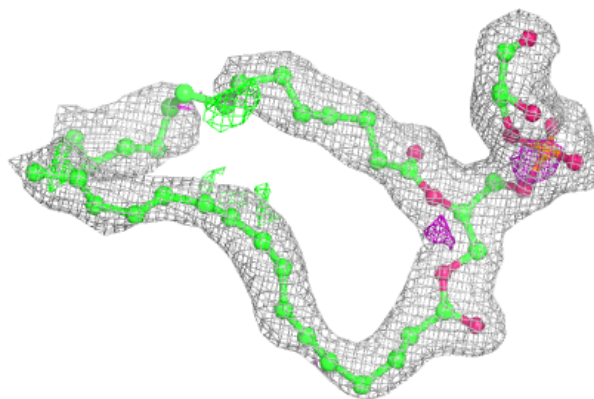


**Electron density around LHG D 409:**

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

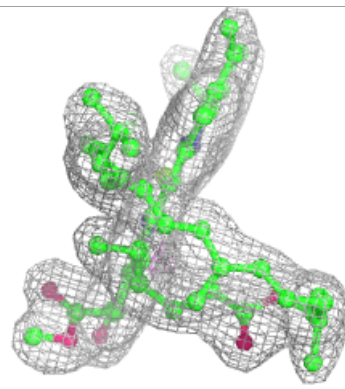
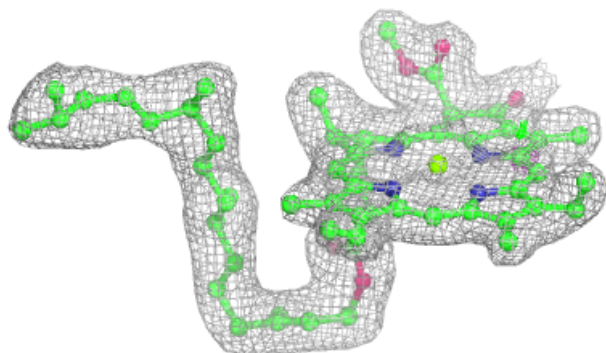
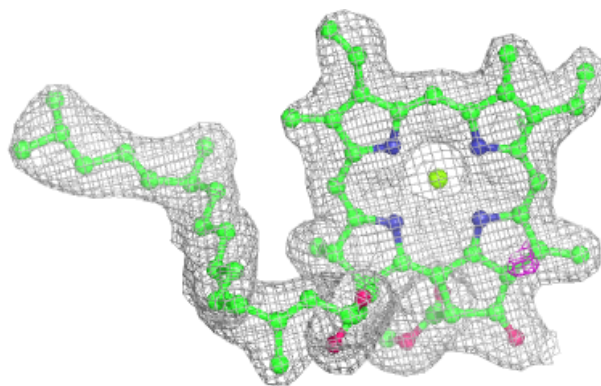
**Electron density around LHG D 410:**

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



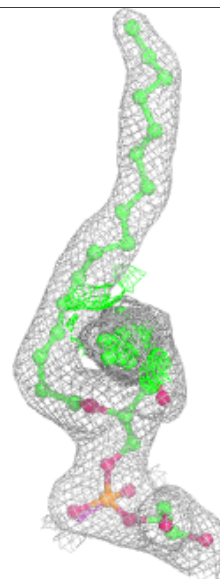
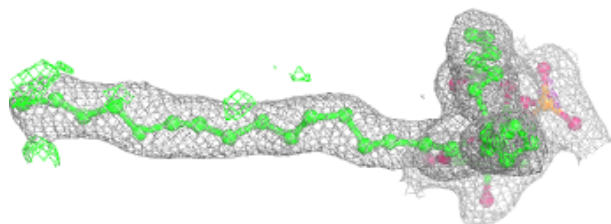
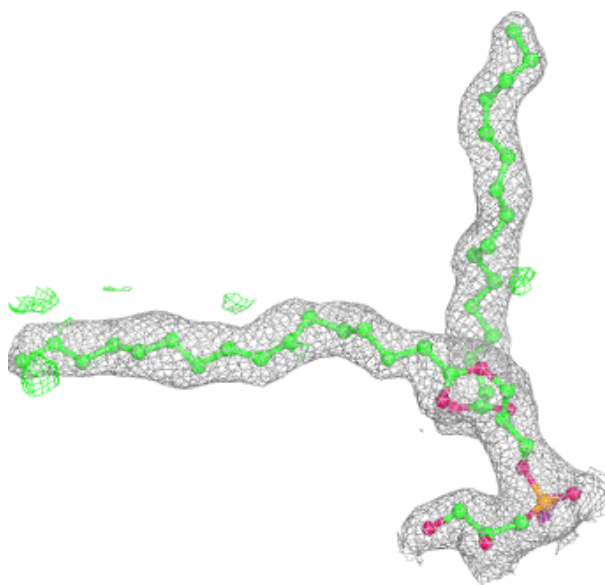
**Electron density around CLA a 611:**

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



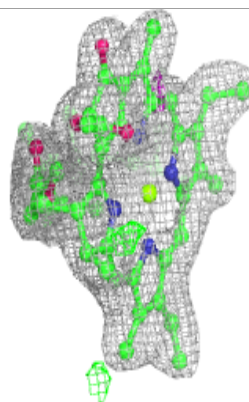
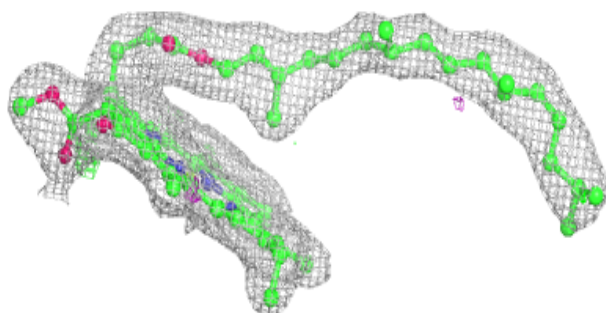
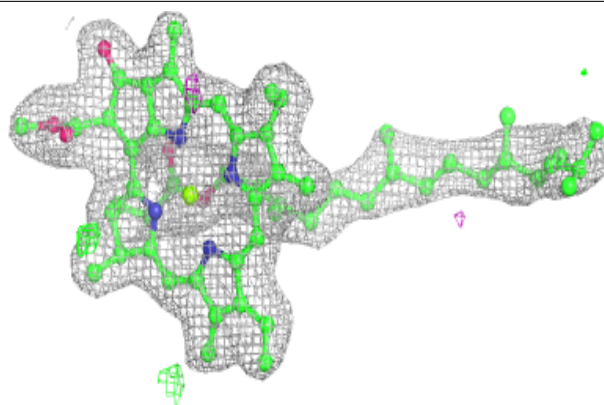
**Electron density around LHG L 101:**

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

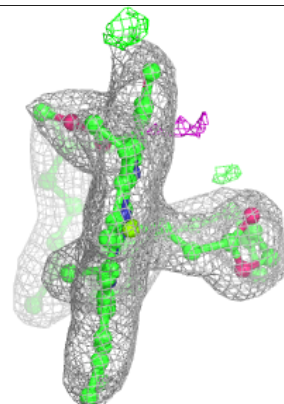
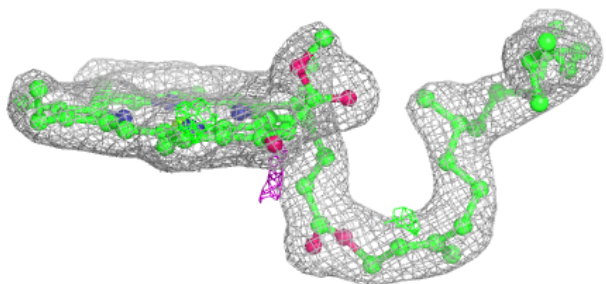
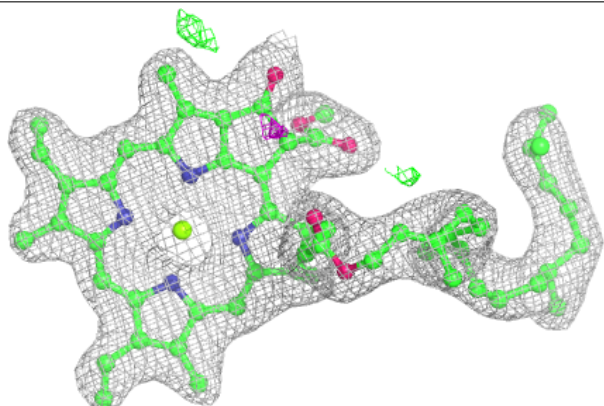


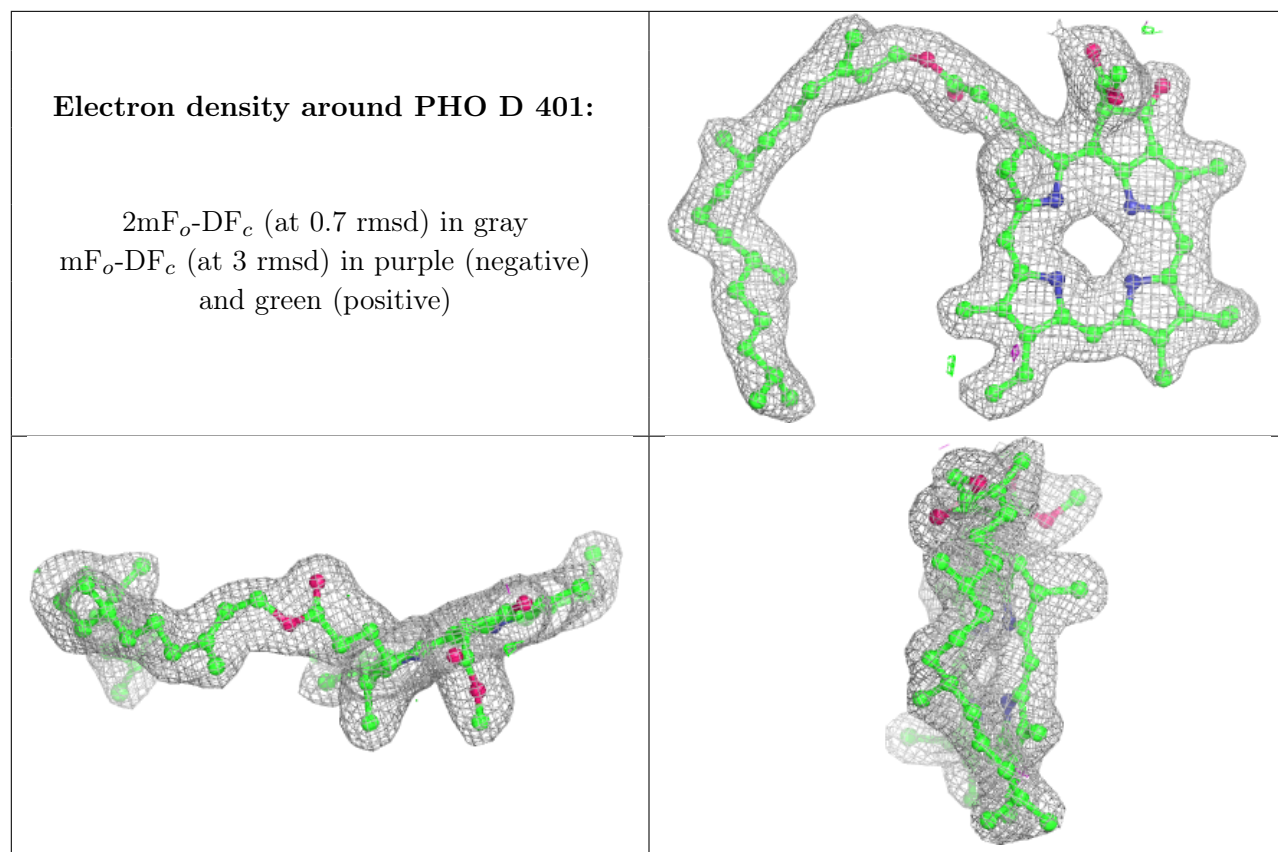
**Electron density around CLA B 608:**

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

**Electron density around CLA B 612:**

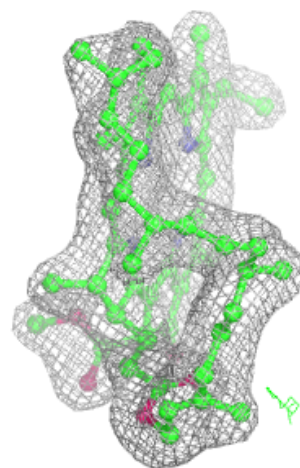
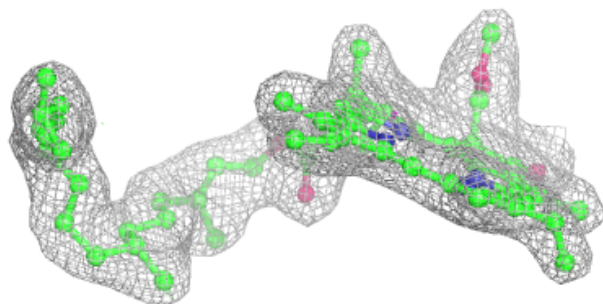
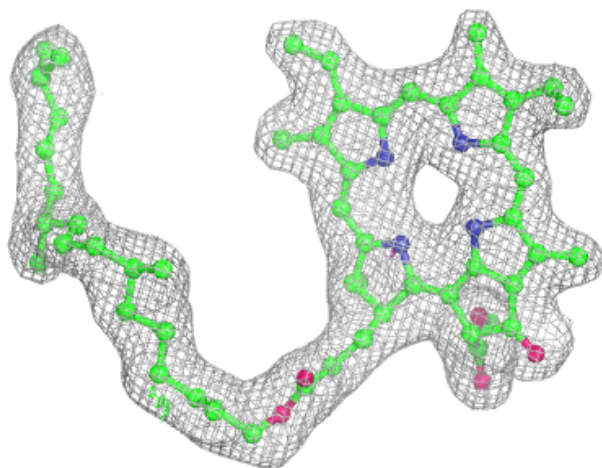
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





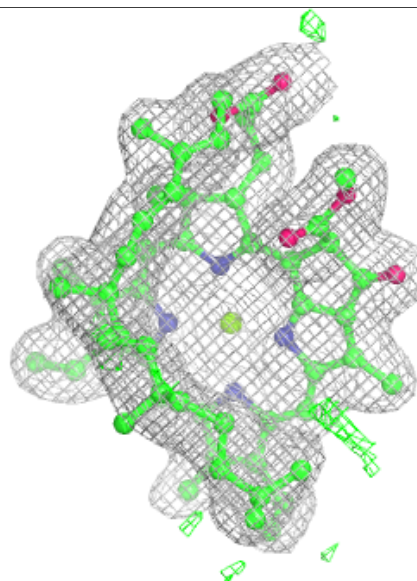
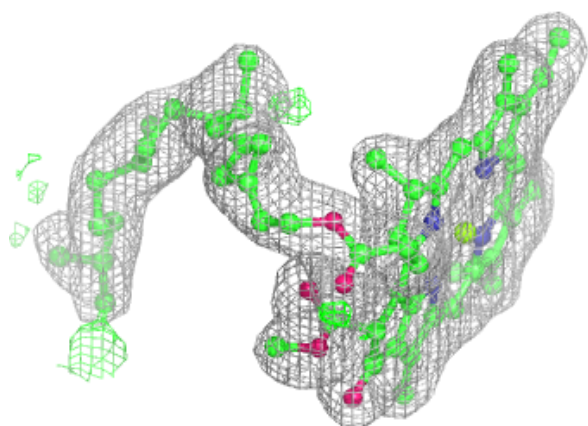
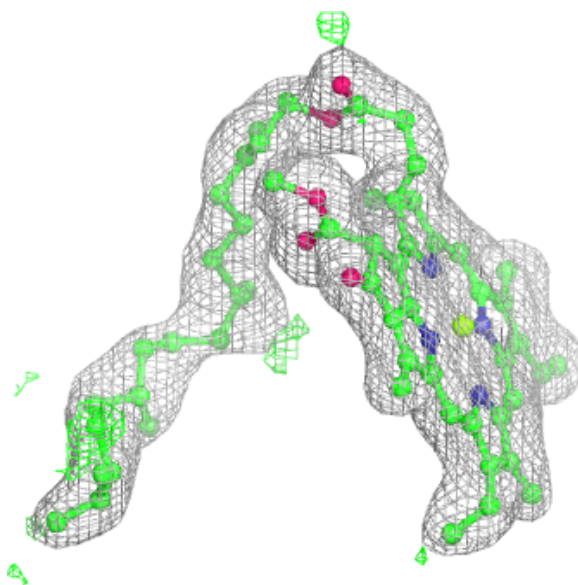
**Electron density around PHO D 402:**

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



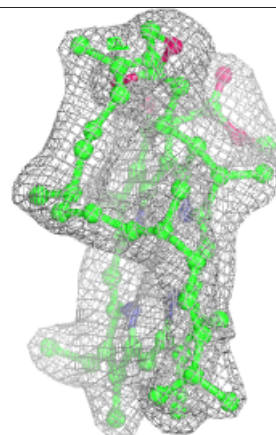
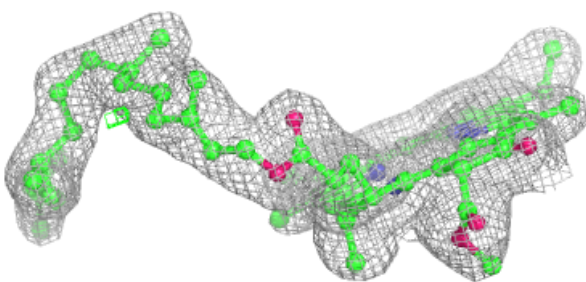
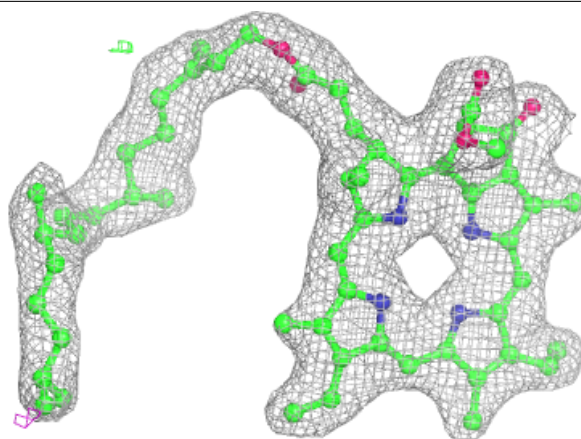
**Electron density around CLA B 613:**

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



**Electron density around PHO d 402:**

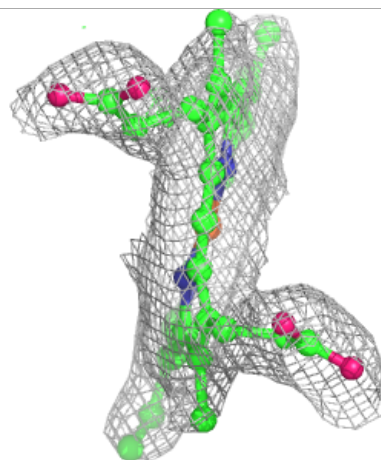
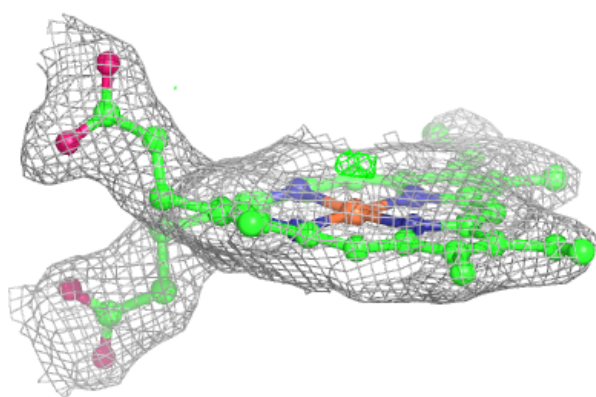
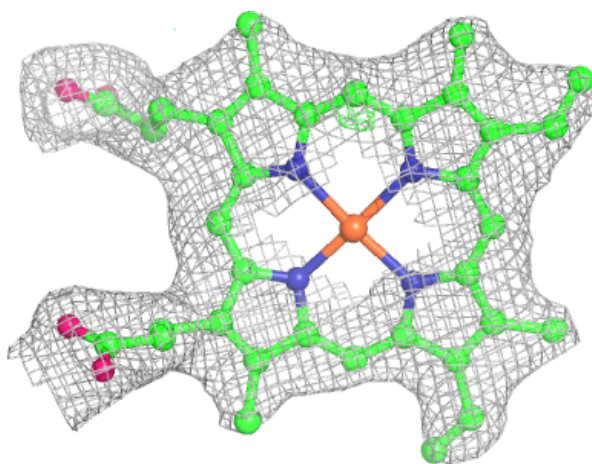
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





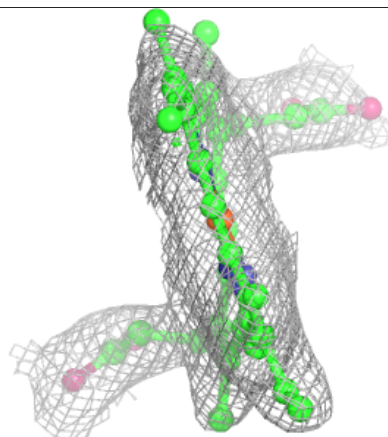
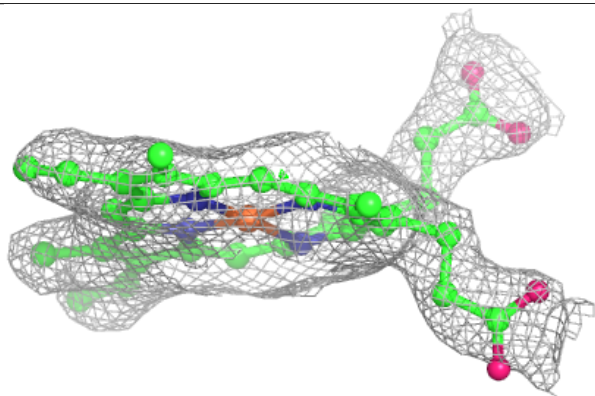
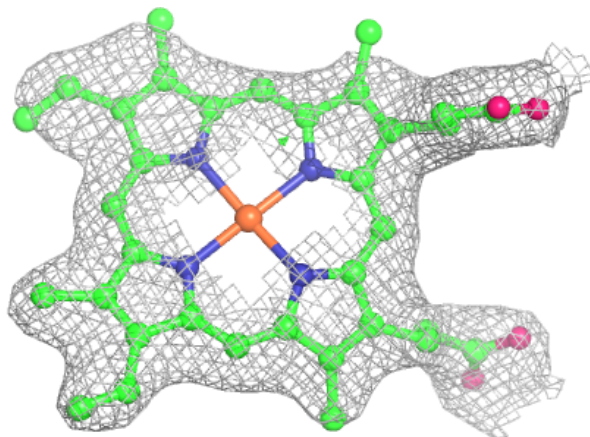
**Electron density around HEM E 101:**

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



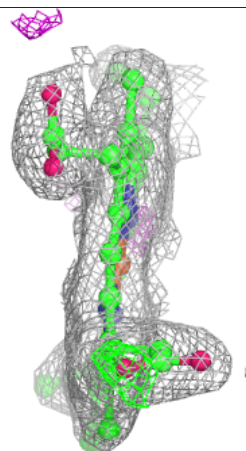
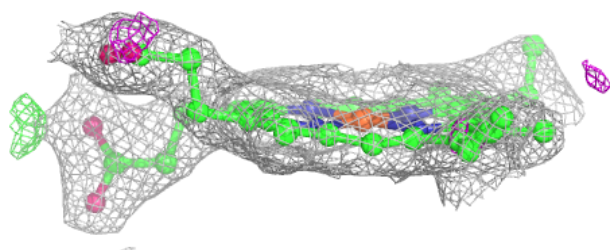
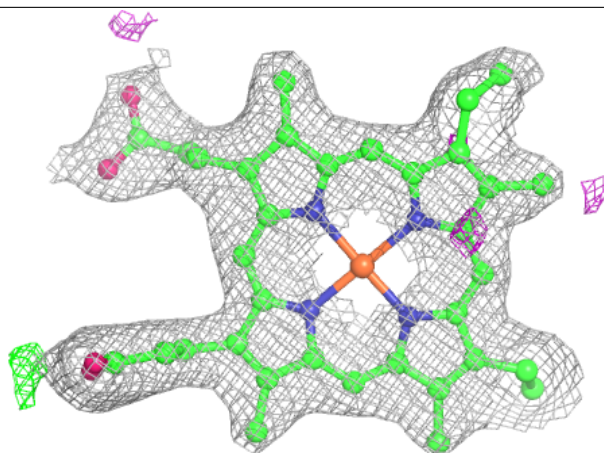
**Electron density around HEM f 101:**

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



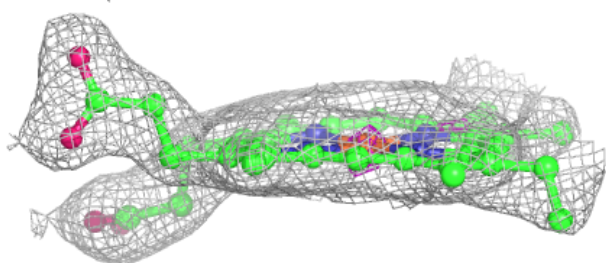
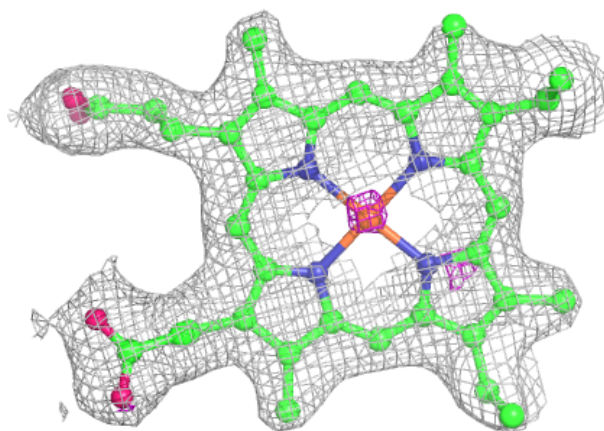
**Electron density around HEC V 201:**

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



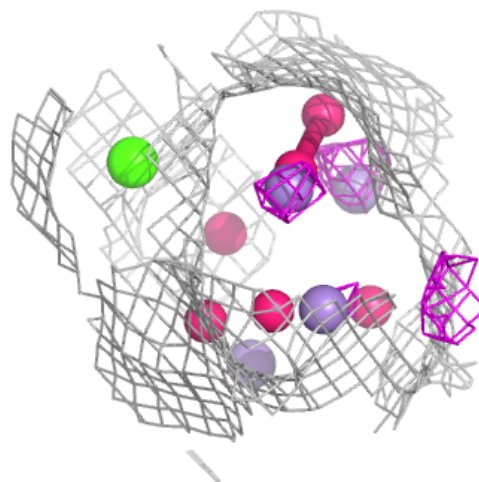
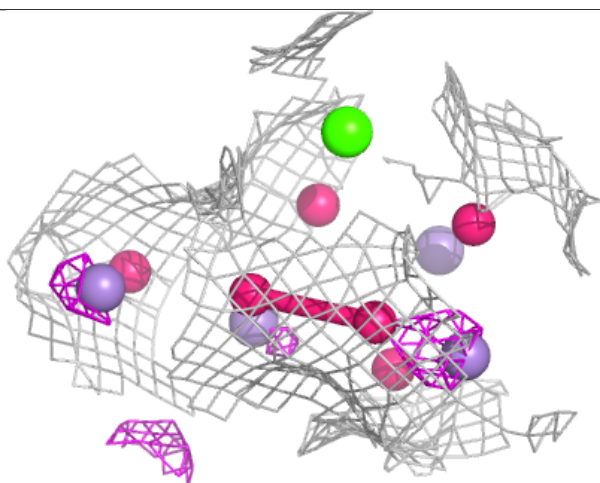
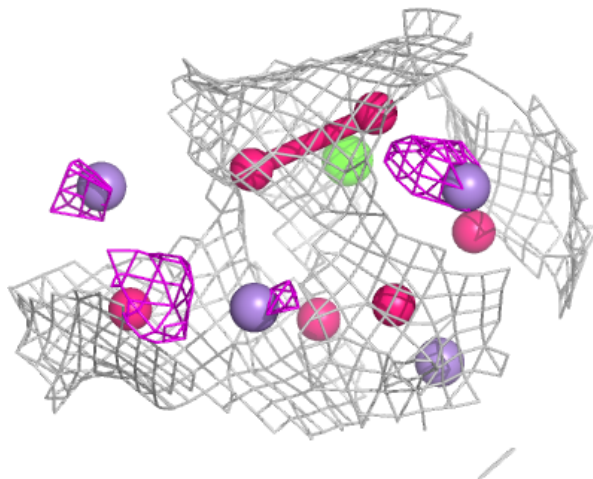
**Electron density around HEC v 201:**

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



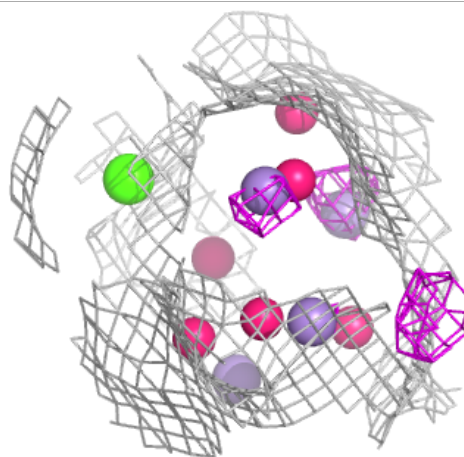
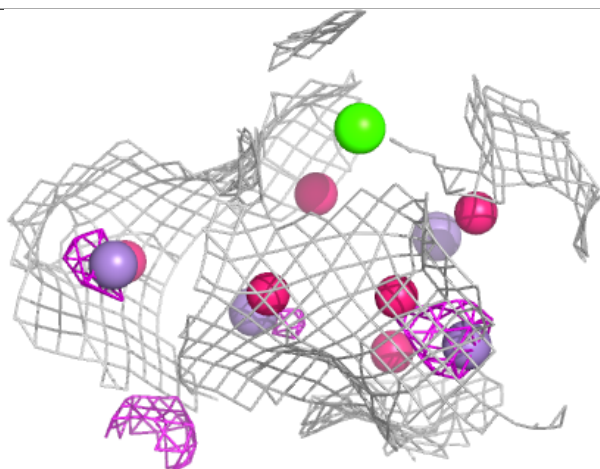
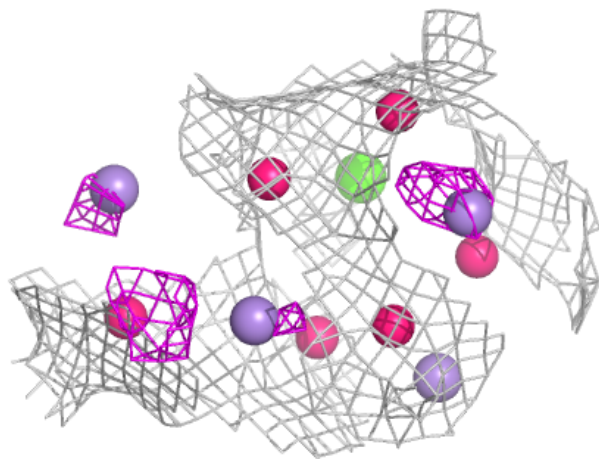
**Electron density around OEY A 601 (B):**

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



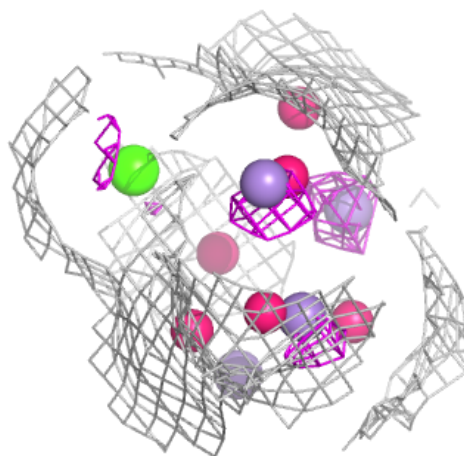
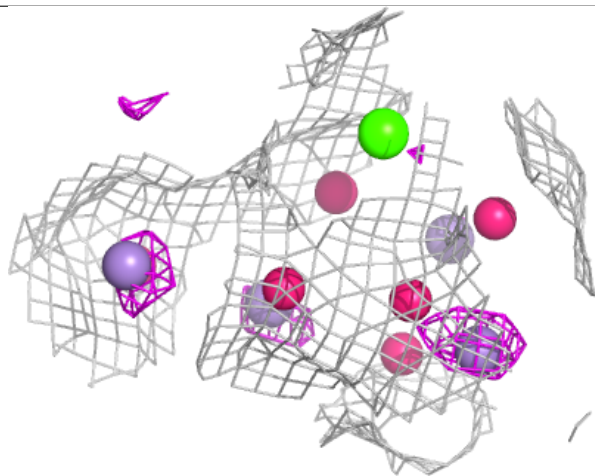
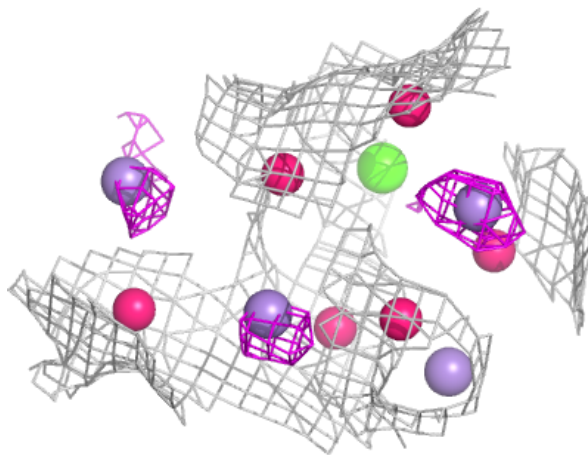
**Electron density around OEY A 601 (A):**

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



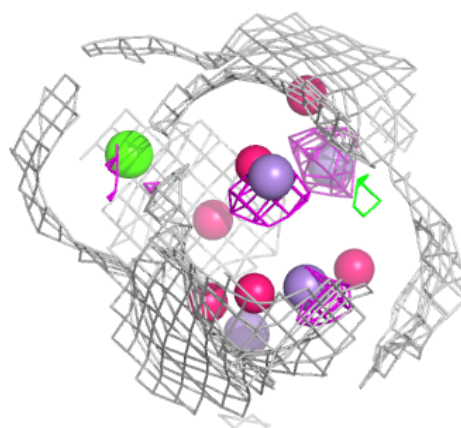
**Electron density around OEY a 601 (A):**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.