



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 11:10 AM BST

PDB ID : 6W1U
Title : RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.09 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)

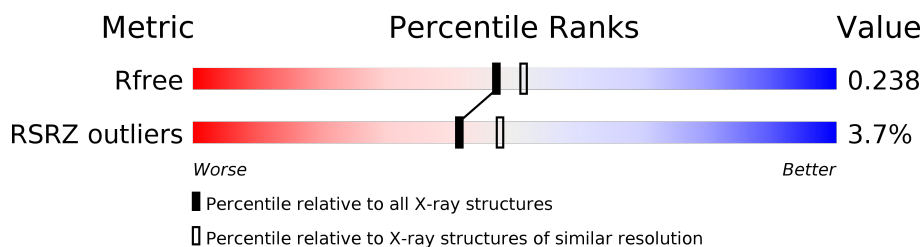
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

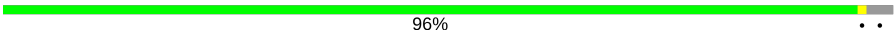

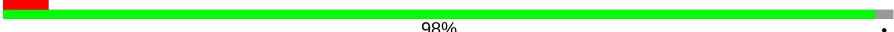











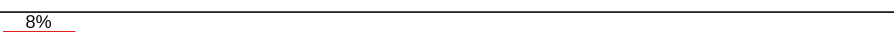
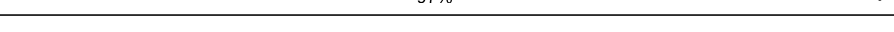
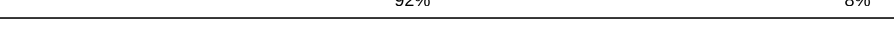

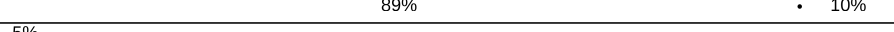






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
2	B	510	<div> <div>2%</div> <div>98%</div> <div>..</div> </div>
2	b	510	<div> <div>3%</div> <div>98%</div> <div>..</div> </div>
3	C	461	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
3	c	461	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
4	D	352	<div> <div>97%</div> <div>.</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

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Mol	Chain	Length	Quality of chain
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	
16	u	134	

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Mol	Chain	Length	Quality of chain
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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	411	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	515	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	h	101	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105950 atoms, of which 52556 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	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
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	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	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	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
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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			
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

- 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
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- 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
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	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
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

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

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

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

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

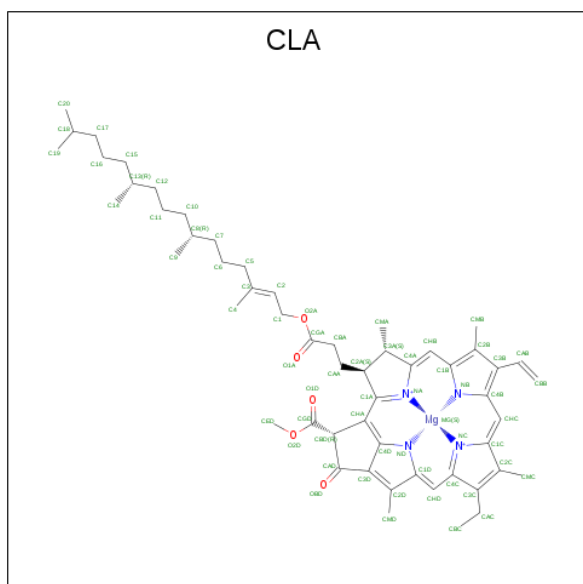
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	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
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0	0
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	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
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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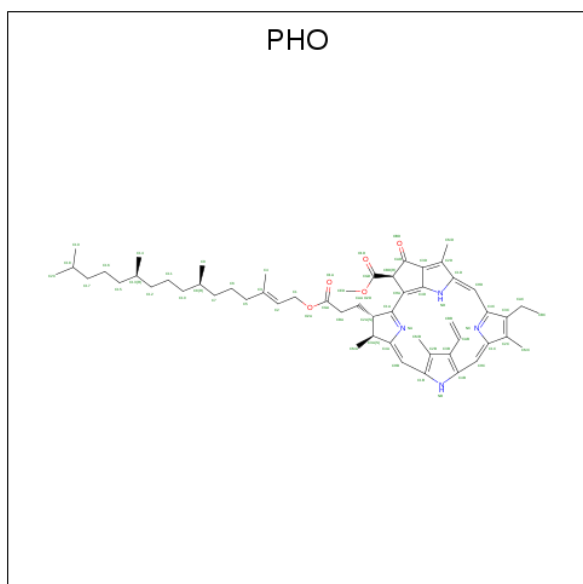
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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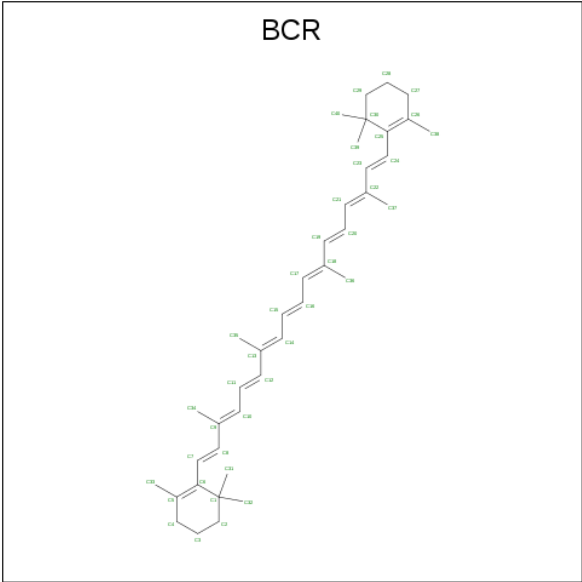
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	h	1	Total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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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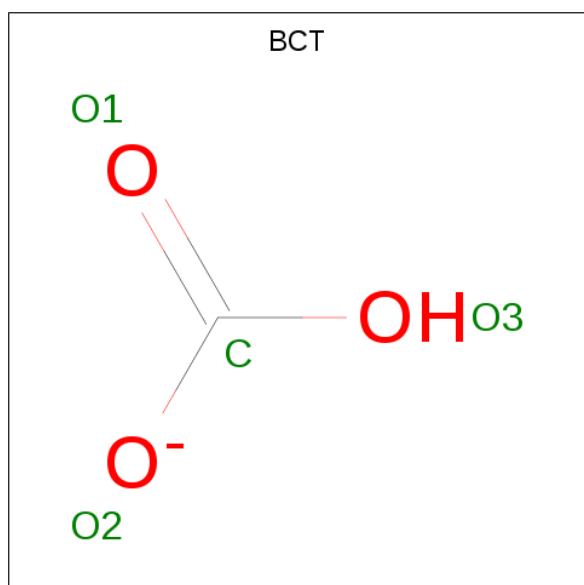
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40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

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

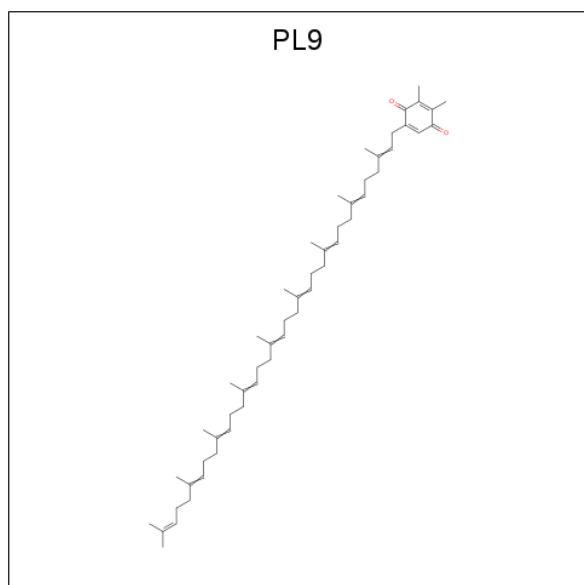
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



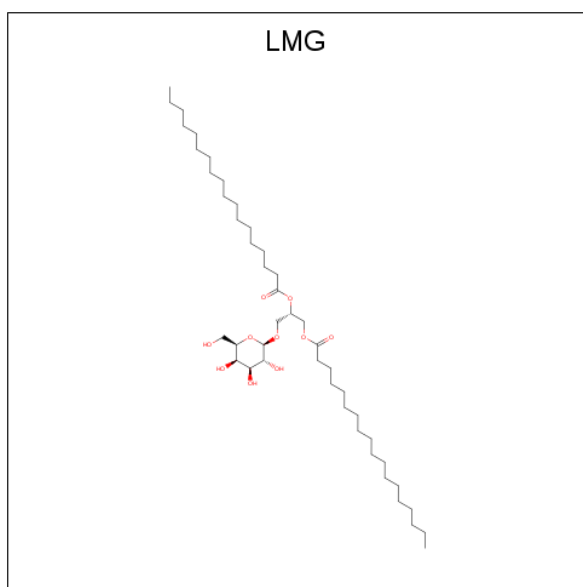
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by author).



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

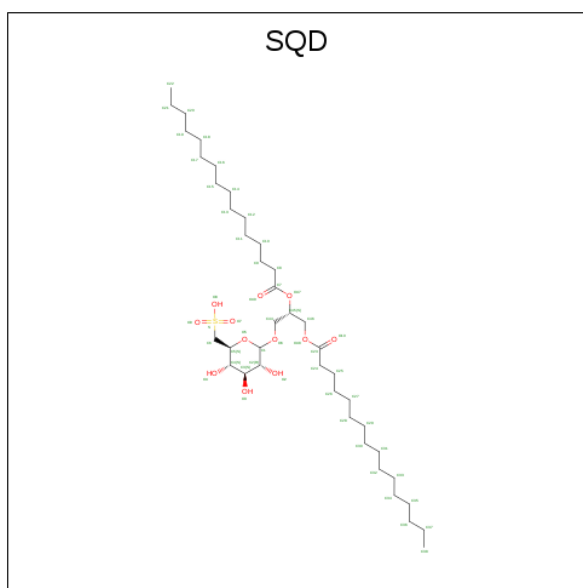
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			141	45	86	10		
28	C	1	Total	C	H	O	0	0
			111	38	63	10		
28	D	1	Total	C	H	O	0	0
			121	41	70	10		
28	D	1	Total	C	H	O	0	0
			78	27	45	6		
28	D	1	Total	C	H	O	0	0
			68	24	40	4		
28	M	1	Total	C	H	O	0	0
			121	41	70	10		
28	b	1	Total	C	H	O	0	0
			122	41	71	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			80	27	43	10		
28	c	1	Total	C	H	O	0	0
			116	38	68	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

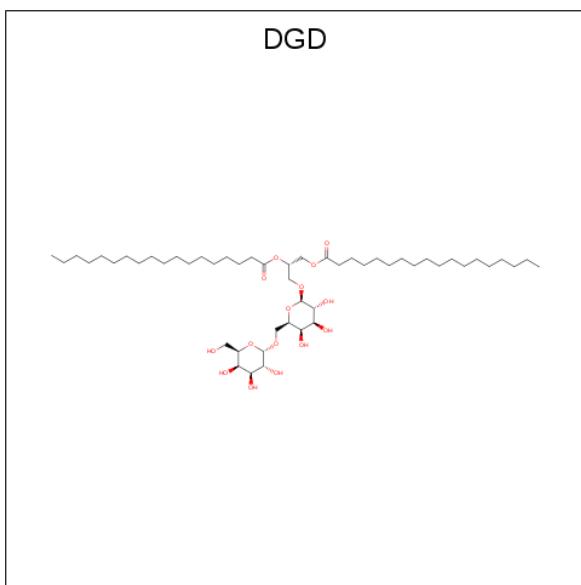
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



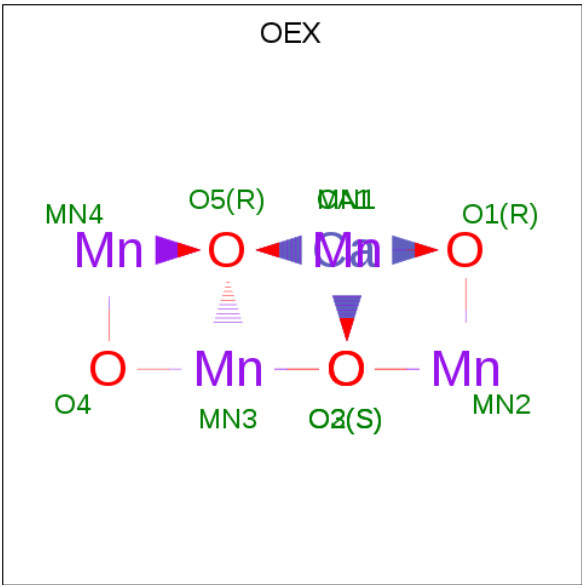
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			87	28	46	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



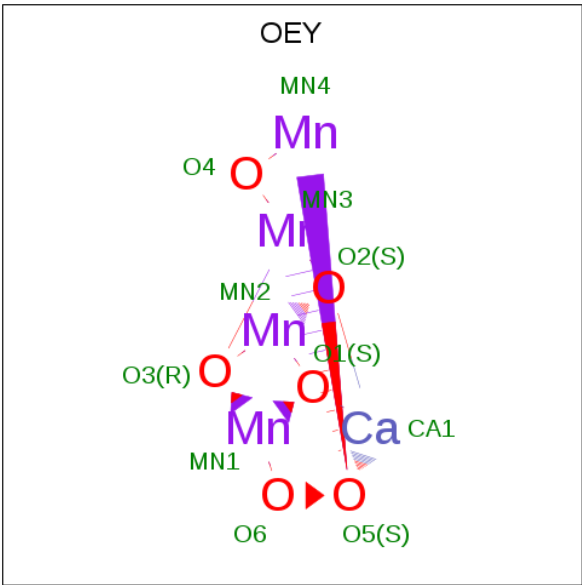
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			159	51	93	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			140	47	78	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			141	47	79	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	h	1	Total	C	H	O	0	0
			140	47	78	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



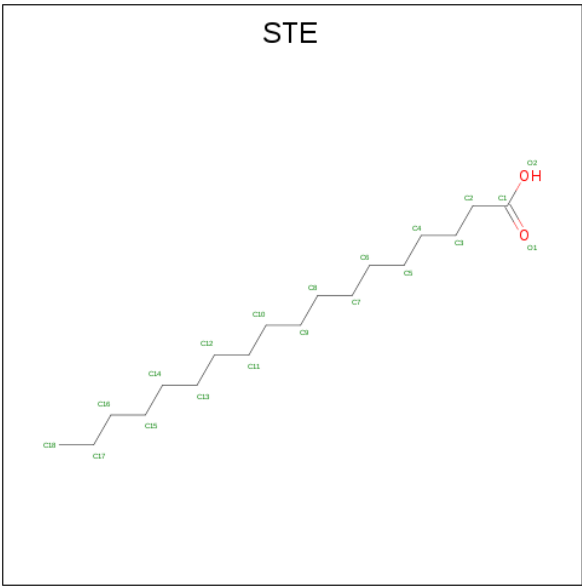
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
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	O	0	0
			46	16	28	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H		0	0
			41	15	26			
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	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			

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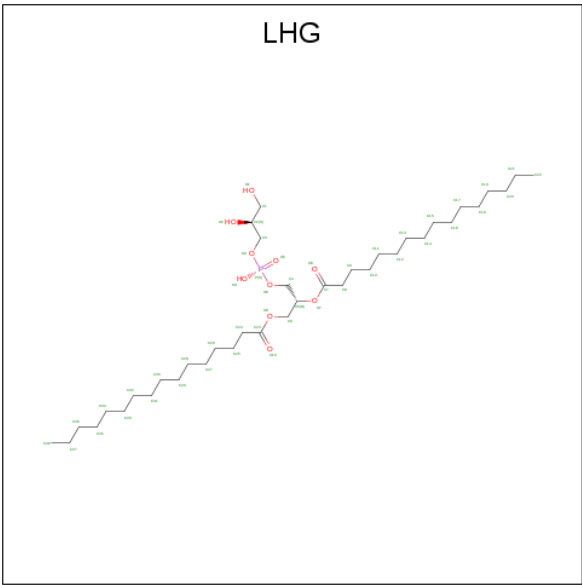
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	L	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		
33	M	1	Total	C	H		0	0
			26	10	16			
33	T	1	Total	C	H		0	0
			44	15	29			
33	X	1	Total	C	H	O	0	0
			55	18	35	2		
33	Z	1	Total	C	H		0	0
			20	8	12			
33	a	1	Total	C	H		0	0
			26	10	16			
33	a	1	Total	C	H	O	0	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
			55	18	35	2		
33	b	1	Total	C	H	O	0	0
			40	14	24	2		
33	b	1	Total	C	H	O	0	0
			55	18	35	2		
33	b	1	Total	C	H		0	0
			26	10	16			
33	c	1	Total	C	H	O	0	0
			28	10	16	2		
33	c	1	Total	C	H	O	0	0
			55	18	35	2		
33	d	1	Total	C	H	O	0	0
			43	15	26	2		
33	d	1	Total	C	H	O	0	0
			55	18	35	2		
33	d	1	Total	C	H	O	0	0
			55	18	35	2		
33	h	1	Total	C	H		0	0
			41	14	27			
33	j	1	Total	C	H	O	0	0
			28	10	16	2		

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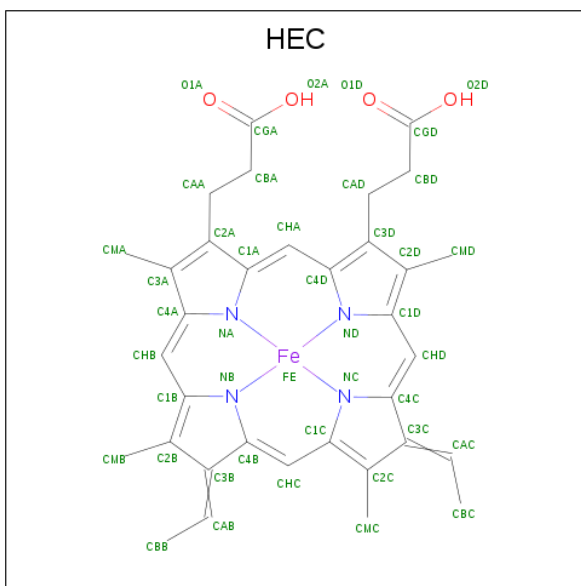
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	1	1	Total	C	H	0	0
			53	18	35		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	B	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
34	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
34	D	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
34	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	E	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
34	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
34	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
34	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

- Molecule 35 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
35	F	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
35	V	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
35	e	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
35	v	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	153	Total O 153 153	0	8
36	B	216	Total O 216 216	0	0
36	C	179	Total O 179 179	0	0
36	D	131	Total O 131 131	0	0
36	E	39	Total O 39 39	0	0
36	F	7	Total O 7 7	0	0
36	H	23	Total O 23 23	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	I	17	Total O 17 17	0	0
36	J	19	Total O 19 19	0	0
36	K	16	Total O 16 16	0	0
36	L	9	Total O 9 9	0	0
36	M	7	Total O 7 7	0	0
36	O	101	Total O 101 101	0	0
36	R	6	Total O 6 6	0	0
36	T	10	Total O 10 10	0	0
36	U	43	Total O 43 43	0	0
36	V	62	Total O 62 62	0	0
36	X	11	Total O 11 11	0	0
36	Y	5	Total O 5 5	0	0
36	Z	10	Total O 10 10	0	0
36	a	137	Total O 137 137	0	8
36	b	186	Total O 186 186	0	0
36	c	179	Total O 179 179	0	0
36	d	110	Total O 110 110	0	0
36	e	29	Total O 29 29	0	0
36	f	7	Total O 7 7	0	0
36	h	31	Total O 31 31	0	0
36	i	8	Total O 8 8	0	0

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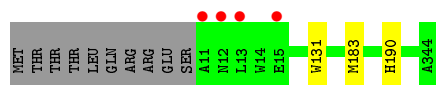
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	16	Total 16	O 16	0	0
36	k	7	Total 7	O 7	0	0
36	l	9	Total 9	O 9	0	0
36	m	7	Total 7	O 7	0	0
36	o	106	Total 106	O 106	0	0
36	r	6	Total 6	O 6	0	0
36	t	6	Total 6	O 6	0	0
36	u	56	Total 56	O 56	0	0
36	v	75	Total 75	O 75	0	0
36	x	12	Total 12	O 12	0	0
36	y	4	Total 4	O 4	0	0
36	z	11	Total 11	O 11	0	0

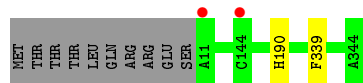
3 Residue-property plots [i](#)

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.

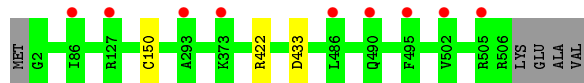
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



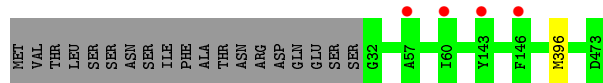
- Molecule 2: Photosystem II CP47 reaction center protein



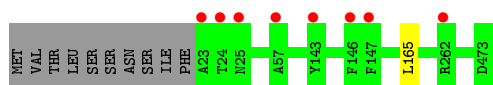
- Molecule 2: Photosystem II CP47 reaction center protein



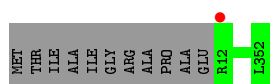
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



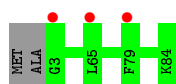
- Molecule 4: Photosystem II D2 protein



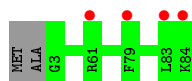
- Molecule 4: Photosystem II D2 protein



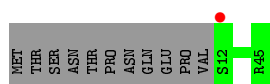
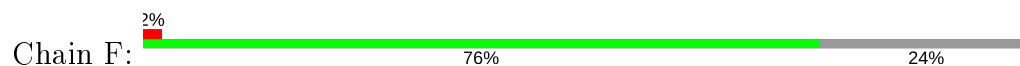
- Molecule 5: Cytochrome b559 subunit alpha



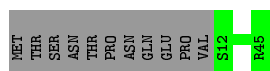
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



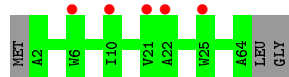
- Molecule 7: Photosystem II reaction center protein H

Chain H:  98%




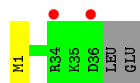
- Molecule 7: Photosystem II reaction center protein H

Chain h:  8% 95% 5%




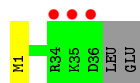
- Molecule 8: Photosystem II reaction center protein I

Chain I:  5% 92% 5%




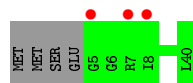
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 92% 5%




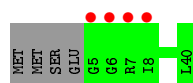
- Molecule 9: Photosystem II reaction center protein J

Chain J:  8% 90% 10%




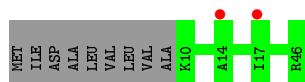
- Molecule 9: Photosystem II reaction center protein J

Chain j:  10% 90% 10%

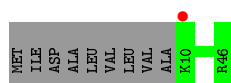
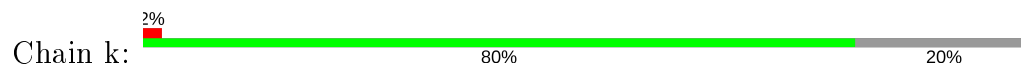


- Molecule 10: Photosystem II reaction center protein K

Chain K:  4% 80% 20%



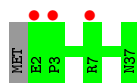
- Molecule 10: Photosystem II reaction center protein K



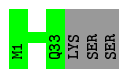
- Molecule 11: Photosystem II reaction center protein L



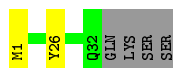
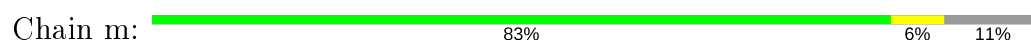
- Molecule 11: Photosystem II reaction center protein L



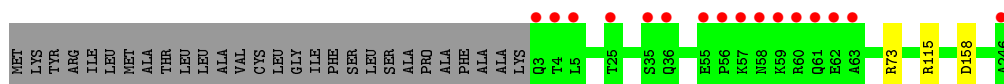
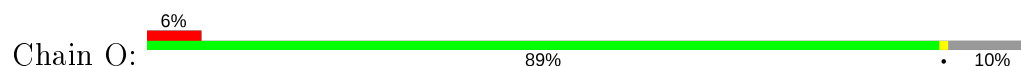
- Molecule 12: Photosystem II reaction center protein M



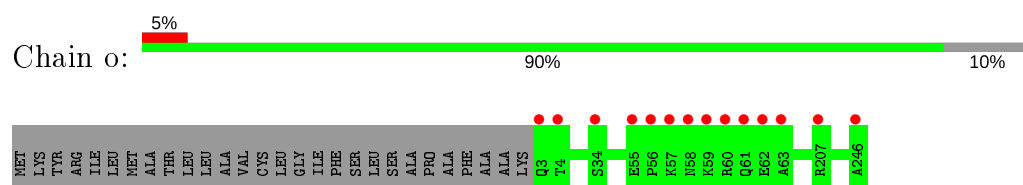
- Molecule 12: Photosystem II reaction center protein M



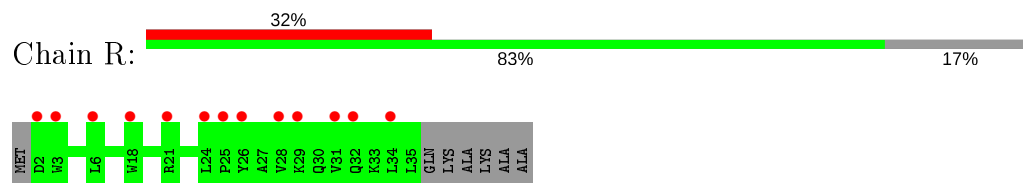
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



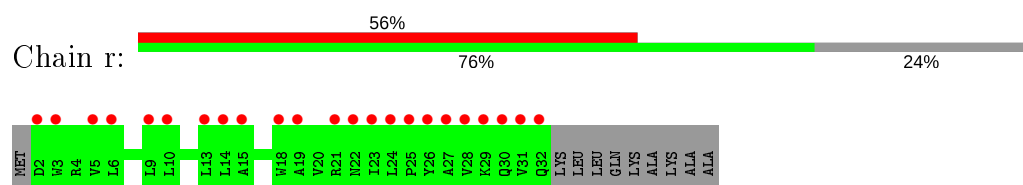
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



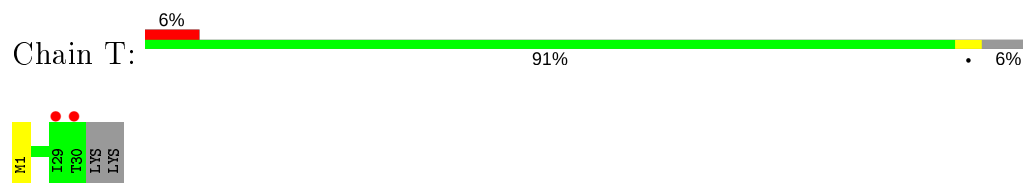
- Molecule 14: Photosystem II protein Y



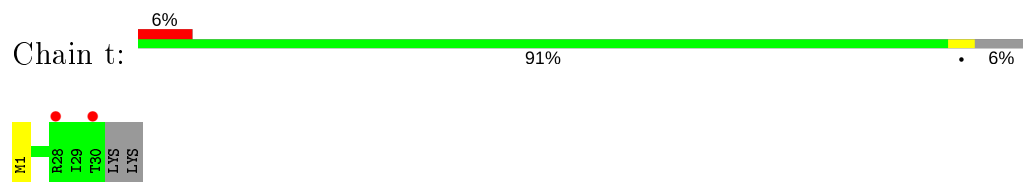
- Molecule 14: Photosystem II protein Y



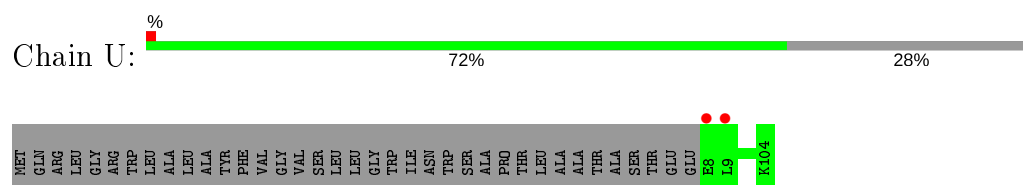
- Molecule 15: Photosystem II reaction center protein T



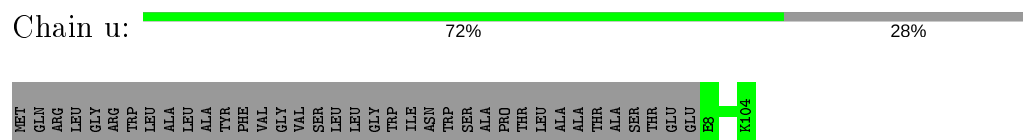
- Molecule 15: Photosystem II reaction center protein T




- Molecule 16: Photosystem II 12 kDa extrinsic protein

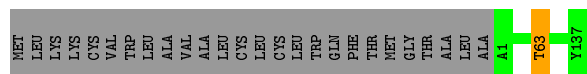


- Molecule 16: Photosystem II 12 kDa extrinsic protein




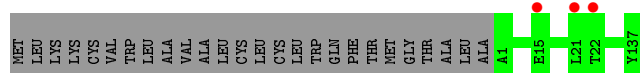
- Molecule 17: Cytochrome c-550

Chain V:  83% 16%



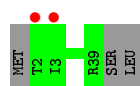
- Molecule 17: Cytochrome c-550

Chain v:  2% 84% 16%



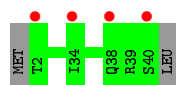
- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 93% 7%



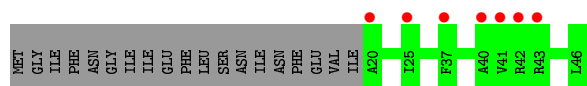
- Molecule 18: Photosystem II reaction center X protein

Chain x:  10% 95% 5%



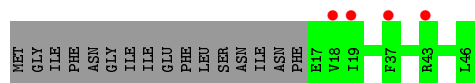
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  15% 59% 41%



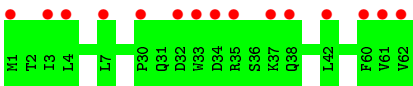
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  9% 65% 35%

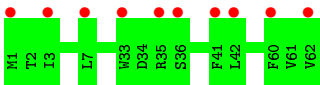


- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  24% 100%



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 86.0 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.180 , 0.239 0.180 , 0.238	Depositor DCC
R_{free} test set	4171 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105950	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.61	0/3187	0.70	3/4342 (0.1%)
1	a	0.62	0/3184	0.81	6/4338 (0.1%)
2	B	0.65	1/4161 (0.0%)	0.69	2/5669 (0.0%)
2	b	0.65	2/4118 (0.0%)	0.69	2/5611 (0.0%)
3	C	0.61	0/3621	0.68	1/4930 (0.0%)
3	c	0.58	0/3693	0.68	1/5026 (0.0%)
4	D	0.68	0/2820	0.70	0/3840
4	d	0.65	0/2829	0.73	3/3852 (0.1%)
5	E	0.60	0/688	0.61	0/940
5	e	0.53	0/683	0.64	0/932
6	F	0.58	0/284	0.52	0/387
6	f	0.50	0/284	0.58	0/387
7	H	0.63	0/523	0.74	0/713
7	h	0.54	0/511	0.69	0/697
8	I	0.63	0/293	0.67	0/396
8	i	0.64	0/293	0.69	0/396
9	J	0.61	0/263	0.63	0/356
9	j	0.55	0/263	0.69	0/356
10	K	0.57	0/303	0.64	0/416
10	k	0.51	0/303	0.69	0/416
11	L	0.63	0/311	0.70	0/422
11	l	0.68	0/303	0.66	0/412
12	M	0.61	0/249	0.63	0/341
12	m	0.85	1/244 (0.4%)	0.72	0/334
13	O	0.62	0/1904	0.75	3/2585 (0.1%)
13	o	0.63	0/1905	0.75	0/2583
14	R	0.46	0/277	0.53	0/380
14	r	0.40	0/245	0.51	0/336
15	T	0.72	0/257	0.77	0/349
15	t	0.67	0/255	0.65	0/346
16	U	0.58	0/785	0.70	0/1064
16	u	0.64	0/785	0.72	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.61	0/1085	0.70	1/1473 (0.1%)
17	v	0.60	0/1085	0.69	0/1473
18	X	0.59	0/284	0.69	0/384
18	x	0.47	0/289	0.60	0/391
19	Y	0.47	0/197	0.54	0/264
19	y	0.42	0/219	0.58	0/294
20	Z	0.46	0/490	0.59	0/669
20	z	0.46	0/488	0.57	0/666
All	All	0.62	4/43961 (0.0%)	0.70	22/59830 (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
1	A	0	1
1	a	0	1
17	V	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	26	TYR	CD1-CE1	-6.90	1.28	1.39
2	B	150	CYS	CB-SG	-6.66	1.71	1.82
2	b	112	CYS	CB-SG	-5.61	1.72	1.81
2	b	486	LEU	C-N	5.06	1.45	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	190[A]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[B]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[A]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[B]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[A]	HIS	C-N-CA	9.85	146.32	121.70
1	a	190[B]	HIS	C-N-CA	9.85	146.32	121.70
17	V	63	THR	C-N-CD	-6.58	106.13	120.60
2	b	385	ARG	NE-CZ-NH2	-6.18	117.21	120.30
4	d	272	LEU	CB-CG-CD1	-5.90	100.97	111.00
4	d	297	ASP	CB-CG-OD1	5.67	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	165	LEU	CA-CB-CG	5.65	128.29	115.30
13	O	73	ARG	NE-CZ-NH2	-5.59	117.50	120.30
3	C	396	MET	CG-SD-CE	-5.32	91.69	100.20
1	A	183[A]	MET	CA-CB-CG	5.31	122.32	113.30
1	A	183[B]	MET	CA-CB-CG	5.31	122.32	113.30
2	B	433	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	422	ARG	NE-CZ-NH1	-5.20	117.70	120.30
2	b	433	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	131	TRP	CA-CB-CG	-5.17	103.88	113.70
4	d	272	LEU	CA-CB-CG	5.16	127.17	115.30
13	O	115	ARG	NE-CZ-NH1	5.14	122.87	120.30
13	O	158	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide
1	a	339[B]	PHE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

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$
8	FME	I	1	8	8,9,10	1.14	1 (12%)	7,9,11	1.46	2 (28%)
8	FME	i	1	8	8,9,10	0.88	0	7,9,11	1.50	2 (28%)
15	FME	T	1	15	8,9,10	1.02	0	7,9,11	1.46	1 (14%)
12	FME	M	1	12	8,9,10	0.86	0	7,9,11	0.93	0
15	FME	t	1	15	8,9,10	1.20	1 (12%)	7,9,11	1.05	0
12	FME	m	1	12	8,9,10	1.04	1 (12%)	7,9,11	1.23	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
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	3/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.98	1.42	1.46
8	I	1	FME	CA-N	-2.83	1.42	1.46
12	m	1	FME	CA-N	-2.21	1.43	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.75	118.60	122.82
15	T	1	FME	O1-CN-N	-2.61	118.39	125.27
8	I	1	FME	CA-N-CN	-2.18	119.46	122.82
8	i	1	FME	C-CA-N	2.04	113.41	109.73
8	I	1	FME	CE-SD-CG	-2.03	93.43	100.40
12	m	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
15	T	1	FME	N-CA-CB-CG
15	T	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	CB-CA-N-CN
12	M	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	$\# Z > 2$
22	CLA	C	512	3	59,73,73	1.84	7 (11%)	67,113,113	1.39	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	602	36	59,73,73	1.61	8 (13%)	67,113,113	2.03	14 (20%)
28	LMG	D	410	-	31,31,55	1.12	3 (9%)	33,33,63	1.15	1 (3%)
22	CLA	b	604	-	59,73,73	1.29	5 (8%)	67,113,113	1.69	13 (19%)
22	CLA	b	615	-	54,68,73	1.30	9 (16%)	61,107,113	1.79	11 (18%)
22	CLA	C	506	-	59,73,73	1.52	5 (8%)	67,113,113	1.43	10 (14%)
30	DGD	C	516	-	63,63,67	1.16	6 (9%)	77,77,81	1.41	19 (24%)
22	CLA	b	607	-	59,73,73	1.52	8 (13%)	67,113,113	1.48	14 (20%)
22	CLA	c	511	-	59,73,73	1.52	5 (8%)	67,113,113	1.76	12 (17%)
33	STE	B	626	-	14,17,19	0.39	0	13,17,19	0.97	0
22	CLA	B	605	-	59,73,73	1.56	7 (11%)	67,113,113	2.03	13 (19%)
34	LHG	d	408	-	38,38,48	0.78	1 (2%)	41,44,54	1.08	3 (7%)
24	BCR	b	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	8 (14%)
33	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.78	0
27	PL9	d	405	-	55,55,55	1.59	7 (12%)	68,69,69	1.66	15 (22%)
22	CLA	b	609	36	59,73,73	1.38	9 (15%)	67,113,113	1.69	14 (20%)
22	CLA	b	603	-	59,73,73	1.38	5 (8%)	67,113,113	1.86	15 (22%)
33	STE	H	103	-	17,17,19	0.48	0	16,16,19	0.63	0
35	HEC	F	101	5,6	26,50,50	2.42	4 (15%)	18,82,82	2.57	7 (38%)
27	PL9	A	410	-	55,55,55	1.15	5 (9%)	68,69,69	1.72	14 (20%)
34	LHG	D	409	-	46,46,48	0.99	2 (4%)	49,52,54	1.32	2 (4%)
31	OEX	a	416[A]	1,3,36	0,15,15	0.00	-	-	-	-
34	LHG	D	408	-	48,48,48	1.09	4 (8%)	51,54,54	1.21	5 (9%)
22	CLA	a	411	36	59,73,73	1.88	7 (11%)	67,113,113	1.42	7 (10%)
22	CLA	D	402	-	59,73,73	1.31	4 (6%)	67,113,113	1.53	9 (13%)
22	CLA	C	513	-	59,73,73	1.48	10 (16%)	67,113,113	1.51	13 (19%)
24	BCR	Z	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
29	SQD	D	407	-	35,36,54	0.97	1 (2%)	42,45,65	2.31	13 (30%)
33	STE	d	411	-	16,19,19	0.46	0	15,19,19	0.51	0
30	DGD	C	517	-	63,63,67	1.32	8 (12%)	77,77,81	1.35	10 (12%)
34	LHG	d	406	-	48,48,48	1.00	3 (6%)	51,54,54	1.37	6 (11%)
35	HEC	V	201	17	26,50,50	2.16	3 (11%)	18,82,82	2.40	6 (33%)
31	OEX	A	416[A]	1,3,36	0,15,15	0.00	-	-	-	-
22	CLA	B	613	-	59,73,73	1.43	4 (6%)	67,113,113	1.71	11 (16%)
22	CLA	b	605	-	59,73,73	1.83	10 (16%)	67,113,113	1.98	19 (28%)
33	STE	E	102	-	8,11,19	0.48	0	7,11,19	0.62	0
33	STE	T	102	-	14,14,19	0.45	0	13,13,19	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	616	-	41,41,41	1.18	5 (12%)	56,56,56	1.44	12 (21%)
29	SQD	b	619	-	48,49,54	0.96	2 (4%)	57,60,65	2.09	14 (24%)
33	STE	B	627	-	15,15,19	0.49	0	14,14,19	0.70	0
22	CLA	B	607	-	59,73,73	1.61	11 (18%)	67,113,113	1.49	12 (17%)
24	BCR	c	517	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	6 (10%)
22	CLA	B	615	-	59,73,73	1.54	7 (11%)	67,113,113	1.78	14 (20%)
22	CLA	b	601	-	59,73,73	1.40	9 (15%)	67,113,113	1.75	9 (13%)
27	PL9	a	410	-	55,55,55	1.09	5 (9%)	68,69,69	1.57	12 (17%)
33	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.87	0
33	STE	B	621	-	13,16,19	0.34	0	12,16,19	1.24	1 (8%)
24	BCR	B	618	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
24	BCR	C	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	7 (12%)
28	LMG	D	411	-	20,26,55	0.55	0	18,26,63	1.13	1 (5%)
22	CLA	a	402	-	59,73,73	1.50	5 (8%)	67,113,113	1.61	12 (17%)
22	CLA	c	504	-	59,73,73	1.65	8 (13%)	67,113,113	1.47	7 (10%)
23	PHO	A	404	-	67,69,69	1.22	8 (11%)	85,99,99	1.26	11 (12%)
34	LHG	B	622	-	48,48,48	1.03	3 (6%)	51,54,54	1.08	2 (3%)
22	CLA	B	609	-	59,73,73	1.26	7 (11%)	67,113,113	1.59	10 (14%)
24	BCR	Y	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	7 (12%)
22	CLA	b	611	-	59,73,73	1.31	6 (10%)	67,113,113	1.63	13 (19%)
30	DGD	A	415	-	67,67,67	1.41	9 (13%)	81,81,81	1.44	13 (16%)
33	STE	M	103	-	9,9,19	0.43	0	8,8,19	0.58	0
22	CLA	C	508	36	59,73,73	1.57	5 (8%)	67,113,113	1.79	14 (20%)
33	STE	C	520	-	8,11,19	0.47	0	7,11,19	0.78	0
22	CLA	b	614	-	59,73,73	1.54	8 (13%)	67,113,113	1.68	13 (19%)
24	BCR	d	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
33	STE	b	625	-	16,19,19	0.52	0	15,19,19	0.60	0
26	BCT	A	409	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	608	36	59,73,73	1.49	9 (15%)	67,113,113	1.66	8 (11%)
22	CLA	A	403	36	59,73,73	1.51	7 (11%)	67,113,113	1.49	10 (14%)
33	STE	I	101	-	14,14,19	0.48	0	13,13,19	0.61	0
30	DGD	c	521	-	63,63,67	1.09	5 (7%)	77,77,81	1.38	10 (12%)
30	DGD	h	102	-	63,63,67	1.15	7 (11%)	77,77,81	1.51	16 (20%)
33	STE	d	412	-	16,19,19	0.42	0	15,19,19	0.84	0
33	STE	B	624	-	10,13,19	0.44	0	9,13,19	0.91	0
29	SQD	a	412	-	53,54,54	0.99	4 (7%)	62,65,65	1.86	11 (17%)
32	OXY	a	417[B]	1,3,36	0,16,16	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	502	-	59,73,73	1.68	9 (15%)	67,113,113	1.51	6 (8%)
29	SQD	A	413	-	51,52,54	0.93	4 (7%)	60,63,65	1.96	11 (18%)
33	STE	b	626	-	9,9,19	0.55	0	8,8,19	0.43	0
29	SQD	B	623	-	53,54,54	0.98	3 (5%)	62,65,65	1.82	10 (16%)
28	LMG	c	524	-	48,48,55	1.12	3 (6%)	56,56,63	1.33	7 (12%)
22	CLA	b	608	-	59,73,73	1.56	8 (13%)	67,113,113	1.55	14 (20%)
22	CLA	C	514	-	59,73,73	1.58	6 (10%)	67,113,113	1.42	10 (14%)
22	CLA	c	513	3	59,73,73	1.47	5 (8%)	67,113,113	1.60	10 (14%)
22	CLA	b	612	-	59,73,73	1.40	10 (16%)	67,113,113	1.67	15 (22%)
27	PL9	D	405	-	55,55,55	1.68	10 (18%)	68,69,69	1.73	16 (23%)
22	CLA	d	403	-	59,73,73	1.53	8 (13%)	67,113,113	1.55	10 (14%)
22	CLA	B	616	-	59,73,73	1.48	8 (13%)	67,113,113	1.43	10 (14%)
34	LHG	E	101	-	48,48,48	0.95	4 (8%)	51,54,54	1.19	5 (9%)
33	STE	h	103	-	13,13,19	0.42	0	12,12,19	0.63	0
33	STE	b	620	-	15,15,19	0.44	0	14,14,19	0.71	0
35	HEC	e	101	5,6	26,50,50	2.55	5 (19%)	18,82,82	2.42	4 (22%)
22	CLA	c	515	-	59,73,73	1.40	6 (10%)	67,113,113	1.25	7 (10%)
24	BCR	T	101	-	41,41,41	1.04	4 (9%)	56,56,56	1.37	6 (10%)
24	BCR	c	518	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	7 (12%)
22	CLA	c	507	-	59,73,73	1.37	7 (11%)	67,113,113	1.51	10 (14%)
22	CLA	B	617	-	54,68,73	1.51	8 (14%)	61,107,113	1.99	17 (27%)
34	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	1.43	8 (15%)
24	BCR	D	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	4 (7%)
24	BCR	b	617	-	41,41,41	1.26	4 (9%)	56,56,56	1.28	8 (14%)
23	PHO	a	404	-	67,69,69	1.14	7 (10%)	85,99,99	1.08	8 (9%)
33	STE	B	601	-	8,11,19	0.37	0	7,11,19	0.65	0
28	LMG	D	406	-	51,51,55	0.88	3 (5%)	59,59,63	1.48	9 (15%)
22	CLA	D	403	-	59,73,73	1.46	9 (15%)	67,113,113	1.47	11 (16%)
24	BCR	x	101	-	41,41,41	1.08	4 (9%)	56,56,56	1.38	10 (17%)
22	CLA	c	508	-	59,73,73	1.36	6 (10%)	67,113,113	1.57	14 (20%)
33	STE	B	625	-	8,11,19	0.31	0	7,11,19	0.92	0
24	BCR	a	406	-	41,41,41	1.07	2 (4%)	56,56,56	1.44	9 (16%)
33	STE	a	414	-	9,9,19	0.51	0	8,8,19	0.43	0
22	CLA	C	503	-	59,73,73	1.27	6 (10%)	67,113,113	1.74	9 (13%)
34	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.13	4 (7%)
24	BCR	c	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	B	628	-	14,14,19	0.41	0	13,13,19	0.87	0
33	STE	Z	102	-	7,7,19	0.30	0	6,6,19	0.75	0
22	CLA	B	603	-	59,73,73	1.47	6 (10%)	67,113,113	1.63	12 (17%)
28	LMG	B	629	-	55,55,55	1.47	6 (10%)	63,63,63	1.47	7 (11%)
22	CLA	C	509	-	59,73,73	1.52	7 (11%)	67,113,113	1.80	14 (20%)
22	CLA	B	610	-	59,73,73	1.50	10 (16%)	67,113,113	1.53	14 (20%)
33	STE	d	410	-	13,16,19	0.37	0	12,16,19	1.03	0
22	CLA	c	510	-	58,72,73	1.54	6 (10%)	65,111,113	1.51	12 (18%)
22	CLA	c	514	-	59,73,73	1.50	9 (15%)	67,113,113	1.68	12 (17%)
30	DGD	C	518	-	63,63,67	0.94	5 (7%)	77,77,81	1.31	7 (9%)
22	CLA	A	402	-	59,73,73	1.43	7 (11%)	67,113,113	1.38	9 (13%)
33	STE	C	522	-	8,11,19	0.31	0	7,11,19	1.19	1 (14%)
22	CLA	B	612	-	59,73,73	1.52	7 (11%)	67,113,113	1.62	13 (19%)
22	CLA	c	505	-	59,73,73	1.58	8 (13%)	67,113,113	1.61	11 (16%)
22	CLA	b	602	-	59,73,73	1.48	9 (15%)	67,113,113	1.75	15 (22%)
33	STE	c	501	-	8,11,19	0.41	0	7,11,19	0.80	0
29	SQD	f	101	-	40,41,54	1.10	5 (12%)	49,52,65	2.02	13 (26%)
28	LMG	c	525	-	49,49,55	1.00	5 (10%)	57,57,63	1.34	5 (8%)
28	LMG	b	623	-	55,55,55	0.93	1 (1%)	63,63,63	1.49	9 (14%)
28	LMG	d	409	-	44,44,55	0.99	3 (6%)	52,52,63	1.40	7 (13%)
28	LMG	M	101	-	51,51,55	0.94	3 (5%)	59,59,63	1.40	11 (18%)
22	CLA	A	405	-	48,62,73	1.48	5 (10%)	53,99,113	1.57	11 (20%)
24	BCR	B	620	-	41,41,41	1.09	3 (7%)	56,56,56	1.34	7 (12%)
28	LMG	A	412	-	48,48,55	1.03	2 (4%)	56,56,63	1.44	8 (14%)
28	LMG	b	621	-	51,51,55	0.98	3 (5%)	59,59,63	1.46	10 (16%)
22	CLA	h	101	36	59,73,73	1.58	8 (13%)	67,113,113	1.77	8 (11%)
28	LMG	C	519	-	48,48,55	1.14	4 (8%)	56,56,63	1.36	6 (10%)
33	STE	b	622	-	16,19,19	0.43	0	15,19,19	0.76	0
22	CLA	b	606	36	59,73,73	1.30	4 (6%)	67,113,113	1.64	10 (14%)
22	CLA	c	512	-	59,73,73	1.46	7 (11%)	67,113,113	1.46	11 (16%)
28	LMG	c	522	-	37,37,55	1.33	6 (16%)	45,45,63	1.26	6 (13%)
22	CLA	c	506	36	54,68,73	1.48	5 (9%)	61,107,113	1.66	15 (24%)
22	CLA	B	614	-	59,73,73	1.64	7 (11%)	67,113,113	1.60	15 (22%)
35	HEC	v	201	17	26,50,50	2.37	3 (11%)	18,82,82	2.21	7 (38%)
33	STE	L	101	-	8,11,19	0.48	0	7,11,19	0.43	0
34	LHG	d	407	-	48,48,48	1.01	3 (6%)	51,54,54	1.24	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	e	102	-	41,41,48	1.04	4 (9%)	44,47,54	1.37	5 (11%)
24	BCR	B	619	-	41,41,41	1.01	2 (4%)	56,56,56	1.40	10 (17%)
22	CLA	b	610	-	59,73,73	1.30	5 (8%)	67,113,113	1.60	11 (16%)
33	STE	j	101	-	8,11,19	0.63	0	7,11,19	0.27	0
22	CLA	C	505	36	53,67,73	1.66	6 (11%)	59,105,113	1.71	12 (20%)
24	BCR	A	406	-	41,41,41	1.05	2 (4%)	56,56,56	1.49	8 (14%)
23	PHO	d	401	-	67,69,69	1.24	7 (10%)	85,99,99	1.11	7 (8%)
22	CLA	C	504	-	59,73,73	1.78	7 (11%)	67,113,113	1.80	11 (16%)
22	CLA	a	405	-	59,73,73	1.57	11 (18%)	67,113,113	1.65	12 (17%)
32	OEY	A	417[B]	1,3,36	0,16,16	0.00	-	-		
22	CLA	B	604	-	59,73,73	1.39	7 (11%)	67,113,113	1.51	14 (20%)
22	CLA	C	510	-	59,73,73	1.31	7 (11%)	67,113,113	1.70	10 (14%)
33	STE	a	415	-	8,11,19	0.55	0	7,11,19	0.86	0
22	CLA	B	606	-	59,73,73	1.28	6 (10%)	67,113,113	1.53	11 (16%)
30	DGD	H	102	-	63,63,67	1.39	11 (17%)	77,77,81	1.46	15 (19%)
29	SQD	A	414	-	38,38,54	1.07	3 (7%)	40,40,65	1.39	3 (7%)
33	STE	b	624	-	12,15,19	0.48	0	11,15,19	0.64	0
30	DGD	c	519	-	63,63,67	1.37	8 (12%)	77,77,81	1.42	15 (19%)
22	CLA	C	511	-	59,73,73	1.36	7 (11%)	67,113,113	1.49	8 (11%)
30	DGD	c	520	-	63,63,67	1.05	4 (6%)	77,77,81	1.43	10 (12%)
29	SQD	a	413	-	35,35,54	1.23	2 (5%)	37,37,65	1.49	6 (16%)
24	BCR	K	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.18	6 (10%)
33	STE	C	521	-	15,15,19	0.46	0	14,14,19	0.67	0
24	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.49	10 (17%)
33	STE	J	101	-	8,11,19	0.34	0	7,11,19	1.11	1 (14%)
22	CLA	c	503	-	59,73,73	1.29	7 (11%)	67,113,113	1.74	12 (17%)
22	CLA	A	411	36	59,73,73	1.55	8 (13%)	67,113,113	1.38	11 (16%)
24	BCR	y	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.09	2 (3%)
22	CLA	B	611	36	59,73,73	1.63	7 (11%)	67,113,113	1.84	13 (19%)
22	CLA	d	402	-	59,73,73	1.53	7 (11%)	67,113,113	1.45	14 (20%)
33	STE	X	101	-	16,19,19	0.33	0	15,19,19	1.13	2 (13%)
33	STE	c	523	-	16,19,19	0.47	0	15,19,19	0.66	0
22	CLA	c	509	36	59,73,73	1.27	4 (6%)	67,113,113	1.62	13 (19%)
24	BCR	t	101	-	41,41,41	0.93	1 (2%)	56,56,56	1.35	5 (8%)
22	CLA	b	613	-	59,73,73	1.48	7 (11%)	67,113,113	1.37	12 (17%)
26	BCT	a	409	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	D	401	-	67,69,69	1.14	6 (8%)	85,99,99	1.24	10 (11%)
22	CLA	C	507	-	59,73,73	1.56	8 (13%)	67,113,113	1.42	10 (14%)
22	CLA	a	403	36	59,73,73	1.48	6 (10%)	67,113,113	1.42	8 (11%)

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
22	CLA	b	607	-	2/2/25/25	10/37/135/135	-
22	CLA	B	602	36	3/3/25/25	17/37/135/135	-
28	LMG	D	410	-	-	15/33/33/70	-
22	CLA	b	615	-	3/3/24/25	9/31/129/135	-
22	CLA	C	506	-	2/2/25/25	13/37/135/135	-
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
22	CLA	C	512	3	3/3/25/25	11/37/135/135	-
33	STE	B	626	-	-	6/13/15/17	-
22	CLA	B	605	-	3/3/25/25	12/37/135/135	-
34	LHG	d	408	-	-	15/43/43/53	-
24	BCR	b	618	-	-	4/29/63/63	0/2/2/2
33	STE	M	102	-	-	4/10/12/17	-
27	PL9	d	405	-	-	13/53/73/73	0/1/1/1
22	CLA	b	609	36	3/3/25/25	5/37/135/135	-
22	CLA	b	603	-	3/3/25/25	6/37/135/135	-
33	STE	H	103	-	-	8/15/15/17	-
35	HEC	F	101	5,6	-	0/6/54/54	-
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
34	LHG	D	409	-	-	25/51/51/53	-
34	LHG	D	408	-	-	22/53/53/53	-
22	CLA	a	411	36	2/2/25/25	4/37/135/135	-
22	CLA	D	402	-	2/2/25/25	5/37/135/135	-
22	CLA	b	606	36	3/3/25/25	12/37/135/135	-
24	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
33	STE	d	411	-	-	10/15/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	C	517	-	-	18/51/91/95	0/2/2/2
34	LHG	d	406	-	-	22/53/53/53	-
22	CLA	B	613	-	3/3/25/25	9/37/135/135	-
22	CLA	C	510	-	3/3/25/25	8/37/135/135	-
33	STE	E	102	-	-	3/7/9/17	-
33	STE	T	102	-	-	7/12/12/17	-
24	BCR	b	616	-	-	6/29/63/63	0/2/2/2
29	SQD	b	619	-	-	19/44/64/69	0/1/1/1
33	STE	B	627	-	-	6/13/13/17	-
22	CLA	B	607	-	3/3/25/25	10/37/135/135	-
24	BCR	c	517	-	-	9/29/63/63	0/2/2/2
22	CLA	B	615	-	3/3/25/25	14/37/135/135	-
22	CLA	C	514	-	2/2/25/25	12/37/135/135	-
27	PL9	a	410	-	-	17/53/73/73	0/1/1/1
35	HEC	V	201	17	-	0/6/54/54	-
33	STE	B	621	-	-	4/12/14/17	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
28	LMG	D	411	-	-	7/18/22/70	-
22	CLA	a	402	-	3/3/25/25	7/37/135/135	-
22	CLA	c	504	-	2/2/25/25	7/37/135/135	-
23	PHO	A	404	-	-	4/53/103/103	0/5/6/6
34	LHG	B	622	-	-	20/53/53/53	-
22	CLA	B	609	-	2/2/25/25	2/37/135/135	-
24	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
22	CLA	b	611	-	3/3/25/25	6/37/135/135	-
30	DGD	A	415	-	-	21/55/95/95	0/2/2/2
33	STE	M	103	-	-	2/7/7/17	-
22	CLA	C	508	36	3/3/25/25	8/37/135/135	-
33	STE	C	520	-	-	3/7/9/17	-
22	CLA	b	614	-	3/3/25/25	11/37/135/135	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
33	STE	b	625	-	-	6/15/17/17	-
22	CLA	B	610	-	-	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	b	623	-	-	21/50/70/70	0/1/1/1
22	CLA	B	608	36	3/3/25/25	10/37/135/135	-
22	CLA	A	403	36	3/3/25/25	10/37/135/135	-
33	STE	I	101	-	-	4/12/12/17	-
30	DGD	c	521	-	-	13/51/91/95	0/2/2/2
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
33	STE	d	412	-	-	7/15/17/17	-
33	STE	B	624	-	-	3/9/11/17	-
29	SQD	a	412	-	-	30/49/69/69	0/1/1/1
22	CLA	c	511	-	3/3/25/25	9/37/135/135	-
22	CLA	C	502	-	2/2/25/25	3/37/135/135	-
35	HEC	e	101	5,6	-	0/6/54/54	-
33	STE	b	626	-	-	5/7/7/17	-
29	SQD	B	623	-	-	21/49/69/69	0/1/1/1
28	LMG	c	524	-	-	23/43/63/70	0/1/1/1
22	CLA	b	608	-	1/1/25/25	6/37/135/135	-
22	CLA	b	601	-	3/3/25/25	8/37/135/135	-
22	CLA	c	513	3	3/3/25/25	11/37/135/135	-
22	CLA	b	612	-	3/3/25/25	4/37/135/135	-
27	PL9	D	405	-	-	9/53/73/73	0/1/1/1
22	CLA	d	403	-	3/3/25/25	7/37/135/135	-
22	CLA	B	616	-	3/3/25/25	8/37/135/135	-
34	LHG	E	101	-	-	29/53/53/53	-
33	STE	b	620	-	-	6/13/13/17	-
33	STE	h	103	-	-	5/11/11/17	-
33	STE	C	522	-	-	3/7/9/17	-
22	CLA	c	515	-	3/3/25/25	8/37/135/135	-
22	CLA	C	511	-	3/3/25/25	9/37/135/135	-
24	BCR	c	518	-	-	11/29/63/63	0/2/2/2
22	CLA	c	507	-	2/2/25/25	5/37/135/135	-
22	CLA	B	617	-	3/3/24/25	6/31/129/135	-
34	LHG	D	412	-	-	17/53/53/53	-
24	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	BCR	b	617	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	a	404	-	-	4/53/103/103	0/5/6/6
33	STE	B	601	-	-	2/7/9/17	-
28	LMG	D	406	-	-	17/46/66/70	0/1/1/1
22	CLA	D	403	-	2/2/25/25	8/37/135/135	-
24	BCR	x	101	-	-	6/29/63/63	0/2/2/2
22	CLA	c	508	-	2/2/25/25	18/37/135/135	-
33	STE	B	625	-	-	3/7/9/17	-
24	BCR	a	406	-	-	8/29/63/63	0/2/2/2
33	STE	a	414	-	-	3/7/7/17	-
22	CLA	C	503	-	3/3/25/25	10/37/135/135	-
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
24	BCR	c	516	-	-	13/29/63/63	0/2/2/2
33	STE	B	628	-	-	7/12/12/17	-
33	STE	Z	102	-	-	2/5/5/17	-
22	CLA	B	603	-	1/1/25/25	5/37/135/135	-
28	LMG	B	629	-	-	29/50/70/70	0/1/1/1
22	CLA	C	509	-	2/2/25/25	6/37/135/135	-
33	STE	l	102	-	-	7/15/15/17	-
33	STE	d	410	-	-	9/12/14/17	-
22	CLA	c	510	-	2/2/24/25	12/36/134/135	-
22	CLA	c	514	-	3/3/25/25	21/37/135/135	-
30	DGD	C	518	-	-	15/51/91/95	0/2/2/2
22	CLA	A	402	-	3/3/25/25	3/37/135/135	-
22	CLA	d	402	-	2/2/25/25	8/37/135/135	-
22	CLA	B	612	-	3/3/25/25	12/37/135/135	-
22	CLA	c	505	-	1/1/25/25	4/37/135/135	-
22	CLA	b	602	-	3/3/25/25	8/37/135/135	-
27	PL9	A	410	-	-	19/53/73/73	0/1/1/1
33	STE	c	501	-	-	3/7/9/17	-
29	SQD	f	101	-	-	13/36/56/69	0/1/1/1
28	LMG	c	525	-	-	18/44/64/70	0/1/1/1
28	LMG	d	409	-	-	12/39/59/70	0/1/1/1
22	CLA	C	505	36	3/3/23/25	9/30/128/135	-
22	CLA	A	405	-	3/3/22/25	6/24/122/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
28	LMG	A	412	-	-	13/43/63/70	0/1/1/1
28	LMG	b	621	-	-	21/46/66/70	0/1/1/1
22	CLA	h	101	36	3/3/25/25	18/37/135/135	-
28	LMG	C	519	-	-	19/43/63/70	0/1/1/1
33	STE	b	622	-	-	9/15/17/17	-
22	CLA	C	513	-	3/3/25/25	-	-
22	CLA	c	512	-	3/3/25/25	12/37/135/135	-
28	LMG	c	522	-	-	9/31/51/70	0/1/1/1
22	CLA	c	506	36	3/3/24/25	9/31/129/135	-
22	CLA	B	614	-	3/3/25/25	10/37/135/135	-
35	HEC	v	201	17	-	0/6/54/54	-
33	STE	L	101	-	-	5/7/9/17	-
34	LHG	d	407	-	-	19/53/53/53	-
34	LHG	e	102	-	-	25/46/46/53	-
24	BCR	B	619	-	-	9/29/63/63	0/2/2/2
22	CLA	b	610	-	2/2/25/25	8/37/135/135	-
28	LMG	M	101	-	-	19/46/66/70	0/1/1/1
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
23	PHO	d	401	-	-	7/53/103/103	0/5/6/6
22	CLA	C	504	-	1/1/25/25	4/37/135/135	-
22	CLA	a	405	-	3/3/25/25	7/37/135/135	-
22	CLA	B	604	-	3/3/25/25	9/37/135/135	-
22	CLA	b	605	-	3/3/25/25	11/37/135/135	-
33	STE	a	415	-	-	3/7/9/17	-
22	CLA	B	606	-	3/3/25/25	9/37/135/135	-
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
29	SQD	A	414	-	-	14/39/39/69	-
33	STE	b	624	-	-	7/11/13/17	-
30	DGD	c	519	-	-	24/51/91/95	0/2/2/2
22	CLA	b	604	-	3/3/25/25	10/37/135/135	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
29	SQD	a	413	-	-	21/37/37/69	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	C	521	-	-	5/13/13/17	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	STE	J	101	-	-	3/7/9/17	-
22	CLA	c	503	-	3/3/25/25	5/37/135/135	-
22	CLA	A	411	36	1/1/25/25	11/37/135/135	-
24	BCR	y	101	-	-	11/29/63/63	0/2/2/2
22	CLA	B	611	36	3/3/25/25	6/37/135/135	-
33	STE	j	101	-	-	4/7/9/17	-
33	STE	X	101	-	-	9/15/17/17	-
33	STE	c	523	-	-	9/15/17/17	-
22	CLA	c	509	36	3/3/25/25	7/37/135/135	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
22	CLA	b	613	-	3/3/25/25	19/37/135/135	-
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
22	CLA	C	507	-	3/3/25/25	14/37/135/135	-
34	LHG	l	101	-	-	20/53/53/53	-
22	CLA	a	403	36	1/1/25/25	14/37/135/135	-

All (776) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	101	HEC	C3B-C2B	-9.06	1.31	1.40
22	a	411	CLA	MG-NA	8.98	2.27	2.06
22	C	512	CLA	MG-NA	8.92	2.27	2.06
22	b	605	CLA	MG-NA	8.78	2.27	2.06
22	B	611	CLA	C4B-NB	8.22	1.42	1.35
22	C	505	CLA	C4B-NB	8.21	1.42	1.35
22	B	614	CLA	C4B-NB	7.93	1.42	1.35
22	B	615	CLA	C4B-NB	7.83	1.42	1.35
22	b	613	CLA	C4B-NB	7.82	1.42	1.35
22	C	504	CLA	C4B-NB	7.79	1.42	1.35
22	B	602	CLA	C4B-NB	7.78	1.42	1.35
22	c	511	CLA	C4B-NB	7.77	1.42	1.35
22	a	411	CLA	C4B-NB	7.77	1.42	1.35
22	C	514	CLA	C4B-NB	7.68	1.42	1.35
22	c	504	CLA	C4B-NB	7.66	1.42	1.35
22	d	403	CLA	C4B-NB	7.62	1.42	1.35
22	B	613	CLA	C4B-NB	7.51	1.41	1.35
22	C	507	CLA	C4B-NB	7.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	C4B-NB	7.42	1.41	1.35
22	c	514	CLA	C4B-NB	7.41	1.41	1.35
22	c	506	CLA	C4B-NB	7.40	1.41	1.35
22	A	411	CLA	C4B-NB	7.38	1.41	1.35
22	C	506	CLA	C4B-NB	7.30	1.41	1.35
35	v	201	HEC	C3B-C2B	-7.29	1.33	1.40
22	A	403	CLA	C4B-NB	7.27	1.41	1.35
22	B	605	CLA	MG-NA	7.25	2.23	2.06
22	b	608	CLA	C4B-NB	7.25	1.41	1.35
22	d	402	CLA	C4B-NB	7.24	1.41	1.35
22	A	402	CLA	C4B-NB	7.23	1.41	1.35
22	B	603	CLA	C4B-NB	7.17	1.41	1.35
22	C	502	CLA	C4B-NB	7.17	1.41	1.35
22	C	504	CLA	MG-NA	7.15	2.23	2.06
22	B	616	CLA	C4B-NB	7.15	1.41	1.35
22	b	607	CLA	C4B-NB	7.12	1.41	1.35
22	C	508	CLA	C4B-NB	7.06	1.41	1.35
22	b	603	CLA	C4B-NB	7.05	1.41	1.35
35	F	101	HEC	C3B-C2B	-7.01	1.33	1.40
22	A	405	CLA	C4B-NB	6.90	1.41	1.35
22	C	509	CLA	C4B-NB	6.88	1.41	1.35
22	c	505	CLA	C4B-NB	6.87	1.41	1.35
22	c	515	CLA	C4B-NB	6.87	1.41	1.35
22	B	610	CLA	C4B-NB	6.86	1.41	1.35
22	a	402	CLA	C4B-NB	6.85	1.41	1.35
22	C	511	CLA	C4B-NB	6.83	1.41	1.35
22	b	601	CLA	C4B-NB	6.79	1.41	1.35
22	h	101	CLA	C4B-NB	6.76	1.41	1.35
22	a	405	CLA	C4B-NB	6.71	1.41	1.35
22	B	612	CLA	MG-NA	6.71	2.22	2.06
22	c	510	CLA	C4B-NB	6.47	1.41	1.35
22	D	403	CLA	C4B-NB	6.45	1.41	1.35
22	C	508	CLA	MG-NA	6.39	2.21	2.06
35	F	101	HEC	C3C-C2C	-6.37	1.34	1.40
22	C	513	CLA	C4B-NB	6.37	1.40	1.35
22	B	608	CLA	C4B-NB	6.36	1.40	1.35
22	D	402	CLA	C4B-NB	6.36	1.40	1.35
22	c	503	CLA	C4B-NB	6.35	1.40	1.35
22	c	509	CLA	C4B-NB	6.34	1.40	1.35
22	B	607	CLA	MG-NA	6.34	2.21	2.06
28	B	629	LMG	C4-C5	6.26	1.66	1.53
22	a	403	CLA	C4B-NB	6.23	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEC	C3B-C2B	-6.21	1.34	1.40
35	V	201	HEC	C3C-C2C	-6.21	1.34	1.40
22	b	611	CLA	C4B-NB	6.18	1.40	1.35
22	c	512	CLA	C4B-NB	6.16	1.40	1.35
22	c	513	CLA	C4B-NB	6.11	1.40	1.35
22	B	604	CLA	MG-NA	6.10	2.20	2.06
22	c	505	CLA	MG-NC	6.09	2.20	2.06
27	d	405	PL9	C6-C1	-6.03	1.37	1.48
22	b	614	CLA	MG-NA	6.02	2.20	2.06
22	c	508	CLA	C4B-NB	5.99	1.40	1.35
27	D	405	PL9	C7-C3	-5.88	1.45	1.51
22	C	510	CLA	C4B-NB	5.87	1.40	1.35
22	C	502	CLA	MG-NA	5.79	2.20	2.06
22	b	614	CLA	C4B-NB	5.79	1.40	1.35
22	c	507	CLA	C4B-NB	5.74	1.40	1.35
22	b	606	CLA	C4B-NB	5.58	1.40	1.35
22	b	610	CLA	C4B-NB	5.55	1.40	1.35
22	h	101	CLA	MG-NA	5.53	2.19	2.06
35	v	201	HEC	C3C-C2C	-5.52	1.35	1.40
22	C	514	CLA	MG-NA	5.51	2.19	2.06
22	b	612	CLA	C4B-NB	5.49	1.40	1.35
22	b	604	CLA	C4B-NB	5.45	1.40	1.35
22	a	403	CLA	MG-NC	5.45	2.19	2.06
22	b	605	CLA	C4B-NB	5.45	1.40	1.35
22	b	602	CLA	C4B-NB	5.26	1.39	1.35
22	c	513	CLA	MG-NA	5.24	2.18	2.06
22	B	617	CLA	C4B-NB	5.20	1.39	1.35
22	B	607	CLA	C4B-NB	5.11	1.39	1.35
22	c	510	CLA	MG-NA	5.10	2.18	2.06
22	c	504	CLA	MG-NA	5.05	2.18	2.06
27	d	405	PL9	C3-C4	-5.04	1.41	1.49
22	B	606	CLA	C4B-NB	5.03	1.39	1.35
35	e	101	HEC	C3C-C2C	-5.01	1.35	1.40
22	B	612	CLA	C4B-NB	4.98	1.39	1.35
22	c	512	CLA	MG-NA	4.84	2.17	2.06
22	B	617	CLA	MG-NA	4.82	2.17	2.06
22	A	411	CLA	MG-NA	4.78	2.17	2.06
35	F	101	HEC	C3D-C2D	4.77	1.51	1.37
22	b	609	CLA	C4B-NB	4.76	1.39	1.35
30	c	519	DGD	C4D-C3D	4.73	1.64	1.52
22	B	609	CLA	C4B-NB	4.73	1.39	1.35
22	C	507	CLA	MG-NA	4.71	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	101	BCR	C30-C25	-4.70	1.47	1.53
24	C	515	BCR	C1-C6	-4.70	1.47	1.53
22	c	511	CLA	MG-NC	4.70	2.17	2.06
34	B	622	LHG	O7-C5	-4.69	1.34	1.46
35	v	201	HEC	C3D-C2D	4.69	1.51	1.37
34	D	408	LHG	O8-C6	-4.68	1.34	1.45
35	e	101	HEC	C3D-C2D	4.66	1.51	1.37
22	a	402	CLA	MG-NA	4.61	2.17	2.06
35	V	201	HEC	C3D-C2D	4.61	1.51	1.37
27	A	410	PL9	C7-C3	-4.57	1.46	1.51
22	C	503	CLA	C4B-NB	4.56	1.39	1.35
24	Y	101	BCR	C30-C25	-4.53	1.47	1.53
22	B	605	CLA	C4B-NB	4.51	1.39	1.35
22	a	405	CLA	MG-NA	4.41	2.16	2.06
22	b	612	CLA	MG-NA	4.39	2.16	2.06
30	A	415	DGD	C3G-C2G	4.39	1.64	1.50
22	b	609	CLA	MG-NC	4.36	2.16	2.06
22	B	614	CLA	MG-NC	4.35	2.16	2.06
22	b	602	CLA	MG-NA	4.31	2.16	2.06
22	b	605	CLA	C1B-NB	4.30	1.39	1.35
22	C	505	CLA	MG-NA	4.26	2.16	2.06
30	H	102	DGD	C4E-C5E	4.24	1.62	1.53
24	D	404	BCR	C30-C25	-4.22	1.48	1.53
28	B	629	LMG	C4-C3	4.19	1.63	1.52
22	b	606	CLA	MG-NA	4.19	2.16	2.06
22	b	608	CLA	MG-NA	4.09	2.16	2.06
22	C	506	CLA	MG-NA	4.08	2.16	2.06
24	b	616	BCR	C1-C6	-4.05	1.48	1.53
27	D	405	PL9	C52-C5	-4.04	1.42	1.50
28	C	519	LMG	C4-C5	4.01	1.61	1.53
22	B	602	CLA	MG-NA	3.97	2.15	2.06
30	C	517	DGD	O5D-C1E	3.91	1.46	1.40
22	C	503	CLA	MG-NA	3.87	2.15	2.06
27	D	405	PL9	C6-C1	-3.85	1.41	1.48
22	B	615	CLA	MG-NA	3.85	2.15	2.06
22	C	509	CLA	MG-NA	3.85	2.15	2.06
22	D	403	CLA	MG-NA	3.83	2.15	2.06
27	D	405	PL9	C41-C39	-3.83	1.43	1.51
22	B	611	CLA	C3B-C2B	-3.82	1.35	1.40
22	b	615	CLA	C4B-NB	3.80	1.38	1.35
22	B	607	CLA	C3B-C2B	-3.78	1.35	1.40
24	c	517	BCR	C1-C6	-3.77	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	CHC-C1C	3.76	1.44	1.35
24	c	516	BCR	C1-C6	-3.74	1.48	1.53
22	c	510	CLA	CHC-C1C	3.73	1.44	1.35
24	x	101	BCR	C30-C25	-3.72	1.48	1.53
24	d	404	BCR	C1-C6	-3.69	1.48	1.53
30	c	521	DGD	O2G-C2G	-3.66	1.37	1.46
30	C	517	DGD	C4D-C3D	3.66	1.61	1.52
22	b	609	CLA	C3B-C2B	-3.66	1.35	1.40
24	A	406	BCR	C1-C6	-3.65	1.48	1.53
22	C	502	CLA	CHC-C1C	3.65	1.44	1.35
22	d	402	CLA	MG-NA	3.61	2.14	2.06
22	C	513	CLA	MG-NA	3.60	2.14	2.06
29	a	413	SQD	O47-C7	3.60	1.44	1.34
24	b	617	BCR	C30-C25	-3.59	1.48	1.53
29	B	623	SQD	O47-C7	3.59	1.44	1.34
22	a	405	CLA	MG-NC	-3.57	1.97	2.06
30	c	519	DGD	O5D-C6D	3.56	1.50	1.43
22	B	614	CLA	MG-NA	3.52	2.14	2.06
29	a	413	SQD	O48-C23	3.51	1.43	1.33
22	B	604	CLA	C4B-NB	3.48	1.38	1.35
27	a	410	PL9	C6-C1	-3.48	1.42	1.48
24	B	618	BCR	C1-C6	-3.47	1.49	1.53
22	C	505	CLA	CHC-C1C	3.47	1.43	1.35
30	A	415	DGD	C4D-C3D	3.47	1.61	1.52
34	D	412	LHG	O7-C5	-3.47	1.37	1.46
29	A	414	SQD	O48-C23	3.46	1.43	1.33
22	b	614	CLA	CHC-C1C	3.46	1.43	1.35
34	d	407	LHG	O7-C5	-3.46	1.37	1.46
24	b	618	BCR	C1-C6	-3.45	1.49	1.53
27	d	405	PL9	C53-C6	-3.44	1.43	1.50
27	d	405	PL9	C46-C44	-3.44	1.44	1.51
22	C	504	CLA	CHC-C1C	3.44	1.43	1.35
22	C	509	CLA	C1D-C2D	3.42	1.50	1.42
22	b	604	CLA	CHC-C1C	3.41	1.43	1.35
22	h	101	CLA	CHC-C1C	3.41	1.43	1.35
22	b	607	CLA	CHC-C1C	3.40	1.43	1.35
28	A	412	LMG	O1-C7	-3.38	1.37	1.43
22	a	402	CLA	CHC-C1C	3.38	1.43	1.35
24	Z	101	BCR	C30-C25	-3.37	1.49	1.53
22	c	514	CLA	CHC-C1C	3.37	1.43	1.35
28	c	524	LMG	C3-C2	3.36	1.60	1.52
24	y	101	BCR	C30-C25	-3.35	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	CHC-C1C	3.35	1.43	1.35
27	D	405	PL9	C11-C9	-3.35	1.44	1.51
29	a	412	SQD	O48-C23	3.34	1.43	1.33
22	B	608	CLA	MG-NC	3.33	2.14	2.06
29	b	619	SQD	O48-C23	3.31	1.43	1.33
22	A	402	CLA	C1D-C2D	3.30	1.50	1.42
22	B	616	CLA	CHC-C1C	3.30	1.43	1.35
22	c	507	CLA	CHC-C1C	3.30	1.43	1.35
30	C	517	DGD	O3E-C3E	-3.29	1.35	1.43
22	c	504	CLA	CHC-C1C	3.29	1.43	1.35
30	c	520	DGD	O3G-C3G	-3.27	1.37	1.43
29	A	414	SQD	O47-C7	3.27	1.43	1.34
24	d	404	BCR	C30-C25	-3.24	1.49	1.53
22	c	513	CLA	CHC-C1C	3.24	1.43	1.35
22	C	511	CLA	CHC-C1C	3.23	1.43	1.35
22	B	606	CLA	CHC-C1C	3.23	1.43	1.35
22	b	615	CLA	C3B-CAB	-3.22	1.41	1.47
22	b	608	CLA	CMB-C2B	-3.22	1.45	1.51
24	y	101	BCR	C1-C6	-3.21	1.49	1.53
22	c	515	CLA	CHC-C1C	3.21	1.43	1.35
30	C	517	DGD	C6E-C5E	3.20	1.62	1.51
24	b	617	BCR	C1-C6	-3.19	1.49	1.53
29	f	101	SQD	O47-C7	3.19	1.43	1.34
22	B	604	CLA	C3B-CAB	-3.18	1.41	1.47
24	B	618	BCR	C30-C25	-3.18	1.49	1.53
22	B	603	CLA	CHC-C1C	3.17	1.43	1.35
30	A	415	DGD	C4E-C5E	3.17	1.59	1.53
34	D	409	LHG	P-O6	3.17	1.72	1.59
22	B	604	CLA	CHC-C1C	3.17	1.43	1.35
22	c	514	CLA	MG-NC	3.15	2.13	2.06
22	C	512	CLA	CHC-C1C	3.15	1.43	1.35
22	C	503	CLA	CHC-C1C	3.14	1.43	1.35
22	B	611	CLA	CMB-C2B	-3.14	1.45	1.51
28	D	410	LMG	C9-C8	3.14	1.60	1.50
22	B	610	CLA	C3B-CAB	-3.14	1.41	1.47
22	a	411	CLA	CMB-C2B	-3.14	1.45	1.51
28	b	623	LMG	C3-C2	3.14	1.60	1.52
28	D	410	LMG	C7-C8	3.13	1.58	1.51
22	c	504	CLA	CMD-C2D	-3.12	1.44	1.51
22	B	614	CLA	CHC-C1C	3.12	1.43	1.35
22	B	603	CLA	MG-NA	3.12	2.13	2.06
28	c	522	LMG	O1-C1	3.12	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	MG-NC	3.11	2.13	2.06
29	D	407	SQD	O48-C23	3.11	1.42	1.33
22	B	607	CLA	CHC-C1C	3.10	1.42	1.35
22	C	509	CLA	CHC-C1C	3.10	1.42	1.35
22	B	609	CLA	C1D-C2D	3.10	1.49	1.42
34	d	406	LHG	O7-C5	-3.10	1.38	1.46
22	B	611	CLA	MG-NC	3.10	2.13	2.06
28	B	629	LMG	O8-C9	-3.09	1.38	1.45
22	a	403	CLA	CHC-C1C	3.09	1.42	1.35
22	B	617	CLA	CMC-C2C	-3.09	1.44	1.50
24	Y	101	BCR	C1-C6	-3.08	1.49	1.53
30	C	518	DGD	O2G-C2G	-3.08	1.38	1.46
34	e	102	LHG	P-O6	3.07	1.71	1.59
22	C	507	CLA	CHC-C1C	3.06	1.42	1.35
30	C	516	DGD	O2E-C2E	-3.06	1.35	1.43
28	c	522	LMG	C1-C2	3.06	1.61	1.52
30	C	516	DGD	C4D-C3D	3.05	1.60	1.52
34	d	407	LHG	C1-C2	-3.05	1.39	1.51
28	c	522	LMG	C3-C2	3.05	1.60	1.52
22	c	513	CLA	C1D-C2D	3.05	1.49	1.42
30	A	415	DGD	C1E-C2E	3.05	1.61	1.52
22	B	615	CLA	CHC-C1C	3.04	1.42	1.35
22	b	612	CLA	MG-NC	-3.04	1.99	2.06
24	K	101	BCR	C30-C25	-3.03	1.49	1.53
22	c	506	CLA	MG-NA	-3.03	1.99	2.06
22	B	603	CLA	C1D-C2D	3.02	1.49	1.42
30	h	102	DGD	C4E-C5E	3.02	1.59	1.53
22	c	508	CLA	CHC-C1C	3.02	1.42	1.35
22	B	611	CLA	CHC-C1C	3.02	1.42	1.35
28	b	621	LMG	C4-C3	3.02	1.60	1.52
24	B	620	BCR	C1-C6	-3.02	1.49	1.53
24	B	620	BCR	C30-C25	-3.01	1.49	1.53
22	b	602	CLA	MG-NC	3.00	2.13	2.06
28	c	525	LMG	O7-C8	-3.00	1.39	1.46
24	B	619	BCR	C30-C25	-3.00	1.49	1.53
22	C	513	CLA	CHC-C1C	2.99	1.42	1.35
22	A	403	CLA	MG-NC	2.99	2.13	2.06
22	b	603	CLA	CHC-C1C	2.99	1.42	1.35
23	A	404	PHO	C4C-NC	2.99	1.43	1.36
22	c	507	CLA	CMB-C2B	-2.98	1.45	1.51
22	A	403	CLA	CHC-C1C	2.98	1.42	1.35
22	d	403	CLA	CMD-C2D	-2.98	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	405	PL9	C36-C34	-2.98	1.45	1.51
22	B	610	CLA	C3B-C2B	-2.97	1.36	1.40
22	C	514	CLA	CHC-C1C	2.97	1.42	1.35
22	b	613	CLA	CMC-C2C	-2.97	1.44	1.50
22	B	602	CLA	C3B-C2B	-2.97	1.36	1.40
24	Z	101	BCR	C1-C6	-2.96	1.49	1.53
30	H	102	DGD	O5D-C1E	2.96	1.45	1.40
22	h	101	CLA	C1D-C2D	2.96	1.49	1.42
22	C	511	CLA	CMC-C2C	-2.96	1.44	1.50
30	c	519	DGD	O3G-C1D	-2.96	1.35	1.40
23	D	401	PHO	CMB-C2B	-2.95	1.44	1.50
23	a	404	PHO	C4C-C3C	2.95	1.50	1.45
22	C	510	CLA	CHC-C1C	2.95	1.42	1.35
30	A	415	DGD	C3D-C2D	2.95	1.59	1.52
22	b	611	CLA	CHC-C1C	2.95	1.42	1.35
22	B	617	CLA	CHC-C1C	2.95	1.42	1.35
22	d	402	CLA	CMB-C2B	-2.94	1.45	1.51
29	a	412	SQD	O47-C7	2.94	1.42	1.34
22	C	504	CLA	C1D-C2D	2.94	1.49	1.42
34	E	101	LHG	P-O6	2.94	1.71	1.59
22	c	512	CLA	CHC-C1C	2.94	1.42	1.35
22	b	607	CLA	C3B-C2B	-2.94	1.36	1.40
29	b	619	SQD	O47-C7	2.93	1.42	1.34
30	c	521	DGD	O3D-C3D	-2.93	1.36	1.43
30	A	415	DGD	C4D-C5D	2.93	1.59	1.53
22	C	513	CLA	CMB-C2B	-2.93	1.45	1.51
28	c	525	LMG	C4-C5	2.92	1.59	1.53
22	a	411	CLA	CHC-C1C	2.92	1.42	1.35
22	C	508	CLA	C1D-C2D	2.92	1.49	1.42
22	c	508	CLA	CMD-C2D	-2.92	1.44	1.51
22	a	405	CLA	CMC-C2C	-2.91	1.44	1.50
28	A	412	LMG	C4-C3	2.91	1.59	1.52
22	b	615	CLA	CMB-C2B	-2.91	1.45	1.51
34	d	407	LHG	O8-C6	-2.90	1.38	1.45
24	c	518	BCR	C1-C6	-2.90	1.49	1.53
22	d	403	CLA	CMB-C2B	-2.90	1.45	1.51
22	b	607	CLA	CMB-C2B	-2.89	1.45	1.51
29	A	414	SQD	O47-C45	-2.89	1.42	1.47
29	B	623	SQD	O48-C23	2.89	1.41	1.33
22	b	614	CLA	CMD-C2D	-2.89	1.44	1.51
34	E	101	LHG	C24-C23	2.89	1.59	1.50
22	B	609	CLA	CMD-C2D	-2.88	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	CMB-C2B	-2.88	1.45	1.51
24	b	618	BCR	C30-C25	-2.87	1.49	1.53
28	C	519	LMG	O7-C8	-2.86	1.39	1.46
22	c	507	CLA	C1B-NB	2.86	1.37	1.35
22	B	610	CLA	CMD-C2D	-2.86	1.44	1.51
24	b	616	BCR	C30-C25	-2.85	1.49	1.53
22	a	402	CLA	CMB-C2B	-2.85	1.45	1.51
22	B	617	CLA	C3B-CAB	-2.84	1.42	1.47
28	c	524	LMG	C4-C3	2.84	1.59	1.52
34	d	406	LHG	C24-C23	2.84	1.59	1.50
22	B	614	CLA	CMD-C2D	-2.84	1.44	1.51
29	f	101	SQD	O48-C23	2.84	1.41	1.33
22	B	604	CLA	C1D-C2D	2.84	1.49	1.42
22	c	512	CLA	CMB-C2B	-2.84	1.45	1.51
22	c	514	CLA	C1D-C2D	2.84	1.49	1.42
22	b	602	CLA	C1D-C2D	2.84	1.49	1.42
22	c	514	CLA	C3B-C2B	-2.83	1.36	1.40
24	c	518	BCR	C30-C25	-2.83	1.49	1.53
22	B	608	CLA	CHC-C1C	2.82	1.42	1.35
22	c	514	CLA	CMB-C2B	-2.82	1.45	1.51
30	c	520	DGD	O2G-C2G	-2.82	1.39	1.46
22	C	502	CLA	C3B-C2B	-2.82	1.36	1.40
30	A	415	DGD	O2G-C1B	2.82	1.42	1.34
22	b	608	CLA	C3B-CAB	-2.82	1.42	1.47
22	b	610	CLA	CHC-C1C	2.82	1.42	1.35
22	c	510	CLA	C3B-C2B	-2.82	1.36	1.40
23	d	401	PHO	C3B-C4B	2.81	1.49	1.43
24	C	515	BCR	C30-C25	-2.81	1.49	1.53
22	D	402	CLA	CHC-C1C	2.81	1.42	1.35
22	B	605	CLA	C1B-NB	2.81	1.37	1.35
22	b	604	CLA	CMD-C2D	-2.81	1.44	1.51
23	d	401	PHO	CHC-C4B	-2.81	1.33	1.40
22	a	402	CLA	C1D-C2D	2.81	1.48	1.42
28	c	522	LMG	C4-C5	2.80	1.58	1.53
34	e	102	LHG	O8-C23	2.80	1.41	1.33
22	B	616	CLA	CMB-C2B	-2.80	1.45	1.51
22	B	602	CLA	C1D-C2D	2.80	1.48	1.42
30	H	102	DGD	O6E-C1E	2.80	1.49	1.41
22	B	608	CLA	CMB-C2B	-2.79	1.45	1.51
22	c	515	CLA	CMB-C2B	-2.79	1.45	1.51
24	C	515	BCR	C36-C18	-2.79	1.45	1.50
22	c	506	CLA	CAC-C3C	-2.79	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	516	DGD	C2A-C1A	-2.78	1.42	1.50
22	B	613	CLA	MG-NA	2.77	2.12	2.06
22	c	505	CLA	CHC-C1C	2.77	1.42	1.35
22	B	612	CLA	CMB-C2B	-2.77	1.45	1.51
22	c	507	CLA	MG-NC	2.77	2.12	2.06
22	C	512	CLA	CMB-C2B	-2.76	1.45	1.51
23	d	401	PHO	CHC-C1C	2.76	1.44	1.38
23	D	401	PHO	C3B-C4B	2.76	1.49	1.43
22	B	615	CLA	C3B-C2B	-2.76	1.36	1.40
22	b	602	CLA	CMD-C2D	-2.75	1.45	1.51
22	b	608	CLA	C1D-C2D	2.75	1.48	1.42
22	c	508	CLA	C1D-C2D	2.75	1.48	1.42
22	d	402	CLA	C3B-C2B	-2.75	1.36	1.40
22	c	515	CLA	C1D-C2D	2.74	1.48	1.42
22	b	607	CLA	CMD-C2D	-2.74	1.45	1.51
30	H	102	DGD	C3D-C2D	2.74	1.59	1.52
22	B	608	CLA	C3B-CAB	-2.74	1.42	1.47
22	b	606	CLA	CHC-C1C	2.73	1.42	1.35
24	T	101	BCR	C1-C6	-2.72	1.50	1.53
22	b	603	CLA	CMC-C2C	-2.72	1.45	1.50
22	C	502	CLA	C1D-C2D	2.71	1.48	1.42
34	E	101	LHG	O7-C5	-2.71	1.39	1.46
22	b	601	CLA	CHC-C1C	2.70	1.41	1.35
22	B	603	CLA	CMB-C2B	-2.70	1.46	1.51
22	b	602	CLA	CHC-C1C	2.70	1.41	1.35
22	C	514	CLA	CMB-C2B	-2.70	1.46	1.51
30	c	521	DGD	C1D-C2D	2.69	1.60	1.52
22	c	509	CLA	C3B-C2B	-2.69	1.36	1.40
22	B	605	CLA	CHC-C1C	2.69	1.41	1.35
22	B	614	CLA	C3B-C2B	-2.68	1.36	1.40
30	H	102	DGD	O1G-C1G	-2.68	1.39	1.45
23	A	404	PHO	C1C-NC	-2.68	1.32	1.38
22	B	617	CLA	C3B-C2B	-2.68	1.36	1.40
22	A	411	CLA	C1D-C2D	2.67	1.48	1.42
22	B	602	CLA	CHC-C1C	2.67	1.41	1.35
24	a	406	BCR	C1-C6	-2.67	1.50	1.53
30	h	102	DGD	O2G-C1B	2.67	1.41	1.34
22	d	402	CLA	CMD-C2D	-2.66	1.45	1.51
22	b	610	CLA	C1D-C2D	2.66	1.48	1.42
23	A	404	PHO	CHC-C1C	2.66	1.43	1.38
22	d	403	CLA	CMC-C2C	-2.65	1.45	1.50
22	B	612	CLA	C3B-C2B	-2.65	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	CMD-C2D	-2.65	1.45	1.51
30	C	518	DGD	O3G-C3G	-2.64	1.38	1.43
22	b	610	CLA	CMD-C2D	-2.64	1.45	1.51
22	B	612	CLA	MG-NC	-2.64	2.00	2.06
22	c	505	CLA	C1D-C2D	2.63	1.48	1.42
27	a	410	PL9	C30-C29	-2.63	1.43	1.50
34	D	409	LHG	O3-C3	-2.63	1.34	1.44
22	C	502	CLA	CMD-C2D	-2.63	1.45	1.51
22	B	610	CLA	MG-NA	2.62	2.12	2.06
22	B	615	CLA	CMB-C2B	-2.62	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.62	1.45	1.51
22	C	506	CLA	CMC-C2C	-2.62	1.45	1.50
22	B	606	CLA	C3B-C2B	-2.62	1.36	1.40
22	b	603	CLA	C1D-C2D	2.62	1.48	1.42
22	c	509	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	615	CLA	CMC-C2C	-2.61	1.45	1.50
24	T	101	BCR	C30-C25	-2.61	1.50	1.53
22	B	605	CLA	C1D-C2D	2.61	1.48	1.42
22	d	402	CLA	C1D-C2D	2.61	1.48	1.42
22	D	403	CLA	CMB-C2B	-2.61	1.46	1.51
22	C	507	CLA	C1D-C2D	2.61	1.48	1.42
23	A	404	PHO	CMC-C2C	-2.61	1.45	1.50
22	b	611	CLA	MG-NA	2.60	2.12	2.06
22	c	506	CLA	CHC-C1C	2.59	1.41	1.35
22	A	405	CLA	CMD-C2D	-2.59	1.45	1.51
22	b	605	CLA	MG-NC	2.59	2.12	2.06
22	C	510	CLA	CMD-C2D	-2.58	1.45	1.51
22	C	513	CLA	CAA-C2A	-2.58	1.49	1.54
22	C	504	CLA	CMD-C2D	-2.58	1.45	1.51
22	C	513	CLA	CMD-C2D	-2.58	1.45	1.51
30	H	102	DGD	C1G-C2G	2.58	1.58	1.50
22	b	615	CLA	C1D-C2D	2.58	1.48	1.42
27	a	410	PL9	C3-C4	-2.57	1.45	1.49
23	A	404	PHO	CHD-C4C	-2.57	1.34	1.40
22	C	504	CLA	CMB-C2B	-2.57	1.46	1.51
30	H	102	DGD	C6E-C5E	2.57	1.60	1.51
22	b	604	CLA	C3B-C2B	-2.56	1.36	1.40
23	A	404	PHO	C3B-C4B	2.56	1.48	1.43
22	C	508	CLA	CHC-C1C	2.56	1.41	1.35
22	A	403	CLA	CMB-C2B	-2.55	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.55	1.45	1.51
24	c	516	BCR	C30-C25	-2.55	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	102	DGD	O3E-C3E	-2.55	1.37	1.43
24	b	617	BCR	C38-C26	-2.55	1.46	1.50
22	b	605	CLA	C1D-C2D	2.55	1.48	1.42
27	A	410	PL9	C3-C4	-2.55	1.45	1.49
27	d	405	PL9	C25-C24	-2.55	1.44	1.50
22	C	512	CLA	C3B-C2B	-2.55	1.36	1.40
24	c	517	BCR	C30-C25	-2.54	1.50	1.53
22	b	608	CLA	CAC-C3C	-2.54	1.44	1.51
22	A	411	CLA	CMB-C2B	-2.52	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.52	1.45	1.51
23	A	404	PHO	C1C-C2C	2.52	1.51	1.45
22	B	607	CLA	C3B-CAB	-2.52	1.42	1.47
22	b	605	CLA	C3B-C2B	-2.52	1.36	1.40
30	C	517	DGD	O3D-C3D	-2.51	1.37	1.43
22	B	613	CLA	C1D-C2D	2.51	1.48	1.42
22	C	509	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	615	CLA	C3B-CAB	-2.51	1.42	1.47
23	D	401	PHO	CHC-C1C	2.51	1.43	1.38
22	b	601	CLA	CMB-C2B	-2.50	1.46	1.51
24	T	101	BCR	C38-C26	-2.50	1.46	1.50
23	a	404	PHO	C4C-NC	2.50	1.42	1.36
22	b	615	CLA	C3B-C2B	-2.50	1.36	1.40
22	a	403	CLA	CMB-C2B	-2.50	1.46	1.51
30	H	102	DGD	C4D-C5D	2.49	1.58	1.53
22	C	514	CLA	C1D-C2D	2.49	1.48	1.42
22	b	608	CLA	C3B-C2B	-2.49	1.36	1.40
22	D	403	CLA	C4B-CHC	-2.49	1.34	1.41
22	c	511	CLA	CHC-C1C	2.48	1.41	1.35
28	d	409	LMG	O1-C7	-2.48	1.39	1.43
34	B	622	LHG	O8-C6	-2.48	1.39	1.45
22	b	605	CLA	CHC-C1C	2.48	1.41	1.35
22	c	503	CLA	CAC-C3C	-2.48	1.44	1.51
22	B	617	CLA	C1D-C2D	2.47	1.48	1.42
22	b	612	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	508	CLA	CAC-C3C	-2.47	1.44	1.51
23	a	404	PHO	C3B-C4B	2.46	1.48	1.43
22	b	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	d	403	CLA	C1D-C2D	2.46	1.48	1.42
22	D	403	CLA	CMD-C2D	-2.46	1.45	1.51
22	b	611	CLA	CMD-C2D	-2.45	1.45	1.51
23	d	401	PHO	C1C-NC	-2.45	1.33	1.38
28	C	519	LMG	C4-C3	2.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C1D-C2D	2.45	1.48	1.42
22	c	510	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	612	CLA	CHC-C1C	2.45	1.41	1.35
22	b	611	CLA	CMC-C2C	-2.45	1.45	1.50
22	C	505	CLA	C1D-C2D	2.44	1.48	1.42
30	c	519	DGD	C3E-C2E	2.44	1.58	1.52
22	D	403	CLA	CMC-C2C	-2.44	1.45	1.50
22	B	611	CLA	C1D-C2D	2.44	1.48	1.42
22	D	403	CLA	C3B-C2B	-2.44	1.37	1.40
28	D	410	LMG	O8-C28	2.44	1.40	1.33
23	d	401	PHO	C1A-NA	2.43	1.42	1.37
30	h	102	DGD	O1G-C1G	-2.43	1.39	1.45
22	d	402	CLA	CMC-C2C	-2.43	1.45	1.50
22	b	607	CLA	C1D-C2D	2.43	1.48	1.42
35	e	101	HEC	C3B-C4B	2.43	1.47	1.43
22	C	510	CLA	CMC-C2C	-2.43	1.45	1.50
22	b	615	CLA	CMC-C2C	-2.43	1.45	1.50
22	a	405	CLA	C1B-NB	2.42	1.37	1.35
22	b	608	CLA	CHC-C1C	2.42	1.41	1.35
22	C	507	CLA	C3B-C2B	-2.42	1.37	1.40
22	C	513	CLA	C3B-C2B	-2.41	1.37	1.40
22	A	411	CLA	CAC-C3C	-2.41	1.44	1.51
22	b	605	CLA	C4B-CHC	-2.41	1.34	1.41
22	B	610	CLA	C1D-C2D	2.41	1.48	1.42
22	c	503	CLA	CHC-C1C	2.41	1.41	1.35
22	b	601	CLA	CAC-C3C	-2.41	1.44	1.51
22	B	613	CLA	CHC-C1C	2.41	1.41	1.35
28	D	406	LMG	C6-C5	2.41	1.59	1.51
22	C	503	CLA	C3B-C2B	-2.41	1.37	1.40
29	A	413	SQD	O48-C23	2.41	1.40	1.33
28	b	621	LMG	O6-C1	2.40	1.48	1.41
22	B	605	CLA	O2D-CGD	2.40	1.39	1.33
22	B	608	CLA	C1D-C2D	2.40	1.48	1.42
22	a	405	CLA	C3B-CAB	-2.40	1.43	1.47
28	M	101	LMG	C9-C8	2.40	1.58	1.50
22	B	616	CLA	MG-NA	2.40	2.12	2.06
29	f	101	SQD	O3-C3	-2.40	1.37	1.43
22	b	607	CLA	C3B-CAB	-2.40	1.43	1.47
24	D	404	BCR	C1-C6	-2.40	1.50	1.53
28	D	406	LMG	C4-C3	2.39	1.58	1.52
22	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
34	D	412	LHG	C24-C23	2.39	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CMA-C3A	-2.39	1.48	1.53
22	c	504	CLA	C1B-NB	2.39	1.37	1.35
22	b	611	CLA	CMB-C2B	-2.39	1.46	1.51
22	a	411	CLA	C1D-C2D	2.39	1.48	1.42
29	A	413	SQD	O2-C2	-2.38	1.37	1.43
22	B	608	CLA	CMC-C2C	-2.38	1.45	1.50
34	D	408	LHG	C4-C5	2.38	1.58	1.50
30	A	415	DGD	C3E-C2E	2.38	1.58	1.52
22	A	403	CLA	C4B-CHC	-2.38	1.34	1.41
22	B	608	CLA	MG-NA	2.38	2.11	2.06
28	C	519	LMG	O8-C9	-2.38	1.39	1.45
22	d	403	CLA	MG-NC	2.38	2.11	2.06
22	A	411	CLA	C3B-C2B	-2.38	1.37	1.40
23	a	404	PHO	O2D-CGD	2.37	1.39	1.33
22	c	504	CLA	C1D-C2D	2.37	1.47	1.42
22	B	607	CLA	CMD-C2D	-2.37	1.45	1.51
22	B	616	CLA	C3B-CAB	-2.37	1.43	1.47
30	h	102	DGD	C4D-C3D	2.36	1.58	1.52
23	a	404	PHO	CHC-C1C	2.36	1.43	1.38
22	b	609	CLA	C3B-CAB	-2.36	1.43	1.47
22	B	616	CLA	C4B-CHC	-2.36	1.34	1.41
24	T	101	BCR	C27-C26	-2.36	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.35	1.46	1.51
30	H	102	DGD	C1E-C2E	2.35	1.59	1.52
22	C	511	CLA	CMD-C2D	-2.35	1.46	1.51
30	C	517	DGD	C1E-C2E	2.35	1.59	1.52
22	b	609	CLA	C1D-C2D	2.35	1.47	1.42
22	C	507	CLA	CAC-C3C	-2.34	1.45	1.51
22	B	604	CLA	CMD-C2D	-2.34	1.46	1.51
22	a	403	CLA	C3B-CAB	-2.34	1.43	1.47
30	C	516	DGD	O6E-C1E	2.34	1.47	1.41
30	C	516	DGD	C3D-C2D	2.34	1.58	1.52
22	b	604	CLA	C1D-C2D	2.34	1.47	1.42
28	c	522	LMG	O2-C2	-2.34	1.37	1.43
29	A	413	SQD	O47-C7	2.33	1.40	1.34
22	b	613	CLA	C1D-C2D	2.33	1.47	1.42
28	c	525	LMG	C1-C2	2.33	1.59	1.52
22	A	402	CLA	CHC-C1C	2.33	1.40	1.35
27	D	405	PL9	C46-C44	-2.33	1.46	1.51
24	b	616	BCR	C4-C5	-2.32	1.46	1.51
30	A	415	DGD	O1G-C1G	-2.32	1.39	1.45
22	C	505	CLA	CMB-C2B	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	C1D-C2D	2.31	1.47	1.42
22	c	505	CLA	CMB-C2B	-2.31	1.46	1.51
35	F	101	HEC	CAD-C3D	2.31	1.55	1.52
28	B	629	LMG	O8-C28	2.31	1.40	1.33
22	b	601	CLA	C4B-CHC	-2.31	1.34	1.41
22	a	403	CLA	C1D-C2D	2.31	1.47	1.42
30	h	102	DGD	O2D-C2D	-2.30	1.37	1.43
22	c	512	CLA	C1D-C2D	2.30	1.47	1.42
22	c	504	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	405	CLA	CMB-C2B	-2.30	1.46	1.51
22	C	509	CLA	C1B-NB	2.29	1.37	1.35
22	c	505	CLA	CMC-C2C	-2.29	1.45	1.50
23	a	404	PHO	CHB-C1B	-2.29	1.34	1.38
22	B	617	CLA	CMB-C2B	-2.29	1.46	1.51
22	D	402	CLA	C1D-C2D	2.29	1.47	1.42
22	A	405	CLA	C1D-C2D	2.29	1.47	1.42
22	A	411	CLA	CHC-C1C	2.29	1.40	1.35
22	h	101	CLA	CMC-C2C	-2.29	1.46	1.50
27	A	410	PL9	C7-C8	-2.29	1.47	1.50
22	D	402	CLA	CAA-C2A	-2.28	1.49	1.54
22	c	506	CLA	CMD-C2D	-2.28	1.46	1.51
30	c	519	DGD	C1D-C2D	2.28	1.59	1.52
22	c	503	CLA	CMD-C2D	-2.28	1.46	1.51
27	d	405	PL9	C16-C14	-2.28	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	513	CLA	CMC-C2C	-2.27	1.46	1.50
22	h	101	CLA	O2A-CGA	2.27	1.40	1.33
22	c	503	CLA	CMB-C2B	-2.27	1.46	1.51
22	A	405	CLA	CHC-C1C	2.27	1.40	1.35
28	c	524	LMG	C1-C2	2.26	1.59	1.52
22	C	503	CLA	CMB-C2B	-2.26	1.46	1.51
22	B	607	CLA	C1B-NB	2.26	1.37	1.35
22	B	607	CLA	C1D-C2D	2.26	1.47	1.42
22	d	403	CLA	C4B-CHC	-2.26	1.34	1.41
27	D	405	PL9	C3-C4	-2.26	1.45	1.49
22	B	612	CLA	CMD-C2D	-2.26	1.46	1.51
22	A	402	CLA	C3B-C2B	-2.25	1.37	1.40
22	a	405	CLA	C4B-CHC	-2.25	1.34	1.41
22	C	512	CLA	CMC-C2C	-2.25	1.46	1.50
29	f	101	SQD	O2-C2	-2.25	1.37	1.43
22	B	609	CLA	CMB-C2B	-2.25	1.47	1.51
22	C	502	CLA	CMC-C2C	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	C1D-C2D	2.25	1.47	1.42
22	C	508	CLA	C3B-CAB	-2.24	1.43	1.47
22	c	515	CLA	MG-NA	-2.24	2.00	2.06
22	C	511	CLA	CMB-C2B	-2.24	1.47	1.51
22	c	503	CLA	C1D-C2D	2.24	1.47	1.42
22	b	612	CLA	C3C-C2C	2.24	1.41	1.36
22	b	614	CLA	CMB-C2B	-2.24	1.47	1.51
22	b	607	CLA	C1B-NB	2.24	1.37	1.35
28	B	629	LMG	O7-C10	2.23	1.40	1.34
22	A	402	CLA	CMB-C2B	-2.23	1.47	1.51
22	C	506	CLA	C3B-CAB	-2.22	1.43	1.47
27	D	405	PL9	C26-C24	-2.22	1.46	1.51
22	c	509	CLA	CHC-C1C	2.22	1.40	1.35
22	b	614	CLA	C3B-C2B	-2.22	1.37	1.40
34	d	408	LHG	P-O6	2.22	1.68	1.59
22	A	402	CLA	O2D-CED	-2.22	1.40	1.45
22	b	601	CLA	CMD-C2D	-2.22	1.46	1.51
22	B	602	CLA	CMC-C2C	-2.22	1.46	1.50
29	f	101	SQD	O4-C4	-2.22	1.37	1.43
22	B	609	CLA	CHC-C1C	2.21	1.40	1.35
24	B	620	BCR	C38-C26	-2.21	1.47	1.50
30	C	518	DGD	O1G-C1G	-2.21	1.40	1.45
28	d	409	LMG	O7-C8	-2.21	1.41	1.46
22	B	610	CLA	CMB-C2B	-2.21	1.47	1.51
30	C	517	DGD	O5D-C6D	-2.20	1.39	1.43
29	a	412	SQD	O3-C3	-2.20	1.37	1.43
22	B	614	CLA	CMB-C2B	-2.20	1.47	1.51
22	A	411	CLA	CMD-C2D	-2.20	1.46	1.51
34	D	408	LHG	C3-C2	2.20	1.59	1.51
24	a	406	BCR	C38-C26	-2.20	1.47	1.50
22	b	613	CLA	C3B-C2B	-2.20	1.37	1.40
35	e	101	HEC	C4D-CHA	-2.19	1.34	1.41
24	K	101	BCR	C1-C6	-2.19	1.50	1.53
22	b	610	CLA	MG-NA	2.19	2.11	2.06
22	B	607	CLA	C4B-CHC	-2.19	1.34	1.41
22	c	504	CLA	C3B-CAB	-2.19	1.43	1.47
30	c	519	DGD	C3G-C2G	2.19	1.57	1.50
22	b	602	CLA	CMB-C2B	-2.19	1.47	1.51
22	B	610	CLA	CHC-C1C	2.19	1.40	1.35
30	h	102	DGD	C1E-C2E	2.18	1.58	1.52
28	c	522	LMG	C7-C8	2.18	1.57	1.50
24	b	616	BCR	C33-C5	-2.18	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1D-C2D	2.18	1.47	1.42
30	C	517	DGD	O2G-C2G	-2.18	1.41	1.46
22	b	606	CLA	CMC-C2C	-2.18	1.46	1.50
22	C	507	CLA	CMB-C2B	-2.18	1.47	1.51
24	x	101	BCR	C33-C5	-2.18	1.47	1.50
23	D	401	PHO	CHC-C4B	-2.18	1.35	1.40
27	d	405	PL9	C51-C49	-2.17	1.44	1.50
28	B	629	LMG	C7-C8	2.17	1.57	1.50
22	b	609	CLA	CHC-C1C	2.17	1.40	1.35
23	d	401	PHO	C4C-C3C	2.17	1.49	1.45
28	M	101	LMG	O6-C1	2.17	1.47	1.41
22	c	505	CLA	C3B-C2B	-2.16	1.37	1.40
22	a	405	CLA	CAC-C3C	-2.16	1.45	1.51
30	c	520	DGD	C4D-C5D	2.16	1.57	1.53
24	x	101	BCR	C36-C18	-2.16	1.46	1.50
22	B	607	CLA	MG-NC	-2.16	2.01	2.06
34	l	101	LHG	P-O6	2.15	1.68	1.59
22	c	513	CLA	CMB-C2B	-2.15	1.47	1.51
27	a	410	PL9	C25-C24	-2.15	1.45	1.50
22	c	503	CLA	C4B-CHC	-2.15	1.35	1.41
29	a	412	SQD	O4-C4	-2.15	1.37	1.43
22	b	612	CLA	C4B-CHC	-2.14	1.35	1.41
22	B	607	CLA	CMB-C2B	-2.14	1.47	1.51
22	B	616	CLA	C3B-C2B	-2.14	1.37	1.40
23	A	404	PHO	C1A-NA	2.14	1.41	1.37
30	C	518	DGD	C6E-C5E	2.14	1.59	1.51
22	b	615	CLA	C4B-CHC	-2.14	1.35	1.41
22	b	614	CLA	CMC-C2C	-2.14	1.46	1.50
30	h	102	DGD	C4E-C3E	2.14	1.57	1.52
22	b	601	CLA	C1D-C2D	2.13	1.47	1.42
22	B	606	CLA	CMC-C2C	-2.13	1.46	1.50
22	b	615	CLA	CHC-C1C	2.13	1.40	1.35
24	C	515	BCR	C27-C26	-2.13	1.46	1.51
22	C	502	CLA	MG-NC	2.13	2.11	2.06
22	c	515	CLA	CMC-C2C	-2.13	1.46	1.50
22	b	605	CLA	CAC-C3C	-2.13	1.45	1.51
22	C	511	CLA	MG-NC	2.13	2.11	2.06
22	b	615	CLA	CMD-C2D	-2.13	1.46	1.51
27	D	405	PL9	C31-C29	-2.13	1.46	1.51
22	d	403	CLA	O1D-CGD	2.13	1.26	1.21
24	t	101	BCR	C30-C25	-2.13	1.50	1.53
23	a	404	PHO	CHD-C4C	-2.13	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C3B-C2B	-2.13	1.37	1.40
24	b	616	BCR	C38-C26	-2.13	1.47	1.50
29	B	623	SQD	O2-C2	-2.12	1.38	1.43
22	B	616	CLA	C1D-C2D	2.12	1.47	1.42
22	b	602	CLA	C1A-CHA	-2.12	1.34	1.43
22	B	605	CLA	MG-NC	2.12	2.11	2.06
28	c	525	LMG	O1-C7	-2.11	1.39	1.43
22	C	512	CLA	CMD-C2D	-2.11	1.46	1.51
22	B	603	CLA	C3C-C2C	2.11	1.41	1.36
28	D	406	LMG	O2-C2	-2.11	1.38	1.43
30	H	102	DGD	C6D-C5D	2.11	1.58	1.51
22	B	604	CLA	C3B-C2B	-2.11	1.37	1.40
22	b	613	CLA	C3B-CAB	-2.11	1.43	1.47
22	D	403	CLA	C3B-CAB	-2.11	1.43	1.47
22	C	504	CLA	CMC-C2C	-2.11	1.46	1.50
24	x	101	BCR	C1-C6	-2.11	1.50	1.53
30	C	516	DGD	C4D-C5D	2.11	1.57	1.53
27	A	410	PL9	C37-C38	2.10	1.57	1.50
22	b	612	CLA	CMC-C2C	-2.10	1.46	1.50
22	h	101	CLA	CMD-C2D	-2.10	1.46	1.51
28	d	409	LMG	C4-C5	2.10	1.57	1.53
22	C	510	CLA	O2D-CGD	2.09	1.38	1.33
27	a	410	PL9	C10-C9	-2.09	1.45	1.50
30	C	518	DGD	C4D-C3D	2.09	1.57	1.52
34	D	408	LHG	O7-C5	-2.09	1.41	1.46
34	d	406	LHG	C4-C5	2.09	1.57	1.50
30	c	520	DGD	O2E-C2E	-2.09	1.38	1.43
22	b	612	CLA	C1D-C2D	2.09	1.47	1.42
22	A	403	CLA	C1D-C2D	2.08	1.47	1.42
22	h	101	CLA	CMB-C2B	-2.08	1.47	1.51
22	b	609	CLA	C4B-CHC	-2.08	1.35	1.41
22	c	510	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	406	BCR	C33-C5	-2.08	1.47	1.50
22	c	514	CLA	C3B-CAB	-2.07	1.43	1.47
22	b	613	CLA	CMB-C2B	-2.07	1.47	1.51
34	E	101	LHG	O8-C23	2.07	1.39	1.33
22	B	608	CLA	C1B-NB	2.07	1.37	1.35
22	B	611	CLA	C1B-NB	2.07	1.37	1.35
34	e	102	LHG	C4-C5	2.07	1.57	1.50
22	B	609	CLA	MG-NC	-2.07	2.01	2.06
22	b	612	CLA	CHC-C1C	2.06	1.40	1.35
22	C	514	CLA	C3B-CAB	-2.06	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	405	CLA	CHC-C1C	2.06	1.40	1.35
22	b	601	CLA	C3B-C2B	-2.06	1.37	1.40
23	D	401	PHO	C4C-NC	2.05	1.41	1.36
30	c	521	DGD	C6D-C5D	2.05	1.58	1.51
28	b	621	LMG	C6-C5	2.05	1.58	1.51
22	a	411	CLA	CMD-C2D	-2.05	1.46	1.51
29	A	413	SQD	O3-C3	-2.05	1.38	1.43
22	C	502	CLA	CAA-C2A	2.05	1.57	1.54
22	a	411	CLA	C1B-NB	2.04	1.37	1.35
22	A	402	CLA	C3C-C2C	2.04	1.41	1.36
22	b	603	CLA	CAC-C3C	-2.04	1.45	1.51
30	c	519	DGD	O1A-C1A	2.04	1.28	1.22
22	c	507	CLA	CMC-C2C	-2.04	1.46	1.50
22	b	614	CLA	C3B-CAB	-2.04	1.43	1.47
28	M	101	LMG	O4-C4	-2.04	1.38	1.43
22	c	511	CLA	C1D-C2D	2.03	1.47	1.42
22	c	505	CLA	CMD-C2D	-2.03	1.46	1.51
30	c	519	DGD	O1G-C1A	2.03	1.39	1.33
22	a	405	CLA	C1D-C2D	2.03	1.47	1.42
22	b	601	CLA	CMC-C2C	-2.03	1.46	1.50
22	C	513	CLA	C1A-CHA	-2.03	1.34	1.43
27	A	410	PL9	C25-C24	-2.02	1.45	1.50
22	A	403	CLA	MG-NA	-2.02	2.01	2.06
22	C	511	CLA	CAA-C2A	-2.02	1.50	1.54
24	b	617	BCR	C36-C18	-2.02	1.46	1.50
30	c	521	DGD	O4E-C4E	-2.02	1.38	1.43
22	C	510	CLA	O2A-CGA	2.02	1.39	1.33
22	B	610	CLA	O2D-CGD	2.02	1.38	1.33
22	c	514	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.02	1.46	1.50
22	c	514	CLA	CMD-C2D	-2.01	1.46	1.51
24	B	619	BCR	C1-C6	-2.01	1.51	1.53
22	B	610	CLA	CMC-C2C	-2.01	1.46	1.50
23	d	401	PHO	CHD-C4C	-2.01	1.35	1.40
22	C	510	CLA	CMB-C2B	-2.01	1.47	1.51
34	e	102	LHG	O7-C5	-2.01	1.41	1.46
34	B	622	LHG	C4-C5	2.01	1.56	1.50
22	c	512	CLA	C3B-C2B	-2.01	1.37	1.40
22	b	602	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	609	CLA	C1B-NB	2.01	1.37	1.35
23	D	401	PHO	CAC-C3C	-2.01	1.46	1.51
28	c	525	LMG	O6-C5	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	MG-NC	2.01	2.11	2.06
22	c	512	CLA	CMD-C2D	-2.00	1.46	1.51

All (1420) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C4A-NA-C1A	11.54	111.89	106.71
22	B	605	CLA	C4A-NA-C1A	10.81	111.56	106.71
22	b	605	CLA	C4A-NA-C1A	9.82	111.12	106.71
22	h	101	CLA	C4A-NA-C1A	9.80	111.11	106.71
22	C	504	CLA	C4A-NA-C1A	9.67	111.05	106.71
29	D	407	SQD	O6-C1-C2	9.00	122.35	108.30
29	b	619	SQD	O6-C1-C2	8.94	122.27	108.30
22	C	508	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	C	509	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	b	606	CLA	C4A-NA-C1A	8.20	110.39	106.71
29	a	412	SQD	O6-C1-C2	8.07	120.90	108.30
29	A	413	SQD	O6-C1-C2	7.83	120.53	108.30
22	B	617	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	C	503	CLA	C4A-NA-C1A	7.55	110.10	106.71
22	b	601	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	b	603	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	c	513	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	c	505	CLA	C4A-NA-C1A	7.30	109.99	106.71
29	B	623	SQD	O6-C1-C2	7.30	119.70	108.30
22	a	405	CLA	C4A-NA-C1A	7.29	109.98	106.71
29	f	101	SQD	O7-S-C6	7.24	115.54	106.94
22	C	512	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	c	511	CLA	C4A-NA-C1A	7.14	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	6.91	109.81	106.71
22	B	608	CLA	C4A-NA-C1A	6.83	109.78	106.71
35	e	101	HEC	CBD-CAD-C3D	-6.80	99.94	112.49
22	c	504	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	C	511	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	c	514	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	b	614	CLA	C4A-NA-C1A	6.38	109.57	106.71
22	B	611	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	B	610	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	B	611	CLA	O2D-CGD-O1D	-6.23	111.67	123.84
22	C	502	CLA	C4A-NA-C1A	6.15	109.47	106.71
29	D	407	SQD	O9-S-C6	6.07	114.16	106.94
22	b	615	CLA	C4A-NA-C1A	6.07	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	a	411	CLA	C4A-NA-C1A	6.01	109.41	106.71
27	D	405	PL9	C7-C3-C4	6.00	121.76	116.88
22	c	510	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	c	503	CLA	O2D-CGD-O1D	-5.85	112.40	123.84
22	b	609	CLA	C4A-NA-C1A	5.79	109.31	106.71
27	A	410	PL9	C7-C3-C4	5.76	121.56	116.88
22	B	603	CLA	O2D-CGD-CBD	5.73	121.45	111.27
22	A	411	CLA	C4A-NA-C1A	5.67	109.25	106.71
22	D	402	CLA	C4A-NA-C1A	5.66	109.25	106.71
22	B	607	CLA	C4A-NA-C1A	5.65	109.25	106.71
27	a	410	PL9	C7-C3-C4	5.60	121.43	116.88
22	C	503	CLA	C4D-C3D-CAD	-5.55	105.38	108.47
35	F	101	HEC	CBA-CAA-C2A	-5.55	102.26	112.48
22	c	509	CLA	C4A-NA-C1A	5.54	109.20	106.71
22	c	503	CLA	C4A-NA-C1A	5.54	109.20	106.71
22	B	612	CLA	C4A-NA-C1A	5.49	109.18	106.71
22	a	402	CLA	CMB-C2B-C1B	-5.46	120.07	128.46
22	B	615	CLA	C4D-C3D-CAD	-5.42	105.44	108.47
22	B	608	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
22	b	615	CLA	O2D-CGD-O1D	-5.33	113.42	123.84
22	d	403	CLA	CMB-C2B-C1B	-5.33	120.28	128.46
35	v	201	HEC	CBD-CAD-C3D	-5.29	102.72	112.49
22	B	603	CLA	O2D-CGD-O1D	-5.24	113.60	123.84
29	b	619	SQD	O7-S-C6	5.17	113.08	106.94
22	B	615	CLA	C4A-NA-C1A	5.15	109.02	106.71
22	C	505	CLA	C4A-NA-C1A	5.15	109.02	106.71
22	b	604	CLA	C4A-NA-C1A	5.13	109.01	106.71
35	F	101	HEC	CBD-CAD-C3D	-5.13	103.03	112.49
28	b	623	LMG	C1-O6-C5	-5.12	103.64	113.69
22	b	612	CLA	C1-C2-C3	-5.09	117.25	126.04
35	e	101	HEC	CBA-CAA-C2A	-5.08	103.12	112.48
22	C	514	CLA	C4A-NA-C1A	5.06	108.98	106.71
29	f	101	SQD	O6-C1-C2	5.03	116.16	108.30
22	B	615	CLA	CMD-C2D-C3D	4.97	133.97	124.68
29	B	623	SQD	O7-S-C6	4.96	112.83	106.94
35	V	201	HEC	CMC-C2C-C1C	-4.93	120.88	128.46
22	b	602	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
22	B	614	CLA	OBD-CAD-CBD	-4.92	118.86	125.89
22	b	614	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
27	d	405	PL9	C7-C3-C4	4.90	120.86	116.88
22	C	505	CLA	CMB-C2B-C1B	-4.90	120.94	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	412	SQD	O7-S-C6	4.88	112.74	106.94
22	A	403	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
29	A	414	SQD	C45-O47-C7	4.78	124.03	117.88
22	C	507	CLA	C4A-NA-C1A	4.78	108.86	106.71
22	a	402	CLA	C4A-NA-C1A	4.77	108.85	106.71
22	c	512	CLA	C4A-NA-C1A	4.77	108.85	106.71
22	C	502	CLA	O2D-CGD-O1D	-4.76	114.54	123.84
22	c	503	CLA	O2D-CGD-CBD	4.70	119.63	111.27
22	b	602	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
35	V	201	HEC	CBD-CAD-C3D	-4.70	103.82	112.49
29	a	413	SQD	O48-C23-O10	-4.69	111.75	123.59
34	D	409	LHG	O4-P-O5	4.68	135.35	112.24
22	d	403	CLA	CMB-C2B-C3B	4.66	133.39	124.68
22	b	610	CLA	O2D-CGD-CBD	4.64	119.52	111.27
29	a	412	SQD	O9-S-C6	4.60	112.41	106.94
22	B	609	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
22	b	610	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
29	A	413	SQD	C1-C2-C3	-4.58	100.45	110.00
22	b	608	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	A	406	BCR	C35-C13-C14	-4.56	116.53	122.92
22	D	403	CLA	C4A-NA-C1A	4.56	108.75	106.71
22	C	509	CLA	CMB-C2B-C1B	-4.55	121.48	128.46
22	c	506	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
22	B	614	CLA	OBD-CAD-C3D	4.52	135.49	127.98
22	B	608	CLA	CMB-C2B-C3B	4.50	133.09	124.68
22	h	101	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
29	A	413	SQD	O47-C7-C8	4.46	121.11	111.50
29	D	407	SQD	O8-S-C6	4.44	112.81	105.74
22	B	605	CLA	CMB-C2B-C1B	-4.42	121.68	128.46
35	V	201	HEC	C1D-C2D-C3D	-4.40	103.93	107.00
22	b	602	CLA	CMB-C2B-C3B	4.39	132.90	124.68
30	c	521	DGD	O3G-C3G-C2G	-4.38	100.32	110.90
22	c	507	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
30	C	517	DGD	O3G-C3G-C2G	-4.37	100.35	110.90
22	C	513	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
22	b	611	CLA	CMD-C2D-C3D	4.34	132.81	124.68
30	C	518	DGD	O3G-C3G-C2G	-4.34	100.44	110.90
23	D	401	PHO	CAC-C3C-C4C	-4.33	120.50	125.22
22	B	616	CLA	C4A-NA-C1A	4.32	108.65	106.71
22	a	402	CLA	CMB-C2B-C3B	4.31	132.75	124.68
22	b	603	CLA	OBD-CAD-CBD	-4.30	119.75	125.89
22	A	403	CLA	CMB-C2B-C3B	4.30	132.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	403	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
29	A	413	SQD	O7-S-C6	4.27	112.01	106.94
22	C	509	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
22	c	515	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
22	B	603	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
28	B	629	LMG	C1-C2-C3	-4.24	101.16	110.00
30	H	102	DGD	O3G-C3G-C2G	-4.24	100.67	110.90
35	F	101	HEC	CMC-C2C-C1C	-4.24	121.95	128.46
22	c	511	CLA	C4D-C3D-CAD	-4.24	106.11	108.47
28	B	629	LMG	C1-O6-C5	-4.24	105.38	113.69
22	A	405	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
29	a	413	SQD	O47-C7-C8	4.22	120.59	111.50
22	b	609	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
29	f	101	SQD	O9-S-O7	-4.19	99.44	113.95
22	B	617	CLA	C4D-C3D-CAD	-4.19	106.13	108.47
29	B	623	SQD	O47-C7-C8	4.19	120.53	111.50
22	b	610	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
29	A	413	SQD	C1-O5-C5	-4.16	105.51	113.69
23	A	404	PHO	CMD-C2D-C1D	4.14	131.44	125.06
29	b	619	SQD	C1-C2-C3	-4.14	101.38	110.00
22	b	603	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
24	H	101	BCR	C16-C15-C14	-4.13	115.01	123.47
34	E	101	LHG	O4-P-O5	4.12	132.62	112.24
22	B	609	CLA	O2D-CGD-O1D	-4.12	115.78	123.84
22	A	402	CLA	C4A-NA-C1A	4.09	108.55	106.71
22	b	601	CLA	O2D-CGD-CBD	4.07	118.51	111.27
22	b	602	CLA	C4A-NA-C1A	4.07	108.54	106.71
22	B	612	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
34	e	102	LHG	O4-P-O5	4.06	132.32	112.24
22	b	601	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
22	C	504	CLA	C7-C6-C5	-4.05	102.37	113.36
34	D	412	LHG	O4-P-O5	4.04	132.24	112.24
22	C	510	CLA	CHB-C4A-NA	4.04	130.10	124.51
22	D	403	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
22	b	612	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
22	a	405	CLA	OBD-CAD-CBD	-4.02	120.15	125.89
22	c	511	CLA	CMD-C2D-C3D	4.02	132.19	124.68
22	b	614	CLA	CMB-C2B-C3B	4.01	132.19	124.68
22	b	615	CLA	CHB-C4A-NA	4.01	130.06	124.51
28	d	409	LMG	O1-C1-C2	-4.01	102.05	108.30
34	l	101	LHG	O4-P-O5	4.00	131.99	112.24
35	v	201	HEC	C1D-C2D-C3D	-3.99	104.22	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	CMB-C2B-C3B	3.98	132.13	124.68
22	c	511	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
27	A	410	PL9	C7-C3-C2	-3.97	118.08	123.30
22	a	411	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
22	B	611	CLA	C1B-CHB-C4A	-3.97	122.26	130.12
34	D	412	LHG	O8-C23-C24	3.96	124.35	111.91
34	B	622	LHG	O4-P-O5	3.96	131.81	112.24
22	C	506	CLA	CMD-C2D-C3D	3.92	132.01	124.68
22	B	602	CLA	CAA-CBA-CGA	-3.92	101.81	113.25
22	b	613	CLA	C4A-NA-C1A	3.91	108.47	106.71
22	b	615	CLA	CMB-C2B-C3B	3.91	131.99	124.68
29	A	413	SQD	O9-S-O7	-3.89	100.47	113.95
22	c	513	CLA	C4D-C3D-CAD	-3.89	106.30	108.47
22	B	615	CLA	OBD-CAD-CBD	-3.89	120.33	125.89
34	d	406	LHG	O8-C23-C24	3.88	124.09	111.91
22	c	514	CLA	C1-C2-C3	-3.88	119.33	126.04
22	c	507	CLA	CMD-C2D-C3D	3.87	131.93	124.68
22	D	402	CLA	CED-O2D-CGD	3.87	124.70	115.94
22	B	615	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
22	b	604	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
22	B	606	CLA	C4D-C3D-CAD	-3.85	106.33	108.47
22	c	511	CLA	O2A-CGA-O1A	-3.84	113.89	123.59
22	B	613	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
35	v	201	HEC	CMB-C2B-C1B	-3.83	122.57	128.46
22	b	601	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
24	t	101	BCR	C3-C4-C5	-3.81	107.27	114.08
22	B	609	CLA	CMB-C2B-C3B	3.80	131.80	124.68
22	a	403	CLA	CMB-C2B-C3B	3.80	131.79	124.68
27	a	410	PL9	C35-C34-C36	3.80	121.67	115.27
22	c	506	CLA	CMB-C2B-C3B	3.80	131.79	124.68
22	c	508	CLA	C4-C3-C5	3.79	121.64	115.27
27	d	405	PL9	C37-C38-C39	-3.79	118.54	127.66
34	d	406	LHG	O4-P-O5	3.78	130.95	112.24
22	B	603	CLA	CMB-C2B-C3B	3.78	131.75	124.68
22	d	403	CLA	C1B-CHB-C4A	-3.77	122.66	130.12
22	B	602	CLA	CAA-C2A-C3A	-3.76	102.49	112.78
29	a	412	SQD	O9-S-O7	-3.75	100.98	113.95
22	b	612	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
29	A	413	SQD	O9-S-C6	3.73	111.38	106.94
22	B	611	CLA	O2A-CGA-O1A	-3.73	114.17	123.59
22	B	609	CLA	O2D-CGD-CBD	3.73	117.89	111.27
22	C	505	CLA	C4D-C3D-CAD	-3.72	106.39	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	b	623	LMG	O2-C2-C1	-3.71	101.02	110.05
22	b	604	CLA	C4-C3-C5	3.71	121.52	115.27
22	B	608	CLA	CED-O2D-CGD	3.71	124.33	115.94
22	D	402	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	c	506	CLA	CMD-C2D-C3D	3.71	131.62	124.68
22	c	508	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	c	520	DGD	O3G-C3G-C2G	-3.70	101.97	110.90
22	c	507	CLA	C4D-C3D-CAD	-3.70	106.41	108.47
22	b	611	CLA	C4A-NA-C1A	3.68	108.36	106.71
22	b	605	CLA	CMB-C2B-C3B	3.67	131.55	124.68
35	F	101	HEC	CMB-C2B-C1B	-3.67	122.82	128.46
22	c	509	CLA	CMD-C2D-C3D	3.67	131.55	124.68
34	d	408	LHG	O4-P-O5	3.67	130.39	112.24
22	b	615	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
34	D	408	LHG	O4-P-O5	3.66	130.34	112.24
27	d	405	PL9	C40-C39-C41	3.66	121.43	115.27
22	C	506	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
30	A	415	DGD	O5D-C1E-C2E	3.66	114.01	108.30
22	B	612	CLA	O2D-CGD-CBD	3.66	117.76	111.27
22	b	608	CLA	CMB-C2B-C3B	3.65	131.51	124.68
22	B	614	CLA	C1-C2-C3	-3.65	119.73	126.04
24	x	101	BCR	C37-C22-C21	-3.65	117.81	122.92
22	b	603	CLA	C1-C2-C3	-3.64	119.74	126.04
27	a	410	PL9	C7-C3-C2	-3.64	118.51	123.30
30	h	102	DGD	O3G-C3G-C2G	-3.62	102.16	110.90
34	d	407	LHG	O4-P-O5	3.62	130.13	112.24
22	B	614	CLA	C4A-NA-C1A	3.62	108.33	106.71
30	A	415	DGD	C4E-C3E-C2E	-3.61	104.52	110.82
34	e	102	LHG	O8-C23-C24	3.61	123.24	111.91
22	b	607	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
22	c	514	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
22	c	515	CLA	CMB-C2B-C3B	3.60	131.41	124.68
22	B	613	CLA	CMB-C2B-C3B	3.59	131.40	124.68
22	b	611	CLA	C4D-C3D-CAD	-3.59	106.47	108.47
22	d	402	CLA	C4A-NA-C1A	3.59	108.32	106.71
24	C	515	BCR	C36-C18-C17	-3.58	117.90	122.92
22	b	610	CLA	CMB-C2B-C3B	3.58	131.38	124.68
22	B	616	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	C	510	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	A	405	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	B	611	CLA	O2D-CGD-CBD	3.57	117.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	O2D-CGD-O1D	-3.57	116.87	123.84
22	C	502	CLA	O2D-CGD-CBD	3.56	117.60	111.27
22	b	606	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	c	512	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
22	C	503	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
22	b	605	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
28	b	621	LMG	O3-C3-C2	-3.54	102.17	110.35
24	C	515	BCR	C15-C16-C17	-3.53	116.24	123.47
22	C	510	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	c	508	CLA	CBC-CAC-C3C	-3.53	102.70	112.43
34	d	406	LHG	O8-C23-O10	-3.52	114.72	123.59
24	b	616	BCR	C2-C1-C6	3.51	115.89	110.48
22	d	402	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
22	A	402	CLA	CMB-C2B-C3B	3.51	131.24	124.68
30	c	520	DGD	O2D-C2D-C1D	-3.50	101.54	110.05
30	h	102	DGD	C1D-C2D-C3D	-3.49	102.72	110.00
24	c	517	BCR	C35-C13-C14	-3.49	118.03	122.92
24	c	518	BCR	C16-C15-C14	-3.49	116.33	123.47
22	b	606	CLA	CMD-C2D-C3D	3.49	131.21	124.68
22	B	609	CLA	C4A-NA-C1A	3.49	108.27	106.71
22	D	402	CLA	CMB-C2B-C3B	3.49	131.20	124.68
22	A	402	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	B	617	CLA	O2A-C1-C2	3.48	117.78	108.64
27	D	405	PL9	C22-C23-C24	-3.48	119.28	127.66
29	f	101	SQD	O47-C7-C8	3.48	120.50	110.80
30	C	516	DGD	O3G-C3G-C2G	-3.48	102.50	110.90
22	b	609	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	T	101	BCR	C7-C8-C9	-3.48	120.98	126.23
22	b	608	CLA	OBD-CAD-CBD	-3.47	120.93	125.89
28	A	412	LMG	O6-C1-O1	-3.47	101.75	109.97
22	C	511	CLA	CMD-C2D-C3D	3.47	131.17	124.68
22	A	403	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
22	a	402	CLA	CAC-C3C-C4C	3.47	129.31	124.81
22	B	615	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
22	B	605	CLA	OBD-CAD-C3D	3.44	133.69	127.98
22	C	507	CLA	OBD-CAD-CBD	-3.44	120.98	125.89
23	D	401	PHO	O2D-CGD-O1D	-3.44	117.12	123.84
22	c	511	CLA	CMB-C2B-C3B	3.44	131.10	124.68
22	B	617	CLA	C1-O2A-CGA	3.43	125.46	116.44
24	Z	101	BCR	C33-C5-C6	-3.43	120.67	124.53
22	B	612	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	B	608	CLA	C1D-CHD-C4C	3.43	127.08	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	BCR	C24-C23-C22	-3.42	121.06	126.23
22	b	603	CLA	OBD-CAD-C3D	3.42	133.66	127.98
28	b	621	LMG	O1-C1-C2	-3.41	102.97	108.30
22	C	505	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
22	B	607	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
29	b	619	SQD	O8-S-C6	3.39	111.14	105.74
22	B	617	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
22	h	101	CLA	CHB-C4A-NA	3.38	129.19	124.51
22	B	613	CLA	CHB-C4A-NA	3.38	129.19	124.51
22	C	513	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	B	617	CLA	OBD-CAD-CBD	-3.38	121.07	125.89
22	C	506	CLA	CAC-C3C-C4C	3.38	129.19	124.81
22	B	613	CLA	CMD-C2D-C3D	3.38	131.00	124.68
22	D	402	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
35	V	201	HEC	CMB-C2B-C1B	-3.37	123.28	128.46
22	B	611	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
22	d	403	CLA	CAC-C3C-C4C	3.37	129.18	124.81
22	c	506	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
27	D	405	PL9	C7-C3-C2	-3.36	118.88	123.30
22	c	507	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	B	605	CLA	OBD-CAD-CBD	-3.35	121.10	125.89
29	A	414	SQD	O48-C23-C24	3.35	122.43	111.91
22	a	403	CLA	CMD-C2D-C3D	3.35	130.94	124.68
22	B	605	CLA	C1D-CHD-C4C	3.35	126.97	122.56
22	B	603	CLA	CHB-C4A-NA	3.34	129.14	124.51
22	B	605	CLA	CMB-C2B-C3B	3.34	130.94	124.68
22	B	613	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
28	D	406	LMG	O1-C7-C8	-3.34	102.84	110.90
22	C	503	CLA	CMD-C2D-C3D	3.34	130.93	124.68
22	B	611	CLA	CMD-C2D-C3D	3.34	130.92	124.68
22	b	610	CLA	CHB-C4A-NA	3.34	129.13	124.51
24	Y	101	BCR	C27-C26-C25	3.34	127.58	122.73
24	Z	101	BCR	C11-C10-C9	-3.33	122.55	127.31
22	b	615	CLA	CMD-C2D-C3D	3.33	130.91	124.68
22	c	508	CLA	C4A-NA-C1A	3.33	108.20	106.71
22	B	602	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
22	b	612	CLA	CED-O2D-CGD	3.32	123.45	115.94
22	C	509	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	B	614	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	C	503	CLA	O1D-CGD-CBD	3.32	131.28	124.48
27	D	405	PL9	C42-C43-C44	-3.32	119.67	127.66
22	B	604	CLA	C4A-NA-C1A	3.31	108.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	102	DGD	O2D-C2D-C1D	-3.30	102.03	110.05
22	b	603	CLA	C4D-C3D-CAD	-3.30	106.63	108.47
27	d	405	PL9	C22-C23-C24	-3.30	119.72	127.66
22	a	402	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
22	c	514	CLA	O2A-CGA-O1A	-3.29	115.29	123.59
22	D	403	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
22	C	505	CLA	C4-C3-C5	3.29	120.80	115.27
22	B	606	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	c	505	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
22	b	613	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
22	B	605	CLA	O2D-CGD-CBD	3.27	117.08	111.27
22	b	605	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	c	505	CLA	C7-C6-C5	-3.27	104.48	113.36
22	C	504	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
22	b	611	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
24	x	101	BCR	C33-C5-C6	-3.26	120.87	124.53
27	A	410	PL9	C22-C23-C24	-3.26	119.82	127.66
22	c	514	CLA	CHB-C4A-NA	3.25	129.01	124.51
22	D	403	CLA	CMB-C2B-C3B	3.25	130.77	124.68
27	A	410	PL9	O2-C1-C6	3.25	126.22	120.59
22	C	513	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	A	402	CLA	CHB-C4A-NA	3.25	129.00	124.51
29	f	101	SQD	C1-C2-C3	-3.25	103.24	110.00
22	b	601	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	c	507	CLA	C1D-CHD-C4C	3.24	126.84	122.56
27	D	405	PL9	C37-C38-C39	-3.24	119.85	127.66
22	c	509	CLA	OBD-CAD-CBD	-3.24	121.27	125.89
22	a	403	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
29	a	412	SQD	O48-C23-C24	3.23	122.05	111.91
30	C	517	DGD	O6D-C1D-O3G	-3.23	102.32	109.97
29	a	412	SQD	C1-C2-C3	-3.23	103.28	110.00
29	D	407	SQD	C1-C2-C3	-3.22	103.29	110.00
22	b	604	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
22	B	606	CLA	CMD-C2D-C3D	3.22	130.70	124.68
22	C	511	CLA	CHB-C4A-NA	3.22	128.96	124.51
22	h	101	CLA	O2D-CGD-CBD	3.22	116.98	111.27
22	b	602	CLA	C7-C6-C5	-3.21	104.63	113.36
22	B	617	CLA	CMB-C2B-C3B	3.21	130.69	124.68
30	C	517	DGD	O2D-C2D-C1D	-3.21	102.25	110.05
29	B	623	SQD	C1-O5-C5	-3.21	107.39	113.69
22	B	604	CLA	OBD-CAD-CBD	-3.20	121.32	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
22	c	512	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	T	101	BCR	C35-C13-C14	-3.20	118.44	122.92
22	c	514	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
22	b	602	CLA	C1D-CHD-C4C	3.20	126.78	122.56
24	B	620	BCR	C2-C1-C6	3.19	115.39	110.48
22	d	402	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
22	C	514	CLA	C4D-C3D-CAD	-3.19	106.69	108.47
22	c	511	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
29	a	412	SQD	C1-O5-C5	-3.18	107.44	113.69
22	b	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
24	H	101	BCR	C35-C13-C14	-3.18	118.47	122.92
24	c	518	BCR	C11-C10-C9	-3.18	122.78	127.31
24	B	619	BCR	C40-C30-C25	3.17	115.45	110.30
22	B	607	CLA	CMD-C2D-C3D	3.17	130.61	124.68
22	c	504	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
22	c	508	CLA	CMB-C2B-C3B	3.17	130.60	124.68
34	D	412	LHG	O3-P-O5	-3.16	96.70	109.07
22	c	503	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	c	514	CLA	CMD-C2D-C3D	3.16	130.59	124.68
22	c	510	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	b	607	CLA	C4A-NA-C1A	3.16	108.13	106.71
34	D	409	LHG	O8-C23-C24	3.16	121.82	111.91
22	B	606	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	B	617	CLA	C5-C3-C2	3.16	127.50	121.12
23	A	404	PHO	CMB-C2B-C1B	-3.15	120.21	125.06
22	b	609	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	b	619	SQD	O47-C7-C8	3.14	118.28	111.50
22	c	505	CLA	CMD-C2D-C3D	3.14	130.56	124.68
23	d	401	PHO	O1D-CGD-CBD	3.14	130.91	124.48
22	B	606	CLA	OBD-CAD-CBD	-3.14	121.41	125.89
22	A	411	CLA	C2C-C1C-NC	3.14	112.91	109.97
24	t	101	BCR	C7-C8-C9	-3.13	121.50	126.23
27	d	405	PL9	C36-C34-C33	-3.13	114.79	121.12
22	C	505	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	b	605	CLA	C4D-C3D-CAD	-3.13	106.73	108.47
22	c	509	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
22	a	403	CLA	C4A-NA-C1A	3.12	108.11	106.71
22	b	613	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	B	604	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
29	D	407	SQD	O5-C1-C2	-3.11	103.76	110.35
22	d	402	CLA	CMD-C2D-C3D	3.11	130.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	C	508	CLA	C1-C2-C3	-3.11	120.66	126.04
24	a	406	BCR	C27-C26-C25	3.11	127.25	122.73
22	C	514	CLA	CMD-C2D-C3D	3.11	130.49	124.68
22	b	607	CLA	O2A-CGA-O1A	-3.10	115.76	123.59
22	b	613	CLA	C1D-CHD-C4C	3.10	126.66	122.56
22	b	612	CLA	C4A-NA-C1A	3.10	108.10	106.71
22	C	504	CLA	O2A-C1-C2	-3.09	100.50	108.64
22	C	508	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
28	b	623	LMG	O1-C1-C2	-3.09	103.48	108.30
22	c	512	CLA	CMD-C2D-C3D	3.09	130.46	124.68
22	b	612	CLA	CMB-C2B-C3B	3.08	130.45	124.68
22	C	513	CLA	C4A-NA-C1A	3.08	108.09	106.71
22	C	514	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
29	a	413	SQD	O48-C23-C24	3.08	121.57	111.91
22	b	612	CLA	CHB-C4A-NA	3.08	128.77	124.51
28	C	519	LMG	O1-C7-C8	-3.08	103.48	110.90
22	c	512	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
30	C	518	DGD	O6D-C1D-O3G	-3.07	102.70	109.97
27	D	405	PL9	C7-C8-C9	-3.07	121.68	126.79
22	b	603	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	b	608	CLA	C4A-NA-C1A	3.07	108.08	106.71
22	d	402	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	b	611	CLA	OBD-CAD-CBD	-3.06	121.52	125.89
22	C	507	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
22	B	611	CLA	O1D-CGD-CBD	3.05	130.72	124.48
22	b	606	CLA	C6-C7-C8	-3.04	106.09	115.92
22	b	601	CLA	CHB-C4A-NA	3.04	128.72	124.51
22	b	604	CLA	O1D-CGD-CBD	3.04	130.71	124.48
22	b	611	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	b	611	CLA	C11-C12-C13	-3.04	106.10	115.92
28	c	525	LMG	O6-C1-O1	-3.03	102.79	109.97
22	C	508	CLA	C4-C3-C5	3.03	120.37	115.27
28	A	412	LMG	C1-O6-C5	-3.03	107.73	113.69
22	B	610	CLA	OBD-CAD-CBD	-3.03	121.56	125.89
22	B	616	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	b	617	BCR	C15-C14-C13	-3.02	123.00	127.31
22	d	403	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
22	B	610	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
29	b	619	SQD	O9-S-O7	-3.01	103.52	113.95
22	B	606	CLA	C1D-CHD-C4C	3.01	126.53	122.56
22	c	509	CLA	CMB-C2B-C3B	3.01	130.31	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	CGD-CBD-CAD	-3.00	101.02	110.73
22	A	403	CLA	CED-O2D-CGD	-3.00	109.16	115.94
30	c	520	DGD	C3G-O3G-C1D	2.99	119.59	113.74
30	c	520	DGD	O3G-C1D-C2D	-2.99	103.63	108.30
22	a	405	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
22	b	611	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
27	a	410	PL9	C22-C23-C24	-2.99	120.47	127.66
22	C	514	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
29	B	623	SQD	O48-C23-C24	2.99	121.28	111.91
22	B	605	CLA	C11-C12-C13	-2.98	106.28	115.92
22	c	513	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
22	h	101	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
30	c	521	DGD	C3D-C4D-C5D	-2.98	104.93	110.24
27	a	410	PL9	C20-C19-C21	2.98	120.28	115.27
24	B	620	BCR	C29-C30-C25	2.98	115.06	110.48
24	a	406	BCR	C30-C25-C26	-2.97	118.43	122.61
22	b	604	CLA	C4D-C3D-CAD	-2.97	106.81	108.47
22	c	504	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	c	504	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
35	v	201	HEC	CMC-C2C-C1C	-2.96	123.92	128.46
35	V	201	HEC	CBA-CAA-C2A	-2.96	107.03	112.48
35	F	101	HEC	CMB-C2B-C3B	2.96	129.30	125.82
29	b	619	SQD	O5-C5-C4	2.95	115.06	109.69
27	A	410	PL9	O2-C1-C2	-2.95	115.02	121.78
22	B	604	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	a	406	BCR	C29-C30-C25	2.94	115.01	110.48
22	c	503	CLA	CMB-C2B-C3B	2.94	130.18	124.68
30	c	519	DGD	O2G-C1B-O1B	-2.94	116.60	123.70
24	x	101	BCR	C27-C26-C25	2.94	127.00	122.73
24	H	101	BCR	C27-C26-C25	2.94	127.00	122.73
34	D	408	LHG	O8-C23-O10	-2.93	116.19	123.59
22	b	605	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
30	A	415	DGD	O2D-C2D-C1D	-2.93	102.94	110.05
22	A	402	CLA	O1D-CGD-CBD	2.92	130.47	124.48
22	B	616	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
22	C	507	CLA	CMD-C2D-C3D	2.92	130.15	124.68
30	h	102	DGD	C3D-C4D-C5D	-2.92	105.03	110.24
22	b	609	CLA	C1-C2-C3	-2.92	120.99	126.04
22	C	510	CLA	C1-C2-C3	-2.92	120.99	126.04
22	b	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	c	509	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	A	411	CLA	CMD-C2D-C3D	2.92	130.14	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	623	LMG	C3-C4-C5	-2.91	105.04	110.24
22	C	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	a	411	CLA	CMB-C2B-C3B	2.91	130.13	124.68
28	b	621	LMG	C38-C37-C36	-2.91	99.66	114.42
22	b	610	CLA	C1D-CHD-C4C	2.91	126.40	122.56
22	c	513	CLA	CHB-C4A-NA	2.91	128.53	124.51
22	B	606	CLA	C7-C6-C5	-2.91	105.47	113.36
28	D	406	LMG	C3-C4-C5	-2.91	105.06	110.24
22	c	515	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	c	513	CLA	CMD-C2D-C3D	2.90	130.11	124.68
22	b	615	CLA	O2D-CGD-CBD	2.90	116.43	111.27
22	c	508	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
22	c	514	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
24	y	101	BCR	C33-C5-C6	-2.90	121.27	124.53
34	D	408	LHG	O8-C23-C24	2.90	121.00	111.91
29	a	413	SQD	O49-C7-C8	-2.90	112.43	123.73
24	H	101	BCR	C2-C1-C6	2.89	114.94	110.48
29	D	407	SQD	O48-C23-C24	2.89	120.99	111.91
22	b	606	CLA	CMB-C2B-C3B	2.89	130.09	124.68
29	D	407	SQD	C1-O5-C5	-2.89	108.02	113.69
24	b	616	BCR	C3-C4-C5	-2.89	108.92	114.08
22	a	403	CLA	CHB-C4A-NA	2.89	128.50	124.51
28	d	409	LMG	O6-C1-O1	-2.88	103.15	109.97
30	c	519	DGD	O6E-C5E-C4E	2.88	114.93	109.69
28	B	629	LMG	O6-C1-C2	-2.88	104.26	110.35
24	T	101	BCR	C28-C27-C26	-2.88	108.94	114.08
22	b	607	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	C	516	DGD	O1G-C1A-C2A	-2.87	102.88	111.91
24	b	617	BCR	C30-C25-C26	-2.87	118.56	122.61
28	b	621	LMG	O7-C10-O9	-2.87	116.76	123.70
22	B	617	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
24	Z	101	BCR	C24-C23-C22	-2.87	121.90	126.23
22	C	510	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
22	A	402	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
23	A	404	PHO	CHD-C1D-ND	-2.86	118.61	124.58
24	b	617	BCR	C27-C26-C25	2.86	126.89	122.73
24	Y	101	BCR	C30-C25-C26	-2.86	118.58	122.61
30	c	519	DGD	O6D-C1D-O3G	-2.86	103.20	109.97
24	A	406	BCR	C38-C26-C25	-2.86	121.32	124.53
30	A	415	DGD	C3G-C2G-C1G	-2.86	105.03	111.79
29	B	623	SQD	O8-S-C6	2.85	110.28	105.74
24	b	618	BCR	C2-C1-C6	2.85	114.87	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	CLA	CHB-C4A-NA	2.84	128.44	124.51
28	d	409	LMG	O2-C2-C1	-2.84	103.15	110.05
22	b	613	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
28	b	621	LMG	C1-O6-C5	-2.83	108.13	113.69
22	C	507	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	B	613	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	T	101	BCR	C27-C26-C25	2.83	126.83	122.73
22	b	607	CLA	OBD-CAD-CBD	-2.83	121.86	125.89
22	b	614	CLA	CMD-C2D-C3D	2.82	129.96	124.68
29	A	413	SQD	O47-C7-O49	-2.82	116.88	123.70
24	c	516	BCR	C11-C10-C9	-2.82	123.28	127.31
34	d	407	LHG	C20-C19-C18	-2.82	100.11	114.42
22	C	507	CLA	CHA-C1A-NA	-2.82	119.95	126.40
27	A	410	PL9	C35-C34-C36	2.82	120.01	115.27
22	B	604	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
22	c	510	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
22	b	605	CLA	O1D-CGD-CBD	2.81	130.24	124.48
22	C	514	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	B	613	CLA	C11-C12-C13	-2.81	106.84	115.92
24	d	404	BCR	C24-C23-C22	-2.81	121.99	126.23
22	C	513	CLA	CMD-C2D-C3D	2.81	129.93	124.68
22	B	602	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	C	513	CLA	C1-C2-C3	-2.80	121.19	126.04
27	A	410	PL9	C36-C34-C33	-2.80	115.45	121.12
22	A	405	CLA	O2D-CGD-CBD	2.80	116.25	111.27
22	B	614	CLA	CHA-C1A-NA	-2.80	119.98	126.40
22	B	604	CLA	O2D-CGD-CBD	2.80	116.24	111.27
22	B	615	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	617	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	b	613	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	b	608	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
22	C	506	CLA	OBD-CAD-CBD	-2.80	121.90	125.89
29	B	623	SQD	O5-C5-C4	2.79	114.77	109.69
28	c	524	LMG	O7-C10-O9	-2.79	116.96	123.70
22	c	505	CLA	C4D-C3D-CAD	-2.79	106.92	108.47
22	B	602	CLA	OBD-CAD-CBD	-2.78	121.92	125.89
27	A	410	PL9	C30-C29-C31	-2.78	110.59	115.27
27	d	405	PL9	C7-C3-C2	-2.78	119.64	123.30
22	D	403	CLA	CMD-C2D-C3D	2.78	129.88	124.68
22	B	614	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	b	601	CLA	CAC-C3C-C4C	2.78	128.42	124.81
22	B	605	CLA	O2A-CGA-O1A	-2.78	116.58	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	619	SQD	O2-C2-C1	2.78	116.79	110.05
22	b	611	CLA	CHB-C4A-NA	2.78	128.35	124.51
30	h	102	DGD	O3E-C3E-C2E	-2.77	103.94	110.35
24	b	616	BCR	C36-C18-C17	-2.77	119.04	122.92
22	c	507	CLA	OBD-CAD-CBD	-2.77	121.93	125.89
24	c	516	BCR	C33-C5-C6	-2.77	121.42	124.53
22	B	612	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	C	505	CLA	C1D-CHD-C4C	2.77	126.21	122.56
22	b	615	CLA	O1D-CGD-CBD	2.77	130.15	124.48
22	a	405	CLA	OBD-CAD-C3D	2.77	132.57	127.98
22	B	613	CLA	C4D-C3D-CAD	-2.76	106.93	108.47
22	B	615	CLA	CHA-C1A-NA	-2.76	120.07	126.40
29	B	623	SQD	O9-S-O7	-2.76	104.39	113.95
22	b	615	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
30	c	521	DGD	O6D-C1D-O3G	-2.76	103.44	109.97
30	h	102	DGD	O6E-C5E-C6E	-2.76	99.57	106.44
28	M	101	LMG	C1-C2-C3	-2.76	104.26	110.00
22	a	403	CLA	O2D-CGD-CBD	2.76	116.17	111.27
27	A	410	PL9	C27-C28-C29	-2.75	121.03	127.66
24	B	618	BCR	C15-C16-C17	-2.75	117.85	123.47
22	C	505	CLA	OBD-CAD-CBD	-2.75	121.97	125.89
28	D	406	LMG	O6-C1-O1	-2.75	103.47	109.97
22	C	513	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
24	c	518	BCR	C37-C22-C21	-2.74	119.08	122.92
24	c	518	BCR	C27-C26-C25	2.74	126.72	122.73
30	A	415	DGD	O1G-C1A-O1A	-2.74	116.67	123.59
22	c	503	CLA	CED-O2D-CGD	-2.74	109.73	115.94
24	b	616	BCR	C8-C7-C6	-2.74	119.50	127.20
22	c	506	CLA	O2D-CGD-CBD	2.74	116.14	111.27
22	a	405	CLA	CMD-C2D-C3D	2.74	129.80	124.68
27	D	405	PL9	C12-C13-C14	-2.74	121.06	127.66
22	b	604	CLA	C1-C2-C3	-2.73	121.33	126.04
22	B	608	CLA	O2A-C1-C2	-2.73	101.47	108.64
24	b	616	BCR	C15-C14-C13	-2.73	123.42	127.31
35	e	101	HEC	CMC-C2C-C1C	-2.72	124.28	128.46
28	C	519	LMG	O1-C1-C2	-2.72	104.06	108.30
22	c	506	CLA	C7-C6-C5	-2.72	105.98	113.36
22	b	604	CLA	CMD-C2D-C3D	2.72	129.76	124.68
22	b	614	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	b	602	CLA	C4-C3-C5	2.72	119.84	115.27
30	c	520	DGD	O5D-C6D-C5D	-2.71	104.03	109.05
22	C	506	CLA	O1D-CGD-CBD	2.71	130.03	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	b	601	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	B	608	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
22	c	506	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	a	405	CLA	C4-C3-C5	2.70	119.81	115.27
30	C	516	DGD	CDB-CCB-CBB	-2.70	100.72	114.42
22	c	503	CLA	CMD-C2D-C3D	2.70	129.73	124.68
22	B	609	CLA	C1D-CHD-C4C	2.70	126.12	122.56
27	D	405	PL9	C32-C33-C34	-2.70	121.17	127.66
28	A	412	LMG	O8-C28-O10	-2.70	116.79	123.59
22	b	608	CLA	OBD-CAD-C3D	2.70	132.46	127.98
22	C	508	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
22	C	506	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
34	d	406	LHG	C11-C10-C9	-2.69	100.75	114.42
22	c	508	CLA	CMC-C2C-C1C	2.69	129.13	125.04
22	B	602	CLA	C2A-C1A-CHA	2.69	128.56	123.86
22	B	609	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	t	101	BCR	C35-C13-C14	-2.69	119.16	122.92
22	B	617	CLA	CMD-C2D-C3D	2.69	129.71	124.68
29	B	623	SQD	C3-C4-C5	2.69	115.03	110.24
30	C	516	DGD	C3G-C2G-C1G	-2.69	105.43	111.79
30	c	519	DGD	C4D-C3D-C2D	-2.69	106.13	110.82
30	H	102	DGD	C3D-C4D-C5D	-2.69	105.44	110.24
30	C	517	DGD	O5D-C6D-C5D	-2.69	104.07	109.05
22	B	615	CLA	C4-C3-C5	2.69	119.79	115.27
22	b	602	CLA	C5-C3-C2	-2.68	115.69	121.12
22	B	612	CLA	C7-C6-C5	-2.68	106.07	113.36
28	c	524	LMG	O3-C3-C2	-2.68	104.15	110.35
22	b	613	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	C	511	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
22	D	403	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
24	b	616	BCR	C11-C10-C9	-2.68	123.49	127.31
23	a	404	PHO	CBD-CHA-C4D	-2.68	105.52	108.54
22	c	510	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
22	b	604	CLA	CHC-C1C-NC	2.67	128.25	124.20
22	D	403	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	b	610	CLA	C7-C6-C5	-2.67	106.11	113.36
28	B	629	LMG	O6-C5-C4	2.67	114.54	109.69
30	c	519	DGD	CDB-CCB-CBB	-2.67	100.88	114.42
23	A	404	PHO	CBD-CHA-C4D	-2.67	105.54	108.54
22	b	612	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
22	A	403	CLA	C1B-CHB-C4A	-2.66	124.85	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	C3B-C4B-NB	-2.66	105.77	109.21
28	c	525	LMG	C1-O6-C5	-2.66	108.47	113.69
22	C	510	CLA	C2A-C1A-CHA	2.66	128.50	123.86
22	C	503	CLA	C1D-CHD-C4C	2.65	126.06	122.56
22	d	403	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	C	508	CLA	CMB-C2B-C3B	2.65	129.64	124.68
24	Z	101	BCR	C28-C27-C26	-2.65	109.34	114.08
29	b	619	SQD	O48-C23-C24	2.65	120.22	111.91
22	B	617	CLA	C1-C2-C3	2.65	130.62	126.04
29	D	407	SQD	O8-S-O9	-2.65	104.80	111.27
22	B	602	CLA	C1-C2-C3	-2.65	121.47	126.04
30	C	517	DGD	C1D-C2D-C3D	-2.65	104.49	110.00
22	C	509	CLA	C4D-C3D-CAD	-2.65	107.00	108.47
24	b	618	BCR	C15-C16-C17	-2.64	118.06	123.47
22	B	605	CLA	CHB-C4A-NA	2.64	128.17	124.51
30	H	102	DGD	C3E-C4E-C5E	-2.64	105.53	110.24
27	D	405	PL9	C50-C49-C48	-2.64	115.01	122.65
22	b	602	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	B	604	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	h	102	DGD	C3G-C2G-C1G	-2.63	105.56	111.79
24	x	101	BCR	C2-C1-C6	2.63	114.53	110.48
22	c	512	CLA	OBD-CAD-C3D	2.63	132.34	127.98
22	c	503	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	A	403	CLA	CMD-C2D-C3D	2.63	129.59	124.68
22	B	612	CLA	CHD-C4C-NC	2.62	128.34	124.20
22	B	610	CLA	OBD-CAD-C3D	2.62	132.33	127.98
24	b	618	BCR	C29-C30-C25	2.62	114.51	110.48
22	c	513	CLA	OBD-CAD-CBD	-2.62	122.15	125.89
22	B	609	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	d	401	PHO	C6-C7-C8	-2.61	107.47	115.92
22	B	607	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
24	A	406	BCR	C27-C26-C25	2.61	126.52	122.73
28	D	406	LMG	O3-C3-C2	-2.61	104.32	110.35
28	c	524	LMG	C1-O6-C5	-2.61	108.57	113.69
30	H	102	DGD	C1D-C2D-C3D	-2.61	104.57	110.00
28	b	623	LMG	O6-C5-C6	2.60	112.91	106.44
22	B	615	CLA	CMB-C2B-C3B	2.60	129.55	124.68
22	d	402	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	c	510	CLA	CMD-C2D-C3D	2.60	129.54	124.68
22	c	506	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	c	513	CLA	C1D-CHD-C4C	2.60	125.98	122.56
22	B	611	CLA	CHB-C4A-NA	2.60	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C38-C26-C27	-2.59	108.63	113.62
29	b	619	SQD	C3-C4-C5	2.59	114.87	110.24
22	b	602	CLA	O2A-C1-C2	-2.59	101.82	108.64
22	c	509	CLA	C4D-C3D-CAD	-2.59	107.03	108.47
24	B	618	BCR	C2-C1-C6	2.59	114.47	110.48
22	b	602	CLA	O2D-CGD-CBD	2.59	115.87	111.27
22	B	604	CLA	C1D-CHD-C4C	2.59	125.97	122.56
24	B	619	BCR	C29-C30-C25	2.59	114.47	110.48
22	B	612	CLA	C2C-C1C-NC	2.59	112.40	109.97
22	C	509	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	B	616	CLA	C5-C3-C2	-2.59	115.89	121.12
22	B	616	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	B	612	CLA	CMD-C2D-C3D	2.58	129.51	124.68
22	B	610	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	b	613	CLA	O2D-CGD-CBD	2.58	115.86	111.27
22	B	610	CLA	O2D-CGD-CBD	2.58	115.85	111.27
22	b	605	CLA	OBD-CAD-CBD	-2.58	122.21	125.89
22	C	510	CLA	CMD-C2D-C3D	2.58	129.51	124.68
24	c	517	BCR	C11-C10-C9	-2.58	123.63	127.31
29	f	101	SQD	O48-C23-O10	-2.58	117.08	123.59
22	d	402	CLA	C4-C3-C5	2.58	119.61	115.27
24	d	404	BCR	C33-C5-C6	-2.58	121.63	124.53
22	c	506	CLA	C1D-CHD-C4C	2.58	125.96	122.56
24	c	517	BCR	C27-C26-C25	2.58	126.47	122.73
30	H	102	DGD	O2G-C1B-O1B	-2.58	117.47	123.70
22	c	515	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
22	B	617	CLA	O1D-CGD-CBD	2.58	129.75	124.48
22	C	508	CLA	C1D-CHD-C4C	2.58	125.96	122.56
24	d	404	BCR	C16-C15-C14	-2.57	118.20	123.47
22	B	607	CLA	C6-C5-C3	-2.57	106.70	113.45
23	d	401	PHO	CMB-C2B-C1B	-2.57	121.10	125.06
22	c	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	D	403	CLA	O1D-CGD-CBD	2.57	129.75	124.48
30	c	521	DGD	O5D-C6D-C5D	-2.57	104.29	109.05
30	c	519	DGD	O6D-C1D-C2D	2.57	115.78	110.35
34	e	102	LHG	C20-C19-C18	-2.57	101.40	114.42
22	A	405	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
28	c	525	LMG	O7-C10-O9	-2.57	117.50	123.70
29	a	413	SQD	C45-O47-C7	2.57	124.11	117.79
24	B	619	BCR	C15-C14-C13	-2.56	123.65	127.31
24	Y	101	BCR	C39-C30-C25	-2.56	106.14	110.30
23	D	401	PHO	CMB-C2B-C1B	-2.56	121.12	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	411	CLA	CMD-C2D-C3D	2.56	129.47	124.68
22	B	604	CLA	OBD-CAD-C3D	2.56	132.23	127.98
22	c	505	CLA	CMB-C2B-C3B	2.56	129.46	124.68
22	c	508	CLA	C4-C3-C2	-2.55	117.12	123.68
24	c	517	BCR	C15-C16-C17	-2.55	118.24	123.47
22	c	510	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
24	b	618	BCR	C32-C1-C6	-2.55	106.16	110.30
22	b	609	CLA	O2D-CGD-CBD	2.55	115.80	111.27
23	D	401	PHO	O1D-CGD-CBD	2.55	129.70	124.48
22	B	602	CLA	O2D-CGD-CBD	2.55	115.79	111.27
22	C	513	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	504	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
24	B	619	BCR	C39-C30-C25	-2.55	106.17	110.30
22	C	512	CLA	CMB-C2B-C1B	-2.54	124.55	128.46
24	b	616	BCR	C35-C13-C12	2.54	122.08	118.08
22	b	603	CLA	CMD-C2D-C3D	2.54	129.44	124.68
30	C	516	DGD	O2G-C1B-C2B	-2.54	106.02	111.50
22	b	606	CLA	OBD-CAD-CBD	-2.54	122.27	125.89
23	a	404	PHO	O2A-CGA-O1A	-2.54	117.18	123.59
22	C	514	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
22	C	511	CLA	C4D-C3D-CAD	-2.54	107.06	108.47
24	a	406	BCR	C7-C8-C9	-2.54	122.40	126.23
22	a	411	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	d	402	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	613	CLA	C1D-CHD-C4C	2.53	125.90	122.56
24	b	617	BCR	C31-C1-C6	2.53	114.40	110.30
24	A	406	BCR	C15-C14-C13	-2.53	123.70	127.31
22	B	602	CLA	C4-C3-C5	2.53	119.52	115.27
22	C	512	CLA	C4-C3-C5	2.53	119.52	115.27
29	b	619	SQD	O5-C1-C2	-2.53	105.00	110.35
27	a	410	PL9	C36-C34-C33	-2.52	116.01	121.12
22	b	605	CLA	C2A-C1A-CHA	2.52	128.27	123.86
22	b	610	CLA	CED-O2D-CGD	-2.52	110.24	115.94
24	C	515	BCR	C33-C5-C6	-2.52	121.70	124.53
28	D	406	LMG	C1-C2-C3	-2.52	104.76	110.00
30	C	518	DGD	O3E-C3E-C2E	-2.51	104.54	110.35
27	a	410	PL9	C7-C8-C9	-2.51	122.61	126.79
22	C	506	CLA	CMB-C2B-C3B	2.51	129.38	124.68
30	c	519	DGD	O5E-C6E-C5E	-2.51	102.67	111.29
22	c	505	CLA	C3A-C2A-C1A	2.51	105.10	101.34
34	E	101	LHG	O8-C23-C24	2.51	119.79	111.91
22	b	608	CLA	C1D-CHD-C4C	2.51	125.87	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	524	LMG	O2-C2-C1	-2.51	103.95	110.05
22	b	614	CLA	C1-O2A-CGA	2.51	123.02	116.44
22	b	603	CLA	C2A-C1A-CHA	2.51	128.24	123.86
22	c	506	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	a	405	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
24	D	404	BCR	C27-C26-C25	2.51	126.37	122.73
28	A	412	LMG	C38-C37-C36	-2.50	101.71	114.42
22	C	508	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	a	406	BCR	C38-C26-C27	-2.50	108.81	113.62
23	D	401	PHO	C3C-C4C-NC	-2.50	106.40	110.28
22	a	402	CLA	C7-C6-C5	-2.50	106.57	113.36
22	B	604	CLA	C3B-C4B-NB	-2.50	105.98	109.21
22	C	507	CLA	OBD-CAD-C3D	2.50	132.13	127.98
22	c	509	CLA	C2C-C1C-NC	2.50	112.31	109.97
22	B	616	CLA	C14-C13-C15	-2.50	102.25	111.29
28	d	409	LMG	C9-C8-C7	-2.50	105.88	111.79
30	C	516	DGD	C3D-C4D-C5D	-2.50	105.79	110.24
22	C	503	CLA	OBD-CAD-CBD	-2.50	122.33	125.89
27	d	405	PL9	C15-C14-C13	-2.49	117.28	123.68
24	c	517	BCR	C34-C9-C10	-2.49	119.43	122.92
22	c	512	CLA	C1D-CHD-C4C	2.49	125.85	122.56
22	C	508	CLA	C2A-C1A-CHA	2.49	128.22	123.86
24	B	619	BCR	C11-C10-C9	-2.49	123.76	127.31
28	c	525	LMG	C40-C39-C38	-2.49	101.79	114.42
22	b	602	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
22	d	403	CLA	O1D-CGD-CBD	2.48	129.57	124.48
28	B	629	LMG	O5-C6-C5	-2.48	102.77	111.29
34	D	412	LHG	O8-C23-O10	-2.48	117.33	123.59
22	c	510	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
28	c	522	LMG	O7-C10-O9	-2.48	118.03	122.96
30	H	102	DGD	C7B-C6B-C5B	-2.48	101.83	114.42
22	A	405	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	B	602	CLA	C3A-C2A-C1A	2.48	105.05	101.34
23	a	404	PHO	CBC-CAC-C3C	2.48	119.27	112.43
22	b	614	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	b	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	c	518	BCR	C8-C7-C6	-2.47	120.25	127.20
22	b	609	CLA	C11-C12-C13	-2.47	107.93	115.92
24	b	616	BCR	C29-C30-C25	2.47	114.29	110.48
22	C	502	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
27	A	410	PL9	C40-C39-C41	2.47	119.43	115.27
30	H	102	DGD	C1E-O6E-C5E	2.46	118.53	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	PHO	O2A-CGA-O1A	-2.46	117.38	123.59
22	D	402	CLA	CHB-C4A-NA	2.46	127.92	124.51
34	d	408	LHG	O8-C23-O10	-2.46	117.38	123.59
22	B	606	CLA	CHD-C4C-C3C	-2.46	121.22	124.84
22	D	402	CLA	OBD-CAD-CBD	-2.46	122.38	125.89
29	f	101	SQD	O5-C1-O6	2.46	115.80	109.97
22	B	615	CLA	C2A-C1A-CHA	2.46	128.16	123.86
22	D	403	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
22	C	508	CLA	C4-C3-C2	-2.46	117.38	123.68
22	b	607	CLA	CMD-C2D-C3D	2.46	129.27	124.68
22	C	504	CLA	CMB-C2B-C3B	2.46	129.27	124.68
24	B	619	BCR	C7-C8-C9	-2.46	122.52	126.23
22	c	503	CLA	C2C-C1C-NC	2.46	112.27	109.97
22	c	507	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	C	504	CLA	CMD-C2D-C3D	2.45	129.26	124.68
22	B	614	CLA	O1D-CGD-CBD	2.45	129.50	124.48
30	C	516	DGD	O6D-C1D-O3G	-2.45	104.18	109.97
22	B	610	CLA	C2C-C1C-NC	2.45	112.27	109.97
22	B	603	CLA	CMD-C2D-C3D	2.45	129.25	124.68
22	c	506	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	x	101	BCR	C38-C26-C25	-2.44	121.79	124.53
22	C	504	CLA	O1D-CGD-CBD	2.44	129.47	124.48
28	c	522	LMG	O6-C1-O1	-2.44	104.21	109.97
22	C	508	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
30	c	519	DGD	O1G-C1A-C2A	-2.43	104.28	111.91
22	C	509	CLA	C1D-CHD-C4C	2.43	125.77	122.56
34	B	622	LHG	C27-C26-C25	-2.43	102.09	114.42
22	A	405	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	B	629	LMG	C9-C8-C7	-2.43	106.05	111.79
35	F	101	HEC	CAD-CBD-CGD	2.43	116.74	112.67
22	B	613	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	b	609	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	D	405	PL9	C41-C39-C38	-2.42	116.21	121.12
22	B	602	CLA	CMD-C2D-C3D	2.42	129.21	124.68
33	C	522	STE	C4-C3-C2	-2.42	104.34	113.76
22	c	508	CLA	OBD-CAD-C3D	2.42	132.00	127.98
24	t	101	BCR	C15-C16-C17	-2.42	118.51	123.47
22	b	613	CLA	OBD-CAD-CBD	-2.42	122.44	125.89
29	D	407	SQD	C44-O6-C1	2.42	117.85	113.84
29	b	619	SQD	C45-O47-C7	2.42	123.75	117.79
30	c	519	DGD	O3G-C3G-C2G	-2.42	105.06	110.90
22	A	405	CLA	CMD-C2D-C3D	2.42	129.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	609	CLA	C6-C7-C8	-2.42	108.11	115.92
22	a	405	CLA	CMB-C2B-C3B	2.41	129.20	124.68
24	A	406	BCR	C24-C23-C22	-2.41	122.59	126.23
22	B	607	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	h	102	DGD	C4D-C3D-C2D	-2.41	106.61	110.82
22	c	512	CLA	CMB-C2B-C3B	2.41	129.19	124.68
23	a	404	PHO	CHC-C4B-NB	2.41	129.98	124.93
33	X	101	STE	C12-C11-C10	-2.41	102.18	114.42
22	A	403	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	607	CLA	O2D-CGD-CBD	2.41	115.55	111.27
29	f	101	SQD	C1-O5-C5	-2.41	108.96	113.69
22	C	502	CLA	C1D-CHD-C4C	2.41	125.73	122.56
28	B	629	LMG	O7-C10-O9	-2.41	117.89	123.70
24	H	101	BCR	C29-C30-C25	2.40	114.18	110.48
24	T	101	BCR	C39-C30-C25	2.40	114.20	110.30
22	B	611	CLA	OBD-CAD-C3D	2.40	131.97	127.98
24	a	406	BCR	C15-C16-C17	-2.40	118.55	123.47
22	b	608	CLA	CED-O2D-CGD	2.40	121.37	115.94
22	b	607	CLA	CHC-C1C-NC	2.40	127.84	124.20
22	A	403	CLA	C4A-NA-C1A	2.40	107.78	106.71
24	B	620	BCR	C28-C27-C26	-2.40	109.80	114.08
28	C	519	LMG	O2-C2-C1	-2.40	104.22	110.05
29	f	101	SQD	O5-C5-C4	2.40	114.05	109.69
30	H	102	DGD	O6D-C1D-O3G	-2.40	104.30	109.97
24	b	616	BCR	C15-C16-C17	-2.40	118.57	123.47
22	b	602	CLA	O1D-CGD-CBD	2.40	129.39	124.48
28	b	623	LMG	O5-C6-C5	-2.40	103.07	111.29
24	B	618	BCR	C27-C26-C25	2.39	126.21	122.73
22	C	504	CLA	C1-O2A-CGA	2.39	122.73	116.44
22	c	513	CLA	CMB-C2B-C3B	2.39	129.16	124.68
23	d	401	PHO	O2D-CGD-O1D	-2.39	119.16	123.84
22	B	603	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	A	405	CLA	C2C-C1C-NC	2.39	112.21	109.97
35	F	101	HEC	CMC-C2C-C3C	-2.39	123.01	125.82
22	b	607	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
34	D	408	LHG	C29-C28-C27	-2.39	102.30	114.42
22	a	405	CLA	O2D-CGD-CBD	2.39	115.51	111.27
22	A	402	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
24	H	101	BCR	C38-C26-C25	-2.39	121.85	124.53
22	c	514	CLA	O1D-CGD-CBD	2.39	129.37	124.48
30	C	516	DGD	C7B-C6B-C5B	-2.38	102.32	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C6-C7-C8	-2.38	108.22	115.92
34	e	102	LHG	C11-C10-C9	-2.38	102.33	114.42
22	c	514	CLA	C1D-CHD-C4C	2.38	125.70	122.56
24	K	101	BCR	C3-C4-C5	-2.38	109.83	114.08
22	b	612	CLA	CMD-C2D-C3D	2.38	129.13	124.68
22	b	611	CLA	CMC-C2C-C1C	-2.38	121.42	125.04
22	b	603	CLA	C6-C7-C8	-2.38	108.23	115.92
24	Z	101	BCR	C35-C13-C14	-2.38	119.59	122.92
30	H	102	DGD	O3E-C3E-C2E	-2.37	104.86	110.35
24	b	616	BCR	C24-C23-C22	-2.37	122.65	126.23
28	d	409	LMG	O3-C3-C2	-2.37	104.87	110.35
22	c	503	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
27	A	410	PL9	C15-C14-C16	-2.37	111.29	115.27
30	c	519	DGD	O2D-C2D-C1D	-2.37	104.30	110.05
22	c	511	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	c	512	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	A	411	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	A	411	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
22	c	506	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
22	c	505	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	c	511	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
34	D	412	LHG	C20-C19-C18	-2.36	102.42	114.42
23	d	401	PHO	C1-C2-C3	-2.36	121.95	126.04
24	A	406	BCR	C35-C13-C12	2.36	121.80	118.08
27	d	405	PL9	C12-C13-C14	-2.36	121.97	127.66
22	D	402	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	d	401	PHO	C1B-NB-C4B	2.36	110.96	106.51
24	b	616	BCR	C38-C26-C25	-2.36	121.88	124.53
22	C	502	CLA	OBD-CAD-CBD	-2.36	122.53	125.89
35	V	201	HEC	CAD-CBD-CGD	-2.36	108.71	112.67
23	A	404	PHO	C1B-NB-C4B	2.36	110.95	106.51
22	b	605	CLA	C2C-C1C-NC	2.36	112.18	109.97
34	e	102	LHG	C15-C14-C13	-2.36	102.46	114.42
22	b	602	CLA	OBD-CAD-CBD	-2.36	122.53	125.89
22	h	101	CLA	CMB-C2B-C3B	2.36	129.09	124.68
22	c	511	CLA	O1D-CGD-CBD	2.36	129.31	124.48
29	A	414	SQD	O48-C23-O10	-2.36	117.64	123.59
22	b	605	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	D	403	CLA	O2A-C1-C2	-2.36	102.44	108.64
30	c	520	DGD	O3D-C3D-C4D	-2.35	104.91	110.35
22	h	101	CLA	C1D-CHD-C4C	2.35	125.66	122.56
22	d	402	CLA	CMA-C3A-C4A	-2.35	105.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	411	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	d	405	PL9	C31-C32-C33	-2.35	104.17	111.88
24	d	404	BCR	C2-C1-C6	2.35	114.09	110.48
27	D	405	PL9	C36-C34-C33	-2.35	116.37	121.12
22	B	604	CLA	CAC-C3C-C4C	2.34	127.85	124.81
22	a	402	CLA	C3A-C2A-C1A	2.34	104.85	101.34
22	d	403	CLA	CHD-C4C-C3C	2.34	128.28	124.84
22	b	609	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
28	A	412	LMG	C1-C2-C3	-2.34	105.12	110.00
24	a	406	BCR	C2-C1-C6	2.34	114.08	110.48
28	A	412	LMG	C35-C34-C33	-2.34	102.55	114.42
22	C	506	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
22	B	602	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
24	x	101	BCR	C36-C18-C17	-2.34	119.65	122.92
22	c	515	CLA	OBD-CAD-CBD	-2.33	122.56	125.89
22	d	403	CLA	C1-C2-C3	-2.33	122.01	126.04
24	c	517	BCR	C36-C18-C17	-2.33	119.65	122.92
28	D	410	LMG	O8-C28-O10	-2.33	117.71	123.59
28	D	406	LMG	O2-C2-C1	-2.33	104.38	110.05
22	b	608	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
23	a	404	PHO	C1B-NB-C4B	2.33	110.90	106.51
22	c	511	CLA	OBD-CAD-CBD	-2.33	122.57	125.89
22	B	607	CLA	C1D-CHD-C4C	2.33	125.63	122.56
22	B	617	CLA	CAC-C3C-C4C	2.33	127.83	124.81
34	l	101	LHG	C11-C10-C9	-2.33	102.61	114.42
29	b	619	SQD	O47-C45-C46	2.33	116.83	108.40
28	b	621	LMG	O1-C7-C8	-2.33	105.29	110.90
28	C	519	LMG	O3-C3-C2	-2.33	104.97	110.35
34	d	407	LHG	O7-C7-C8	-2.32	106.49	111.50
27	a	410	PL9	C42-C43-C44	-2.32	122.06	127.66
22	c	505	CLA	C11-C12-C13	-2.32	108.41	115.92
22	d	402	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	C	504	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
27	d	405	PL9	C20-C19-C21	2.32	119.17	115.27
30	C	517	DGD	CDB-CCB-CBB	-2.32	102.67	114.42
22	c	515	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
28	C	519	LMG	C38-C37-C36	-2.32	102.67	114.42
24	H	101	BCR	C37-C22-C21	-2.32	119.68	122.92
22	c	508	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	h	101	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	d	402	CLA	C6-C7-C8	-2.31	108.45	115.92
22	a	403	CLA	CAC-C3C-C4C	2.31	127.81	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	c	520	DGD	O6D-C1D-O3G	-2.31	104.51	109.97
22	b	606	CLA	C4D-C3D-CAD	-2.31	107.18	108.47
22	b	611	CLA	O2A-C1-C2	-2.31	102.57	108.64
27	A	410	PL9	C20-C19-C21	2.31	119.15	115.27
35	e	101	HEC	C1D-C2D-C3D	-2.30	105.39	107.00
24	b	618	BCR	C31-C1-C6	2.30	114.03	110.30
22	B	606	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	b	612	CLA	CHA-C1A-NA	-2.30	121.13	126.40
28	M	101	LMG	C4-C3-C2	-2.30	106.81	110.82
24	d	404	BCR	C38-C26-C25	-2.30	121.95	124.53
22	C	505	CLA	C6-C5-C3	2.30	119.48	113.45
22	b	610	CLA	CHA-C1A-NA	-2.30	121.14	126.40
35	v	201	HEC	CBA-CAA-C2A	-2.29	108.25	112.48
22	b	615	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
22	b	612	CLA	O1D-CGD-CBD	2.29	129.17	124.48
24	K	101	BCR	C7-C8-C9	-2.29	122.77	126.23
22	C	513	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
34	d	406	LHG	C27-C26-C25	-2.29	102.80	114.42
29	D	407	SQD	O5-C5-C4	2.29	113.85	109.69
22	c	503	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
22	D	402	CLA	CMD-C2D-C3D	2.29	128.96	124.68
29	b	619	SQD	O48-C23-O10	-2.29	117.82	123.59
22	C	509	CLA	O1D-CGD-CBD	2.29	129.16	124.48
22	B	603	CLA	C1-C2-C3	-2.29	122.09	126.04
34	d	407	LHG	C18-C17-C16	-2.29	102.82	114.42
28	M	101	LMG	C1-O6-C5	-2.28	109.20	113.69
28	D	406	LMG	O1-C1-C2	-2.28	104.74	108.30
22	b	601	CLA	CHC-C1C-NC	2.28	127.67	124.20
24	B	620	BCR	C30-C25-C26	-2.28	119.40	122.61
30	C	516	DGD	C9B-C8B-C7B	-2.28	102.84	114.42
28	b	621	LMG	C9-C8-C7	-2.28	106.39	111.79
27	d	405	PL9	C42-C43-C44	-2.28	122.18	127.66
22	c	505	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	C	509	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
22	c	504	CLA	C1-C2-C3	-2.27	122.11	126.04
34	D	412	LHG	C11-C10-C9	-2.27	102.88	114.42
22	C	514	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
34	d	407	LHG	C11-C10-C9	-2.27	102.89	114.42
22	C	503	CLA	CHD-C4C-NC	2.27	127.78	124.20
30	C	516	DGD	C6B-C5B-C4B	-2.27	102.89	114.42
28	c	524	LMG	C3-C4-C5	-2.27	106.19	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	519	DGD	O3E-C3E-C2E	-2.27	105.11	110.35
30	c	521	DGD	CAB-C9B-C8B	-2.27	102.92	114.42
22	b	610	CLA	C4A-NA-C1A	2.27	107.72	106.71
24	Y	101	BCR	C38-C26-C27	-2.27	109.26	113.62
24	t	101	BCR	C29-C30-C25	2.26	113.97	110.48
30	C	516	DGD	CCB-CBB-CAB	-2.26	102.94	114.42
24	b	618	BCR	C36-C18-C17	-2.26	119.76	122.92
30	C	516	DGD	O3E-C3E-C2E	-2.26	105.13	110.35
30	C	518	DGD	CDB-CCB-CBB	-2.26	102.97	114.42
22	C	504	CLA	C6-C7-C8	-2.25	108.63	115.92
22	C	514	CLA	O1D-CGD-CBD	2.25	129.10	124.48
22	c	507	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	c	509	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
22	a	402	CLA	CGD-CBD-CAD	-2.25	103.44	110.73
24	a	406	BCR	C11-C10-C9	-2.25	124.10	127.31
22	B	610	CLA	CHA-C1A-NA	-2.25	121.24	126.40
24	B	620	BCR	C1-C6-C5	-2.25	119.44	122.61
30	c	521	DGD	C1D-C2D-C3D	-2.25	105.31	110.00
22	B	616	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
29	f	101	SQD	O9-S-C6	2.25	109.61	106.94
24	B	619	BCR	C2-C1-C6	2.25	113.94	110.48
22	c	514	CLA	O2A-C1-C2	-2.25	102.73	108.64
28	b	623	LMG	C40-C39-C38	-2.25	103.03	114.42
24	c	516	BCR	C12-C13-C14	-2.25	115.50	118.94
22	b	607	CLA	O2D-CGD-CBD	2.24	115.26	111.27
28	c	525	LMG	C38-C37-C36	-2.24	103.03	114.42
29	A	413	SQD	O5-C1-O6	2.24	115.29	109.97
30	c	519	DGD	C3D-C4D-C5D	-2.24	106.23	110.24
22	a	411	CLA	O2D-CGD-CBD	2.24	115.26	111.27
28	b	621	LMG	O2-C2-C1	-2.24	104.60	110.05
22	B	607	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	K	101	BCR	C29-C30-C25	2.24	113.93	110.48
30	c	521	DGD	O3E-C3E-C2E	-2.24	105.17	110.35
24	Z	101	BCR	C36-C18-C17	-2.24	119.79	122.92
30	C	517	DGD	O3D-C3D-C4D	-2.24	105.18	110.35
22	B	614	CLA	CMD-C2D-C3D	2.24	128.86	124.68
24	b	617	BCR	C8-C7-C6	-2.23	120.92	127.20
28	C	519	LMG	C40-C39-C38	-2.23	103.09	114.42
22	B	611	CLA	C3A-C2A-C1A	2.23	104.68	101.34
30	A	415	DGD	CDB-CCB-CBB	-2.23	103.09	114.42
22	B	614	CLA	O2D-CGD-CBD	-2.23	107.30	111.27
29	a	412	SQD	O47-C7-C8	2.23	116.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
33	J	101	STE	C4-C3-C2	-2.23	105.09	113.76
22	c	509	CLA	OBD-CAD-C3D	2.23	131.68	127.98
24	x	101	BCR	C8-C9-C10	2.23	122.36	118.94
22	B	603	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
27	D	405	PL9	C8-C7-C3	2.23	118.28	111.98
30	H	102	DGD	CCB-CBB-CAB	-2.23	103.12	114.42
28	b	621	LMG	O8-C28-O10	-2.23	117.97	123.59
30	h	102	DGD	C7B-C6B-C5B	-2.23	103.12	114.42
24	y	101	BCR	C27-C26-C25	2.23	125.96	122.73
24	B	619	BCR	C15-C16-C17	-2.22	118.92	123.47
22	a	402	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	K	101	BCR	C15-C16-C17	-2.22	118.92	123.47
34	l	101	LHG	O8-C23-C24	2.22	118.89	111.91
22	C	507	CLA	C1D-CHD-C4C	2.22	125.49	122.56
22	B	604	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	D	406	LMG	O8-C28-O10	-2.22	117.98	123.59
29	f	101	SQD	C46-C45-C44	-2.22	106.54	111.79
30	C	518	DGD	O3D-C3D-C4D	-2.22	105.22	110.35
27	A	410	PL9	C12-C13-C14	-2.22	122.31	127.66
22	c	508	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	A	405	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	b	610	CLA	C11-C10-C8	-2.22	108.75	115.92
22	B	612	CLA	CMB-C2B-C3B	2.22	128.83	124.68
24	b	618	BCR	C33-C5-C6	-2.22	122.04	124.53
28	M	101	LMG	O6-C1-O1	-2.22	104.72	109.97
22	c	503	CLA	C1C-C2C-C3C	-2.22	104.63	106.96
35	v	201	HEC	CMB-C2B-C3B	2.22	128.43	125.82
34	l	101	LHG	O8-C23-O10	-2.22	118.00	123.59
22	B	607	CLA	C2A-C1A-CHA	2.21	127.73	123.86
22	B	610	CLA	C2A-C3A-C4A	2.21	105.44	101.87
24	B	618	BCR	C11-C10-C9	-2.21	124.15	127.31
22	a	411	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
22	b	602	CLA	CMA-C3A-C4A	2.21	117.72	111.77
22	a	402	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	C	509	CLA	O2D-CGD-CBD	2.21	115.19	111.27
29	D	407	SQD	O2-C2-C1	2.21	115.41	110.05
22	c	510	CLA	C7-C6-C5	-2.21	107.36	113.36
22	b	609	CLA	C2A-C1A-CHA	2.21	127.72	123.86
24	c	516	BCR	C28-C27-C26	-2.20	110.14	114.08
22	B	612	CLA	CHD-C4C-C3C	-2.20	121.60	124.84
22	C	513	CLA	C1D-CHD-C4C	2.20	125.47	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	621	LMG	C36-C35-C34	-2.20	103.24	114.42
30	C	516	DGD	CBB-CAB-C9B	-2.20	103.25	114.42
22	B	614	CLA	CMA-C3A-C4A	-2.20	105.86	111.77
29	D	407	SQD	O48-C23-O10	-2.20	118.04	123.59
22	B	610	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	A	411	CLA	C2A-C1A-CHA	2.20	127.70	123.86
22	c	504	CLA	O2D-CGD-CBD	2.20	115.17	111.27
22	b	605	CLA	CHA-C1A-NA	-2.20	121.36	126.40
22	b	608	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
22	B	605	CLA	C1-O2A-CGA	-2.19	110.69	116.44
22	B	614	CLA	C2A-C1A-CHA	2.19	127.70	123.86
33	B	621	STE	C6-C5-C4	-2.19	103.28	114.42
28	c	522	LMG	C40-C39-C38	-2.19	103.28	114.42
30	C	516	DGD	C6D-O5D-C1E	2.19	118.02	113.74
23	D	401	PHO	CMD-C2D-C1D	2.19	128.44	125.06
34	E	101	LHG	C20-C19-C18	-2.19	103.31	114.42
24	c	516	BCR	C7-C8-C9	-2.19	122.93	126.23
28	c	524	LMG	O6-C1-O1	-2.19	104.79	109.97
28	M	101	LMG	C22-C21-C20	-2.19	103.31	114.42
22	d	402	CLA	C6-C5-C3	2.19	119.19	113.45
30	A	415	DGD	O6D-C1D-O3G	-2.19	104.80	109.97
24	x	101	BCR	C35-C13-C14	-2.18	119.86	122.92
28	c	524	LMG	O1-C1-C2	-2.18	104.90	108.30
22	C	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	c	508	CLA	CMD-C2D-C3D	2.18	128.76	124.68
22	b	603	CLA	CHD-C4C-NC	2.18	127.64	124.20
29	B	623	SQD	C1-C2-C3	-2.18	105.46	110.00
22	c	505	CLA	CMA-C3A-C4A	2.18	117.63	111.77
27	a	410	PL9	C11-C12-C13	-2.18	104.72	111.88
30	c	520	DGD	C1D-O6D-C5D	-2.18	109.41	113.69
22	b	606	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
24	B	618	BCR	C8-C7-C6	-2.18	121.09	127.20
24	B	618	BCR	C33-C5-C6	-2.18	122.08	124.53
22	c	513	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
27	d	405	PL9	C35-C34-C36	2.17	118.93	115.27
27	d	405	PL9	C7-C8-C9	-2.17	123.17	126.79
22	b	613	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
28	d	409	LMG	C38-C37-C36	-2.17	103.39	114.42
28	c	522	LMG	O2-C2-C1	-2.17	104.77	110.05
22	A	403	CLA	O1D-CGD-CBD	2.17	128.93	124.48
22	B	615	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
34	E	101	LHG	C11-C10-C9	-2.17	103.40	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	CHA-C1A-NA	-2.17	121.43	126.40
30	h	102	DGD	C1E-O6E-C5E	2.17	117.95	113.69
24	H	101	BCR	C16-C17-C18	-2.17	124.22	127.31
22	C	505	CLA	O1A-CGA-CBA	2.17	132.19	123.73
22	b	614	CLA	C16-C15-C13	-2.17	108.91	115.92
28	M	101	LMG	C37-C36-C35	-2.17	103.42	114.42
22	b	603	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
27	d	405	PL9	C46-C47-C48	-2.16	104.77	111.88
30	A	415	DGD	O6E-C5E-C4E	2.16	113.62	109.69
22	B	607	CLA	CHA-C1A-NA	-2.16	121.44	126.40
24	c	518	BCR	C15-C16-C17	-2.16	119.04	123.47
23	a	404	PHO	OBD-CAD-C3D	2.16	133.72	128.52
22	b	608	CLA	CHD-C4C-NC	2.16	127.61	124.20
28	A	412	LMG	O1-C7-C8	-2.16	105.69	110.90
28	M	101	LMG	O3-C3-C2	-2.16	105.35	110.35
34	D	408	LHG	C27-C26-C25	-2.16	103.46	114.42
22	C	511	CLA	CMB-C2B-C3B	2.16	128.72	124.68
22	B	611	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
22	C	505	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	b	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	h	102	DGD	C4E-C3E-C2E	-2.16	107.06	110.82
30	C	516	DGD	O2D-C2D-C1D	-2.16	104.80	110.05
22	b	605	CLA	C7-C6-C5	-2.16	107.50	113.36
30	c	521	DGD	O2D-C2D-C1D	-2.16	104.81	110.05
22	C	506	CLA	CGD-CBD-CAD	-2.15	103.75	110.73
24	D	404	BCR	C3-C4-C5	-2.15	110.23	114.08
22	b	604	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
22	C	512	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	C	508	CLA	O2D-CGD-CBD	2.15	115.09	111.27
22	b	614	CLA	C14-C13-C15	-2.15	103.50	111.29
23	a	404	PHO	C1-C2-C3	-2.15	122.32	126.04
27	a	410	PL9	C31-C29-C28	2.15	125.47	121.12
22	b	607	CLA	OBD-CAD-C3D	2.15	131.55	127.98
24	C	515	BCR	C15-C14-C13	-2.15	124.25	127.31
24	Y	101	BCR	C16-C15-C14	-2.15	119.08	123.47
27	a	410	PL9	C27-C28-C29	-2.15	122.49	127.66
28	b	623	LMG	C38-C37-C36	-2.14	103.54	114.42
22	c	510	CLA	CHB-C4A-NA	2.14	127.48	124.51
24	Z	101	BCR	C2-C1-C6	2.14	113.78	110.48
22	C	503	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
22	A	411	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	A	411	CLA	CMB-C2B-C1B	-2.14	125.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	516	BCR	C35-C13-C14	-2.14	119.92	122.92
22	b	608	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	A	413	SQD	O48-C23-O10	-2.14	118.19	123.59
22	C	510	CLA	C1D-CHD-C4C	2.14	125.38	122.56
22	C	505	CLA	CMD-C2D-C3D	2.14	128.68	124.68
22	c	509	CLA	CHB-C4A-NA	2.14	127.47	124.51
28	M	101	LMG	C38-C37-C36	-2.14	103.58	114.42
22	a	405	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
22	B	605	CLA	CMD-C2D-C3D	2.14	128.67	124.68
22	c	508	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	b	613	CLA	C1-C2-C3	-2.13	122.35	126.04
23	a	404	PHO	C7-C6-C5	-2.13	107.56	113.36
29	a	412	SQD	C9-C8-C7	-2.13	105.86	113.62
27	A	410	PL9	C32-C33-C34	-2.13	122.52	127.66
24	x	101	BCR	C15-C16-C17	-2.13	119.11	123.47
22	b	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	C	510	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	B	610	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
24	C	515	BCR	C32-C1-C6	-2.13	106.85	110.30
28	M	101	LMG	C40-C39-C38	-2.13	103.63	114.42
28	M	101	LMG	O8-C28-O10	-2.13	118.23	123.59
22	b	615	CLA	CED-O2D-CGD	-2.13	111.13	115.94
22	C	508	CLA	C2C-C1C-NC	2.13	111.96	109.97
22	B	615	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
29	D	407	SQD	O9-S-O7	-2.12	106.60	113.95
24	b	617	BCR	C15-C16-C17	-2.12	119.12	123.47
22	B	603	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
22	A	402	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
22	b	609	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
30	c	520	DGD	C4E-C3E-C2E	-2.12	107.12	110.82
24	c	516	BCR	C27-C26-C25	2.12	125.81	122.73
22	C	506	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
27	D	405	PL9	C20-C19-C21	2.12	118.83	115.27
24	D	404	BCR	C30-C25-C26	-2.12	119.63	122.61
29	a	412	SQD	O8-S-C6	2.12	109.11	105.74
22	A	405	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
22	d	402	CLA	O1D-CGD-CBD	2.12	128.81	124.48
23	D	401	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
23	D	401	PHO	C1B-NB-C4B	2.11	110.48	106.51
22	c	512	CLA	O1D-CGD-CBD	2.11	128.79	124.48
24	b	617	BCR	C39-C30-C25	2.11	113.72	110.30
30	c	519	DGD	C4E-C3E-C2E	-2.11	107.15	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	516	DGD	C4E-C3E-C2E	-2.10	107.15	110.82
29	a	412	SQD	C45-O47-C7	2.10	122.97	117.79
22	B	606	CLA	O1D-CGD-CBD	2.10	128.79	124.48
22	a	405	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	A	415	DGD	O4D-C4D-C3D	2.10	115.21	110.35
30	c	520	DGD	C3E-C4E-C5E	-2.10	106.49	110.24
22	b	614	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	B	610	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	b	614	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
30	c	521	DGD	CDB-CCB-CBB	-2.10	103.78	114.42
23	D	401	PHO	C2B-C1B-NB	-2.10	106.63	109.79
30	C	517	DGD	C7B-C6B-C5B	-2.10	103.78	114.42
22	B	616	CLA	CMD-C2D-C3D	2.10	128.60	124.68
24	B	618	BCR	C3-C4-C5	-2.10	110.33	114.08
34	d	408	LHG	C26-C25-C24	2.10	120.72	113.19
30	h	102	DGD	O6D-C1D-O3G	-2.10	105.01	109.97
22	B	607	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
22	b	605	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
24	B	620	BCR	C2-C3-C4	-2.09	106.70	111.38
22	b	613	CLA	C4D-C3D-CAD	-2.09	107.30	108.47
24	c	518	BCR	C38-C26-C25	-2.09	122.18	124.53
22	c	515	CLA	CMD-C2D-C3D	2.09	128.59	124.68
22	B	614	CLA	C1D-CHD-C4C	2.09	125.32	122.56
22	C	509	CLA	C5-C3-C2	-2.09	116.89	121.12
22	b	614	CLA	CHD-C4C-NC	2.09	127.50	124.20
22	c	506	CLA	C4A-NA-C1A	2.09	107.64	106.71
22	c	507	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
22	B	614	CLA	CED-O2D-CGD	2.09	120.66	115.94
30	H	102	DGD	C4D-C3D-C2D	-2.09	107.18	110.82
24	K	101	BCR	C38-C26-C25	-2.09	122.19	124.53
22	B	606	CLA	OBD-CAD-C3D	2.08	131.44	127.98
22	b	605	CLA	C3C-C4C-NC	-2.08	108.23	110.57
22	D	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	B	609	CLA	OBD-CAD-CBD	-2.08	122.92	125.89
28	d	409	LMG	C3-C4-C5	-2.08	106.53	110.24
24	B	619	BCR	C40-C30-C29	-2.08	100.58	108.91
22	b	607	CLA	C3B-C4B-NB	-2.08	106.52	109.21
22	C	514	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	a	402	CLA	O1D-CGD-CBD	2.08	128.74	124.48
22	B	608	CLA	C6-C5-C3	-2.08	108.00	113.45
28	D	406	LMG	C38-C37-C36	-2.08	103.87	114.42
22	b	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	C7-C6-C5	-2.08	107.72	113.36
24	d	404	BCR	C27-C26-C25	2.08	125.75	122.73
23	A	404	PHO	O2D-CGD-O1D	-2.08	119.78	123.84
28	b	623	LMG	O7-C10-O9	-2.08	118.68	123.70
30	H	102	DGD	CAB-C9B-C8B	-2.08	103.89	114.42
22	c	510	CLA	CHD-C4C-NC	2.08	127.47	124.20
22	B	615	CLA	O1D-CGD-CBD	2.07	128.73	124.48
22	B	605	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
28	c	522	LMG	C1-O6-C5	-2.07	109.62	113.69
23	A	404	PHO	O2A-C1-C2	2.07	114.08	108.64
22	b	607	CLA	C11-C10-C8	-2.07	109.22	115.92
22	b	612	CLA	C16-C15-C13	-2.07	109.22	115.92
22	B	614	CLA	CAC-C3C-C4C	2.07	127.50	124.81
27	D	405	PL9	C11-C12-C13	-2.07	105.08	111.88
24	b	616	BCR	C27-C26-C25	2.07	125.74	122.73
22	C	511	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	h	102	DGD	O6E-C1E-O5D	-2.07	105.07	109.97
24	A	406	BCR	C37-C22-C21	-2.07	120.02	122.92
22	c	511	CLA	C3A-C2A-C1A	2.07	104.44	101.34
30	C	516	DGD	O6E-C5E-C4E	2.07	113.45	109.69
24	H	101	BCR	C35-C13-C12	2.07	121.33	118.08
24	C	515	BCR	C10-C11-C12	-2.07	116.77	123.22
22	B	610	CLA	CHD-C4C-NC	2.07	127.46	124.20
24	H	101	BCR	C36-C18-C17	-2.06	120.03	122.92
24	Y	101	BCR	C15-C16-C17	-2.06	119.25	123.47
30	C	516	DGD	C5B-C4B-C3B	-2.06	103.95	114.42
22	c	510	CLA	CAC-C3C-C4C	-2.06	122.14	124.81
22	c	510	CLA	O2D-CGD-CBD	2.06	114.93	111.27
22	b	605	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	A	406	BCR	C33-C5-C6	-2.06	122.22	124.53
22	B	612	CLA	C17-C16-C15	-2.06	103.78	113.24
23	A	404	PHO	CBC-CAC-C3C	2.06	118.10	112.43
22	C	509	CLA	C3A-C2A-C1A	2.06	104.42	101.34
22	b	606	CLA	CHB-C4A-NA	2.06	127.36	124.51
33	X	101	STE	C10-C9-C8	-2.06	103.99	114.42
22	B	612	CLA	CHB-C4A-NA	2.06	127.35	124.51
22	b	604	CLA	C4-C3-C2	-2.06	118.41	123.68
30	C	517	DGD	O3G-C1D-C2D	-2.05	105.10	108.30
22	B	602	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
24	C	515	BCR	C27-C26-C25	2.05	125.71	122.73
22	A	411	CLA	CMB-C2B-C3B	2.05	128.52	124.68
22	c	512	CLA	O2A-CGA-O1A	-2.05	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CHB-C4A-NA	2.05	127.35	124.51
28	c	522	LMG	C3-C4-C5	-2.05	106.58	110.24
24	Y	101	BCR	C8-C7-C6	-2.05	121.45	127.20
22	C	513	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
22	B	604	CLA	O1A-CGA-CBA	2.05	131.72	123.73
22	d	402	CLA	C1-C2-C3	-2.05	122.50	126.04
30	c	519	DGD	CBB-CAB-C9B	-2.05	104.04	114.42
22	C	507	CLA	O1D-CGD-CBD	2.04	128.66	124.48
29	f	101	SQD	O5-C1-C2	-2.04	106.03	110.35
23	A	404	PHO	CAC-C3C-C2C	2.04	131.02	127.53
30	h	102	DGD	C3E-C4E-C5E	-2.04	106.60	110.24
24	b	618	BCR	C16-C15-C14	-2.04	119.29	123.47
24	B	620	BCR	C38-C26-C25	-2.04	122.24	124.53
23	A	404	PHO	CAB-C3B-C4B	-2.04	118.67	126.21
22	b	605	CLA	C1D-CHD-C4C	2.04	125.25	122.56
30	A	415	DGD	O5E-C6E-C5E	-2.04	104.30	111.29
27	d	405	PL9	C47-C48-C49	-2.04	120.79	127.75
22	B	611	CLA	O1A-CGA-CBA	2.04	131.67	123.73
30	C	516	DGD	C4A-C3A-C2A	-2.04	105.87	113.19
22	a	402	CLA	CAC-C3C-C2C	-2.04	124.05	127.53
22	c	506	CLA	O1A-CGA-CBA	2.03	131.67	123.73
30	A	415	DGD	O3G-C3G-C2G	-2.03	105.99	110.90
22	b	608	CLA	O1D-CGD-CBD	2.03	128.64	124.48
30	H	102	DGD	C1D-O6D-C5D	-2.03	109.70	113.69
30	c	521	DGD	C6B-C5B-C4B	-2.03	104.12	114.42
28	D	411	LMG	C36-C35-C34	-2.03	104.12	114.42
22	b	606	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	c	519	DGD	C3G-C2G-C1G	-2.03	106.99	111.79
30	C	518	DGD	C6B-C5B-C4B	-2.03	104.13	114.42
23	D	401	PHO	CBA-CAA-C2A	-2.03	107.88	113.86
28	A	412	LMG	C3-C4-C5	-2.03	106.62	110.24
22	b	609	CLA	CMD-C2D-C3D	2.03	128.47	124.68
22	C	508	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	B	603	CLA	C4A-NA-C1A	2.03	107.62	106.71
28	M	101	LMG	C33-C32-C31	-2.03	104.14	114.42
22	c	507	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	a	413	SQD	C46-O48-C23	2.03	124.62	117.12
22	B	617	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
22	B	617	CLA	C4-C3-C2	-2.02	118.49	123.68
34	d	406	LHG	C20-C19-C18	-2.02	104.16	114.42
22	A	403	CLA	O1A-CGA-CBA	2.02	131.62	123.73
22	b	611	CLA	CMC-C2C-C3C	2.02	131.61	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	412	LHG	C27-C26-C25	-2.02	104.17	114.42
35	v	201	HEC	CMA-C3A-C2A	2.02	128.75	124.94
24	B	619	BCR	C27-C26-C25	2.02	125.66	122.73
30	h	102	DGD	O5D-C6D-C5D	-2.02	105.31	109.05
22	b	608	CLA	C3C-C4C-NC	-2.02	108.31	110.57
22	A	402	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	B	610	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
24	b	617	BCR	C38-C26-C27	-2.02	109.74	113.62
24	K	101	BCR	C37-C22-C21	-2.02	120.10	122.92
29	f	101	SQD	C45-O47-C7	2.02	122.75	117.79
34	D	412	LHG	C18-C17-C16	-2.02	104.19	114.42
30	C	517	DGD	CBB-CAB-C9B	-2.01	104.20	114.42
24	c	516	BCR	C20-C21-C22	-2.01	124.44	127.31
22	C	513	CLA	C11-C12-C13	-2.01	109.41	115.92
30	h	102	DGD	C1D-O6D-C5D	-2.01	109.74	113.69
22	A	405	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	c	516	BCR	C15-C16-C17	-2.01	119.35	123.47
22	b	612	CLA	C2C-C1C-NC	2.01	111.86	109.97
22	b	604	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
22	c	508	CLA	C1D-CHD-C4C	2.01	125.21	122.56
34	E	101	LHG	O8-C23-O10	-2.01	118.52	123.59
30	A	415	DGD	CBB-CAB-C9B	-2.01	104.24	114.42
22	C	509	CLA	CMD-C2D-C3D	2.01	128.43	124.68
30	h	102	DGD	C4B-C3B-C2B	-2.01	105.98	113.19
22	C	507	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
29	A	413	SQD	O8-S-O9	2.01	116.18	111.27
27	a	410	PL9	C21-C19-C18	-2.01	117.06	121.12
24	a	406	BCR	C37-C22-C21	-2.00	120.11	122.92
30	A	415	DGD	CAB-C9B-C8B	-2.00	104.25	114.42
27	D	405	PL9	C35-C34-C36	2.00	118.64	115.27
30	H	102	DGD	CBB-CAB-C9B	-2.00	104.25	114.42
22	c	514	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
22	B	603	CLA	C1D-CHD-C4C	2.00	125.20	122.56
22	b	605	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
23	d	401	PHO	CHC-C1C-C2C	-2.00	120.69	125.73
30	C	518	DGD	C5B-C4B-C3B	-2.00	104.26	114.42
24	x	101	BCR	C35-C13-C12	2.00	121.23	118.08
24	Z	101	BCR	C7-C8-C9	-2.00	123.21	126.23
22	A	411	CLA	OBD-CAD-CBD	2.00	128.75	125.89
27	D	405	PL9	C11-C9-C8	-2.00	117.07	121.12

All (180) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	b	615	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	607	CLA	ND
22	b	607	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	b	609	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	a	411	CLA	ND
22	a	411	CLA	NA
22	D	402	CLA	ND
22	D	402	CLA	NA
22	C	513	CLA	NC
22	C	513	CLA	ND
22	C	513	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	615	CLA	NA
22	b	601	CLA	NC
22	b	601	CLA	ND
22	b	601	CLA	NA
22	a	402	CLA	NC
22	a	402	CLA	ND
22	a	402	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	NA
22	b	611	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	A	403	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	NA
22	b	608	CLA	NC
22	C	514	CLA	NC
22	C	514	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	ND
22	c	513	CLA	NA
22	b	612	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	d	403	CLA	NC
22	d	403	CLA	ND

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Mol	Chain	Res	Type	Atom
22	d	403	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	c	515	CLA	NC
22	c	515	CLA	ND
22	c	515	CLA	NA
22	c	507	CLA	ND
22	c	507	CLA	NA
22	B	617	CLA	NA
22	B	617	CLA	NC
22	B	617	CLA	ND
22	D	403	CLA	NC
22	D	403	CLA	NA
22	c	508	CLA	ND
22	c	508	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	B	603	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	NA
22	c	514	CLA	NC
22	c	514	CLA	ND
22	c	514	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	d	402	CLA	ND
22	d	402	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	c	505	CLA	NC
22	b	602	CLA	NC
22	b	602	CLA	ND
22	b	602	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA

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Mol	Chain	Res	Type	Atom
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	h	101	CLA	NC
22	h	101	CLA	ND
22	h	101	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	B	614	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	b	610	CLA	NC
22	b	610	CLA	NA
22	C	504	CLA	NC
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	A	411	CLA	NA
22	B	611	CLA	NA
22	B	611	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	611	CLA	ND
22	c	509	CLA	NC
22	c	509	CLA	NA
22	c	509	CLA	ND
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	a	403	CLA	NA

All (1772) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	D	410	LMG	O1-C7-C8-C9
28	D	410	LMG	O1-C7-C8-O7
28	D	410	LMG	C11-C10-O7-C8
22	b	604	CLA	C4-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
34	B	622	LHG	C3-O3-P-O4
34	B	622	LHG	C4-O6-P-O4
34	B	622	LHG	C4-O6-P-O5
24	b	618	BCR	C37-C22-C23-C24
27	d	405	PL9	C32-C33-C34-C36
27	d	405	PL9	C42-C43-C44-C45
27	d	405	PL9	C42-C43-C44-C46
34	D	408	LHG	O1-C1-C2-C3
34	D	408	LHG	C1-C2-C3-O3
34	D	408	LHG	O2-C2-C3-O3
34	D	408	LHG	C3-O3-P-O4
34	D	408	LHG	C4-O6-P-O4
22	a	411	CLA	CHA-CBD-CGD-O1D
22	a	411	CLA	CHA-CBD-CGD-O2D
24	Z	101	BCR	C11-C12-C13-C35
24	Z	101	BCR	C35-C13-C14-C15
24	Z	101	BCR	C16-C17-C18-C19
24	Z	101	BCR	C16-C17-C18-C36
24	Z	101	BCR	C17-C18-C19-C20
24	Z	101	BCR	C21-C22-C23-C24
24	Z	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	D	407	SQD	O5-C1-O6-C44
33	d	411	STE	C1-C2-C3-C4
34	d	406	LHG	O1-C1-C2-C3
34	d	406	LHG	C4-O6-P-O5
22	b	605	CLA	CHA-CBD-CGD-O1D
22	b	605	CLA	CHA-CBD-CGD-O2D
33	E	102	STE	C1-C2-C3-C4
24	b	616	BCR	C36-C18-C19-C20
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	CHA-CBD-CGD-O2D
27	a	410	PL9	C17-C18-C19-C21
27	a	410	PL9	C22-C23-C24-C25
27	a	410	PL9	C22-C23-C24-C26
27	a	410	PL9	C42-C43-C44-C45
33	B	621	STE	C1-C2-C3-C4
24	C	515	BCR	C36-C18-C19-C20
24	C	515	BCR	C20-C21-C22-C37
28	D	411	LMG	C28-C29-C30-C31
24	c	517	BCR	C35-C13-C14-C15
24	c	517	BCR	C18-C19-C20-C21
24	c	517	BCR	C20-C21-C22-C37
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
33	d	412	STE	C1-C2-C3-C4
29	a	412	SQD	O6-C44-C45-O47
29	a	412	SQD	C5-C6-S-O7
29	a	412	SQD	C5-C6-S-O8
29	a	412	SQD	C5-C6-S-O9
27	A	410	PL9	C12-C13-C14-C15
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
28	c	524	LMG	C11-C10-O7-C8
22	C	514	CLA	O2A-C1-C2-C3
22	c	513	CLA	C14-C13-C15-C16
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C32-C33-C34-C36
34	E	101	LHG	O1-C1-C2-C3
34	E	101	LHG	C4-O6-P-O4
24	T	101	BCR	C18-C19-C20-C21
24	c	518	BCR	C35-C13-C14-C15
24	c	518	BCR	C36-C18-C19-C20
24	c	518	BCR	C37-C22-C23-C24
34	D	412	LHG	O1-C1-C2-O2
34	D	412	LHG	O1-C1-C2-C3
24	D	404	BCR	C23-C24-C25-C26
24	D	404	BCR	C23-C24-C25-C30
33	B	625	STE	C1-C2-C3-C4
24	a	406	BCR	C11-C10-C9-C34
24	a	406	BCR	C35-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C37
34	l	101	LHG	C4-O6-P-O3
34	l	101	LHG	C4-O6-P-O4
34	l	101	LHG	C4-O6-P-O5
24	c	516	BCR	C7-C8-C9-C10
24	c	516	BCR	C7-C8-C9-C34
24	c	516	BCR	C11-C12-C13-C35
24	c	516	BCR	C12-C13-C14-C15
24	c	516	BCR	C35-C13-C14-C15
24	c	516	BCR	C18-C19-C20-C21
22	C	509	CLA	CHA-CBD-CGD-O1D
33	d	410	STE	C1-C2-C3-C4
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
28	c	525	LMG	O6-C1-O1-C7
28	b	623	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	b	623	LMG	C11-C10-O7-C8
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
28	A	412	LMG	O9-C10-O7-C8
33	b	622	STE	C1-C2-C3-C4
22	c	512	CLA	C12-C13-C15-C16
33	L	101	STE	C1-C2-C3-C4
34	d	407	LHG	O1-C1-C2-C3
34	d	407	LHG	C3-O3-P-O4
34	d	407	LHG	C4-O6-P-O3
34	d	407	LHG	C4-O6-P-O4
34	d	407	LHG	C4-O6-P-O5
34	e	102	LHG	C3-O3-P-O5
34	e	102	LHG	O10-C23-O8-C6
34	e	102	LHG	C24-C23-O8-C6
24	B	619	BCR	C11-C10-C9-C34
24	B	619	BCR	C37-C22-C23-C24
24	A	406	BCR	C20-C21-C22-C37
33	b	624	STE	C1-C2-C3-C4
29	a	413	SQD	O6-C44-C45-C46
29	a	413	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
24	K	101	BCR	C17-C18-C19-C20
24	K	101	BCR	C36-C18-C19-C20
24	K	101	BCR	C37-C22-C23-C24
22	A	411	CLA	CHA-CBD-CGD-O1D
22	A	411	CLA	CHA-CBD-CGD-O2D
24	y	101	BCR	C1-C6-C7-C8
24	y	101	BCR	C5-C6-C7-C8
24	y	101	BCR	C36-C18-C19-C20
33	j	101	STE	C1-C2-C3-C4
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C4-C3-C5-C6
24	t	101	BCR	C17-C18-C19-C20
24	t	101	BCR	C36-C18-C19-C20
22	b	613	CLA	CHA-CBD-CGD-O1D
22	b	613	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
28	c	524	LMG	O10-C28-O8-C9
34	E	101	LHG	O10-C23-O8-C6
28	c	525	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	M	101	LMG	O10-C28-O8-C9
29	D	407	SQD	C24-C23-O48-C46
34	E	101	LHG	C24-C23-O8-C6
22	B	602	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
29	D	407	SQD	O10-C23-O48-C46
29	b	619	SQD	O10-C23-O48-C46
29	a	413	SQD	O10-C23-O48-C46
22	B	604	CLA	CBD-CGD-O2D-CED
28	D	410	LMG	O9-C10-O7-C8
28	c	524	LMG	O9-C10-O7-C8
29	a	413	SQD	O49-C7-O47-C45
22	b	601	CLA	C3-C5-C6-C7
22	A	405	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
29	b	619	SQD	C24-C23-O48-C46
28	c	524	LMG	C29-C28-O8-C9
29	f	101	SQD	C24-C23-O48-C46
28	c	525	LMG	C29-C28-O8-C9
29	a	413	SQD	C24-C23-O48-C46
28	A	412	LMG	C11-C10-O7-C8
29	B	623	SQD	O10-C23-O48-C46
30	A	415	DGD	O6E-C5E-C6E-O5E
27	a	410	PL9	C35-C34-C36-C37
27	A	410	PL9	C20-C19-C21-C22
22	c	508	CLA	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
27	d	405	PL9	C38-C39-C41-C42
22	A	405	CLA	C2-C3-C5-C6
22	a	402	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
33	C	522	STE	C4-C5-C6-C7
22	B	602	CLA	CBA-CGA-O2A-C1
29	B	623	SQD	C24-C23-O48-C46
28	b	621	LMG	C29-C28-O8-C9
28	M	101	LMG	C29-C28-O8-C9
27	d	405	PL9	C12-C13-C14-C15
22	c	514	CLA	CBD-CGD-O2D-CED
27	a	410	PL9	C42-C43-C44-C46
29	f	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	c	522	LMG	O9-C10-O7-C8
22	c	513	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
34	d	406	LHG	O2-C2-C3-O3
34	e	102	LHG	O2-C2-C3-O3
22	B	606	CLA	C3-C5-C6-C7
29	b	619	SQD	C8-C7-O47-C45
30	C	516	DGD	C1B-C2B-C3B-C4B
22	h	101	CLA	CBD-CGD-O2D-CED
34	B	622	LHG	C7-C8-C9-C10
28	d	409	LMG	C10-C11-C12-C13
33	X	101	STE	C13-C14-C15-C16
22	B	602	CLA	O1A-CGA-O2A-C1
27	D	405	PL9	C47-C48-C49-C51
22	B	615	CLA	C4-C3-C5-C6
22	C	508	CLA	C4-C3-C5-C6
30	A	415	DGD	C4E-C5E-C6E-O5E
30	H	102	DGD	C4E-C5E-C6E-O5E
22	b	604	CLA	C2-C3-C5-C6
22	B	615	CLA	C2-C3-C5-C6
22	C	508	CLA	C2-C3-C5-C6
22	b	602	CLA	C2-C3-C5-C6
29	A	413	SQD	C7-C8-C9-C10
22	B	607	CLA	C2A-CAA-CBA-CGA
27	a	410	PL9	C19-C21-C22-C23
27	a	410	PL9	C24-C26-C27-C28
27	a	410	PL9	C34-C36-C37-C38
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C39-C41-C42-C43
22	B	605	CLA	C3-C5-C6-C7
22	d	402	CLA	C3-C5-C6-C7
23	d	401	PHO	CBD-CGD-O2D-CED
29	A	413	SQD	C11-C12-C13-C14
27	a	410	PL9	C7-C8-C9-C10
27	a	410	PL9	C17-C18-C19-C20
27	D	405	PL9	C27-C28-C29-C30
34	d	406	LHG	C1-C2-C3-O3
34	e	102	LHG	C1-C2-C3-O3
22	B	617	CLA	C3-C5-C6-C7
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	A	415	DGD	C2A-C1A-O1G-C1G
22	c	508	CLA	CBA-CGA-O2A-C1
28	B	629	LMG	C29-C28-O8-C9
22	h	101	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C10-C11-C12-C13
22	D	402	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
22	B	616	CLA	C5-C6-C7-C8
22	B	603	CLA	C13-C15-C16-C17
22	B	612	CLA	C8-C10-C11-C12
22	C	507	CLA	C5-C6-C7-C8
22	c	511	CLA	C3-C5-C6-C7
29	B	623	SQD	C2-C1-O6-C44
28	c	524	LMG	C4-C5-C6-O5
27	a	410	PL9	C33-C34-C36-C37
22	b	613	CLA	C2-C3-C5-C6
22	C	512	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	b	615	CLA	C6-C7-C8-C9
22	D	402	CLA	C11-C10-C8-C9
23	A	404	PHO	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	A	403	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
22	B	617	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	h	101	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	b	613	CLA	C6-C7-C8-C9
22	B	608	CLA	C10-C11-C12-C13
22	C	507	CLA	C13-C15-C16-C17
22	b	605	CLA	C2A-CAA-CBA-CGA
24	d	404	BCR	C37-C22-C23-C24
24	T	101	BCR	C36-C18-C19-C20
28	b	623	LMG	O6-C5-C6-O5
34	E	101	LHG	C7-C8-C9-C10
28	d	409	LMG	C28-C29-C30-C31
22	c	508	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C8-C10-C11-C12
30	H	102	DGD	O6E-C5E-C6E-O5E
28	c	522	LMG	C11-C10-O7-C8
22	B	615	CLA	C8-C10-C11-C12
22	C	514	CLA	C15-C16-C17-C18
22	c	508	CLA	C13-C15-C16-C17
22	c	514	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	510	CLA	C10-C11-C12-C13
34	d	406	LHG	C23-C24-C25-C26
28	D	406	LMG	C10-C11-C12-C13
28	M	101	LMG	C28-C29-C30-C31
22	b	603	CLA	C15-C16-C17-C18
22	a	402	CLA	C15-C16-C17-C18
22	C	508	CLA	C10-C11-C12-C13
22	b	614	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
22	C	503	CLA	C15-C16-C17-C18
22	c	505	CLA	C8-C10-C11-C12
22	B	614	CLA	C8-C10-C11-C12
22	C	511	CLA	C15-C16-C17-C18
27	d	405	PL9	C32-C33-C34-C35
30	c	521	DGD	C1A-C2A-C3A-C4A
29	B	623	SQD	C23-C24-C25-C26
28	C	519	LMG	C28-C29-C30-C31
28	c	522	LMG	C28-C29-C30-C31
28	M	101	LMG	C10-C11-C12-C13
22	B	602	CLA	C5-C6-C7-C8
22	b	608	CLA	C15-C16-C17-C18
22	c	514	CLA	C13-C15-C16-C17
22	b	602	CLA	C5-C6-C7-C8
22	b	610	CLA	C13-C15-C16-C17
22	C	504	CLA	C5-C6-C7-C8
28	D	410	LMG	C10-C11-C12-C13
34	D	409	LHG	C7-C8-C9-C10
28	b	623	LMG	C28-C29-C30-C31
29	A	413	SQD	C30-C31-C32-C33
22	c	513	CLA	C15-C16-C17-C18
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	C11-C10-C8-C7
22	B	612	CLA	C12-C13-C15-C16
22	h	101	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	411	CLA	C11-C12-C13-C15
22	a	403	CLA	C6-C7-C8-C10
28	D	410	LMG	O10-C28-O8-C9
22	c	508	CLA	O1A-CGA-O2A-C1
28	B	629	LMG	O10-C28-O8-C9
22	c	514	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C10-C11-C12-C13
22	B	608	CLA	C5-C6-C7-C8
22	c	514	CLA	C8-C10-C11-C12
22	C	505	CLA	C8-C10-C11-C12
22	B	606	CLA	C13-C15-C16-C17
22	h	101	CLA	O1A-CGA-O2A-C1
28	C	519	LMG	O10-C28-O8-C9
22	c	513	CLA	C13-C15-C16-C17
22	A	402	CLA	C15-C16-C17-C18
27	d	405	PL9	C34-C36-C37-C38
27	A	410	PL9	C29-C31-C32-C33
27	A	410	PL9	C34-C36-C37-C38
24	B	618	BCR	C10-C11-C12-C13
24	d	404	BCR	C10-C11-C12-C13
24	a	406	BCR	C18-C19-C20-C21
24	B	620	BCR	C10-C11-C12-C13
22	b	603	CLA	C10-C11-C12-C13
22	B	613	CLA	C10-C11-C12-C13
22	b	614	CLA	C15-C16-C17-C18
22	B	616	CLA	C13-C15-C16-C17
22	B	603	CLA	C8-C10-C11-C12
29	a	412	SQD	C7-C8-C9-C10
34	l	101	LHG	C7-C8-C9-C10
22	B	609	CLA	C13-C15-C16-C17
22	B	608	CLA	C8-C10-C11-C12
22	c	508	CLA	C8-C10-C11-C12
22	c	505	CLA	C5-C6-C7-C8
22	h	101	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
30	A	415	DGD	CEB-CFB-CGB-CHB
22	a	402	CLA	O1D-CGD-O2D-CED
30	c	520	DGD	C4E-C5E-C6E-O5E
28	C	519	LMG	C11-C10-O7-C8
22	B	607	CLA	C15-C16-C17-C18
22	c	511	CLA	C8-C10-C11-C12
22	d	403	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C15-C16-C17-C18
22	c	512	CLA	C8-C10-C11-C12
22	b	610	CLA	C15-C16-C17-C18
34	B	622	LHG	C4-O6-P-O3
34	D	409	LHG	C3-O3-P-O6
34	D	408	LHG	C3-O3-P-O6
34	d	407	LHG	C3-O3-P-O6
22	C	514	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C29-C28-O8-C9
22	b	613	CLA	C4-C3-C5-C6
22	b	601	CLA	C16-C17-C18-C20
22	c	507	CLA	C15-C16-C17-C18
24	B	619	BCR	C14-C15-C16-C17
30	c	520	DGD	O6E-C5E-C6E-O5E
34	E	101	LHG	C11-C12-C13-C14
34	D	412	LHG	C29-C30-C31-C32
30	C	518	DGD	C6A-C7A-C8A-C9A
28	c	522	LMG	C36-C37-C38-C39
29	a	413	SQD	C10-C11-C12-C13
28	B	629	LMG	C11-C10-O7-C8
24	b	618	BCR	C35-C13-C14-C15
24	Z	101	BCR	C20-C21-C22-C37
24	b	616	BCR	C16-C17-C18-C36
24	b	616	BCR	C20-C21-C22-C37
24	B	618	BCR	C11-C10-C9-C34
24	B	618	BCR	C35-C13-C14-C15
24	B	618	BCR	C16-C17-C18-C36
24	Y	101	BCR	C11-C10-C9-C34
24	Y	101	BCR	C16-C17-C18-C36
24	c	518	BCR	C20-C21-C22-C37
24	D	404	BCR	C20-C21-C22-C37
24	b	617	BCR	C16-C17-C18-C36
24	b	617	BCR	C20-C21-C22-C37
24	x	101	BCR	C11-C10-C9-C34
24	x	101	BCR	C20-C21-C22-C37
24	B	620	BCR	C11-C10-C9-C34
24	B	620	BCR	C20-C21-C22-C37
24	B	619	BCR	C16-C17-C18-C36
24	B	619	BCR	C20-C21-C22-C37
24	A	406	BCR	C35-C13-C14-C15
24	t	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
34	B	622	LHG	C31-C32-C33-C34
34	D	408	LHG	C11-C12-C13-C14
34	d	406	LHG	C32-C33-C34-C35
33	E	102	STE	C3-C4-C5-C6
33	B	627	STE	C11-C12-C13-C14
28	D	411	LMG	C30-C31-C32-C33
33	b	625	STE	C12-C13-C14-C15
33	B	624	STE	C11-C10-C9-C8
28	c	524	LMG	C34-C35-C36-C37
33	h	103	STE	C9-C10-C11-C12
33	b	620	STE	C6-C7-C8-C9
34	D	412	LHG	C12-C13-C14-C15
28	D	406	LMG	C21-C22-C23-C24
34	l	101	LHG	C17-C18-C19-C20
28	B	629	LMG	C36-C37-C38-C39
33	d	410	STE	C5-C6-C7-C8
33	b	622	STE	C7-C8-C9-C10
34	e	102	LHG	C14-C15-C16-C17
29	a	413	SQD	C11-C10-C9-C8
22	d	402	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C20
29	A	413	SQD	C13-C14-C15-C16
34	D	408	LHG	C10-C11-C12-C13
29	D	407	SQD	C31-C32-C33-C34
33	b	625	STE	C14-C15-C16-C17
30	h	102	DGD	C2B-C3B-C4B-C5B
34	D	412	LHG	C9-C10-C11-C12
28	D	406	LMG	C35-C36-C37-C38
28	c	525	LMG	C15-C16-C17-C18
28	C	519	LMG	C32-C33-C34-C35
30	c	519	DGD	C6B-C7B-C8B-C9B
33	c	523	STE	C9-C10-C11-C12
29	b	619	SQD	C46-C45-O47-C7
22	c	514	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	C13-C15-C16-C17
22	B	604	CLA	C15-C16-C17-C18
22	C	502	CLA	CBD-CGD-O2D-CED
30	C	517	DGD	C9A-CAA-CBA-CCA
30	A	415	DGD	CBA-CCA-CDA-CEA
30	A	415	DGD	CBB-CCB-CDB-CEB
29	B	623	SQD	C33-C34-C35-C36
28	B	629	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	l	102	STE	C14-C15-C16-C17
28	b	623	LMG	C30-C31-C32-C33
30	H	102	DGD	C7A-C8A-C9A-CAA
30	c	519	DGD	C4B-C5B-C6B-C7B
30	C	516	DGD	C5A-C6A-C7A-C8A
34	B	622	LHG	C29-C30-C31-C32
34	D	409	LHG	C25-C26-C27-C28
29	a	412	SQD	C15-C16-C17-C18
33	b	620	STE	C7-C8-C9-C10
22	b	606	CLA	O1D-CGD-O2D-CED
34	D	409	LHG	O2-C2-C3-O3
33	H	103	STE	C13-C14-C15-C16
33	d	412	STE	C9-C10-C11-C12
29	B	623	SQD	C13-C14-C15-C16
28	c	524	LMG	C31-C32-C33-C34
34	E	101	LHG	C34-C35-C36-C37
28	b	623	LMG	C32-C33-C34-C35
28	A	412	LMG	C16-C17-C18-C19
24	Z	101	BCR	C12-C13-C14-C15
30	C	517	DGD	C2E-C1E-O5D-C6D
24	c	517	BCR	C20-C21-C22-C23
24	c	518	BCR	C16-C17-C18-C19
24	x	101	BCR	C11-C10-C9-C8
24	a	406	BCR	C20-C21-C22-C23
24	c	516	BCR	C20-C21-C22-C23
30	c	520	DGD	C2E-C1E-O5D-C6D
24	y	101	BCR	C20-C21-C22-C23
24	t	101	BCR	C20-C21-C22-C23
33	d	412	STE	C14-C15-C16-C17
28	c	524	LMG	C16-C17-C18-C19
34	D	412	LHG	C18-C19-C20-C21
34	d	407	LHG	C29-C30-C31-C32
22	B	615	CLA	C13-C15-C16-C17
22	C	514	CLA	O1A-CGA-O2A-C1
28	b	621	LMG	O10-C28-O8-C9
22	B	613	CLA	C16-C17-C18-C20
22	B	607	CLA	C16-C17-C18-C19
22	c	514	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C19
34	B	622	LHG	C17-C18-C19-C20
34	d	406	LHG	C10-C11-C12-C13
28	c	525	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	A	412	LMG	C38-C39-C40-C41
22	c	508	CLA	C2-C3-C5-C6
22	c	507	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C9
28	c	524	LMG	C28-C29-C30-C31
34	E	101	LHG	C23-C24-C25-C26
28	A	412	LMG	C28-C29-C30-C31
34	D	408	LHG	C30-C31-C32-C33
30	C	517	DGD	C7B-C8B-C9B-CAB
33	b	626	STE	C6-C7-C8-C9
29	B	623	SQD	C11-C12-C13-C14
34	l	101	LHG	C32-C33-C34-C35
29	f	101	SQD	C32-C33-C34-C35
28	A	412	LMG	C12-C13-C14-C15
34	e	102	LHG	C16-C17-C18-C19
33	c	523	STE	C11-C12-C13-C14
22	b	605	CLA	C15-C16-C17-C18
30	c	521	DGD	O1A-C1A-O1G-C1G
22	c	514	CLA	O1A-CGA-O2A-C1
24	b	617	BCR	C37-C22-C23-C24
33	h	103	STE	C11-C12-C13-C14
33	b	622	STE	C14-C15-C16-C17
28	M	101	LMG	C36-C37-C38-C39
34	d	408	LHG	O1-C1-C2-C3
34	D	409	LHG	O1-C1-C2-C3
24	d	404	BCR	C21-C22-C23-C24
34	D	408	LHG	C34-C35-C36-C37
33	B	627	STE	C4-C5-C6-C7
33	l	102	STE	C10-C11-C12-C13
33	d	410	STE	C10-C11-C12-C13
29	f	101	SQD	C29-C30-C31-C32
28	d	409	LMG	C32-C33-C34-C35
34	d	408	LHG	C23-C24-C25-C26
34	d	406	LHG	C7-C8-C9-C10
28	b	621	LMG	C28-C29-C30-C31
34	d	408	LHG	C32-C33-C34-C35
28	D	411	LMG	C14-C15-C16-C17
30	A	415	DGD	C6B-C7B-C8B-C9B
29	a	412	SQD	C29-C30-C31-C32
33	b	626	STE	C2-C3-C4-C5
28	B	629	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	l	102	STE	C4-C5-C6-C7
34	d	407	LHG	C11-C12-C13-C14
30	H	102	DGD	C5B-C6B-C7B-C8B
29	a	413	SQD	C15-C16-C17-C18
22	a	402	CLA	C16-C17-C18-C20
22	c	506	CLA	C11-C12-C13-C14
22	C	511	CLA	C16-C17-C18-C19
22	C	511	CLA	C16-C17-C18-C20
30	c	520	DGD	O6E-C1E-O5D-C6D
22	c	511	CLA	C10-C11-C12-C13
22	c	515	CLA	C5-C6-C7-C8
22	C	507	CLA	C8-C10-C11-C12
34	D	409	LHG	C32-C33-C34-C35
30	A	415	DGD	C4B-C5B-C6B-C7B
33	b	625	STE	C4-C5-C6-C7
28	B	629	LMG	C16-C17-C18-C19
28	c	525	LMG	C17-C18-C19-C20
28	c	525	LMG	C39-C40-C41-C42
33	L	101	STE	C4-C5-C6-C7
30	c	519	DGD	C3B-C4B-C5B-C6B
30	c	519	DGD	C5B-C6B-C7B-C8B
29	a	413	SQD	C11-C12-C13-C14
34	B	622	LHG	C12-C13-C14-C15
34	D	409	LHG	C30-C31-C32-C33
34	D	408	LHG	C32-C33-C34-C35
30	C	517	DGD	C5A-C6A-C7A-C8A
30	C	517	DGD	CBA-CCA-CDA-CEA
33	B	627	STE	C5-C6-C7-C8
33	B	621	STE	C4-C5-C6-C7
30	c	521	DGD	C2A-C3A-C4A-C5A
30	h	102	DGD	CBA-CCA-CDA-CEA
28	D	406	LMG	C17-C18-C19-C20
28	D	406	LMG	C39-C40-C41-C42
34	l	101	LHG	C26-C27-C28-C29
33	d	410	STE	C4-C5-C6-C7
30	C	518	DGD	C5A-C6A-C7A-C8A
34	d	407	LHG	C12-C13-C14-C15
28	B	629	LMG	C14-C15-C16-C17
33	l	102	STE	C9-C10-C11-C12
28	b	621	LMG	C33-C34-C35-C36
34	D	409	LHG	C9-C10-C11-C12
29	b	619	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	X	101	STE	C4-C5-C6-C7
22	c	514	CLA	C3A-C2A-CAA-CBA
29	A	413	SQD	C16-C17-C18-C19
29	A	413	SQD	C28-C29-C30-C31
34	D	408	LHG	C12-C13-C14-C15
28	D	411	LMG	C31-C32-C33-C34
30	h	102	DGD	C9A-CAA-CBA-CCA
34	E	101	LHG	C32-C33-C34-C35
28	b	621	LMG	C32-C33-C34-C35
22	a	402	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
34	d	406	LHG	C34-C35-C36-C37
34	l	101	LHG	C27-C28-C29-C30
28	M	101	LMG	C16-C17-C18-C19
30	c	520	DGD	C6B-C7B-C8B-C9B
34	D	409	LHG	C11-C10-C9-C8
28	d	409	LMG	C33-C34-C35-C36
30	c	520	DGD	C5B-C6B-C7B-C8B
30	c	519	DGD	O6D-C5D-C6D-O5D
24	c	517	BCR	C14-C15-C16-C17
24	A	406	BCR	C14-C15-C16-C17
28	D	410	LMG	C28-C29-C30-C31
33	B	626	STE	C9-C10-C11-C12
33	h	103	STE	C7-C8-C9-C10
22	B	610	CLA	C4-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
27	A	410	PL9	C28-C29-C31-C32
27	D	405	PL9	C13-C14-C16-C17
27	D	405	PL9	C28-C29-C31-C32
22	c	512	CLA	C2-C3-C5-C6
34	D	409	LHG	C31-C32-C33-C34
33	a	414	STE	C2-C3-C4-C5
33	b	622	STE	C2-C3-C4-C5
30	c	520	DGD	CBB-CCB-CDB-CEB
34	d	406	LHG	O1-C1-C2-O2
34	E	101	LHG	O1-C1-C2-O2
34	d	407	LHG	O1-C1-C2-O2
33	M	102	STE	C11-C10-C9-C8
33	T	102	STE	C5-C6-C7-C8
28	D	411	LMG	C32-C33-C34-C35
30	A	415	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
33	b	624	STE	C3-C4-C5-C6
33	C	521	STE	C4-C5-C6-C7
30	C	518	DGD	O1A-C1A-O1G-C1G
22	c	514	CLA	C16-C17-C18-C20
30	c	521	DGD	C9B-CAB-CBB-CCB
28	B	629	LMG	C32-C33-C34-C35
28	c	525	LMG	C12-C13-C14-C15
28	c	525	LMG	C30-C31-C32-C33
22	C	505	CLA	C11-C12-C13-C14
29	D	407	SQD	C30-C31-C32-C33
33	c	501	STE	C5-C6-C7-C8
28	b	623	LMG	C11-C12-C13-C14
28	C	519	LMG	C18-C19-C20-C21
28	c	522	LMG	C33-C34-C35-C36
30	c	520	DGD	CAB-CBB-CCB-CDB
33	H	103	STE	C7-C8-C9-C10
34	D	408	LHG	C13-C14-C15-C16
33	T	102	STE	C12-C13-C14-C15
28	D	406	LMG	C30-C31-C32-C33
29	A	414	SQD	C12-C13-C14-C15
29	b	619	SQD	O49-C7-O47-C45
28	b	621	LMG	O9-C10-O7-C8
22	c	508	CLA	C2-C1-O2A-CGA
34	D	409	LHG	C10-C11-C12-C13
33	d	411	STE	C3-C4-C5-C6
28	b	623	LMG	C16-C17-C18-C19
28	b	621	LMG	C37-C38-C39-C40
33	c	523	STE	C2-C3-C4-C5
22	C	506	CLA	C5-C6-C7-C8
28	D	410	LMG	C14-C15-C16-C17
29	A	413	SQD	C9-C10-C11-C12
34	D	409	LHG	C24-C25-C26-C27
33	c	501	STE	C6-C7-C8-C9
28	b	623	LMG	C34-C35-C36-C37
28	A	412	LMG	C34-C35-C36-C37
33	b	622	STE	C9-C10-C11-C12
22	b	601	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
30	c	520	DGD	C1A-C2A-C3A-C4A
24	Z	101	BCR	C23-C24-C25-C26
24	T	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	516	BCR	C1-C6-C7-C8
24	c	516	BCR	C5-C6-C7-C8
28	c	524	LMG	O6-C5-C6-O5
34	D	408	LHG	C33-C34-C35-C36
34	d	406	LHG	C31-C32-C33-C34
34	d	406	LHG	C33-C34-C35-C36
22	b	613	CLA	C5-C6-C7-C8
30	A	415	DGD	CCA-CDA-CEA-CFA
33	b	626	STE	C5-C6-C7-C8
28	c	525	LMG	C33-C34-C35-C36
28	B	629	LMG	C30-C31-C32-C33
22	B	602	CLA	C8-C10-C11-C12
22	d	403	CLA	C8-C10-C11-C12
22	B	617	CLA	C5-C6-C7-C8
22	A	411	CLA	C15-C16-C17-C18
30	A	415	DGD	C4A-C5A-C6A-C7A
28	b	621	LMG	C18-C19-C20-C21
33	j	101	STE	C4-C5-C6-C7
22	C	506	CLA	C4-C3-C5-C6
22	C	511	CLA	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
22	c	504	CLA	C11-C12-C13-C15
22	b	611	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C12-C13-C15
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	d	403	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	b	610	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	511	CLA	C2-C3-C5-C6
22	b	613	CLA	C6-C7-C8-C10
22	h	101	CLA	C3-C5-C6-C7
22	A	402	CLA	C2C-C3C-CAC-CBC
22	B	612	CLA	C13-C15-C16-C17
22	c	509	CLA	C5-C6-C7-C8
22	c	513	CLA	C16-C17-C18-C19
34	B	622	LHG	O9-C7-O7-C5
33	b	622	STE	C10-C11-C12-C13
33	T	102	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C32-C33-C34-C35
34	l	101	LHG	C29-C30-C31-C32
30	H	102	DGD	C9A-CAA-CBA-CCA
22	c	513	CLA	O1D-CGD-O2D-CED
33	d	410	STE	C11-C12-C13-C14
33	L	101	STE	C5-C6-C7-C8
34	e	102	LHG	C7-C8-C9-C10
30	C	516	DGD	CCB-CDB-CEB-CFB
29	B	623	SQD	C35-C36-C37-C38
34	E	101	LHG	C24-C25-C26-C27
33	b	622	STE	C13-C14-C15-C16
30	H	102	DGD	C7B-C8B-C9B-CAB
22	h	101	CLA	O1D-CGD-O2D-CED
30	c	521	DGD	C6A-C7A-C8A-C9A
22	B	607	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
22	C	503	CLA	C16-C17-C18-C20
30	C	517	DGD	O6E-C1E-O5D-C6D
22	B	610	CLA	C15-C16-C17-C18
22	A	411	CLA	C13-C15-C16-C17
34	B	622	LHG	C18-C19-C20-C21
33	H	103	STE	C10-C11-C12-C13
34	d	406	LHG	C16-C17-C18-C19
28	c	524	LMG	C30-C31-C32-C33
28	C	519	LMG	C31-C32-C33-C34
30	c	519	DGD	C4A-C5A-C6A-C7A
29	A	414	SQD	C7-C8-C9-C10
22	a	405	CLA	C10-C11-C12-C13
27	D	405	PL9	C47-C48-C49-C50
34	D	409	LHG	C27-C28-C29-C30
33	d	411	STE	C10-C11-C12-C13
30	C	517	DGD	C9B-CAB-CBB-CCB
34	d	406	LHG	C18-C19-C20-C21
28	D	411	LMG	C16-C17-C18-C19
34	d	407	LHG	C17-C18-C19-C20
29	A	414	SQD	C18-C19-C20-C21
29	a	412	SQD	O49-C7-O47-C45
34	d	407	LHG	C14-C15-C16-C17
29	D	407	SQD	C2-C1-O6-C44
30	A	415	DGD	O2G-C2G-C3G-O3G
30	c	519	DGD	O6E-C5E-C6E-O5E
34	D	408	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C3A-C4A-C5A-C6A
30	c	519	DGD	C7A-C8A-C9A-CAA
29	f	101	SQD	C24-C25-C26-C27
28	A	412	LMG	C33-C34-C35-C36
22	c	512	CLA	C4-C3-C5-C6
27	d	405	PL9	C13-C14-C16-C17
27	A	410	PL9	C23-C24-C26-C27
33	B	628	STE	C5-C6-C7-C8
22	A	403	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	d	403	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C14
22	h	101	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
22	a	405	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	A	411	CLA	C11-C12-C13-C14
30	h	102	DGD	C5B-C6B-C7B-C8B
29	a	412	SQD	C24-C25-C26-C27
28	D	406	LMG	C12-C13-C14-C15
33	B	628	STE	C10-C11-C12-C13
30	C	516	DGD	C9A-CAA-CBA-CCA
33	H	103	STE	C5-C6-C7-C8
34	D	408	LHG	C25-C26-C27-C28
29	b	619	SQD	C25-C26-C27-C28
33	B	627	STE	C9-C10-C11-C12
30	h	102	DGD	C6B-C7B-C8B-C9B
33	a	414	STE	C4-C5-C6-C7
33	Z	102	STE	C11-C12-C13-C14
28	B	629	LMG	C39-C40-C41-C42
28	b	623	LMG	C31-C32-C33-C34
28	b	621	LMG	C31-C32-C33-C34
28	D	410	LMG	C29-C28-O8-C9
24	y	101	BCR	C7-C8-C9-C34
34	B	622	LHG	C14-C15-C16-C17
29	A	413	SQD	C26-C27-C28-C29
34	D	412	LHG	C24-C25-C26-C27
28	b	623	LMG	C40-C41-C42-C43
30	c	520	DGD	C4A-C5A-C6A-C7A
29	a	413	SQD	C9-C10-C11-C12
34	d	408	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	510	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C20
30	c	519	DGD	O1B-C1B-O2G-C2G
33	E	102	STE	C4-C5-C6-C7
33	M	103	STE	C4-C5-C6-C7
29	a	412	SQD	C17-C18-C19-C20
29	B	623	SQD	C34-C35-C36-C37
28	b	623	LMG	C17-C18-C19-C20
34	B	622	LHG	C34-C35-C36-C37
30	h	102	DGD	C7A-C8A-C9A-CAA
28	d	409	LMG	C14-C15-C16-C17
29	B	623	SQD	C9-C10-C11-C12
34	D	412	LHG	C27-C28-C29-C30
28	D	406	LMG	C19-C20-C21-C22
34	l	101	LHG	C34-C35-C36-C37
30	H	102	DGD	CCA-CDA-CEA-CFA
34	d	406	LHG	C25-C26-C27-C28
33	d	412	STE	C11-C12-C13-C14
29	a	412	SQD	C12-C13-C14-C15
28	c	524	LMG	C41-C42-C43-C44
29	f	101	SQD	C31-C32-C33-C34
30	C	516	DGD	C2A-C3A-C4A-C5A
29	B	623	SQD	C18-C19-C20-C21
28	B	629	LMG	C37-C38-C39-C40
28	b	623	LMG	C18-C19-C20-C21
28	C	519	LMG	C30-C31-C32-C33
27	D	405	PL9	C30-C29-C31-C32
30	A	415	DGD	CCB-CDB-CEB-CFB
34	E	101	LHG	C15-C16-C17-C18
33	h	103	STE	C6-C7-C8-C9
33	C	520	STE	C2-C3-C4-C5
33	B	601	STE	C2-C3-C4-C5
33	d	410	STE	C9-C10-C11-C12
34	d	407	LHG	C11-C10-C9-C8
28	M	101	LMG	C29-C30-C31-C32
29	A	413	SQD	C34-C35-C36-C37
29	a	412	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	b	620	STE	C10-C11-C12-C13
34	e	102	LHG	C24-C25-C26-C27
22	h	101	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20
34	d	408	LHG	C4-C5-C6-O8
33	H	103	STE	C3-C4-C5-C6
30	A	415	DGD	C1G-C2G-C3G-O3G
29	B	623	SQD	O6-C44-C45-C46
28	B	629	LMG	O1-C7-C8-C9
30	c	519	DGD	O1G-C1G-C2G-C3G
22	b	604	CLA	C15-C16-C17-C18
29	A	413	SQD	C17-C18-C19-C20
30	C	517	DGD	CDA-CEA-CFA-CGA
30	C	517	DGD	C2G-C3G-O3G-C1D
30	C	517	DGD	C5D-C6D-O5D-C1E
28	B	629	LMG	C8-C7-O1-C1
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C5D-C6D-O5D-C1E
22	C	512	CLA	O1D-CGD-O2D-CED
28	b	623	LMG	C42-C43-C44-C45
29	a	413	SQD	C19-C20-C21-C22
22	c	503	CLA	O1D-CGD-O2D-CED
34	d	406	LHG	C27-C28-C29-C30
33	I	101	STE	C1-C2-C3-C4
33	B	628	STE	C11-C10-C9-C8
33	d	410	STE	C12-C13-C14-C15
33	b	622	STE	C5-C6-C7-C8
34	d	407	LHG	C16-C17-C18-C19
28	M	101	LMG	C14-C15-C16-C17
30	c	520	DGD	CBA-CCA-CDA-CEA
30	C	516	DGD	O6E-C5E-C6E-O5E
28	c	522	LMG	O6-C5-C6-O5
33	H	103	STE	C1-C2-C3-C4
33	B	624	STE	C4-C5-C6-C7
33	B	628	STE	C6-C7-C8-C9
22	B	604	CLA	C5-C6-C7-C8
33	b	626	STE	C1-C2-C3-C4
28	d	409	LMG	C38-C39-C40-C41
34	D	408	LHG	O1-C1-C2-O2
28	D	410	LMG	C33-C34-C35-C36
30	c	519	DGD	C3A-C4A-C5A-C6A
22	a	403	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C26-C27-C28-C29
34	D	412	LHG	C19-C20-C21-C22
29	A	414	SQD	C19-C20-C21-C22
34	D	409	LHG	C35-C36-C37-C38
34	d	406	LHG	C19-C20-C21-C22
22	b	606	CLA	C8-C10-C11-C12
28	D	406	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
34	D	409	LHG	C14-C15-C16-C17
34	l	101	LHG	C13-C14-C15-C16
30	H	102	DGD	CAA-CBA-CCA-CDA
30	h	102	DGD	O6E-C5E-C6E-O5E
30	h	102	DGD	CDB-CEB-CFB-CGB
22	c	510	CLA	C16-C17-C18-C19
28	M	101	LMG	C12-C13-C14-C15
30	H	102	DGD	C3B-C4B-C5B-C6B
33	C	521	STE	C3-C4-C5-C6
28	c	522	LMG	C34-C35-C36-C37
28	D	410	LMG	C9-C8-O7-C10
28	B	629	LMG	O6-C5-C6-O5
30	c	521	DGD	C5A-C6A-C7A-C8A
29	a	412	SQD	C10-C11-C12-C13
30	h	102	DGD	CAB-CBB-CCB-CDB
28	B	629	LMG	C33-C34-C35-C36
23	d	401	PHO	C2C-C3C-CAC-CBC
23	d	401	PHO	O1D-CGD-O2D-CED
22	c	506	CLA	C5-C6-C7-C8
34	B	622	LHG	C27-C28-C29-C30
30	A	415	DGD	CFA-CGA-CHA-CIA
33	d	411	STE	C2-C3-C4-C5
29	a	412	SQD	C19-C20-C21-C22
33	X	101	STE	C2-C3-C4-C5
30	c	519	DGD	CDB-CEB-CFB-CGB
30	C	517	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C4-C5-C6-C7
29	a	412	SQD	C35-C36-C37-C38
28	B	629	LMG	C34-C35-C36-C37
34	e	102	LHG	C13-C14-C15-C16
34	D	412	LHG	C7-C8-C9-C10
34	e	102	LHG	C23-C24-C25-C26
24	b	616	BCR	C20-C21-C22-C23
24	C	515	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	c	516	BCR	C16-C17-C18-C19
28	c	525	LMG	C2-C1-O1-C7
24	B	619	BCR	C11-C10-C9-C8
34	E	101	LHG	C28-C29-C30-C31
29	A	413	SQD	O6-C44-C45-O47
29	b	619	SQD	O47-C45-C46-O48
28	c	524	LMG	O1-C7-C8-O7
28	c	525	LMG	O1-C7-C8-O7
33	B	627	STE	C3-C4-C5-C6
22	A	405	CLA	C6-C7-C8-C9
30	c	520	DGD	C7A-C8A-C9A-CAA
33	l	102	STE	C2-C3-C4-C5
27	a	410	PL9	C40-C39-C41-C42
27	A	410	PL9	C42-C43-C44-C45
34	D	409	LHG	C26-C27-C28-C29
22	C	506	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
22	B	605	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	C	514	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C12-C13-C15
22	c	515	CLA	C11-C12-C13-C15
22	c	507	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C12-C13-C15
22	h	101	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C15
22	a	405	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
34	l	101	LHG	C33-C34-C35-C36
28	b	621	LMG	C39-C40-C41-C42
22	C	506	CLA	C14-C13-C15-C16
22	B	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C14
22	b	611	CLA	C6-C7-C8-C9
22	B	608	CLA	C11-C10-C8-C9
22	A	403	CLA	C11-C12-C13-C14
22	c	511	CLA	C6-C7-C8-C9
22	c	515	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9
33	B	626	STE	C11-C12-C13-C14
34	l	101	LHG	C15-C16-C17-C18
22	b	607	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	CBA-CGA-O2A-C1
33	L	101	STE	C7-C8-C9-C10
30	c	519	DGD	C4D-C5D-C6D-O5D
34	e	102	LHG	C27-C28-C29-C30
34	d	408	LHG	C35-C36-C37-C38
30	A	415	DGD	CAA-CBA-CCA-CDA
34	e	102	LHG	C11-C10-C9-C8
22	A	405	CLA	CBA-CGA-O2A-C1
22	a	405	CLA	CBA-CGA-O2A-C1
28	b	623	LMG	C4-C5-C6-O5
29	D	407	SQD	C25-C26-C27-C28
30	H	102	DGD	CAB-CBB-CCB-CDB
33	c	523	STE	C7-C8-C9-C10
33	b	625	STE	C11-C10-C9-C8
33	L	101	STE	C3-C4-C5-C6
22	C	503	CLA	C16-C17-C18-C19
22	a	403	CLA	C16-C17-C18-C20
34	d	407	LHG	O6-C4-C5-C6
33	M	102	STE	C9-C10-C11-C12
30	C	518	DGD	CCA-CDA-CEA-CFA
34	d	406	LHG	C15-C16-C17-C18
33	b	624	STE	C9-C10-C11-C12
27	a	410	PL9	C20-C19-C21-C22
22	c	514	CLA	C4-C3-C5-C6
22	c	514	CLA	C2-C3-C5-C6
28	D	406	LMG	C36-C37-C38-C39
34	B	622	LHG	C19-C20-C21-C22
30	c	521	DGD	C7A-C8A-C9A-CAA
34	D	412	LHG	C28-C29-C30-C31
22	C	506	CLA	C16-C17-C18-C20
29	a	413	SQD	C31-C32-C33-C34
33	X	101	STE	C11-C10-C9-C8
33	c	523	STE	C4-C5-C6-C7
33	c	523	STE	C12-C13-C14-C15
33	C	521	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	X	101	STE	C10-C11-C12-C13
33	a	415	STE	C6-C7-C8-C9
22	B	611	CLA	C16-C17-C18-C19
33	H	103	STE	C12-C13-C14-C15
22	c	512	CLA	C5-C6-C7-C8
29	a	412	SQD	O6-C44-C45-C46
28	c	524	LMG	O1-C7-C8-C9
28	c	524	LMG	C7-C8-C9-O8
34	E	101	LHG	C4-C5-C6-O8
28	c	525	LMG	O1-C7-C8-C9
30	c	521	DGD	C3B-C4B-C5B-C6B
28	M	101	LMG	C18-C19-C20-C21
29	a	413	SQD	C14-C15-C16-C17
30	A	415	DGD	O1A-C1A-O1G-C1G
34	D	409	LHG	C33-C34-C35-C36
28	A	412	LMG	C40-C41-C42-C43
28	C	519	LMG	C15-C16-C17-C18
28	C	519	LMG	C19-C20-C21-C22
34	E	101	LHG	C16-C17-C18-C19
34	d	407	LHG	C25-C26-C27-C28
29	a	413	SQD	C18-C19-C20-C21
23	A	404	PHO	C4-C3-C5-C6
22	C	506	CLA	C16-C17-C18-C19
22	a	403	CLA	C16-C17-C18-C19
33	d	410	STE	C7-C8-C9-C10
28	c	525	LMG	C31-C32-C33-C34
34	D	408	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O3
34	e	102	LHG	C4-O6-P-O3
28	b	621	LMG	C38-C39-C40-C41
34	d	408	LHG	O1-C1-C2-O2
28	b	621	LMG	C13-C14-C15-C16
34	d	407	LHG	C32-C33-C34-C35
34	D	412	LHG	O9-C7-O7-C5
33	d	411	STE	C9-C10-C11-C12
33	a	414	STE	C7-C8-C9-C10
27	d	405	PL9	C37-C38-C39-C40
22	c	513	CLA	O1A-CGA-O2A-C1
30	c	519	DGD	C1A-C2A-C3A-C4A
22	c	504	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
34	e	102	LHG	C10-C11-C12-C13
30	C	516	DGD	O1G-C1A-C2A-C3A
28	B	629	LMG	O8-C28-C29-C30
33	M	102	STE	C4-C5-C6-C7
29	B	623	SQD	C27-C28-C29-C30
33	b	622	STE	C6-C7-C8-C9
28	b	621	LMG	C11-C12-C13-C14
29	a	412	SQD	O47-C45-C46-O48
28	b	621	LMG	O7-C8-C9-O8
28	M	101	LMG	O7-C8-C9-O8
29	a	413	SQD	O47-C45-C46-O48
33	B	628	STE	C2-C3-C4-C5
28	b	621	LMG	C14-C15-C16-C17
30	c	519	DGD	C2A-C3A-C4A-C5A
33	b	624	STE	C11-C10-C9-C8
33	X	101	STE	C3-C4-C5-C6
22	c	515	CLA	C13-C15-C16-C17
33	C	520	STE	C3-C4-C5-C6
22	C	511	CLA	C10-C11-C12-C13
22	C	512	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	614	CLA	C6-C7-C8-C9
22	b	608	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	c	514	CLA	C6-C7-C8-C9
22	c	514	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	B	606	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
29	A	414	SQD	C30-C31-C32-C33
28	M	101	LMG	C13-C14-C15-C16
22	B	602	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
34	d	408	LHG	C2-C3-O3-P
34	E	101	LHG	C2-C3-O3-P
29	D	407	SQD	O6-C44-C45-C46
22	A	402	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	h	101	CLA	C16-C17-C18-C19
22	c	506	CLA	C11-C12-C13-C15
24	b	616	BCR	C1-C6-C7-C8
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C5-C6-C7-C8
24	Y	101	BCR	C23-C24-C25-C30
24	T	101	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	K	101	BCR	C23-C24-C25-C30
28	b	621	LMG	C16-C17-C18-C19
24	B	619	BCR	C11-C12-C13-C35
30	C	517	DGD	C6A-C7A-C8A-C9A
28	c	524	LMG	C15-C16-C17-C18
24	B	618	BCR	C11-C12-C13-C14
24	Y	101	BCR	C11-C12-C13-C14
24	T	101	BCR	C7-C8-C9-C10
24	c	518	BCR	C11-C12-C13-C14
24	A	406	BCR	C17-C18-C19-C20
33	J	101	STE	C3-C4-C5-C6
34	d	408	LHG	C30-C31-C32-C33
22	a	411	CLA	C2C-C3C-CAC-CBC
33	C	522	STE	C5-C6-C7-C8
33	l	102	STE	C15-C16-C17-C18
22	B	612	CLA	C16-C17-C18-C20
22	B	615	CLA	C15-C16-C17-C18
34	l	101	LHG	O6-C4-C5-C6
29	B	623	SQD	C30-C31-C32-C33
28	c	525	LMG	C19-C20-C21-C22
30	c	520	DGD	C3A-C4A-C5A-C6A
33	c	523	STE	C10-C11-C12-C13
22	B	602	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	b	603	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C12-C13-C15
22	B	608	CLA	C11-C10-C8-C7
22	A	403	CLA	C11-C12-C13-C15
22	b	608	CLA	C12-C13-C15-C16
22	c	513	CLA	C12-C13-C15-C16
22	B	617	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C12-C13-C15
22	C	503	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	514	CLA	C11-C12-C13-C15
22	c	514	CLA	C12-C13-C15-C16
22	d	402	CLA	C6-C7-C8-C10
22	B	612	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C10-C8-C7
22	b	613	CLA	C12-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
24	c	518	BCR	C19-C20-C21-C22
24	y	101	BCR	C19-C20-C21-C22
22	c	504	CLA	C16-C17-C18-C19
30	C	518	DGD	C3A-C4A-C5A-C6A
28	d	409	LMG	C30-C31-C32-C33
22	c	504	CLA	C13-C15-C16-C17
22	B	605	CLA	C2C-C3C-CAC-CBC
30	c	520	DGD	CCA-CDA-CEA-CFA
24	B	618	BCR	C20-C21-C22-C37
24	H	101	BCR	C35-C13-C14-C15
24	y	101	BCR	C16-C17-C18-C36
24	y	101	BCR	C20-C21-C22-C37
22	b	606	CLA	C16-C17-C18-C20
22	A	411	CLA	C16-C17-C18-C19
22	C	506	CLA	CBA-CGA-O2A-C1
29	a	412	SQD	C24-C23-O48-C46
28	M	101	LMG	C39-C40-C41-C42
30	H	102	DGD	CBA-CCA-CDA-CEA
28	D	410	LMG	C13-C14-C15-C16
34	D	409	LHG	C17-C18-C19-C20
34	E	101	LHG	C19-C20-C21-C22
22	C	512	CLA	C15-C16-C17-C18
29	a	412	SQD	O10-C23-O48-C46
33	d	412	STE	C2-C3-C4-C5
30	C	518	DGD	C9B-CAB-CBB-CCB
22	b	609	CLA	CAD-CBD-CGD-O2D
22	C	514	CLA	CAD-CBD-CGD-O2D
22	c	515	CLA	CAD-CBD-CGD-O2D
28	B	629	LMG	C9-C8-O7-C10
22	c	505	CLA	CAD-CBD-CGD-O2D
29	f	101	SQD	C46-C45-O47-C7
22	B	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	X	101	STE	C12-C13-C14-C15
33	j	101	STE	C5-C6-C7-C8
24	y	101	BCR	C22-C23-C24-C25
22	b	611	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C20
30	c	521	DGD	C8B-C9B-CAB-CBB
33	C	521	STE	C7-C8-C9-C10
27	a	410	PL9	C9-C11-C12-C13
28	D	406	LMG	C32-C33-C34-C35
33	l	102	STE	C7-C8-C9-C10
29	A	413	SQD	O6-C44-C45-C46
29	f	101	SQD	C44-C45-C46-O48
28	b	621	LMG	C7-C8-C9-O8
22	d	403	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	O1A-CGA-O2A-C1
22	c	515	CLA	C3-C5-C6-C7
29	b	619	SQD	C28-C29-C30-C31
33	I	101	STE	C7-C8-C9-C10
33	h	103	STE	C10-C11-C12-C13
30	C	518	DGD	CAB-CBB-CCB-CDB
34	e	102	LHG	C28-C29-C30-C31
28	C	519	LMG	O9-C10-O7-C8
22	c	504	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
29	f	101	SQD	C28-C29-C30-C31
30	c	520	DGD	C9A-CAA-CBA-CCA
22	b	607	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	O1A-CGA-O2A-C1
30	C	516	DGD	CBA-CCA-CDA-CEA
28	D	406	LMG	C15-C16-C17-C18
24	Z	101	BCR	C11-C10-C9-C8
33	T	102	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	c	524	LMG	O7-C8-C9-O8
34	E	101	LHG	O7-C5-C6-O8
29	f	101	SQD	O47-C45-C46-O48
28	B	629	LMG	C38-C39-C40-C41
28	b	623	LMG	O10-C28-O8-C9
33	X	101	STE	C7-C8-C9-C10
29	a	413	SQD	C28-C29-C30-C31
27	A	410	PL9	C11-C12-C13-C14
28	c	524	LMG	C12-C13-C14-C15
22	C	506	CLA	O1A-CGA-O2A-C1
27	A	410	PL9	C13-C14-C16-C17
27	a	410	PL9	C4-C3-C7-C8
22	c	508	CLA	C6-C7-C8-C9
22	c	514	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	a	403	CLA	C14-C13-C15-C16
33	B	621	STE	C7-C8-C9-C10
34	D	412	LHG	C25-C26-C27-C28
34	D	412	LHG	C31-C32-C33-C34
22	b	608	CLA	C13-C15-C16-C17
22	b	610	CLA	C8-C10-C11-C12
30	C	518	DGD	CDB-CEB-CFB-CGB
28	C	519	LMG	C39-C40-C41-C42
24	x	101	BCR	C37-C22-C23-C24
29	D	407	SQD	C32-C33-C34-C35
22	c	506	CLA	C8-C10-C11-C12
30	C	517	DGD	CAB-CBB-CCB-CDB
34	d	406	LHG	C13-C14-C15-C16
28	B	629	LMG	C18-C19-C20-C21
30	H	102	DGD	C6B-C7B-C8B-C9B
30	c	519	DGD	CBB-CCB-CDB-CEB
22	b	607	CLA	C16-C17-C18-C19
22	B	604	CLA	C16-C17-C18-C19
34	D	409	LHG	O9-C7-O7-C5
33	C	520	STE	C4-C5-C6-C7
22	B	617	CLA	C2-C1-O2A-CGA
28	B	629	LMG	C23-C24-C25-C26
29	a	413	SQD	C12-C13-C14-C15
33	j	101	STE	C3-C4-C5-C6
22	B	607	CLA	C5-C6-C7-C8
34	D	409	LHG	C2-C3-O3-P
27	A	410	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C4-O6-P-O4
34	D	409	LHG	C3-O3-P-O5
34	l	101	LHG	C3-O3-P-O4
22	C	514	CLA	C10-C11-C12-C13
34	D	412	LHG	C30-C31-C32-C33
28	b	623	LMG	C37-C38-C39-C40
33	a	415	STE	C3-C4-C5-C6
34	l	101	LHG	C14-C15-C16-C17
22	b	605	CLA	C5-C6-C7-C8
22	C	507	CLA	C3-C5-C6-C7
34	E	101	LHG	C30-C31-C32-C33
28	c	522	LMG	C30-C31-C32-C33
22	C	508	CLA	C16-C17-C18-C20
33	b	620	STE	C3-C4-C5-C6
33	d	410	STE	C6-C7-C8-C9
33	c	523	STE	C3-C4-C5-C6
22	B	608	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	h	101	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
29	A	414	SQD	C15-C16-C17-C18
22	C	512	CLA	C11-C12-C13-C15
22	C	506	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C12-C13-C15
22	C	508	CLA	C11-C10-C8-C7
22	d	403	CLA	C11-C12-C13-C15
23	a	404	PHO	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C7
22	B	614	CLA	C6-C7-C8-C10
34	d	407	LHG	O6-C4-C5-O7
22	c	503	CLA	C11-C12-C13-C15
22	A	411	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C15
22	a	403	CLA	C12-C13-C15-C16
33	B	621	STE	C6-C7-C8-C9
30	h	102	DGD	C7B-C8B-C9B-CAB
29	a	412	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	C	519	LMG	C16-C17-C18-C19
24	c	516	BCR	C13-C14-C15-C16
30	h	102	DGD	O2G-C1B-C2B-C3B
30	H	102	DGD	C5A-C6A-C7A-C8A
33	d	411	STE	C12-C13-C14-C15
30	A	415	DGD	C5B-C6B-C7B-C8B
28	c	525	LMG	C35-C36-C37-C38
28	d	409	LMG	C36-C37-C38-C39
28	b	621	LMG	C35-C36-C37-C38
30	C	516	DGD	CDB-CEB-CFB-CGB
28	A	412	LMG	C7-C8-C9-O8
28	M	101	LMG	C7-C8-C9-O8
29	a	413	SQD	C44-C45-C46-O48
30	C	516	DGD	O1G-C1G-C2G-O2G
34	d	408	LHG	O7-C5-C6-O8
29	b	619	SQD	O6-C44-C45-O47
28	B	629	LMG	O1-C7-C8-O7
28	A	412	LMG	O7-C8-C9-O8
30	c	519	DGD	O1G-C1G-C2G-O2G
28	D	410	LMG	C34-C35-C36-C37
30	C	516	DGD	C2B-C3B-C4B-C5B
34	E	101	LHG	C11-C10-C9-C8
33	T	102	STE	C10-C11-C12-C13
30	H	102	DGD	O2G-C1B-C2B-C3B
22	b	614	CLA	C8-C10-C11-C12
30	C	516	DGD	C5B-C6B-C7B-C8B
34	E	101	LHG	C9-C10-C11-C12
22	b	604	CLA	C5-C6-C7-C8
23	A	404	PHO	C2-C3-C5-C6
27	A	410	PL9	C33-C34-C36-C37
28	c	524	LMG	C13-C14-C15-C16
22	B	611	CLA	C8-C10-C11-C12
22	b	607	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C12-C13-C14
22	B	617	CLA	C6-C7-C8-C9
22	C	503	CLA	C14-C13-C15-C16
22	d	402	CLA	C6-C7-C8-C9
22	B	612	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C12-C13-C14
24	b	618	BCR	C6-C7-C8-C9
34	B	622	LHG	C32-C33-C34-C35
22	b	606	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C26-C27-C28-C29
33	B	628	STE	C4-C5-C6-C7
34	D	409	LHG	O1-C1-C2-O2
33	I	101	STE	C11-C10-C9-C8
33	T	102	STE	C14-C15-C16-C17
33	M	103	STE	C5-C6-C7-C8
24	c	517	BCR	C7-C8-C9-C34
24	T	101	BCR	C7-C8-C9-C34
22	D	402	CLA	C2C-C3C-CAC-CBC
30	A	415	DGD	C2A-C3A-C4A-C5A
28	D	406	LMG	C33-C34-C35-C36
29	A	414	SQD	C10-C11-C12-C13
24	Z	101	BCR	C11-C12-C13-C14
22	B	610	CLA	C13-C15-C16-C17
22	d	402	CLA	C2C-C3C-CAC-CBC
33	J	101	STE	C6-C7-C8-C9
33	c	501	STE	C7-C8-C9-C10
28	b	621	LMG	C19-C20-C21-C22
24	c	517	BCR	C11-C10-C9-C34
33	Z	102	STE	C14-C15-C16-C17
33	X	101	STE	C6-C7-C8-C9
33	b	625	STE	C2-C3-C4-C5
29	a	413	SQD	C24-C25-C26-C27
29	a	412	SQD	C44-C45-O47-C7
29	B	623	SQD	C46-C45-O47-C7
22	c	503	CLA	C2A-CAA-CBA-CGA
34	e	102	LHG	O9-C7-O7-C5
22	a	402	CLA	C2-C1-O2A-CGA
22	B	614	CLA	C2-C1-O2A-CGA
29	A	414	SQD	C32-C33-C34-C35
22	c	511	CLA	CAA-CBA-CGA-O2A
33	C	522	STE	C6-C7-C8-C9
28	C	519	LMG	C14-C15-C16-C17
28	c	524	LMG	C35-C36-C37-C38
34	l	101	LHG	O6-C4-C5-O7
33	a	415	STE	C4-C5-C6-C7
33	B	625	STE	C6-C7-C8-C9
24	b	616	BCR	C5-C6-C7-C8
24	c	518	BCR	C1-C6-C7-C8
30	c	521	DGD	CBA-CCA-CDA-CEA
28	D	410	LMG	C15-C16-C17-C18
30	c	520	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
30	c	519	DGD	O1G-C1A-C2A-C3A
29	A	413	SQD	C31-C32-C33-C34
28	d	409	LMG	C37-C38-C39-C40
28	M	101	LMG	C15-C16-C17-C18
29	A	414	SQD	C28-C29-C30-C31
22	C	508	CLA	C16-C17-C18-C19
29	b	619	SQD	O5-C1-O6-C44
24	c	517	BCR	C12-C13-C14-C15
24	B	620	BCR	C11-C10-C9-C8
24	B	619	BCR	C16-C17-C18-C19
24	y	101	BCR	C11-C10-C9-C8
34	e	102	LHG	O7-C5-C6-O8
22	c	510	CLA	C8-C10-C11-C12
30	h	102	DGD	CDA-CEA-CFA-CGA
29	a	412	SQD	C28-C29-C30-C31
33	b	626	STE	C4-C5-C6-C7
34	l	101	LHG	C9-C10-C11-C12
34	E	101	LHG	C35-C36-C37-C38
30	C	518	DGD	O6D-C5D-C6D-O5D
22	a	405	CLA	C15-C16-C17-C18
33	d	411	STE	C11-C12-C13-C14
30	C	518	DGD	C9A-CAA-CBA-CCA
29	A	414	SQD	C46-C45-O47-C7
30	C	516	DGD	O1G-C1G-C2G-C3G
28	C	519	LMG	O1-C7-C8-C9
34	D	412	LHG	C26-C27-C28-C29
28	D	406	LMG	C34-C35-C36-C37
22	c	507	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C12-C13-C15
27	d	405	PL9	C47-C48-C49-C50
22	b	605	CLA	C11-C10-C8-C9
22	d	403	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C12-C13-C14
22	b	606	CLA	C6-C7-C8-C9
22	B	614	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
24	Z	101	BCR	C9-C10-C11-C12
24	Z	101	BCR	C15-C16-C17-C18
30	C	516	DGD	C6B-C7B-C8B-C9B
28	D	406	LMG	C37-C38-C39-C40
28	C	519	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
33	b	624	STE	C6-C7-C8-C9
30	C	517	DGD	C6B-C7B-C8B-C9B
33	B	628	STE	C7-C8-C9-C10
33	d	412	STE	C3-C4-C5-C6
22	b	610	CLA	C10-C11-C12-C13
33	b	620	STE	C15-C16-C17-C18
29	b	619	SQD	C14-C15-C16-C17
22	C	509	CLA	C16-C17-C18-C19
30	c	521	DGD	C2A-C1A-O1G-C1G
29	a	412	SQD	C9-C10-C11-C12
22	B	615	CLA	CBD-CGD-O2D-CED
33	d	411	STE	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
28	b	623	LMG	O6-C1-O1-C7
24	y	101	BCR	C9-C10-C11-C12
30	C	516	DGD	C3A-C4A-C5A-C6A
29	b	619	SQD	C13-C14-C15-C16
33	B	626	STE	C13-C14-C15-C16
30	c	519	DGD	C6A-C7A-C8A-C9A
23	d	401	PHO	C5-C6-C7-C8
34	d	408	LHG	C9-C10-C11-C12
29	b	619	SQD	C29-C30-C31-C32
34	e	102	LHG	O6-C4-C5-O7
24	d	404	BCR	C18-C19-C20-C21
22	b	608	CLA	C3-C5-C6-C7
34	B	622	LHG	C11-C12-C13-C14
34	l	101	LHG	C18-C19-C20-C21
33	d	411	STE	C4-C5-C6-C7
22	B	612	CLA	C2-C3-C5-C6
33	T	102	STE	C15-C16-C17-C18
22	D	402	CLA	C10-C11-C12-C13
22	d	402	CLA	C2-C1-O2A-CGA
30	C	518	DGD	CBA-CCA-CDA-CEA
29	D	407	SQD	C44-C45-C46-O48
34	d	406	LHG	C17-C18-C19-C20
28	c	522	LMG	C31-C32-C33-C34
33	d	412	STE	C15-C16-C17-C18
30	C	518	DGD	C2A-C3A-C4A-C5A
28	B	629	LMG	C21-C22-C23-C24
28	b	623	LMG	C12-C13-C14-C15
30	C	518	DGD	C4B-C5B-C6B-C7B
22	B	602	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C3A-C2A-CAA-CBA
23	d	401	PHO	C4C-C3C-CAC-CBC
22	B	605	CLA	C13-C15-C16-C17
27	A	410	PL9	C4-C3-C7-C8
28	D	411	LMG	C29-C30-C31-C32
28	C	519	LMG	C4-C5-C6-O5
22	C	512	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	B	612	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
24	c	516	BCR	C16-C17-C18-C36
34	e	102	LHG	C4-C5-C6-O8
28	M	101	LMG	C11-C12-C13-C14
22	B	605	CLA	O2A-C1-C2-C3
22	h	101	CLA	O2A-C1-C2-C3
30	C	517	DGD	O6D-C1D-O3G-C3G
24	Z	101	BCR	C14-C15-C16-C17
28	d	409	LMG	C12-C13-C14-C15
30	c	519	DGD	CBA-CCA-CDA-CEA
29	a	412	SQD	C46-C45-O47-C7
22	b	613	CLA	C10-C11-C12-C13
22	c	515	CLA	C1A-C2A-CAA-CBA
28	A	412	LMG	C14-C15-C16-C17
30	c	519	DGD	C8A-C9A-CAA-CBA
22	b	607	CLA	C11-C10-C8-C7
22	B	607	CLA	C6-C7-C8-C10
23	A	404	PHO	C12-C13-C15-C16
22	A	403	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
30	C	517	DGD	C4A-C5A-C6A-C7A
29	a	412	SQD	C11-C10-C9-C8
22	C	514	CLA	C8-C10-C11-C12
22	B	615	CLA	C16-C17-C18-C19
33	b	620	STE	C12-C13-C14-C15
22	b	613	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C15-C16-C17-C18
22	b	611	CLA	C8-C10-C11-C12
30	C	518	DGD	C3B-C4B-C5B-C6B
22	b	607	CLA	C2C-C3C-CAC-CBC
33	H	103	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	B	625	STE	C7-C8-C9-C10
34	e	102	LHG	O6-C4-C5-C6
22	B	610	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
34	D	408	LHG	C29-C30-C31-C32
34	d	406	LHG	C29-C30-C31-C32
33	C	521	STE	C11-C12-C13-C14
22	D	403	CLA	C4-C3-C5-C6
22	b	615	CLA	C8-C10-C11-C12
22	D	403	CLA	C13-C15-C16-C17
28	c	525	LMG	C28-C29-C30-C31
22	D	403	CLA	C3-C5-C6-C7
22	h	101	CLA	C10-C11-C12-C13
28	B	629	LMG	O7-C8-C9-O8
24	c	516	BCR	C9-C10-C11-C12
22	b	602	CLA	C13-C15-C16-C17
33	B	627	STE	C7-C8-C9-C10
30	H	102	DGD	CDA-CEA-CFA-CGA
30	C	516	DGD	O6E-C1E-O5D-C6D
33	b	625	STE	C6-C7-C8-C9
22	A	411	CLA	C4C-C3C-CAC-CBC
22	B	602	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
34	E	101	LHG	C18-C19-C20-C21
34	D	408	LHG	C17-C18-C19-C20
22	B	602	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C12-C13-C14
29	b	619	SQD	C10-C11-C12-C13
29	A	413	SQD	C10-C11-C12-C13
24	c	518	BCR	C23-C24-C25-C26
24	c	518	BCR	C23-C24-C25-C30
24	x	101	BCR	C23-C24-C25-C30
24	a	406	BCR	C1-C6-C7-C8
22	a	411	CLA	C4C-C3C-CAC-CBC
33	B	624	STE	C7-C8-C9-C10
28	b	623	LMG	C33-C34-C35-C36
24	Y	101	BCR	C13-C14-C15-C16
22	D	403	CLA	C10-C11-C12-C13
29	f	101	SQD	C35-C36-C37-C38
28	B	629	LMG	C35-C36-C37-C38
28	M	101	LMG	C22-C23-C24-C25
23	D	401	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C12-C13-C14-C15
22	B	609	CLA	C16-C17-C18-C19
22	b	601	CLA	C8-C10-C11-C12
22	b	603	CLA	C4-C3-C5-C6
33	M	102	STE	C5-C6-C7-C8
22	b	604	CLA	C11-C12-C13-C15
22	b	615	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C10-C8-C7
27	a	410	PL9	C38-C39-C41-C42
22	c	508	CLA	C6-C7-C8-C10
22	b	613	CLA	C11-C10-C8-C7
22	B	605	CLA	C4C-C3C-CAC-CBC
34	d	408	LHG	C11-C10-C9-C8
29	a	412	SQD	C16-C17-C18-C19
28	b	623	LMG	C2-C1-O1-C7
22	A	411	CLA	C16-C17-C18-C20
29	b	619	SQD	C19-C20-C21-C22
34	e	102	LHG	C19-C20-C21-C22
28	b	621	LMG	C12-C13-C14-C15
34	D	408	LHG	C14-C15-C16-C17
22	b	604	CLA	C10-C11-C12-C13
33	B	626	STE	C4-C5-C6-C7
22	c	511	CLA	C15-C16-C17-C18
22	B	610	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C20
28	D	410	LMG	C37-C38-C39-C40
22	C	512	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	CAA-CBA-CGA-O2A
28	B	629	LMG	O10-C28-C29-C30
27	d	405	PL9	C40-C39-C41-C42
22	C	514	CLA	C4-C3-C5-C6
28	B	629	LMG	C22-C23-C24-C25
22	B	613	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	A	403	CLA	C11-C10-C8-C9
23	a	404	PHO	C6-C7-C8-C9
22	c	508	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C14
22	A	411	CLA	C14-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C14
30	C	516	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	a	402	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	C	511	CLA	CAD-CBD-CGD-O2D
30	H	102	DGD	C4A-C5A-C6A-C7A
29	A	414	SQD	C24-C25-C26-C27
28	c	524	LMG	C36-C37-C38-C39
30	H	102	DGD	CCB-CDB-CEB-CFB
30	h	102	DGD	O1B-C1B-C2B-C3B
24	D	404	BCR	C22-C23-C24-C25
22	C	507	CLA	C4-C3-C5-C6
22	B	604	CLA	C16-C17-C18-C20
22	C	514	CLA	C2-C3-C5-C6
22	B	602	CLA	CAA-CBA-CGA-O2A
34	B	622	LHG	O7-C7-C8-C9
34	D	409	LHG	O8-C23-C24-C25
28	d	409	LMG	O7-C10-C11-C12
22	B	614	CLA	CAA-CBA-CGA-O2A
24	c	517	BCR	C21-C22-C23-C24
24	a	406	BCR	C21-C22-C23-C24
22	b	609	CLA	O1D-CGD-O2D-CED
29	b	619	SQD	C44-C45-C46-O48
28	M	101	LMG	O1-C7-C8-C9
22	c	514	CLA	C15-C16-C17-C18
22	B	602	CLA	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
22	D	403	CLA	O2A-C1-C2-C3
22	d	402	CLA	O2A-C1-C2-C3
22	C	510	CLA	O2A-C1-C2-C3
22	b	609	CLA	C2A-CAA-CBA-CGA
33	B	626	STE	C7-C8-C9-C10
28	D	406	LMG	C38-C39-C40-C41
30	C	517	DGD	C8A-C9A-CAA-CBA
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	A	403	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	c	505	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
29	A	414	SQD	O48-C23-C24-C25
22	b	615	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C11-C12-C13-C14
33	d	411	STE	C5-C6-C7-C8
29	A	413	SQD	O47-C45-C46-O48
28	C	519	LMG	O1-C7-C8-O7
30	C	518	DGD	C8A-C9A-CAA-CBA
29	A	414	SQD	C31-C32-C33-C34
22	C	514	CLA	C13-C15-C16-C17
28	b	621	LMG	O8-C28-C29-C30
34	E	101	LHG	C10-C11-C12-C13
30	H	102	DGD	CBB-CCB-CDB-CEB
22	C	512	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	614	CLA	C12-C13-C15-C16
22	B	616	CLA	C12-C13-C15-C16
22	B	606	CLA	C2-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
29	a	412	SQD	C34-C35-C36-C37
28	A	412	LMG	O6-C1-O1-C7
33	B	626	STE	C11-C10-C9-C8
29	B	623	SQD	C11-C10-C9-C8
34	e	102	LHG	C17-C18-C19-C20
22	C	506	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	B	605	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	c	509	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
27	A	410	PL9	C44-C46-C47-C48
22	B	611	CLA	C15-C16-C17-C18
33	b	624	STE	C10-C11-C12-C13
29	a	412	SQD	O47-C7-C8-C9
22	B	613	CLA	CAA-CBA-CGA-O1A
29	b	619	SQD	C11-C12-C13-C14
22	C	512	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	CDB-CEB-CFB-CGB
34	d	408	LHG	C24-C25-C26-C27
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
33	B	601	STE	C1-C2-C3-C4
22	B	603	CLA	C1A-C2A-CAA-CBA
33	c	523	STE	C1-C2-C3-C4
33	b	624	STE	C7-C8-C9-C10
34	B	622	LHG	C30-C31-C32-C33
34	D	412	LHG	C10-C11-C12-C13
30	c	520	DGD	C8B-C9B-CAB-CBB
34	D	409	LHG	C28-C29-C30-C31
28	D	406	LMG	C16-C17-C18-C19
22	B	602	CLA	CAA-CBA-CGA-O1A
29	B	623	SQD	O10-C23-C24-C25
29	A	414	SQD	O10-C23-C24-C25
30	c	519	DGD	O1B-C1B-C2B-C3B
30	c	521	DGD	C2B-C3B-C4B-C5B
28	c	524	LMG	C38-C39-C40-C41
33	J	101	STE	C5-C6-C7-C8
34	D	408	LHG	C4-O6-P-O5
34	E	101	LHG	C4-O6-P-O5
34	e	102	LHG	C4-O6-P-O4
34	e	102	LHG	C4-O6-P-O5
22	B	615	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
34	B	622	LHG	C26-C27-C28-C29
24	c	518	BCR	C5-C6-C7-C8
24	x	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	a	406	BCR	C5-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C26
22	B	614	CLA	CAA-CBA-CGA-O1A
22	b	611	CLA	CAA-CBA-CGA-O2A
29	a	413	SQD	C30-C31-C32-C33
24	D	404	BCR	C18-C19-C20-C21
22	h	101	CLA	C2A-CAA-CBA-CGA
22	B	611	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6
22	B	612	CLA	C4-C3-C5-C6
27	D	405	PL9	C46-C47-C48-C49
28	c	524	LMG	C40-C41-C42-C43
22	B	613	CLA	CAD-CBD-CGD-O1D
22	B	610	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
34	D	409	LHG	O10-C23-C24-C25
22	a	403	CLA	C13-C15-C16-C17
22	b	604	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	c	515	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
30	H	102	DGD	C8B-C9B-CAB-CBB
29	b	619	SQD	C23-C24-C25-C26
30	h	102	DGD	C1A-C2A-C3A-C4A
30	C	516	DGD	O2G-C1B-C2B-C3B
29	A	413	SQD	O47-C7-C8-C9
28	B	629	LMG	O7-C10-C11-C12
34	l	101	LHG	O9-C7-C8-C9
34	d	406	LHG	C35-C36-C37-C38
30	c	521	DGD	O1G-C1A-C2A-C3A
22	C	508	CLA	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
27	d	405	PL9	C45-C44-C46-C47
34	d	407	LHG	C26-C27-C28-C29
22	C	512	CLA	C11-C10-C8-C7
22	b	604	CLA	C12-C13-C15-C16
27	d	405	PL9	C33-C34-C36-C37

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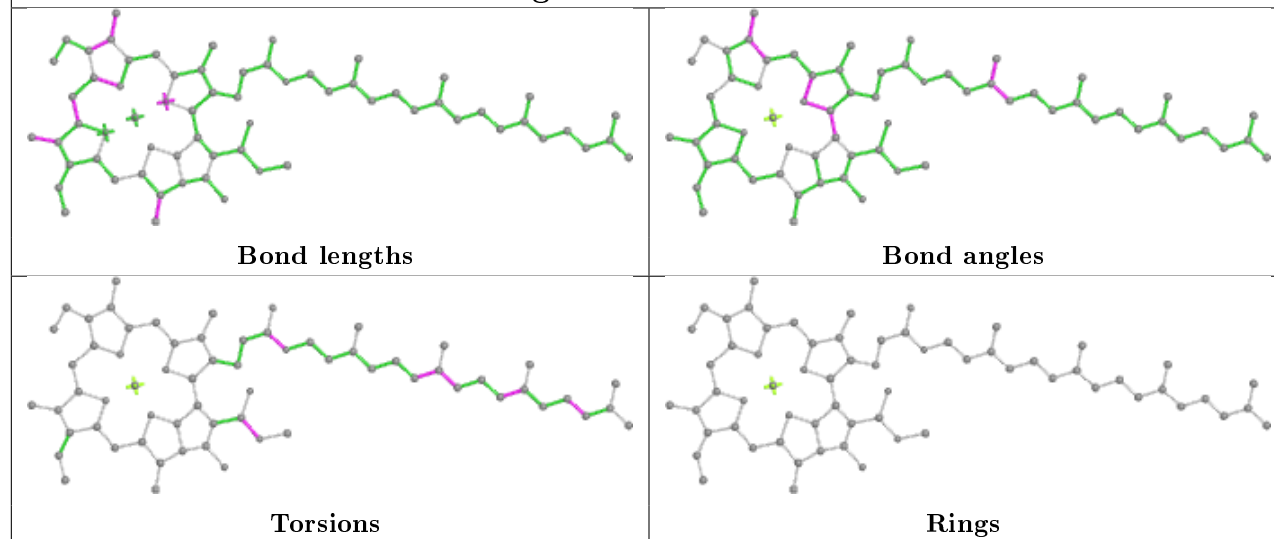
Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C3A-C2A-CAA-CBA
22	c	510	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	b	602	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C12-C13-C15
22	c	509	CLA	C12-C13-C15-C16
29	A	413	SQD	O49-C7-C8-C9
28	M	101	LMG	C34-C35-C36-C37
30	c	519	DGD	O2G-C1B-C2B-C3B
24	b	618	BCR	C17-C18-C19-C20
24	B	619	BCR	C7-C8-C9-C10
22	b	605	CLA	C16-C17-C18-C19
30	c	519	DGD	O6E-C1E-O5D-C6D
22	b	609	CLA	C15-C16-C17-C18
22	C	510	CLA	C8-C10-C11-C12
22	c	512	CLA	CAA-CBA-CGA-O1A
22	b	607	CLA	C13-C15-C16-C17
22	C	507	CLA	C15-C16-C17-C18
28	c	525	LMG	C8-C9-O8-C28
22	c	512	CLA	CAA-CBA-CGA-O2A
29	a	412	SQD	O49-C7-C8-C9
23	a	404	PHO	C4-C3-C5-C6
34	E	101	LHG	C14-C15-C16-C17

There are no ring outliers.

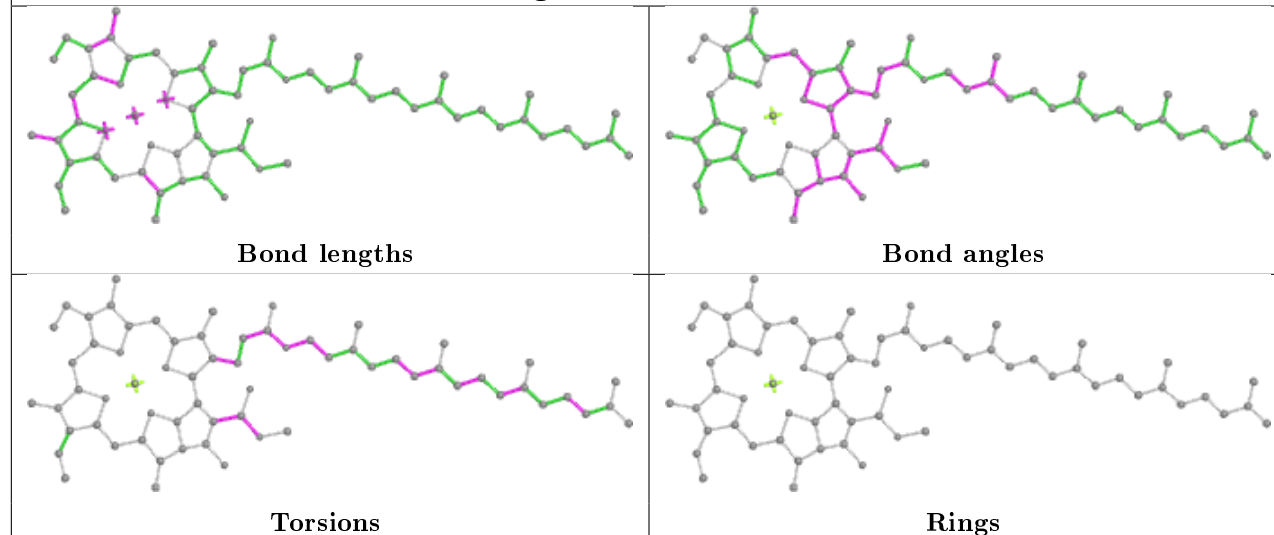
No monomer is involved in short contacts.

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.

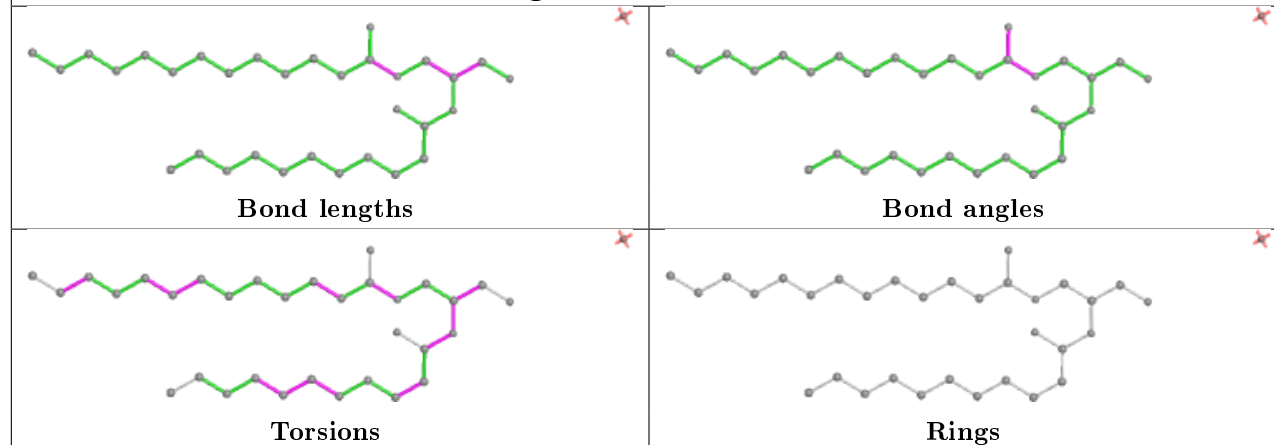
Ligand CLA C 512



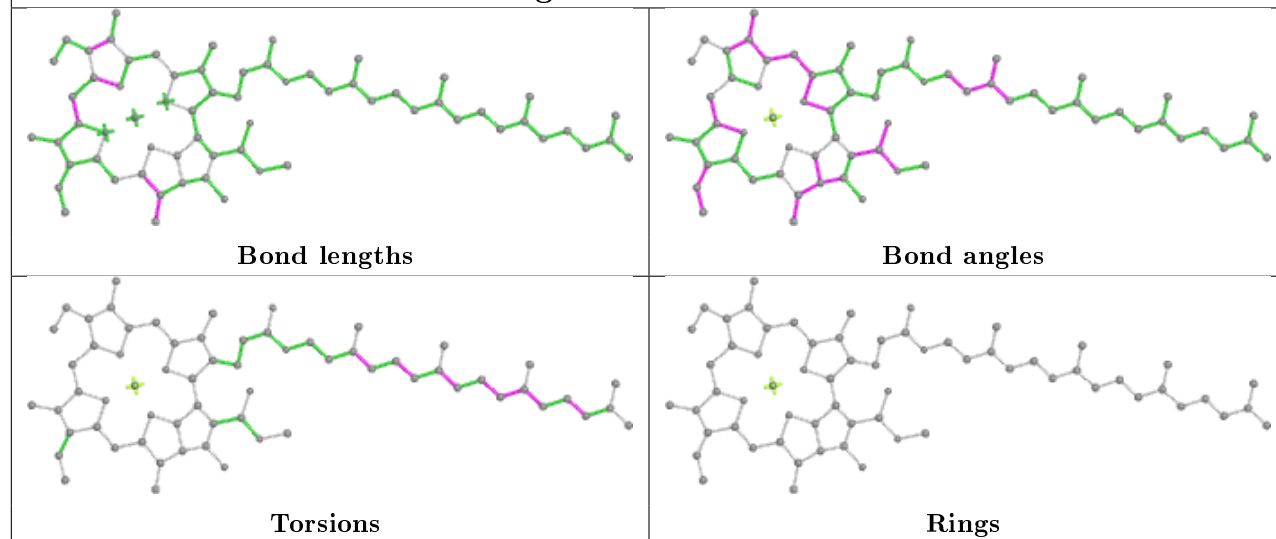
Ligand CLA B 602



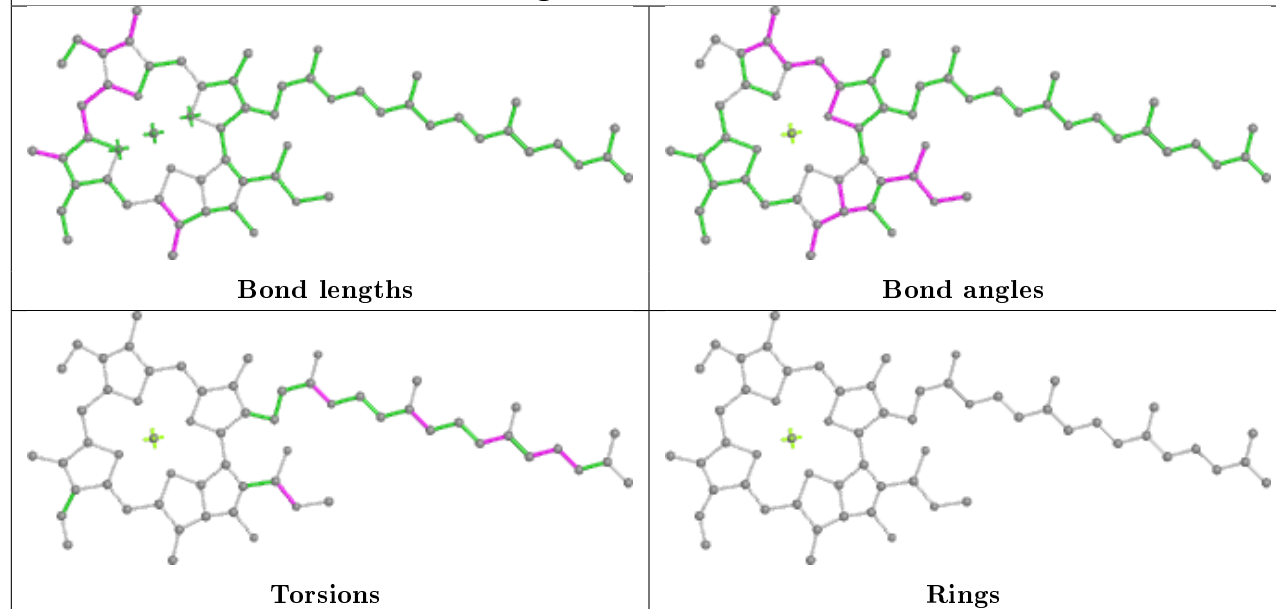
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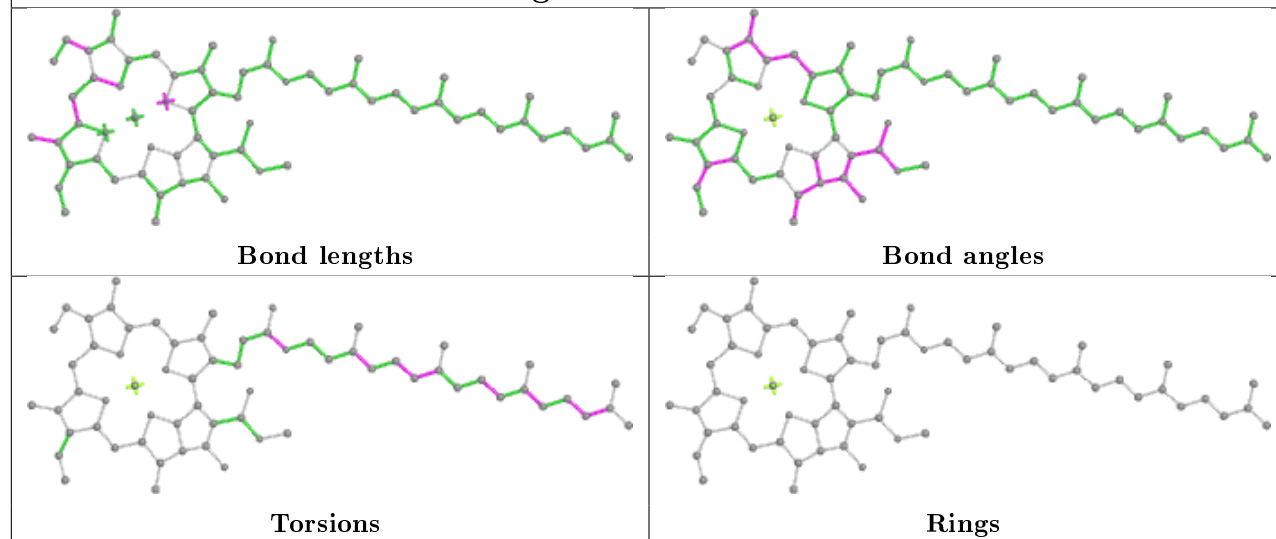
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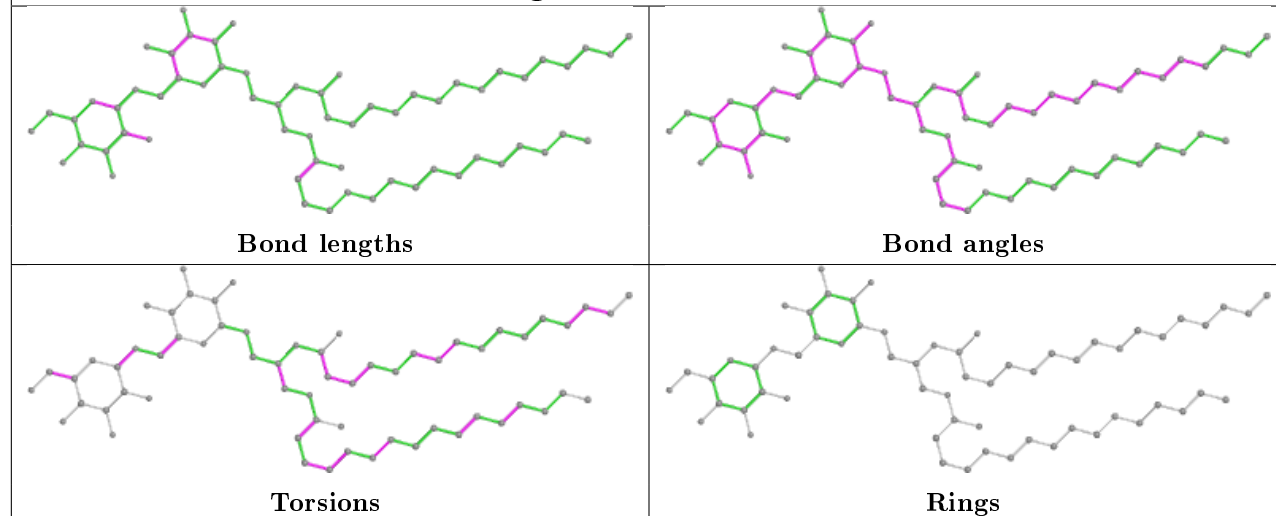
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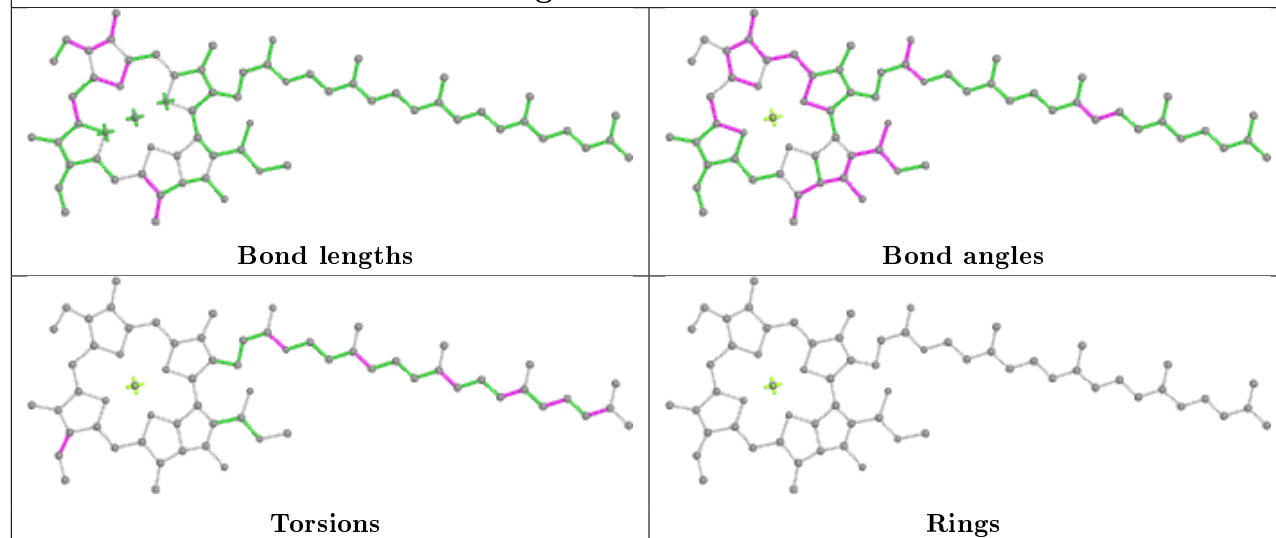
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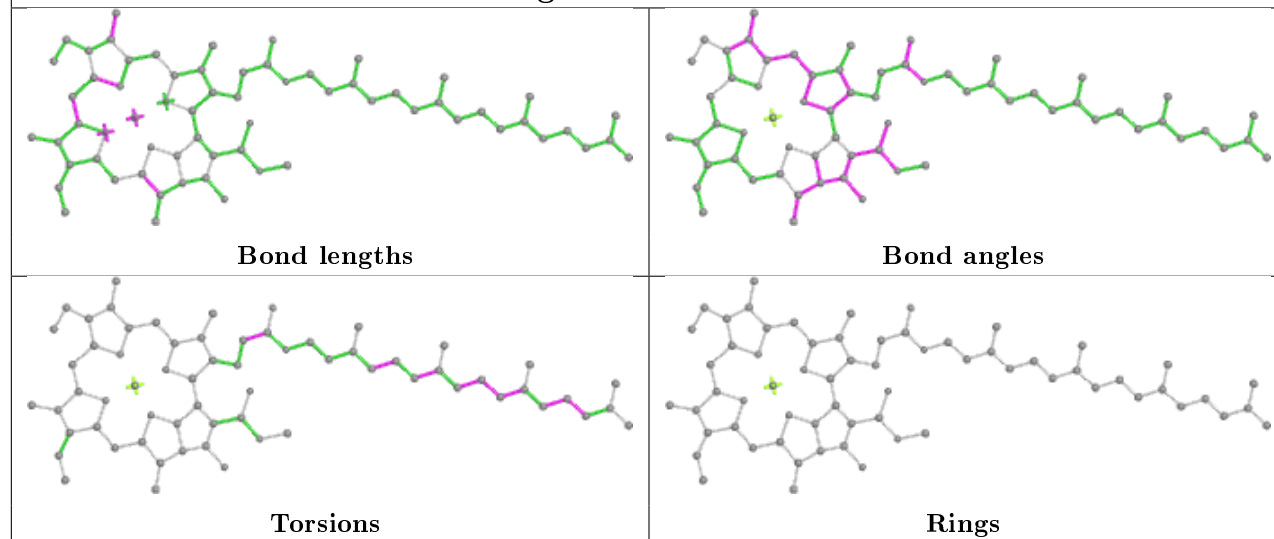
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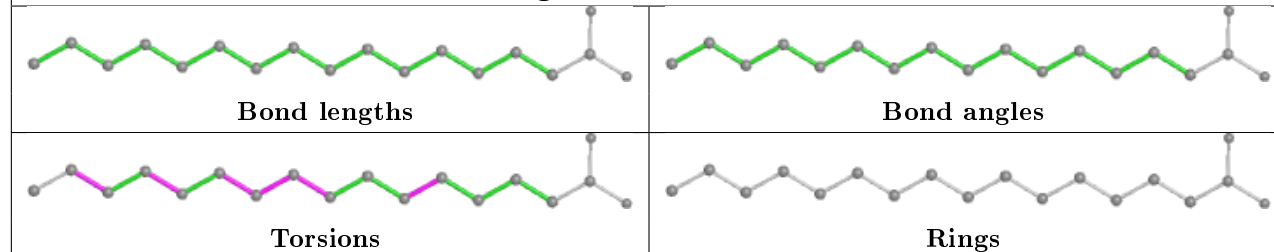
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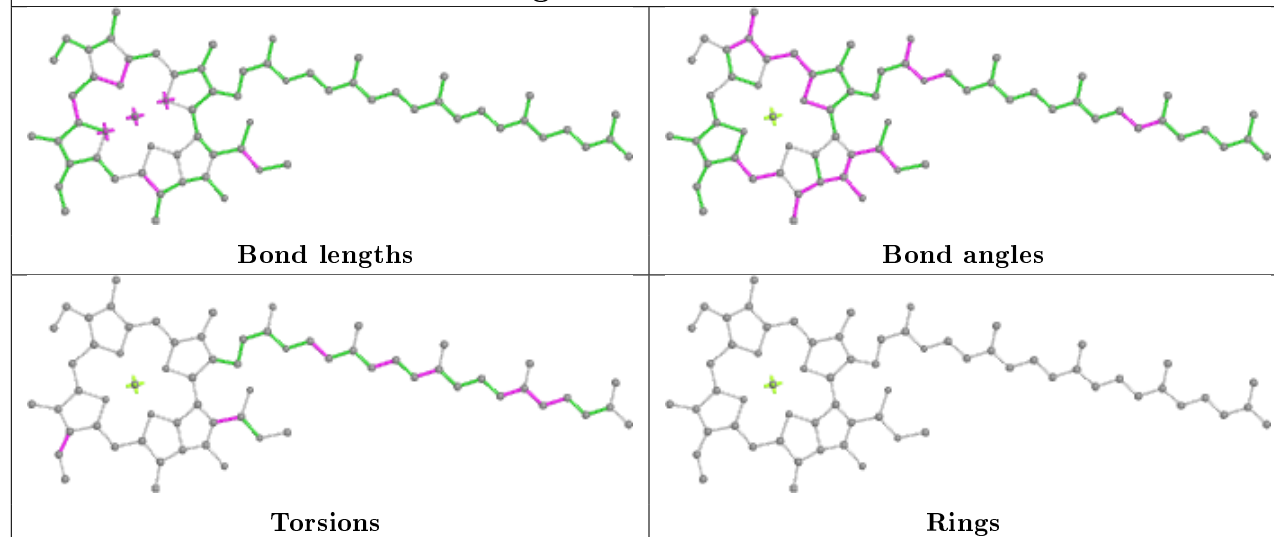
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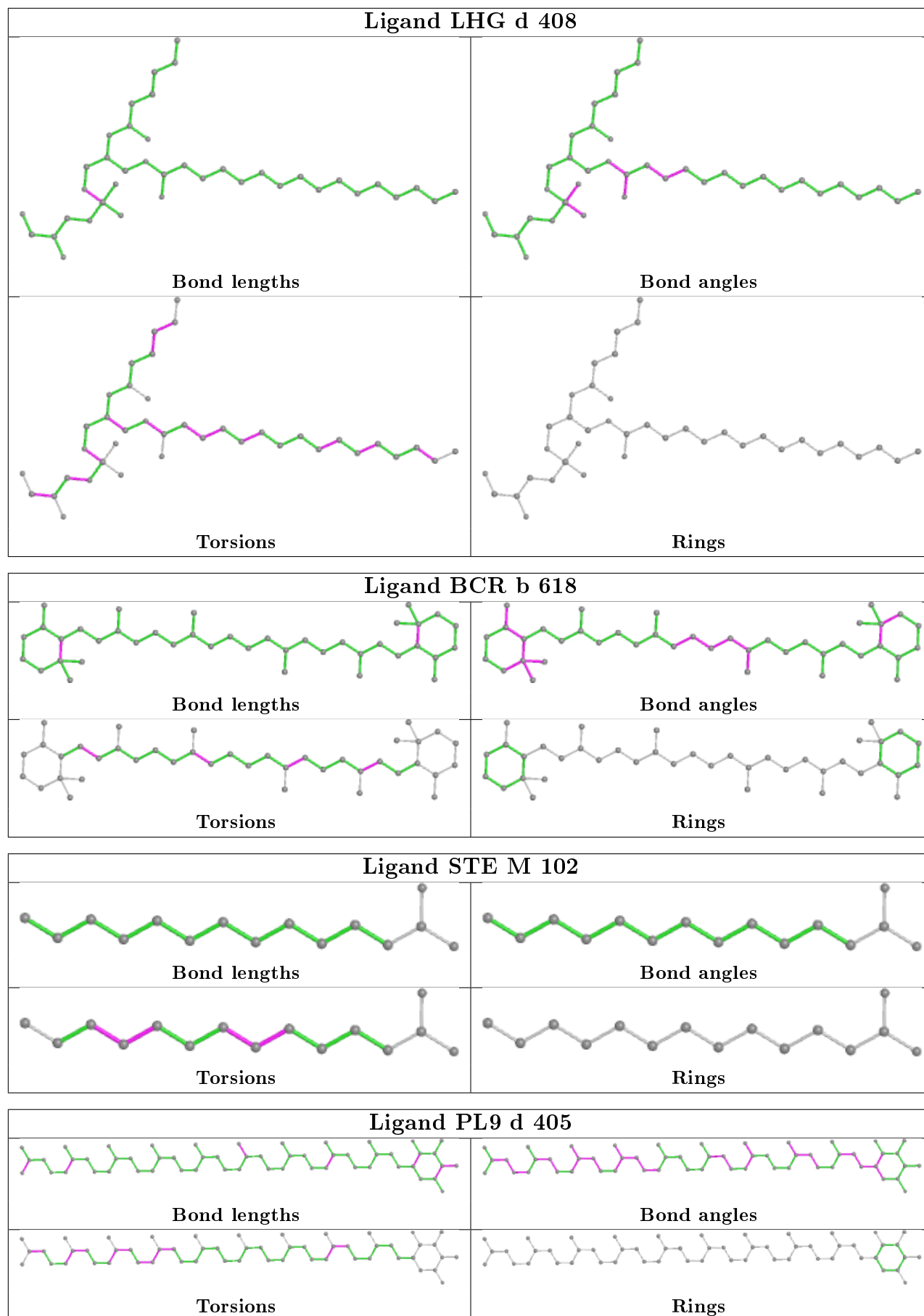


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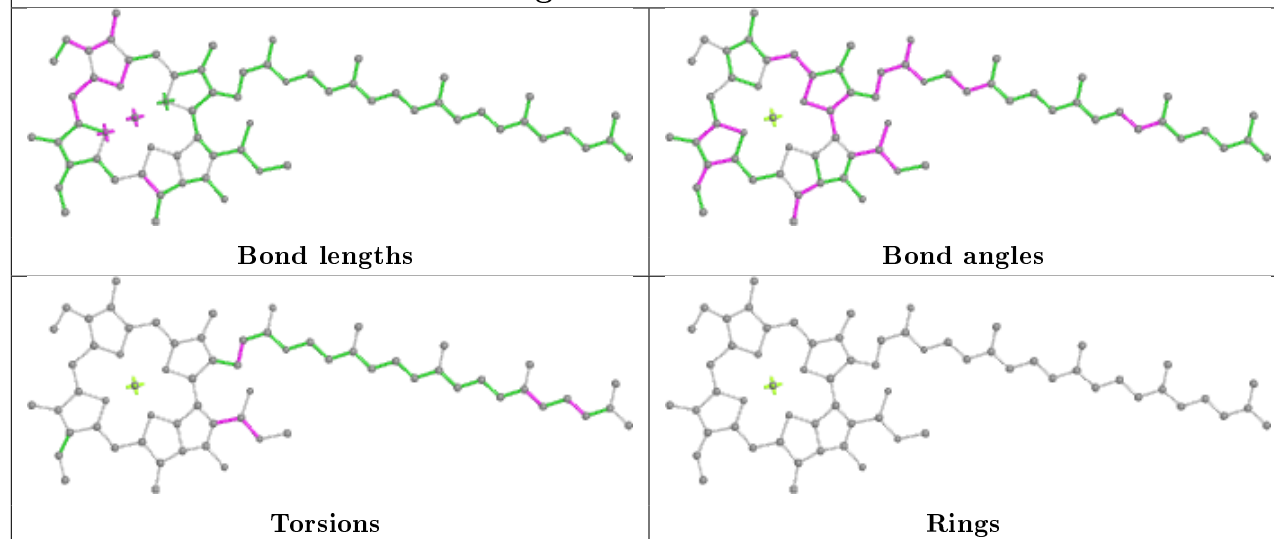


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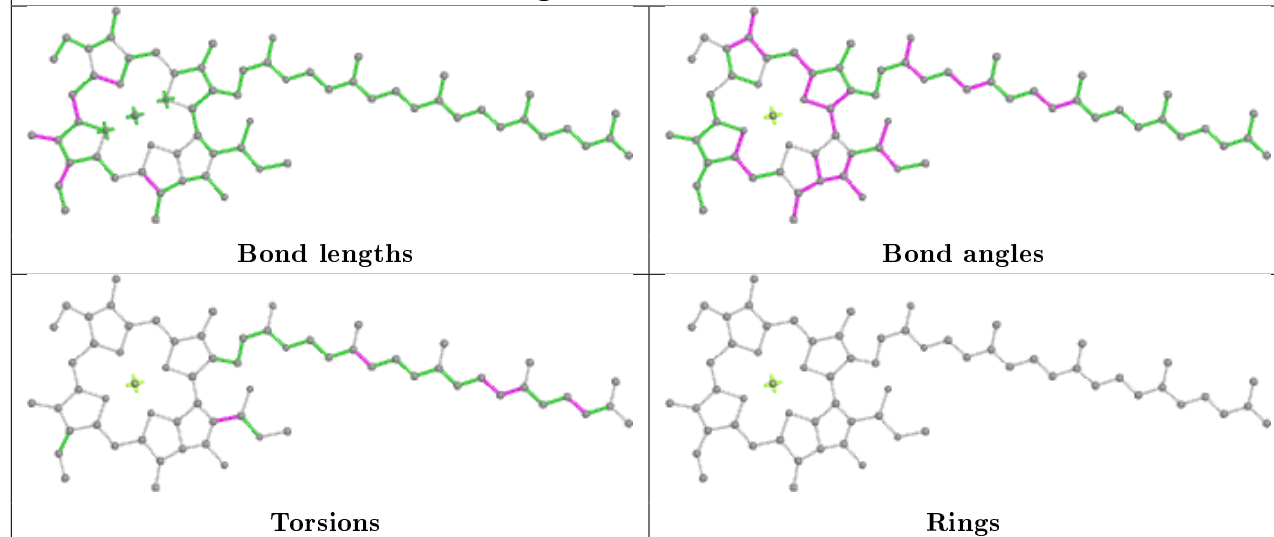




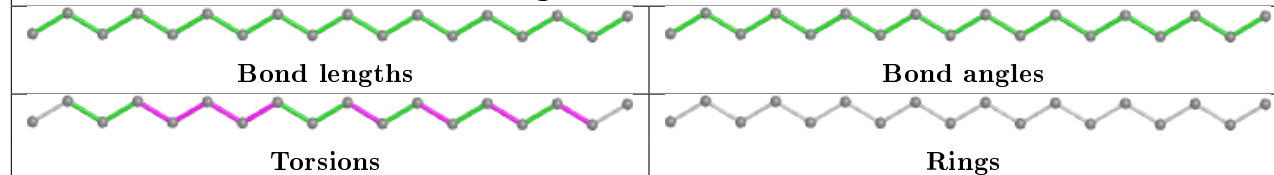
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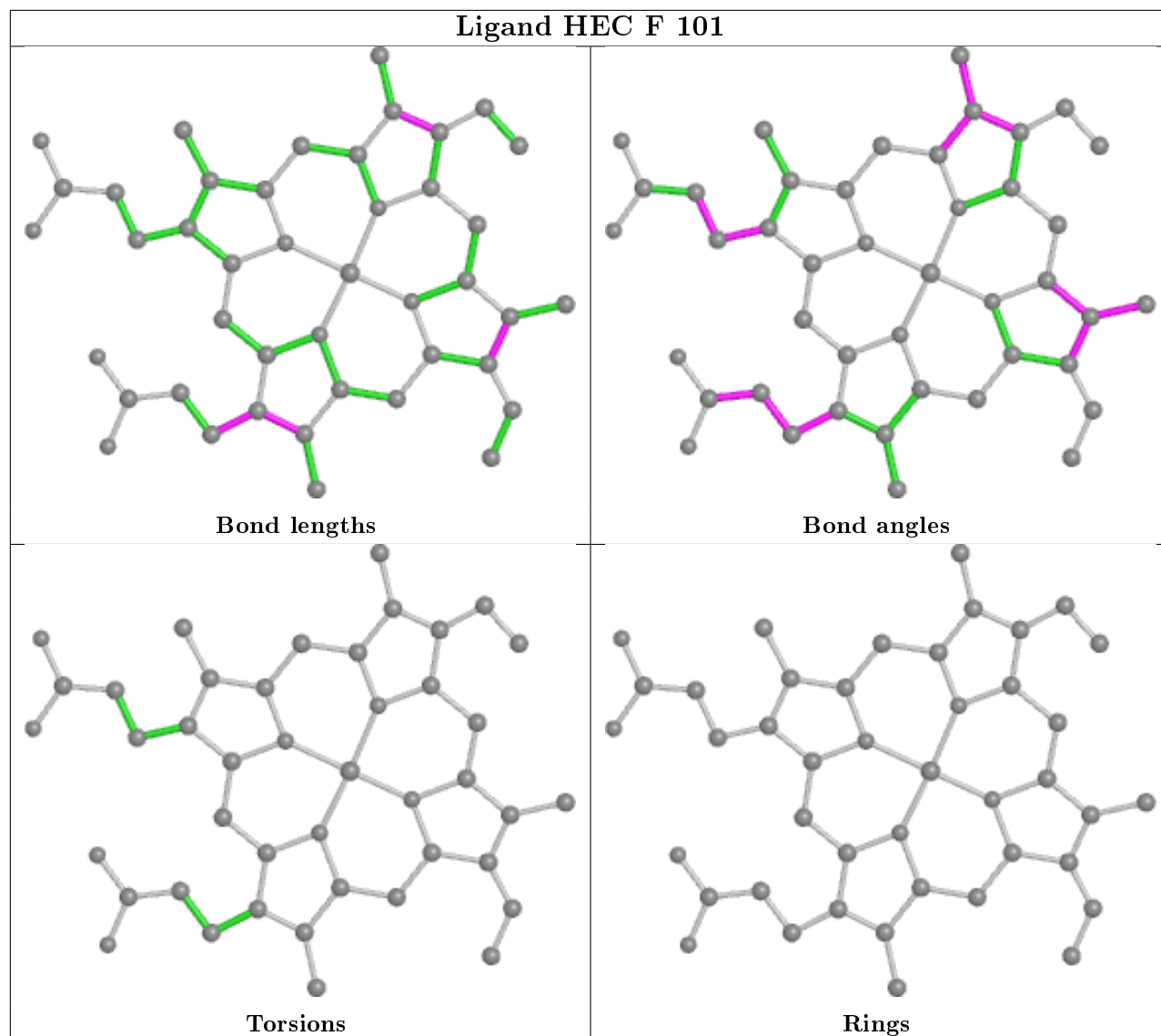
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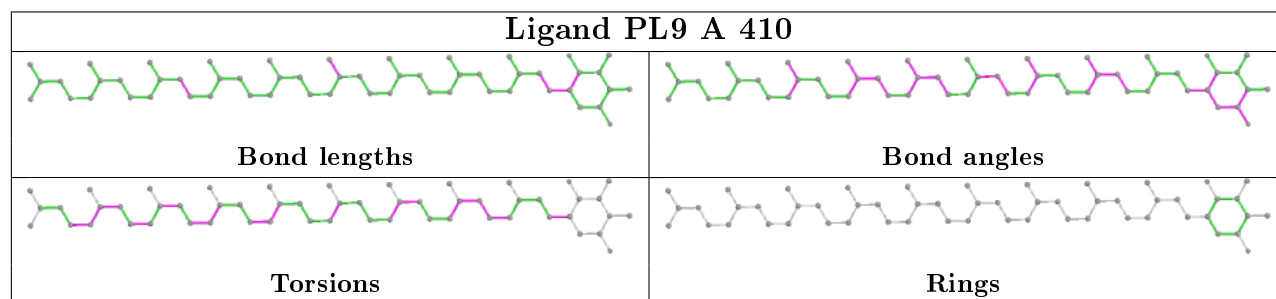
Ligand STE H 103

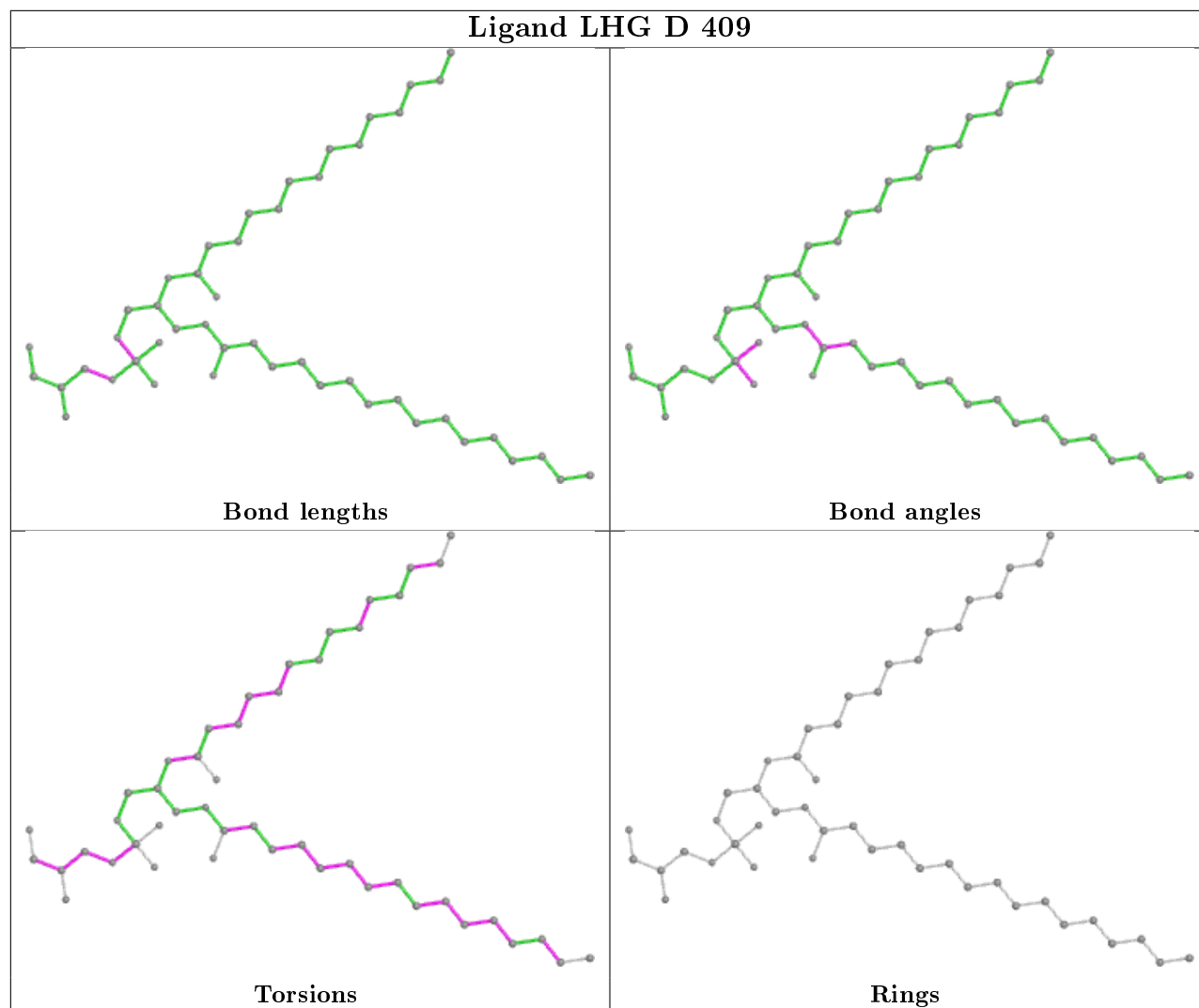


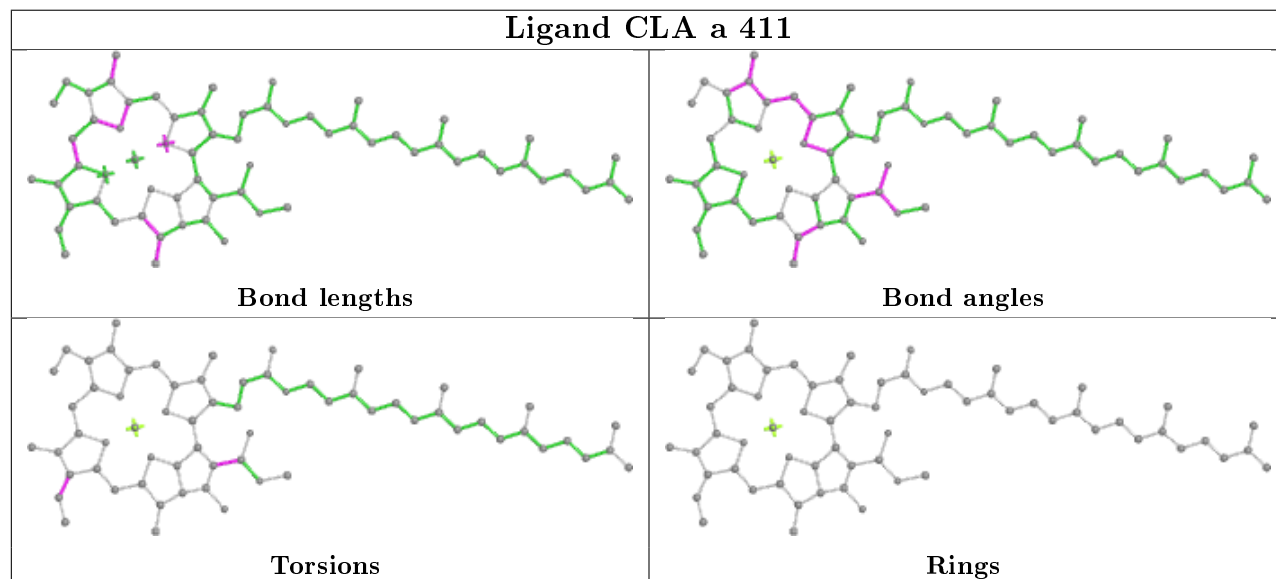
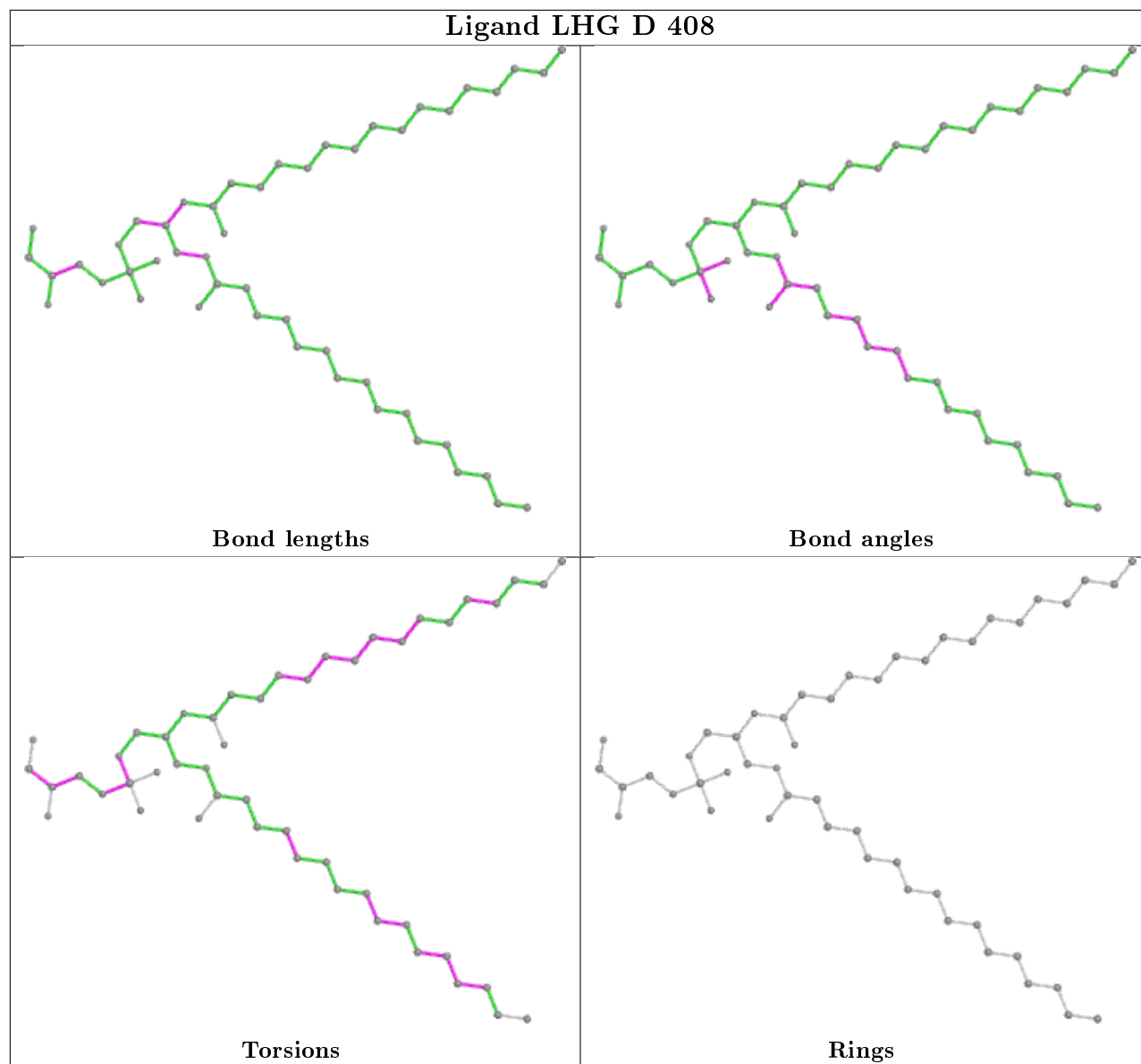
Ligand HEC F 101



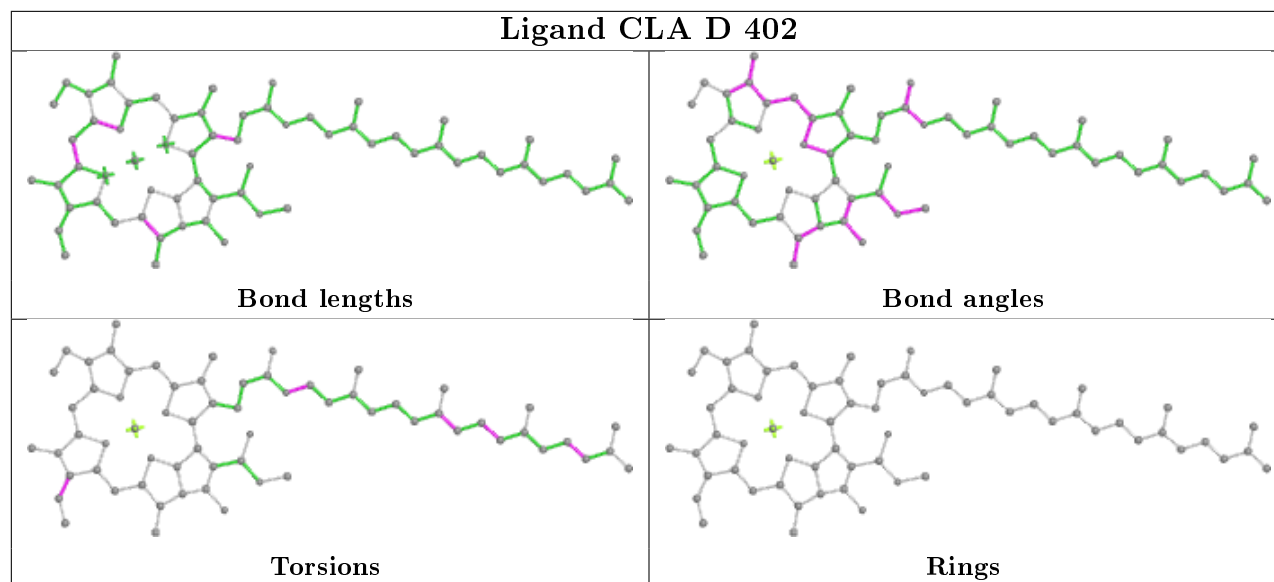
Ligand PL9 A 410



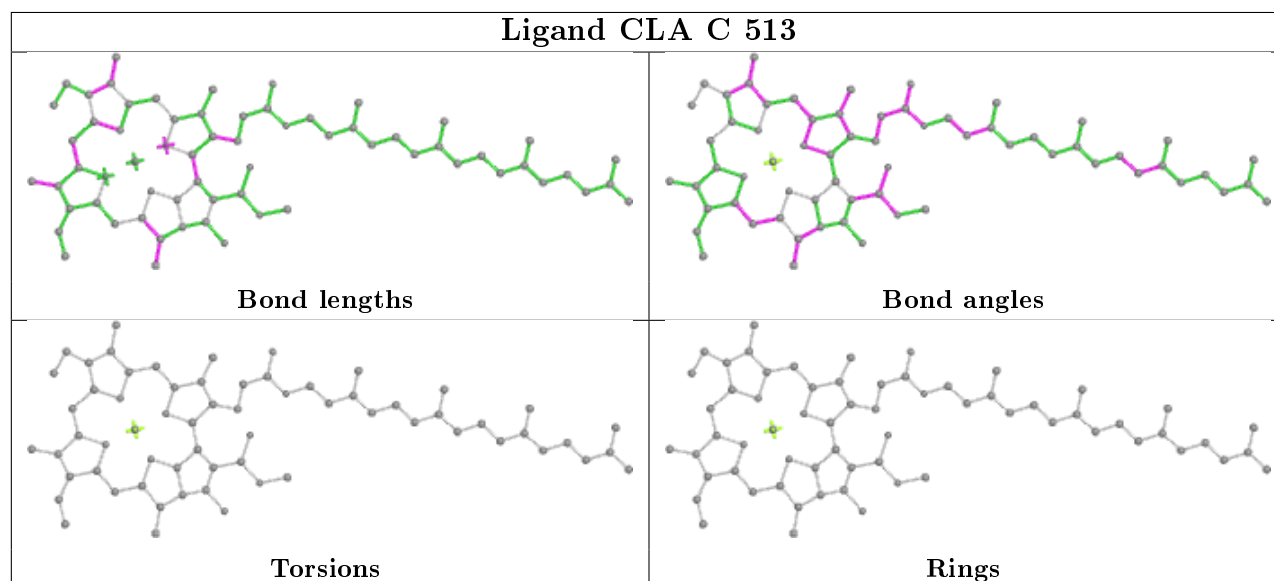




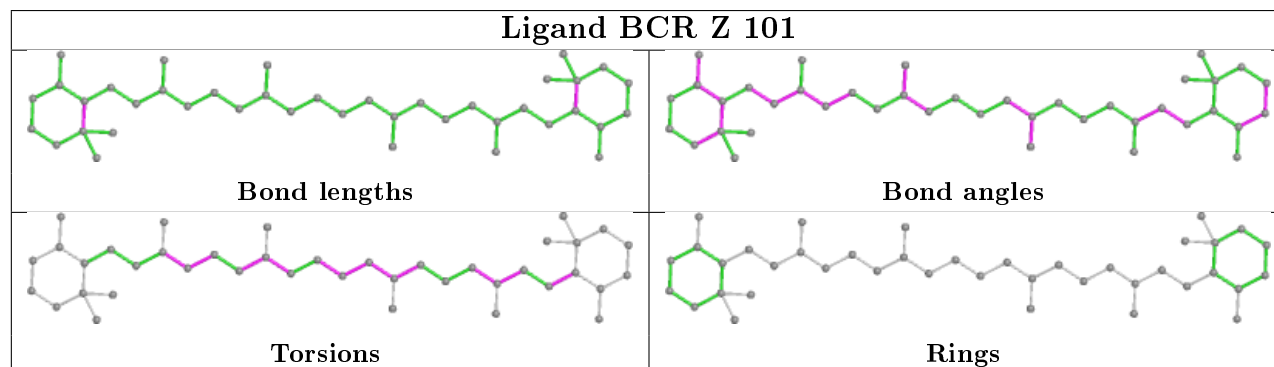
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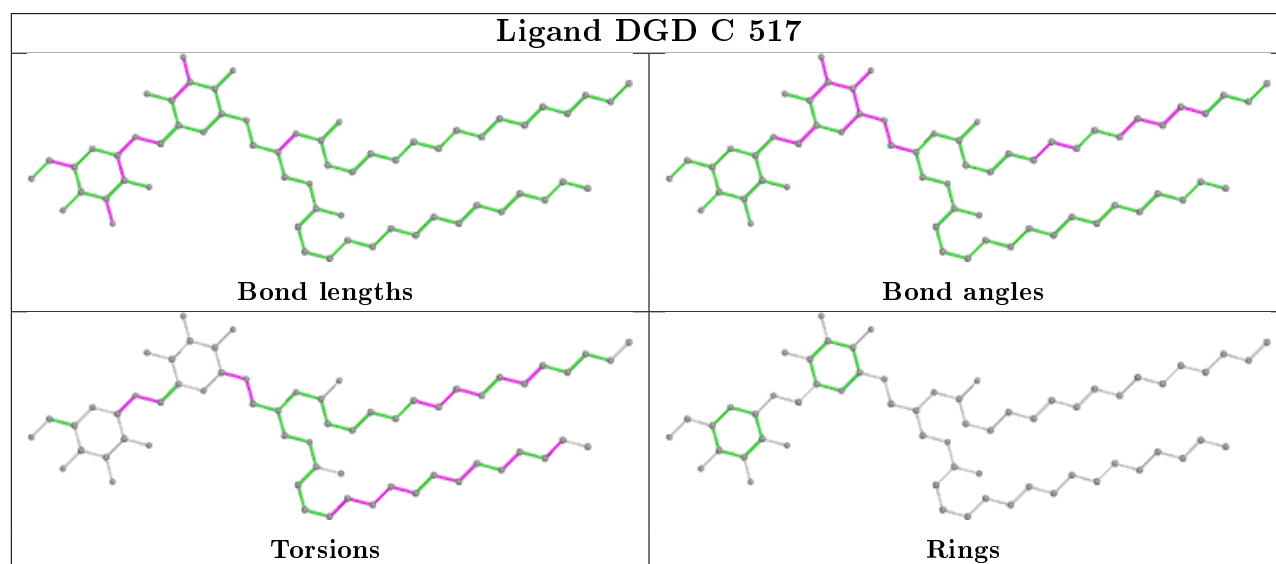
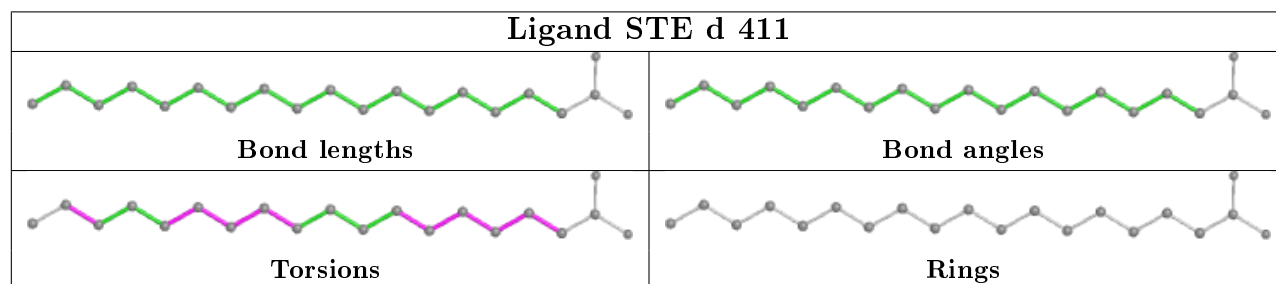
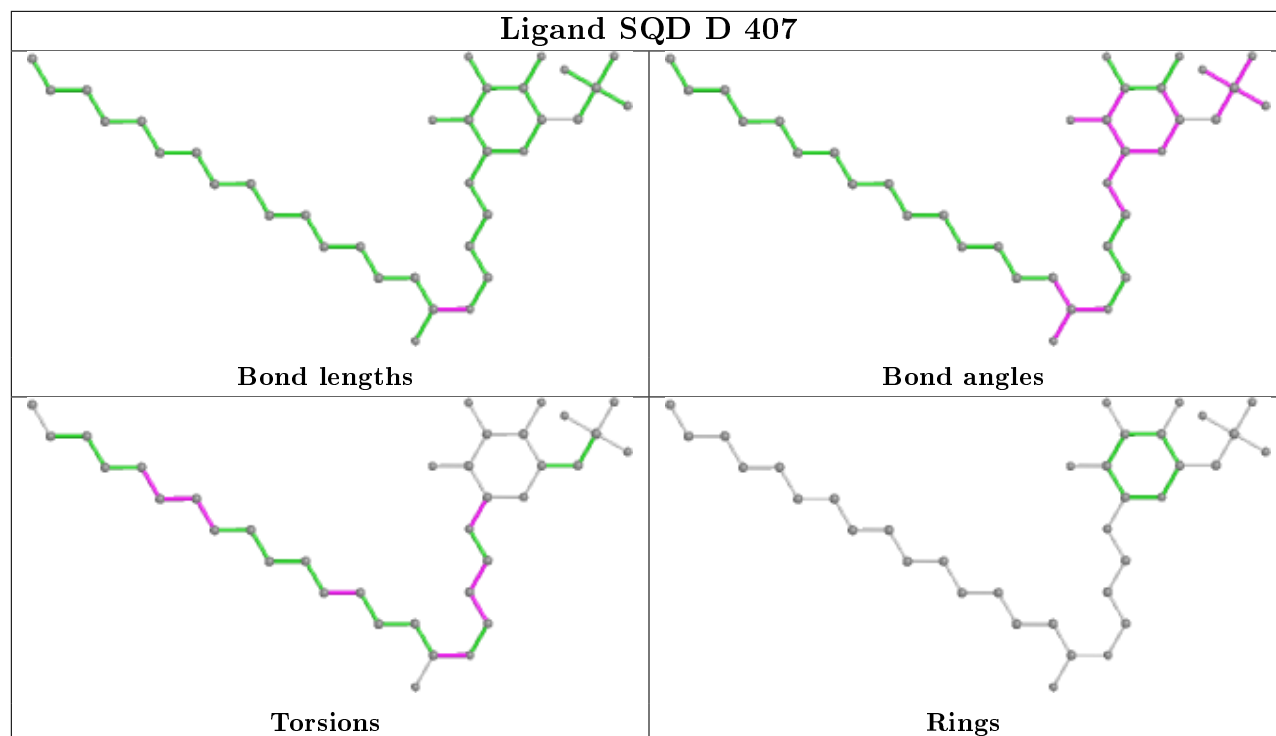


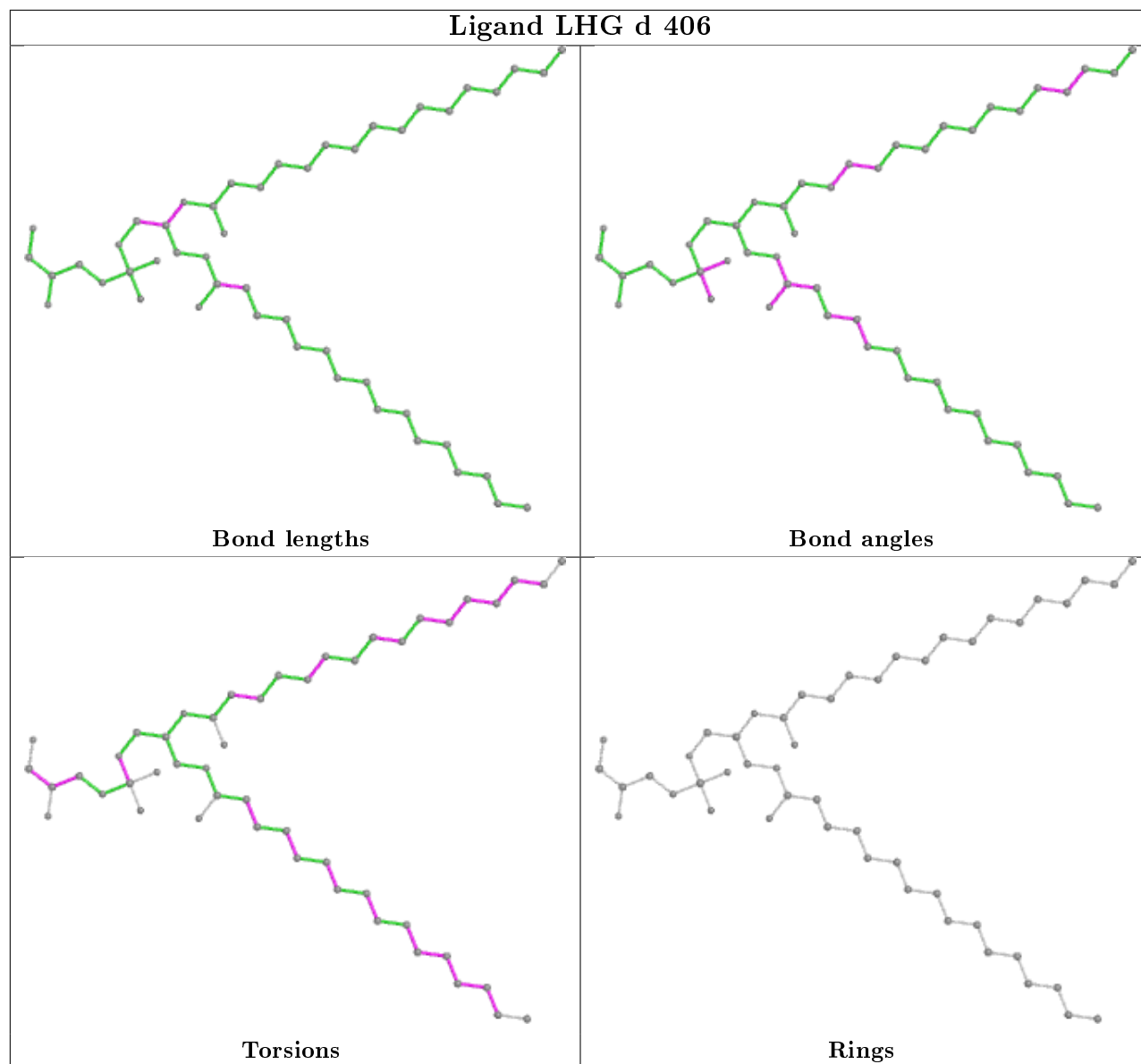
Ligand CLA C 513



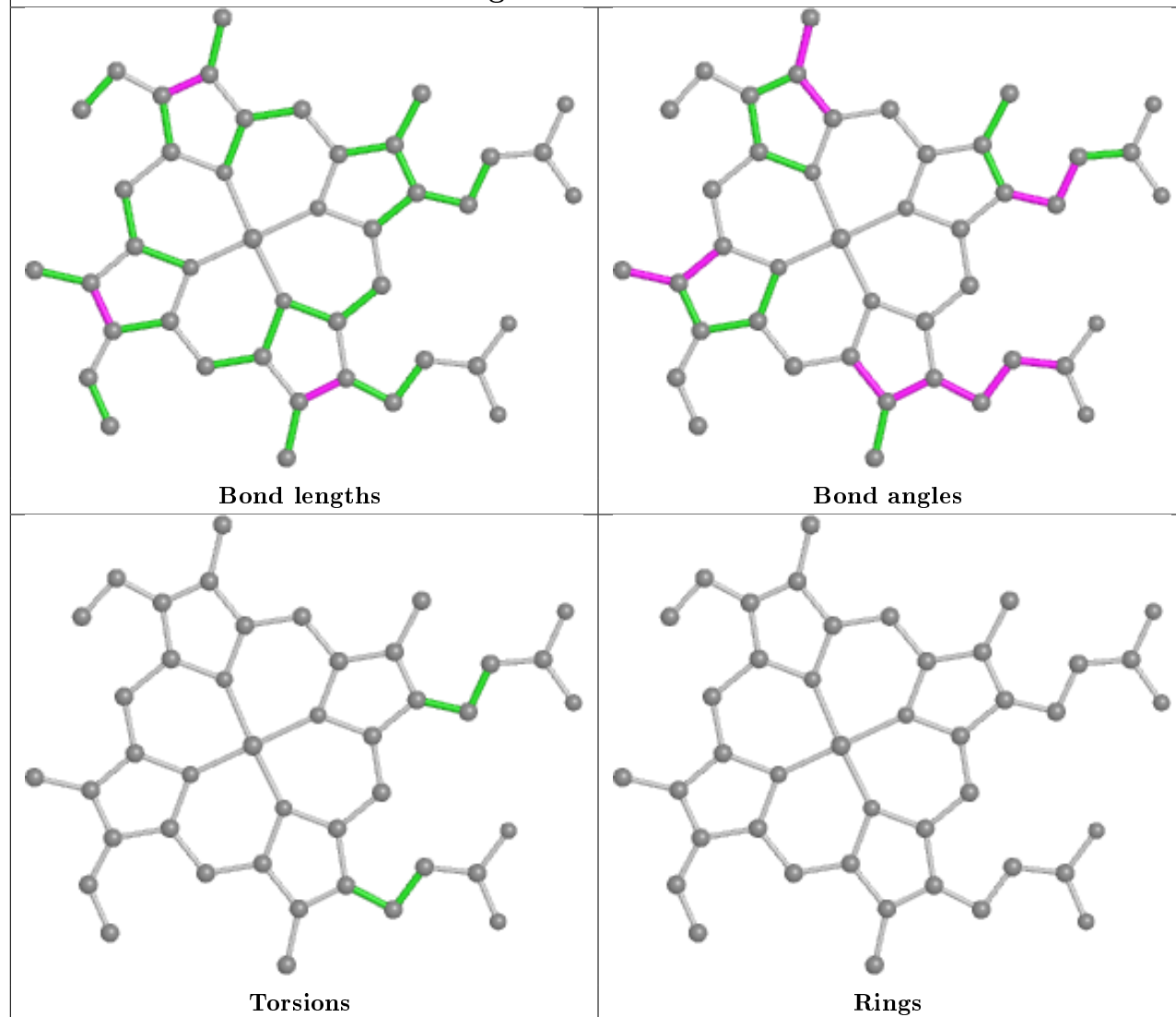
Ligand BCR Z 101



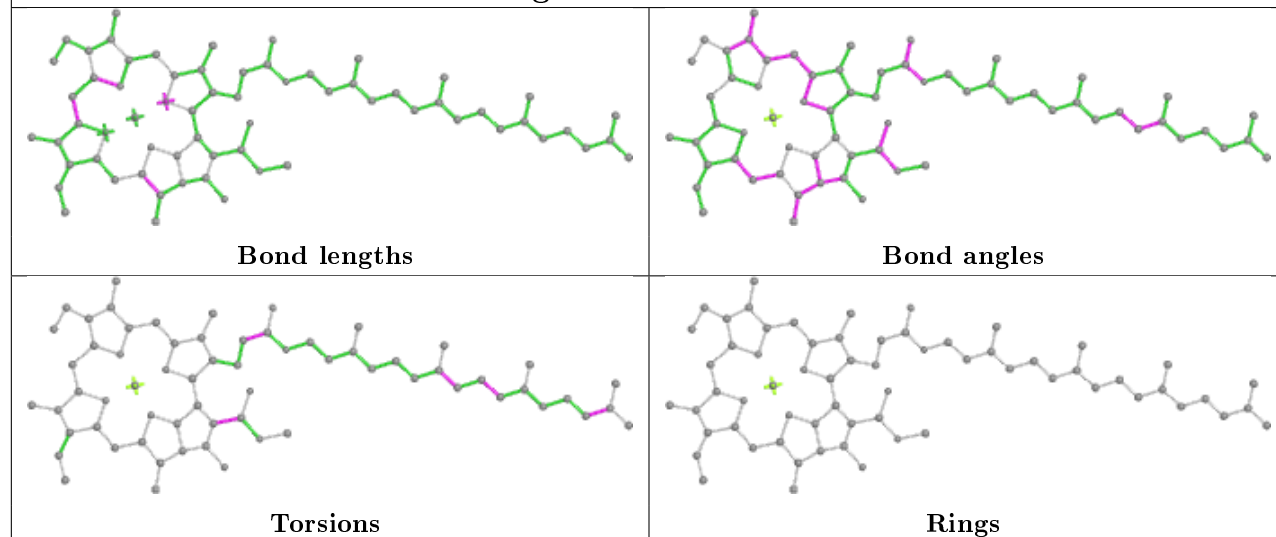




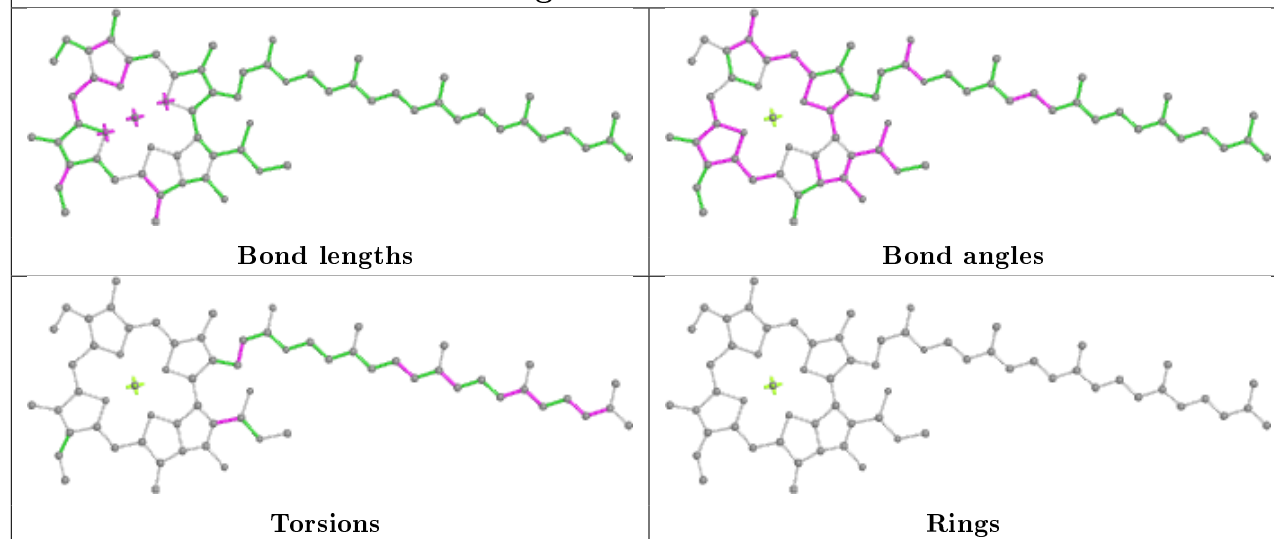
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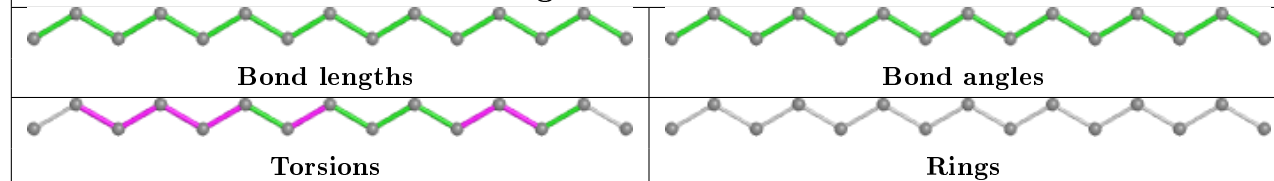
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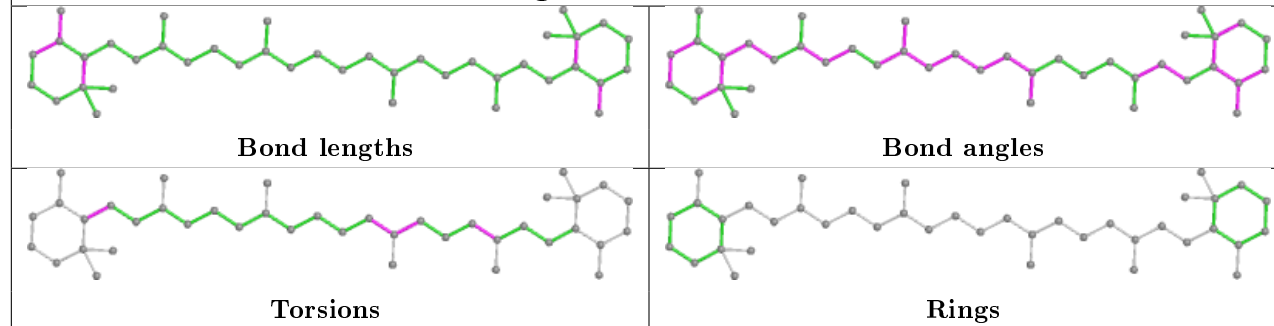
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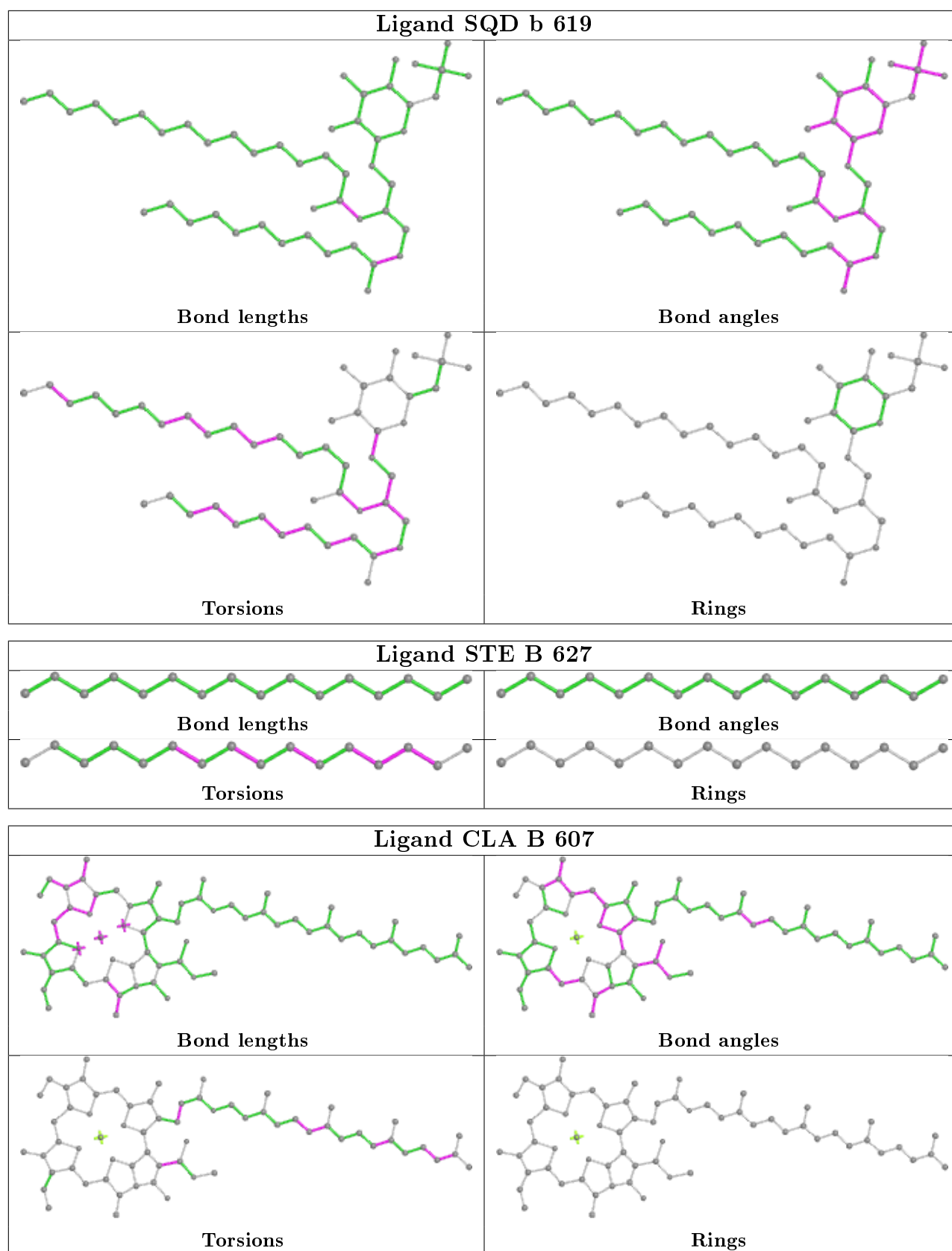


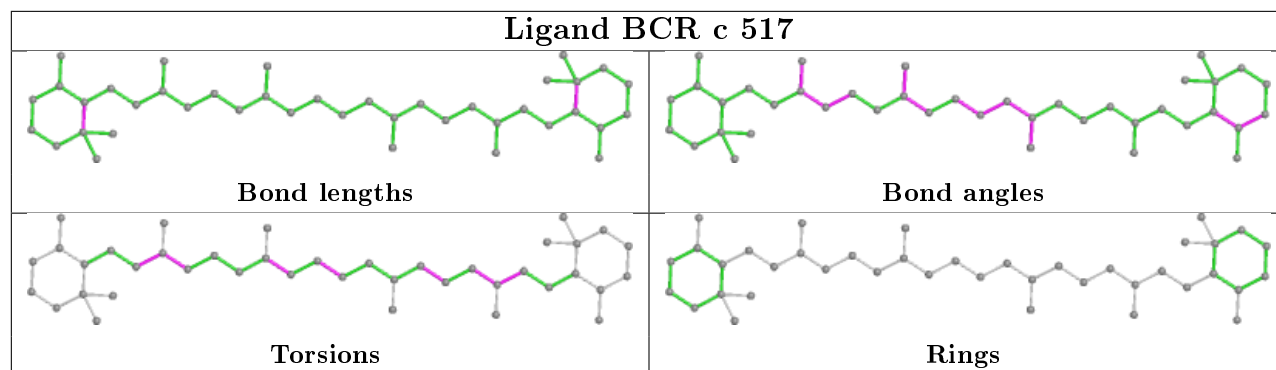
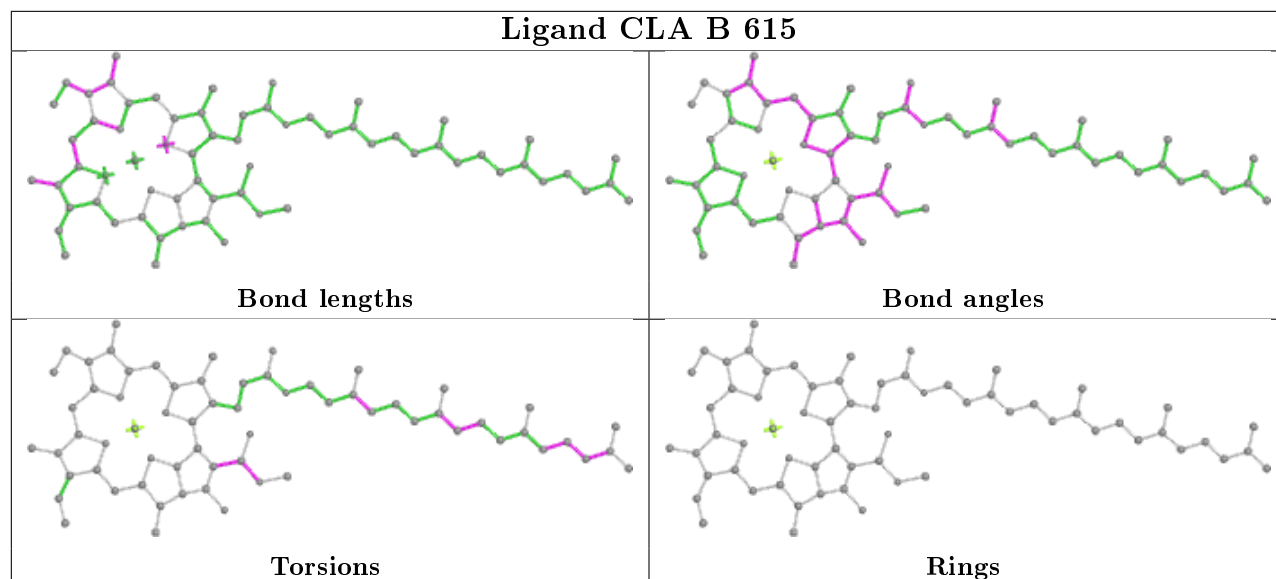
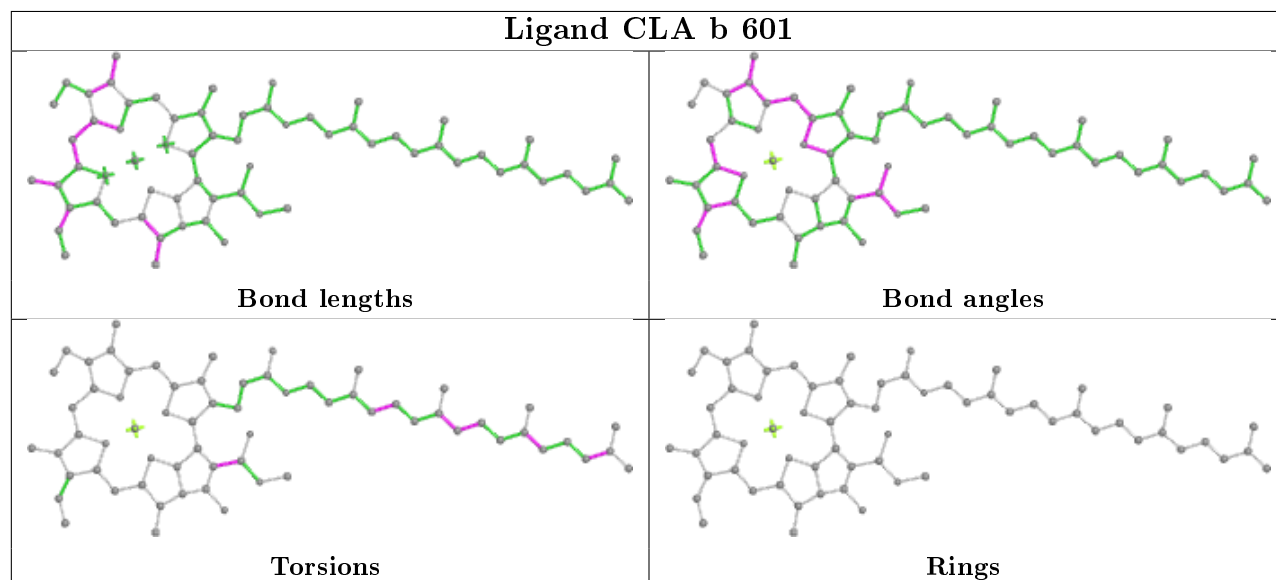
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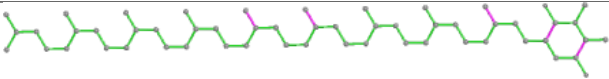
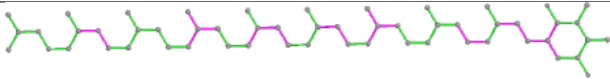
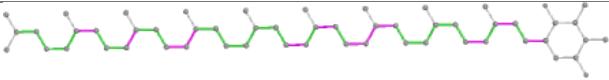
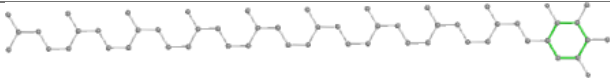




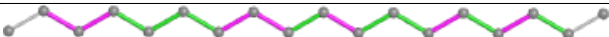
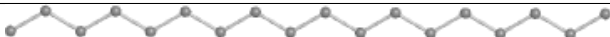
Ligand BCR b 616

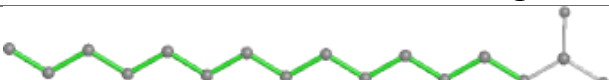
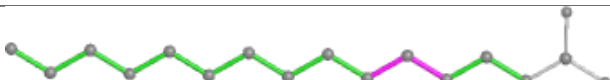
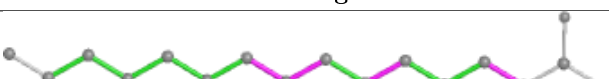
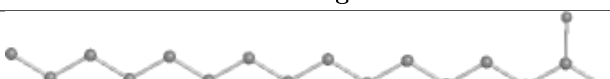


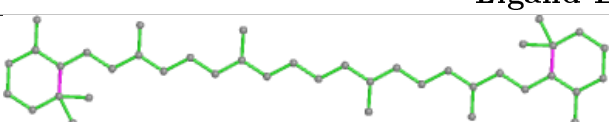

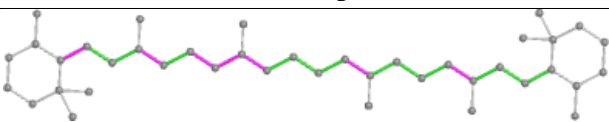
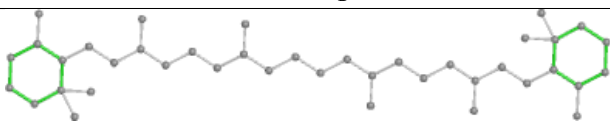


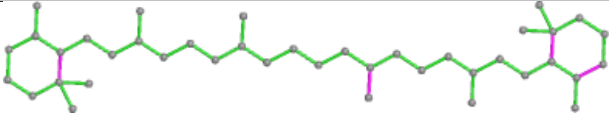
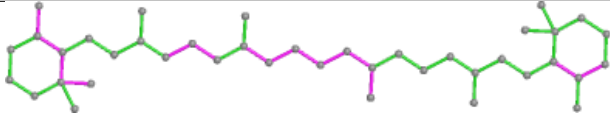
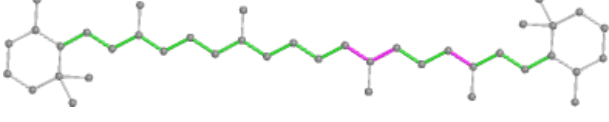
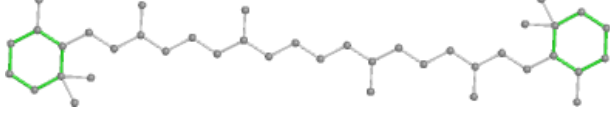
Ligand BCR c 517**Ligand CLA B 615****Ligand CLA b 601**

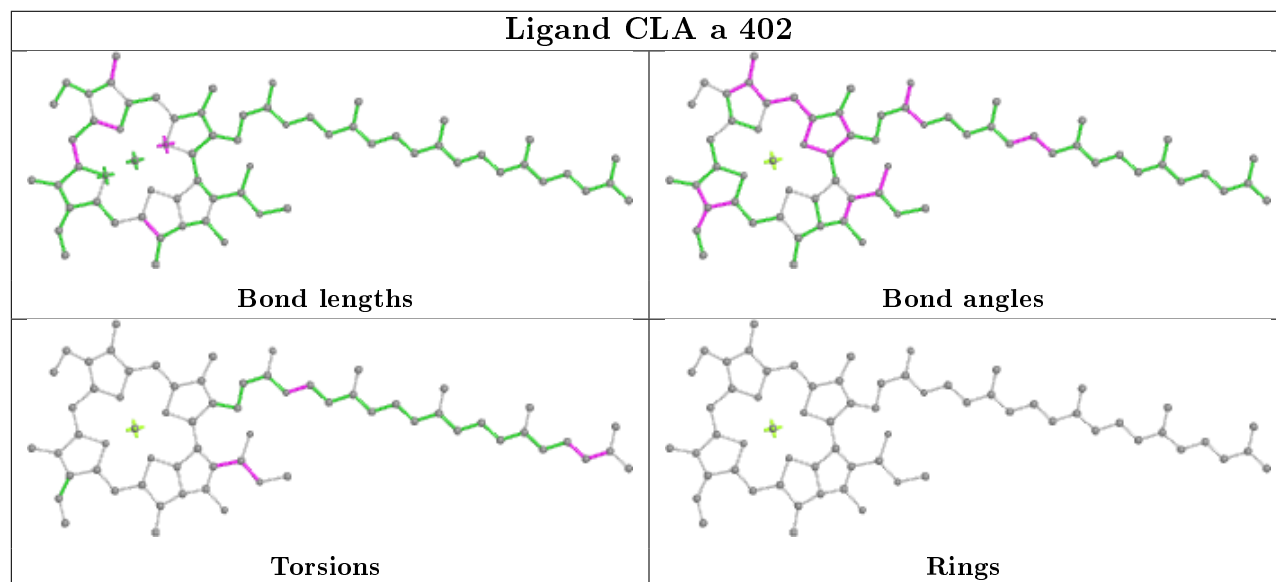
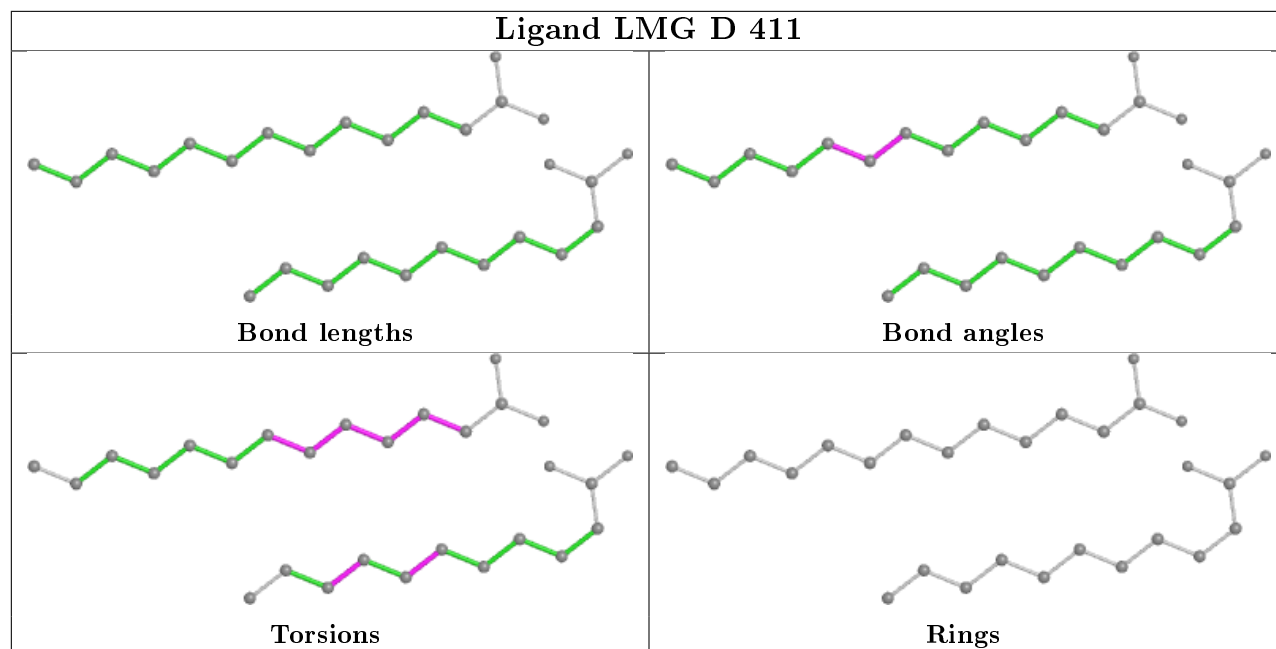
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 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand STE 1 102			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

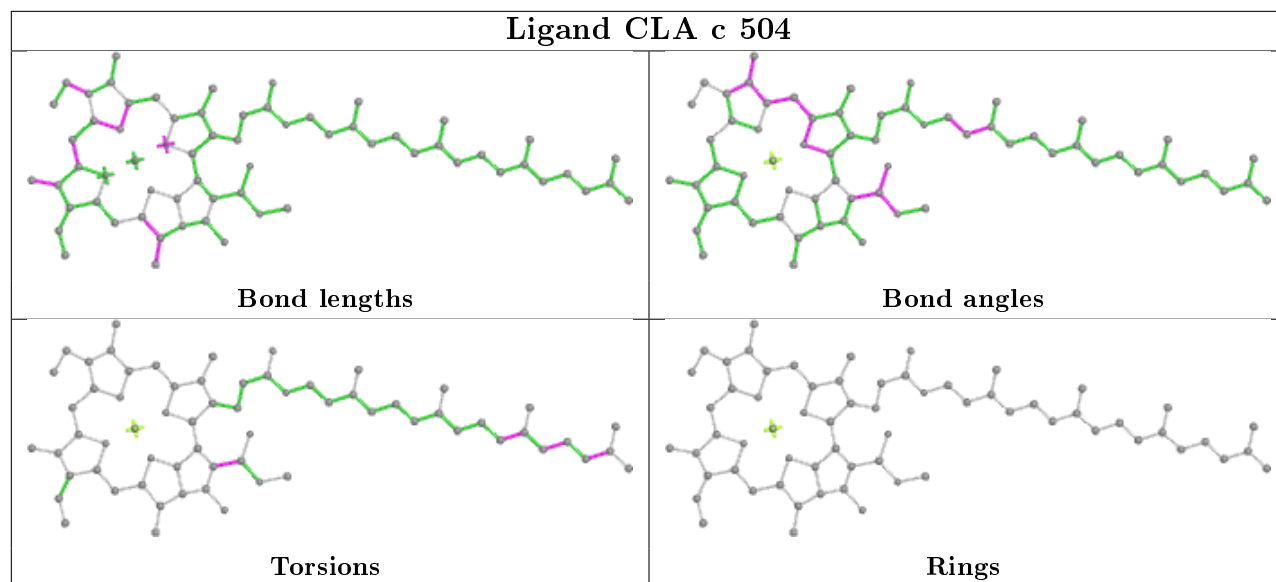
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 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand BCR B 618			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

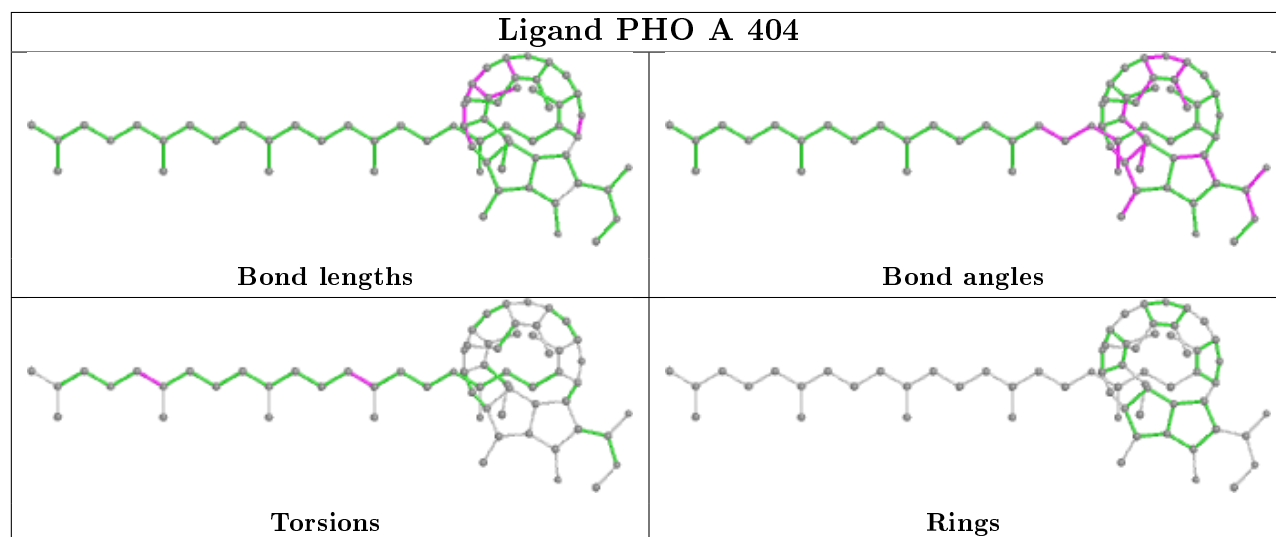
Ligand BCR C 515			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

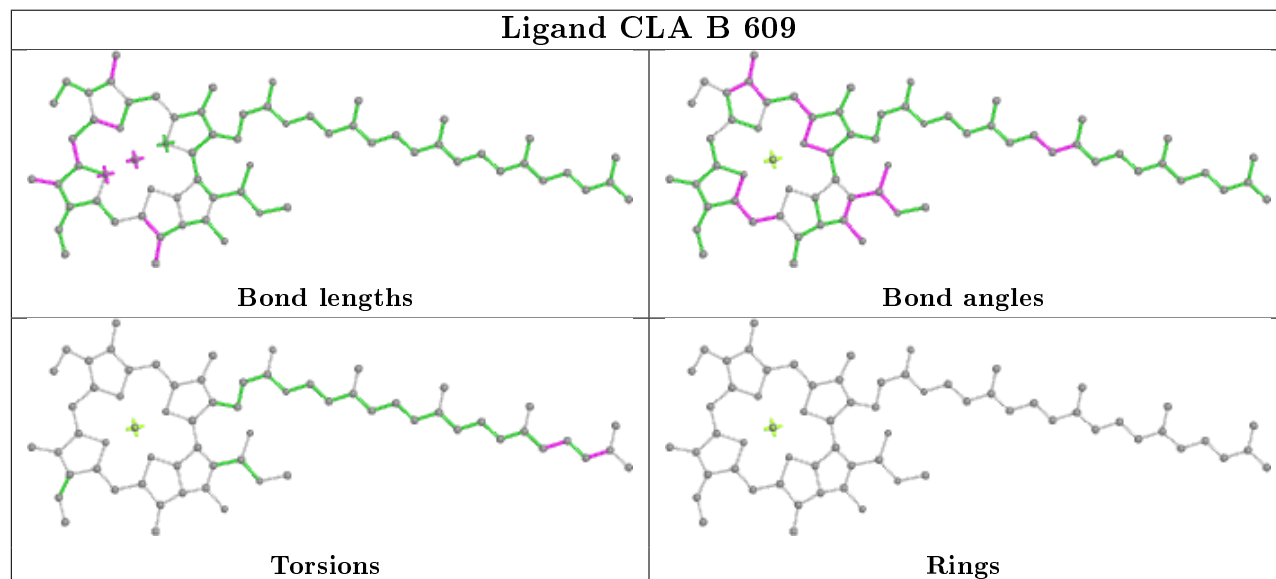
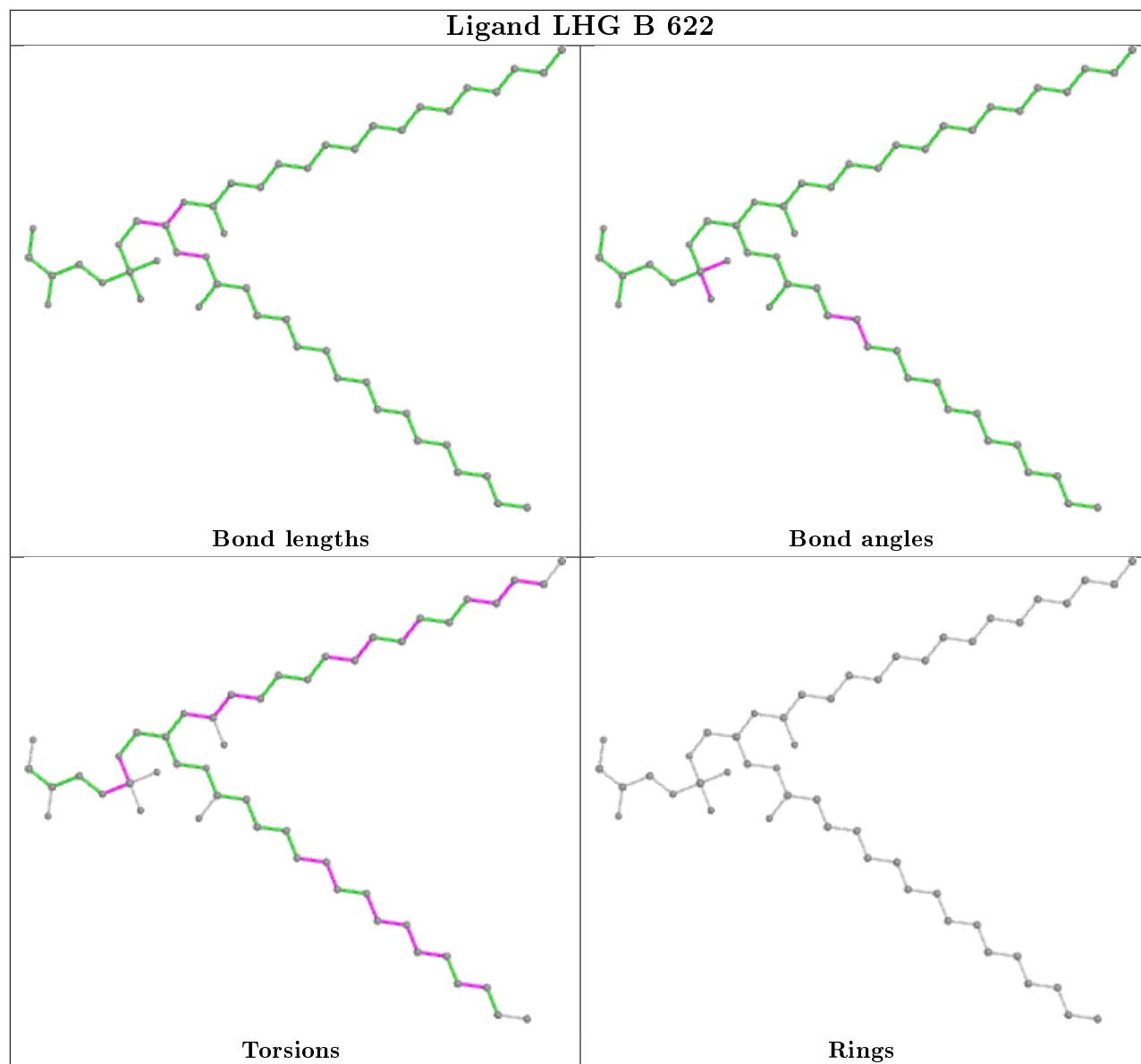


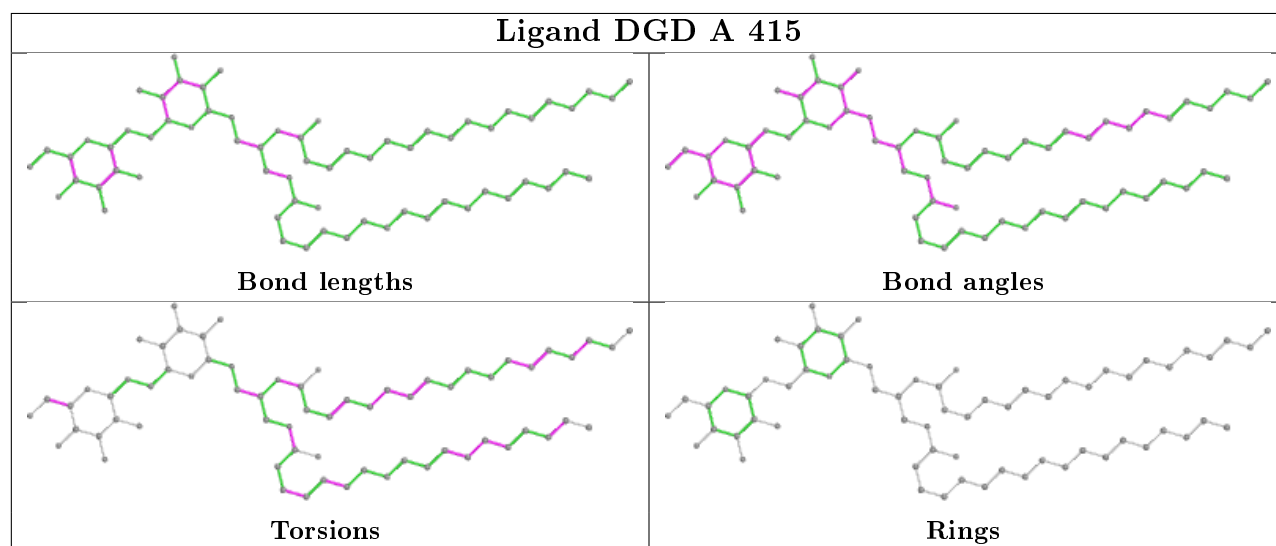
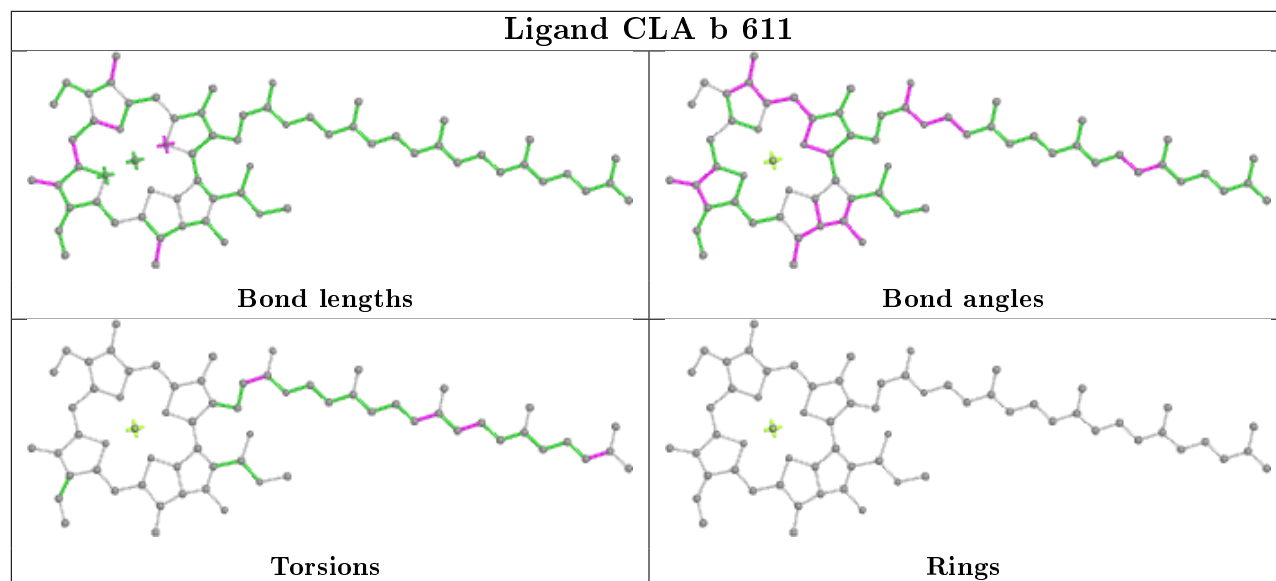
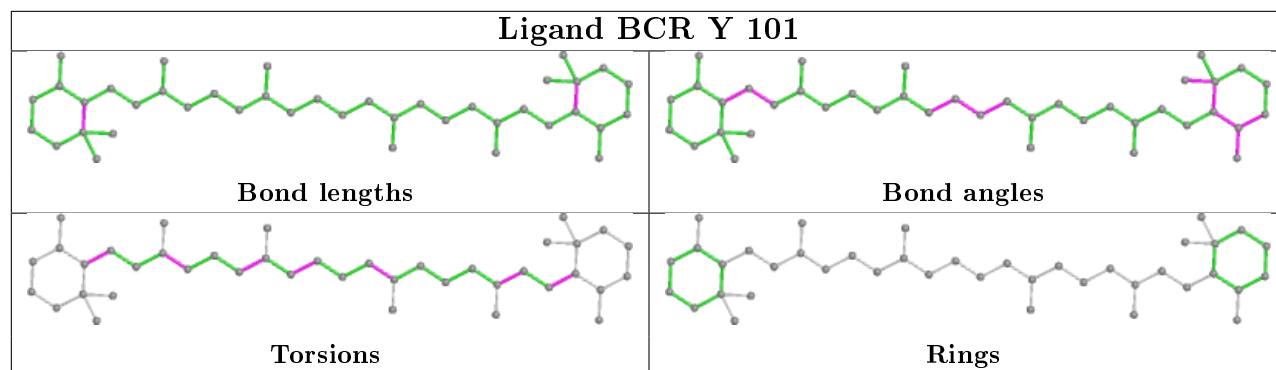
Ligand CLA c 504

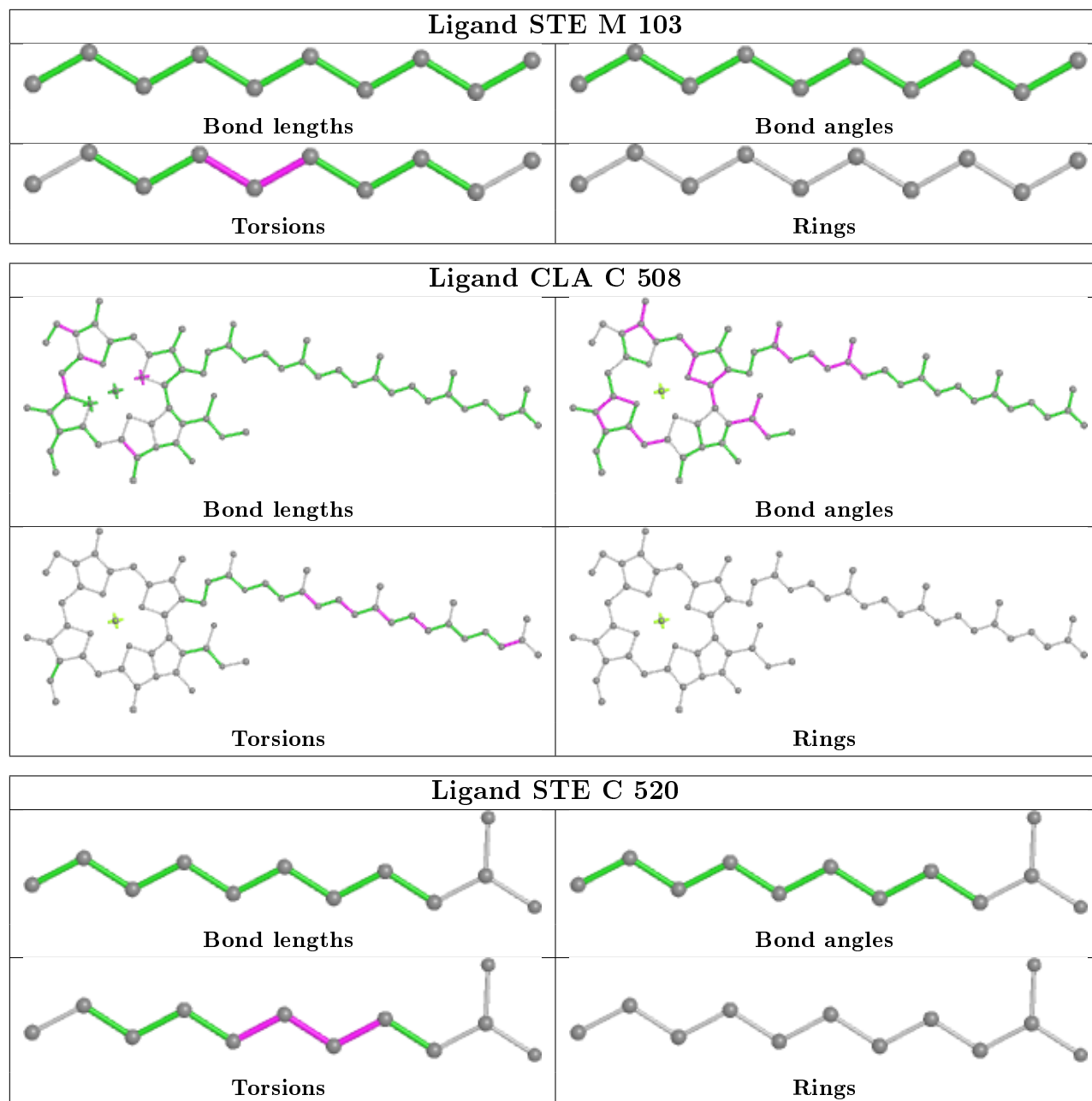


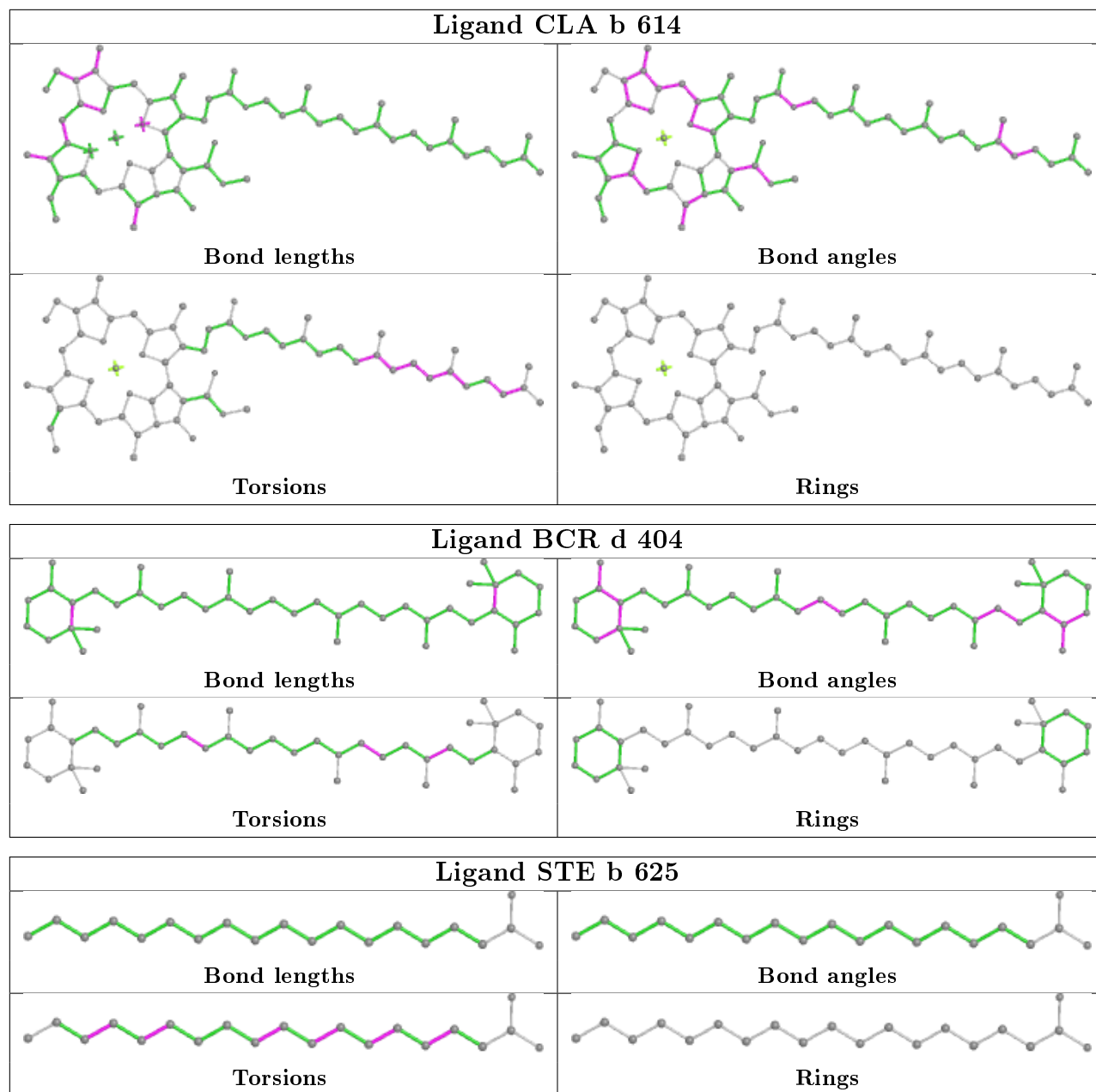
Ligand PHO A 404



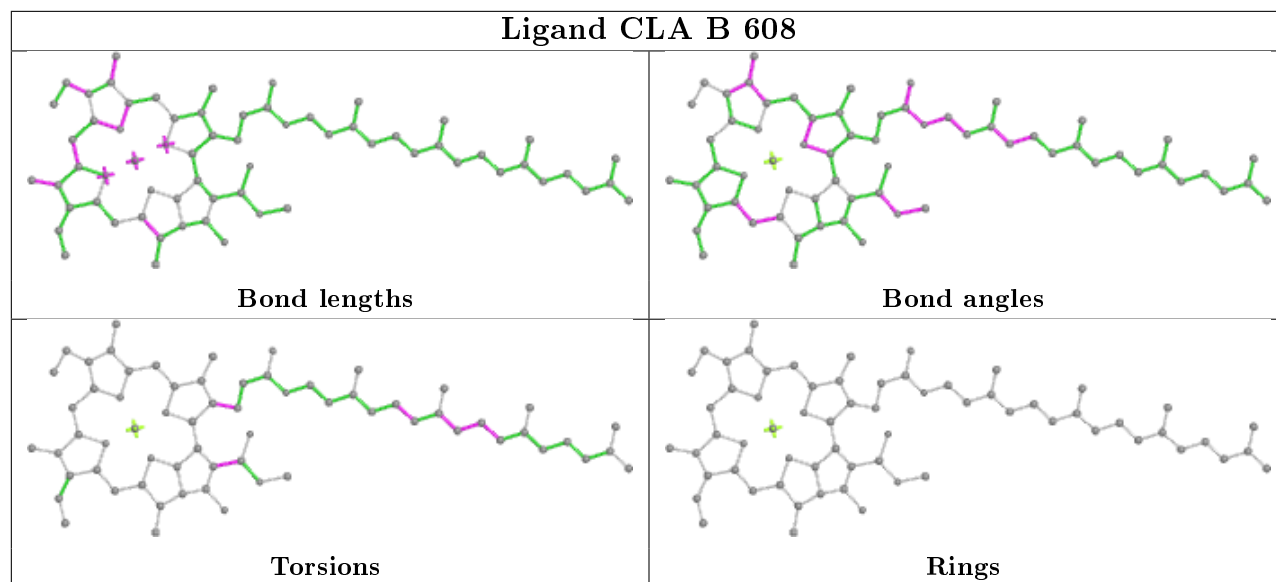




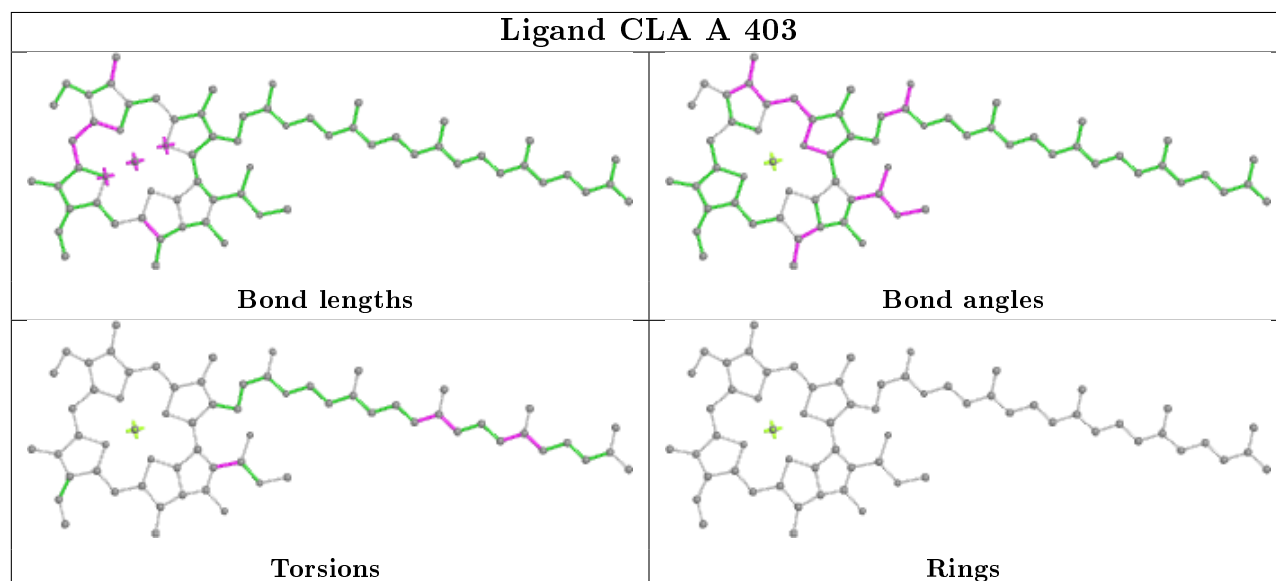




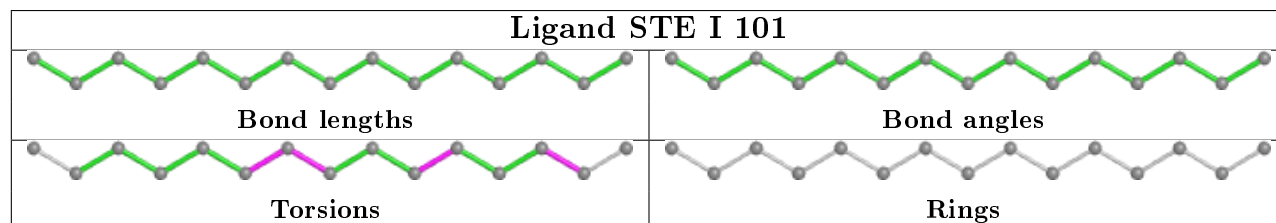
Ligand CLA B 608



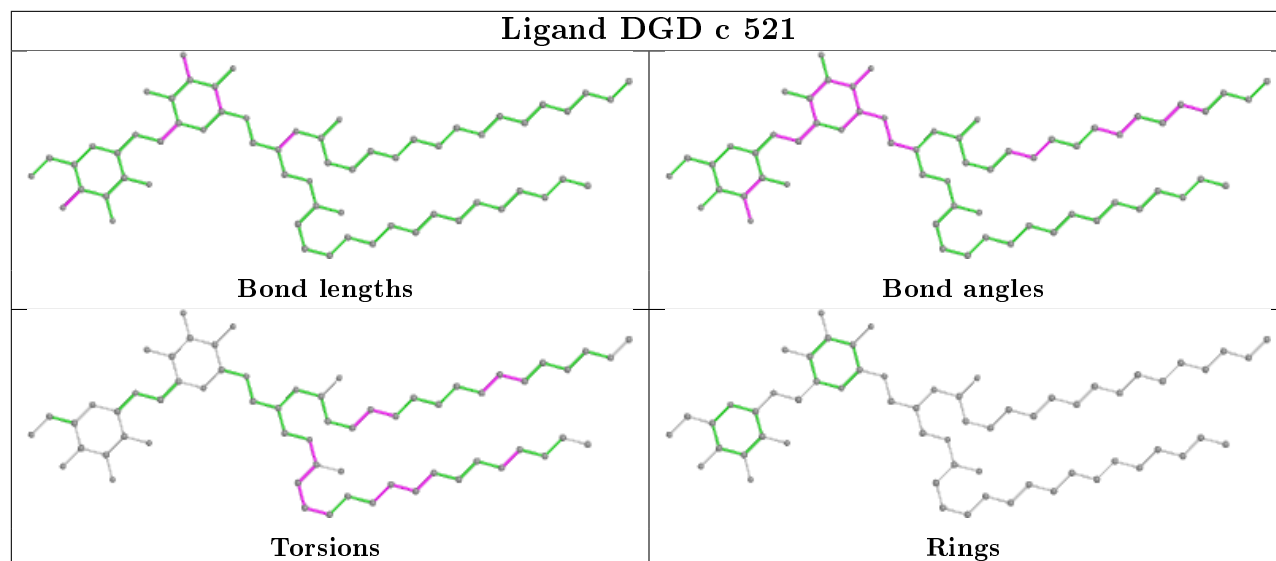
Ligand CLA A 403



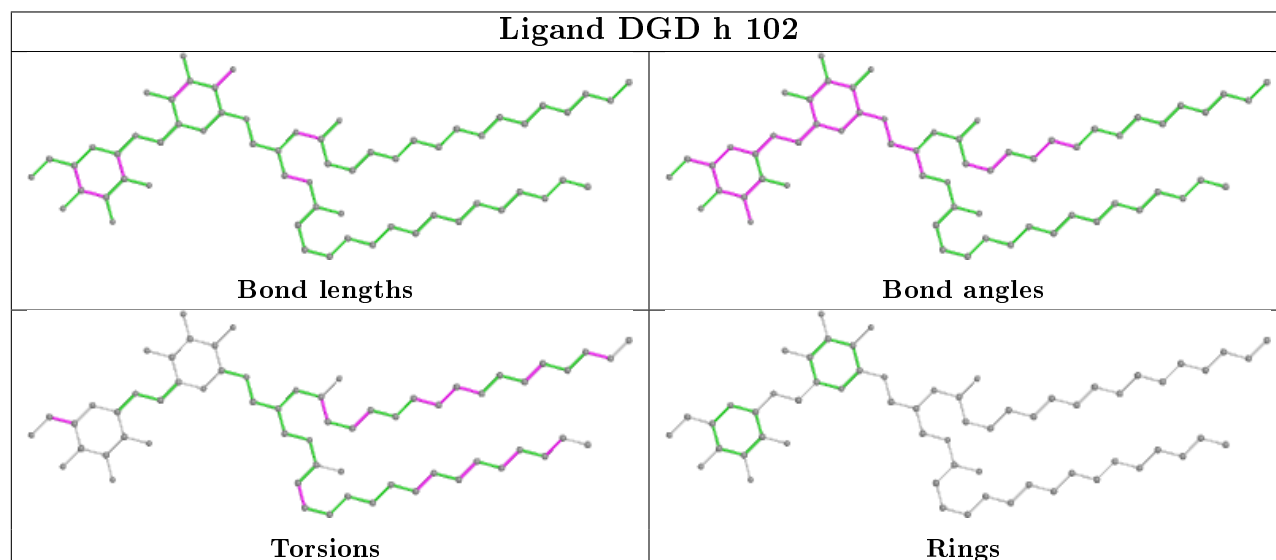
Ligand STE I 101



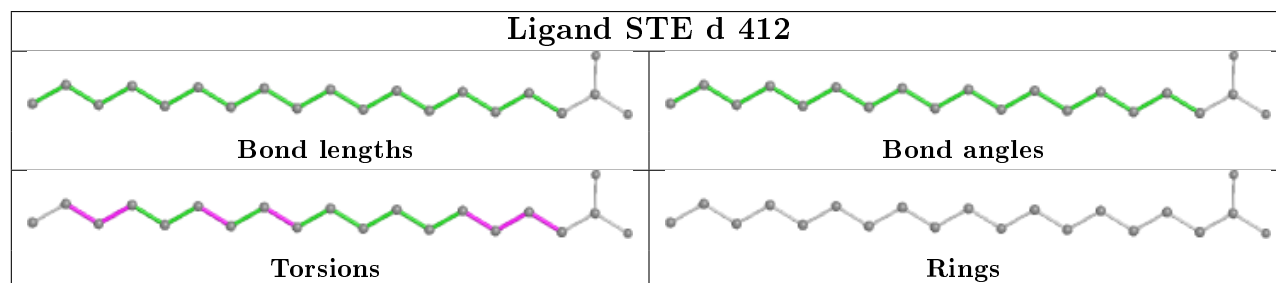
Ligand DGD c 521



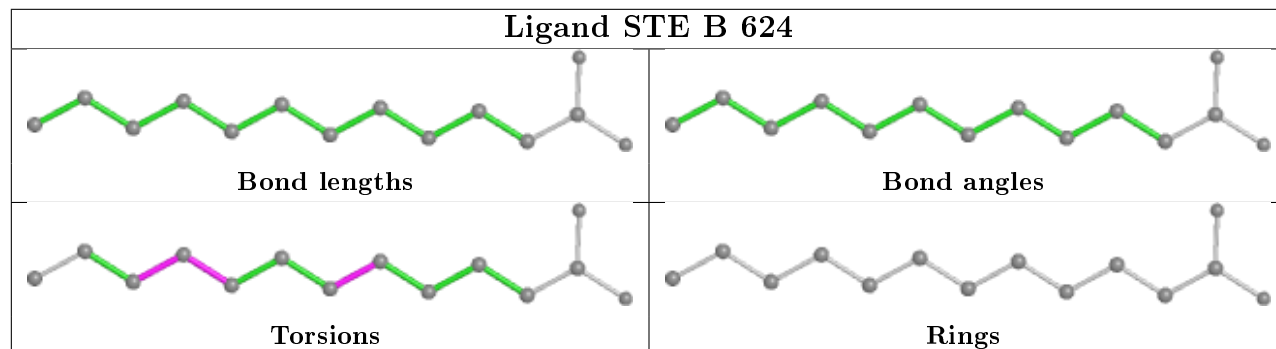
Ligand DGD h 102

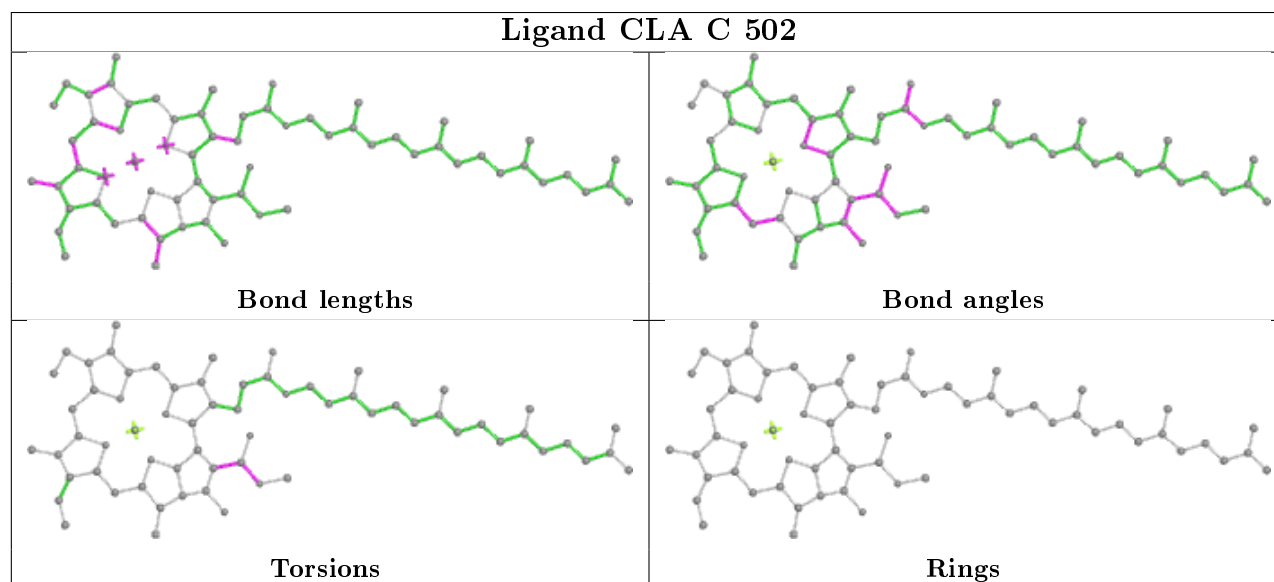
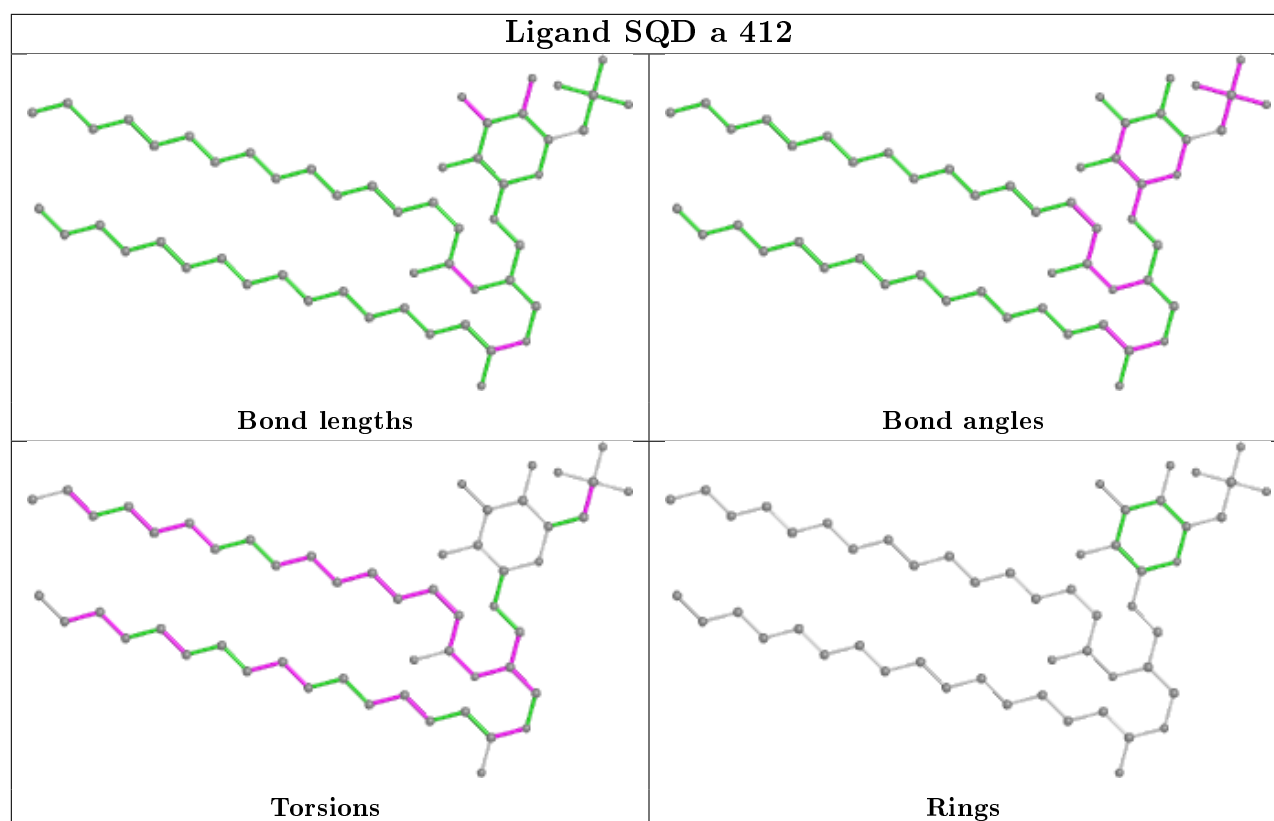


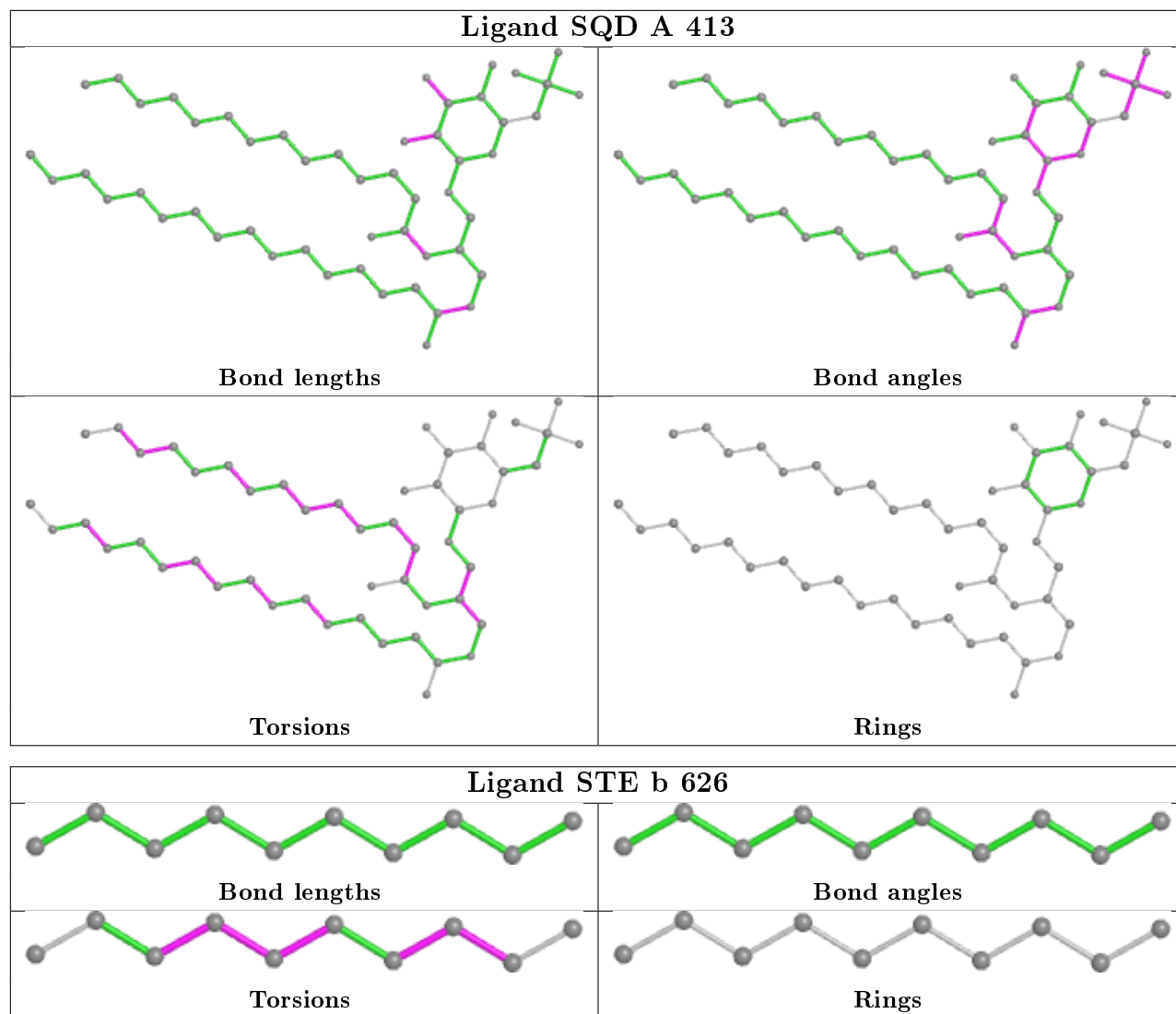
Ligand STE d 412

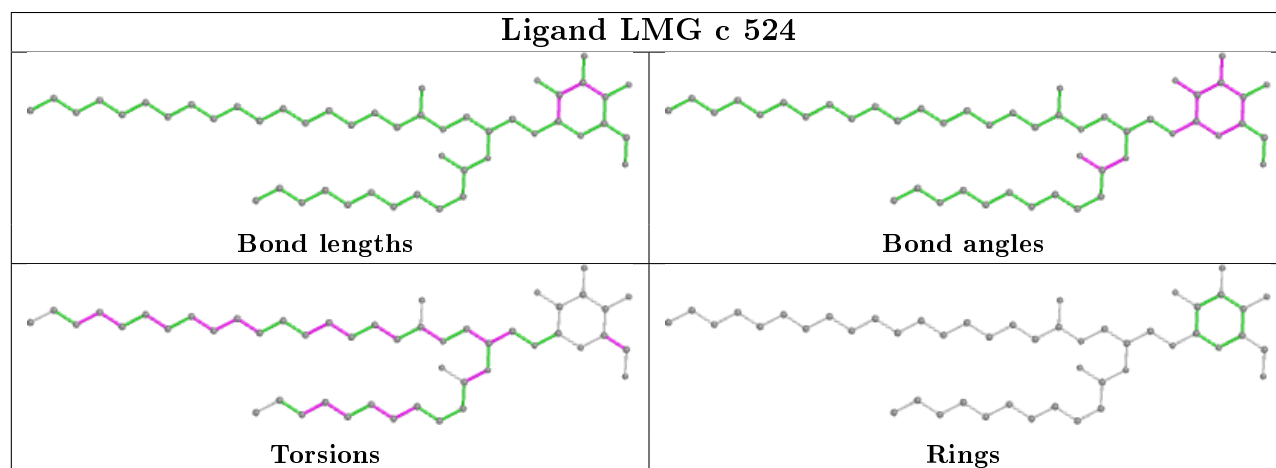
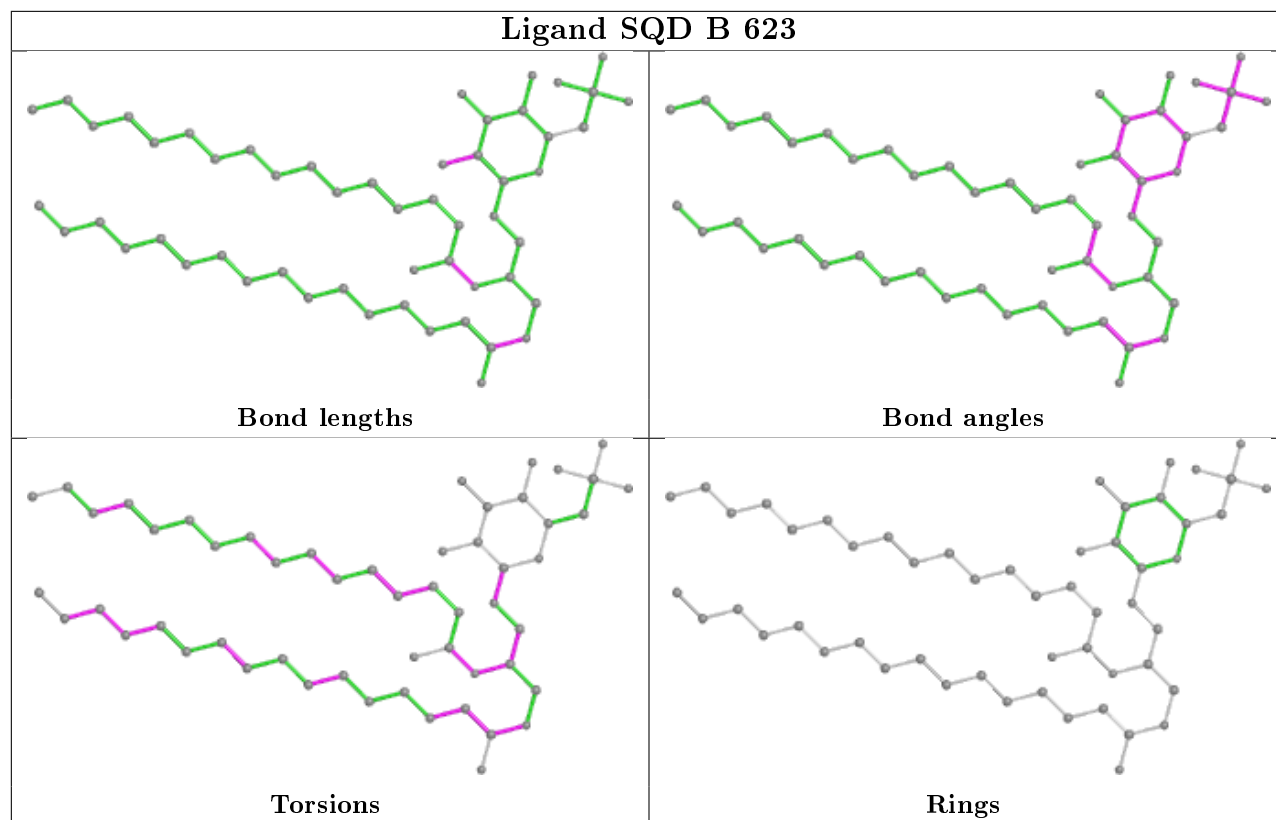


Ligand STE B 624

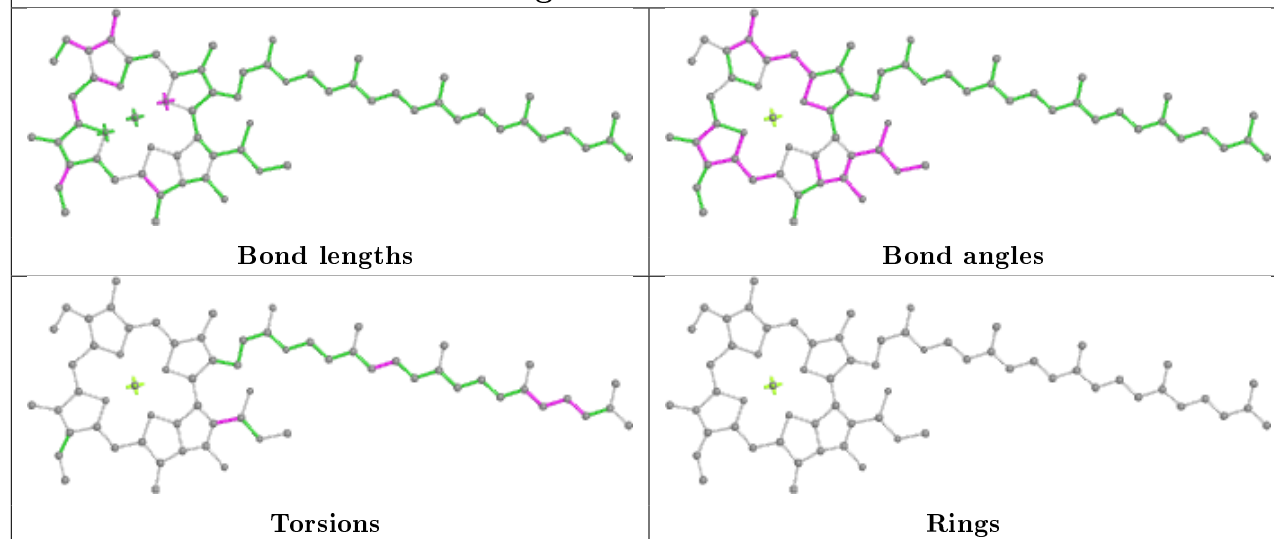




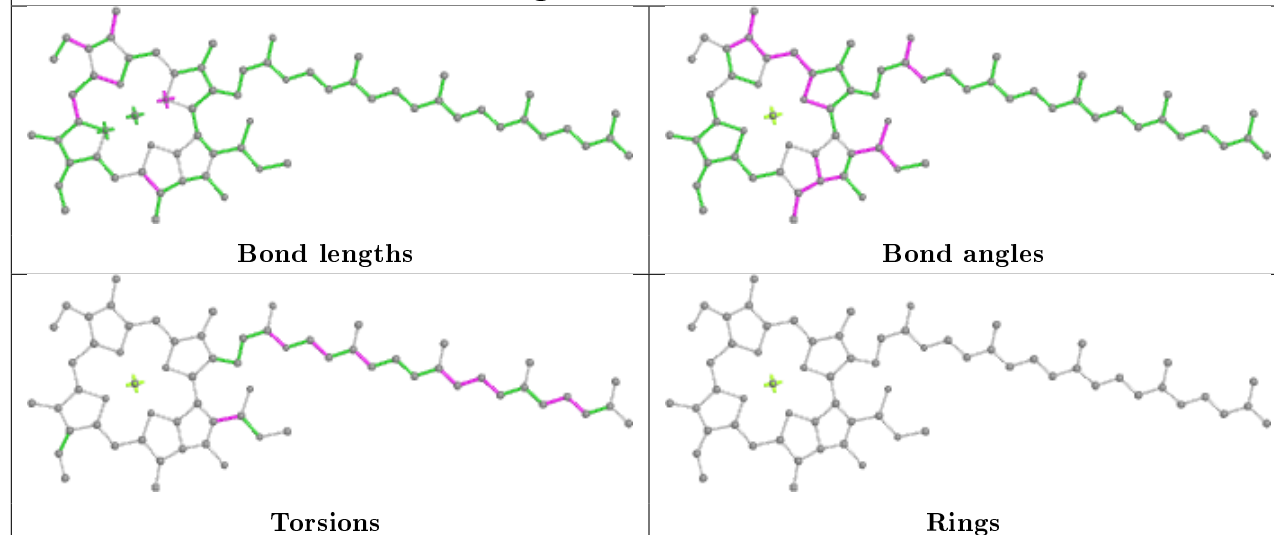




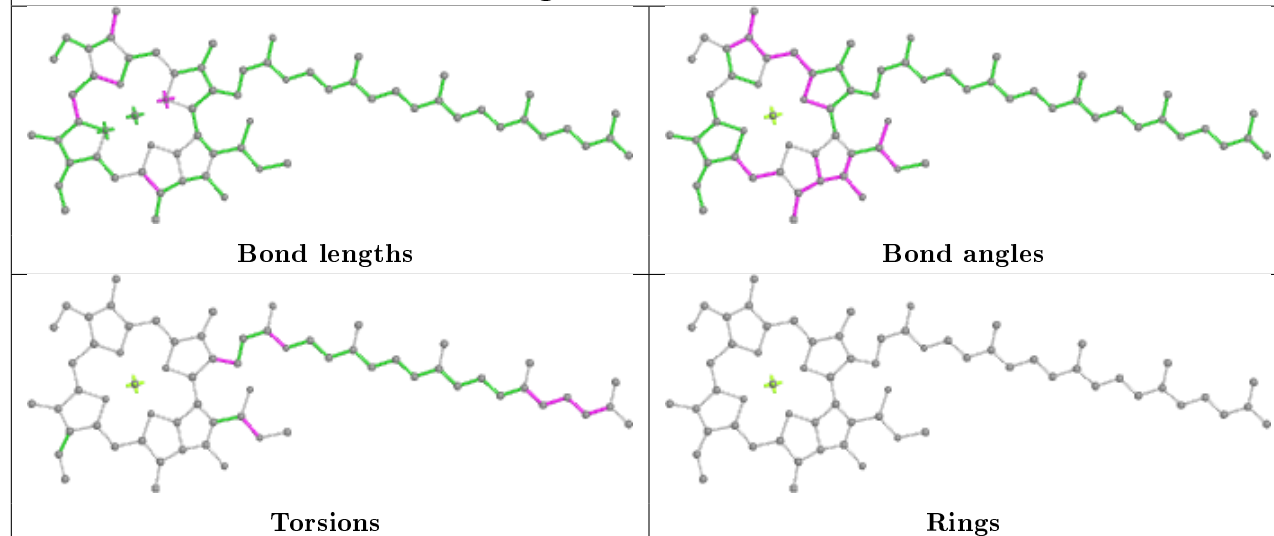
Ligand CLA b 608

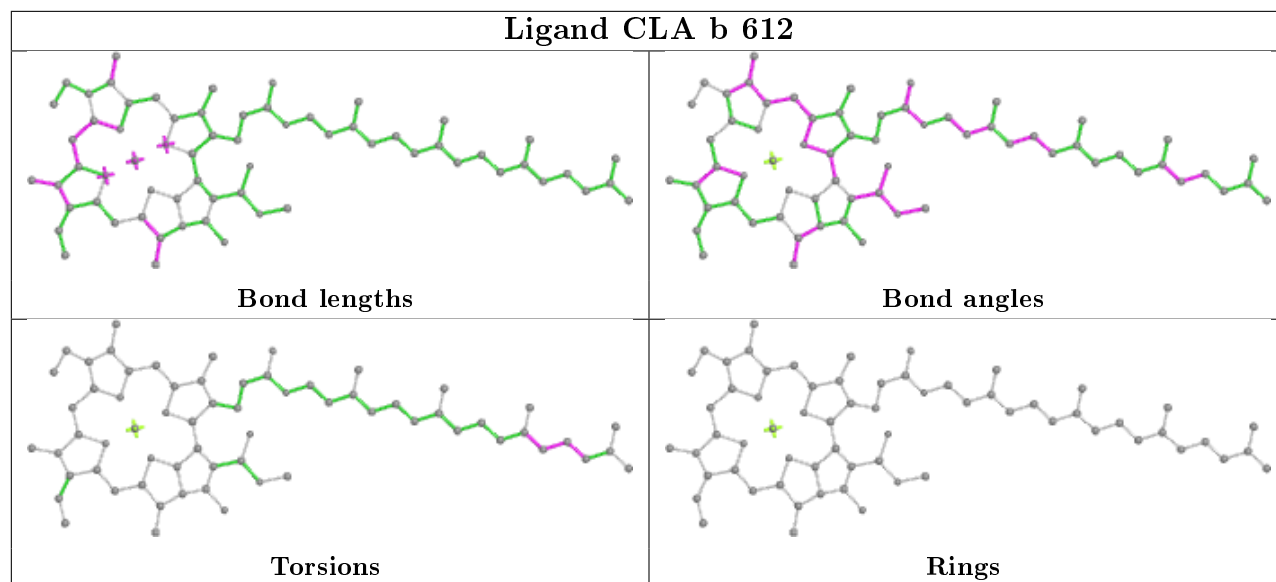
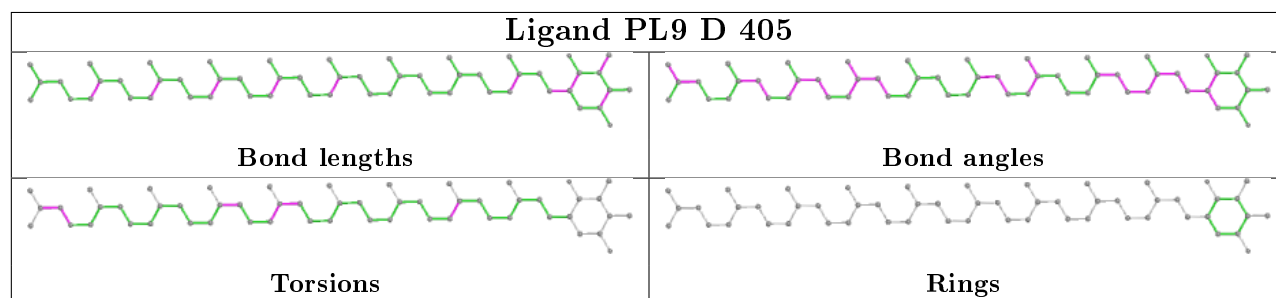
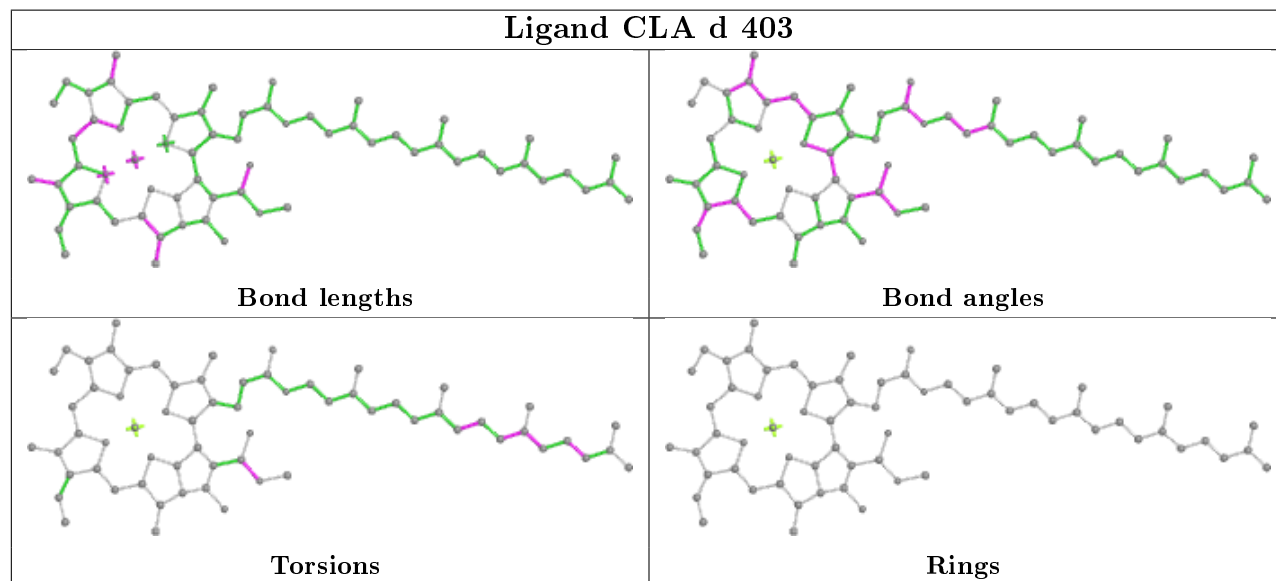


Ligand CLA C 514

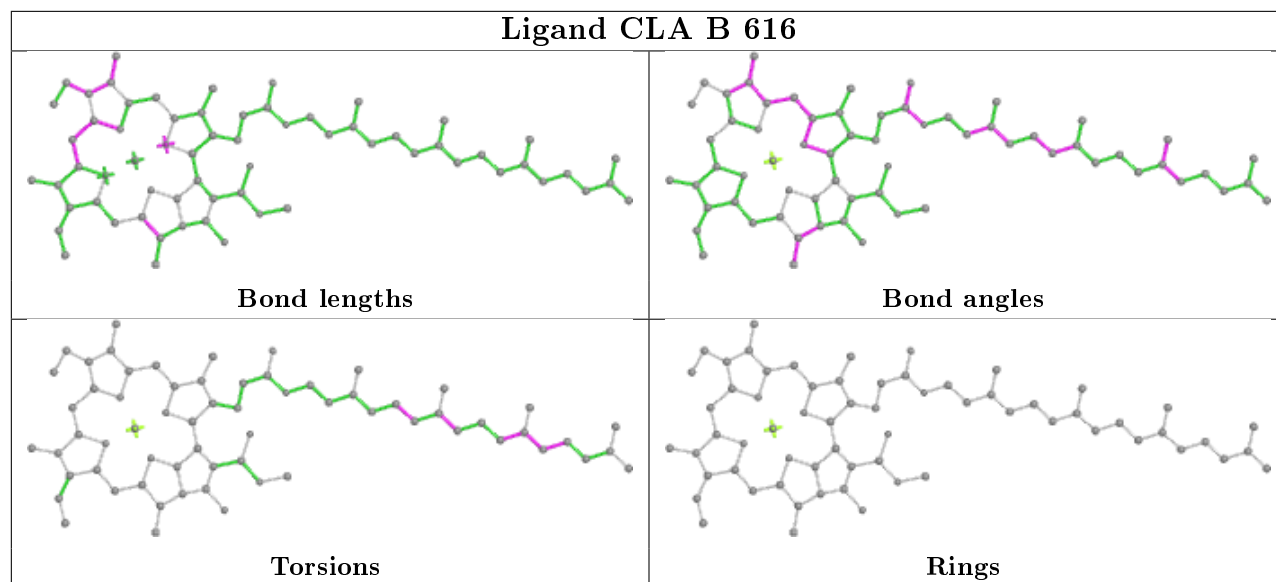


Ligand CLA c 513

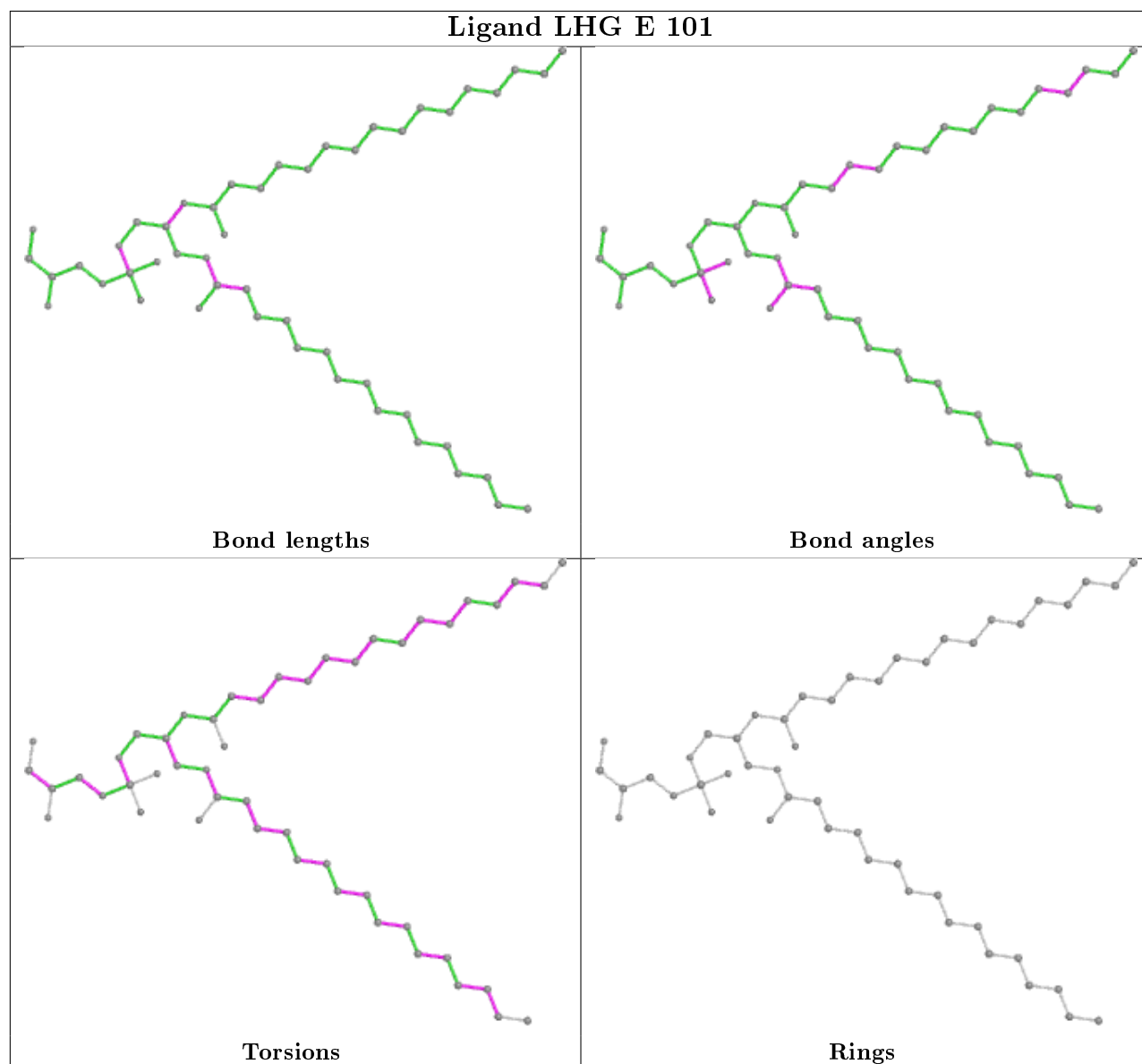


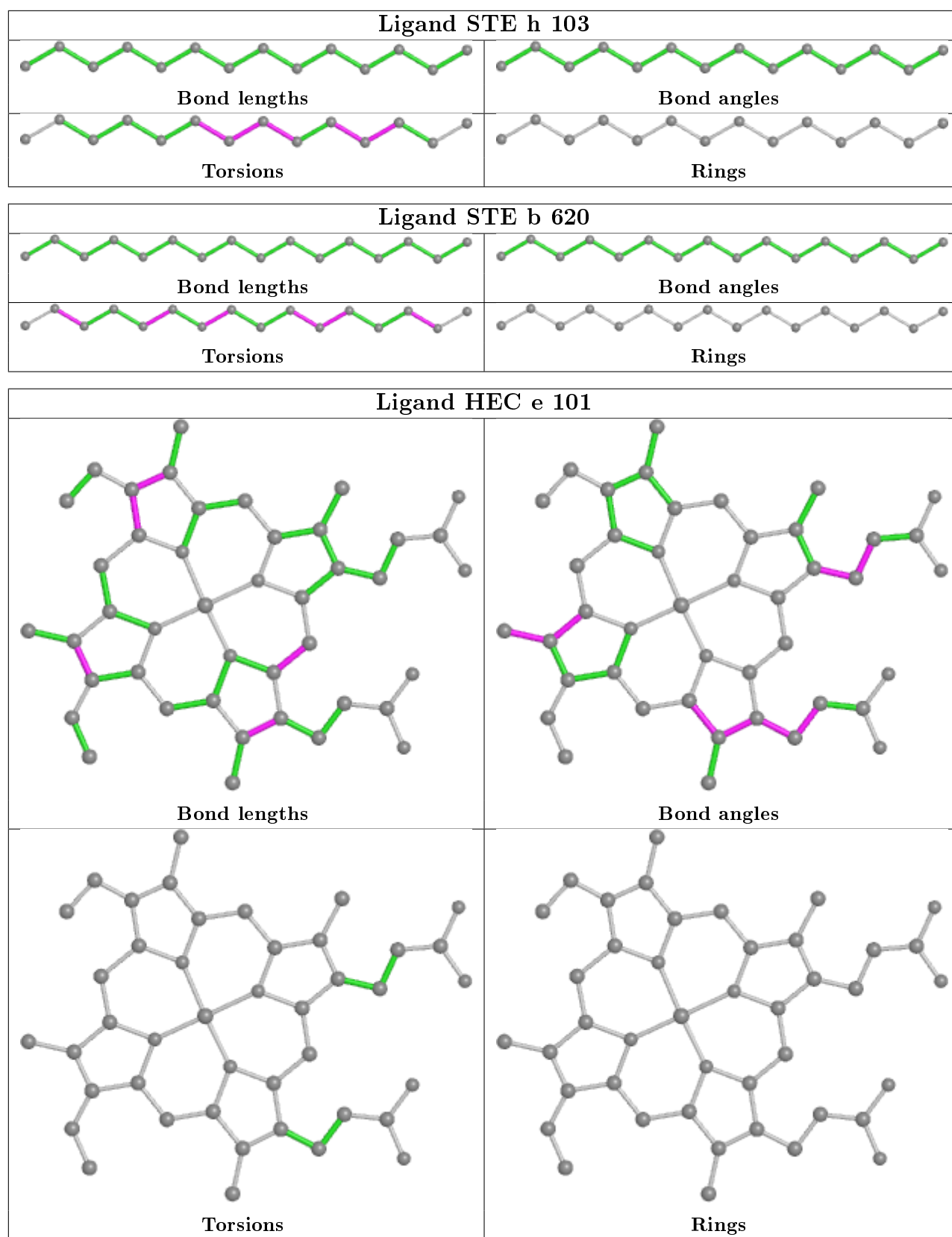
Ligand CLA b 612**Ligand PL9 D 405****Ligand CLA d 403**

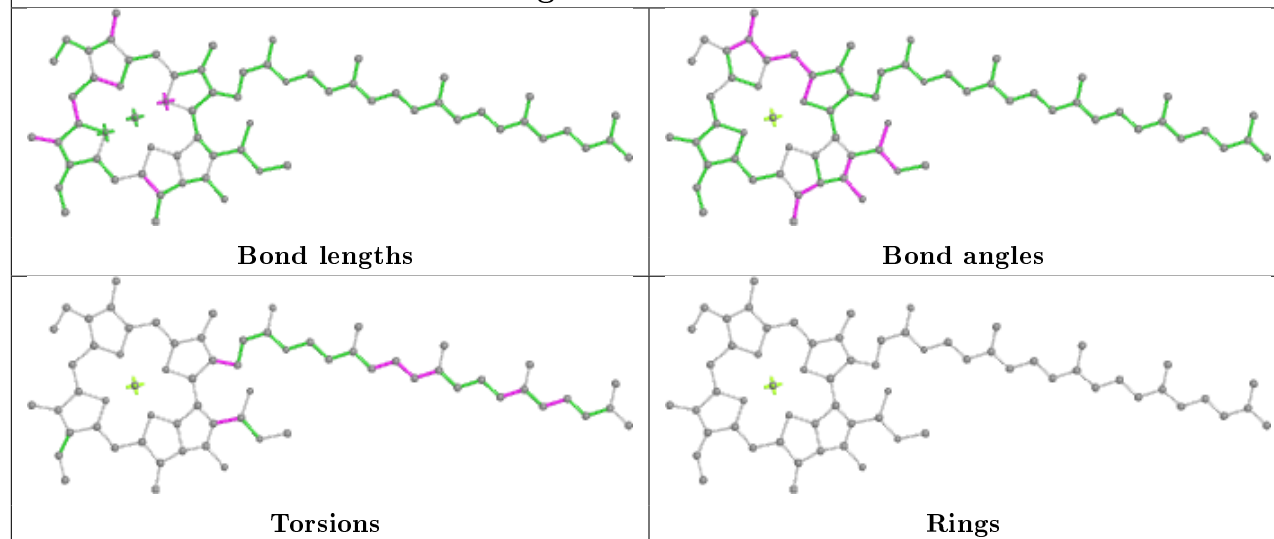
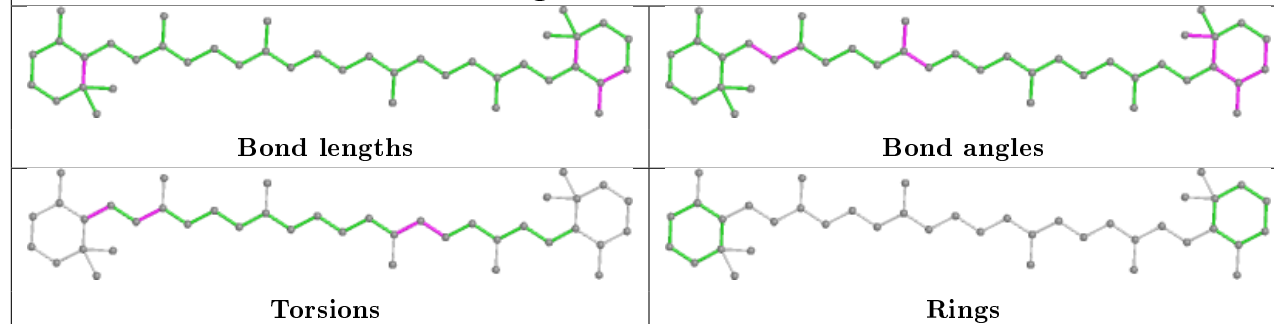
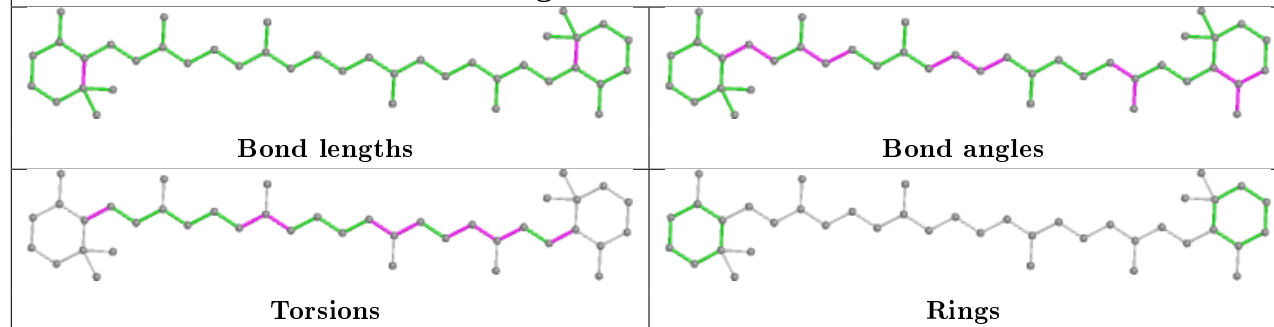
Ligand CLA B 616



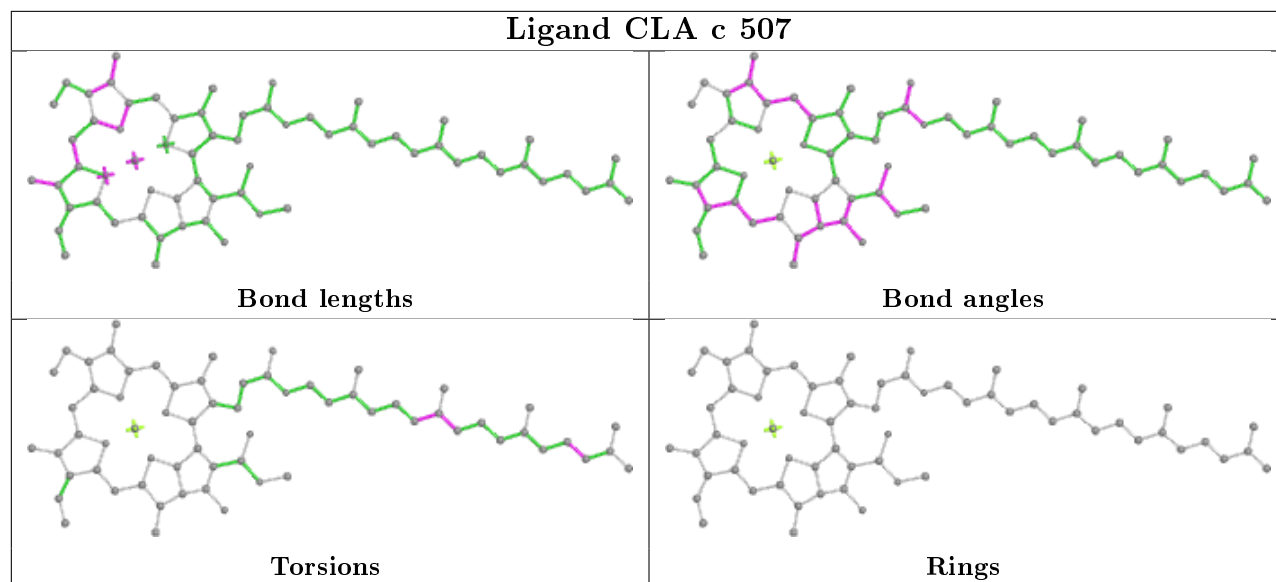
Ligand LHG E 101



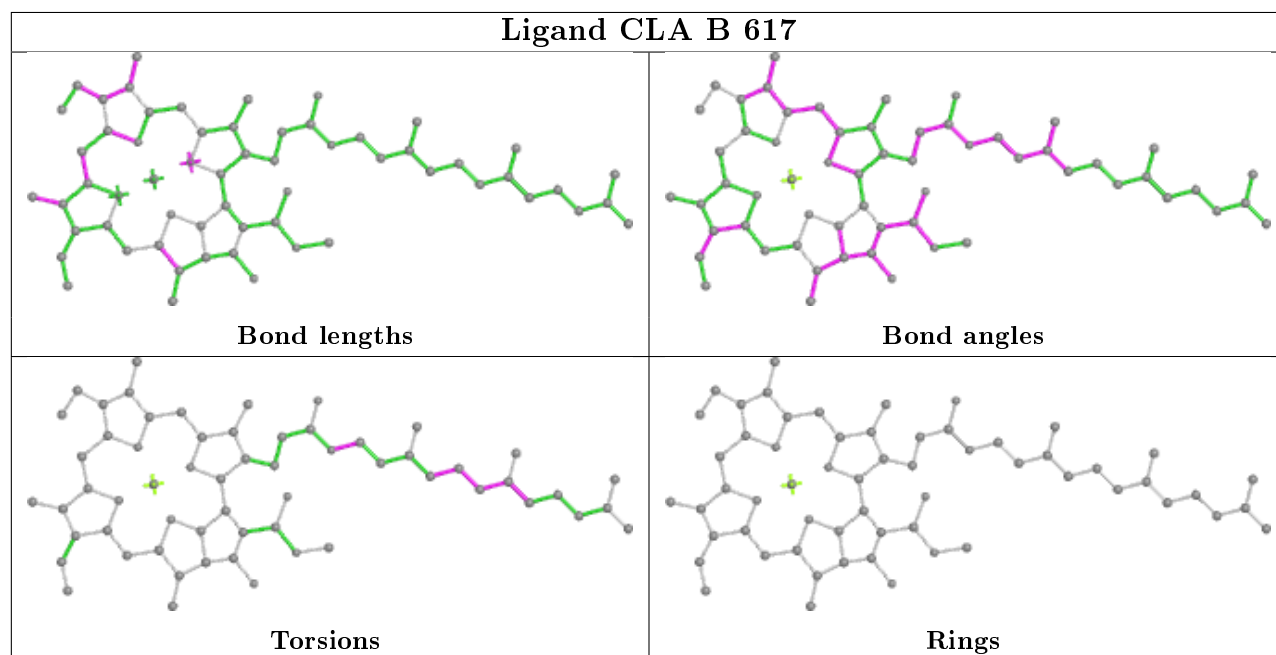


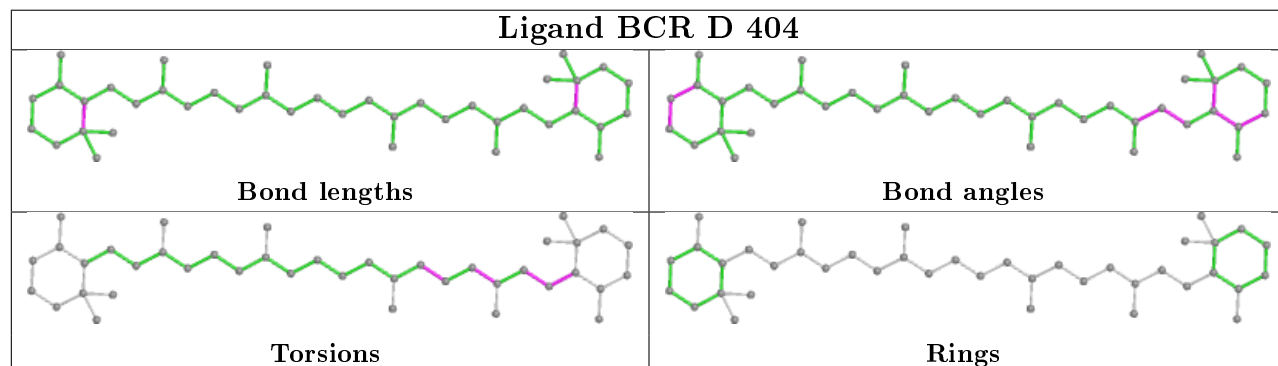
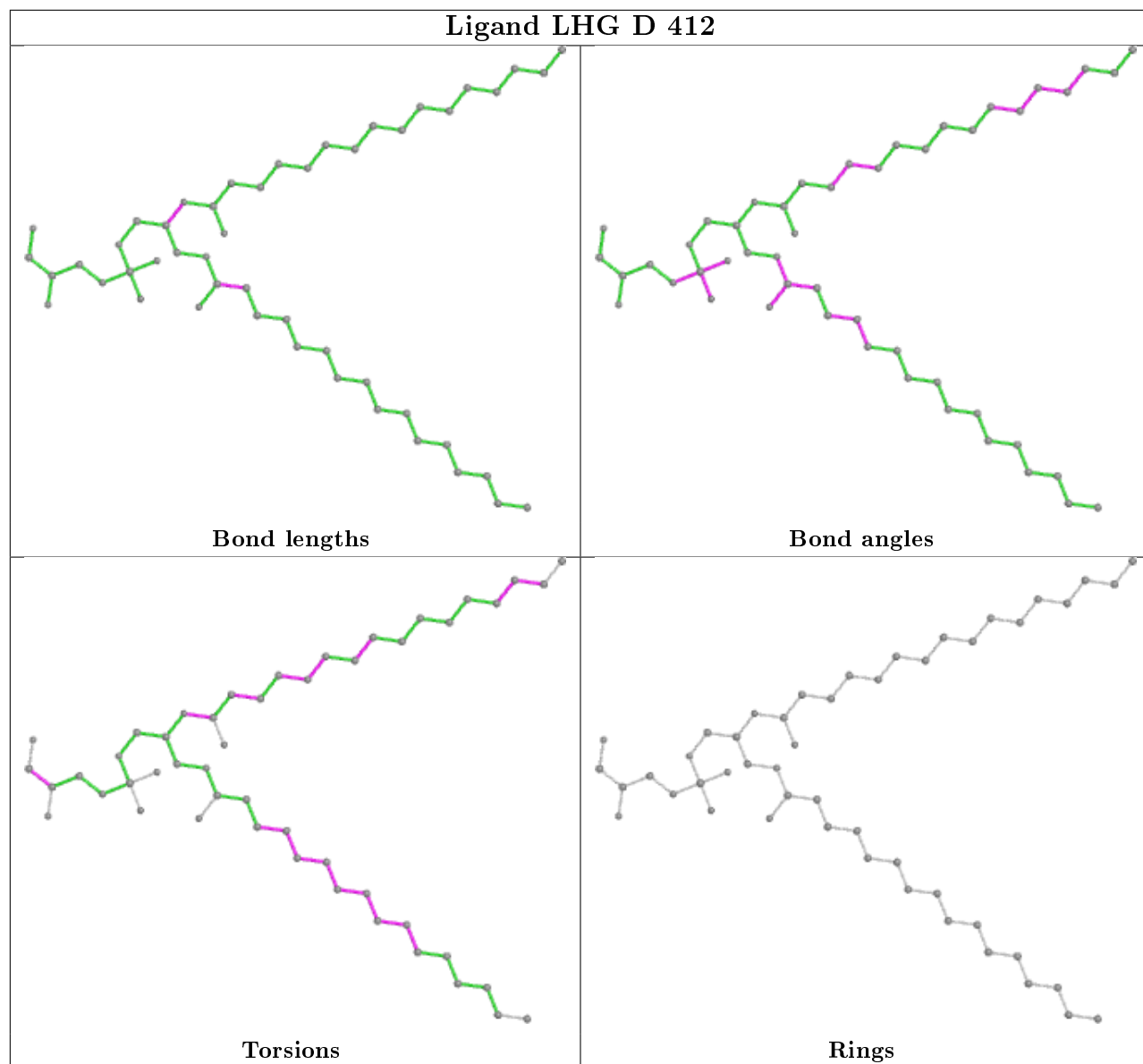
Ligand CLA c 515**Ligand BCR T 101****Ligand BCR c 518**

Ligand CLA c 507

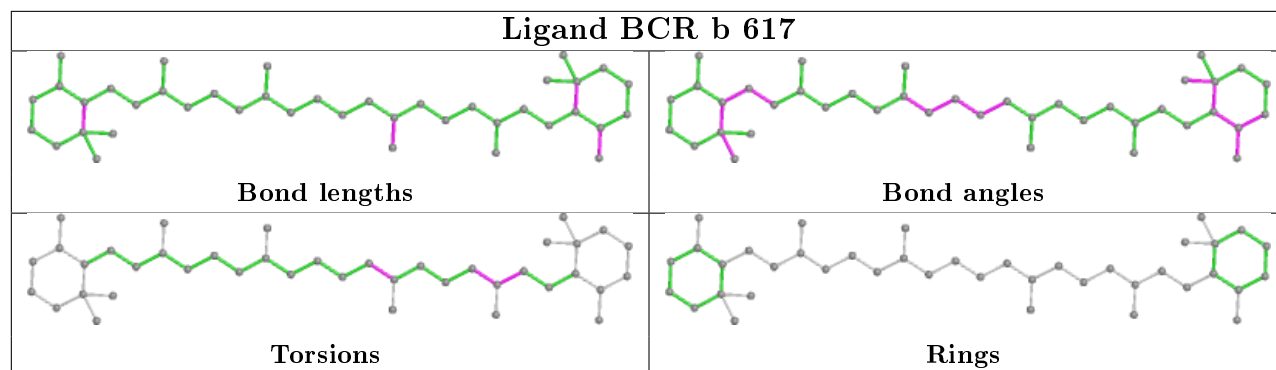


Ligand CLA B 617

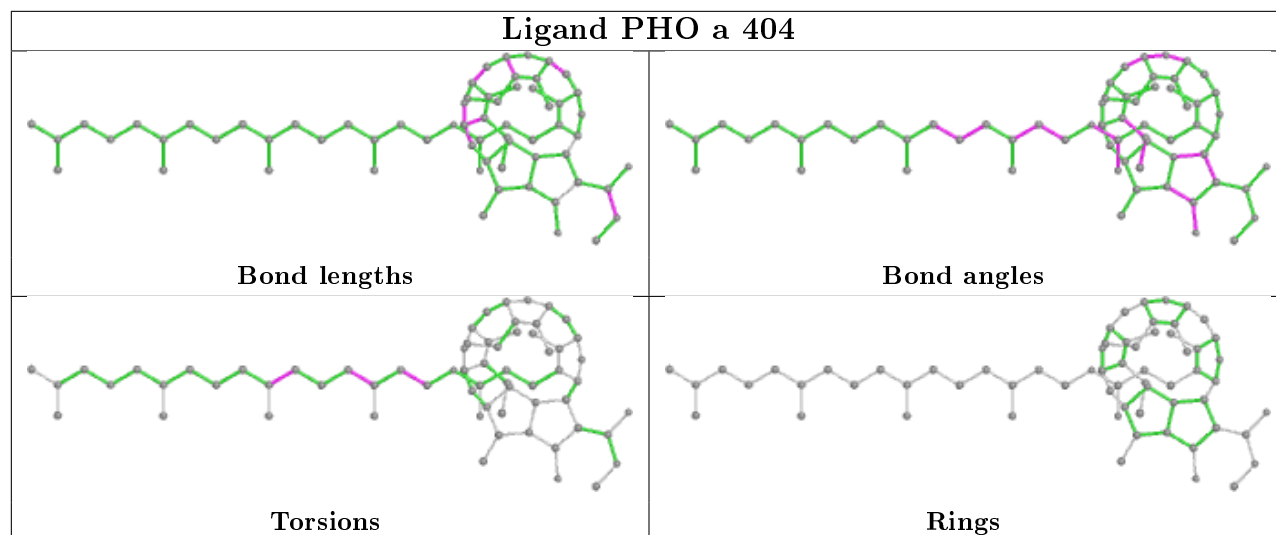




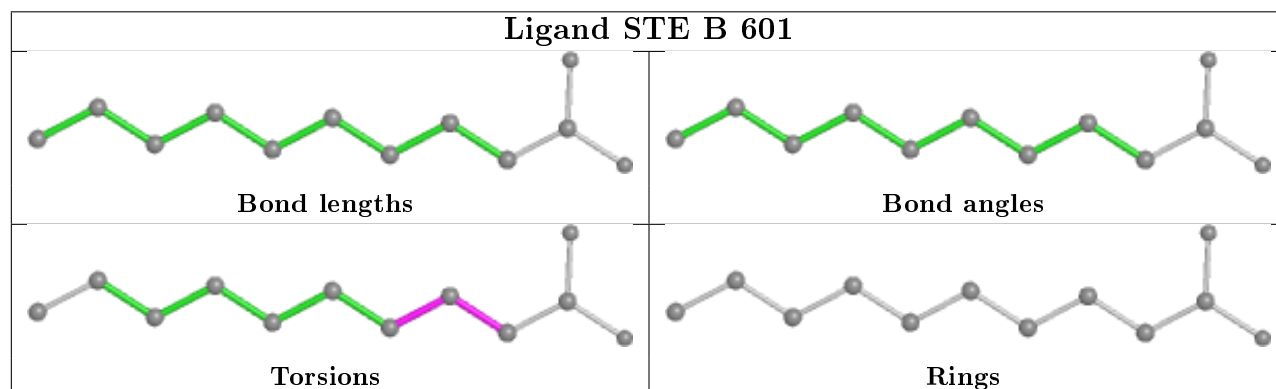
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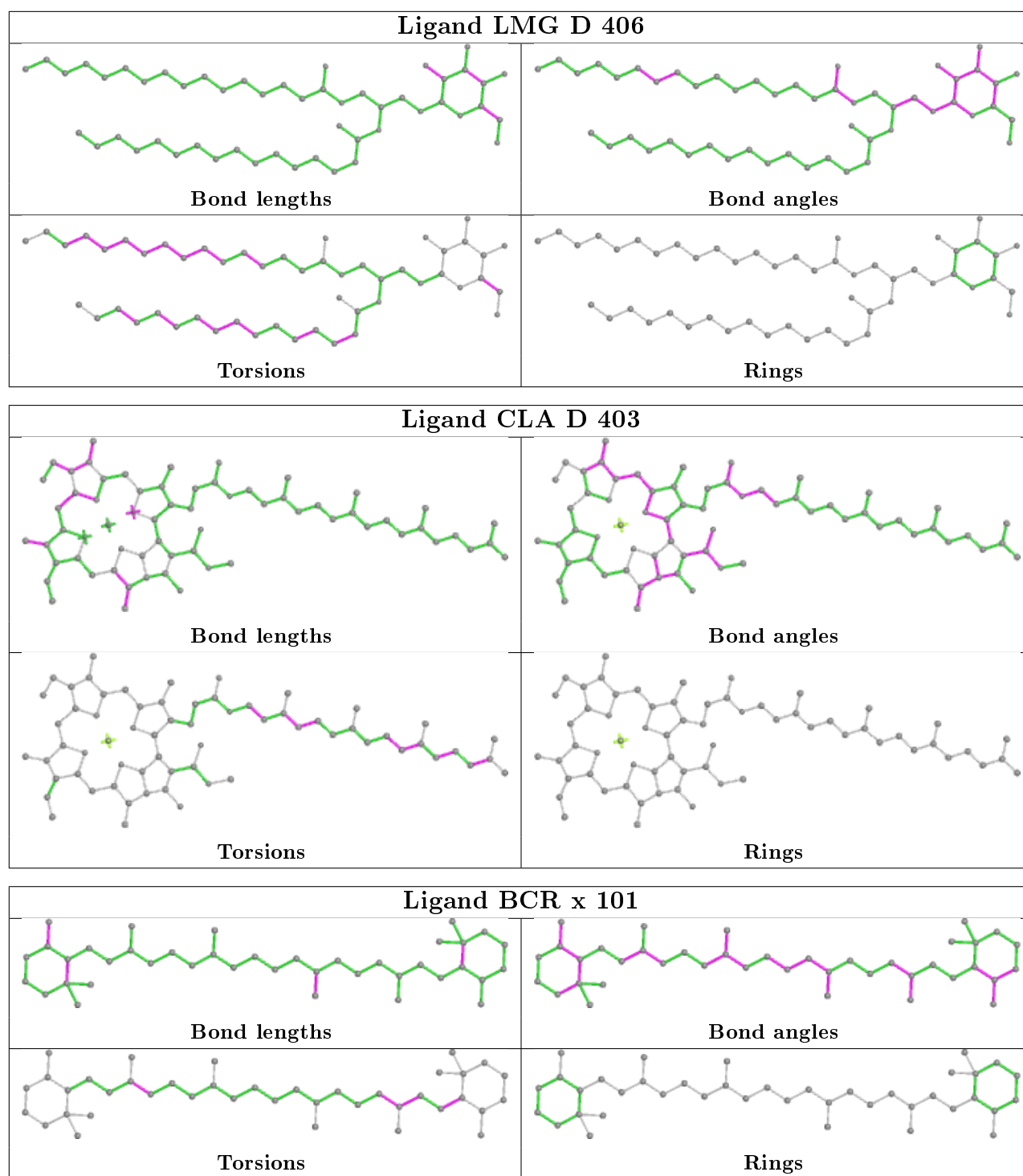


Ligand PHO a 404

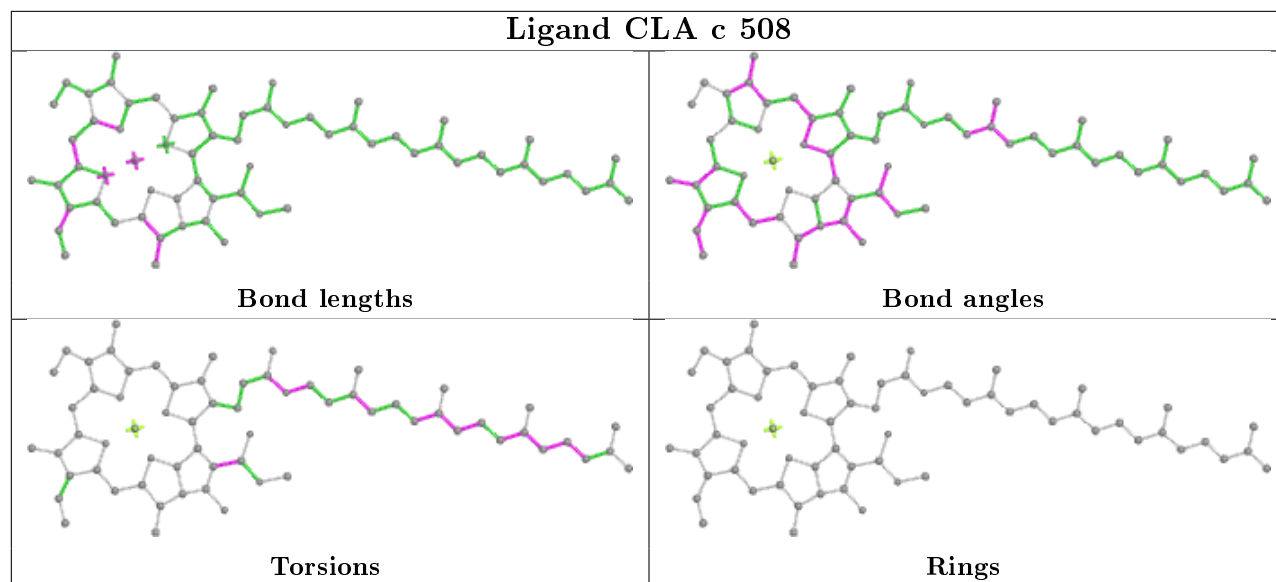


Ligand STE B 601

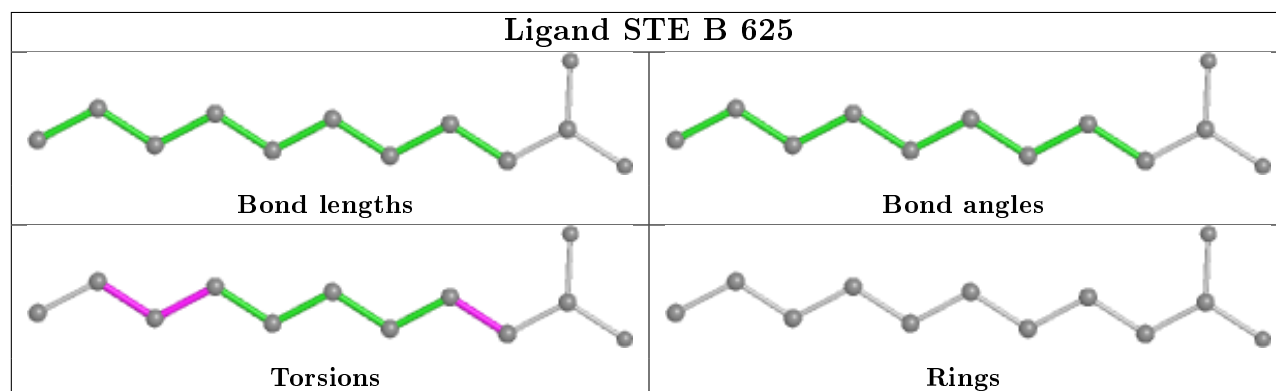




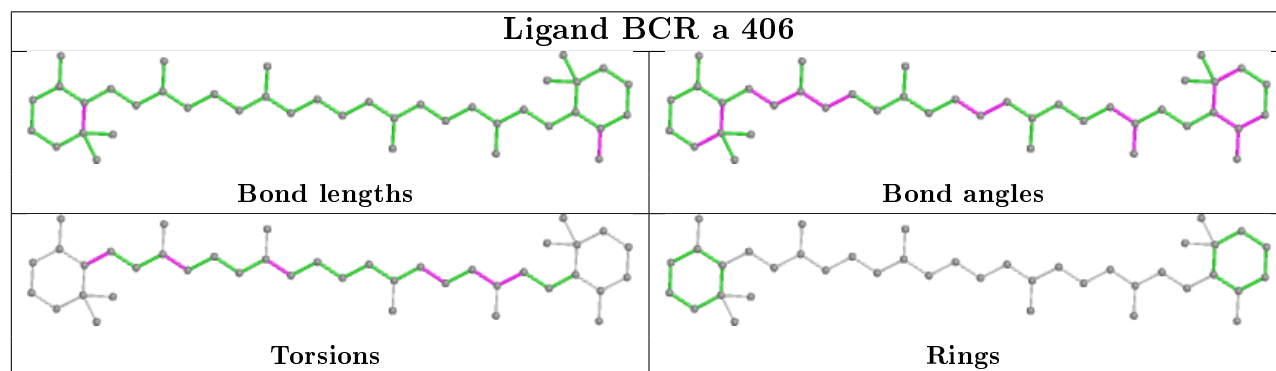
Ligand CLA c 508



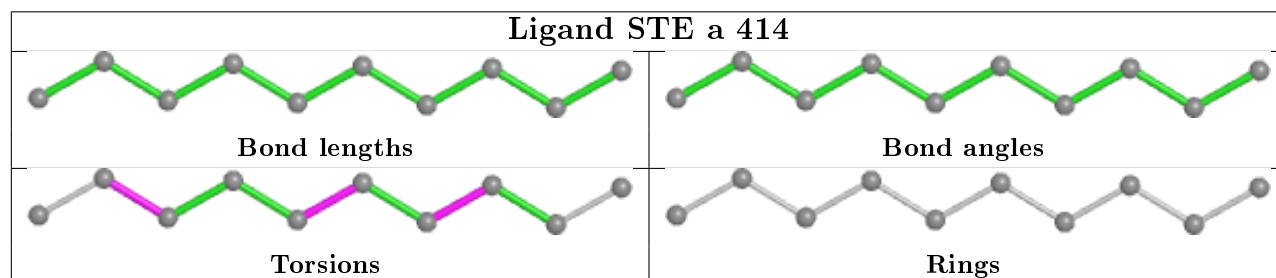
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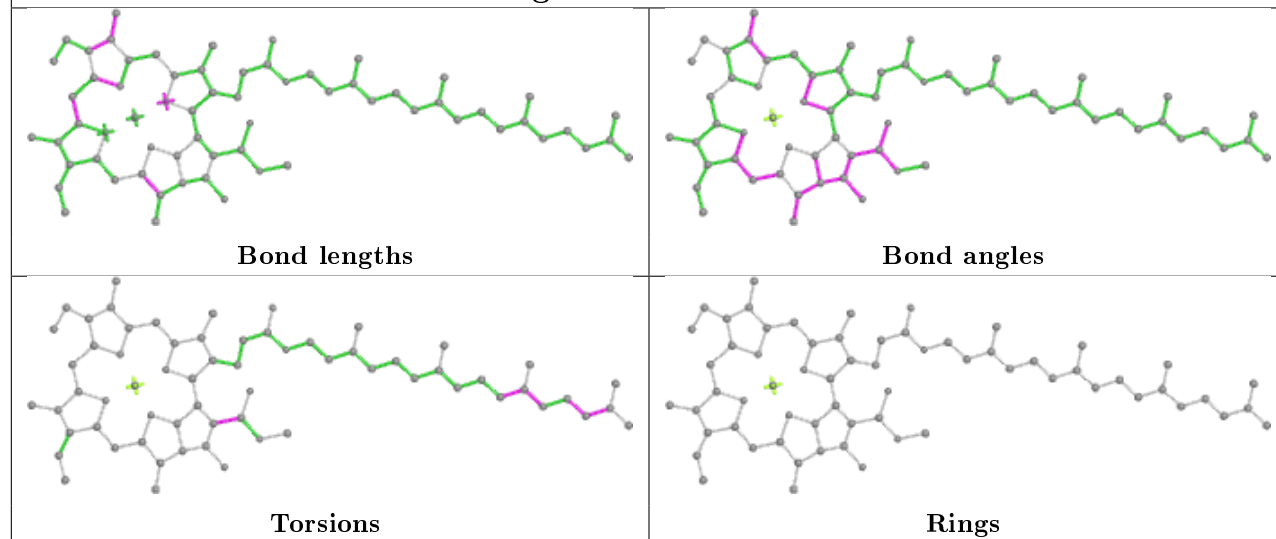
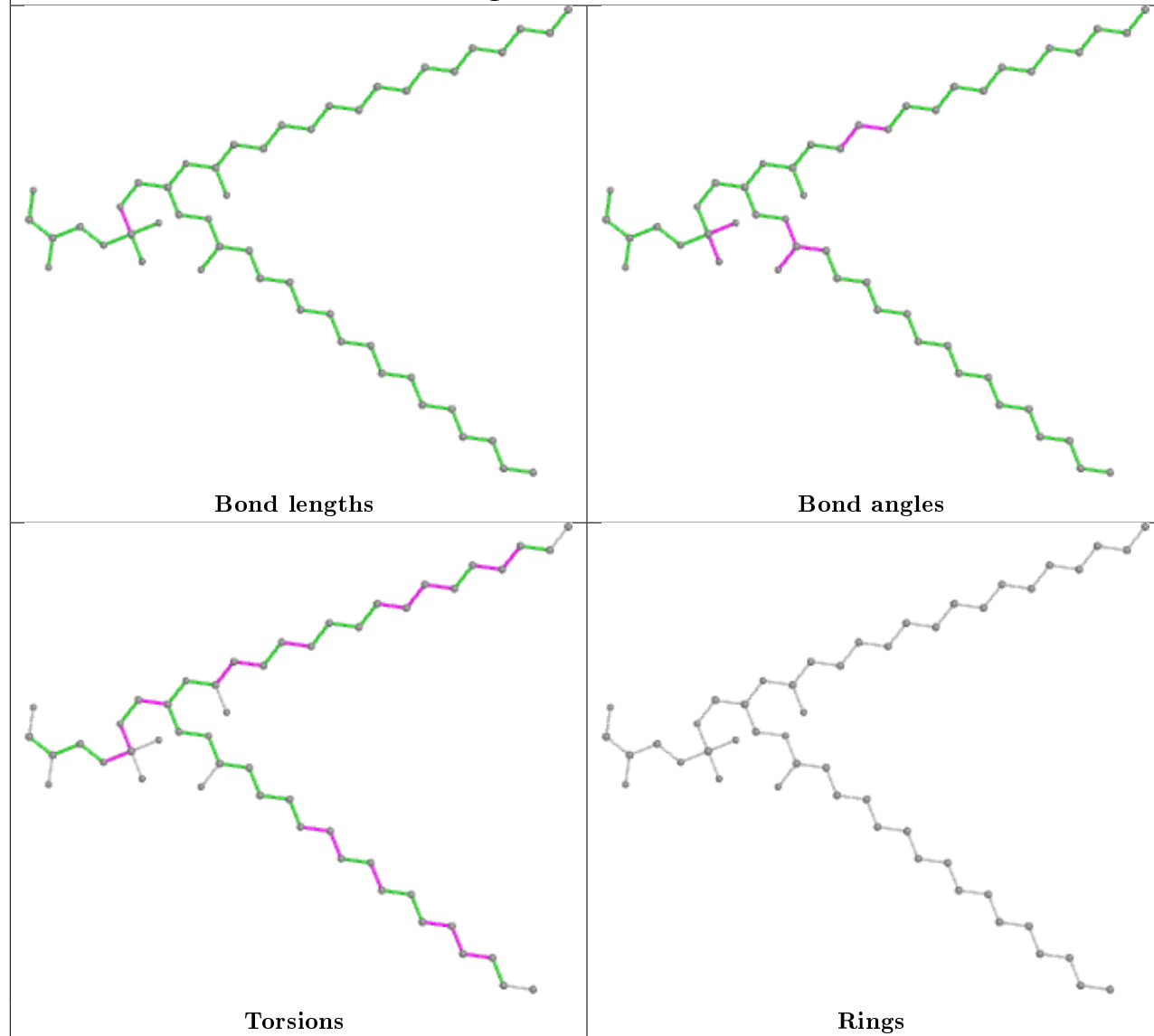


Ligand BCR a 406

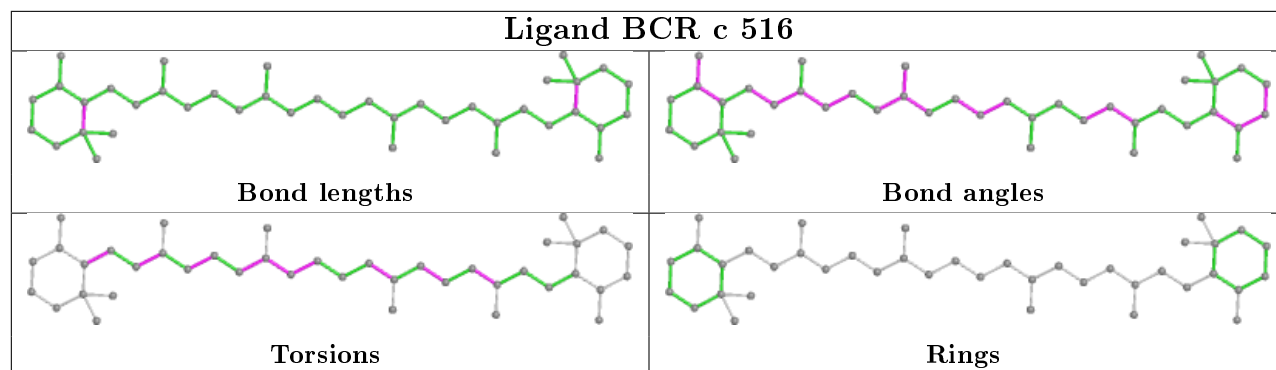


Ligand STE a 414

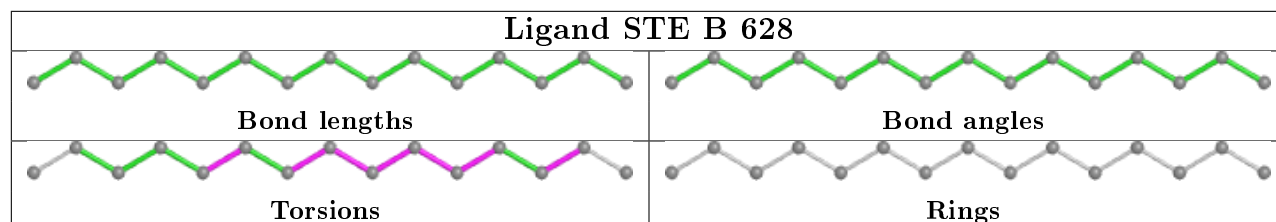


Ligand CLA C 503**Ligand LHG 1 101**

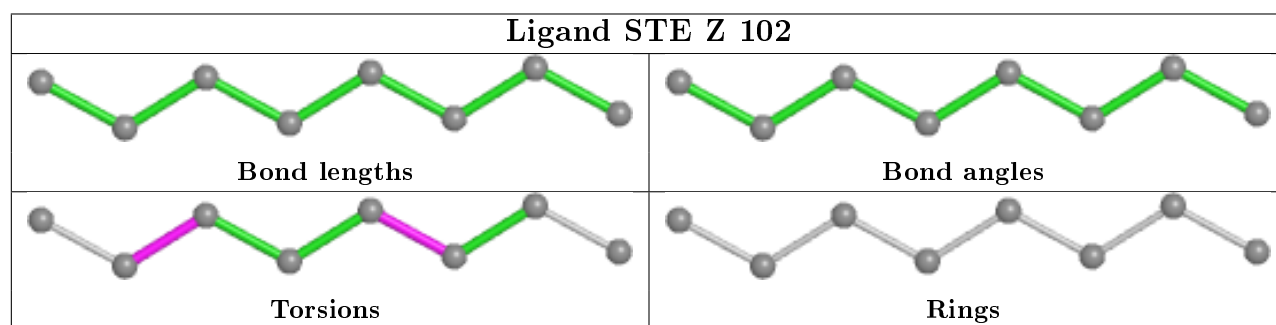
Ligand BCR c 516



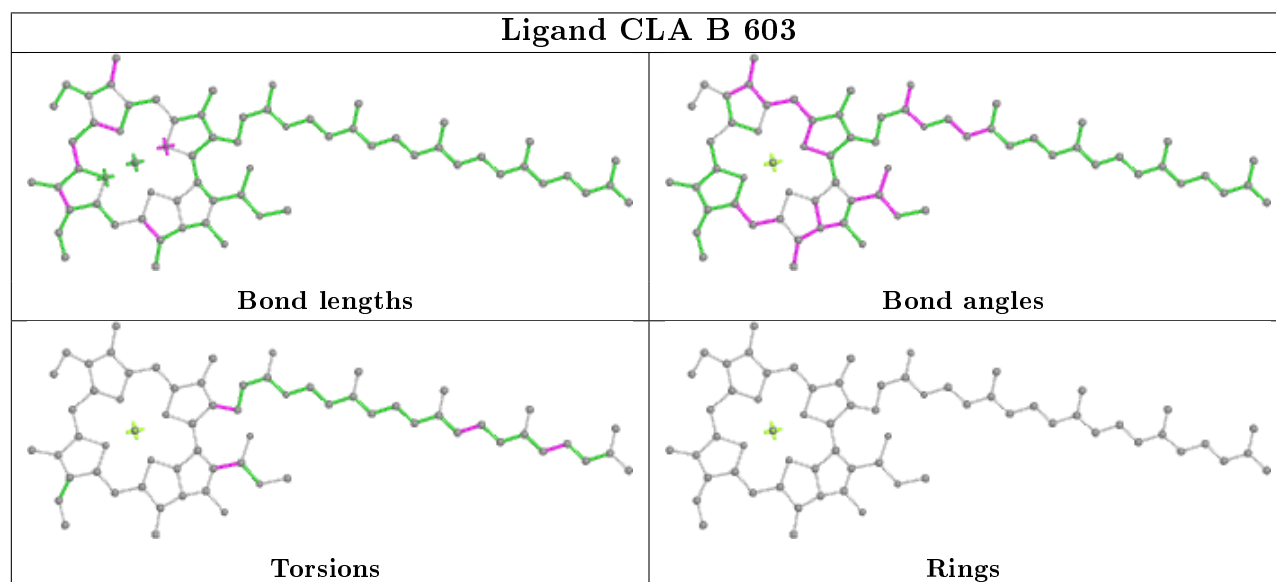
Ligand STE B 628

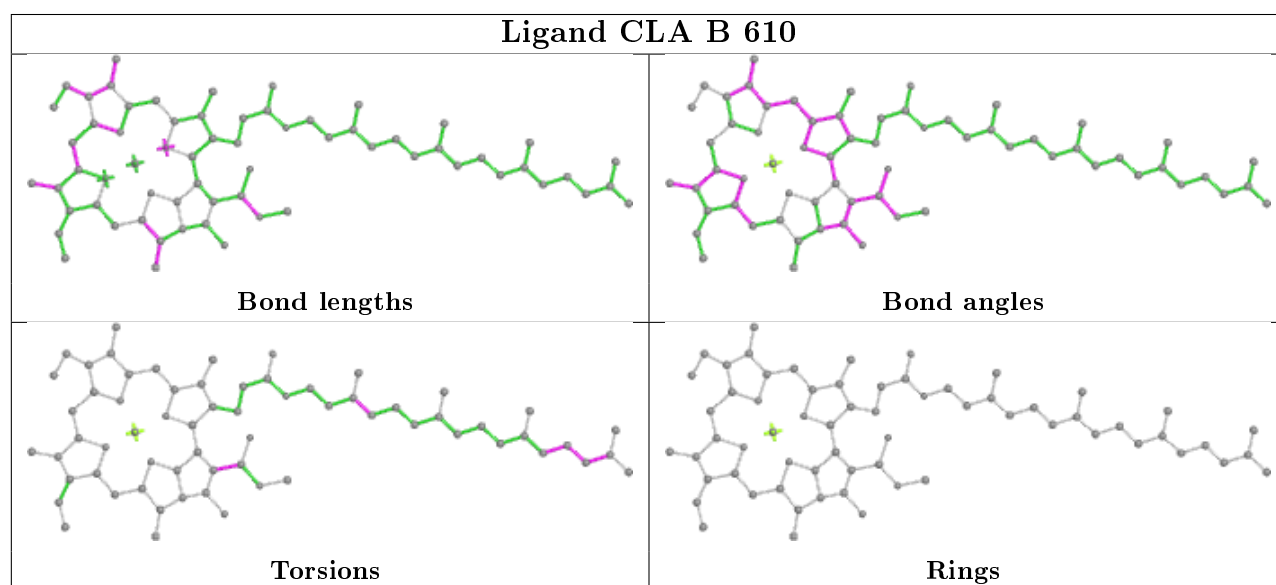
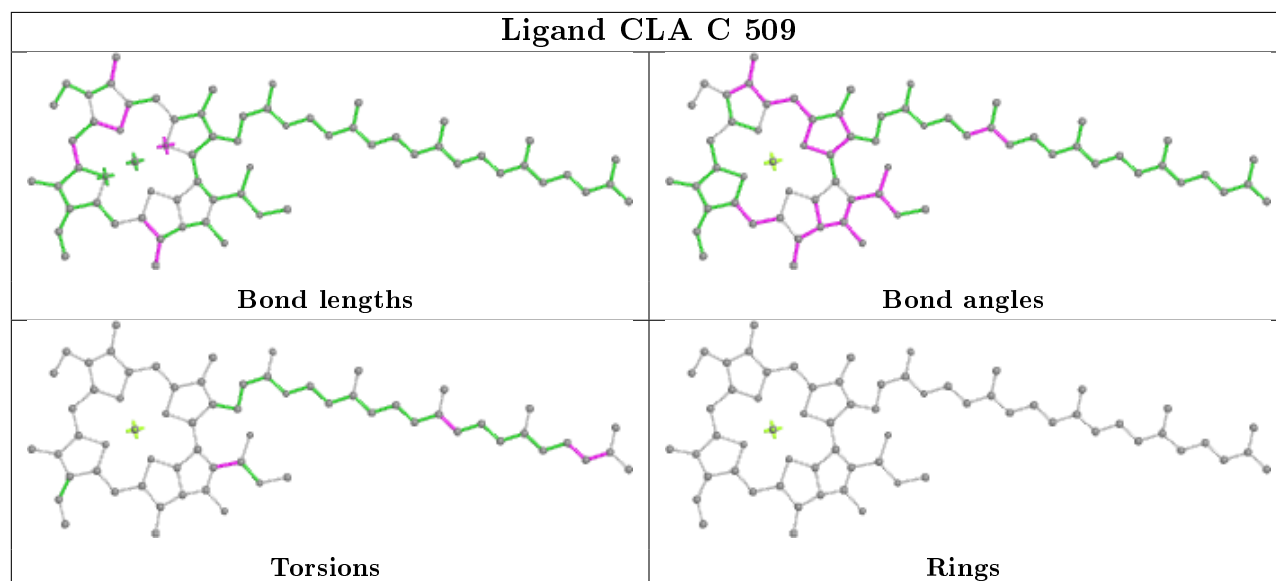
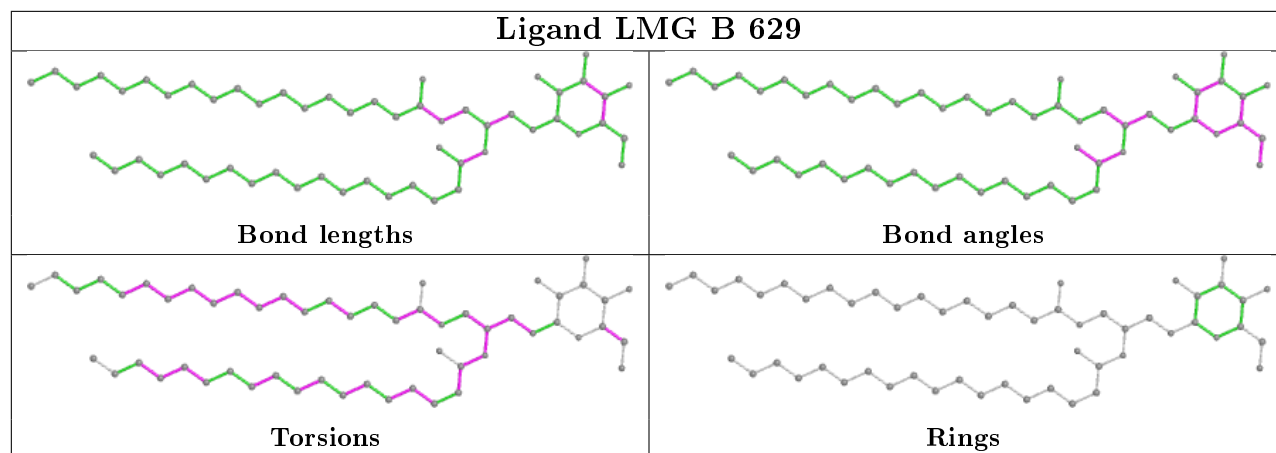


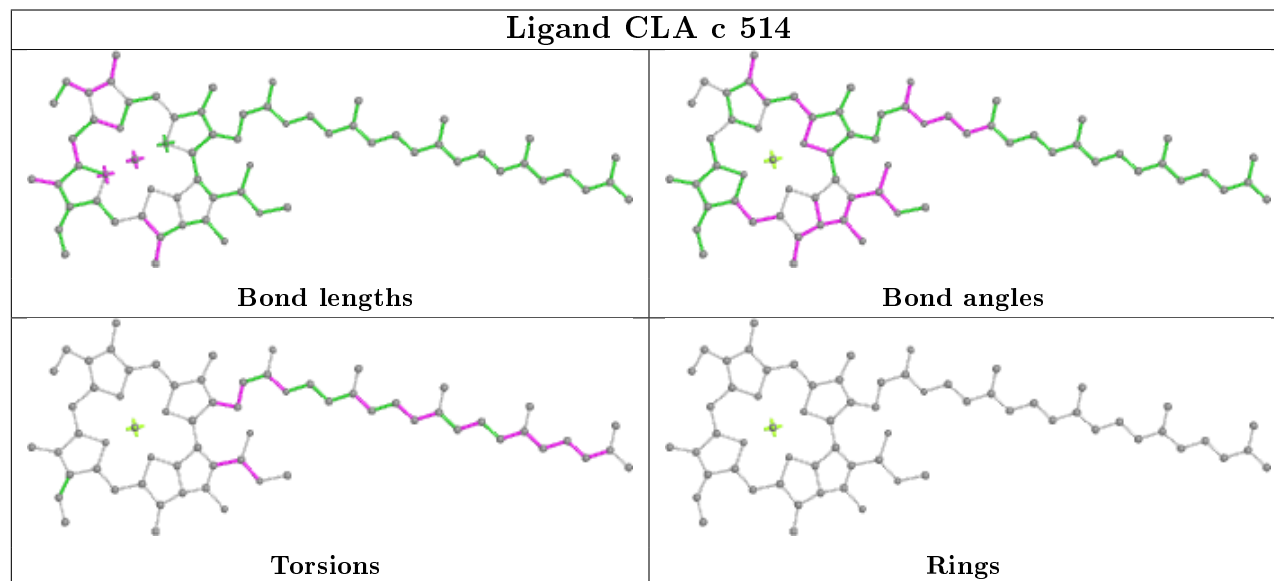
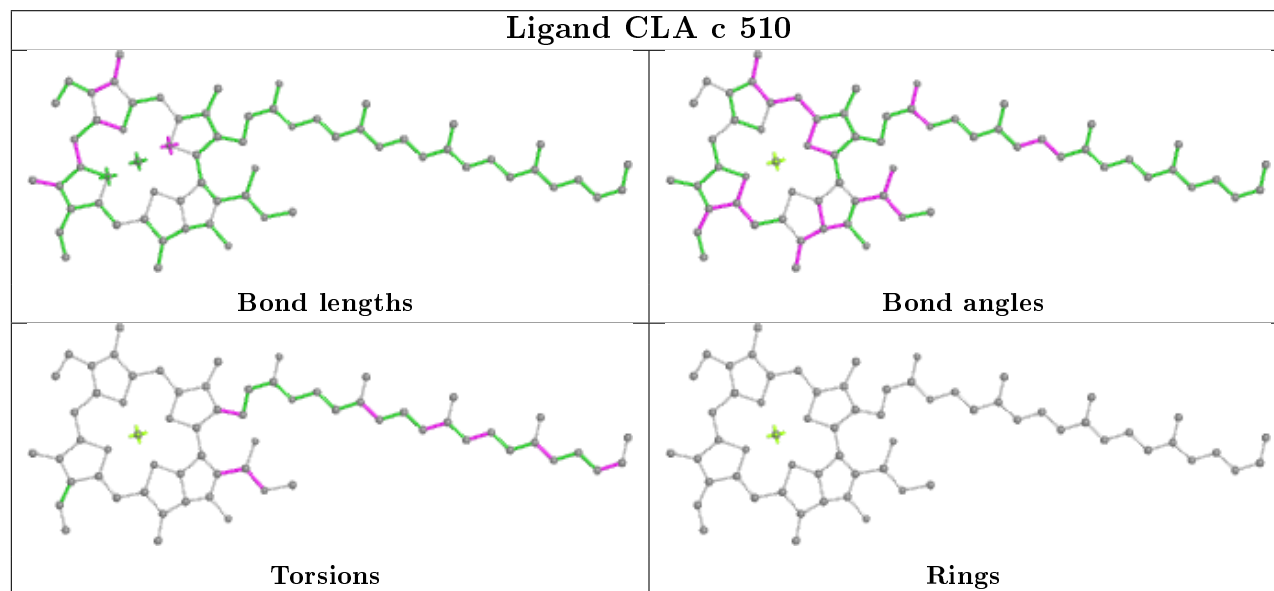
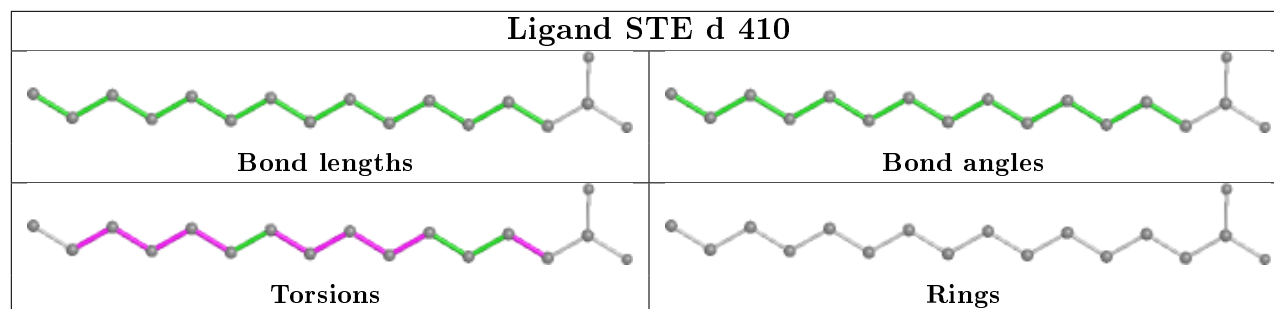
Ligand STE Z 102

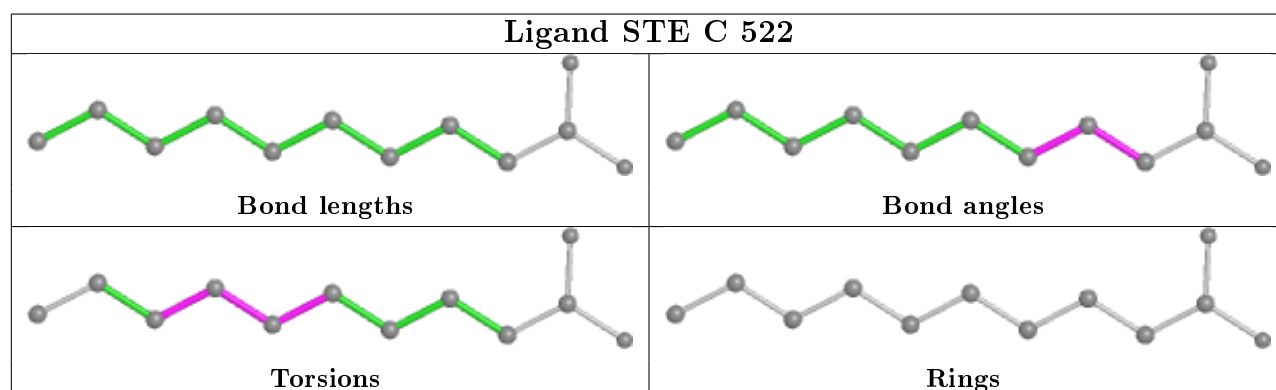
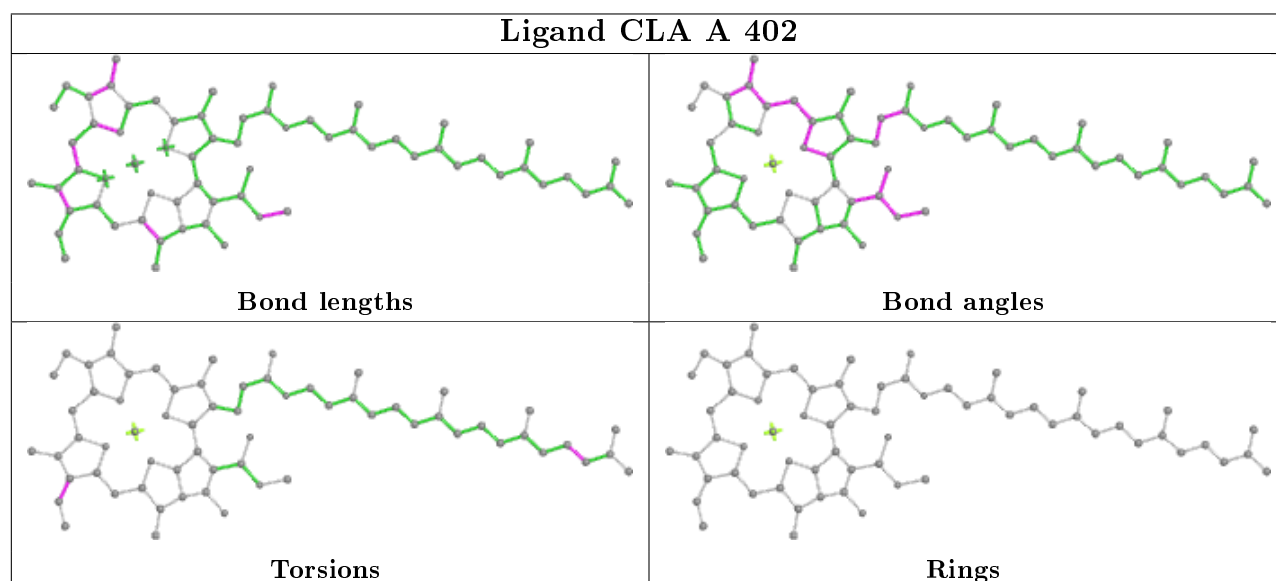
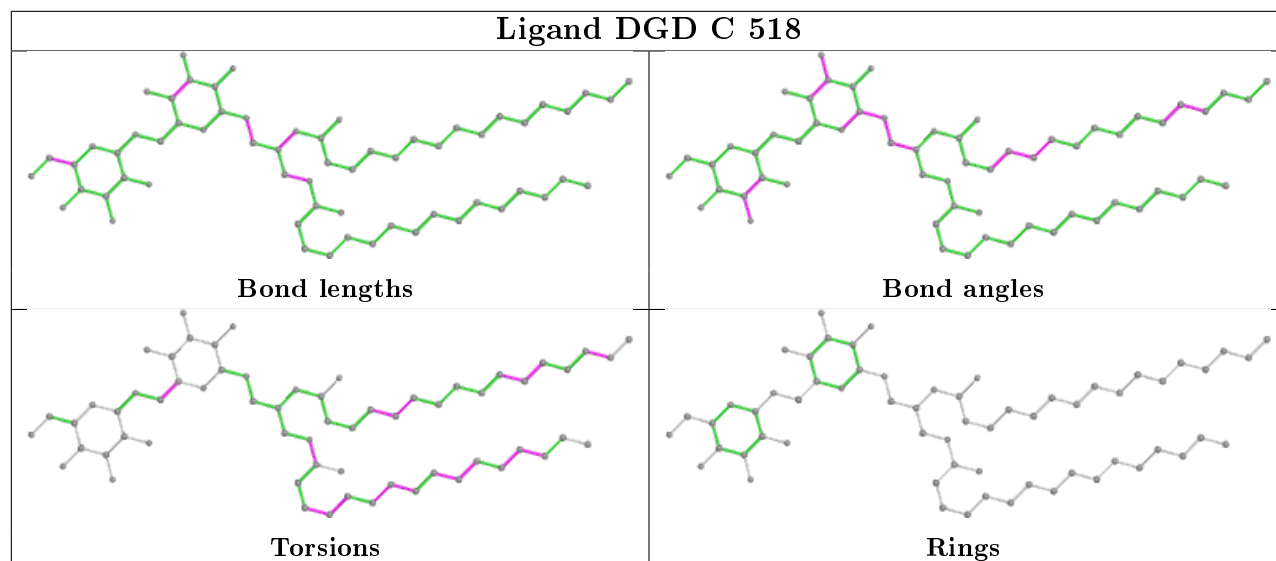


Ligand CLA B 603

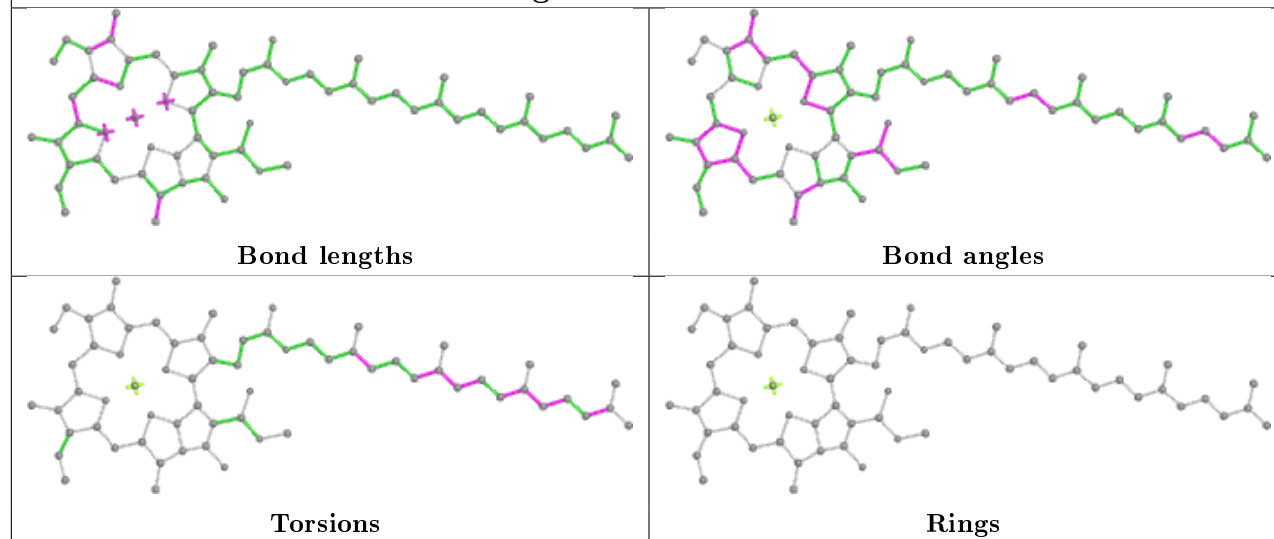




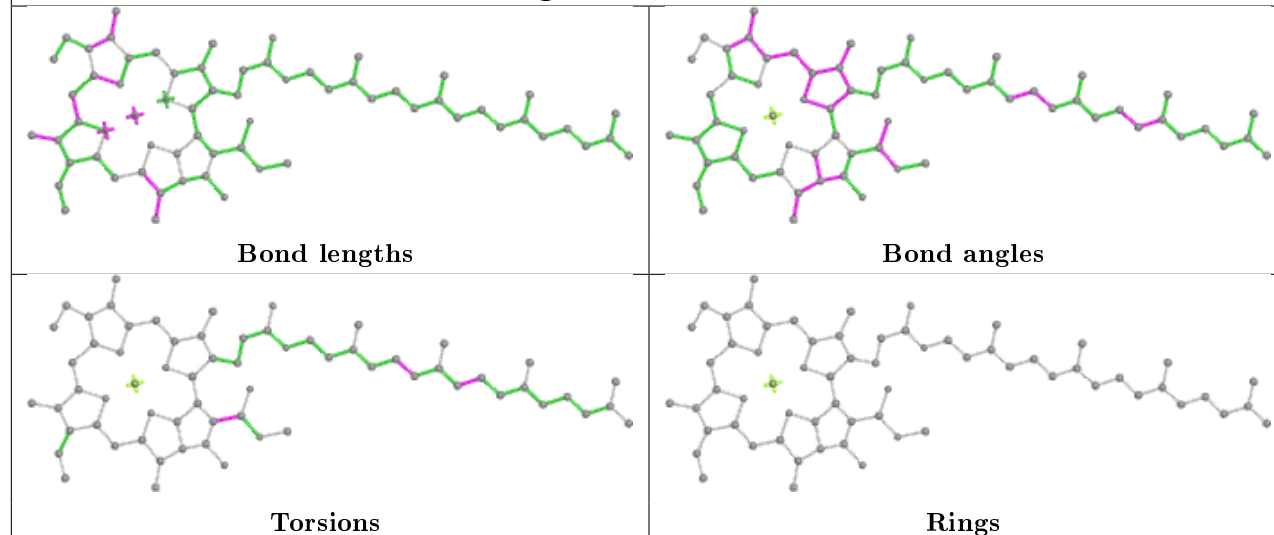




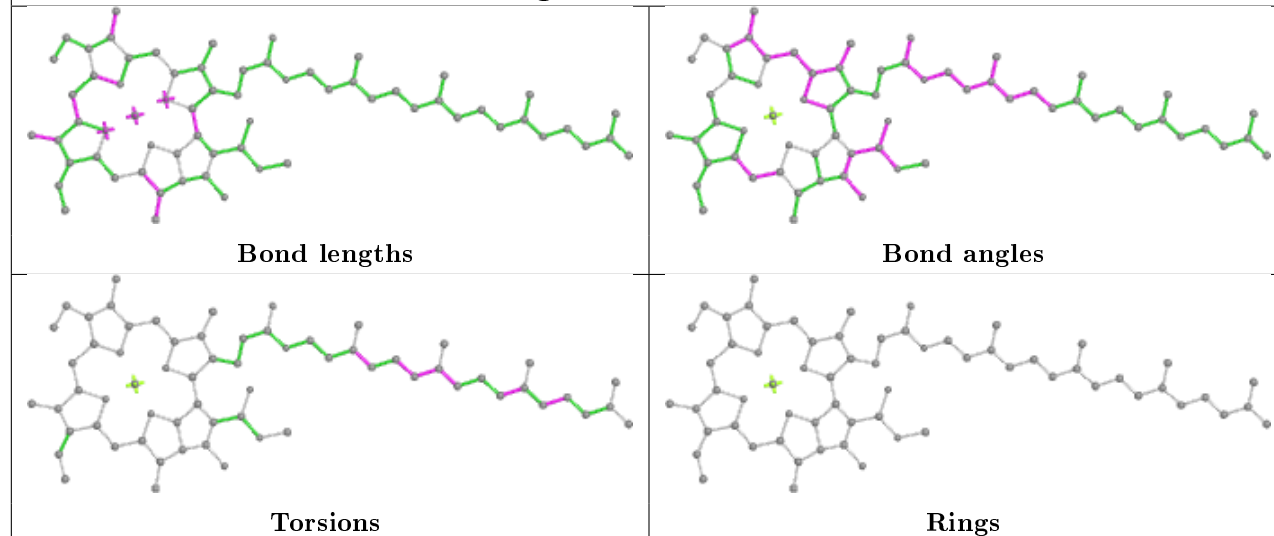
Ligand CLA B 612

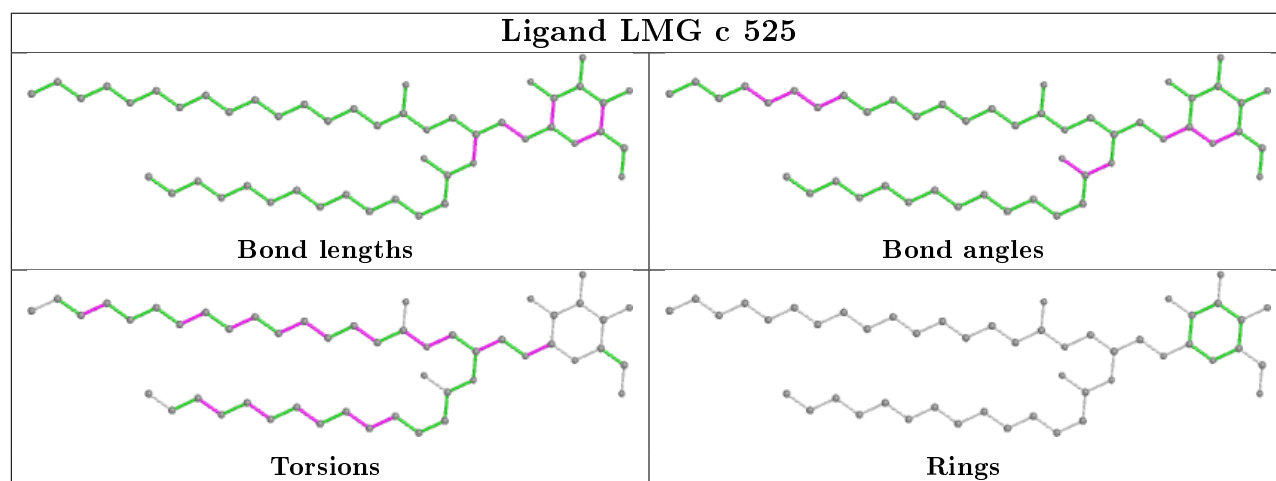
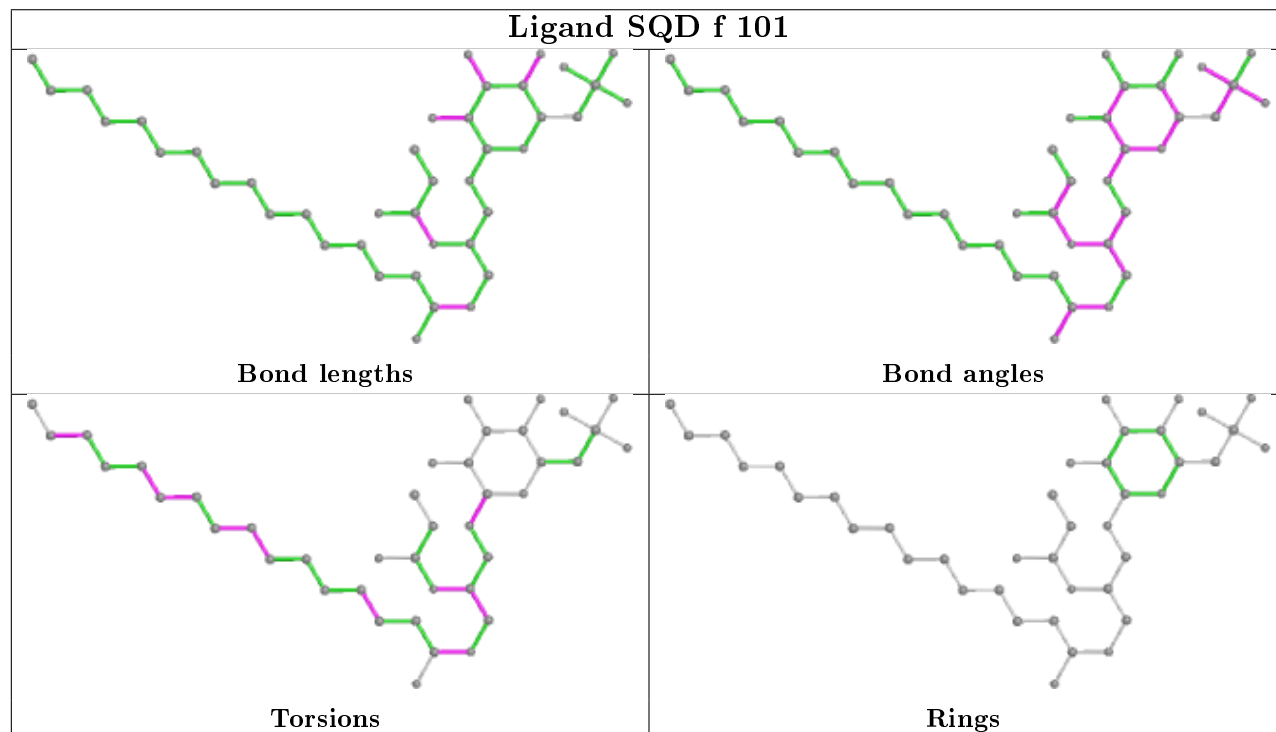
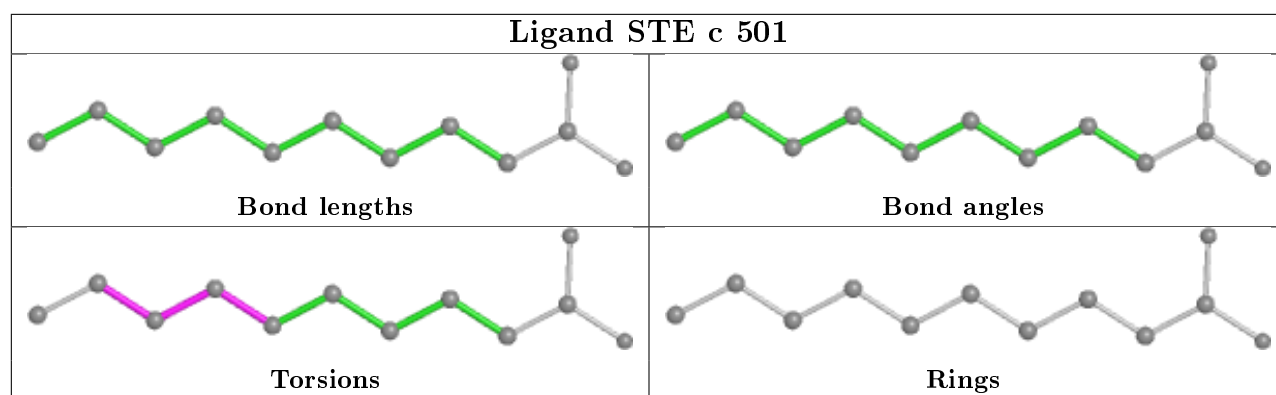


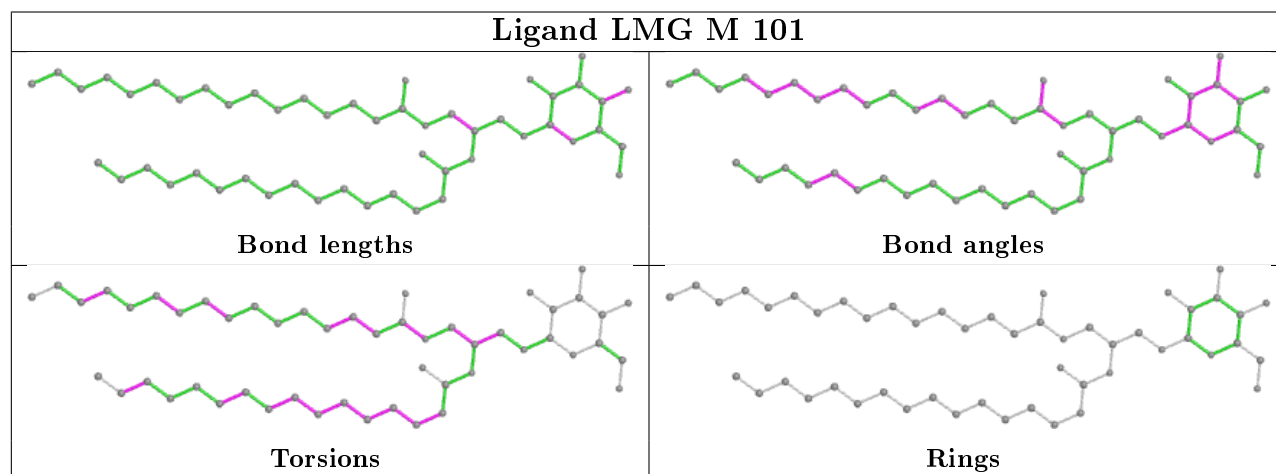
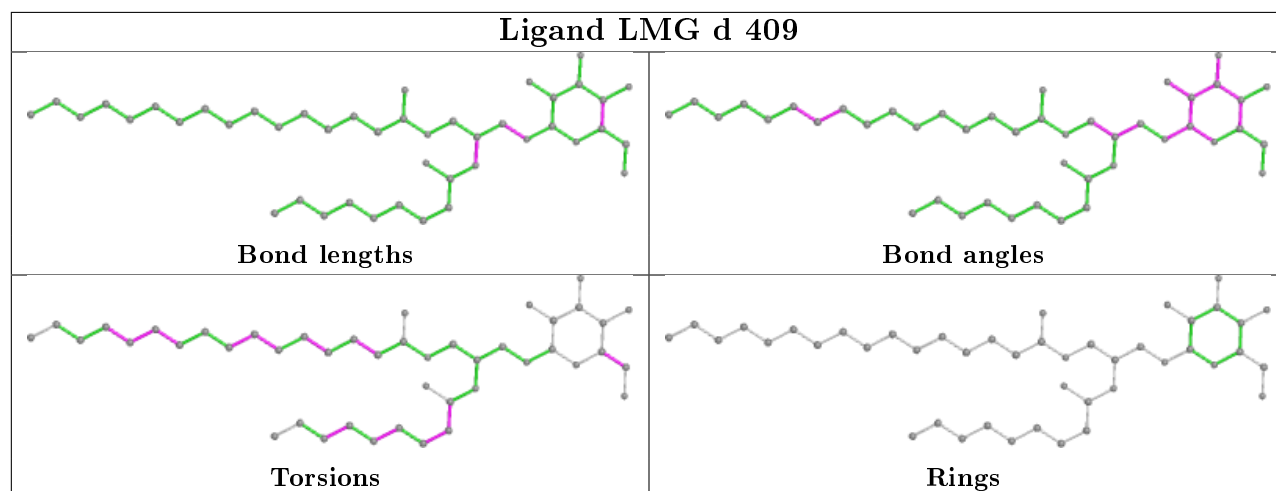
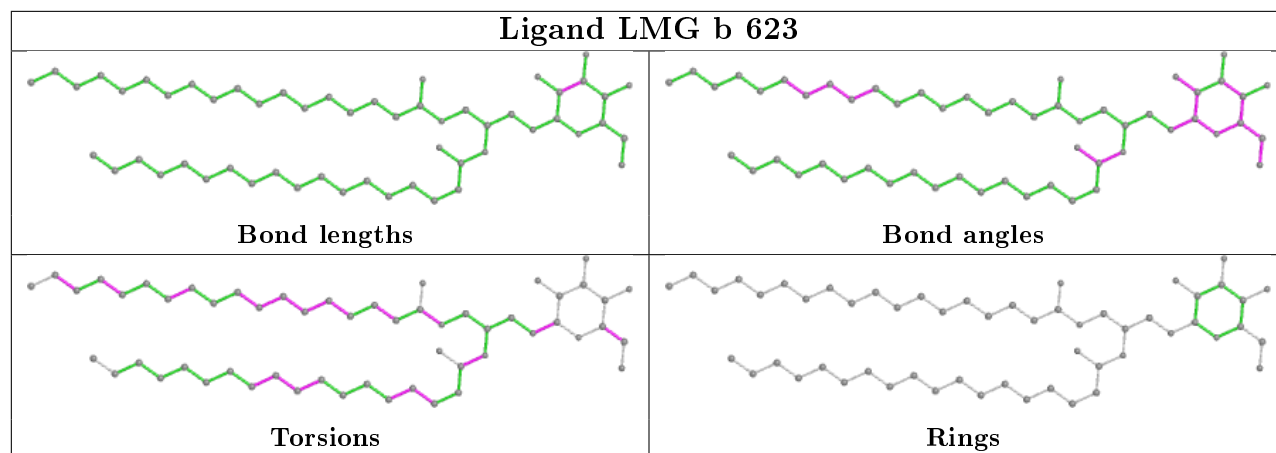
Ligand CLA c 505

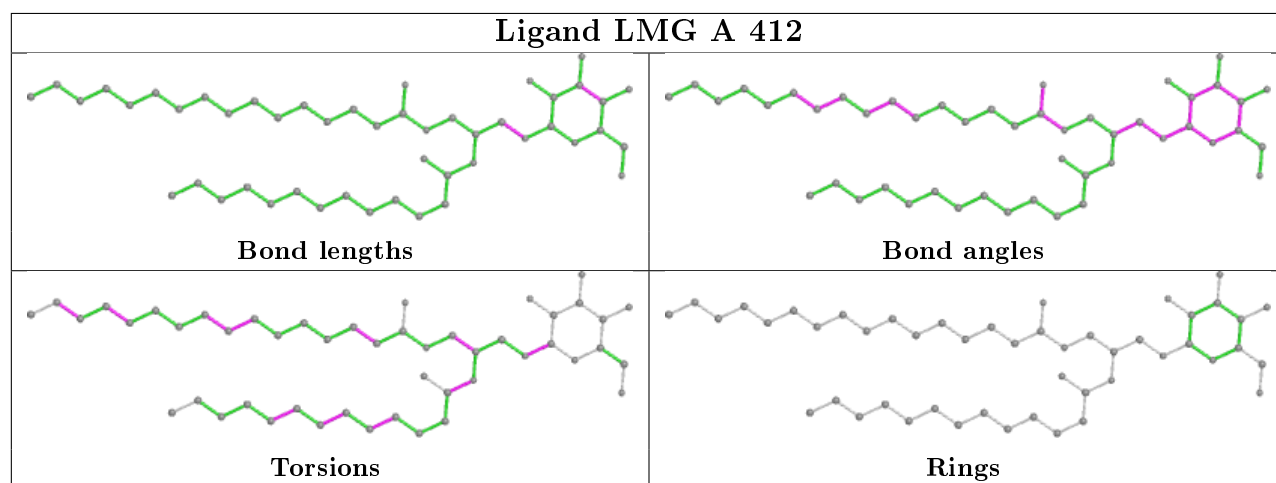
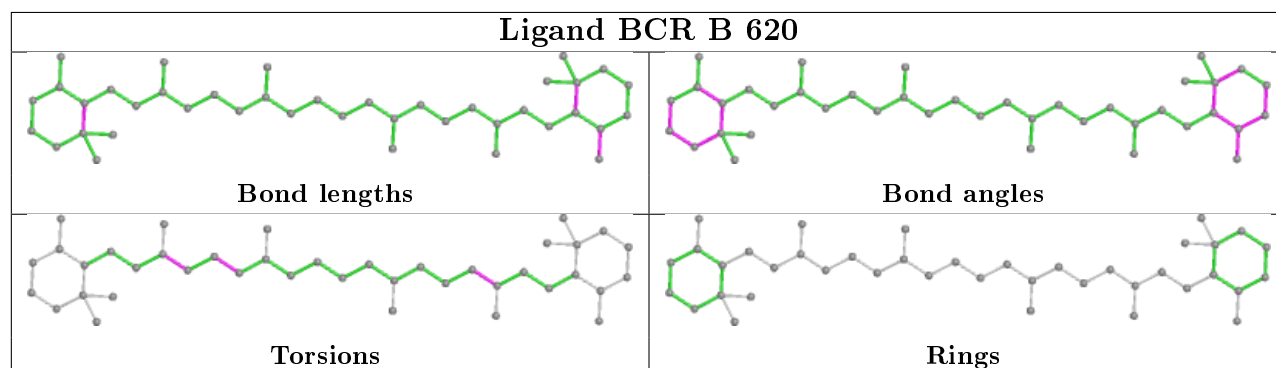
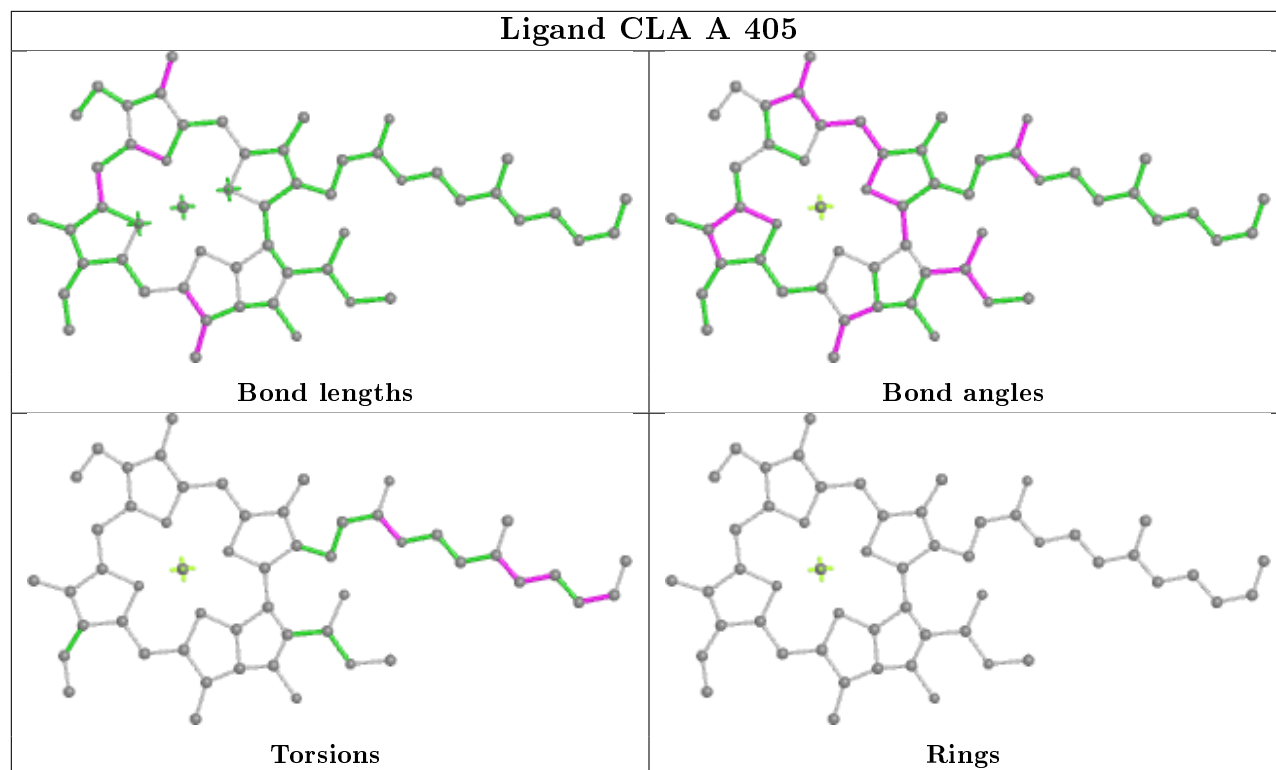


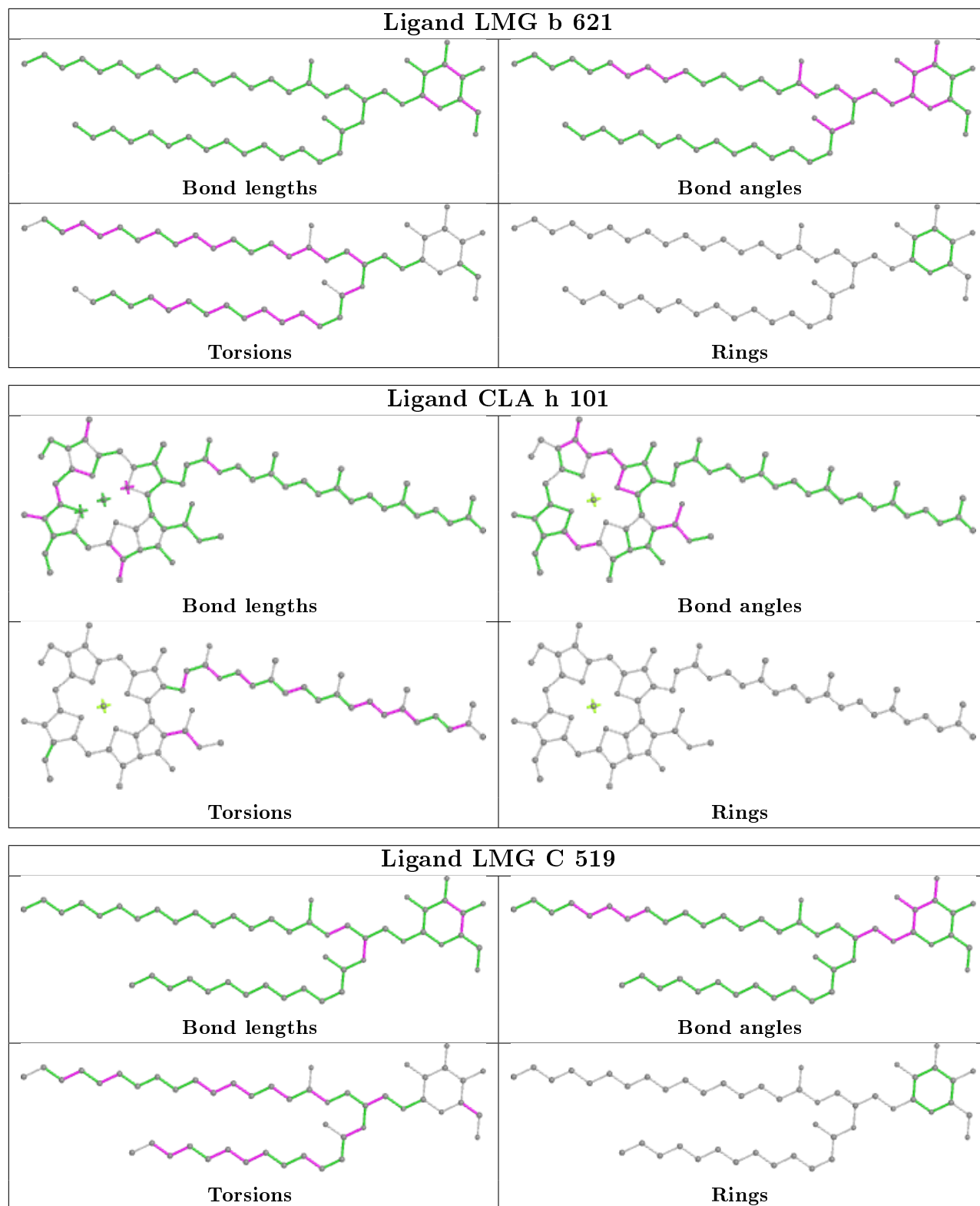
Ligand CLA b 602

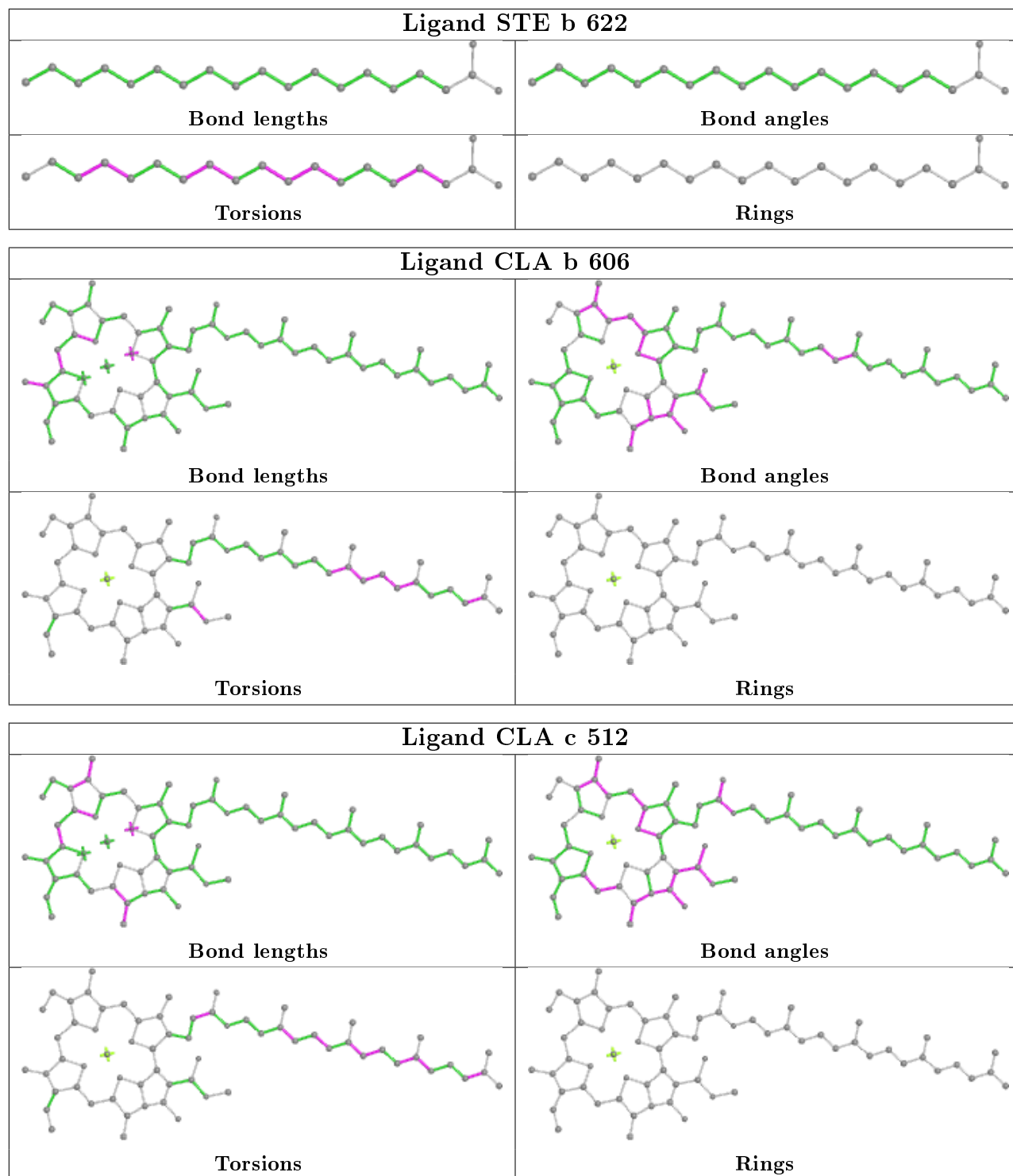




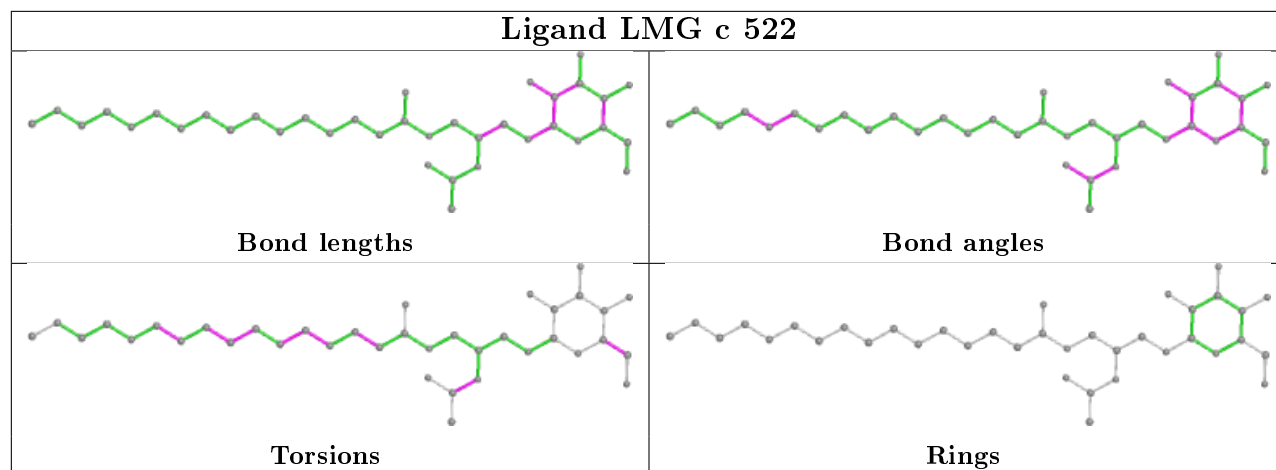




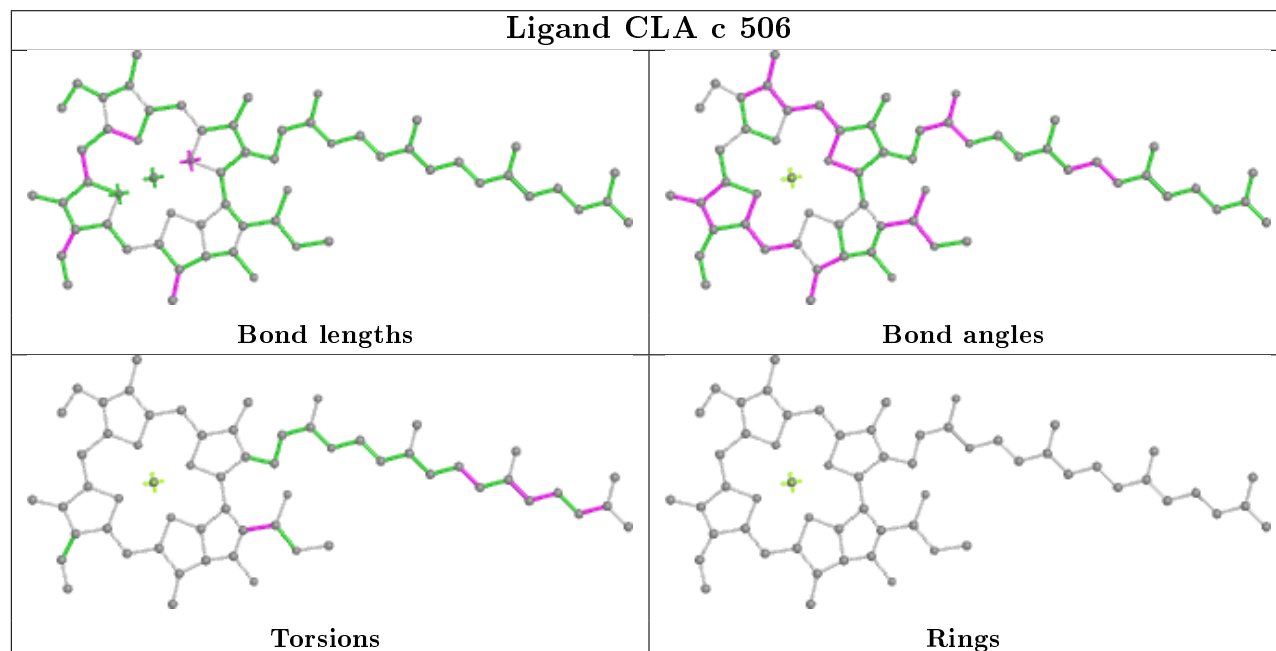




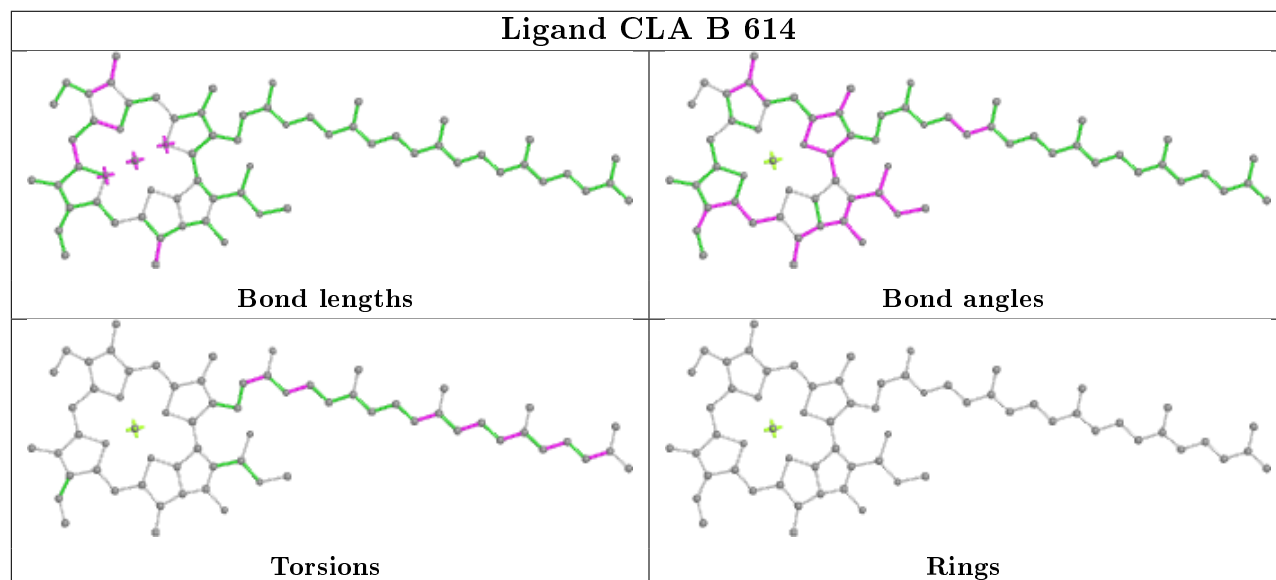
Ligand LMG c 522



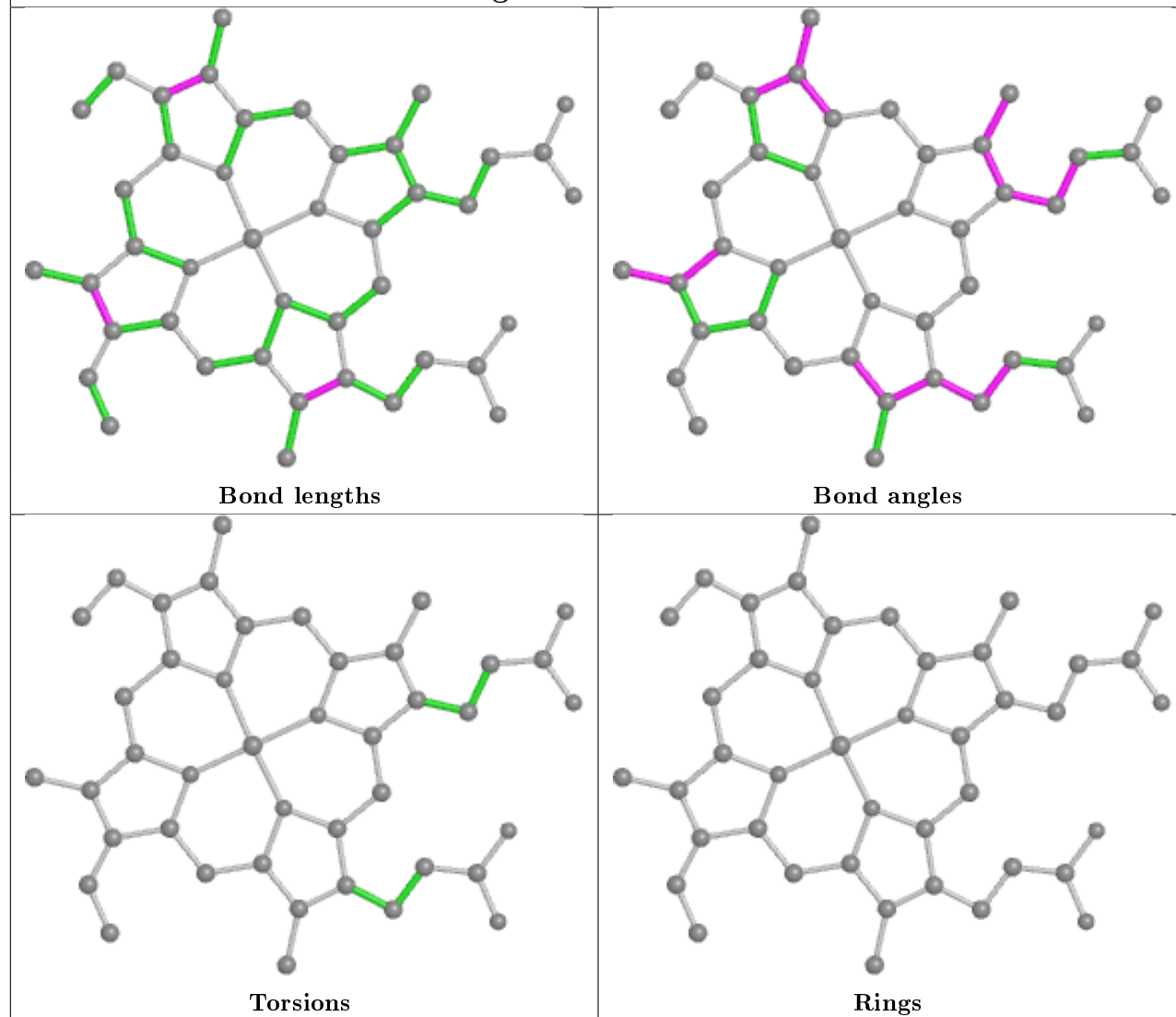
Ligand CLA c 506



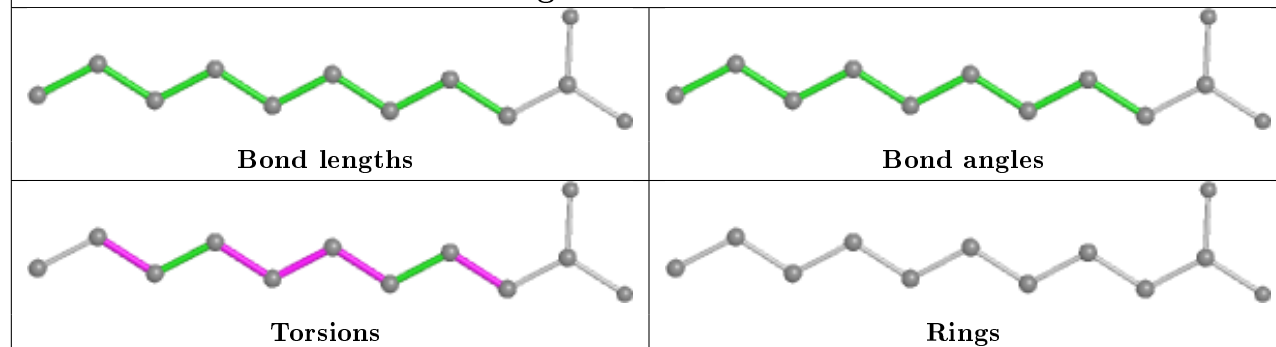
Ligand CLA B 614

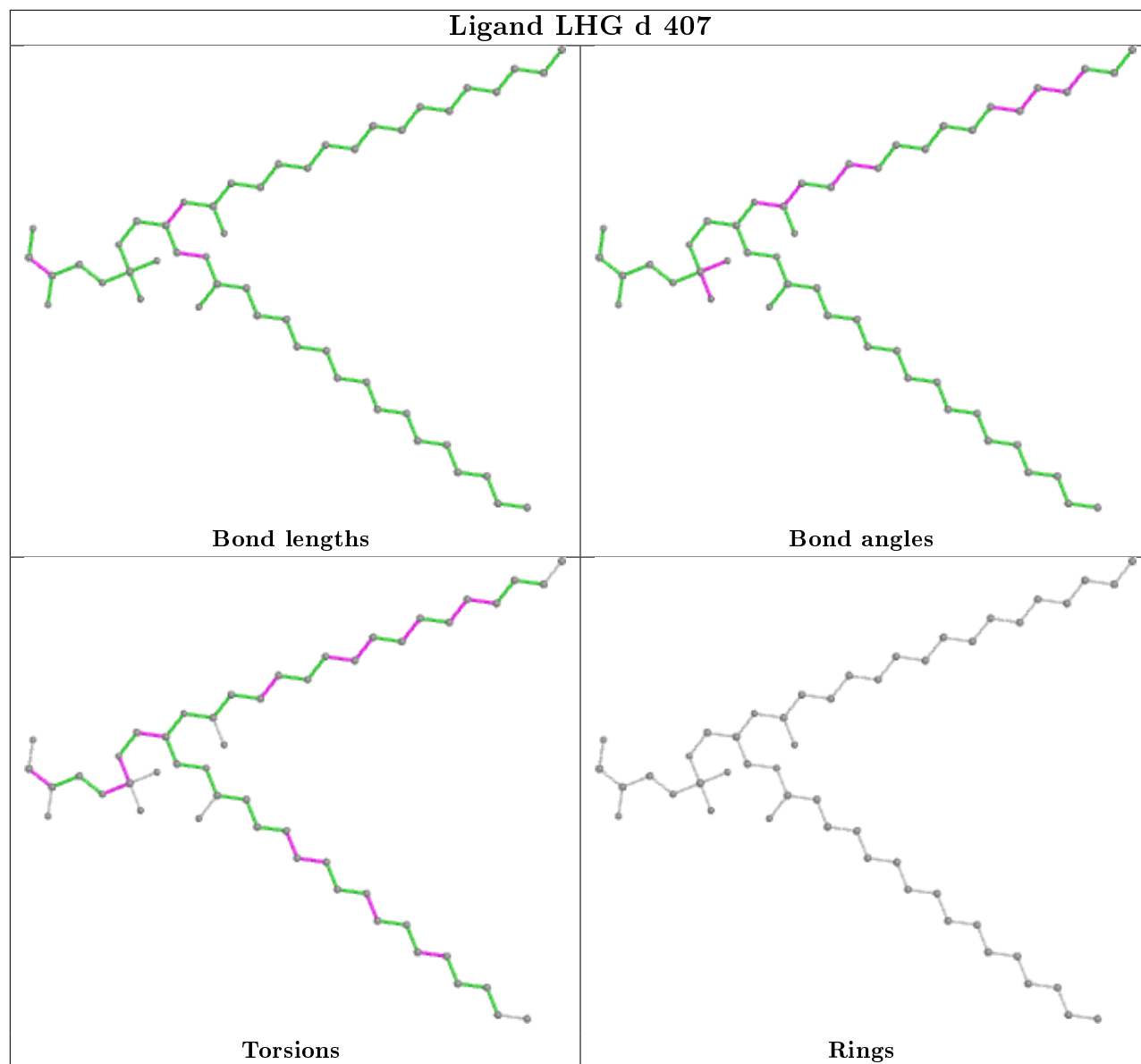


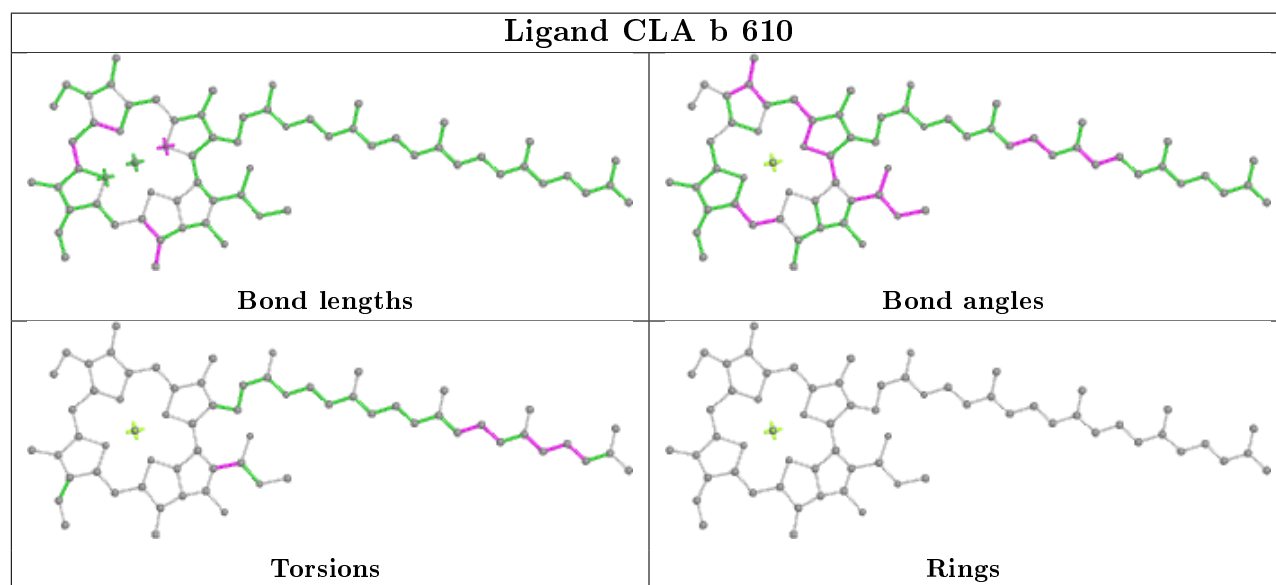
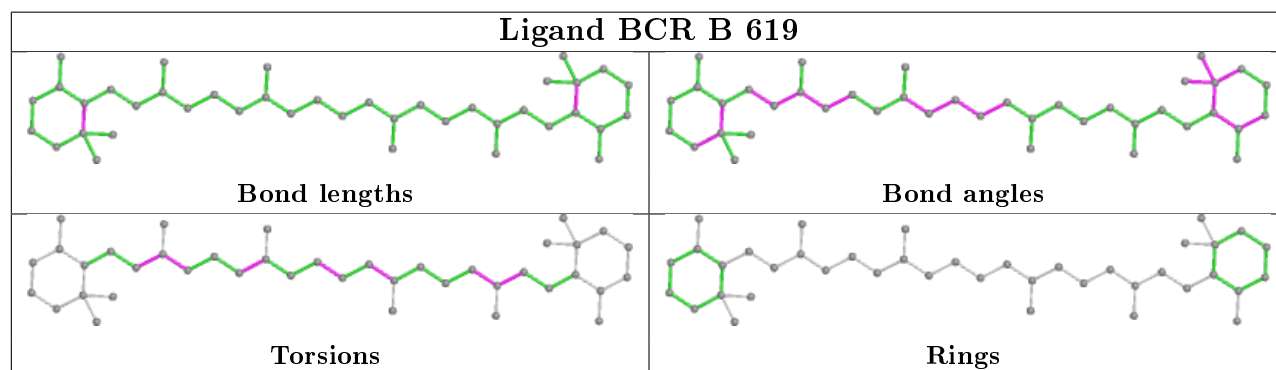
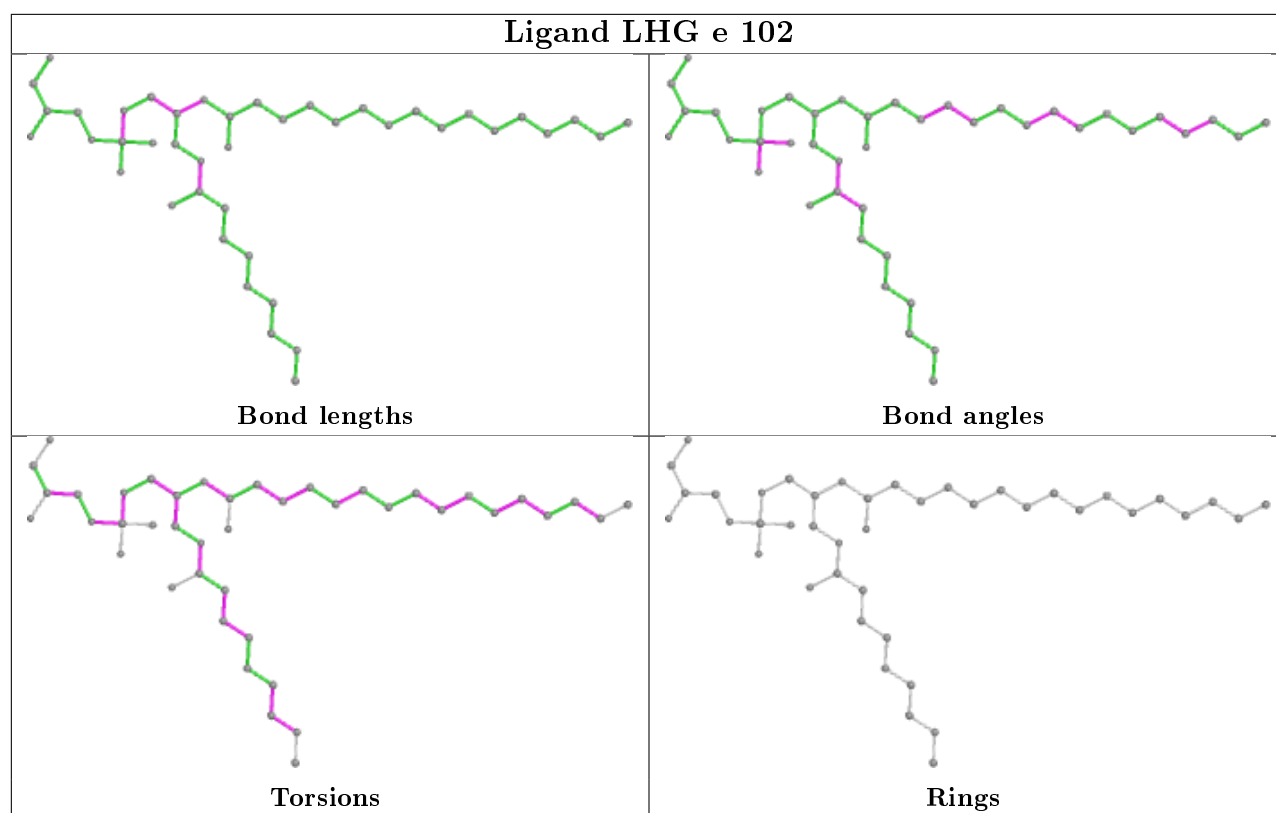
Ligand HEC v 201

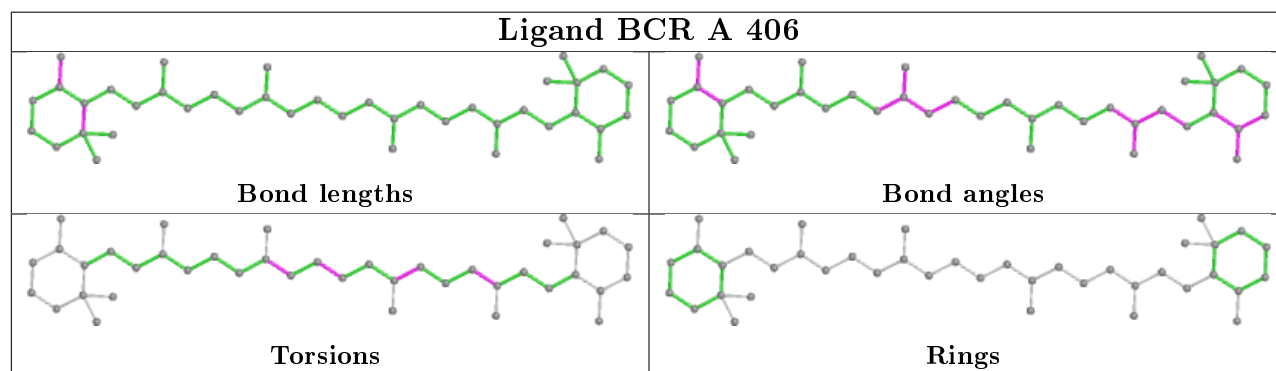
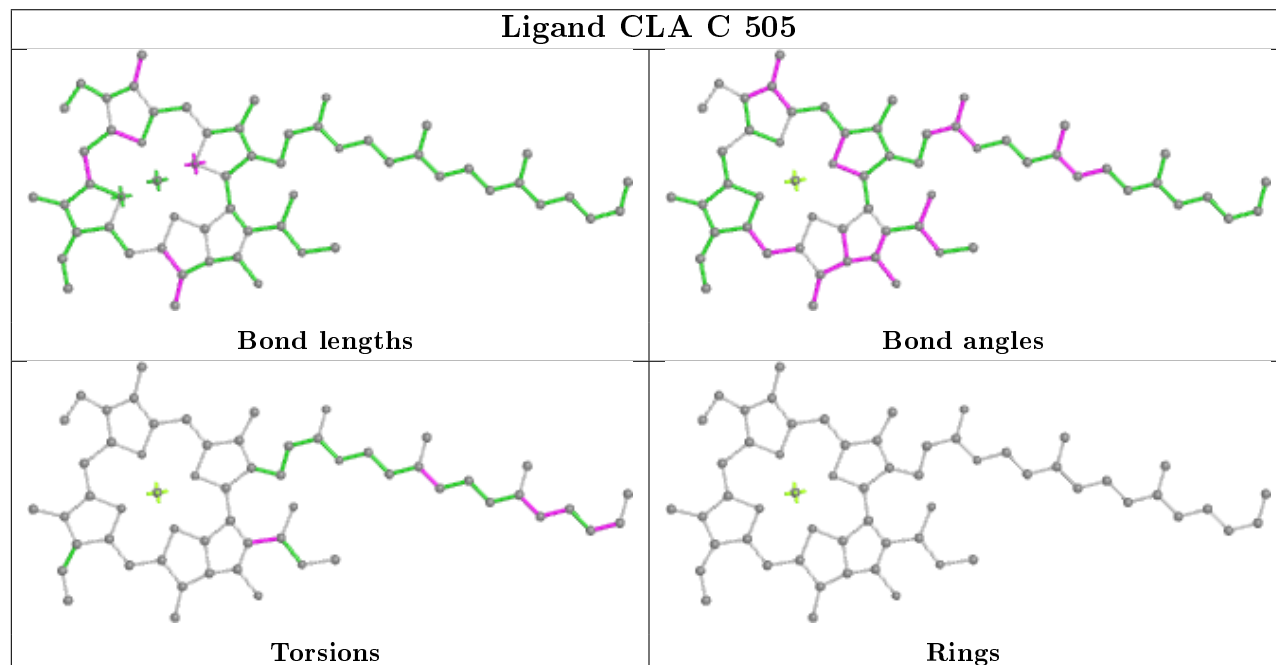
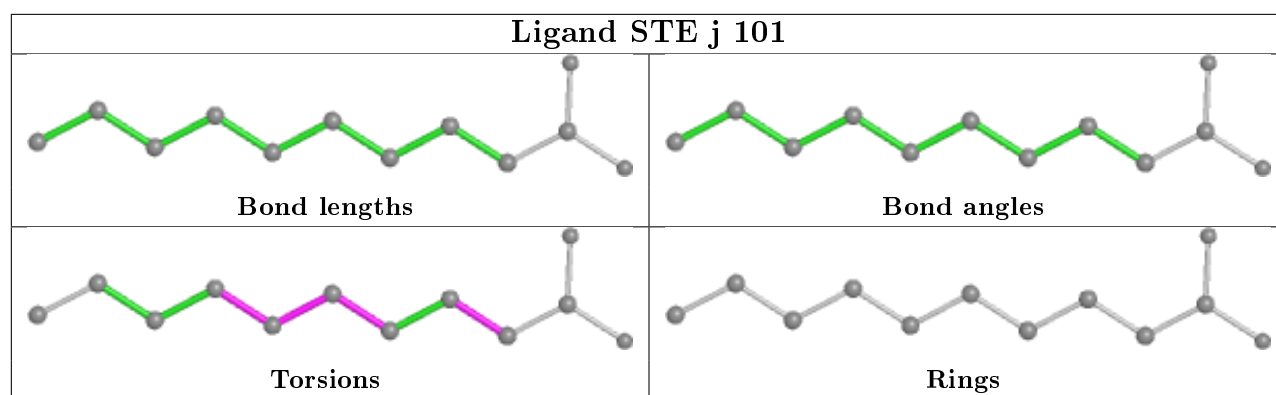


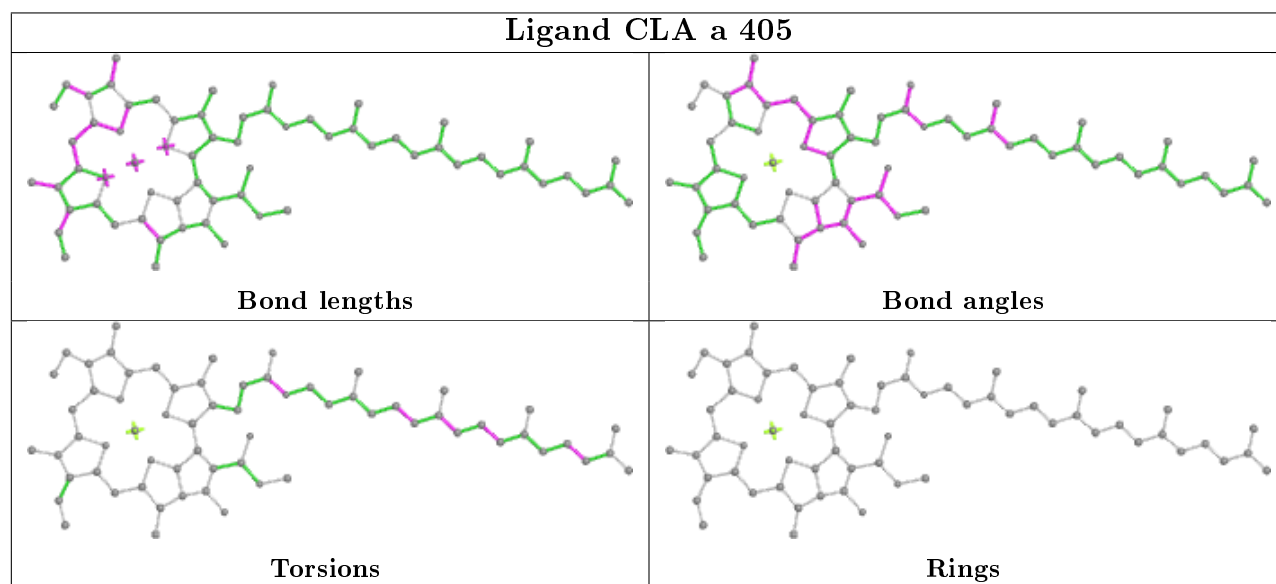
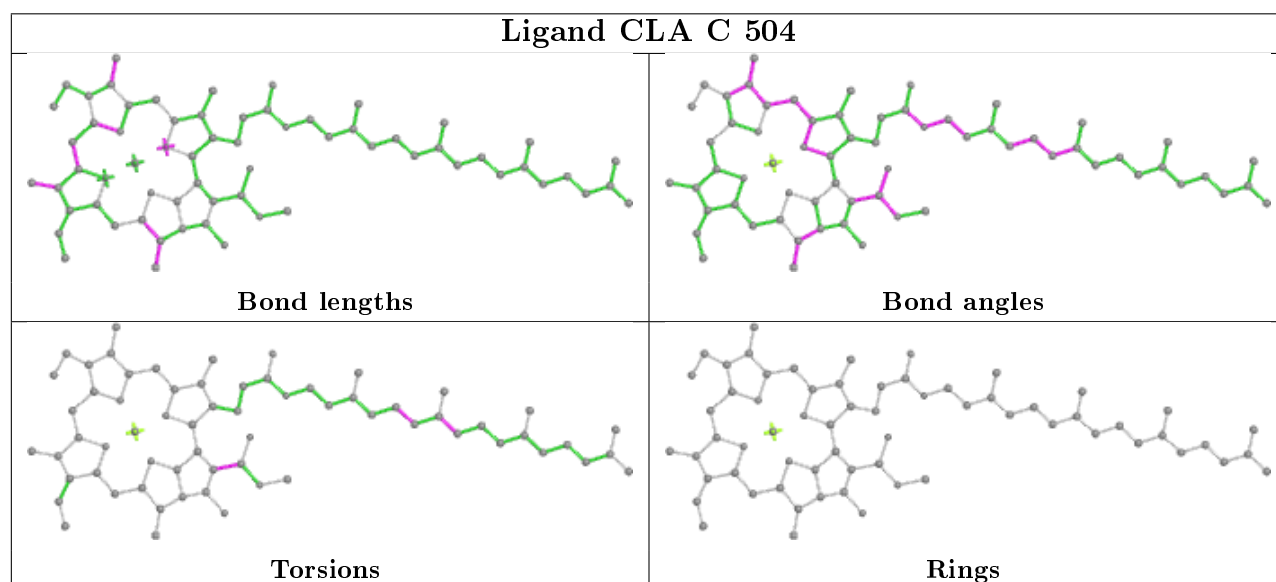
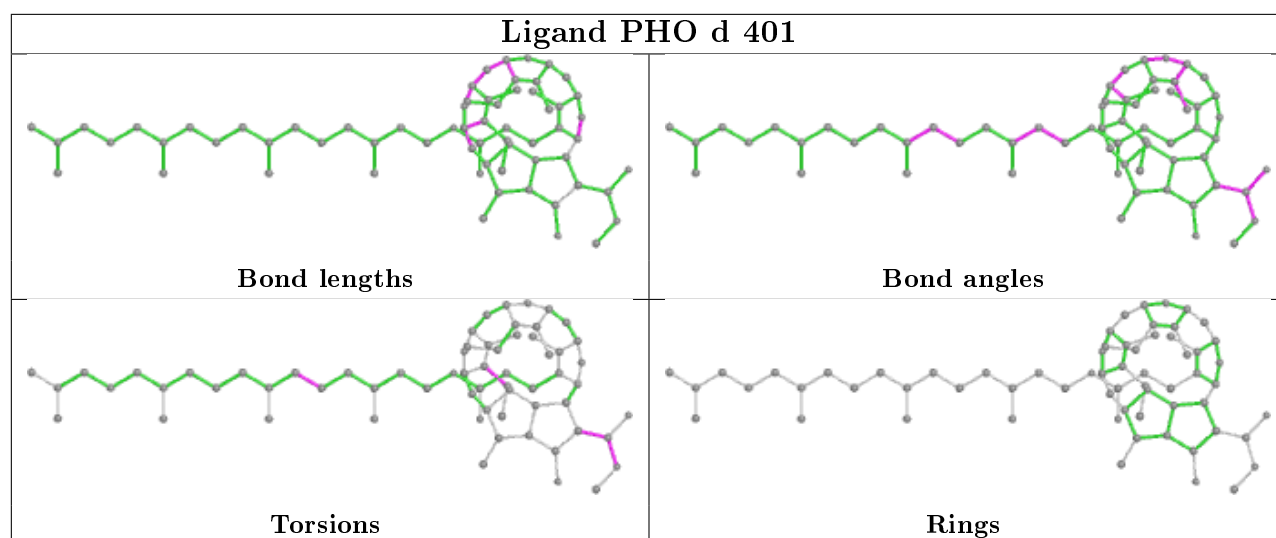
Ligand STE L 101



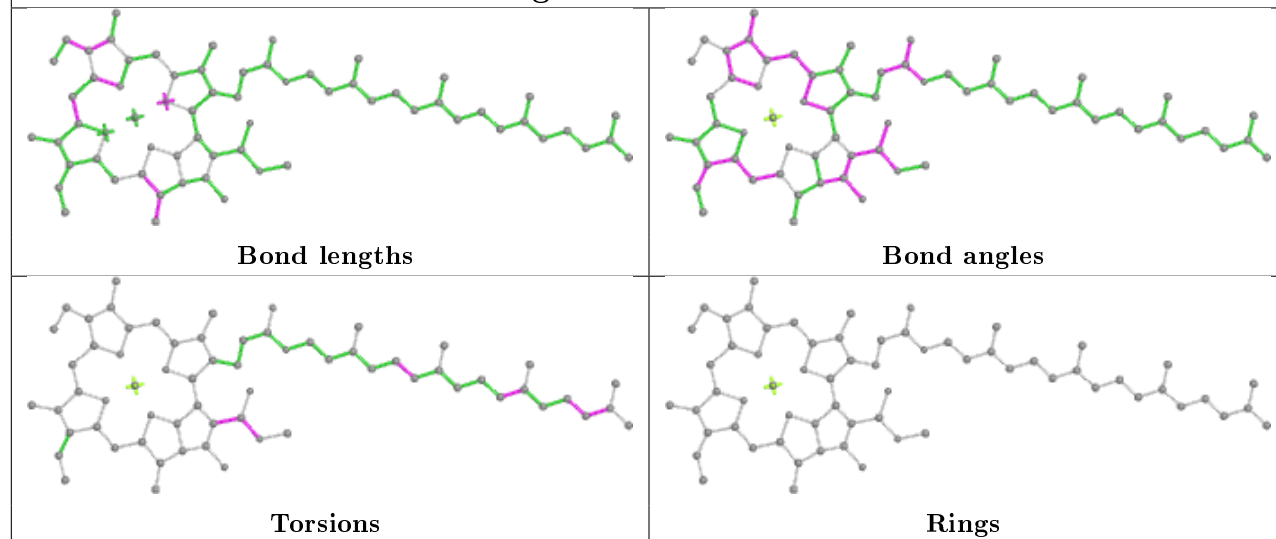




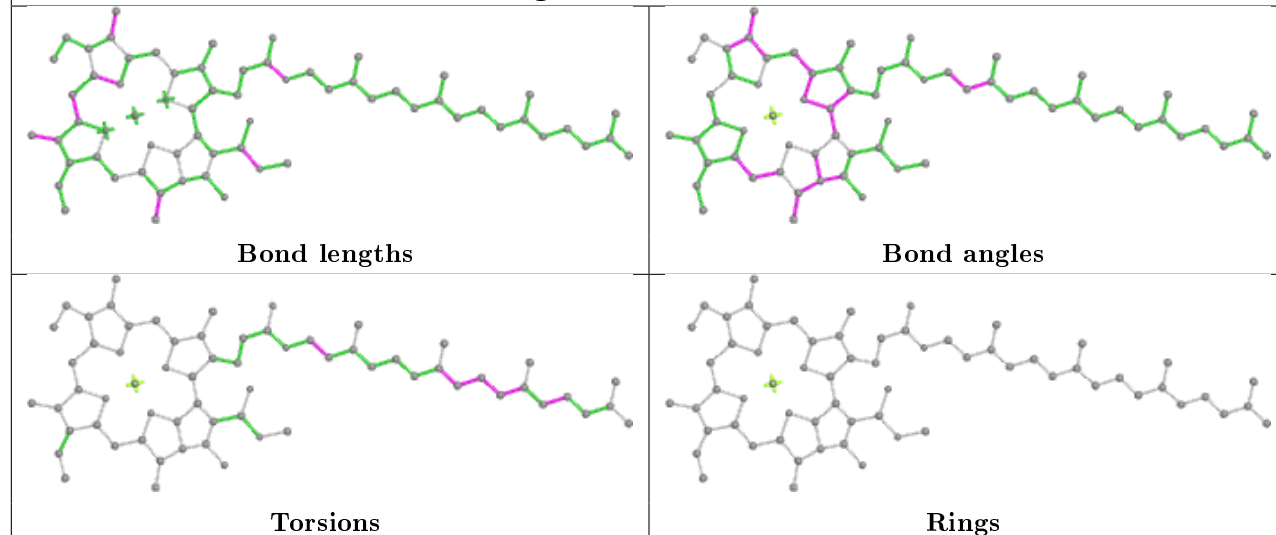




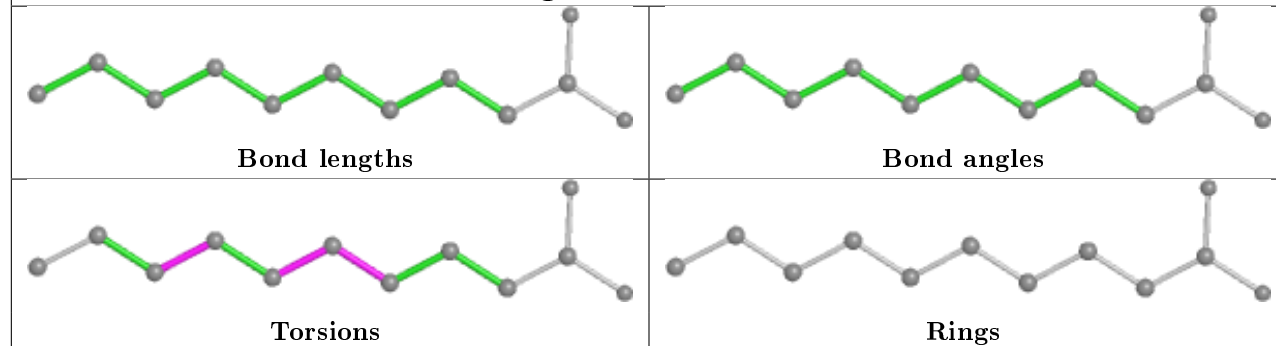
Ligand CLA B 604

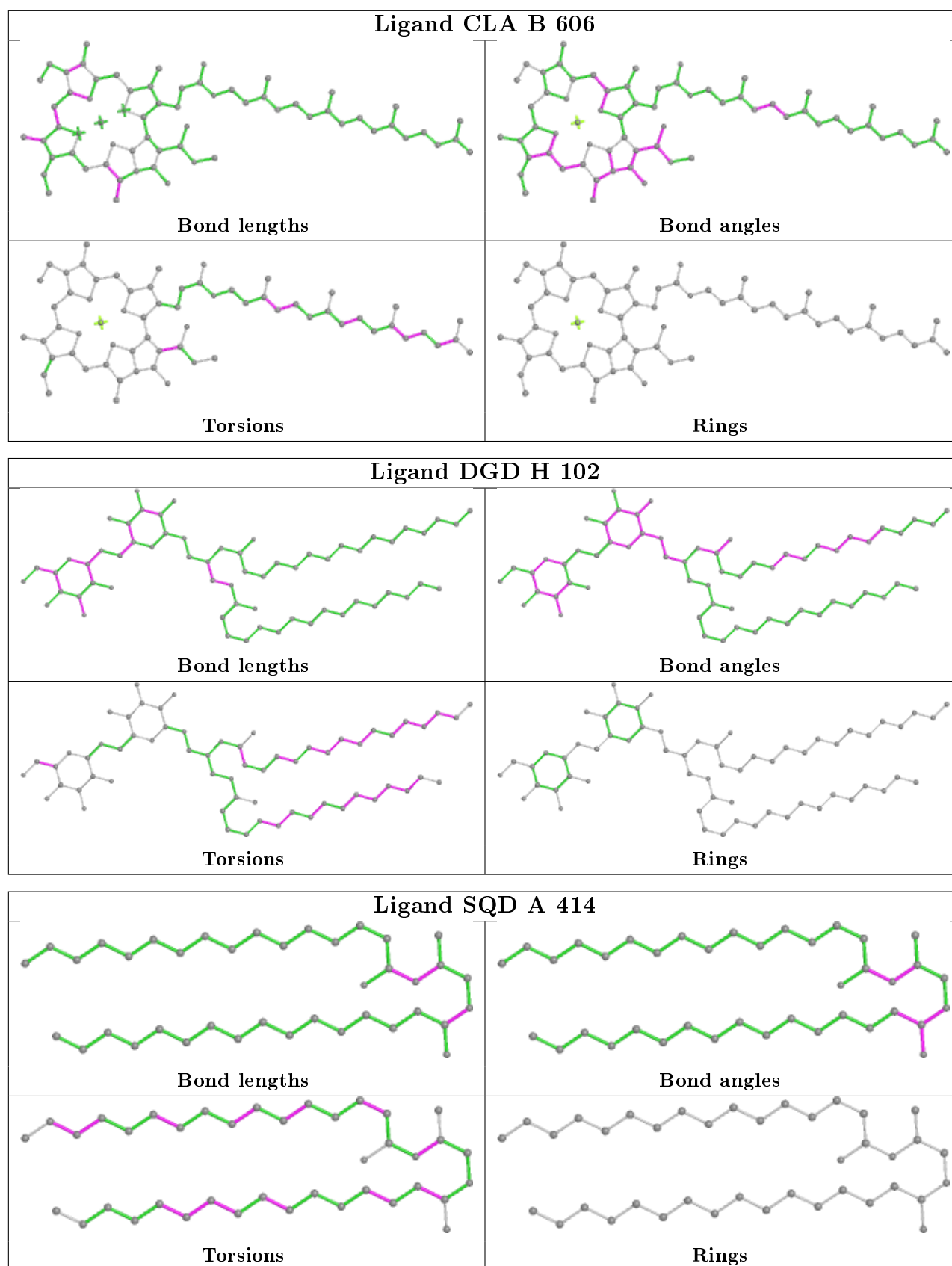


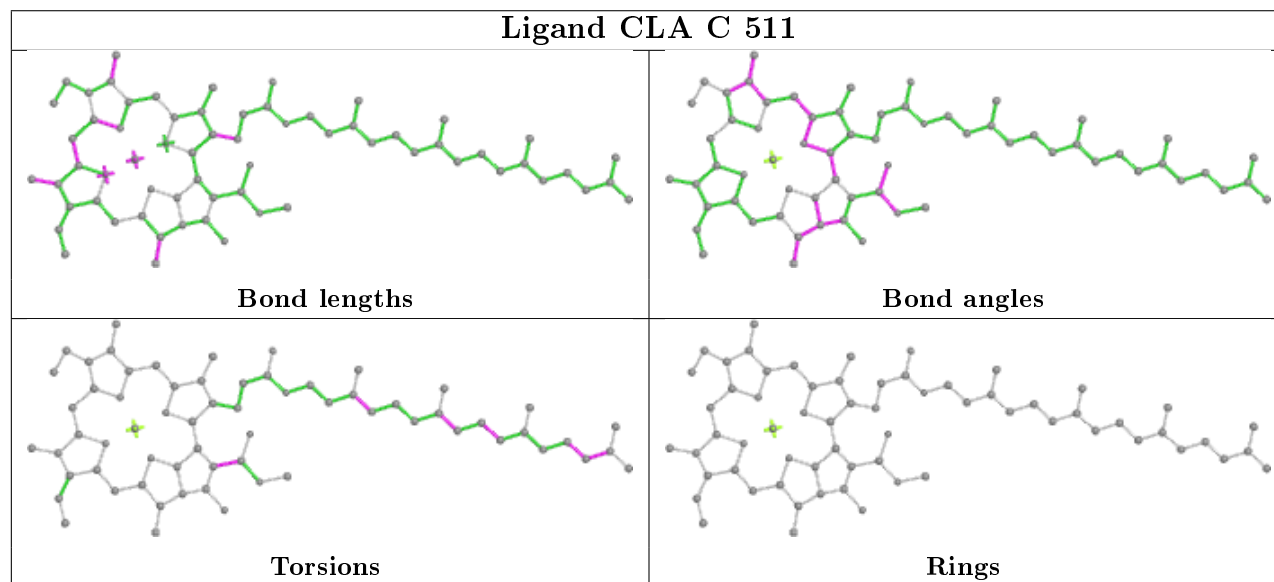
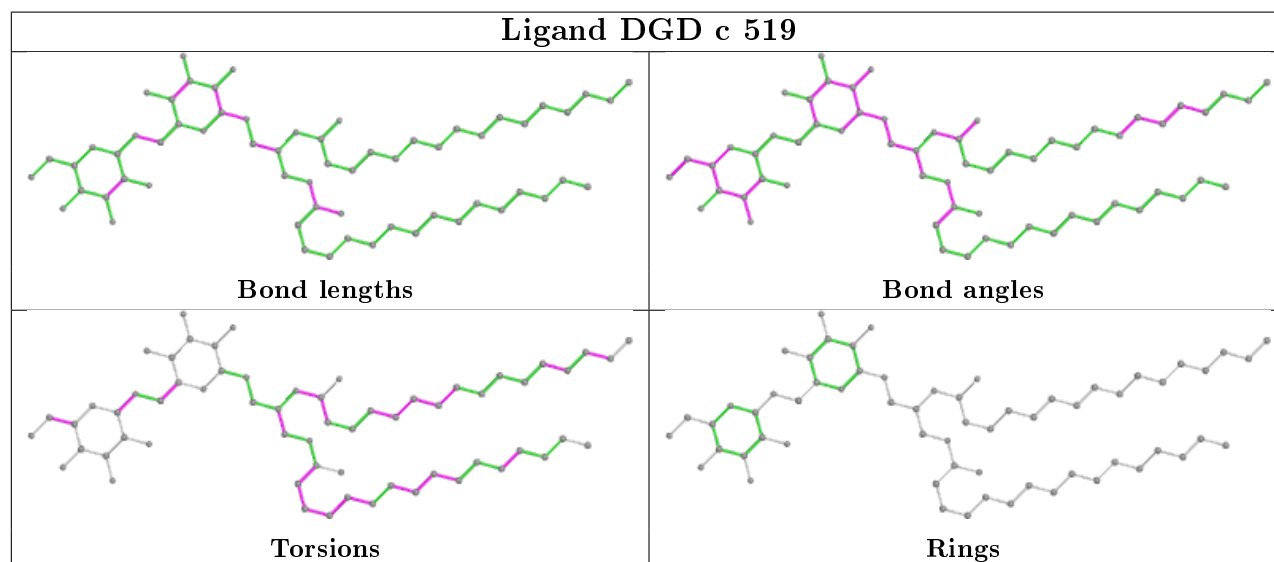
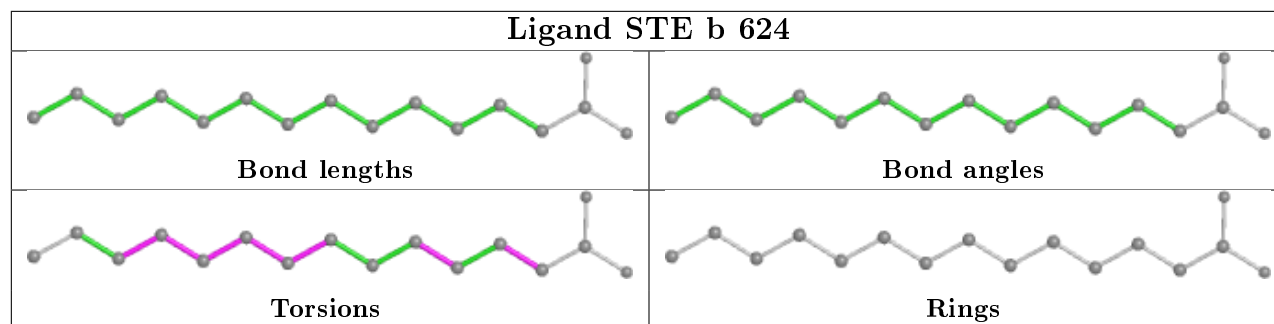
Ligand CLA C 510



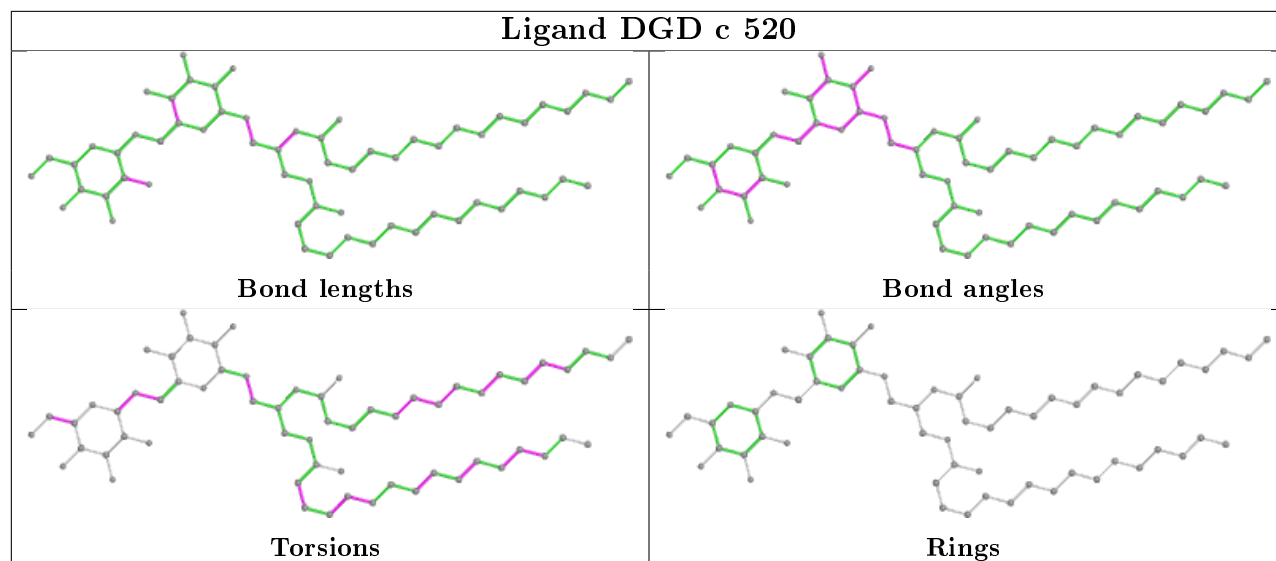
Ligand STE a 415



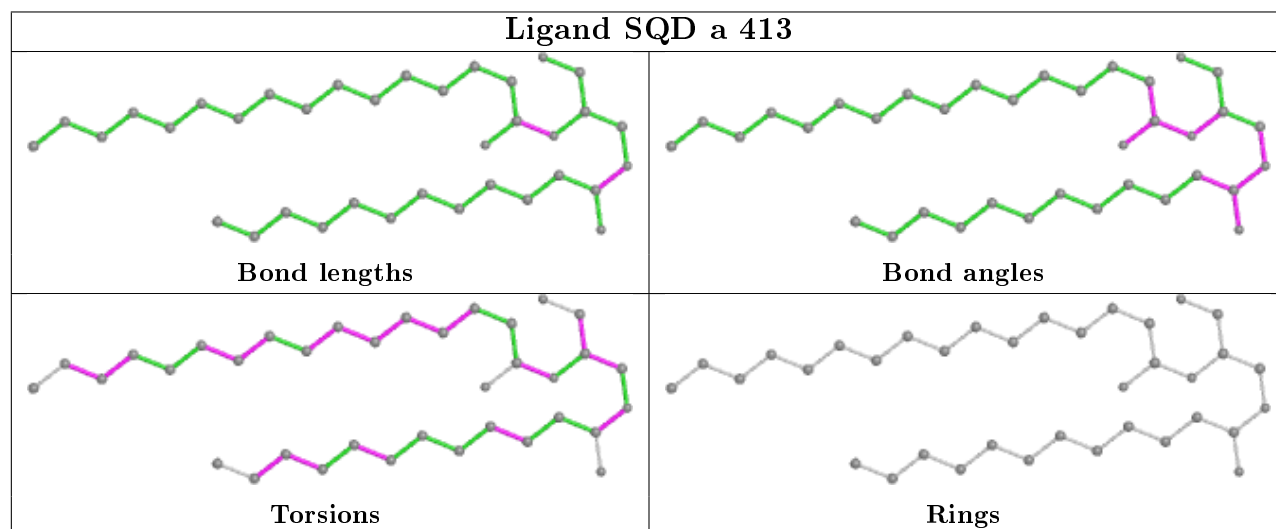




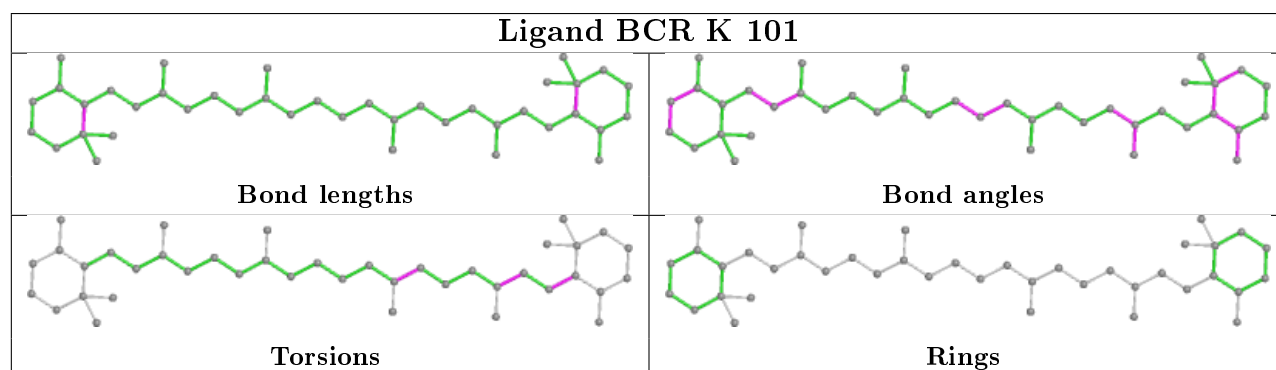
Ligand DGD c 520



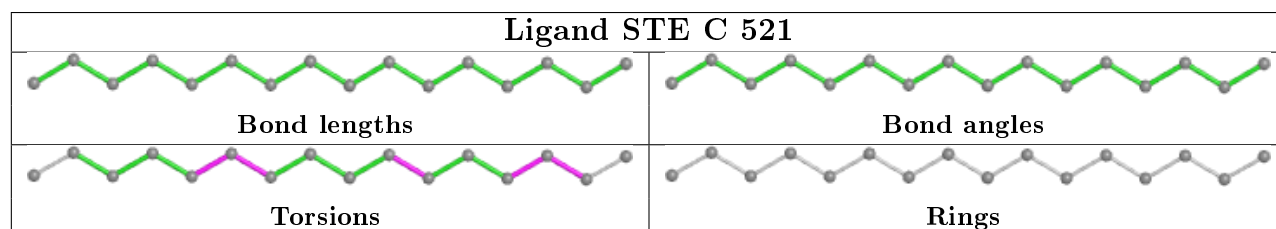
Ligand SQD a 413

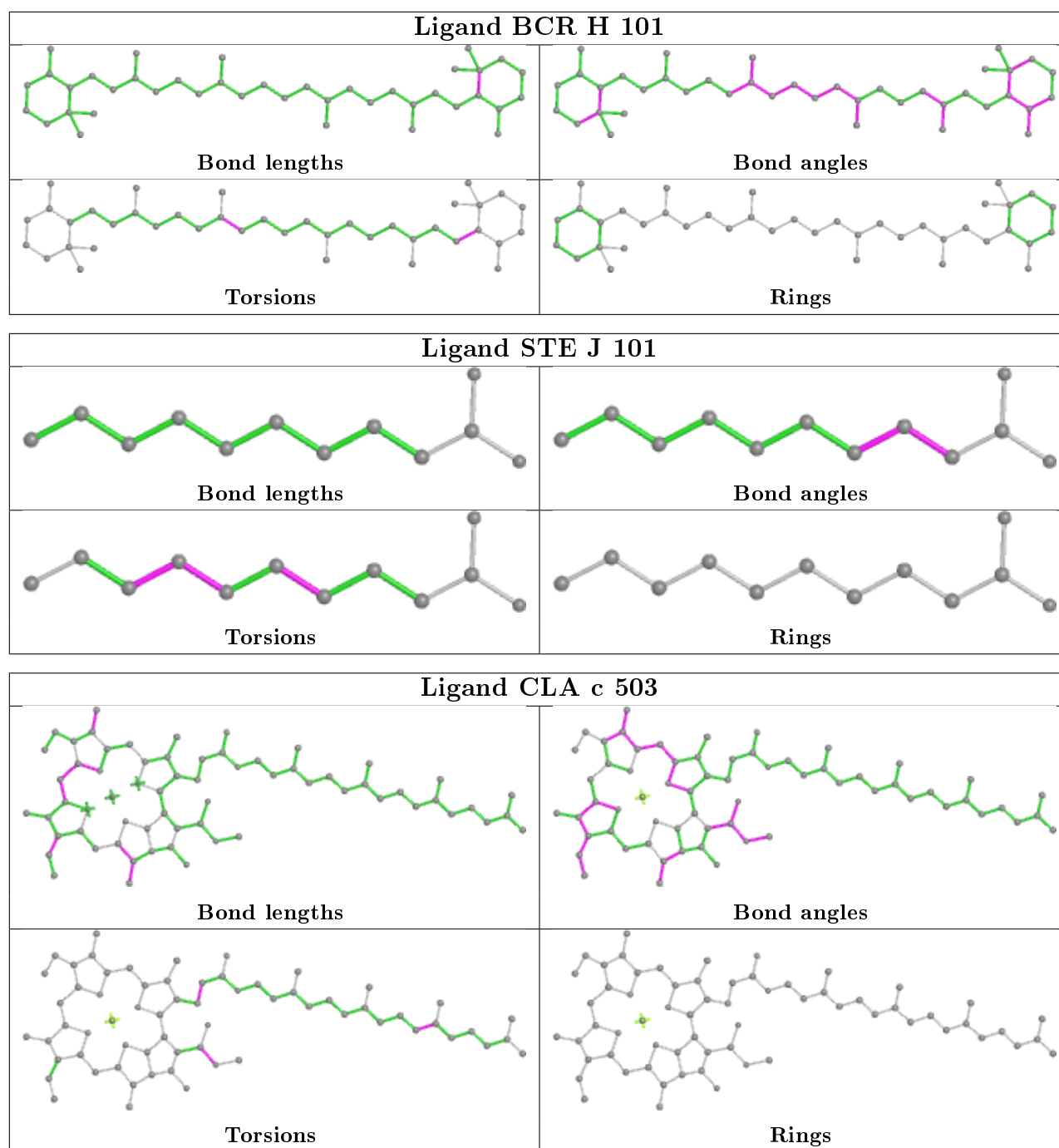


Ligand BCR K 101

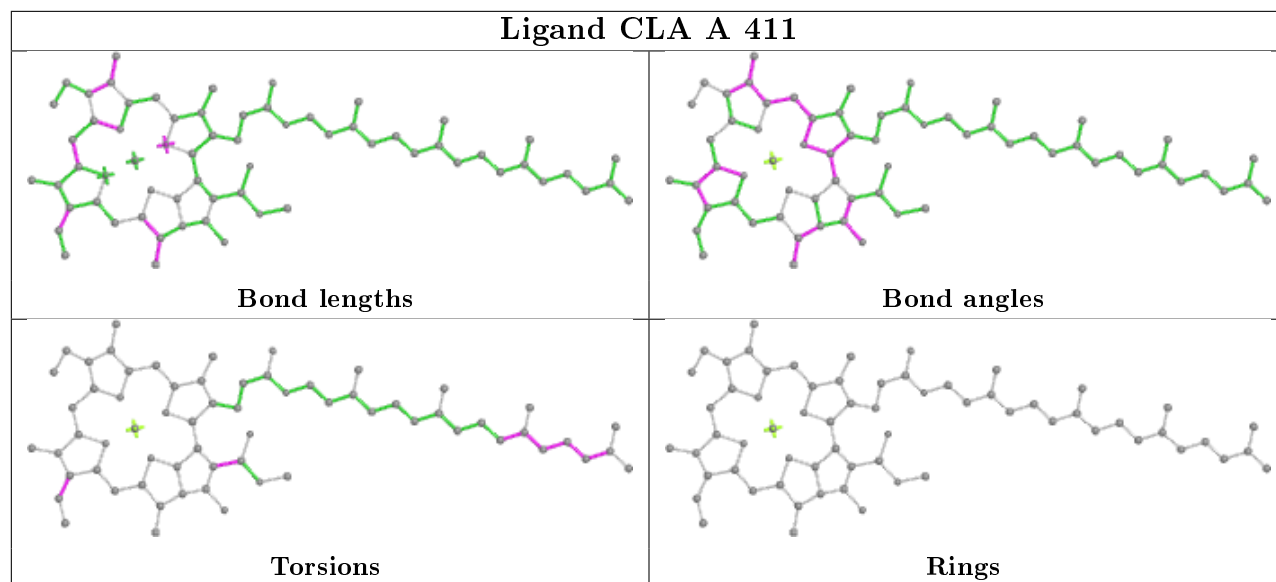


Ligand STE C 521

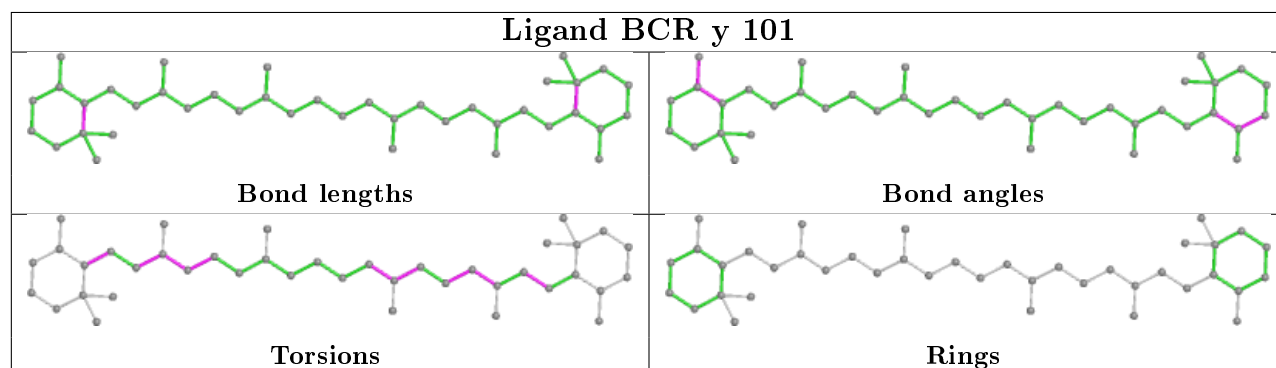




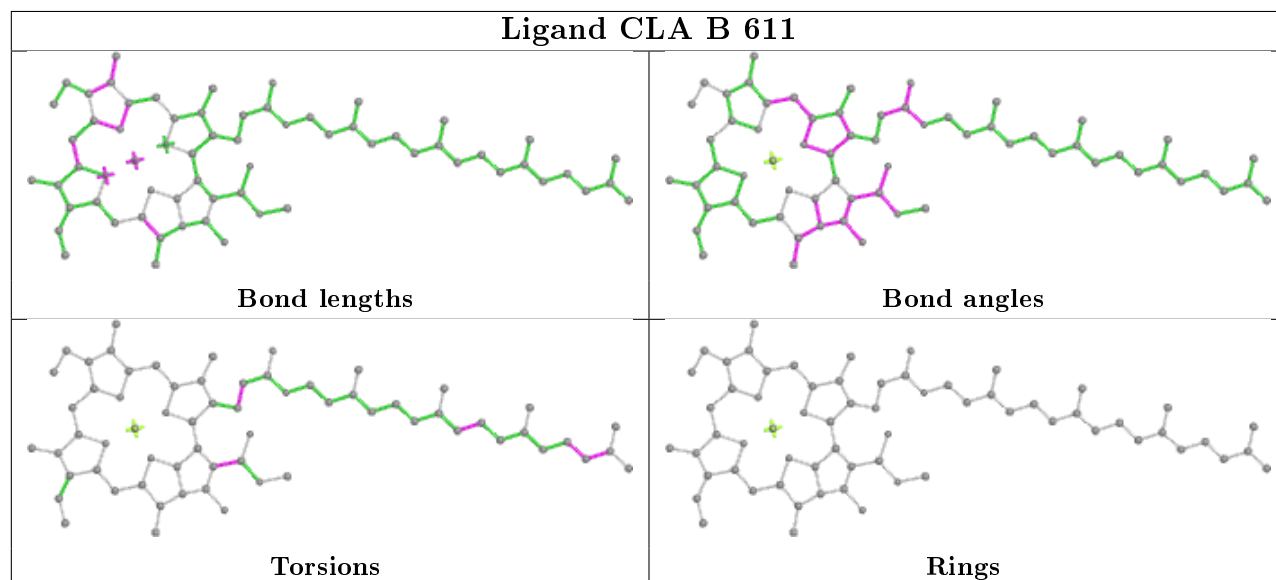
Ligand CLA A 411



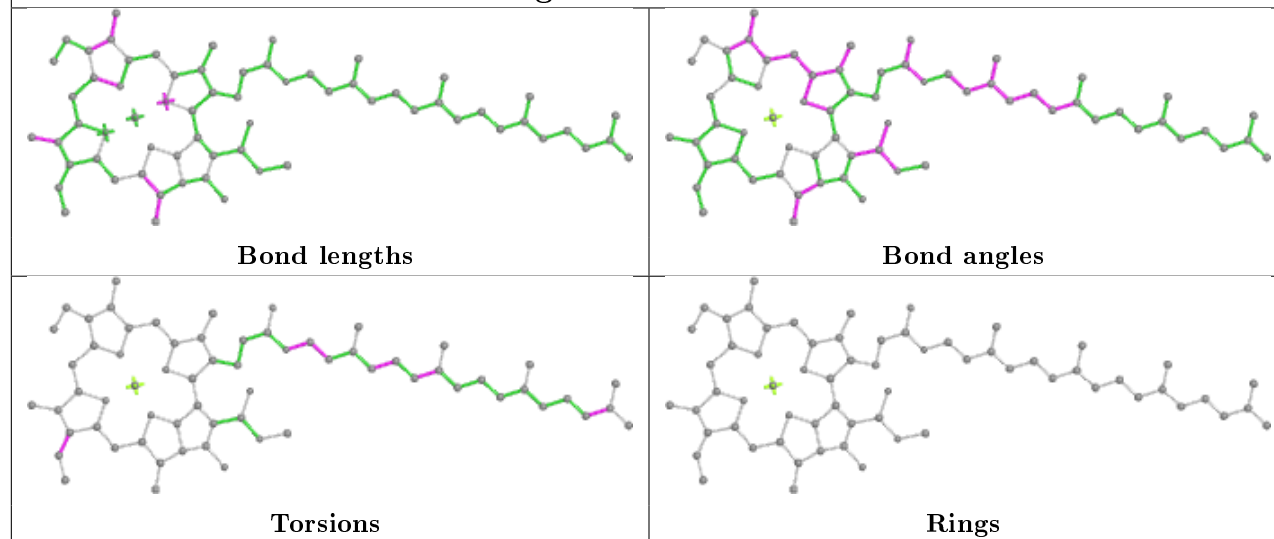
Ligand BCR y 101



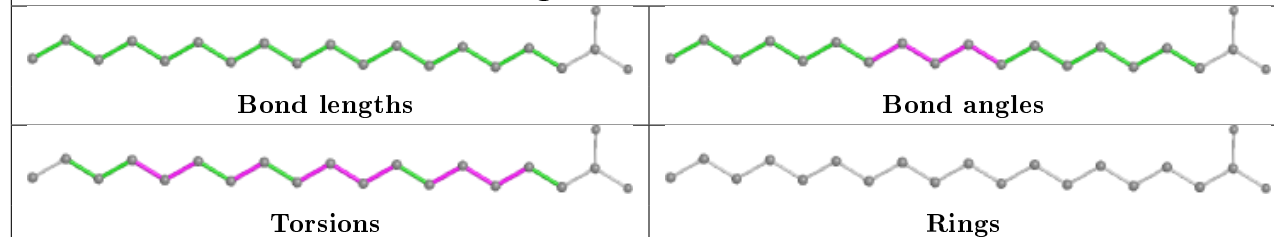
Ligand CLA B 611



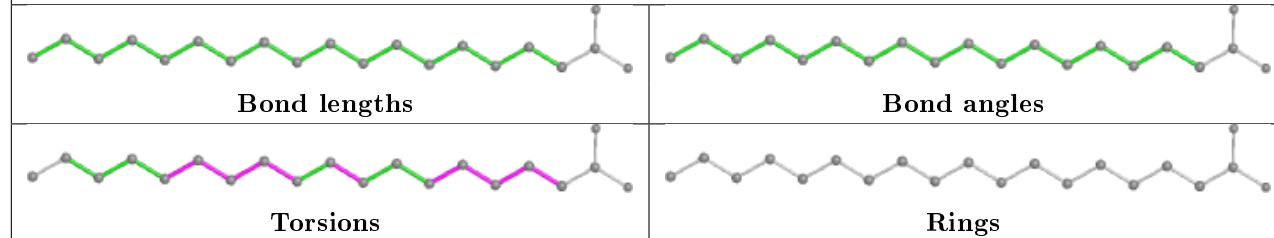
Ligand CLA d 402



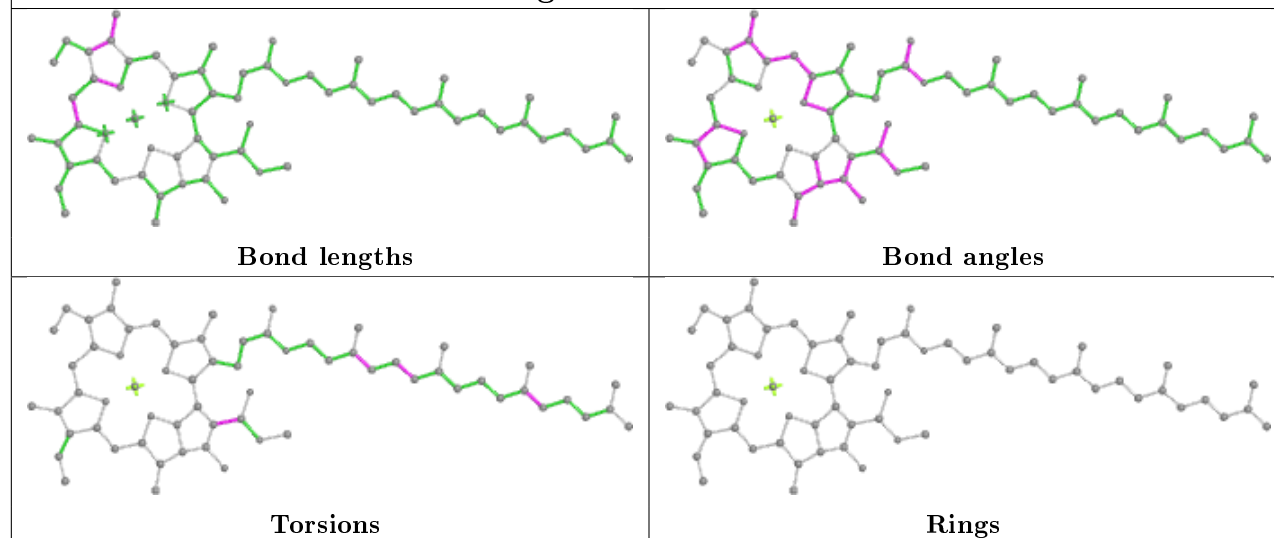
Ligand STE X 101

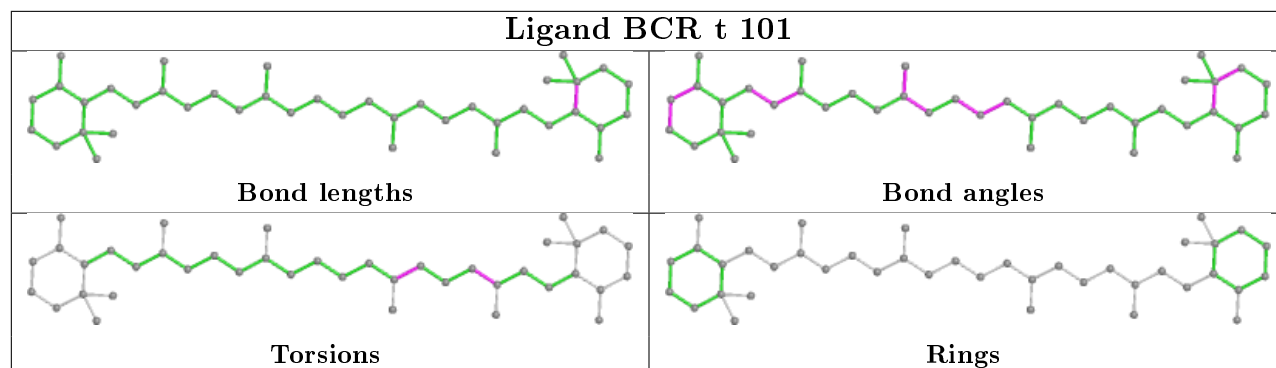
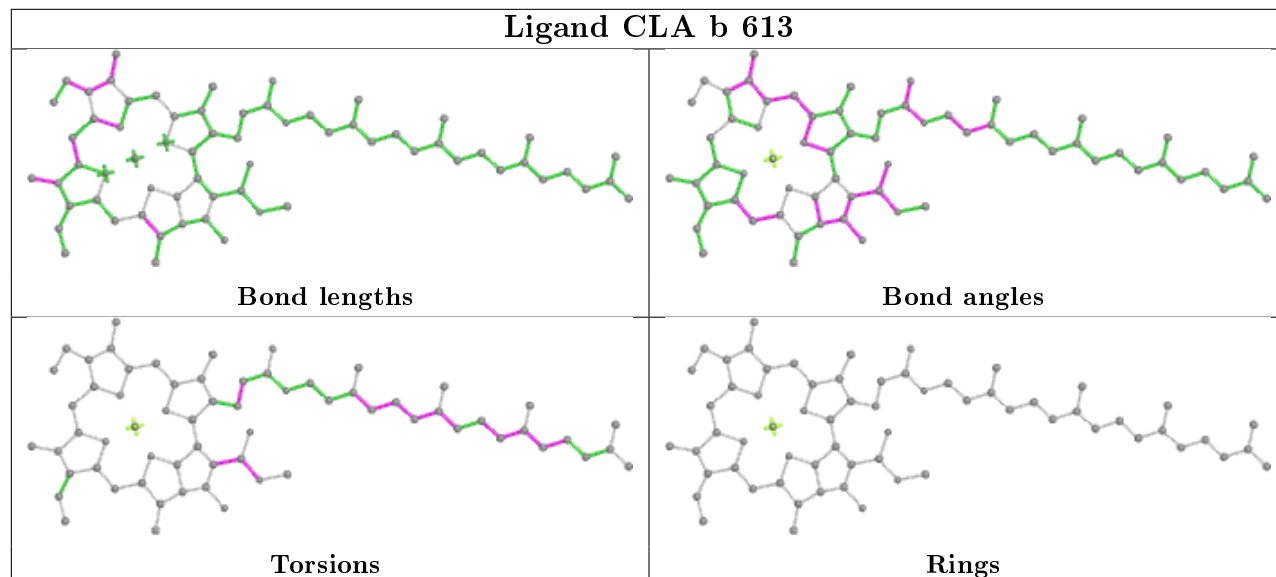
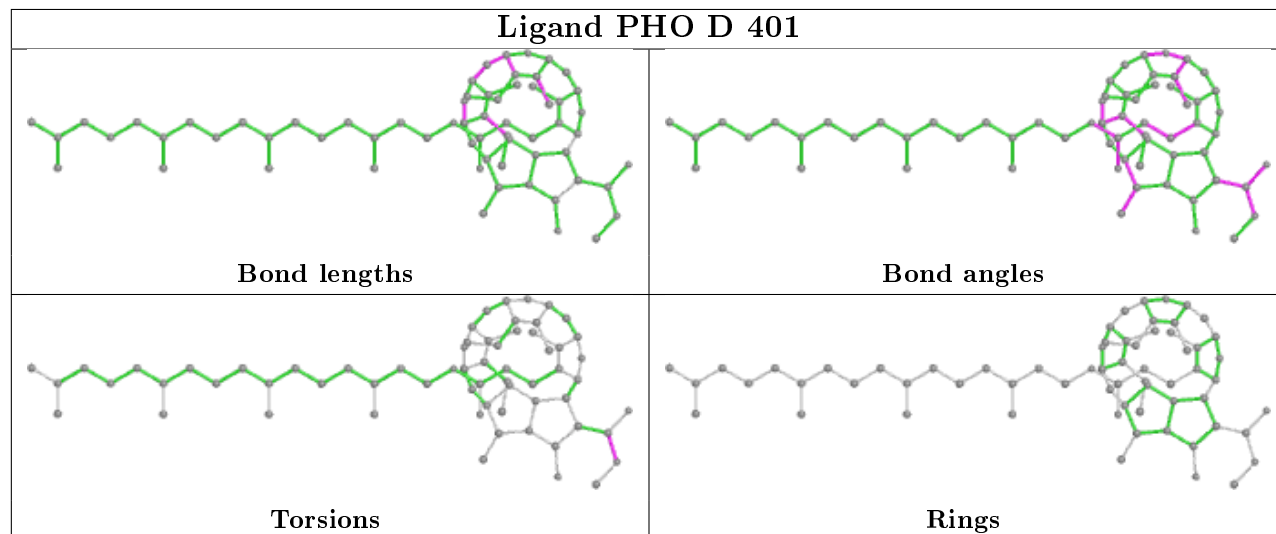


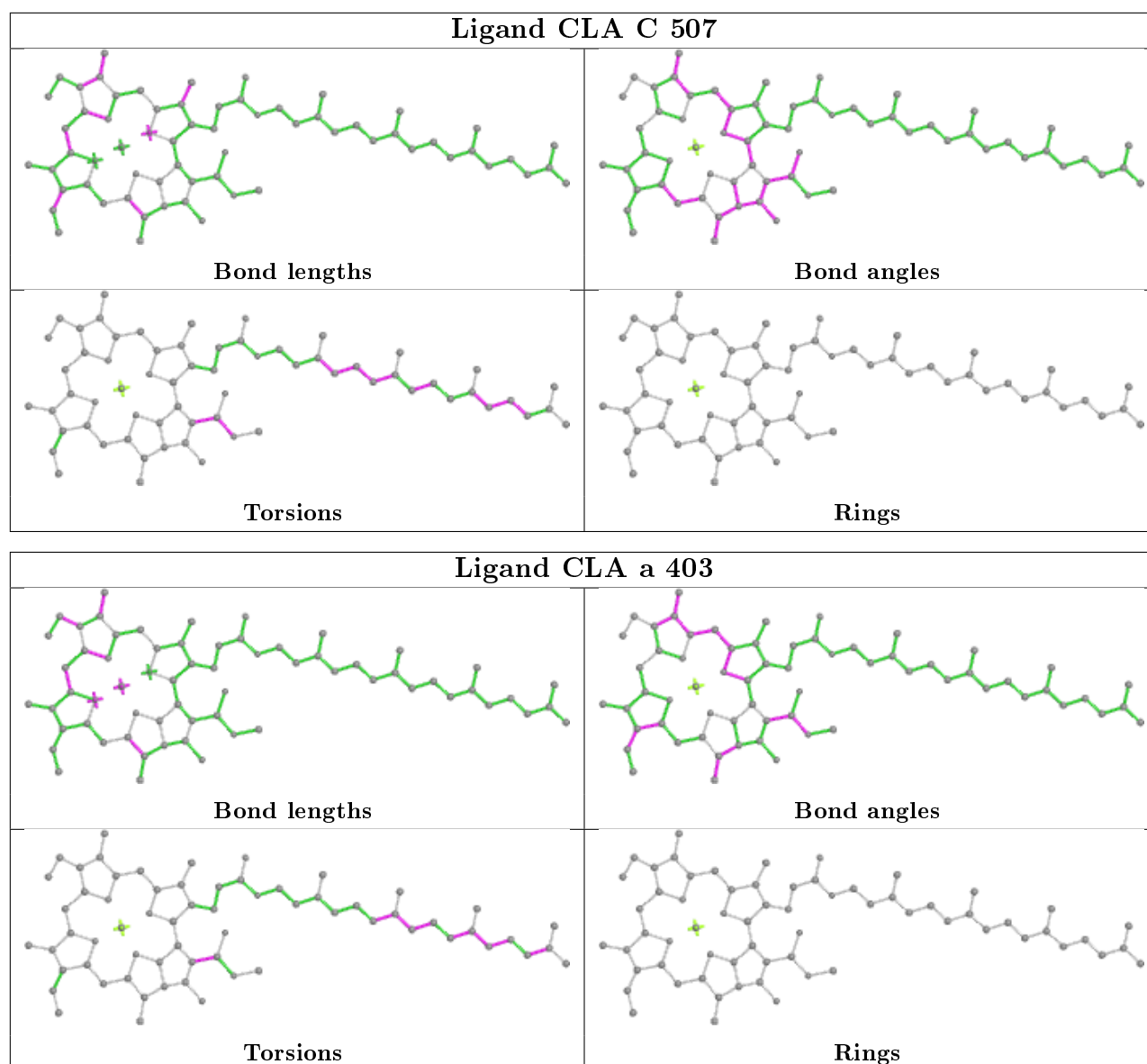
Ligand STE c 523



Ligand CLA c 509



Ligand BCR t 101**Ligand CLA b 613****Ligand PHO D 401**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	30:GLN	C	31:VAL	N	3.77

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.37	4 (1%) 79 82	21, 28, 44, 78	0
1	a	334/344 (97%)	-0.39	2 (0%) 89 91	22, 30, 52, 81	0
2	B	505/510 (99%)	-0.39	9 (1%) 68 72	24, 32, 58, 85	0
2	b	505/510 (99%)	-0.19	16 (3%) 47 54	22, 35, 68, 92	0
3	C	442/461 (95%)	-0.28	4 (0%) 84 86	25, 34, 49, 69	0
3	c	451/461 (97%)	-0.22	8 (1%) 68 72	26, 37, 59, 91	0
4	D	341/352 (96%)	-0.34	1 (0%) 94 94	23, 29, 44, 75	0
4	d	341/352 (96%)	-0.32	1 (0%) 94 94	24, 33, 53, 74	0
5	E	82/84 (97%)	-0.03	3 (3%) 41 48	31, 48, 66, 80	0
5	e	82/84 (97%)	0.17	4 (4%) 29 35	37, 54, 72, 78	0
6	F	34/45 (75%)	-0.43	1 (2%) 51 57	33, 39, 57, 79	0
6	f	34/45 (75%)	-0.30	0 100 100	37, 46, 67, 83	0
7	H	65/66 (98%)	-0.09	0 100 100	30, 38, 55, 66	0
7	h	63/66 (95%)	0.26	5 (7%) 12 16	36, 45, 61, 67	0
8	I	35/38 (92%)	-0.18	2 (5%) 23 29	31, 37, 67, 78	0
8	i	35/38 (92%)	-0.12	3 (8%) 10 13	30, 38, 73, 84	0
9	J	36/40 (90%)	-0.03	3 (8%) 11 14	32, 46, 67, 85	0
9	j	36/40 (90%)	0.01	4 (11%) 5 7	33, 47, 82, 90	0
10	K	37/46 (80%)	0.10	2 (5%) 25 31	38, 48, 64, 70	0
10	k	37/46 (80%)	-0.05	1 (2%) 54 60	42, 50, 66, 72	0
11	L	37/37 (100%)	-0.47	1 (2%) 54 60	25, 29, 60, 70	0
11	l	36/37 (97%)	-0.25	3 (8%) 11 14	25, 29, 73, 83	0
12	M	32/36 (88%)	-0.12	0 100 100	27, 33, 60, 69	0
12	m	31/36 (86%)	-0.17	0 100 100	25, 33, 54, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.00	16 (6%) 18 23	24, 41, 79, 128	0
13	o	244/272 (89%)	-0.08	14 (5%) 23 29	26, 39, 77, 117	0
14	R	34/41 (82%)	1.64	13 (38%) 0 0	54, 63, 84, 102	0
14	r	31/41 (75%)	3.41	23 (74%) 0 0	65, 81, 96, 107	0
15	T	29/32 (90%)	-0.42	2 (6%) 16 21	25, 30, 59, 78	0
15	t	29/32 (90%)	-0.22	2 (6%) 16 21	28, 31, 80, 88	0
16	U	97/134 (72%)	-0.28	2 (2%) 63 68	31, 42, 65, 84	0
16	u	97/134 (72%)	-0.45	0 100 100	30, 39, 58, 77	0
17	V	137/163 (84%)	-0.49	0 100 100	30, 39, 54, 78	0
17	v	137/163 (84%)	-0.25	3 (2%) 62 66	31, 44, 64, 80	0
18	X	38/41 (92%)	-0.12	2 (5%) 26 32	35, 46, 67, 74	0
18	x	39/41 (95%)	0.26	4 (10%) 6 8	44, 51, 81, 94	0
19	Y	27/46 (58%)	1.13	7 (25%) 0 0	50, 65, 85, 98	0
19	y	30/46 (65%)	0.37	4 (13%) 3 4	56, 64, 82, 90	0
20	Z	62/62 (100%)	0.84	15 (24%) 0 0	49, 60, 102, 112	0
20	z	62/62 (100%)	0.75	10 (16%) 1 2	52, 65, 100, 110	0
All	All	5302/5700 (93%)	-0.18	194 (3%) 41 48	21, 36, 69, 128	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	8.5
13	o	58	ASN	8.4
20	Z	33	TRP	7.6
13	o	3	GLN	7.0
14	r	29	LYS	6.5
13	O	56	PRO	6.3
14	r	3	TRP	6.2
1	A	13	LEU	6.1
13	O	3	GLN	5.9
20	z	33	TRP	5.9
14	r	6	LEU	5.7
2	b	495	PHE	5.4
14	r	10	LEU	5.3
13	O	4	THR	5.2
9	j	5	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
14	r	25	PRO	5.2
13	o	57	LYS	5.1
13	O	59	LYS	5.1
14	r	31	VAL	5.1
14	R	3	TRP	5.1
20	Z	3	ILE	5.1
14	R	6	LEU	5.0
13	o	60	ARG	5.0
2	b	127	ARG	4.9
13	O	60	ARG	4.9
20	Z	61	VAL	4.8
14	r	28	VAL	4.7
13	O	61	GLN	4.6
20	Z	62	VAL	4.6
14	r	27	ALA	4.6
13	O	62	GLU	4.5
15	t	30	THR	4.5
20	z	35	ARG	4.5
14	r	9	LEU	4.4
13	o	56	PRO	4.4
5	e	79	PHE	4.4
1	a	11	ALA	4.3
9	J	5	GLY	4.3
13	O	57	LYS	4.3
3	c	143	TYR	4.3
18	X	2	THR	4.2
20	Z	35	ARG	4.2
14	R	32	GLN	4.2
13	o	4	THR	4.1
15	T	30	THR	4.1
14	r	24	LEU	4.1
1	A	11	ALA	4.1
14	r	13	LEU	4.0
7	h	21	VAL	4.0
3	c	24	THR	3.9
20	z	3	ILE	3.9
14	r	15	ALA	3.8
9	j	7	ARG	3.8
3	c	23	ALA	3.8
13	o	61	GLN	3.8
20	z	1	MET	3.7
13	O	5	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
13	O	63	ALA	3.6
19	Y	20	ALA	3.6
8	I	36	ASP	3.6
3	c	147	PHE	3.6
19	Y	43	ARG	3.6
19	Y	25	ILE	3.6
20	z	7	LEU	3.6
3	C	146	PHE	3.5
14	r	18	TRP	3.5
2	b	486	LEU	3.5
13	O	246	ALA	3.5
3	c	146	PHE	3.5
9	J	7	ARG	3.5
20	Z	42	LEU	3.4
18	x	38	GLN	3.4
14	r	14	LEU	3.3
20	Z	1	MET	3.3
13	o	207	ARG	3.3
8	I	34	ARG	3.3
20	Z	7	LEU	3.3
9	J	8	ILE	3.3
19	y	18	VAL	3.3
20	Z	32	ASP	3.2
18	x	40	SER	3.2
13	O	35	SER	3.2
2	b	487	SER	3.2
20	z	41	PHE	3.2
5	E	3	GLY	3.1
14	r	5	VAL	3.1
19	Y	40	ALA	3.1
13	o	62	GLU	3.1
5	E	79	PHE	3.1
14	R	28	VAL	3.1
20	Z	4	LEU	3.0
14	r	23	ILE	3.0
14	r	26	TYR	3.0
20	Z	34	ASP	3.0
13	O	58	ASN	3.0
14	R	21	ARG	3.0
8	i	36	ASP	2.9
14	r	2	ASP	2.9
2	b	506	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
5	e	61	ARG	2.9
2	b	505	ARG	2.9
13	O	55	GLU	2.9
20	z	62	VAL	2.9
13	o	63	ALA	2.9
15	t	28	ARG	2.9
20	z	36	SER	2.8
7	h	6	TRP	2.8
1	A	12	ASN	2.8
19	Y	37	PHE	2.8
20	z	60	PHE	2.8
2	b	293	ALA	2.8
2	B	486	LEU	2.8
2	B	502	VAL	2.7
3	c	25	ASN	2.7
7	h	10	ILE	2.7
2	b	491	VAL	2.7
11	l	2	GLU	2.7
11	l	3	PRO	2.6
19	Y	41	VAL	2.6
8	i	35	LYS	2.6
8	i	34	ARG	2.6
6	F	12	SER	2.6
14	R	25	PRO	2.6
13	o	246	ALA	2.6
17	v	15	GLU	2.6
20	Z	30	PRO	2.6
19	y	19	ILE	2.6
20	Z	37	LYS	2.5
3	C	57	ALA	2.5
18	x	34	ILE	2.5
16	U	8	GLU	2.5
2	b	128	THR	2.5
2	B	373	LYS	2.5
9	j	8	ILE	2.5
10	K	17	ILE	2.5
2	B	293	ALA	2.5
2	B	127	ARG	2.4
5	e	83	LEU	2.4
2	b	502	VAL	2.4
2	B	86	ILE	2.4
3	C	143	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
17	v	21	LEU	2.4
14	r	21	ARG	2.4
2	B	490	GLN	2.3
2	b	289	GLN	2.3
15	T	29	ILE	2.3
14	R	34	LEU	2.3
20	Z	38	GLN	2.3
2	b	295	GLY	2.3
13	o	59	LYS	2.3
7	h	25	TRP	2.3
18	X	3	ILE	2.3
14	R	2	ASP	2.3
2	b	503	THR	2.3
14	R	18	TRP	2.3
14	R	24	LEU	2.3
7	h	22	ALA	2.3
2	b	492	GLU	2.3
13	O	36	GLN	2.2
1	A	15	GLU	2.2
14	R	26	TYR	2.2
2	B	495	PHE	2.2
4	d	227[A]	GLU	2.2
16	U	9	LEU	2.2
20	Z	60	PHE	2.2
9	j	6	GLY	2.2
14	r	19	ALA	2.2
2	b	292	LEU	2.2
20	z	42	LEU	2.2
14	r	22	ASN	2.2
2	B	505	ARG	2.1
10	K	14	ALA	2.1
13	o	55	GLU	2.1
14	R	31	VAL	2.1
13	o	34	SER	2.1
19	y	37	PHE	2.1
3	c	57	ALA	2.1
5	e	84	LYS	2.1
18	x	2	THR	2.1
1	a	144	CYS	2.1
19	Y	42	ARG	2.1
13	O	25	THR	2.1
5	E	65	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
11	l	7	ARG	2.1
14	r	30	GLN	2.1
17	v	22	THR	2.1
3	C	60	ILE	2.0
4	D	12	ARG	2.0
19	y	43	ARG	2.0
10	k	10	LYS	2.0
14	R	29	LYS	2.0
11	L	2	GLU	2.0
3	c	262	ARG	2.0
2	b	161	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	FME	T	1	10/11	0.93	0.11	29,40,67,67	0
8	FME	i	1	10/11	0.96	0.17	37,46,63,63	0
15	FME	t	1	10/11	0.96	0.08	27,43,73,73	0
12	FME	M	1	10/11	0.97	0.12	42,52,69,73	0
8	FME	I	1	10/11	0.97	0.15	35,42,57,69	0
12	FME	m	1	10/11	0.97	0.13	32,49,65,76	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	STE	L	101	12/20	0.72	0.17	45,61,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	STE	b	626	10/20	0.74	0.24	43,58,68,71	0
33	STE	E	102	12/20	0.74	0.28	42,72,79,86	0
33	STE	H	103	18/20	0.75	0.25	49,70,84,84	0
33	STE	b	625	20/20	0.78	0.20	47,64,79,85	0
33	STE	a	415	12/20	0.78	0.26	39,68,76,84	0
33	STE	B	627	16/20	0.79	0.23	42,64,79,80	0
33	STE	h	103	14/20	0.80	0.23	50,65,88,91	0
29	SQD	a	413	36/54	0.80	0.17	31,61,87,90	0
30	DGD	A	415	66/66	0.81	0.16	41,62,85,89	0
34	LHG	E	101	49/49	0.81	0.20	46,74,98,118	0
33	STE	B	626	18/20	0.82	0.14	39,63,82,84	0
28	LMG	c	524	48/55	0.82	0.22	47,71,106,116	0
33	STE	c	501	12/20	0.82	0.26	45,66,83,85	0
34	LHG	e	102	42/49	0.83	0.23	61,78,99,119	0
28	LMG	D	410	33/55	0.83	0.18	33,53,78,93	0
29	SQD	A	414	39/54	0.83	0.17	38,63,93,102	0
22	CLA	C	513	65/65	0.83	0.17	33,54,85,98	0
33	STE	j	101	12/20	0.83	0.13	38,54,72,78	0
33	STE	c	523	20/20	0.83	0.18	40,59,79,87	0
33	STE	a	414	10/20	0.84	0.19	34,65,74,75	0
28	LMG	B	629	55/55	0.84	0.15	35,58,81,93	0
33	STE	d	411	20/20	0.84	0.22	33,57,73,77	0
24	BCR	H	101	40/40	0.84	0.15	22,44,58,70	0
24	BCR	x	101	40/40	0.84	0.13	29,48,66,73	0
33	STE	B	625	12/20	0.84	0.12	42,55,66,66	0
33	STE	B	628	15/20	0.85	0.14	39,62,75,80	0
28	LMG	b	623	55/55	0.85	0.29	49,77,101,110	0
22	CLA	h	101	65/65	0.86	0.15	37,64,87,99	0
33	STE	b	622	20/20	0.86	0.22	39,58,75,78	0
33	STE	B	601	12/20	0.86	0.38	44,63,83,88	0
28	LMG	c	525	49/55	0.86	0.15	35,54,95,112	0
33	STE	l	102	18/20	0.86	0.15	33,50,77,89	0
33	STE	b	620	16/20	0.87	0.17	35,50,75,81	0
33	STE	C	522	12/20	0.87	0.09	35,48,54,55	0
22	CLA	c	514	65/65	0.87	0.15	36,55,95,110	0
27	PL9	A	410	55/55	0.87	0.21	35,65,88,95	0
33	STE	b	624	16/20	0.87	0.14	45,61,80,82	0
24	BCR	Y	101	40/40	0.87	0.12	34,49,67,72	0
33	STE	C	521	16/20	0.87	0.12	38,51,63,70	0
29	SQD	b	619	49/54	0.87	0.15	42,60,97,99	0
24	BCR	y	101	40/40	0.87	0.12	38,59,75,79	0
27	PL9	a	410	55/55	0.87	0.19	36,67,87,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	STE	d	412	20/20	0.87	0.14	39,63,81,82	0
29	SQD	B	623	54/54	0.88	0.15	38,58,94,100	0
33	STE	I	101	15/20	0.88	0.15	38,55,74,78	0
33	STE	T	102	15/20	0.88	0.17	41,57,79,85	0
22	CLA	B	602	65/65	0.88	0.15	30,57,92,101	0
33	STE	B	621	17/20	0.88	0.18	35,49,69,71	0
24	BCR	Z	101	40/40	0.89	0.14	38,56,69,70	0
22	CLA	C	514	65/65	0.89	0.17	39,62,91,98	0
28	LMG	A	412	48/55	0.89	0.14	36,54,79,101	0
22	CLA	c	515	65/65	0.89	0.18	39,66,105,110	0
33	STE	M	102	15/20	0.90	0.13	34,48,62,68	0
22	CLA	c	504	65/65	0.90	0.14	27,42,62,69	0
33	STE	M	103	10/20	0.90	0.15	33,49,60,63	0
28	LMG	c	522	37/55	0.90	0.16	42,64,82,91	0
33	STE	X	101	20/20	0.90	0.14	27,50,73,76	0
24	BCR	d	404	40/40	0.90	0.12	28,48,86,102	0
22	CLA	d	403	65/65	0.91	0.15	26,46,89,103	0
22	CLA	c	510	64/65	0.91	0.14	30,45,86,105	0
22	CLA	C	503	65/65	0.91	0.14	24,39,61,66	0
24	BCR	c	516	40/40	0.91	0.15	43,58,71,73	0
22	CLA	b	614	65/65	0.91	0.13	23,39,56,60	0
33	STE	C	520	12/20	0.91	0.11	45,56,65,65	0
28	LMG	M	101	51/55	0.91	0.12	26,48,73,85	0
22	CLA	a	405	65/65	0.91	0.13	18,38,79,87	0
24	BCR	B	620	40/40	0.91	0.10	26,41,58,69	0
33	STE	d	410	17/20	0.92	0.10	38,52,60,66	0
22	CLA	D	403	65/65	0.92	0.12	21,42,102,116	0
22	CLA	b	615	60/65	0.92	0.13	26,42,84,93	0
22	CLA	B	607	65/65	0.92	0.11	21,35,74,78	0
29	SQD	f	101	41/54	0.92	0.17	47,78,110,116	0
33	STE	B	624	14/20	0.92	0.09	32,49,66,66	0
24	BCR	C	515	40/40	0.92	0.11	25,41,53,65	0
24	BCR	c	518	40/40	0.92	0.15	39,51,61,68	0
24	BCR	D	404	40/40	0.92	0.12	24,42,81,90	0
28	LMG	b	621	51/55	0.92	0.12	29,51,77,92	0
33	STE	Z	102	8/20	0.92	0.14	43,56,67,67	0
28	LMG	C	519	48/55	0.92	0.13	34,67,87,93	0
28	LMG	D	411	28/55	0.92	0.13	25,49,62,67	0
28	LMG	D	406	51/55	0.92	0.16	28,54,88,96	0
22	CLA	c	509	65/65	0.92	0.14	27,43,57,64	0
22	CLA	C	508	65/65	0.93	0.13	21,38,53,59	0
22	CLA	B	616	65/65	0.93	0.12	22,36,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	508	65/65	0.93	0.12	27,46,95,106	0
22	CLA	B	615	65/65	0.93	0.16	22,35,80,90	0
29	SQD	a	412	54/54	0.93	0.15	38,64,93,96	0
22	CLA	b	601	65/65	0.93	0.15	25,42,62,70	0
30	DGD	C	517	62/66	0.93	0.12	27,50,99,120	0
24	BCR	b	618	40/40	0.93	0.10	26,44,66,67	0
22	CLA	C	506	65/65	0.93	0.17	23,40,69,82	0
33	STE	J	101	12/20	0.93	0.09	45,60,72,73	0
22	CLA	b	608	65/65	0.93	0.14	29,43,57,64	0
24	BCR	b	617	40/40	0.93	0.11	25,40,55,61	0
22	CLA	c	512	65/65	0.93	0.15	30,46,62,71	0
30	DGD	h	102	62/66	0.93	0.11	24,49,65,74	0
22	CLA	c	513	65/65	0.93	0.12	38,53,68,75	0
22	CLA	C	507	65/65	0.93	0.12	22,40,87,99	0
22	CLA	c	505	65/65	0.94	0.15	30,43,53,59	0
24	BCR	B	619	40/40	0.94	0.09	23,38,49,57	0
22	CLA	b	607	65/65	0.94	0.13	23,39,59,62	0
22	CLA	C	504	65/65	0.94	0.14	24,40,54,56	0
30	DGD	c	521	62/66	0.94	0.13	28,52,93,108	0
22	CLA	b	605	65/65	0.94	0.11	25,39,73,80	0
22	CLA	C	512	65/65	0.94	0.11	27,48,66,70	0
28	LMG	d	409	44/55	0.94	0.12	28,50,79,91	0
30	DGD	c	520	62/66	0.94	0.10	32,50,88,94	0
22	CLA	c	507	65/65	0.94	0.15	25,39,67,76	0
24	BCR	K	101	40/40	0.94	0.14	30,48,58,62	0
22	CLA	B	617	60/65	0.94	0.13	21,38,87,94	0
29	SQD	D	407	36/54	0.94	0.14	43,66,86,99	0
27	PL9	D	405	55/55	0.94	0.10	20,33,48,49	0
22	CLA	C	509	65/65	0.94	0.12	25,43,98,114	0
24	BCR	c	517	40/40	0.94	0.11	25,43,60,62	0
22	CLA	c	511	65/65	0.94	0.16	30,45,62,67	0
22	CLA	B	605	65/65	0.94	0.11	19,34,72,81	0
22	CLA	c	506	60/65	0.94	0.11	29,42,79,84	0
24	BCR	t	101	40/40	0.94	0.10	23,38,51,53	0
22	CLA	b	611	65/65	0.94	0.16	21,35,52,56	0
22	CLA	a	403	65/65	0.94	0.13	24,41,95,107	0
22	CLA	b	604	65/65	0.95	0.12	18,35,50,58	0
30	DGD	C	518	62/66	0.95	0.11	26,46,75,85	0
22	CLA	b	610	65/65	0.95	0.13	21,34,53,59	0
22	CLA	d	402	65/65	0.95	0.11	18,35,52,67	0
24	BCR	A	406	40/40	0.95	0.08	22,34,47,51	0
23	PHO	d	401	64/64	0.95	0.10	26,37,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	BCR	B	618	40/40	0.95	0.11	27,39,57,69	0
22	CLA	C	502	65/65	0.95	0.12	20,34,53,55	0
22	CLA	C	510	65/65	0.95	0.17	24,43,64,68	0
24	BCR	b	616	40/40	0.95	0.10	21,41,52,59	0
30	DGD	H	102	62/66	0.95	0.10	26,43,58,61	0
24	BCR	a	406	40/40	0.95	0.08	19,33,47,52	0
22	CLA	b	609	65/65	0.95	0.17	23,39,51,57	0
22	CLA	C	511	65/65	0.95	0.13	26,43,58,66	0
22	CLA	b	603	65/65	0.95	0.13	17,37,85,98	0
22	CLA	C	505	59/65	0.95	0.12	27,40,78,90	0
22	CLA	A	405	54/65	0.95	0.10	18,33,61,69	0
34	LHG	l	101	49/49	0.95	0.10	31,43,60,69	0
24	BCR	T	101	40/40	0.95	0.09	21,38,55,67	0
22	CLA	A	403	65/65	0.95	0.13	22,36,90,100	0
22	CLA	c	503	65/65	0.95	0.12	22,40,53,61	0
22	CLA	A	411	65/65	0.95	0.10	16,27,54,64	0
34	LHG	d	408	39/49	0.95	0.11	28,45,68,75	0
22	CLA	B	611	65/65	0.95	0.14	19,33,46,47	0
22	CLA	B	603	65/65	0.95	0.14	22,37,54,60	0
22	CLA	B	610	65/65	0.95	0.12	23,37,58,69	0
22	CLA	B	613	65/65	0.95	0.15	17,33,49,53	0
22	CLA	b	612	65/65	0.95	0.14	19,33,72,90	0
29	SQD	A	413	52/54	0.95	0.14	28,56,88,98	0
22	CLA	b	613	65/65	0.95	0.12	22,40,81,91	0
22	CLA	B	614	65/65	0.95	0.14	18,31,67,71	0
30	DGD	C	516	62/66	0.95	0.11	21,39,75,91	0
30	DGD	c	519	62/66	0.96	0.10	22,41,74,96	0
34	LHG	D	412	49/49	0.96	0.12	27,43,71,77	0
22	CLA	b	602	65/65	0.96	0.13	22,36,67,77	0
22	CLA	B	608	65/65	0.96	0.10	17,34,65,74	0
35	HEC	F	101	43/43	0.96	0.11	26,44,64,66	0
23	PHO	a	404	64/64	0.96	0.12	17,31,42,45	0
27	PL9	d	405	55/55	0.96	0.10	19,34,45,46	0
34	LHG	D	409	47/49	0.96	0.11	27,48,87,104	0
22	CLA	a	411	65/65	0.96	0.10	19,29,45,50	0
35	HEC	e	101	43/43	0.96	0.12	36,52,72,81	0
22	CLA	a	402	65/65	0.96	0.10	18,29,47,59	0
22	CLA	D	402	65/65	0.96	0.10	13,30,52,59	0
23	PHO	A	404	64/64	0.96	0.10	18,28,37,39	0
22	CLA	B	604	65/65	0.96	0.14	17,34,61,63	0
34	LHG	d	406	49/49	0.96	0.12	32,48,82,87	0
22	CLA	A	402	65/65	0.96	0.09	15,27,42,61	0

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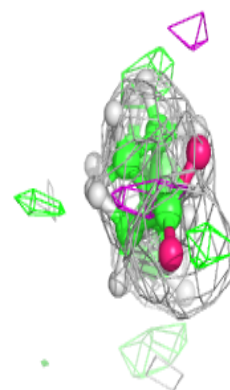
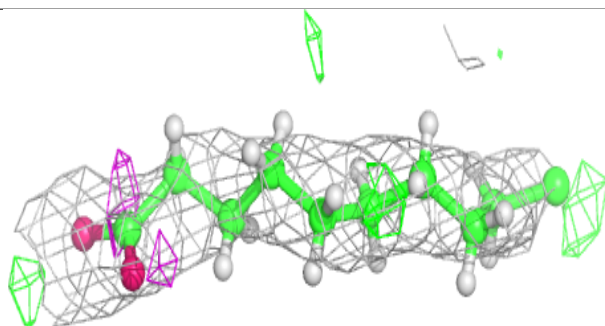
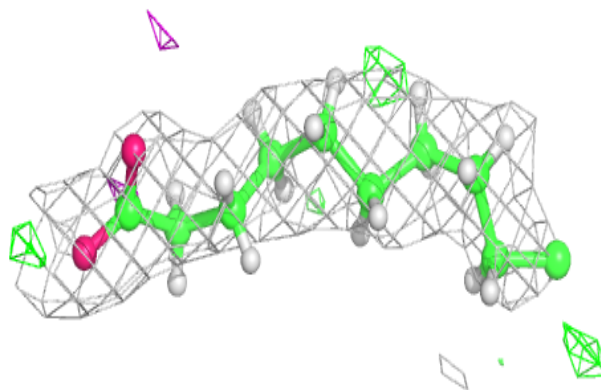
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	606	65/65	0.96	0.13	21,33,47,52	0
22	CLA	B	609	65/65	0.96	0.11	21,36,57,63	0
26	BCT	a	409	4/4	0.96	0.19	26,33,40,48	0
23	PHO	D	401	64/64	0.96	0.12	23,34,44,48	0
22	CLA	b	606	65/65	0.96	0.12	19,36,71,78	0
22	CLA	B	612	65/65	0.96	0.14	21,32,51,52	0
35	HEC	v	201	43/43	0.97	0.13	25,37,45,48	0
34	LHG	D	408	49/49	0.97	0.10	18,41,53,59	0
34	LHG	d	407	49/49	0.97	0.10	25,42,55,61	0
34	LHG	B	622	49/49	0.97	0.10	25,41,56,64	0
35	HEC	V	201	43/43	0.98	0.11	21,31,44,53	0
31	OEX	A	416[A]	10/10	0.99	0.13	25,30,31,31	10
26	BCT	A	409	4/4	0.99	0.18	31,33,36,43	0
25	CL	A	408	1/1	0.99	0.02	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.08	28,28,28,28	0
25	CL	a	408	1/1	0.99	0.03	28,28,28,28	0
21	FE2	a	401	1/1	0.99	0.08	34,34,34,34	0
25	CL	A	407	1/1	0.99	0.06	27,27,27,27	0
31	OEX	a	416[A]	10/10	0.99	0.11	27,28,30,30	10
32	OXY	A	417[B]	11/11	0.99	0.13	21,27,31,34	11
32	OXY	a	417[B]	11/11	0.99	0.11	22,26,28,31	11
21	FE2	A	401	1/1	1.00	0.08	26,26,26,26	0

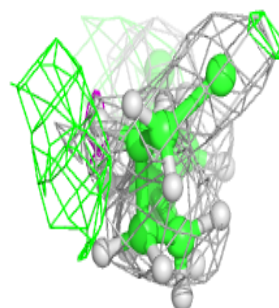
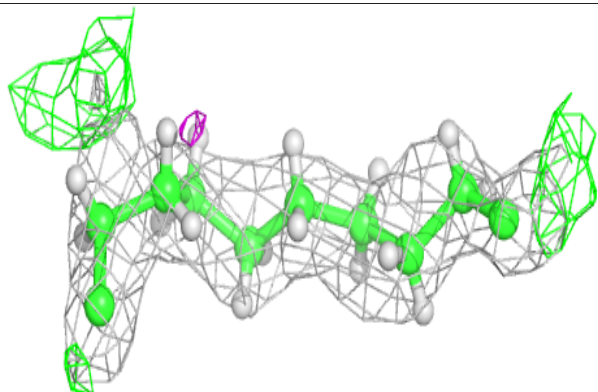
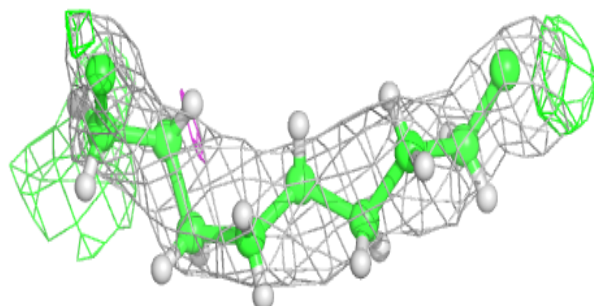
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE L 101:

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

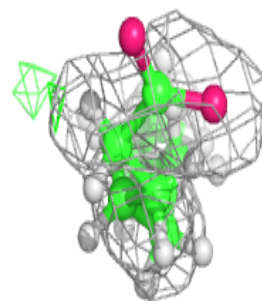
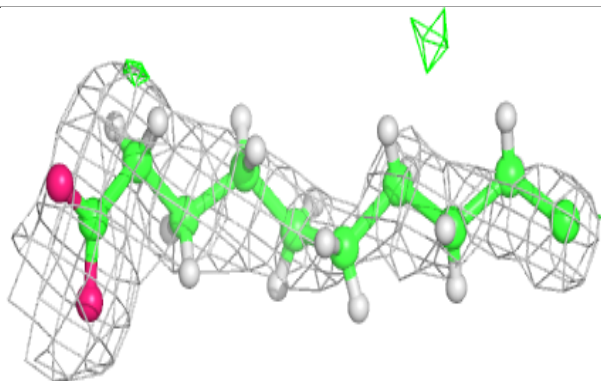
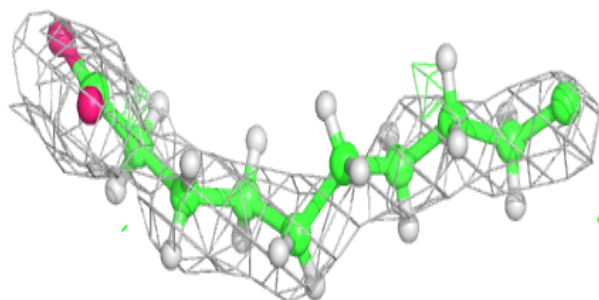
**Electron density around STE b 626:**

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

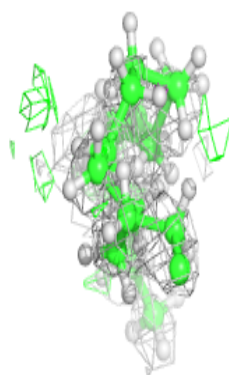
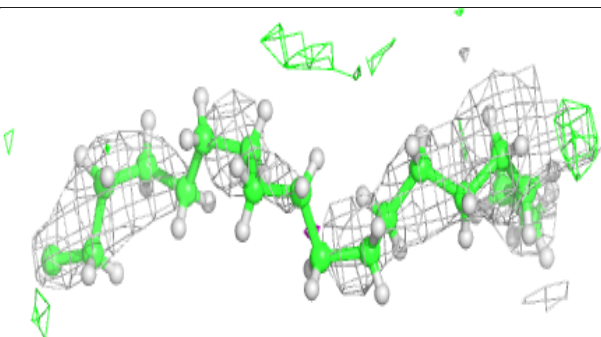
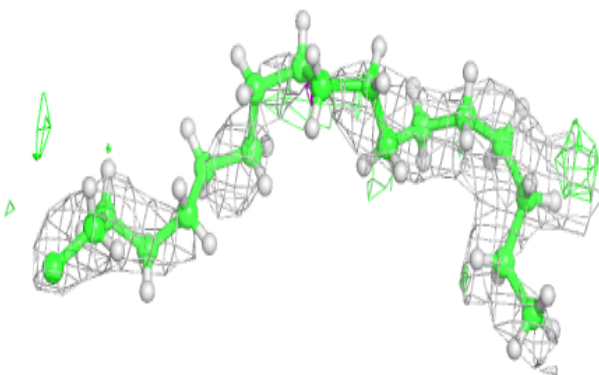


Electron density around STE E 102:

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

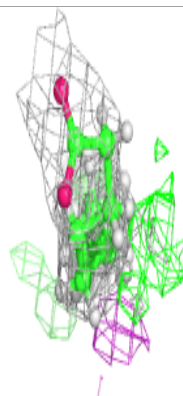
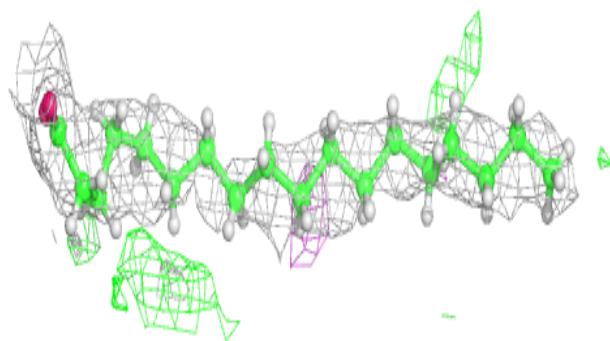
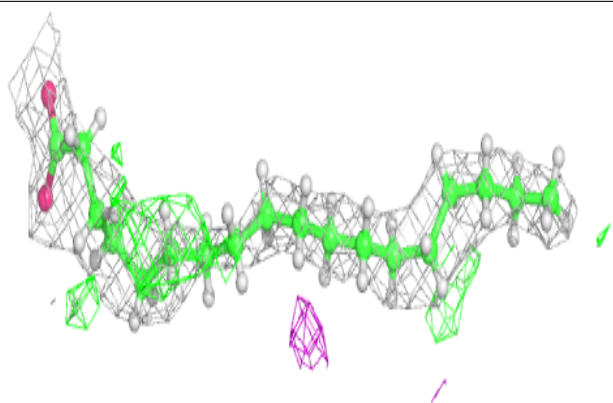
**Electron density around STE H 103:**

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

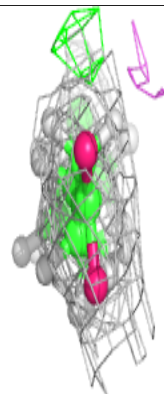
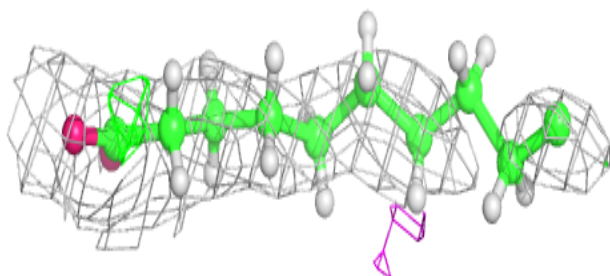
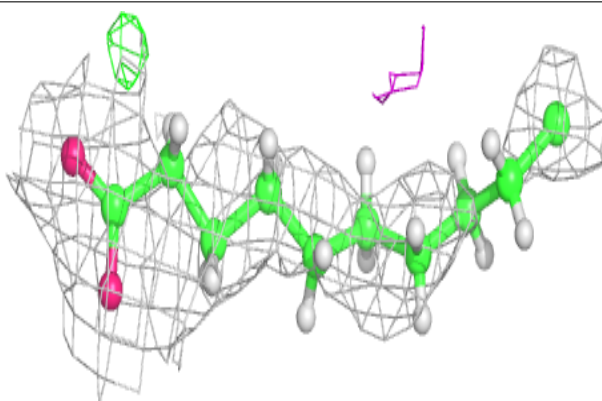


Electron density around STE b 625:

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

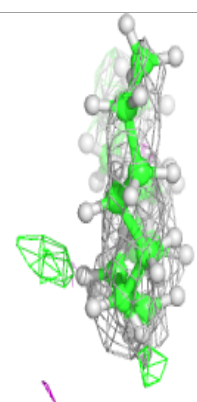
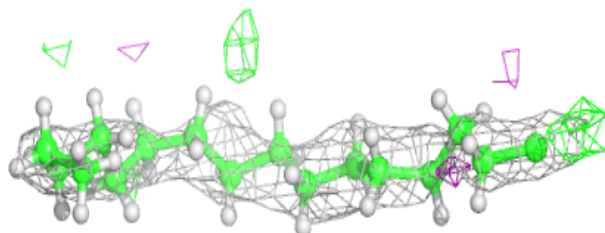
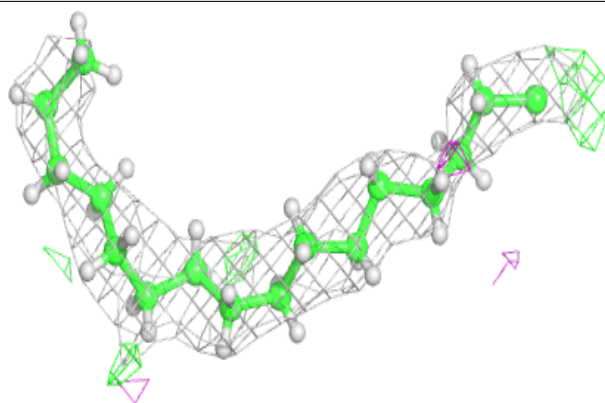
**Electron density around STE a 415:**

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

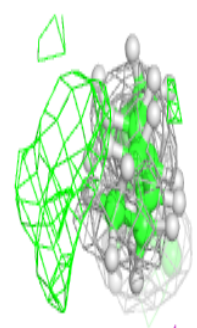
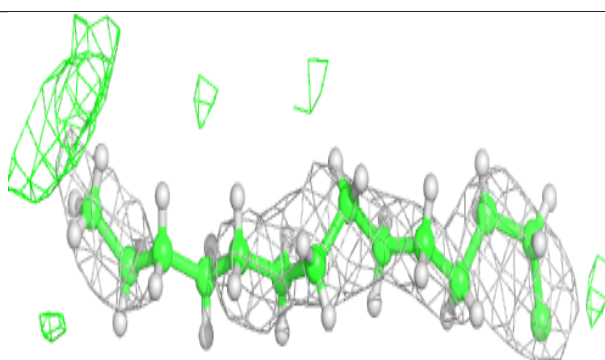
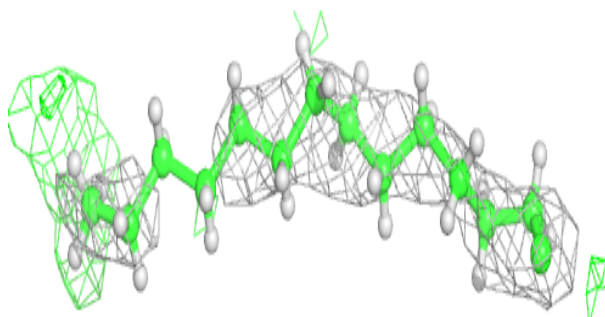


Electron density around STE B 627:

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

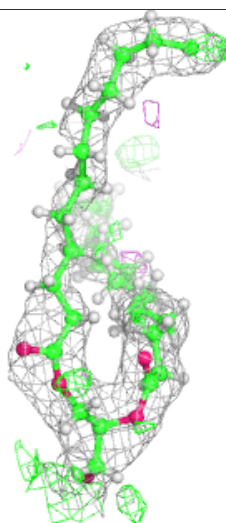
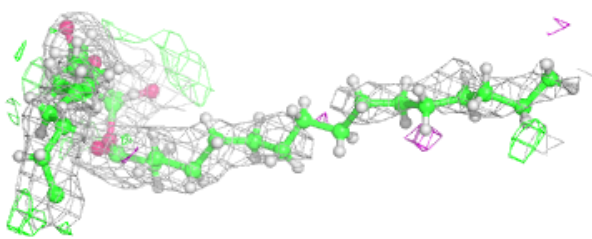
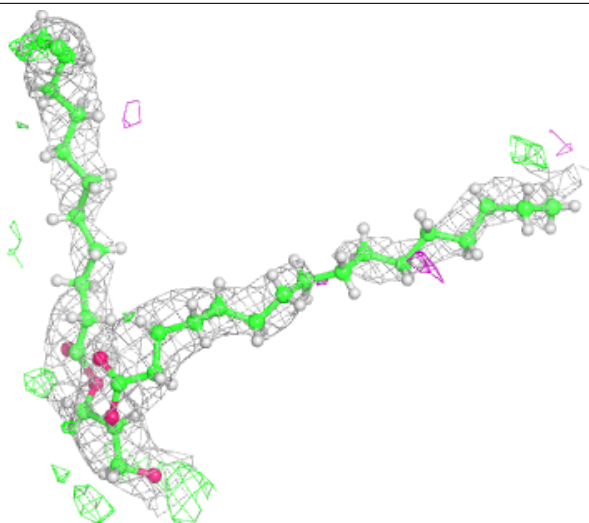
**Electron density around STE h 103:**

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



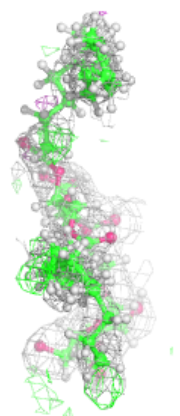
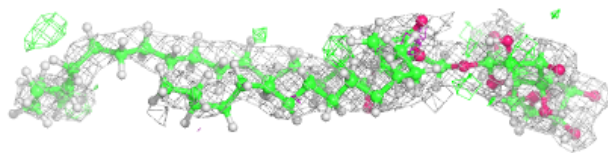
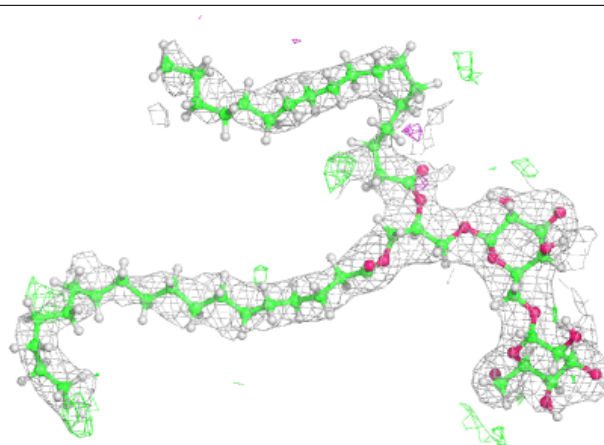
Electron density around SQD a 413:

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



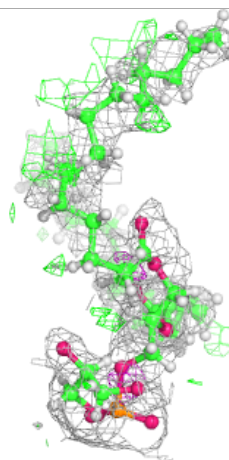
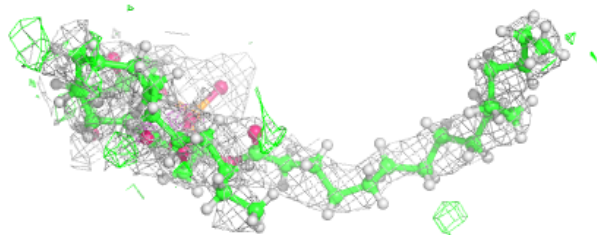
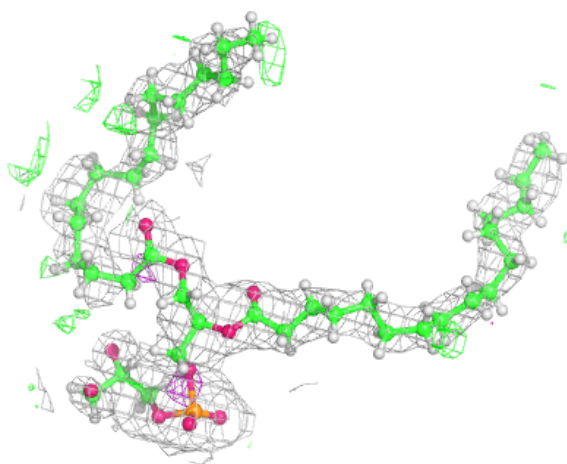
Electron density around DGD A 415:

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



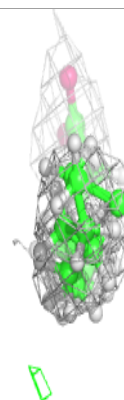
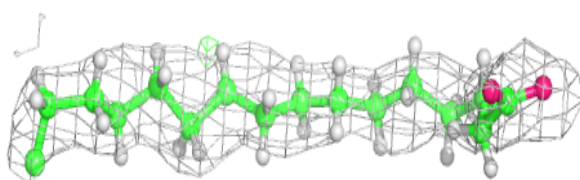
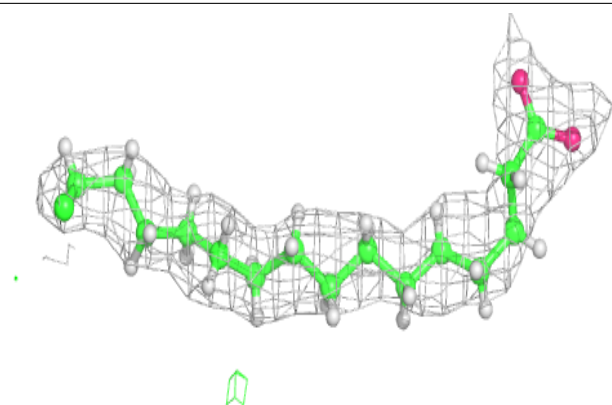
Electron density around LHG E 101:

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

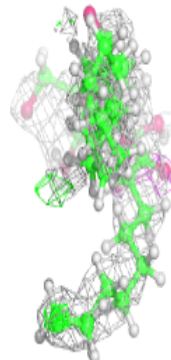
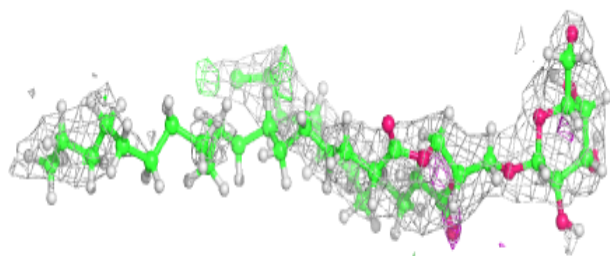
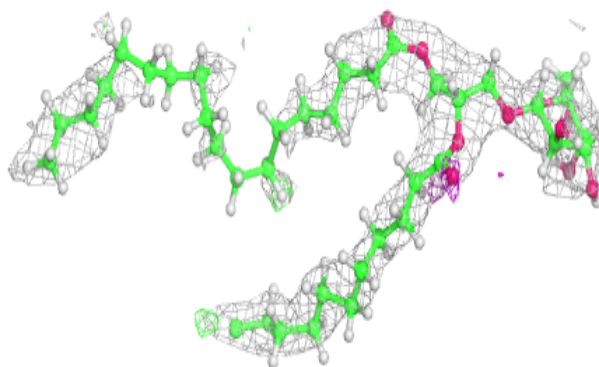


Electron density around STE B 626:

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

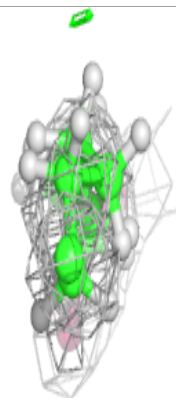
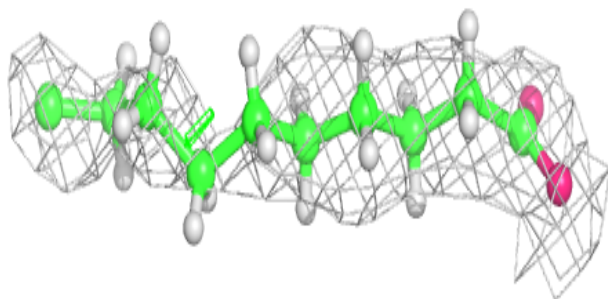
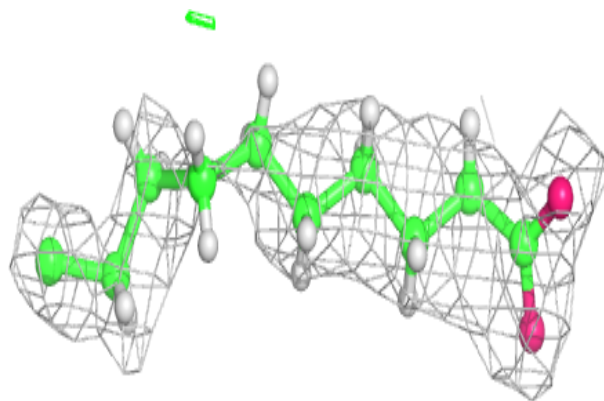
**Electron density around LMG c 524:**

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

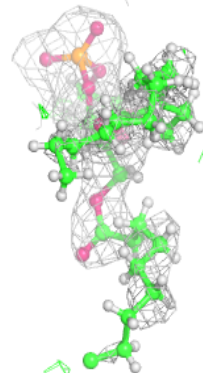
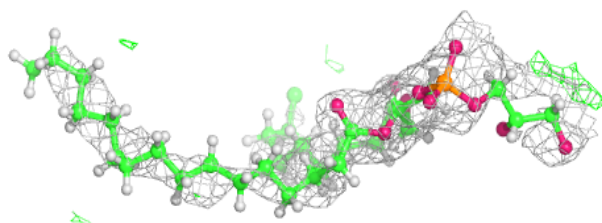
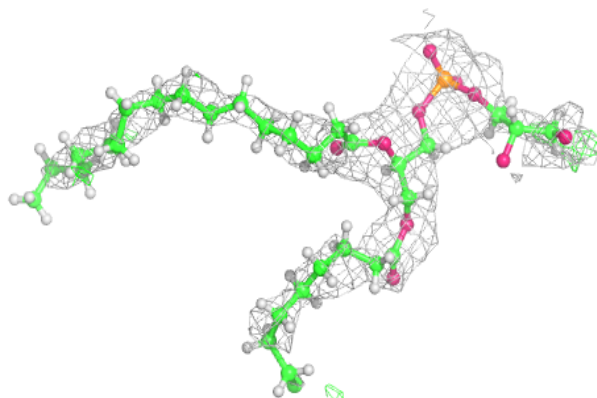


Electron density around STE c 501:

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

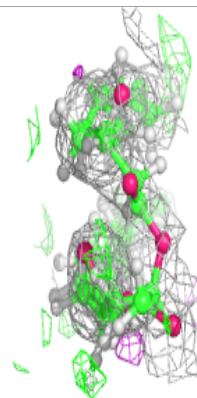
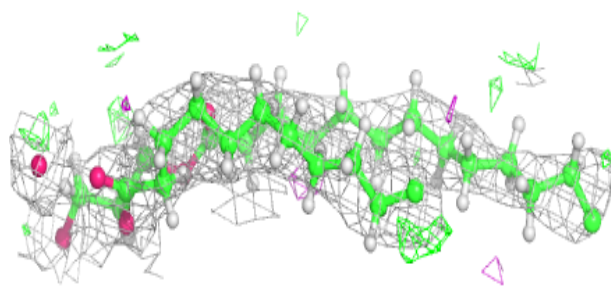
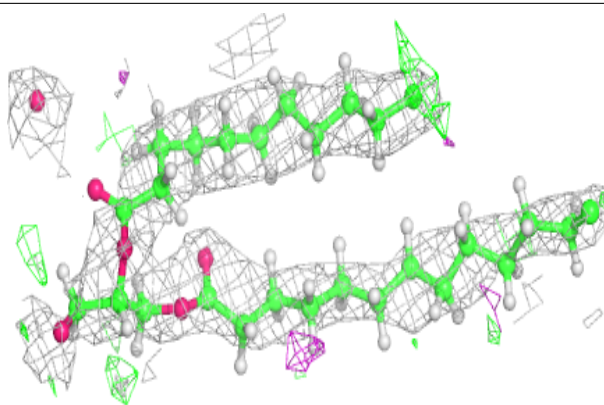
**Electron density around LHG e 102:**

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



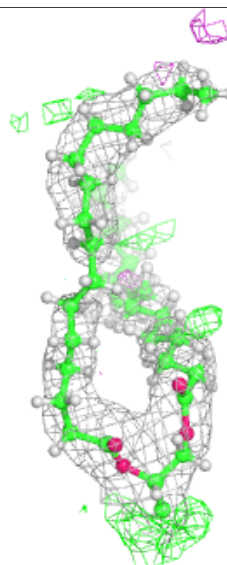
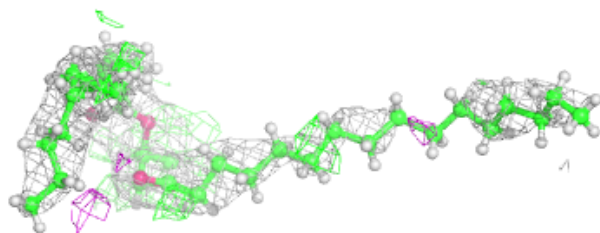
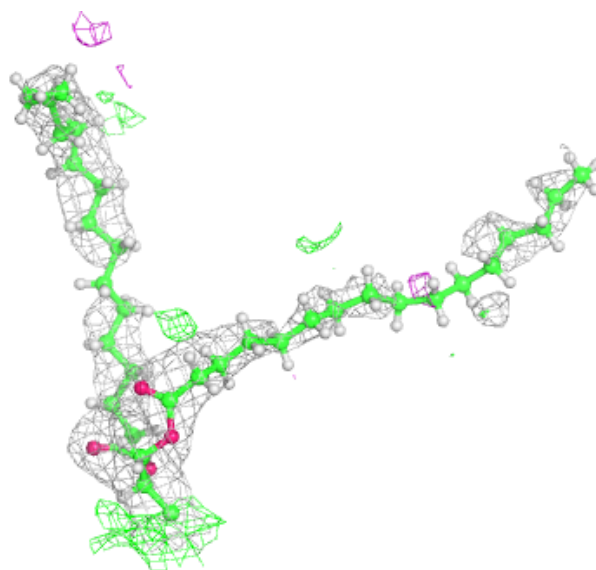
Electron density around LMG D 410:

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



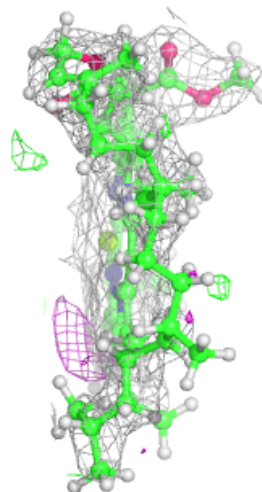
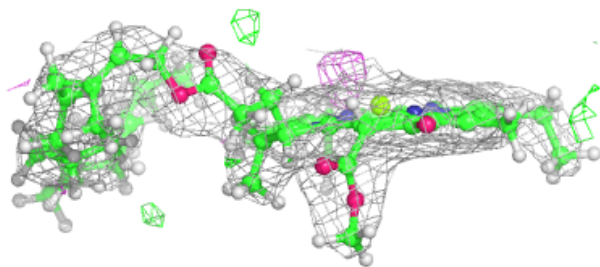
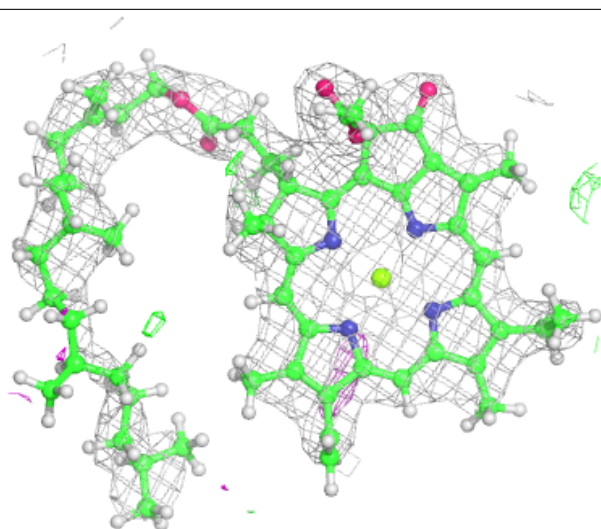
Electron density around SQD A 414:

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



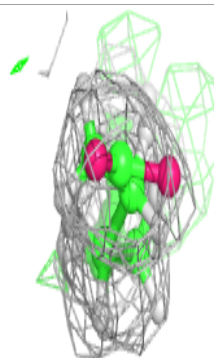
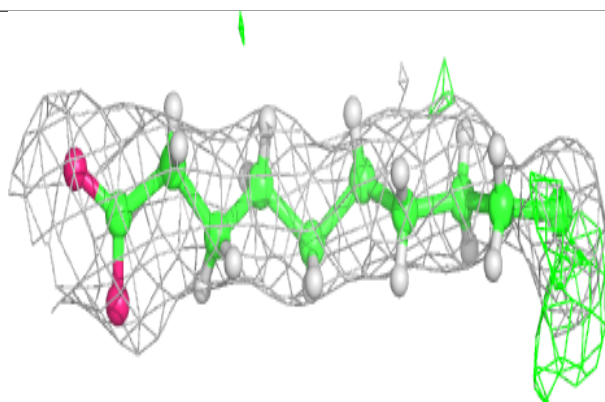
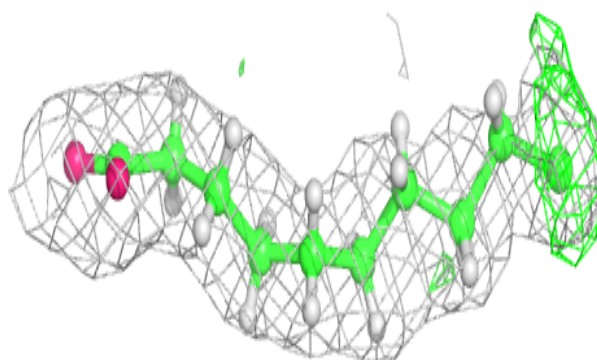
Electron density around CLA C 513:

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

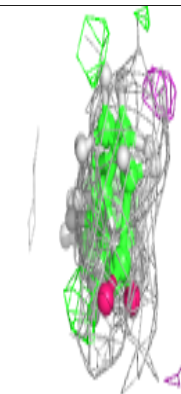
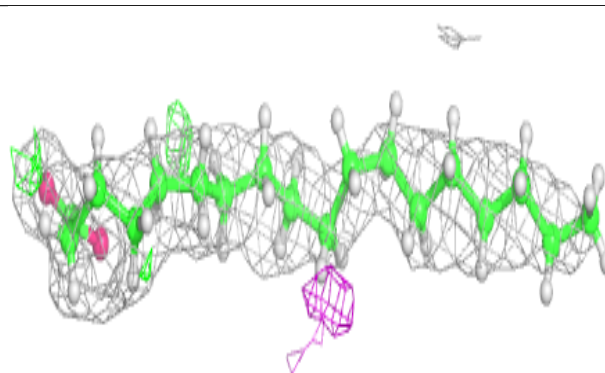
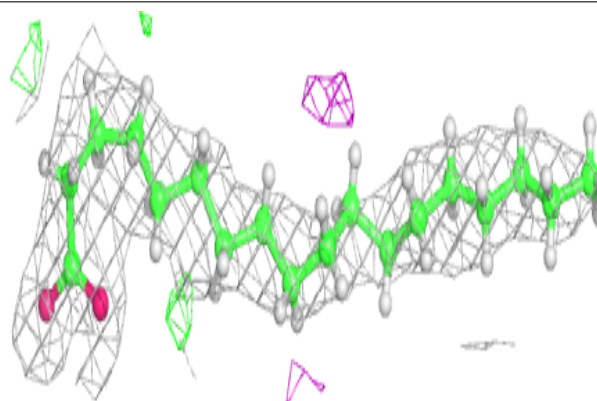


Electron density around STE j 101:

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

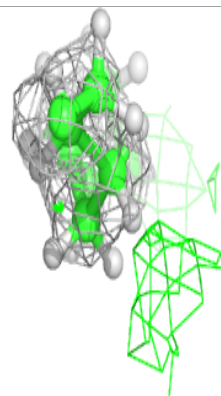
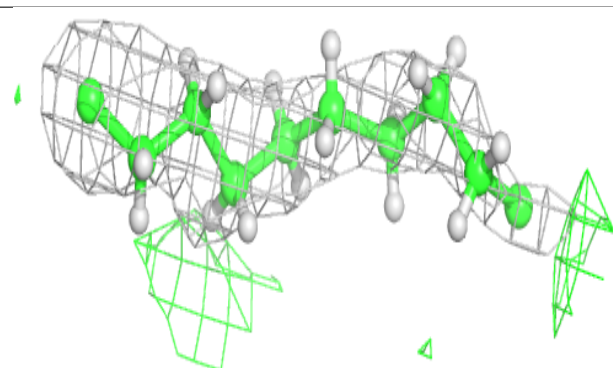
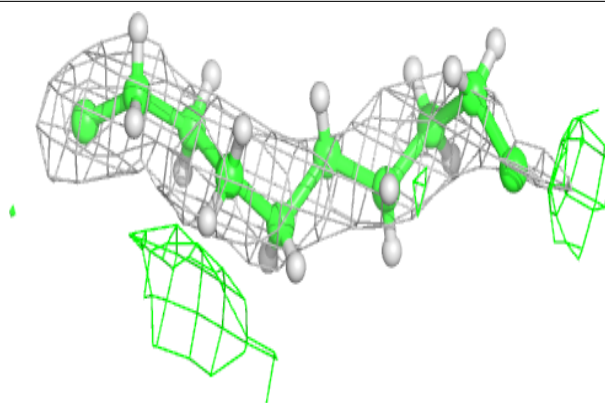
**Electron density around STE c 523:**

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

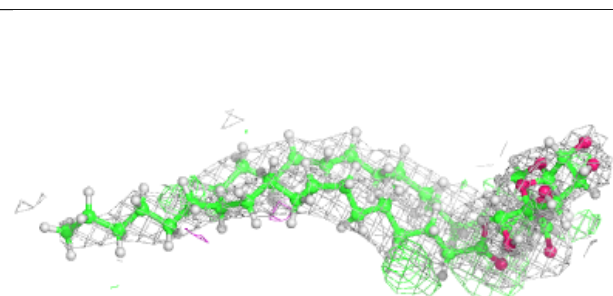
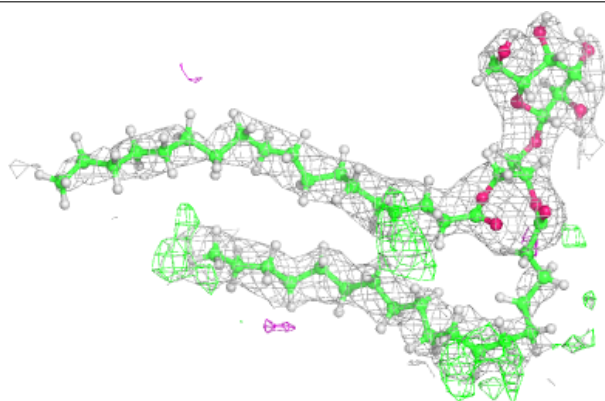


Electron density around STE a 414:

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

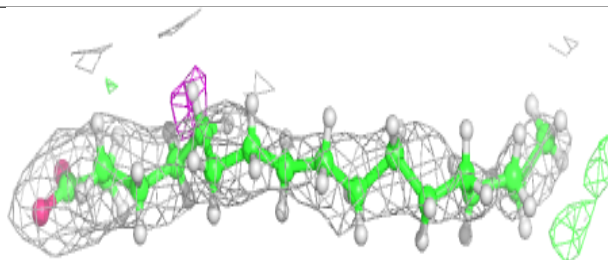
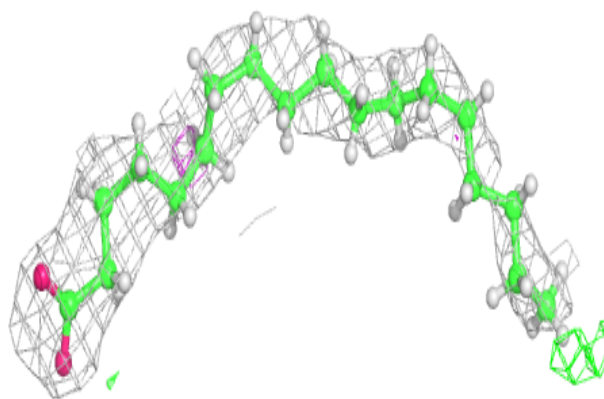
**Electron density around LMG B 629:**

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

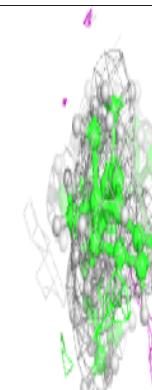
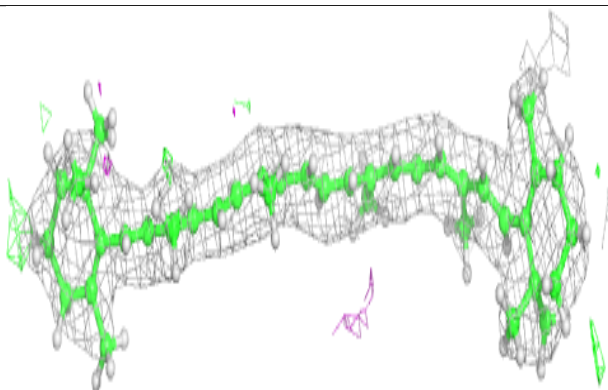
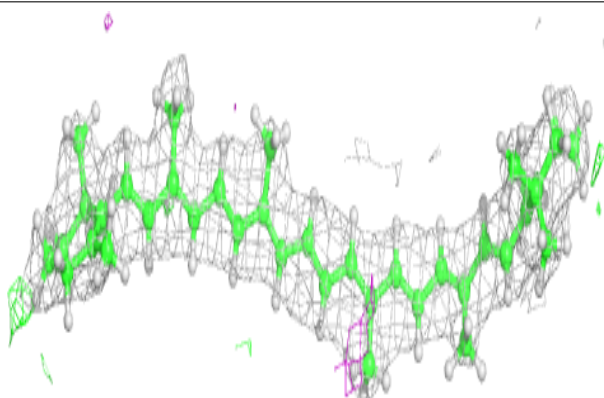


Electron density around STE d 411:

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

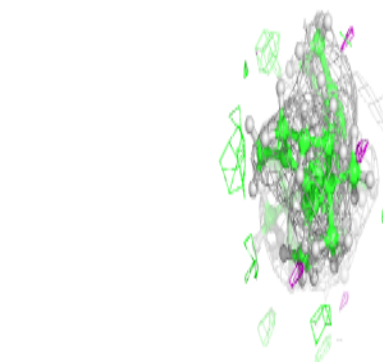
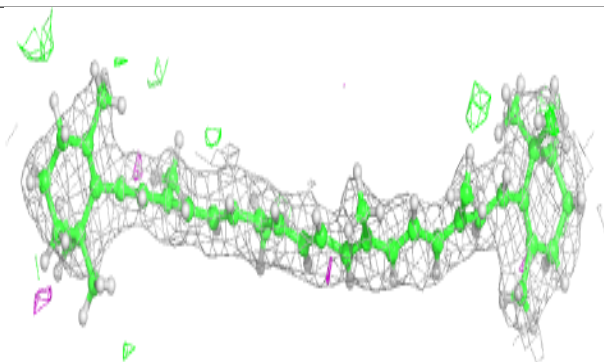
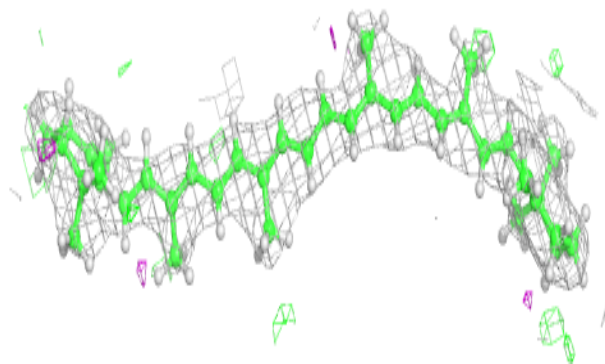
**Electron density around BCR H 101:**

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

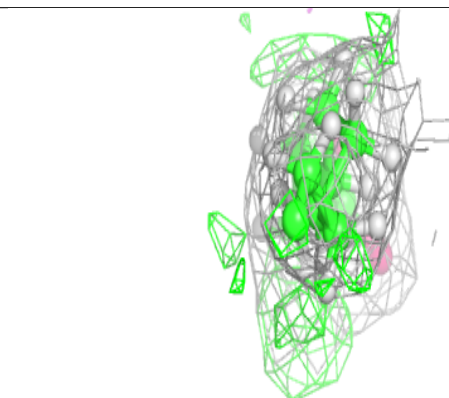
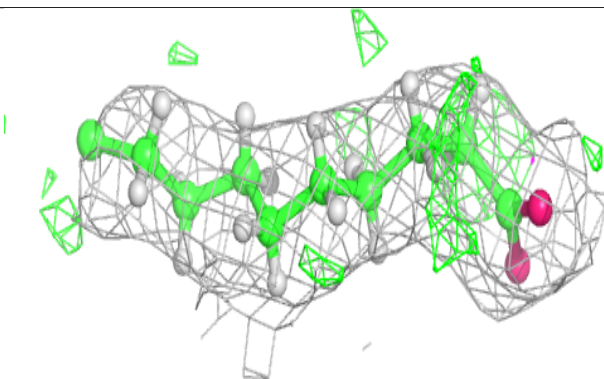
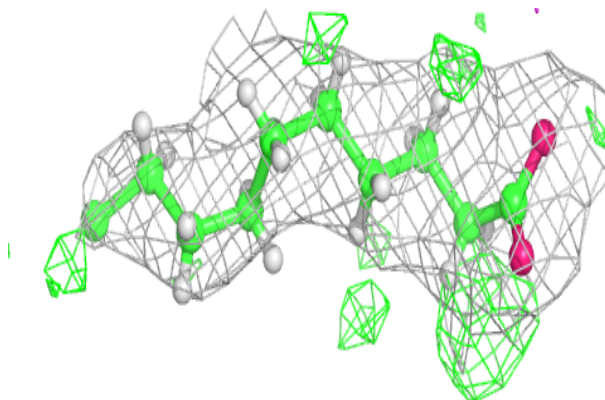


Electron density around BCR x 101:

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

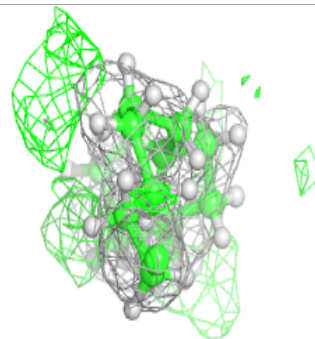
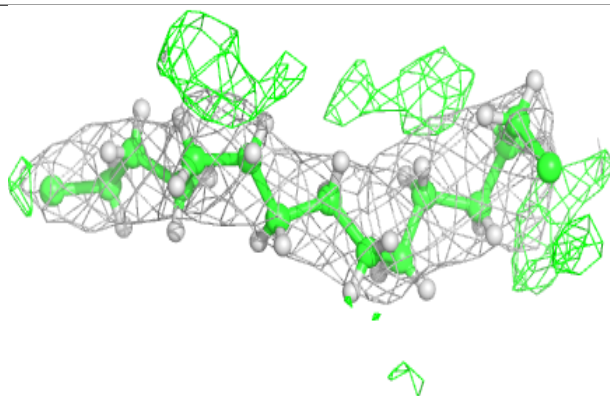
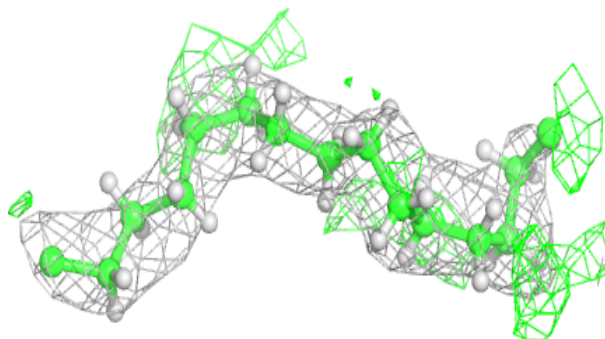
**Electron density around STE B 625:**

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

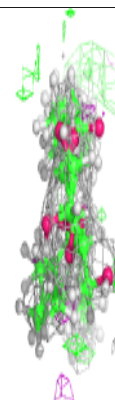
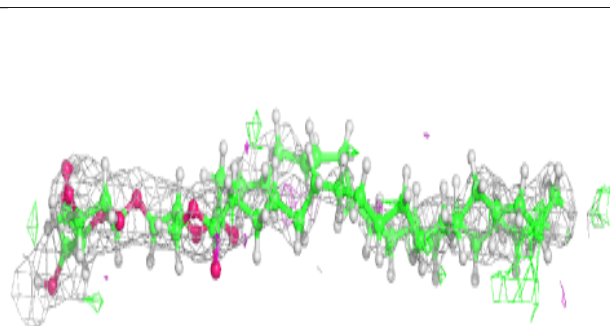
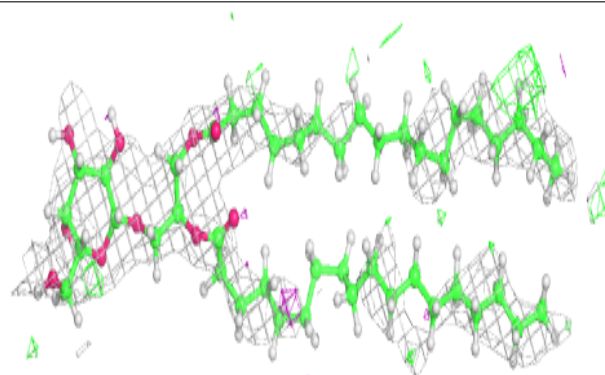


Electron density around STE B 628:

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

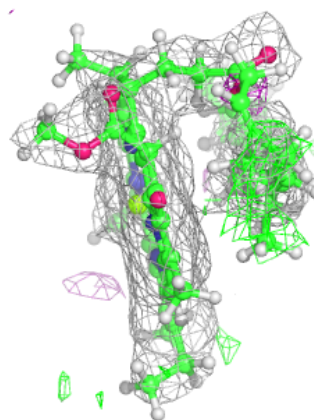
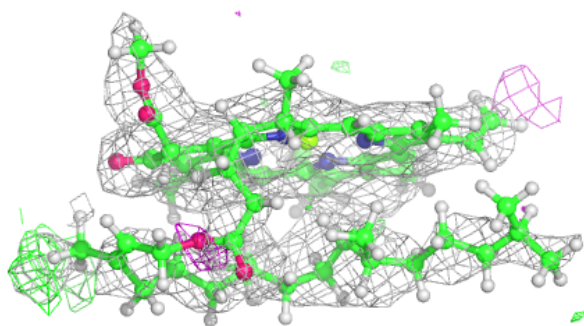
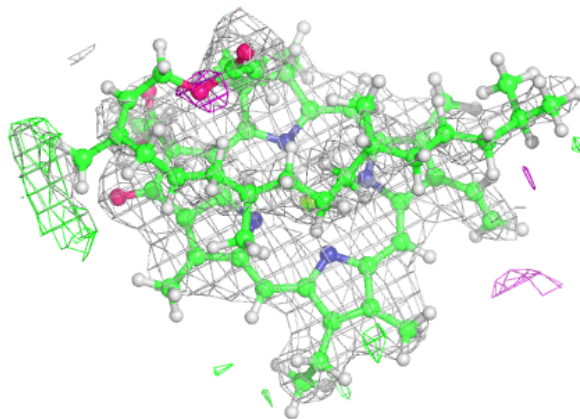
**Electron density around LMG b 623:**

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



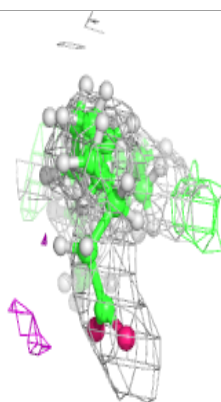
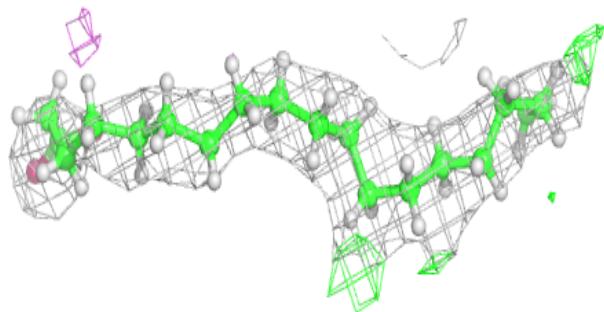
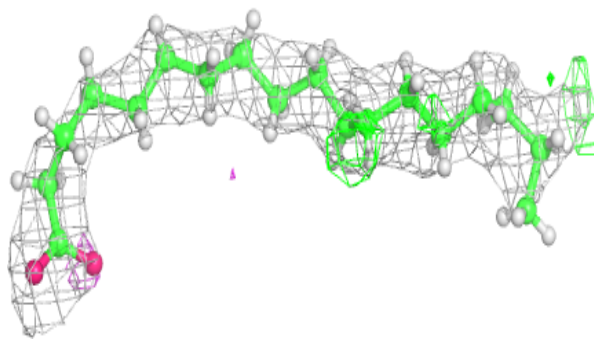
Electron density around CLA h 101:

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

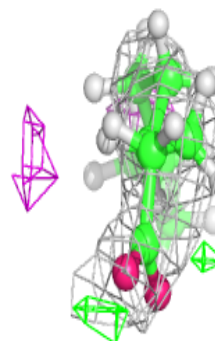
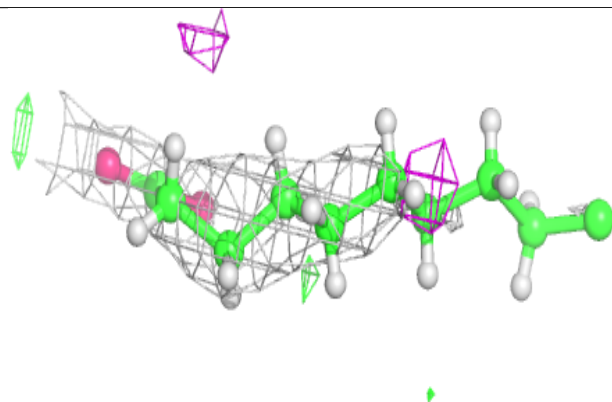
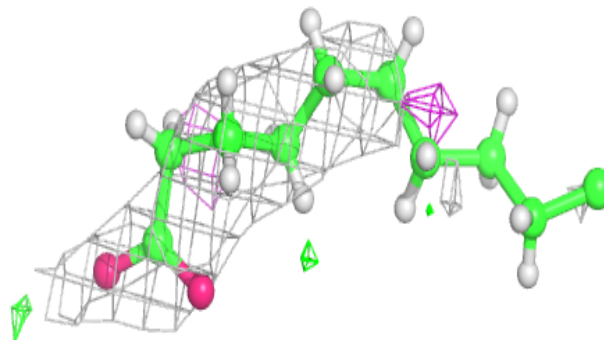


Electron density around STE b 622:

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

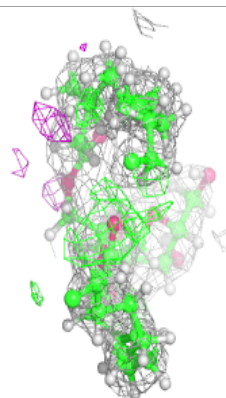
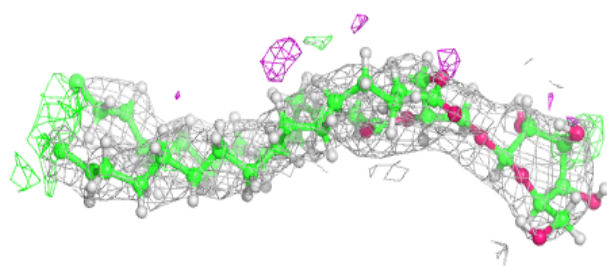
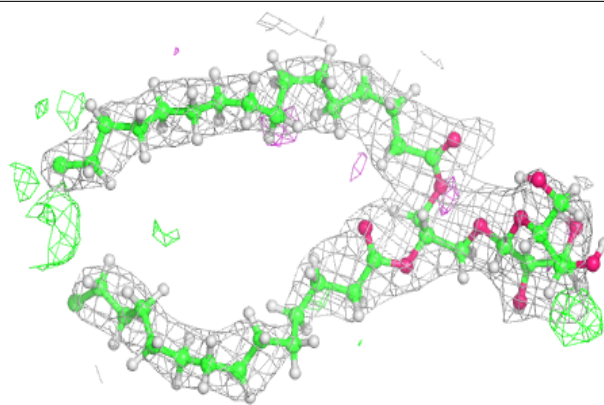
**Electron density around STE B 601:**

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

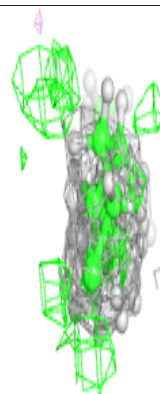
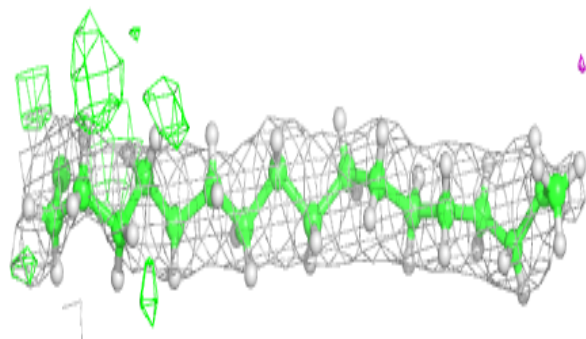
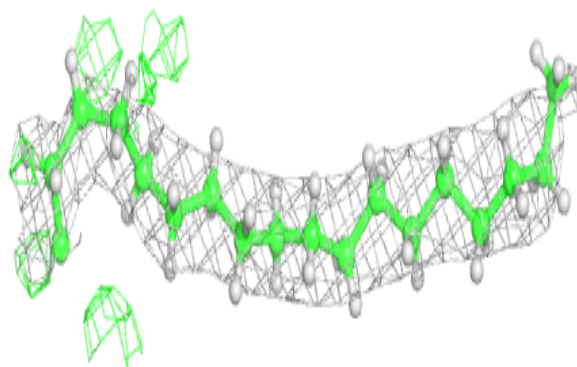


Electron density around LMG c 525:

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

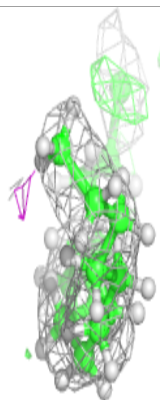
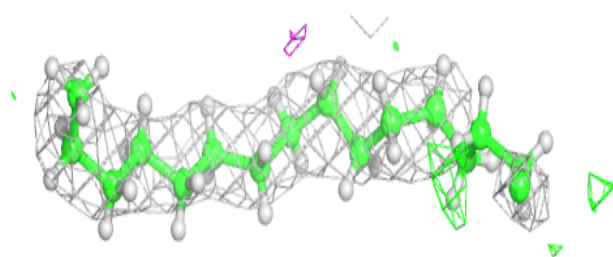
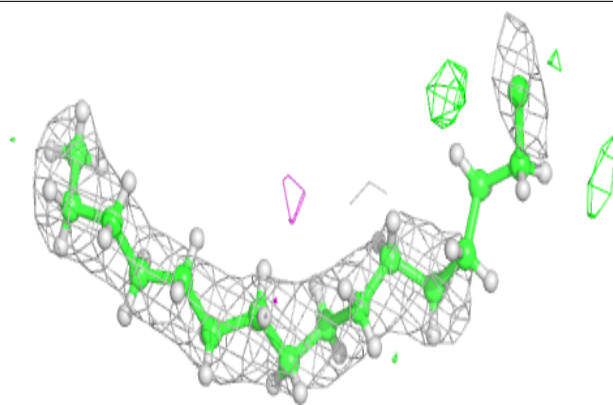
**Electron density around STE l 102:**

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

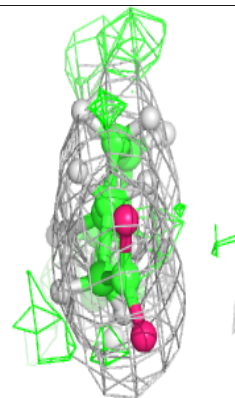
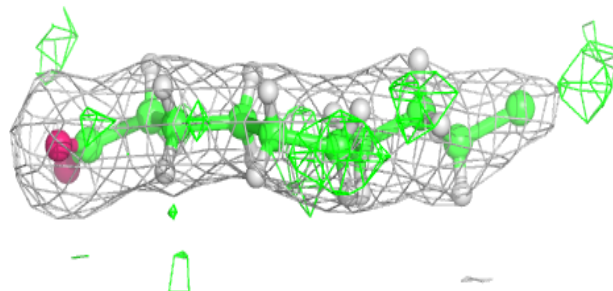
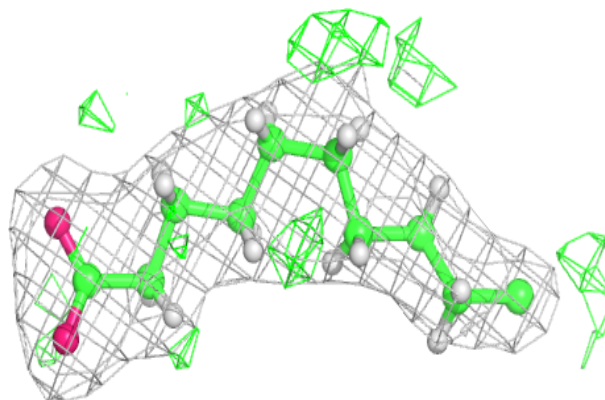


Electron density around STE b 620:

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

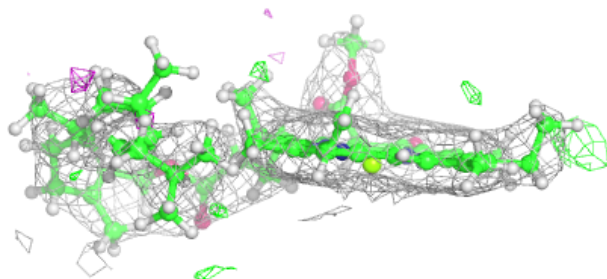
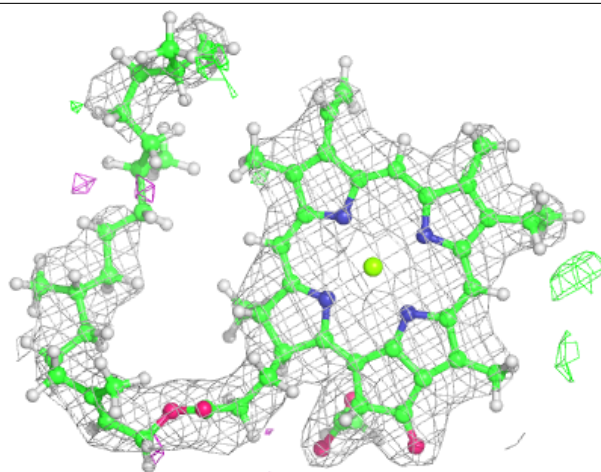
**Electron density around STE C 522:**

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



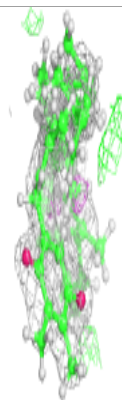
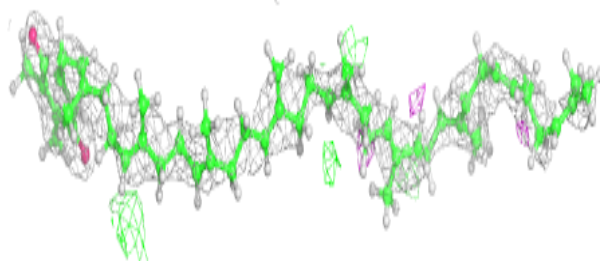
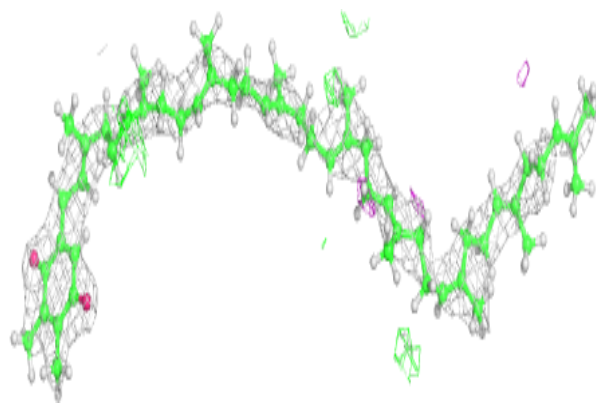
Electron density around CLA c 514:

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

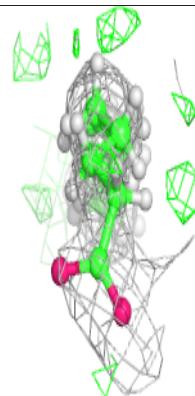
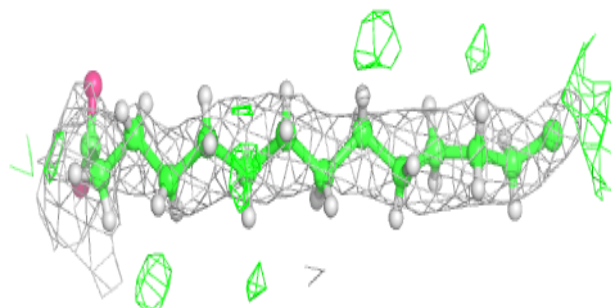
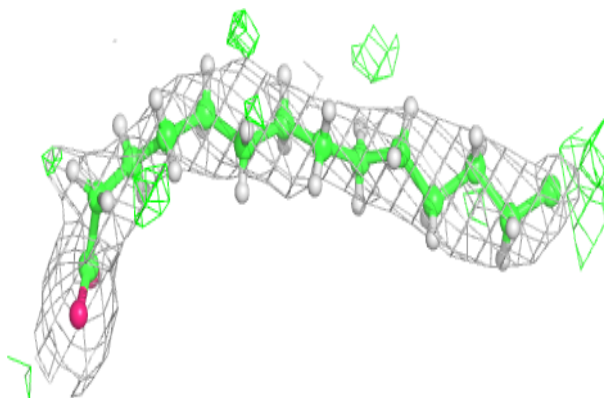


Electron density around PL9 A 410:

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

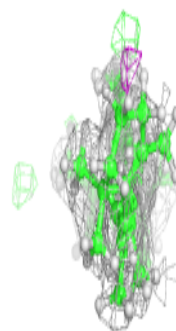
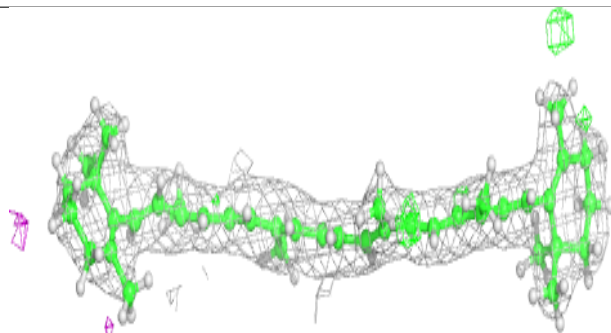
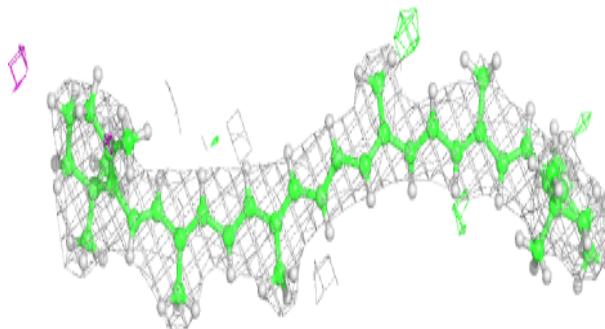
**Electron density around STE b 624:**

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

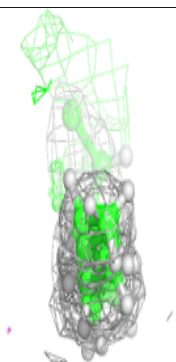
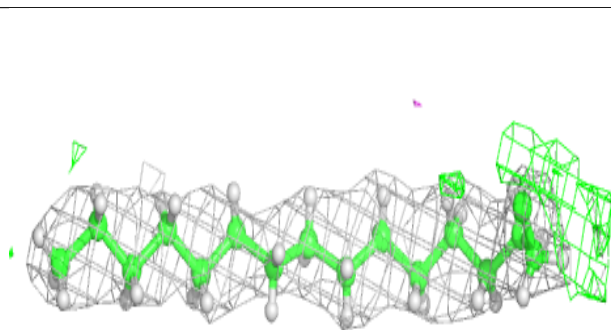
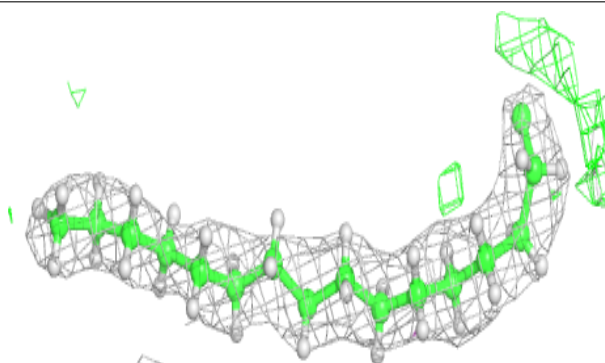


Electron density around BCR Y 101:

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

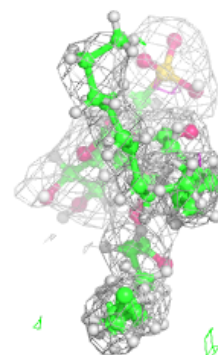
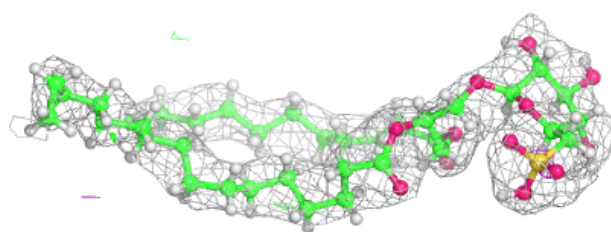
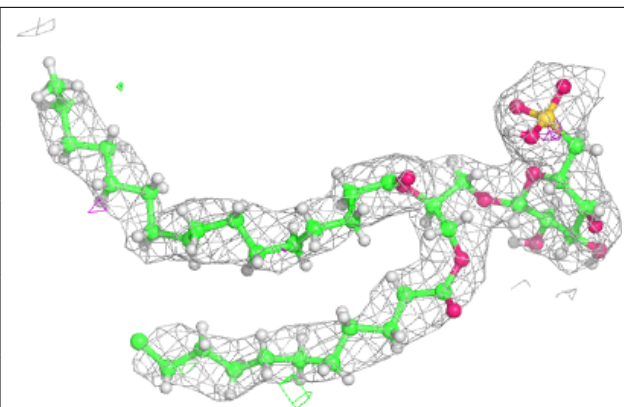
**Electron density around STE C 521:**

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

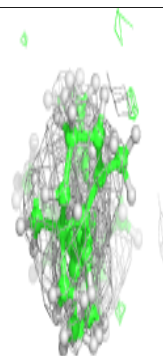
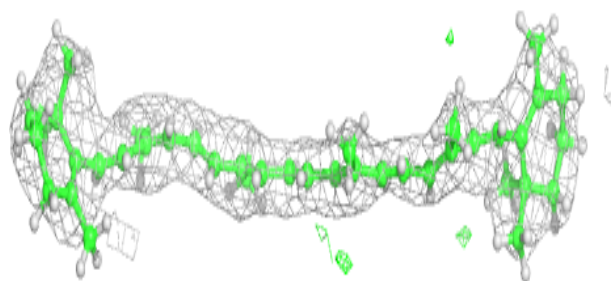
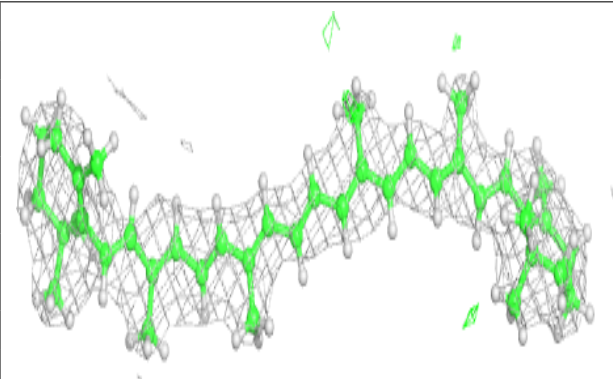


Electron density around SQD b 619:

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

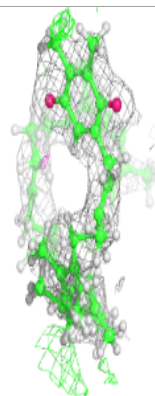
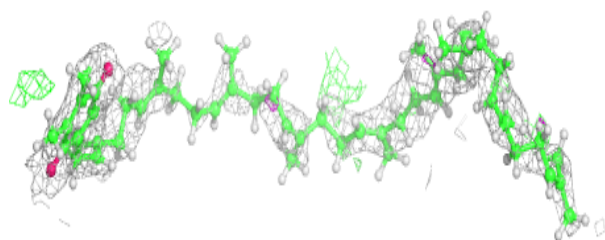
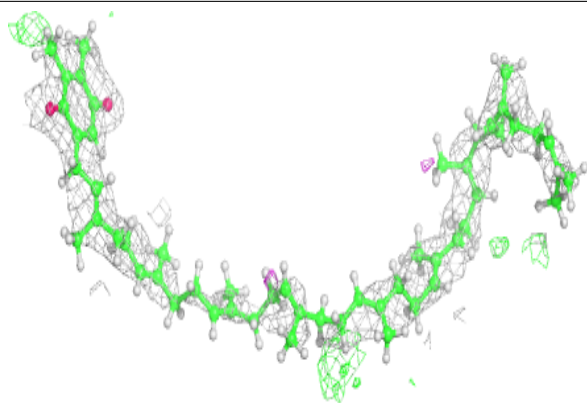
**Electron density around BCR y 101:**

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

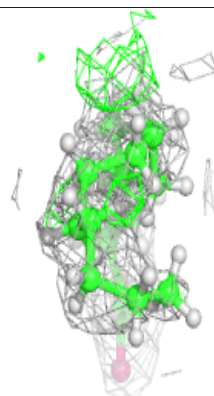
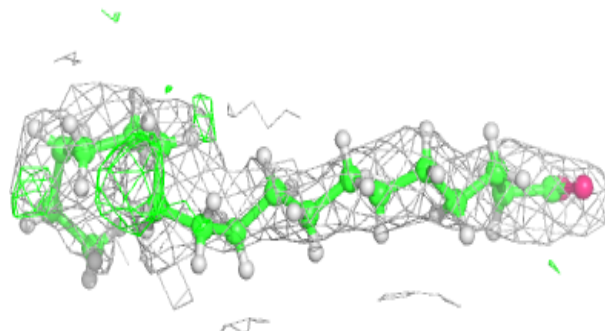
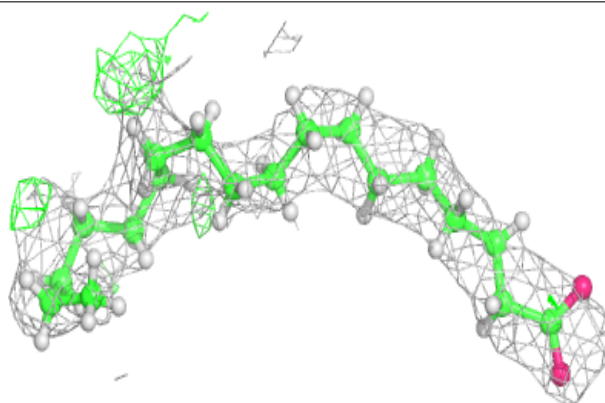


Electron density around PL9 a 410:

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

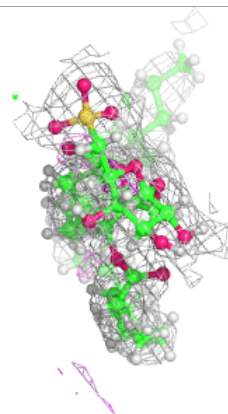
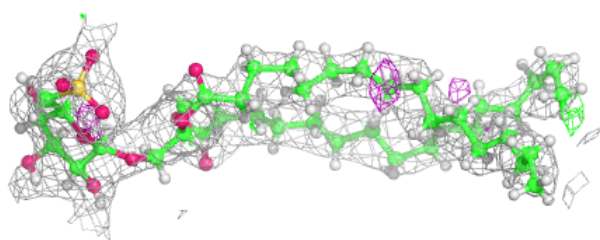
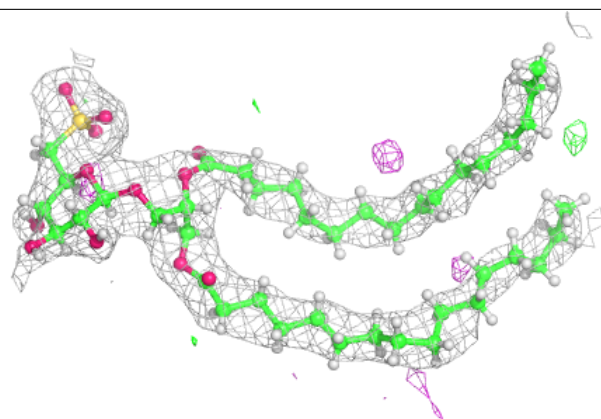
**Electron density around STE d 412:**

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

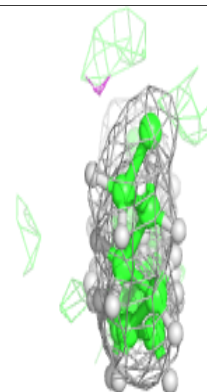
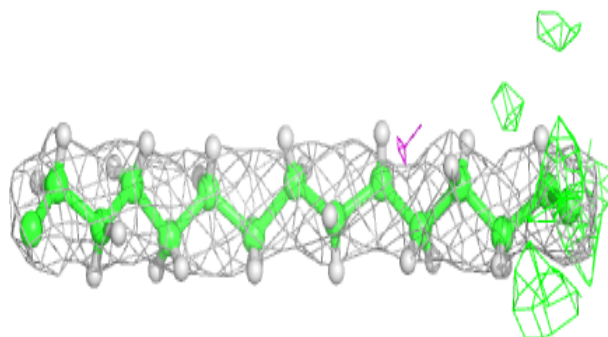
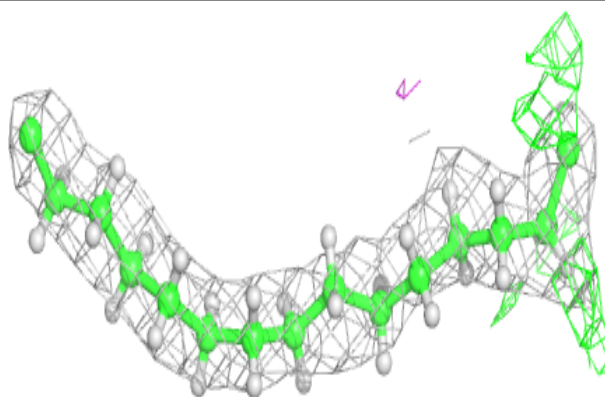


Electron density around SQD B 623:

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

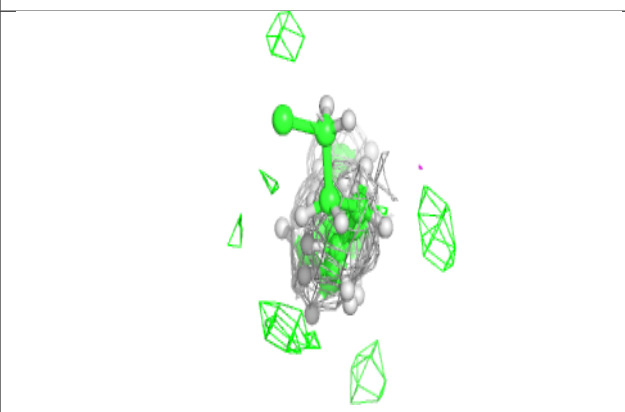
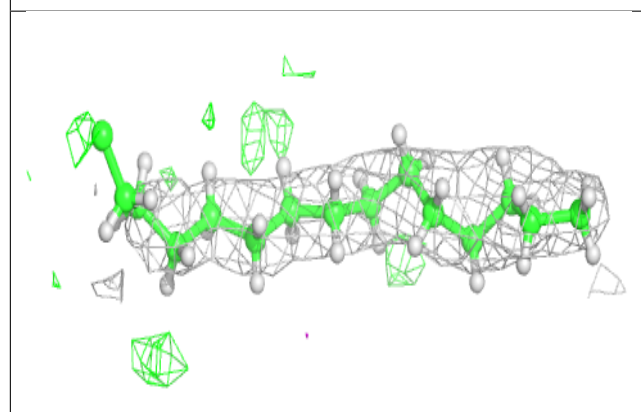
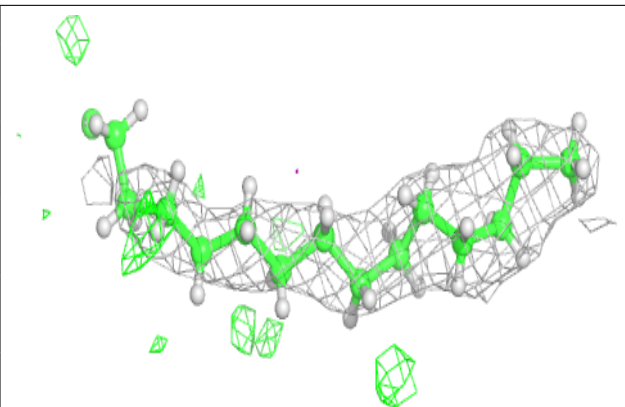
**Electron density around STE I 101:**

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



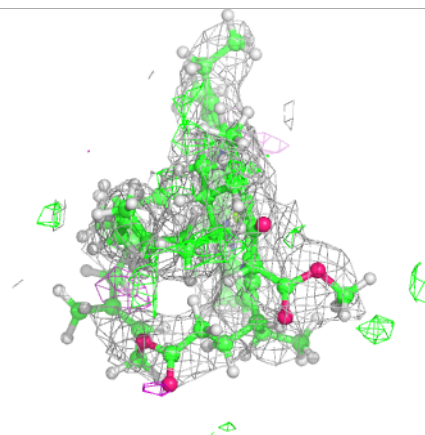
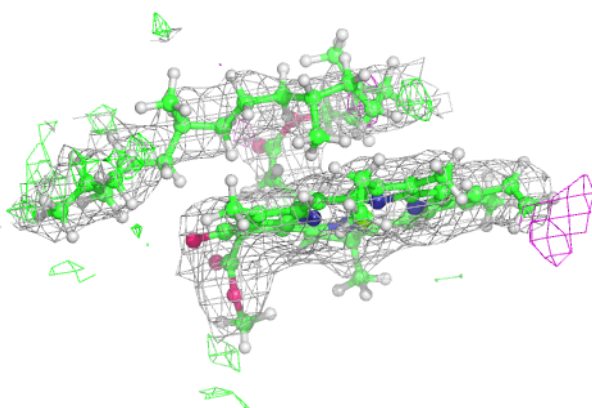
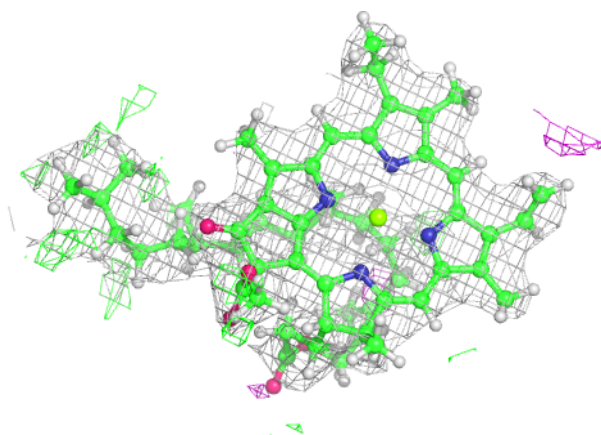
Electron density around STE T 102:

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



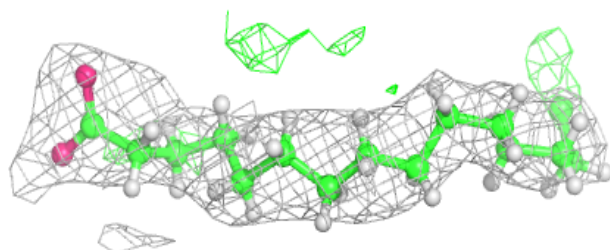
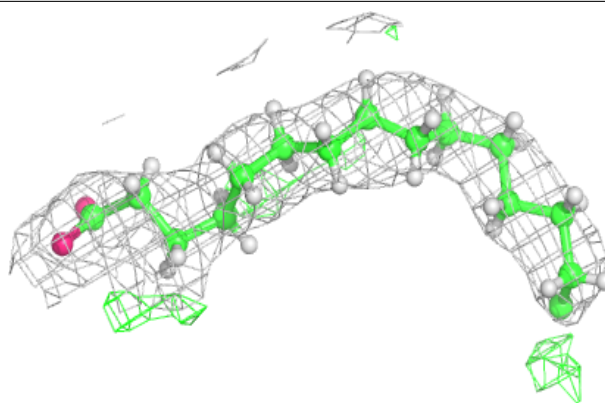
Electron density around CLA B 602:

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

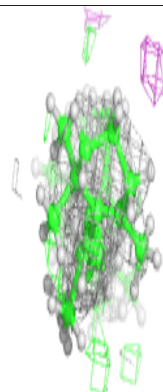
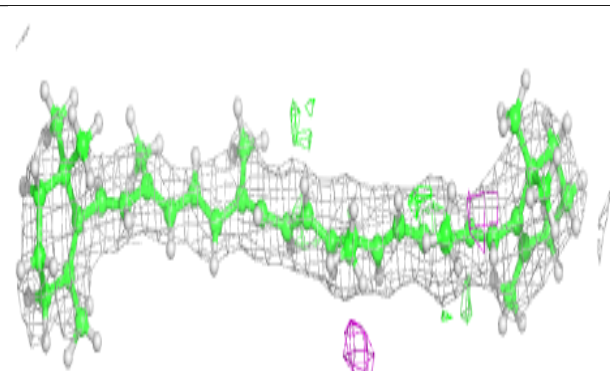
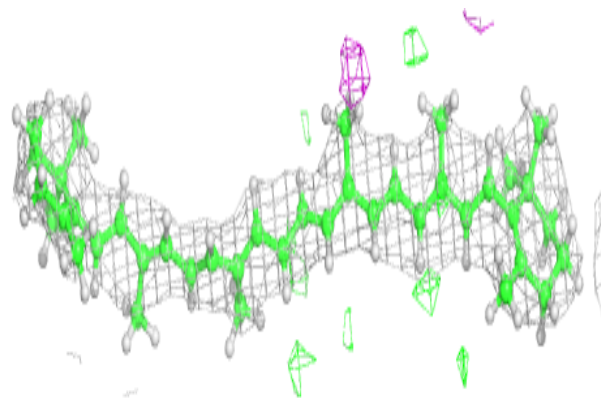


Electron density around STE B 621:

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

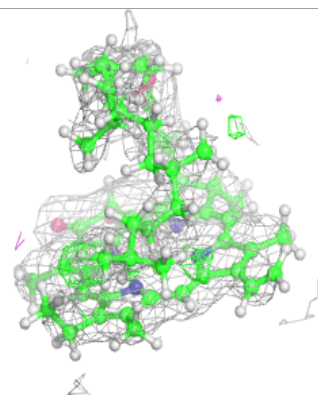
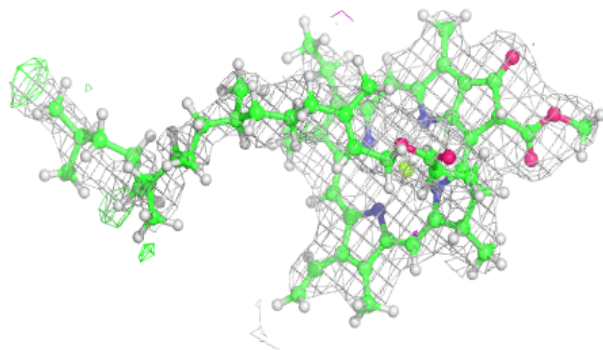
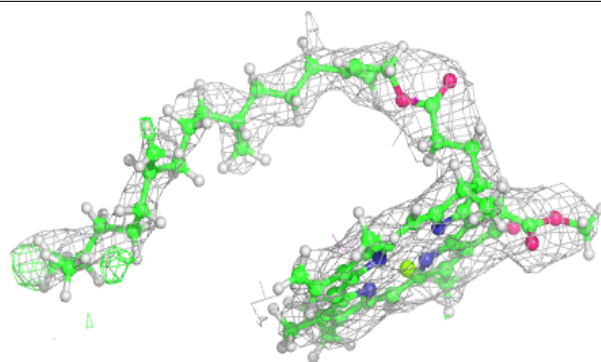
**Electron density around BCR Z 101:**

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

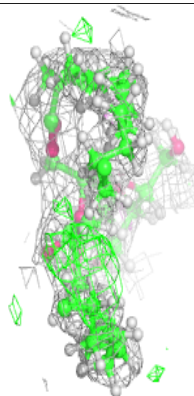
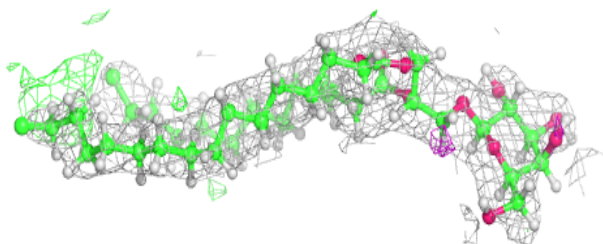
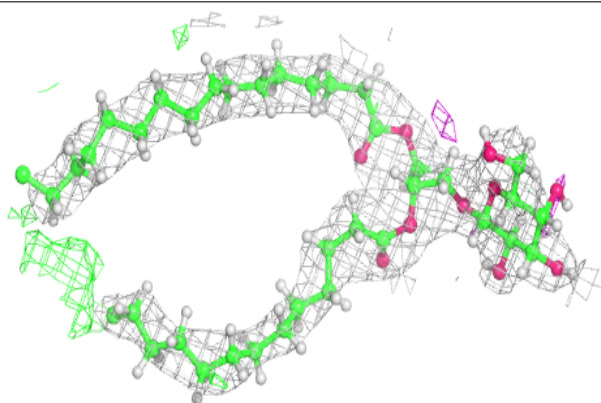


Electron density around CLA C 514:

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

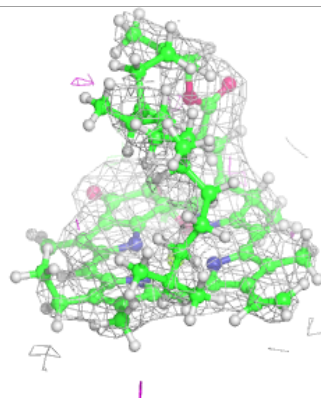
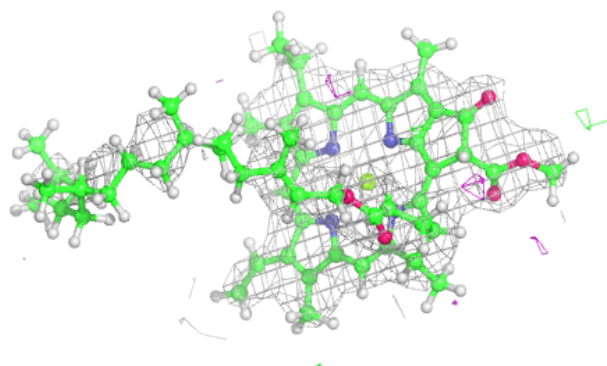
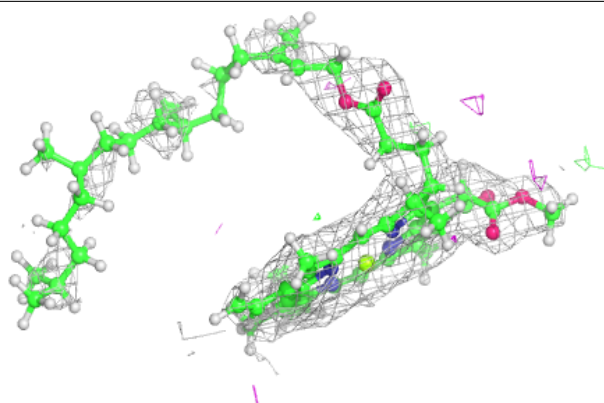
**Electron density around LMG A 412:**

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

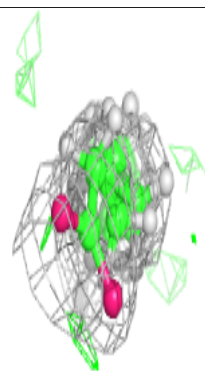
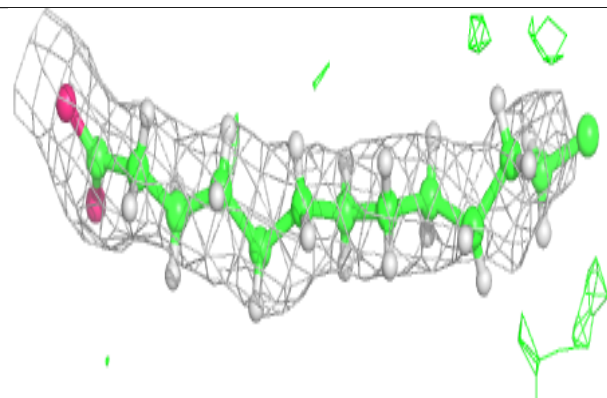
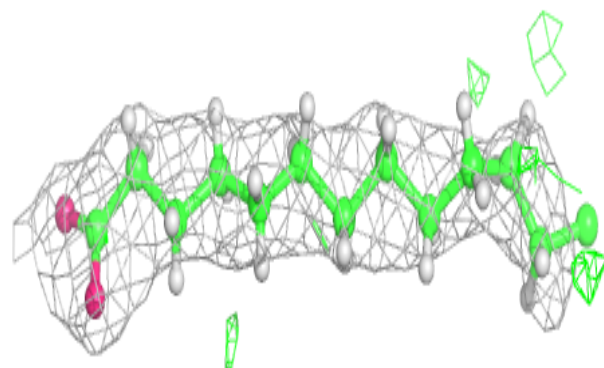


Electron density around CLA c 515:

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

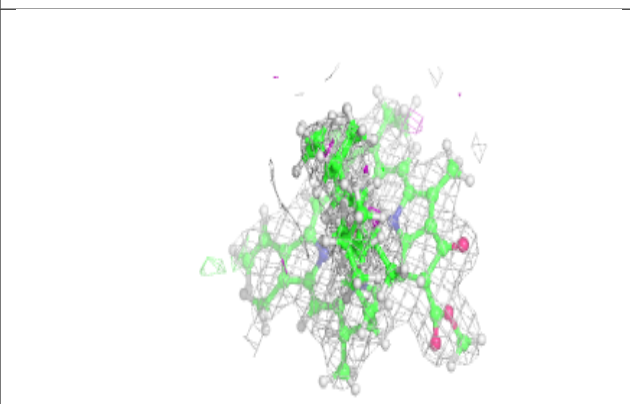
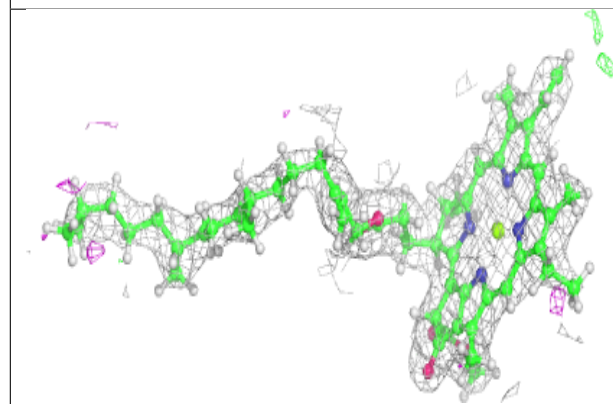
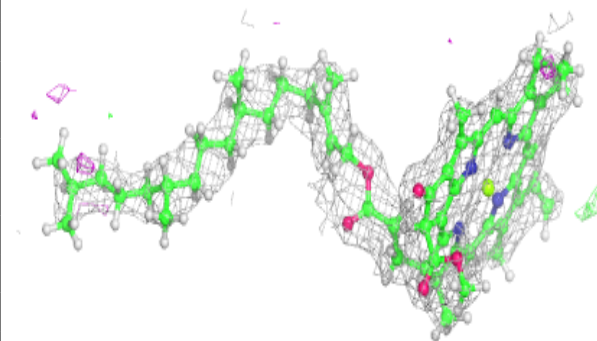
**Electron density around STE M 102:**

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

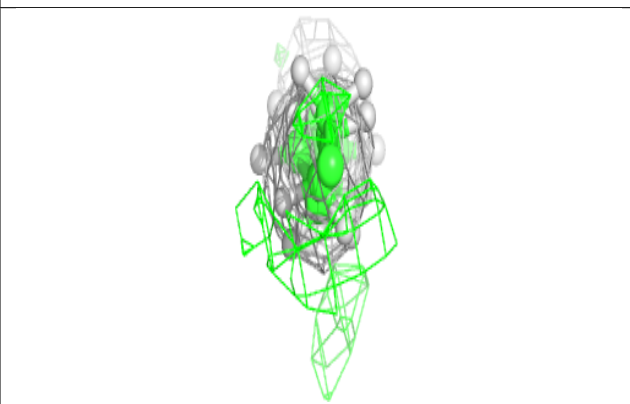
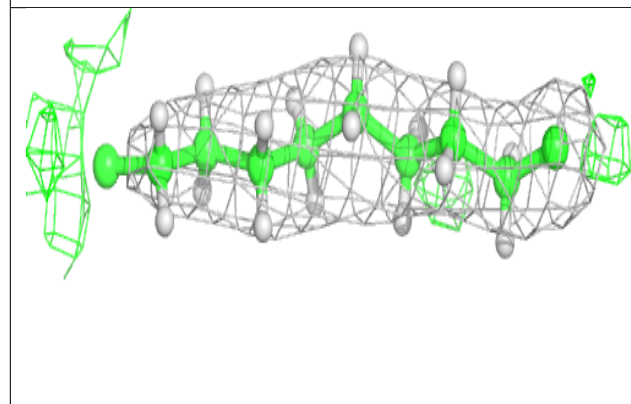
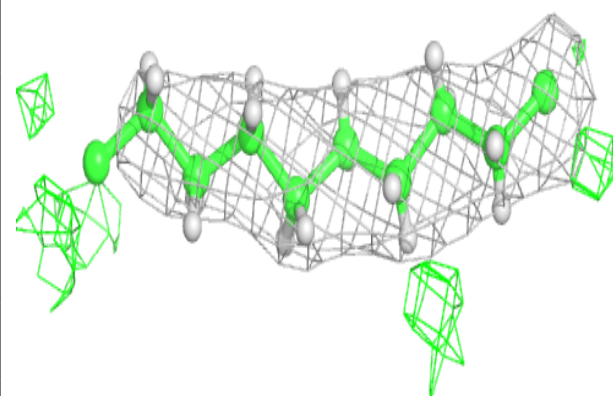


Electron density around CLA c 504:

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

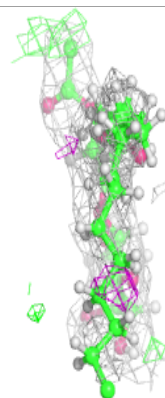
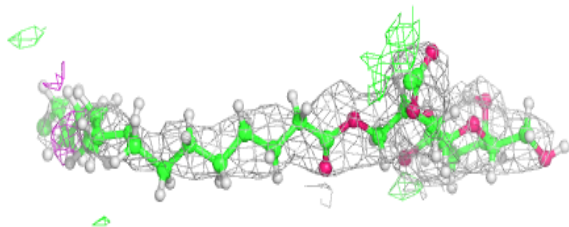
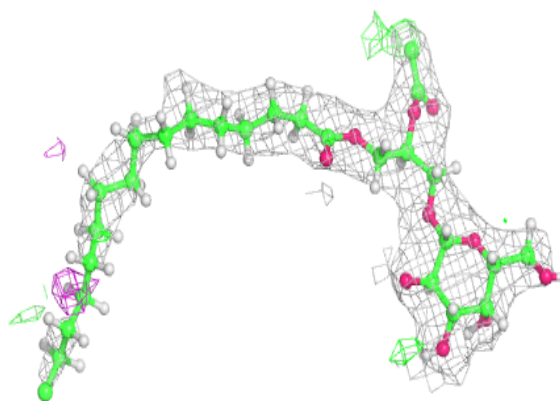
**Electron density around STE M 103:**

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

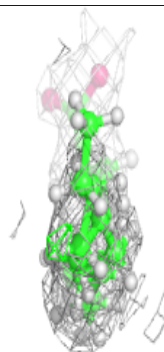
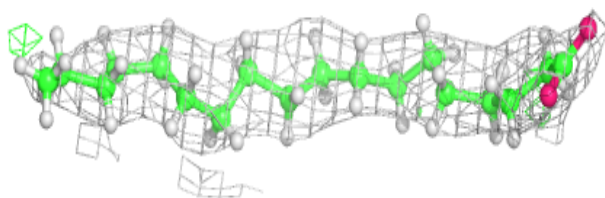
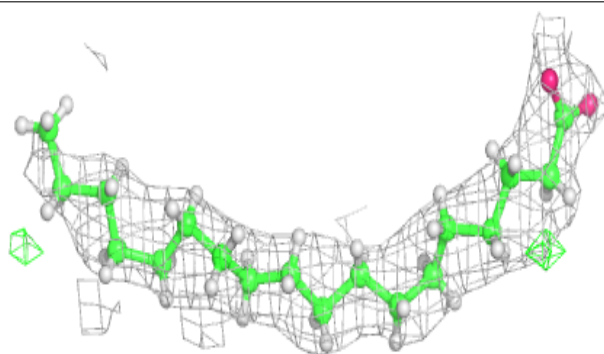


Electron density around LMG c 522:

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

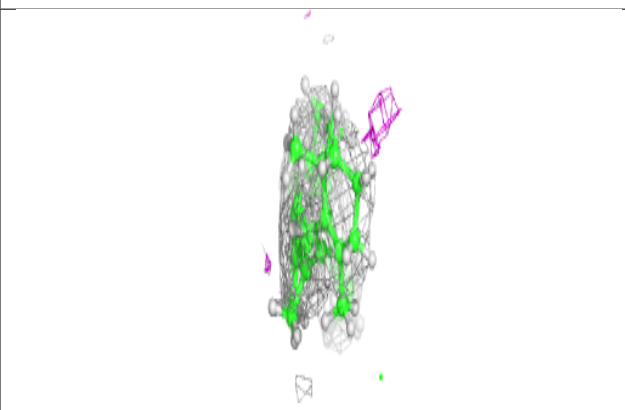
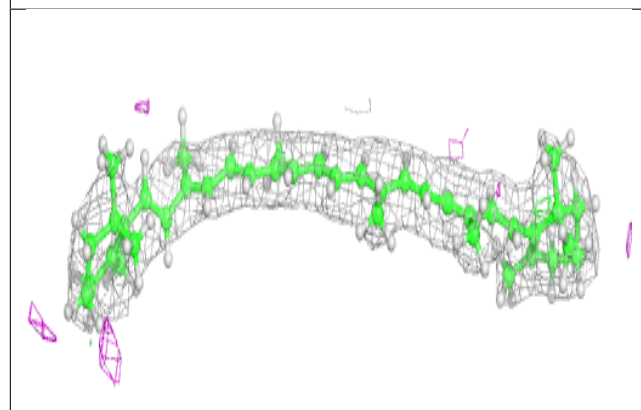
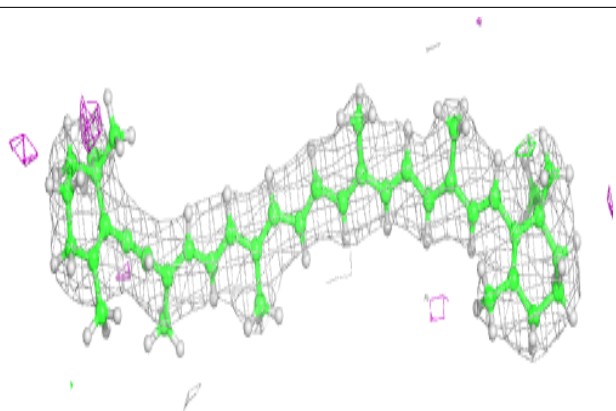
**Electron density around STE X 101:**

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

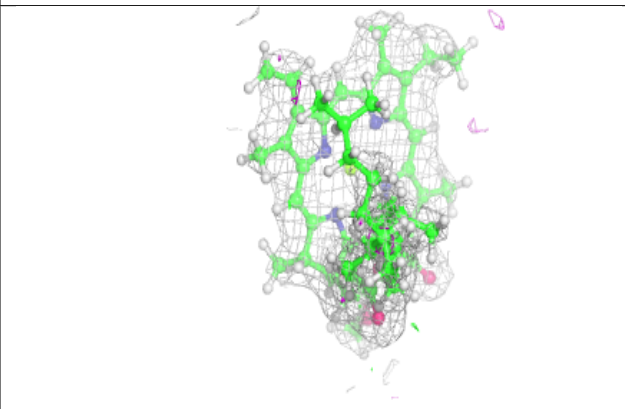
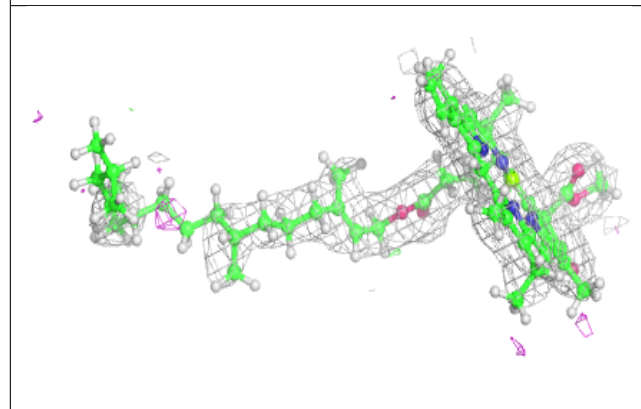
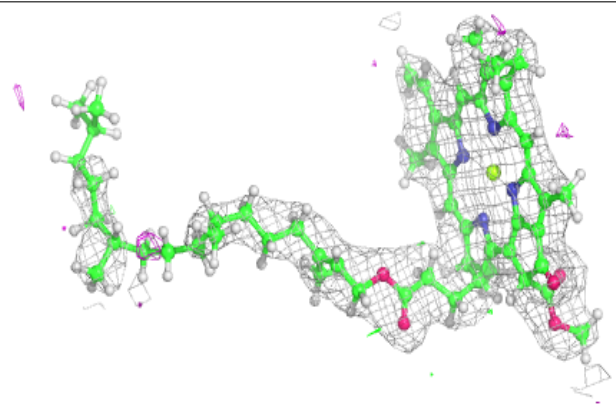


Electron density around BCR d 404:

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

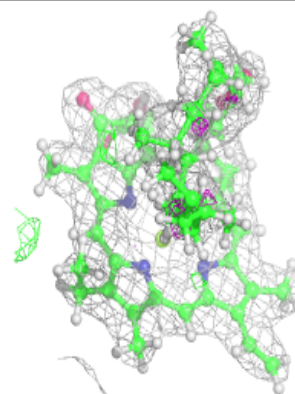
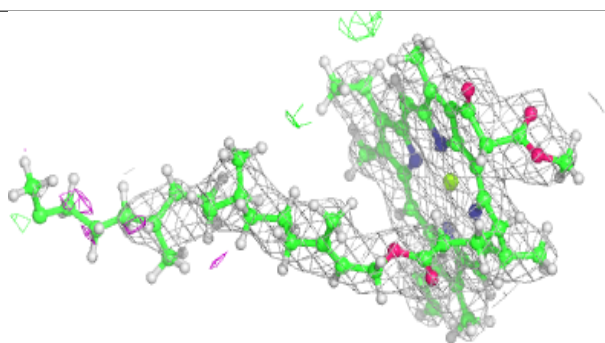
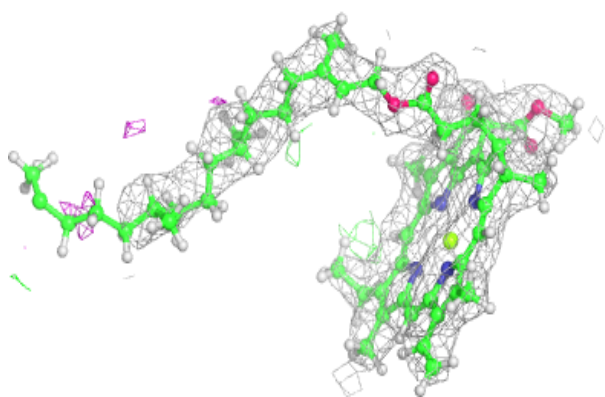
**Electron density around CLA d 403:**

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

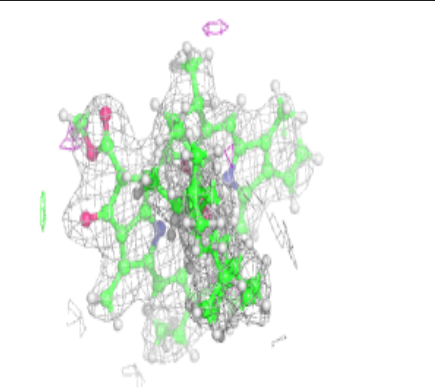
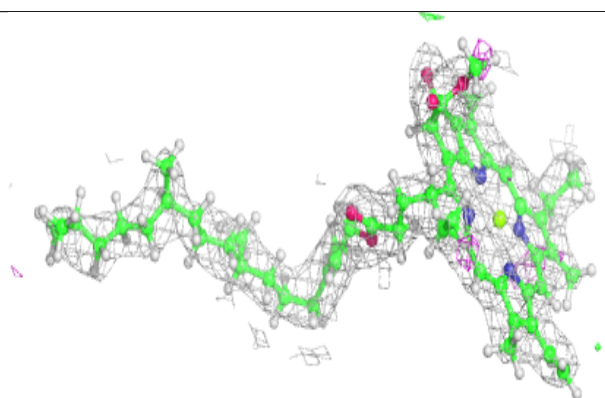
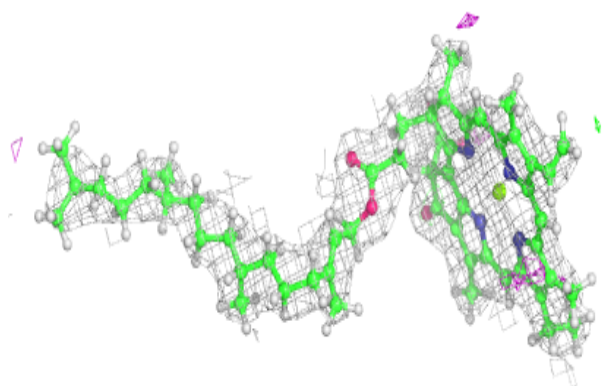


Electron density around CLA c 510:

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

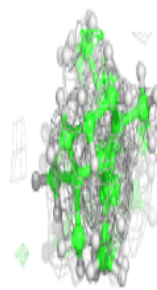
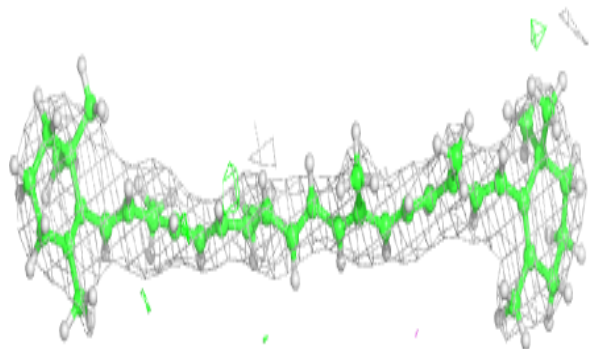
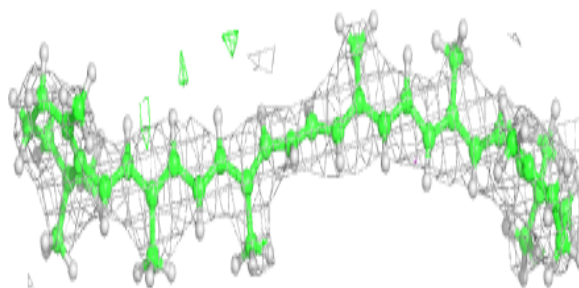
**Electron density around CLA C 503:**

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



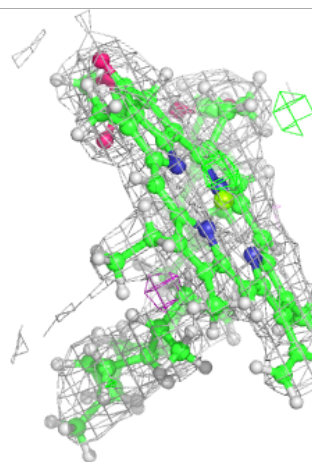
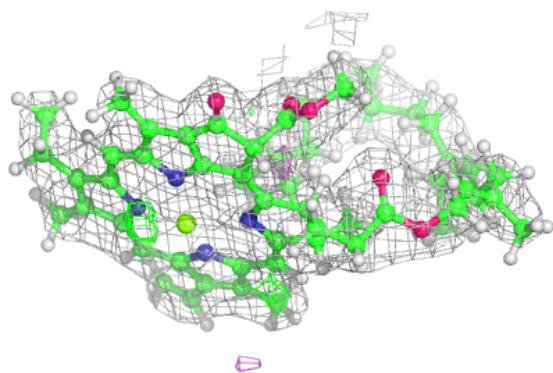
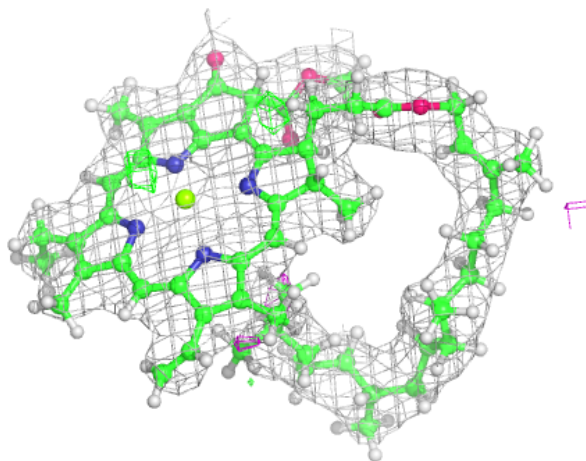
Electron density around BCR c 516:

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



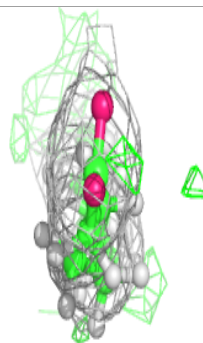
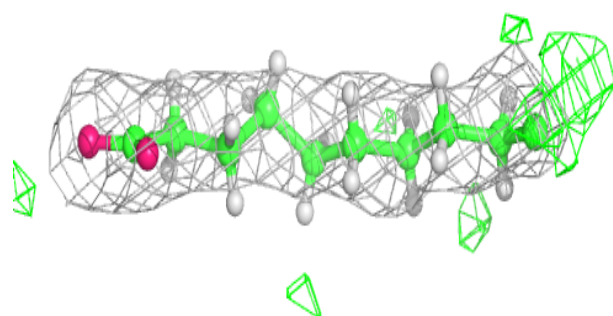
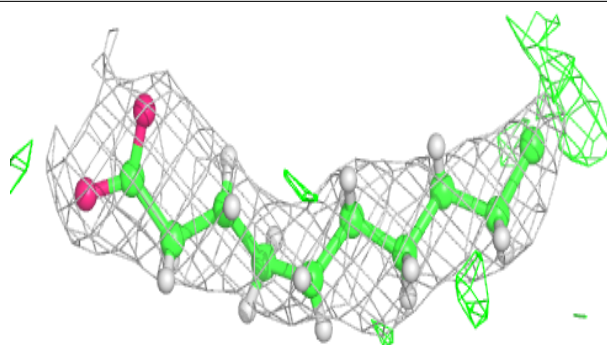
Electron density around CLA b 614:

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

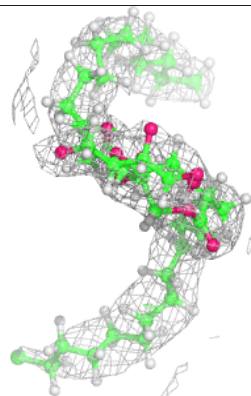
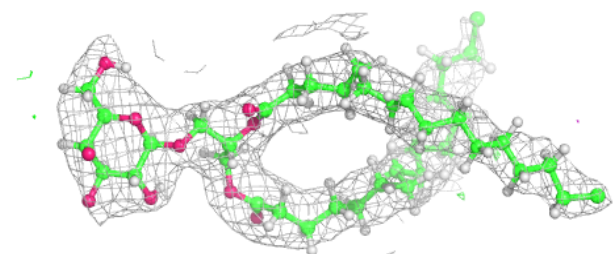
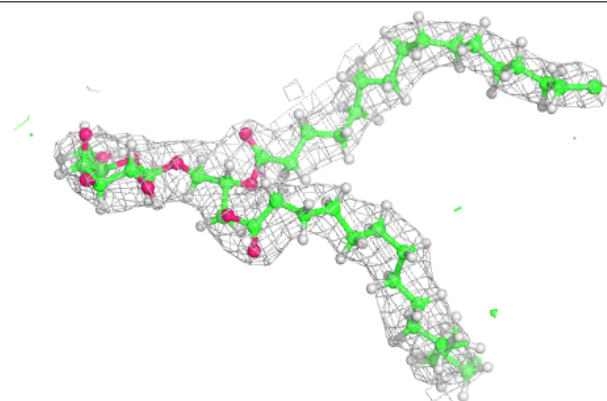


Electron density around STE C 520:

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

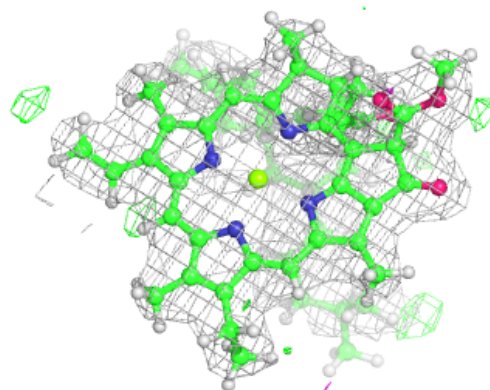
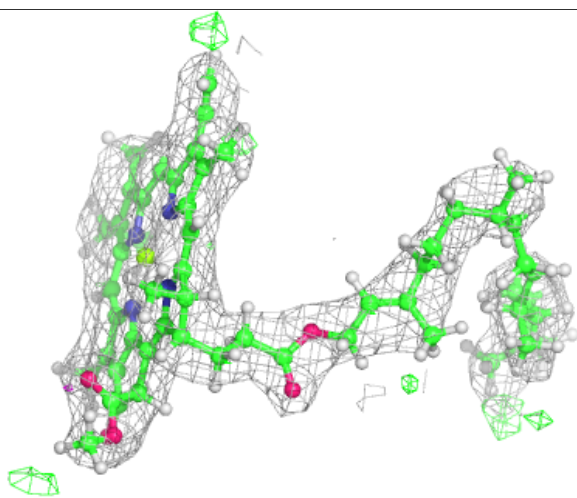
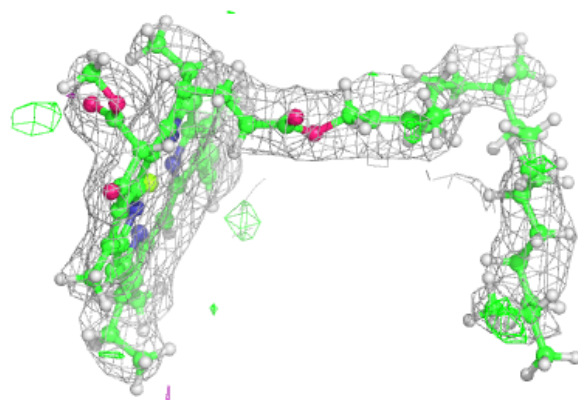
**Electron density around LMG M 101:**

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



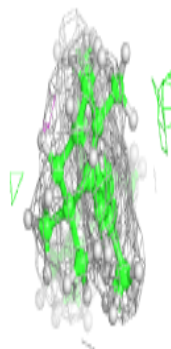
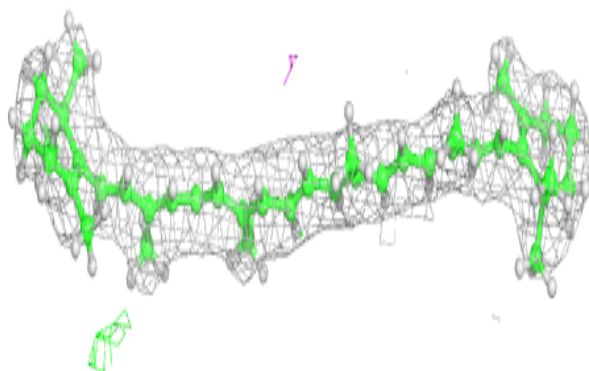
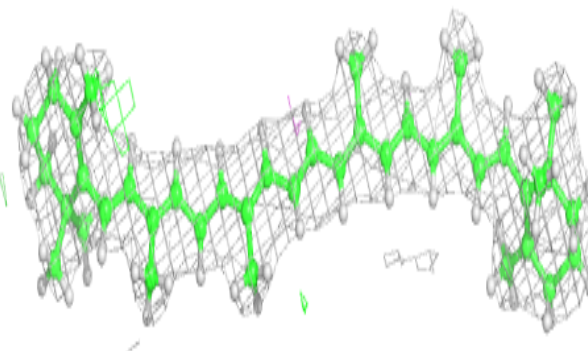
Electron density around CLA a 405:

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

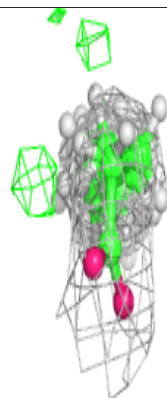
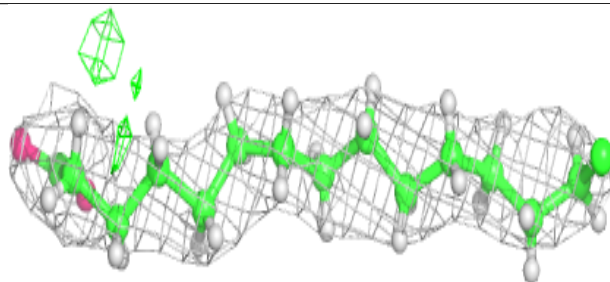
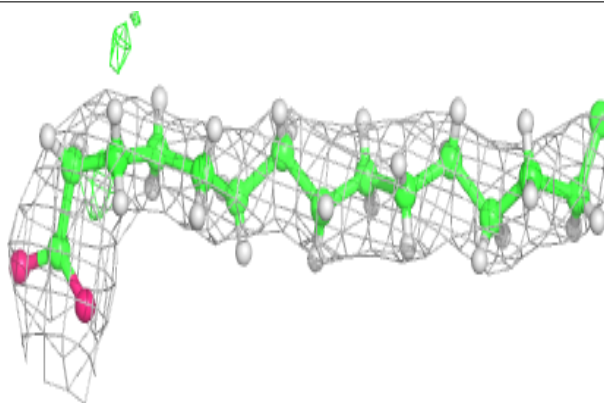


Electron density around BCR B 620:

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

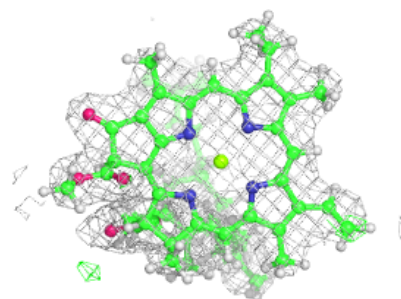
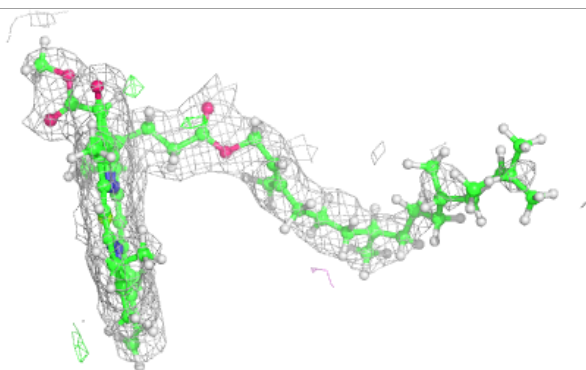
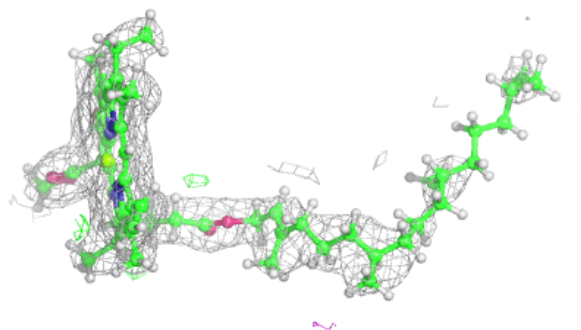
**Electron density around STE d 410:**

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



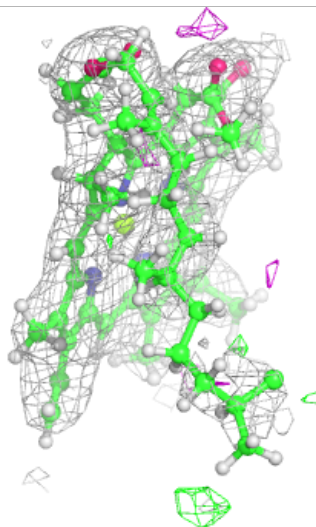
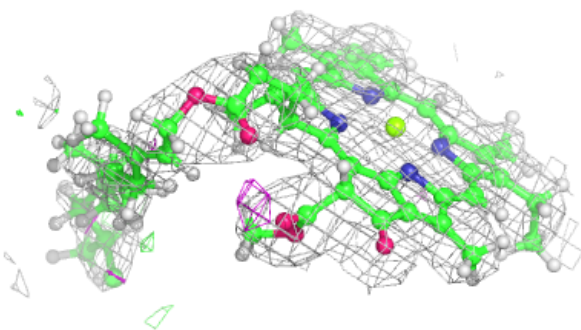
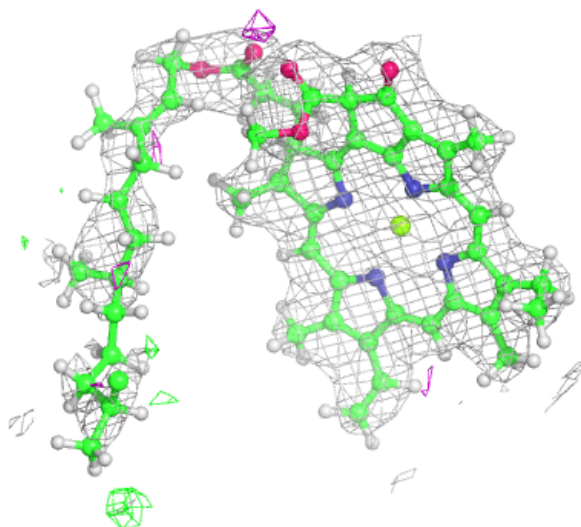
Electron density around CLA D 403:

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



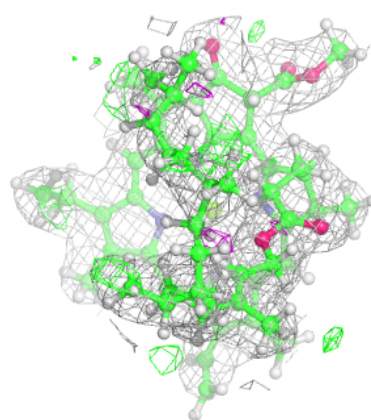
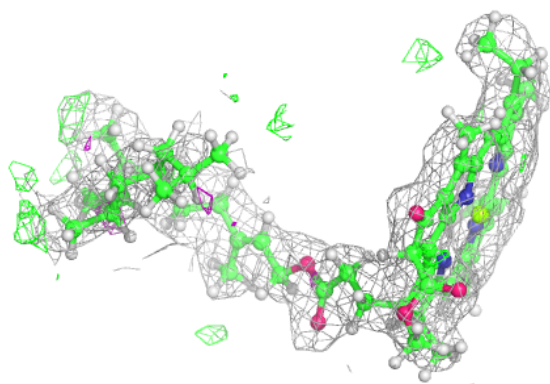
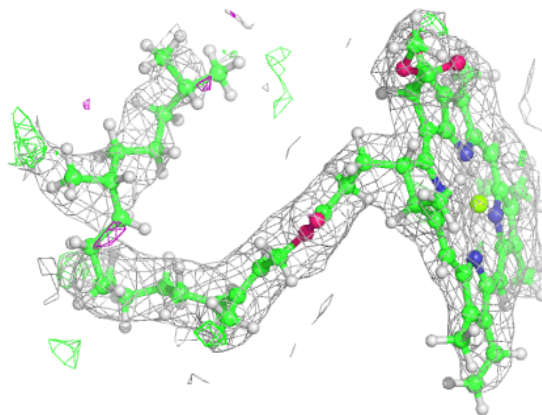
Electron density around CLA b 615:

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



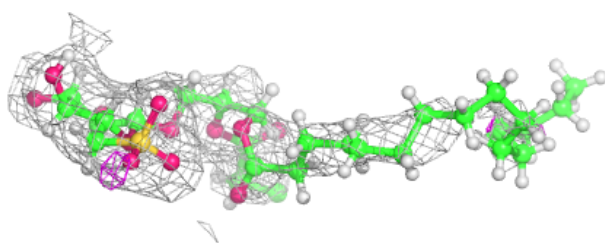
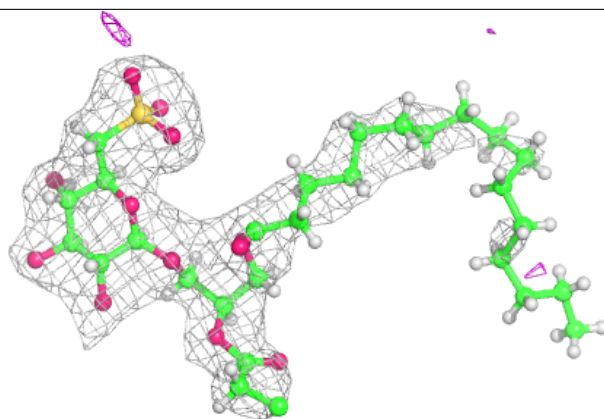
Electron density around CLA B 607:

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

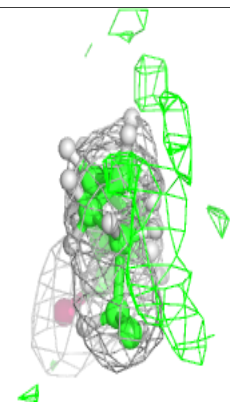
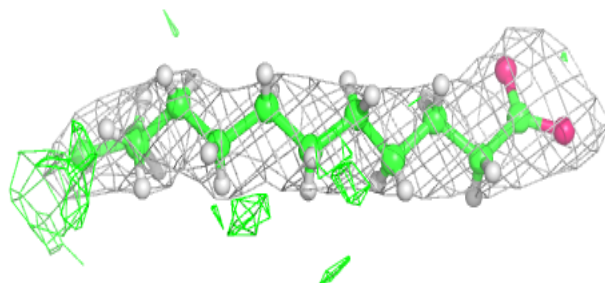
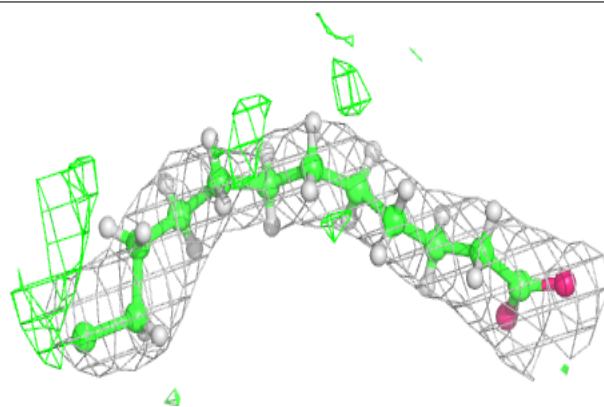


Electron density around SQD f 101:

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

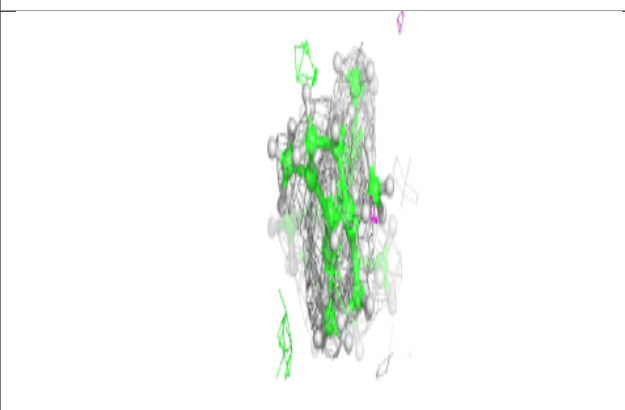
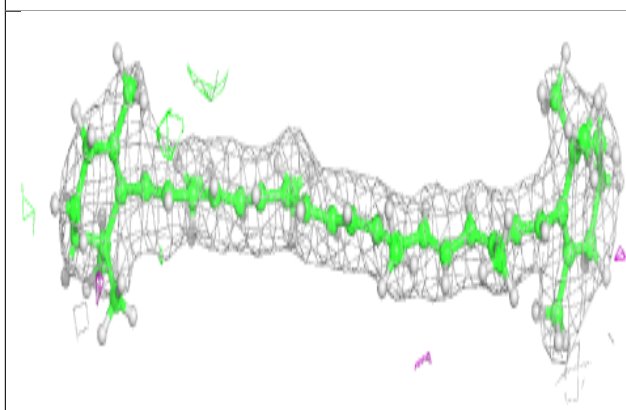
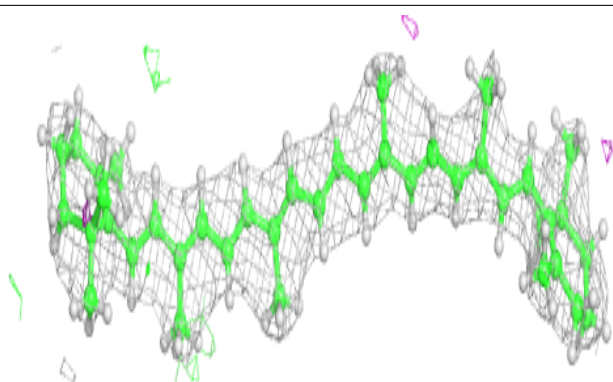
**Electron density around STE B 624:**

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

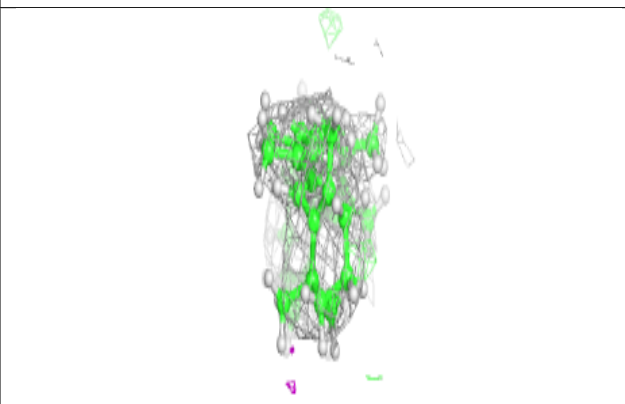
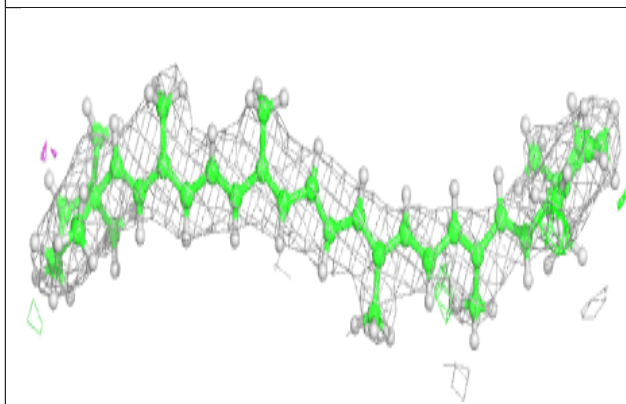
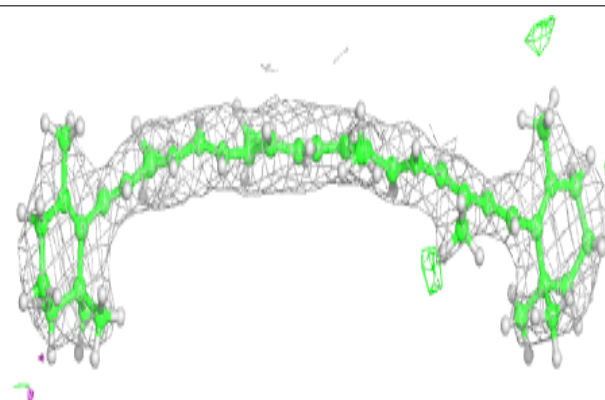


Electron density around BCR C 515:

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

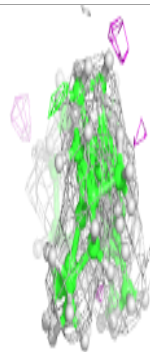
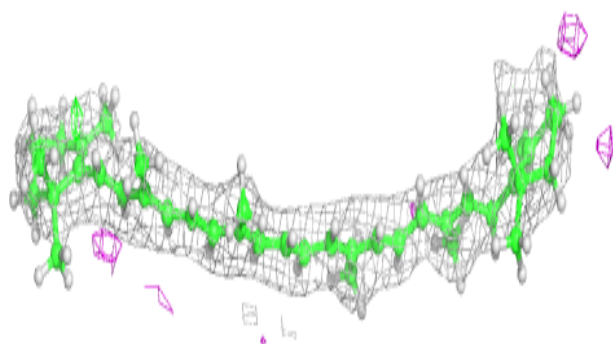
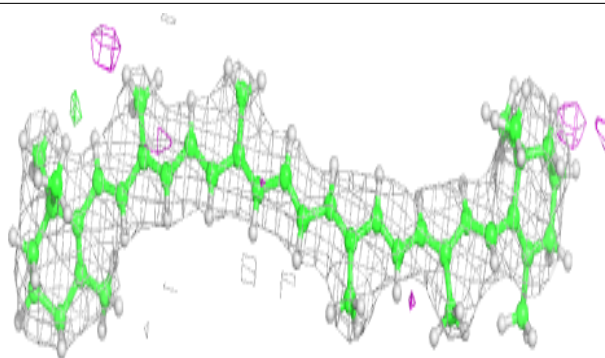
**Electron density around BCR c 518:**

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

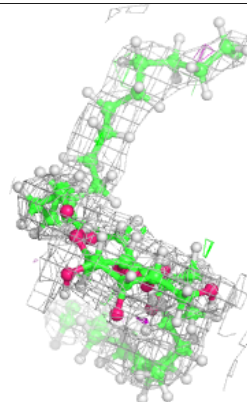
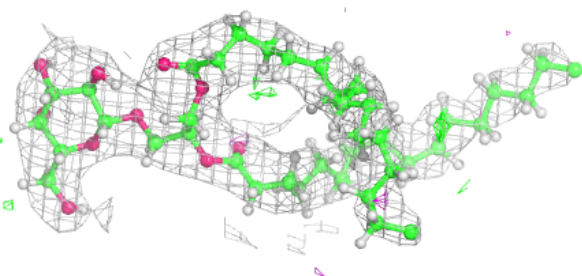
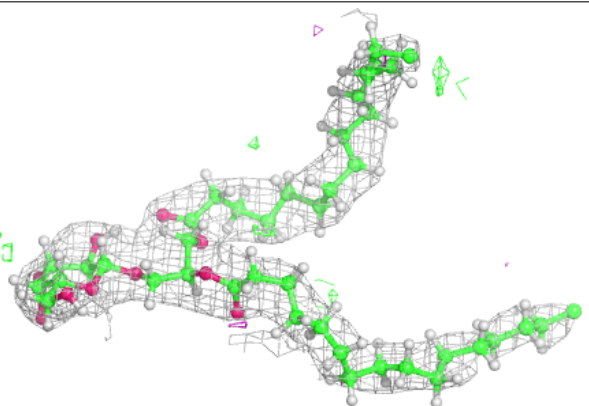


Electron density around BCR D 404:

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

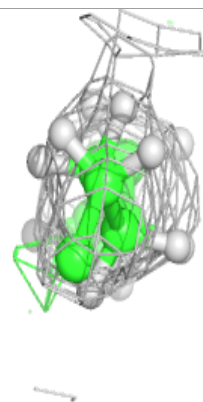
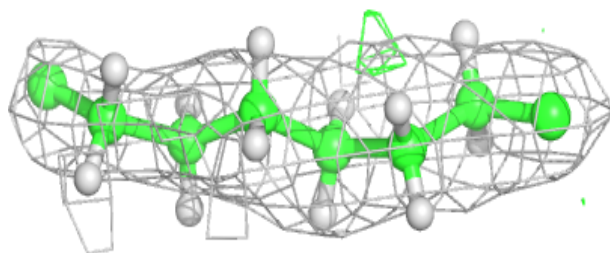
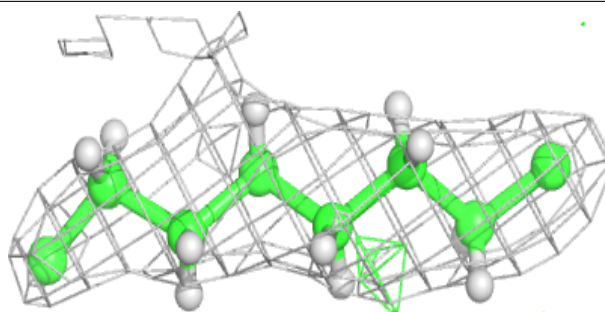
**Electron density around LMG b 621:**

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



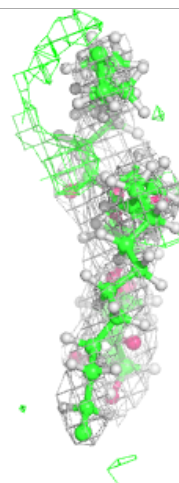
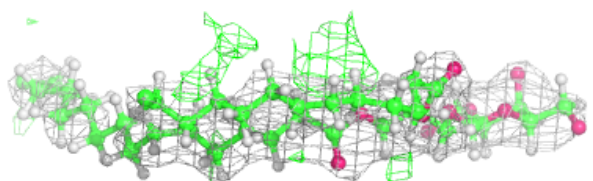
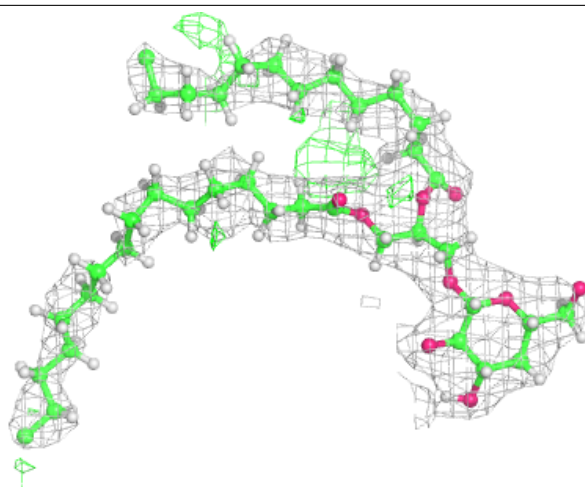
Electron density around STE Z 102:

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



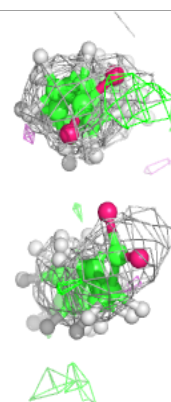
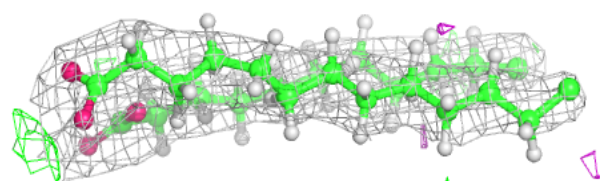
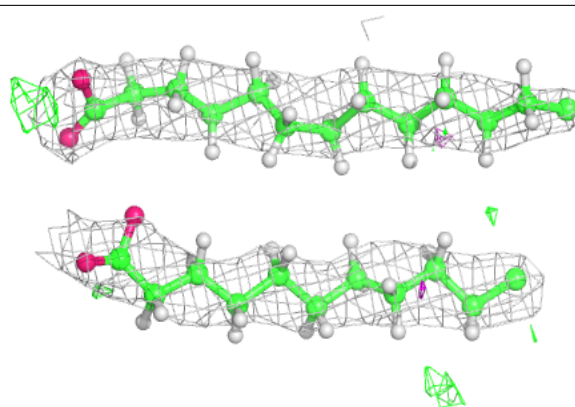
Electron density around LMG C 519:

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

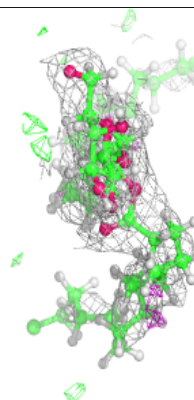
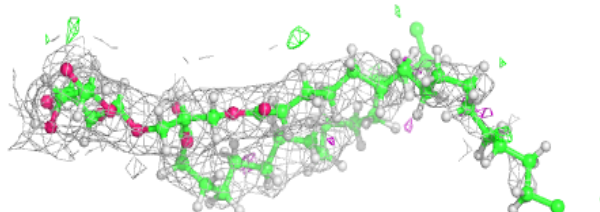
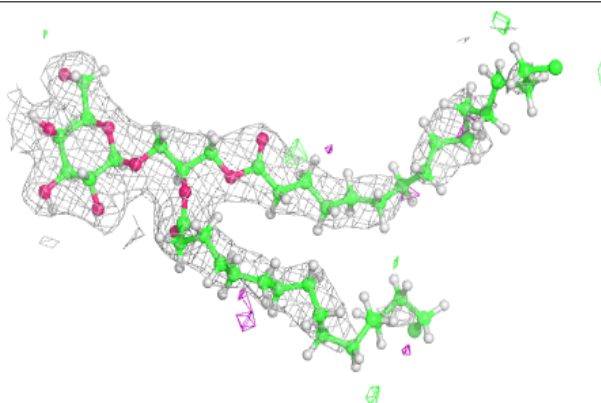


Electron density around LMG D 411:

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

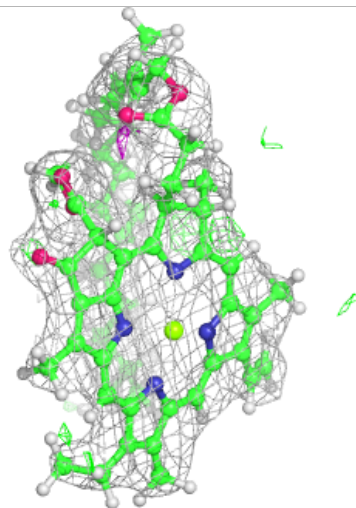
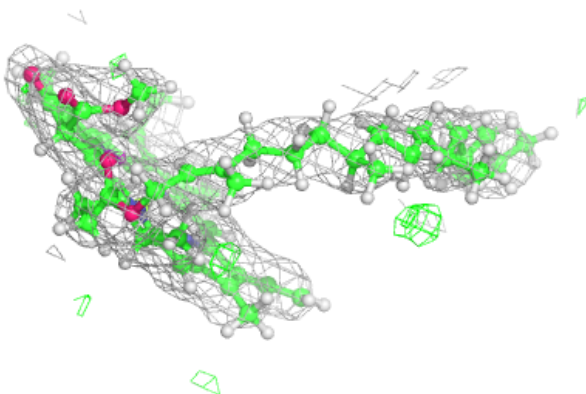
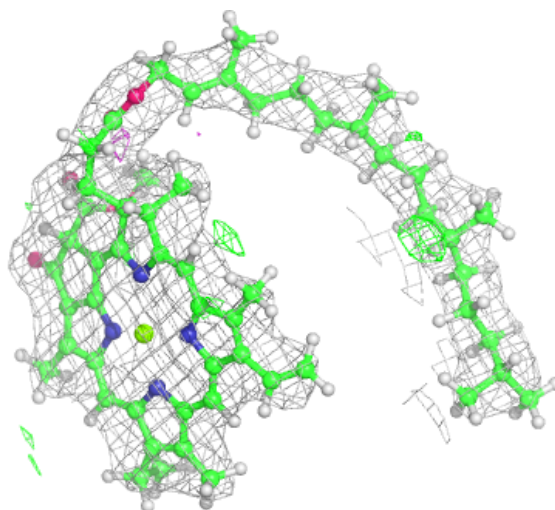
**Electron density around LMG D 406:**

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



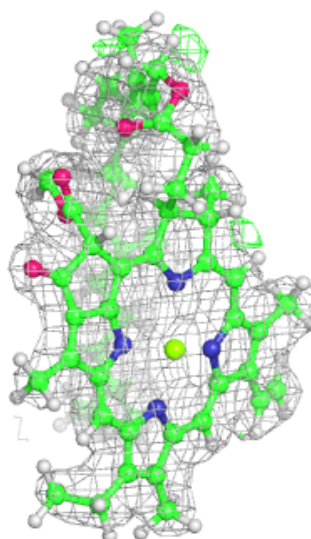
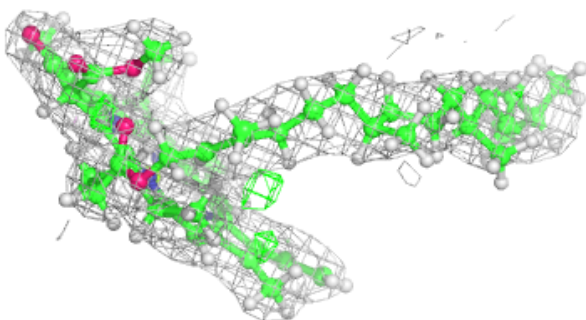
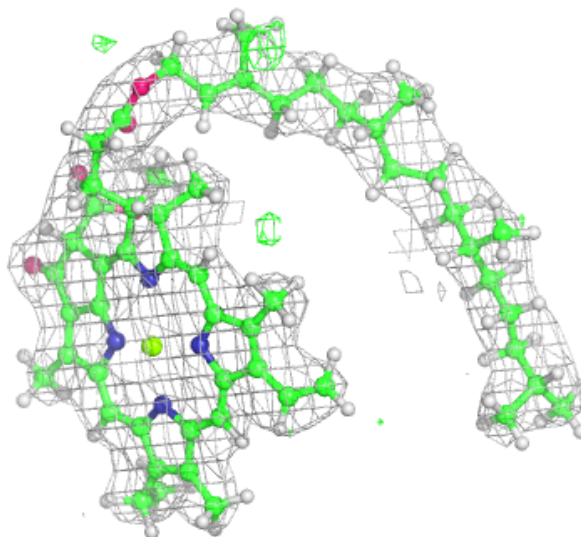
Electron density around CLA c 509:

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



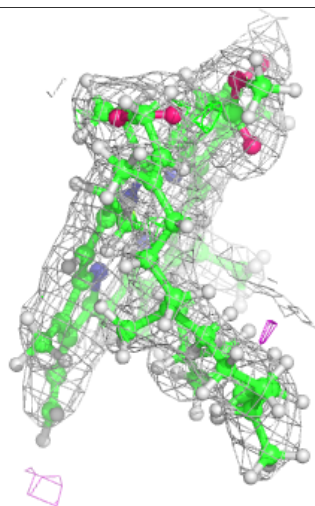
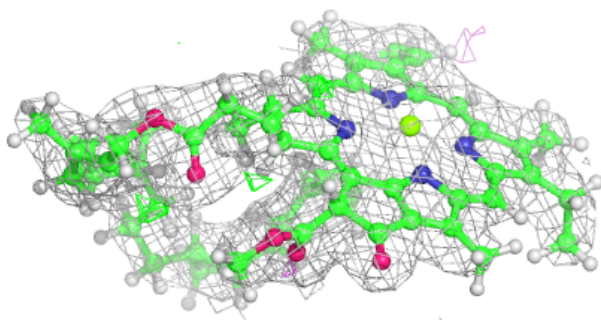
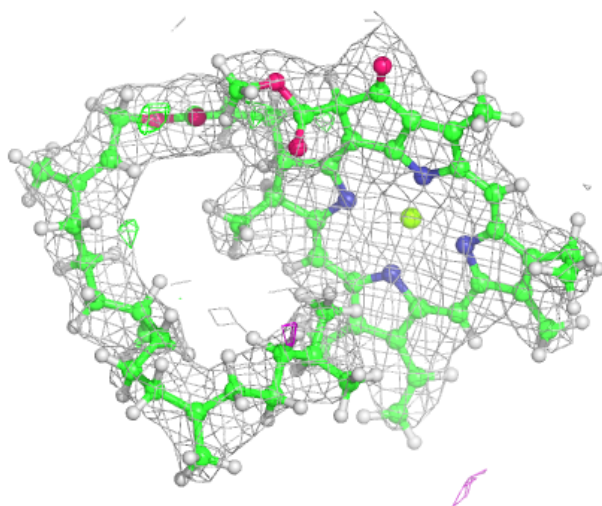
Electron density around CLA C 508:

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



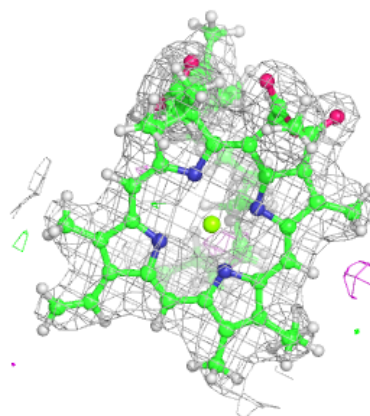
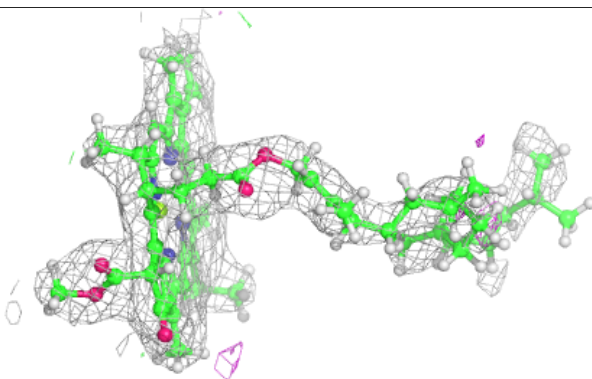
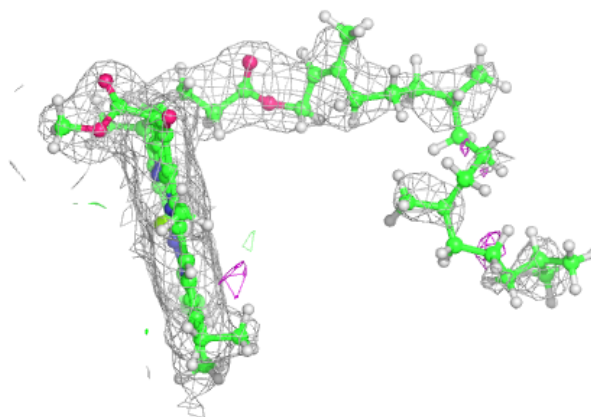
Electron density around CLA B 616:

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

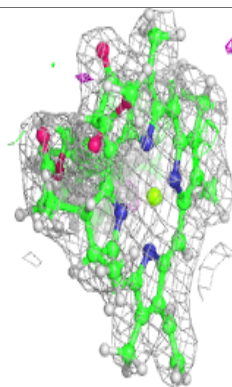
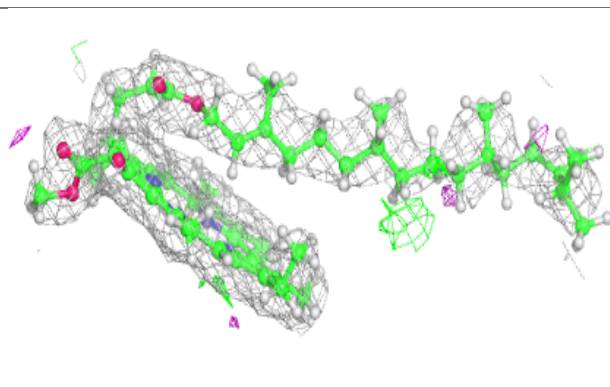
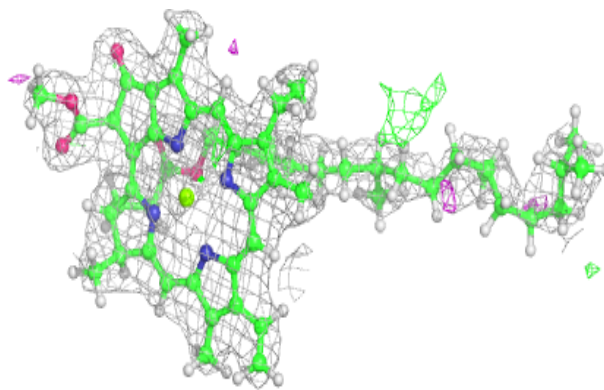


Electron density around CLA c 508:

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

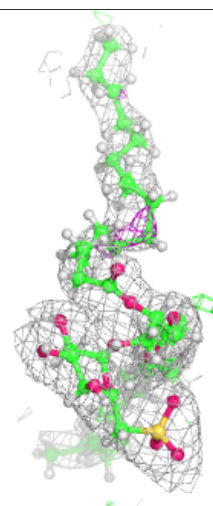
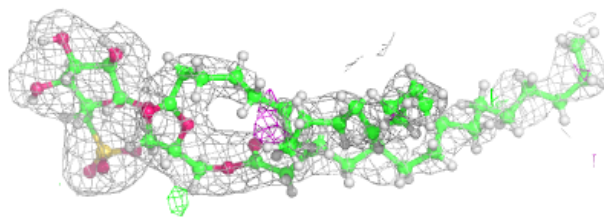
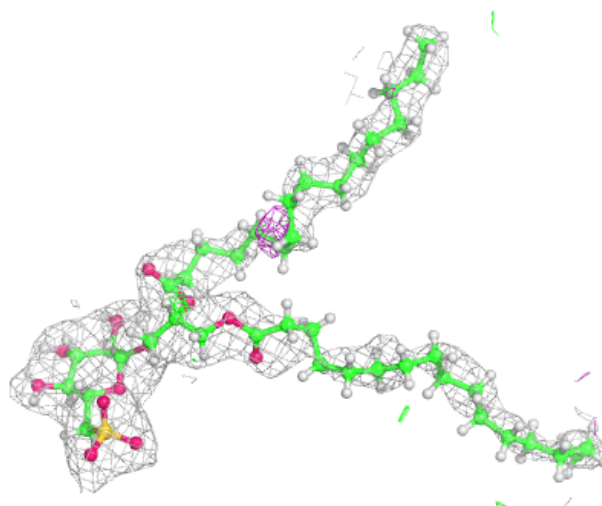
**Electron density around CLA B 615:**

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



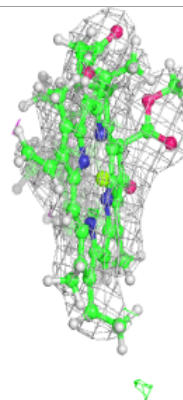
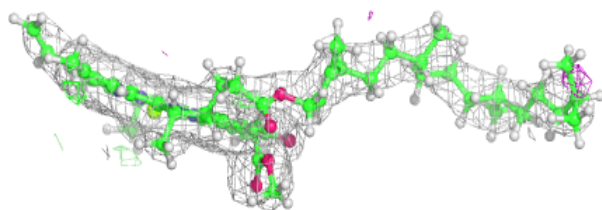
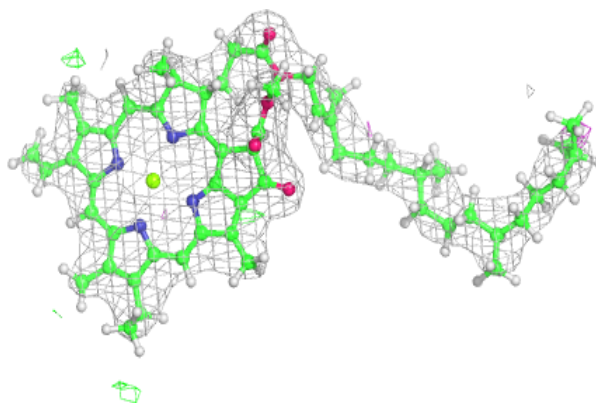
Electron density around SQD a 412:

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

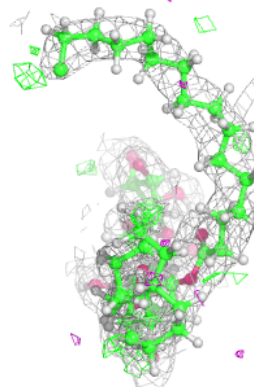
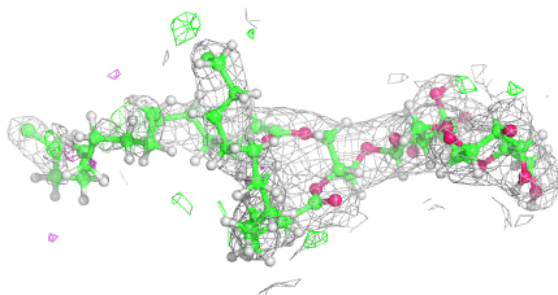
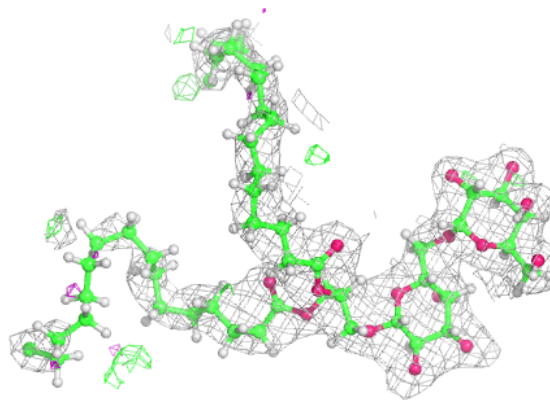


Electron density around CLA b 601:

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

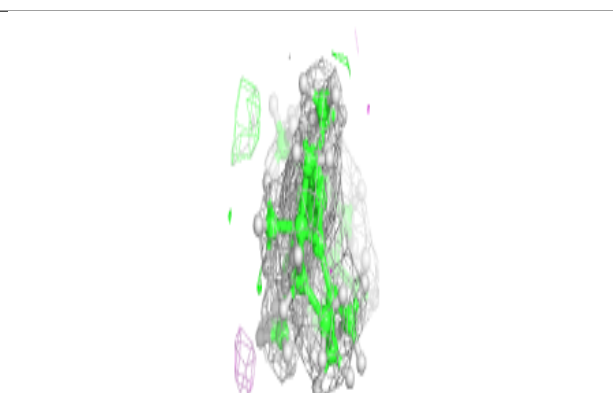
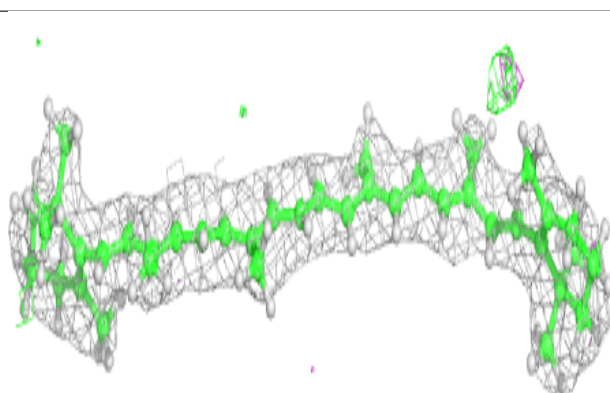
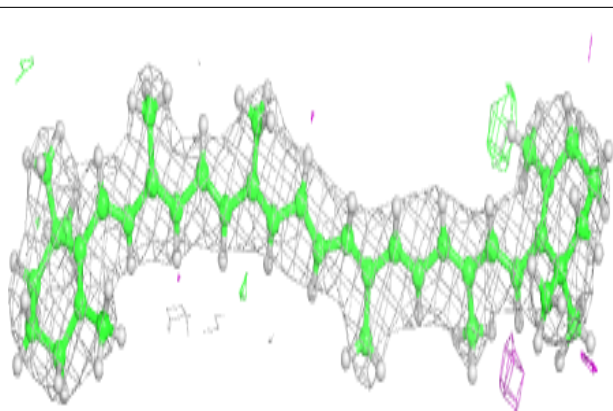
**Electron density around DGD C 517:**

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

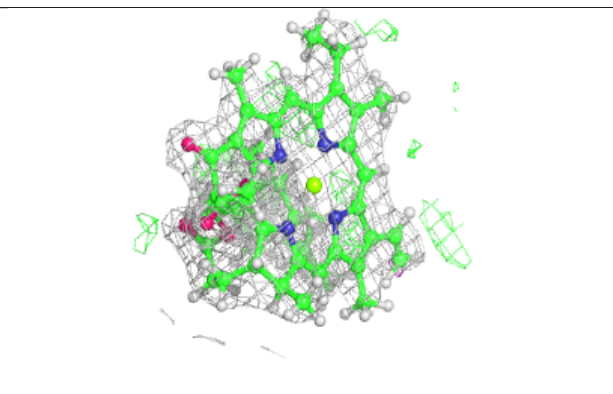
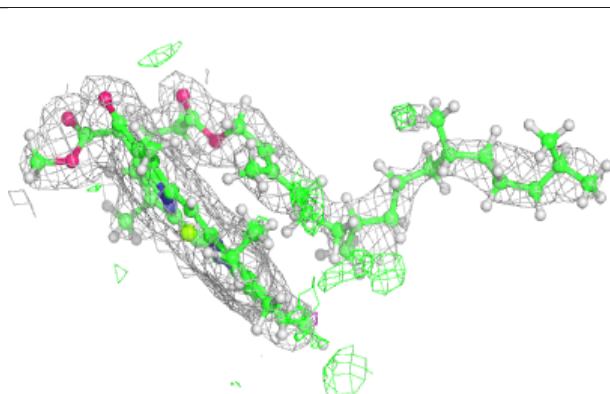
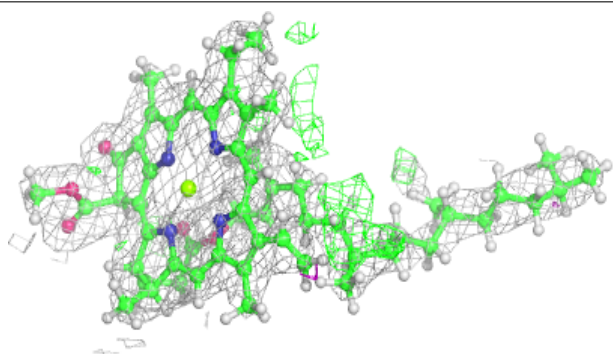


Electron density around BCR b 618:

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

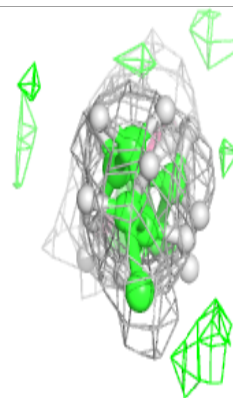
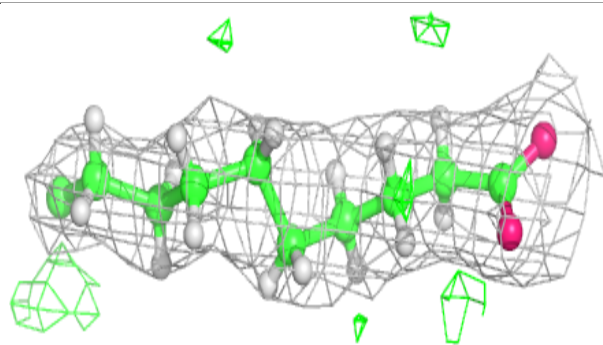
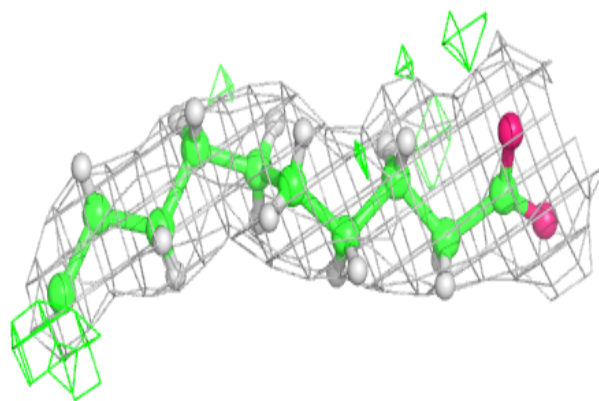
**Electron density around CLA C 506:**

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

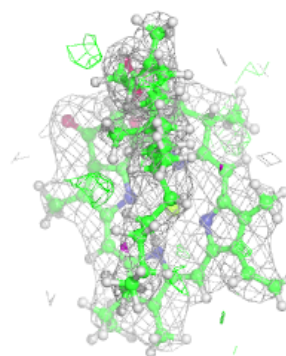
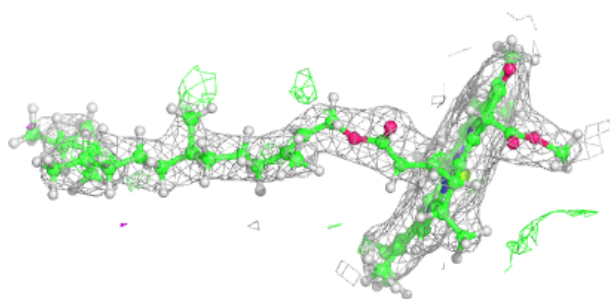
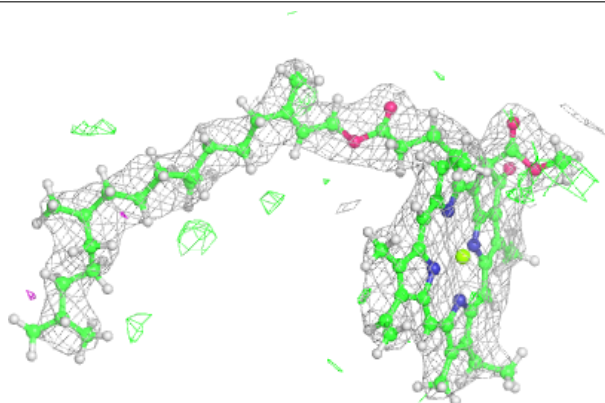


Electron density around STE J 101:

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

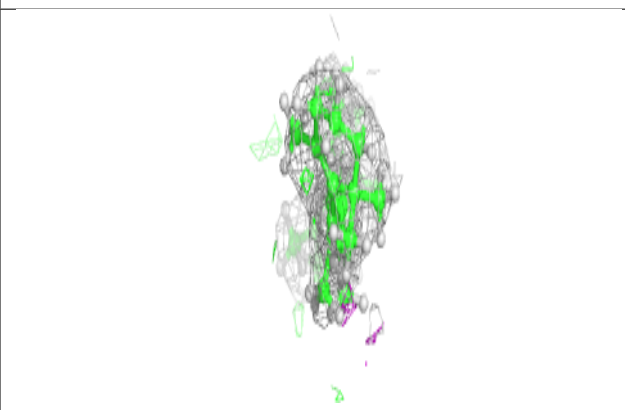
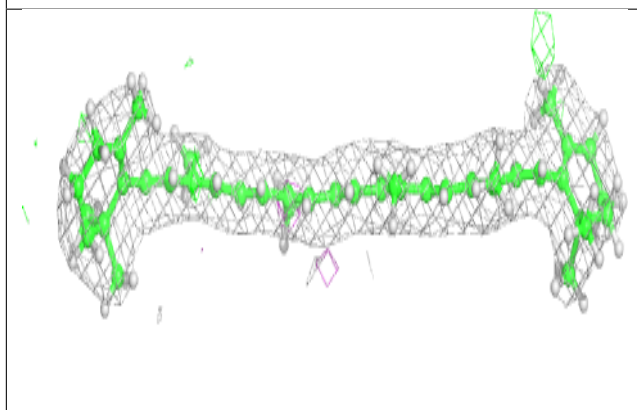
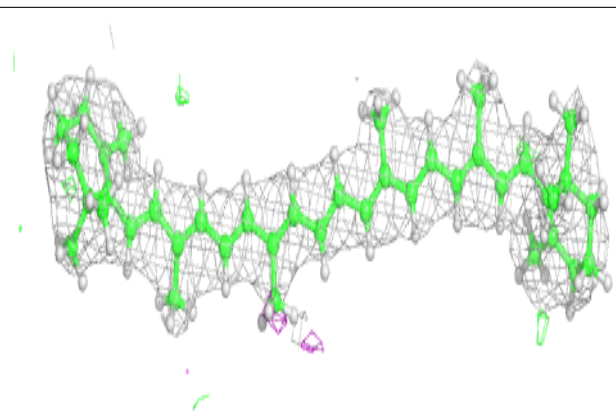
**Electron density around CLA b 608:**

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



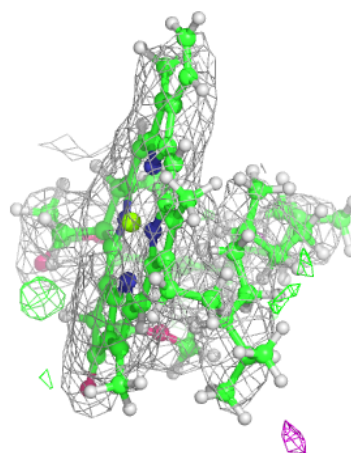
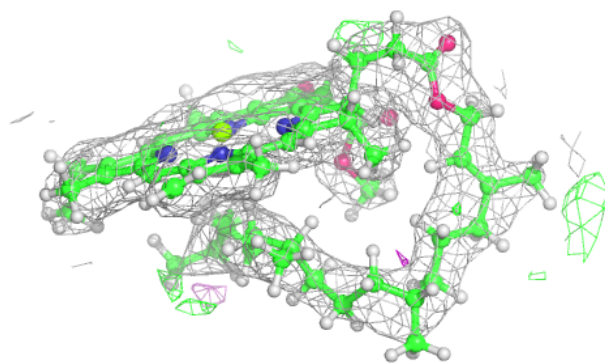
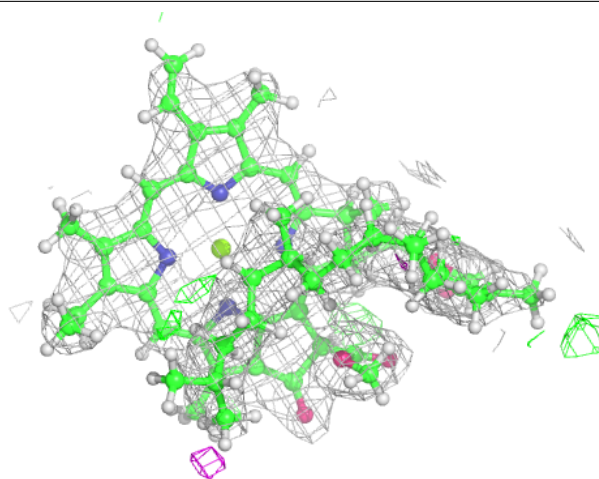
Electron density around BCR b 617:

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



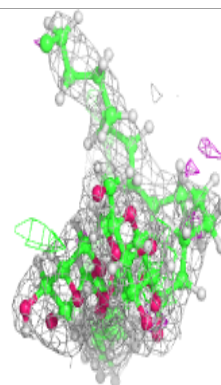
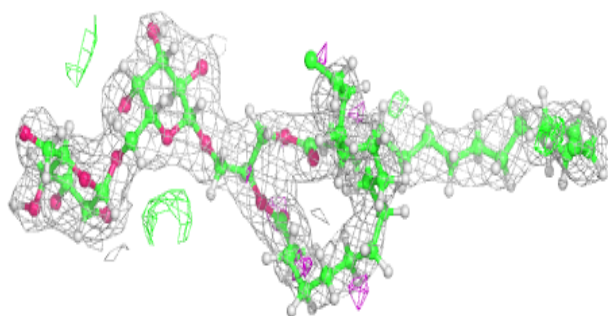
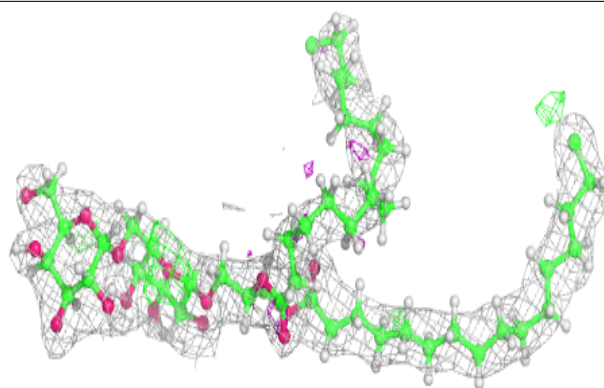
Electron density around CLA c 512:

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

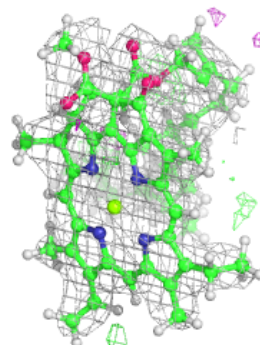
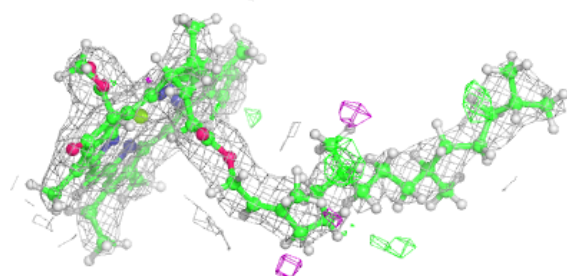
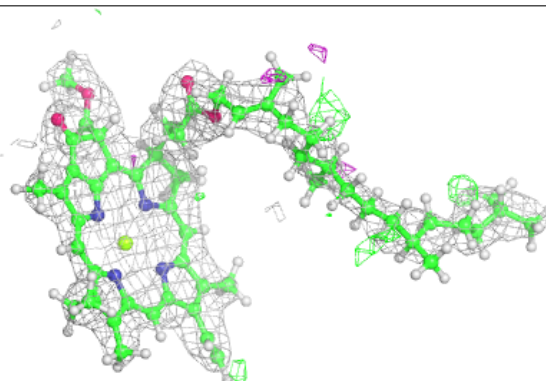


Electron density around DGD h 102:

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

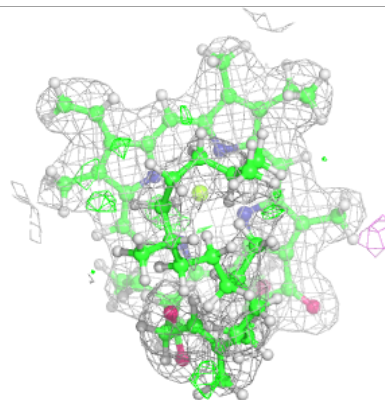
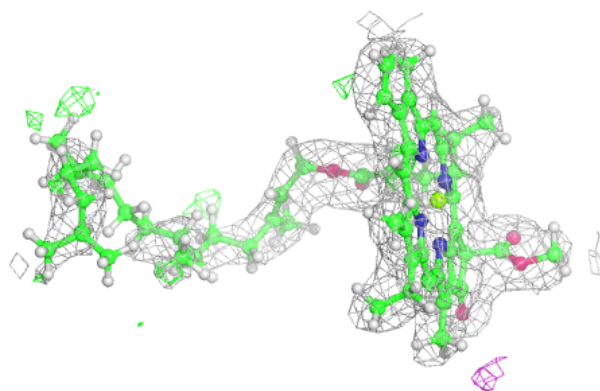
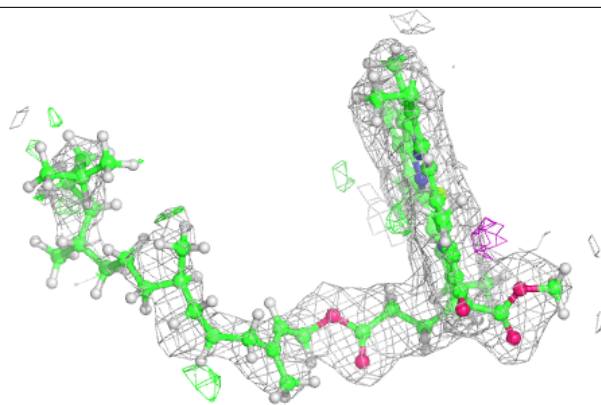
**Electron density around CLA c 513:**

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



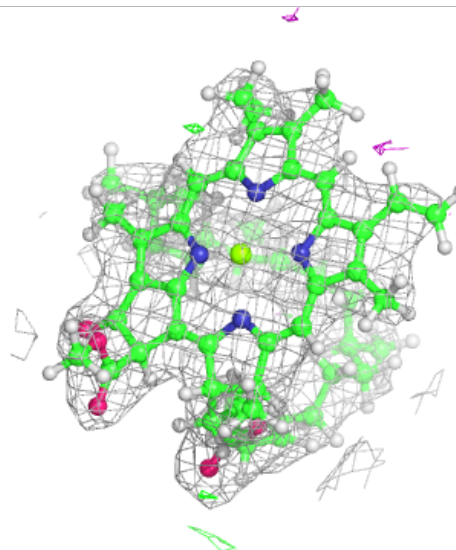
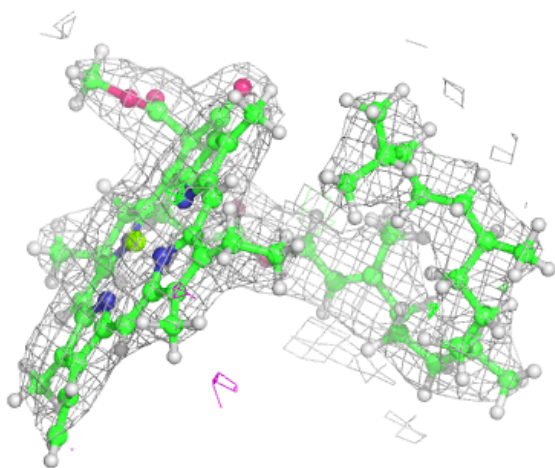
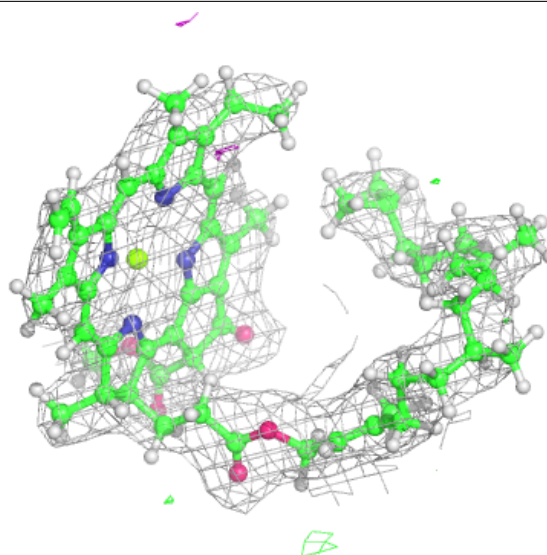
Electron density around CLA C 507:

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



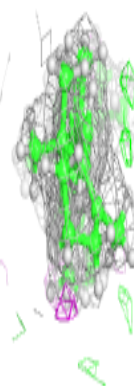
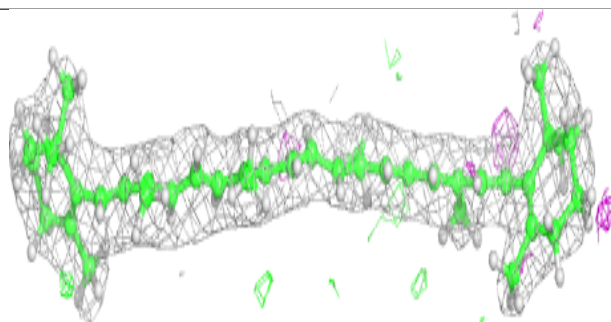
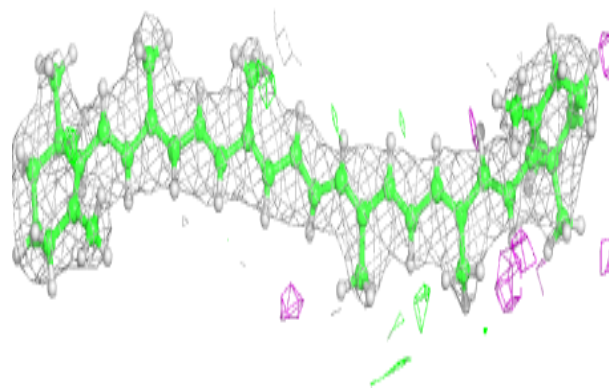
Electron density around CLA c 505:

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

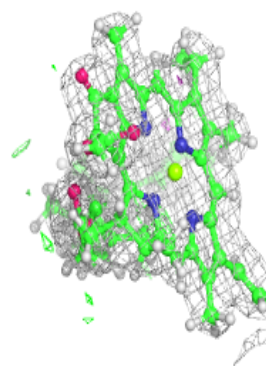
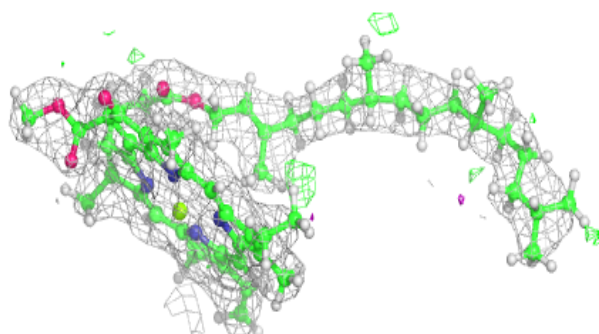
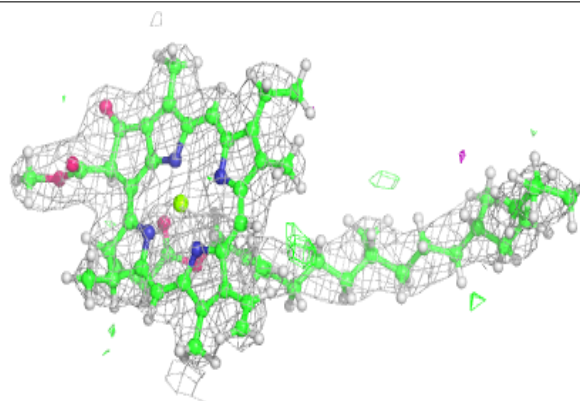


Electron density around BCR B 619:

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

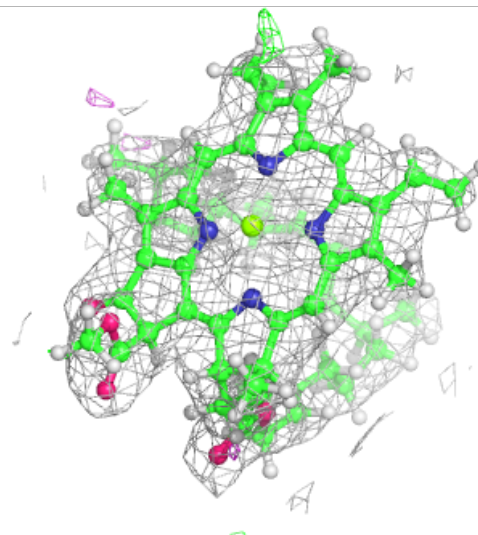
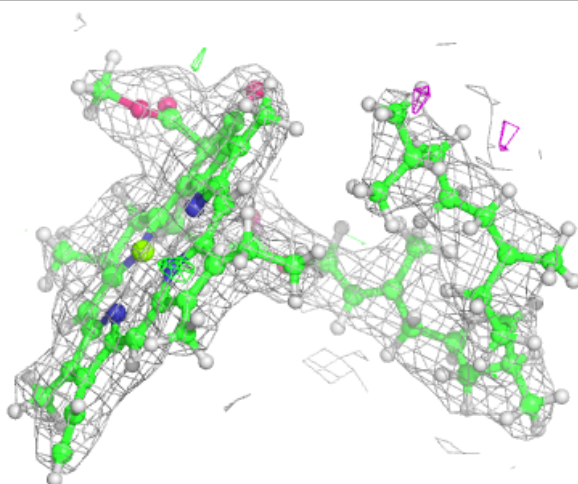
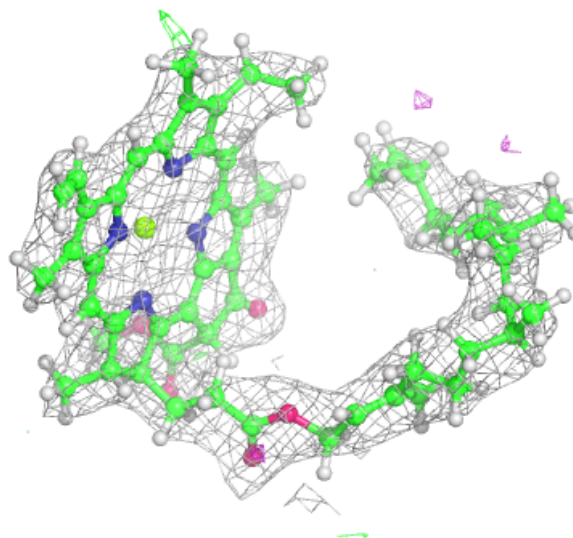
**Electron density around CLA b 607:**

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



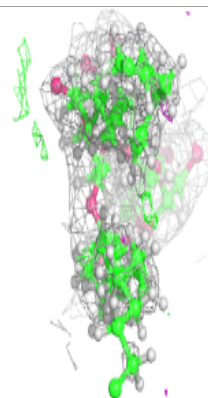
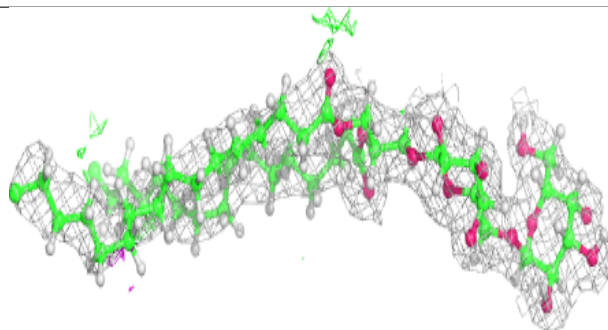
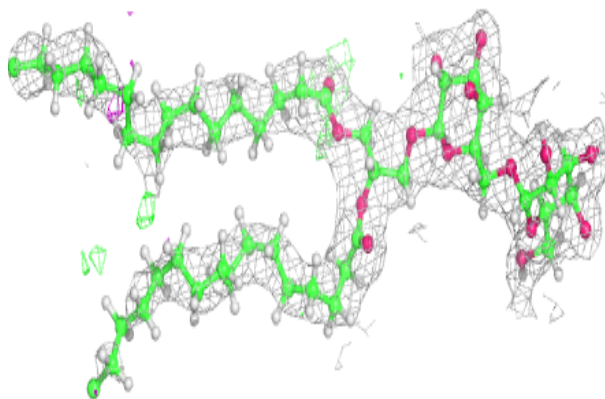
Electron density around CLA C 504:

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

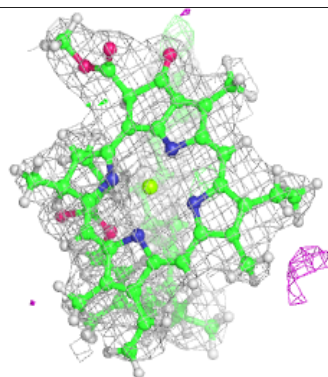
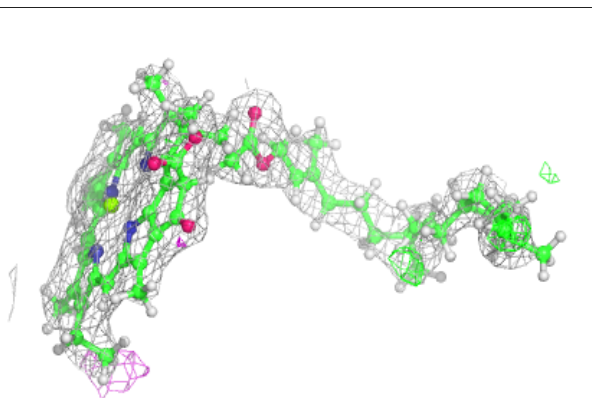
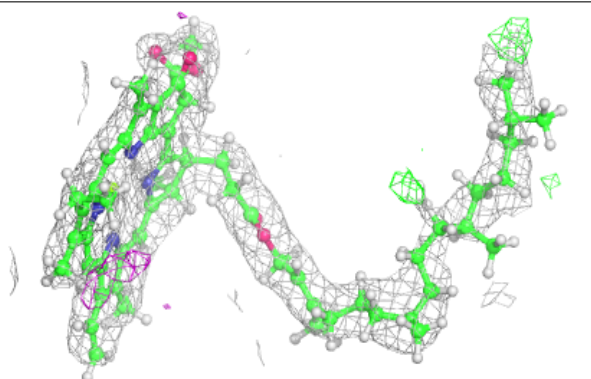


Electron density around DGD c 521:

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

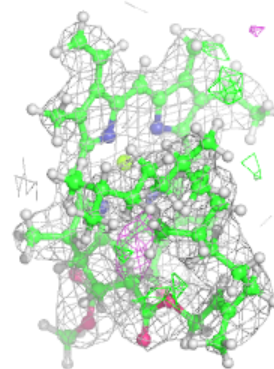
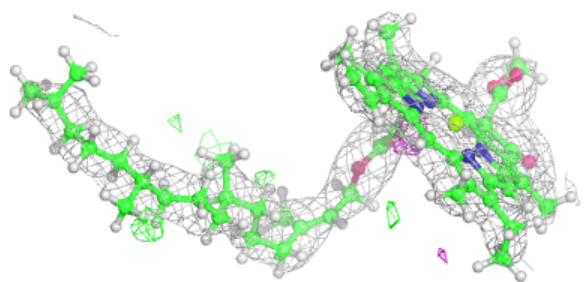
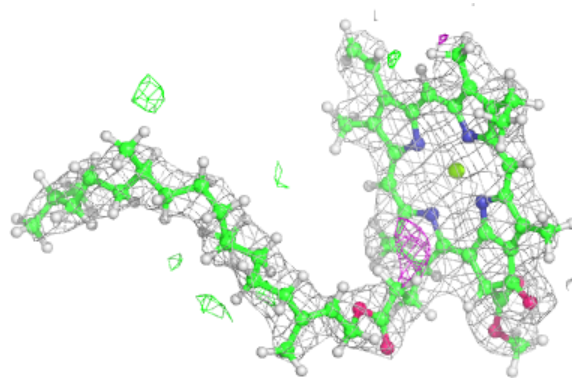
**Electron density around CLA b 605:**

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

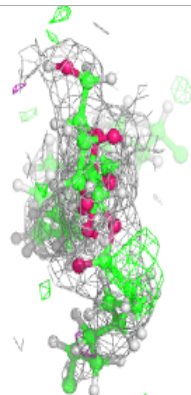
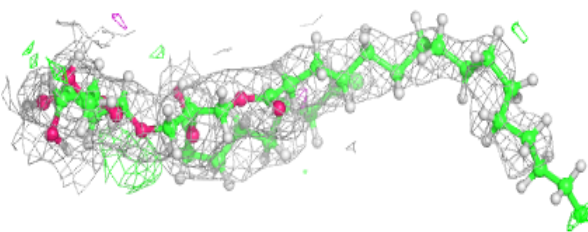
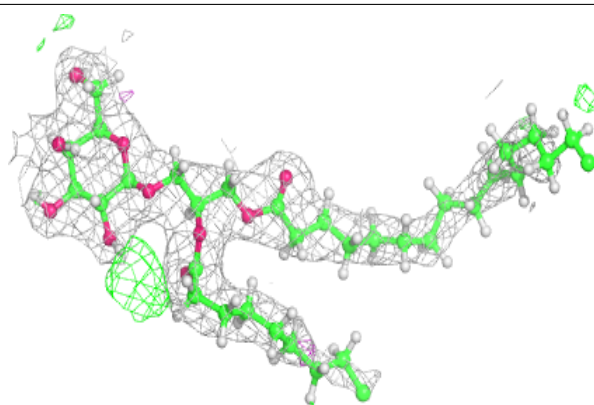


Electron density around CLA C 512:

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

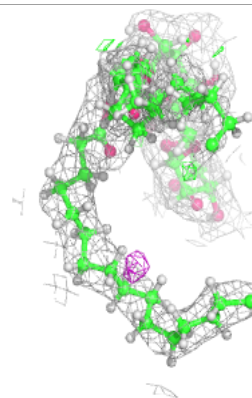
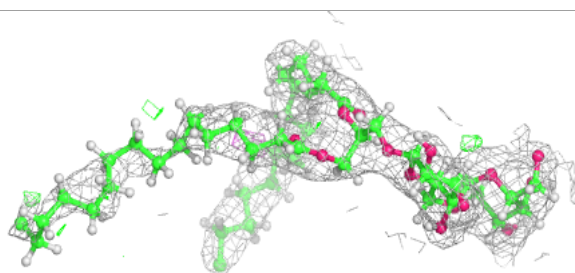
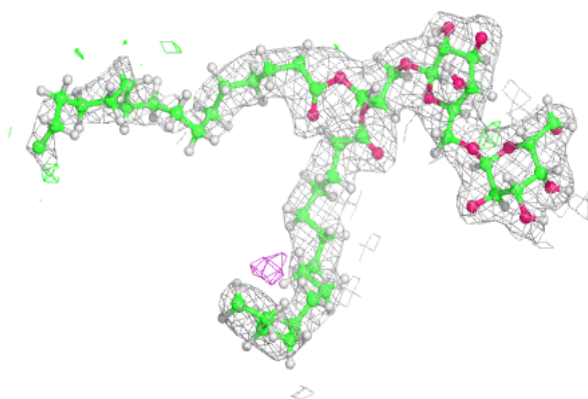
**Electron density around LMG d 409:**

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

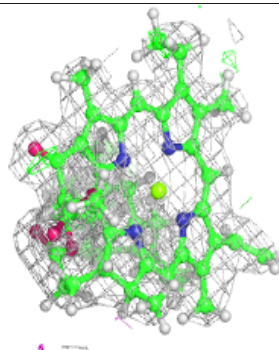
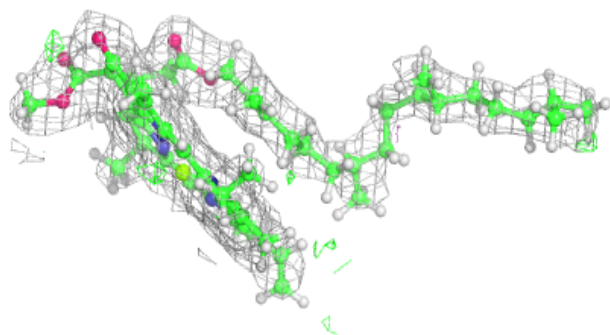
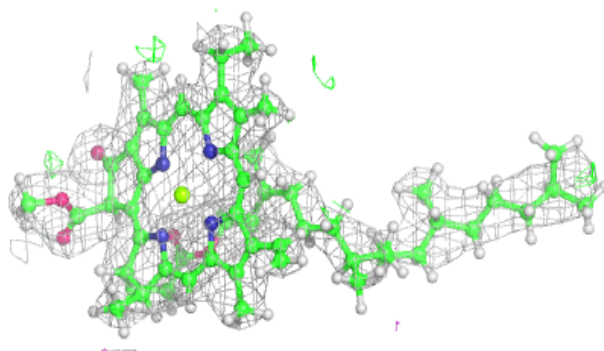


Electron density around DGD c 520:

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

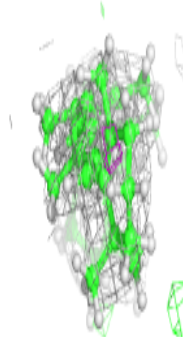
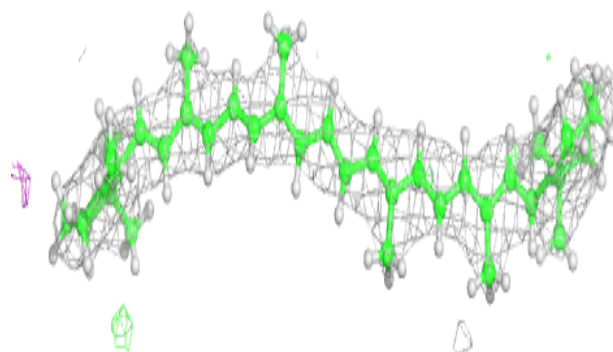
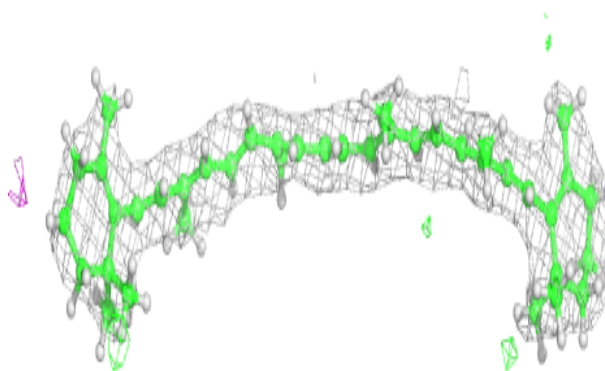
**Electron density around CLA c 507:**

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



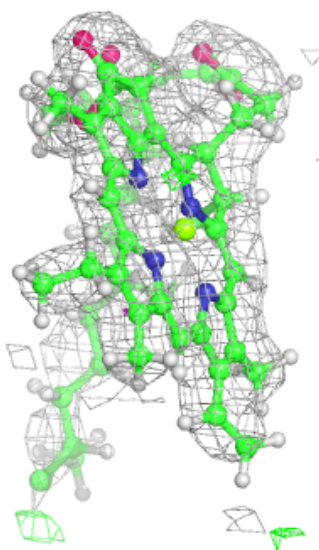
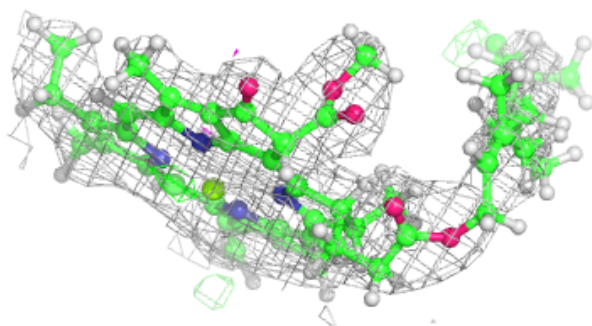
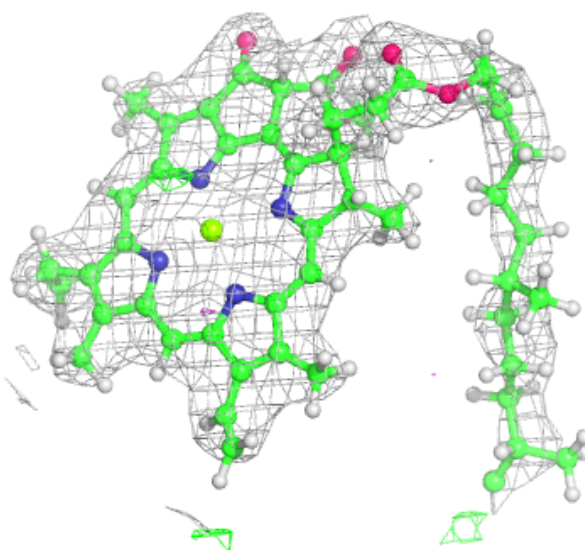
Electron density around BCR K 101:

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



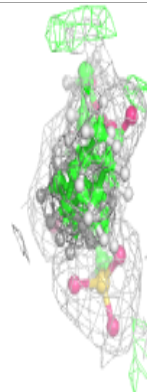
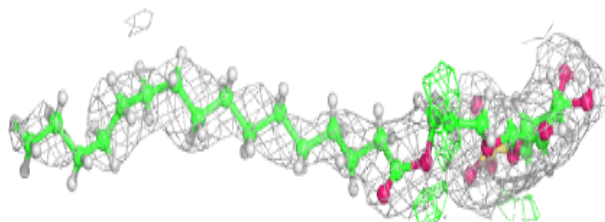
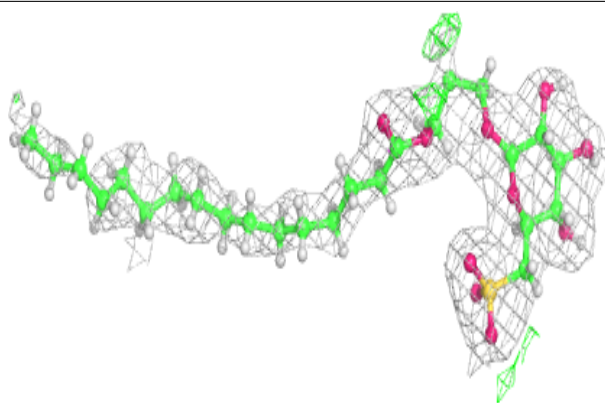
Electron density around CLA B 617:

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

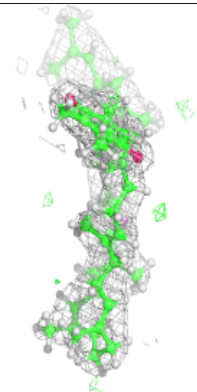
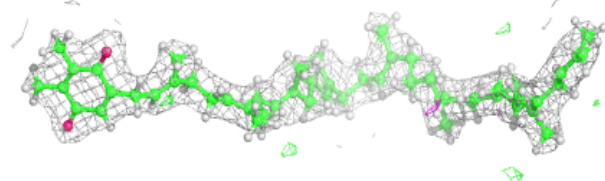
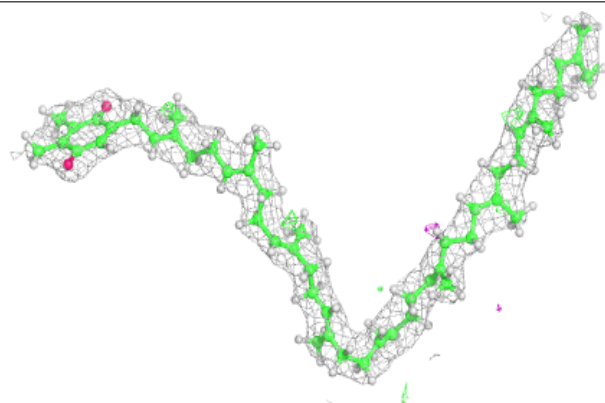


Electron density around SQD D 407:

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

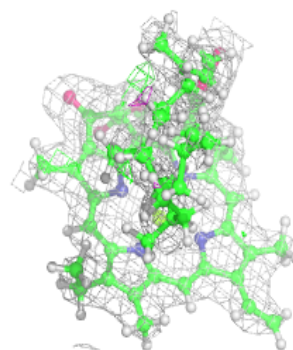
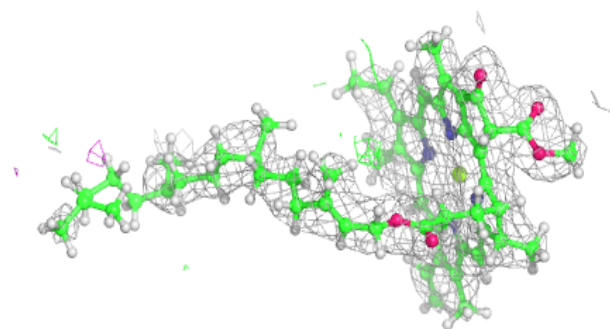
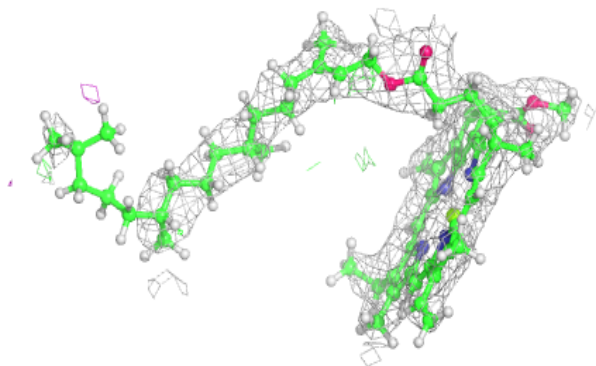
**Electron density around PL9 D 405:**

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

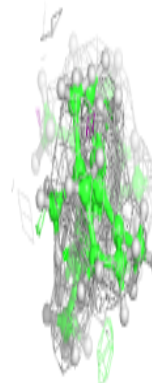
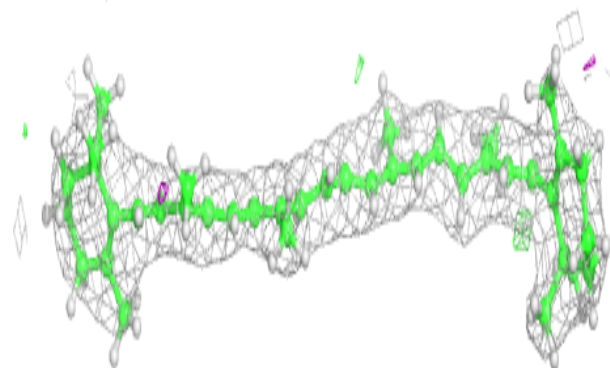
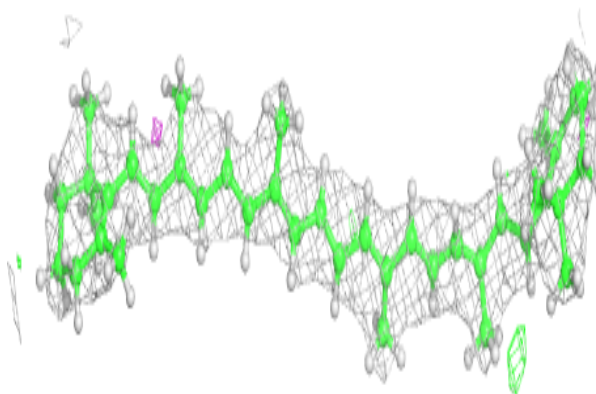


Electron density around CLA C 509:

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

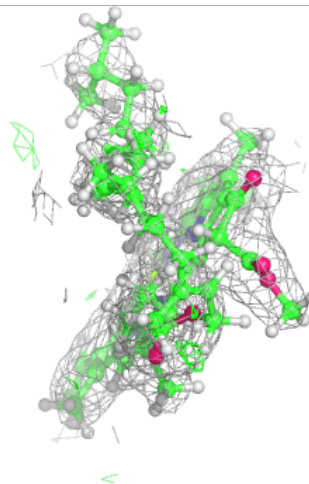
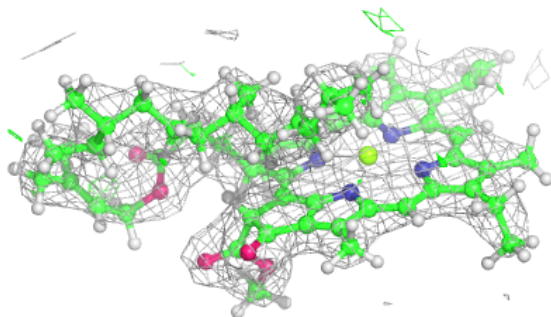
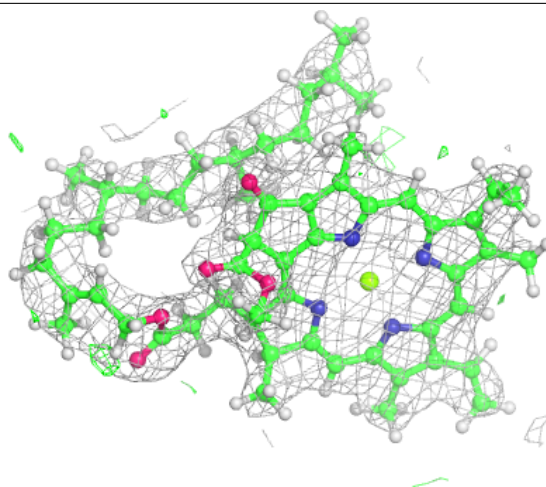
**Electron density around BCR c 517:**

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



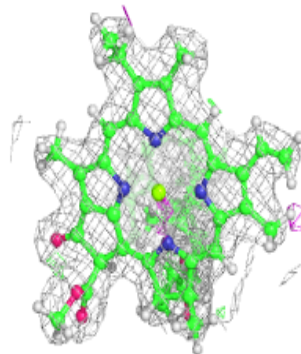
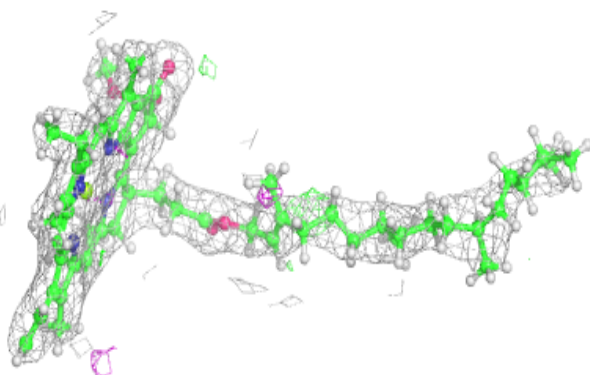
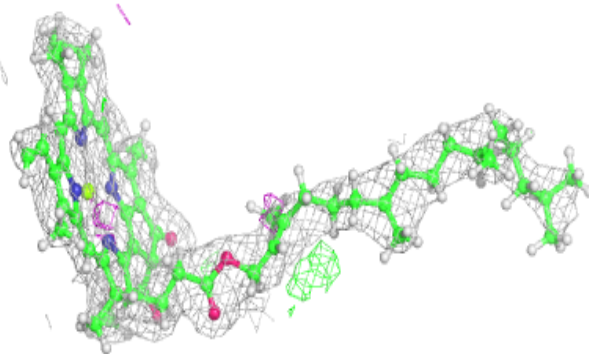
Electron density around CLA c 511:

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

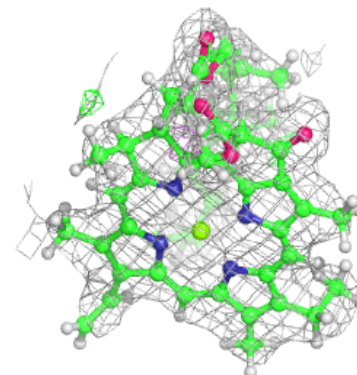
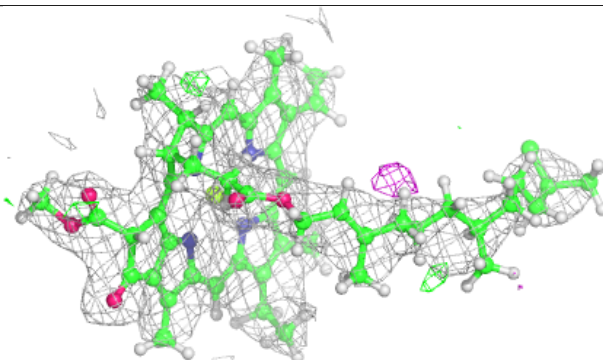
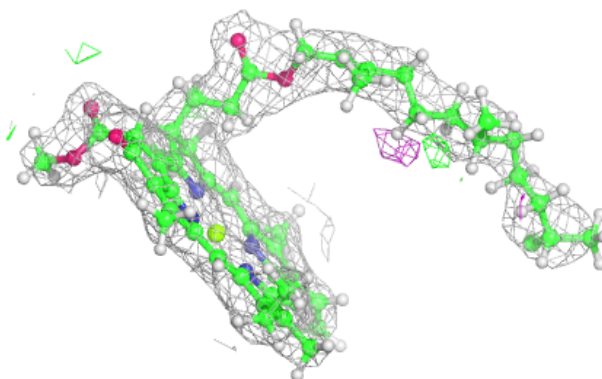


Electron density around CLA B 605:

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

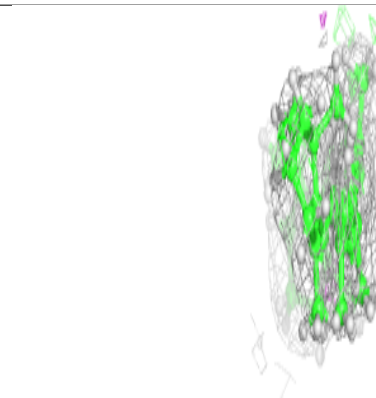
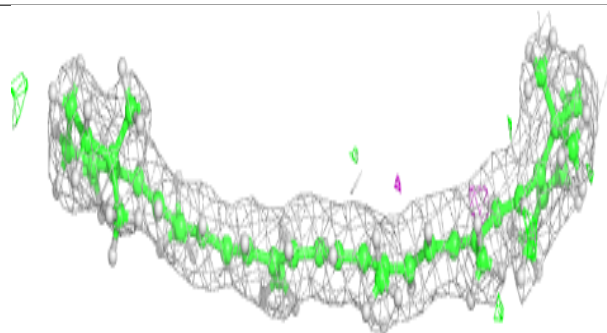
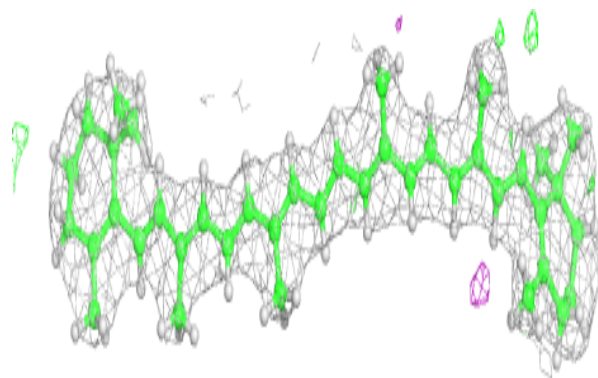
**Electron density around CLA c 506:**

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

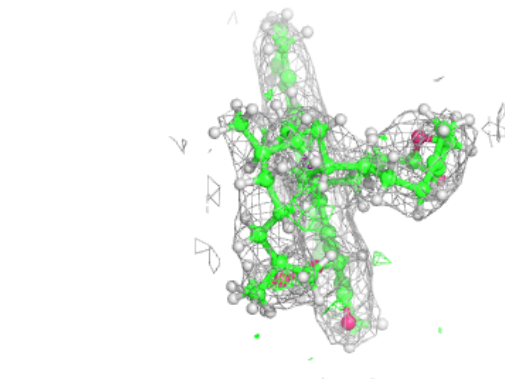
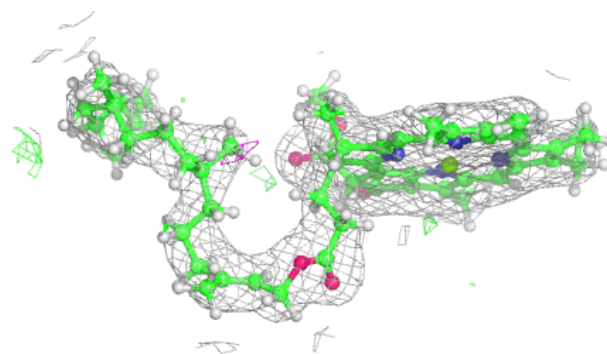
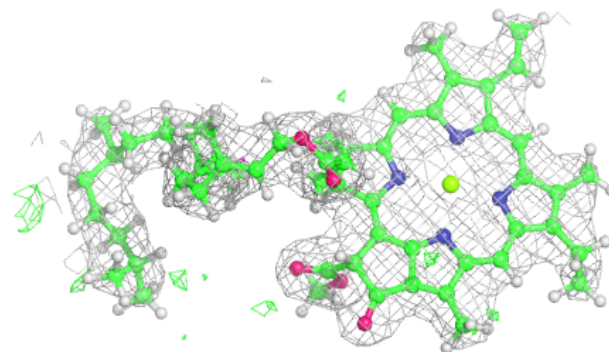


Electron density around BCR t 101:

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

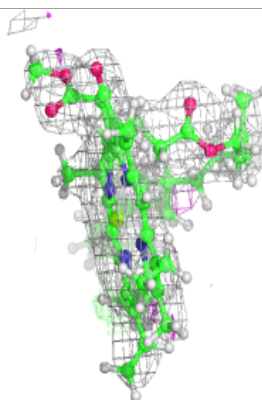
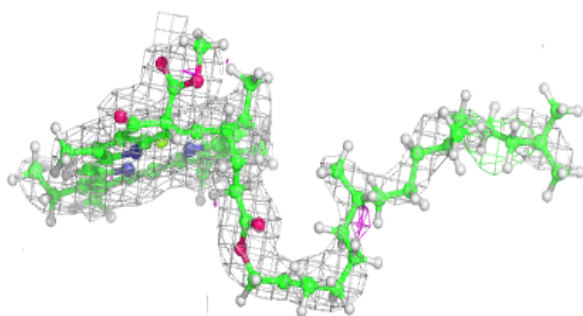
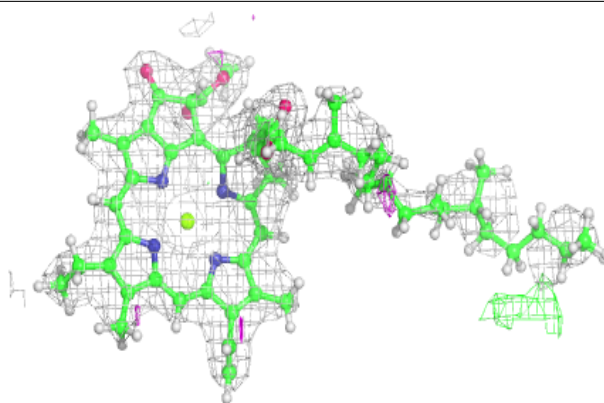
**Electron density around CLA b 611:**

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

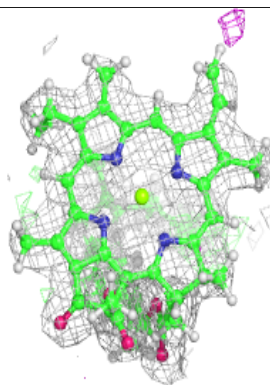
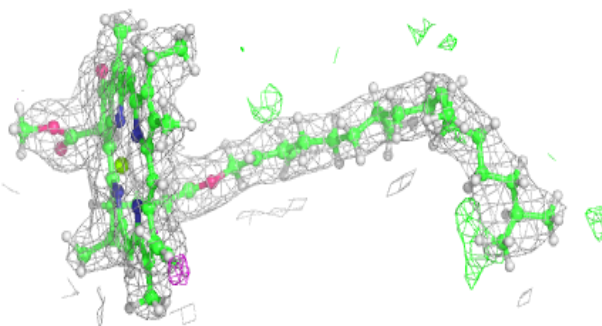
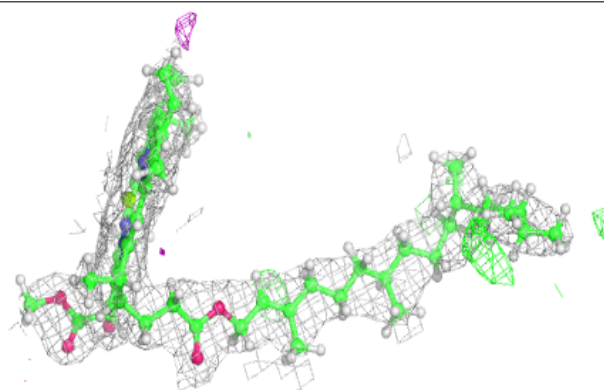


Electron density around CLA a 403:

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

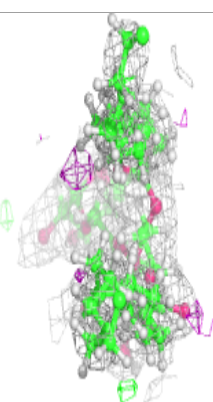
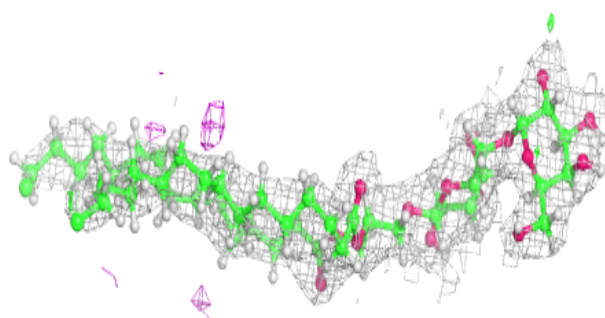
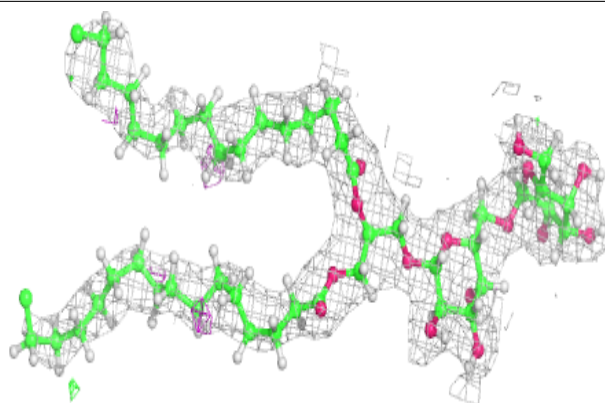
**Electron density around CLA b 604:**

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

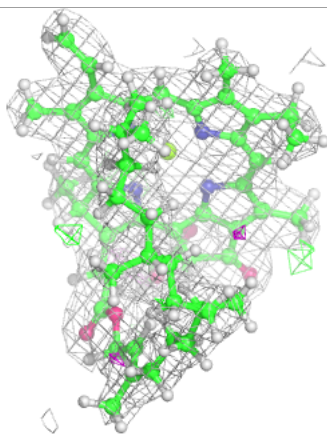
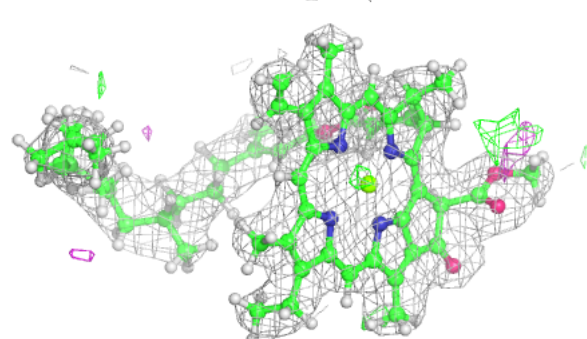
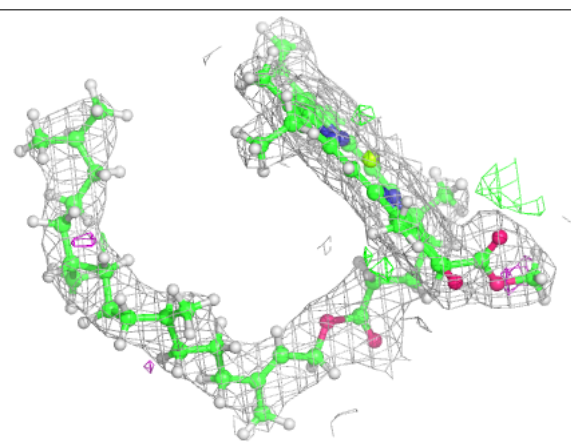


Electron density around DGD C 518:

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

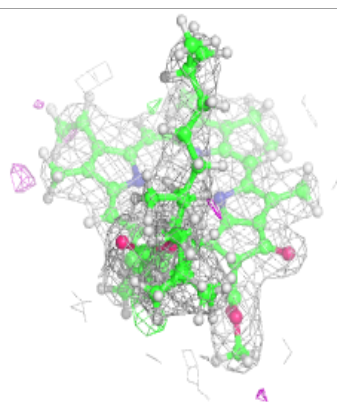
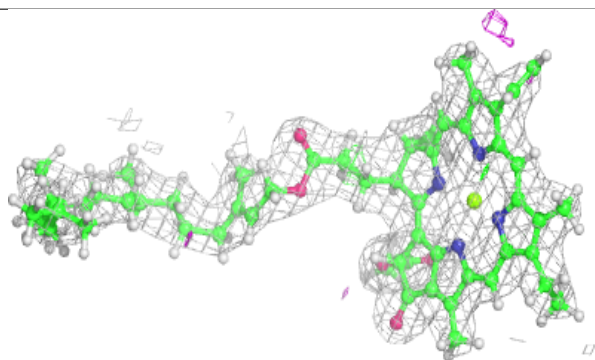
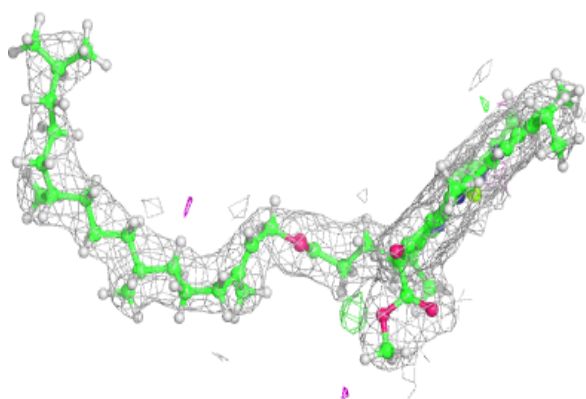
**Electron density around CLA b 610:**

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

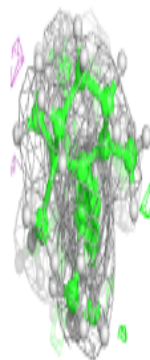
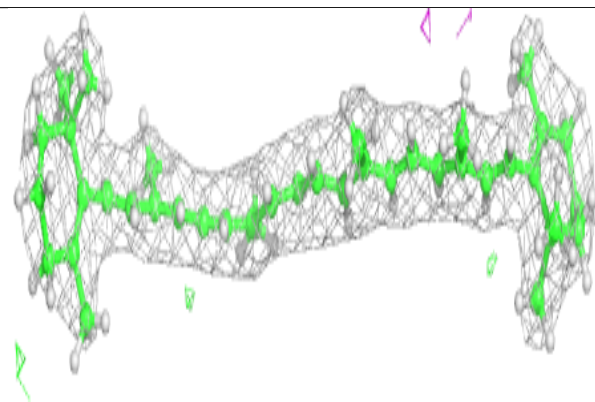
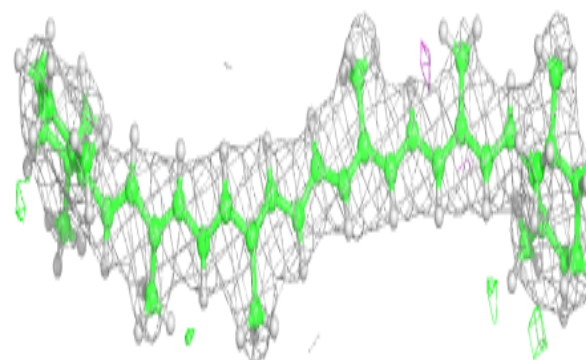


Electron density around CLA d 402:

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

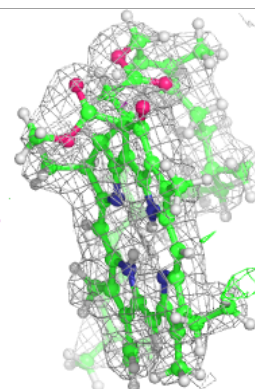
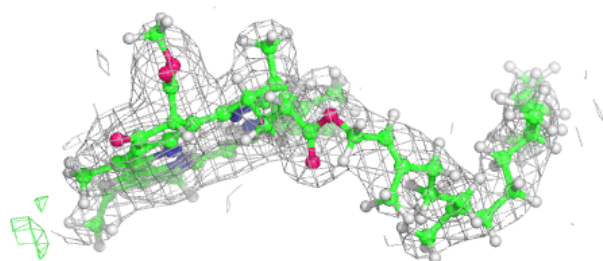
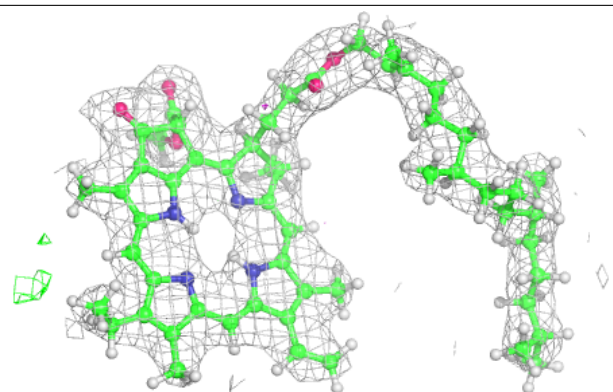
**Electron density around BCR A 406:**

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

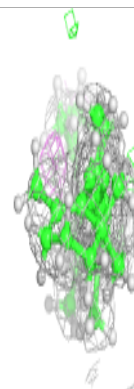
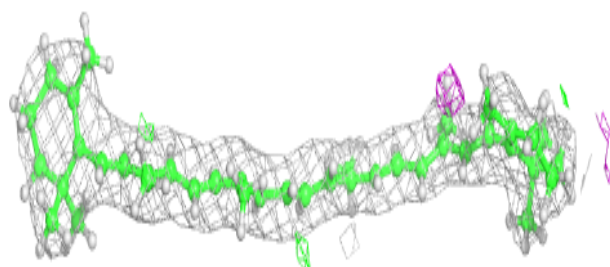
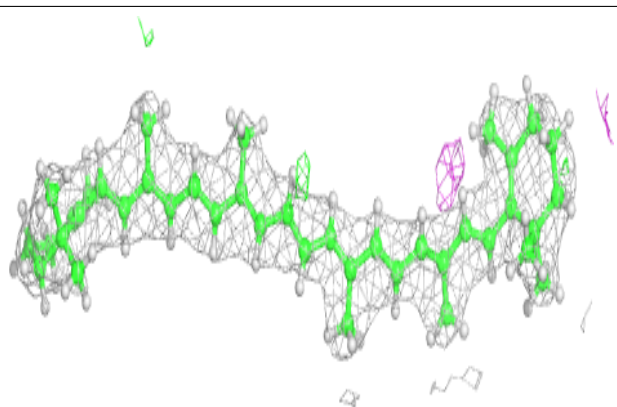


Electron density around PHO d 401:

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

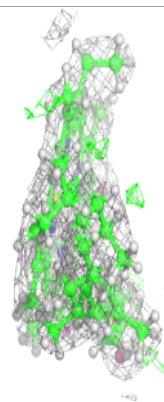
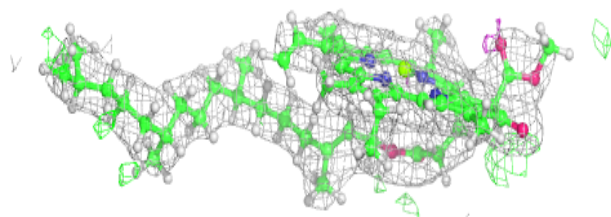
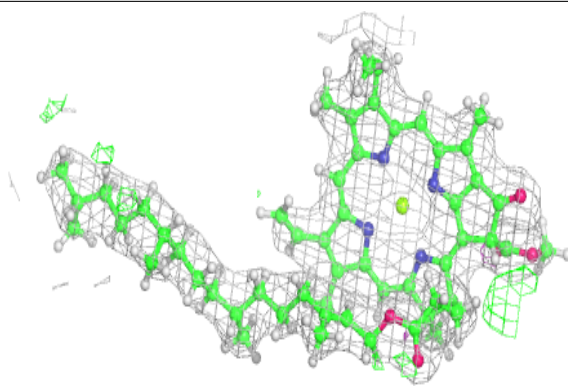
**Electron density around BCR B 618:**

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



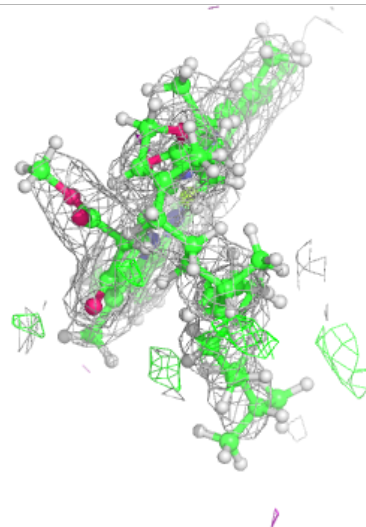
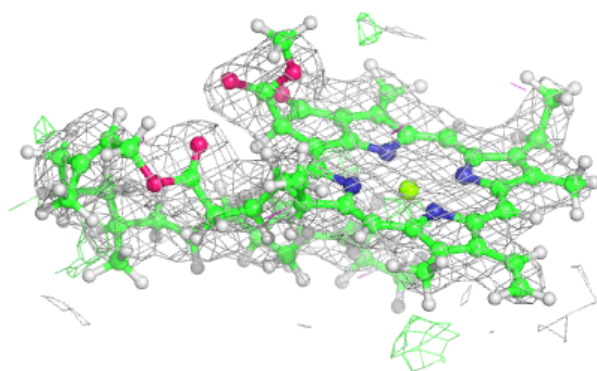
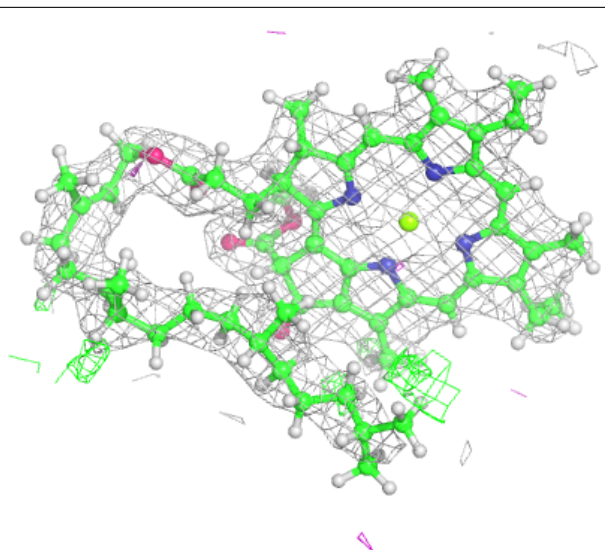
Electron density around CLA C 502:

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



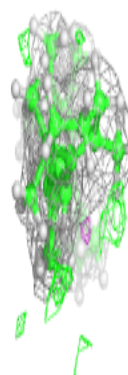
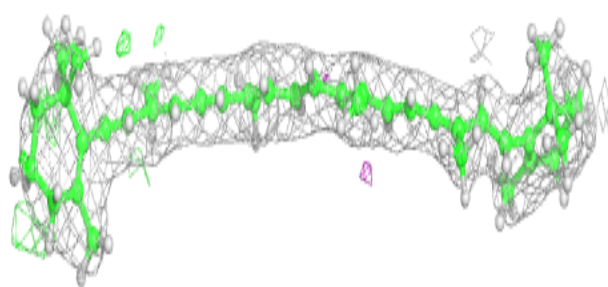
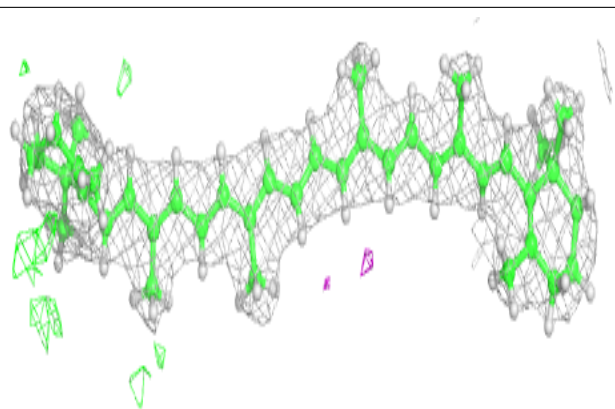
Electron density around CLA C 510:

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

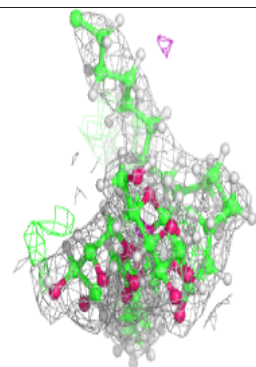
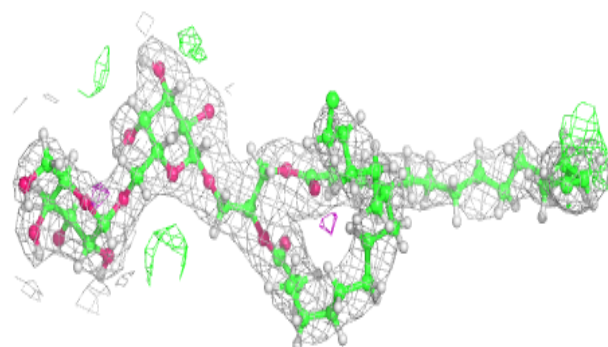
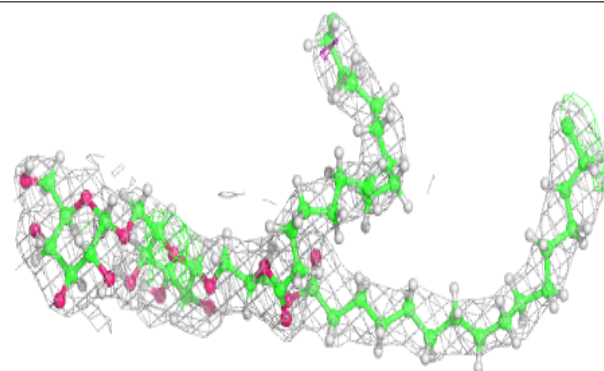


Electron density around BCR b 616:

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

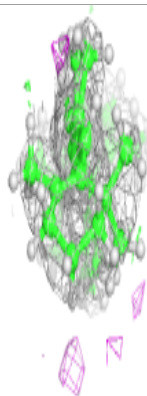
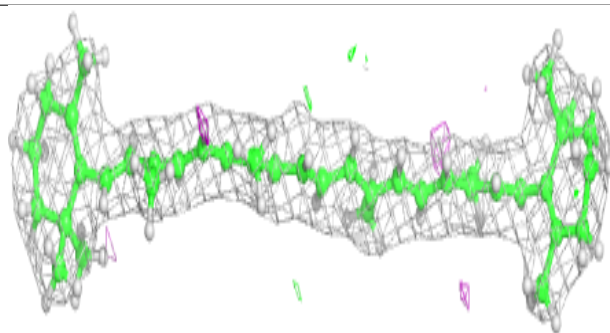
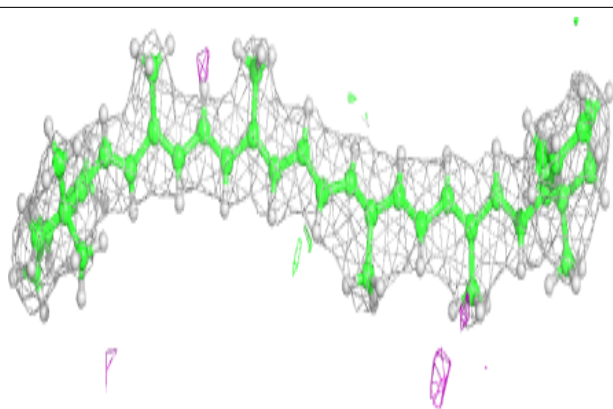
**Electron density around DGD H 102:**

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

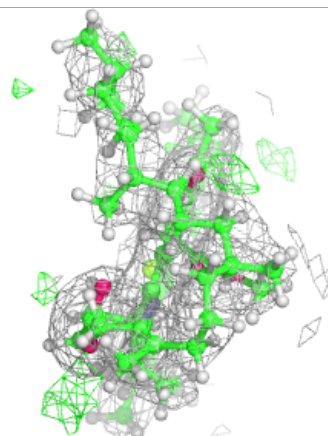
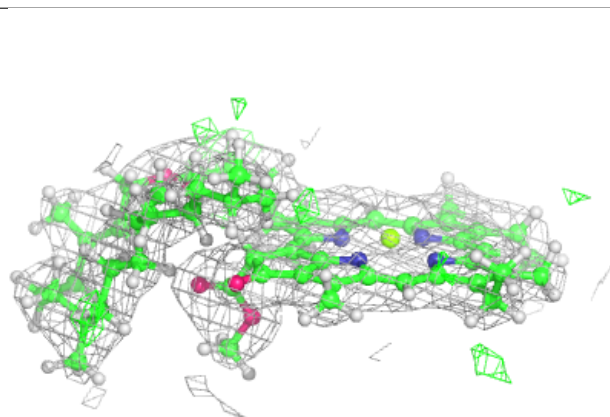
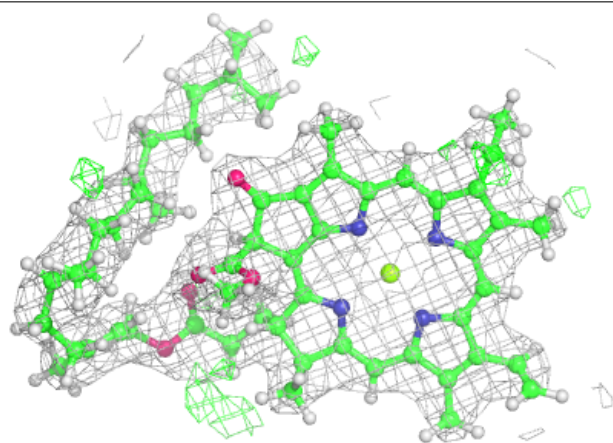


Electron density around BCR a 406:

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

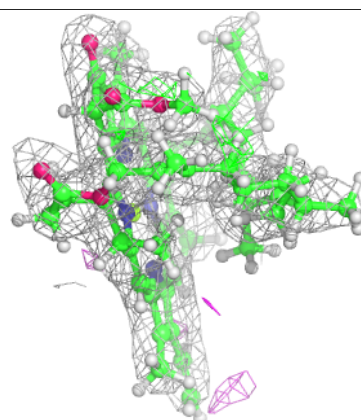
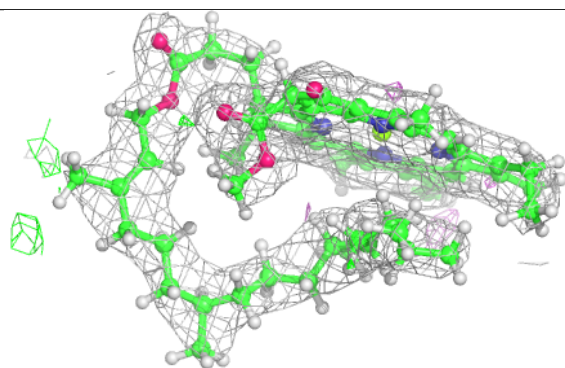
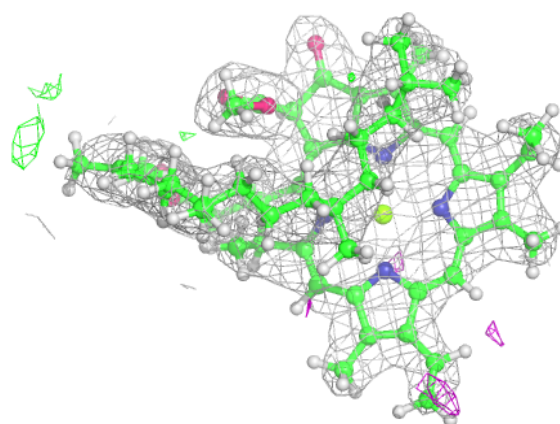
**Electron density around CLA b 609:**

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

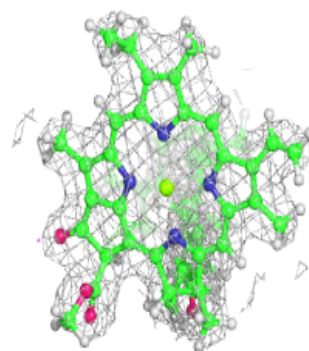
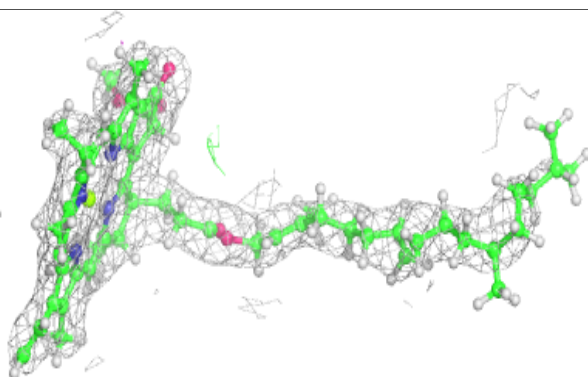
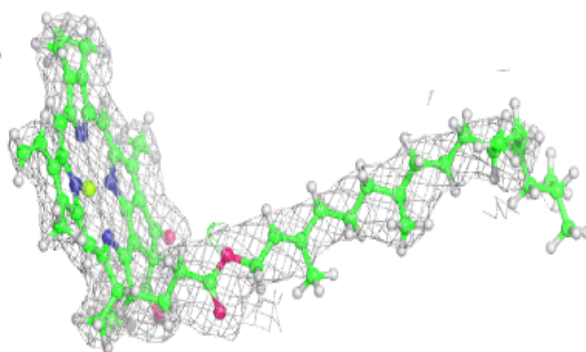


Electron density around CLA C 511:

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

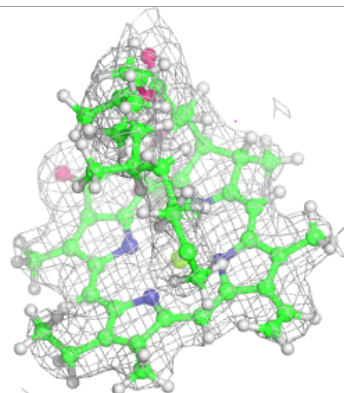
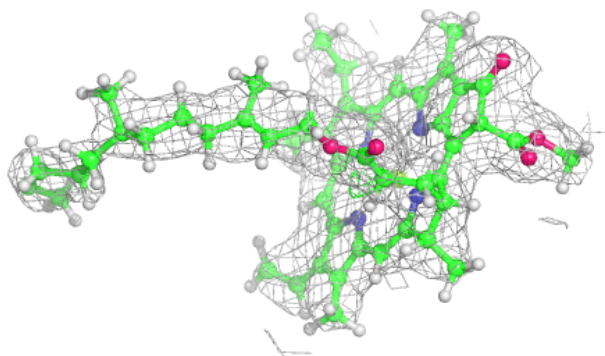
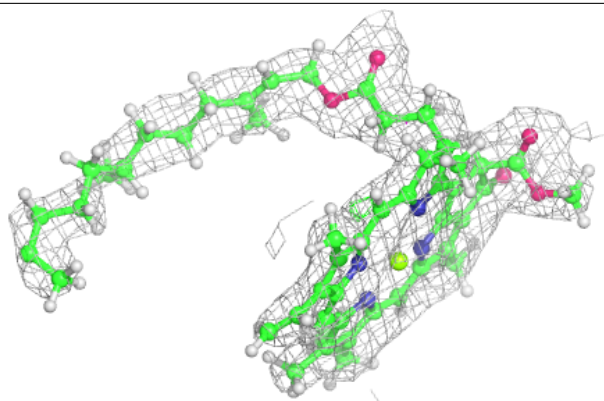
**Electron density around CLA b 603:**

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



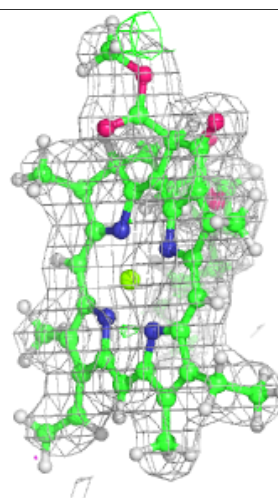
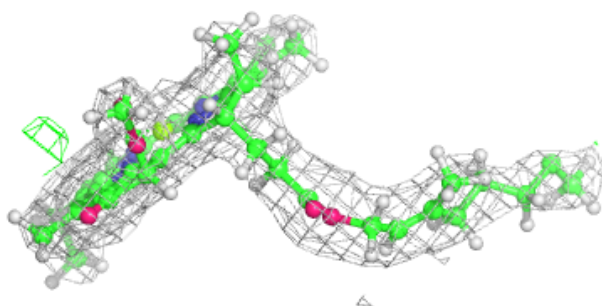
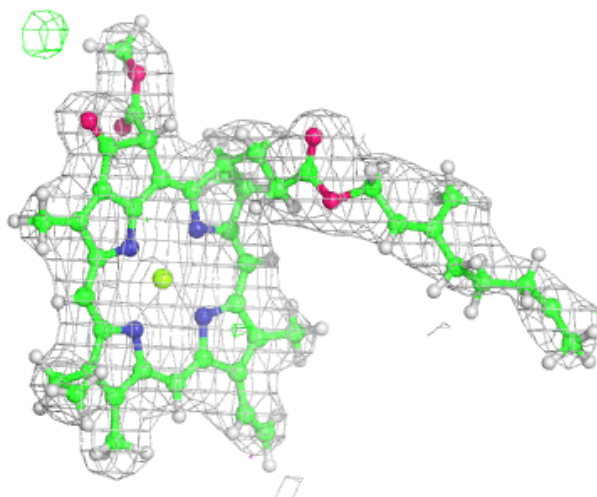
Electron density around CLA C 505:

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



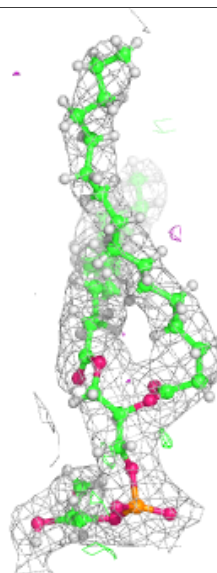
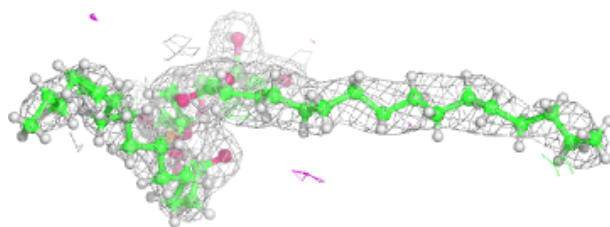
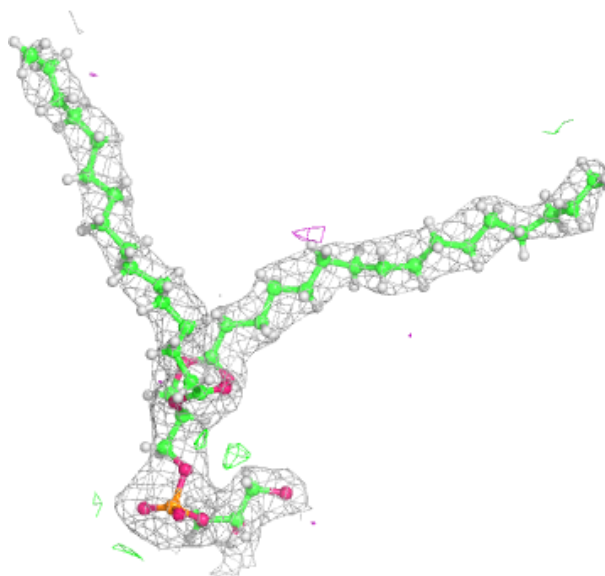
Electron density around CLA A 405:

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



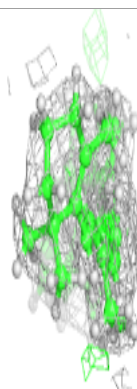
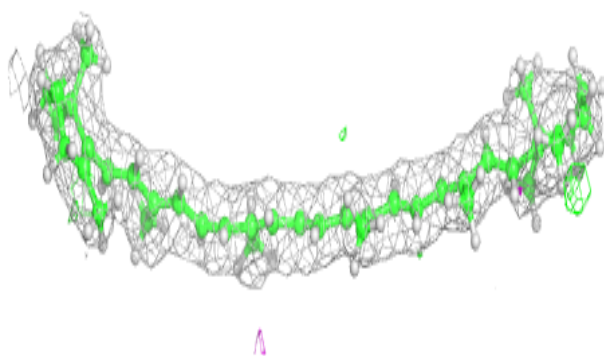
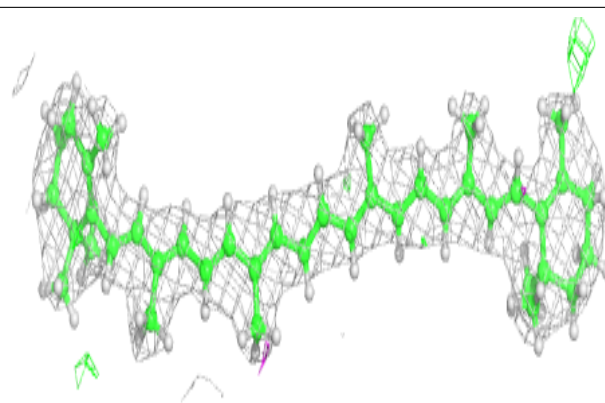
Electron density around LHG 1 101:

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

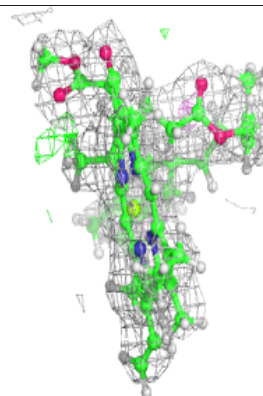
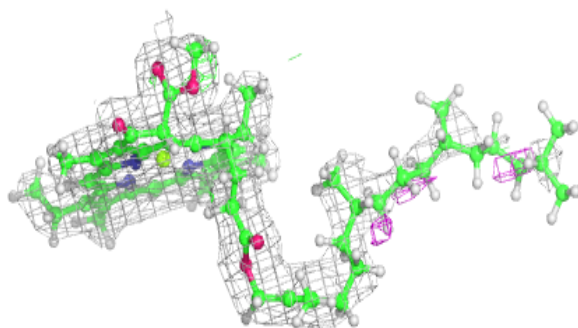
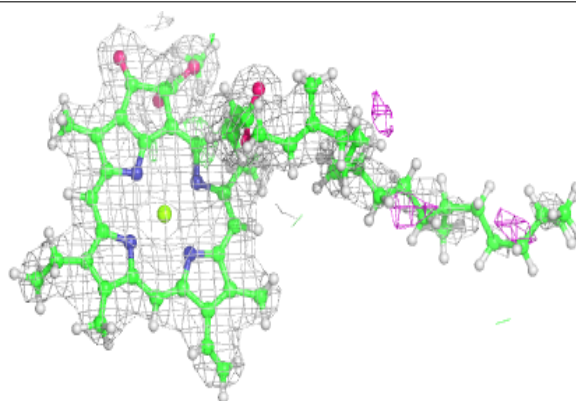


Electron density around BCR T 101:

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

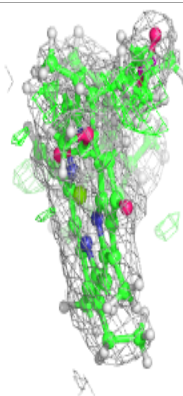
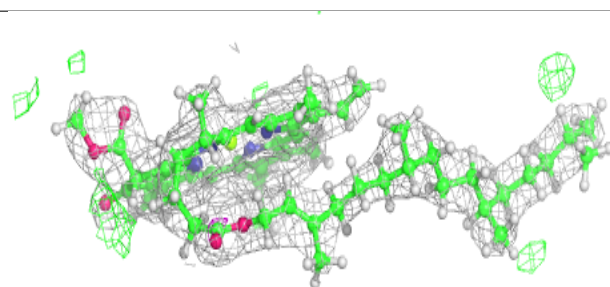
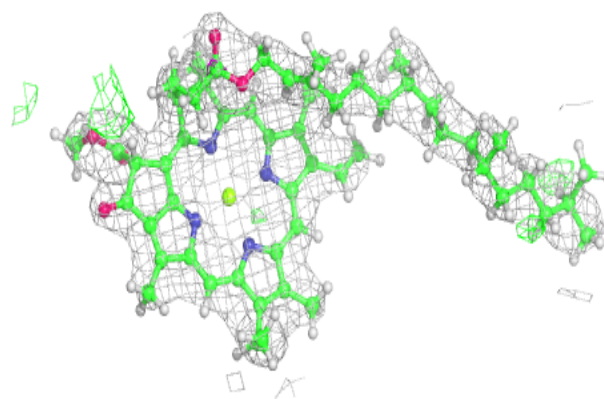
**Electron density around CLA A 403:**

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

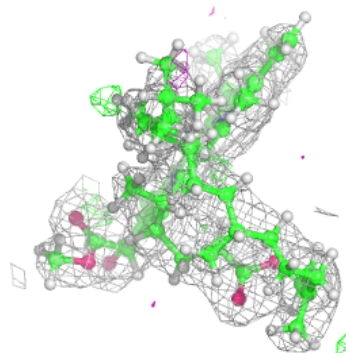
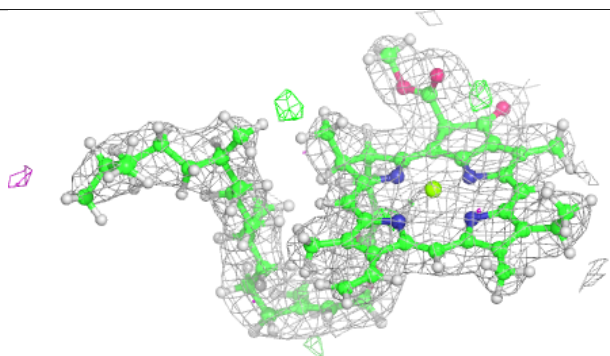
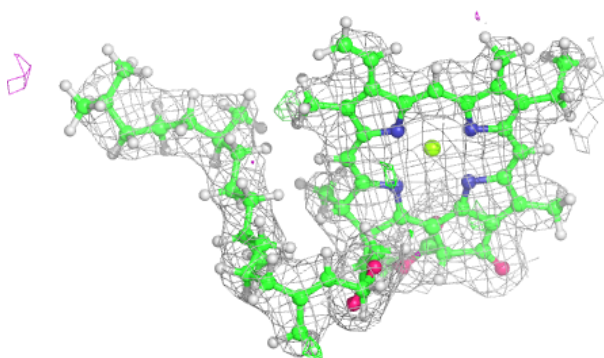


Electron density around CLA c 503:

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

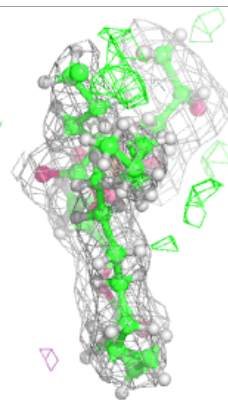
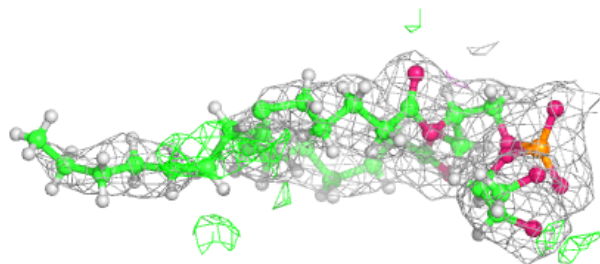
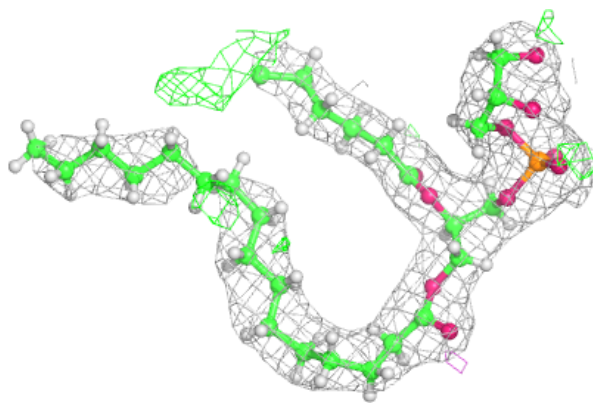
**Electron density around CLA A 411:**

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

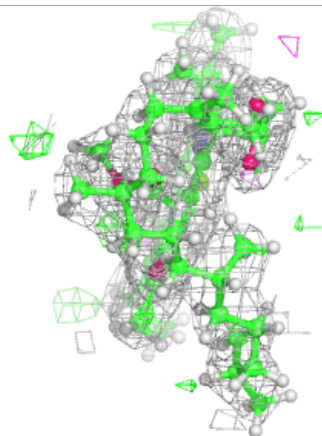
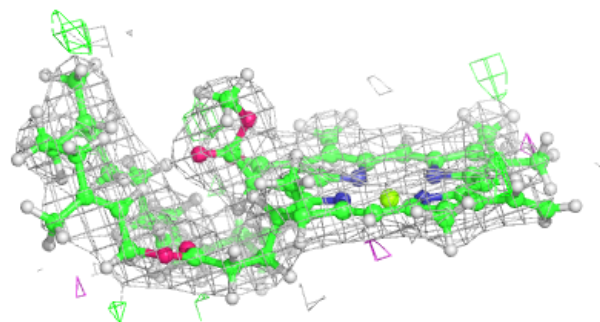
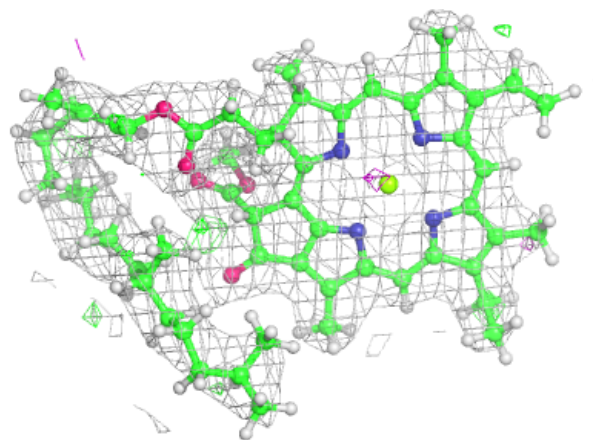


Electron density around LHG d 408:

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

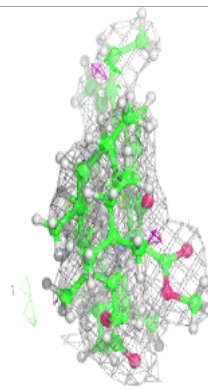
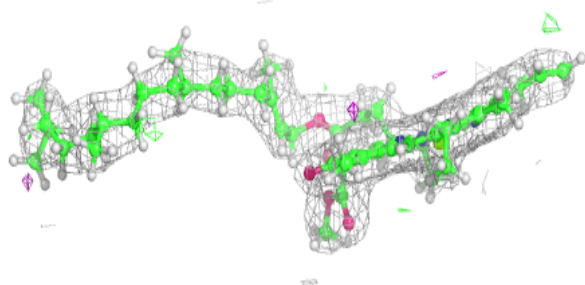
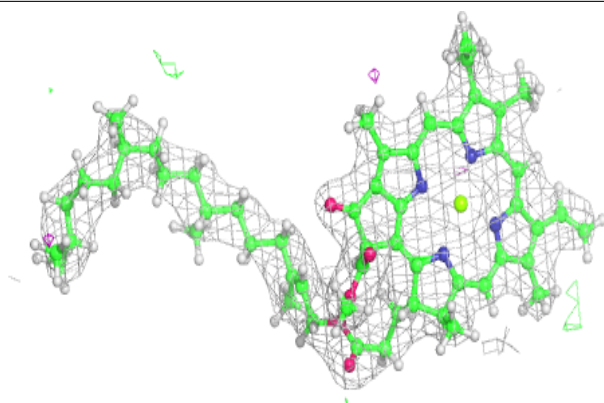
**Electron density around CLA B 611:**

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

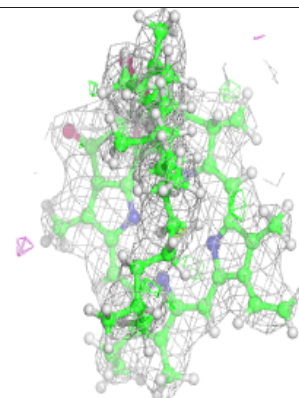
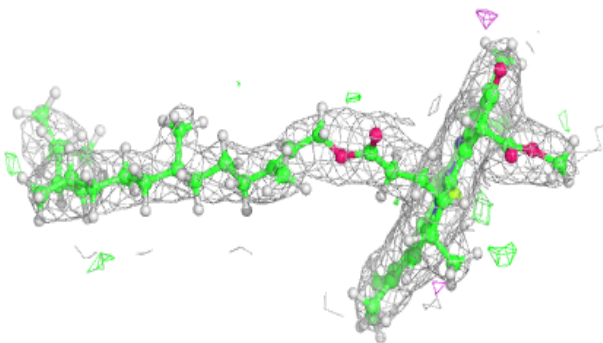
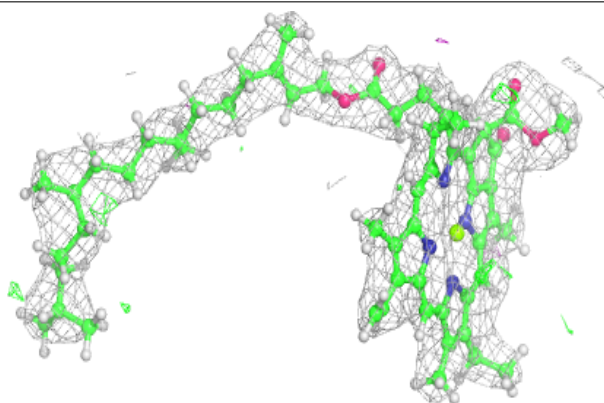


Electron density around CLA B 603:

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

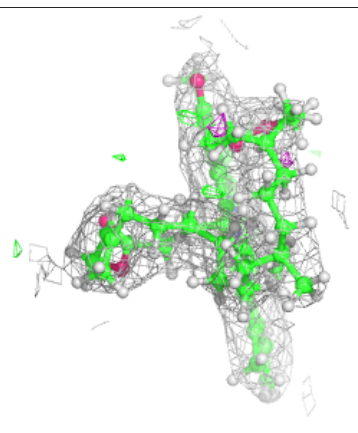
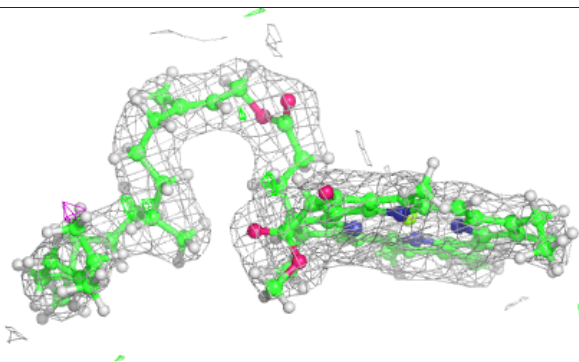
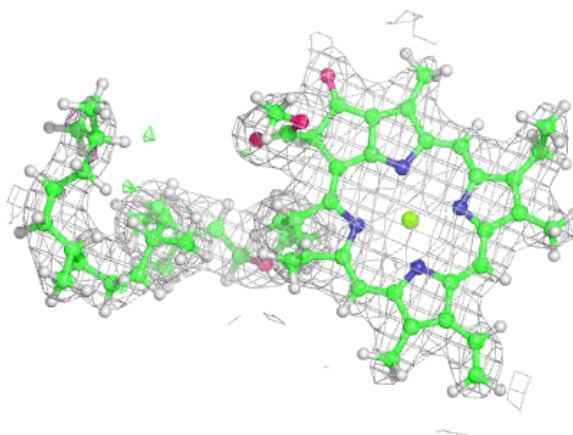
**Electron density around CLA B 610:**

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



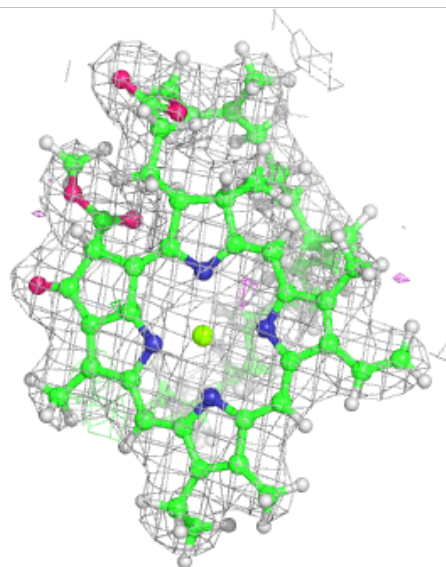
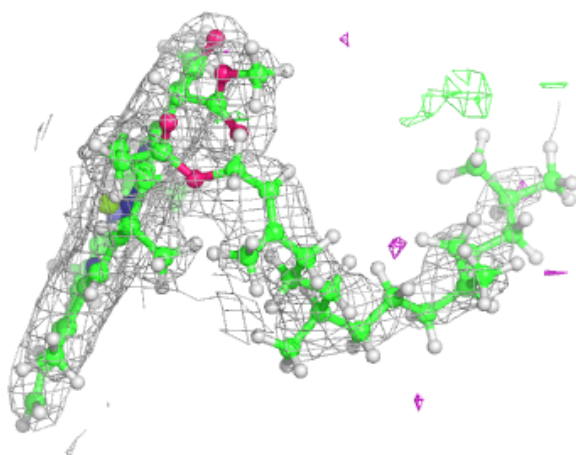
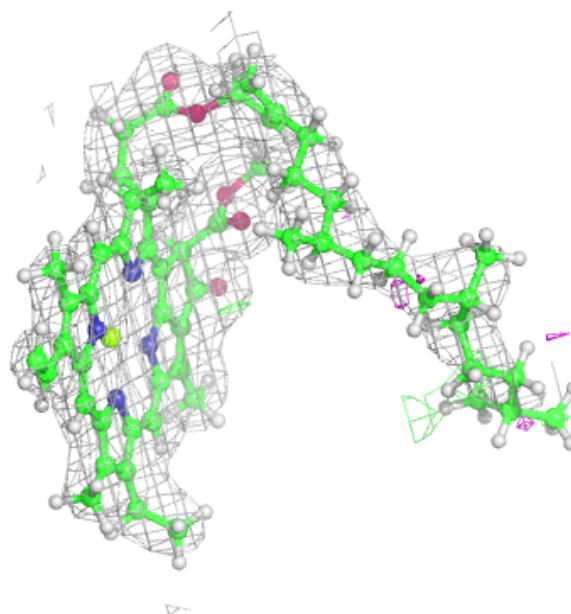
Electron density around CLA B 613:

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



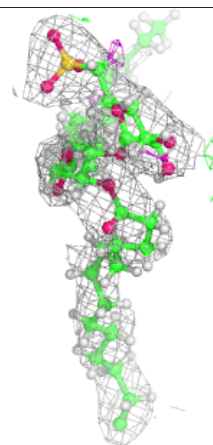
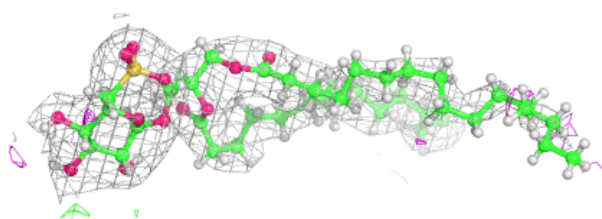
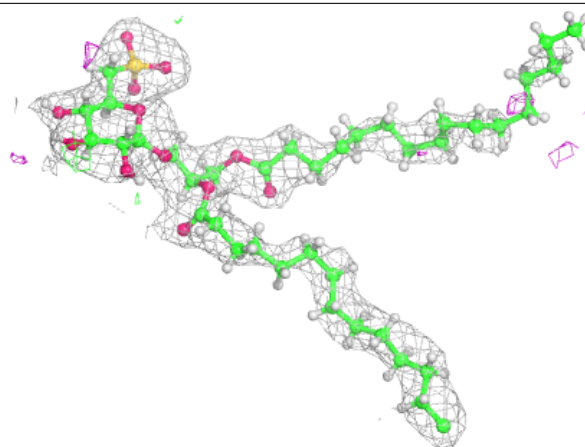
Electron density around CLA b 612:

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

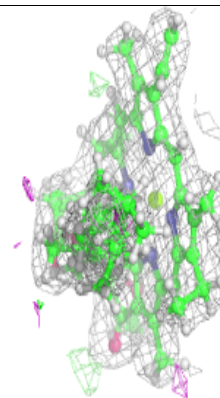
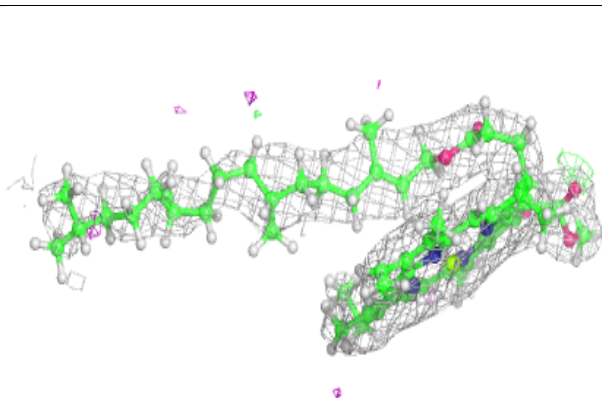
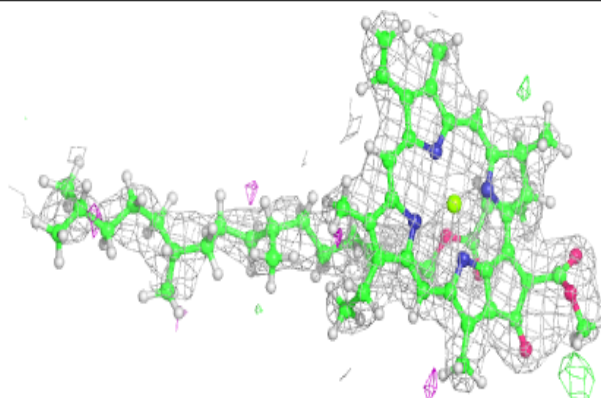


Electron density around SQD A 413:

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

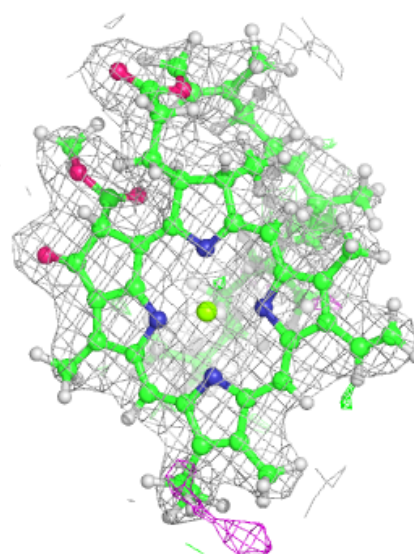
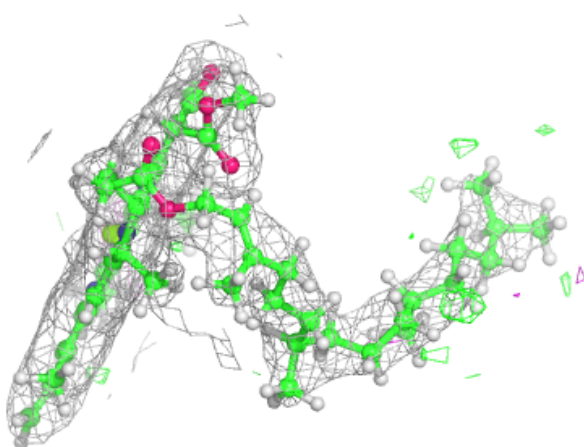
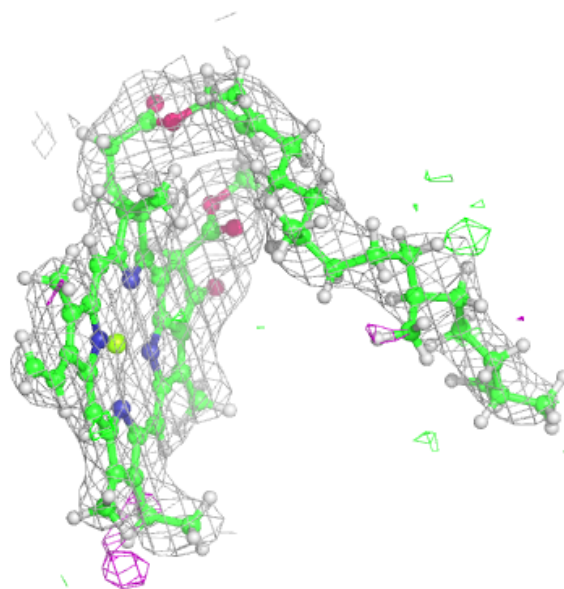
**Electron density around CLA b 613:**

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



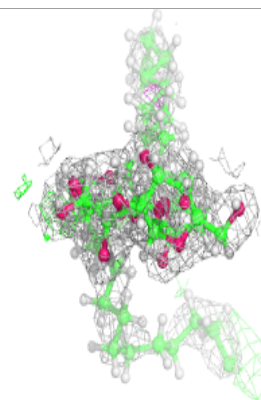
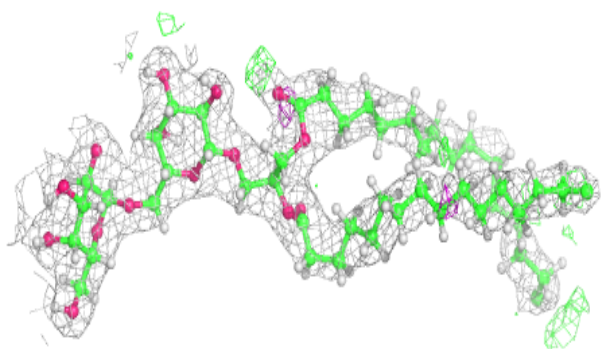
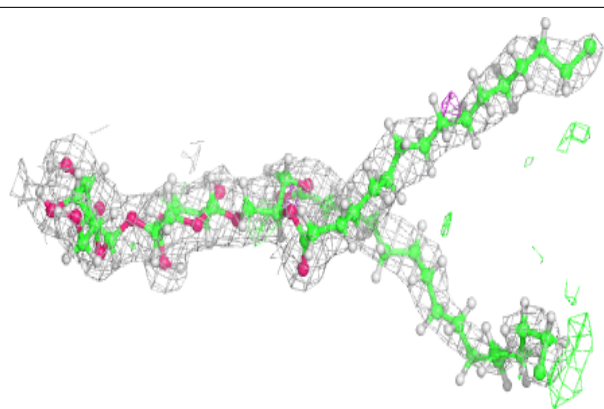
Electron density around CLA B 614:

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

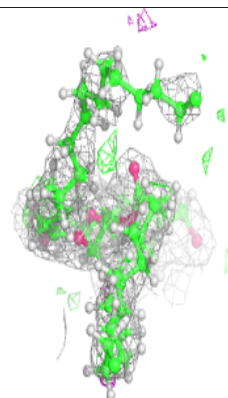
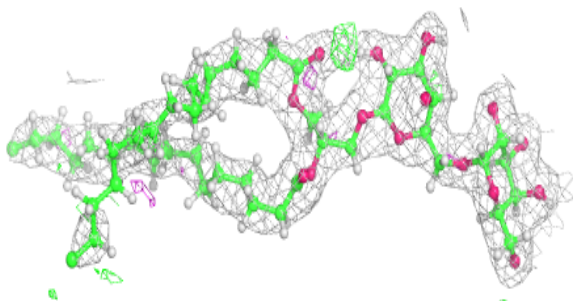
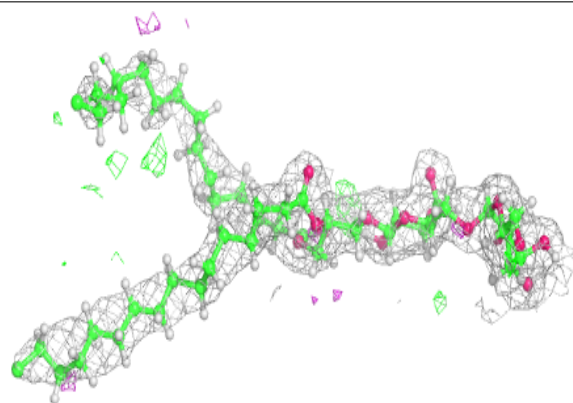


Electron density around DGD C 516:

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

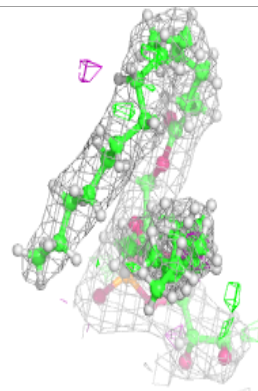
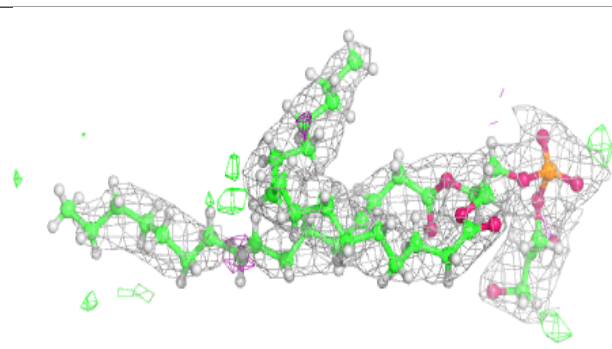
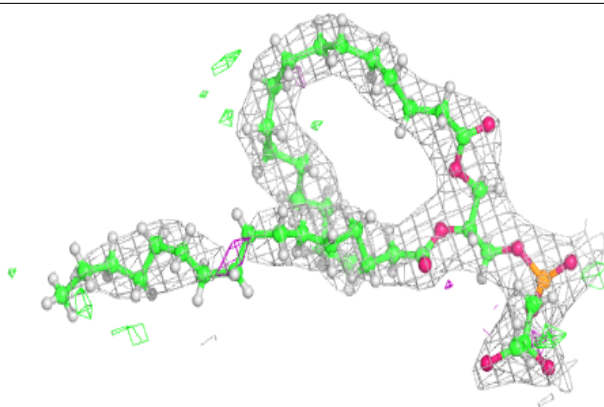
**Electron density around DGD c 519:**

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

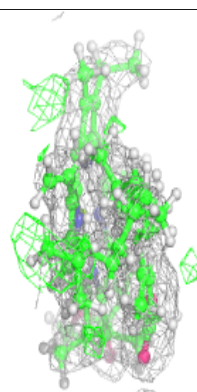
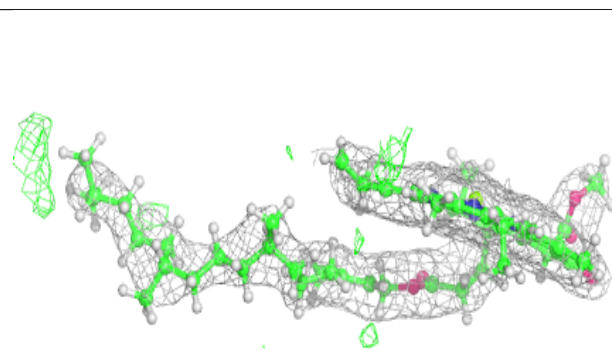
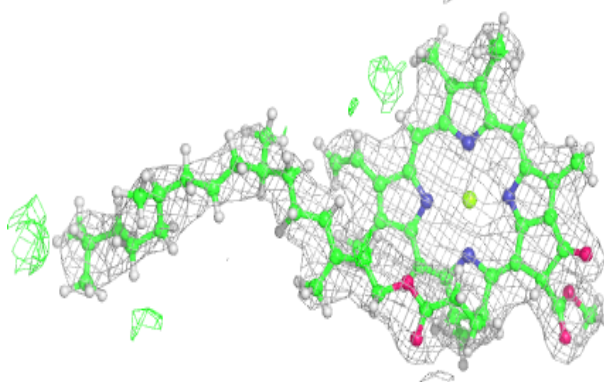


Electron density around LHG D 412:

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

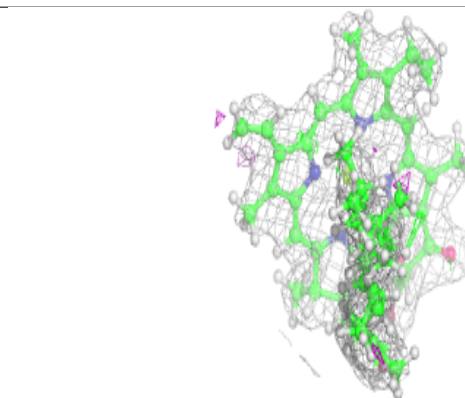
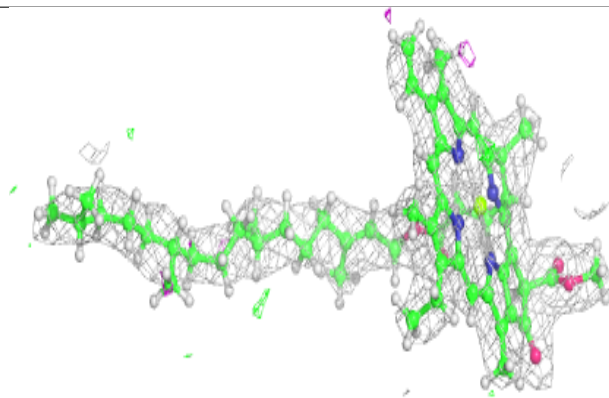
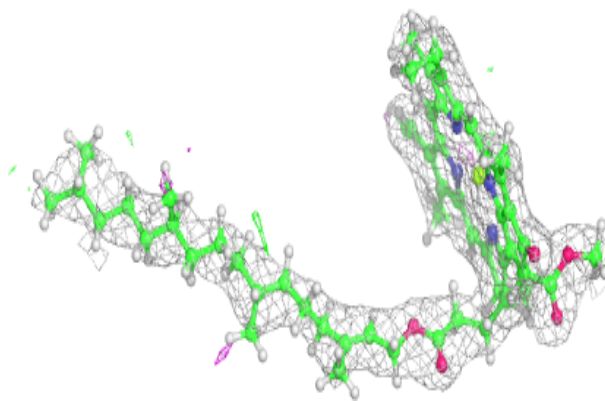
**Electron density around CLA b 602:**

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

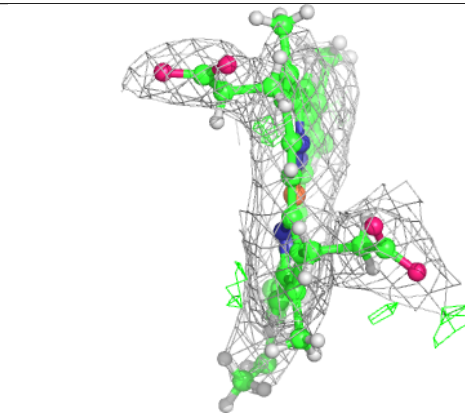
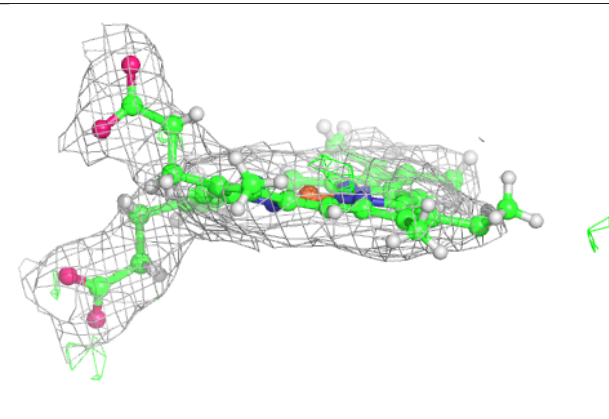
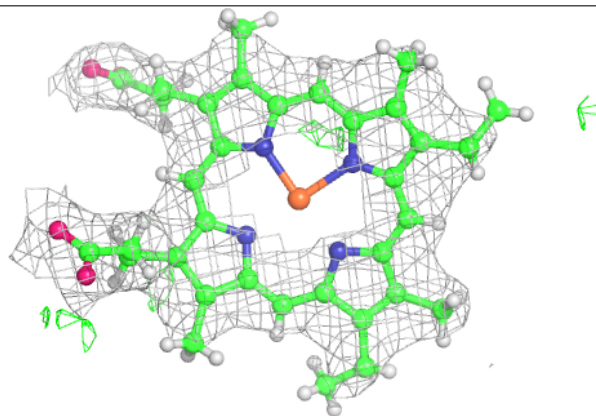


Electron density around CLA B 608:

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

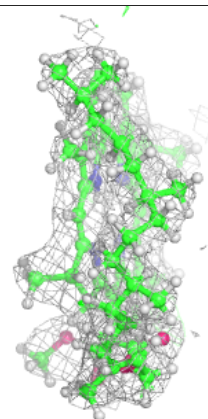
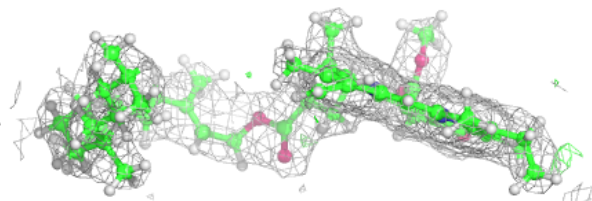
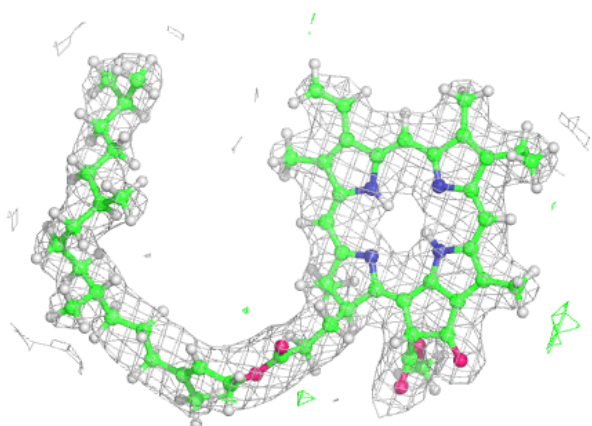
**Electron density around HEC F 101:**

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

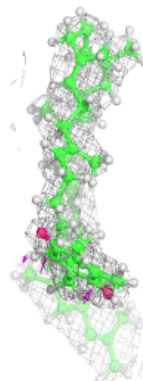
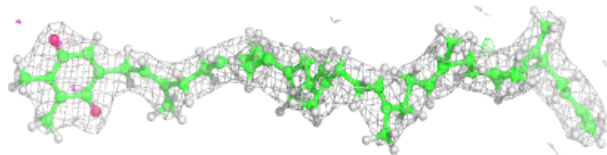
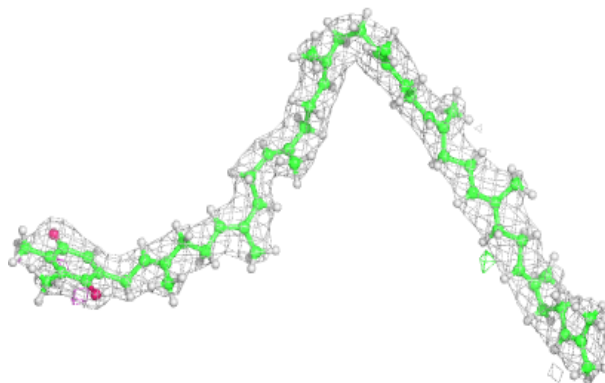


Electron density around PHO a 404:

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

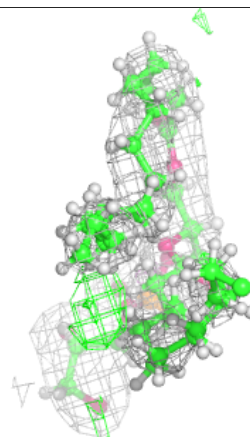
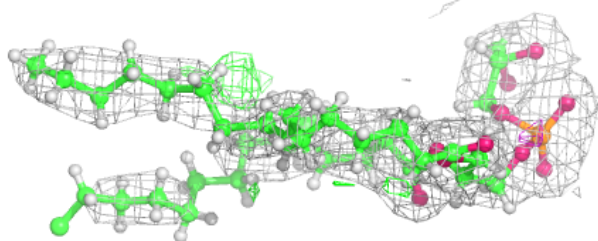
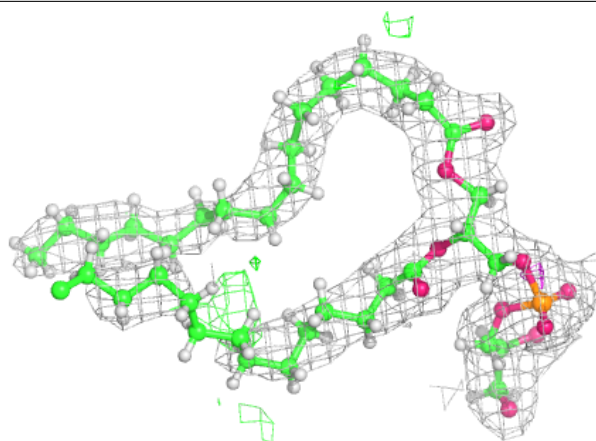
**Electron density around PL9 d 405:**

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

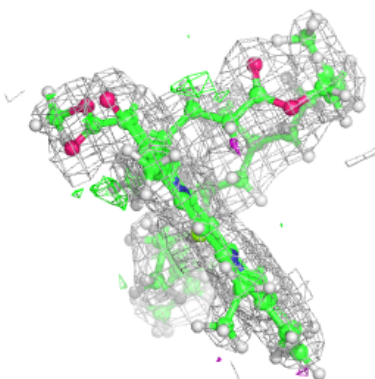
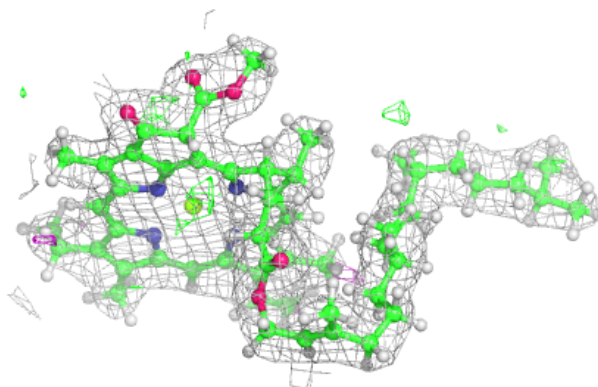
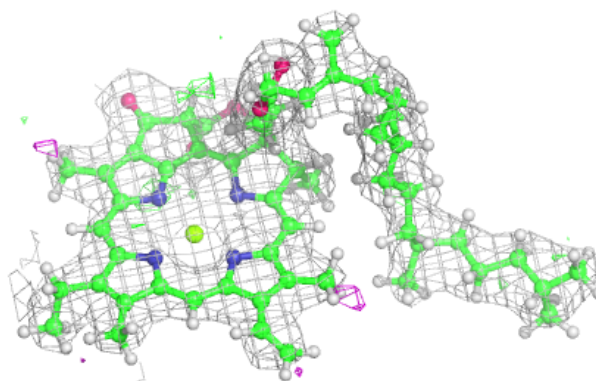


Electron density around LHG D 409:

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

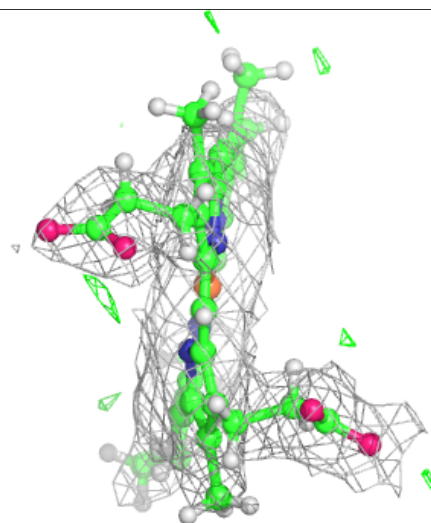
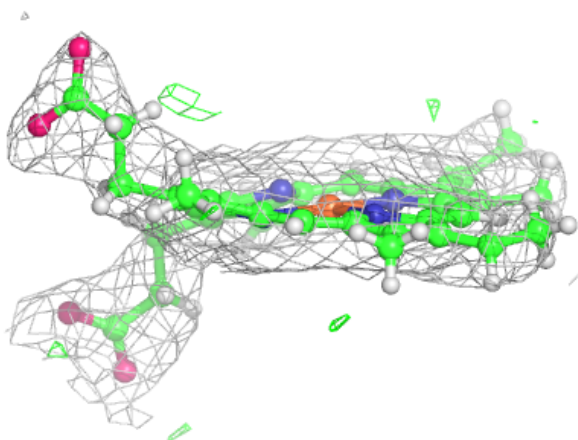
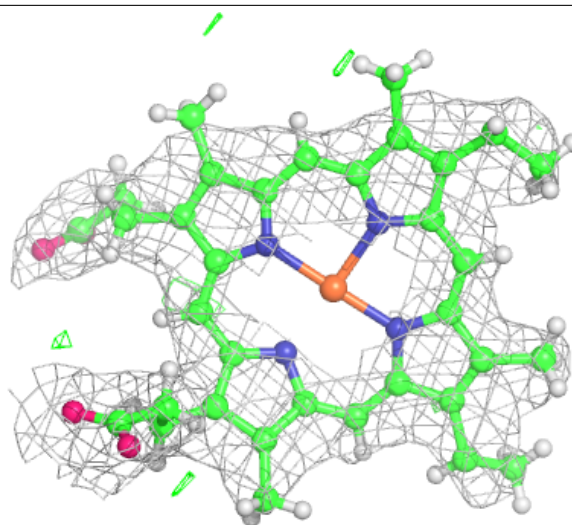
**Electron density around CLA a 411:**

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



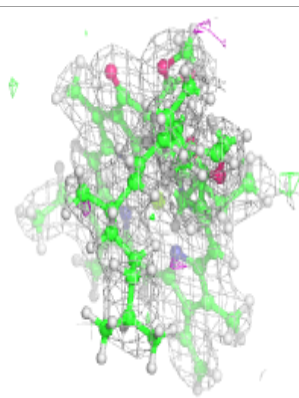
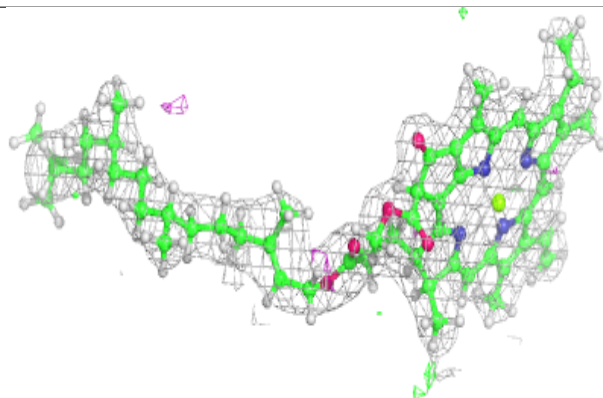
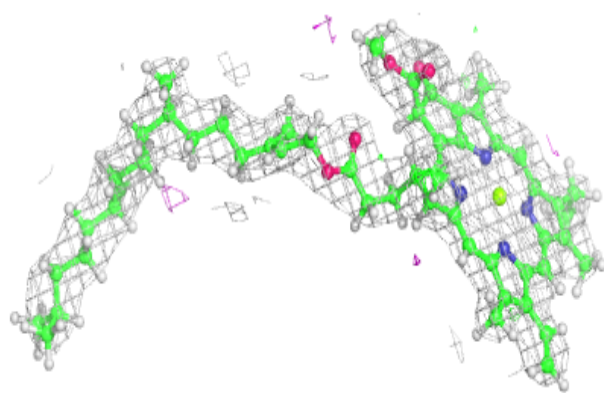
Electron density around HEC e 101:

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

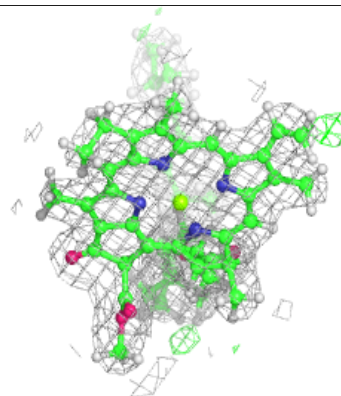
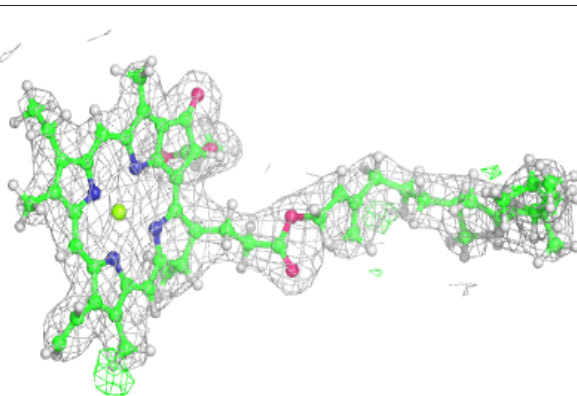
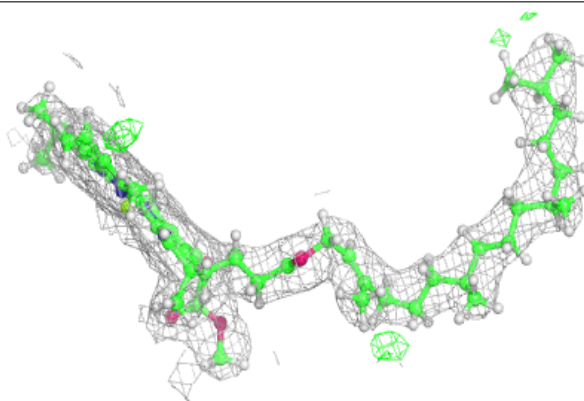


Electron density around CLA a 402:

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

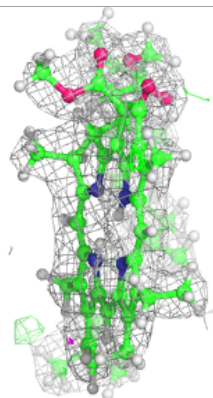
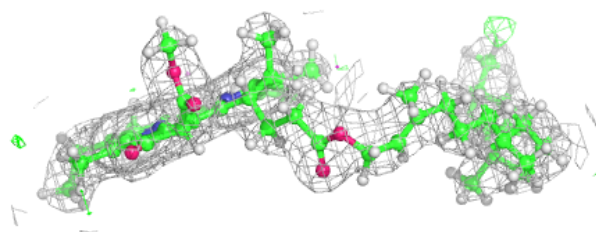
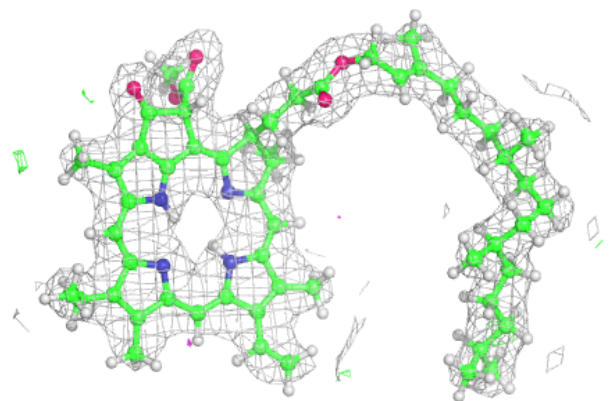
**Electron density around CLA D 402:**

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

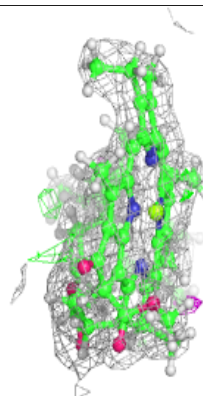
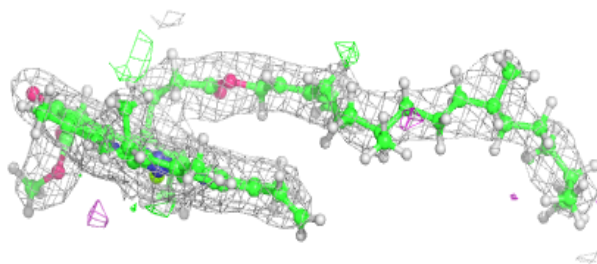
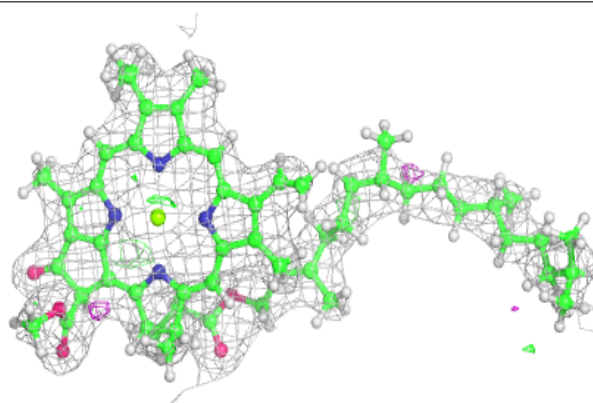


Electron density around PHO A 404:

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

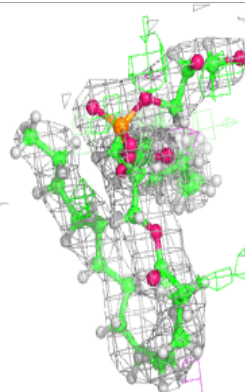
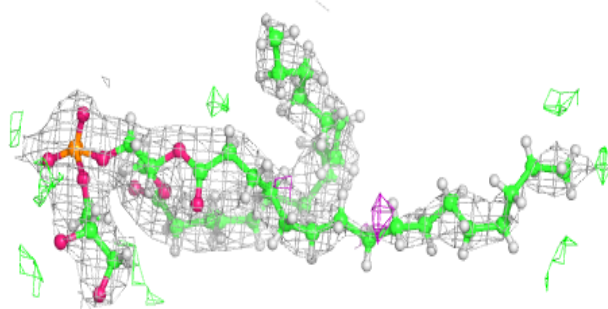
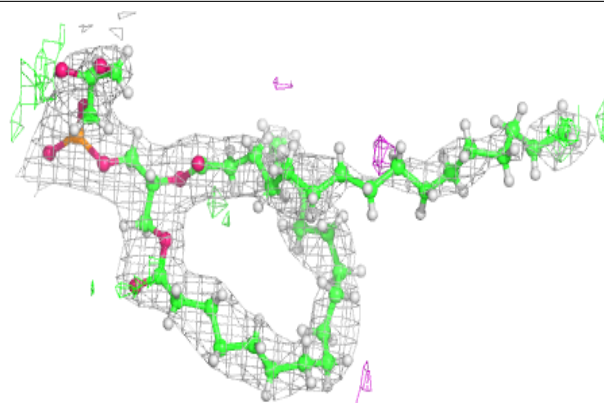
**Electron density around CLA B 604:**

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

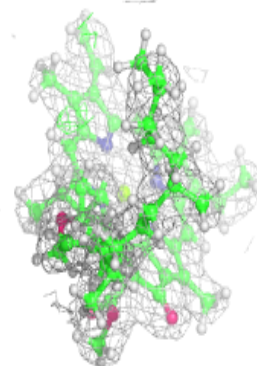
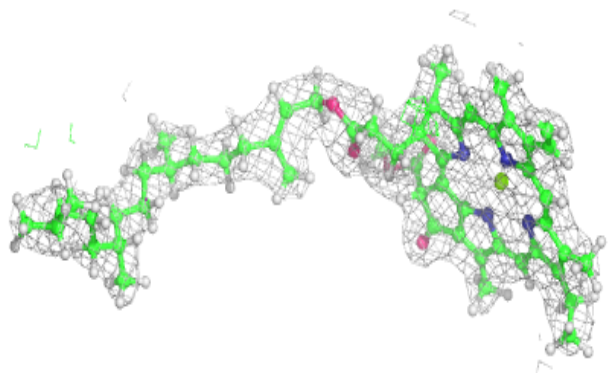
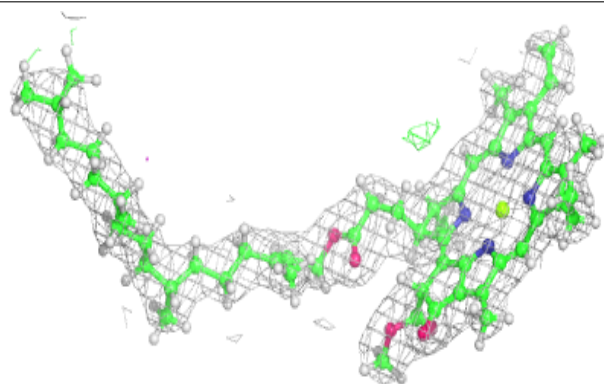


Electron density around LHG d 406:

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

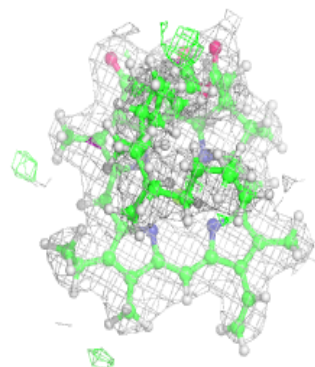
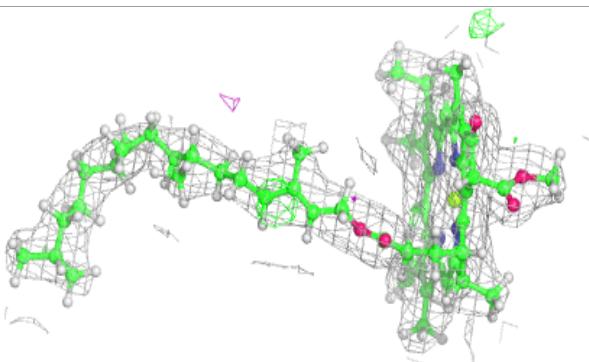
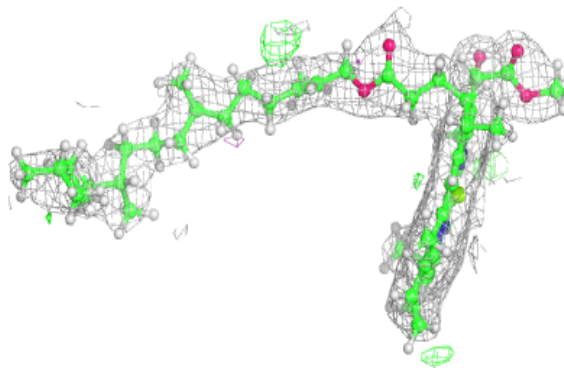
**Electron density around CLA A 402:**

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

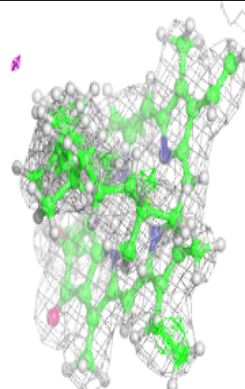
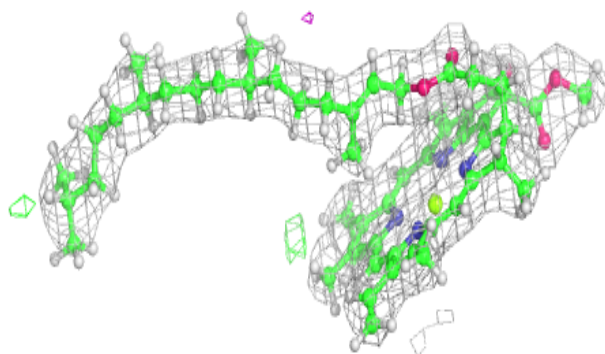
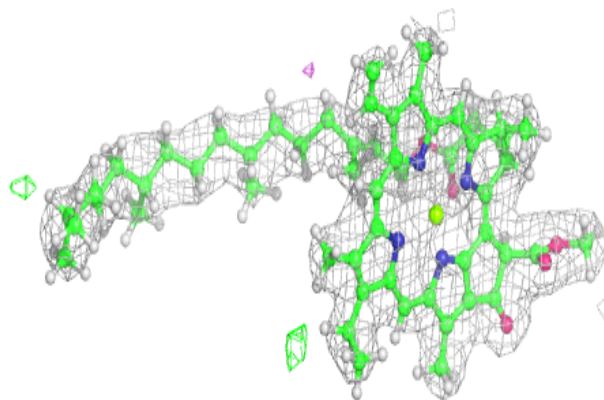


Electron density around CLA B 606:

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

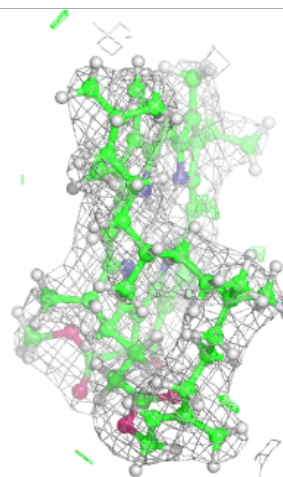
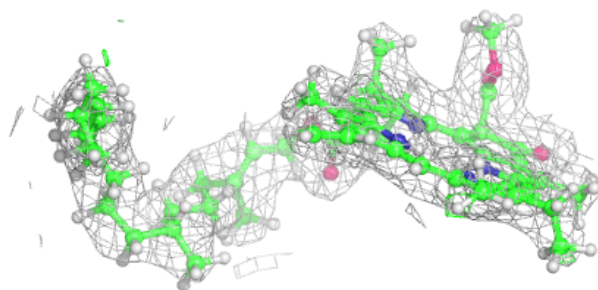
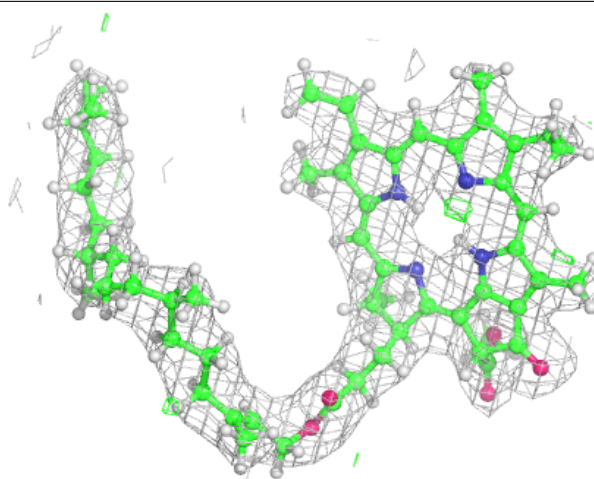
**Electron density around CLA B 609:**

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



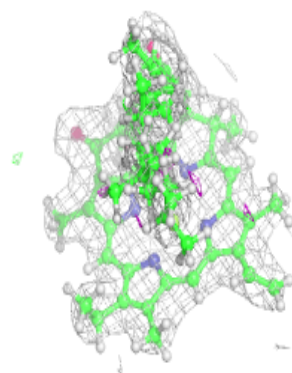
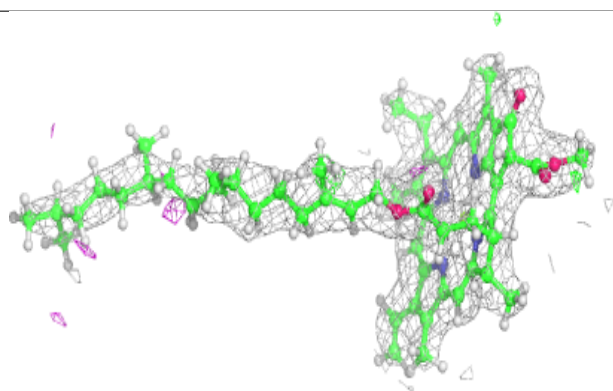
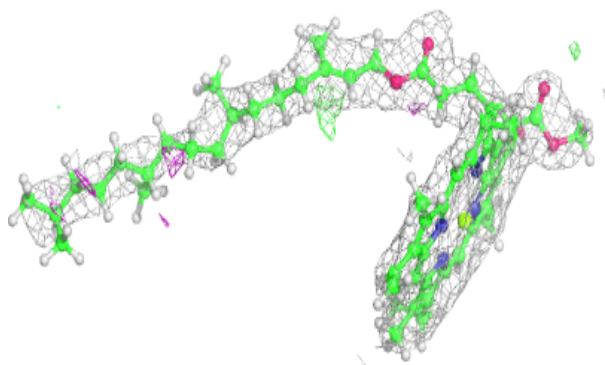
Electron density around PHO D 401:

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



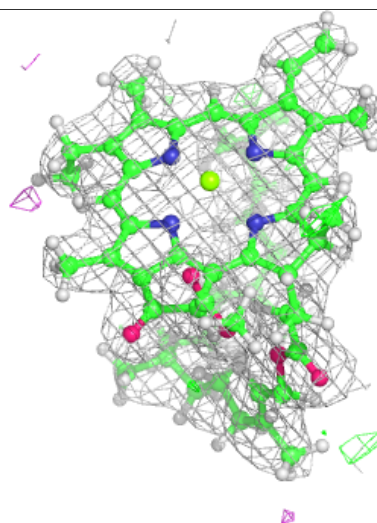
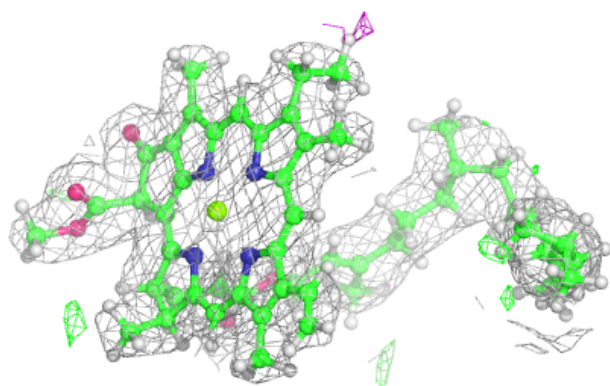
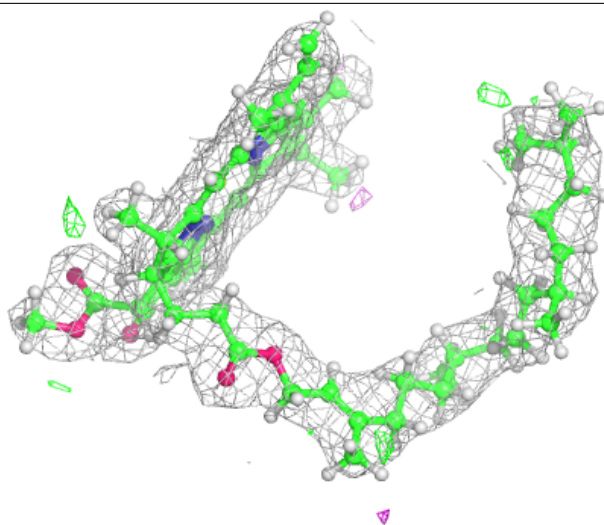
Electron density around CLA b 606:

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



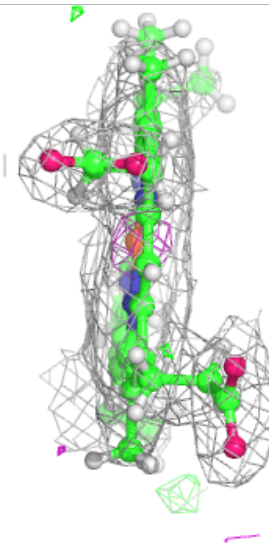
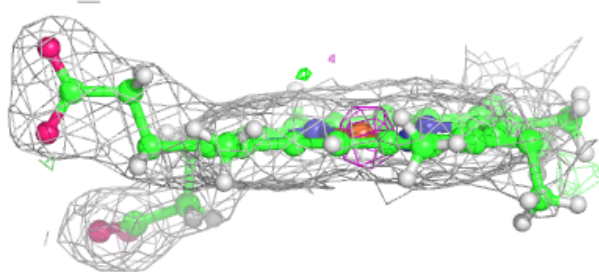
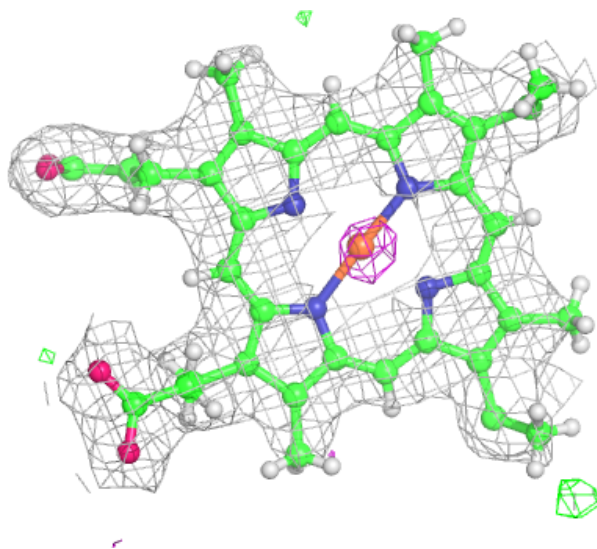
Electron density around CLA B 612:

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



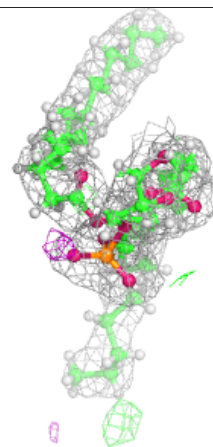
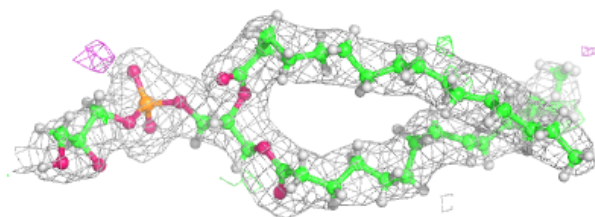
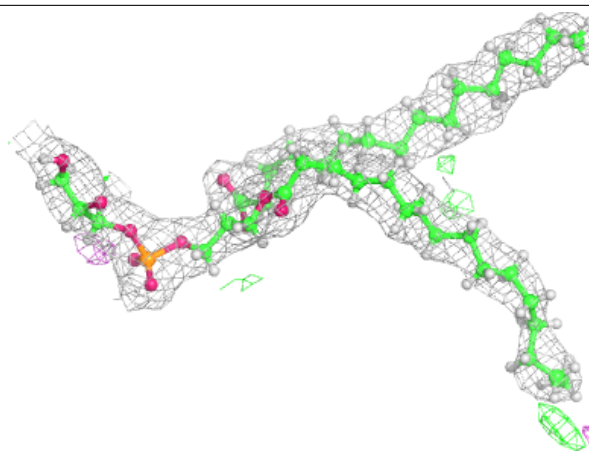
Electron density around HEC v 201:

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

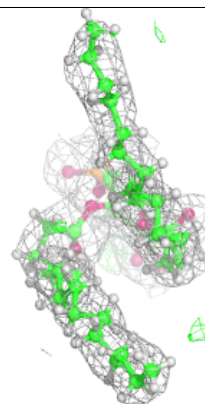
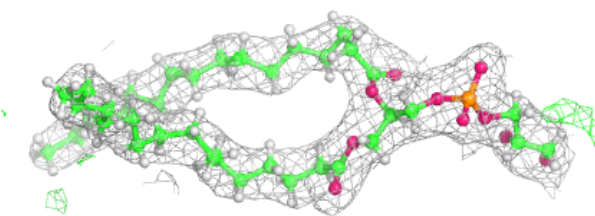
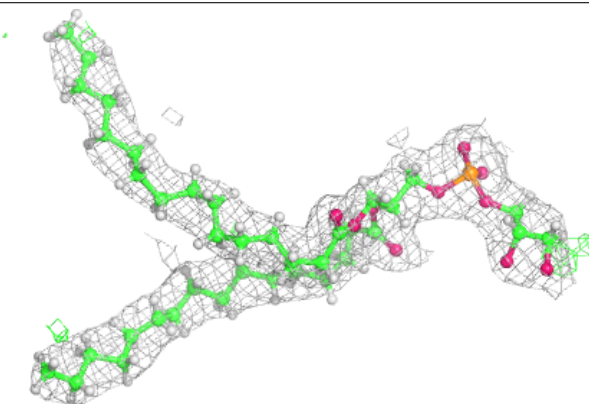


Electron density around LHG D 408:

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

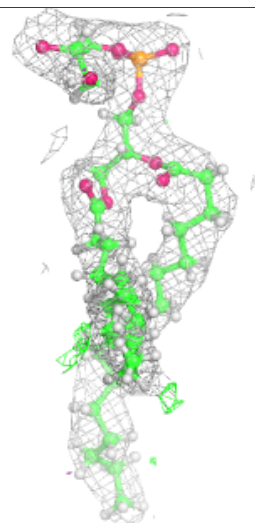
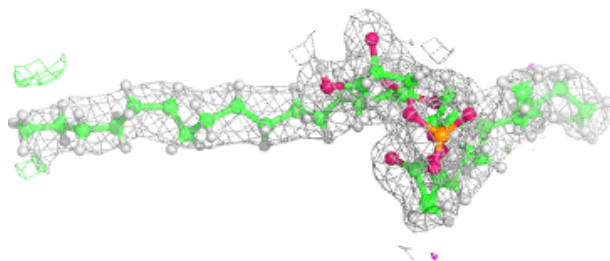
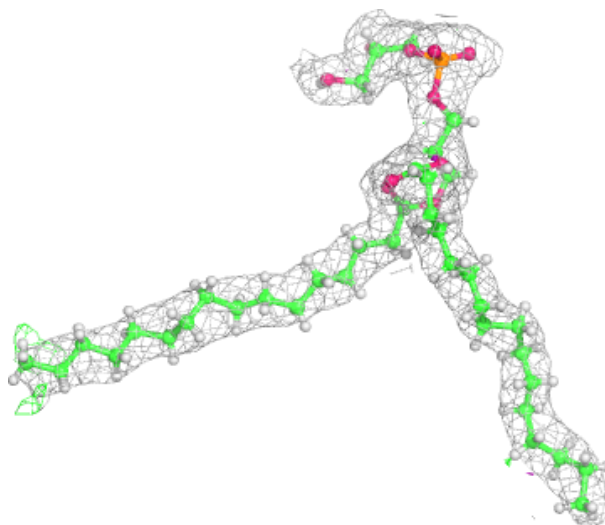
**Electron density around LHG d 407:**

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



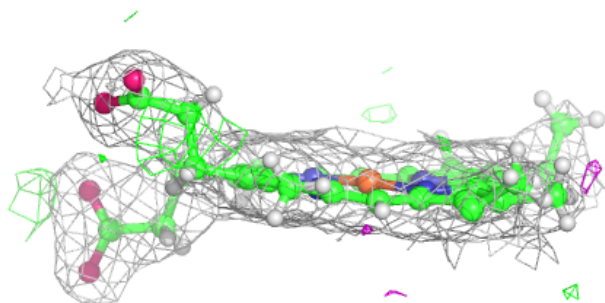
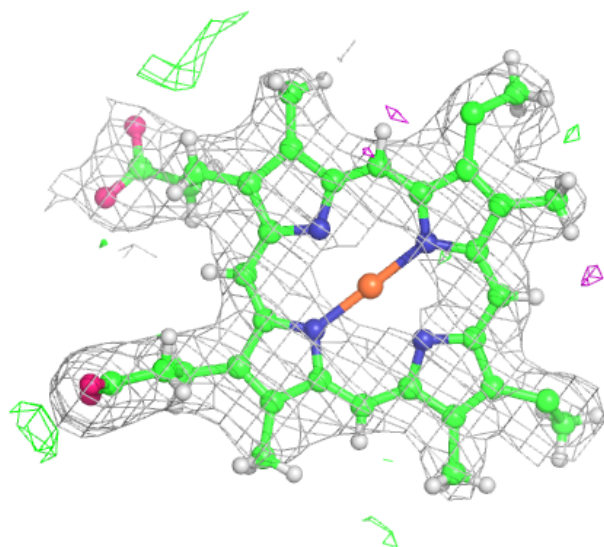
Electron density around LHG B 622:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.