



## Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 04:49 PM EDT

PDB ID : 7RF6  
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 2.01 Å(reported)

This is a 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.

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The following versions of software and data (see [references](#) ①) 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	:	2.23.2
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)	:	2.23.2



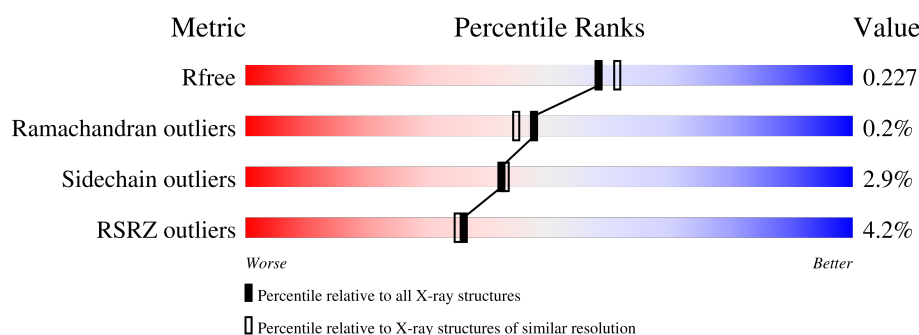
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 Å.

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



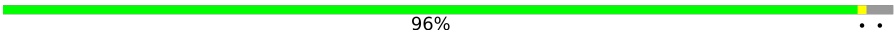
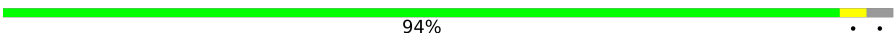

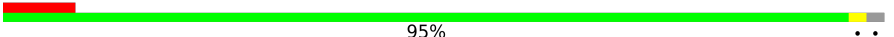






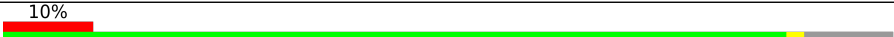


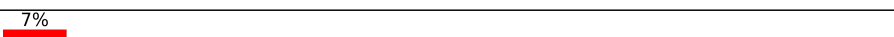
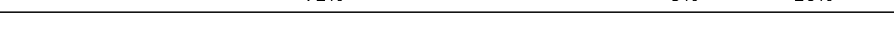
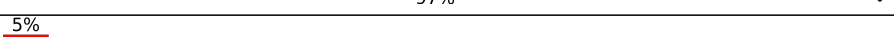



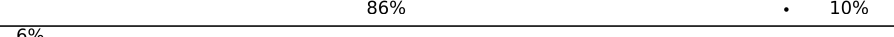





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>0%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>94%</div> <div>...</div> </div>
2	B	510	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
2	b	510	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
3	C	461	<div> <div>94%</div> <div>..</div> </div>
3	c	461	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

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Mol	Chain	Length	Quality of chain
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	608	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	612	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106128 atoms, of which 52762 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

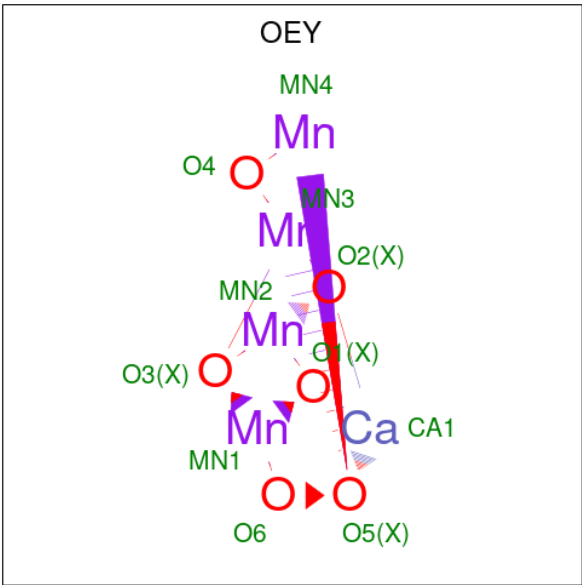
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

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

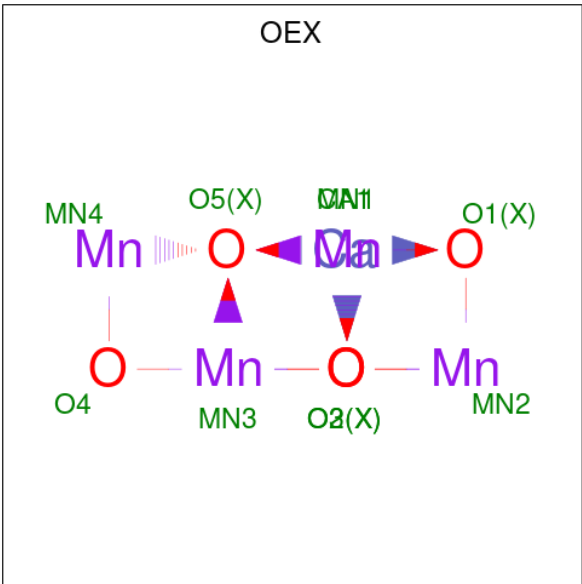
- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



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

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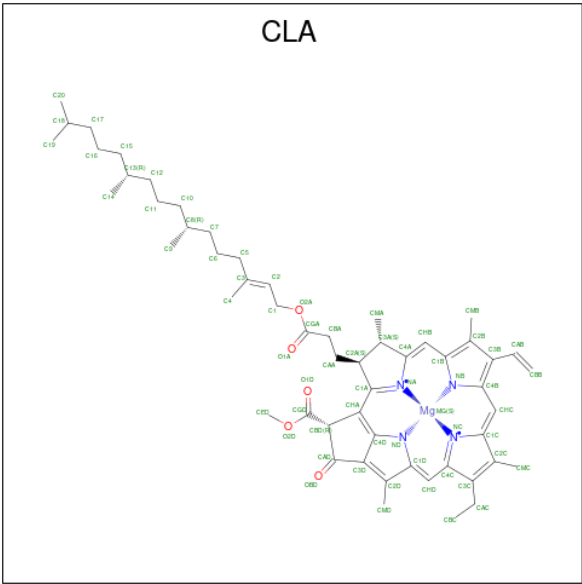
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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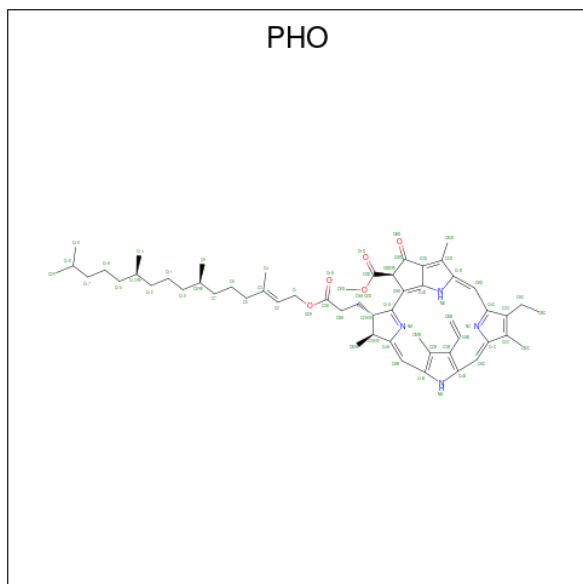
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total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

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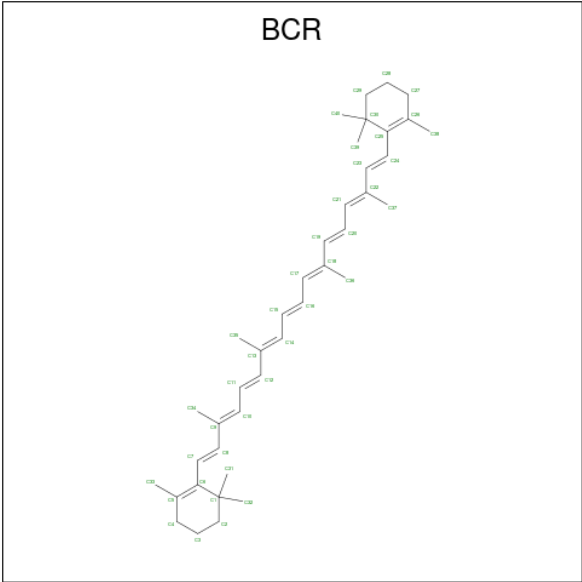
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

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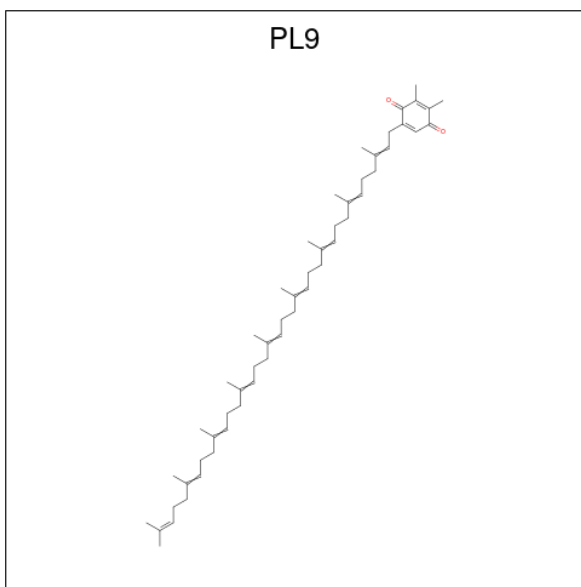
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		
26	x	1	Total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

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

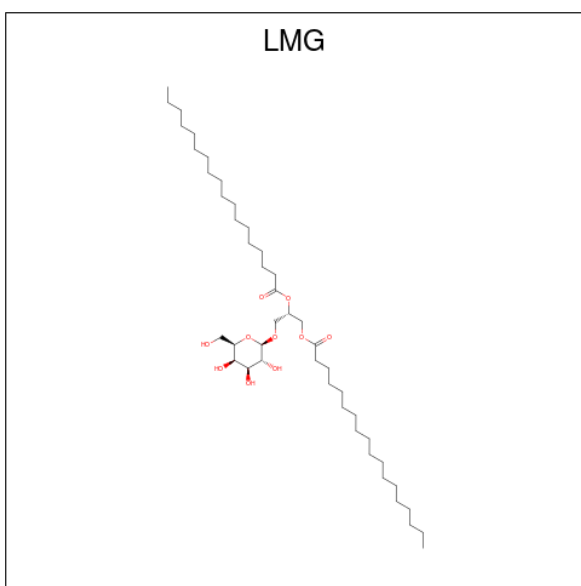
- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





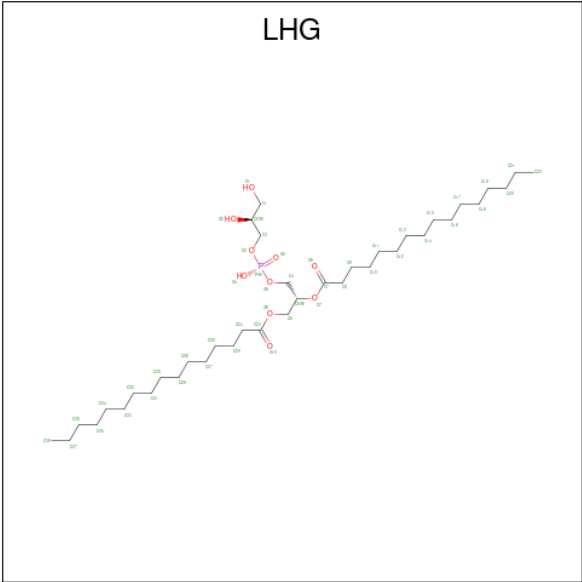
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



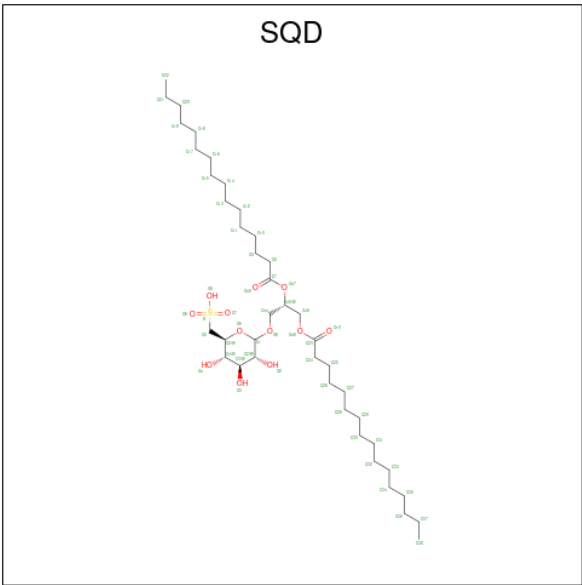
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			123	41	72	10		
29	D	1	Total	C	H	O	0	0
			78	27	45	6		
29	D	1	Total	C	H	O	0	0
			68	24	40	4		
29	M	1	Total	C	H	O	0	0
			123	41	72	10		
29	a	1	Total	C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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



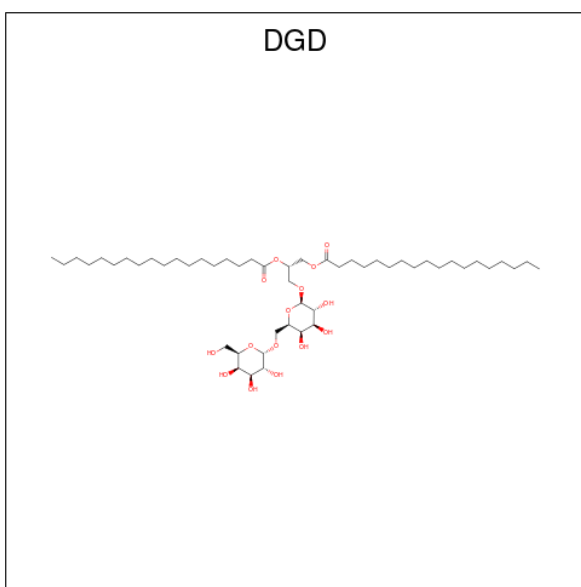
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 31 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).



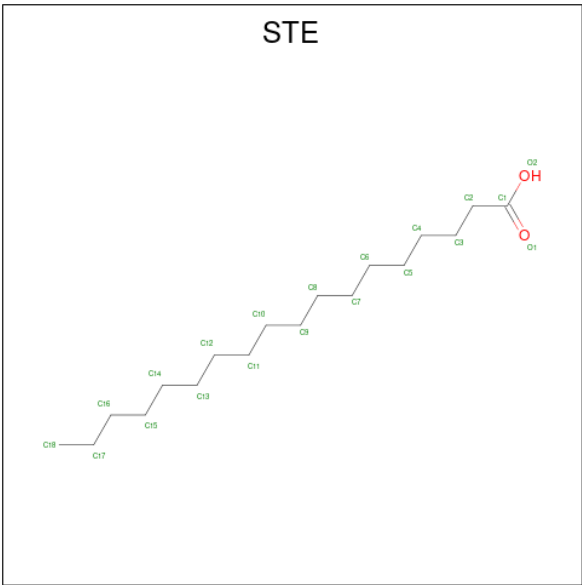
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
31	A	1	Total	C	H	O		0	0
			104	35	65	4			
31	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
31	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	a	1	Total	C	H	O		0	0
			92	31	56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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



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

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



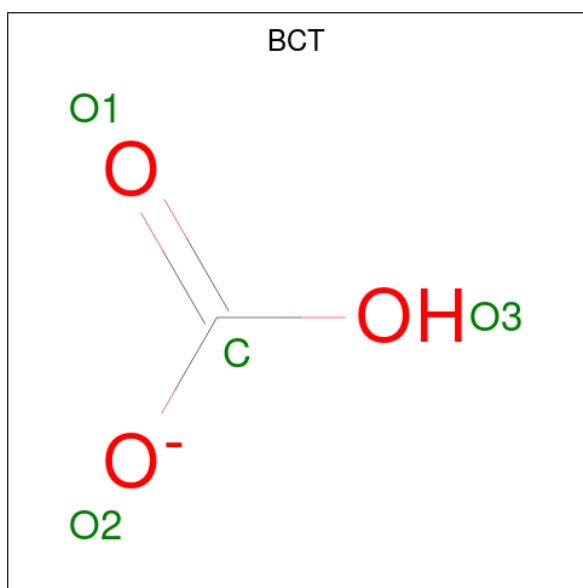
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
		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

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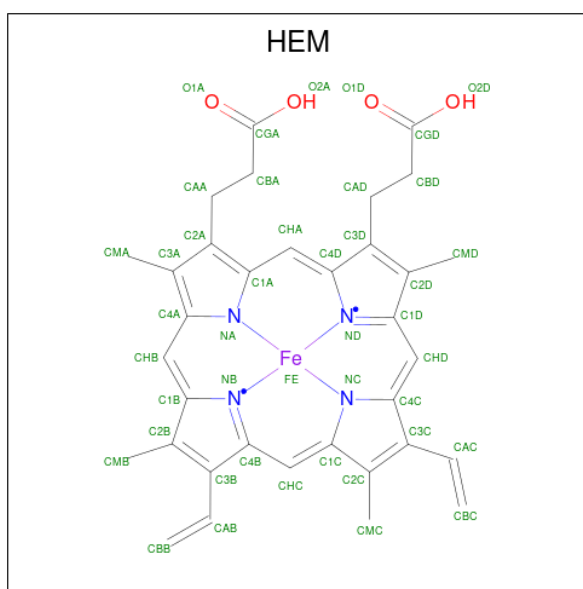
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	M	1	Total	C	H	0	0
			26	10	16		
33	T	1	Total	C	H	0	0
			47	16	31		
33	T	1	Total	C	H	0	0
			44	15	29		
33	Z	1	Total	C	H	0	0
			20	8	12		
33	a	1	Total	C	H	0	0
			26	10	16		
33	a	1	Total	C	H	O	0
			28	10	16	2	0
33	a	1	Total	C	H	0	0
			41	15	26		
33	b	1	Total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

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

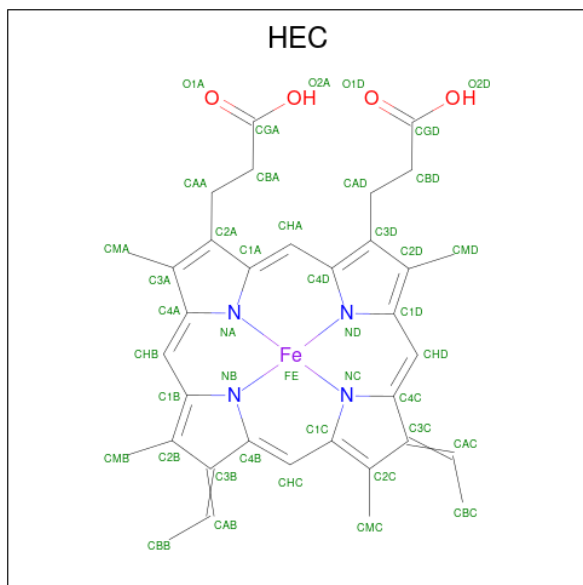
- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





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

- Molecule 36 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



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

- Molecule 37 is water.

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

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

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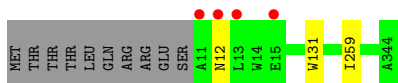
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	7	Total 7	O 7	0	0
37	j	8	Total 8	O 8	0	0
37	k	11	Total 11	O 11	0	0
37	l	8	Total 8	O 8	0	0
37	m	9	Total 9	O 9	0	0
37	o	104	Total 104	O 104	0	0
37	r	5	Total 5	O 5	0	0
37	t	9	Total 9	O 9	0	0
37	u	68	Total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

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

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

- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



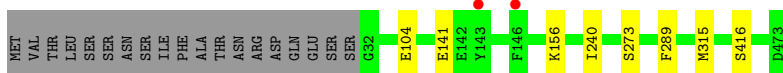
- Molecule 2: Photosystem II CP47 reaction center protein



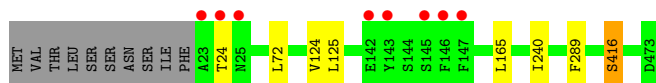
- Molecule 2: Photosystem II CP47 reaction center protein



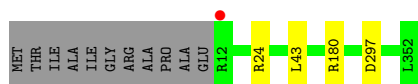
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



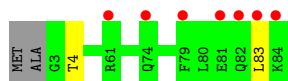
- Molecule 4: Photosystem II D2 protein



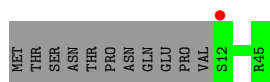
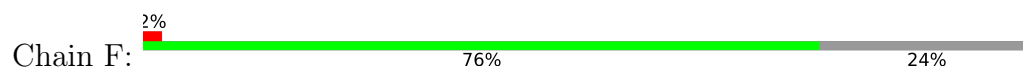
- Molecule 5: Cytochrome b559 subunit alpha



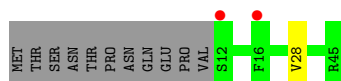
- Molecule 5: Cytochrome b559 subunit alpha



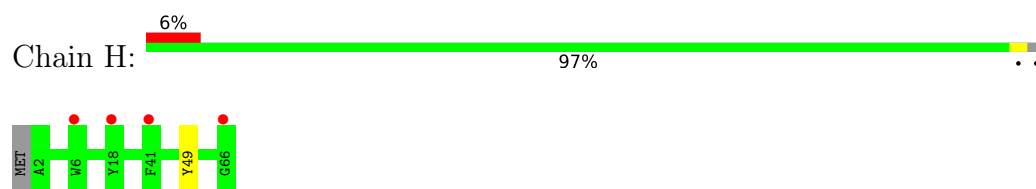
- Molecule 6: Cytochrome b559 subunit beta



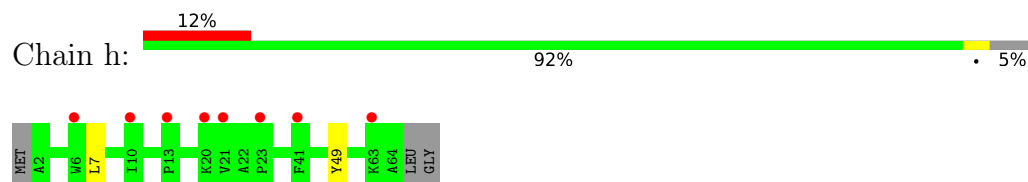
- Molecule 6: Cytochrome b559 subunit beta



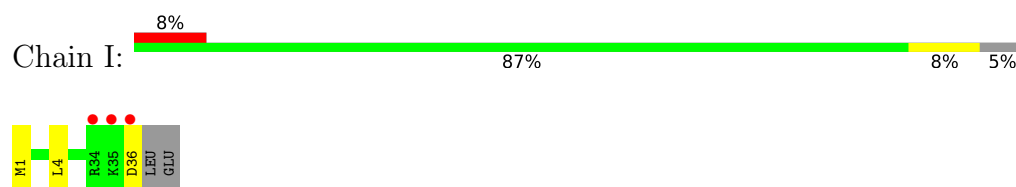
- Molecule 7: Photosystem II reaction center protein H



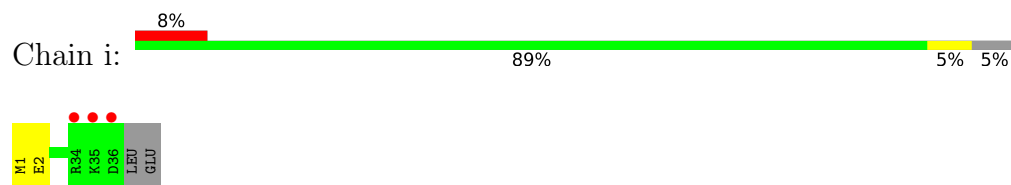
- Molecule 7: Photosystem II reaction center protein H



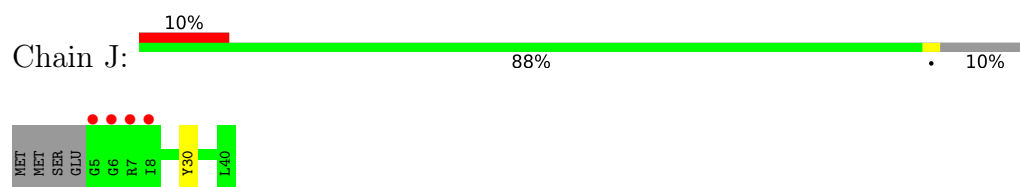
- Molecule 8: Photosystem II reaction center protein I



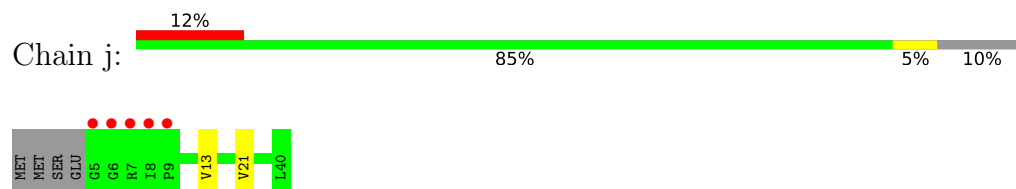
- Molecule 8: Photosystem II reaction center protein I



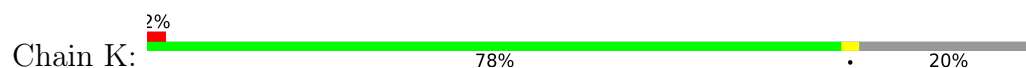
- Molecule 9: Photosystem II reaction center protein J

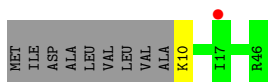


- Molecule 9: Photosystem II reaction center protein J

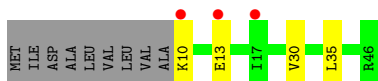


- Molecule 10: Photosystem II reaction center protein K





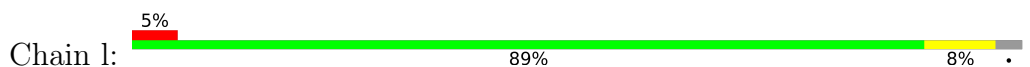
- Molecule 10: Photosystem II reaction center protein K



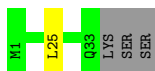
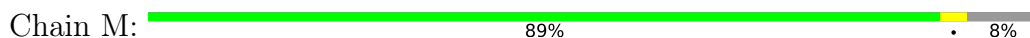
- Molecule 11: Photosystem II reaction center protein L



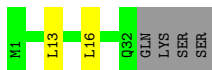
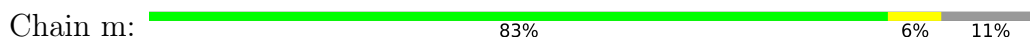
- Molecule 11: Photosystem II reaction center protein L



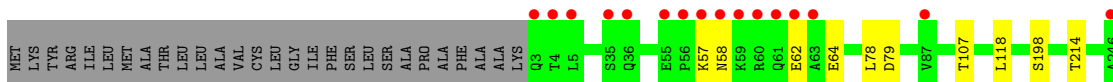
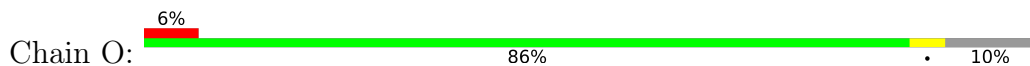
- Molecule 12: Photosystem II reaction center protein M



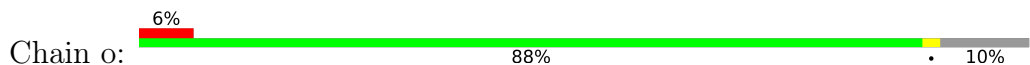
- Molecule 12: Photosystem II reaction center protein M

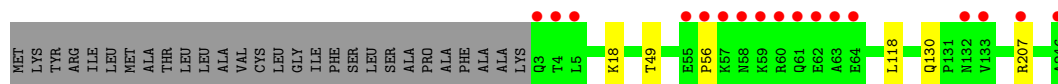


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





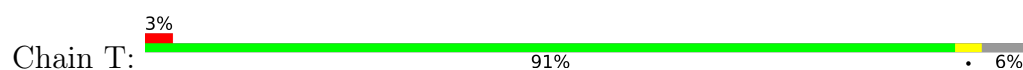
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y



- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein




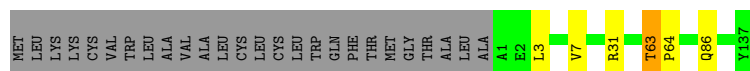
- Molecule 16: Photosystem II 12 kDa extrinsic protein




- Molecule 17: Cytochrome c-550

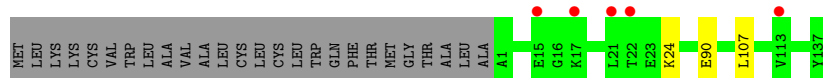


Chain V:  80% 16%




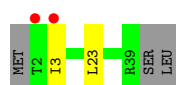
• Molecule 17: Cytochrome c-550

Chain v:  82% 16%



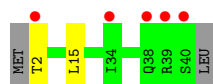
• Molecule 18: Photosystem II reaction center X protein

Chain X:  88% 5% 7%



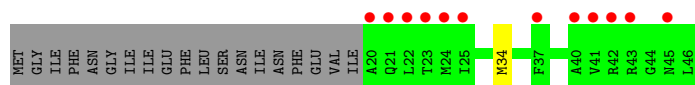
• Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5%



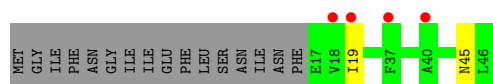
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  57% 26% 17%




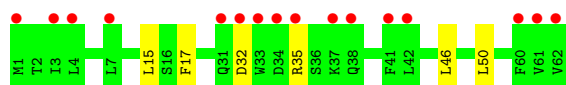
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  61% 35% 9%

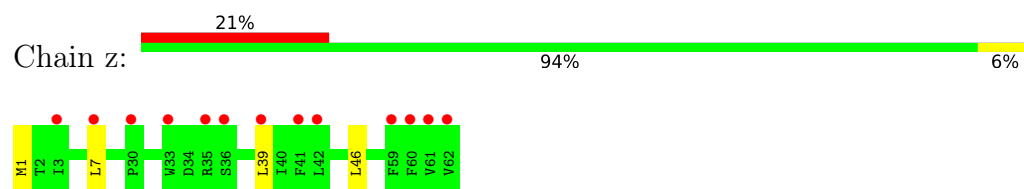


• Molecule 20: Photosystem II reaction center protein Z

Chain Z:  90% 10% 26%



- Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.7 (33.59-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.180 , 0.227 0.180 , 0.227	Depositor DCC
$R_{free}$ test set	4767 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	106128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

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

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, DGD, FME, SQD, OEX, CL, PL9, CLA, LHG, OEY, FE2, LMG, BCT, PHO, HEM, STE, 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	0.58	0/3227	0.64	1/4397 (0.0%)
1	a	0.57	0/3224	0.65	3/4393 (0.1%)
2	B	0.61	0/4161	0.67	0/5669
2	b	0.58	0/4118	0.66	0/5611
3	C	0.58	0/3647	0.65	0/4965
3	c	0.55	0/3719	0.65	0/5061
4	D	0.63	0/2825	0.67	1/3847 (0.0%)
4	d	0.59	0/2834	0.68	0/3859
5	E	0.54	0/688	0.62	0/940
5	e	0.48	0/683	0.61	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.50	0/284	0.61	0/387
7	H	0.63	0/523	0.66	0/713
7	h	0.57	0/511	0.67	0/697
8	I	0.58	0/293	0.64	0/396
8	i	0.63	0/293	0.65	0/396
9	J	0.44	0/263	0.62	0/356
9	j	0.48	0/263	0.62	0/356
10	K	0.45	0/303	0.60	0/416
10	k	0.47	0/303	0.59	0/416
11	L	0.57	0/311	0.65	0/422
11	l	0.60	0/303	0.68	0/412
12	M	0.60	0/249	0.63	0/341
12	m	0.65	0/244	0.68	0/334
13	O	0.57	0/1904	0.70	1/2585 (0.0%)
13	o	0.58	0/1905	0.71	0/2583
14	R	0.41	0/227	0.54	0/313
14	r	0.36	0/227	0.54	0/313
15	T	0.69	0/257	0.64	0/349
15	t	0.71	0/255	0.61	0/346
16	U	0.53	0/785	0.66	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.57	0/785	0.67	0/1064
17	V	0.55	0/1085	0.68	1/1473 (0.1%)
17	v	0.53	0/1085	0.63	0/1473
18	X	0.47	0/284	0.57	0/384
18	x	0.43	0/289	0.53	0/391
19	Y	0.42	0/197	0.60	0/264
19	y	0.39	0/219	0.55	0/294
20	Z	0.43	0/490	0.54	0/669
20	z	0.37	0/488	0.48	0/666
All	All	0.57	0/44035	0.65	7/59934 (0.0%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-6.37	106.59	120.60
1	a	42	LEU	CA-CB-CG	5.69	128.39	115.30
1	a	131	TRP	CA-CB-CG	-5.25	103.73	113.70
4	D	297	ASP	CB-CG-OD1	5.15	122.94	118.30
13	O	79	ASP	CB-CG-OD1	5.15	122.93	118.30
1	a	200	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	131	TRP	CA-CB-CG	-5.07	104.06	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	392 (99%)	4 (1%)	1 (0%)	41	37
1	a	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	41	37
2	B	508/510 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	442 (97%)	11 (2%)	1 (0%)	47	44
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	47	44
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	230 (95%)	11 (4%)	2 (1%)	19	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	34	30
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	16
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
All	All	5387/5700 (94%)	5245 (97%)	134 (2%)	8 (0%)	47	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	58	ASN
13	O	62	GLU
1	A	259	ILE
1	a	259	ILE
13	o	56	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	323 (100%)	1 (0%)	92	95
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	40
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	58
2	b	402/407 (99%)	393 (98%)	9 (2%)	52	55
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	58
3	c	364/362 (101%)	356 (98%)	8 (2%)	52	55
4	D	277/283 (98%)	274 (99%)	3 (1%)	73	78
4	d	278/283 (98%)	268 (96%)	10 (4%)	35	34
5	E	72/73 (99%)	67 (93%)	5 (7%)	15	11
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	44
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	34
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	51 (96%)	2 (4%)	33	31
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	40
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	27
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	7
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	37
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	43
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	34
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	37	36
13	o	207/228 (91%)	202 (98%)	5 (2%)	49	51
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	5
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	83 (99%)	1 (1%)	71	76
16	u	84/112 (75%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	113 (97%)	4 (3%)	37	36
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	48
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	12
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	18
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	47 (92%)	4 (8%)	12	8
All	All	4451/4654 (96%)	4324 (97%)	127 (3%)	42	43

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	76	SER
2	B	79	SER
2	B	127	ARG
2	B	240	SER
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	141	GLU
3	C	156	LYS
3	C	240	ILE
3	C	273	SER
3	C	289	PHE
3	C	315	MET
4	D	24	ARG
4	D	43	LEU
4	D	180	ARG
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
5	E	81	GLU
7	H	49	TYR
8	I	4	LEU

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Mol	Chain	Res	Type
8	I	36	ASP
9	J	30	TYR
10	K	10	LYS
11	L	2	GLU
12	M	25	LEU
13	O	57	LYS
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	198	SER
13	O	214	THR
14	R	10	LEU
14	R	21	ARG
14	R	29	LYS
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	31	ARG
17	V	86	GLN
18	X	3	ILE
18	X	23	LEU
19	Y	34	MET
20	Z	15	LEU
20	Z	17	PHE
20	Z	32	ASP
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	83	GLU
2	b	128	THR
2	b	149	LEU

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Mol	Chain	Res	Type
2	b	236	THR
2	b	362	PHE
2	b	485	GLU
2	b	492	GLU
2	b	495	PHE
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	289	PHE
3	c	416	SER
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	233	ARG
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	4	THR
5	e	83	LEU
6	f	28	VAL
7	h	7	LEU
7	h	49	TYR
8	i	2	GLU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS

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Mol	Chain	Res	Type
13	o	49	THR
13	o	118	LEU
13	o	130	GLN
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
17	v	24	LYS
17	v	90	GLU
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	45	ASN
20	z	1	MET
20	z	7	LEU
20	z	39	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
13	O	36	GLN
13	O	88	ASN
17	V	86	GLN
20	Z	31	GLN
1	a	234	ASN
2	b	179	GLN
3	c	378	ASN
5	e	60	GLN
5	e	82	GLN
7	h	59	ASN
18	x	33	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	M	1	12	8,9,10	0.98	0	7,9,11	0.90	0
15	FME	t	1	15	8,9,10	1.45	1 (12%)	7,9,11	0.71	0
8	FME	i	1	8	8,9,10	1.03	1 (12%)	7,9,11	0.78	0
8	FME	I	1	8	8,9,10	0.97	1 (12%)	7,9,11	0.78	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.96	0	7,9,11	1.41	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
12	FME	M	1	12	-	1/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.48	1.41	1.46
8	i	1	FME	CA-N	-2.16	1.43	1.46
8	I	1	FME	CA-N	-2.02	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.37	119.02	125.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	SQD	B	623	-	53,54,54	0.98	3 (5%)	62,65,65	2.00	15 (24%)
24	CLA	A	605	37	56,73,73	1.53	3 (5%)	55,113,113	1.83	12 (21%)
26	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.24	6 (10%)
26	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	8 (14%)
24	CLA	C	510	-	56,73,73	1.58	8 (14%)	55,113,113	1.88	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMG	a	618	-	55,55,55	1.06	5 (9%)	63,63,63	1.45	5 (7%)
24	CLA	C	511	3	56,73,73	1.79	6 (10%)	55,113,113	1.66	10 (18%)
24	CLA	B	602	-	56,73,73	1.76	7 (12%)	55,113,113	1.62	11 (20%)
24	CLA	c	512	-	56,73,73	1.41	5 (8%)	55,113,113	1.60	11 (20%)
24	CLA	B	609	-	56,73,73	1.68	7 (12%)	55,113,113	1.61	9 (16%)
32	DGD	c	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.43	14 (18%)
30	LHG	l	101	-	48,48,48	0.85	1 (2%)	51,54,54	1.27	8 (15%)
24	CLA	C	508	-	56,73,73	1.70	7 (12%)	55,113,113	1.86	12 (21%)
33	STE	B	624	-	10,13,19	0.42	0	9,13,19	0.80	0
30	LHG	E	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.26	5 (9%)
24	CLA	B	606	-	56,73,73	1.74	8 (14%)	55,113,113	1.65	10 (18%)
33	STE	B	627	-	8,11,19	0.47	0	7,11,19	0.62	0
26	BCR	A	609	-	41,41,41	1.21	5 (12%)	56,56,56	1.43	7 (12%)
24	CLA	a	604	-	56,73,73	1.58	4 (7%)	55,113,113	1.59	6 (10%)
26	BCR	b	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.20	5 (8%)
24	CLA	c	511	3	56,73,73	1.86	8 (14%)	55,113,113	1.63	9 (16%)
24	CLA	b	608	-	56,73,73	1.70	8 (14%)	55,113,113	1.55	10 (18%)
29	LMG	c	522	-	49,49,55	0.87	1 (2%)	57,57,63	1.30	6 (10%)
26	BCR	c	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	7 (12%)
34	BCT	a	610	23	0,3,3	-	-	0,3,3	-	-
33	STE	b	625	-	16,19,19	0.40	0	15,19,19	0.98	1 (6%)
31	SQD	A	617	-	38,38,54	0.96	3 (7%)	40,40,65	1.51	4 (10%)
24	CLA	b	616	-	51,68,73	1.59	12 (23%)	49,107,113	1.85	10 (20%)
33	STE	C	522	-	8,11,19	0.36	0	7,11,19	1.04	1 (14%)
24	CLA	b	613	-	56,73,73	1.58	6 (10%)	55,113,113	1.67	13 (23%)
24	CLA	b	614	-	56,73,73	1.54	7 (12%)	55,113,113	1.88	13 (23%)
22	OEX	A	602[A]	1,37,3	0,15,15	-	-	-	-	-
24	CLA	d	403	-	56,73,73	1.77	9 (16%)	55,113,113	1.82	11 (20%)
30	LHG	d	409	-	38,38,48	0.91	1 (2%)	41,44,54	1.17	2 (4%)
31	SQD	a	613	-	53,54,54	1.07	5 (9%)	62,65,65	1.89	11 (17%)
24	CLA	C	509	-	56,73,73	1.43	7 (12%)	55,113,113	1.92	10 (18%)
21	OEY	a	601[B]	1,37,3	0,16,16	-	-	-	-	-
26	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.03	3 (5%)
24	CLA	b	611	-	56,73,73	1.54	7 (12%)	55,113,113	1.54	8 (14%)
33	STE	x	102	-	16,19,19	0.39	0	15,19,19	0.75	0
33	STE	a	616	-	8,11,19	0.52	0	7,11,19	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	b	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.38	8 (14%)
24	CLA	c	507	37	56,73,73	1.44	5 (8%)	55,113,113	1.72	11 (20%)
24	CLA	B	611	-	56,73,73	1.58	8 (14%)	55,113,113	2.10	17 (30%)
29	LMG	D	409	-	31,31,55	0.95	2 (6%)	33,33,63	1.10	1 (3%)
33	STE	d	412	-	16,19,19	0.30	0	15,19,19	1.03	0
24	CLA	b	604	-	56,73,73	1.49	6 (10%)	55,113,113	1.75	17 (30%)
26	BCR	t	101	-	41,41,41	1.13	4 (9%)	56,56,56	1.37	7 (12%)
24	CLA	b	601	37	56,73,73	1.63	6 (10%)	55,113,113	1.70	7 (12%)
24	CLA	A	608	-	45,62,73	1.64	6 (13%)	41,99,113	1.74	11 (26%)
24	CLA	b	612	-	56,73,73	1.62	6 (10%)	55,113,113	1.76	10 (18%)
32	DGD	C	518	-	63,63,67	1.10	5 (7%)	77,77,81	1.34	7 (9%)
26	BCR	C	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	9 (16%)
29	LMG	D	410	-	20,26,55	0.36	0	18,26,63	1.18	0
33	STE	M	102	-	11,14,19	0.28	0	10,14,19	1.05	0
33	STE	t	102	-	14,17,19	0.32	0	13,17,19	1.02	0
26	BCR	K	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	2 (3%)
30	LHG	B	622	-	48,48,48	0.89	3 (6%)	51,54,54	1.32	8 (15%)
31	SQD	f	101	-	40,41,54	1.13	4 (10%)	49,52,65	2.01	12 (24%)
32	DGD	H	102	-	63,63,67	1.35	13 (20%)	77,77,81	1.38	8 (10%)
32	DGD	C	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.37	9 (11%)
33	STE	D	411	-	16,19,19	0.24	0	15,19,19	1.01	0
24	CLA	c	505	-	56,73,73	1.58	5 (8%)	55,113,113	1.72	9 (16%)
24	CLA	b	610	37	56,73,73	1.46	8 (14%)	55,113,113	1.72	14 (25%)
30	LHG	d	407	-	48,48,48	0.86	3 (6%)	51,54,54	1.44	7 (13%)
24	CLA	a	606	-	56,73,73	1.71	8 (14%)	55,113,113	1.60	11 (20%)
30	LHG	A	615	-	46,46,48	1.12	4 (8%)	49,52,54	1.36	5 (10%)
33	STE	b	626	-	9,9,19	0.44	0	8,8,19	0.63	0
33	STE	j	101	-	8,11,19	0.48	0	7,11,19	0.68	0
24	CLA	b	602	-	56,73,73	1.40	8 (14%)	55,113,113	2.04	13 (23%)
29	LMG	M	101	-	51,51,55	1.06	4 (7%)	59,59,63	1.50	7 (11%)
33	STE	m	101	-	8,11,19	0.38	0	7,11,19	0.84	0
32	DGD	c	517	-	63,63,67	1.22	8 (12%)	77,77,81	1.40	15 (19%)
33	STE	Z	101	-	7,7,19	0.45	0	6,6,19	0.46	0
33	STE	c	520	-	16,19,19	0.31	0	15,19,19	0.85	0
24	CLA	B	603	-	56,73,73	1.65	8 (14%)	55,113,113	1.92	14 (25%)
24	CLA	b	615	-	56,73,73	1.75	7 (12%)	55,113,113	1.92	11 (20%)
24	CLA	B	614	-	56,73,73	1.67	9 (16%)	55,113,113	1.63	12 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	509	-	56,73,73	1.54	2 (3%)	55,113,113	1.88	10 (18%)
28	PL9	a	611	-	55,55,55	1.09	6 (10%)	68,69,69	1.70	16 (23%)
32	DGD	A	618	-	67,67,67	1.21	7 (10%)	81,81,81	1.39	9 (11%)
30	LHG	D	408	-	48,48,48	1.10	4 (8%)	51,54,54	1.25	5 (9%)
24	CLA	b	606	-	56,73,73	1.86	6 (10%)	55,113,113	2.07	11 (20%)
24	CLA	B	605	-	56,73,73	1.26	5 (8%)	55,113,113	1.50	10 (18%)
26	BCR	B	619	-	41,41,41	1.23	4 (9%)	56,56,56	1.27	5 (8%)
32	DGD	c	516	-	63,63,67	1.16	8 (12%)	77,77,81	1.38	10 (12%)
24	CLA	c	510	-	56,73,73	1.96	8 (14%)	55,113,113	1.88	11 (20%)
33	STE	T	102	-	15,15,19	0.39	0	14,14,19	0.83	0
26	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	9 (16%)
26	BCR	B	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.32	8 (14%)
35	HEM	F	101	6,5	27,50,50	1.89	4 (14%)	17,82,82	2.37	9 (52%)
24	CLA	C	504	37	50,67,73	1.44	5 (10%)	47,105,113	1.64	8 (17%)
32	DGD	C	516	-	63,63,67	1.28	9 (14%)	77,77,81	1.40	9 (11%)
24	CLA	B	607	37	56,73,73	1.31	8 (14%)	55,113,113	1.52	5 (9%)
33	STE	a	615	-	9,9,19	0.53	0	8,8,19	0.47	0
24	CLA	D	403	-	56,73,73	1.60	7 (12%)	55,113,113	1.67	11 (20%)
24	CLA	c	502	-	56,73,73	1.54	6 (10%)	55,113,113	1.63	8 (14%)
26	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
24	CLA	B	604	-	56,73,73	1.29	5 (8%)	55,113,113	1.82	12 (21%)
24	CLA	C	502	-	56,73,73	1.72	7 (12%)	55,113,113	1.53	7 (12%)
25	PHO	A	607	-	67,69,69	1.22	6 (8%)	85,99,99	1.14	8 (9%)
25	PHO	d	402	-	67,69,69	1.28	9 (13%)	85,99,99	1.06	6 (7%)
24	CLA	b	609	-	56,73,73	1.70	6 (10%)	55,113,113	2.07	15 (27%)
33	STE	B	620	-	13,16,19	0.36	0	12,16,19	1.09	0
33	STE	H	103	-	17,17,19	0.48	0	16,16,19	0.69	0
24	CLA	b	607	37	56,73,73	1.43	8 (14%)	55,113,113	1.50	10 (18%)
26	BCR	x	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
29	LMG	c	519	-	37,37,55	1.24	6 (16%)	45,45,63	1.33	6 (13%)
21	OEY	A	601[B]	1,37,3	0,16,16	-	-	-	-	-
29	LMG	A	614	-	48,48,55	1.03	4 (8%)	56,56,63	1.41	6 (10%)
24	CLA	B	608	-	56,73,73	1.46	7 (12%)	55,113,113	1.51	11 (20%)
24	CLA	C	503	-	56,73,73	1.65	6 (10%)	55,113,113	2.03	11 (20%)
29	LMG	D	406	-	51,51,55	0.96	4 (7%)	59,59,63	1.27	4 (6%)
24	CLA	D	402	-	56,73,73	1.43	6 (10%)	55,113,113	1.72	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LHG	d	408	-	48,48,48	0.83	2 (4%)	51,54,54	1.20	4 (7%)
31	SQD	D	407	-	35,36,54	1.02	3 (8%)	42,45,65	2.16	10 (23%)
33	STE	T	103	-	14,14,19	0.43	0	13,13,19	0.78	0
36	HEC	v	201	17	26,50,50	2.42	3 (11%)	18,82,82	1.88	6 (33%)
36	HEC	V	201	17	26,50,50	2.09	4 (15%)	18,82,82	2.04	7 (38%)
32	DGD	h	101	-	63,63,67	1.18	6 (9%)	77,77,81	1.37	11 (14%)
24	CLA	B	616	-	51,68,73	1.79	9 (17%)	49,107,113	2.08	8 (16%)
25	PHO	A	606	-	67,69,69	1.11	6 (8%)	85,99,99	1.10	5 (5%)
24	CLA	B	615	-	56,73,73	1.74	7 (12%)	55,113,113	1.46	6 (10%)
24	CLA	C	507	37	56,73,73	1.51	7 (12%)	55,113,113	1.79	13 (23%)
33	STE	a	617	-	14,14,19	0.41	0	13,13,19	0.80	0
34	BCT	D	401	23	0,3,3	-	-	0,3,3	-	-
35	HEM	e	101	6,5	27,50,50	1.95	5 (18%)	17,82,82	2.16	5 (29%)
26	BCR	C	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	6 (10%)
25	PHO	a	605	-	67,69,69	1.17	9 (13%)	85,99,99	1.10	5 (5%)
26	BCR	B	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.15	4 (7%)
33	STE	d	411	-	13,16,19	0.30	0	12,16,19	1.18	0
24	CLA	d	404	-	56,73,73	1.67	9 (16%)	55,113,113	1.53	9 (16%)
28	PL9	A	612	-	55,55,55	1.13	5 (9%)	68,69,69	1.62	11 (16%)
24	CLA	A	604	-	56,73,73	1.56	5 (8%)	55,113,113	1.56	11 (20%)
33	STE	J	101	-	8,11,19	0.33	0	7,11,19	0.99	0
31	SQD	a	614	-	35,35,54	1.02	2 (5%)	37,37,65	1.51	6 (16%)
33	STE	C	521	-	15,15,19	0.35	0	14,14,19	0.86	0
24	CLA	c	504	37	51,68,73	1.65	7 (13%)	49,107,113	1.57	10 (20%)
33	STE	I	101	-	14,14,19	0.43	0	13,13,19	0.64	0
33	STE	b	624	-	12,15,19	0.39	0	11,15,19	0.72	0
24	CLA	a	612	37	56,73,73	1.79	6 (10%)	55,113,113	1.92	9 (16%)
24	CLA	A	613	37	56,73,73	1.61	8 (14%)	55,113,113	1.71	10 (18%)
33	STE	k	103	-	8,11,19	0.46	0	7,11,19	0.72	0
29	LMG	b	621	-	51,51,55	0.94	3 (5%)	59,59,63	1.48	10 (16%)
29	LMG	b	623	-	55,55,55	0.88	3 (5%)	63,63,63	1.40	8 (12%)
24	CLA	C	506	-	56,73,73	1.55	9 (16%)	55,113,113	1.51	8 (14%)
31	SQD	A	616	-	51,52,54	1.11	6 (11%)	60,63,65	2.14	11 (18%)
24	CLA	B	613	-	56,73,73	1.64	6 (10%)	55,113,113	1.40	8 (14%)
29	LMG	C	519	-	48,48,55	0.89	3 (6%)	56,56,63	1.37	8 (14%)
24	CLA	c	506	-	56,73,73	1.51	11 (19%)	55,113,113	1.79	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	508	-	55,72,73	1.61	7 (12%)	53,111,113	1.76	10 (18%)
22	OEX	a	602[A]	1,37,3	0,15,15	-	-	-		
26	BCR	Y	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.15	5 (8%)
30	LHG	e	102	-	41,41,48	0.88	2 (4%)	44,47,54	1.31	5 (11%)
24	CLA	B	601	37	56,73,73	1.64	7 (12%)	55,113,113	1.61	9 (16%)
29	LMG	d	410	-	44,44,55	1.02	3 (6%)	52,52,63	1.26	6 (11%)
33	STE	B	625	-	8,11,19	0.37	0	7,11,19	0.93	0
33	STE	b	627	-	13,13,19	0.46	0	12,12,19	0.53	0
24	CLA	B	612	-	56,73,73	1.48	3 (5%)	55,113,113	1.92	11 (20%)
24	CLA	C	512	-	56,73,73	1.40	8 (14%)	55,113,113	1.76	11 (20%)
24	CLA	b	603	-	56,73,73	1.85	8 (14%)	55,113,113	1.77	11 (20%)
33	STE	E	102	-	8,11,19	0.44	0	7,11,19	0.59	0
28	PL9	D	405	-	55,55,55	1.52	9 (16%)	68,69,69	1.71	17 (25%)
30	LHG	B	621	-	48,48,48	0.82	1 (2%)	51,54,54	1.17	5 (9%)
31	SQD	b	620	-	48,49,54	1.00	4 (8%)	57,60,65	1.92	14 (24%)
24	CLA	b	605	-	56,73,73	1.33	7 (12%)	55,113,113	1.79	13 (23%)
33	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.87	0
26	BCR	d	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.23	6 (10%)
33	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.89	0
24	CLA	B	610	37	56,73,73	1.65	9 (16%)	55,113,113	1.75	11 (20%)
24	CLA	d	401	37	56,73,73	1.63	9 (16%)	55,113,113	1.50	9 (16%)
29	LMG	c	521	-	48,48,55	1.09	6 (12%)	56,56,63	1.27	3 (5%)
33	STE	B	626	-	15,15,19	0.44	0	14,14,19	0.67	0
28	PL9	d	406	-	55,55,55	1.50	7 (12%)	68,69,69	1.78	16 (23%)
24	CLA	c	513	-	56,73,73	1.53	7 (12%)	55,113,113	1.59	8 (14%)
26	BCR	D	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	4 (7%)
33	STE	b	622	-	16,19,19	0.34	0	15,19,19	0.83	0
24	CLA	C	505	-	56,73,73	1.62	4 (7%)	55,113,113	1.88	9 (16%)
24	CLA	C	501	-	56,73,73	1.78	8 (14%)	55,113,113	1.83	9 (16%)
24	CLA	C	513	-	56,73,73	1.42	7 (12%)	55,113,113	1.77	9 (16%)
26	BCR	a	607	-	41,41,41	1.05	4 (9%)	56,56,56	1.22	5 (8%)
24	CLA	c	503	-	56,73,73	1.59	8 (14%)	55,113,113	1.57	9 (16%)
33	STE	C	520	-	8,11,19	0.52	0	7,11,19	0.51	0
24	CLA	c	501	-	56,73,73	1.41	5 (8%)	55,113,113	1.78	10 (18%)

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
31	SQD	B	623	-	-	22/49/69/69	0/1/1/1
24	CLA	A	605	37	1/1/20/20	14/37/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	510	-	1/1/20/20	10/37/115/115	-
29	LMG	a	618	-	-	30/50/70/70	0/1/1/1
24	CLA	C	511	3	1/1/20/20	5/37/115/115	-
24	CLA	B	602	-	1/1/20/20	6/37/115/115	-
24	CLA	c	512	-	1/1/20/20	19/37/115/115	-
24	CLA	B	609	-	-	5/37/115/115	-
32	DGD	c	518	-	-	12/51/91/95	0/2/2/2
30	LHG	l	101	-	-	15/53/53/53	-
24	CLA	C	508	-	-	9/37/115/115	-
33	STE	B	624	-	-	3/9/11/17	-
30	LHG	E	101	-	-	22/53/53/53	-
24	CLA	B	606	-	1/1/20/20	12/37/115/115	-
33	STE	B	627	-	-	5/7/9/17	-
26	BCR	A	609	-	-	8/29/63/63	0/2/2/2
24	CLA	a	604	-	1/1/20/20	5/37/115/115	-
26	BCR	b	618	-	-	4/29/63/63	0/2/2/2
24	CLA	c	511	3	1/1/20/20	11/37/115/115	-
24	CLA	b	608	-	-	1/37/115/115	-
29	LMG	c	522	-	-	20/44/64/70	0/1/1/1
26	BCR	c	515	-	-	3/29/63/63	0/2/2/2
33	STE	b	625	-	-	10/15/17/17	-
24	CLA	b	616	-	1/1/19/20	8/31/109/115	-
33	STE	C	522	-	-	3/7/9/17	-
24	CLA	b	613	-	1/1/20/20	8/37/115/115	-
24	CLA	b	614	-	1/1/20/20	15/37/115/115	-
24	CLA	d	403	-	1/1/20/20	5/37/115/115	-
30	LHG	d	409	-	-	14/43/43/53	-
31	SQD	a	613	-	-	21/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	509	-	1/1/20/20	15/37/115/115	-
26	BCR	k	101	-	-	12/29/63/63	0/2/2/2
24	CLA	b	611	-	1/1/20/20	5/37/115/115	-
33	STE	x	102	-	-	6/15/17/17	-
33	STE	a	616	-	-	3/7/9/17	-
26	BCR	b	617	-	-	6/29/63/63	0/2/2/2
24	CLA	c	507	37	1/1/20/20	12/37/115/115	-
24	CLA	B	611	-	1/1/20/20	7/37/115/115	-
29	LMG	D	409	-	-	16/33/33/70	-
33	STE	d	412	-	-	11/15/17/17	-
24	CLA	b	604	-	1/1/20/20	8/37/115/115	-
26	BCR	t	101	-	-	6/29/63/63	0/2/2/2
24	CLA	b	601	37	1/1/20/20	14/37/115/115	-
24	CLA	A	608	-	1/1/17/20	2/24/102/115	-
24	CLA	b	612	-	1/1/20/20	7/37/115/115	-
32	DGD	C	518	-	-	18/51/91/95	0/2/2/2
26	BCR	C	514	-	-	8/29/63/63	0/2/2/2
29	LMG	D	410	-	-	10/18/22/70	-
33	STE	M	102	-	-	3/10/12/17	-
33	STE	t	102	-	-	7/13/15/17	-
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
30	LHG	B	622	-	-	16/53/53/53	-
31	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
32	DGD	C	517	-	-	24/51/91/95	0/2/2/2
33	STE	D	411	-	-	11/15/17/17	-
24	CLA	c	505	-	1/1/20/20	11/37/115/115	-
24	CLA	b	610	37	1/1/20/20	3/37/115/115	-
30	LHG	d	407	-	-	21/53/53/53	-
24	CLA	a	606	-	1/1/20/20	9/37/115/115	-
30	LHG	A	615	-	-	20/51/51/53	-
33	STE	b	626	-	-	5/7/7/17	-
33	STE	j	101	-	-	4/7/9/17	-
24	CLA	b	602	-	-	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	M	101	-	-	23/46/66/70	0/1/1/1
33	STE	m	101	-	-	3/7/9/17	-
32	DGD	c	517	-	-	19/51/91/95	0/2/2/2
33	STE	Z	101	-	-	2/5/5/17	-
33	STE	c	520	-	-	8/15/17/17	-
24	CLA	B	603	-	1/1/20/20	7/37/115/115	-
24	CLA	b	615	-	1/1/20/20	8/37/115/115	-
24	CLA	B	614	-	1/1/20/20	17/37/115/115	-
24	CLA	c	509	-	1/1/20/20	12/37/115/115	-
28	PL9	a	611	-	-	23/53/73/73	0/1/1/1
32	DGD	A	618	-	-	26/55/95/95	0/2/2/2
30	LHG	D	408	-	-	23/53/53/53	-
24	CLA	b	606	-	1/1/20/20	12/37/115/115	-
24	CLA	B	605	-	1/1/20/20	8/37/115/115	-
26	BCR	B	619	-	-	5/29/63/63	0/2/2/2
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
24	CLA	c	510	-	1/1/20/20	10/37/115/115	-
33	STE	T	102	-	-	8/13/13/17	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	0/6/54/54	-
24	CLA	C	504	37	1/1/18/20	6/30/108/115	-
32	DGD	C	516	-	-	18/51/91/95	0/2/2/2
24	CLA	B	607	37	1/1/20/20	5/37/115/115	-
33	STE	a	615	-	-	4/7/7/17	-
24	CLA	D	403	-	-	10/37/115/115	-
24	CLA	c	502	-	-	4/37/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
24	CLA	B	604	-	1/1/20/20	12/37/115/115	-
24	CLA	C	502	-	-	8/37/115/115	-
25	PHO	A	607	-	-	1/53/103/103	0/5/6/6
25	PHO	d	402	-	-	1/53/103/103	0/5/6/6
24	CLA	b	609	-	-	11/37/115/115	-
33	STE	B	620	-	-	6/12/14/17	-
33	STE	H	103	-	-	9/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	607	37	1/1/20/20	13/37/115/115	-
26	BCR	x	101	-	-	7/29/63/63	0/2/2/2
29	LMG	c	519	-	-	11/31/51/70	0/1/1/1
29	LMG	A	614	-	-	21/43/63/70	0/1/1/1
24	CLA	C	503	-	1/1/20/20	5/37/115/115	-
24	CLA	B	608	-	-	2/37/115/115	-
29	LMG	D	406	-	-	14/46/66/70	0/1/1/1
24	CLA	D	402	-	1/1/20/20	6/37/115/115	-
30	LHG	d	408	-	-	18/53/53/53	-
31	SQD	D	407	-	-	15/28/48/69	0/1/1/1
33	STE	T	103	-	-	11/12/12/17	-
36	HEC	v	201	17	-	0/6/54/54	-
36	HEC	V	201	17	-	0/6/54/54	-
32	DGD	h	101	-	-	15/51/91/95	0/2/2/2
24	CLA	B	616	-	1/1/19/20	8/31/109/115	-
25	PHO	A	606	-	-	3/53/103/103	0/5/6/6
24	CLA	B	615	-	1/1/20/20	11/37/115/115	-
24	CLA	C	507	37	1/1/20/20	10/37/115/115	-
33	STE	a	617	-	-	8/12/12/17	-
35	HEM	e	101	6,5	-	0/6/54/54	-
26	BCR	C	515	-	-	3/29/63/63	0/2/2/2
25	PHO	a	605	-	-	2/53/103/103	0/5/6/6
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
33	STE	d	411	-	-	7/12/14/17	-
24	CLA	d	404	-	1/1/20/20	11/37/115/115	-
28	PL9	A	612	-	-	23/53/73/73	0/1/1/1
24	CLA	A	604	-	1/1/20/20	4/37/115/115	-
33	STE	J	101	-	-	5/7/9/17	-
31	SQD	a	614	-	-	18/37/37/69	-
33	STE	C	521	-	-	7/13/13/17	-
24	CLA	c	504	37	1/1/19/20	8/31/109/115	-
33	STE	I	101	-	-	4/12/12/17	-
33	STE	b	624	-	-	8/11/13/17	-
24	CLA	a	612	37	1/1/20/20	5/37/115/115	-
24	CLA	A	613	37	-	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	k	103	-	-	4/7/9/17	-
29	LMG	b	621	-	-	24/46/66/70	0/1/1/1
29	LMG	b	623	-	-	27/50/70/70	0/1/1/1
24	CLA	C	506	-	1/1/20/20	11/37/115/115	-
31	SQD	A	616	-	-	15/47/67/69	0/1/1/1
24	CLA	B	613	-	1/1/20/20	14/37/115/115	-
29	LMG	C	519	-	-	17/43/63/70	0/1/1/1
24	CLA	c	506	-	1/1/20/20	14/37/115/115	-
24	CLA	c	508	-	-	9/36/114/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
30	LHG	e	102	-	-	27/46/46/53	-
24	CLA	B	601	37	1/1/20/20	15/37/115/115	-
29	LMG	d	410	-	-	11/39/59/70	0/1/1/1
33	STE	B	625	-	-	4/7/9/17	-
33	STE	b	627	-	-	6/11/11/17	-
24	CLA	B	612	-	1/1/20/20	8/37/115/115	-
24	CLA	C	512	-	1/1/20/20	12/37/115/115	-
24	CLA	b	603	-	1/1/20/20	9/37/115/115	-
33	STE	E	102	-	-	4/7/9/17	-
28	PL9	D	405	-	-	12/53/73/73	0/1/1/1
30	LHG	B	621	-	-	25/53/53/53	-
31	SQD	b	620	-	-	19/44/64/69	0/1/1/1
24	CLA	b	605	-	1/1/20/20	6/37/115/115	-
33	STE	M	103	-	-	1/7/7/17	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
33	STE	l	102	-	-	9/15/15/17	-
24	CLA	B	610	37	1/1/20/20	6/37/115/115	-
24	CLA	d	401	37	-	12/37/115/115	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
33	STE	B	626	-	-	8/13/13/17	-
28	PL9	d	406	-	-	11/53/73/73	0/1/1/1
24	CLA	c	513	-	1/1/20/20	7/37/115/115	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
33	STE	b	622	-	-	9/15/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	505	-	1/1/20/20	10/37/115/115	-
24	CLA	C	501	-	1/1/20/20	3/37/115/115	-
24	CLA	C	513	-	1/1/20/20	6/37/115/115	-
26	BCR	a	607	-	-	1/29/63/63	0/2/2/2
24	CLA	c	503	-	1/1/20/20	8/37/115/115	-
33	STE	C	520	-	-	6/7/9/17	-
24	CLA	c	501	-	1/1/20/20	2/37/115/115	-

All (783) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	MG-NA	9.48	2.28	2.06
24	d	403	CLA	C4B-NB	9.31	1.43	1.35
24	c	504	CLA	C4B-NB	8.70	1.43	1.35
24	b	603	CLA	C4B-NB	8.65	1.42	1.35
24	B	612	CLA	C4B-NB	8.34	1.42	1.35
24	B	602	CLA	C4B-NB	8.06	1.42	1.35
24	A	604	CLA	C4B-NB	8.01	1.42	1.35
24	B	614	CLA	C4B-NB	7.84	1.42	1.35
24	B	613	CLA	C4B-NB	7.84	1.42	1.35
24	B	615	CLA	C4B-NB	7.78	1.42	1.35
24	a	612	CLA	MG-NA	7.78	2.24	2.06
24	c	511	CLA	MG-NA	7.69	2.24	2.06
36	v	201	HEC	C3B-C2B	-7.66	1.32	1.40
24	A	605	CLA	C4B-NB	7.57	1.42	1.35
24	c	509	CLA	C4C-NC	7.52	1.41	1.35
24	C	502	CLA	C4C-NC	7.50	1.41	1.35
24	B	601	CLA	C4B-NB	7.49	1.41	1.35
24	b	612	CLA	C4C-NC	7.46	1.41	1.35
24	b	613	CLA	C4B-NB	7.44	1.41	1.35
24	c	510	CLA	MG-NA	7.43	2.23	2.06
24	b	608	CLA	C4C-NC	7.41	1.41	1.35
24	b	615	CLA	C4B-NB	7.41	1.41	1.35
24	C	505	CLA	C4B-NB	7.40	1.41	1.35
24	B	609	CLA	C4B-NB	7.34	1.41	1.35
24	c	505	CLA	C4B-NB	7.24	1.41	1.35
24	B	610	CLA	C4B-NB	7.23	1.41	1.35
24	C	501	CLA	C4B-NB	7.15	1.41	1.35
24	c	510	CLA	C4C-NC	7.14	1.41	1.35
24	B	611	CLA	MG-NA	7.14	2.23	2.06
24	D	403	CLA	C4B-NB	7.09	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C4B-NB	7.07	1.41	1.35
24	a	606	CLA	C4C-NC	7.06	1.41	1.35
24	b	601	CLA	C4B-NB	7.01	1.41	1.35
24	c	513	CLA	C4B-NB	6.99	1.41	1.35
24	b	611	CLA	C4C-NC	6.97	1.41	1.35
24	b	604	CLA	C4B-NB	6.93	1.41	1.35
24	d	401	CLA	C4B-NB	6.90	1.41	1.35
24	a	604	CLA	C4B-NB	6.88	1.41	1.35
24	B	606	CLA	C4B-NB	6.87	1.41	1.35
24	a	606	CLA	C4B-NB	6.86	1.41	1.35
24	D	402	CLA	C4B-NB	6.84	1.41	1.35
24	b	609	CLA	C4B-NB	6.76	1.41	1.35
24	c	510	CLA	C4B-NB	6.69	1.41	1.35
24	d	404	CLA	C4B-NB	6.67	1.41	1.35
24	C	511	CLA	C4C-NC	6.64	1.41	1.35
24	C	501	CLA	MG-NA	6.56	2.21	2.06
24	C	510	CLA	C4B-NB	6.52	1.41	1.35
24	c	503	CLA	C4B-NB	6.49	1.41	1.35
24	C	506	CLA	C4B-NB	6.44	1.41	1.35
24	A	608	CLA	C4B-NB	6.44	1.41	1.35
24	c	511	CLA	C4B-NB	6.44	1.41	1.35
24	c	507	CLA	C4C-NC	6.43	1.40	1.35
36	V	201	HEC	C3B-C2B	-6.41	1.34	1.40
24	b	614	CLA	C4B-NB	6.41	1.40	1.35
24	B	602	CLA	C4C-NC	6.38	1.40	1.35
24	c	502	CLA	C4B-NB	6.36	1.40	1.35
24	C	503	CLA	C4B-NB	6.35	1.40	1.35
24	C	508	CLA	C4C-NC	6.34	1.40	1.35
24	A	613	CLA	C4B-NB	6.24	1.40	1.35
24	b	609	CLA	MG-NA	6.23	2.21	2.06
24	B	611	CLA	C4B-NB	6.16	1.40	1.35
24	a	612	CLA	C4B-NB	6.13	1.40	1.35
24	c	511	CLA	C4C-NC	6.07	1.40	1.35
24	C	511	CLA	MG-NA	6.03	2.20	2.06
24	C	509	CLA	C4B-NB	6.02	1.40	1.35
35	e	101	HEM	C3B-C2B	-6.01	1.32	1.40
24	C	505	CLA	MG-NA	5.97	2.20	2.06
24	B	616	CLA	C4B-NB	5.96	1.40	1.35
24	B	616	CLA	MG-NA	5.94	2.20	2.06
24	C	508	CLA	MG-NA	5.93	2.20	2.06
24	B	609	CLA	MG-NA	5.93	2.20	2.06
24	C	502	CLA	C4B-NB	5.91	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C4B-NB	5.91	1.40	1.35
24	c	501	CLA	C4B-NB	5.90	1.40	1.35
24	a	604	CLA	C4C-NC	5.89	1.40	1.35
24	A	613	CLA	C4C-NC	5.86	1.40	1.35
24	c	502	CLA	C4C-NC	5.86	1.40	1.35
24	C	510	CLA	C4C-NC	5.83	1.40	1.35
24	c	505	CLA	C4C-NC	5.82	1.40	1.35
24	C	503	CLA	MG-NA	5.81	2.20	2.06
24	B	603	CLA	C4C-NC	5.80	1.40	1.35
24	B	608	CLA	C4C-NC	5.80	1.40	1.35
24	c	506	CLA	C4B-NB	5.75	1.40	1.35
36	v	201	HEC	C3C-C2C	-5.75	1.34	1.40
24	d	401	CLA	C4C-NC	5.72	1.40	1.35
24	c	509	CLA	C4B-NB	5.66	1.40	1.35
24	b	608	CLA	C4B-NB	5.61	1.40	1.35
24	C	513	CLA	C4B-NB	5.59	1.40	1.35
28	d	406	PL9	C6-C1	-5.57	1.38	1.48
24	B	616	CLA	C4C-NC	5.56	1.40	1.35
24	C	507	CLA	C4B-NB	5.43	1.40	1.35
24	b	602	CLA	C4C-NC	5.42	1.40	1.35
24	B	603	CLA	C4B-NB	5.37	1.40	1.35
24	c	501	CLA	C4C-NC	5.35	1.40	1.35
24	B	610	CLA	C4C-NC	5.34	1.40	1.35
24	C	501	CLA	C4C-NC	5.31	1.39	1.35
24	c	512	CLA	C4B-NB	5.28	1.39	1.35
24	B	614	CLA	C4C-NC	5.28	1.39	1.35
24	C	507	CLA	MG-NA	5.28	2.18	2.06
24	D	403	CLA	C4C-NC	5.28	1.39	1.35
24	c	503	CLA	C4C-NC	5.28	1.39	1.35
24	C	504	CLA	C4B-NB	5.27	1.39	1.35
24	b	616	CLA	C4C-NC	5.27	1.39	1.35
24	b	605	CLA	C4B-NB	5.26	1.39	1.35
24	b	601	CLA	C4C-NC	5.25	1.39	1.35
24	b	610	CLA	C4C-NC	5.25	1.39	1.35
24	b	613	CLA	C4C-NC	5.24	1.39	1.35
24	c	508	CLA	C4C-NC	5.21	1.39	1.35
24	c	512	CLA	C4C-NC	5.21	1.39	1.35
24	A	608	CLA	C4C-NC	5.18	1.39	1.35
24	b	610	CLA	C4B-NB	5.17	1.39	1.35
24	b	612	CLA	C4B-NB	5.17	1.39	1.35
24	C	512	CLA	C4B-NB	5.16	1.39	1.35
24	b	615	CLA	C4C-NC	5.13	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C4C-NC	5.10	1.39	1.35
24	a	612	CLA	C4C-NC	5.09	1.39	1.35
35	F	101	HEM	C3B-C2B	-5.01	1.33	1.40
36	v	201	HEC	C3D-C2D	5.00	1.52	1.37
24	b	606	CLA	C4C-NC	5.00	1.39	1.35
36	V	201	HEC	C3C-C2C	-5.00	1.35	1.40
24	B	604	CLA	C4B-NB	4.96	1.39	1.35
24	d	404	CLA	MG-NA	4.95	2.18	2.06
24	B	615	CLA	C4C-NC	4.91	1.39	1.35
24	B	601	CLA	C4C-NC	4.90	1.39	1.35
24	C	508	CLA	C4B-NB	4.89	1.39	1.35
24	C	504	CLA	C4C-NC	4.88	1.39	1.35
24	b	607	CLA	C4B-NB	4.86	1.39	1.35
35	F	101	HEM	C3C-C2C	-4.85	1.33	1.40
24	C	513	CLA	C4C-NC	4.84	1.39	1.35
24	c	508	CLA	MG-NA	4.83	2.17	2.06
24	B	603	CLA	MG-NA	4.81	2.17	2.06
24	c	513	CLA	C4C-NC	4.79	1.39	1.35
24	b	616	CLA	C4B-NB	4.75	1.39	1.35
24	B	606	CLA	C4C-NC	4.74	1.39	1.35
24	b	615	CLA	MG-NA	4.73	2.17	2.06
24	b	606	CLA	C4B-NB	4.73	1.39	1.35
24	B	613	CLA	C4C-NC	4.70	1.39	1.35
28	D	405	PL9	C7-C3	-4.67	1.46	1.51
24	C	507	CLA	C4C-NC	4.60	1.39	1.35
24	C	509	CLA	C4C-NC	4.58	1.39	1.35
24	b	603	CLA	MG-NA	4.55	2.17	2.06
24	B	606	CLA	C3B-C2B	-4.55	1.34	1.40
24	b	614	CLA	C4C-NC	4.54	1.39	1.35
24	b	604	CLA	C4C-NC	4.52	1.39	1.35
24	b	609	CLA	C4C-NC	4.52	1.39	1.35
28	d	406	PL9	C53-C6	-4.49	1.41	1.50
30	D	408	LHG	O7-C5	-4.46	1.35	1.46
24	b	602	CLA	C4B-NB	4.42	1.39	1.35
24	d	403	CLA	C4C-NC	4.39	1.39	1.35
24	C	502	CLA	MG-NA	4.39	2.16	2.06
24	b	611	CLA	C4B-NB	4.36	1.39	1.35
24	B	606	CLA	MG-NA	4.35	2.16	2.06
24	A	605	CLA	C4C-NC	4.34	1.39	1.35
24	C	506	CLA	MG-NA	4.32	2.16	2.06
36	V	201	HEC	C3D-C2D	4.30	1.50	1.37
24	B	605	CLA	C4C-NC	4.25	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C4B-NB	4.25	1.39	1.35
24	B	605	CLA	C4B-NB	4.22	1.39	1.35
32	A	618	DGD	O5D-C6D	-4.14	1.36	1.43
24	d	404	CLA	C4C-NC	4.09	1.38	1.35
24	C	505	CLA	C4C-NC	4.07	1.38	1.35
30	A	615	LHG	O3-C3	-4.07	1.29	1.44
26	c	515	BCR	C1-C6	-4.06	1.48	1.53
26	B	618	BCR	C30-C25	-4.02	1.48	1.53
24	b	601	CLA	MG-NA	4.01	2.15	2.06
26	Y	101	BCR	C30-C25	-4.01	1.48	1.53
29	a	618	LMG	C4-C5	3.97	1.61	1.53
24	c	506	CLA	C4C-NC	3.96	1.38	1.35
24	B	615	CLA	MG-NA	3.93	2.15	2.06
24	C	512	CLA	C4C-NC	3.92	1.38	1.35
24	c	507	CLA	C3B-C2B	-3.92	1.34	1.40
24	B	612	CLA	C4C-NC	3.91	1.38	1.35
24	B	608	CLA	C4B-NB	3.88	1.38	1.35
24	C	503	CLA	C4C-NC	3.84	1.38	1.35
26	C	515	BCR	C1-C6	-3.83	1.48	1.53
24	B	609	CLA	C4C-NC	3.81	1.38	1.35
28	D	405	PL9	C3-C4	-3.80	1.43	1.49
24	b	605	CLA	C4C-NC	3.80	1.38	1.35
24	C	506	CLA	C4C-NC	3.77	1.38	1.35
35	e	101	HEM	C3C-C2C	-3.76	1.35	1.40
29	D	409	LMG	C7-C8	3.76	1.60	1.51
32	C	518	DGD	O2G-C2G	-3.76	1.37	1.46
31	b	620	SQD	O48-C23	3.69	1.44	1.33
26	c	514	BCR	C1-C6	-3.69	1.48	1.53
24	b	607	CLA	C4C-NC	3.69	1.38	1.35
26	H	101	BCR	C30-C25	-3.67	1.48	1.53
26	D	404	BCR	C30-C25	-3.66	1.48	1.53
24	b	615	CLA	C3B-C2B	-3.66	1.35	1.40
25	A	607	PHO	C3B-C4B	3.63	1.50	1.43
25	d	402	PHO	C3B-C4B	3.62	1.50	1.43
24	C	508	CLA	C1D-C2D	3.58	1.50	1.42
24	D	402	CLA	C4C-NC	3.58	1.38	1.35
26	C	514	BCR	C1-C6	-3.58	1.48	1.53
31	a	613	SQD	O48-C23	3.56	1.43	1.33
26	B	619	BCR	C1-C6	-3.55	1.48	1.53
31	a	614	SQD	O48-C23	3.55	1.43	1.33
28	d	406	PL9	C31-C29	-3.54	1.43	1.51
26	K	101	BCR	C30-C25	-3.54	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C30-C25	-3.52	1.48	1.53
26	d	405	BCR	C30-C25	-3.52	1.48	1.53
32	c	518	DGD	O3G-C3G	-3.52	1.37	1.43
29	c	519	LMG	C1-C2	3.51	1.62	1.52
24	b	612	CLA	MG-NA	3.51	2.14	2.06
24	d	401	CLA	C3B-C2B	-3.49	1.35	1.40
25	A	607	PHO	C1C-NC	-3.46	1.31	1.38
32	C	517	DGD	C4D-C3D	3.46	1.61	1.52
30	B	621	LHG	O7-C5	-3.45	1.38	1.46
24	B	603	CLA	CMB-C2B	-3.45	1.44	1.51
30	A	615	LHG	P-O6	3.44	1.73	1.59
25	A	607	PHO	C1A-NA	3.44	1.44	1.37
26	C	514	BCR	C30-C25	-3.43	1.49	1.53
28	D	405	PL9	C26-C24	-3.43	1.44	1.51
32	C	517	DGD	O5D-C6D	-3.41	1.37	1.43
29	c	521	LMG	O1-C1	3.40	1.46	1.40
24	c	507	CLA	C4B-NB	3.39	1.38	1.35
24	b	610	CLA	C3B-C2B	-3.39	1.35	1.40
32	h	101	DGD	O2D-C2D	-3.38	1.35	1.43
29	A	614	LMG	O1-C7	-3.37	1.37	1.43
26	k	101	BCR	C30-C25	-3.36	1.49	1.53
24	B	601	CLA	C3B-C2B	-3.34	1.35	1.40
24	B	615	CLA	CMB-C2B	-3.33	1.44	1.51
30	d	407	LHG	C24-C23	3.33	1.60	1.50
31	B	623	SQD	O47-C7	3.33	1.43	1.34
32	c	517	DGD	C3E-C2E	3.33	1.60	1.52
32	H	102	DGD	O2D-C2D	-3.32	1.35	1.43
31	D	407	SQD	O48-C23	3.30	1.43	1.33
24	c	505	CLA	MG-NA	3.29	2.14	2.06
29	d	410	LMG	C4-C5	3.29	1.60	1.53
28	D	405	PL9	C6-C1	-3.28	1.42	1.48
24	c	504	CLA	C4C-NC	3.26	1.38	1.35
24	B	602	CLA	MG-NA	3.25	2.14	2.06
24	B	606	CLA	C3B-CAB	-3.25	1.41	1.47
26	k	102	BCR	C30-C25	-3.24	1.49	1.53
26	b	618	BCR	C1-C6	-3.24	1.49	1.53
26	c	514	BCR	C30-C25	-3.23	1.49	1.53
32	A	618	DGD	C4D-C3D	3.22	1.60	1.52
24	B	615	CLA	C1D-C2D	3.21	1.49	1.42
24	b	615	CLA	CMB-C2B	-3.21	1.45	1.51
24	B	614	CLA	C3B-C2B	-3.20	1.35	1.40
31	a	614	SQD	O47-C7	3.20	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	613	CLA	MG-NA	3.20	2.13	2.06
25	a	605	PHO	C4C-NC	3.19	1.44	1.36
32	A	618	DGD	C3E-C2E	3.19	1.60	1.52
35	F	101	HEM	C3B-CAB	3.18	1.54	1.47
24	b	608	CLA	CMB-C2B	-3.18	1.45	1.51
24	b	612	CLA	CMB-C2B	-3.18	1.45	1.51
31	B	623	SQD	O48-C23	3.16	1.42	1.33
24	B	607	CLA	MG-NA	3.16	2.13	2.06
26	B	617	BCR	C1-C6	-3.16	1.49	1.53
24	B	602	CLA	CMB-C2B	-3.16	1.45	1.51
28	A	612	PL9	C7-C8	-3.16	1.46	1.50
26	C	515	BCR	C30-C25	-3.15	1.49	1.53
24	B	604	CLA	MG-NA	3.15	2.13	2.06
24	B	601	CLA	CMB-C2B	-3.15	1.45	1.51
31	a	613	SQD	O2-C2	-3.14	1.35	1.43
24	B	607	CLA	C4C-NC	3.13	1.38	1.35
26	b	618	BCR	C30-C25	-3.13	1.49	1.53
31	A	617	SQD	O47-C7	3.13	1.43	1.34
24	c	510	CLA	CMB-C2B	-3.13	1.45	1.51
28	d	406	PL9	C3-C4	-3.12	1.44	1.49
32	C	516	DGD	O2E-C2E	-3.11	1.35	1.43
32	H	102	DGD	O3G-C1D	3.10	1.45	1.40
26	b	617	BCR	C30-C25	-3.10	1.49	1.53
30	E	101	LHG	P-O6	3.09	1.71	1.59
24	B	604	CLA	C4C-NC	3.09	1.38	1.35
24	B	613	CLA	CMD-C2D	-3.09	1.44	1.51
24	a	612	CLA	CMB-C2B	-3.08	1.45	1.51
31	A	616	SQD	O48-C23	3.08	1.42	1.33
24	b	601	CLA	C1D-C2D	3.08	1.49	1.42
26	x	101	BCR	C30-C25	-3.07	1.49	1.53
31	f	101	SQD	O48-C23	3.07	1.42	1.33
26	c	515	BCR	C30-C25	-3.07	1.49	1.53
24	D	403	CLA	CMB-C2B	-3.06	1.45	1.51
32	H	102	DGD	O5D-C1E	3.06	1.45	1.40
24	A	604	CLA	C1D-C2D	3.05	1.49	1.42
26	A	609	BCR	C33-C5	-3.05	1.45	1.50
32	C	516	DGD	C6D-C5D	3.05	1.61	1.51
24	B	610	CLA	C3B-C2B	-3.04	1.36	1.40
29	a	618	LMG	C4-C3	3.03	1.60	1.52
32	C	516	DGD	C6E-C5E	3.02	1.62	1.51
24	b	603	CLA	CMB-C2B	-3.02	1.45	1.51
32	C	517	DGD	C6E-C5E	3.01	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	611	PL9	C3-C4	-3.01	1.44	1.49
24	c	512	CLA	C1D-C2D	3.00	1.49	1.42
32	C	516	DGD	O5D-C1E	2.99	1.45	1.40
32	H	102	DGD	C3E-C2E	2.99	1.59	1.52
26	Y	101	BCR	C1-C6	-2.99	1.49	1.53
24	c	506	CLA	CAC-C3C	-2.98	1.44	1.52
31	b	620	SQD	O47-C7	2.98	1.42	1.34
30	B	622	LHG	O7-C5	-2.98	1.39	1.46
24	b	602	CLA	CAC-C3C	-2.98	1.44	1.52
32	H	102	DGD	C4E-C5E	2.97	1.59	1.53
24	b	608	CLA	C1D-C2D	2.96	1.49	1.42
24	C	513	CLA	MG-NA	2.96	2.13	2.06
31	f	101	SQD	O47-C7	2.96	1.42	1.34
24	b	607	CLA	C3B-C2B	-2.96	1.36	1.40
24	B	608	CLA	C1D-C2D	2.96	1.49	1.42
31	A	617	SQD	O48-C23	2.96	1.42	1.33
24	B	616	CLA	C3B-CAB	-2.95	1.41	1.47
26	b	619	BCR	C30-C25	-2.93	1.49	1.53
32	h	101	DGD	C4E-C5E	2.93	1.59	1.53
24	b	614	CLA	CMB-C2B	-2.92	1.45	1.51
24	C	503	CLA	C1D-C2D	2.92	1.49	1.42
26	d	405	BCR	C1-C6	-2.92	1.49	1.53
32	c	516	DGD	O2E-C2E	-2.91	1.36	1.43
26	t	101	BCR	C30-C25	-2.91	1.49	1.53
24	b	603	CLA	C1D-C2D	2.91	1.49	1.42
28	a	611	PL9	C52-C5	-2.91	1.44	1.50
32	h	101	DGD	C4D-C3D	2.90	1.59	1.52
29	c	521	LMG	C3-C2	2.90	1.59	1.52
25	A	606	PHO	C4C-NC	2.90	1.43	1.36
24	C	512	CLA	MG-NA	2.89	2.13	2.06
32	C	516	DGD	C4D-C3D	2.89	1.59	1.52
26	b	619	BCR	C1-C6	-2.89	1.49	1.53
28	a	611	PL9	C53-C6	-2.89	1.44	1.50
32	c	516	DGD	O2G-C2G	-2.88	1.39	1.46
24	B	603	CLA	C3B-C2B	-2.87	1.36	1.40
32	C	518	DGD	O5D-C1E	2.87	1.45	1.40
24	b	614	CLA	MG-NA	2.87	2.13	2.06
24	B	610	CLA	C1D-C2D	2.87	1.49	1.42
24	c	502	CLA	CMD-C2D	-2.85	1.44	1.51
31	D	407	SQD	O2-C2	-2.84	1.36	1.43
28	d	406	PL9	C21-C19	-2.84	1.45	1.51
31	A	616	SQD	O2-C2	-2.84	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C1B-NB	-2.83	1.32	1.35
24	b	613	CLA	CMB-C2B	-2.83	1.45	1.51
26	A	609	BCR	C1-C6	-2.83	1.49	1.53
24	c	503	CLA	C1D-C2D	2.82	1.49	1.42
26	B	619	BCR	C30-C25	-2.82	1.49	1.53
25	d	402	PHO	C1A-NA	2.82	1.43	1.37
26	B	617	BCR	C33-C5	-2.82	1.46	1.50
24	C	502	CLA	CMB-C2B	-2.81	1.45	1.51
24	d	401	CLA	CMB-C2B	-2.81	1.45	1.51
24	b	607	CLA	MG-NA	2.80	2.12	2.06
31	a	613	SQD	O47-C7	2.80	1.42	1.34
24	c	511	CLA	C1D-C2D	2.80	1.48	1.42
26	b	617	BCR	C1-C6	-2.79	1.49	1.53
24	a	606	CLA	CMC-C2C	-2.79	1.44	1.51
26	k	102	BCR	C1-C6	-2.79	1.49	1.53
30	d	409	LHG	P-O6	2.79	1.70	1.59
31	A	617	SQD	O47-C45	-2.79	1.42	1.47
24	b	610	CLA	CMB-C2B	-2.79	1.45	1.51
28	A	612	PL9	C3-C4	-2.79	1.45	1.49
31	f	101	SQD	O2-C2	-2.78	1.36	1.43
24	b	616	CLA	C3B-CAB	-2.78	1.42	1.47
24	b	616	CLA	C3B-C2B	-2.78	1.36	1.40
24	b	603	CLA	CMC-C2C	-2.78	1.45	1.51
32	c	517	DGD	O3E-C3E	-2.78	1.36	1.43
24	b	607	CLA	CMD-C2D	-2.77	1.45	1.51
24	a	606	CLA	CMD-C2D	-2.76	1.45	1.51
29	b	621	LMG	C4-C3	2.76	1.59	1.52
35	e	101	HEM	C3B-CAB	2.76	1.53	1.47
32	c	518	DGD	O2G-C2G	-2.76	1.39	1.46
26	b	617	BCR	C33-C5	-2.76	1.46	1.50
24	C	511	CLA	CMB-C2B	-2.76	1.45	1.51
31	B	623	SQD	O2-C2	-2.75	1.36	1.43
24	b	615	CLA	CMD-C2D	-2.75	1.45	1.51
24	C	512	CLA	CMD-C2D	-2.75	1.45	1.51
29	M	101	LMG	C4-C5	2.75	1.58	1.53
24	c	506	CLA	C3B-CAB	-2.75	1.42	1.47
24	d	404	CLA	CMD-C2D	-2.75	1.45	1.51
24	B	610	CLA	C1B-NB	2.75	1.37	1.35
29	D	406	LMG	C4-C5	2.74	1.58	1.53
24	B	615	CLA	C3B-C2B	-2.74	1.36	1.40
25	a	605	PHO	CHD-C4C	-2.72	1.34	1.40
24	B	605	CLA	C1D-C2D	2.70	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	CMB-C2B	-2.70	1.46	1.51
24	B	616	CLA	CMC-C2C	-2.70	1.45	1.51
24	b	608	CLA	MG-NA	2.70	2.12	2.06
26	D	404	BCR	C1-C6	-2.70	1.50	1.53
26	T	101	BCR	C1-C6	-2.70	1.50	1.53
26	B	617	BCR	C30-C25	-2.69	1.50	1.53
24	B	603	CLA	CMC-C2C	-2.69	1.45	1.51
24	B	608	CLA	MG-NA	2.69	2.12	2.06
32	C	516	DGD	O2G-C1B	2.69	1.41	1.34
25	a	605	PHO	O2D-CGD	2.69	1.39	1.33
24	B	613	CLA	C3B-CAB	-2.69	1.42	1.47
24	b	616	CLA	CMB-C2B	-2.68	1.46	1.51
24	d	403	CLA	CMB-C2B	-2.68	1.46	1.51
25	d	402	PHO	CMC-C2C	-2.68	1.45	1.50
24	B	607	CLA	CAC-C3C	-2.68	1.45	1.52
24	d	403	CLA	MG-NA	2.68	2.12	2.06
32	H	102	DGD	C1E-C2E	2.67	1.60	1.52
24	A	605	CLA	CMD-C2D	-2.67	1.45	1.51
32	c	517	DGD	C4D-C3D	2.67	1.59	1.52
30	l	101	LHG	O7-C5	-2.66	1.39	1.46
32	c	516	DGD	C4D-C5D	2.66	1.58	1.53
24	d	404	CLA	CMC-C2C	-2.66	1.45	1.51
29	c	522	LMG	C4-C5	2.66	1.58	1.53
30	D	408	LHG	P-O3	2.66	1.70	1.59
28	D	405	PL9	C30-C29	-2.66	1.43	1.50
24	C	501	CLA	CMC-C2C	-2.65	1.45	1.51
32	C	517	DGD	C1E-C2E	2.65	1.60	1.52
25	d	402	PHO	CHC-C1C	2.65	1.43	1.38
24	D	402	CLA	CMD-C2D	-2.65	1.45	1.51
32	h	101	DGD	O2E-C2E	-2.65	1.36	1.43
31	A	616	SQD	O3-C3	-2.65	1.36	1.43
25	d	402	PHO	CAA-C2A	-2.65	1.49	1.54
24	A	613	CLA	CMB-C2B	-2.64	1.46	1.51
24	C	512	CLA	CMB-C2B	-2.64	1.46	1.51
24	b	610	CLA	CMD-C2D	-2.64	1.45	1.51
24	b	608	CLA	C3B-CAB	-2.64	1.42	1.47
24	B	611	CLA	C3B-C2B	-2.64	1.36	1.40
24	b	616	CLA	CMC-C2C	-2.63	1.45	1.51
24	B	608	CLA	CMD-C2D	-2.63	1.45	1.51
24	c	513	CLA	CMB-C2B	-2.63	1.46	1.51
24	B	610	CLA	CMB-C2B	-2.63	1.46	1.51
30	A	615	LHG	O7-C7	2.62	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	CAC-C3C	-2.62	1.45	1.52
30	e	102	LHG	P-O6	2.62	1.69	1.59
29	c	519	LMG	C4-C3	2.62	1.59	1.52
26	a	607	BCR	C27-C26	-2.62	1.45	1.51
24	b	612	CLA	CMC-C2C	-2.61	1.45	1.51
24	c	503	CLA	CMB-C2B	-2.61	1.46	1.51
24	b	616	CLA	CAC-C3C	-2.61	1.45	1.52
32	A	618	DGD	C3G-C2G	2.60	1.58	1.50
24	b	604	CLA	C1D-C2D	2.60	1.48	1.42
24	c	506	CLA	C1B-NB	-2.60	1.32	1.35
24	B	613	CLA	CMC-C2C	-2.60	1.45	1.51
24	b	610	CLA	C4B-CHC	-2.60	1.33	1.41
31	A	616	SQD	O47-C7	2.60	1.41	1.34
24	C	510	CLA	CMB-C2B	-2.60	1.46	1.51
32	C	516	DGD	O5D-C6D	-2.60	1.39	1.43
29	c	521	LMG	C4-C3	2.59	1.58	1.52
24	C	502	CLA	C1C-C2C	2.59	1.48	1.42
24	c	510	CLA	CMC-C2C	-2.59	1.45	1.51
24	c	513	CLA	C1D-C2D	2.59	1.48	1.42
24	C	507	CLA	CMB-C2B	-2.59	1.46	1.51
24	a	612	CLA	C1C-C2C	2.58	1.48	1.42
26	a	607	BCR	C1-C6	-2.58	1.50	1.53
24	d	404	CLA	CAC-C3C	-2.58	1.45	1.52
28	D	405	PL9	C7-C8	-2.58	1.46	1.50
29	b	623	LMG	C7-C8	2.58	1.58	1.50
31	a	613	SQD	O4-C4	-2.57	1.36	1.43
24	B	615	CLA	C4B-CHC	-2.57	1.33	1.41
29	A	614	LMG	C4-C3	2.57	1.58	1.52
35	e	101	HEM	C3C-CAC	2.57	1.53	1.47
28	A	612	PL9	C7-C3	-2.57	1.48	1.51
24	D	403	CLA	C1D-C2D	2.57	1.48	1.42
31	b	620	SQD	O2-C2	-2.57	1.36	1.43
28	d	406	PL9	C7-C3	-2.56	1.48	1.51
24	c	511	CLA	CMB-C2B	-2.56	1.46	1.51
24	d	404	CLA	C3B-C2B	-2.55	1.36	1.40
24	d	403	CLA	CMD-C2D	-2.55	1.45	1.51
30	A	615	LHG	C8-C7	-2.55	1.43	1.50
32	c	517	DGD	O3G-C1D	-2.55	1.35	1.40
24	b	609	CLA	CMB-C2B	-2.55	1.46	1.51
24	a	612	CLA	C1D-C2D	2.54	1.48	1.42
28	D	405	PL9	C10-C9	-2.54	1.44	1.50
24	C	513	CLA	C1D-C2D	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	606	PHO	CMC-C2C	-2.54	1.45	1.50
24	b	602	CLA	MG-NA	-2.54	2.00	2.06
24	C	509	CLA	C1B-NB	2.53	1.37	1.35
24	c	503	CLA	C5-C3	-2.53	1.46	1.51
24	B	606	CLA	C4B-CHC	-2.53	1.33	1.41
24	C	503	CLA	CAC-C3C	-2.53	1.45	1.52
24	c	505	CLA	CMB-C2B	-2.53	1.46	1.51
24	C	510	CLA	O2A-CGA	2.53	1.40	1.33
24	A	604	CLA	C4C-NC	2.53	1.37	1.35
28	A	612	PL9	C6-C1	-2.52	1.44	1.48
32	c	516	DGD	C6D-C5D	2.52	1.59	1.51
24	B	603	CLA	C1D-C2D	2.51	1.48	1.42
26	A	609	BCR	C30-C25	-2.51	1.50	1.53
24	a	604	CLA	C1D-C2D	2.51	1.48	1.42
32	H	102	DGD	C6E-C5E	2.51	1.60	1.51
24	A	608	CLA	C1D-C2D	2.50	1.48	1.42
25	a	605	PHO	C4C-C3C	2.50	1.49	1.45
30	B	622	LHG	C24-C23	2.50	1.58	1.50
24	C	504	CLA	CMD-C2D	-2.50	1.45	1.51
32	A	618	DGD	C4D-C5D	2.50	1.58	1.53
26	K	101	BCR	C33-C5	-2.50	1.46	1.50
26	k	101	BCR	C1-C6	-2.49	1.50	1.53
31	f	101	SQD	O3-C3	-2.49	1.37	1.43
32	c	517	DGD	C4D-C5D	2.49	1.58	1.53
24	c	510	CLA	CAC-C3C	-2.49	1.46	1.52
29	D	406	LMG	C7-C8	2.49	1.58	1.50
24	b	614	CLA	CMC-C2C	-2.49	1.45	1.51
29	C	519	LMG	C4-C5	2.48	1.58	1.53
24	B	609	CLA	O2D-CGD	2.48	1.39	1.33
35	e	101	HEM	C4A-CHB	-2.48	1.34	1.41
29	b	621	LMG	O7-C8	-2.48	1.40	1.46
29	M	101	LMG	O7-C8	-2.48	1.40	1.46
24	B	611	CLA	CMC-C2C	-2.48	1.45	1.51
24	b	603	CLA	C3B-CAB	-2.47	1.42	1.47
26	t	101	BCR	C33-C5	-2.47	1.46	1.50
24	b	611	CLA	CMC-C2C	-2.47	1.45	1.51
25	A	607	PHO	CMB-C2B	-2.47	1.45	1.50
24	B	601	CLA	C3B-CAB	-2.47	1.42	1.47
26	K	101	BCR	C1-C6	-2.47	1.50	1.53
24	c	508	CLA	C1D-C2D	2.47	1.48	1.42
24	c	503	CLA	C3B-C2B	-2.46	1.37	1.40
28	a	611	PL9	C6-C1	-2.46	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	CMC-C2C	-2.46	1.45	1.51
28	D	405	PL9	C5-C4	-2.46	1.38	1.47
32	c	517	DGD	C6E-C5E	2.46	1.60	1.51
24	B	606	CLA	CMB-C2B	-2.45	1.46	1.51
24	b	607	CLA	C1D-C2D	2.45	1.48	1.42
24	C	506	CLA	CMB-C2B	-2.45	1.46	1.51
24	b	608	CLA	C3B-C2B	-2.45	1.37	1.40
24	D	402	CLA	CAA-C2A	-2.44	1.49	1.54
24	C	510	CLA	C1D-C2D	2.44	1.48	1.42
30	E	101	LHG	O7-C5	-2.44	1.40	1.46
24	C	504	CLA	C1D-C2D	2.43	1.48	1.42
25	A	607	PHO	CHC-C1C	2.43	1.43	1.38
30	D	408	LHG	C8-C7	-2.43	1.43	1.50
24	C	509	CLA	CMB-C2B	-2.43	1.46	1.51
24	c	508	CLA	CMD-C2D	-2.43	1.45	1.51
32	c	516	DGD	O3D-C3D	-2.42	1.37	1.43
24	a	606	CLA	C4B-CHC	-2.42	1.34	1.41
25	d	402	PHO	C1C-NC	-2.42	1.33	1.38
26	k	101	BCR	C33-C5	-2.42	1.47	1.50
25	A	606	PHO	CHC-C4B	-2.42	1.34	1.40
24	C	506	CLA	C3B-CAB	-2.42	1.43	1.47
24	b	613	CLA	C3B-C2B	-2.41	1.37	1.40
24	C	501	CLA	C1D-C2D	2.41	1.48	1.42
24	B	609	CLA	CMD-C2D	-2.41	1.45	1.51
32	c	518	DGD	O3D-C3D	-2.41	1.37	1.43
32	A	618	DGD	O3D-C3D	-2.41	1.37	1.43
24	b	603	CLA	C1B-NB	2.41	1.37	1.35
24	B	616	CLA	CMD-C2D	-2.40	1.45	1.51
24	C	506	CLA	C1D-C2D	2.40	1.48	1.42
24	b	606	CLA	CAC-C3C	-2.40	1.46	1.52
24	C	506	CLA	C3B-C2B	-2.40	1.37	1.40
29	M	101	LMG	C29-C28	-2.40	1.43	1.50
25	a	605	PHO	C1C-NC	-2.40	1.33	1.38
24	C	510	CLA	CMC-C2C	-2.39	1.45	1.51
24	c	506	CLA	CMB-C2B	-2.39	1.46	1.51
26	c	515	BCR	C33-C5	-2.39	1.47	1.50
24	d	401	CLA	C1D-C2D	2.39	1.48	1.42
24	B	609	CLA	C3B-CAB	-2.39	1.43	1.47
24	d	403	CLA	C4B-CHC	-2.39	1.34	1.41
24	b	606	CLA	CMB-C2B	-2.38	1.46	1.51
29	M	101	LMG	O1-C7	-2.38	1.39	1.43
24	C	508	CLA	C1C-C2C	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C4B-CHC	-2.38	1.34	1.41
29	c	519	LMG	O2-C2	-2.38	1.37	1.43
32	C	518	DGD	O3G-C1D	-2.38	1.36	1.40
24	c	506	CLA	C1D-C2D	2.38	1.47	1.42
32	c	518	DGD	O1G-C1G	-2.38	1.39	1.45
29	A	614	LMG	C4-C5	2.38	1.58	1.53
24	D	403	CLA	C4B-CHC	-2.37	1.34	1.41
24	b	611	CLA	C1D-C2D	2.37	1.47	1.42
24	c	512	CLA	CMB-C2B	-2.37	1.46	1.51
24	b	605	CLA	MG-NA	2.37	2.11	2.06
29	c	519	LMG	O1-C1	2.37	1.44	1.40
26	a	607	BCR	C30-C25	-2.37	1.50	1.53
24	B	609	CLA	C1D-C2D	2.37	1.47	1.42
28	d	406	PL9	C45-C44	-2.36	1.44	1.50
24	C	513	CLA	CMB-C2B	-2.36	1.46	1.51
24	C	509	CLA	CMD-C2D	-2.36	1.45	1.51
24	A	613	CLA	CMD-C2D	-2.36	1.45	1.51
29	b	623	LMG	C3-C2	2.36	1.58	1.52
29	b	621	LMG	C1-C2	2.36	1.59	1.52
24	c	504	CLA	CMD-C2D	-2.36	1.46	1.51
32	C	517	DGD	C6D-C5D	2.36	1.58	1.51
24	B	611	CLA	CMB-C2B	-2.35	1.46	1.51
24	A	613	CLA	C1D-C2D	2.35	1.47	1.42
24	b	604	CLA	C3B-CAB	-2.35	1.43	1.47
24	c	506	CLA	CMC-C2C	-2.34	1.46	1.51
24	c	507	CLA	CMB-C2B	-2.34	1.46	1.51
31	A	616	SQD	O47-C45	-2.34	1.40	1.46
25	d	402	PHO	CHD-C4C	-2.34	1.35	1.40
32	H	102	DGD	O2G-C2G	-2.33	1.40	1.46
30	d	408	LHG	O7-C5	-2.33	1.40	1.46
24	c	512	CLA	CMD-C2D	-2.33	1.46	1.51
24	B	607	CLA	C1D-C2D	2.32	1.47	1.42
24	C	512	CLA	CMC-C2C	-2.32	1.46	1.51
32	c	516	DGD	O3E-C3E	-2.32	1.37	1.43
24	A	604	CLA	CMD-C2D	-2.32	1.46	1.51
24	d	404	CLA	C4B-CHC	-2.31	1.34	1.41
24	b	616	CLA	CMD-C2D	-2.31	1.46	1.51
24	c	501	CLA	CAC-C3C	-2.30	1.46	1.52
24	a	606	CLA	C1D-C2D	2.30	1.47	1.42
26	a	607	BCR	C33-C5	-2.30	1.47	1.50
24	C	507	CLA	C1D-C2D	2.30	1.47	1.42
32	C	518	DGD	C6D-C5D	2.30	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C1B-NB	2.30	1.37	1.35
24	C	513	CLA	C3B-CAB	-2.30	1.43	1.47
24	C	502	CLA	C1D-C2D	2.30	1.47	1.42
24	c	506	CLA	CMD-C2D	-2.30	1.46	1.51
24	A	613	CLA	C3B-C2B	-2.30	1.37	1.40
24	a	604	CLA	CMB-C2B	-2.30	1.46	1.51
24	d	403	CLA	C1D-C2D	2.30	1.47	1.42
24	b	613	CLA	CMC-C2C	-2.30	1.46	1.51
24	B	603	CLA	C3B-CAB	-2.29	1.43	1.47
24	A	613	CLA	CAC-C3C	-2.29	1.46	1.52
32	H	102	DGD	C4D-C5D	2.29	1.57	1.53
32	C	516	DGD	C3G-C2G	2.29	1.57	1.50
24	b	604	CLA	CMB-C2B	-2.29	1.46	1.51
24	b	609	CLA	CAC-C3C	-2.29	1.46	1.52
24	b	616	CLA	MG-NA	2.29	2.11	2.06
25	d	402	PHO	CMD-C2D	-2.29	1.46	1.50
24	b	602	CLA	C1D-C2D	2.28	1.47	1.42
24	c	504	CLA	CMB-C2B	-2.28	1.46	1.51
32	c	518	DGD	O5D-C6D	-2.28	1.39	1.43
24	b	611	CLA	O2D-CGD	2.28	1.38	1.33
24	c	508	CLA	C3B-C2B	-2.28	1.37	1.40
24	B	612	CLA	C1D-C2D	2.28	1.47	1.42
24	B	614	CLA	C3B-CAB	-2.28	1.43	1.47
31	A	616	SQD	O4-C4	-2.28	1.37	1.43
24	b	601	CLA	O2A-CGA	2.28	1.40	1.33
24	B	611	CLA	C4C-NC	2.27	1.37	1.35
29	a	618	LMG	C7-C8	2.27	1.57	1.50
24	D	402	CLA	C1D-C2D	2.27	1.47	1.42
24	c	505	CLA	CMC-C2C	-2.27	1.46	1.51
28	a	611	PL9	C46-C44	-2.27	1.46	1.51
31	D	407	SQD	O3-C3	-2.27	1.37	1.43
32	c	516	DGD	O3G-C3G	-2.27	1.39	1.43
24	B	608	CLA	C3B-C2B	-2.27	1.37	1.40
24	b	602	CLA	CMD-C2D	-2.27	1.46	1.51
24	d	404	CLA	C3B-CAB	-2.26	1.43	1.47
24	d	401	CLA	CAC-C3C	-2.26	1.46	1.52
24	B	601	CLA	C1D-C2D	2.26	1.47	1.42
24	B	604	CLA	CMC-C2C	-2.26	1.46	1.51
24	A	608	CLA	CAC-C3C	-2.25	1.46	1.52
24	d	401	CLA	C4B-CHC	-2.25	1.34	1.41
24	C	508	CLA	CMC-C2C	-2.25	1.46	1.51
24	B	608	CLA	CAC-C3C	-2.25	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	CLA	C4B-CHC	-2.25	1.34	1.41
29	d	410	LMG	O1-C1	2.25	1.44	1.40
24	C	507	CLA	CMD-C2D	-2.25	1.46	1.51
24	C	511	CLA	CMC-C2C	-2.25	1.46	1.51
24	B	604	CLA	C3B-C2B	-2.24	1.37	1.40
24	b	610	CLA	C3B-CAB	-2.24	1.43	1.47
24	C	504	CLA	CMB-C2B	-2.24	1.47	1.51
24	c	510	CLA	C4B-CHC	-2.24	1.34	1.41
26	A	609	BCR	C38-C26	-2.24	1.47	1.50
24	A	608	CLA	CMD-C2D	-2.24	1.46	1.51
24	D	402	CLA	C1C-C2C	2.23	1.47	1.42
24	c	503	CLA	C3B-CAB	-2.23	1.43	1.47
24	B	616	CLA	C1D-C2D	2.23	1.47	1.42
32	c	517	DGD	O3D-C3D	-2.23	1.37	1.43
24	b	616	CLA	C1D-C2D	2.23	1.47	1.42
24	c	504	CLA	CAC-C3C	-2.23	1.46	1.52
24	B	610	CLA	MG-NA	2.23	2.11	2.06
24	B	602	CLA	C1C-C2C	2.22	1.47	1.42
24	c	504	CLA	CMC-C2C	-2.22	1.46	1.51
24	c	506	CLA	O2D-CGD	2.22	1.38	1.33
30	D	408	LHG	O8-C6	-2.22	1.40	1.45
29	a	618	LMG	C1-C2	2.22	1.58	1.52
24	c	513	CLA	CMC-C2C	-2.22	1.46	1.51
25	A	606	PHO	C1C-NC	-2.22	1.33	1.38
24	C	510	CLA	CMD-C2D	-2.22	1.46	1.51
24	b	612	CLA	C1C-C2C	2.22	1.47	1.42
24	D	403	CLA	CMD-C2D	-2.21	1.46	1.51
24	B	602	CLA	C1D-C2D	2.21	1.47	1.42
29	D	406	LMG	O7-C10	2.21	1.40	1.34
25	A	606	PHO	CHB-C1B	-2.21	1.34	1.38
29	c	519	LMG	C7-C8	2.21	1.57	1.50
32	h	101	DGD	O4D-C4D	-2.21	1.37	1.43
29	c	521	LMG	C7-C8	2.21	1.57	1.50
28	A	612	PL9	C37-C38	2.21	1.57	1.50
24	C	503	CLA	CMD-C2D	-2.21	1.46	1.51
35	F	101	HEM	C3C-CAC	2.21	1.52	1.47
32	h	101	DGD	C1E-C2E	2.20	1.58	1.52
24	c	502	CLA	CMB-C2B	-2.20	1.47	1.51
29	b	623	LMG	O6-C1	2.20	1.47	1.41
31	a	613	SQD	O3-C3	-2.20	1.37	1.43
30	B	622	LHG	P-O4	-2.20	1.45	1.55
24	C	513	CLA	C4B-CHC	-2.19	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C3B-C2B	-2.19	1.37	1.40
24	b	607	CLA	CMB-C2B	-2.19	1.47	1.51
25	a	605	PHO	CAA-C2A	-2.19	1.50	1.54
32	H	102	DGD	C4E-C3E	2.19	1.57	1.52
24	b	604	CLA	C3B-C2B	-2.19	1.37	1.40
32	H	102	DGD	C6D-C5D	2.19	1.58	1.51
24	b	609	CLA	C3B-CAB	-2.19	1.43	1.47
24	C	505	CLA	CMC-C2C	-2.19	1.46	1.51
24	d	401	CLA	CMD-C2D	-2.19	1.46	1.51
26	C	515	BCR	C33-C5	-2.19	1.47	1.50
26	t	101	BCR	C27-C26	-2.19	1.46	1.51
26	B	619	BCR	C31-C1	-2.18	1.49	1.53
30	d	407	LHG	O7-C5	-2.18	1.41	1.46
24	B	611	CLA	C1D-C2D	2.18	1.47	1.42
24	b	611	CLA	CAC-C3C	-2.18	1.46	1.52
26	x	101	BCR	C1-C6	-2.18	1.50	1.53
24	b	602	CLA	CMB-C2B	-2.17	1.47	1.51
24	B	614	CLA	CMB-C2B	-2.17	1.47	1.51
24	C	512	CLA	C1D-C2D	2.17	1.47	1.42
32	C	517	DGD	O1G-C1G	-2.17	1.40	1.45
24	c	511	CLA	C3B-CAB	-2.17	1.43	1.47
24	d	403	CLA	C1C-C2C	2.17	1.47	1.42
24	c	503	CLA	CMC-C2C	-2.17	1.46	1.51
24	A	604	CLA	C4B-CHC	-2.17	1.35	1.41
24	b	611	CLA	CMD-C2D	-2.16	1.46	1.51
32	c	516	DGD	O4D-C4D	-2.16	1.37	1.43
24	B	601	CLA	CMC-C2C	-2.16	1.46	1.51
24	b	616	CLA	C4B-CHC	-2.16	1.35	1.41
24	a	606	CLA	CMA-C3A	-2.15	1.48	1.53
24	B	616	CLA	CAC-C3C	-2.15	1.46	1.52
24	b	610	CLA	C1D-C2D	2.15	1.47	1.42
24	B	614	CLA	MG-NA	2.14	2.11	2.06
29	a	618	LMG	C3-C2	2.14	1.57	1.52
24	c	513	CLA	CMD-C2D	-2.14	1.46	1.51
29	C	519	LMG	C4-C3	2.14	1.57	1.52
29	c	521	LMG	O7-C8	-2.14	1.41	1.46
24	b	614	CLA	C1D-C2D	2.14	1.47	1.42
26	B	618	BCR	C27-C26	-2.14	1.46	1.51
32	c	518	DGD	O3E-C3E	-2.13	1.38	1.43
32	H	102	DGD	O6E-C1E	2.13	1.47	1.41
24	B	614	CLA	C1C-C2C	2.13	1.47	1.42
24	b	605	CLA	CAC-C3C	-2.13	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	519	LMG	C3-C2	2.13	1.57	1.52
25	a	605	PHO	CHC-C1C	2.12	1.42	1.38
24	B	607	CLA	CMD-C2D	-2.12	1.46	1.51
24	C	501	CLA	C3B-CAB	-2.12	1.43	1.47
32	H	102	DGD	O1G-C1G	-2.12	1.40	1.45
32	A	618	DGD	O6E-C5E	-2.12	1.39	1.44
28	D	405	PL9	C52-C5	-2.12	1.46	1.50
24	C	507	CLA	CAC-C3C	-2.12	1.47	1.52
24	c	502	CLA	CMC-C2C	-2.11	1.46	1.51
24	B	606	CLA	C1B-NB	2.11	1.37	1.35
24	C	502	CLA	CMC-C2C	-2.11	1.46	1.51
30	e	102	LHG	O8-C23	2.11	1.39	1.33
24	c	504	CLA	C1D-C2D	2.11	1.47	1.42
26	d	405	BCR	C33-C5	-2.11	1.47	1.50
26	t	101	BCR	C31-C1	-2.10	1.49	1.53
26	b	618	BCR	C27-C26	-2.10	1.46	1.51
24	C	506	CLA	CAC-C3C	-2.10	1.47	1.52
24	B	602	CLA	CAC-C3C	-2.10	1.47	1.52
29	c	521	LMG	O2-C2	2.10	1.47	1.43
24	C	510	CLA	C1C-C2C	2.10	1.47	1.42
24	d	401	CLA	CMC-C2C	-2.09	1.46	1.51
25	A	606	PHO	CHC-C1C	2.09	1.42	1.38
24	B	614	CLA	CAA-C2A	-2.09	1.50	1.54
24	c	506	CLA	C3B-C2B	-2.08	1.37	1.40
26	A	609	BCR	C37-C22	-2.08	1.46	1.50
24	B	616	CLA	CMB-C2B	-2.08	1.47	1.51
24	c	511	CLA	CAC-C3C	-2.08	1.47	1.52
30	d	407	LHG	P-O6	2.08	1.67	1.59
24	C	512	CLA	C4B-CHC	-2.08	1.35	1.41
26	b	618	BCR	C33-C5	-2.08	1.47	1.50
29	d	410	LMG	O2-C2	-2.08	1.38	1.43
24	B	611	CLA	CAC-C3C	-2.07	1.47	1.52
24	c	502	CLA	C1D-C2D	2.07	1.47	1.42
24	b	608	CLA	CMD-C2D	-2.07	1.46	1.51
24	b	605	CLA	CMB-C2B	-2.07	1.47	1.51
32	C	516	DGD	O1G-C1A	2.07	1.39	1.33
24	b	615	CLA	CMC-C2C	-2.07	1.46	1.51
30	d	408	LHG	C4-C5	2.06	1.57	1.50
24	b	606	CLA	C3B-C2B	-2.06	1.37	1.40
24	b	616	CLA	O2D-CED	-2.06	1.40	1.45
24	c	507	CLA	C3B-CAB	-2.05	1.43	1.47
24	C	508	CLA	CMB-C2B	-2.05	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	606	CLA	CMB-C2B	-2.05	1.47	1.51
24	c	501	CLA	C4B-CHC	-2.05	1.35	1.41
24	B	613	CLA	C1D-C2D	2.05	1.47	1.42
32	C	518	DGD	C1D-C2D	2.05	1.58	1.52
29	A	614	LMG	O7-C8	-2.05	1.41	1.46
24	C	501	CLA	C3B-C2B	-2.05	1.37	1.40
25	A	607	PHO	C4B-NB	2.05	1.41	1.36
24	b	613	CLA	C1D-C2D	2.05	1.47	1.42
28	a	611	PL9	C30-C29	-2.04	1.45	1.50
24	C	509	CLA	C1D-C2D	2.04	1.47	1.42
24	B	610	CLA	C1A-CHA	-2.04	1.34	1.43
24	B	614	CLA	CMC-C2C	-2.04	1.46	1.51
24	C	511	CLA	C1D-C2D	2.04	1.47	1.42
32	c	517	DGD	C4E-C5E	2.04	1.57	1.53
36	V	201	HEC	CMB-C2B	2.04	1.56	1.51
26	B	618	BCR	C1-C6	-2.04	1.51	1.53
25	a	605	PHO	C3B-C4B	2.03	1.47	1.43
24	B	610	CLA	CMC-C2C	-2.03	1.46	1.51
25	d	402	PHO	C4C-C3C	2.03	1.48	1.45
24	c	501	CLA	CMD-C2D	-2.03	1.46	1.51
24	c	510	CLA	C1D-C2D	2.03	1.47	1.42
24	C	501	CLA	CMB-C2B	-2.03	1.47	1.51
25	a	605	PHO	CHC-C4B	-2.02	1.35	1.40
24	C	509	CLA	CMC-C2C	-2.02	1.46	1.51
26	c	514	BCR	C33-C5	-2.02	1.47	1.50
29	C	519	LMG	O7-C8	-2.02	1.41	1.46
29	D	406	LMG	C4-C3	2.02	1.57	1.52
24	b	602	CLA	C4B-CHC	-2.02	1.35	1.41
24	c	508	CLA	C4B-CHC	-2.02	1.35	1.41
24	c	513	CLA	CAC-C3C	-2.02	1.47	1.52
29	D	409	LMG	O8-C28	2.02	1.39	1.33
24	C	506	CLA	CMD-C2D	-2.02	1.46	1.51
24	B	605	CLA	CMC-C2C	-2.01	1.46	1.51
31	b	620	SQD	O3-C3	-2.01	1.38	1.43
24	B	605	CLA	CMD-C2D	-2.01	1.46	1.51
26	B	619	BCR	C27-C26	-2.01	1.47	1.51
24	b	601	CLA	CAC-C3C	-2.01	1.47	1.52
24	b	605	CLA	C1A-CHA	-2.00	1.34	1.43
24	c	511	CLA	C1C-C2C	2.00	1.47	1.42

All (1270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4A-NA-C1A	10.06	111.23	106.71
24	b	615	CLA	C4A-NA-C1A	9.37	110.92	106.71
24	B	611	CLA	C4A-NA-C1A	9.23	110.86	106.71
31	a	613	SQD	O6-C1-C2	8.97	122.30	108.30
31	A	616	SQD	O7-S-C6	8.91	117.53	106.94
24	B	603	CLA	C4A-NA-C1A	8.60	110.57	106.71
24	b	606	CLA	C4A-NA-C1A	8.47	110.52	106.71
24	B	616	CLA	C4A-NA-C1A	8.46	110.51	106.71
24	B	604	CLA	C4A-NA-C1A	8.36	110.46	106.71
31	D	407	SQD	O6-C1-C2	8.12	120.98	108.30
24	C	507	CLA	C4A-NA-C1A	8.08	110.34	106.71
24	b	601	CLA	C4A-NA-C1A	8.03	110.32	106.71
24	d	403	CLA	C4A-NA-C1A	7.99	110.30	106.71
31	B	623	SQD	O6-C1-C2	7.88	120.61	108.30
24	B	612	CLA	C4A-NA-C1A	7.88	110.25	106.71
24	b	609	CLA	C4A-NA-C1A	7.85	110.23	106.71
24	A	613	CLA	C4A-NA-C1A	7.81	110.22	106.71
24	c	510	CLA	C4A-NA-C1A	7.66	110.15	106.71
24	C	501	CLA	C4A-NA-C1A	7.56	110.11	106.71
24	C	511	CLA	C4A-NA-C1A	7.42	110.04	106.71
24	A	605	CLA	C4A-NA-C1A	7.40	110.03	106.71
24	c	509	CLA	C4A-NA-C1A	7.34	110.00	106.71
24	c	511	CLA	C4A-NA-C1A	7.33	110.00	106.71
24	B	601	CLA	C4A-NA-C1A	7.19	109.94	106.71
24	C	509	CLA	C4A-NA-C1A	7.13	109.91	106.71
24	b	614	CLA	C4A-NA-C1A	7.10	109.90	106.71
24	b	616	CLA	C4A-NA-C1A	6.90	109.81	106.71
24	c	508	CLA	C4A-NA-C1A	6.88	109.80	106.71
31	b	620	SQD	O6-C1-C2	6.76	118.86	108.30
24	a	612	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	C	513	CLA	C4A-NA-C1A	6.71	109.72	106.71
31	f	101	SQD	O6-C1-C2	6.59	118.60	108.30
24	D	403	CLA	C4A-NA-C1A	6.46	109.61	106.71
24	C	502	CLA	C4A-NA-C1A	6.43	109.60	106.71
31	f	101	SQD	O7-S-C6	6.40	114.54	106.94
35	e	101	HEM	CBD-CAD-C3D	-6.40	100.69	112.48
31	A	616	SQD	O6-C1-C2	6.37	118.26	108.30
24	B	606	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	c	502	CLA	C4A-NA-C1A	6.29	109.53	106.71
24	c	506	CLA	C4A-NA-C1A	6.21	109.50	106.71
24	B	609	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	b	602	CLA	C4A-NA-C1A	6.11	109.45	106.71
24	C	510	CLA	C4A-NA-C1A	6.09	109.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	612	CLA	CMB-C2B-C1B	-6.02	119.21	128.46
24	C	508	CLA	C4A-NA-C1A	6.02	109.41	106.71
24	C	505	CLA	C4A-NA-C1A	6.00	109.40	106.71
24	C	505	CLA	CMB-C2B-C1B	-6.00	119.24	128.46
31	A	617	SQD	C45-O47-C7	5.96	125.55	117.88
24	b	609	CLA	CMB-C2B-C1B	-5.96	119.31	128.46
24	C	509	CLA	CMB-C2B-C1B	-5.92	119.36	128.46
35	F	101	HEM	CBD-CAD-C3D	-5.90	101.61	112.48
24	B	607	CLA	C4A-NA-C1A	5.88	109.35	106.71
28	d	406	PL9	C7-C3-C4	5.79	121.58	116.88
28	a	611	PL9	C7-C3-C4	5.69	121.51	116.88
24	d	401	CLA	C4A-NA-C1A	5.67	109.25	106.71
24	a	604	CLA	C4A-NA-C1A	5.62	109.23	106.71
24	b	614	CLA	CMB-C2B-C1B	-5.61	119.83	128.46
24	B	615	CLA	C4A-NA-C1A	5.57	109.21	106.71
24	C	512	CLA	C4A-NA-C1A	5.57	109.21	106.71
24	B	616	CLA	CMB-C2B-C1B	-5.46	120.08	128.46
24	C	509	CLA	CMB-C2B-C3B	5.42	134.81	124.68
24	b	608	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
24	c	501	CLA	O2D-CGD-O1D	-5.27	113.53	123.84
24	c	512	CLA	C4A-NA-C1A	5.25	109.07	106.71
31	A	616	SQD	O9-S-O7	-5.24	95.80	113.95
24	b	606	CLA	O2D-CGD-O1D	-5.22	113.62	123.84
24	b	610	CLA	C4A-NA-C1A	5.20	109.05	106.71
24	B	610	CLA	O2D-CGD-O1D	-5.20	113.68	123.84
24	d	404	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
28	d	406	PL9	C40-C39-C41	5.14	123.92	115.27
24	b	602	CLA	CMB-C2B-C1B	-5.13	120.59	128.46
24	C	501	CLA	O2D-CGD-O1D	-5.12	113.82	123.84
24	B	602	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
24	B	605	CLA	C4A-NA-C1A	5.08	108.99	106.71
24	a	604	CLA	CMB-C2B-C1B	-5.07	120.66	128.46
31	a	614	SQD	O47-C7-C8	5.07	122.44	111.50
31	A	616	SQD	C1-C2-C3	-5.06	99.47	110.00
31	D	407	SQD	O8-S-C6	5.03	113.76	105.74
24	C	512	CLA	CMB-C2B-C1B	-5.02	120.74	128.46
24	b	603	CLA	CMB-C2B-C1B	-5.02	120.74	128.46
31	b	620	SQD	O7-S-C6	5.01	112.89	106.94
24	c	501	CLA	C4A-NA-C1A	5.00	108.95	106.71
24	B	616	CLA	CMB-C2B-C3B	4.99	134.01	124.68
24	C	510	CLA	O2D-CGD-O1D	-4.98	114.10	123.84
24	b	607	CLA	C4A-NA-C1A	4.98	108.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
24	b	604	CLA	C4A-NA-C1A	4.95	108.93	106.71
24	D	402	CLA	CMD-C2D-C3D	4.93	133.90	124.68
24	c	504	CLA	C4A-NA-C1A	4.92	108.92	106.71
24	B	611	CLA	O2D-CGD-O1D	-4.91	114.24	123.84
24	A	605	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
24	c	513	CLA	CMB-C2B-C1B	-4.87	120.97	128.46
24	c	505	CLA	C4A-NA-C1A	4.87	108.90	106.71
24	C	510	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
31	D	407	SQD	O9-S-C6	4.85	112.71	106.94
24	c	505	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
24	b	612	CLA	C4D-C3D-CAD	-4.83	105.78	108.47
29	a	618	LMG	C1-C2-C3	-4.82	99.95	110.00
24	b	613	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
24	D	402	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	b	608	CLA	CMB-C2B-C3B	4.79	133.64	124.68
24	C	508	CLA	C4D-C3D-CAD	-4.78	105.81	108.47
36	V	201	HEC	CMC-C2C-C1C	-4.77	121.13	128.46
24	c	507	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	c	503	CLA	C4D-C3D-CAD	-4.74	105.83	108.47
24	b	602	CLA	CMB-C2B-C3B	4.74	133.55	124.68
24	b	606	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
24	b	602	CLA	O2D-CGD-O1D	-4.71	114.62	123.84
24	d	404	CLA	CMB-C2B-C3B	4.65	133.39	124.68
24	b	612	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
24	c	510	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
24	b	609	CLA	CMB-C2B-C3B	4.62	133.31	124.68
24	D	403	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
24	C	501	CLA	O2D-CGD-CBD	4.59	119.42	111.27
24	C	505	CLA	CMB-C2B-C3B	4.58	133.25	124.68
24	b	605	CLA	O2D-CGD-O1D	-4.57	114.90	123.84
24	b	612	CLA	CMD-C2D-C3D	4.52	133.14	124.68
24	b	616	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
24	c	502	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
24	c	505	CLA	C4D-C3D-CAD	-4.48	105.97	108.47
24	b	615	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
24	b	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	C	508	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
24	b	605	CLA	CMB-C2B-C1B	-4.44	121.65	128.46
30	A	615	LHG	O4-P-O5	4.42	134.08	112.24
28	a	611	PL9	C35-C34-C36	4.40	122.67	115.27
24	c	513	CLA	C4A-NA-C1A	4.39	108.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
24	c	509	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
24	C	506	CLA	C4A-NA-C1A	4.38	108.67	106.71
24	C	513	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
24	A	604	CLA	CMB-C2B-C3B	4.37	132.85	124.68
24	c	509	CLA	CHB-C4A-NA	4.37	130.55	124.51
31	A	616	SQD	C1-O5-C5	-4.37	105.12	113.69
24	b	616	CLA	CMB-C2B-C3B	4.35	132.81	124.68
36	V	201	HEC	CBD-CAD-C3D	-4.33	104.49	112.49
30	E	101	LHG	O4-P-O5	4.33	133.62	112.24
24	C	512	CLA	CMB-C2B-C3B	4.32	132.75	124.68
31	B	623	SQD	O7-S-C6	4.29	112.04	106.94
24	C	508	CLA	OBD-CAD-CBD	-4.29	119.76	125.89
24	A	605	CLA	CMB-C2B-C3B	4.29	132.70	124.68
24	B	610	CLA	C4A-NA-C1A	4.27	108.62	106.71
24	a	612	CLA	CMB-C2B-C3B	4.26	132.66	124.68
24	B	610	CLA	C1B-CHB-C4A	-4.24	121.72	130.12
24	c	507	CLA	C4D-C3D-CAD	-4.24	106.11	108.47
24	a	606	CLA	C4A-NA-C1A	4.24	108.61	106.71
24	b	610	CLA	O2D-CGD-O1D	-4.23	115.57	123.84
24	c	505	CLA	CMD-C2D-C3D	4.22	132.57	124.68
24	B	612	CLA	CMB-C2B-C3B	4.21	132.56	124.68
24	C	510	CLA	CMB-C2B-C3B	4.20	132.54	124.68
24	b	607	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
24	c	513	CLA	CMB-C2B-C3B	4.18	132.51	124.68
24	C	513	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
24	a	604	CLA	CMB-C2B-C3B	4.17	132.49	124.68
24	b	614	CLA	CMB-C2B-C3B	4.15	132.45	124.68
31	f	101	SQD	O9-S-O7	-4.14	99.62	113.95
30	d	409	LHG	O4-P-O5	4.13	132.65	112.24
24	b	603	CLA	C4A-NA-C1A	4.12	108.56	106.71
24	c	501	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
24	B	608	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
24	C	513	CLA	CMB-C2B-C3B	4.11	132.37	124.68
24	C	510	CLA	O2D-CGD-CBD	4.11	118.57	111.27
24	A	604	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
24	B	613	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
29	b	621	LMG	O7-C10-O9	-4.08	113.83	123.70
30	e	102	LHG	O4-P-O5	4.08	132.43	112.24
30	B	622	LHG	O4-P-O5	4.08	132.41	112.24
24	B	608	CLA	CMB-C2B-C3B	4.07	132.30	124.68
32	H	102	DGD	O3G-C3G-C2G	-4.07	101.08	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	CMB-C2B-C3B	4.06	132.28	124.68
30	d	408	LHG	O4-P-O5	4.03	132.19	112.24
24	c	501	CLA	CMB-C2B-C3B	4.03	132.22	124.68
24	b	605	CLA	O1D-CGD-CBD	4.03	132.73	124.48
24	B	608	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
24	c	504	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
24	c	503	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
24	B	614	CLA	O2D-CGD-O1D	-4.01	116.01	123.84
24	C	505	CLA	C4D-C3D-CAD	-4.00	106.24	108.47
24	b	602	CLA	O2D-CGD-CBD	3.99	118.36	111.27
24	C	508	CLA	CMB-C2B-C3B	3.99	132.15	124.68
32	C	518	DGD	O6D-C1D-O3G	-3.99	100.54	109.97
28	A	612	PL9	C40-C39-C41	3.98	121.97	115.27
30	d	407	LHG	O4-P-O5	3.98	131.92	112.24
29	b	623	LMG	C1-O6-C5	-3.97	105.90	113.69
26	A	609	BCR	C37-C22-C21	-3.97	117.37	122.92
24	b	602	CLA	CHB-C4A-NA	3.96	129.99	124.51
24	b	603	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
30	D	408	LHG	O4-P-O5	3.96	131.80	112.24
24	c	502	CLA	CMB-C2B-C3B	3.95	132.06	124.68
31	B	623	SQD	O8-S-C6	3.94	112.01	105.74
24	B	607	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
32	C	518	DGD	O3G-C3G-C2G	-3.92	101.44	110.90
24	B	614	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
24	A	608	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
24	C	503	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
28	a	611	PL9	C25-C24-C26	3.91	121.84	115.27
24	c	507	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
24	B	602	CLA	O2D-CGD-CBD	3.90	118.19	111.27
24	b	603	CLA	CMB-C2B-C3B	3.89	131.95	124.68
24	b	611	CLA	C4A-NA-C1A	3.88	108.45	106.71
24	A	613	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
24	C	504	CLA	C4A-NA-C1A	3.87	108.44	106.71
24	b	612	CLA	CMB-C2B-C3B	3.87	131.91	124.68
24	B	612	CLA	C4D-C3D-CAD	-3.86	106.31	108.47
24	D	402	CLA	C4D-C3D-CAD	-3.86	106.32	108.47
31	A	616	SQD	O47-C7-C8	3.86	119.81	111.50
24	A	605	CLA	CED-O2D-CGD	-3.85	107.22	115.94
24	B	606	CLA	OBD-CAD-CBD	-3.85	120.39	125.89
26	b	617	BCR	C2-C1-C6	3.85	116.41	110.48
32	C	516	DGD	O3G-C3G-C2G	-3.84	101.62	110.90
26	C	515	BCR	C15-C16-C17	-3.83	115.63	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
24	a	612	CLA	CMD-C2D-C3D	3.82	131.83	124.68
24	b	609	CLA	C4D-C3D-CAD	-3.82	106.34	108.47
30	d	407	LHG	O8-C23-O10	-3.81	113.98	123.59
28	D	405	PL9	C36-C34-C33	-3.80	113.43	121.12
24	c	507	CLA	CMB-C2B-C3B	3.80	131.79	124.68
32	c	518	DGD	O3G-C3G-C2G	-3.77	101.79	110.90
24	B	615	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
24	b	605	CLA	C4-C3-C5	3.75	121.58	115.27
32	c	516	DGD	O3G-C3G-C2G	-3.75	101.85	110.90
24	b	606	CLA	CMB-C2B-C3B	3.74	131.67	124.68
26	B	619	BCR	C2-C1-C6	3.74	116.23	110.48
24	c	506	CLA	OBD-CAD-CBD	-3.73	120.56	125.89
28	a	611	PL9	C7-C3-C2	-3.73	118.40	123.30
30	l	101	LHG	O4-P-O5	3.73	130.66	112.24
24	C	506	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
24	B	611	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	B	606	CLA	OBD-CAD-C3D	3.71	134.14	127.98
28	D	405	PL9	C30-C29-C31	-3.71	109.03	115.27
24	c	506	CLA	OBD-CAD-C3D	3.68	134.09	127.98
25	d	402	PHO	C1-C2-C3	-3.68	119.69	126.04
31	b	620	SQD	O9-S-C6	3.66	111.29	106.94
24	c	506	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
24	d	401	CLA	CHB-C4A-NA	3.66	129.57	124.51
26	T	101	BCR	C35-C13-C14	-3.66	117.80	122.92
24	b	604	CLA	OBD-CAD-CBD	-3.65	120.68	125.89
24	d	403	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	b	606	CLA	CMD-C2D-C3D	3.64	131.49	124.68
24	B	601	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
24	c	513	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
31	a	613	SQD	O7-S-C6	3.64	111.26	106.94
24	c	508	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
24	B	602	CLA	CMB-C2B-C3B	3.63	131.47	124.68
28	A	612	PL9	C7-C3-C4	3.62	119.82	116.88
24	d	403	CLA	O2D-CGD-CBD	3.62	117.69	111.27
31	a	613	SQD	O9-S-C6	3.61	111.23	106.94
30	B	621	LHG	O4-P-O5	3.61	130.08	112.24
29	M	101	LMG	C1-O6-C5	-3.61	106.61	113.69
28	D	405	PL9	C7-C3-C4	3.60	119.81	116.88
24	C	503	CLA	CMB-C2B-C3B	3.60	131.41	124.68
24	b	607	CLA	CMB-C2B-C3B	3.60	131.41	124.68
24	b	606	CLA	C4D-C3D-CAD	-3.60	106.47	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	623	SQD	C1-O5-C5	-3.59	106.64	113.69
24	a	612	CLA	O2D-CGD-CBD	3.59	117.65	111.27
24	d	403	CLA	CMD-C2D-C3D	3.59	131.39	124.68
28	A	612	PL9	C20-C19-C21	3.59	121.31	115.27
31	B	623	SQD	O5-C5-C4	3.59	116.21	109.69
24	C	505	CLA	CMD-C2D-C3D	3.58	131.38	124.68
31	B	623	SQD	O47-C7-C8	3.57	119.19	111.50
24	b	612	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
24	C	508	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	b	601	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
24	c	508	CLA	CMB-C2B-C3B	3.56	131.33	124.68
31	f	101	SQD	C1-C2-C3	-3.55	102.61	110.00
24	B	609	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
24	b	613	CLA	CMB-C2B-C3B	3.54	131.30	124.68
24	d	403	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
24	b	609	CLA	OBD-CAD-CBD	-3.53	120.85	125.89
24	C	511	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
31	a	614	SQD	O48-C23-C24	3.52	122.94	111.91
25	A	607	PHO	O2D-CGD-O1D	-3.51	116.97	123.84
24	c	501	CLA	CED-O2D-CGD	-3.51	108.00	115.94
24	c	506	CLA	CMB-C2B-C3B	3.50	131.23	124.68
24	c	509	CLA	O2A-CGA-O1A	-3.50	114.76	123.59
28	D	405	PL9	C27-C28-C29	-3.50	119.24	127.66
24	A	608	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
24	a	606	CLA	CMB-C2B-C3B	3.49	131.22	124.68
24	B	603	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
24	b	603	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
24	c	510	CLA	CMB-C2B-C3B	3.48	131.19	124.68
24	c	512	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
24	b	602	CLA	C4D-C3D-CAD	-3.47	106.53	108.47
24	B	613	CLA	CMB-C2B-C3B	3.47	131.17	124.68
26	A	609	BCR	C27-C26-C25	3.47	127.77	122.73
24	a	606	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
36	v	201	HEC	CMC-C2C-C1C	-3.47	123.14	128.46
24	b	603	CLA	OBD-CAD-CBD	-3.46	120.95	125.89
24	C	506	CLA	CMB-C2B-C3B	3.46	131.15	124.68
24	c	505	CLA	CMB-C2B-C3B	3.45	131.14	124.68
24	b	611	CLA	CMB-C2B-C3B	3.45	131.14	124.68
24	b	613	CLA	CHB-C4A-NA	3.44	129.27	124.51
24	B	611	CLA	OBD-CAD-CBD	-3.44	120.98	125.89
24	B	602	CLA	C4A-NA-C1A	3.43	108.25	106.71
26	c	515	BCR	C27-C26-C25	3.43	127.70	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406	PL9	C7-C3-C2	-3.42	118.80	123.30
24	b	605	CLA	CMB-C2B-C3B	3.42	131.08	124.68
24	b	601	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
24	b	613	CLA	CMC-C2C-C3C	3.41	131.37	124.94
24	A	604	CLA	C4A-NA-C1A	3.41	108.24	106.71
30	e	102	LHG	O8-C23-C24	3.41	122.59	111.91
24	C	507	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
24	D	403	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
24	D	403	CLA	CMB-C2B-C3B	3.40	131.03	124.68
24	b	604	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
24	c	510	CLA	CMD-C2D-C3D	3.39	131.02	124.68
30	d	407	LHG	O8-C23-C24	3.38	122.51	111.91
28	A	612	PL9	C36-C34-C33	-3.38	114.28	121.12
24	B	611	CLA	CMB-C2B-C3B	3.37	130.99	124.68
24	A	608	CLA	O2D-CGD-CBD	3.37	117.25	111.27
24	A	613	CLA	CMB-C2B-C3B	3.37	130.98	124.68
24	A	604	CLA	CHB-C4A-NA	3.36	129.16	124.51
31	B	623	SQD	O48-C23-C24	3.36	122.47	111.91
24	c	504	CLA	CMB-C2B-C3B	3.36	130.97	124.68
28	A	612	PL9	O1-C4-C3	-3.36	117.02	120.72
31	a	613	SQD	O9-S-O7	-3.36	102.33	113.95
26	C	514	BCR	C2-C1-C6	3.35	115.64	110.48
29	c	522	LMG	O6-C1-O1	-3.35	102.04	109.97
31	B	623	SQD	O48-C23-O10	-3.35	115.14	123.59
32	h	101	DGD	O2D-C2D-C1D	-3.35	101.91	110.05
24	A	608	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
28	D	405	PL9	C35-C34-C36	3.34	120.90	115.27
24	c	510	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
24	B	614	CLA	CMB-C2B-C3B	3.34	130.93	124.68
31	a	613	SQD	C1-C2-C3	-3.34	103.04	110.00
24	B	616	CLA	CMD-C2D-C3D	3.34	130.93	124.68
24	C	504	CLA	C4-C3-C5	3.34	120.89	115.27
24	c	509	CLA	C4D-C3D-CAD	-3.34	106.61	108.47
24	C	512	CLA	C1-C2-C3	-3.34	120.27	126.04
24	c	508	CLA	CHB-C4A-NA	3.33	129.12	124.51
32	h	101	DGD	O3G-C3G-C2G	-3.33	102.86	110.90
24	C	503	CLA	O2A-C1-C2	-3.32	99.90	108.64
28	d	406	PL9	C37-C38-C39	-3.32	119.66	127.66
24	B	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
24	B	613	CLA	C1-C2-C3	-3.31	120.31	126.04
24	b	612	CLA	CHB-C4A-NA	3.31	129.09	124.51
25	d	402	PHO	O1D-CGD-CBD	3.30	131.24	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	517	DGD	C6D-O5D-C1E	3.30	120.19	113.74
32	C	517	DGD	O3G-C3G-C2G	-3.30	102.94	110.90
26	B	617	BCR	C2-C1-C6	3.30	115.56	110.48
24	B	609	CLA	CMB-C2B-C3B	3.30	130.84	124.68
24	b	601	CLA	CMB-C2B-C3B	3.29	130.84	124.68
24	b	601	CLA	CHB-C4A-NA	3.29	129.06	124.51
24	c	502	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
24	B	603	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
24	C	503	CLA	C7-C6-C5	-3.29	104.43	113.36
28	A	612	PL9	C22-C23-C24	-3.28	119.76	127.66
32	C	516	DGD	C3D-C4D-C5D	-3.28	104.38	110.24
24	B	603	CLA	C4-C3-C5	3.28	120.79	115.27
26	C	515	BCR	C36-C18-C17	-3.27	118.34	122.92
24	B	614	CLA	O1D-CGD-CBD	3.27	131.18	124.48
30	d	409	LHG	C26-C25-C24	3.27	124.93	113.19
29	A	614	LMG	O6-C1-O1	-3.26	102.25	109.97
24	a	612	CLA	CHB-C4A-NA	3.26	129.02	124.51
24	C	503	CLA	O1D-CGD-CBD	3.26	131.15	124.48
29	M	101	LMG	O1-C1-C2	-3.26	103.22	108.30
31	B	623	SQD	C3-C4-C5	3.25	116.04	110.24
24	B	611	CLA	O2D-CGD-CBD	3.24	117.03	111.27
24	A	608	CLA	CMB-C2B-C3B	3.24	130.75	124.68
24	B	604	CLA	CHB-C4A-NA	3.24	129.00	124.51
29	D	406	LMG	O6-C1-O1	-3.24	102.30	109.97
24	a	612	CLA	C4D-C3D-CAD	-3.24	106.66	108.47
24	b	611	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
24	B	605	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	b	613	CLA	C1-C2-C3	-3.24	120.45	126.04
24	b	615	CLA	CHB-C4A-NA	3.23	128.99	124.51
24	c	509	CLA	CMD-C2D-C3D	3.23	130.73	124.68
24	b	614	CLA	C4-C3-C5	3.23	120.71	115.27
24	b	614	CLA	O2A-CGA-O1A	-3.23	115.44	123.59
24	C	504	CLA	CMB-C2B-C3B	3.22	130.69	124.68
24	B	614	CLA	C4D-C3D-CAD	-3.21	106.68	108.47
24	c	501	CLA	O2D-CGD-CBD	3.21	116.97	111.27
28	d	406	PL9	C7-C8-C9	-3.21	121.45	126.79
26	A	609	BCR	C36-C18-C17	-3.21	118.43	122.92
24	b	606	CLA	O2D-CGD-CBD	3.21	116.97	111.27
24	A	604	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
24	c	501	CLA	CMD-C2D-C3D	3.19	130.65	124.68
24	c	512	CLA	C1-C2-C3	-3.19	120.53	126.04
24	b	616	CLA	CHB-C4A-NA	3.19	128.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CMB-C2B-C3B	3.18	130.64	124.68
24	b	610	CLA	O1D-CGD-CBD	3.18	130.99	124.48
24	B	610	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
24	b	605	CLA	C4D-C3D-CAD	-3.18	106.70	108.47
24	c	507	CLA	CHB-C4A-NA	3.17	128.90	124.51
31	b	620	SQD	O8-S-C6	3.17	110.80	105.74
24	c	512	CLA	CHB-C4A-NA	3.17	128.90	124.51
28	D	405	PL9	C42-C43-C44	-3.17	120.04	127.66
31	a	613	SQD	C1-O5-C5	-3.16	107.49	113.69
24	B	615	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
25	A	607	PHO	CAC-C3C-C4C	-3.15	121.79	125.22
24	a	606	CLA	CHB-C4A-NA	3.15	128.87	124.51
24	c	507	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
24	D	402	CLA	CED-O2D-CGD	3.14	123.04	115.94
31	b	620	SQD	O5-C5-C4	3.14	115.40	109.69
32	C	516	DGD	O6D-C1D-O3G	-3.14	102.54	109.97
24	c	503	CLA	CMD-C2D-C3D	3.14	130.55	124.68
24	A	613	CLA	CMD-C2D-C3D	3.14	130.55	124.68
24	C	506	CLA	O1D-CGD-CBD	3.14	130.90	124.48
26	H	101	BCR	C2-C1-C6	3.13	115.31	110.48
24	C	510	CLA	CMD-C2D-C3D	3.13	130.53	124.68
24	B	602	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
31	D	407	SQD	C1-C2-C3	-3.12	103.49	110.00
32	C	517	DGD	O5D-C6D-C5D	-3.12	103.27	109.05
32	c	517	DGD	O3G-C3G-C2G	-3.12	103.37	110.90
24	B	616	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
31	b	620	SQD	C1-C2-C3	-3.12	103.50	110.00
24	C	512	CLA	CHB-C4A-NA	3.12	128.82	124.51
24	C	512	CLA	CMD-C2D-C3D	3.12	130.51	124.68
26	b	618	BCR	C37-C22-C21	-3.12	118.56	122.92
26	d	405	BCR	C27-C26-C25	3.11	127.25	122.73
26	b	619	BCR	C29-C30-C25	3.11	115.27	110.48
26	H	101	BCR	C37-C22-C21	-3.10	118.57	122.92
36	v	201	HEC	CBA-CAA-C2A	-3.10	106.76	112.48
32	c	518	DGD	C3D-C4D-C5D	-3.10	104.71	110.24
24	C	502	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
24	b	602	CLA	CMD-C2D-C3D	3.09	130.46	124.68
24	c	503	CLA	C7-C6-C5	-3.09	104.96	113.36
24	b	602	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
24	C	507	CLA	CMB-C2B-C3B	3.09	130.45	124.68
24	b	611	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	A	607	PHO	CMB-C2B-C1B	-3.08	120.32	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	C	504	CLA	O2A-CGA-O1A	-3.07	115.83	123.59
29	a	618	LMG	C9-C8-C7	-3.07	104.52	111.79
24	c	503	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	t	101	BCR	C1-C6-C5	-3.05	118.31	122.61
36	v	201	HEC	CBD-CAD-C3D	-3.05	106.86	112.49
32	C	516	DGD	O5D-C6D-C5D	-3.05	103.40	109.05
35	e	101	HEM	C4C-C3C-C2C	3.05	109.03	106.90
31	b	620	SQD	O48-C23-C24	3.05	121.47	111.91
24	b	605	CLA	C4A-NA-C1A	3.05	108.08	106.71
24	C	502	CLA	C4D-C3D-CAD	-3.04	106.78	108.47
24	a	606	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
31	a	613	SQD	O47-C7-C8	3.04	118.04	111.50
24	b	616	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
25	A	607	PHO	O1D-CGD-CBD	3.03	130.69	124.48
24	c	506	CLA	CBC-CAC-C3C	-3.02	104.56	112.27
29	b	623	LMG	O1-C1-C2	-3.02	103.59	108.30
24	D	402	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
24	b	605	CLA	CMD-C2D-C3D	3.02	130.33	124.68
31	A	616	SQD	O5-C1-O6	3.02	117.12	109.97
25	A	606	PHO	CBD-CHA-C4D	-3.02	105.14	108.54
29	c	521	LMG	O3-C3-C2	-3.01	103.38	110.35
31	A	617	SQD	O48-C23-C24	3.01	121.36	111.91
24	c	511	CLA	CMD-C2D-C3D	3.01	130.31	124.68
24	c	511	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
24	D	402	CLA	CMB-C2B-C3B	3.01	130.30	124.68
24	c	508	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
30	d	407	LHG	C11-C10-C9	-3.00	99.19	114.42
32	C	517	DGD	O6D-C1D-O3G	-3.00	102.87	109.97
26	T	101	BCR	C7-C8-C9	-2.99	121.72	126.23
24	B	614	CLA	C4A-NA-C1A	2.99	108.05	106.71
32	A	618	DGD	O3G-C3G-C2G	-2.99	103.69	110.90
24	a	612	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	B	602	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	c	506	CLA	CHB-C4A-NA	2.99	128.64	124.51
24	c	503	CLA	C4A-NA-C1A	2.99	108.05	106.71
24	b	613	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
24	C	507	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	B	610	CLA	O2D-CGD-CBD	2.98	116.56	111.27
24	d	404	CLA	CMD-C2D-C3D	2.98	130.25	124.68
24	b	610	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
28	D	405	PL9	C22-C23-C24	-2.97	120.50	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	614	SQD	O48-C23-O10	-2.97	116.09	123.59
35	F	101	HEM	CAD-CBD-CGD	2.97	117.66	112.67
28	D	405	PL9	C20-C19-C21	2.97	120.26	115.27
24	C	509	CLA	CHB-C4A-NA	2.96	128.61	124.51
29	b	621	LMG	C9-C8-C7	-2.96	104.79	111.79
29	d	410	LMG	O2-C2-C1	-2.95	102.88	110.05
24	b	615	CLA	CMB-C2B-C3B	2.94	130.19	124.68
24	c	504	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
31	b	620	SQD	C3-C4-C5	2.94	115.48	110.24
32	A	618	DGD	C3G-C2G-C1G	-2.94	104.84	111.79
24	c	507	CLA	C4-C3-C5	2.94	120.21	115.27
24	c	504	CLA	CHB-C4A-NA	2.93	128.57	124.51
24	a	606	CLA	O2D-CGD-CBD	2.93	116.48	111.27
24	B	614	CLA	C4-C3-C5	2.93	120.20	115.27
24	b	613	CLA	C4A-NA-C1A	2.93	108.02	106.71
24	c	510	CLA	O2A-CGA-O1A	-2.93	116.20	123.59
26	T	101	BCR	C27-C26-C25	2.93	126.98	122.73
24	C	501	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
28	d	406	PL9	C42-C43-C44	-2.92	120.62	127.66
32	C	518	DGD	O3D-C3D-C4D	-2.92	103.59	110.35
24	c	508	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
24	b	604	CLA	OBD-CAD-C3D	2.92	132.83	127.98
24	b	609	CLA	O1D-CGD-CBD	2.92	130.46	124.48
24	C	507	CLA	O2D-CGD-CBD	2.91	116.45	111.27
24	B	616	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
24	C	512	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	b	617	BCR	C27-C26-C25	2.91	126.95	122.73
24	a	604	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
29	b	623	LMG	C3-C4-C5	-2.90	105.06	110.24
24	C	504	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
35	F	101	HEM	CBA-CAA-C2A	-2.90	107.14	112.49
26	d	405	BCR	C38-C26-C25	-2.89	121.28	124.53
29	b	621	LMG	C38-C37-C36	-2.89	99.76	114.42
32	c	516	DGD	O2D-C2D-C3D	-2.88	103.68	110.35
24	B	601	CLA	CMD-C2D-C3D	2.88	130.07	124.68
24	B	610	CLA	CMB-C2B-C3B	2.88	130.07	124.68
24	C	506	CLA	CHB-C4A-NA	2.87	128.48	124.51
24	B	603	CLA	OBD-CAD-CBD	-2.87	121.79	125.89
24	A	613	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
30	B	622	LHG	O8-C23-C24	2.87	120.91	111.91
24	a	606	CLA	CMD-C2D-C3D	2.87	130.04	124.68
24	B	604	CLA	CMB-C2B-C1B	-2.86	124.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	CMB-C2B-C1B	-2.86	124.07	128.46
24	B	615	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	b	612	CLA	C1-C2-C3	-2.86	121.10	126.04
24	b	614	CLA	OBD-CAD-CBD	-2.86	121.81	125.89
24	b	610	CLA	CHB-C4A-NA	2.86	128.46	124.51
24	B	609	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
24	b	606	CLA	OBD-CAD-CBD	-2.85	121.82	125.89
31	D	407	SQD	C1-O5-C5	-2.85	108.09	113.69
24	C	503	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	b	621	LMG	O3-C3-C2	-2.84	103.78	110.35
29	d	410	LMG	O1-C1-C2	-2.84	103.88	108.30
32	A	618	DGD	O5D-C6D-C5D	-2.83	103.80	109.05
31	D	407	SQD	O48-C23-C24	2.83	120.80	111.91
24	A	605	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	c	505	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	Y	101	BCR	C27-C26-C25	2.83	126.84	122.73
29	A	614	LMG	C9-C8-C7	-2.83	105.09	111.79
26	D	404	BCR	C27-C26-C25	2.83	126.84	122.73
24	b	615	CLA	C11-C10-C8	-2.83	106.77	115.92
31	b	620	SQD	O9-S-O7	-2.83	104.16	113.95
26	x	101	BCR	C38-C26-C25	-2.83	121.35	124.53
24	c	513	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	b	610	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
29	C	519	LMG	O6-C1-O1	-2.82	103.28	109.97
24	d	403	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	B	603	CLA	CMB-C2B-C3B	2.82	129.96	124.68
26	t	101	BCR	C7-C8-C9	-2.82	121.97	126.23
28	A	612	PL9	C27-C28-C29	-2.82	120.88	127.66
24	b	615	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	B	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
32	C	518	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
24	c	511	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	a	613	SQD	O48-C23-C24	2.81	120.73	111.91
24	B	605	CLA	C16-C15-C13	-2.81	106.83	115.92
26	C	514	BCR	C27-C26-C25	2.81	126.81	122.73
30	E	101	LHG	O8-C23-C24	2.81	120.72	111.91
26	x	101	BCR	C37-C22-C21	-2.81	118.99	122.92
24	b	608	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
24	C	513	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
24	B	606	CLA	CHA-C1A-NA	-2.80	119.99	126.40
29	M	101	LMG	O3-C3-C2	-2.79	103.89	110.35
24	b	614	CLA	C1-C2-C3	-2.79	121.22	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	609	BCR	C2-C1-C6	2.78	114.77	110.48
26	a	607	BCR	C37-C22-C21	-2.78	119.03	122.92
28	D	405	PL9	C40-C39-C38	-2.78	116.54	123.68
24	c	512	CLA	CMB-C2B-C3B	2.78	129.88	124.68
32	c	518	DGD	O6D-C1D-O3G	-2.78	103.40	109.97
31	A	616	SQD	O47-C7-O49	-2.77	117.00	123.70
24	c	503	CLA	OBD-CAD-CBD	-2.77	121.93	125.89
24	b	615	CLA	O2D-CGD-CBD	2.77	116.19	111.27
24	b	614	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
24	C	513	CLA	C1-O2A-CGA	-2.77	109.18	116.44
24	C	509	CLA	CMC-C2C-C3C	2.77	130.16	124.94
24	B	613	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	d	403	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
24	B	614	CLA	CMD-C2D-C3D	2.77	129.85	124.68
24	c	512	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
24	c	505	CLA	C1-C2-C3	-2.76	121.26	126.04
29	b	623	LMG	O6-C5-C6	2.76	113.30	106.44
24	B	605	CLA	CMB-C2B-C3B	2.76	129.84	124.68
28	d	406	PL9	C20-C19-C21	2.75	119.89	115.27
35	F	101	HEM	C4C-C3C-C2C	2.74	108.81	106.90
32	A	618	DGD	C4E-C3E-C2E	-2.74	106.03	110.82
24	c	506	CLA	CMD-C2D-C3D	2.74	129.81	124.68
32	H	102	DGD	C3D-C4D-C5D	-2.74	105.35	110.24
31	a	613	SQD	C3-C4-C5	2.74	115.12	110.24
26	c	514	BCR	C27-C26-C25	2.74	126.70	122.73
24	b	616	CLA	CMD-C2D-C3D	2.73	129.79	124.68
26	b	617	BCR	C15-C16-C17	-2.73	117.88	123.47
24	a	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	b	621	LMG	C1-O6-C5	-2.73	108.33	113.69
24	B	602	CLA	C1-C2-C3	-2.73	121.32	126.04
24	c	512	CLA	C4D-C3D-CAD	-2.73	106.95	108.47
26	c	515	BCR	C7-C8-C9	-2.73	122.12	126.23
24	A	605	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
24	a	612	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
24	B	611	CLA	CMD-C2D-C3D	2.72	129.76	124.68
31	D	407	SQD	O5-C1-C2	-2.72	104.60	110.35
24	c	507	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
24	B	612	CLA	CMD-C2D-C3D	2.71	129.75	124.68
29	b	621	LMG	O1-C7-C8	-2.71	104.36	110.90
28	A	612	PL9	C31-C32-C33	-2.71	102.97	111.88
25	d	402	PHO	O2D-CGD-O1D	-2.71	118.55	123.84
32	H	102	DGD	O3E-C3E-C2E	-2.71	104.09	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
30	D	408	LHG	O8-C23-C24	2.70	120.39	111.91
24	a	606	CLA	OBD-CAD-CBD	-2.70	122.03	125.89
26	b	618	BCR	C36-C18-C17	-2.70	119.14	122.92
31	b	620	SQD	C45-O47-C7	2.70	124.44	117.79
29	b	623	LMG	O2-C2-C1	-2.70	103.49	110.05
24	b	605	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
24	b	612	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
24	A	604	CLA	O1D-CGD-CBD	2.70	130.00	124.48
24	C	511	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
32	A	618	DGD	C1D-C2D-C3D	-2.70	104.38	110.00
26	B	617	BCR	C36-C18-C17	-2.69	119.15	122.92
31	f	101	SQD	O5-C1-C2	-2.69	104.65	110.35
24	B	613	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
24	c	509	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	k	101	BCR	C38-C26-C25	-2.69	121.51	124.53
32	c	518	DGD	O3D-C3D-C4D	-2.69	104.14	110.35
24	C	501	CLA	OBD-CAD-CBD	-2.69	122.06	125.89
24	A	613	CLA	CHB-C4A-NA	2.69	128.22	124.51
26	C	514	BCR	C11-C10-C9	-2.69	123.48	127.31
24	D	402	CLA	OBD-CAD-CBD	-2.68	122.06	125.89
25	a	605	PHO	CBD-CHA-C4D	-2.68	105.52	108.54
31	a	614	SQD	O49-C7-C8	-2.68	113.26	123.73
24	C	509	CLA	CED-O2D-CGD	2.68	122.00	115.94
31	b	620	SQD	O2-C2-C1	2.68	116.56	110.05
32	C	516	DGD	O2D-C2D-C1D	-2.68	103.53	110.05
36	V	201	HEC	C1D-C2D-C3D	-2.68	105.13	107.00
26	t	101	BCR	C36-C18-C19	2.68	122.30	118.08
30	l	101	LHG	C20-C19-C18	-2.68	100.83	114.42
24	b	610	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
32	A	618	DGD	CDB-CCB-CBB	-2.68	100.83	114.42
26	b	617	BCR	C36-C18-C17	-2.68	119.17	122.92
24	B	604	CLA	CMB-C2B-C3B	2.67	129.68	124.68
31	a	613	SQD	O8-S-C6	2.67	110.00	105.74
24	b	608	CLA	C4A-NA-C1A	2.67	107.91	106.71
24	c	512	CLA	CMD-C2D-C3D	2.67	129.67	124.68
24	d	401	CLA	C4D-C3D-CAD	-2.67	106.98	108.47
26	d	405	BCR	C2-C1-C6	2.66	114.58	110.48
31	f	101	SQD	O47-C7-C8	2.66	118.22	110.80
26	T	101	BCR	C38-C26-C27	-2.66	108.51	113.62
24	b	615	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
26	A	609	BCR	C38-C26-C25	-2.66	121.54	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	C1D-C2D-C3D	-2.66	105.15	107.00
32	H	102	DGD	O2D-C2D-C1D	-2.66	103.59	110.05
26	b	617	BCR	C38-C26-C25	-2.65	121.55	124.53
32	C	517	DGD	C3E-C4E-C5E	-2.65	105.52	110.24
24	b	612	CLA	C11-C12-C13	-2.65	107.36	115.92
24	B	612	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
24	B	603	CLA	C4D-C3D-CAD	-2.65	107.00	108.47
26	C	514	BCR	C38-C26-C25	-2.64	121.56	124.53
29	A	614	LMG	O3-C3-C2	-2.64	104.24	110.35
26	B	619	BCR	C36-C18-C17	-2.64	119.22	122.92
24	b	609	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
24	B	605	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
24	A	608	CLA	C4-C3-C5	2.64	119.71	115.27
24	b	610	CLA	OBD-CAD-CBD	-2.63	122.13	125.89
31	f	101	SQD	C3-C4-C5	2.63	114.94	110.24
32	c	517	DGD	O6D-C1D-O3G	-2.63	103.74	109.97
32	C	517	DGD	C1D-C2D-C3D	-2.63	104.51	110.00
24	B	611	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	B	606	CLA	C4-C3-C5	2.63	119.69	115.27
24	B	612	CLA	C11-C12-C13	-2.63	107.43	115.92
24	B	603	CLA	CMD-C2D-C3D	2.63	129.59	124.68
24	c	508	CLA	CMD-C2D-C3D	2.63	129.59	124.68
24	b	613	CLA	C7-C6-C5	-2.62	106.23	113.36
24	B	616	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	Y	101	BCR	C39-C30-C25	-2.62	106.05	110.30
24	C	511	CLA	CMD-C2D-C3D	2.62	129.58	124.68
24	c	501	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	b	603	CLA	O2D-CGD-CBD	2.61	115.91	111.27
24	c	510	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
30	d	408	LHG	O8-C23-C24	2.61	120.10	111.91
29	c	519	LMG	O6-C1-O1	-2.61	103.79	109.97
24	d	401	CLA	OBD-CAD-CBD	-2.61	122.17	125.89
28	A	612	PL9	C26-C24-C23	-2.61	115.84	121.12
26	t	101	BCR	C15-C16-C17	-2.61	118.13	123.47
30	l	101	LHG	C11-C10-C9	-2.61	101.19	114.42
29	b	621	LMG	O1-C1-C2	-2.61	104.23	108.30
24	b	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	D	402	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	c	515	BCR	C2-C1-C6	2.60	114.48	110.48
26	k	102	BCR	C29-C30-C25	2.60	114.48	110.48
32	c	516	DGD	O6E-C5E-C4E	2.60	114.41	109.69
30	l	101	LHG	C18-C17-C16	-2.60	101.25	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CMC-C2C-C3C	2.59	129.83	124.94
26	K	101	BCR	C37-C22-C21	-2.59	119.30	122.92
24	b	604	CLA	CMC-C2C-C3C	2.59	129.82	124.94
26	H	101	BCR	C16-C15-C14	-2.58	118.18	123.47
26	a	607	BCR	C37-C22-C23	2.58	122.15	118.08
30	D	408	LHG	C11-C10-C9	-2.58	101.31	114.42
26	c	514	BCR	C15-C16-C17	-2.58	118.19	123.47
31	D	407	SQD	O5-C5-C4	2.58	114.38	109.69
26	c	515	BCR	C36-C18-C17	-2.58	119.31	122.92
24	c	511	CLA	OBD-CAD-CBD	-2.58	122.21	125.89
24	c	513	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
24	B	610	CLA	O1D-CGD-CBD	2.58	129.76	124.48
24	B	606	CLA	CGD-CBD-CAD	-2.58	102.39	110.73
24	b	607	CLA	OBD-CAD-CBD	-2.58	122.22	125.89
24	B	609	CLA	CMD-C2D-C3D	2.58	129.50	124.68
24	b	604	CLA	C6-C5-C3	-2.57	106.71	113.45
32	C	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.42
24	c	510	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	C	504	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	C	510	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
24	C	508	CLA	CMC-C2C-C3C	2.57	129.79	124.94
24	B	605	CLA	OBD-CAD-CBD	-2.57	122.22	125.89
30	D	408	LHG	C20-C19-C18	-2.57	101.39	114.42
24	c	507	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
32	H	102	DGD	C3E-C4E-C5E	-2.56	105.67	110.24
24	B	604	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
24	d	404	CLA	OBD-CAD-CBD	-2.56	122.24	125.89
26	B	619	BCR	C29-C30-C25	2.55	114.41	110.48
24	B	604	CLA	CMC-C2C-C3C	2.55	129.76	124.94
24	C	513	CLA	CMD-C2D-C3D	2.55	129.45	124.68
26	D	404	BCR	C38-C26-C25	-2.55	121.66	124.53
24	b	610	CLA	C1-C2-C3	-2.55	121.63	126.04
35	e	101	HEM	CMC-C2C-C3C	2.55	129.45	124.68
24	C	501	CLA	OBD-CAD-C3D	2.55	132.22	127.98
24	C	509	CLA	OBD-CAD-CBD	-2.55	122.26	125.89
28	a	611	PL9	C36-C34-C33	-2.55	115.96	121.12
24	B	601	CLA	O2D-CGD-CBD	2.55	115.79	111.27
24	c	502	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
26	B	618	BCR	C7-C8-C9	-2.54	122.39	126.23
24	B	605	CLA	C7-C6-C5	-2.54	106.46	113.36
24	C	513	CLA	O2D-CGD-CBD	2.54	115.78	111.27
32	c	516	DGD	CDB-CCB-CBB	-2.54	101.53	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	CMC-C2C-C3C	2.54	129.73	124.94
24	d	403	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	A	607	PHO	C1B-NB-C4B	2.54	111.29	106.51
29	c	519	LMG	C9-C8-C7	-2.54	105.79	111.79
24	C	511	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
30	B	622	LHG	C11-C10-C9	-2.54	101.55	114.42
29	b	623	LMG	O1-C7-C8	-2.54	104.78	110.90
24	b	609	CLA	CMD-C2D-C3D	2.53	129.42	124.68
24	C	505	CLA	OBD-CAD-CBD	-2.53	122.28	125.89
32	h	101	DGD	C3D-C4D-C5D	-2.53	105.72	110.24
24	a	606	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
24	D	403	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	B	623	SQD	O5-C1-C2	-2.52	105.01	110.35
24	b	604	CLA	C1-C2-C3	-2.52	121.68	126.04
24	c	510	CLA	C7-C6-C5	-2.52	106.51	113.36
24	c	511	CLA	C4D-C3D-CAD	-2.52	107.06	108.47
24	B	602	CLA	CMD-C2D-C3D	2.52	129.40	124.68
24	B	613	CLA	CHA-C1A-NA	-2.52	120.63	126.40
24	C	509	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
32	h	101	DGD	C4E-C3E-C2E	-2.52	106.43	110.82
29	d	410	LMG	O6-C1-O1	-2.52	104.01	109.97
24	B	606	CLA	C1-C2-C3	-2.52	121.69	126.04
24	B	614	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
24	d	401	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
24	b	604	CLA	CMD-C2D-C3D	2.51	129.38	124.68
24	A	605	CLA	O2D-CGD-CBD	2.51	115.73	111.27
35	e	101	HEM	CBA-CAA-C2A	-2.51	107.86	112.49
26	c	515	BCR	C8-C9-C10	2.51	122.79	118.94
24	c	507	CLA	CMC-C2C-C3C	2.51	129.67	124.94
24	B	604	CLA	OBD-CAD-CBD	-2.51	122.31	125.89
31	f	101	SQD	O9-S-C6	2.50	109.92	106.94
26	B	617	BCR	C29-C30-C25	2.50	114.34	110.48
24	b	610	CLA	CHA-C1A-NA	-2.50	120.66	126.40
26	H	101	BCR	C1-C6-C5	-2.50	119.09	122.61
24	d	401	CLA	CMD-C2D-C3D	2.50	129.35	124.68
24	b	604	CLA	CMA-C3A-C4A	2.50	118.49	111.77
32	h	101	DGD	O3E-C3E-C2E	-2.50	104.58	110.35
24	b	607	CLA	C1-O2A-CGA	2.49	122.99	116.44
24	b	616	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
24	b	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	b	617	BCR	C36-C18-C19	2.49	122.00	118.08
24	b	610	CLA	C2A-C1A-CHA	2.49	128.21	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	OBD-CAD-C3D	2.49	132.11	127.98
24	b	614	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	B	603	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
26	D	404	BCR	C2-C1-C6	2.48	114.30	110.48
24	b	603	CLA	CMC-C2C-C3C	2.48	129.62	124.94
26	b	619	BCR	C36-C18-C17	-2.48	119.45	122.92
29	c	519	LMG	C3-C4-C5	-2.47	105.83	110.24
31	b	620	SQD	O47-C45-C46	2.47	117.36	108.40
28	D	405	PL9	C37-C38-C39	-2.47	121.70	127.66
31	A	616	SQD	O48-C23-C24	2.47	119.66	111.91
24	C	507	CLA	C2A-C1A-CHA	2.47	128.18	123.86
24	C	508	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	b	610	CLA	CMD-C2D-C3D	2.47	129.29	124.68
24	d	404	CLA	CHA-C1A-NA	-2.46	120.75	126.40
24	c	511	CLA	O2D-CGD-CBD	2.46	115.65	111.27
24	B	602	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
30	d	407	LHG	C18-C17-C16	-2.46	101.91	114.42
24	C	508	CLA	C1-C2-C3	-2.46	121.79	126.04
24	C	508	CLA	OBD-CAD-C3D	2.46	132.06	127.98
24	b	613	CLA	CMD-C2D-C3D	2.46	129.28	124.68
24	C	507	CLA	CHB-C4A-NA	2.46	127.91	124.51
28	a	611	PL9	C11-C12-C13	-2.46	103.81	111.88
32	C	518	DGD	C1D-C2D-C3D	-2.46	104.88	110.00
24	c	508	CLA	O2D-CGD-CBD	2.45	115.63	111.27
26	B	617	BCR	C3-C4-C5	-2.45	109.69	114.08
24	B	611	CLA	C1-C2-C3	-2.45	121.80	126.04
24	b	604	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
35	F	101	HEM	C1D-C2D-C3D	2.45	108.70	107.00
24	B	608	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	d	403	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	B	623	SQD	O9-S-C6	-2.45	104.03	106.94
32	c	518	DGD	O5D-C1E-C2E	2.44	112.12	108.30
24	A	608	CLA	CHB-C4A-NA	2.44	127.89	124.51
28	D	405	PL9	C8-C7-C3	2.44	118.88	111.98
30	d	408	LHG	C20-C19-C18	-2.44	102.04	114.42
26	c	514	BCR	C37-C22-C23	2.44	121.92	118.08
24	B	616	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
26	C	514	BCR	C33-C5-C6	-2.43	121.79	124.53
32	c	517	DGD	C3E-C4E-C5E	-2.43	105.90	110.24
24	c	505	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
29	c	522	LMG	C38-C37-C36	-2.43	102.07	114.42
24	C	506	CLA	CMD-C2D-C3D	2.43	129.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	615	LHG	O8-C6-C5	-2.43	101.35	108.43
24	C	506	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
31	A	617	SQD	O47-C7-C8	2.43	116.73	111.50
32	H	102	DGD	O5D-C1E-C2E	2.43	112.09	108.30
24	C	501	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
24	A	613	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
24	c	506	CLA	C4-C3-C2	-2.43	117.45	123.68
24	a	604	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
24	b	604	CLA	C11-C12-C13	-2.42	108.09	115.92
28	d	406	PL9	C31-C32-C33	-2.42	103.92	111.88
24	b	604	CLA	CMB-C2B-C3B	2.42	129.21	124.68
24	d	401	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
24	B	604	CLA	CGD-CBD-CAD	-2.42	102.90	110.73
26	C	515	BCR	C27-C26-C25	2.42	126.24	122.73
24	b	602	CLA	C4-C3-C5	2.42	119.34	115.27
29	A	614	LMG	C12-C11-C10	-2.42	104.83	113.62
35	F	101	HEM	CMD-C2D-C1D	-2.41	124.75	128.46
26	C	514	BCR	C36-C18-C17	-2.41	119.55	122.92
24	C	502	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	c	501	CLA	O1D-CGD-CBD	2.41	129.41	124.48
26	H	101	BCR	C27-C26-C25	2.41	126.23	122.73
29	a	618	LMG	C40-C39-C38	-2.41	102.20	114.42
28	D	405	PL9	C31-C32-C33	-2.41	103.97	111.88
26	c	514	BCR	C2-C1-C6	2.41	114.18	110.48
29	A	614	LMG	O8-C28-O10	-2.40	117.52	123.59
31	D	407	SQD	O9-S-O7	-2.40	105.64	113.95
26	c	514	BCR	C37-C22-C21	-2.40	119.56	122.92
31	D	407	SQD	C44-O6-C1	2.40	117.82	113.84
29	M	101	LMG	O1-C7-C8	-2.40	105.11	110.90
24	B	604	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
28	D	405	PL9	C11-C12-C13	-2.40	104.00	111.88
32	c	518	DGD	O6E-C1E-O5D	-2.40	104.29	109.97
24	c	508	CLA	C7-C6-C5	-2.40	106.84	113.36
24	C	510	CLA	C11-C10-C8	-2.40	108.17	115.92
24	b	604	CLA	O1D-CGD-CBD	2.40	129.38	124.48
24	b	606	CLA	CMC-C2C-C3C	2.39	129.45	124.94
31	A	616	SQD	O9-S-C6	2.39	109.78	106.94
24	A	604	CLA	O2D-CGD-CBD	-2.39	107.02	111.27
24	C	513	CLA	CHB-C4A-NA	2.39	127.81	124.51
29	D	406	LMG	O3-C3-C2	-2.39	104.83	110.35
32	H	102	DGD	CDB-CCB-CBB	-2.38	102.32	114.42
28	a	611	PL9	C27-C28-C29	-2.38	121.92	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C7-C8-C9	-2.38	122.63	126.23
29	c	519	LMG	O2-C2-C1	-2.38	104.26	110.05
26	c	515	BCR	C1-C6-C5	-2.38	119.26	122.61
24	C	502	CLA	CMD-C2D-C3D	2.38	129.13	124.68
32	c	517	DGD	C3D-C4D-C5D	-2.38	105.99	110.24
26	Y	101	BCR	C38-C26-C25	-2.38	121.86	124.53
32	A	618	DGD	CBB-CAB-C9B	-2.38	102.36	114.42
26	a	607	BCR	C29-C30-C25	2.37	114.13	110.48
24	c	513	CLA	O2D-CGD-CBD	2.37	115.48	111.27
26	k	102	BCR	C27-C26-C25	2.37	126.17	122.73
26	b	619	BCR	C27-C26-C25	2.37	126.17	122.73
26	x	101	BCR	C27-C26-C25	2.36	126.16	122.73
32	c	518	DGD	CDB-CCB-CBB	-2.36	102.42	114.42
32	c	516	DGD	O3E-C3E-C2E	-2.36	104.89	110.35
28	a	611	PL9	C20-C19-C21	2.36	119.25	115.27
26	b	619	BCR	C7-C8-C9	-2.36	122.67	126.23
35	F	101	HEM	CMC-C2C-C3C	2.36	129.09	124.68
30	B	622	LHG	C20-C19-C18	-2.36	102.44	114.42
24	B	603	CLA	O1D-CGD-CBD	2.36	129.31	124.48
24	b	613	CLA	CHA-C1A-NA	-2.36	121.00	126.40
32	c	518	DGD	O6E-C5E-C4E	2.36	113.97	109.69
24	C	502	CLA	CHA-C1A-NA	-2.36	121.00	126.40
24	B	603	CLA	C5-C3-C2	-2.36	116.35	121.12
30	E	101	LHG	C18-C17-C16	-2.36	102.47	114.42
24	b	603	CLA	C4-C3-C5	2.35	119.23	115.27
24	A	613	CLA	C3B-C4B-NB	-2.35	106.17	109.21
28	D	405	PL9	C31-C29-C28	2.35	125.87	121.12
25	a	605	PHO	O2A-CGA-O1A	-2.35	117.66	123.59
25	d	402	PHO	C1B-NB-C4B	2.35	110.94	106.51
24	B	605	CLA	CHB-C4A-NA	2.35	127.76	124.51
36	V	201	HEC	CMB-C2B-C1B	-2.35	124.85	128.46
26	k	101	BCR	C27-C26-C25	2.35	126.14	122.73
24	B	608	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
30	e	102	LHG	C11-C10-C9	-2.35	102.51	114.42
24	b	604	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
24	c	502	CLA	C1-C2-C3	-2.35	121.99	126.04
24	d	401	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
24	B	605	CLA	O1D-CGD-CBD	2.34	129.28	124.48
32	c	517	DGD	O3G-C1D-C2D	-2.34	104.64	108.30
24	b	609	CLA	CHA-C1A-NA	-2.34	121.03	126.40
26	B	617	BCR	C15-C16-C17	-2.34	118.68	123.47
29	b	621	LMG	O6-C1-O1	-2.34	104.43	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	521	LMG	O6-C1-O1	-2.34	104.43	109.97
31	a	614	SQD	O48-C46-C45	2.34	115.25	108.43
26	B	618	BCR	C29-C30-C25	2.34	114.08	110.48
24	b	610	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
33	C	522	STE	C4-C3-C2	-2.34	104.66	113.76
26	d	405	BCR	C3-C4-C5	-2.34	109.90	114.08
29	C	519	LMG	O2-C2-C1	-2.34	104.37	110.05
24	b	610	CLA	CMC-C2C-C3C	2.34	129.35	124.94
24	C	508	CLA	O2D-CGD-CBD	2.33	115.42	111.27
24	b	603	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
29	C	519	LMG	O7-C10-O9	-2.33	118.07	123.70
24	C	502	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	B	606	CLA	C2A-C1A-CHA	2.33	127.93	123.86
24	C	511	CLA	CMB-C2B-C3B	2.33	129.04	124.68
29	c	521	LMG	O2-C2-C1	-2.33	104.39	110.05
24	b	609	CLA	C11-C10-C8	-2.33	108.40	115.92
24	c	502	CLA	O1D-CGD-CBD	2.33	129.25	124.48
24	b	613	CLA	OBD-CAD-CBD	-2.33	122.57	125.89
28	a	611	PL9	C7-C8-C9	-2.33	122.92	126.79
32	C	516	DGD	O1G-C1A-C2A	-2.33	104.61	111.91
26	A	609	BCR	C15-C16-C17	-2.32	118.72	123.47
26	B	617	BCR	C27-C26-C25	2.32	126.10	122.73
32	h	101	DGD	O5E-C6E-C5E	-2.32	103.33	111.29
30	B	622	LHG	O8-C23-O10	-2.32	117.73	123.59
26	C	514	BCR	C34-C9-C10	-2.32	119.67	122.92
24	c	501	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
24	B	612	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	b	602	CLA	OBD-CAD-CBD	-2.32	122.58	125.89
26	C	514	BCR	C15-C16-C17	-2.32	118.72	123.47
24	B	608	CLA	C4A-NA-C1A	2.32	107.75	106.71
24	D	403	CLA	CMC-C2C-C3C	2.31	129.30	124.94
26	K	101	BCR	C27-C26-C25	2.31	126.09	122.73
24	b	602	CLA	C1-C2-C3	-2.31	122.04	126.04
29	a	618	LMG	O6-C5-C4	2.31	113.89	109.69
24	B	604	CLA	O2D-CGD-CBD	2.31	115.38	111.27
24	b	613	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	T	101	BCR	C1-C6-C5	-2.31	119.36	122.61
28	d	406	PL9	C36-C34-C33	-2.31	116.44	121.12
28	d	406	PL9	C22-C23-C24	-2.31	122.10	127.66
24	B	608	CLA	CMC-C2C-C3C	2.31	129.29	124.94
24	b	609	CLA	CMC-C2C-C3C	2.31	129.29	124.94
31	b	620	SQD	O10-C23-C24	-2.30	114.75	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	A	615	LHG	C27-C26-C25	-2.30	102.75	114.42
33	b	625	STE	C4-C3-C2	-2.30	104.82	113.76
25	A	606	PHO	O2D-CGD-O1D	-2.30	119.34	123.84
29	M	101	LMG	C1-C2-C3	-2.30	105.21	110.00
24	C	509	CLA	C1-C2-C3	-2.30	122.07	126.04
26	H	101	BCR	C37-C22-C23	2.30	121.70	118.08
32	c	517	DGD	C4E-C3E-C2E	-2.30	106.81	110.82
35	F	101	HEM	CMB-C2B-C3B	2.30	128.98	124.68
32	C	517	DGD	CDB-CCB-CBB	-2.29	102.78	114.42
32	c	516	DGD	CBB-CAB-C9B	-2.29	102.78	114.42
24	B	609	CLA	CHA-C1A-NA	-2.29	121.15	126.40
24	B	611	CLA	OBD-CAD-C3D	2.29	131.78	127.98
28	D	405	PL9	C50-C49-C48	-2.29	116.03	122.65
26	b	619	BCR	C2-C1-C6	2.29	114.00	110.48
24	C	512	CLA	OBD-CAD-CBD	-2.29	122.63	125.89
24	B	604	CLA	O2A-C1-C2	2.28	114.64	108.64
28	a	611	PL9	C12-C13-C14	-2.28	122.16	127.66
28	a	611	PL9	C22-C23-C24	-2.28	122.16	127.66
26	a	607	BCR	C27-C26-C25	2.28	126.04	122.73
24	C	501	CLA	CMB-C2B-C3B	2.28	128.94	124.68
31	f	101	SQD	O5-C5-C4	2.28	113.83	109.69
32	c	517	DGD	C8B-C7B-C6B	-2.28	102.85	114.42
29	A	614	LMG	C1-O6-C5	-2.28	109.22	113.69
25	A	606	PHO	C1B-NB-C4B	2.28	110.80	106.51
29	M	101	LMG	C31-C30-C29	-2.27	105.02	113.19
24	C	509	CLA	C2A-C3A-C4A	2.27	105.54	101.87
26	t	101	BCR	C2-C1-C6	2.27	113.98	110.48
30	E	101	LHG	C11-C10-C9	-2.27	102.90	114.42
24	b	615	CLA	C1-O2A-CGA	2.27	122.40	116.44
29	D	409	LMG	O1-C7-C8	-2.27	105.76	111.78
24	B	615	CLA	C6-C7-C8	-2.27	108.58	115.92
24	A	613	CLA	O2D-CGD-CBD	2.27	115.30	111.27
24	b	604	CLA	C6-C7-C8	-2.27	108.59	115.92
32	h	101	DGD	O6E-C5E-C4E	2.26	113.81	109.69
26	d	405	BCR	C24-C23-C22	-2.26	122.82	126.23
24	b	607	CLA	CHA-C1A-NA	-2.26	121.22	126.40
32	C	518	DGD	O3E-C3E-C2E	-2.26	105.13	110.35
24	b	607	CLA	C2A-C1A-CHA	2.26	127.81	123.86
32	C	516	DGD	C5B-C4B-C3B	-2.26	102.97	114.42
26	b	618	BCR	C15-C16-C17	-2.26	118.85	123.47
24	b	616	CLA	CMC-C2C-C3C	2.25	129.19	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	518	DGD	CBB-CAB-C9B	-2.25	102.99	114.42
36	V	201	HEC	CMC-C2C-C3C	2.25	128.47	125.82
24	c	504	CLA	O1A-CGA-CBA	2.25	132.52	123.73
30	D	408	LHG	C27-C26-C25	-2.25	103.00	114.42
30	d	408	LHG	C18-C17-C16	-2.25	103.00	114.42
24	c	506	CLA	C4-C3-C5	2.25	119.05	115.27
24	c	506	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
24	B	601	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	d	403	CLA	C2A-C1A-CHA	2.25	127.79	123.86
24	b	606	CLA	O1D-CGD-CBD	2.25	129.08	124.48
32	h	101	DGD	CDB-CCB-CBB	-2.25	103.03	114.42
24	c	512	CLA	O1D-CGD-CBD	2.24	129.08	124.48
24	b	605	CLA	CMC-C2C-C3C	2.24	129.17	124.94
35	F	101	HEM	C3C-C4C-NC	-2.24	106.71	110.94
24	C	504	CLA	CMC-C2C-C3C	2.24	129.17	124.94
26	b	619	BCR	C38-C26-C25	-2.24	122.01	124.53
29	D	406	LMG	C38-C37-C36	-2.24	103.06	114.42
26	C	515	BCR	C2-C1-C6	2.24	113.93	110.48
24	C	507	CLA	C1-C2-C3	-2.24	122.17	126.04
24	b	605	CLA	O1A-CGA-CBA	2.24	132.46	123.73
26	B	618	BCR	C15-C16-C17	-2.24	118.89	123.47
24	B	603	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	b	618	BCR	C15-C14-C13	-2.23	124.12	127.31
32	h	101	DGD	C6D-C5D-C4D	2.23	116.75	112.09
24	C	507	CLA	CMC-C2C-C3C	2.23	129.15	124.94
32	c	516	DGD	C5B-C4B-C3B	-2.23	103.10	114.42
24	c	504	CLA	CMD-C2D-C3D	2.23	128.85	124.68
32	c	518	DGD	O2D-C2D-C1D	-2.23	104.63	110.05
24	b	608	CLA	C6-C7-C8	-2.23	108.71	115.92
24	d	404	CLA	O2A-C1-C2	-2.23	102.78	108.64
36	V	201	HEC	CAD-CBD-CGD	-2.23	108.93	112.67
24	C	511	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	A	605	CLA	C3D-CAD-CBD	-2.23	104.67	107.61
24	b	614	CLA	OBD-CAD-C3D	2.23	131.68	127.98
24	c	511	CLA	CMB-C2B-C3B	2.23	128.84	124.68
30	l	101	LHG	C27-C26-C25	-2.22	103.16	114.42
28	a	611	PL9	O2-C1-C2	-2.22	116.69	121.78
24	c	512	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
26	b	617	BCR	C29-C30-C25	2.22	113.90	110.48
24	B	608	CLA	O1D-CGD-CBD	2.22	129.02	124.48
32	c	517	DGD	O4E-C4E-C3E	-2.22	105.22	110.35
24	D	402	CLA	C1B-CHB-C4A	-2.22	125.72	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	407	LHG	C20-C19-C18	-2.22	103.17	114.42
29	a	618	LMG	C42-C41-C40	-2.22	103.17	114.42
24	B	611	CLA	C9-C8-C10	-2.22	103.27	111.29
31	f	101	SQD	C46-C45-C44	-2.21	106.55	111.79
24	A	605	CLA	C1-O2A-CGA	2.21	122.25	116.44
24	c	502	CLA	CHB-C4A-NA	2.21	127.57	124.51
26	Y	101	BCR	C30-C25-C26	-2.21	119.50	122.61
24	b	609	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	b	608	CLA	C11-C10-C8	-2.21	108.78	115.92
24	b	611	CLA	CHB-C4A-NA	2.21	127.56	124.51
24	C	510	CLA	CMC-C2C-C3C	2.21	129.10	124.94
24	B	608	CLA	CMD-C2D-C3D	2.21	128.81	124.68
24	c	509	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
25	A	607	PHO	C1-C2-C3	-2.20	122.23	126.04
26	x	101	BCR	C36-C18-C17	-2.20	119.84	122.92
30	E	101	LHG	C20-C19-C18	-2.20	103.24	114.42
24	B	612	CLA	C1-C2-C3	-2.20	122.23	126.04
24	B	606	CLA	CMD-C2D-C3D	2.20	128.80	124.68
28	A	612	PL9	O2-C1-C2	-2.20	116.74	121.78
24	B	601	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	b	604	CLA	C3A-C2A-C1A	2.20	104.63	101.34
24	b	606	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	A	607	PHO	CAC-C3C-C2C	2.20	131.29	127.53
29	c	519	LMG	C1-O6-C5	-2.20	109.38	113.69
24	A	605	CLA	CHB-C4A-NA	2.19	127.55	124.51
24	b	616	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	b	607	CLA	OBD-CAD-C3D	2.19	131.62	127.98
24	C	507	CLA	CMD-C2D-C3D	2.19	128.78	124.68
24	B	612	CLA	C16-C15-C13	-2.19	108.84	115.92
24	B	601	CLA	C2A-C1A-CHA	2.19	127.69	123.86
29	b	623	LMG	C40-C39-C38	-2.19	103.31	114.42
30	B	621	LHG	C20-C19-C18	-2.19	103.31	114.42
32	c	517	DGD	O2E-C2E-C1E	-2.19	104.73	110.05
32	c	516	DGD	O1G-C1A-C2A	-2.19	105.04	111.91
30	A	615	LHG	O8-C23-C24	2.19	118.77	111.91
24	a	604	CLA	CMD-C2D-C3D	2.18	128.76	124.68
32	c	517	DGD	O3E-C3E-C4E	-2.18	105.30	110.35
24	c	509	CLA	CMC-C2C-C3C	2.18	129.06	124.94
24	B	614	CLA	C3B-C4B-NB	-2.18	106.39	109.21
24	C	503	CLA	CMC-C2C-C3C	2.18	129.06	124.94
28	D	405	PL9	C32-C33-C34	-2.18	122.41	127.66
30	B	622	LHG	O3-P-O5	-2.18	100.55	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	518	DGD	O5E-C6E-C5E	-2.18	103.82	111.29
26	k	102	BCR	C37-C22-C21	-2.18	119.88	122.92
32	H	102	DGD	C1E-O6E-C5E	2.18	117.96	113.69
29	d	410	LMG	O3-C3-C2	-2.18	105.32	110.35
24	B	602	CLA	CMC-C2C-C3C	2.17	129.04	124.94
25	A	606	PHO	C2B-C1B-NB	-2.17	106.51	109.79
24	d	404	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
24	b	607	CLA	CMC-C2C-C3C	2.17	129.04	124.94
24	B	610	CLA	C1-C2-C3	-2.17	122.29	126.04
26	C	514	BCR	C24-C23-C22	-2.17	122.95	126.23
26	t	101	BCR	C4-C5-C6	2.17	125.88	122.73
26	x	101	BCR	C16-C15-C14	-2.17	119.03	123.47
24	A	604	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
24	c	504	CLA	O2D-CGD-CBD	2.17	115.12	111.27
24	A	613	CLA	C7-C6-C5	-2.17	107.47	113.36
28	a	611	PL9	O2-C1-C6	2.17	124.34	120.59
24	B	611	CLA	C11-C12-C13	-2.16	108.92	115.92
24	C	510	CLA	C16-C15-C13	-2.16	108.92	115.92
24	b	614	CLA	O1A-CGA-CBA	2.16	132.17	123.73
24	c	505	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
32	c	517	DGD	O5D-C6D-C5D	-2.16	105.04	109.05
24	a	606	CLA	CHA-C1A-NA	-2.16	121.44	126.40
25	d	402	PHO	CMB-C2B-C1B	-2.16	121.73	125.06
24	C	512	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	A	604	CLA	CMD-C2D-C3D	2.16	128.72	124.68
24	B	609	CLA	C6-C5-C3	2.16	119.12	113.45
26	b	617	BCR	C3-C4-C5	-2.16	110.22	114.08
30	l	101	LHG	O8-C23-C24	2.16	118.68	111.91
26	x	101	BCR	C2-C1-C6	2.16	113.80	110.48
32	c	517	DGD	C1D-C2D-C3D	-2.16	105.51	110.00
26	c	514	BCR	C33-C5-C6	-2.16	122.11	124.53
32	h	101	DGD	C4D-C3D-C2D	-2.15	107.06	110.82
24	c	510	CLA	O1A-CGA-CBA	2.15	132.13	123.73
24	B	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	C	503	CLA	C3A-C2A-C1A	2.15	104.56	101.34
24	b	611	CLA	C11-C12-C13	-2.15	108.97	115.92
31	f	101	SQD	O5-C1-O6	2.15	115.07	109.97
25	d	402	PHO	CBD-CHA-C4D	-2.15	106.12	108.54
31	B	623	SQD	C25-C24-C23	-2.15	105.81	113.62
24	b	604	CLA	CGD-CBD-CAD	-2.15	103.78	110.73
29	C	519	LMG	O1-C7-C8	-2.15	105.72	110.90
26	c	515	BCR	C15-C16-C17	-2.15	119.08	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	C6-C5-C3	2.15	119.08	113.45
24	A	604	CLA	CAA-CBA-CGA	-2.14	106.98	113.25
24	B	611	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
26	C	515	BCR	C34-C9-C10	-2.14	119.92	122.92
28	d	406	PL9	C8-C7-C3	2.14	118.04	111.98
24	C	511	CLA	C4-C3-C5	2.14	118.88	115.27
31	A	616	SQD	O8-S-O9	2.14	116.51	111.27
30	d	407	LHG	O3-P-O5	-2.14	100.69	109.07
24	B	611	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
25	a	605	PHO	C1B-NB-C4B	2.14	110.54	106.51
36	v	201	HEC	CMD-C2D-C3D	2.14	128.97	124.94
36	V	201	HEC	CBA-CAA-C2A	-2.14	108.54	112.48
29	c	522	LMG	C40-C39-C38	-2.14	103.59	114.42
25	a	605	PHO	O2D-CGD-O1D	-2.13	119.66	123.84
24	b	601	CLA	CMC-C2C-C3C	2.13	128.97	124.94
30	A	615	LHG	C3-C2-C1	-2.13	104.08	111.67
24	C	507	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	A	605	CLA	CMC-C2C-C3C	2.13	128.96	124.94
24	c	507	CLA	CMD-C2D-C3D	2.13	128.67	124.68
24	B	614	CLA	CHB-C4A-NA	2.13	127.46	124.51
29	c	522	LMG	C8-O7-C10	2.13	123.04	117.79
24	c	510	CLA	OBD-CAD-CBD	-2.13	122.86	125.89
24	d	404	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
29	C	519	LMG	O8-C28-O10	-2.13	118.23	123.59
24	A	605	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
32	c	518	DGD	C3G-C2G-C1G	-2.12	106.77	111.79
24	B	611	CLA	C14-C13-C15	-2.12	103.61	111.29
29	c	522	LMG	O2-C2-C3	-2.12	105.45	110.35
30	B	622	LHG	C13-C12-C11	-2.12	103.67	114.42
24	B	607	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
24	b	601	CLA	O2D-CGD-CBD	2.12	115.03	111.27
28	a	611	PL9	C37-C38-C39	-2.12	122.56	127.66
31	B	623	SQD	C27-C26-C25	-2.12	103.69	114.42
24	b	614	CLA	C4-C3-C2	-2.12	118.25	123.68
29	d	410	LMG	C40-C39-C38	-2.11	103.69	114.42
29	M	101	LMG	C6-C5-C4	-2.11	108.05	113.00
26	d	405	BCR	C30-C25-C26	-2.11	119.64	122.61
26	B	617	BCR	C11-C10-C9	-2.11	124.30	127.31
26	c	514	BCR	C38-C26-C25	-2.11	122.16	124.53
24	c	503	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
24	C	501	CLA	C3A-C2A-C1A	2.11	104.50	101.34
26	D	404	BCR	C7-C8-C9	-2.11	123.05	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CBC-CAC-C3C	-2.11	106.90	112.27
24	B	609	CLA	OBD-CAD-CBD	-2.11	122.89	125.89
28	A	612	PL9	C36-C37-C38	-2.11	104.96	111.88
24	b	608	CLA	CHA-C1A-NA	-2.11	121.58	126.40
24	B	608	CLA	O2D-CGD-CBD	2.11	115.01	111.27
32	c	516	DGD	CAB-C9B-C8B	-2.10	103.74	114.42
25	A	607	PHO	CHB-C1B-NB	2.10	128.96	124.58
24	A	608	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
24	d	401	CLA	CMA-C3A-C4A	-2.10	106.12	111.77
24	C	505	CLA	C11-C10-C8	-2.10	109.13	115.92
24	C	508	CLA	CMD-C2D-C3D	2.10	128.60	124.68
30	B	622	LHG	C18-C17-C16	-2.10	103.79	114.42
24	c	504	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
26	c	514	BCR	C36-C18-C17	-2.09	119.99	122.92
24	c	511	CLA	CMC-C2C-C3C	2.09	128.89	124.94
24	B	601	CLA	C4-C3-C5	2.09	118.79	115.27
24	B	603	CLA	CMC-C2C-C3C	2.09	128.89	124.94
28	d	406	PL9	C40-C39-C38	-2.09	118.31	123.68
24	B	606	CLA	O1A-CGA-CBA	2.09	131.89	123.73
26	t	101	BCR	C15-C14-C13	-2.09	124.33	127.31
31	a	614	SQD	C9-C8-C7	-2.09	106.02	113.62
24	C	511	CLA	C1-C2-C3	-2.09	122.43	126.04
24	D	403	CLA	O2D-CGD-CBD	2.09	114.98	111.27
32	c	516	DGD	C8B-C7B-C6B	-2.09	103.81	114.42
24	D	403	CLA	OBD-CAD-CBD	-2.09	122.91	125.89
24	C	507	CLA	C4D-C3D-CAD	-2.09	107.31	108.47
24	D	403	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	D	403	CLA	C11-C10-C8	-2.09	109.18	115.92
24	b	616	CLA	C2A-C3A-C4A	2.08	105.23	101.87
24	B	615	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	B	602	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	d	403	CLA	C4-C3-C5	2.08	118.77	115.27
29	d	410	LMG	C38-C37-C36	-2.08	103.86	114.42
30	e	102	LHG	C20-C19-C18	-2.08	103.86	114.42
28	D	405	PL9	C12-C13-C14	-2.08	122.65	127.66
24	b	609	CLA	CHB-C4A-NA	2.08	127.39	124.51
26	b	618	BCR	C7-C8-C9	-2.08	123.09	126.23
28	d	406	PL9	C35-C34-C36	2.08	118.77	115.27
26	C	515	BCR	C1-C6-C5	-2.08	119.69	122.61
24	C	511	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
32	A	618	DGD	O5E-C6E-C5E	-2.07	104.17	111.29
24	A	608	CLA	C1-C2-C3	-2.07	122.46	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	CMD-C2D-C3D	2.07	128.55	124.68
24	D	402	CLA	C3B-C4B-NB	-2.07	106.54	109.21
29	C	519	LMG	C40-C39-C38	-2.07	103.93	114.42
26	H	101	BCR	C38-C26-C25	-2.07	122.21	124.53
28	d	406	PL9	C17-C16-C14	2.07	119.78	112.98
24	b	605	CLA	C1-C2-C3	-2.06	122.47	126.04
24	D	403	CLA	OBD-CAD-C3D	2.06	131.41	127.98
26	k	101	BCR	C1-C6-C5	-2.06	119.71	122.61
32	c	517	DGD	CBB-CAB-C9B	-2.06	103.97	114.42
24	b	608	CLA	O2D-CGD-CBD	2.06	114.93	111.27
30	B	621	LHG	C18-C17-C16	-2.06	103.97	114.42
29	b	623	LMG	C38-C37-C36	-2.06	103.98	114.42
30	e	102	LHG	O8-C23-O10	-2.06	118.40	123.59
24	D	402	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
31	a	613	SQD	O4-C4-C3	-2.06	105.59	110.35
24	c	508	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
24	B	614	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	B	601	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
31	B	623	SQD	C1-C2-C3	-2.05	105.73	110.00
24	B	613	CLA	O1D-CGD-CBD	2.05	128.67	124.48
32	C	518	DGD	O5E-C6E-C5E	-2.05	104.27	111.29
26	B	619	BCR	C38-C26-C25	-2.05	122.23	124.53
30	l	101	LHG	C5-O7-C7	-2.05	112.75	117.79
26	Y	101	BCR	C1-C6-C5	-2.05	119.73	122.61
29	c	519	LMG	C40-C39-C38	-2.05	104.04	114.42
25	a	605	PHO	C3A-C4A-CHB	-2.05	118.29	121.83
24	B	609	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
30	l	101	LHG	C29-C28-C27	-2.04	104.05	114.42
24	B	611	CLA	O1D-CGD-CBD	2.04	128.66	124.48
24	B	611	CLA	C7-C6-C5	-2.04	107.81	113.36
24	C	512	CLA	C6-C5-C3	-2.04	108.10	113.45
32	c	518	DGD	CAB-C9B-C8B	-2.04	104.06	114.42
24	C	512	CLA	CMC-C2C-C3C	2.04	128.79	124.94
26	T	101	BCR	C4-C5-C6	2.04	125.69	122.73
24	b	605	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	c	504	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
24	c	503	CLA	CMC-C2C-C3C	2.04	128.78	124.94
32	C	516	DGD	C6B-C5B-C4B	-2.04	104.08	114.42
32	c	517	DGD	O2D-C2D-C1D	-2.04	105.10	110.05
24	b	608	CLA	CMC-C2C-C3C	2.04	128.78	124.94
32	c	518	DGD	C5B-C4B-C3B	-2.03	104.10	114.42
24	b	607	CLA	O2D-CGD-O1D	-2.03	119.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C2A-C1A-CHA	2.03	127.42	123.86
26	B	618	BCR	C2-C1-C6	2.03	113.61	110.48
28	a	611	PL9	C21-C19-C18	-2.03	117.01	121.12
24	b	611	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
24	B	604	CLA	C11-C10-C8	-2.03	109.36	115.92
26	H	101	BCR	C29-C30-C25	2.03	113.60	110.48
24	A	608	CLA	OBD-CAD-C3D	2.03	131.35	127.98
26	a	607	BCR	C8-C7-C6	-2.03	121.51	127.20
24	c	513	CLA	CMD-C2D-C3D	2.03	128.47	124.68
32	c	517	DGD	CDB-CCB-CBB	-2.02	104.14	114.42
24	B	608	CLA	CED-O2D-CGD	-2.02	111.36	115.94
31	A	617	SQD	O48-C23-O10	-2.02	118.48	123.59
24	b	615	CLA	C6-C5-C3	-2.02	108.15	113.45
25	A	606	PHO	O2D-CGD-CBD	2.02	114.86	111.27
31	f	101	SQD	O48-C23-C24	2.02	118.25	111.91
24	C	505	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	D	402	CLA	CBA-CAA-C2A	-2.02	107.90	113.86
24	C	510	CLA	CHB-C4A-NA	2.02	127.31	124.51
26	k	102	BCR	C1-C6-C5	-2.02	119.77	122.61
29	C	519	LMG	C6-C5-C4	-2.02	108.28	113.00
29	C	519	LMG	C38-C37-C36	-2.02	104.18	114.42
31	B	623	SQD	O9-S-O7	-2.02	106.96	113.95
26	A	609	BCR	C16-C15-C14	-2.02	119.34	123.47
26	B	617	BCR	C8-C7-C6	-2.02	121.54	127.20
30	B	621	LHG	O7-C7-O9	-2.02	118.83	123.70
32	C	517	DGD	C3D-C4D-C5D	-2.02	106.64	110.24
24	b	609	CLA	OBD-CAD-C3D	2.02	131.33	127.98
30	B	621	LHG	C27-C26-C25	-2.01	104.20	114.42
28	d	406	PL9	C32-C33-C34	-2.01	122.81	127.66
28	a	611	PL9	C26-C24-C23	-2.01	117.04	121.12
35	e	101	HEM	CMD-C2D-C1D	-2.01	125.37	128.46
24	B	613	CLA	OBD-CAD-CBD	-2.01	123.02	125.89
31	b	620	SQD	O48-C23-O10	-2.01	118.52	123.59
28	d	406	PL9	C12-C13-C14	-2.01	122.82	127.66
24	b	609	CLA	C7-C6-C5	-2.01	107.90	113.36
32	C	517	DGD	O2D-C2D-C1D	-2.01	105.16	110.05
24	B	607	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	b	615	CLA	CMD-C2D-C3D	2.01	128.44	124.68
32	h	101	DGD	O3G-C1D-C2D	-2.01	105.17	108.30
29	b	621	LMG	C22-C21-C20	-2.01	104.23	114.42
24	d	404	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
29	b	621	LMG	O8-C28-O10	-2.01	118.53	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	608	CLA	C3D-CAD-CBD	-2.01	104.96	107.61
24	A	604	CLA	C7-C6-C5	-2.01	107.91	113.36
29	D	406	LMG	C3-C4-C5	-2.01	106.66	110.24
32	A	618	DGD	C8B-C7B-C6B	-2.00	104.25	114.42
26	B	619	BCR	C3-C4-C5	-2.00	110.50	114.08
24	c	512	CLA	OBD-CAD-CBD	-2.00	123.03	125.89
29	c	522	LMG	C30-C29-C28	-2.00	106.34	113.62
24	b	614	CLA	O2A-C1-C2	-2.00	103.38	108.64
24	B	605	CLA	CMD-C2D-C3D	2.00	128.42	124.68

All (58) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	608	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	501	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	402	CLA	ND

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

All (1767) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	608	CLA	C2-C3-C5-C6
24	A	608	CLA	C4-C3-C5-C6
24	A	613	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C2C-C3C-CAC-CBC
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	C2-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	C	507	CLA	C11-C10-C8-C9
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	513	CLA	O2A-C1-C2-C3
24	a	612	CLA	CHA-CBD-CGD-O1D
24	a	612	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	C4-C3-C5-C6
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	C4-C3-C5-C6
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	CHA-CBD-CGD-O2D
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C35-C13-C14-C15
26	C	514	BCR	C11-C12-C13-C35
26	C	515	BCR	C11-C12-C13-C14
26	C	515	BCR	C36-C18-C19-C20
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	H	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C36-C18-C19-C20
26	K	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C11-C12-C13-C35
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C37-C22-C23-C24
26	b	617	BCR	C21-C22-C23-C24
26	b	619	BCR	C11-C12-C13-C35
26	b	619	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	c	514	BCR	C20-C21-C22-C37
26	d	405	BCR	C37-C22-C23-C24
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C7-C8-C9-C34
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
26	x	101	BCR	C7-C8-C9-C34
28	A	612	PL9	C9-C11-C12-C13
28	A	612	PL9	C12-C13-C14-C15
28	A	612	PL9	C12-C13-C14-C16
28	A	612	PL9	C22-C23-C24-C26
28	A	612	PL9	C37-C38-C39-C40
28	A	612	PL9	C37-C38-C39-C41
28	A	612	PL9	C40-C39-C41-C42
28	A	612	PL9	C43-C44-C46-C47
28	D	405	PL9	C32-C33-C34-C36
28	D	405	PL9	C33-C34-C36-C37
28	D	405	PL9	C37-C38-C39-C40
28	a	611	PL9	C12-C13-C14-C15
28	a	611	PL9	C17-C18-C19-C21
28	a	611	PL9	C20-C19-C21-C22
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C25-C24-C26-C27
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C35-C34-C36-C37
28	d	406	PL9	C32-C33-C34-C36
28	d	406	PL9	C38-C39-C41-C42
28	d	406	PL9	C40-C39-C41-C42
28	d	406	PL9	C42-C43-C44-C45
29	A	614	LMG	O9-C10-O7-C8
29	D	409	LMG	O1-C7-C8-C9
29	D	409	LMG	O1-C7-C8-O7
29	D	410	LMG	C28-C29-C30-C31
29	b	623	LMG	C11-C10-O7-C8
29	c	522	LMG	O6-C1-O1-C7
30	B	621	LHG	C4-O6-P-O3
30	B	621	LHG	C4-O6-P-O5
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	O2-C2-C3-O3
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C4-O6-P-O4
30	E	101	LHG	O1-C1-C2-C3
30	E	101	LHG	O10-C23-O8-C6
30	E	101	LHG	C24-C23-O8-C6
30	d	407	LHG	C3-O3-P-O4
30	d	408	LHG	O1-C1-C2-C3
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C4-O6-P-O4
30	d	409	LHG	C4-O6-P-O4
30	e	102	LHG	C1-C2-C3-O3
30	e	102	LHG	C3-O3-P-O5
30	e	102	LHG	C4-O6-P-O5
30	e	102	LHG	O6-C4-C5-O7
30	e	102	LHG	O10-C23-O8-C6
30	e	102	LHG	C24-C23-O8-C6
31	B	623	SQD	O5-C1-O6-C44
31	B	623	SQD	O6-C44-C45-O47
31	B	623	SQD	O49-C7-O47-C45
31	D	407	SQD	O5-C1-O6-C44
31	D	407	SQD	O10-C23-O48-C46
31	a	613	SQD	O6-C44-C45-O47
31	a	614	SQD	O6-C44-C45-C46
31	a	614	SQD	O6-C44-C45-O47
31	a	614	SQD	C8-C7-O47-C45
31	a	614	SQD	O10-C23-O48-C46
31	a	614	SQD	C24-C23-O48-C46
31	f	101	SQD	C2-C1-O6-C44
31	f	101	SQD	O5-C1-O6-C44
32	A	618	DGD	C2B-C1B-O2G-C2G
32	A	618	DGD	O1B-C1B-O2G-C2G
33	B	627	STE	C1-C2-C3-C4
33	C	520	STE	C1-C2-C3-C4
33	E	102	STE	C1-C2-C3-C4
33	J	101	STE	C1-C2-C3-C4
33	b	624	STE	C1-C2-C3-C4
33	d	412	STE	C1-C2-C3-C4
33	j	101	STE	C1-C2-C3-C4
33	m	101	STE	C1-C2-C3-C4
33	x	102	STE	C1-C2-C3-C4
24	B	614	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	CBD-CGD-O2D-CED
29	c	522	LMG	O10-C28-O8-C9
31	D	407	SQD	C24-C23-O48-C46
31	f	101	SQD	C24-C23-O48-C46
24	C	509	CLA	CBD-CGD-O2D-CED
29	M	101	LMG	O10-C28-O8-C9
29	c	521	LMG	O10-C28-O8-C9
31	f	101	SQD	O10-C23-O48-C46
29	D	409	LMG	O9-C10-O7-C8
29	b	623	LMG	O9-C10-O7-C8
31	a	614	SQD	O49-C7-O47-C45
24	B	614	CLA	C3-C5-C6-C7
29	c	522	LMG	C29-C28-O8-C9
31	b	620	SQD	C24-C23-O48-C46
29	A	614	LMG	C11-C10-O7-C8
29	a	618	LMG	C11-C10-O7-C8
31	B	623	SQD	C8-C7-O47-C45
28	A	612	PL9	C47-C48-C49-C51
24	C	511	CLA	CBD-CGD-O2D-CED
31	b	620	SQD	O10-C23-O48-C46
24	C	507	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	C	507	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	c	507	CLA	C2-C3-C5-C6
28	a	611	PL9	C23-C24-C26-C27
24	b	606	CLA	C2A-CAA-CBA-CGA
24	b	601	CLA	C3-C5-C6-C7
24	b	602	CLA	C3-C5-C6-C7
24	d	404	CLA	C3-C5-C6-C7
24	B	616	CLA	CBA-CGA-O2A-C1
29	c	521	LMG	C29-C28-O8-C9
28	A	612	PL9	C22-C23-C24-C25
28	d	406	PL9	C32-C33-C34-C35
24	C	501	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	O1D-CGD-O2D-CED
28	a	611	PL9	C42-C43-C44-C46
31	B	623	SQD	O10-C23-O48-C46
33	T	102	STE	C5-C6-C7-C8
30	e	102	LHG	O2-C2-C3-O3
24	B	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C11-C10-O7-C8
29	D	409	LMG	C11-C10-O7-C8
24	B	612	CLA	CBD-CGD-O2D-CED
24	c	508	CLA	CBD-CGD-O2D-CED
32	A	618	DGD	O6E-C5E-C6E-O5E
30	d	409	LHG	C24-C25-C26-C27
32	A	618	DGD	C4E-C5E-C6E-O5E
30	d	409	LHG	C30-C31-C32-C33
29	M	101	LMG	C29-C28-O8-C9
29	A	614	LMG	O6-C5-C6-O5
29	a	618	LMG	O6-C5-C6-O5
28	A	612	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C51
24	b	614	CLA	C4-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
28	A	612	PL9	C23-C24-C26-C27
28	a	611	PL9	C33-C34-C36-C37
24	B	616	CLA	O1A-CGA-O2A-C1
28	A	612	PL9	C34-C36-C37-C38
28	a	611	PL9	C19-C21-C22-C23
28	a	611	PL9	C34-C36-C37-C38
31	B	623	SQD	C24-C23-O48-C46
24	B	601	CLA	O1A-CGA-O2A-C1
29	A	614	LMG	C4-C5-C6-O5
33	C	522	STE	C4-C5-C6-C7
28	D	405	PL9	C27-C28-C29-C30
24	c	506	CLA	CBA-CGA-O2A-C1
32	C	518	DGD	C8A-C9A-CAA-CBA
33	D	411	STE	C11-C12-C13-C14
24	C	509	CLA	O1D-CGD-O2D-CED
24	B	611	CLA	C13-C15-C16-C17
24	C	513	CLA	C15-C16-C17-C18
29	d	410	LMG	C10-C11-C12-C13
29	c	522	LMG	C2-C1-O1-C7
31	B	623	SQD	C2-C1-O6-C44
31	D	407	SQD	C2-C1-O6-C44
29	a	618	LMG	C4-C5-C6-O5
24	A	605	CLA	C14-C13-C15-C16
24	B	610	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C14
24	B	614	CLA	C6-C7-C8-C9
24	B	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C12-C13-C14
24	b	601	CLA	C14-C13-C15-C16
24	b	602	CLA	C11-C10-C8-C9
24	b	613	CLA	C11-C12-C13-C14
24	b	616	CLA	C11-C10-C8-C9
24	c	509	CLA	C6-C7-C8-C9
24	c	509	CLA	C11-C12-C13-C14
24	c	512	CLA	C6-C7-C8-C9
24	d	404	CLA	C6-C7-C8-C9
24	C	510	CLA	C15-C16-C17-C18
24	B	606	CLA	C2A-CAA-CBA-CGA
26	A	609	BCR	C36-C18-C19-C20
26	A	609	BCR	C37-C22-C23-C24
26	B	619	BCR	C11-C12-C13-C35
26	B	619	BCR	C37-C22-C23-C24
26	C	515	BCR	C11-C12-C13-C35
26	b	618	BCR	C37-C22-C23-C24
26	k	101	BCR	C37-C22-C23-C24
33	d	412	STE	C7-C8-C9-C10
24	B	605	CLA	C15-C16-C17-C18
24	c	503	CLA	C8-C10-C11-C12
24	B	613	CLA	C8-C10-C11-C12
24	D	402	CLA	C15-C16-C17-C18
24	c	512	CLA	C13-C15-C16-C17
30	E	101	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
24	A	604	CLA	C15-C16-C17-C18
24	B	601	CLA	C5-C6-C7-C8
24	B	602	CLA	C13-C15-C16-C17
24	B	614	CLA	C13-C15-C16-C17
24	C	503	CLA	C5-C6-C7-C8
24	C	506	CLA	C8-C10-C11-C12
24	C	510	CLA	C10-C11-C12-C13
24	a	606	CLA	C15-C16-C17-C18
24	b	614	CLA	C5-C6-C7-C8
24	c	505	CLA	C5-C6-C7-C8
24	c	511	CLA	C15-C16-C17-C18
29	D	409	LMG	C28-C29-C30-C31
29	b	623	LMG	C28-C29-C30-C31
29	c	521	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	B	622	LHG	C23-C24-C25-C26
30	d	407	LHG	C23-C24-C25-C26
32	c	518	DGD	C1A-C2A-C3A-C4A
24	c	511	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C15-C16-C17-C18
24	B	609	CLA	C13-C15-C16-C17
24	B	616	CLA	C5-C6-C7-C8
24	a	606	CLA	C10-C11-C12-C13
24	b	611	CLA	C15-C16-C17-C18
24	c	509	CLA	C13-C15-C16-C17
31	B	623	SQD	C45-C46-O48-C23
31	B	623	SQD	C29-C30-C31-C32
28	A	612	PL9	C32-C33-C34-C36
24	B	612	CLA	C13-C15-C16-C17
24	C	508	CLA	C15-C16-C17-C18
24	b	615	CLA	C10-C11-C12-C13
29	D	406	LMG	C10-C11-C12-C13
29	c	519	LMG	C28-C29-C30-C31
30	d	407	LHG	C7-C8-C9-C10
29	c	521	LMG	C11-C10-O7-C8
24	b	611	CLA	C13-C15-C16-C17
24	c	511	CLA	C13-C15-C16-C17
24	A	605	CLA	C6-C7-C8-C10
24	B	611	CLA	C12-C13-C15-C16
24	b	603	CLA	C6-C7-C8-C10
24	b	613	CLA	C11-C10-C8-C7
24	c	505	CLA	C11-C10-C8-C7
24	C	506	CLA	C15-C16-C17-C18
24	b	607	CLA	C10-C11-C12-C13
24	c	506	CLA	C13-C15-C16-C17
24	c	509	CLA	C10-C11-C12-C13
24	c	512	CLA	C8-C10-C11-C12
24	C	512	CLA	C13-C15-C16-C17
28	A	612	PL9	C44-C46-C47-C48
29	d	410	LMG	C28-C29-C30-C31
30	e	102	LHG	C7-C8-C9-C10
26	B	619	BCR	C10-C11-C12-C13
26	c	514	BCR	C18-C19-C20-C21
30	d	407	LHG	O2-C2-C3-O3
24	C	509	CLA	C10-C11-C12-C13
24	C	512	CLA	C10-C11-C12-C13
24	D	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C15-C16-C17-C18
24	c	506	CLA	O1A-CGA-O2A-C1
29	b	621	LMG	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	b	601	CLA	C8-C10-C11-C12
24	b	611	CLA	C8-C10-C11-C12
24	b	615	CLA	C15-C16-C17-C18
24	b	607	CLA	C8-C10-C11-C12
24	c	503	CLA	C5-C6-C7-C8
30	A	615	LHG	C3-O3-P-O6
30	D	408	LHG	C3-O3-P-O6
30	D	408	LHG	C4-O6-P-O3
30	d	408	LHG	C3-O3-P-O6
30	d	408	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O3
32	c	516	DGD	C1A-C2A-C3A-C4A
29	a	618	LMG	C29-C28-O8-C9
31	D	407	SQD	C44-C45-C46-O48
32	c	518	DGD	O1A-C1A-O1G-C1G
30	d	407	LHG	C1-C2-C3-O3
29	M	101	LMG	O9-C10-O7-C8
30	e	102	LHG	O9-C7-O7-C5
24	a	606	CLA	C5-C6-C7-C8
24	B	606	CLA	C16-C17-C18-C19
24	C	513	CLA	CBA-CGA-O2A-C1
26	c	514	BCR	C13-C14-C15-C16
29	c	521	LMG	C33-C34-C35-C36
33	T	102	STE	C7-C8-C9-C10
31	b	620	SQD	C8-C7-O47-C45
24	b	614	CLA	C8-C10-C11-C12
26	A	609	BCR	C11-C10-C9-C34
26	A	609	BCR	C35-C13-C14-C15
26	A	609	BCR	C20-C21-C22-C37
26	B	617	BCR	C11-C10-C9-C34
26	D	404	BCR	C20-C21-C22-C37
26	K	101	BCR	C11-C10-C9-C34
26	b	617	BCR	C20-C21-C22-C37
26	b	618	BCR	C16-C17-C18-C36
26	c	514	BCR	C16-C17-C18-C36
26	k	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
29	a	618	LMG	C12-C13-C14-C15
30	A	615	LHG	C11-C12-C13-C14
30	B	621	LHG	C31-C32-C33-C34
30	E	101	LHG	C9-C10-C11-C12
30	d	407	LHG	C10-C11-C12-C13
31	a	614	SQD	C12-C13-C14-C15
32	c	516	DGD	C7A-C8A-C9A-CAA
33	B	620	STE	C4-C5-C6-C7
33	T	103	STE	C13-C14-C15-C16
33	b	627	STE	C11-C12-C13-C14
33	t	102	STE	C2-C3-C4-C5
24	B	614	CLA	C16-C17-C18-C20
24	B	615	CLA	C16-C17-C18-C20
24	D	403	CLA	C16-C17-C18-C19
24	a	604	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C19
29	b	621	LMG	C32-C33-C34-C35
29	c	519	LMG	C33-C34-C35-C36
29	c	521	LMG	C40-C41-C42-C43
29	c	522	LMG	C12-C13-C14-C15
29	d	410	LMG	C36-C37-C38-C39
30	D	408	LHG	C30-C31-C32-C33
30	E	101	LHG	C27-C28-C29-C30
30	d	408	LHG	C32-C33-C34-C35
31	a	614	SQD	C10-C11-C12-C13
32	c	517	DGD	CCA-CDA-CEA-CFA
32	c	517	DGD	CAB-CBB-CCB-CDB
32	c	517	DGD	CBB-CCB-CDB-CEB
32	h	101	DGD	C9A-CAA-CBA-CCA
32	h	101	DGD	C5B-C6B-C7B-C8B
33	C	520	STE	C6-C7-C8-C9
33	x	102	STE	C11-C12-C13-C14
24	b	603	CLA	C13-C15-C16-C17
29	A	614	LMG	C13-C14-C15-C16
29	M	101	LMG	C36-C37-C38-C39
29	c	519	LMG	C39-C40-C41-C42
29	c	521	LMG	C30-C31-C32-C33
30	E	101	LHG	C28-C29-C30-C31
31	a	613	SQD	C25-C26-C27-C28
33	T	102	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	b	627	STE	C9-C10-C11-C12
29	A	614	LMG	C14-C15-C16-C17
29	D	410	LMG	C14-C15-C16-C17
29	a	618	LMG	C36-C37-C38-C39
30	A	615	LHG	C12-C13-C14-C15
33	B	626	STE	C4-C5-C6-C7
33	b	624	STE	C10-C11-C12-C13
33	b	625	STE	C4-C5-C6-C7
33	l	102	STE	C14-C15-C16-C17
24	C	511	CLA	O1D-CGD-O2D-CED
29	b	623	LMG	C11-C12-C13-C14
29	d	410	LMG	C33-C34-C35-C36
30	A	615	LHG	C32-C33-C34-C35
30	B	621	LHG	C12-C13-C14-C15
30	B	621	LHG	C17-C18-C19-C20
30	E	101	LHG	C33-C34-C35-C36
32	C	518	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	C8B-C9B-CAB-CBB
33	M	102	STE	C11-C10-C9-C8
26	B	618	BCR	C20-C21-C22-C23
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C12-C13-C14-C15
26	C	514	BCR	C11-C10-C9-C8
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C20-C21-C22-C23
26	T	101	BCR	C12-C13-C14-C15
26	b	617	BCR	C20-C21-C22-C23
26	b	618	BCR	C20-C21-C22-C23
26	c	514	BCR	C20-C21-C22-C23
26	k	101	BCR	C11-C10-C9-C8
26	k	102	BCR	C11-C10-C9-C8
26	x	101	BCR	C11-C10-C9-C8
26	x	101	BCR	C12-C13-C14-C15
26	x	101	BCR	C16-C17-C18-C19
32	C	517	DGD	C2E-C1E-O5D-C6D
32	c	517	DGD	C2E-C1E-O5D-C6D
29	d	410	LMG	C32-C33-C34-C35
30	E	101	LHG	C24-C25-C26-C27
32	c	516	DGD	C4B-C5B-C6B-C7B
33	b	627	STE	C7-C8-C9-C10
33	d	412	STE	C14-C15-C16-C17
33	k	103	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
33	k	103	STE	C6-C7-C8-C9
33	t	102	STE	C5-C6-C7-C8
24	B	611	CLA	C8-C10-C11-C12
24	b	607	CLA	C16-C17-C18-C20
24	c	504	CLA	C11-C12-C13-C14
24	d	403	CLA	C16-C17-C18-C20
24	C	501	CLA	O1D-CGD-O2D-CED
29	A	614	LMG	C17-C18-C19-C20
29	b	621	LMG	C14-C15-C16-C17
29	c	521	LMG	C39-C40-C41-C42
29	c	521	LMG	C41-C42-C43-C44
30	l	101	LHG	C29-C30-C31-C32
32	C	516	DGD	C3B-C4B-C5B-C6B
32	H	102	DGD	C6B-C7B-C8B-C9B
32	H	102	DGD	CCB-CDB-CEB-CFB
32	c	517	DGD	C7B-C8B-C9B-CAB
33	B	624	STE	C6-C7-C8-C9
33	D	411	STE	C2-C3-C4-C5
33	H	103	STE	C11-C12-C13-C14
33	b	622	STE	C14-C15-C16-C17
24	B	606	CLA	C11-C12-C13-C14
24	C	503	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	a	606	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
25	A	607	PHO	C6-C7-C8-C9
29	b	623	LMG	C10-C11-C12-C13
32	c	516	DGD	C1B-C2B-C3B-C4B
29	D	410	LMG	C30-C31-C32-C33
29	a	618	LMG	C13-C14-C15-C16
29	b	621	LMG	C33-C34-C35-C36
29	c	519	LMG	C38-C39-C40-C41
30	d	407	LHG	C30-C31-C32-C33
30	d	409	LHG	C26-C27-C28-C29
30	d	409	LHG	C32-C33-C34-C35
31	A	616	SQD	C9-C10-C11-C12
31	B	623	SQD	C34-C35-C36-C37
32	A	618	DGD	C5B-C6B-C7B-C8B
32	C	516	DGD	C8A-C9A-CAA-CBA
32	C	517	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	C6A-C7A-C8A-C9A
33	C	521	STE	C7-C8-C9-C10
24	C	505	CLA	C10-C11-C12-C13
24	b	607	CLA	C5-C6-C7-C8
24	c	512	CLA	C2A-CAA-CBA-CGA
26	k	101	BCR	C36-C18-C19-C20
29	A	614	LMG	C38-C39-C40-C41
29	c	521	LMG	C16-C17-C18-C19
30	B	622	LHG	C29-C30-C31-C32
30	e	102	LHG	C26-C27-C28-C29
31	B	623	SQD	C33-C34-C35-C36
31	a	613	SQD	C24-C25-C26-C27
32	c	516	DGD	C5B-C6B-C7B-C8B
33	d	411	STE	C4-C5-C6-C7
33	j	101	STE	C4-C5-C6-C7
30	d	407	LHG	O1-C1-C2-C3
30	d	409	LHG	O1-C1-C2-C3
26	C	514	BCR	C11-C12-C13-C14
26	T	101	BCR	C7-C8-C9-C10
26	Y	101	BCR	C21-C22-C23-C24
29	c	521	LMG	O9-C10-O7-C8
24	C	505	CLA	C5-C6-C7-C8
29	c	522	LMG	C11-C10-O7-C8
29	b	623	LMG	C13-C14-C15-C16
31	A	616	SQD	C30-C31-C32-C33
31	B	623	SQD	C11-C12-C13-C14
31	f	101	SQD	C29-C30-C31-C32
32	C	516	DGD	CCB-CDB-CEB-CFB
33	a	617	STE	C5-C6-C7-C8
29	A	614	LMG	C28-C29-C30-C31
29	A	614	LMG	C31-C32-C33-C34
29	D	406	LMG	C17-C18-C19-C20
29	M	101	LMG	C17-C18-C19-C20
29	M	101	LMG	C29-C30-C31-C32
29	b	623	LMG	C21-C22-C23-C24
29	b	623	LMG	C41-C42-C43-C44
29	d	410	LMG	C30-C31-C32-C33
30	A	615	LHG	C27-C28-C29-C30
30	B	622	LHG	C27-C28-C29-C30
30	D	408	LHG	C11-C12-C13-C14
30	D	408	LHG	C34-C35-C36-C37
30	d	408	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	A	618	DGD	C2A-C3A-C4A-C5A
32	A	618	DGD	C4B-C5B-C6B-C7B
32	C	517	DGD	C9A-CAA-CBA-CCA
32	C	517	DGD	CAB-CBB-CCB-CDB
32	c	516	DGD	C2A-C3A-C4A-C5A
32	c	518	DGD	C3A-C4A-C5A-C6A
33	B	620	STE	C11-C12-C13-C14
33	H	103	STE	C10-C11-C12-C13
33	J	101	STE	C5-C6-C7-C8
33	T	103	STE	C5-C6-C7-C8
33	b	625	STE	C5-C6-C7-C8
33	c	520	STE	C9-C10-C11-C12
33	d	412	STE	C9-C10-C11-C12
24	a	604	CLA	C16-C17-C18-C20
24	b	601	CLA	C16-C17-C18-C20
24	c	511	CLA	C16-C17-C18-C20
32	C	517	DGD	O6E-C1E-O5D-C6D
32	c	517	DGD	O6E-C1E-O5D-C6D
24	b	613	CLA	C13-C15-C16-C17
24	c	506	CLA	C8-C10-C11-C12
24	d	401	CLA	C8-C10-C11-C12
29	A	614	LMG	C11-C12-C13-C14
29	A	614	LMG	C35-C36-C37-C38
29	C	519	LMG	C32-C33-C34-C35
30	l	101	LHG	C14-C15-C16-C17
31	a	613	SQD	C34-C35-C36-C37
32	H	102	DGD	C5B-C6B-C7B-C8B
33	B	626	STE	C5-C6-C7-C8
33	B	626	STE	C14-C15-C16-C17
33	x	102	STE	C3-C4-C5-C6
29	A	614	LMG	C16-C17-C18-C19
29	D	410	LMG	C29-C30-C31-C32
29	M	101	LMG	C11-C12-C13-C14
29	c	522	LMG	C15-C16-C17-C18
30	d	408	LHG	C29-C30-C31-C32
30	e	102	LHG	C16-C17-C18-C19
31	D	407	SQD	C32-C33-C34-C35
32	h	101	DGD	CCA-CDA-CEA-CFA
33	B	620	STE	C9-C10-C11-C12
33	a	617	STE	C12-C13-C14-C15
33	b	625	STE	C7-C8-C9-C10
29	M	101	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	B	622	LHG	C7-C8-C9-C10
29	A	614	LMG	C36-C37-C38-C39
29	b	621	LMG	C12-C13-C14-C15
30	D	408	LHG	C25-C26-C27-C28
31	a	614	SQD	C11-C12-C13-C14
32	h	101	DGD	C6B-C7B-C8B-C9B
33	C	522	STE	C6-C7-C8-C9
33	H	103	STE	C13-C14-C15-C16
33	d	411	STE	C10-C11-C12-C13
33	d	411	STE	C11-C12-C13-C14
29	d	410	LMG	O6-C5-C6-O5
29	b	621	LMG	C29-C28-O8-C9
29	c	522	LMG	C33-C34-C35-C36
30	A	615	LHG	C29-C30-C31-C32
32	H	102	DGD	C7A-C8A-C9A-CAA
24	B	612	CLA	O1D-CGD-O2D-CED
24	c	512	CLA	C3A-C2A-CAA-CBA
31	D	407	SQD	C45-C44-O6-C1
29	A	614	LMG	C33-C34-C35-C36
29	M	101	LMG	C14-C15-C16-C17
29	b	621	LMG	C18-C19-C20-C21
29	c	521	LMG	C14-C15-C16-C17
29	c	522	LMG	C30-C31-C32-C33
30	e	102	LHG	C11-C10-C9-C8
31	B	623	SQD	C28-C29-C30-C31
32	C	516	DGD	C5B-C6B-C7B-C8B
32	c	516	DGD	C3A-C4A-C5A-C6A
33	B	627	STE	C5-C6-C7-C8
33	E	102	STE	C3-C4-C5-C6
29	a	618	LMG	O10-C28-O8-C9
24	B	607	CLA	C16-C17-C18-C20
29	b	623	LMG	C37-C38-C39-C40
32	C	517	DGD	C5A-C6A-C7A-C8A
33	a	617	STE	C10-C11-C12-C13
33	c	520	STE	C2-C3-C4-C5
24	c	508	CLA	O1D-CGD-O2D-CED
29	c	521	LMG	C31-C32-C33-C34
30	A	615	LHG	C30-C31-C32-C33
33	t	102	STE	C7-C8-C9-C10
33	x	102	STE	C6-C7-C8-C9
26	C	514	BCR	C14-C15-C16-C17
32	c	517	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
29	D	409	LMG	C14-C15-C16-C17
33	t	102	STE	C11-C12-C13-C14
24	C	505	CLA	C4-C3-C5-C6
24	c	505	CLA	C4-C3-C5-C6
24	c	505	CLA	C2-C3-C5-C6
31	b	620	SQD	C25-C26-C27-C28
30	D	408	LHG	O1-C1-C2-O2
30	E	101	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
29	D	409	LMG	C31-C32-C33-C34
29	D	410	LMG	C16-C17-C18-C19
29	b	621	LMG	C17-C18-C19-C20
31	a	613	SQD	C29-C30-C31-C32
33	H	103	STE	C2-C3-C4-C5
33	t	102	STE	C4-C5-C6-C7
32	h	101	DGD	O6E-C5E-C6E-O5E
24	B	606	CLA	C16-C17-C18-C20
24	B	614	CLA	C16-C17-C18-C19
24	C	509	CLA	C16-C17-C18-C19
33	T	103	STE	C11-C10-C9-C8
29	c	522	LMG	C17-C18-C19-C20
30	e	102	LHG	C27-C28-C29-C30
33	B	624	STE	C11-C10-C9-C8
24	C	510	CLA	CBD-CGD-O2D-CED
29	b	623	LMG	C16-C17-C18-C19
29	c	519	LMG	C36-C37-C38-C39
30	B	621	LHG	C14-C15-C16-C17
30	e	102	LHG	C18-C19-C20-C21
32	A	618	DGD	C5A-C6A-C7A-C8A
33	T	103	STE	C6-C7-C8-C9
30	e	102	LHG	C13-C14-C15-C16
32	A	618	DGD	CAA-CBA-CCA-CDA
32	H	102	DGD	C7B-C8B-C9B-CAB
33	T	103	STE	C14-C15-C16-C17
24	B	603	CLA	C8-C10-C11-C12
24	B	612	CLA	C10-C11-C12-C13
24	C	513	CLA	O1A-CGA-O2A-C1
29	C	519	LMG	C15-C16-C17-C18
29	D	406	LMG	C32-C33-C34-C35
29	a	618	LMG	C35-C36-C37-C38
30	A	615	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	B	622	LHG	C14-C15-C16-C17
30	d	407	LHG	C25-C26-C27-C28
30	l	101	LHG	C27-C28-C29-C30
31	D	407	SQD	C31-C32-C33-C34
24	C	512	CLA	C3-C5-C6-C7
26	B	617	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	Y	101	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C30
26	k	101	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
31	a	613	SQD	C17-C18-C19-C20
29	M	101	LMG	C11-C10-O7-C8
30	e	102	LHG	C8-C7-O7-C5
29	b	621	LMG	C30-C31-C32-C33
29	b	623	LMG	C23-C24-C25-C26
30	B	621	LHG	C29-C30-C31-C32
30	B	622	LHG	C28-C29-C30-C31
32	C	517	DGD	CBA-CCA-CDA-CEA
32	h	101	DGD	C2B-C3B-C4B-C5B
29	b	621	LMG	C16-C17-C18-C19
32	C	518	DGD	CBA-CCA-CDA-CEA
32	c	517	DGD	C7A-C8A-C9A-CAA
33	b	622	STE	C5-C6-C7-C8
24	A	613	CLA	C13-C15-C16-C17
30	B	621	LHG	C27-C28-C29-C30
28	D	405	PL9	C45-C44-C46-C47
28	a	611	PL9	C40-C39-C41-C42
24	A	604	CLA	C12-C13-C15-C16
24	B	602	CLA	C11-C12-C13-C15
24	B	606	CLA	C11-C12-C13-C15
24	B	614	CLA	C6-C7-C8-C10
24	C	505	CLA	C2-C3-C5-C6
24	C	512	CLA	C11-C12-C13-C15
24	a	606	CLA	C11-C10-C8-C7
24	b	601	CLA	C11-C12-C13-C15
24	c	504	CLA	C11-C10-C8-C7
24	c	511	CLA	C12-C13-C15-C16
24	d	401	CLA	C6-C7-C8-C10
28	a	611	PL9	C38-C39-C41-C42
24	A	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	b	602	CLA	C8-C10-C11-C12
31	f	101	SQD	O49-C7-O47-C45
31	a	613	SQD	C24-C23-O48-C46
24	C	513	CLA	C5-C6-C7-C8
24	b	604	CLA	C5-C6-C7-C8
29	D	406	LMG	C30-C31-C32-C33
29	D	409	LMG	C15-C16-C17-C18
30	B	621	LHG	C34-C35-C36-C37
32	c	518	DGD	C8B-C9B-CAB-CBB
29	D	409	LMG	C16-C17-C18-C19
29	c	522	LMG	C37-C38-C39-C40
30	E	101	LHG	C32-C33-C34-C35
30	d	408	LHG	C28-C29-C30-C31
32	C	517	DGD	C6A-C7A-C8A-C9A
33	B	625	STE	C3-C4-C5-C6
29	C	519	LMG	C17-C18-C19-C20
32	C	517	DGD	C4A-C5A-C6A-C7A
32	c	516	DGD	CBB-CCB-CDB-CEB
24	b	609	CLA	CBD-CGD-O2D-CED
24	b	616	CLA	C11-C12-C13-C14
24	c	512	CLA	C16-C17-C18-C19
32	c	517	DGD	C8B-C9B-CAB-CBB
32	h	101	DGD	C3B-C4B-C5B-C6B
33	b	622	STE	C7-C8-C9-C10
33	d	412	STE	C12-C13-C14-C15
32	c	517	DGD	C1A-C2A-C3A-C4A
26	c	514	BCR	C10-C11-C12-C13
30	D	408	LHG	C17-C18-C19-C20
32	C	518	DGD	C5A-C6A-C7A-C8A
33	D	411	STE	C5-C6-C7-C8
26	b	617	BCR	C14-C15-C16-C17
29	b	621	LMG	O9-C10-O7-C8
29	c	522	LMG	O9-C10-O7-C8
30	d	407	LHG	C14-C15-C16-C17
33	a	617	STE	C11-C12-C13-C14
31	A	616	SQD	O6-C44-C45-O47
32	A	618	DGD	O2G-C2G-C3G-O3G
29	b	623	LMG	C32-C33-C34-C35
30	A	615	LHG	C25-C26-C27-C28
24	D	403	CLA	C16-C17-C18-C20
29	C	519	LMG	C16-C17-C18-C19
29	C	519	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	B	623	SQD	C9-C10-C11-C12
32	C	516	DGD	C3A-C4A-C5A-C6A
33	d	412	STE	C2-C3-C4-C5
29	b	623	LMG	O6-C5-C6-O5
28	A	612	PL9	C18-C19-C21-C22
29	a	618	LMG	C30-C31-C32-C33
32	c	516	DGD	C6B-C7B-C8B-C9B
24	A	604	CLA	C14-C13-C15-C16
24	A	605	CLA	C6-C7-C8-C9
24	B	602	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
24	C	510	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	b	601	CLA	C11-C12-C13-C14
24	c	504	CLA	C11-C10-C8-C9
24	c	505	CLA	C11-C10-C8-C9
24	d	401	CLA	C6-C7-C8-C9
29	M	101	LMG	C31-C32-C33-C34
32	h	101	DGD	C7A-C8A-C9A-CAA
24	B	605	CLA	C3-C5-C6-C7
24	B	616	CLA	C3-C5-C6-C7
32	A	618	DGD	CEB-CFB-CGB-CHB
33	b	627	STE	C10-C11-C12-C13
29	D	406	LMG	O6-C5-C6-O5
24	B	608	CLA	C15-C16-C17-C18
24	c	507	CLA	C5-C6-C7-C8
30	E	101	LHG	C11-C12-C13-C14
24	c	513	CLA	C1A-C2A-CAA-CBA
24	b	616	CLA	C11-C12-C13-C15
24	c	510	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C20
29	C	519	LMG	O9-C10-O7-C8
29	a	618	LMG	O9-C10-O7-C8
31	a	613	SQD	C18-C19-C20-C21
32	A	618	DGD	C9B-CAB-CBB-CCB
32	C	516	DGD	C8B-C9B-CAB-CBB
32	C	517	DGD	C9B-CAB-CBB-CCB
33	B	627	STE	C2-C3-C4-C5
24	C	509	CLA	C5-C6-C7-C8
30	d	407	LHG	C3-O3-P-O6
30	e	102	LHG	C3-O3-P-O6
30	B	621	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	a	613	SQD	C23-C24-C25-C26
30	B	621	LHG	O6-C4-C5-C6
29	b	621	LMG	C37-C38-C39-C40
33	C	522	STE	C5-C6-C7-C8
31	D	407	SQD	C30-C31-C32-C33
24	C	509	CLA	C16-C17-C18-C20
29	b	621	LMG	C11-C12-C13-C14
31	A	616	SQD	C16-C17-C18-C19
33	C	521	STE	C4-C5-C6-C7
33	E	102	STE	C4-C5-C6-C7
33	b	622	STE	C13-C14-C15-C16
32	C	516	DGD	O6E-C5E-C6E-O5E
29	b	621	LMG	C39-C40-C41-C42
30	E	101	LHG	C16-C17-C18-C19
32	A	618	DGD	C2B-C3B-C4B-C5B
33	B	626	STE	C6-C7-C8-C9
24	B	605	CLA	C8-C10-C11-C12
29	c	521	LMG	C11-C12-C13-C14
29	c	522	LMG	C31-C32-C33-C34
28	d	406	PL9	C45-C44-C46-C47
29	c	521	LMG	C34-C35-C36-C37
29	c	521	LMG	C38-C39-C40-C41
30	D	408	LHG	C28-C29-C30-C31
33	d	411	STE	C5-C6-C7-C8
24	b	609	CLA	C15-C16-C17-C18
31	b	620	SQD	C27-C28-C29-C30
32	C	518	DGD	CAB-CBB-CCB-CDB
33	Z	101	STE	C12-C13-C14-C15
29	b	623	LMG	O10-C28-O8-C9
29	A	614	LMG	C34-C35-C36-C37
30	B	622	LHG	C18-C19-C20-C21
33	J	101	STE	C6-C7-C8-C9
33	a	615	STE	C5-C6-C7-C8
24	B	616	CLA	C11-C12-C13-C15
24	b	607	CLA	C16-C17-C18-C19
29	M	101	LMG	C7-C8-C9-O8
29	c	521	LMG	O1-C7-C8-C9
29	c	522	LMG	O1-C7-C8-C9
30	l	101	LHG	C13-C14-C15-C16
31	A	616	SQD	O6-C44-C45-C46
31	B	623	SQD	O6-C44-C45-C46
31	a	613	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
31	b	620	SQD	C44-C45-C46-O48
32	A	618	DGD	C1G-C2G-C3G-O3G
32	C	518	DGD	CDA-CEA-CFA-CGA
32	c	516	DGD	O1G-C1G-C2G-C3G
33	T	102	STE	C9-C10-C11-C12
24	b	601	CLA	C13-C15-C16-C17
24	b	615	CLA	C5-C6-C7-C8
29	D	406	LMG	C34-C35-C36-C37
30	B	622	LHG	C19-C20-C21-C22
33	b	626	STE	C4-C5-C6-C7
29	a	618	LMG	C8-C7-O1-C1
32	C	517	DGD	C2G-C3G-O3G-C1D
32	c	517	DGD	C5D-C6D-O5D-C1E
31	B	623	SQD	C13-C14-C15-C16
31	a	614	SQD	C31-C32-C33-C34
32	C	518	DGD	CCA-CDA-CEA-CFA
32	c	516	DGD	C3B-C4B-C5B-C6B
33	B	620	STE	C2-C3-C4-C5
33	b	622	STE	C10-C11-C12-C13
24	D	402	CLA	C10-C11-C12-C13
24	b	614	CLA	C15-C16-C17-C18
29	b	621	LMG	C22-C23-C24-C25
33	T	103	STE	C11-C12-C13-C14
33	a	615	STE	C2-C3-C4-C5
30	E	101	LHG	C19-C20-C21-C22
33	B	625	STE	C7-C8-C9-C10
33	C	521	STE	C3-C4-C5-C6
33	d	412	STE	C6-C7-C8-C9
33	m	101	STE	C7-C8-C9-C10
24	C	509	CLA	C8-C10-C11-C12
29	a	618	LMG	C16-C17-C18-C19
29	c	519	LMG	C31-C32-C33-C34
31	A	616	SQD	C17-C18-C19-C20
31	D	407	SQD	C27-C28-C29-C30
31	a	613	SQD	C27-C28-C29-C30
32	C	516	DGD	C2A-C3A-C4A-C5A
32	C	517	DGD	CDB-CEB-CFB-CGB
32	H	102	DGD	CDB-CEB-CFB-CGB
32	c	518	DGD	C5B-C6B-C7B-C8B
33	M	102	STE	C9-C10-C11-C12
28	a	611	PL9	C42-C43-C44-C45
32	c	518	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
32	h	101	DGD	CBA-CCA-CDA-CEA
24	b	601	CLA	C10-C11-C12-C13
24	d	404	CLA	C13-C15-C16-C17
26	D	404	BCR	C11-C10-C9-C34
32	c	516	DGD	O6E-C5E-C6E-O5E
28	a	611	PL9	C45-C44-C46-C47
29	C	519	LMG	C31-C32-C33-C34
29	D	409	LMG	C34-C35-C36-C37
29	b	623	LMG	C42-C43-C44-C45
30	D	408	LHG	C33-C34-C35-C36
31	B	623	SQD	C35-C36-C37-C38
33	b	624	STE	C6-C7-C8-C9
24	B	607	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C19
24	c	512	CLA	CBA-CGA-O2A-C1
30	e	102	LHG	C28-C29-C30-C31
24	b	609	CLA	O1D-CGD-O2D-CED
29	b	621	LMG	C38-C39-C40-C41
32	C	516	DGD	C9B-CAB-CBB-CCB
29	a	618	LMG	C9-C8-O7-C10
30	d	408	LHG	C12-C13-C14-C15
29	a	618	LMG	C34-C35-C36-C37
29	b	623	LMG	C22-C23-C24-C25
33	b	625	STE	C11-C10-C9-C8
24	c	510	CLA	C8-C10-C11-C12
29	a	618	LMG	C33-C34-C35-C36
30	B	621	LHG	C30-C31-C32-C33
24	B	613	CLA	C16-C17-C18-C20
29	a	618	LMG	C17-C18-C19-C20
31	b	620	SQD	C19-C20-C21-C22
33	Z	101	STE	C13-C14-C15-C16
33	d	412	STE	C5-C6-C7-C8
24	C	506	CLA	C13-C15-C16-C17
29	D	406	LMG	C38-C39-C40-C41
24	C	510	CLA	O1D-CGD-O2D-CED
29	A	614	LMG	C40-C41-C42-C43
33	b	625	STE	C3-C4-C5-C6
24	b	612	CLA	C10-C11-C12-C13
24	c	504	CLA	C5-C6-C7-C8
26	a	607	BCR	C12-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C19
33	C	520	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
33	T	102	STE	C15-C16-C17-C18
31	a	613	SQD	O47-C45-C46-O48
29	b	623	LMG	C18-C19-C20-C21
30	B	622	LHG	C25-C26-C27-C28
32	H	102	DGD	CCA-CDA-CEA-CFA
33	I	101	STE	C4-C5-C6-C7
32	C	516	DGD	O6D-C5D-C6D-O5D
29	A	614	LMG	C30-C31-C32-C33
29	D	406	LMG	C14-C15-C16-C17
30	d	407	LHG	C28-C29-C30-C31
31	b	620	SQD	C11-C12-C13-C14
32	C	517	DGD	C6B-C7B-C8B-C9B
32	h	101	DGD	C5A-C6A-C7A-C8A
28	a	611	PL9	C17-C18-C19-C20
32	c	517	DGD	C5B-C6B-C7B-C8B
32	h	101	DGD	CAB-CBB-CCB-CDB
24	B	610	CLA	C15-C16-C17-C18
24	A	605	CLA	C11-C12-C13-C15
24	A	605	CLA	C12-C13-C15-C16
24	B	603	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	510	CLA	C12-C13-C15-C16
24	C	512	CLA	C12-C13-C15-C16
24	b	601	CLA	C12-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C10
24	b	614	CLA	C12-C13-C15-C16
24	c	505	CLA	C6-C7-C8-C10
24	c	505	CLA	C12-C13-C15-C16
24	c	513	CLA	C11-C12-C13-C15
24	d	401	CLA	C11-C10-C8-C7
24	d	404	CLA	C11-C12-C13-C15
24	d	404	CLA	C12-C13-C15-C16
29	D	406	LMG	C21-C22-C23-C24
32	C	518	DGD	C8B-C9B-CAB-CBB
24	A	605	CLA	C11-C12-C13-C14
24	A	613	CLA	C14-C13-C15-C16
24	B	603	CLA	C14-C13-C15-C16
24	B	604	CLA	C11-C12-C13-C14
24	C	509	CLA	C11-C12-C13-C14
24	D	402	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	a	604	CLA	C14-C13-C15-C16
24	b	603	CLA	C11-C12-C13-C14
24	b	604	CLA	C14-C13-C15-C16
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	607	CLA	C14-C13-C15-C16
24	b	609	CLA	C14-C13-C15-C16
24	b	613	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	c	510	CLA	C11-C10-C8-C9
24	d	401	CLA	C11-C10-C8-C9
24	d	404	CLA	C11-C12-C13-C14
24	d	404	CLA	C14-C13-C15-C16
30	d	407	LHG	C15-C16-C17-C18
30	e	102	LHG	C10-C11-C12-C13
33	M	102	STE	C4-C5-C6-C7
24	C	512	CLA	C15-C16-C17-C18
24	C	507	CLA	C16-C17-C18-C20
26	k	101	BCR	C17-C18-C19-C20
29	a	618	LMG	C23-C24-C25-C26
31	a	614	SQD	C19-C20-C21-C22
29	c	522	LMG	C8-C9-O8-C28
30	d	408	LHG	O9-C7-O7-C5
24	C	507	CLA	C10-C11-C12-C13
32	C	516	DGD	CDA-CEA-CFA-CGA
33	T	102	STE	C3-C4-C5-C6
29	b	621	LMG	C20-C21-C22-C23
33	E	102	STE	C6-C7-C8-C9
24	C	512	CLA	C8-C10-C11-C12
24	D	403	CLA	C5-C6-C7-C8
29	M	101	LMG	C38-C39-C40-C41
30	D	408	LHG	C11-C10-C9-C8
30	E	101	LHG	C29-C30-C31-C32
30	e	102	LHG	C14-C15-C16-C17
31	a	613	SQD	C28-C29-C30-C31
32	C	516	DGD	CBA-CCA-CDA-CEA
32	c	516	DGD	O6D-C5D-C6D-O5D
32	c	517	DGD	C9B-CAB-CBB-CCB
24	b	601	CLA	C16-C17-C18-C19
30	e	102	LHG	O6-C4-C5-C6
29	C	519	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	b	622	STE	C4-C5-C6-C7
29	c	519	LMG	O6-C5-C6-O5
29	c	519	LMG	C4-C5-C6-O5
29	M	101	LMG	C39-C40-C41-C42
32	C	517	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	CDA-CEA-CFA-CGA
33	b	624	STE	C11-C10-C9-C8
33	l	102	STE	C2-C3-C4-C5
24	c	511	CLA	O1D-CGD-O2D-CED
30	E	101	LHG	O2-C2-C3-O3
30	B	621	LHG	O9-C7-O7-C5
24	c	512	CLA	O1A-CGA-O2A-C1
31	a	614	SQD	C17-C18-C19-C20
33	T	103	STE	C7-C8-C9-C10
33	j	101	STE	C2-C3-C4-C5
24	C	509	CLA	C3-C5-C6-C7
24	b	604	CLA	C13-C15-C16-C17
29	C	519	LMG	C29-C28-O8-C9
32	c	517	DGD	C5A-C6A-C7A-C8A
32	c	516	DGD	O1A-C1A-O1G-C1G
31	a	613	SQD	C11-C10-C9-C8
33	b	625	STE	C6-C7-C8-C9
26	T	101	BCR	C13-C14-C15-C16
33	d	412	STE	C4-C5-C6-C7
24	B	616	CLA	C11-C12-C13-C14
24	C	507	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
30	d	407	LHG	C32-C33-C34-C35
32	C	518	DGD	C3A-C4A-C5A-C6A
30	E	101	LHG	C4-C5-C6-O8
31	a	613	SQD	O6-C44-C45-C46
32	A	618	DGD	O1G-C1G-C2G-C3G
30	l	101	LHG	C32-C33-C34-C35
30	A	615	LHG	C11-C10-C9-C8
32	C	518	DGD	C3B-C4B-C5B-C6B
31	D	407	SQD	O6-C44-C45-C46
33	D	411	STE	C12-C13-C14-C15
24	b	616	CLA	O1D-CGD-O2D-CED
29	D	406	LMG	C39-C40-C41-C42
30	A	615	LHG	C33-C34-C35-C36
30	B	621	LHG	C10-C11-C12-C13
31	A	616	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	d	409	LHG	O1-C1-C2-O2
29	d	410	LMG	C38-C39-C40-C41
30	B	621	LHG	C11-C12-C13-C14
33	l	102	STE	C1-C2-C3-C4
32	C	516	DGD	C4D-C5D-C6D-O5D
24	a	606	CLA	CBA-CGA-O2A-C1
29	b	623	LMG	C24-C25-C26-C27
30	D	408	LHG	C29-C30-C31-C32
33	l	102	STE	C7-C8-C9-C10
29	D	409	LMG	C11-C12-C13-C14
29	M	101	LMG	C40-C41-C42-C43
30	A	615	LHG	C34-C35-C36-C37
31	A	616	SQD	C11-C12-C13-C14
29	c	519	LMG	C30-C31-C32-C33
33	H	103	STE	C9-C10-C11-C12
29	c	521	LMG	O1-C7-C8-O7
29	c	521	LMG	O7-C8-C9-O8
29	c	522	LMG	O1-C7-C8-O7
31	b	620	SQD	O6-C44-C45-O47
24	b	616	CLA	CBD-CGD-O2D-CED
24	B	613	CLA	C10-C11-C12-C13
24	c	509	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	C10-C11-C12-C13
33	M	103	STE	C1-C2-C3-C4
24	A	605	CLA	C16-C17-C18-C19
24	B	610	CLA	C16-C17-C18-C19
32	A	618	DGD	CDB-CEB-CFB-CGB
28	d	406	PL9	C34-C36-C37-C38
29	a	618	LMG	C29-C30-C31-C32
32	A	618	DGD	CCB-CDB-CEB-CFB
33	b	625	STE	C10-C11-C12-C13
24	B	613	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
28	D	405	PL9	C47-C48-C49-C51
30	d	407	LHG	C16-C17-C18-C19
30	d	408	LHG	C26-C27-C28-C29
33	x	102	STE	C2-C3-C4-C5
24	B	611	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	b	607	CLA	C6-C7-C8-C9
24	b	609	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C11-C12-C13-C14
24	d	401	CLA	C14-C13-C15-C16
29	D	409	LMG	C33-C34-C35-C36
29	D	410	LMG	C37-C38-C39-C40
33	d	411	STE	C12-C13-C14-C15
29	a	618	LMG	C32-C33-C34-C35
33	d	412	STE	C11-C10-C9-C8
33	t	102	STE	C10-C11-C12-C13
24	B	602	CLA	C8-C10-C11-C12
24	b	616	CLA	C8-C10-C11-C12
29	a	618	LMG	C19-C20-C21-C22
32	C	517	DGD	C8B-C9B-CAB-CBB
33	c	520	STE	C4-C5-C6-C7
33	d	411	STE	C7-C8-C9-C10
24	B	604	CLA	C16-C17-C18-C20
24	c	504	CLA	C11-C12-C13-C15
26	A	609	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	K	101	BCR	C23-C24-C25-C26
26	K	101	BCR	C23-C24-C25-C30
26	b	617	BCR	C1-C6-C7-C8
26	c	514	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
26	k	102	BCR	C23-C24-C25-C26
26	k	102	BCR	C23-C24-C25-C30
26	x	101	BCR	C23-C24-C25-C26
26	x	101	BCR	C23-C24-C25-C30
29	a	618	LMG	C21-C22-C23-C24
29	d	410	LMG	C14-C15-C16-C17
30	l	101	LHG	C19-C20-C21-C22
33	H	103	STE	C12-C13-C14-C15
33	T	103	STE	C12-C13-C14-C15
29	b	623	LMG	C34-C35-C36-C37
26	K	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C21-C22-C23-C24
30	B	621	LHG	C18-C19-C20-C21
26	A	609	BCR	C14-C15-C16-C17
29	D	410	LMG	C34-C35-C36-C37
30	d	408	LHG	C11-C12-C13-C14
24	c	513	CLA	C13-C15-C16-C17
24	B	611	CLA	C16-C17-C18-C20
24	B	615	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	D	411	STE	C6-C7-C8-C9
24	b	606	CLA	C8-C10-C11-C12
29	b	623	LMG	C19-C20-C21-C22
30	E	101	LHG	C31-C32-C33-C34
32	A	618	DGD	CFA-CGA-CHA-CIA
33	H	103	STE	C1-C2-C3-C4
30	D	408	LHG	C32-C33-C34-C35
31	b	620	SQD	C12-C13-C14-C15
33	a	616	STE	C5-C6-C7-C8
24	B	604	CLA	C11-C12-C13-C15
24	B	605	CLA	C11-C10-C8-C7
24	B	613	CLA	C12-C13-C15-C16
24	B	614	CLA	C12-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C10
24	C	509	CLA	C11-C12-C13-C15
24	C	510	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	b	602	CLA	C11-C10-C8-C7
24	b	604	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	b	615	CLA	C11-C10-C8-C7
24	b	616	CLA	C11-C10-C8-C7
24	c	506	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
24	c	509	CLA	C6-C7-C8-C10
24	c	512	CLA	C12-C13-C15-C16
24	d	401	CLA	C12-C13-C15-C16
33	C	520	STE	C3-C4-C5-C6
33	D	411	STE	C9-C10-C11-C12
26	T	101	BCR	C9-C10-C11-C12
24	B	613	CLA	C16-C17-C18-C19
33	C	521	STE	C10-C11-C12-C13
33	a	617	STE	C7-C8-C9-C10
33	C	521	STE	C11-C10-C9-C8
33	I	101	STE	C11-C10-C9-C8
33	T	102	STE	C10-C11-C12-C13
29	M	101	LMG	C12-C13-C14-C15
31	a	614	SQD	C24-C25-C26-C27
26	C	514	BCR	C16-C17-C18-C36
26	k	101	BCR	C11-C10-C9-C34
26	x	101	BCR	C16-C17-C18-C36
29	D	406	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	C7A-C8A-C9A-CAA
33	b	622	STE	C3-C4-C5-C6
24	B	609	CLA	C16-C17-C18-C19
32	c	516	DGD	O1G-C1A-C2A-C3A
30	d	409	LHG	C35-C36-C37-C38
29	a	618	LMG	C22-C23-C24-C25
24	a	604	CLA	C15-C16-C17-C18
32	C	518	DGD	O1A-C1A-O1G-C1G
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	512	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
25	a	605	PHO	CAD-CBD-CGD-O2D
29	c	522	LMG	C9-C8-O7-C10
24	B	612	CLA	C15-C16-C17-C18
24	c	509	CLA	C15-C16-C17-C18
29	b	621	LMG	C31-C32-C33-C34
31	f	101	SQD	C33-C34-C35-C36
33	b	627	STE	C5-C6-C7-C8
24	c	512	CLA	C4-C3-C5-C6
28	A	612	PL9	C25-C24-C26-C27
30	B	622	LHG	C9-C10-C11-C12
32	C	517	DGD	CBB-CCB-CDB-CEB
33	B	626	STE	C9-C10-C11-C12
28	D	405	PL9	C43-C44-C46-C47
28	A	612	PL9	C39-C41-C42-C43
30	B	622	LHG	C32-C33-C34-C35
29	a	618	LMG	O1-C7-C8-C9
29	c	521	LMG	C7-C8-C9-O8
29	b	623	LMG	C12-C13-C14-C15
30	A	615	LHG	C17-C18-C19-C20
30	l	101	LHG	O6-C4-C5-O7
24	b	604	CLA	C3-C5-C6-C7
29	b	623	LMG	C20-C21-C22-C23
33	l	102	STE	C4-C5-C6-C7
24	A	613	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O1D
31	a	614	SQD	O47-C45-C46-O48
32	A	618	DGD	O1G-C1G-C2G-O2G
32	c	516	DGD	O1G-C1G-C2G-O2G
32	C	517	DGD	O1A-C1A-O1G-C1G
32	A	618	DGD	CBA-CCA-CDA-CEA
33	l	102	STE	C10-C11-C12-C13
33	I	101	STE	C7-C8-C9-C10
24	C	506	CLA	C4-C3-C5-C6
31	D	407	SQD	C29-C30-C31-C32
28	a	611	PL9	C4-C3-C7-C8
33	D	411	STE	C11-C10-C9-C8
33	b	624	STE	C11-C12-C13-C14
24	B	604	CLA	C14-C13-C15-C16
24	B	613	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C12-C13-C14
24	c	512	CLA	C14-C13-C15-C16
29	D	406	LMG	C37-C38-C39-C40
32	H	102	DGD	C5A-C6A-C7A-C8A
32	c	516	DGD	CBA-CCA-CDA-CEA
24	B	606	CLA	C8-C10-C11-C12
33	H	103	STE	C14-C15-C16-C17
33	I	101	STE	C2-C3-C4-C5
30	d	409	LHG	C29-C30-C31-C32
33	a	617	STE	C13-C14-C15-C16
32	c	516	DGD	C4D-C5D-C6D-O5D
26	B	617	BCR	C11-C12-C13-C35
31	D	407	SQD	C33-C34-C35-C36
24	d	403	CLA	C3-C5-C6-C7
31	A	616	SQD	C14-C15-C16-C17
33	T	103	STE	C9-C10-C11-C12
24	C	508	CLA	C1A-C2A-CAA-CBA
24	c	511	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	D	411	STE	C1-C2-C3-C4
33	c	520	STE	C1-C2-C3-C4
33	k	103	STE	C1-C2-C3-C4
24	d	404	CLA	C16-C17-C18-C19
24	c	506	CLA	C2-C1-O2A-CGA
33	a	615	STE	C4-C5-C6-C7
26	c	514	BCR	C15-C16-C17-C18
32	H	102	DGD	CBA-CCA-CDA-CEA
32	c	516	DGD	C6A-C7A-C8A-C9A
33	a	617	STE	C3-C4-C5-C6
29	C	519	LMG	C37-C38-C39-C40
32	A	618	DGD	CEA-CFA-CGA-CHA
24	b	609	CLA	C4-C3-C5-C6
28	D	405	PL9	C35-C34-C36-C37
24	C	506	CLA	C2-C3-C5-C6
29	M	101	LMG	C13-C14-C15-C16
30	d	407	LHG	C29-C30-C31-C32
31	a	614	SQD	C13-C14-C15-C16
33	C	521	STE	C12-C13-C14-C15
30	A	615	LHG	C3-O3-P-O5
30	B	622	LHG	C3-O3-P-O4
30	D	408	LHG	C3-O3-P-O4
30	D	408	LHG	C4-O6-P-O5
30	d	407	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	l	101	LHG	C4-O6-P-O5
24	B	610	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
31	B	623	SQD	C18-C19-C20-C21
32	H	102	DGD	C2B-C3B-C4B-C5B
33	b	625	STE	C14-C15-C16-C17
24	c	505	CLA	C15-C16-C17-C18
30	l	101	LHG	O6-C4-C5-C6
30	d	409	LHG	C27-C28-C29-C30
24	c	510	CLA	C15-C16-C17-C18
29	a	618	LMG	C37-C38-C39-C40
24	B	607	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
31	A	616	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C35-C36-C37-C38
29	c	519	LMG	C35-C36-C37-C38
30	d	408	LHG	C31-C32-C33-C34
29	a	618	LMG	C41-C42-C43-C44
32	c	518	DGD	C5A-C6A-C7A-C8A
24	c	503	CLA	CBA-CGA-O2A-C1
32	C	518	DGD	O6D-C5D-C6D-O5D
24	b	604	CLA	C8-C10-C11-C12
24	A	605	CLA	C11-C10-C8-C7
24	B	604	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C15
24	B	615	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C12-C13-C15
24	B	616	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C10-C8-C7
24	C	509	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C12-C13-C15
24	b	609	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C7
24	c	512	CLA	C6-C7-C8-C10
24	c	512	CLA	C11-C12-C13-C15
24	d	404	CLA	C6-C7-C8-C10
29	b	621	LMG	C28-C29-C30-C31
30	l	101	LHG	C23-C24-C25-C26
33	J	101	STE	C3-C4-C5-C6
32	C	516	DGD	O1G-C1A-C2A-C3A
33	t	102	STE	C13-C14-C15-C16
24	A	605	CLA	C15-C16-C17-C18
30	D	408	LHG	C23-C24-C25-C26
33	b	625	STE	C11-C12-C13-C14
29	b	623	LMG	C17-C18-C19-C20
30	A	615	LHG	C14-C15-C16-C17
30	d	409	LHG	C9-C10-C11-C12
32	h	101	DGD	O2G-C1B-C2B-C3B
31	a	614	SQD	C44-C45-C46-O48
32	C	518	DGD	C4B-C5B-C6B-C7B
30	E	101	LHG	O7-C5-C6-O8
25	a	605	PHO	O2A-C1-C2-C3
33	b	624	STE	C3-C4-C5-C6
32	C	517	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C5-C6-C7-C8
24	C	511	CLA	C8-C10-C11-C12
24	b	616	CLA	C10-C11-C12-C13
24	c	511	CLA	C8-C10-C11-C12
33	c	520	STE	C3-C4-C5-C6
30	d	409	LHG	C25-C26-C27-C28
24	B	605	CLA	C6-C7-C8-C9
24	B	605	CLA	C11-C10-C8-C9
24	C	505	CLA	C6-C7-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	c	512	CLA	C11-C12-C13-C14
24	a	606	CLA	O1A-CGA-O2A-C1
24	B	604	CLA	C16-C17-C18-C19
32	C	518	DGD	C9B-CAB-CBB-CCB
29	D	410	LMG	C13-C14-C15-C16
29	b	621	LMG	C4-C5-C6-O5
32	H	102	DGD	O2G-C1B-C2B-C3B
31	A	616	SQD	C29-C30-C31-C32
33	C	521	STE	C11-C12-C13-C14
29	C	519	LMG	C13-C14-C15-C16
30	B	621	LHG	C13-C14-C15-C16
33	b	624	STE	C5-C6-C7-C8
33	l	102	STE	C15-C16-C17-C18
29	b	621	LMG	O6-C5-C6-O5
26	c	515	BCR	C21-C22-C23-C24
29	b	621	LMG	C19-C20-C21-C22
33	b	625	STE	C12-C13-C14-C15
26	d	405	BCR	C20-C21-C22-C37
30	e	102	LHG	C12-C13-C14-C15
28	d	406	PL9	C13-C14-C16-C17
24	c	505	CLA	C16-C17-C18-C20
33	x	102	STE	C10-C11-C12-C13
30	e	102	LHG	C11-C12-C13-C14
29	D	409	LMG	C9-C8-O7-C10
31	B	623	SQD	C46-C45-O47-C7
31	b	620	SQD	C46-C45-O47-C7
24	c	503	CLA	O1A-CGA-O2A-C1
24	D	402	CLA	C2-C1-O2A-CGA
33	d	412	STE	C13-C14-C15-C16
24	d	404	CLA	C16-C17-C18-C20
32	C	518	DGD	C2A-C3A-C4A-C5A
32	c	518	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
26	C	514	BCR	C9-C10-C11-C12
30	B	621	LHG	O6-C4-C5-O7
24	C	507	CLA	C5-C6-C7-C8
30	e	102	LHG	C24-C25-C26-C27
26	A	609	BCR	C23-C24-C25-C30
26	B	618	BCR	C23-C24-C25-C26
26	B	618	BCR	C23-C24-C25-C30
26	c	514	BCR	C1-C6-C7-C8
28	A	612	PL9	C38-C39-C41-C42
29	c	522	LMG	C36-C37-C38-C39
32	A	618	DGD	CBB-CCB-CDB-CEB
31	a	613	SQD	C8-C7-O47-C45
30	A	615	LHG	C24-C25-C26-C27
33	B	626	STE	C7-C8-C9-C10
26	B	617	BCR	C12-C13-C14-C15
26	C	514	BCR	C12-C13-C14-C15
26	H	101	BCR	C12-C13-C14-C15
29	M	101	LMG	O7-C8-C9-O8
29	a	618	LMG	O1-C7-C8-O7
31	b	620	SQD	O47-C45-C46-O48
30	l	101	LHG	C12-C13-C14-C15
31	f	101	SQD	C32-C33-C34-C35
24	A	605	CLA	C16-C17-C18-C20
33	T	102	STE	C12-C13-C14-C15
24	C	505	CLA	C15-C16-C17-C18
29	d	410	LMG	C15-C16-C17-C18
29	C	519	LMG	O1-C7-C8-C9
30	l	101	LHG	C4-C5-C6-O8
29	C	519	LMG	C18-C19-C20-C21
29	b	623	LMG	C31-C32-C33-C34
24	b	606	CLA	C15-C16-C17-C18
24	B	615	CLA	C12-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C10
24	D	402	CLA	C12-C13-C15-C16
24	a	604	CLA	C12-C13-C15-C16
24	b	603	CLA	C11-C12-C13-C15
24	b	607	CLA	C11-C10-C8-C7
24	b	612	CLA	C11-C10-C8-C7
24	b	613	CLA	C11-C12-C13-C15
24	b	615	CLA	C11-C12-C13-C15
24	c	512	CLA	C2-C3-C5-C6
30	B	621	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	c	518	DGD	C8A-C9A-CAA-CBA
24	B	616	CLA	C6-C7-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	b	614	CLA	C14-C13-C15-C16
24	c	505	CLA	C6-C7-C8-C9
24	c	507	CLA	C11-C10-C8-C9
30	d	408	LHG	C19-C20-C21-C22
31	a	613	SQD	C10-C11-C12-C13
31	D	407	SQD	C23-C24-C25-C26
24	B	609	CLA	C16-C17-C18-C20
24	b	611	CLA	C16-C17-C18-C19
30	A	615	LHG	C2-C3-O3-P
30	d	409	LHG	C2-C3-O3-P
29	c	522	LMG	C34-C35-C36-C37
30	B	621	LHG	C24-C25-C26-C27
31	A	616	SQD	C26-C27-C28-C29
30	E	101	LHG	C1-C2-C3-O3
28	a	611	PL9	C21-C22-C23-C24
29	C	519	LMG	C28-C29-C30-C31
29	D	409	LMG	C29-C28-O8-C9
32	H	102	DGD	C9A-CAA-CBA-CCA
33	D	411	STE	C4-C5-C6-C7
29	c	521	LMG	C42-C43-C44-C45
31	b	620	SQD	C30-C31-C32-C33
33	b	624	STE	C9-C10-C11-C12
30	l	101	LHG	C17-C18-C19-C20
31	a	614	SQD	C30-C31-C32-C33
24	c	506	CLA	C16-C17-C18-C19
26	C	514	BCR	C13-C14-C15-C16
33	b	626	STE	C7-C8-C9-C10
31	a	613	SQD	C19-C20-C21-C22
26	d	405	BCR	C18-C19-C20-C21
32	C	516	DGD	O1A-C1A-O1G-C1G
32	A	618	DGD	C6A-C7A-C8A-C9A
29	a	618	LMG	O8-C28-C29-C30
24	b	609	CLA	C2-C3-C5-C6
28	D	405	PL9	C13-C14-C16-C17
32	c	516	DGD	CDB-CEB-CFB-CGB
29	M	101	LMG	C20-C21-C22-C23
33	B	620	STE	C7-C8-C9-C10
33	b	626	STE	C1-C2-C3-C4
32	h	101	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C19-C20-C21-C22
33	l	102	STE	C12-C13-C14-C15
24	B	601	CLA	C3A-C2A-CAA-CBA
24	c	507	CLA	C15-C16-C17-C18
24	d	401	CLA	C16-C17-C18-C20
32	H	102	DGD	C4E-C5E-C6E-O5E
32	c	516	DGD	C5A-C6A-C7A-C8A
33	C	520	STE	C4-C5-C6-C7
31	b	620	SQD	C11-C10-C9-C8
33	k	103	STE	C4-C5-C6-C7
28	A	612	PL9	C4-C3-C7-C8
24	A	605	CLA	C11-C10-C8-C9
24	B	606	CLA	C11-C10-C8-C9
24	C	507	CLA	C14-C13-C15-C16
24	b	605	CLA	C11-C10-C8-C9
24	c	507	CLA	C14-C13-C15-C16
24	c	511	CLA	C11-C10-C8-C9
24	B	601	CLA	C16-C17-C18-C19
33	a	616	STE	C4-C5-C6-C7
32	C	516	DGD	O1G-C1G-C2G-C3G
24	b	601	CLA	C2A-CAA-CBA-CGA
33	b	627	STE	C6-C7-C8-C9
24	B	611	CLA	C16-C17-C18-C19
24	B	604	CLA	O2A-C1-C2-C3
24	C	512	CLA	O2A-C1-C2-C3
24	a	612	CLA	CBA-CGA-O2A-C1
32	C	517	DGD	O6D-C1D-O3G-C3G
32	c	516	DGD	O6E-C1E-O5D-C6D
24	b	605	CLA	C15-C16-C17-C18
31	B	623	SQD	C10-C11-C12-C13
33	B	627	STE	C3-C4-C5-C6
33	B	626	STE	C11-C12-C13-C14
26	k	101	BCR	C7-C8-C9-C10
29	D	406	LMG	C20-C21-C22-C23
33	j	101	STE	C5-C6-C7-C8
32	A	618	DGD	O6D-C5D-C6D-O5D
24	c	508	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C12-C13-C15-C16
24	C	508	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C12-C13-C15
24	b	614	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
30	e	102	LHG	C25-C26-C27-C28
30	B	621	LHG	C9-C10-C11-C12
30	e	102	LHG	C4-O6-P-O3
29	A	614	LMG	C19-C20-C21-C22
31	a	614	SQD	C15-C16-C17-C18
24	B	614	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	c	501	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C10-C11-C12-C13
33	H	103	STE	C7-C8-C9-C10
33	J	101	STE	C7-C8-C9-C10
33	D	411	STE	C15-C16-C17-C18
30	D	408	LHG	O6-C4-C5-C6
24	D	403	CLA	C13-C15-C16-C17
32	C	517	DGD	C5B-C6B-C7B-C8B
33	C	520	STE	C5-C6-C7-C8
32	C	517	DGD	C1B-C2B-C3B-C4B
31	a	613	SQD	C35-C36-C37-C38
33	c	520	STE	C10-C11-C12-C13
26	B	617	BCR	C11-C10-C9-C8
24	B	614	CLA	C8-C10-C11-C12
33	b	626	STE	C5-C6-C7-C8
25	d	402	PHO	C2C-C3C-CAC-CBC
31	b	620	SQD	C10-C11-C12-C13
30	B	621	LHG	C23-C24-C25-C26
29	a	618	LMG	C24-C25-C26-C27
30	d	408	LHG	C14-C15-C16-C17
30	E	101	LHG	C10-C11-C12-C13
32	C	518	DGD	C4A-C5A-C6A-C7A
32	A	618	DGD	O6D-C1D-O3G-C3G
24	b	606	CLA	C10-C11-C12-C13
24	c	510	CLA	C10-C11-C12-C13
24	c	508	CLA	C4-C3-C5-C6
28	D	405	PL9	C40-C39-C41-C42
31	A	616	SQD	C31-C32-C33-C34
32	H	102	DGD	O6E-C5E-C6E-O5E
24	C	506	CLA	C2-C1-O2A-CGA
32	C	518	DGD	C2B-C3B-C4B-C5B
24	c	502	CLA	C6-C7-C8-C9
26	T	101	BCR	C1-C6-C7-C8
26	b	618	BCR	C23-C24-C25-C30
26	t	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	c	515	BCR	C7-C8-C9-C34
24	d	404	CLA	C10-C11-C12-C13
30	B	622	LHG	C31-C32-C33-C34
33	T	103	STE	C15-C16-C17-C18
28	D	405	PL9	C30-C29-C31-C32
24	d	401	CLA	C15-C16-C17-C18
28	a	611	PL9	C43-C44-C46-C47
28	d	406	PL9	C43-C44-C46-C47
24	B	612	CLA	O1A-CGA-O2A-C1
32	c	516	DGD	C5D-C6D-O5D-C1E
33	B	625	STE	C6-C7-C8-C9
24	C	508	CLA	C16-C17-C18-C19
24	c	508	CLA	C10-C11-C12-C13
32	C	518	DGD	C1B-C2B-C3B-C4B
28	a	611	PL9	C47-C48-C49-C50
29	D	410	LMG	C17-C18-C19-C20
31	b	620	SQD	C13-C14-C15-C16
32	C	516	DGD	O6E-C1E-O5D-C6D
24	a	612	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	C4-C3-C5-C6
24	a	606	CLA	C4-C3-C5-C6
28	A	612	PL9	C30-C29-C31-C32
24	B	606	CLA	C11-C10-C8-C7
24	C	502	CLA	C11-C12-C13-C15
24	C	503	CLA	C11-C10-C8-C7
24	C	505	CLA	C11-C10-C8-C7
24	b	606	CLA	C11-C10-C8-C7
24	b	606	CLA	C12-C13-C15-C16
24	c	509	CLA	C11-C12-C13-C15
28	A	612	PL9	C33-C34-C36-C37
24	b	611	CLA	C16-C17-C18-C20
29	D	406	LMG	C18-C19-C20-C21
33	D	411	STE	C13-C14-C15-C16
32	h	101	DGD	CDA-CEA-CFA-CGA
32	c	518	DGD	C7B-C8B-C9B-CAB
30	A	615	LHG	C35-C36-C37-C38
30	B	621	LHG	C35-C36-C37-C38
24	d	401	CLA	C16-C17-C18-C19
26	Y	101	BCR	C16-C17-C18-C36
30	B	621	LHG	O7-C7-C8-C9
32	c	518	DGD	O6D-C5D-C6D-O5D
24	B	615	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C2-C3-C5-C6
24	B	604	CLA	C11-C10-C8-C9
24	B	615	CLA	C6-C7-C8-C9
24	C	502	CLA	C14-C13-C15-C16
24	b	604	CLA	C11-C10-C8-C9
24	b	606	CLA	C11-C12-C13-C14
24	b	612	CLA	C11-C10-C8-C9
24	c	503	CLA	C11-C10-C8-C9
31	f	101	SQD	C24-C25-C26-C27
33	l	102	STE	C9-C10-C11-C12
24	B	602	CLA	C3A-C2A-CAA-CBA
24	B	601	CLA	C13-C15-C16-C17
24	b	614	CLA	C13-C15-C16-C17
24	C	508	CLA	O1A-CGA-O2A-C1
24	b	601	CLA	O1A-CGA-O2A-C1
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	609	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	601	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
29	D	409	LMG	C37-C38-C39-C40
24	B	613	CLA	C5-C6-C7-C8
24	B	603	CLA	C2A-CAA-CBA-CGA
24	B	610	CLA	C2A-CAA-CBA-CGA
32	C	517	DGD	O1B-C1B-O2G-C2G
24	B	601	CLA	O1D-CGD-O2D-CED
24	b	612	CLA	C8-C10-C11-C12
31	A	616	SQD	C25-C26-C27-C28
30	d	407	LHG	C17-C18-C19-C20
33	B	627	STE	C4-C5-C6-C7
28	a	611	PL9	C39-C41-C42-C43
24	A	605	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	D	402	CLA	C2C-C3C-CAC-CBC
24	a	612	CLA	C2C-C3C-CAC-CBC
29	A	614	LMG	C7-C8-C9-O8
31	b	620	SQD	O6-C44-C45-C46
30	E	101	LHG	C26-C27-C28-C29
31	a	613	SQD	O47-C7-C8-C9
24	B	601	CLA	CBD-CGD-O2D-CED
29	D	410	LMG	C33-C34-C35-C36
24	C	509	CLA	O2A-C1-C2-C3
24	D	403	CLA	O2A-C1-C2-C3
24	d	403	CLA	O2A-C1-C2-C3
25	A	606	PHO	O2A-C1-C2-C3
29	C	519	LMG	C39-C40-C41-C42
30	d	407	LHG	C33-C34-C35-C36
24	C	501	CLA	C2A-CAA-CBA-CGA
24	b	605	CLA	C10-C11-C12-C13
32	c	517	DGD	C6B-C7B-C8B-C9B
32	c	518	DGD	CAA-CBA-CCA-CDA
33	a	616	STE	C6-C7-C8-C9
24	A	605	CLA	CHA-CBD-CGD-O1D
24	A	605	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	609	CLA	CHA-CBD-CGD-O1D
24	b	609	CLA	CHA-CBD-CGD-O2D
24	c	503	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	b	608	CLA	C4-C3-C5-C6
32	c	517	DGD	C3B-C4B-C5B-C6B
33	B	624	STE	C3-C4-C5-C6
31	A	616	SQD	O47-C7-C8-C9
31	b	620	SQD	O47-C7-C8-C9
32	c	516	DGD	O2G-C1B-C2B-C3B
29	A	614	LMG	O1-C7-C8-O7
29	C	519	LMG	O1-C7-C8-O7
30	l	101	LHG	O7-C5-C6-O8
31	f	101	SQD	O6-C44-C45-O47
29	c	522	LMG	C18-C19-C20-C21
31	B	623	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	CAA-CBA-CGA-O1A
30	d	407	LHG	C18-C19-C20-C21
33	T	103	STE	C4-C5-C6-C7
24	c	509	CLA	C2A-CAA-CBA-CGA
32	H	102	DGD	CBB-CCB-CDB-CEB
33	a	615	STE	C3-C4-C5-C6
29	M	101	LMG	C10-C11-C12-C13
24	b	603	CLA	C11-C10-C8-C7
24	b	612	CLA	C6-C7-C8-C10
25	A	606	PHO	C2-C3-C5-C6
28	A	612	PL9	C13-C14-C16-C17
31	b	620	SQD	C26-C27-C28-C29
24	B	611	CLA	C6-C7-C8-C9
24	B	613	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C10-C8-C9
24	a	606	CLA	C6-C7-C8-C9
24	b	603	CLA	C11-C10-C8-C9
26	k	101	BCR	C19-C20-C21-C22
33	b	622	STE	C9-C10-C11-C12
30	A	615	LHG	C23-C24-C25-C26
32	H	102	DGD	CDA-CEA-CFA-CGA
31	a	613	SQD	C5-C6-S-O8
24	b	613	CLA	CBD-CGD-O2D-CED
24	b	612	CLA	CAA-CBA-CGA-O2A
29	M	101	LMG	C33-C34-C35-C36
32	A	618	DGD	CCA-CDA-CEA-CFA
30	B	622	LHG	O1-C1-C2-C3
30	e	102	LHG	O1-C1-C2-C3
24	c	510	CLA	C2-C3-C5-C6
33	c	520	STE	C11-C10-C9-C8
24	B	602	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
33	B	625	STE	C1-C2-C3-C4
33	b	622	STE	C1-C2-C3-C4
33	d	411	STE	C1-C2-C3-C4
24	A	604	CLA	C2-C1-O2A-CGA
24	b	601	CLA	CBA-CGA-O2A-C1
29	c	519	LMG	O1-C7-C8-C9
31	f	101	SQD	O6-C44-C45-C46
32	c	516	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
32	c	516	DGD	C2B-C3B-C4B-C5B
25	A	606	PHO	C4-C3-C5-C6
24	b	613	CLA	CAA-CBA-CGA-O2A
24	B	612	CLA	C8-C10-C11-C12
32	H	102	DGD	CAA-CBA-CCA-CDA
32	c	516	DGD	O1B-C1B-C2B-C3B
24	A	613	CLA	C16-C17-C18-C19
24	b	610	CLA	C15-C16-C17-C18
31	f	101	SQD	C25-C26-C27-C28
26	T	101	BCR	C5-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
29	c	521	LMG	C35-C36-C37-C38
33	a	617	STE	C4-C5-C6-C7
24	B	613	CLA	CAA-CBA-CGA-O2A
29	b	621	LMG	O8-C28-C29-C30
30	A	615	LHG	C10-C11-C12-C13
24	b	612	CLA	CAA-CBA-CGA-O1A
29	D	409	LMG	C36-C37-C38-C39
29	a	618	LMG	O7-C10-C11-C12
24	B	601	CLA	C4-C3-C5-C6
24	B	609	CLA	C4-C3-C5-C6
28	D	405	PL9	C15-C14-C16-C17
30	B	622	LHG	C16-C17-C18-C19
24	b	613	CLA	C15-C16-C17-C18
24	B	605	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	b	602	CLA	CAD-CBD-CGD-O1D
24	b	607	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
32	h	101	DGD	O1B-C1B-C2B-C3B
33	b	626	STE	C3-C4-C5-C6
24	c	512	CLA	C5-C6-C7-C8
24	C	502	CLA	C11-C12-C13-C14
24	b	614	CLA	C11-C10-C8-C9
24	c	507	CLA	C6-C7-C8-C9
24	c	507	CLA	C11-C12-C13-C14
33	c	520	STE	C11-C12-C13-C14
29	b	623	LMG	O10-C28-C29-C30
24	B	606	CLA	C3-C5-C6-C7
24	C	504	CLA	C10-C11-C12-C13
24	b	606	CLA	C5-C6-C7-C8
30	B	621	LHG	C16-C17-C18-C19

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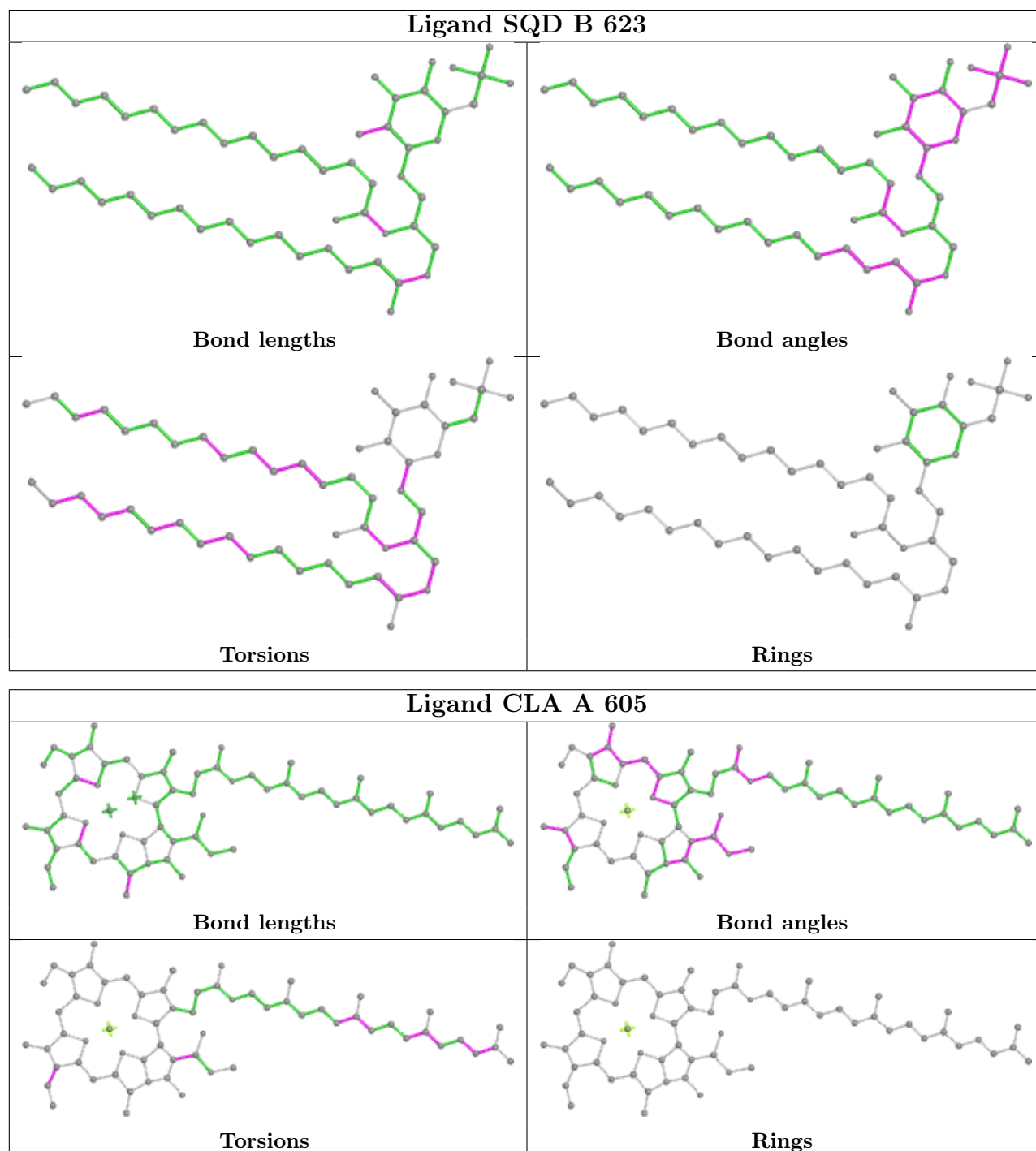
Mol	Chain	Res	Type	Atoms
32	H	102	DGD	C3A-C4A-C5A-C6A
29	c	521	LMG	C15-C16-C17-C18
29	d	410	LMG	C37-C38-C39-C40
24	B	612	CLA	CAA-CBA-CGA-O2A
30	B	622	LHG	C1-C2-C3-O3
31	B	623	SQD	O10-C23-C24-C25
24	B	604	CLA	C11-C10-C8-C7
24	B	608	CLA	C6-C7-C8-C10
24	B	613	CLA	C6-C7-C8-C10
24	B	613	CLA	C11-C10-C8-C7
24	B	615	CLA	C2-C3-C5-C6
24	b	614	CLA	C11-C10-C8-C7
24	c	503	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C10-C8-C7
24	c	510	CLA	C11-C10-C8-C7
28	d	406	PL9	C18-C19-C21-C22
32	c	516	DGD	CAA-CBA-CCA-CDA
26	d	405	BCR	C21-C22-C23-C24
29	b	621	LMG	O9-C10-C11-C12
29	b	623	LMG	O9-C10-C11-C12
32	c	517	DGD	O1B-C1B-C2B-C3B
26	c	515	BCR	C13-C14-C15-C16
26	k	102	BCR	C19-C20-C21-C22
29	b	623	LMG	O7-C10-C11-C12
24	B	603	CLA	C10-C11-C12-C13
24	c	509	CLA	C8-C10-C11-C12
33	B	620	STE	C5-C6-C7-C8
32	C	517	DGD	O1G-C1A-C2A-C3A
33	m	101	STE	C6-C7-C8-C9
24	B	604	CLA	C13-C15-C16-C17
33	B	626	STE	C3-C4-C5-C6
24	C	505	CLA	CBD-CGD-O2D-CED
24	c	506	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
31	D	407	SQD	C45-C46-O48-C23
24	B	601	CLA	CAA-CBA-CGA-O2A

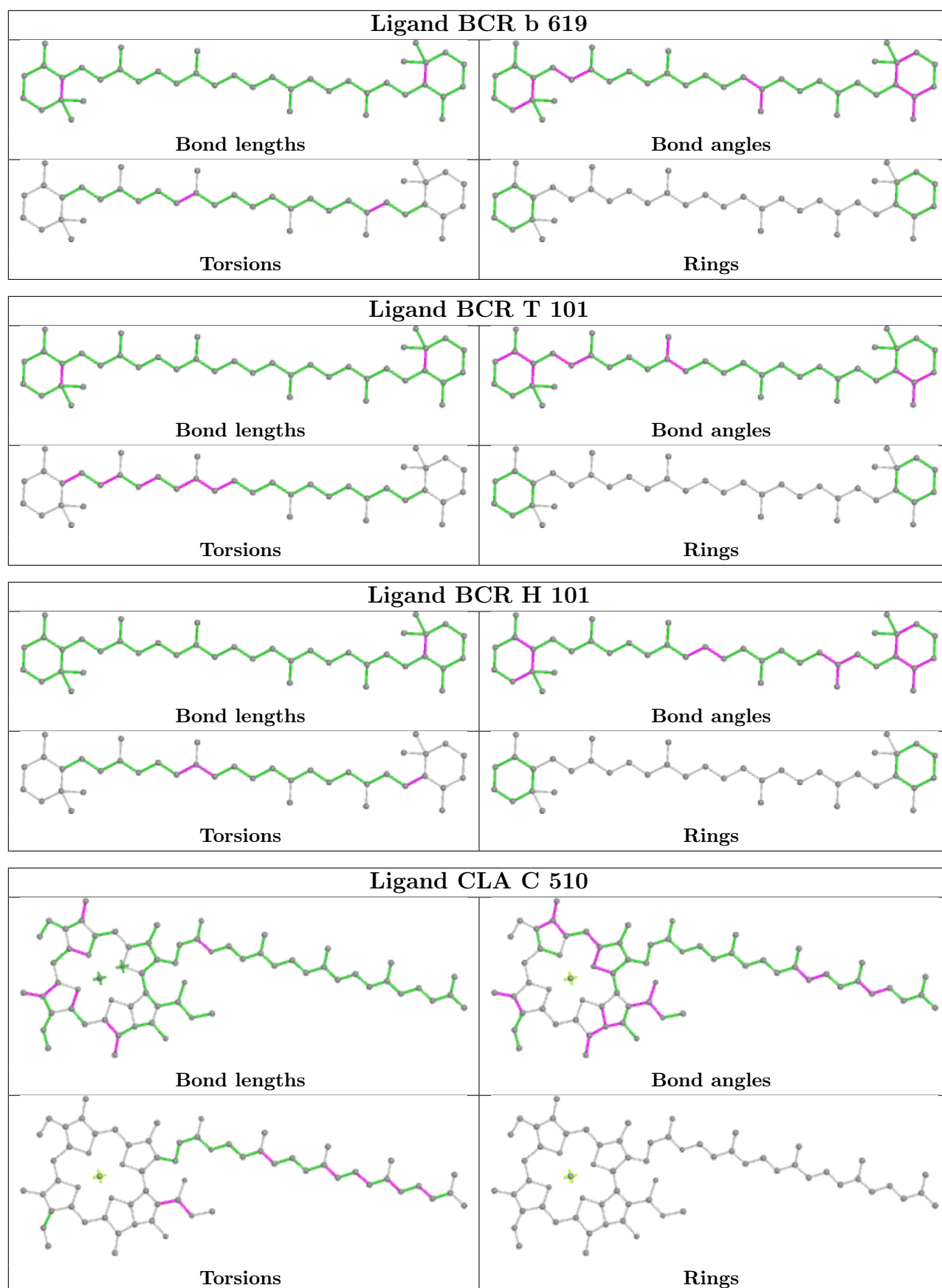
There are no ring outliers.

No monomer is involved in short contacts.

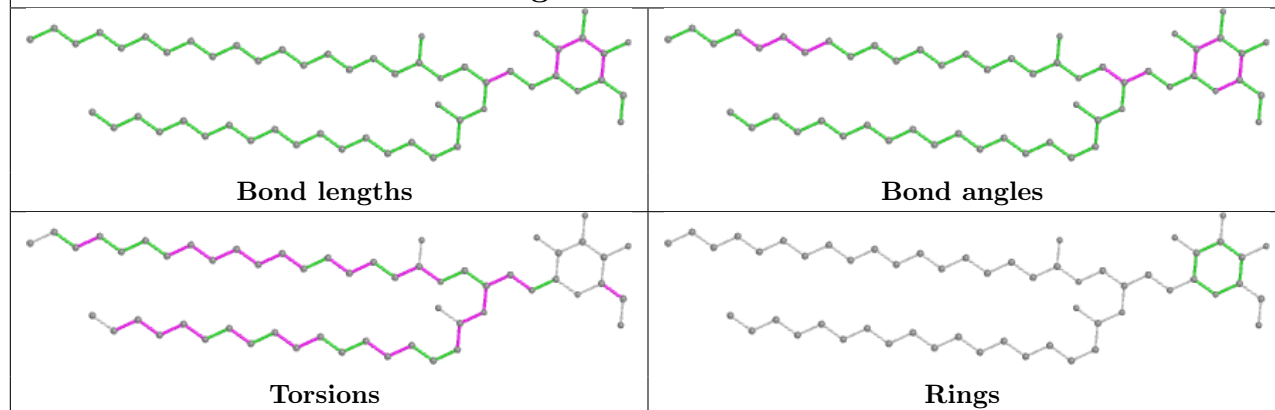
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

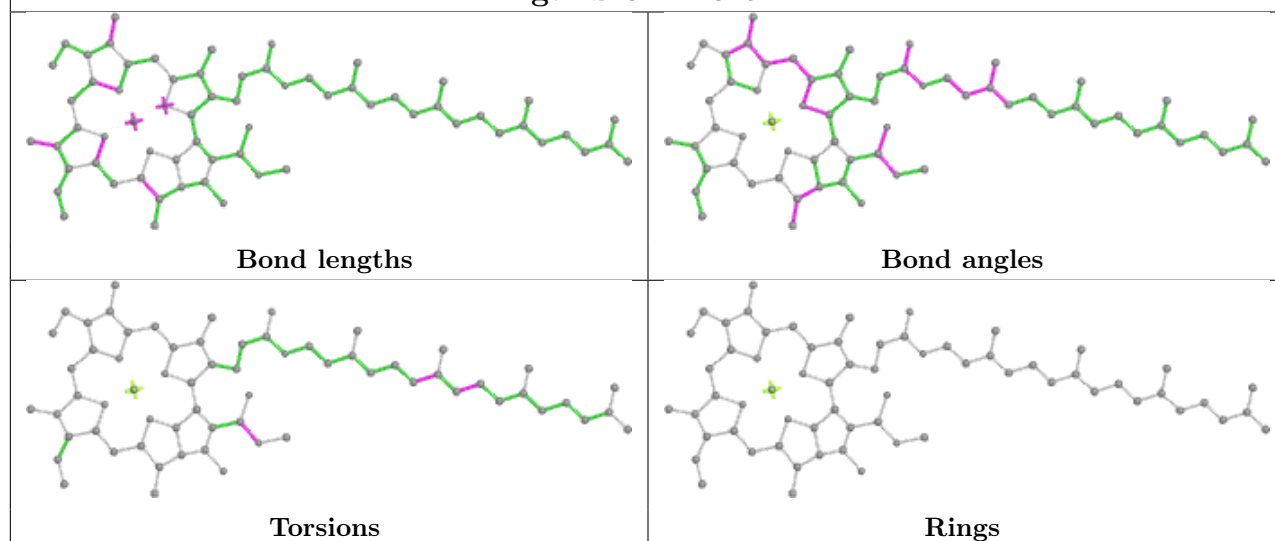




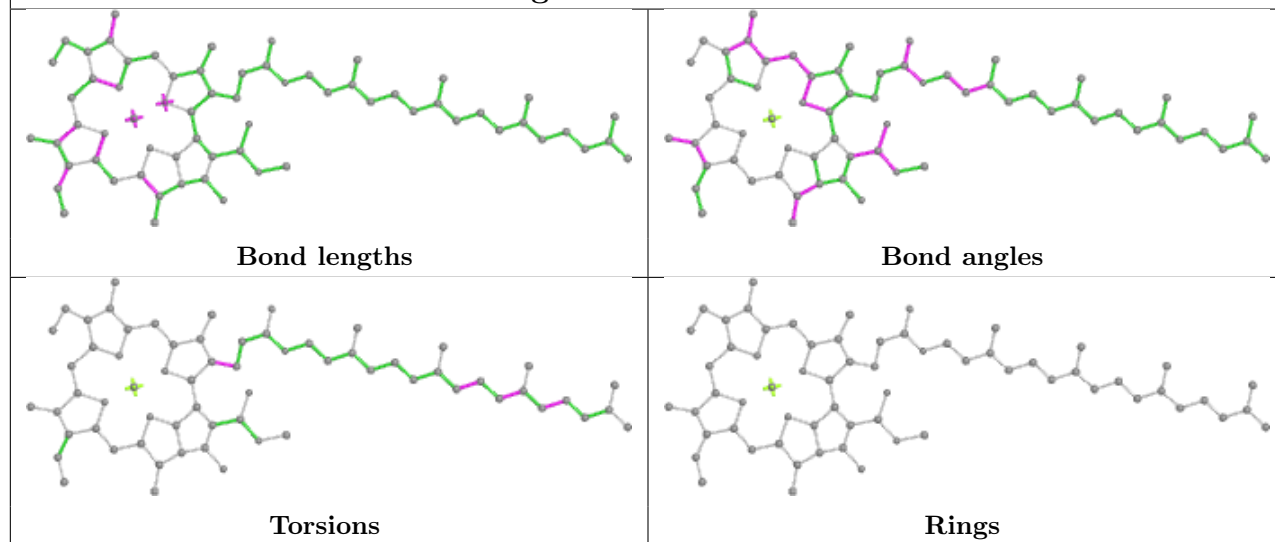
## Ligand LMG a 618



## Ligand CLA C 511

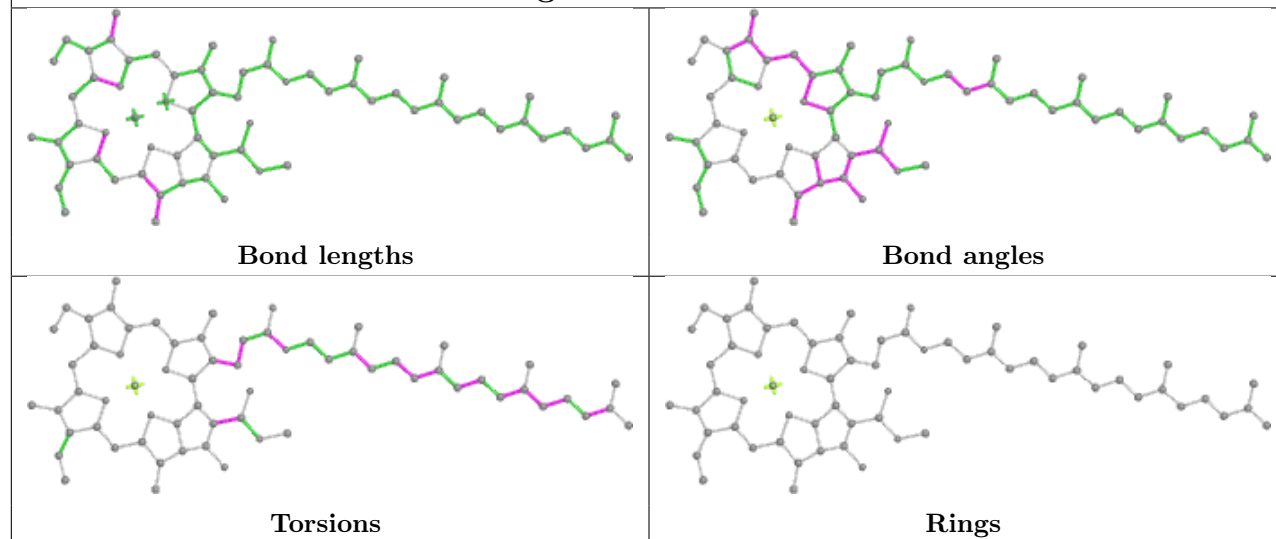


## Ligand CLA B 602

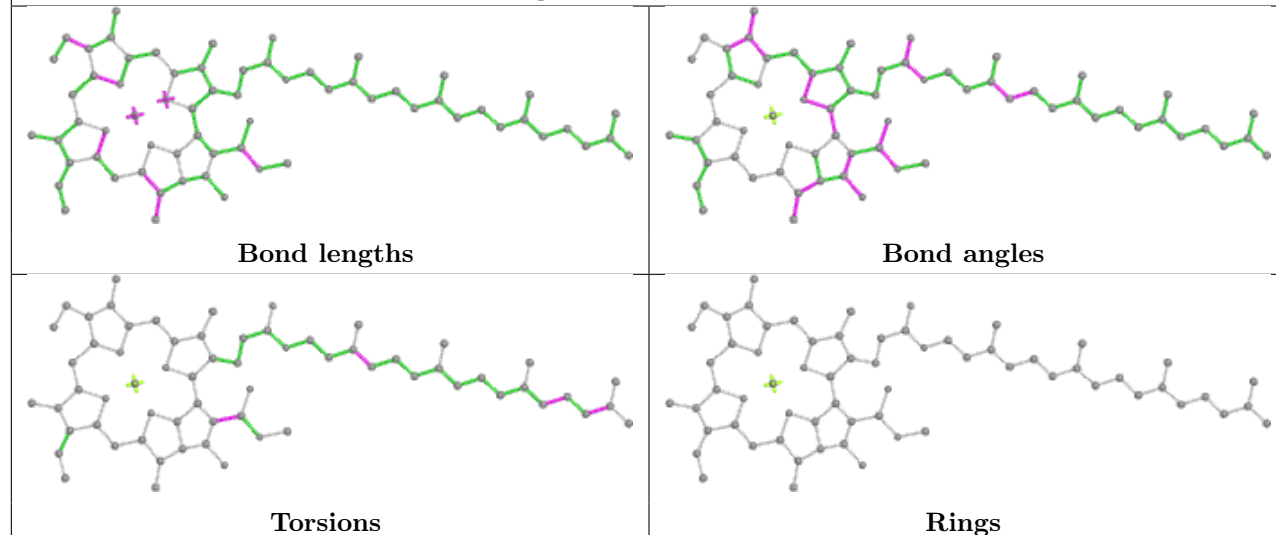




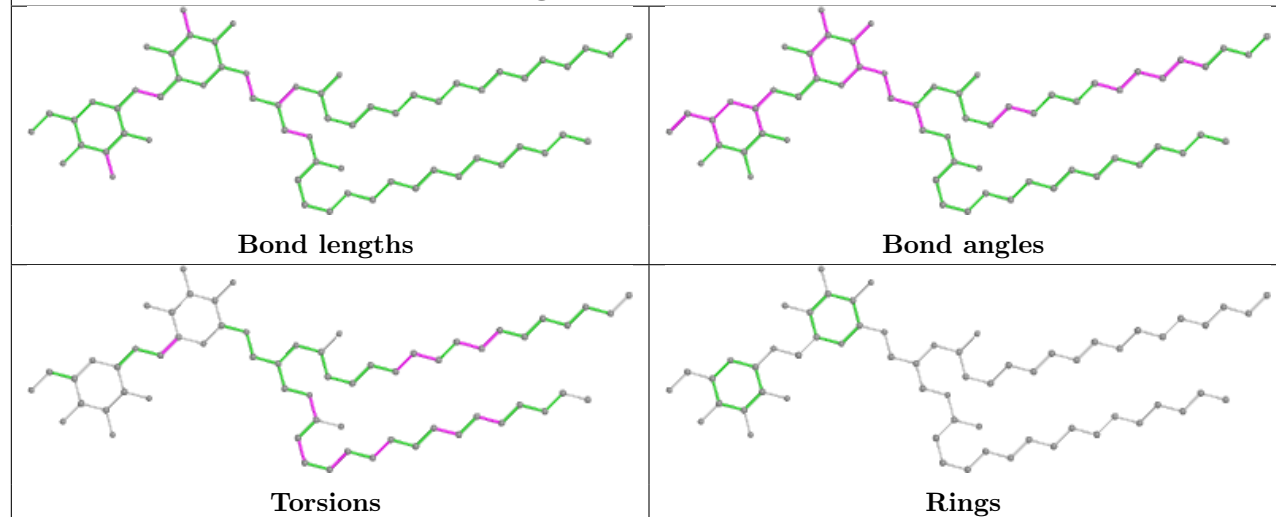
## Ligand CLA c 512

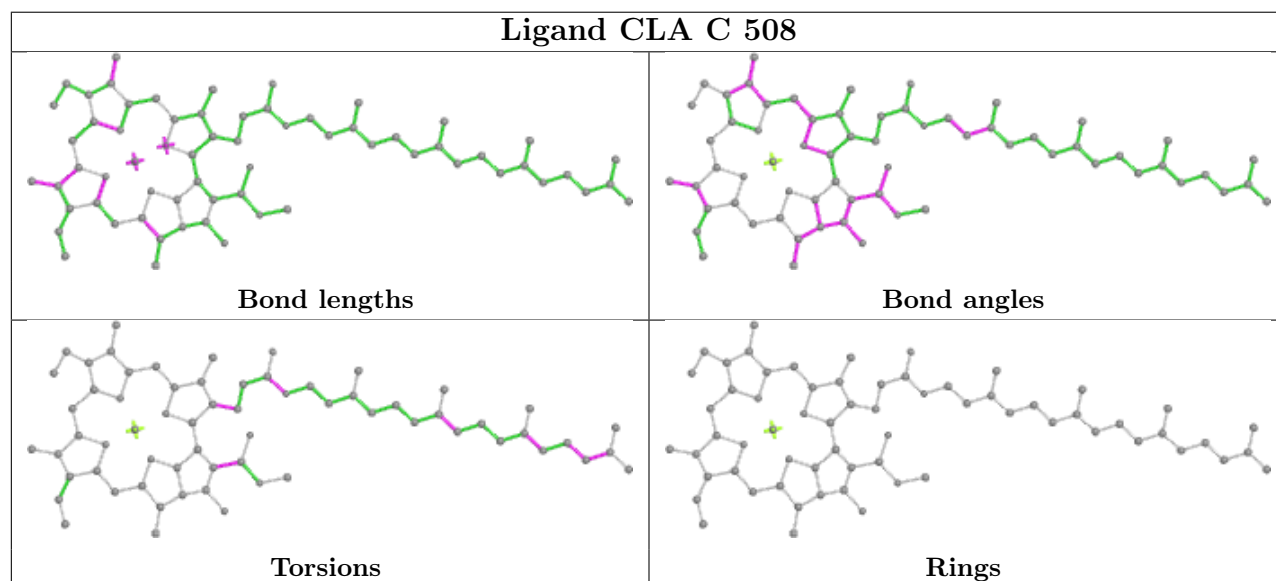
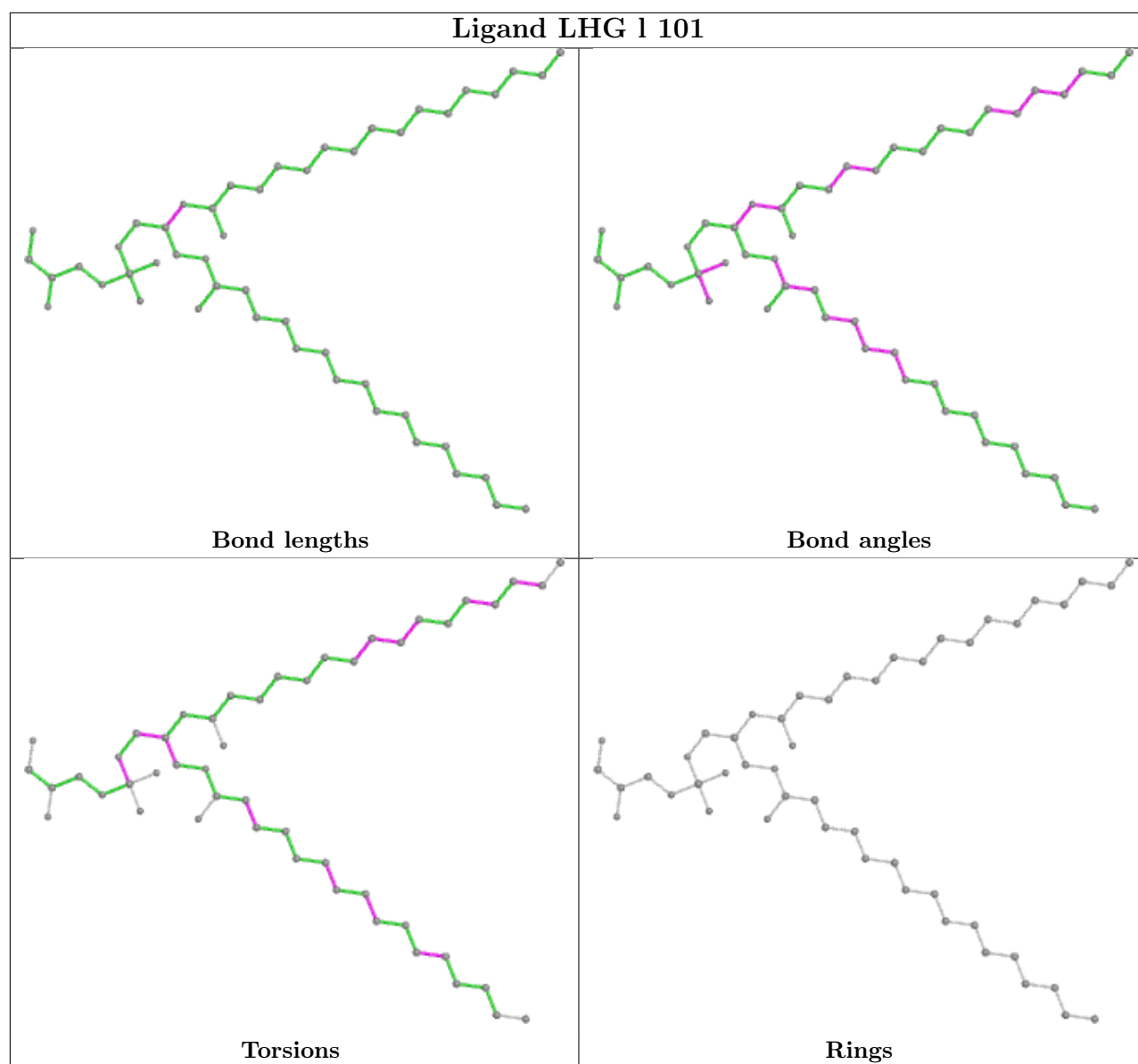


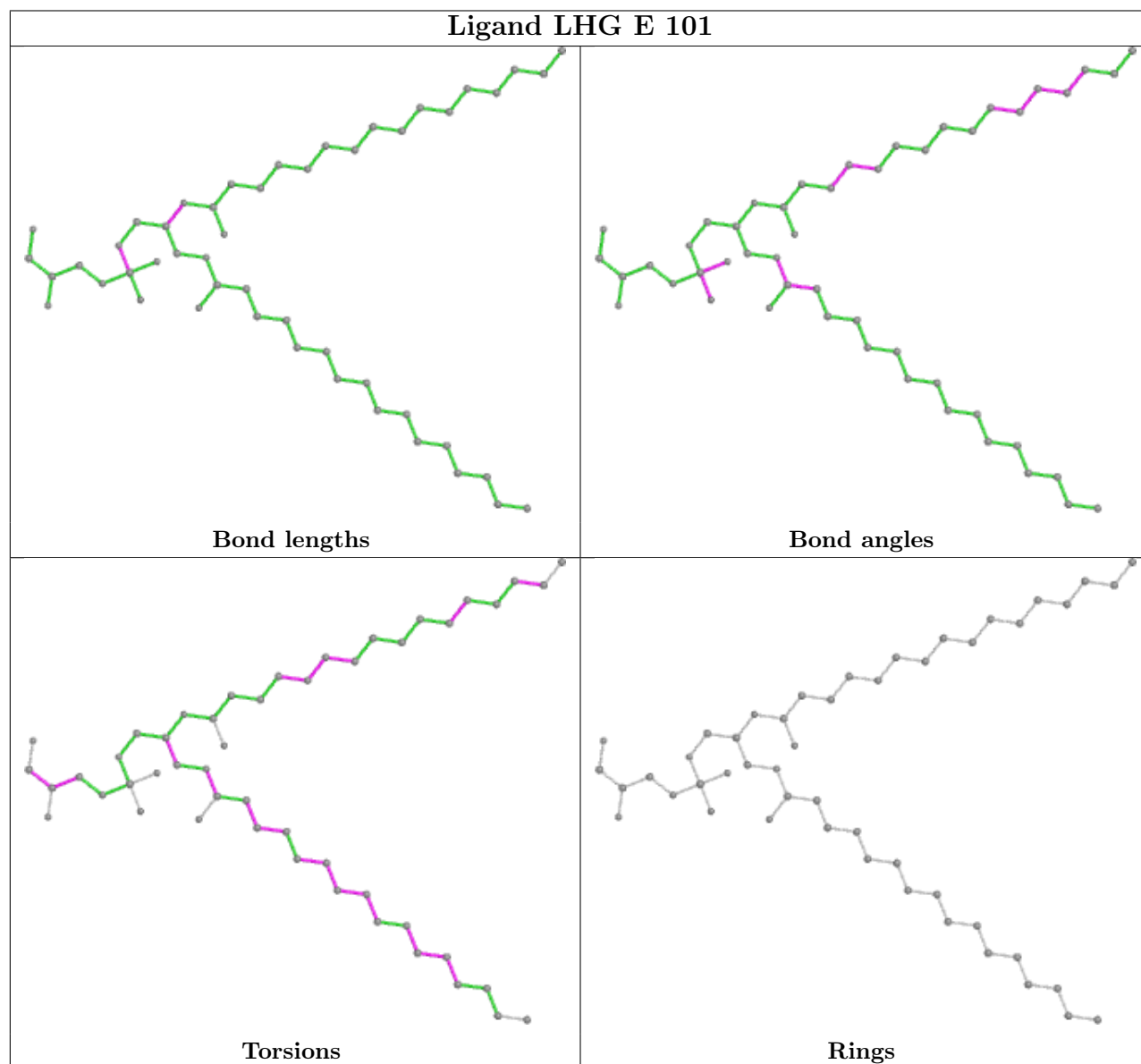
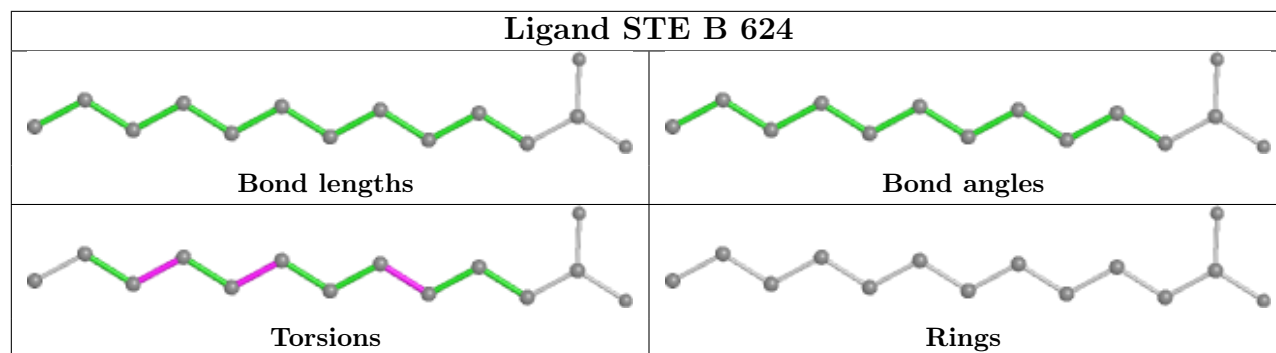
## Ligand CLA B 609

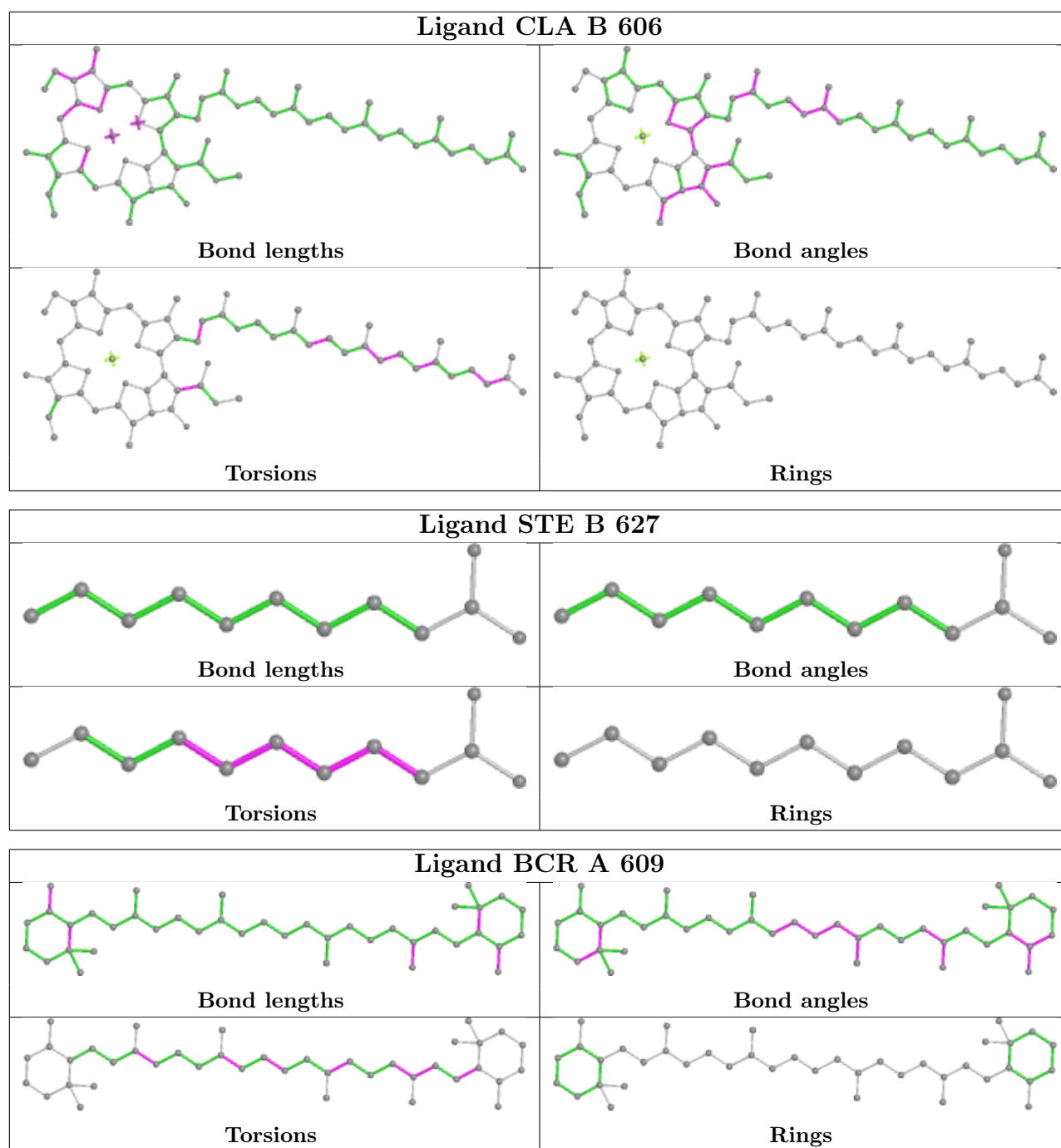


## Ligand DGD c 518

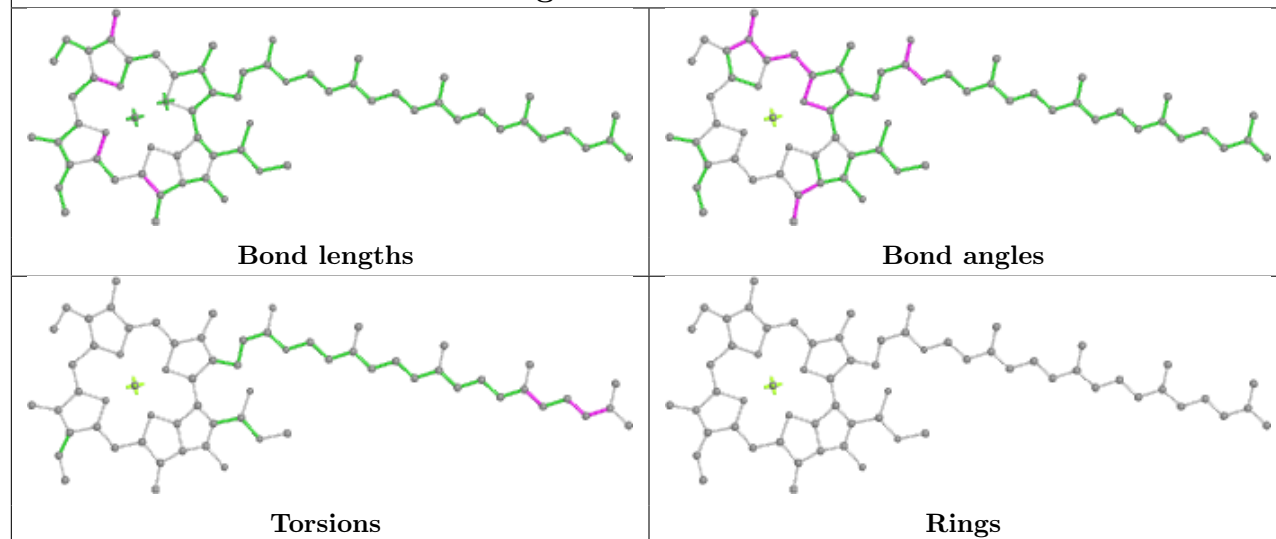




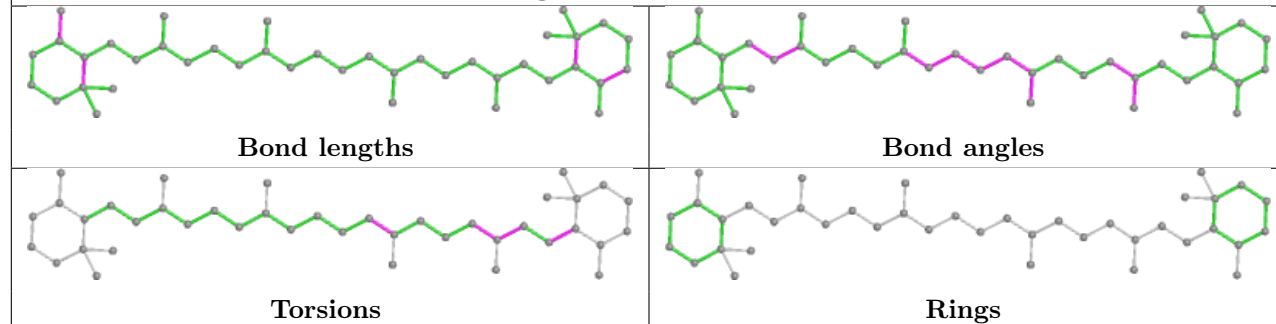




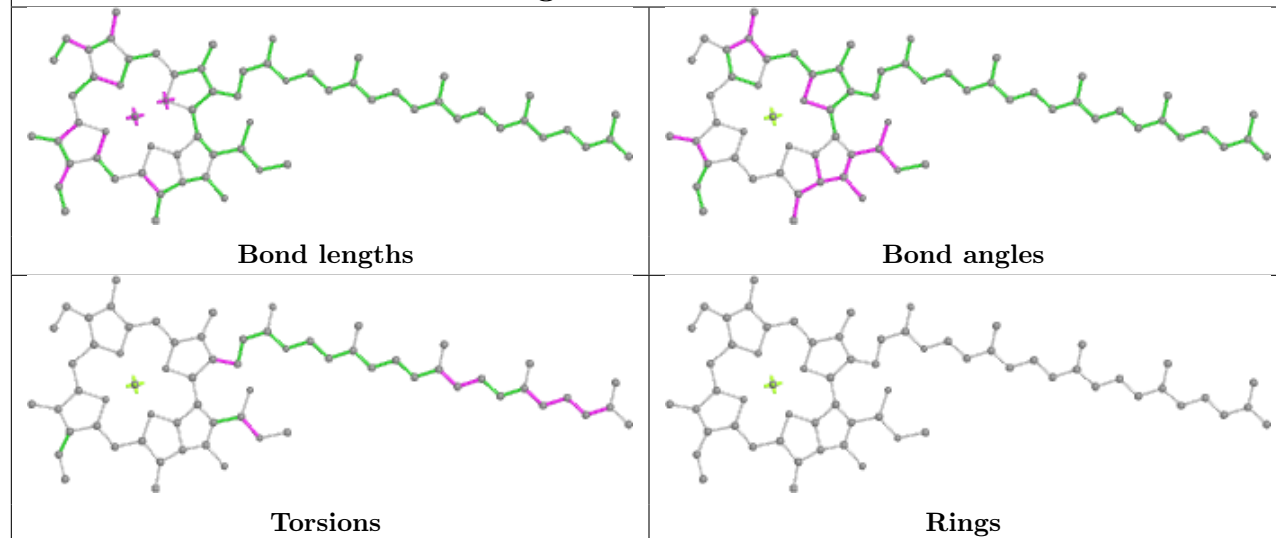
## Ligand CLA a 604



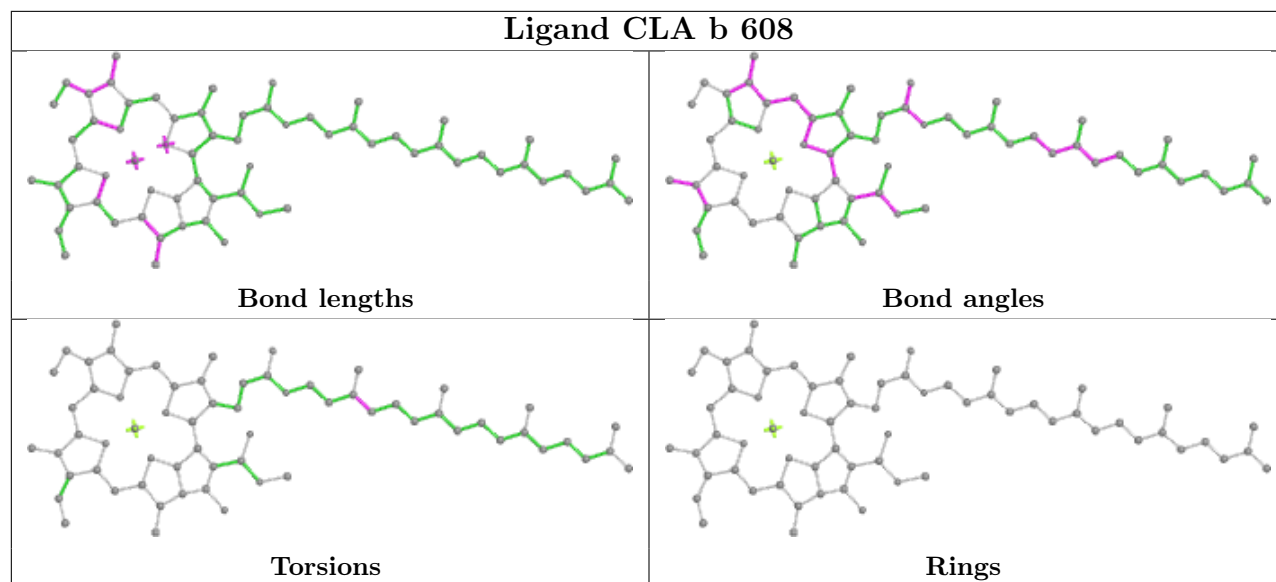
## Ligand BCR b 618



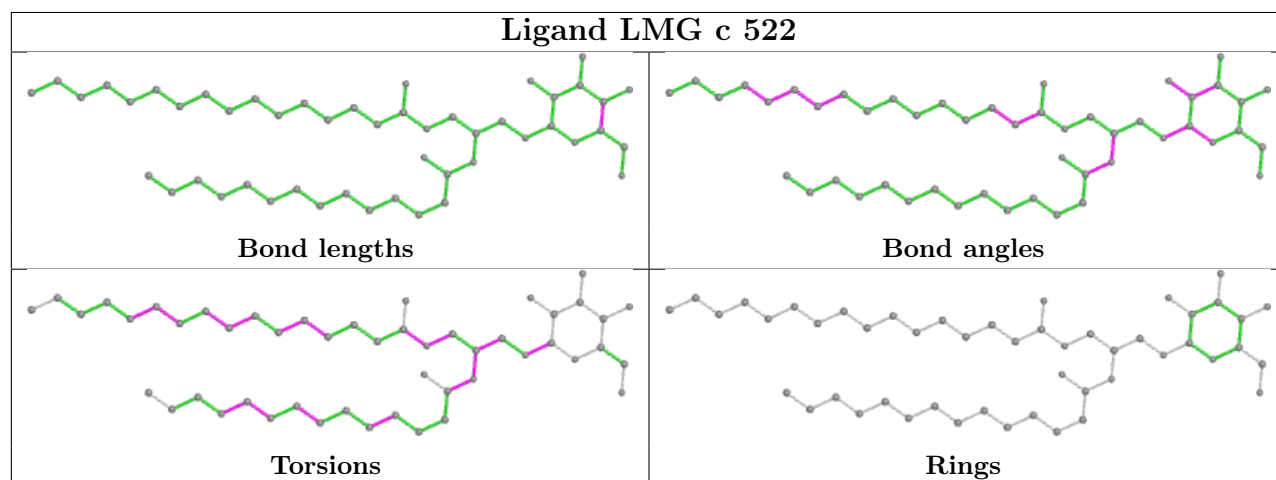
## Ligand CLA c 511



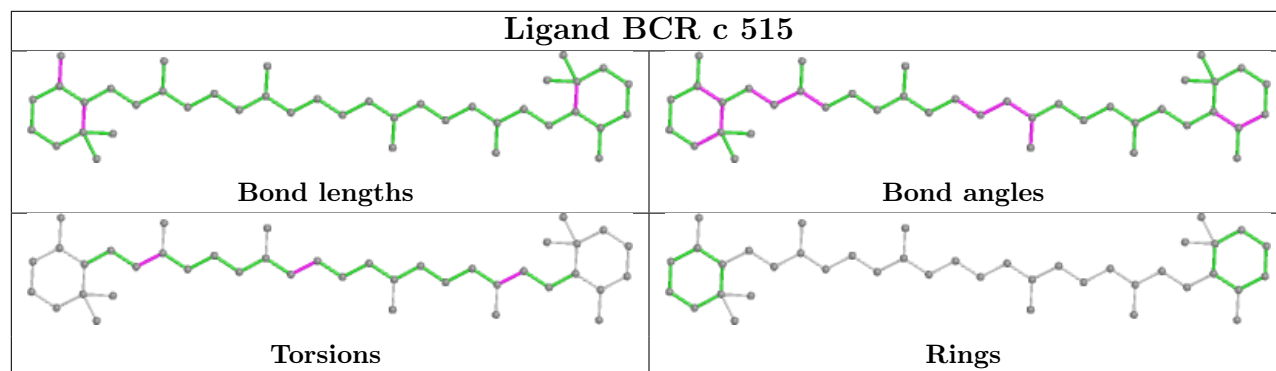
## Ligand CLA b 608



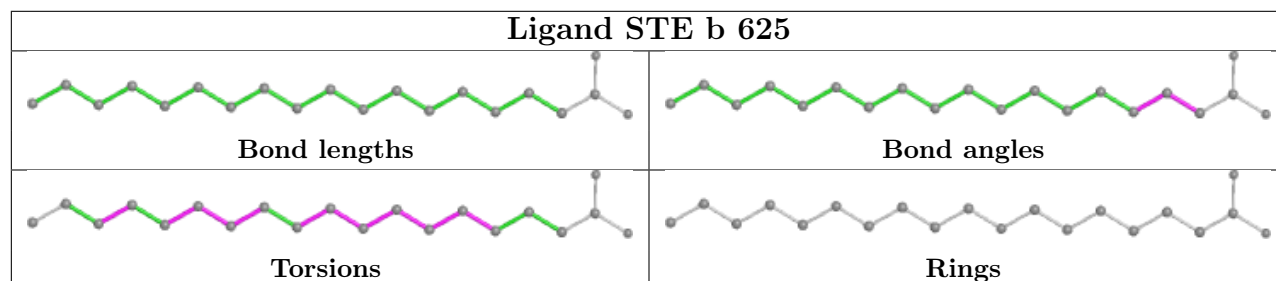
## Ligand LMG c 522

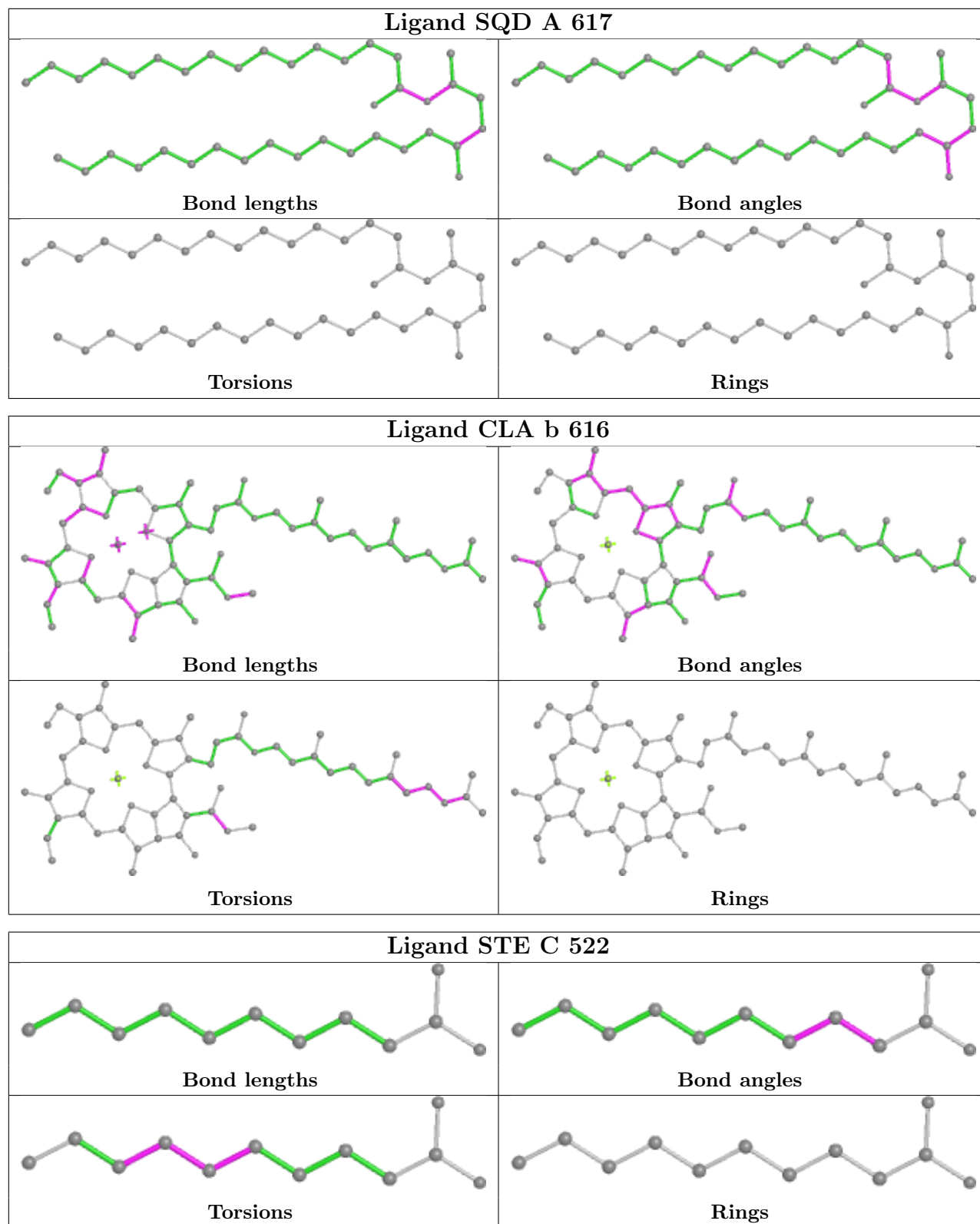


## Ligand BCR c 515

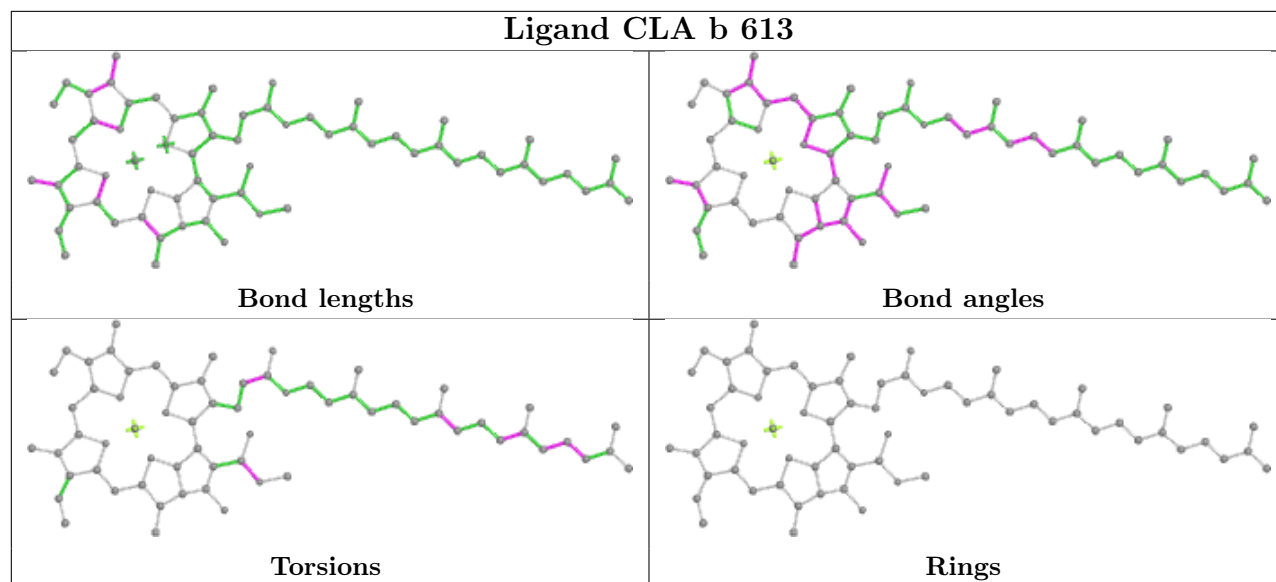


## Ligand STE b 625

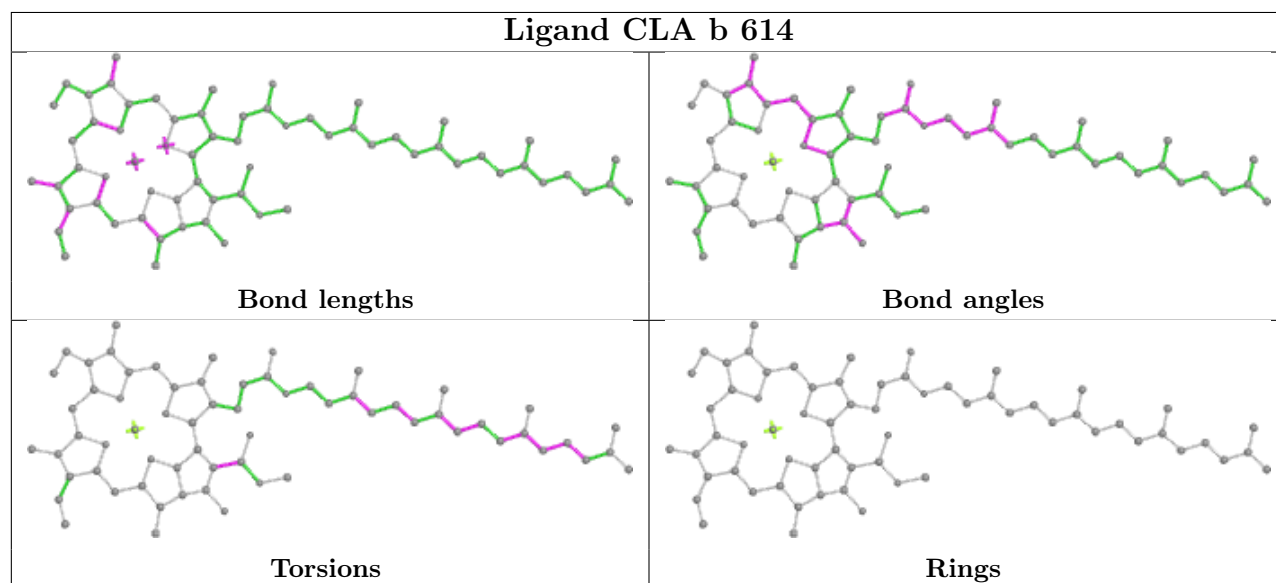




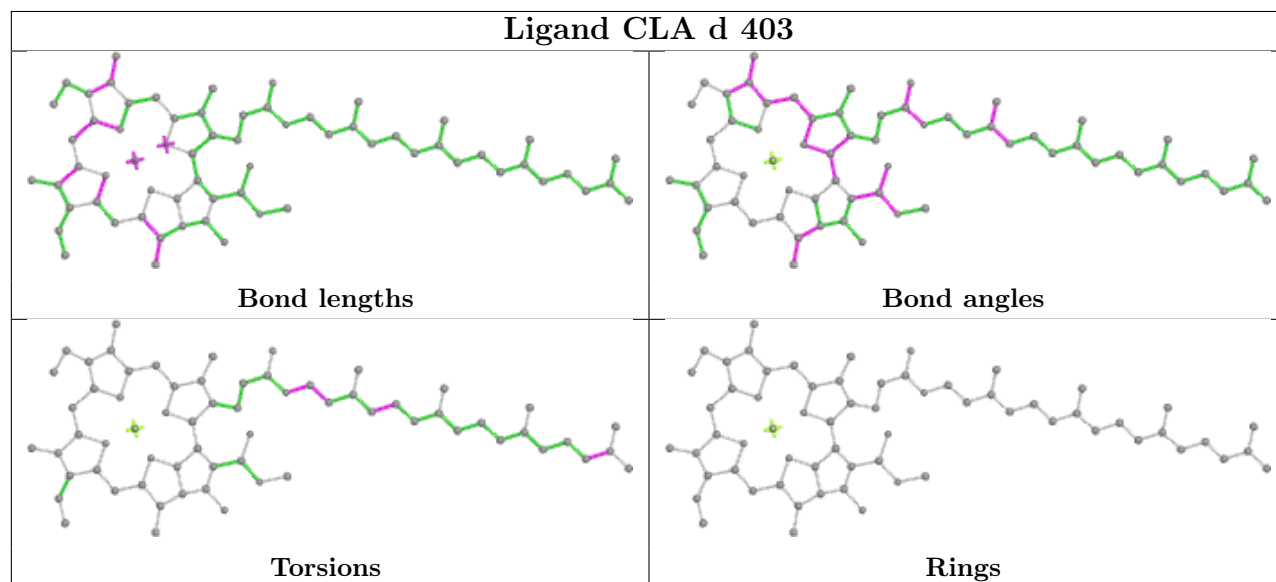
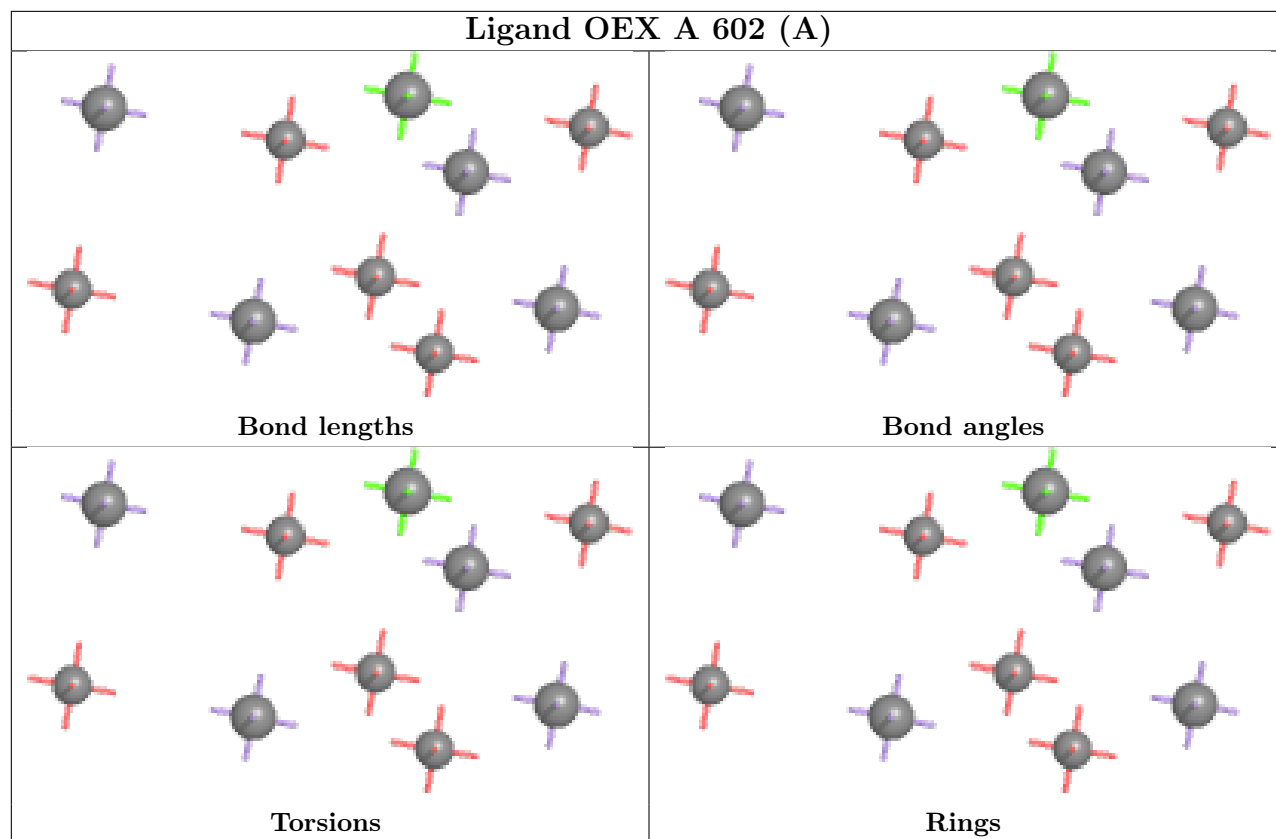
## Ligand CLA b 613

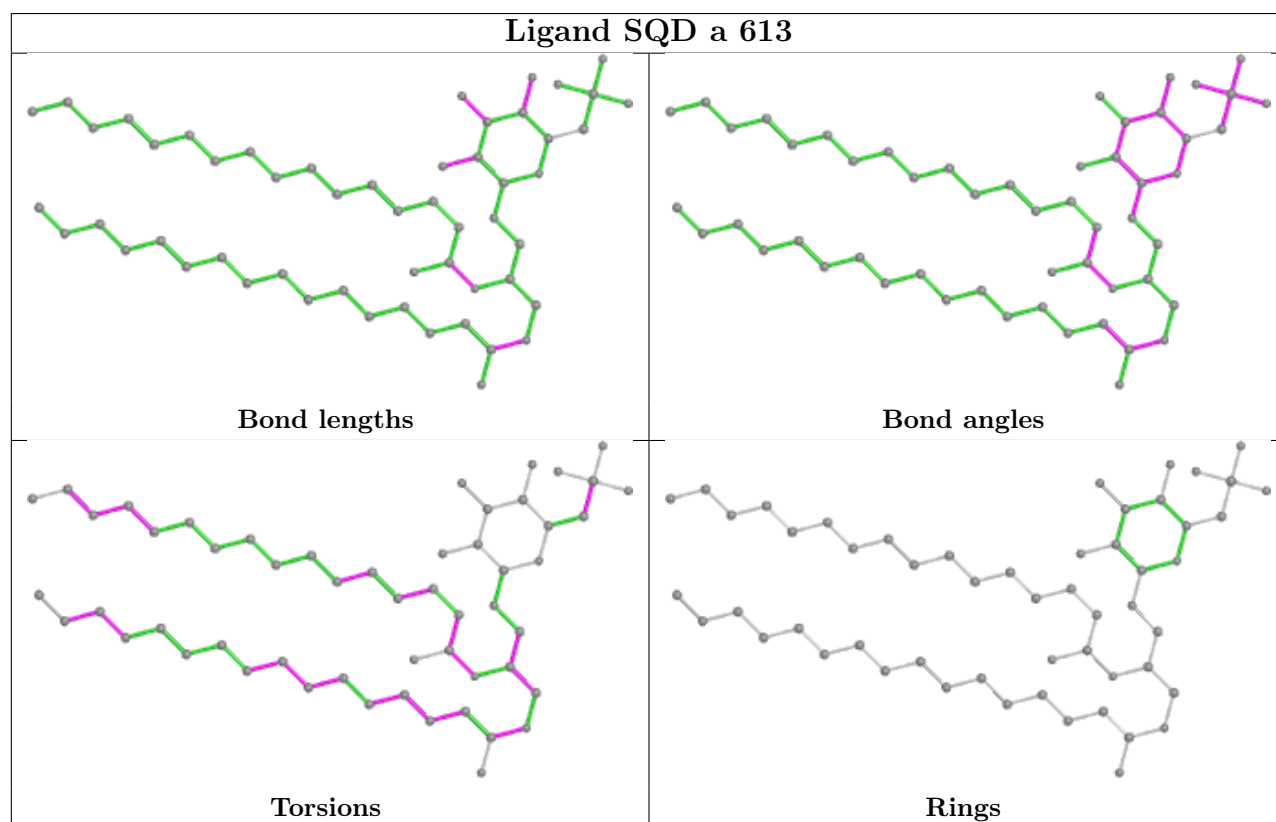
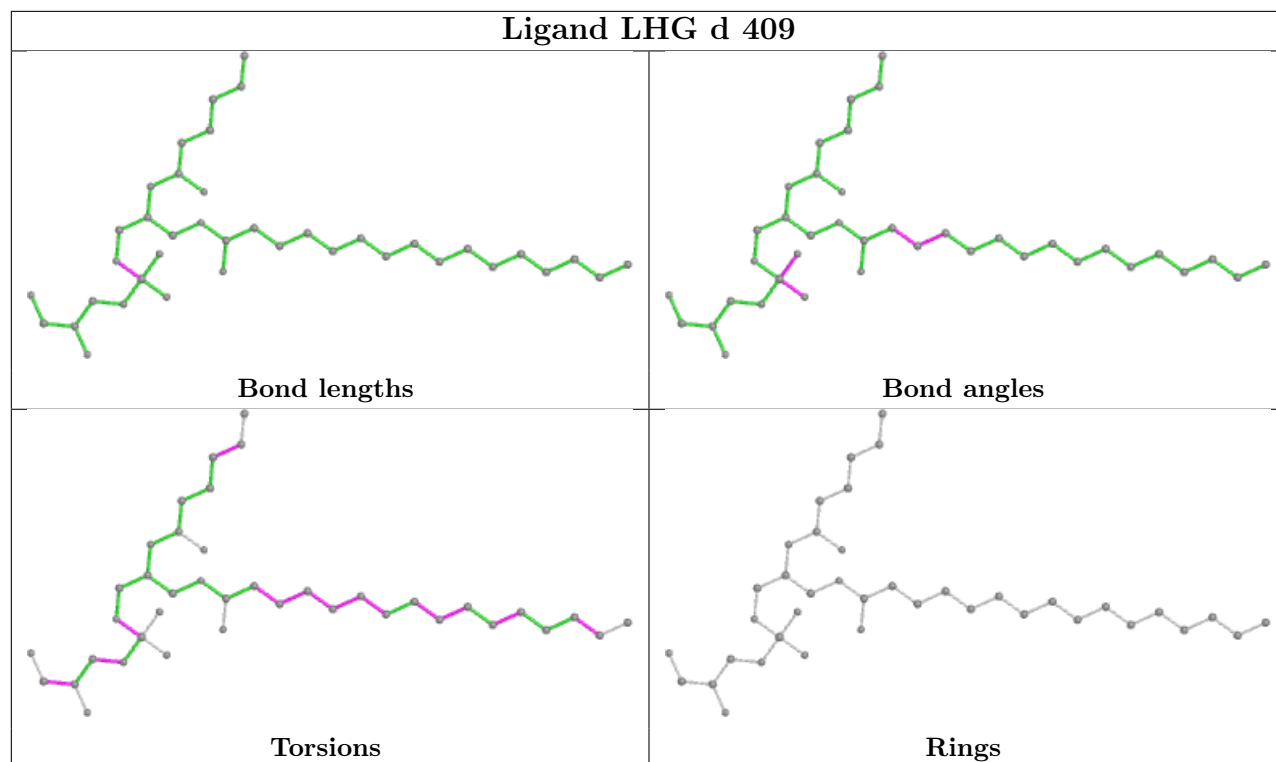


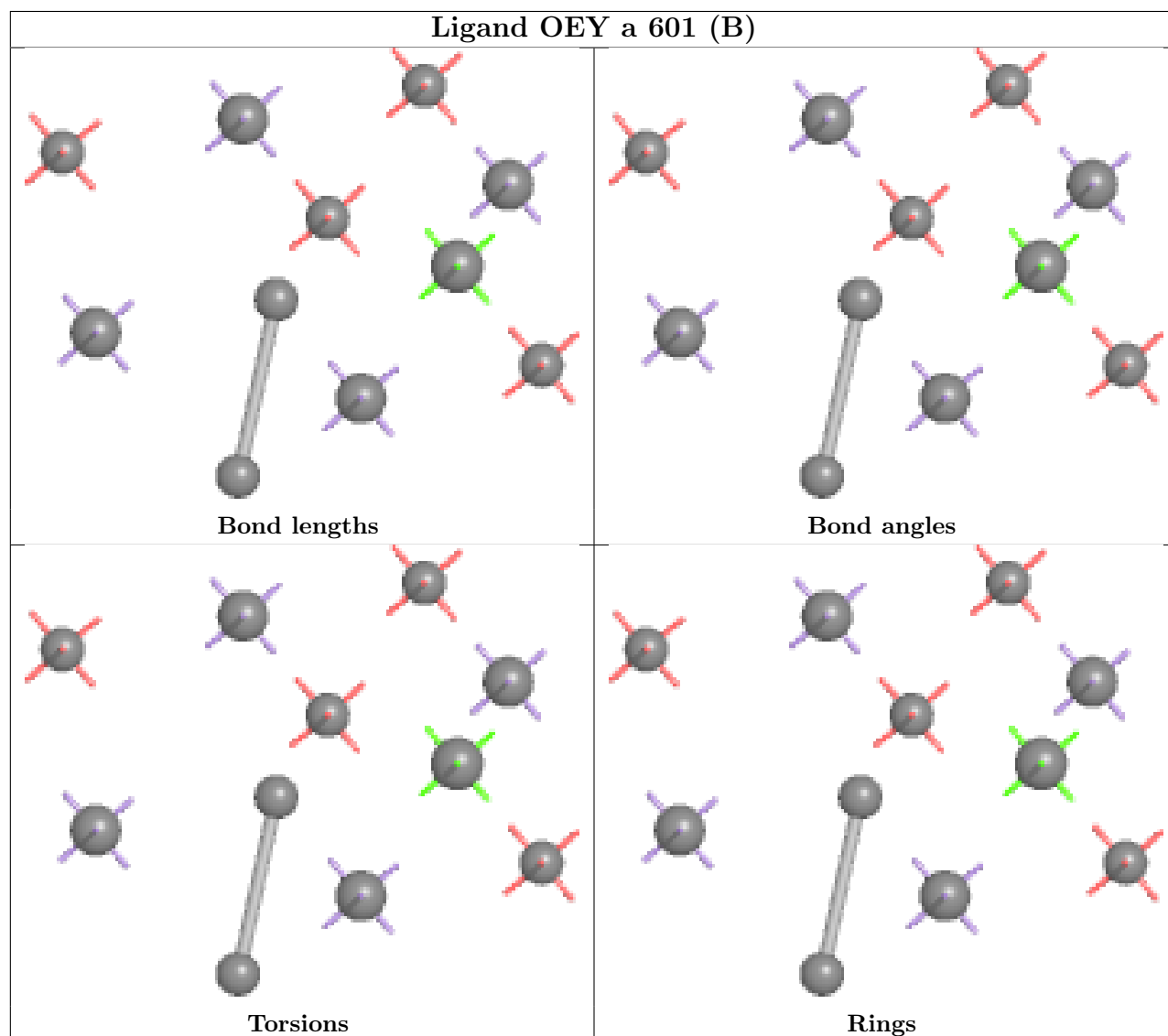
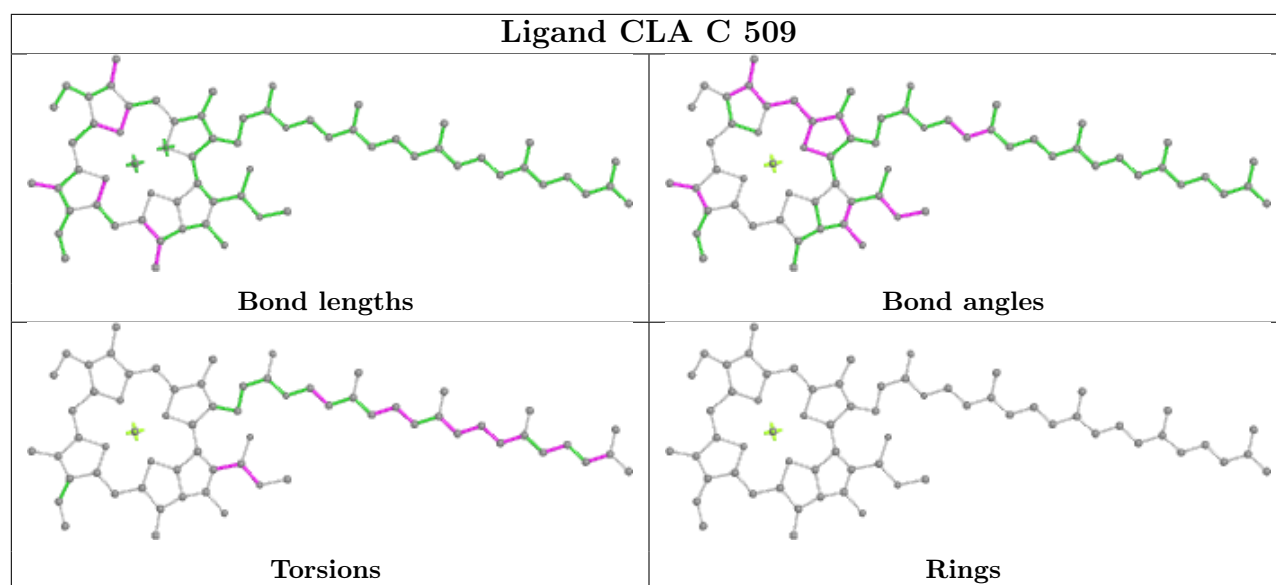
## Ligand CLA b 614

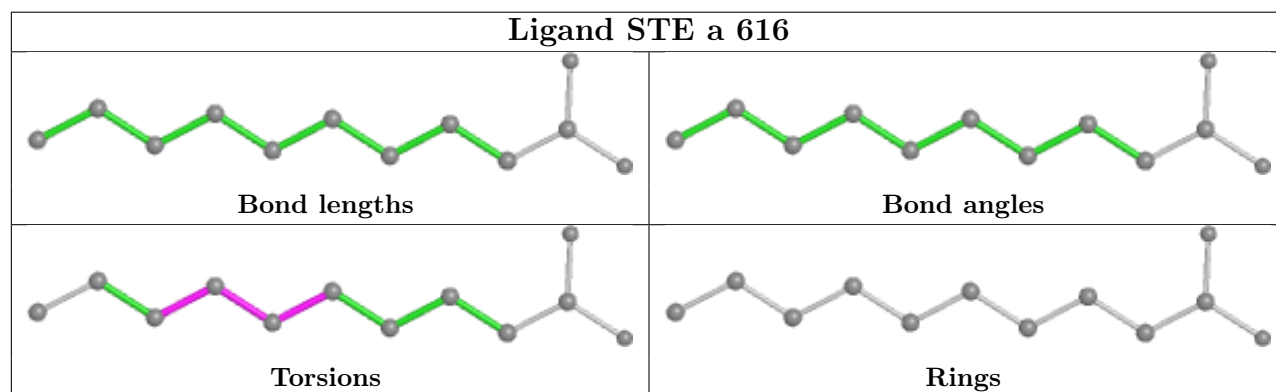
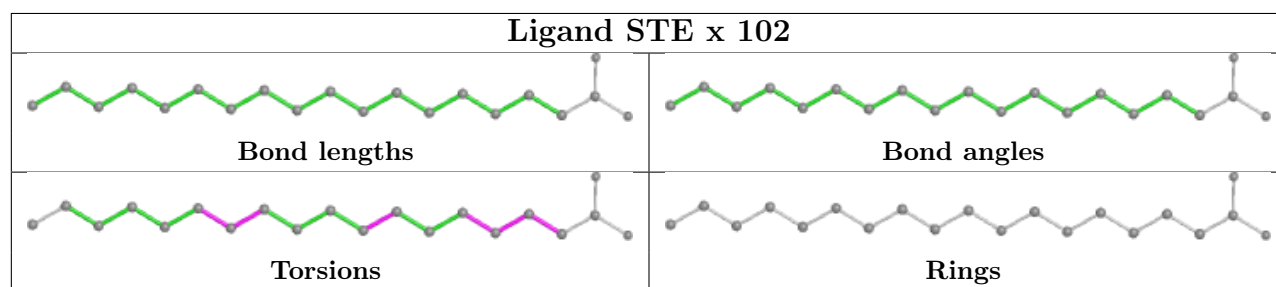
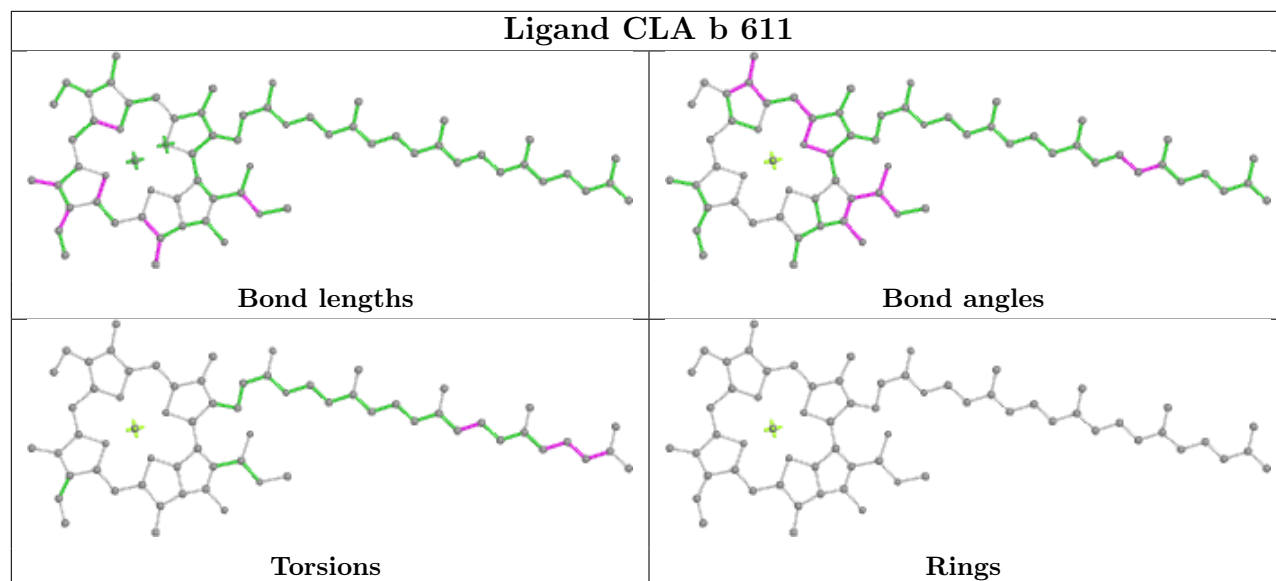
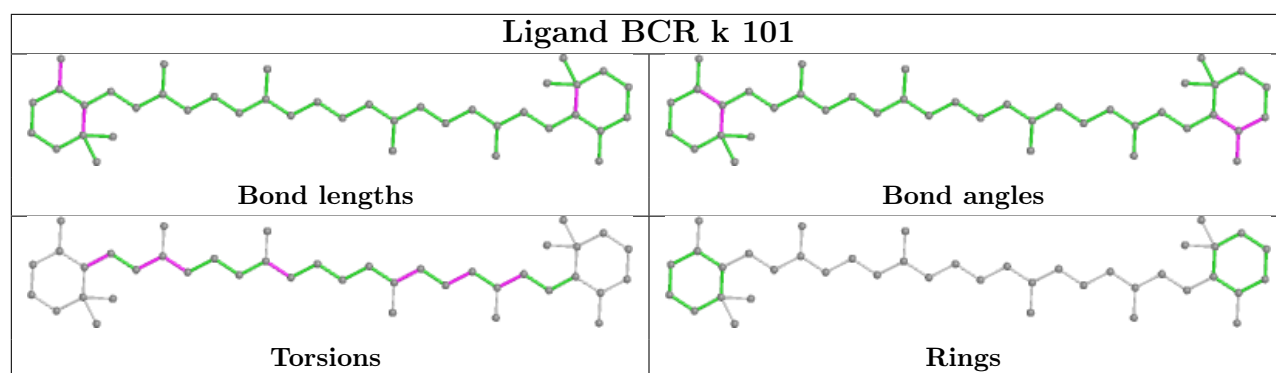




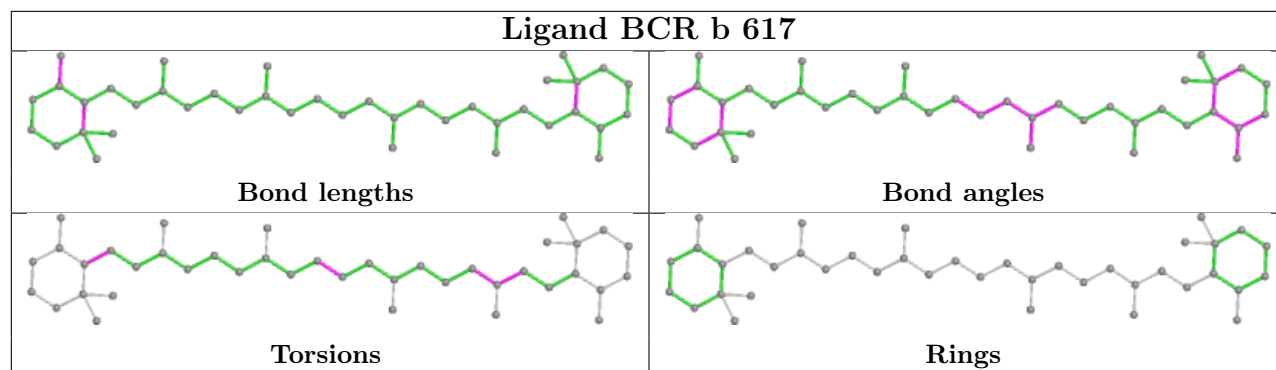




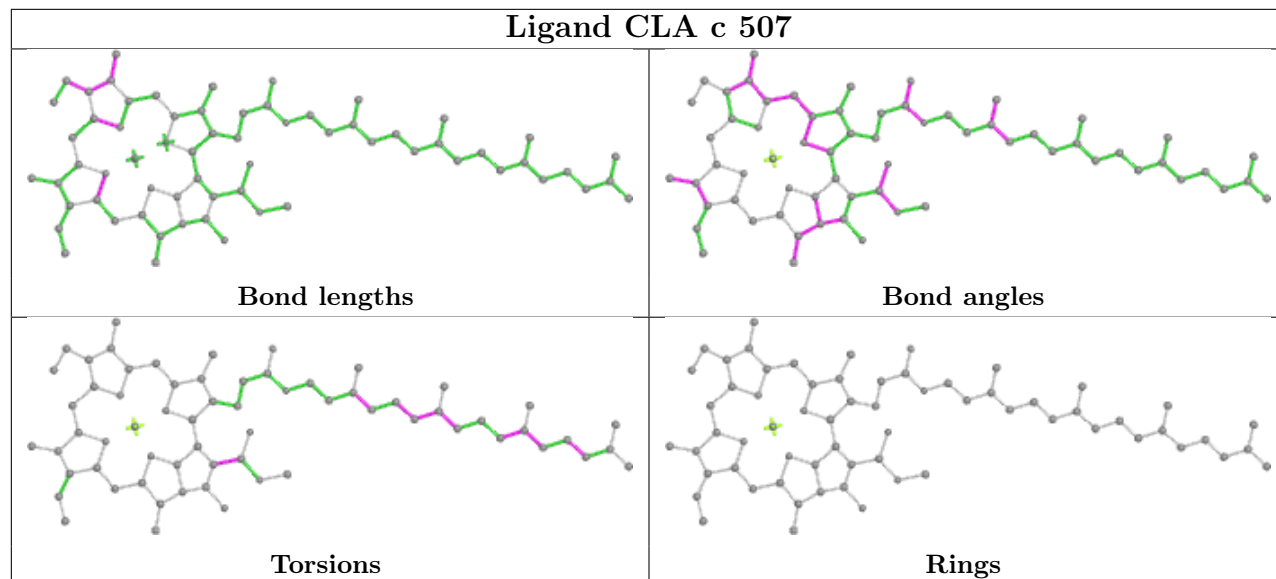




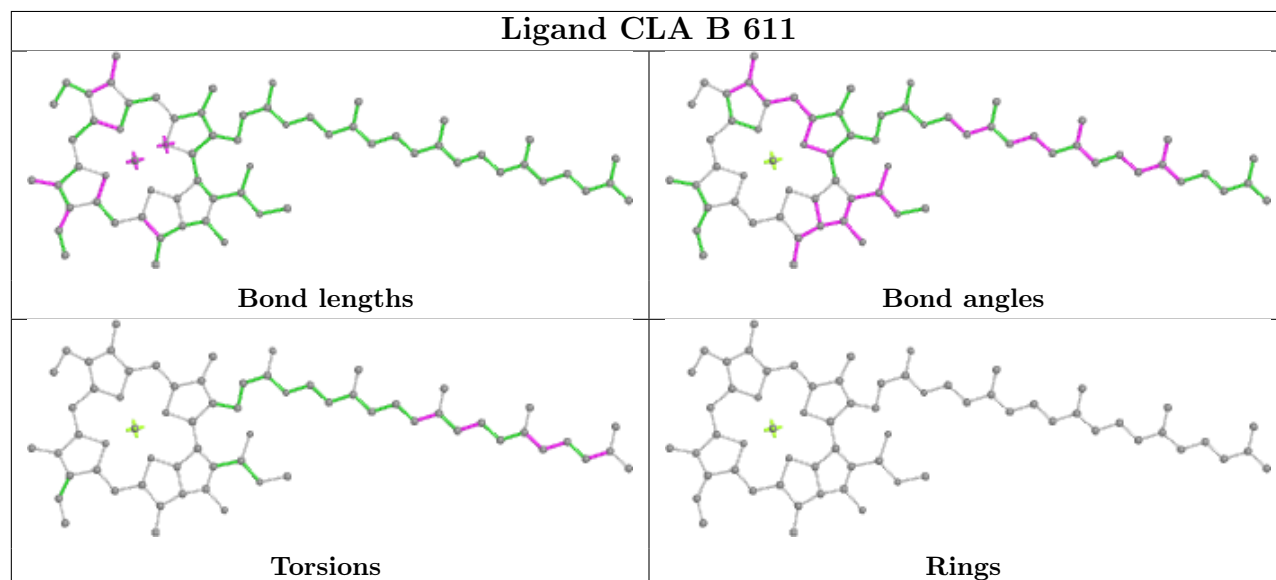
## Ligand BCR b 617

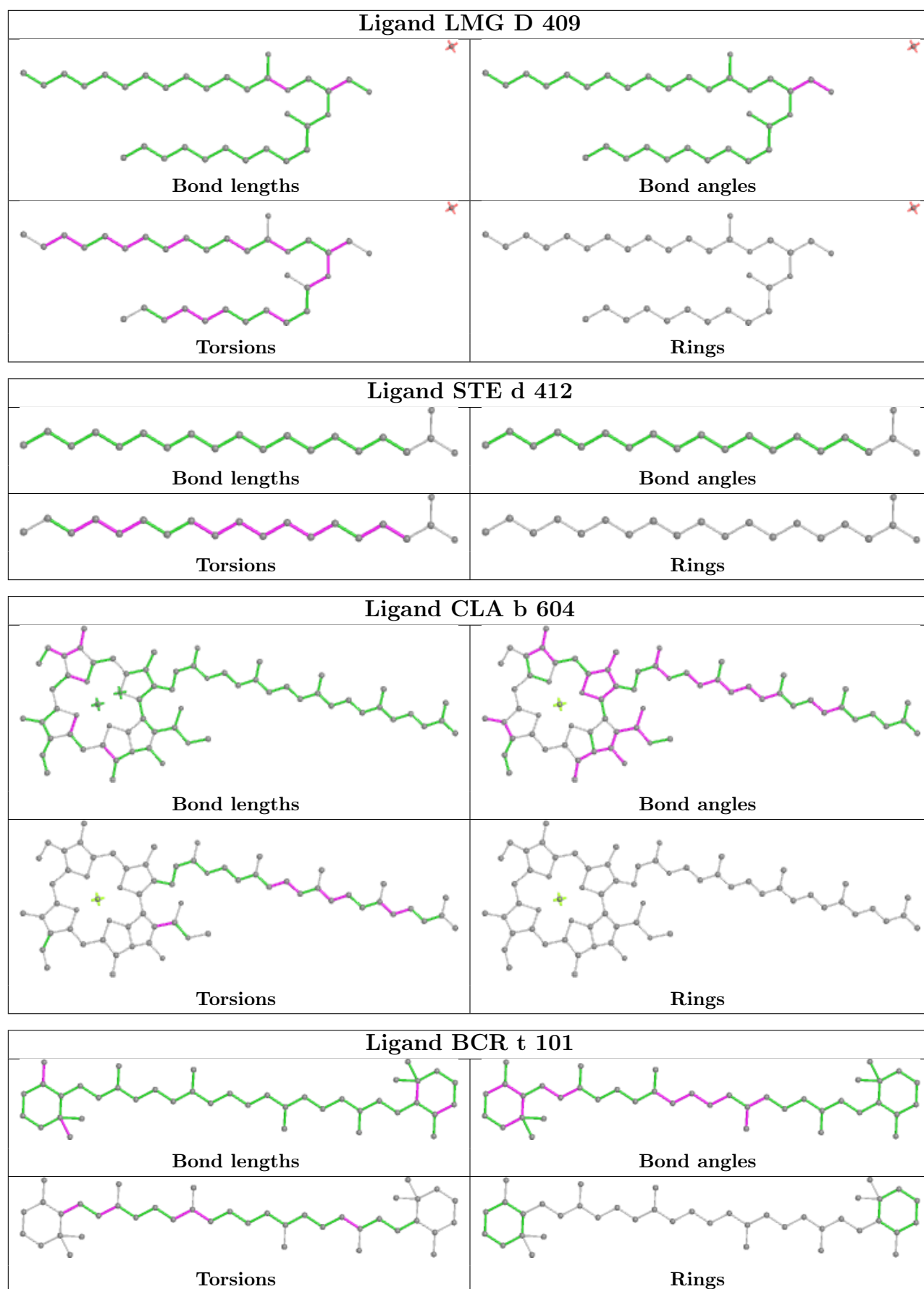


## Ligand CLA c 507

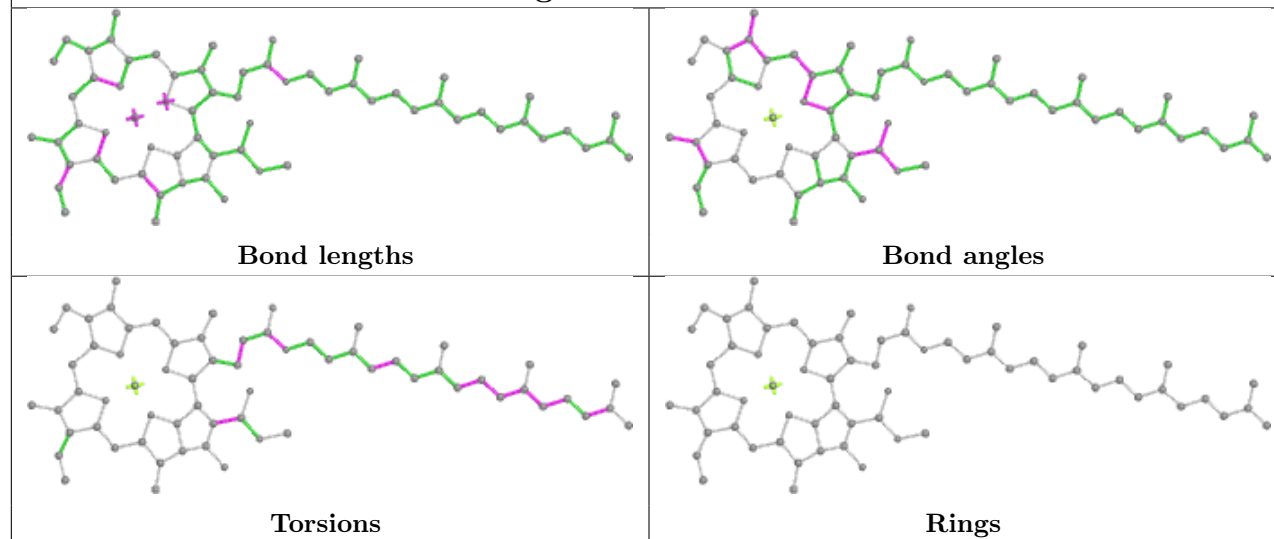


## Ligand CLA B 611

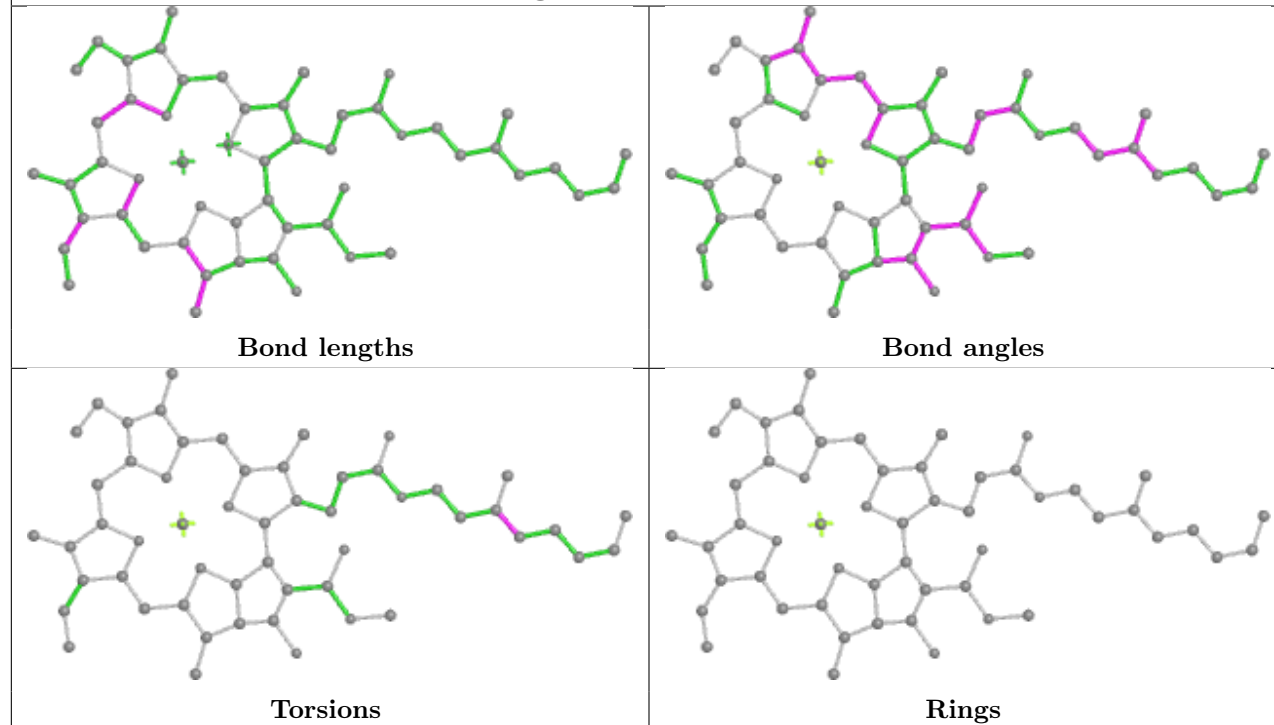




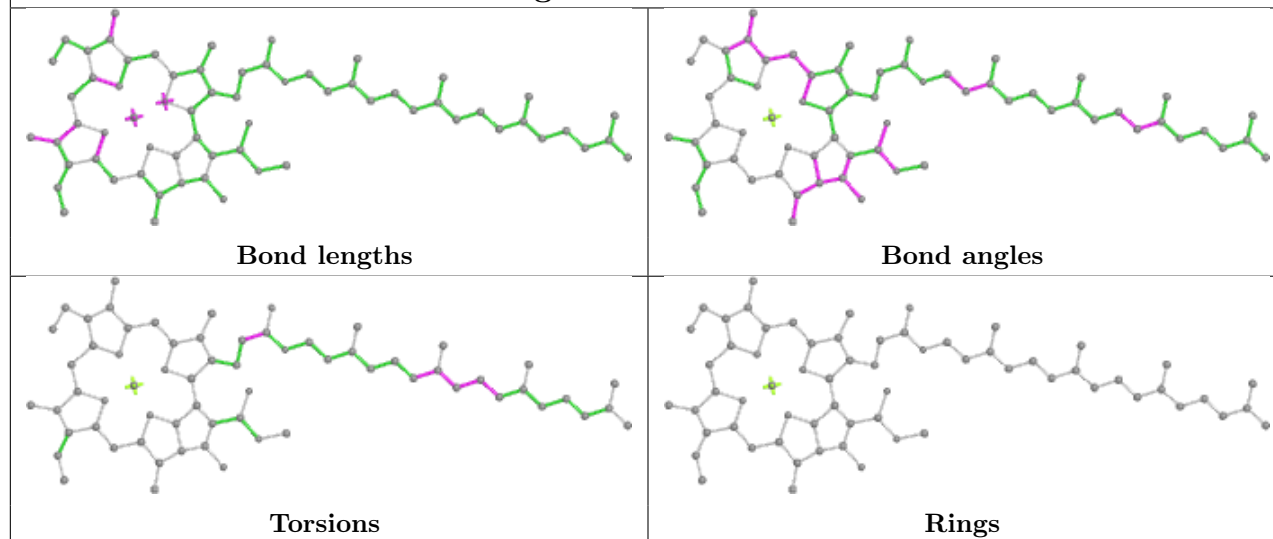
## Ligand CLA b 601



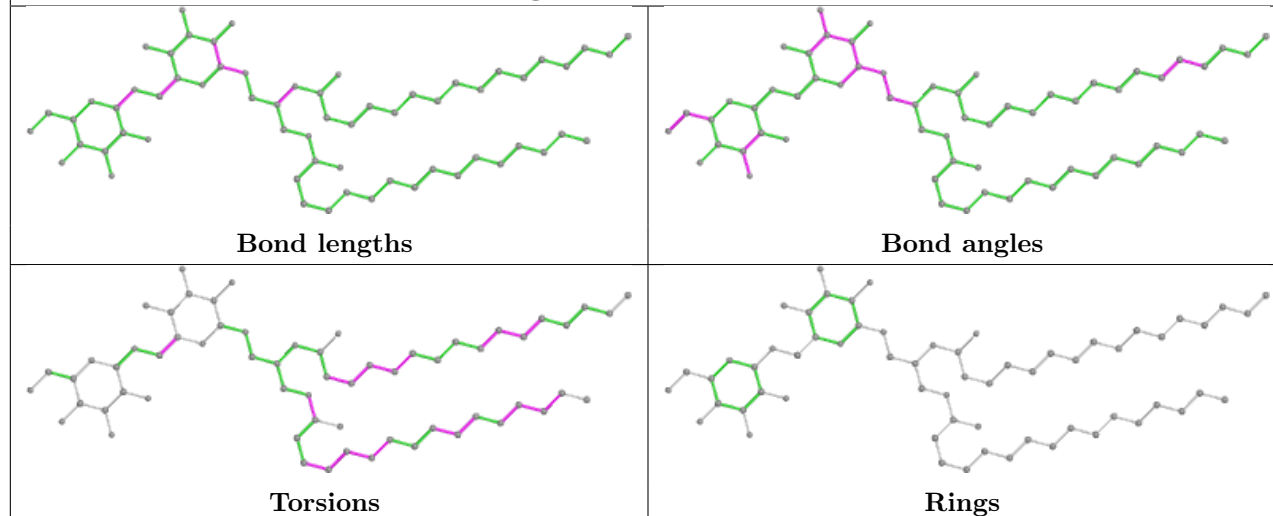
## Ligand CLA A 608



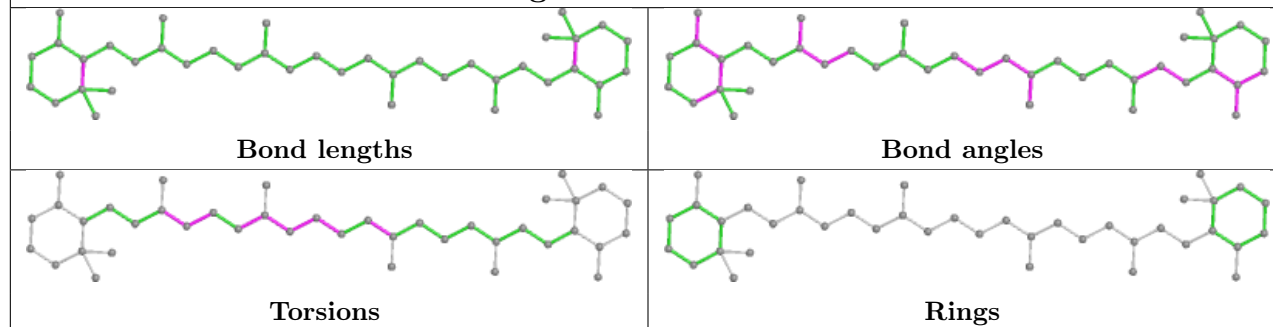
## Ligand CLA b 612



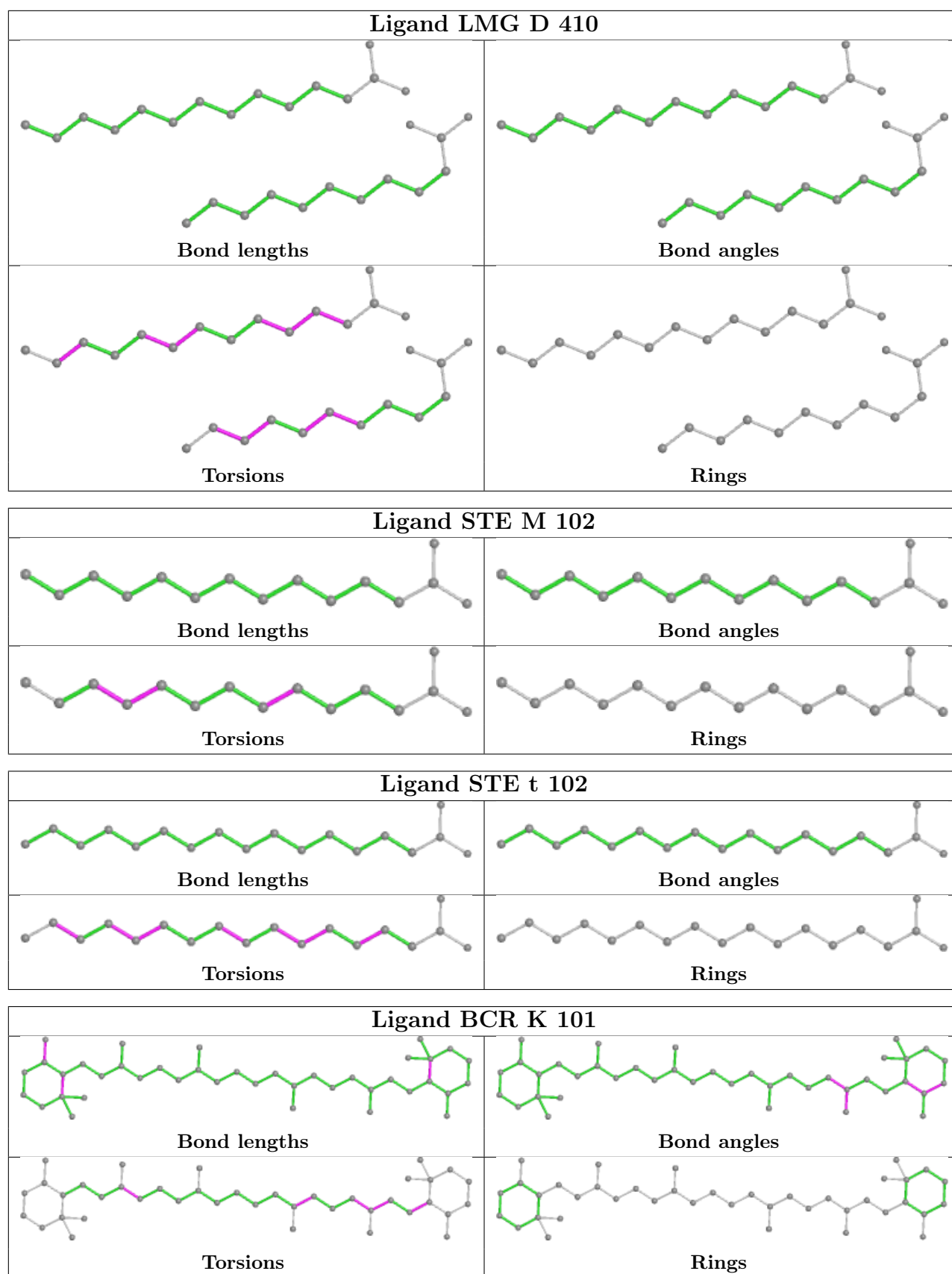
## Ligand DGD C 518

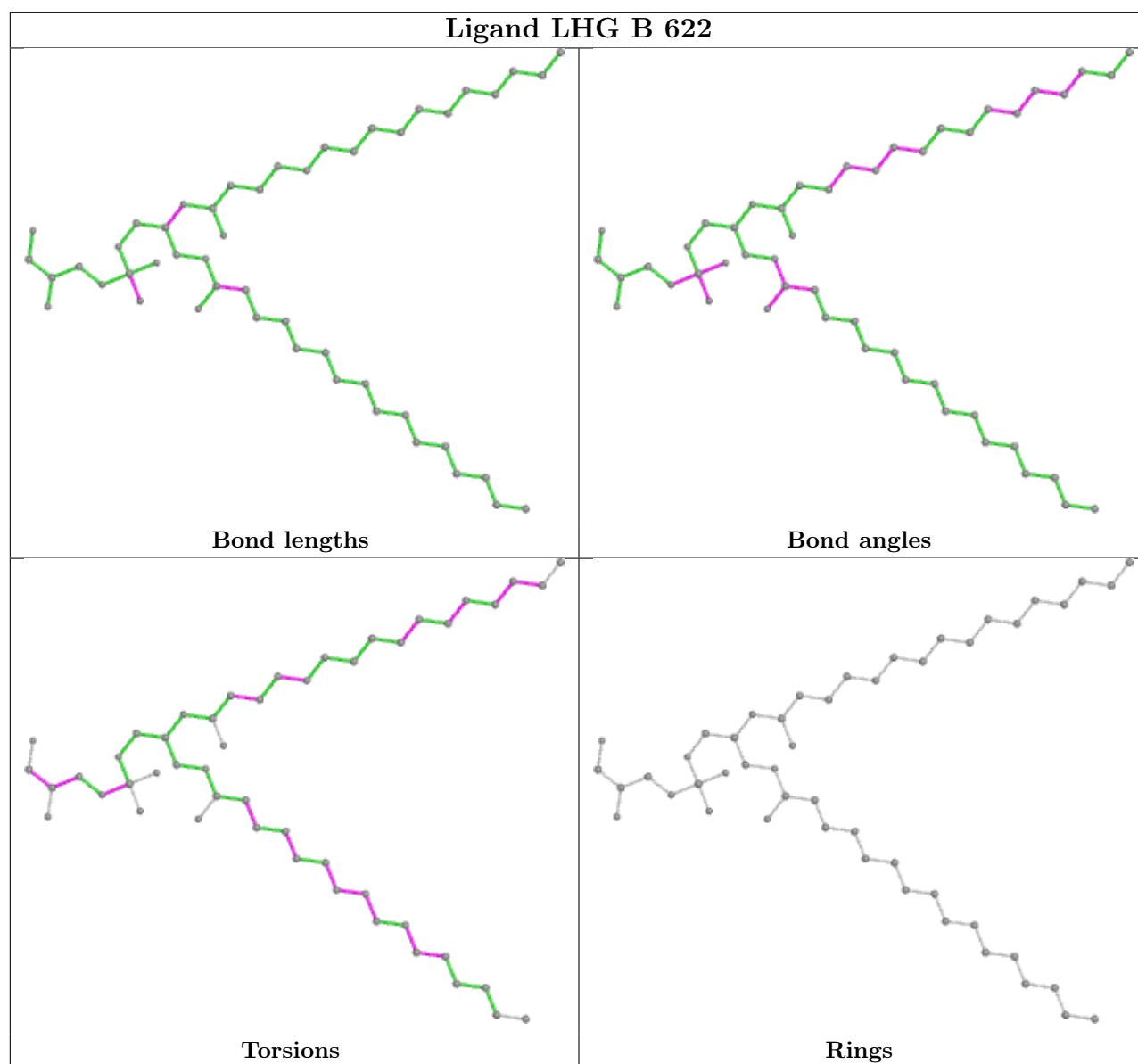


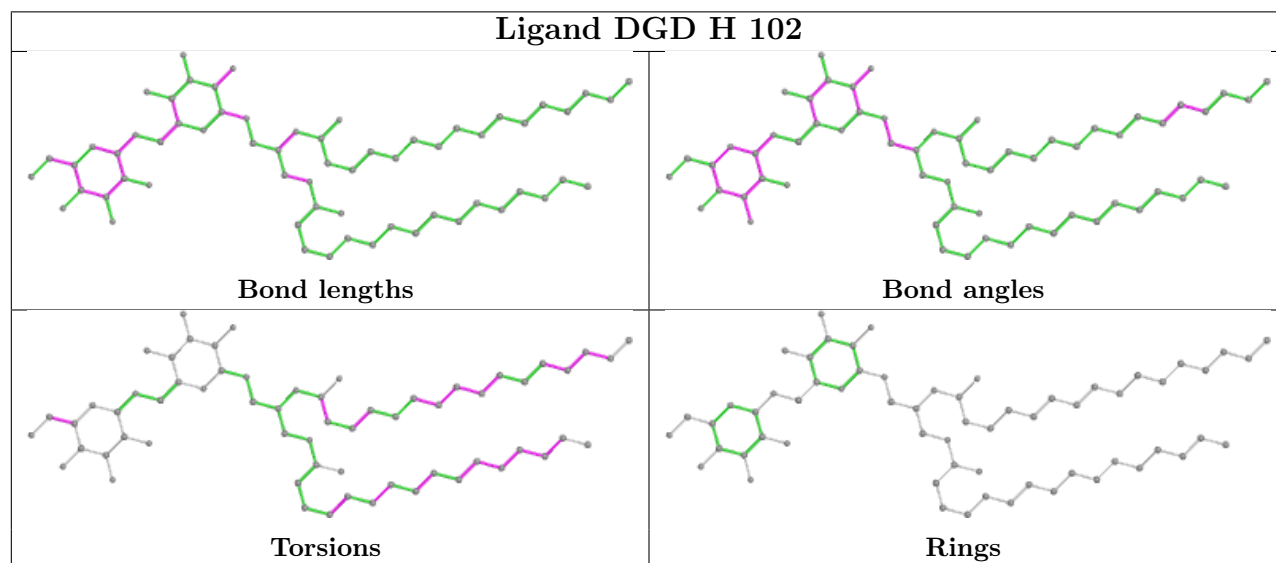
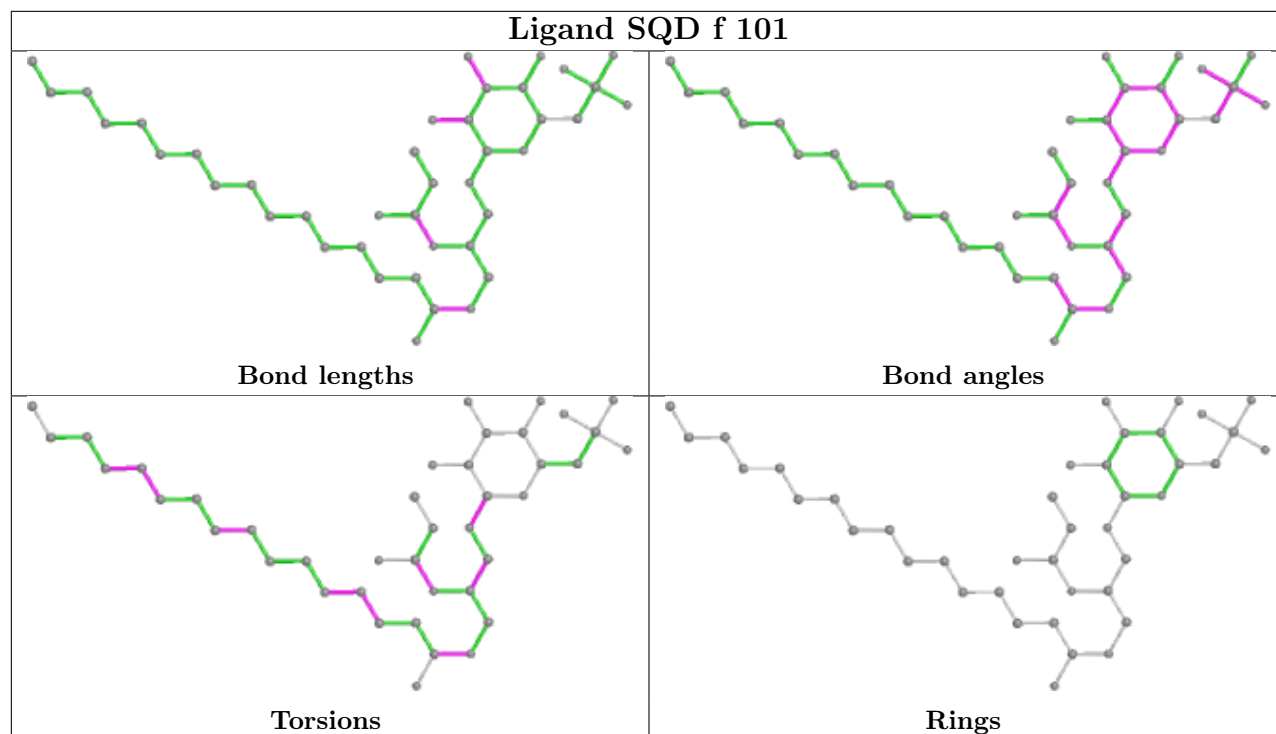
## Ligand BCR C 514

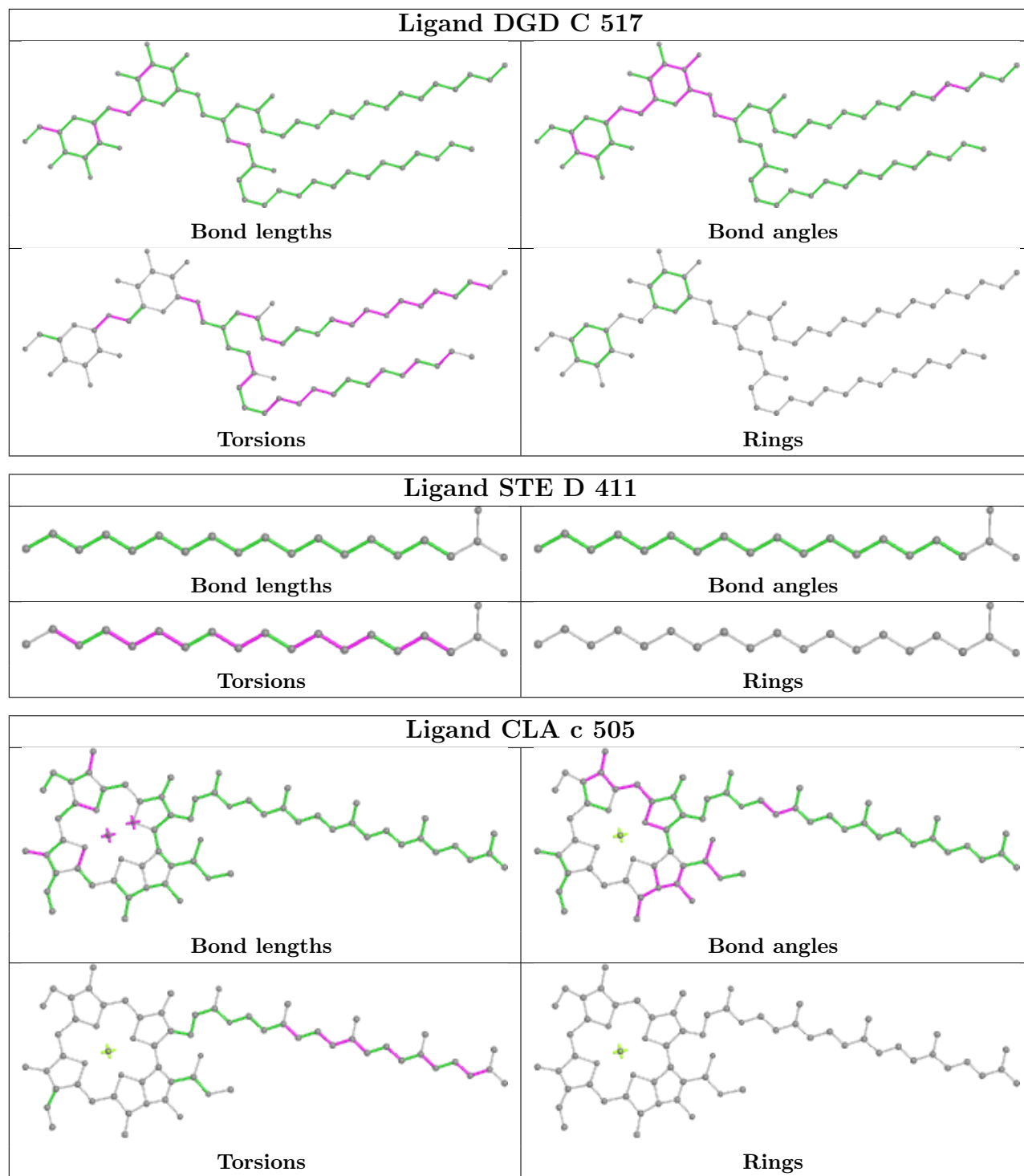




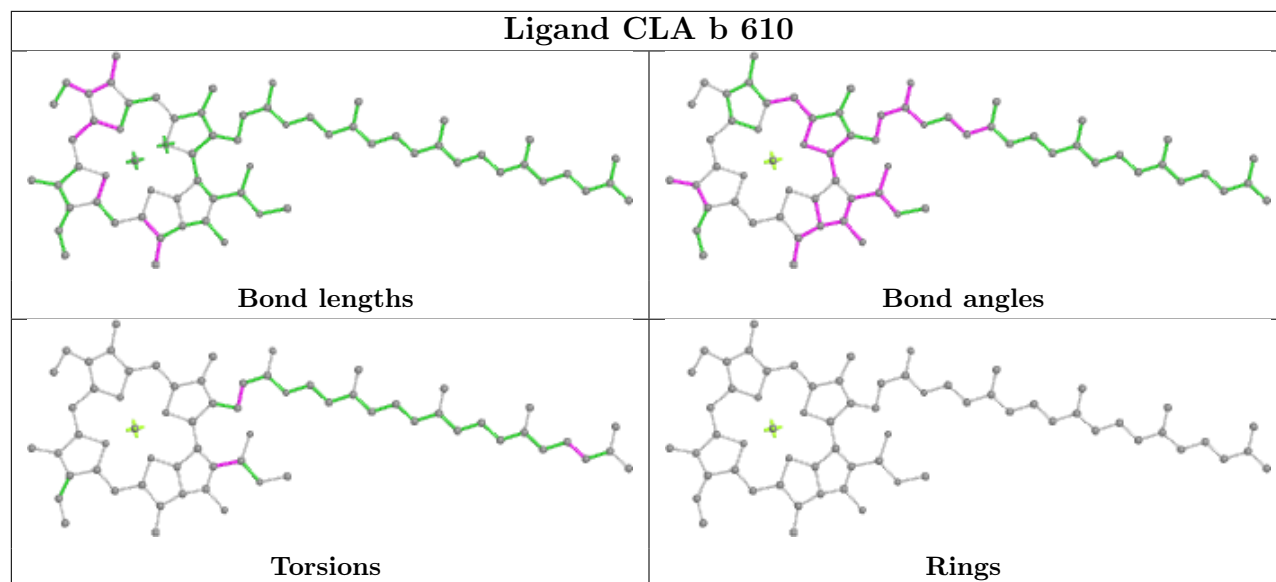




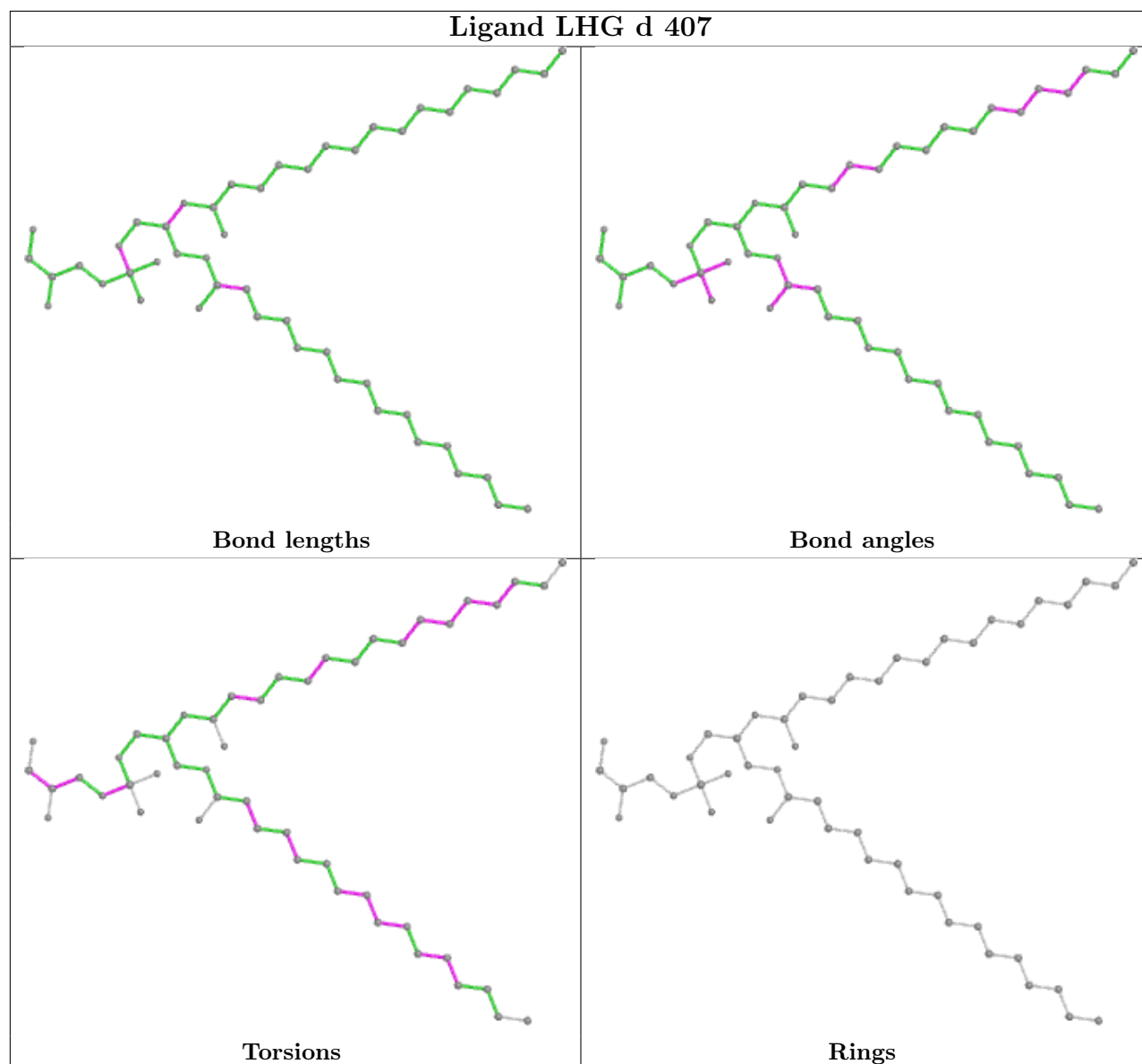




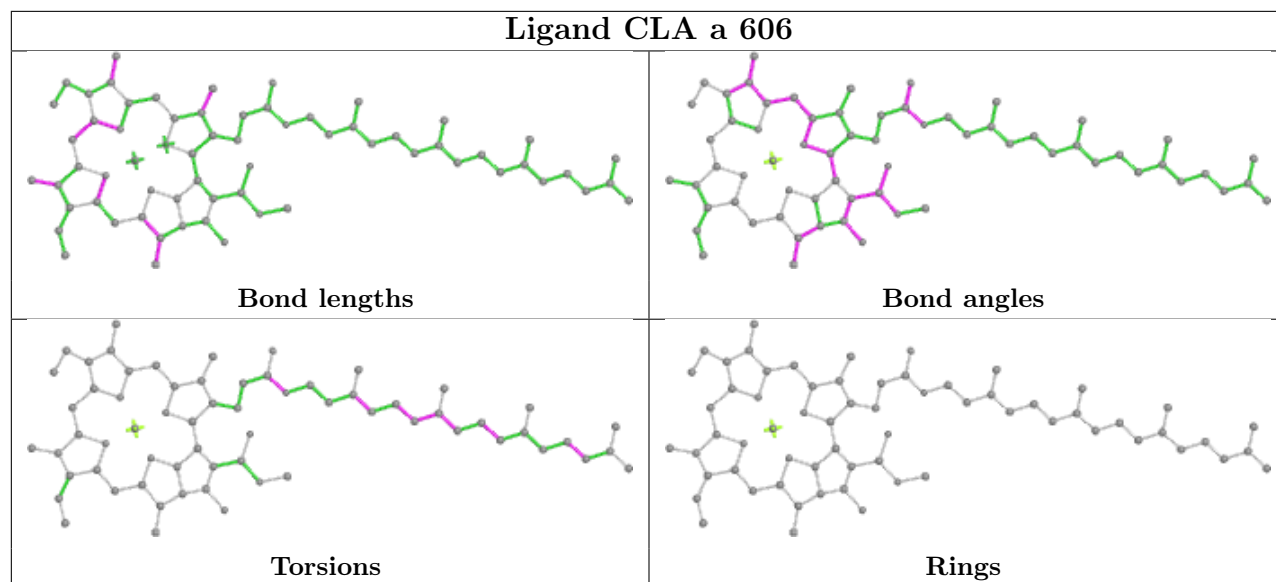
## Ligand CLA b 610



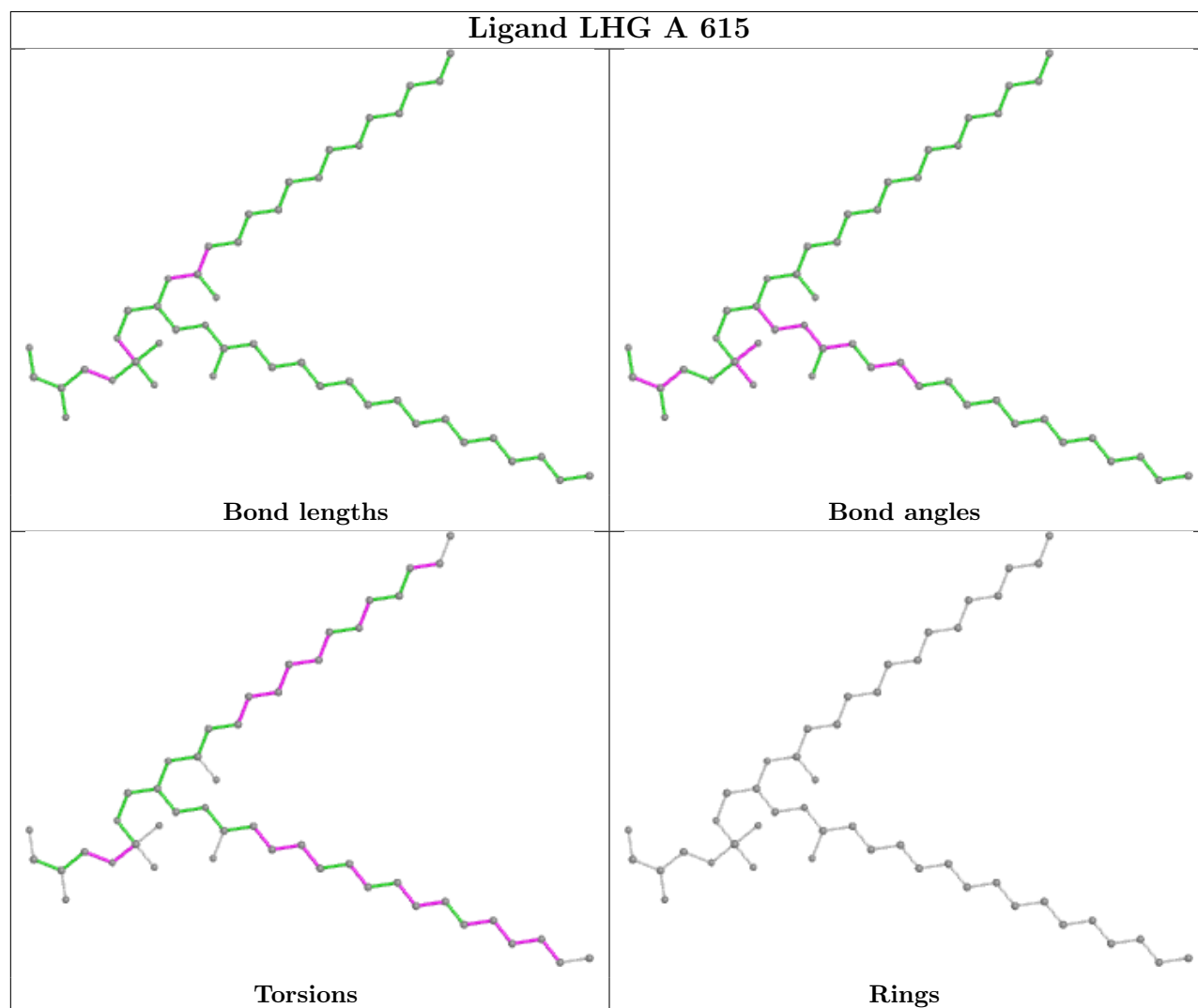
## Ligand LHG d 407

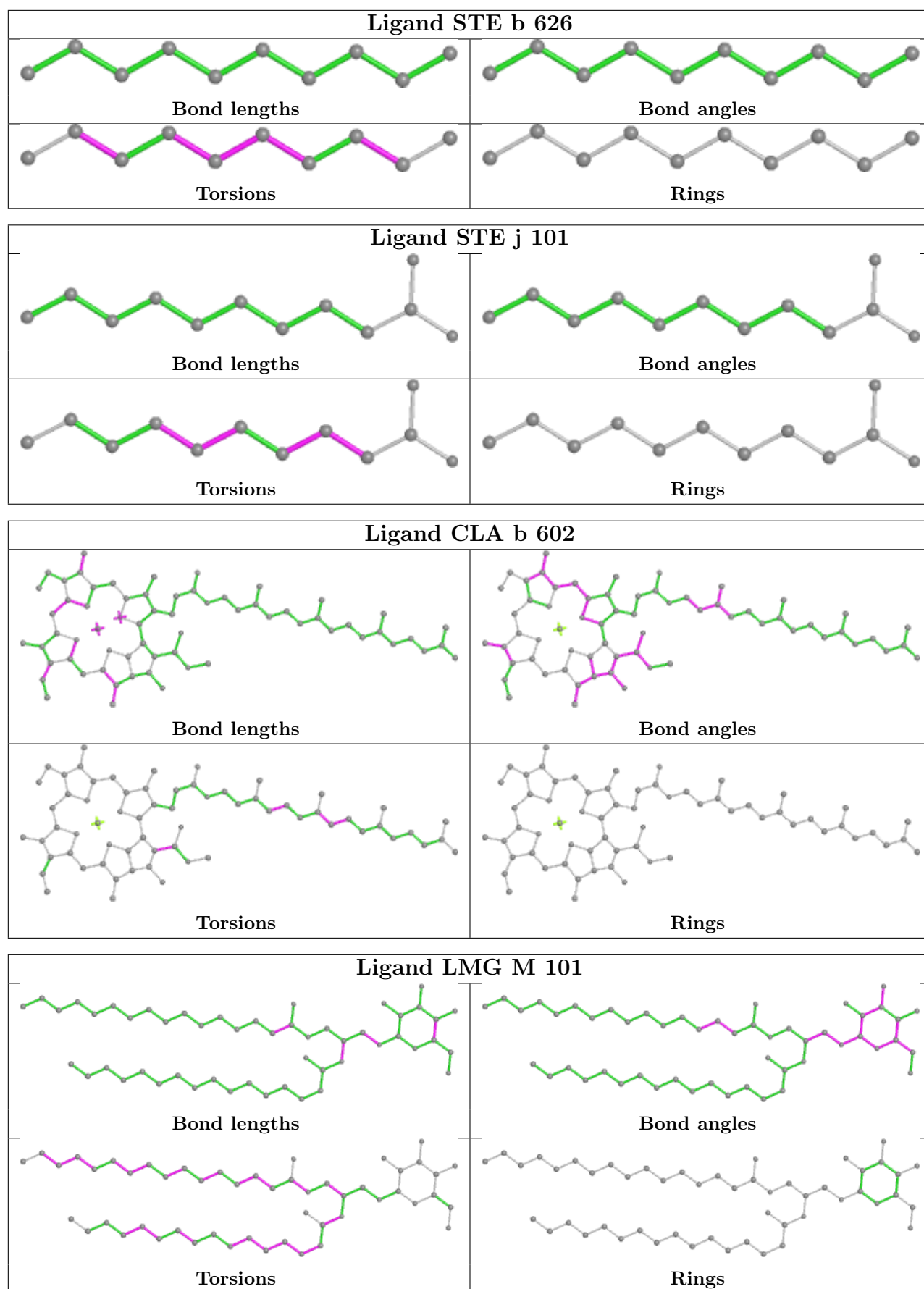


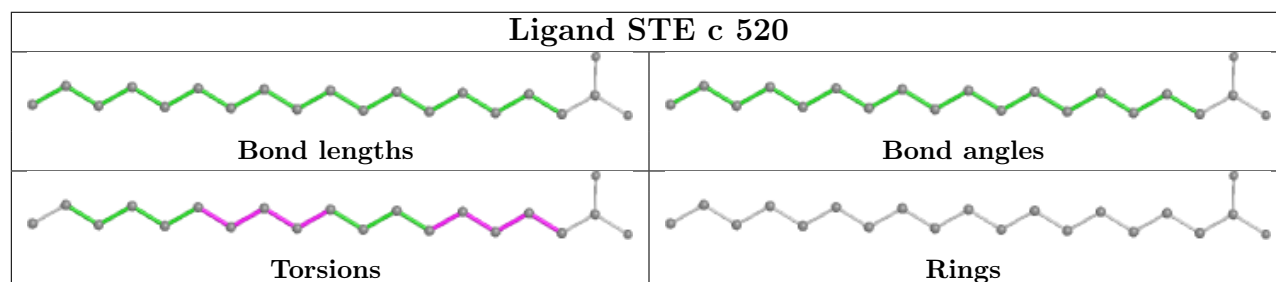
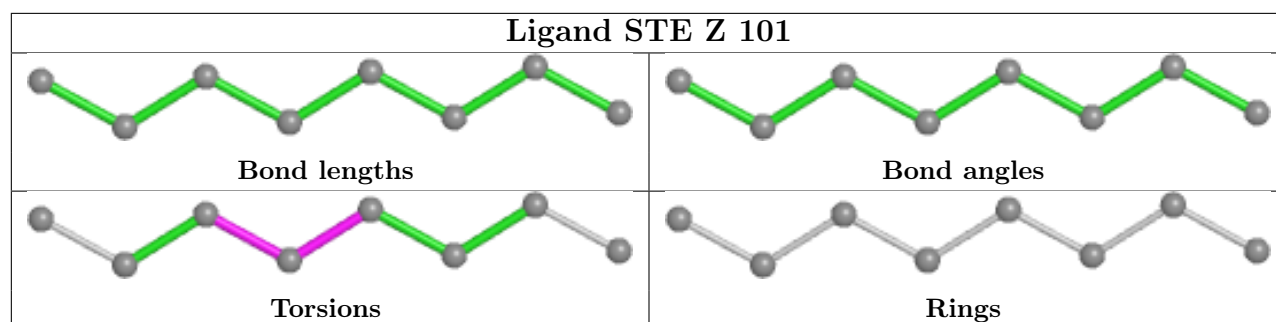
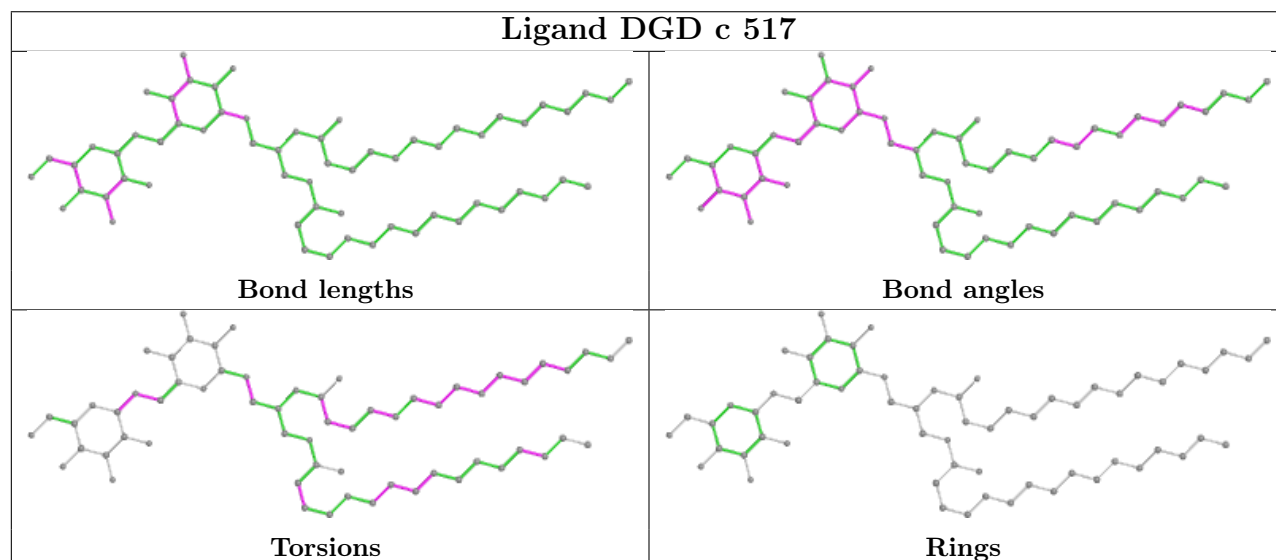
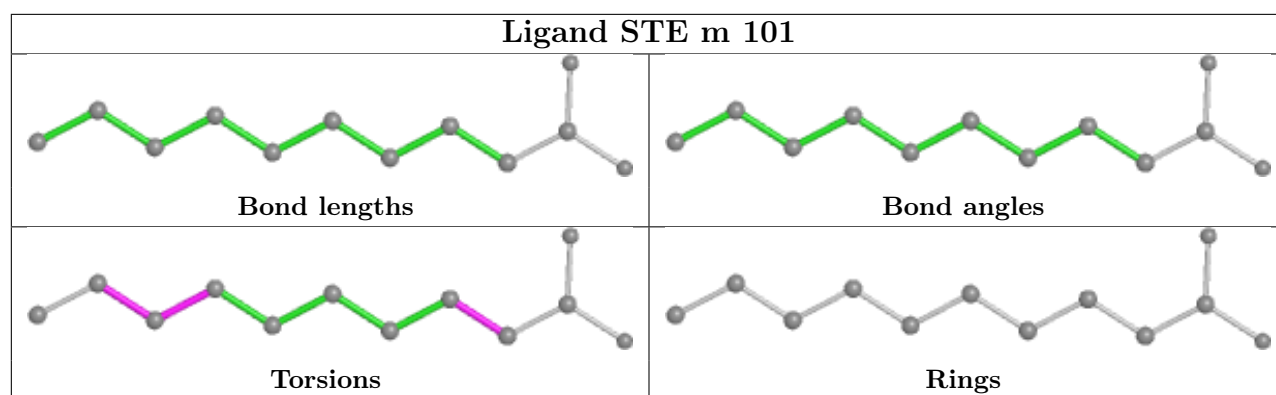
## Ligand CLA a 606



## Ligand LHG A 615

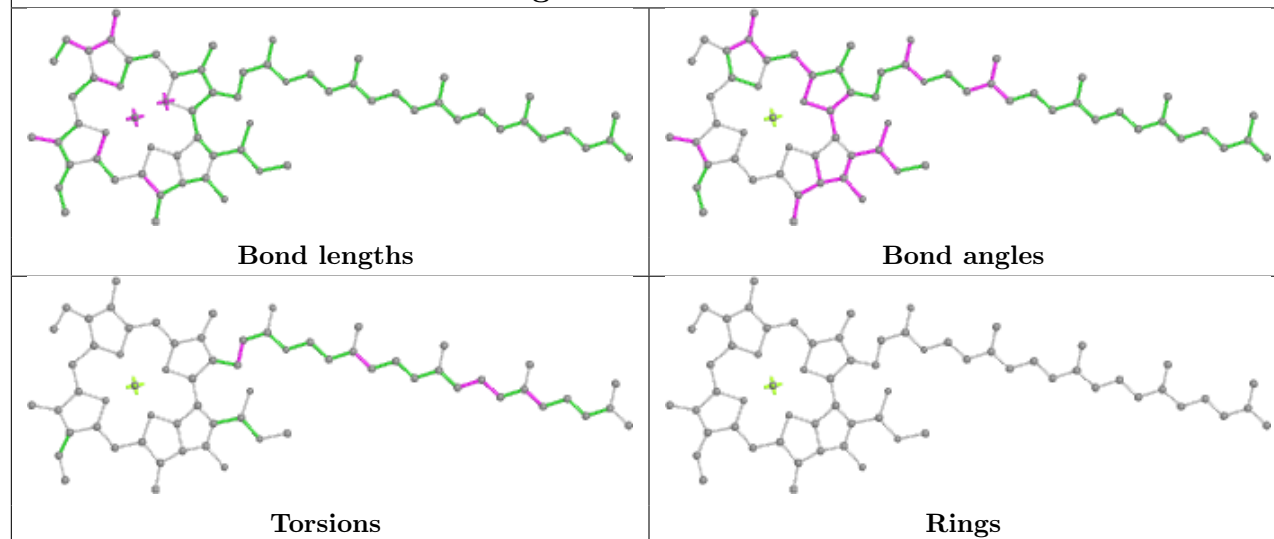




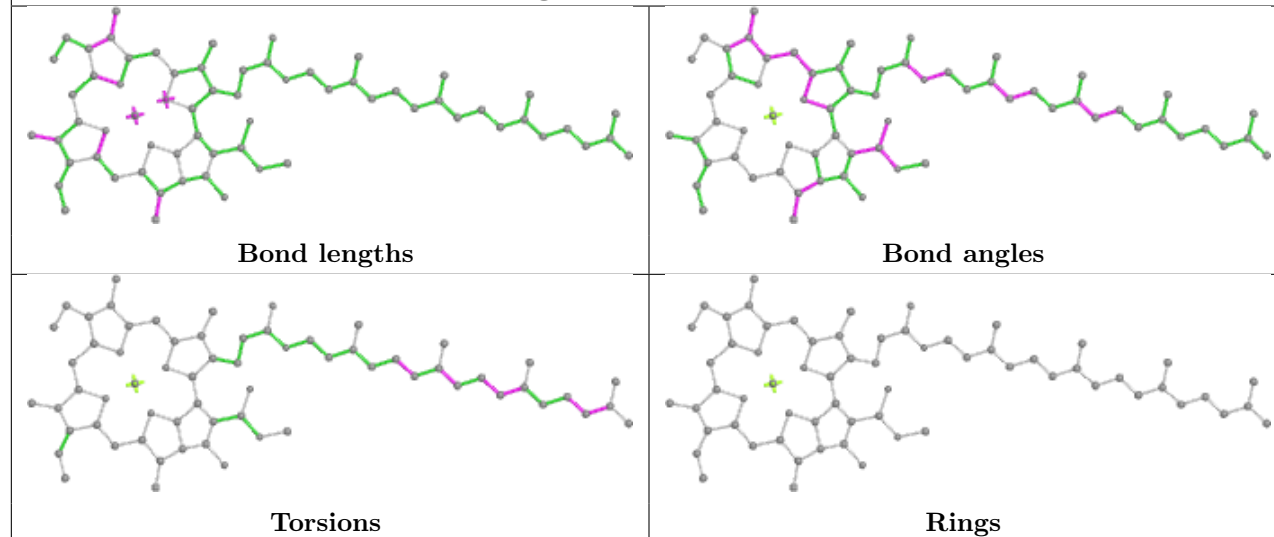




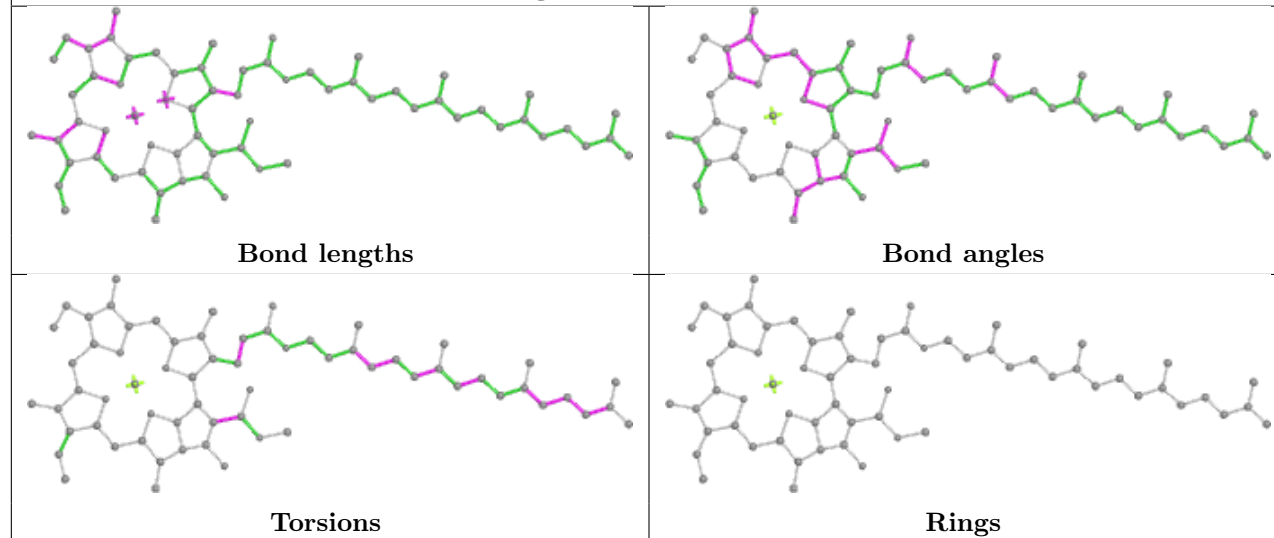
## Ligand CLA B 603



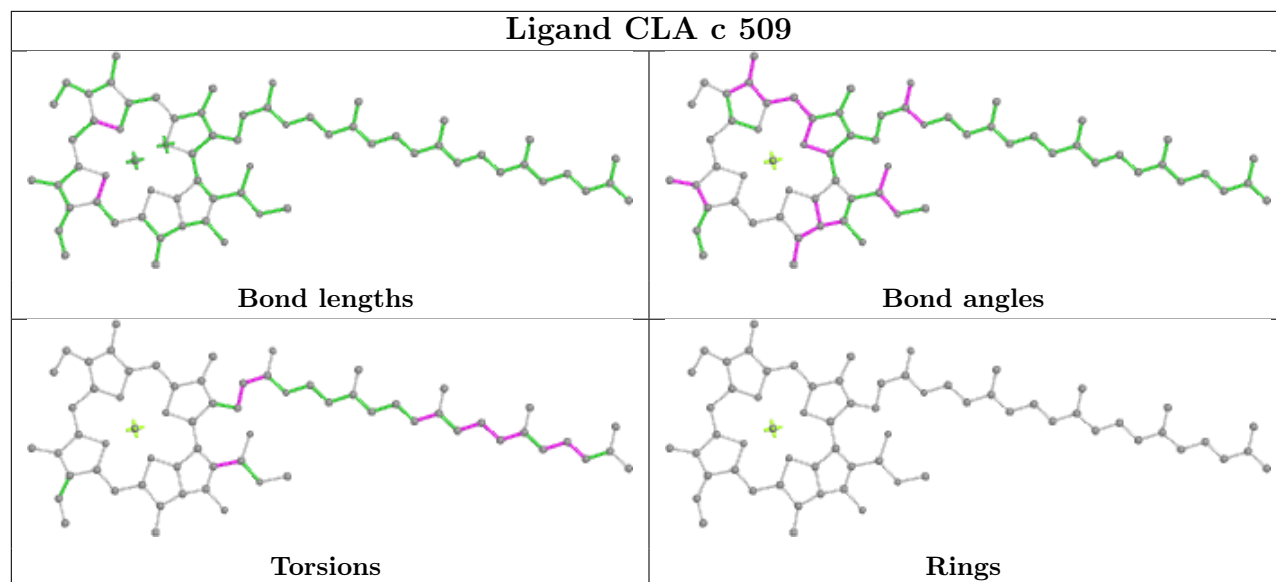
## Ligand CLA b 615



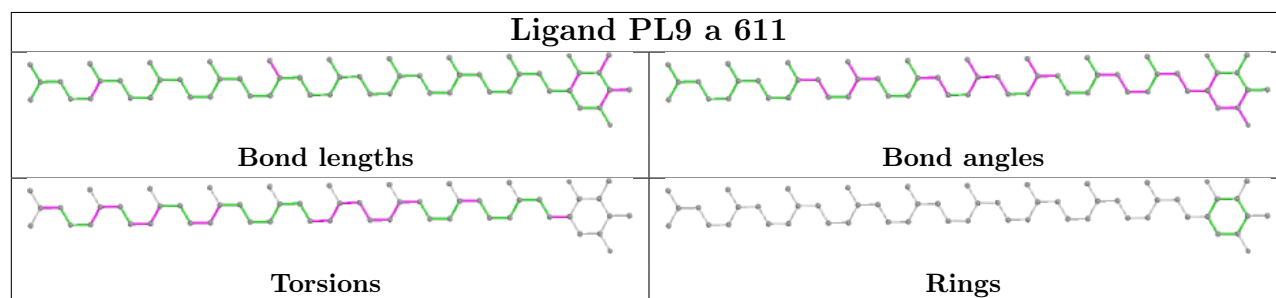
## Ligand CLA B 614



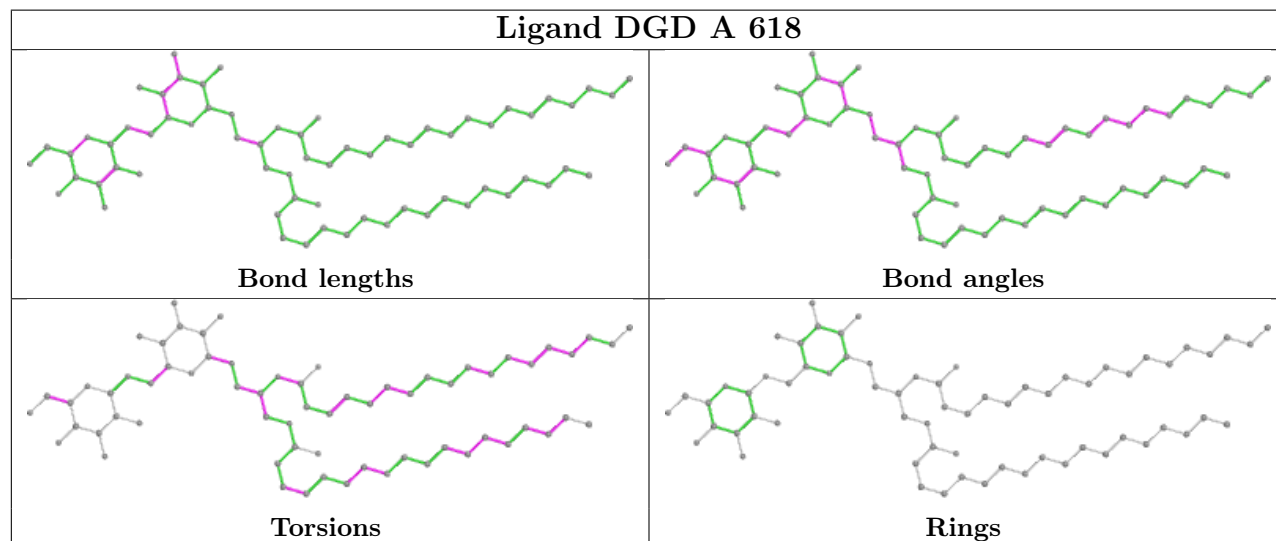
## Ligand CLA c 509

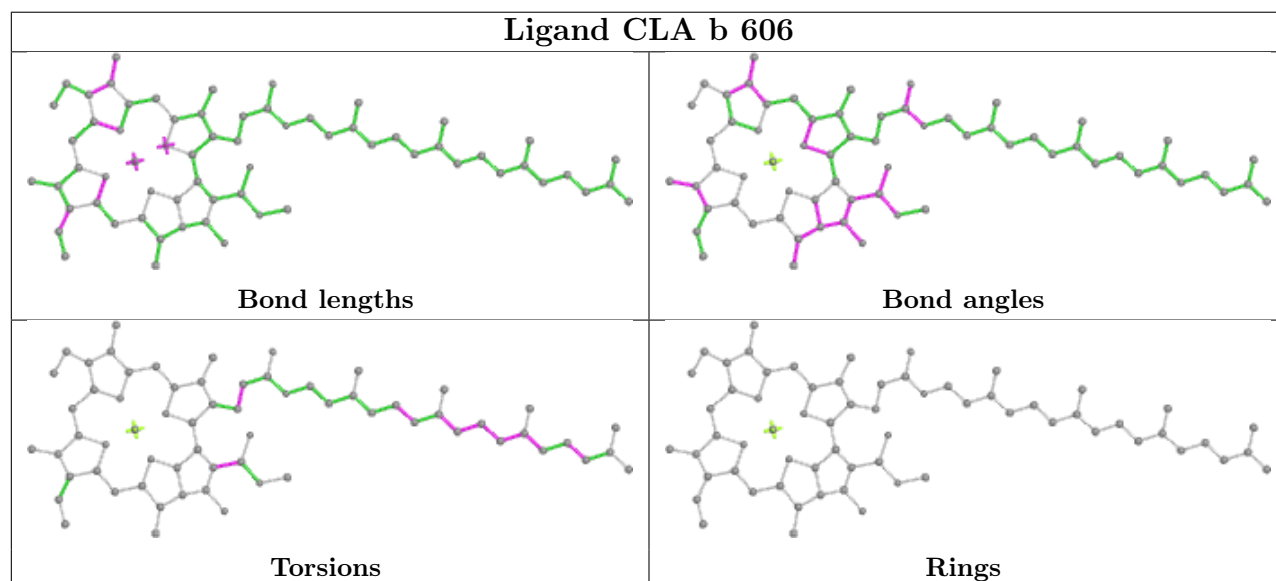
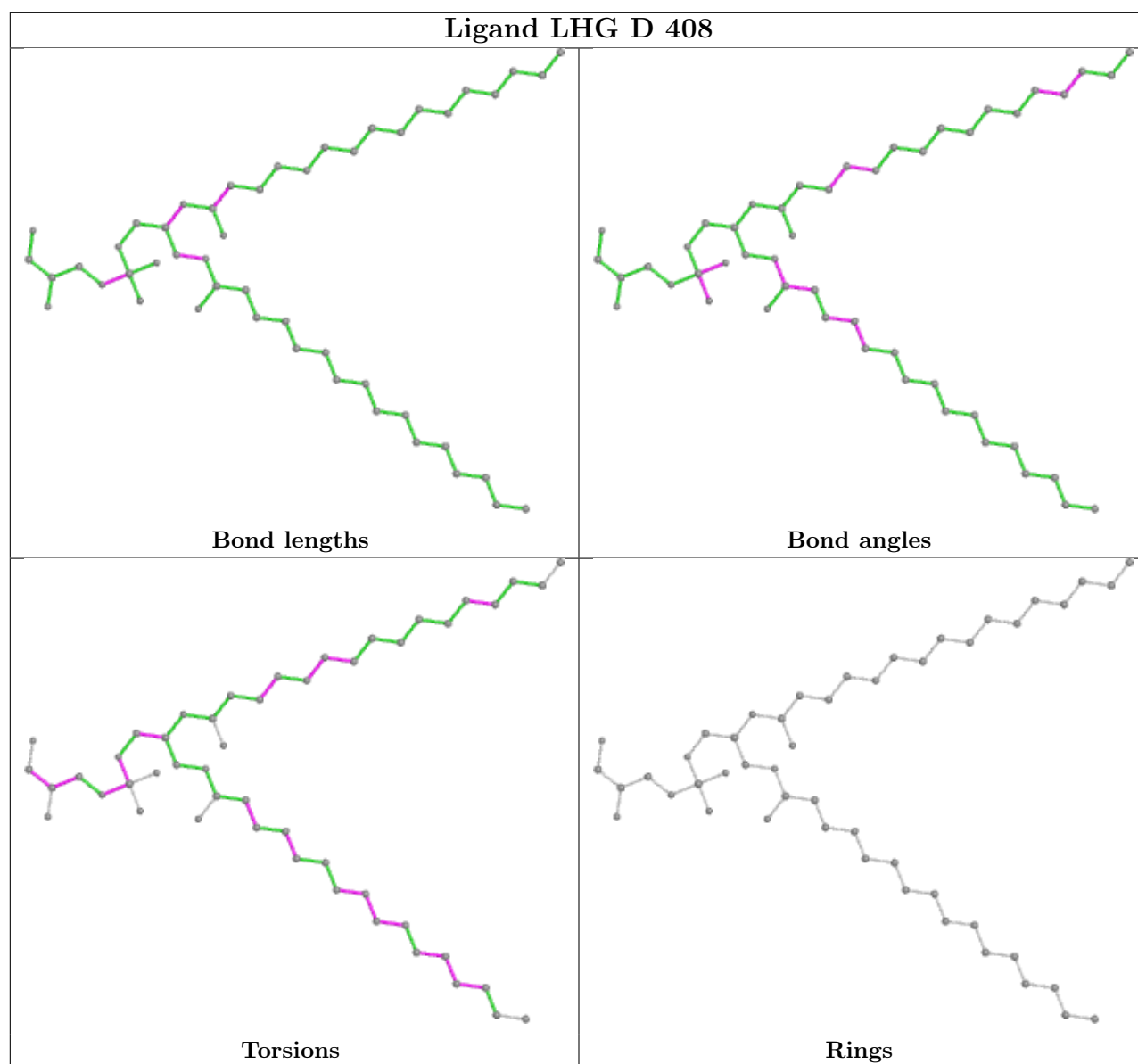


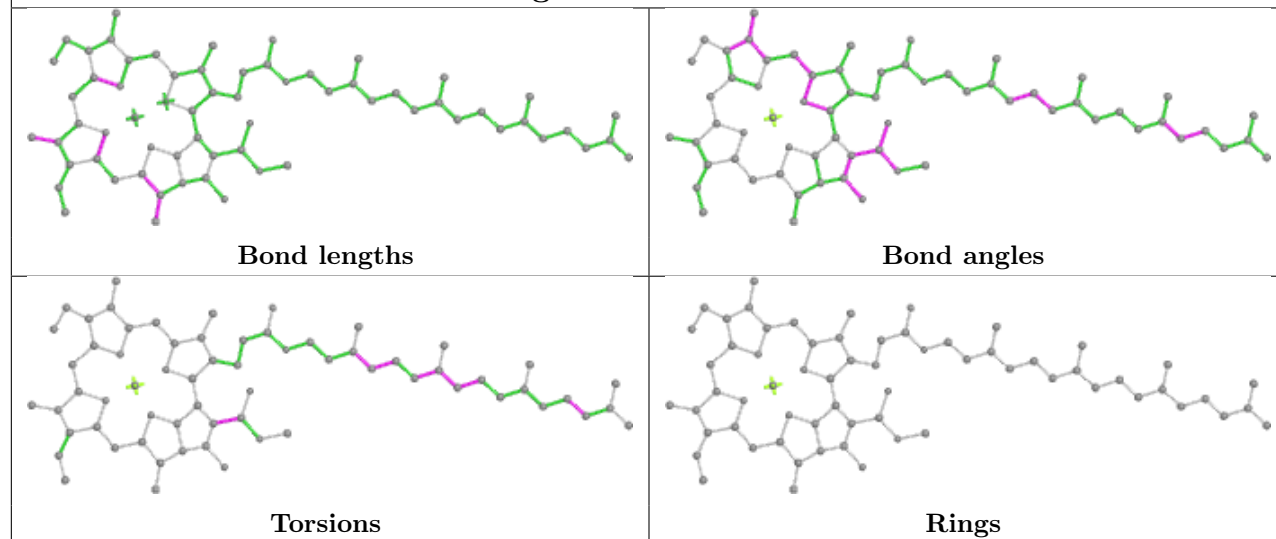
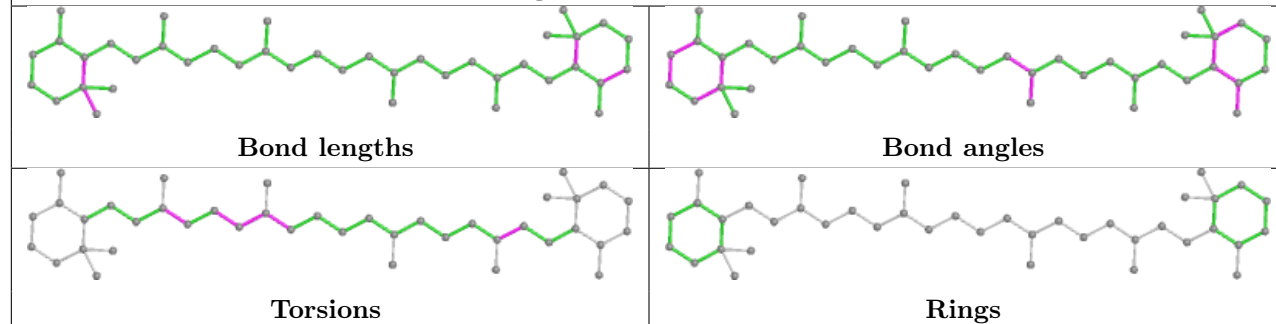
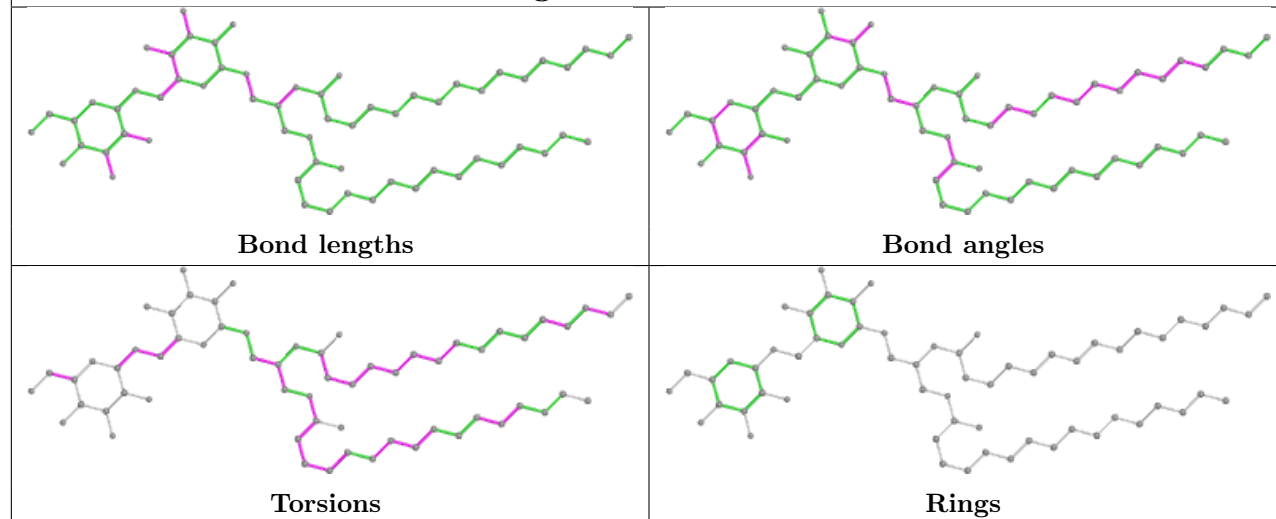
## Ligand PL9 a 611



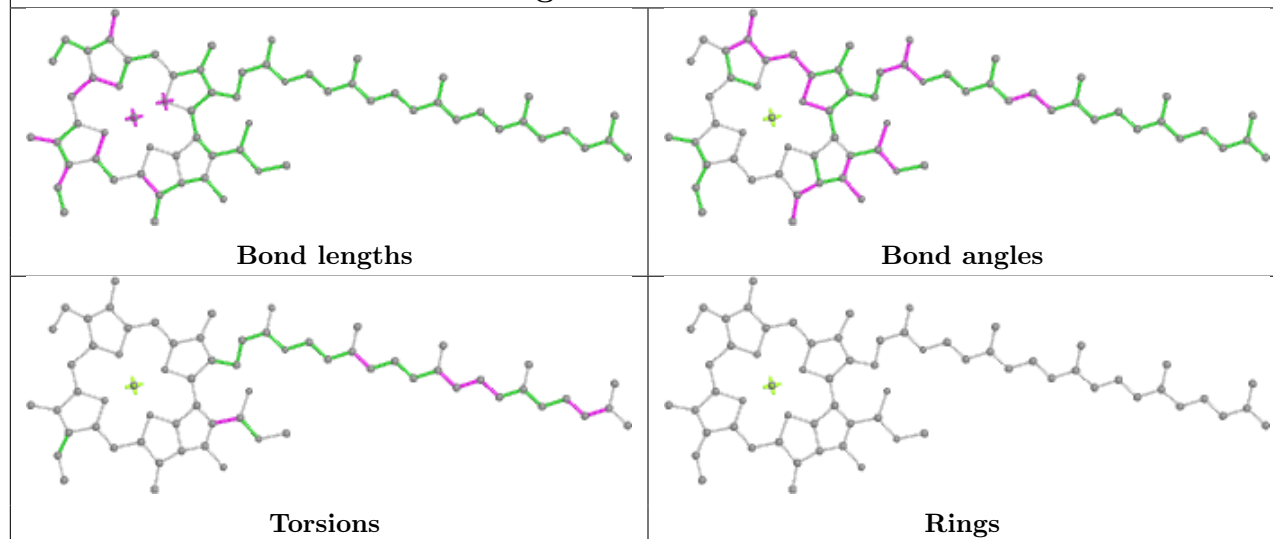
## Ligand DGD A 618



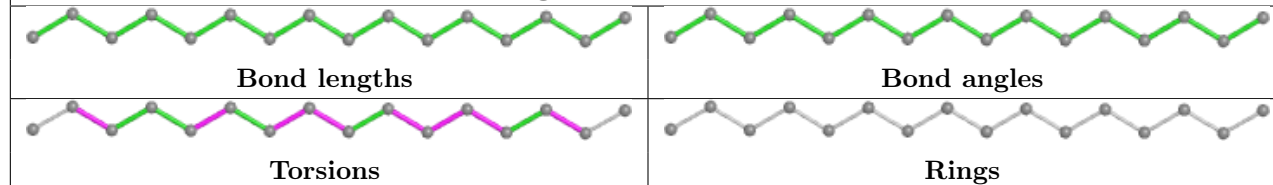


**Ligand CLA B 605****Ligand BCR B 619****Ligand DGD c 516**

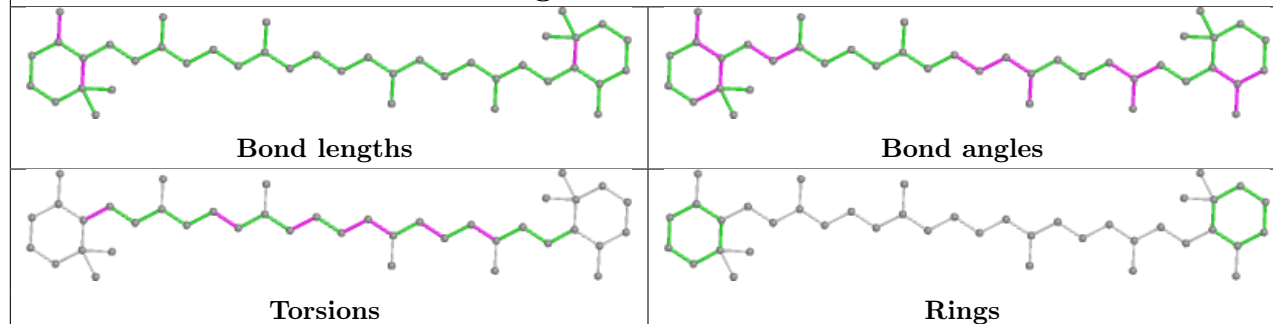
## Ligand CLA c 510



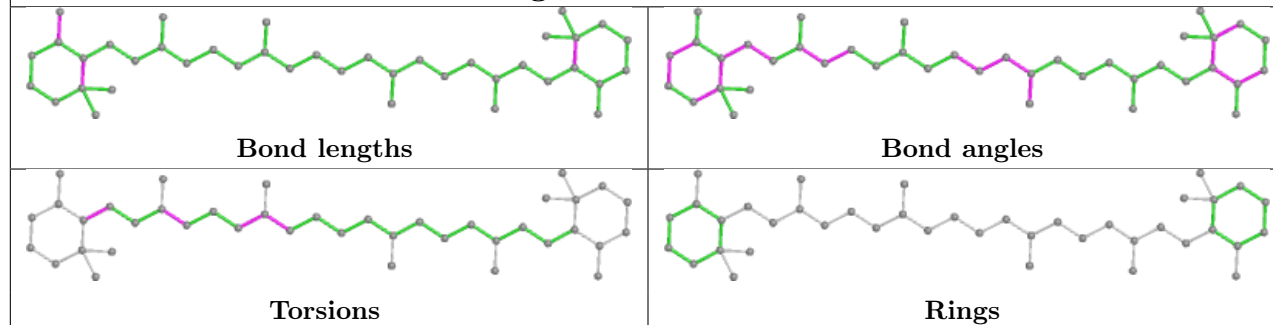
## Ligand STE T 102

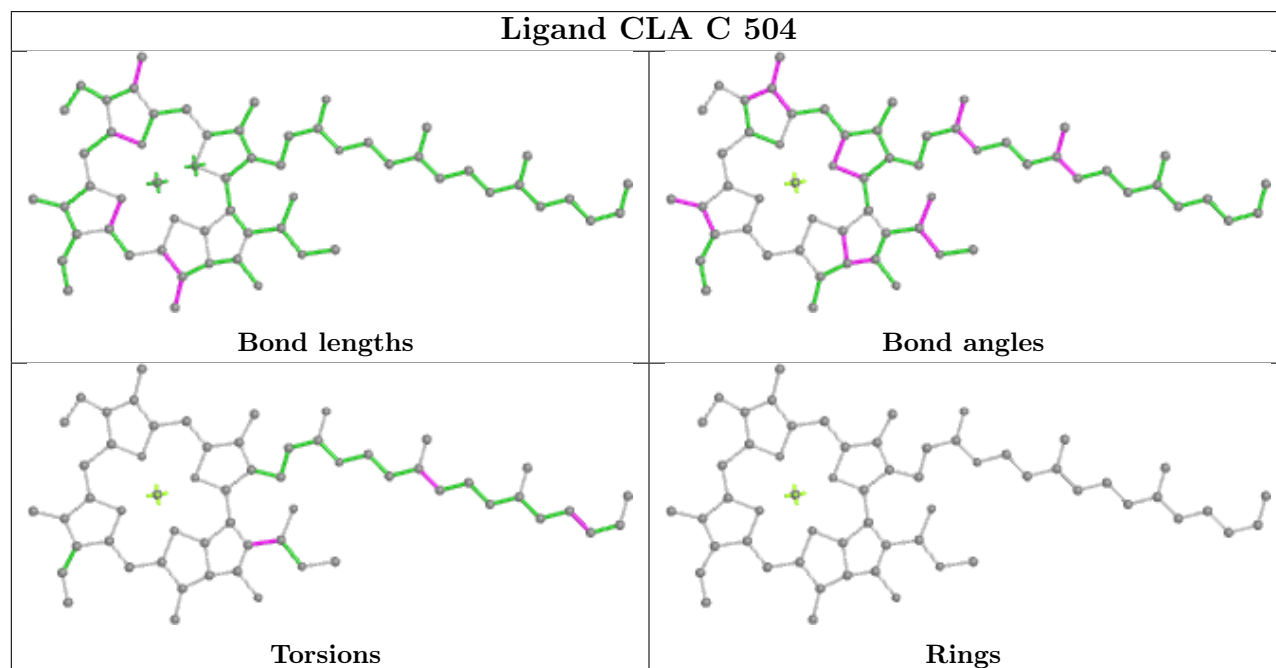
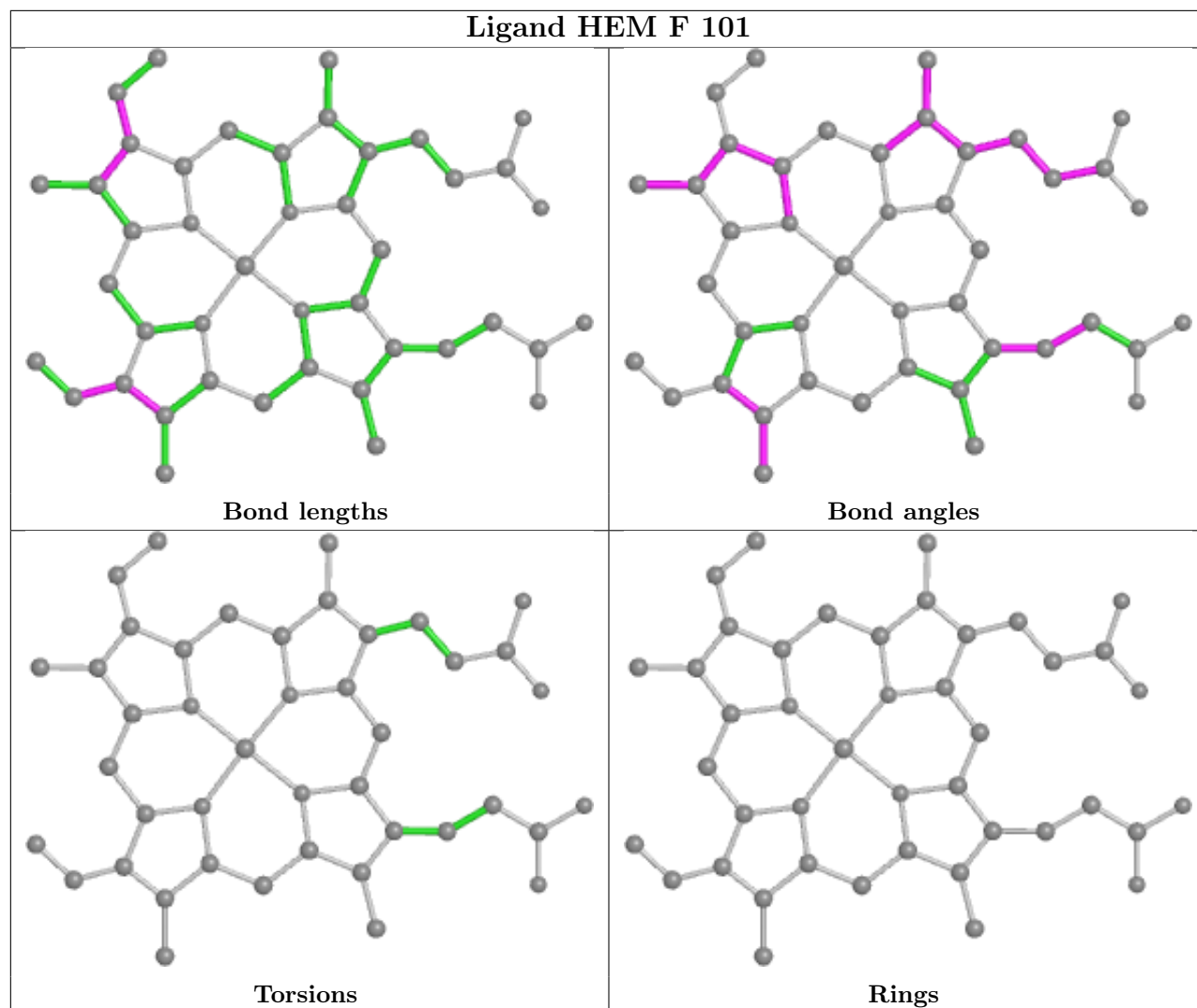


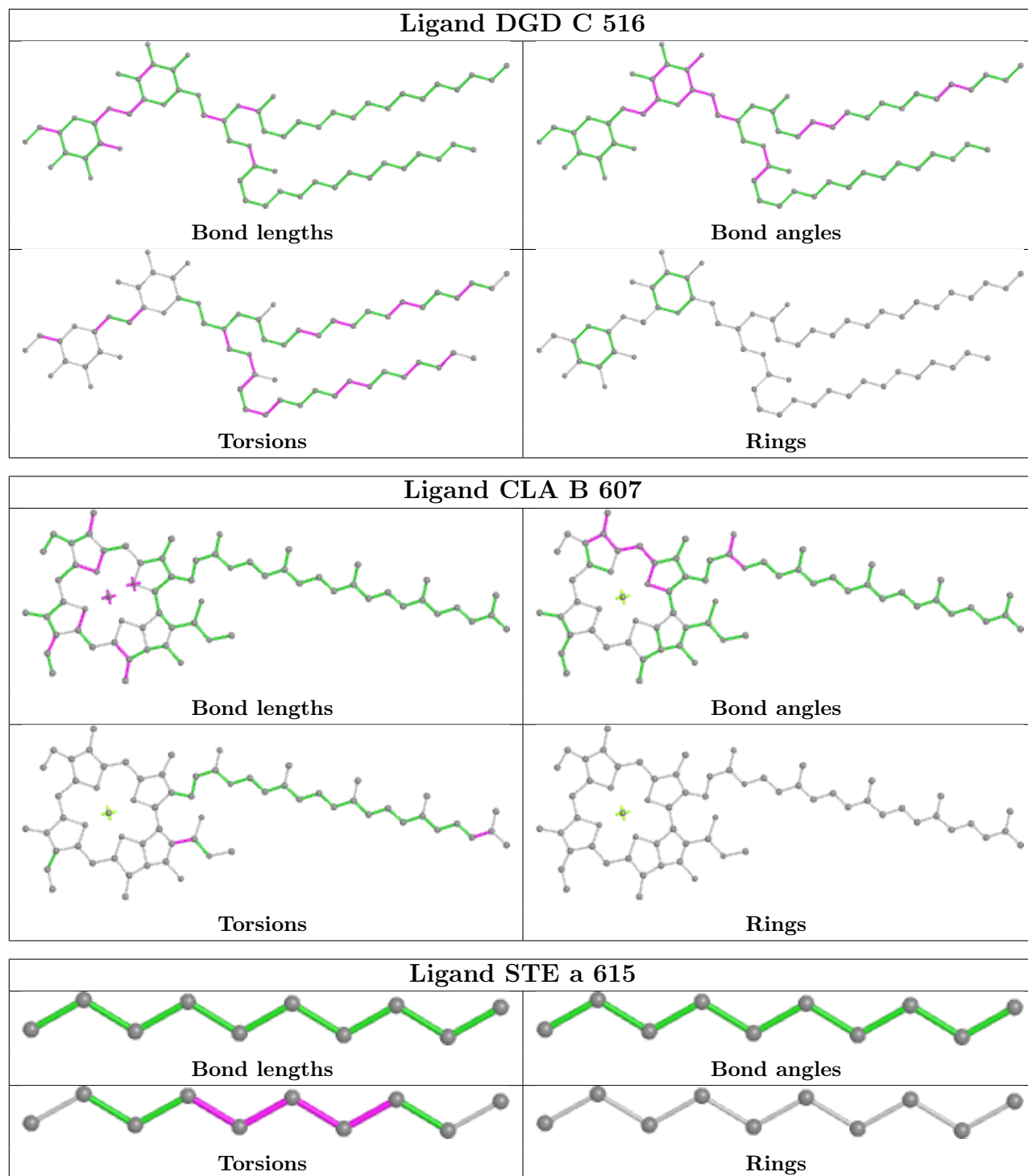
## Ligand BCR c 514



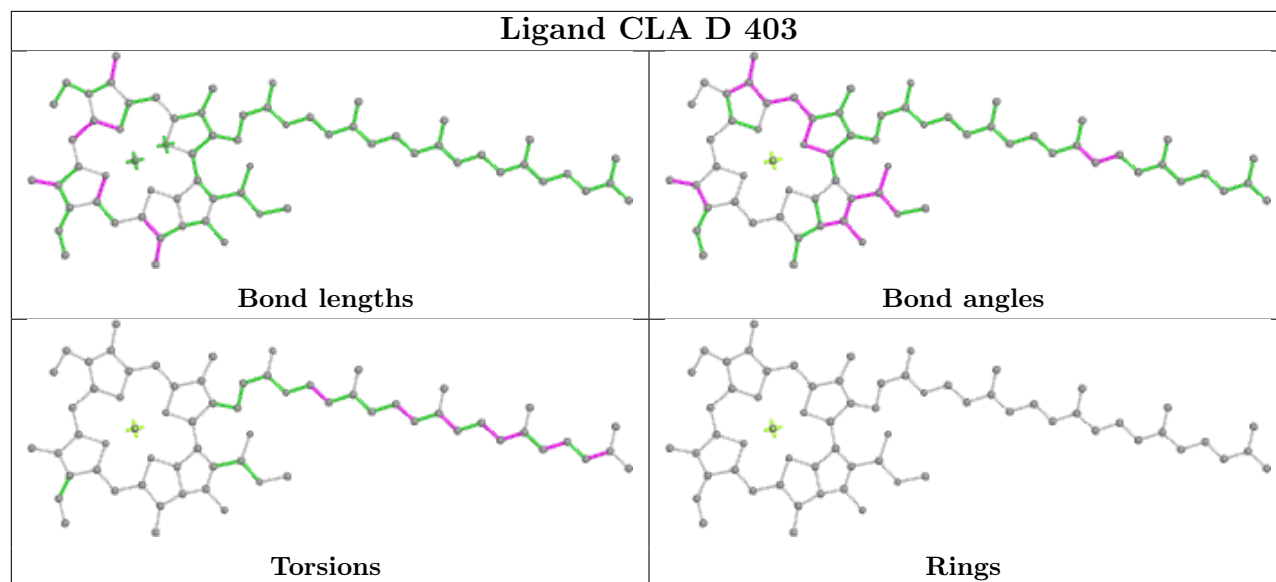
## Ligand BCR B 617



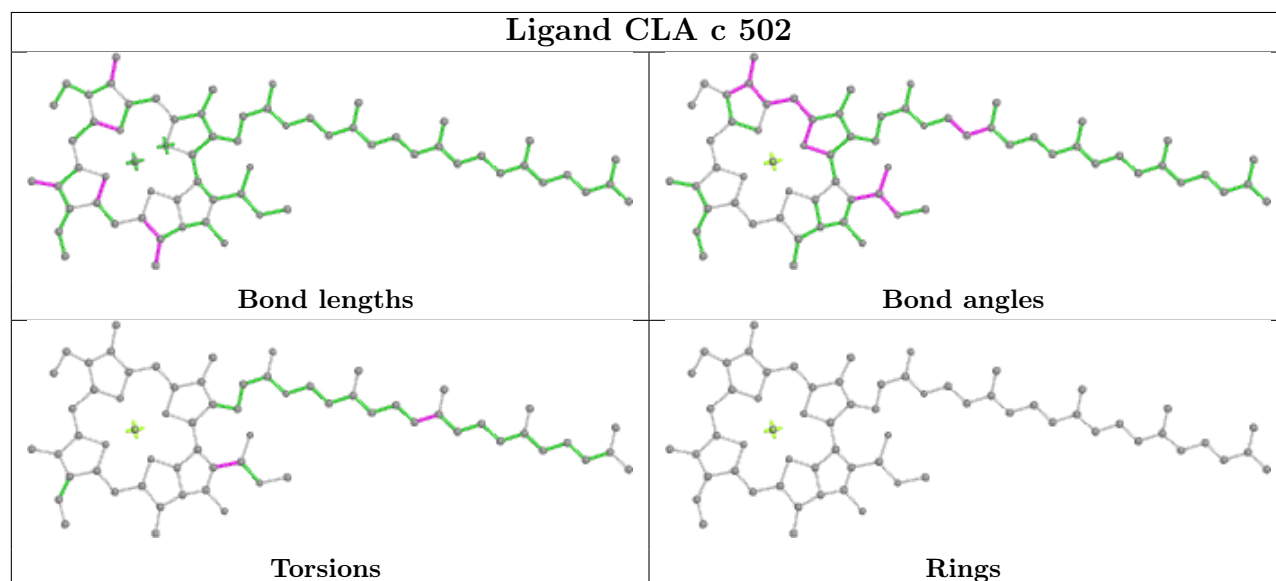




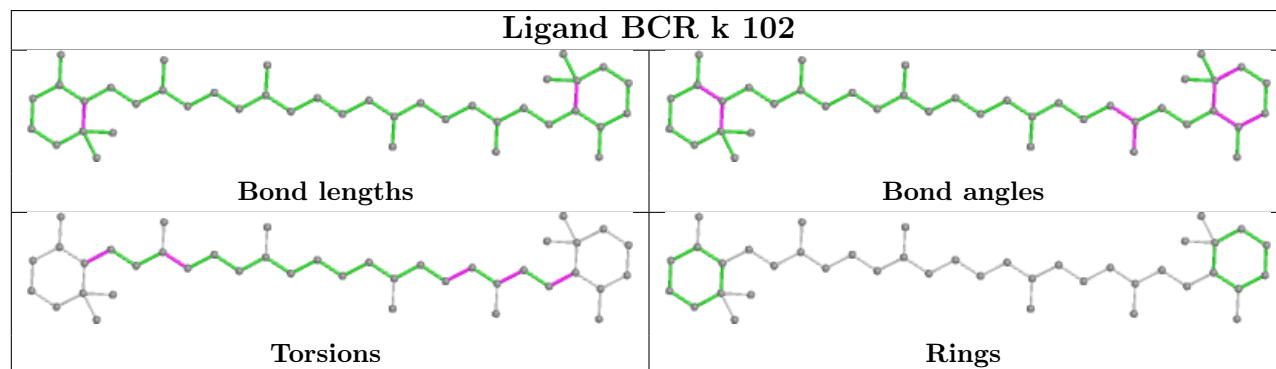
## Ligand CLA D 403



## Ligand CLA c 502

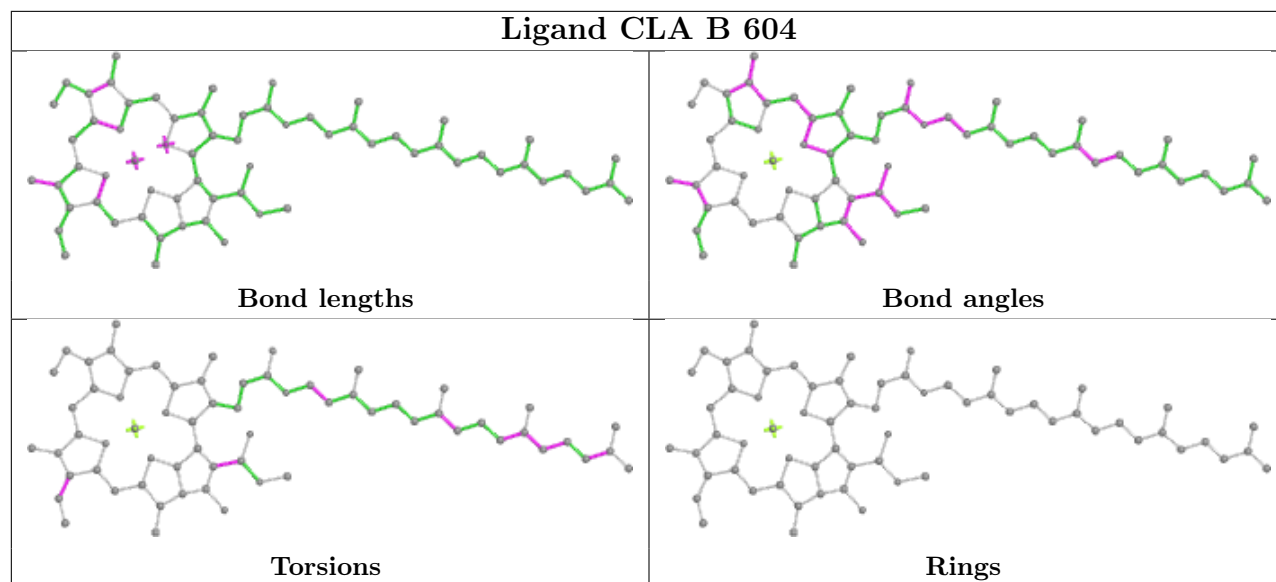


## Ligand BCR k 102

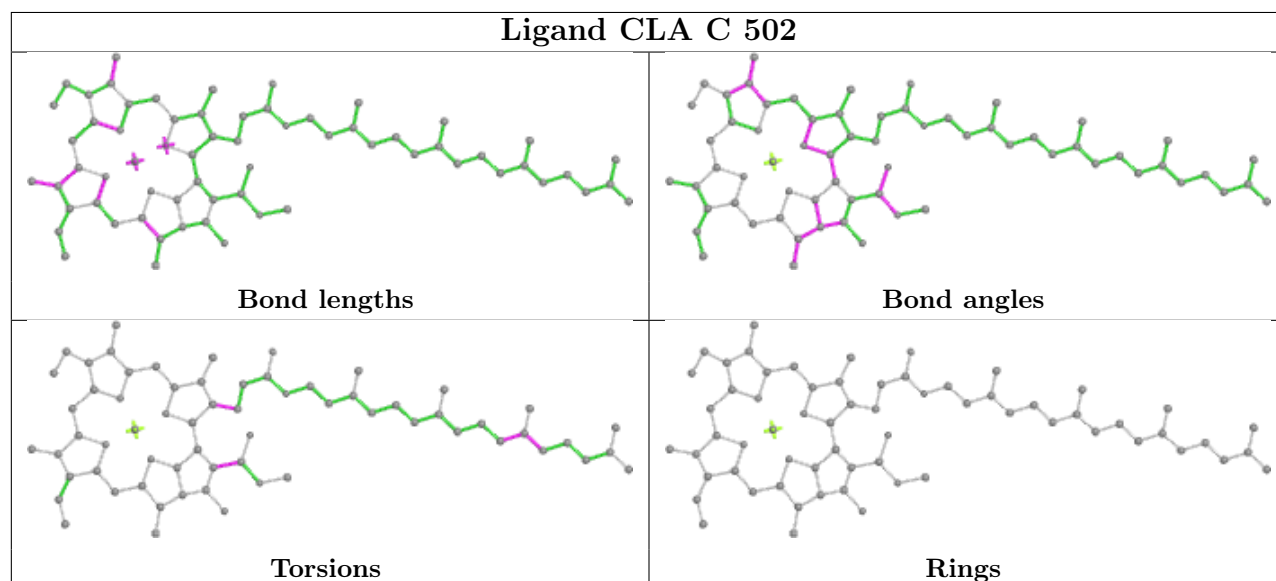




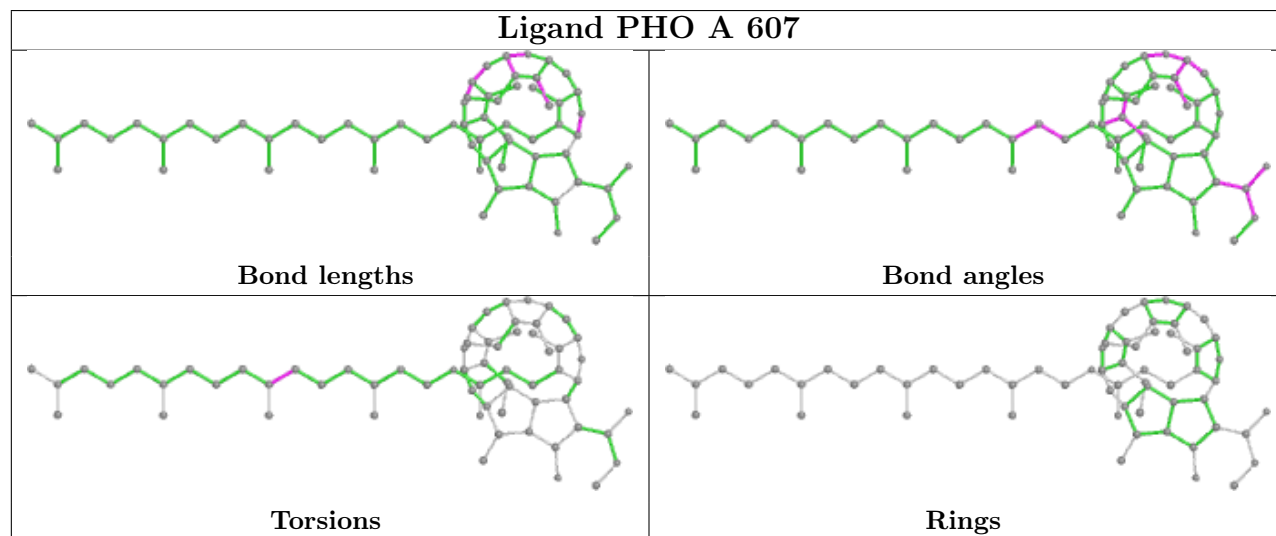
## Ligand CLA B 604

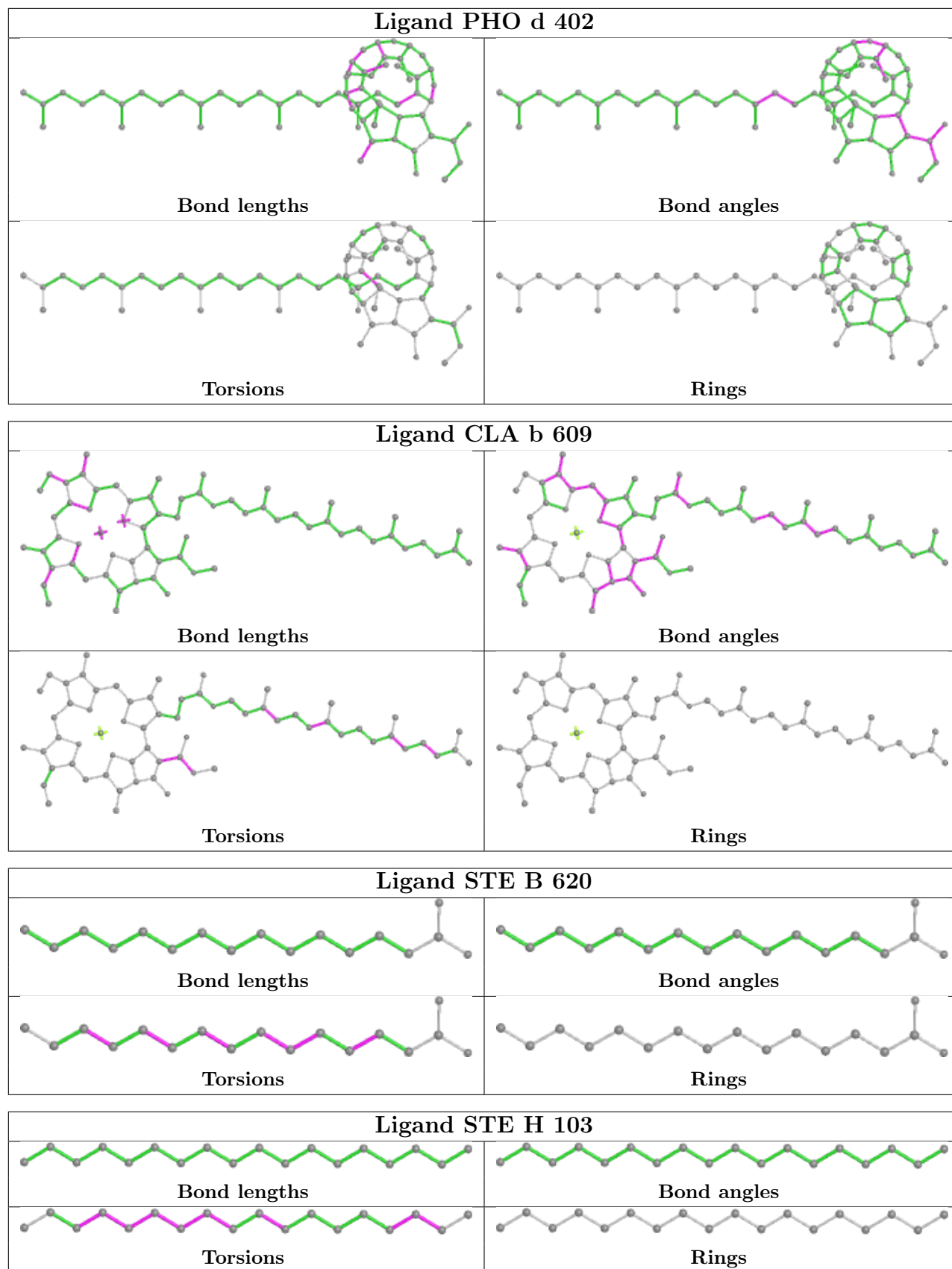


## Ligand CLA C 502

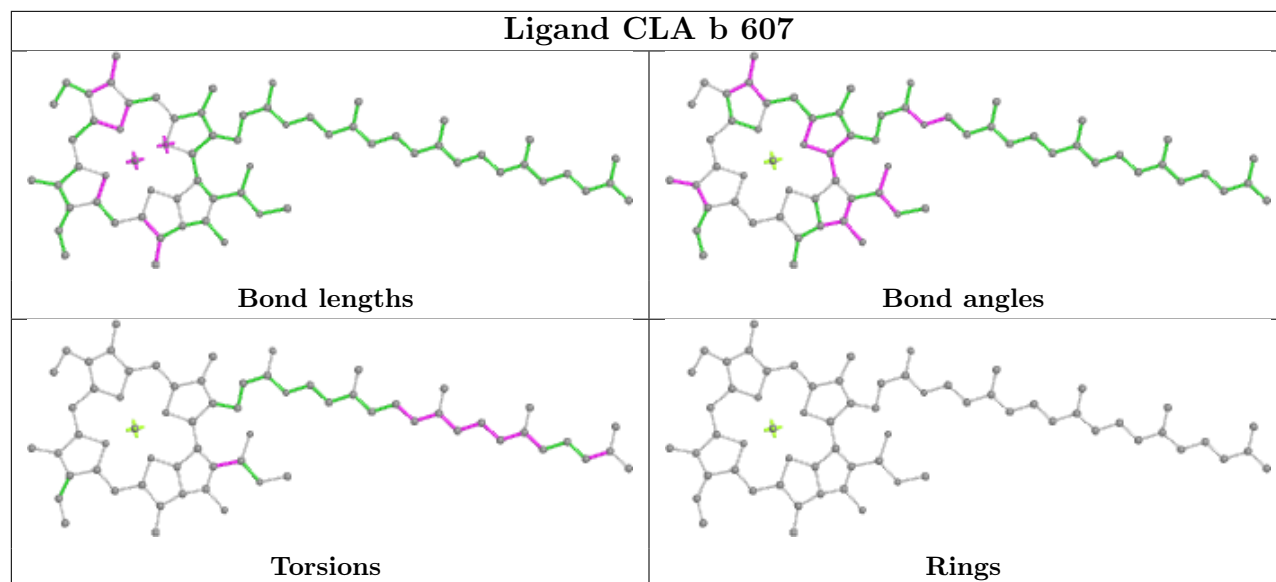


## Ligand PHO A 607

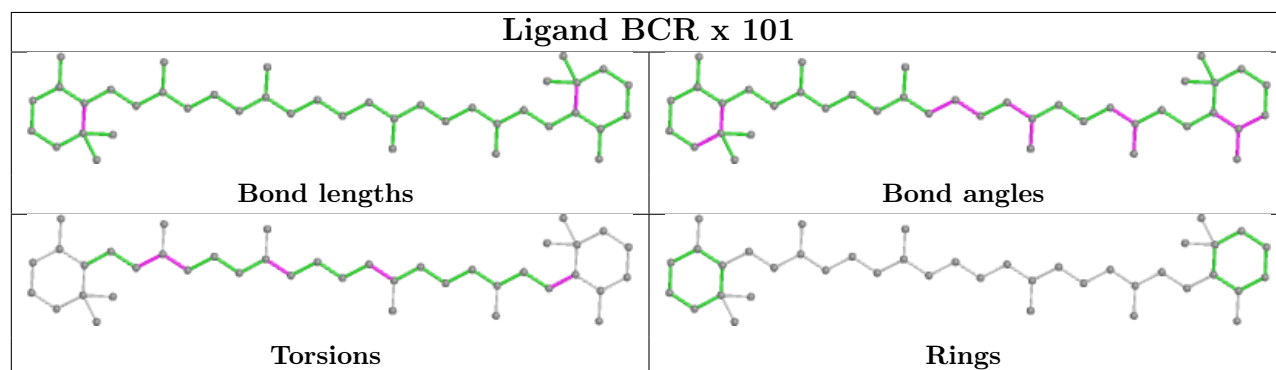




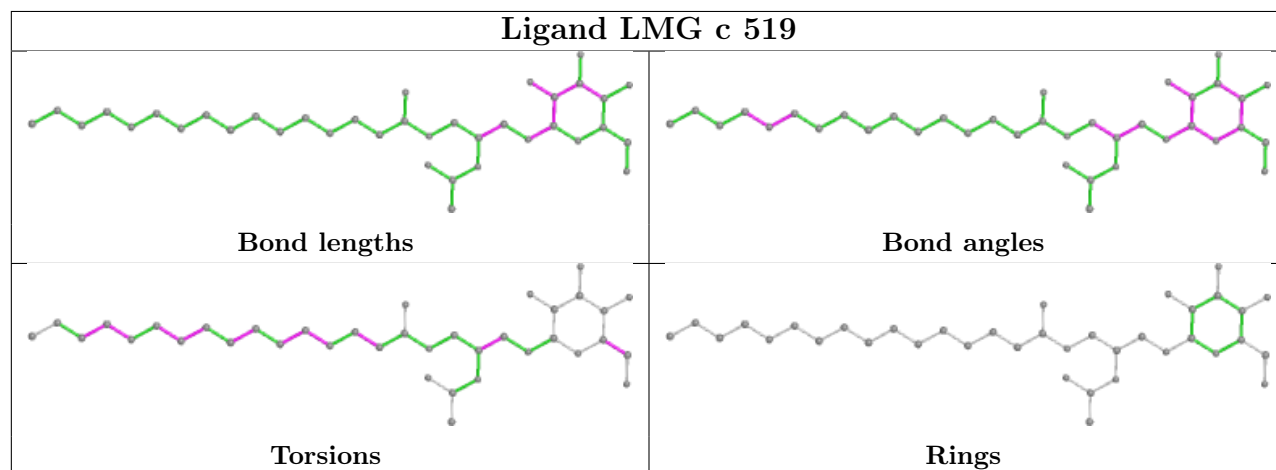
## Ligand CLA b 607

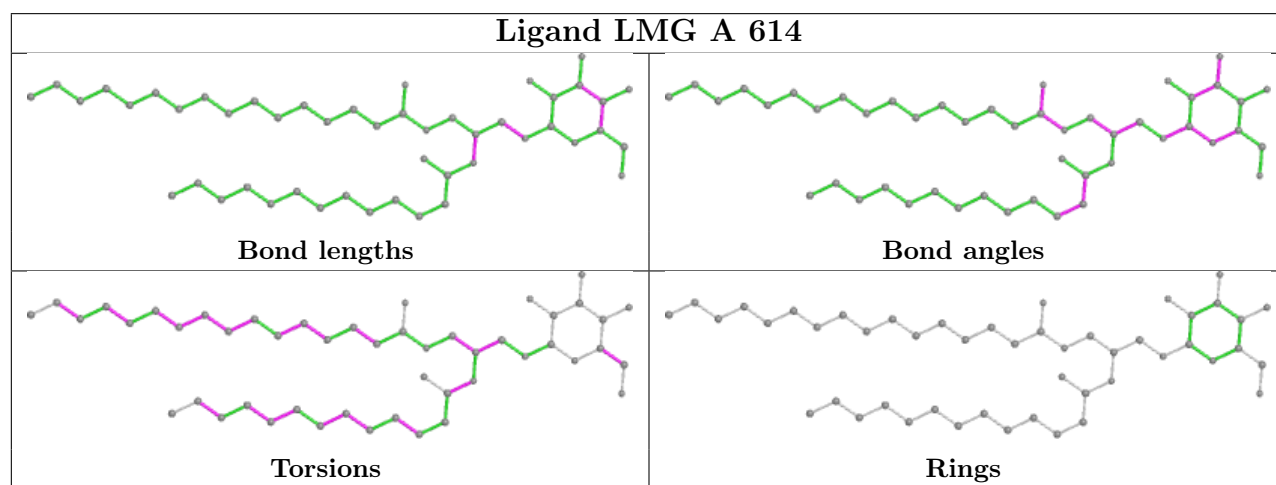
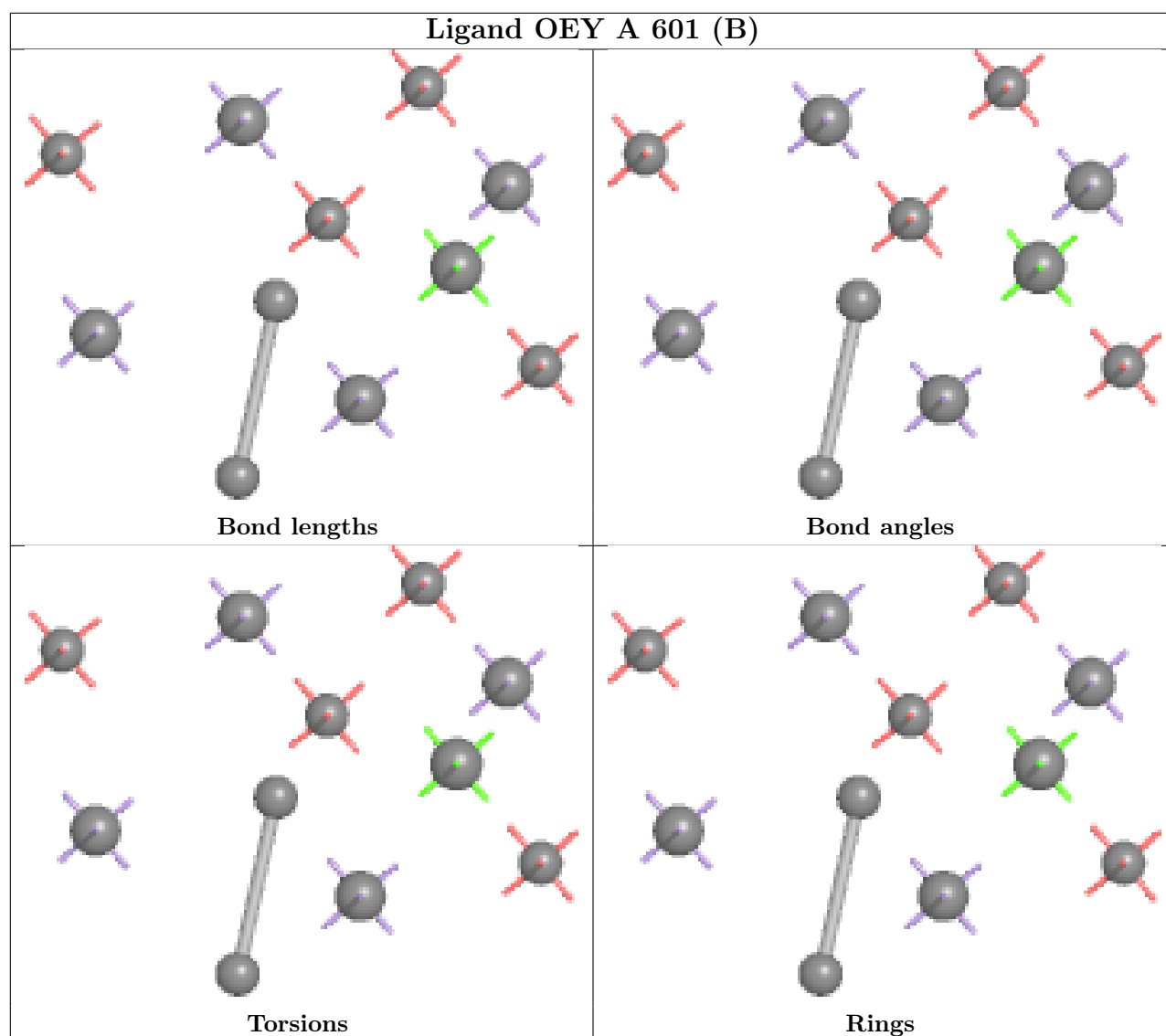


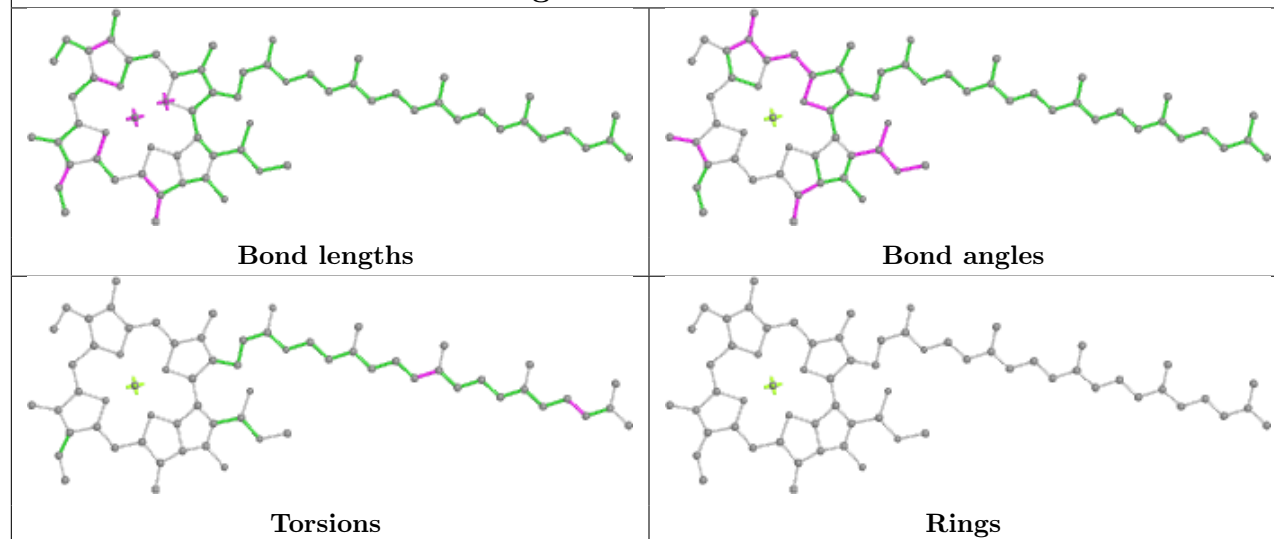
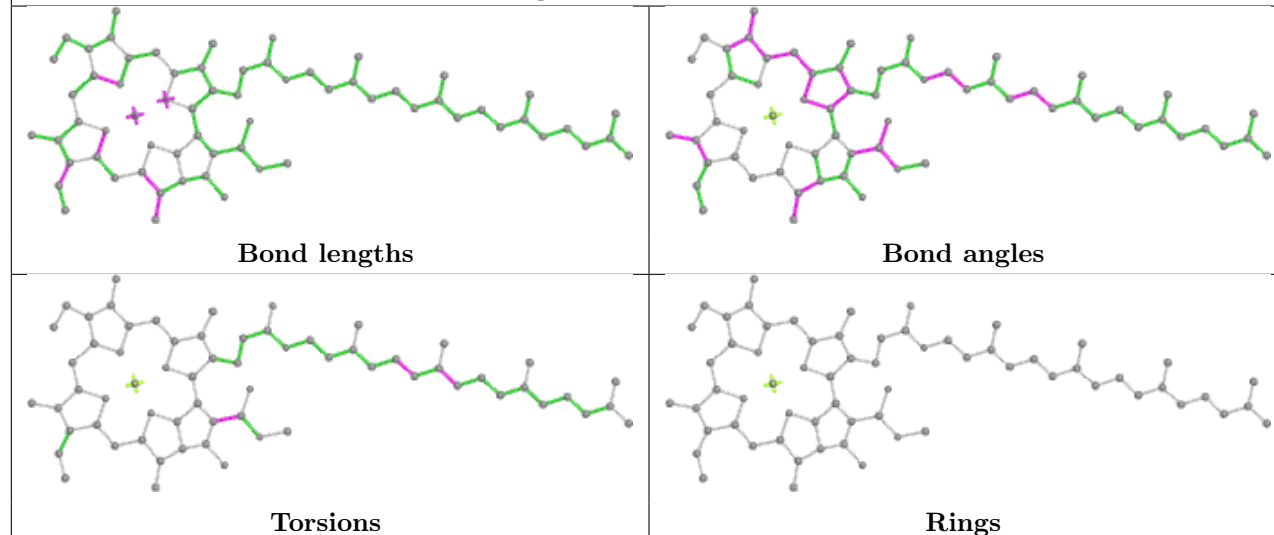
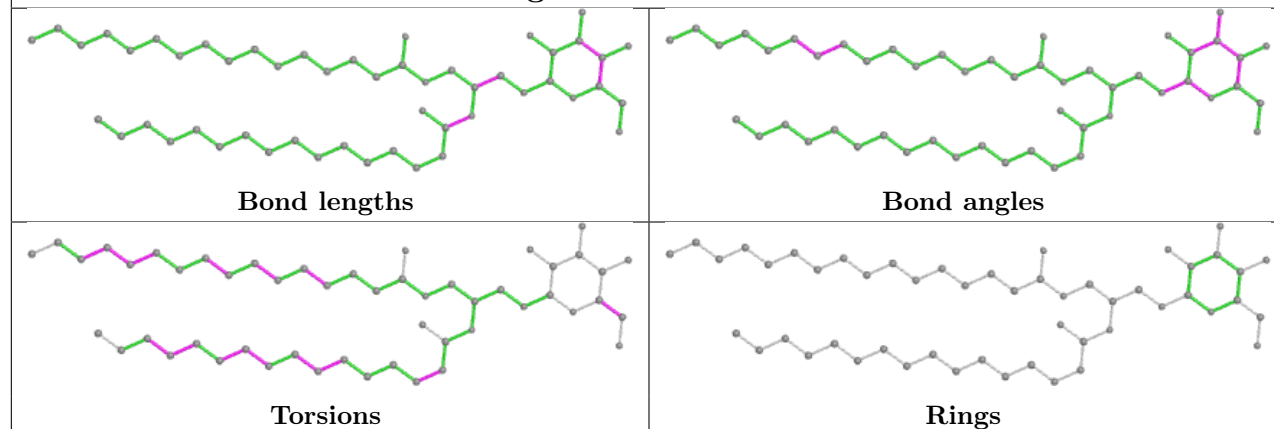
## Ligand BCR x 101



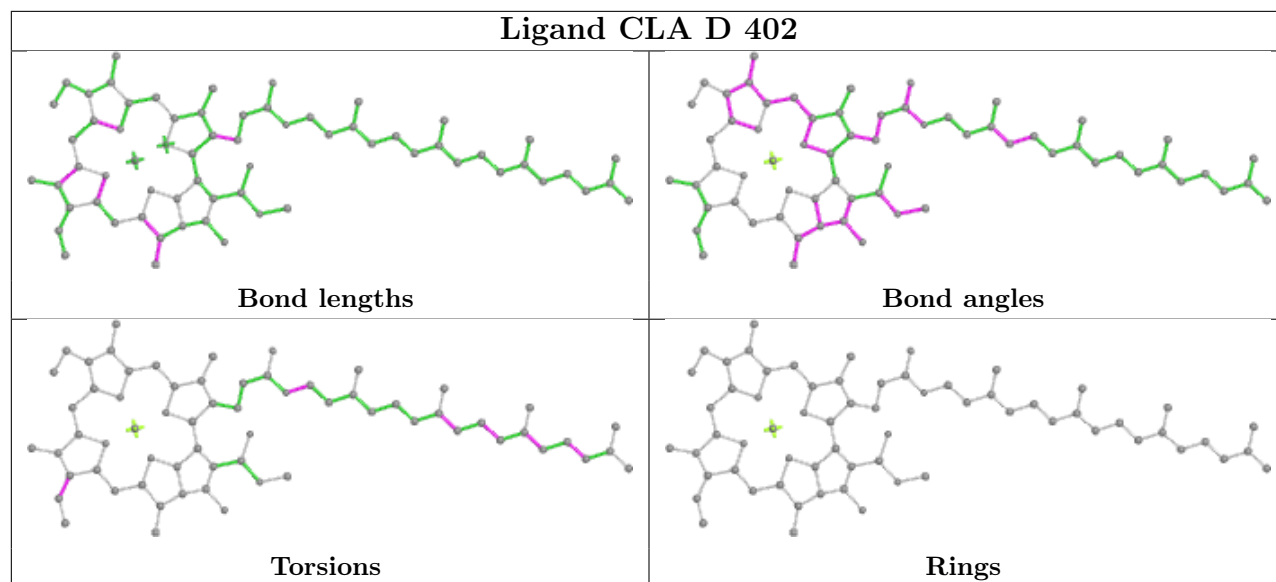
## Ligand LMG c 519



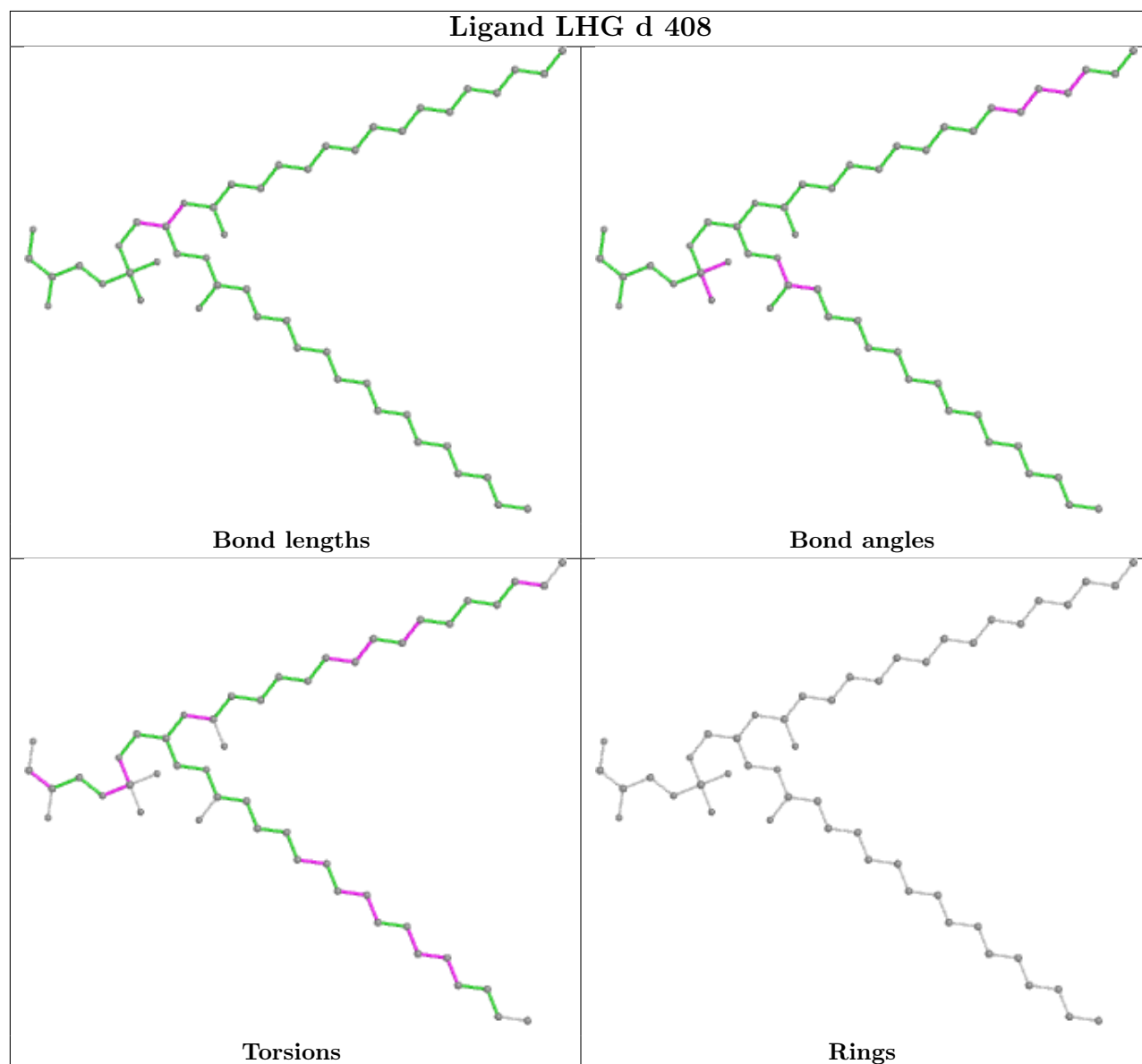


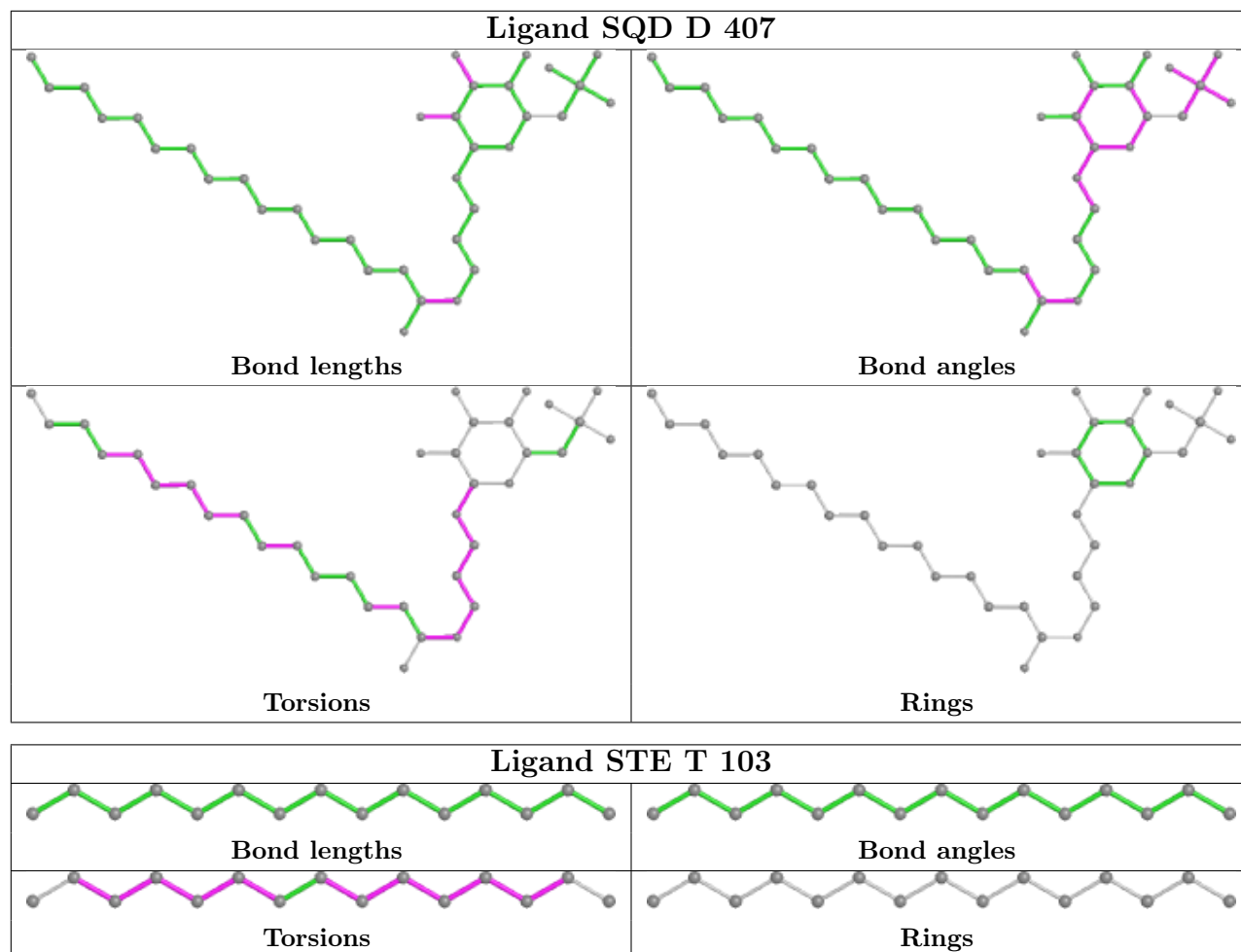
**Ligand CLA B 608****Ligand CLA C 503****Ligand LMG D 406**

## Ligand CLA D 402

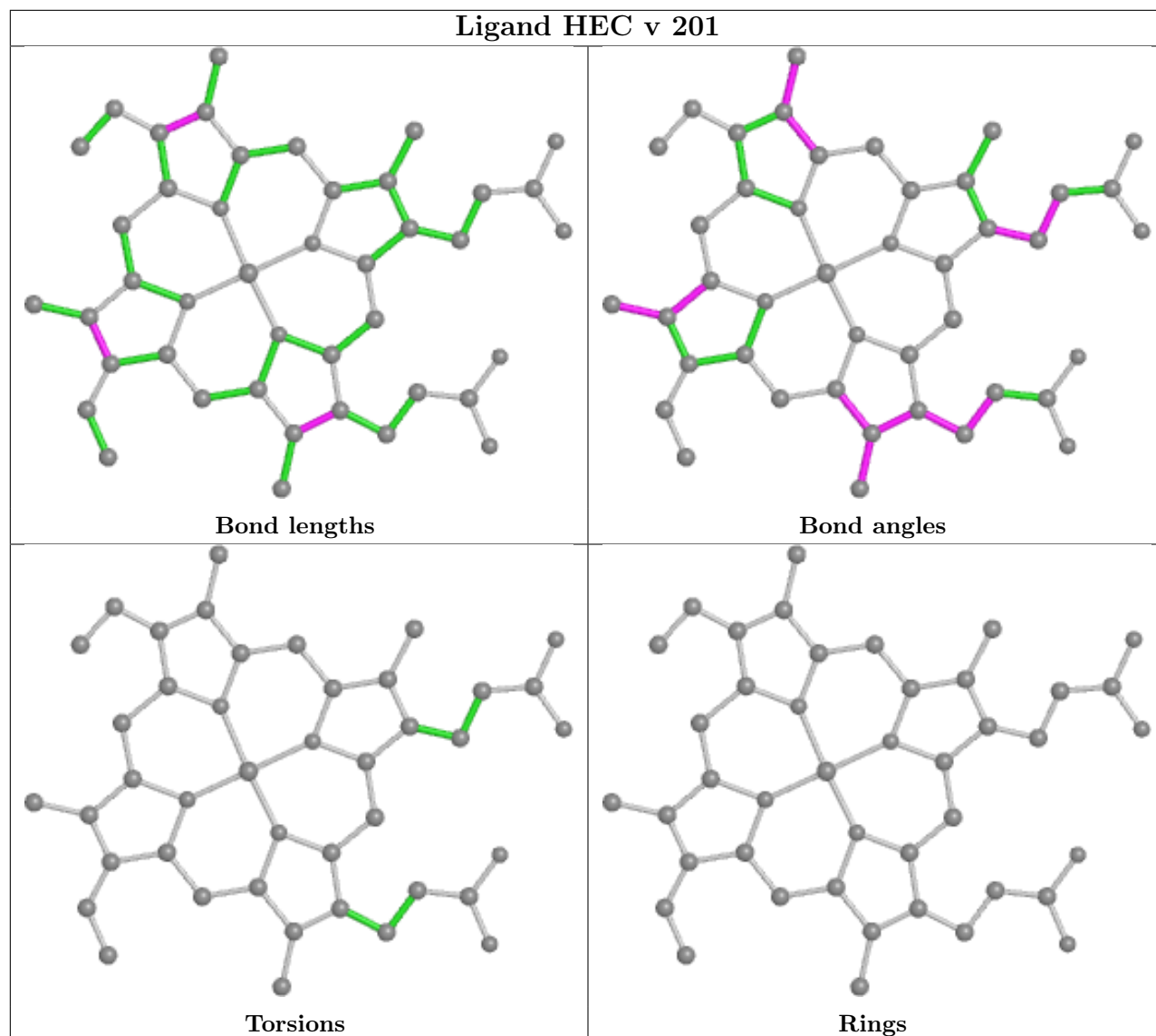


## Ligand LHG d 408

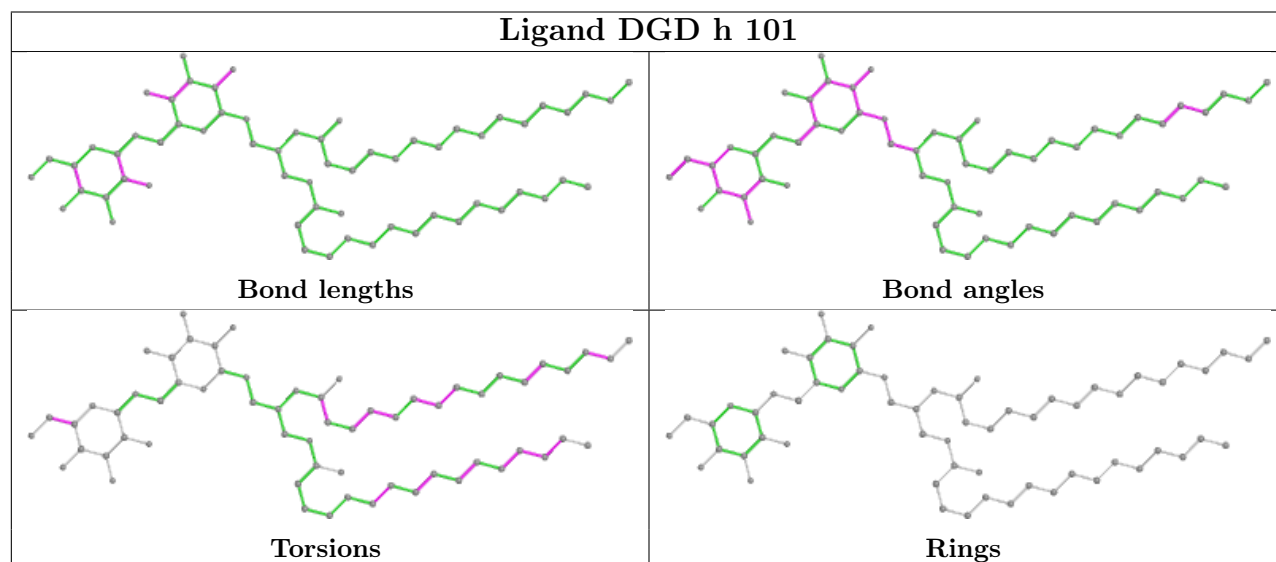
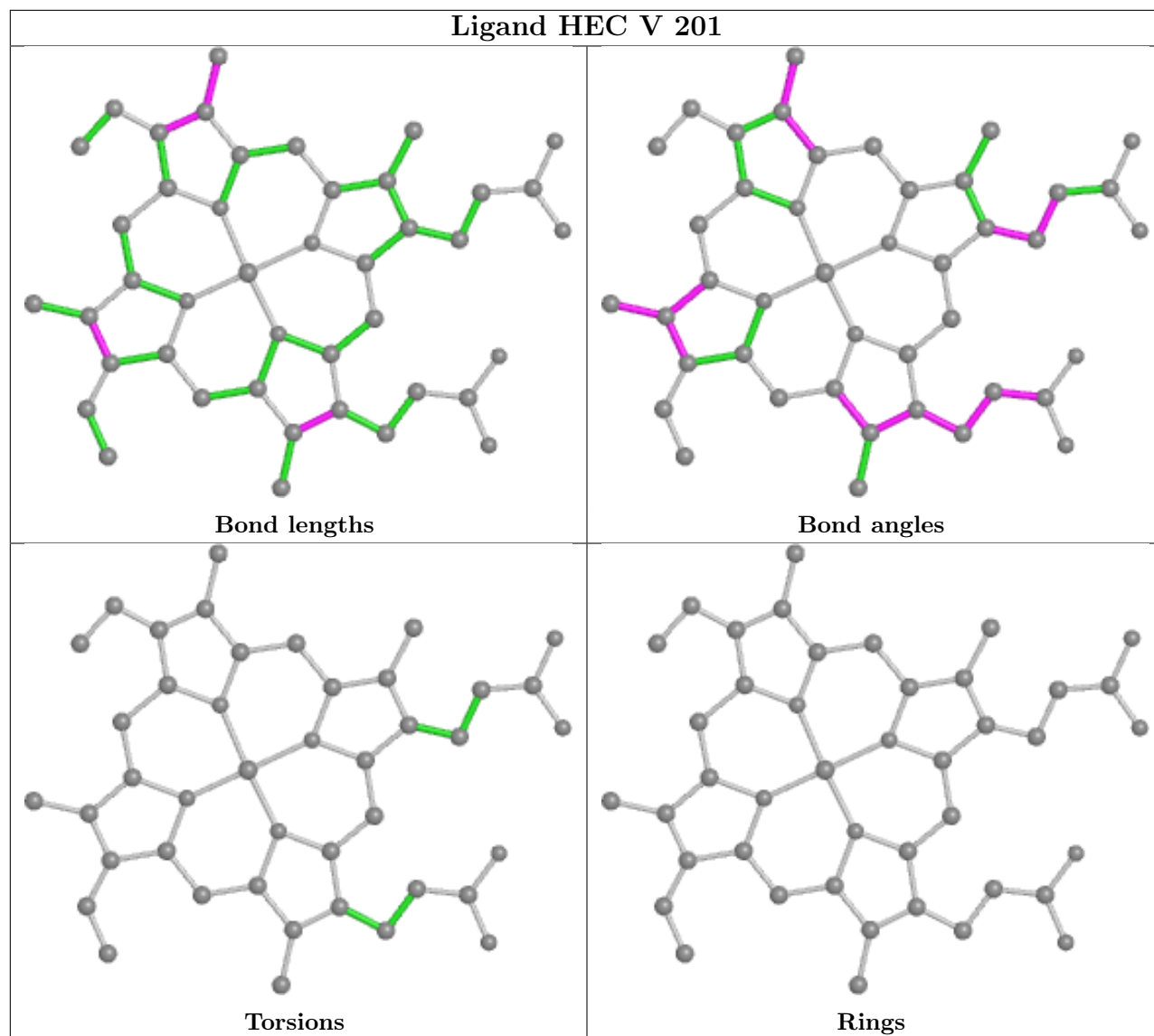




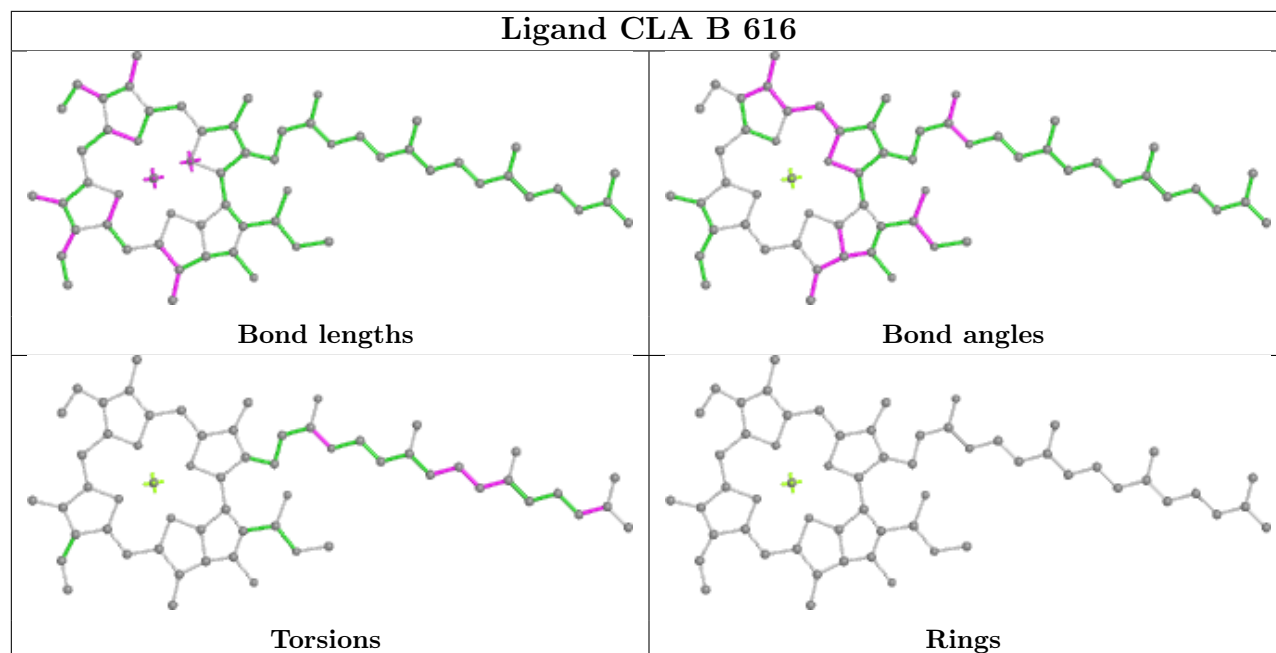
## Ligand HEC v 201



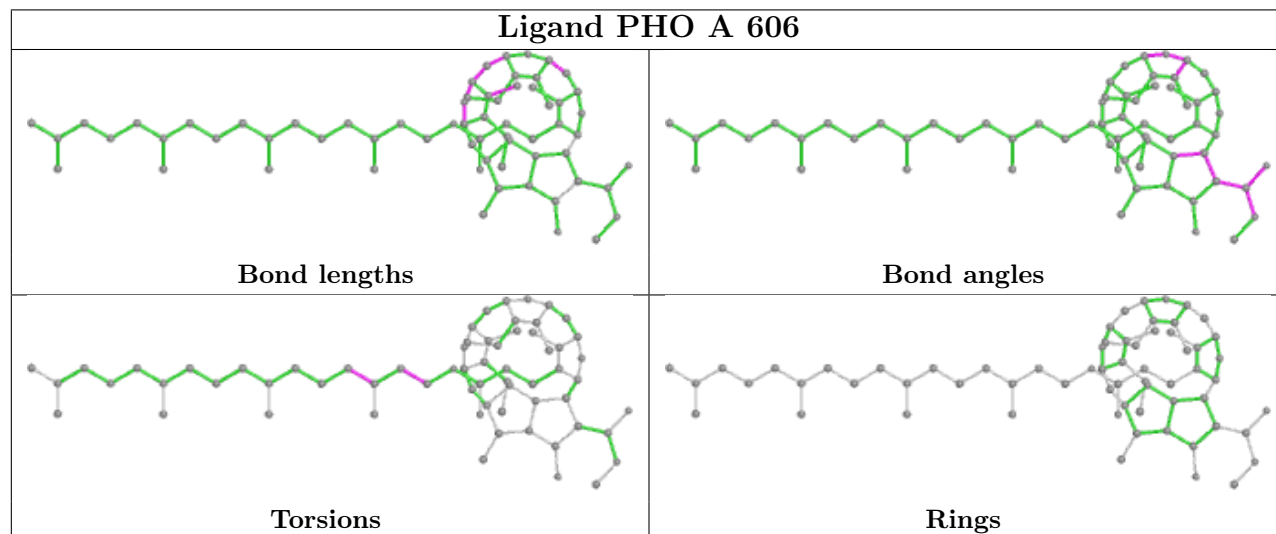




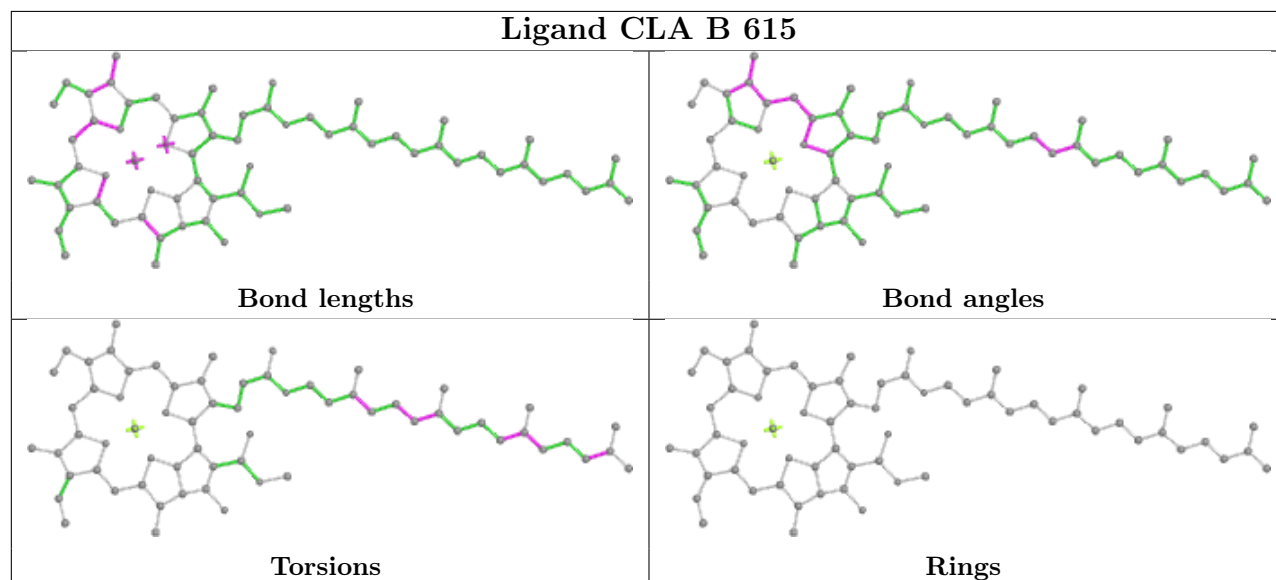
## Ligand CLA B 616

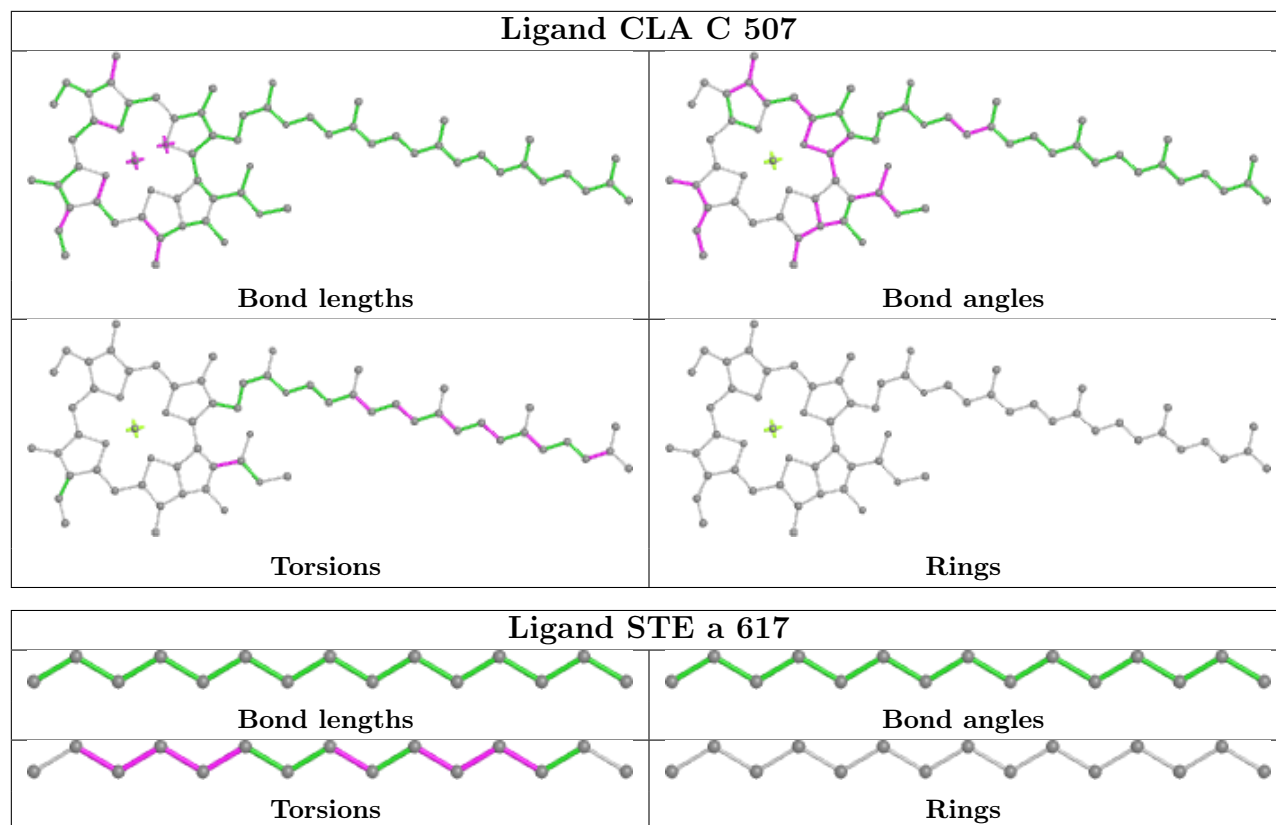


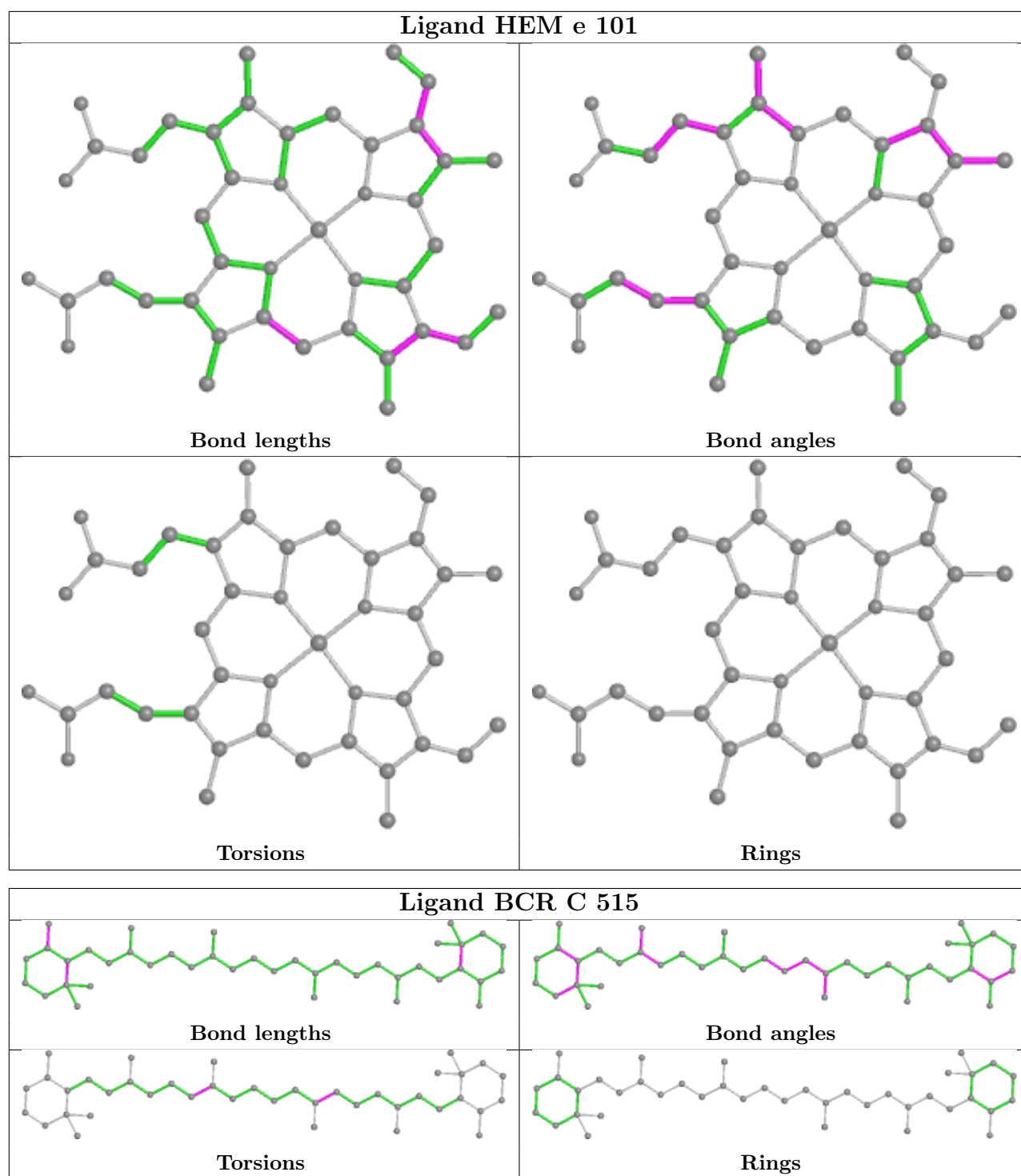
## Ligand PHO A 606

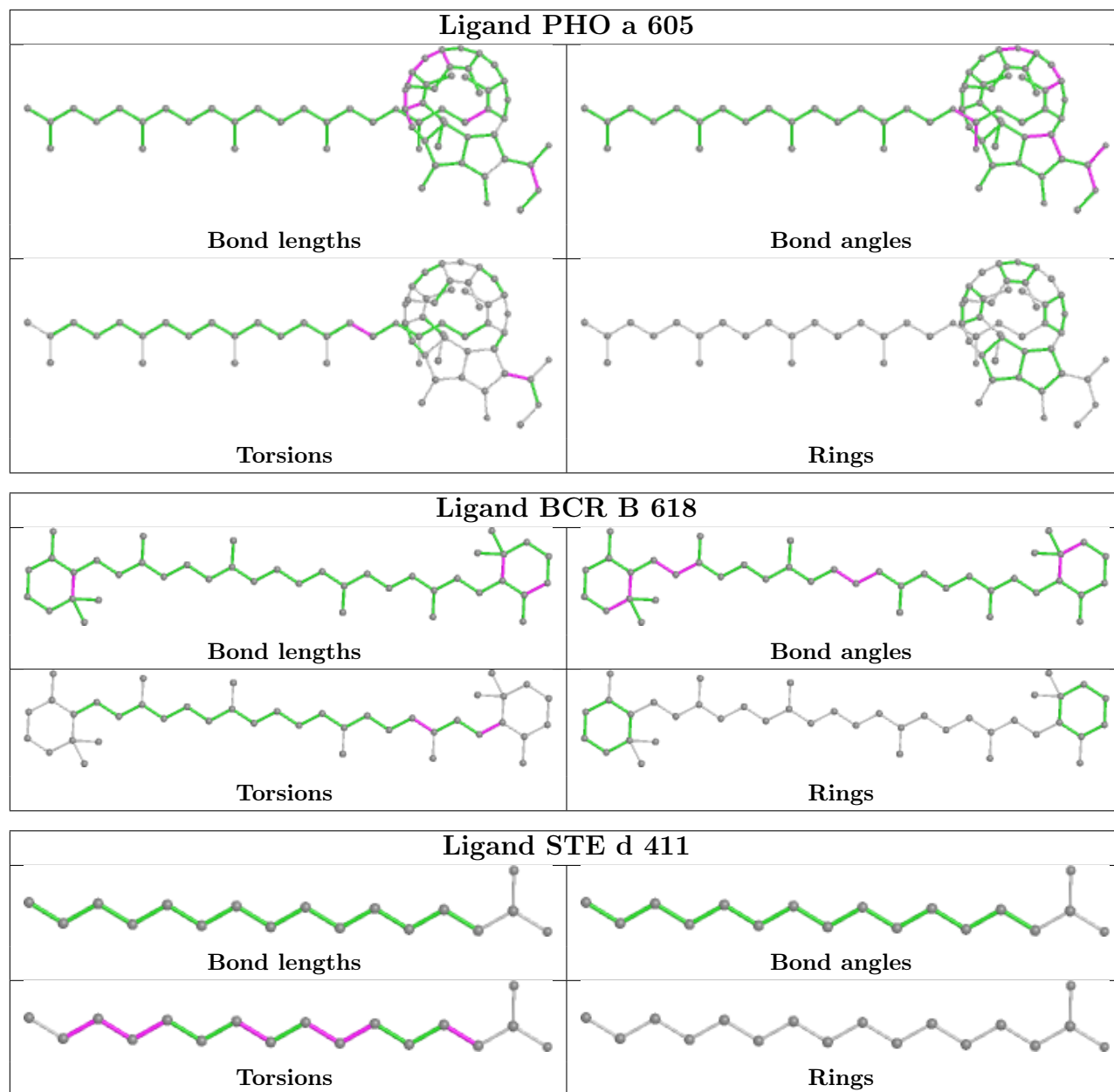


## Ligand CLA B 615

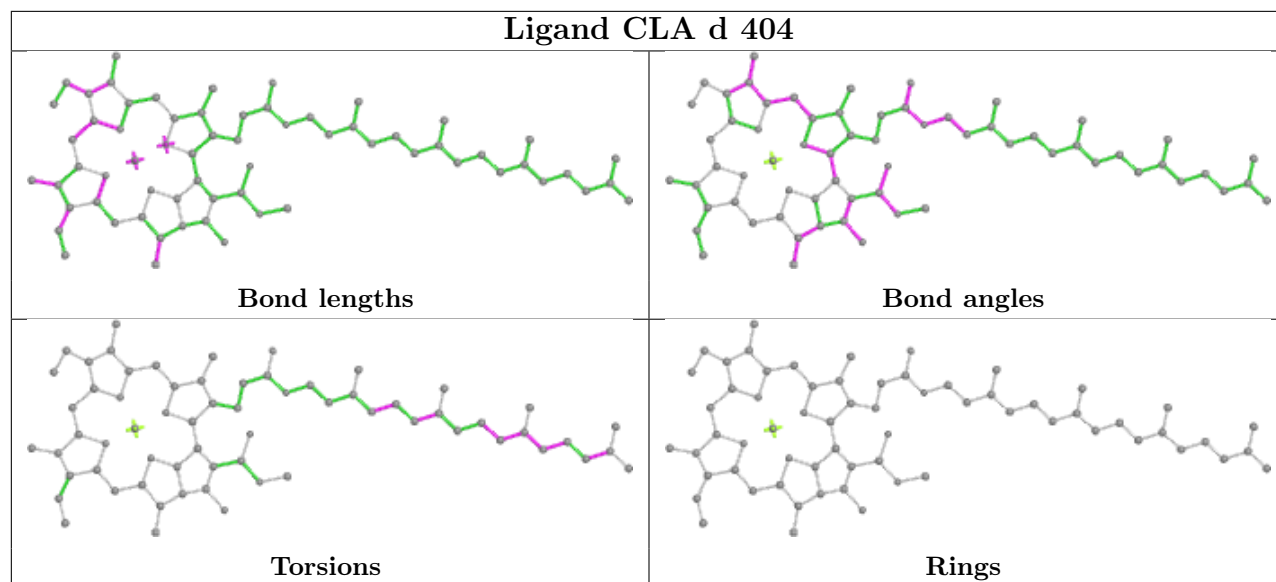




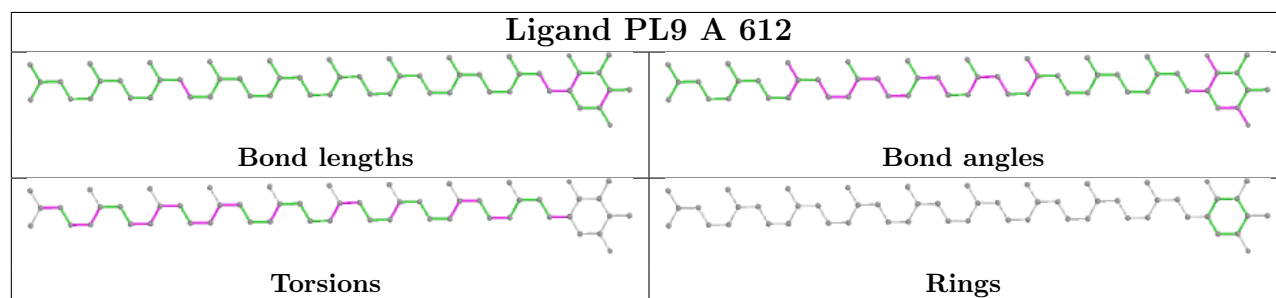




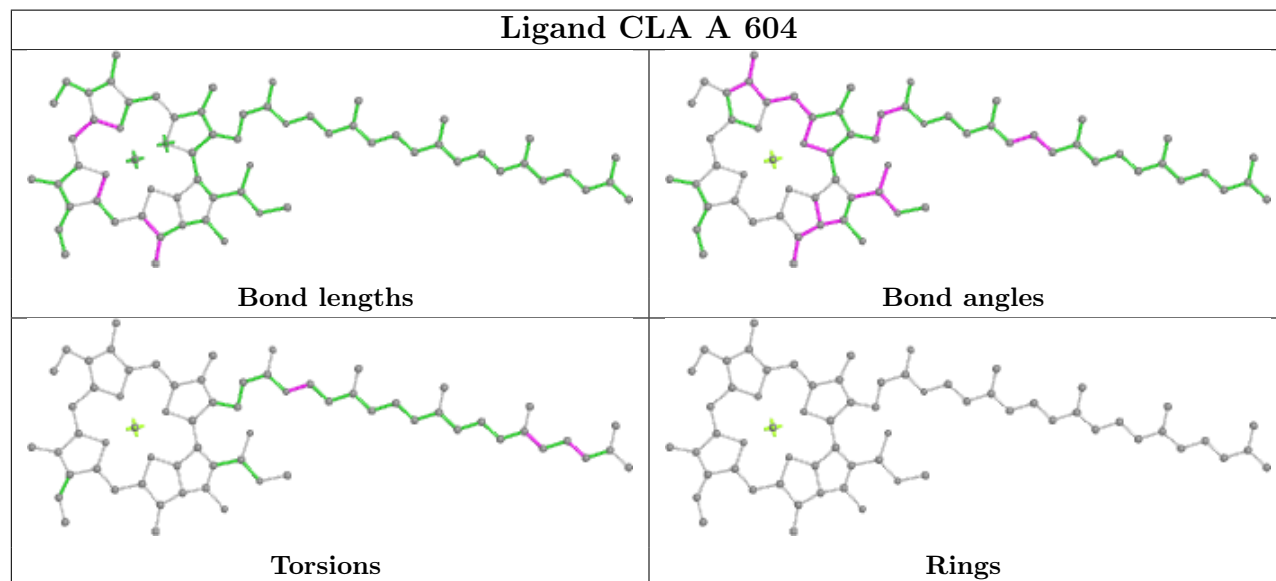
## Ligand CLA d 404

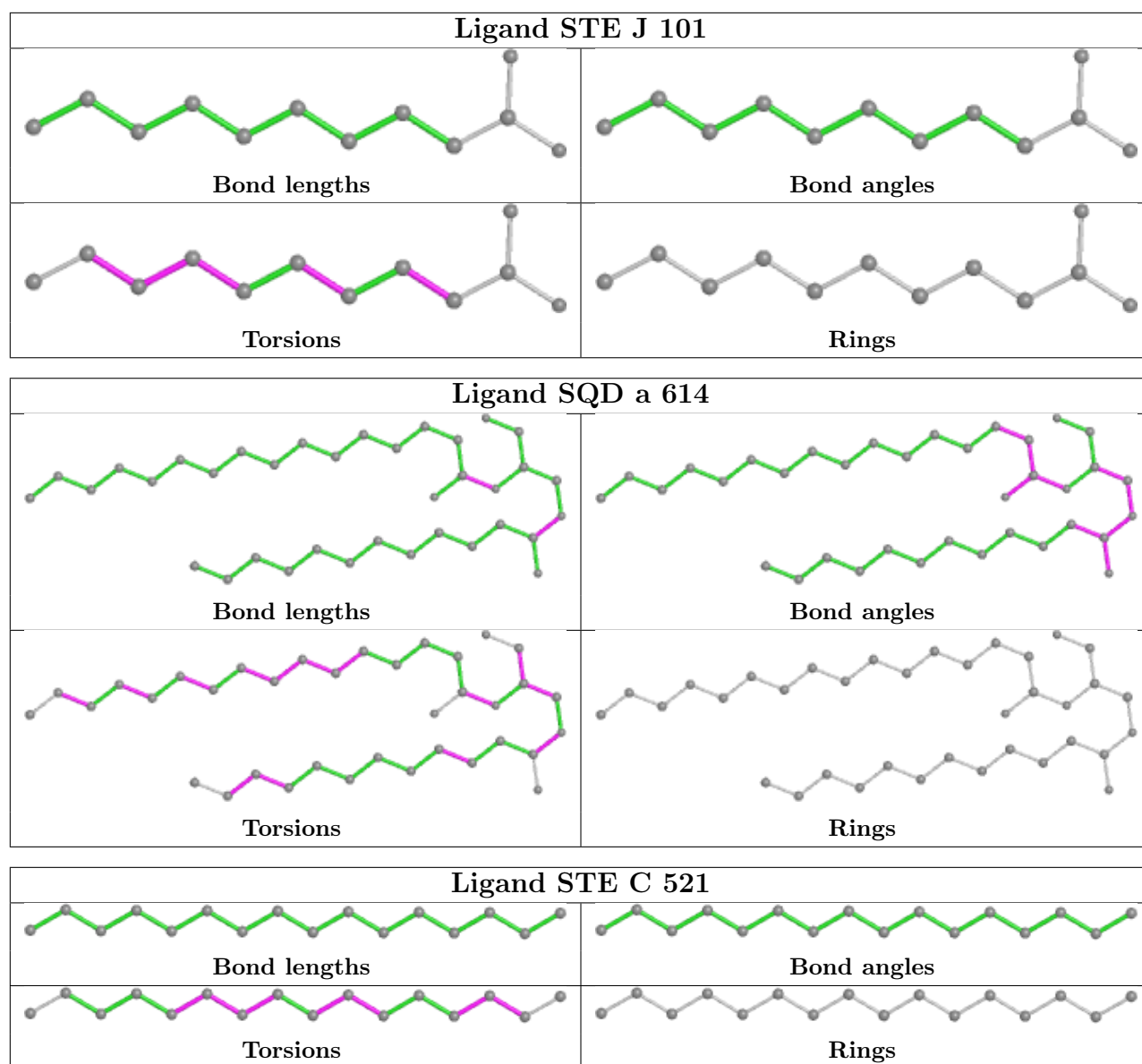


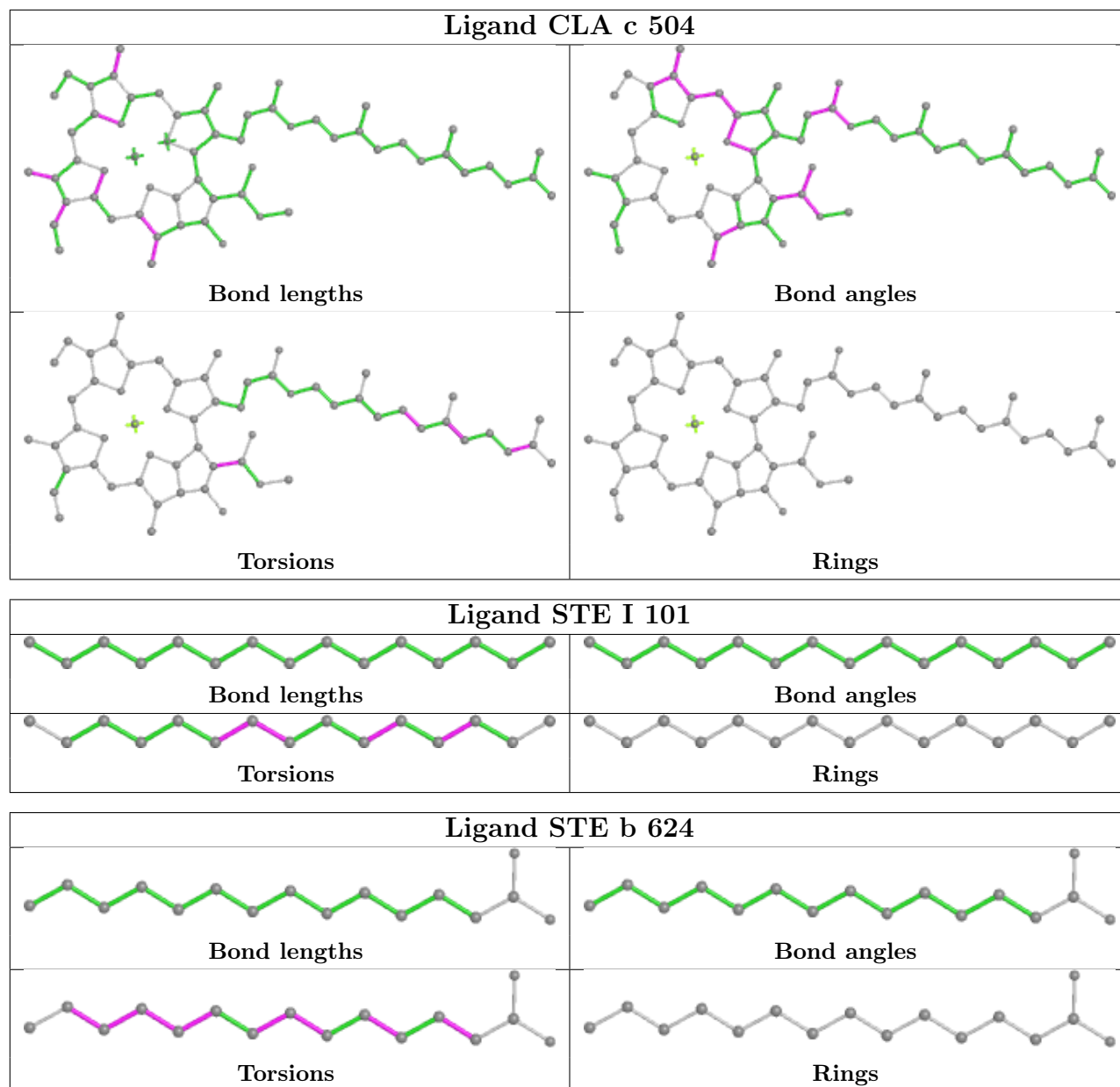
## Ligand PL9 A 612



## Ligand CLA A 604

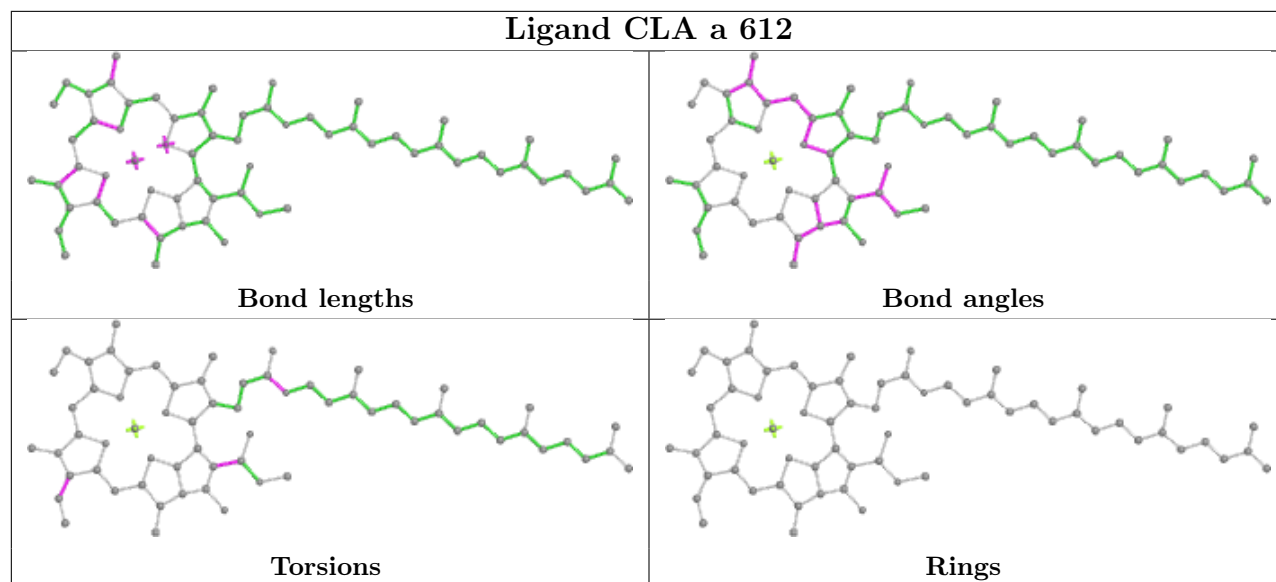




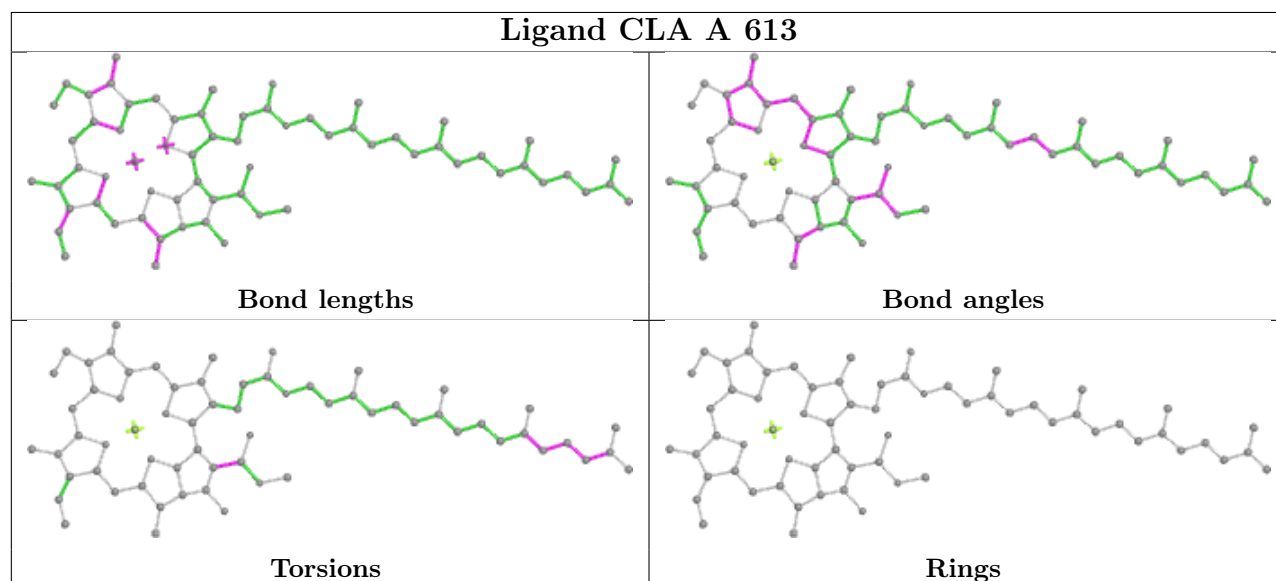




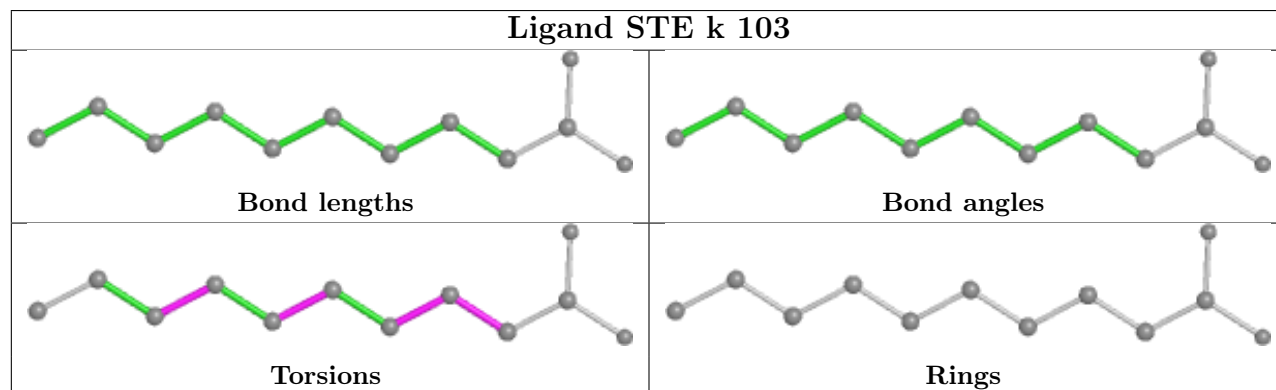
## Ligand CLA a 612

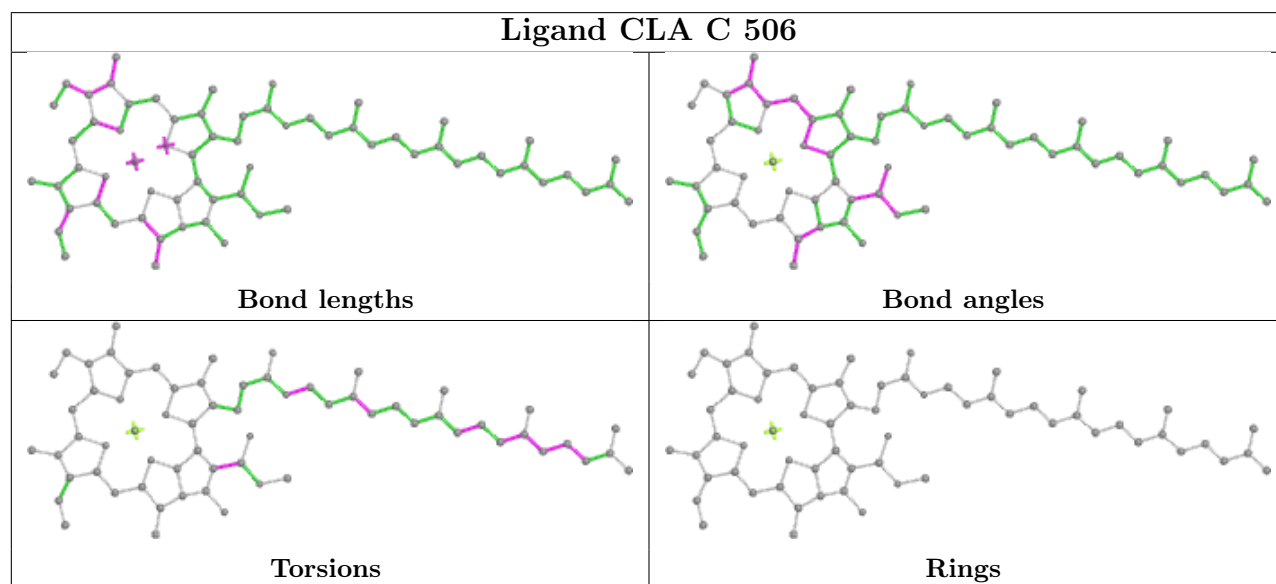
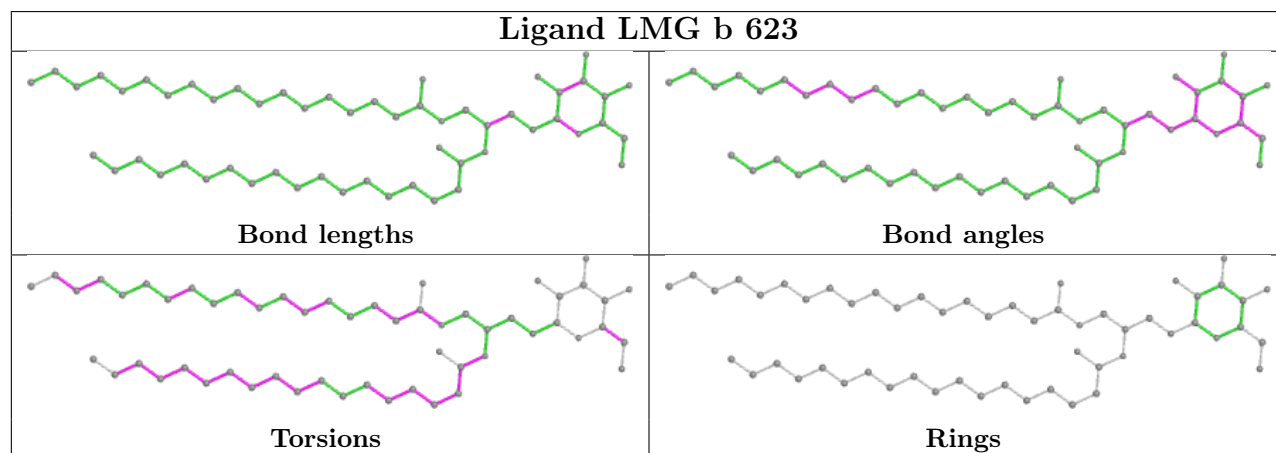
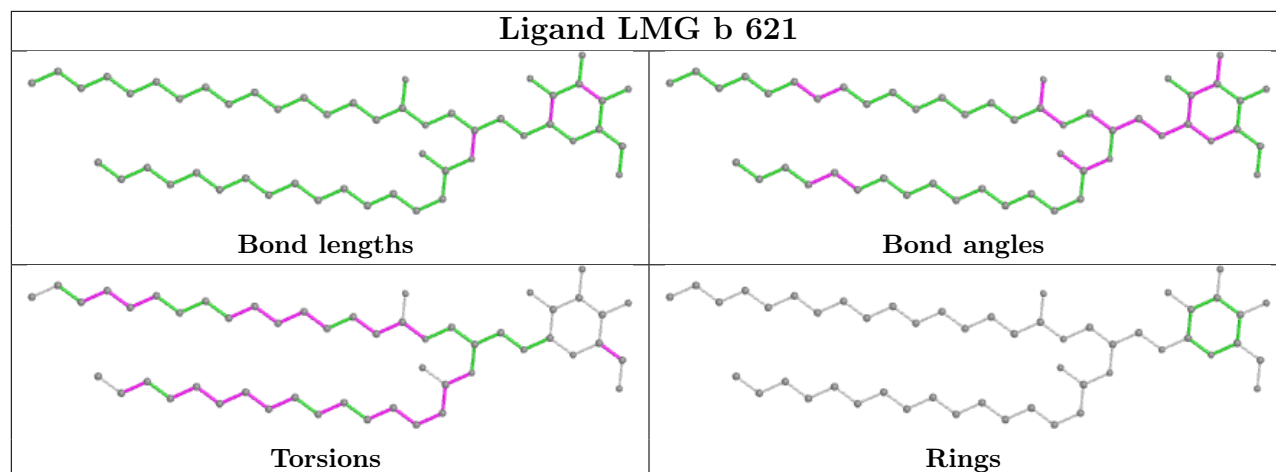


## Ligand CLA A 613

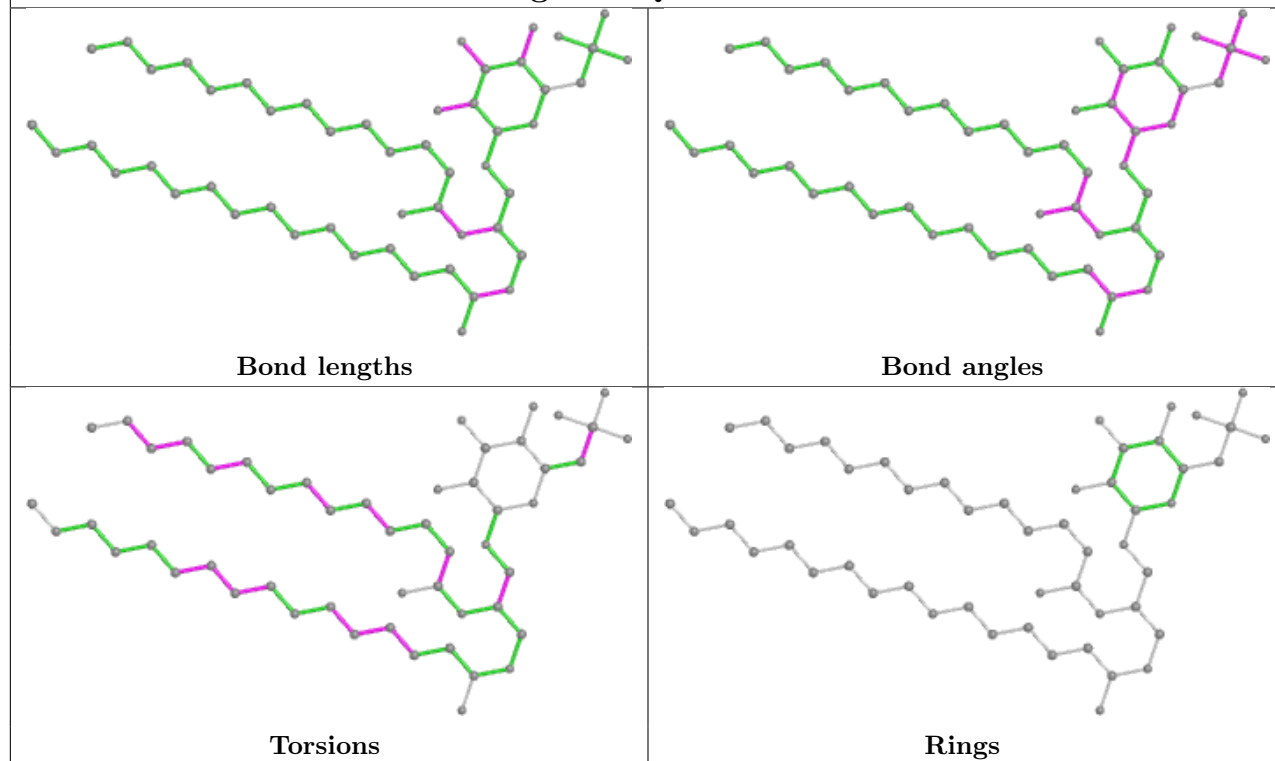


## Ligand STE k 103

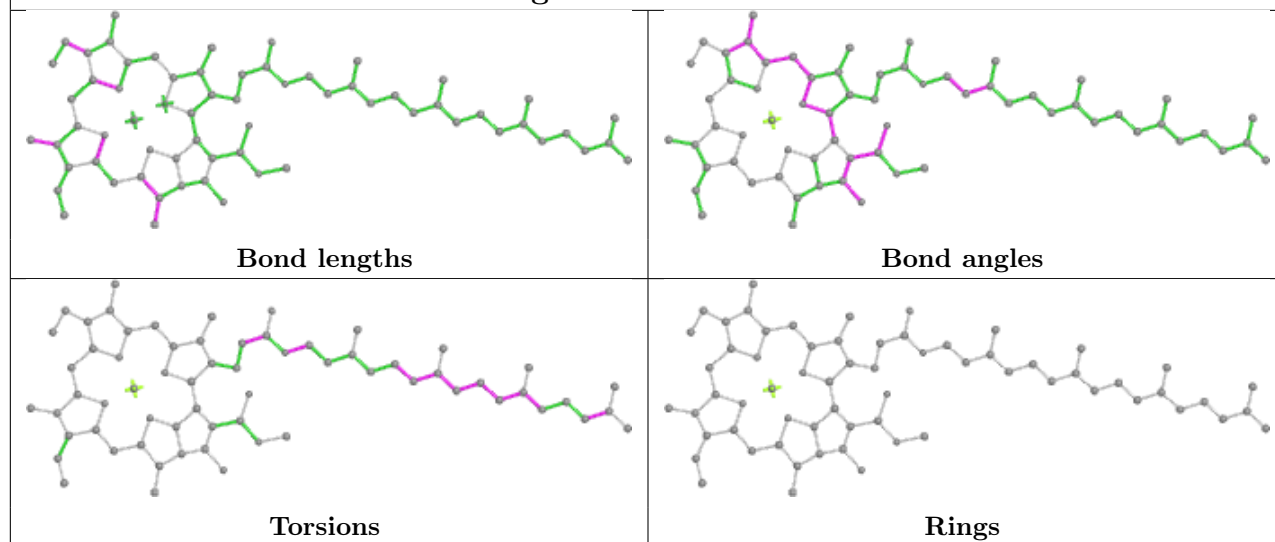


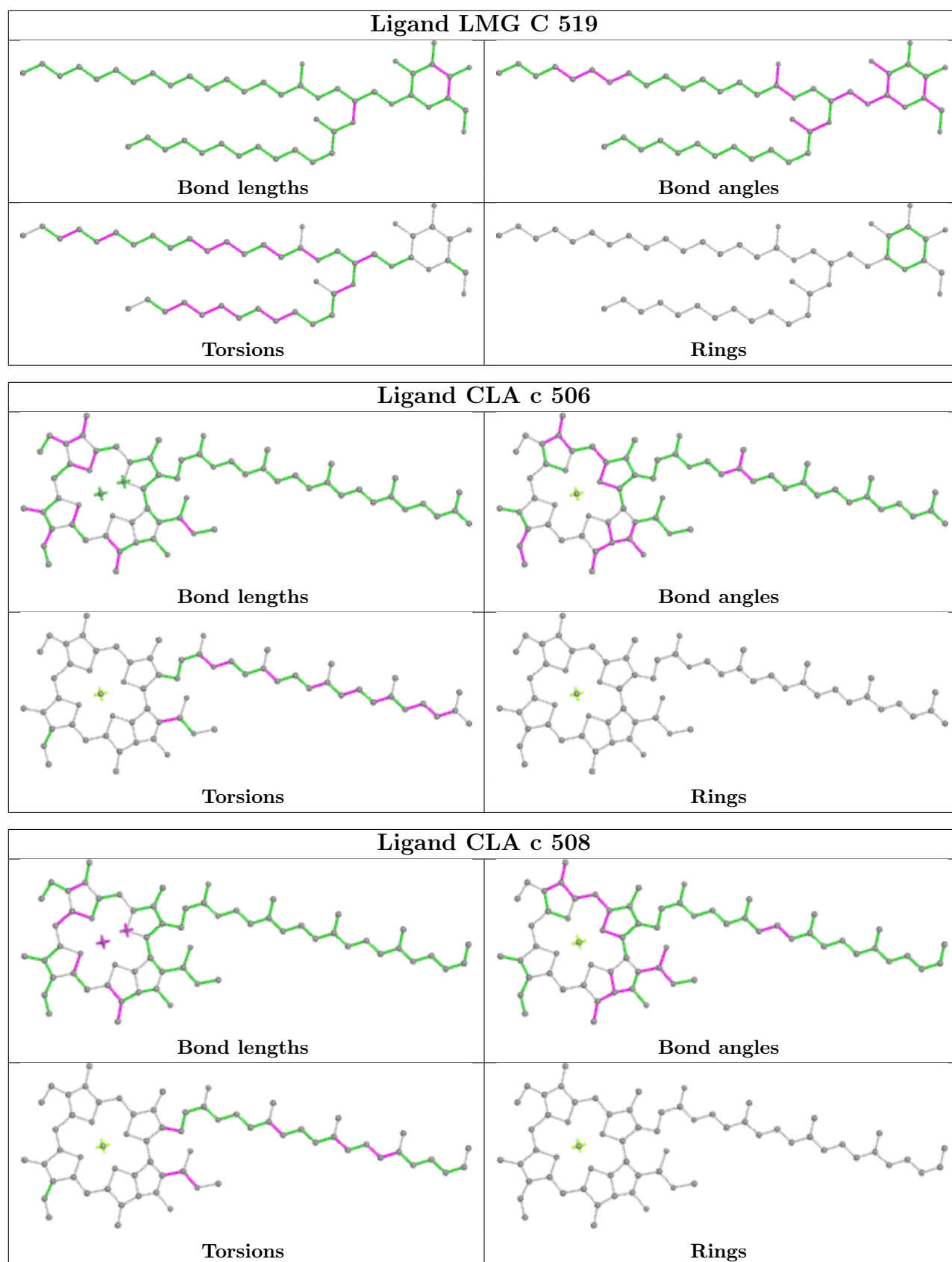


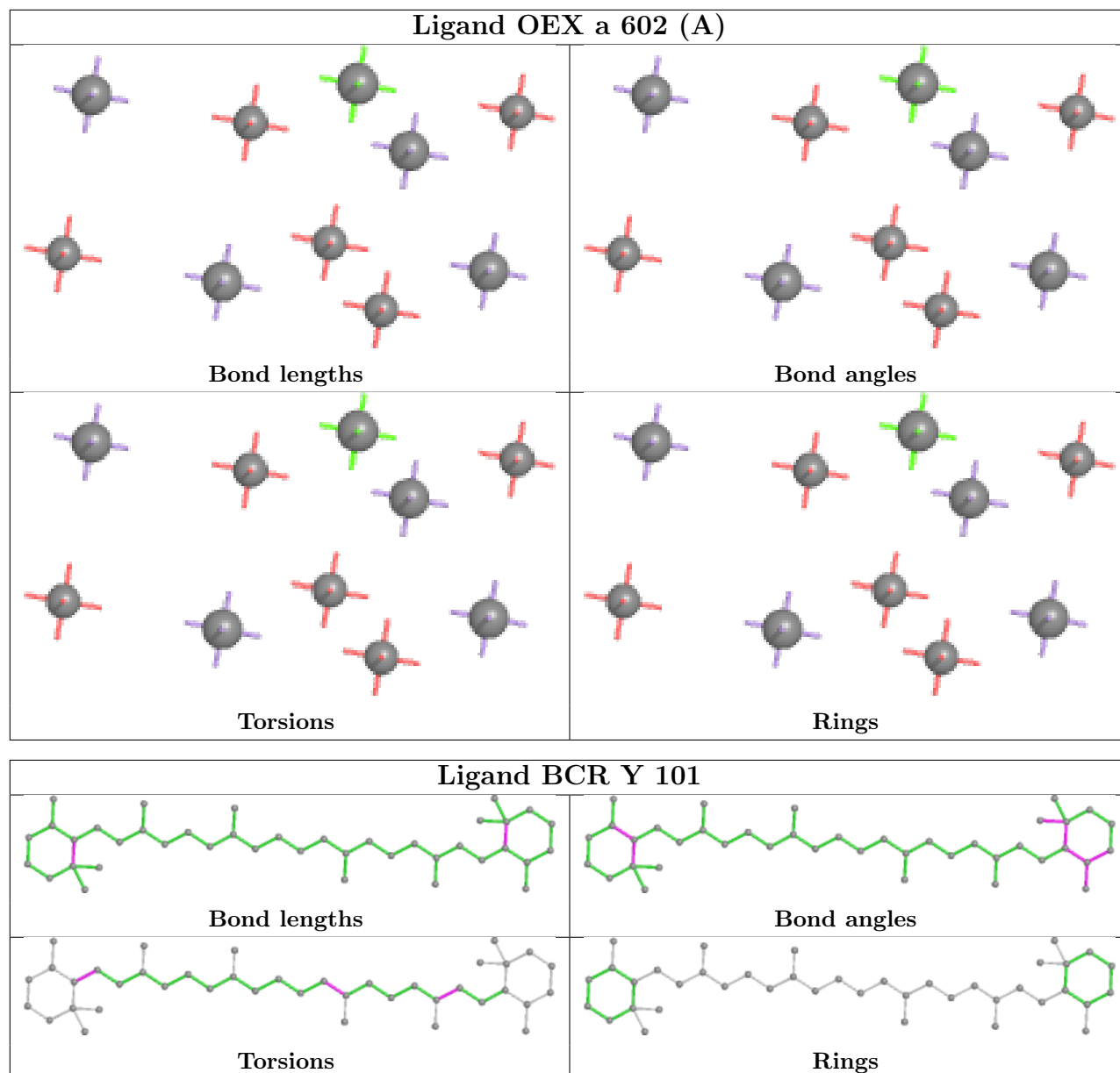
## Ligand SQD A 616

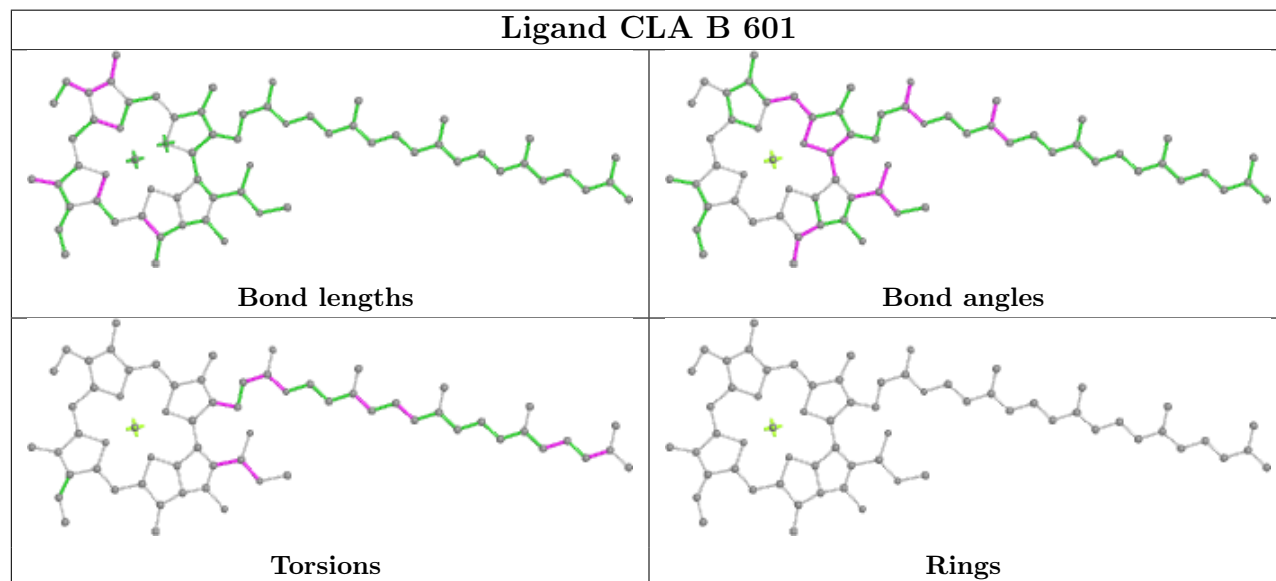
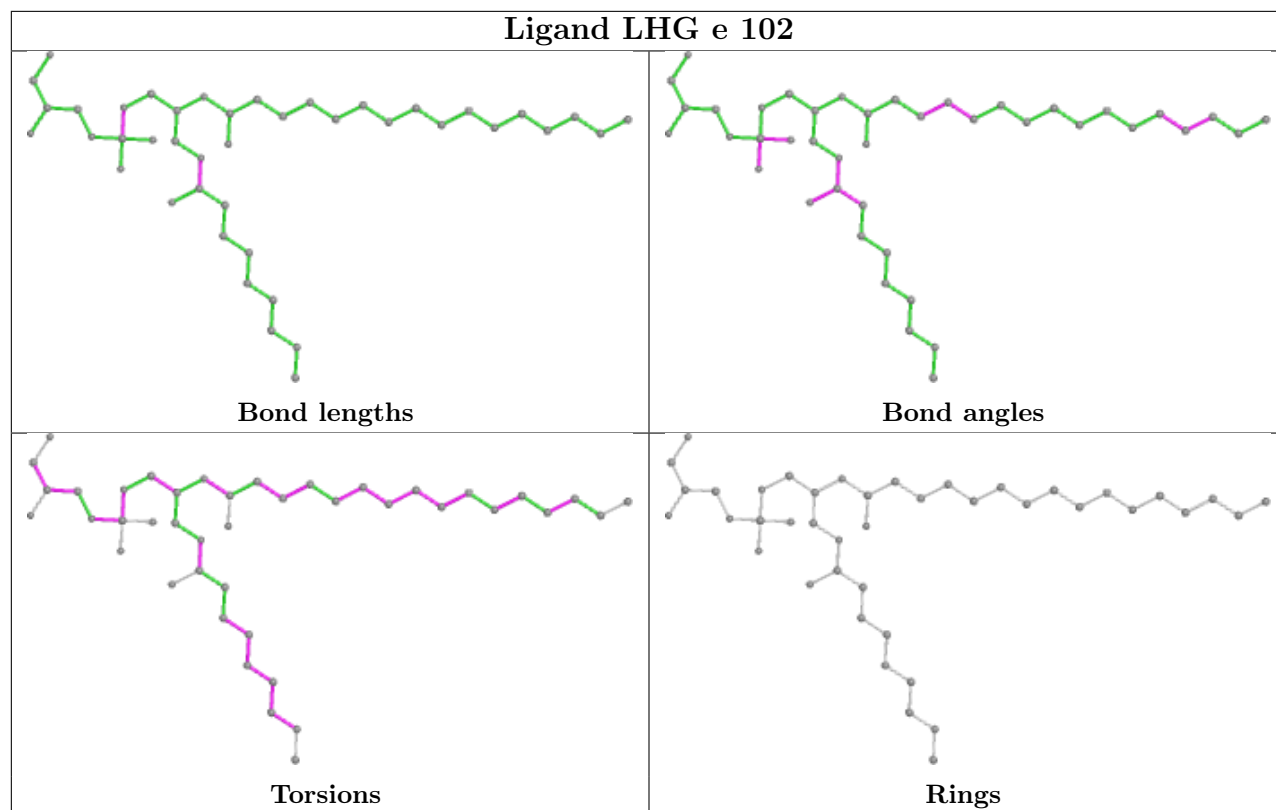


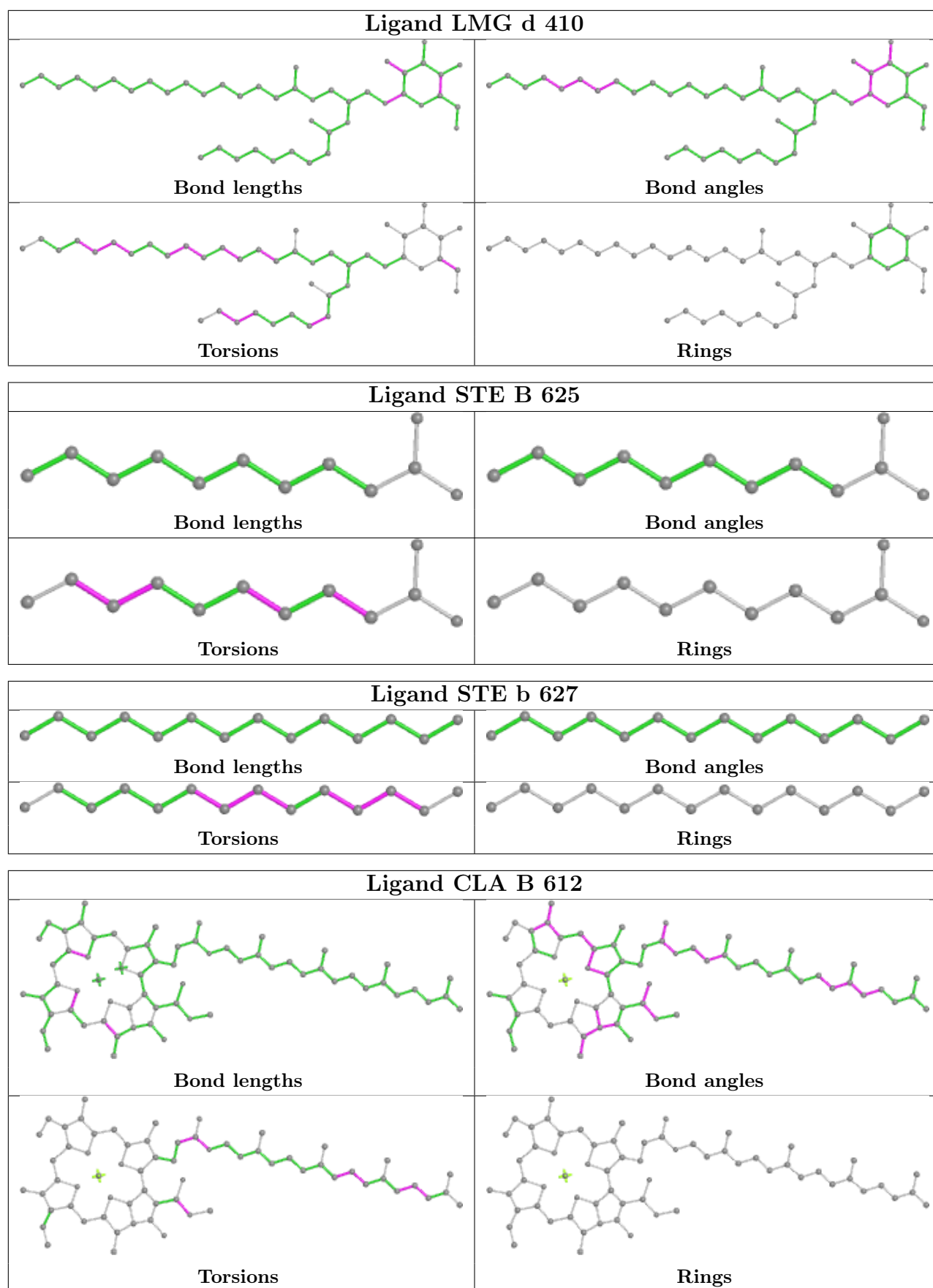
## Ligand CLA B 613



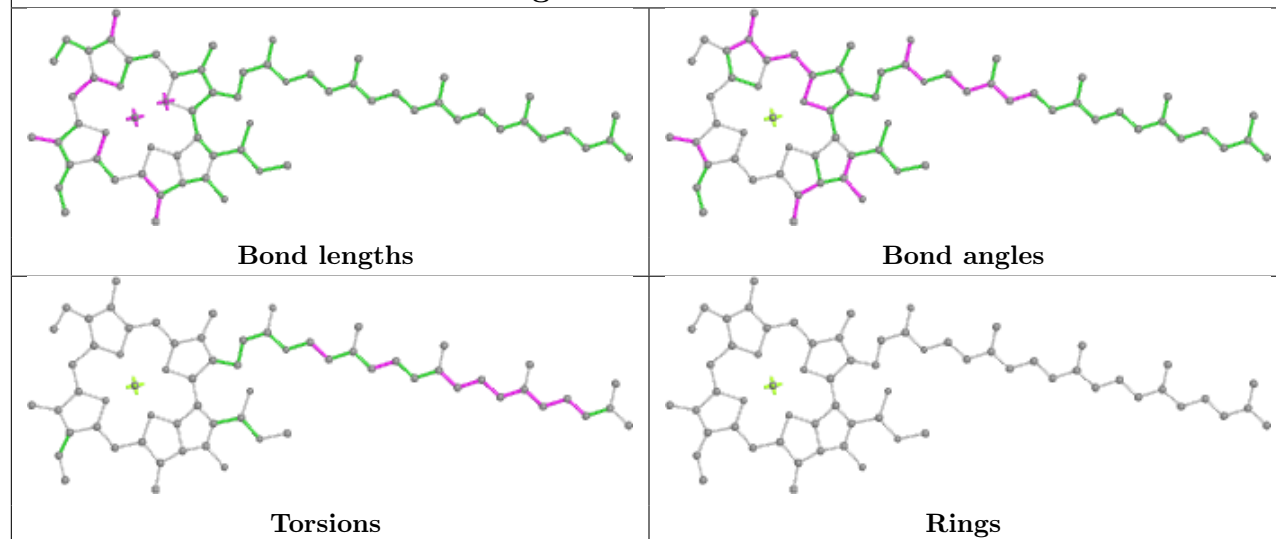




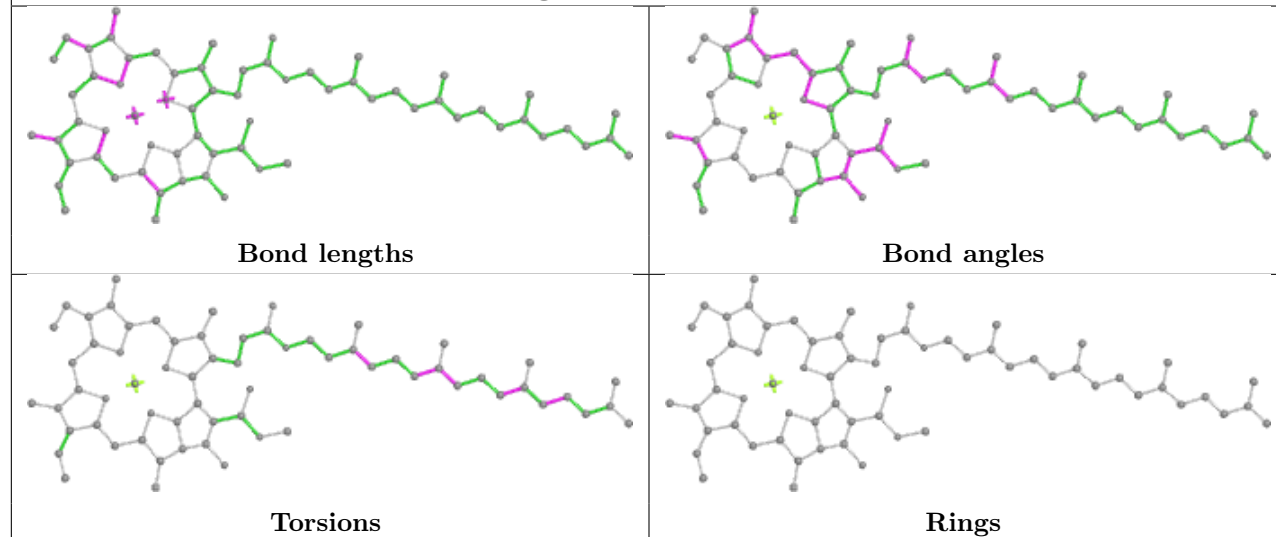




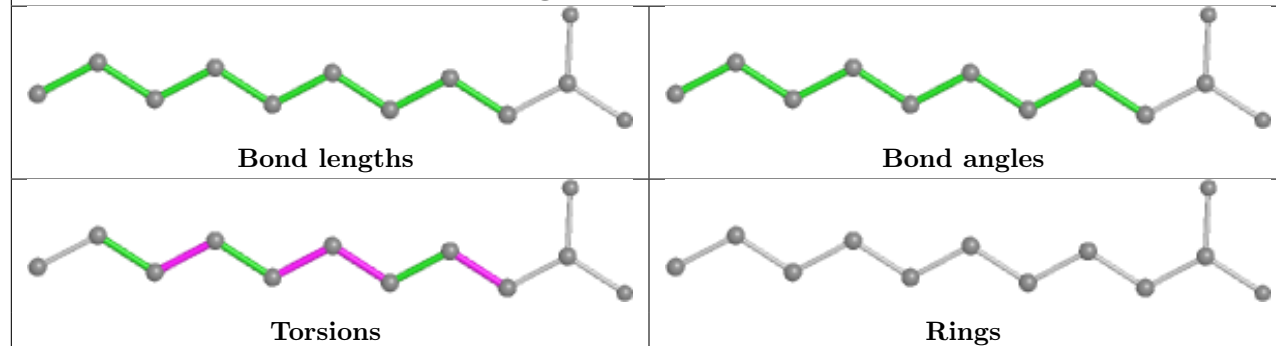
## Ligand CLA C 512



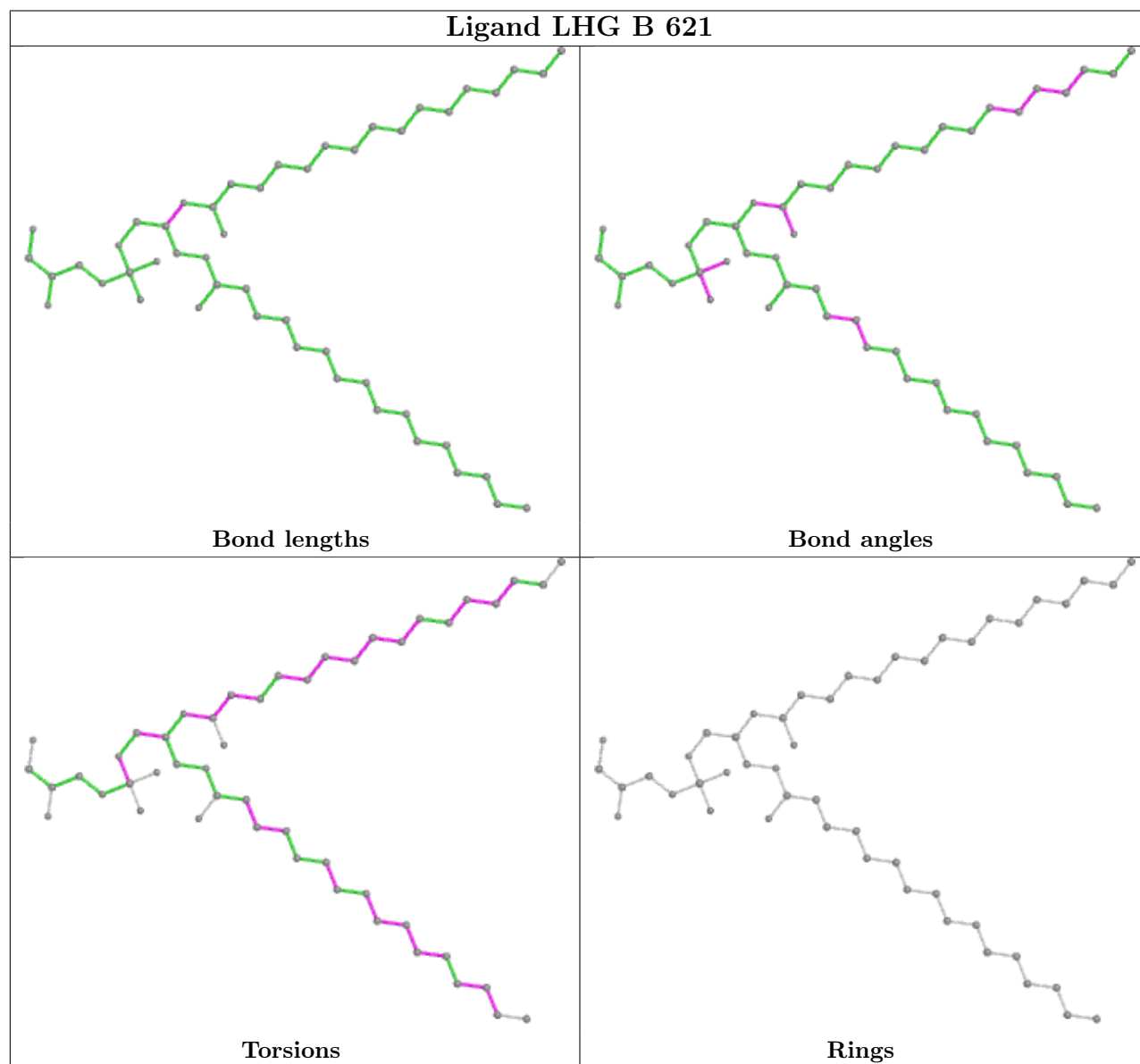
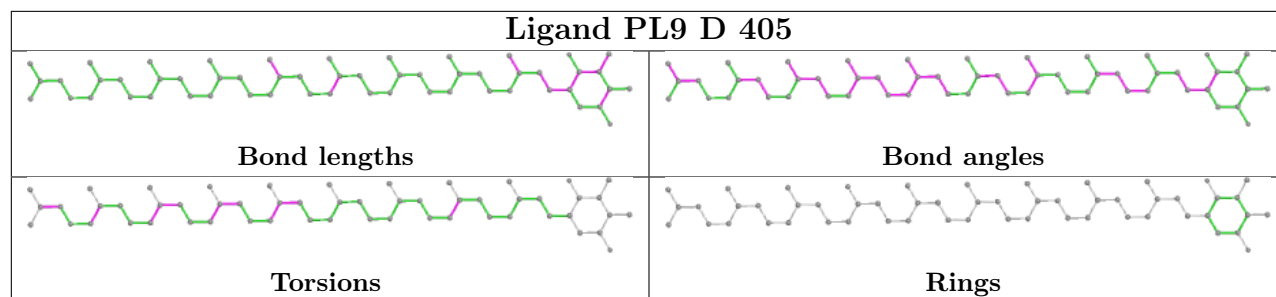
## Ligand CLA b 603

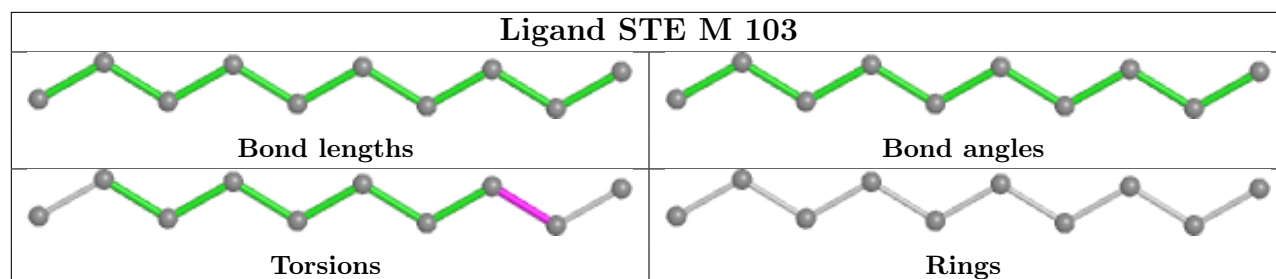
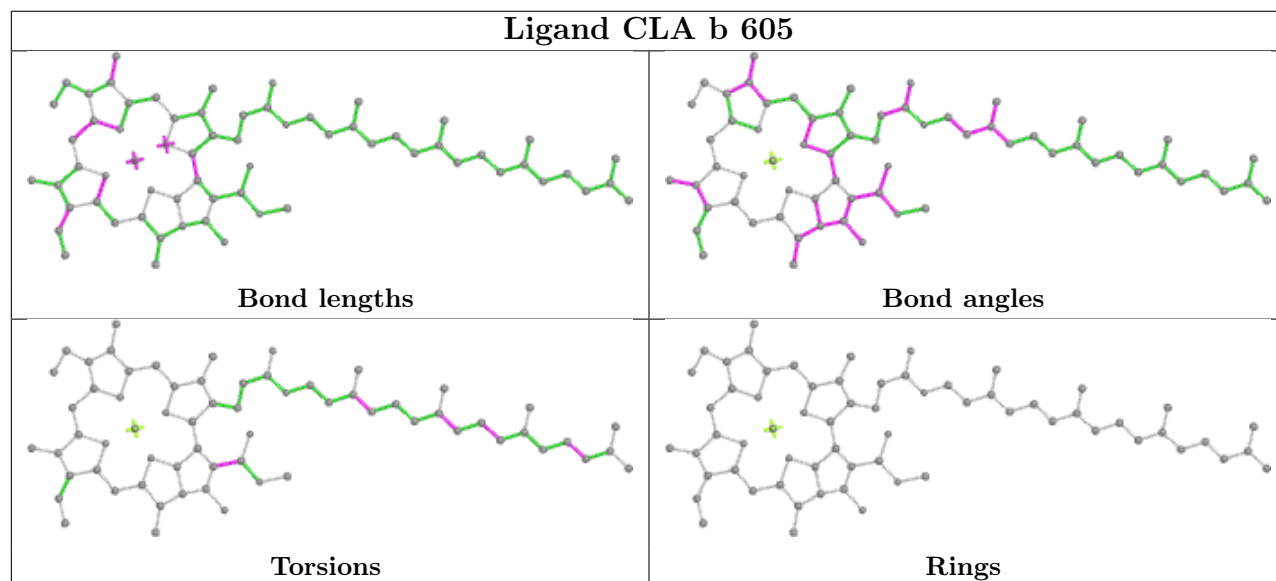
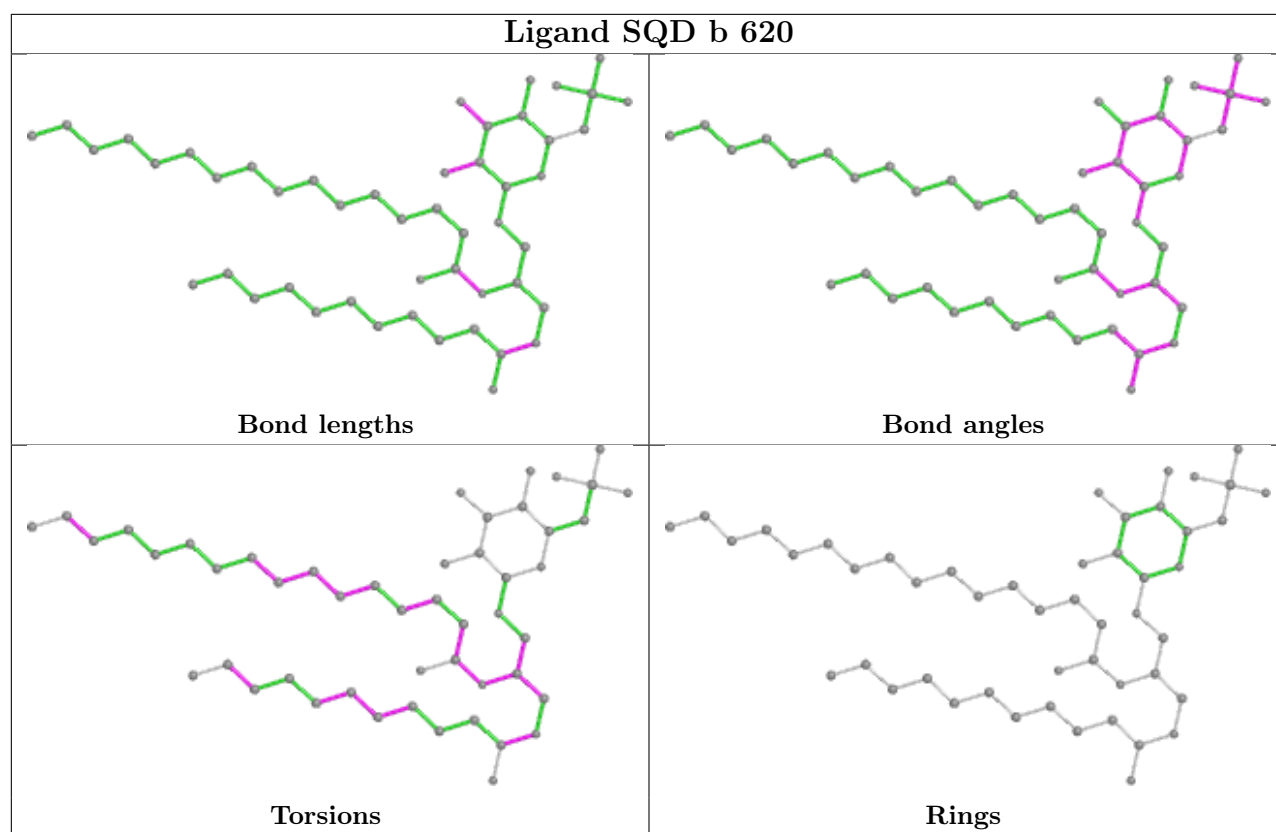


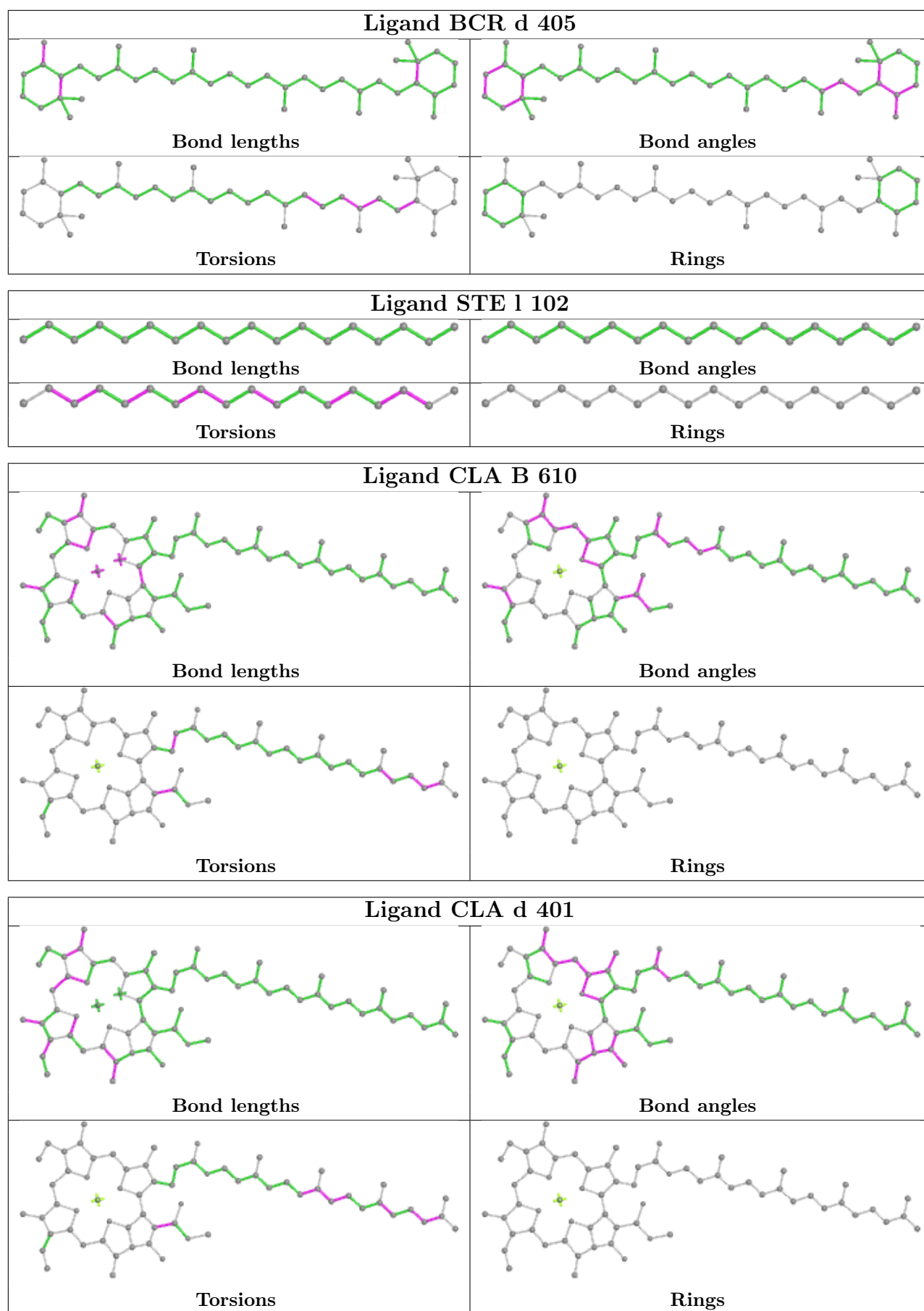
## Ligand STE E 102

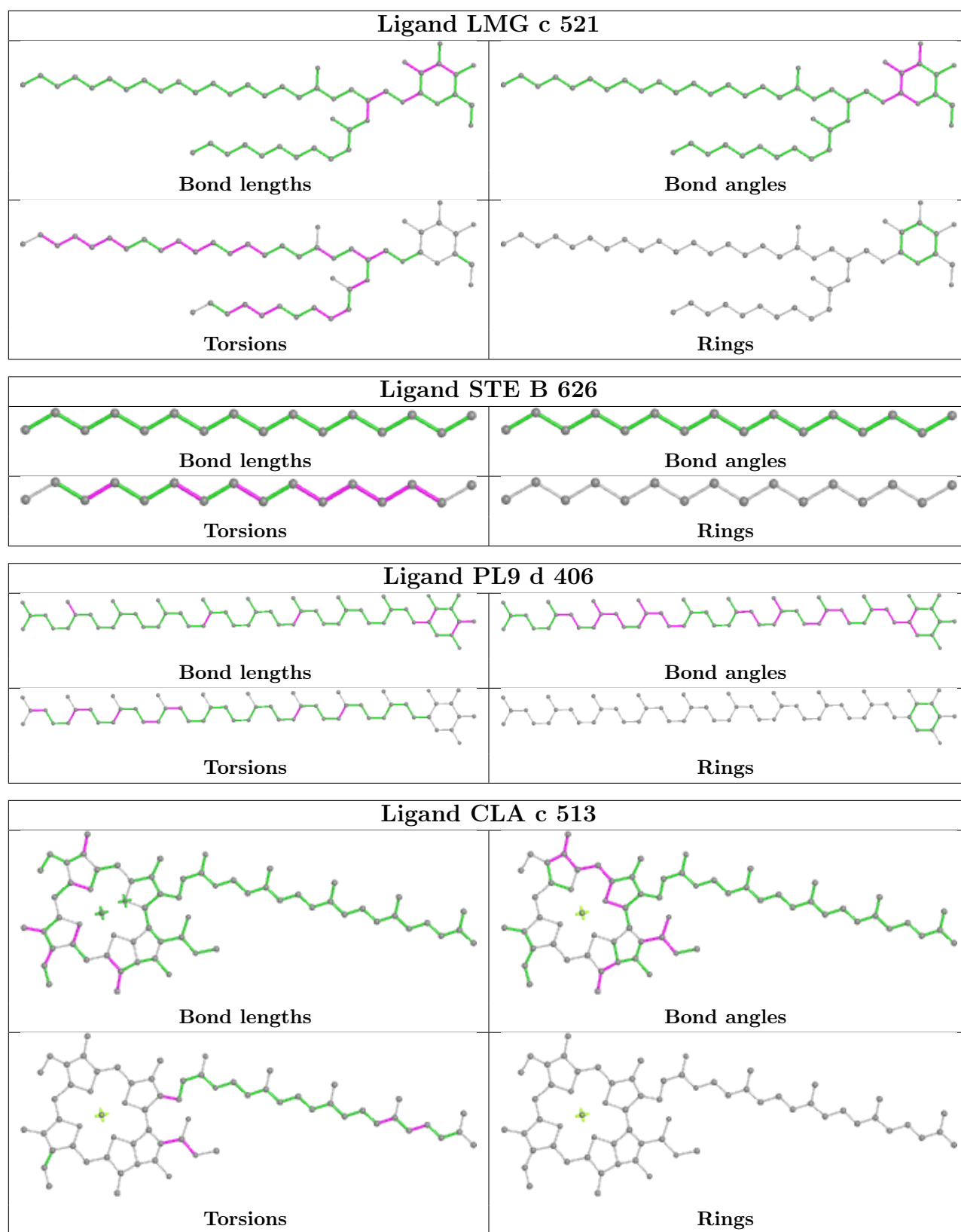


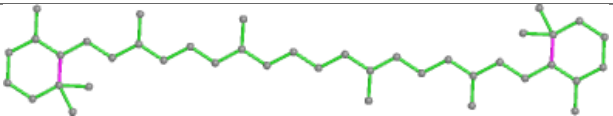
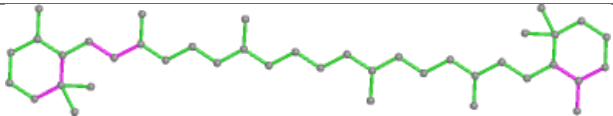
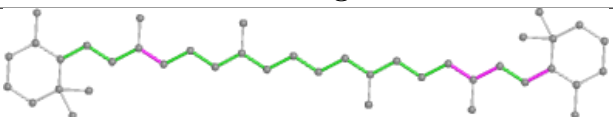
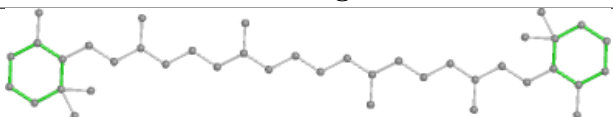



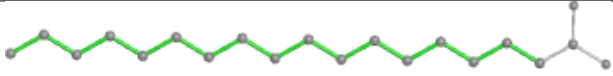
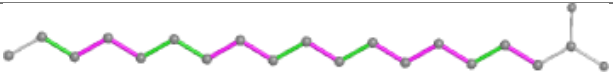
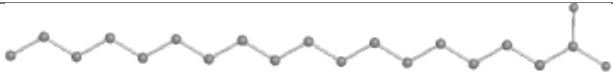


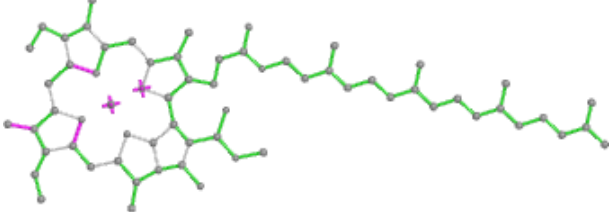
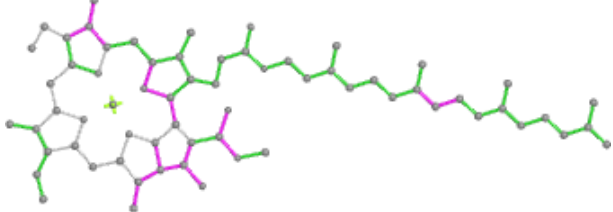
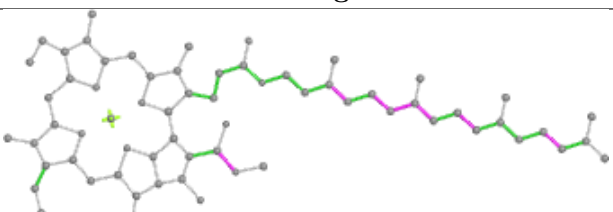
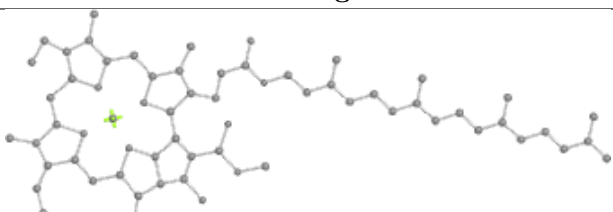




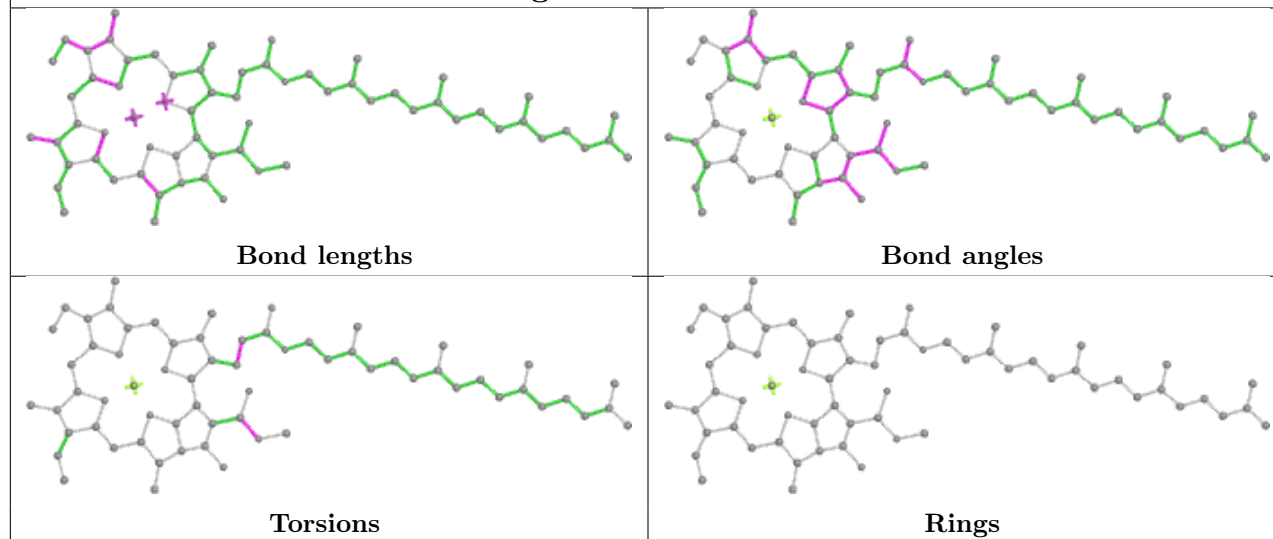


Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

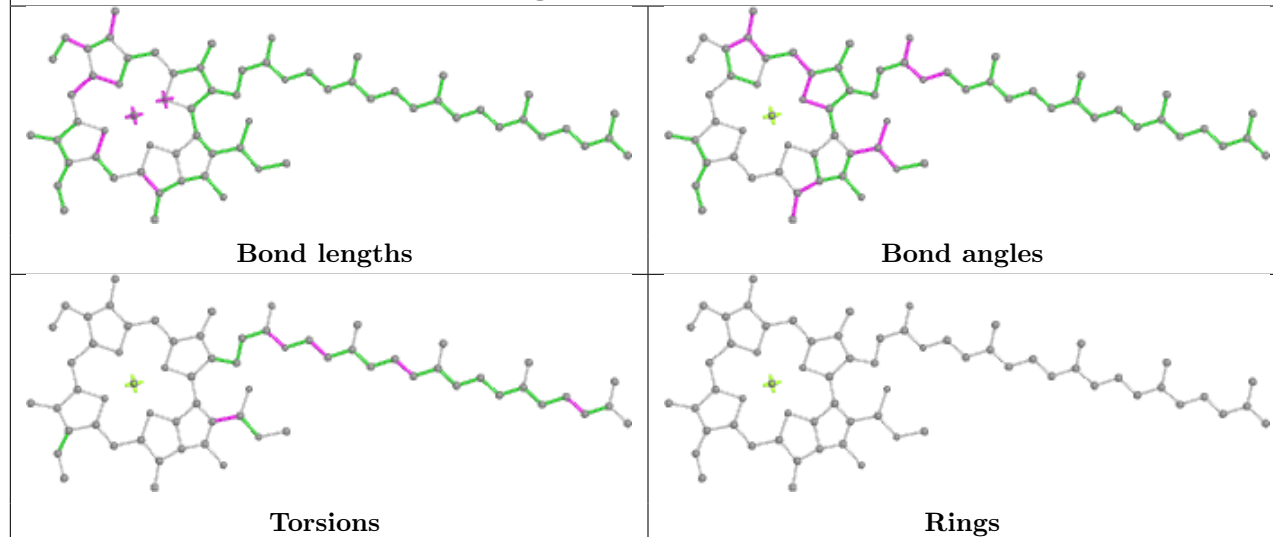
Ligand STE b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

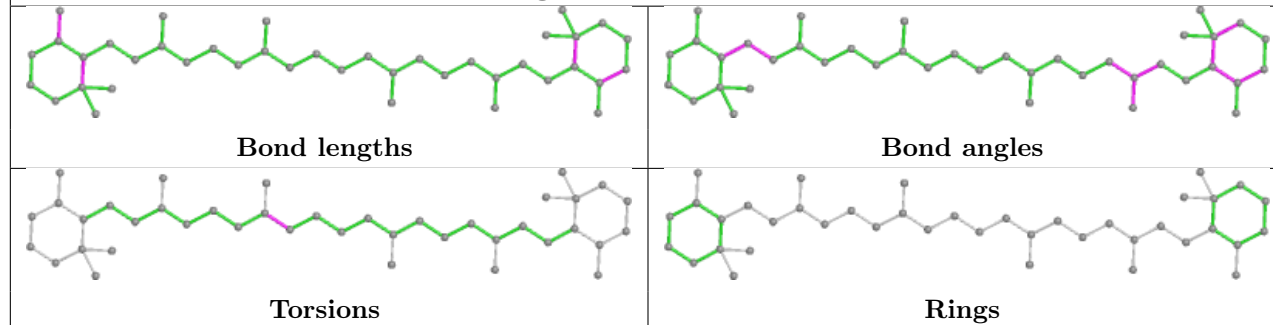
## Ligand CLA C 501

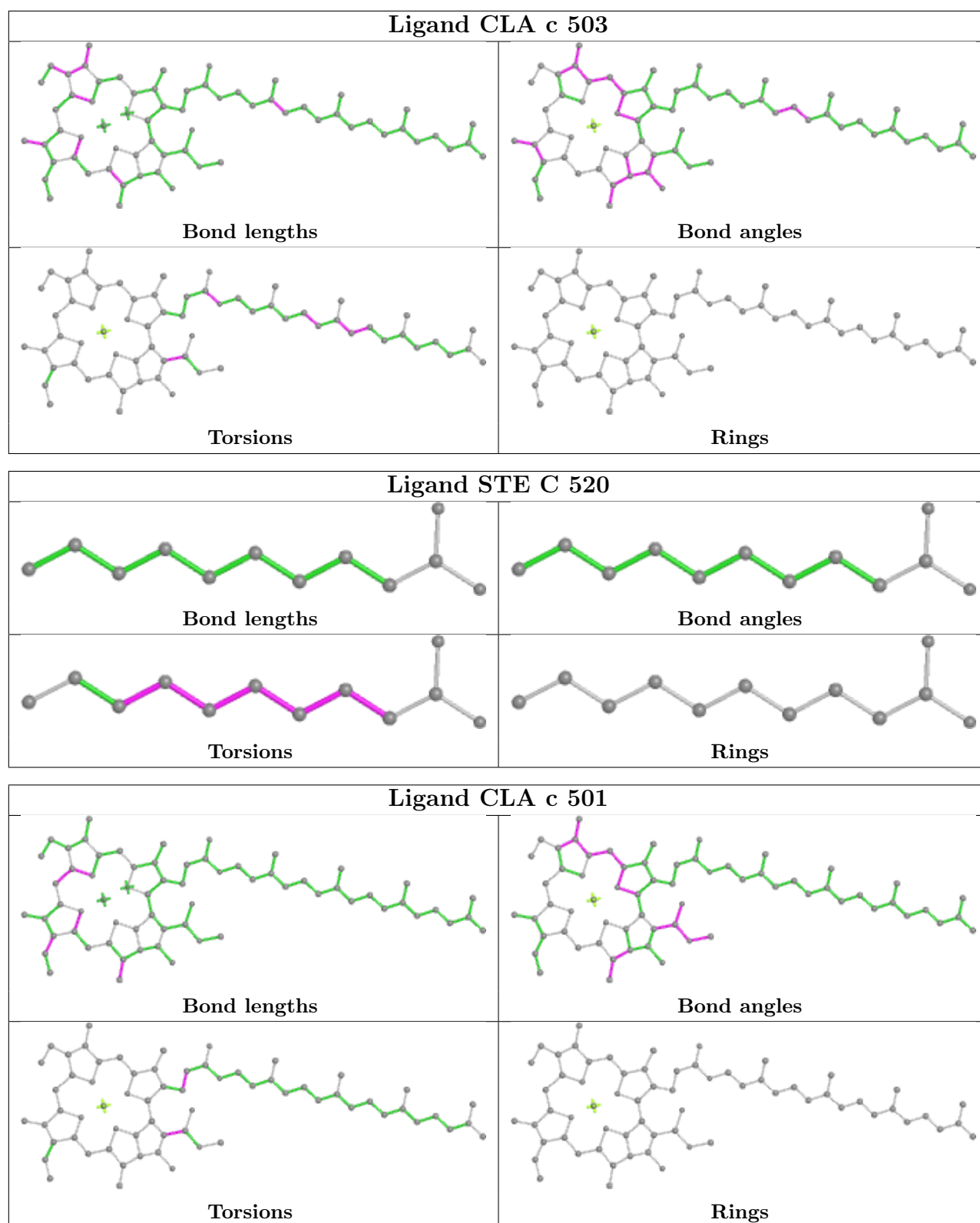


## Ligand CLA C 513



## Ligand BCR a 607





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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.30	4 (1%) 79 78	19, 27, 44, 77	0
1	a	334/344 (97%)	-0.31	1 (0%) 94 93	22, 29, 52, 77	0
2	B	505/510 (99%)	-0.27	9 (1%) 68 66	22, 31, 57, 80	0
2	b	505/510 (99%)	-0.08	18 (3%) 42 42	22, 34, 65, 97	0
3	C	442/461 (95%)	-0.18	2 (0%) 91 90	23, 33, 48, 70	0
3	c	451/461 (97%)	-0.10	8 (1%) 68 66	24, 37, 56, 94	0
4	D	341/352 (96%)	-0.30	1 (0%) 94 93	21, 28, 43, 74	0
4	d	341/352 (96%)	-0.20	1 (0%) 94 93	22, 31, 52, 73	0
5	E	82/84 (97%)	0.09	3 (3%) 41 41	32, 47, 63, 80	0
5	e	82/84 (97%)	0.36	7 (8%) 10 10	37, 54, 70, 81	0
6	F	34/45 (75%)	-0.29	1 (2%) 51 50	33, 39, 56, 78	0
6	f	34/45 (75%)	-0.12	2 (5%) 22 21	38, 44, 68, 84	0
7	H	65/66 (98%)	0.07	4 (6%) 20 19	30, 37, 52, 67	0
7	h	63/66 (95%)	0.43	8 (12%) 3 3	36, 46, 58, 64	0
8	I	35/38 (92%)	-0.13	3 (8%) 10 9	28, 36, 65, 77	0
8	i	35/38 (92%)	0.06	3 (8%) 10 9	29, 37, 68, 85	0
9	J	36/40 (90%)	0.11	4 (11%) 5 4	31, 46, 67, 81	0
9	j	36/40 (90%)	0.21	5 (13%) 2 2	36, 50, 86, 95	0
10	K	37/46 (80%)	0.15	1 (2%) 54 53	37, 48, 65, 73	0
10	k	37/46 (80%)	0.19	3 (8%) 12 11	44, 50, 64, 76	0
11	L	37/37 (100%)	-0.31	0 100 100	23, 28, 54, 63	0
11	l	36/37 (97%)	-0.10	2 (5%) 24 23	25, 28, 66, 83	0
12	M	32/36 (88%)	0.10	0 100 100	25, 32, 54, 65	0
12	m	31/36 (86%)	-0.04	0 100 100	24, 33, 47, 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%)	0.12	16 (6%) 18 17	24, 40, 76, 127	0
13	o	244/272 (89%)	-0.02	17 (6%) 16 15	25, 38, 74, 121	0
14	R	28/41 (68%)	1.68	12 (42%) 0 0	56, 63, 77, 81	0
14	r	28/41 (68%)	3.52	22 (78%) 0 0	65, 80, 95, 99	0
15	T	29/32 (90%)	-0.27	1 (3%) 45 44	25, 29, 54, 68	0
15	t	29/32 (90%)	-0.19	2 (6%) 16 16	25, 29, 70, 80	0
16	U	97/134 (72%)	-0.12	3 (3%) 49 48	29, 39, 65, 82	0
16	u	97/134 (72%)	-0.28	0 100 100	28, 37, 52, 81	0
17	V	137/163 (84%)	-0.35	0 100 100	28, 37, 51, 73	0
17	v	137/163 (84%)	-0.04	5 (3%) 42 42	31, 44, 62, 82	0
18	X	38/41 (92%)	0.26	2 (5%) 26 25	34, 45, 62, 70	0
18	x	39/41 (95%)	0.53	5 (12%) 3 3	44, 52, 79, 92	0
19	Y	27/46 (58%)	1.54	12 (44%) 0 0	49, 63, 90, 93	0
19	y	30/46 (65%)	0.66	4 (13%) 3 2	55, 66, 81, 89	0
20	Z	62/62 (100%)	1.05	16 (25%) 0 0	50, 62, 105, 118	0
20	z	62/62 (100%)	0.97	13 (20%) 1 0	54, 67, 103, 108	0
All	All	5293/5700 (92%)	-0.06	220 (4%) 36 35	19, 35, 67, 127	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.0
2	b	495	PHE	8.0
13	O	56	PRO	7.1
14	r	6	LEU	6.8
14	r	13	LEU	6.5
13	O	4	THR	6.4
14	r	10	LEU	6.3
14	r	28	VAL	6.2
14	r	3	TRP	6.1
1	A	13	LEU	5.8
14	R	3	TRP	5.8
9	j	6	GLY	5.8
13	O	3	GLN	5.7
13	O	60	ARG	5.6
13	o	3	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
13	o	60	ARG	5.5
3	c	23	ALA	5.4
5	e	79	PHE	5.4
14	r	29	LYS	5.4
3	c	24	THR	5.3
20	Z	62	VAL	5.3
14	r	25	PRO	5.2
15	T	30	THR	5.2
13	O	59	LYS	5.2
15	t	30	THR	5.2
20	Z	1	MET	5.1
14	r	24	LEU	5.0
14	r	14	LEU	4.9
14	R	6	LEU	4.8
20	z	30	PRO	4.7
20	Z	34	ASP	4.6
20	z	35	ARG	4.5
20	z	33	TRP	4.5
14	r	9	LEU	4.5
18	X	2	THR	4.5
19	Y	21	GLN	4.4
13	o	4	THR	4.3
2	b	487	SER	4.3
14	r	7	VAL	4.2
20	Z	35	ARG	4.2
2	b	127	ARG	4.2
13	o	5	LEU	4.1
1	A	11	ALA	4.1
20	Z	38	GLN	4.0
13	o	57	LYS	4.0
20	z	3	ILE	4.0
14	r	26	TYR	4.0
20	Z	33	TRP	4.0
6	F	12	SER	4.0
13	o	59	LYS	4.0
5	e	61	ARG	3.9
2	b	486	LEU	3.9
19	Y	20	ALA	3.8
13	o	62	GLU	3.8
5	E	79	PHE	3.7
1	a	11	ALA	3.7
9	j	7	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
18	x	2	THR	3.7
9	J	5	GLY	3.6
8	i	36	ASP	3.6
19	Y	43	ARG	3.6
19	Y	41	VAL	3.6
18	X	3	ILE	3.5
5	E	83	LEU	3.5
13	O	5	LEU	3.5
18	x	34	ILE	3.5
2	B	127	ARG	3.5
20	Z	3	ILE	3.4
7	H	66	GLY	3.4
20	Z	60	PHE	3.4
20	z	36	SER	3.4
9	J	7	ARG	3.4
3	c	143	TYR	3.4
7	h	21	VAL	3.4
20	Z	7	LEU	3.3
13	O	61	GLN	3.3
13	o	207	ARG	3.3
20	Z	41	PHE	3.3
2	b	292	LEU	3.3
3	c	25	ASN	3.3
2	b	295	GLY	3.2
14	R	21	ARG	3.2
2	B	490	GLN	3.2
9	j	8	ILE	3.2
3	c	146	PHE	3.2
2	b	506	ARG	3.2
8	i	34	ARG	3.1
18	x	38	GLN	3.1
2	b	505	ARG	3.1
20	Z	37	LYS	3.1
13	o	63	ALA	3.1
14	r	23	ILE	3.1
19	Y	37	PHE	3.1
2	b	502	VAL	3.1
7	h	6	TRP	3.1
11	l	3	PRO	3.1
9	j	5	GLY	3.0
8	I	34	ARG	3.0
13	O	58	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
20	z	60	PHE	3.0
14	r	5	VAL	3.0
14	r	18	TRP	3.0
20	z	41	PHE	3.0
3	C	143	TYR	3.0
19	Y	22	LEU	3.0
14	r	21	ARG	2.9
14	R	26	TYR	2.9
20	Z	32	ASP	2.9
2	b	289	GLN	2.9
19	Y	40	ALA	2.9
10	k	17	ILE	2.9
14	r	12	VAL	2.9
14	r	4	ARG	2.9
14	r	27	ALA	2.9
19	y	18	VAL	2.8
13	o	61	GLN	2.8
14	R	28	VAL	2.8
20	Z	61	VAL	2.8
2	b	293	ALA	2.8
2	B	495	PHE	2.8
17	v	15	GLU	2.8
9	J	6	GLY	2.8
20	Z	4	LEU	2.8
20	Z	42	LEU	2.8
8	I	35	LYS	2.8
7	h	10	ILE	2.8
8	I	36	ASP	2.8
13	O	57	LYS	2.8
17	v	21	LEU	2.8
13	O	62	GLU	2.7
5	e	83	LEU	2.7
13	o	56	PRO	2.7
10	k	13	GLU	2.7
20	Z	31	GLN	2.7
8	i	35	LYS	2.7
19	y	37	PHE	2.7
19	Y	42	ARG	2.7
7	h	20	LYS	2.7
19	Y	25	ILE	2.7
13	O	55	GLU	2.7
5	e	84	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
14	R	29	LYS	2.6
2	B	505	ARG	2.6
13	o	246	ALA	2.6
17	v	113	VAL	2.6
16	U	8	GLU	2.6
13	O	63	ALA	2.6
19	Y	23	THR	2.6
3	C	146	PHE	2.6
2	b	496	TYR	2.6
5	E	82	GLN	2.6
2	B	295	GLY	2.5
15	t	29	ILE	2.5
9	J	8	ILE	2.5
11	l	7	ARG	2.5
2	b	296	ALA	2.5
5	e	82	GLN	2.4
2	B	294	SER	2.4
10	K	17	ILE	2.4
17	v	22	THR	2.4
2	b	128	THR	2.4
2	B	487	SER	2.4
20	z	42	LEU	2.4
2	b	490	GLN	2.4
14	R	25	PRO	2.4
14	r	22	ASN	2.4
14	r	15	ALA	2.4
6	f	12	SER	2.4
7	h	41	PHE	2.4
16	U	9	LEU	2.4
13	O	87	VAL	2.4
13	o	55	GLU	2.4
3	c	147	PHE	2.3
7	H	41	PHE	2.3
18	x	40	SER	2.3
1	A	15	GLU	2.3
14	r	11	PRO	2.3
13	O	36	GLN	2.3
7	h	63	LYS	2.3
2	b	494	GLY	2.3
5	e	74	GLN	2.3
18	x	39	ARG	2.3
2	B	502	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
14	R	14	LEU	2.2
7	H	18	TYR	2.2
14	R	24	LEU	2.2
5	e	81	GLU	2.2
13	O	35	SER	2.2
1	A	12	ASN	2.2
19	y	40	ALA	2.2
20	z	59	PHE	2.2
19	Y	45	ASN	2.2
17	v	17	LYS	2.2
19	y	19	ILE	2.1
4	d	227[A]	GLU	2.1
6	f	16	PHE	2.1
14	R	20	VAL	2.1
20	z	61	VAL	2.1
20	z	39	LEU	2.1
7	H	6	TRP	2.1
13	O	246	ALA	2.1
10	k	10	LYS	2.1
20	z	7	LEU	2.1
3	c	145	SER	2.1
2	B	506	ARG	2.1
4	D	12	ARG	2.1
9	j	9	PRO	2.1
14	R	5	VAL	2.1
16	U	68	THR	2.1
13	o	132	ASN	2.0
7	h	13	PRO	2.0
2	b	485	GLU	2.0
3	c	142	GLU	2.0
20	z	62	VAL	2.0
7	h	23	PRO	2.0
19	Y	24	MET	2.0
13	o	64	GLU	2.0
2	b	161	LEU	2.0
13	o	133	VAL	2.0
14	R	2	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.94	0.13	37,48,67,75	0
15	FME	t	1	10/11	0.94	0.10	31,44,66,66	0
8	FME	I	1	10/11	0.95	0.19	35,46,65,66	0
8	FME	i	1	10/11	0.96	0.16	33,48,59,64	0
12	FME	m	1	10/11	0.96	0.14	34,42,59,71	0
15	FME	T	1	10/11	0.96	0.08	28,45,61,61	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
33	STE	E	102	12/20	0.68	0.29	56,72,77,83	0
33	STE	H	103	18/20	0.71	0.30	49,67,78,81	0
33	STE	a	616	12/20	0.75	0.26	45,61,68,71	0
33	STE	B	627	12/20	0.76	0.35	47,60,73,74	0
33	STE	k	103	12/20	0.77	0.21	49,67,78,80	0
33	STE	b	625	20/20	0.78	0.23	47,62,72,76	0
29	LMG	c	521	48/55	0.78	0.26	50,71,93,96	0
33	STE	a	615	10/20	0.79	0.23	40,60,68,69	0
33	STE	a	617	15/20	0.79	0.20	38,57,69,77	0
33	STE	b	626	10/20	0.81	0.23	42,54,62,63	0
31	SQD	a	614	36/54	0.81	0.19	33,61,81,83	0
33	STE	m	101	12/20	0.81	0.20	45,61,75,76	0
33	STE	d	412	20/20	0.82	0.20	41,65,84,85	0
33	STE	j	101	12/20	0.82	0.16	45,58,67,70	0
29	LMG	a	618	55/55	0.82	0.17	38,58,72,83	0
32	DGD	A	618	66/66	0.82	0.18	43,61,74,82	0
29	LMG	c	522	49/55	0.83	0.18	37,56,81,96	0
24	CLA	b	601	65/65	0.83	0.18	47,65,83,96	0
26	BCR	H	101	40/40	0.83	0.15	30,46,59,63	0
33	STE	b	624	16/20	0.84	0.15	45,61,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	PL9	A	612	55/55	0.84	0.24	33,62,82,85	0
30	LHG	e	102	42/49	0.84	0.26	52,77,103,111	0
33	STE	b	627	14/20	0.84	0.23	50,65,77,78	0
31	SQD	A	617	39/54	0.84	0.19	40,59,87,92	0
29	LMG	b	623	55/55	0.84	0.29	51,68,87,91	0
29	LMG	D	409	33/55	0.84	0.20	37,56,77,84	0
33	STE	B	620	17/20	0.84	0.22	36,51,64,65	0
30	LHG	E	101	49/49	0.85	0.21	46,71,102,108	0
29	LMG	A	614	48/55	0.85	0.16	37,55,74,84	0
33	STE	B	626	16/20	0.85	0.27	45,58,70,74	0
24	CLA	C	512	65/65	0.85	0.17	33,51,81,86	0
33	STE	C	522	12/20	0.85	0.14	39,49,57,58	0
33	STE	l	102	18/20	0.85	0.16	36,49,76,78	0
24	CLA	B	601	65/65	0.85	0.16	32,58,84,95	0
28	PL9	a	611	55/55	0.86	0.19	32,65,80,88	0
24	CLA	c	513	65/65	0.86	0.21	44,65,100,105	0
24	CLA	C	513	65/65	0.86	0.19	41,62,84,92	0
26	BCR	d	405	40/40	0.86	0.14	37,52,87,93	0
26	BCR	x	101	40/40	0.86	0.15	37,52,71,75	0
24	CLA	c	512	65/65	0.86	0.17	41,56,88,94	0
33	STE	I	101	15/20	0.87	0.17	40,55,75,80	0
33	STE	B	624	14/20	0.87	0.14	36,51,61,63	0
31	SQD	B	623	54/54	0.87	0.16	39,57,81,90	0
26	BCR	Y	101	40/40	0.87	0.13	32,50,62,69	0
33	STE	c	520	20/20	0.87	0.21	36,55,71,76	0
33	STE	J	101	12/20	0.88	0.14	45,55,63,65	0
33	STE	M	103	10/20	0.88	0.16	33,43,52,58	0
33	STE	T	103	15/20	0.88	0.20	43,55,68,71	0
33	STE	Z	101	8/20	0.88	0.16	41,57,64,64	0
33	STE	D	411	20/20	0.88	0.19	35,49,68,72	0
26	BCR	C	514	40/40	0.88	0.15	38,55,68,71	0
26	BCR	k	101	40/40	0.88	0.14	39,56,68,69	0
33	STE	b	622	20/20	0.88	0.22	38,53,67,67	0
31	SQD	f	101	41/54	0.88	0.20	54,77,98,101	0
33	STE	t	102	18/20	0.88	0.15	42,55,72,77	0
33	STE	T	102	16/20	0.89	0.17	30,48,62,65	0
33	STE	C	521	16/20	0.89	0.12	37,51,64,71	0
29	LMG	C	519	48/55	0.89	0.18	39,67,85,89	0
33	STE	x	102	20/20	0.89	0.22	38,55,68,71	0
29	LMG	b	621	51/55	0.90	0.13	35,51,70,76	0
26	BCR	D	404	40/40	0.90	0.14	28,43,79,87	0
33	STE	d	411	17/20	0.90	0.14	41,52,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LMG	c	519	37/55	0.90	0.15	44,63,80,85	0
24	CLA	D	403	65/65	0.90	0.14	22,42,105,112	0
29	LMG	D	406	51/55	0.90	0.19	26,52,75,84	0
24	CLA	d	404	65/65	0.90	0.16	28,47,81,87	0
29	LMG	D	410	28/55	0.90	0.16	36,50,61,63	0
24	CLA	a	606	65/65	0.90	0.14	19,36,78,84	0
33	STE	C	520	12/20	0.90	0.12	44,56,64,64	0
29	LMG	M	101	51/55	0.91	0.14	31,47,64,73	0
26	BCR	k	102	40/40	0.91	0.19	39,51,63,68	0
24	CLA	c	508	64/65	0.91	0.16	29,43,83,98	0
26	BCR	c	514	40/40	0.91	0.15	46,59,68,70	0
31	SQD	b	620	49/54	0.91	0.15	38,54,87,97	0
33	STE	B	625	12/20	0.92	0.10	37,51,59,66	0
24	CLA	C	502	65/65	0.92	0.14	25,39,52,59	0
26	BCR	B	618	40/40	0.92	0.10	23,38,49,49	0
26	BCR	B	619	40/40	0.92	0.12	25,41,54,62	0
24	CLA	b	615	65/65	0.92	0.14	26,39,57,63	0
32	DGD	c	518	62/66	0.92	0.15	25,49,80,86	0
24	CLA	c	502	65/65	0.92	0.14	29,40,55,62	0
31	SQD	D	407	36/54	0.92	0.17	41,65,80,82	0
32	DGD	c	517	62/66	0.93	0.13	31,51,87,90	0
24	CLA	c	510	65/65	0.93	0.15	28,45,58,71	0
24	CLA	C	506	65/65	0.93	0.12	26,42,78,84	0
24	CLA	C	511	65/65	0.93	0.12	30,48,65,70	0
24	CLA	b	602	65/65	0.93	0.15	27,41,57,62	0
29	LMG	d	410	44/55	0.93	0.14	33,51,79,86	0
24	CLA	b	606	65/65	0.93	0.13	25,39,70,73	0
24	CLA	b	609	65/65	0.93	0.15	29,43,62,68	0
24	CLA	B	615	65/65	0.93	0.12	22,36,59,63	0
24	CLA	b	616	60/65	0.93	0.14	26,41,81,83	0
24	CLA	B	616	60/65	0.93	0.14	23,37,88,95	0
31	SQD	a	613	54/54	0.93	0.17	38,60,79,84	0
24	CLA	c	506	65/65	0.93	0.12	31,48,89,90	0
26	BCR	b	619	40/40	0.93	0.12	26,47,61,69	0
24	CLA	c	507	65/65	0.93	0.14	26,43,58,64	0
24	CLA	B	604	65/65	0.93	0.13	21,32,68,71	0
32	DGD	C	517	62/66	0.93	0.13	27,47,92,108	0
32	DGD	H	102	62/66	0.93	0.11	25,43,55,60	0
24	CLA	d	401	65/65	0.94	0.14	24,37,86,90	0
28	PL9	D	405	55/55	0.94	0.11	19,31,46,47	0
24	CLA	C	505	65/65	0.94	0.15	23,39,65,81	0
33	STE	M	102	15/20	0.94	0.11	36,47,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	614	65/65	0.94	0.16	20,35,70,80	0
24	CLA	c	503	65/65	0.94	0.15	28,42,53,61	0
24	CLA	c	504	60/65	0.94	0.12	31,43,78,85	0
26	BCR	C	515	40/40	0.94	0.12	27,40,50,61	0
32	DGD	C	516	62/66	0.94	0.12	21,40,77,80	0
24	CLA	c	505	65/65	0.94	0.18	25,38,66,72	0
32	DGD	C	518	62/66	0.94	0.13	24,46,75,85	0
24	CLA	C	507	65/65	0.94	0.14	25,38,53,57	0
26	BCR	T	101	40/40	0.94	0.10	25,37,50,52	0
24	CLA	C	510	65/65	0.94	0.14	26,41,61,62	0
32	DGD	h	101	62/66	0.94	0.11	31,45,57,64	0
26	BCR	b	617	40/40	0.94	0.12	29,40,51,54	0
26	BCR	b	618	40/40	0.94	0.10	26,39,51,54	0
24	CLA	B	602	65/65	0.94	0.15	23,35,54,61	0
24	CLA	c	509	65/65	0.94	0.18	32,46,61,69	0
24	CLA	b	608	65/65	0.94	0.15	25,42,61,66	0
30	LHG	A	615	47/49	0.94	0.13	27,48,77,88	0
24	CLA	c	511	65/65	0.94	0.13	33,50,70,75	0
24	CLA	B	606	65/65	0.94	0.11	23,34,65,71	0
31	SQD	A	616	52/54	0.94	0.16	34,54,90,95	0
24	CLA	B	610	65/65	0.94	0.15	20,32,42,45	0
24	CLA	A	605	65/65	0.95	0.13	23,33,83,91	0
24	CLA	A	608	54/65	0.95	0.11	17,32,67,69	0
30	LHG	d	407	49/49	0.95	0.13	34,47,70,74	0
24	CLA	b	603	65/65	0.95	0.14	23,36,60,68	0
26	BCR	c	515	40/40	0.95	0.11	27,42,58,61	0
24	CLA	b	604	65/65	0.95	0.13	19,35,79,89	0
24	CLA	b	605	65/65	0.95	0.12	21,34,49,54	0
24	CLA	C	508	65/65	0.95	0.12	26,38,98,109	0
26	BCR	t	101	40/40	0.95	0.10	27,37,50,54	0
24	CLA	b	607	65/65	0.95	0.12	20,35,62,68	0
24	CLA	C	509	65/65	0.95	0.18	26,42,60,64	0
24	CLA	B	609	65/65	0.95	0.12	24,36,58,66	0
24	CLA	b	610	65/65	0.95	0.19	22,37,50,54	0
28	PL9	d	406	55/55	0.95	0.11	20,34,42,44	0
24	CLA	b	611	65/65	0.95	0.14	22,33,52,62	0
26	BCR	B	617	40/40	0.95	0.12	26,38,56,60	0
24	CLA	b	612	65/65	0.95	0.17	21,34,47,56	0
32	DGD	c	516	62/66	0.95	0.11	21,41,67,74	0
24	CLA	b	613	65/65	0.95	0.14	17,33,66,74	0
24	CLA	b	614	65/65	0.95	0.12	24,38,68,76	0
24	CLA	C	501	65/65	0.95	0.14	21,35,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	603	65/65	0.95	0.15	20,32,61,63	0
24	CLA	c	501	65/65	0.95	0.13	28,39,51,55	0
26	BCR	K	101	40/40	0.95	0.15	34,49,65,65	0
24	CLA	C	503	65/65	0.95	0.13	27,39,48,51	0
24	CLA	C	504	59/65	0.95	0.12	28,40,79,80	0
26	BCR	a	607	40/40	0.95	0.09	23,33,43,49	0
24	CLA	B	613	65/65	0.95	0.14	17,31,65,70	0
24	CLA	a	604	65/65	0.96	0.10	18,28,45,55	0
30	LHG	B	621	49/49	0.96	0.11	26,40,54,61	0
30	LHG	B	622	49/49	0.96	0.11	29,43,64,69	0
24	CLA	B	605	65/65	0.96	0.14	20,31,47,50	0
24	CLA	a	612	65/65	0.96	0.11	20,29,46,51	0
30	LHG	d	409	39/49	0.96	0.11	30,44,67,68	0
24	CLA	d	403	65/65	0.96	0.11	20,32,54,64	0
30	LHG	l	101	49/49	0.96	0.10	30,42,51,57	0
24	CLA	B	611	65/65	0.96	0.14	19,31,49,52	0
25	PHO	A	606	64/64	0.96	0.10	17,27,35,41	0
25	PHO	A	607	64/64	0.96	0.11	22,31,40,42	0
25	PHO	a	605	64/64	0.96	0.12	18,29,37,46	0
25	PHO	d	402	64/64	0.96	0.11	26,35,45,49	0
26	BCR	A	609	40/40	0.96	0.10	21,34,42,44	0
24	CLA	B	612	65/65	0.96	0.15	19,32,49,53	0
24	CLA	A	604	65/65	0.96	0.11	15,26,44,54	0
24	CLA	B	607	65/65	0.96	0.11	17,32,57,67	0
24	CLA	B	608	65/65	0.96	0.13	18,33,54,56	0
24	CLA	D	402	65/65	0.96	0.11	17,28,54,56	0
24	CLA	A	613	65/65	0.96	0.10	18,28,47,53	0
34	BCT	a	610	4/4	0.96	0.21	28,33,39,47	0
35	HEM	F	101	43/43	0.96	0.11	34,46,60,62	0
30	LHG	d	408	49/49	0.97	0.09	24,41,51,60	0
30	LHG	D	408	49/49	0.97	0.10	21,40,52,57	0
35	HEM	e	101	43/43	0.97	0.12	41,53,73,73	0
34	BCT	D	401	4/4	0.98	0.19	27,28,31,38	0
36	HEC	V	201	43/43	0.98	0.12	23,31,40,40	0
36	HEC	v	201	43/43	0.98	0.13	26,36,46,46	0
21	OEY	A	601[B]	11/11	0.99	0.13	15,20,23,26	11
27	CL	A	610	1/1	0.99	0.06	28,28,28,28	0
27	CL	A	611	1/1	0.99	0.04	27,27,27,27	0
27	CL	a	608	1/1	0.99	0.05	25,25,25,25	0
27	CL	a	609	1/1	0.99	0.03	25,25,25,25	0
21	OEY	a	601[B]	11/11	0.99	0.10	15,21,24,26	11
22	OEX	A	602[A]	10/10	0.99	0.13	29,31,35,35	10

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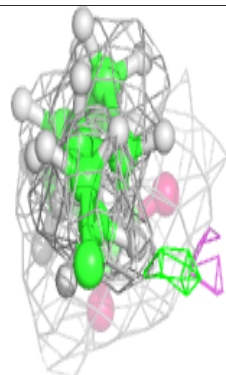
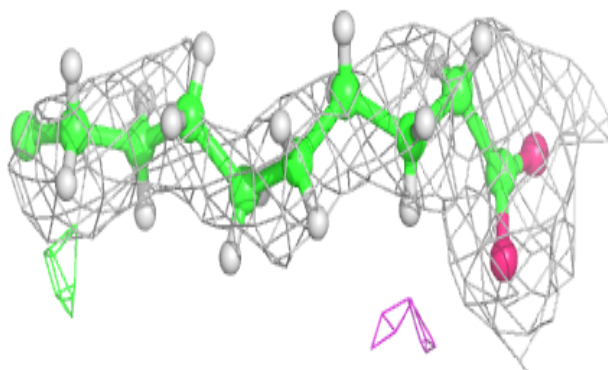
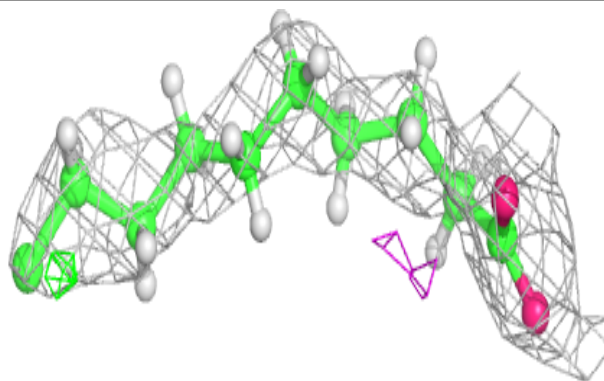
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	OEX	a	602[A]	10/10	0.99	0.10	27,32,35,35	10
23	FE2	a	603	1/1	0.99	0.05	29,29,29,29	0
23	FE2	A	603	1/1	1.00	0.08	24,24,24,24	0

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

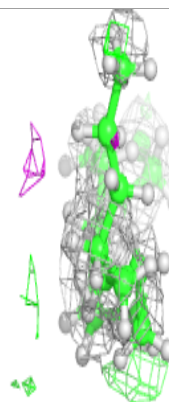
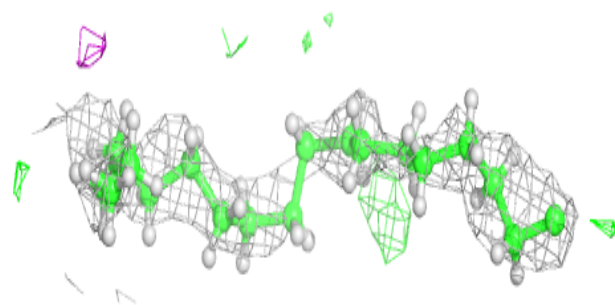
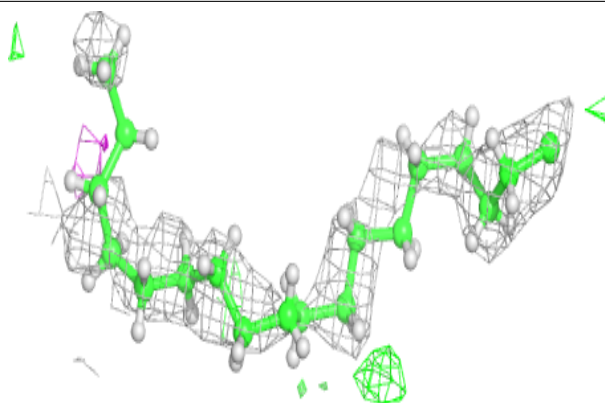
**Electron density around STE E 102:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

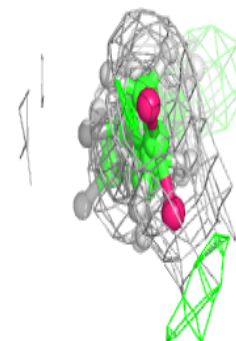
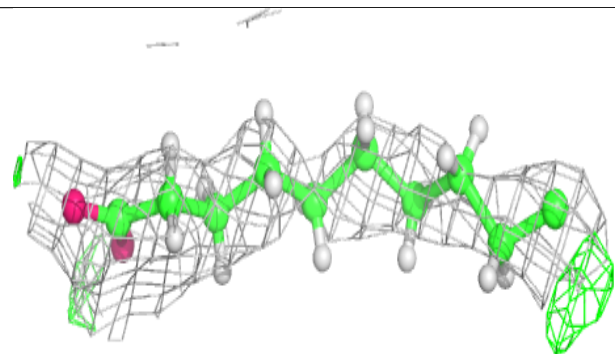
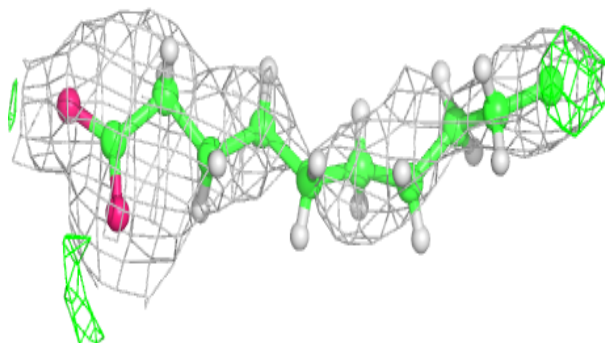


**Electron density around STE H 103:**

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

**Electron density around STE a 616:**

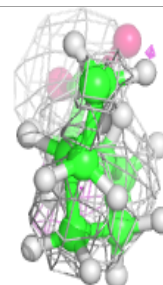
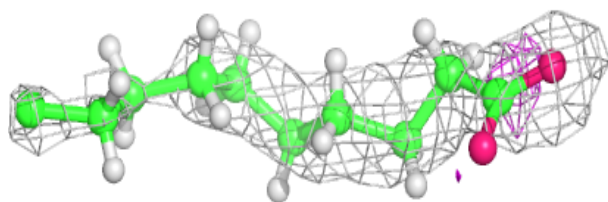
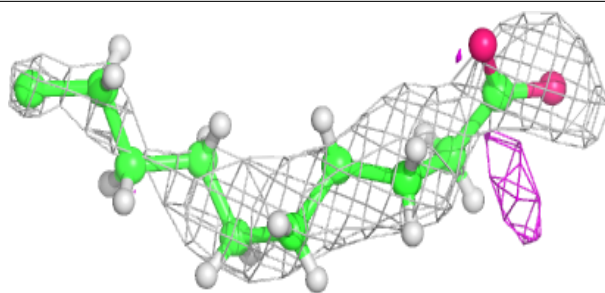
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



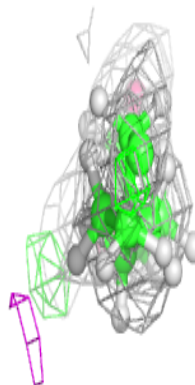
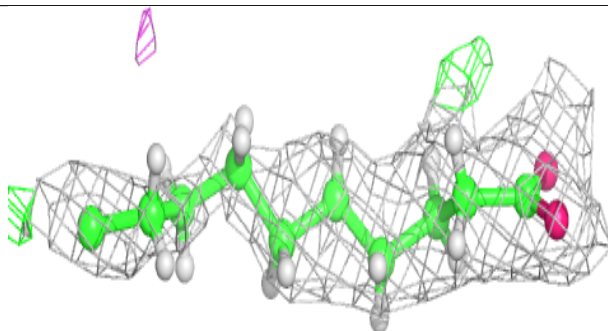
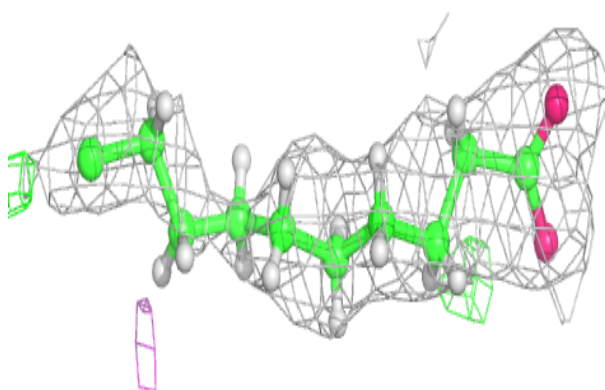


**Electron density around STE B 627:**

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

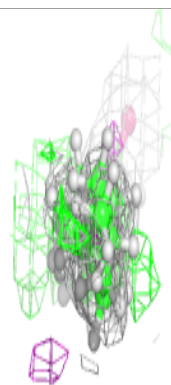
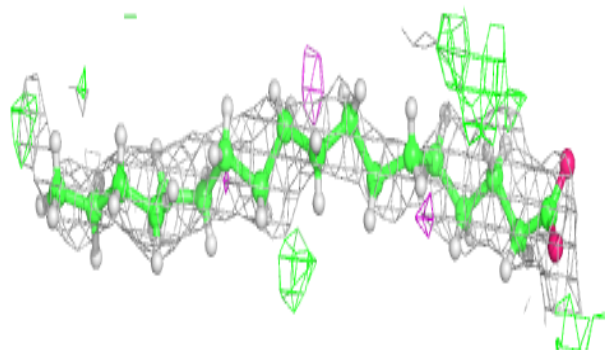
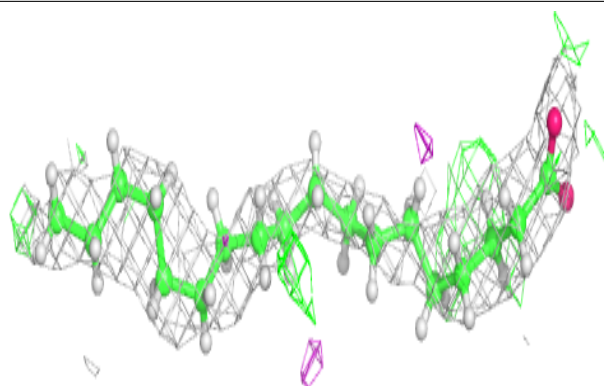
**Electron density around STE k 103:**

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

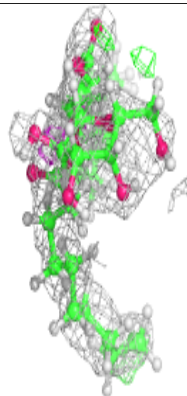
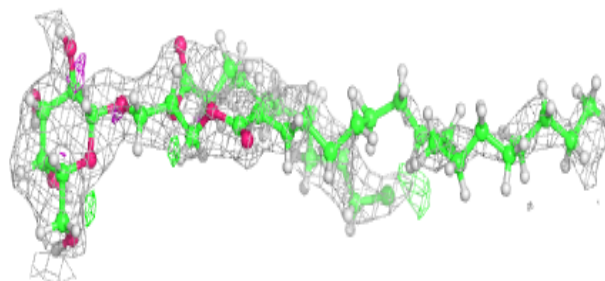
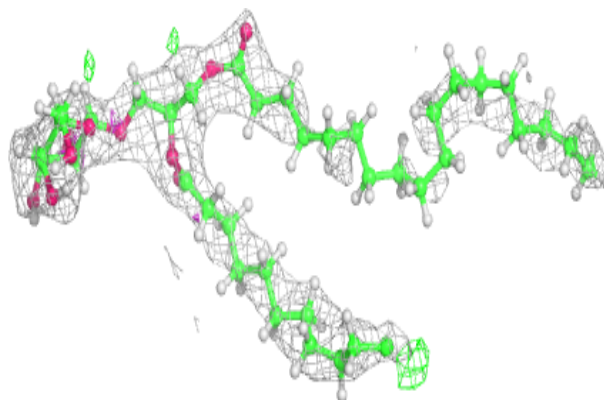


**Electron density around STE b 625:**

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

**Electron density around LMG c 521:**

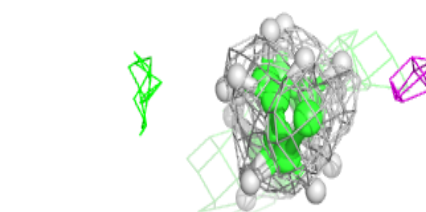
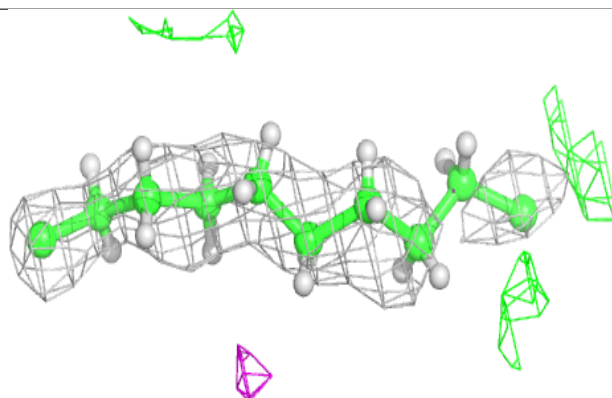
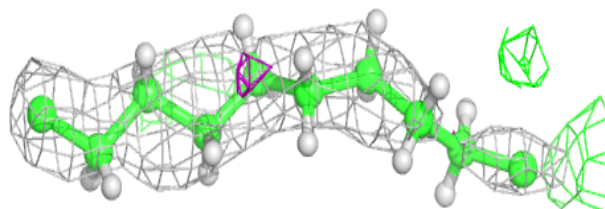
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



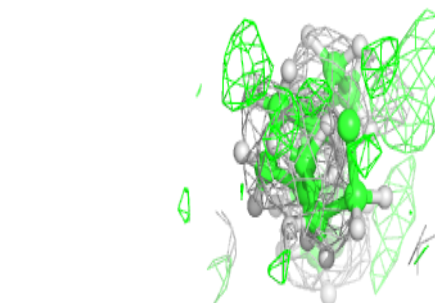
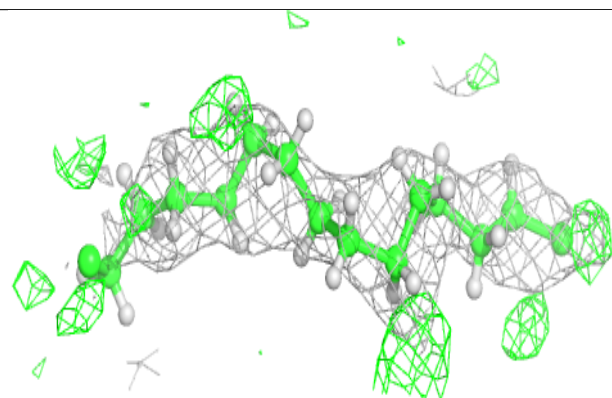
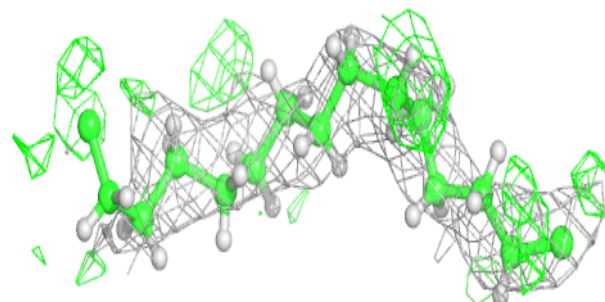


**Electron density around STE a 615:**

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

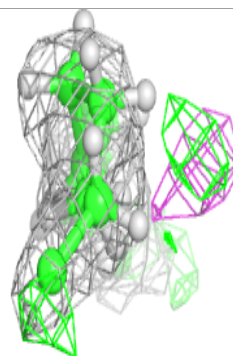
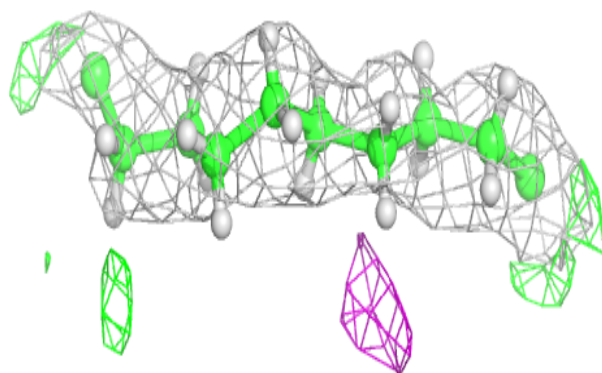
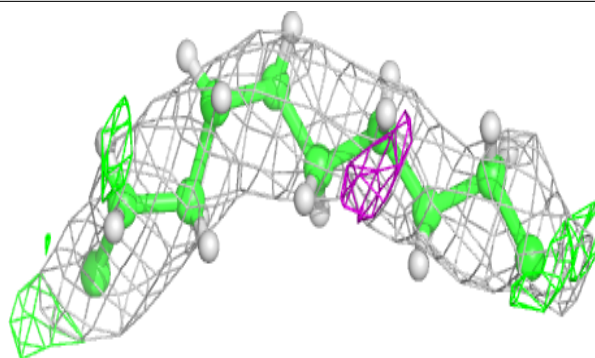
**Electron density around STE a 617:**

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



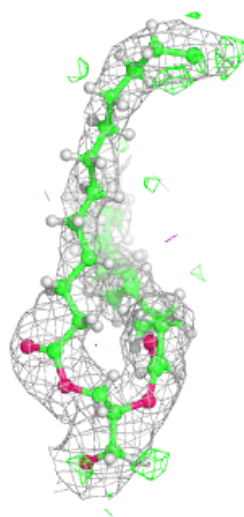
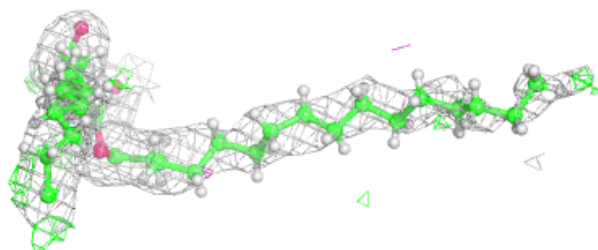
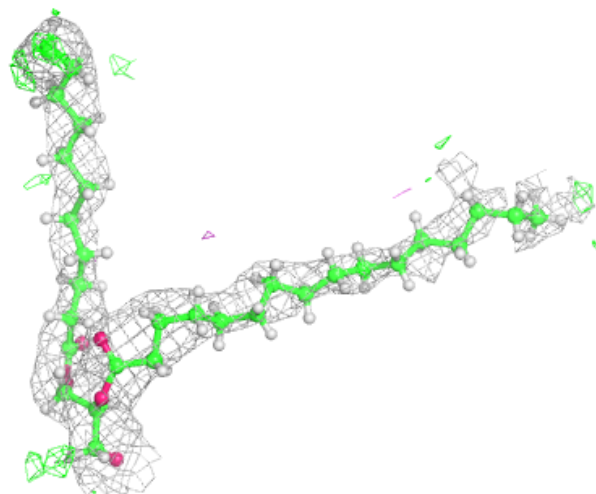
**Electron density around STE b 626:**

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



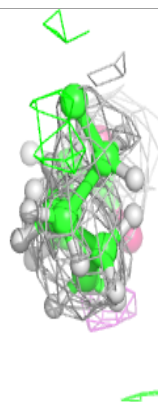
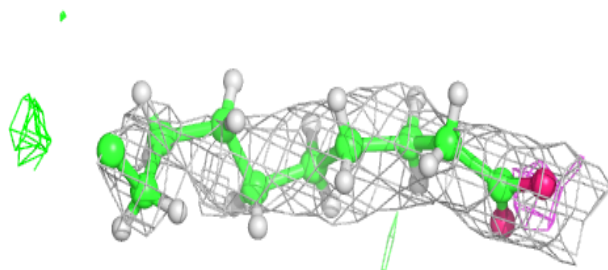
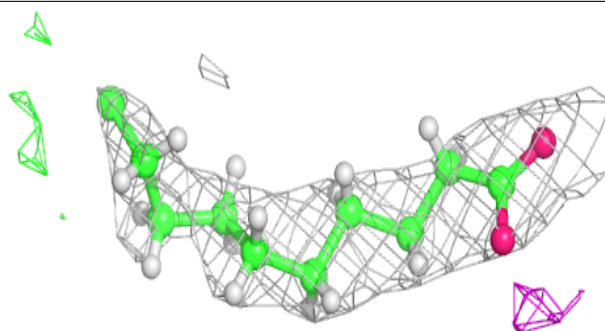
**Electron density around SQD a 614:**

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

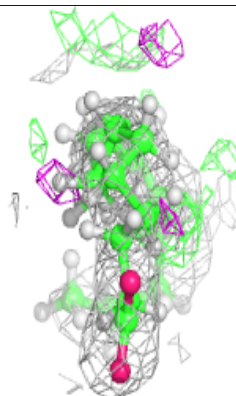
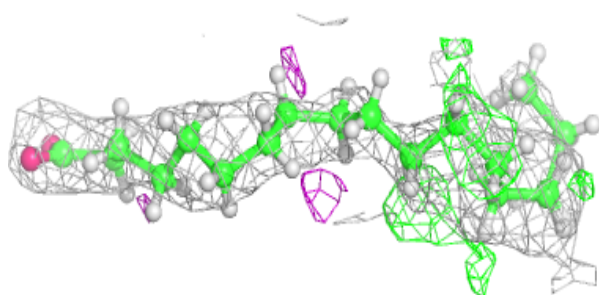
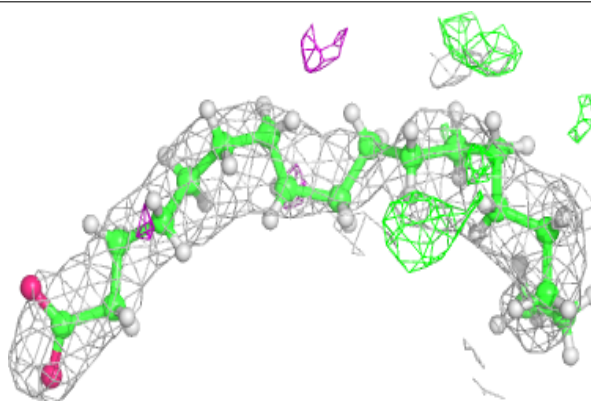


**Electron density around STE m 101:**

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

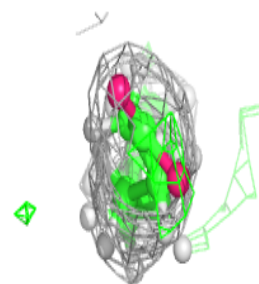
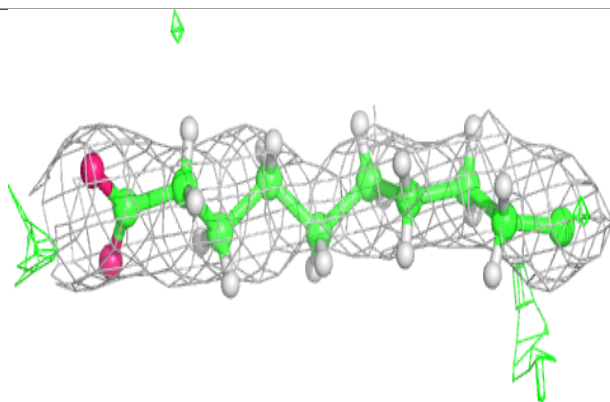
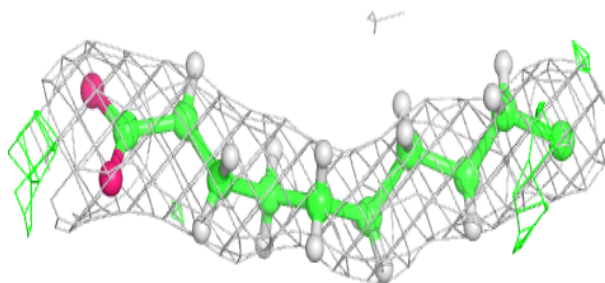
**Electron density around STE d 412:**

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

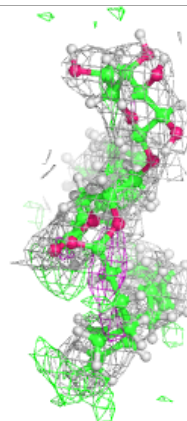
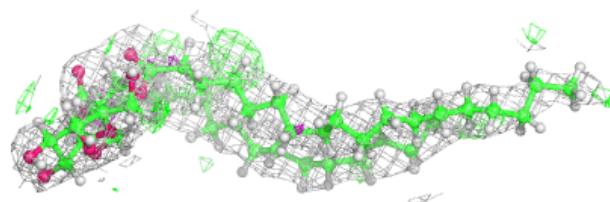
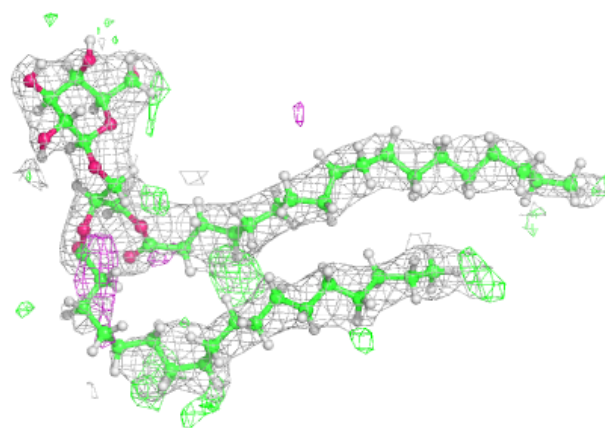


**Electron density around STE j 101:**

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

**Electron density around LMG a 618:**

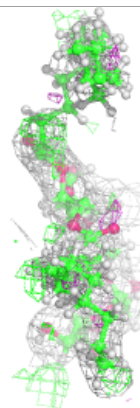
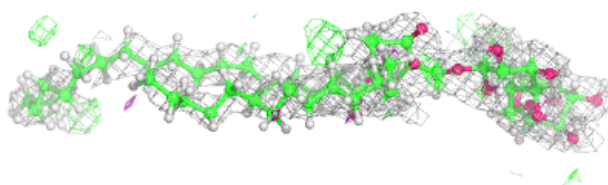
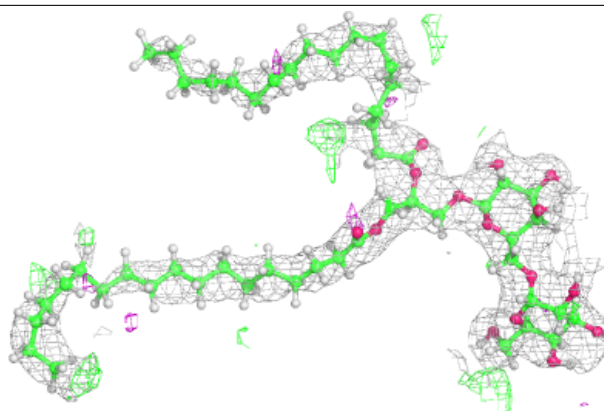
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



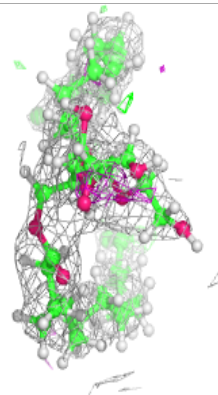
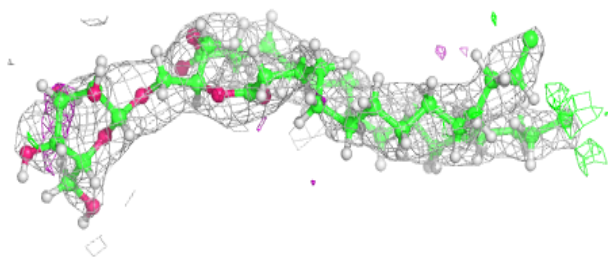
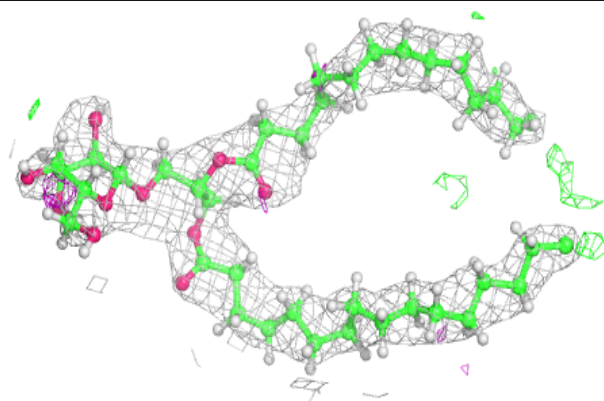


**Electron density around DGD A 618:**

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

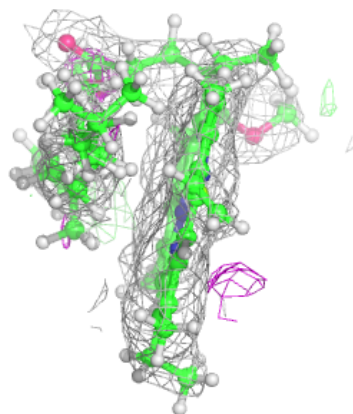
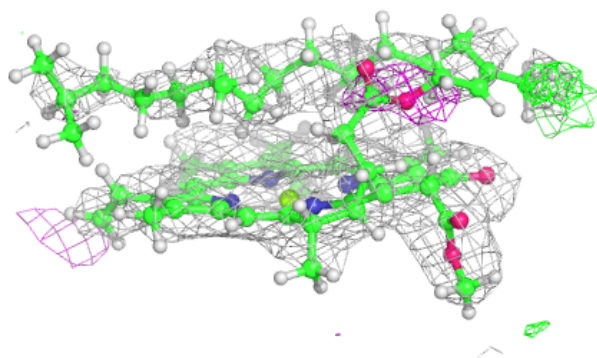
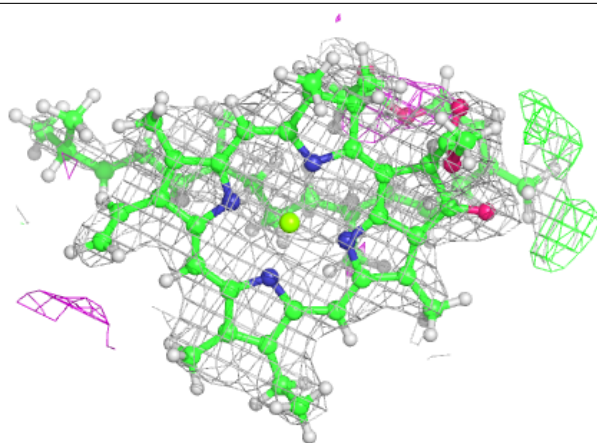
**Electron density around LMG c 522:**

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

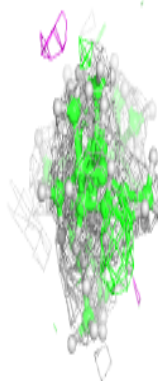
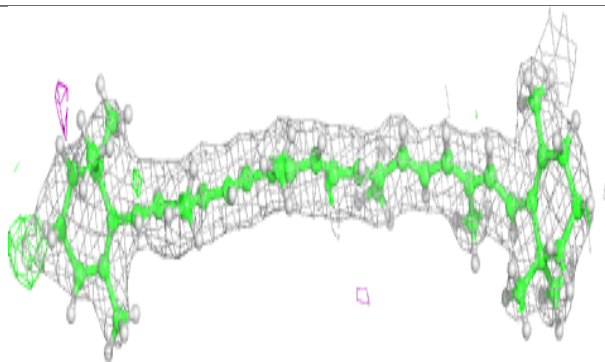
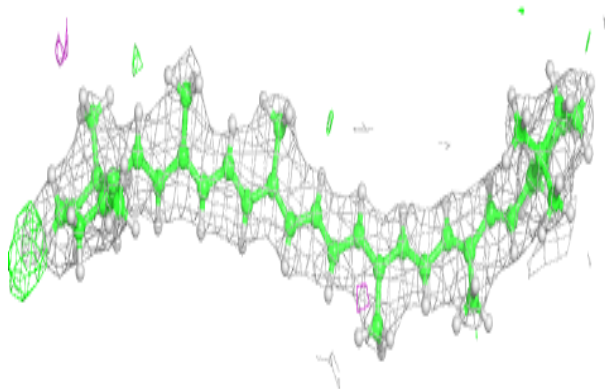


**Electron density around CLA b 601:**

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

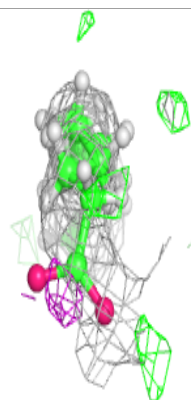
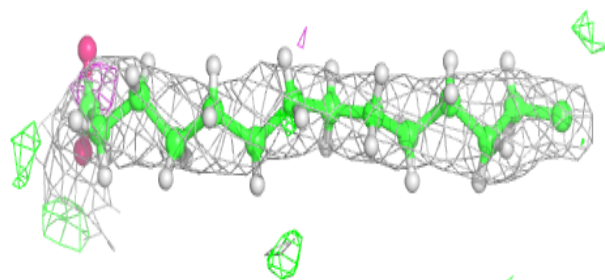
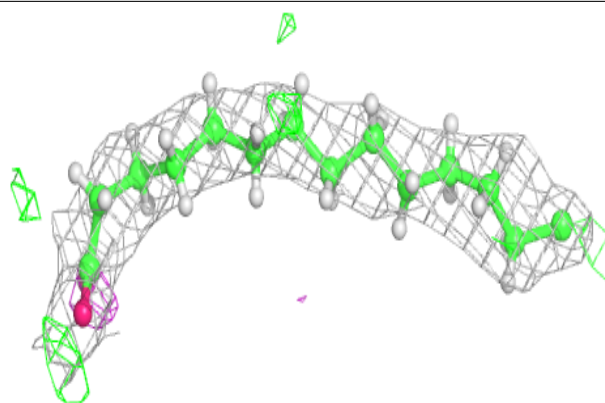
**Electron density around BCR H 101:**

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

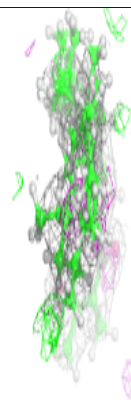
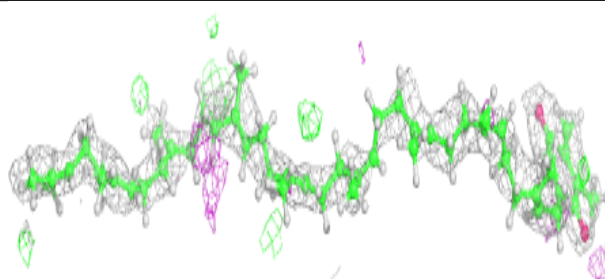
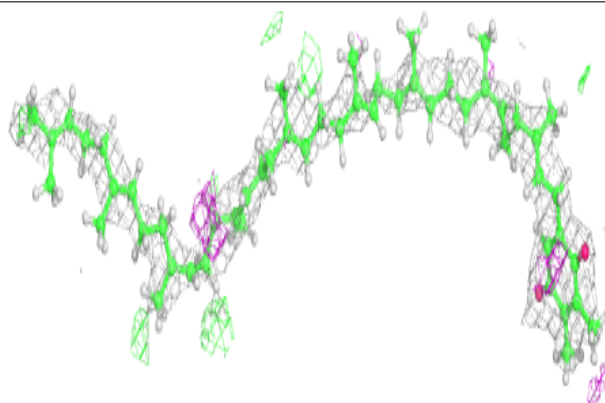


**Electron density around STE b 624:**

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

**Electron density around PL9 A 612:**

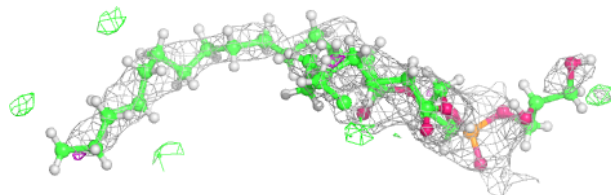
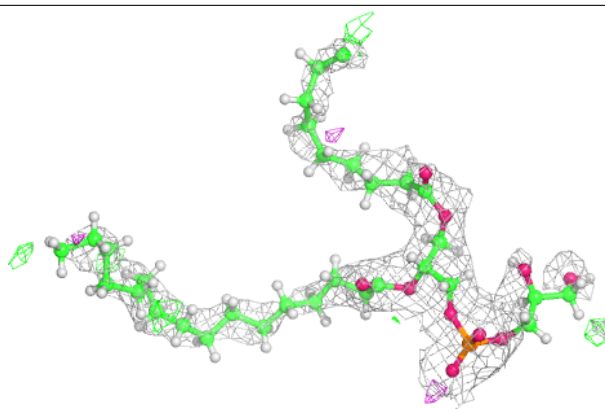
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



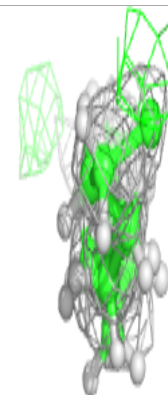
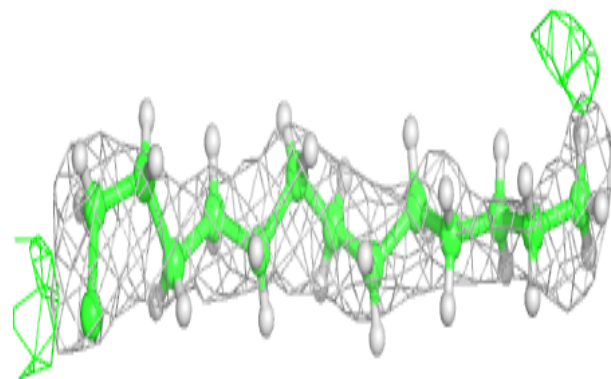
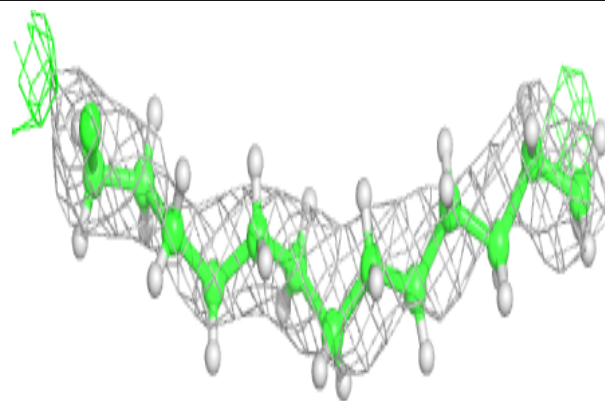


**Electron density around LHG e 102:**

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

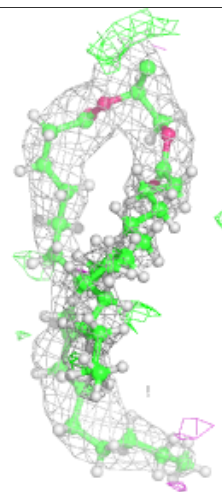
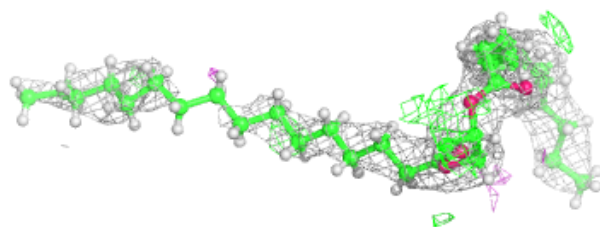
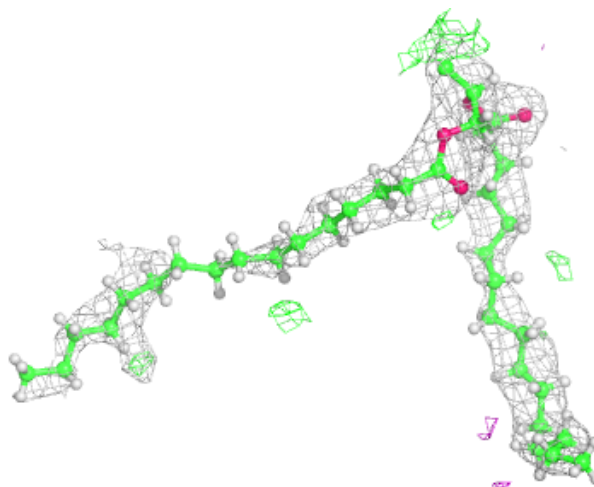
**Electron density around STE b 627:**

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



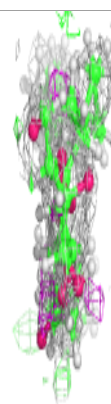
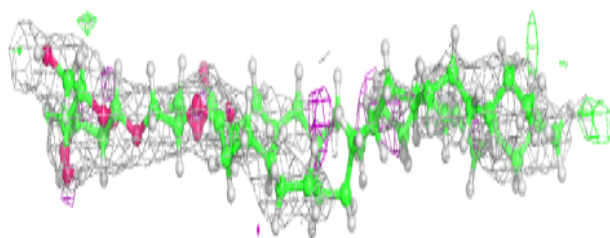
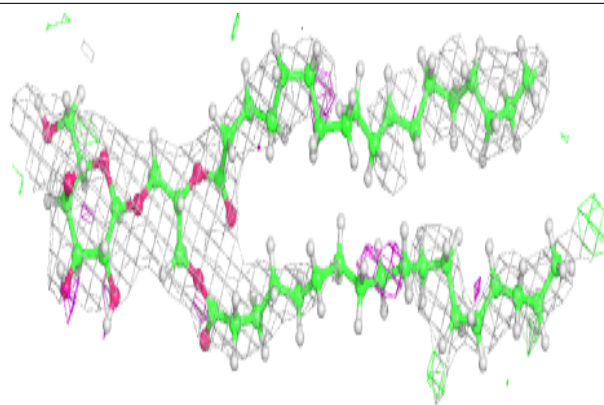
**Electron density around SQD A 617:**

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

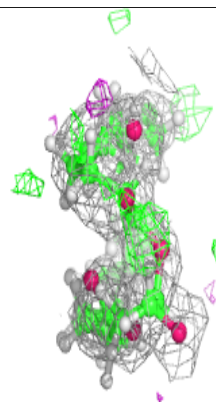
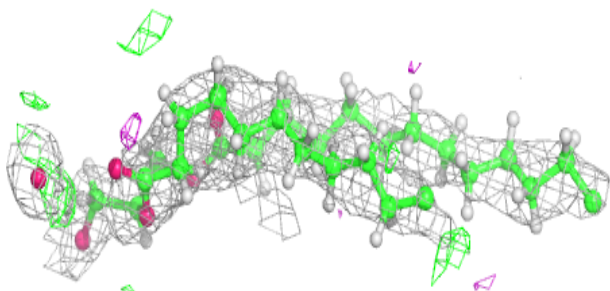
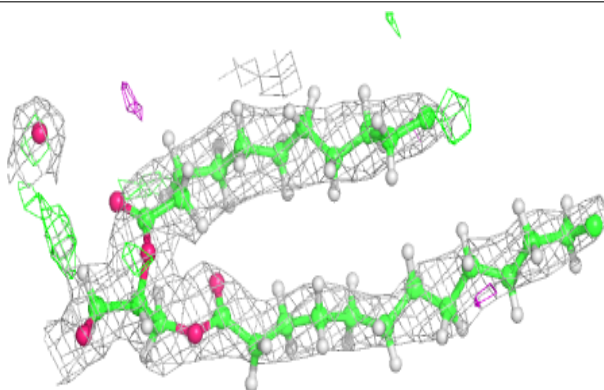


**Electron density around LMG b 623:**

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

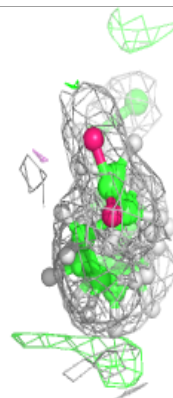
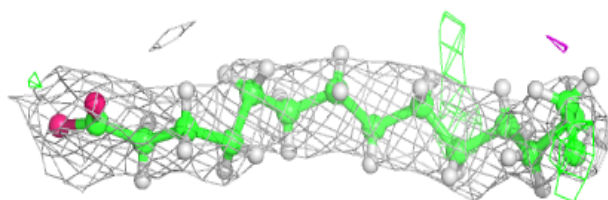
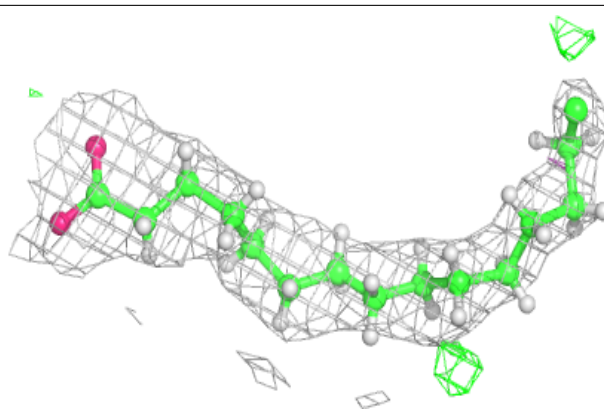
**Electron density around LMG D 409:**

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



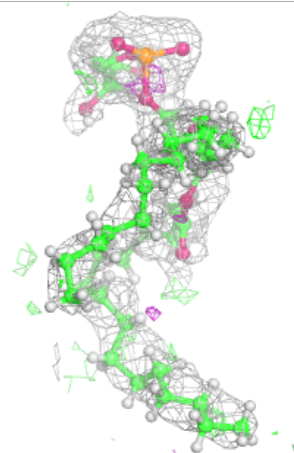
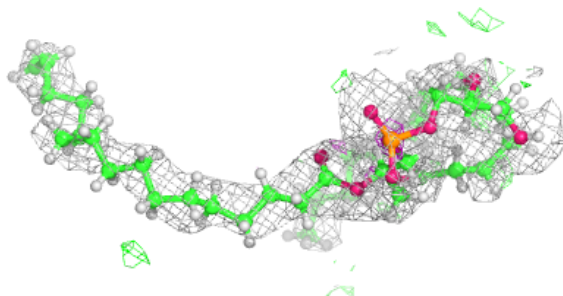
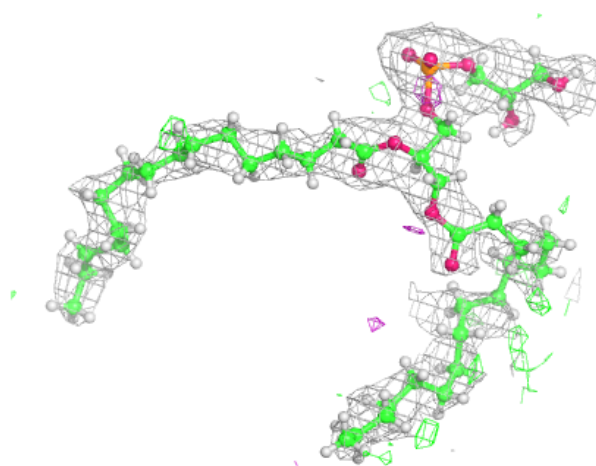
**Electron density around STE B 620:**

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



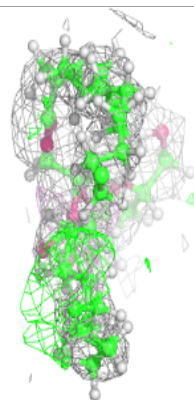
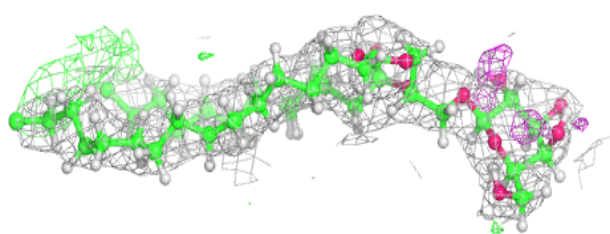
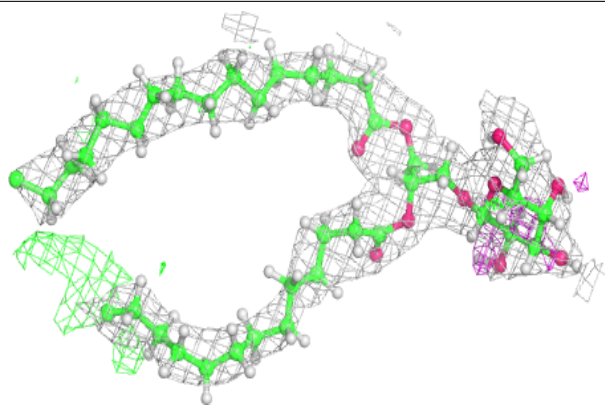
**Electron density around LHG E 101:**

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

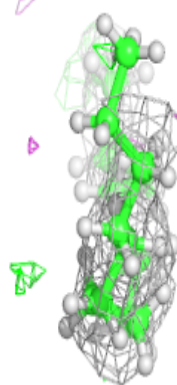
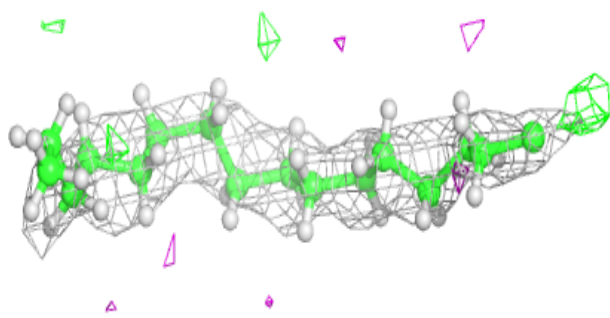
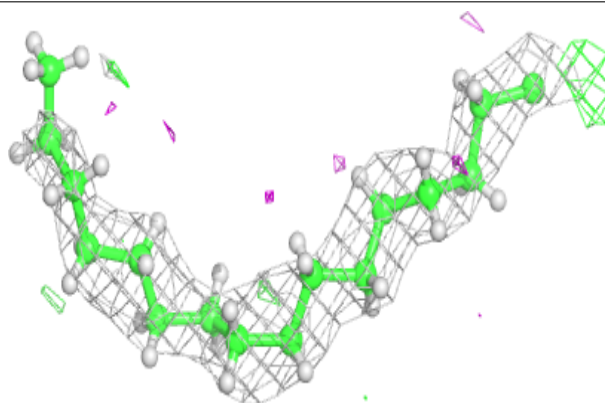


**Electron density around LMG A 614:**

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

**Electron density around STE B 626:**

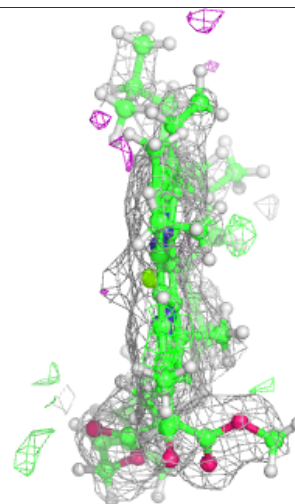
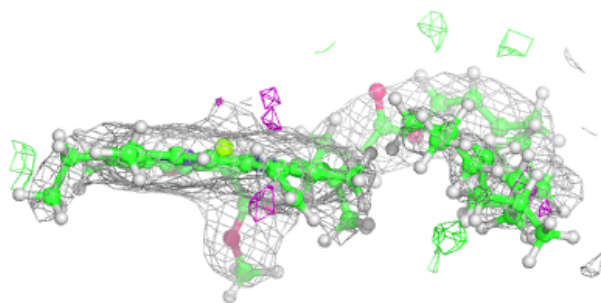
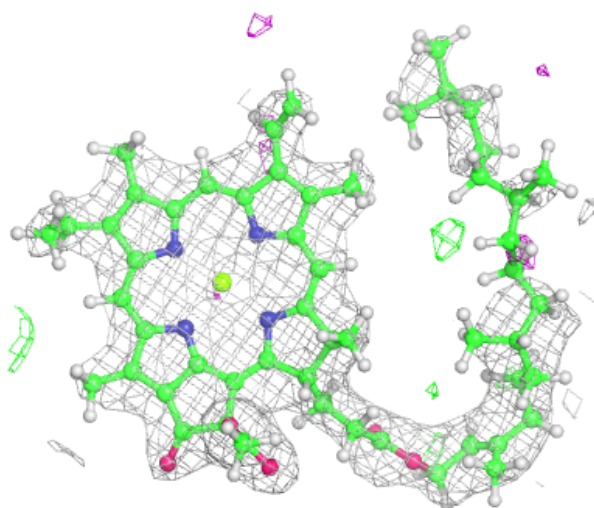
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





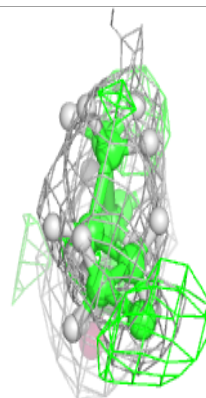
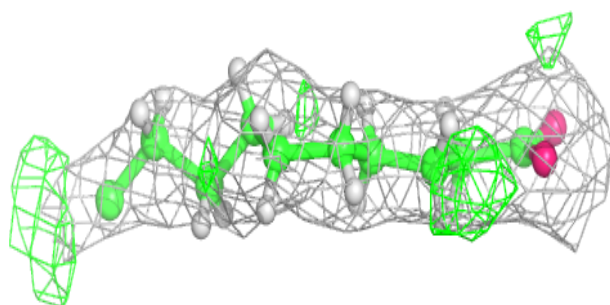
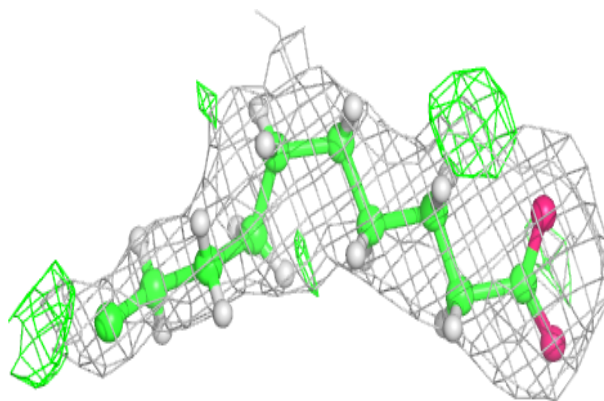
**Electron density around CLA C 512:**

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

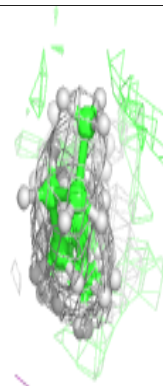
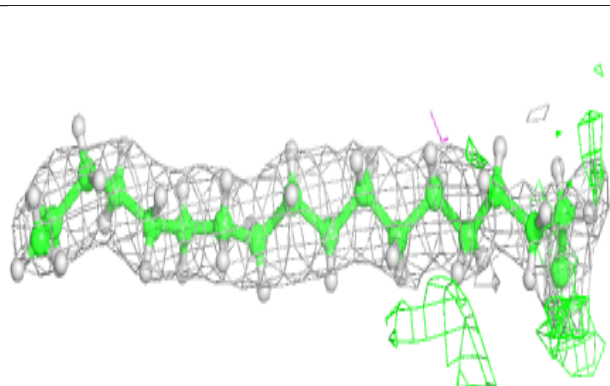
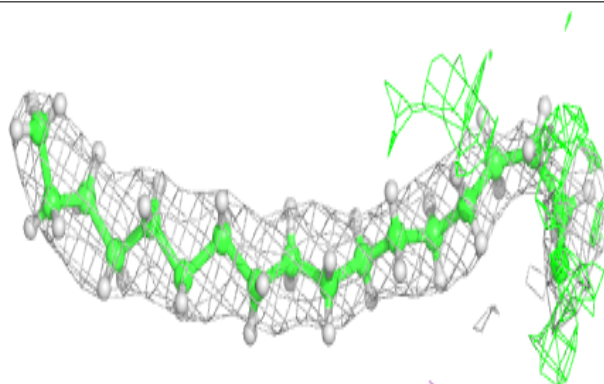


**Electron density around STE C 522:**

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

**Electron density around STE I 102:**

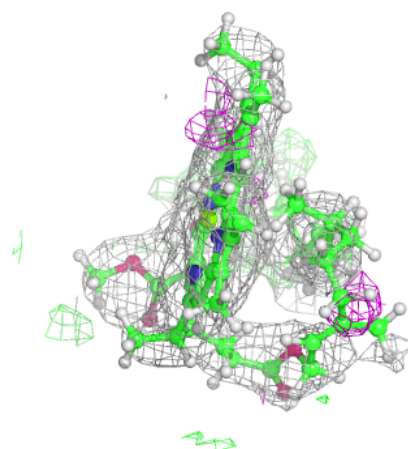
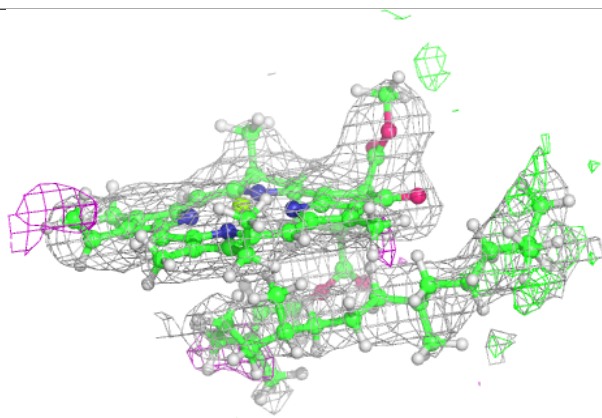
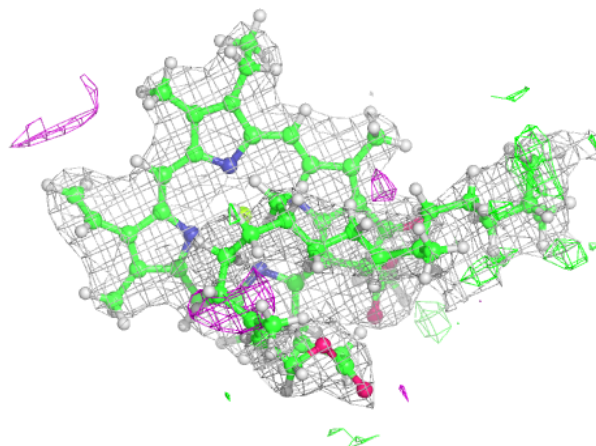
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





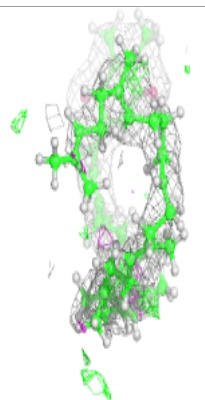
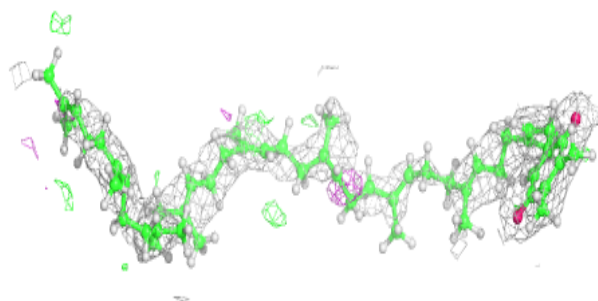
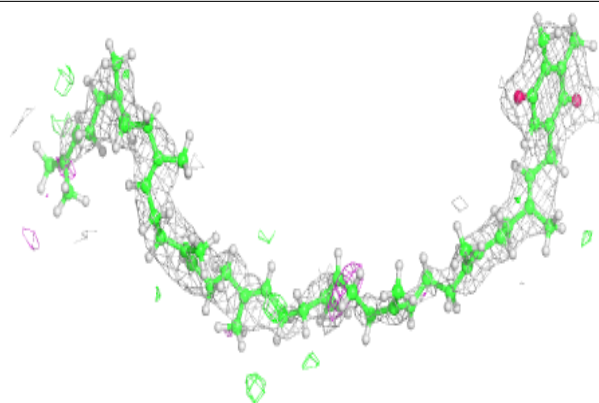
**Electron density around CLA B 601:**

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

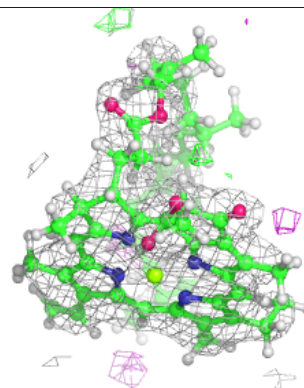
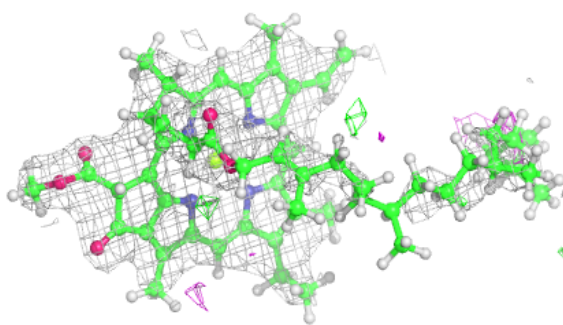
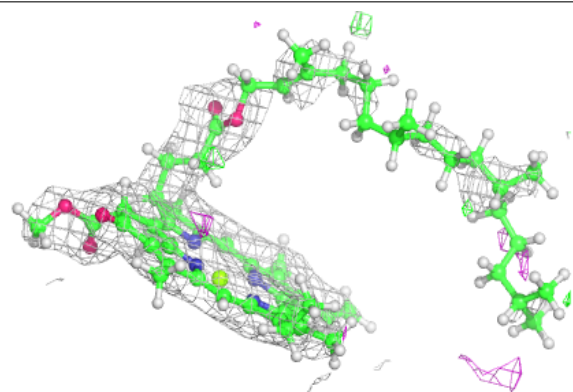


**Electron density around PL9 a 611:**

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

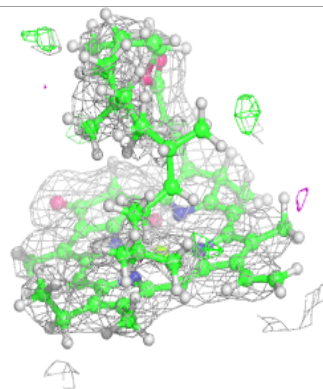
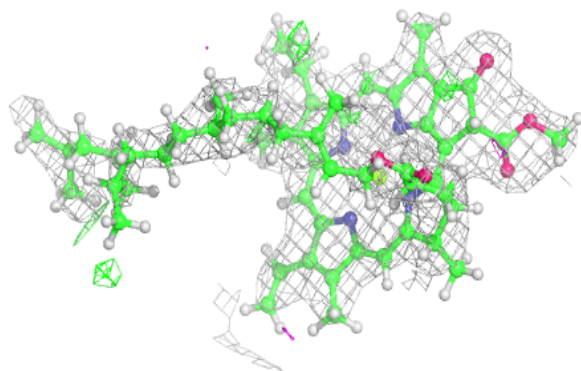
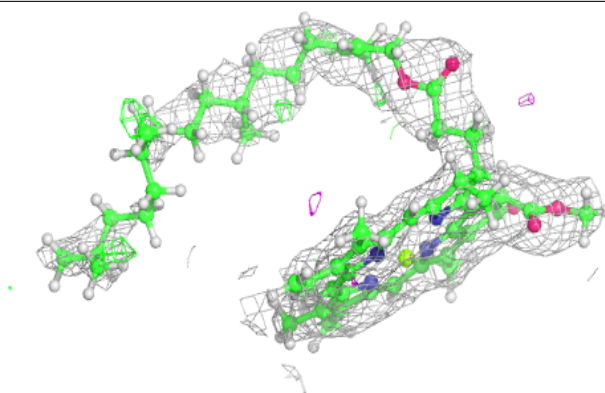
**Electron density around CLA c 513:**

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

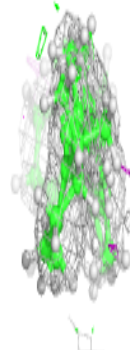
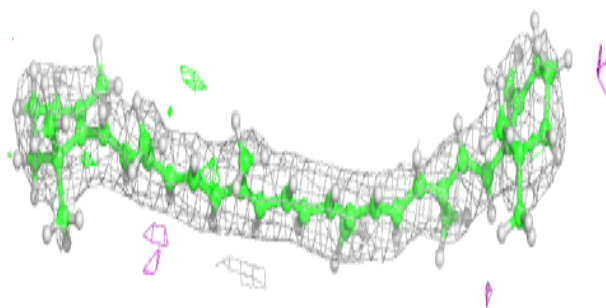
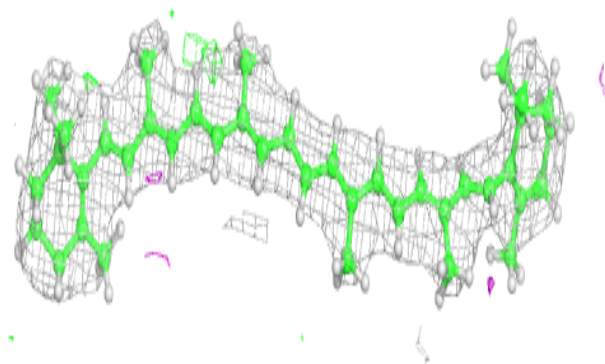


**Electron density around CLA C 513:**

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

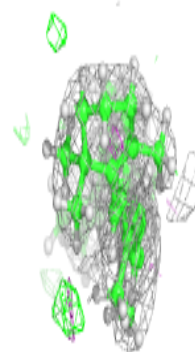
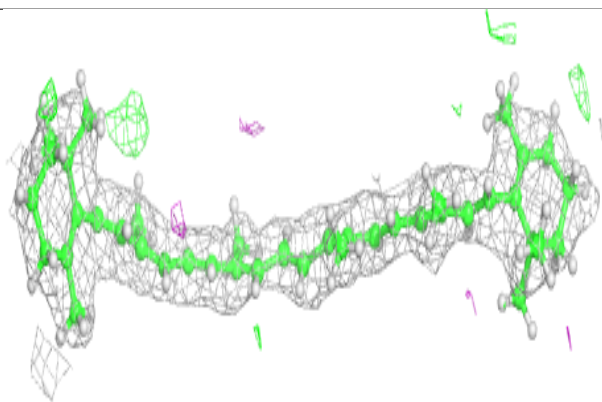
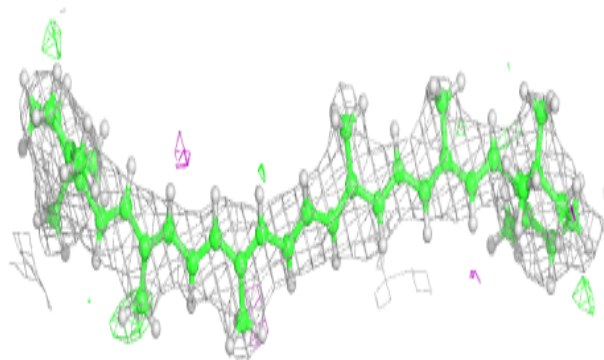
**Electron density around BCR d 405:**

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



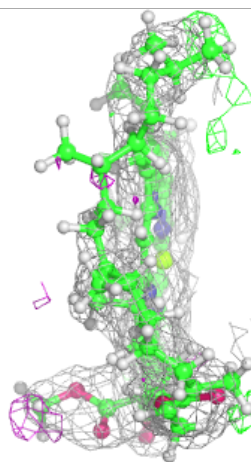
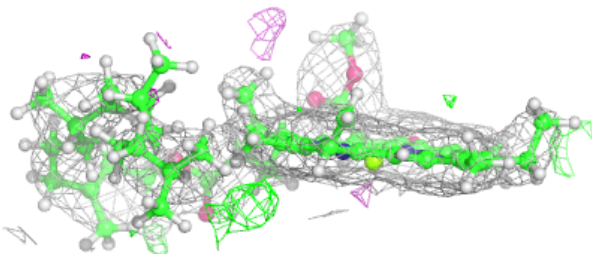
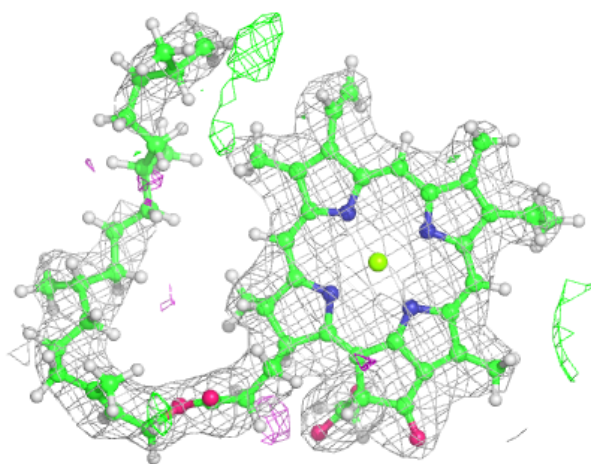
**Electron density around BCR x 101:**

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



**Electron density around CLA c 512:**

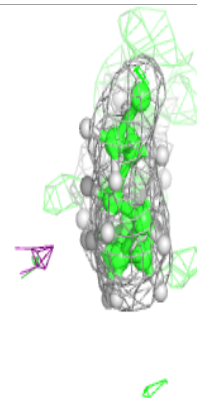
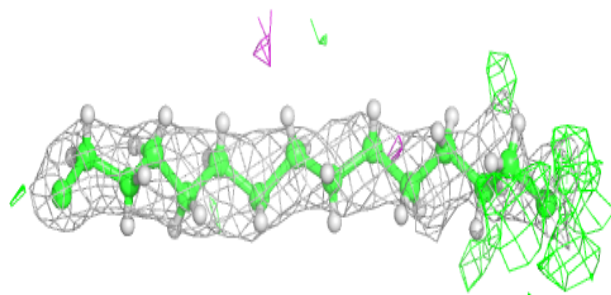
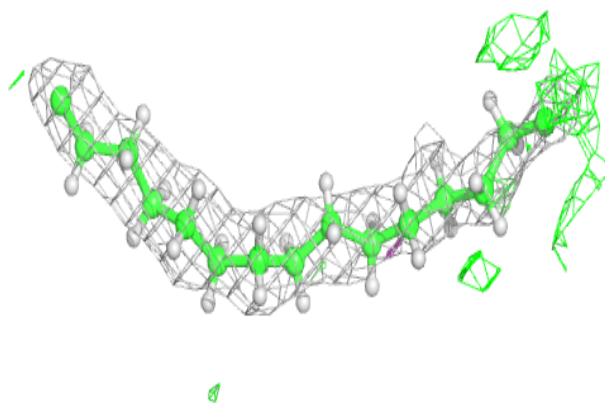
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



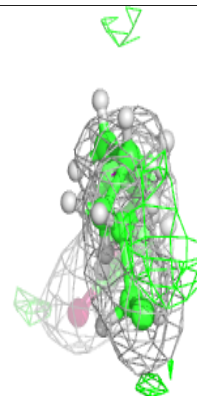
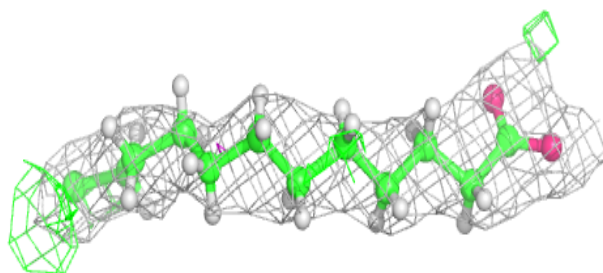
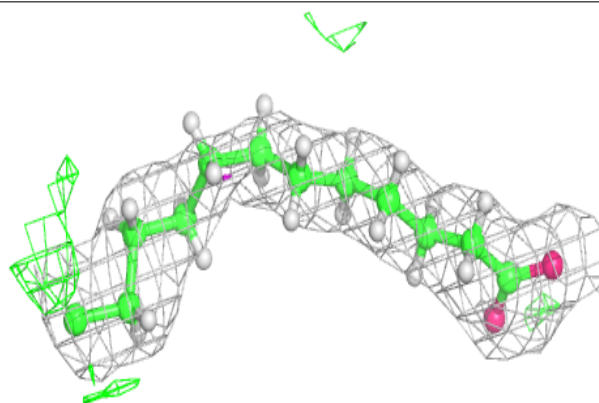


**Electron density around STE I 101:**

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

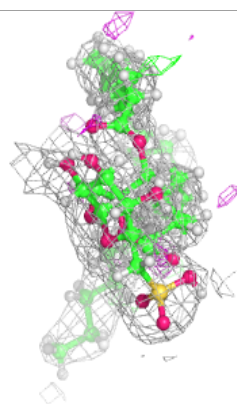
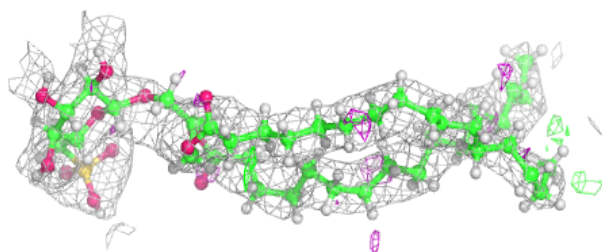
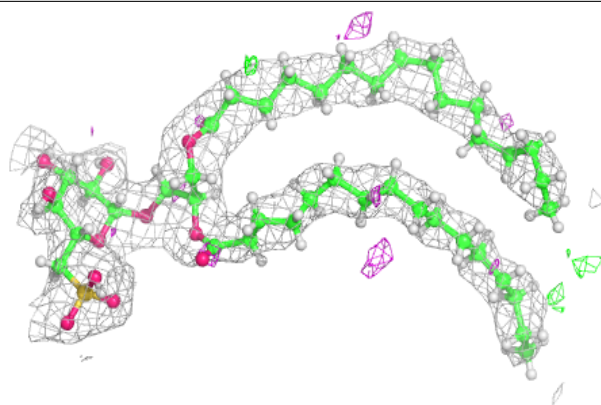
**Electron density around STE B 624:**

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

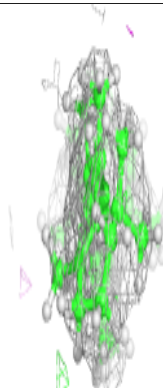
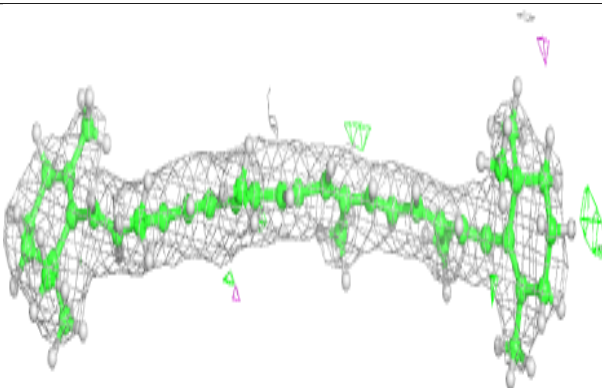
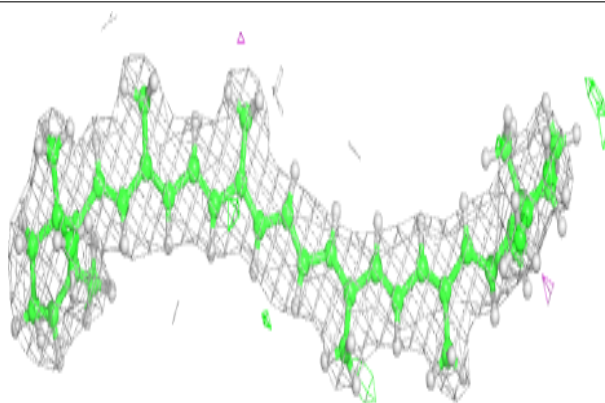


**Electron density around SQD B 623:**

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

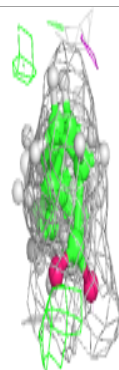
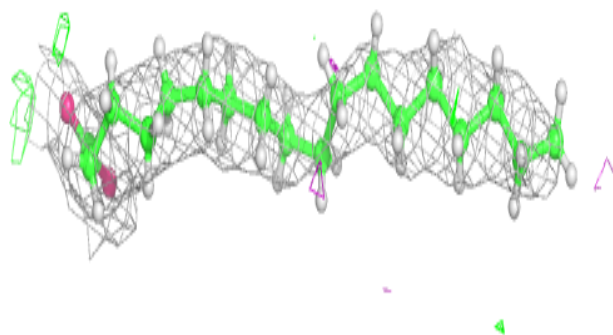
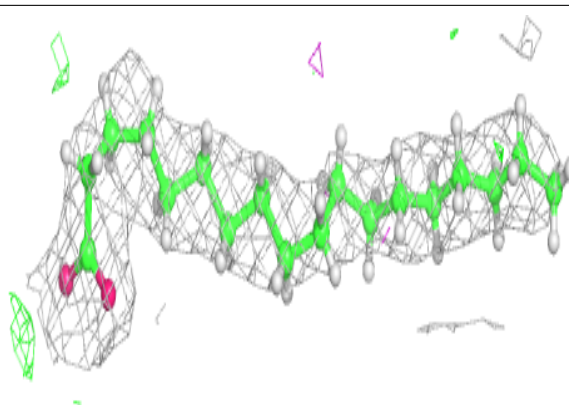
**Electron density around BCR Y 101:**

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

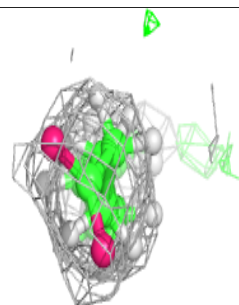
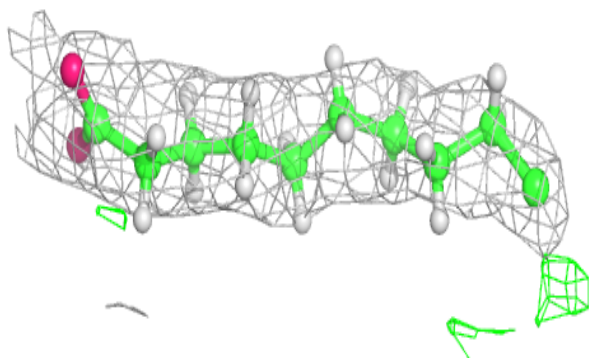
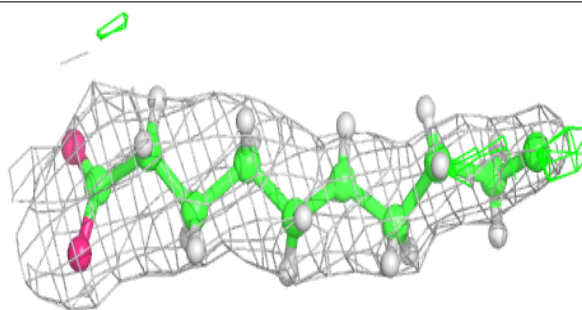


**Electron density around STE c 520:**

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

**Electron density around STE J 101:**

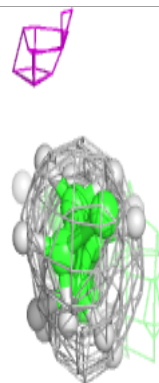
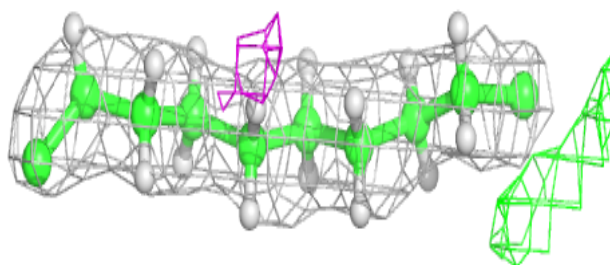
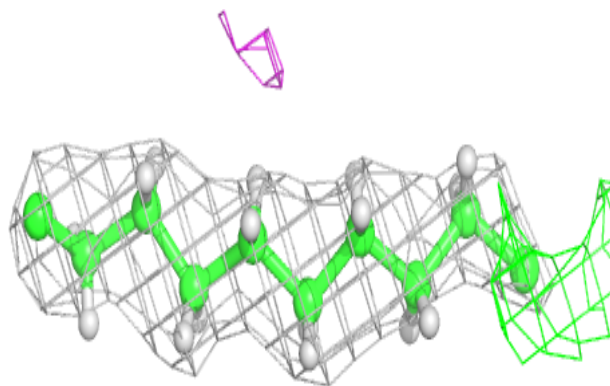
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



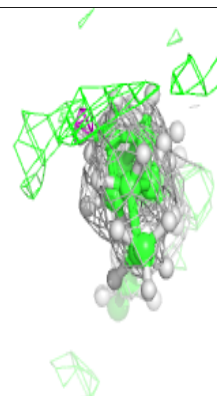
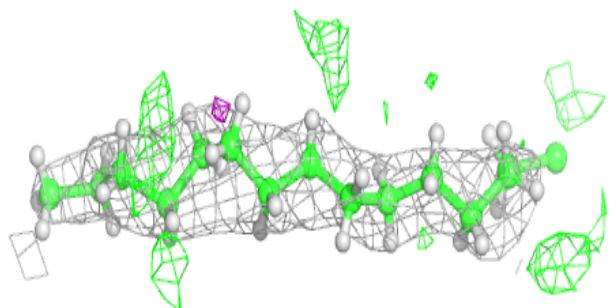
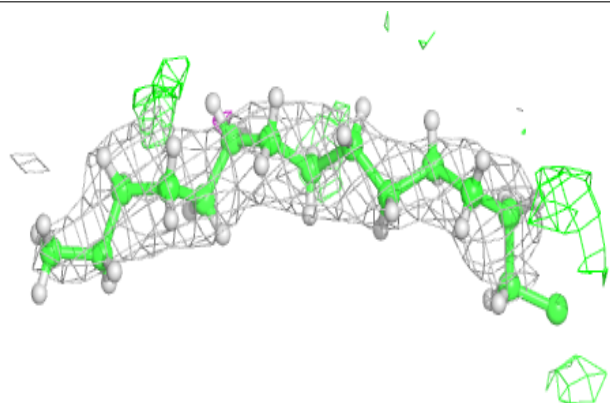


**Electron density around STE M 103:**

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

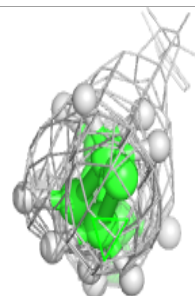
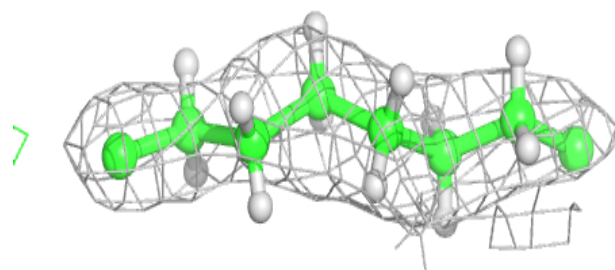
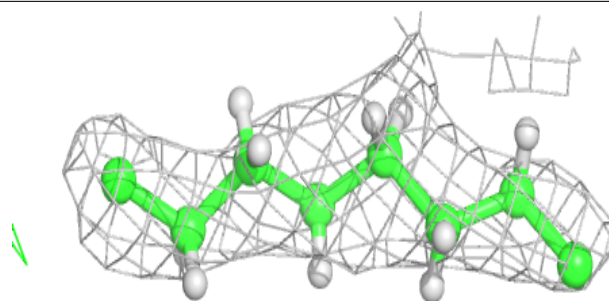
**Electron density around STE T 103:**

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

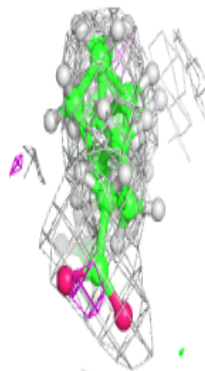
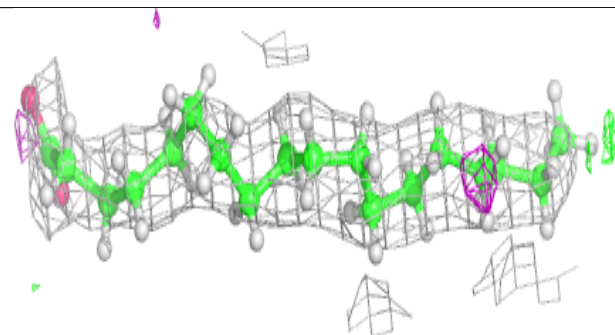
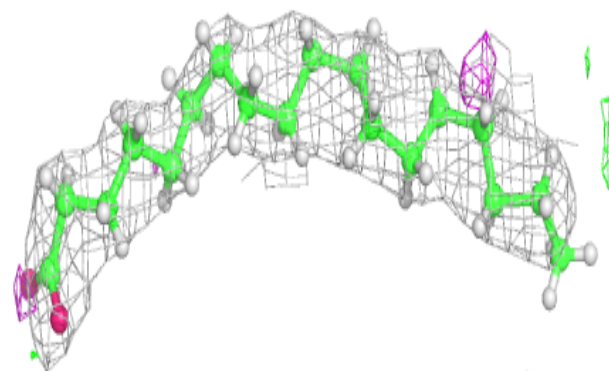


**Electron density around STE Z 101:**

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

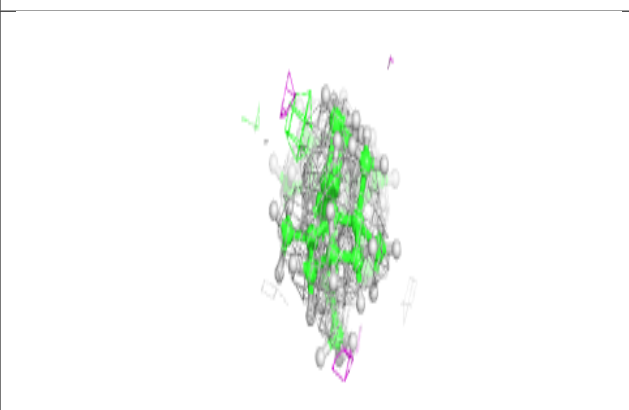
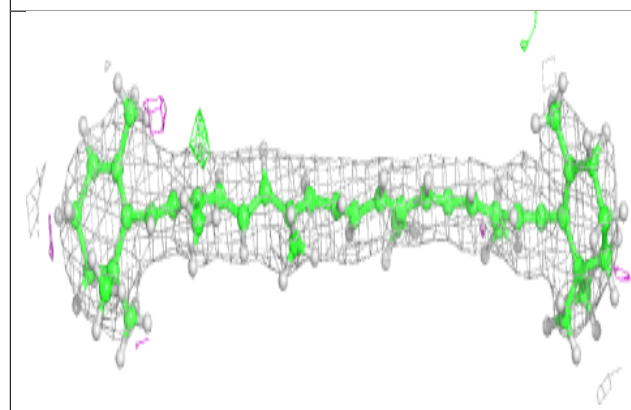
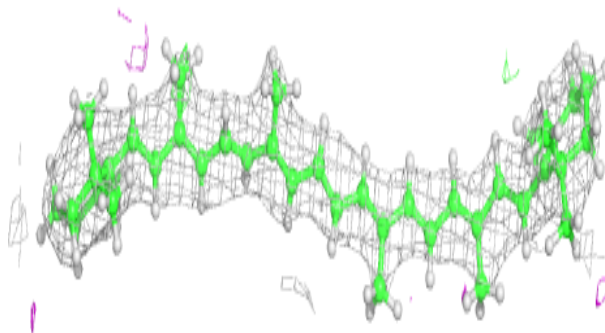
**Electron density around STE D 411:**

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

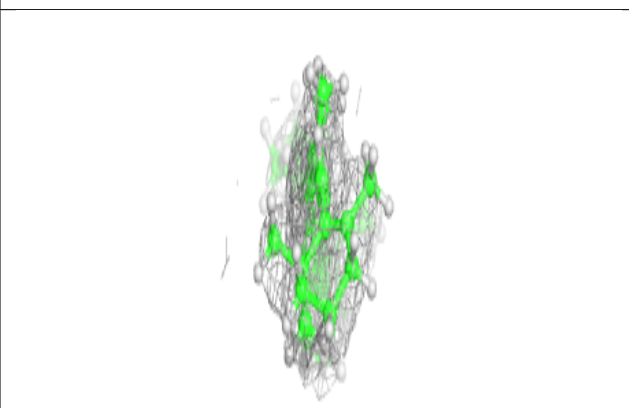
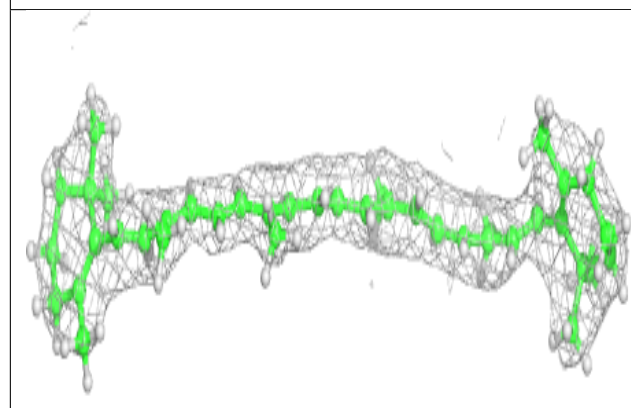
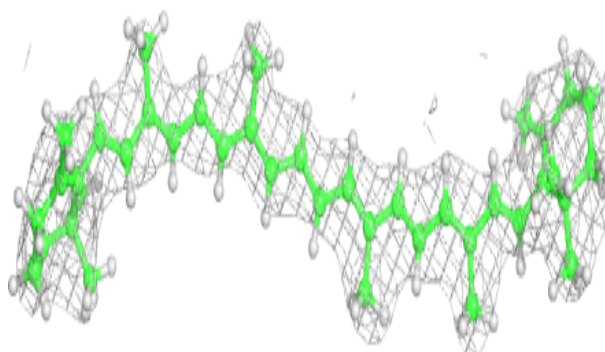


**Electron density around BCR C 514:**

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

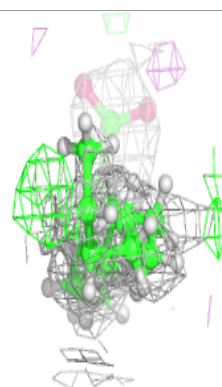
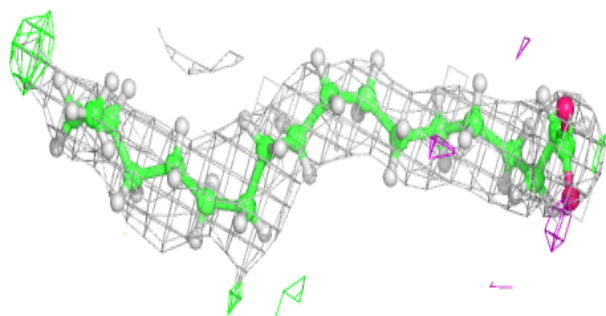
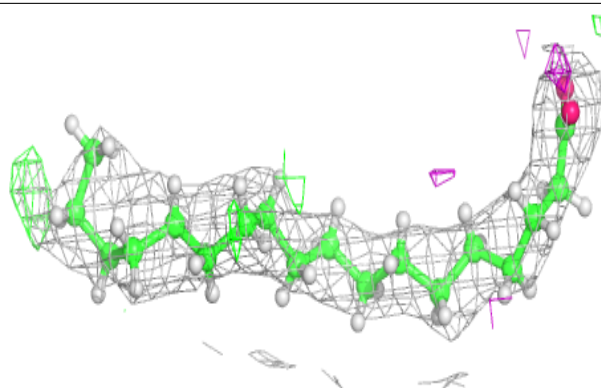
**Electron density around BCR k 101:**

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

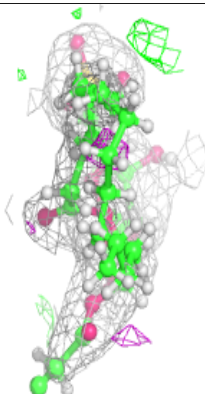
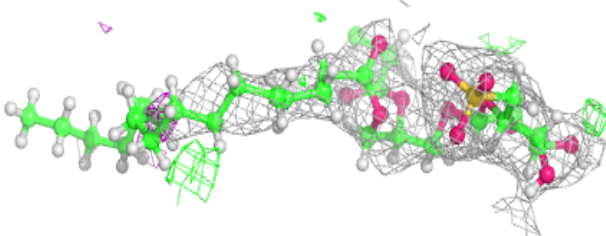
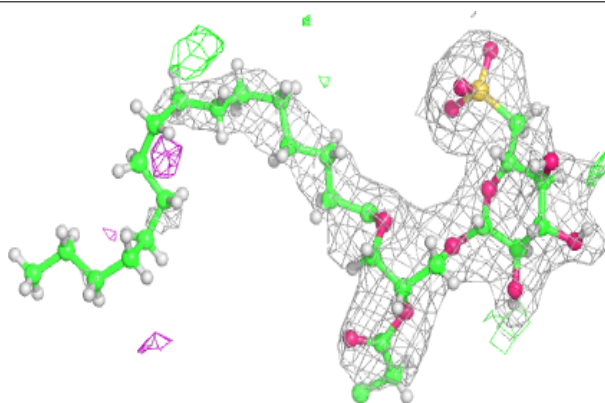


**Electron density around STE b 622:**

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

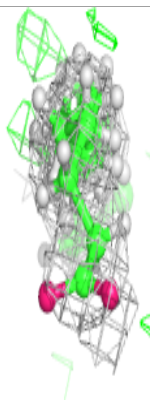
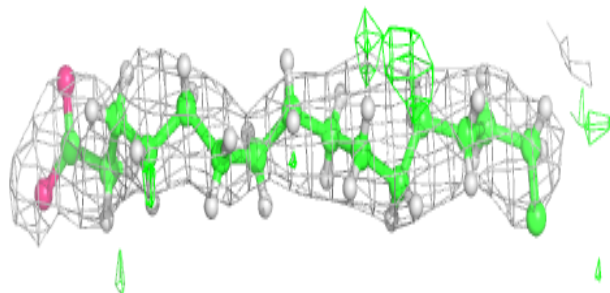
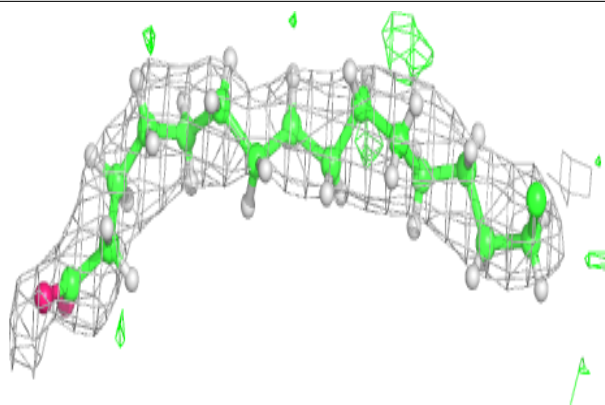
**Electron density around SQD f 101:**

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

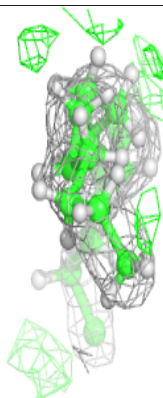
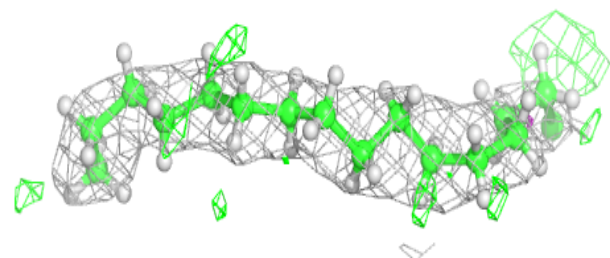
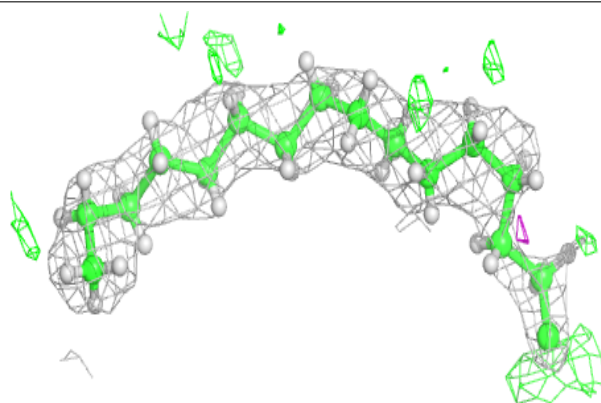


**Electron density around STE t 102:**

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

**Electron density around STE T 102:**

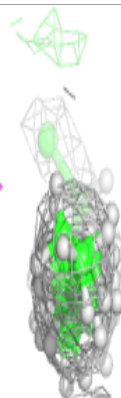
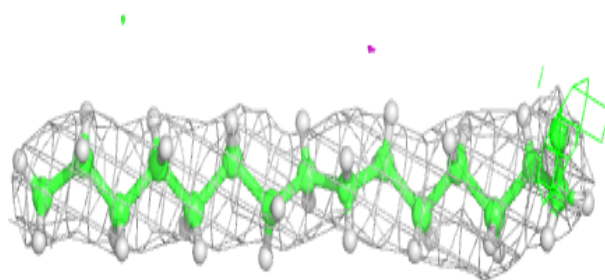
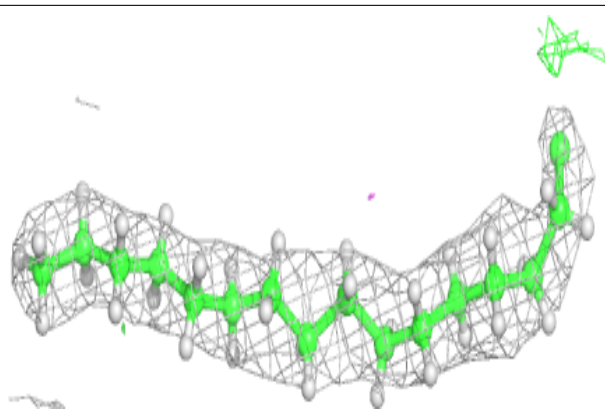
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





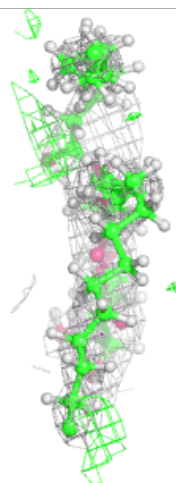
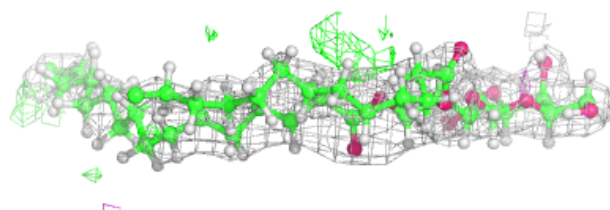
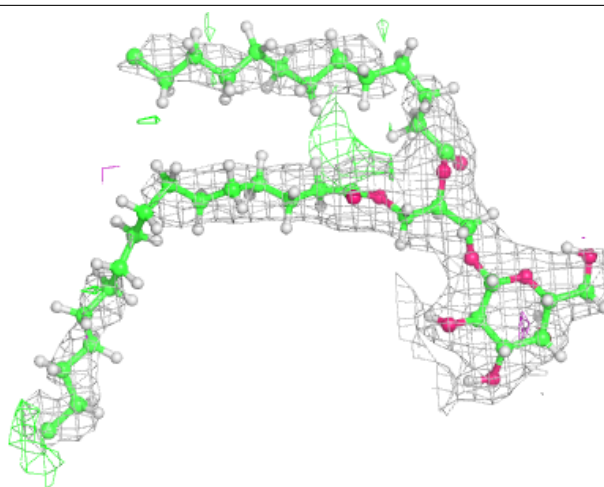
**Electron density around STE C 521:**

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



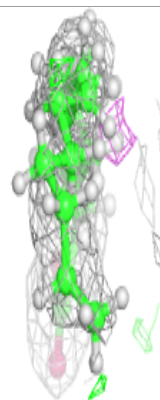
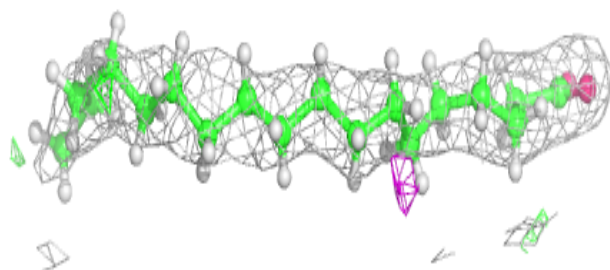
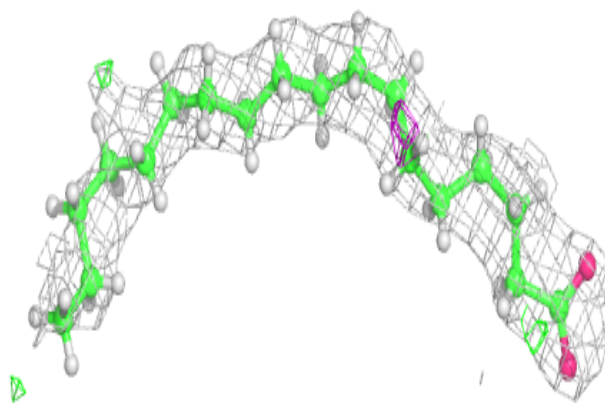
**Electron density around LMG C 519:**

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

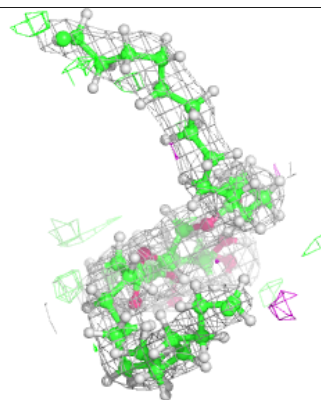
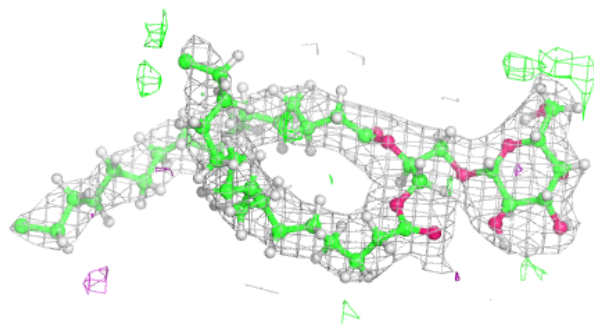
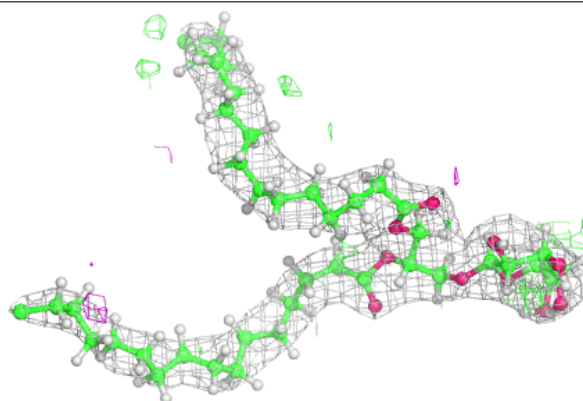


**Electron density around STE x 102:**

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

**Electron density around LMG b 621:**

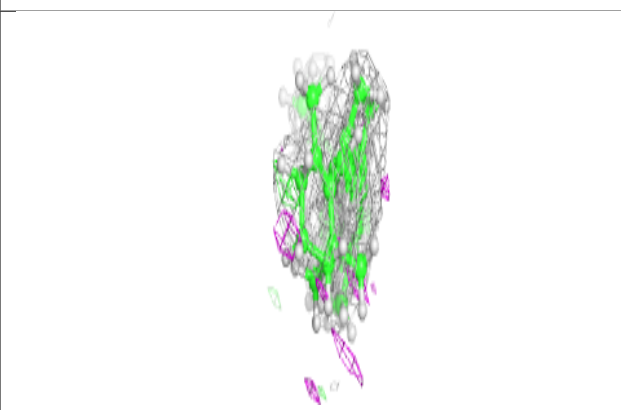
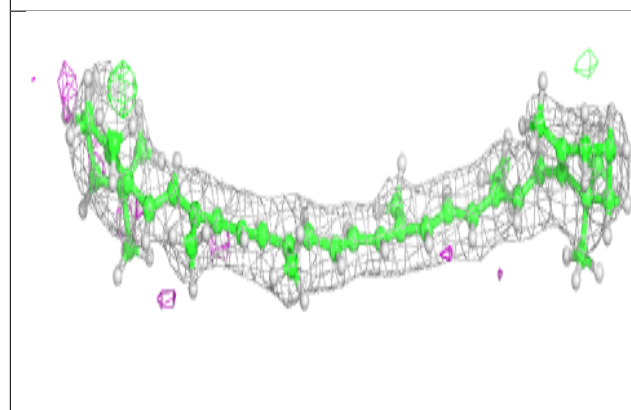
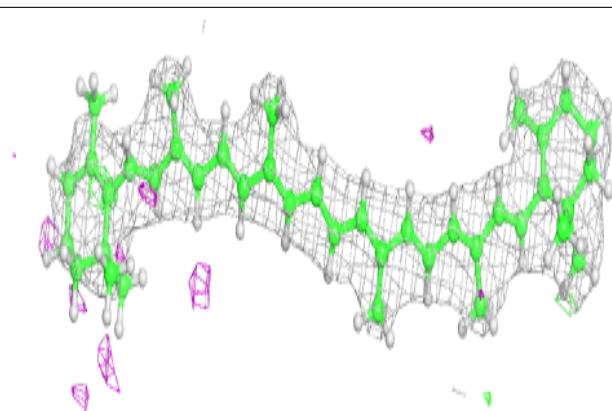
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



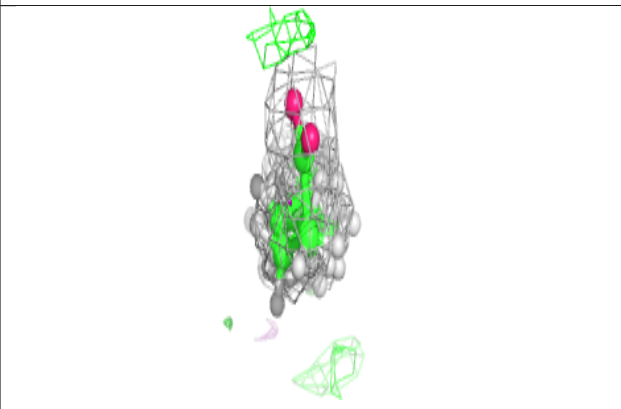
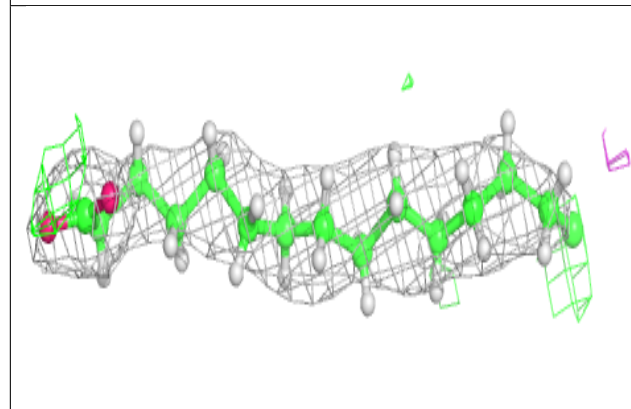
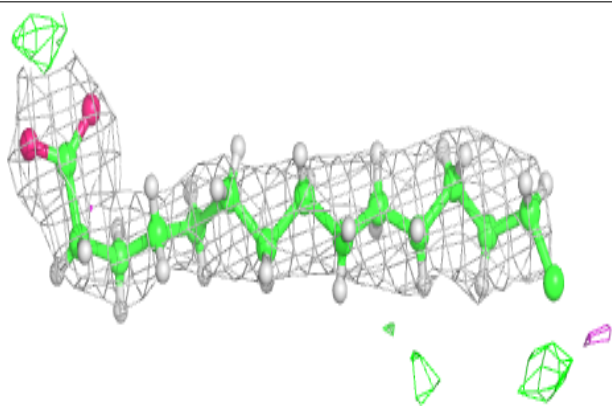


**Electron density around BCR D 404:**

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

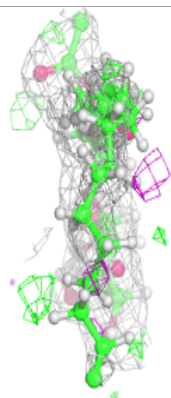
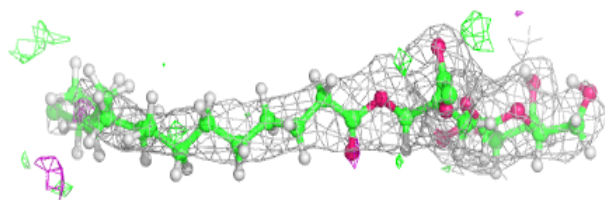
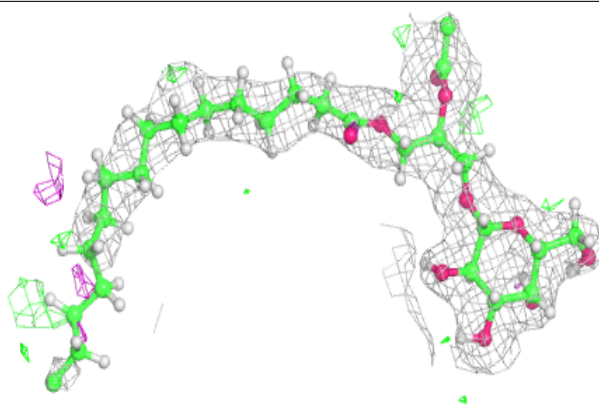
**Electron density around STE d 411:**

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

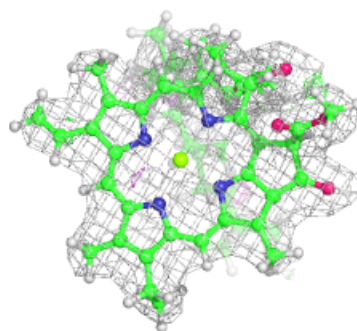
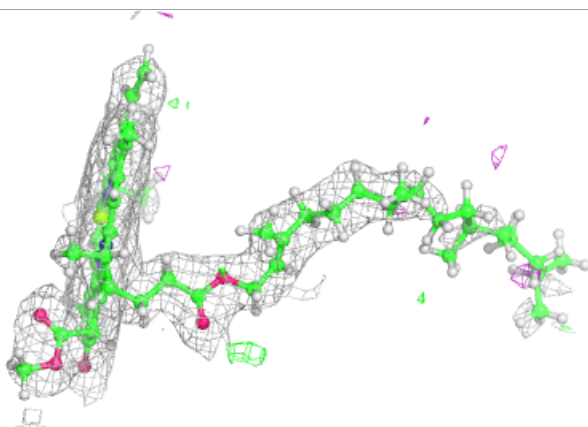
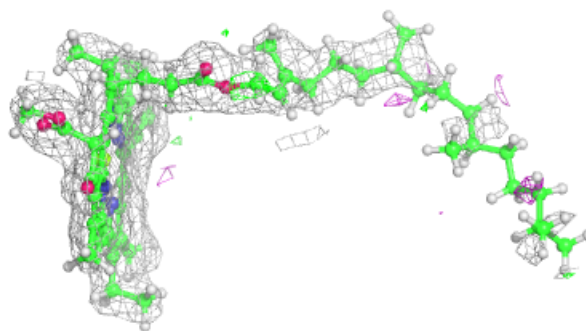


**Electron density around LMG c 519:**

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

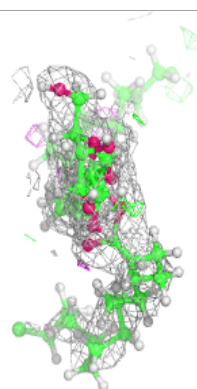
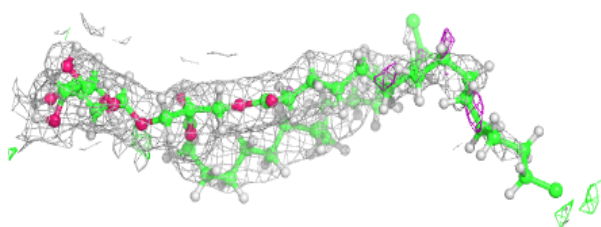
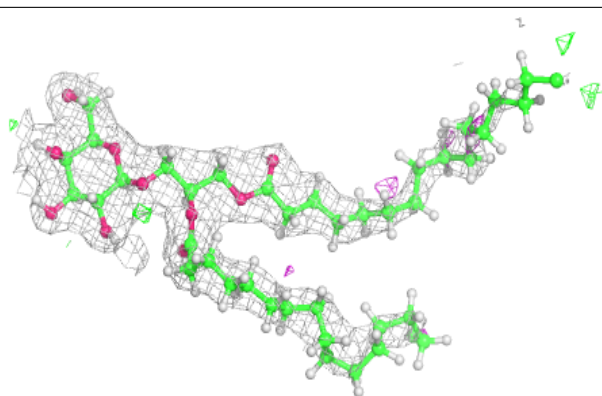
**Electron density around CLA D 403:**

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

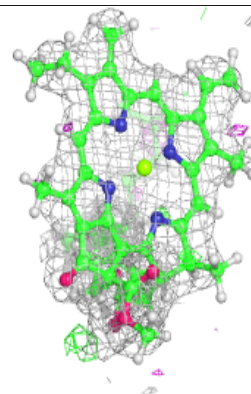
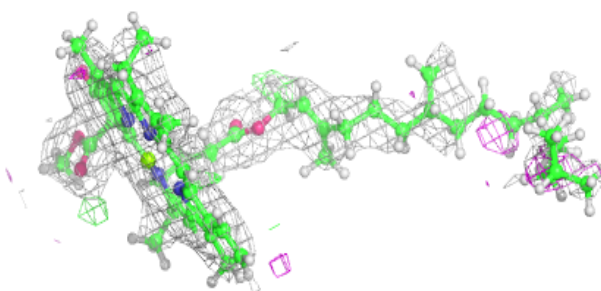
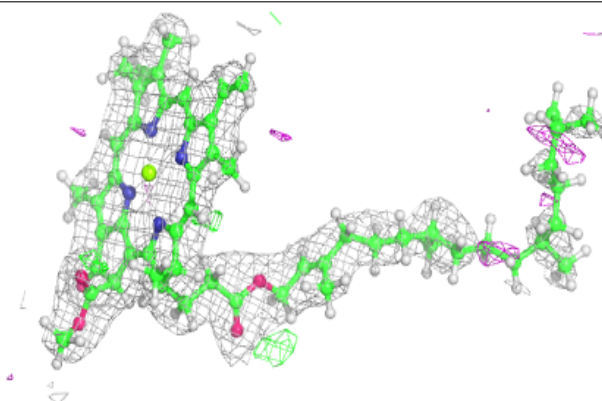


**Electron density around LMG D 406:**

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

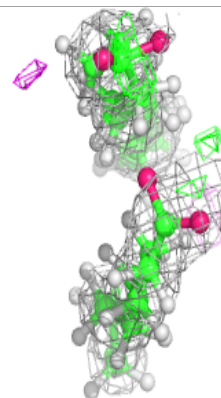
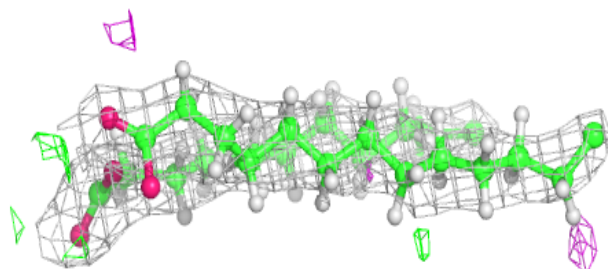
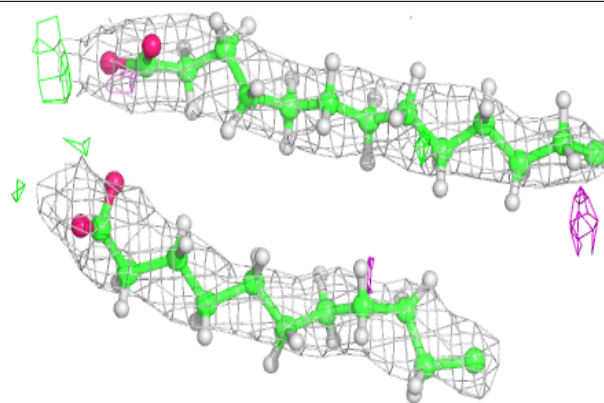
**Electron density around CLA d 404:**

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



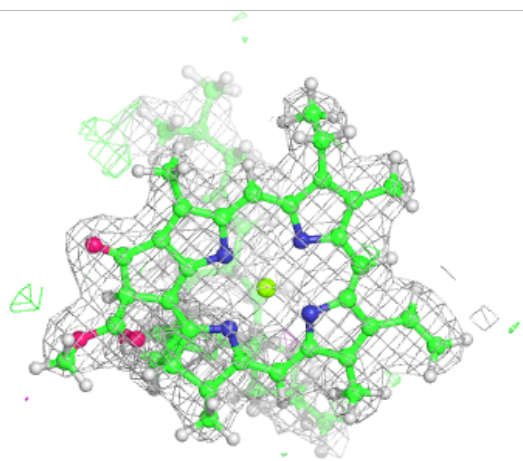
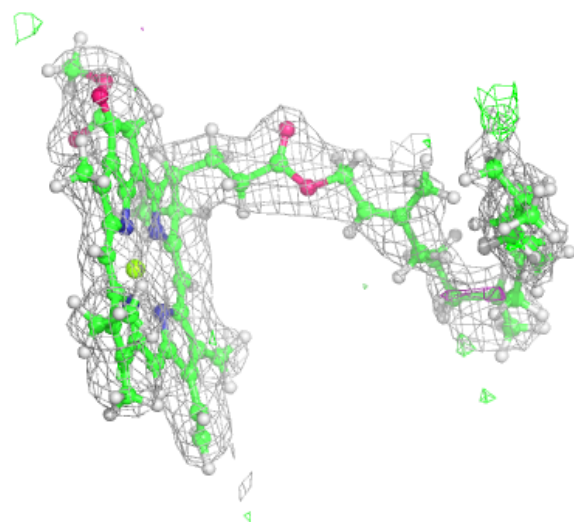
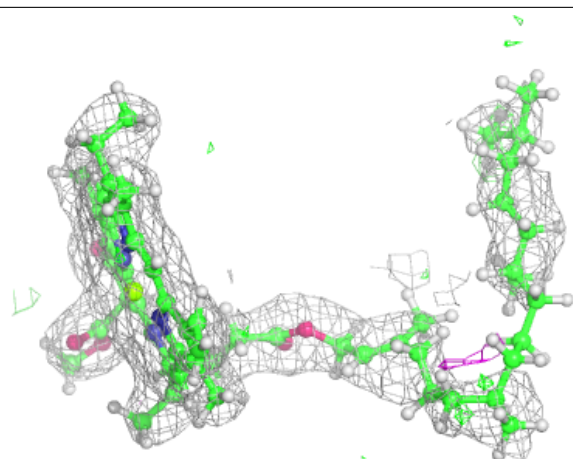
**Electron density around LMG D 410:**

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



**Electron density around CLA a 606:**

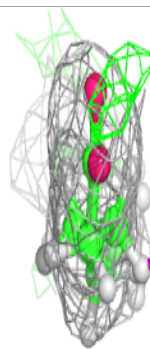
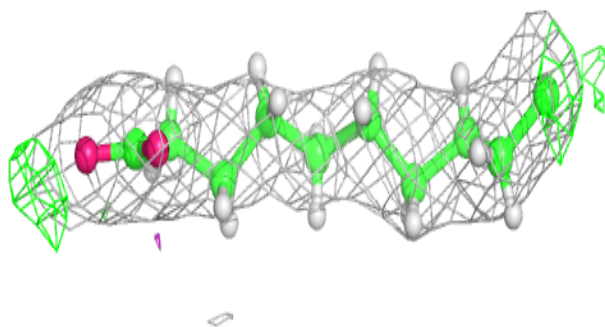
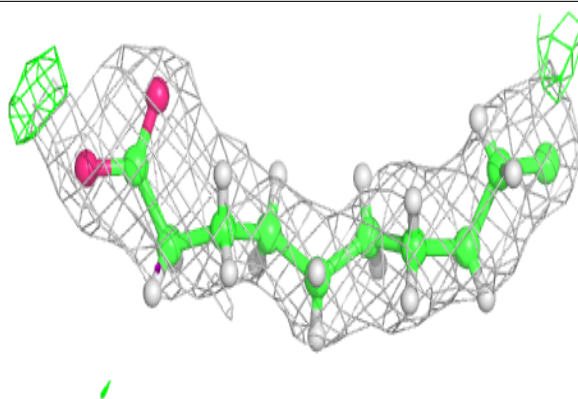
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



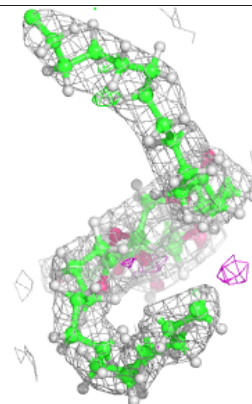
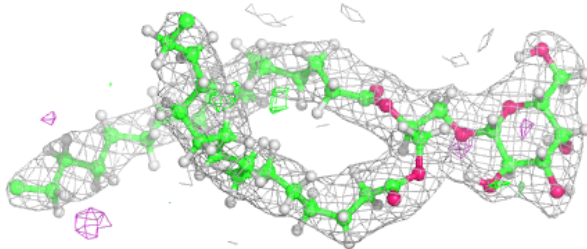
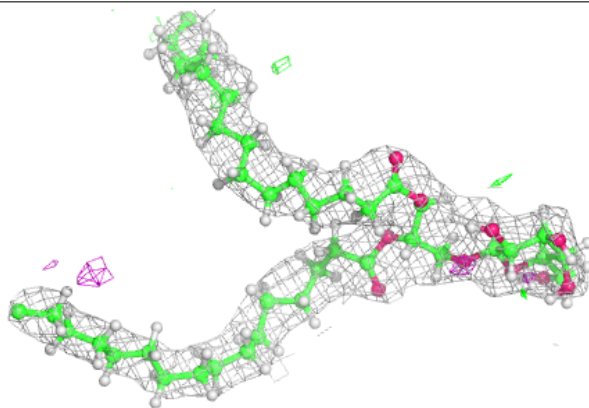


**Electron density around STE C 520:**

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

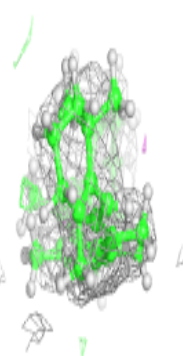
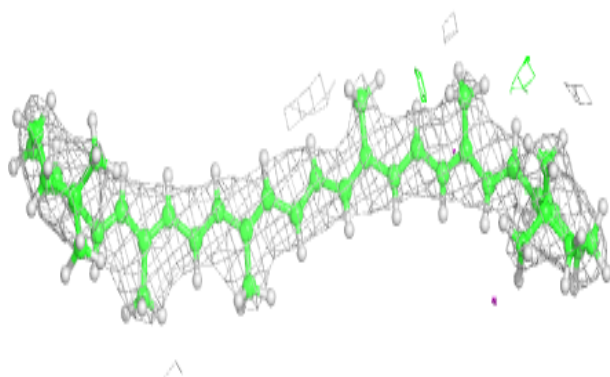
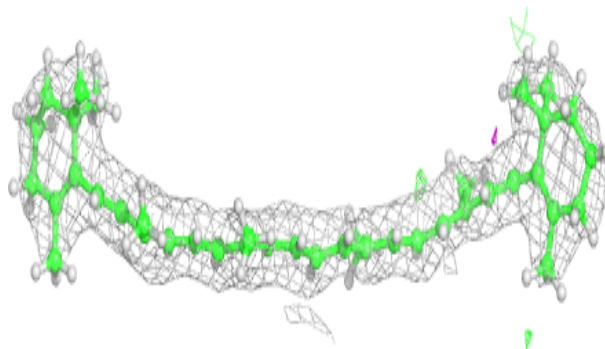
**Electron density around LMG M 101:**

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

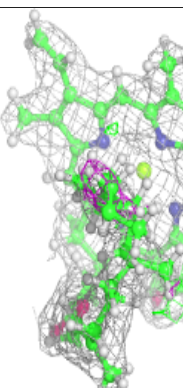
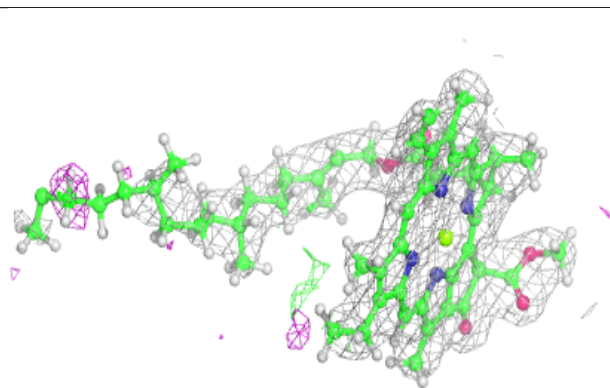
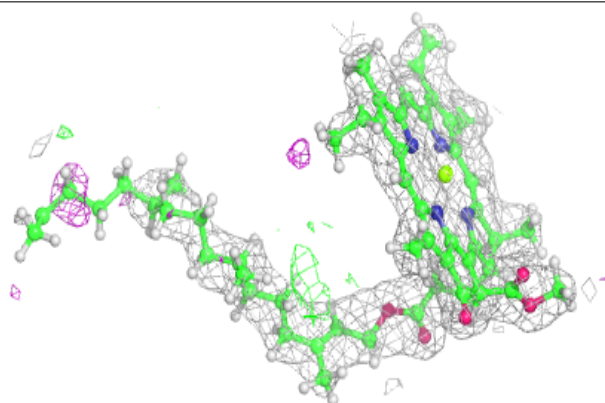


**Electron density around BCR k 102:**

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

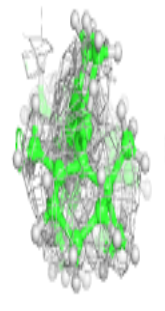
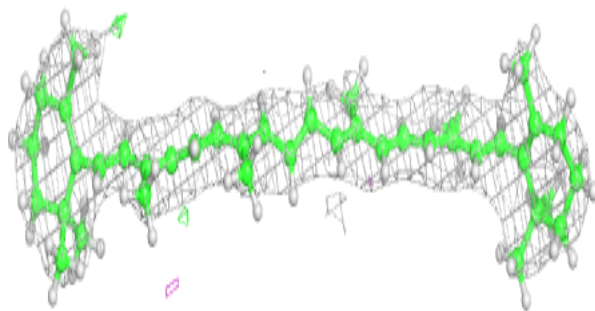
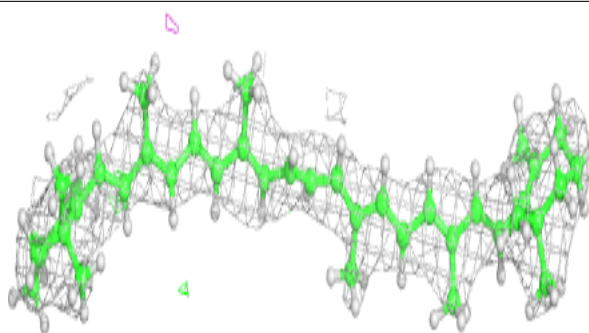
**Electron density around CLA c 508:**

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

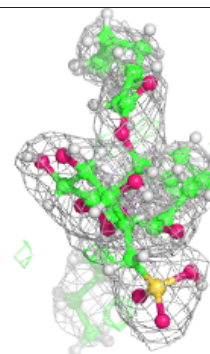
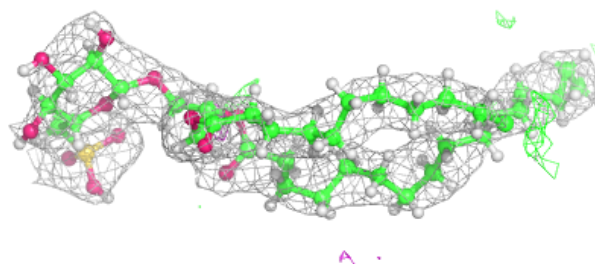
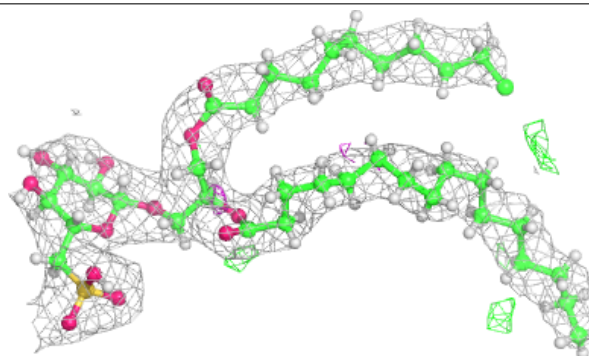


**Electron density around BCR c 514:**

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

**Electron density around SQD b 620:**

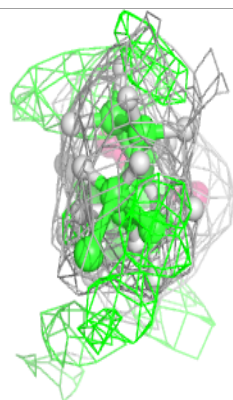
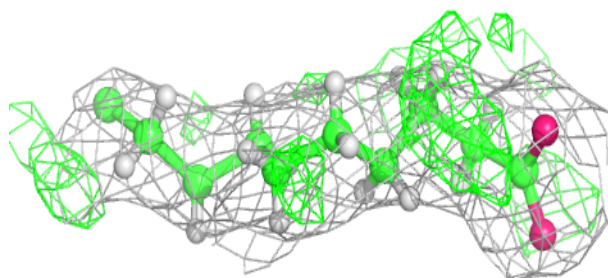
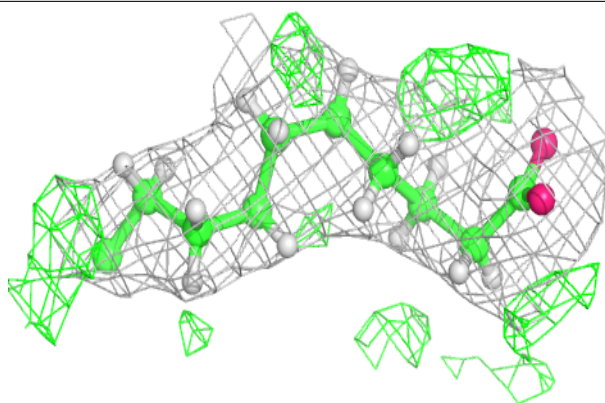
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



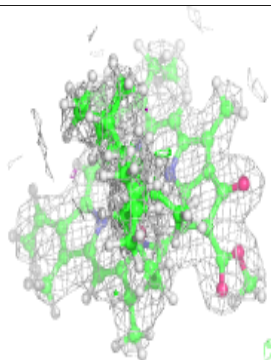
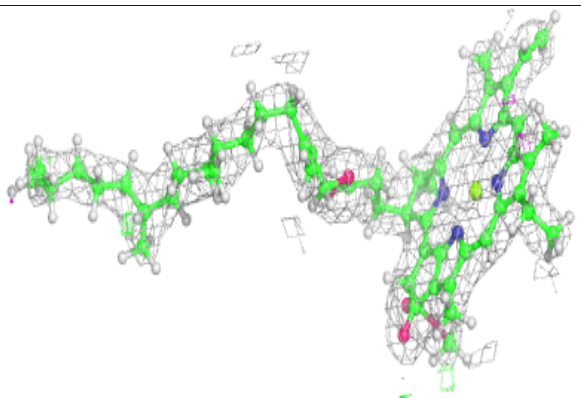
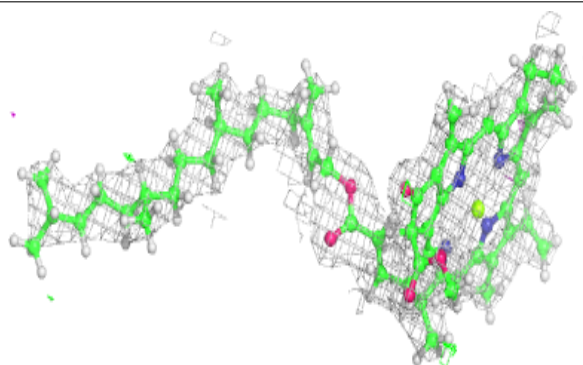


**Electron density around STE B 625:**

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

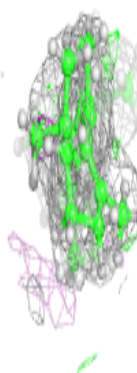
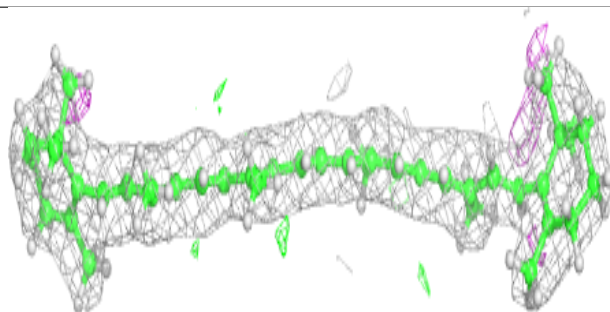
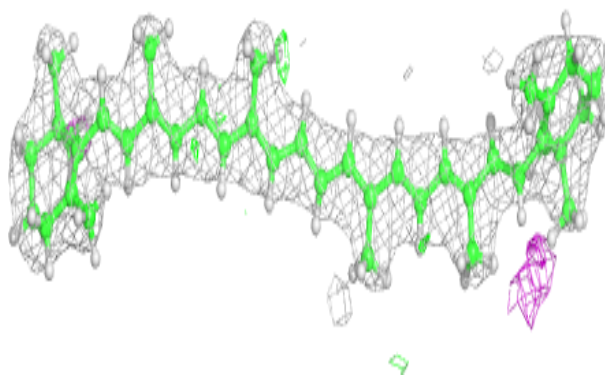
**Electron density around CLA C 502:**

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

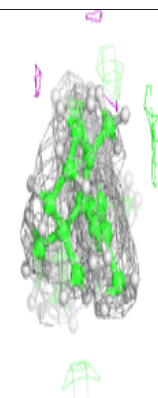
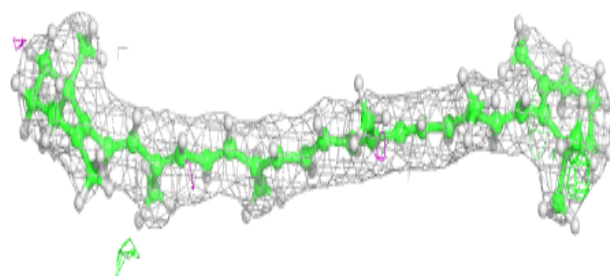
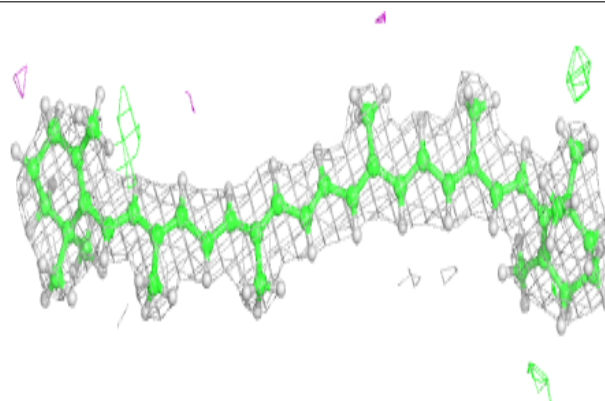


**Electron density around BCR B 618:**

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

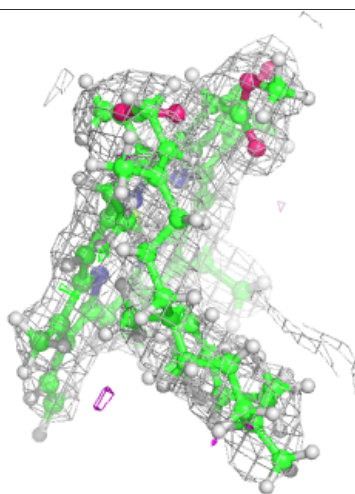
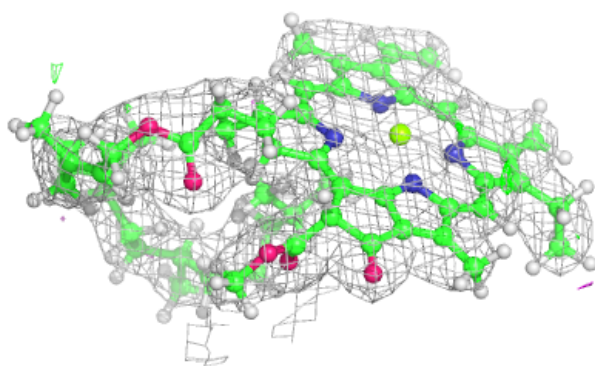
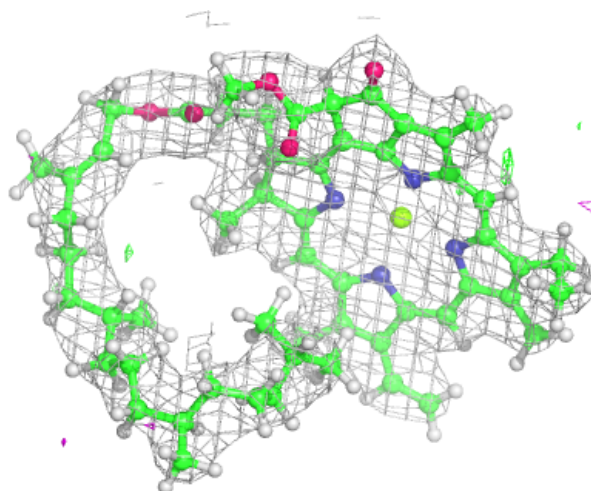
**Electron density around BCR B 619:**

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



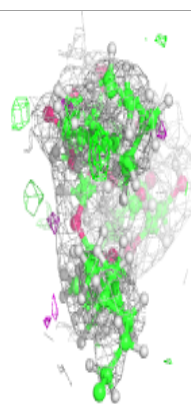
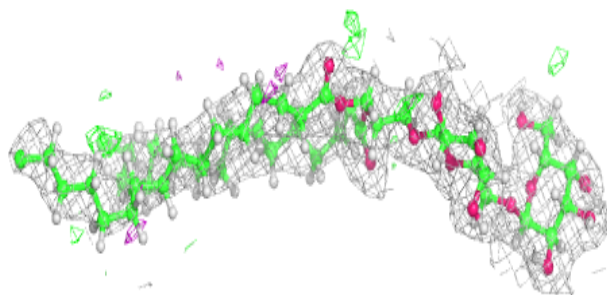
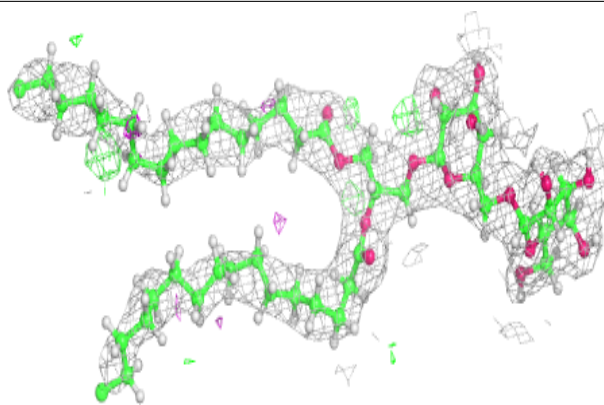
**Electron density around CLA b 615:**

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

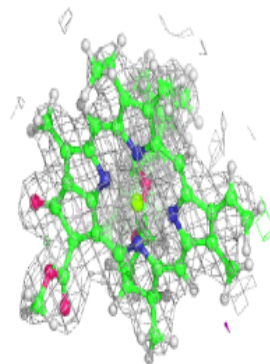
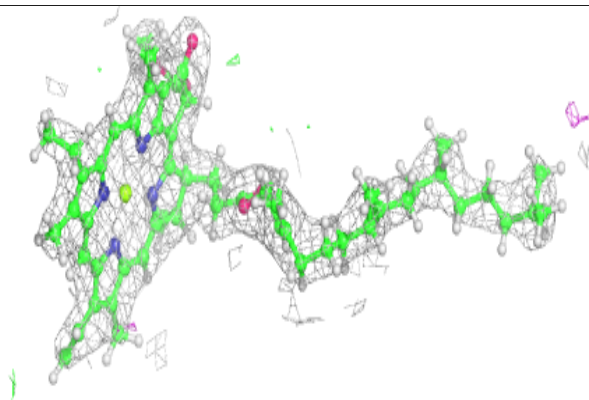
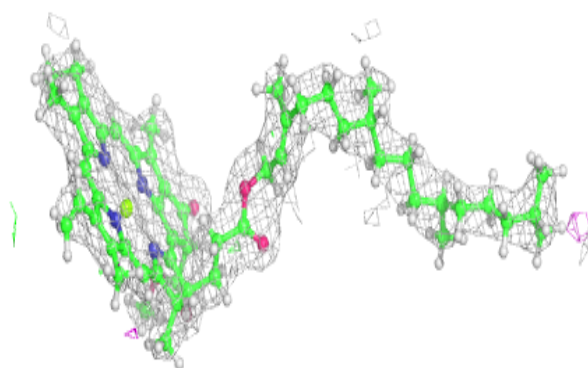


**Electron density around DGD c 518:**

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

**Electron density around CLA c 502:**

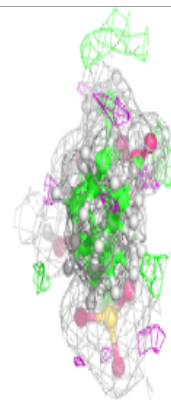
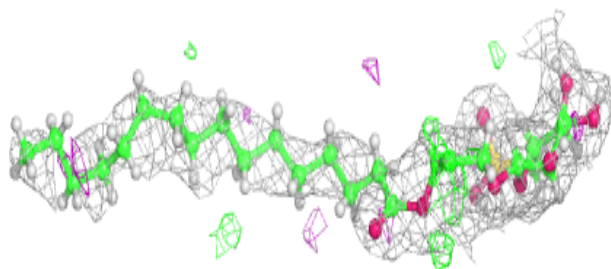
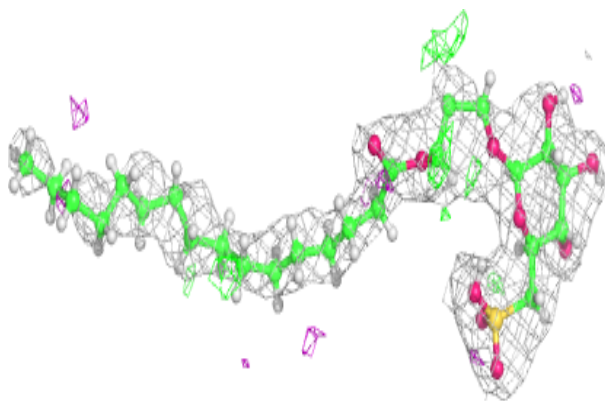
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



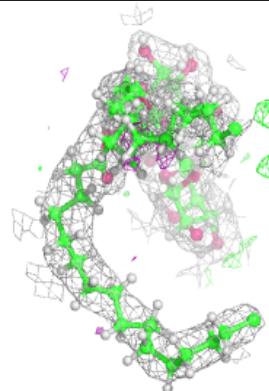
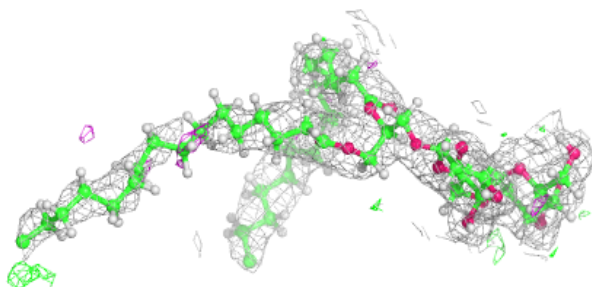
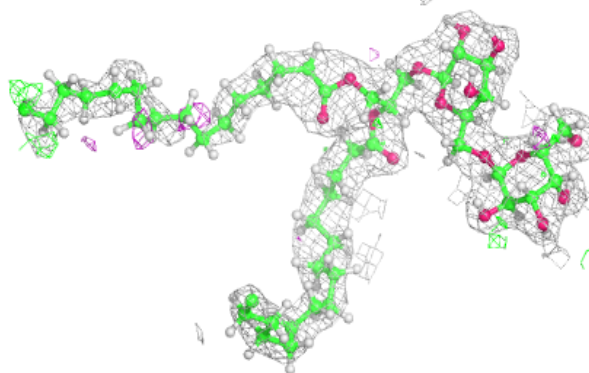


**Electron density around SQD D 407:**

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

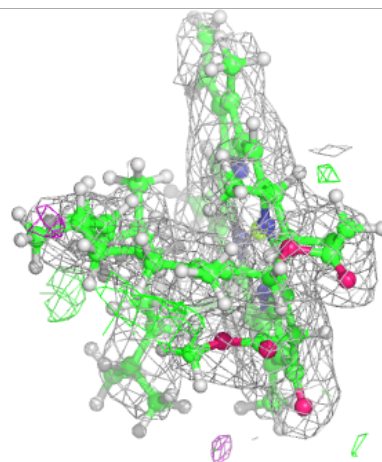
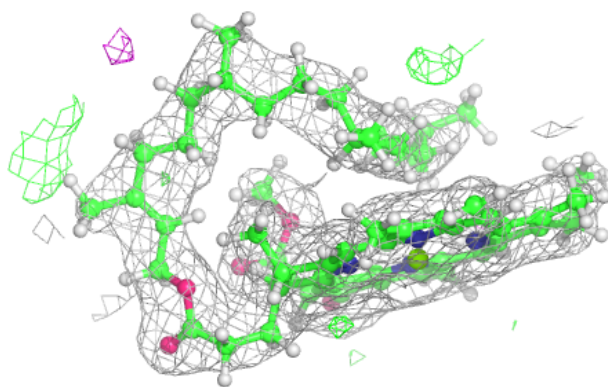
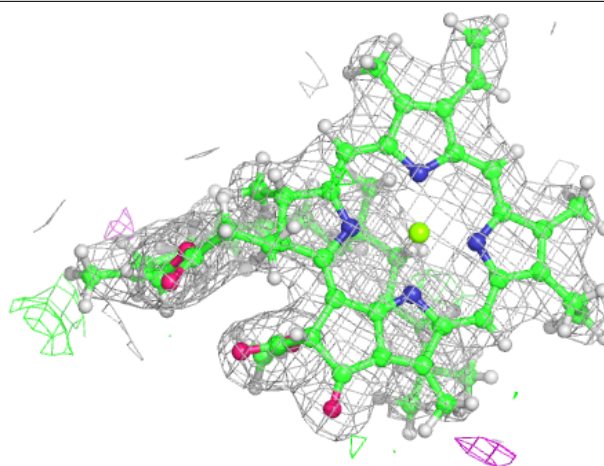
**Electron density around DGD c 517:**

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



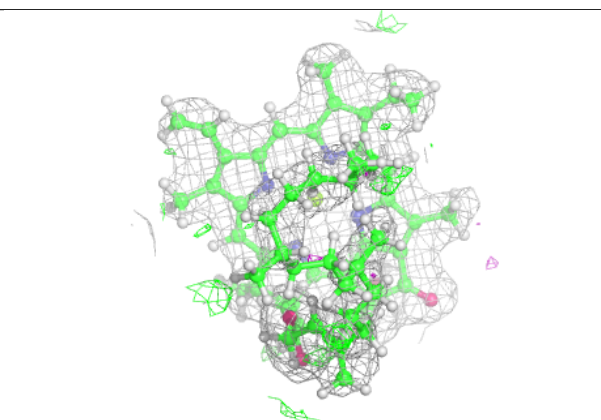
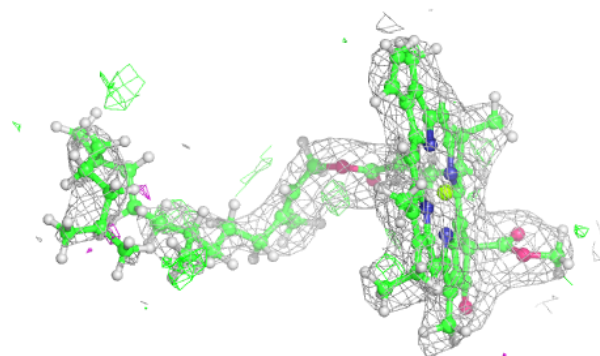
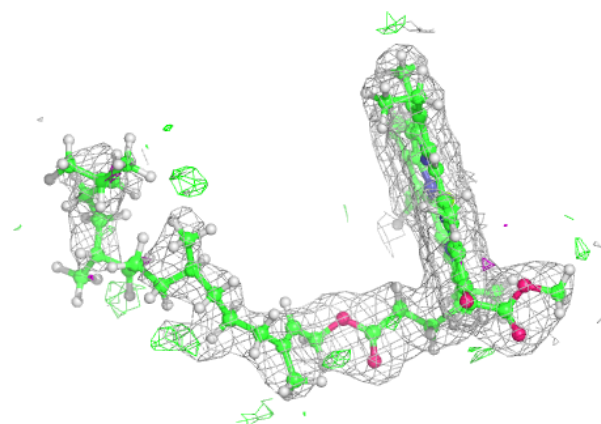
**Electron density around CLA c 510:**

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

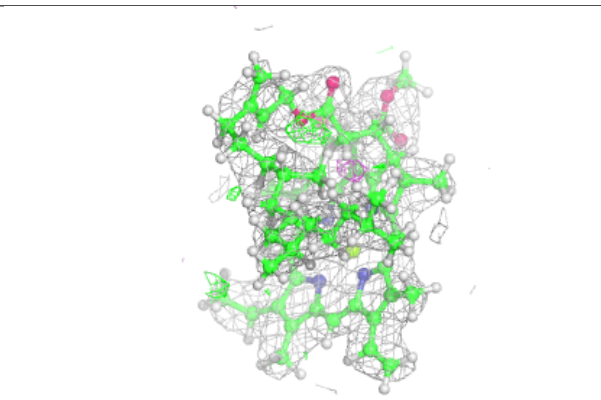
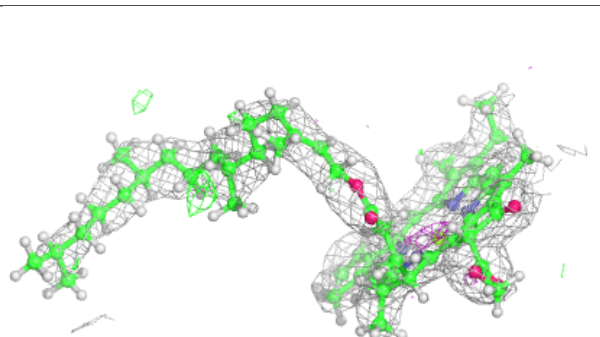
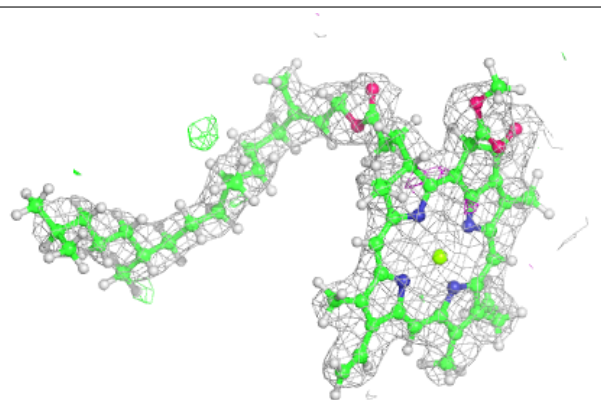


**Electron density around CLA C 506:**

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

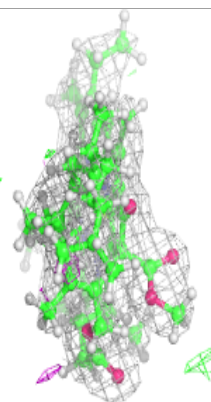
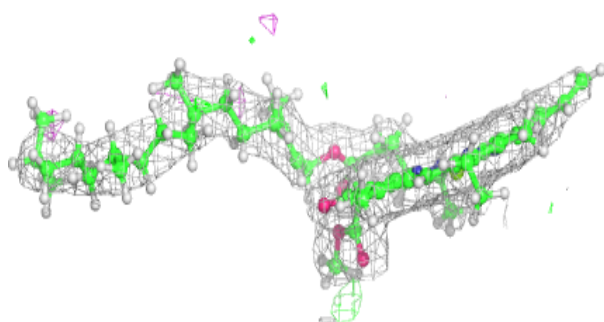
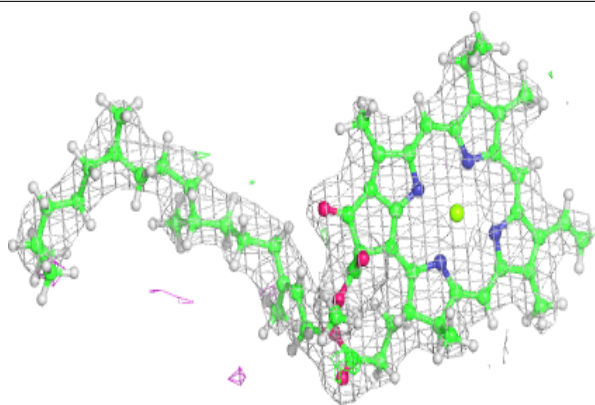
**Electron density around CLA C 511:**

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

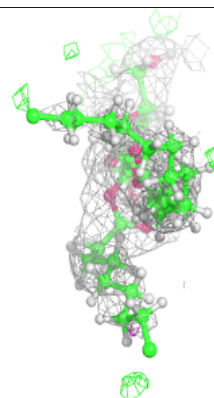
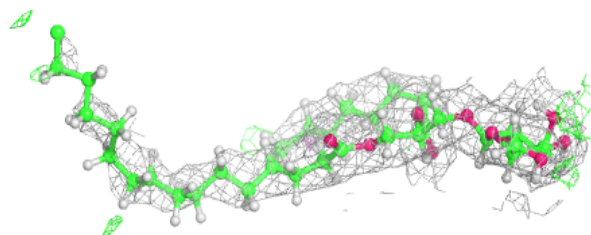
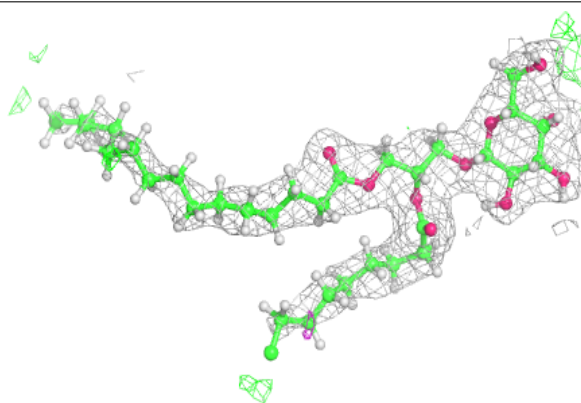


**Electron density around CLA b 602:**

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

**Electron density around LMG d 410:**

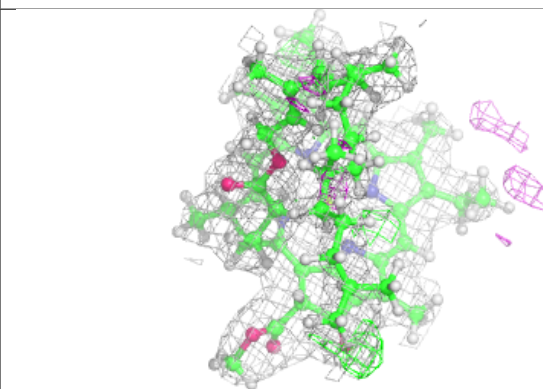
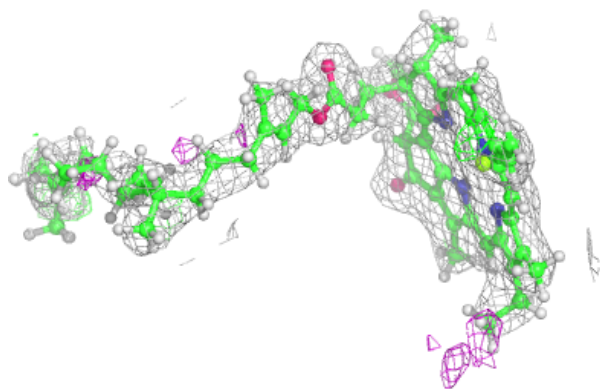
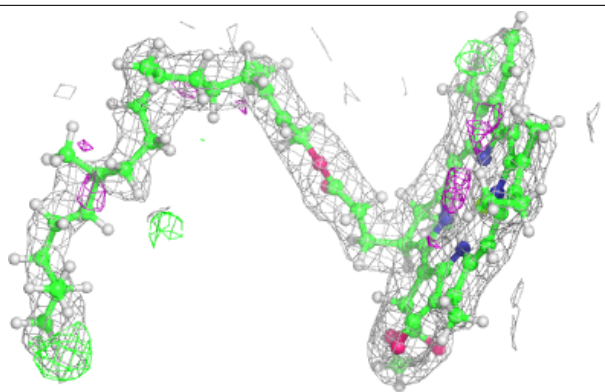
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



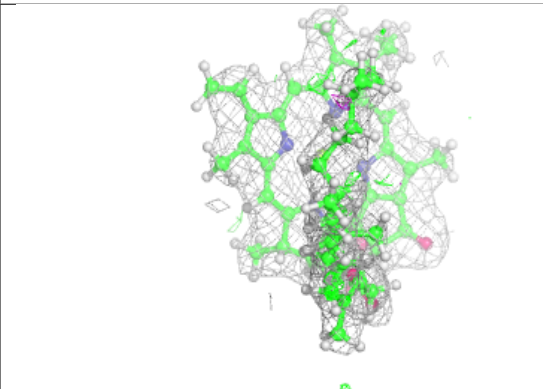
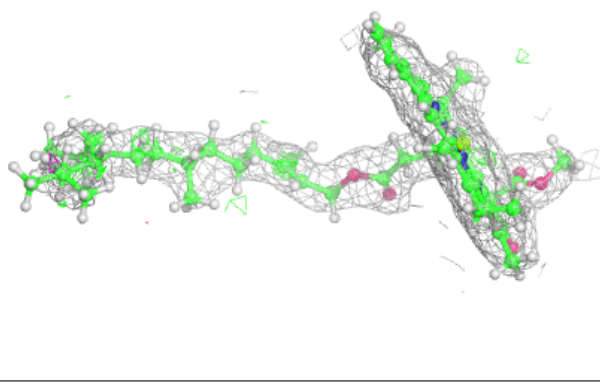
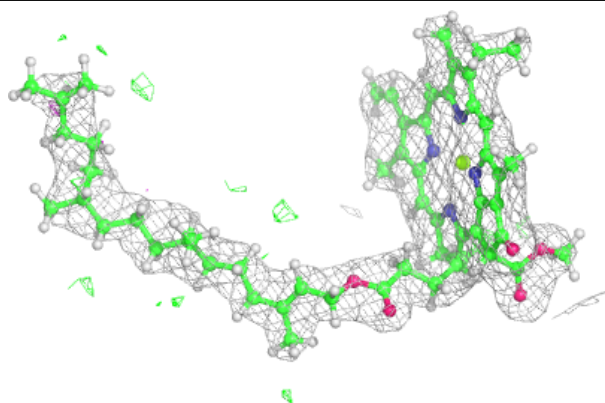


**Electron density around CLA b 606:**

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

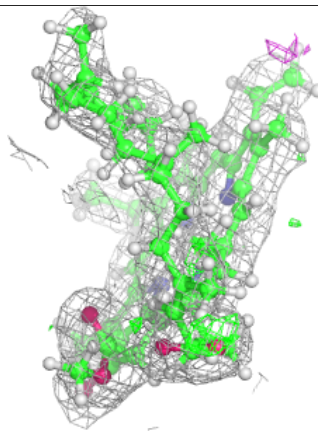
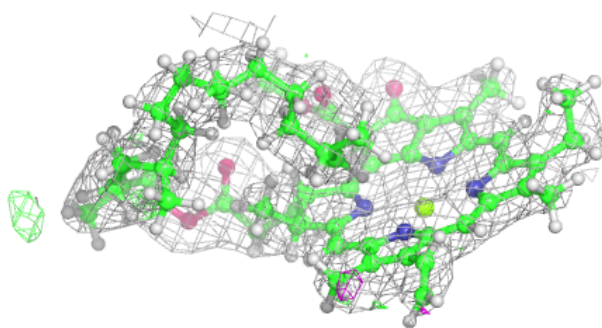
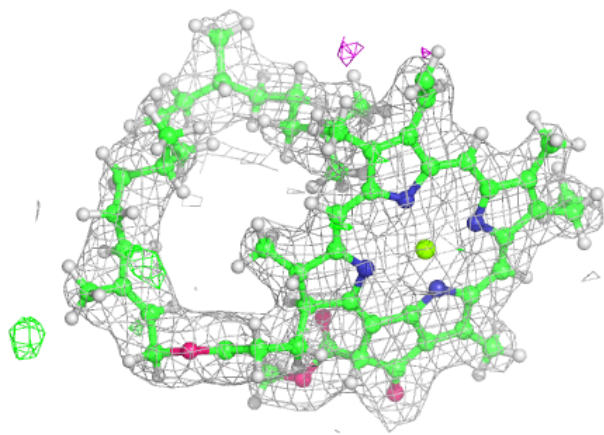
**Electron density around CLA b 609:**

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



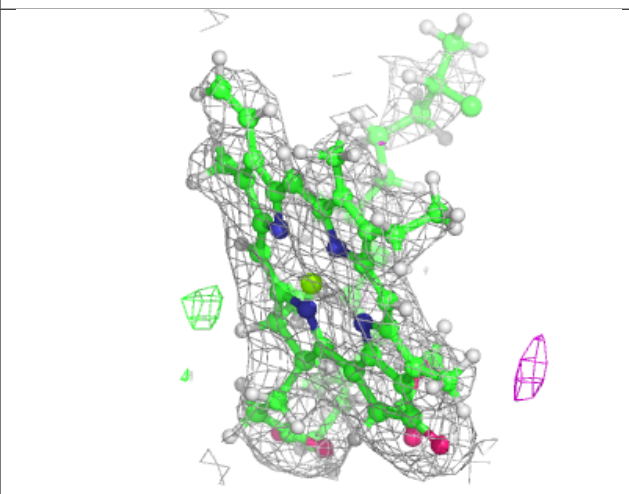
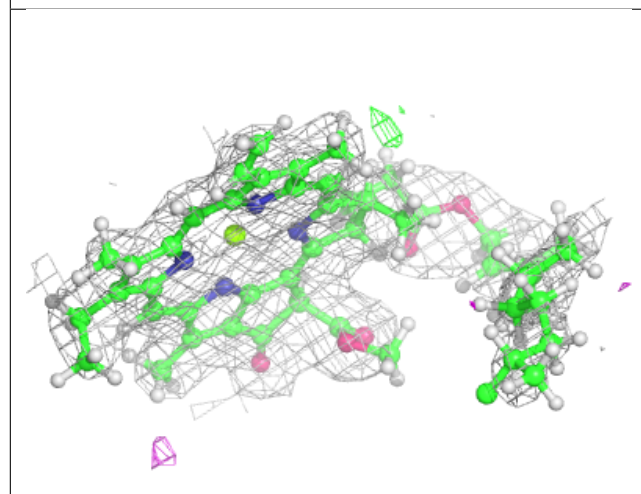
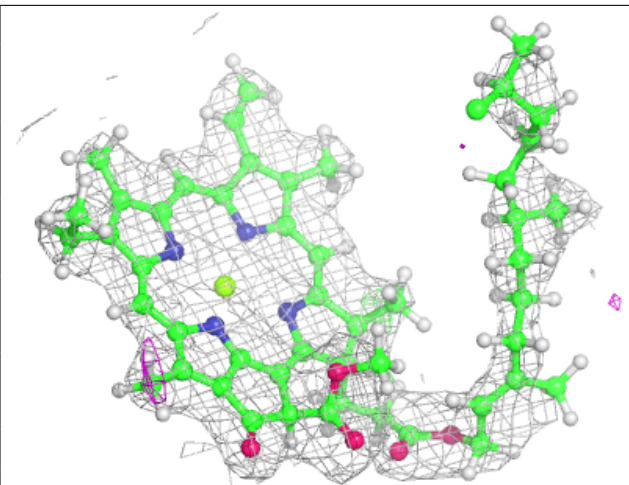
**Electron density around CLA B 615:**

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



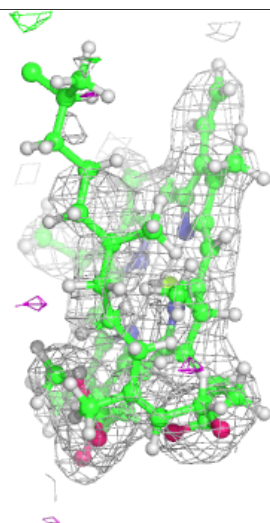
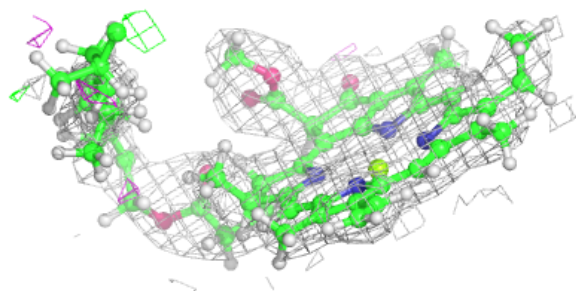
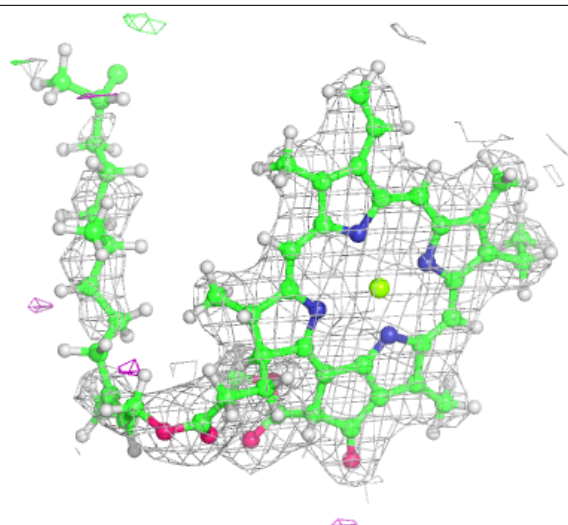
**Electron density around CLA b 616:**

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



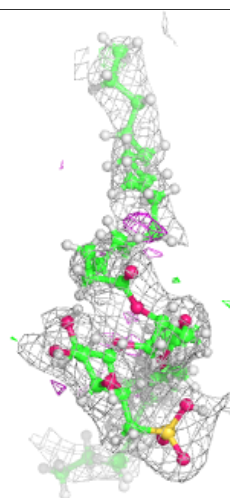
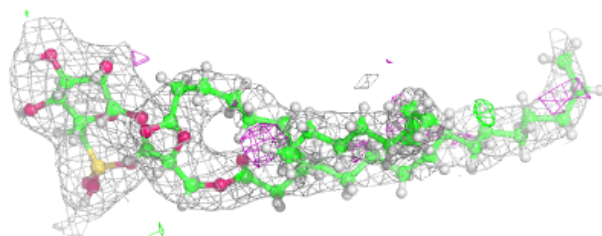
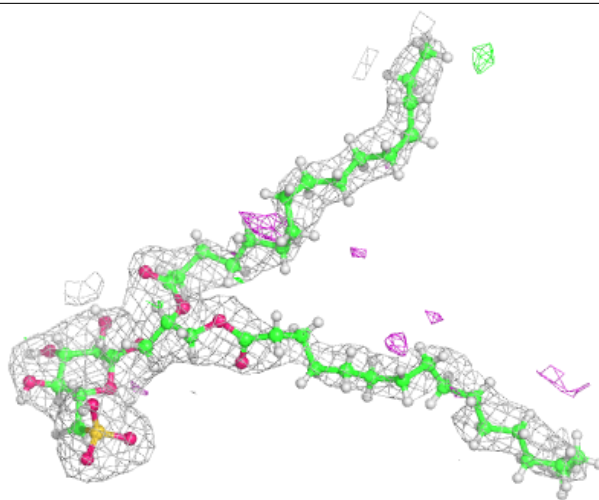
**Electron density around CLA B 616:**

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



**Electron density around SQD a 613:**

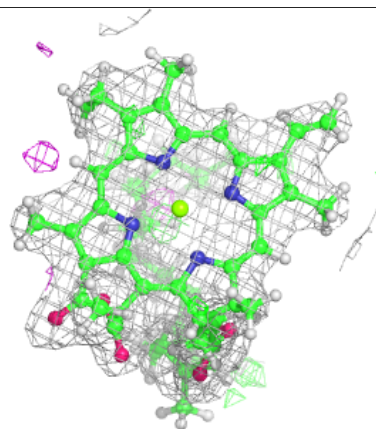
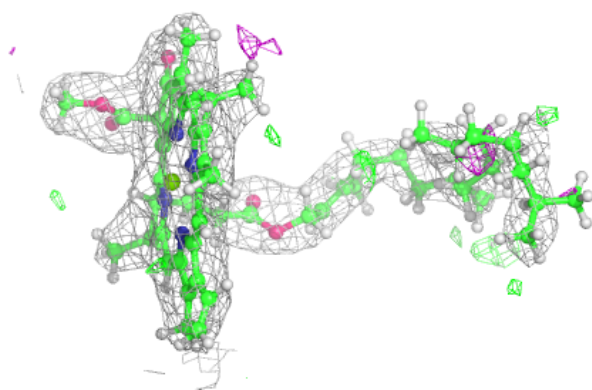
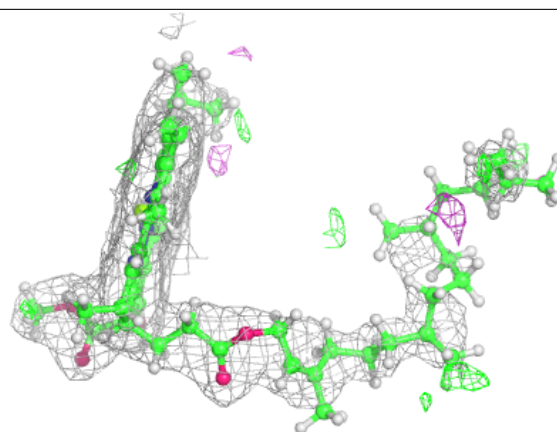
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



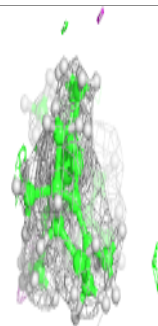
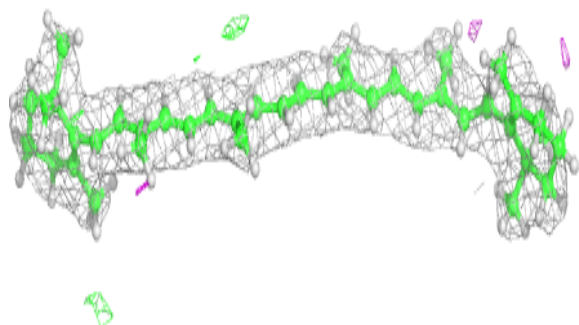
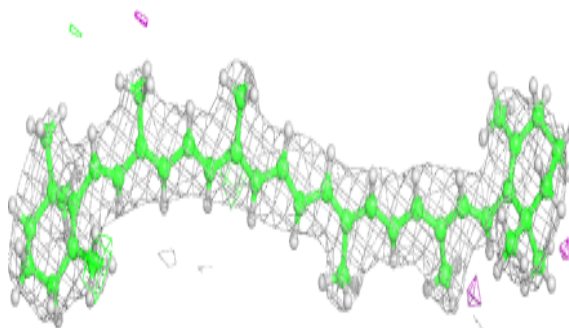


**Electron density around CLA c 506:**

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

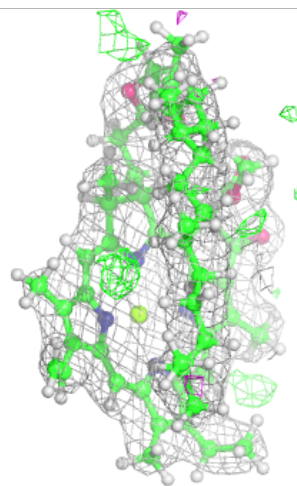
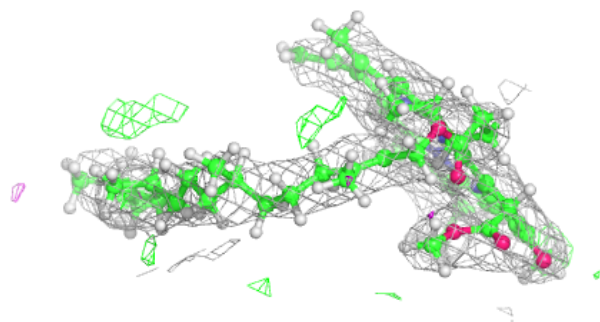
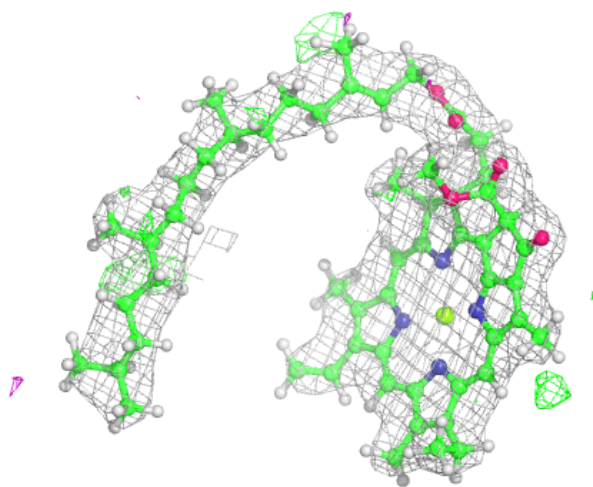
**Electron density around BCR b 619:**

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



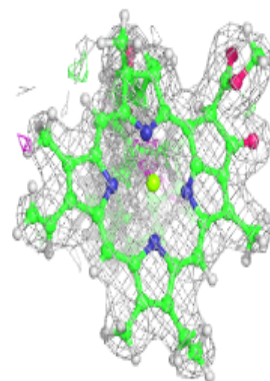
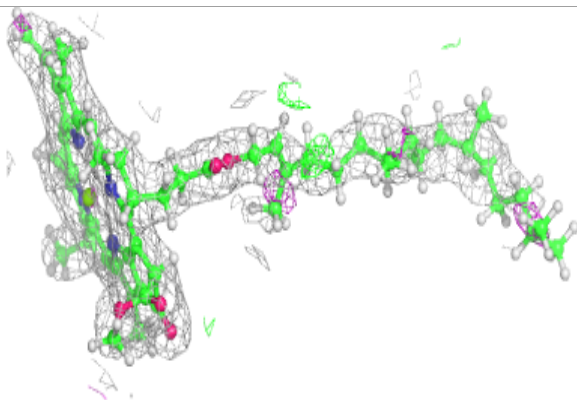
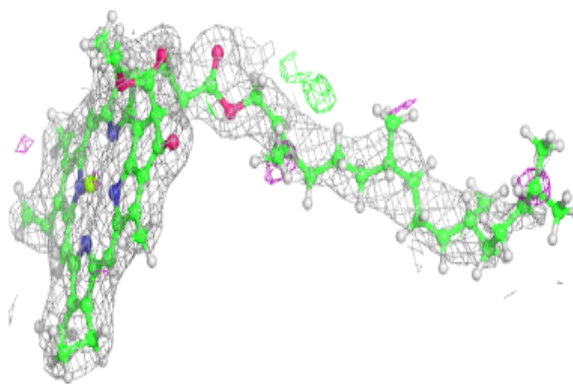
**Electron density around CLA c 507:**

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

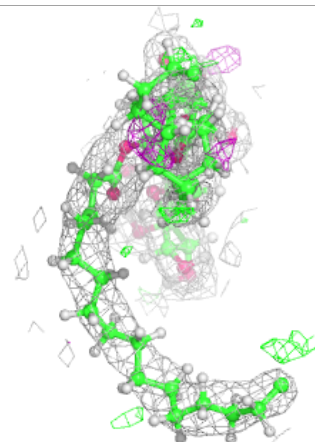
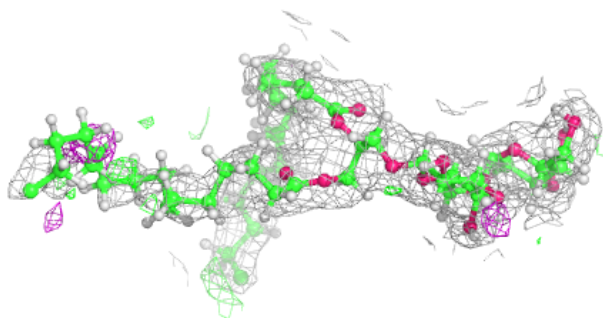
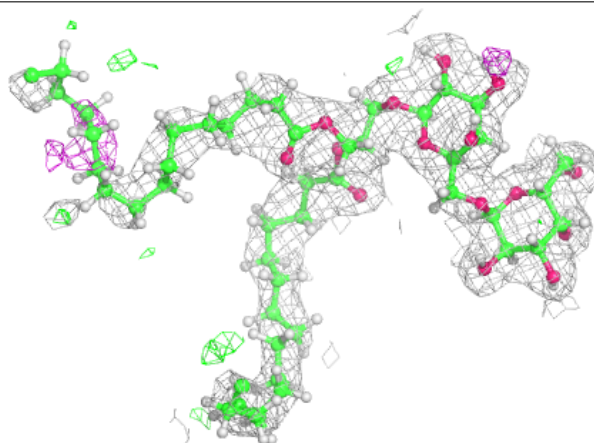


**Electron density around CLA B 604:**

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

**Electron density around DGD C 517:**

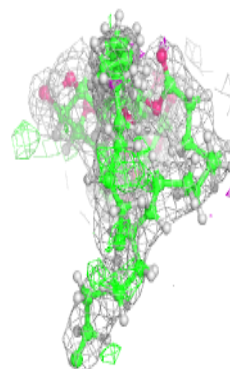
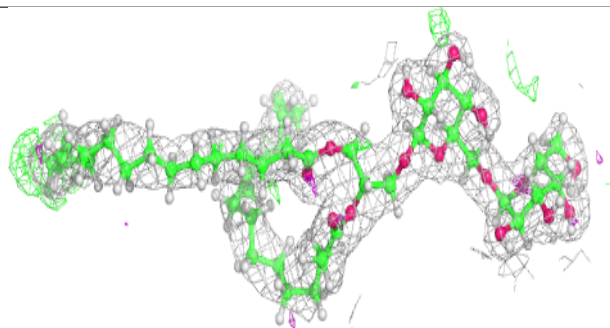
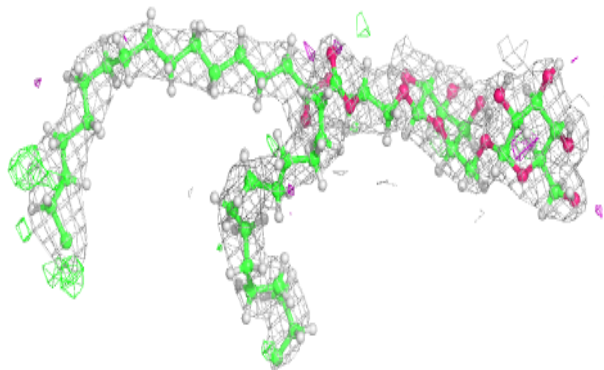
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



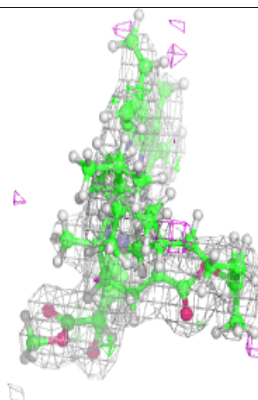
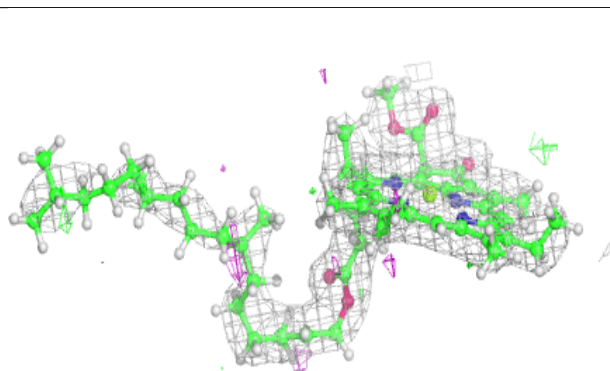
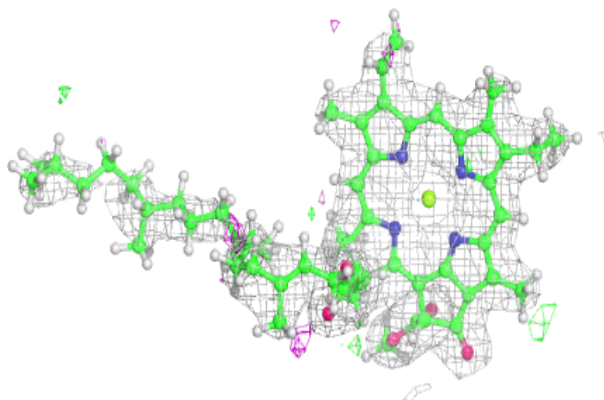


**Electron density around DGD H 102:**

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

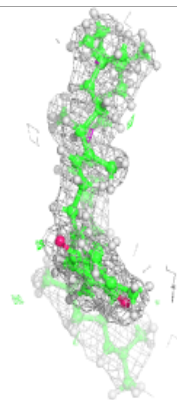
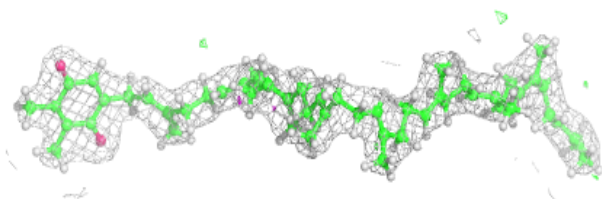
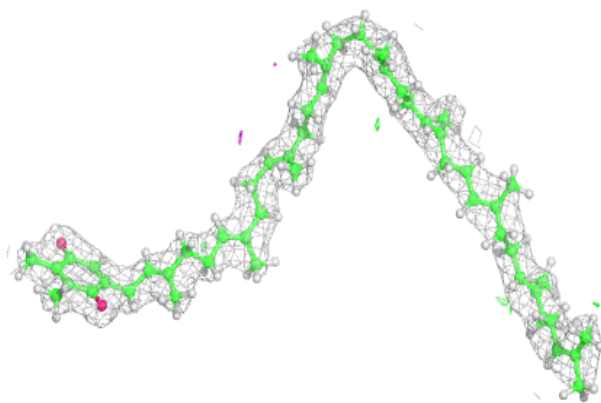
**Electron density around CLA d 401:**

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

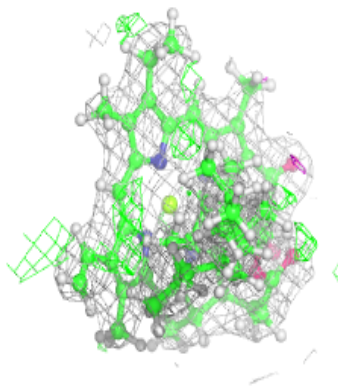
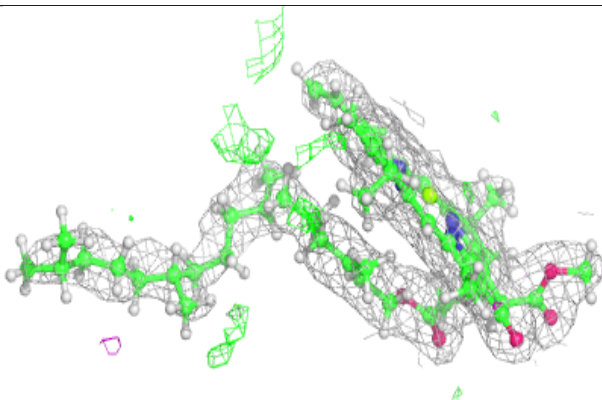
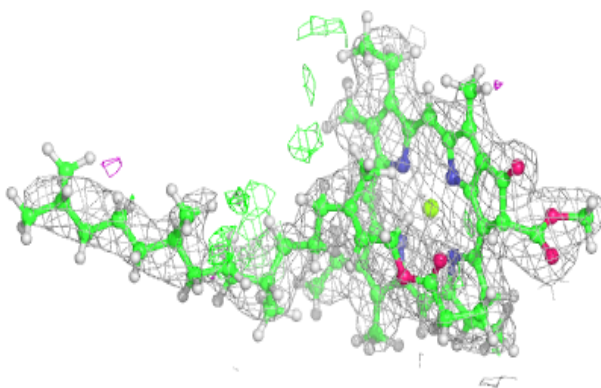


**Electron density around PL9 D 405:**

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

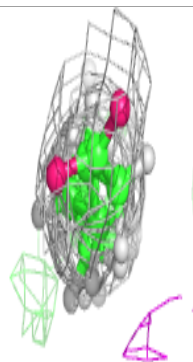
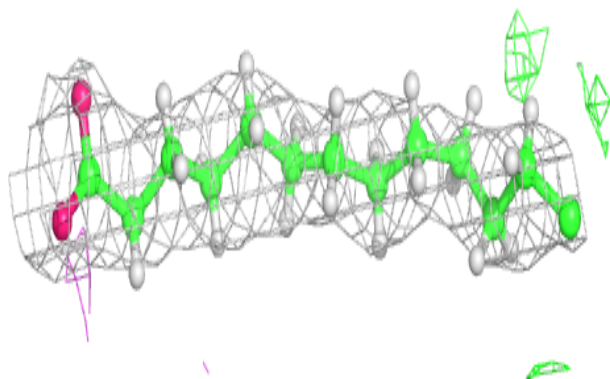
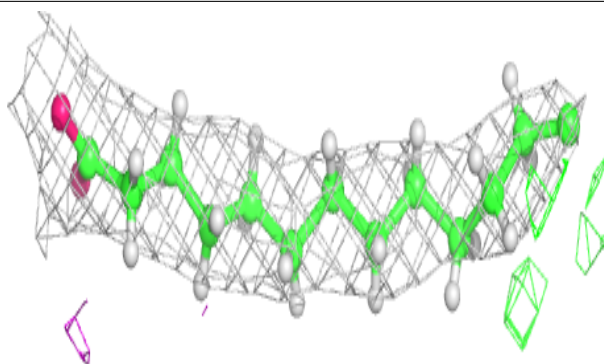
**Electron density around CLA C 505:**

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

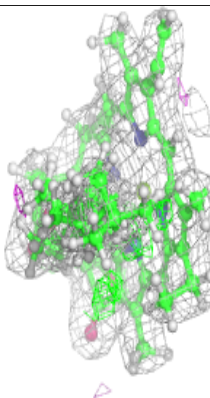
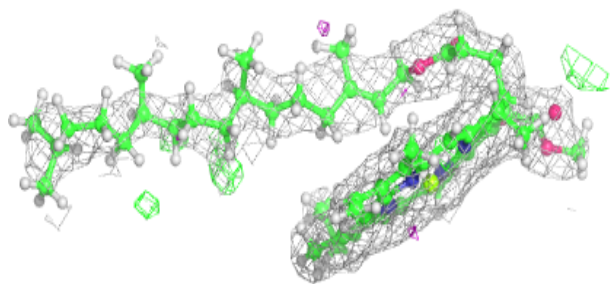
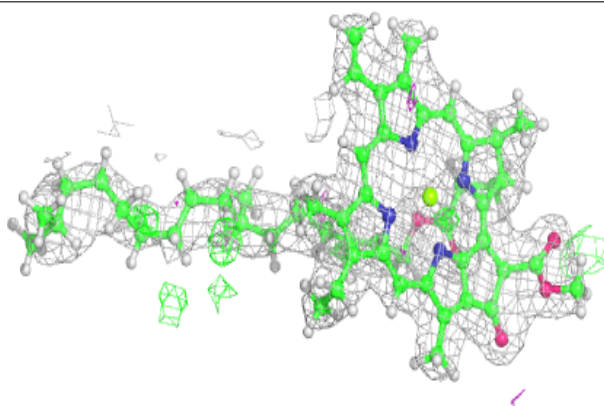


**Electron density around STE M 102:**

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

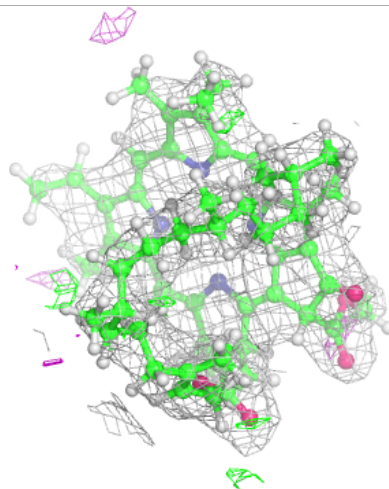
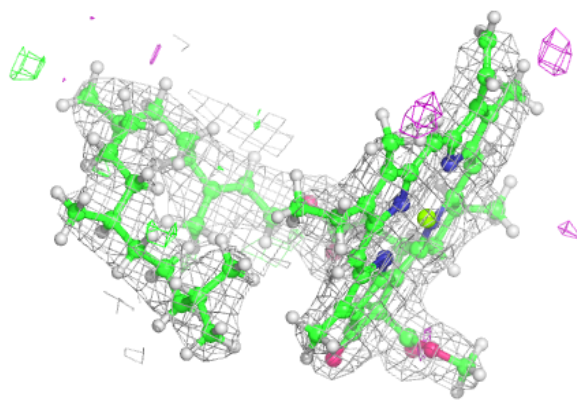
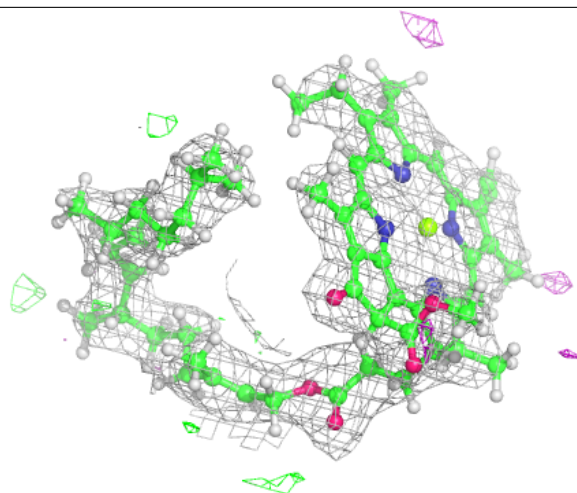
**Electron density around CLA B 614:**

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



**Electron density around CLA c 503:**

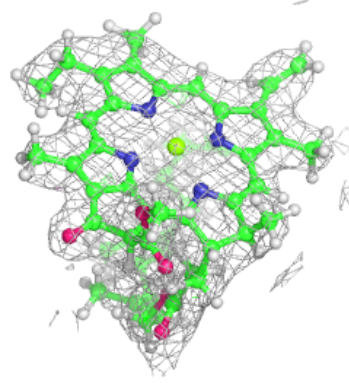
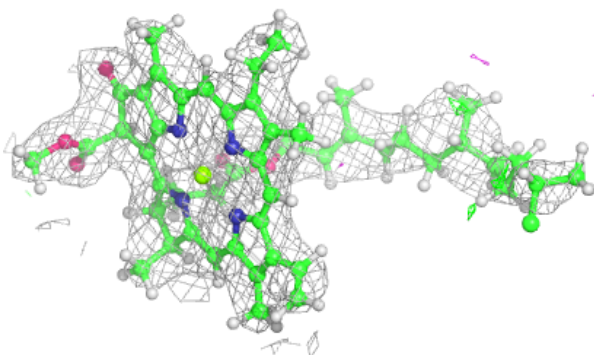
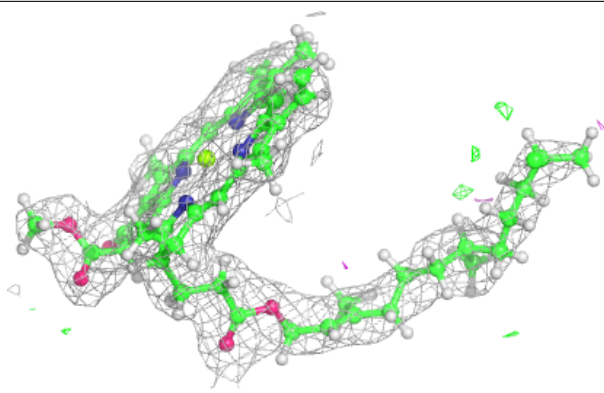
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



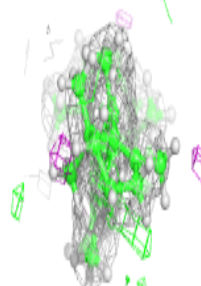
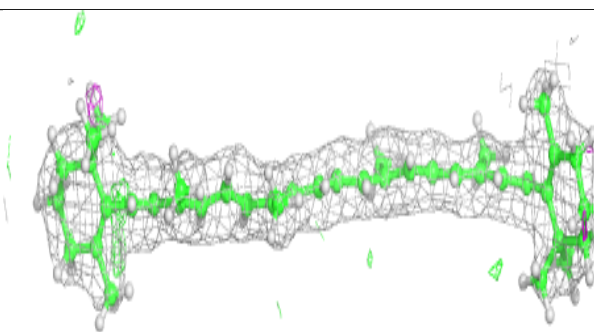
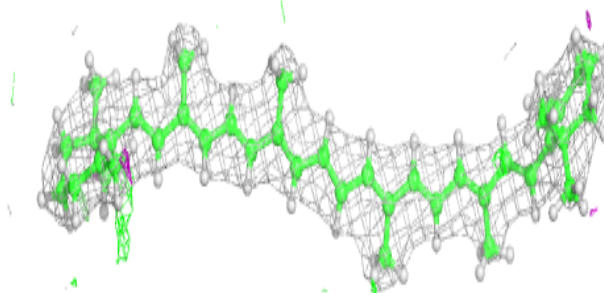


**Electron density around CLA c 504:**

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

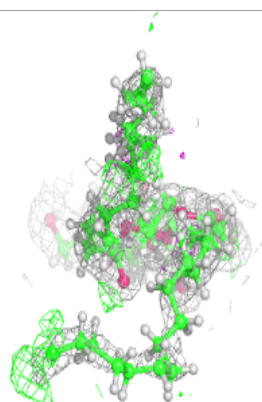
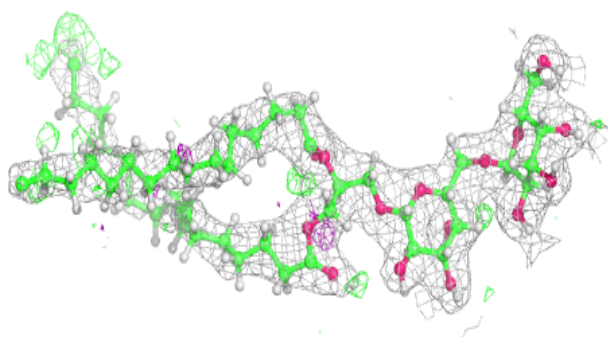
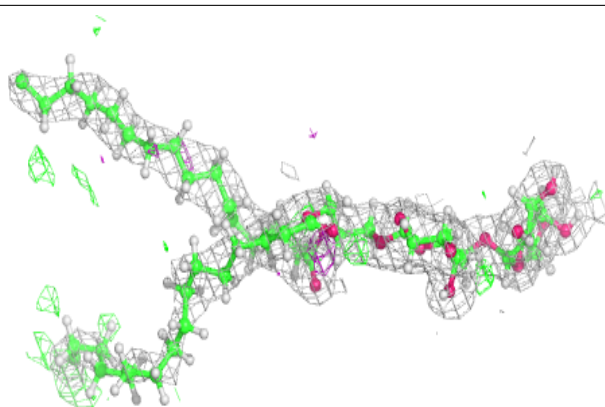
**Electron density around BCR C 515:**

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

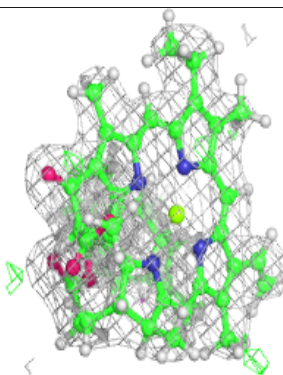
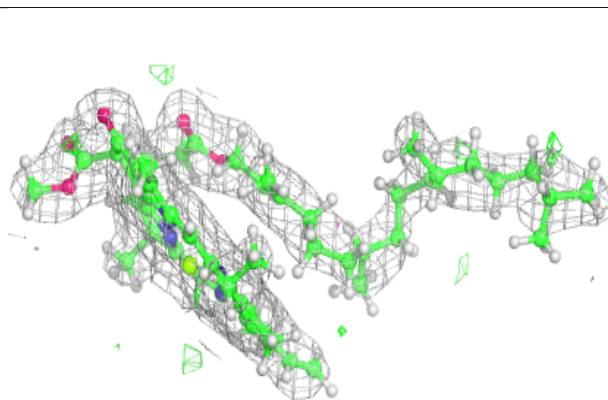
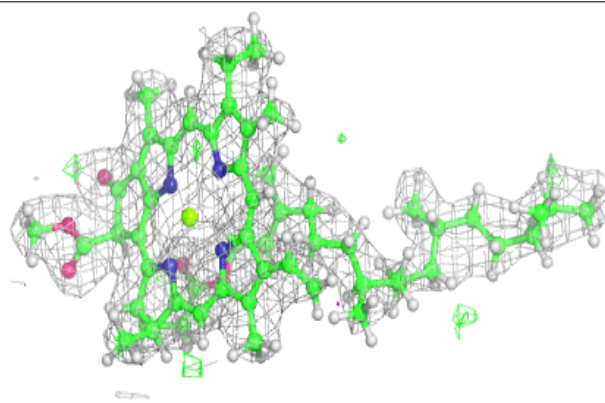


**Electron density around DGD C 516:**

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

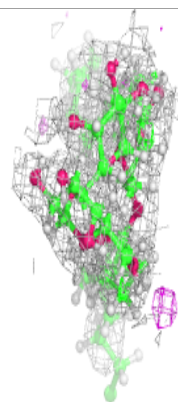
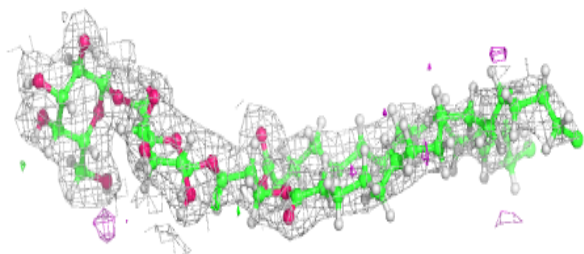
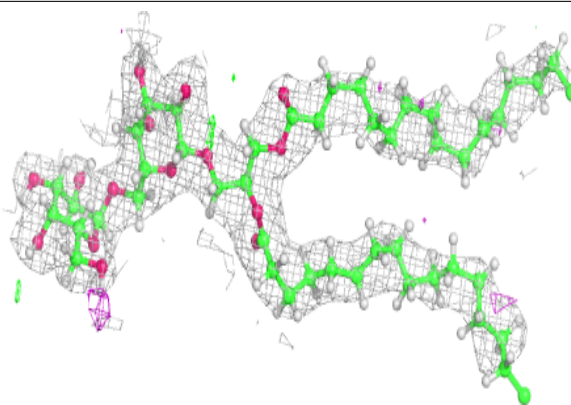
**Electron density around CLA c 505:**

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



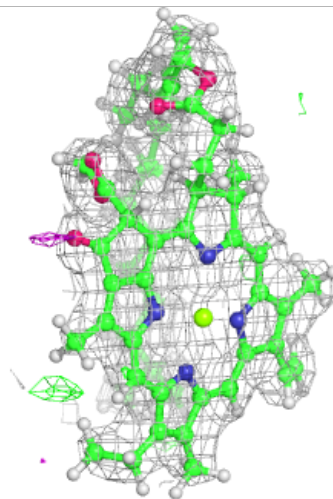
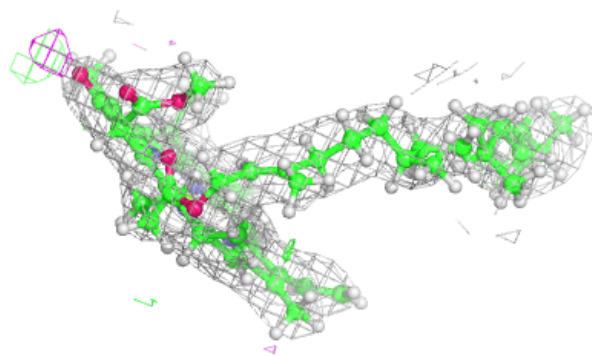
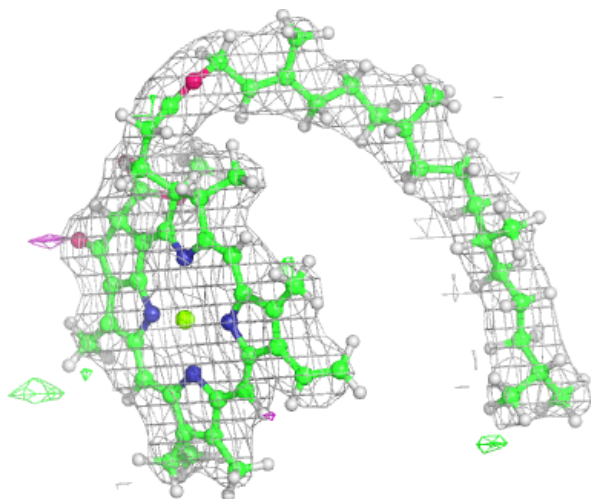
**Electron density around DGD C 518:**

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



**Electron density around CLA C 507:**

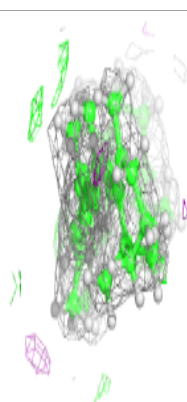
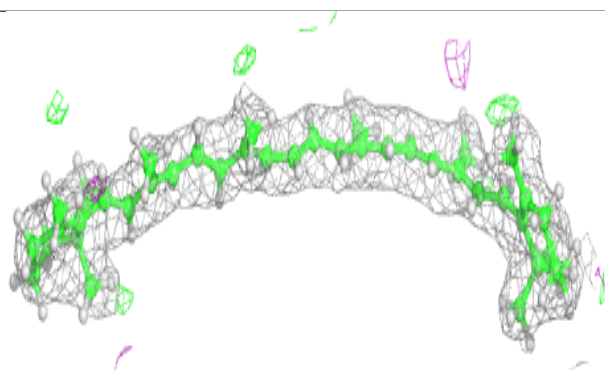
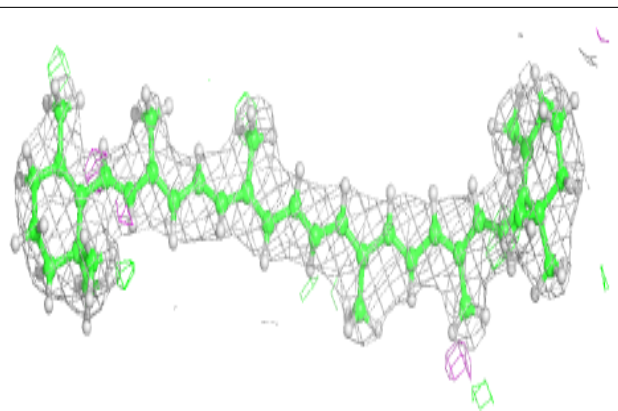
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





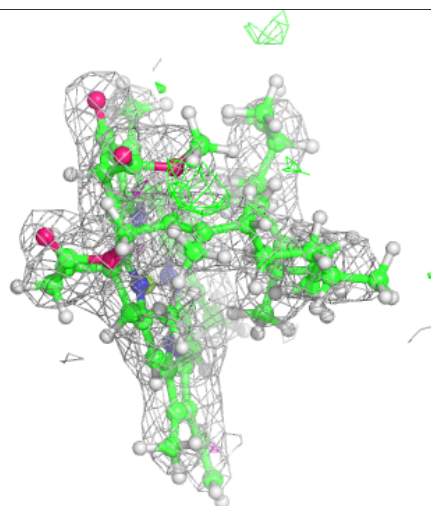
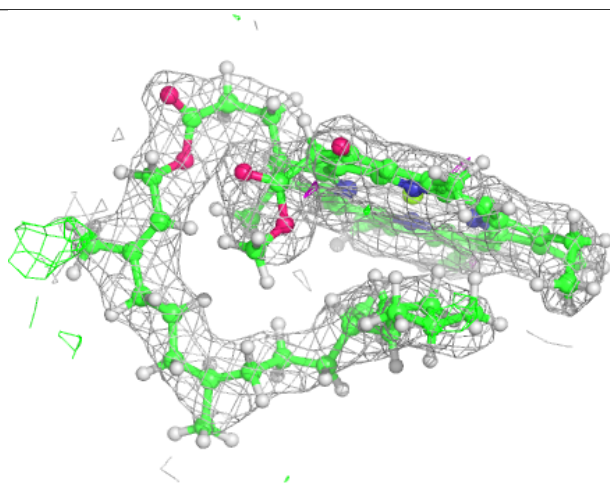
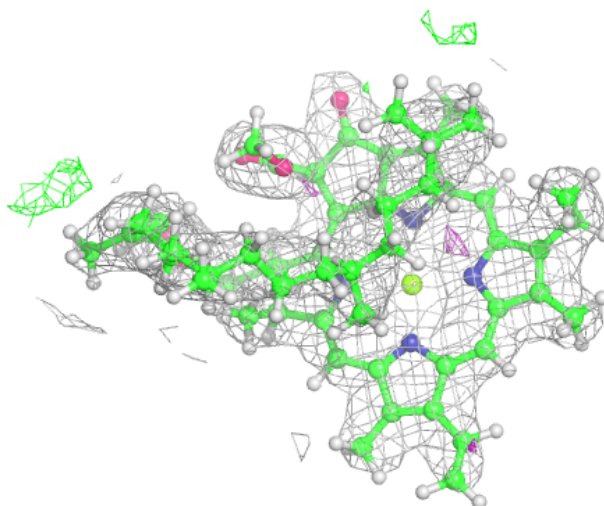
**Electron density around BCR T 101:**

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



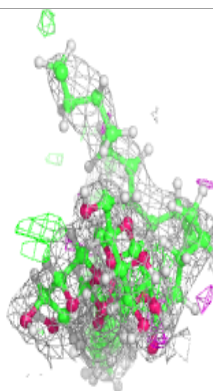
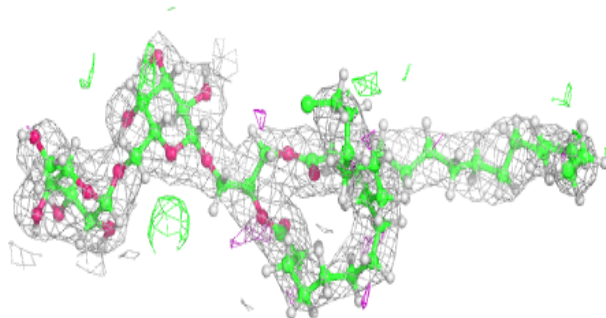
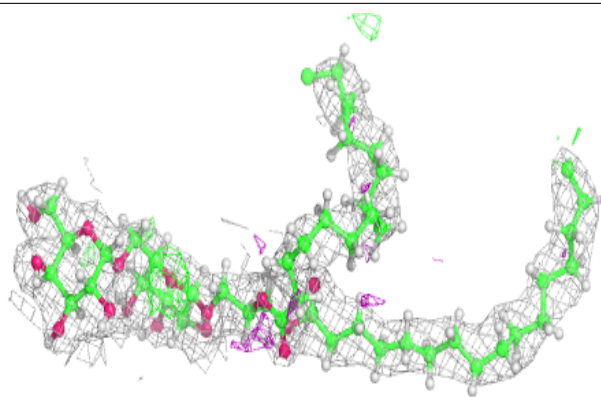
**Electron density around CLA C 510:**

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

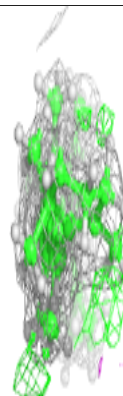
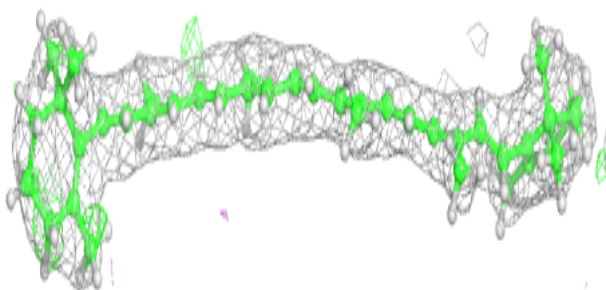
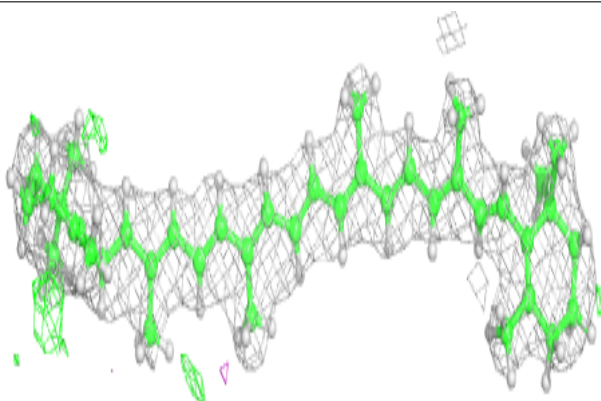


**Electron density around DGD h 101:**

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

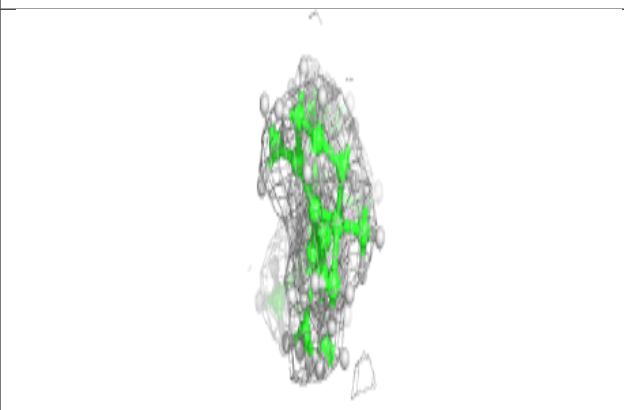
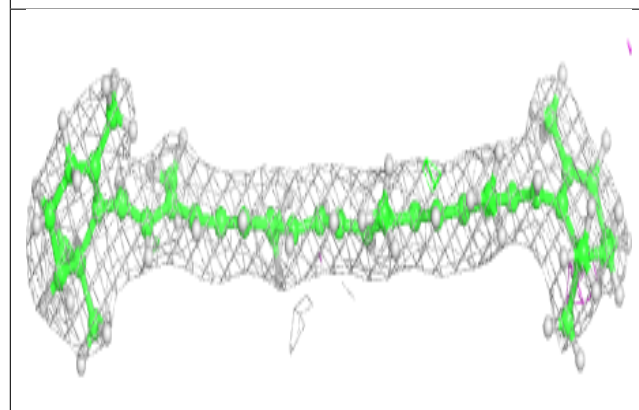
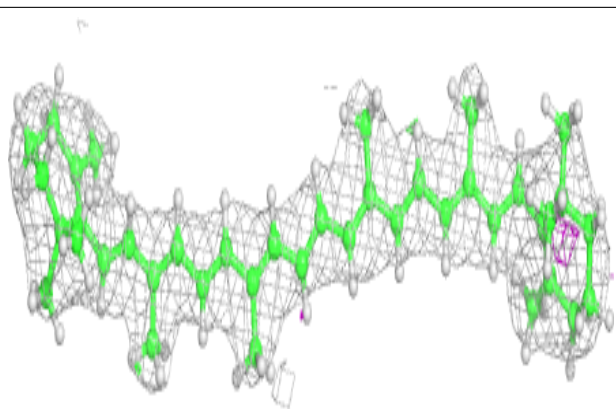
**Electron density around BCR b 617:**

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

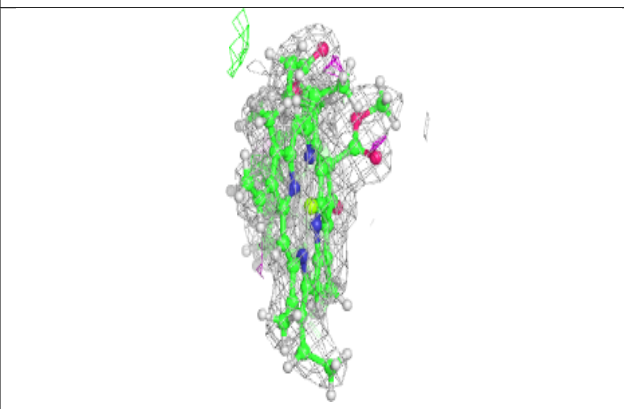
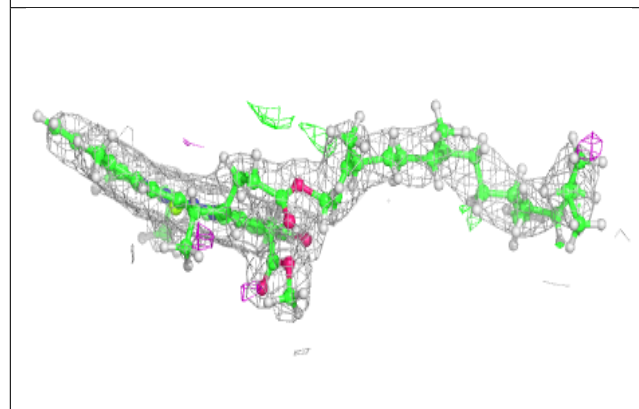
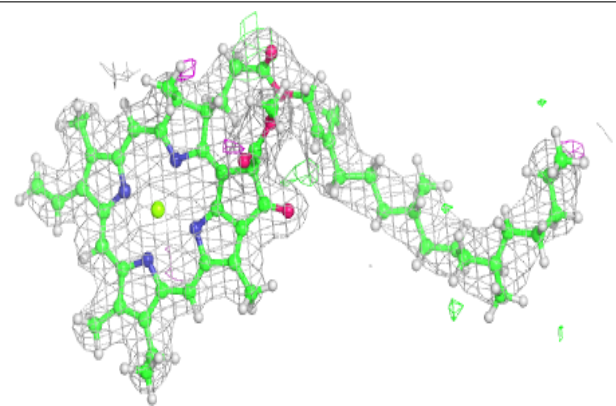


**Electron density around BCR b 618:**

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

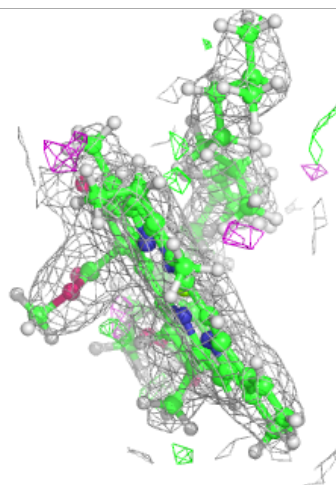
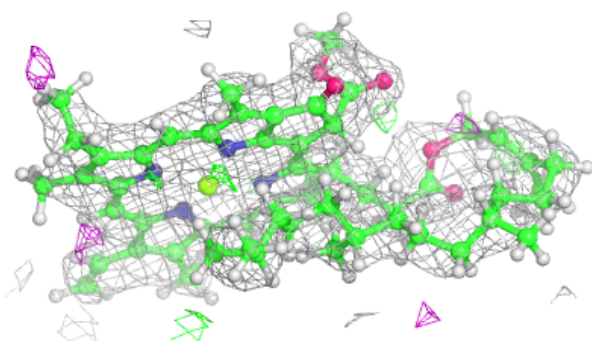
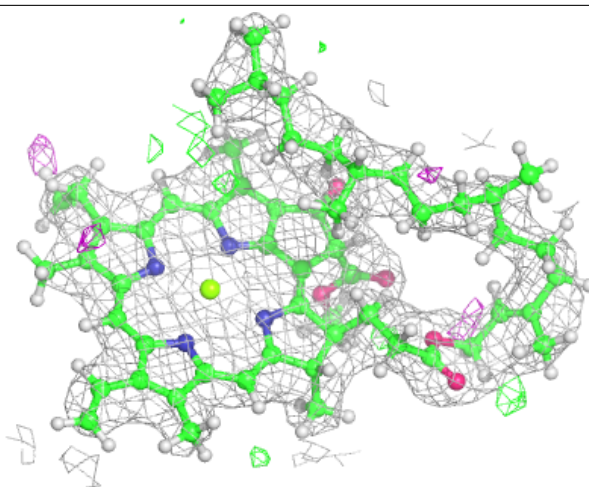
**Electron density around CLA B 602:**

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



**Electron density around CLA c 509:**

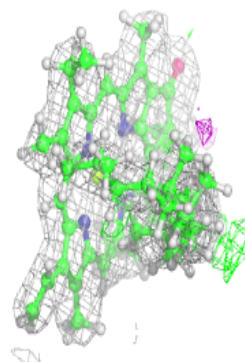
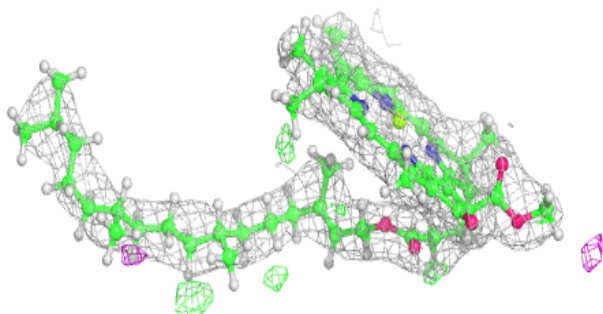
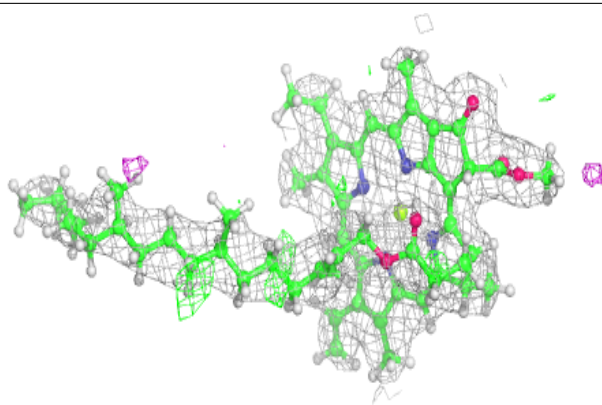
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



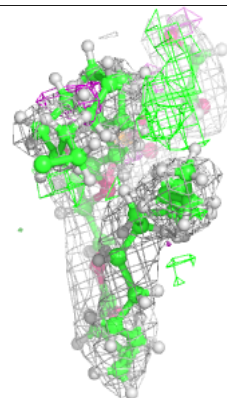
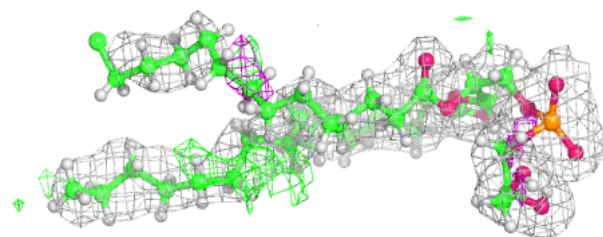
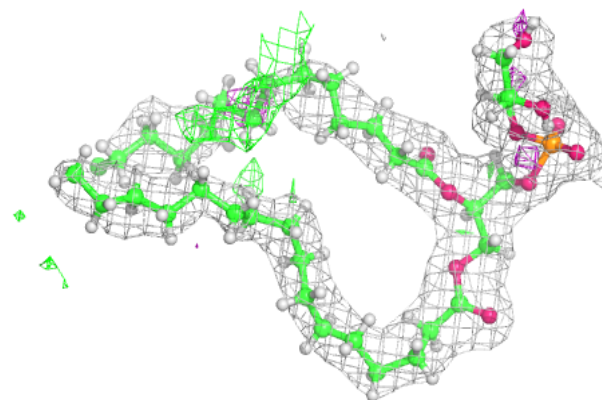


**Electron density around CLA b 608:**

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

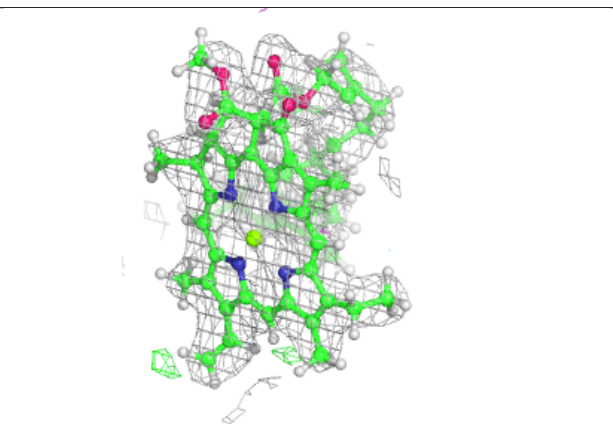
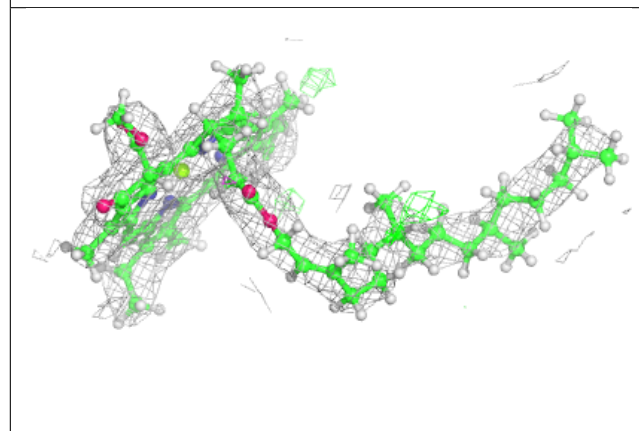
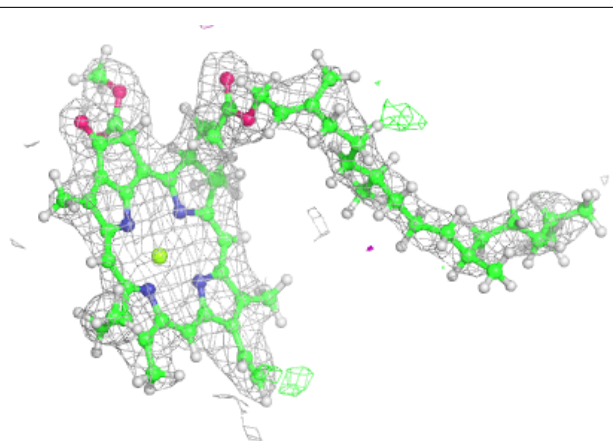
**Electron density around LHG A 615:**

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



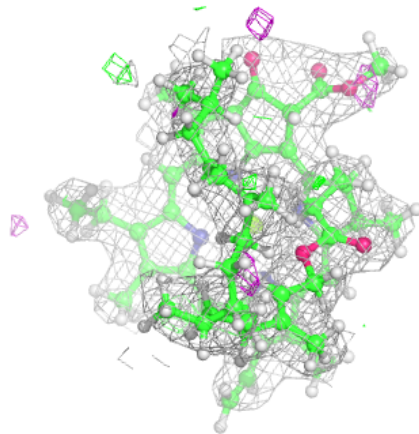
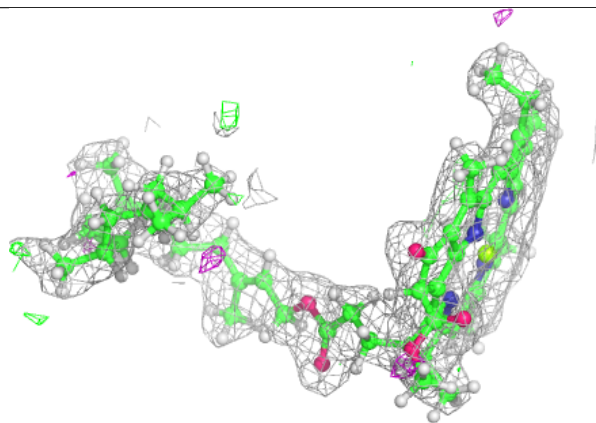
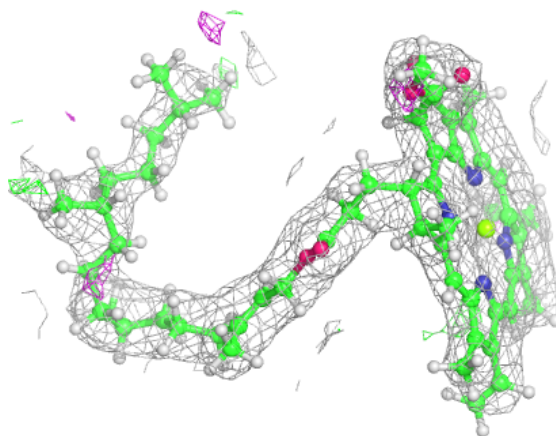
**Electron density around CLA c 511:**

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



**Electron density around CLA B 606:**

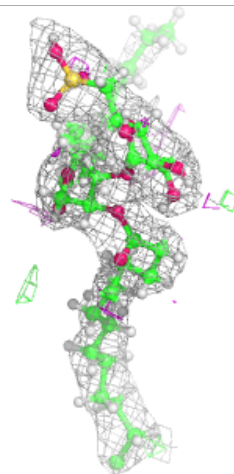
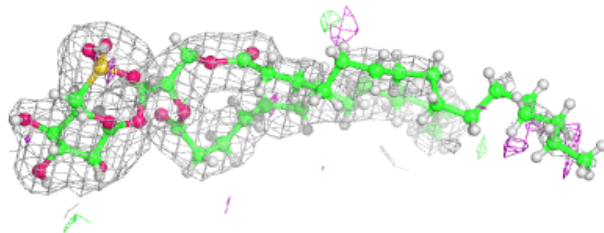
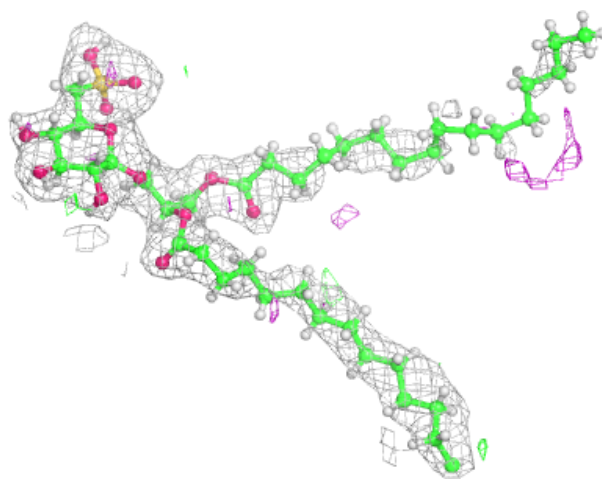
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





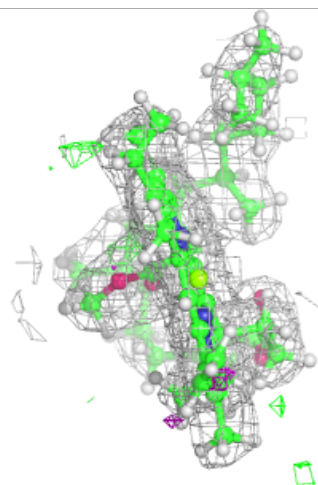
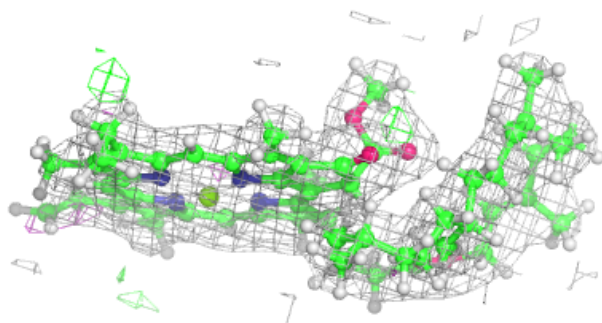
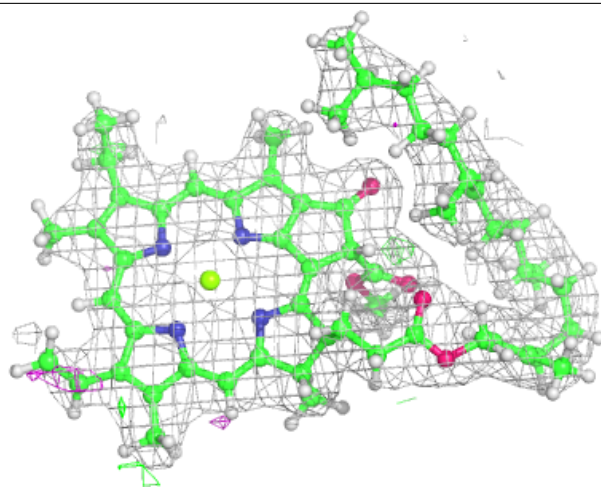
**Electron density around SQD A 616:**

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



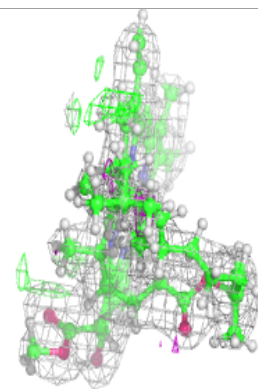
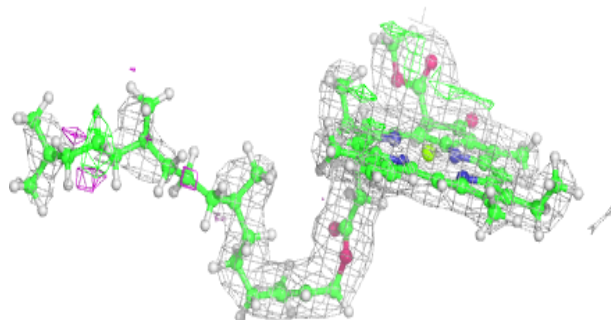
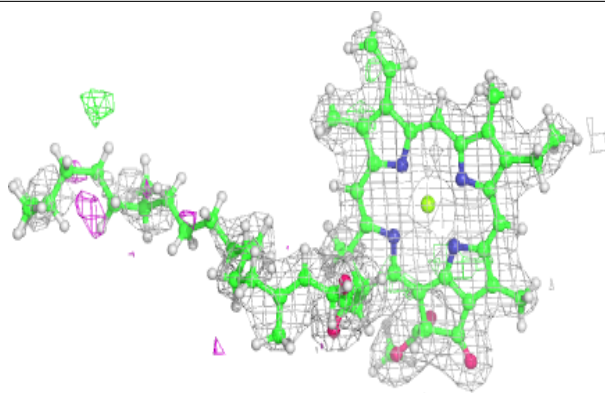
**Electron density around CLA B 610:**

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

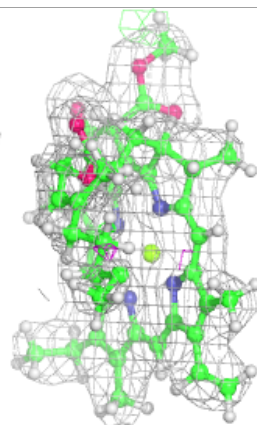
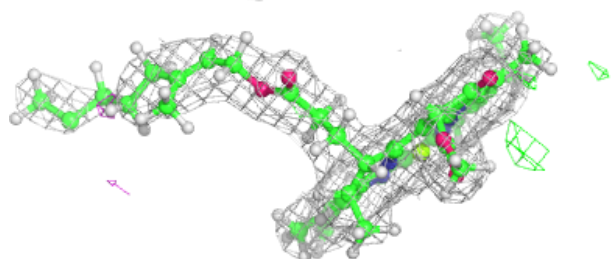
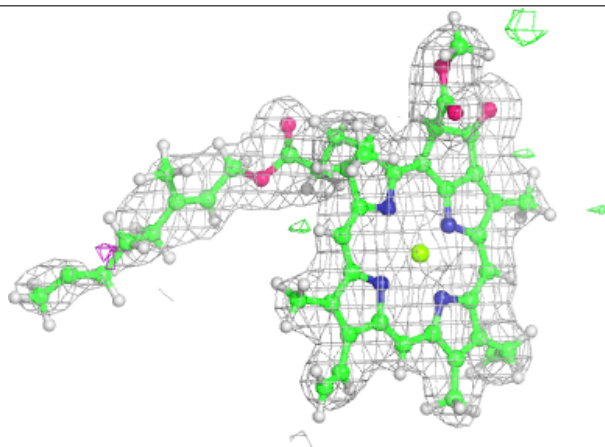


**Electron density around CLA A 605:**

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

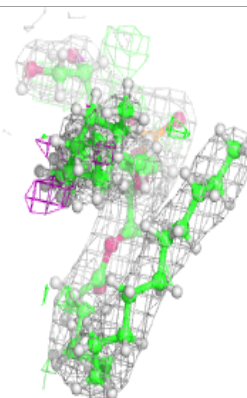
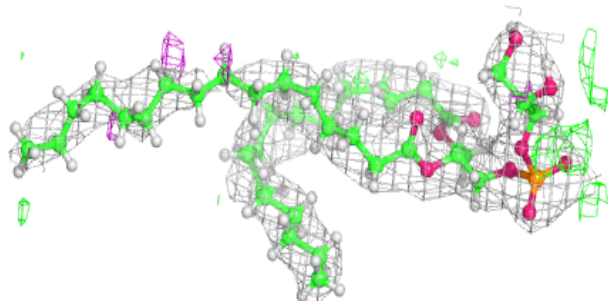
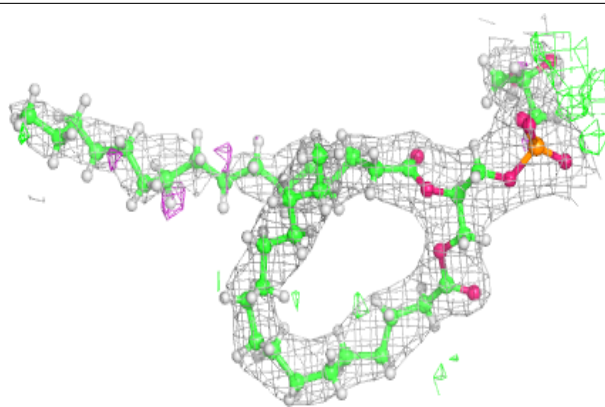
**Electron density around CLA A 608:**

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

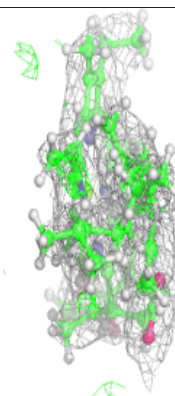
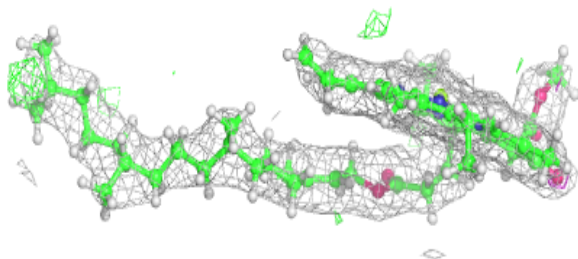
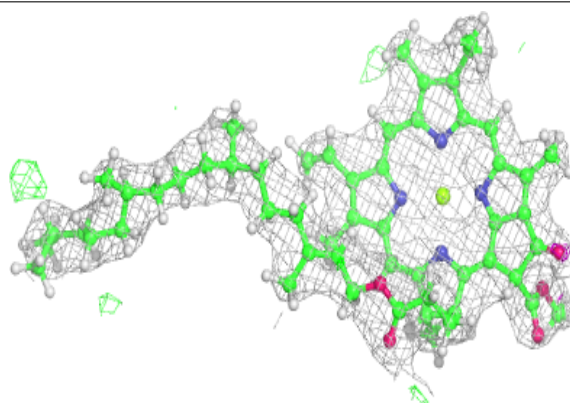


**Electron density around LHG d 407:**

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

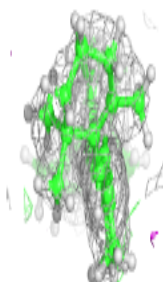
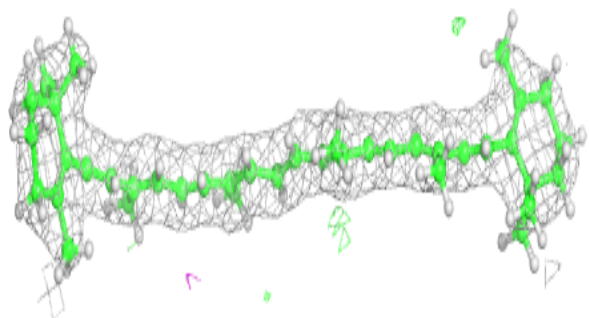
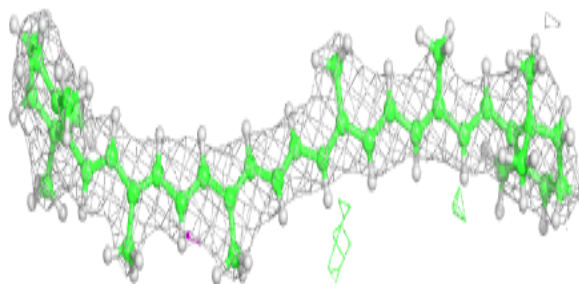
**Electron density around CLA b 603:**

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

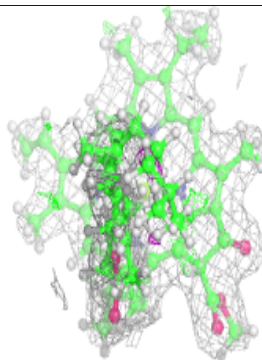
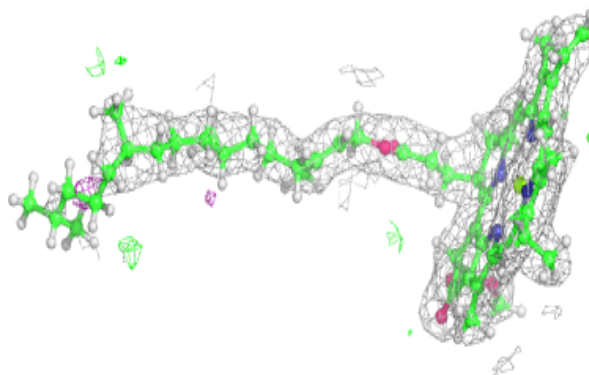
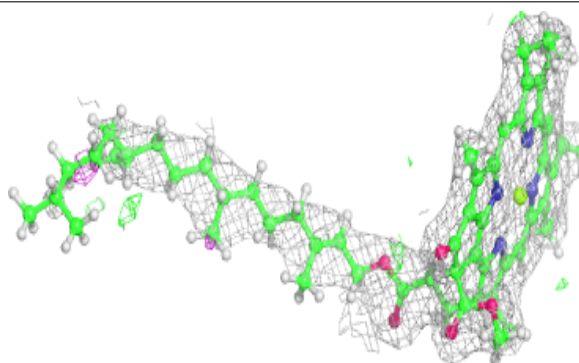


**Electron density around BCR c 515:**

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

**Electron density around CLA b 604:**

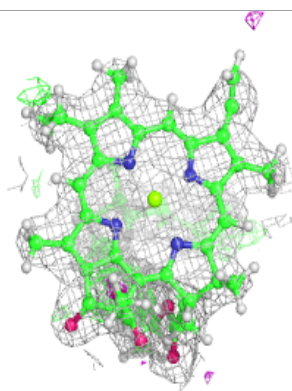
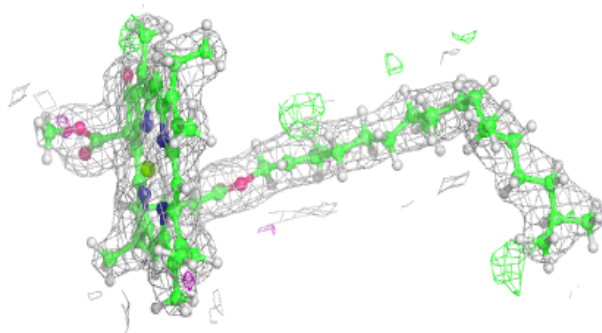
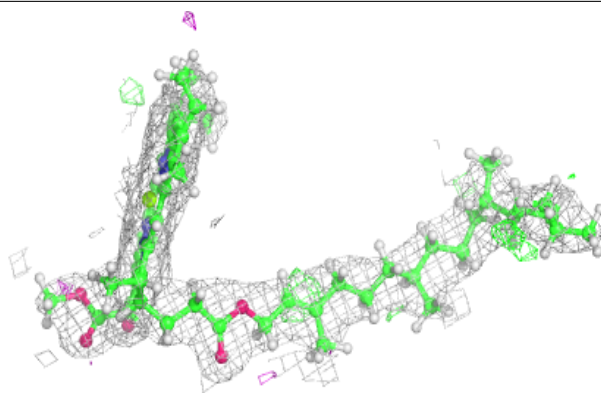
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



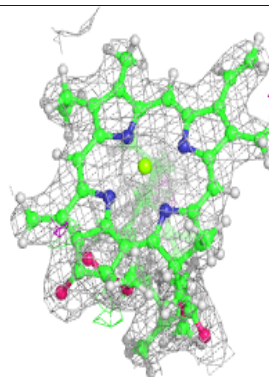
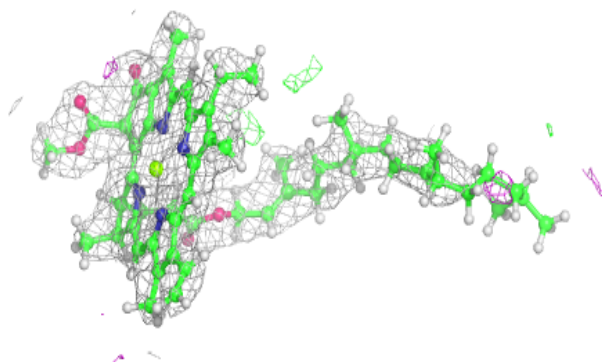
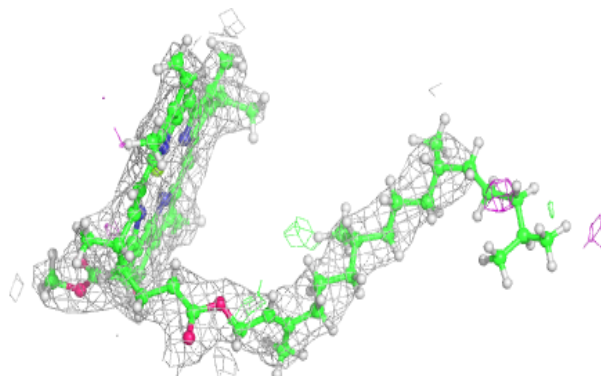


**Electron density around CLA b 605:**

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

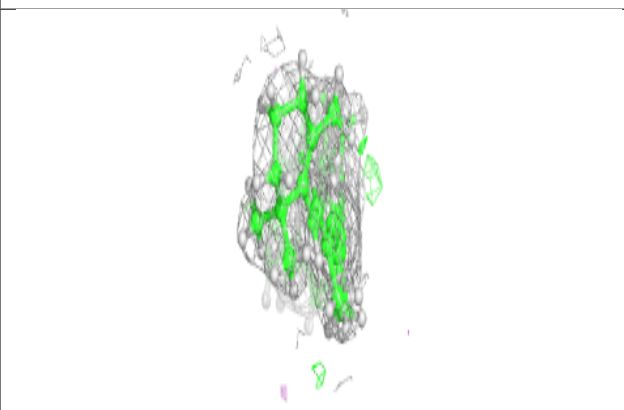
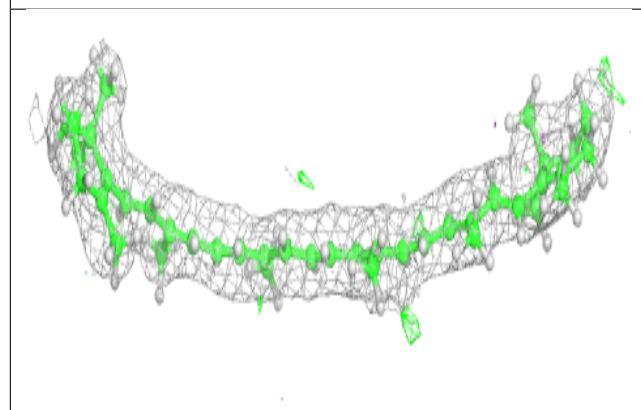
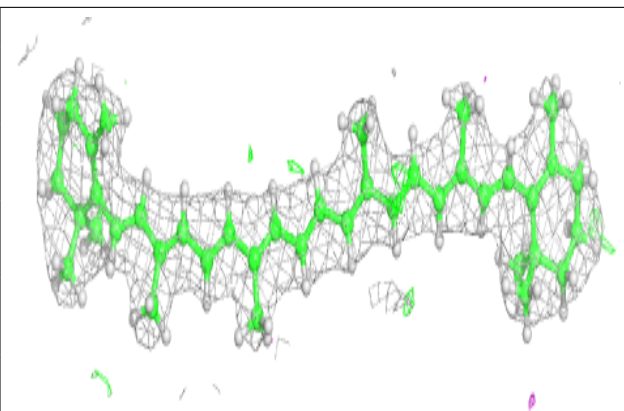
**Electron density around CLA C 508:**

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

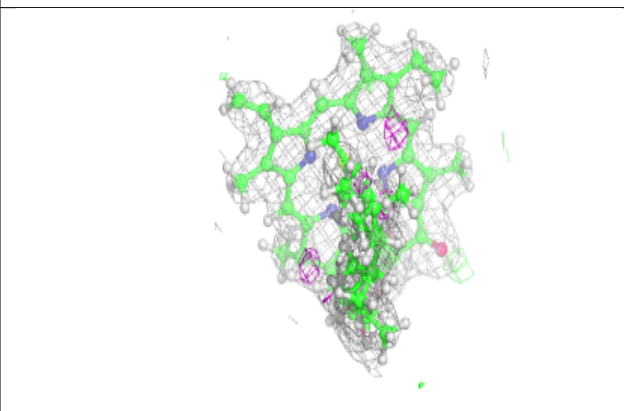
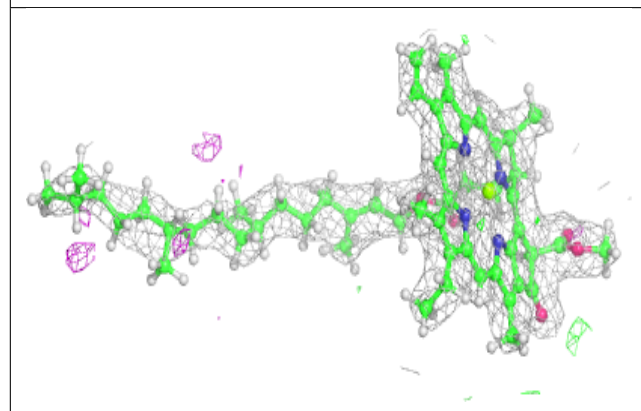
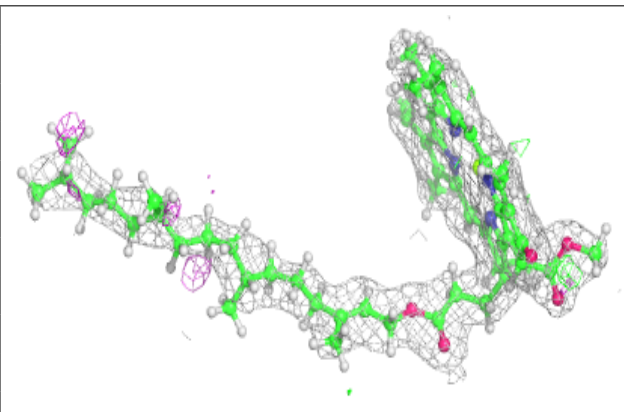


**Electron density around BCR t 101:**

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

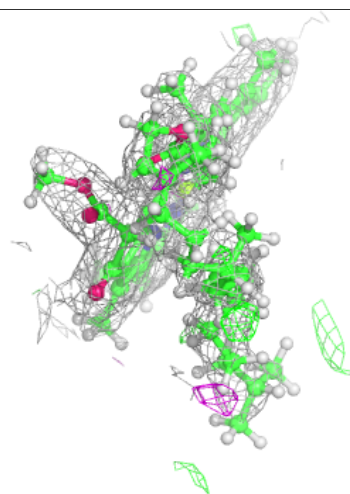
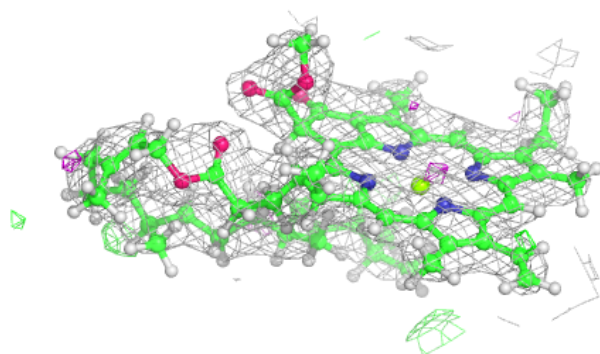
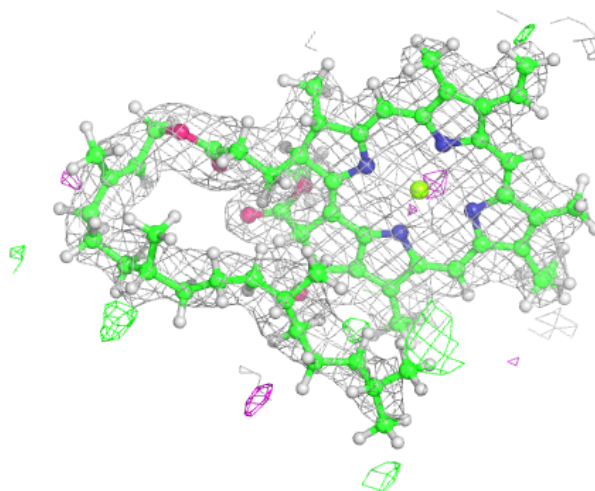
**Electron density around CLA b 607:**

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



**Electron density around CLA C 509:**

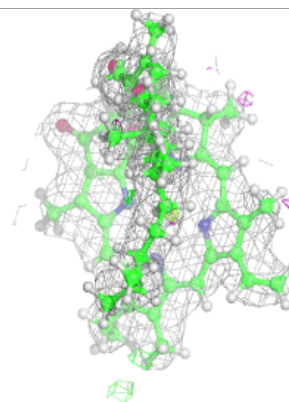
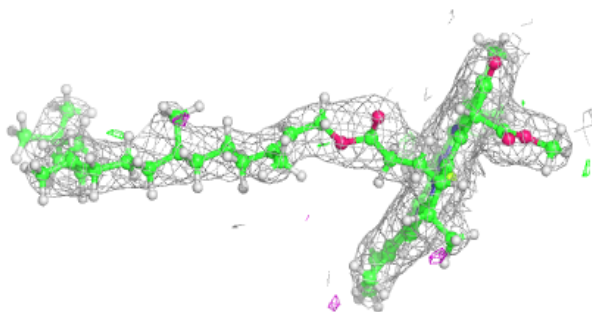
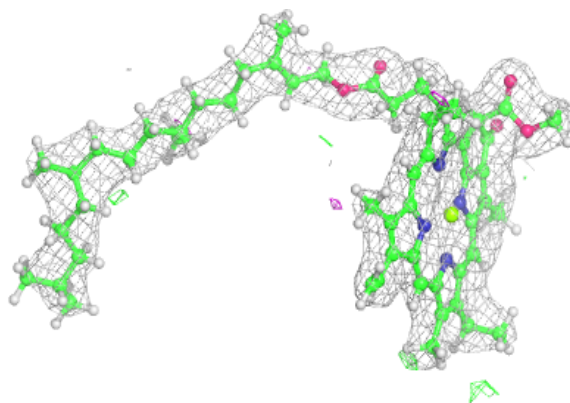
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





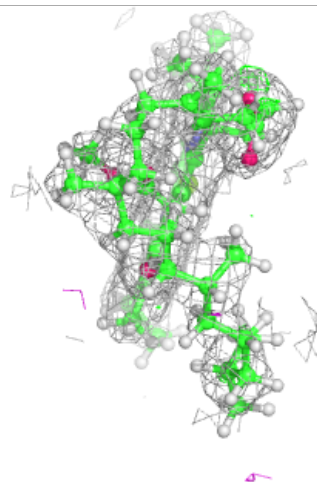
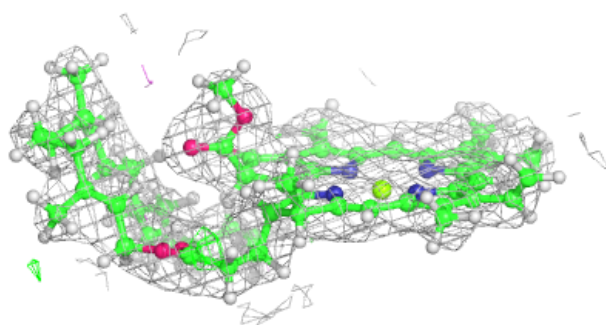
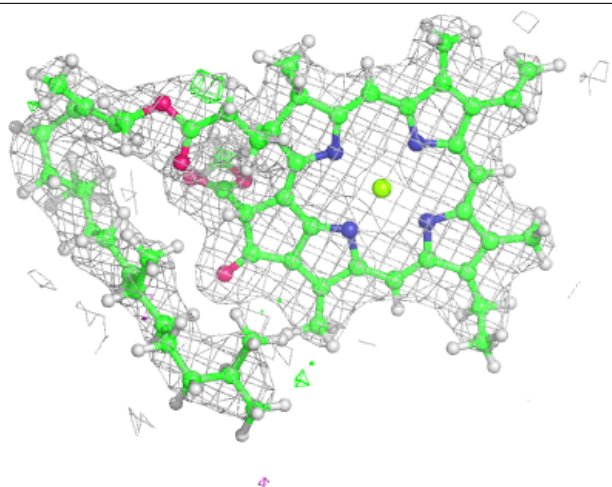
**Electron density around CLA B 609:**

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



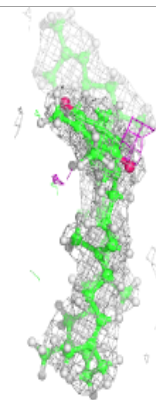
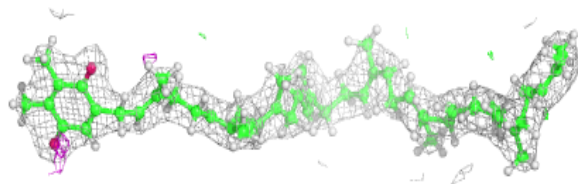
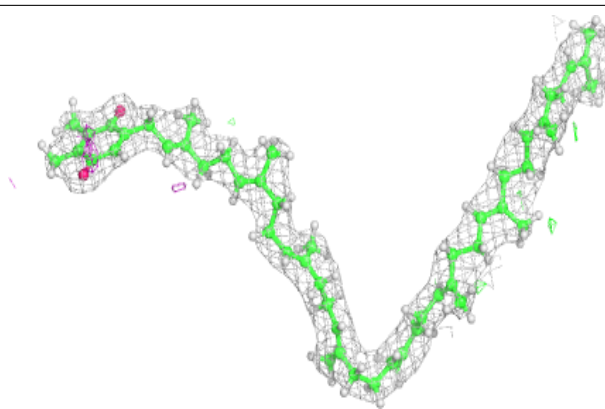
**Electron density around CLA b 610:**

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



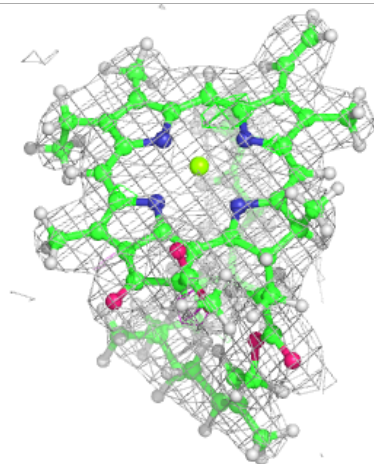
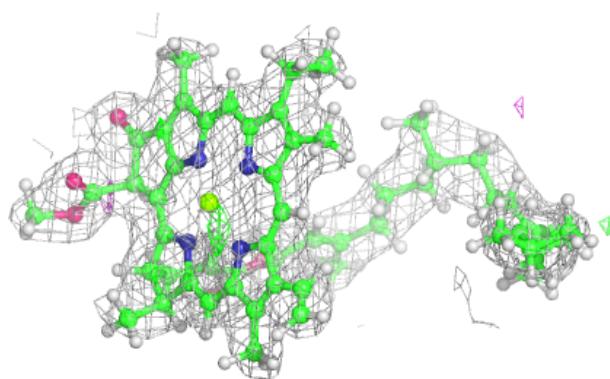
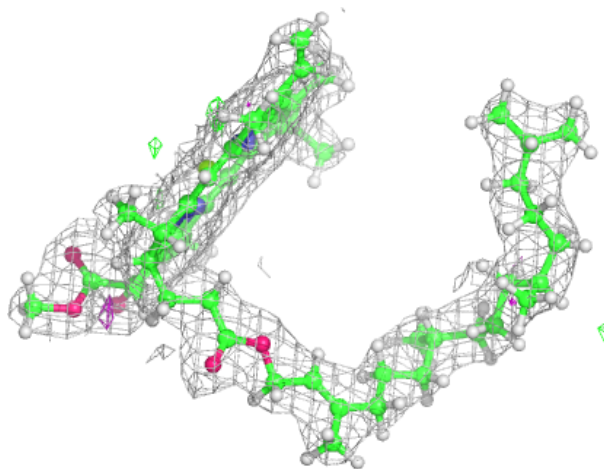
**Electron density around PL9 d 406:**

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



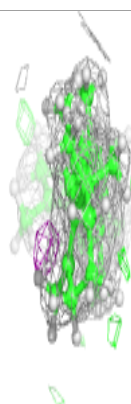
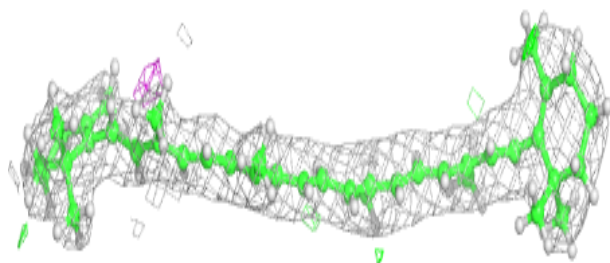
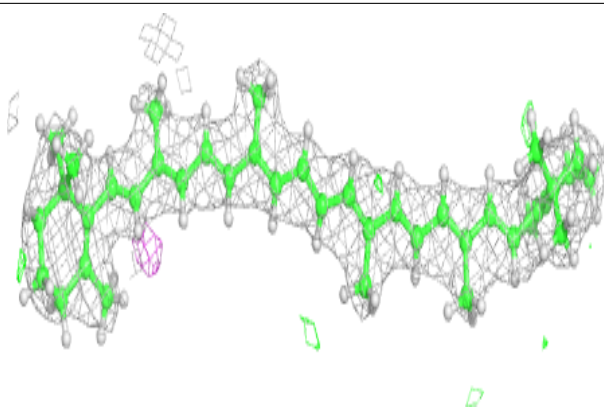
**Electron density around CLA b 611:**

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

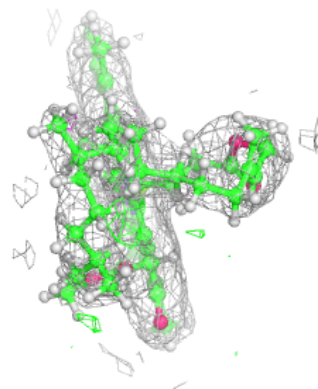
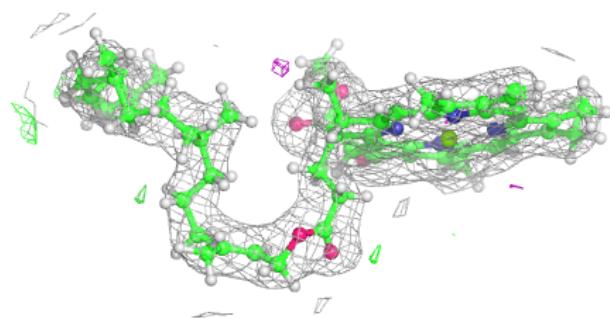
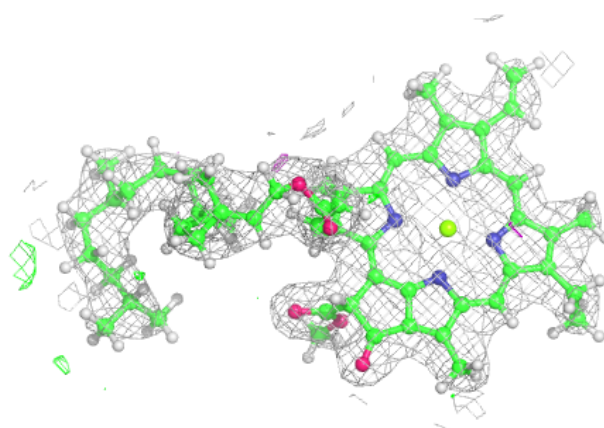


**Electron density around BCR B 617:**

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

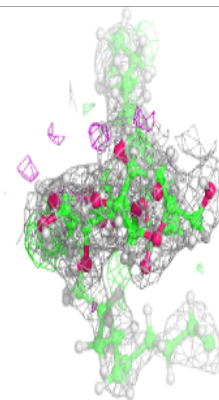
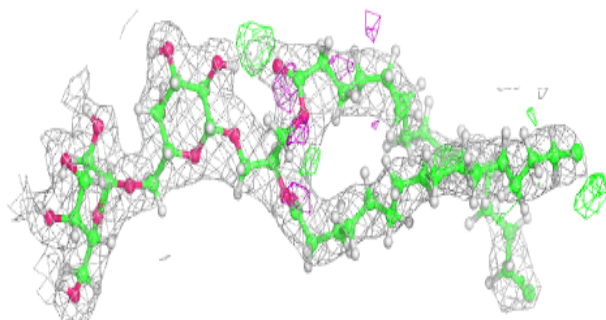
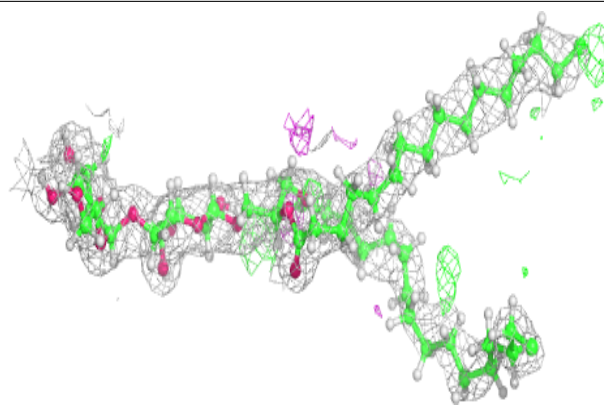
**Electron density around CLA b 612:**

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



**Electron density around DGD c 516:**

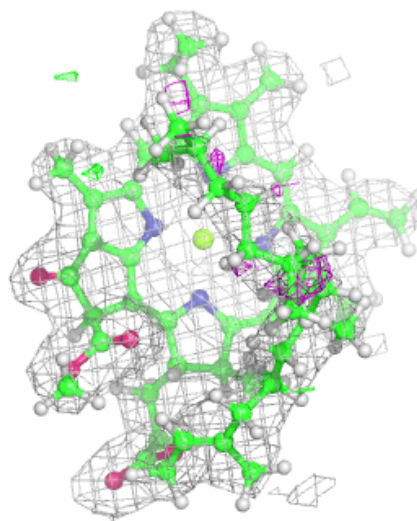
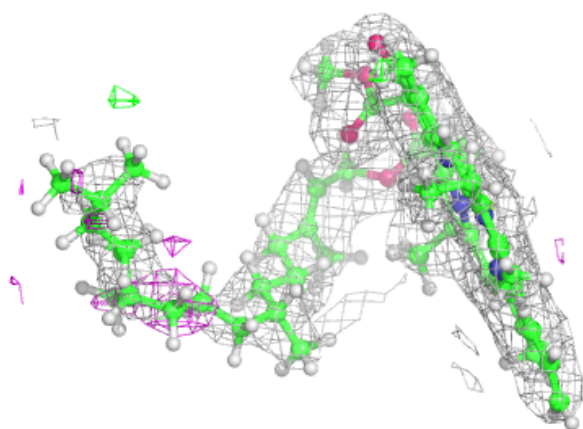
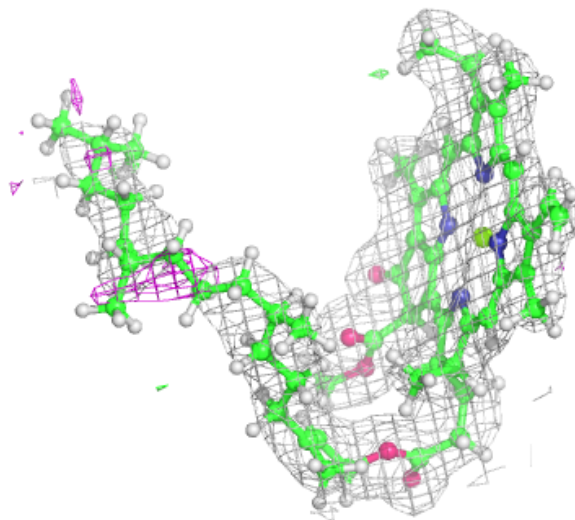
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





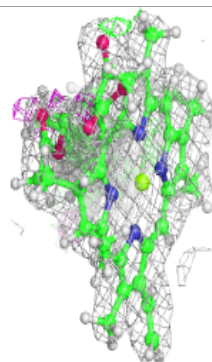
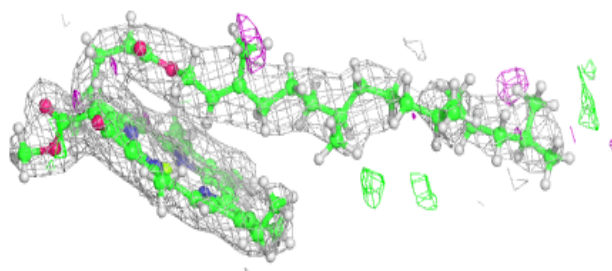
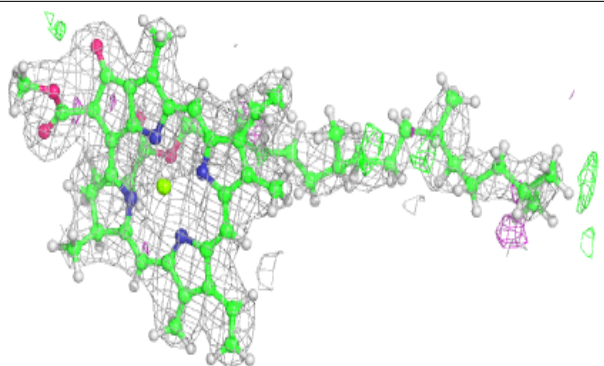
**Electron density around CLA b 613:**

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

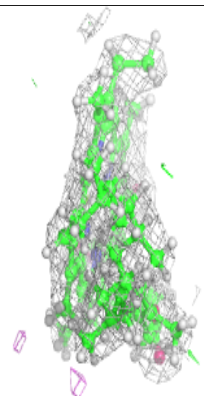
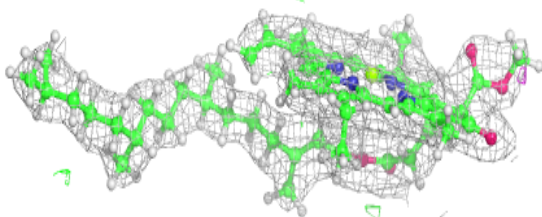
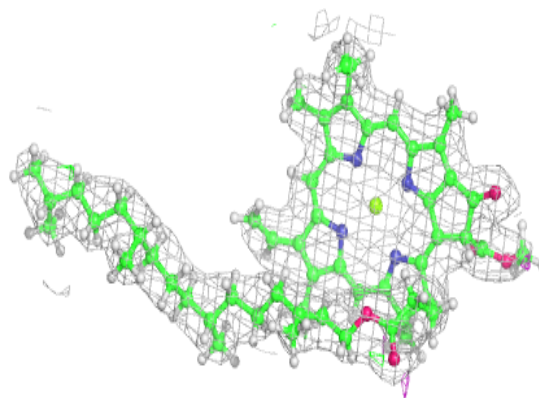


**Electron density around CLA b 614:**

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

**Electron density around CLA C 501:**

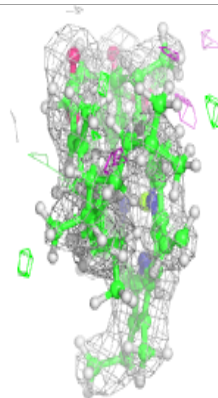
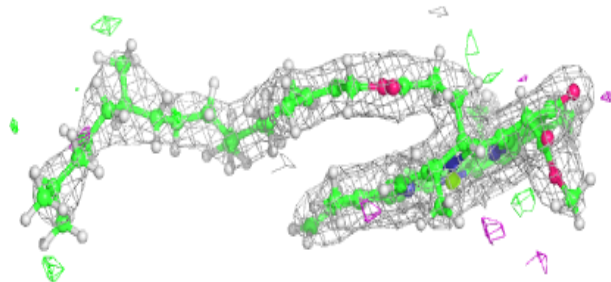
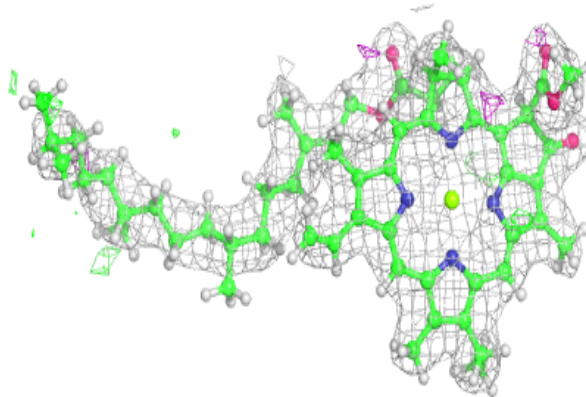
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



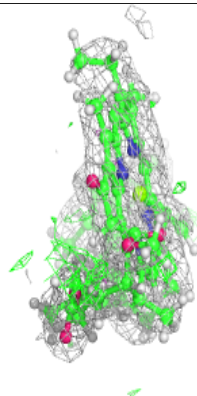
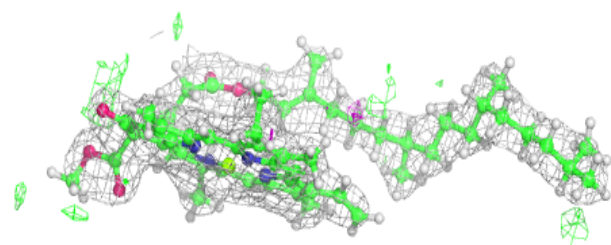
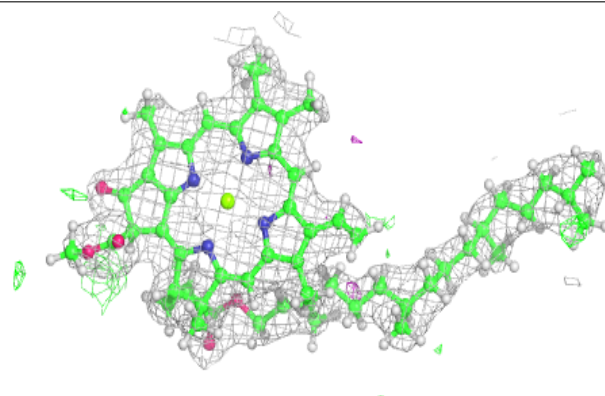


**Electron density around CLA B 603:**

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

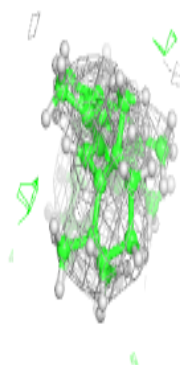
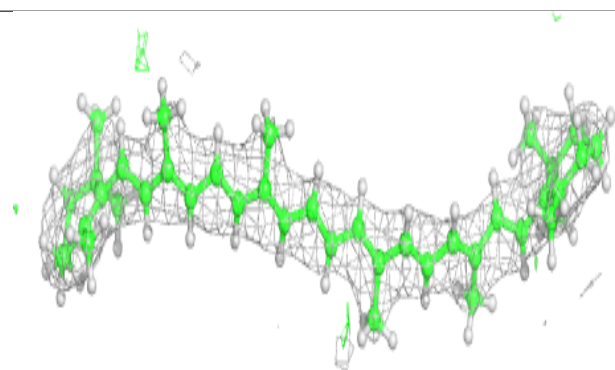
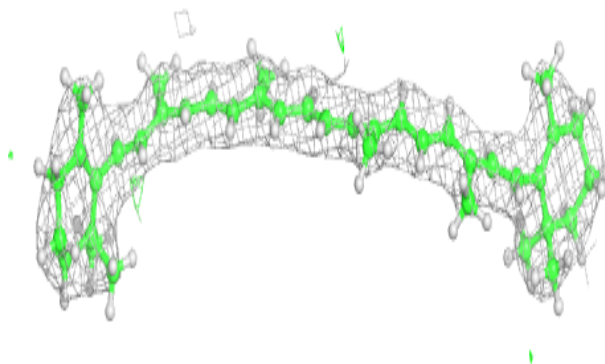
**Electron density around CLA c 501:**

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



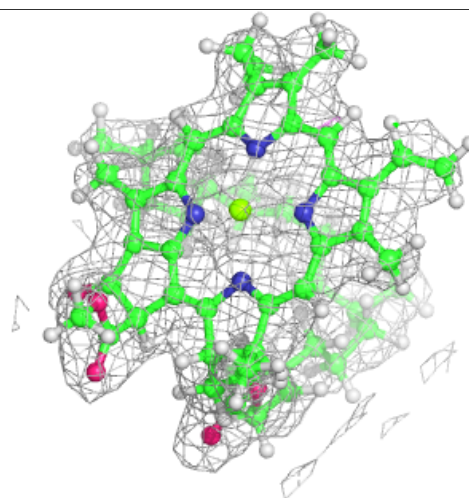
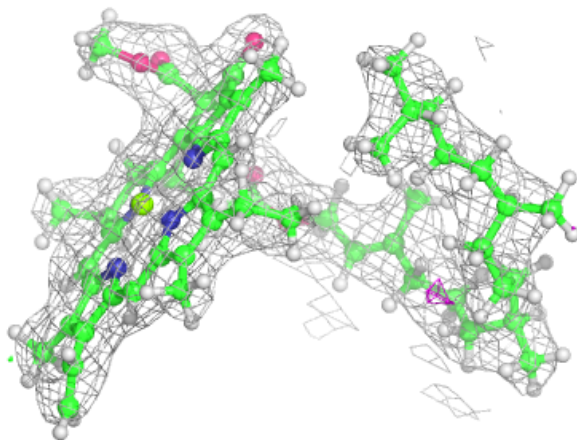
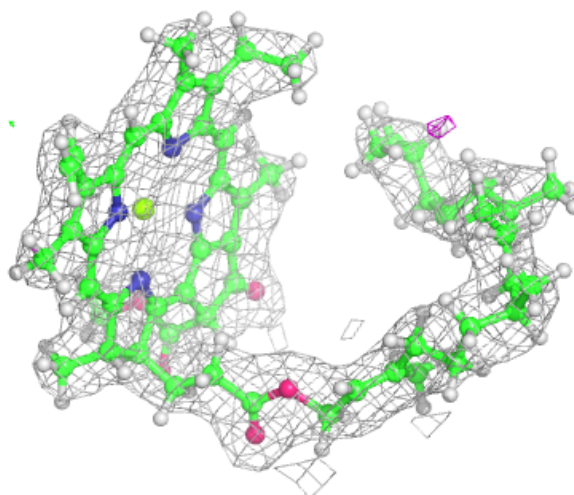
**Electron density around BCR K 101:**

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



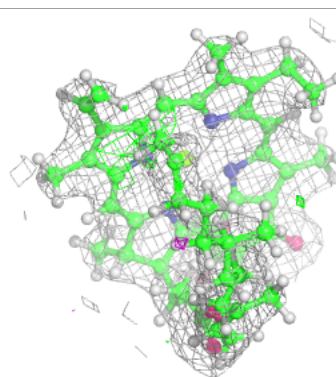
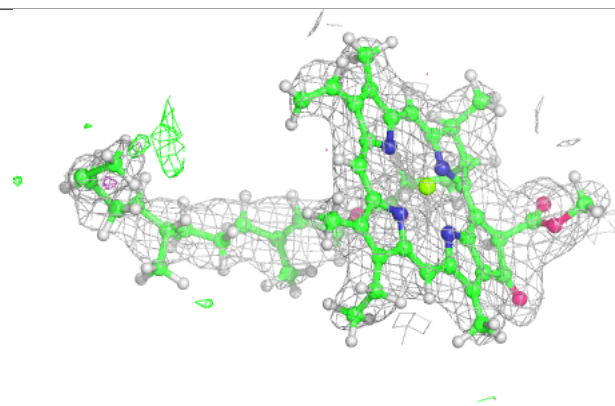
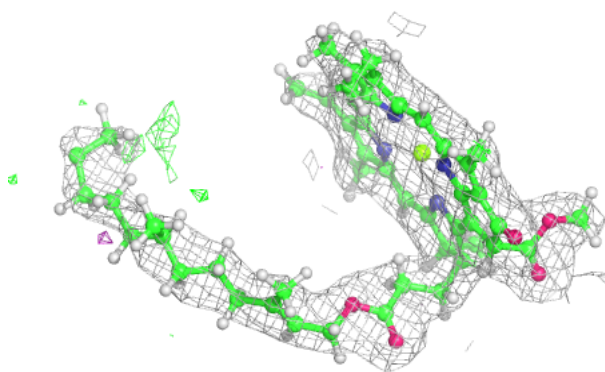
**Electron density around CLA C 503:**

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

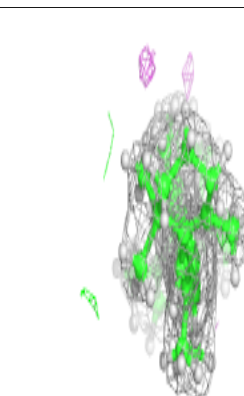
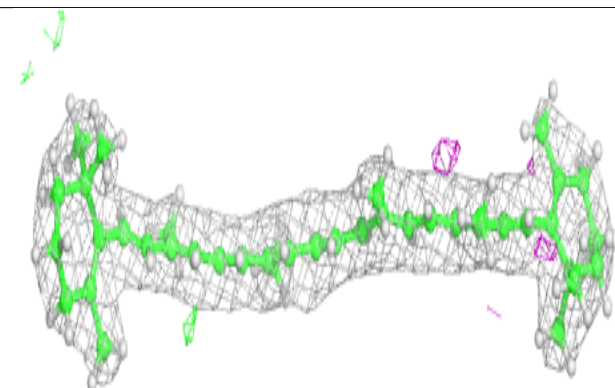
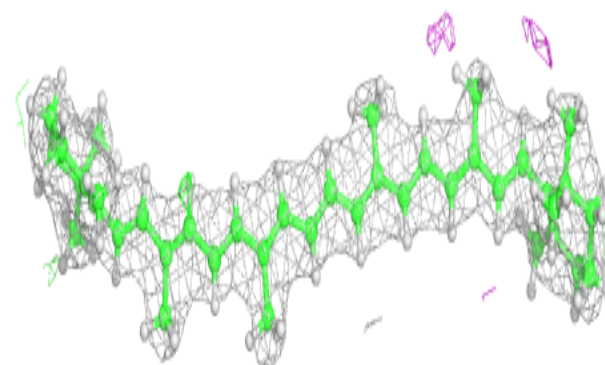


**Electron density around CLA C 504:**

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

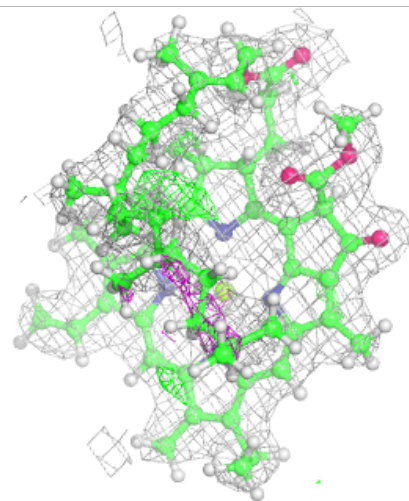
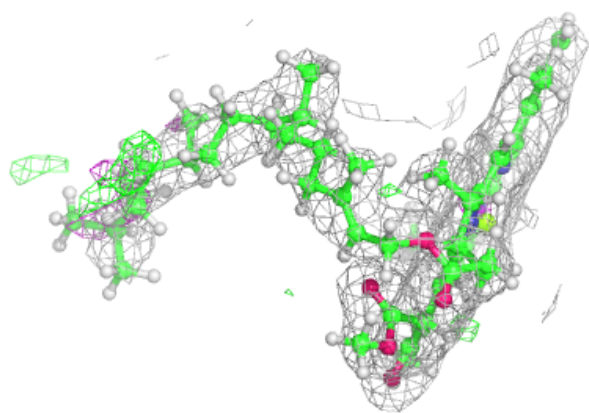
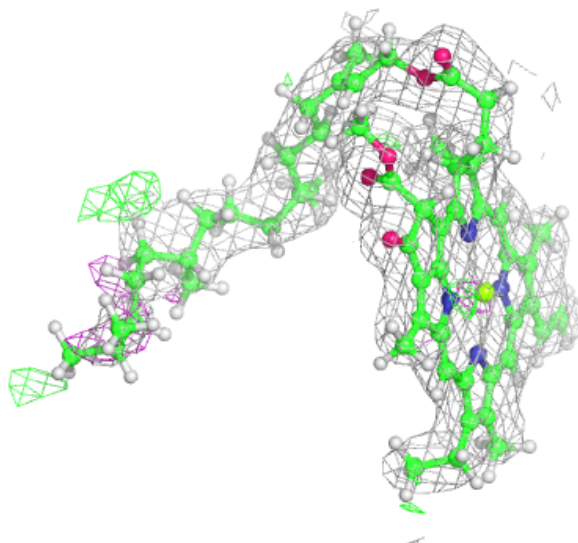
**Electron density around BCR a 607:**

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



**Electron density around CLA B 613:**

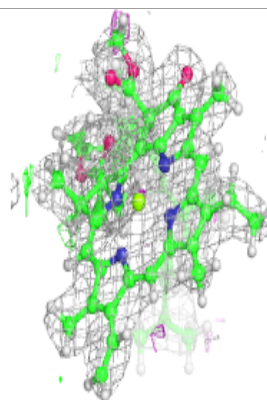
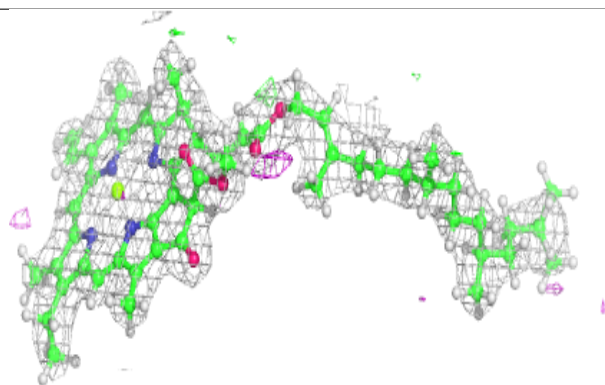
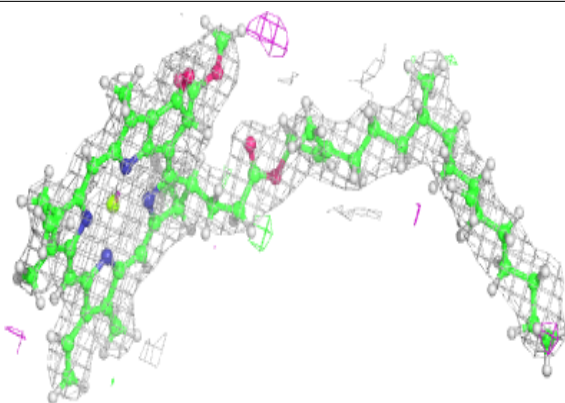
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





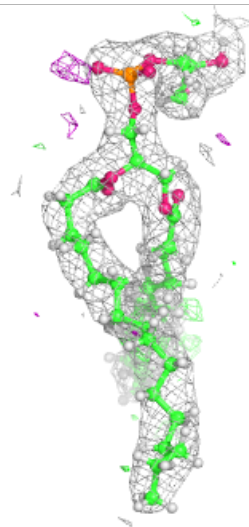
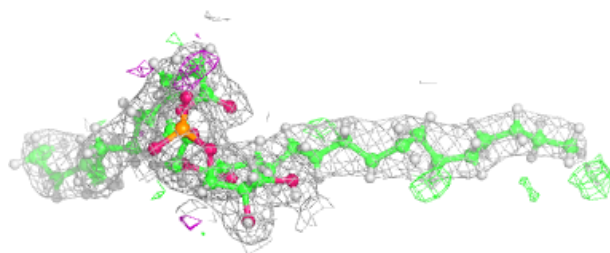
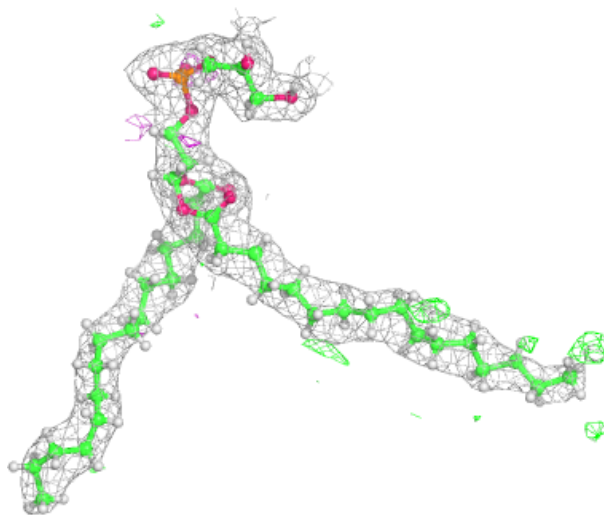
**Electron density around CLA a 604:**

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



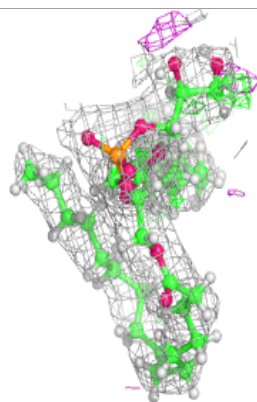
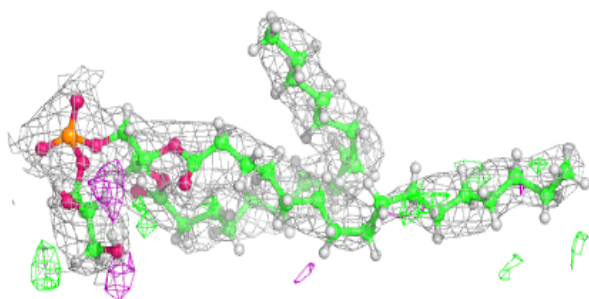
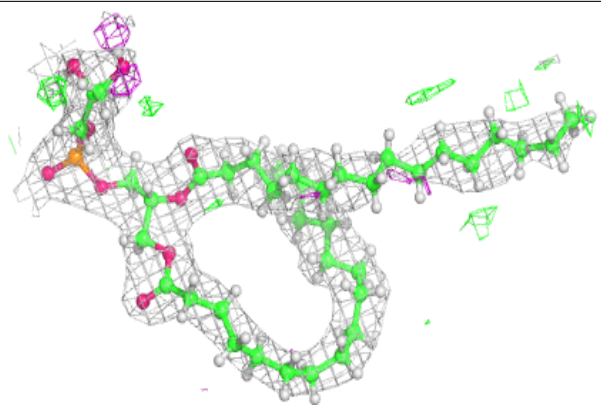
**Electron density around LHG B 621:**

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

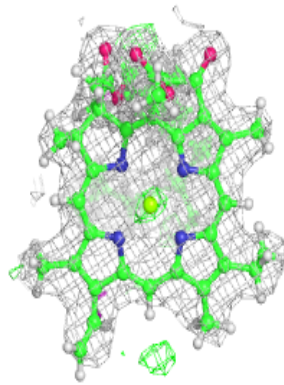
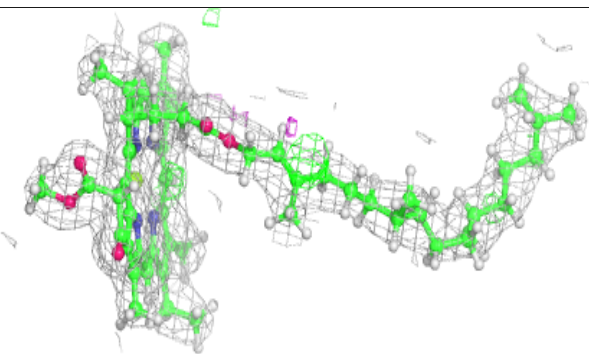
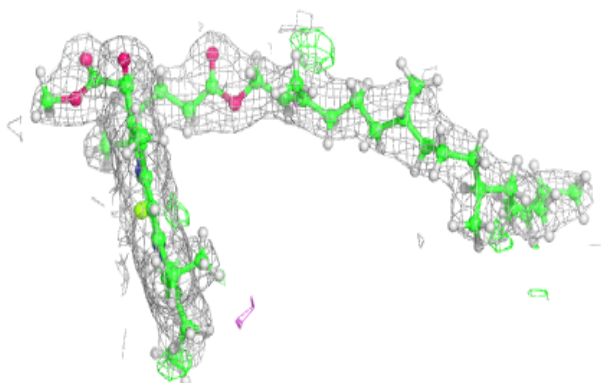


**Electron density around LHG B 622:**

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

**Electron density around CLA B 605:**

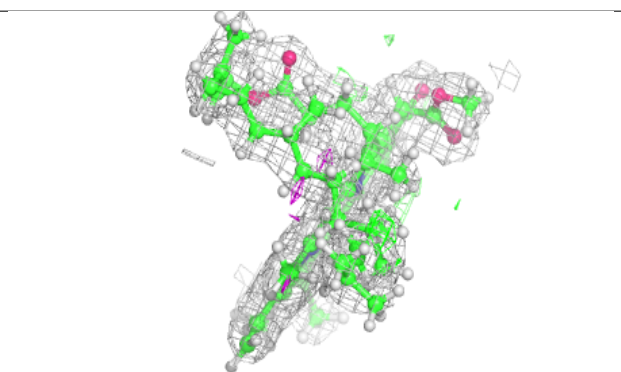
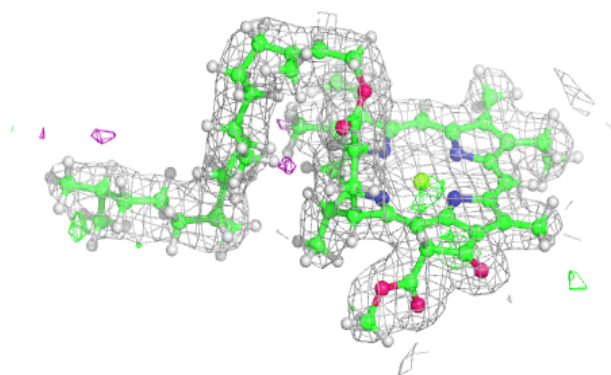
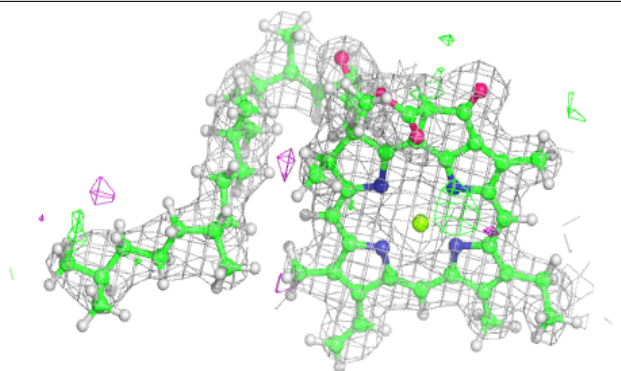
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



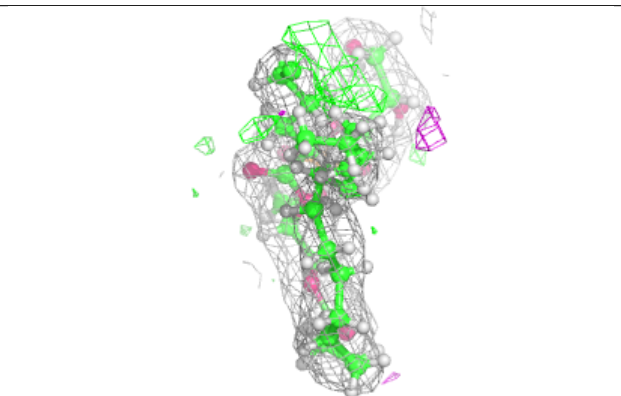
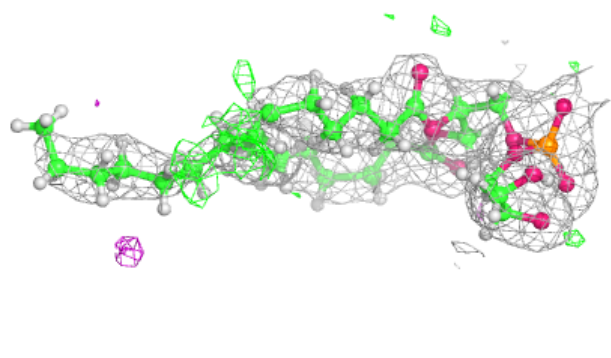
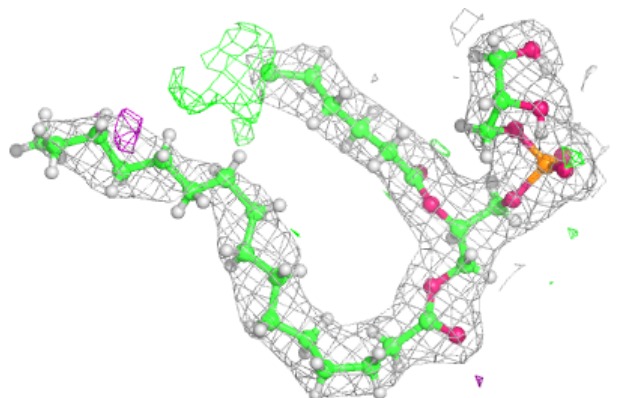


**Electron density around CLA a 612:**

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

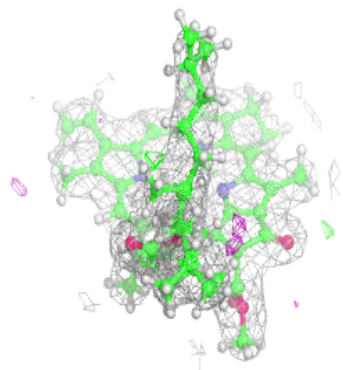
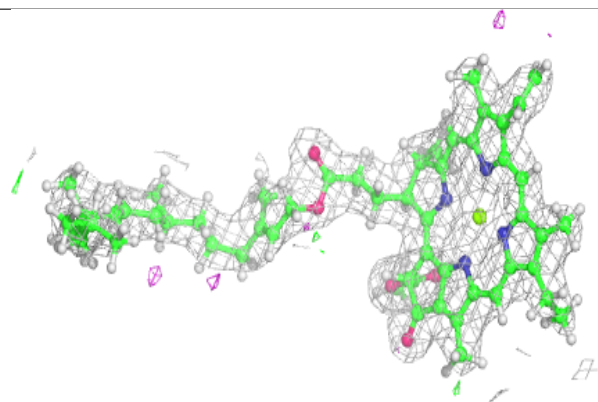
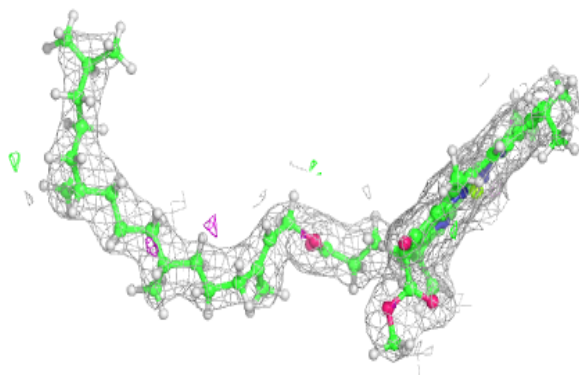
**Electron density around LHG d 409:**

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



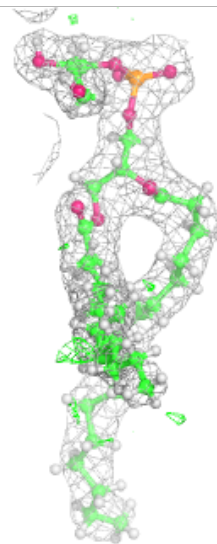
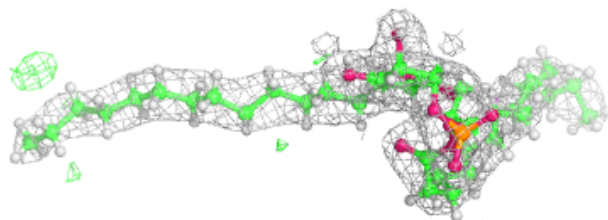
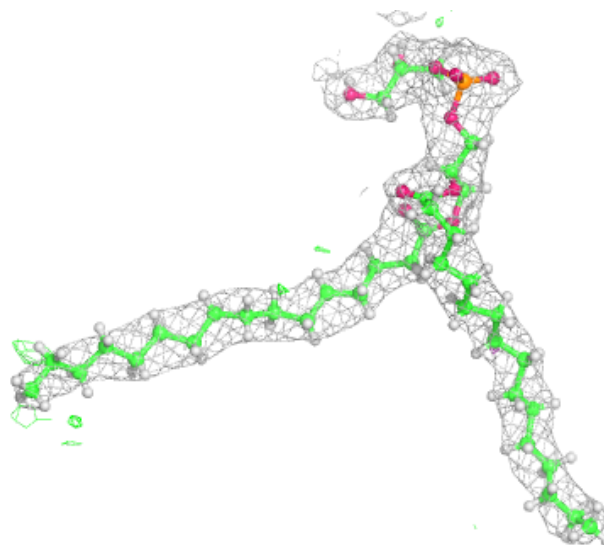
**Electron density around CLA d 403:**

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



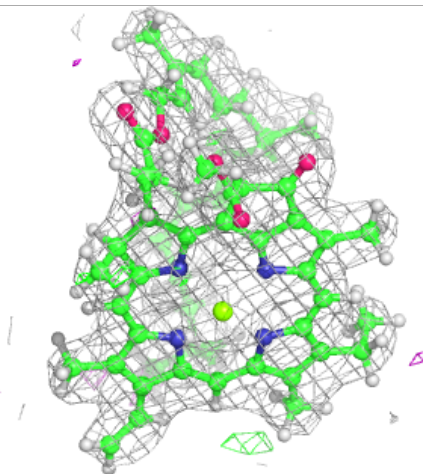
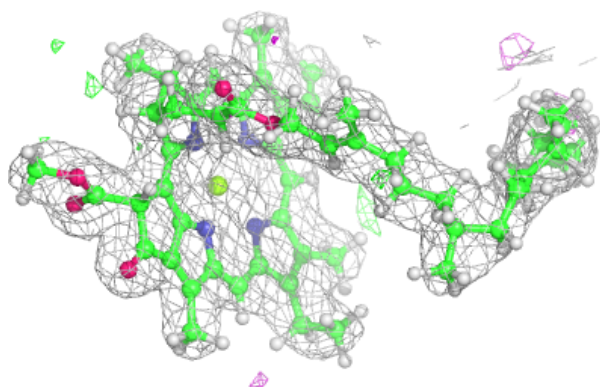
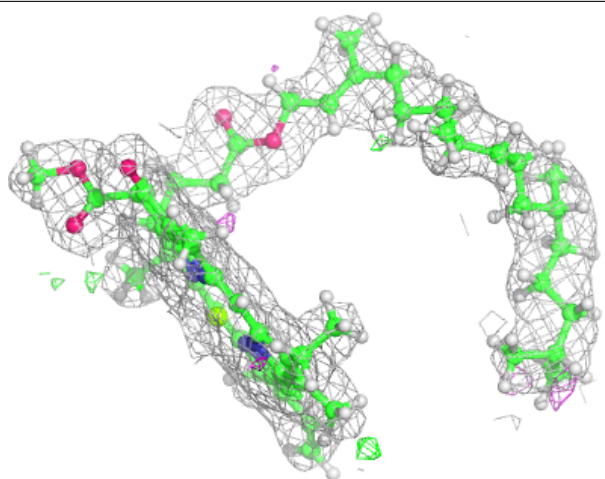
**Electron density around LHG 1 101:**

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



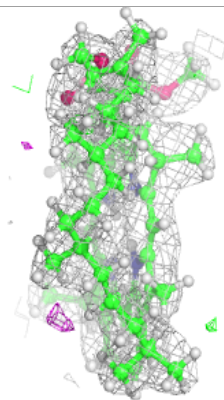
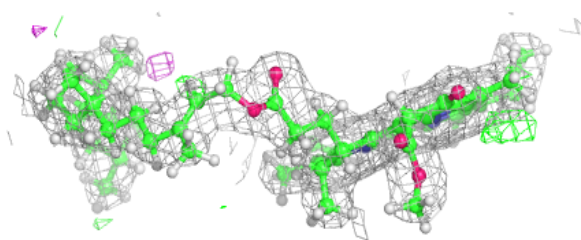
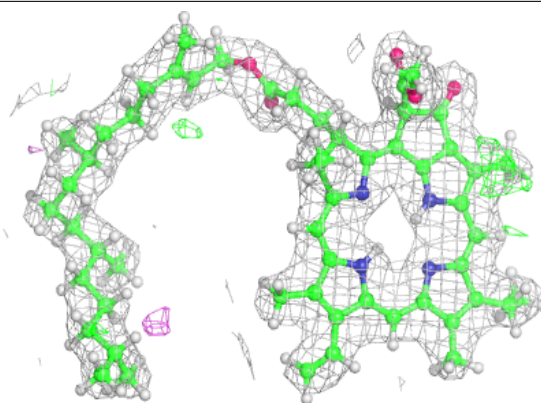
**Electron density around CLA B 611:**

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



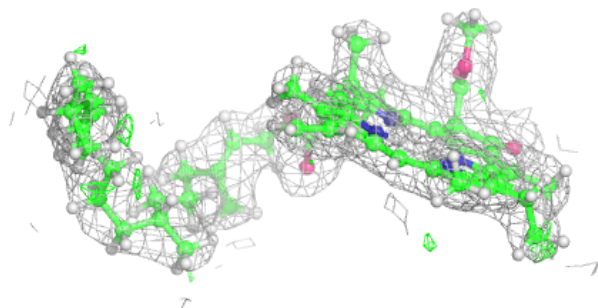
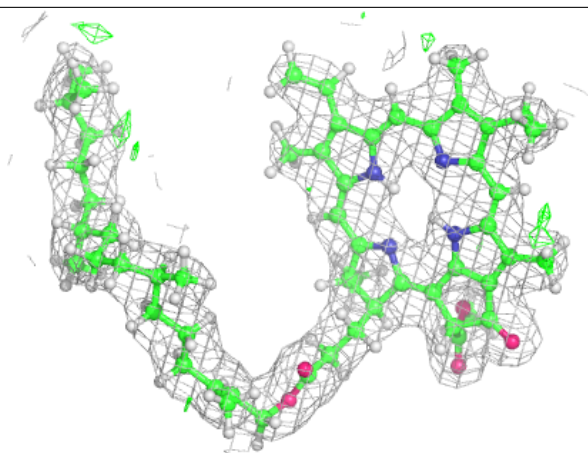
**Electron density around PHO A 606:**

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



**Electron density around PHO A 607:**

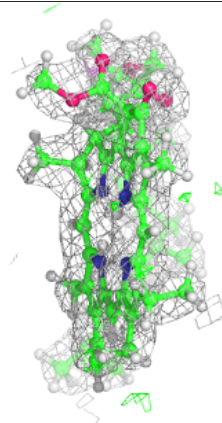
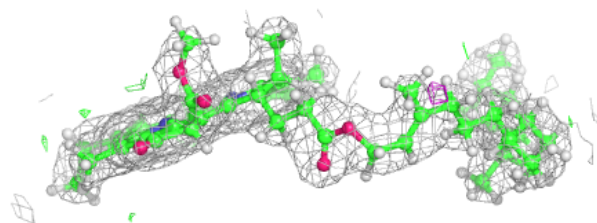
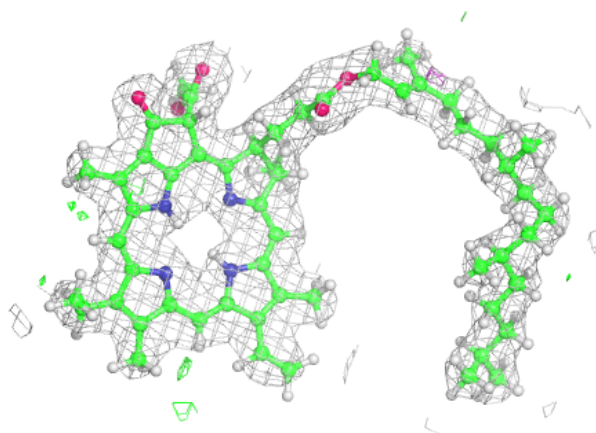
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





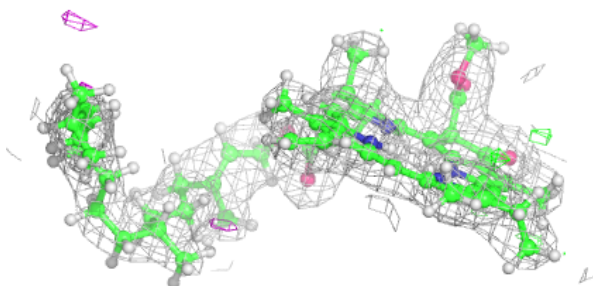
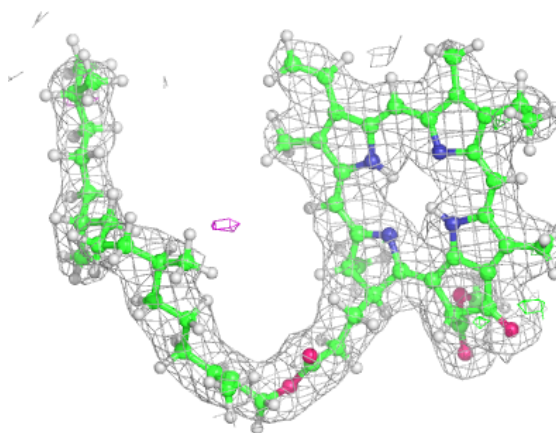
**Electron density around PHO a 605:**

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

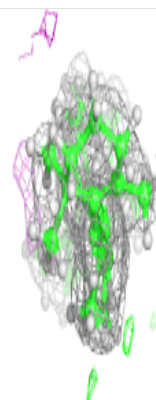
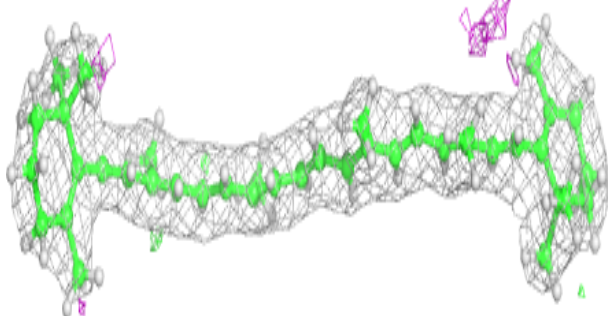
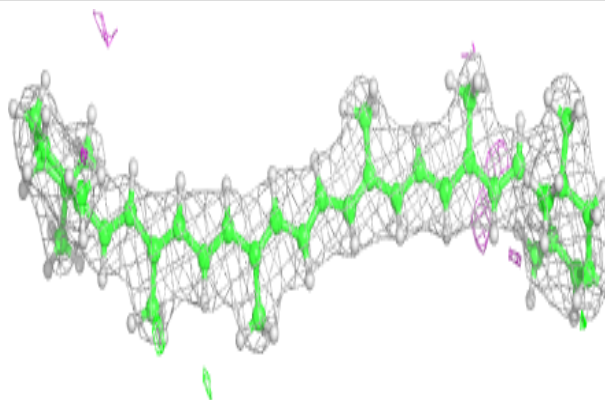


**Electron density around PHO d 402:**

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

**Electron density around BCR A 609:**

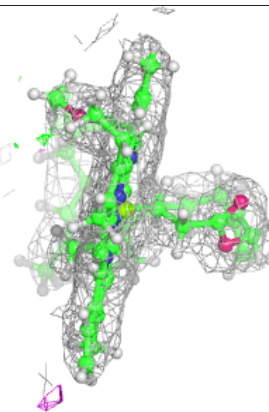
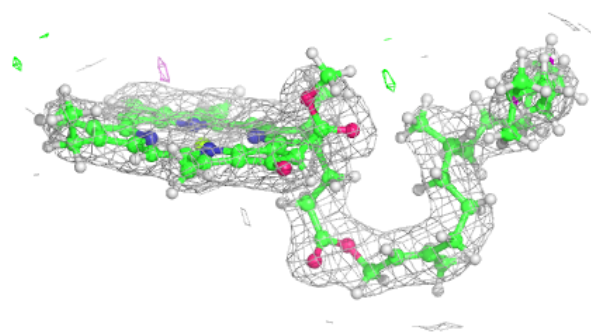
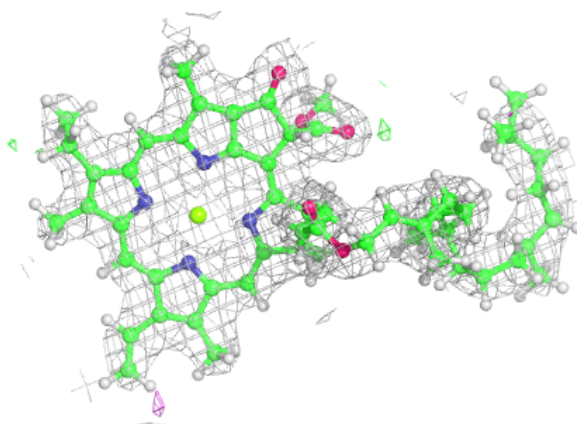
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



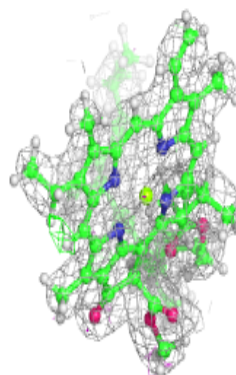
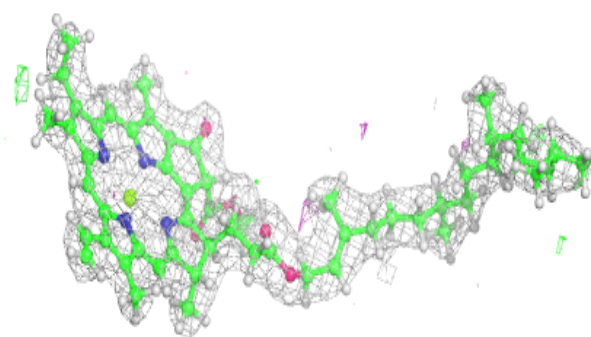
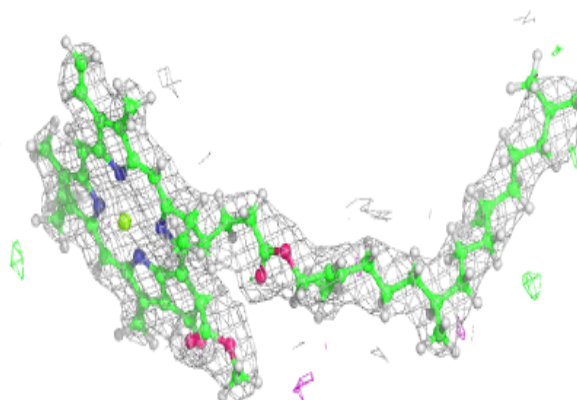


**Electron density around CLA B 612:**

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

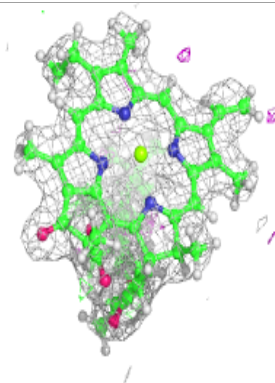
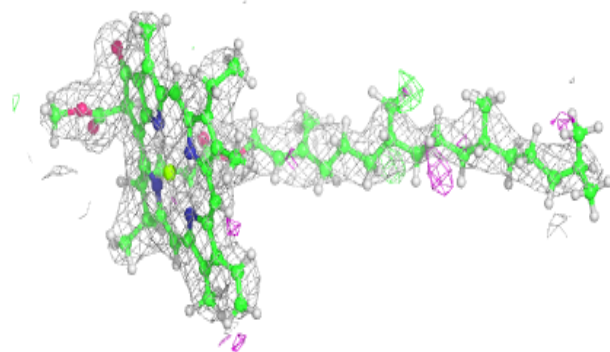
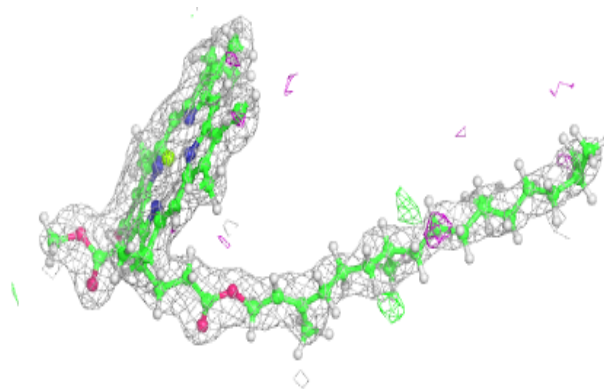
**Electron density around CLA A 604:**

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

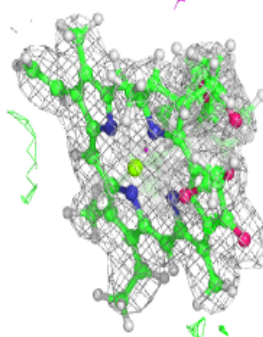
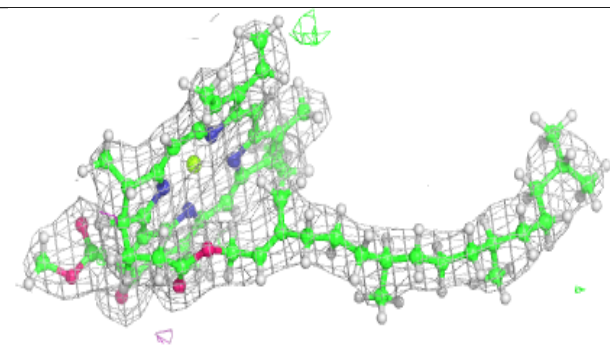
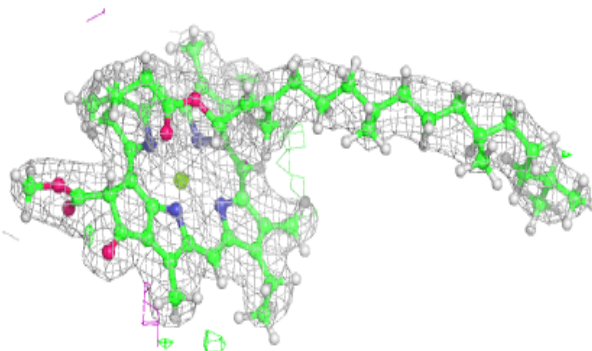


**Electron density around CLA B 607:**

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

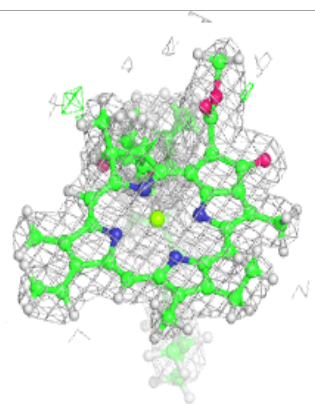
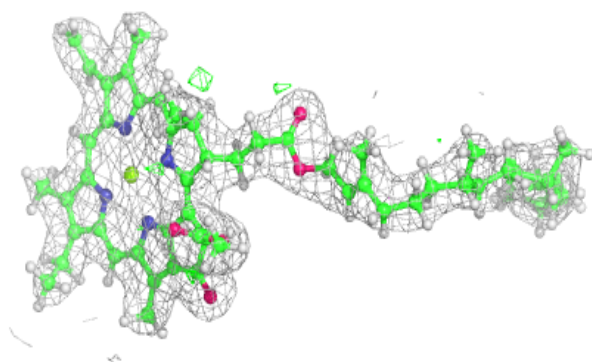
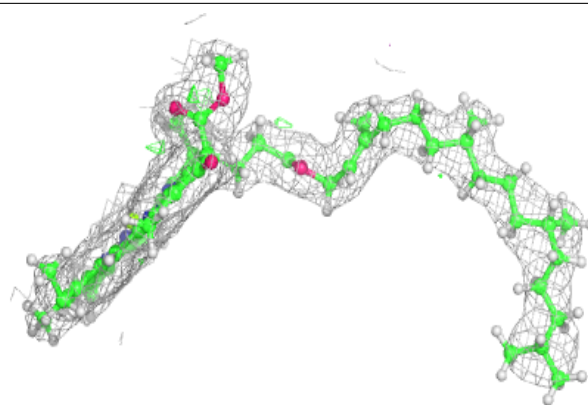
**Electron density around CLA B 608:**

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

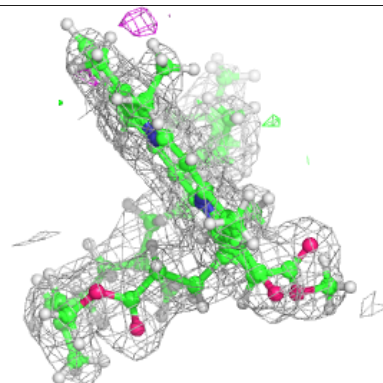
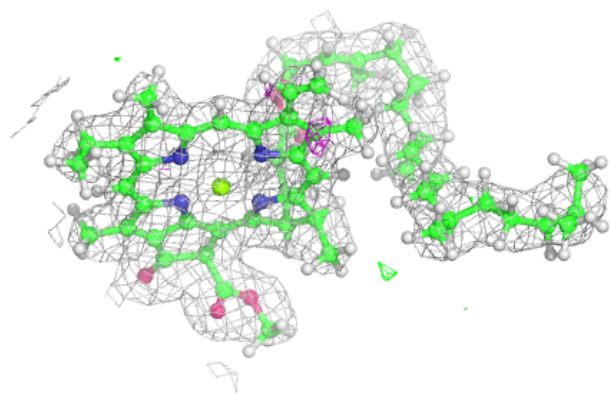
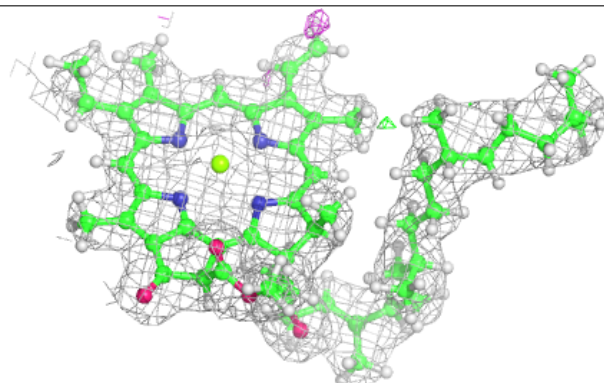


**Electron density around CLA D 402:**

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

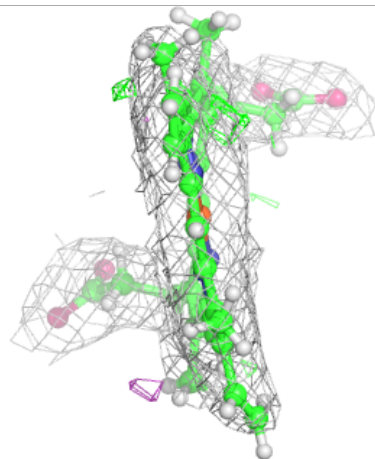
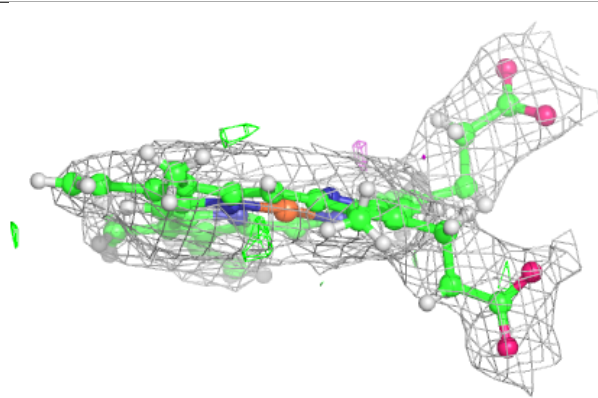
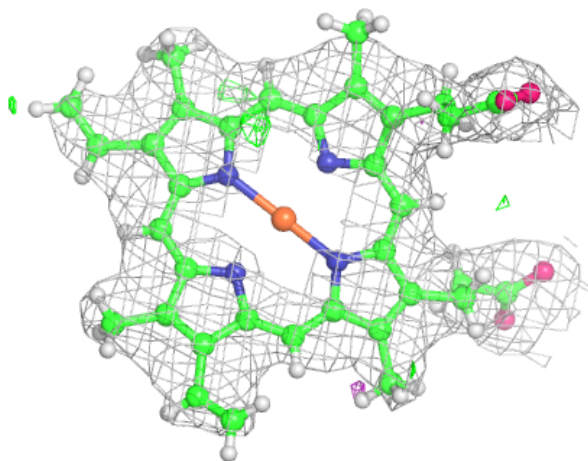
**Electron density around CLA A 613:**

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



**Electron density around HEM F 101:**

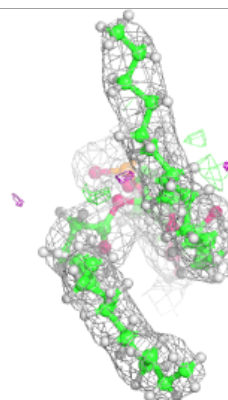
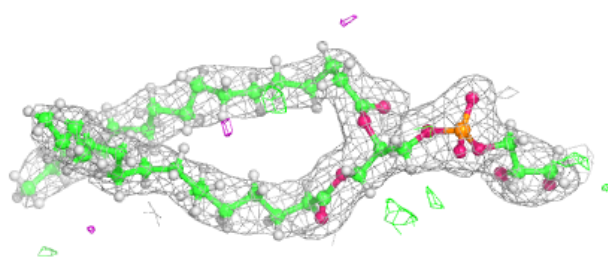
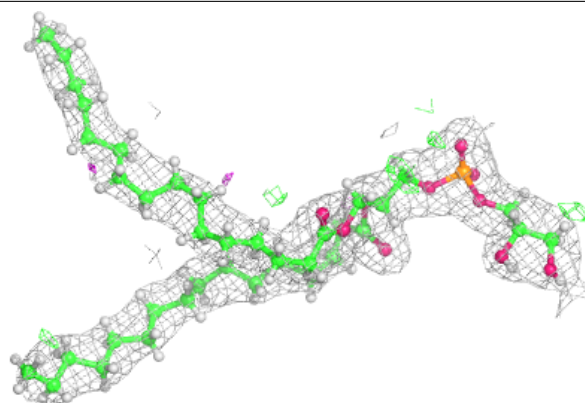
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



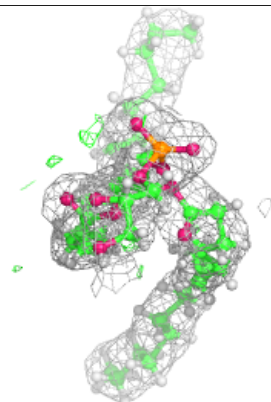
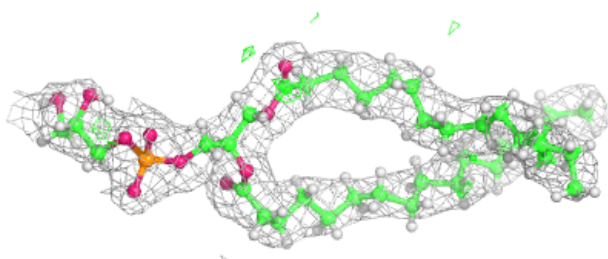
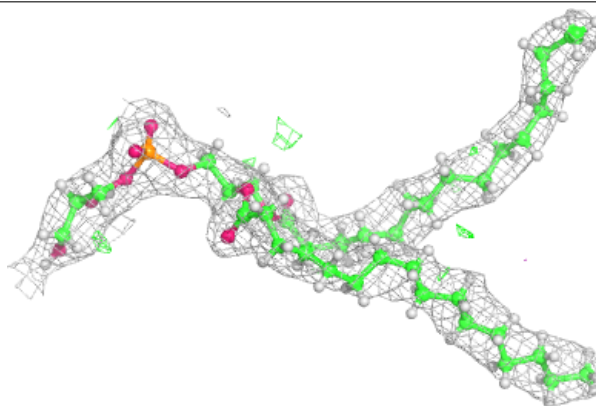


**Electron density around LHG d 408:**

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

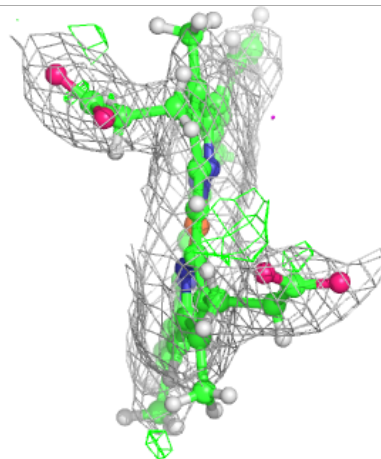
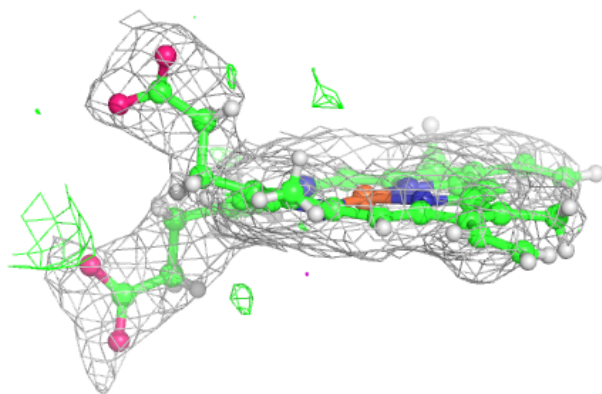
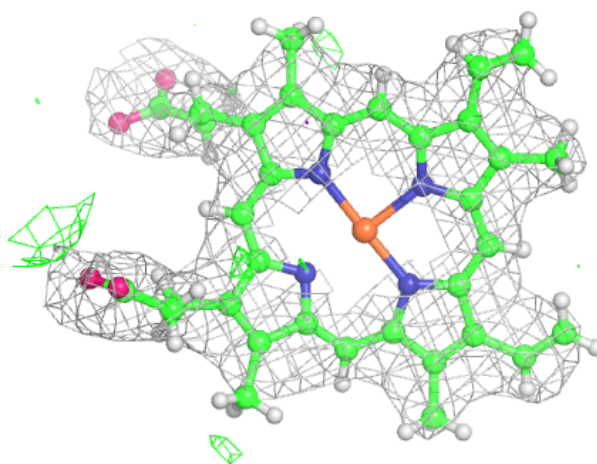
**Electron density around LHG D 408:**

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



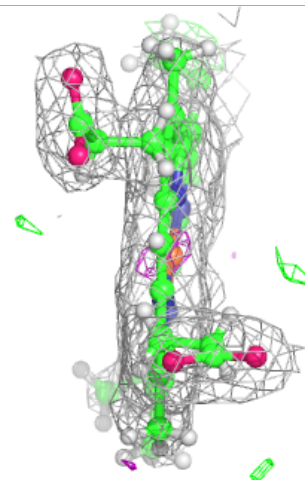
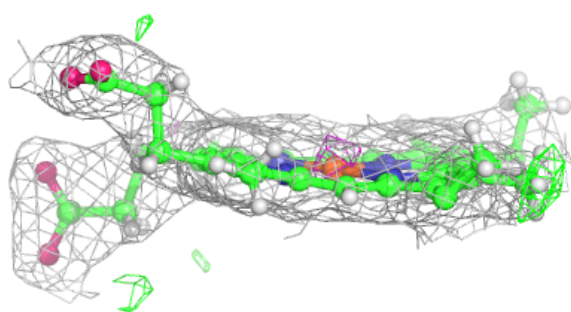
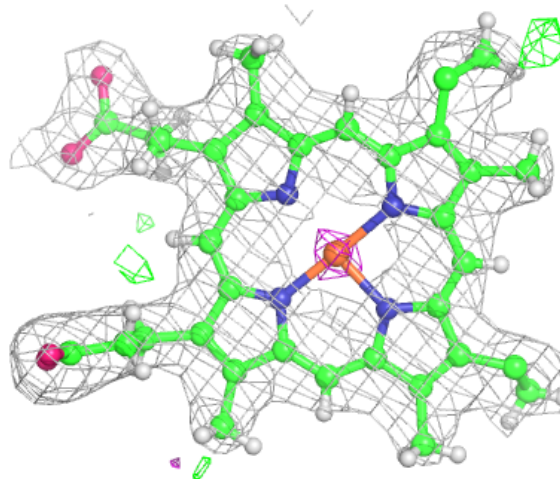
**Electron density around HEM e 101:**

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



**Electron density around HEC V 201:**

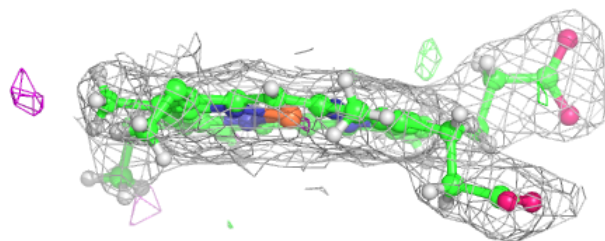
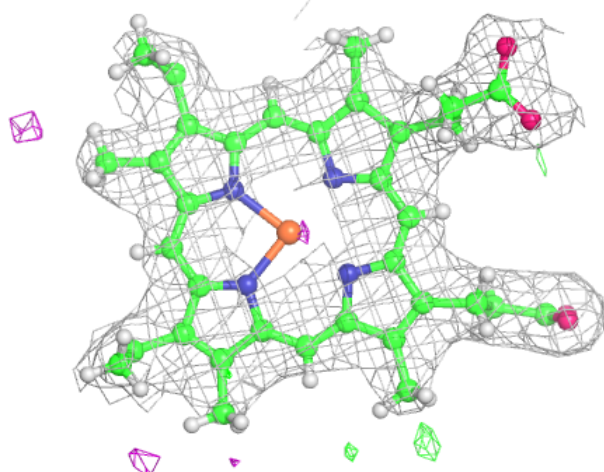
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





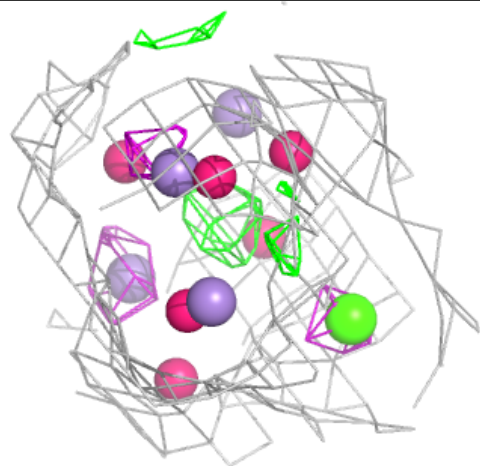
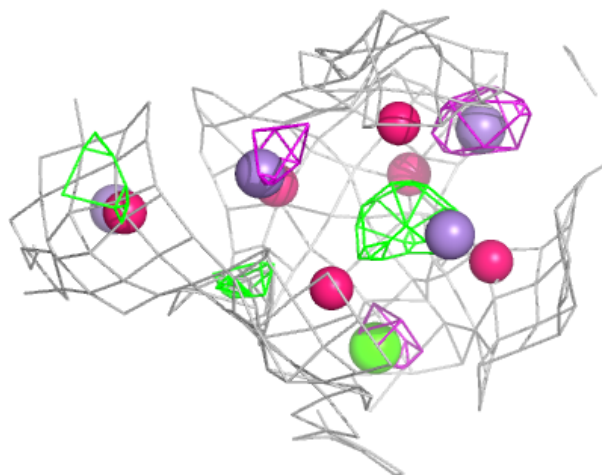
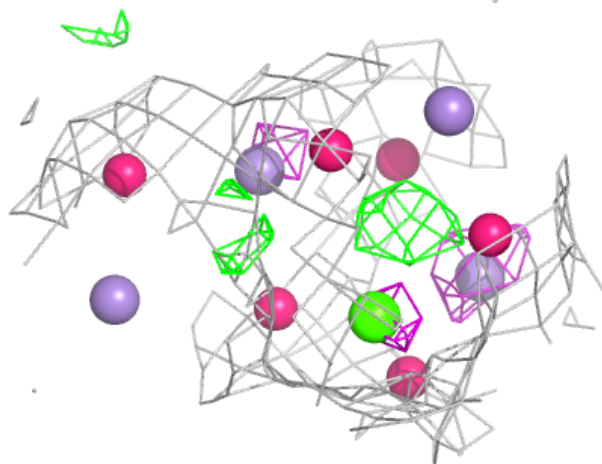
**Electron density around HEC v 201:**

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



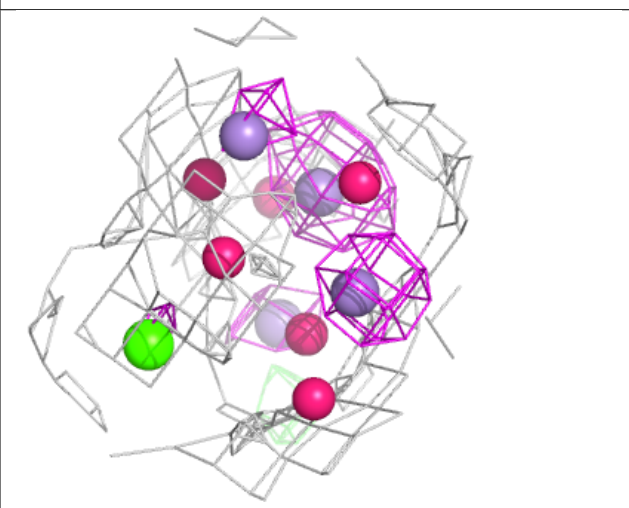
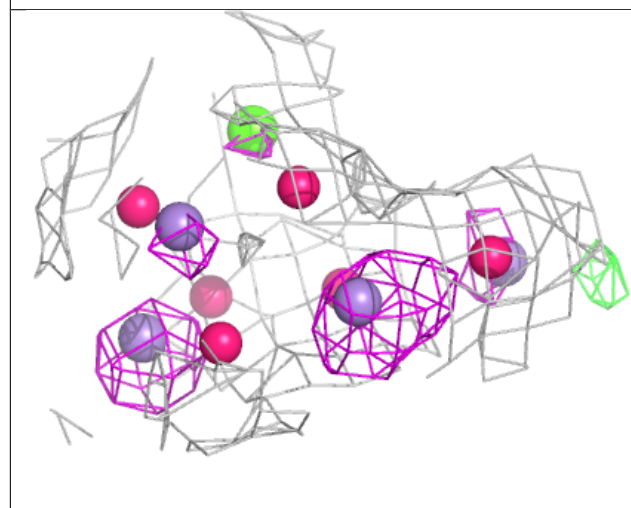
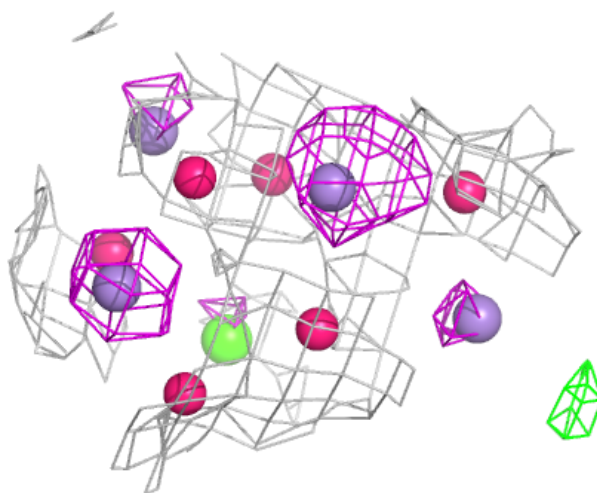
**Electron density around OEY A 601 (B):**

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



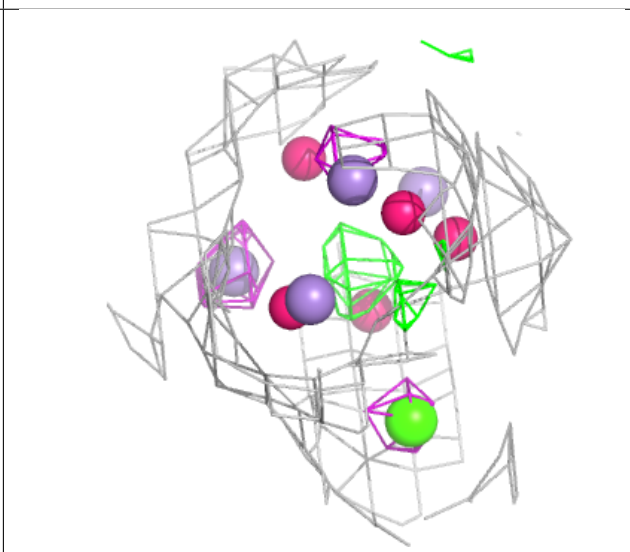
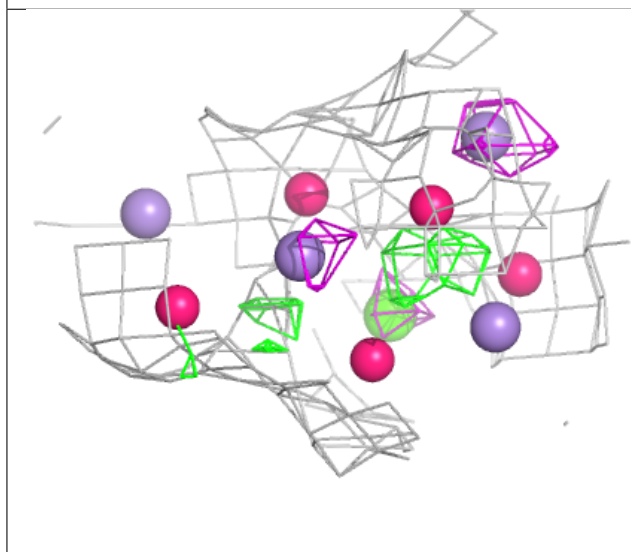
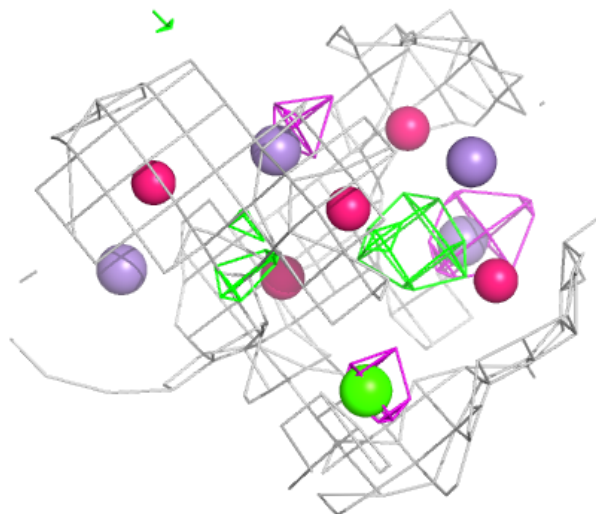
**Electron density around OEY a 601 (B):**

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



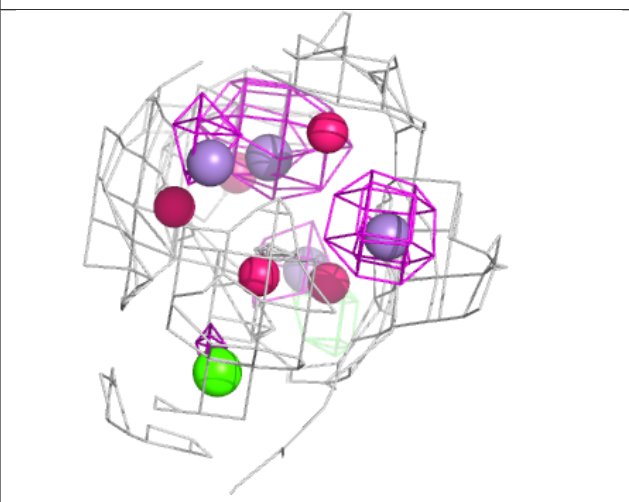
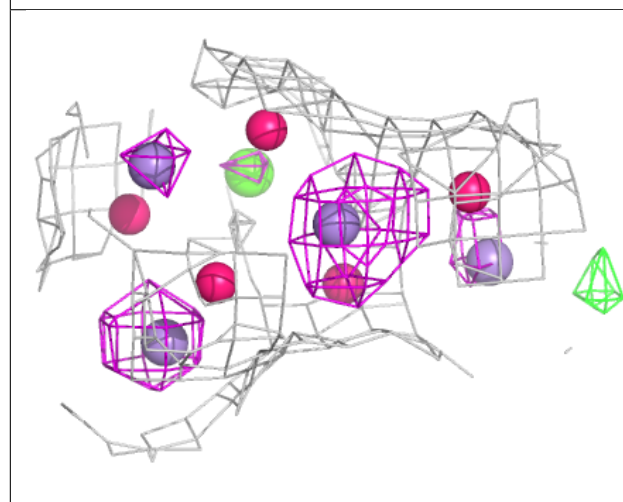
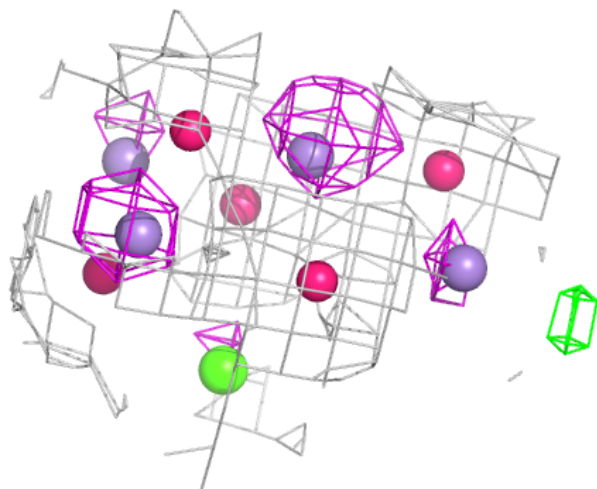
**Electron density around OEX A 602 (A):**

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



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

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.